wwPDB EM Validation Summary Report

Oct 1, 2026 – 10:48 AM JST

PDB ID	:	6K33 / pdb_00006k33
EMDB ID	:	EMD-9908
Title	:	Structure of PSI-isiA supercomplex from Thermosynechococcus vulcanus
Authors	:	Akita, F.; Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.
Deposited on	:	2019-05-16
Resolution	:	2.74 Å(reported)
Based on initial model	:	1JB0

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

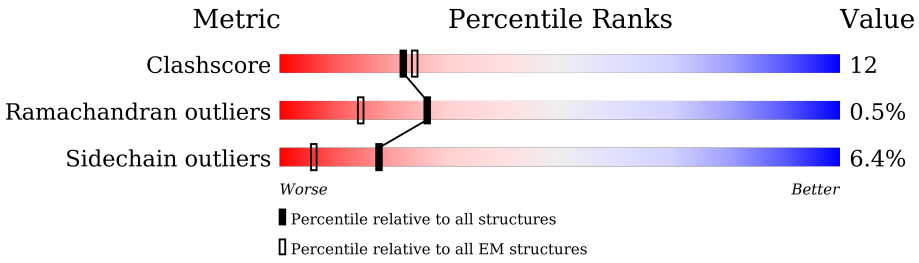
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

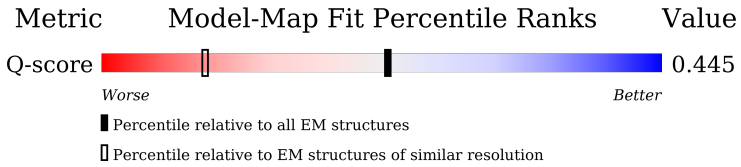
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





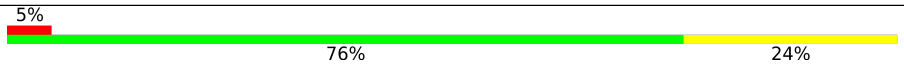
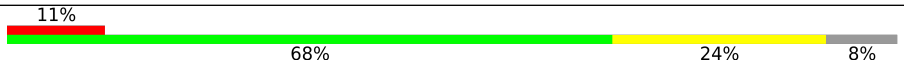
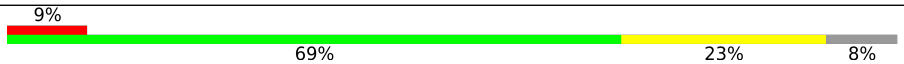
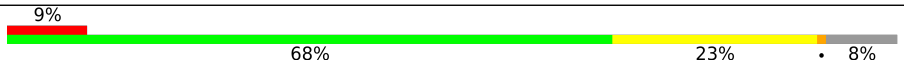
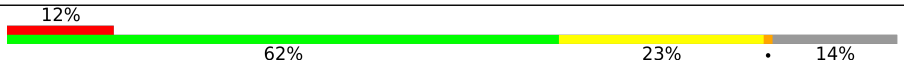
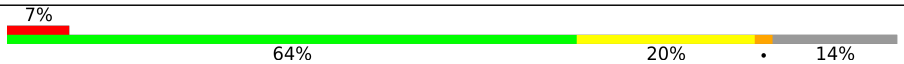
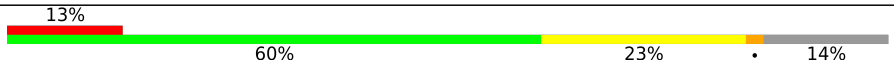
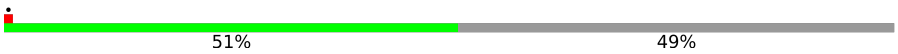
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	aA	755	75% 21%
1	bA	755	75% 21%
1	cA	755	74% 22%
2	aB	740	77% 21%

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Mol	Chain	Length	Quality of chain
2	bB	740	
2	cB	740	
3	aC	80	
3	bC	80	
3	cC	80	
4	aD	138	
4	bD	138	
4	cD	138	
5	aE	75	
5	bE	75	
5	cE	75	
6	aF	164	
6	bF	164	
6	cF	164	
7	aI	38	
7	bI	38	
7	cI	38	
8	aJ	41	
8	bJ	41	
8	cJ	41	
9	aK	85	
9	bK	85	
9	cK	85	
10	aL	154	
10	bL	154	

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Mol	Chain	Length	Quality of chain
10	cL	154	78% 19%
11	aM	31	65% 29% 6%
11	bM	31	65% 29% 6%
11	cM	31	68% 29%
12	aX	35	77% 17%
12	bX	35	77% 6% 17%
12	cX	35	71% 11% 17%
13	a1	358	48% 66% 23% 8%
13	a2	358	52% 63% 26% 9%
13	a3	358	37% 67% 23% 7%
13	a4	358	41% 67% 24% 6%
13	a5	358	48% 67% 23% 7%
13	a6	358	54% 66% 22% 8%
13	b1	358	49% 68% 22% 8%
13	b2	358	53% 65% 23% 9%
13	b3	358	38% 67% 23% 7%
13	b4	358	39% 68% 22% 6%
13	b5	358	48% 69% 21% 7%
13	b6	358	53% 66% 22% 8%
13	c1	358	50% 68% 22% 8%
13	c2	358	52% 64% 24% 9%
13	c3	358	39% 68% 22% 7%
13	c4	358	40% 69% 22% 6%
13	c5	358	48% 66% 23% 7%
13	c6	358	54% 66% 22% 8%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 137634 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	bA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	cA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	bB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	cB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	bC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	cC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	cD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	69	Total	C	N	O	0	0
			539	342	93	104		
5	bE	69	Total	C	N	O	0	0
			539	342	93	104		
5	cE	69	Total	C	N	O	0	0
			539	342	93	104		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	bF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	cF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	bI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	cI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		
8	bJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	cJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	aK	43	Total	C	N	O	0	0
			208	122	43	43		
9	bK	43	Total	C	N	O	0	0
			208	122	43	43		
9	cK	43	Total	C	N	O	0	0
			208	122	43	43		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	bL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	cL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	bM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	cM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

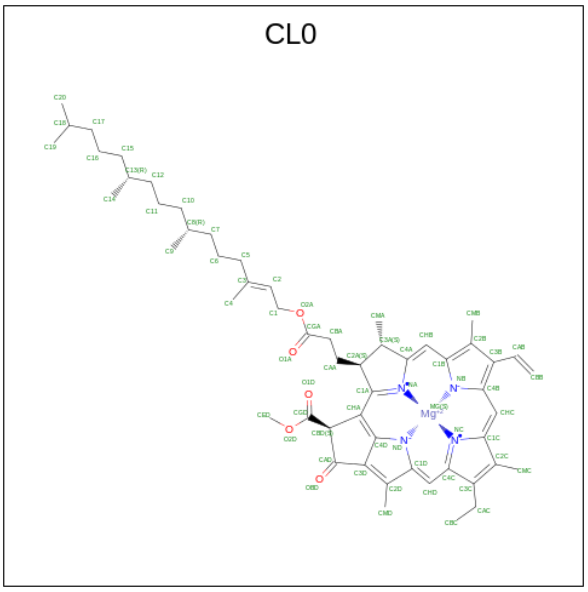
- Molecule 12 is a protein called Photosystem I reaction center subunit psaX.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	29	Total	C	N	O	0	0
			233	164	34	35		
12	bX	29	Total	C	N	O	0	0
			233	164	34	35		
12	cX	29	Total	C	N	O	0	0
			233	164	34	35		

- Molecule 13 is a protein called Iron stress in-duced protein A.

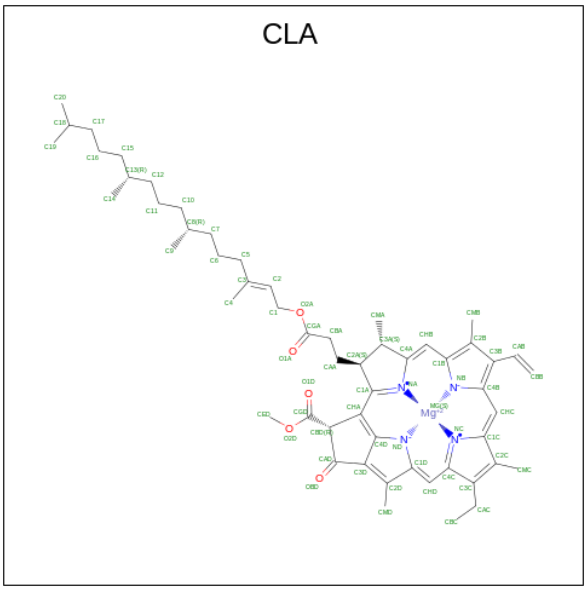
Mol	Chain	Residues	Atoms					AltConf	Trace
13	a1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	a2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	a3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	a5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	b3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	b5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	c3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	c5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		

- Molecule 14 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	aK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	a1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	bA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	bK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	cA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	cK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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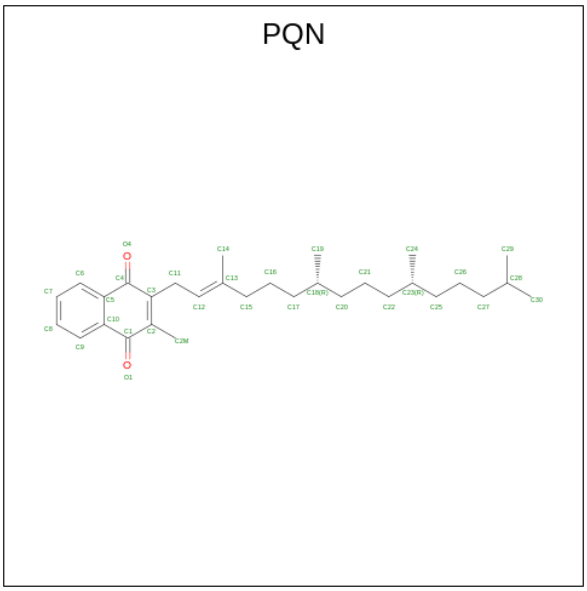
Mol	Chain	Residues	Atoms					AltConf
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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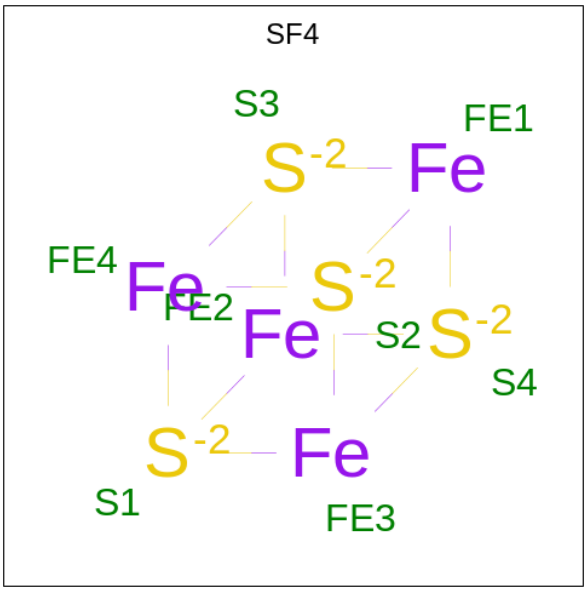
Mol	Chain	Residues	Atoms					AltConf
15	c5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



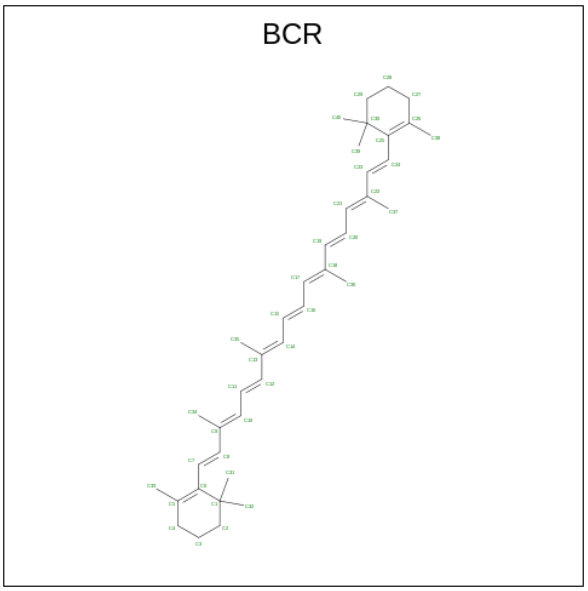
Mol	Chain	Residues	Atoms	AltConf
16	aA	1	Total C O 33 31 2	0
16	aB	1	Total C O 33 31 2	0
16	bA	1	Total C O 33 31 2	0
16	bB	1	Total C O 33 31 2	0
16	cA	1	Total C O 33 31 2	0
16	cB	1	Total C O 33 31 2	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total Fe S 8 4 4	0
17	aC	1	Total Fe S 8 4 4	0
17	aC	1	Total Fe S 8 4 4	0
17	bA	1	Total Fe S 8 4 4	0
17	bC	1	Total Fe S 8 4 4	0
17	bC	1	Total Fe S 8 4 4	0
17	cA	1	Total Fe S 8 4 4	0
17	cC	1	Total Fe S 8 4 4	0
17	cC	1	Total Fe S 8 4 4	0

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 25 25	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aF	1	Total C 40 40	0
18	aF	1	Total C 40 40	0
18	aF	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	aI	1	Total C 40 40	0
18	aI	1	Total C 40 40	0
18	aI	1	Total C 40 40	0
18	aJ	1	Total C 40 40	0
18	aJ	1	Total C 40 40	0
18	aK	1	Total C 40 40	0
18	aL	1	Total C 40 40	0
18	aM	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	bB	1	Total C 25 25	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bF	1	Total C 40 40	0
18	bI	1	Total C 40 40	0
18	bI	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bM	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b2	1	Total C 40 40	0
18	b2	1	Total C 40 40	0
18	b2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	b2	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0

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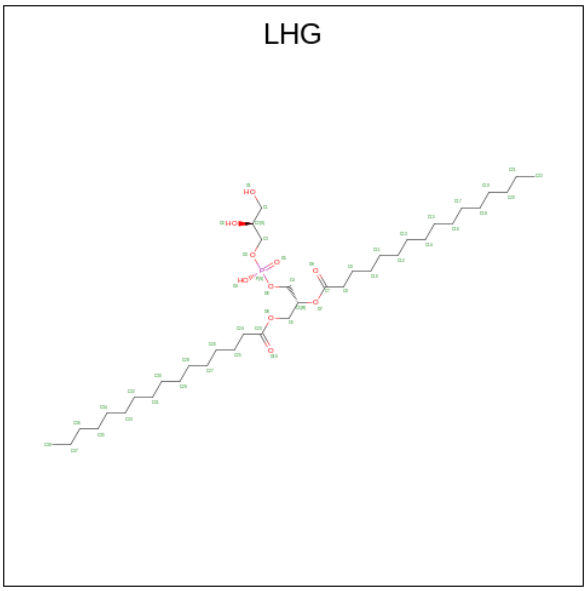
Mol	Chain	Residues	Atoms	AltConf
18	cA	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 25 25	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cI	1	Total C 40 40	0
18	cI	1	Total C 40 40	0
18	cJ	1	Total C 40 40	0
18	cJ	1	Total C 40 40	0
18	cK	1	Total C 40 40	0
18	cL	1	Total C 40 40	0
18	cM	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0

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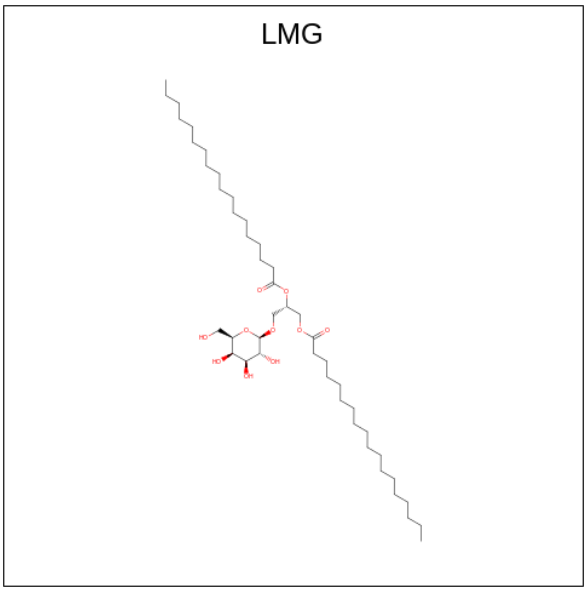
Mol	Chain	Residues	Atoms	AltConf
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
19	aA	1	Total	C	O	P	0
			49	38	10	1	
19	aA	1	Total	C	O	P	0
			27	16	10	1	
19	aX	1	Total	C	O	P	0
			23	12	10	1	
19	bA	1	Total	C	O	P	0
			49	38	10	1	
19	bA	1	Total	C	O	P	0
			27	16	10	1	
19	bX	1	Total	C	O	P	0
			23	12	10	1	
19	cA	1	Total	C	O	P	0
			49	38	10	1	
19	cA	1	Total	C	O	P	0
			27	16	10	1	
19	cX	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
20	aB	1	Total C O 55 45 10	0
20	bB	1	Total C O 55 45 10	0
20	cB	1	Total C O 55 45 10	0

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
21	aL	1	Total Ca 1 1	0
21	bL	1	Total Ca 1 1	0
21	cL	1	Total Ca 1 1	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	aA	3	Total O 3 3	0
22	aB	3	Total O 3 3	0
22	aL	1	Total O 1 1	0

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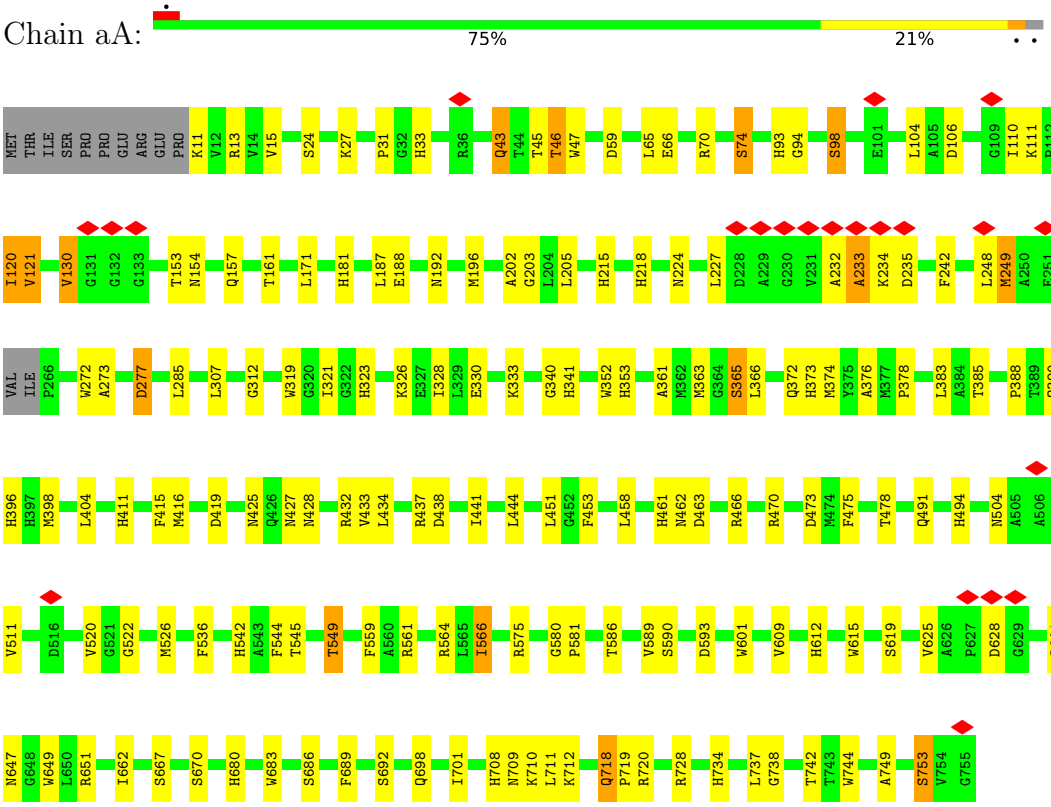
Mol	Chain	Residues	Atoms	AltConf
22	bA	3	Total O 3 3	0
22	bB	3	Total O 3 3	0
22	bL	1	Total O 1 1	0
22	cA	2	Total O 2 2	0
22	cB	3	Total O 3 3	0
22	cF	1	Total O 1 1	0
22	cL	1	Total O 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

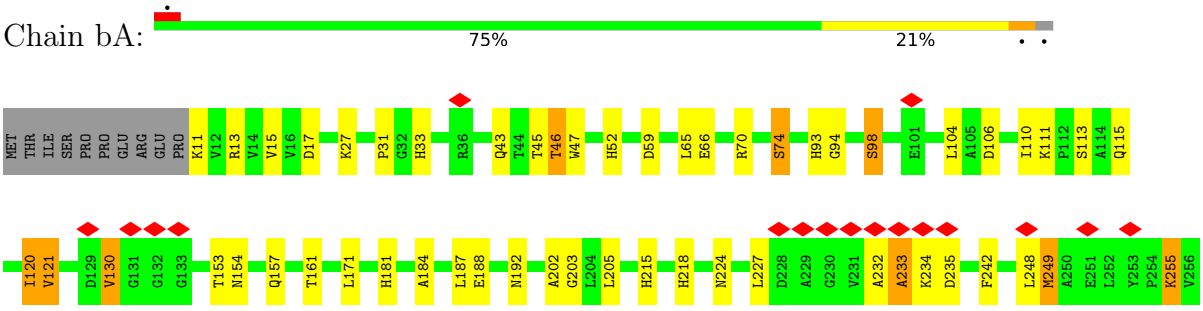
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

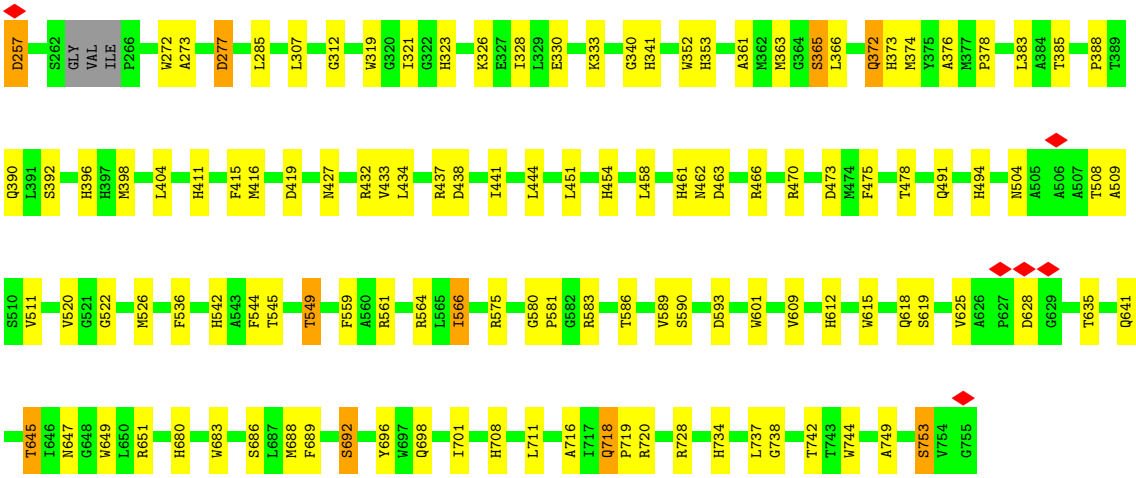
Chain aA:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain bA:

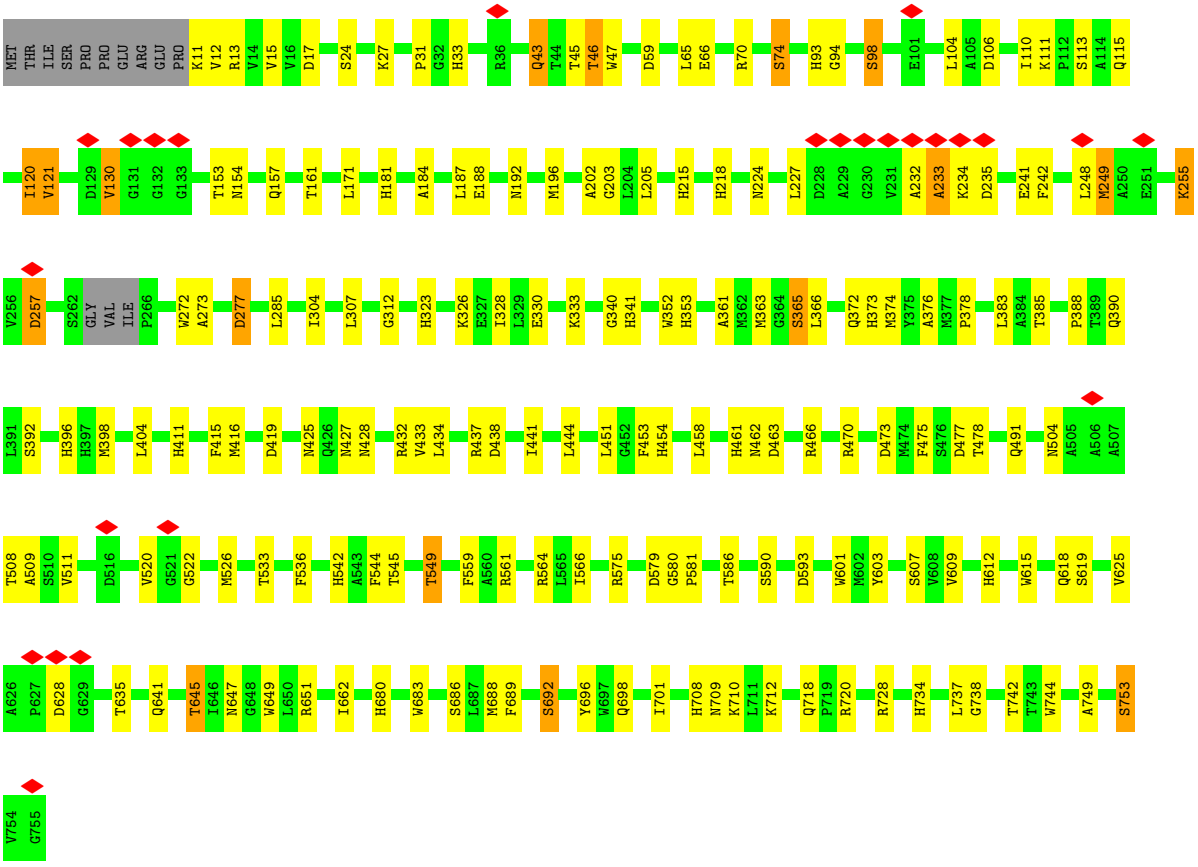




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:

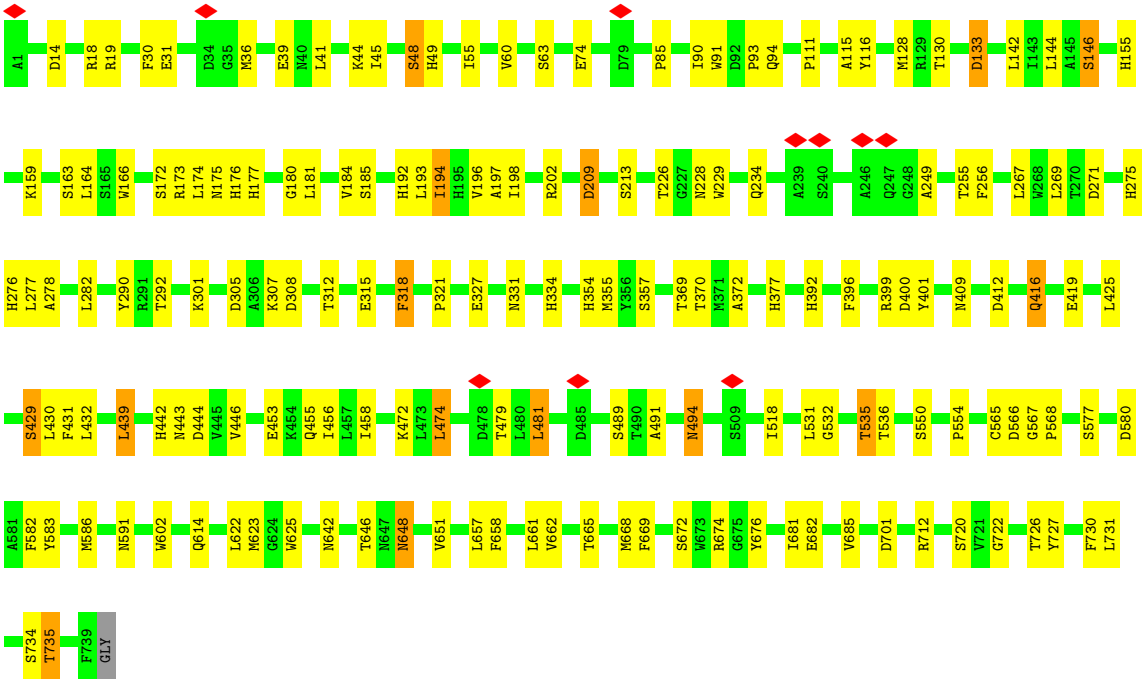




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain aB:

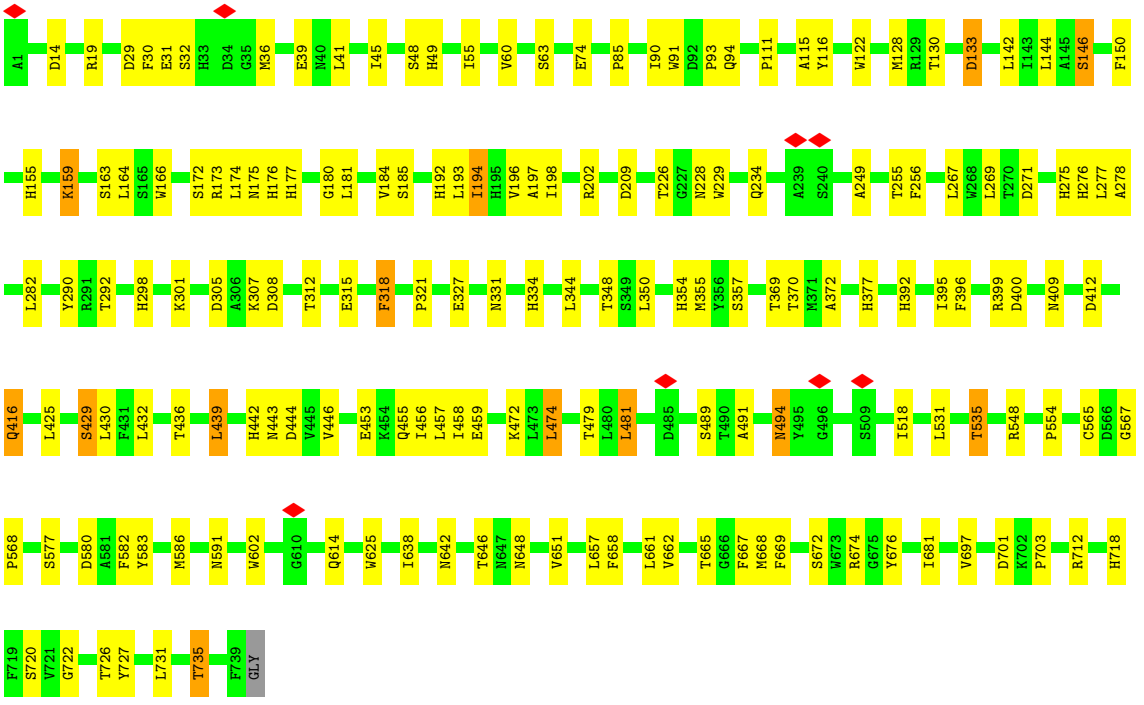




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB:

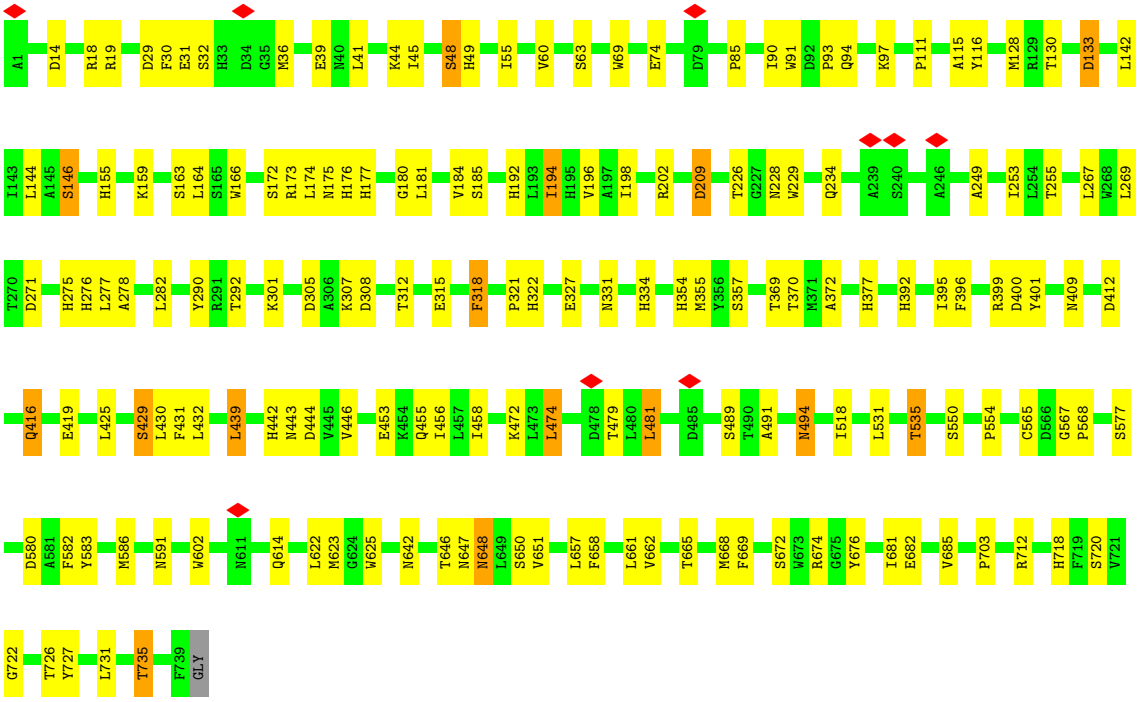




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB:

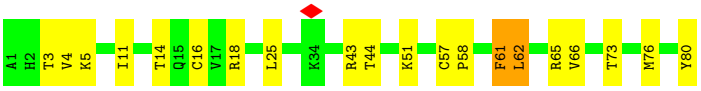




• Molecule 3: Photosystem I iron-sulfur center

Chain aC:

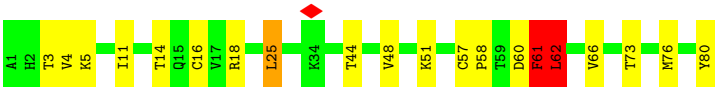




• Molecule 3: Photosystem I iron-sulfur center

Chain bC:

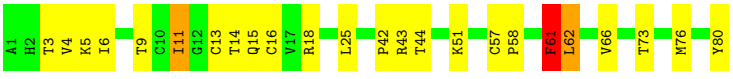




• Molecule 3: Photosystem I iron-sulfur center

Chain cC:

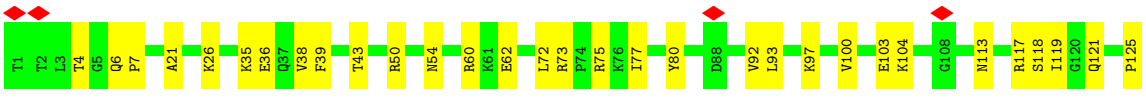


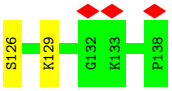


• Molecule 4: Photosystem I reaction center subunit II

Chain aD:

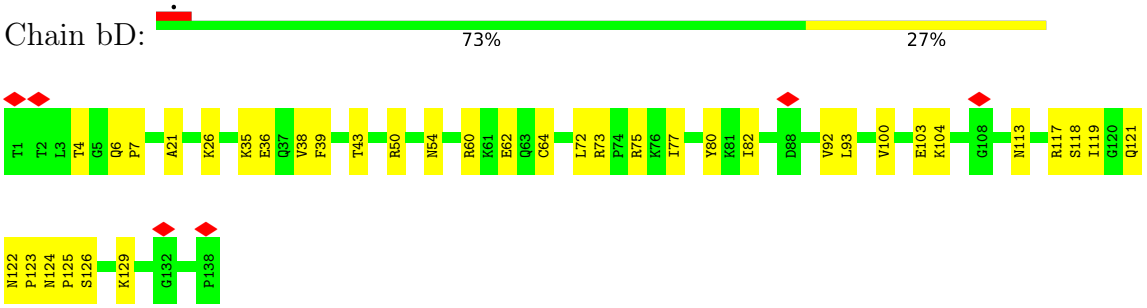






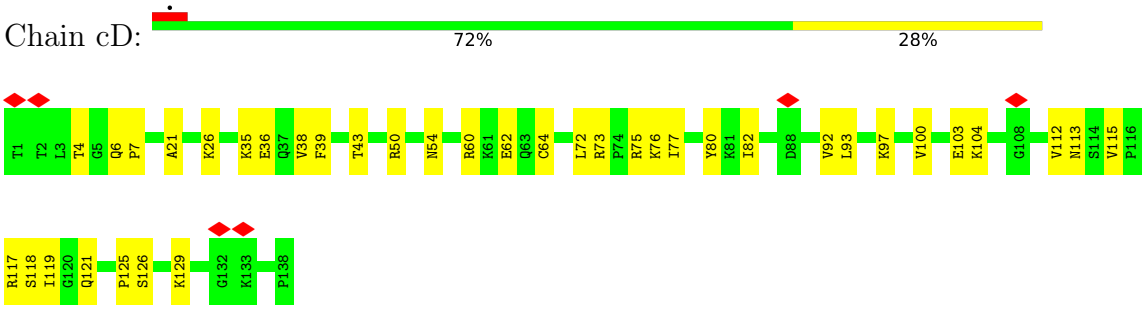
• Molecule 4: Photosystem I reaction center subunit II

Chain bD:



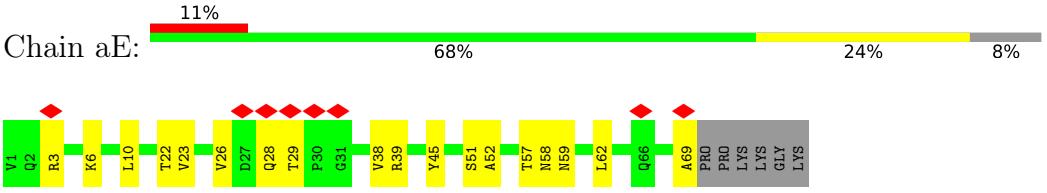
• Molecule 4: Photosystem I reaction center subunit II

Chain cD:



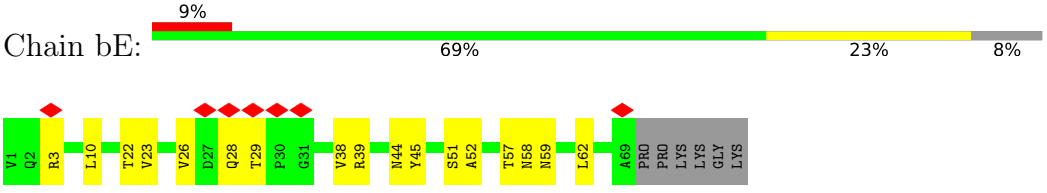
• Molecule 5: Photosystem I reaction center subunit IV

Chain aE:



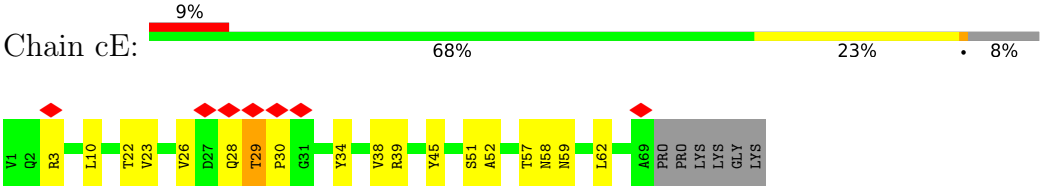
• Molecule 5: Photosystem I reaction center subunit IV

Chain bE:



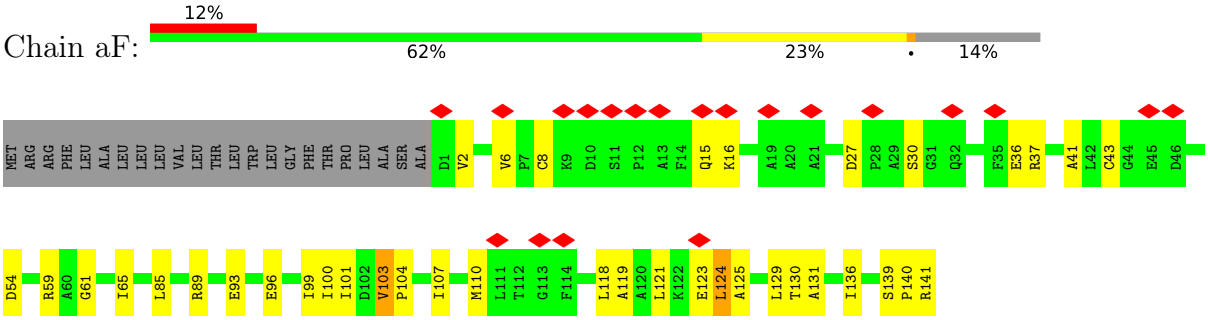
• Molecule 5: Photosystem I reaction center subunit IV

Chain cE:



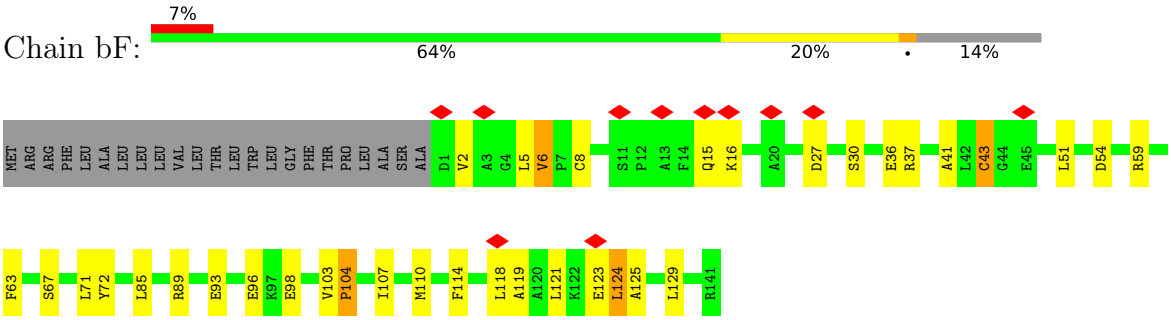
• Molecule 6: Photosystem I reaction center subunit III

Chain aF:



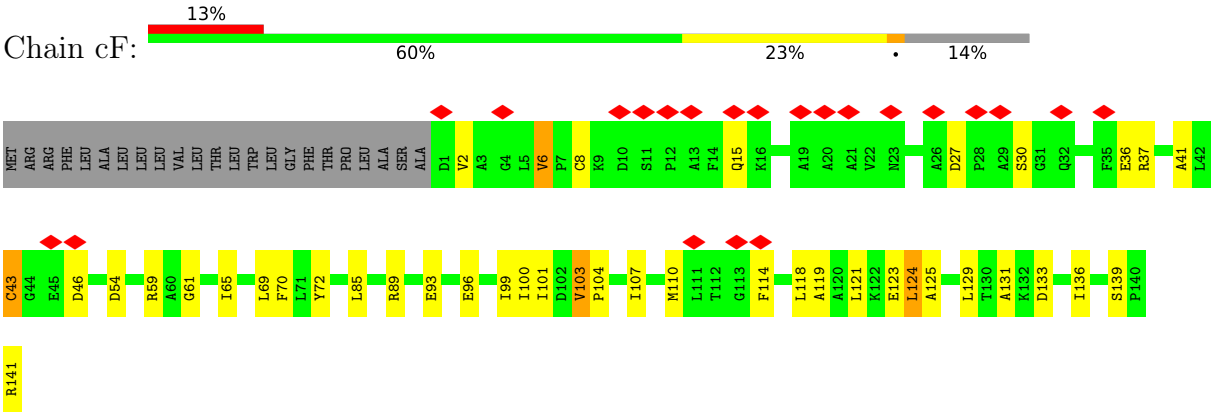
• Molecule 6: Photosystem I reaction center subunit III

Chain bF:



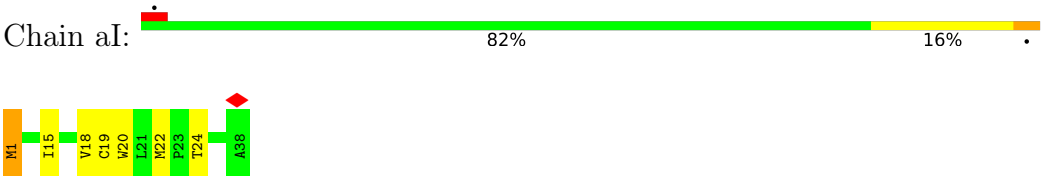
• Molecule 6: Photosystem I reaction center subunit III

Chain cF:



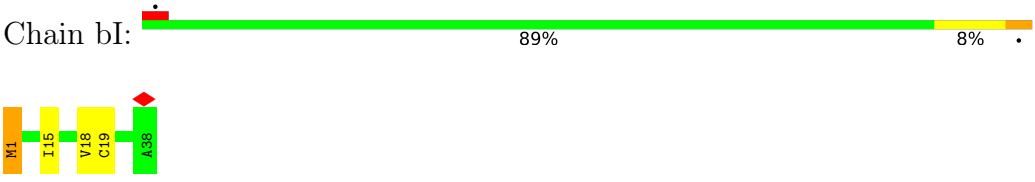
• Molecule 7: Photosystem I reaction center subunit VIII

Chain aI:



• Molecule 7: Photosystem I reaction center subunit VIII

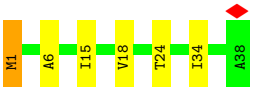
Chain bI:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain cI:

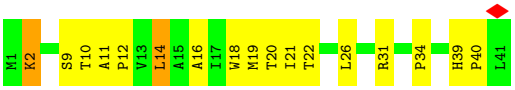




• Molecule 8: Photosystem I reaction center subunit IX

Chain aJ:

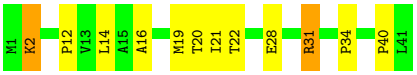




• Molecule 8: Photosystem I reaction center subunit IX

Chain bJ:

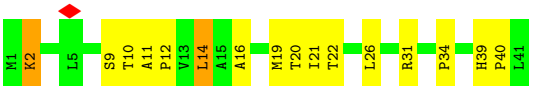




• Molecule 8: Photosystem I reaction center subunit IX

Chain cJ:

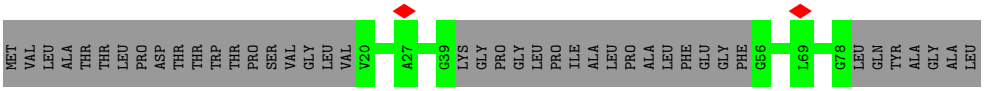




• Molecule 9: Photosystem I reaction center subunit PsaK

Chain aK:

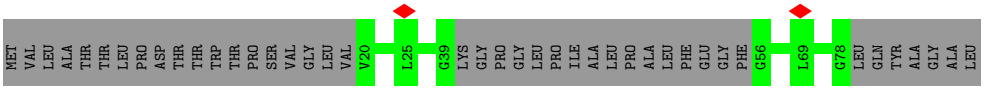




• Molecule 9: Photosystem I reaction center subunit PsaK

Chain bK:

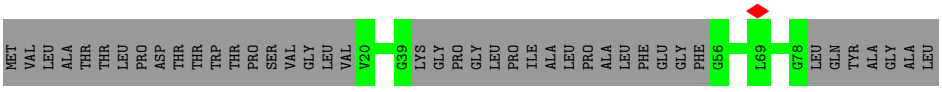




• Molecule 9: Photosystem I reaction center subunit PsaK

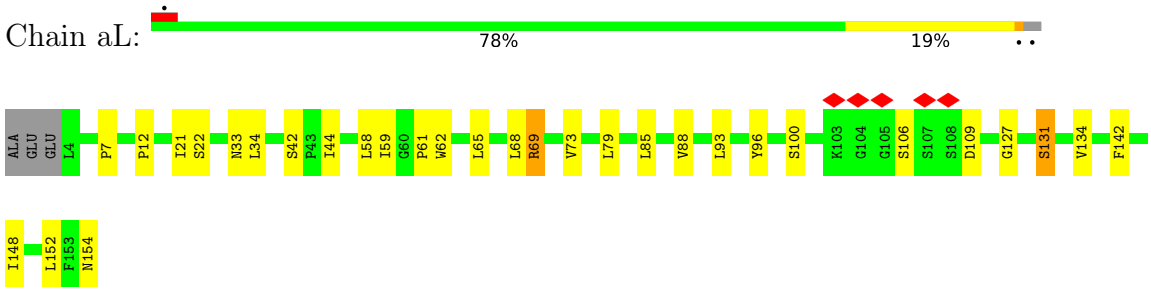
Chain cK:





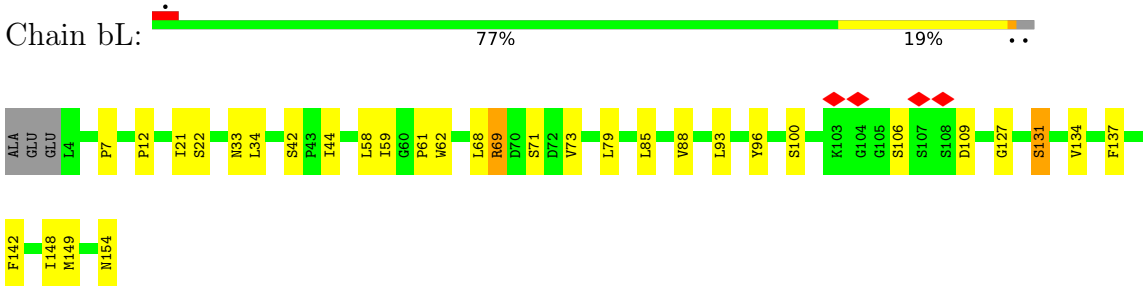
• Molecule 10: Photosystem I reaction center subunit XI

Chain aL:



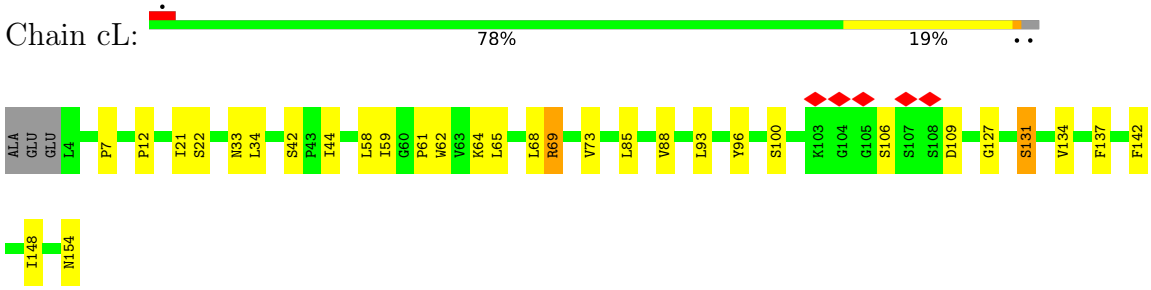
• Molecule 10: Photosystem I reaction center subunit XI

Chain bL:



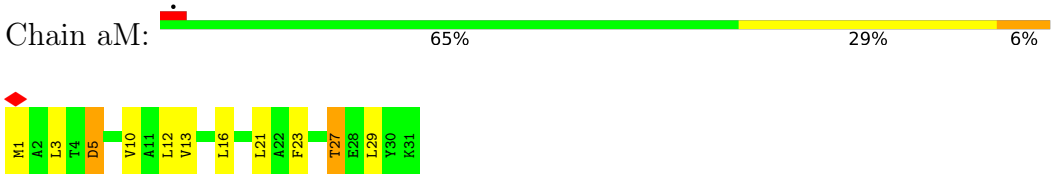
• Molecule 10: Photosystem I reaction center subunit XI

Chain cL:



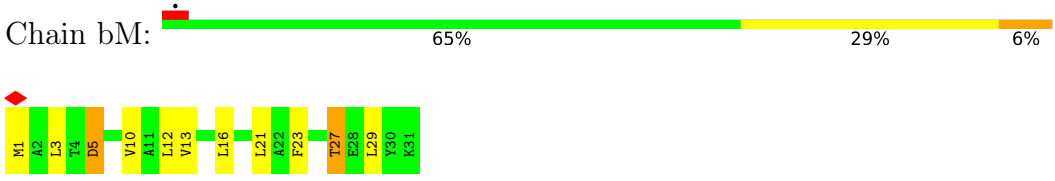
• Molecule 11: Photosystem I reaction center subunit XII

Chain aM:



• Molecule 11: Photosystem I reaction center subunit XII

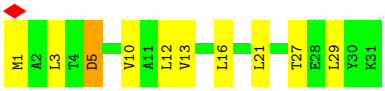
Chain bM:



• Molecule 11: Photosystem I reaction center subunit XII

Chain cM:

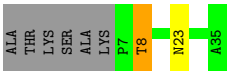




• Molecule 12: Photosystem I reaction center subunit psaX

Chain aX:

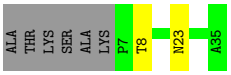




• Molecule 12: Photosystem I reaction center subunit psaX

Chain bX:

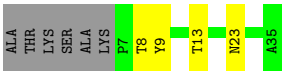




• Molecule 12: Photosystem I reaction center subunit psaX

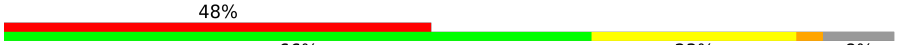
Chain cX:

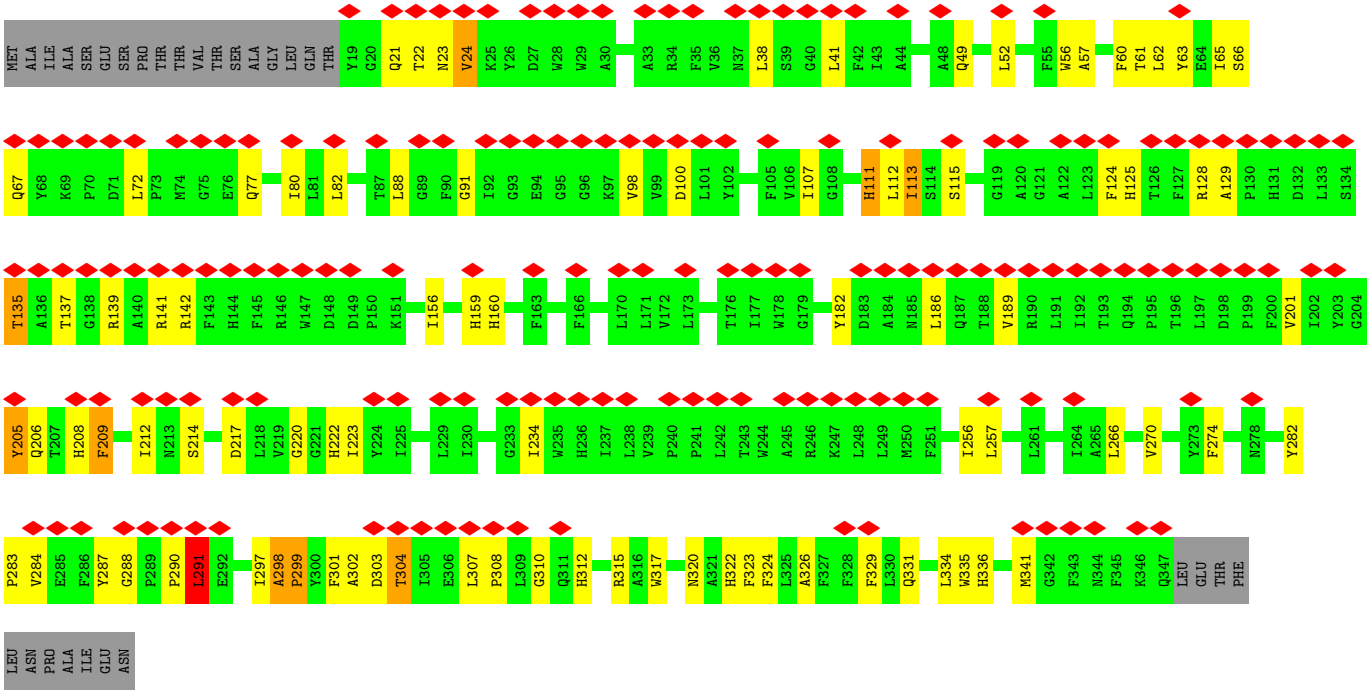




• Molecule 13: Iron stress in-duced protein A

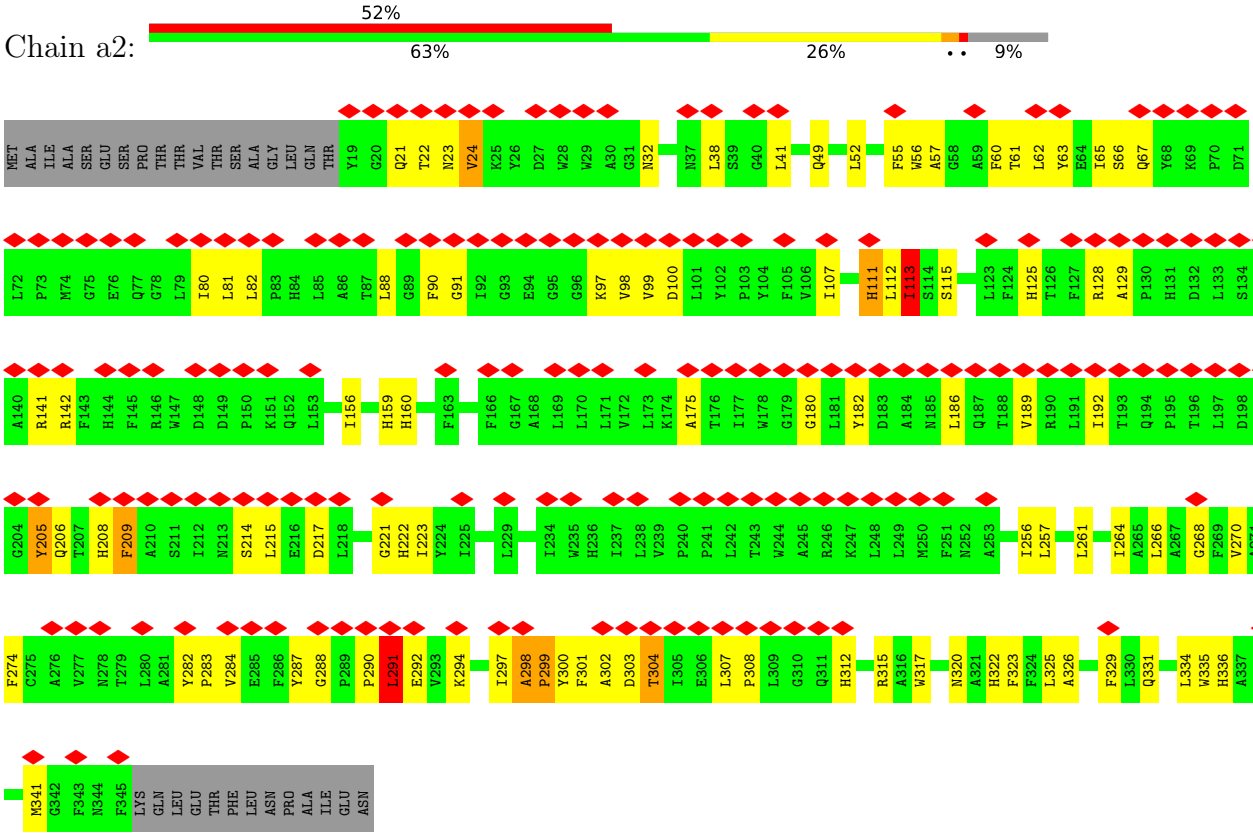
Chain a1:





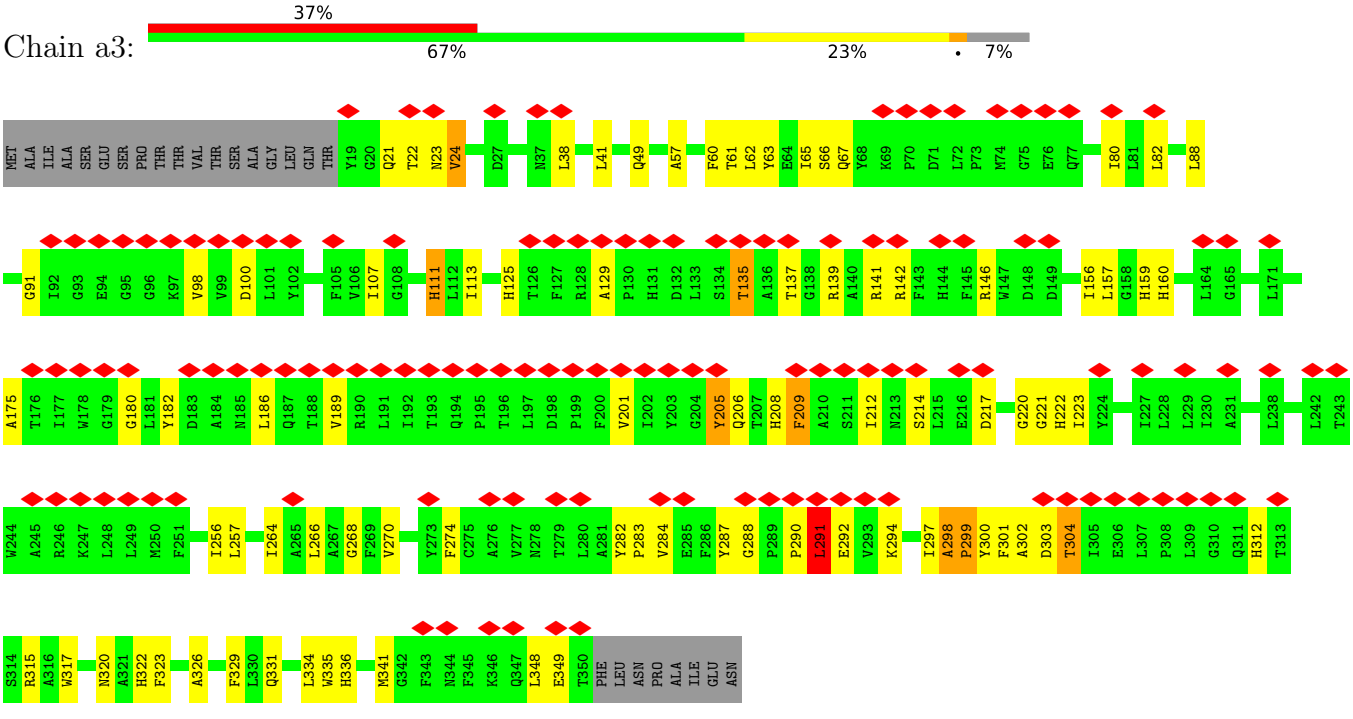
• Molecule 13: Iron stress in-duced protein A

Chain a2:



• Molecule 13: Iron stress in-duced protein A

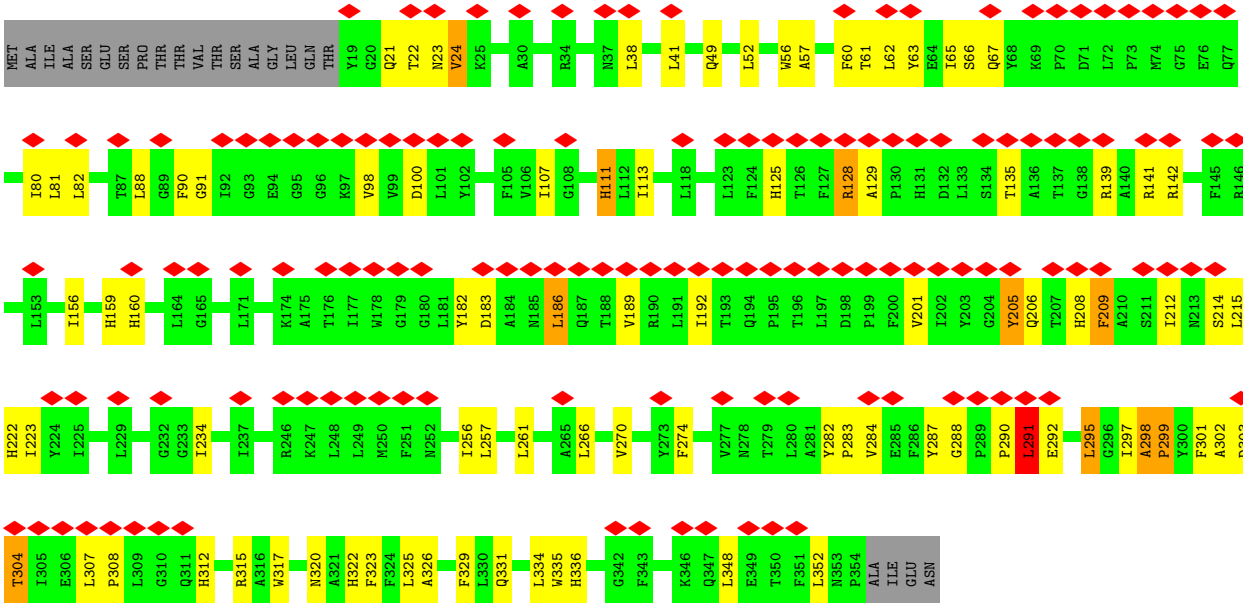
Chain a3:



• Molecule 13: Iron stress in-duced protein A

Chain a4:

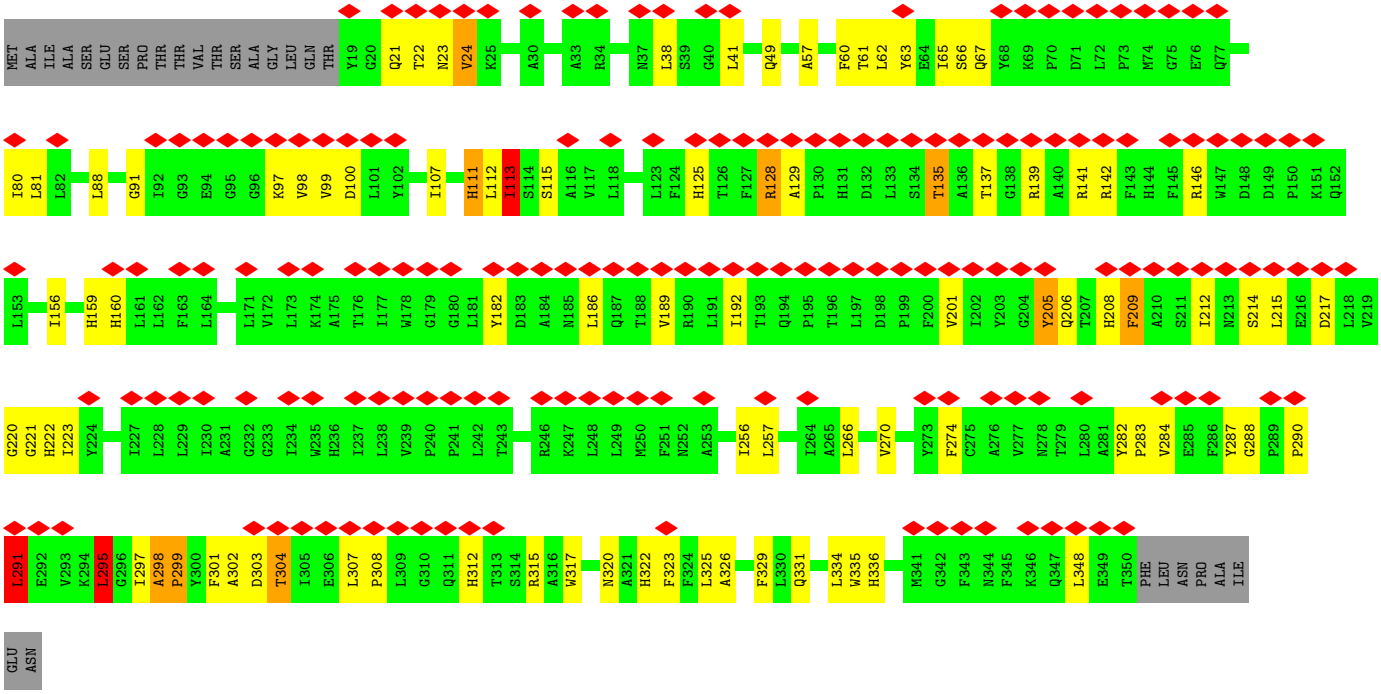




• Molecule 13: Iron stress in-duced protein A

Chain a5:

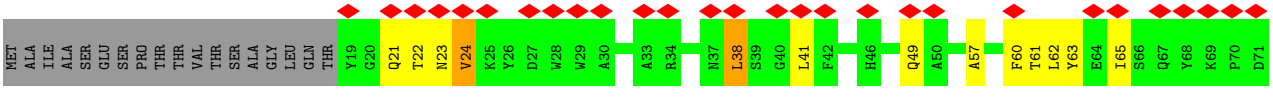


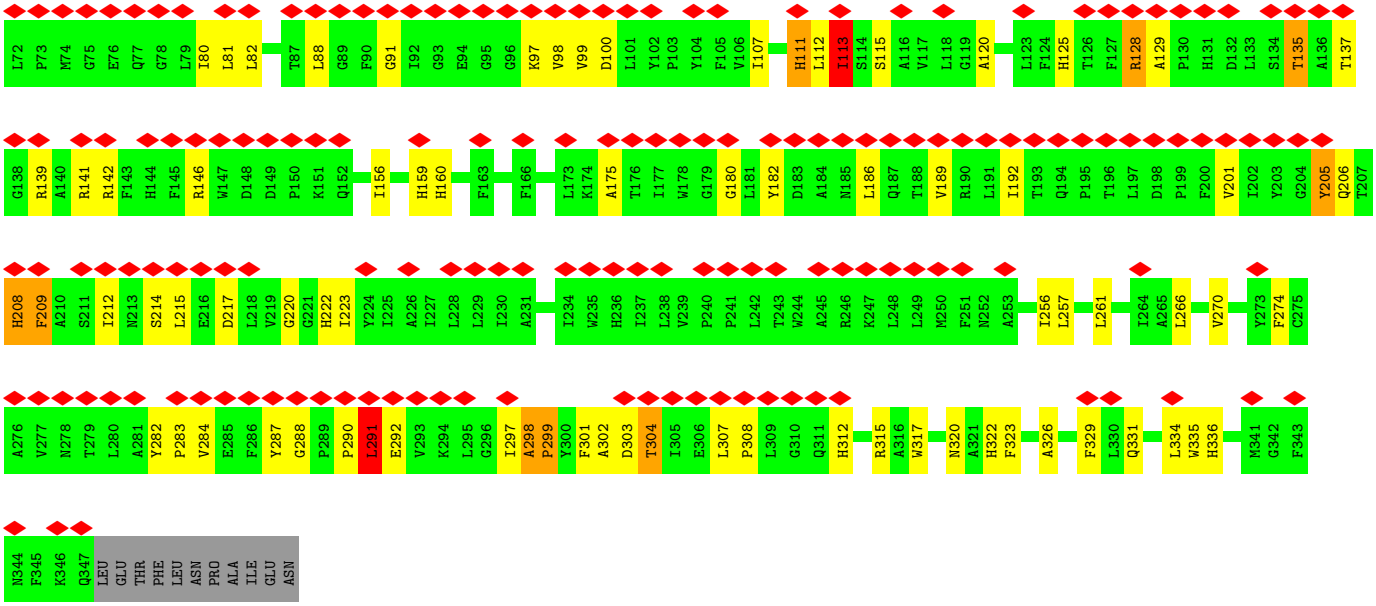


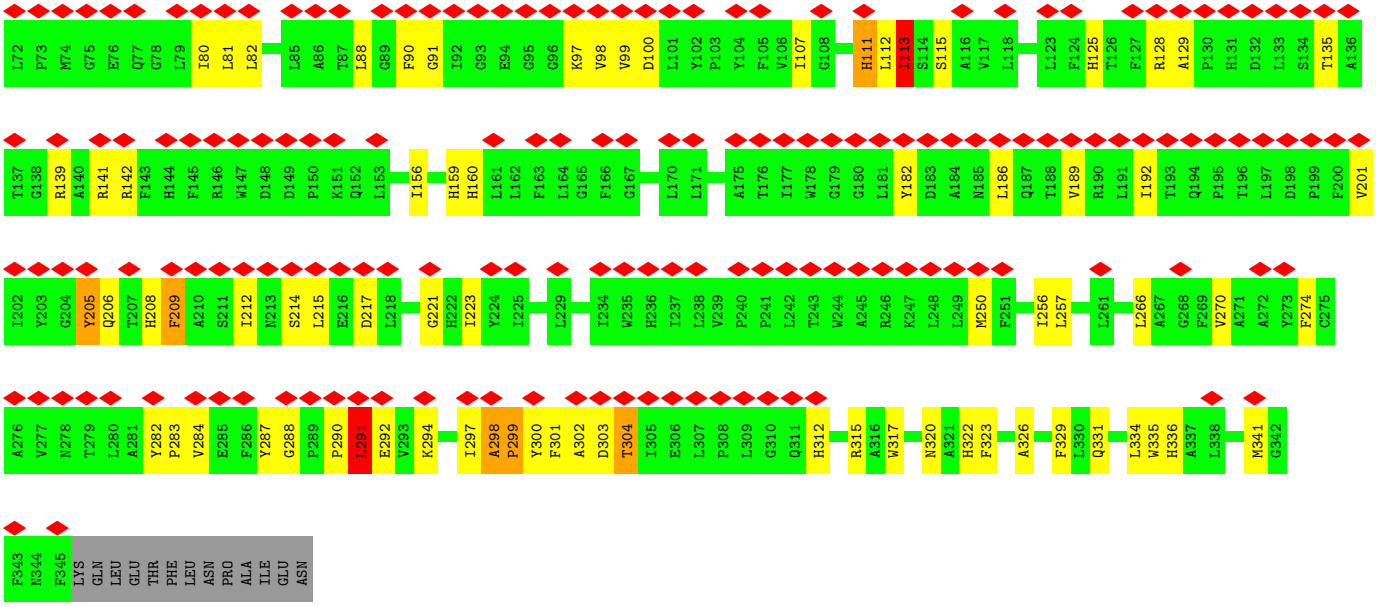
• Molecule 13: Iron stress in-duced protein A

Chain a6:





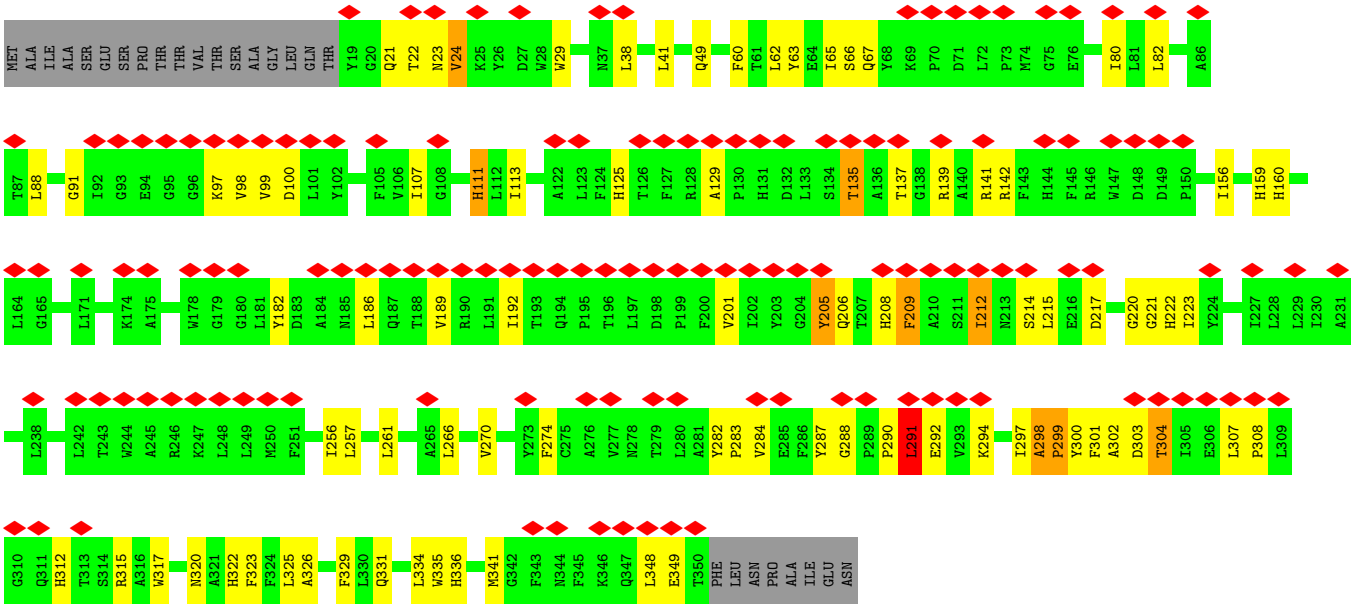




• Molecule 13: Iron stress in-duced protein A

Chain b3:

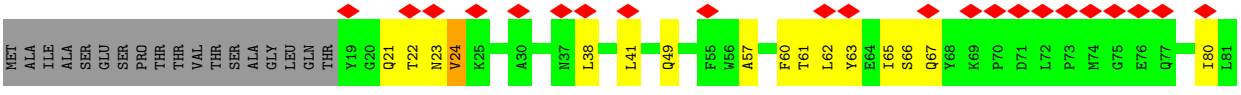


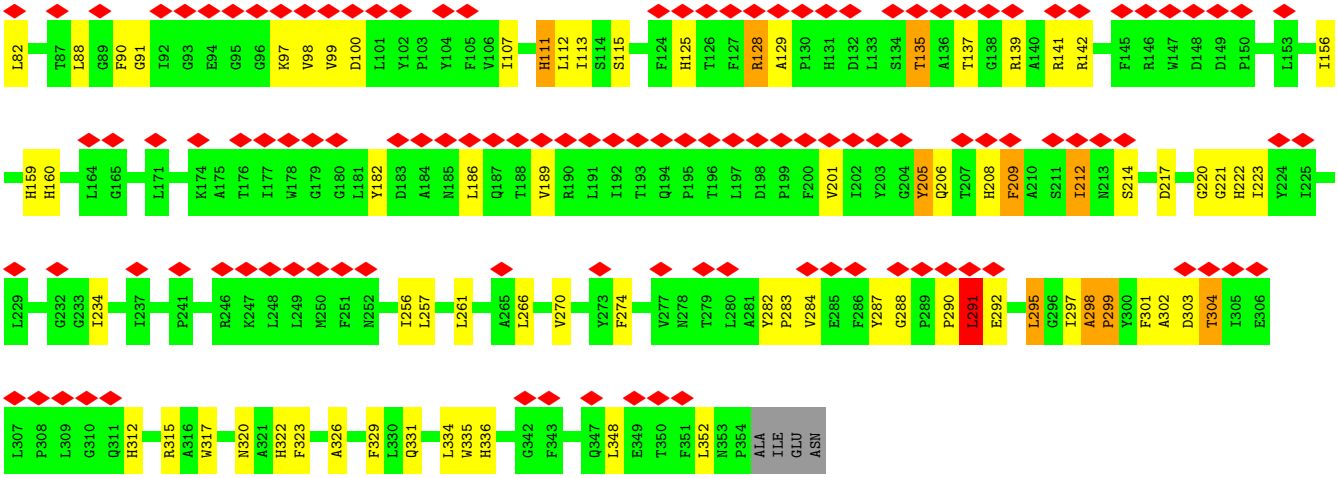


• Molecule 13: Iron stress in-duced protein A

Chain b4:



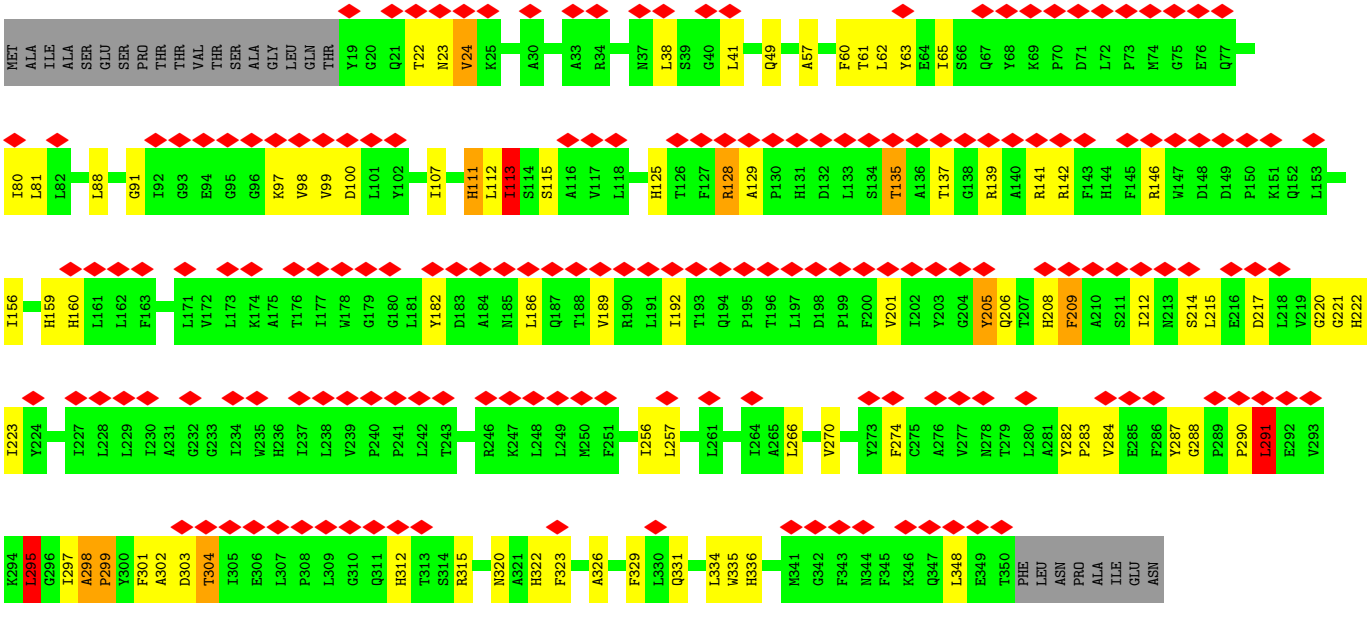




• Molecule 13: Iron stress in-duced protein A

Chain b5:

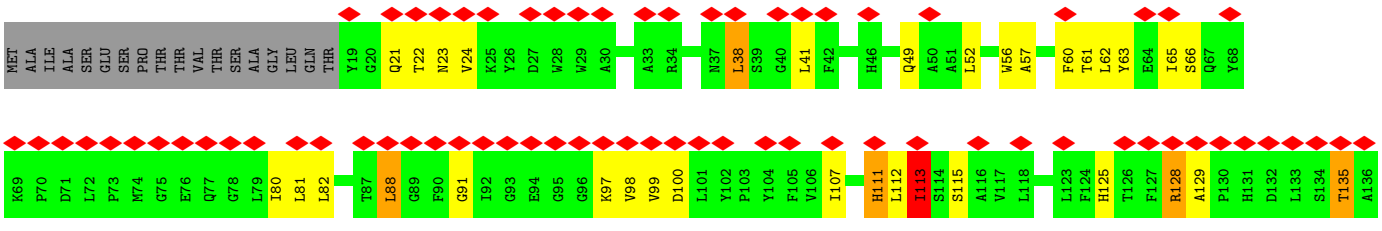


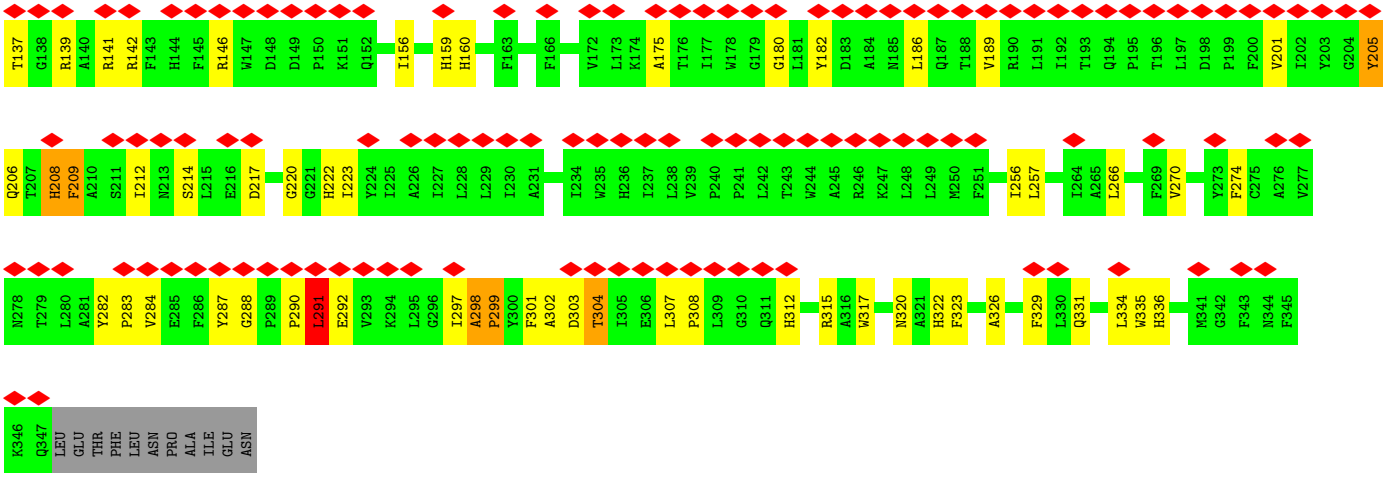


• Molecule 13: Iron stress in-duced protein A

Chain b6:



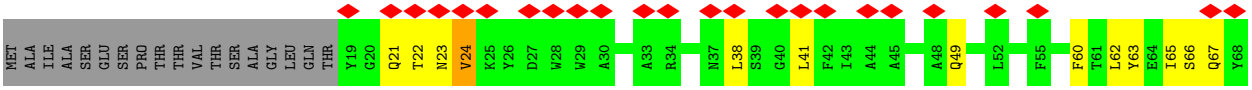


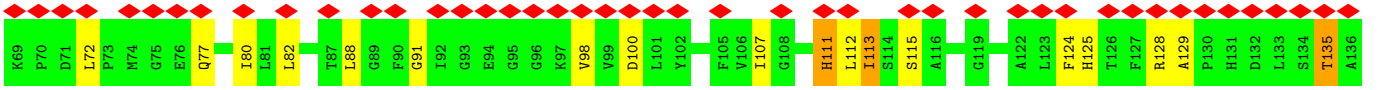


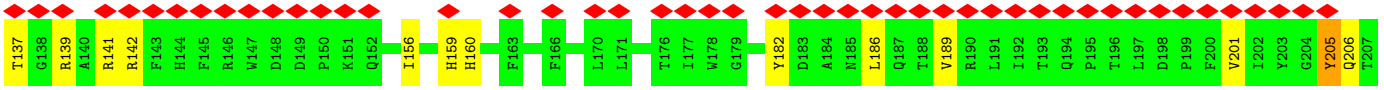
• Molecule 13: Iron stress in-duced protein A

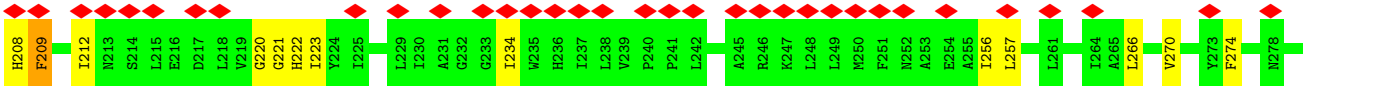
Chain c1:

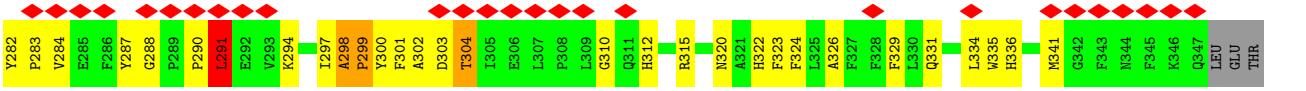








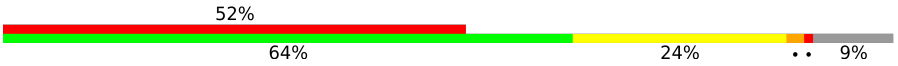


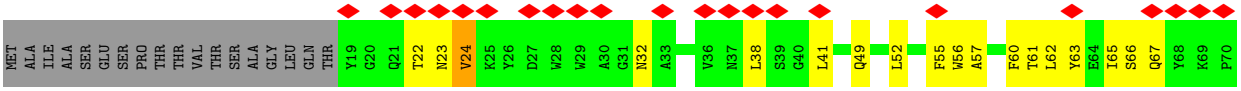


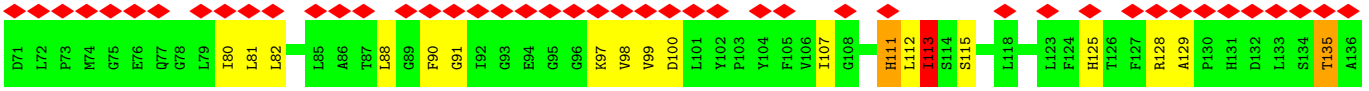


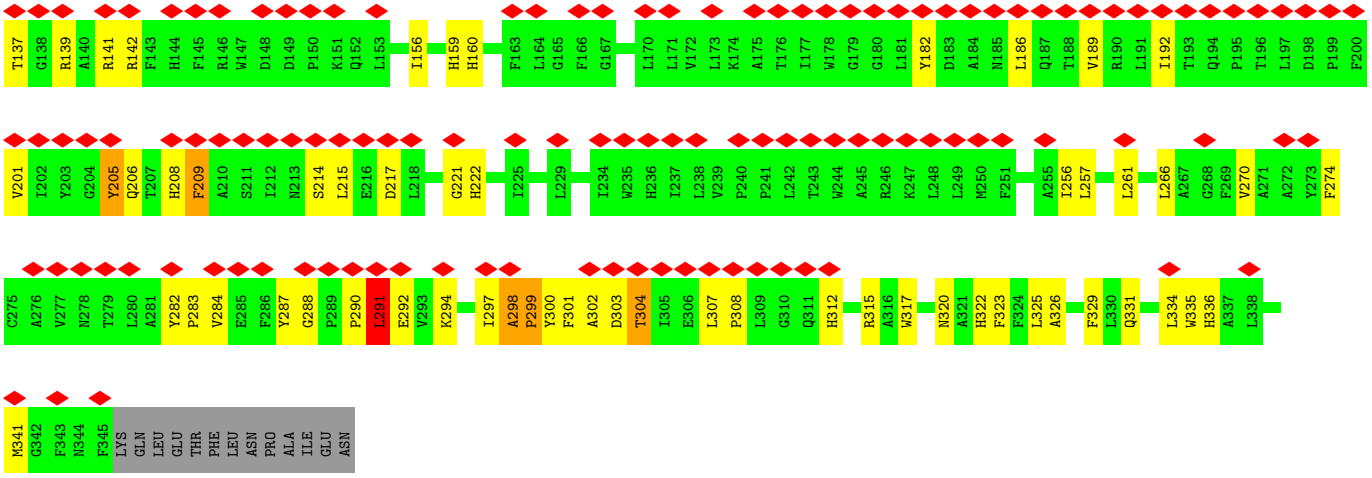
• Molecule 13: Iron stress in-duced protein A

Chain c2:





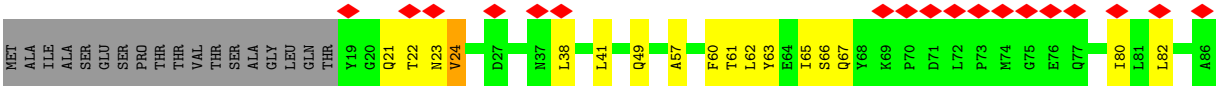


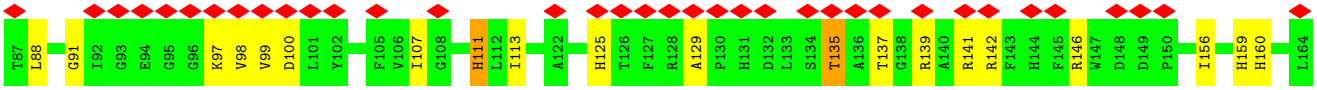


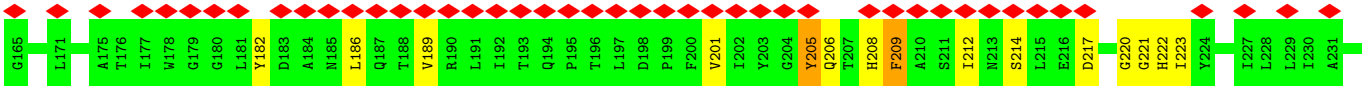
• Molecule 13: Iron stress in-duced protein A

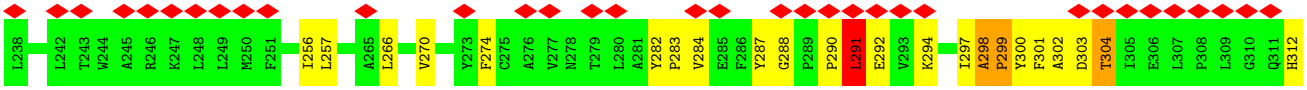
Chain c3:

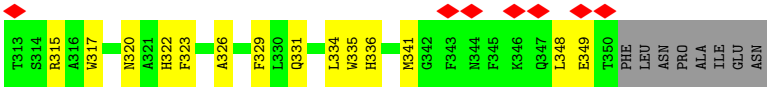








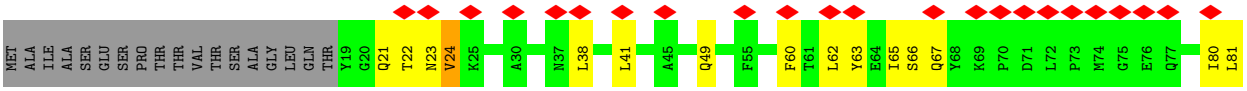




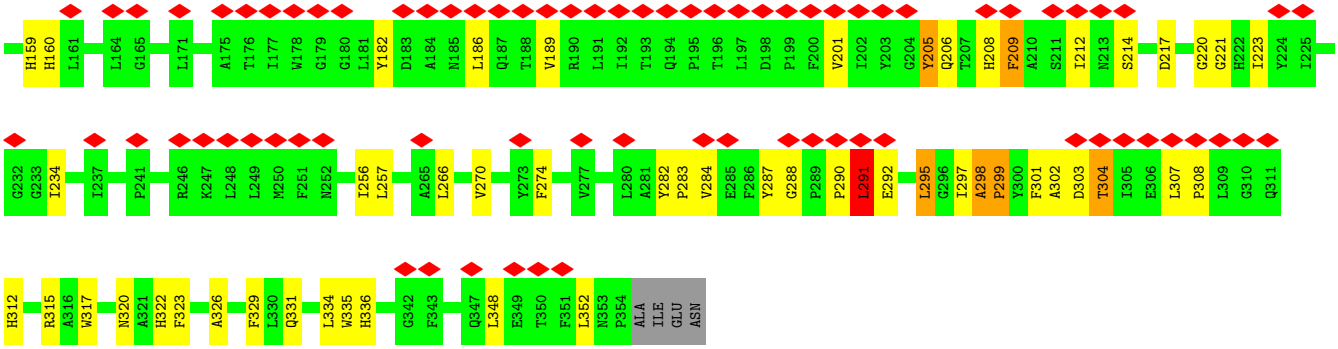
• Molecule 13: Iron stress in-duced protein A

Chain c4:





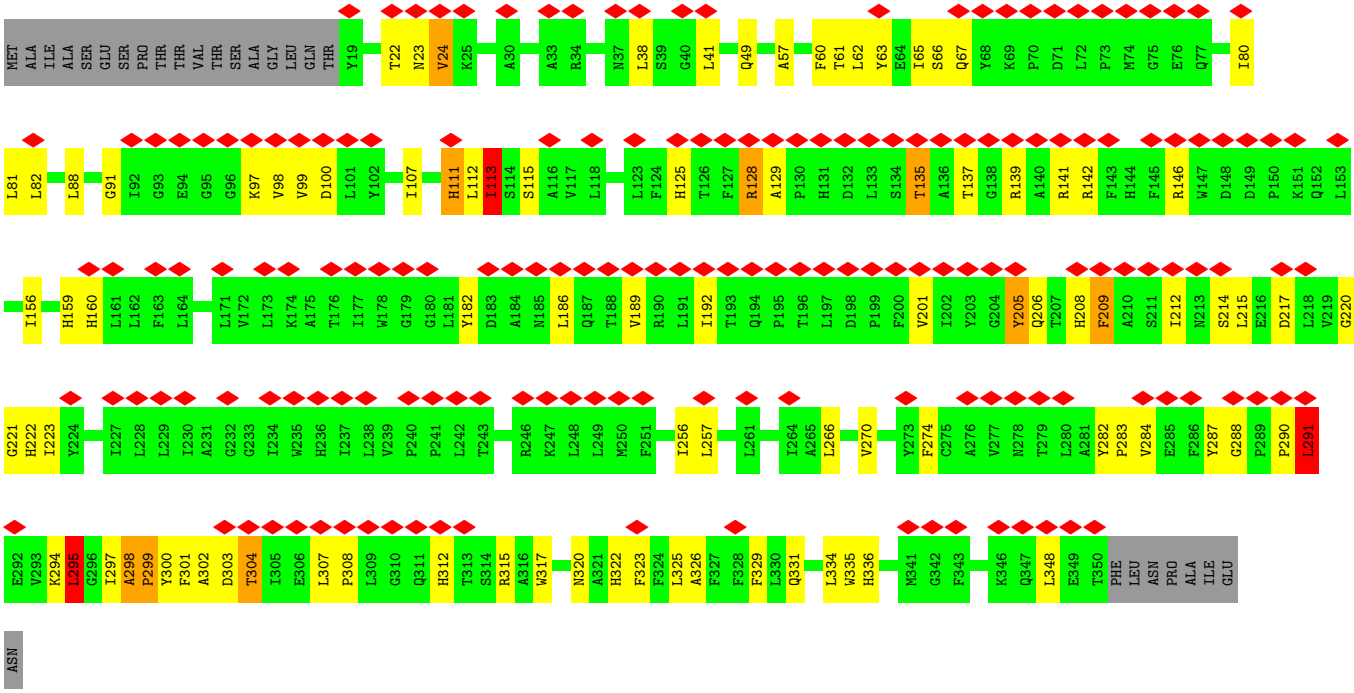




• Molecule 13: Iron stress in-duced protein A

Chain c5:

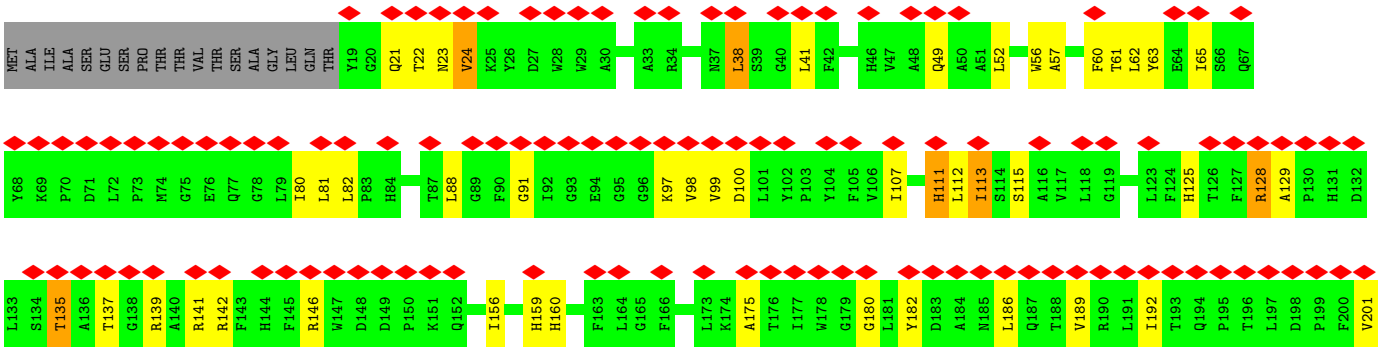


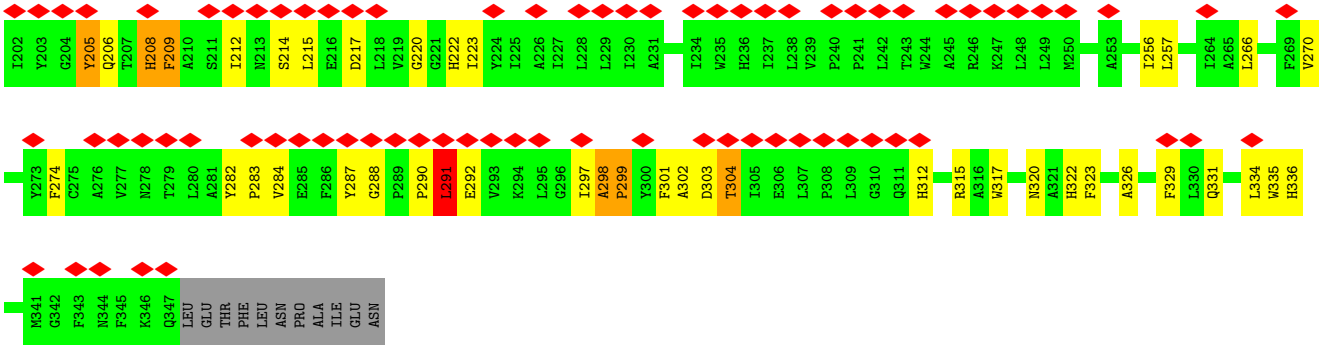


• Molecule 13: Iron stress in-duced protein A

Chain c6:






I202 Y203 G204 Y205 Q206 T207 H208 F209 A210 S211 I212 N213 S214 L215 E216 D217 L218 V219 G220 G221 H222 I223 Y224 I225 A226 I227 L228 L229 I230 A231 I234 W235 H236 I237 L238 V239 P240 P241 L242 T243 W244 A245 R246 K247 L248 L249 M250 A253 I256 L257 I264 A265 L266 F269 V270
Y273 F274 C275 A276 V277 N278 T279 L280 A281 Y282 P283 V284 E285 F286 Y287 G288 P289 P290 L291 E292 V293 K294 L295 G296 I297 A298 P299 Y300 F301 A302 D303 T304 I305 E306 L307 P308 L309 G310 Q311 H312 R315 A316 W317 N320 A321 H322 F323 A326 F329 L330 Q331 L334 W335 H336
M341 G342 F343 N344 F345 K346 Q347 LEU GLU THR PHE LEU ASN PRO ALA ILE GLU ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	303983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.291	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	534.24, 534.24, 534.24	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, LMG, CLA, CA, PQN, SF4, BCR, LHG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	aA	0.53	0/6000	0.54	0/8180
1	bA	0.53	0/6000	0.54	0/8180
1	cA	0.53	0/6000	0.54	0/8180
2	aB	0.52	0/6096	0.57	0/8332
2	bB	0.52	0/6096	0.56	0/8332
2	cB	0.52	0/6096	0.57	0/8332
3	aC	0.52	0/608	0.70	2/824 (0.2%)
3	bC	0.52	0/608	0.70	2/824 (0.2%)
3	cC	0.52	0/608	0.70	2/824 (0.2%)
4	aD	0.42	0/1101	0.51	0/1492
4	bD	0.42	0/1101	0.51	0/1492
4	cD	0.42	0/1101	0.51	0/1492
5	aE	0.35	0/551	0.44	0/750
5	bE	0.35	0/551	0.44	0/750
5	cE	0.35	0/551	0.44	0/750
6	aF	0.41	0/1087	0.56	0/1476
6	bF	0.40	0/1087	0.55	0/1476
6	cF	0.41	0/1087	0.55	0/1476
7	aI	0.55	0/312	0.70	0/425
7	bI	0.55	0/312	0.70	0/425
7	cI	0.55	0/312	0.70	0/425
8	aJ	0.47	0/350	0.64	0/477
8	bJ	0.47	0/350	0.64	0/477
8	cJ	0.47	0/350	0.64	0/477
9	aK	0.23	0/206	0.34	0/281
9	bK	0.23	0/206	0.34	0/281
9	cK	0.23	0/206	0.34	0/281
10	aL	0.52	0/1148	0.54	0/1558
10	bL	0.52	0/1148	0.55	0/1558
10	cL	0.52	0/1148	0.54	0/1558
11	aM	0.44	0/244	0.60	0/332
11	bM	0.44	0/244	0.60	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	cM	0.44	0/244	0.60	0/332
12	aX	0.37	0/242	0.42	0/332
12	bX	0.37	0/242	0.42	0/332
12	cX	0.37	0/242	0.42	0/332
13	a1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	a2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	a3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	a4	0.42	1/2731 (0.0%)	0.73	14/3730 (0.4%)
13	a5	0.41	1/2695 (0.0%)	0.75	15/3680 (0.4%)
13	a6	0.40	1/2671 (0.0%)	0.74	15/3647 (0.4%)
13	b1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	b2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	b3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	b4	0.42	1/2731 (0.0%)	0.73	14/3730 (0.4%)
13	b5	0.41	1/2695 (0.0%)	0.75	16/3680 (0.4%)
13	b6	0.40	1/2671 (0.0%)	0.74	15/3647 (0.4%)
13	c1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	c2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	c3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	c4	0.42	1/2731 (0.0%)	0.72	14/3730 (0.4%)
13	c5	0.41	1/2695 (0.0%)	0.75	16/3680 (0.4%)
13	c6	0.40	1/2671 (0.0%)	0.72	14/3647 (0.4%)
All	All	0.46	18/102183 (0.0%)	0.64	256/139401 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	aB	0	1
2	bB	0	1
2	cB	0	1
6	aF	0	1
6	bF	0	1
6	cF	0	1
11	aM	0	1
11	bM	0	1
11	cM	0	1
13	a1	0	3
13	a2	0	3
13	a3	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	a4	0	3
13	a5	0	3
13	a6	0	3
13	b1	0	3
13	b2	0	3
13	b3	0	3
13	b4	0	3
13	b5	0	3
13	b6	0	3
13	c1	0	3
13	c2	0	3
13	c3	0	3
13	c4	0	3
13	c5	0	3
13	c6	0	3
All	All	0	63

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	297	ILE	CB-CG2	-6.66	1.30	1.52
13	b1	297	ILE	CB-CG2	-6.66	1.30	1.52
13	c4	297	ILE	CB-CG2	-6.66	1.30	1.52
13	a4	297	ILE	CB-CG2	-6.64	1.30	1.52
13	b4	297	ILE	CB-CG2	-6.64	1.30	1.52

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a1	113	ILE	N-CA-CB	-7.92	103.50	112.21
13	c1	113	ILE	N-CA-CB	-7.87	103.55	112.21
13	b6	113	ILE	N-CA-CB	-7.86	103.56	112.21
13	b5	113	ILE	N-CA-CB	-7.62	103.26	112.33
13	a6	113	ILE	N-CA-CB	-7.61	103.84	112.21

There are no chirality outliers.

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	a1	282	TYR	Peptide
13	a1	290	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	aB	234	GLN	Peptide
6	aF	125	ALA	Peptide
11	aM	29	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5801	0	5660	126	0
1	bA	5801	0	5660	126	0
1	cA	5801	0	5660	128	0
2	aB	5879	0	5627	119	0
2	bB	5879	0	5627	120	0
2	cB	5879	0	5627	121	0
3	aC	598	0	580	11	0
3	bC	598	0	580	12	0
3	cC	598	0	580	17	0
4	aD	1075	0	1077	20	0
4	bD	1075	0	1077	22	0
4	cD	1075	0	1077	24	0
5	aE	539	0	528	8	0
5	bE	539	0	528	8	0
5	cE	539	0	528	9	0
6	aF	1065	0	1077	29	0
6	bF	1065	0	1077	21	0
6	cF	1065	0	1077	30	0
7	aI	301	0	306	7	0
7	bI	301	0	306	3	0
7	cI	301	0	306	6	0
8	aJ	338	0	347	20	0
8	bJ	338	0	347	9	0
8	cJ	338	0	347	17	0
9	aK	208	0	106	0	0
9	bK	208	0	106	0	0
9	cK	208	0	106	0	0
10	aL	1119	0	1125	21	0
10	bL	1119	0	1125	23	0
10	cL	1119	0	1125	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	aM	241	0	264	6	0
11	bM	241	0	264	5	0
11	cM	241	0	264	5	0
12	aX	233	0	231	2	0
12	bX	233	0	231	2	0
12	cX	233	0	231	2	0
13	a1	2583	0	2568	69	0
13	a2	2565	0	2545	77	0
13	a3	2607	0	2590	64	0
13	a4	2641	0	2624	67	0
13	a5	2607	0	2591	67	0
13	a6	2583	0	2567	73	0
13	b1	2583	0	2568	69	0
13	b2	2565	0	2545	73	0
13	b3	2607	0	2590	65	0
13	b4	2641	0	2624	67	0
13	b5	2607	0	2591	62	0
13	b6	2583	0	2567	73	0
13	c1	2583	0	2568	69	0
13	c2	2565	0	2545	73	0
13	c3	2607	0	2590	62	0
13	c4	2641	0	2624	63	0
13	c5	2607	0	2591	68	0
13	c6	2583	0	2567	69	0
14	aA	65	0	72	4	0
14	bA	65	0	72	4	0
14	cA	65	0	72	3	0
15	a1	830	0	720	40	0
15	a2	960	0	862	64	0
15	a3	895	0	790	49	0
15	a4	895	0	792	53	0
15	a5	895	0	792	52	0
15	a6	895	0	790	53	0
15	aA	2557	0	2532	109	0
15	aB	2414	0	2369	111	0
15	aJ	127	0	91	5	0
15	aK	45	0	33	0	0
15	aL	195	0	216	11	0
15	aX	45	0	33	2	0
15	b1	830	0	720	41	0
15	b2	960	0	862	67	0
15	b3	895	0	790	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b4	895	0	792	54	0
15	b5	895	0	792	56	0
15	b6	895	0	790	53	0
15	bA	2557	0	2532	113	0
15	bB	2414	0	2369	113	0
15	bF	45	0	33	2	0
15	bJ	82	0	58	1	0
15	bK	45	0	33	0	0
15	bL	195	0	216	11	0
15	bX	45	0	33	3	0
15	c1	830	0	720	40	0
15	c2	960	0	862	65	0
15	c3	895	0	790	48	0
15	c4	895	0	792	47	0
15	c5	895	0	792	52	0
15	c6	895	0	790	51	0
15	cA	2506	0	2491	112	0
15	cB	2414	0	2369	109	0
15	cF	96	0	74	6	0
15	cJ	82	0	58	1	0
15	cK	45	0	33	0	0
15	cL	195	0	216	13	0
15	cX	45	0	33	2	0
16	aA	33	0	46	3	0
16	aB	33	0	46	3	0
16	bA	33	0	46	3	0
16	bB	33	0	46	4	0
16	cA	33	0	46	4	0
16	cB	33	0	46	3	0
17	aA	8	0	0	0	0
17	aC	16	0	0	0	0
17	bA	8	0	0	0	0
17	bC	16	0	0	0	0
17	cA	8	0	0	0	0
17	cC	16	0	0	0	0
18	a1	200	0	280	15	0
18	a2	160	0	224	14	0
18	a3	160	0	224	9	0
18	a4	160	0	224	13	0
18	a5	120	0	168	10	0
18	a6	200	0	280	14	0
18	aA	200	0	278	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	aB	225	0	313	16	0
18	aF	120	0	168	15	0
18	aI	120	0	168	10	0
18	aJ	80	0	112	8	0
18	aK	40	0	56	1	0
18	aL	40	0	56	1	0
18	aM	40	0	56	3	0
18	b1	160	0	224	13	0
18	b2	160	0	224	14	0
18	b3	160	0	224	11	0
18	b4	160	0	224	12	0
18	b5	120	0	168	9	0
18	b6	200	0	280	11	0
18	bA	240	0	334	15	0
18	bB	265	0	369	25	0
18	bF	40	0	56	5	0
18	bI	80	0	112	4	0
18	bJ	120	0	168	14	0
18	bL	120	0	168	6	0
18	bM	40	0	56	4	0
18	c1	160	0	224	12	0
18	c2	160	0	224	11	0
18	c3	160	0	224	9	0
18	c4	160	0	224	13	0
18	c5	120	0	168	9	0
18	c6	160	0	224	10	0
18	cA	200	0	278	13	0
18	cB	225	0	313	16	0
18	cF	120	0	168	17	0
18	cI	80	0	112	4	0
18	cJ	80	0	112	9	0
18	cK	40	0	56	1	0
18	cL	40	0	56	3	0
18	cM	40	0	56	4	0
19	aA	76	0	98	3	0
19	aX	23	0	16	1	0
19	bA	76	0	98	3	0
19	bX	23	0	16	0	0
19	cA	76	0	98	3	0
19	cX	23	0	16	0	0
20	aB	55	0	86	1	0
20	bB	55	0	86	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	cB	55	0	86	1	0
21	aL	1	0	0	0	0
21	bL	1	0	0	0	0
21	cL	1	0	0	0	0
22	aA	3	0	0	0	0
22	aB	3	0	0	0	0
22	aL	1	0	0	0	0
22	bA	3	0	0	0	0
22	bB	3	0	0	0	0
22	bL	1	0	0	0	0
22	cA	2	0	0	0	0
22	cB	3	0	0	0	0
22	cF	1	0	0	0	0
22	cL	1	0	0	0	0
All	All	137634	0	136044	3155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 3155 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a1:331:GLN:HE22	15:a1:414:CLA:C1B	1.70	1.04
13:c1:331:GLN:HE22	15:c1:415:CLA:C1B	1.70	1.04
13:b1:331:GLN:HE22	15:b1:415:CLA:C1B	1.71	1.03
13:b3:331:GLN:HE22	15:b3:415:CLA:C1B	1.73	1.01
13:c5:331:GLN:HE22	15:c5:415:CLA:C1B	1.74	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	69
1	bA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	69
1	cA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	69
2	aB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
2	bB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
2	cB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
3	aC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	6
3	bC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	6
3	cC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	6
4	aD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
4	bD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
4	cD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
5	aE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	bE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	cE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
6	aF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
6	bF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
6	cF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
7	aI	36/38 (95%)	36 (100%)	0	0	100	100
7	bI	36/38 (95%)	36 (100%)	0	0	100	100
7	cI	36/38 (95%)	36 (100%)	0	0	100	100
8	aJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	bJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	cJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	aK	39/85 (46%)	39 (100%)	0	0	100	100
9	bK	39/85 (46%)	39 (100%)	0	0	100	100
9	cK	39/85 (46%)	39 (100%)	0	0	100	100
10	aL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	bL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	cL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
11	aM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	bM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	cM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	aX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	bX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	cX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
13	a1	327/358 (91%)	301 (92%)	24 (7%)	2 (1%)	21	36
13	a2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	26
13	a3	330/358 (92%)	303 (92%)	24 (7%)	3 (1%)	14	26
13	a4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	a5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	21	36
13	a6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	26
13	b1	327/358 (91%)	299 (91%)	26 (8%)	2 (1%)	21	36
13	b2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	26
13	b3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	26
13	b4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	b5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	21	36
13	b6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	26
13	c1	327/358 (91%)	300 (92%)	25 (8%)	2 (1%)	21	36
13	c2	325/358 (91%)	298 (92%)	24 (7%)	3 (1%)	14	26
13	c3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	26
13	c4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	c5	330/358 (92%)	302 (92%)	26 (8%)	2 (1%)	21	36
13	c6	327/358 (91%)	298 (91%)	26 (8%)	3 (1%)	14	26
All	All	12561/13452 (93%)	11740 (94%)	764 (6%)	57 (0%)	26	40

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	aA	233	ALA
13	a1	283	PRO
13	a2	283	PRO
13	a3	283	PRO
13	a4	283	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	592/604 (98%)	555 (94%)	37 (6%)	16	29
1	bA	592/604 (98%)	555 (94%)	37 (6%)	16	29
1	cA	592/604 (98%)	554 (94%)	38 (6%)	16	29
2	aB	595/597 (100%)	559 (94%)	36 (6%)	17	30
2	bB	595/597 (100%)	559 (94%)	36 (6%)	17	30
2	cB	595/597 (100%)	559 (94%)	36 (6%)	17	30
3	aC	67/67 (100%)	61 (91%)	6 (9%)	9	17
3	bC	67/67 (100%)	60 (90%)	7 (10%)	7	13
3	cC	67/67 (100%)	61 (91%)	6 (9%)	9	17
4	aD	115/115 (100%)	110 (96%)	5 (4%)	26	46
4	bD	115/115 (100%)	110 (96%)	5 (4%)	26	46
4	cD	115/115 (100%)	110 (96%)	5 (4%)	26	46
5	aE	59/64 (92%)	53 (90%)	6 (10%)	7	13
5	bE	59/64 (92%)	53 (90%)	6 (10%)	7	13
5	cE	59/64 (92%)	53 (90%)	6 (10%)	7	13
6	aF	109/128 (85%)	101 (93%)	8 (7%)	13	24
6	bF	109/128 (85%)	101 (93%)	8 (7%)	13	24
6	cF	109/128 (85%)	101 (93%)	8 (7%)	13	24
7	aI	32/32 (100%)	30 (94%)	2 (6%)	16	29
7	bI	32/32 (100%)	30 (94%)	2 (6%)	16	29
7	cI	32/32 (100%)	30 (94%)	2 (6%)	16	29
8	aJ	36/36 (100%)	32 (89%)	4 (11%)	6	11
8	bJ	36/36 (100%)	32 (89%)	4 (11%)	6	11
8	cJ	36/36 (100%)	32 (89%)	4 (11%)	6	11
10	aL	117/119 (98%)	110 (94%)	7 (6%)	17	31
10	bL	117/119 (98%)	110 (94%)	7 (6%)	17	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	cL	117/119 (98%)	110 (94%)	7 (6%)	17 31
11	aM	26/26 (100%)	21 (81%)	5 (19%)	1 2
11	bM	26/26 (100%)	21 (81%)	5 (19%)	1 2
11	cM	26/26 (100%)	21 (81%)	5 (19%)	1 2
12	aX	20/24 (83%)	19 (95%)	1 (5%)	22 40
12	bX	20/24 (83%)	19 (95%)	1 (5%)	22 40
12	cX	20/24 (83%)	19 (95%)	1 (5%)	22 40
13	a1	255/279 (91%)	240 (94%)	15 (6%)	18 32
13	a2	253/279 (91%)	238 (94%)	15 (6%)	18 32
13	a3	258/279 (92%)	242 (94%)	16 (6%)	16 30
13	a4	262/279 (94%)	246 (94%)	16 (6%)	17 30
13	a5	258/279 (92%)	241 (93%)	17 (7%)	15 28
13	a6	255/279 (91%)	239 (94%)	16 (6%)	16 29
13	b1	255/279 (91%)	240 (94%)	15 (6%)	18 32
13	b2	253/279 (91%)	238 (94%)	15 (6%)	18 32
13	b3	258/279 (92%)	243 (94%)	15 (6%)	18 33
13	b4	262/279 (94%)	246 (94%)	16 (6%)	17 30
13	b5	258/279 (92%)	241 (93%)	17 (7%)	15 28
13	b6	255/279 (91%)	239 (94%)	16 (6%)	16 29
13	c1	255/279 (91%)	240 (94%)	15 (6%)	18 32
13	c2	253/279 (91%)	239 (94%)	14 (6%)	19 35
13	c3	258/279 (92%)	242 (94%)	16 (6%)	16 30
13	c4	262/279 (94%)	246 (94%)	16 (6%)	17 30
13	c5	258/279 (92%)	240 (93%)	18 (7%)	14 26
13	c6	255/279 (91%)	240 (94%)	15 (6%)	18 32
All	All	9927/10458 (95%)	9291 (94%)	636 (6%)	18 29

5 of 636 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	cB	63	SER
13	c3	88	LEU
2	cB	357	SER

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Mol	Chain	Res	Type
2	cB	48	SER
6	cF	104	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
2	bB	614	GLN
13	b4	320	ASN
13	c6	320	ASN
4	cD	70	GLN
2	bB	639	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 759 ligands modelled in this entry, 3 are monoatomic - leaving 756 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	cA	818	1	58,62,73	1.33	10 (17%)	69,99,113	1.60	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a4	407	-	49,53,73	1.47	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	c4	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	b1	411	13	49,53,73	1.49	9 (18%)	59,89,113	1.66	9 (15%)
16	PQN	aA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	c3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)
15	CLA	a3	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
15	CLA	c2	405	-	49,53,73	1.58	9 (18%)	59,89,113	1.94	19 (32%)
15	CLA	c2	414	13	49,53,73	1.52	10 (20%)	59,89,113	1.52	6 (10%)
15	CLA	bA	838	1	55,59,73	1.46	10 (18%)	66,96,113	1.69	12 (18%)
15	CLA	aA	835	1	69,73,73	1.28	10 (14%)	83,113,113	1.56	10 (12%)
15	CLA	a6	415	13	45,49,73	1.52	9 (20%)	54,84,113	1.59	6 (11%)
15	CLA	bA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.49	10 (15%)
16	PQN	cB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
18	BCR	b3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
15	CLA	a3	413	13	49,53,73	1.51	11 (22%)	59,89,113	1.50	6 (10%)
15	CLA	aA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	6 (10%)
15	CLA	bB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	b2	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	cA	831	1	69,73,73	1.37	10 (14%)	83,113,113	1.63	13 (15%)
15	CLA	cB	835	2	49,53,73	1.42	9 (18%)	59,89,113	1.72	6 (10%)
19	LHG	bX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	a6	411	13	68,72,73	1.32	11 (16%)	81,111,113	1.57	15 (18%)
15	CLA	cB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	a2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.47	7 (11%)
15	CLA	a6	414	13	49,53,73	1.50	12 (24%)	59,89,113	1.68	10 (16%)
15	CLA	cA	815	1	49,53,73	1.49	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	bA	842	22	55,59,73	1.41	10 (18%)	66,96,113	1.33	8 (12%)
15	CLA	bA	815	1	49,53,73	1.49	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	b5	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.93	16 (22%)
15	CLA	a1	413	13	45,49,73	1.49	9 (20%)	54,84,113	1.58	7 (12%)
15	CLA	c2	415	13	45,49,73	1.51	7 (15%)	54,84,113	1.60	5 (9%)
17	SF4	aC	101	3	0,12,12	-	-	-		
15	CLA	c2	413	13	49,53,73	1.58	10 (20%)	59,89,113	1.63	15 (25%)
15	CLA	aA	840	1	51,55,73	1.52	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	bB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.53	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c5	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	22 (37%)
15	CLA	c5	409	13	69,73,73	1.27	10 (14%)	83,113,113	1.32	8 (9%)
15	CLA	a6	412	13	49,53,73	1.48	11 (22%)	59,89,113	1.64	11 (18%)
15	CLA	b6	414	13	49,53,73	1.53	10 (20%)	59,89,113	1.69	10 (16%)
15	CLA	aB	836	2	64,68,73	1.37	9 (14%)	77,107,113	1.49	10 (12%)
15	CLA	bA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.46	6 (9%)
15	CLA	cA	810	1	69,73,73	1.25	11 (15%)	83,113,113	1.46	6 (7%)
15	CLA	c2	411	13	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	a4	421	13	69,73,73	1.40	15 (21%)	83,113,113	1.68	16 (19%)
18	BCR	a3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	aA	836	1	58,62,73	1.35	10 (17%)	69,99,113	1.41	6 (8%)
15	CLA	b2	402	13	69,73,73	1.25	8 (11%)	83,113,113	1.35	6 (7%)
15	CLA	aB	841	-	49,53,73	1.52	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	b5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.37	6 (7%)
18	BCR	b1	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	8 (14%)
15	CLA	aA	834	1	69,73,73	1.33	12 (17%)	83,113,113	1.58	11 (13%)
15	CLA	aB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.49	8 (11%)
15	CLA	cB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.58	12 (14%)
15	CLA	aA	818	1	58,62,73	1.34	10 (17%)	69,99,113	1.62	8 (11%)
15	CLA	b5	403	13	69,73,73	1.22	9 (13%)	83,113,113	1.42	11 (13%)
15	CLA	b2	415	13	45,49,73	1.51	8 (17%)	54,84,113	1.61	5 (9%)
18	BCR	c1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.65	12 (21%)
15	CLA	b5	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.84	12 (20%)
15	CLA	a3	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.93	18 (25%)
15	CLA	bB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.50	8 (11%)
15	CLA	bB	841	-	49,53,73	1.52	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	aA	838	1	55,59,73	1.45	10 (18%)	66,96,113	1.68	12 (18%)
15	CLA	aJ	203	8	42,45,73	1.52	11 (26%)	50,78,113	1.66	5 (10%)
18	BCR	b4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	b2	417	-	54,58,73	1.57	11 (20%)	65,95,113	2.32	18 (27%)
15	CLA	bB	817	2	59,63,73	1.36	8 (13%)	71,101,113	1.63	14 (19%)
15	CLA	a2	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.93	15 (21%)
15	CLA	c3	416	-	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
15	CLA	b2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	cA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.48	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	aB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	16 (19%)
15	CLA	aL	202	10	69,73,73	1.26	10 (14%)	83,113,113	1.59	11 (13%)
15	CLA	a4	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.95	16 (22%)
15	CLA	cL	202	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
18	BCR	b3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
19	LHG	aA	854	15	26,26,48	0.97	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	bA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	12 (16%)
15	CLA	a5	408	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	cF	201	22	55,59,73	1.42	10 (18%)	66,96,113	1.33	8 (12%)
15	CLA	aA	842	22	55,59,73	1.41	9 (16%)	66,96,113	1.33	8 (12%)
15	CLA	aB	816	2	49,53,73	1.40	10 (20%)	59,89,113	1.73	7 (11%)
15	CLA	a5	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.94	15 (21%)
15	CLA	c1	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.92	17 (23%)
18	BCR	aB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
15	CLA	aB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.77	15 (18%)
18	BCR	aB	847	-	25,25,41	1.18	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	bB	819	2	64,68,73	1.31	11 (17%)	77,107,113	1.60	10 (12%)
15	CLA	bA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
15	CLA	b3	416	-	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
18	BCR	c2	401	-	41,41,41	1.25	4 (9%)	56,56,56	1.84	11 (19%)
15	CLA	a3	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.60	11 (18%)
15	CLA	b3	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.52	5 (8%)
15	CLA	c6	401	13	69,73,73	1.42	14 (20%)	83,113,113	1.98	20 (24%)
18	BCR	c1	401	-	41,41,41	1.16	3 (7%)	56,56,56	1.54	9 (16%)
15	CLA	a4	416	-	54,58,73	1.54	9 (16%)	65,95,113	2.26	17 (26%)
15	CLA	cA	820	1	69,73,73	1.30	10 (14%)	83,113,113	1.51	11 (13%)
15	CLA	cB	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.48	13 (17%)
15	CLA	c2	418	13	59,63,73	1.59	8 (13%)	71,101,113	1.93	15 (21%)
15	CLA	cA	812	1	69,73,73	1.26	10 (14%)	83,113,113	1.36	9 (10%)
15	CLA	b2	408	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	11 (18%)
15	CLA	c1	405	-	49,53,73	1.55	9 (18%)	59,89,113	1.91	19 (32%)
15	CLA	c1	409	13	69,73,73	1.25	8 (11%)	83,113,113	1.29	8 (9%)
15	CLA	b6	416	13	49,53,73	1.51	9 (18%)	59,89,113	1.83	11 (18%)
18	BCR	a6	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
18	BCR	b2	401	-	41,41,41	1.24	4 (9%)	56,56,56	1.82	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	b3	418	-	41,41,41	1.43	5 (12%)	56,56,56	1.55	10 (17%)
18	BCR	b4	420	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	10 (17%)
15	CLA	aA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	11 (13%)
18	BCR	a6	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	a3	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.64	10 (16%)
15	CLA	a2	414	13	49,53,73	1.51	9 (18%)	59,89,113	1.52	5 (8%)
15	CLA	bA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.49	10 (12%)
19	LHG	aA	853	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	b3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	bB	820	22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	bB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.47	10 (12%)
15	CLA	a6	406	-	49,53,73	1.57	8 (16%)	59,89,113	1.92	19 (32%)
15	CLA	b3	414	13	45,49,73	1.50	10 (22%)	54,84,113	1.63	6 (11%)
18	BCR	a1	419	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
19	LHG	cA	852	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
18	BCR	a3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.67	9 (16%)
15	CLA	cA	832	1	54,58,73	1.36	10 (18%)	65,95,113	1.70	8 (12%)
15	CLA	c6	416	13	45,49,73	1.52	8 (17%)	54,84,113	1.60	6 (11%)
15	CLA	bA	821	1	65,69,73	1.30	12 (18%)	78,108,113	1.41	7 (8%)
15	CLA	aB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.53	8 (9%)
15	CLA	c2	402	13	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
15	CLA	c2	416	13	49,53,73	1.49	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	c6	408	13	49,53,73	1.45	9 (18%)	59,89,113	1.49	7 (11%)
15	CLA	b6	406	-	49,53,73	1.58	8 (16%)	59,89,113	1.92	19 (32%)
15	CLA	b4	415	13	49,53,73	1.48	9 (18%)	59,89,113	1.86	13 (22%)
19	LHG	bA	855	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	bB	836	2	64,68,73	1.38	9 (14%)	77,107,113	1.49	10 (12%)
15	CLA	bB	832	2	53,57,73	1.43	8 (15%)	62,93,113	1.52	9 (14%)
15	CLA	bB	803	-	69,73,73	1.32	8 (11%)	83,113,113	1.51	14 (16%)
15	CLA	a2	415	13	45,49,73	1.51	8 (17%)	54,84,113	1.60	5 (9%)
15	CLA	c2	408	-	49,53,73	1.48	9 (18%)	59,89,113	1.49	10 (16%)
15	CLA	a4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.61	14 (23%)
18	BCR	cA	851	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
15	CLA	cB	827	2	69,73,73	1.29	10 (14%)	83,113,113	1.55	14 (16%)
15	CLA	bA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	aL	203	22	69,73,73	1.31	9 (13%)	83,113,113	1.32	9 (10%)
15	CLA	aA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.50	12 (14%)
15	CLA	a2	417	-	54,58,73	1.57	11 (20%)	65,95,113	2.36	20 (30%)
18	BCR	a1	418	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
15	CLA	bB	839	22	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
17	SF4	aC	102	3	0,12,12	-	-	-		
15	CLA	b5	413	13	49,53,73	1.50	10 (20%)	59,89,113	1.49	5 (8%)
17	SF4	cA	846	1,2	0,12,12	-	-	-		
18	BCR	c2	420	-	41,41,41	1.12	3 (7%)	56,56,56	1.45	8 (14%)
15	CLA	bJ	101	8	49,53,73	1.46	12 (24%)	59,89,113	1.66	7 (11%)
15	CLA	c4	406	13	49,53,73	1.43	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	cA	840	1	51,55,73	1.53	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	b6	407	13	49,53,73	1.46	9 (18%)	59,89,113	1.49	7 (11%)
18	BCR	a4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	cA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
18	BCR	b5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	10 (17%)
18	BCR	c4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.49	10 (17%)
15	CLA	c5	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.84	12 (20%)
15	CLA	aA	812	1	69,73,73	1.26	11 (15%)	83,113,113	1.35	9 (10%)
15	CLA	c5	413	13	49,53,73	1.50	11 (22%)	59,89,113	1.51	5 (8%)
14	CL0	aA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	aB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	11 (13%)
15	CLA	aA	845	19	56,60,73	1.41	12 (21%)	67,97,113	2.02	18 (26%)
18	BCR	b3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	10 (17%)
15	CLA	bL	204	22	69,73,73	1.31	9 (13%)	83,113,113	1.31	9 (10%)
15	CLA	cA	807	1	69,73,73	1.36	11 (15%)	83,113,113	1.49	14 (16%)
15	CLA	bB	840	2	69,73,73	1.31	11 (15%)	83,113,113	1.67	12 (14%)
15	CLA	bB	811	2	69,73,73	1.29	10 (14%)	83,113,113	1.70	12 (14%)
15	CLA	cL	204	22	69,73,73	1.31	9 (13%)	83,113,113	1.31	9 (10%)
18	BCR	bA	850	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	cA	809	1	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
15	CLA	c5	411	13	49,53,73	1.49	9 (18%)	59,89,113	1.65	10 (16%)
15	CLA	c4	416	-	54,58,73	1.54	9 (16%)	65,95,113	2.27	17 (26%)
17	SF4	bA	847	1,2	0,12,12	-	-	-		
18	BCR	a6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c6	413	13	49,53,73	1.49	10 (20%)	59,89,113	1.64	11 (18%)
15	CLA	aA	809	1	69,73,73	1.24	11 (15%)	83,113,113	1.43	9 (10%)
15	CLA	b4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.61	14 (23%)
15	CLA	c2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.48	7 (11%)
18	BCR	bA	852	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	cB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	9 (10%)
15	CLA	cA	834	1	69,73,73	1.33	12 (17%)	83,113,113	1.56	11 (13%)
15	CLA	c6	411	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	9 (10%)
15	CLA	aA	816	1	49,53,73	1.46	11 (22%)	59,89,113	1.65	6 (10%)
15	CLA	c2	404	13	69,73,73	1.26	10 (14%)	83,113,113	1.39	9 (10%)
15	CLA	c5	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.64	7 (12%)
15	CLA	aB	818	2	63,67,73	1.30	10 (15%)	75,105,113	1.48	13 (17%)
18	BCR	a2	401	-	41,41,41	1.26	4 (9%)	56,56,56	1.83	12 (21%)
15	CLA	a1	410	13	49,53,73	1.49	11 (22%)	59,89,113	1.65	8 (13%)
18	BCR	b6	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.53	8 (14%)
15	CLA	c3	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.92	18 (25%)
15	CLA	b1	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	15 (18%)
15	CLA	b4	403	13	69,73,73	1.22	8 (11%)	83,113,113	1.40	8 (9%)
15	CLA	bA	844	-	46,49,73	1.47	9 (19%)	55,83,113	1.59	5 (9%)
15	CLA	bB	834	2	62,66,73	1.32	11 (17%)	74,104,113	1.49	9 (12%)
19	LHG	bA	854	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	bJ	102	8	42,45,73	1.51	11 (26%)	50,78,113	1.64	5 (10%)
15	CLA	b6	422	13	69,73,73	1.45	13 (18%)	83,113,113	2.00	20 (24%)
15	CLA	c6	418	-	54,58,73	1.52	10 (18%)	65,95,113	2.28	18 (27%)
18	BCR	b6	402	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
15	CLA	a3	412	13	49,53,73	1.56	10 (20%)	59,89,113	1.62	14 (23%)
15	CLA	cA	838	1	55,59,73	1.45	10 (18%)	66,96,113	1.69	12 (18%)
15	CLA	a3	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	10 (16%)
18	BCR	c6	421	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	c3	402	13	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
15	CLA	bB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.64	8 (13%)
18	BCR	cM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.34	9 (16%)
15	CLA	b5	409	13	69,73,73	1.27	10 (14%)	83,113,113	1.32	8 (9%)
15	CLA	bB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.44	7 (8%)
15	CLA	b6	412	13	49,53,73	1.48	10 (20%)	59,89,113	1.64	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	bA	832	1	54,58,73	1.37	10 (18%)	65,95,113	1.69	8 (12%)
18	BCR	c6	402	-	41,41,41	1.18	4 (9%)	56,56,56	1.53	11 (19%)
15	CLA	c4	414	13	45,49,73	1.53	9 (20%)	54,84,113	1.59	5 (9%)
15	CLA	aB	819	2	64,68,73	1.30	11 (17%)	77,107,113	1.60	10 (12%)
18	BCR	a1	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.59	9 (16%)
15	CLA	cB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
15	CLA	aB	839	22	69,73,73	1.24	11 (15%)	83,113,113	1.42	9 (10%)
18	BCR	bJ	104	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	c6	405	13	69,73,73	1.23	8 (11%)	83,113,113	1.42	10 (12%)
18	BCR	aJ	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	bA	834	1	69,73,73	1.34	12 (17%)	83,113,113	1.56	11 (13%)
15	CLA	a6	418	13	59,63,73	1.59	8 (13%)	71,101,113	1.91	14 (19%)
15	CLA	bB	842	-	49,53,73	1.47	7 (14%)	59,89,113	1.40	3 (5%)
15	CLA	cB	817	2	59,63,73	1.35	8 (13%)	71,101,113	1.62	13 (18%)
15	CLA	c6	414	13	49,53,73	1.56	10 (20%)	59,89,113	1.60	14 (23%)
15	CLA	bB	826	22	50,54,73	1.43	11 (22%)	60,90,113	1.75	11 (18%)
15	CLA	aA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.49	10 (12%)
15	CLA	bA	818	1	58,62,73	1.34	11 (18%)	69,99,113	1.61	9 (13%)
15	CLA	c5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.85	17 (20%)
15	CLA	cA	836	1	58,62,73	1.35	10 (17%)	69,99,113	1.41	6 (8%)
15	CLA	c1	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.45	5 (8%)
15	CLA	aA	821	1	65,69,73	1.32	12 (18%)	78,108,113	1.41	7 (8%)
18	BCR	cF	202	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	9 (16%)
15	CLA	cB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.56	5 (8%)
18	BCR	b6	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.41	10 (17%)
18	BCR	c5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.53	12 (21%)
15	CLA	cA	835	1	69,73,73	1.27	9 (13%)	83,113,113	1.55	10 (12%)
18	BCR	bJ	105	-	41,41,41	1.20	5 (12%)	56,56,56	1.35	9 (16%)
15	CLA	a5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.84	17 (20%)
15	CLA	cA	803	-	69,73,73	1.28	12 (17%)	83,113,113	1.74	15 (18%)
18	BCR	cI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.28	5 (8%)
15	CLA	aB	806	2	69,73,73	1.26	11 (15%)	83,113,113	1.52	9 (10%)
15	CLA	cA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	11 (13%)
18	BCR	c1	418	-	41,41,41	1.37	5 (12%)	56,56,56	1.54	11 (19%)
14	CL0	cA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	bB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	9 (10%)
15	CLA	b4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.32	10 (12%)
15	CLA	b5	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.50	8 (13%)
15	CLA	b4	410	13	68,72,73	1.31	11 (16%)	81,111,113	1.60	14 (17%)
18	BCR	b6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	b3	403	13	69,73,73	1.21	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	a3	414	13	45,49,73	1.50	10 (22%)	54,84,113	1.62	6 (11%)
15	CLA	bB	812	2	49,53,73	1.46	10 (20%)	59,89,113	1.47	8 (13%)
18	BCR	c1	420	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
15	CLA	aB	804	-	69,73,73	1.35	10 (14%)	83,113,113	1.87	16 (19%)
18	BCR	bB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	9 (16%)
15	CLA	c3	404	13	69,73,73	1.26	9 (13%)	83,113,113	1.37	7 (8%)
18	BCR	a3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	9 (16%)
15	CLA	a4	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.40	9 (10%)
15	CLA	bB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	12 (20%)
15	CLA	aB	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.56	14 (16%)
15	CLA	a5	415	13	49,53,73	1.49	10 (20%)	59,89,113	1.85	12 (20%)
15	CLA	aB	815	2	69,73,73	1.23	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	a5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.39	6 (7%)
15	CLA	b5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.84	17 (20%)
18	BCR	aF	203	-	41,41,41	1.20	4 (9%)	56,56,56	1.35	9 (16%)
15	CLA	b5	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.64	6 (11%)
15	CLA	cA	811	1	49,53,73	1.46	11 (22%)	59,89,113	1.47	7 (11%)
15	CLA	b4	421	13	69,73,73	1.40	15 (21%)	83,113,113	1.69	16 (19%)
15	CLA	cB	822	2	49,53,73	1.44	7 (14%)	59,89,113	1.63	8 (13%)
15	CLA	c5	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.42	11 (13%)
15	CLA	a5	411	13	49,53,73	1.49	10 (20%)	59,89,113	1.65	10 (16%)
15	CLA	c3	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.50	6 (10%)
18	BCR	cB	846	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
15	CLA	bB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.57	12 (14%)
15	CLA	bA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	10 (12%)
18	BCR	aL	205	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	c1	415	13	49,53,73	1.47	9 (18%)	59,89,113	1.83	11 (18%)
15	CLA	c3	412	13	49,53,73	1.56	10 (20%)	59,89,113	1.62	14 (23%)
18	BCR	c4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LHG	cX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
18	BCR	cB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	9 (16%)
18	BCR	c3	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.54	10 (17%)
15	CLA	a2	411	13	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
14	CL0	bA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	a1	409	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	14 (17%)
15	CLA	bA	845	19	56,60,73	1.41	12 (21%)	67,97,113	2.02	17 (25%)
15	CLA	b6	410	13	69,73,73	1.25	9 (13%)	83,113,113	1.33	9 (10%)
15	CLA	cB	823	-	59,63,73	1.30	9 (15%)	71,101,113	1.50	7 (9%)
15	CLA	a5	414	13	45,49,73	1.49	9 (20%)	54,84,113	1.62	7 (12%)
15	CLA	c3	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.62	14 (17%)
15	CLA	aA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
15	CLA	bB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.55	9 (10%)
15	CLA	aB	802	2	69,73,73	1.37	10 (14%)	83,113,113	1.51	9 (10%)
15	CLA	a1	414	13	49,53,73	1.48	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	aJ	202	8	49,53,73	1.45	12 (24%)	59,89,113	1.65	7 (11%)
15	CLA	a2	405	-	49,53,73	1.58	8 (16%)	59,89,113	1.95	19 (32%)
15	CLA	b2	411	13	68,72,73	1.30	11 (16%)	81,111,113	1.58	15 (18%)
18	BCR	bB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
15	CLA	bA	813	1	58,62,73	1.43	10 (17%)	69,99,113	1.42	9 (13%)
18	BCR	c4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)
15	CLA	b1	414	13	45,49,73	1.51	9 (20%)	54,84,113	1.57	8 (14%)
15	CLA	c5	412	13	49,53,73	1.55	9 (18%)	59,89,113	1.62	14 (23%)
15	CLA	bB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	bA	810	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	6 (7%)
18	BCR	a2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	bA	827	22	69,73,73	1.30	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	cA	823	1	53,57,73	1.39	9 (16%)	62,93,113	1.47	6 (9%)
15	CLA	b3	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.61	12 (20%)
15	CLA	a2	416	13	49,53,73	1.48	9 (18%)	59,89,113	1.81	11 (18%)
18	BCR	bB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	a6	417	-	54,58,73	1.52	10 (18%)	65,95,113	2.28	17 (26%)
15	CLA	b3	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	14 (17%)
18	BCR	cA	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
20	LMG	bB	851	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	bA	853	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	6 (10%)
15	CLA	bA	809	1	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
15	CLA	a4	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	b6	408	-	49,53,73	1.47	9 (18%)	59,89,113	1.55	9 (15%)
15	CLA	c2	412	13	49,53,73	1.51	11 (22%)	59,89,113	1.66	10 (16%)
15	CLA	cA	842	1	69,73,73	1.32	10 (14%)	83,113,113	1.51	8 (9%)
15	CLA	cA	805	1	63,67,73	1.34	11 (17%)	75,105,113	1.53	11 (14%)
15	CLA	c5	404	13	69,73,73	1.26	10 (14%)	83,113,113	1.37	9 (10%)
15	CLA	aA	807	1	69,73,73	1.35	11 (15%)	83,113,113	1.49	14 (16%)
15	CLA	c5	408	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	10 (16%)
20	LMG	cB	850	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)
15	CLA	b1	413	13	49,53,73	1.52	10 (20%)	59,89,113	1.43	4 (6%)
15	CLA	bB	816	2	49,53,73	1.41	10 (20%)	59,89,113	1.74	7 (11%)
15	CLA	b6	417	-	54,58,73	1.52	10 (18%)	65,95,113	2.28	18 (27%)
18	BCR	cF	204	-	41,41,41	1.20	3 (7%)	56,56,56	1.43	10 (17%)
15	CLA	b1	405	-	49,53,73	1.55	8 (16%)	59,89,113	1.91	20 (33%)
15	CLA	c1	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.59	6 (11%)
15	CLA	c5	410	13	68,72,73	1.31	11 (16%)	81,111,113	1.63	15 (18%)
15	CLA	c2	417	-	54,58,73	1.58	11 (20%)	65,95,113	2.35	19 (29%)
15	CLA	c6	404	13	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
15	CLA	aA	823	1	53,57,73	1.40	9 (16%)	62,93,113	1.46	6 (9%)
15	CLA	cB	836	2	64,68,73	1.38	10 (15%)	77,107,113	1.49	10 (12%)
15	CLA	c6	410	13	49,53,73	1.46	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	a6	416	13	49,53,73	1.51	9 (18%)	59,89,113	1.82	11 (18%)
18	BCR	b4	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.56	9 (16%)
19	LHG	cA	853	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	a4	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.58	8 (13%)
15	CLA	a3	416	-	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
15	CLA	c6	419	13	59,63,73	1.60	8 (13%)	71,101,113	1.93	14 (19%)
18	BCR	cF	205	-	41,41,41	1.21	5 (12%)	56,56,56	1.34	8 (14%)
18	BCR	a2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.44	8 (14%)
15	CLA	a1	401	13	69,73,73	1.23	9 (13%)	83,113,113	1.36	7 (8%)
15	CLA	c1	403	13	69,73,73	1.24	9 (13%)	83,113,113	1.43	10 (12%)
18	BCR	a5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	11 (19%)
15	CLA	bA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c3	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.63	6 (11%)
15	CLA	aA	820	1	69,73,73	1.29	10 (14%)	83,113,113	1.52	10 (12%)
15	CLA	a4	411	13	49,53,73	1.50	11 (22%)	59,89,113	1.64	9 (15%)
15	CLA	aB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	c4	417	13	59,63,73	1.57	9 (15%)	71,101,113	1.95	16 (22%)
15	CLA	cA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.50	11 (13%)
15	CLA	a1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	bL	203	10	69,73,73	1.26	10 (14%)	83,113,113	1.60	11 (13%)
15	CLA	c5	407	-	49,53,73	1.46	8 (16%)	59,89,113	1.54	9 (15%)
15	CLA	c3	421	13	69,73,73	1.39	11 (15%)	83,113,113	1.61	15 (18%)
18	BCR	cL	205	-	41,41,41	1.30	4 (9%)	56,56,56	1.45	9 (16%)
15	CLA	b3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	cA	821	1	65,69,73	1.31	12 (18%)	78,108,113	1.41	7 (8%)
15	CLA	b6	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
15	CLA	cA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	6 (10%)
18	BCR	aB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	b1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.36	7 (8%)
15	CLA	bA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.50	12 (14%)
15	CLA	b5	408	13	49,53,73	1.45	11 (22%)	59,89,113	1.62	9 (15%)
18	BCR	aB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	8 (14%)
15	CLA	aB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.55	5 (8%)
15	CLA	a5	403	13	69,73,73	1.23	10 (14%)	83,113,113	1.42	10 (12%)
15	CLA	b6	405	13	69,73,73	1.27	10 (14%)	83,113,113	1.38	9 (10%)
15	CLA	aA	814	1	64,68,73	1.36	11 (17%)	77,107,113	1.38	7 (9%)
15	CLA	b2	406	13	69,73,73	1.41	12 (17%)	83,113,113	1.89	21 (25%)
15	CLA	b6	409	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	bB	821	2	51,55,73	1.45	11 (21%)	61,91,113	1.46	4 (6%)
18	BCR	c6	420	-	41,41,41	1.36	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	c3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.81	11 (18%)
18	BCR	a1	417	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	8 (14%)
15	CLA	bA	835	1	69,73,73	1.28	10 (14%)	83,113,113	1.56	10 (12%)
15	CLA	cB	803	-	69,73,73	1.31	8 (11%)	83,113,113	1.51	14 (16%)
15	CLA	aB	821	2	51,55,73	1.46	11 (21%)	61,91,113	1.48	4 (6%)
15	CLA	b4	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.49	5 (8%)
15	CLA	c6	409	-	49,53,73	1.46	9 (18%)	59,89,113	1.52	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	PQN	bB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
18	BCR	bI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)
15	CLA	cJ	101	8	49,53,73	1.46	11 (22%)	59,89,113	1.64	7 (11%)
15	CLA	aA	805	1	63,67,73	1.33	10 (15%)	75,105,113	1.54	11 (14%)
15	CLA	aA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.51	11 (13%)
18	BCR	bI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
15	CLA	a5	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.51	8 (13%)
15	CLA	b2	412	13	49,53,73	1.50	12 (24%)	59,89,113	1.67	10 (16%)
15	CLA	c3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	bB	835	2	49,53,73	1.42	10 (20%)	59,89,113	1.72	6 (10%)
15	CLA	c4	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.59	8 (13%)
18	BCR	aA	850	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
18	BCR	a6	402	-	41,41,41	1.24	4 (9%)	56,56,56	1.71	10 (17%)
18	BCR	b1	401	-	41,41,41	1.16	4 (9%)	56,56,56	1.54	10 (17%)
15	CLA	bA	820	1	69,73,73	1.29	10 (14%)	83,113,113	1.52	11 (13%)
15	CLA	c2	409	13	49,53,73	1.43	9 (18%)	59,89,113	1.58	9 (15%)
17	SF4	aA	847	1,2	0,12,12	-	-	-		
15	CLA	aB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	bA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
15	CLA	b6	413	13	49,53,73	1.55	10 (20%)	59,89,113	1.59	14 (23%)
15	CLA	a6	413	13	49,53,73	1.56	10 (20%)	59,89,113	1.61	14 (23%)
15	CLA	c4	405	-	49,53,73	1.55	11 (22%)	59,89,113	1.96	21 (35%)
18	BCR	aA	852	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
15	CLA	cA	844	19	56,60,73	1.41	12 (21%)	67,97,113	2.01	17 (25%)
15	CLA	c1	410	13	68,72,73	1.29	11 (16%)	81,111,113	1.60	15 (18%)
15	CLA	cK	102	-	49,53,73	1.47	11 (22%)	59,89,113	1.51	10 (16%)
18	BCR	bA	849	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	b2	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.39	9 (10%)
18	BCR	a4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)
15	CLA	bA	831	1	69,73,73	1.38	10 (14%)	83,113,113	1.63	13 (15%)
15	CLA	aA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	7 (8%)
15	CLA	cA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
15	CLA	cB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	13 (22%)
15	CLA	bB	807	2	69,73,73	1.38	12 (17%)	83,113,113	1.49	9 (10%)
15	CLA	b1	415	13	49,53,73	1.48	8 (16%)	59,89,113	1.79	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a5	407	-	49,53,73	1.46	9 (18%)	59,89,113	1.55	10 (16%)
15	CLA	b6	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.92	15 (21%)
15	CLA	cB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	aA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
15	CLA	bB	823	-	59,63,73	1.30	10 (16%)	71,101,113	1.51	7 (9%)
15	CLA	b3	411	13	49,53,73	1.49	10 (20%)	59,89,113	1.63	10 (16%)
15	CLA	b2	422	13	69,73,73	1.37	11 (15%)	83,113,113	1.82	19 (22%)
15	CLA	a2	412	13	49,53,73	1.50	12 (24%)	59,89,113	1.67	10 (16%)
18	BCR	aA	848	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	a6	422	13	69,73,73	1.50	15 (21%)	83,113,113	2.17	21 (25%)
15	CLA	b5	407	-	49,53,73	1.45	8 (16%)	59,89,113	1.55	10 (16%)
15	CLA	a2	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.42	8 (9%)
15	CLA	cF	203	-	49,53,73	1.51	10 (20%)	59,89,113	1.67	11 (18%)
18	BCR	bB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	c1	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.59	8 (13%)
15	CLA	a4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.35	8 (9%)
15	CLA	c4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.33	10 (12%)
18	BCR	bF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
15	CLA	b2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.48	7 (11%)
15	CLA	b4	406	13	49,53,73	1.44	9 (18%)	59,89,113	1.49	7 (11%)
15	CLA	cA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	cB	806	2	69,73,73	1.26	11 (15%)	83,113,113	1.53	9 (10%)
15	CLA	cB	834	2	62,66,73	1.31	11 (17%)	74,104,113	1.48	9 (12%)
18	BCR	cK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
18	BCR	bJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	aA	802	22	69,73,73	1.41	11 (15%)	83,113,113	1.44	11 (13%)
15	CLA	cA	814	1	64,68,73	1.35	10 (15%)	77,107,113	1.38	7 (9%)
15	CLA	bA	812	1	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
15	CLA	b2	405	-	49,53,73	1.59	8 (16%)	59,89,113	1.94	19 (32%)
15	CLA	bA	823	1	53,57,73	1.41	10 (18%)	62,93,113	1.46	6 (9%)
15	CLA	aA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
15	CLA	a4	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	20 (33%)
18	BCR	b2	419	-	41,41,41	1.36	5 (12%)	56,56,56	1.55	9 (16%)
15	CLA	b5	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.66	10 (16%)
15	CLA	a6	409	13	49,53,73	1.45	10 (20%)	59,89,113	1.62	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	bA	816	1	49,53,73	1.47	10 (20%)	59,89,113	1.65	6 (10%)
15	CLA	a1	415	-	54,58,73	1.54	11 (20%)	65,95,113	2.28	18 (27%)
18	BCR	bL	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.45	9 (16%)
15	CLA	b4	402	13	69,73,73	1.22	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	a6	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.33	7 (8%)
18	BCR	b5	419	-	41,41,41	1.16	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	aB	823	-	59,63,73	1.30	9 (15%)	71,101,113	1.50	7 (9%)
15	CLA	aX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.67	12 (20%)
15	CLA	a5	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	22 (37%)
18	BCR	c2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.52	9 (16%)
18	BCR	c3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
15	CLA	cA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.49	12 (14%)
15	CLA	bB	827	2	69,73,73	1.29	11 (15%)	83,113,113	1.55	14 (16%)
15	CLA	a1	411	13	49,53,73	1.56	11 (22%)	59,89,113	1.70	14 (23%)
15	CLA	cA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.48	10 (15%)
15	CLA	cB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.48	9 (10%)
18	BCR	a3	418	-	41,41,41	1.44	5 (12%)	56,56,56	1.55	10 (17%)
15	CLA	c5	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.94	15 (21%)
15	CLA	aA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.54	9 (13%)
15	CLA	a2	413	13	49,53,73	1.57	11 (22%)	59,89,113	1.65	15 (25%)
15	CLA	a1	406	-	49,53,73	1.46	9 (18%)	59,89,113	1.57	9 (15%)
18	BCR	aI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)
15	CLA	b4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.34	7 (8%)
15	CLA	b3	402	13	69,73,73	1.23	8 (11%)	83,113,113	1.33	7 (8%)
15	CLA	c3	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.60	10 (16%)
15	CLA	a2	409	13	49,53,73	1.44	9 (18%)	59,89,113	1.57	8 (13%)
18	BCR	aA	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	a4	402	13	69,73,73	1.22	9 (13%)	83,113,113	1.37	8 (9%)
15	CLA	bA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.37	7 (8%)
15	CLA	cA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	cX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.67	11 (18%)
15	CLA	a2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	b3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	aB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	13 (22%)
15	CLA	b5	405	-	49,53,73	1.54	10 (20%)	59,89,113	1.97	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b2	414	13	49,53,73	1.52	9 (18%)	59,89,113	1.53	6 (10%)
15	CLA	b1	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.47	8 (13%)
15	CLA	c5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.36	6 (7%)
15	CLA	c5	416	-	54,58,73	1.53	9 (16%)	65,95,113	2.26	16 (24%)
18	BCR	a1	420	-	41,41,41	1.14	3 (7%)	56,56,56	1.51	10 (17%)
20	LMG	aB	850	-	55,55,55	1.07	4 (7%)	63,63,63	1.62	8 (12%)
15	CLA	bA	836	1	58,62,73	1.34	10 (17%)	69,99,113	1.40	6 (8%)
15	CLA	aA	844	-	46,49,73	1.46	8 (17%)	55,83,113	1.60	4 (7%)
15	CLA	b6	415	13	45,49,73	1.52	8 (17%)	54,84,113	1.60	6 (11%)
15	CLA	a2	422	13	69,73,73	1.37	11 (15%)	83,113,113	1.82	19 (22%)
15	CLA	bA	803	-	69,73,73	1.28	13 (18%)	83,113,113	1.74	15 (18%)
15	CLA	aB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.59	7 (11%)
15	CLA	a4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.32	10 (12%)
15	CLA	b4	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	cA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	7 (8%)
15	CLA	aB	832	2	53,57,73	1.43	8 (15%)	62,93,113	1.53	8 (12%)
15	CLA	b6	411	13	68,72,73	1.31	12 (17%)	81,111,113	1.57	15 (18%)
18	BCR	a2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	b3	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.62	14 (23%)
15	CLA	c1	411	13	49,53,73	1.48	11 (22%)	59,89,113	1.64	9 (15%)
15	CLA	aA	813	1	58,62,73	1.43	10 (17%)	69,99,113	1.42	10 (14%)
15	CLA	aB	803	-	69,73,73	1.32	8 (11%)	83,113,113	1.52	15 (18%)
15	CLA	aA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	c5	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.50	6 (10%)
15	CLA	a6	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.34	9 (10%)
15	CLA	b3	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.55	10 (16%)
15	CLA	c6	415	13	49,53,73	1.52	7 (14%)	59,89,113	1.64	8 (13%)
18	BCR	bB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
15	CLA	a3	421	13	69,73,73	1.40	11 (15%)	83,113,113	1.62	15 (18%)
15	CLA	cB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.54	8 (9%)
15	CLA	cB	811	2	69,73,73	1.28	8 (11%)	83,113,113	1.70	12 (14%)
15	CLA	cA	802	22	69,73,73	1.41	11 (15%)	83,113,113	1.44	11 (13%)
15	CLA	aB	834	2	62,66,73	1.32	11 (17%)	74,104,113	1.48	9 (12%)
15	CLA	aA	843	1	69,73,73	1.31	10 (14%)	83,113,113	1.52	8 (9%)
15	CLA	a1	403	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.60	14 (23%)
15	CLA	aA	811	1	49,53,73	1.46	11 (22%)	59,89,113	1.48	7 (11%)
15	CLA	cB	815	2	69,73,73	1.22	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	b1	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	b1	403	13	69,73,73	1.24	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	aB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.58	12 (14%)
15	CLA	cB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.60	7 (11%)
18	BCR	b1	420	-	41,41,41	1.20	4 (9%)	56,56,56	1.45	11 (19%)
18	BCR	cA	847	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	cB	832	2	53,57,73	1.44	8 (15%)	62,93,113	1.53	8 (12%)
15	CLA	bB	802	2	69,73,73	1.38	10 (14%)	83,113,113	1.50	9 (10%)
15	CLA	b3	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	cA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	11 (14%)
18	BCR	bL	206	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	a6	408	-	49,53,73	1.47	9 (18%)	59,89,113	1.54	9 (15%)
15	CLA	a4	415	13	49,53,73	1.48	8 (16%)	59,89,113	1.86	13 (22%)
15	CLA	bA	840	1	51,55,73	1.52	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	c6	412	13	68,72,73	1.31	11 (16%)	81,111,113	1.57	15 (18%)
15	CLA	a5	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.62	15 (18%)
15	CLA	b1	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.30	8 (9%)
15	CLA	b3	417	13	59,63,73	1.57	8 (13%)	71,101,113	1.93	18 (25%)
18	BCR	bA	848	-	41,41,41	1.21	3 (7%)	56,56,56	1.41	9 (16%)
18	BCR	cJ	104	-	41,41,41	1.31	3 (7%)	56,56,56	1.43	7 (12%)
15	CLA	cA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.55	9 (13%)
15	CLA	a3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.83	12 (20%)
15	CLA	cA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
15	CLA	aK	102	-	49,53,73	1.47	11 (22%)	59,89,113	1.51	10 (16%)
15	CLA	aB	840	2	69,73,73	1.30	11 (15%)	83,113,113	1.67	12 (14%)
15	CLA	a4	414	13	45,49,73	1.52	9 (20%)	54,84,113	1.60	6 (11%)
18	BCR	c4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	b3	405	-	49,53,73	1.55	11 (22%)	59,89,113	1.93	18 (30%)
15	CLA	bA	805	1	63,67,73	1.33	11 (17%)	75,105,113	1.54	11 (14%)
15	CLA	cB	812	2	49,53,73	1.46	9 (18%)	59,89,113	1.47	7 (11%)
15	CLA	cA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	5 (8%)
15	CLA	cB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a3	405	-	49,53,73	1.56	11 (22%)	59,89,113	1.93	19 (32%)
15	CLA	cB	839	22	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
15	CLA	c6	407	-	49,53,73	1.57	9 (18%)	59,89,113	1.93	19 (32%)
15	CLA	cB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.49	8 (11%)
15	CLA	cA	816	1	49,53,73	1.47	10 (20%)	59,89,113	1.66	6 (10%)
15	CLA	a1	407	13	49,53,73	1.45	10 (20%)	59,89,113	1.59	8 (13%)
18	BCR	aJ	204	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	a3	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.60	14 (17%)
15	CLA	aA	815	1	49,53,73	1.48	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	cB	804	-	69,73,73	1.35	10 (14%)	83,113,113	1.87	16 (19%)
15	CLA	bA	802	22	69,73,73	1.41	12 (17%)	83,113,113	1.44	10 (12%)
15	CLA	aB	807	2	69,73,73	1.39	11 (15%)	83,113,113	1.49	10 (12%)
15	CLA	b1	407	-	49,53,73	1.46	9 (18%)	59,89,113	1.56	8 (13%)
15	CLA	cB	816	2	49,53,73	1.41	10 (20%)	59,89,113	1.72	6 (10%)
15	CLA	aA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.49	10 (15%)
15	CLA	cB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.78	15 (18%)
18	BCR	bA	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
15	CLA	c6	417	13	49,53,73	1.51	8 (16%)	59,89,113	1.82	11 (18%)
15	CLA	cB	841	-	49,53,73	1.52	11 (22%)	59,89,113	1.55	9 (15%)
15	CLA	c4	415	13	49,53,73	1.47	8 (16%)	59,89,113	1.85	12 (20%)
15	CLA	b5	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	15 (18%)
15	CLA	aB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	9 (10%)
15	CLA	bB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.79	15 (18%)
15	CLA	b5	416	-	54,58,73	1.53	9 (16%)	65,95,113	2.27	16 (24%)
15	CLA	cB	840	2	69,73,73	1.30	11 (15%)	83,113,113	1.68	12 (14%)
15	CLA	c3	405	-	49,53,73	1.56	11 (22%)	59,89,113	1.93	19 (32%)
15	CLA	c4	413	13	49,53,73	1.52	10 (20%)	59,89,113	1.49	6 (10%)
18	BCR	b6	401	-	41,41,41	1.18	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	a1	404	-	49,53,73	1.54	9 (18%)	59,89,113	1.91	19 (32%)
18	BCR	aI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
18	BCR	bL	201	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
18	BCR	cB	848	-	41,41,41	1.33	4 (9%)	56,56,56	1.50	8 (14%)
15	CLA	b2	416	13	49,53,73	1.49	9 (18%)	59,89,113	1.81	11 (18%)
15	CLA	c4	411	13	49,53,73	1.49	11 (22%)	59,89,113	1.66	9 (15%)
18	BCR	b1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	c3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.40	8 (14%)
15	CLA	bL	202	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
15	CLA	bB	806	2	69,73,73	1.26	12 (17%)	83,113,113	1.53	9 (10%)
15	CLA	b5	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.63	13 (22%)
18	BCR	aK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
15	CLA	cB	807	2	69,73,73	1.38	12 (17%)	83,113,113	1.50	10 (12%)
18	BCR	b5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)
18	BCR	aI	103	-	41,41,41	1.31	4 (9%)	56,56,56	1.44	9 (16%)
15	CLA	b4	414	13	45,49,73	1.52	9 (20%)	54,84,113	1.60	6 (11%)
15	CLA	cJ	102	8	42,45,73	1.52	11 (26%)	50,78,113	1.66	5 (10%)
15	CLA	b4	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.60	8 (13%)
15	CLA	c1	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.45	8 (13%)
15	CLA	a5	416	-	54,58,73	1.53	9 (16%)	65,95,113	2.26	16 (24%)
15	CLA	aA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	a3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)
15	CLA	bB	822	2	49,53,73	1.44	8 (16%)	59,89,113	1.62	8 (13%)
15	CLA	cB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.40	9 (10%)
15	CLA	cB	802	2	69,73,73	1.38	11 (15%)	83,113,113	1.51	10 (12%)
15	CLA	c3	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.54	10 (16%)
15	CLA	a5	413	13	49,53,73	1.50	9 (18%)	59,89,113	1.50	5 (8%)
15	CLA	cA	843	-	46,49,73	1.47	8 (17%)	55,83,113	1.59	5 (9%)
15	CLA	aB	820	22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	cA	827	22	69,73,73	1.31	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	bA	807	1	69,73,73	1.35	12 (17%)	83,113,113	1.49	14 (16%)
15	CLA	aB	826	22	50,54,73	1.43	11 (22%)	60,90,113	1.75	11 (18%)
15	CLA	c4	421	13	69,73,73	1.38	14 (20%)	83,113,113	1.69	16 (19%)
18	BCR	bB	849	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	10 (17%)
15	CLA	a4	406	13	49,53,73	1.43	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	bB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
15	CLA	bB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.61	7 (11%)
18	BCR	a5	418	-	41,41,41	1.39	6 (14%)	56,56,56	1.53	10 (17%)
18	BCR	a5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)
15	CLA	c1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
15	CLA	c1	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	c1	416	-	54,58,73	1.52	11 (20%)	65,95,113	2.27	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.65	10 (16%)
15	CLA	c2	406	13	69,73,73	1.41	11 (15%)	83,113,113	1.89	20 (24%)
16	PQN	bA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
18	BCR	cA	849	-	41,41,41	1.19	2 (4%)	56,56,56	1.44	9 (16%)
18	BCR	cB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	bB	815	2	69,73,73	1.23	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	cB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.43	7 (8%)
15	CLA	b2	409	13	49,53,73	1.43	9 (18%)	59,89,113	1.59	10 (16%)
15	CLA	a6	407	13	49,53,73	1.45	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	b4	411	13	49,53,73	1.50	11 (22%)	59,89,113	1.66	9 (15%)
18	BCR	c3	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	9 (16%)
15	CLA	cB	819	2	64,68,73	1.31	11 (17%)	77,107,113	1.60	10 (12%)
18	BCR	c5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	b2	413	13	49,53,73	1.57	10 (20%)	59,89,113	1.66	15 (25%)
15	CLA	aA	831	1	69,73,73	1.38	10 (14%)	83,113,113	1.62	13 (15%)
15	CLA	a5	404	13	69,73,73	1.25	9 (13%)	83,113,113	1.38	8 (9%)
16	PQN	aB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
15	CLA	cB	842	-	49,53,73	1.47	8 (16%)	59,89,113	1.40	3 (5%)
15	CLA	c1	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
18	BCR	cA	850	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	cB	826	22	50,54,73	1.43	10 (20%)	60,90,113	1.75	11 (18%)
15	CLA	c2	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.42	9 (10%)
15	CLA	b3	421	13	69,73,73	1.39	11 (15%)	83,113,113	1.60	15 (18%)
15	CLA	aA	810	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	6 (7%)
15	CLA	a1	405	13	49,53,73	1.46	9 (18%)	59,89,113	1.47	8 (13%)
15	CLA	cB	821	2	51,55,73	1.47	11 (21%)	61,91,113	1.46	4 (6%)
17	SF4	bC	101	3	0,12,12	-	-	-		
15	CLA	aJ	201	-	49,53,73	1.52	10 (20%)	59,89,113	1.66	11 (18%)
19	LHG	aX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	a6	404	13	69,73,73	1.22	9 (13%)	83,113,113	1.42	10 (12%)
17	SF4	bC	102	3	0,12,12	-	-	-		
18	BCR	aF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
15	CLA	aB	812	2	49,53,73	1.46	10 (20%)	59,89,113	1.47	8 (13%)
15	CLA	aA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	12 (16%)
15	CLA	c6	406	13	69,73,73	1.27	10 (14%)	83,113,113	1.39	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	bA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.54	9 (13%)
18	BCR	a4	401	-	41,41,41	1.18	3 (7%)	56,56,56	1.49	11 (19%)
18	BCR	aB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.35	9 (16%)
15	CLA	aB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.47	11 (13%)
18	BCR	c5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.41	11 (19%)
15	CLA	bA	843	1	69,73,73	1.32	10 (14%)	83,113,113	1.50	8 (9%)
15	CLA	aB	822	2	49,53,73	1.44	7 (14%)	59,89,113	1.62	8 (13%)
15	CLA	a3	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.37	8 (9%)
15	CLA	aA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.45	6 (9%)
15	CLA	a3	403	13	69,73,73	1.21	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	c1	412	13	49,53,73	1.56	11 (22%)	59,89,113	1.67	13 (22%)
15	CLA	bA	811	1	49,53,73	1.45	11 (22%)	59,89,113	1.47	7 (11%)
15	CLA	c2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	bB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	16 (19%)
18	BCR	b2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.45	8 (14%)
15	CLA	aB	811	2	69,73,73	1.29	9 (13%)	83,113,113	1.69	12 (14%)
15	CLA	a3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	bB	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.48	13 (17%)
15	CLA	bB	804	-	69,73,73	1.36	10 (14%)	83,113,113	1.87	16 (19%)
15	CLA	b6	404	13	69,73,73	1.23	8 (11%)	83,113,113	1.42	10 (12%)
15	CLA	b4	417	13	59,63,73	1.57	9 (15%)	71,101,113	1.95	16 (22%)
18	BCR	b2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	c2	422	13	69,73,73	1.36	11 (15%)	83,113,113	1.80	19 (22%)
18	BCR	a6	421	-	41,41,41	1.11	4 (9%)	56,56,56	1.55	9 (16%)
18	BCR	bB	850	-	41,41,41	1.41	5 (12%)	56,56,56	1.30	8 (14%)
15	CLA	c4	402	13	69,73,73	1.22	8 (11%)	83,113,113	1.38	8 (9%)
18	BCR	bM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	aB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	9 (10%)
18	BCR	cI	102	-	41,41,41	1.37	3 (7%)	56,56,56	1.41	9 (16%)
15	CLA	c3	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.63	10 (16%)
15	CLA	a2	406	13	69,73,73	1.41	11 (15%)	83,113,113	1.89	20 (24%)
15	CLA	c4	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.40	8 (9%)
15	CLA	a5	409	13	69,73,73	1.28	10 (14%)	83,113,113	1.33	8 (9%)
15	CLA	b1	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.92	16 (22%)
15	CLA	bA	814	1	64,68,73	1.36	10 (15%)	77,107,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	aB	845	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	6 (10%)
18	BCR	aA	851	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	a4	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.48	5 (8%)
18	BCR	aF	201	-	41,41,41	1.31	4 (9%)	56,56,56	1.37	9 (16%)
15	CLA	bA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
17	SF4	cC	101	3	0,12,12	-	-	-		
15	CLA	a2	408	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	11 (18%)
18	BCR	b4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.50	9 (16%)
18	BCR	cB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	bA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	7 (11%)
17	SF4	cC	102	3	0,12,12	-	-	-		
15	CLA	aB	835	2	49,53,73	1.42	10 (20%)	59,89,113	1.72	6 (10%)
15	CLA	b4	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	18 (30%)
15	CLA	bA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	bK	101	-	49,53,73	1.48	11 (22%)	59,89,113	1.52	10 (16%)
15	CLA	b5	404	13	69,73,73	1.26	9 (13%)	83,113,113	1.36	8 (9%)
15	CLA	c4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.34	8 (9%)
15	CLA	aL	201	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
15	CLA	a6	405	13	69,73,73	1.27	10 (14%)	83,113,113	1.37	8 (9%)
15	CLA	bA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.51	11 (13%)
15	CLA	aB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.65	10 (16%)
15	CLA	a2	402	13	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
15	CLA	aB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.44	7 (8%)
15	CLA	a5	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.63	13 (22%)
15	CLA	c4	410	13	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	a1	416	13	59,63,73	1.54	9 (15%)	71,101,113	1.93	17 (23%)
15	CLA	b2	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.92	15 (21%)
15	CLA	cB	820	22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	cL	203	10	69,73,73	1.26	10 (14%)	83,113,113	1.59	11 (13%)
18	BCR	cJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
18	BCR	cB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
15	CLA	aB	817	2	59,63,73	1.35	8 (13%)	71,101,113	1.62	13 (18%)
15	CLA	a1	412	13	49,53,73	1.51	10 (20%)	59,89,113	1.45	4 (6%)
15	CLA	b1	416	-	54,58,73	1.52	9 (16%)	65,95,113	2.25	17 (26%)
18	BCR	a4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cA	813	1	58,62,73	1.42	10 (17%)	69,99,113	1.42	10 (14%)
15	CLA	a1	408	13	69,73,73	1.26	8 (11%)	83,113,113	1.30	9 (10%)
15	CLA	aA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	4 (6%)
15	CLA	c3	403	13	69,73,73	1.22	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	b1	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.66	14 (23%)
15	CLA	aB	842	-	49,53,73	1.47	8 (16%)	59,89,113	1.40	3 (5%)
16	PQN	cA	845	-	34,34,34	1.40	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	b4	416	-	54,58,73	1.54	9 (16%)	65,95,113	2.26	17 (26%)
15	CLA	a2	404	13	69,73,73	1.27	10 (14%)	83,113,113	1.40	9 (10%)
15	CLA	b1	408	13	49,53,73	1.44	9 (18%)	59,89,113	1.60	9 (15%)
18	BCR	c2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
18	BCR	c6	403	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
18	BCR	aM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	bB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.55	5 (8%)
15	CLA	bF	201	-	49,53,73	1.52	10 (20%)	59,89,113	1.66	11 (18%)
15	CLA	aA	827	22	69,73,73	1.30	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	bX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.68	11 (18%)
15	CLA	aA	832	1	54,58,73	1.37	10 (18%)	65,95,113	1.70	8 (12%)
15	CLA	cA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.46	6 (9%)
15	CLA	aA	803	-	69,73,73	1.27	12 (17%)	83,113,113	1.74	15 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cA	818	1	-	6/26/102/115	-
15	CLA	a4	407	-	-	8/15/91/115	-
15	CLA	c4	407	-	-	8/15/91/115	-
15	CLA	b1	411	13	-	5/15/91/115	-
16	PQN	aA	846	-	-	5/23/43/43	0/2/2/2
15	CLA	c3	406	13	-	4/15/91/115	-
15	CLA	a3	402	13	-	17/39/115/115	-
15	CLA	c2	405	-	-	3/15/91/115	-
15	CLA	c2	414	13	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bA	838	1	-	8/23/99/115	-
15	CLA	aA	835	1	-	14/39/115/115	-
15	CLA	a6	415	13	-	4/10/86/115	-
15	CLA	bA	808	1	-	4/23/99/115	-
16	PQN	cB	843	-	-	10/23/43/43	0/2/2/2
18	BCR	b3	401	-	-	13/29/63/63	0/2/2/2
15	CLA	a3	413	13	-	3/15/91/115	-
15	CLA	aA	837	1	-	7/15/91/115	-
15	CLA	bB	825	2	-	10/26/102/115	-
15	CLA	b2	403	13	-	14/39/115/115	-
15	CLA	cA	831	1	-	8/39/115/115	-
15	CLA	cB	835	2	-	9/15/91/115	-
19	LHG	bX	101	-	-	11/26/26/53	-
15	CLA	a6	411	13	-	13/38/114/115	-
15	CLA	cB	833	2	-	18/39/115/115	-
15	CLA	a2	407	13	-	4/15/91/115	-
15	CLA	a6	414	13	-	4/15/91/115	-
15	CLA	cA	815	1	-	4/15/91/115	-
15	CLA	bA	842	22	-	10/23/99/115	-
15	CLA	bA	815	1	-	4/15/91/115	-
15	CLA	b5	417	13	-	10/27/103/115	-
15	CLA	a1	413	13	-	4/10/86/115	-
15	CLA	c2	415	13	-	4/10/86/115	-
17	SF4	aC	101	3	-	-	0/6/5/5
15	CLA	c2	413	13	-	9/15/91/115	-
15	CLA	aA	840	1	-	4/18/94/115	-
15	CLA	bB	828	2	-	21/39/115/115	-
15	CLA	c5	405	-	-	4/15/91/115	-
15	CLA	c5	409	13	-	6/39/115/115	-
15	CLA	a6	412	13	-	4/15/91/115	-
15	CLA	b6	414	13	-	4/15/91/115	-
15	CLA	aB	836	2	-	11/33/109/115	-
15	CLA	bA	824	1	-	14/23/99/115	-
15	CLA	cA	810	1	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c2	411	13	-	12/38/114/115	-
15	CLA	a4	421	13	-	13/39/115/115	-
18	BCR	a3	419	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	836	1	-	8/26/102/115	-
15	CLA	b2	402	13	-	17/39/115/115	-
15	CLA	aB	841	-	-	4/15/91/115	-
15	CLA	b5	402	13	-	17/39/115/115	-
18	BCR	b1	418	-	-	9/29/63/63	0/2/2/2
15	CLA	aA	834	1	-	12/39/115/115	-
15	CLA	aB	805	2	-	5/26/102/115	-
15	CLA	cB	810	2	-	16/39/115/115	-
15	CLA	aA	818	1	-	6/26/102/115	-
15	CLA	b5	403	13	-	14/39/115/115	-
15	CLA	b2	415	13	-	4/10/86/115	-
18	BCR	c1	419	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	415	13	-	7/15/91/115	-
15	CLA	a3	417	13	-	12/27/103/115	-
15	CLA	bB	805	2	-	5/26/102/115	-
15	CLA	bB	841	-	-	4/15/91/115	-
15	CLA	aA	838	1	-	8/23/99/115	-
15	CLA	aJ	203	8	-	2/4/76/115	-
18	BCR	b4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	417	-	-	9/21/97/115	-
15	CLA	bB	817	2	-	12/27/103/115	-
15	CLA	a2	418	13	-	11/27/103/115	-
15	CLA	c3	416	-	-	11/21/97/115	-
15	CLA	b2	410	13	-	7/39/115/115	-
15	CLA	cA	826	-	-	10/39/115/115	-
15	CLA	aB	814	2	-	25/39/115/115	-
15	CLA	aL	202	10	-	10/39/115/115	-
15	CLA	a4	417	13	-	9/27/103/115	-
15	CLA	cL	202	10	-	15/39/115/115	-
18	BCR	b3	419	-	-	11/29/63/63	0/2/2/2
19	LHG	aA	854	15	-	15/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bA	825	1	-	17/32/108/115	-
15	CLA	a5	408	13	-	5/15/91/115	-
15	CLA	cF	201	22	-	10/23/99/115	-
15	CLA	aA	842	22	-	10/23/99/115	-
15	CLA	aB	816	2	-	6/15/91/115	-
15	CLA	a5	417	13	-	9/27/103/115	-
15	CLA	c1	417	13	-	9/27/103/115	-
18	BCR	aB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	830	2	-	6/39/115/115	-
18	BCR	aB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	bB	819	2	-	12/33/109/115	-
15	CLA	bA	841	1	-	17/39/115/115	-
15	CLA	b3	416	-	-	11/21/97/115	-
18	BCR	c2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a3	408	13	-	5/15/91/115	-
15	CLA	b3	413	13	-	3/15/91/115	-
15	CLA	c6	401	13	-	16/39/115/115	-
18	BCR	c1	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a4	416	-	-	11/21/97/115	-
15	CLA	cA	820	1	-	18/39/115/115	-
15	CLA	cB	818	2	-	10/32/108/115	-
15	CLA	c2	418	13	-	11/27/103/115	-
15	CLA	cA	812	1	-	13/39/115/115	-
15	CLA	b2	408	-	-	7/15/91/115	-
15	CLA	c1	405	-	-	3/15/91/115	-
15	CLA	c1	409	13	-	6/39/115/115	-
15	CLA	b6	416	13	-	7/15/91/115	-
18	BCR	a6	420	-	-	12/29/63/63	0/2/2/2
18	BCR	b2	401	-	-	12/29/63/63	0/2/2/2
18	BCR	b3	418	-	-	10/29/63/63	0/2/2/2
18	BCR	b4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	806	1	-	23/39/115/115	-
18	BCR	a6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	a3	411	13	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a2	414	13	-	3/15/91/115	-
15	CLA	bA	826	-	-	10/39/115/115	-
19	LHG	aA	853	-	-	19/53/53/53	-
15	CLA	b3	406	13	-	4/15/91/115	-
15	CLA	bB	820	22	-	10/39/115/115	-
15	CLA	bB	837	2	-	15/39/115/115	-
15	CLA	a6	406	-	-	3/15/91/115	-
15	CLA	b3	414	13	-	4/10/86/115	-
18	BCR	a1	419	-	-	12/29/63/63	0/2/2/2
19	LHG	cA	852	-	-	19/53/53/53	-
18	BCR	a3	401	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	832	1	-	8/21/97/115	-
15	CLA	c6	416	13	-	4/10/86/115	-
15	CLA	bA	821	1	-	15/35/111/115	-
15	CLA	aB	828	2	-	21/39/115/115	-
15	CLA	c2	402	13	-	17/39/115/115	-
15	CLA	c2	416	13	-	7/15/91/115	-
15	CLA	c6	408	13	-	4/15/91/115	-
15	CLA	b6	406	-	-	3/15/91/115	-
15	CLA	b4	415	13	-	7/15/91/115	-
19	LHG	bA	855	15	-	15/31/31/53	-
15	CLA	bB	836	2	-	11/33/109/115	-
15	CLA	bB	832	2	-	8/20/96/115	-
15	CLA	bB	803	-	-	11/39/115/115	-
15	CLA	a2	415	13	-	4/10/86/115	-
15	CLA	c2	408	-	-	8/15/91/115	-
15	CLA	a4	412	13	-	9/15/91/115	-
18	BCR	cA	851	-	-	22/29/63/63	0/2/2/2
15	CLA	cB	827	2	-	15/39/115/115	-
15	CLA	bA	833	1	-	11/39/115/115	-
15	CLA	aL	203	22	-	15/39/115/115	-
15	CLA	aA	829	1	-	22/39/115/115	-
15	CLA	a2	417	-	-	9/21/97/115	-
18	BCR	a1	418	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	839	22	-	10/39/115/115	-
17	SF4	aC	102	3	-	-	0/6/5/5
15	CLA	b5	413	13	-	3/15/91/115	-
18	BCR	c2	420	-	-	11/29/63/63	0/2/2/2
17	SF4	cA	846	1,2	-	-	0/6/5/5
15	CLA	bJ	101	8	-	8/15/91/115	-
15	CLA	c4	406	13	-	4/15/91/115	-
15	CLA	cA	840	1	-	5/18/94/115	-
15	CLA	b6	407	13	-	4/15/91/115	-
18	BCR	a4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	822	-	-	18/39/115/115	-
18	BCR	b5	418	-	-	11/29/63/63	0/2/2/2
18	BCR	c4	401	-	-	13/29/63/63	0/2/2/2
15	CLA	c5	415	13	-	7/15/91/115	-
15	CLA	aA	812	1	-	13/39/115/115	-
15	CLA	c5	413	13	-	3/15/91/115	-
14	CL0	aA	801	1	-	6/39/115/115	-
15	CLA	aB	801	-	-	12/39/115/115	-
15	CLA	aA	845	19	-	13/24/100/115	-
18	BCR	b3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	bL	204	22	-	15/39/115/115	-
15	CLA	cA	807	1	-	11/39/115/115	-
15	CLA	bB	840	2	-	16/39/115/115	-
15	CLA	bB	811	2	-	13/39/115/115	-
15	CLA	cL	204	22	-	15/39/115/115	-
18	BCR	bA	850	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	809	1	-	21/39/115/115	-
15	CLA	c5	411	13	-	3/15/91/115	-
15	CLA	c4	416	-	-	11/21/97/115	-
17	SF4	bA	847	1,2	-	-	0/6/5/5
18	BCR	a6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	c6	413	13	-	4/15/91/115	-
15	CLA	aA	809	1	-	21/39/115/115	-
15	CLA	b4	412	13	-	9/15/91/115	-
15	CLA	c2	407	13	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	bA	852	-	-	8/29/63/63	0/2/2/2
15	CLA	cB	809	2	-	13/39/115/115	-
15	CLA	cA	834	1	-	12/39/115/115	-
15	CLA	c6	411	13	-	6/39/115/115	-
15	CLA	aA	816	1	-	3/15/91/115	-
15	CLA	c2	404	13	-	11/39/115/115	-
15	CLA	c5	414	13	-	4/10/86/115	-
15	CLA	aB	818	2	-	10/32/108/115	-
18	BCR	a2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a1	410	13	-	4/15/91/115	-
18	BCR	b6	421	-	-	13/29/63/63	0/2/2/2
15	CLA	c3	417	13	-	11/27/103/115	-
15	CLA	b1	410	13	-	14/38/114/115	-
15	CLA	b4	403	13	-	14/39/115/115	-
15	CLA	bA	844	-	-	7/9/81/115	-
15	CLA	bB	834	2	-	15/31/107/115	-
19	LHG	bA	854	-	-	19/53/53/53	-
15	CLA	bJ	102	8	-	2/4/76/115	-
15	CLA	b6	422	13	-	17/39/115/115	-
15	CLA	c6	418	-	-	11/21/97/115	-
18	BCR	b6	402	-	-	14/29/63/63	0/2/2/2
15	CLA	a3	412	13	-	9/15/91/115	-
15	CLA	cA	838	1	-	8/23/99/115	-
15	CLA	a3	407	-	-	7/15/91/115	-
18	BCR	c6	421	-	-	12/29/63/63	0/2/2/2
15	CLA	c3	402	13	-	17/39/115/115	-
15	CLA	bB	838	2	-	2/18/94/115	-
18	BCR	cM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	409	13	-	6/39/115/115	-
15	CLA	bB	808	2	-	14/39/115/115	-
15	CLA	b6	412	13	-	4/15/91/115	-
15	CLA	bA	832	1	-	8/21/97/115	-
18	BCR	c6	402	-	-	11/29/63/63	0/2/2/2
15	CLA	c4	414	13	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	819	2	-	12/33/109/115	-
18	BCR	a1	421	-	-	14/29/63/63	0/2/2/2
15	CLA	cB	801	-	-	12/39/115/115	-
15	CLA	aB	839	22	-	10/39/115/115	-
18	BCR	bJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	c6	405	13	-	14/39/115/115	-
18	BCR	aJ	205	-	-	10/29/63/63	0/2/2/2
15	CLA	bA	834	1	-	12/39/115/115	-
15	CLA	a6	418	13	-	11/27/103/115	-
15	CLA	bB	842	-	-	2/15/91/115	-
15	CLA	cB	817	2	-	12/27/103/115	-
15	CLA	c6	414	13	-	9/15/91/115	-
15	CLA	bB	826	22	-	8/17/93/115	-
15	CLA	aA	826	-	-	10/39/115/115	-
15	CLA	bA	818	1	-	6/26/102/115	-
15	CLA	c5	420	13	-	12/39/115/115	-
15	CLA	cA	836	1	-	8/26/102/115	-
15	CLA	c1	413	13	-	4/15/91/115	-
15	CLA	aA	821	1	-	15/35/111/115	-
18	BCR	cF	202	-	-	14/29/63/63	0/2/2/2
15	CLA	cB	831	2	-	8/15/91/115	-
18	BCR	b6	420	-	-	12/29/63/63	0/2/2/2
18	BCR	c5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	835	1	-	14/39/115/115	-
18	BCR	bJ	105	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	420	13	-	12/39/115/115	-
15	CLA	cA	803	-	-	16/39/115/115	-
18	BCR	cI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	806	2	-	21/39/115/115	-
15	CLA	cA	806	1	-	23/39/115/115	-
18	BCR	c1	418	-	-	8/29/63/63	0/2/2/2
14	CL0	cA	801	1	-	6/39/115/115	-
15	CLA	bB	829	2	-	16/39/115/115	-
15	CLA	b4	409	13	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b5	406	13	-	4/15/91/115	-
15	CLA	b4	410	13	-	13/38/114/115	-
18	BCR	b6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	b3	403	13	-	13/39/115/115	-
15	CLA	a3	414	13	-	4/10/86/115	-
15	CLA	bB	812	2	-	3/15/91/115	-
18	BCR	c1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	804	-	-	12/39/115/115	-
18	BCR	bB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	c3	404	13	-	12/39/115/115	-
18	BCR	a3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	a4	403	13	-	14/39/115/115	-
15	CLA	bB	824	2	-	5/15/91/115	-
15	CLA	aB	827	2	-	15/39/115/115	-
15	CLA	a5	415	13	-	7/15/91/115	-
15	CLA	aB	815	2	-	17/39/115/115	-
15	CLA	a5	402	13	-	17/39/115/115	-
15	CLA	b5	420	13	-	12/39/115/115	-
18	BCR	aF	203	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	414	13	-	4/10/86/115	-
15	CLA	cA	811	1	-	10/15/91/115	-
15	CLA	b4	421	13	-	13/39/115/115	-
15	CLA	cB	822	2	-	2/15/91/115	-
15	CLA	c5	403	13	-	14/39/115/115	-
15	CLA	a5	411	13	-	3/15/91/115	-
15	CLA	c3	413	13	-	4/15/91/115	-
18	BCR	cB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	bB	810	2	-	16/39/115/115	-
15	CLA	bA	806	1	-	23/39/115/115	-
18	BCR	aL	205	-	-	14/29/63/63	0/2/2/2
15	CLA	c1	415	13	-	7/15/91/115	-
15	CLA	c3	412	13	-	9/15/91/115	-
18	BCR	c4	419	-	-	11/29/63/63	0/2/2/2
19	LHG	cX	101	-	-	11/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	cB	849	-	-	11/29/63/63	0/2/2/2
18	BCR	c3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	a2	411	13	-	13/38/114/115	-
14	CL0	bA	801	1	-	6/39/115/115	-
15	CLA	a1	409	13	-	14/38/114/115	-
15	CLA	bA	845	19	-	13/24/100/115	-
15	CLA	b6	410	13	-	6/39/115/115	-
15	CLA	cB	823	-	-	5/27/103/115	-
15	CLA	a5	414	13	-	4/10/86/115	-
15	CLA	c3	410	13	-	12/38/114/115	-
15	CLA	aA	839	1	-	16/39/115/115	-
15	CLA	bB	809	2	-	13/39/115/115	-
15	CLA	aB	802	2	-	13/39/115/115	-
15	CLA	a1	414	13	-	7/15/91/115	-
15	CLA	aJ	202	8	-	8/15/91/115	-
15	CLA	a2	405	-	-	4/15/91/115	-
15	CLA	b2	411	13	-	13/38/114/115	-
18	BCR	bB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	813	1	-	8/26/102/115	-
18	BCR	c4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	b1	414	13	-	4/10/86/115	-
15	CLA	c5	412	13	-	9/15/91/115	-
15	CLA	bB	833	2	-	18/39/115/115	-
15	CLA	bA	810	1	-	18/39/115/115	-
18	BCR	a2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	bA	827	22	-	10/39/115/115	-
15	CLA	cA	823	1	-	6/20/96/115	-
15	CLA	b3	408	13	-	5/15/91/115	-
15	CLA	a2	416	13	-	7/15/91/115	-
18	BCR	bB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	a6	417	-	-	11/21/97/115	-
15	CLA	b3	410	13	-	12/38/114/115	-
18	BCR	cA	848	-	-	13/29/63/63	0/2/2/2
20	LMG	bB	851	-	-	26/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	bA	853	-	-	22/29/63/63	0/2/2/2
15	CLA	bA	809	1	-	21/39/115/115	-
15	CLA	a4	410	13	-	13/38/114/115	-
15	CLA	b6	408	-	-	7/15/91/115	-
15	CLA	c2	412	13	-	3/15/91/115	-
15	CLA	cA	842	1	-	14/39/115/115	-
15	CLA	cA	805	1	-	11/32/108/115	-
15	CLA	c5	404	13	-	11/39/115/115	-
15	CLA	aA	807	1	-	11/39/115/115	-
15	CLA	c5	408	13	-	5/15/91/115	-
20	LMG	cB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	b1	413	13	-	4/15/91/115	-
15	CLA	bB	816	2	-	6/15/91/115	-
15	CLA	b6	417	-	-	11/21/97/115	-
18	BCR	cF	204	-	-	12/29/63/63	0/2/2/2
15	CLA	b1	405	-	-	3/15/91/115	-
15	CLA	c1	414	13	-	4/10/86/115	-
15	CLA	c5	410	13	-	13/38/114/115	-
15	CLA	c2	417	-	-	9/21/97/115	-
15	CLA	c6	404	13	-	17/39/115/115	-
15	CLA	aA	823	1	-	6/20/96/115	-
15	CLA	cB	836	2	-	11/33/109/115	-
15	CLA	c6	410	13	-	5/15/91/115	-
15	CLA	a6	416	13	-	7/15/91/115	-
18	BCR	b4	418	-	-	9/29/63/63	0/2/2/2
19	LHG	cA	853	15	-	15/31/31/53	-
15	CLA	a4	408	13	-	5/15/91/115	-
15	CLA	a3	416	-	-	11/21/97/115	-
15	CLA	c6	419	13	-	11/27/103/115	-
18	BCR	cF	205	-	-	11/29/63/63	0/2/2/2
18	BCR	a2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	a1	401	13	-	17/39/115/115	-
15	CLA	c1	403	13	-	14/39/115/115	-
18	BCR	a5	419	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bA	817	-	-	6/20/96/115	-
15	CLA	c3	414	13	-	4/10/86/115	-
15	CLA	aA	820	1	-	18/39/115/115	-
15	CLA	a4	411	13	-	5/15/91/115	-
15	CLA	aB	833	2	-	18/39/115/115	-
15	CLA	c4	417	13	-	9/27/103/115	-
15	CLA	cA	830	1	-	13/39/115/115	-
15	CLA	a1	402	13	-	14/39/115/115	-
15	CLA	bL	203	10	-	10/39/115/115	-
15	CLA	c5	407	-	-	8/15/91/115	-
15	CLA	c3	421	13	-	12/39/115/115	-
18	BCR	cL	205	-	-	9/29/63/63	0/2/2/2
15	CLA	b3	409	13	-	5/39/115/115	-
15	CLA	cA	821	1	-	15/35/111/115	-
15	CLA	b6	403	13	-	17/39/115/115	-
15	CLA	cA	837	1	-	7/15/91/115	-
18	BCR	aB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	b1	402	13	-	17/39/115/115	-
15	CLA	bA	829	1	-	22/39/115/115	-
15	CLA	b5	408	13	-	5/15/91/115	-
18	BCR	aB	849	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	831	2	-	8/15/91/115	-
15	CLA	a5	403	13	-	14/39/115/115	-
15	CLA	b6	405	13	-	11/39/115/115	-
15	CLA	aA	814	1	-	16/33/109/115	-
15	CLA	b2	406	13	-	10/39/115/115	-
15	CLA	b6	409	13	-	5/15/91/115	-
15	CLA	bB	821	2	-	13/18/94/115	-
18	BCR	c6	420	-	-	10/29/63/63	0/2/2/2
15	CLA	c3	415	13	-	7/15/91/115	-
18	BCR	a1	417	-	-	9/29/63/63	0/2/2/2
15	CLA	bA	835	1	-	14/39/115/115	-
15	CLA	cB	803	-	-	11/39/115/115	-
15	CLA	aB	821	2	-	13/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b4	413	13	-	4/15/91/115	-
15	CLA	c6	409	-	-	7/15/91/115	-
16	PQN	bB	843	-	-	10/23/43/43	0/2/2/2
18	BCR	bI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	cJ	101	8	-	8/15/91/115	-
15	CLA	aA	805	1	-	11/32/108/115	-
15	CLA	aA	830	1	-	13/39/115/115	-
18	BCR	bI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	406	13	-	4/15/91/115	-
15	CLA	b2	412	13	-	3/15/91/115	-
15	CLA	c3	409	13	-	6/39/115/115	-
15	CLA	bB	835	2	-	9/15/91/115	-
15	CLA	c4	408	13	-	5/15/91/115	-
18	BCR	aA	850	-	-	13/29/63/63	0/2/2/2
18	BCR	a6	402	-	-	14/29/63/63	0/2/2/2
18	BCR	b1	401	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	820	1	-	18/39/115/115	-
15	CLA	c2	409	13	-	5/15/91/115	-
17	SF4	aA	847	1,2	-	-	0/6/5/5
15	CLA	aB	825	2	-	10/26/102/115	-
15	CLA	bA	822	-	-	18/39/115/115	-
15	CLA	b6	413	13	-	9/15/91/115	-
15	CLA	a6	413	13	-	9/15/91/115	-
15	CLA	c4	405	-	-	4/15/91/115	-
18	BCR	aA	852	-	-	22/29/63/63	0/2/2/2
15	CLA	cA	844	19	-	13/24/100/115	-
15	CLA	c1	410	13	-	15/38/114/115	-
15	CLA	cK	102	-	-	10/15/91/115	-
18	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	404	13	-	11/39/115/115	-
18	BCR	a4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	bA	831	1	-	8/39/115/115	-
15	CLA	aA	828	1	-	14/39/115/115	-
15	CLA	cA	839	1	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	824	2	-	5/15/91/115	-
15	CLA	bB	807	2	-	15/39/115/115	-
15	CLA	b1	415	13	-	7/15/91/115	-
15	CLA	a5	407	-	-	8/15/91/115	-
15	CLA	b6	418	13	-	11/27/103/115	-
15	CLA	cB	825	2	-	10/26/102/115	-
15	CLA	aA	841	1	-	17/39/115/115	-
15	CLA	bB	823	-	-	5/27/103/115	-
15	CLA	b3	411	13	-	5/15/91/115	-
15	CLA	b2	422	13	-	12/39/115/115	-
15	CLA	a2	412	13	-	3/15/91/115	-
18	BCR	aA	848	-	-	11/29/63/63	0/2/2/2
15	CLA	a6	422	13	-	19/39/115/115	-
15	CLA	b5	407	-	-	8/15/91/115	-
15	CLA	a2	403	13	-	14/39/115/115	-
15	CLA	cF	203	-	-	10/15/91/115	-
18	BCR	bB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	c1	408	13	-	5/15/91/115	-
15	CLA	a4	404	13	-	12/39/115/115	-
15	CLA	c4	409	13	-	6/39/115/115	-
18	BCR	bF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	b2	407	13	-	4/15/91/115	-
15	CLA	b4	406	13	-	4/15/91/115	-
15	CLA	cA	833	1	-	11/39/115/115	-
15	CLA	cB	806	2	-	21/39/115/115	-
15	CLA	cB	834	2	-	15/31/107/115	-
18	BCR	cK	101	-	-	10/29/63/63	0/2/2/2
18	BCR	bJ	103	-	-	14/29/63/63	0/2/2/2
15	CLA	aA	802	22	-	16/39/115/115	-
15	CLA	cA	814	1	-	16/33/109/115	-
15	CLA	bA	812	1	-	13/39/115/115	-
15	CLA	b2	405	-	-	4/15/91/115	-
15	CLA	bA	823	1	-	6/20/96/115	-
15	CLA	aA	822	-	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a4	405	-	-	4/15/91/115	-
18	BCR	b2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	b5	411	13	-	3/15/91/115	-
15	CLA	a6	409	13	-	5/15/91/115	-
15	CLA	bA	816	1	-	3/15/91/115	-
15	CLA	a1	415	-	-	11/21/97/115	-
18	BCR	bL	205	-	-	9/29/63/63	0/2/2/2
15	CLA	b4	402	13	-	17/39/115/115	-
15	CLA	a6	403	13	-	17/39/115/115	-
18	BCR	b5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	823	-	-	5/27/103/115	-
15	CLA	aX	102	12	-	8/15/91/115	-
15	CLA	a5	405	-	-	4/15/91/115	-
18	BCR	c2	419	-	-	10/29/63/63	0/2/2/2
18	BCR	c3	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	829	1	-	22/39/115/115	-
15	CLA	bB	827	2	-	15/39/115/115	-
15	CLA	a1	411	13	-	9/15/91/115	-
15	CLA	cA	808	1	-	4/23/99/115	-
15	CLA	cB	837	2	-	15/39/115/115	-
18	BCR	a3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	c5	417	13	-	10/27/103/115	-
15	CLA	aA	819	1	-	10/26/102/115	-
15	CLA	a2	413	13	-	9/15/91/115	-
15	CLA	a1	406	-	-	8/15/91/115	-
18	BCR	aI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	b4	404	13	-	12/39/115/115	-
15	CLA	b3	402	13	-	17/39/115/115	-
15	CLA	c3	408	13	-	5/15/91/115	-
15	CLA	a2	409	13	-	5/15/91/115	-
18	BCR	aA	849	-	-	13/29/63/63	0/2/2/2
15	CLA	a4	402	13	-	17/39/115/115	-
15	CLA	bA	828	1	-	14/39/115/115	-
15	CLA	cA	804	1	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cX	102	12	-	8/15/91/115	-
15	CLA	a2	410	13	-	6/39/115/115	-
15	CLA	b3	415	13	-	7/15/91/115	-
15	CLA	aB	824	2	-	5/15/91/115	-
15	CLA	b5	405	-	-	4/15/91/115	-
15	CLA	b2	414	13	-	3/15/91/115	-
15	CLA	b1	406	13	-	4/15/91/115	-
15	CLA	c5	402	13	-	17/39/115/115	-
15	CLA	c5	416	-	-	11/21/97/115	-
18	BCR	a1	420	-	-	12/29/63/63	0/2/2/2
20	LMG	aB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	bA	836	1	-	8/26/102/115	-
15	CLA	aA	844	-	-	7/9/81/115	-
15	CLA	b6	415	13	-	4/10/86/115	-
15	CLA	a2	422	13	-	13/39/115/115	-
15	CLA	bA	803	-	-	16/39/115/115	-
15	CLA	aB	813	2	-	4/15/91/115	-
15	CLA	a4	409	13	-	5/39/115/115	-
15	CLA	b4	407	-	-	8/15/91/115	-
15	CLA	cA	828	1	-	14/39/115/115	-
15	CLA	aB	832	2	-	8/20/96/115	-
15	CLA	b6	411	13	-	14/38/114/115	-
18	BCR	a2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	b3	412	13	-	9/15/91/115	-
15	CLA	c1	411	13	-	5/15/91/115	-
15	CLA	aA	813	1	-	8/26/102/115	-
15	CLA	aB	803	-	-	11/39/115/115	-
15	CLA	aA	804	1	-	10/39/115/115	-
15	CLA	c5	406	13	-	4/15/91/115	-
15	CLA	a6	410	13	-	6/39/115/115	-
15	CLA	b3	407	-	-	7/15/91/115	-
15	CLA	c6	415	13	-	4/15/91/115	-
18	BCR	bB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	a3	421	13	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	828	2	-	21/39/115/115	-
15	CLA	cB	811	2	-	13/39/115/115	-
15	CLA	cA	802	22	-	16/39/115/115	-
15	CLA	aB	834	2	-	15/31/107/115	-
15	CLA	aA	843	1	-	14/39/115/115	-
15	CLA	a1	403	13	-	13/39/115/115	-
15	CLA	c4	412	13	-	9/15/91/115	-
15	CLA	aA	811	1	-	10/15/91/115	-
15	CLA	cB	815	2	-	17/39/115/115	-
15	CLA	b1	404	13	-	14/39/115/115	-
15	CLA	b1	403	13	-	14/39/115/115	-
15	CLA	aB	810	2	-	16/39/115/115	-
15	CLA	cB	813	2	-	4/15/91/115	-
18	BCR	b1	420	-	-	12/29/63/63	0/2/2/2
18	BCR	cA	847	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	832	2	-	8/20/96/115	-
15	CLA	bB	802	2	-	13/39/115/115	-
15	CLA	b3	404	13	-	12/39/115/115	-
15	CLA	cA	825	1	-	17/32/108/115	-
18	BCR	bL	206	-	-	14/29/63/63	0/2/2/2
15	CLA	a6	408	-	-	7/15/91/115	-
15	CLA	a4	415	13	-	7/15/91/115	-
15	CLA	bA	840	1	-	5/18/94/115	-
15	CLA	c6	412	13	-	12/38/114/115	-
15	CLA	a5	410	13	-	14/38/114/115	-
15	CLA	b1	409	13	-	6/39/115/115	-
15	CLA	b3	417	13	-	11/27/103/115	-
18	BCR	bA	848	-	-	10/29/63/63	0/2/2/2
18	BCR	cJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	cA	819	1	-	10/26/102/115	-
15	CLA	a3	415	13	-	7/15/91/115	-
15	CLA	cA	841	1	-	17/39/115/115	-
15	CLA	aK	102	-	-	10/15/91/115	-
15	CLA	aB	840	2	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a4	414	13	-	4/10/86/115	-
18	BCR	c4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b3	405	-	-	3/15/91/115	-
15	CLA	bA	805	1	-	11/32/108/115	-
15	CLA	cB	812	2	-	3/15/91/115	-
15	CLA	cA	817	-	-	6/20/96/115	-
15	CLA	cB	814	2	-	25/39/115/115	-
15	CLA	a3	405	-	-	3/15/91/115	-
15	CLA	cB	839	22	-	10/39/115/115	-
15	CLA	c6	407	-	-	3/15/91/115	-
15	CLA	cB	805	2	-	5/26/102/115	-
15	CLA	cA	816	1	-	3/15/91/115	-
15	CLA	a1	407	13	-	5/15/91/115	-
18	BCR	aJ	204	-	-	14/29/63/63	0/2/2/2
15	CLA	a3	410	13	-	12/38/114/115	-
15	CLA	aA	815	1	-	4/15/91/115	-
15	CLA	cB	804	-	-	12/39/115/115	-
15	CLA	bA	802	22	-	16/39/115/115	-
15	CLA	aB	807	2	-	15/39/115/115	-
15	CLA	b1	407	-	-	7/15/91/115	-
15	CLA	cB	816	2	-	6/15/91/115	-
15	CLA	aA	808	1	-	4/23/99/115	-
15	CLA	cB	830	2	-	6/39/115/115	-
18	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
15	CLA	c6	417	13	-	7/15/91/115	-
15	CLA	cB	841	-	-	4/15/91/115	-
15	CLA	c4	415	13	-	7/15/91/115	-
15	CLA	b5	410	13	-	14/38/114/115	-
15	CLA	aB	829	2	-	16/39/115/115	-
15	CLA	bB	830	2	-	6/39/115/115	-
15	CLA	b5	416	-	-	11/21/97/115	-
15	CLA	cB	840	2	-	16/39/115/115	-
15	CLA	c3	405	-	-	3/15/91/115	-
15	CLA	c4	413	13	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	b6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	a1	404	-	-	3/15/91/115	-
18	BCR	aI	102	-	-	11/29/63/63	0/2/2/2
18	BCR	bL	201	-	-	14/29/63/63	0/2/2/2
18	BCR	cB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	b2	416	13	-	7/15/91/115	-
15	CLA	c4	411	13	-	4/15/91/115	-
18	BCR	b1	419	-	-	11/29/63/63	0/2/2/2
18	BCR	c3	419	-	-	10/29/63/63	0/2/2/2
15	CLA	bL	202	10	-	15/39/115/115	-
15	CLA	bB	806	2	-	21/39/115/115	-
15	CLA	b5	412	13	-	9/15/91/115	-
18	BCR	aK	101	-	-	10/29/63/63	0/2/2/2
15	CLA	cB	807	2	-	15/39/115/115	-
18	BCR	b5	401	-	-	14/29/63/63	0/2/2/2
18	BCR	aI	103	-	-	9/29/63/63	0/2/2/2
15	CLA	b4	414	13	-	4/10/86/115	-
15	CLA	cJ	102	8	-	2/4/76/115	-
15	CLA	b4	408	13	-	5/15/91/115	-
15	CLA	c1	406	13	-	4/15/91/115	-
15	CLA	a5	416	-	-	11/21/97/115	-
15	CLA	aA	833	1	-	11/39/115/115	-
15	CLA	a3	406	13	-	4/15/91/115	-
15	CLA	bB	822	2	-	2/15/91/115	-
15	CLA	cB	829	2	-	16/39/115/115	-
15	CLA	cB	802	2	-	13/39/115/115	-
15	CLA	c3	407	-	-	7/15/91/115	-
15	CLA	a5	413	13	-	3/15/91/115	-
15	CLA	cA	843	-	-	7/9/81/115	-
15	CLA	aB	820	22	-	10/39/115/115	-
15	CLA	cA	827	22	-	10/39/115/115	-
15	CLA	bA	807	1	-	11/39/115/115	-
15	CLA	aB	826	22	-	8/17/93/115	-
15	CLA	c4	421	13	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	bB	849	-	-	14/29/63/63	0/2/2/2
15	CLA	a4	406	13	-	4/15/91/115	-
15	CLA	bB	801	-	-	12/39/115/115	-
15	CLA	bB	813	2	-	4/15/91/115	-
18	BCR	a5	418	-	-	11/29/63/63	0/2/2/2
18	BCR	a5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	c1	402	13	-	17/39/115/115	-
15	CLA	c1	407	-	-	8/15/91/115	-
15	CLA	c1	416	-	-	11/21/97/115	-
15	CLA	cB	838	2	-	2/18/94/115	-
15	CLA	c2	406	13	-	11/39/115/115	-
16	PQN	bA	846	-	-	5/23/43/43	0/2/2/2
18	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
18	BCR	cB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	bB	815	2	-	17/39/115/115	-
15	CLA	cB	808	2	-	14/39/115/115	-
15	CLA	b2	409	13	-	5/15/91/115	-
15	CLA	a6	407	13	-	4/15/91/115	-
15	CLA	b4	411	13	-	5/15/91/115	-
18	BCR	c3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cB	819	2	-	12/33/109/115	-
18	BCR	c5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	413	13	-	9/15/91/115	-
15	CLA	aA	831	1	-	8/39/115/115	-
15	CLA	a5	404	13	-	11/39/115/115	-
16	PQN	aB	843	-	-	10/23/43/43	0/2/2/2
15	CLA	cB	842	-	-	2/15/91/115	-
15	CLA	c1	404	13	-	13/39/115/115	-
18	BCR	cA	850	-	-	8/29/63/63	0/2/2/2
15	CLA	cB	826	22	-	8/17/93/115	-
15	CLA	c2	403	13	-	14/39/115/115	-
15	CLA	b3	421	13	-	12/39/115/115	-
15	CLA	aA	810	1	-	18/39/115/115	-
15	CLA	a1	405	13	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	821	2	-	13/18/94/115	-
17	SF4	bC	101	3	-	-	0/6/5/5
15	CLA	aJ	201	-	-	10/15/91/115	-
19	LHG	aX	101	-	-	11/26/26/53	-
15	CLA	a6	404	13	-	14/39/115/115	-
17	SF4	bC	102	3	-	-	0/6/5/5
18	BCR	aF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	812	2	-	3/15/91/115	-
15	CLA	aA	825	1	-	17/32/108/115	-
15	CLA	c6	406	13	-	11/39/115/115	-
15	CLA	bA	819	1	-	10/26/102/115	-
18	BCR	a4	401	-	-	13/29/63/63	0/2/2/2
18	BCR	aB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	837	2	-	15/39/115/115	-
18	BCR	c5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	843	1	-	14/39/115/115	-
15	CLA	aB	822	2	-	2/15/91/115	-
15	CLA	a3	404	13	-	12/39/115/115	-
15	CLA	aA	824	1	-	14/23/99/115	-
15	CLA	a3	403	13	-	13/39/115/115	-
15	CLA	c1	412	13	-	9/15/91/115	-
15	CLA	bA	811	1	-	10/15/91/115	-
15	CLA	c2	410	13	-	6/39/115/115	-
15	CLA	bB	814	2	-	25/39/115/115	-
18	BCR	b2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	811	2	-	13/39/115/115	-
15	CLA	a3	409	13	-	5/39/115/115	-
15	CLA	bB	818	2	-	10/32/108/115	-
15	CLA	bB	804	-	-	12/39/115/115	-
15	CLA	b6	404	13	-	14/39/115/115	-
15	CLA	b4	417	13	-	9/27/103/115	-
18	BCR	b2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	c2	422	13	-	13/39/115/115	-
18	BCR	a6	421	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	bB	850	-	-	11/29/63/63	0/2/2/2
15	CLA	c4	402	13	-	17/39/115/115	-
18	BCR	bM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	809	2	-	13/39/115/115	-
18	BCR	cI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	c3	411	13	-	5/15/91/115	-
15	CLA	a2	406	13	-	11/39/115/115	-
15	CLA	c4	403	13	-	14/39/115/115	-
15	CLA	a5	409	13	-	6/39/115/115	-
15	CLA	b1	417	13	-	12/27/103/115	-
15	CLA	bA	814	1	-	16/33/109/115	-
18	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
18	BCR	aA	851	-	-	8/29/63/63	0/2/2/2
15	CLA	a4	413	13	-	4/15/91/115	-
18	BCR	aF	201	-	-	14/29/63/63	0/2/2/2
15	CLA	bA	839	1	-	16/39/115/115	-
18	BCR	b4	401	-	-	13/29/63/63	0/2/2/2
15	CLA	a2	408	-	-	8/15/91/115	-
18	BCR	cB	847	-	-	9/18/35/63	0/1/1/2
17	SF4	cC	101	3	-	-	0/6/5/5
15	CLA	bA	837	1	-	7/15/91/115	-
17	SF4	cC	102	3	-	-	0/6/5/5
15	CLA	aB	835	2	-	9/15/91/115	-
15	CLA	b4	405	-	-	4/15/91/115	-
15	CLA	bA	804	1	-	10/39/115/115	-
15	CLA	bK	101	-	-	10/15/91/115	-
15	CLA	b5	404	13	-	11/39/115/115	-
15	CLA	c4	404	13	-	11/39/115/115	-
15	CLA	aL	201	10	-	15/39/115/115	-
15	CLA	a6	405	13	-	11/39/115/115	-
15	CLA	bA	830	1	-	13/39/115/115	-
15	CLA	aB	838	2	-	2/18/94/115	-
15	CLA	a2	402	13	-	17/39/115/115	-
15	CLA	aB	808	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a5	412	13	-	9/15/91/115	-
15	CLA	c4	410	13	-	13/38/114/115	-
15	CLA	a1	416	13	-	10/27/103/115	-
15	CLA	b2	418	13	-	11/27/103/115	-
15	CLA	cB	820	22	-	10/39/115/115	-
15	CLA	cL	203	10	-	10/39/115/115	-
18	BCR	cJ	103	-	-	14/29/63/63	0/2/2/2
18	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	817	2	-	12/27/103/115	-
15	CLA	a1	412	13	-	4/15/91/115	-
15	CLA	b1	416	-	-	11/21/97/115	-
18	BCR	a4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	813	1	-	8/26/102/115	-
15	CLA	a1	408	13	-	6/39/115/115	-
15	CLA	aA	817	-	-	6/20/96/115	-
15	CLA	c3	403	13	-	13/39/115/115	-
15	CLA	b1	412	13	-	9/15/91/115	-
15	CLA	aB	842	-	-	2/15/91/115	-
16	PQN	cA	845	-	-	5/23/43/43	0/2/2/2
15	CLA	b4	416	-	-	11/21/97/115	-
15	CLA	a2	404	13	-	12/39/115/115	-
15	CLA	b1	408	13	-	5/15/91/115	-
18	BCR	c2	421	-	-	12/29/63/63	0/2/2/2
18	BCR	c6	403	-	-	13/29/63/63	0/2/2/2
18	BCR	aM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	831	2	-	8/15/91/115	-
15	CLA	bF	201	-	-	10/15/91/115	-
15	CLA	aA	827	22	-	10/39/115/115	-
15	CLA	bX	102	12	-	8/15/91/115	-
15	CLA	aA	832	1	-	8/21/97/115	-
15	CLA	cA	824	1	-	14/23/99/115	-
15	CLA	aA	803	-	-	16/39/115/115	-

The worst 5 of 6339 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	aA	846	PQN	C3-C2	6.92	1.47	1.35
16	bA	846	PQN	C3-C2	6.88	1.47	1.35
16	cA	845	PQN	C3-C2	6.86	1.47	1.35
16	cB	843	PQN	C3-C2	6.78	1.47	1.35
16	aB	843	PQN	C3-C2	6.78	1.47	1.35

The worst 5 of 7568 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	bB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	aB	804	CLA	C4A-NA-C1A	10.44	111.40	106.71
15	aA	803	CLA	C4A-NA-C1A	9.96	111.19	106.71
15	cA	803	CLA	C4A-NA-C1A	9.91	111.16	106.71

There are no chirality outliers.

5 of 7649 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	aA	803	CLA	CBA-CGA-O2A-C1
15	aA	803	CLA	O1A-CGA-O2A-C1
15	aA	804	CLA	C1A-C2A-CAA-CBA
15	aA	804	CLA	CHA-CBD-CGD-O1D
15	aA	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

660 monomers are involved in 1881 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cA	818	CLA	2	0
15	b1	411	CLA	1	0
16	aA	846	PQN	3	0
15	a3	402	CLA	9	0
15	c2	405	CLA	1	0
15	bA	838	CLA	1	0
15	aA	835	CLA	5	0
15	a6	415	CLA	1	0
15	bA	808	CLA	2	0
16	cB	843	PQN	3	0
18	b3	401	BCR	1	0
15	aA	837	CLA	1	0
15	bB	825	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b2	403	CLA	5	0
15	cA	831	CLA	5	0
15	cB	835	CLA	2	0
15	a6	411	CLA	3	0
15	cB	833	CLA	9	0
15	cA	815	CLA	2	0
15	bA	842	CLA	3	0
15	bA	815	CLA	1	0
15	b5	417	CLA	6	0
15	a1	413	CLA	1	0
15	c2	415	CLA	1	0
15	c2	413	CLA	3	0
15	aA	840	CLA	2	0
15	bB	828	CLA	5	0
15	c5	405	CLA	1	0
15	c5	409	CLA	3	0
15	a6	412	CLA	1	0
15	cA	810	CLA	6	0
15	c2	411	CLA	4	0
15	a4	421	CLA	7	0
18	a3	419	BCR	2	0
15	aA	836	CLA	3	0
15	b2	402	CLA	8	0
15	aB	841	CLA	1	0
15	b5	402	CLA	9	0
18	b1	418	BCR	3	0
15	aA	834	CLA	5	0
15	cB	810	CLA	4	0
15	aA	818	CLA	1	0
15	b5	403	CLA	4	0
15	b2	415	CLA	1	0
18	c1	419	BCR	4	0
15	b5	415	CLA	8	0
15	a3	417	CLA	5	0
15	bB	841	CLA	1	0
15	aA	838	CLA	1	0
18	b4	419	BCR	3	0
15	b2	417	CLA	6	0
15	bB	817	CLA	4	0
15	a2	418	CLA	4	0
15	c3	416	CLA	4	0
15	b2	410	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cA	826	CLA	3	0
15	aB	814	CLA	7	0
15	aL	202	CLA	4	0
15	a4	417	CLA	6	0
15	cL	202	CLA	5	0
18	b3	419	BCR	3	0
15	bA	825	CLA	5	0
15	a5	408	CLA	1	0
15	cF	201	CLA	3	0
15	aA	842	CLA	3	0
15	aB	816	CLA	1	0
15	a5	417	CLA	4	0
15	c1	417	CLA	2	0
18	aB	848	BCR	3	0
15	aB	830	CLA	3	0
18	aB	847	BCR	3	0
15	bB	819	CLA	4	0
15	bA	841	CLA	3	0
15	b3	416	CLA	4	0
18	c2	401	BCR	5	0
15	a3	408	CLA	1	0
15	c6	401	CLA	8	0
18	c1	401	BCR	2	0
15	a4	416	CLA	5	0
15	cA	820	CLA	3	0
15	cB	818	CLA	3	0
15	c2	418	CLA	4	0
15	cA	812	CLA	5	0
15	c1	405	CLA	1	0
15	c1	409	CLA	3	0
15	b6	416	CLA	8	0
18	a6	420	BCR	3	0
18	b2	401	BCR	4	0
18	b3	418	BCR	2	0
18	b4	420	BCR	5	0
15	aA	806	CLA	5	0
18	a6	401	BCR	3	0
15	a3	411	CLA	1	0
15	bA	826	CLA	3	0
19	aA	853	LHG	3	0
15	bB	820	CLA	1	0
15	bB	837	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a6	406	CLA	1	0
15	b3	414	CLA	1	0
18	a1	419	BCR	3	0
19	cA	852	LHG	3	0
18	a3	401	BCR	2	0
15	cA	832	CLA	1	0
15	c6	416	CLA	1	0
15	bA	821	CLA	3	0
15	aB	828	CLA	6	0
15	c2	402	CLA	9	0
15	c2	416	CLA	8	0
15	b6	406	CLA	1	0
15	b4	415	CLA	8	0
15	bB	836	CLA	1	0
15	bB	832	CLA	4	0
15	bB	803	CLA	4	0
15	a2	415	CLA	1	0
15	a4	412	CLA	2	0
18	cA	851	BCR	4	0
15	cB	827	CLA	3	0
15	bA	833	CLA	3	0
15	aL	203	CLA	4	0
15	aA	829	CLA	4	0
15	a2	417	CLA	6	0
18	a1	418	BCR	4	0
15	bB	839	CLA	4	0
18	c2	420	BCR	2	0
15	bJ	101	CLA	1	0
15	cA	840	CLA	2	0
18	a4	420	BCR	5	0
15	cA	822	CLA	3	0
18	b5	418	BCR	1	0
18	c4	401	BCR	4	0
15	c5	415	CLA	8	0
15	aA	812	CLA	5	0
14	aA	801	CL0	4	0
15	aB	801	CLA	4	0
15	aA	845	CLA	1	0
18	b3	420	BCR	5	0
15	bL	204	CLA	5	0
15	cA	807	CLA	5	0
15	bB	840	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bB	811	CLA	7	0
15	cL	204	CLA	5	0
18	bA	850	BCR	3	0
15	cA	809	CLA	2	0
15	c5	411	CLA	1	0
15	c4	416	CLA	2	0
18	a6	419	BCR	2	0
15	c6	413	CLA	1	0
15	aA	809	CLA	2	0
15	b4	412	CLA	1	0
18	bA	852	BCR	3	0
15	cB	809	CLA	3	0
15	cA	834	CLA	5	0
15	c6	411	CLA	3	0
15	aA	816	CLA	1	0
15	c2	404	CLA	3	0
15	c5	414	CLA	1	0
15	aB	818	CLA	4	0
18	a2	401	BCR	6	0
15	a1	410	CLA	1	0
18	b6	421	BCR	1	0
15	c3	417	CLA	6	0
15	b1	410	CLA	3	0
15	b4	403	CLA	5	0
15	bA	844	CLA	1	0
15	bB	834	CLA	1	0
19	bA	854	LHG	3	0
15	b6	422	CLA	9	0
15	c6	418	CLA	5	0
18	b6	402	BCR	3	0
15	a3	412	CLA	2	0
15	cA	838	CLA	1	0
15	a3	407	CLA	1	0
18	c6	421	BCR	2	0
15	c3	402	CLA	9	0
15	bB	838	CLA	1	0
18	cM	101	BCR	4	0
15	b5	409	CLA	3	0
15	bB	808	CLA	2	0
15	b6	412	CLA	1	0
15	bA	832	CLA	1	0
18	c6	402	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c4	414	CLA	1	0
15	aB	819	CLA	3	0
18	a1	421	BCR	2	0
15	cB	801	CLA	5	0
15	aB	839	CLA	4	0
18	bJ	104	BCR	5	0
15	c6	405	CLA	4	0
18	aJ	205	BCR	3	0
15	bA	834	CLA	5	0
15	a6	418	CLA	4	0
15	bB	842	CLA	2	0
15	cB	817	CLA	4	0
15	c6	414	CLA	3	0
15	bB	826	CLA	2	0
15	aA	826	CLA	3	0
15	bA	818	CLA	2	0
15	c5	420	CLA	8	0
15	cA	836	CLA	2	0
15	c1	413	CLA	1	0
15	aA	821	CLA	4	0
18	cF	202	BCR	5	0
15	cB	831	CLA	3	0
18	b6	420	BCR	3	0
18	c5	401	BCR	3	0
15	cA	835	CLA	3	0
18	bJ	105	BCR	4	0
15	a5	420	CLA	10	0
15	cA	803	CLA	5	0
18	cI	101	BCR	1	0
15	aB	806	CLA	2	0
15	cA	806	CLA	4	0
18	c1	418	BCR	2	0
14	cA	801	CL0	3	0
15	bB	829	CLA	5	0
15	b4	409	CLA	3	0
15	b4	410	CLA	4	0
18	b6	419	BCR	1	0
15	b3	403	CLA	4	0
15	a3	414	CLA	1	0
15	bB	812	CLA	2	0
18	c1	420	BCR	4	0
15	aB	804	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	bB	846	BCR	2	0
15	c3	404	CLA	3	0
18	a3	420	BCR	4	0
15	a4	403	CLA	5	0
15	bB	824	CLA	1	0
15	aB	827	CLA	3	0
15	a5	415	CLA	8	0
15	aB	815	CLA	5	0
15	a5	402	CLA	9	0
15	b5	420	CLA	10	0
18	aF	203	BCR	6	0
15	b5	414	CLA	1	0
15	b4	421	CLA	10	0
15	c5	403	CLA	4	0
15	a5	411	CLA	1	0
18	cB	846	BCR	2	0
15	bB	810	CLA	3	0
15	bA	806	CLA	4	0
18	aL	205	BCR	1	0
15	c1	415	CLA	8	0
15	c3	412	CLA	2	0
18	c4	419	BCR	3	0
18	cB	849	BCR	5	0
18	c3	418	BCR	1	0
15	a2	411	CLA	3	0
14	bA	801	CL0	4	0
15	a1	409	CLA	4	0
15	bA	845	CLA	1	0
15	b6	410	CLA	4	0
15	a5	414	CLA	1	0
15	c3	410	CLA	3	0
15	aA	839	CLA	5	0
15	bB	809	CLA	3	0
15	aB	802	CLA	2	0
15	a1	414	CLA	7	0
15	aJ	202	CLA	1	0
15	a2	405	CLA	1	0
15	b2	411	CLA	3	0
18	bB	845	BCR	3	0
15	bA	813	CLA	2	0
18	c4	418	BCR	1	0
15	b1	414	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c5	412	CLA	3	0
15	bB	833	CLA	4	0
15	bA	810	CLA	6	0
18	a2	419	BCR	1	0
15	bA	827	CLA	4	0
15	b3	408	CLA	1	0
15	a2	416	CLA	8	0
18	bB	844	BCR	3	0
15	a6	417	CLA	5	0
15	b3	410	CLA	4	0
18	cA	848	BCR	3	0
20	bB	851	LMG	1	0
18	bA	853	BCR	4	0
15	bA	809	CLA	2	0
15	a4	410	CLA	4	0
15	c2	412	CLA	2	0
15	cA	842	CLA	11	0
15	cA	805	CLA	2	0
15	c5	404	CLA	3	0
15	aA	807	CLA	5	0
15	c5	408	CLA	1	0
20	cB	850	LMG	1	0
15	bB	816	CLA	1	0
15	b6	417	CLA	4	0
18	cF	204	BCR	5	0
15	b1	405	CLA	1	0
15	c1	414	CLA	1	0
15	c5	410	CLA	4	0
15	c2	417	CLA	6	0
15	c6	404	CLA	9	0
15	c6	410	CLA	1	0
15	a6	416	CLA	8	0
18	b4	418	BCR	1	0
15	a4	408	CLA	1	0
15	a3	416	CLA	4	0
15	c6	419	CLA	4	0
18	cF	205	BCR	8	0
18	a2	420	BCR	3	0
15	a1	401	CLA	9	0
15	c1	403	CLA	4	0
18	a5	419	BCR	5	0
15	c3	414	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	aA	820	CLA	2	0
15	a4	411	CLA	1	0
15	aB	833	CLA	8	0
15	c4	417	CLA	5	0
15	cA	830	CLA	1	0
15	a1	402	CLA	4	0
15	bL	203	CLA	4	0
15	c3	421	CLA	6	0
18	cL	205	BCR	3	0
15	b3	409	CLA	3	0
15	cA	821	CLA	4	0
15	b6	403	CLA	9	0
15	cA	837	CLA	1	0
18	aB	844	BCR	2	0
15	b1	402	CLA	9	0
15	bA	829	CLA	6	0
15	b5	408	CLA	1	0
18	aB	849	BCR	4	0
15	aB	831	CLA	2	0
15	a5	403	CLA	4	0
15	b6	405	CLA	3	0
15	aA	814	CLA	2	0
15	b2	406	CLA	16	0
15	b6	409	CLA	1	0
15	bB	821	CLA	2	0
18	c6	420	BCR	2	0
15	c3	415	CLA	7	0
18	a1	417	BCR	4	0
15	bA	835	CLA	6	0
15	cB	803	CLA	2	0
15	aB	821	CLA	2	0
16	bB	843	PQN	4	0
15	cJ	101	CLA	1	0
15	aA	805	CLA	3	0
15	aA	830	CLA	1	0
18	bI	102	BCR	4	0
15	b2	412	CLA	2	0
15	c3	409	CLA	3	0
15	bB	835	CLA	2	0
15	c4	408	CLA	1	0
18	aA	850	BCR	3	0
18	a6	402	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b1	401	BCR	2	0
15	bA	820	CLA	3	0
15	c2	409	CLA	1	0
15	aB	825	CLA	1	0
15	bA	822	CLA	3	0
15	b6	413	CLA	3	0
15	a6	413	CLA	3	0
15	c4	405	CLA	1	0
18	aA	852	BCR	4	0
15	cA	844	CLA	3	0
15	c1	410	CLA	4	0
18	bA	849	BCR	3	0
15	b2	404	CLA	2	0
18	a4	418	BCR	1	0
15	bA	831	CLA	5	0
15	aA	828	CLA	3	0
15	cA	839	CLA	6	0
15	cB	824	CLA	2	0
15	bB	807	CLA	4	0
15	b1	415	CLA	8	0
15	b6	418	CLA	5	0
15	cB	825	CLA	1	0
15	aA	841	CLA	5	0
15	b3	411	CLA	1	0
15	b2	422	CLA	9	0
15	a2	412	CLA	3	0
18	aA	848	BCR	4	0
15	a6	422	CLA	11	0
15	a2	403	CLA	5	0
15	cF	203	CLA	3	0
18	bB	847	BCR	4	0
15	c1	408	CLA	1	0
15	a4	404	CLA	3	0
15	c4	409	CLA	3	0
18	bF	202	BCR	5	0
15	cA	833	CLA	3	0
15	cB	806	CLA	2	0
15	cB	834	CLA	1	0
18	cK	101	BCR	1	0
18	bJ	103	BCR	5	0
15	aA	802	CLA	2	0
15	cA	814	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bA	812	CLA	5	0
15	b2	405	CLA	1	0
15	aA	822	CLA	4	0
15	a4	405	CLA	1	0
18	b2	419	BCR	3	0
15	b5	411	CLA	1	0
15	a6	409	CLA	1	0
15	bA	816	CLA	1	0
15	a1	415	CLA	5	0
18	bL	205	BCR	3	0
15	b4	402	CLA	9	0
15	a6	403	CLA	9	0
18	b5	419	BCR	5	0
15	aX	102	CLA	2	0
15	a5	405	CLA	1	0
18	c2	419	BCR	1	0
18	c3	401	BCR	1	0
15	cA	829	CLA	4	0
15	bB	827	CLA	3	0
15	a1	411	CLA	2	0
15	cA	808	CLA	2	0
15	cB	837	CLA	5	0
18	a3	418	BCR	1	0
15	c5	417	CLA	4	0
15	aA	819	CLA	1	0
15	a2	413	CLA	3	0
15	b4	404	CLA	3	0
15	b3	402	CLA	9	0
15	c3	408	CLA	1	0
15	a2	409	CLA	1	0
18	aA	849	BCR	2	0
15	a4	402	CLA	9	0
15	bA	828	CLA	3	0
15	cA	804	CLA	8	0
15	cX	102	CLA	2	0
15	a2	410	CLA	3	0
15	b3	415	CLA	7	0
15	aB	824	CLA	1	0
15	b5	405	CLA	1	0
15	c5	402	CLA	9	0
15	c5	416	CLA	5	0
18	a1	420	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	aB	850	LMG	1	0
15	bA	836	CLA	3	0
15	aA	844	CLA	1	0
15	b6	415	CLA	1	0
15	a2	422	CLA	8	0
15	bA	803	CLA	8	0
15	aB	813	CLA	3	0
15	a4	409	CLA	3	0
15	cA	828	CLA	3	0
15	aB	832	CLA	2	0
15	b6	411	CLA	3	0
18	a2	421	BCR	4	0
15	b3	412	CLA	2	0
15	c1	411	CLA	1	0
15	aA	813	CLA	2	0
15	aB	803	CLA	1	0
15	aA	804	CLA	6	0
15	a6	410	CLA	3	0
18	bB	848	BCR	2	0
15	a3	421	CLA	6	0
15	cB	828	CLA	4	0
15	cB	811	CLA	4	0
15	cA	802	CLA	2	0
15	aB	834	CLA	1	0
15	aA	843	CLA	11	0
15	a1	403	CLA	2	0
15	c4	412	CLA	2	0
15	cB	815	CLA	5	0
15	b1	404	CLA	3	0
15	b1	403	CLA	4	0
15	aB	810	CLA	2	0
15	cB	813	CLA	3	0
18	b1	420	BCR	5	0
18	cA	847	BCR	3	0
15	cB	832	CLA	2	0
15	bB	802	CLA	3	0
15	b3	404	CLA	3	0
15	cA	825	CLA	5	0
18	bL	206	BCR	2	0
15	a4	415	CLA	8	0
15	bA	840	CLA	2	0
15	c6	412	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a5	410	CLA	3	0
15	b1	409	CLA	3	0
15	b3	417	CLA	5	0
18	bA	848	BCR	2	0
18	cJ	104	BCR	3	0
15	cA	819	CLA	1	0
15	a3	415	CLA	8	0
15	cA	841	CLA	6	0
15	aB	840	CLA	1	0
15	a4	414	CLA	1	0
18	c4	420	BCR	5	0
15	b3	405	CLA	1	0
15	bA	805	CLA	3	0
15	cB	812	CLA	2	0
15	cB	814	CLA	7	0
15	a3	405	CLA	1	0
15	cB	839	CLA	5	0
15	c6	407	CLA	1	0
15	cA	816	CLA	1	0
15	a1	407	CLA	1	0
18	aJ	204	BCR	5	0
15	a3	410	CLA	4	0
15	aA	815	CLA	2	0
15	cB	804	CLA	4	0
15	bA	802	CLA	1	0
15	aB	807	CLA	2	0
15	cB	816	CLA	1	0
15	aA	808	CLA	2	0
15	cB	830	CLA	3	0
18	bA	851	BCR	2	0
15	c6	417	CLA	8	0
15	cB	841	CLA	1	0
15	c4	415	CLA	9	0
15	b5	410	CLA	4	0
15	aB	829	CLA	5	0
15	bB	830	CLA	3	0
15	b5	416	CLA	5	0
15	cB	840	CLA	2	0
15	c3	405	CLA	1	0
18	b6	401	BCR	3	0
15	a1	404	CLA	1	0
18	aI	102	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	bL	201	BCR	1	0
18	cB	848	BCR	2	0
15	b2	416	CLA	8	0
15	c4	411	CLA	1	0
18	b1	419	BCR	3	0
18	c3	419	BCR	1	0
15	bL	202	CLA	2	0
15	bB	806	CLA	2	0
15	b5	412	CLA	3	0
18	aK	101	BCR	1	0
15	cB	807	CLA	3	0
18	b5	401	BCR	3	0
18	aI	103	BCR	4	0
15	b4	414	CLA	1	0
15	b4	408	CLA	1	0
15	a5	416	CLA	5	0
15	aA	833	CLA	2	0
15	bB	822	CLA	1	0
15	cB	829	CLA	4	0
15	cB	802	CLA	3	0
15	cA	843	CLA	1	0
15	aB	820	CLA	1	0
15	cA	827	CLA	2	0
15	bA	807	CLA	5	0
15	aB	826	CLA	3	0
15	c4	421	CLA	7	0
18	bB	849	BCR	6	0
15	bB	801	CLA	6	0
15	bB	813	CLA	3	0
18	a5	418	BCR	1	0
18	a5	401	BCR	4	0
15	c1	402	CLA	9	0
15	c1	416	CLA	4	0
15	cB	838	CLA	3	0
15	c2	406	CLA	13	0
16	bA	846	PQN	3	0
18	cA	849	BCR	2	0
18	cB	844	BCR	2	0
15	bB	815	CLA	5	0
15	cB	808	CLA	5	0
15	b2	409	CLA	1	0
15	b4	411	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	c3	420	BCR	6	0
15	cB	819	CLA	3	0
18	c5	418	BCR	1	0
15	b2	413	CLA	2	0
15	aA	831	CLA	4	0
15	a5	404	CLA	2	0
16	aB	843	PQN	3	0
15	cB	842	CLA	2	0
15	c1	404	CLA	2	0
18	cA	850	BCR	3	0
15	cB	826	CLA	3	0
15	c2	403	CLA	5	0
15	b3	421	CLA	5	0
15	aA	810	CLA	6	0
15	cB	821	CLA	2	0
15	aJ	201	CLA	4	0
19	aX	101	LHG	1	0
15	a6	404	CLA	4	0
18	aF	202	BCR	7	0
15	aB	812	CLA	2	0
15	aA	825	CLA	5	0
15	c6	406	CLA	3	0
15	bA	819	CLA	1	0
18	a4	401	BCR	4	0
18	aB	846	BCR	1	0
15	aB	837	CLA	8	0
18	c5	419	BCR	5	0
15	bA	843	CLA	10	0
15	a3	404	CLA	3	0
15	a3	403	CLA	4	0
15	c1	412	CLA	2	0
15	c2	410	CLA	2	0
15	bB	814	CLA	8	0
18	b2	420	BCR	3	0
15	aB	811	CLA	10	0
15	a3	409	CLA	2	0
15	bB	818	CLA	4	0
15	bB	804	CLA	4	0
15	b6	404	CLA	4	0
15	b4	417	CLA	5	0
18	b2	421	BCR	4	0
15	c2	422	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a6	421	BCR	1	0
18	bB	850	BCR	5	0
15	c4	402	CLA	8	0
18	bM	101	BCR	4	0
15	aB	809	CLA	3	0
18	cI	102	BCR	3	0
15	c3	411	CLA	1	0
15	a2	406	CLA	11	0
15	c4	403	CLA	4	0
15	a5	409	CLA	3	0
15	b1	417	CLA	4	0
15	bA	814	CLA	1	0
18	aB	845	BCR	3	0
18	aA	851	BCR	2	0
18	aF	201	BCR	3	0
15	bA	839	CLA	5	0
18	b4	401	BCR	3	0
18	cB	847	BCR	2	0
15	bA	837	CLA	1	0
15	aB	835	CLA	2	0
15	b4	405	CLA	1	0
15	bA	804	CLA	8	0
15	b5	404	CLA	3	0
15	c4	404	CLA	2	0
15	aL	201	CLA	3	0
15	a6	405	CLA	2	0
15	aB	838	CLA	3	0
15	a2	402	CLA	9	0
15	aB	808	CLA	5	0
15	a5	412	CLA	3	0
15	c4	410	CLA	4	0
15	a1	416	CLA	2	0
15	b2	418	CLA	4	0
15	cB	820	CLA	1	0
15	cL	203	CLA	3	0
18	cJ	103	BCR	6	0
18	cB	845	BCR	3	0
15	aB	817	CLA	4	0
15	a1	412	CLA	1	0
15	b1	416	CLA	4	0
18	a4	419	BCR	3	0
15	cA	813	CLA	2	0

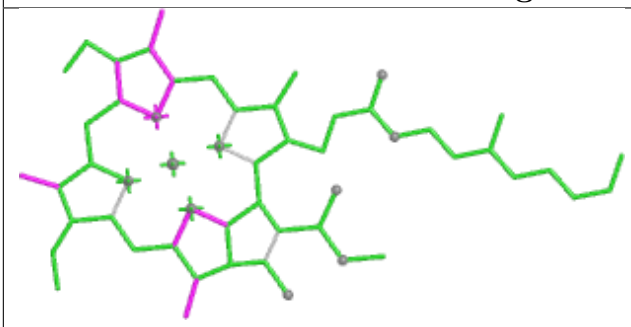
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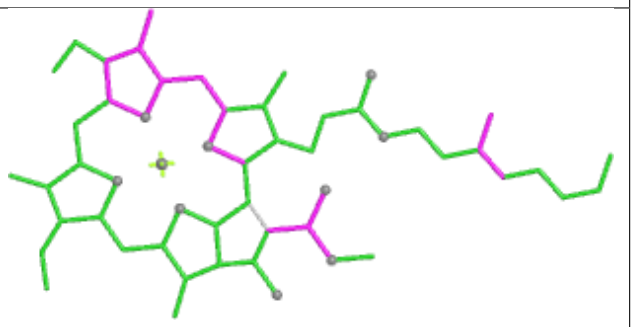
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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15	c3	403	CLA	4	0
15	b1	412	CLA	2	0
15	aB	842	CLA	2	0
16	cA	845	PQN	4	0
15	b4	416	CLA	5	0
15	a2	404	CLA	2	0
15	b1	408	CLA	1	0
18	c2	421	BCR	3	0
18	c6	403	BCR	3	0
18	aM	101	BCR	3	0
15	bB	831	CLA	3	0
15	bF	201	CLA	2	0
15	aA	827	CLA	2	0
15	bX	102	CLA	3	0
15	aA	832	CLA	1	0
15	aA	803	CLA	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

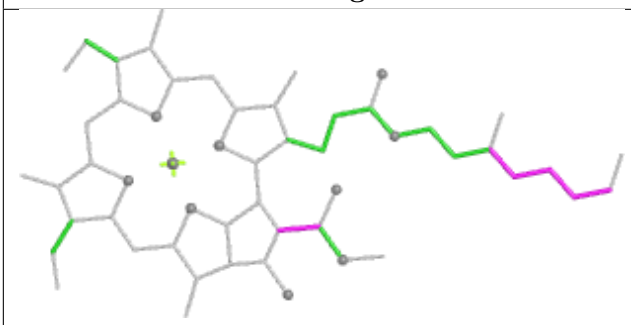
Ligand CLA cA 818



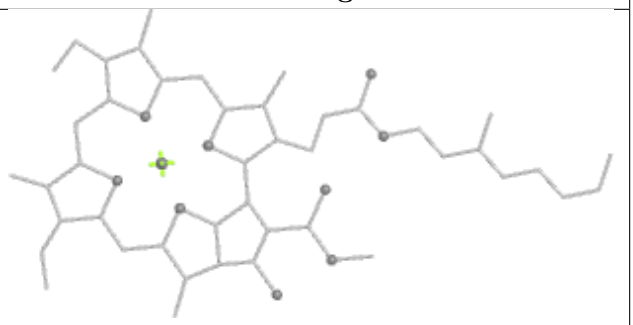
Bond lengths



Bond angles

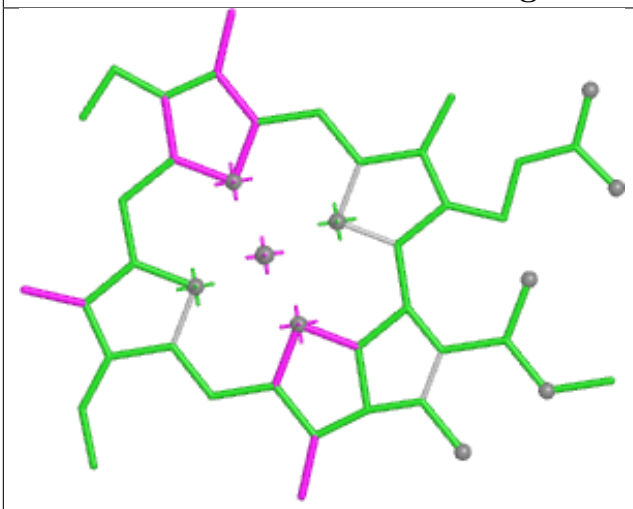


Torsions

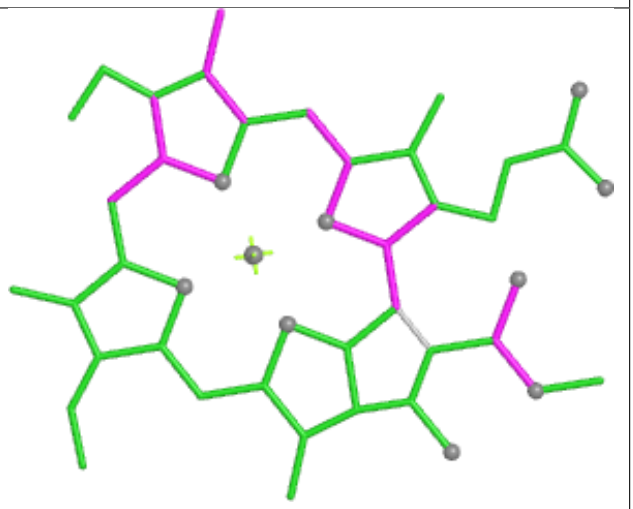


Rings

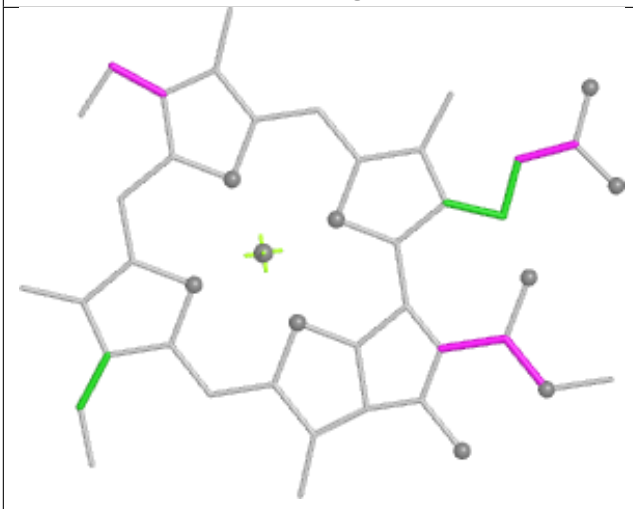
Ligand CLA a4 407



Bond lengths



Bond angles

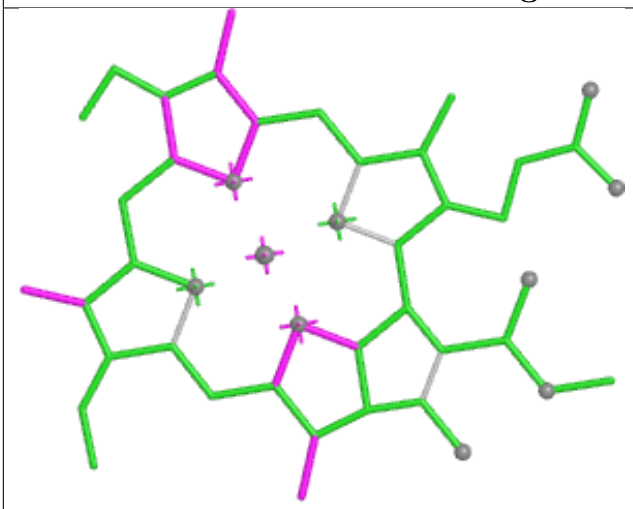


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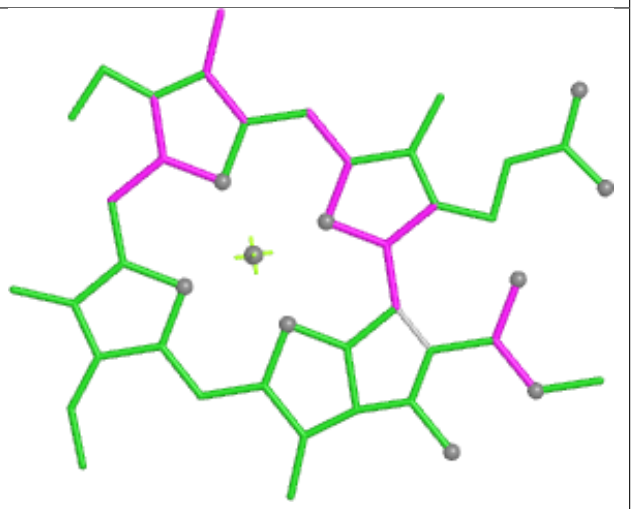


Rings

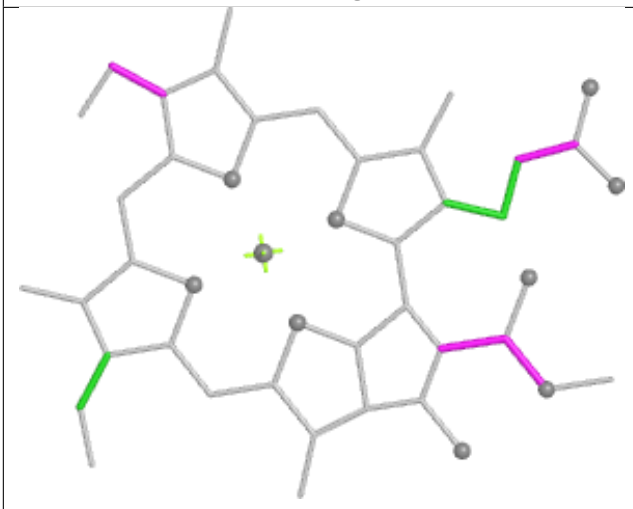
Ligand CLA c4 407



Bond lengths



Bond angles

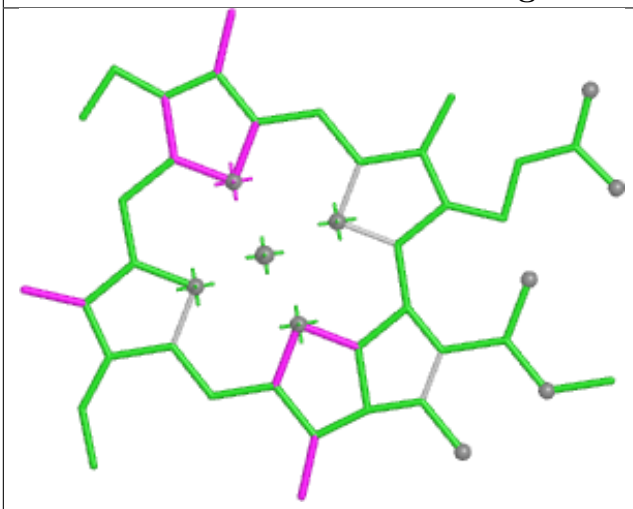


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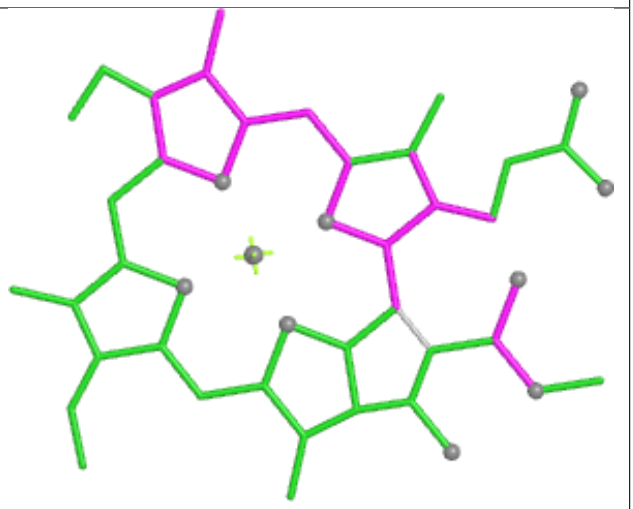


Rings

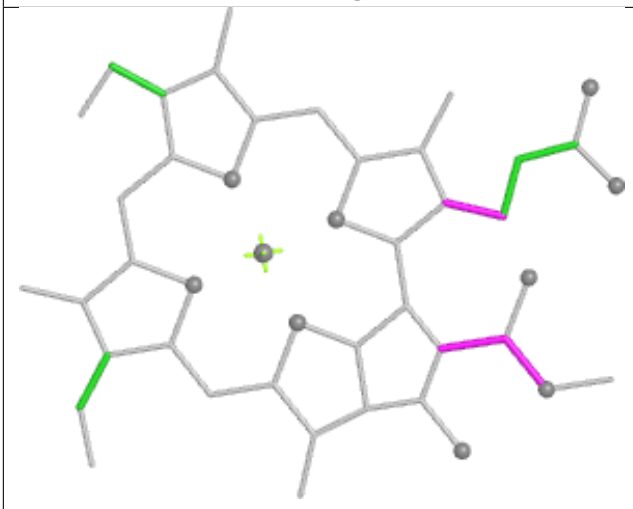
Ligand CLA b1 411



Bond lengths



Bond angles

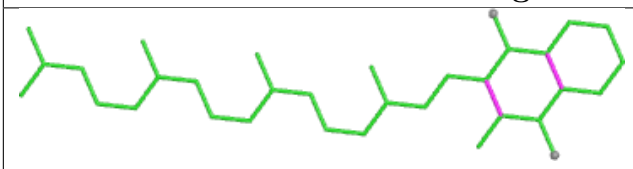


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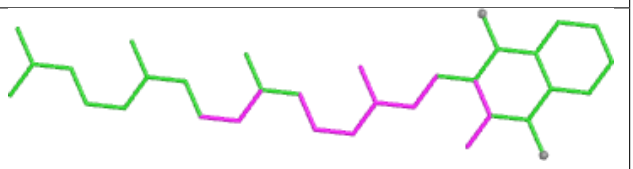


Rings

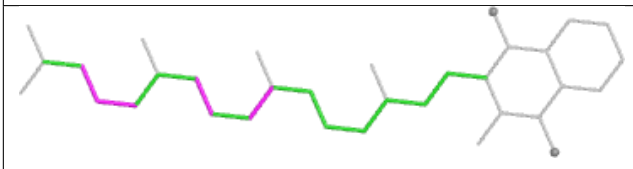
Ligand PQN aA 846



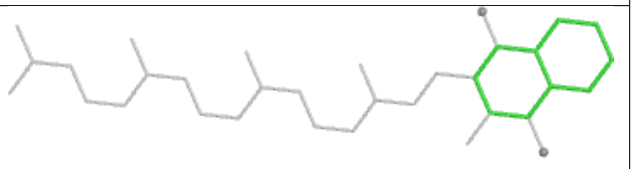
Bond lengths



Bond angles

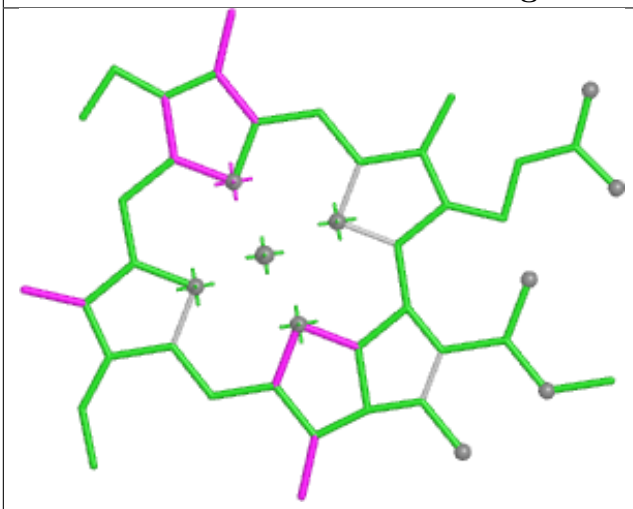


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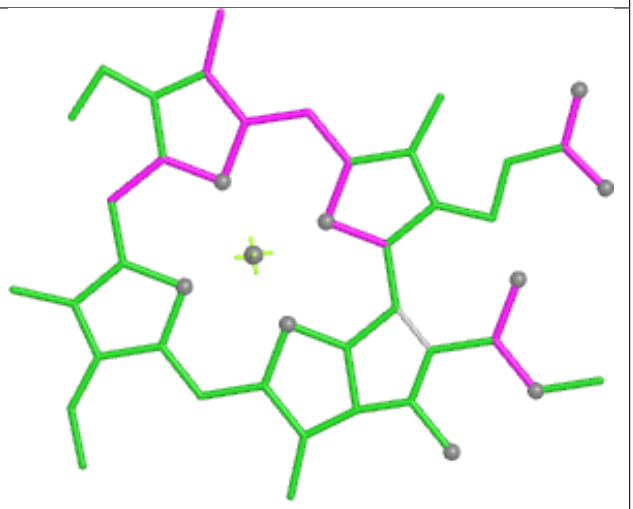


Rings

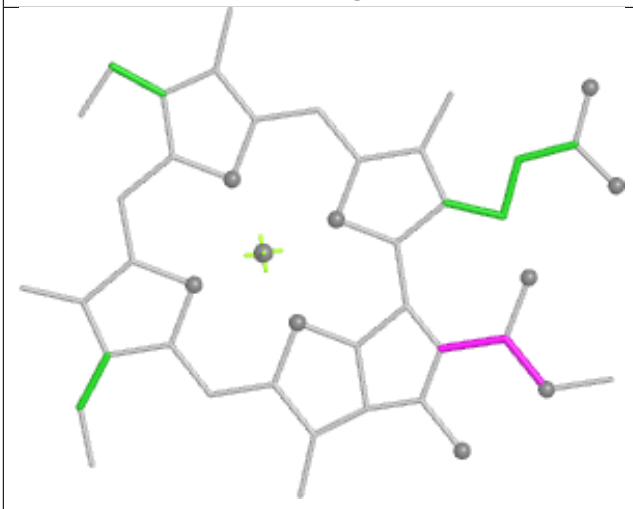
Ligand CLA c3 406



Bond lengths



Bond angles

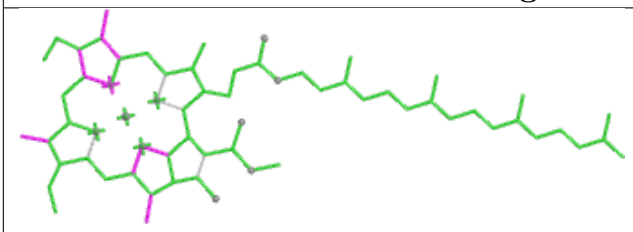


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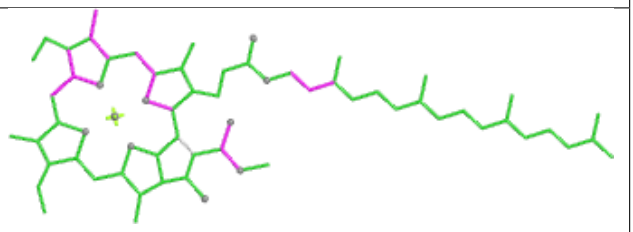


Rings

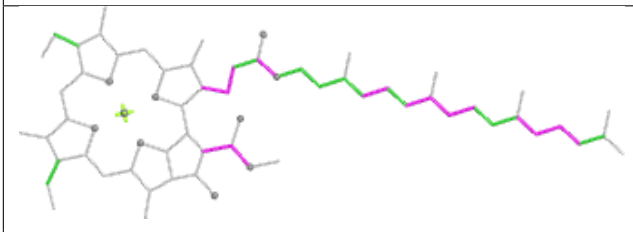
Ligand CLA a3 402



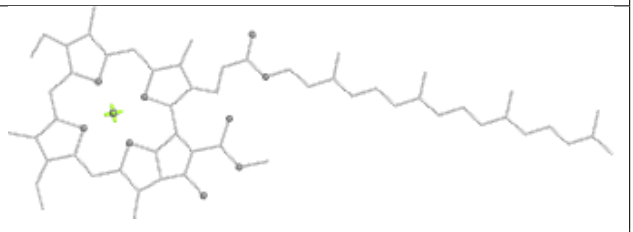
Bond lengths



Bond angles

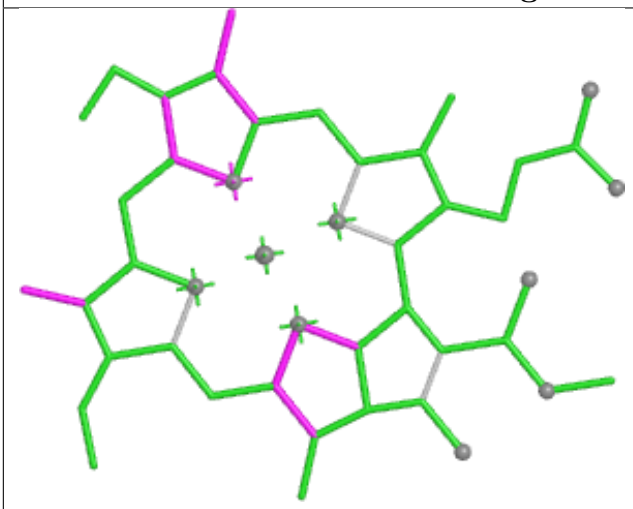


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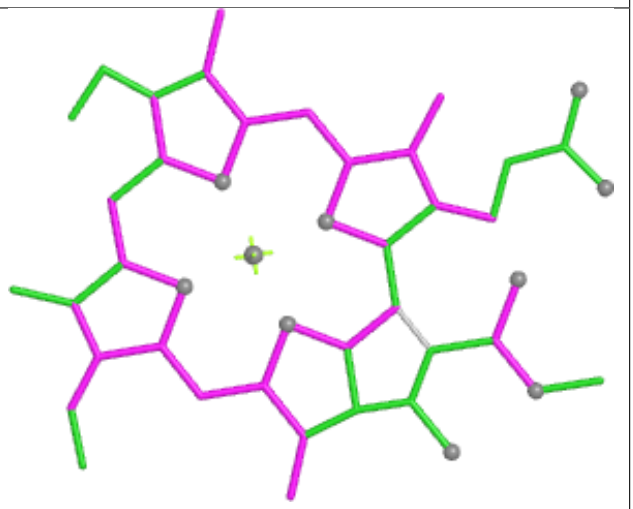


Rings

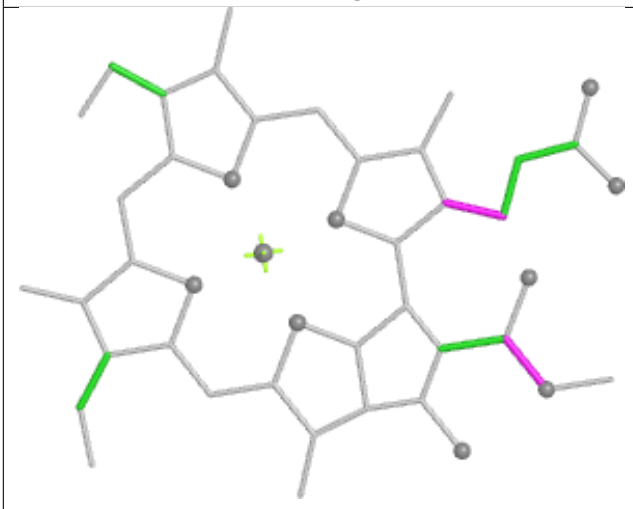
Ligand CLA c2 405



Bond lengths



Bond angles

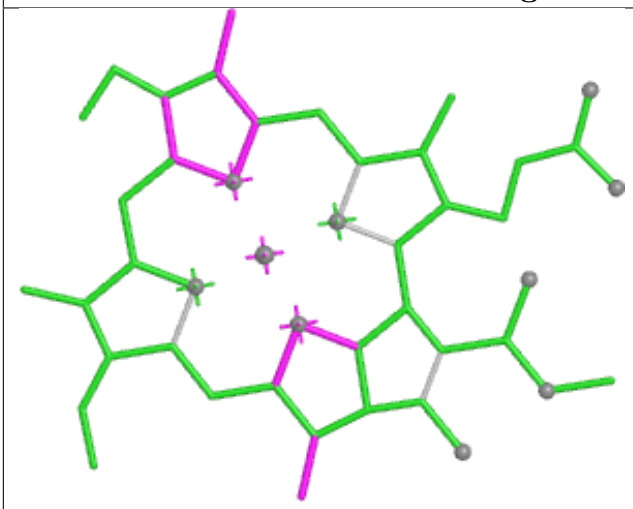


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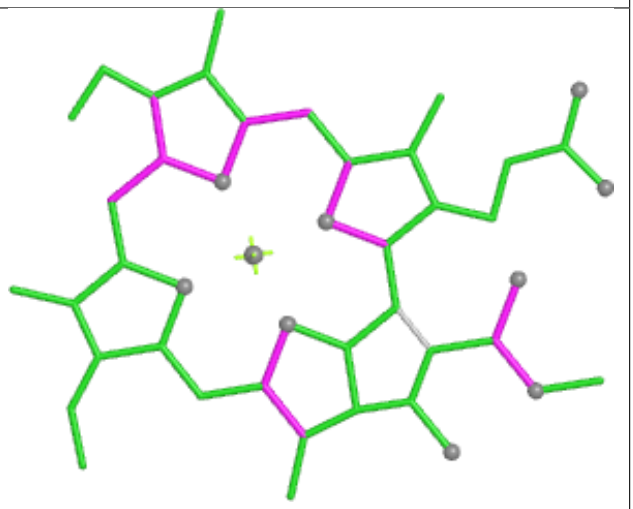


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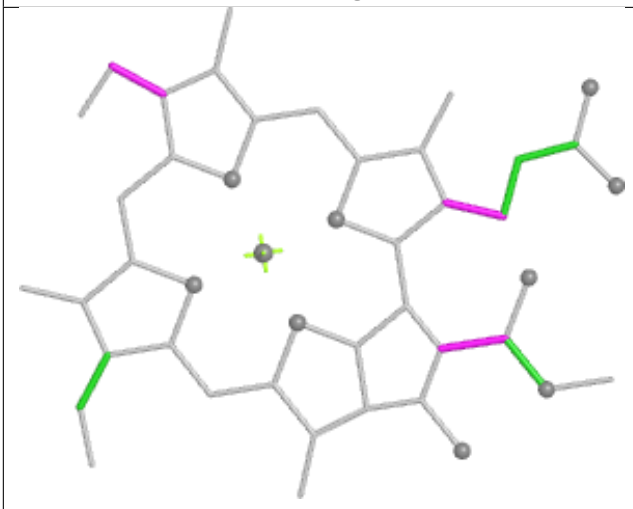
Ligand CLA c2 414



Bond lengths



Bond angles

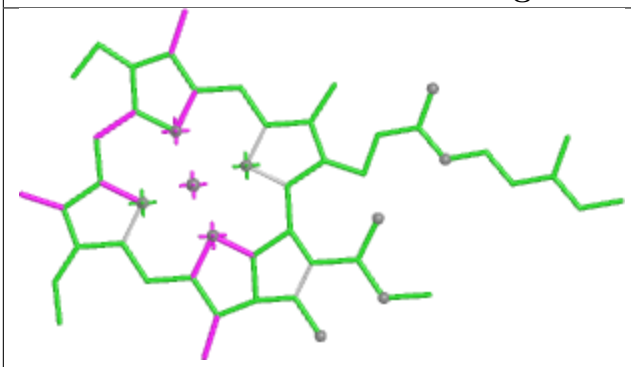


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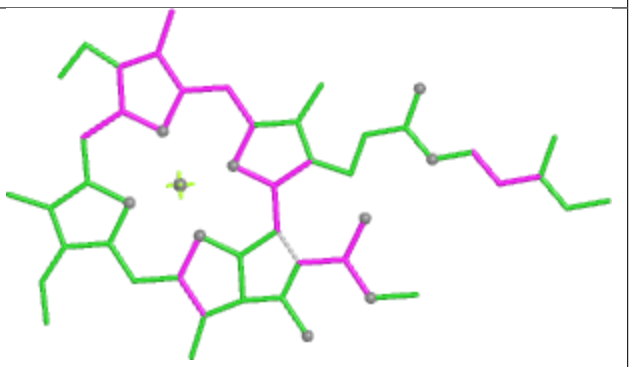


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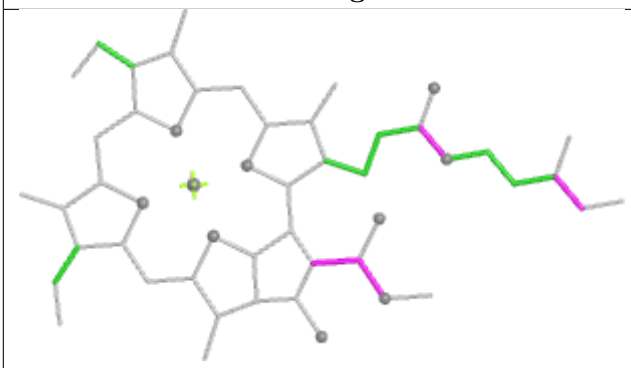
Ligand CLA bA 838



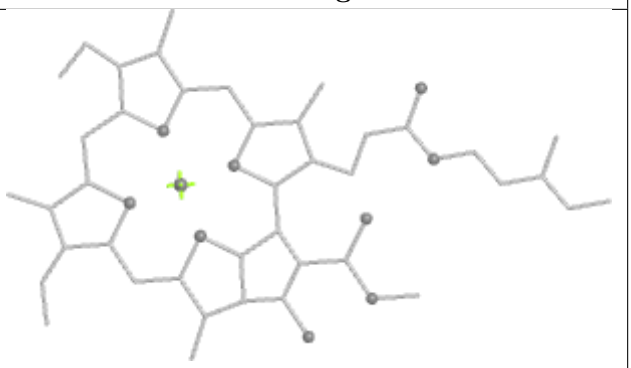
Bond lengths



Bond angles

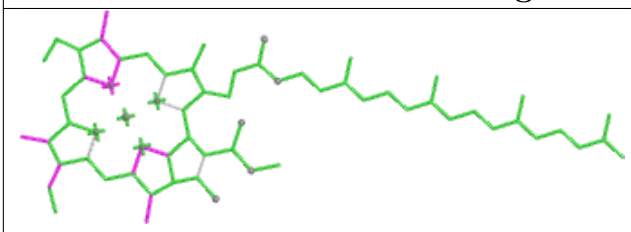


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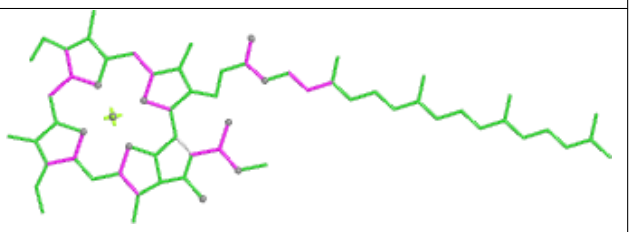


Rings

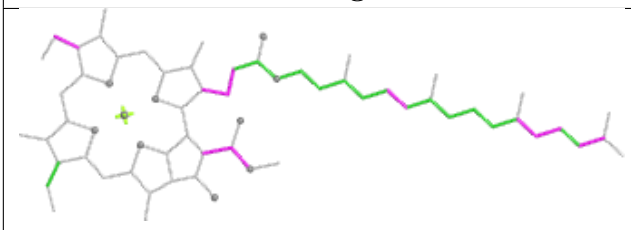
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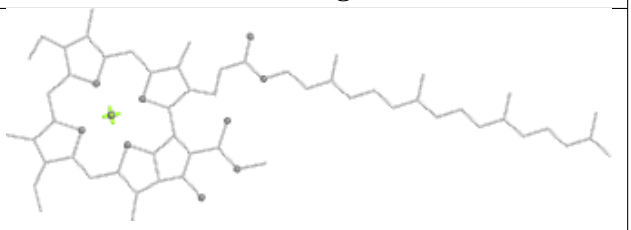
Bond lengths



Bond angles

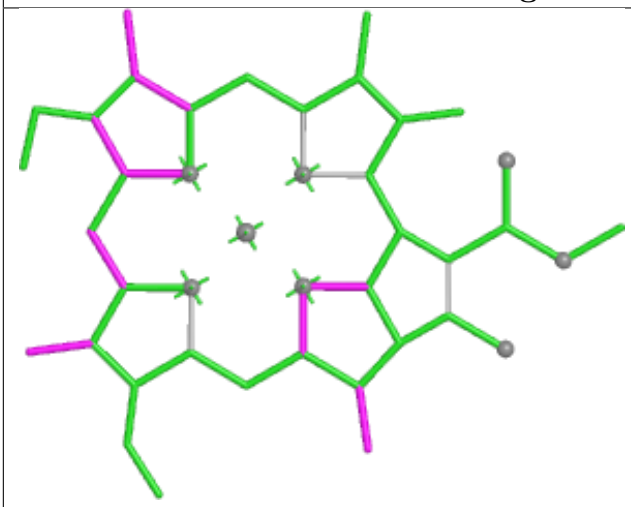


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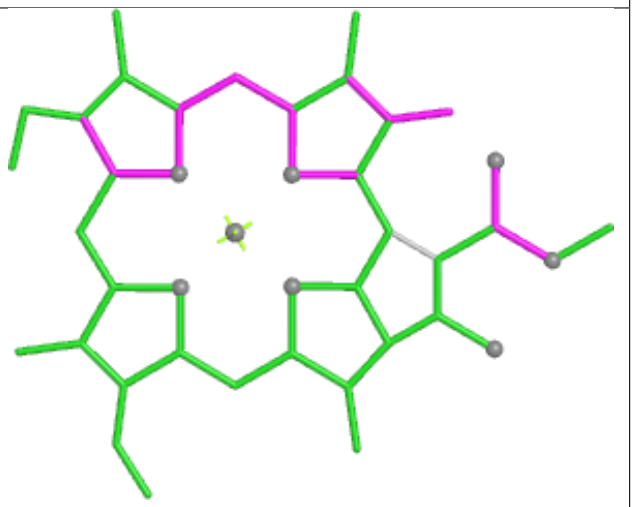


Rings

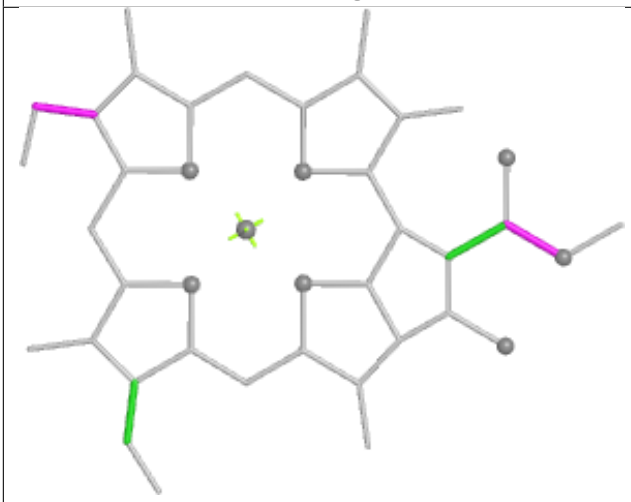
Ligand CLA a6 415



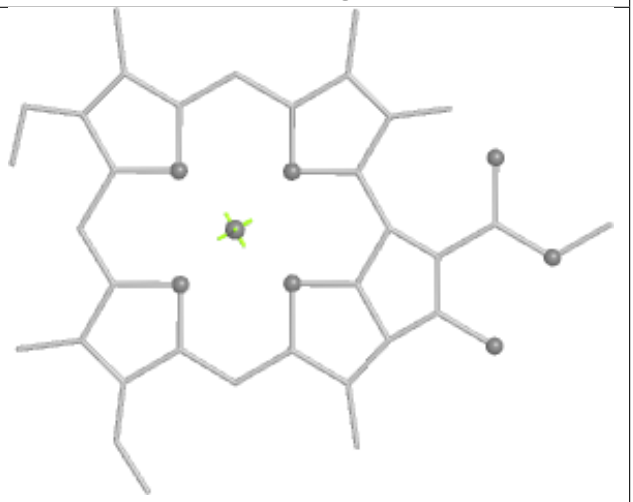
Bond lengths



Bond angles

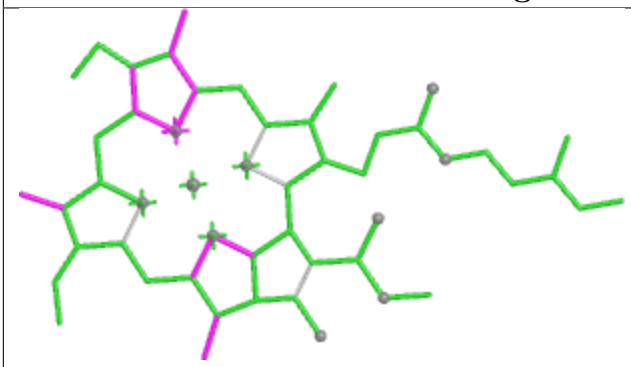


Torsions

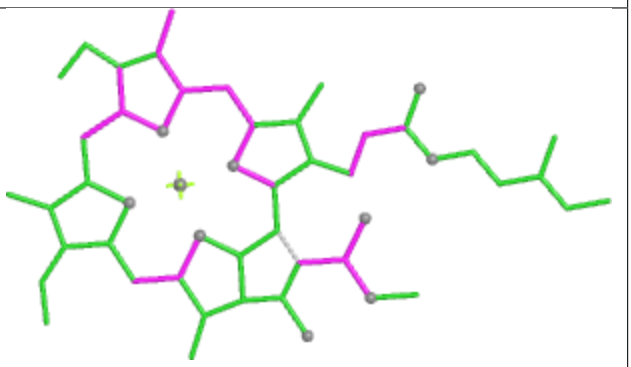


Rings

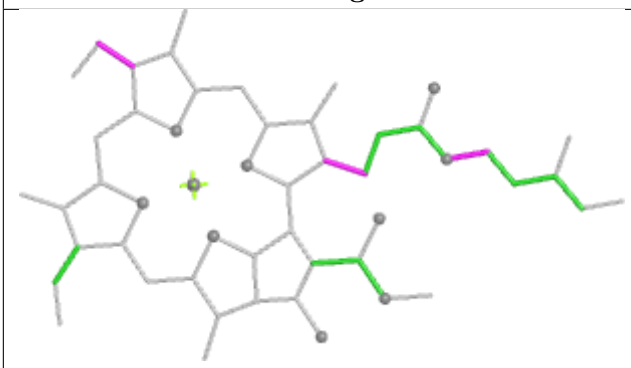
Ligand CLA bA 808



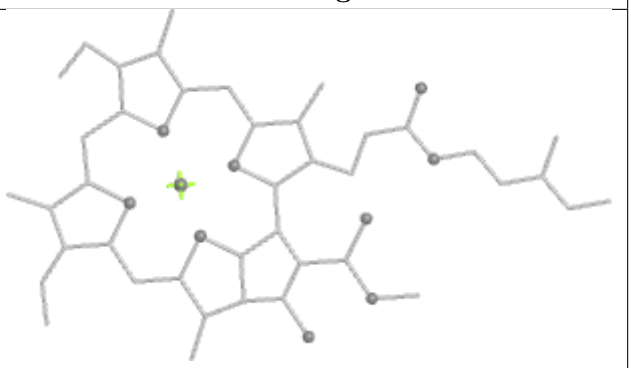
Bond lengths



Bond angles

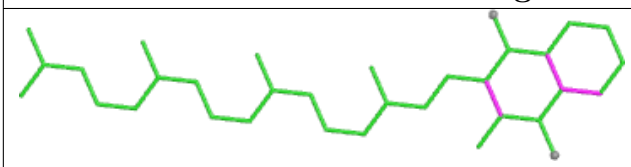


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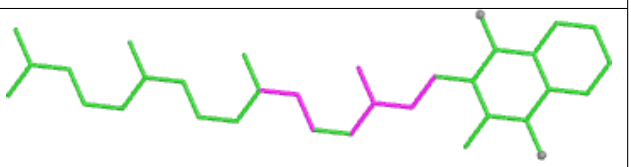


Rings

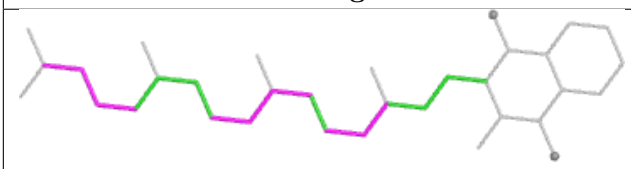
Ligand PQN cB 843



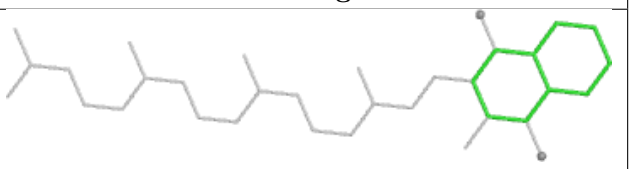
Bond lengths



Bond angles

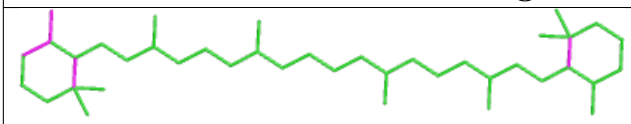


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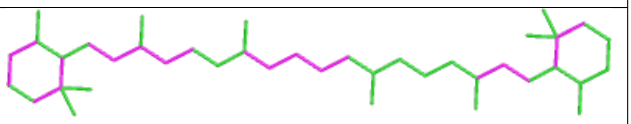


Rings

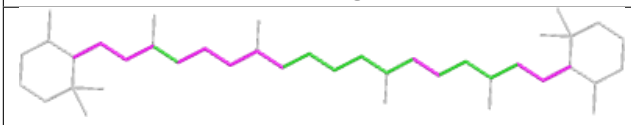
Ligand BCR b3 401



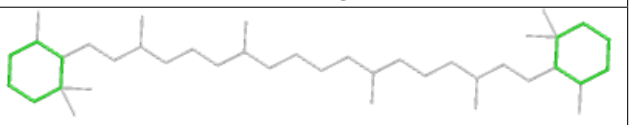
Bond lengths



Bond angles

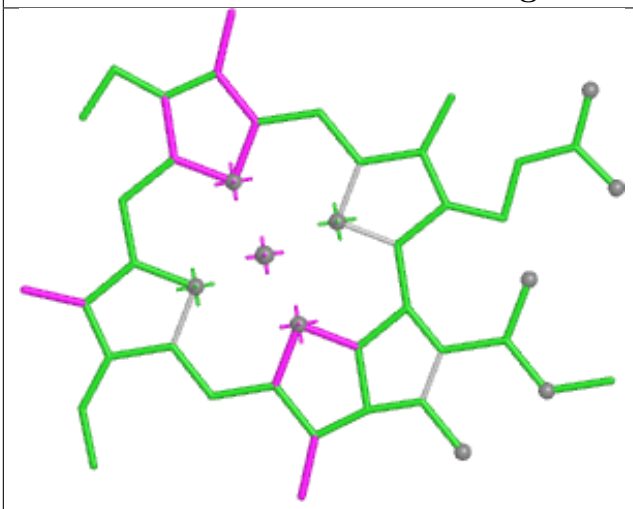


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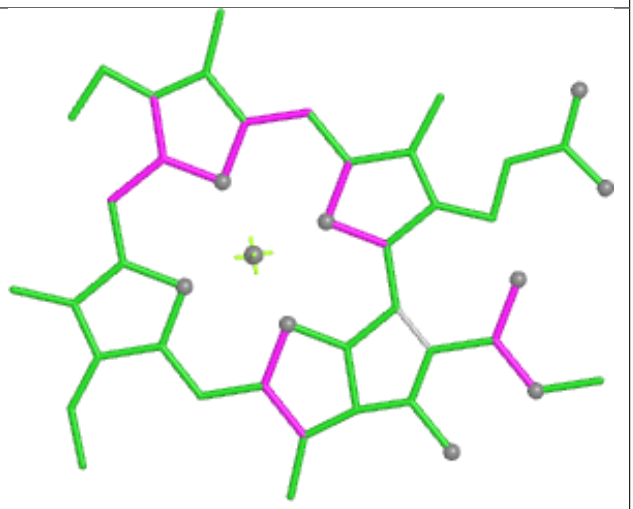


Rings

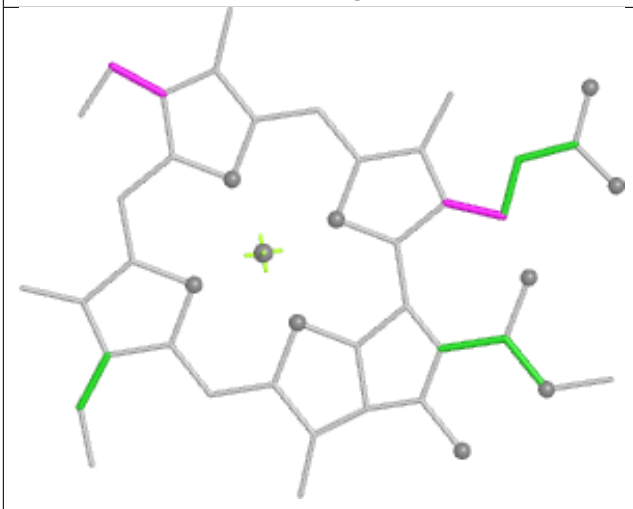
Ligand CLA a3 413



Bond lengths



Bond angles

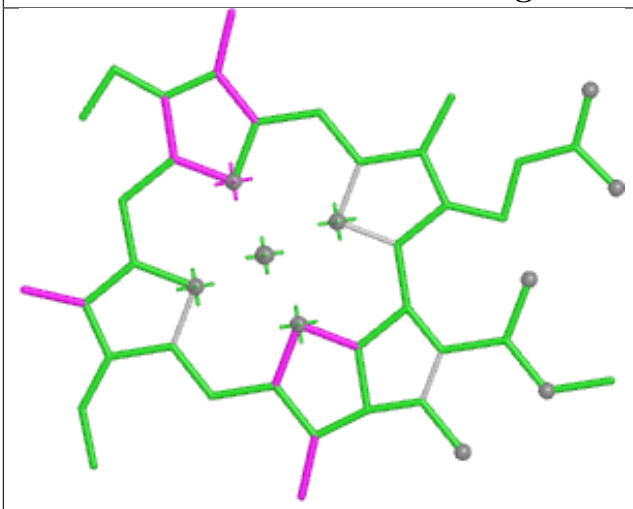


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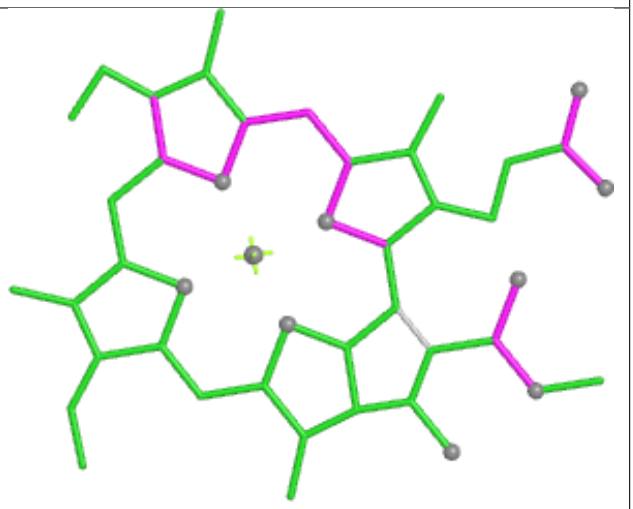


Rings

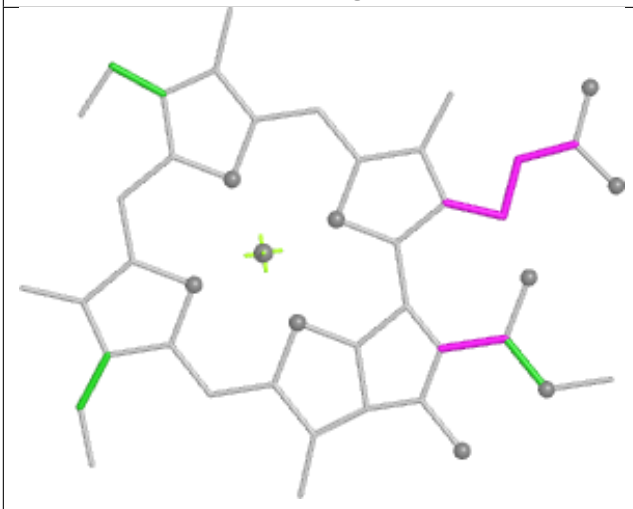
Ligand CLA aA 837



Bond lengths



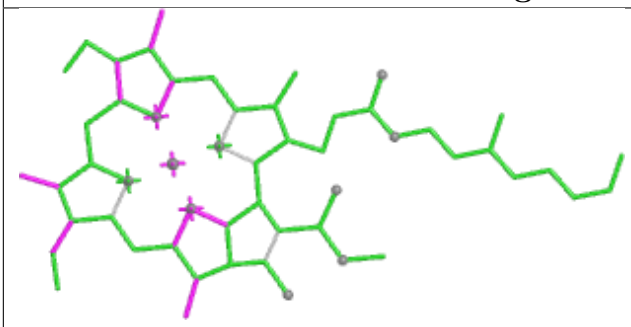
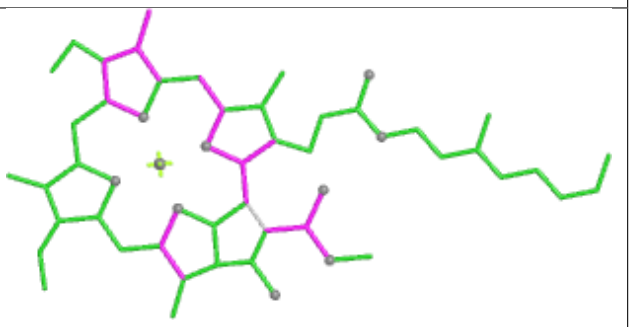
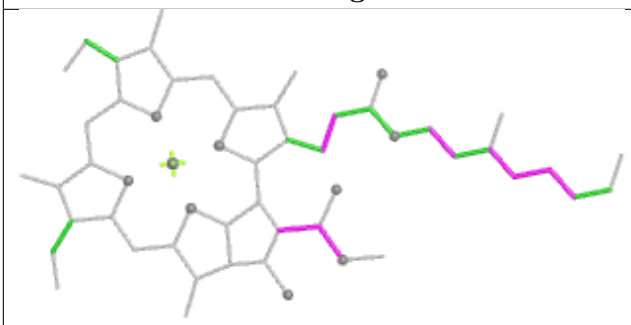
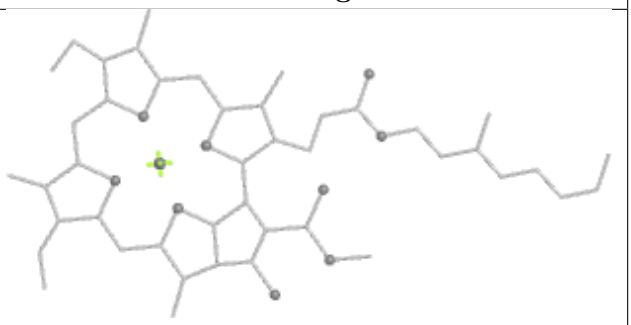
Bond angles

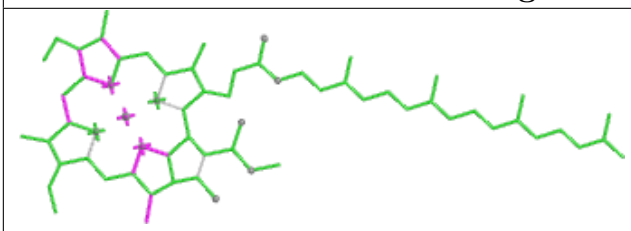
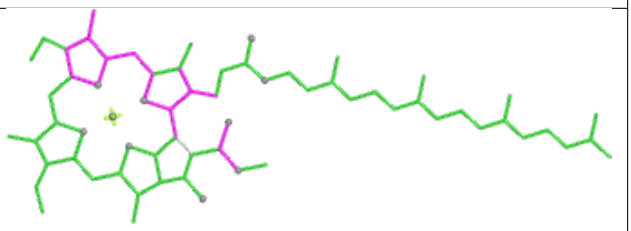
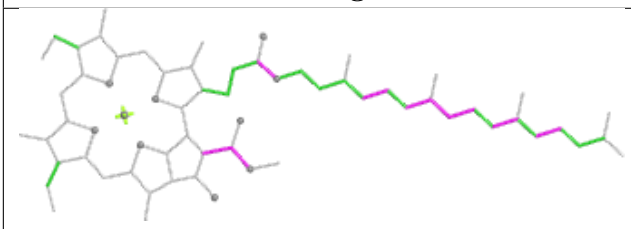
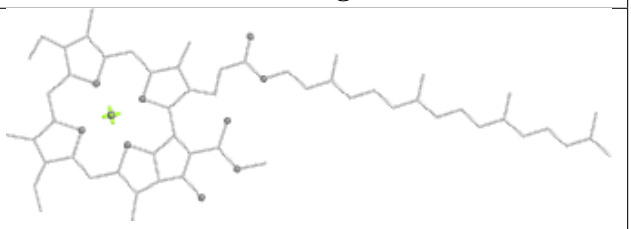


Torsions

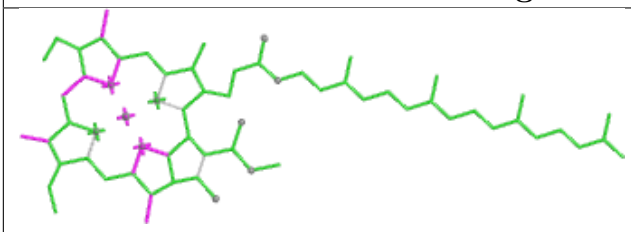


Rings

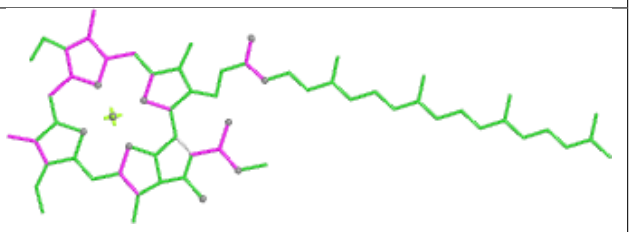
Ligand CLA bB 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b2 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

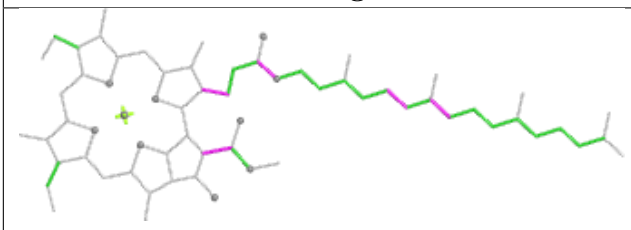
Ligand CLA cA 831



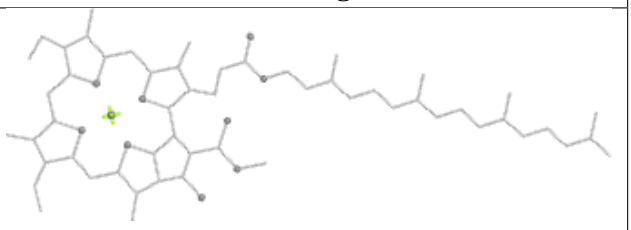
Bond lengths



Bond angles

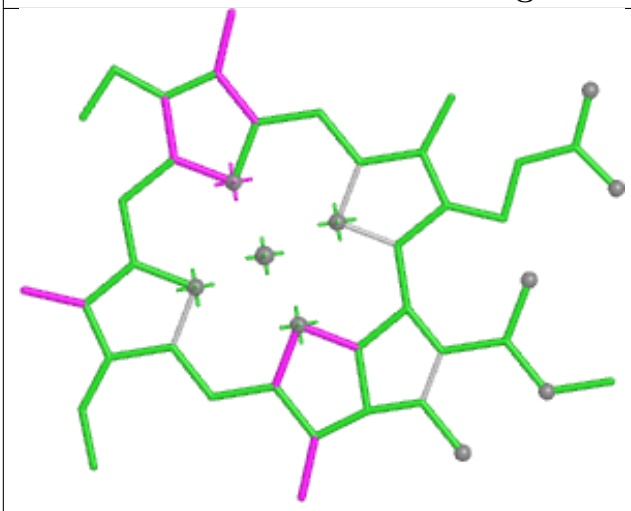


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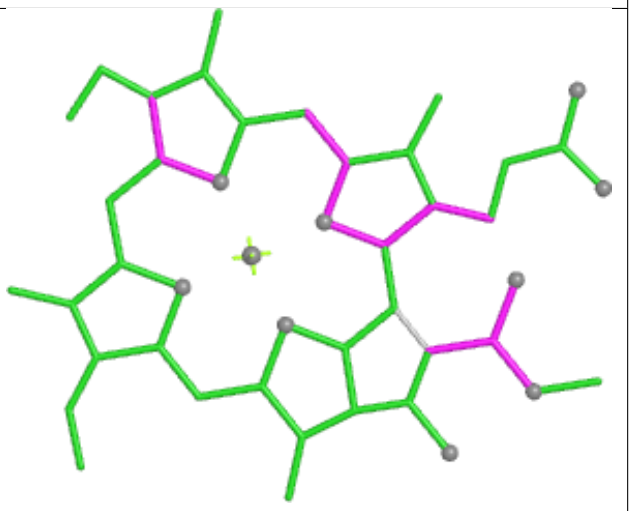


Rings

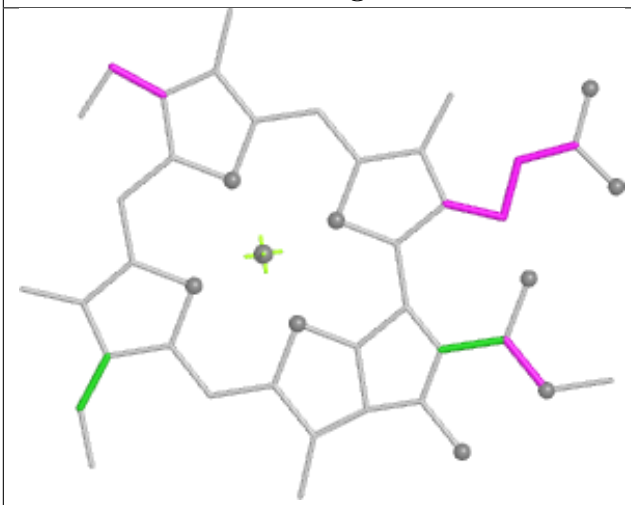
Ligand CLA cB 835



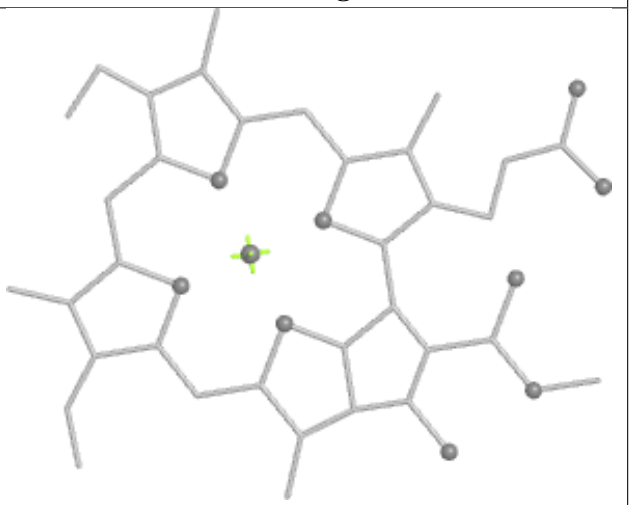
Bond lengths



Bond angles

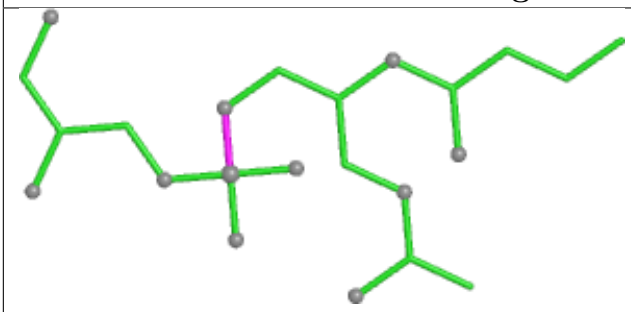


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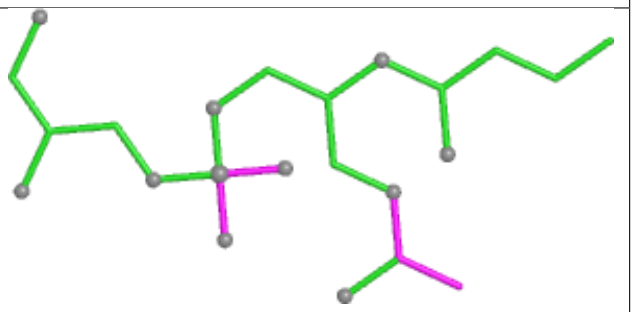


Rings

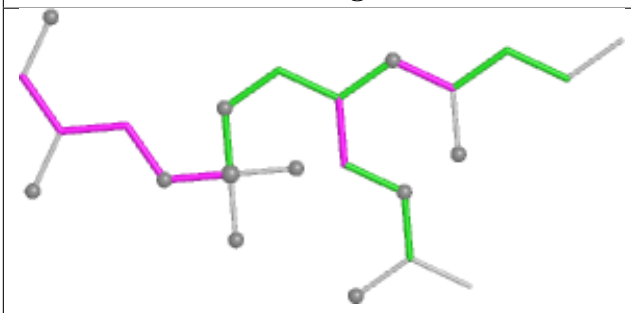
Ligand LHG bX 101



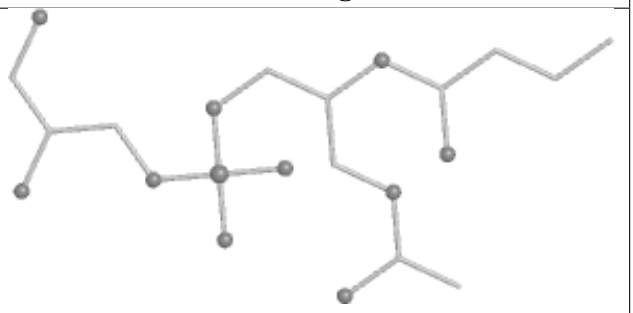
Bond lengths



Bond angles

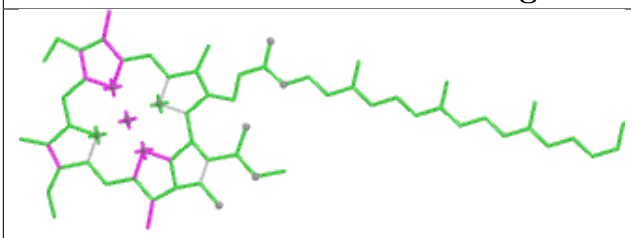


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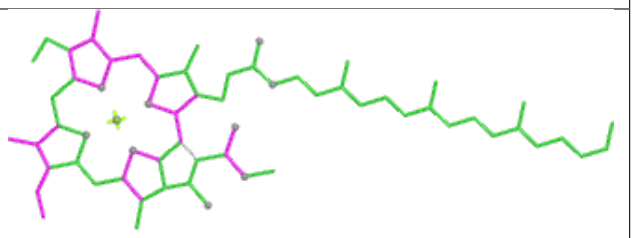


Rings

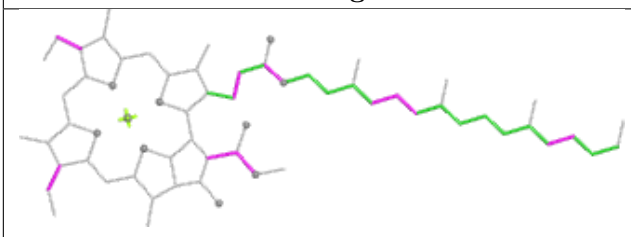
Ligand CLA a6 411



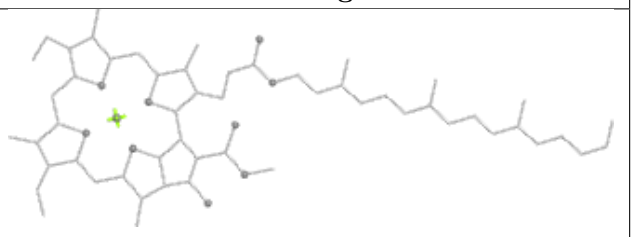
Bond lengths



Bond angles

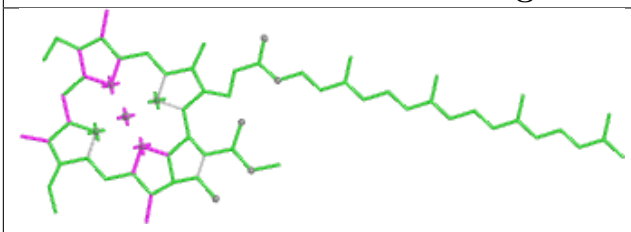


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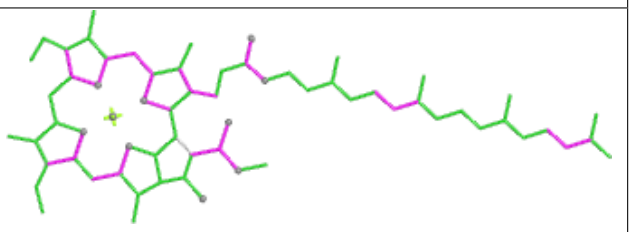


Rings

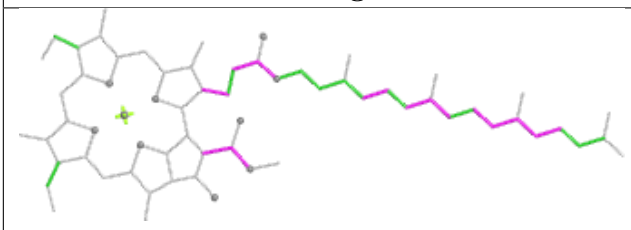
Ligand CLA cB 833



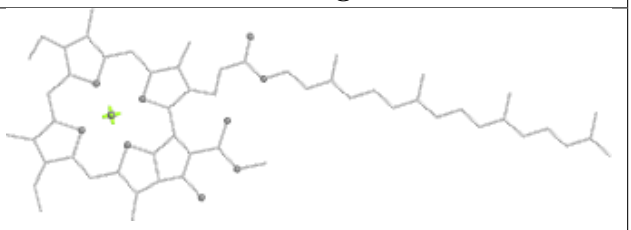
Bond lengths



Bond angles

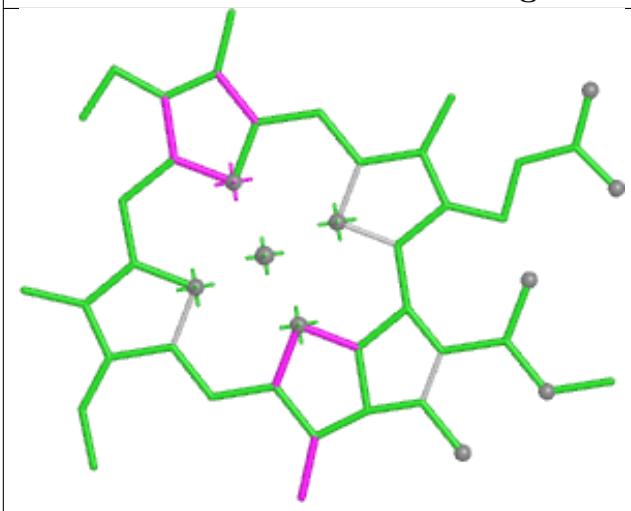


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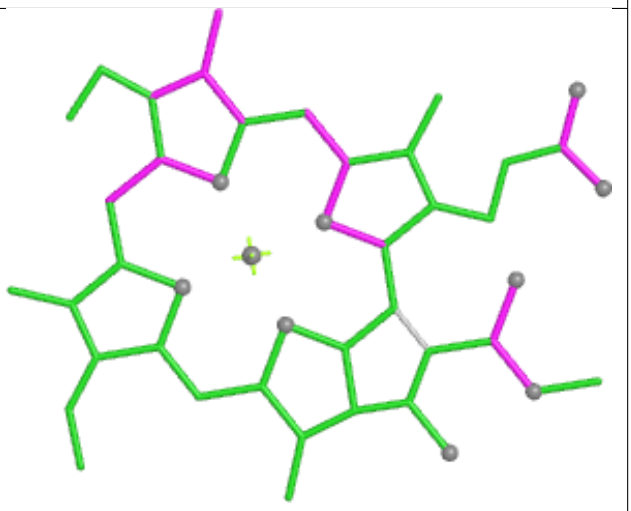


Rings

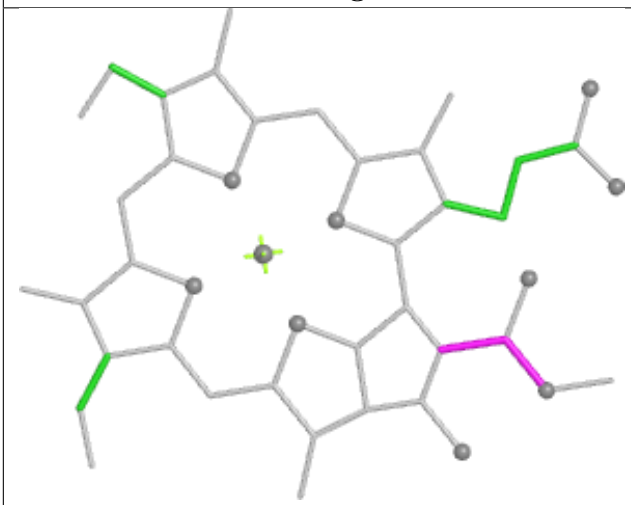
Ligand CLA a2 407



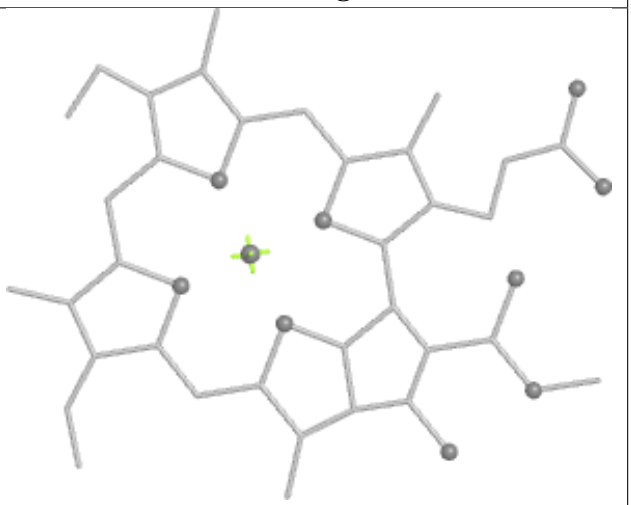
Bond lengths



Bond angles

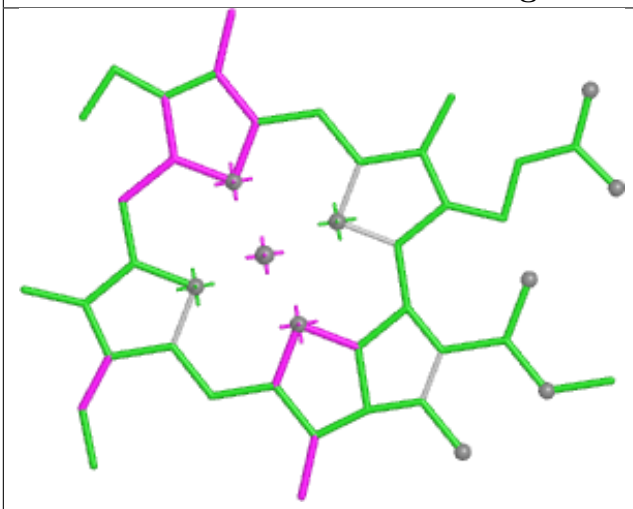


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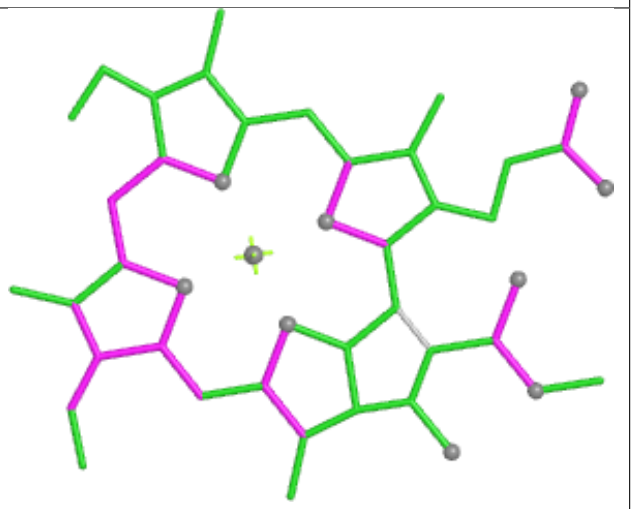


Rings

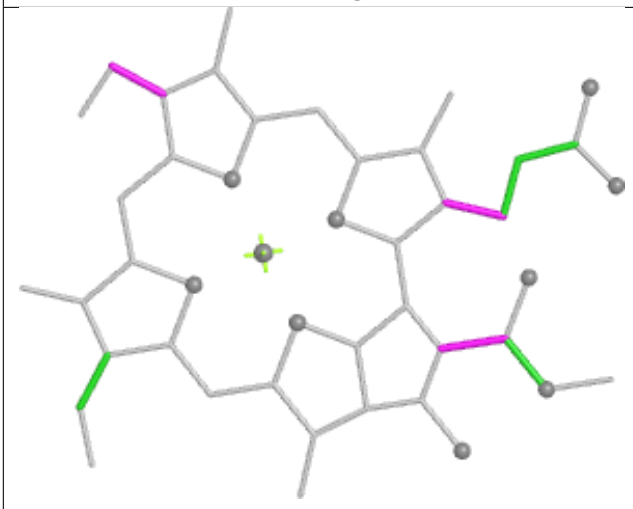
Ligand CLA a6 414



Bond lengths



Bond angles

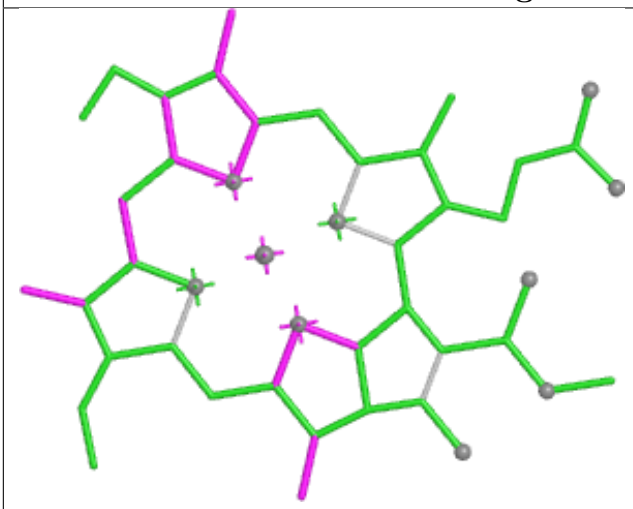


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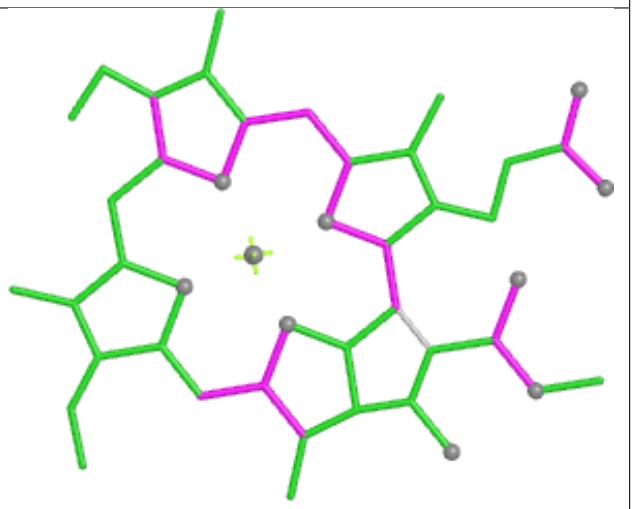


Rings

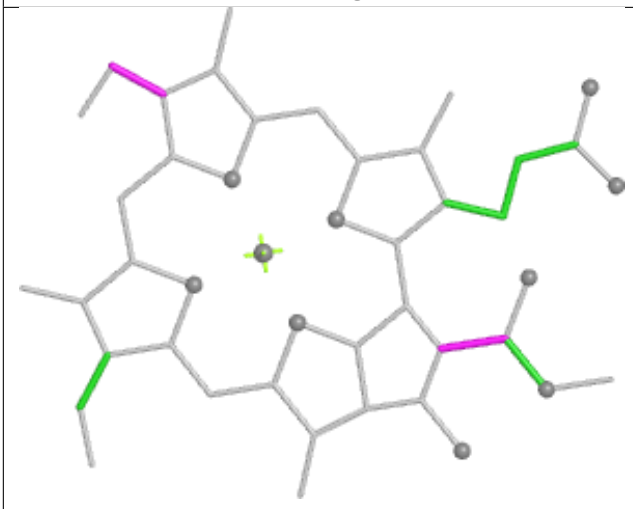
Ligand CLA cA 815



Bond lengths



Bond angles

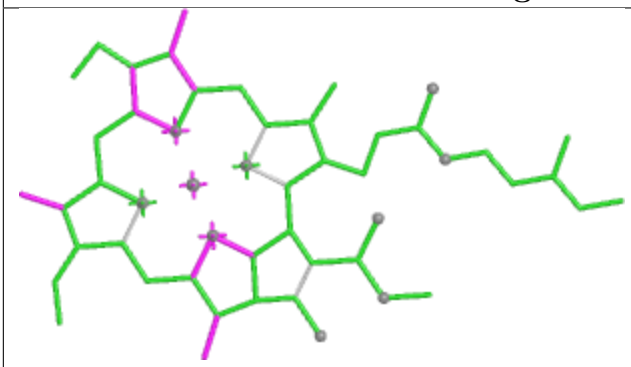


Torsions

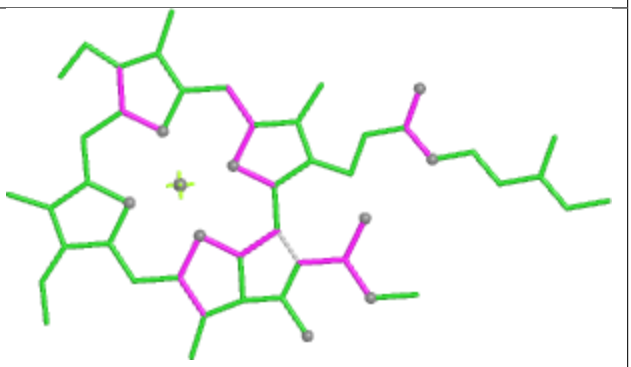


Rings

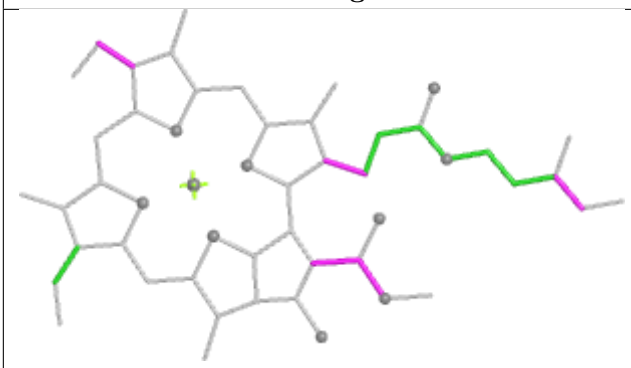
Ligand CLA bA 842



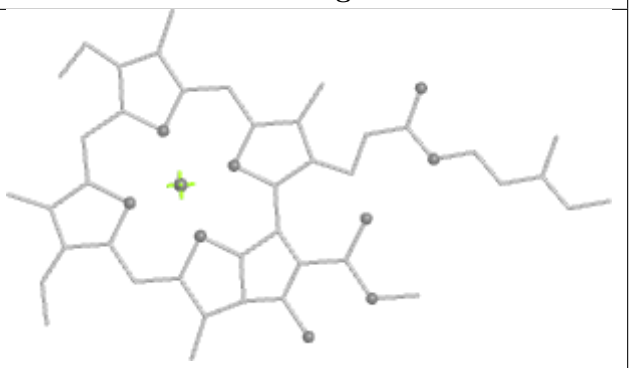
Bond lengths



Bond angles

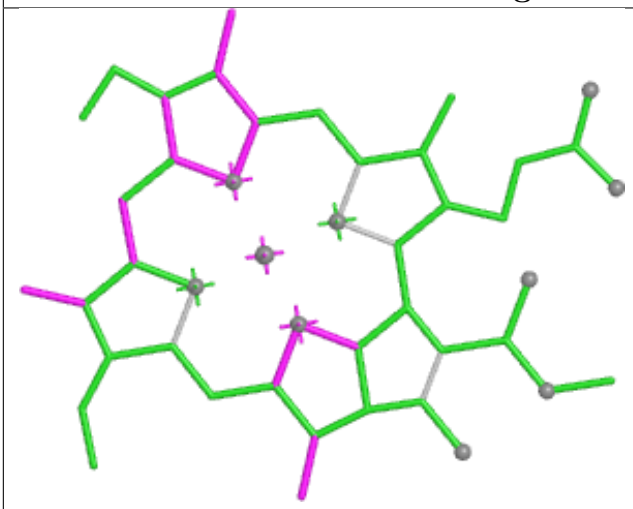


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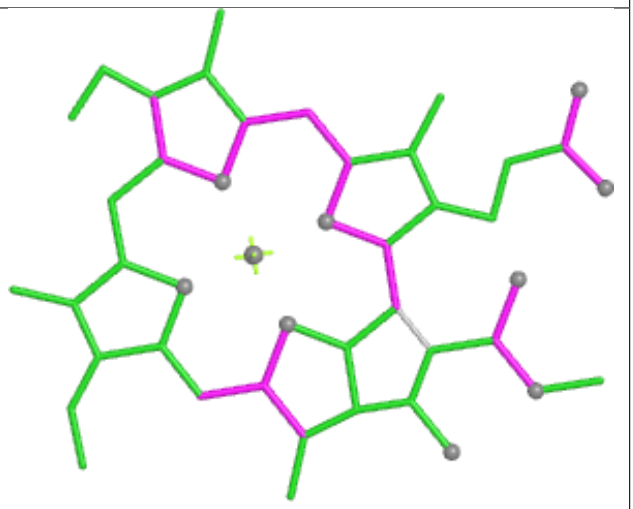


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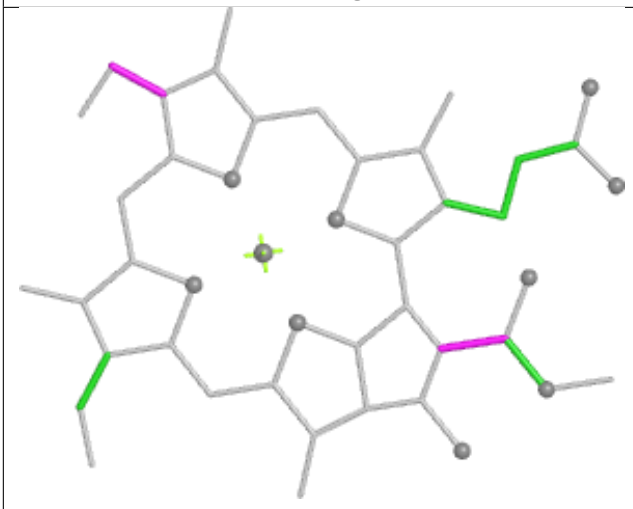
Ligand CLA bA 815



Bond lengths



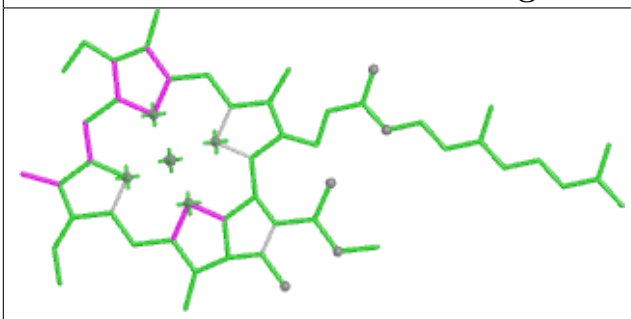
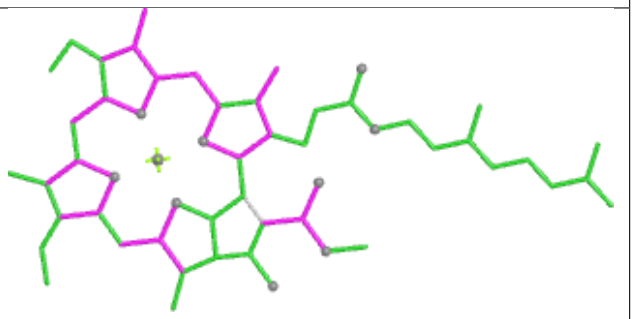
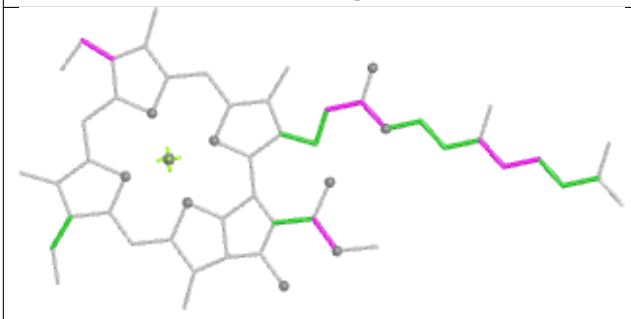
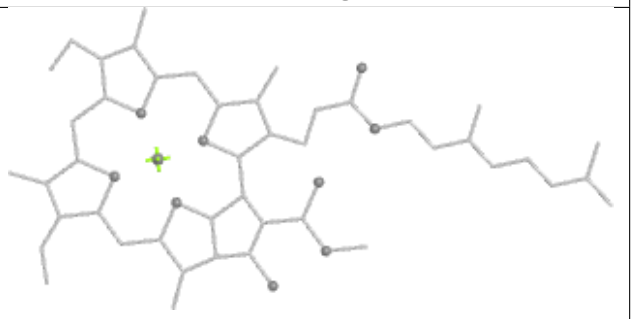
Bond angles



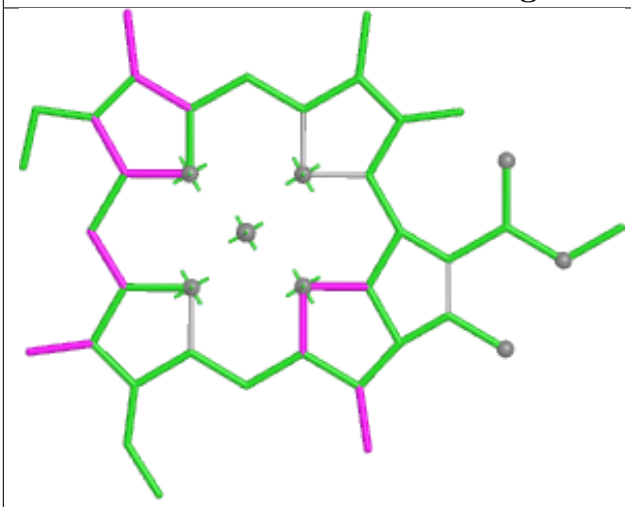
Torsions



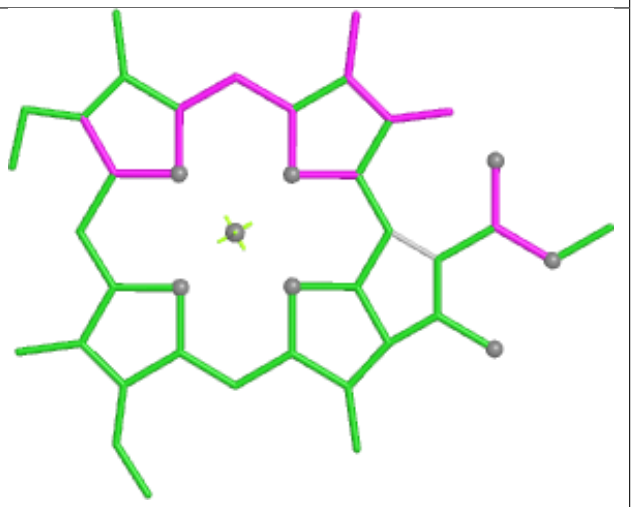
Rings

Ligand CLA b5 417	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

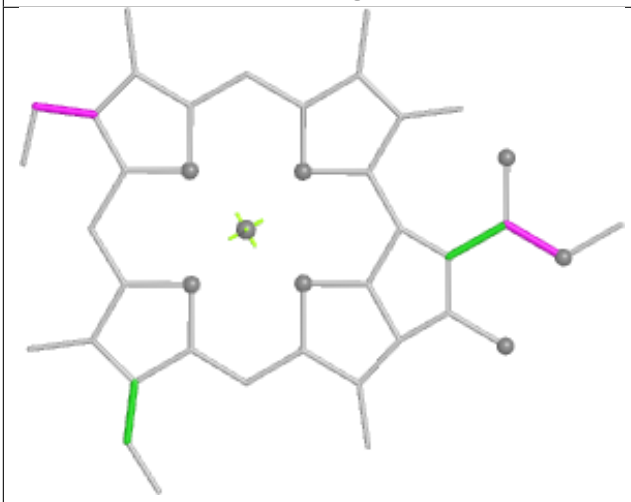
Ligand CLA a1 413



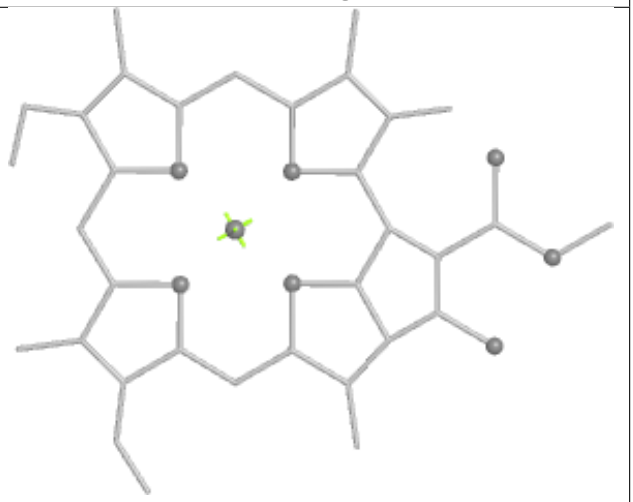
Bond lengths



Bond angles

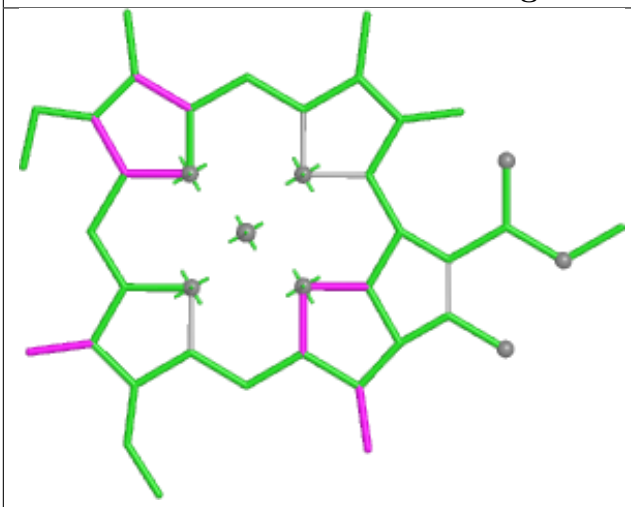


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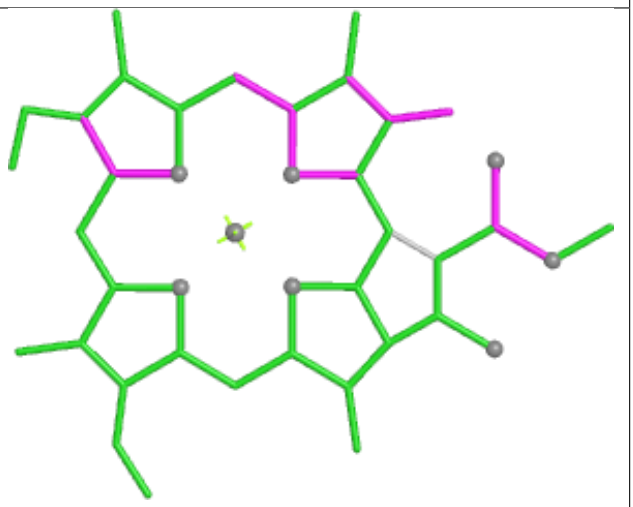


Rings

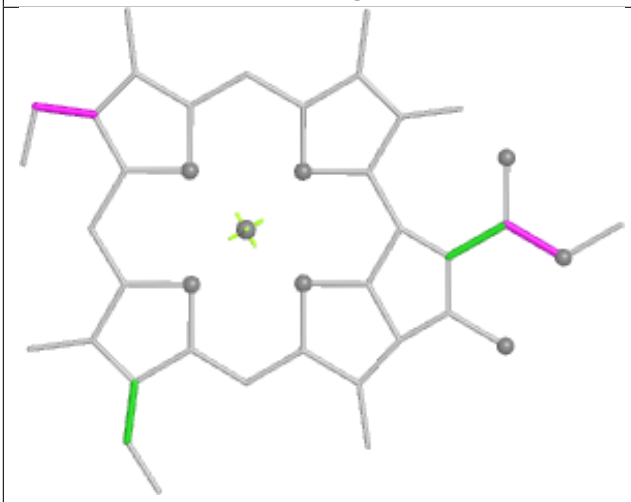
Ligand CLA c2 415



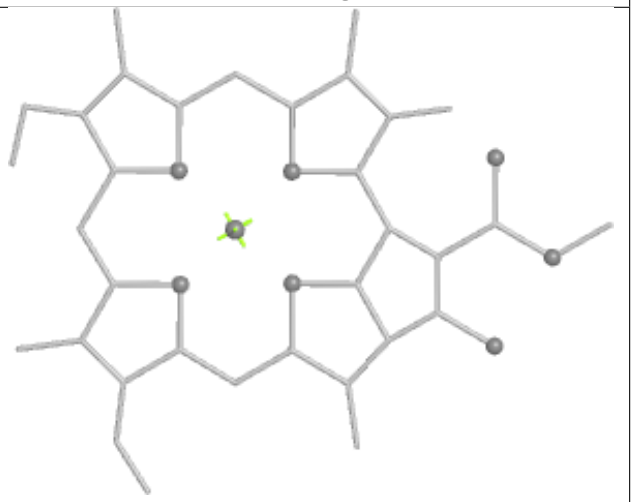
Bond lengths



Bond angles

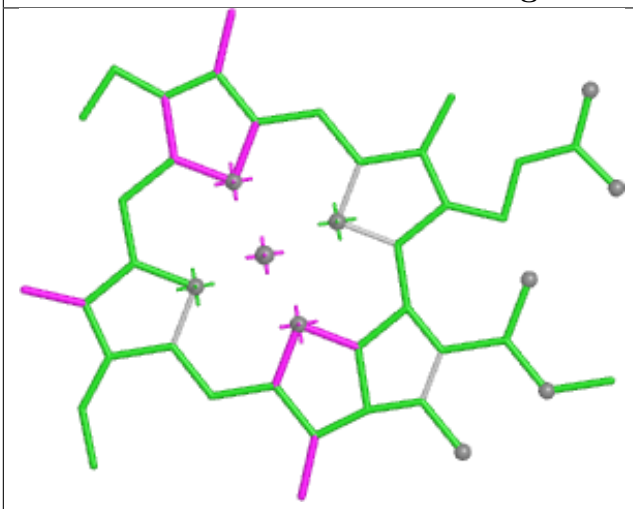


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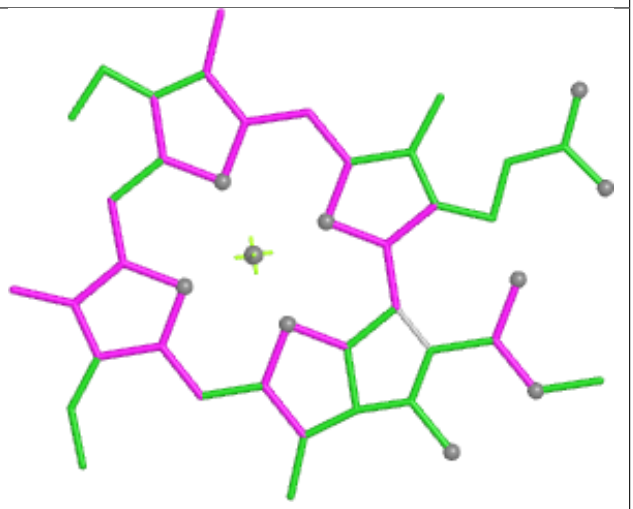


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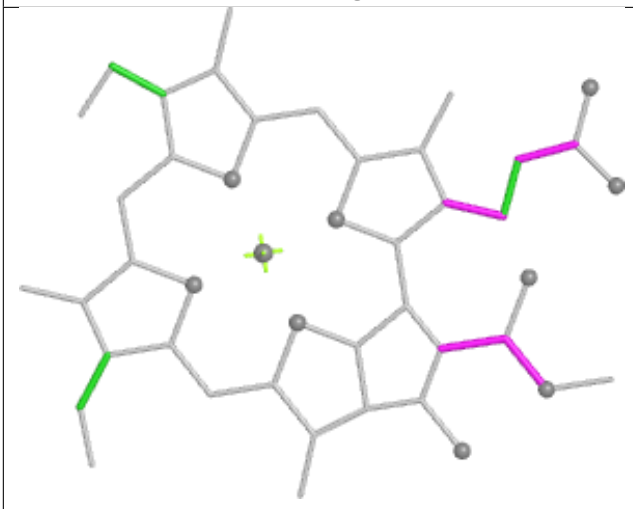
Ligand CLA c2 413



Bond lengths



Bond angles

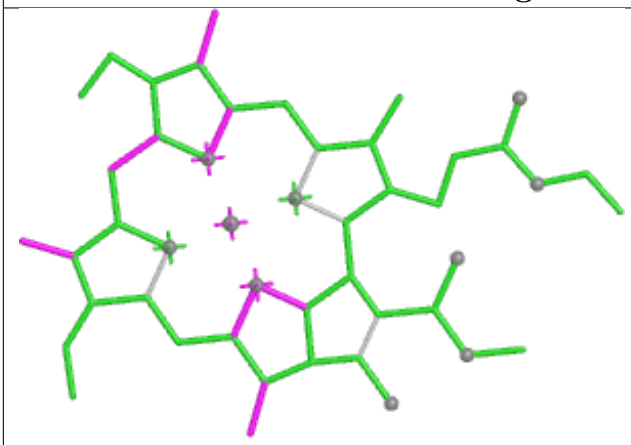


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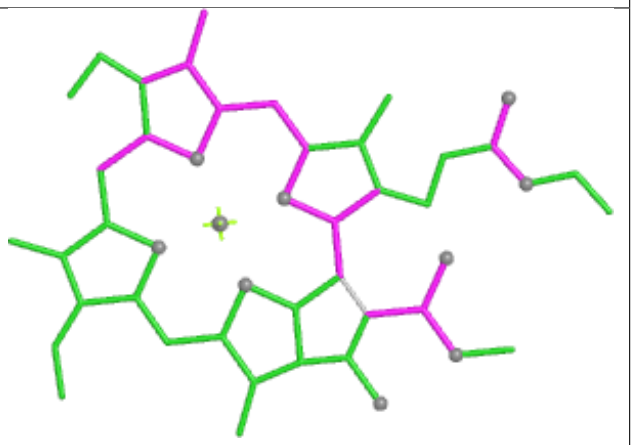


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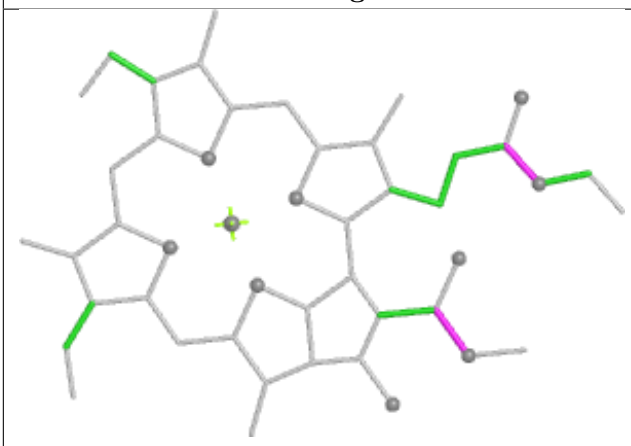
Ligand CLA aA 840



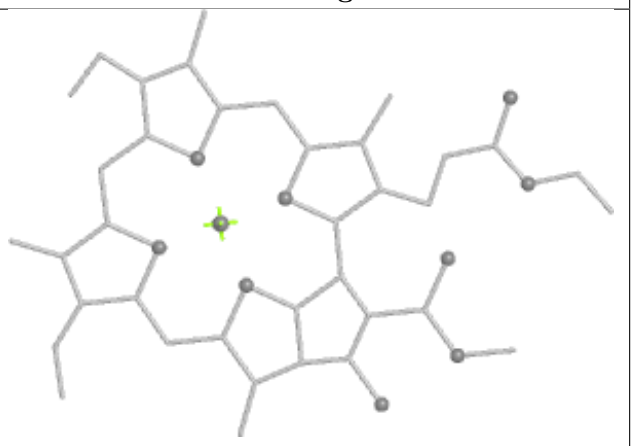
Bond lengths



Bond angles

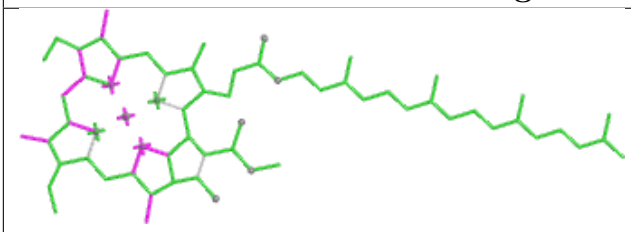


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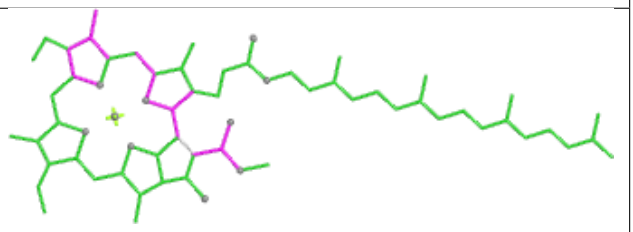


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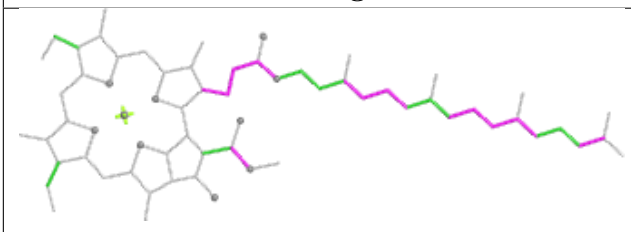
Ligand CLA bB 828



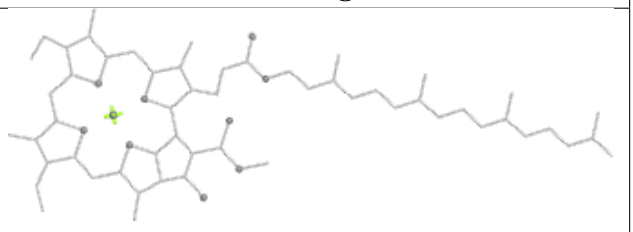
Bond lengths



Bond angles

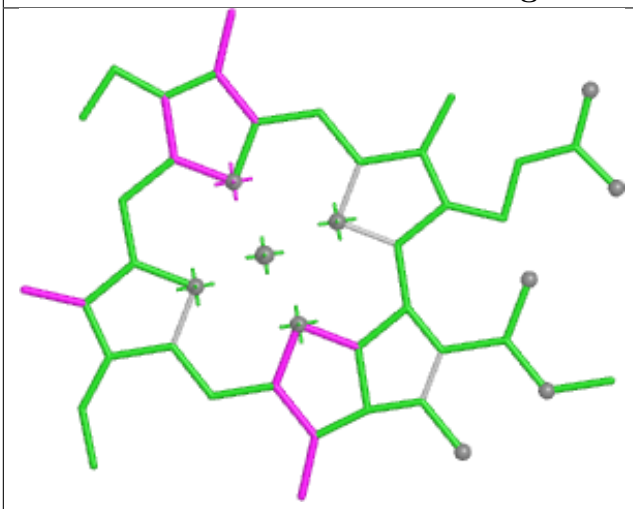


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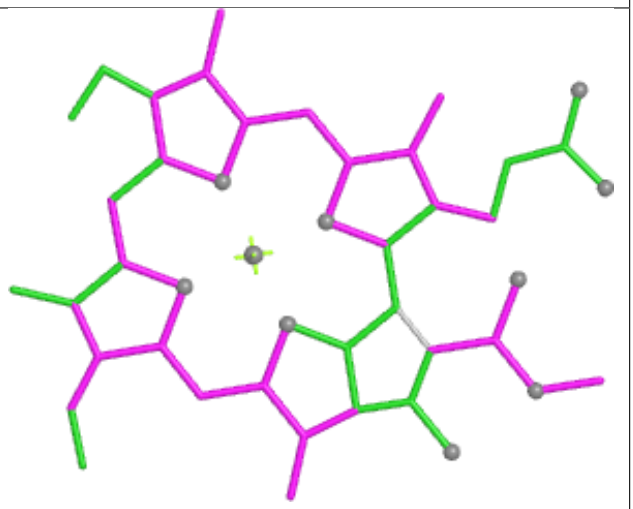


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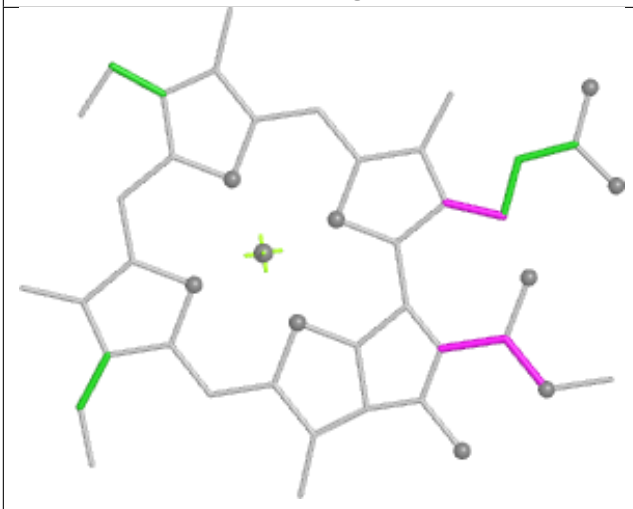
Ligand CLA c5 405



Bond lengths



Bond angles

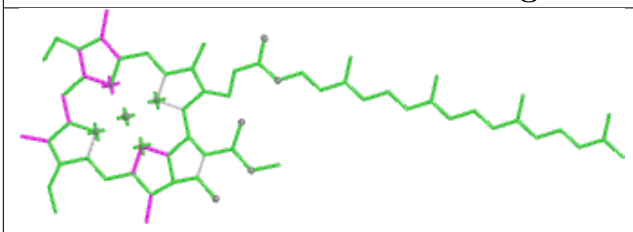


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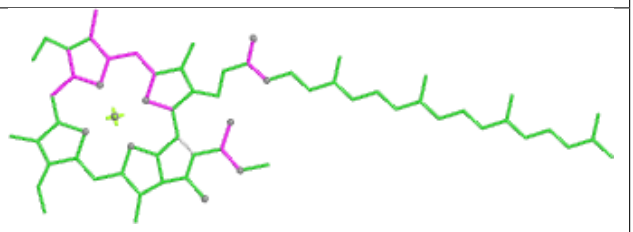


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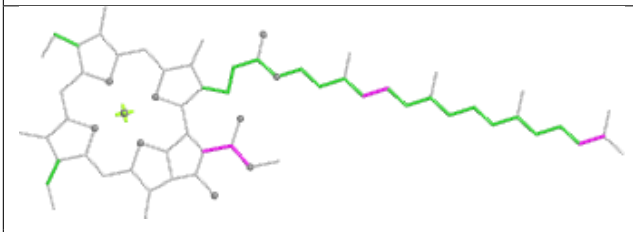
Ligand CLA c5 409



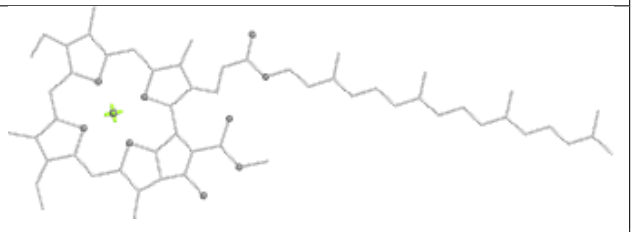
Bond lengths



Bond angles

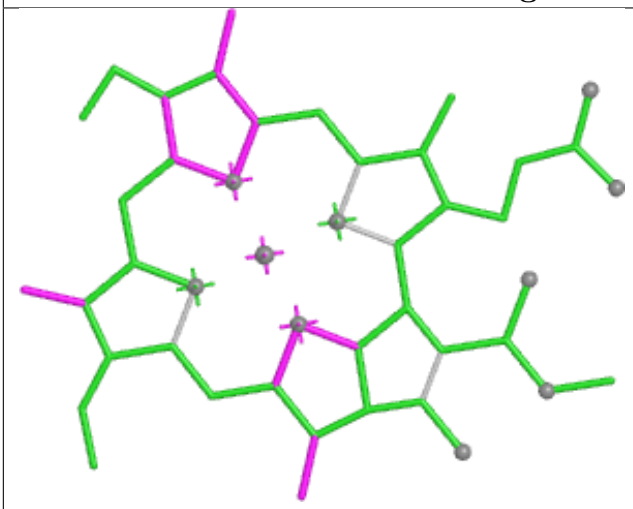


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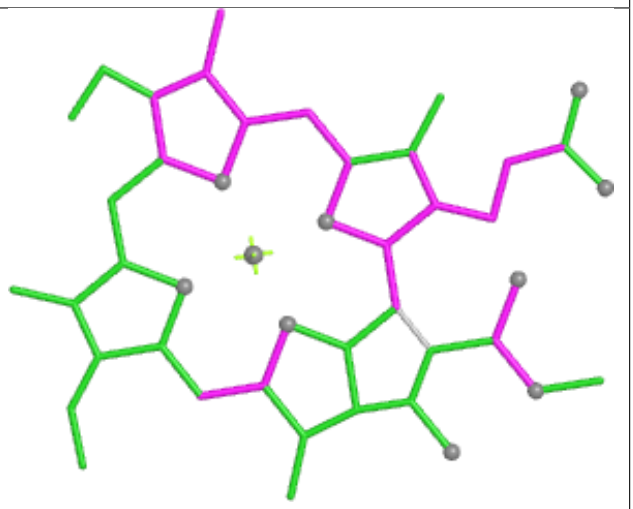


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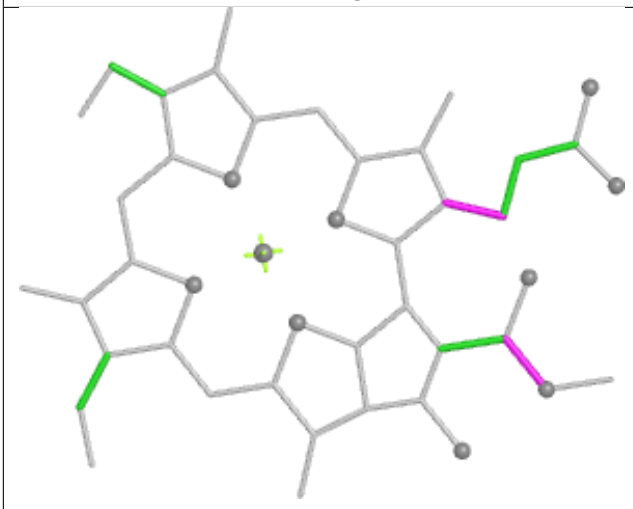
Ligand CLA a6 412



Bond lengths



Bond angles

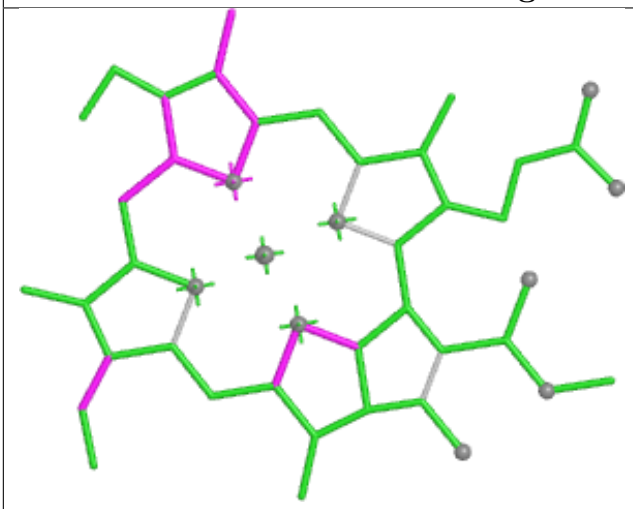


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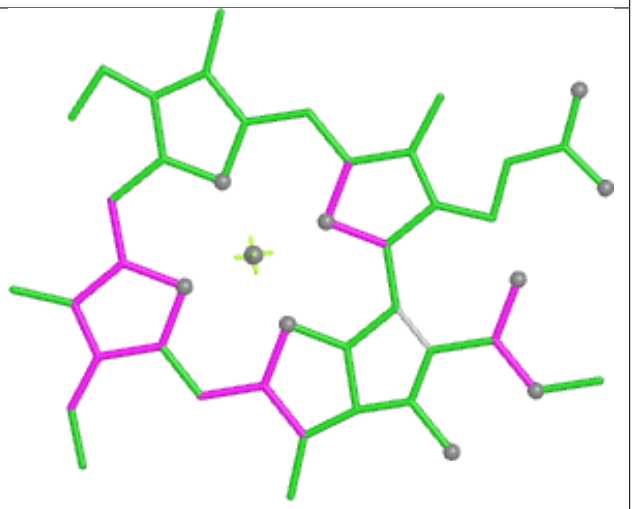


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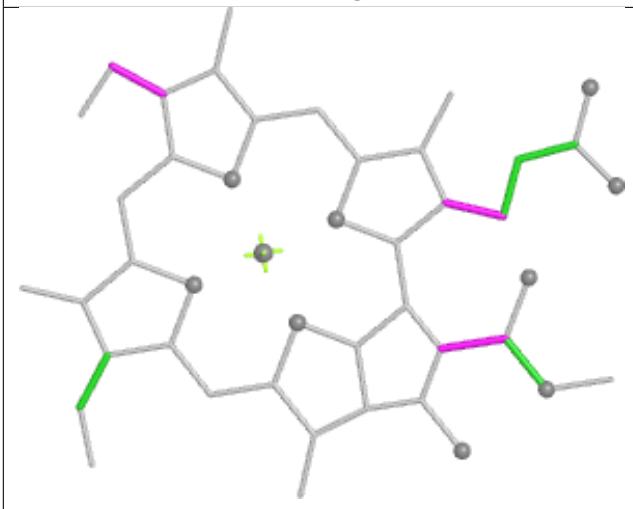
Ligand CLA b6 414



Bond lengths



Bond angles

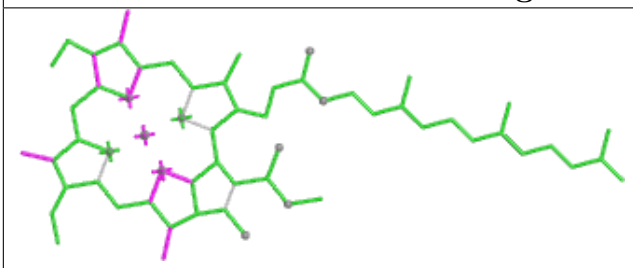


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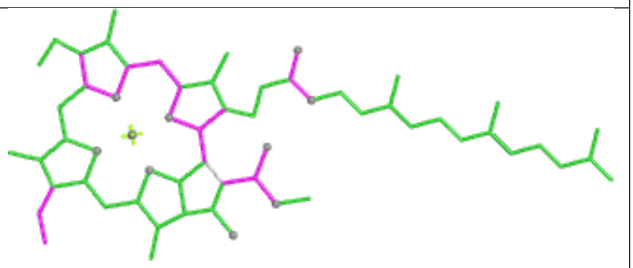


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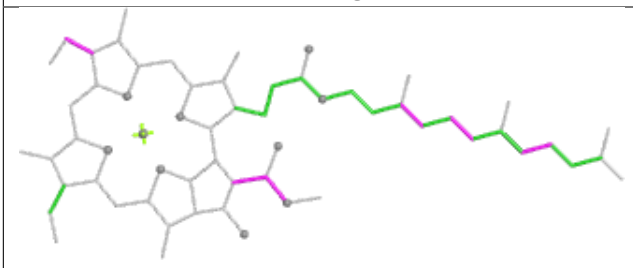
Ligand CLA aB 836



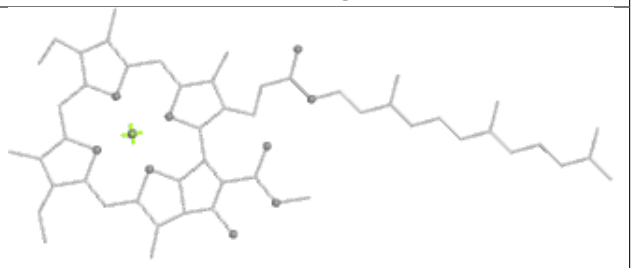
Bond lengths



Bond angles

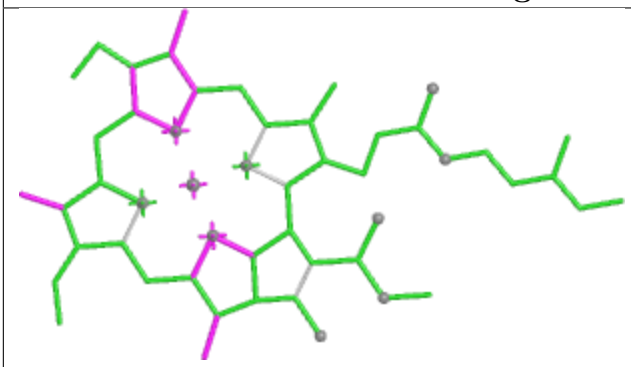


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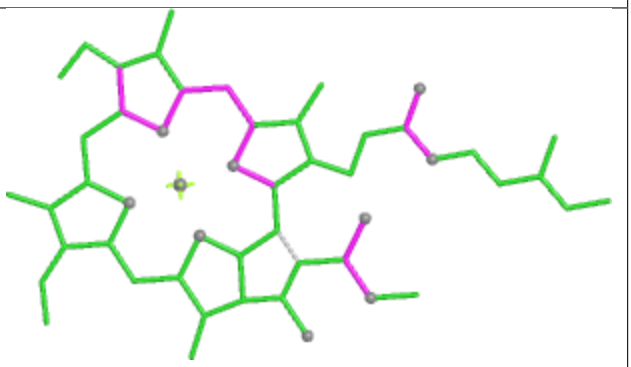


Rings

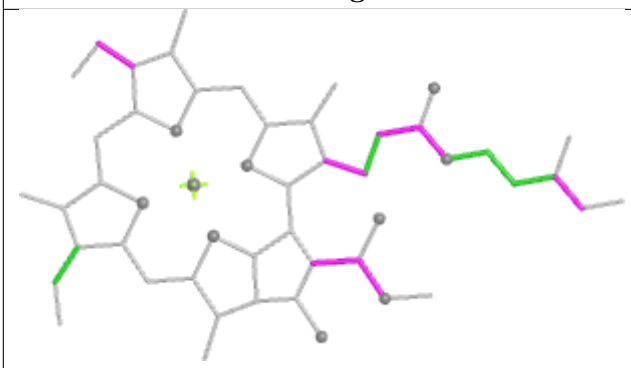
Ligand CLA bA 824



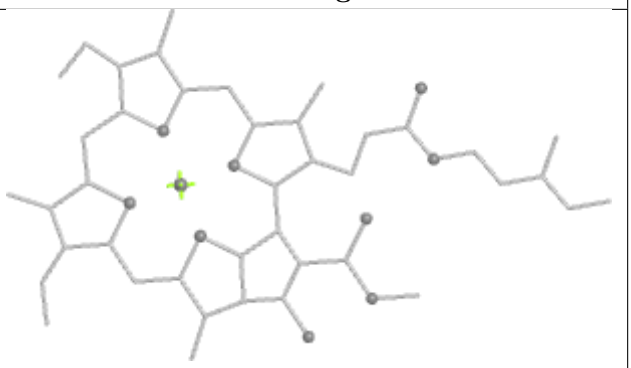
Bond lengths



Bond angles

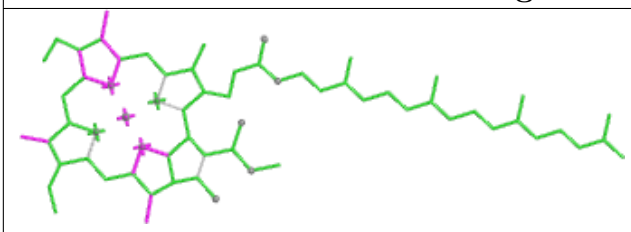


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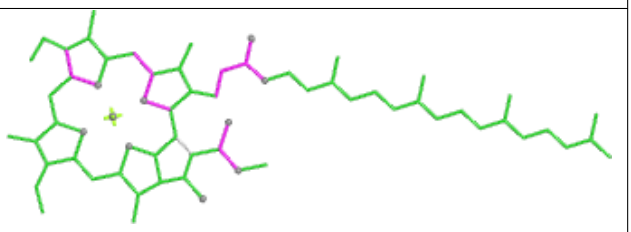


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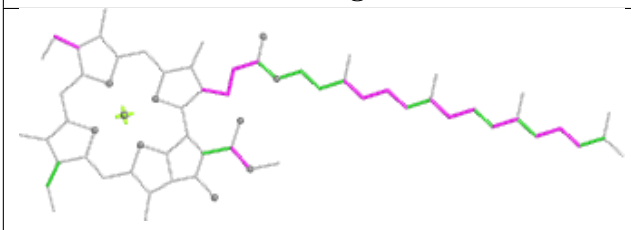
Ligand CLA cA 810



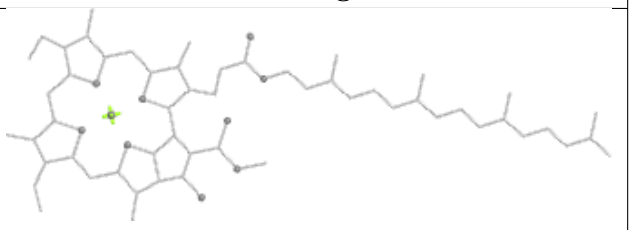
Bond lengths



Bond angles

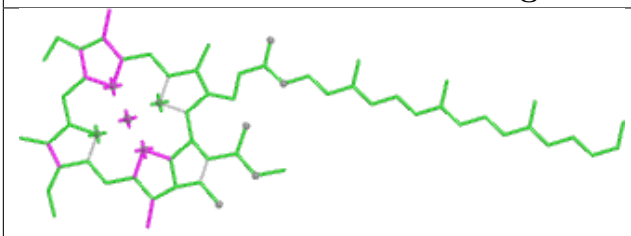


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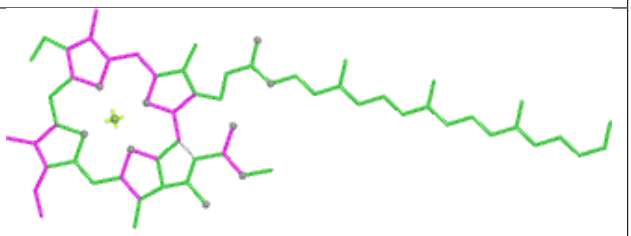


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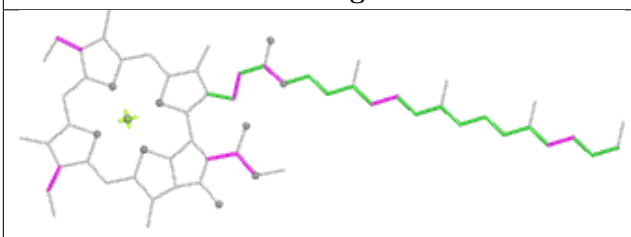
Ligand CLA c2 411



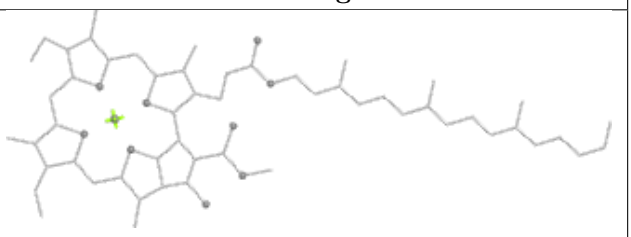
Bond lengths



Bond angles

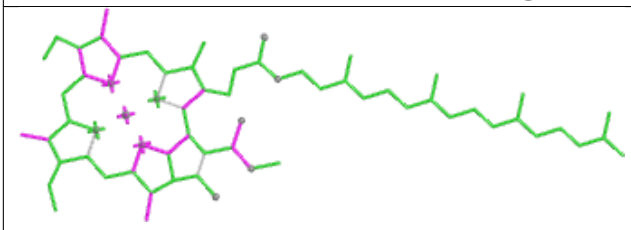


Torsions

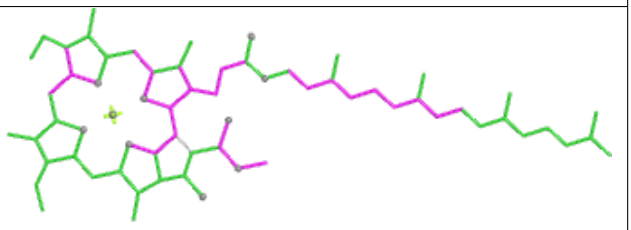


Rings

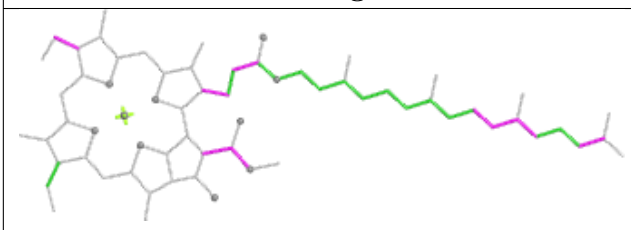
Ligand CLA a4 421



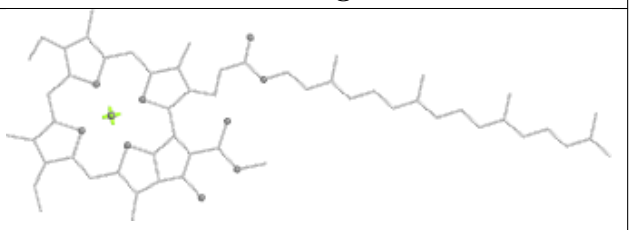
Bond lengths



Bond angles



Torsions

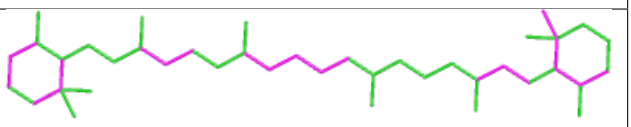


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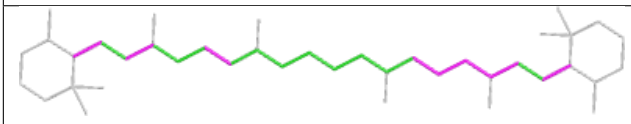
Ligand BCR a3 419



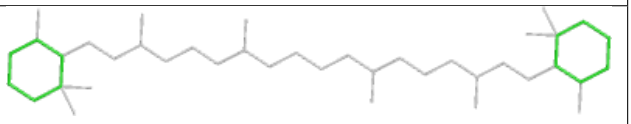
Bond lengths



Bond angles

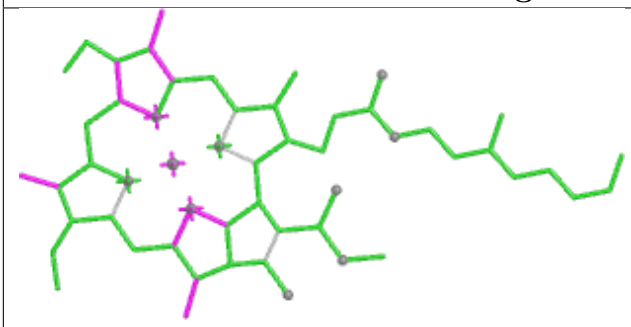


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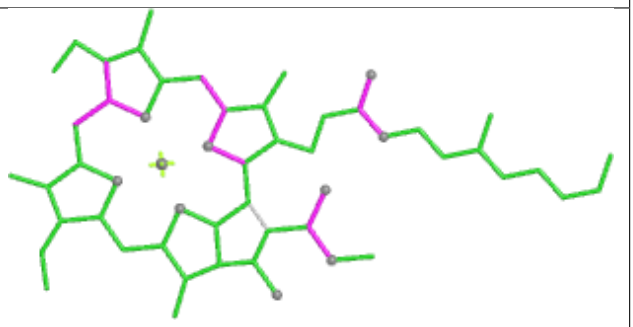


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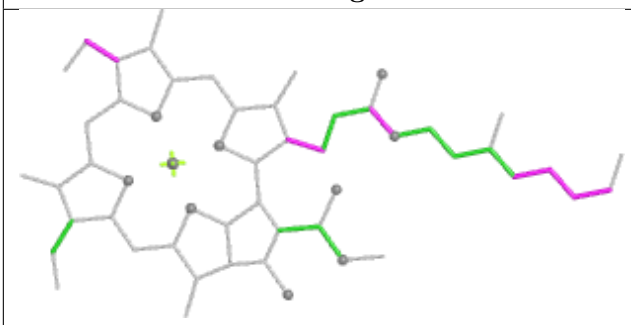
Ligand CLA aA 836



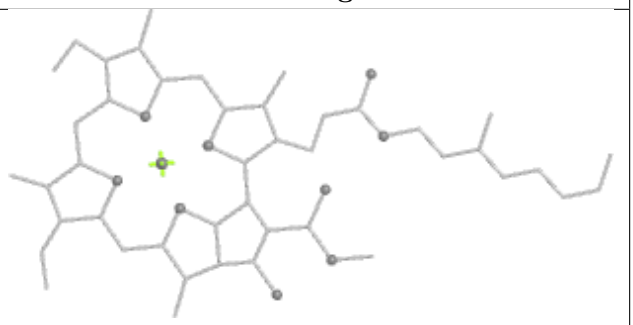
Bond lengths



Bond angles

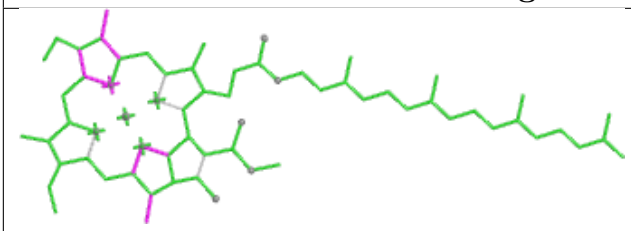


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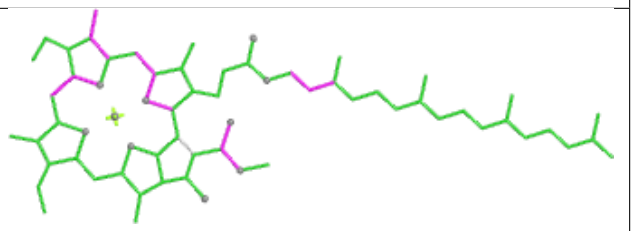


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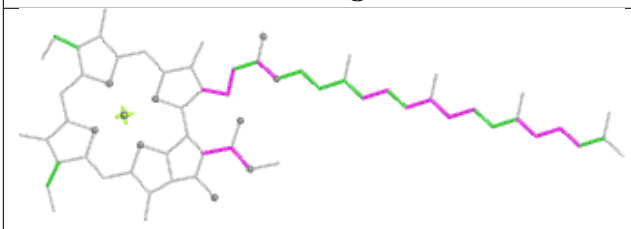
Ligand CLA b2 402



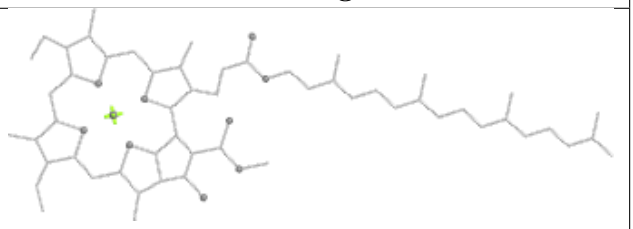
Bond lengths



Bond angles

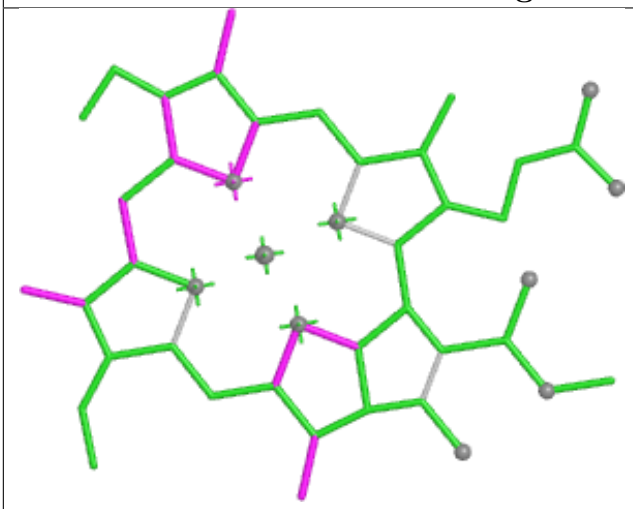


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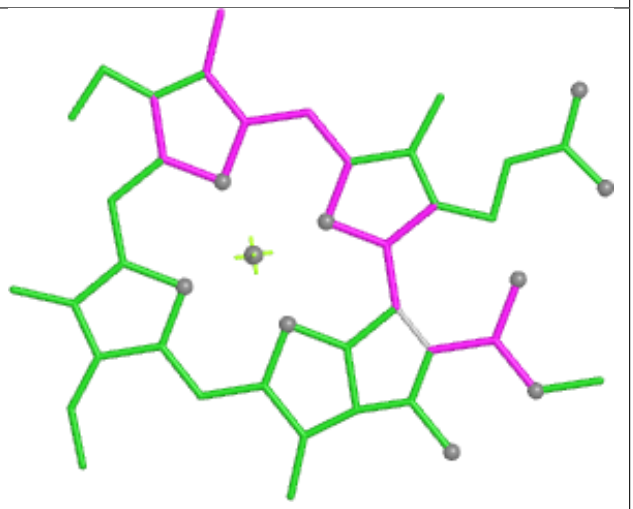


Rings

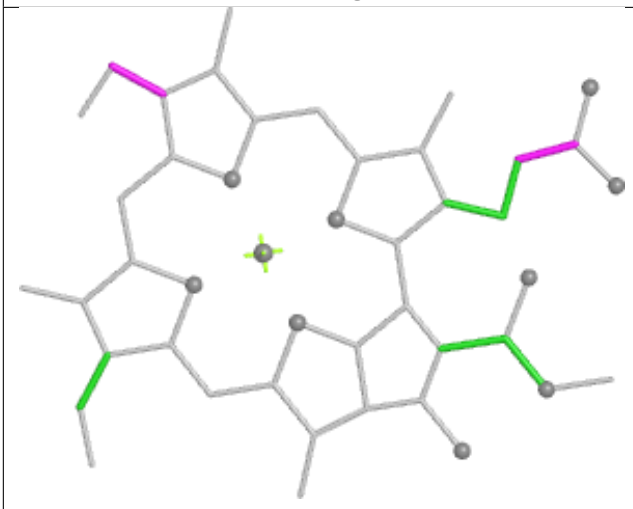
Ligand CLA aB 841



Bond lengths



Bond angles

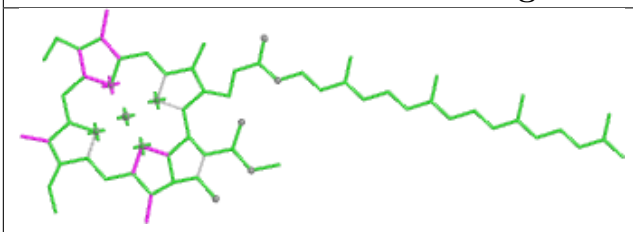


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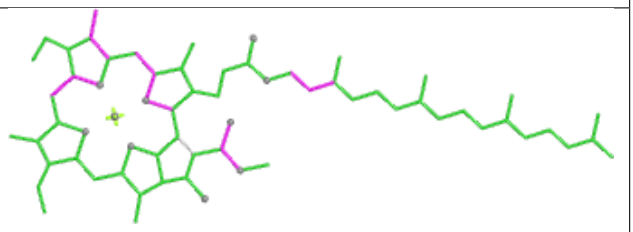


Rings

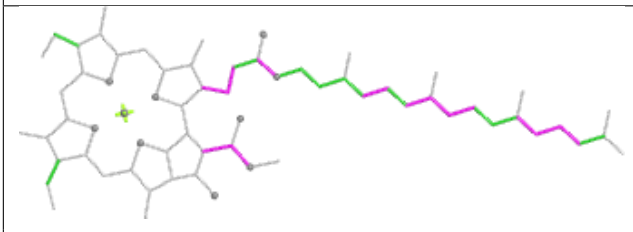
Ligand CLA b5 402



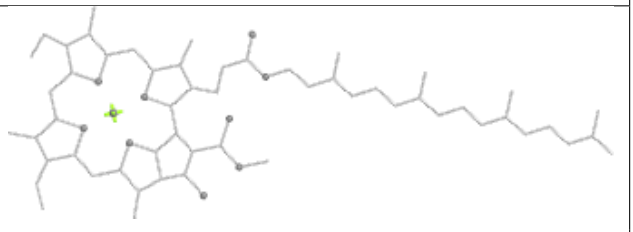
Bond lengths



Bond angles

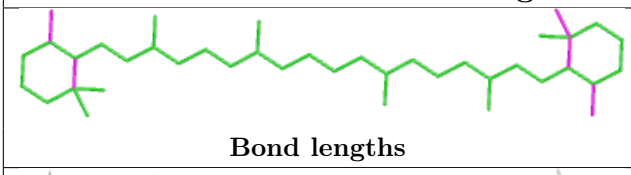


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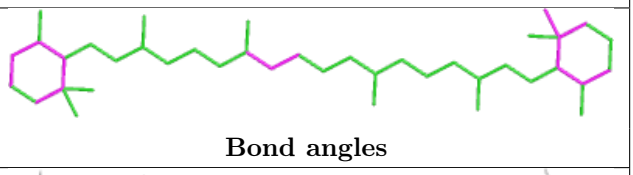


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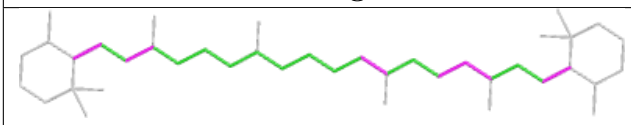
Ligand BCR b1 418



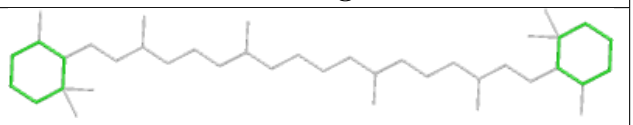
Bond lengths



Bond angles

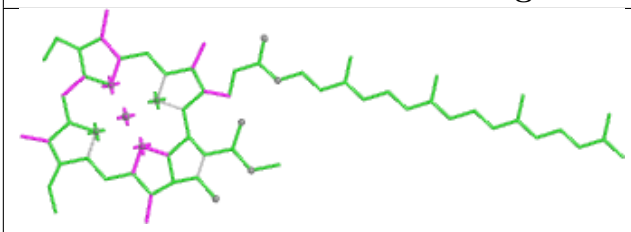


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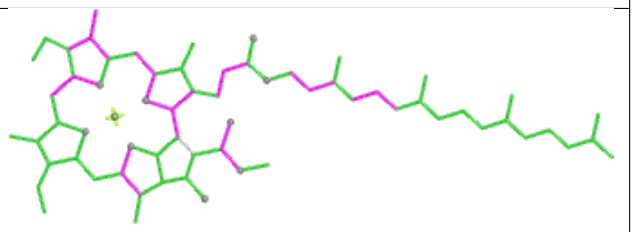


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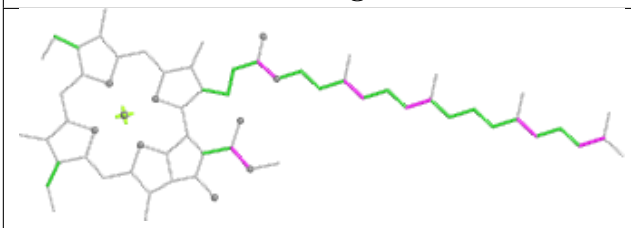
Ligand CLA aA 834



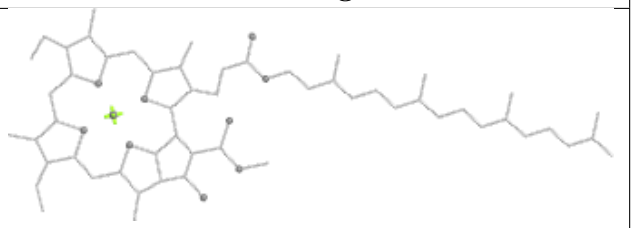
Bond lengths



Bond angles

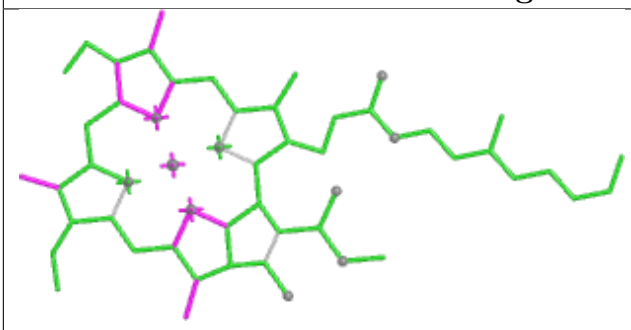


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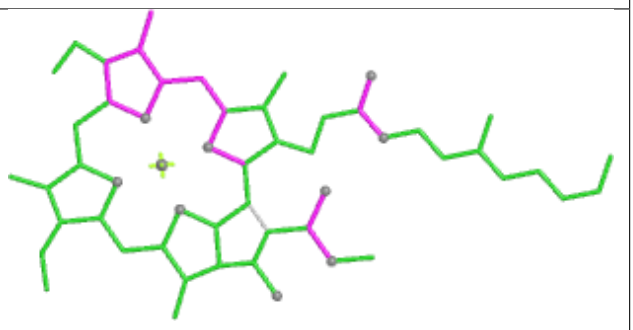


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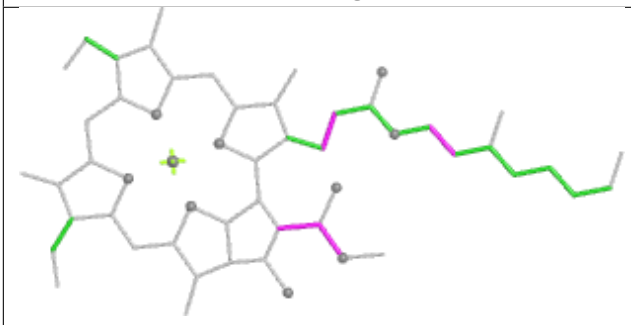
Ligand CLA aB 805



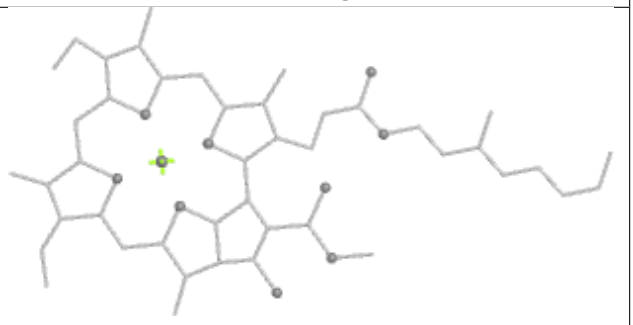
Bond lengths



Bond angles

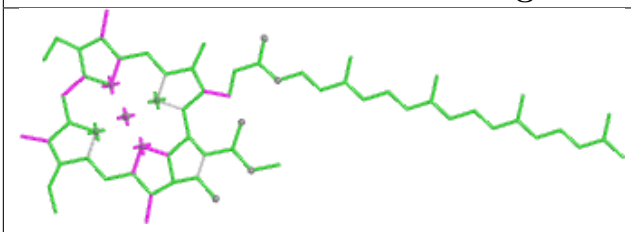


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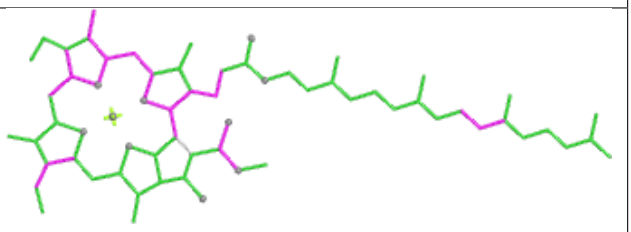


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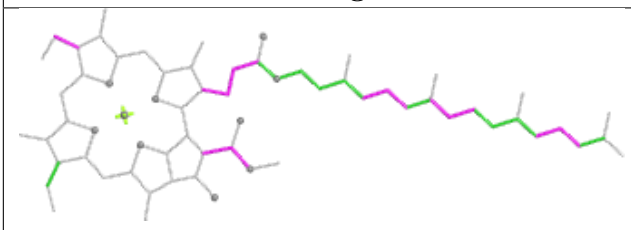
Ligand CLA cB 810



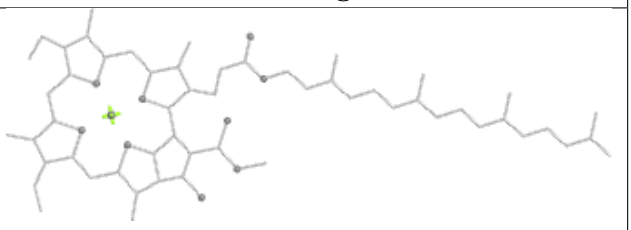
Bond lengths



Bond angles

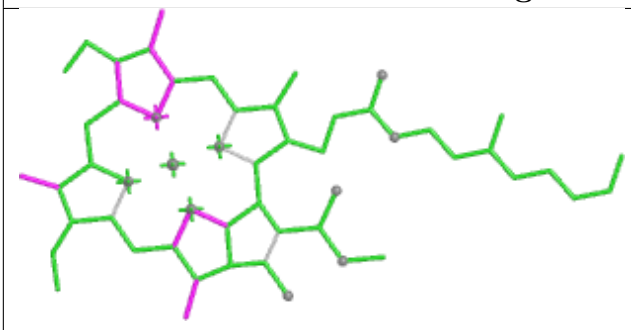


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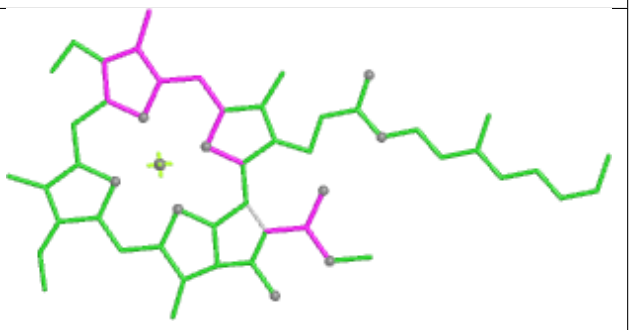


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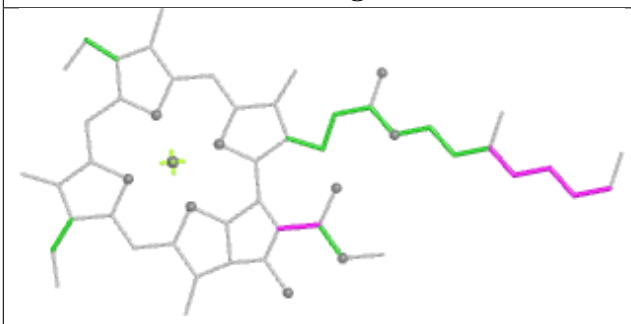
Ligand CLA aA 818



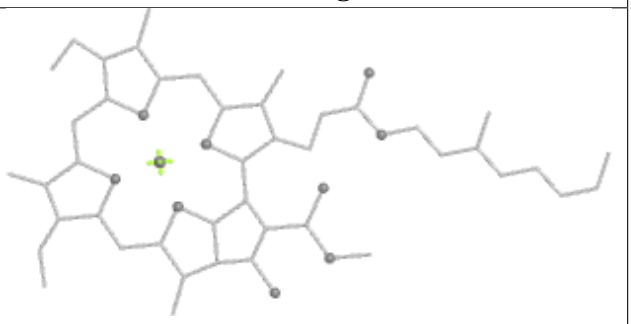
Bond lengths



Bond angles

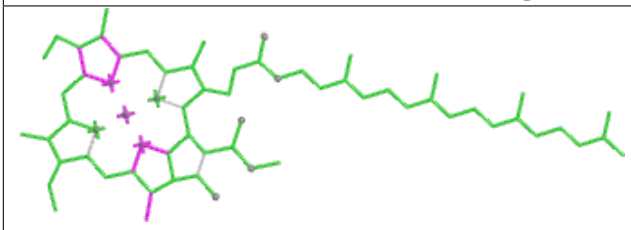


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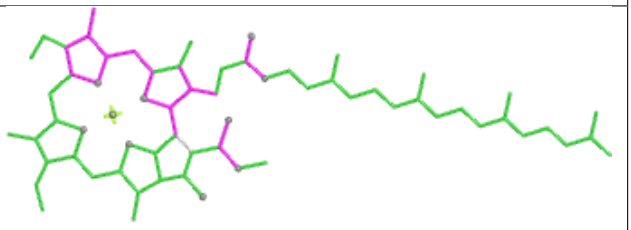


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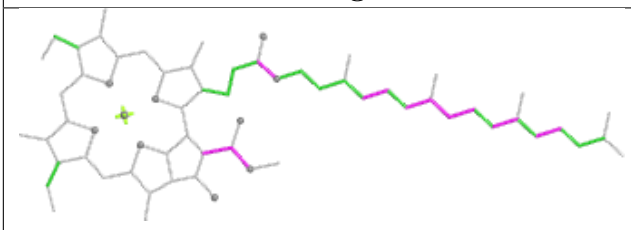
Ligand CLA b5 403



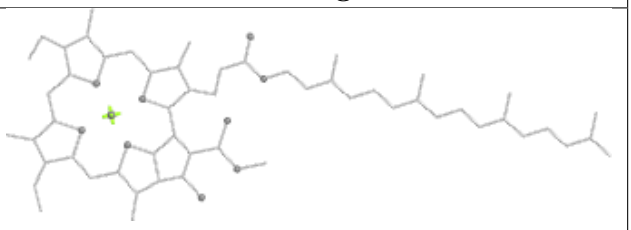
Bond lengths



Bond angles

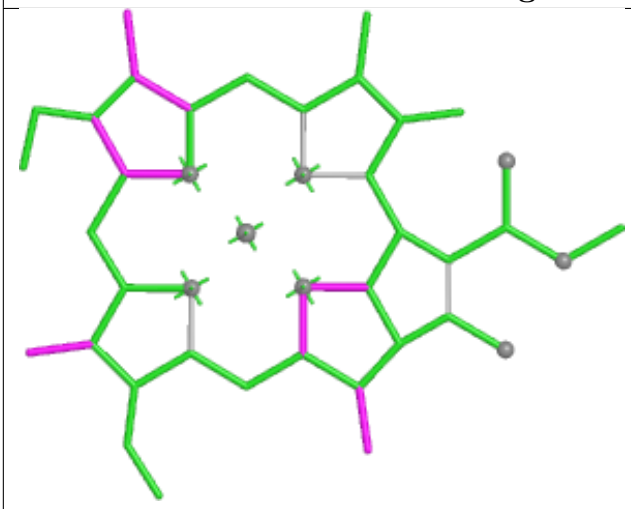


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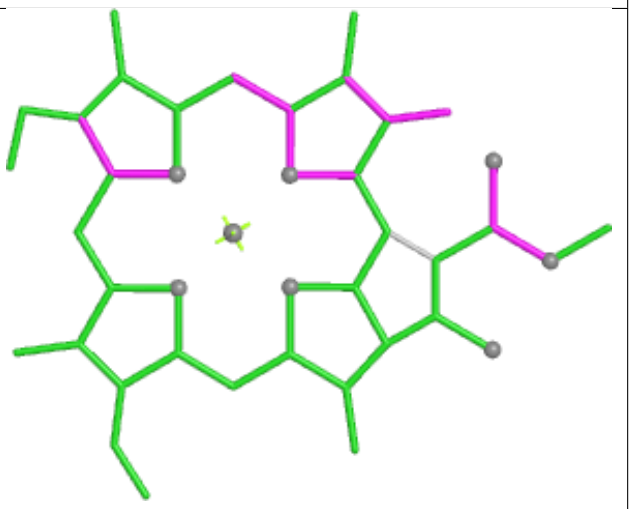


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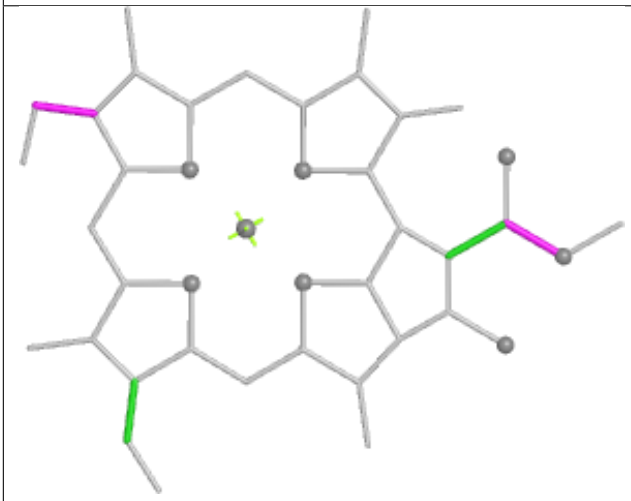
Ligand CLA b2 415



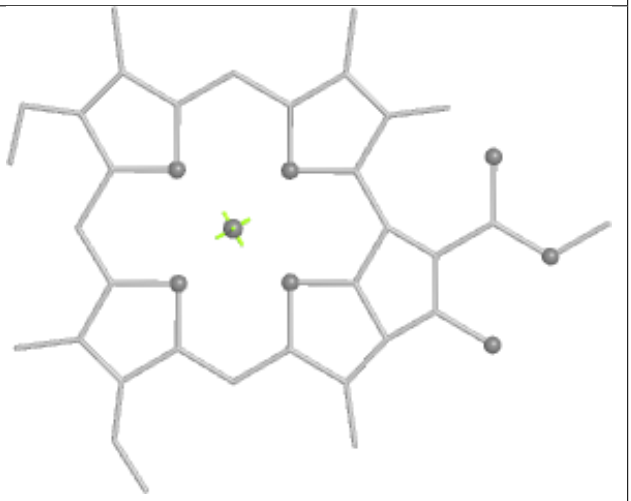
Bond lengths



Bond angles

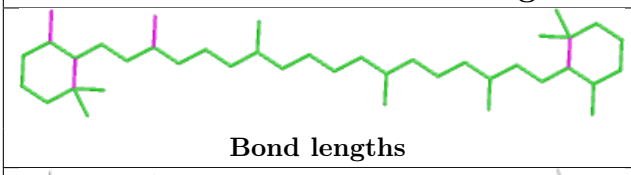


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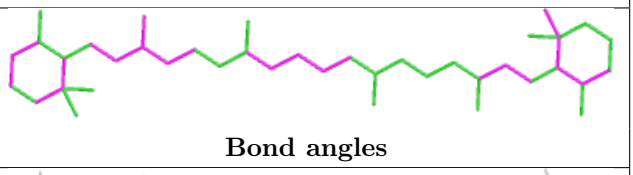


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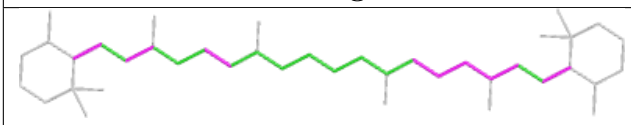
Ligand BCR c1 419



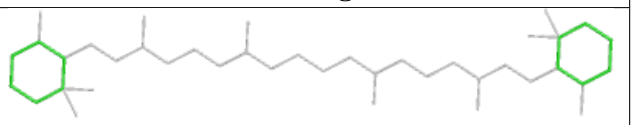
Bond lengths



Bond angles

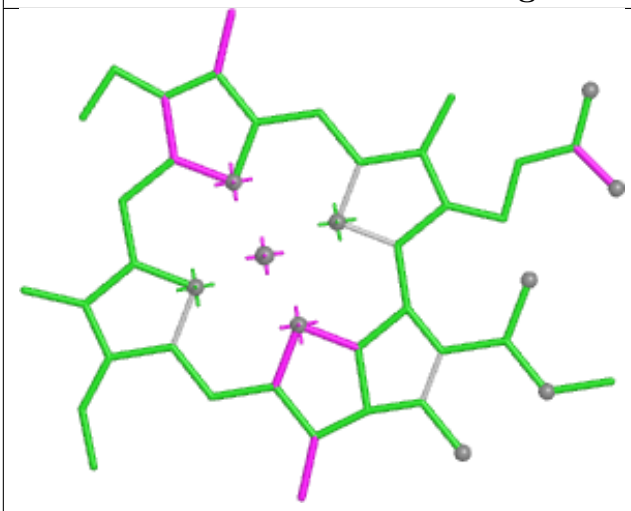


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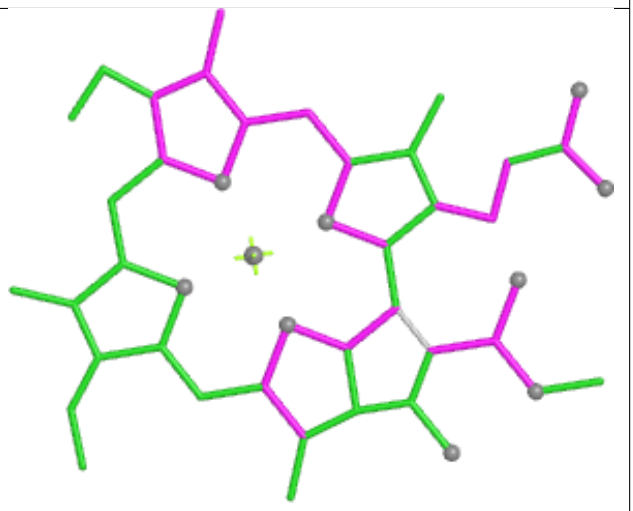


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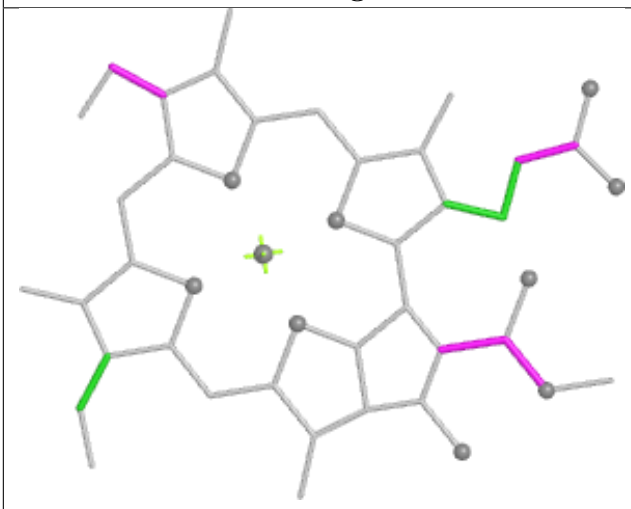
Ligand CLA b5 415



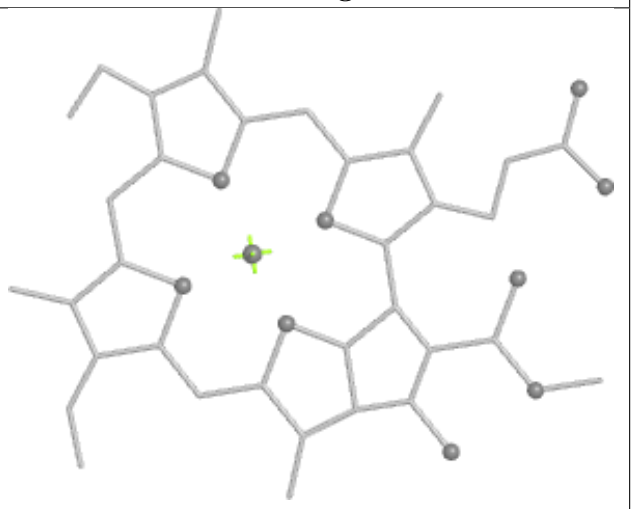
Bond lengths



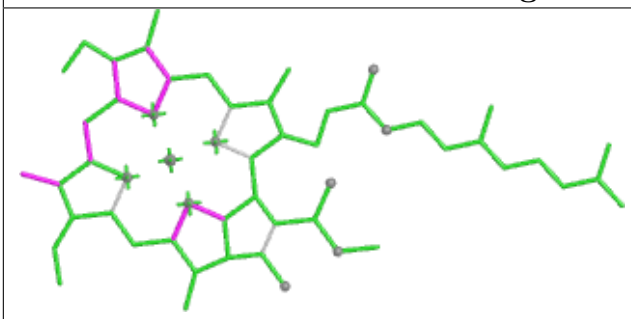
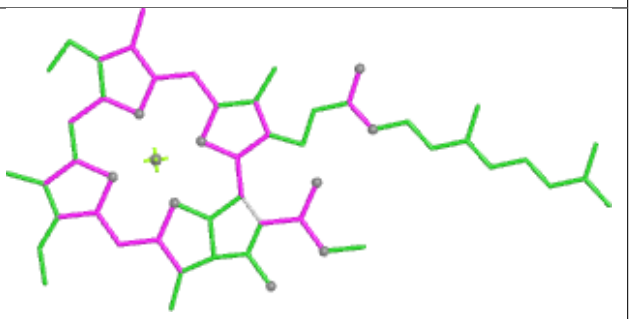
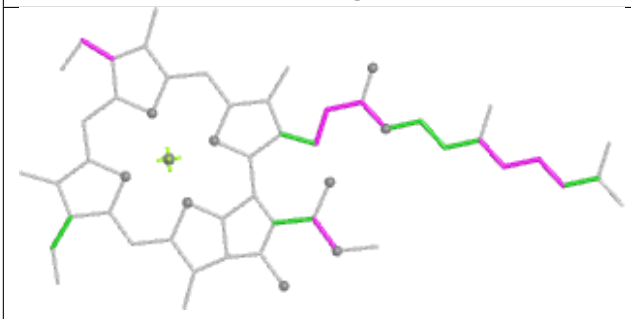
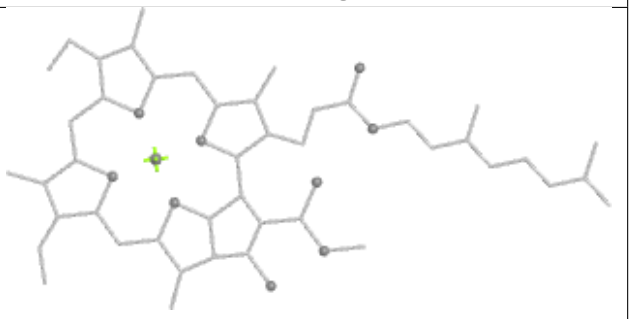
Bond angles

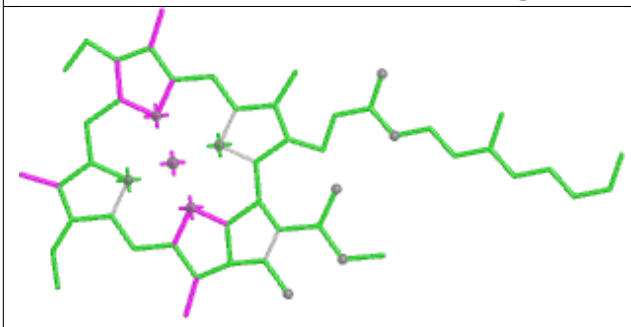
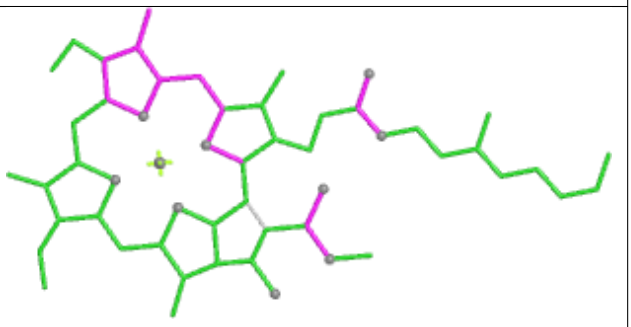
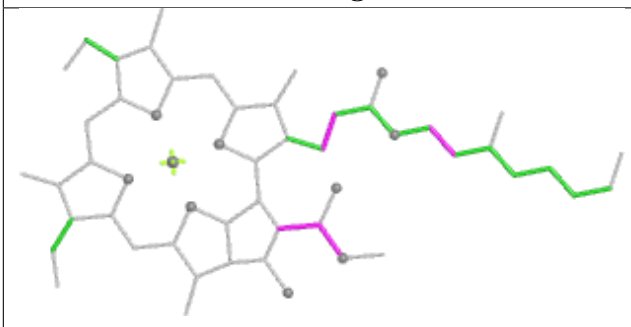
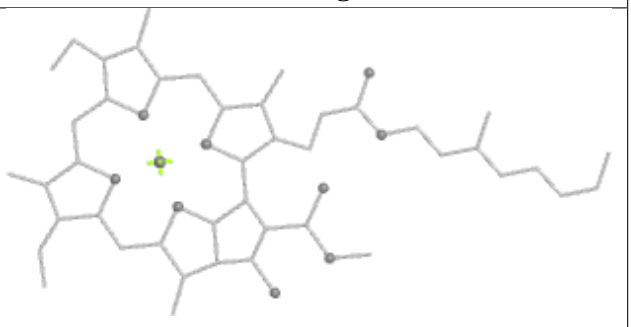


Torsions

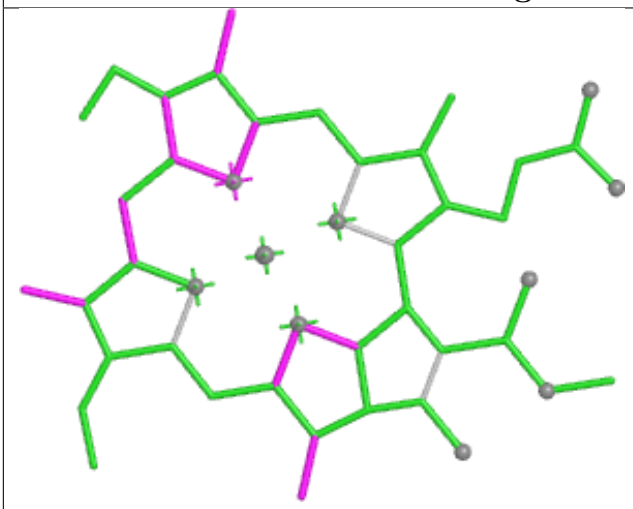


Rings

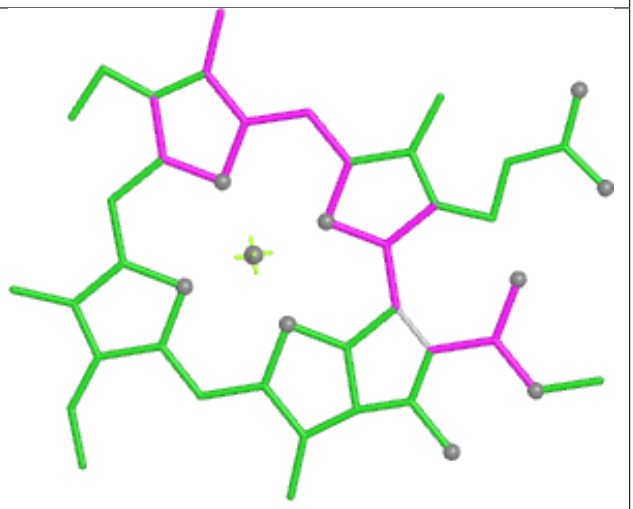
Ligand CLA a3 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bB 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

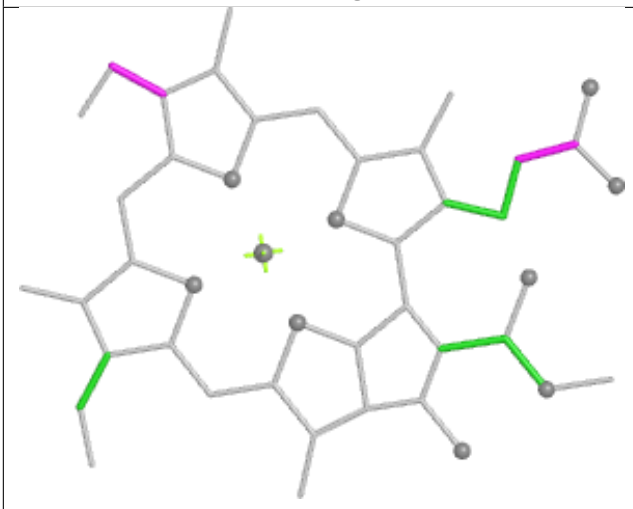
Ligand CLA bB 841



Bond lengths



Bond angles

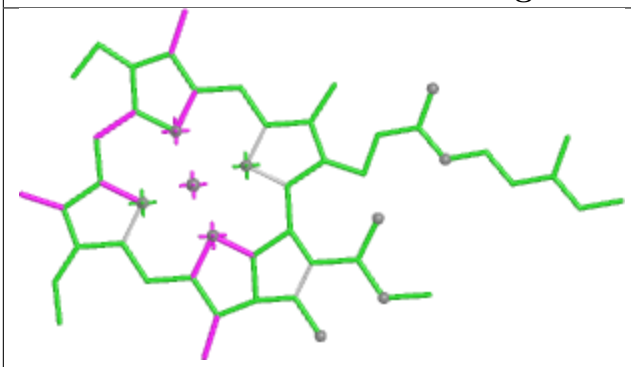


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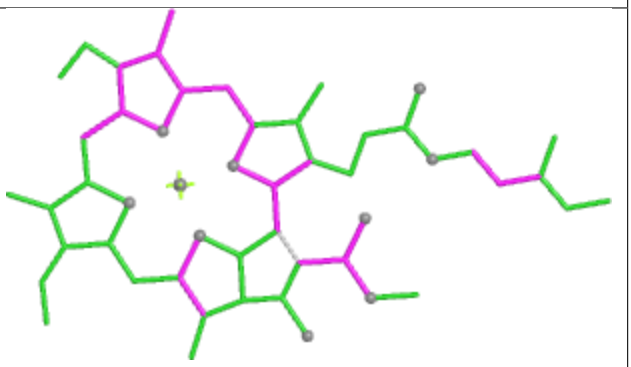


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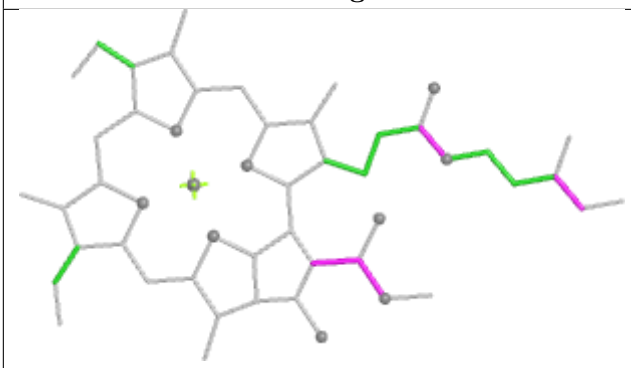
Ligand CLA aA 838



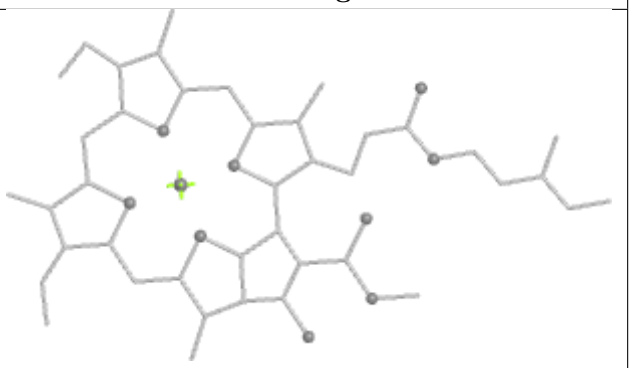
Bond lengths



Bond angles

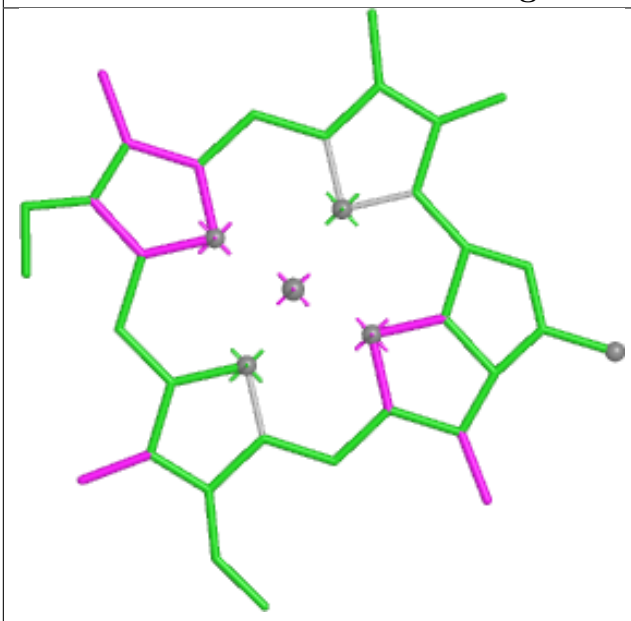


Torsions



Rings

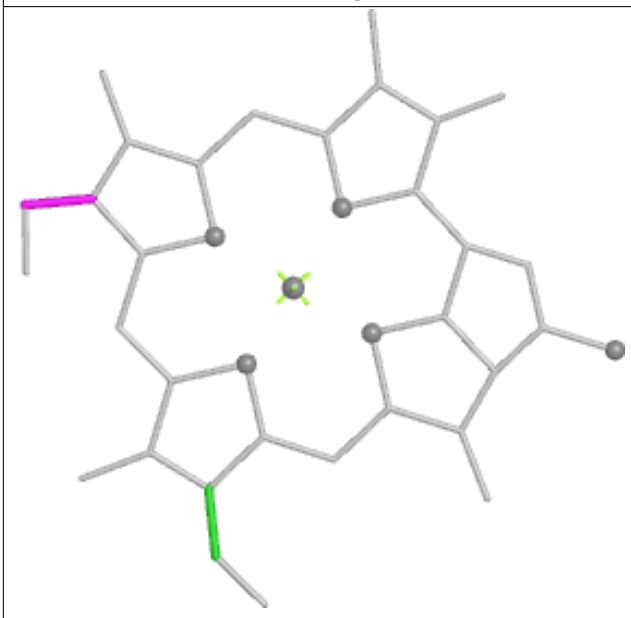
Ligand CLA aJ 203



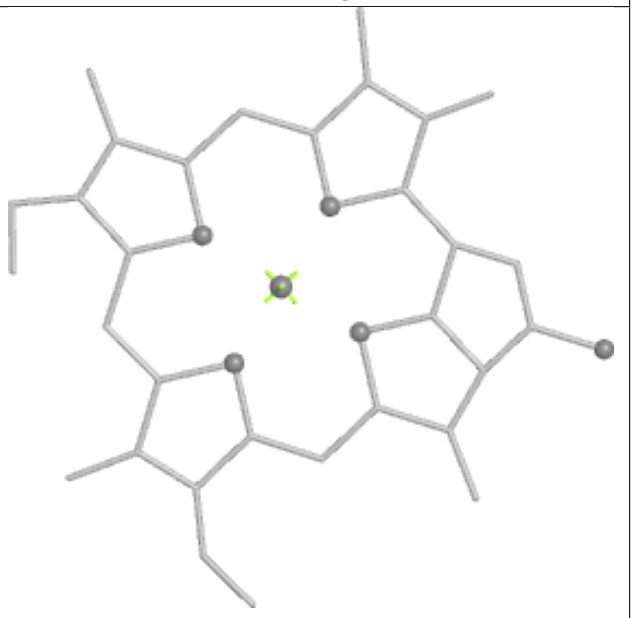
Bond lengths



Bond angles

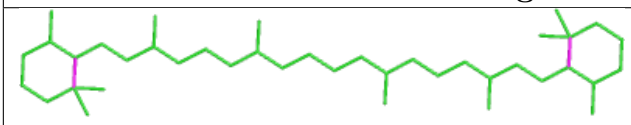


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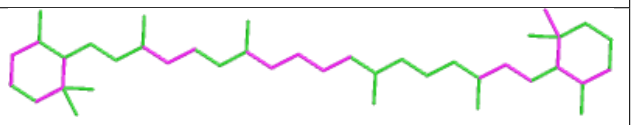


Rings

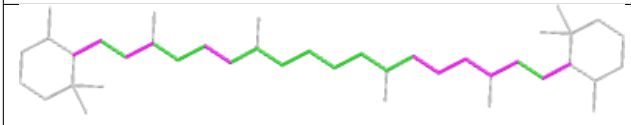
Ligand BCR b4 419



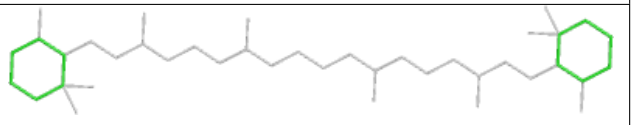
Bond lengths



Bond angles

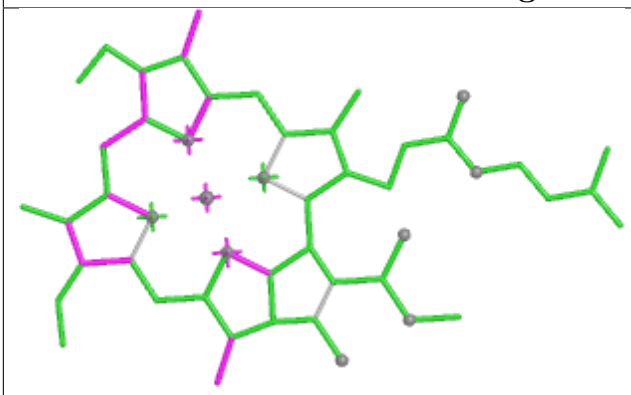


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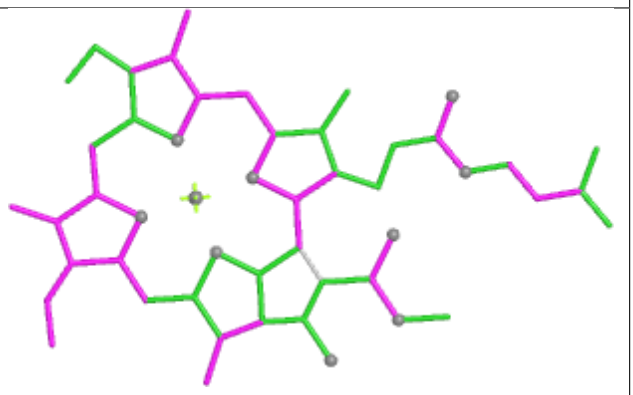


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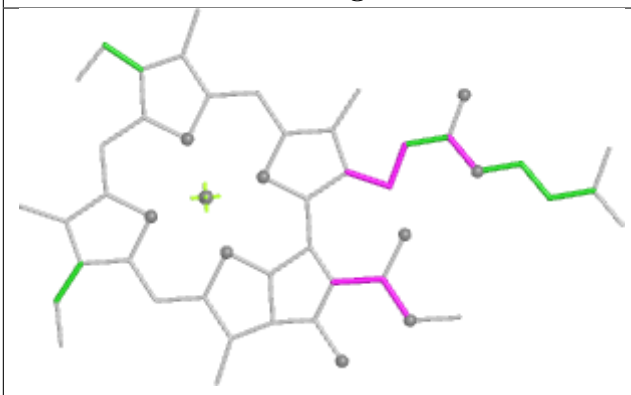
Ligand CLA b2 417



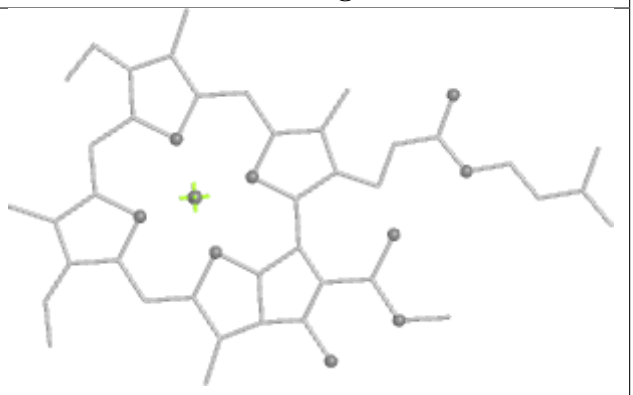
Bond lengths



Bond angles

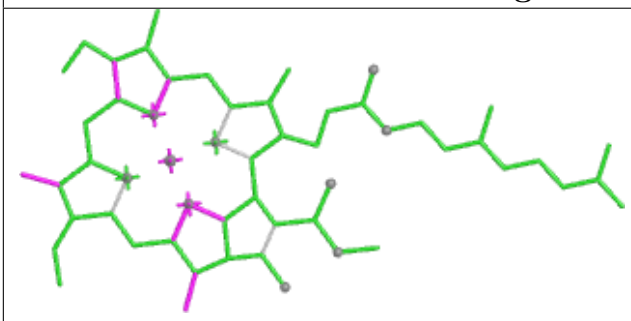


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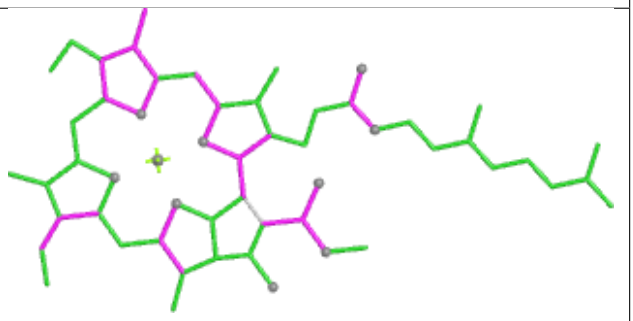


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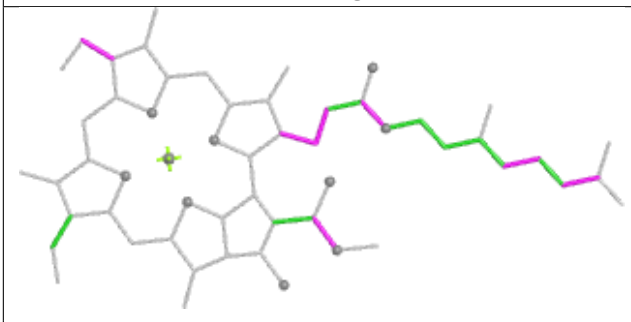
Ligand CLA bB 817



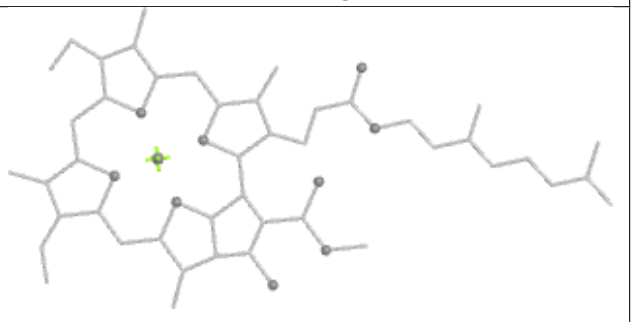
Bond lengths



Bond angles

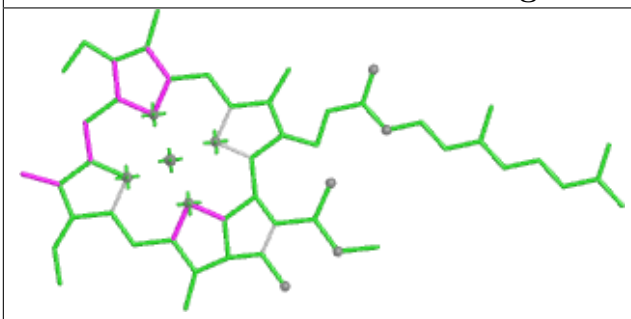


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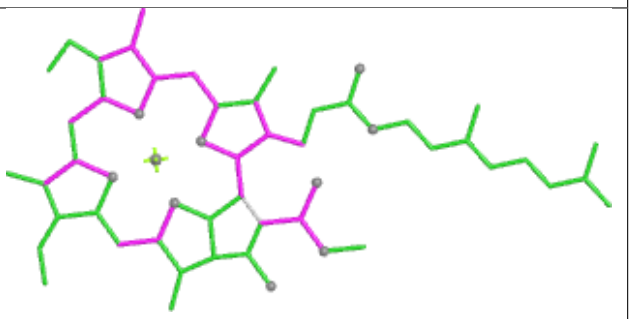


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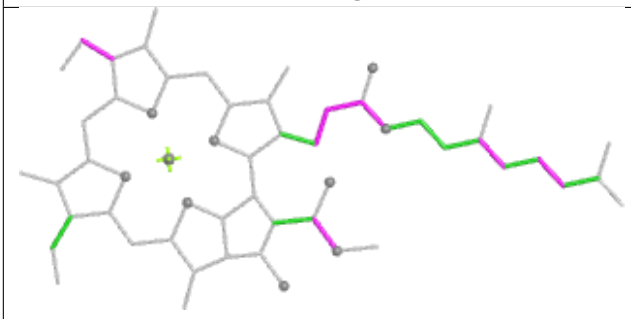
Ligand CLA a2 418



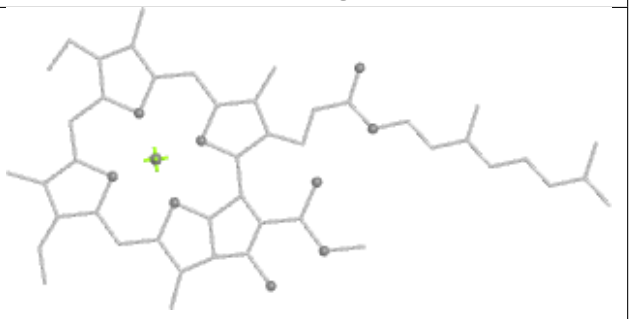
Bond lengths



Bond angles

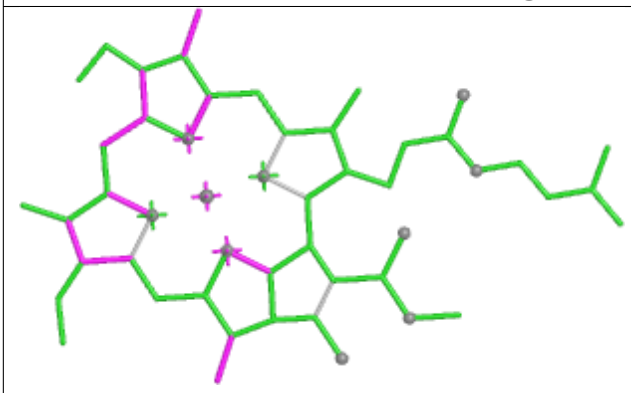


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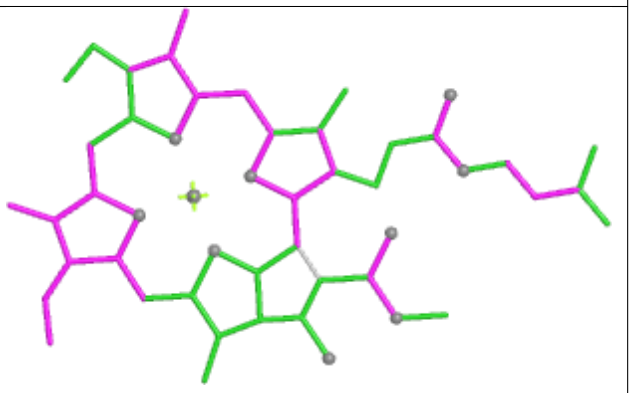


Rings

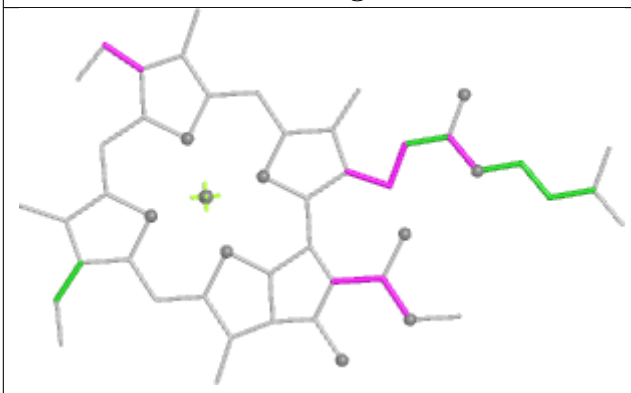
Ligand CLA c3 416



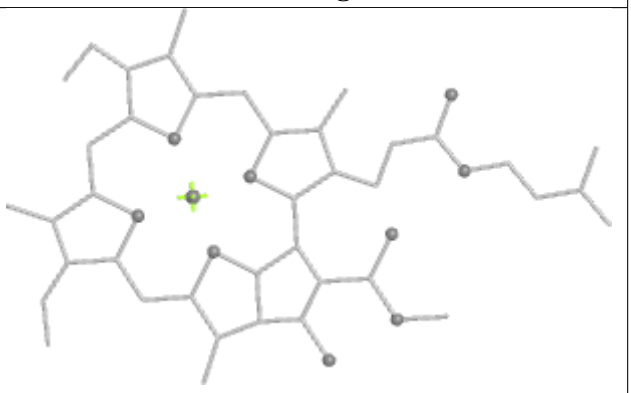
Bond lengths



Bond angles

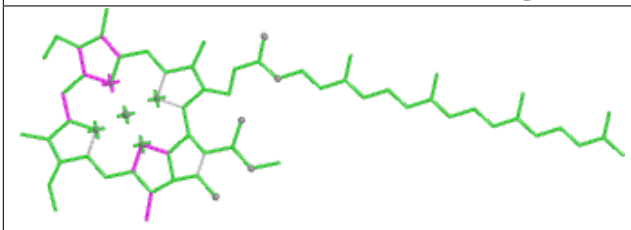


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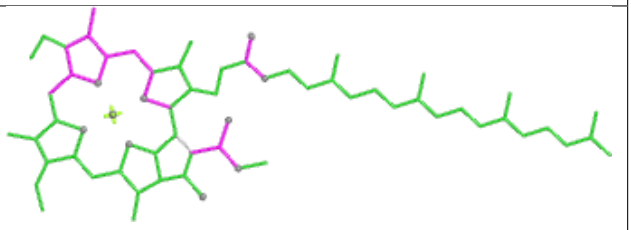


Rings

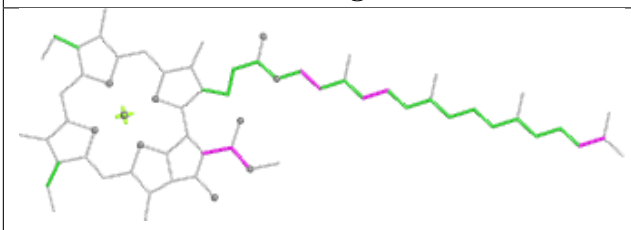
Ligand CLA b2 410



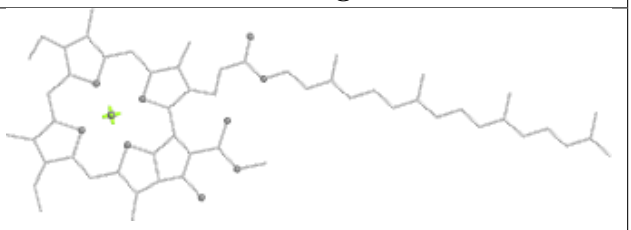
Bond lengths



Bond angles

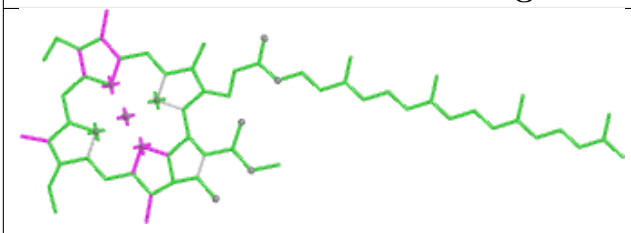


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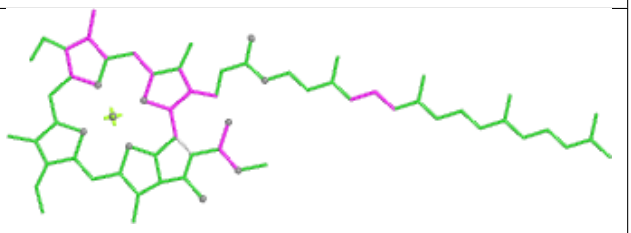


Rings

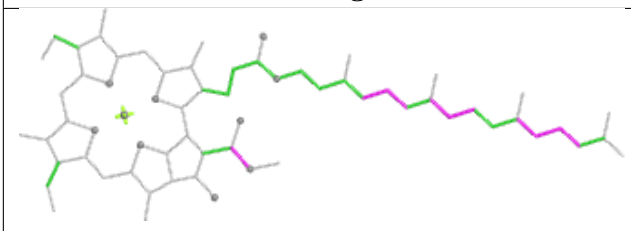
Ligand CLA cA 826



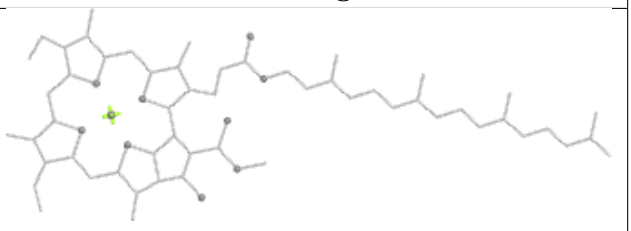
Bond lengths



Bond angles

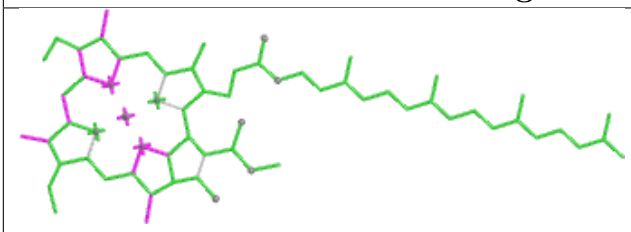


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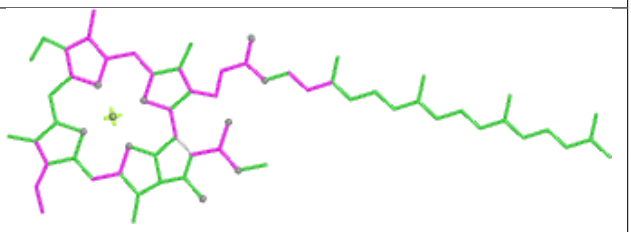


Rings

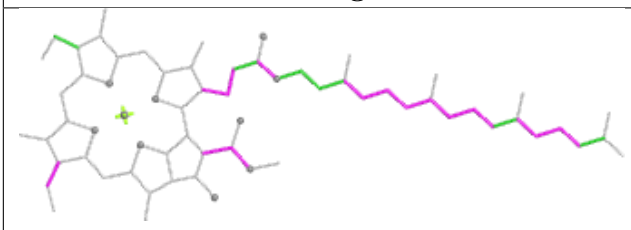
Ligand CLA aB 814



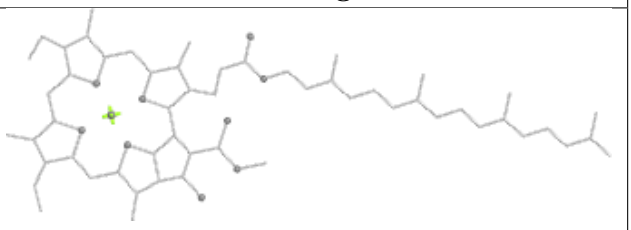
Bond lengths



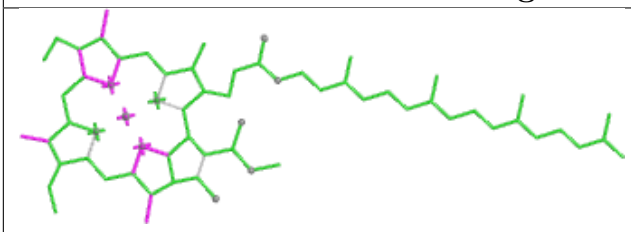
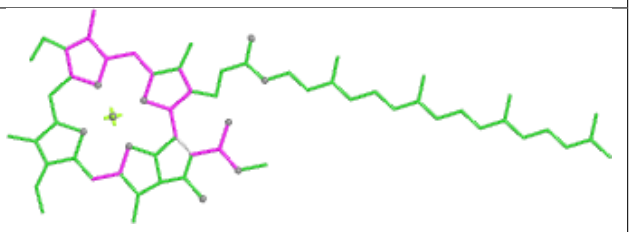
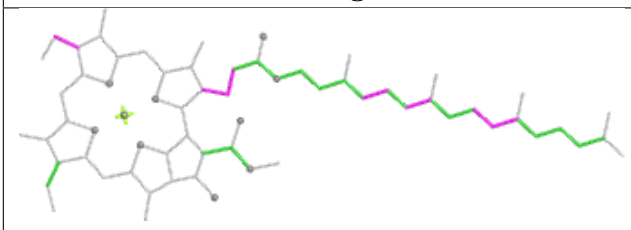
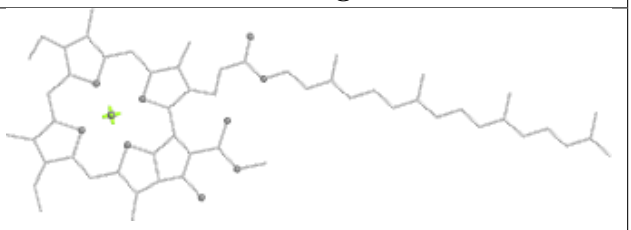
Bond angles

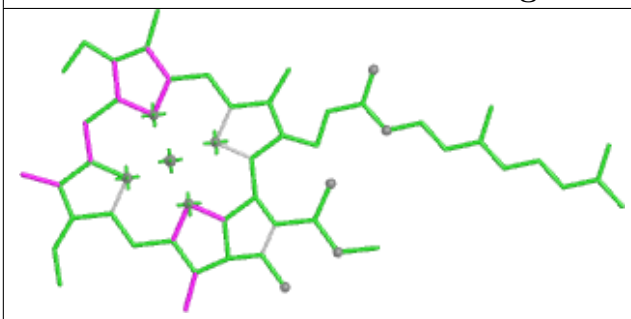
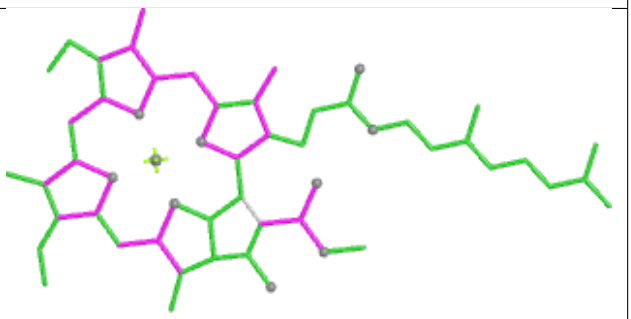
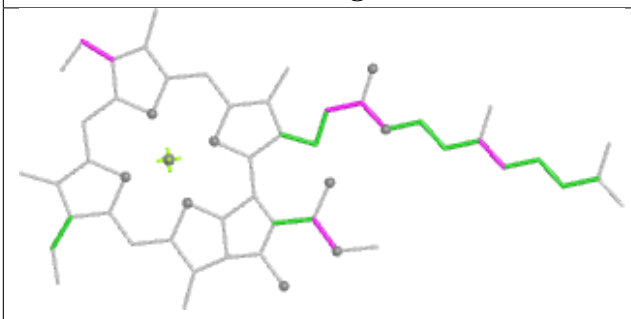
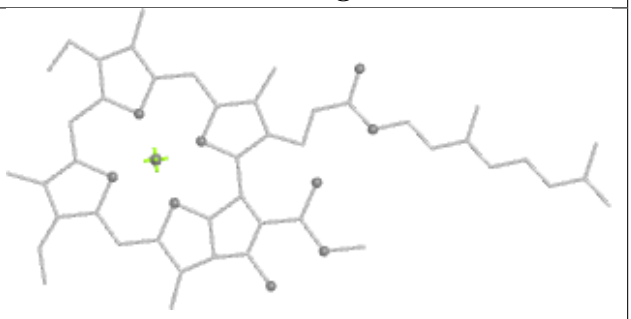


Torsions

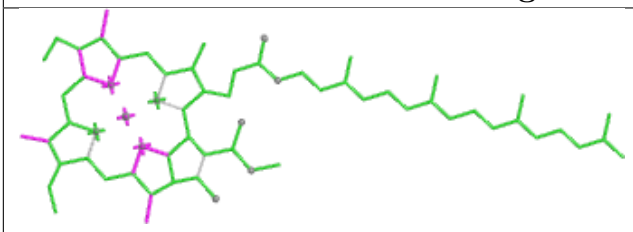


Rings

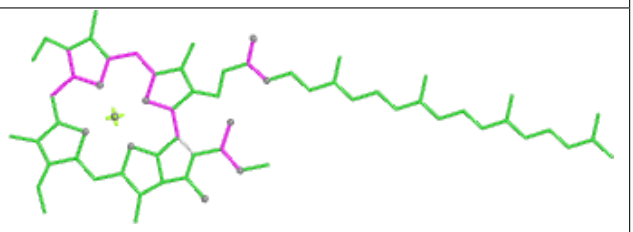
Ligand CLA aL 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a4 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

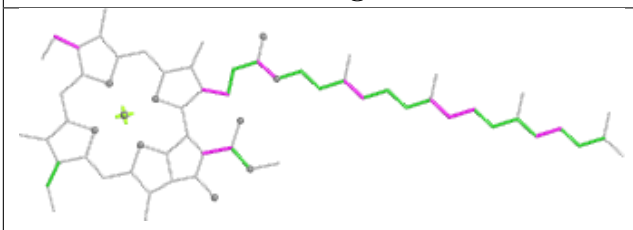
Ligand CLA cL 202



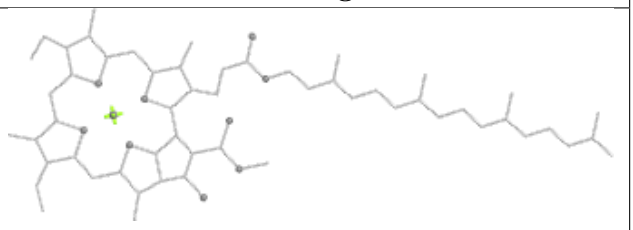
Bond lengths



Bond angles



Torsions

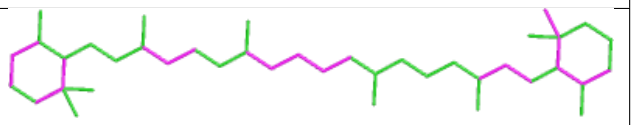


Rings

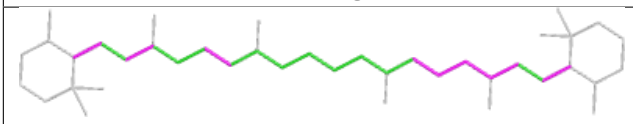
Ligand BCR b3 419



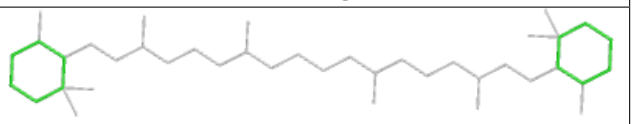
Bond lengths



Bond angles

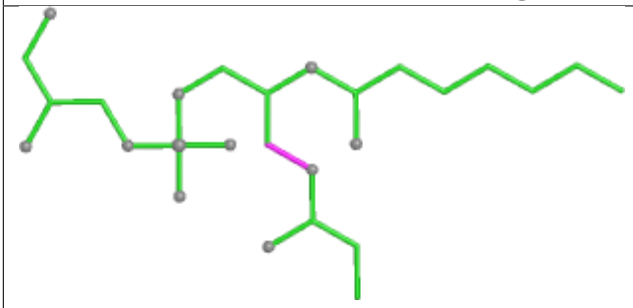


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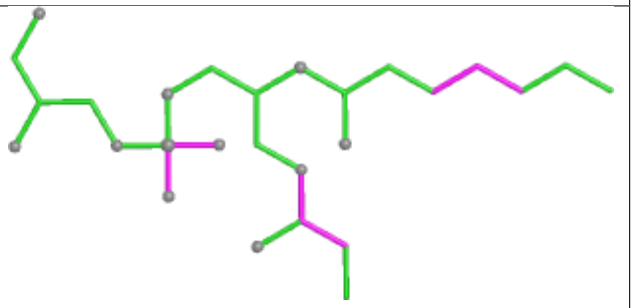


Rings

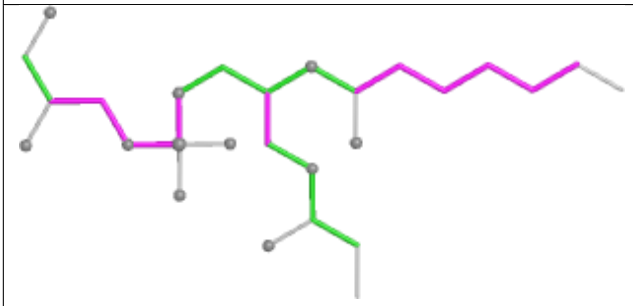
Ligand LHG aA 854



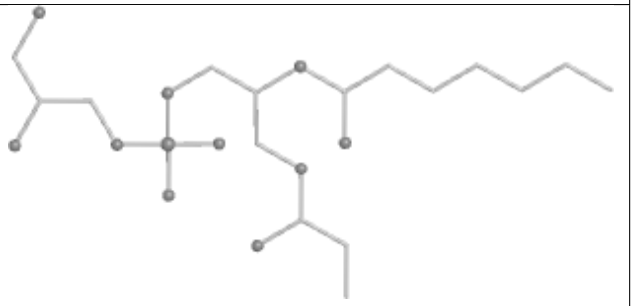
Bond lengths



Bond angles

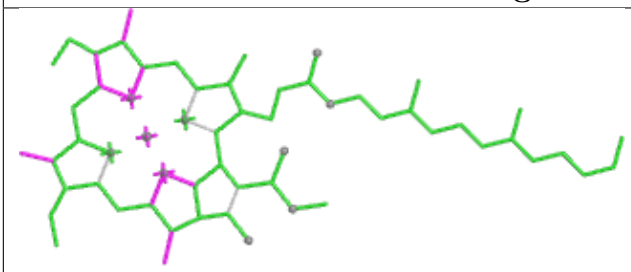


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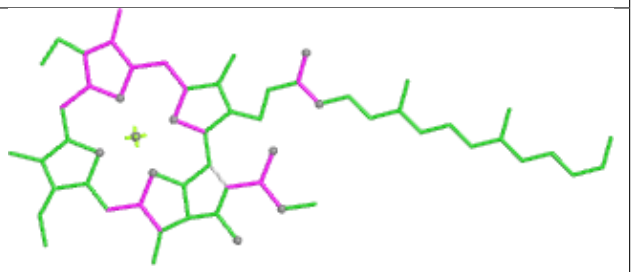


Rings

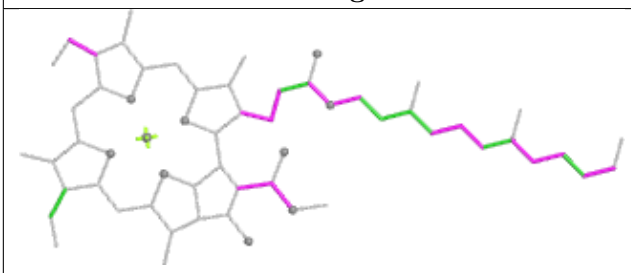
Ligand CLA bA 825



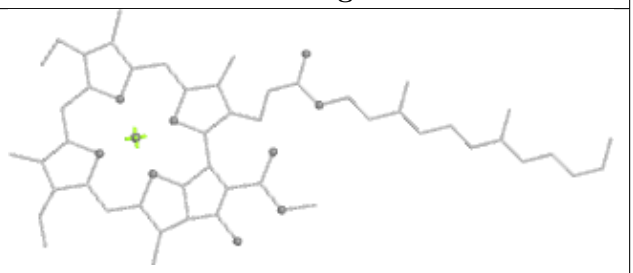
Bond lengths



Bond angles

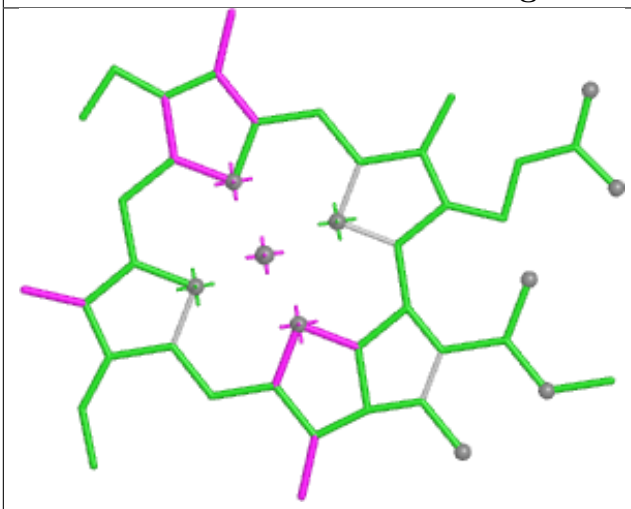


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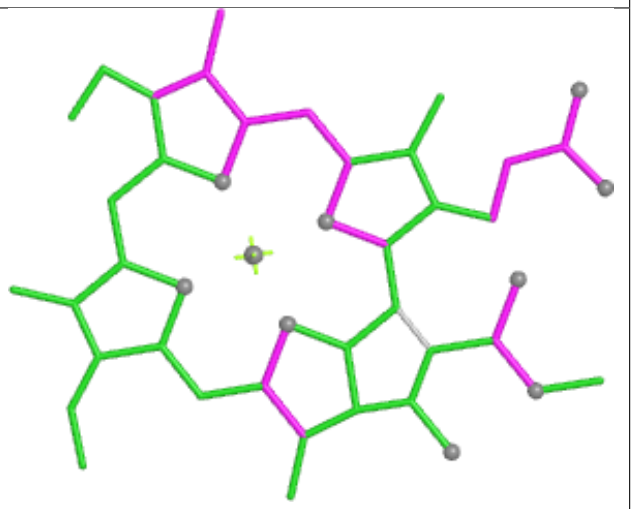


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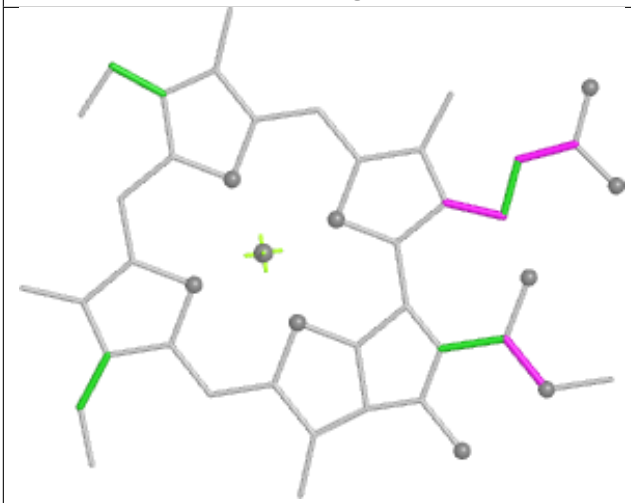
Ligand CLA a5 408



Bond lengths



Bond angles

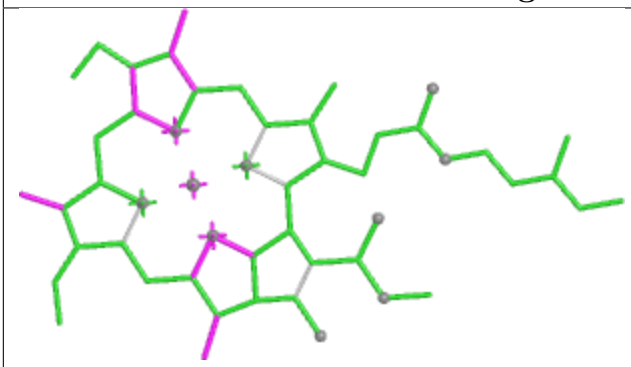


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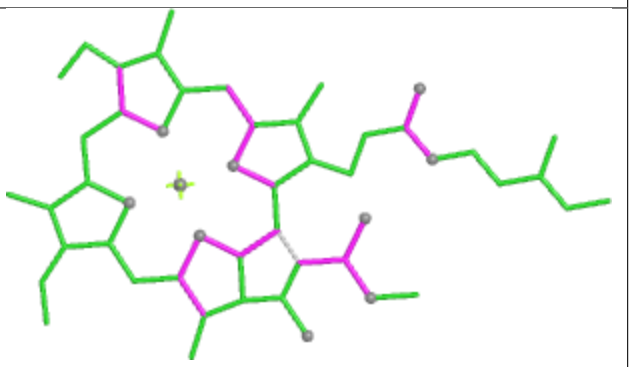


Rings

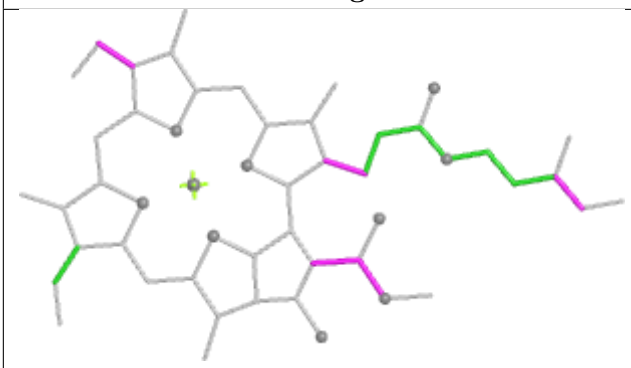
Ligand CLA cF 201



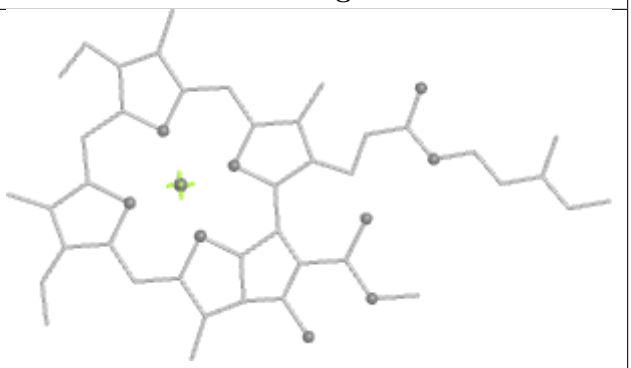
Bond lengths



Bond angles

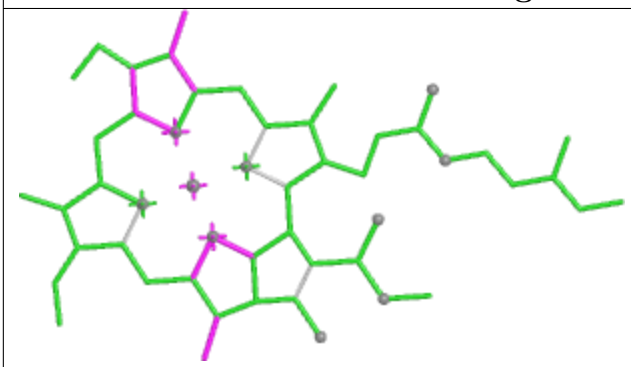


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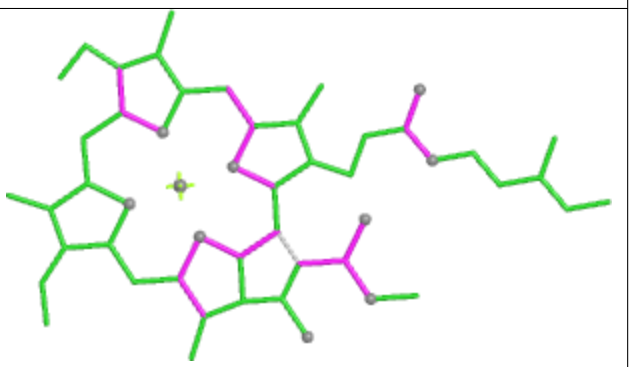


Rings

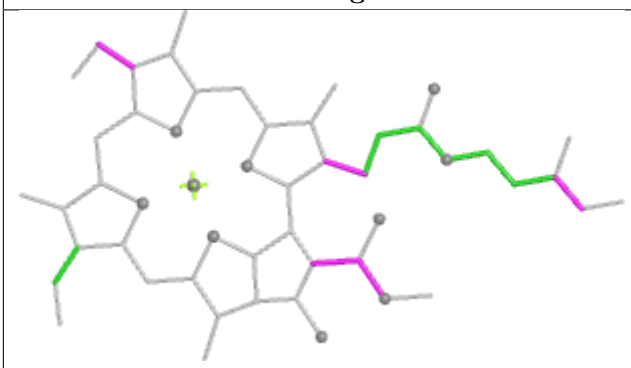
Ligand CLA aA 842



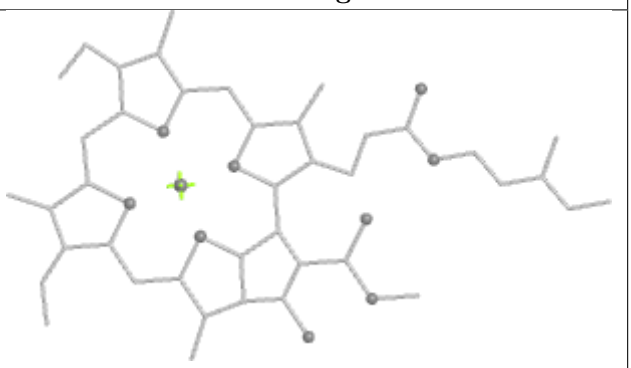
Bond lengths



Bond angles

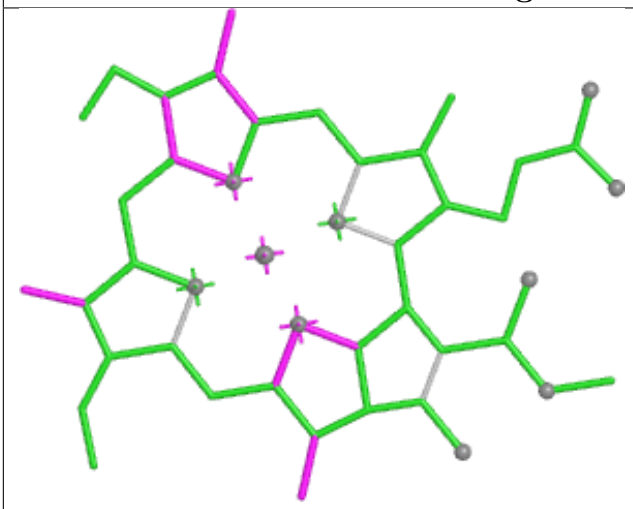


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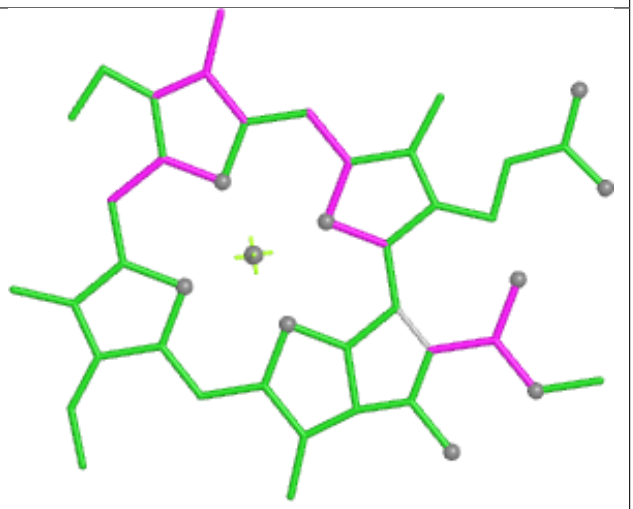


Rings

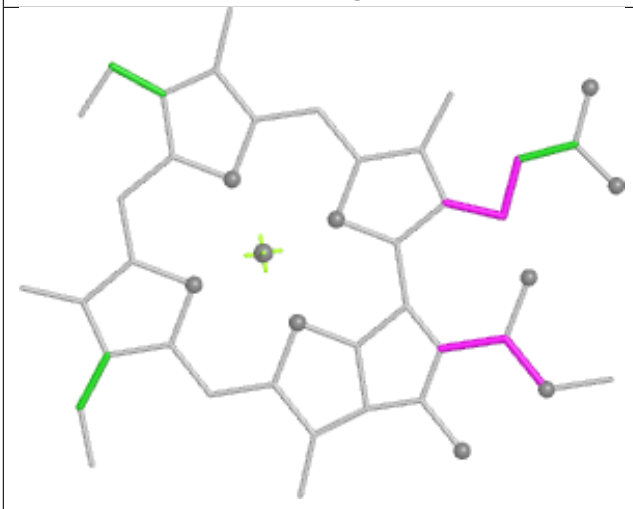
Ligand CLA aB 816



Bond lengths



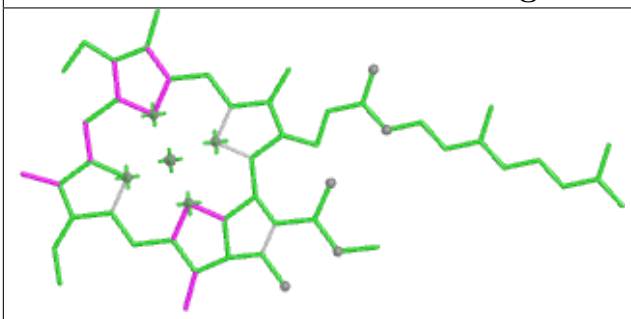
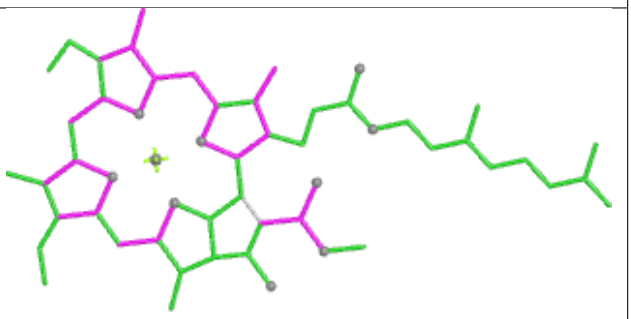
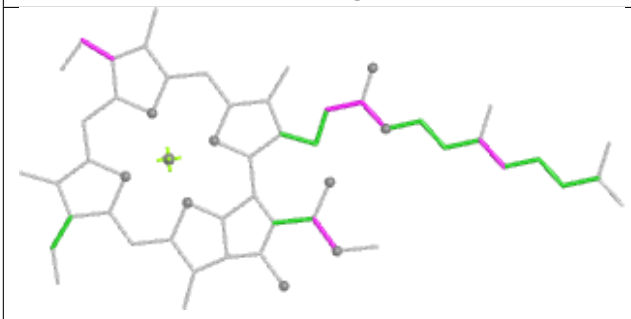
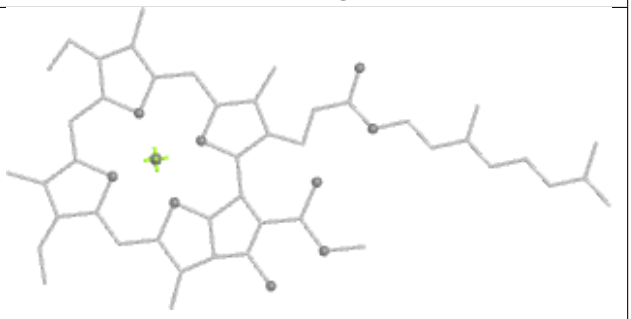
Bond angles

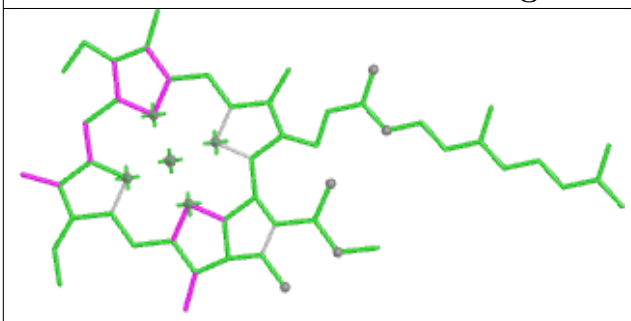
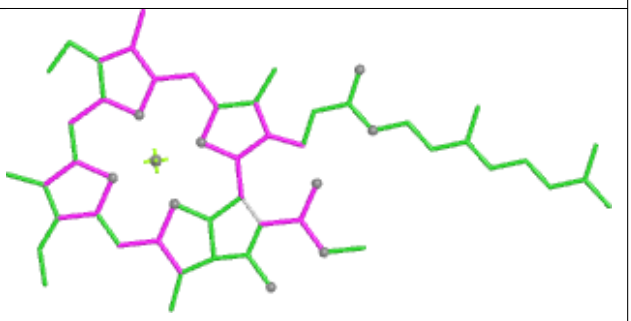
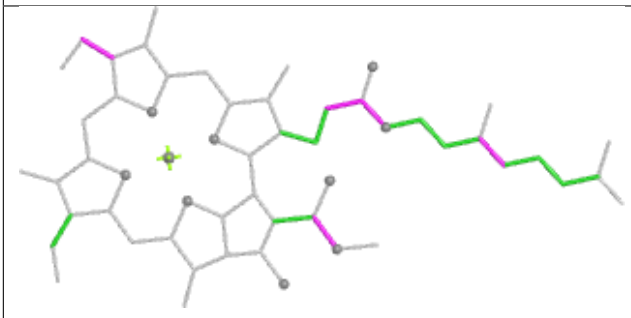
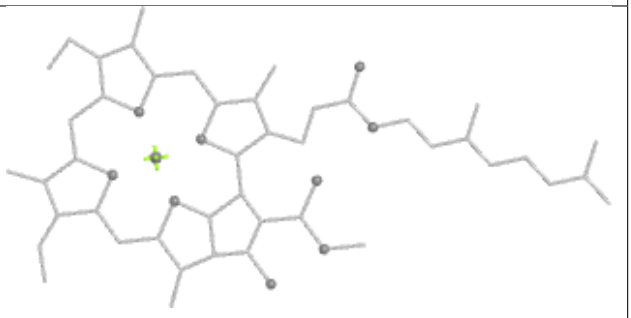


Torsions

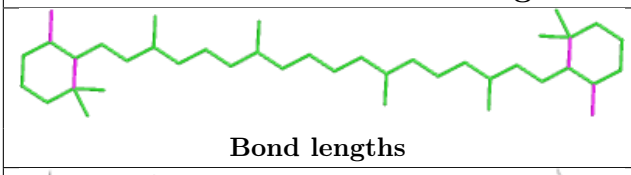


Rings

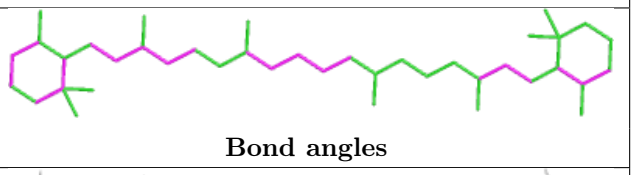
Ligand CLA a5 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c1 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

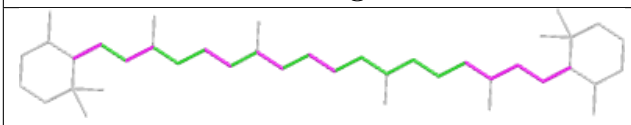
Ligand BCR aB 848



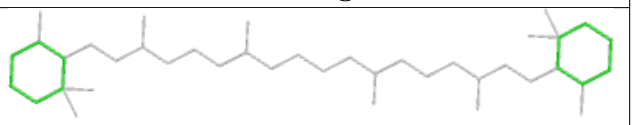
Bond lengths



Bond angles

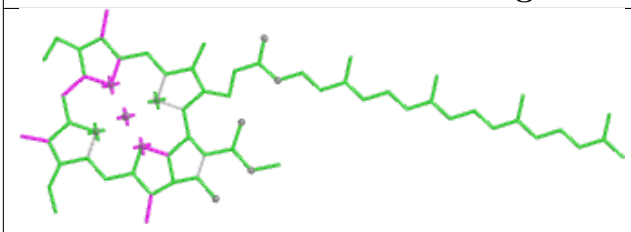


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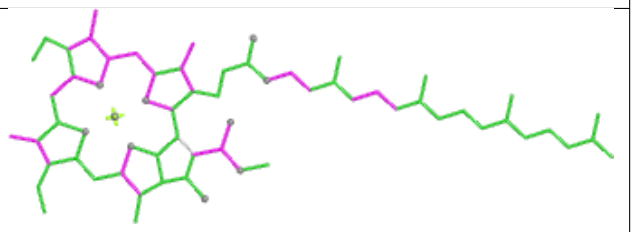


Rings

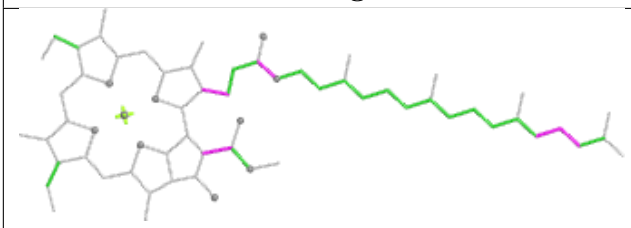
Ligand CLA aB 830



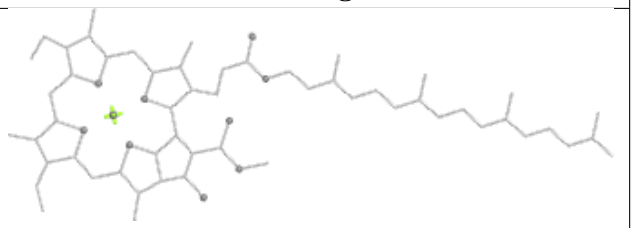
Bond lengths



Bond angles

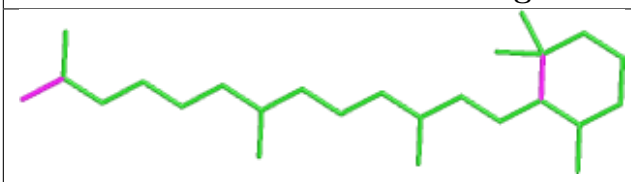


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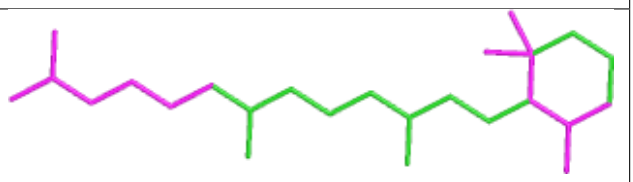


Rings

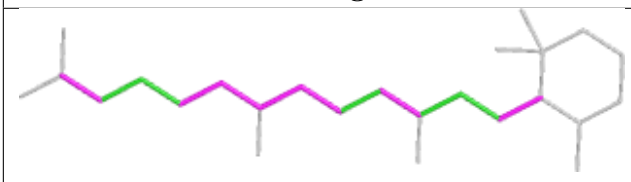
Ligand BCR aB 847



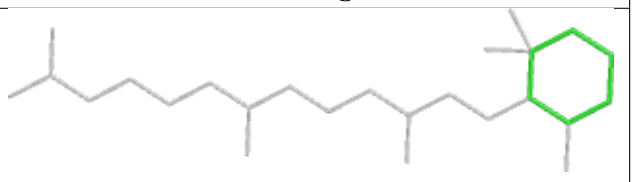
Bond lengths



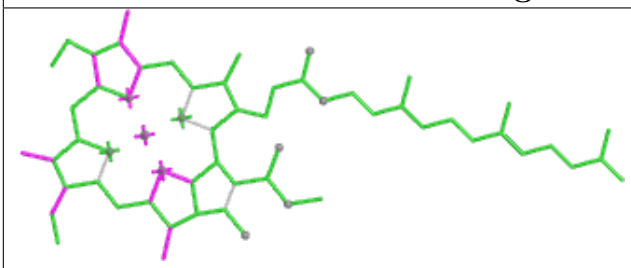
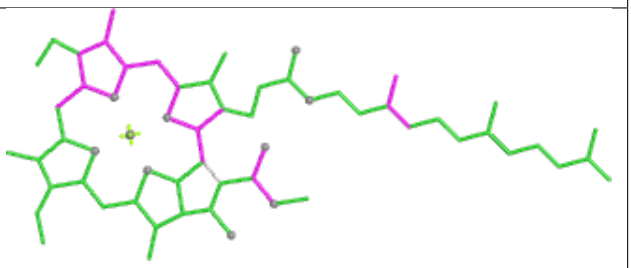
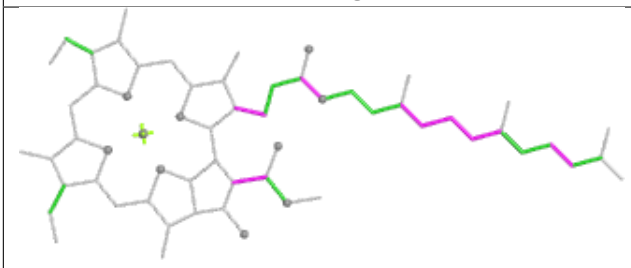
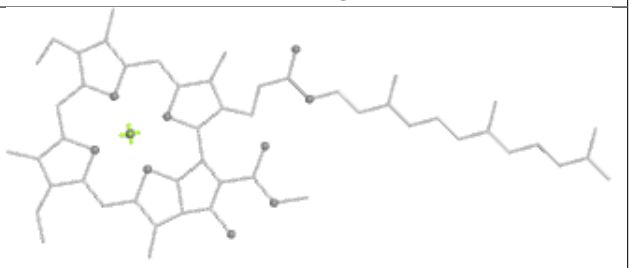
Bond angles

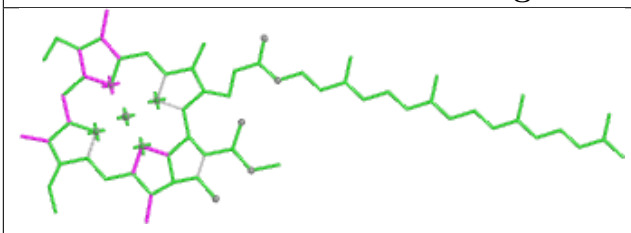
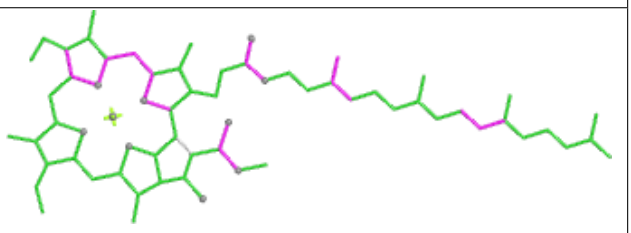
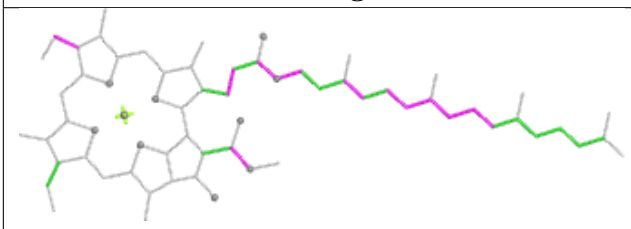
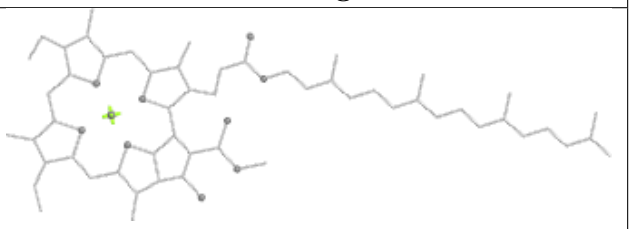


Torsions

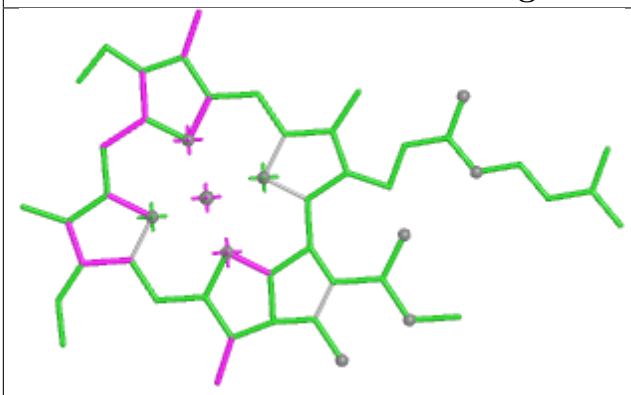


Rings

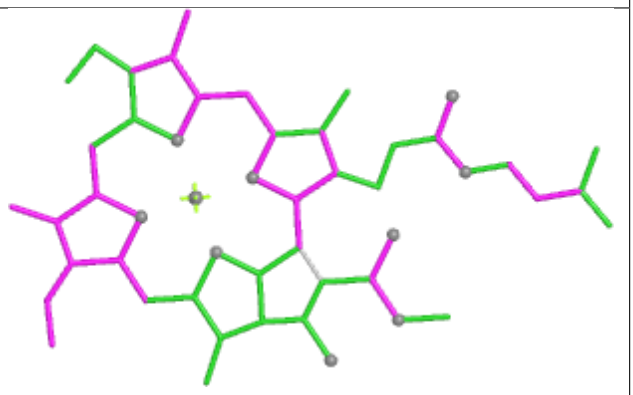
Ligand CLA bB 819	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA bA 841	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

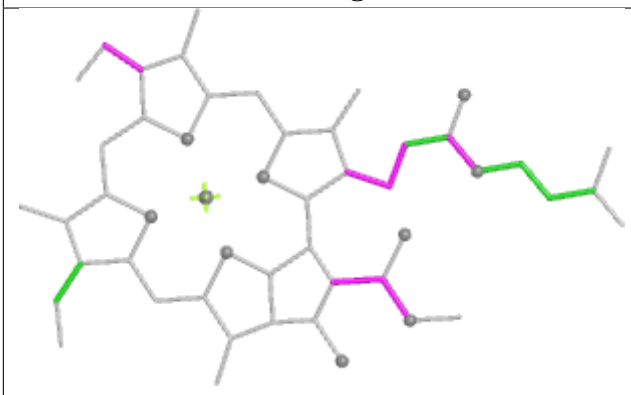
Ligand CLA b3 416



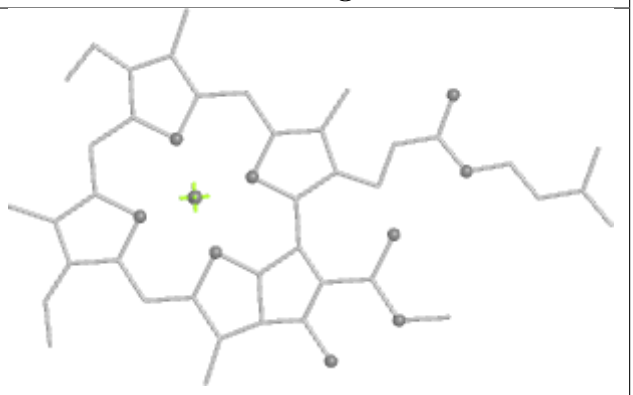
Bond lengths



Bond angles



Torsions

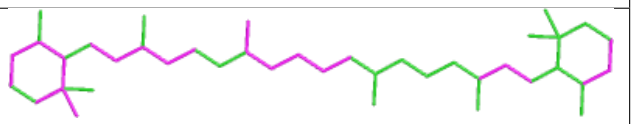


Rings

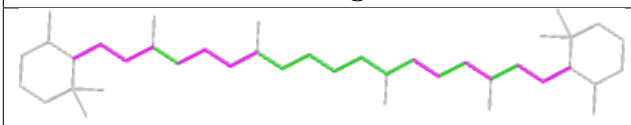
Ligand BCR c2 401



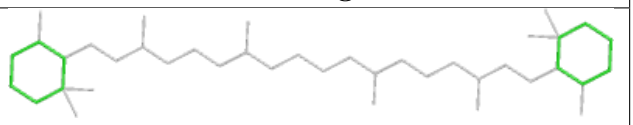
Bond lengths



Bond angles

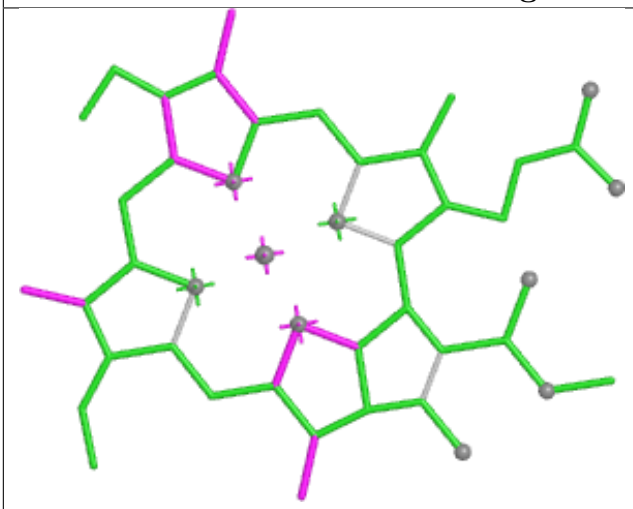


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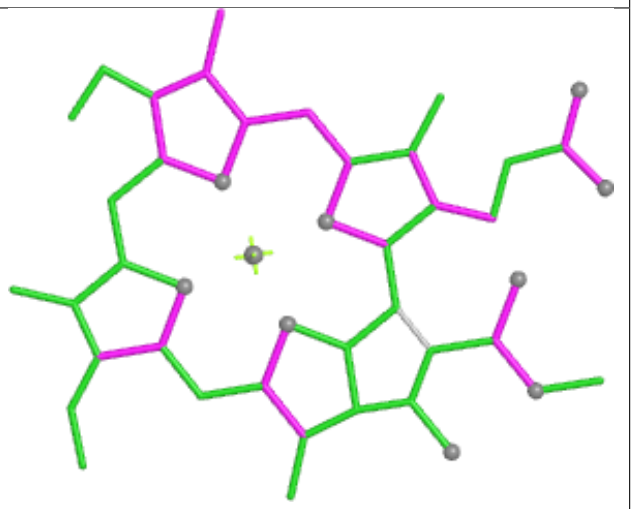


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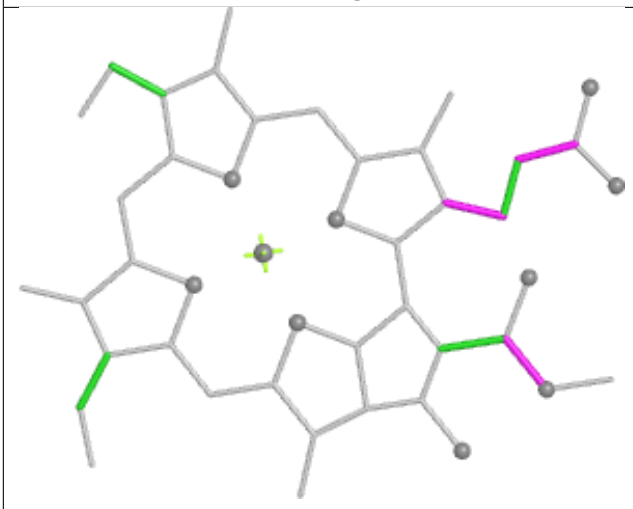
Ligand CLA a3 408



Bond lengths



Bond angles

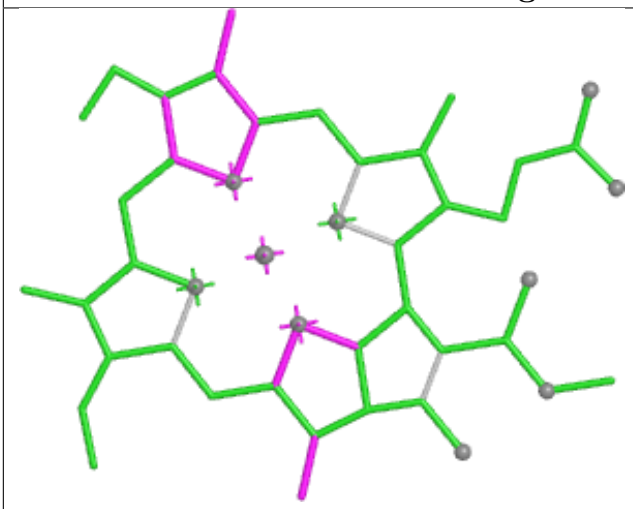


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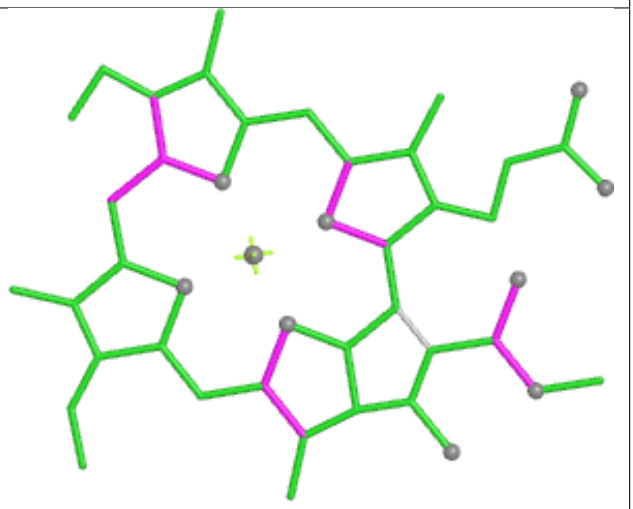


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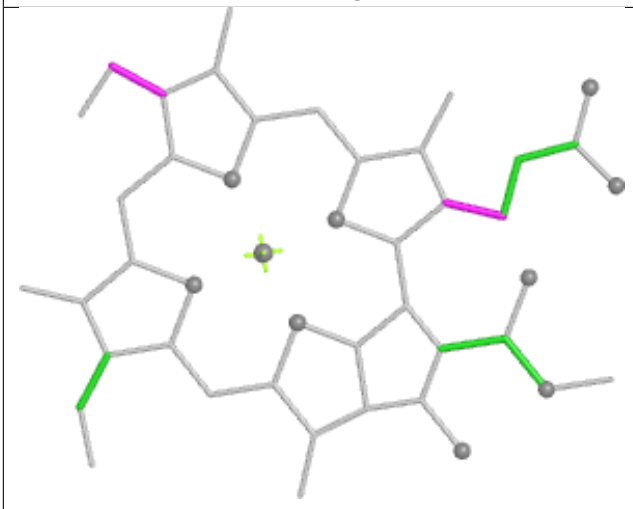
Ligand CLA b3 413



Bond lengths



Bond angles

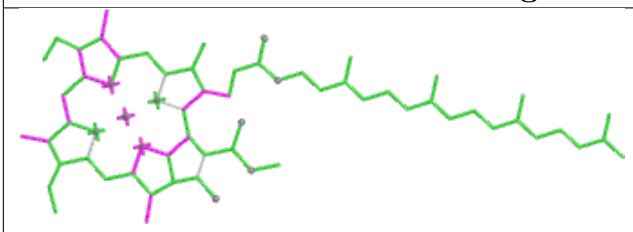


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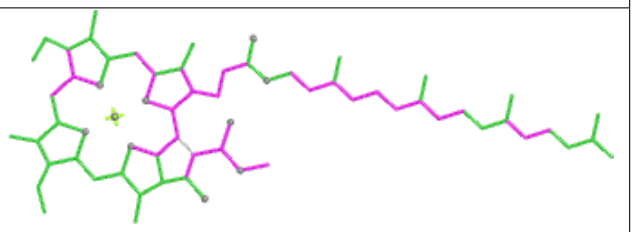


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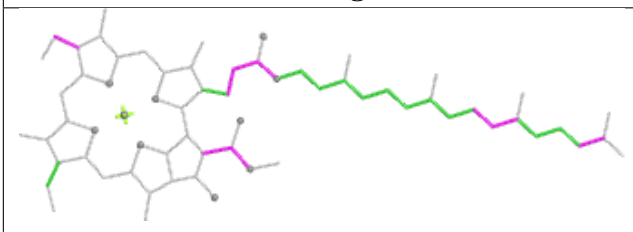
Ligand CLA c6 401



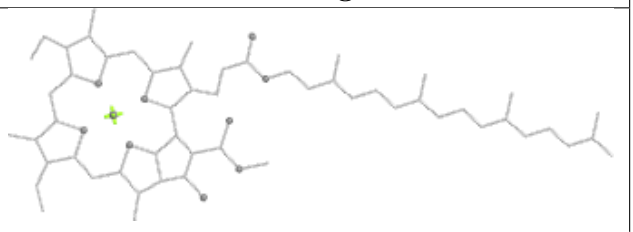
Bond lengths



Bond angles

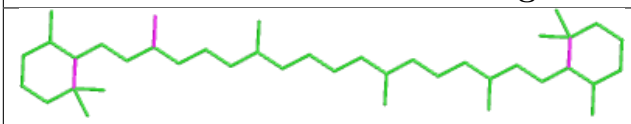


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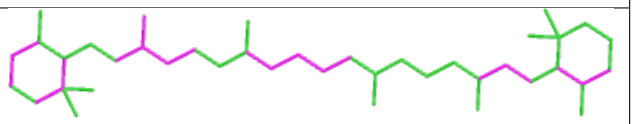


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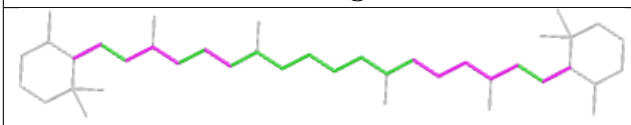
Ligand BCR c1 401



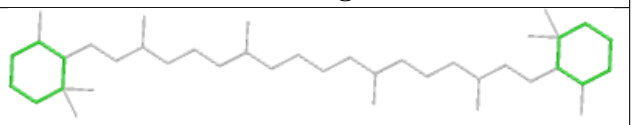
Bond lengths



Bond angles

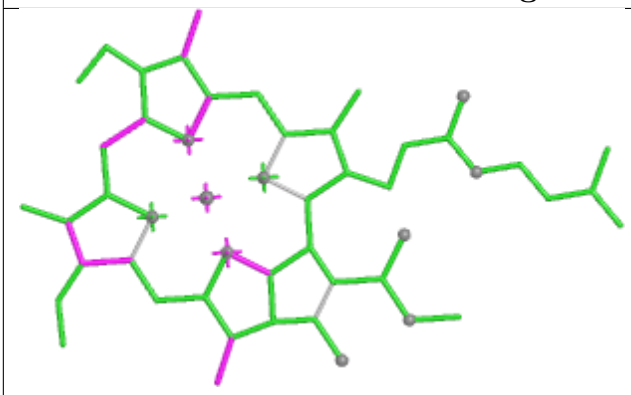


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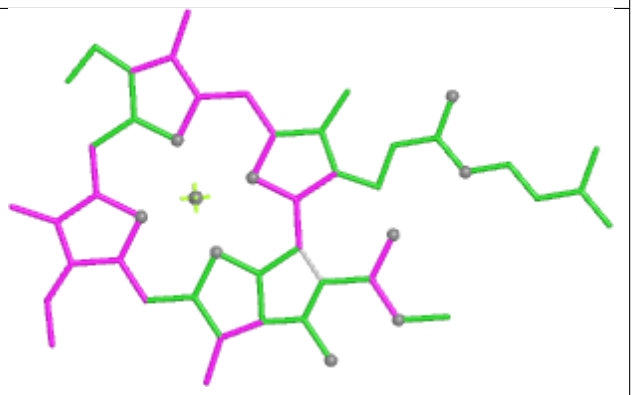


Rings

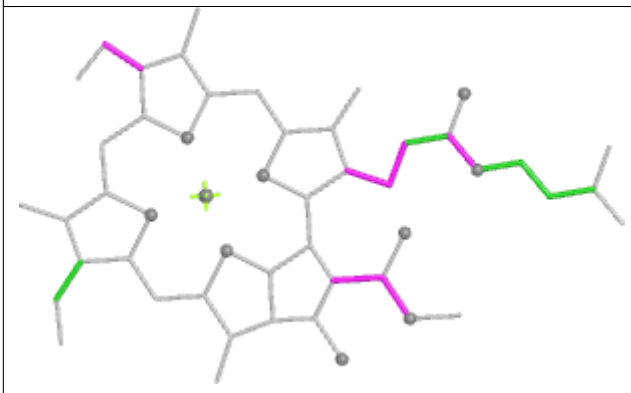
Ligand CLA a4 416



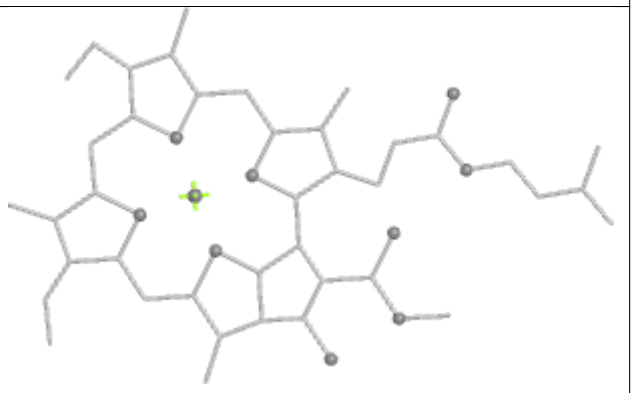
Bond lengths



Bond angles

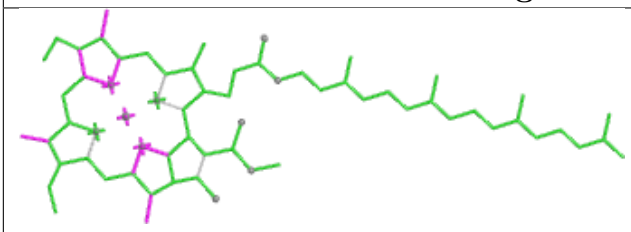


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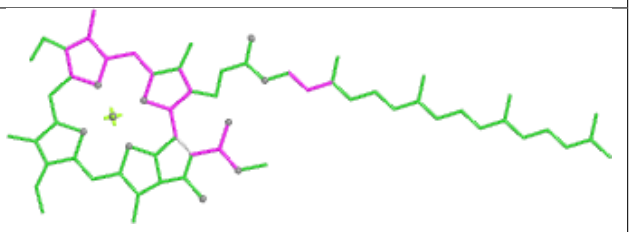


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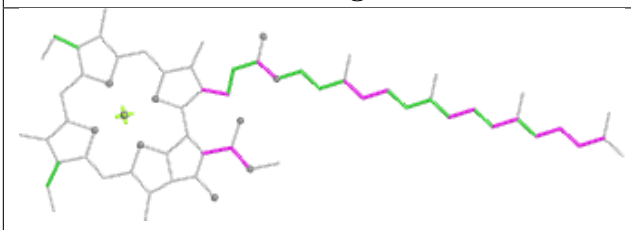
Ligand CLA cA 820



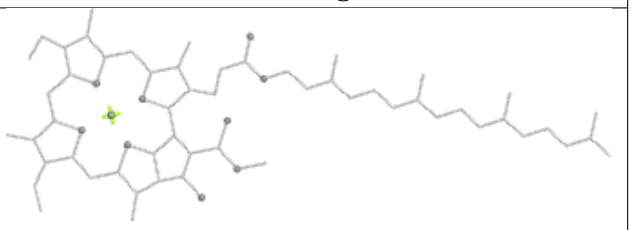
Bond lengths



Bond angles

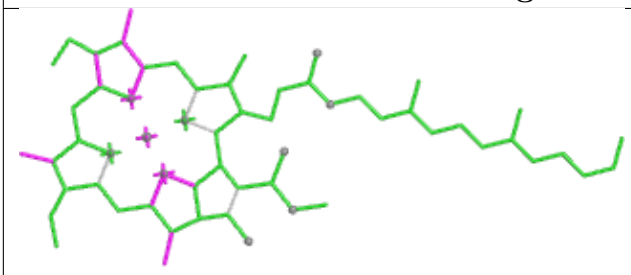


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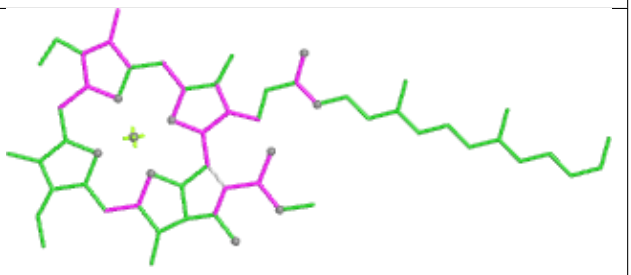


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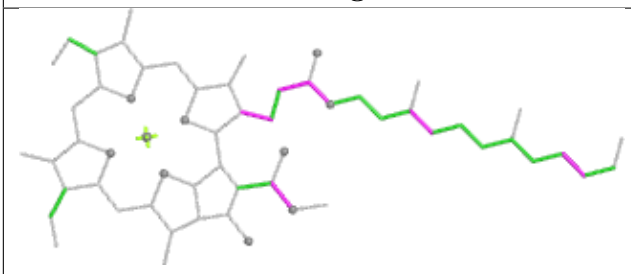
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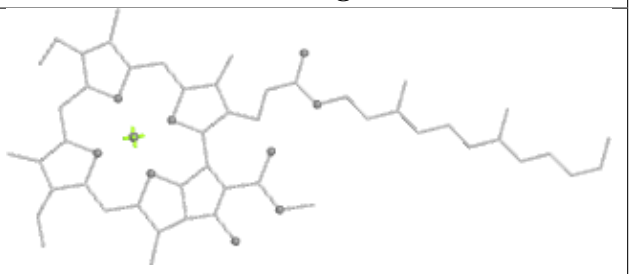
Bond lengths



Bond angles

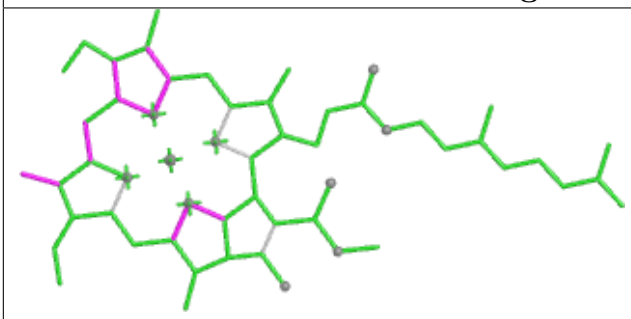


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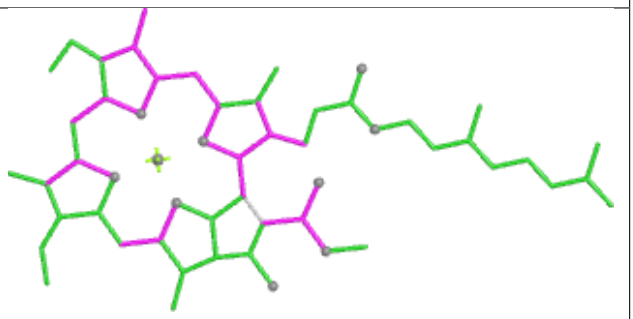


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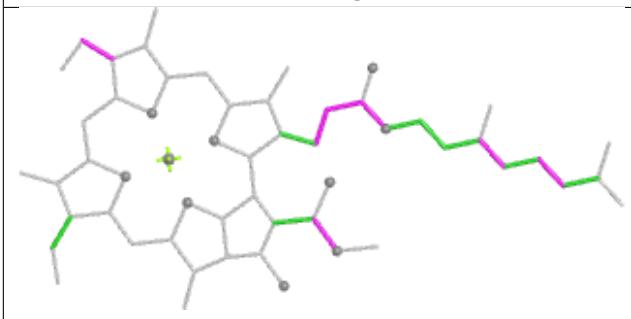
Ligand CLA c2 418



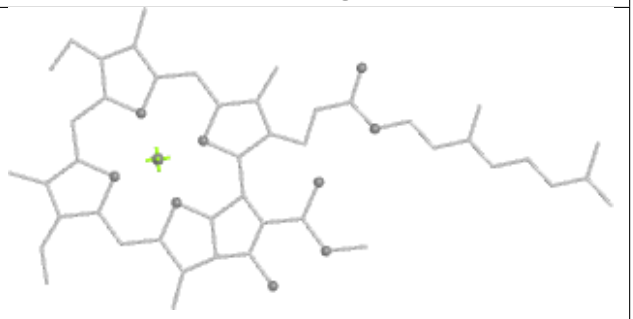
Bond lengths



Bond angles

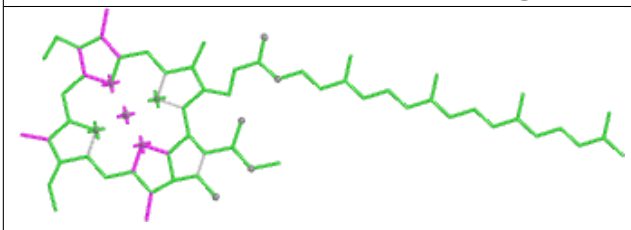


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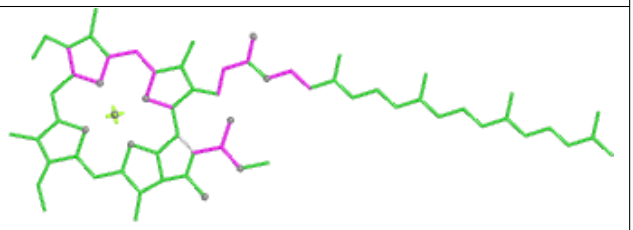


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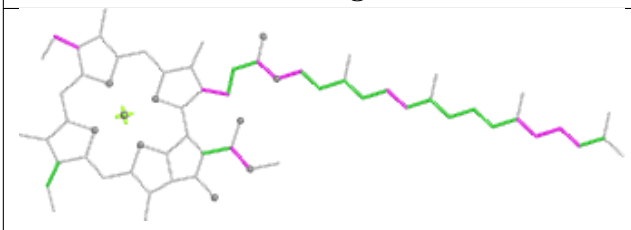
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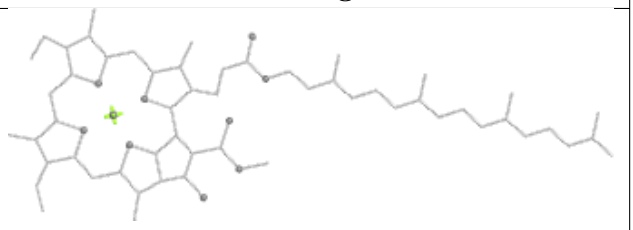
Bond lengths



Bond angles

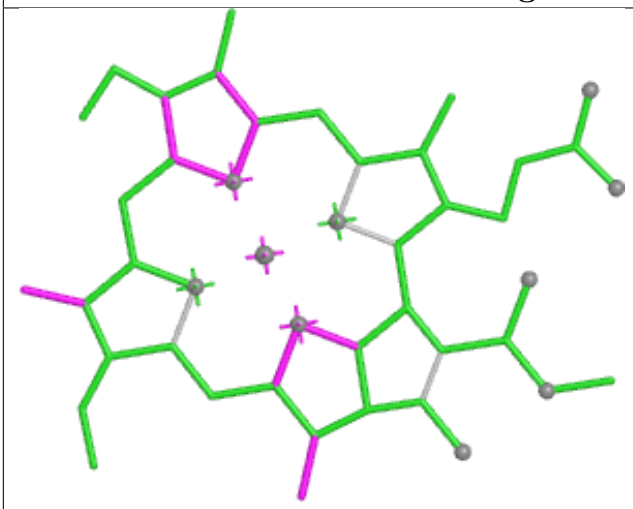


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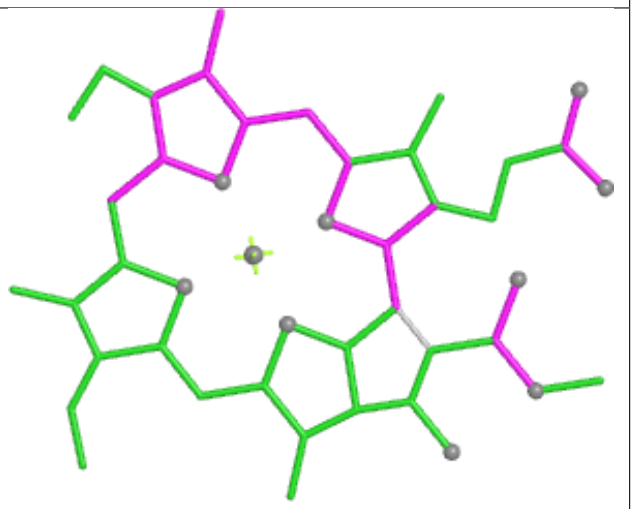


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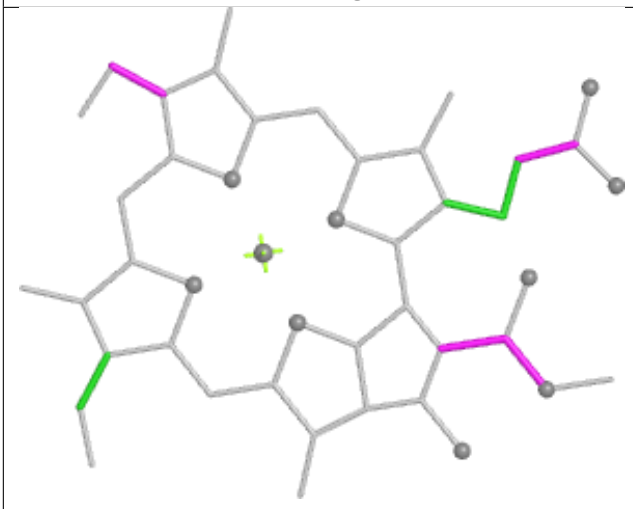
Ligand CLA b2 408



Bond lengths



Bond angles

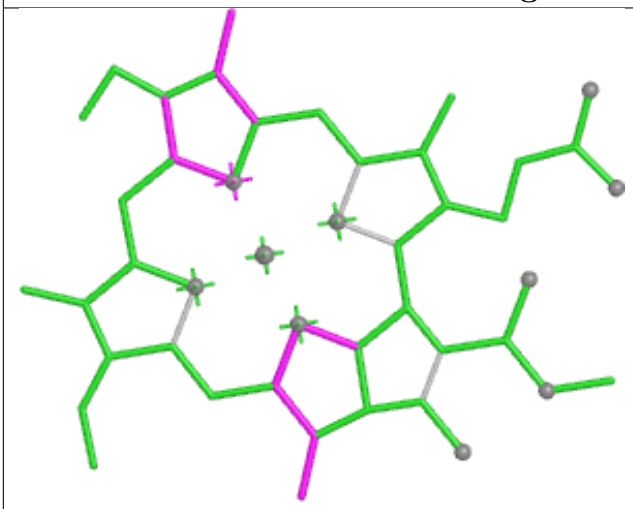


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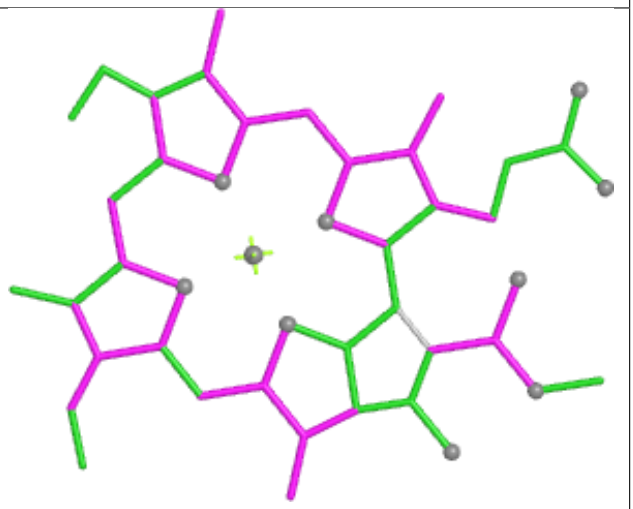


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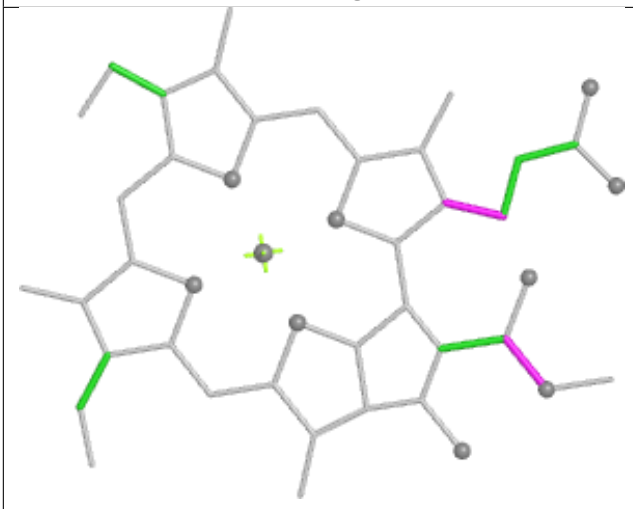
Ligand CLA c1 405



Bond lengths



Bond angles

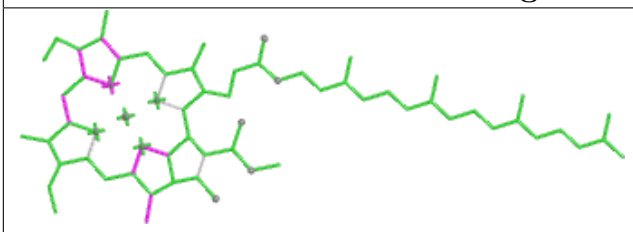


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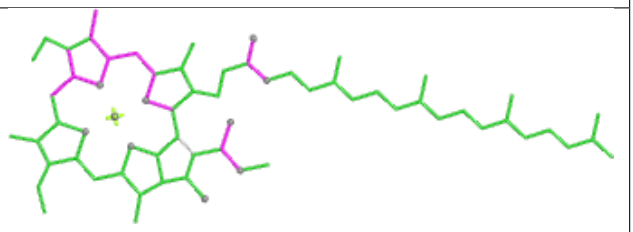


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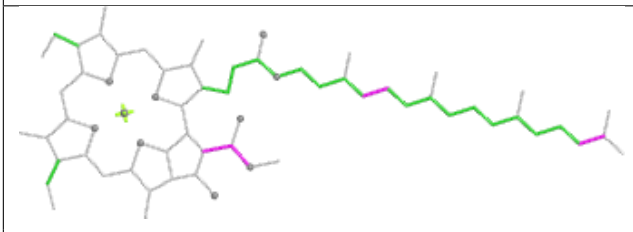
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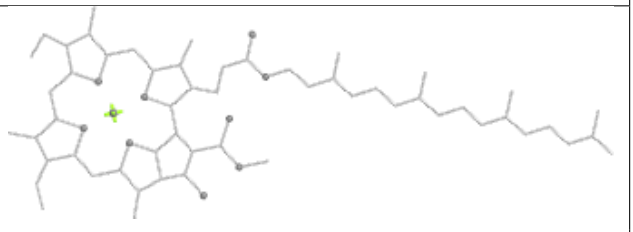
Bond lengths



Bond angles

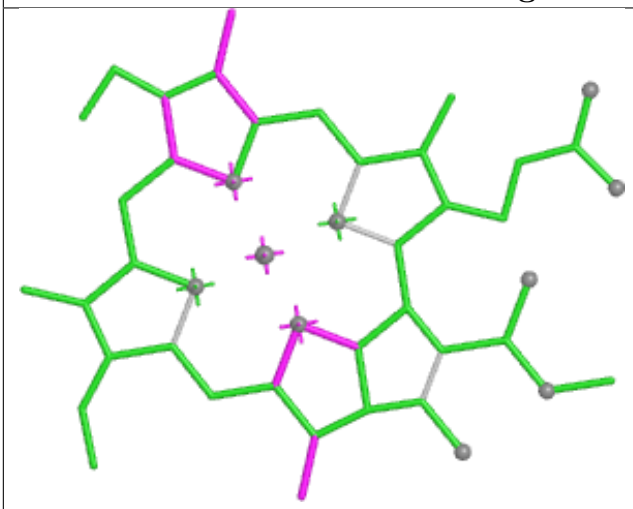


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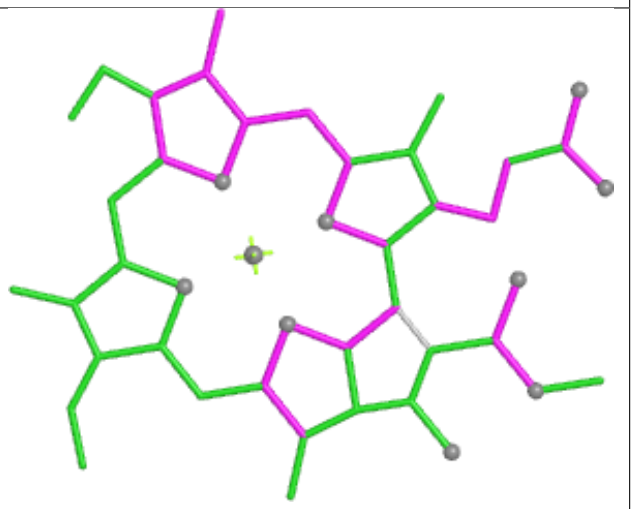


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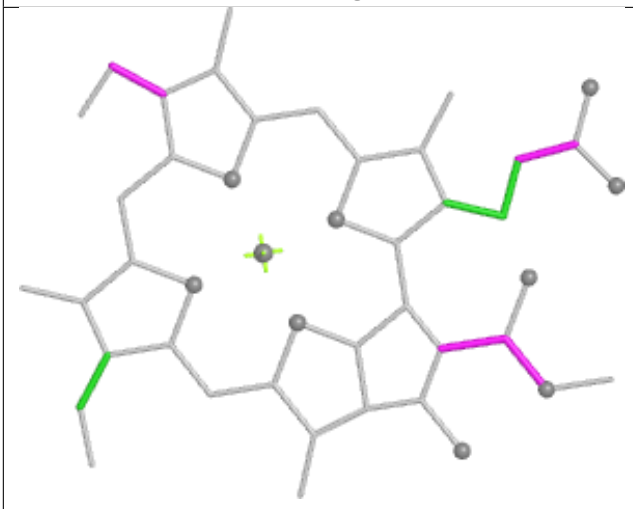
Ligand CLA b6 416



Bond lengths



Bond angles

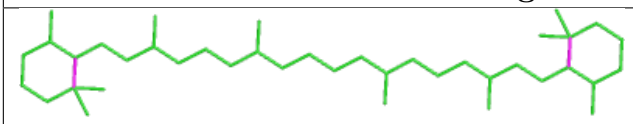


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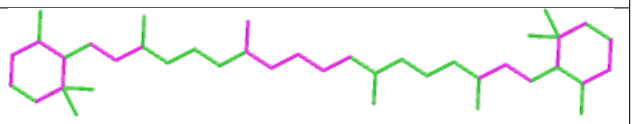


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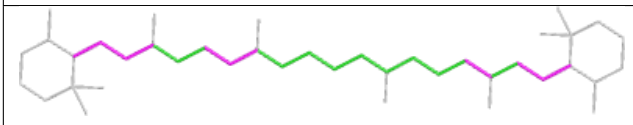
Ligand BCR a6 420



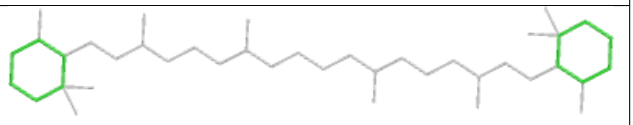
Bond lengths



Bond angles

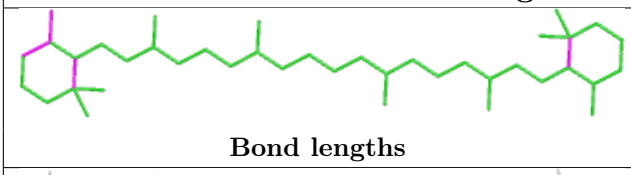


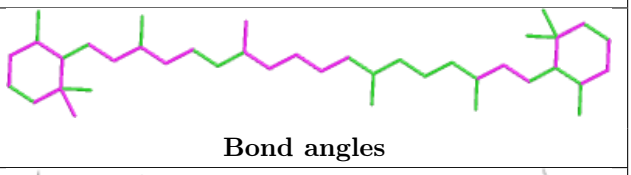
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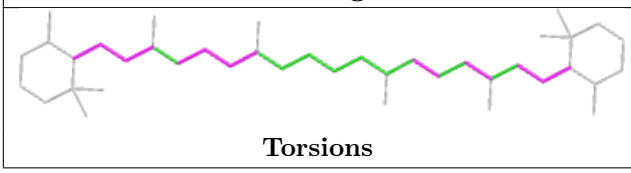


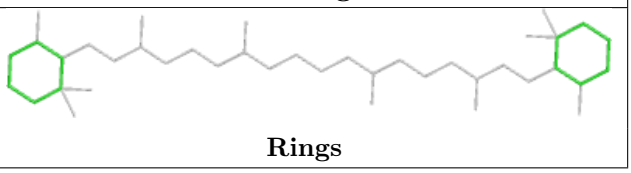
Rings

Ligand BCR b2 401

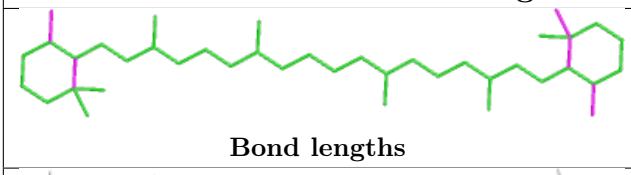

Bond lengths

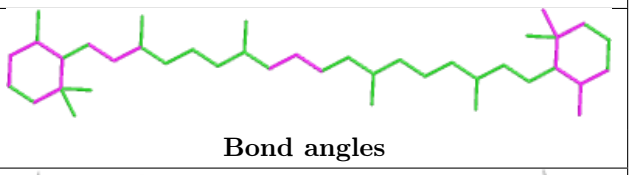

Bond angles

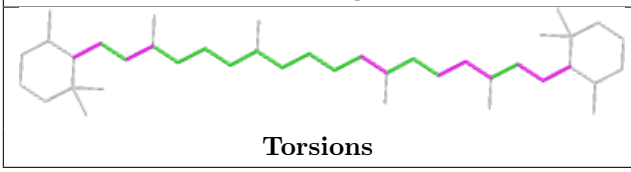

Torsions

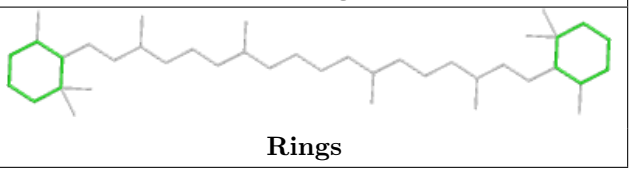

Rings

Ligand BCR b3 418

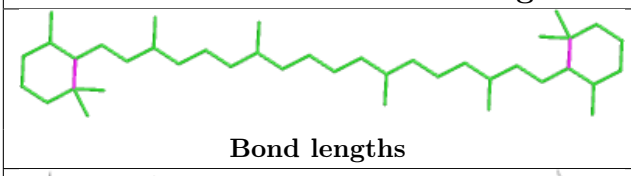

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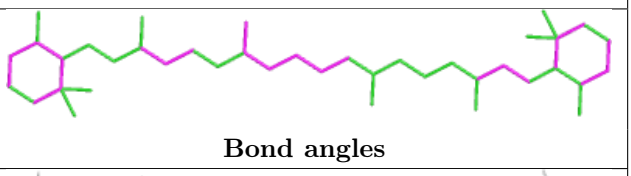

Bond angles

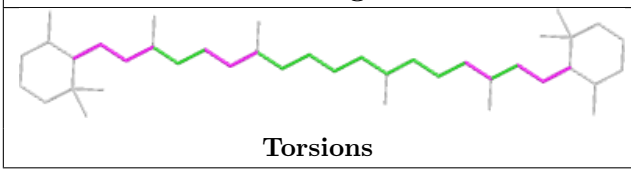

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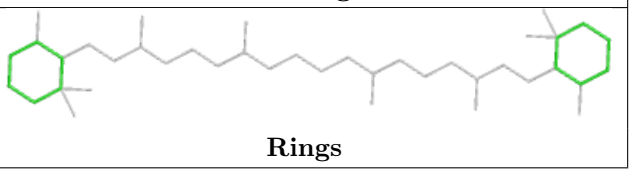

Rings

Ligand BCR b4 420

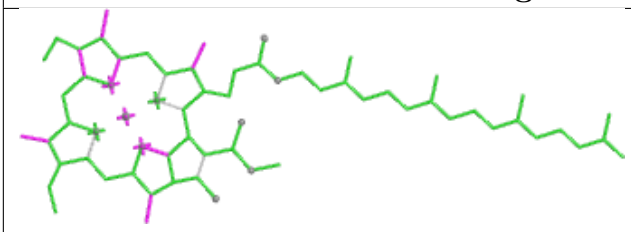

Bond lengths

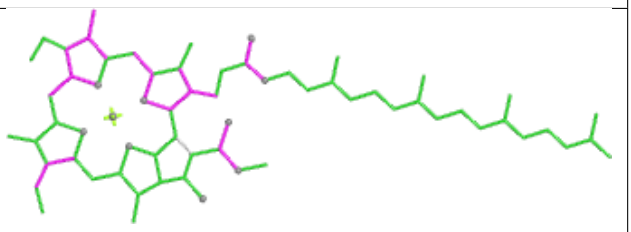

Bond angles

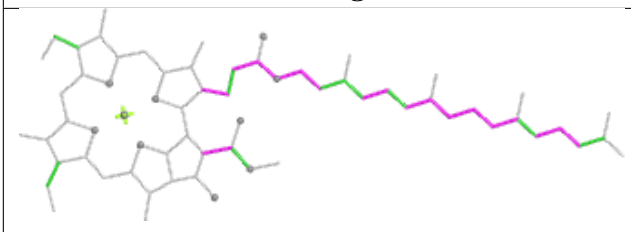

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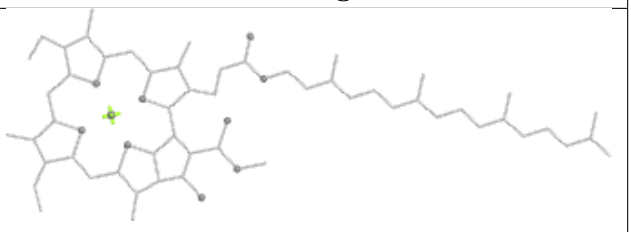

Rings

Ligand CLA aA 806

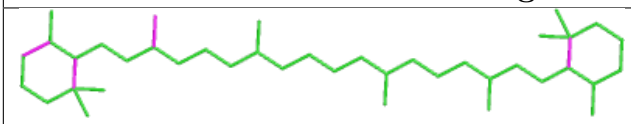

Bond lengths


Bond angles

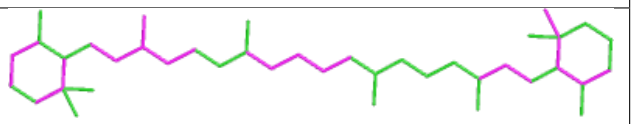

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Rings

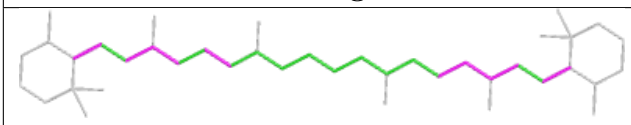
Ligand BCR a6 401



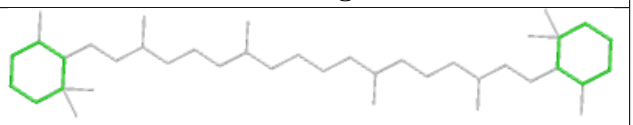
Bond lengths



Bond angles

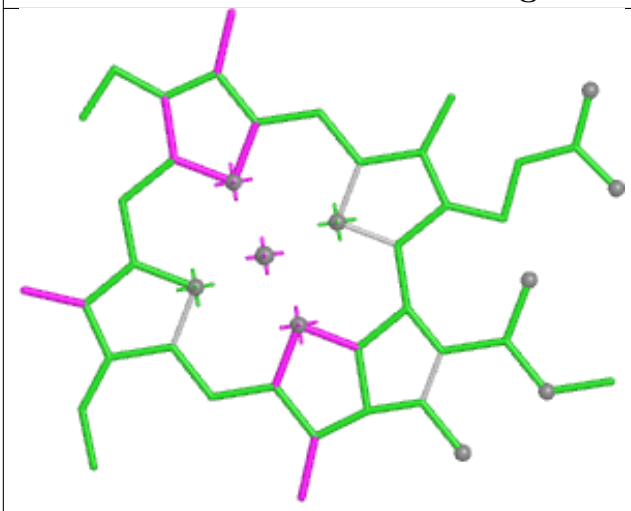


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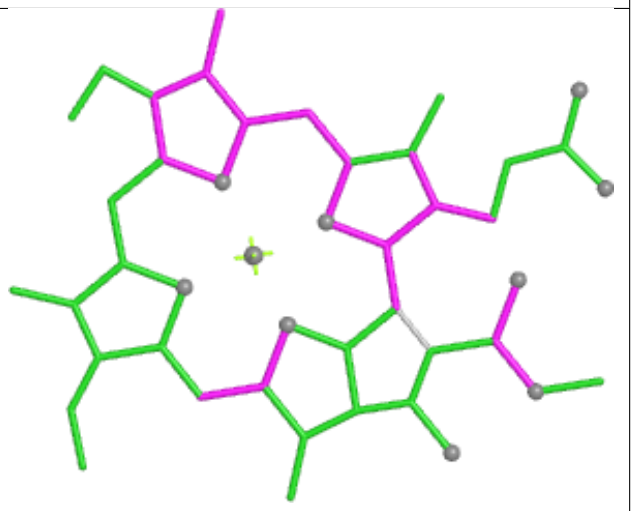


Rings

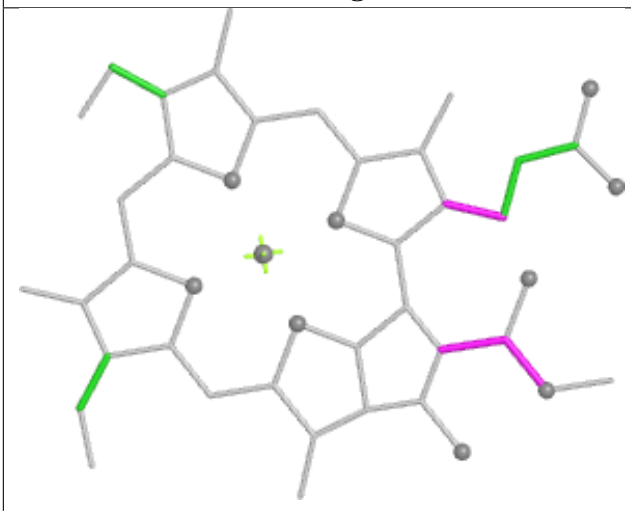
Ligand CLA a3 411



Bond lengths



Bond angles

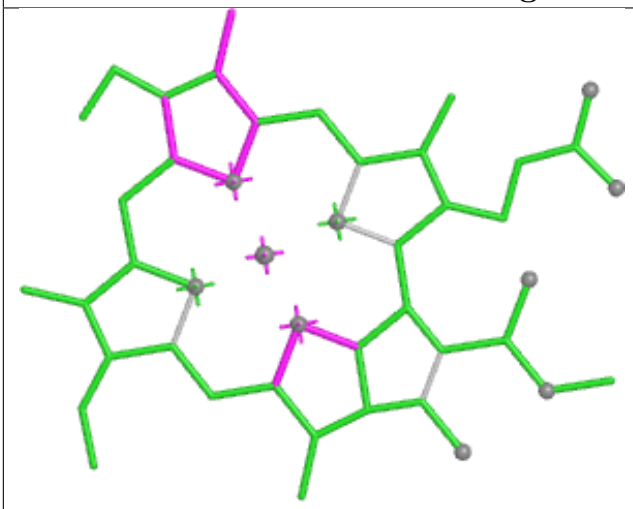


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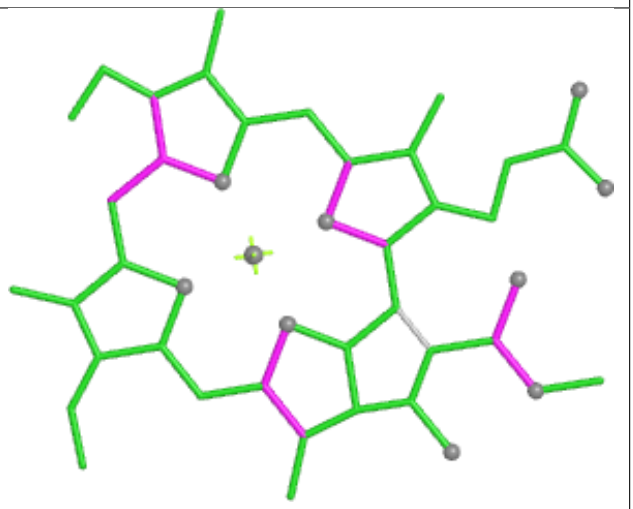


Rings

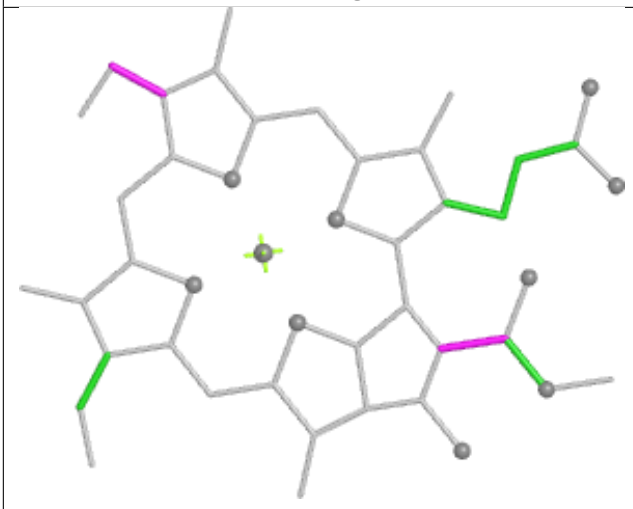
Ligand CLA a2 414



Bond lengths



Bond angles

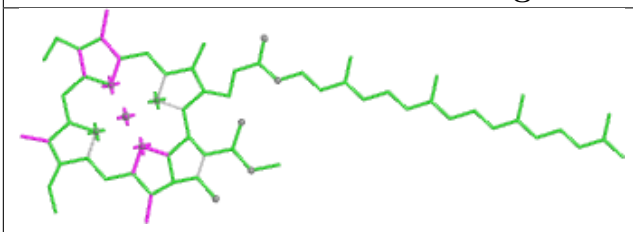


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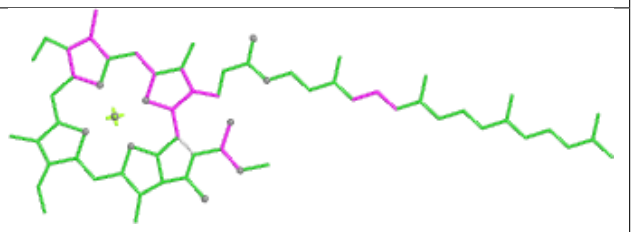


Rings

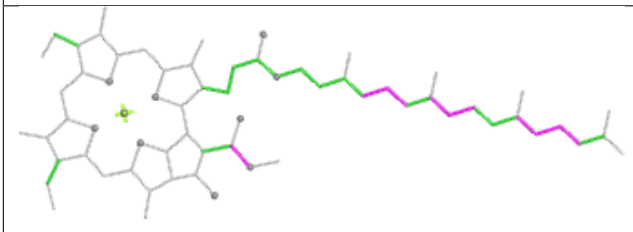
Ligand CLA bA 826



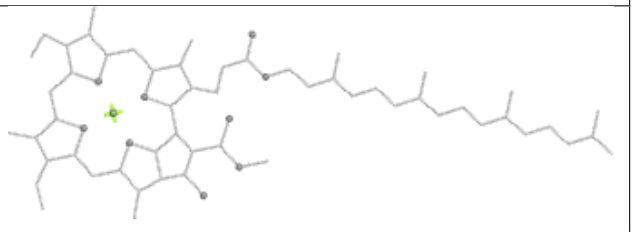
Bond lengths



Bond angles

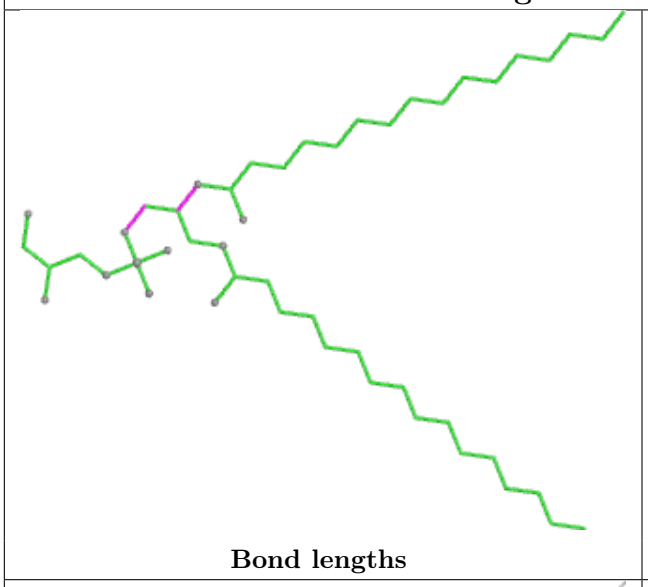


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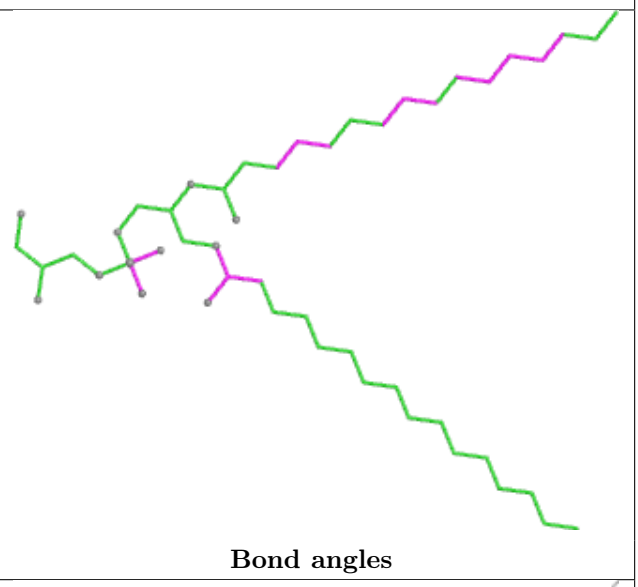


Rings

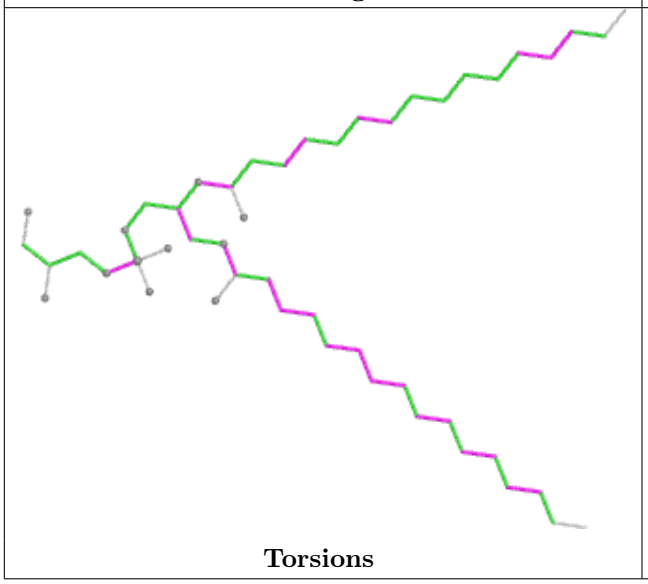
Ligand LHG aA 853



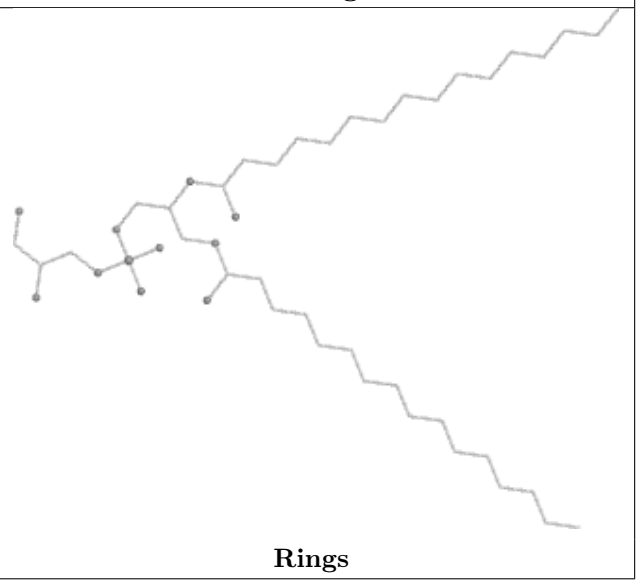
Bond lengths



Bond angles

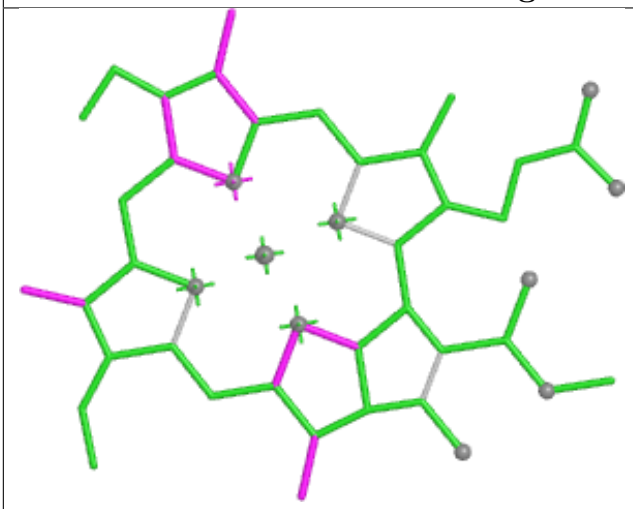


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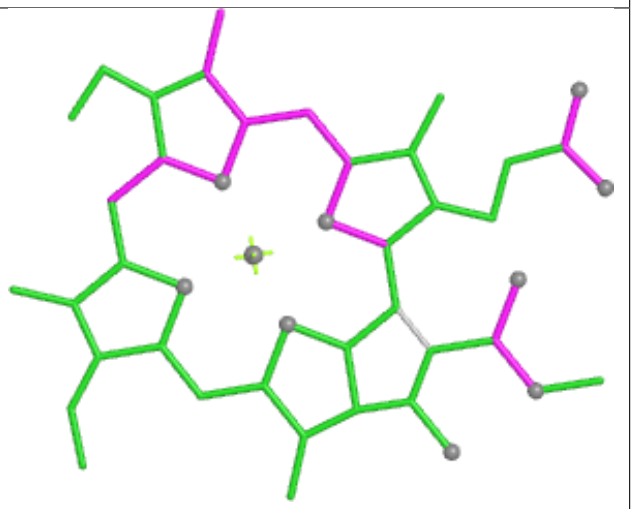


Rings

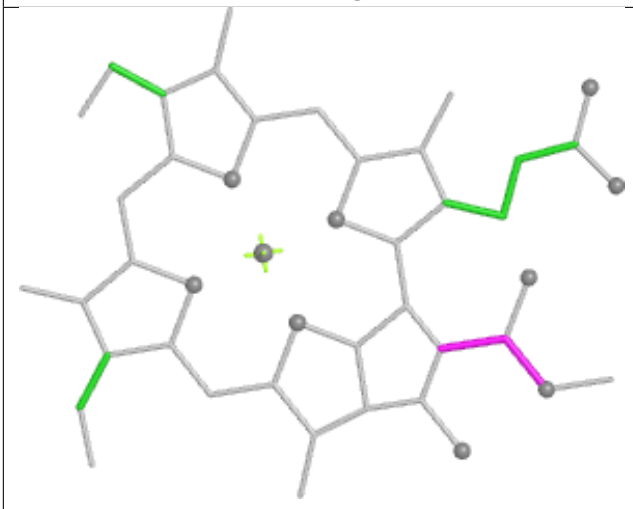
Ligand CLA b3 406



Bond lengths



Bond angles

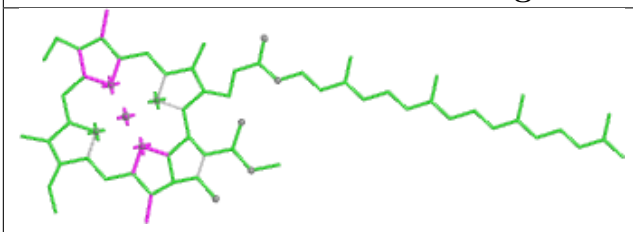


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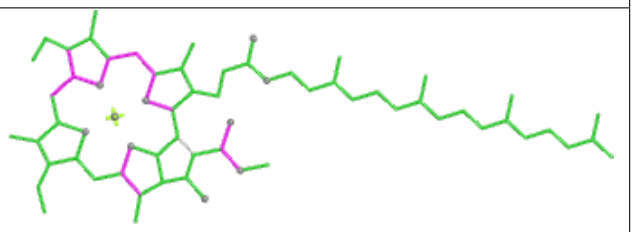


Rings

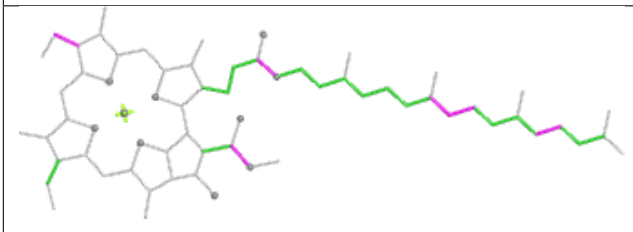
Ligand CLA bB 820



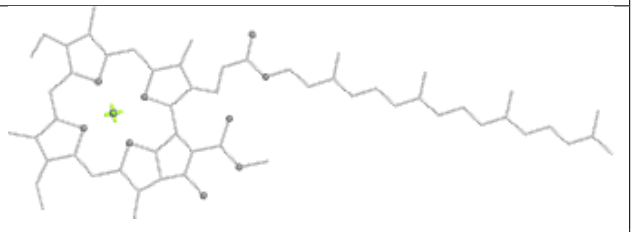
Bond lengths



Bond angles

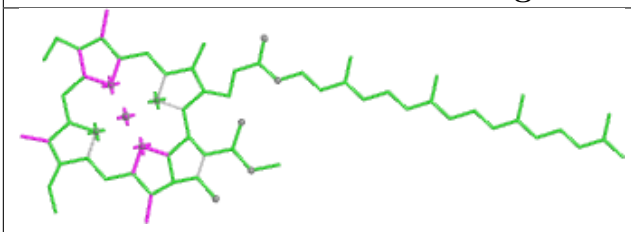


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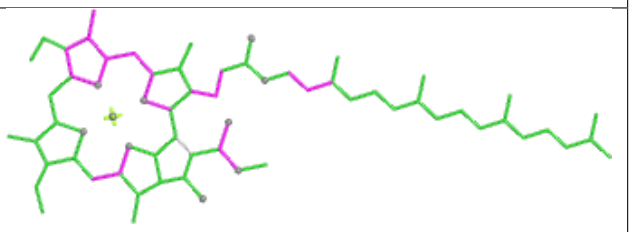


Rings

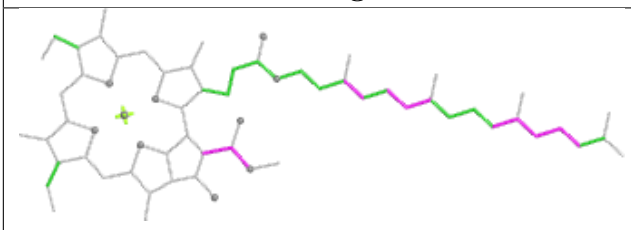
Ligand CLA bB 837



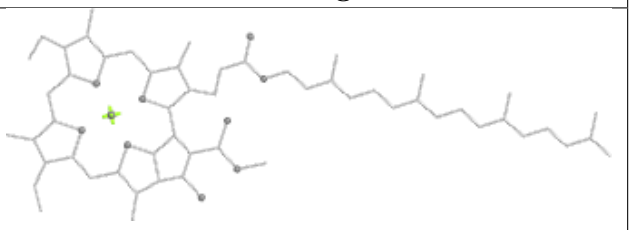
Bond lengths



Bond angles

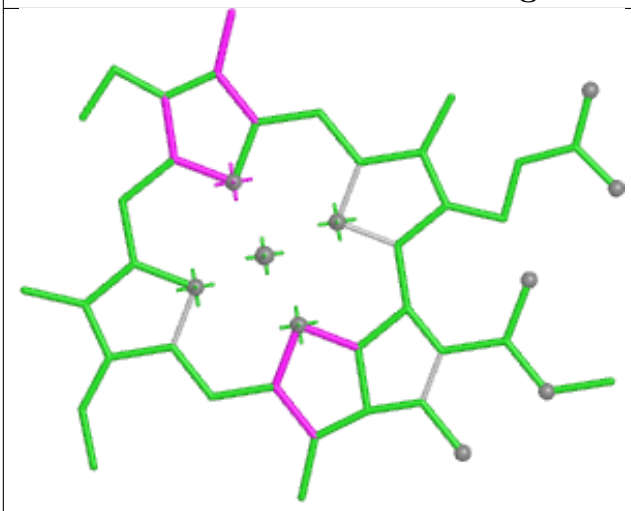


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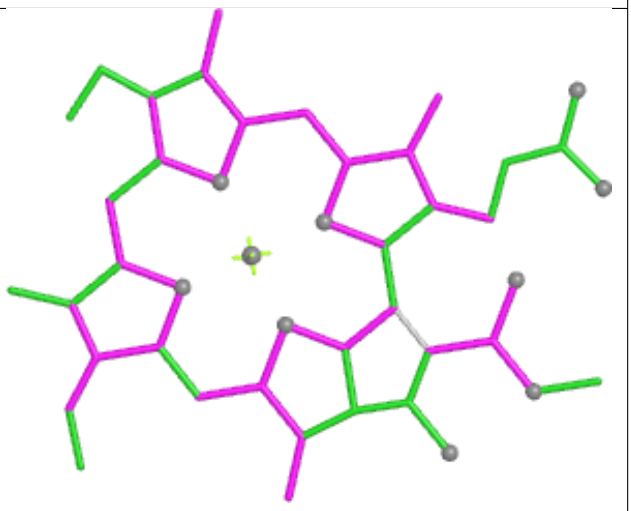


Rings

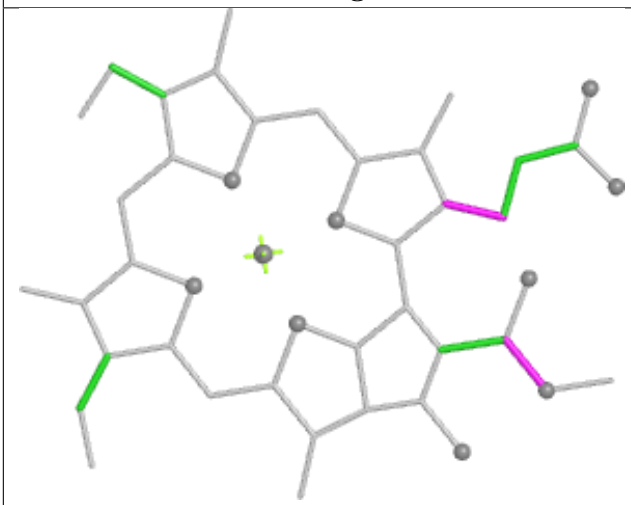
Ligand CLA a6 406



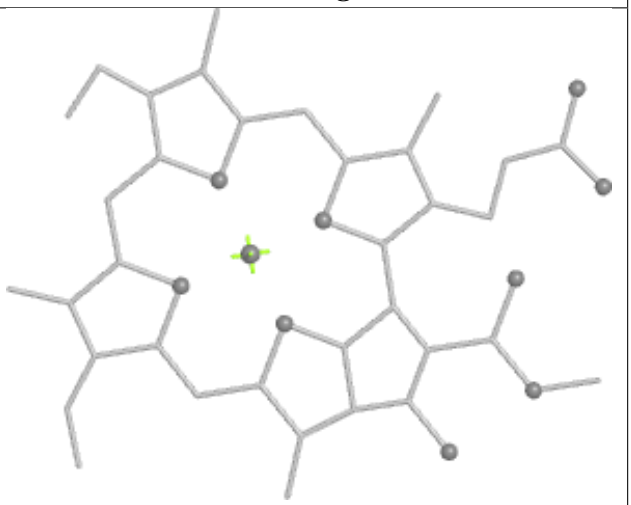
Bond lengths



Bond angles

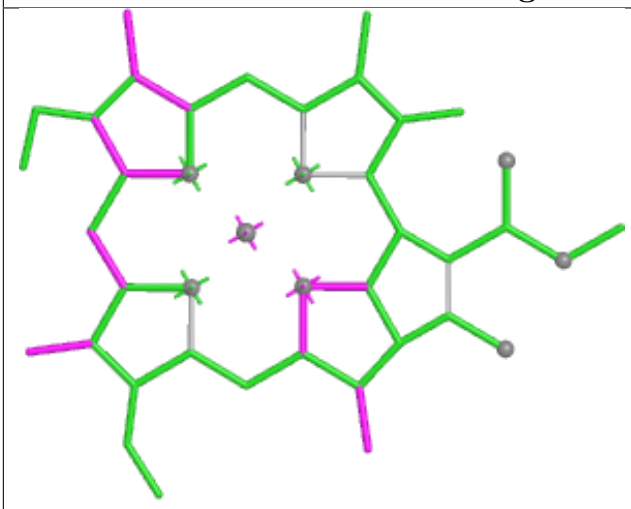


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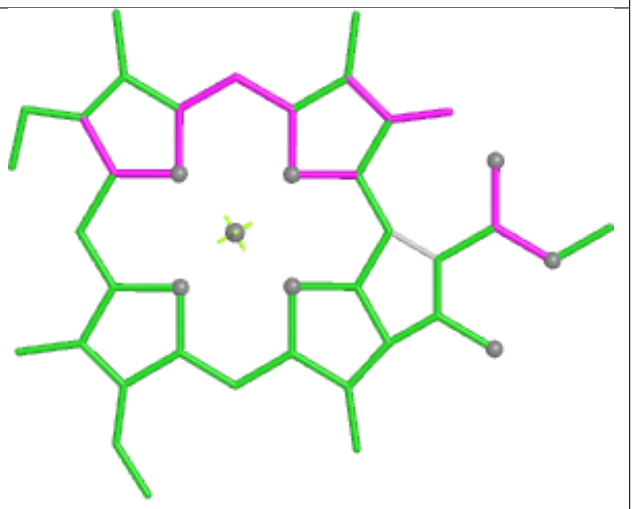


Rings

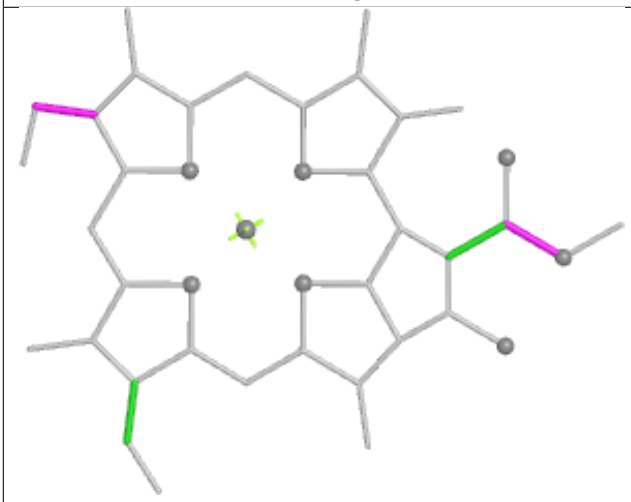
Ligand CLA b3 414



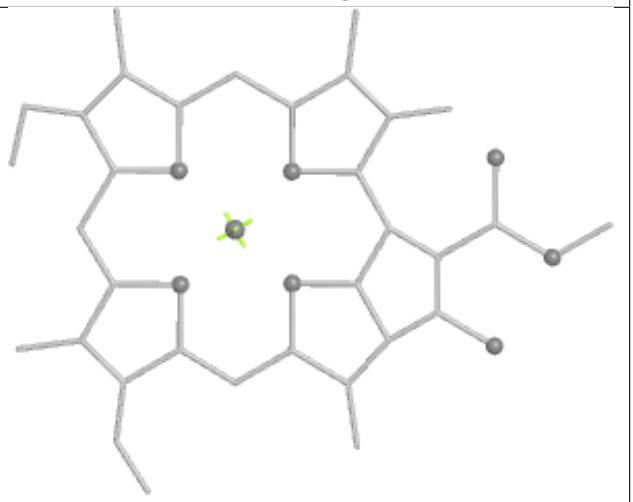
Bond lengths



Bond angles

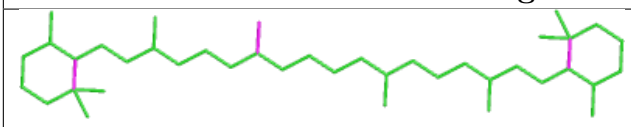


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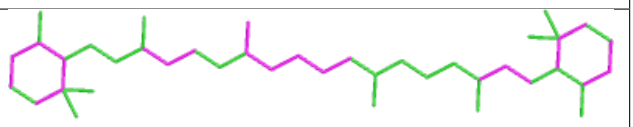


Rings

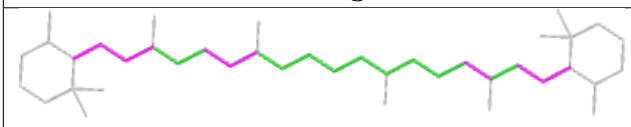
Ligand BCR a1 419



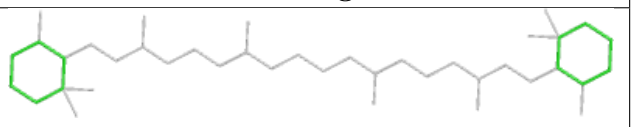
Bond lengths



Bond angles

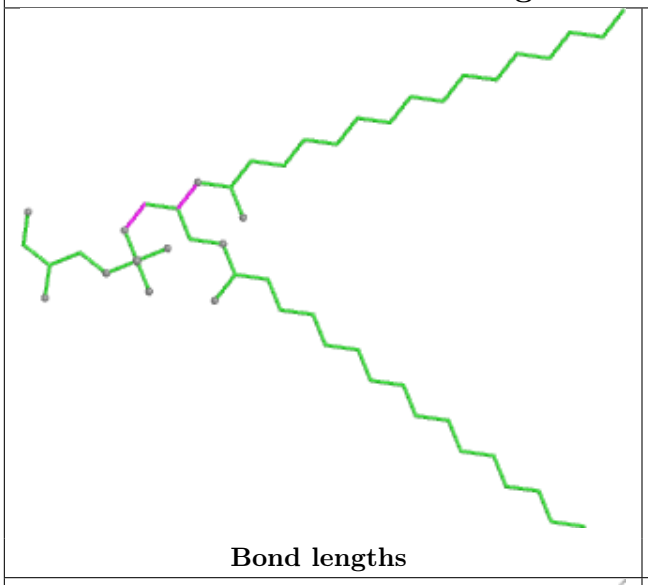


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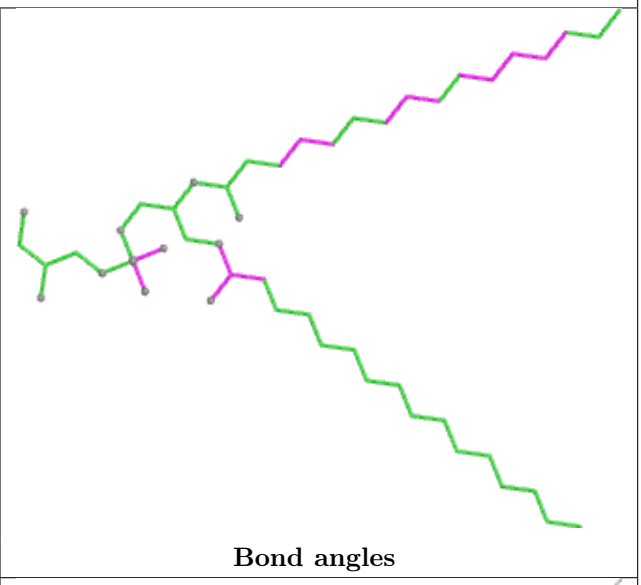


Rings

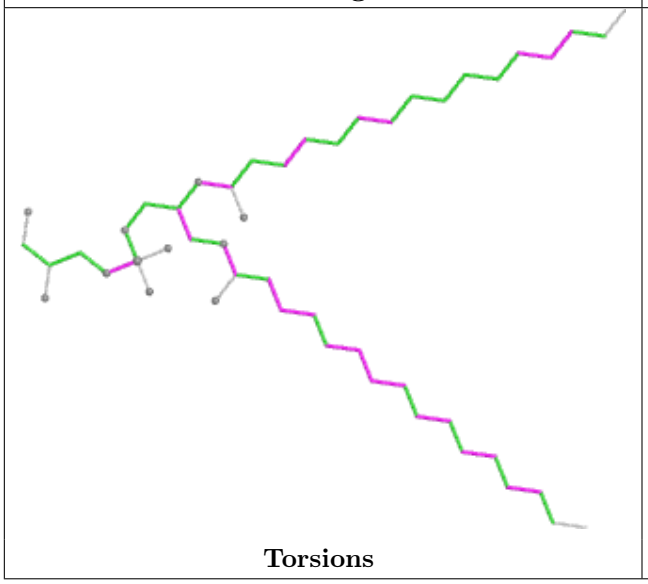
Ligand LHG cA 852



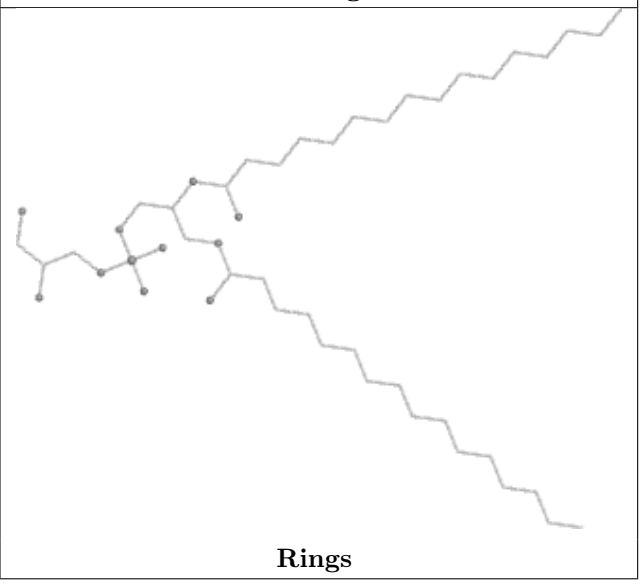
Bond lengths



Bond angles



Torsions

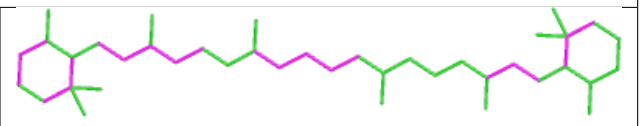


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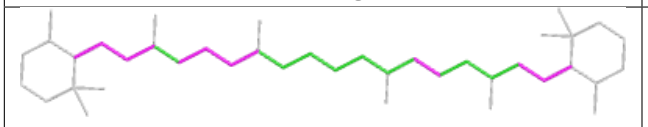
Ligand BCR a3 401



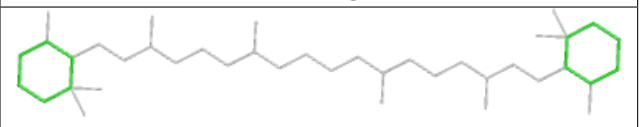
Bond lengths



Bond angles

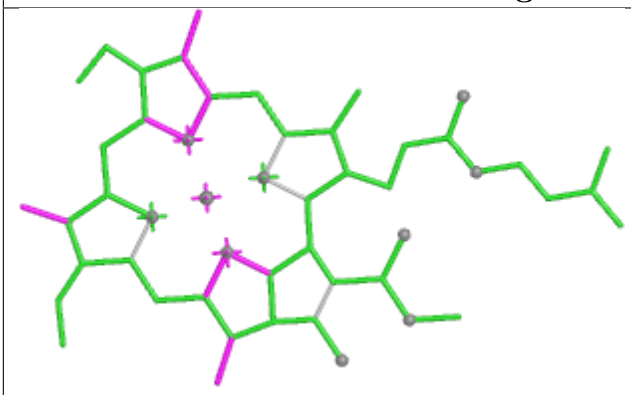


Torsions

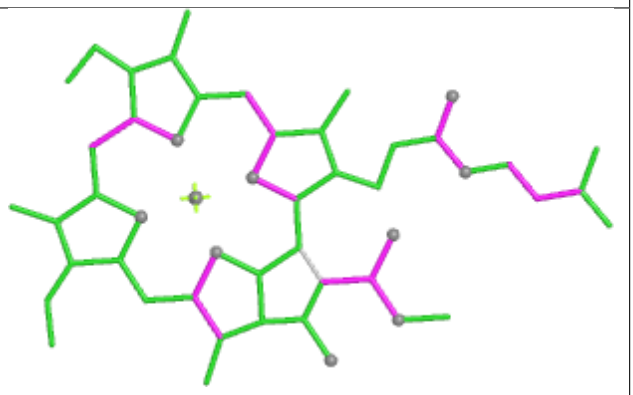


Rings

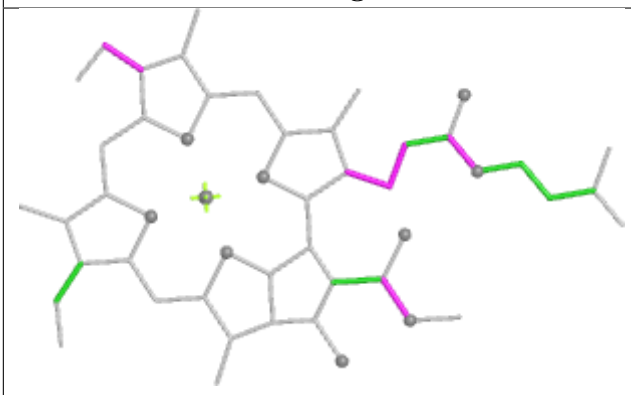
Ligand CLA cA 832



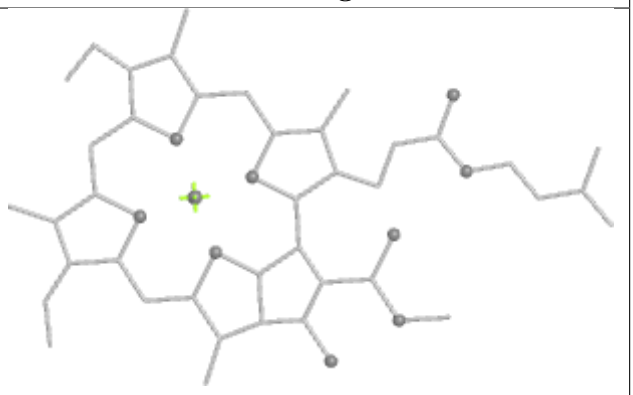
Bond lengths



Bond angles

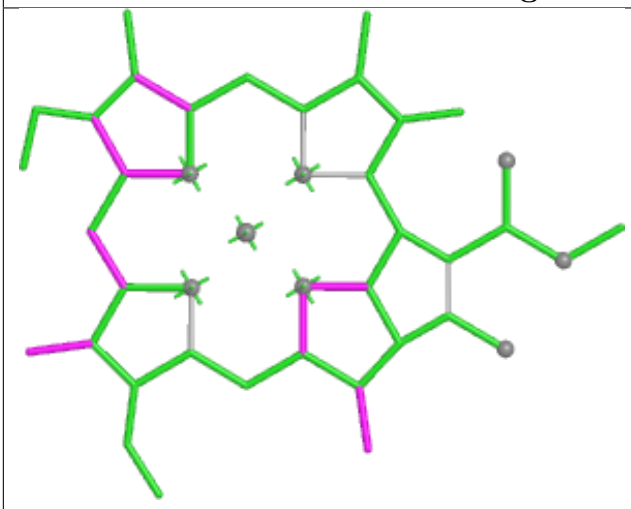


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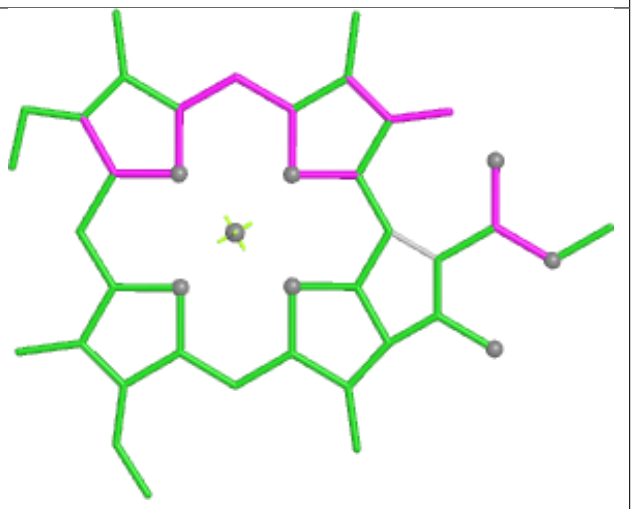


Rings

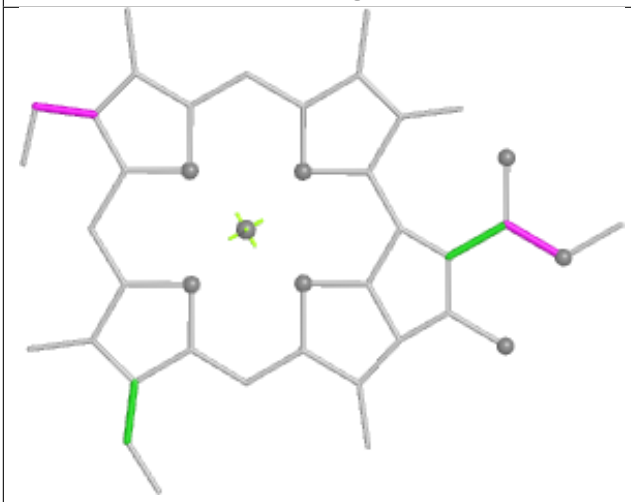
Ligand CLA c6 416



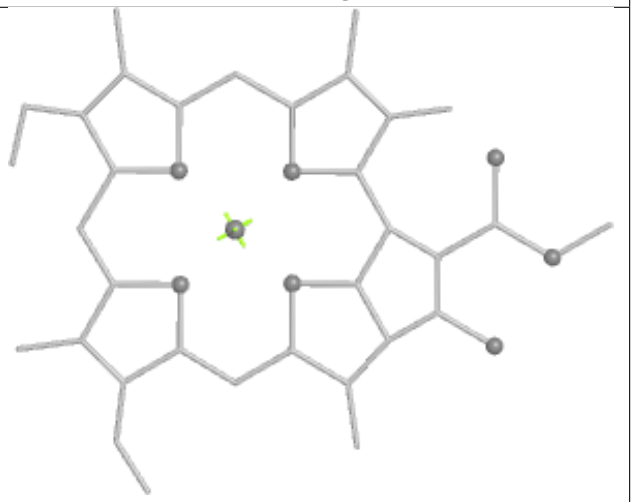
Bond lengths



Bond angles

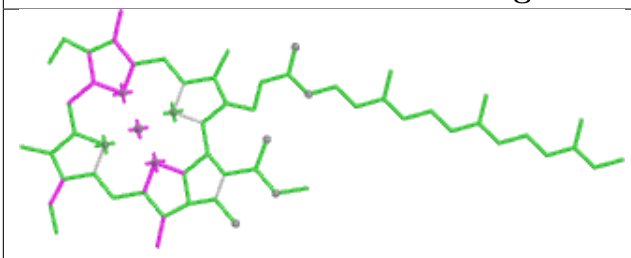


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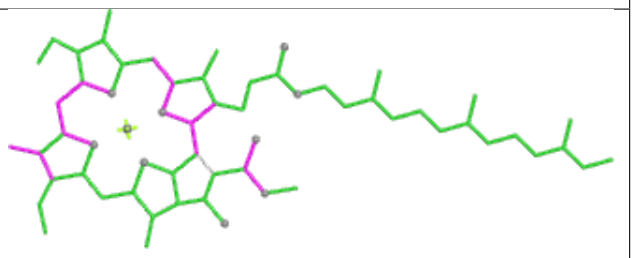


Rings

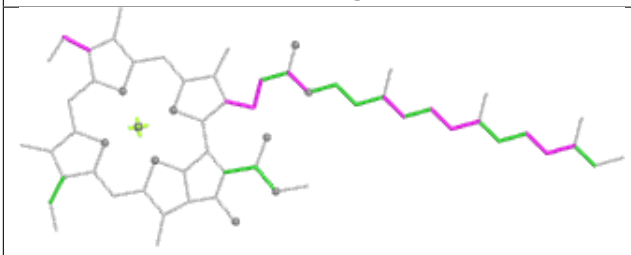
Ligand CLA bA 821



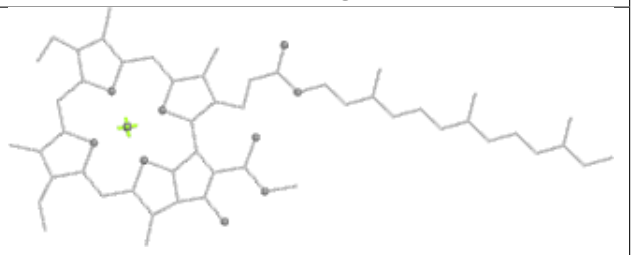
Bond lengths



Bond angles

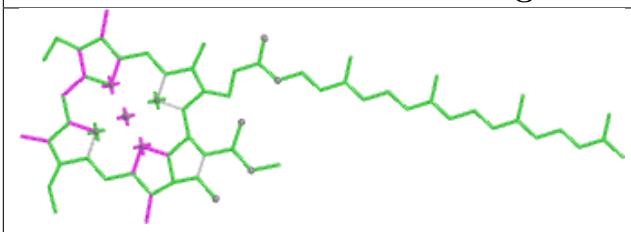


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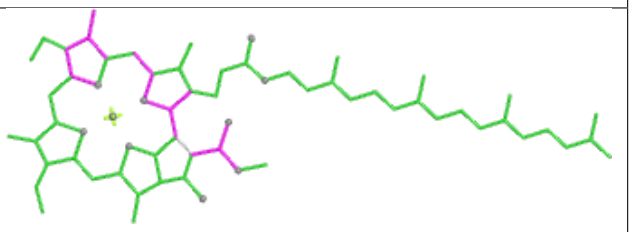


Rings

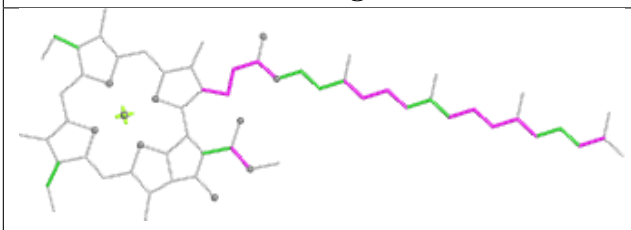
Ligand CLA aB 828



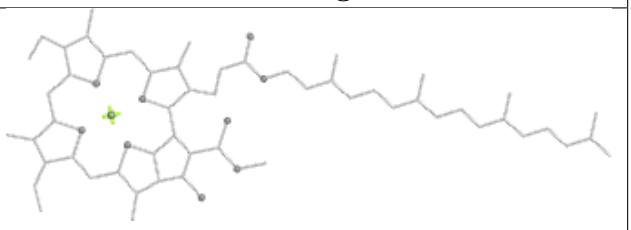
Bond lengths



Bond angles

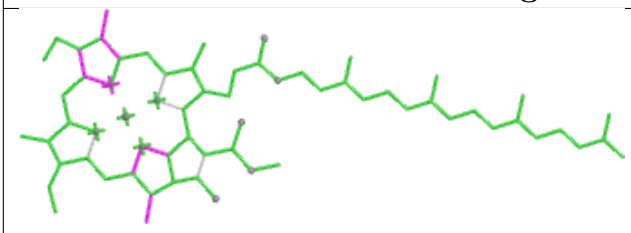


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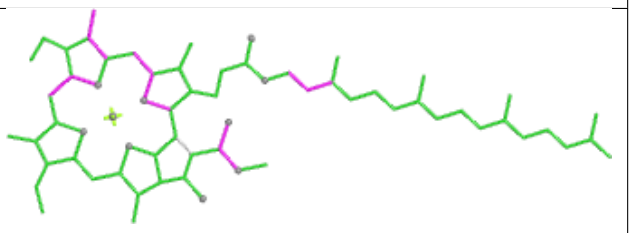


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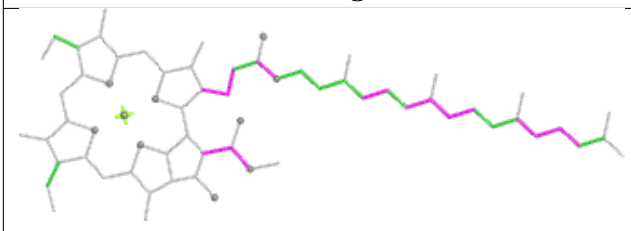
Ligand CLA c2 402



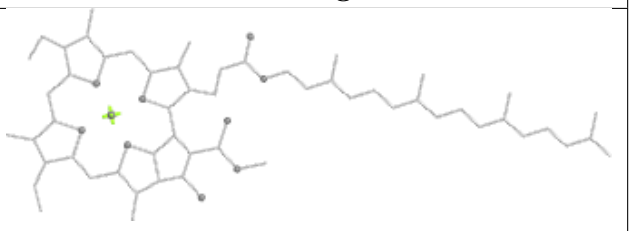
Bond lengths



Bond angles

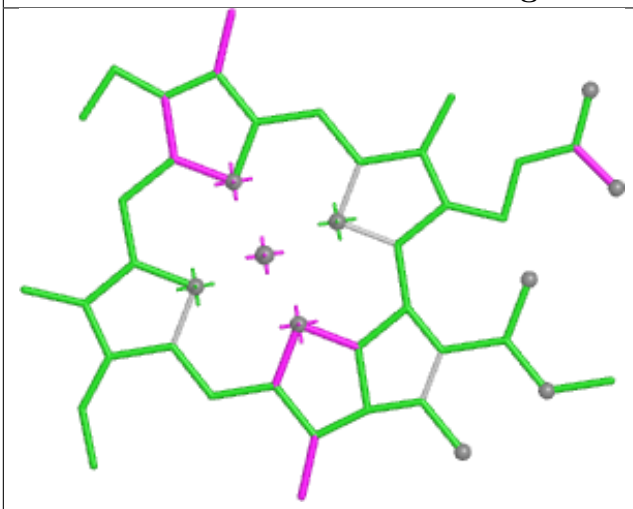


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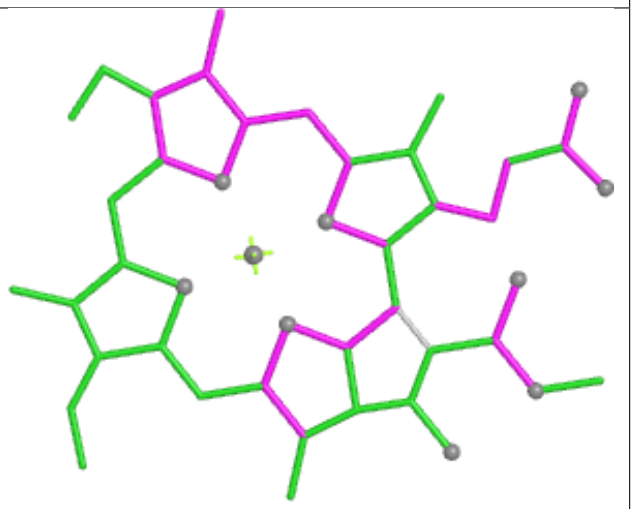


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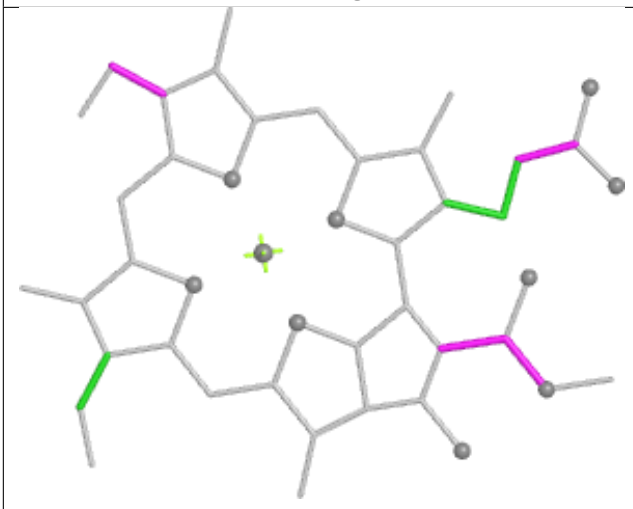
Ligand CLA c2 416



Bond lengths



Bond angles

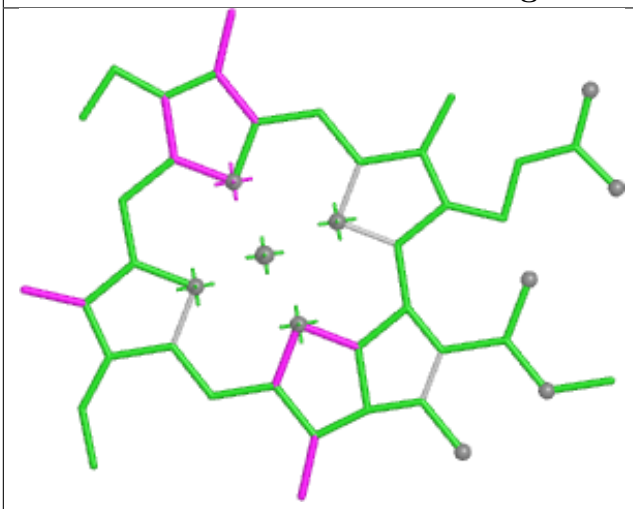


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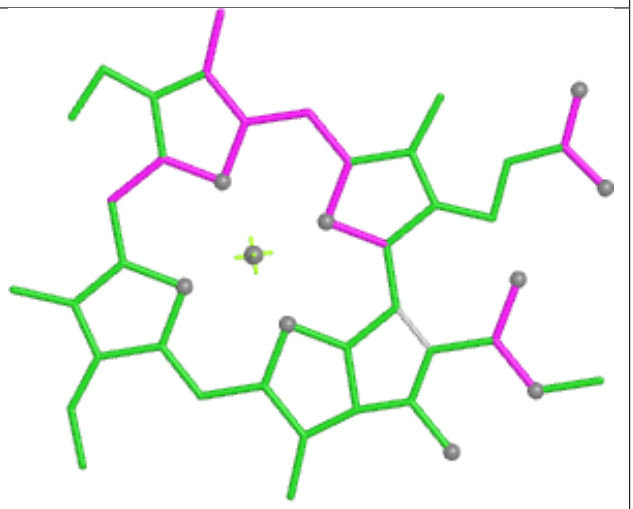


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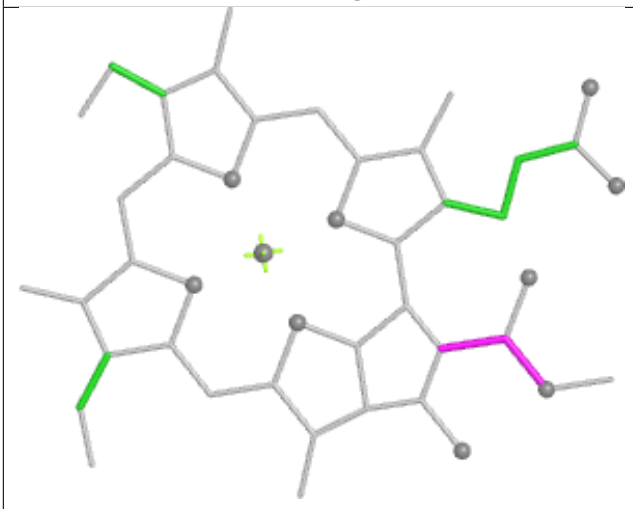
Ligand CLA c6 408



Bond lengths



Bond angles

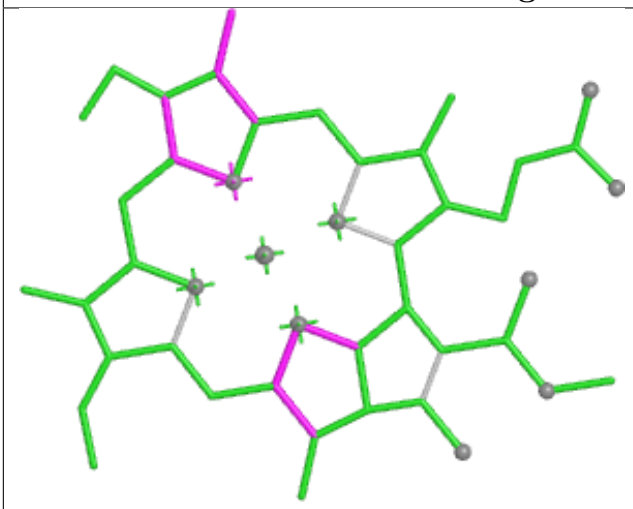


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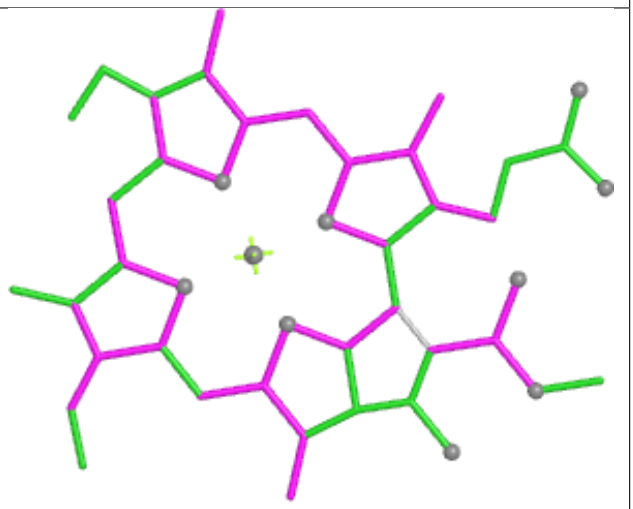


Rings

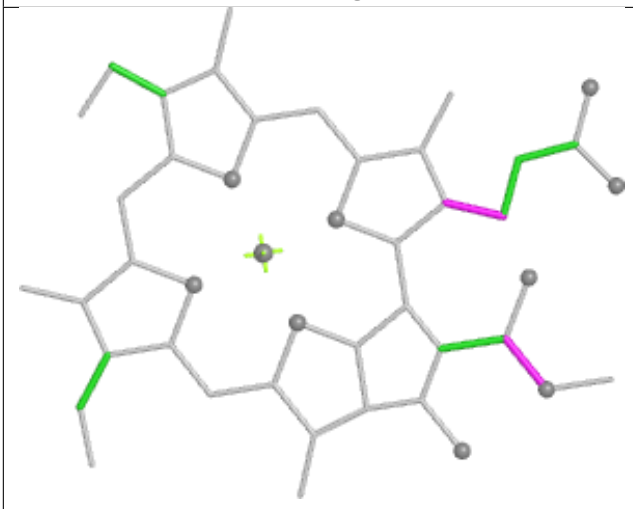
Ligand CLA b6 406



Bond lengths



Bond angles

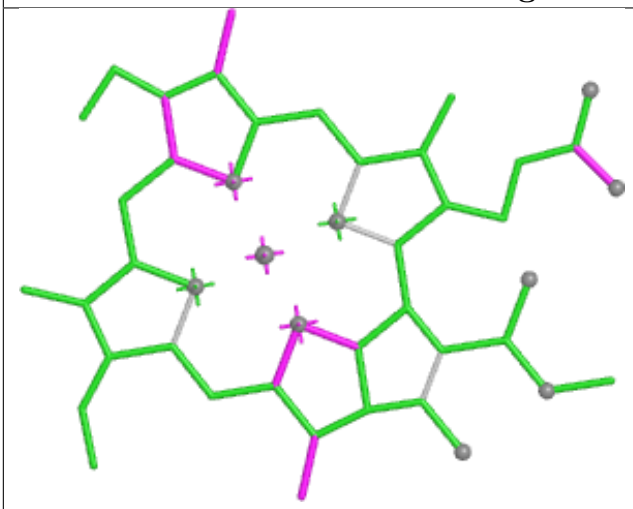


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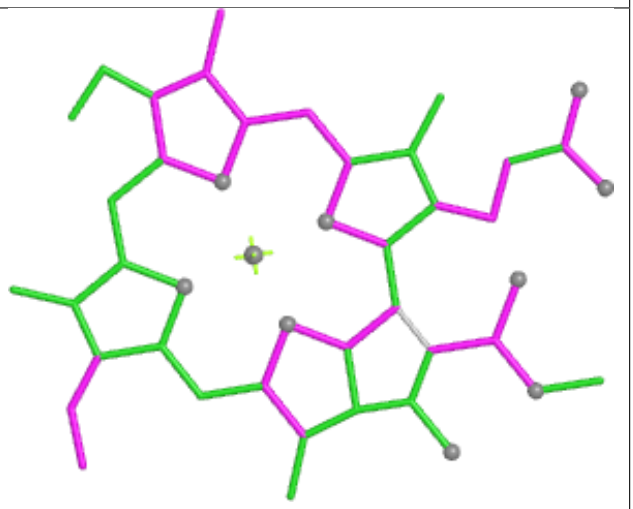


Rings

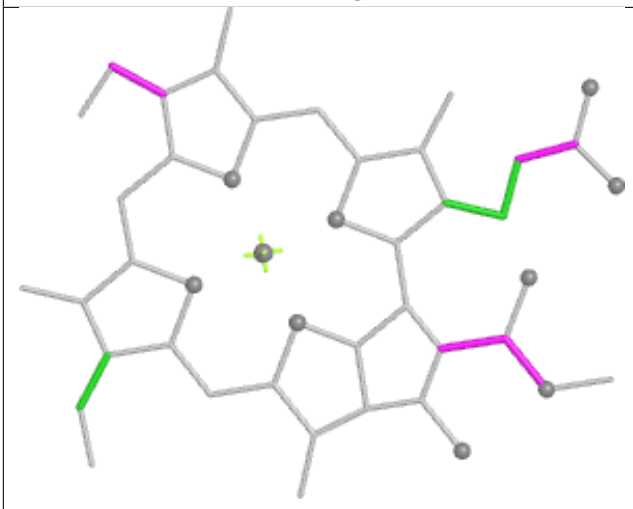
Ligand CLA b4 415



Bond lengths



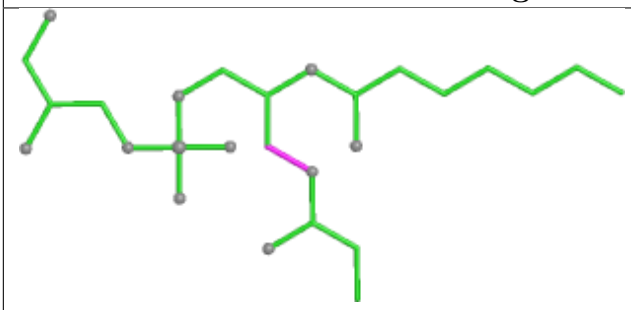
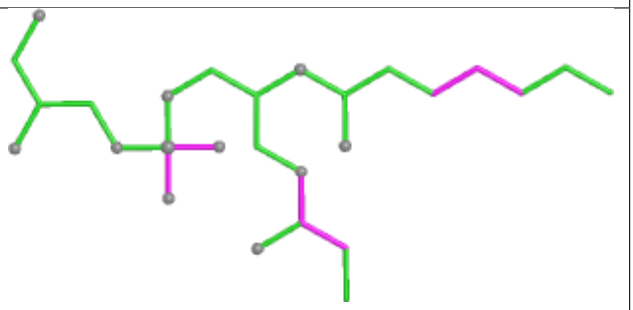
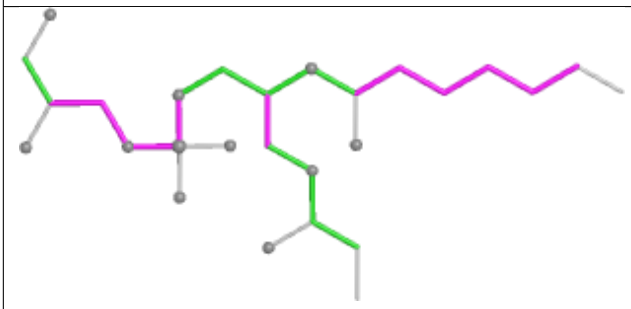
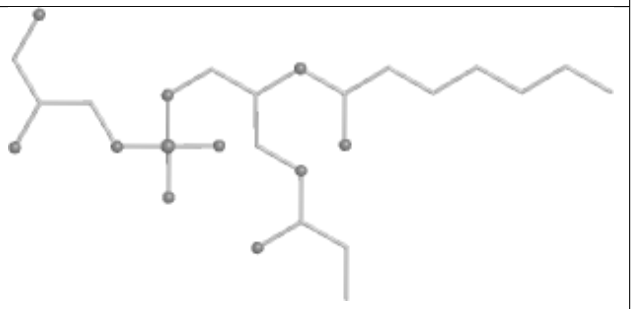
Bond angles

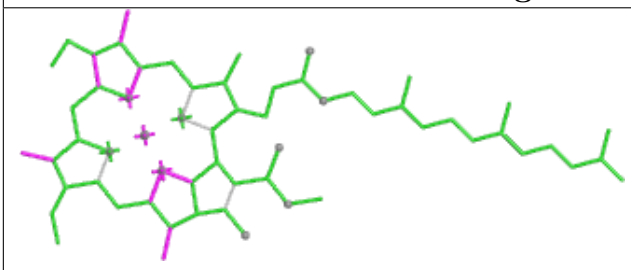
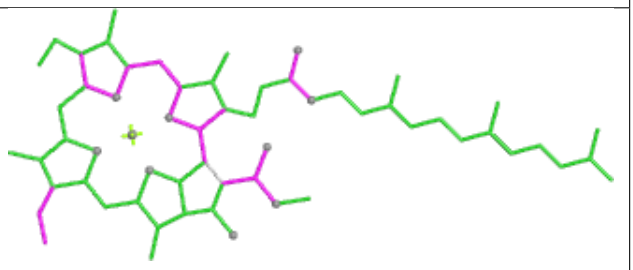
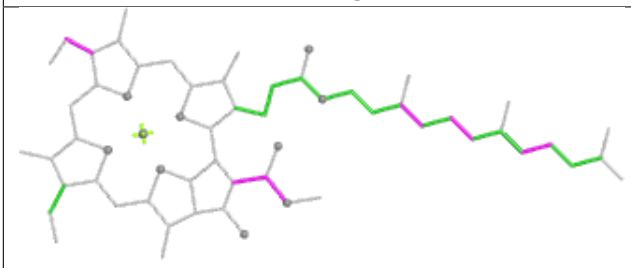
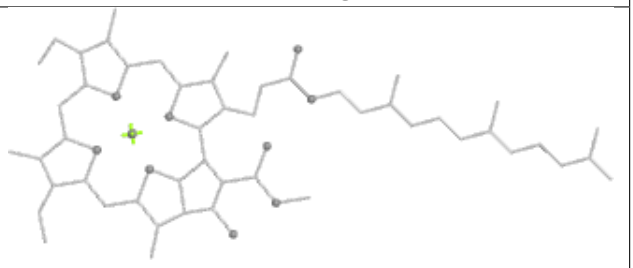


Torsions

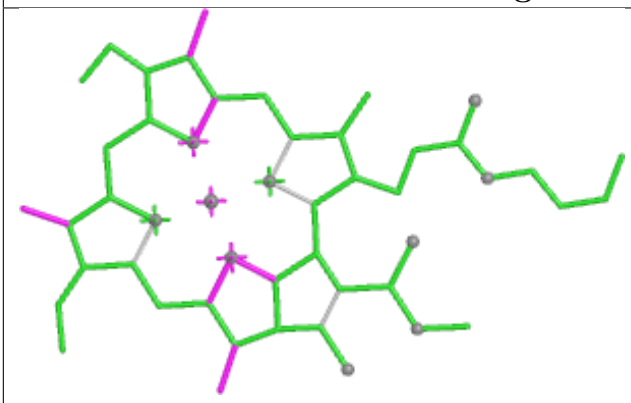


Rings

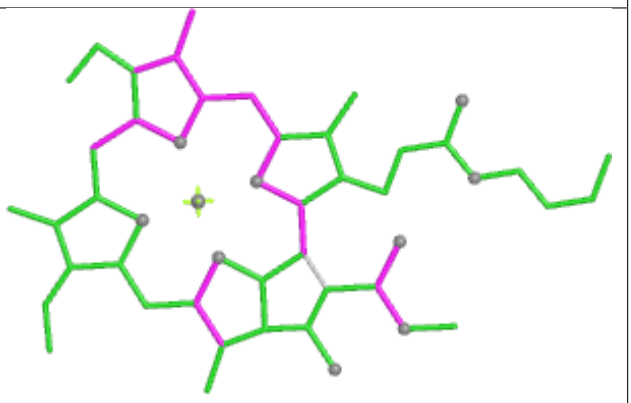
Ligand LHG bA 855	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bB 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

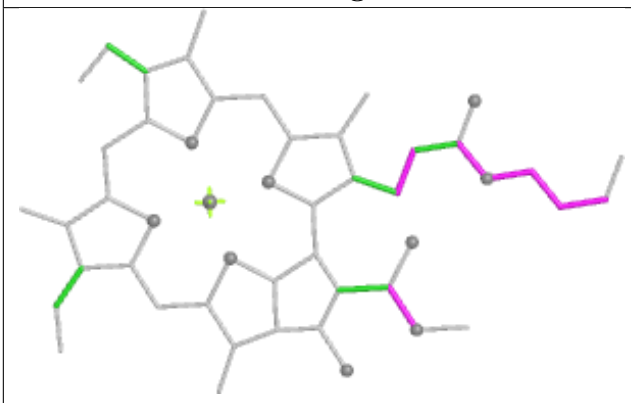
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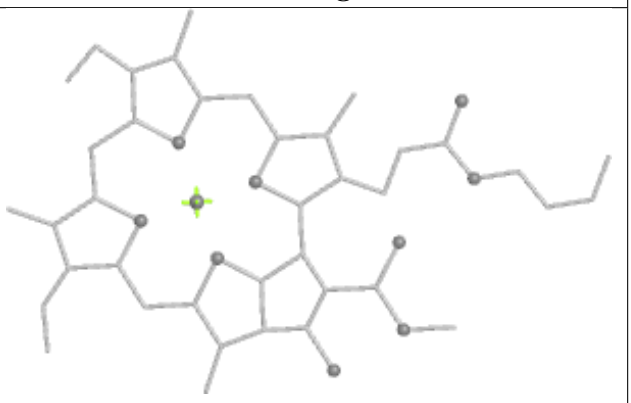
Bond lengths



Bond angles

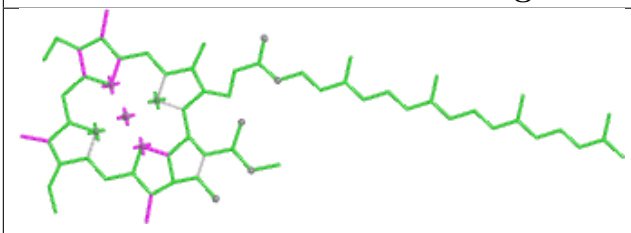


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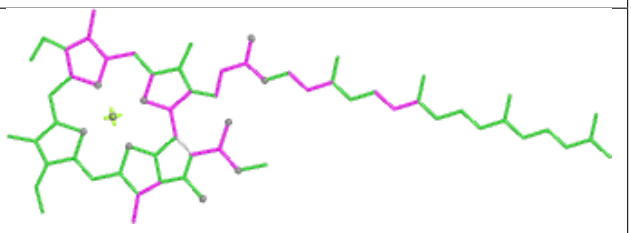


Rings

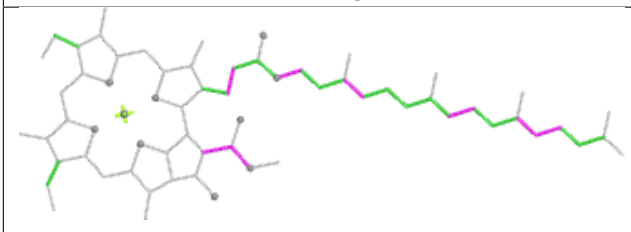
Ligand CLA bB 803



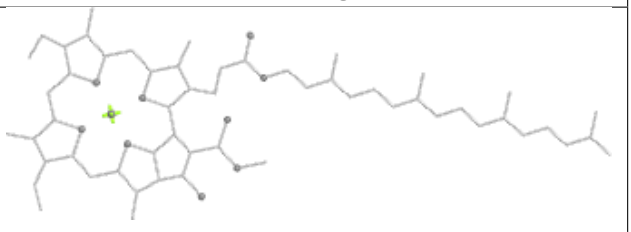
Bond lengths



Bond angles

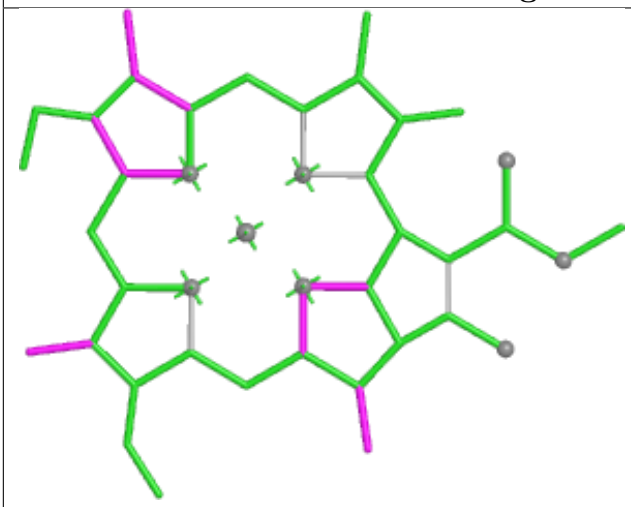


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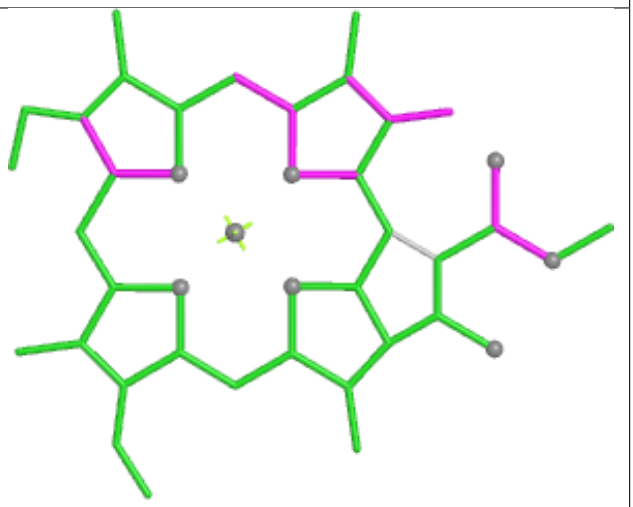


Rings

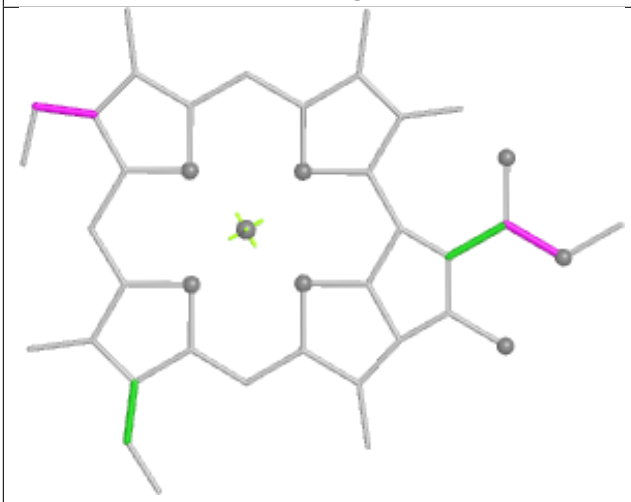
Ligand CLA a2 415



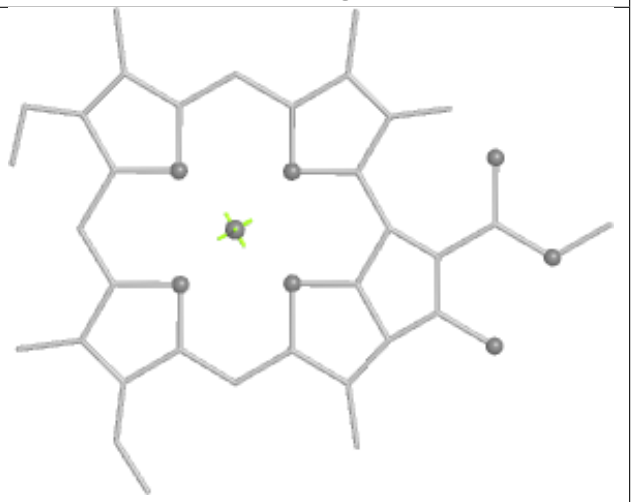
Bond lengths



Bond angles

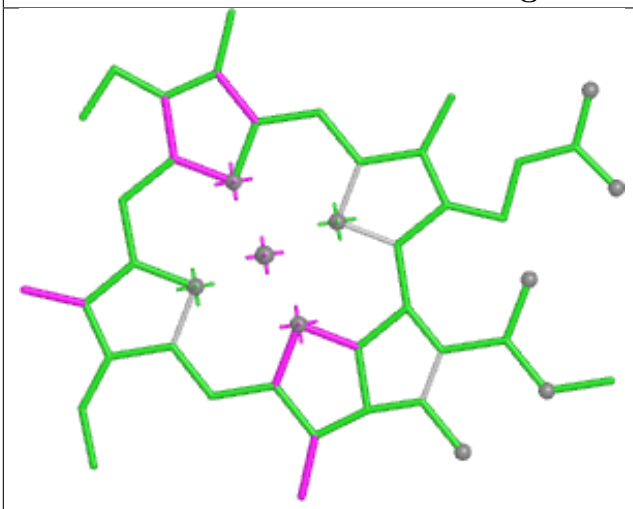


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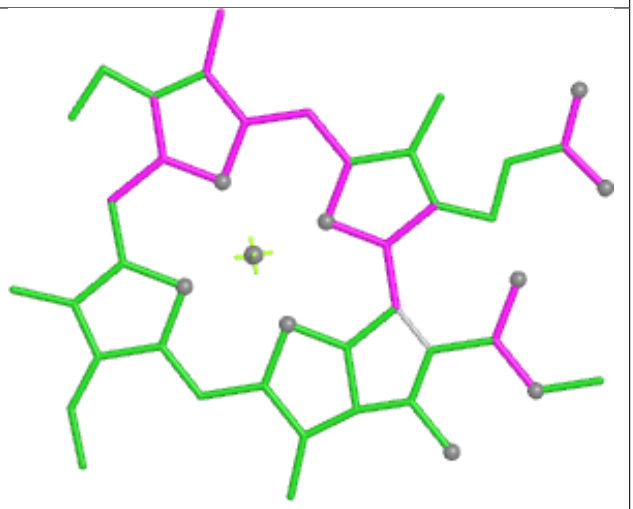


Rings

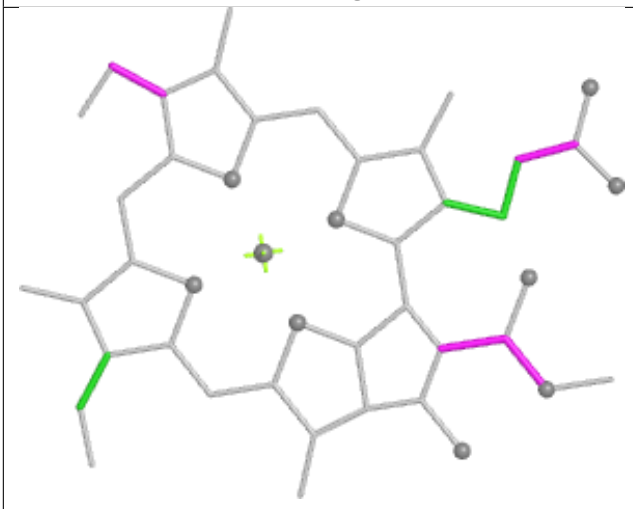
Ligand CLA c2 408



Bond lengths



Bond angles

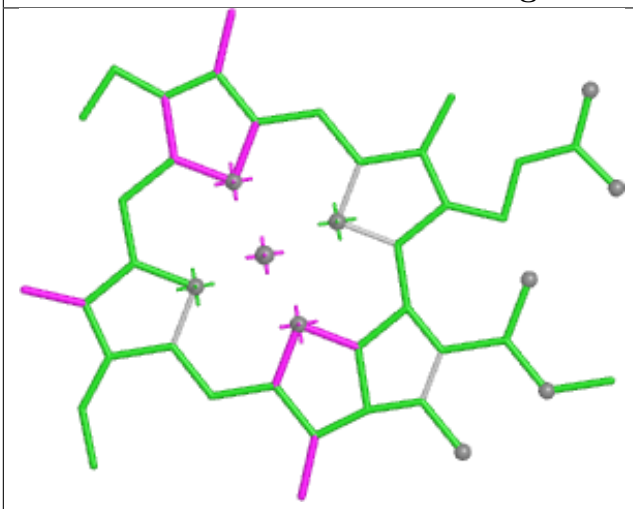


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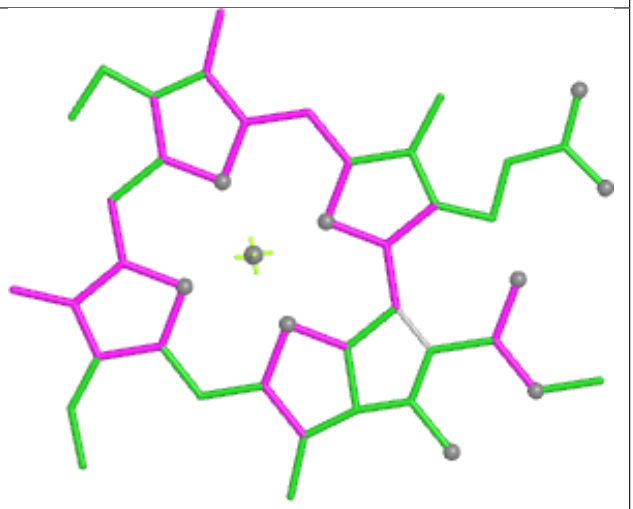


Rings

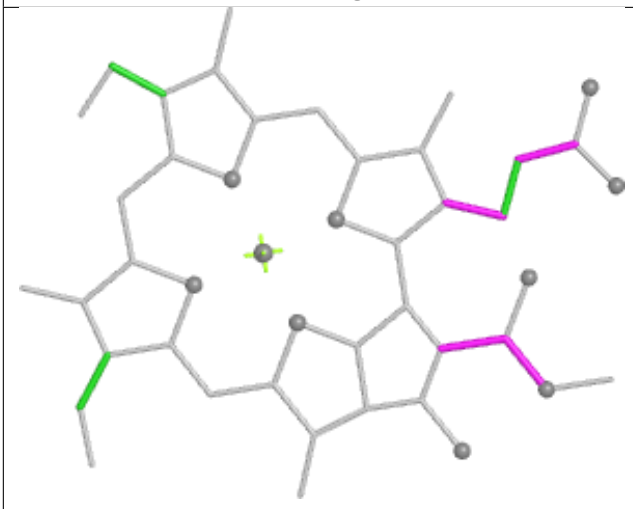
Ligand CLA a4 412



Bond lengths



Bond angles

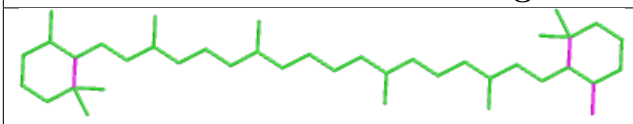


Torsions

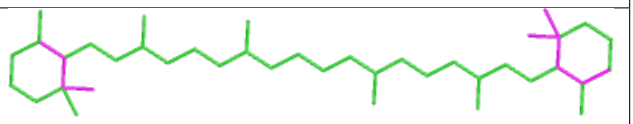


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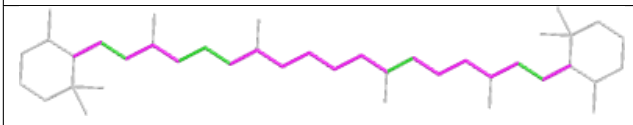
Ligand BCR cA 851



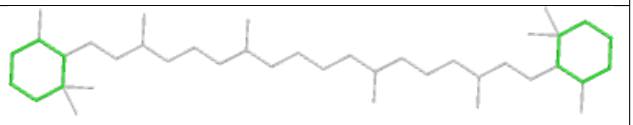
Bond lengths



Bond angles

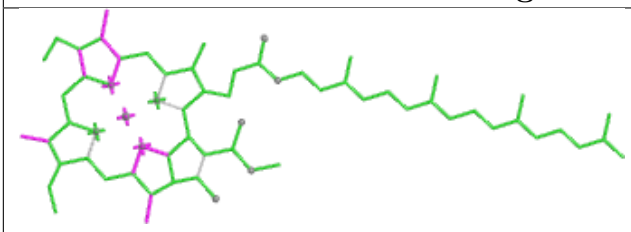


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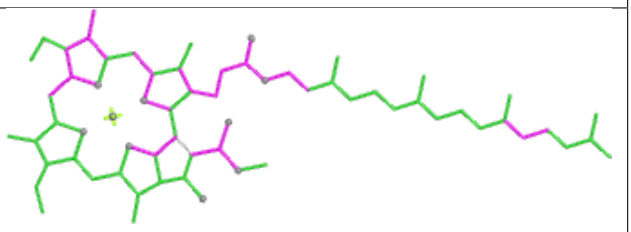


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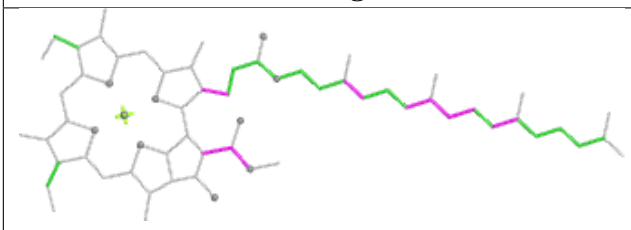
Ligand CLA cB 827



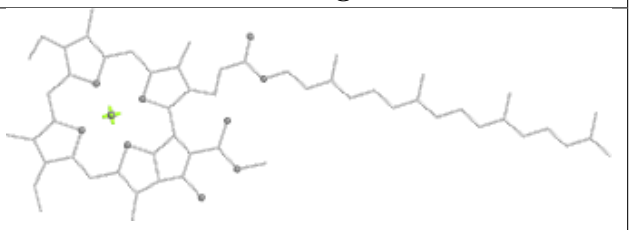
Bond lengths



Bond angles

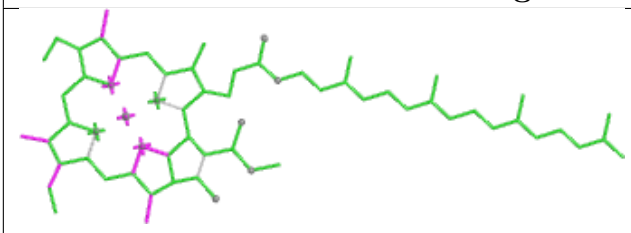


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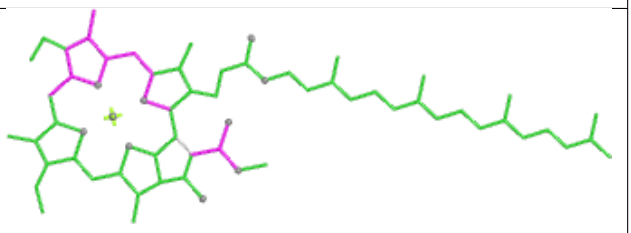


Rings

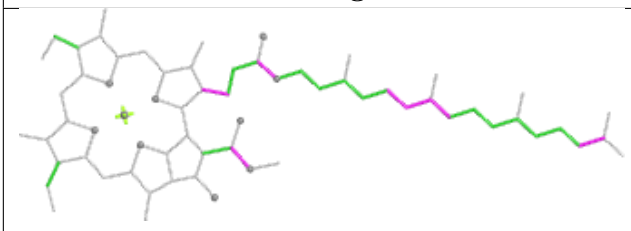
Ligand CLA bA 833



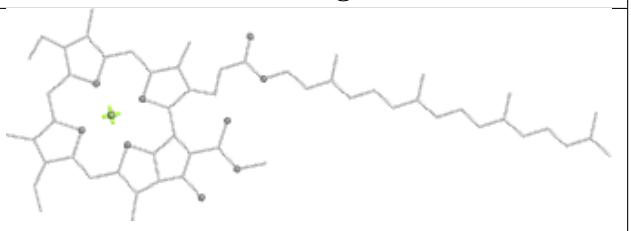
Bond lengths



Bond angles

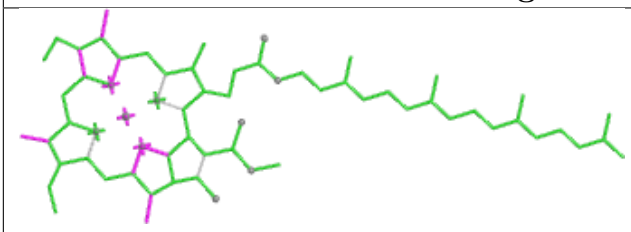


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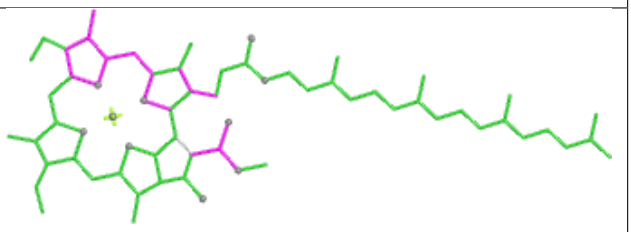


Rings

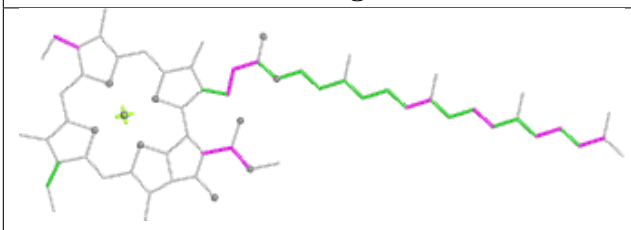
Ligand CLA aL 203



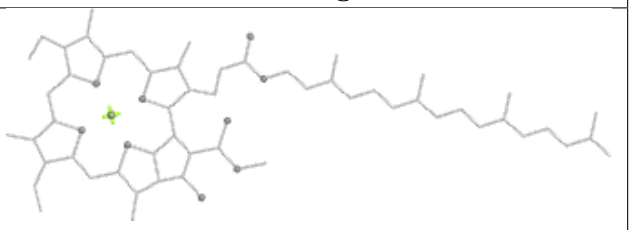
Bond lengths



Bond angles

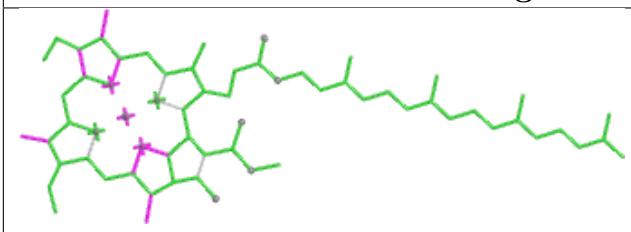


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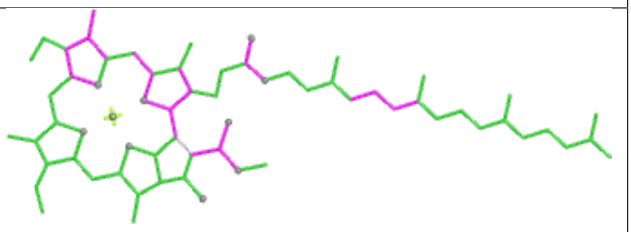


Rings

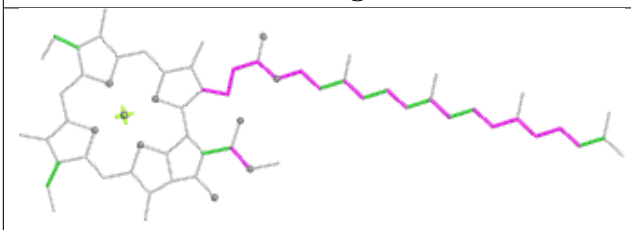
Ligand CLA aA 829



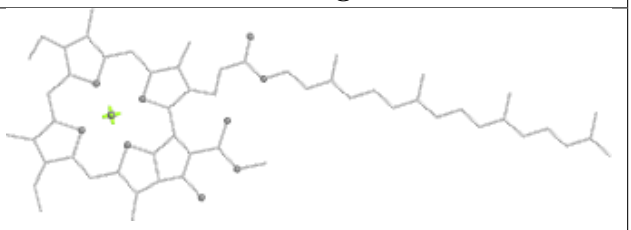
Bond lengths



Bond angles

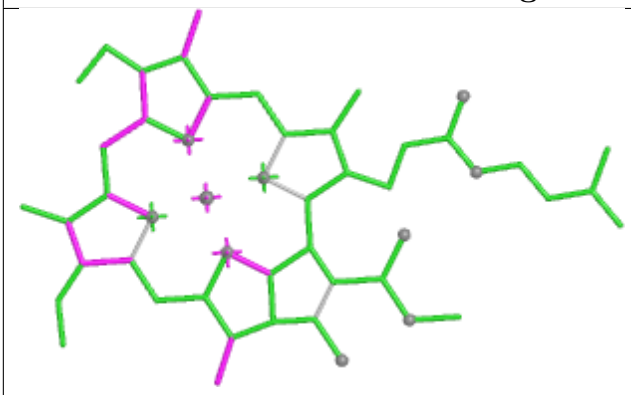


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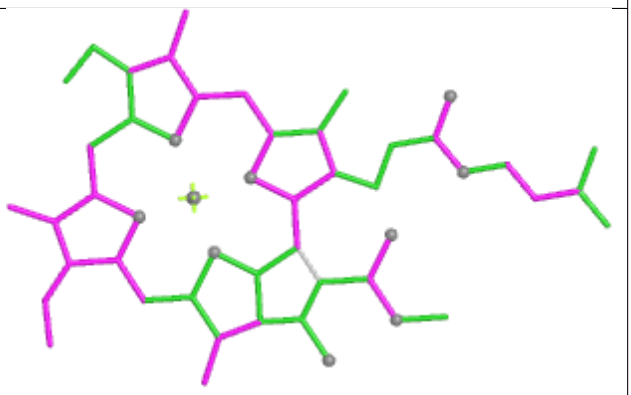


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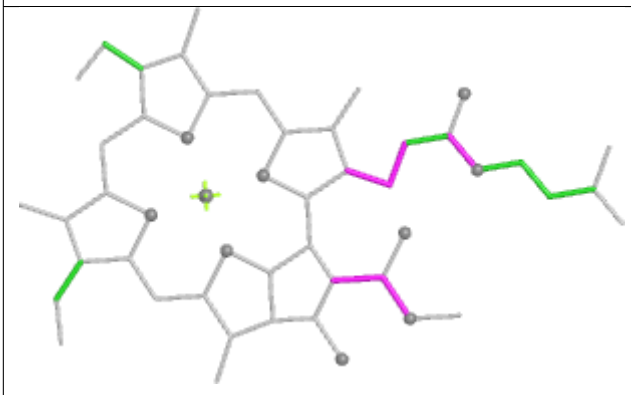
Ligand CLA a2 417



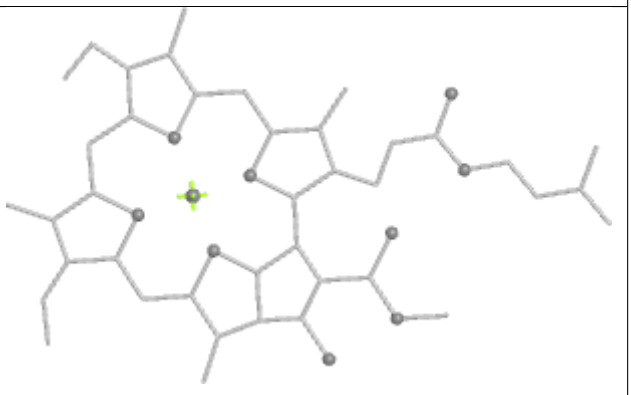
Bond lengths



Bond angles

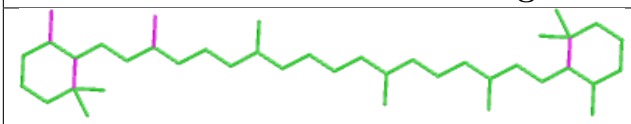


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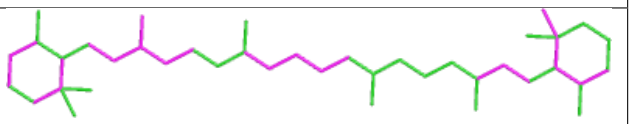


Rings

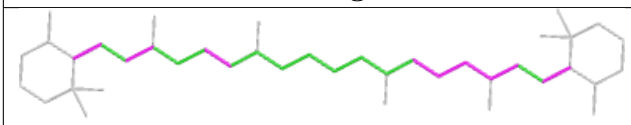
Ligand BCR a1 418



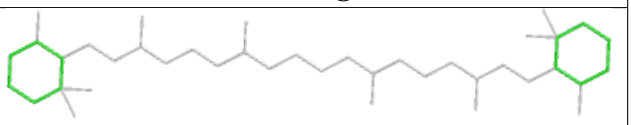
Bond lengths



Bond angles

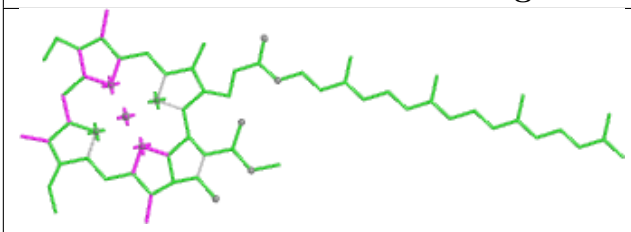


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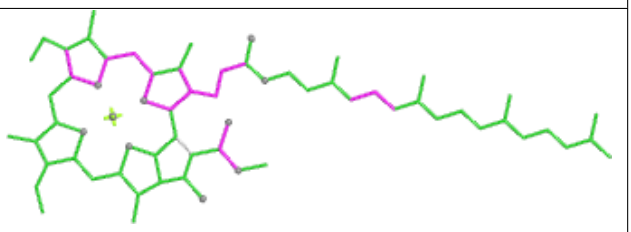


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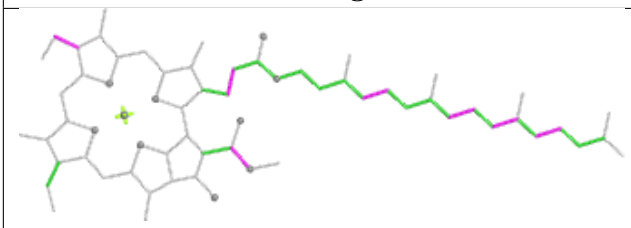
Ligand CLA bB 839



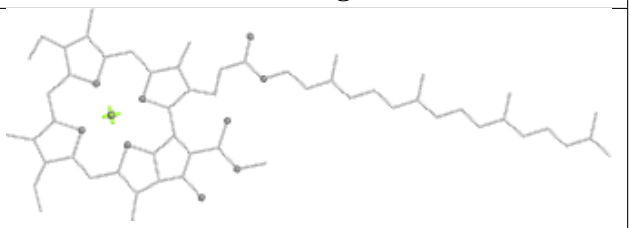
Bond lengths



Bond angles

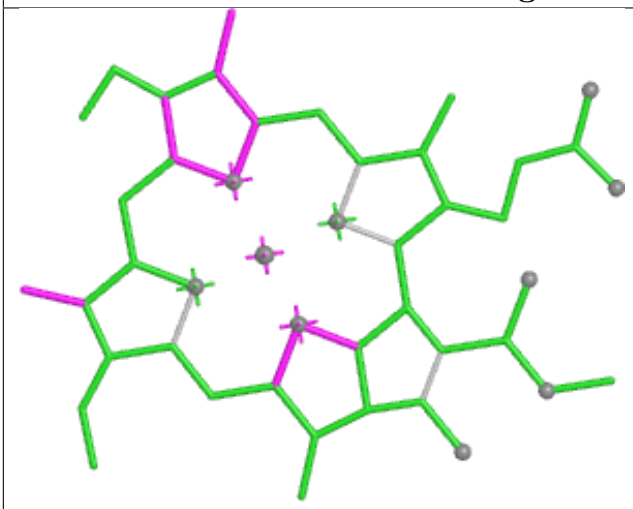


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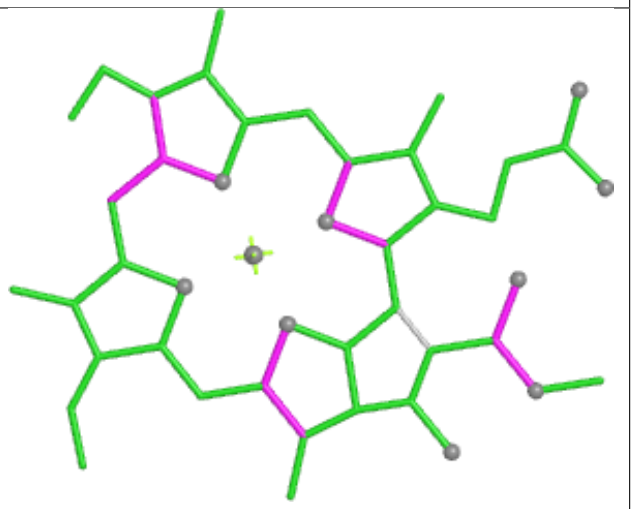


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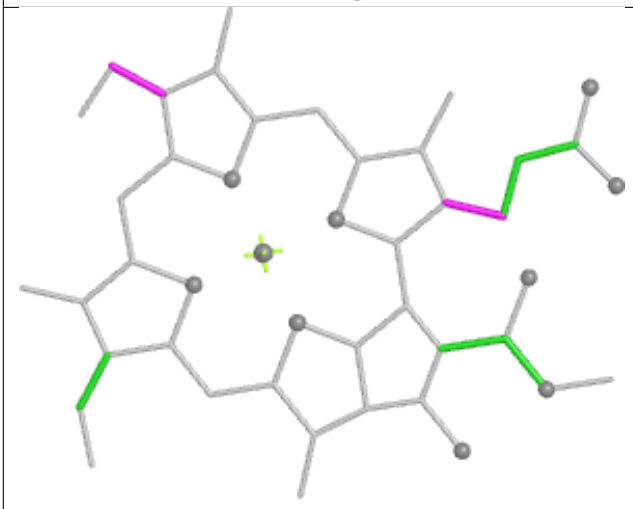
Ligand CLA b5 413



Bond lengths



Bond angles

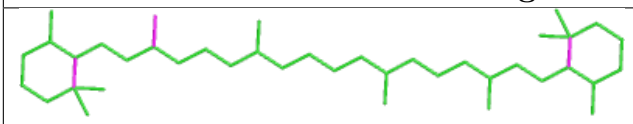


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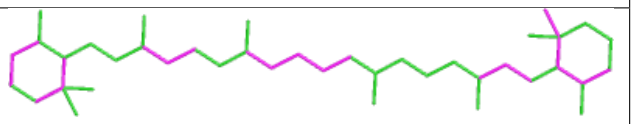


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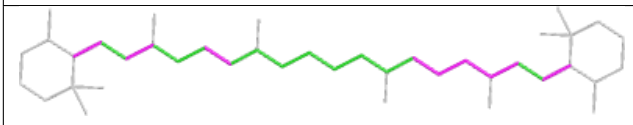
Ligand BCR c2 420



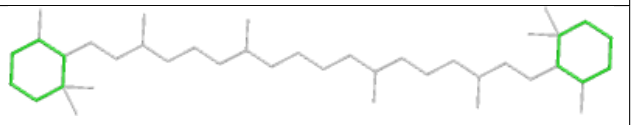
Bond lengths



Bond angles

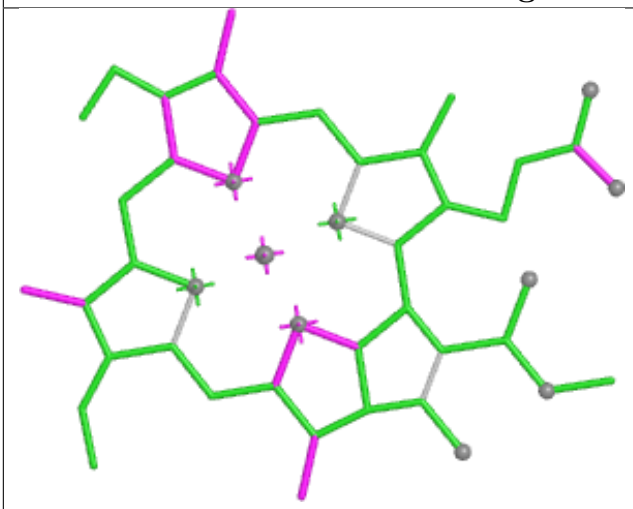


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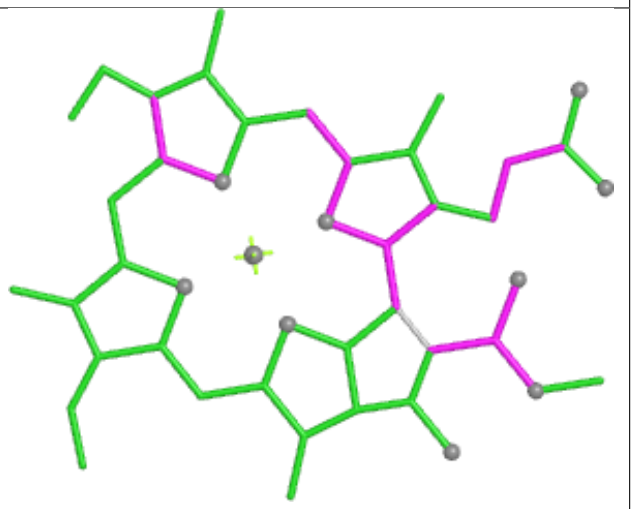


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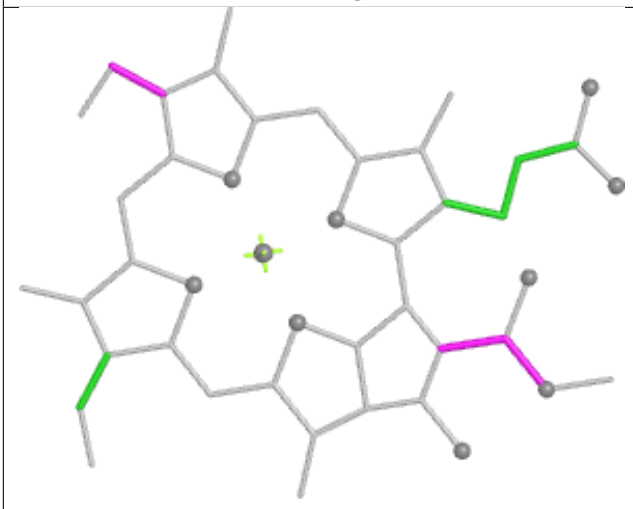
Ligand CLA bJ 101



Bond lengths



Bond angles

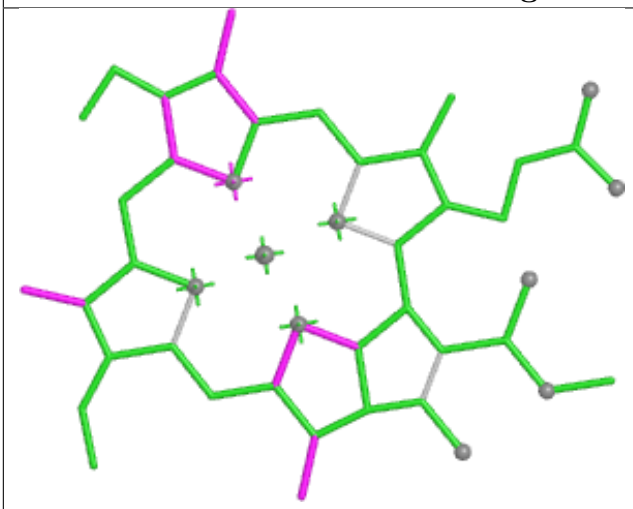


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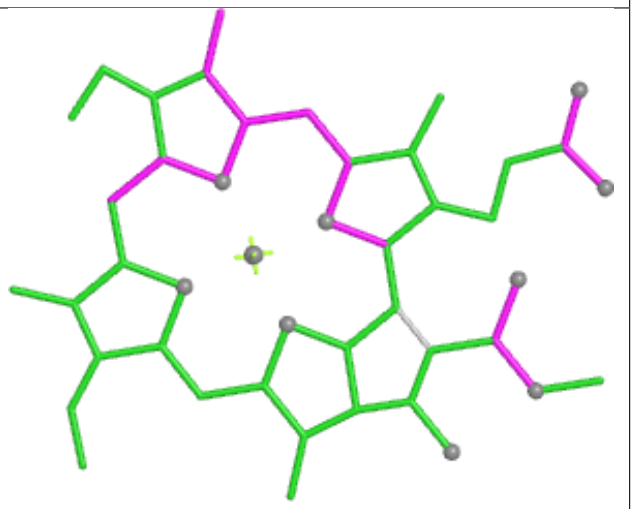


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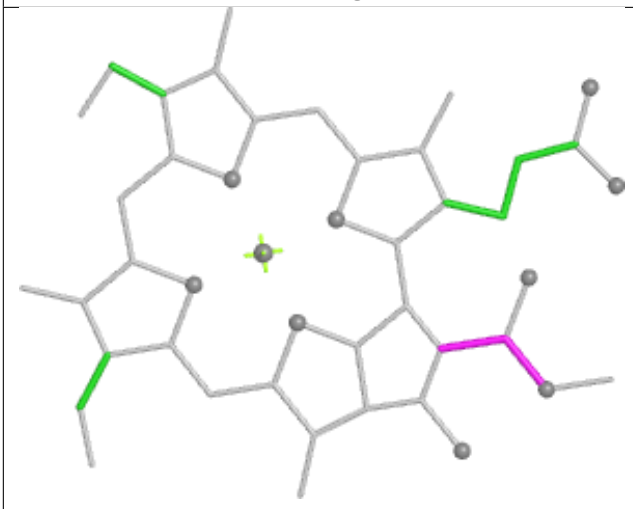
Ligand CLA c4 406



Bond lengths



Bond angles

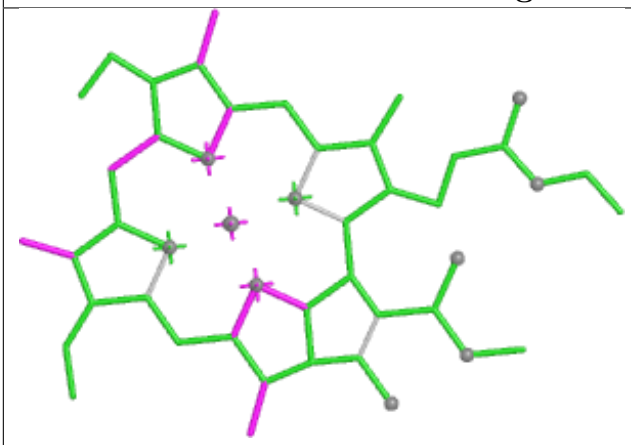


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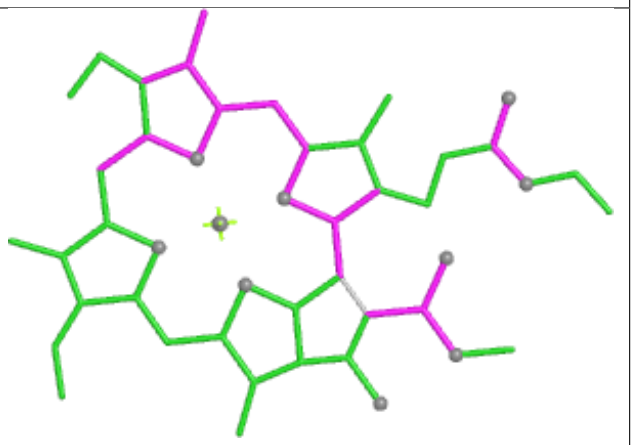


Rings

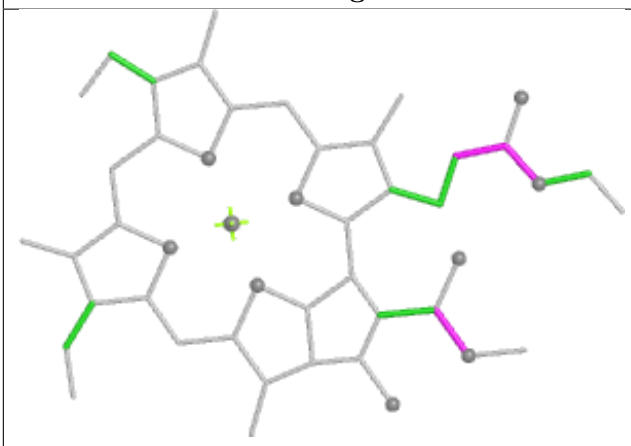
Ligand CLA cA 840



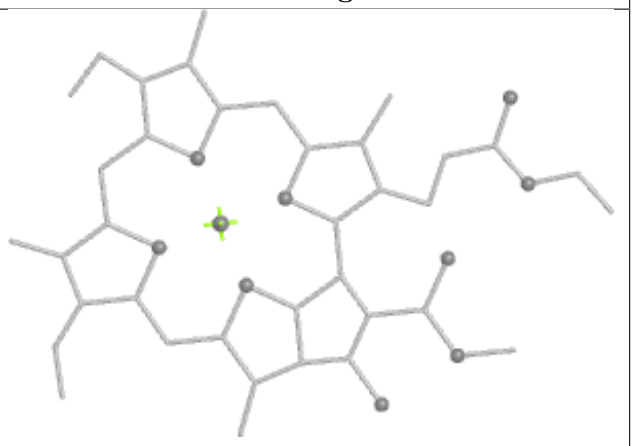
Bond lengths



Bond angles

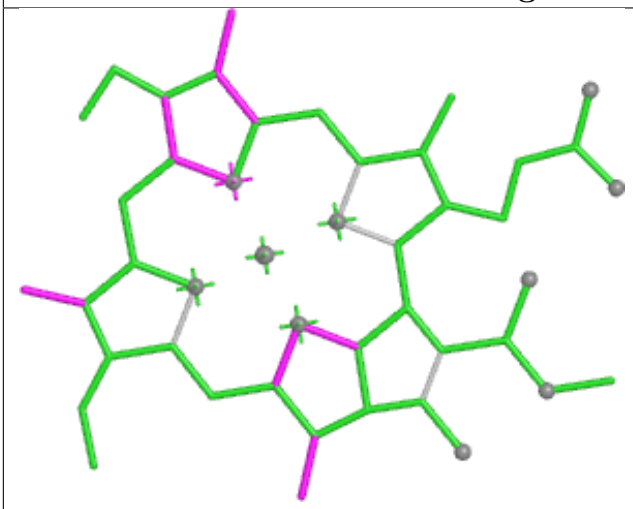


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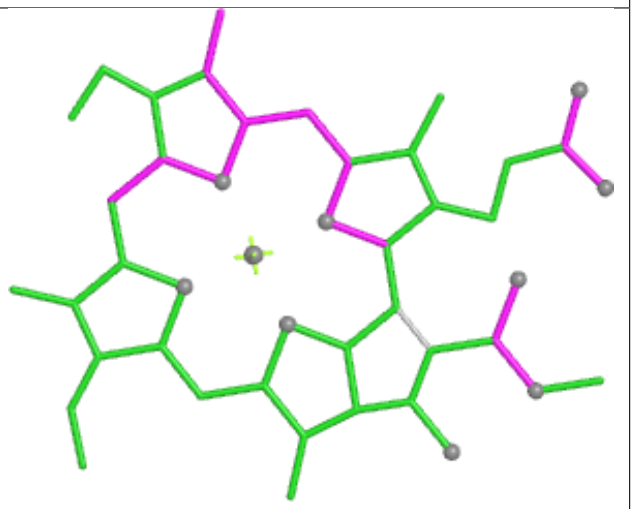


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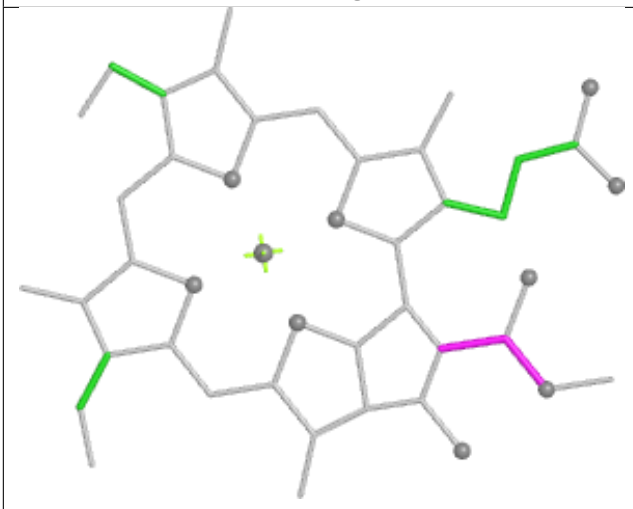
Ligand CLA b6 407



Bond lengths



Bond angles

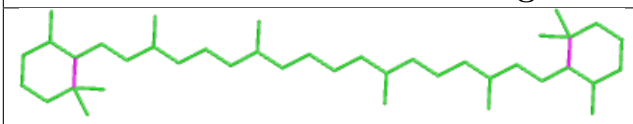


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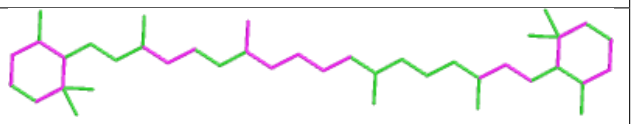


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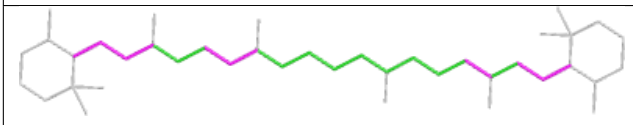
Ligand BCR a4 420



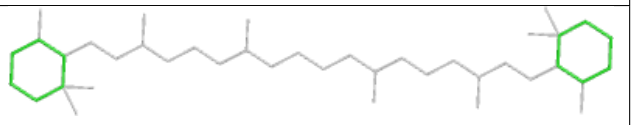
Bond lengths



Bond angles

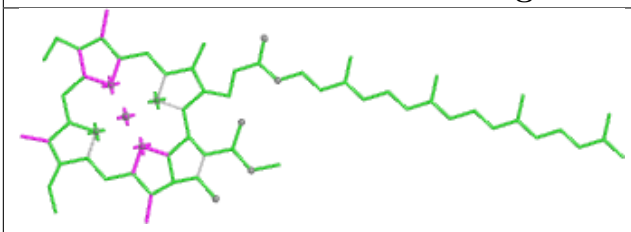


Torsions

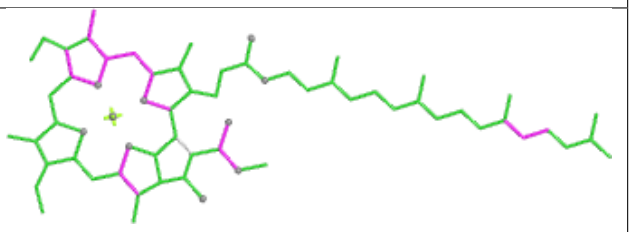


Rings

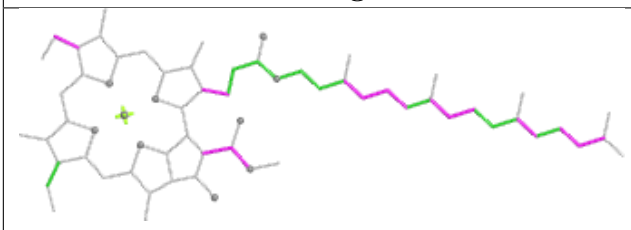
Ligand CLA cA 822



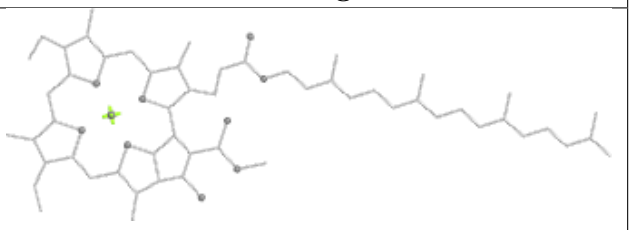
Bond lengths



Bond angles



Torsions

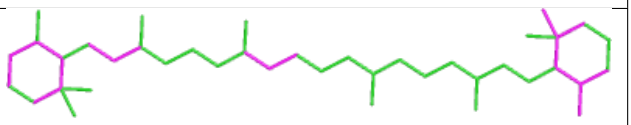


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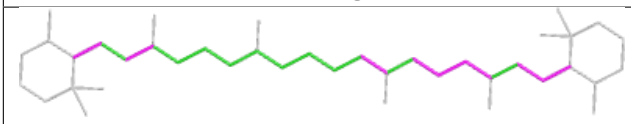
Ligand BCR b5 418



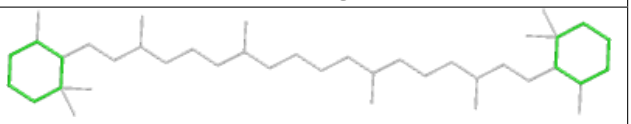
Bond lengths



Bond angles

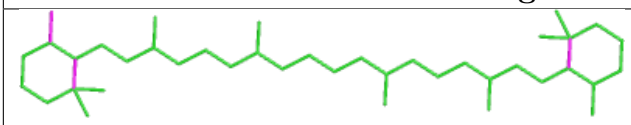


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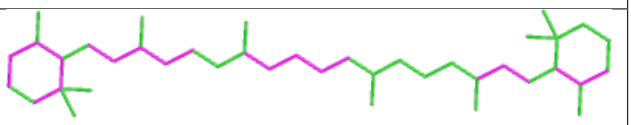


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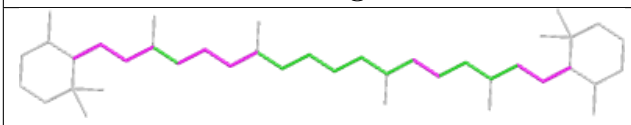
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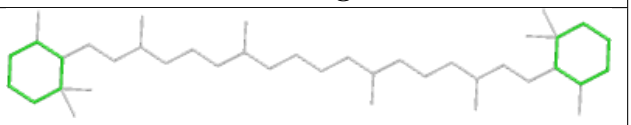
Bond lengths



Bond angles

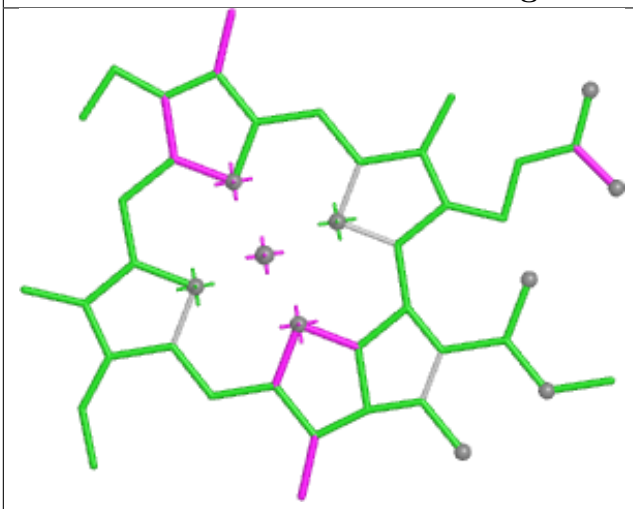


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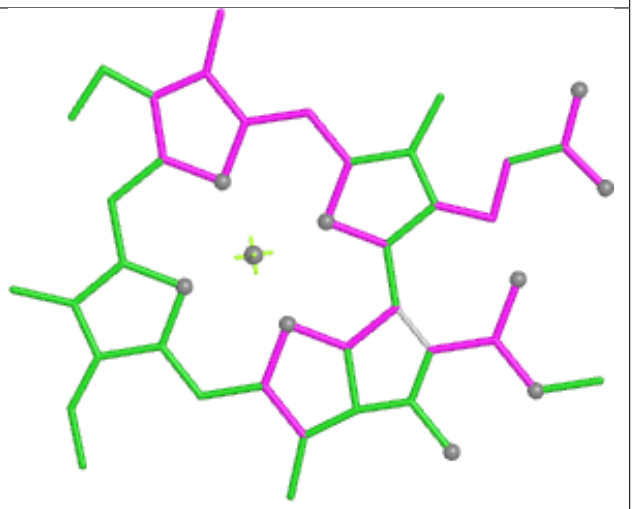


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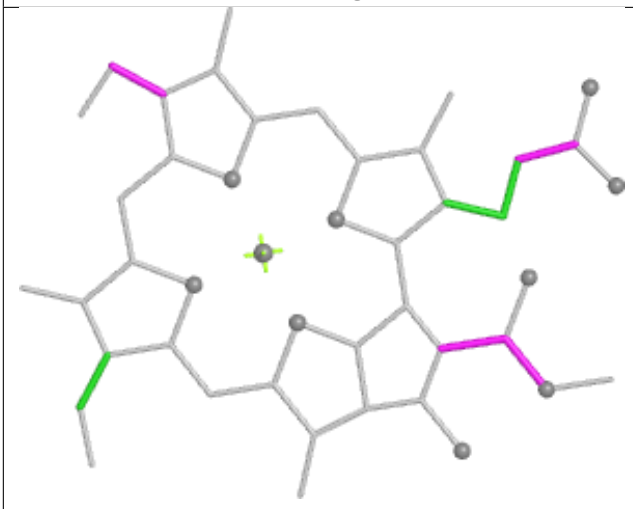
Ligand CLA c5 415



Bond lengths



Bond angles

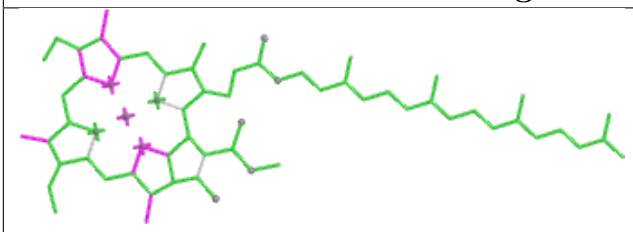


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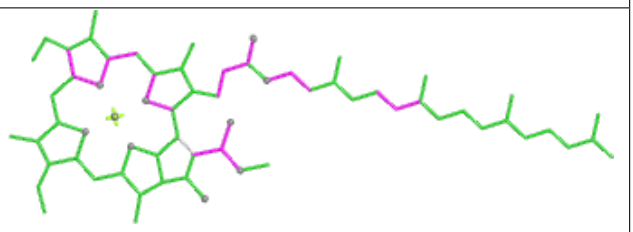


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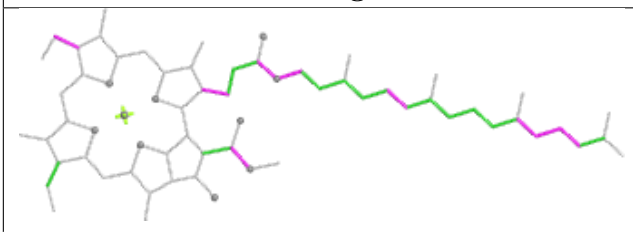
Ligand CLA aA 812



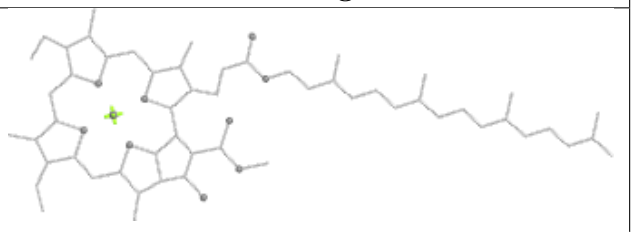
Bond lengths



Bond angles

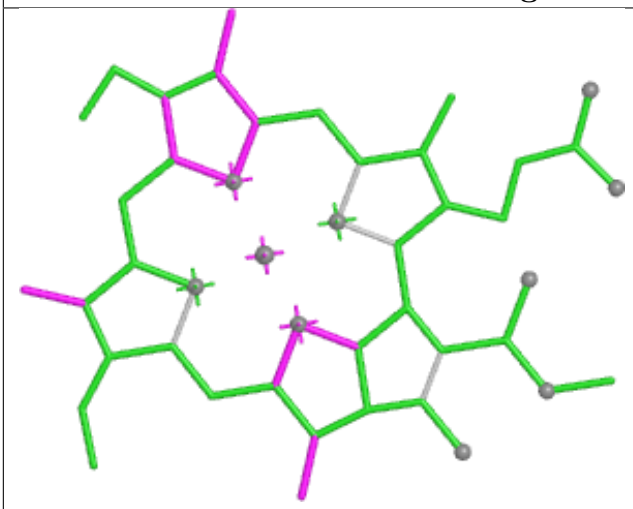


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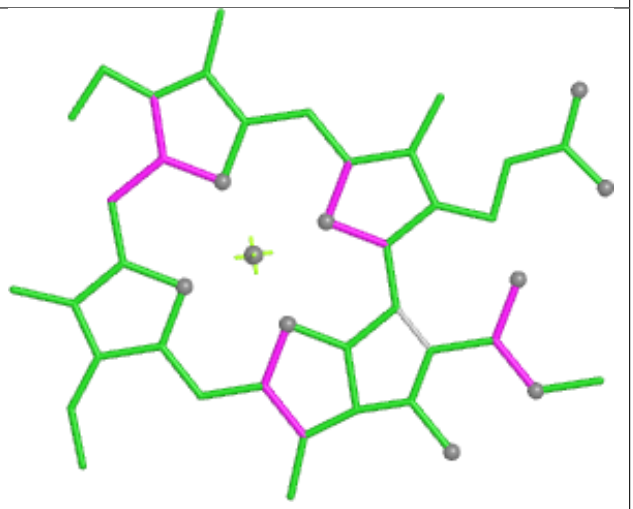


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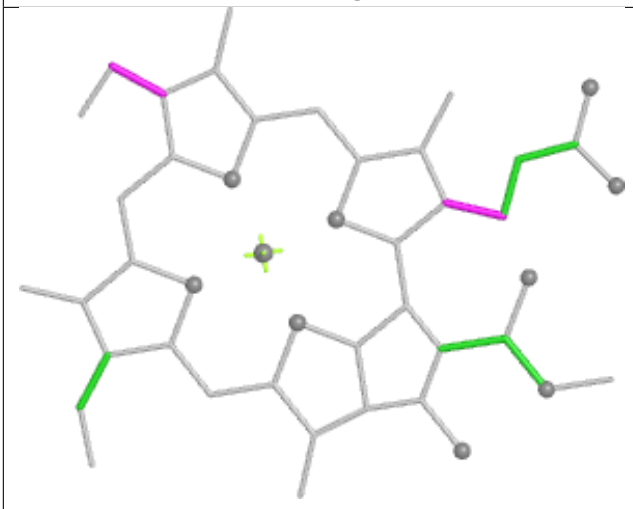
Ligand CLA c5 413



Bond lengths



Bond angles

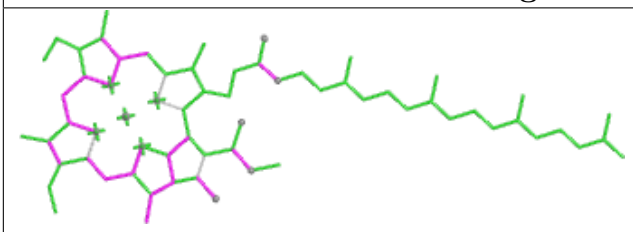


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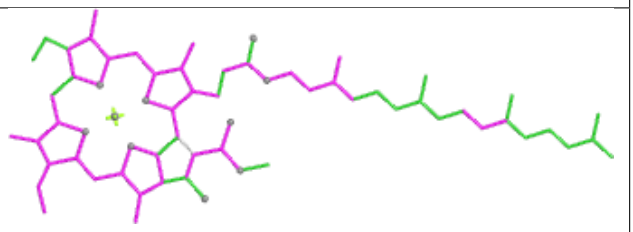


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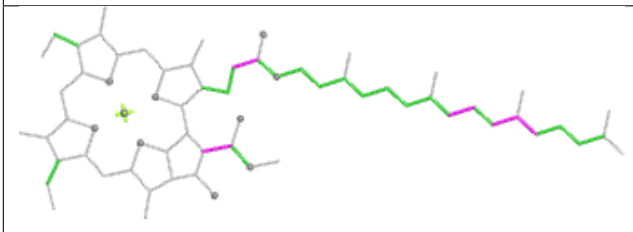
Ligand CL0 aA 801



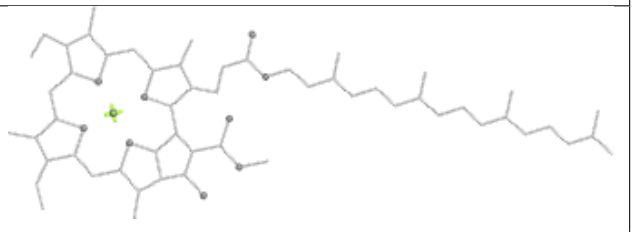
Bond lengths



Bond angles

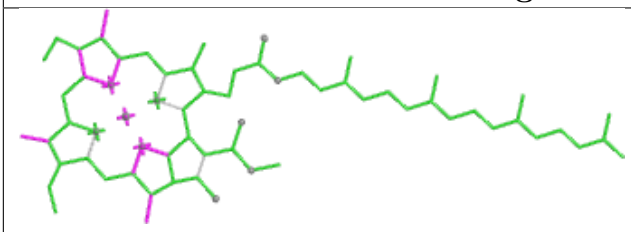


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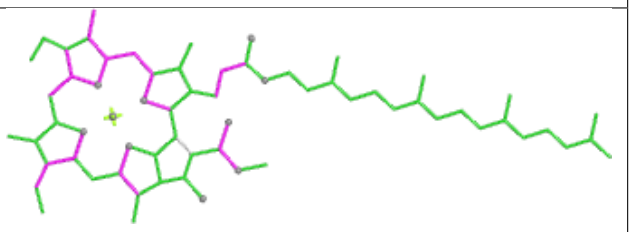


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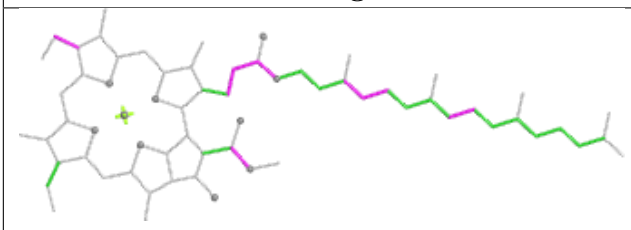
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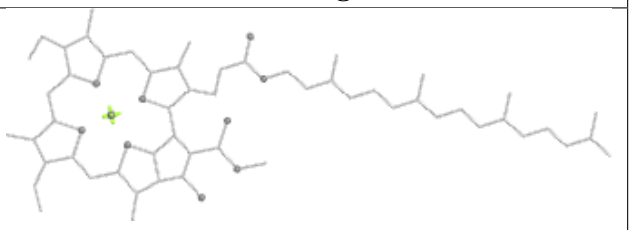
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Bond angles

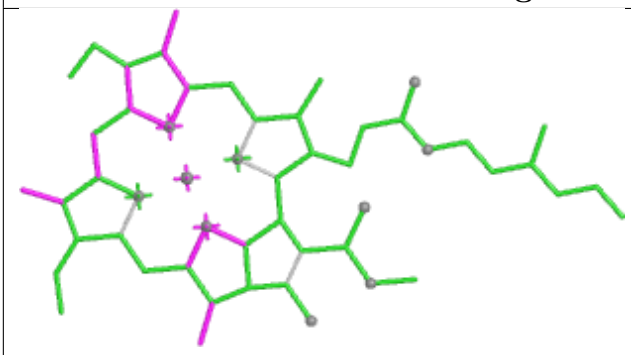


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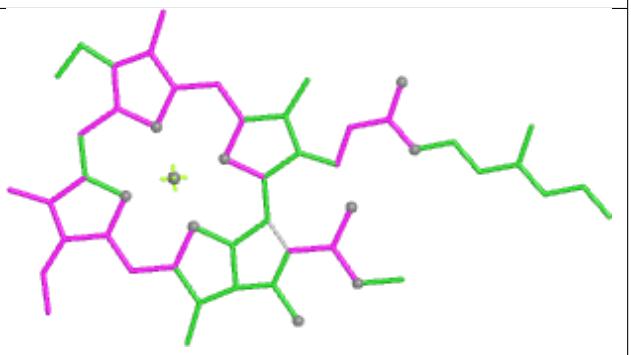


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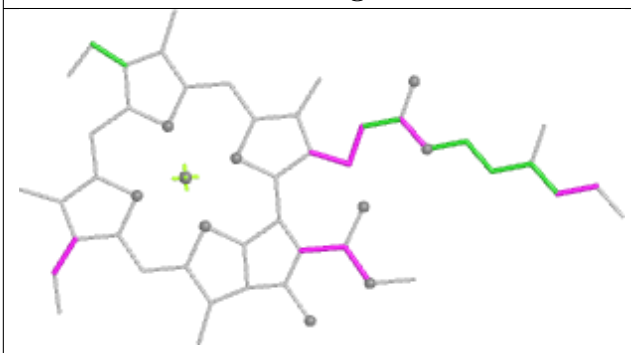
Ligand CLA aA 845



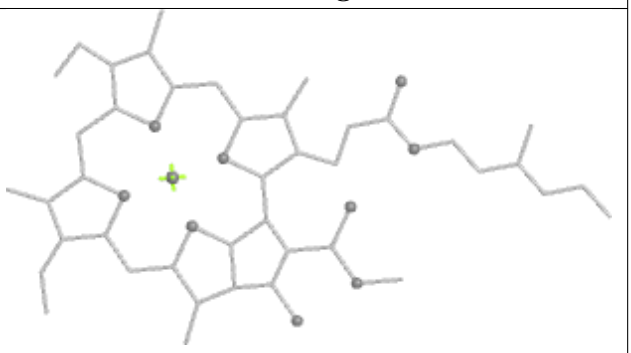
Bond lengths



Bond angles



Torsions

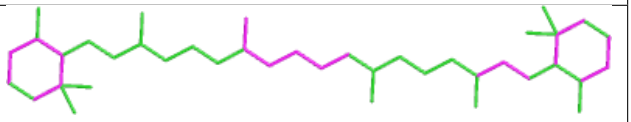


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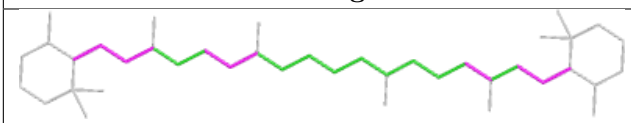
Ligand BCR b3 420



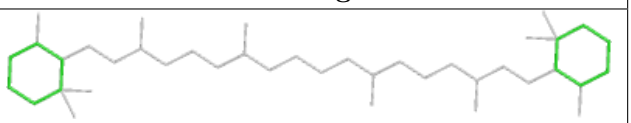
Bond lengths



Bond angles

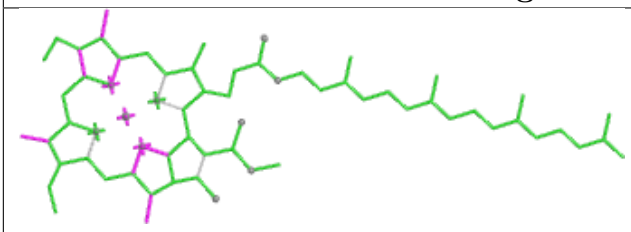


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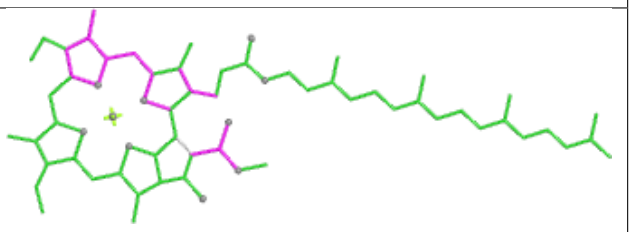


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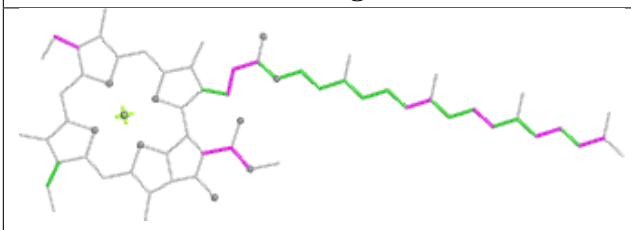
Ligand CLA bL 204



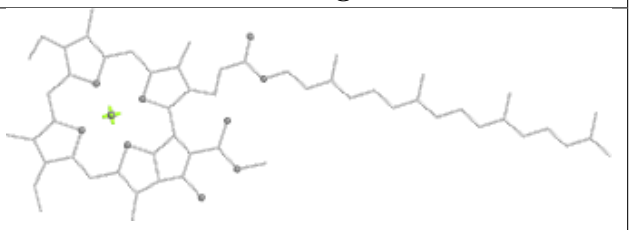
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Bond angles

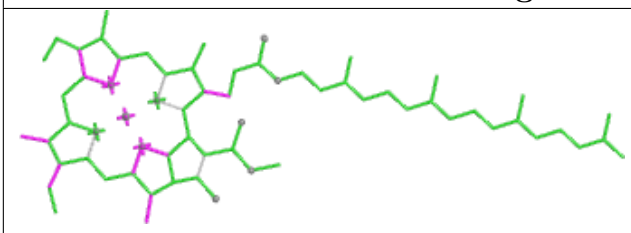


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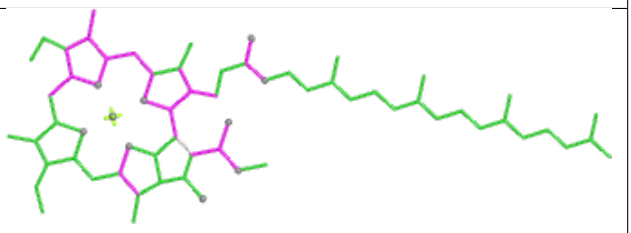


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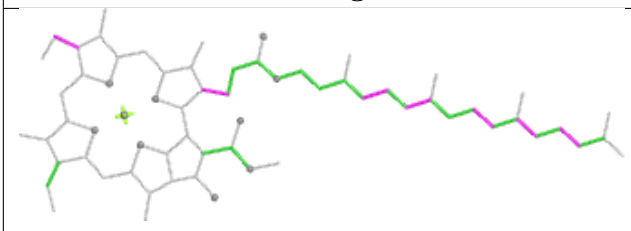
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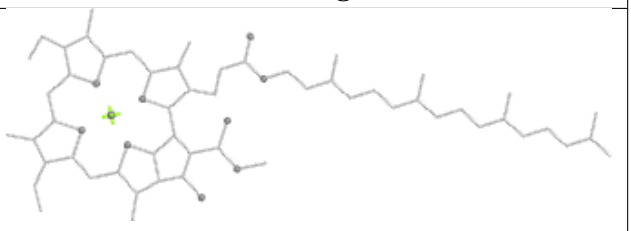
Bond lengths



Bond angles

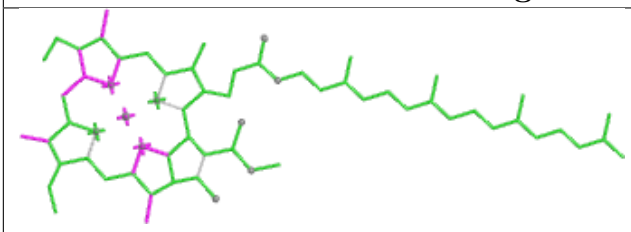


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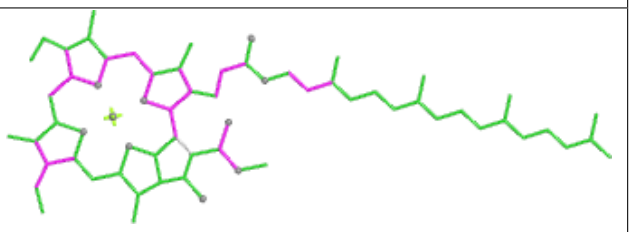


Rings

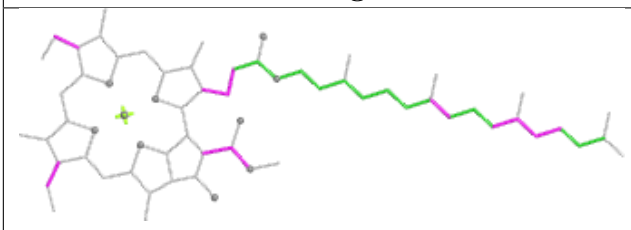
Ligand CLA bB 840



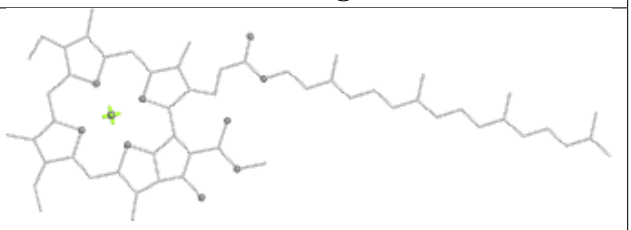
Bond lengths



Bond angles

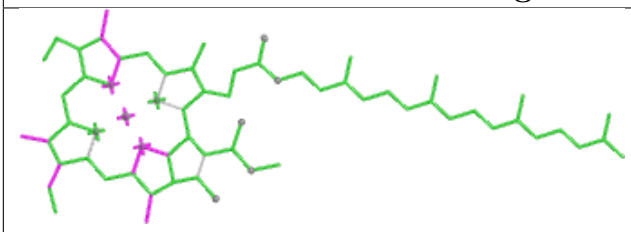


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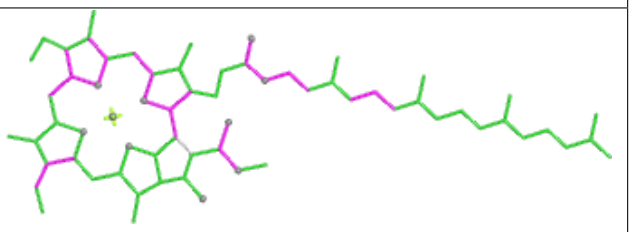


Rings

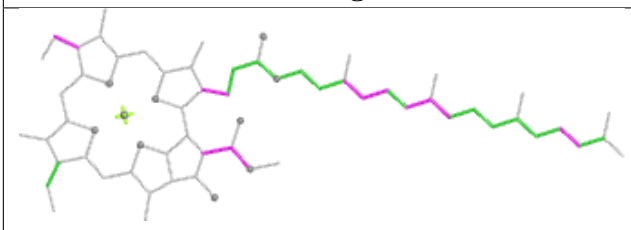
Ligand CLA bB 811



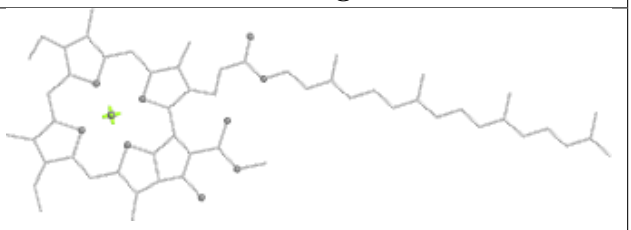
Bond lengths



Bond angles

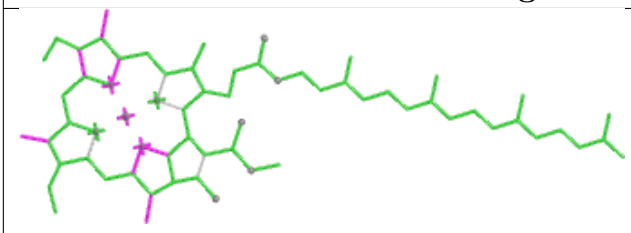


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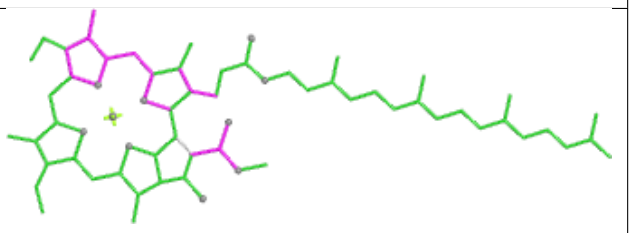


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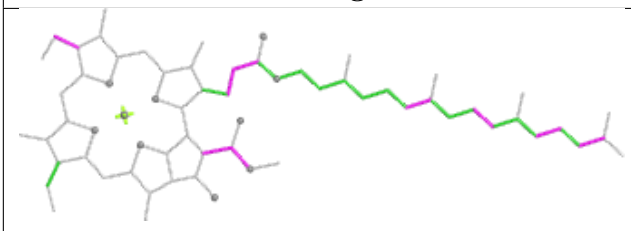
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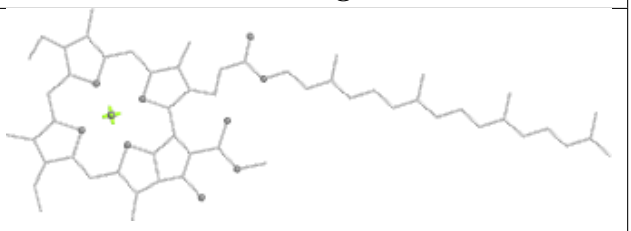
Bond lengths



Bond angles

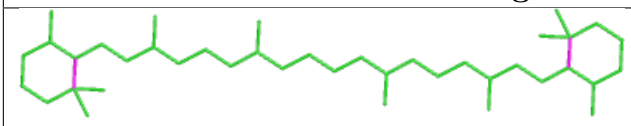


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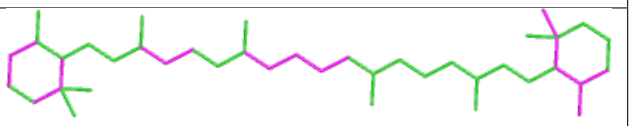


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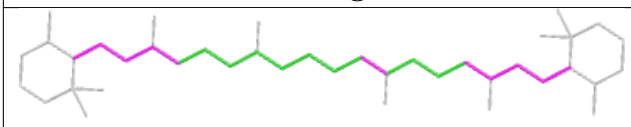
Ligand BCR bA 850



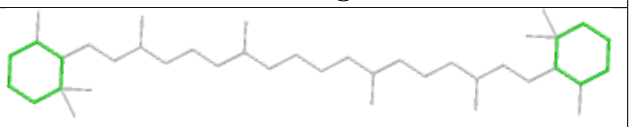
Bond lengths



Bond angles

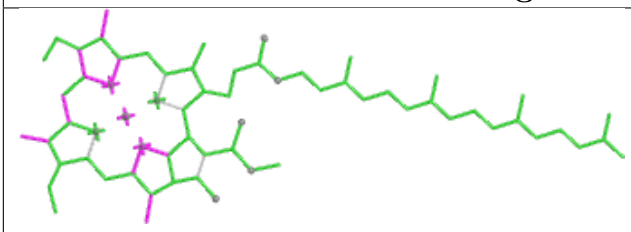


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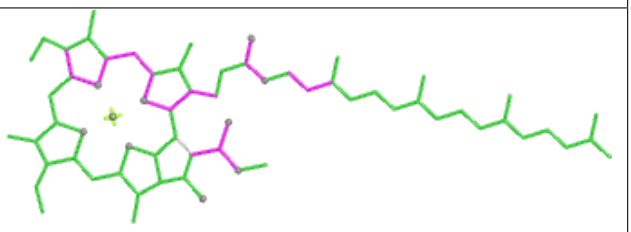


Rings

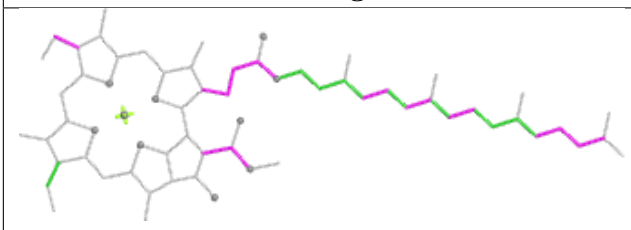
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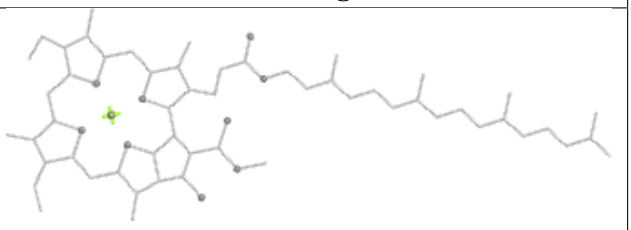
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Bond angles

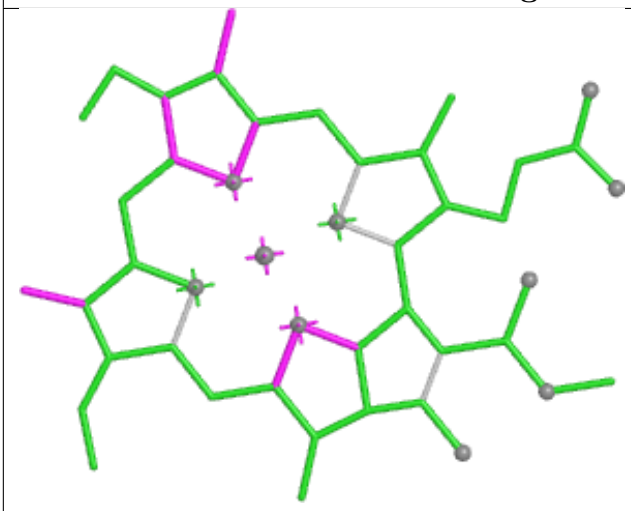


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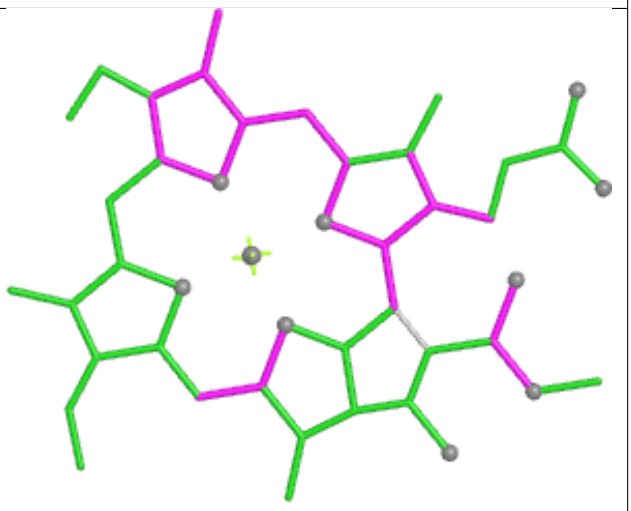


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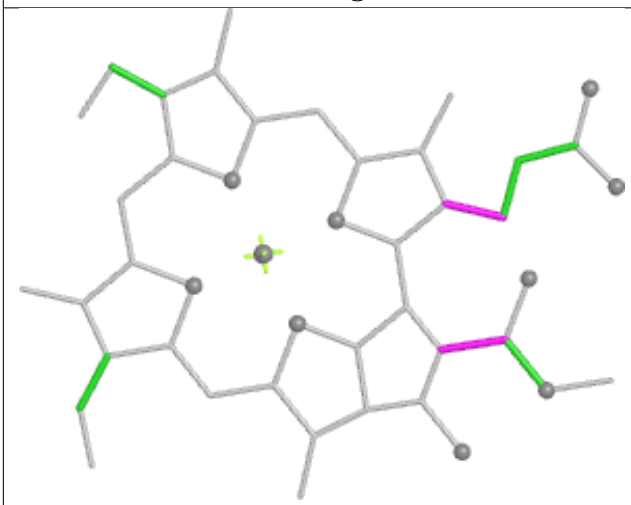
Ligand CLA c5 411



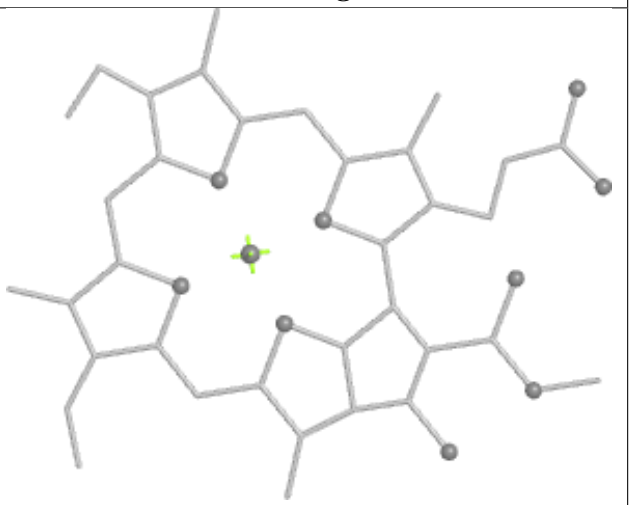
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Bond angles

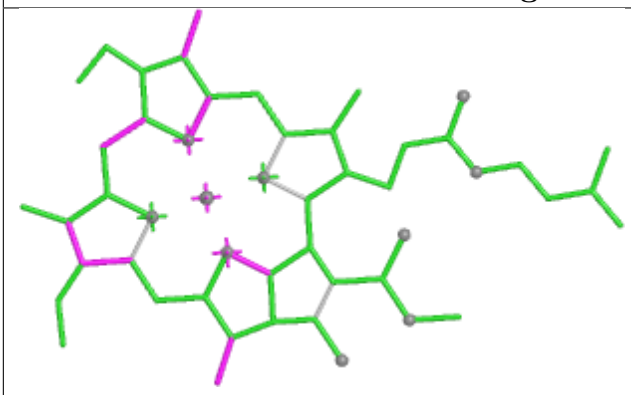


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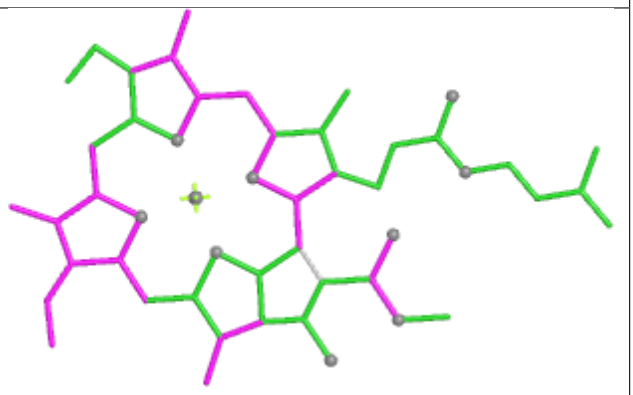


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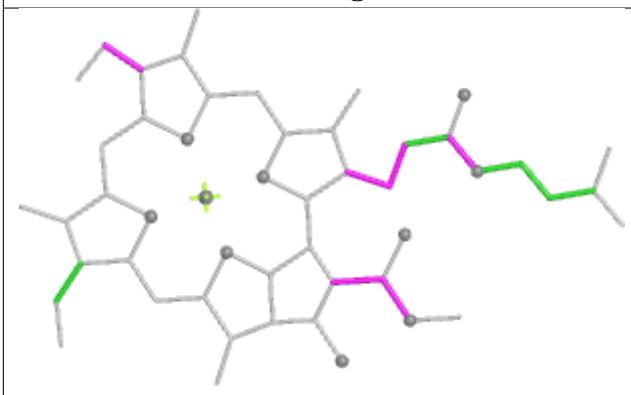
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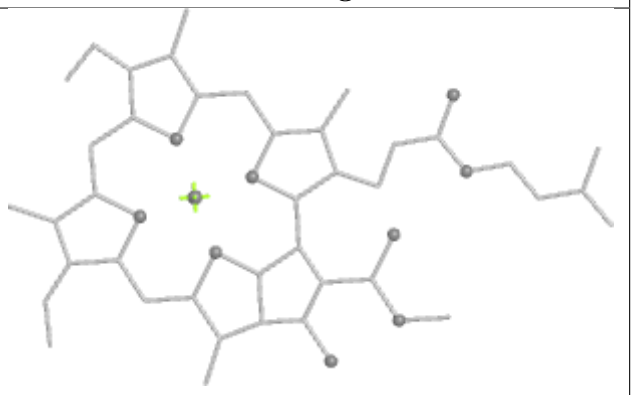
Bond lengths



Bond angles



Torsions

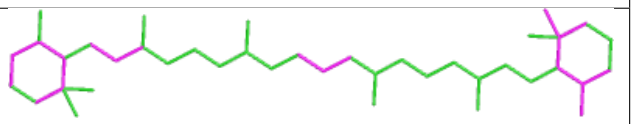


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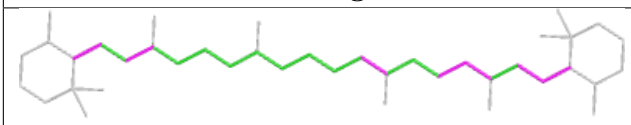
Ligand BCR a6 419



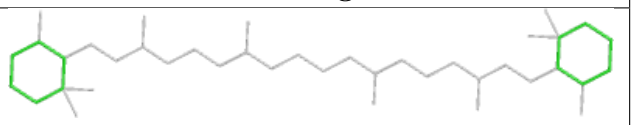
Bond lengths



Bond angles

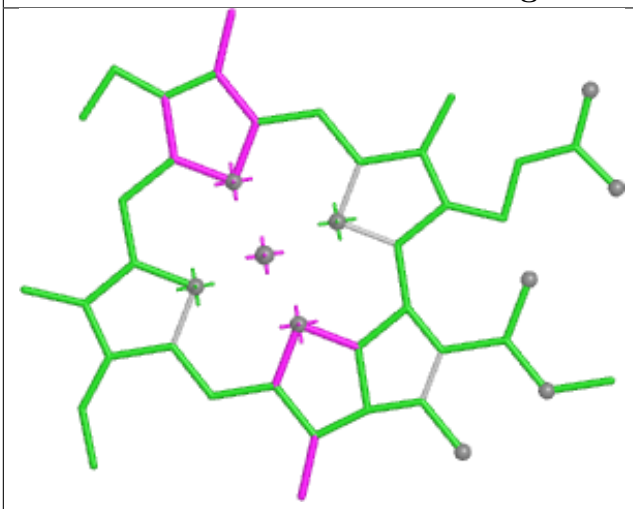


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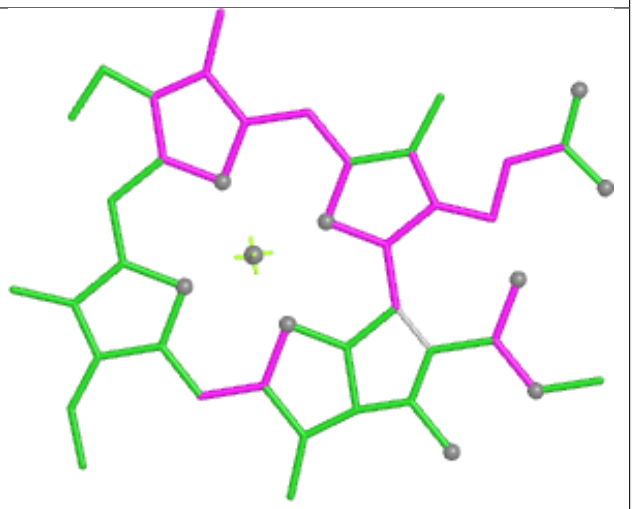


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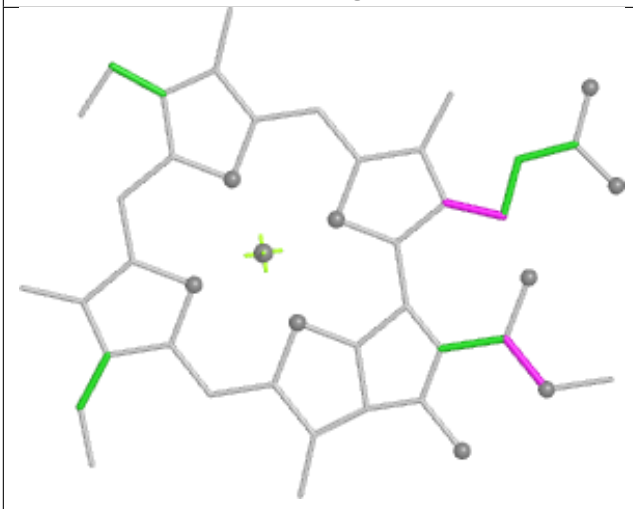
Ligand CLA c6 413



Bond lengths



Bond angles

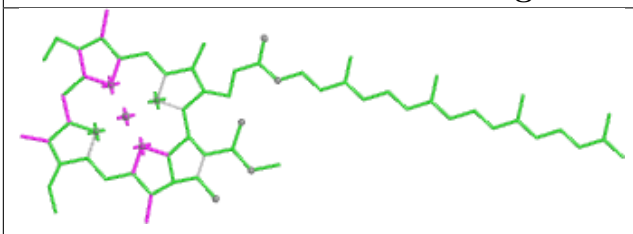


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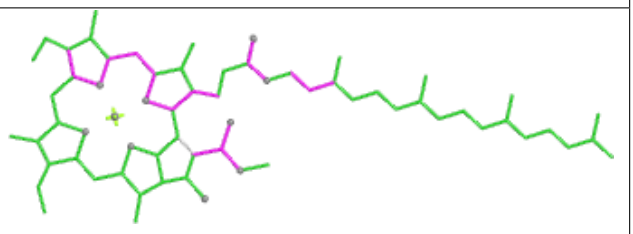


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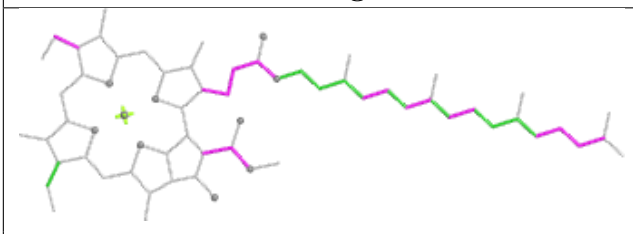
Ligand CLA aA 809



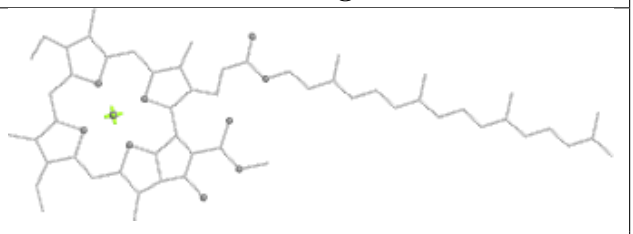
Bond lengths



Bond angles

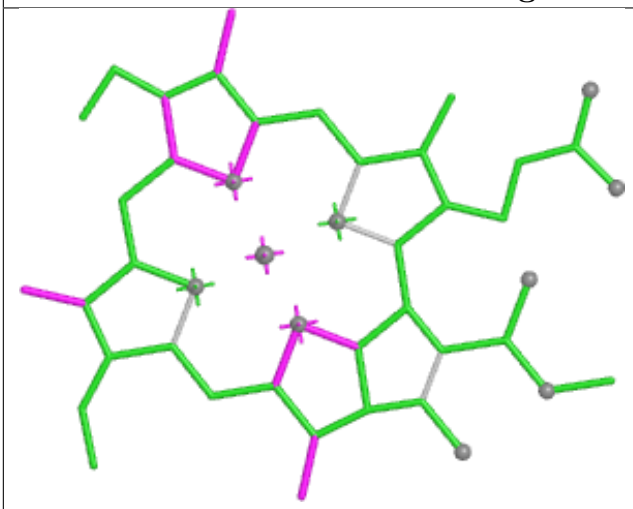


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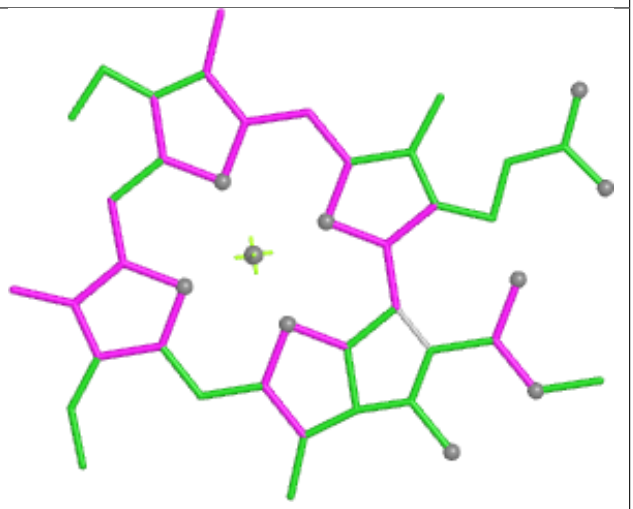


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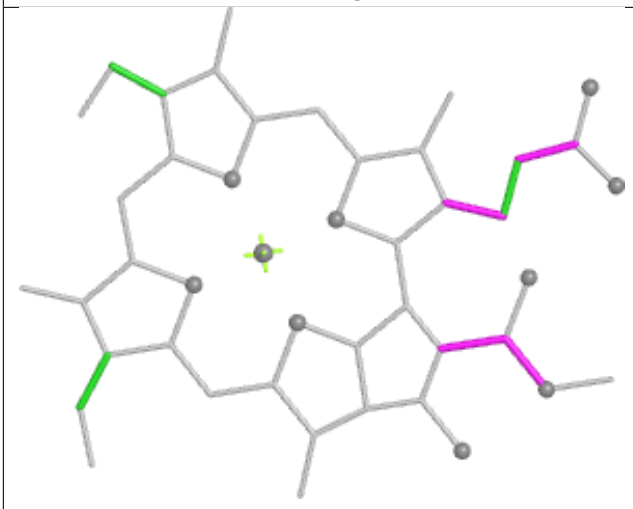
Ligand CLA b4 412



Bond lengths



Bond angles

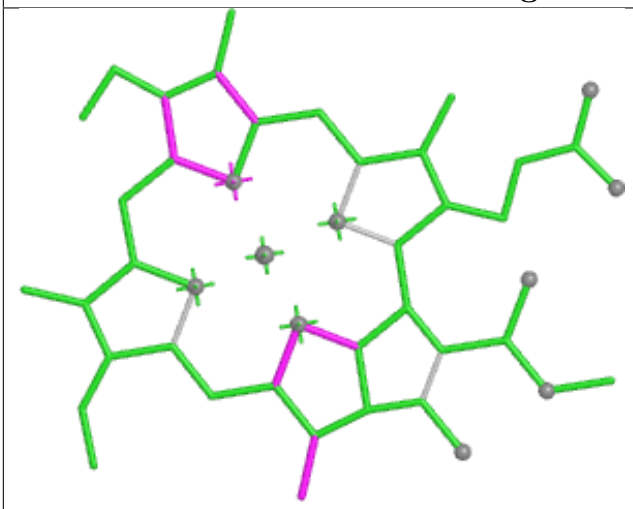


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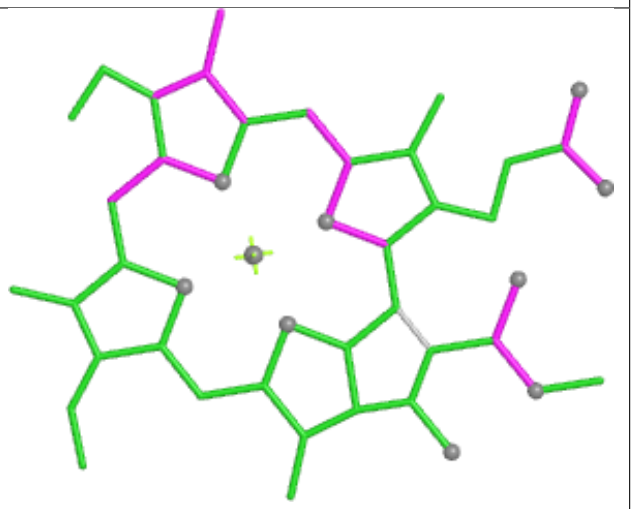


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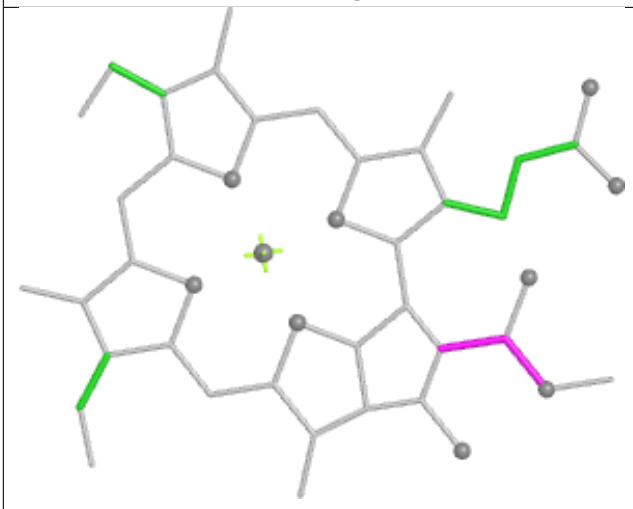
Ligand CLA c2 407



Bond lengths



Bond angles

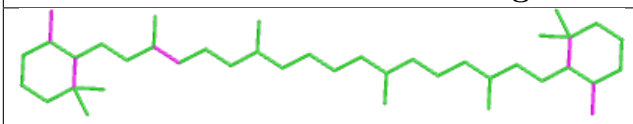


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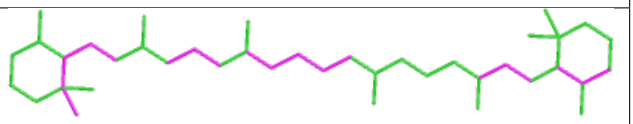


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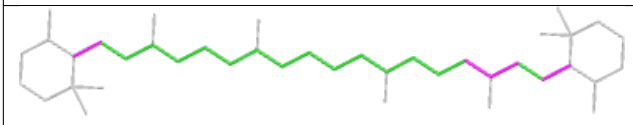
Ligand BCR bA 852



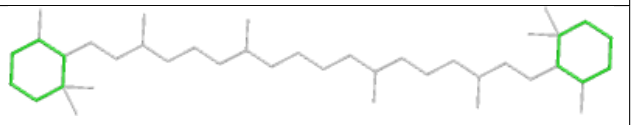
Bond lengths



Bond angles

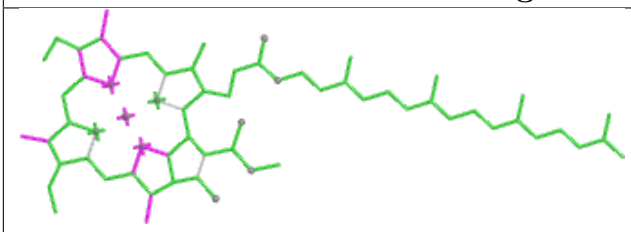


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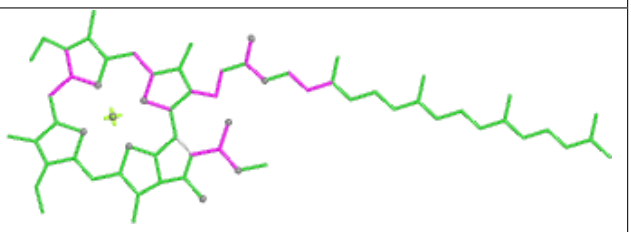


Rings

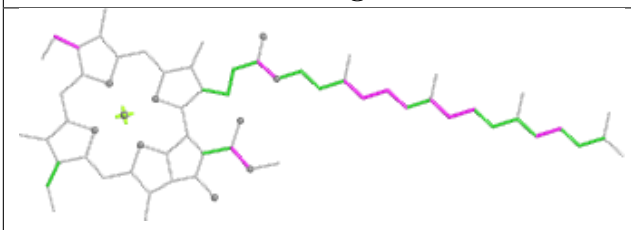
Ligand CLA cB 809



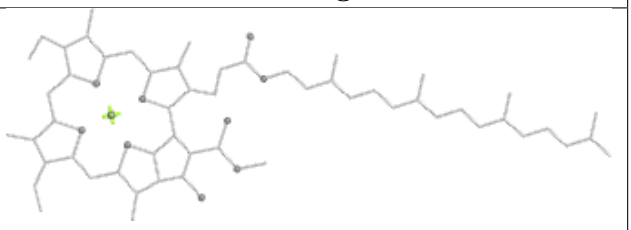
Bond lengths



Bond angles

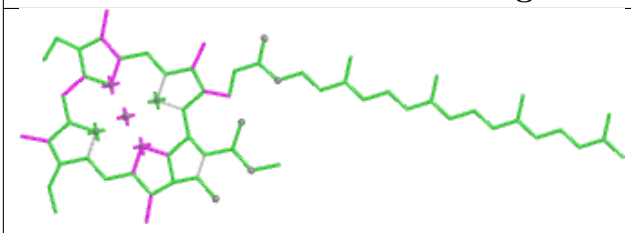


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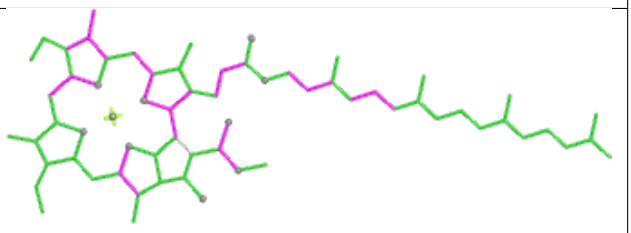


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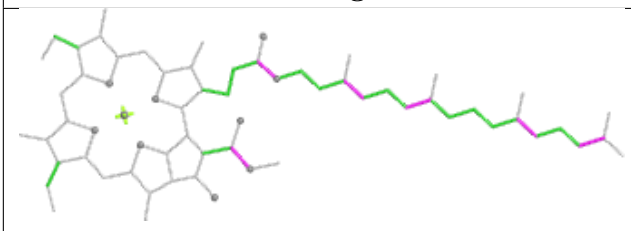
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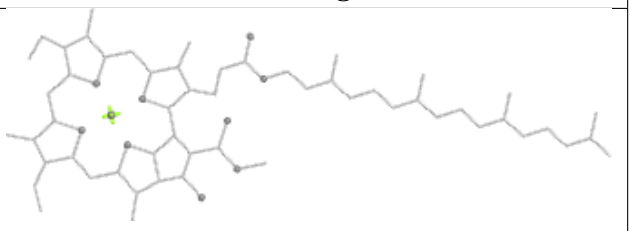
Bond lengths



Bond angles

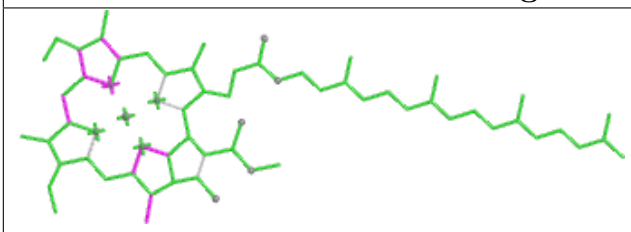


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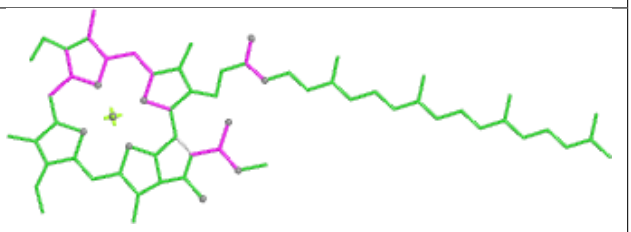


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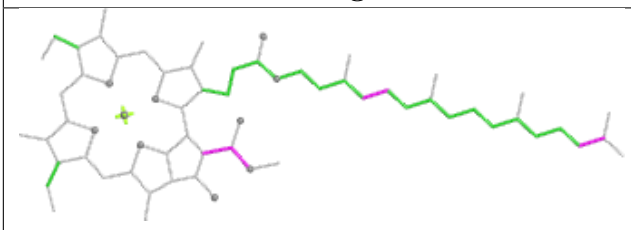
Ligand CLA c6 411



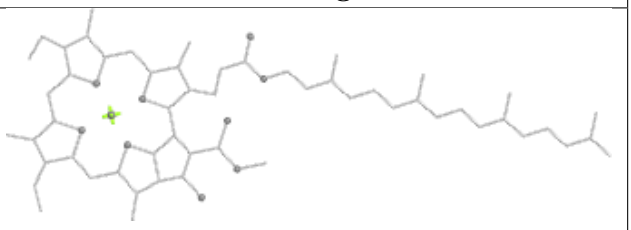
Bond lengths



Bond angles

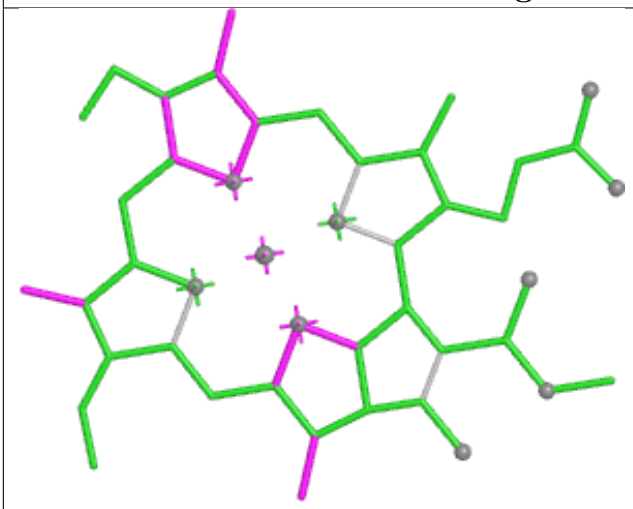


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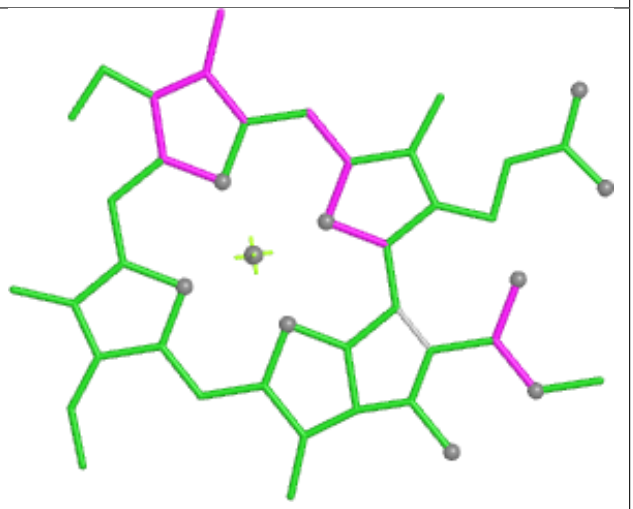


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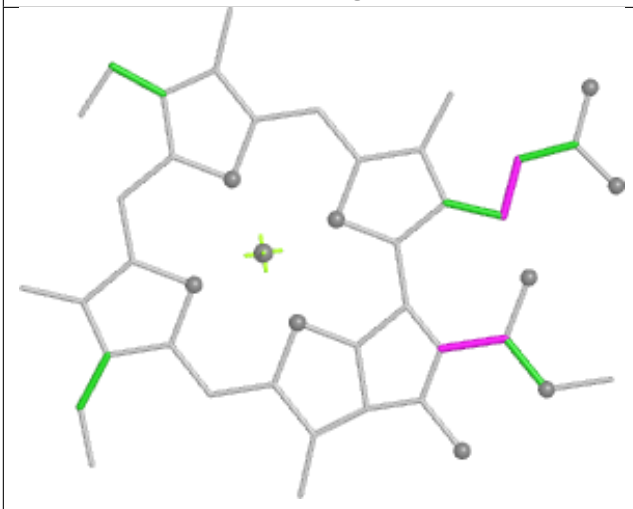
Ligand CLA aA 816



Bond lengths



Bond angles

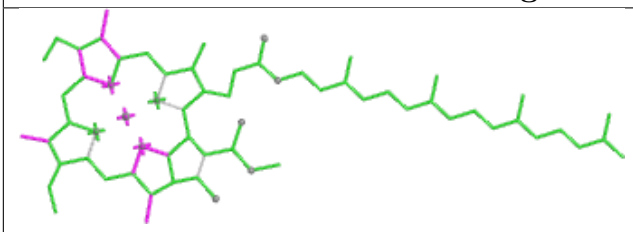


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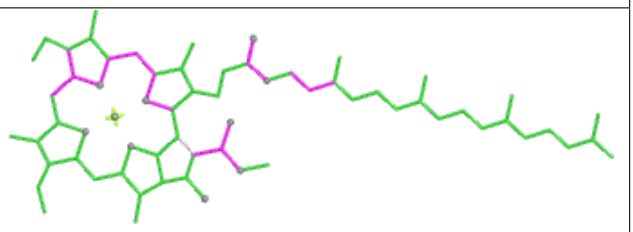


Rings

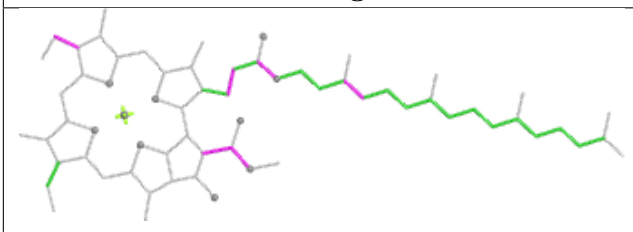
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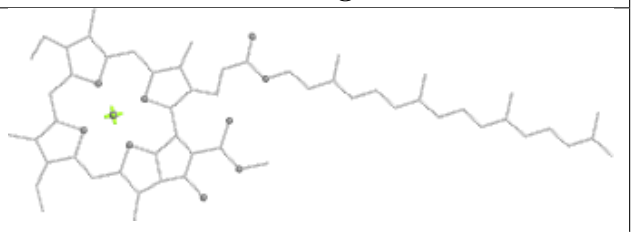
Bond lengths



Bond angles

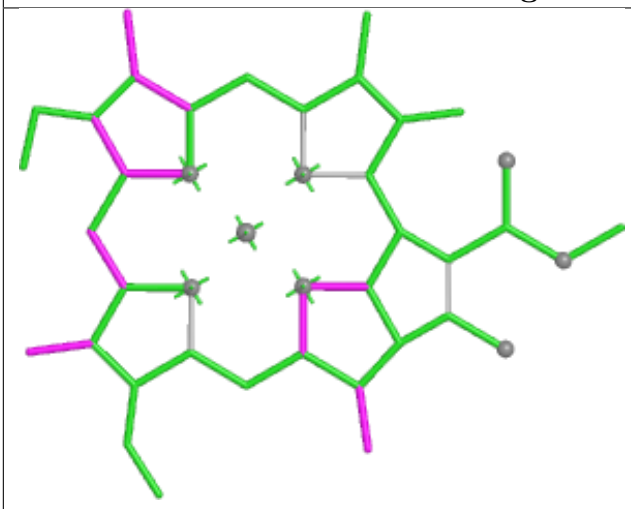


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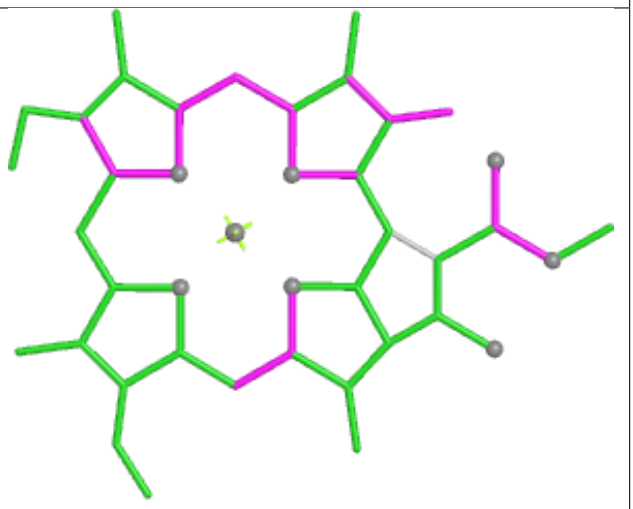


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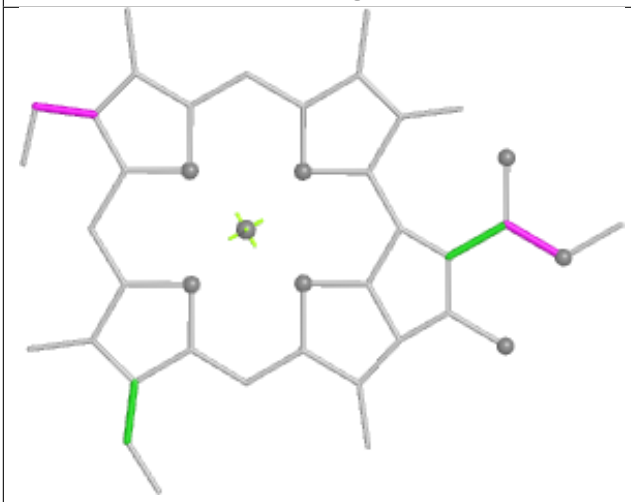
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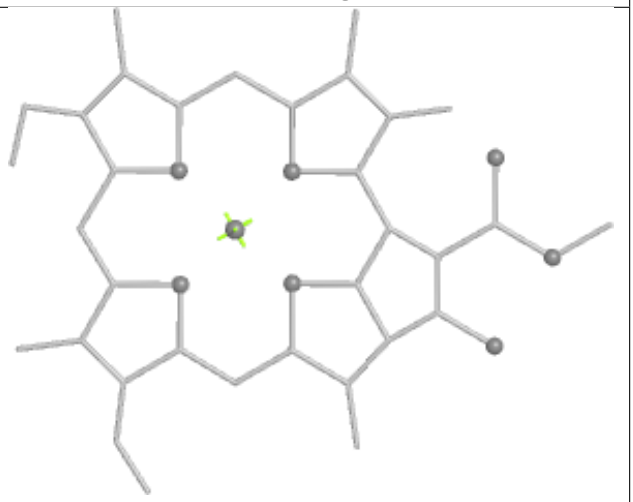
Bond lengths



Bond angles

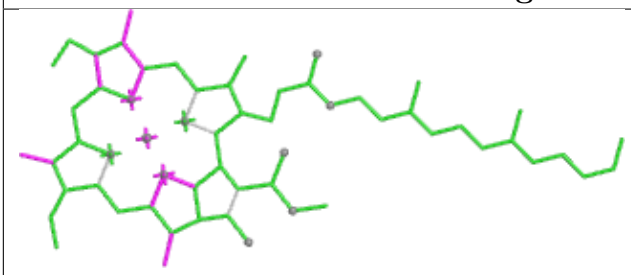


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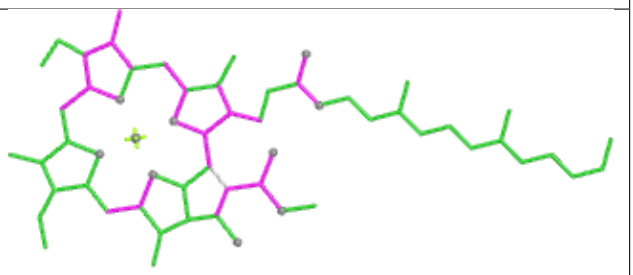


Rings

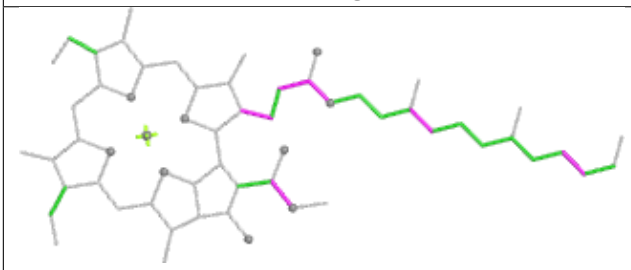
Ligand CLA aB 818



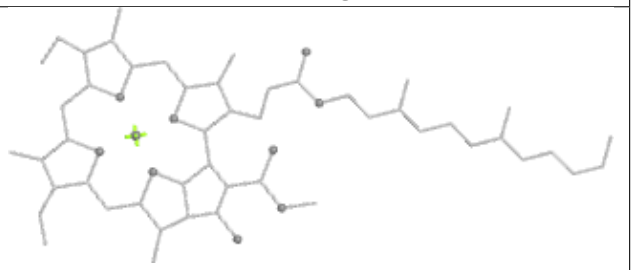
Bond lengths



Bond angles

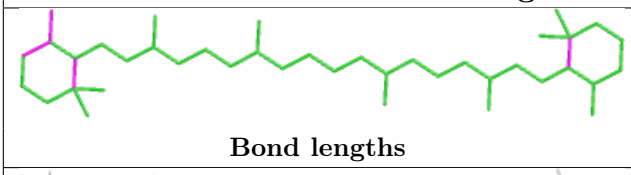


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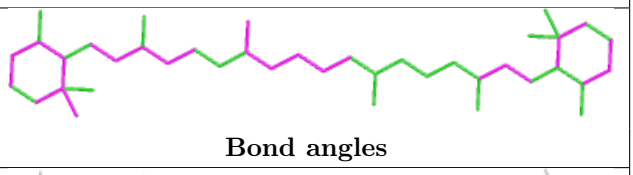


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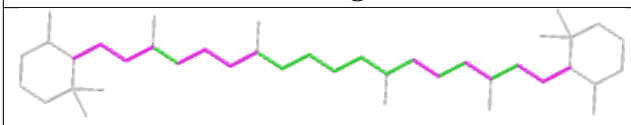
Ligand BCR a2 401



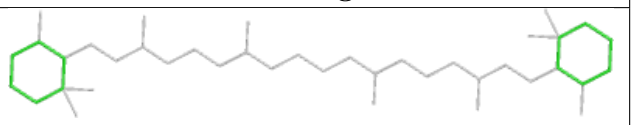
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Bond angles

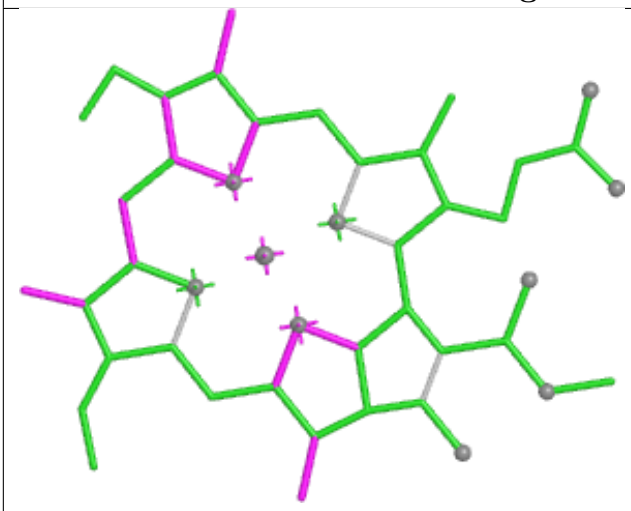


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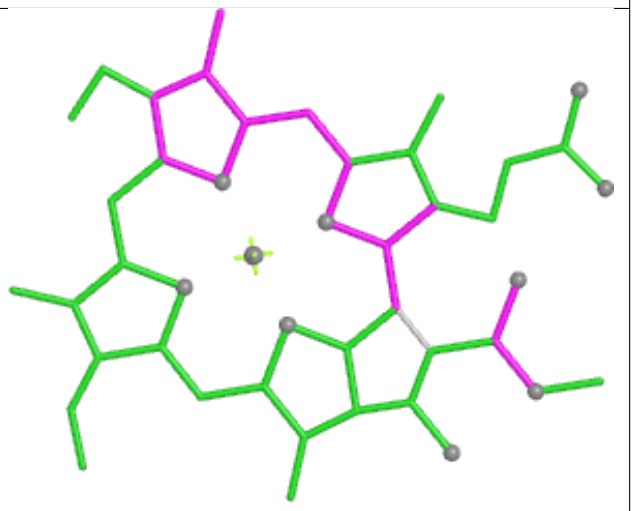


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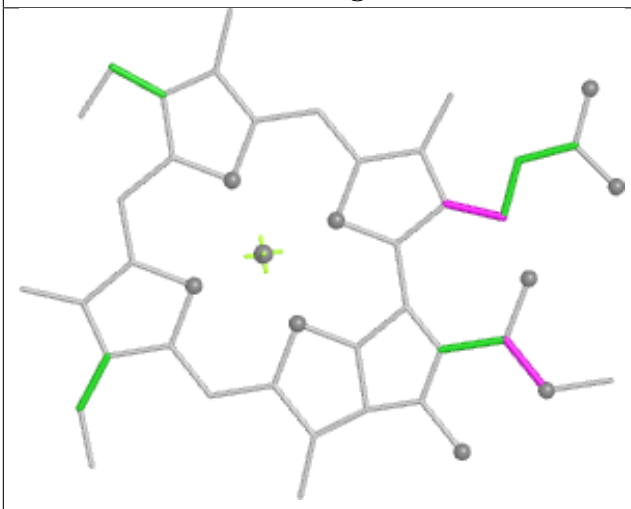
Ligand CLA a1 410



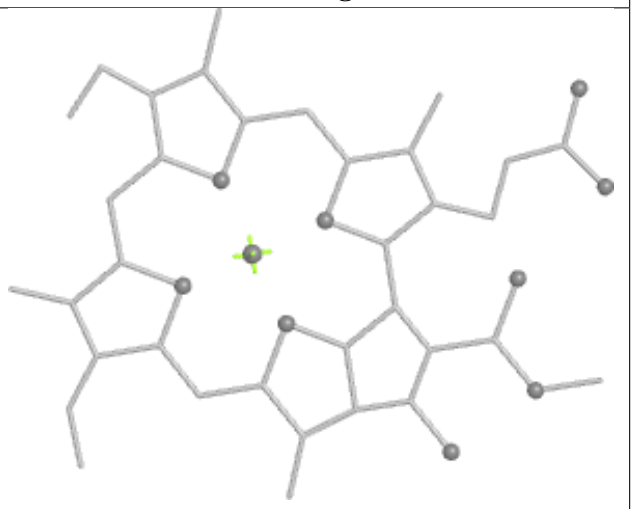
Bond lengths



Bond angles

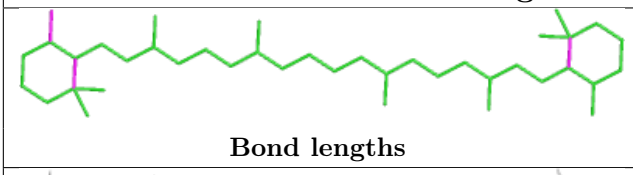


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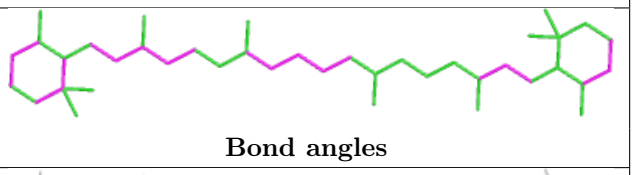


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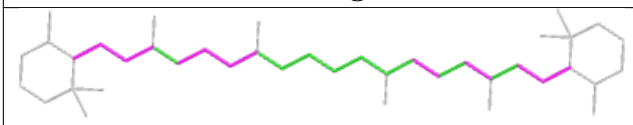
Ligand BCR b6 421



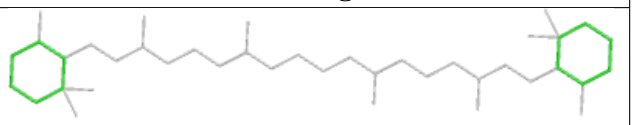
Bond lengths



Bond angles

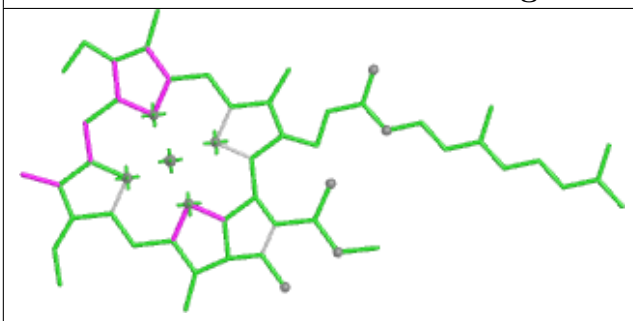


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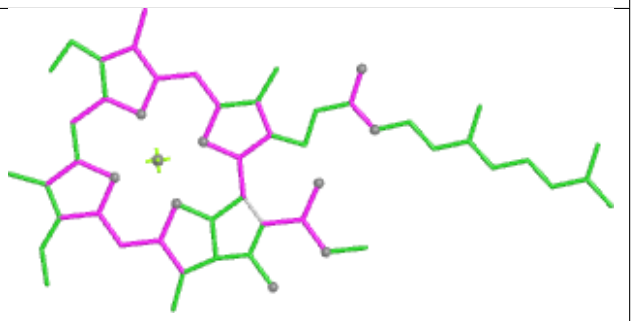


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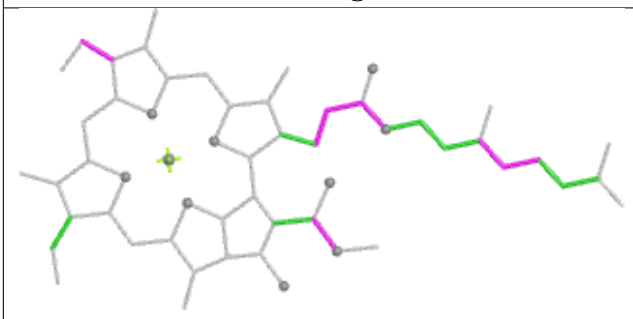
Ligand CLA c3 417



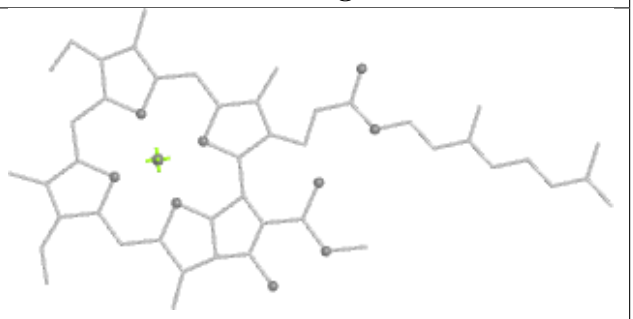
Bond lengths



Bond angles

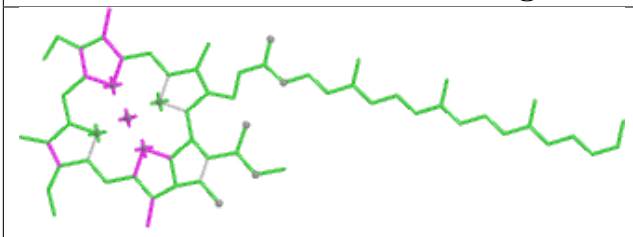


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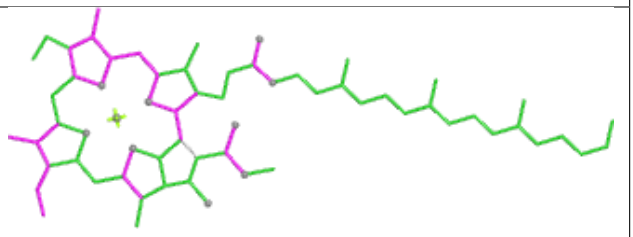


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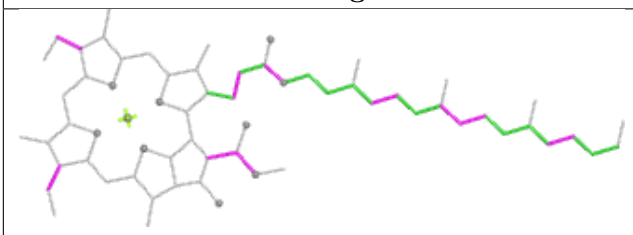
Ligand CLA b1 410



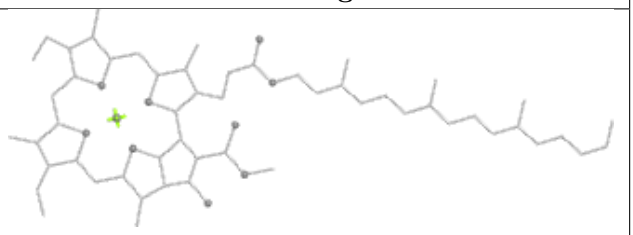
Bond lengths



Bond angles

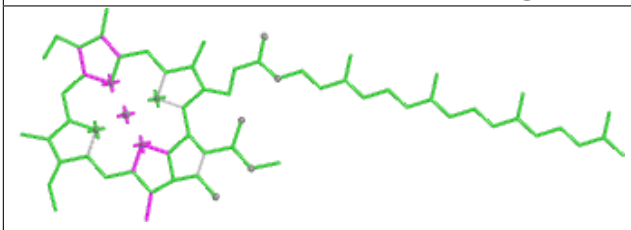


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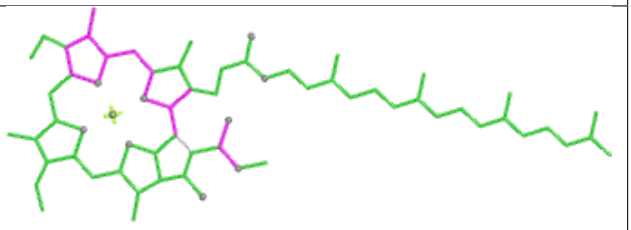


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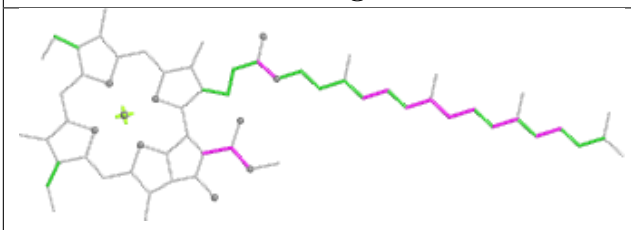
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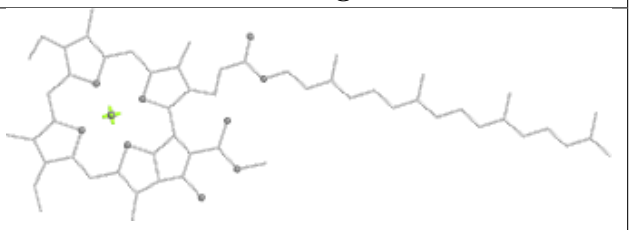
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Bond angles

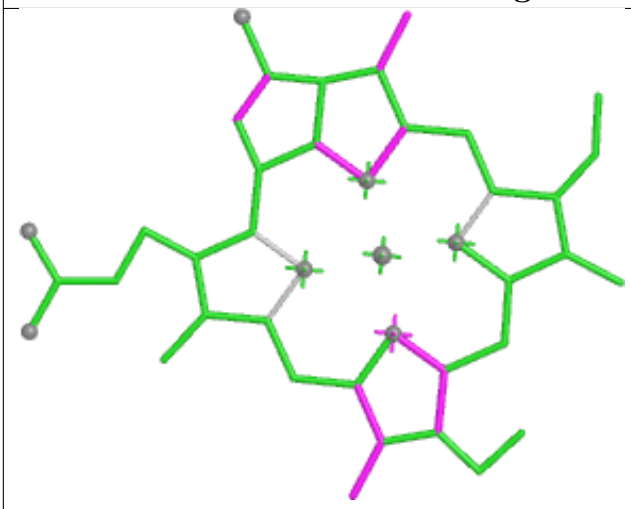


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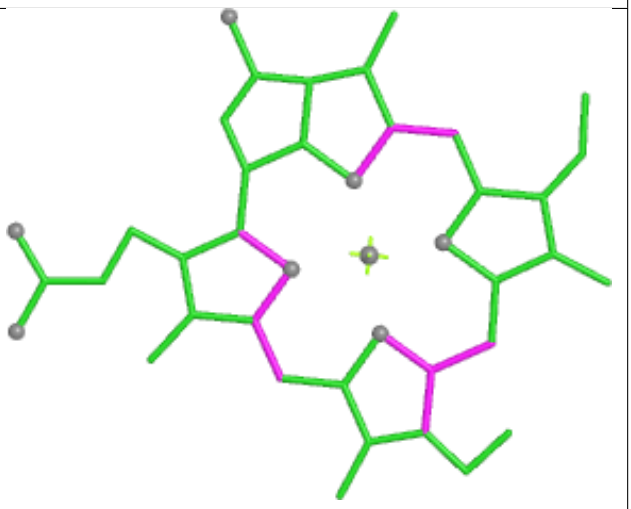


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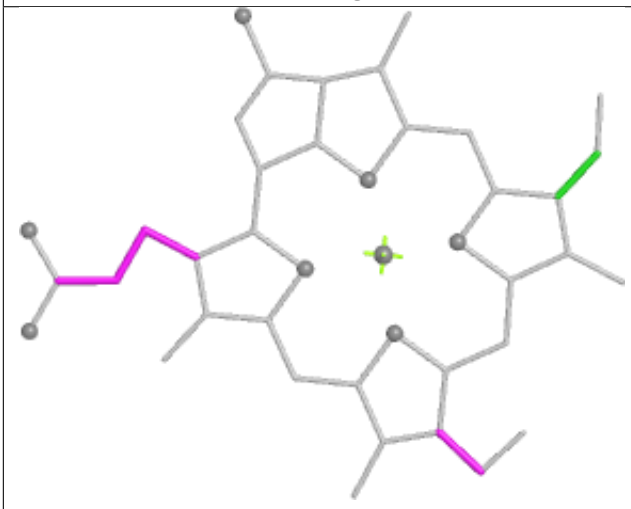
Ligand CLA bA 844



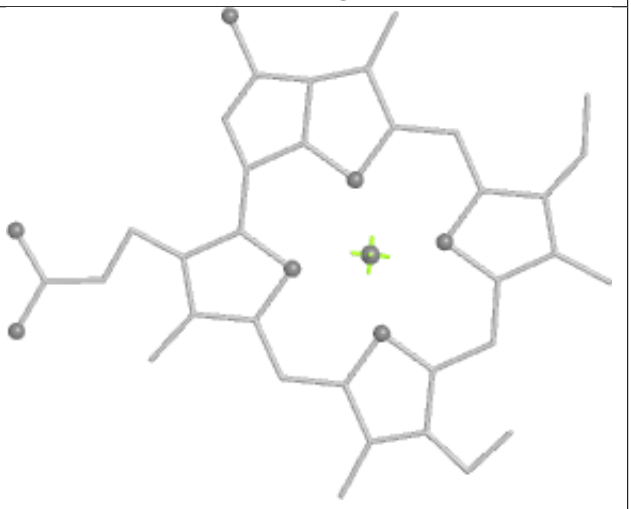
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Bond angles

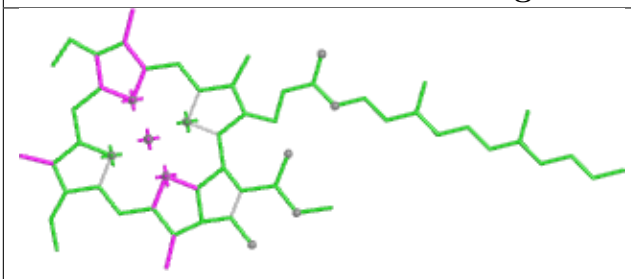


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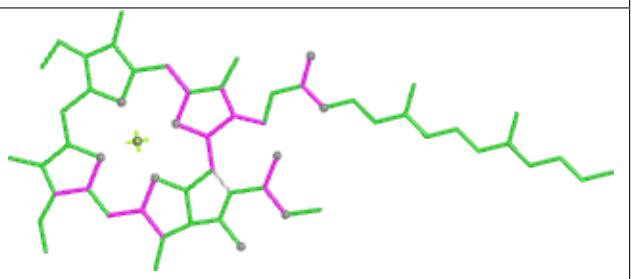


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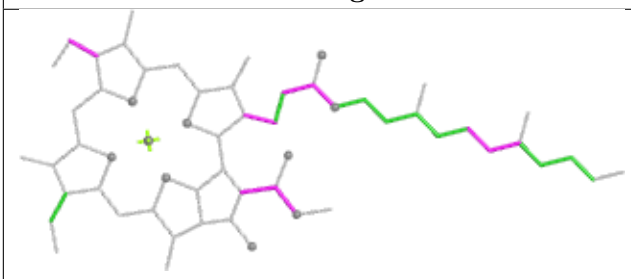
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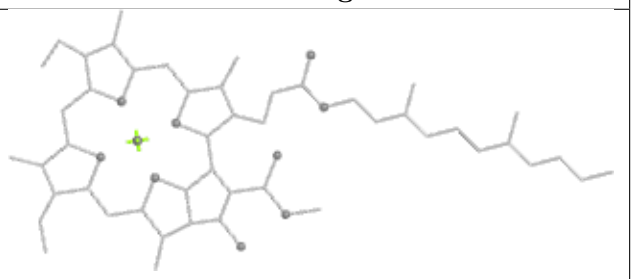
Bond lengths



Bond angles

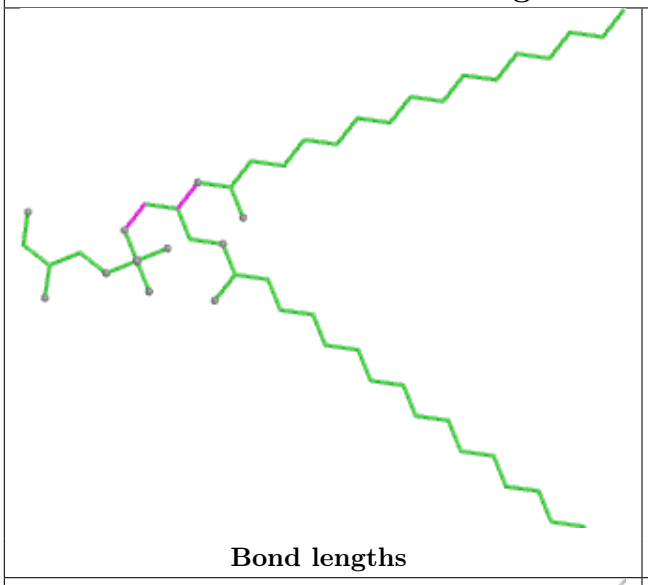


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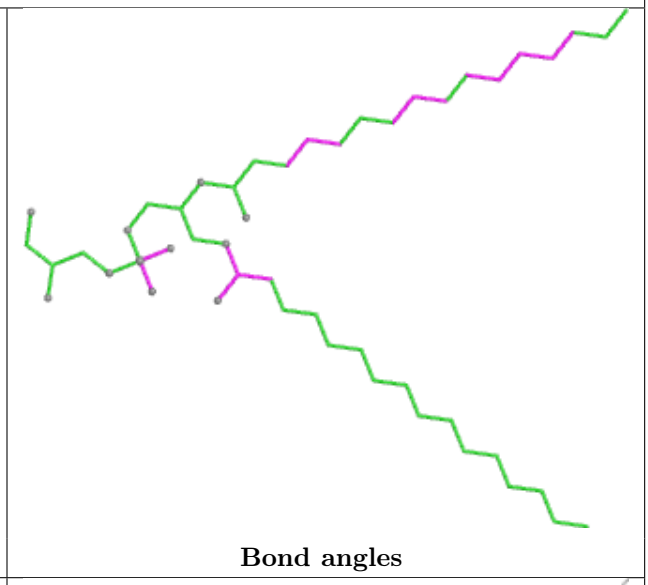


Rings

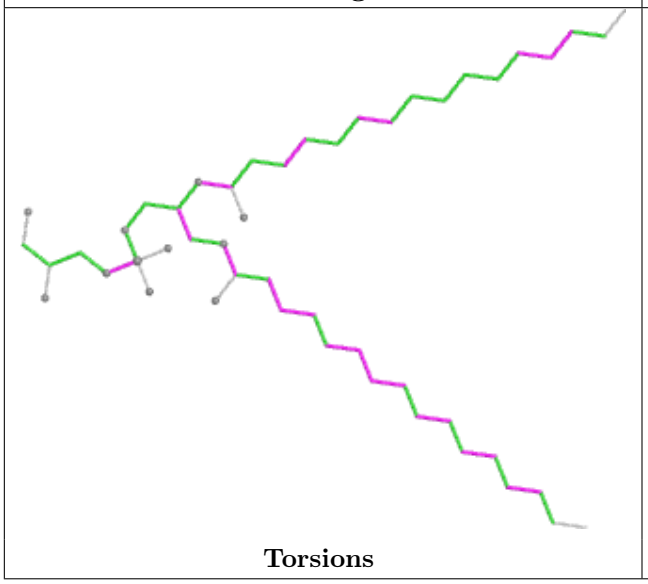
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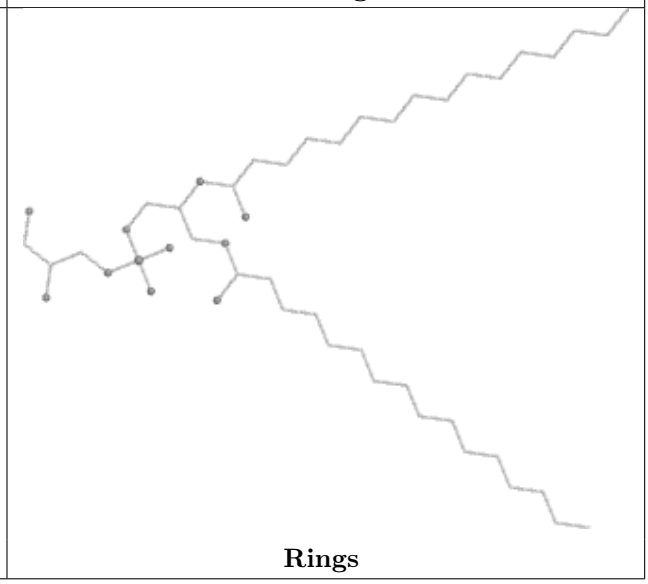
Bond lengths



Bond angles

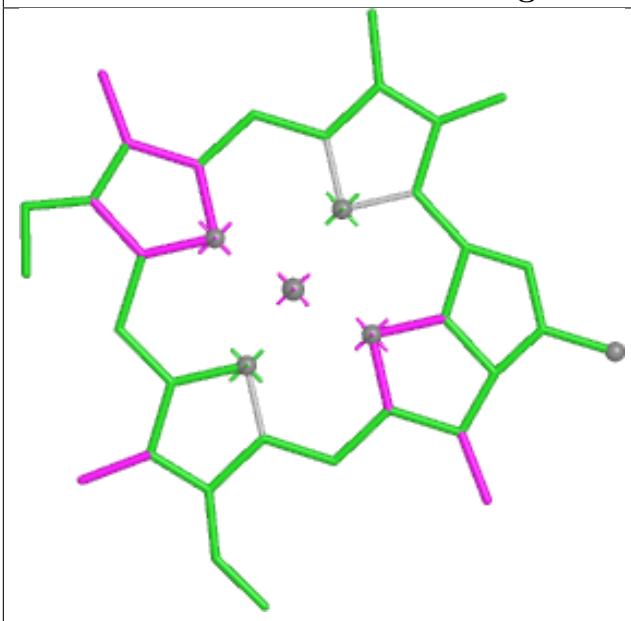


Torsions



Rings

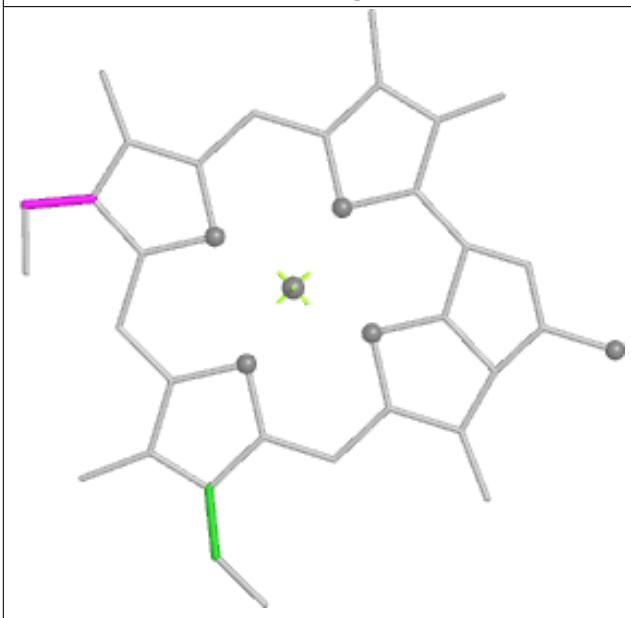
Ligand CLA bJ 102



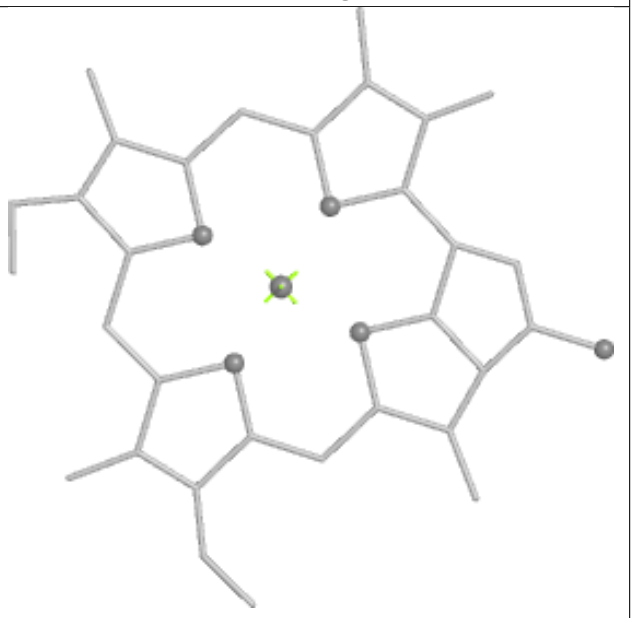
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Bond angles

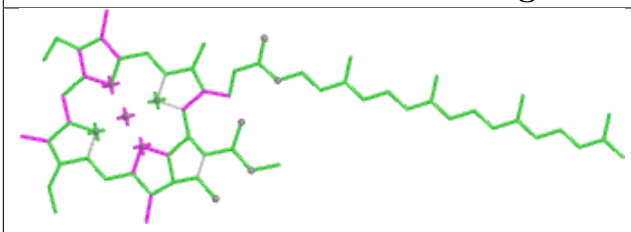


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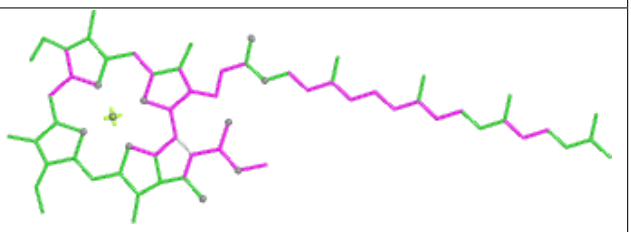


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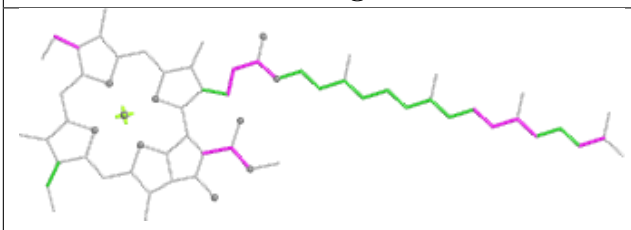
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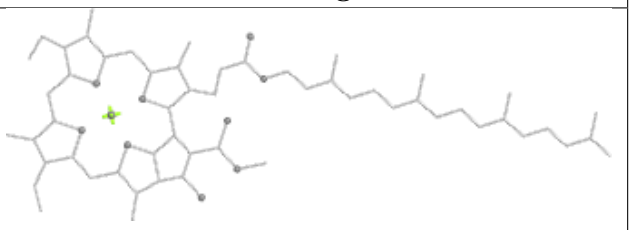
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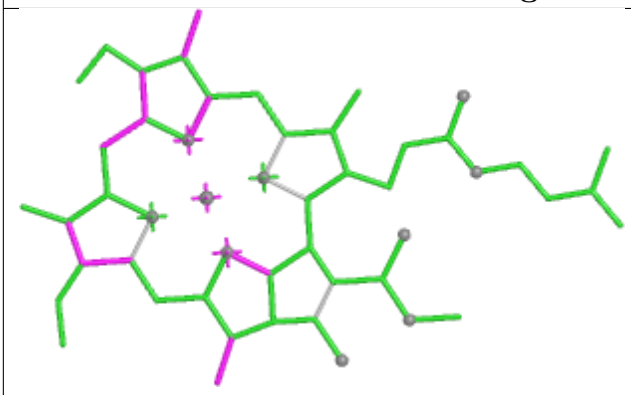


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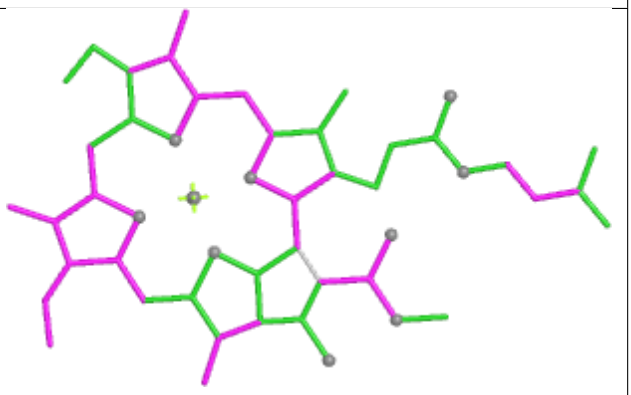


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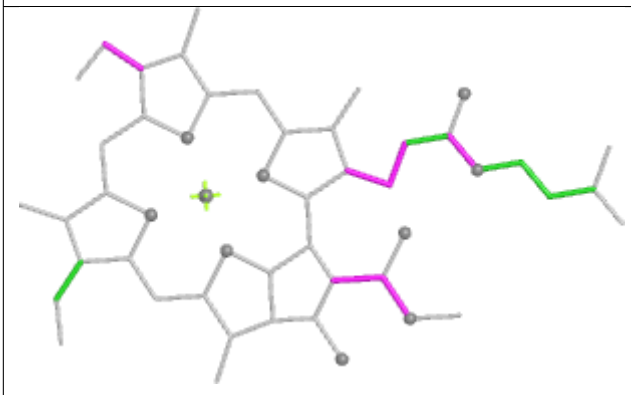
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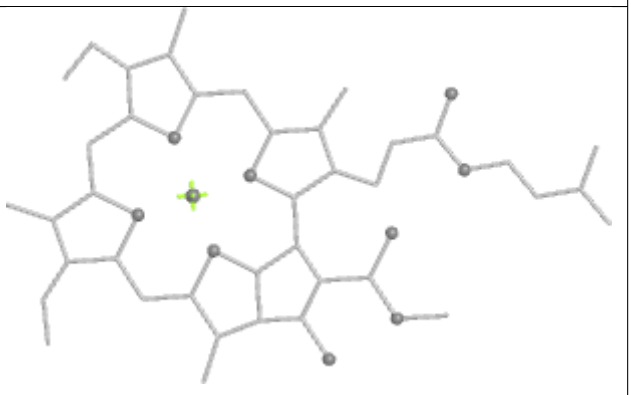
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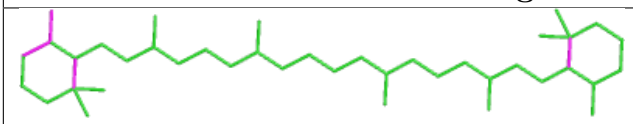


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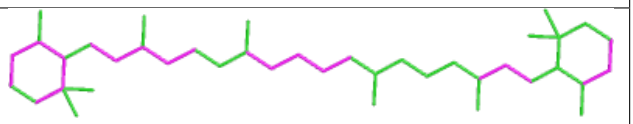


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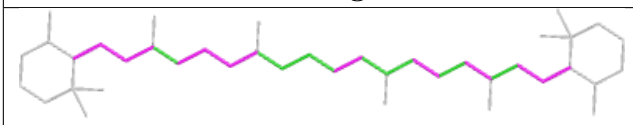
Ligand BCR b6 402



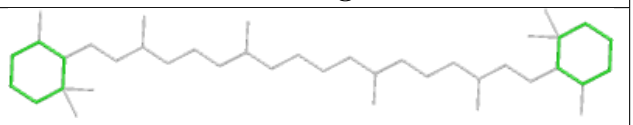
Bond lengths



Bond angles

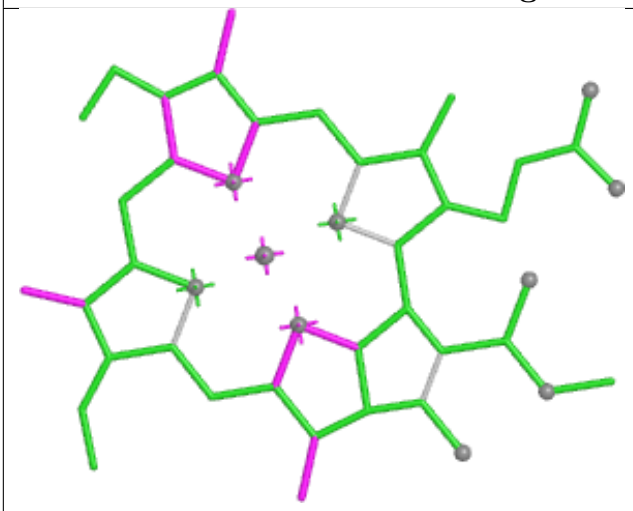


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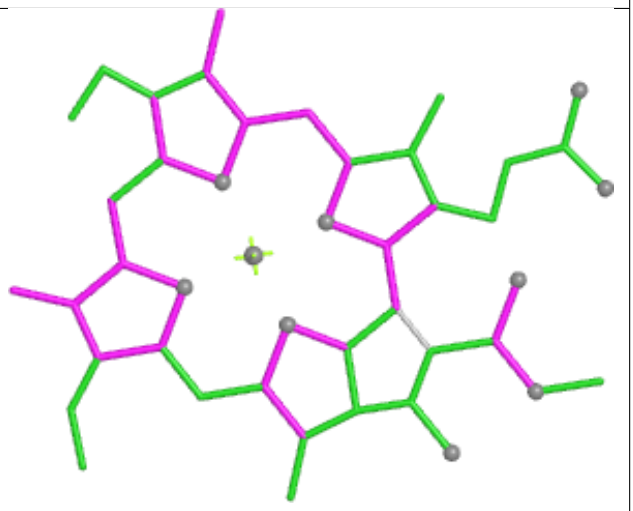


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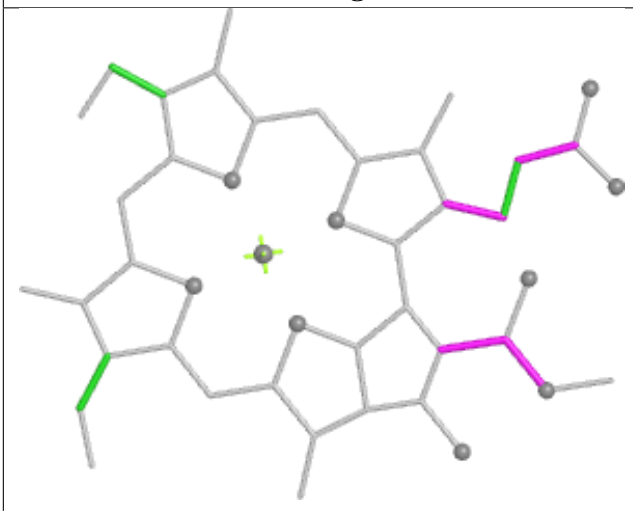
Ligand CLA a3 412



Bond lengths



Bond angles

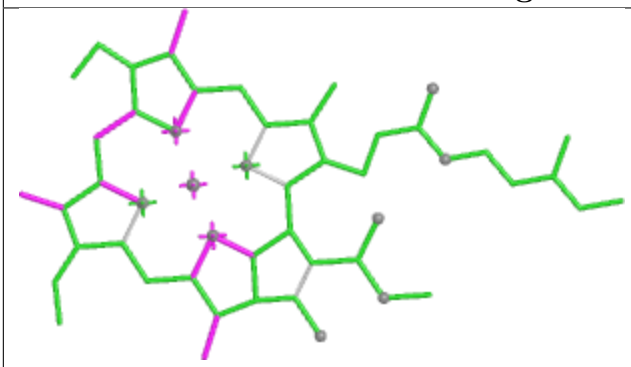


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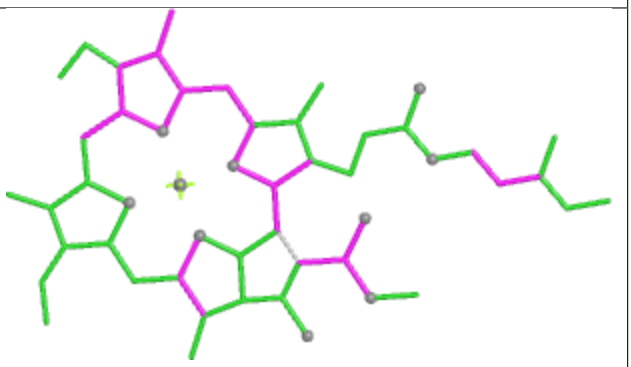


Rings

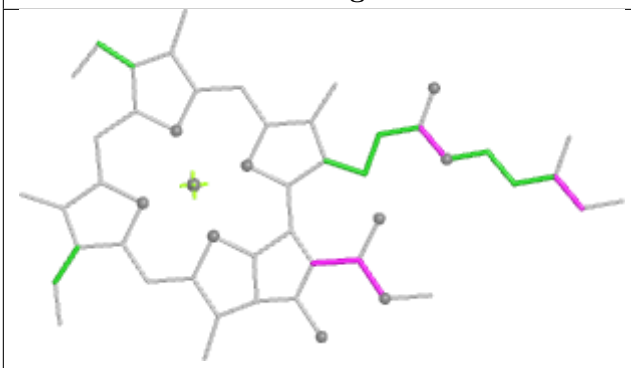
Ligand CLA cA 838



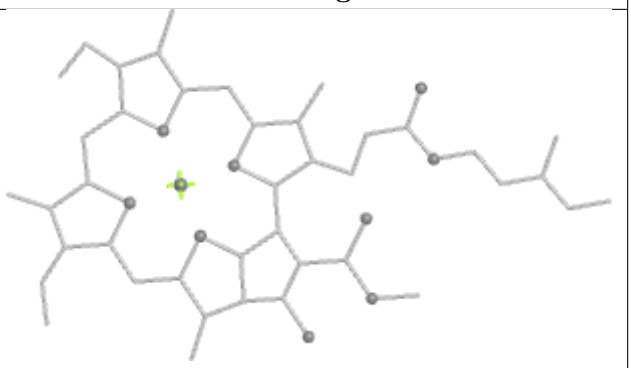
Bond lengths



Bond angles

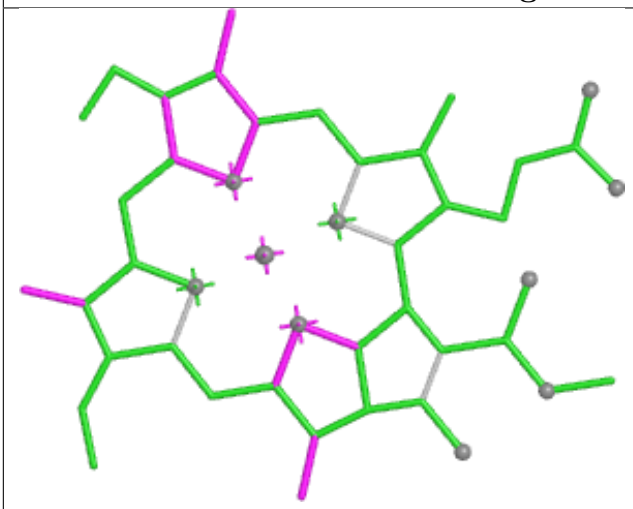


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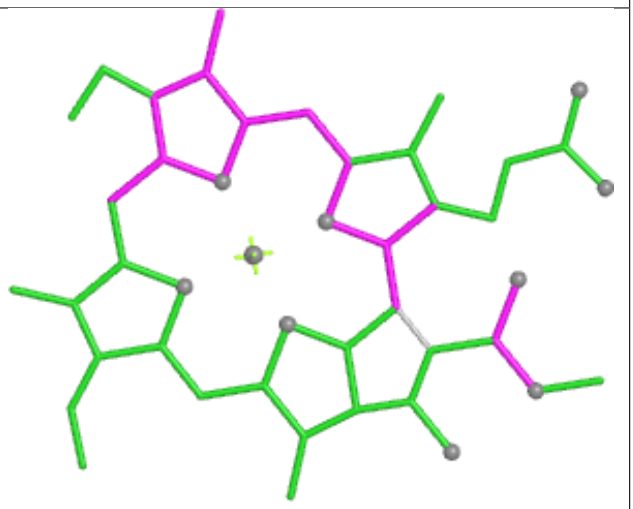


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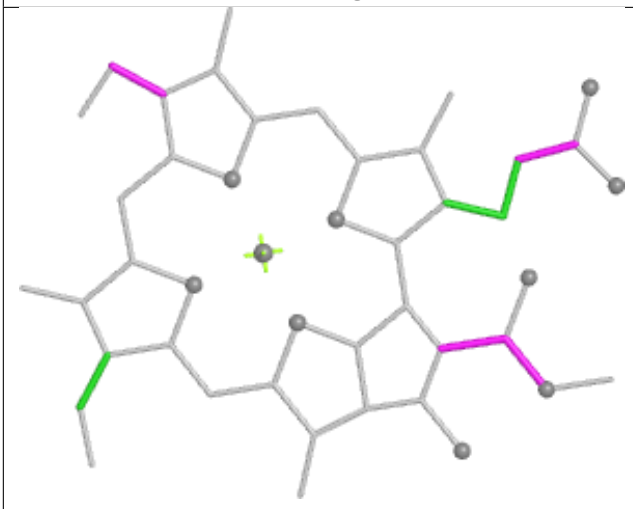
Ligand CLA a3 407



Bond lengths



Bond angles

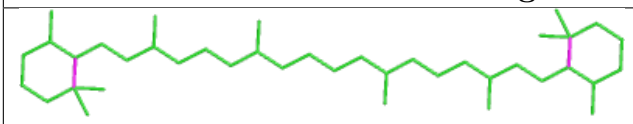


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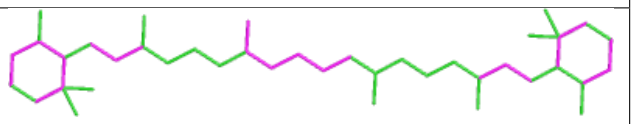


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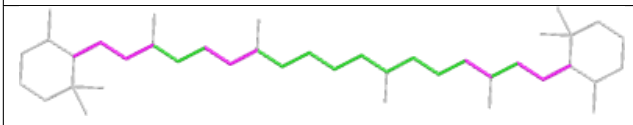
Ligand BCR c6 421



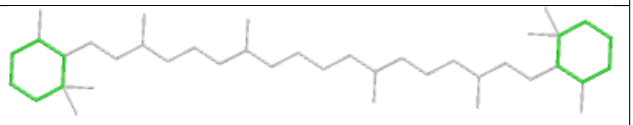
Bond lengths



Bond angles

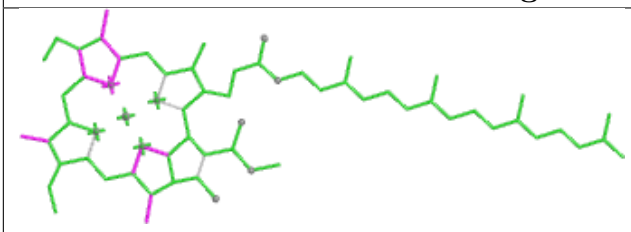


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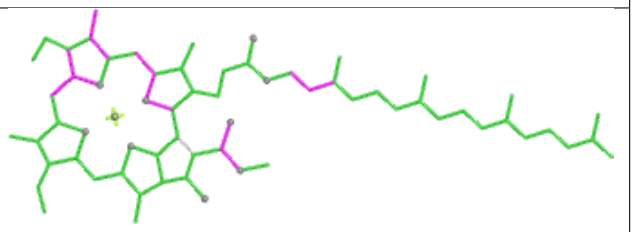


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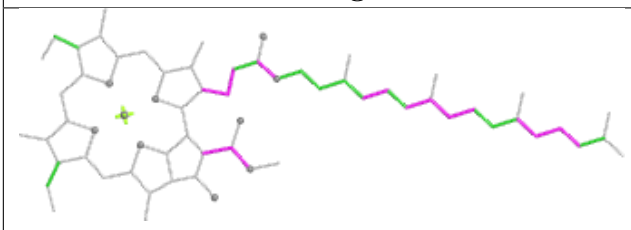
Ligand CLA c3 402



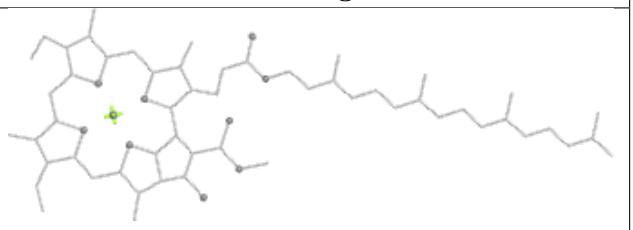
Bond lengths



Bond angles

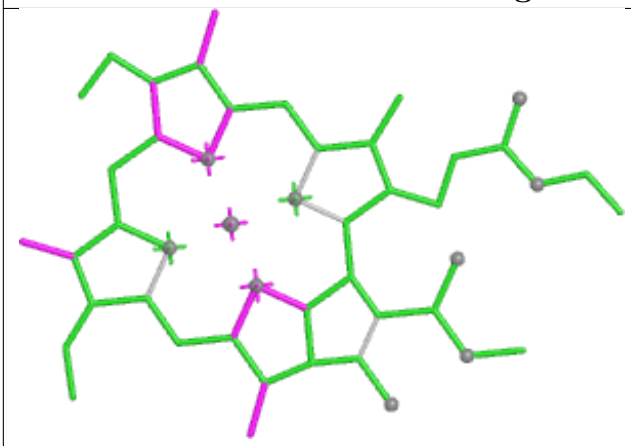


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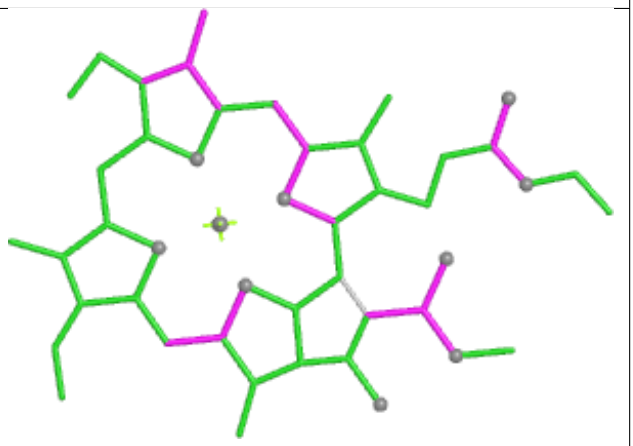


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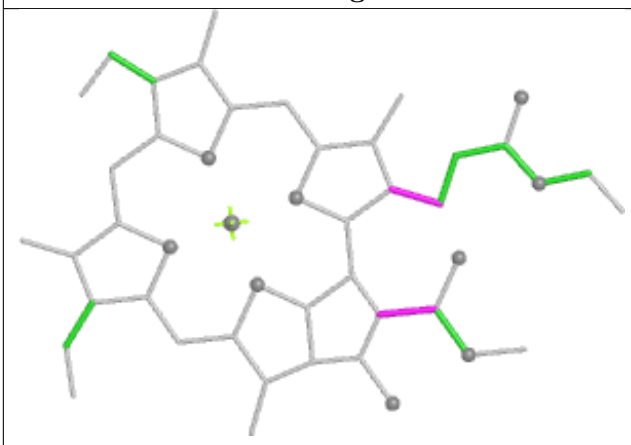
Ligand CLA bB 838



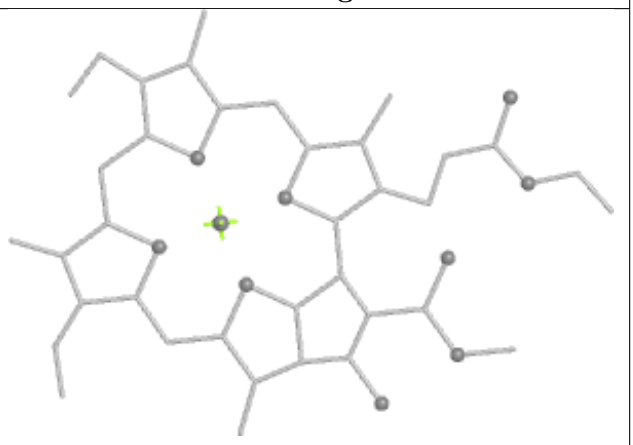
Bond lengths



Bond angles

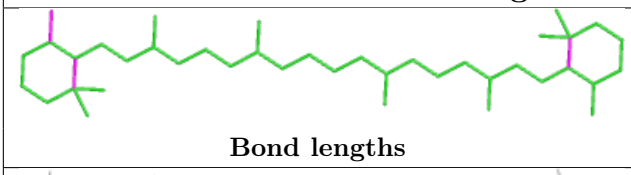


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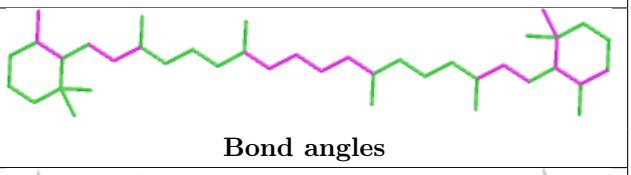


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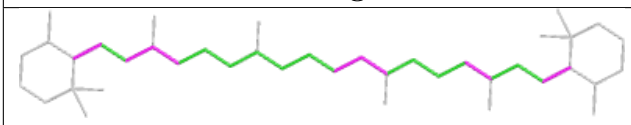
Ligand BCR cM 101



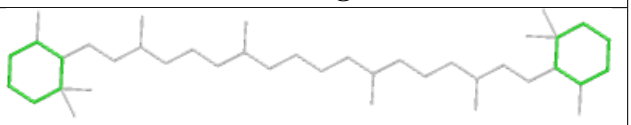
Bond lengths



Bond angles

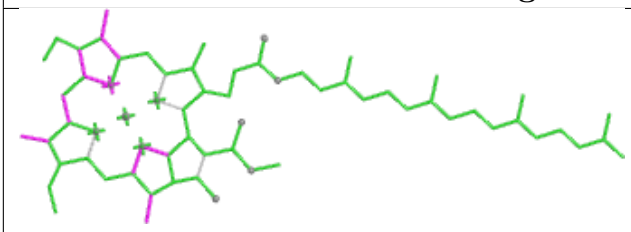


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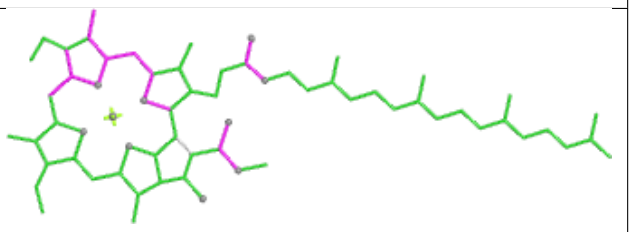


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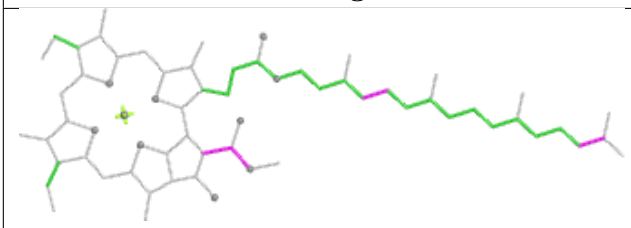
Ligand CLA b5 409



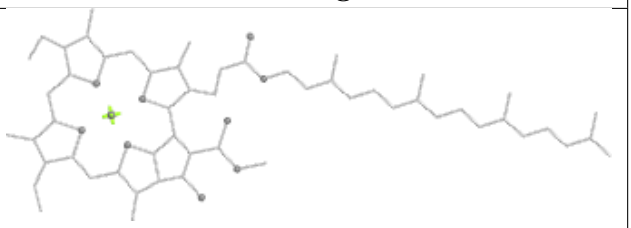
Bond lengths



Bond angles

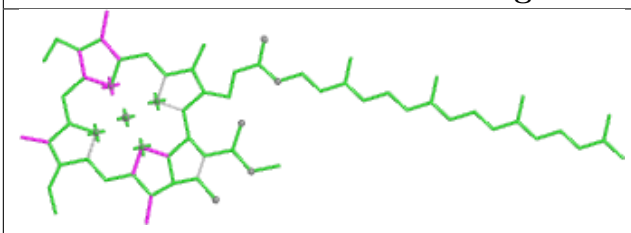


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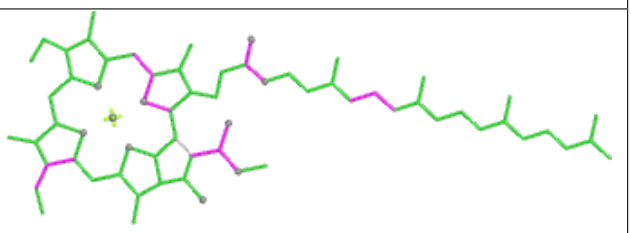


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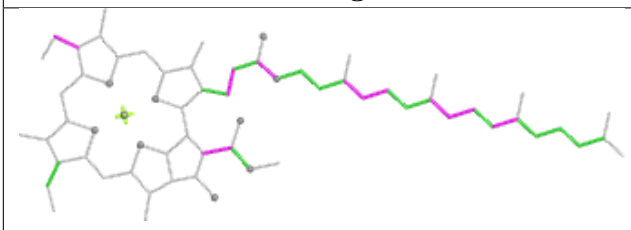
Ligand CLA bB 808



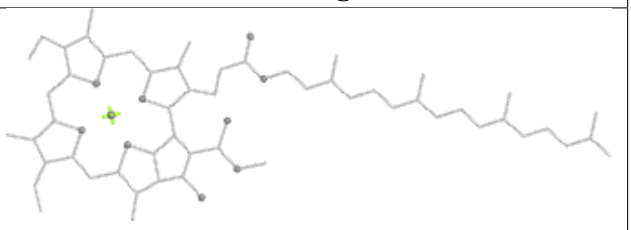
Bond lengths



Bond angles

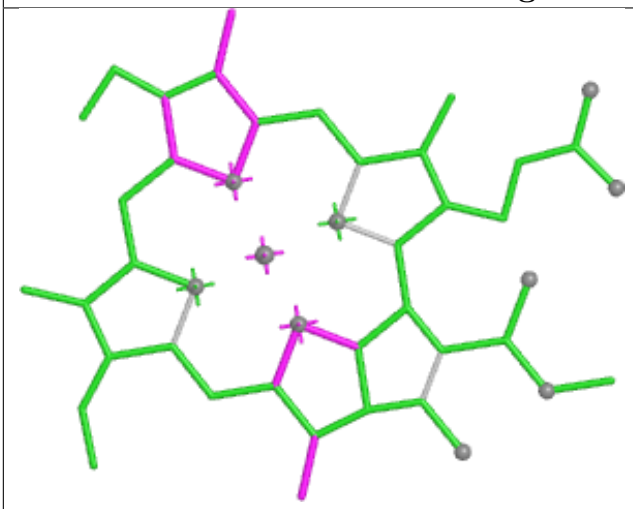


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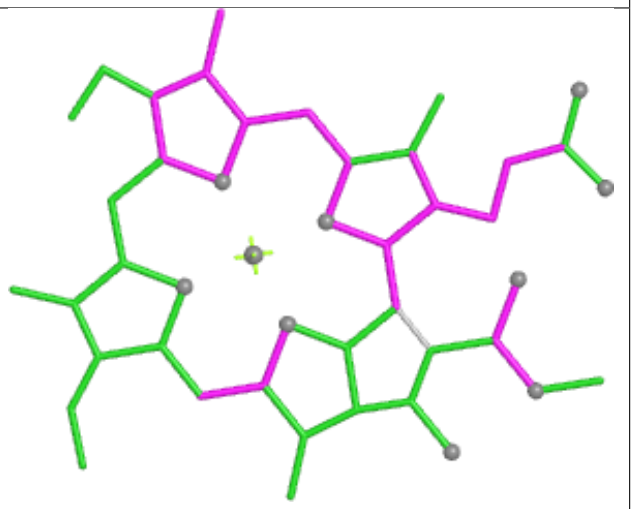


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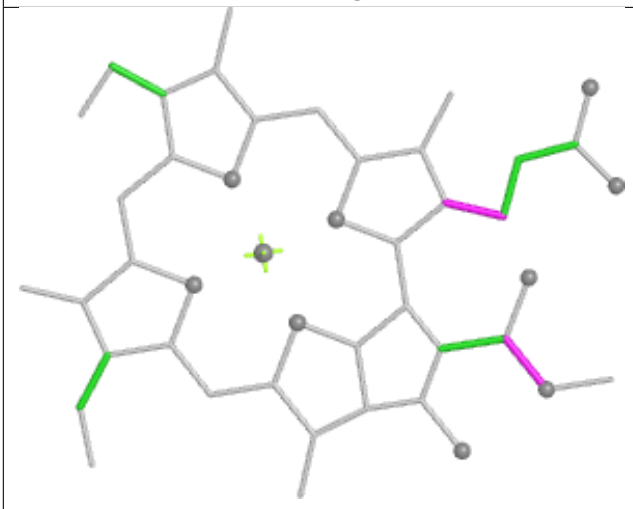
Ligand CLA b6 412



Bond lengths



Bond angles

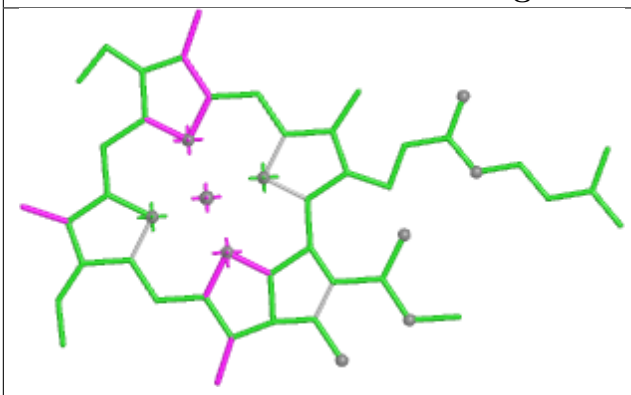


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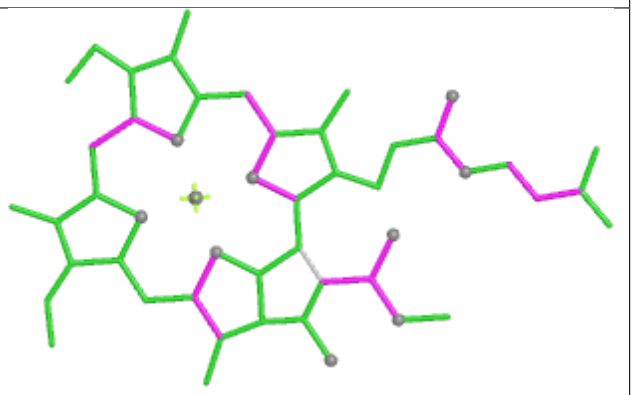


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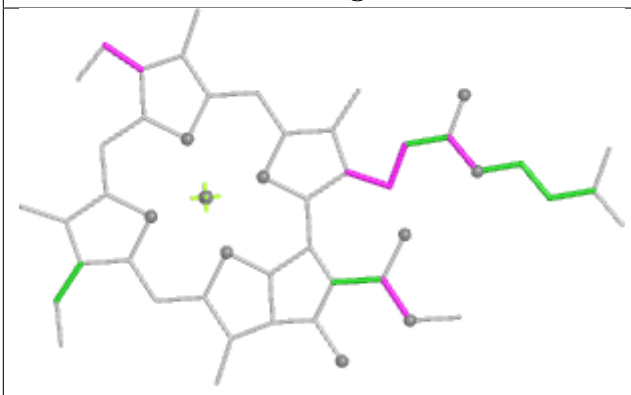
Ligand CLA bA 832



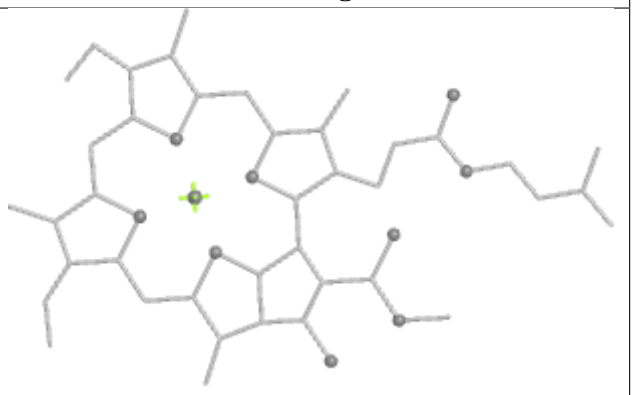
Bond lengths



Bond angles



Torsions

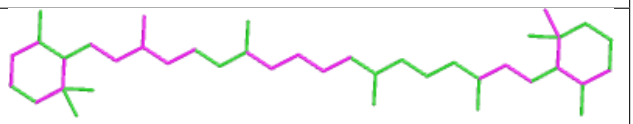


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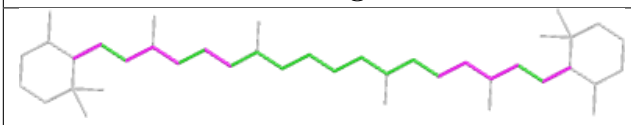
Ligand BCR c6 402



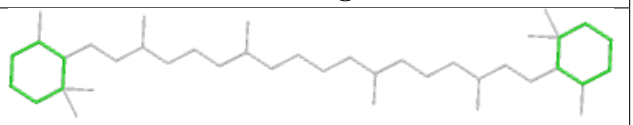
Bond lengths



Bond angles

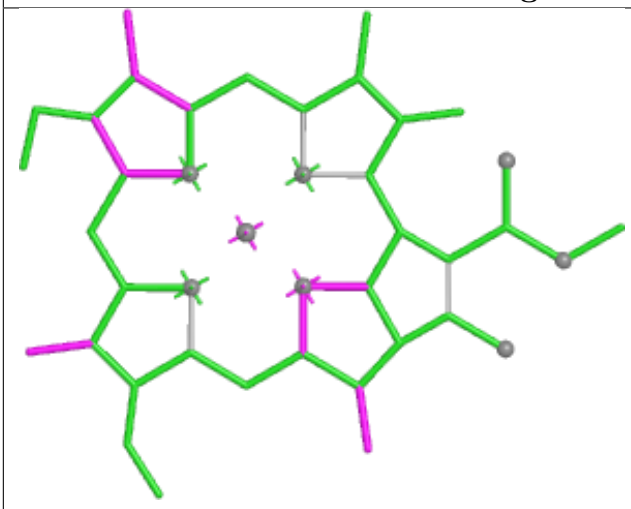


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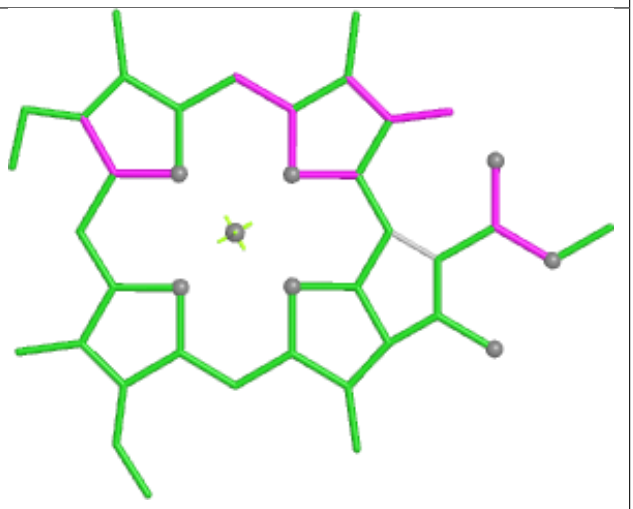


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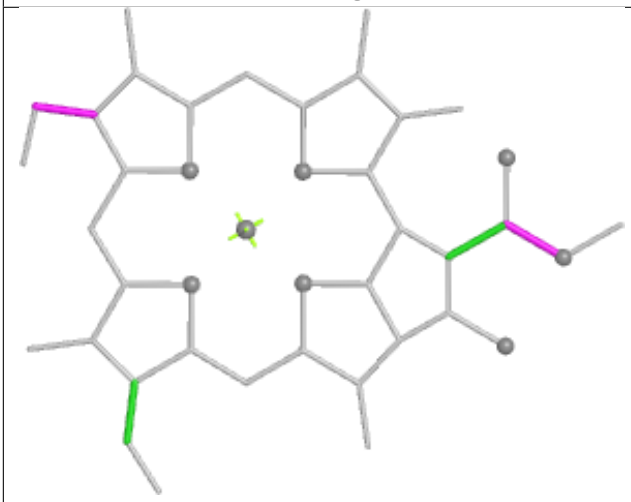
Ligand CLA c4 414



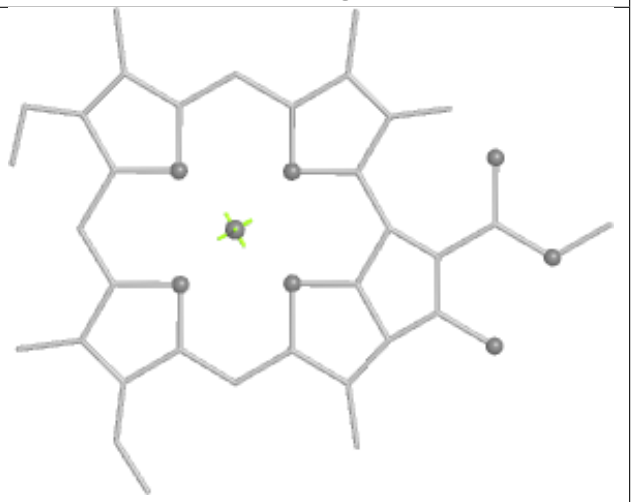
Bond lengths



Bond angles

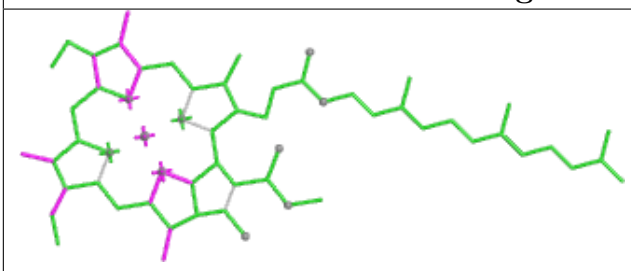


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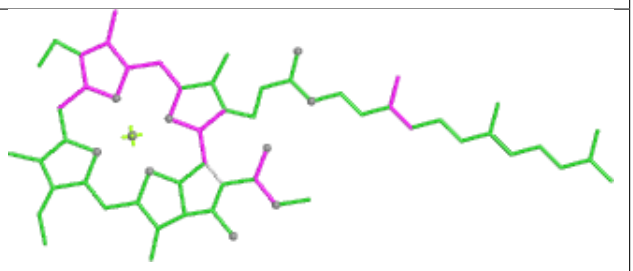


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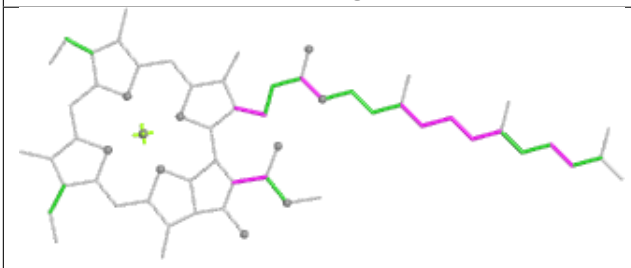
Ligand CLA aB 819



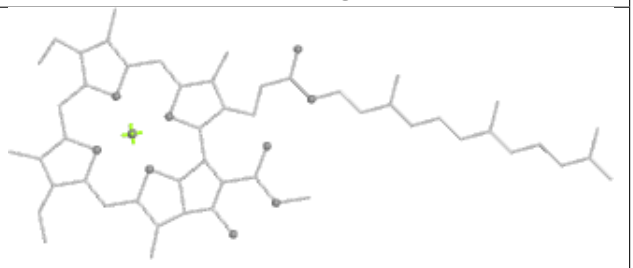
Bond lengths



Bond angles

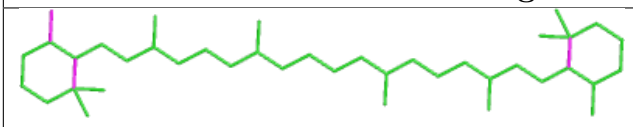


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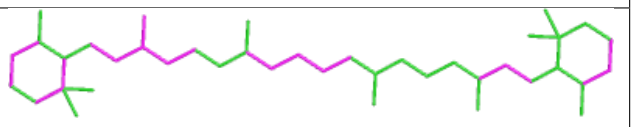


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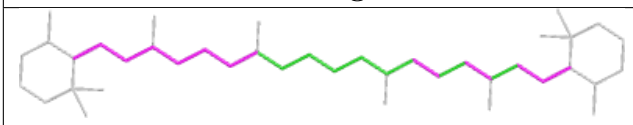
Ligand BCR a1 421



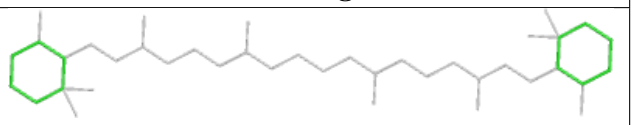
Bond lengths



Bond angles

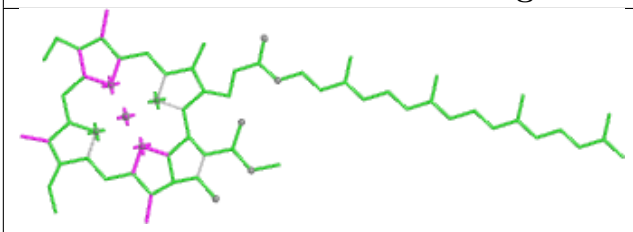


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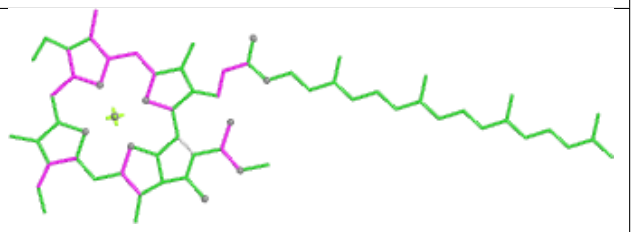


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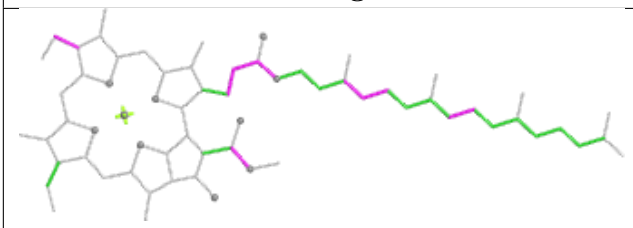
Ligand CLA cB 801



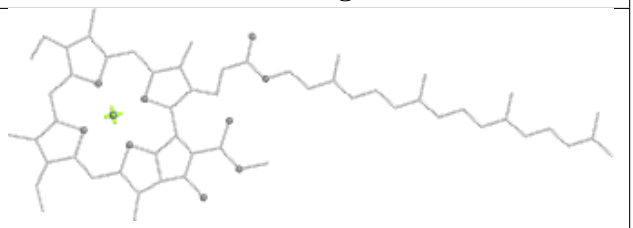
Bond lengths



Bond angles

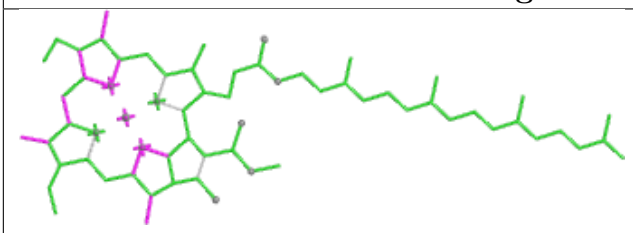


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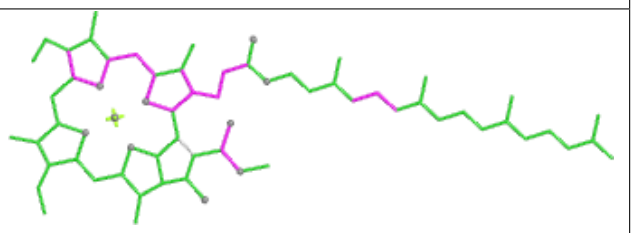


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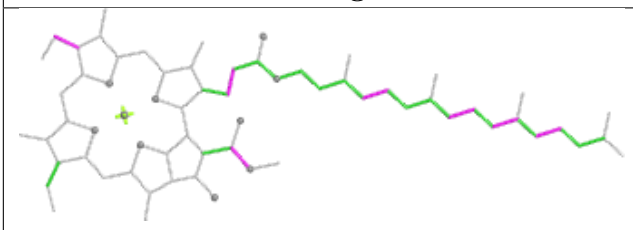
Ligand CLA aB 839



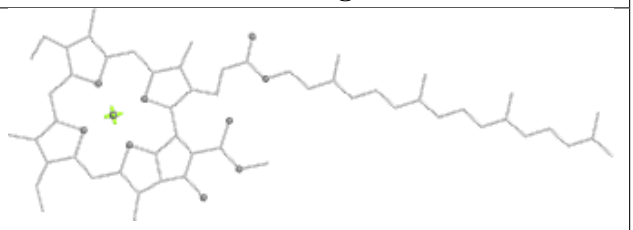
Bond lengths



Bond angles

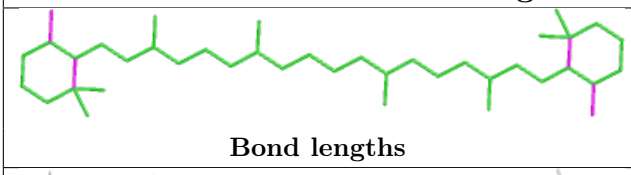


Torsions

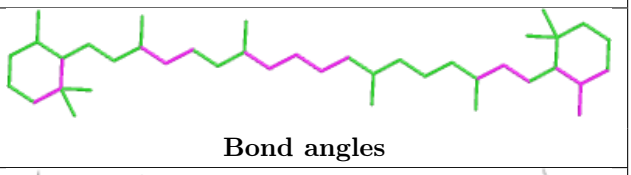


Rings

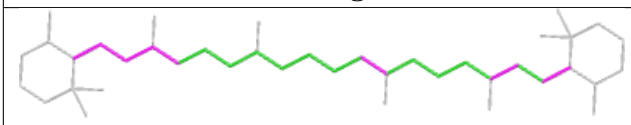
Ligand BCR bJ 104



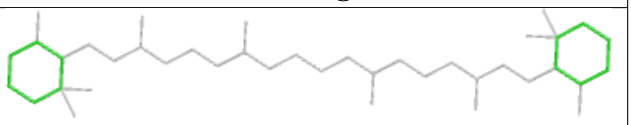
Bond lengths



Bond angles

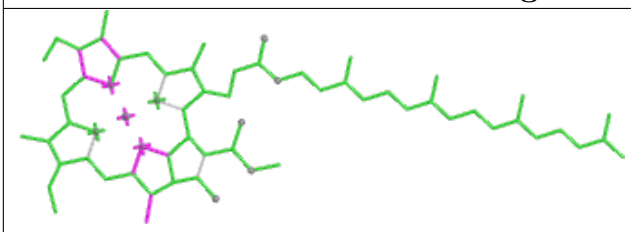


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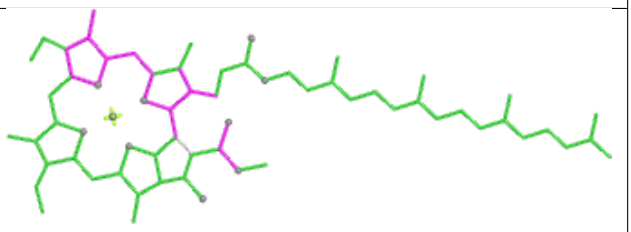


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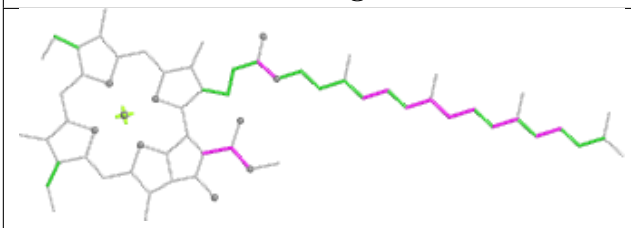
Ligand CLA c6 405



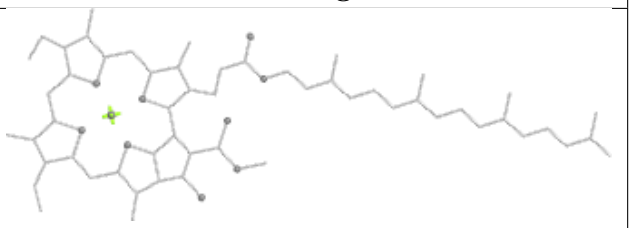
Bond lengths



Bond angles

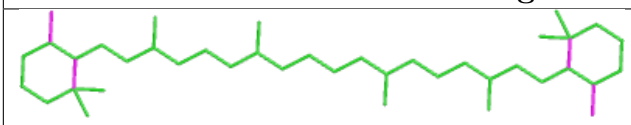


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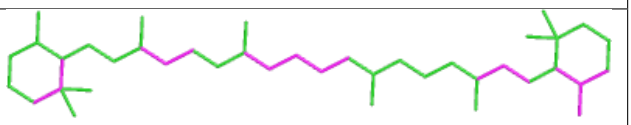


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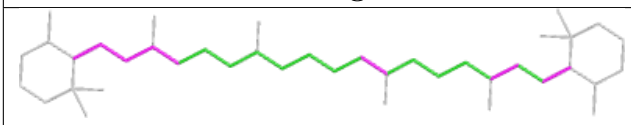
Ligand BCR aJ 205



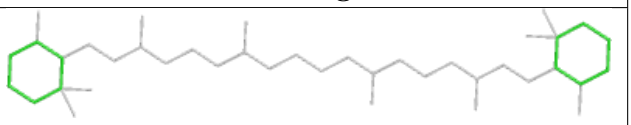
Bond lengths



Bond angles

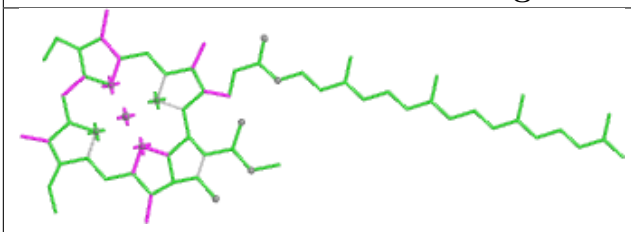


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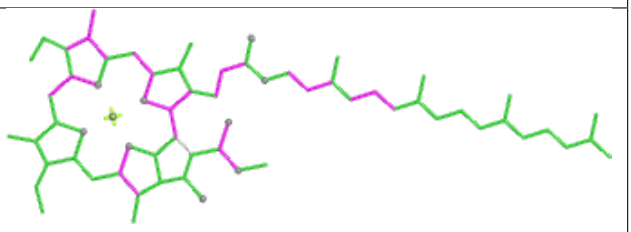


Rings

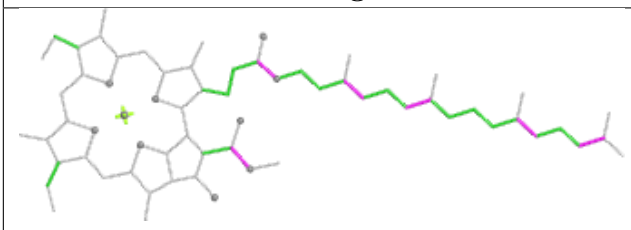
Ligand CLA bA 834



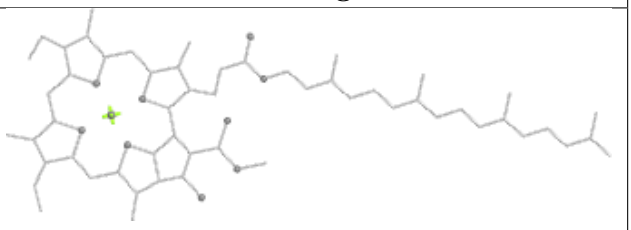
Bond lengths



Bond angles

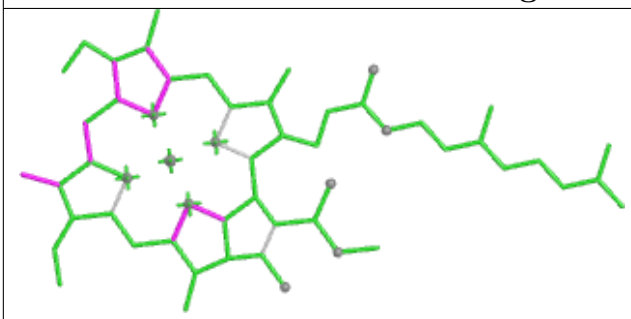


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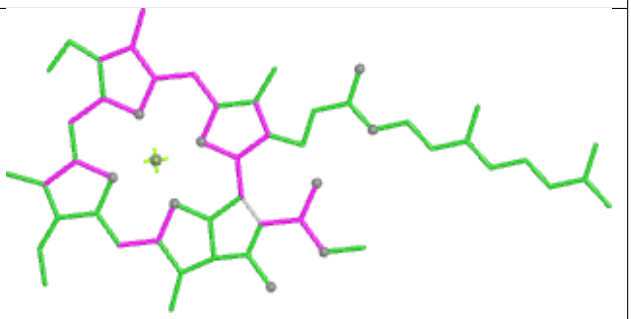


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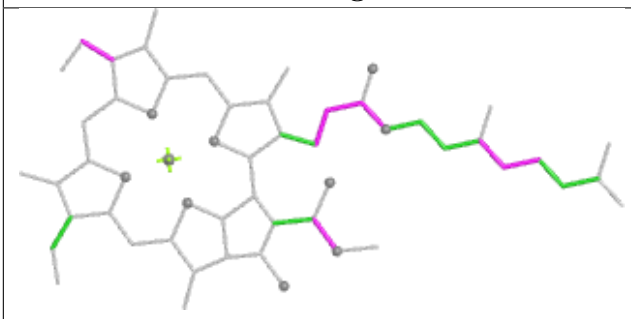
Ligand CLA a6 418



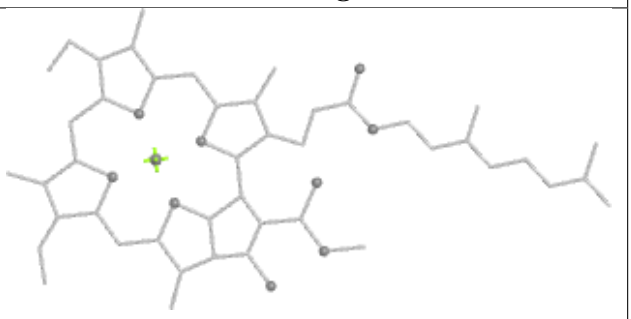
Bond lengths



Bond angles

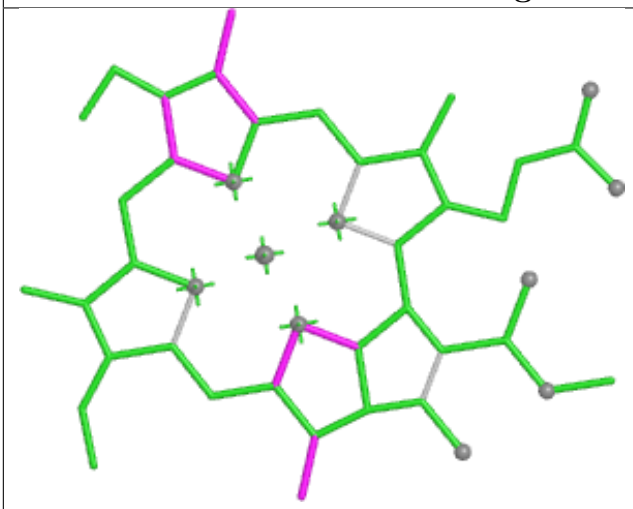


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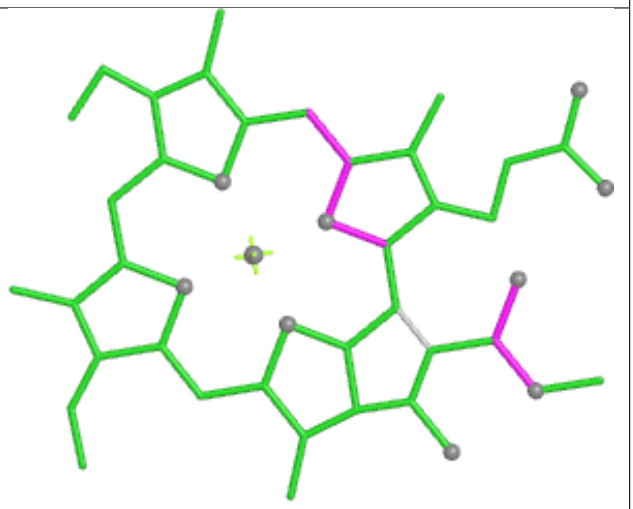


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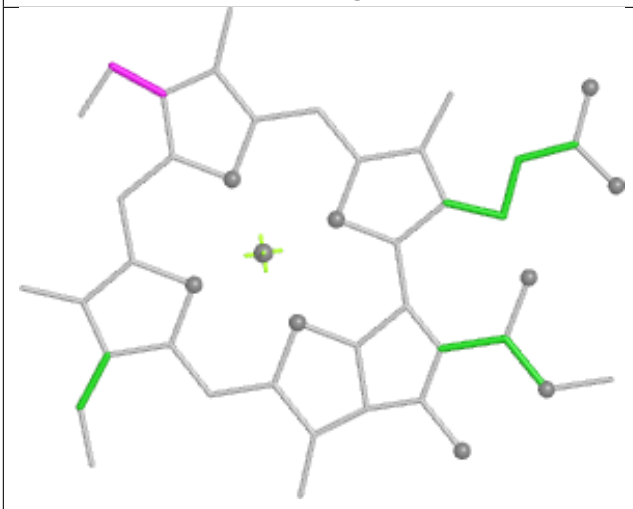
Ligand CLA bB 842



Bond lengths



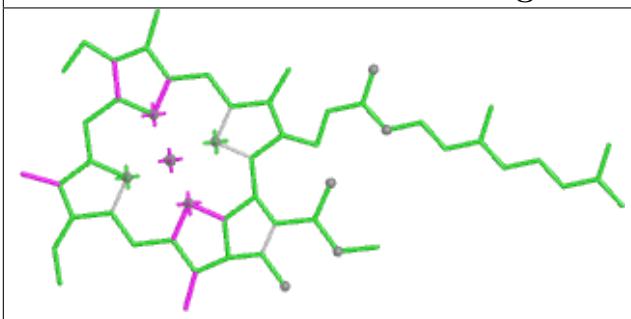
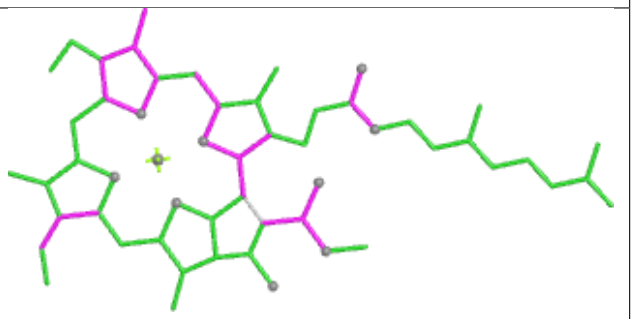
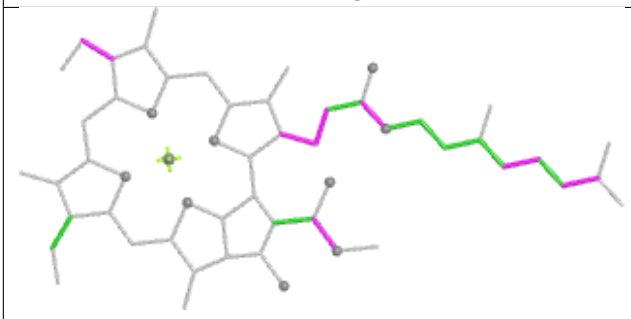
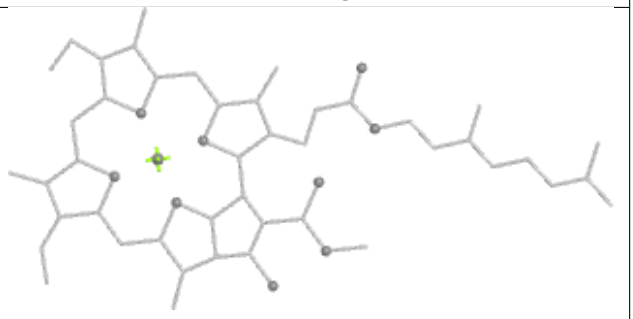
Bond angles



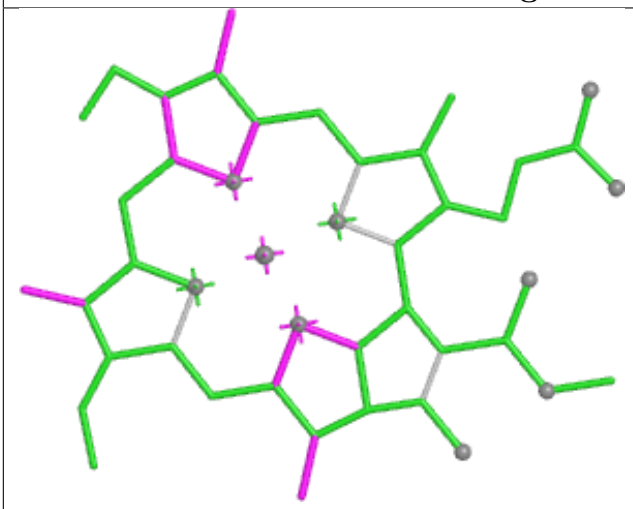
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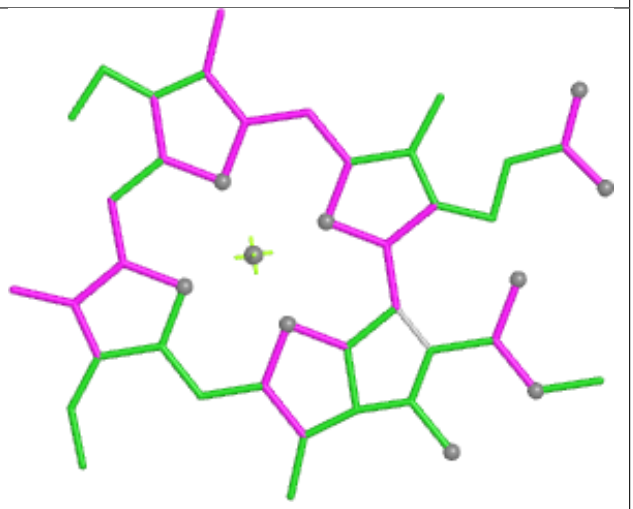
Rings

Ligand CLA cB 817	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

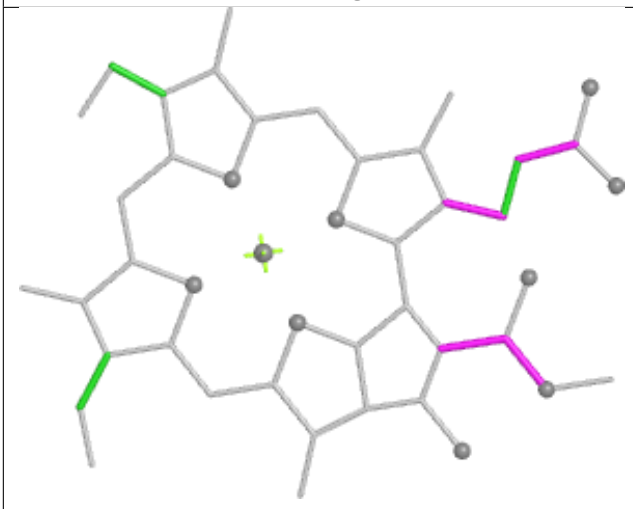
Ligand CLA c6 414



Bond lengths



Bond angles

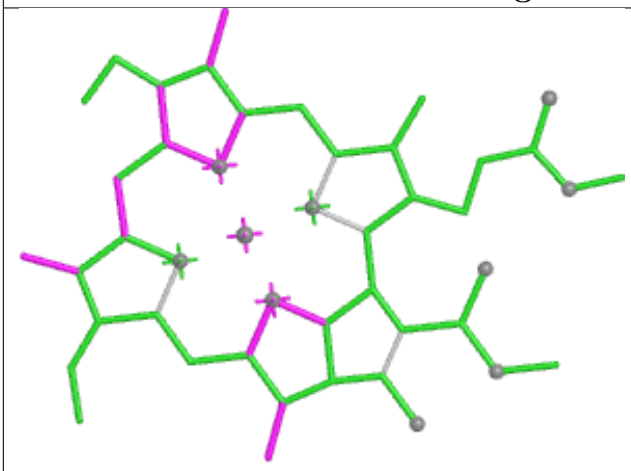


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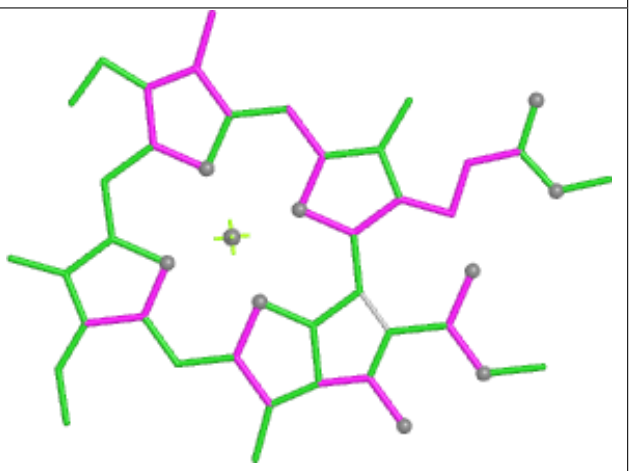


Rings

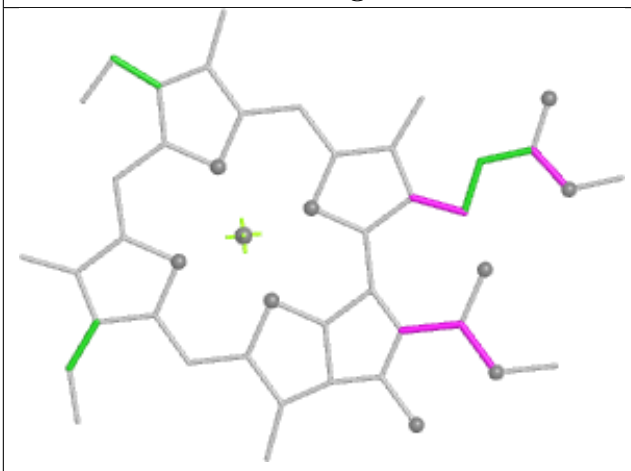
Ligand CLA bB 826



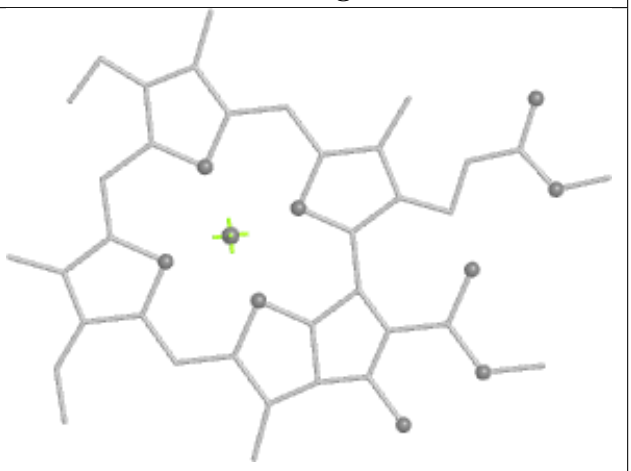
Bond lengths



Bond angles

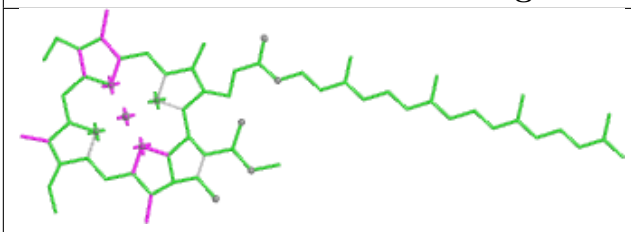


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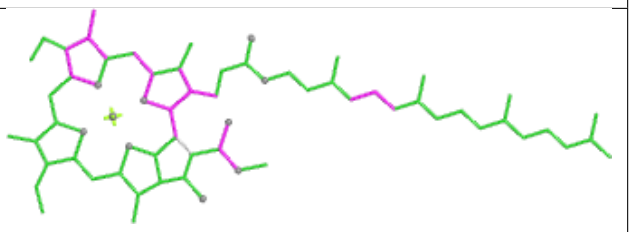


Rings

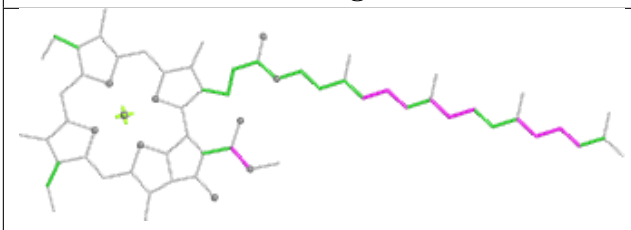
Ligand CLA aA 826



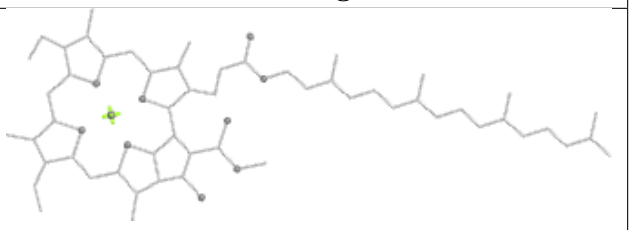
Bond lengths



Bond angles

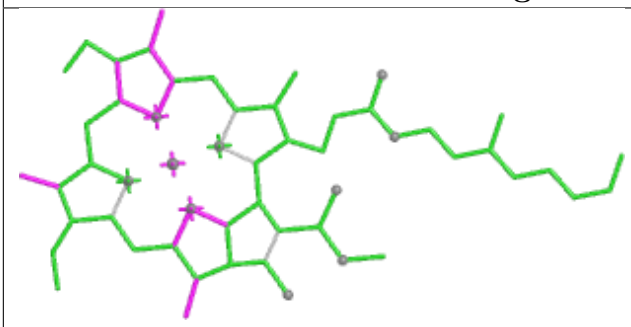


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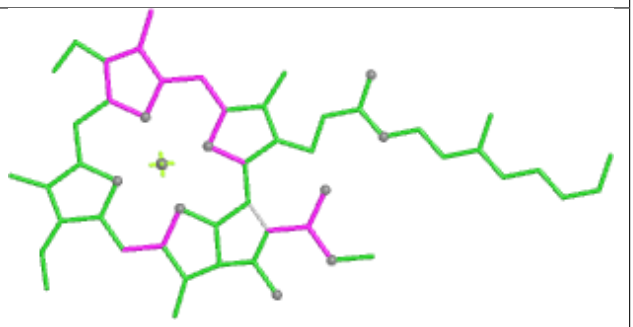


Rings

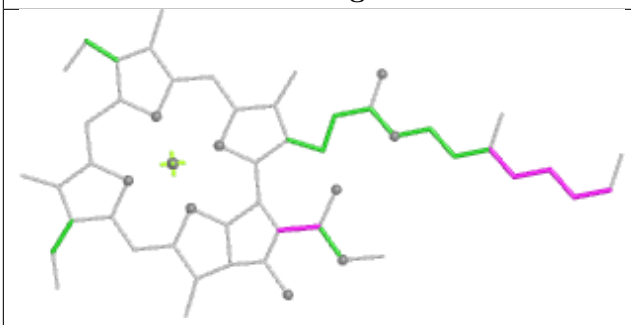
Ligand CLA bA 818



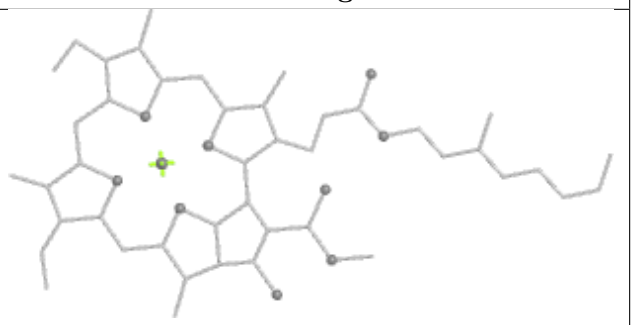
Bond lengths



Bond angles

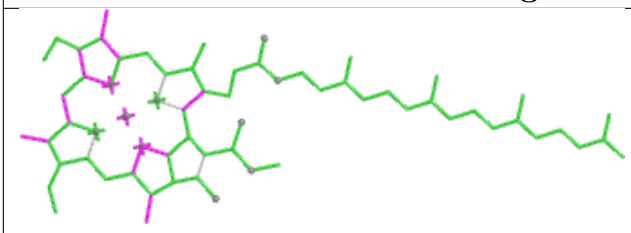


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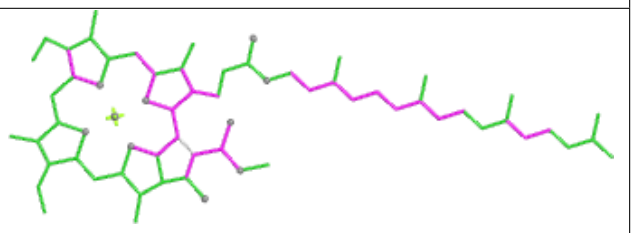


Rings

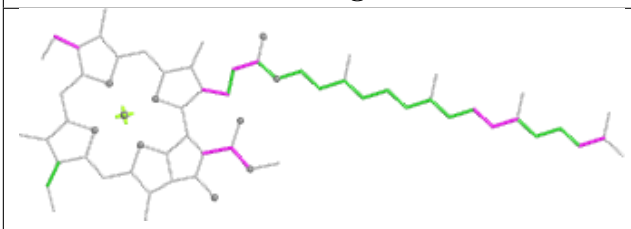
Ligand CLA c5 420



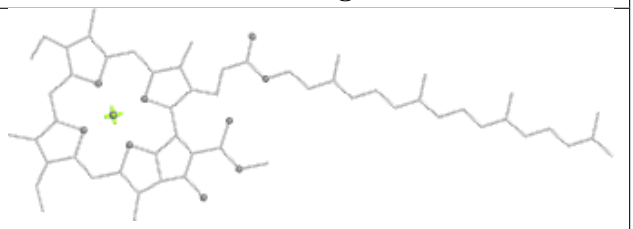
Bond lengths



Bond angles

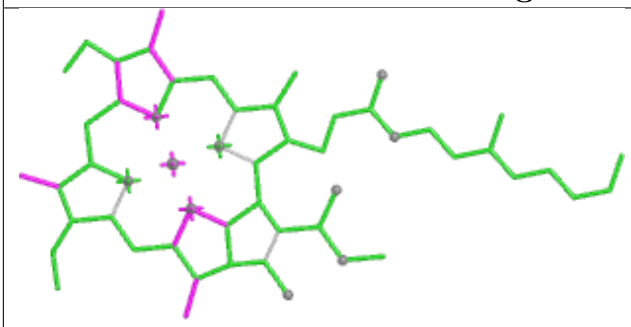


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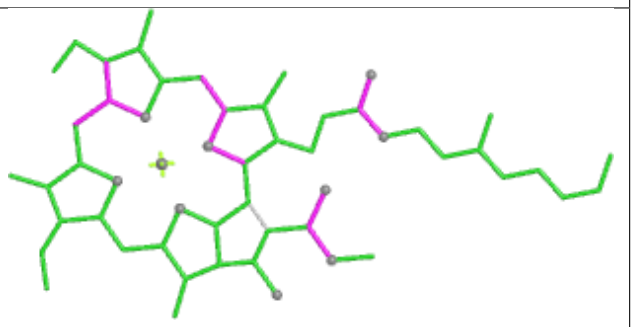


Rings

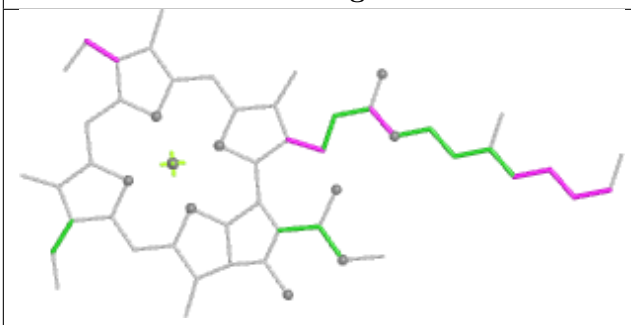
Ligand CLA cA 836



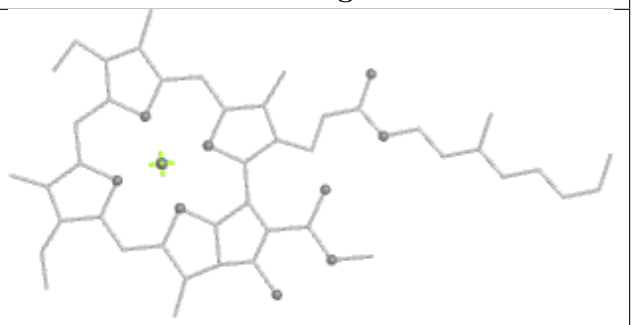
Bond lengths



Bond angles

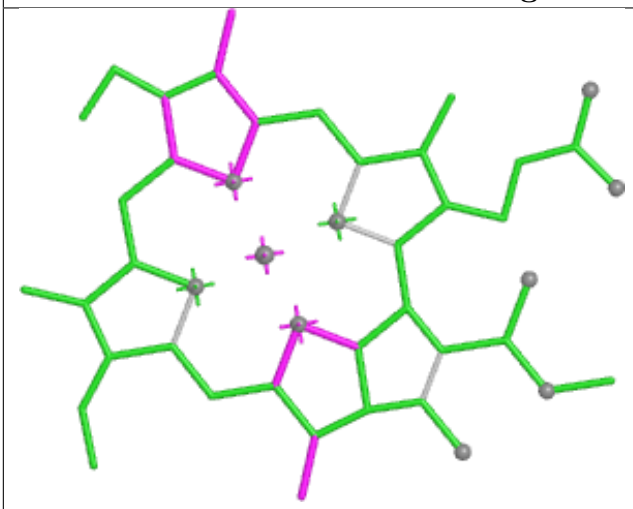


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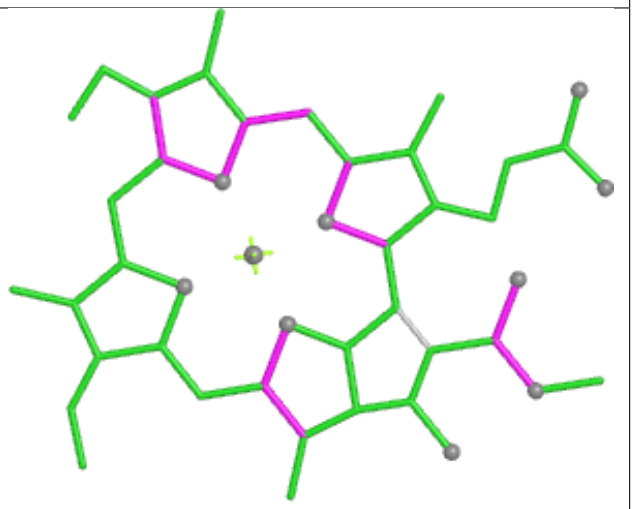


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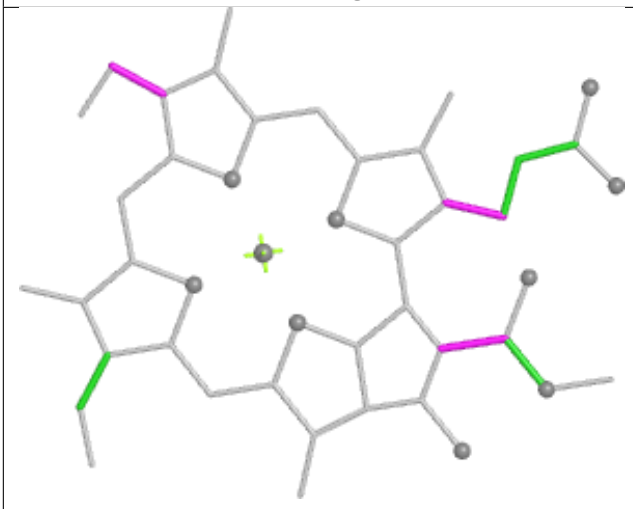
Ligand CLA c1 413



Bond lengths



Bond angles

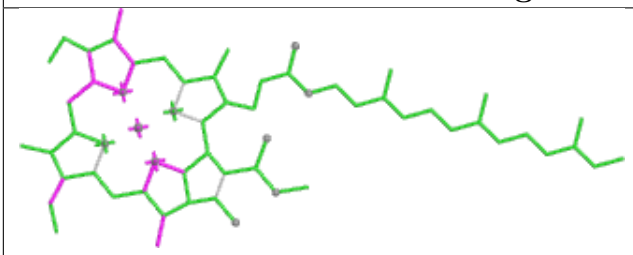


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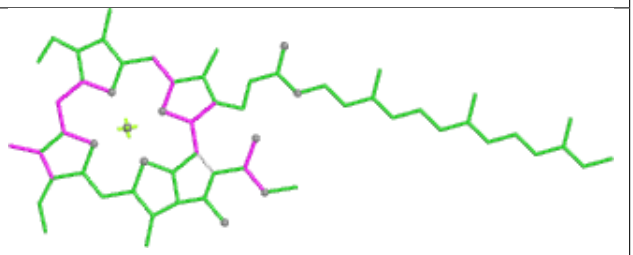


Rings

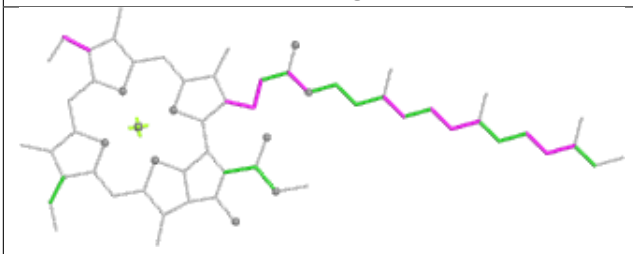
Ligand CLA aA 821



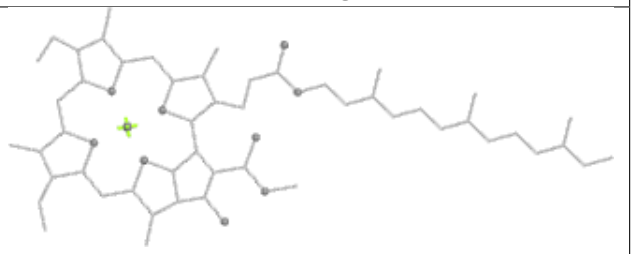
Bond lengths



Bond angles

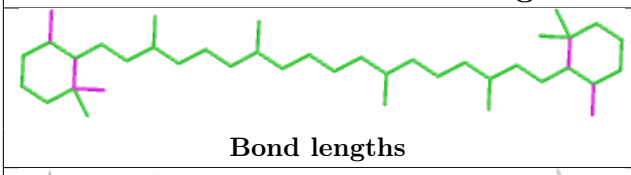


Torsions

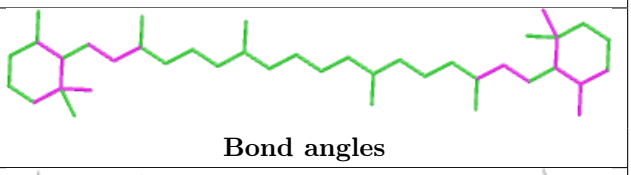


Rings

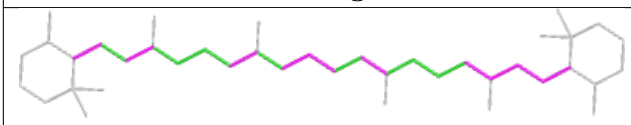
Ligand BCR cF 202



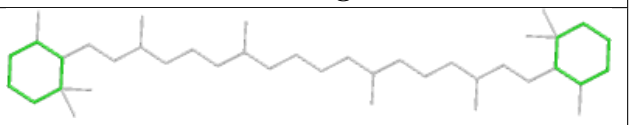
Bond lengths



Bond angles

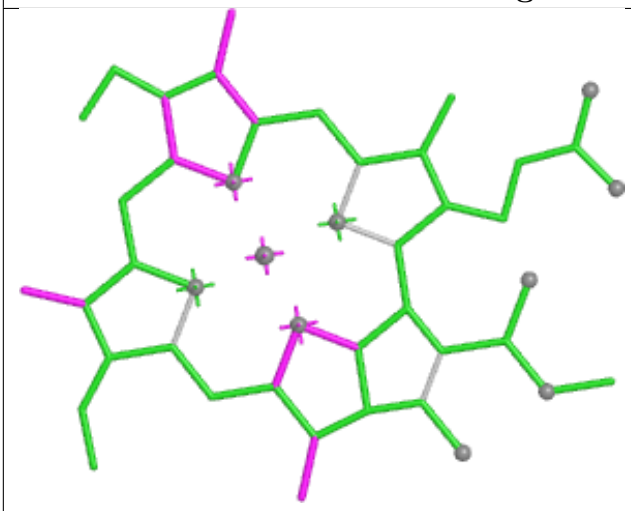


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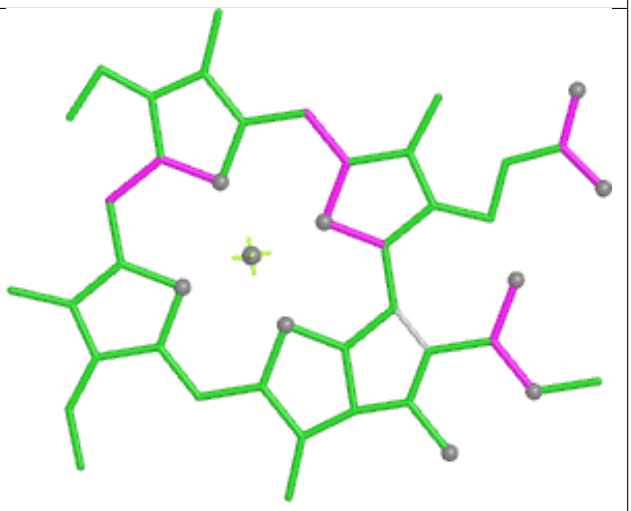


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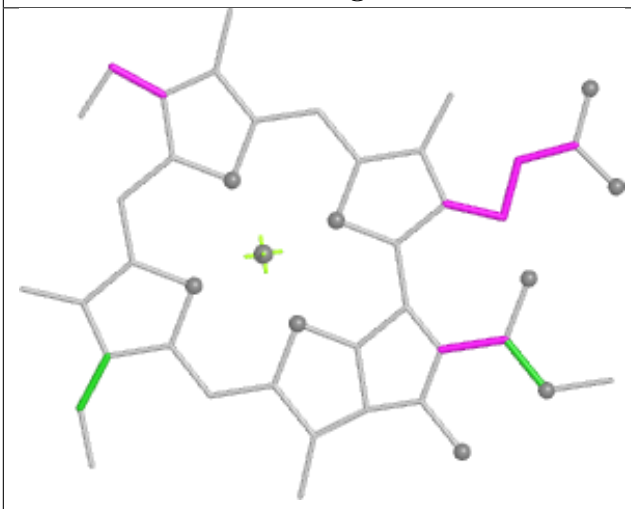
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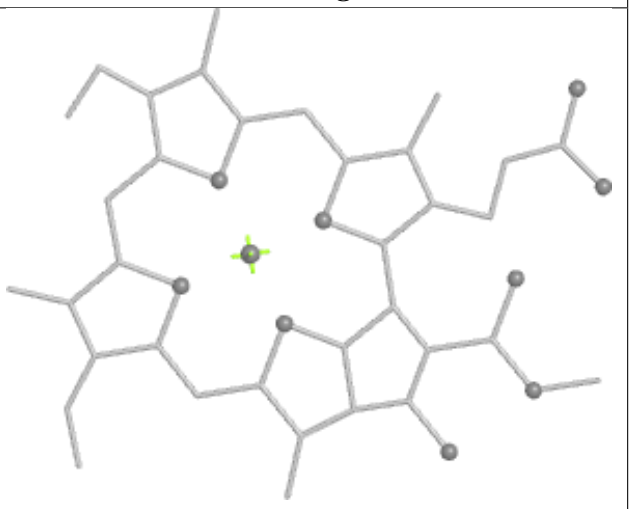
Bond lengths



Bond angles

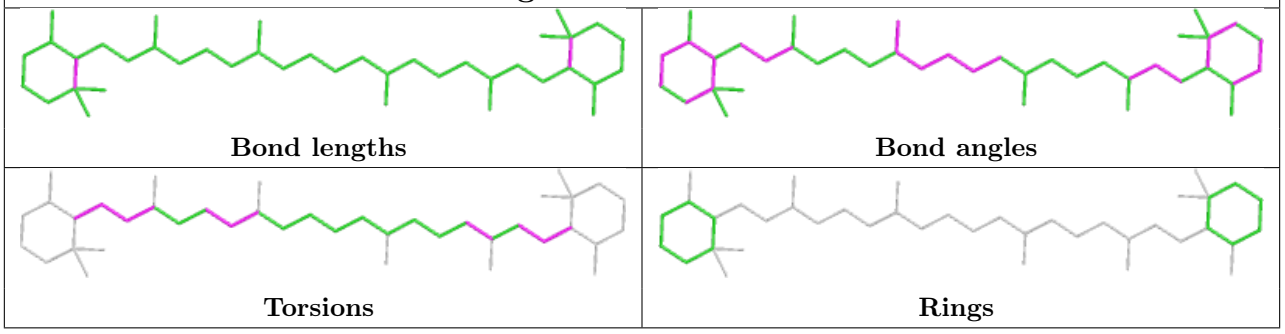


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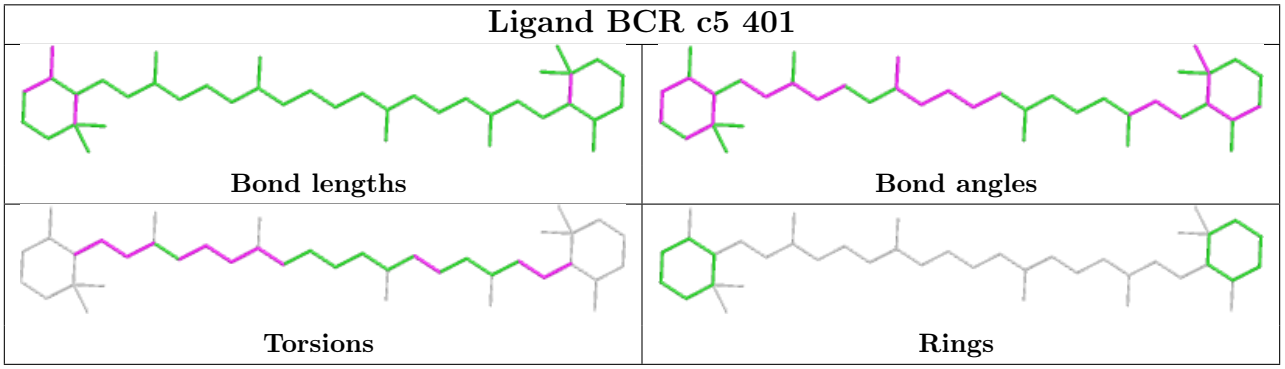


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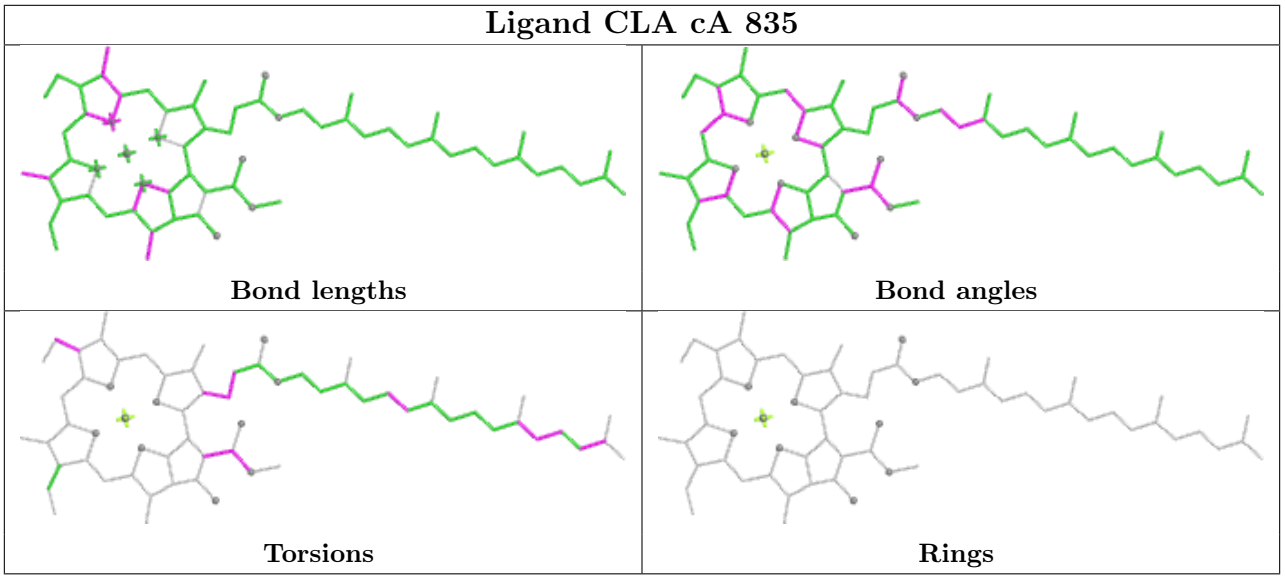
Ligand BCR b6 420



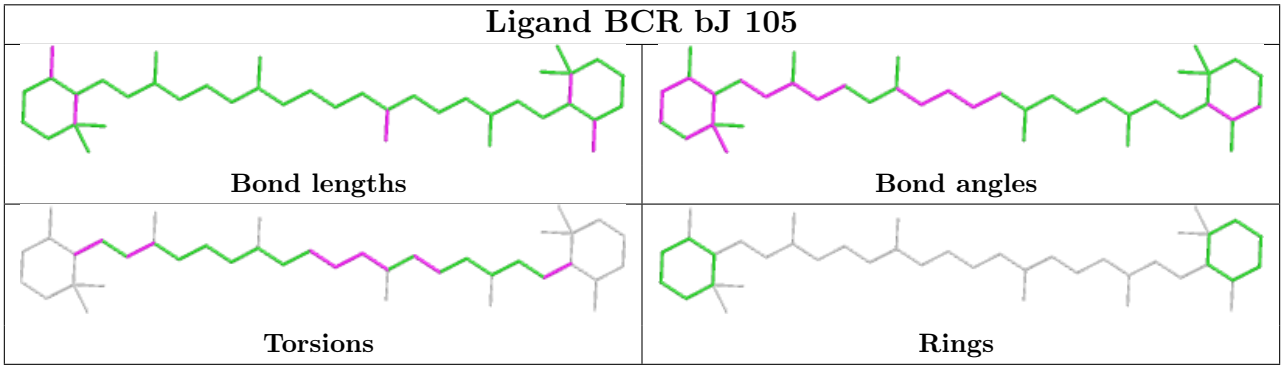
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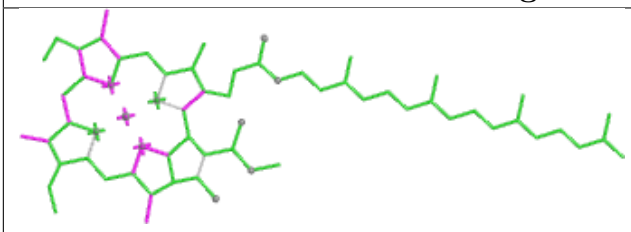
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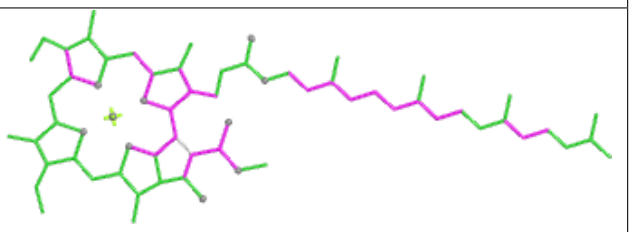
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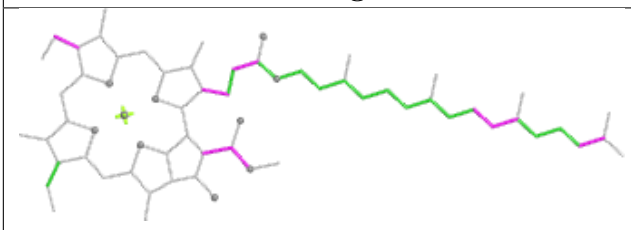
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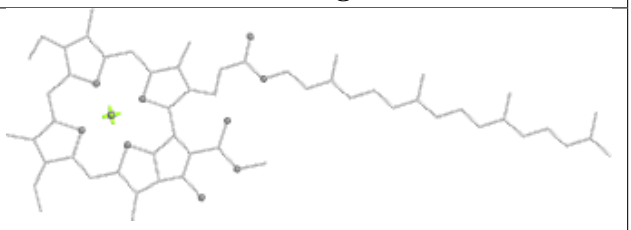
Bond lengths



Bond angles

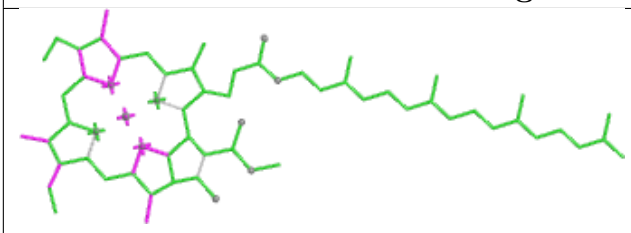


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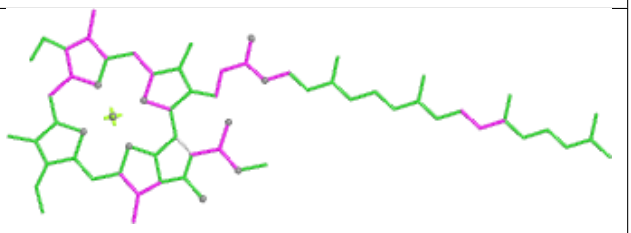


Rings

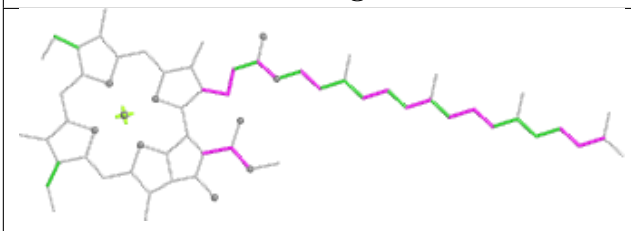
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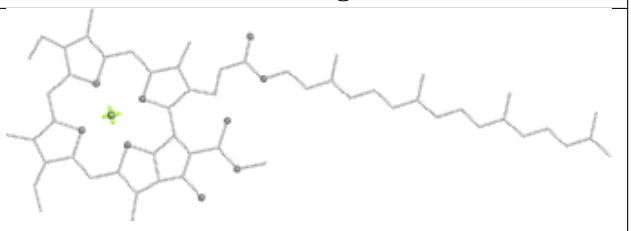
Bond lengths



Bond angles

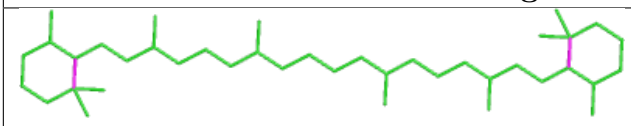


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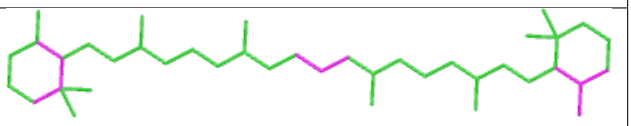


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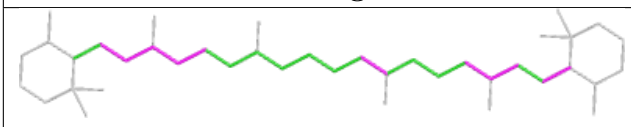
Ligand BCR cI 101



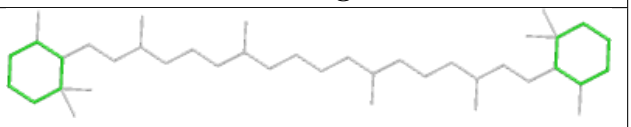
Bond lengths



Bond angles

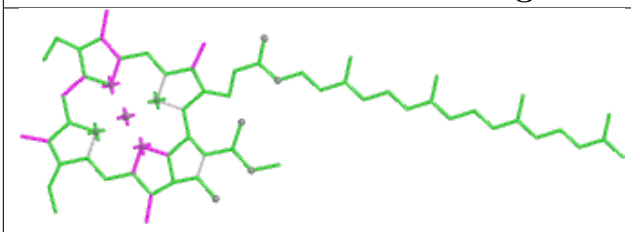


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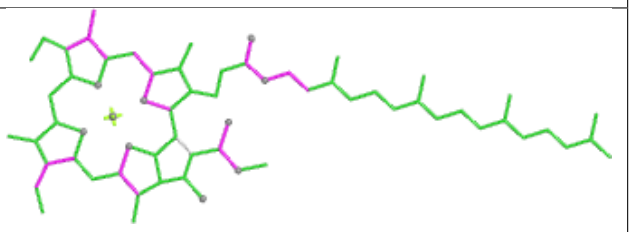


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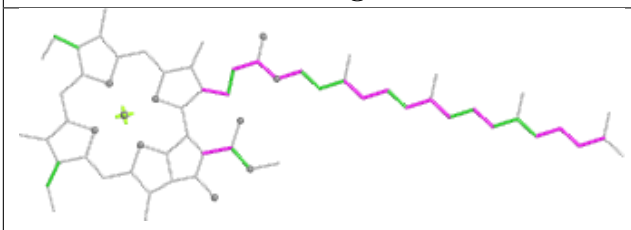
Ligand CLA aB 806



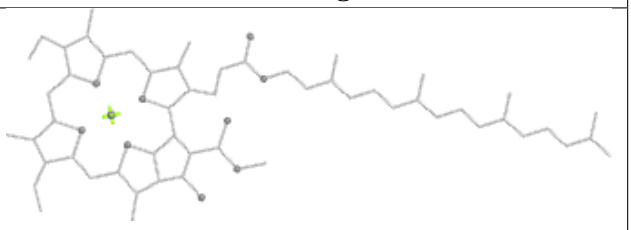
Bond lengths



Bond angles

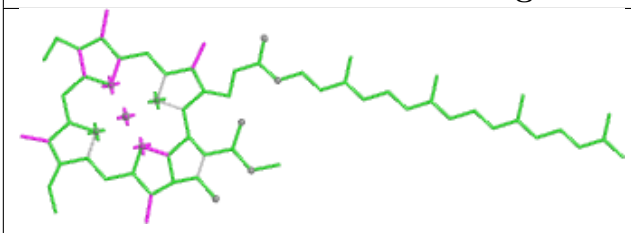


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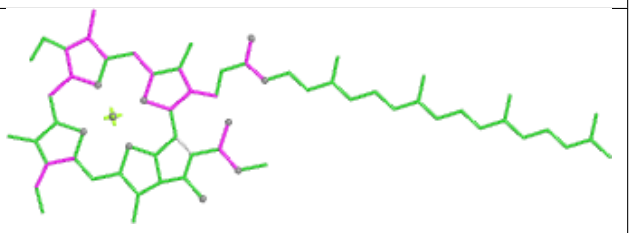


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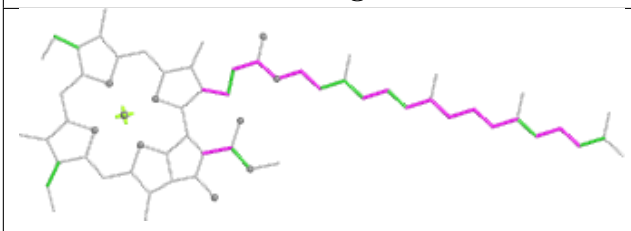
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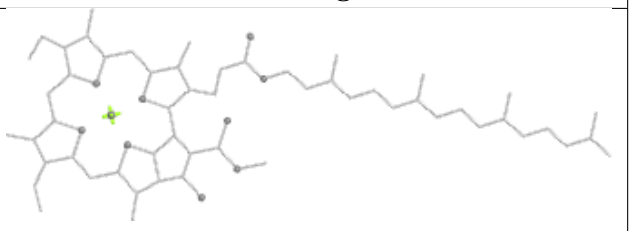
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Bond angles

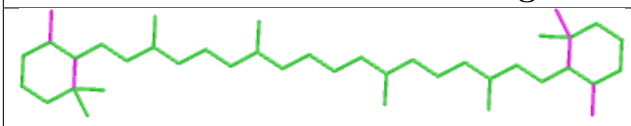


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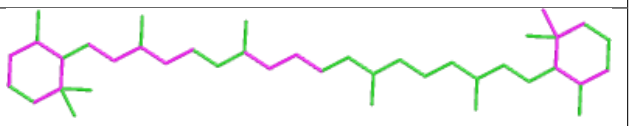


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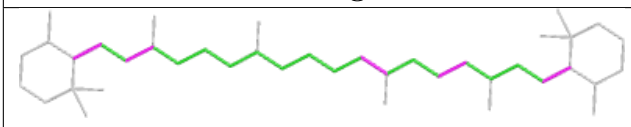
Ligand BCR c1 418



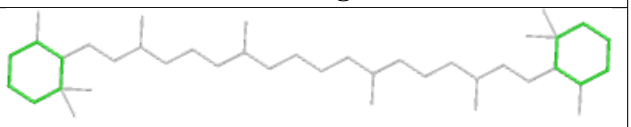
Bond lengths



Bond angles

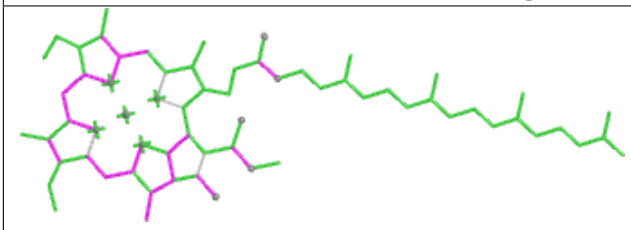


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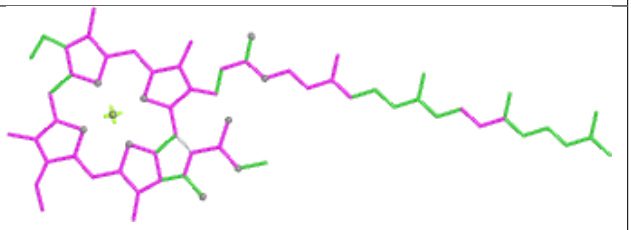


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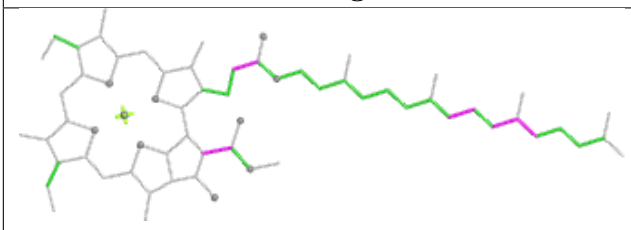
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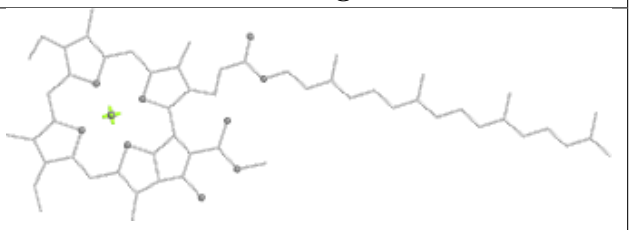
Bond lengths



Bond angles

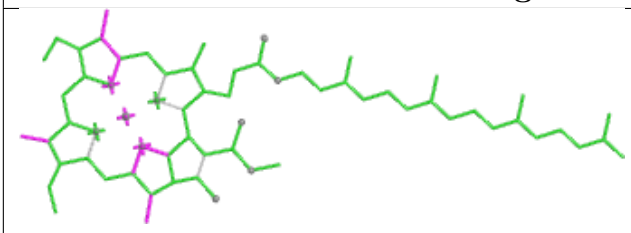


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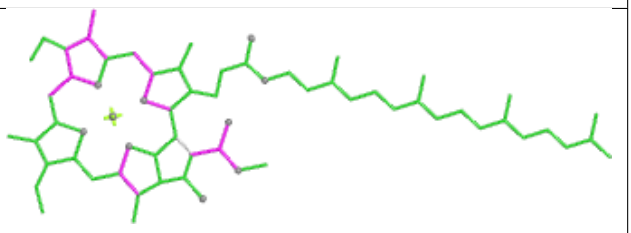


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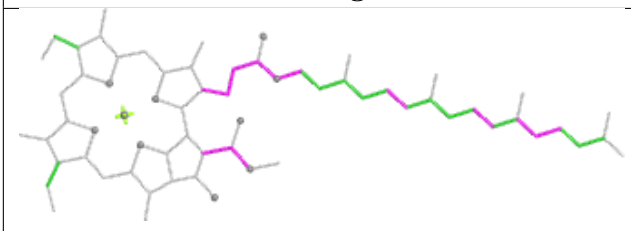
Ligand CLA bB 829



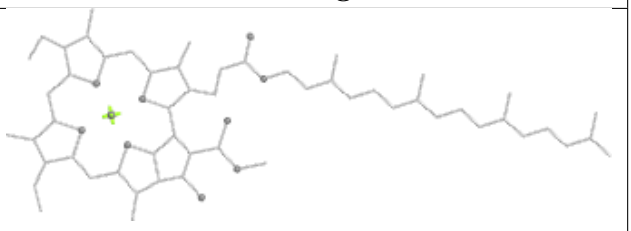
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Bond angles

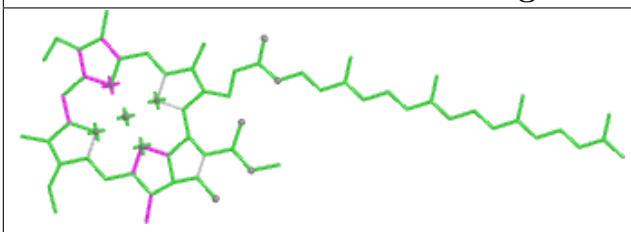


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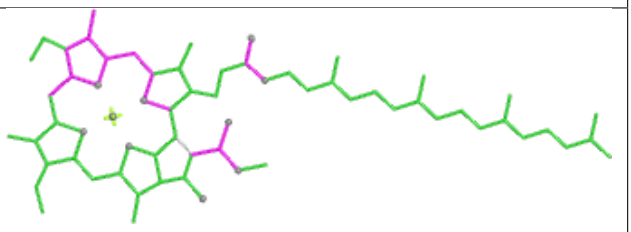


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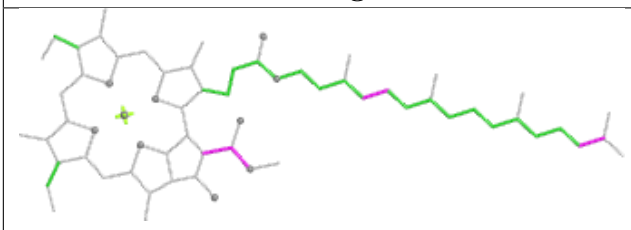
Ligand CLA b4 409



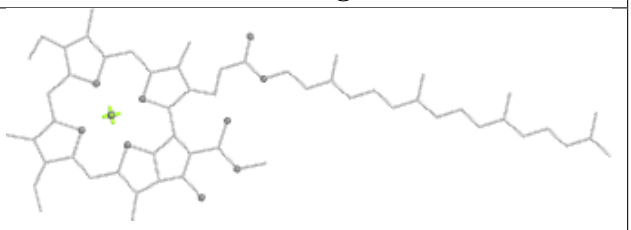
Bond lengths



Bond angles

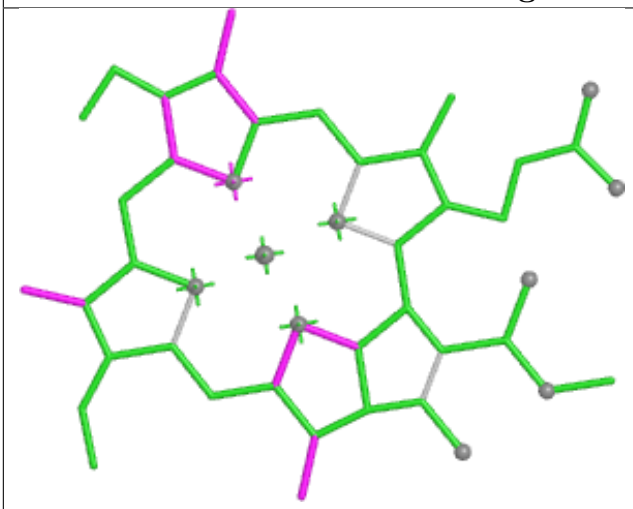


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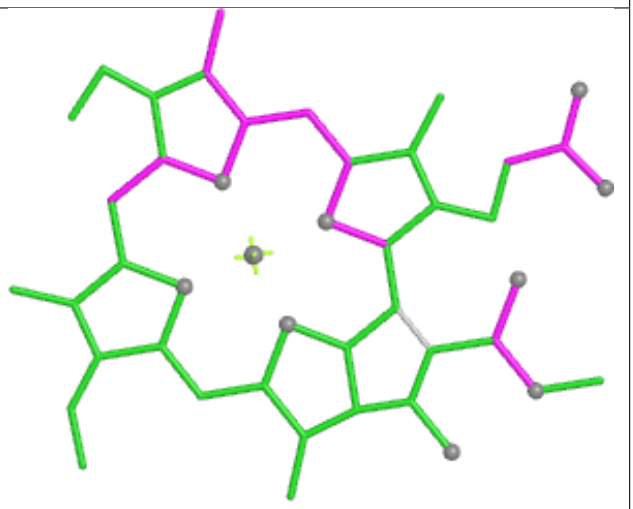


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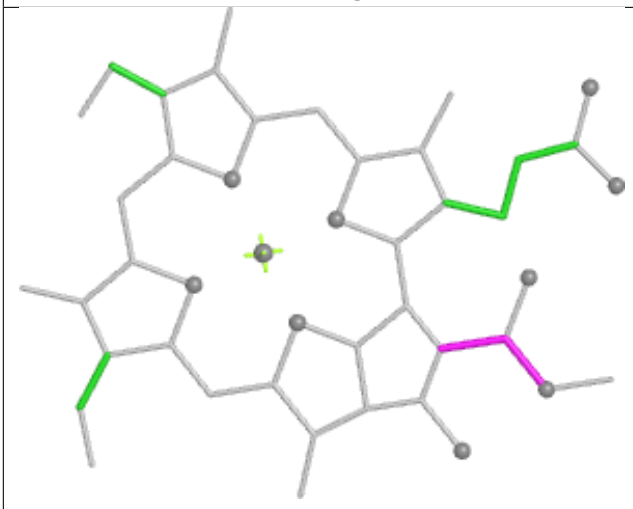
Ligand CLA b5 406



Bond lengths



Bond angles

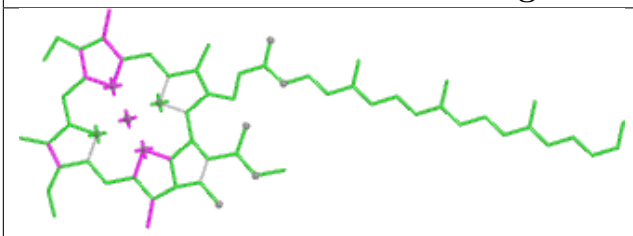


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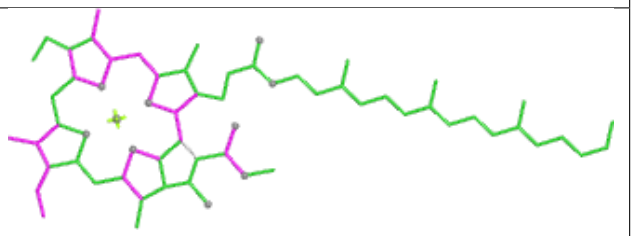


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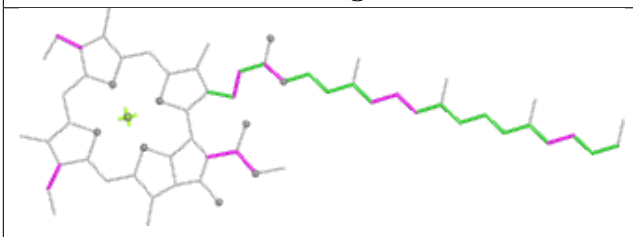
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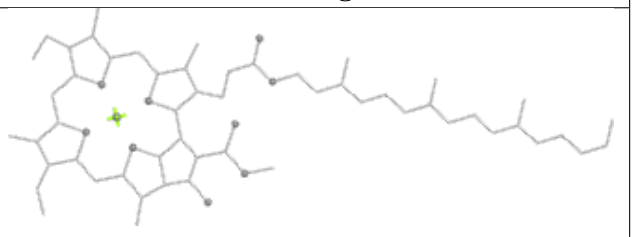
Bond lengths



Bond angles

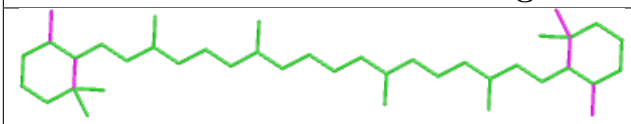


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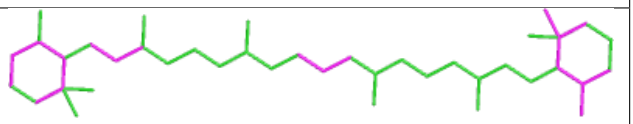


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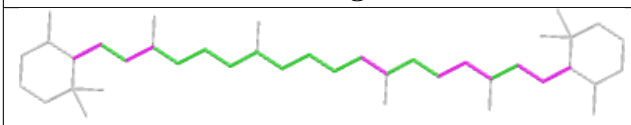
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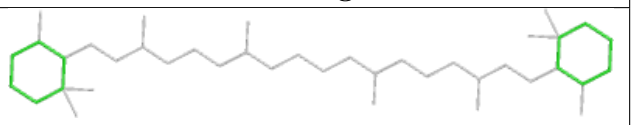
Bond lengths



Bond angles

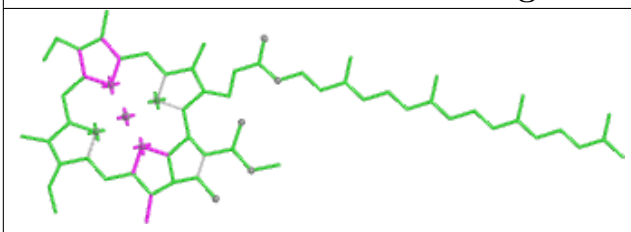


Torsions

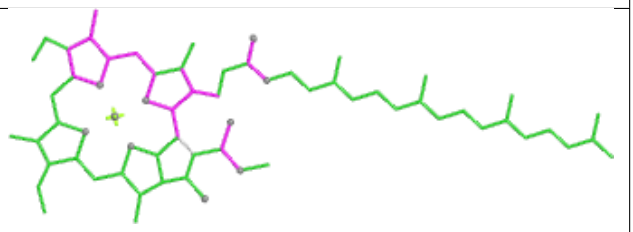


Rings

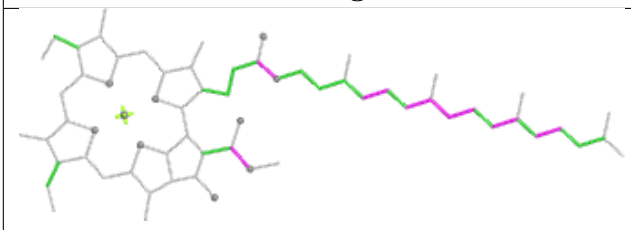
Ligand CLA b3 403



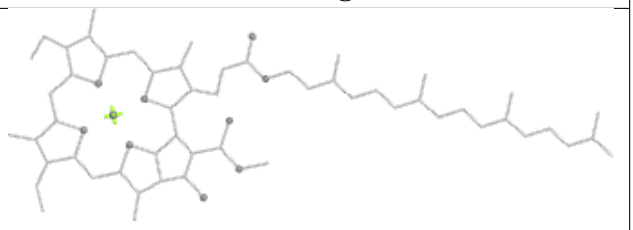
Bond lengths



Bond angles

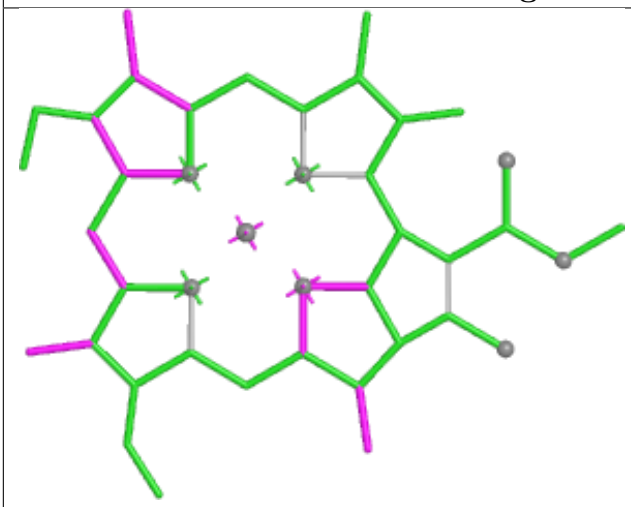


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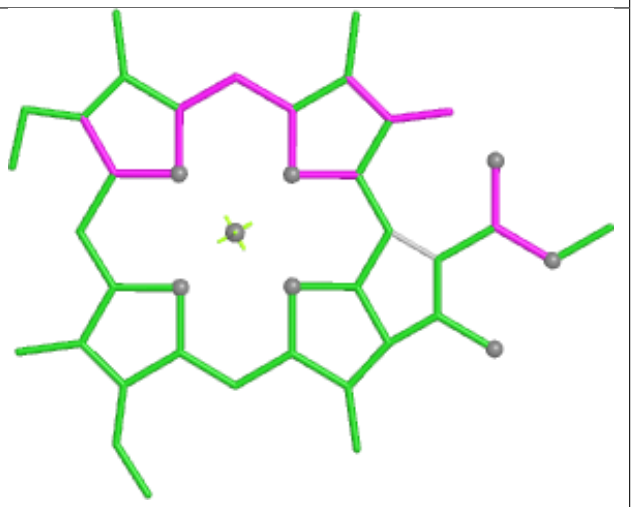


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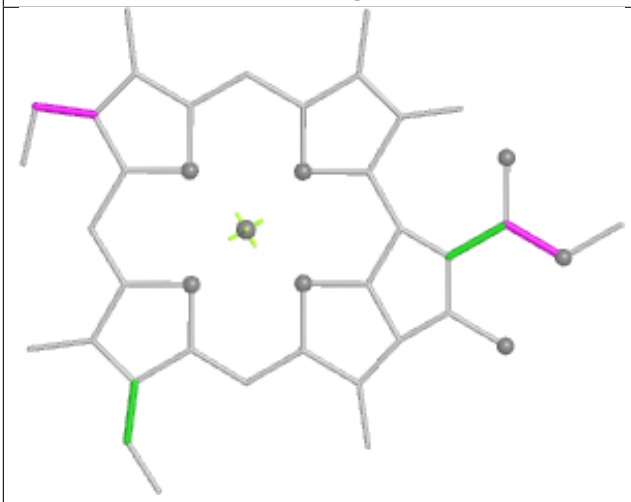
Ligand CLA a3 414



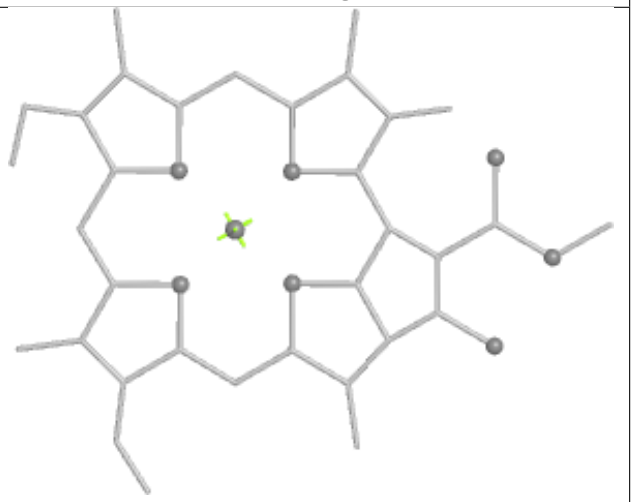
Bond lengths



Bond angles

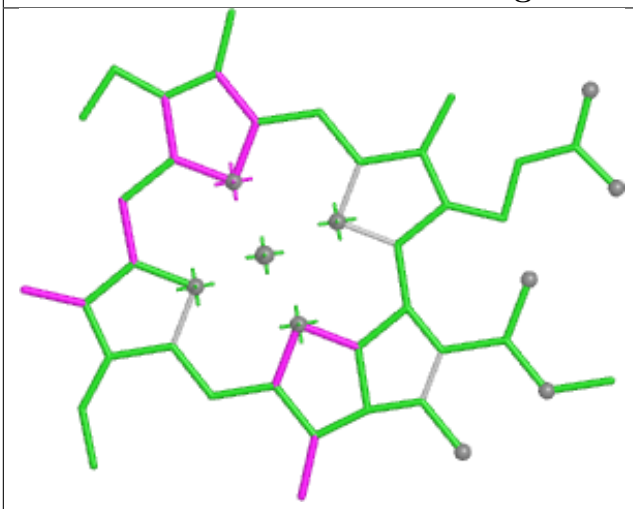


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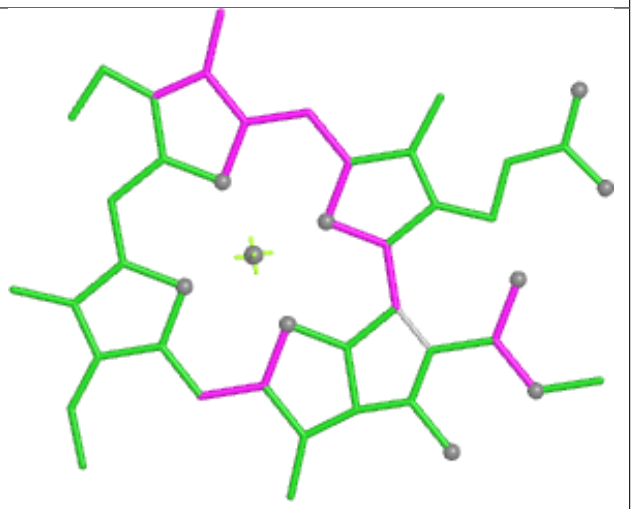


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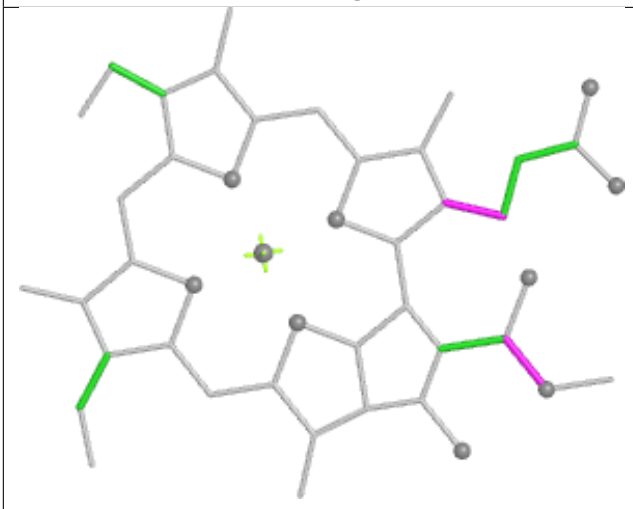
Ligand CLA bB 812



Bond lengths



Bond angles

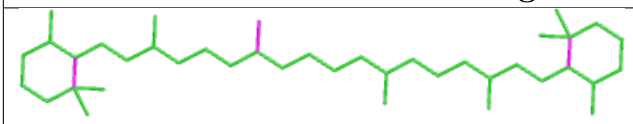


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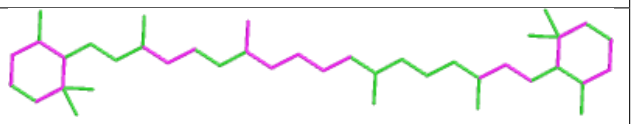


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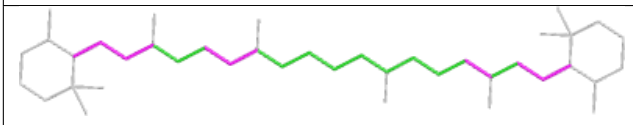
Ligand BCR c1 420



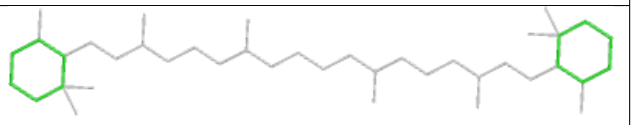
Bond lengths



Bond angles

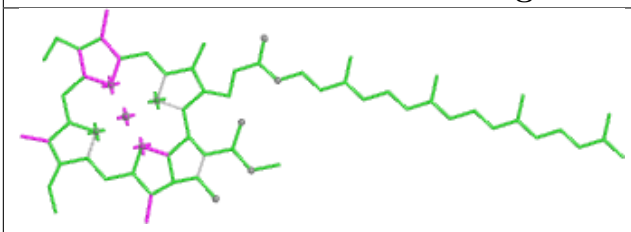


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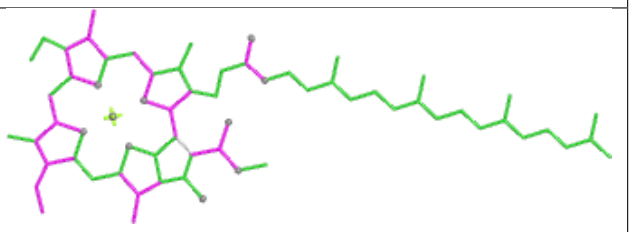


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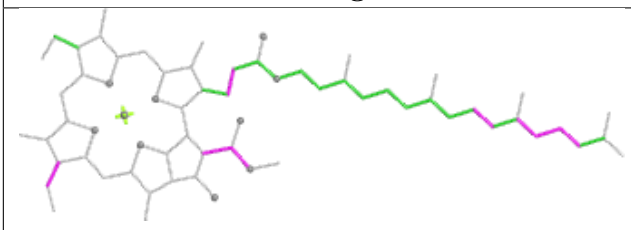
Ligand CLA aB 804



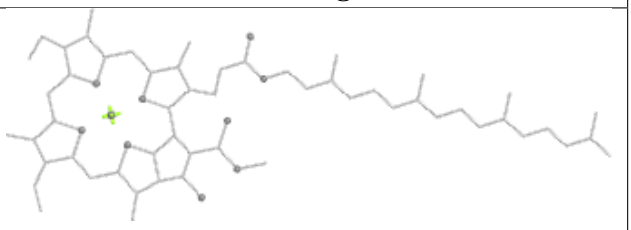
Bond lengths



Bond angles



Torsions

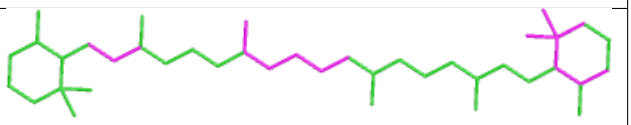


Rings

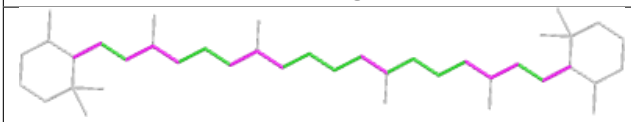
Ligand BCR bB 846



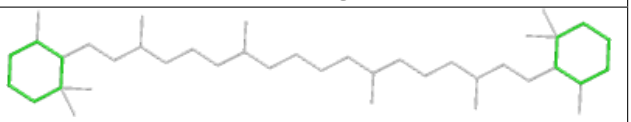
Bond lengths



Bond angles

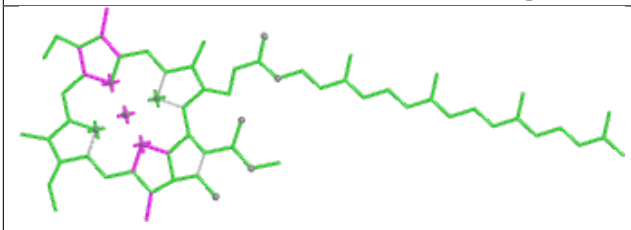


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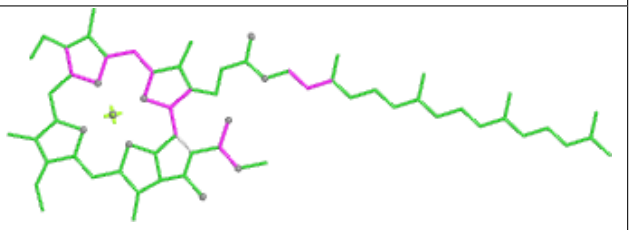


Rings

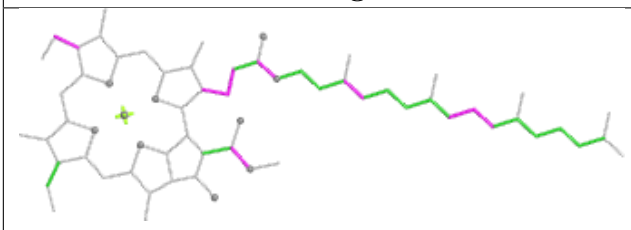
Ligand CLA c3 404



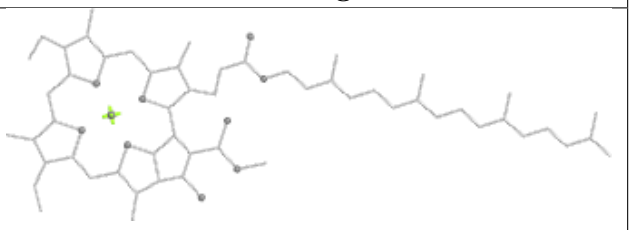
Bond lengths



Bond angles

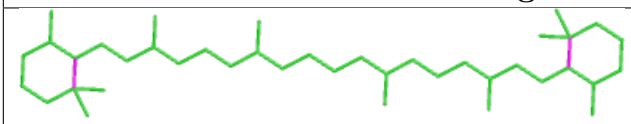


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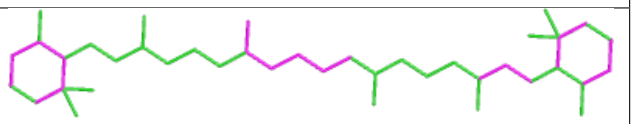


Rings

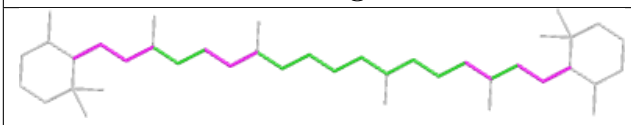
Ligand BCR a3 420



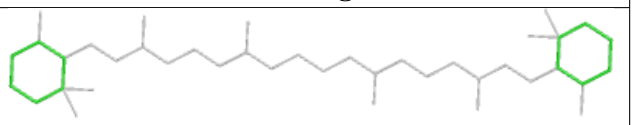
Bond lengths



Bond angles

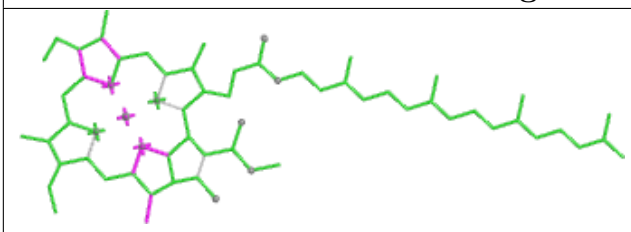


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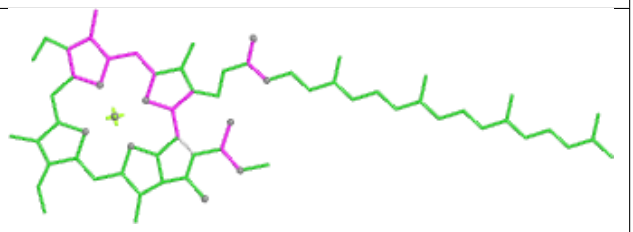


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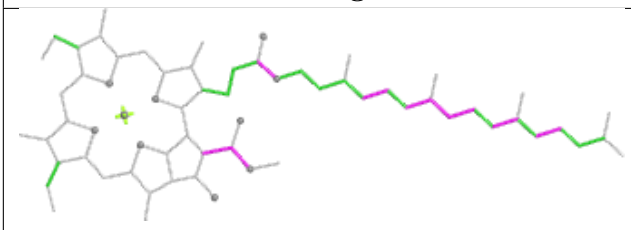
Ligand CLA a4 403



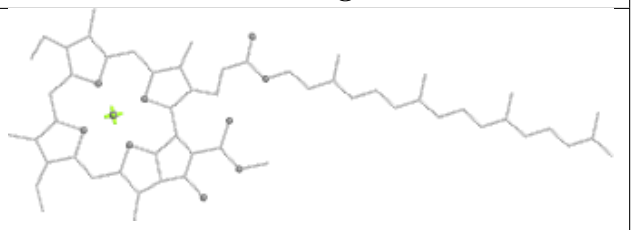
Bond lengths



Bond angles

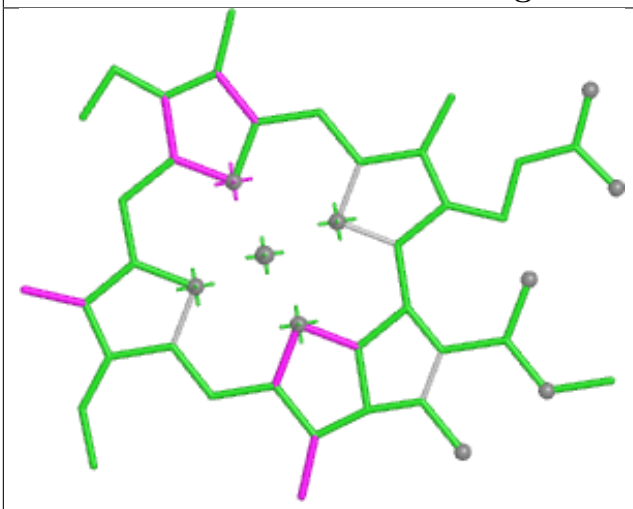


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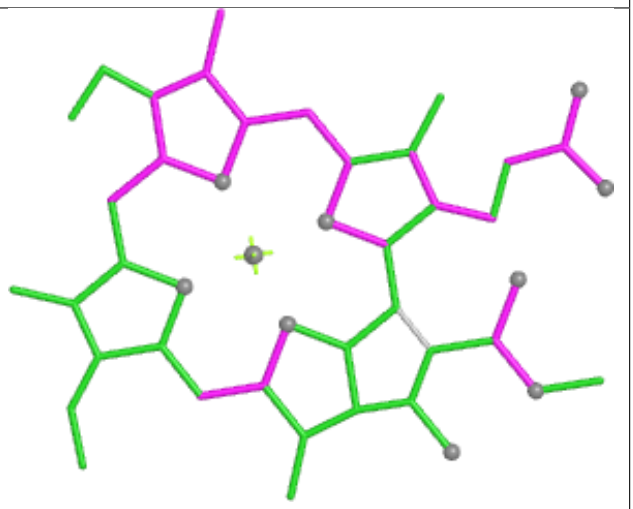


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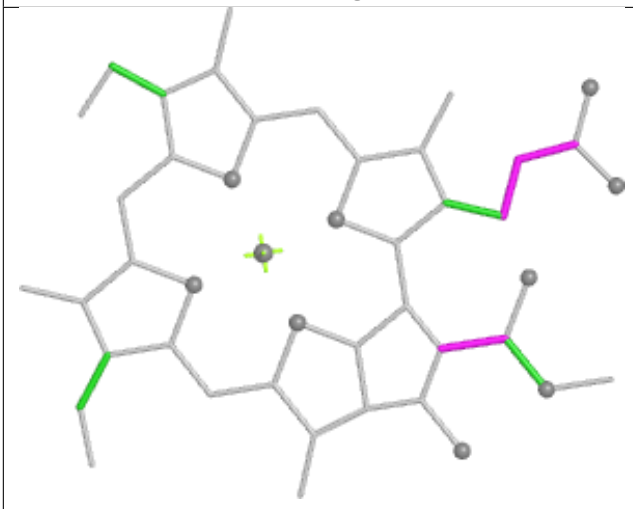
Ligand CLA bB 824



Bond lengths



Bond angles

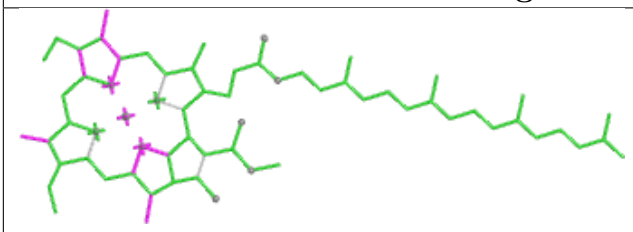


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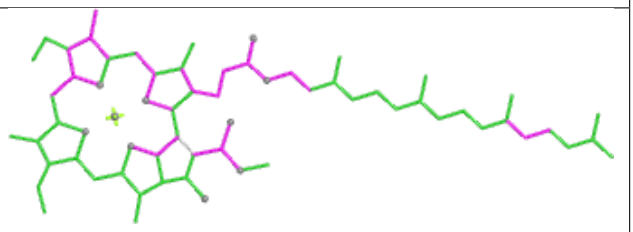


Rings

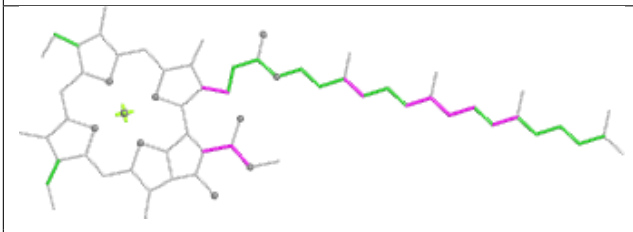
Ligand CLA aB 827



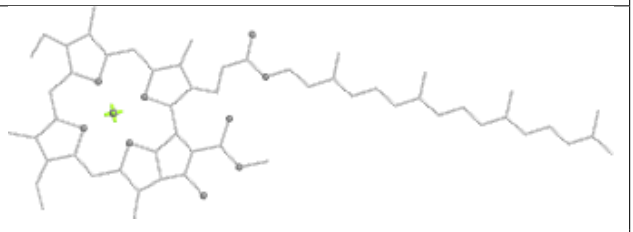
Bond lengths



Bond angles

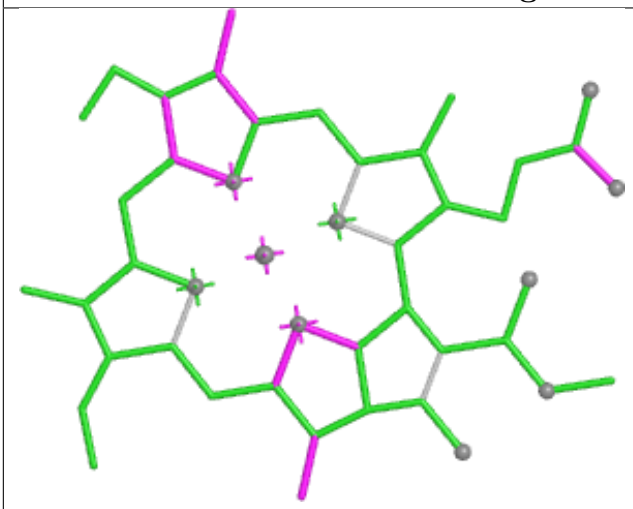


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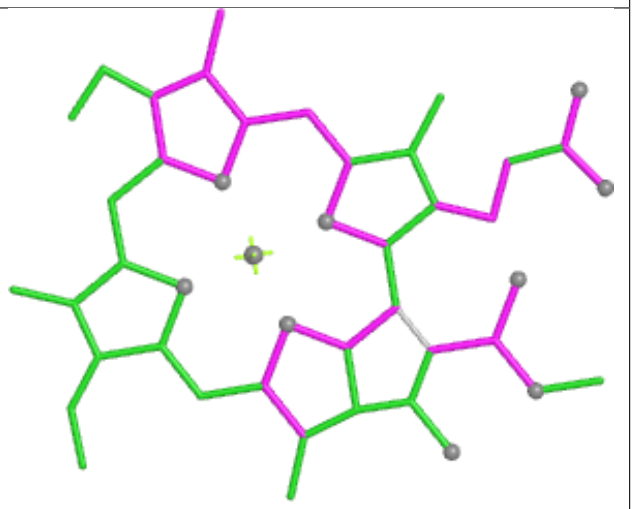


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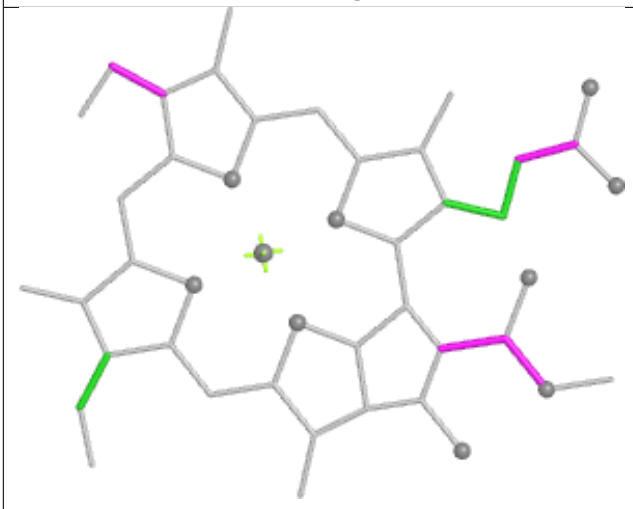
Ligand CLA a5 415



Bond lengths



Bond angles

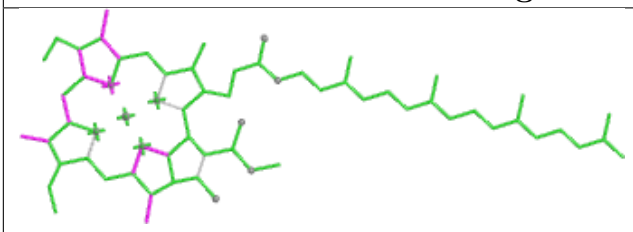


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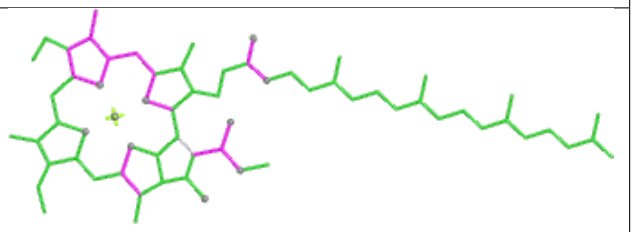


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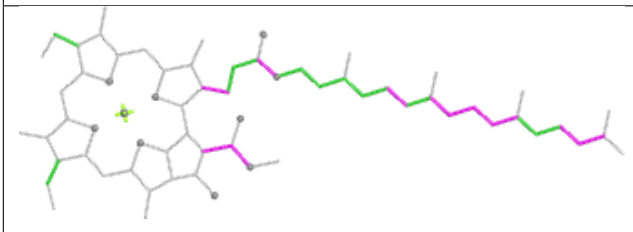
Ligand CLA aB 815



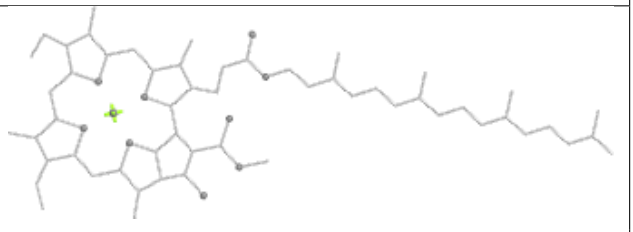
Bond lengths



Bond angles

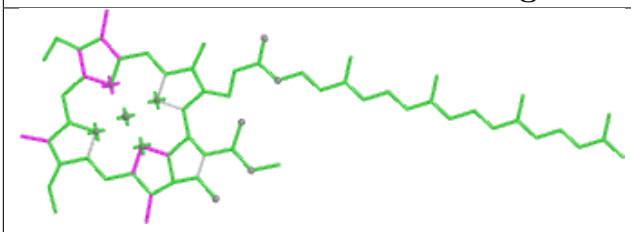


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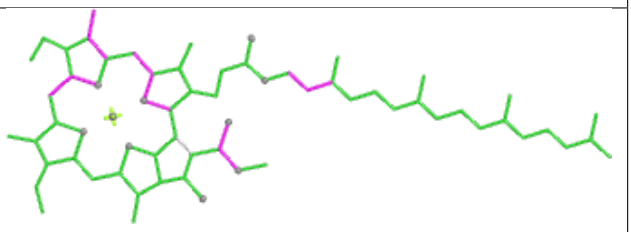


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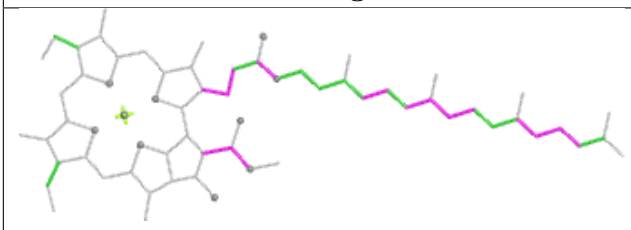
Ligand CLA a5 402



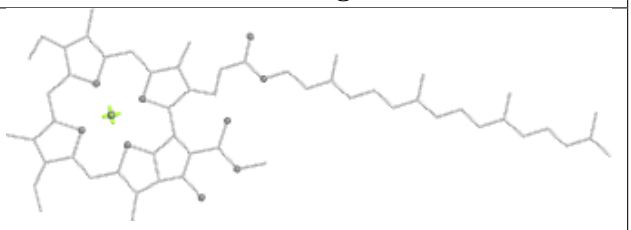
Bond lengths



Bond angles

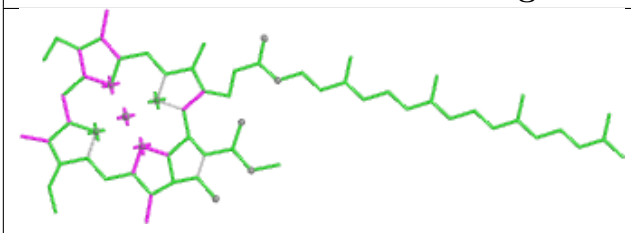


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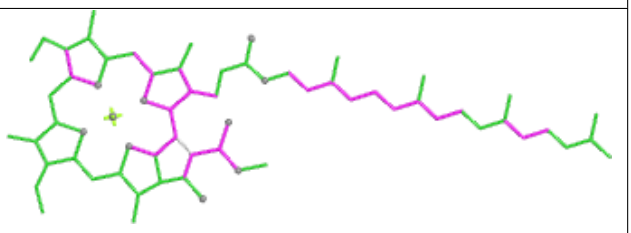


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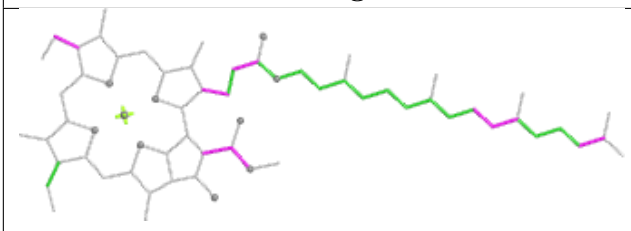
Ligand CLA b5 420



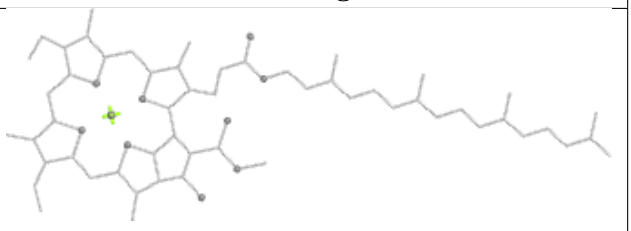
Bond lengths



Bond angles

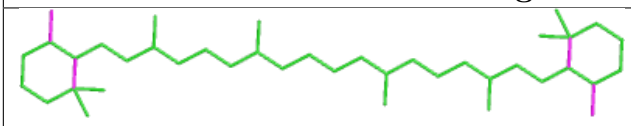


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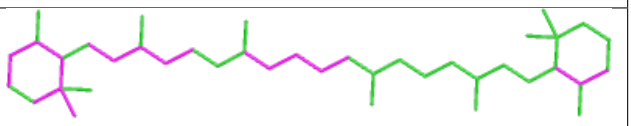


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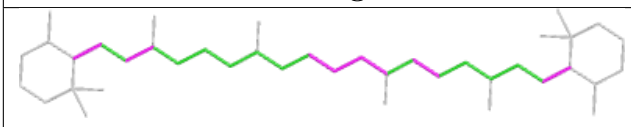
Ligand BCR aF 203



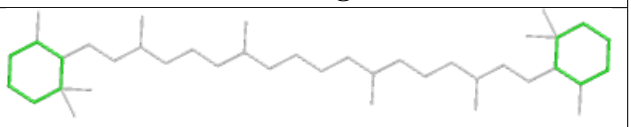
Bond lengths



Bond angles

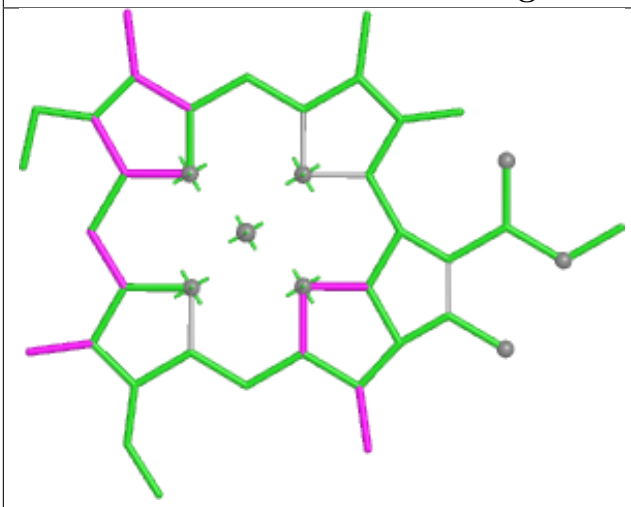


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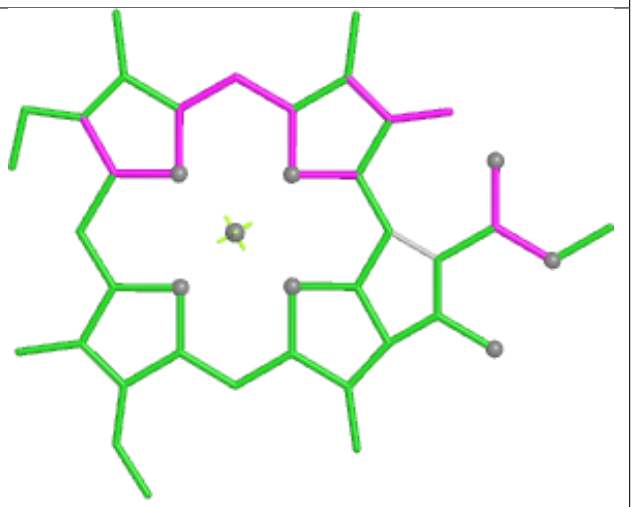


Rings

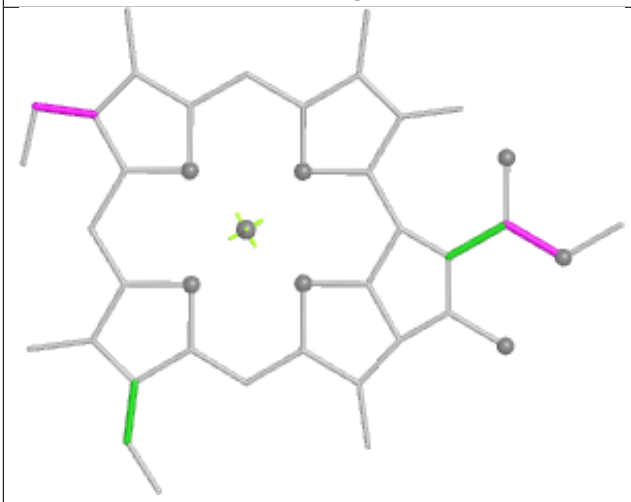
Ligand CLA b5 414



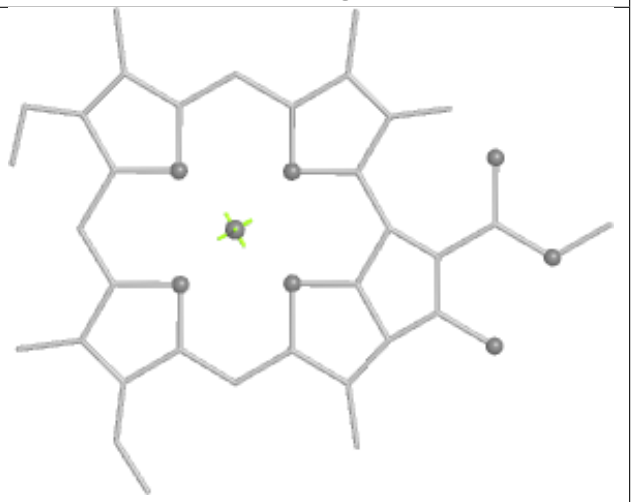
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Bond angles

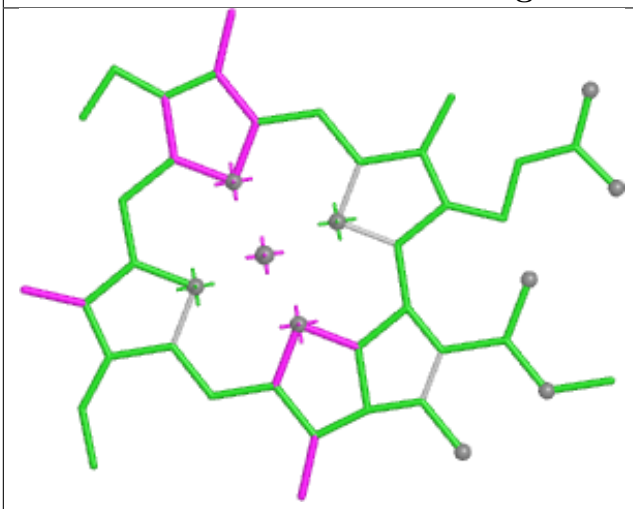


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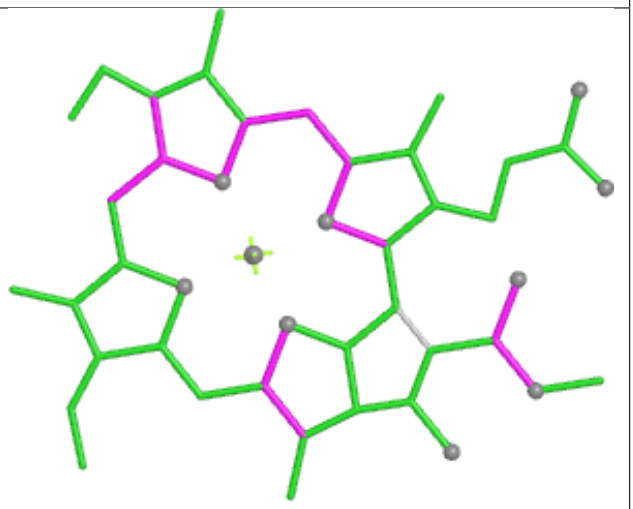


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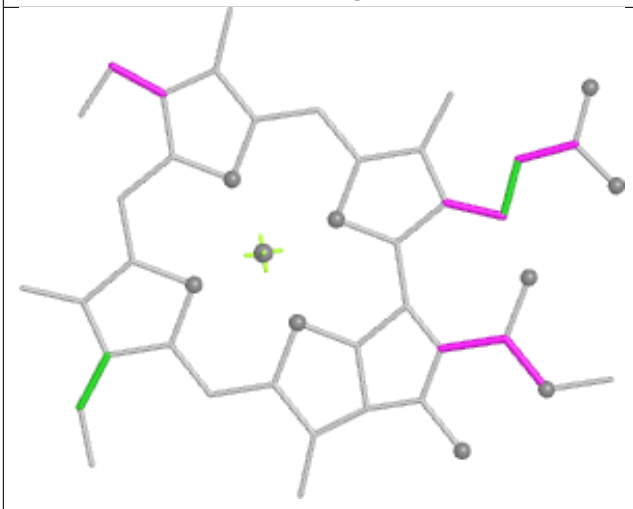
Ligand CLA cA 811



Bond lengths



Bond angles

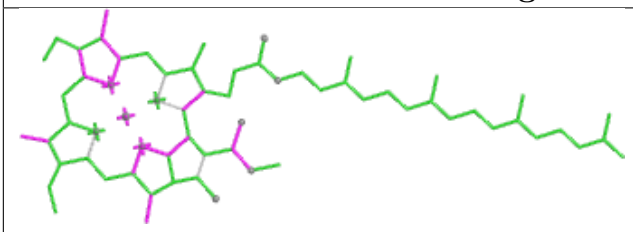


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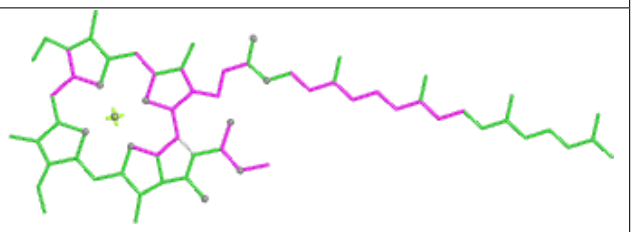


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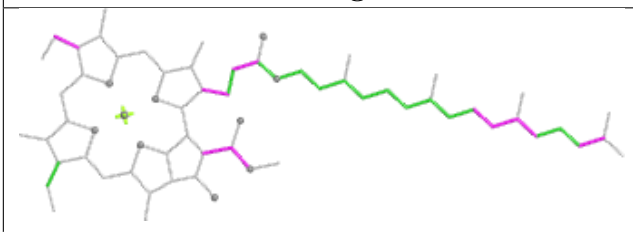
Ligand CLA b4 421



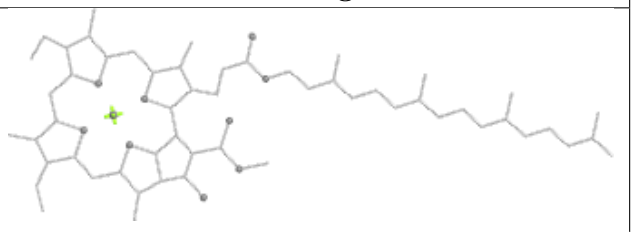
Bond lengths



Bond angles

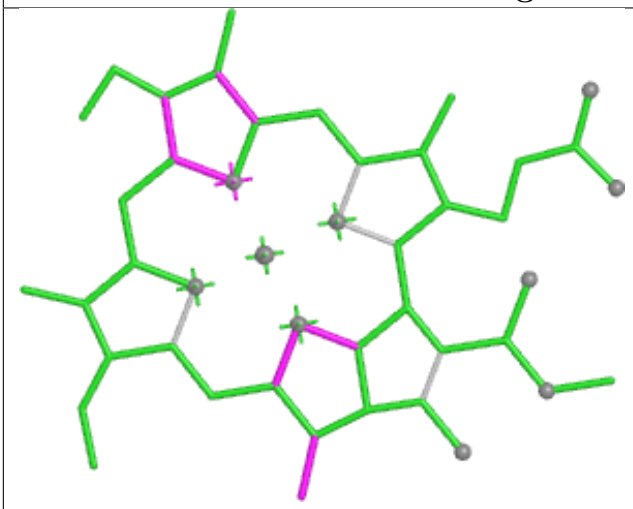


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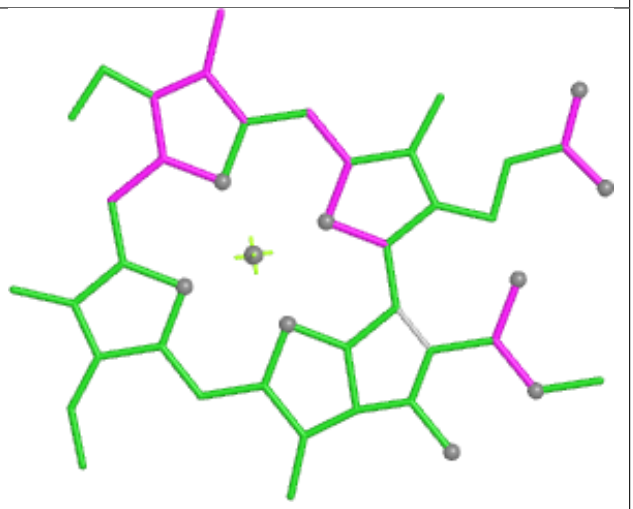


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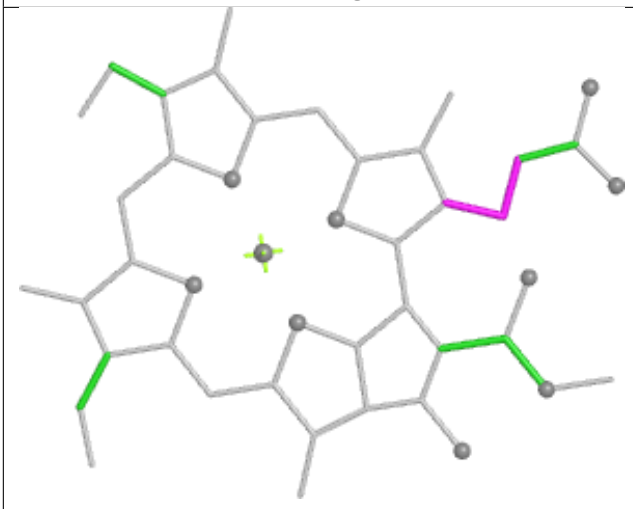
Ligand CLA cB 822



Bond lengths



Bond angles

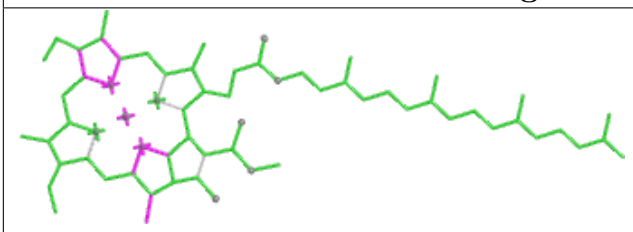


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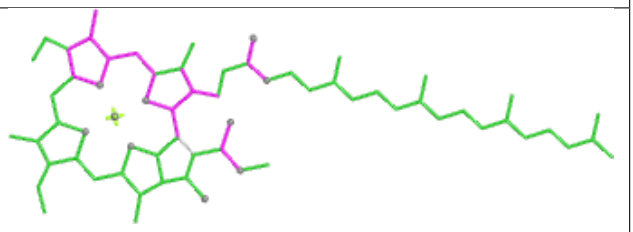


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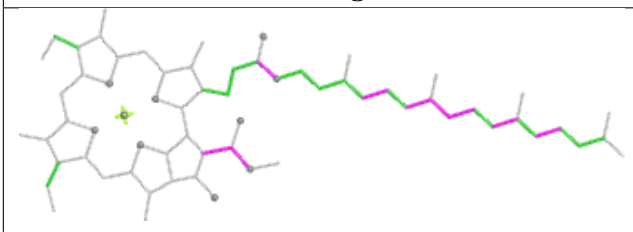
Ligand CLA c5 403



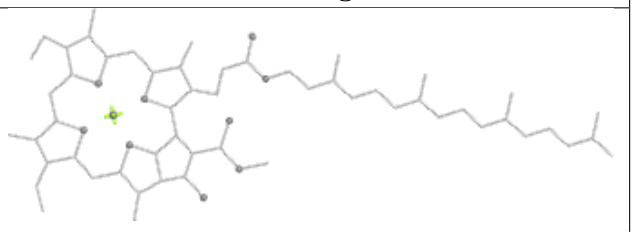
Bond lengths



Bond angles

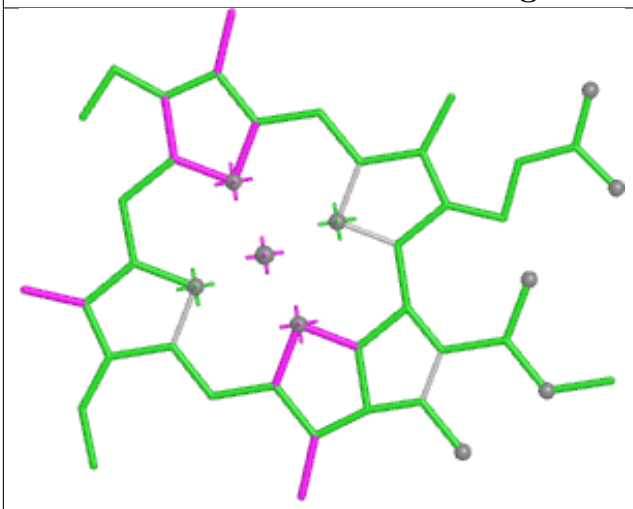


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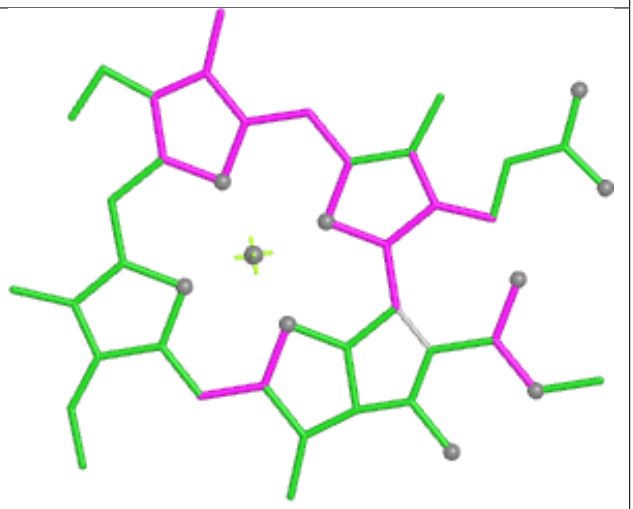


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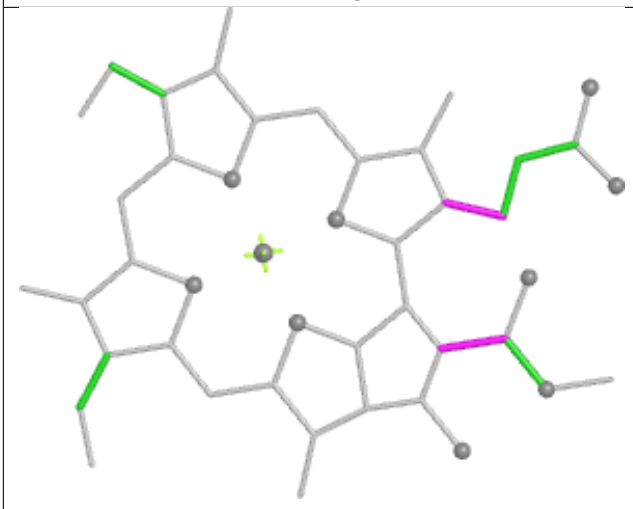
Ligand CLA a5 411



Bond lengths



Bond angles

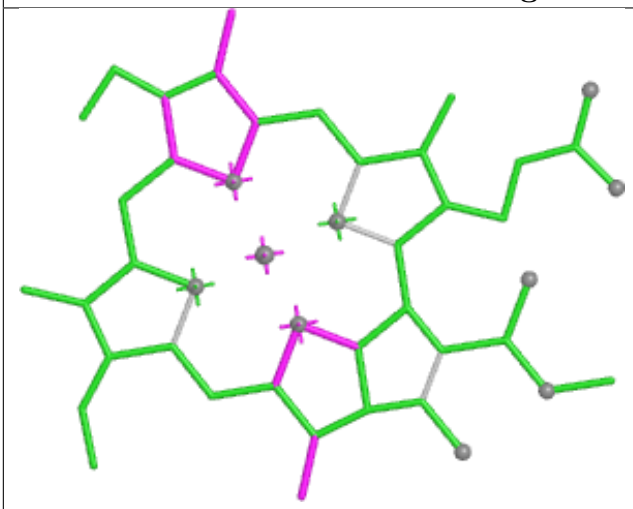


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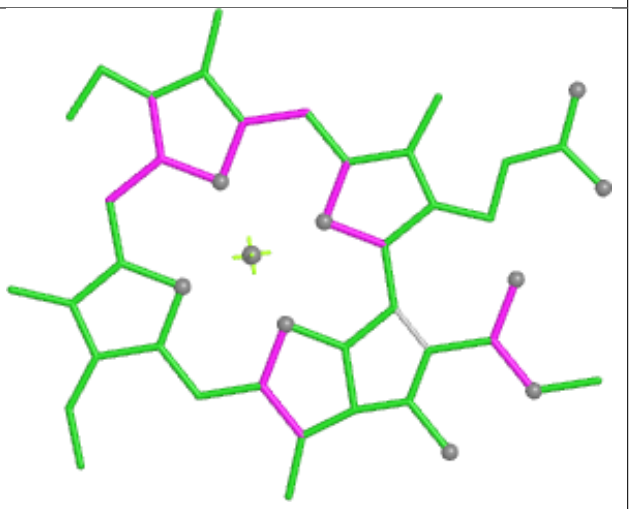


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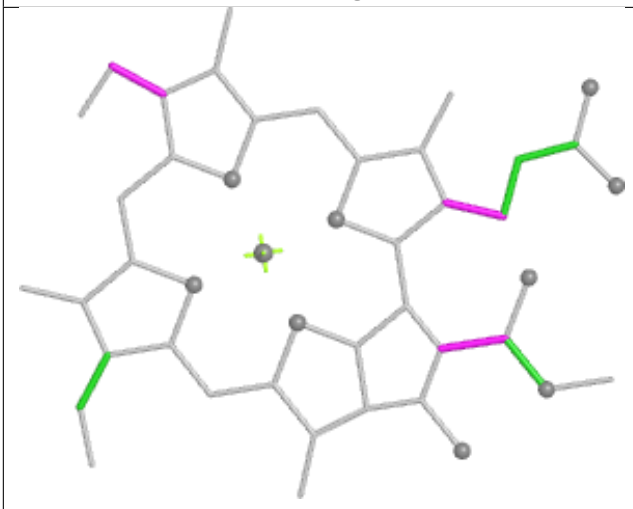
Ligand CLA c3 413



Bond lengths



Bond angles

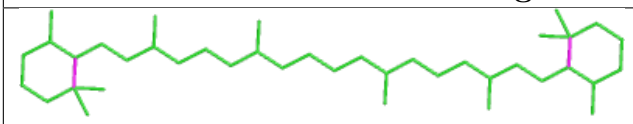


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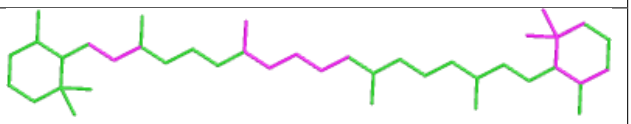


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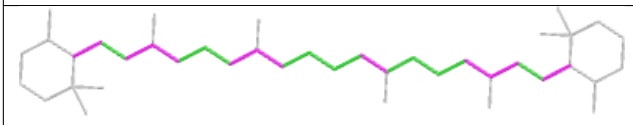
Ligand BCR cB 846



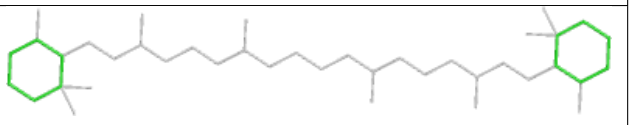
Bond lengths



Bond angles

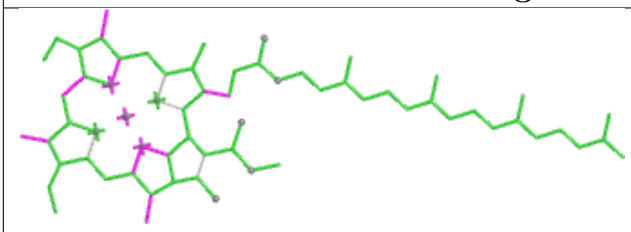


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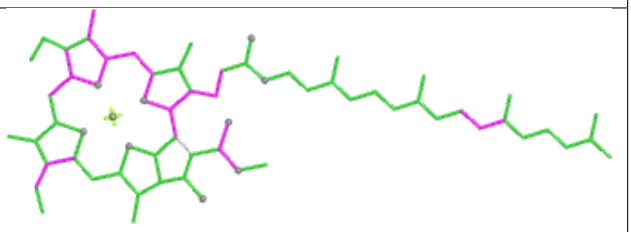


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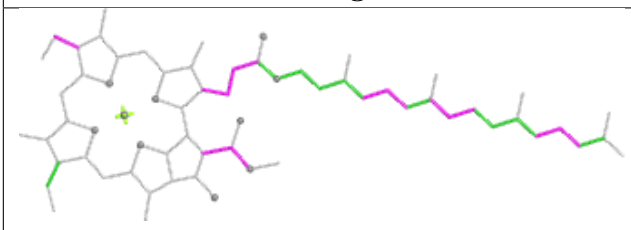
Ligand CLA bB 810



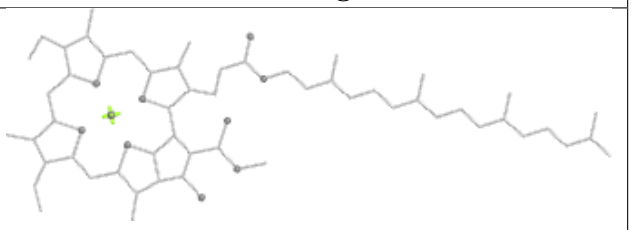
Bond lengths



Bond angles

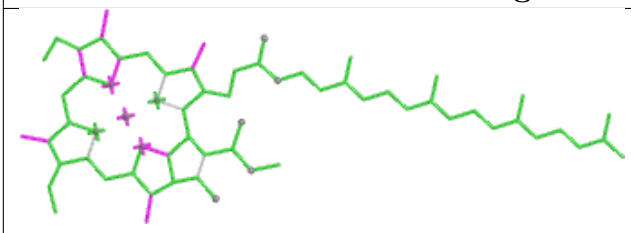


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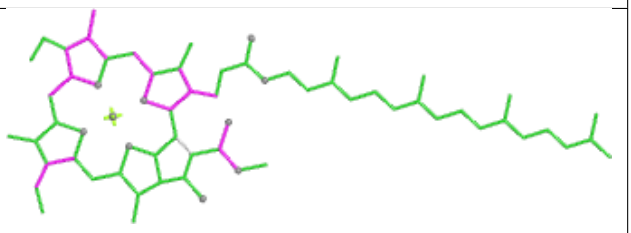


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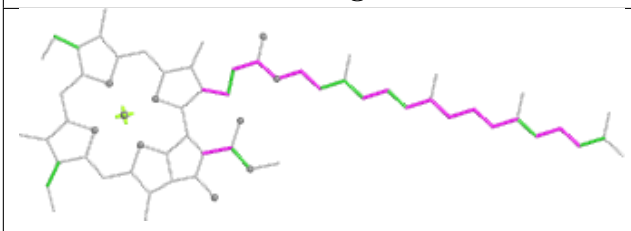
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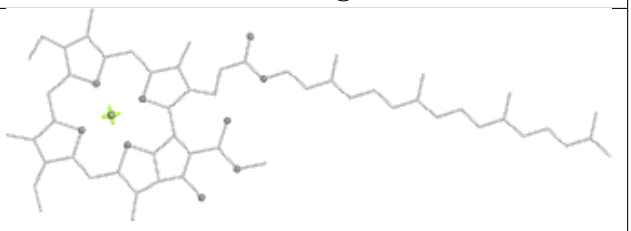
Bond lengths



Bond angles

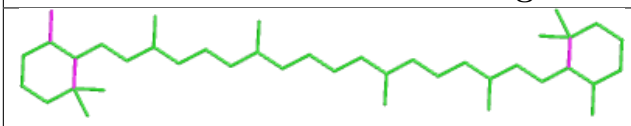


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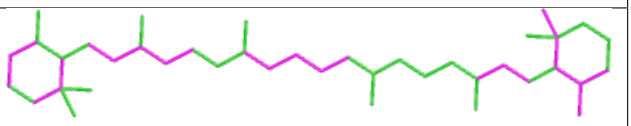


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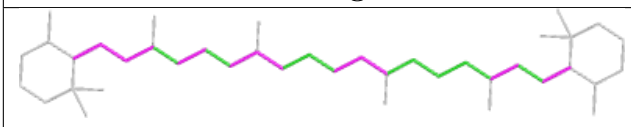
Ligand BCR aL 205



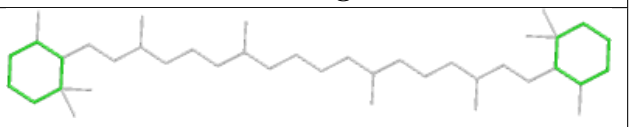
Bond lengths



Bond angles

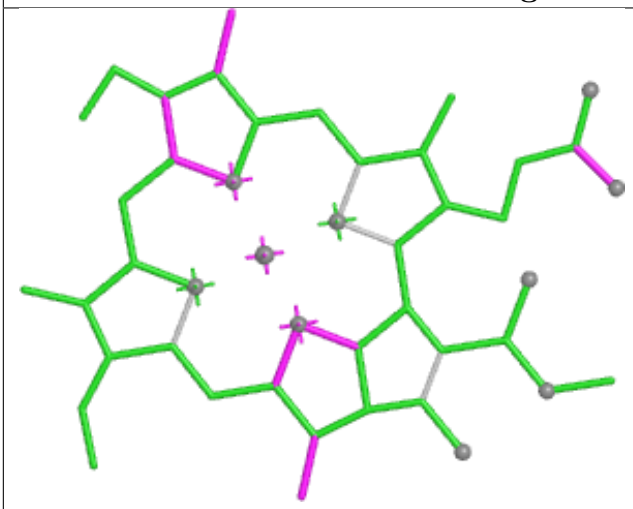


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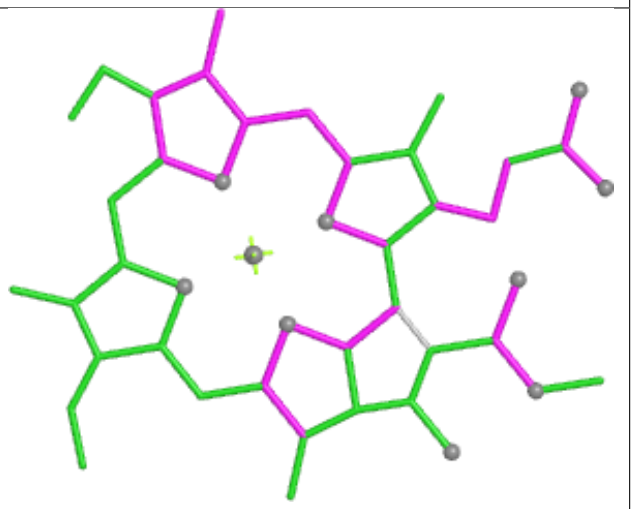


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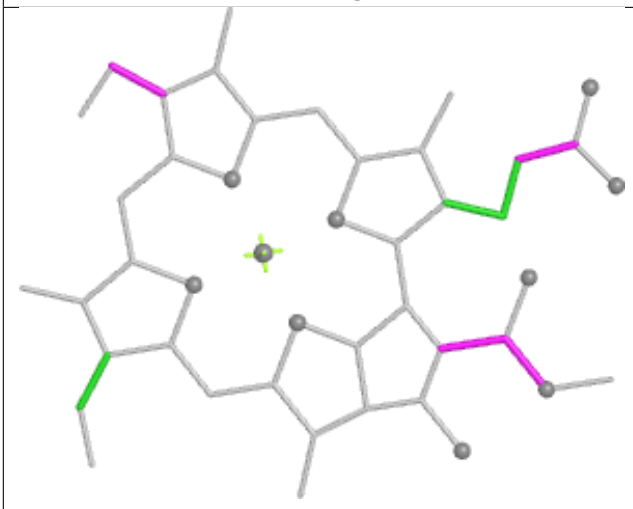
Ligand CLA c1 415



Bond lengths



Bond angles

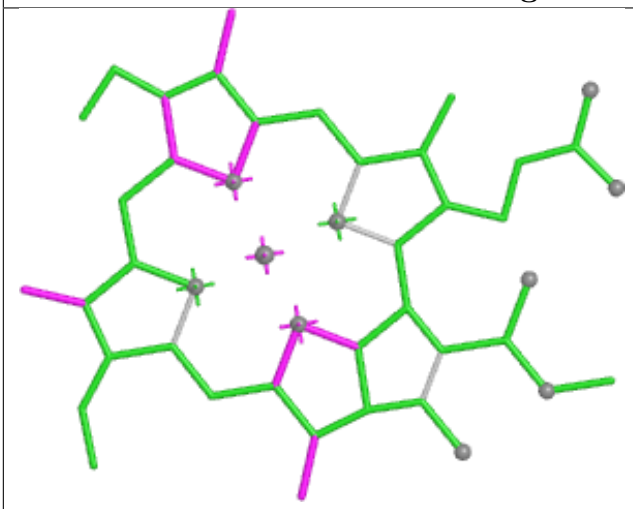


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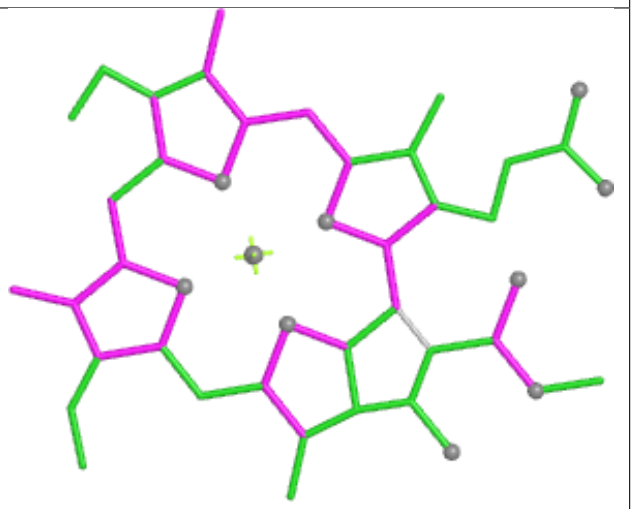


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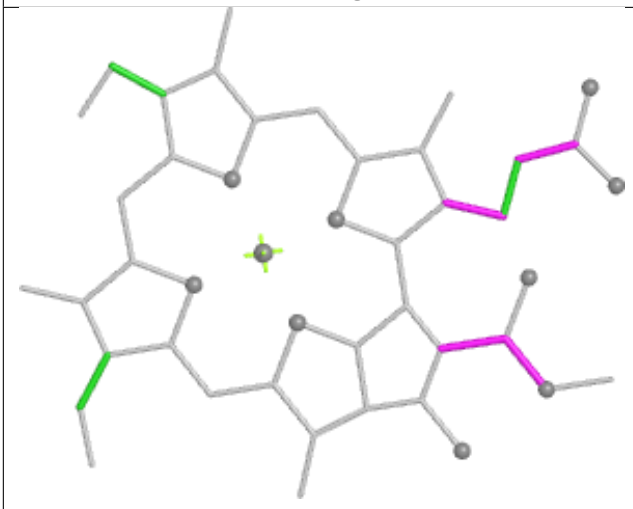
Ligand CLA c3 412



Bond lengths



Bond angles

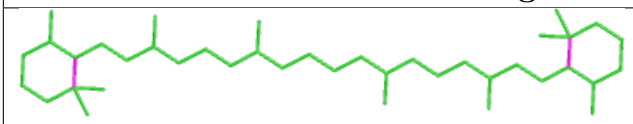


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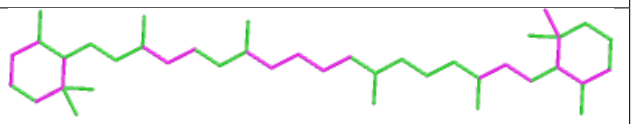


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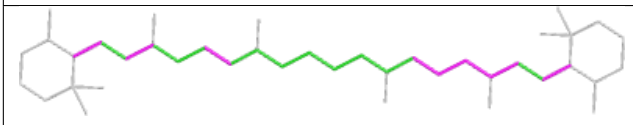
Ligand BCR c4 419



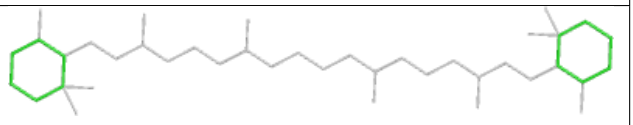
Bond lengths



Bond angles

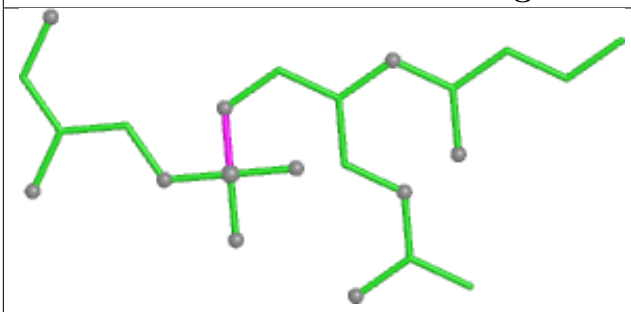


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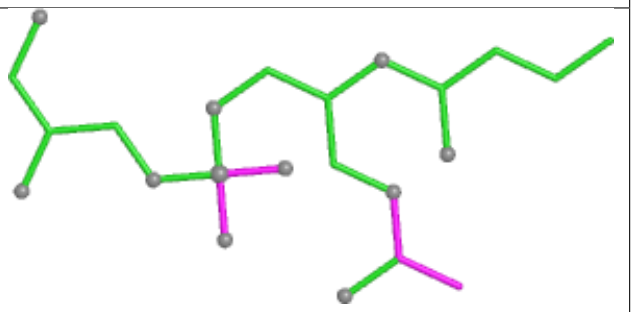


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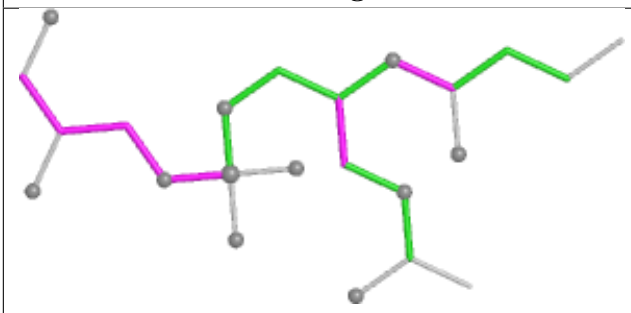
Ligand LHG cX 101



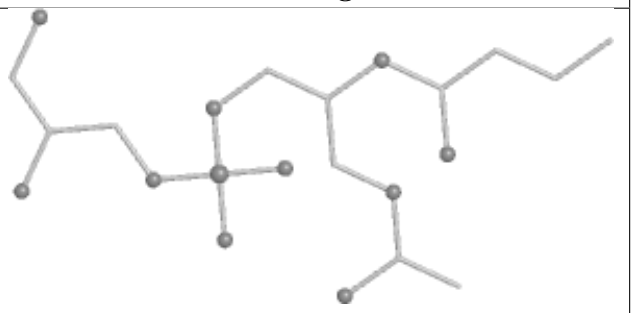
Bond lengths



Bond angles



Torsions

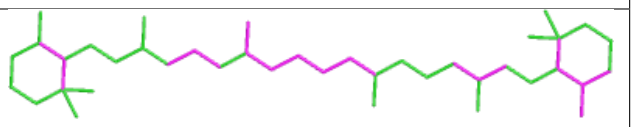


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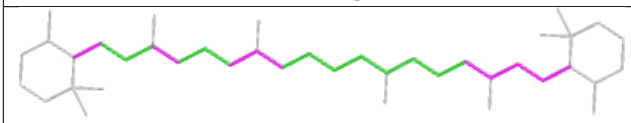
Ligand BCR cB 849



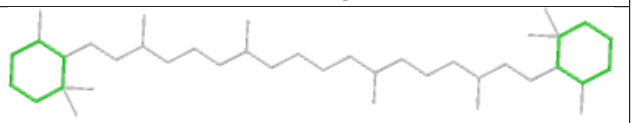
Bond lengths



Bond angles

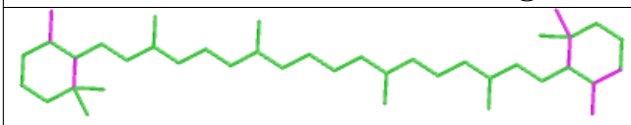


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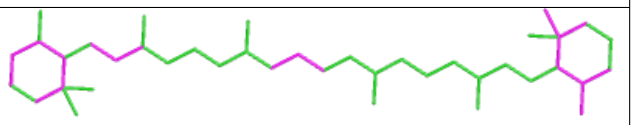


Rings

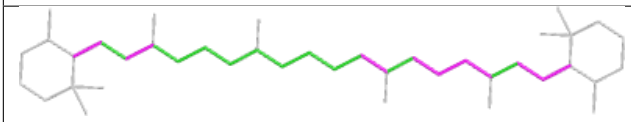
Ligand BCR c3 418



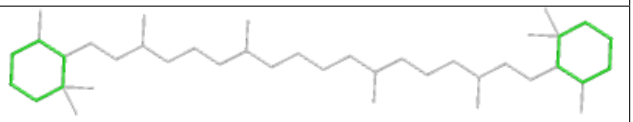
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Bond angles

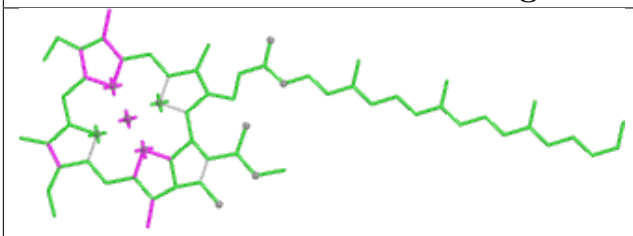


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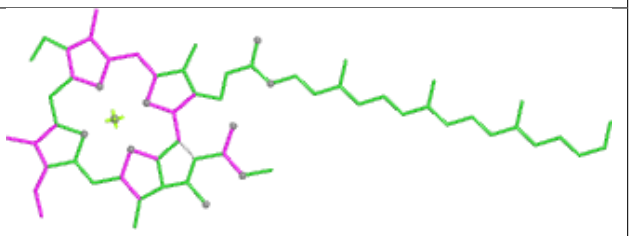


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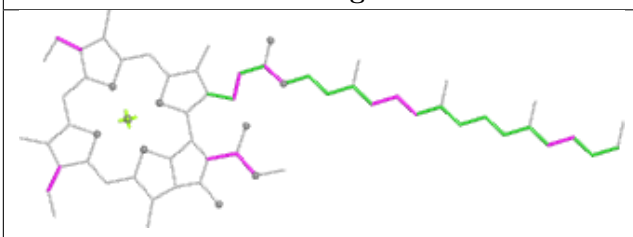
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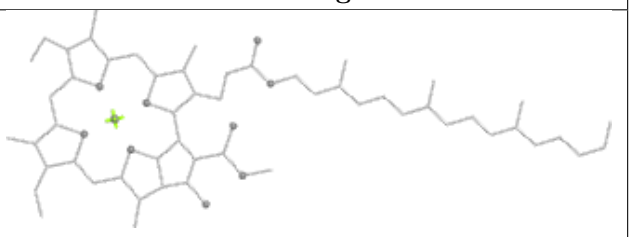
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Bond angles

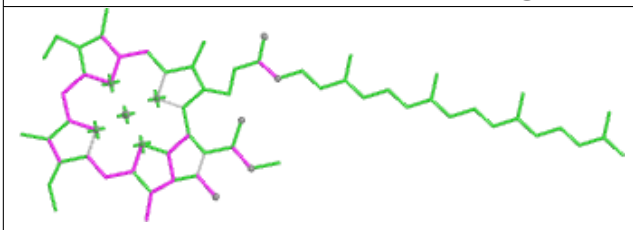


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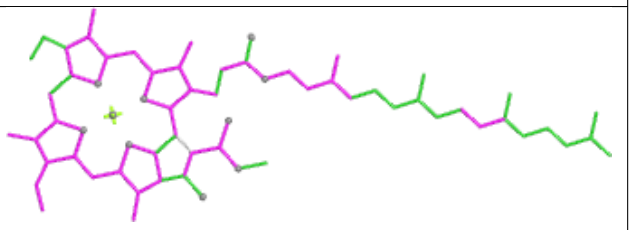


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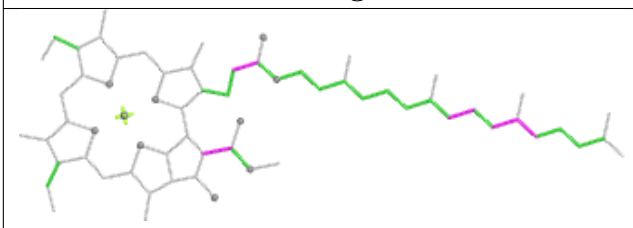
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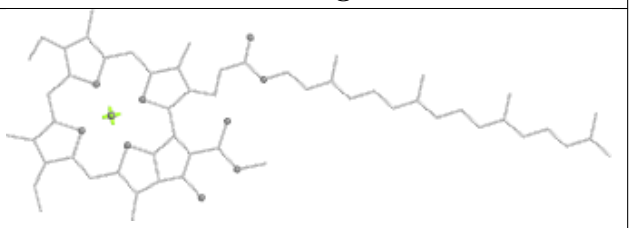
Bond lengths



Bond angles

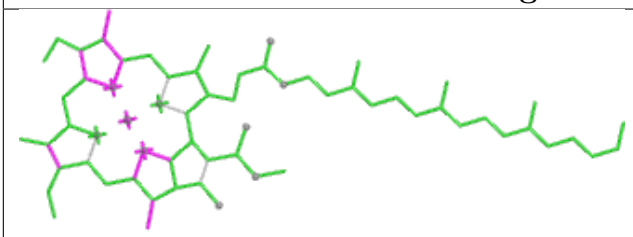


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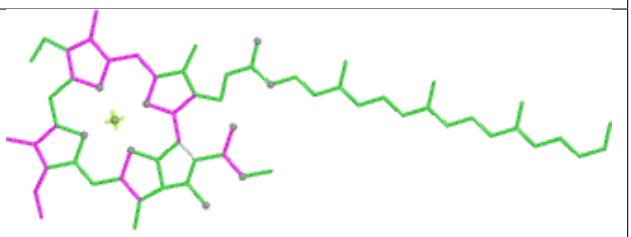


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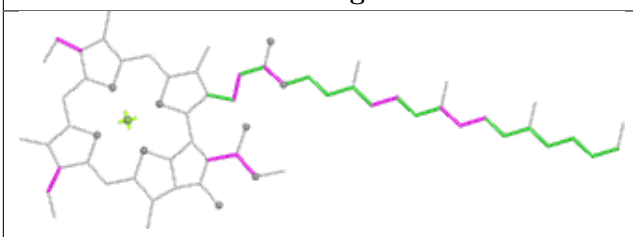
Ligand CLA a1 409



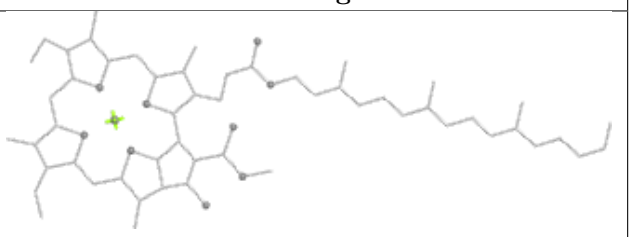
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Bond angles

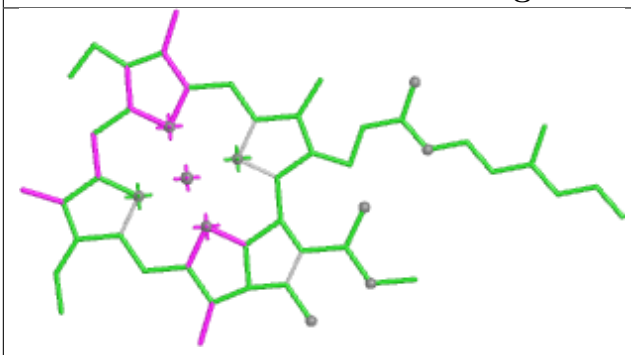


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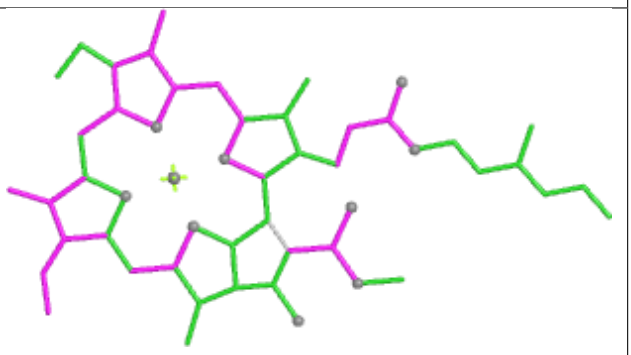


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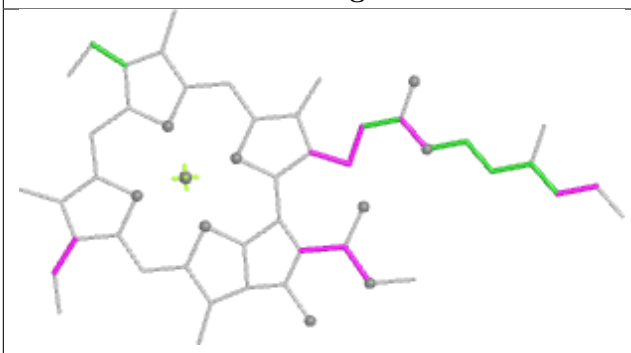
Ligand CLA bA 845



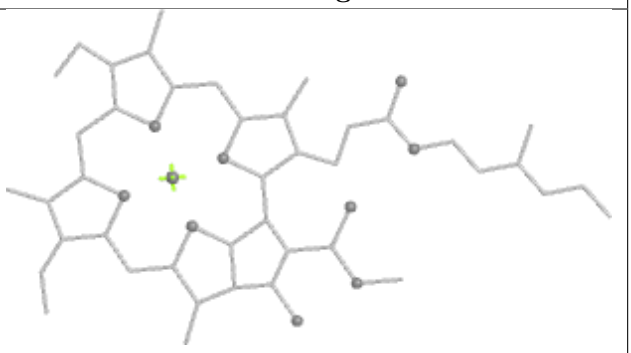
Bond lengths



Bond angles

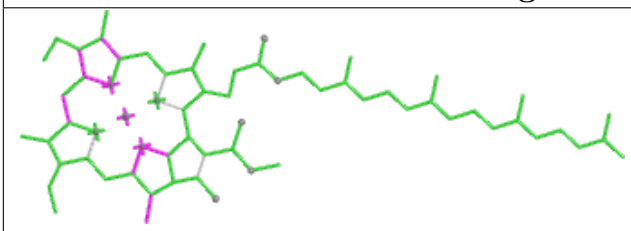


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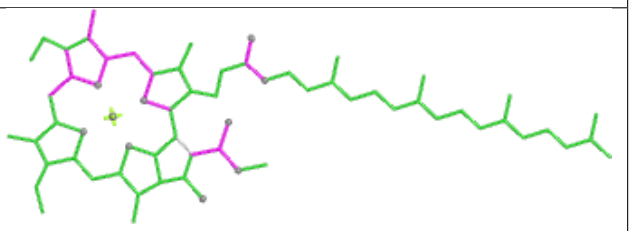


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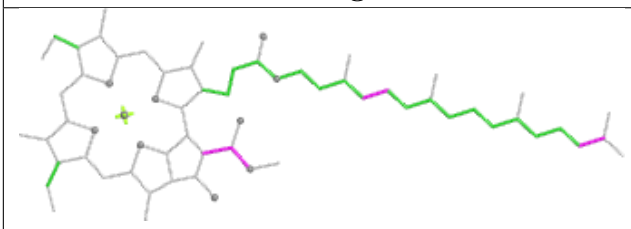
Ligand CLA b6 410



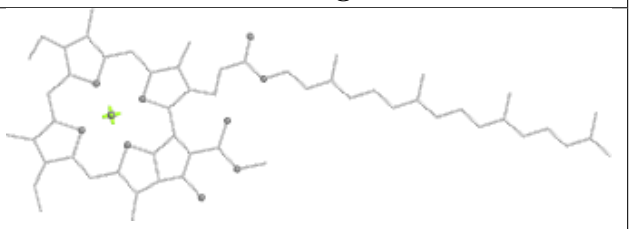
Bond lengths



Bond angles

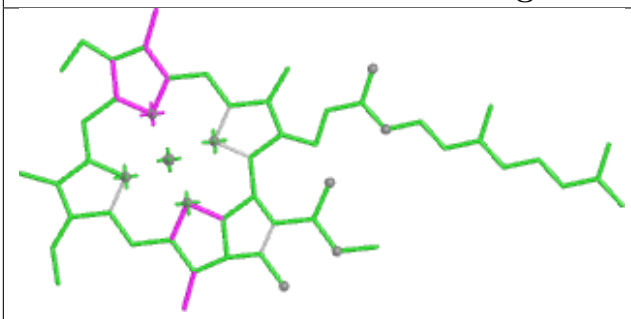


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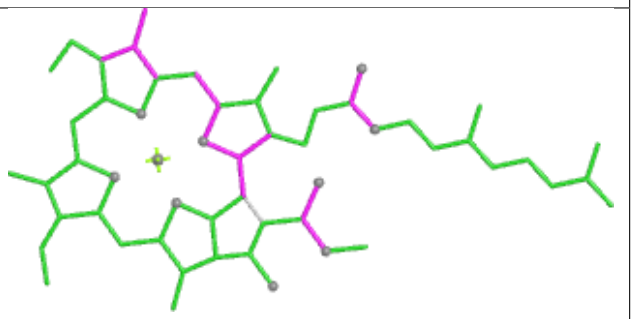


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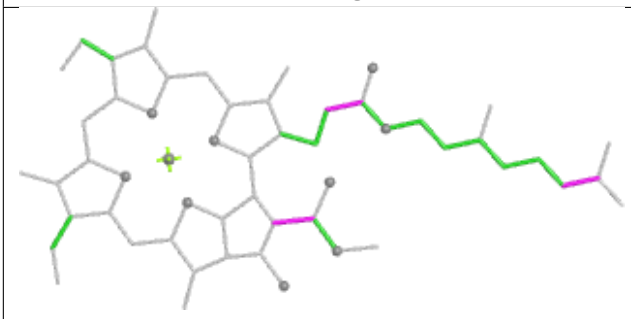
Ligand CLA cB 823



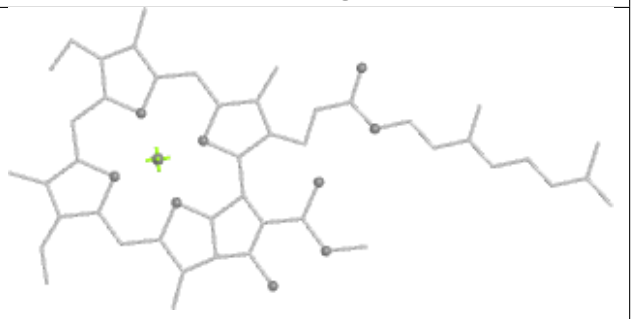
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Bond angles

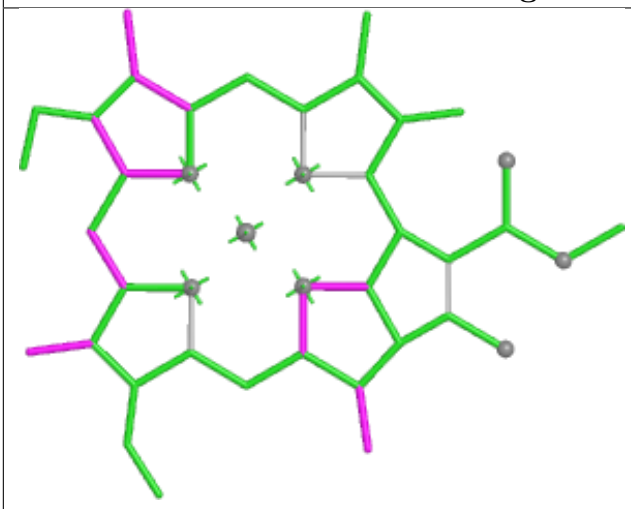


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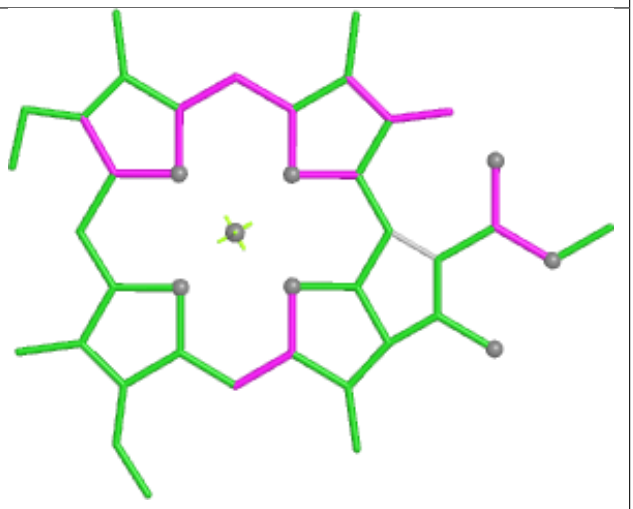


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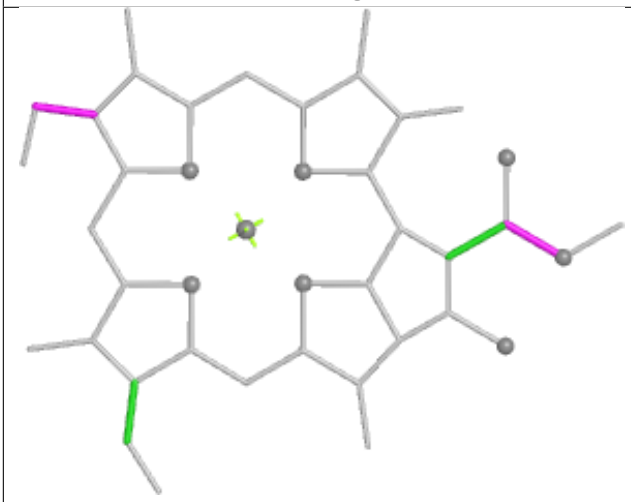
Ligand CLA a5 414



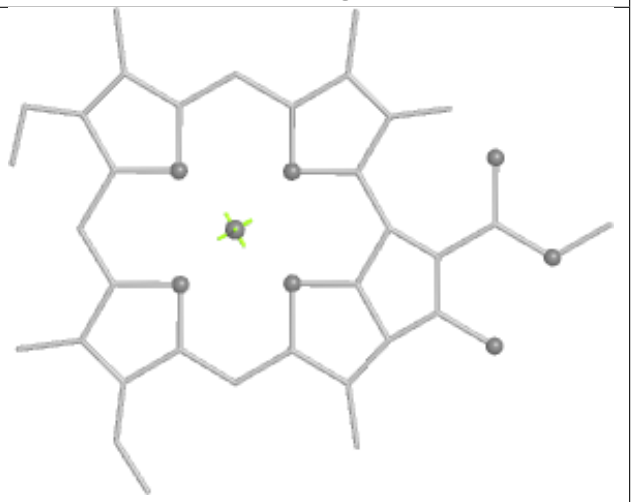
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Bond angles

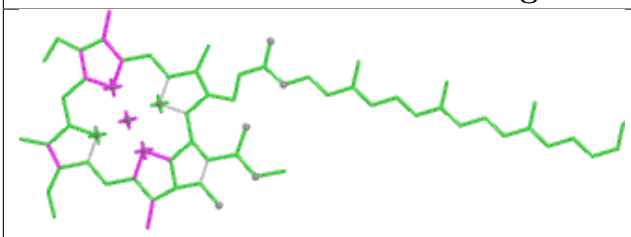


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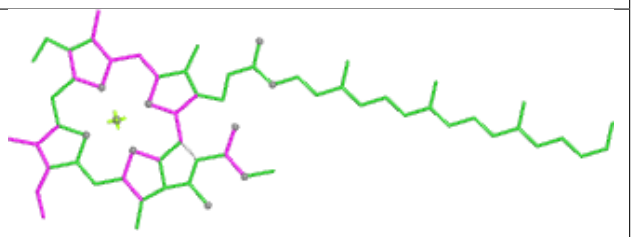


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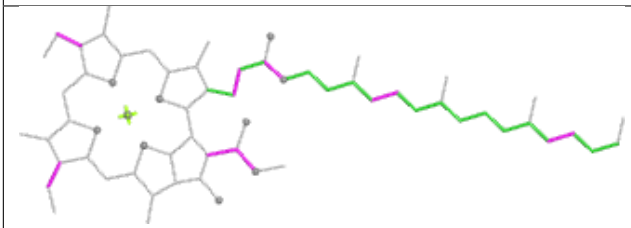
Ligand CLA c3 410



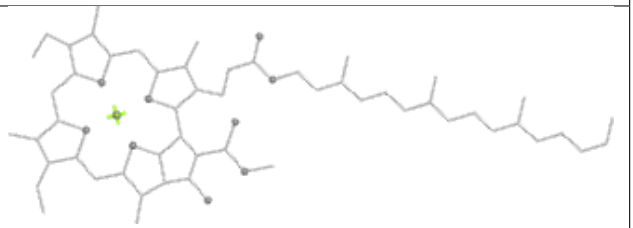
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Bond angles

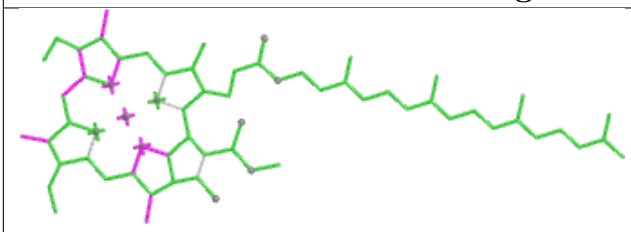


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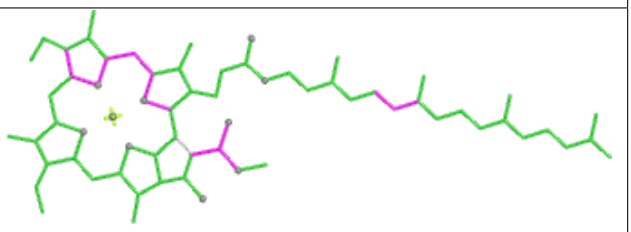


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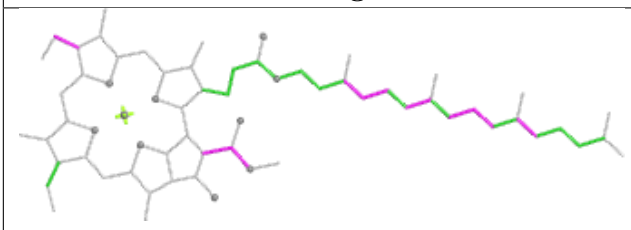
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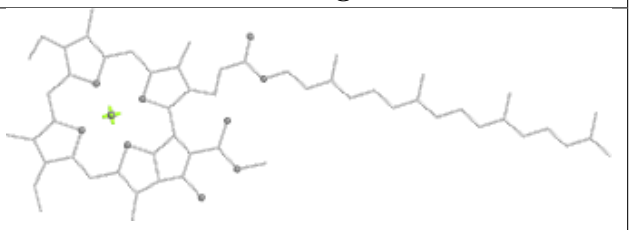
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Bond angles

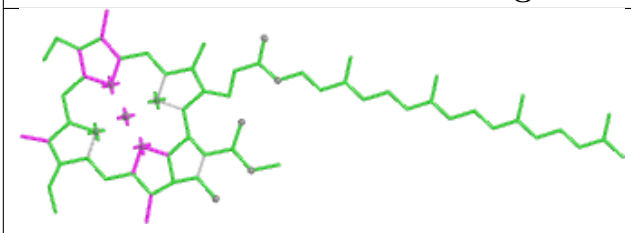


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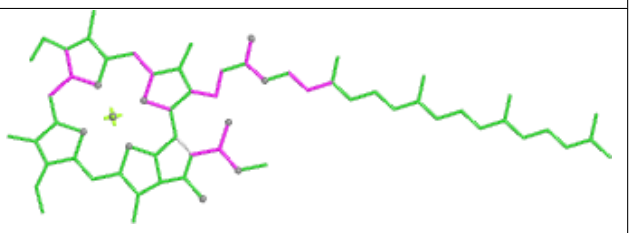


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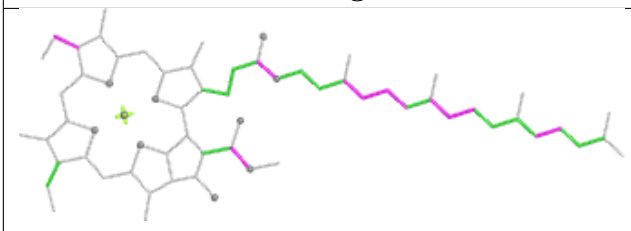
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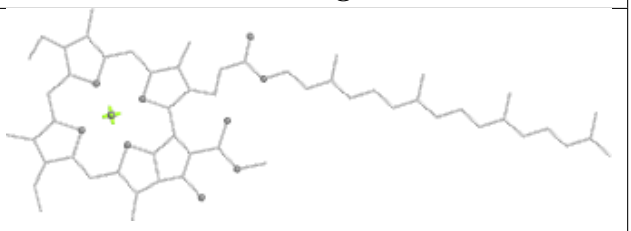
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Bond angles

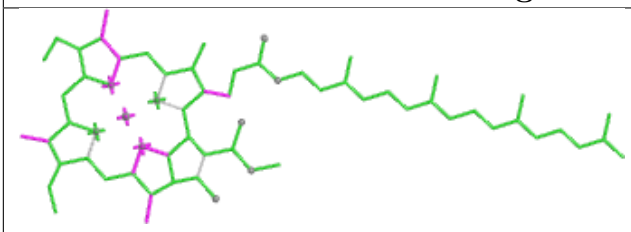


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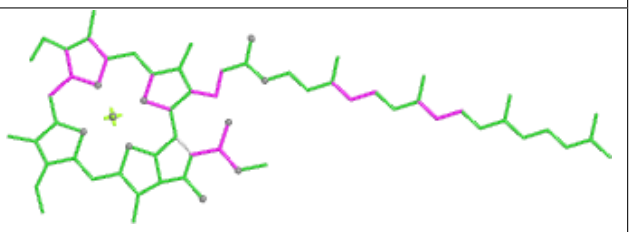


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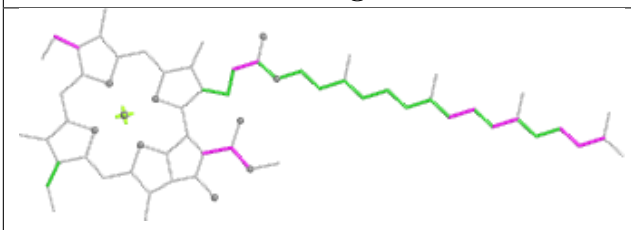
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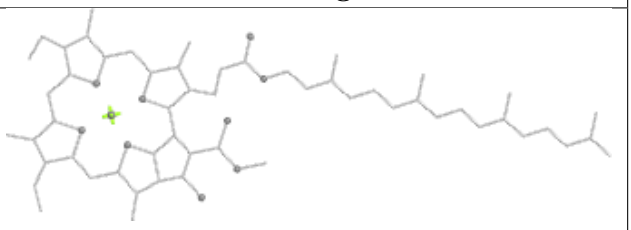
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Bond angles

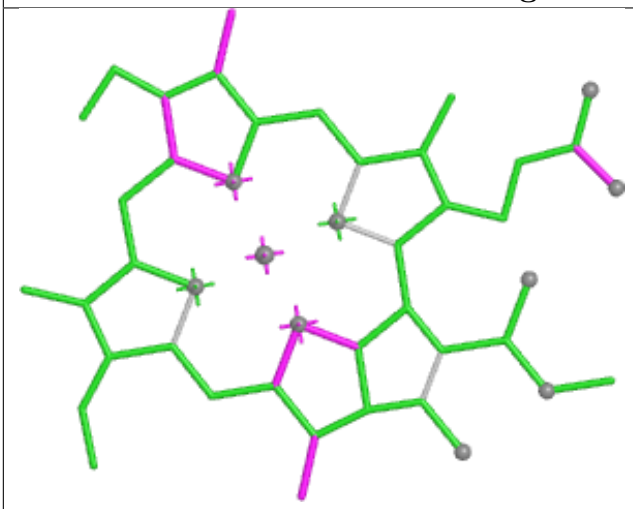


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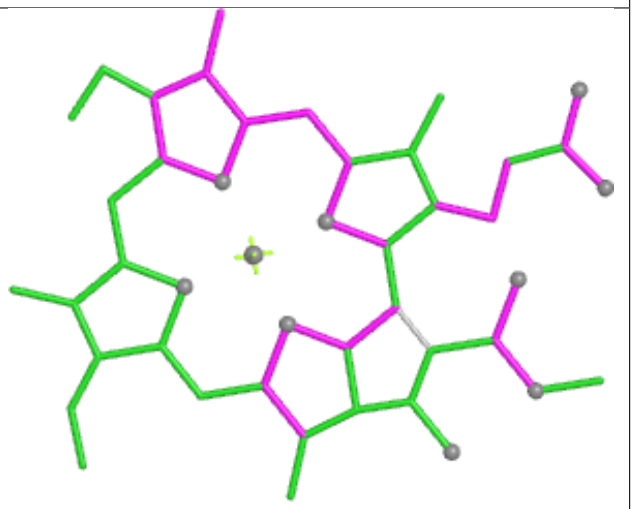


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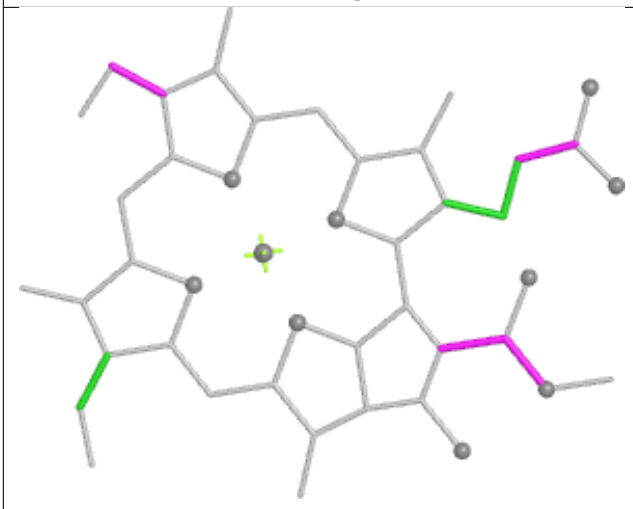
Ligand CLA a1 414



Bond lengths



Bond angles

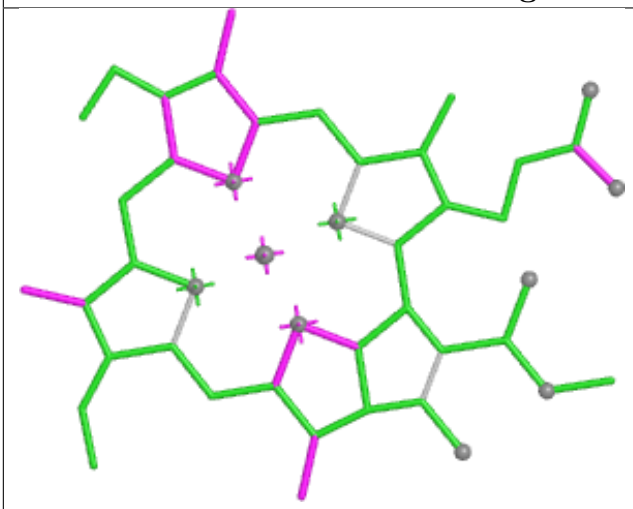


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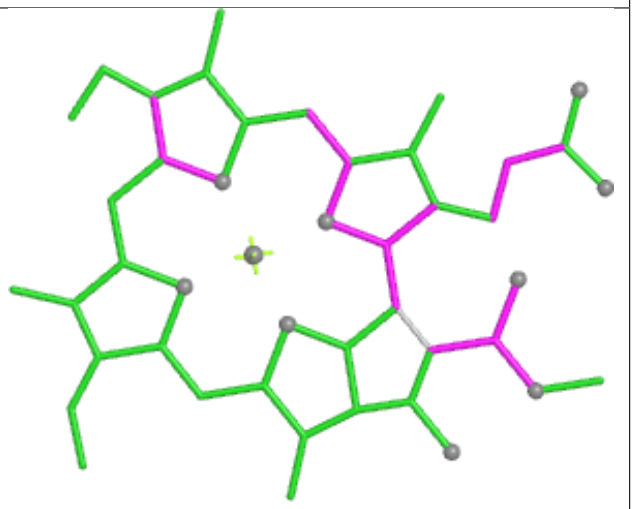


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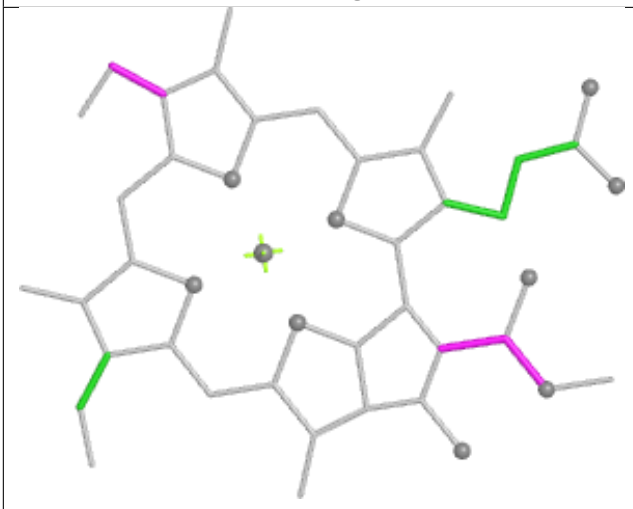
Ligand CLA aJ 202



Bond lengths



Bond angles

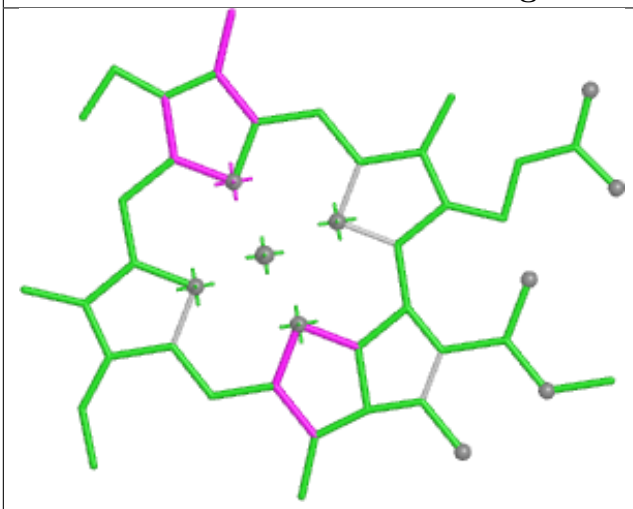


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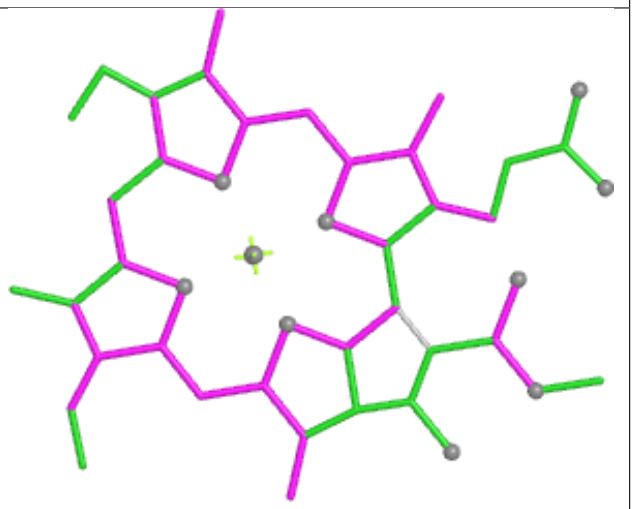


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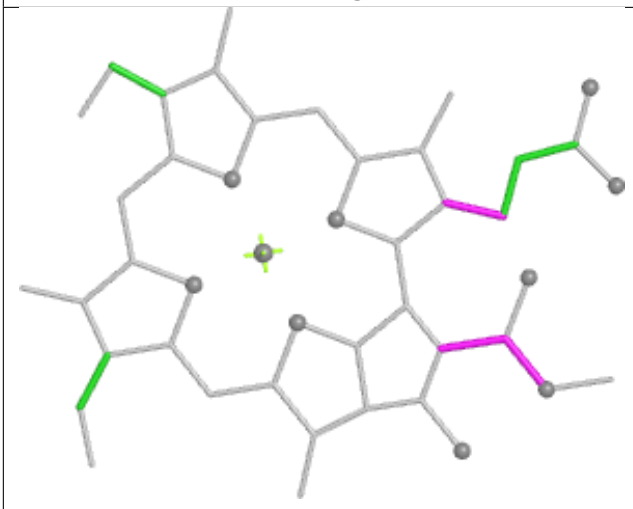
Ligand CLA a2 405



Bond lengths



Bond angles

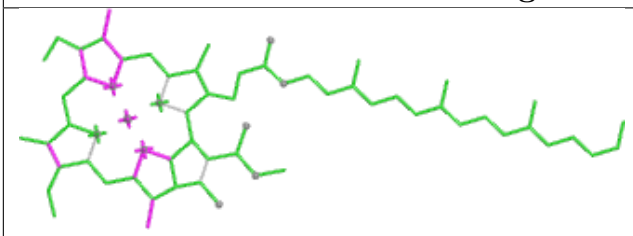


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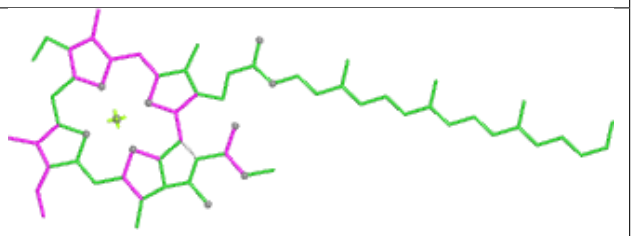


Rings

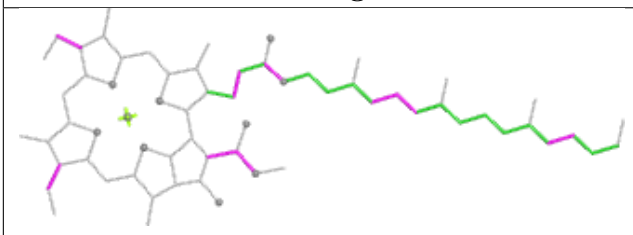
Ligand CLA b2 411



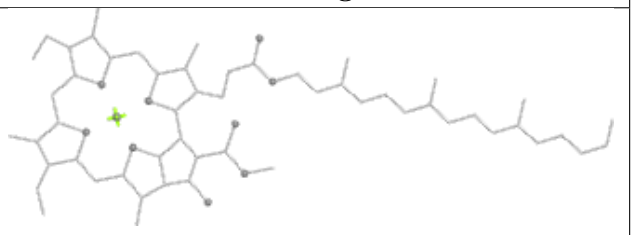
Bond lengths



Bond angles

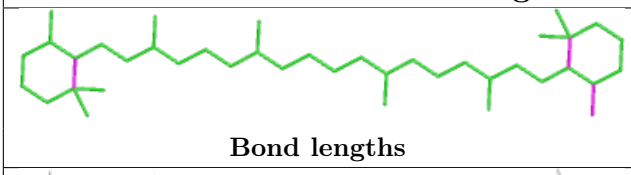


Torsions

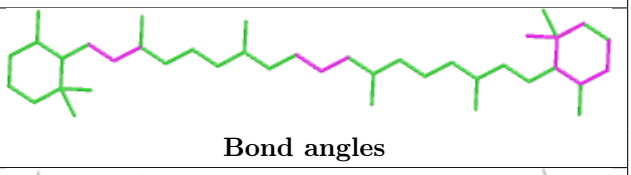


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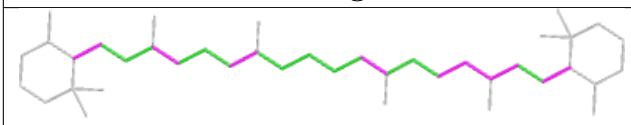
Ligand BCR bB 845



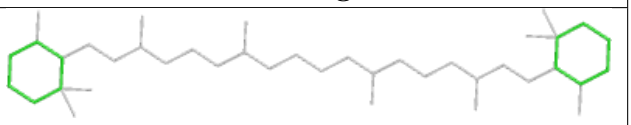
Bond lengths



Bond angles

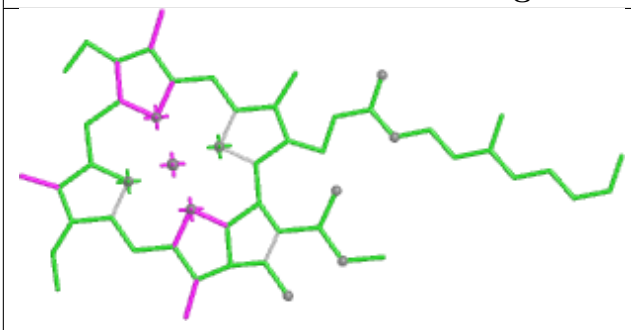


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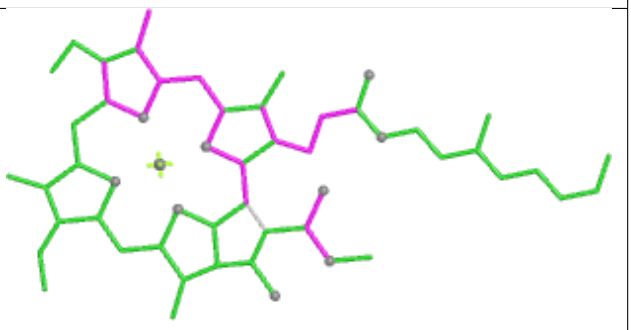


Rings

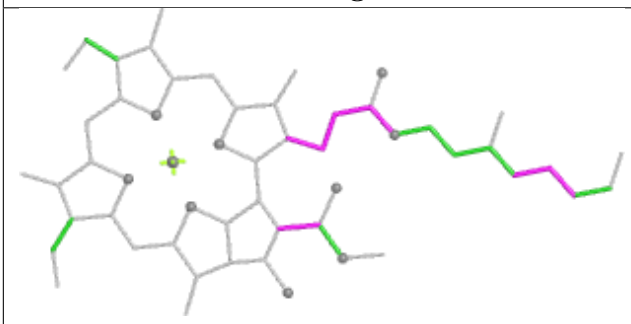
Ligand CLA bA 813



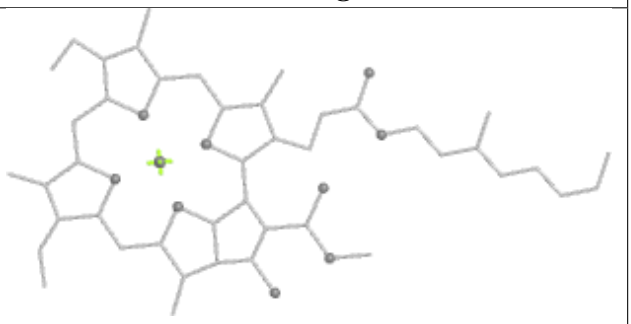
Bond lengths



Bond angles

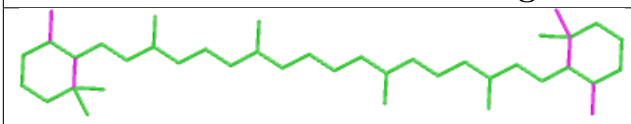


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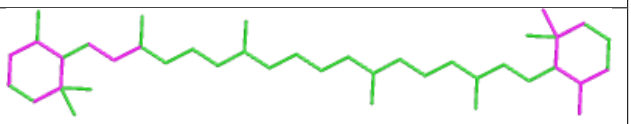


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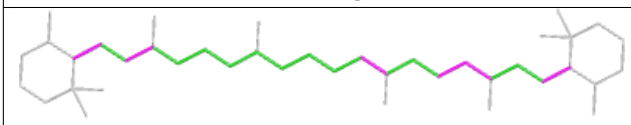
Ligand BCR c4 418



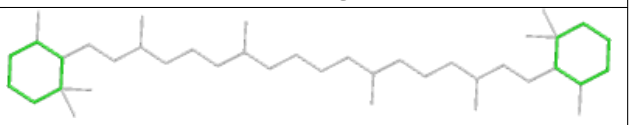
Bond lengths



Bond angles

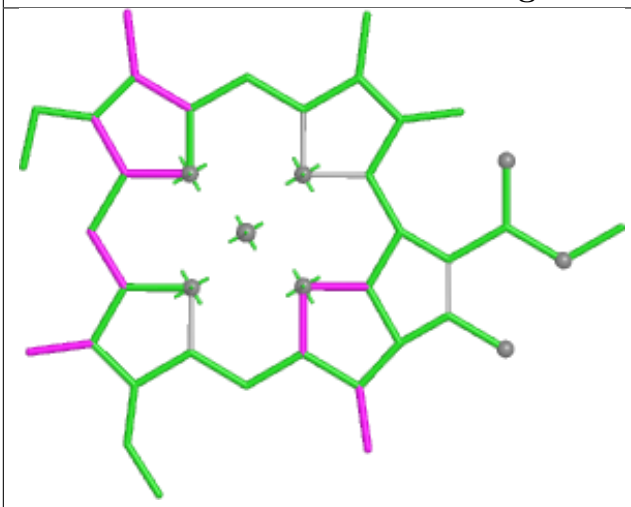


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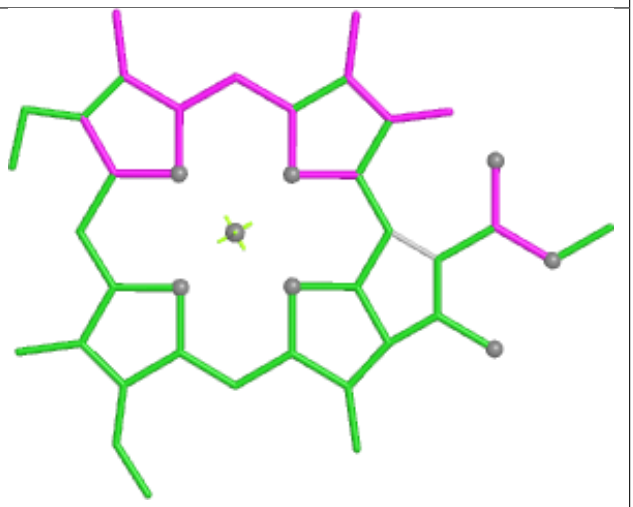


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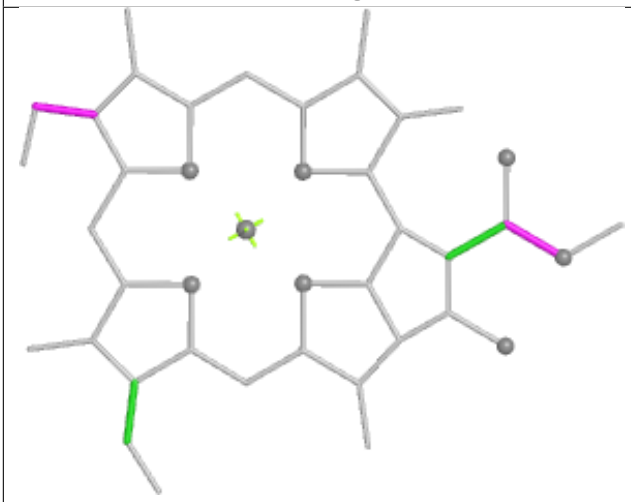
Ligand CLA b1 414



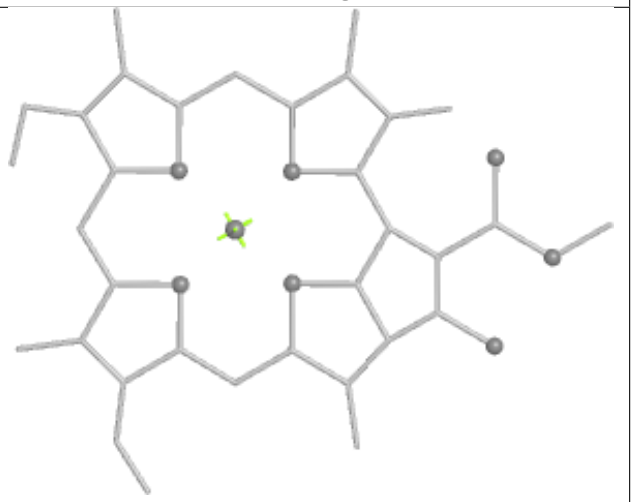
Bond lengths



Bond angles

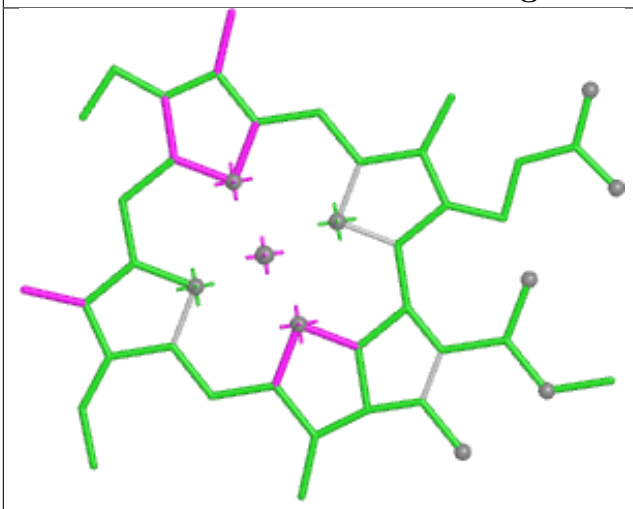


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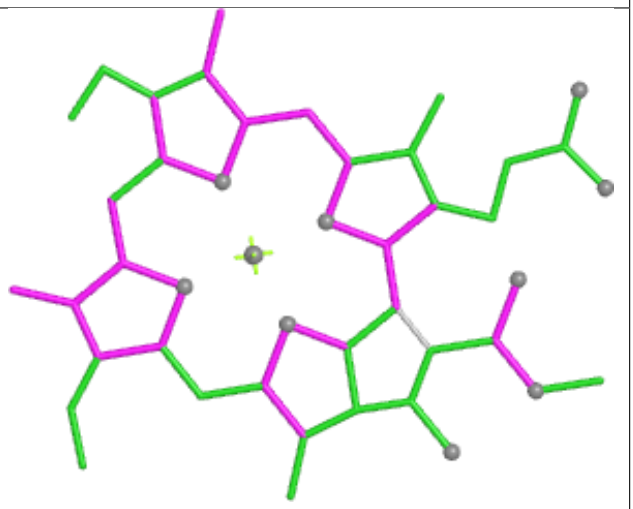


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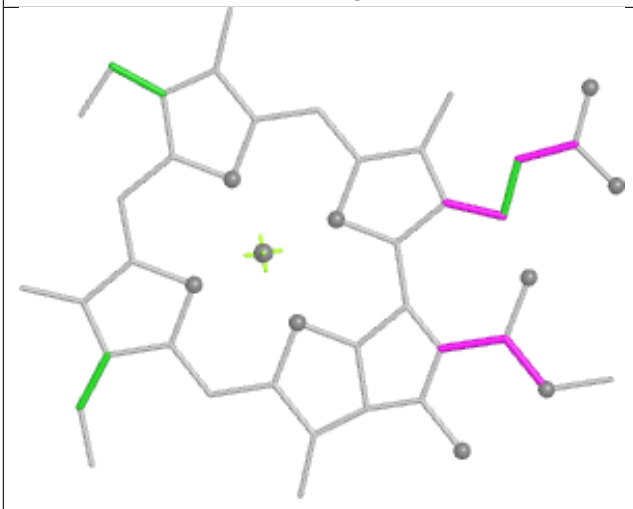
Ligand CLA c5 412



Bond lengths



Bond angles

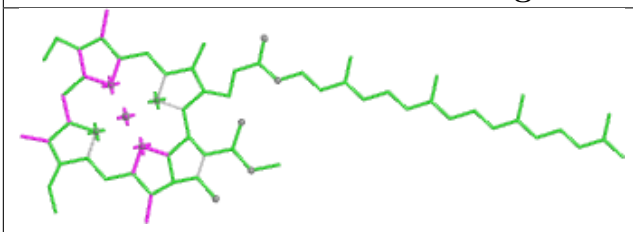


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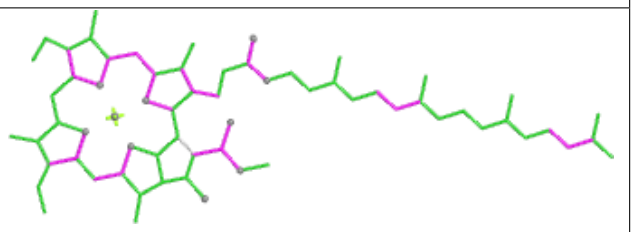


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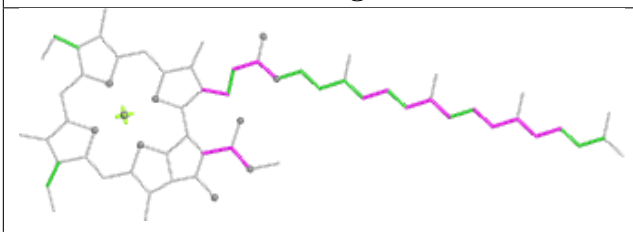
Ligand CLA bB 833



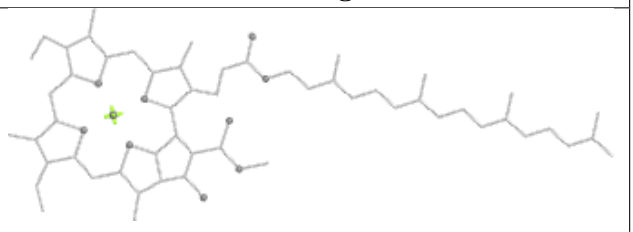
Bond lengths



Bond angles

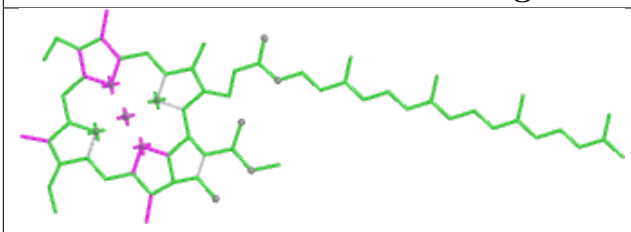


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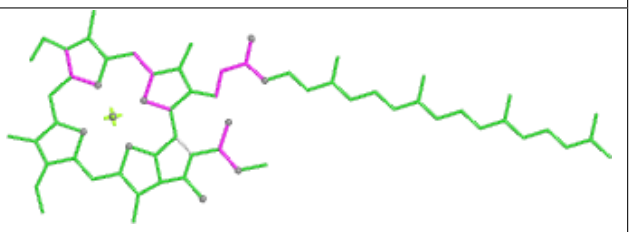


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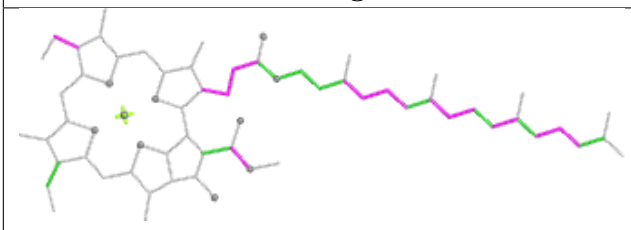
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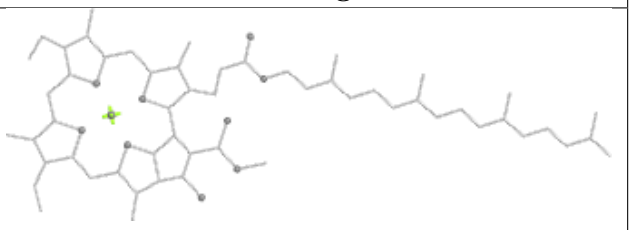
Bond lengths



Bond angles



Torsions

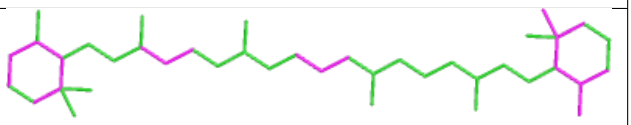


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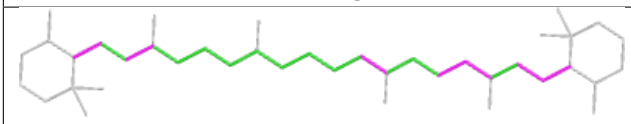
Ligand BCR a2 419



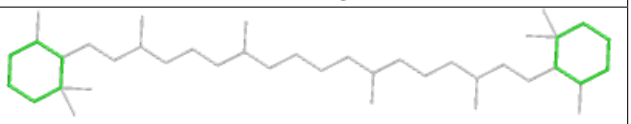
Bond lengths



Bond angles

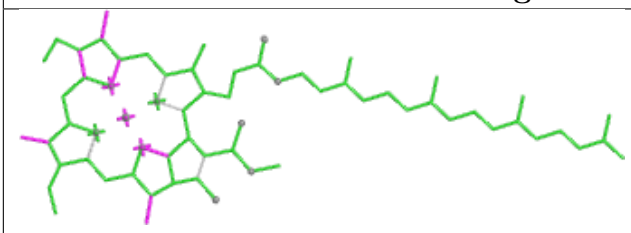


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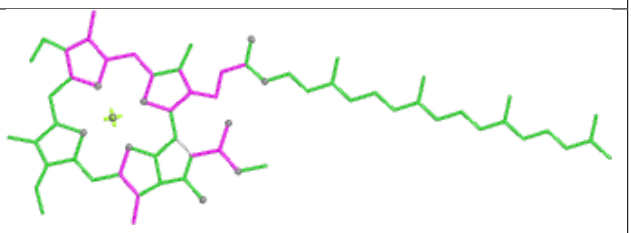


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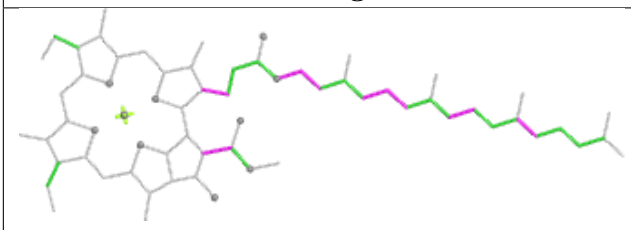
Ligand CLA bA 827



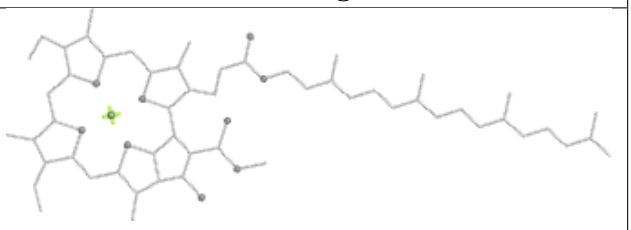
Bond lengths



Bond angles

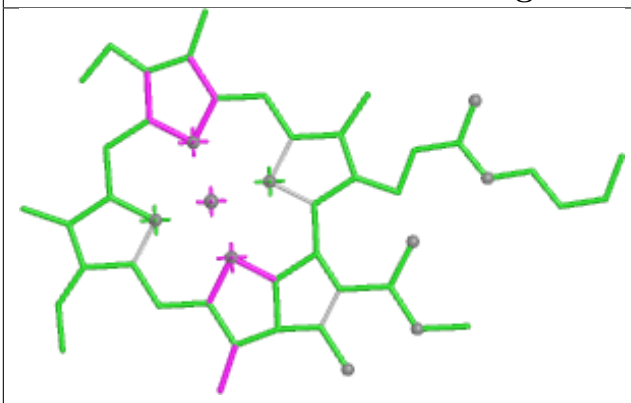


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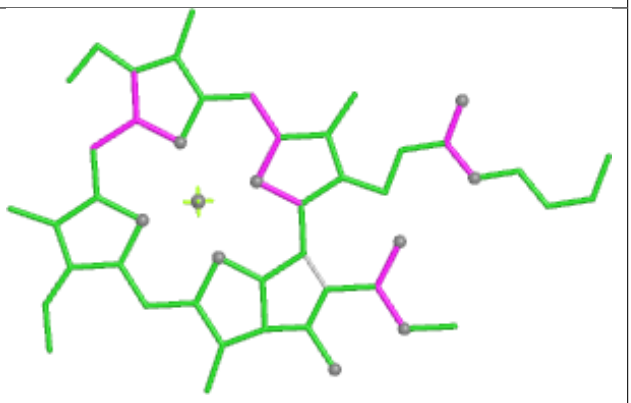


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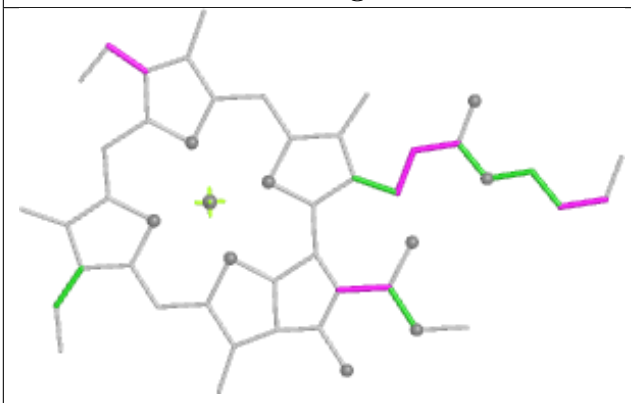
Ligand CLA cA 823



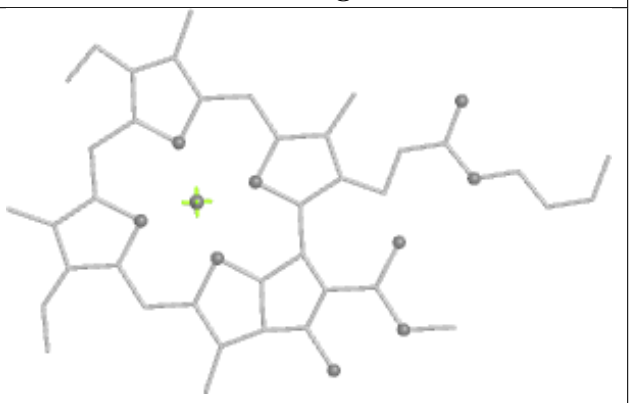
Bond lengths



Bond angles

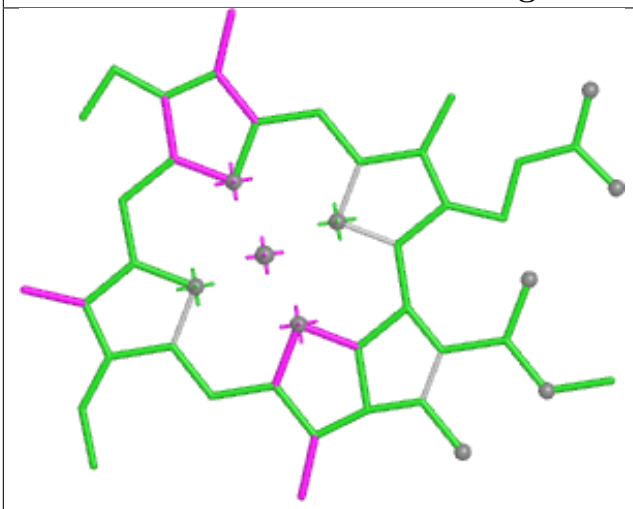


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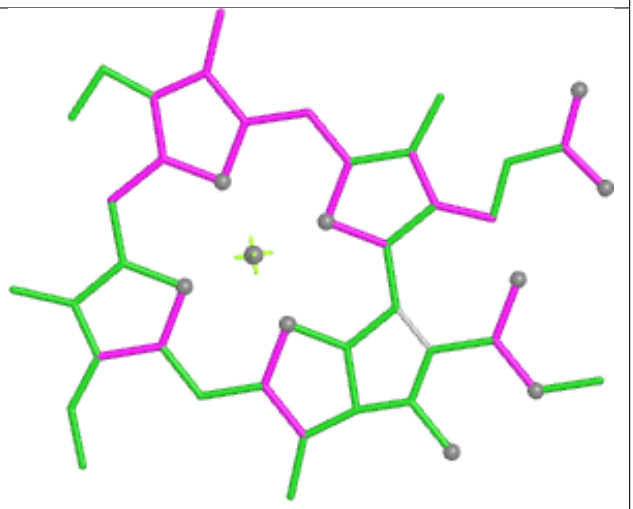


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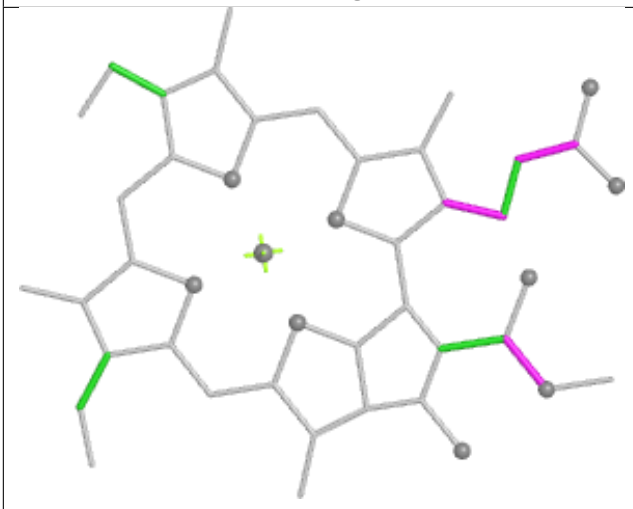
Ligand CLA b3 408



Bond lengths



Bond angles

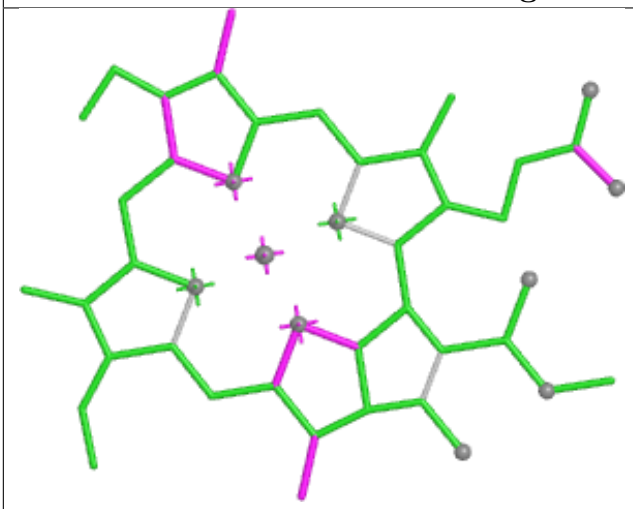


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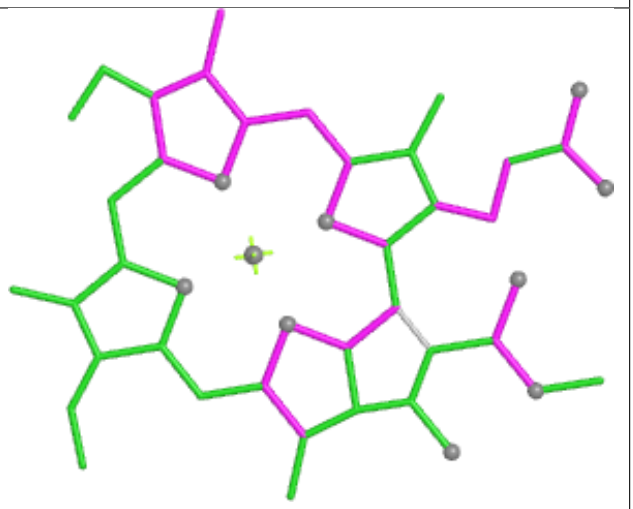


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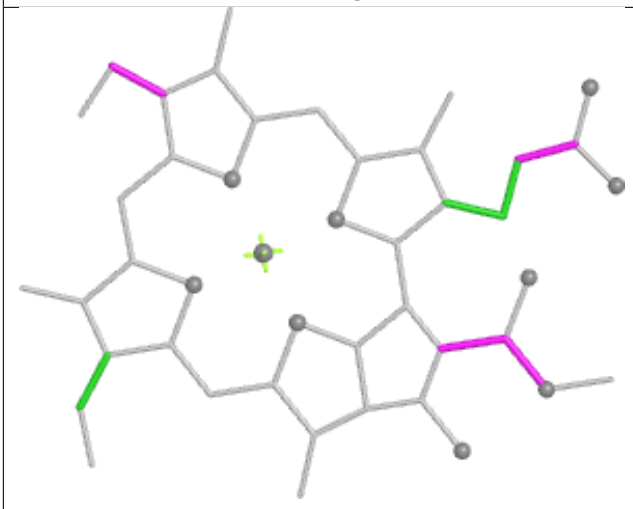
Ligand CLA a2 416



Bond lengths



Bond angles

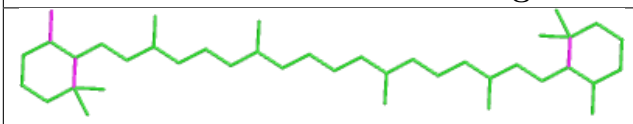


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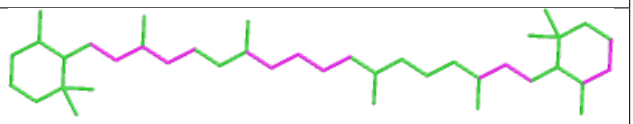


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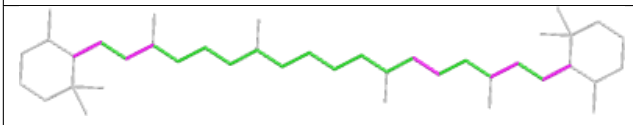
Ligand BCR bB 844



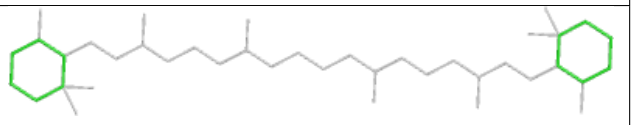
Bond lengths



Bond angles

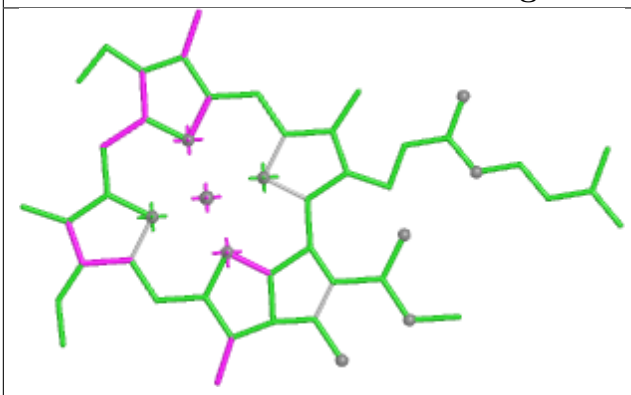


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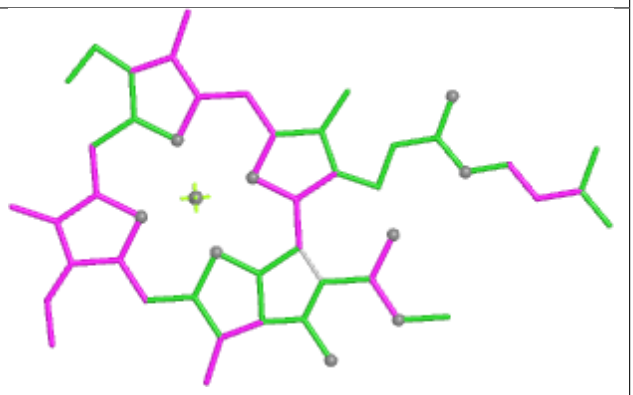


Rings

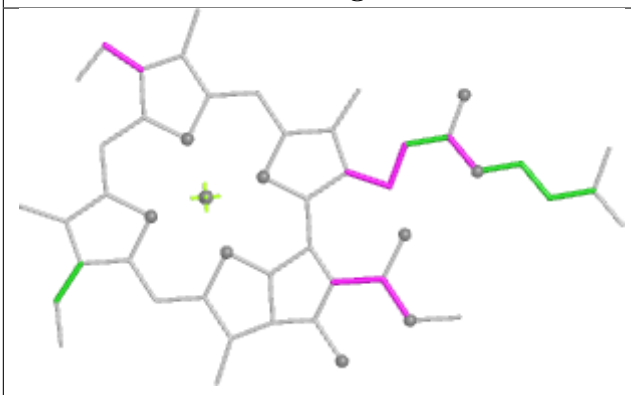
Ligand CLA a6 417



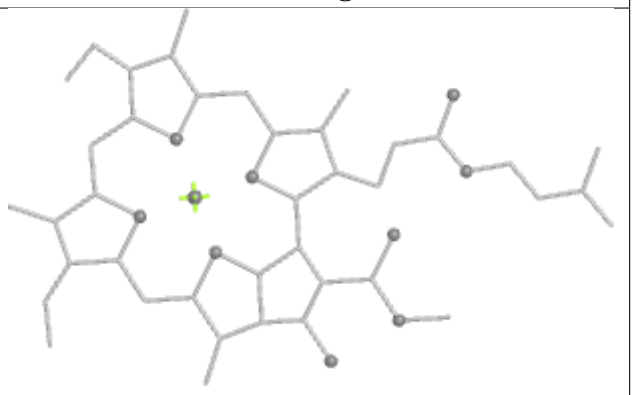
Bond lengths



Bond angles

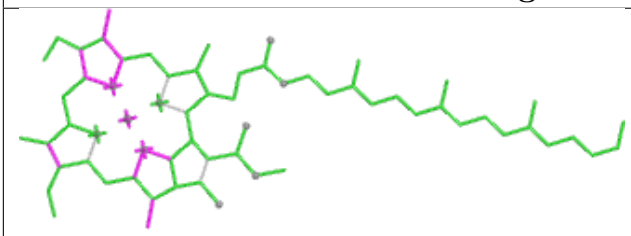


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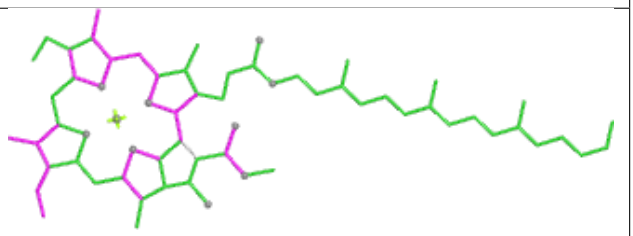


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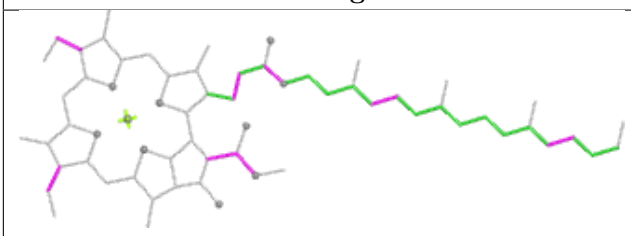
Ligand CLA b3 410



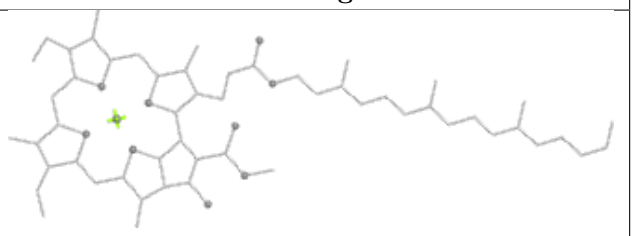
Bond lengths



Bond angles

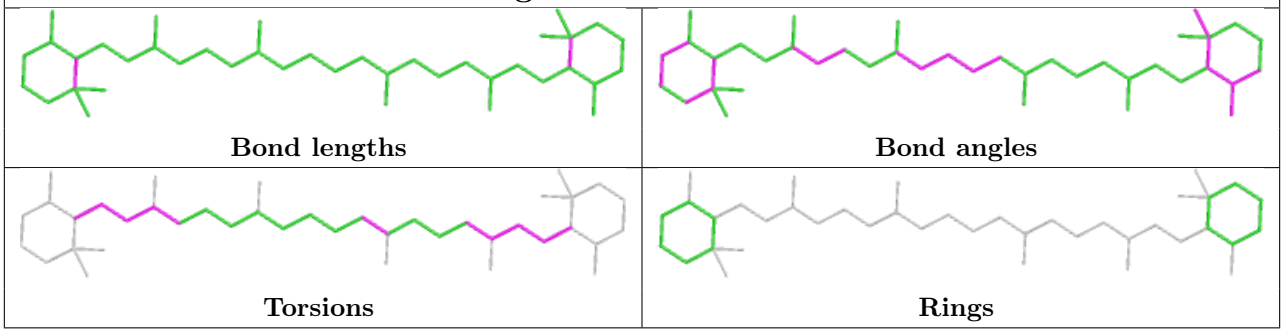


Torsions

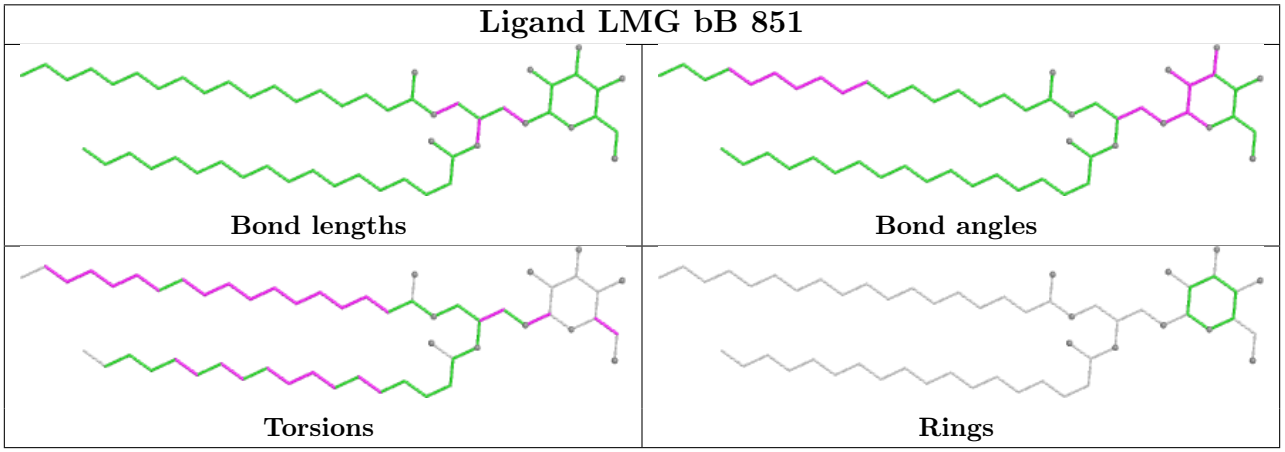


Rings

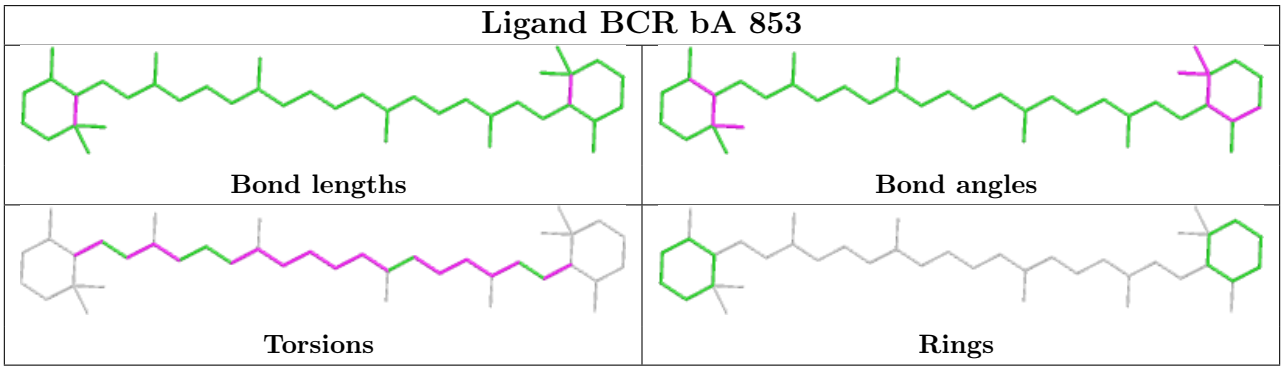
Ligand BCR cA 848



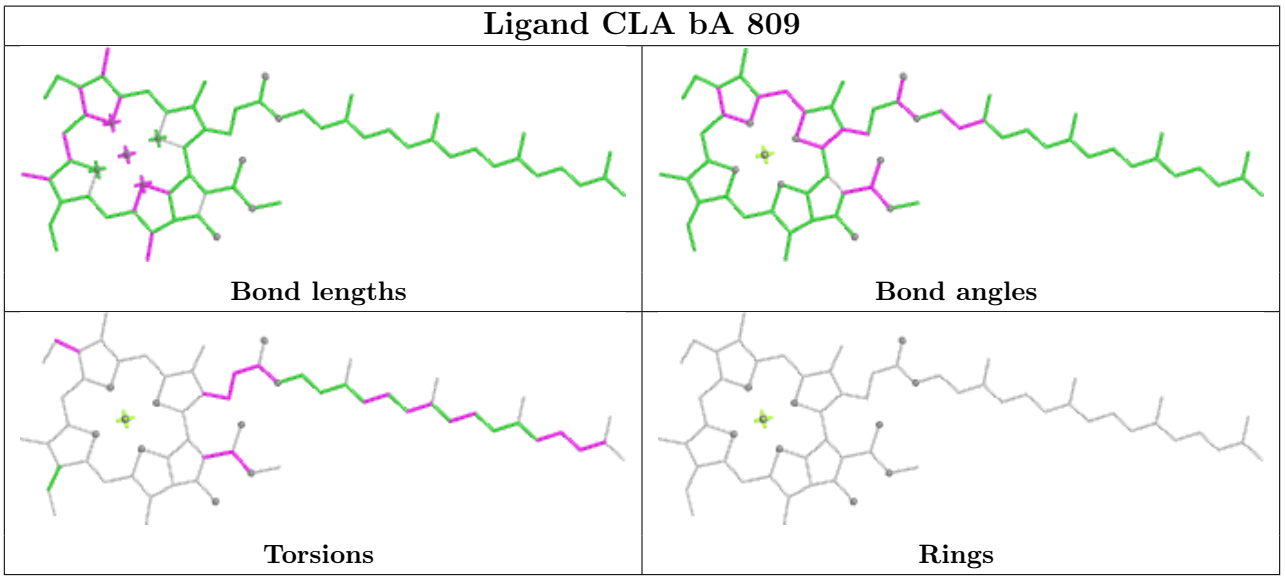
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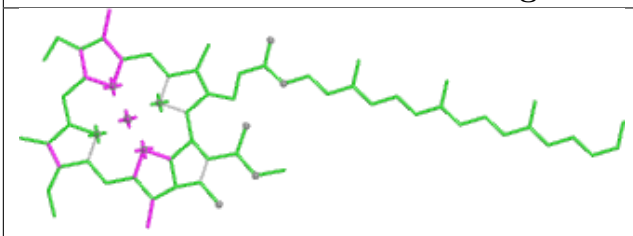
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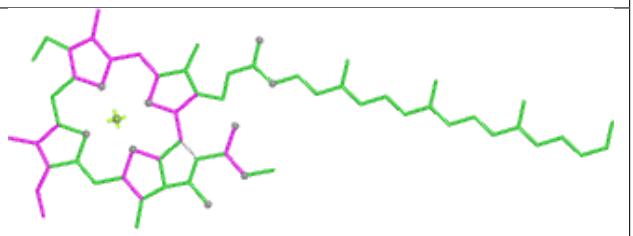
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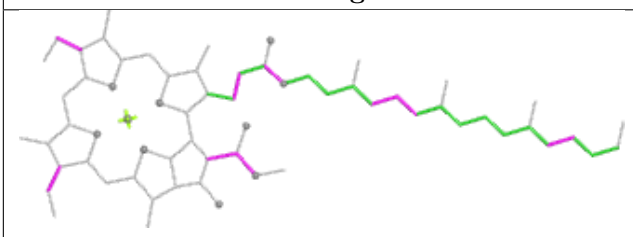
Ligand CLA a4 410



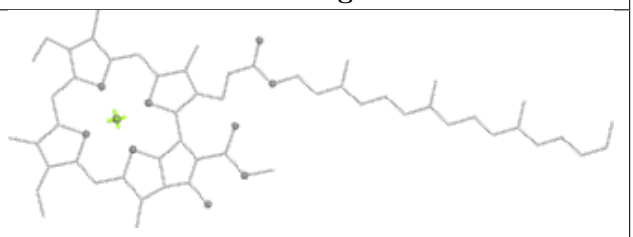
Bond lengths



Bond angles

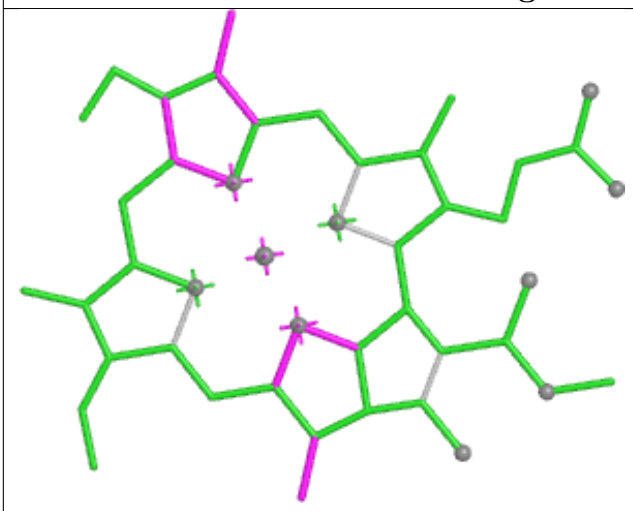


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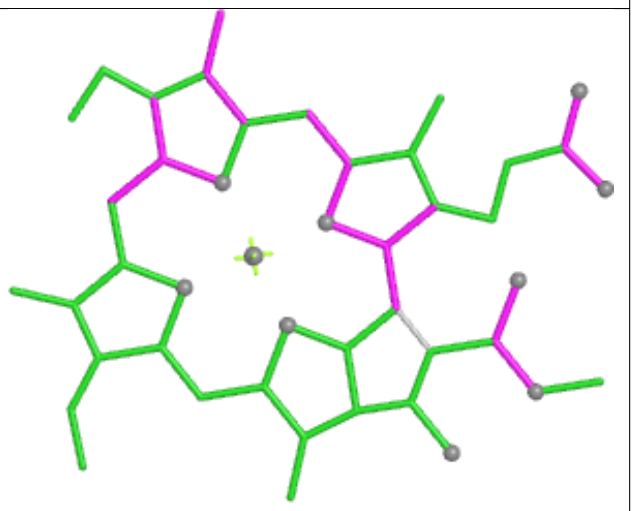


Rings

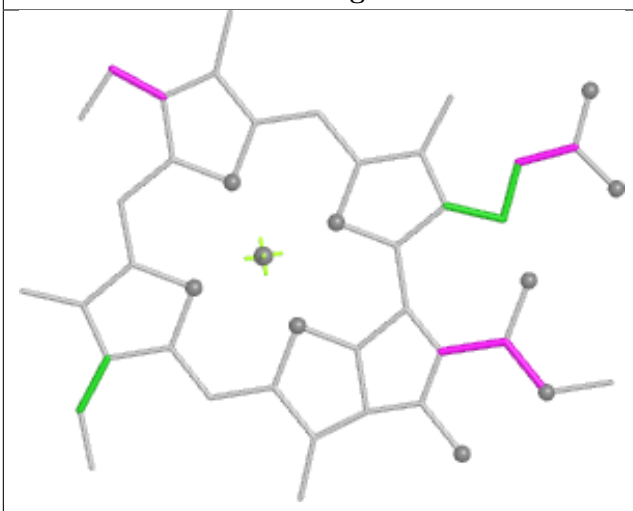
Ligand CLA b6 408



Bond lengths



Bond angles

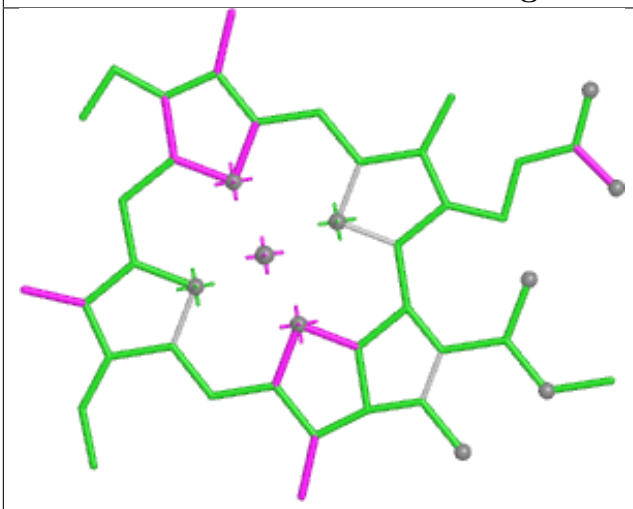


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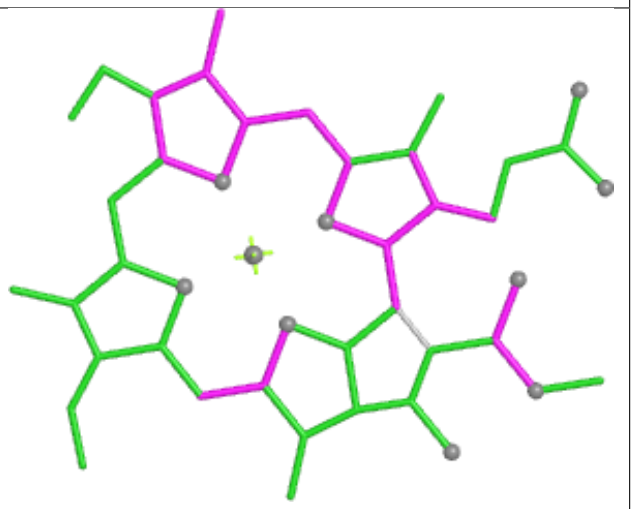


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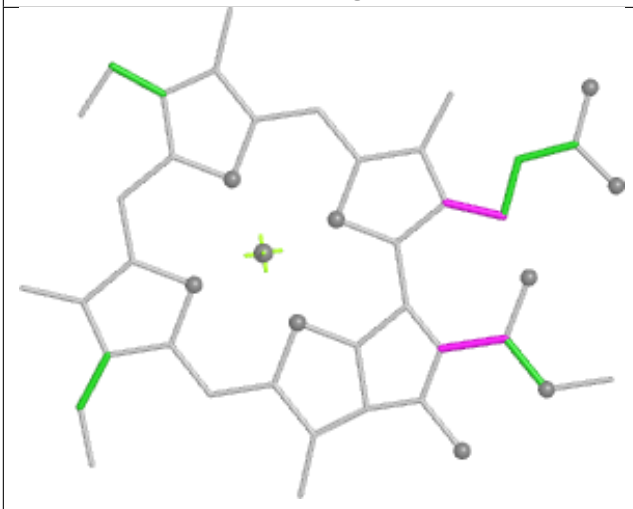
Ligand CLA c2 412



Bond lengths



Bond angles

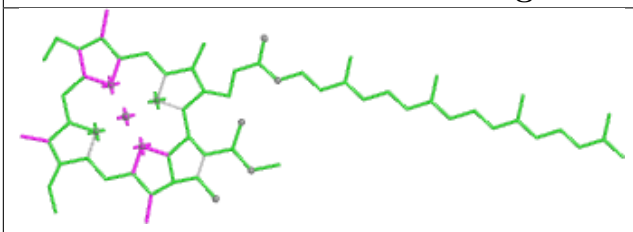


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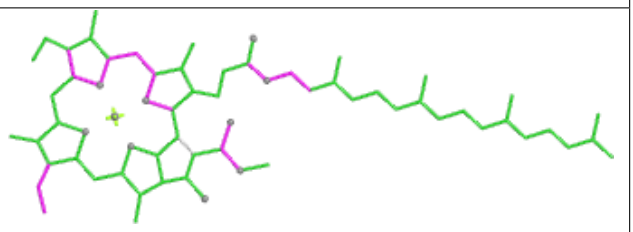


Rings

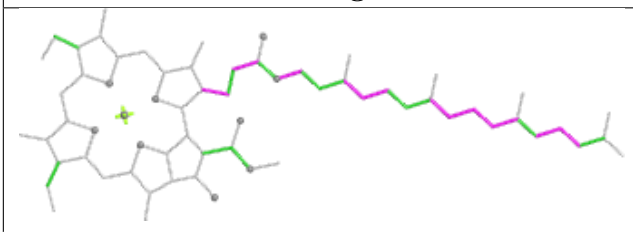
Ligand CLA cA 842



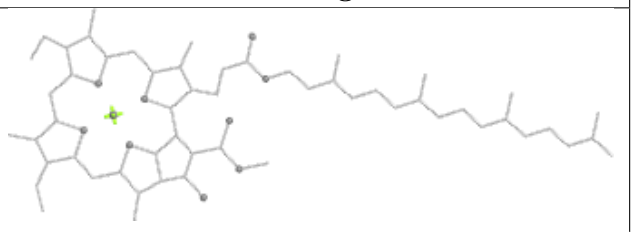
Bond lengths



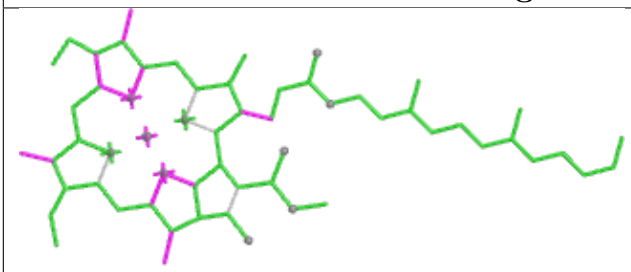
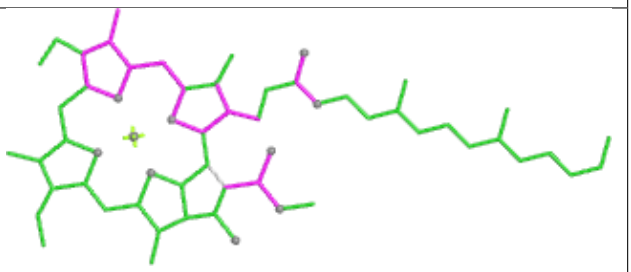
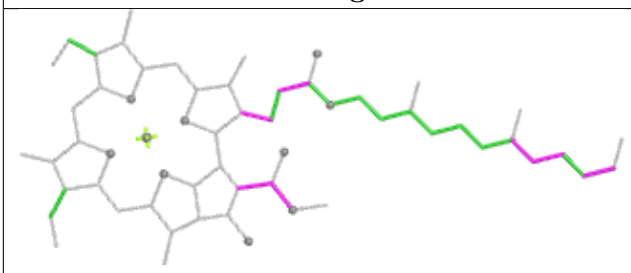
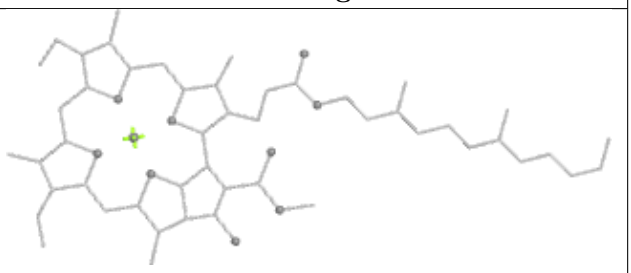
Bond angles

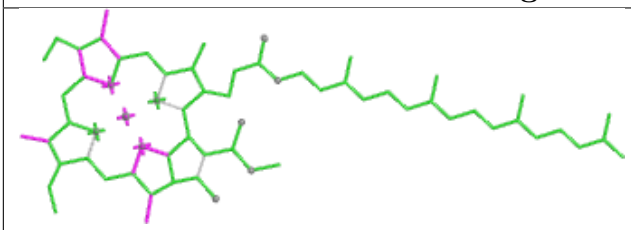
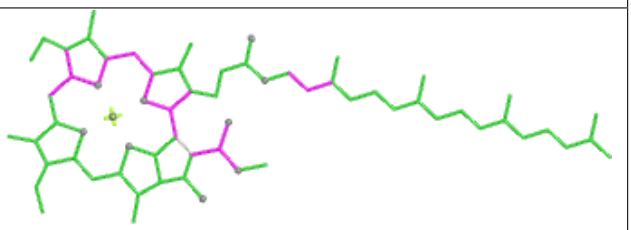
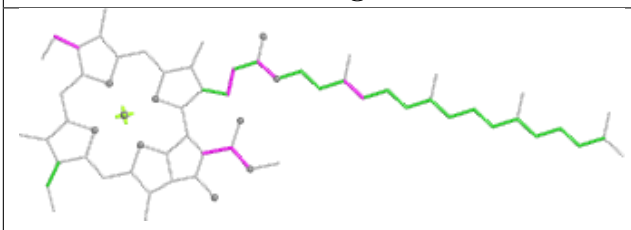
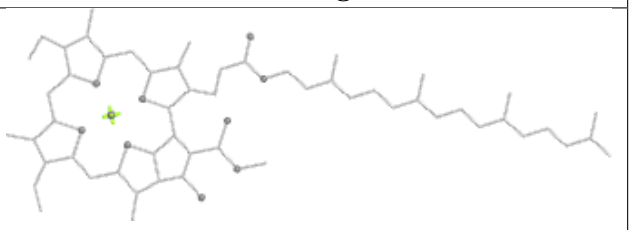


Torsions

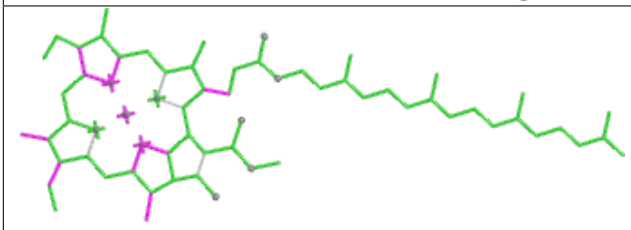


Rings

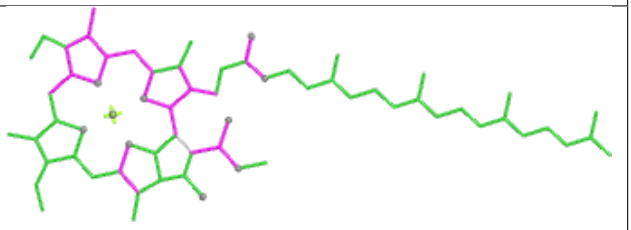
Ligand CLA cA 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c5 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

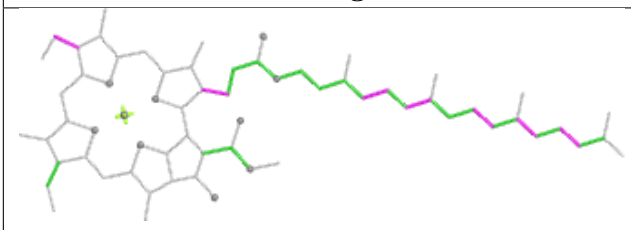
Ligand CLA aA 807



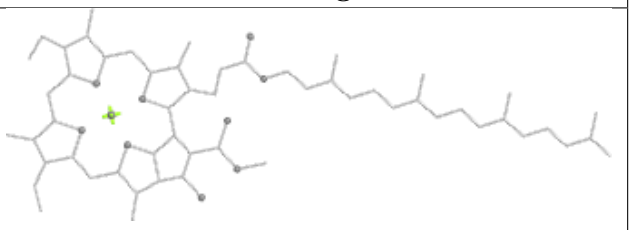
Bond lengths



Bond angles

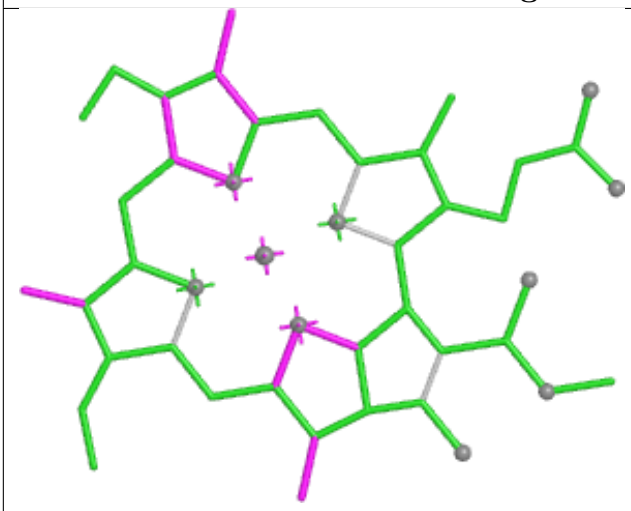


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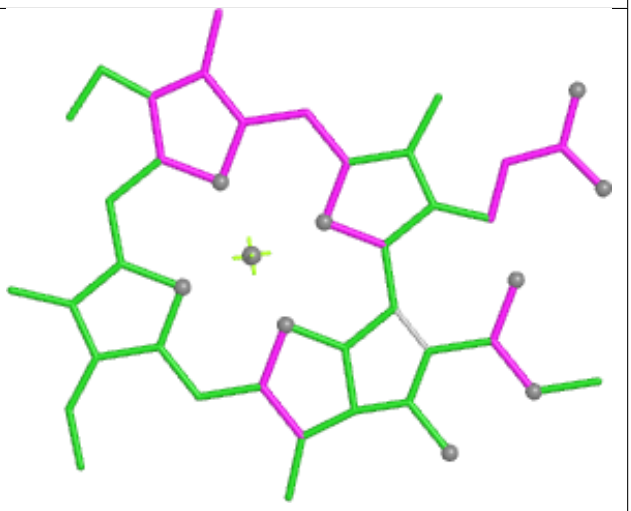


Rings

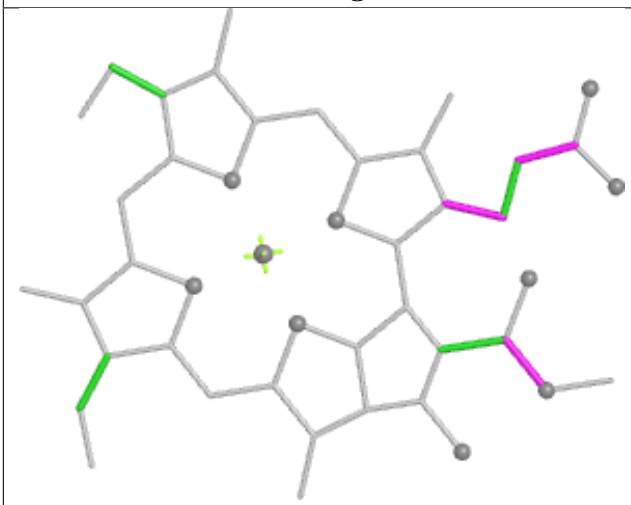
Ligand CLA c5 408



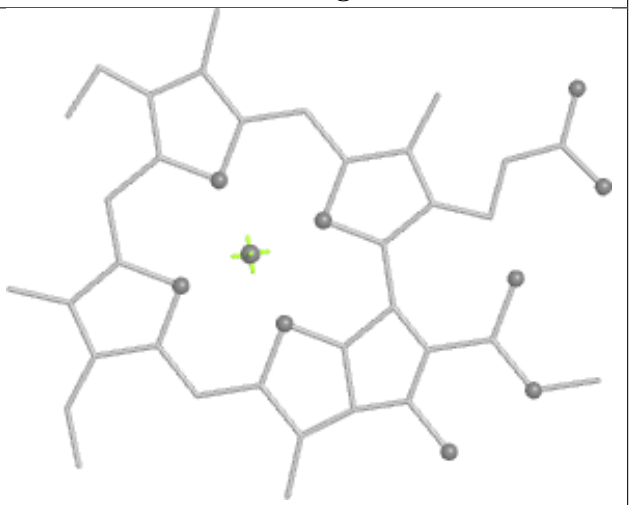
Bond lengths



Bond angles

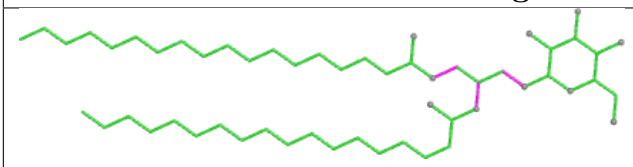


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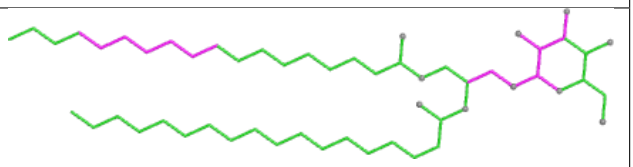


Rings

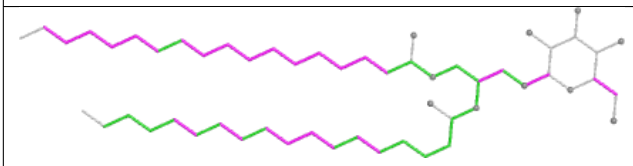
Ligand LMG cB 850



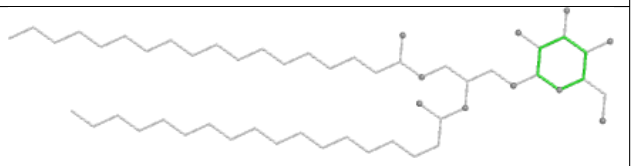
Bond lengths



Bond angles

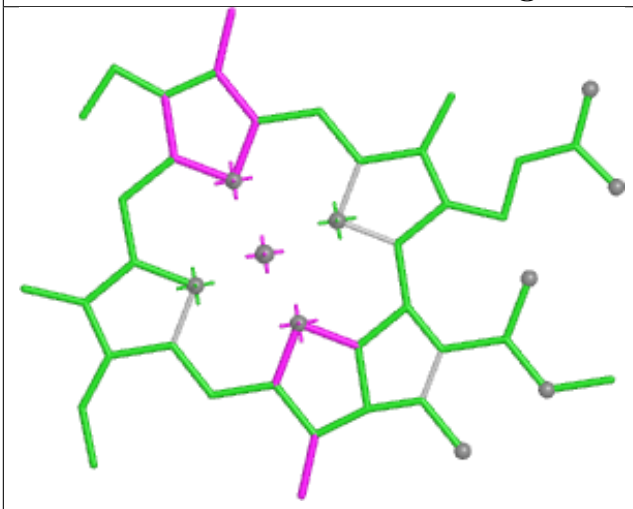


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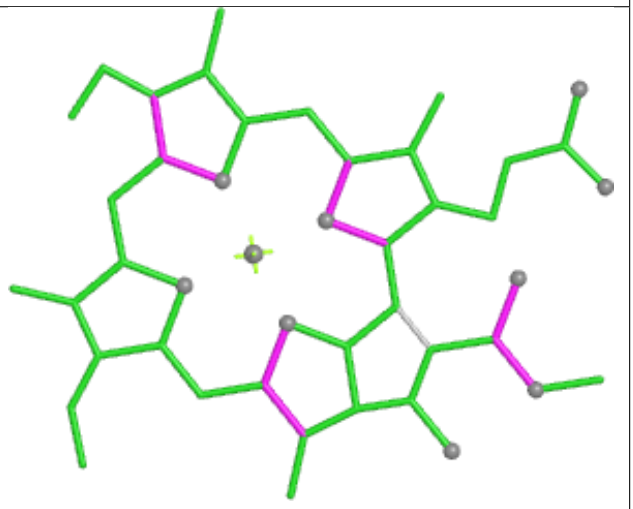


Rings

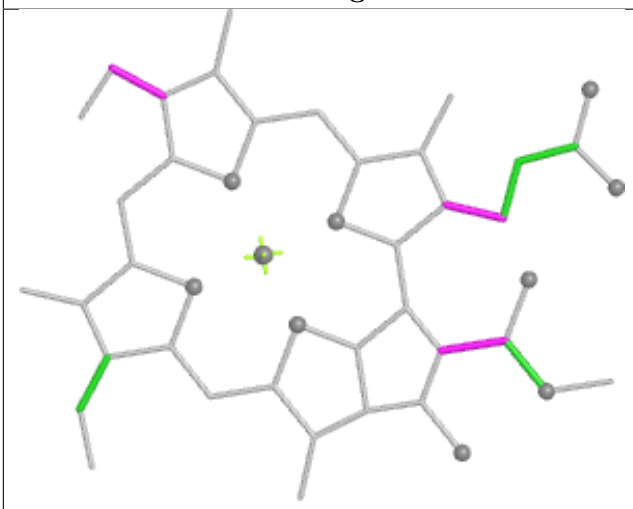
Ligand CLA b1 413



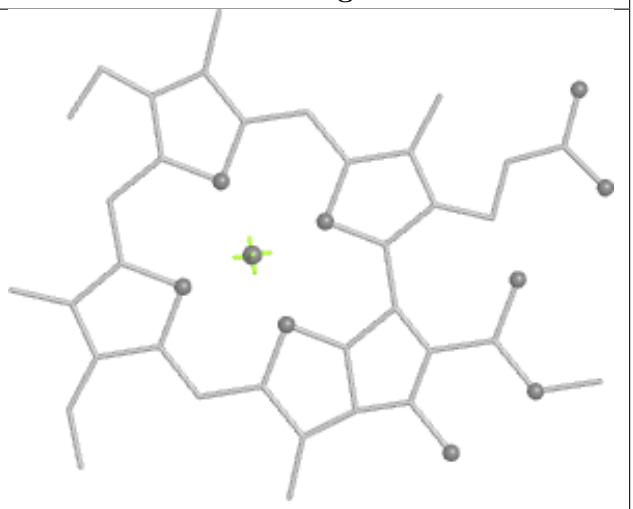
Bond lengths



Bond angles

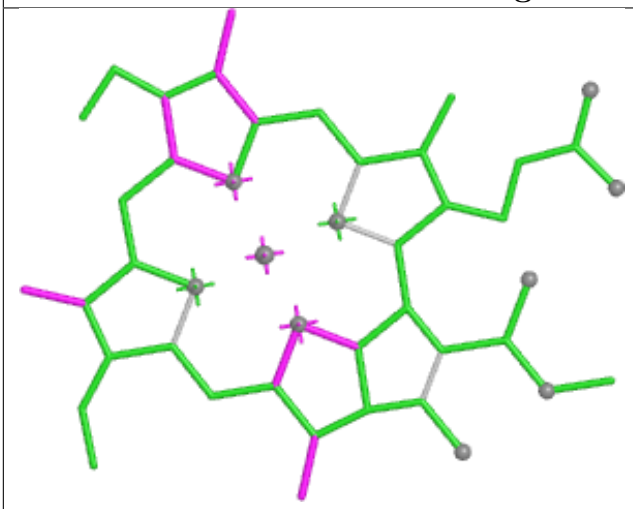


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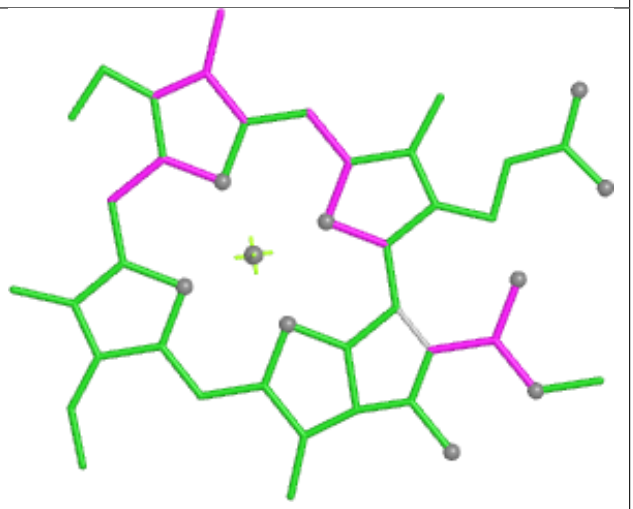


Rings

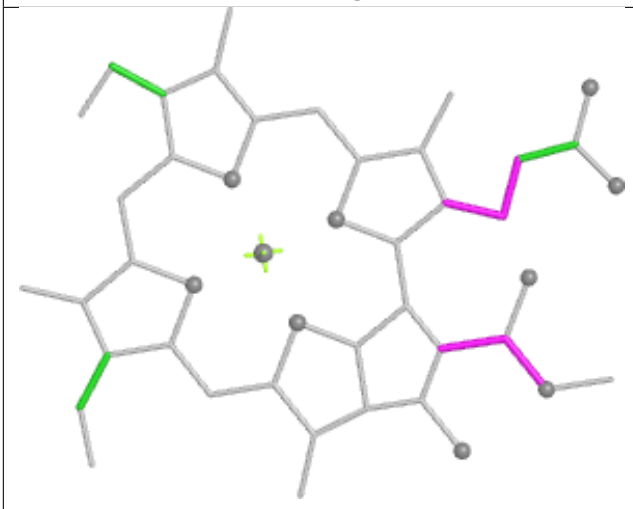
Ligand CLA bB 816



Bond lengths



Bond angles

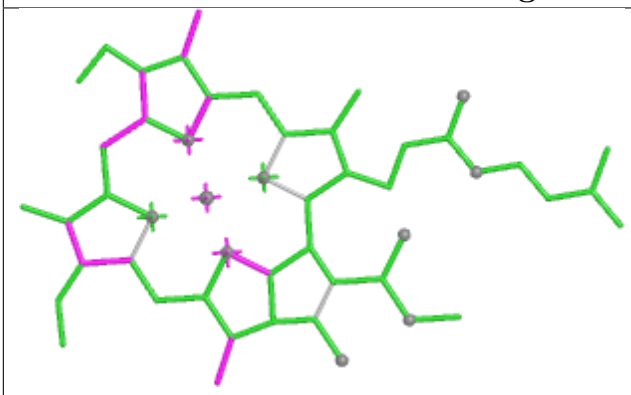


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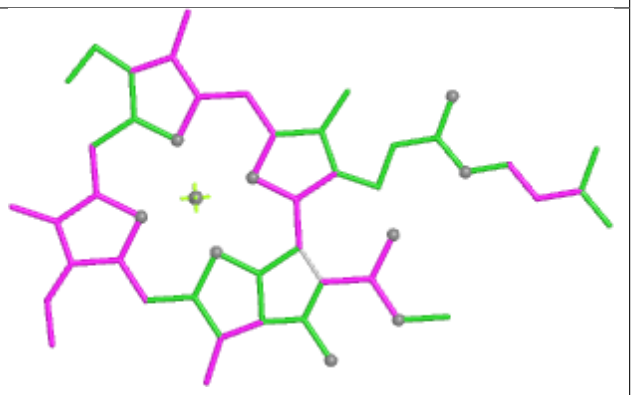


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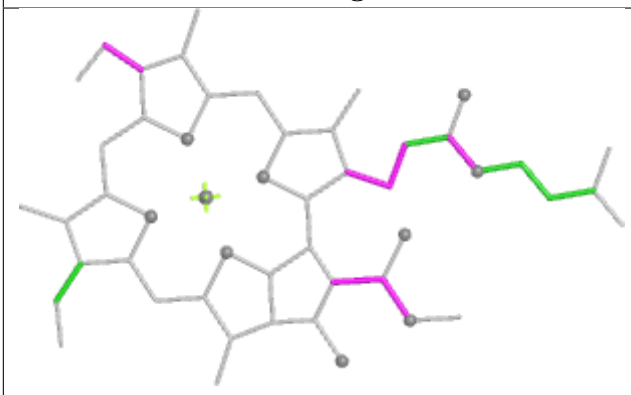
Ligand CLA b6 417



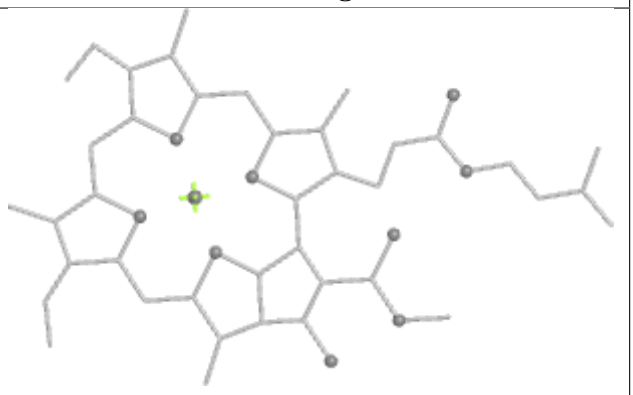
Bond lengths



Bond angles



Torsions

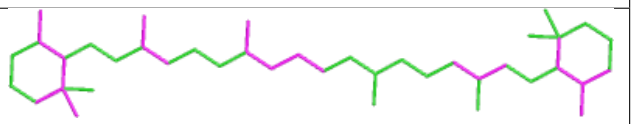


Rings

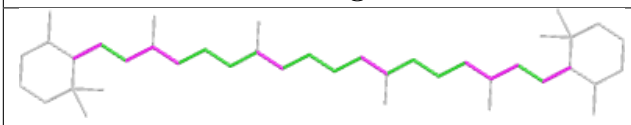
Ligand BCR cF 204



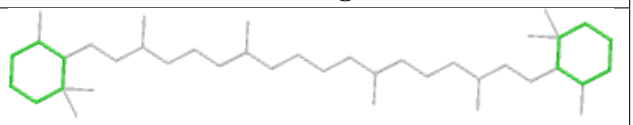
Bond lengths



Bond angles

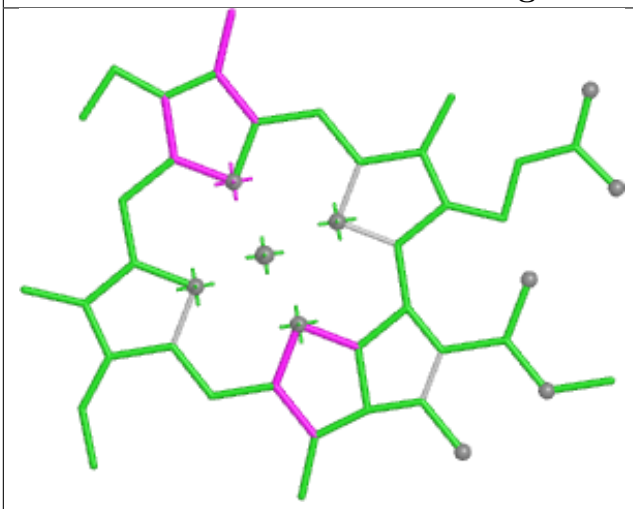


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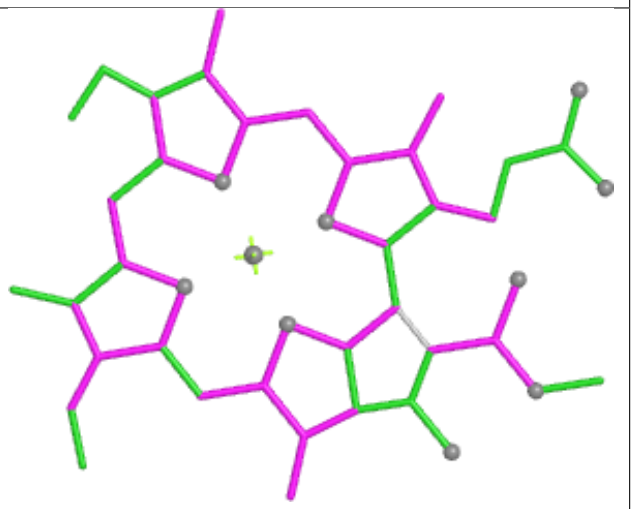


Rings

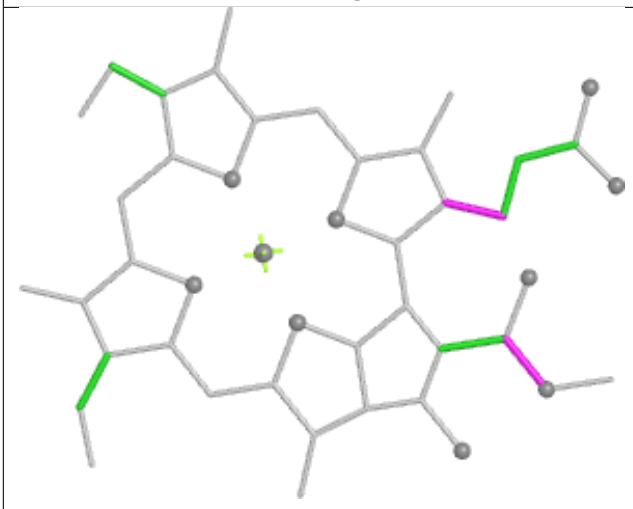
Ligand CLA b1 405



Bond lengths



Bond angles

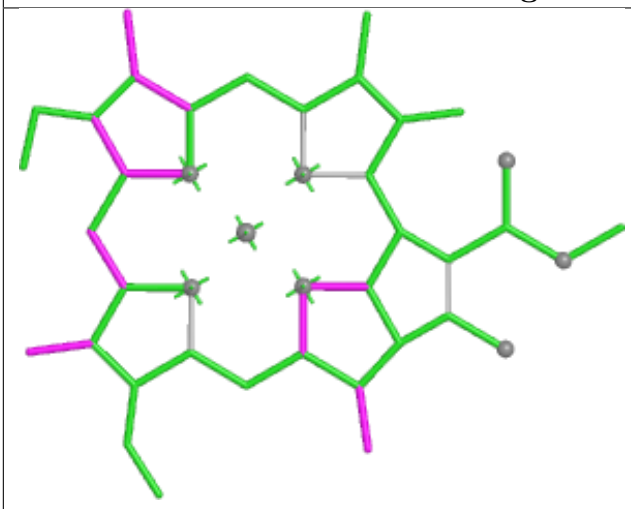


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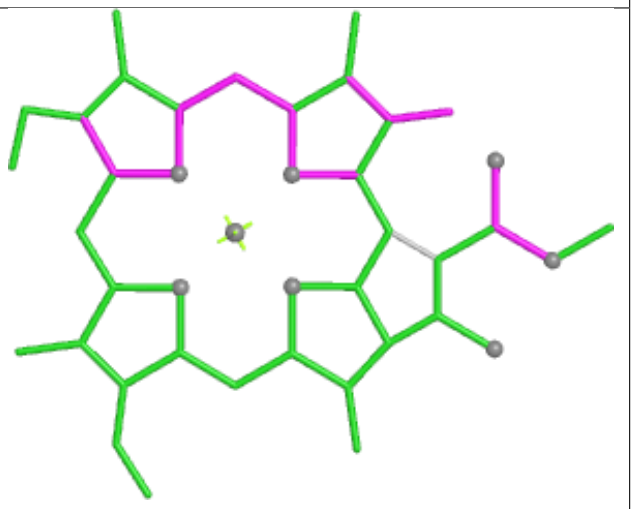


Rings

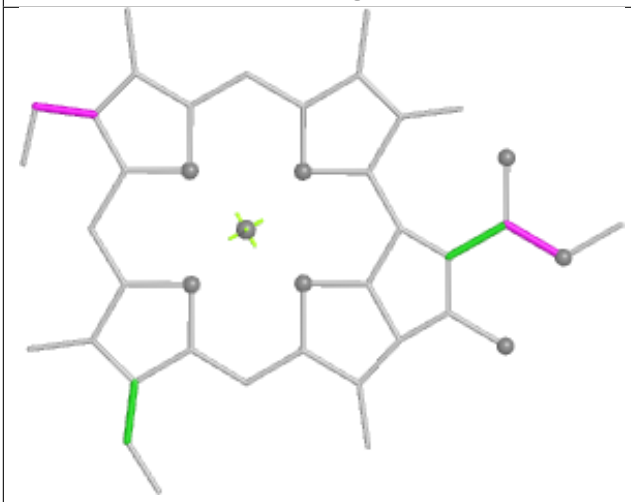
Ligand CLA c1 414



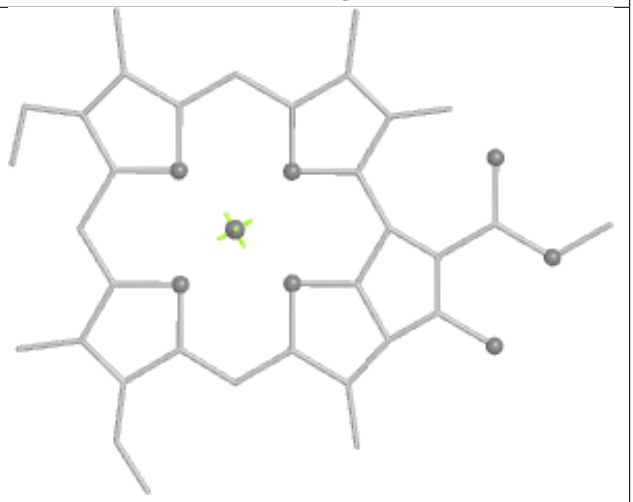
Bond lengths



Bond angles

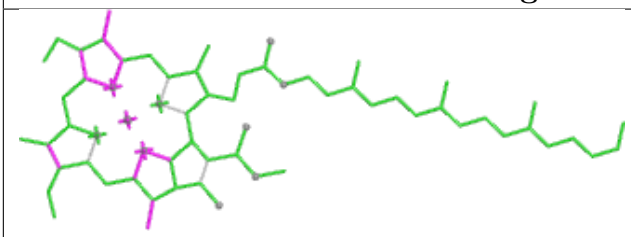


Torsions

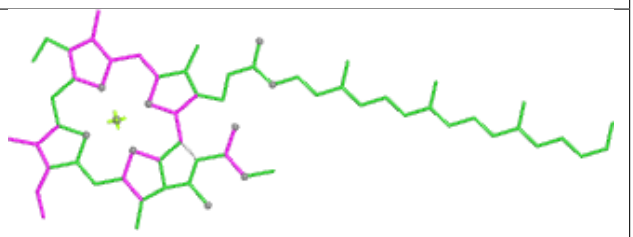


Rings

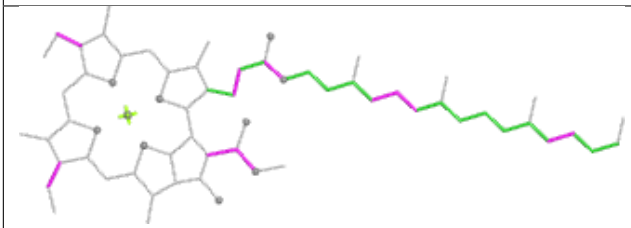
Ligand CLA c5 410



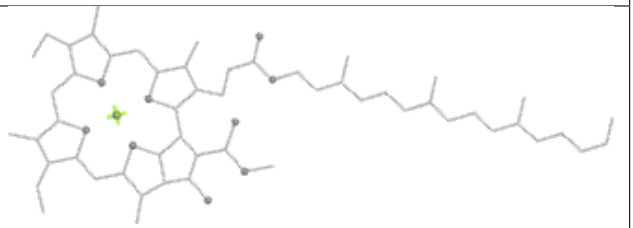
Bond lengths



Bond angles

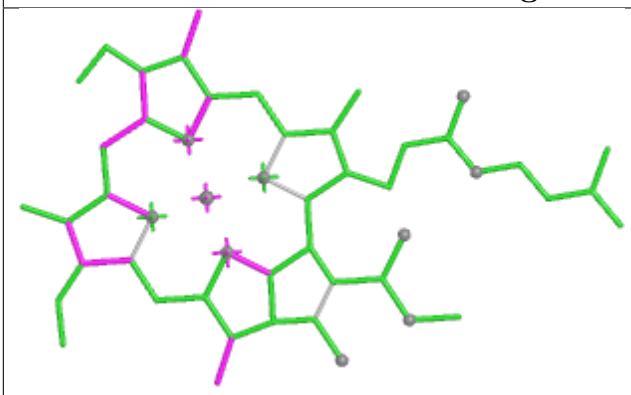


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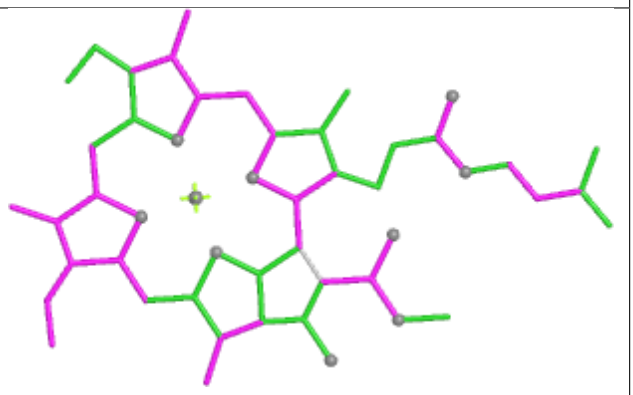


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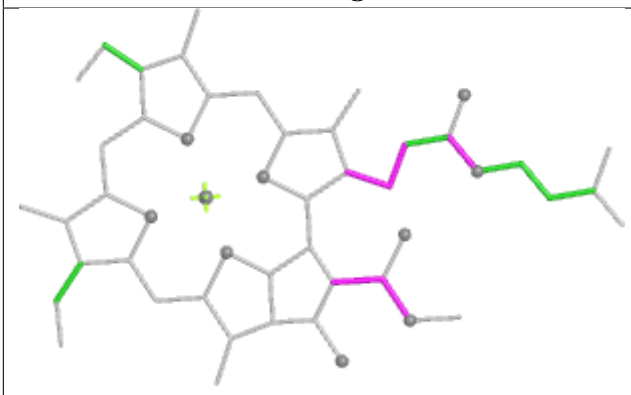
Ligand CLA c2 417



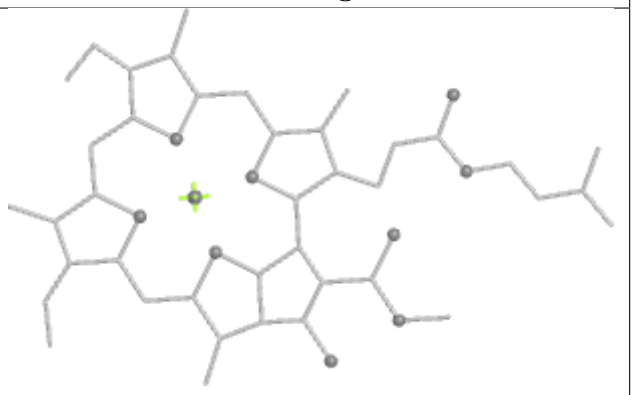
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Bond angles

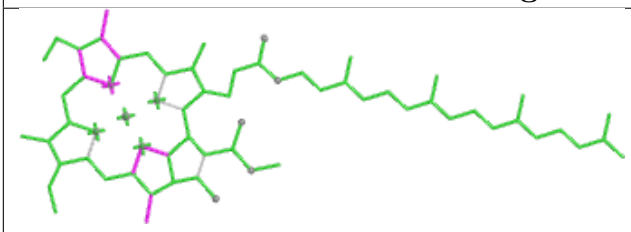


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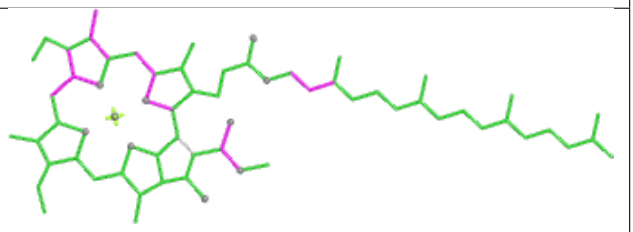


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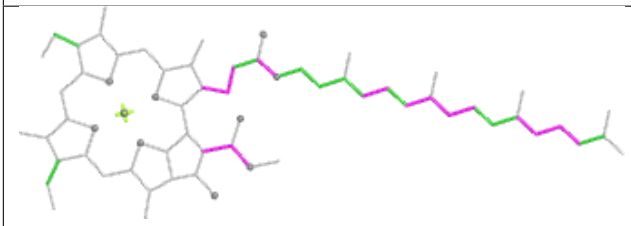
Ligand CLA c6 404



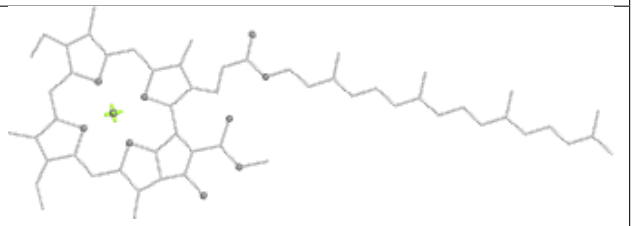
Bond lengths



Bond angles

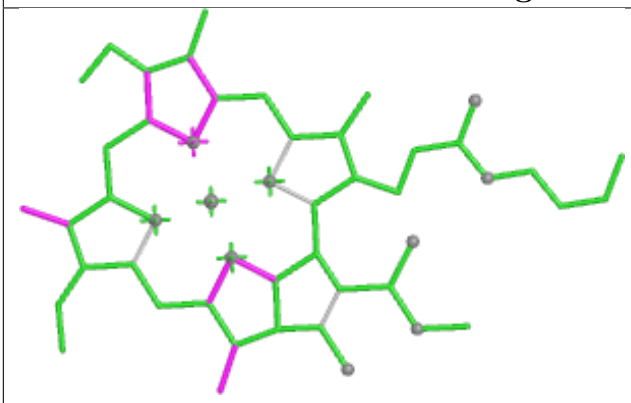


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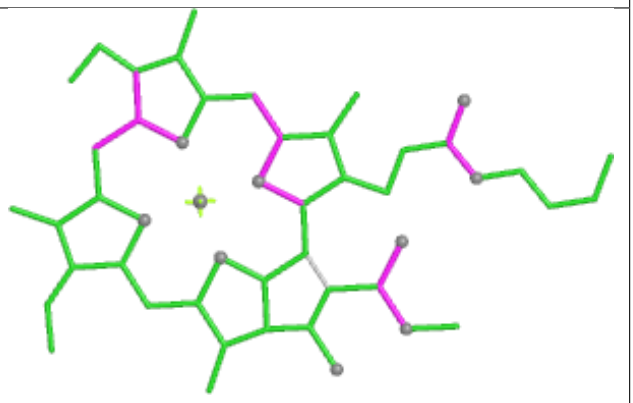


Rings

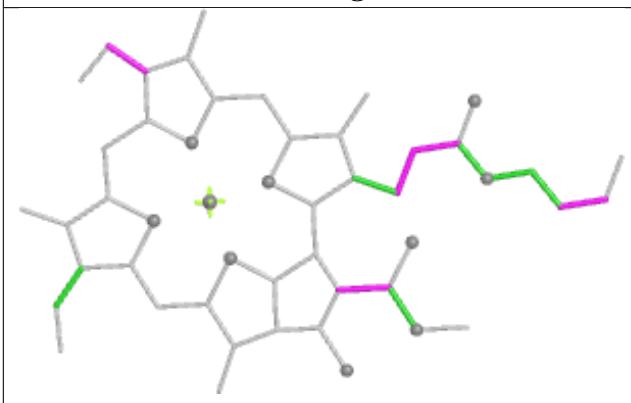
Ligand CLA aA 823



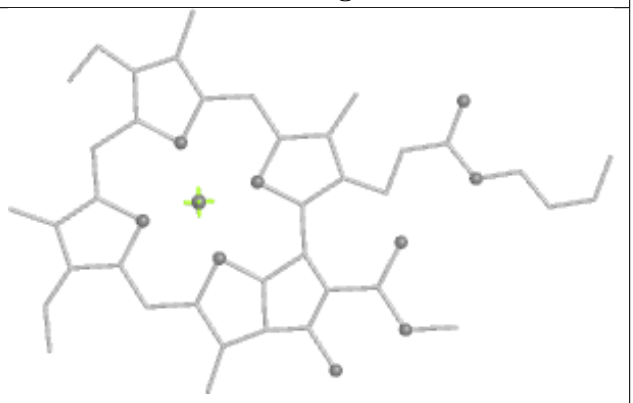
Bond lengths



Bond angles

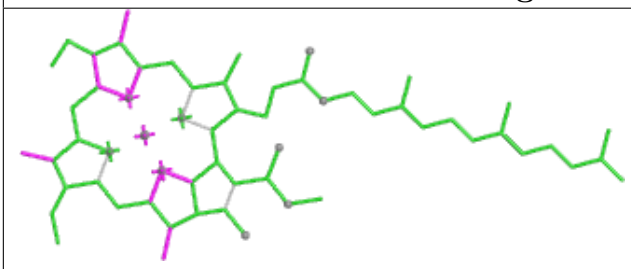


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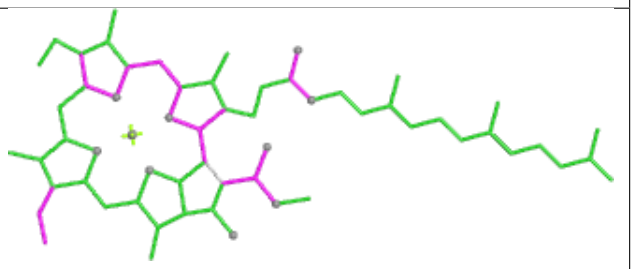


Rings

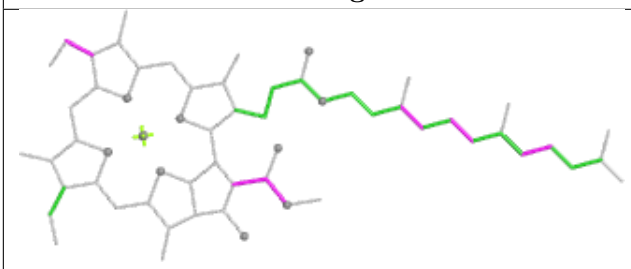
Ligand CLA cB 836



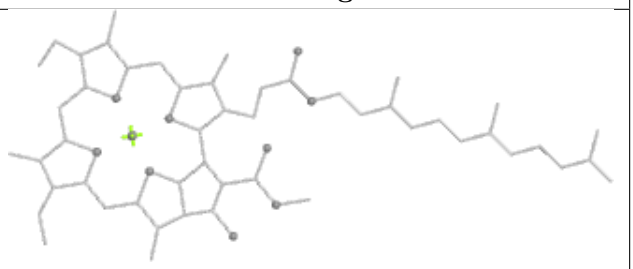
Bond lengths



Bond angles

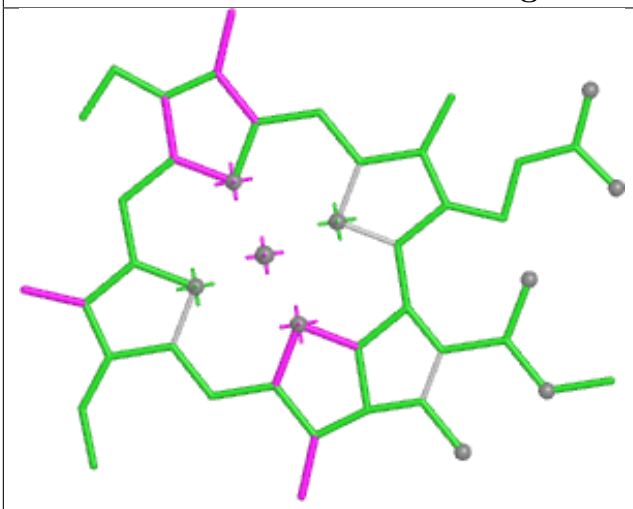


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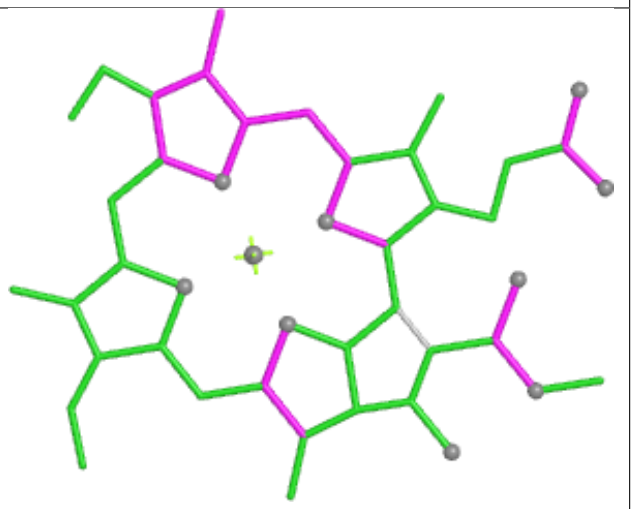


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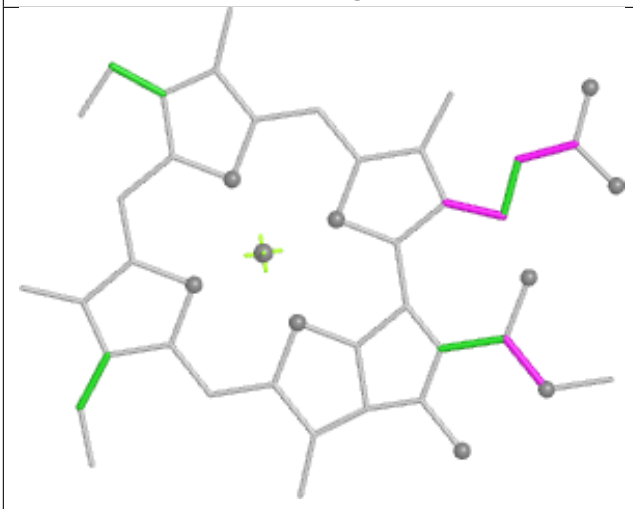
Ligand CLA c6 410



Bond lengths



Bond angles

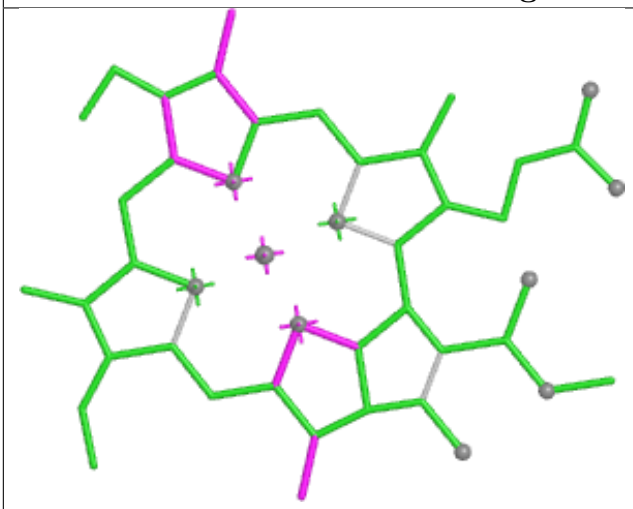


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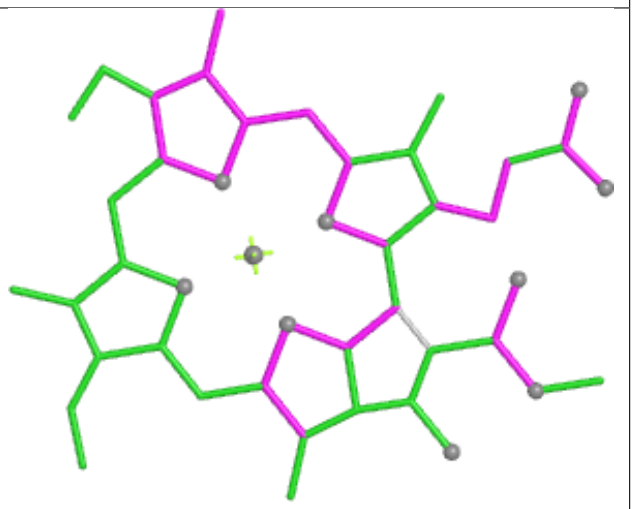


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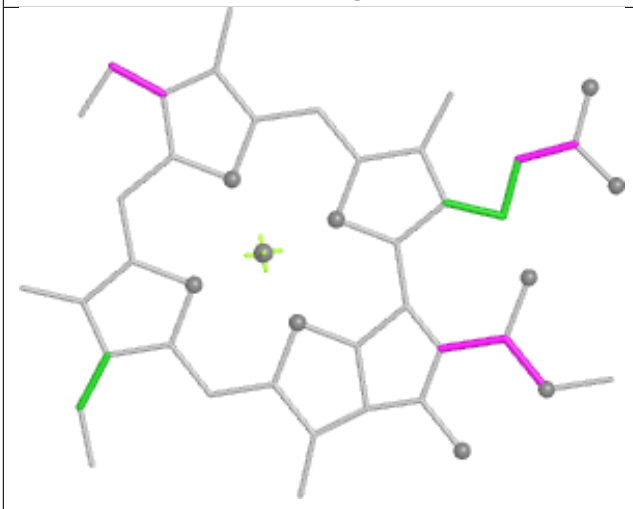
Ligand CLA a6 416



Bond lengths



Bond angles

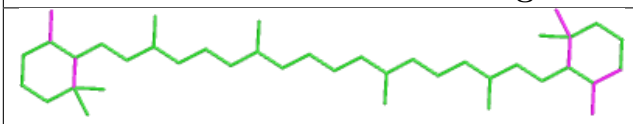


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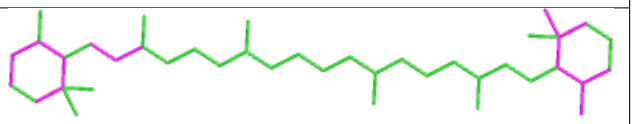


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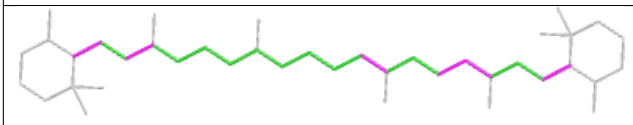
Ligand BCR b4 418



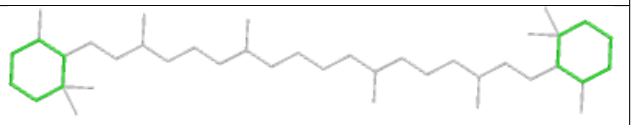
Bond lengths



Bond angles

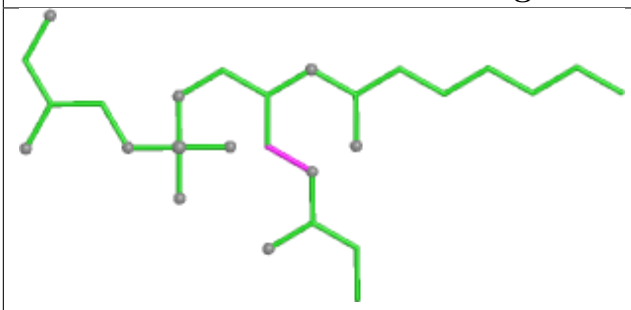


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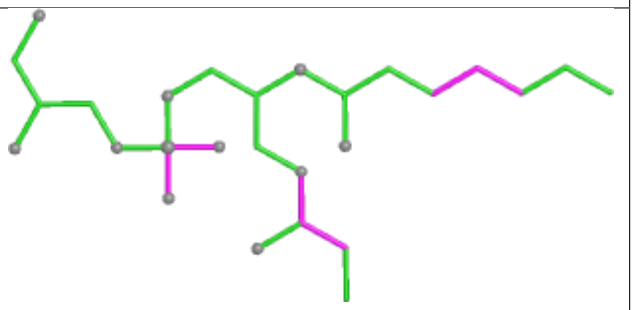


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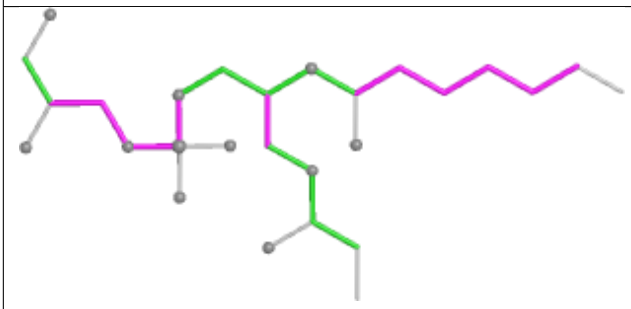
Ligand LHG cA 853



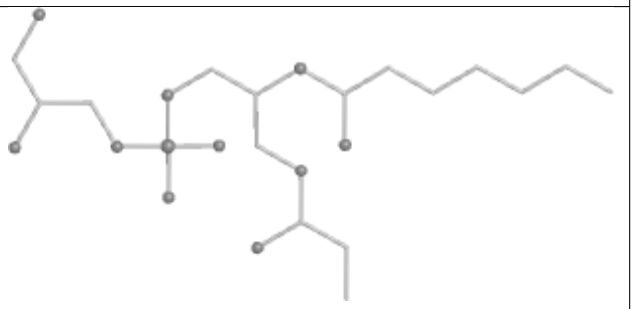
Bond lengths



Bond angles

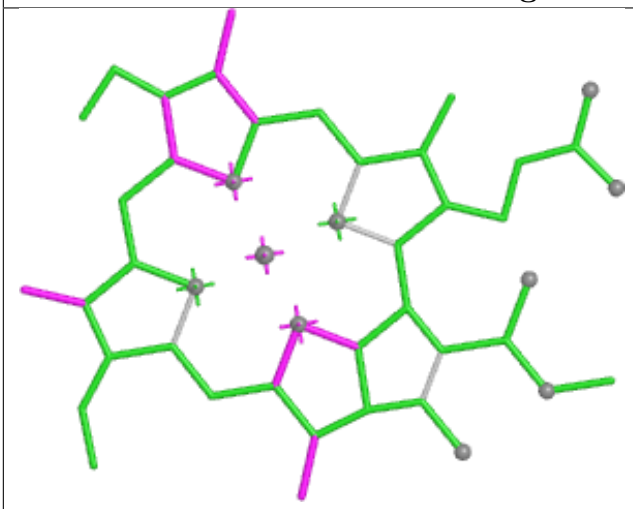


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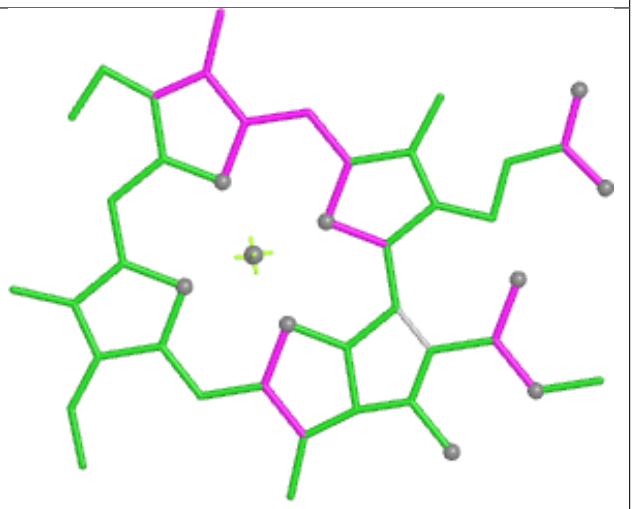


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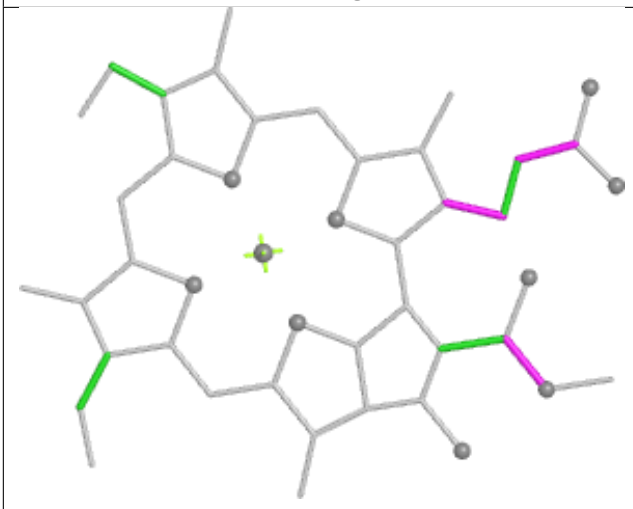
Ligand CLA a4 408



Bond lengths



Bond angles

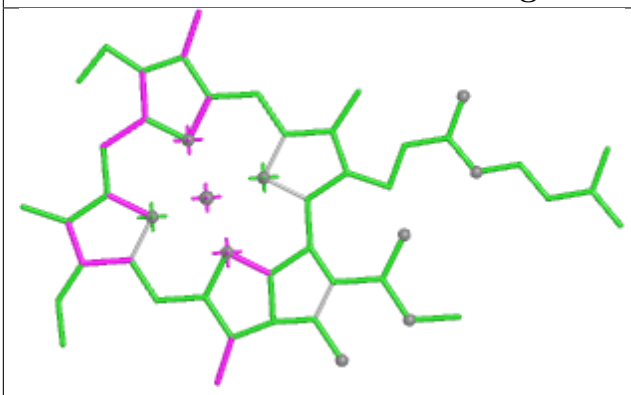


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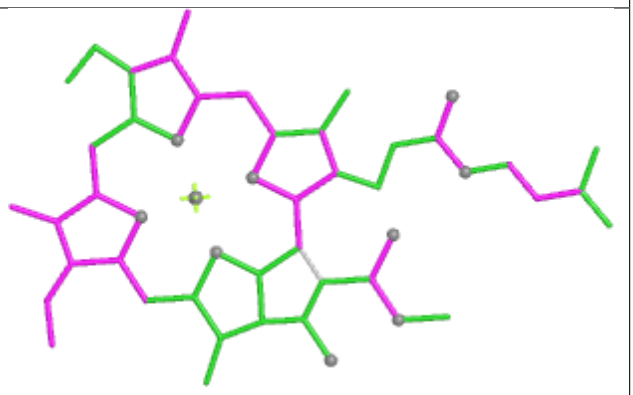


Rings

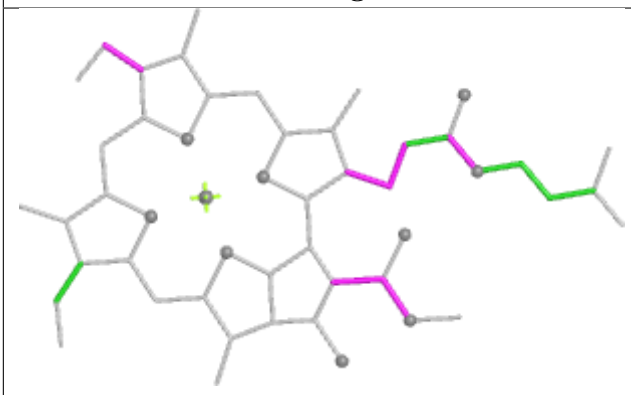
Ligand CLA a3 416



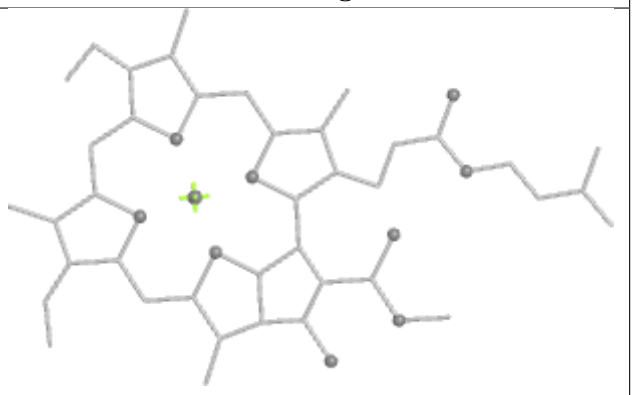
Bond lengths



Bond angles

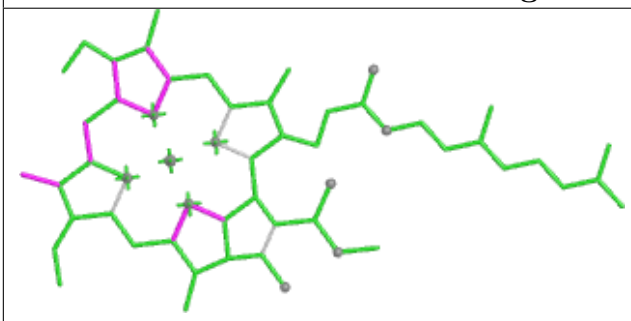


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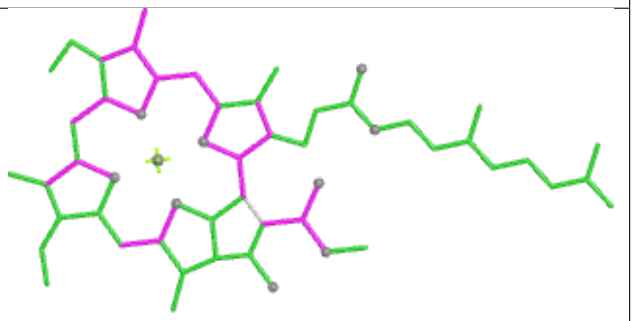


Rings

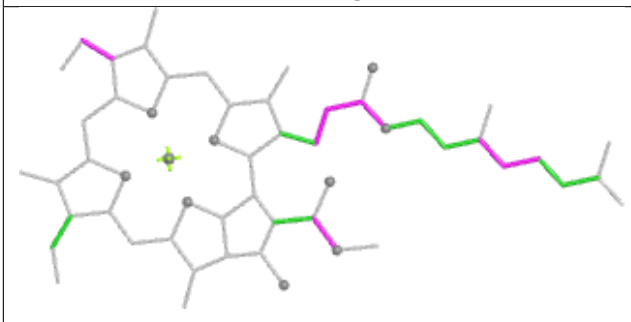
Ligand CLA c6 419



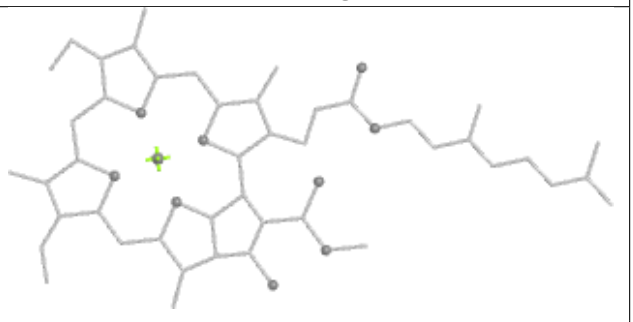
Bond lengths



Bond angles

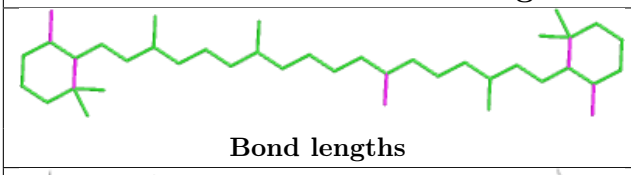


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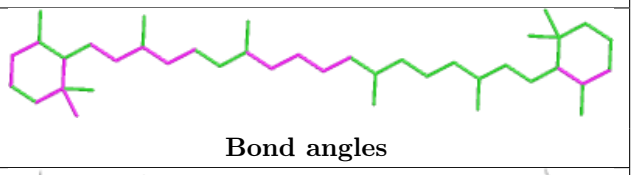


Rings

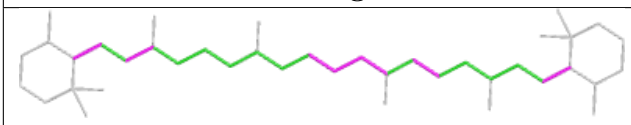
Ligand BCR cF 205



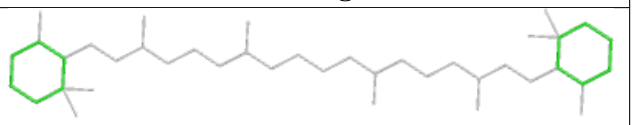
Bond lengths



Bond angles



Torsions

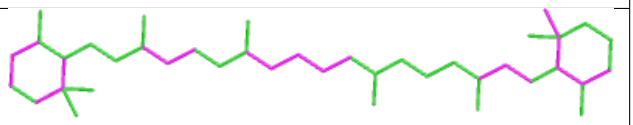


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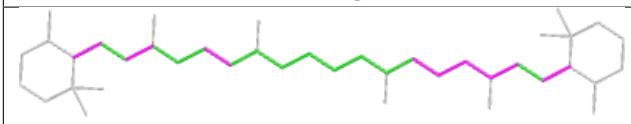
Ligand BCR a2 420



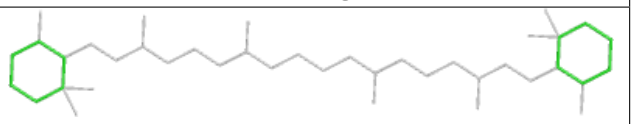
Bond lengths



Bond angles

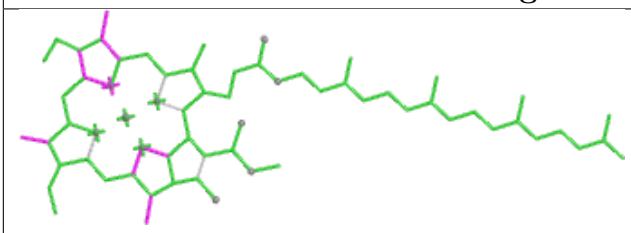


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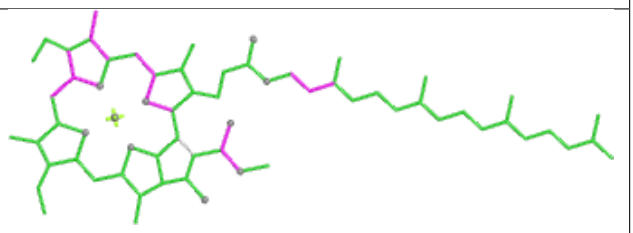


Rings

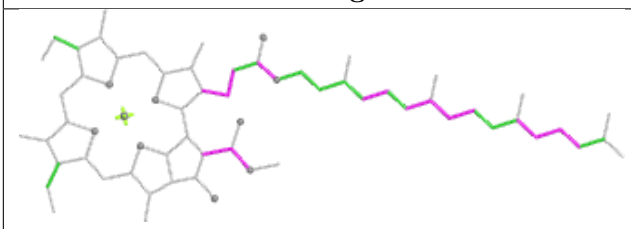
Ligand CLA a1 401



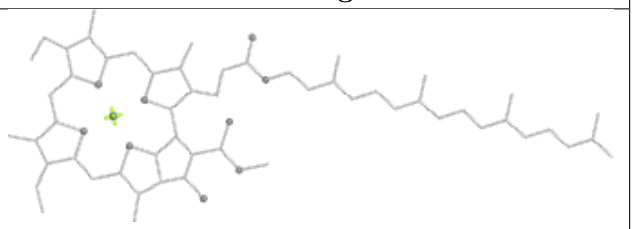
Bond lengths



Bond angles

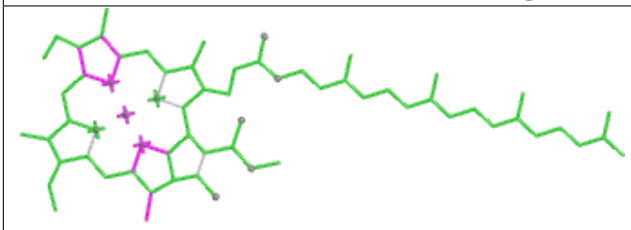


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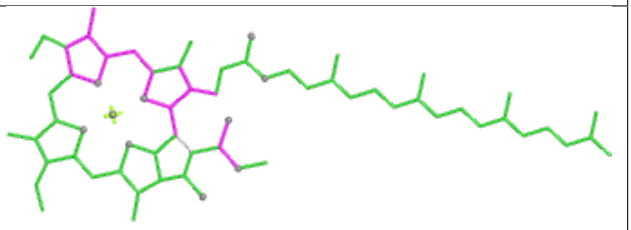


Rings

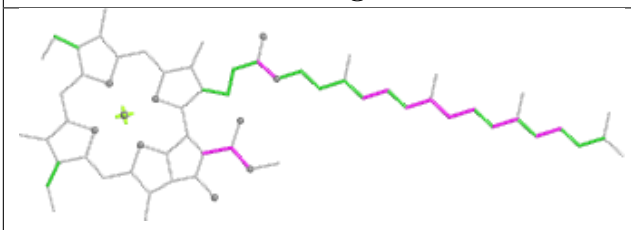
Ligand CLA c1 403



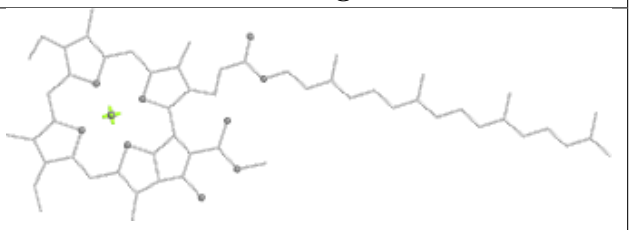
Bond lengths



Bond angles



Torsions

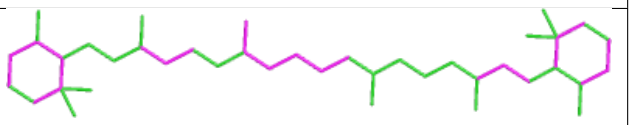


Rings

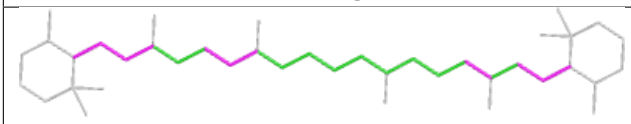
Ligand BCR a5 419



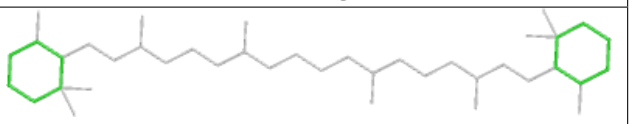
Bond lengths



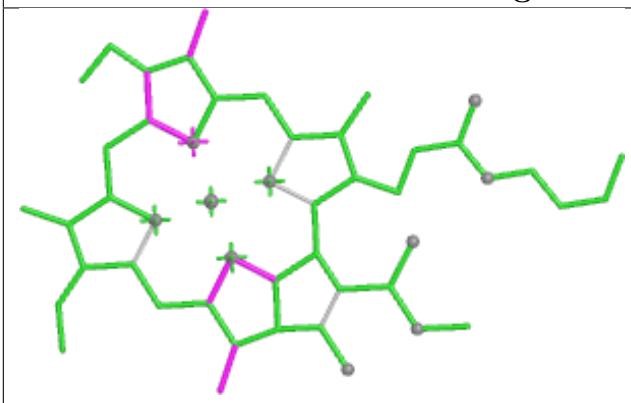
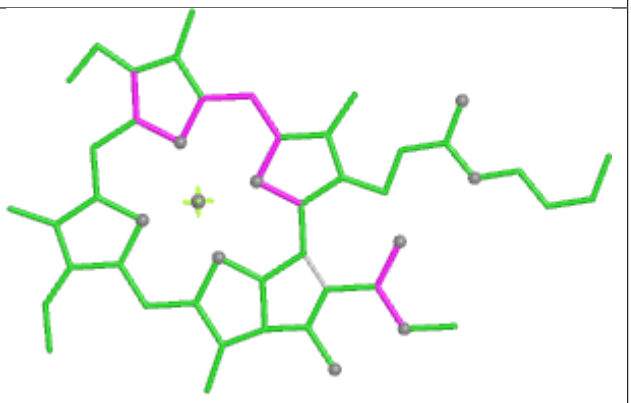
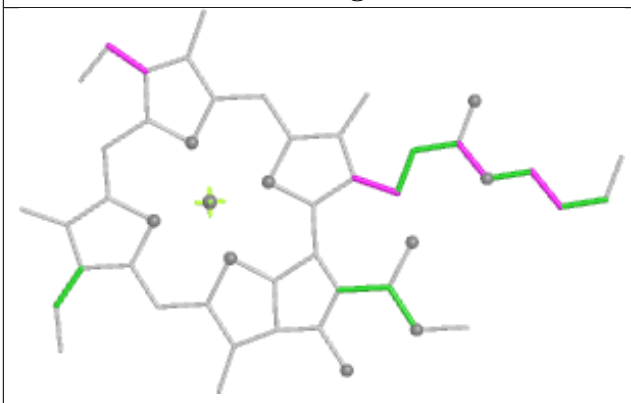
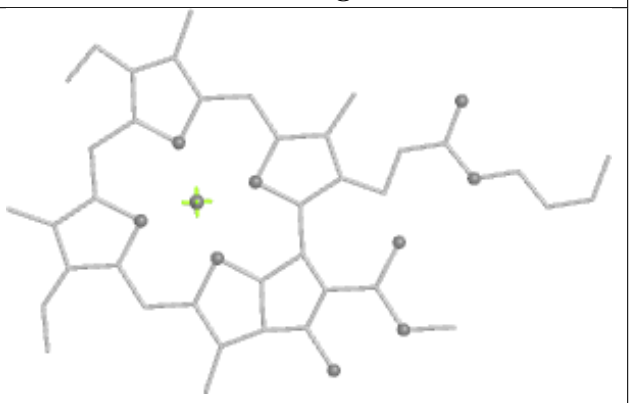
Bond angles



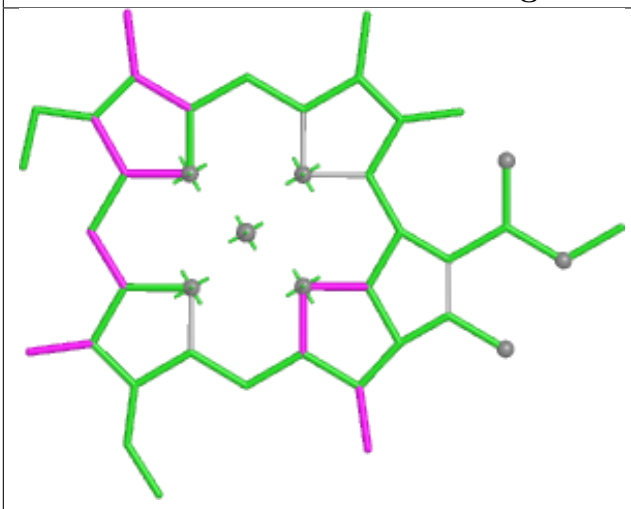
Torsions



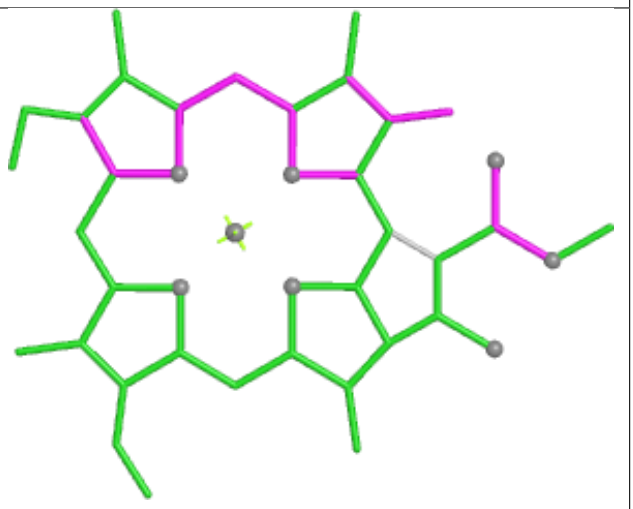
Rings

Ligand CLA bA 817	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

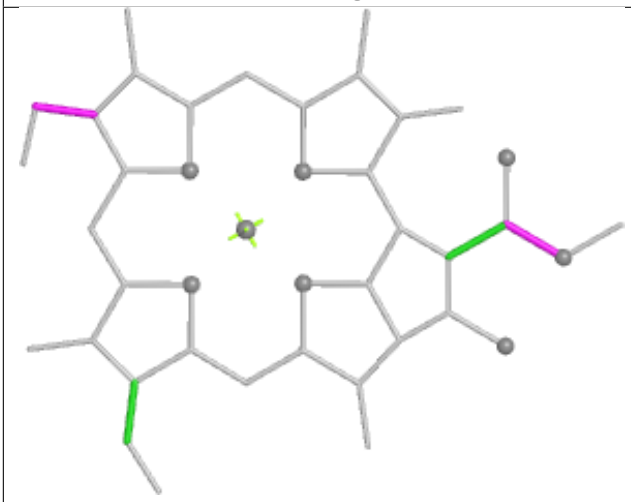
Ligand CLA c3 414



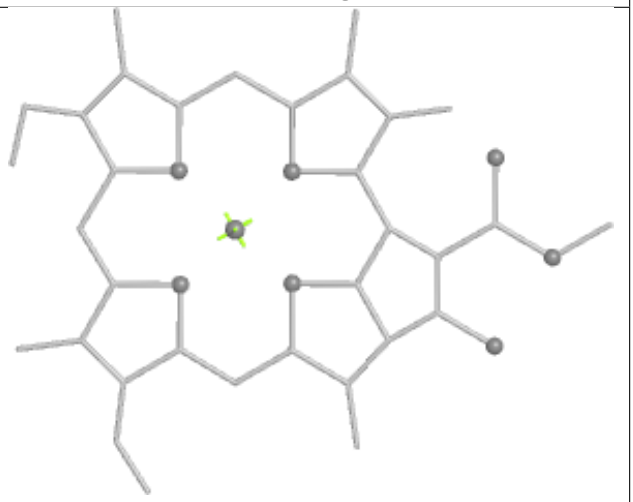
Bond lengths



Bond angles

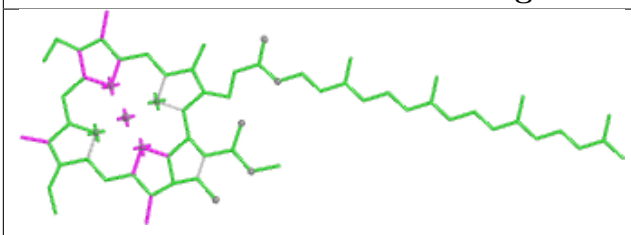


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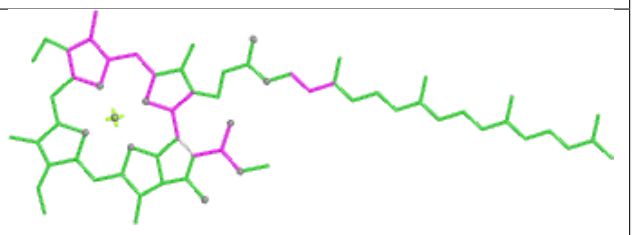


Rings

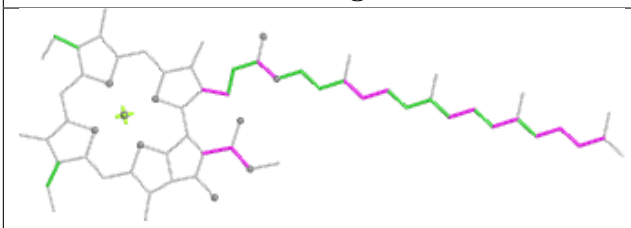
Ligand CLA aA 820



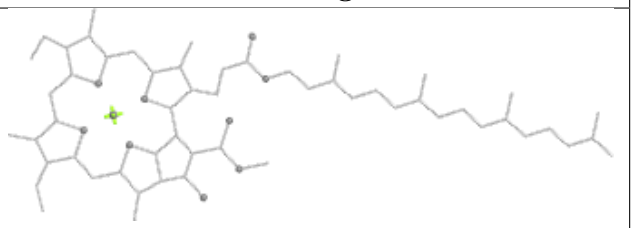
Bond lengths



Bond angles

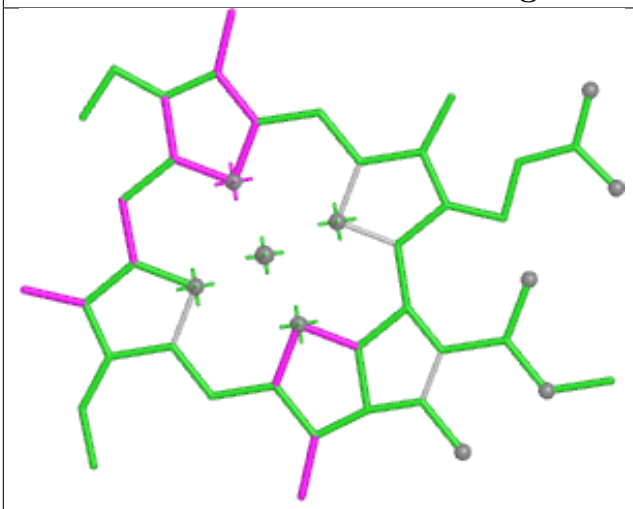


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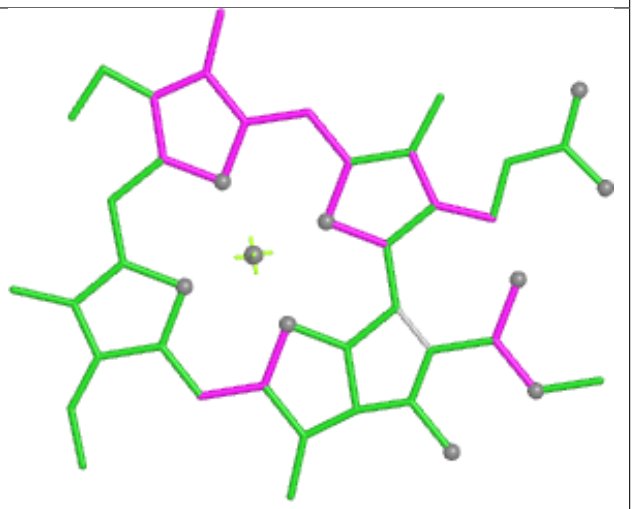


Rings

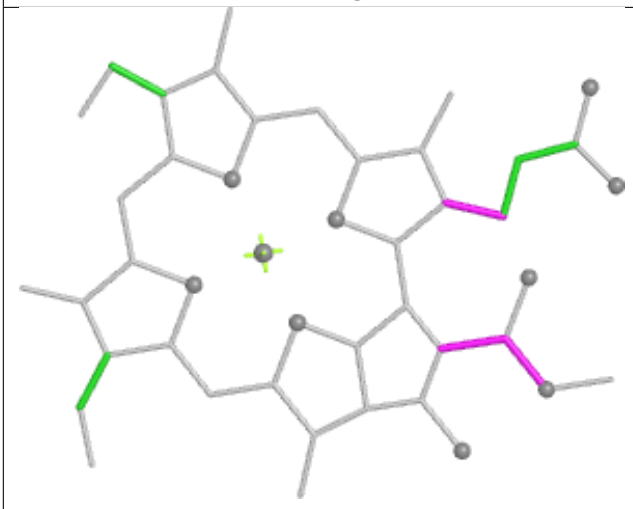
Ligand CLA a4 411



Bond lengths



Bond angles

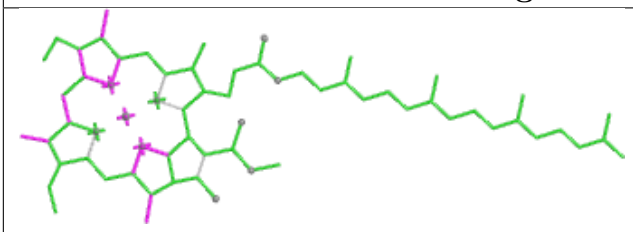


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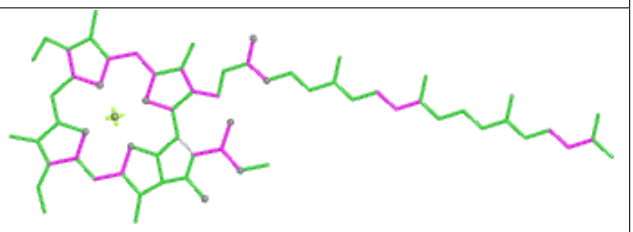


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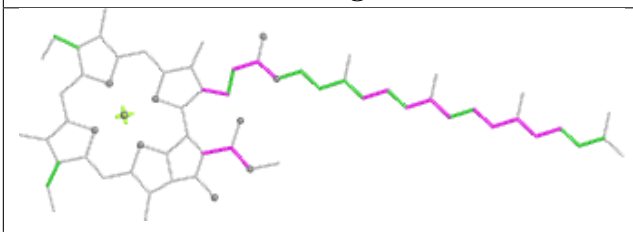
Ligand CLA aB 833



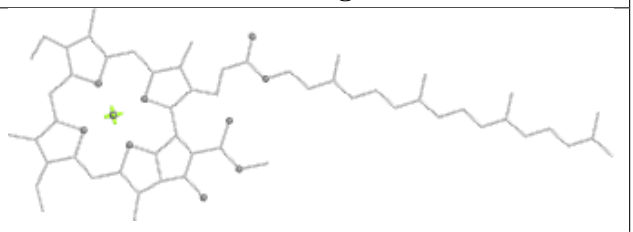
Bond lengths



Bond angles

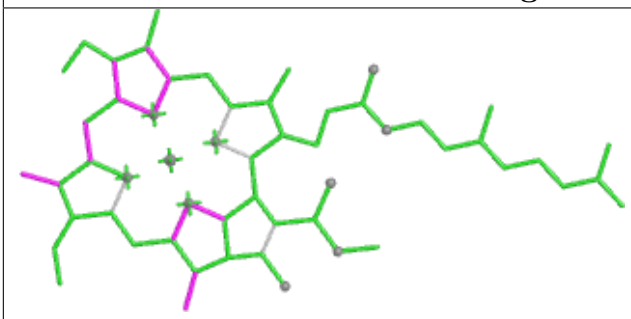


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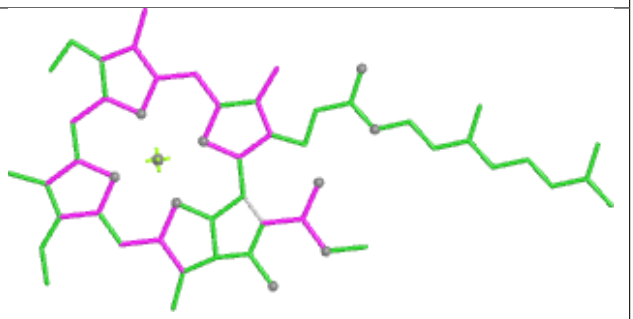


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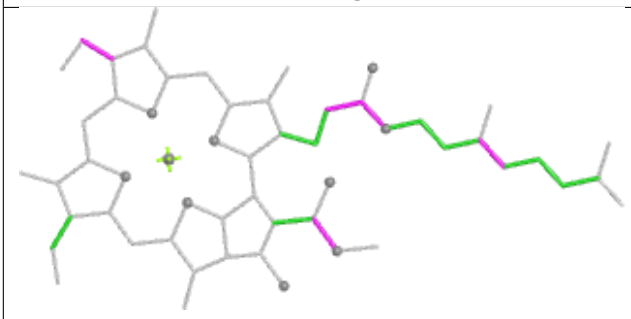
Ligand CLA c4 417



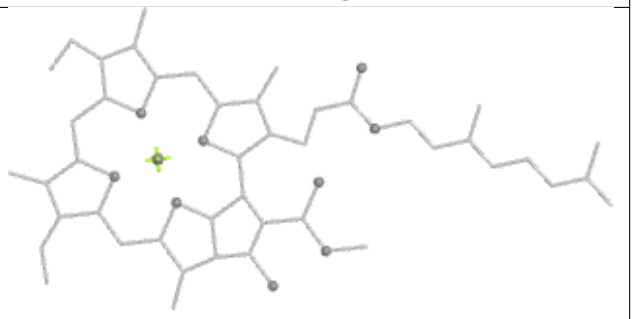
Bond lengths



Bond angles

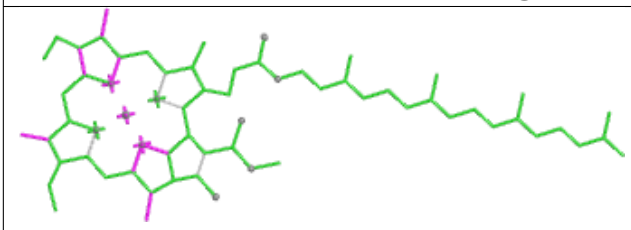


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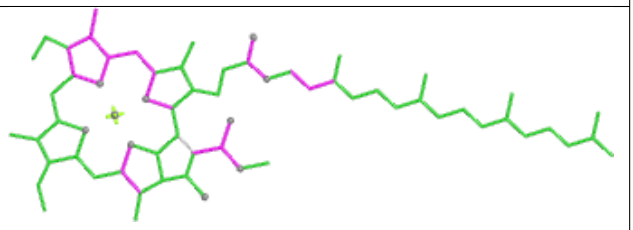


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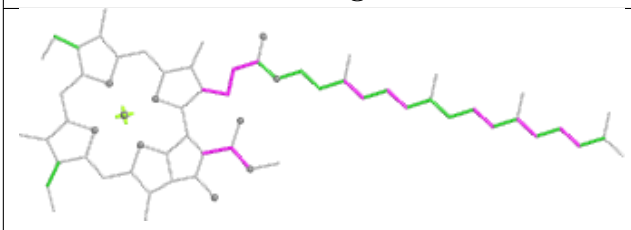
Ligand CLA cA 830



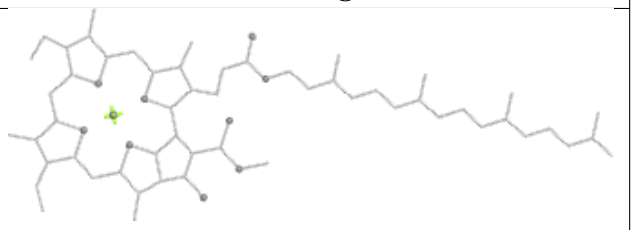
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Bond angles

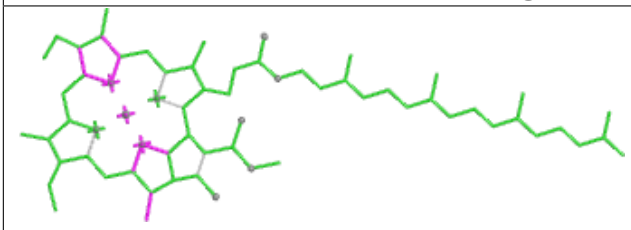


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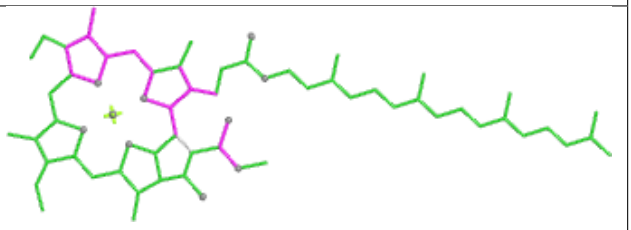


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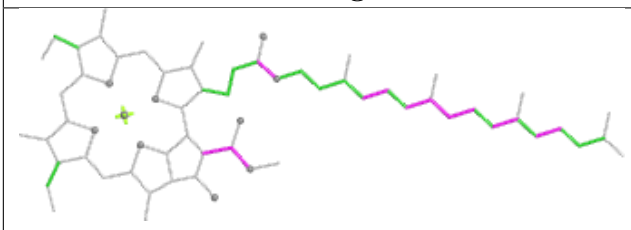
Ligand CLA a1 402



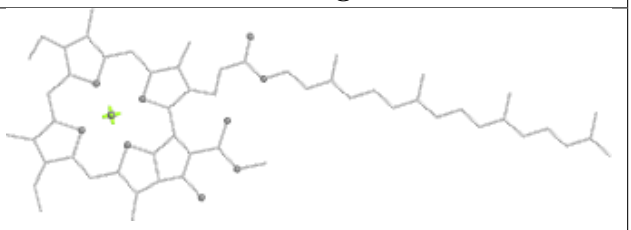
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Bond angles

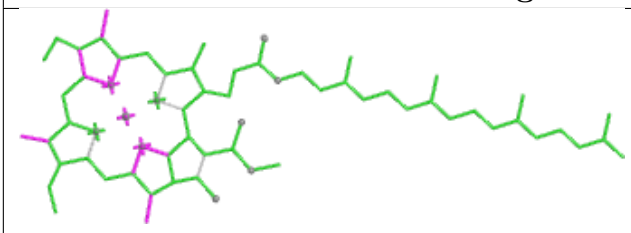


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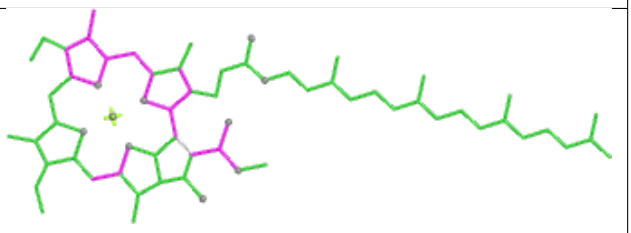


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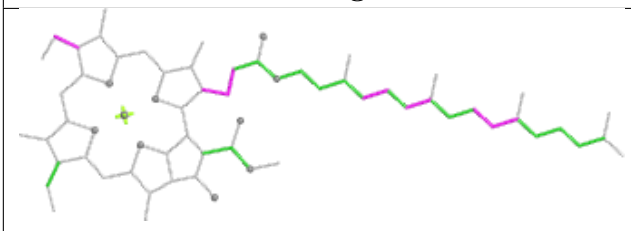
Ligand CLA bL 203



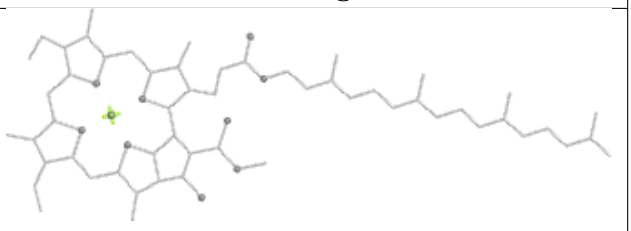
Bond lengths



Bond angles

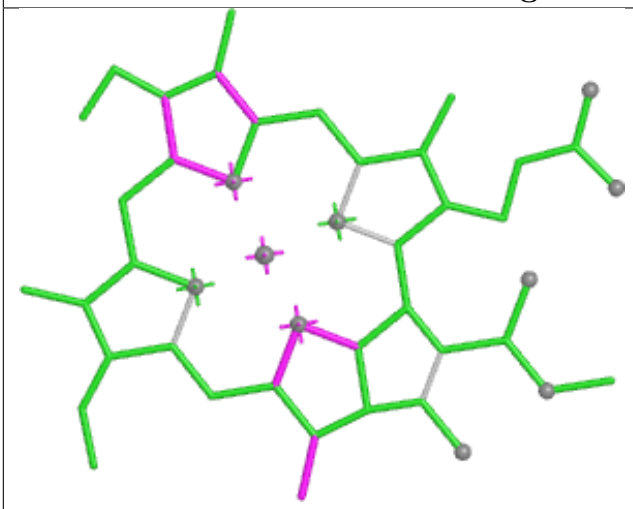


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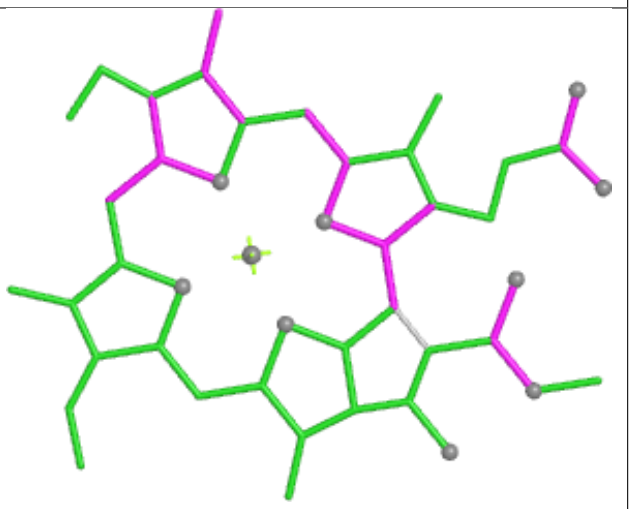


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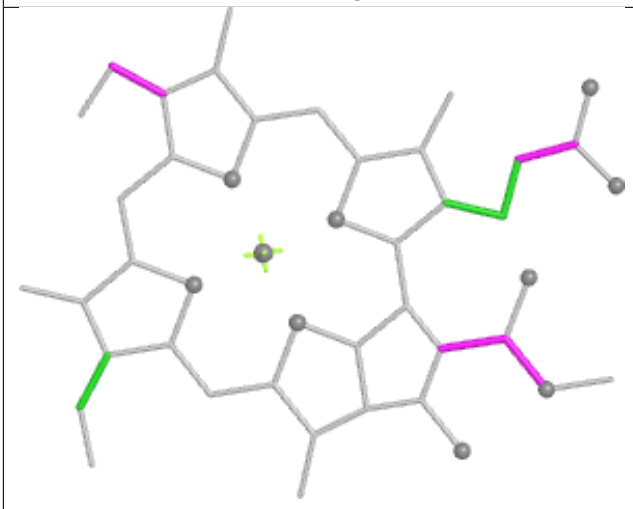
Ligand CLA c5 407



Bond lengths



Bond angles

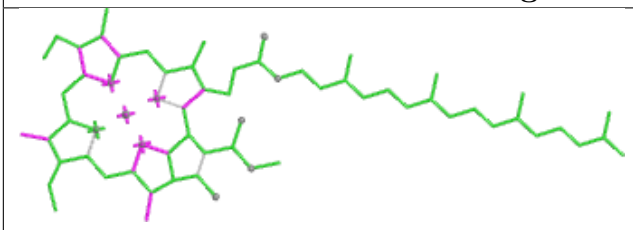


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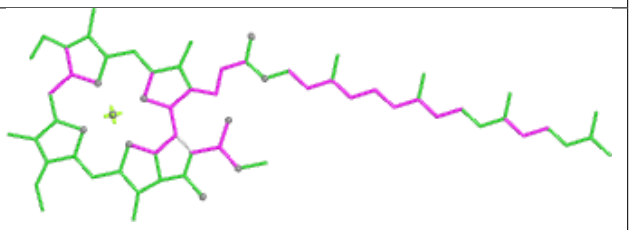


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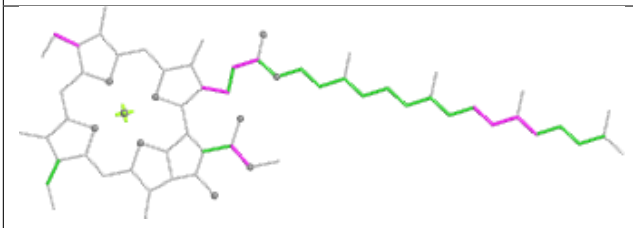
Ligand CLA c3 421



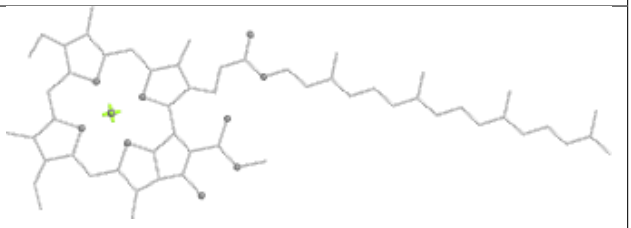
Bond lengths



Bond angles

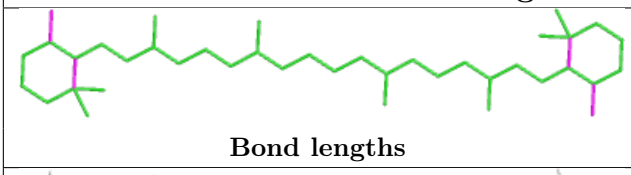


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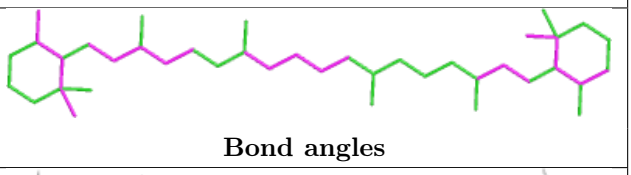


Rings

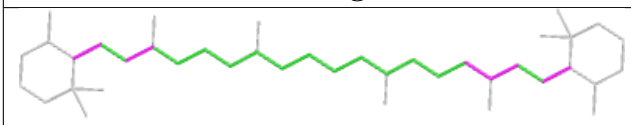
Ligand BCR cL 205



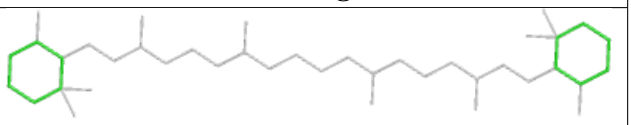
Bond lengths



Bond angles

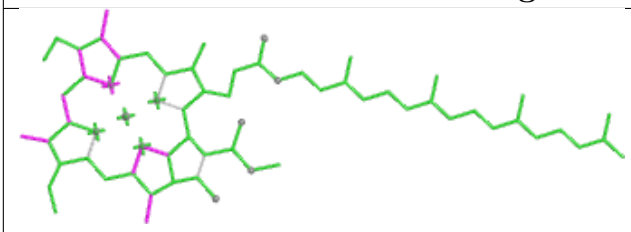


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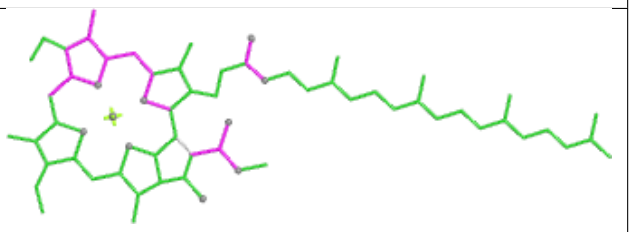


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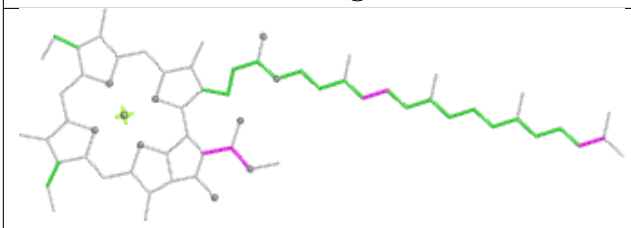
Ligand CLA b3 409



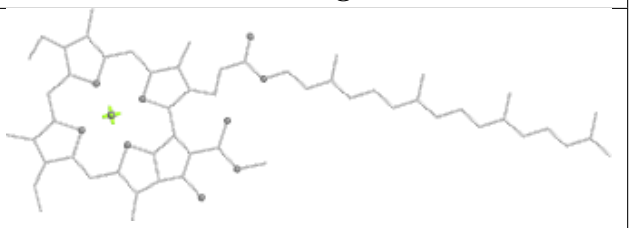
Bond lengths



Bond angles

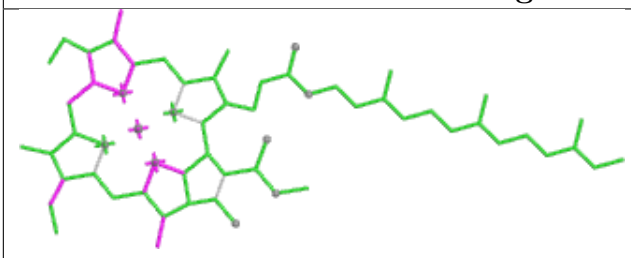


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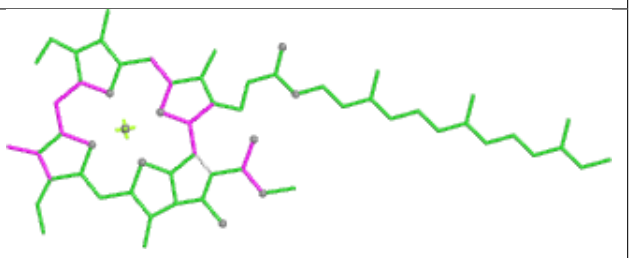


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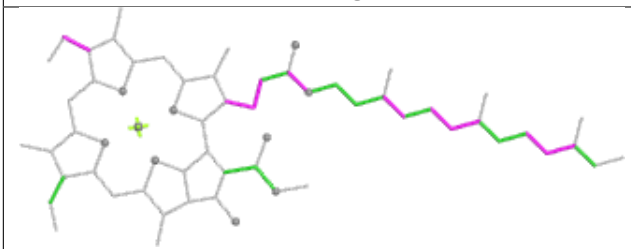
Ligand CLA cA 821



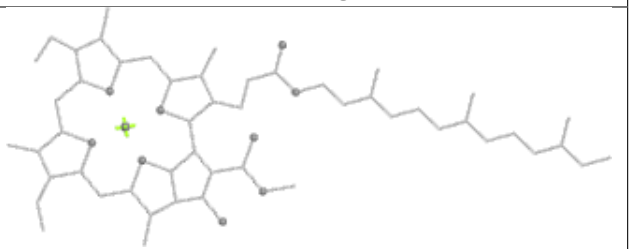
Bond lengths



Bond angles

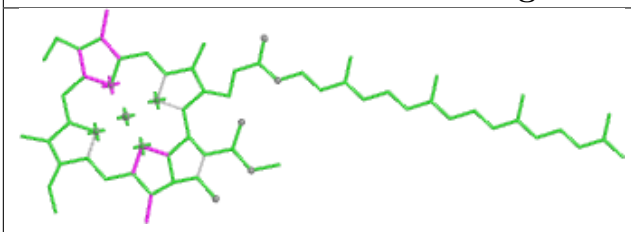


Torsions

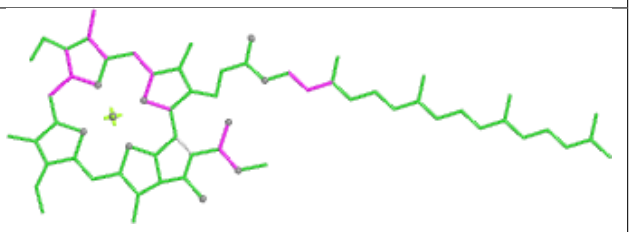


Rings

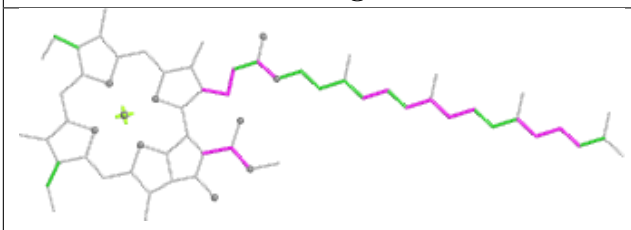
Ligand CLA b6 403



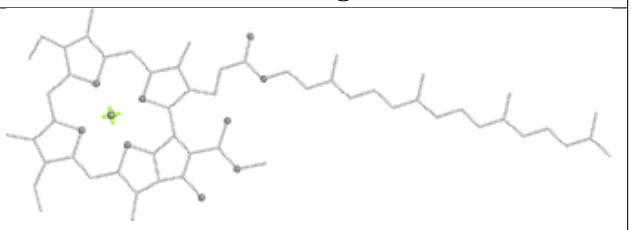
Bond lengths



Bond angles

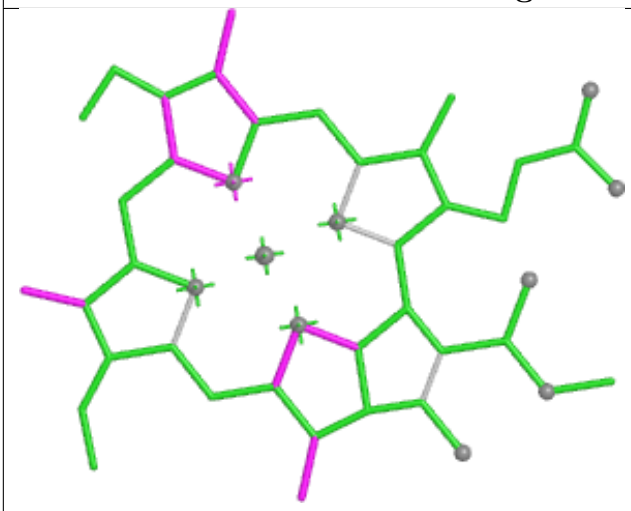


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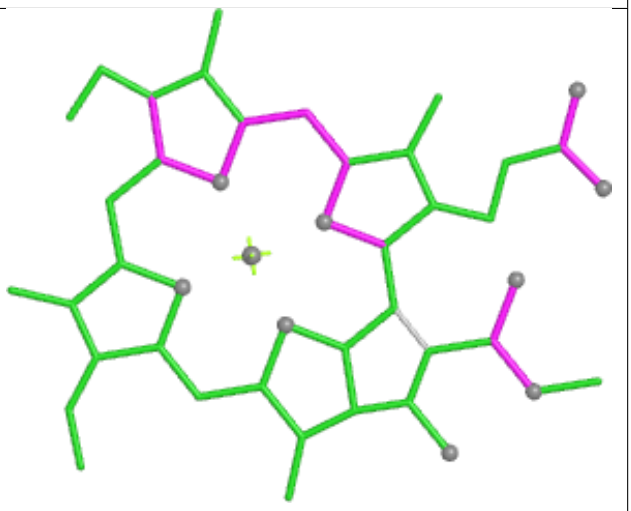


Rings

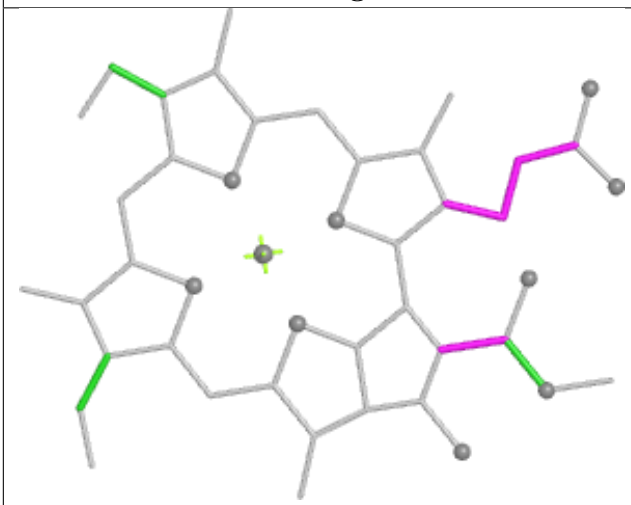
Ligand CLA cA 837



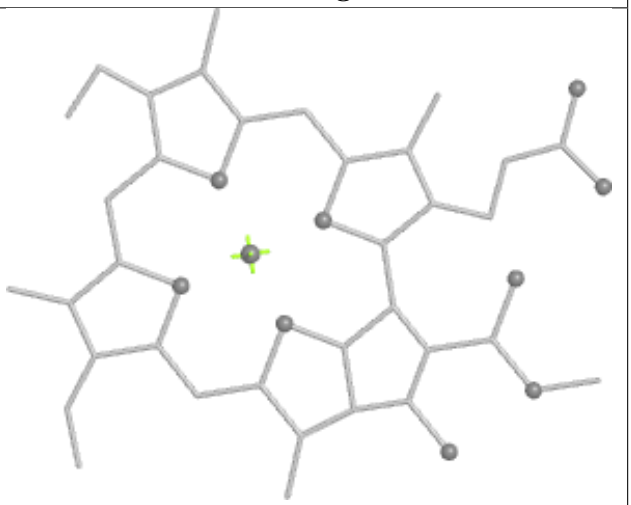
Bond lengths



Bond angles

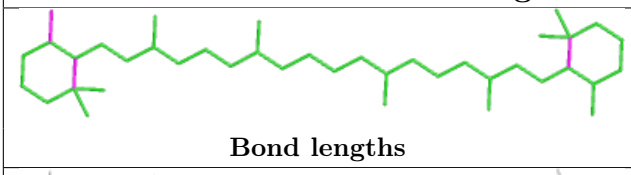


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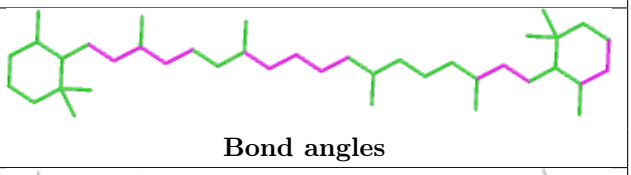


Rings

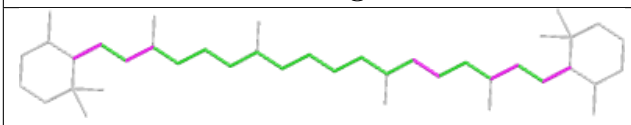
Ligand BCR aB 844



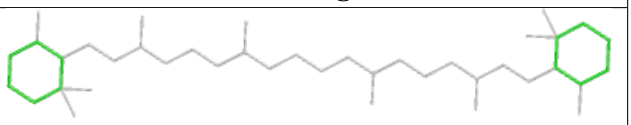
Bond lengths



Bond angles

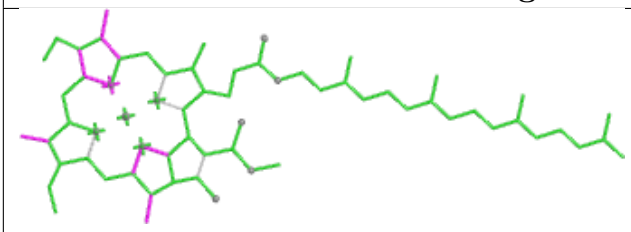


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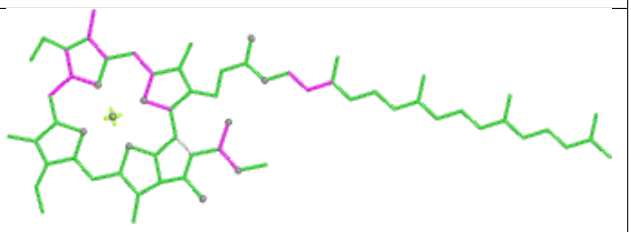


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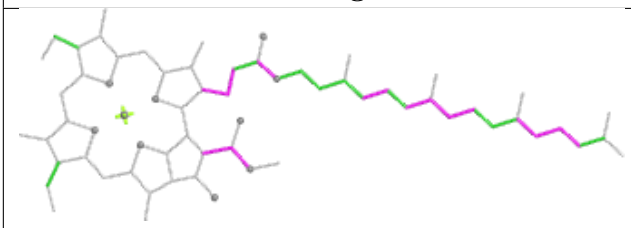
Ligand CLA b1 402



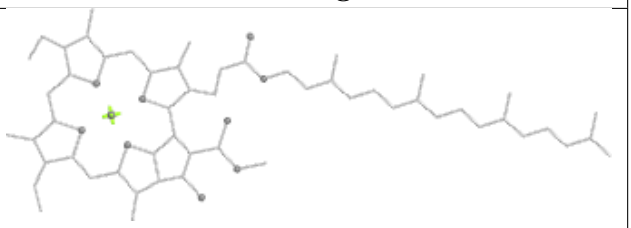
Bond lengths



Bond angles

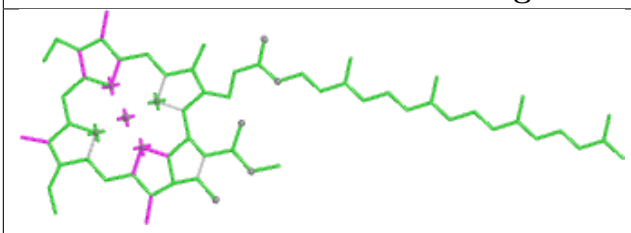


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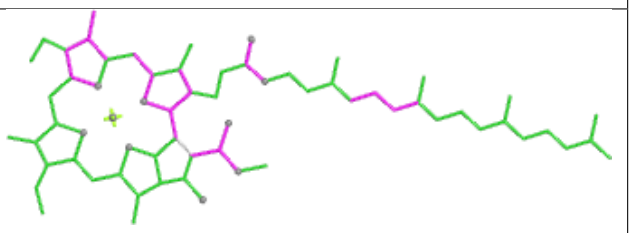


Rings

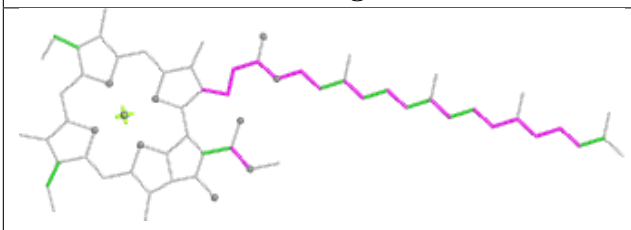
Ligand CLA bA 829



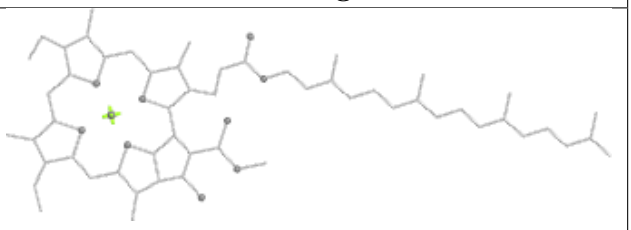
Bond lengths



Bond angles

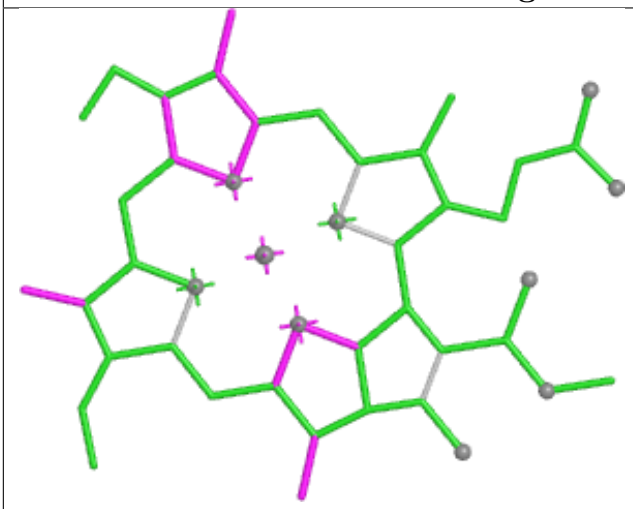


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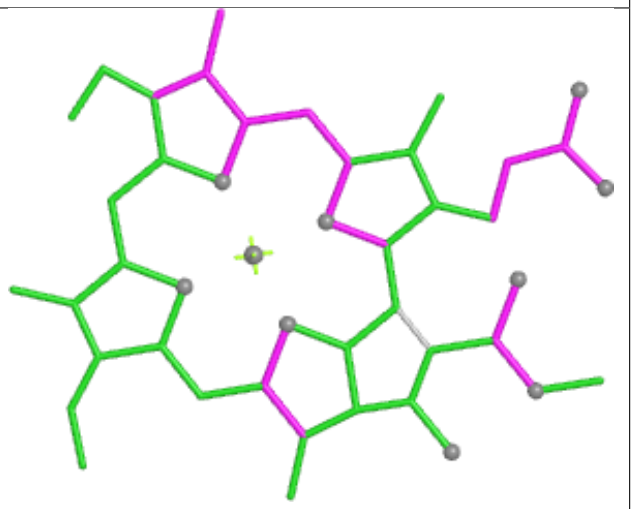


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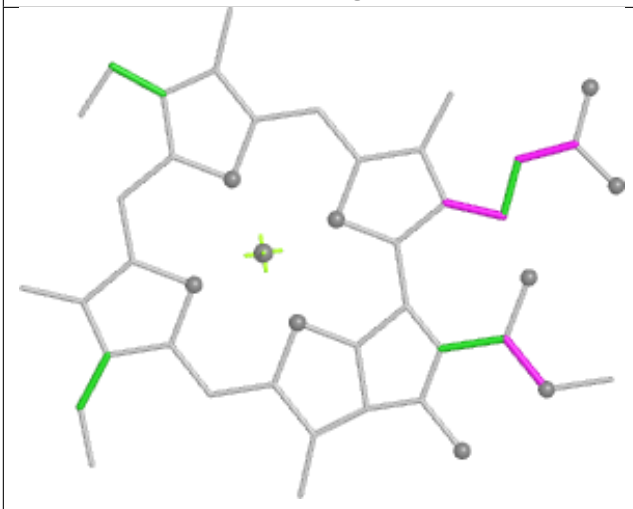
Ligand CLA b5 408



Bond lengths



Bond angles

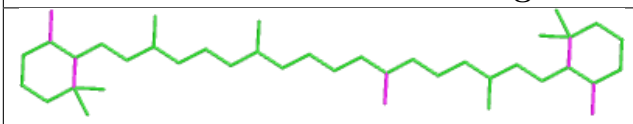


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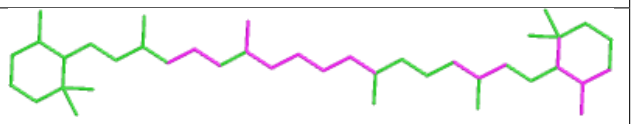


Rings

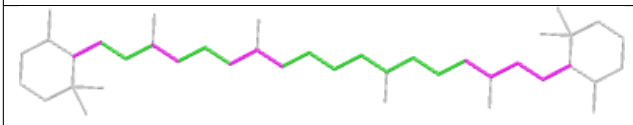
Ligand BCR aB 849



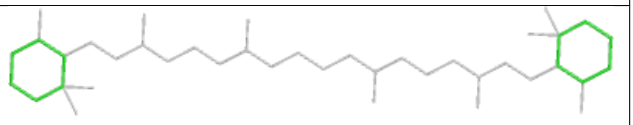
Bond lengths



Bond angles

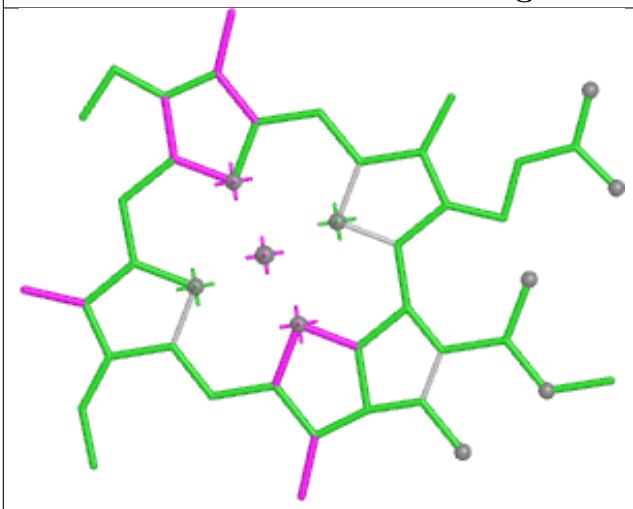


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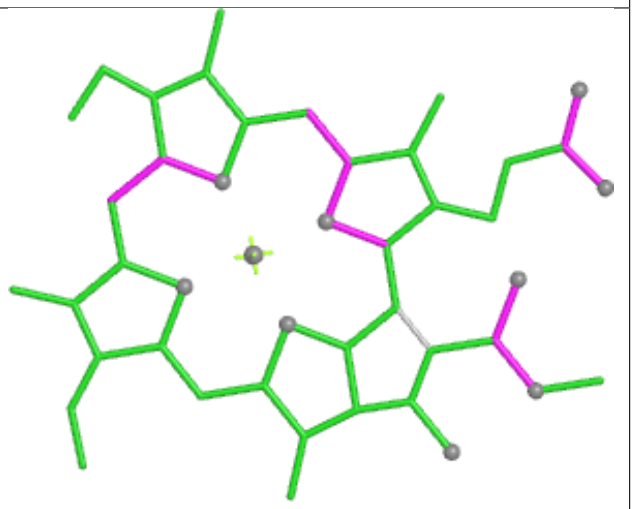


Rings

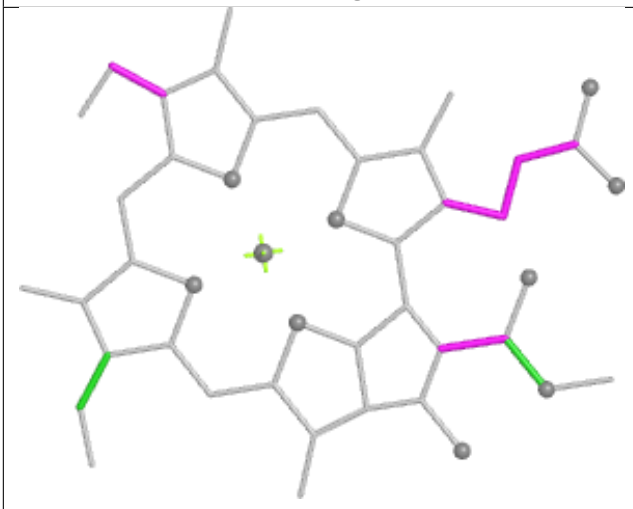
Ligand CLA aB 831



Bond lengths



Bond angles

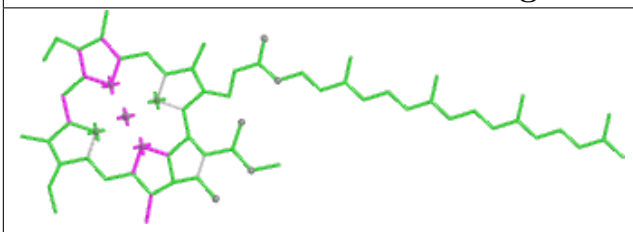


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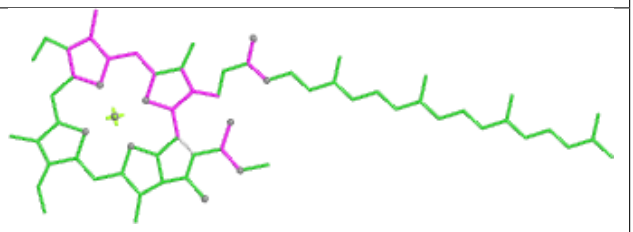


Rings

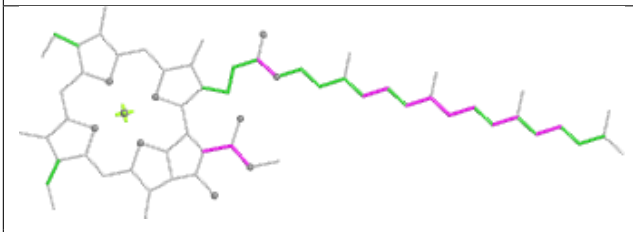
Ligand CLA a5 403



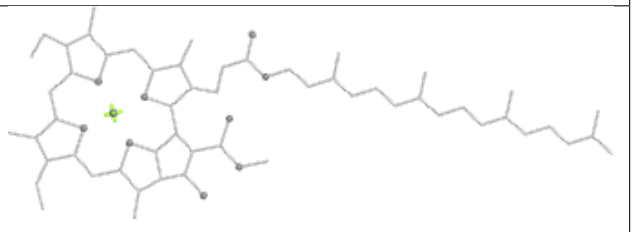
Bond lengths



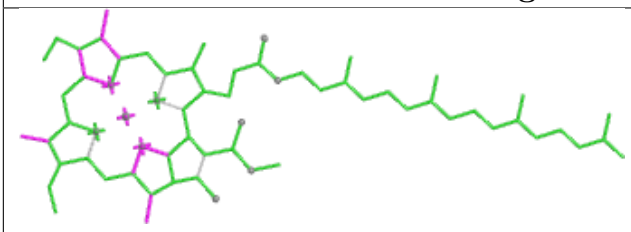
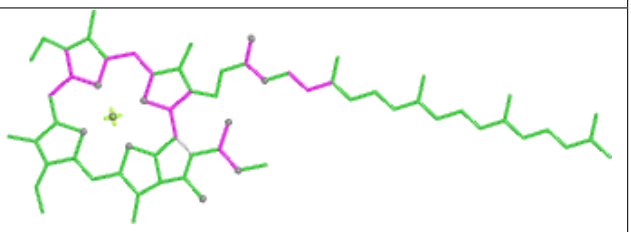
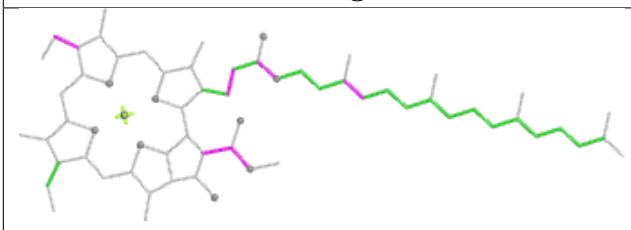
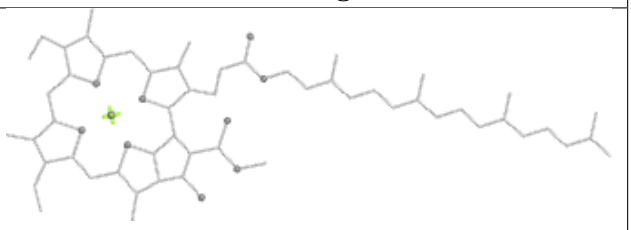
Bond angles

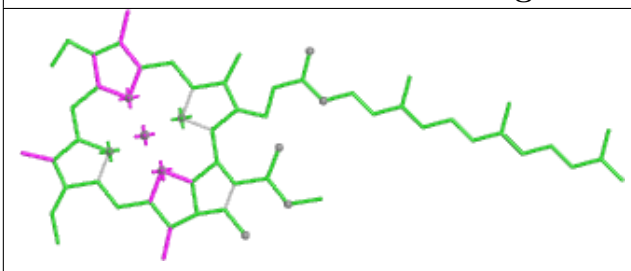
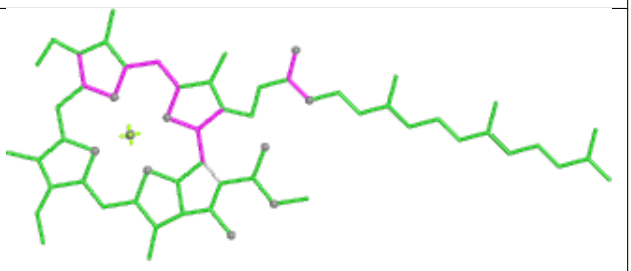
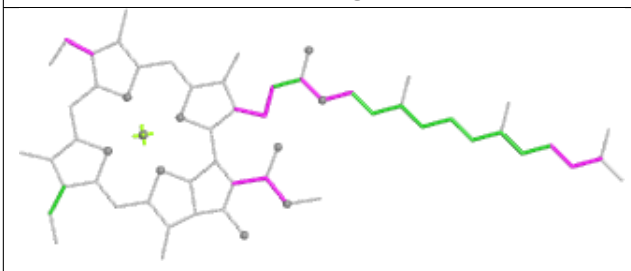
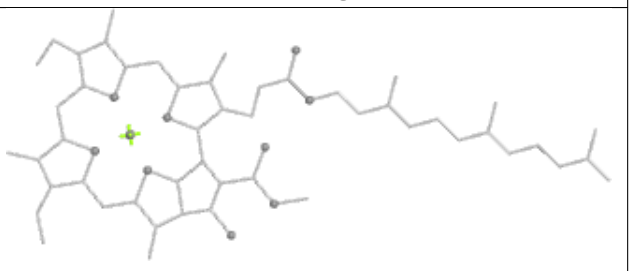


Torsions

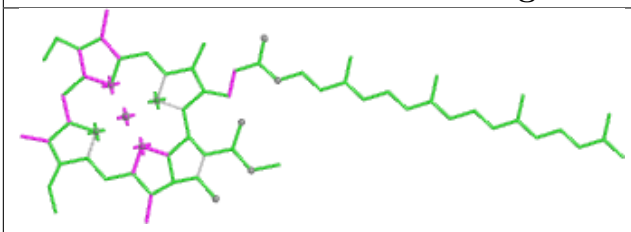


Rings

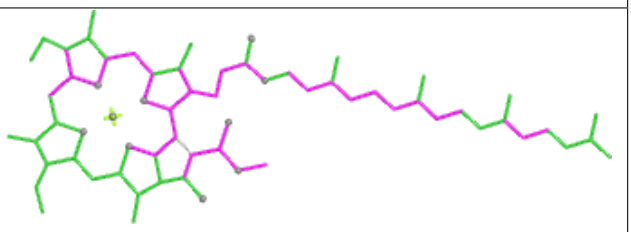
Ligand CLA b6 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aA 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

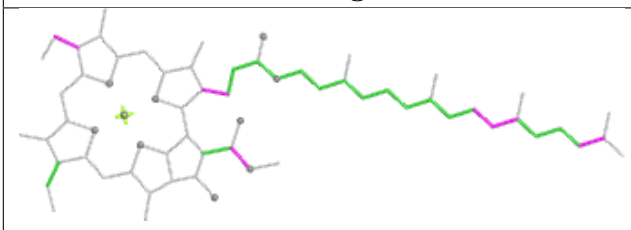
Ligand CLA b2 406



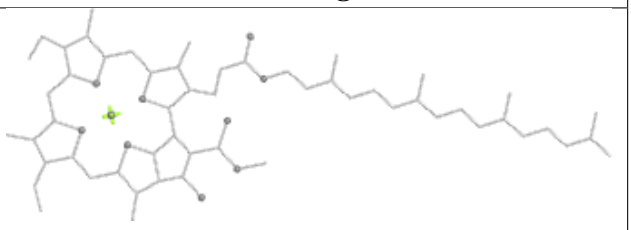
Bond lengths



Bond angles

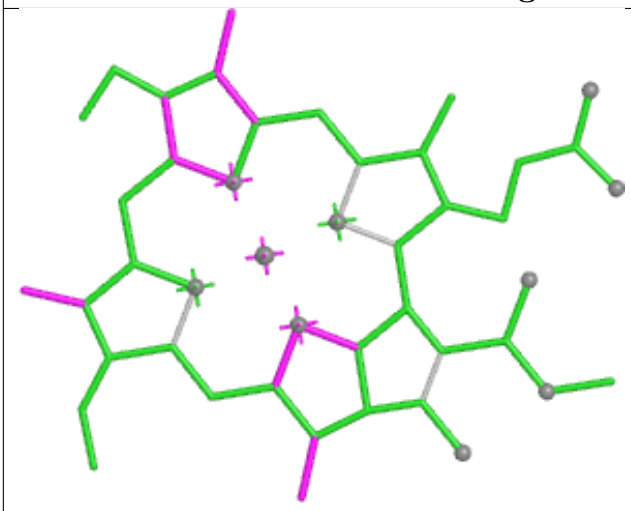


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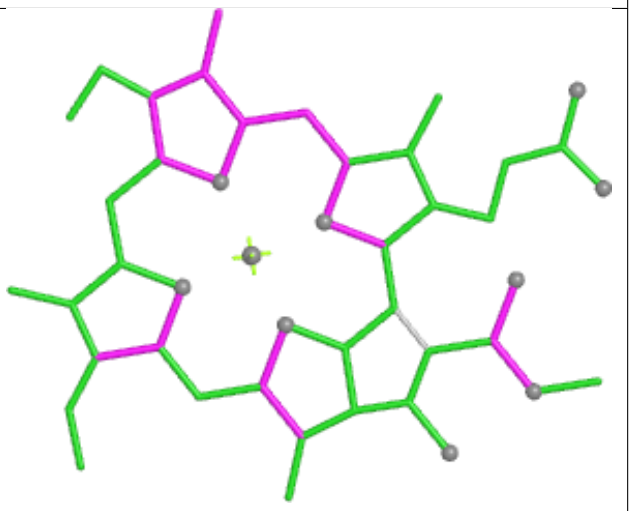


Rings

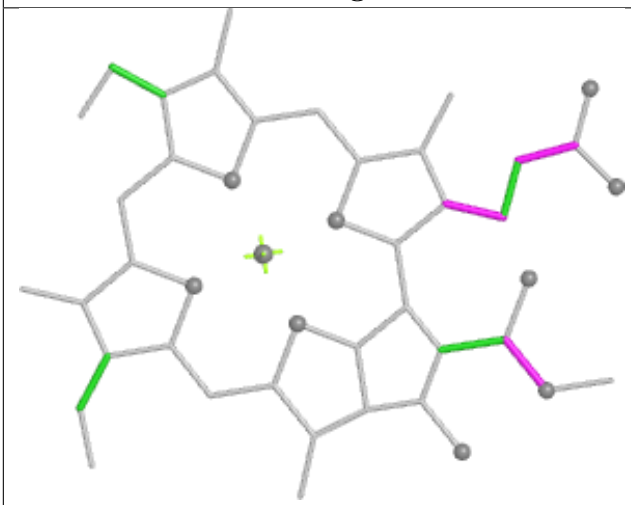
Ligand CLA b6 409



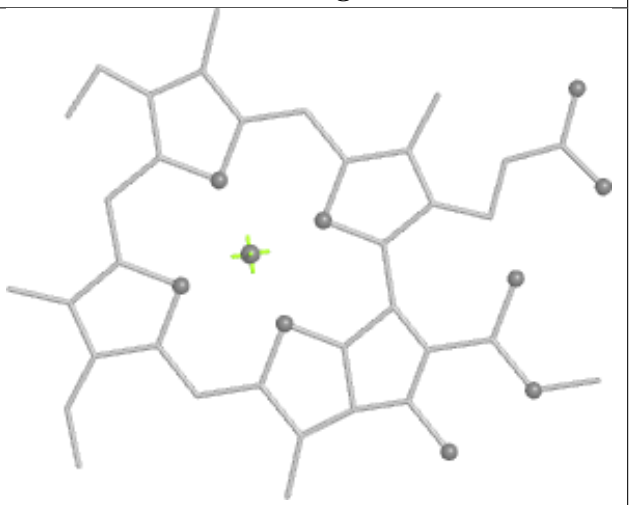
Bond lengths



Bond angles

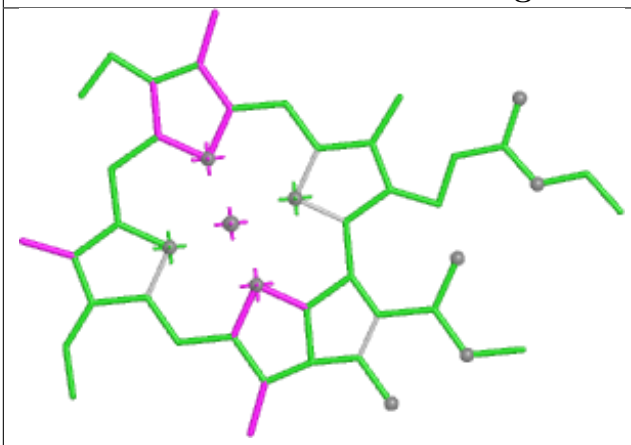


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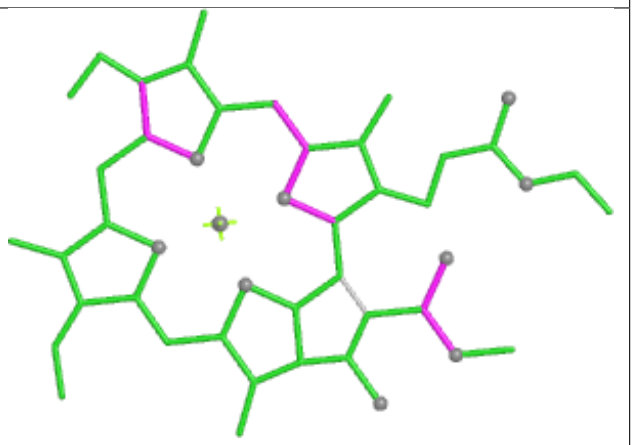


Rings

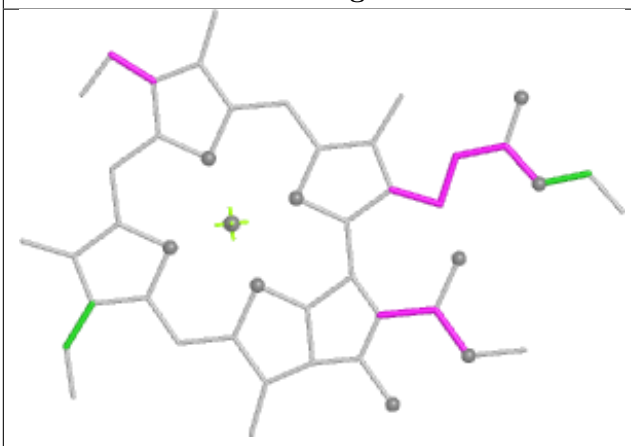
Ligand CLA bB 821



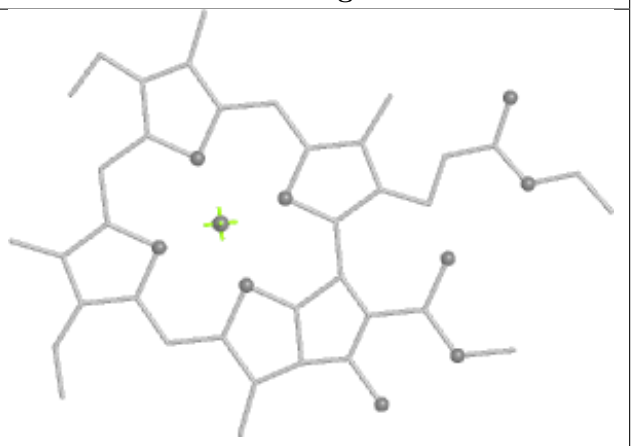
Bond lengths



Bond angles



Torsions

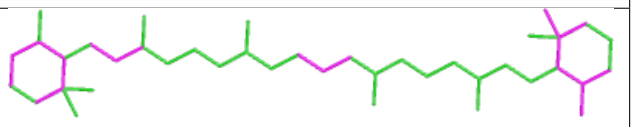


Rings

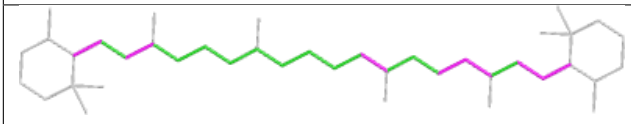
Ligand BCR c6 420



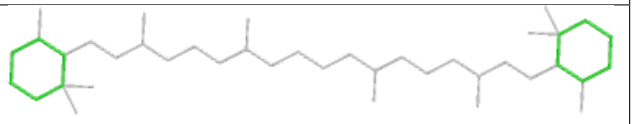
Bond lengths



Bond angles

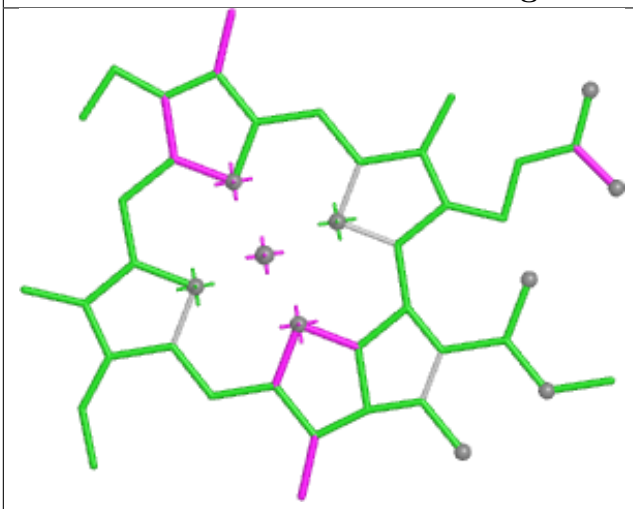


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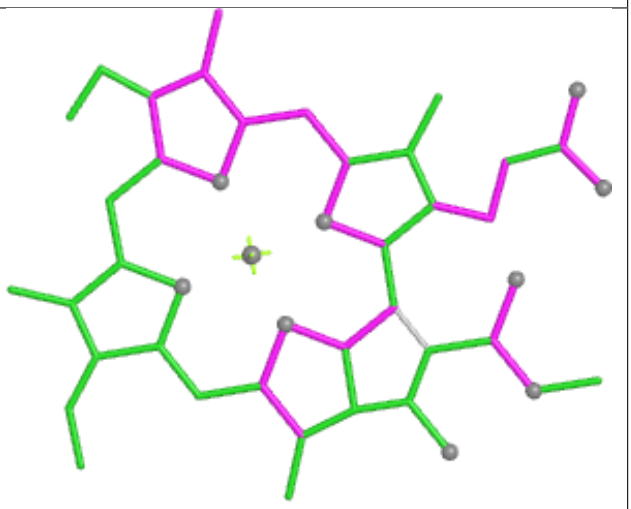


Rings

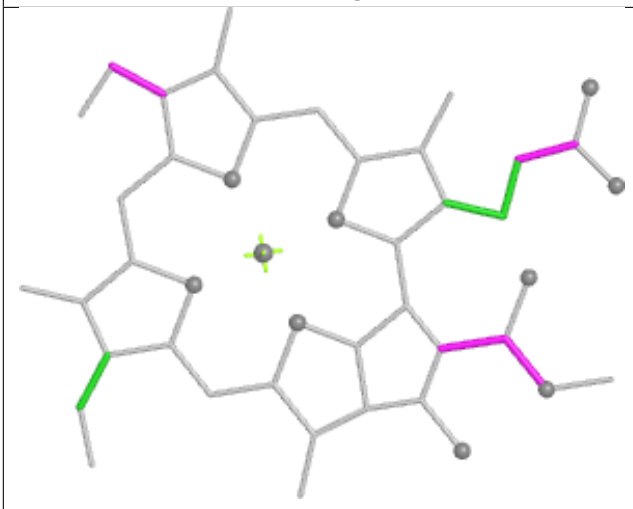
Ligand CLA c3 415



Bond lengths



Bond angles

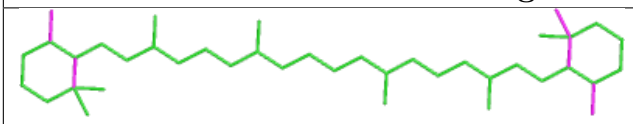


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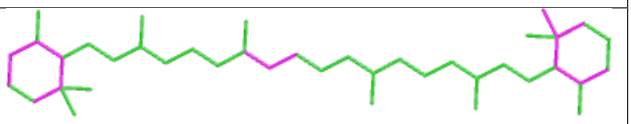


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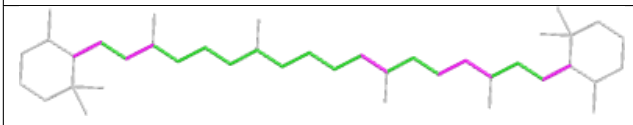
Ligand BCR a1 417



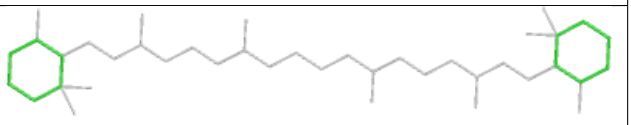
Bond lengths



Bond angles

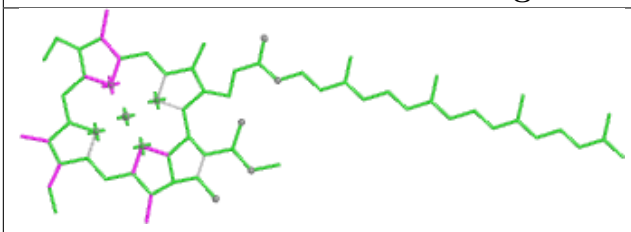


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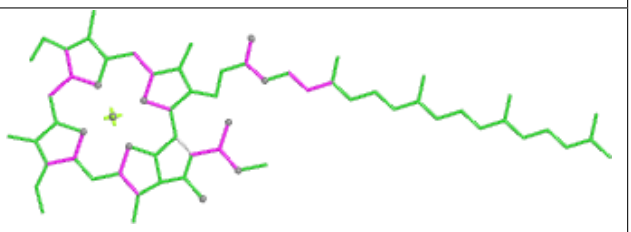


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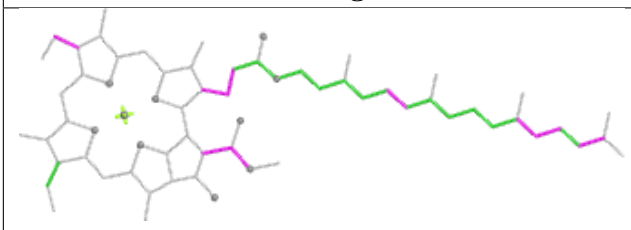
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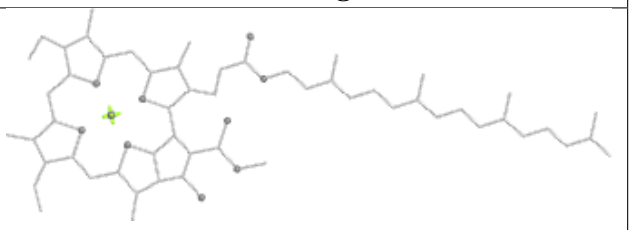
Bond lengths



Bond angles

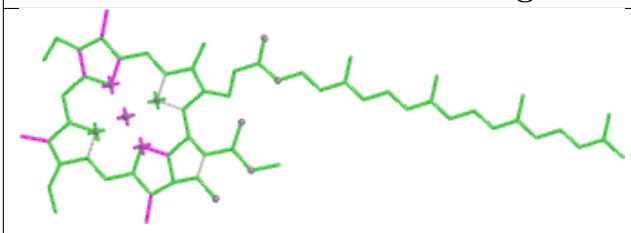


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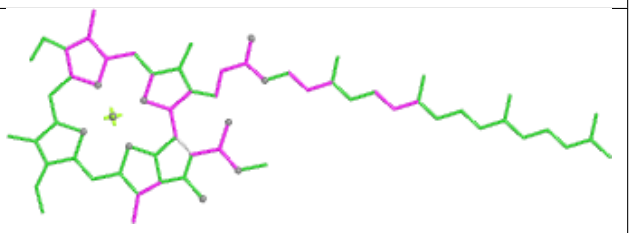


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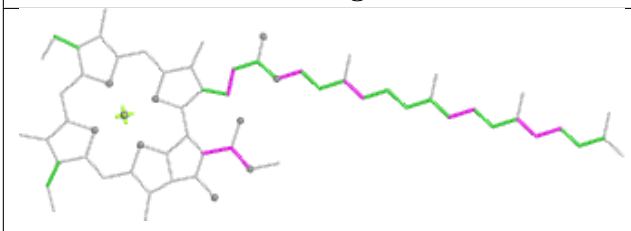
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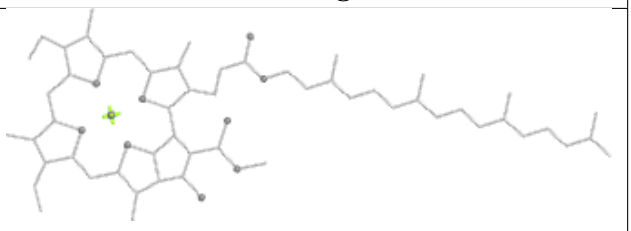
Bond lengths



Bond angles

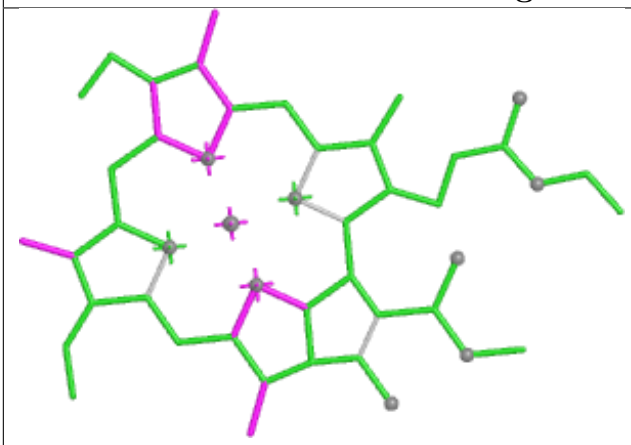


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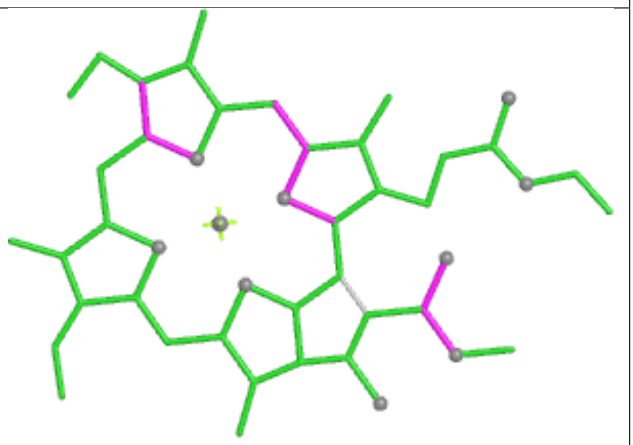


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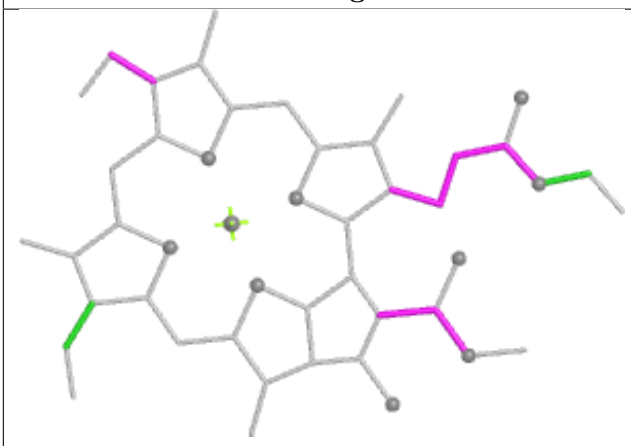
Ligand CLA aB 821



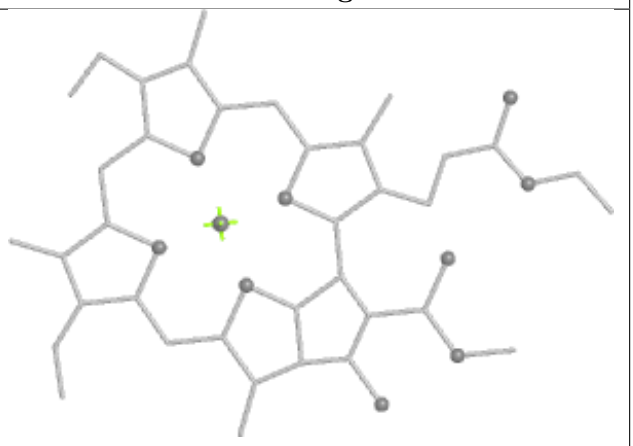
Bond lengths



Bond angles

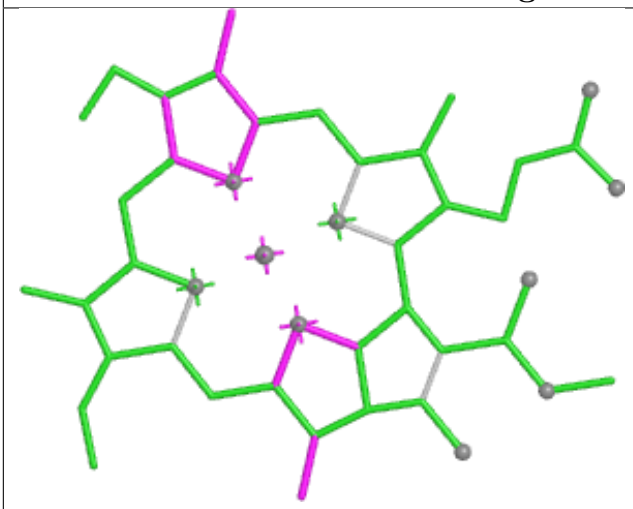


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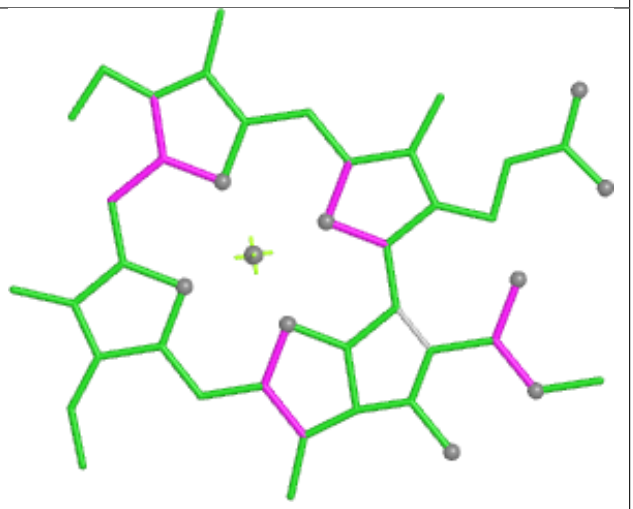


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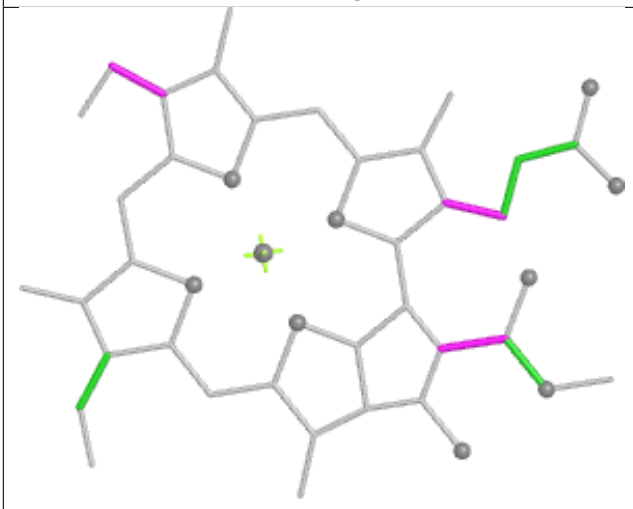
Ligand CLA b4 413



Bond lengths



Bond angles

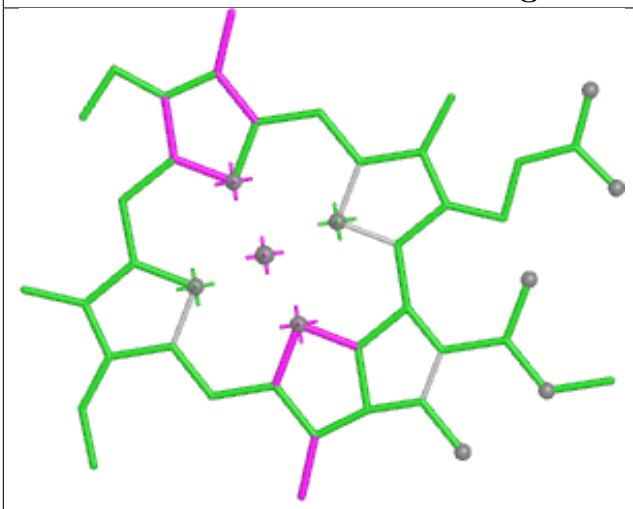


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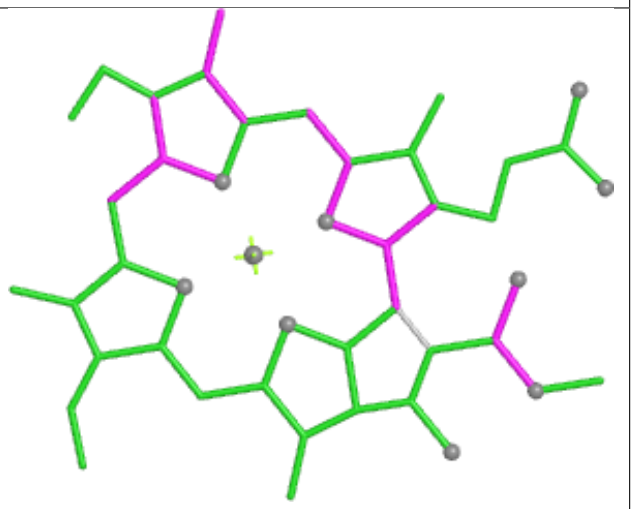


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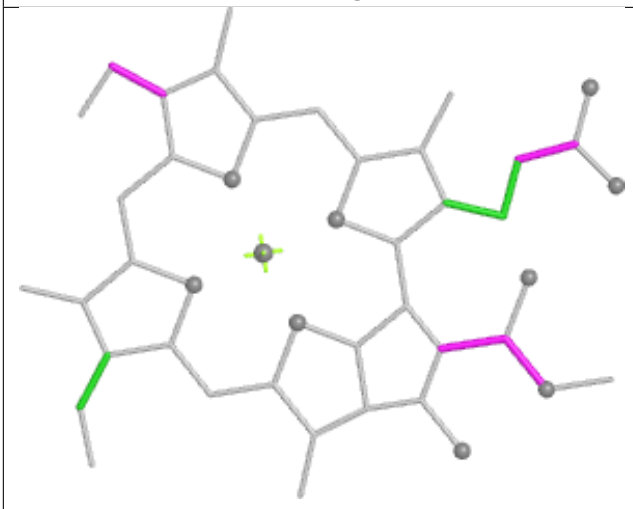
Ligand CLA c6 409



Bond lengths



Bond angles

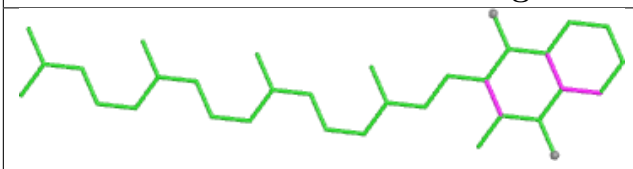


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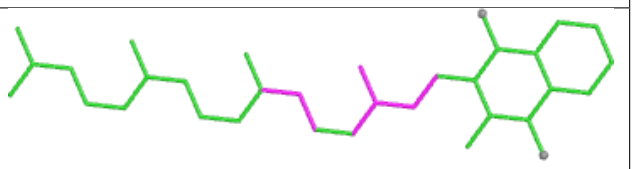


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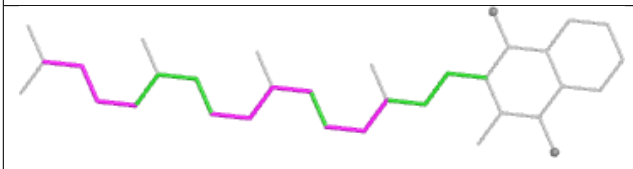
Ligand PQN bB 843



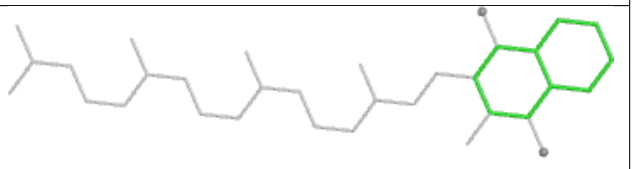
Bond lengths



Bond angles

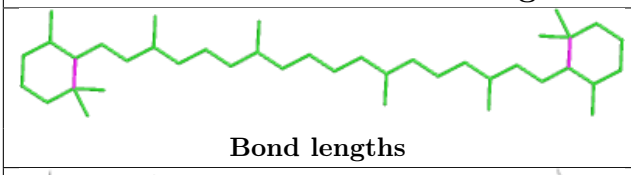


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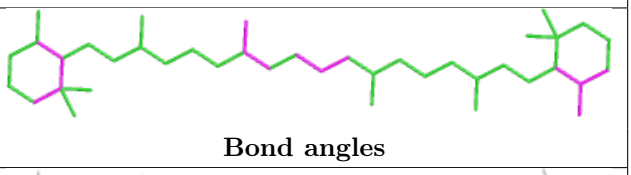


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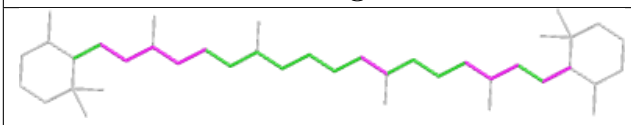
Ligand BCR bI 101



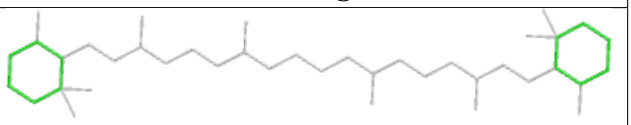
Bond lengths



Bond angles

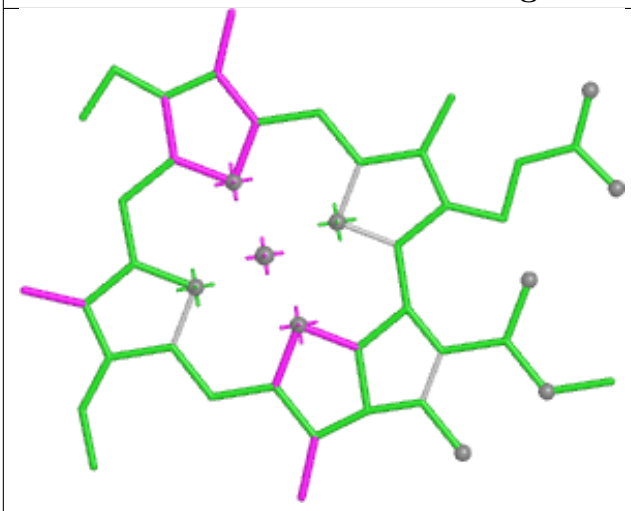


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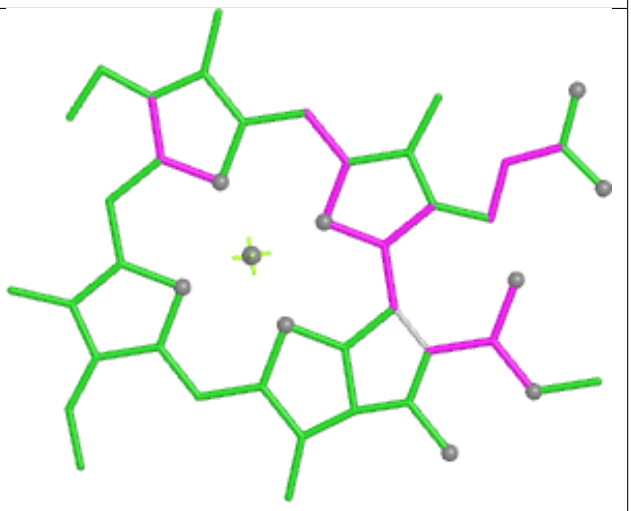


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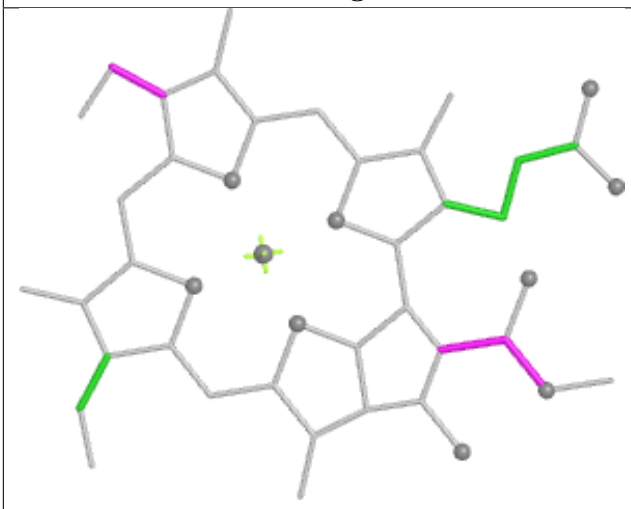
Ligand CLA cJ 101



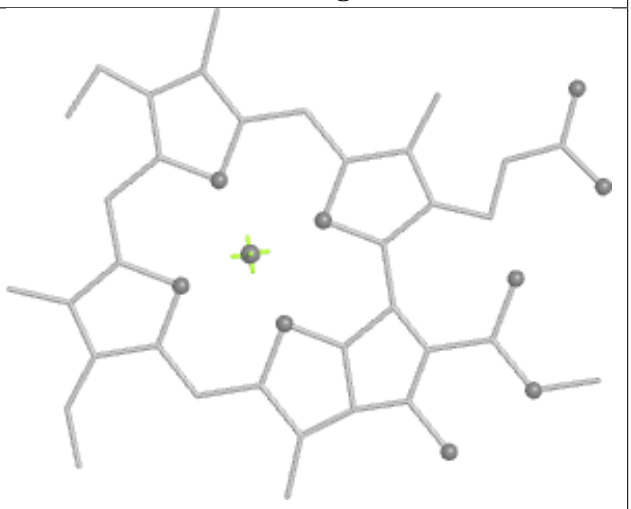
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Bond angles

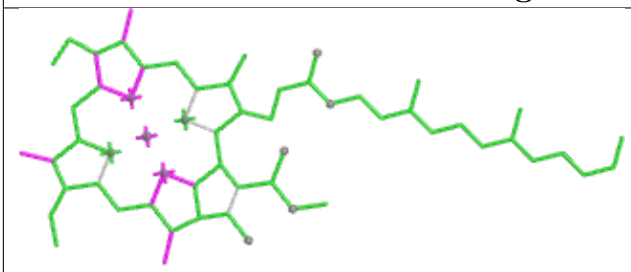


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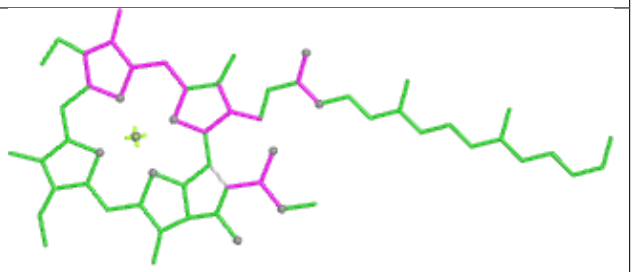


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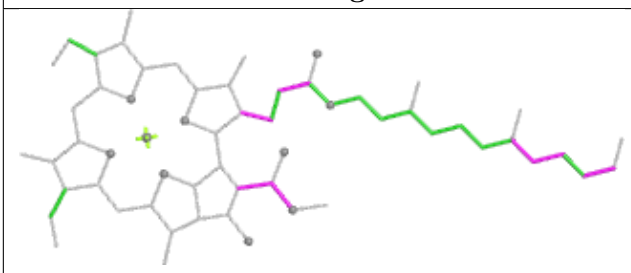
Ligand CLA aA 805



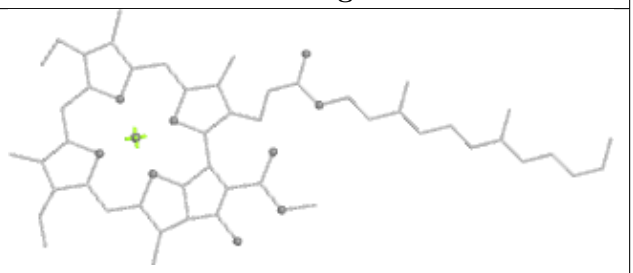
Bond lengths



Bond angles

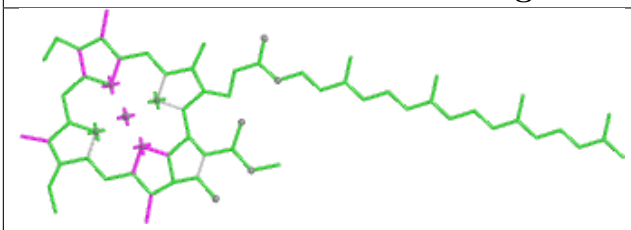


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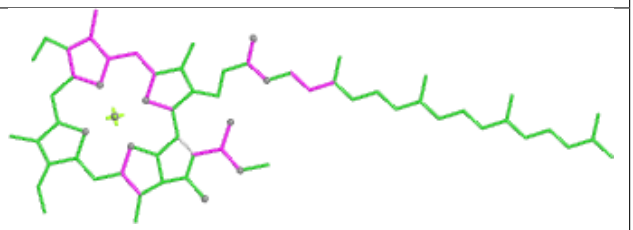


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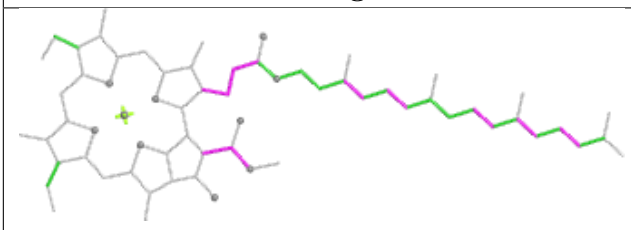
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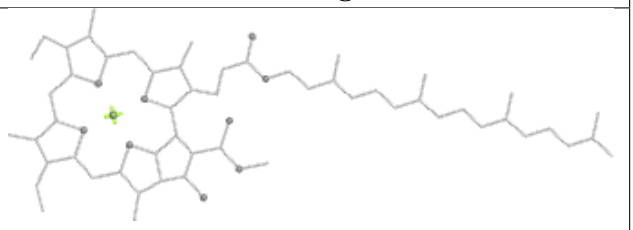
Bond lengths



Bond angles

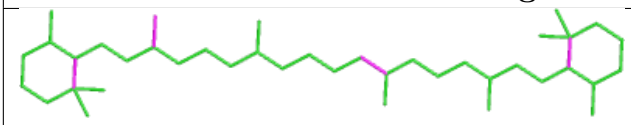


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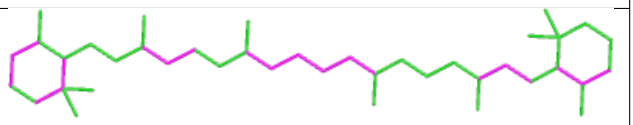


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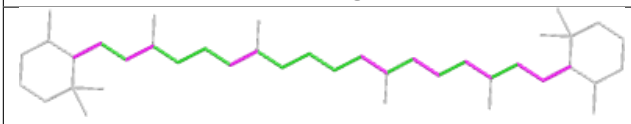
Ligand BCR bI 102



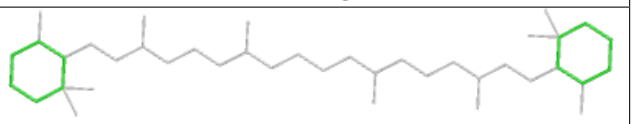
Bond lengths



Bond angles

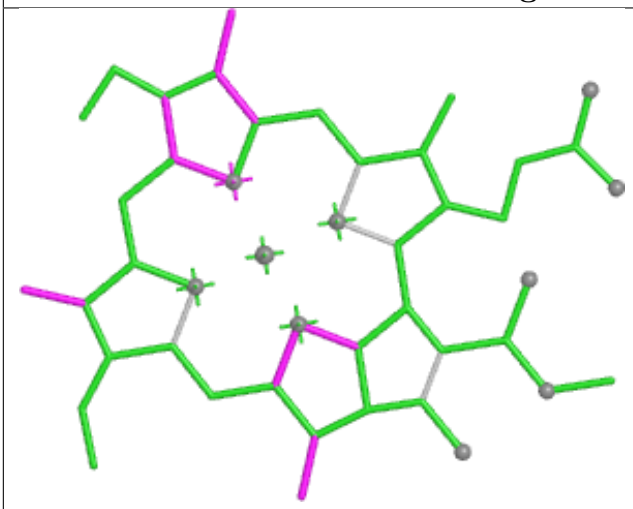


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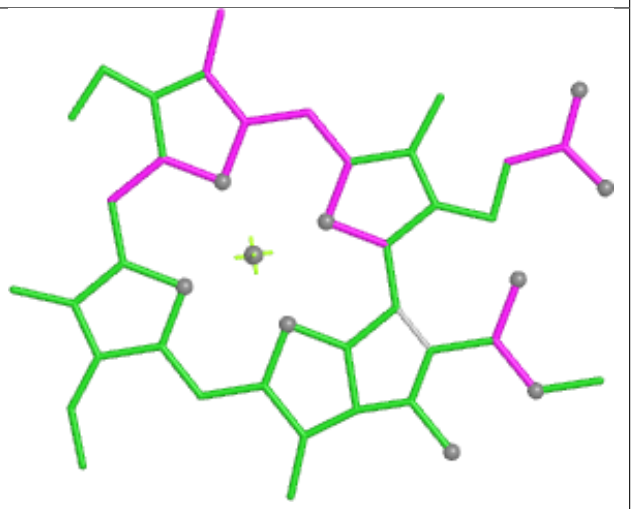


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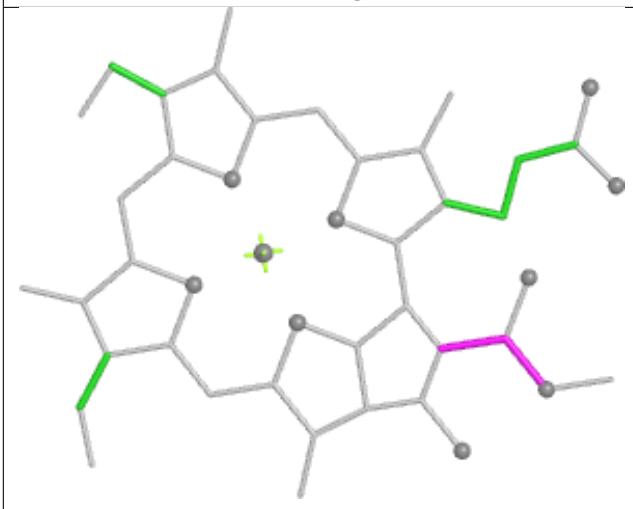
Ligand CLA a5 406



Bond lengths



Bond angles

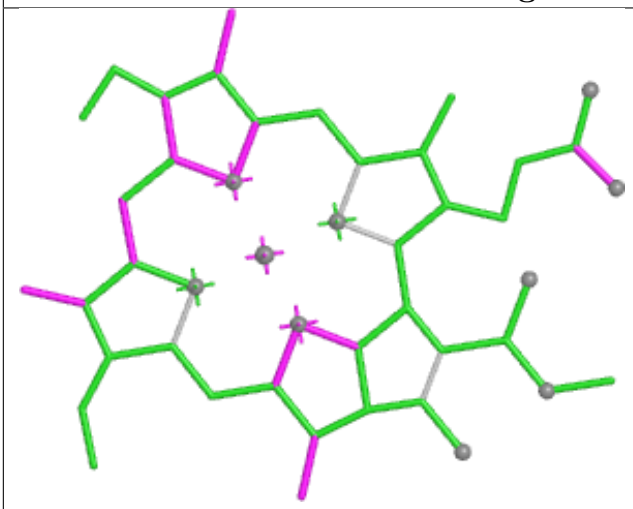


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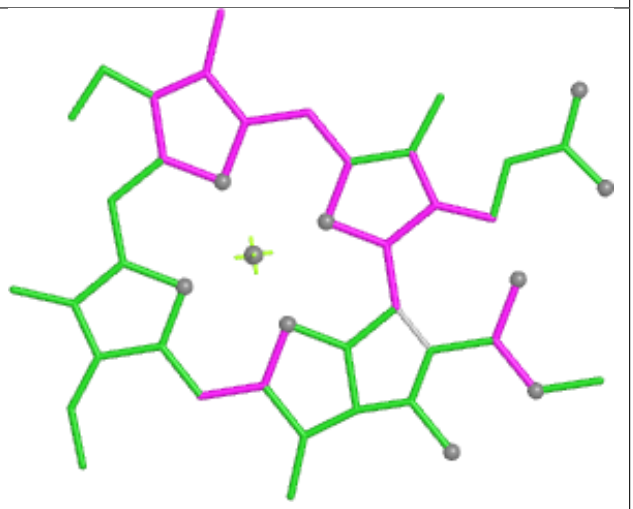


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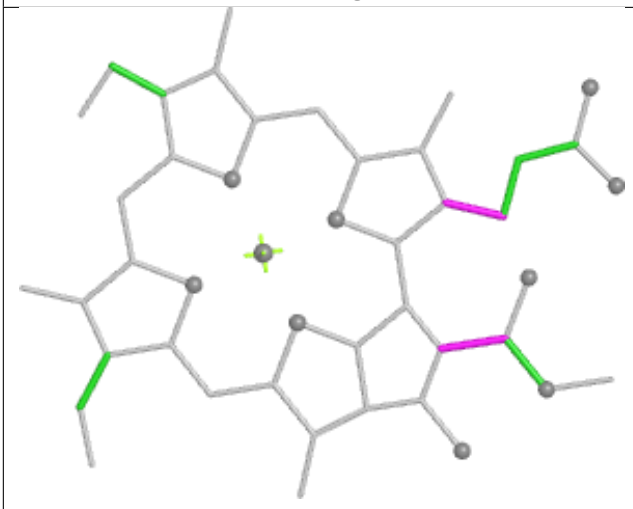
Ligand CLA b2 412



Bond lengths



Bond angles

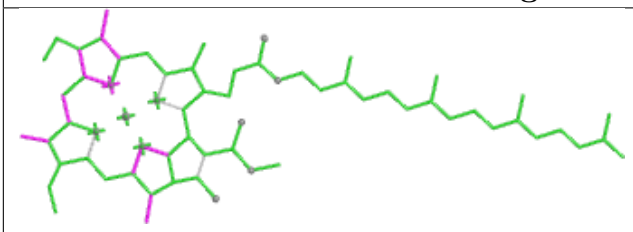


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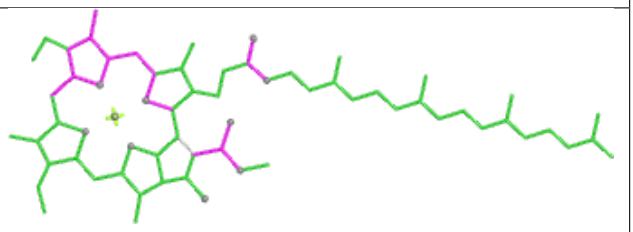


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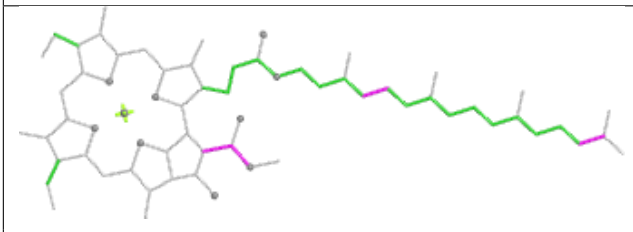
Ligand CLA c3 409



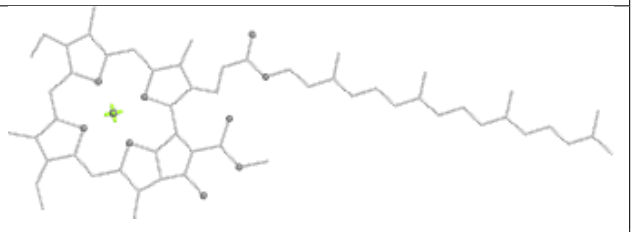
Bond lengths



Bond angles

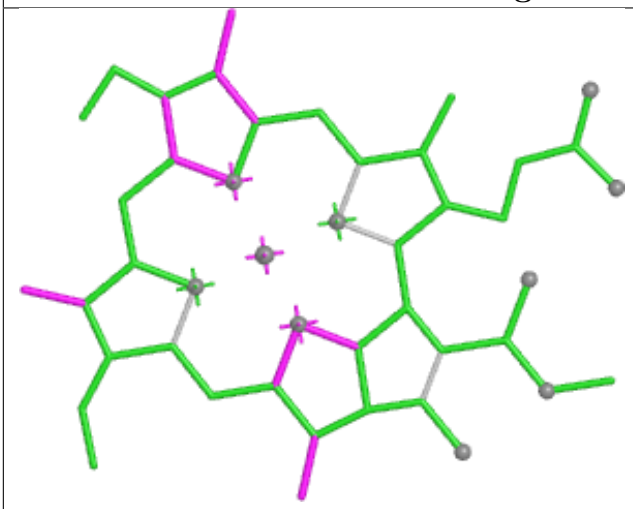


Torsions

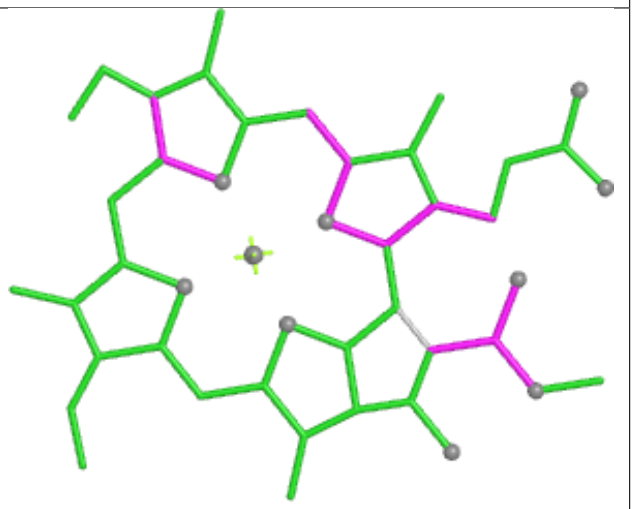


Rings

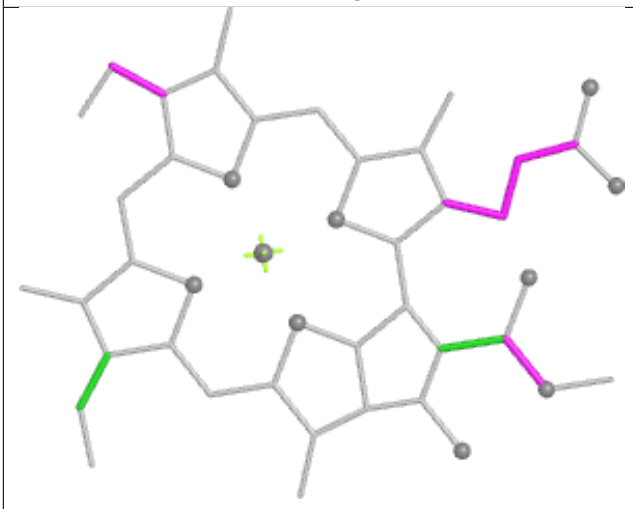
Ligand CLA bB 835



Bond lengths



Bond angles

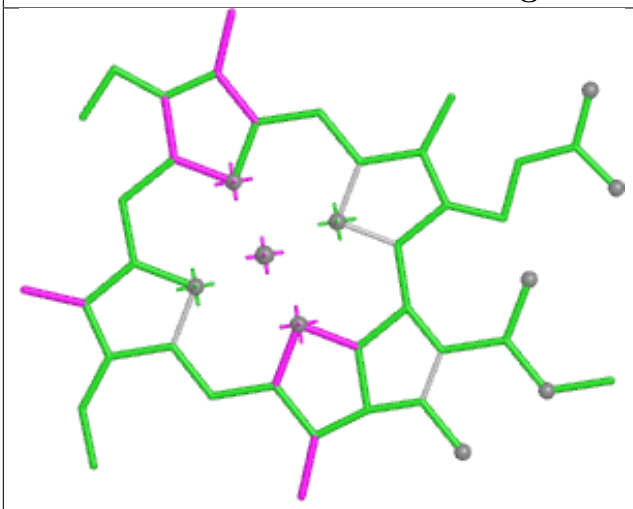


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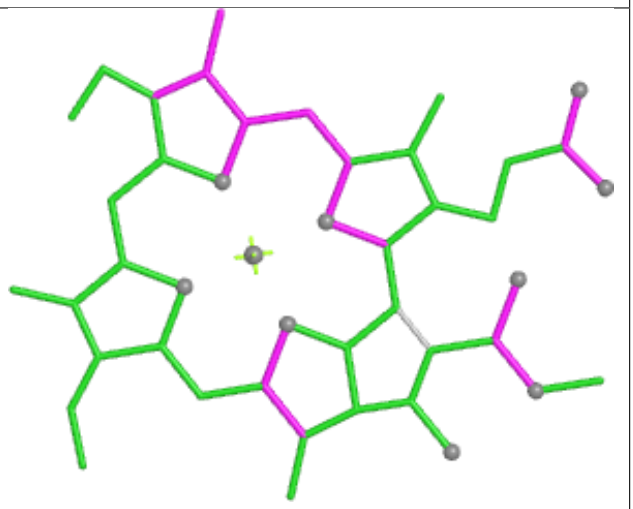


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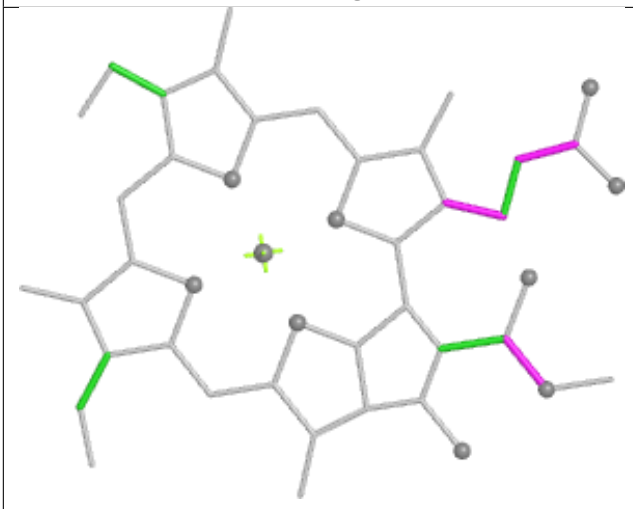
Ligand CLA c4 408



Bond lengths



Bond angles

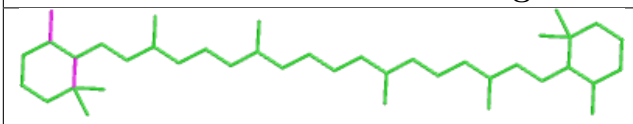


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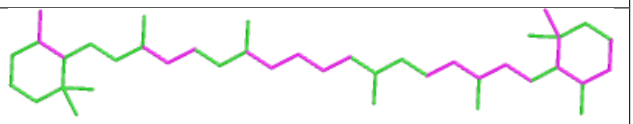


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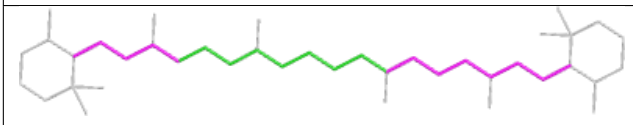
Ligand BCR aA 850



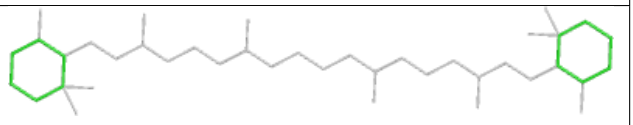
Bond lengths



Bond angles

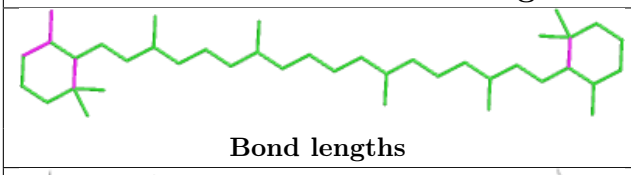


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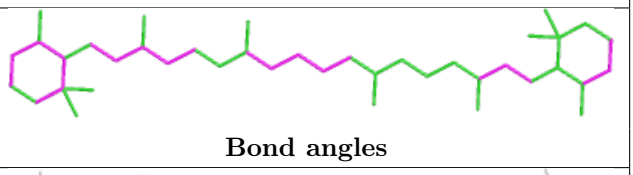


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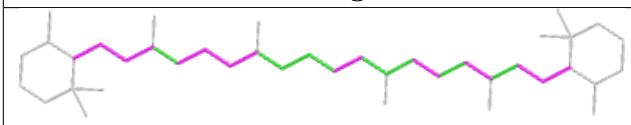
Ligand BCR a6 402



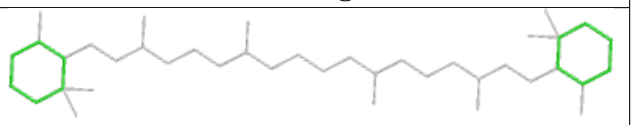
Bond lengths



Bond angles



Torsions

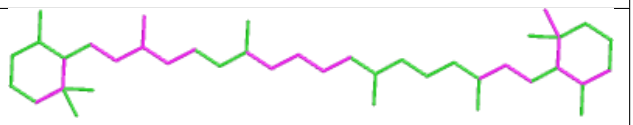


Rings

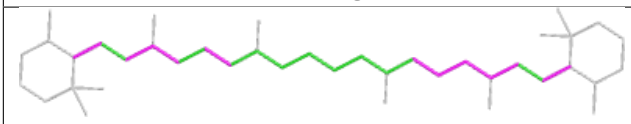
Ligand BCR b1 401



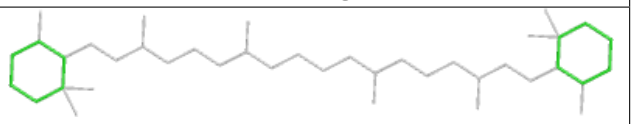
Bond lengths



Bond angles

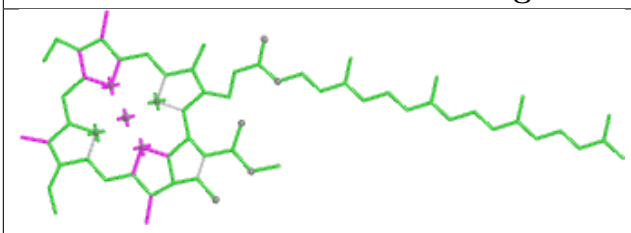


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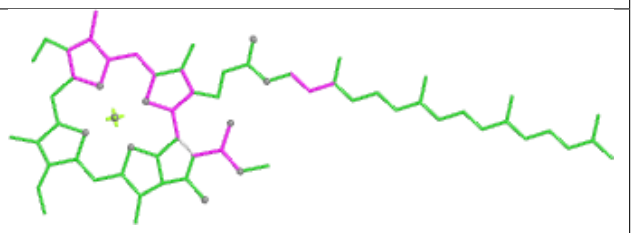


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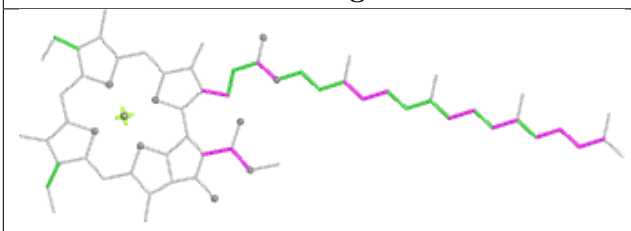
Ligand CLA bA 820



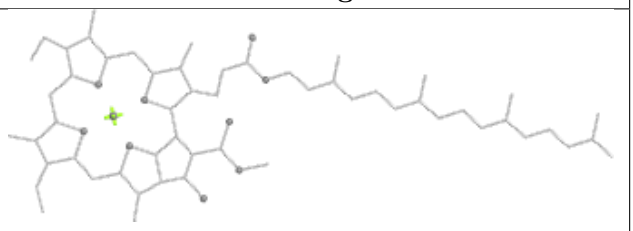
Bond lengths



Bond angles

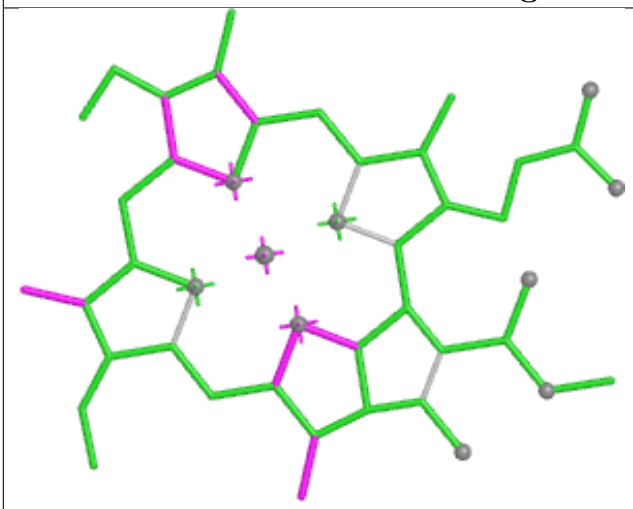


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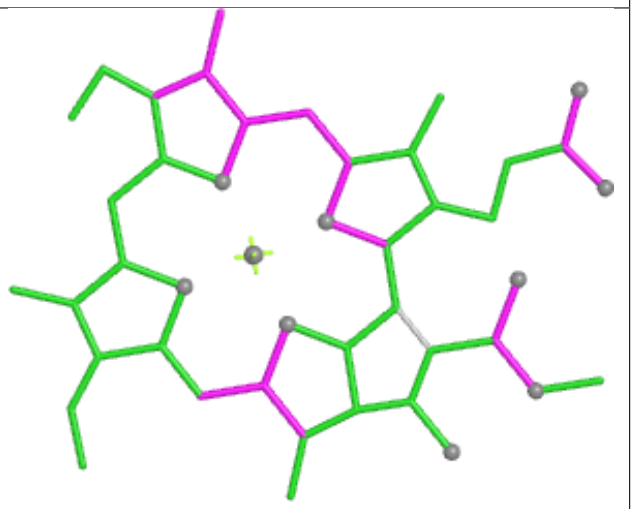


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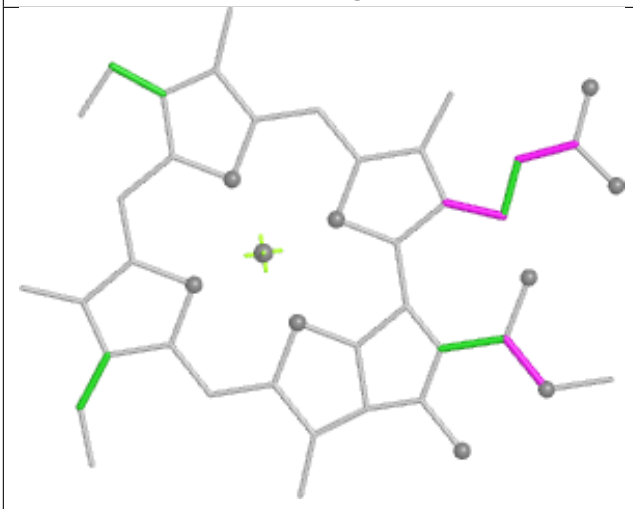
Ligand CLA c2 409



Bond lengths



Bond angles

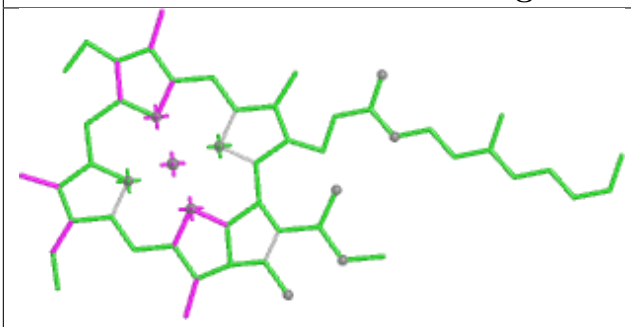


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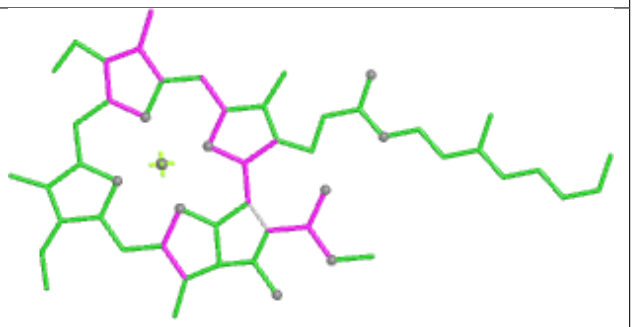


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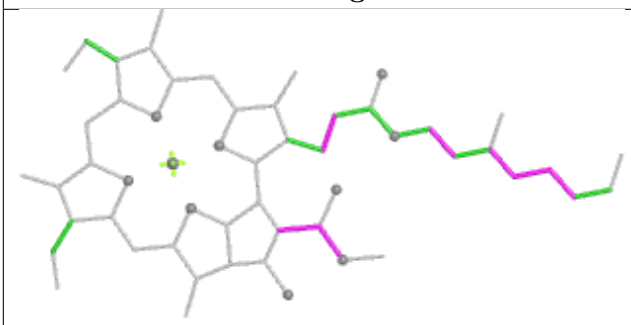
Ligand CLA aB 825



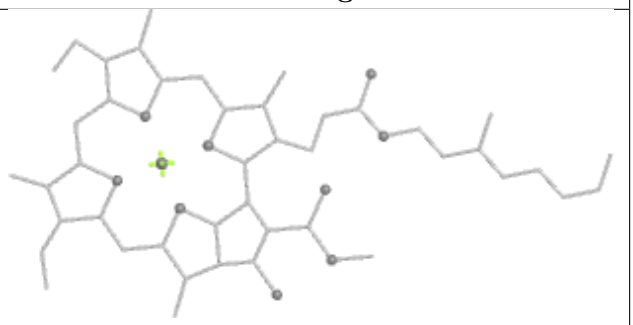
Bond lengths



Bond angles

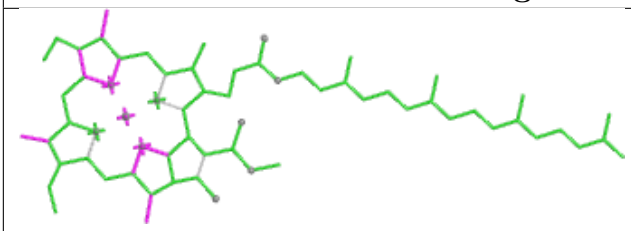


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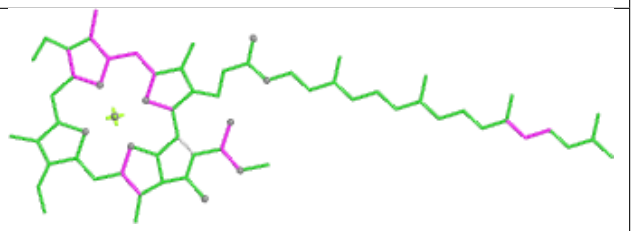


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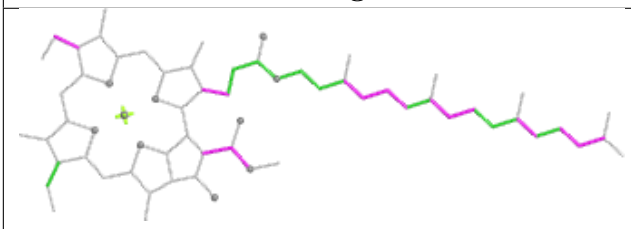
Ligand CLA bA 822



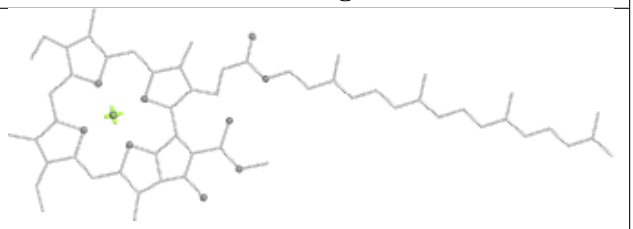
Bond lengths



Bond angles

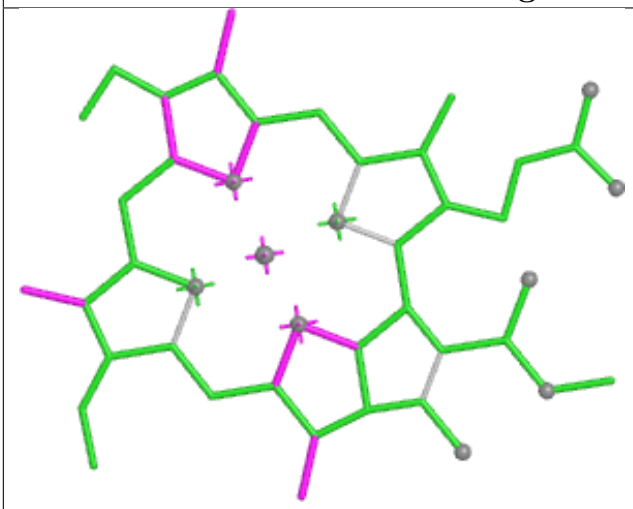


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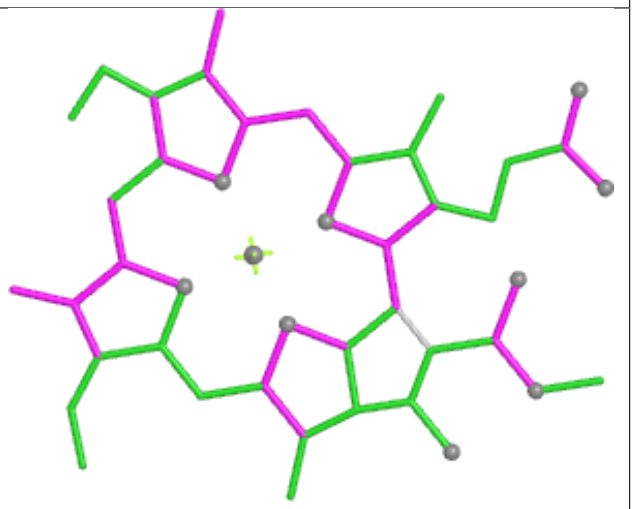


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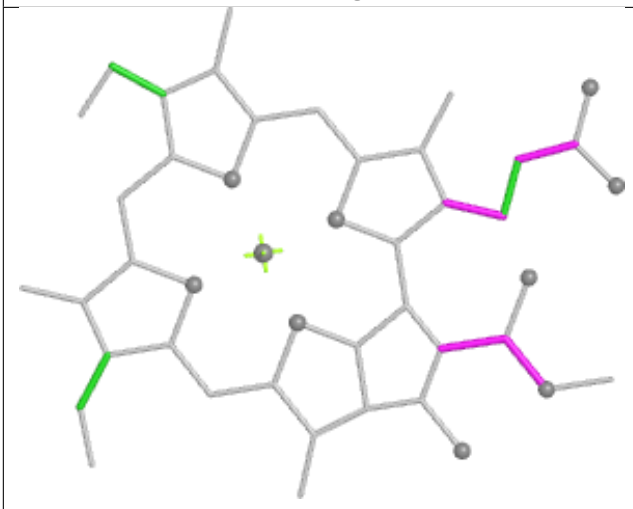
Ligand CLA b6 413



Bond lengths



Bond angles

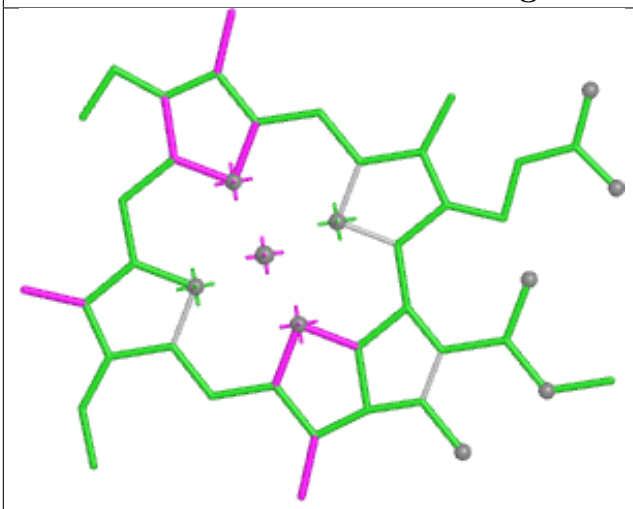


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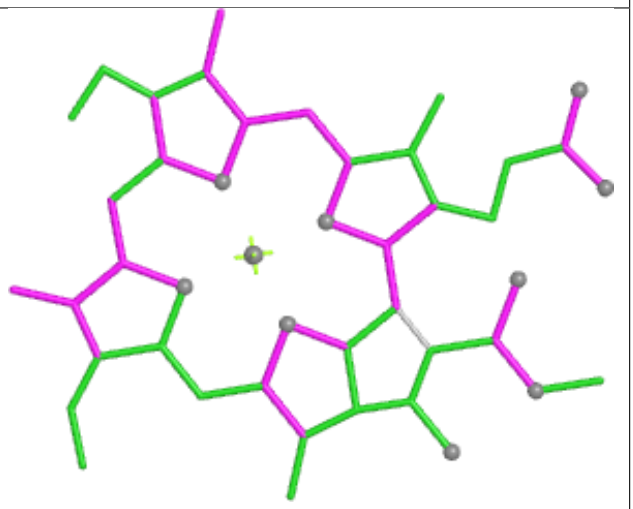


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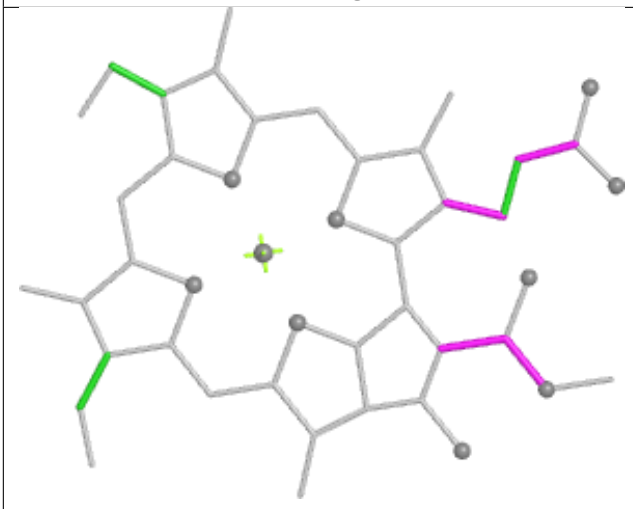
Ligand CLA a6 413



Bond lengths



Bond angles

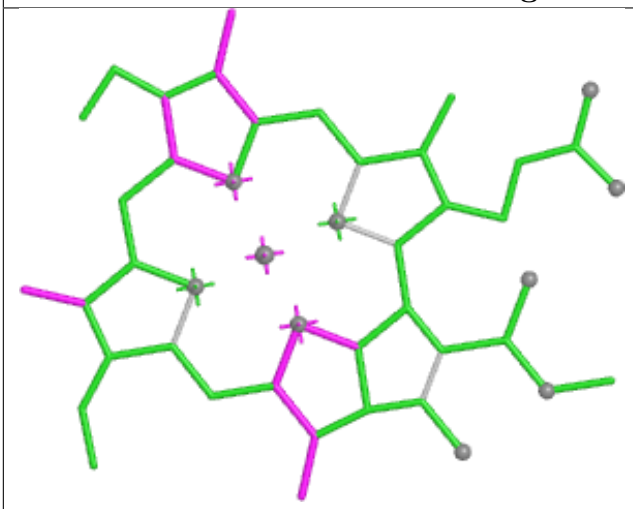


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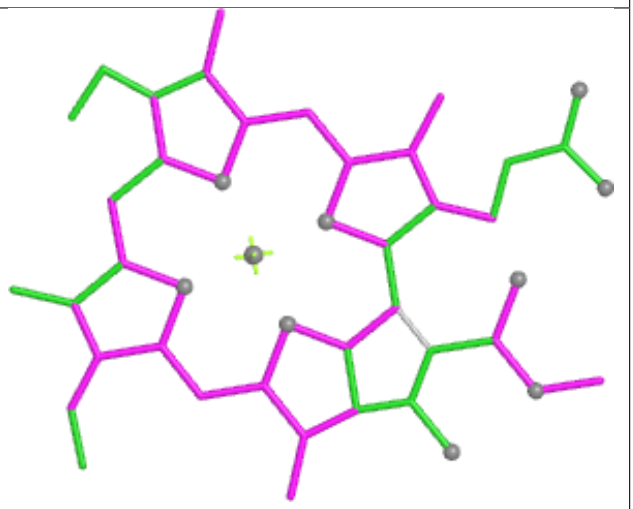


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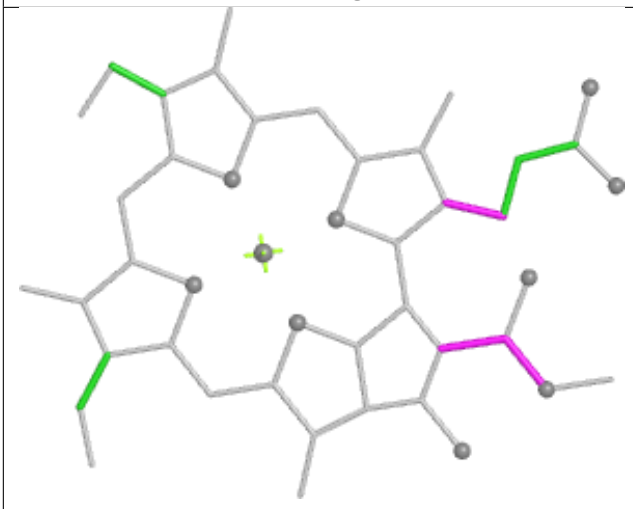
Ligand CLA c4 405



Bond lengths



Bond angles

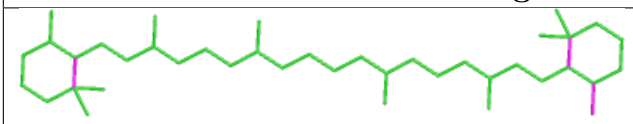


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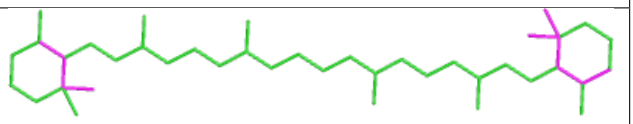


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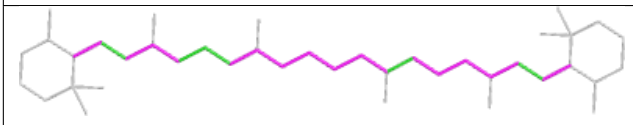
Ligand BCR aA 852



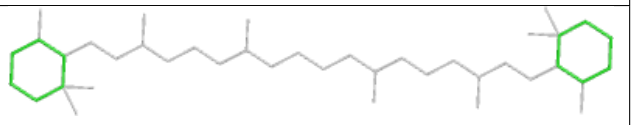
Bond lengths



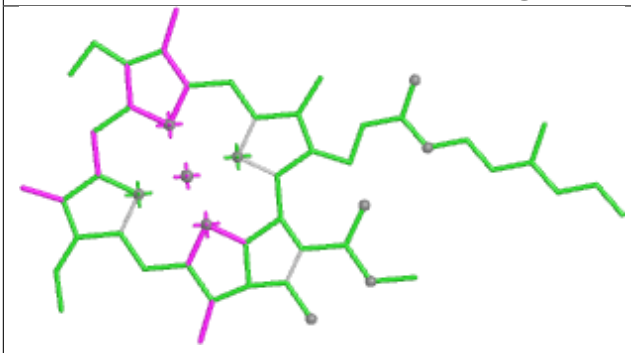
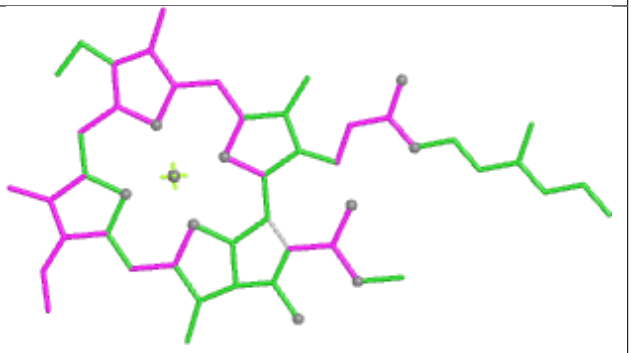
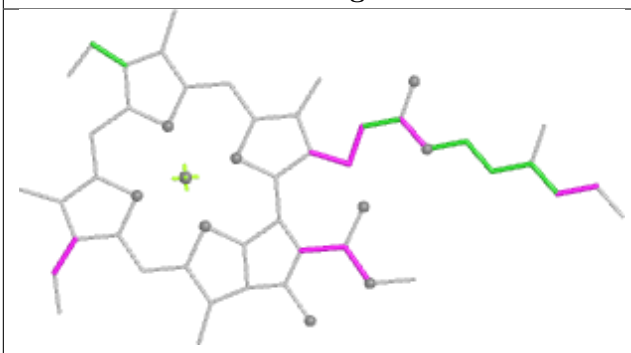
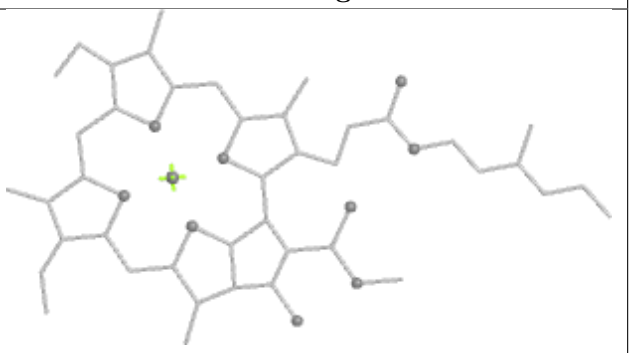
Bond angles

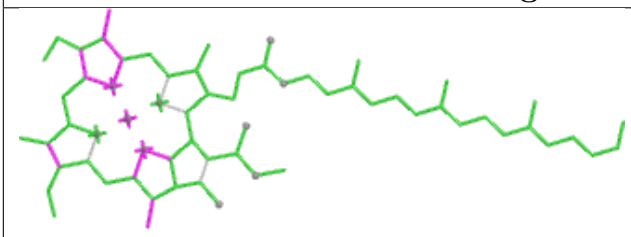
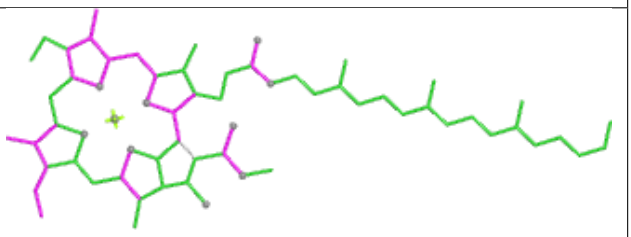
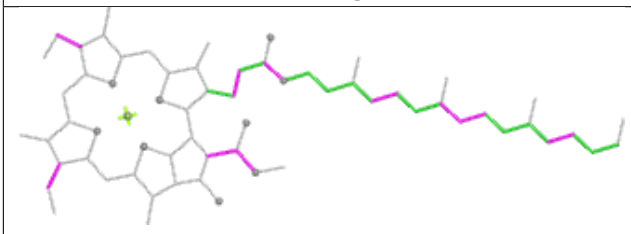
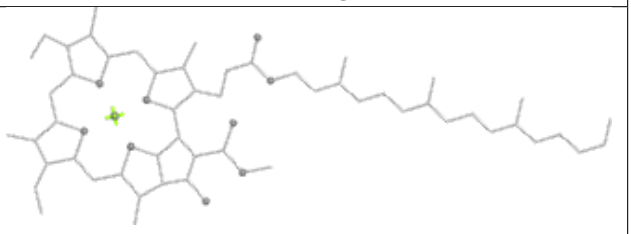


Torsions

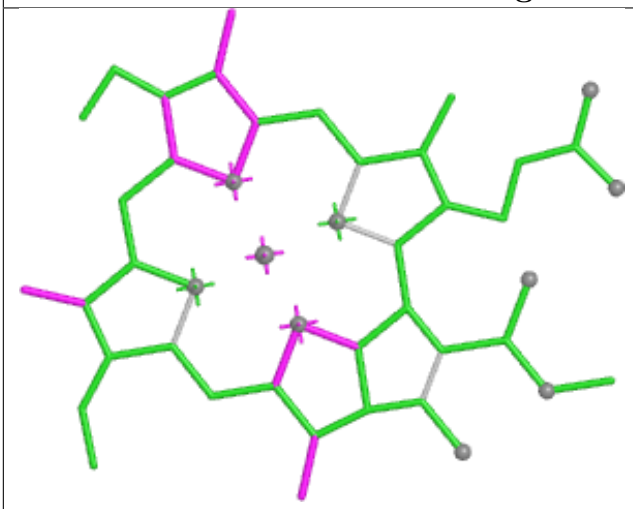


Rings

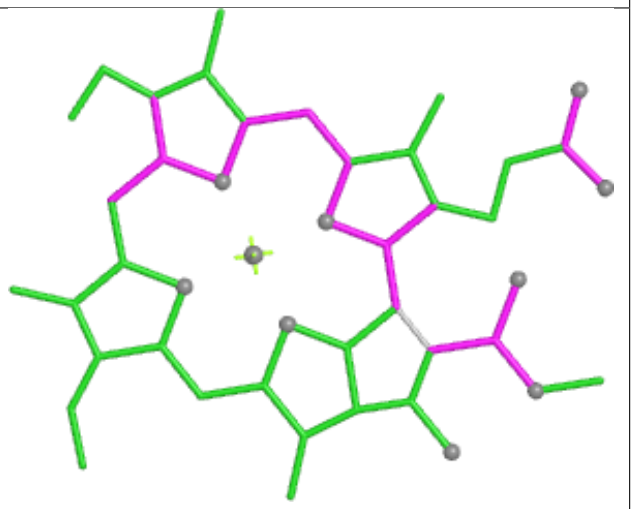
Ligand CLA cA 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c1 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

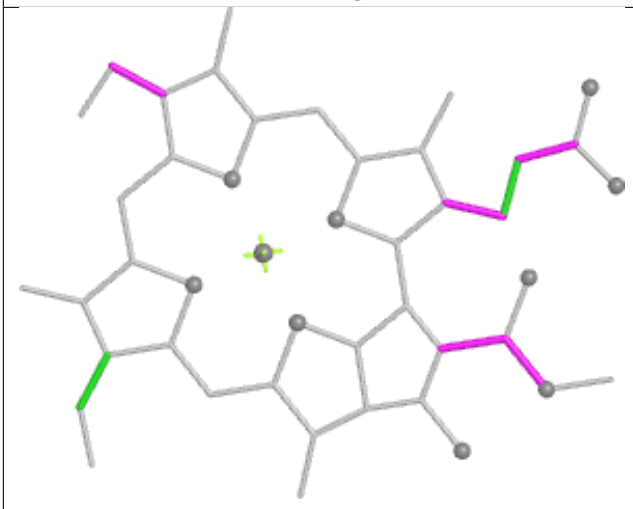
Ligand CLA cK 102



Bond lengths



Bond angles

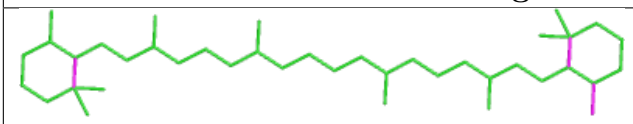


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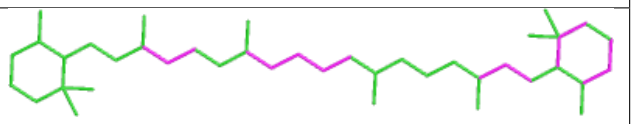


Rings

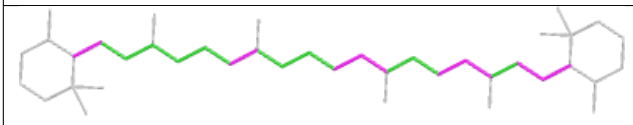
Ligand BCR bA 849



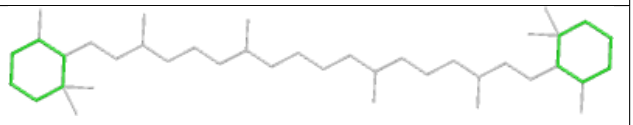
Bond lengths



Bond angles

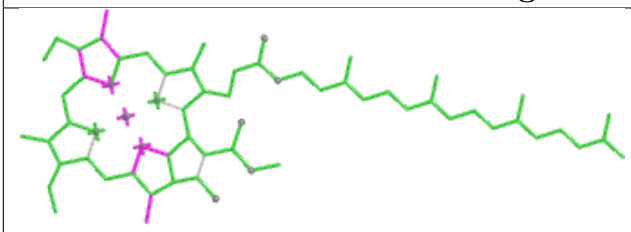


Torsions

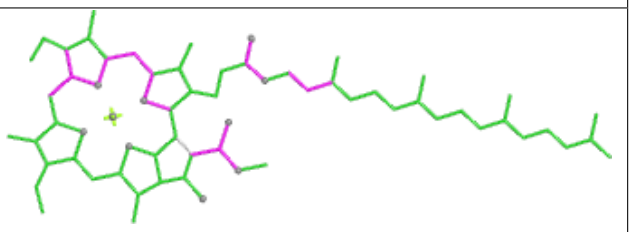


Rings

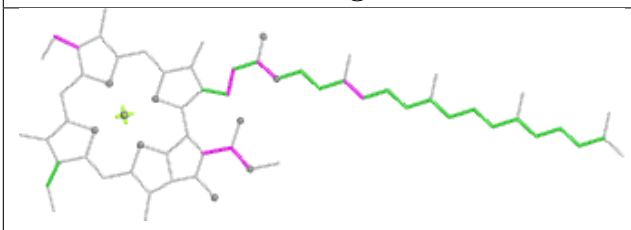
Ligand CLA b2 404



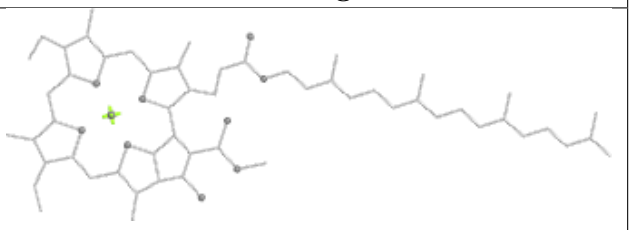
Bond lengths



Bond angles



Torsions

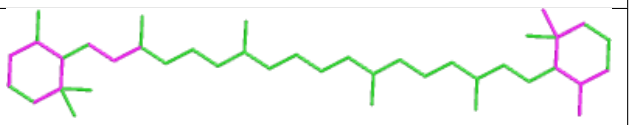


Rings

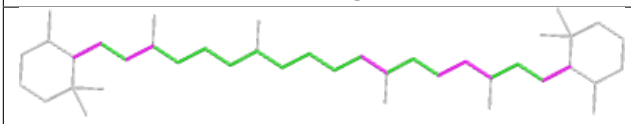
Ligand BCR a4 418



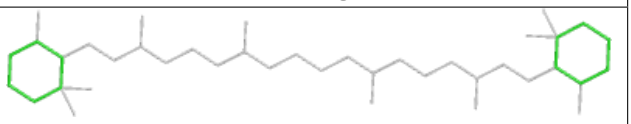
Bond lengths



Bond angles

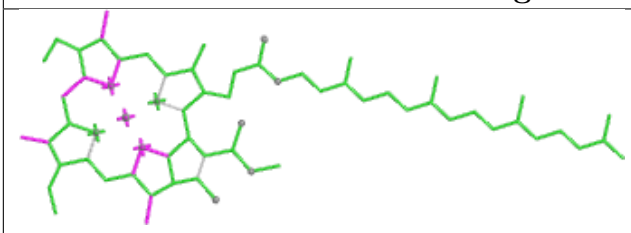


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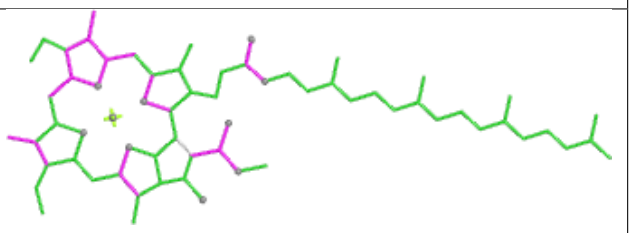


Rings

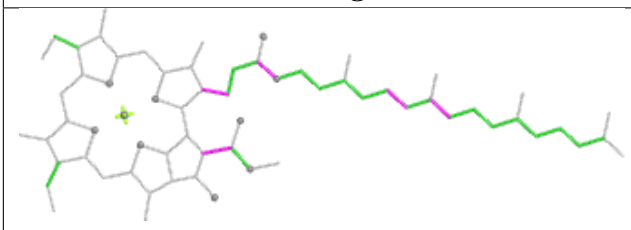
Ligand CLA bA 831



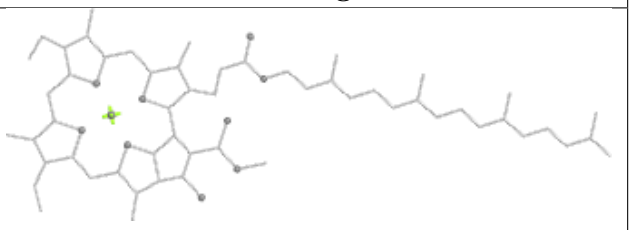
Bond lengths



Bond angles

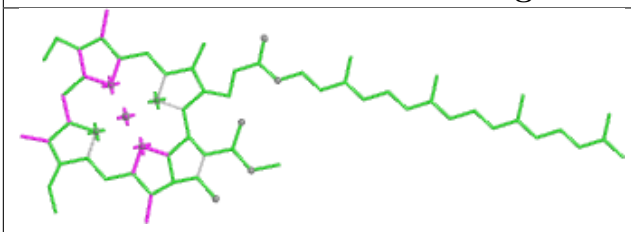


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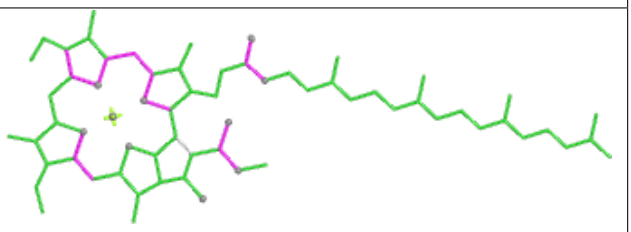


Rings

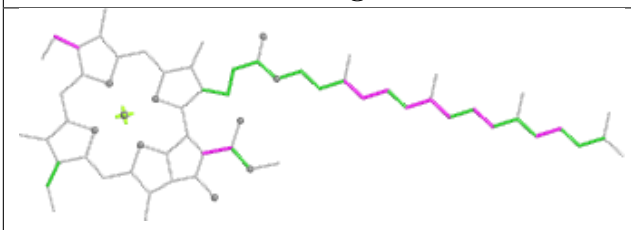
Ligand CLA aA 828



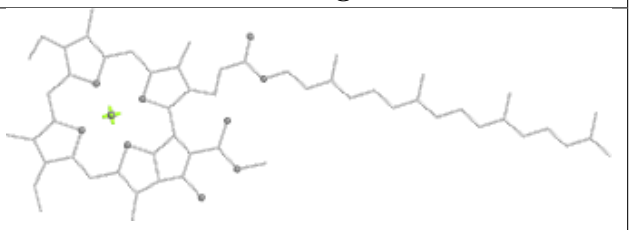
Bond lengths



Bond angles

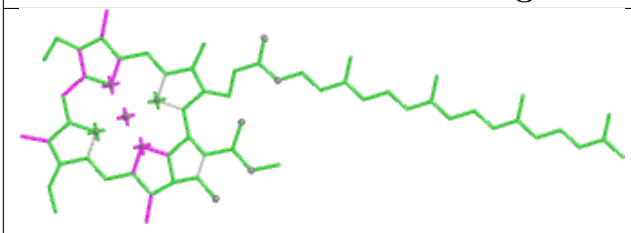


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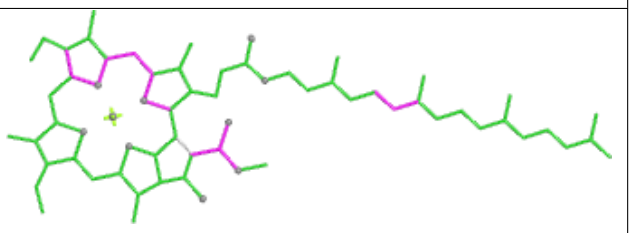


Rings

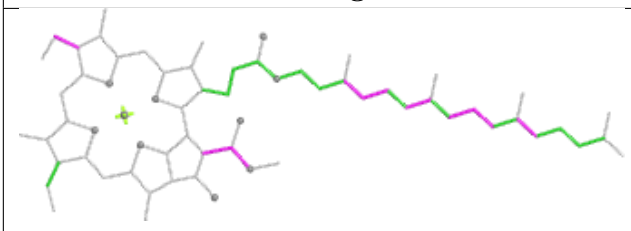
Ligand CLA cA 839



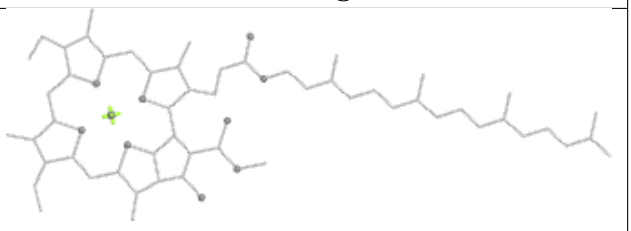
Bond lengths



Bond angles

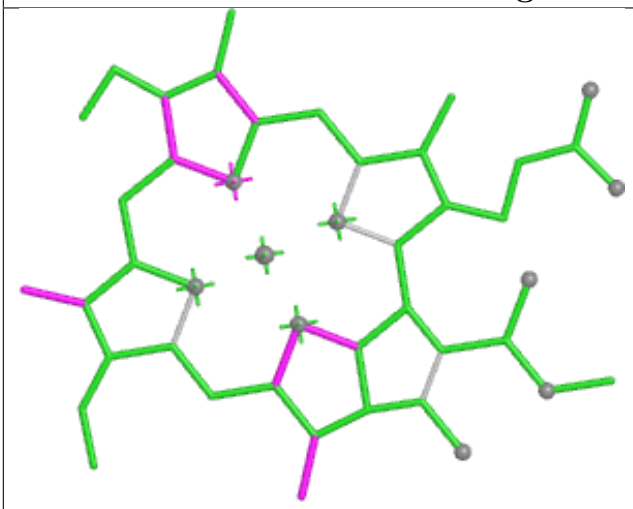


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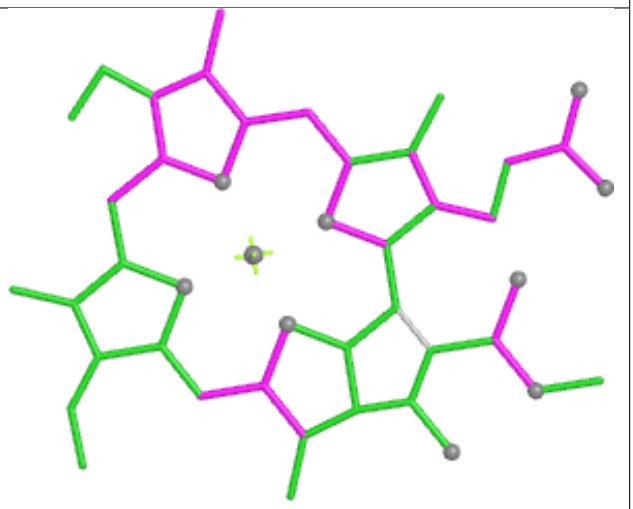


Rings

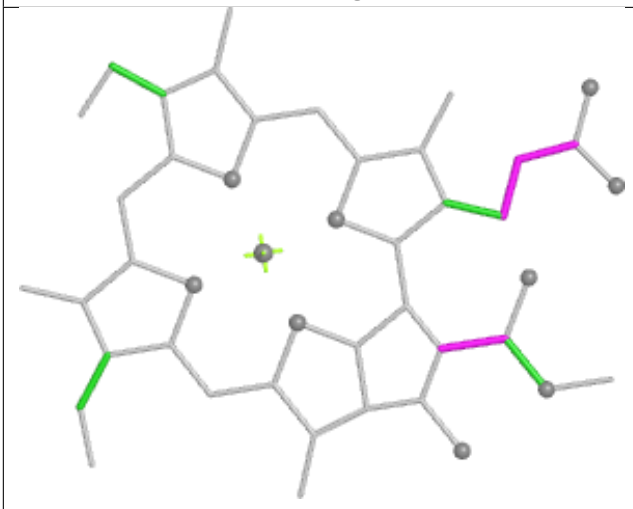
Ligand CLA cB 824



Bond lengths



Bond angles

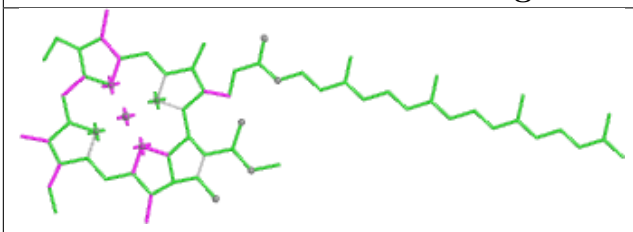


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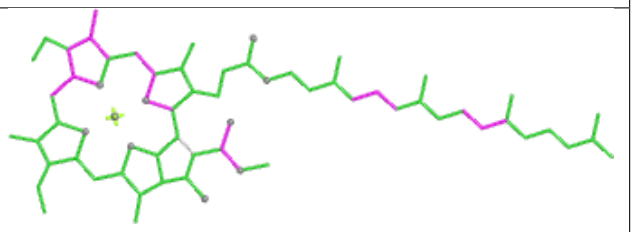


Rings

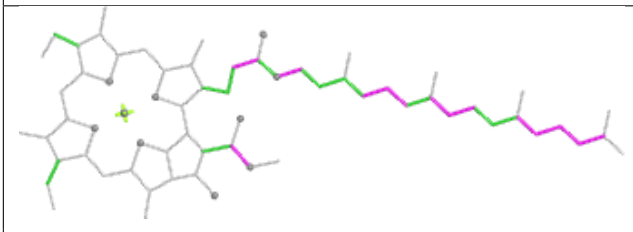
Ligand CLA bB 807



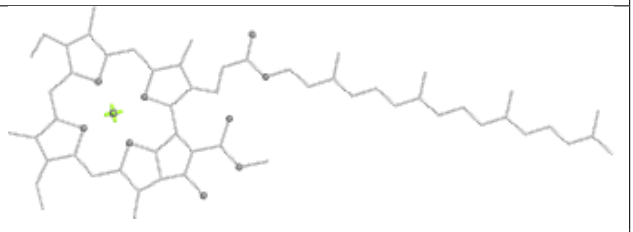
Bond lengths



Bond angles

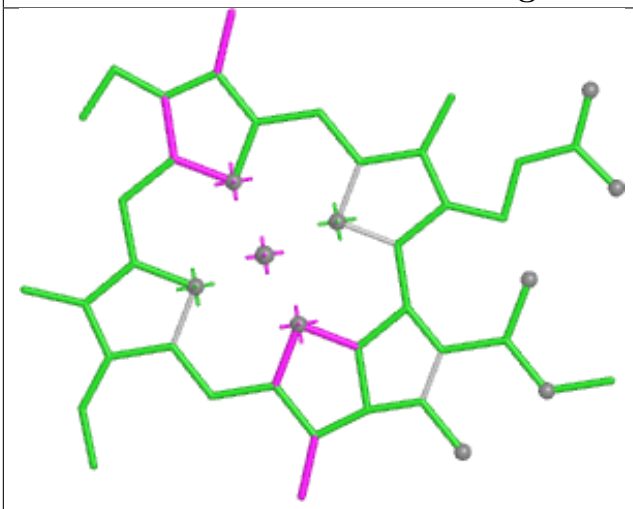


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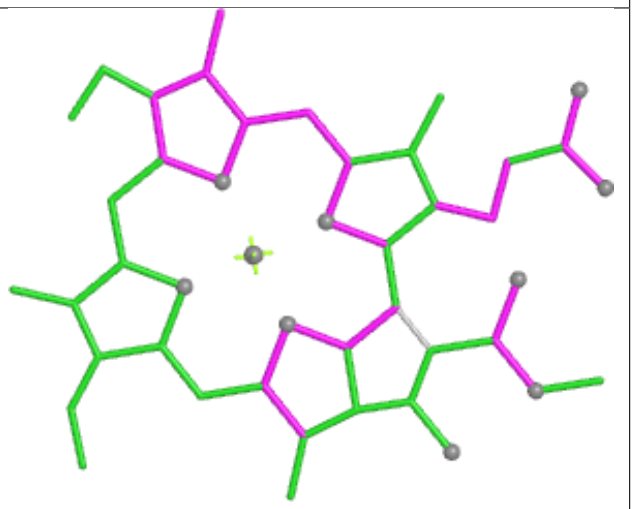


Rings

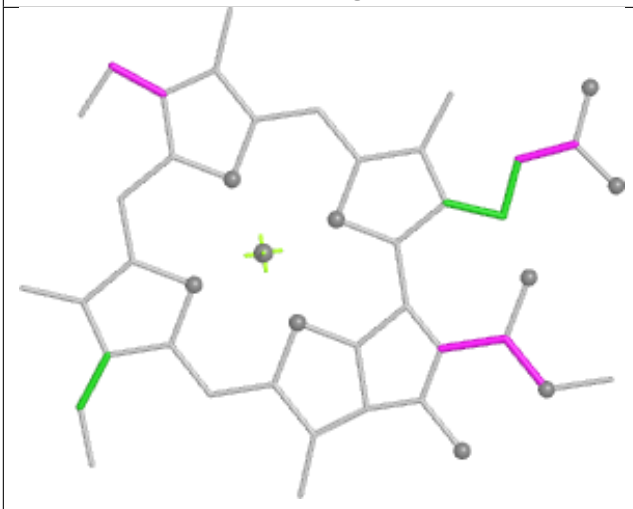
Ligand CLA b1 415



Bond lengths



Bond angles

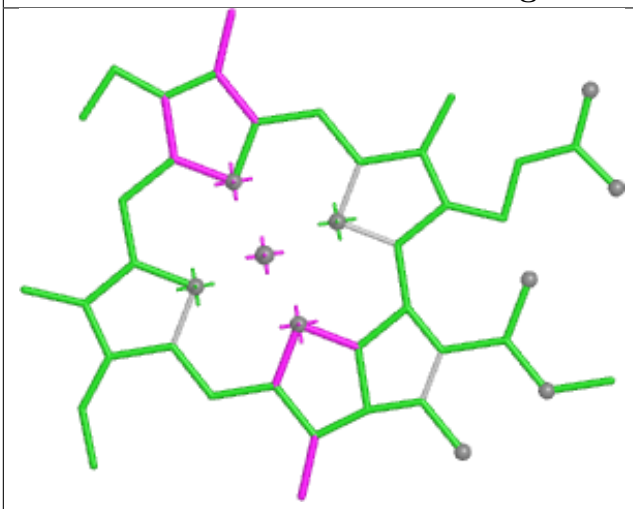


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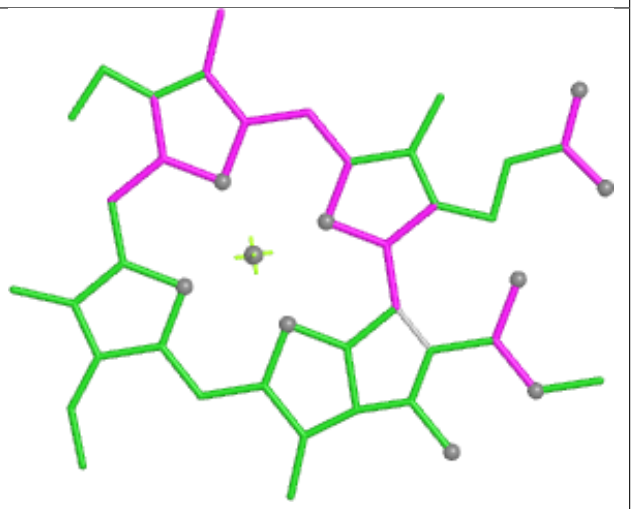


Rings

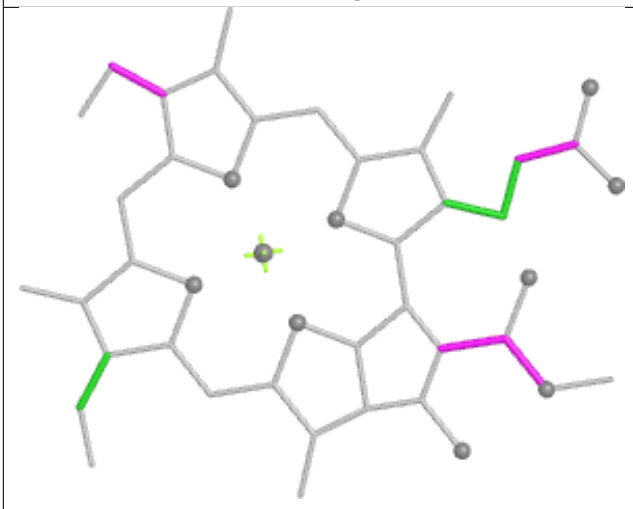
Ligand CLA a5 407



Bond lengths



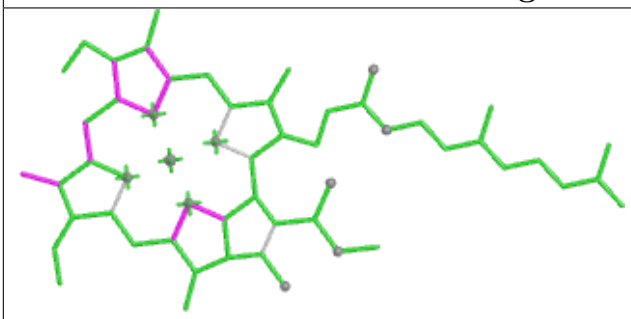
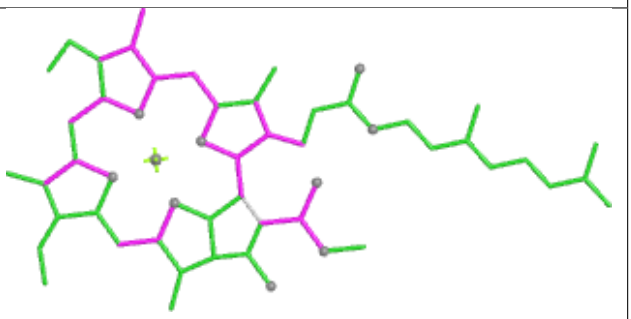
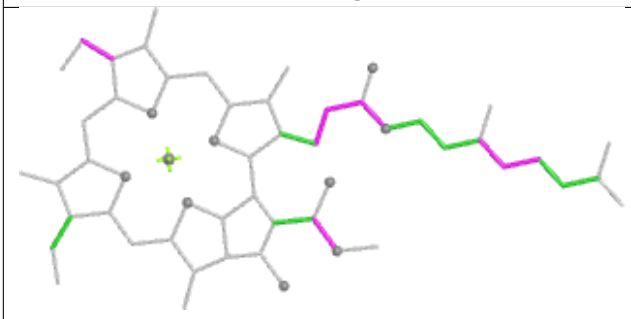
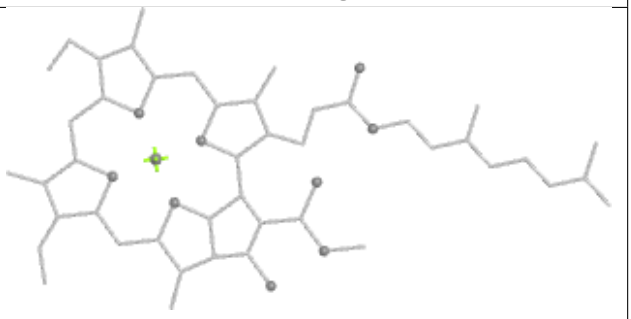
Bond angles

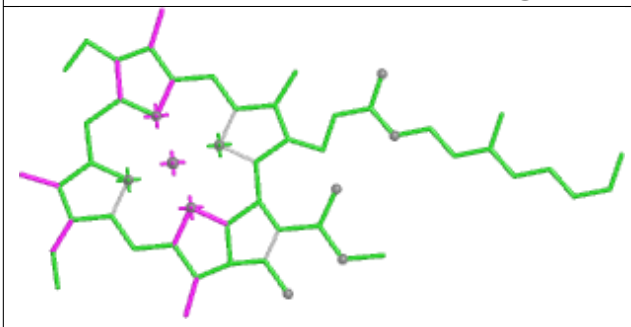
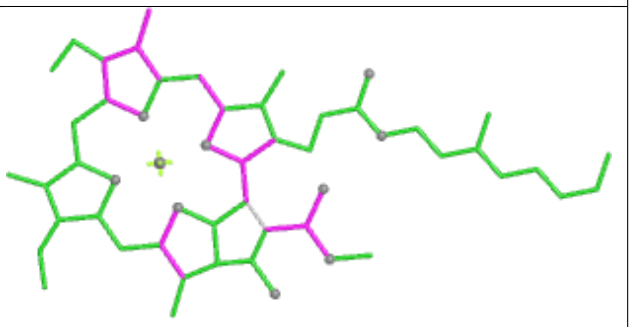
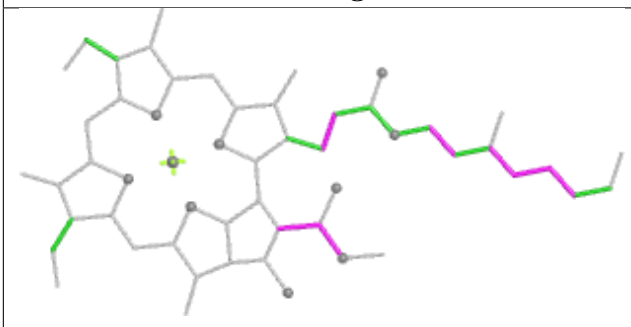
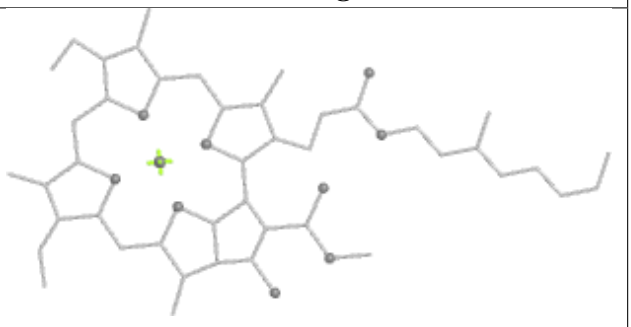


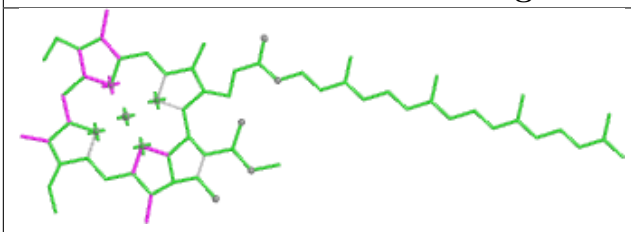
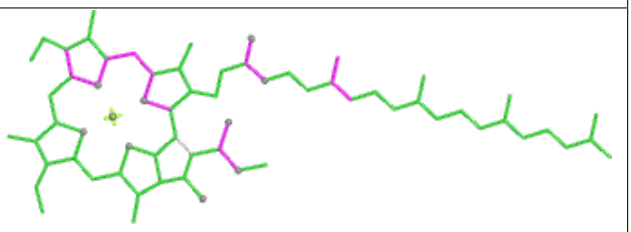
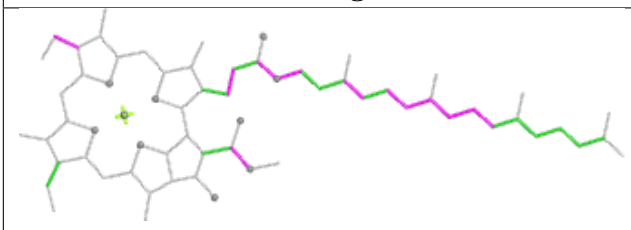
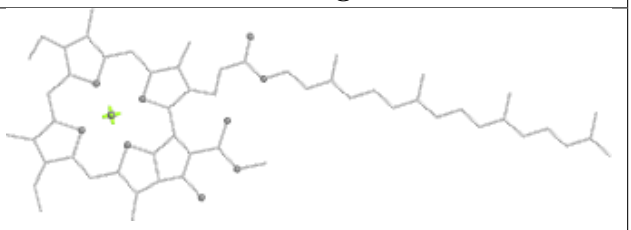
Torsions

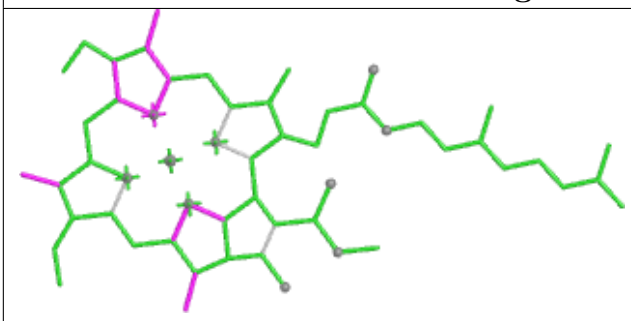
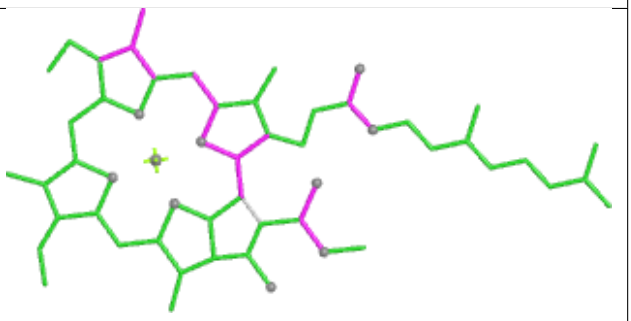
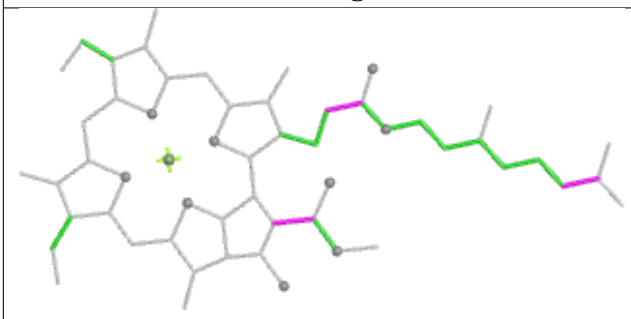
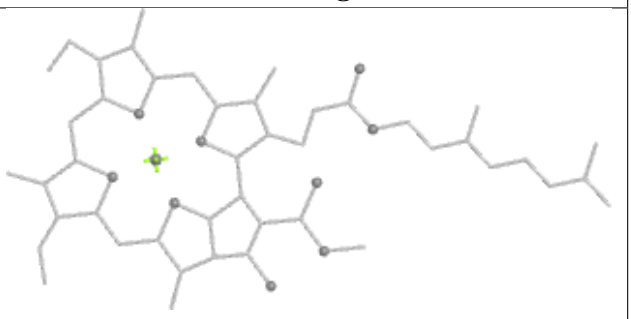


Rings

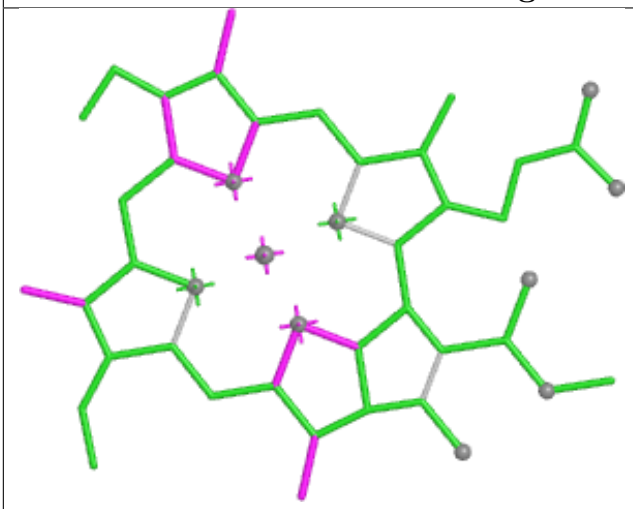
Ligand CLA b6 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cB 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

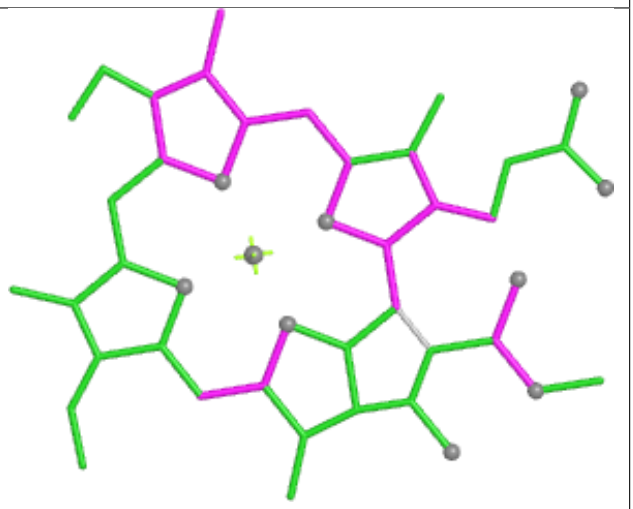
Ligand CLA aA 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bB 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

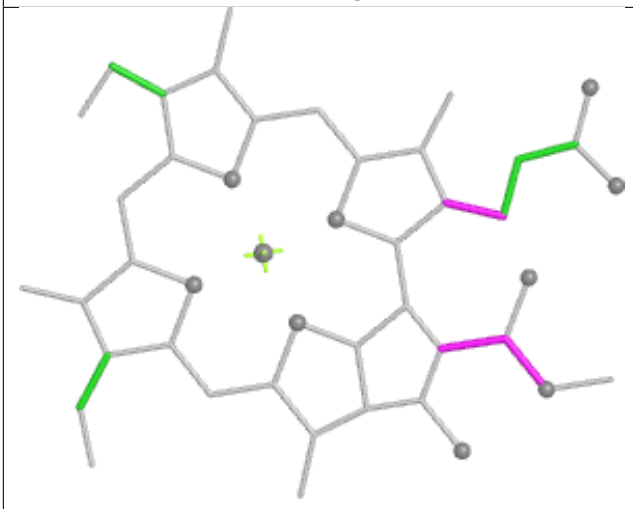
Ligand CLA b3 411



Bond lengths



Bond angles

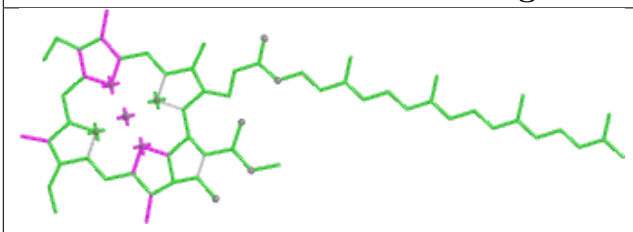


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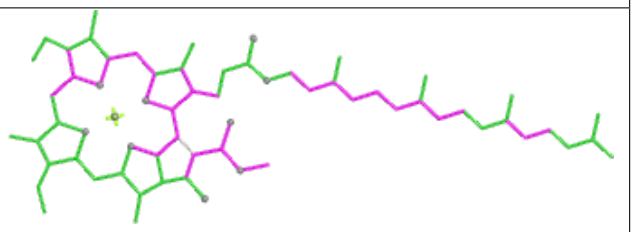


Rings

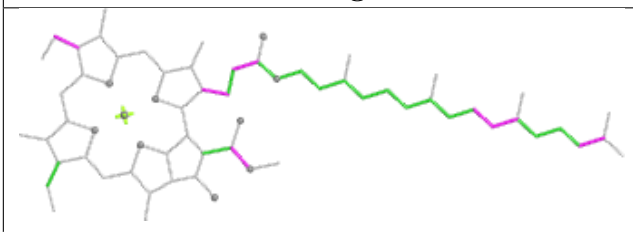
Ligand CLA b2 422



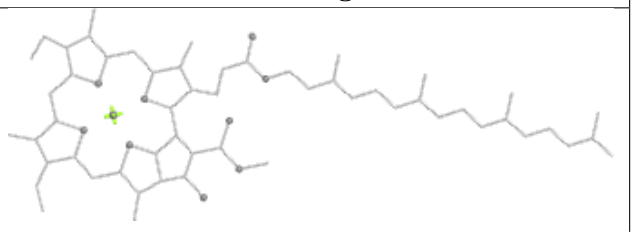
Bond lengths



Bond angles

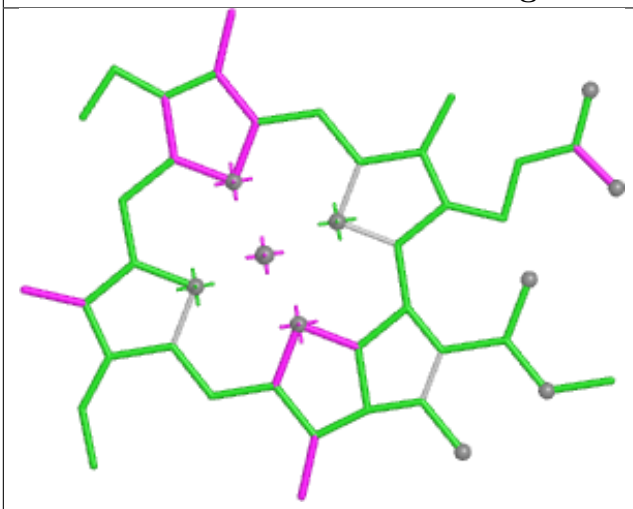


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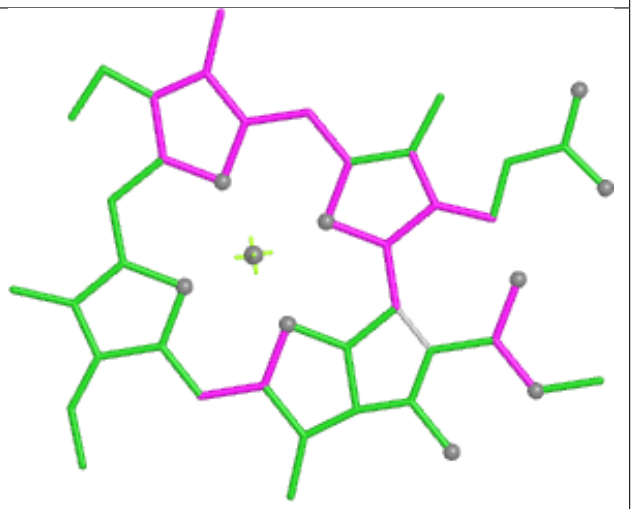


Rings

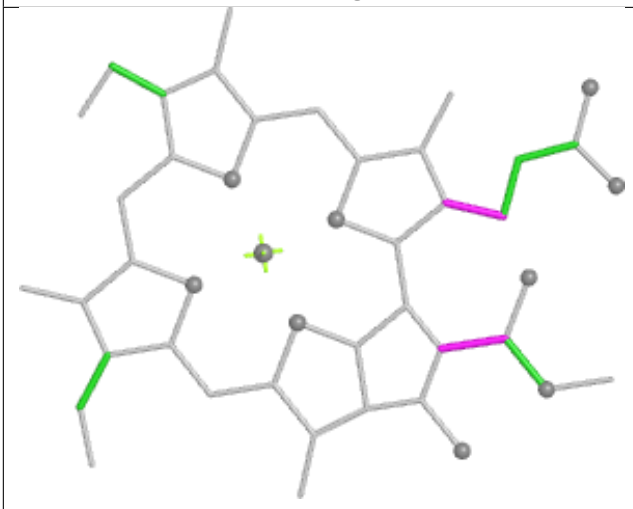
Ligand CLA a2 412



Bond lengths



Bond angles

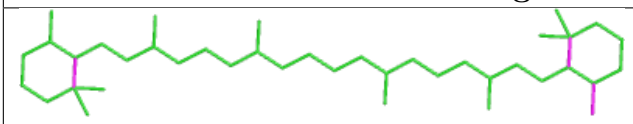


Torsions

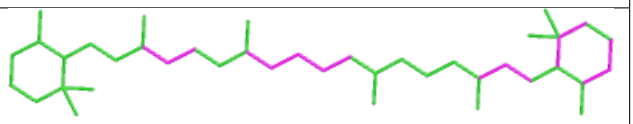


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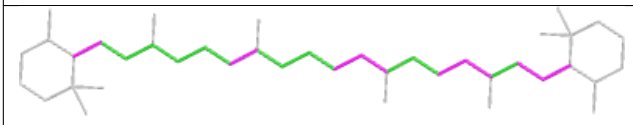
Ligand BCR aA 848



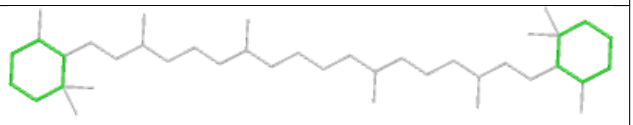
Bond lengths



Bond angles

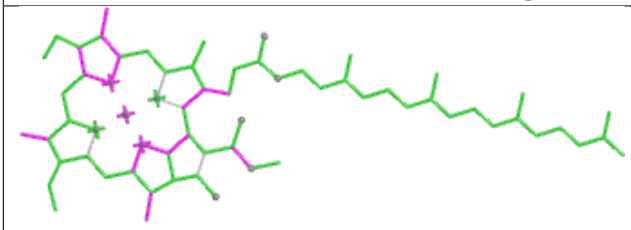


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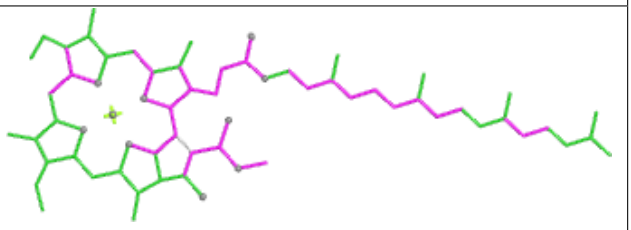


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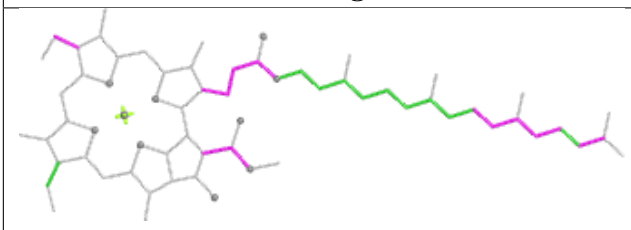
Ligand CLA a6 422



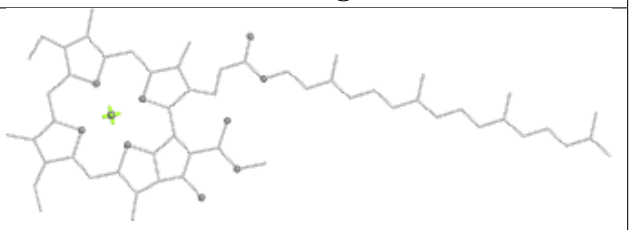
Bond lengths



Bond angles

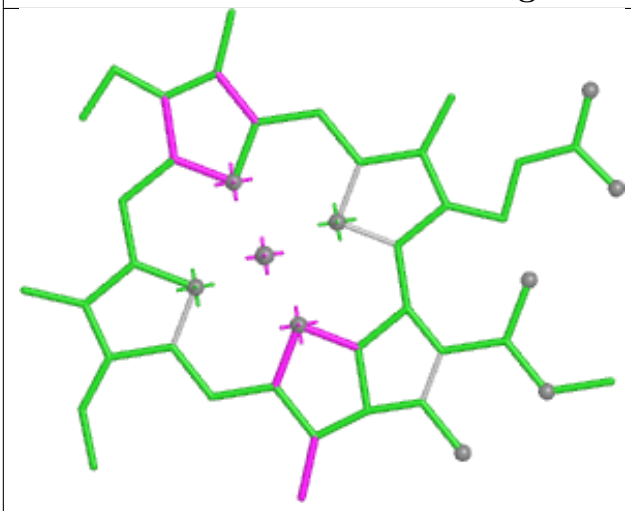


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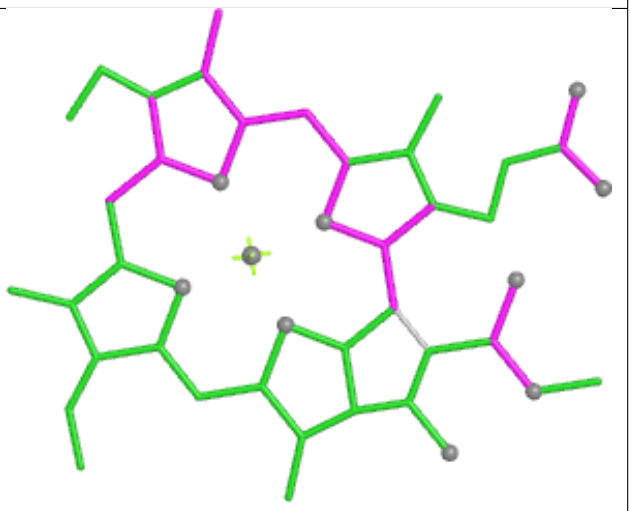


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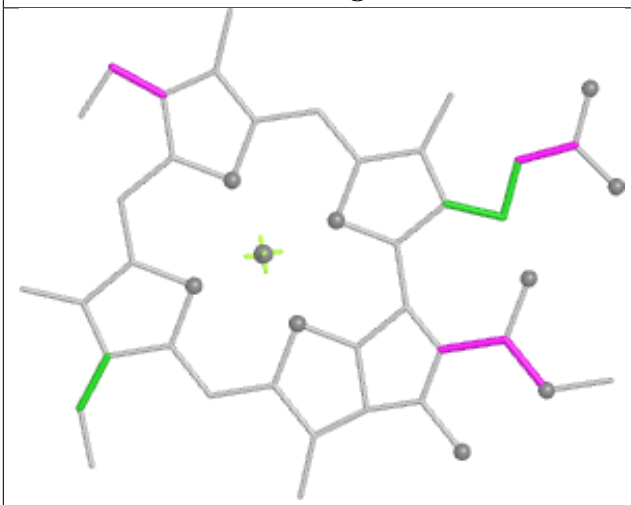
Ligand CLA b5 407



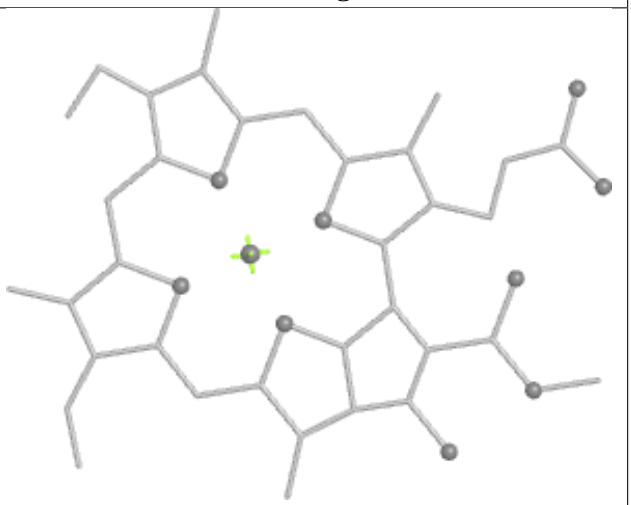
Bond lengths



Bond angles

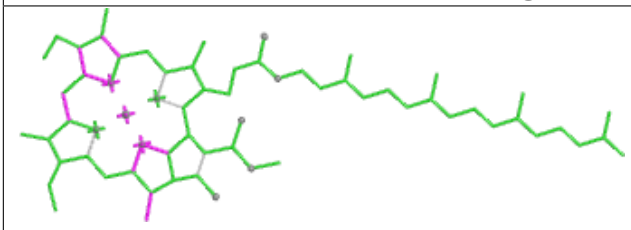


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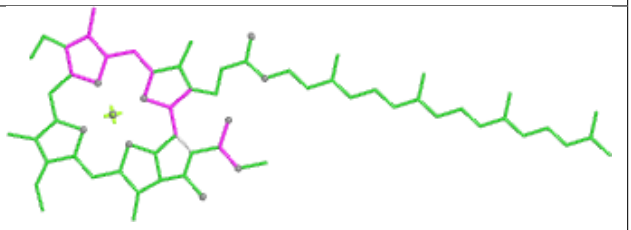


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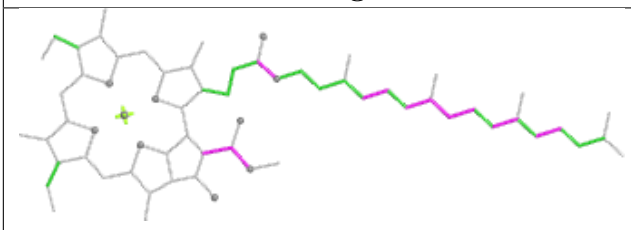
Ligand CLA a2 403



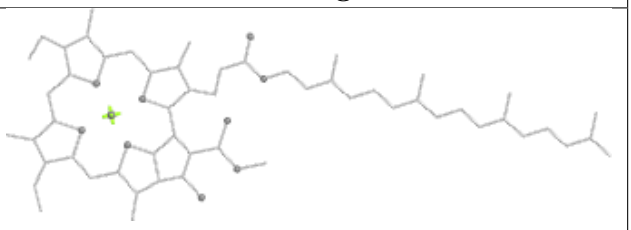
Bond lengths



Bond angles

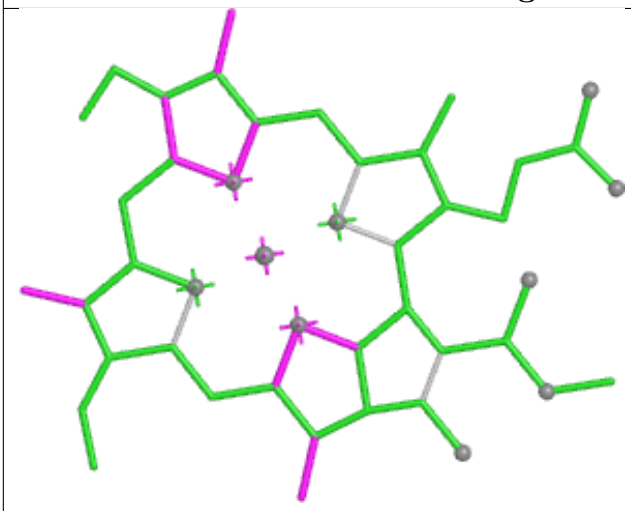


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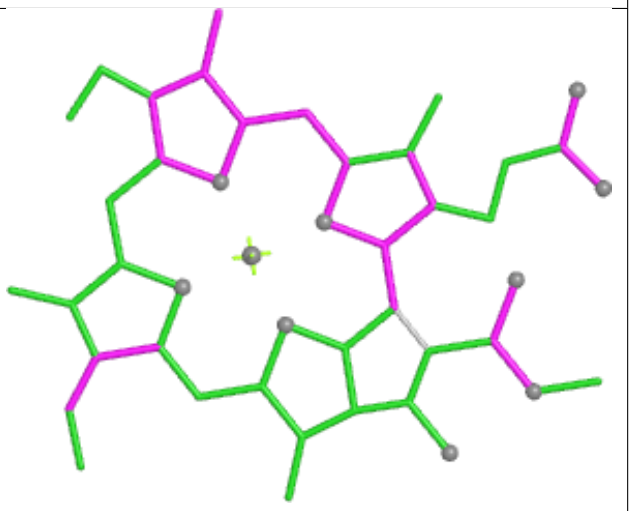


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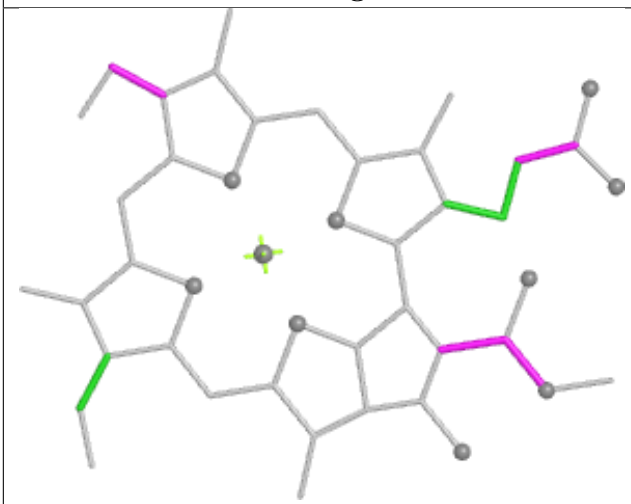
Ligand CLA cF 203



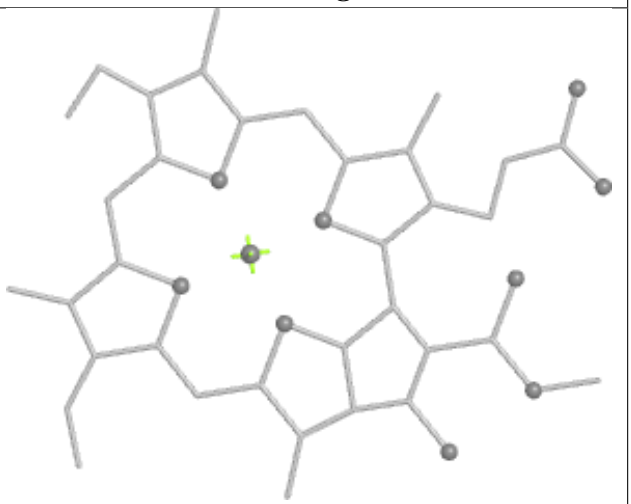
Bond lengths



Bond angles

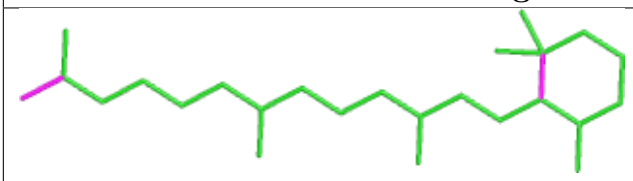


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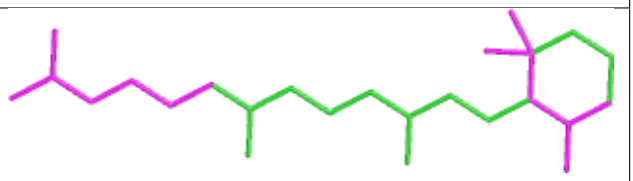


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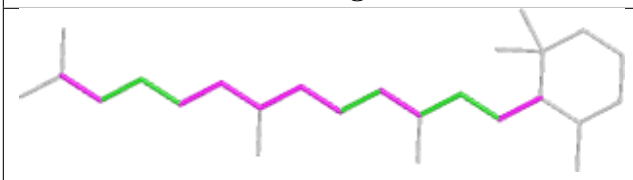
Ligand BCR bB 847



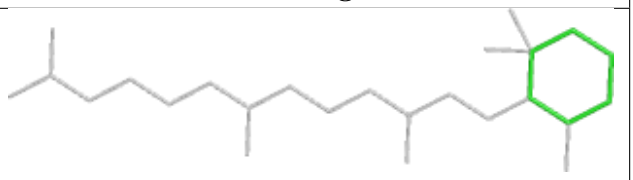
Bond lengths



Bond angles

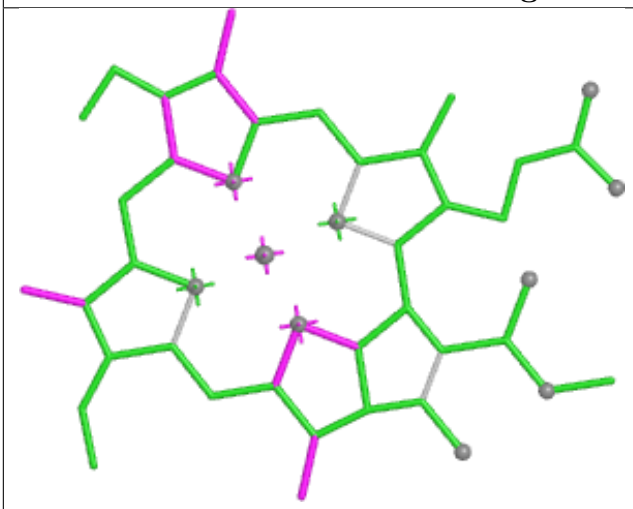


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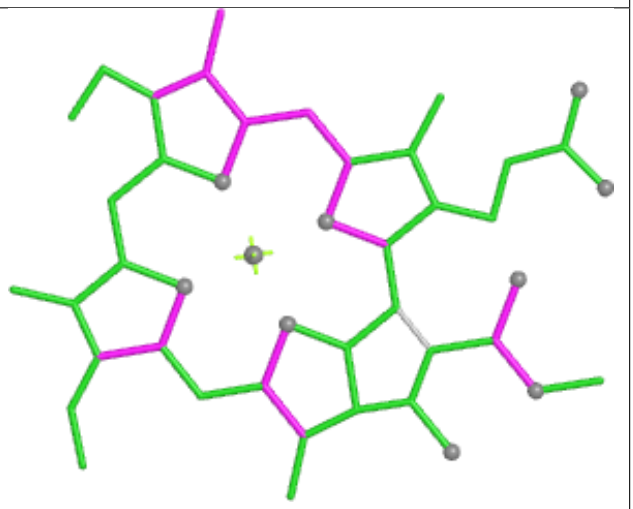


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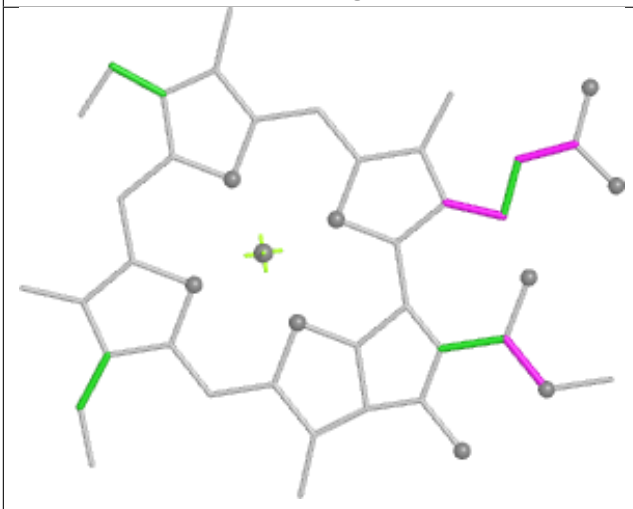
Ligand CLA c1 408



Bond lengths



Bond angles

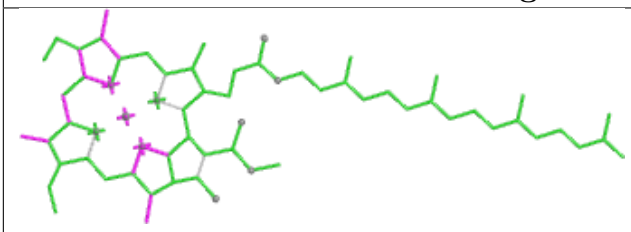


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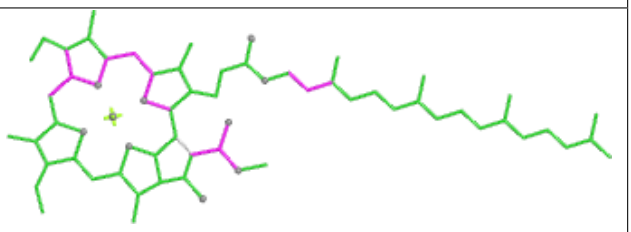


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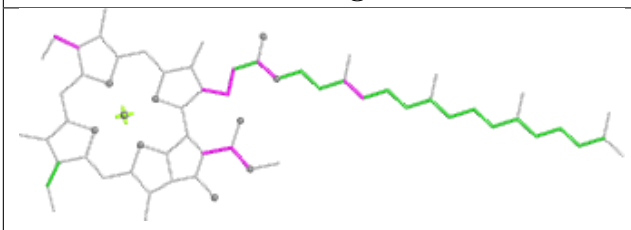
Ligand CLA a4 404



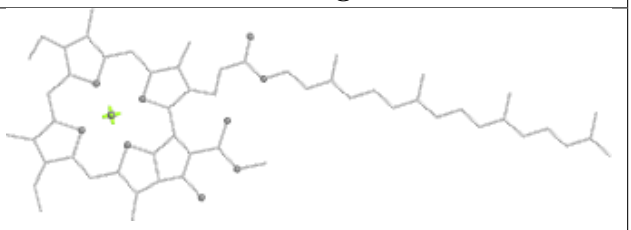
Bond lengths



Bond angles

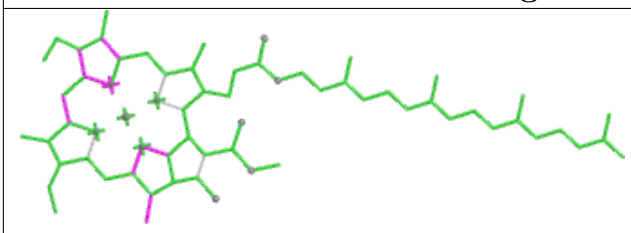


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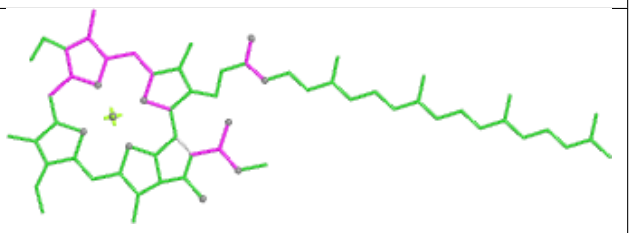


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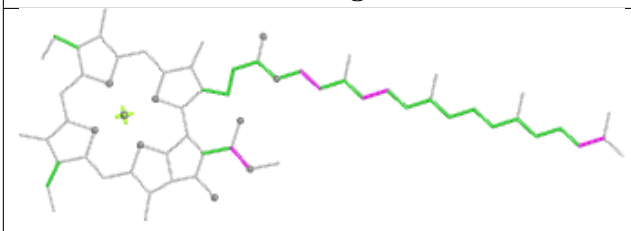
Ligand CLA c4 409



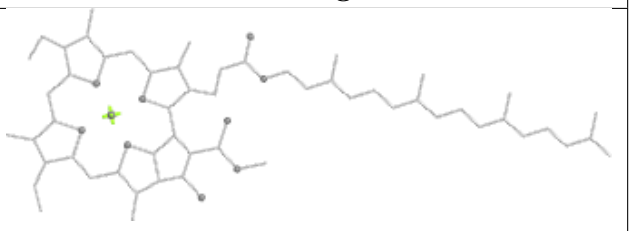
Bond lengths



Bond angles

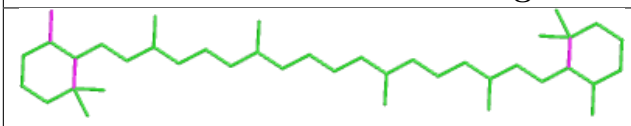


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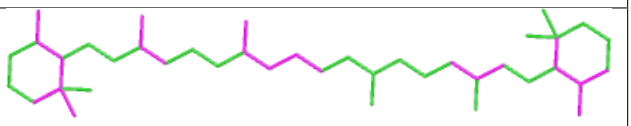


Rings

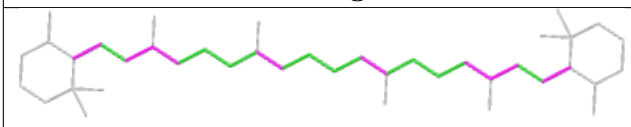
Ligand BCR bF 202



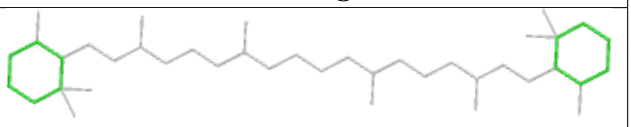
Bond lengths



Bond angles

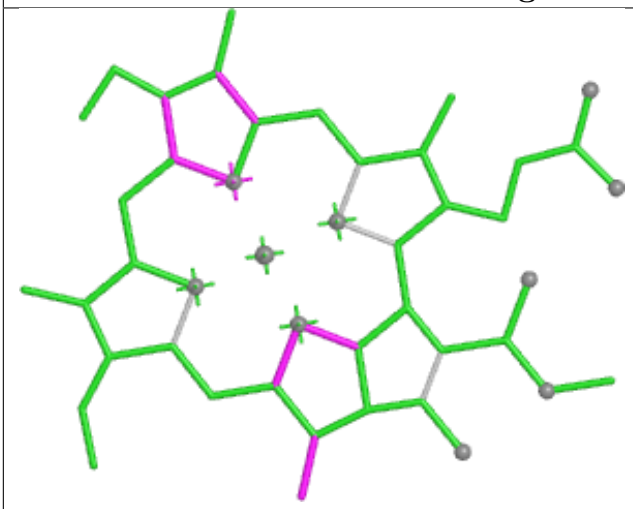


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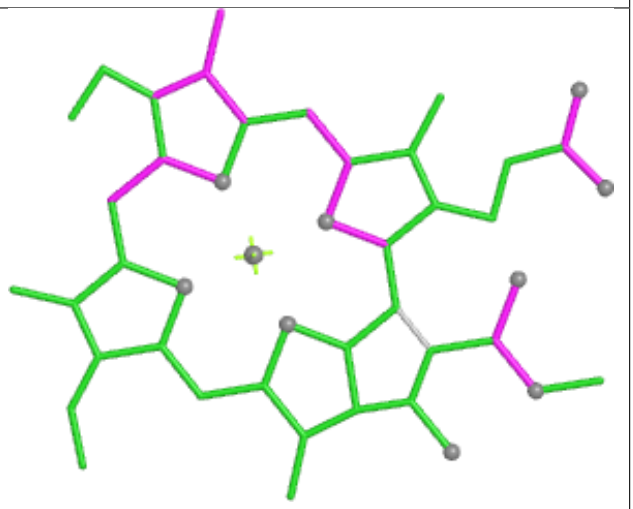


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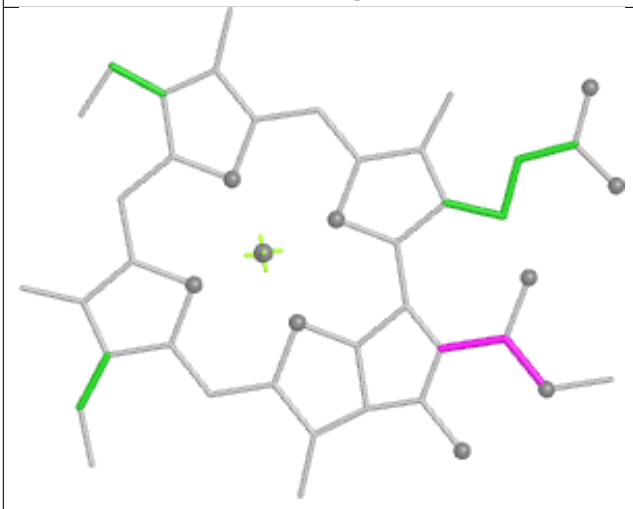
Ligand CLA b2 407



Bond lengths



Bond angles

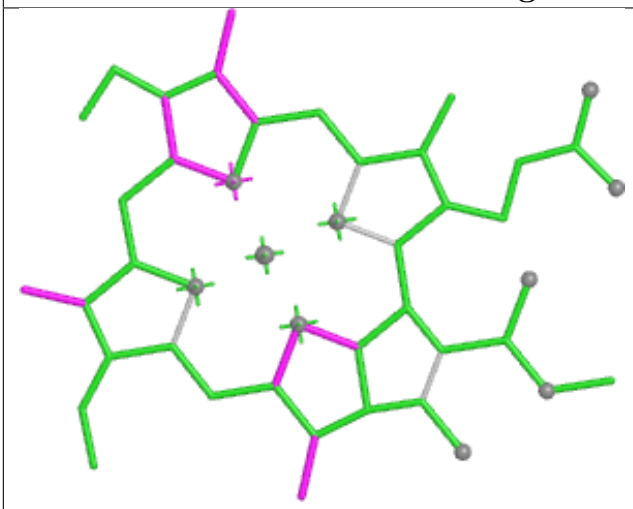


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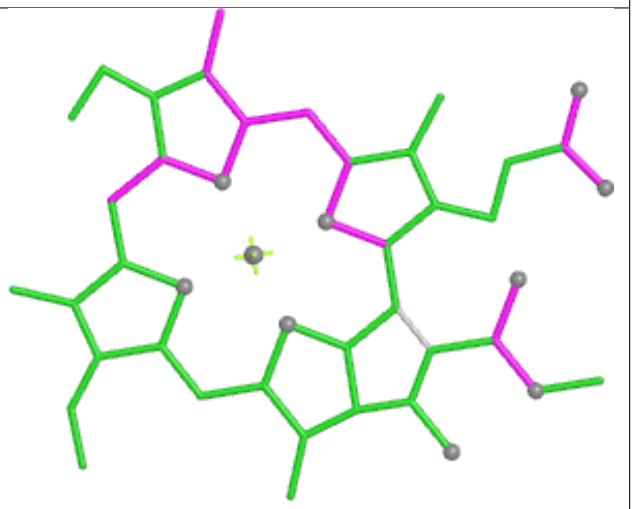


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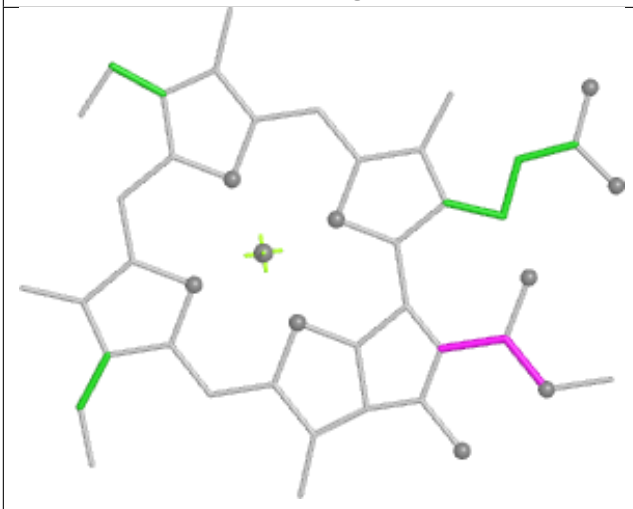
Ligand CLA b4 406



Bond lengths



Bond angles

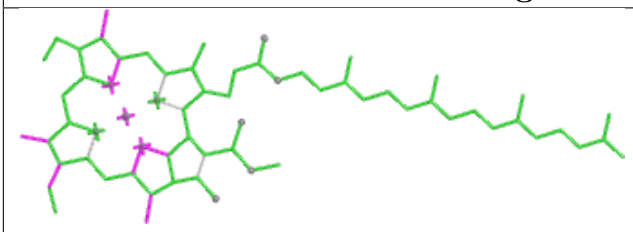


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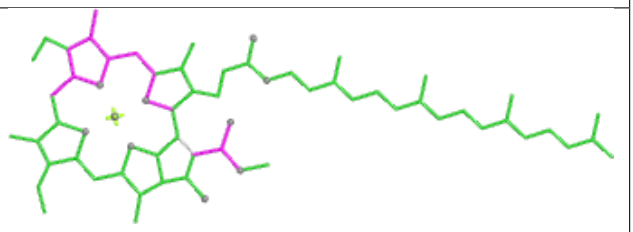


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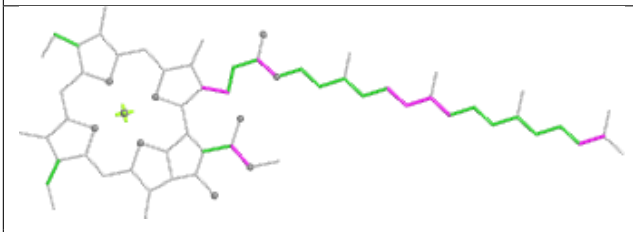
Ligand CLA cA 833



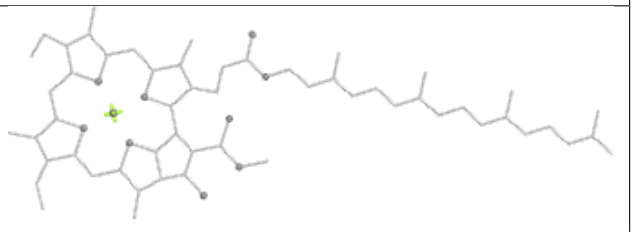
Bond lengths



Bond angles

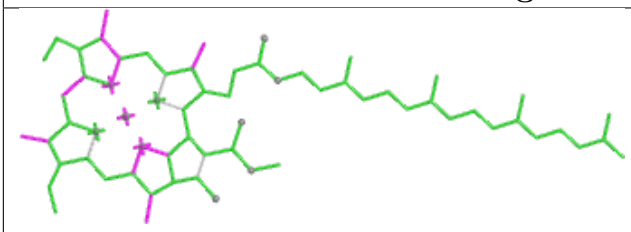


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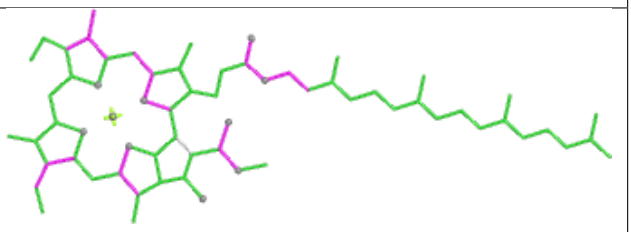


Rings

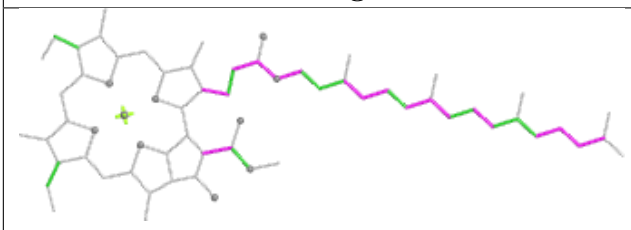
Ligand CLA cB 806



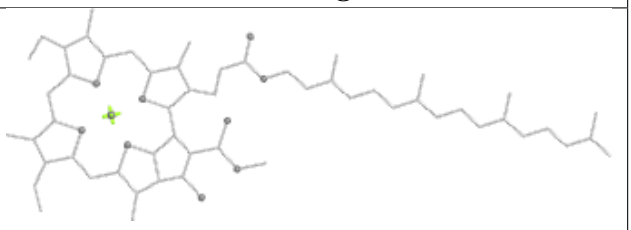
Bond lengths



Bond angles

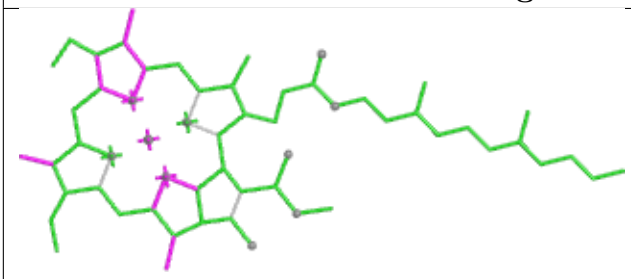


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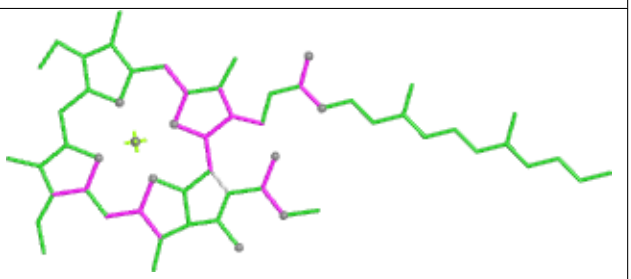


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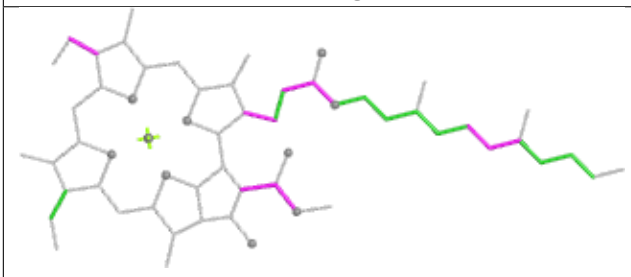
Ligand CLA cB 834



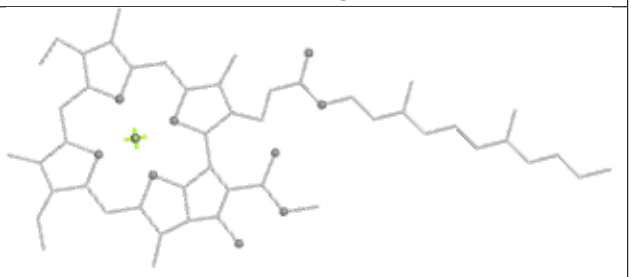
Bond lengths



Bond angles

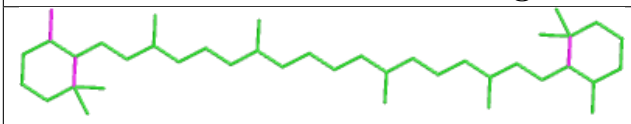


Torsions

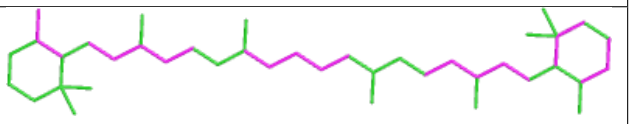


Rings

Ligand BCR cK 101



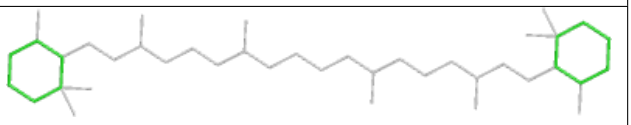
Bond lengths



Bond angles

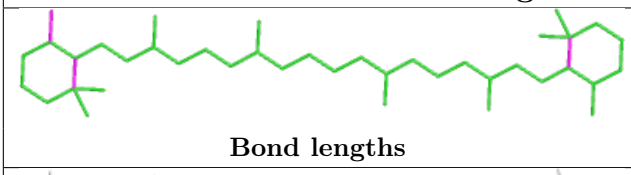


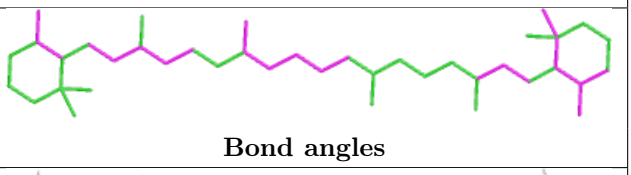
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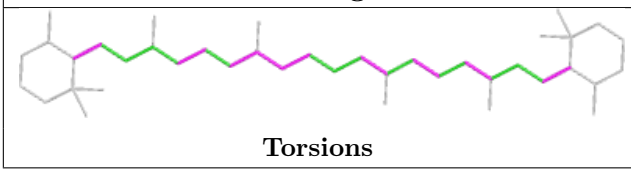


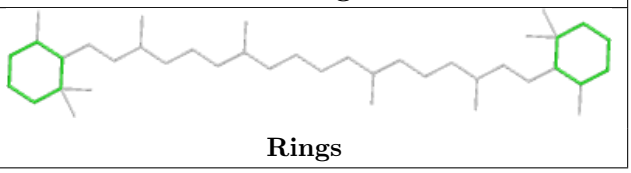
Rings

Ligand BCR bJ 103

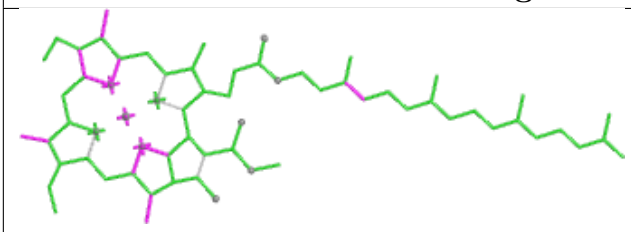

Bond lengths

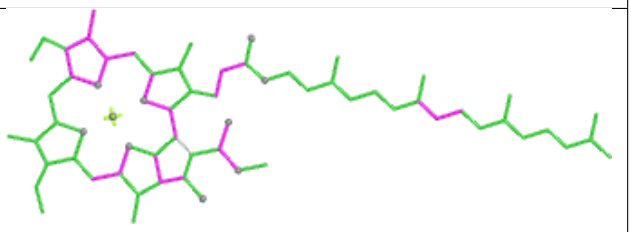

Bond angles

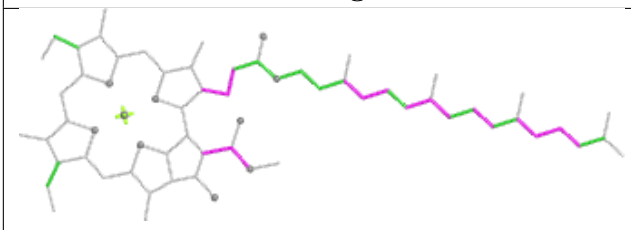

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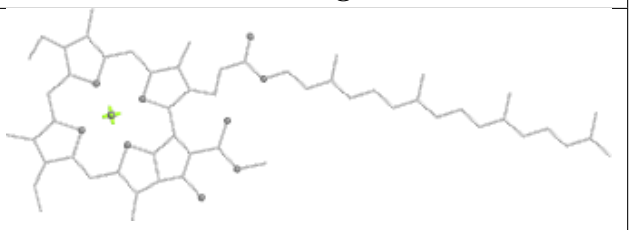

Rings

Ligand CLA aA 802

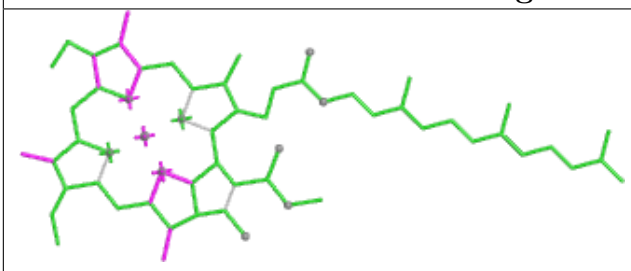

Bond lengths

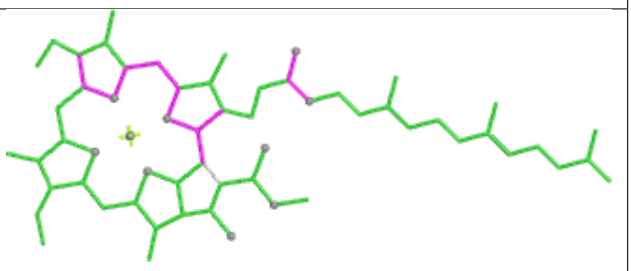

Bond angles

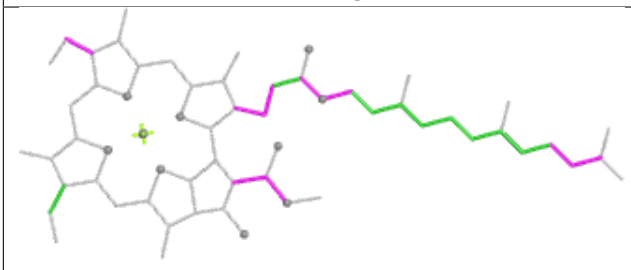

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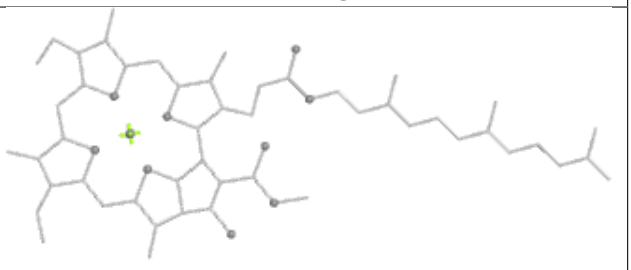

Rings

Ligand CLA cA 814

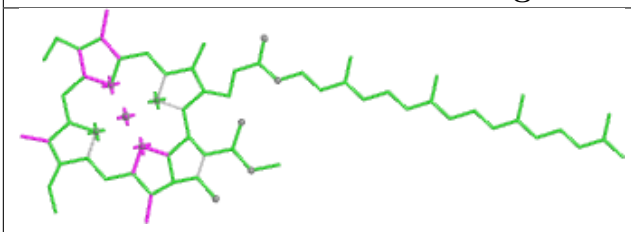

Bond lengths


Bond angles

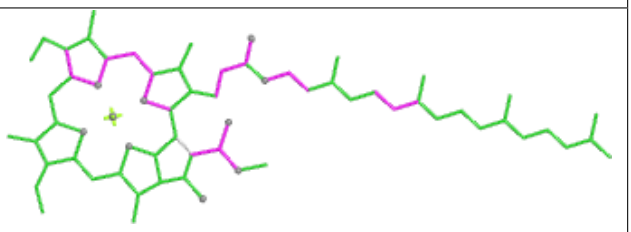

Torsions


Rings

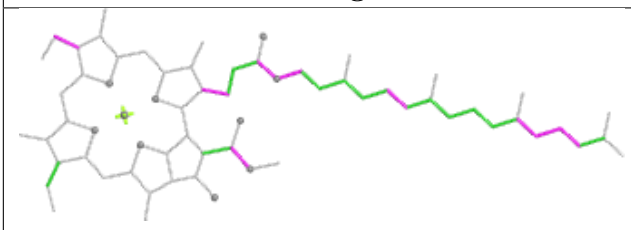
Ligand CLA bA 812



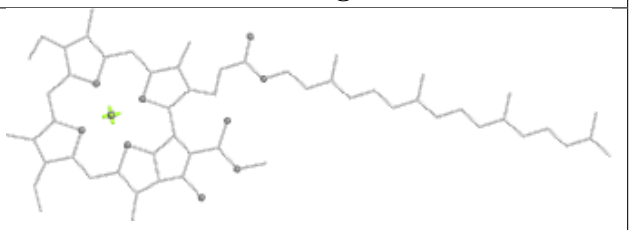
Bond lengths



Bond angles

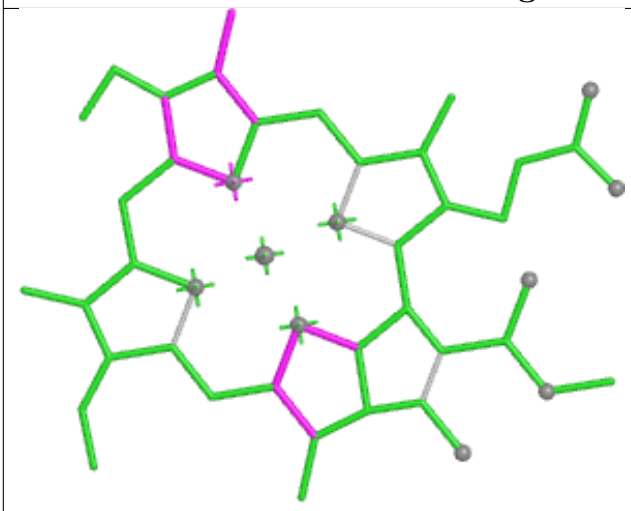


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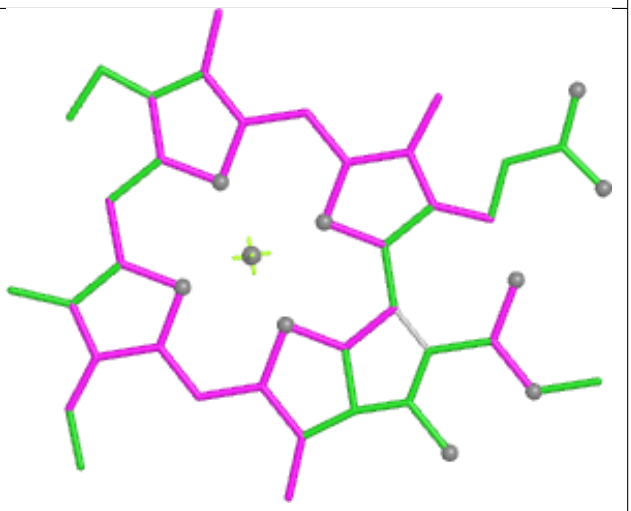


Rings

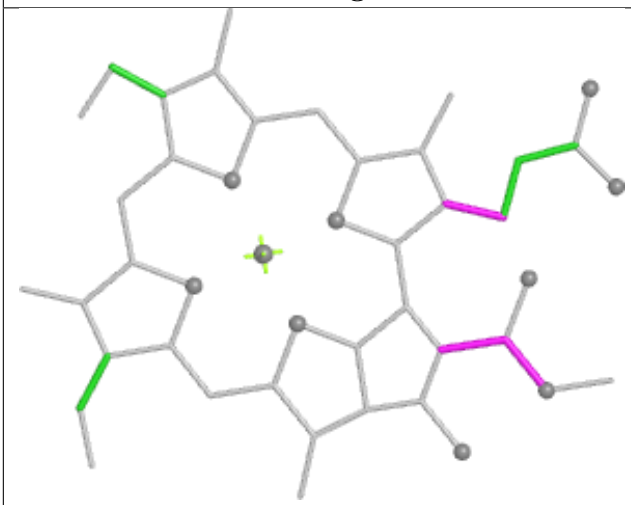
Ligand CLA b2 405



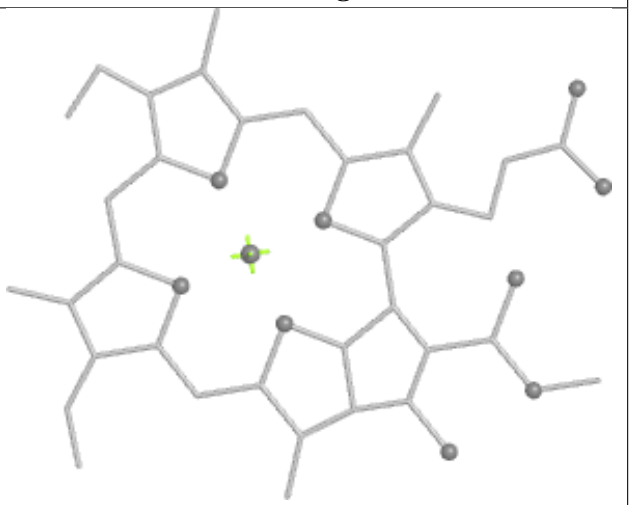
Bond lengths



Bond angles

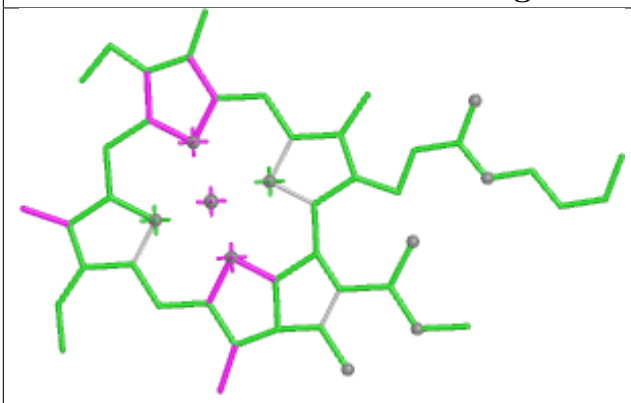


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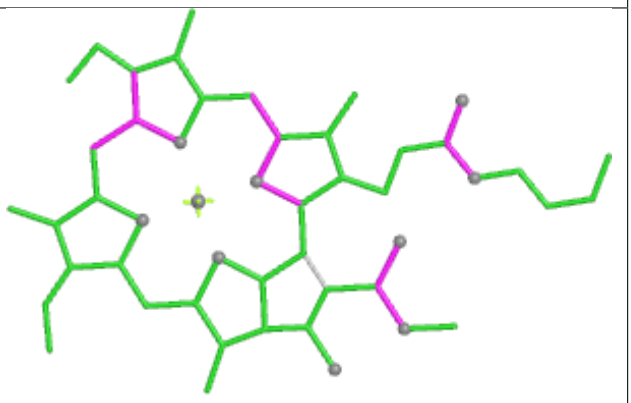


Rings

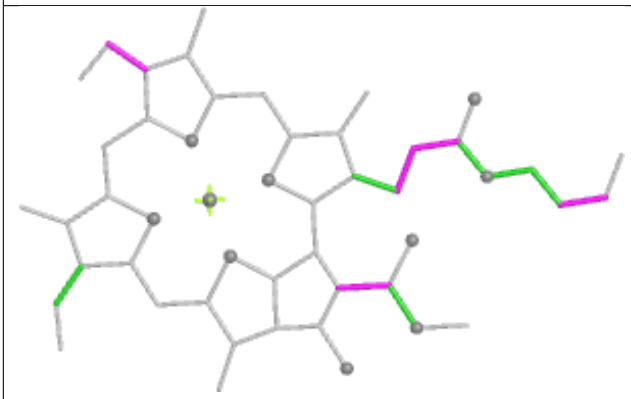
Ligand CLA bA 823



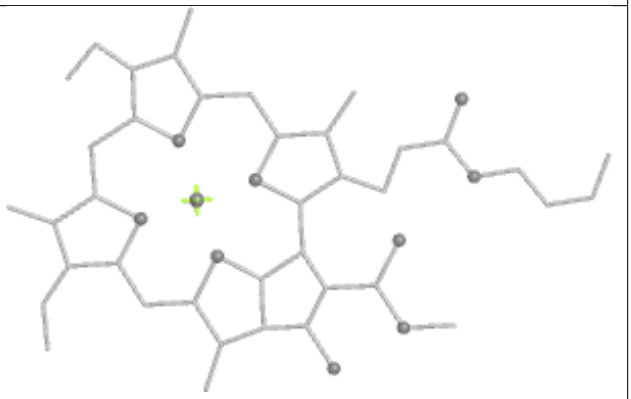
Bond lengths



Bond angles

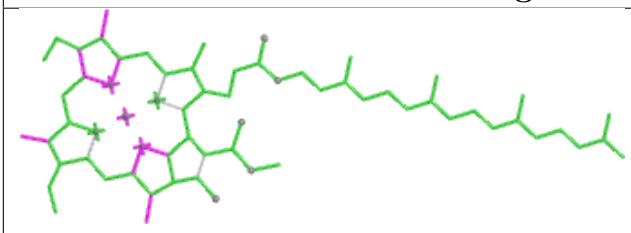


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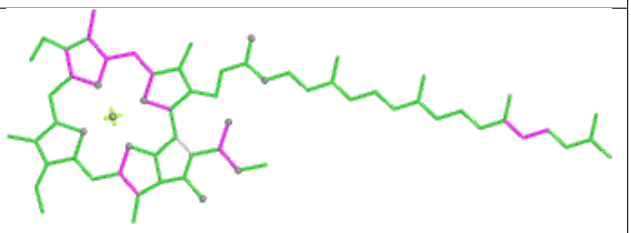


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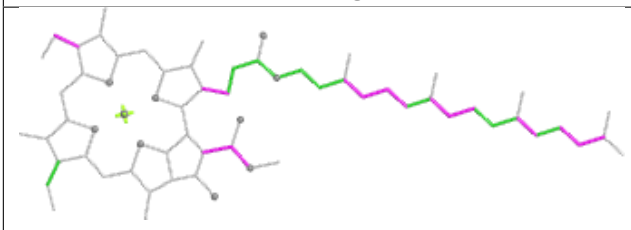
Ligand CLA aA 822



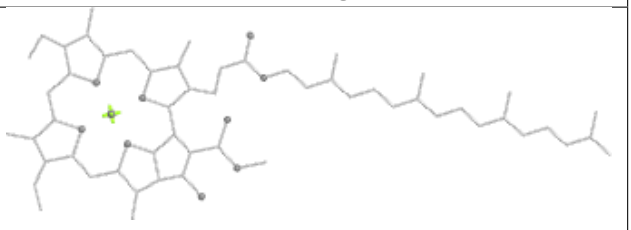
Bond lengths



Bond angles

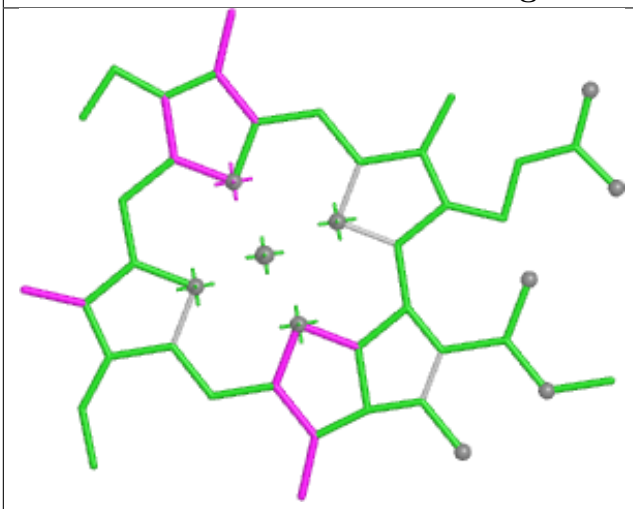


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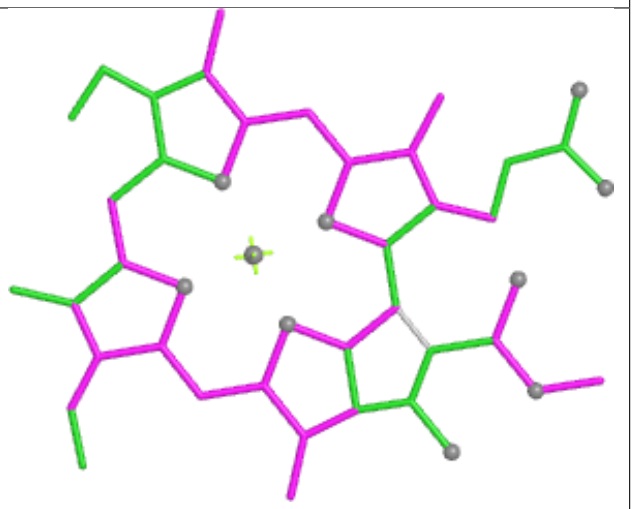


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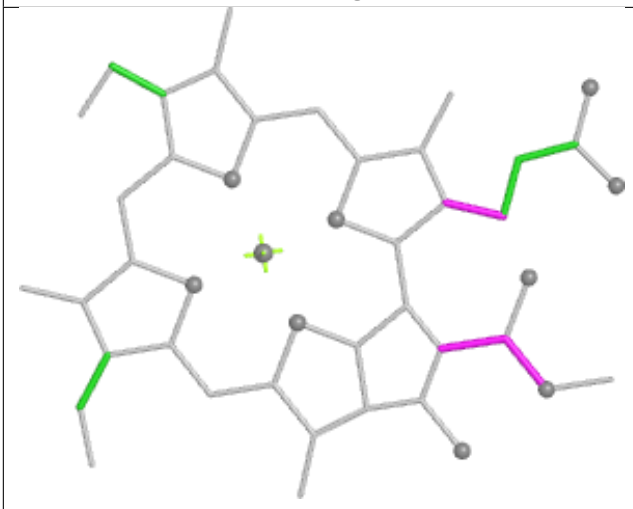
Ligand CLA a4 405



Bond lengths



Bond angles

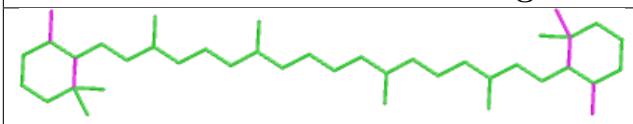


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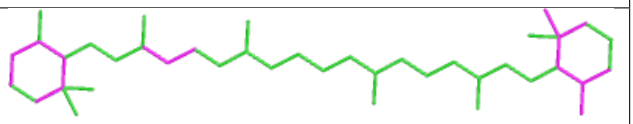


Rings

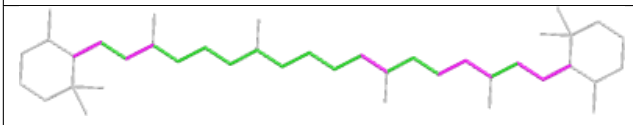
Ligand BCR b2 419



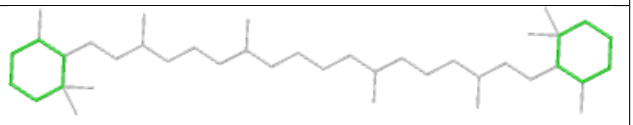
Bond lengths



Bond angles

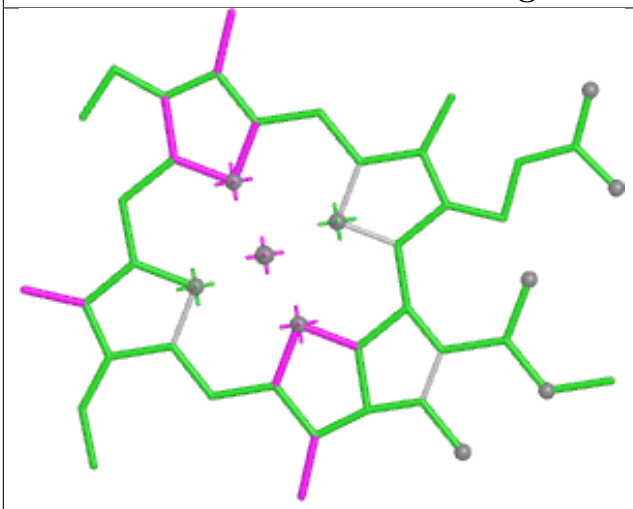


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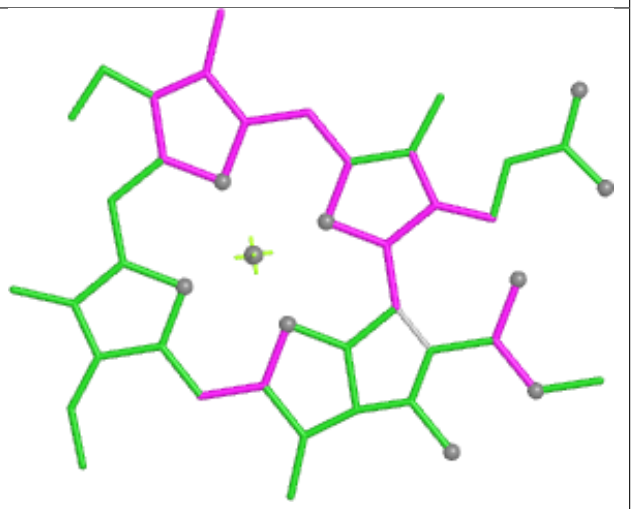


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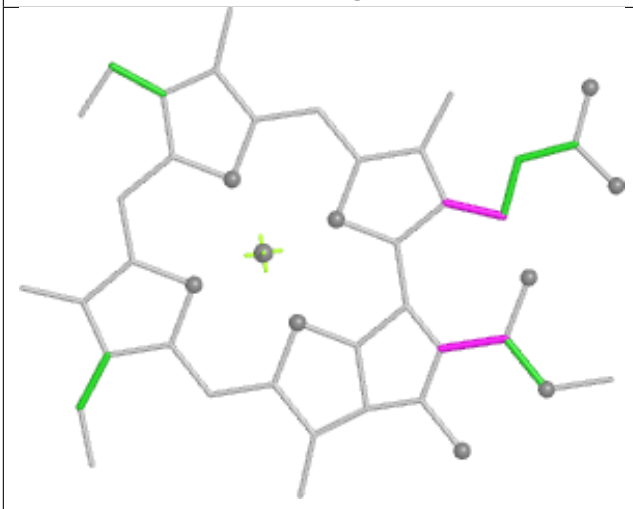
Ligand CLA b5 411



Bond lengths



Bond angles

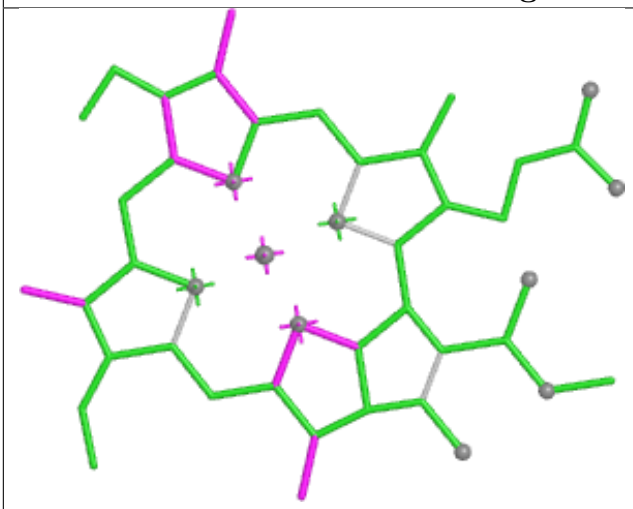


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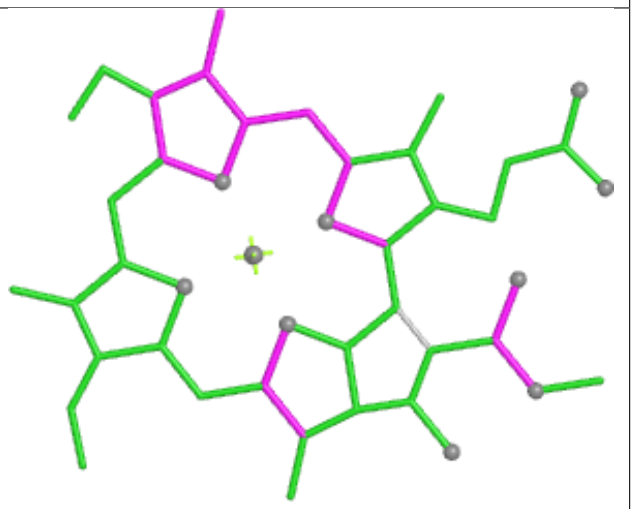


Rings

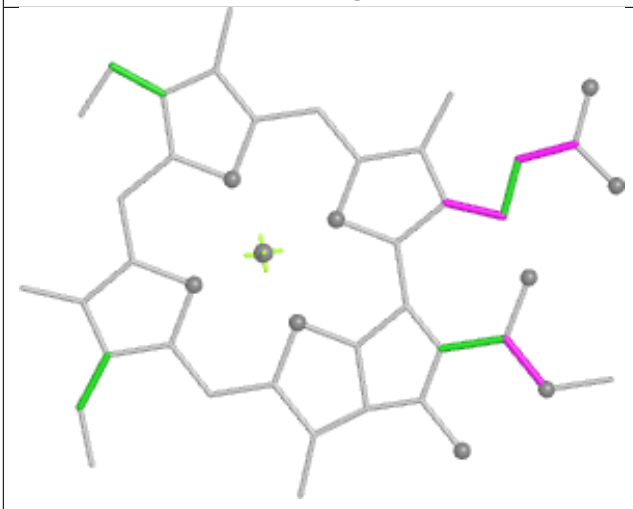
Ligand CLA a6 409



Bond lengths



Bond angles

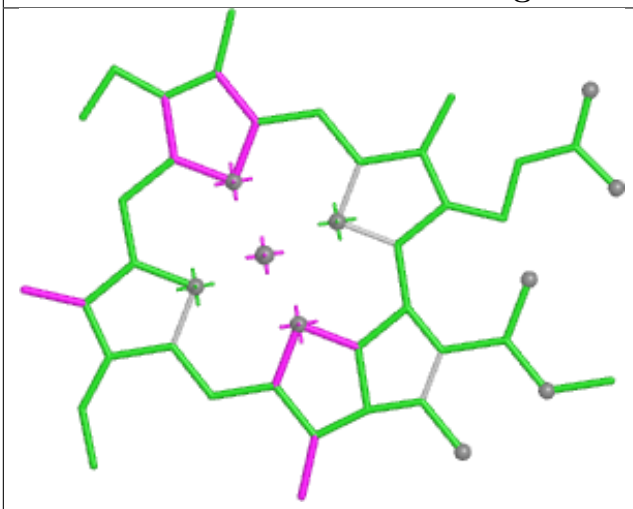


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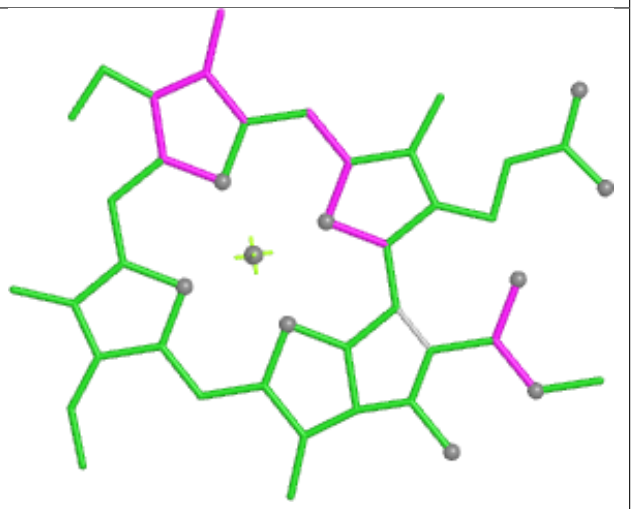


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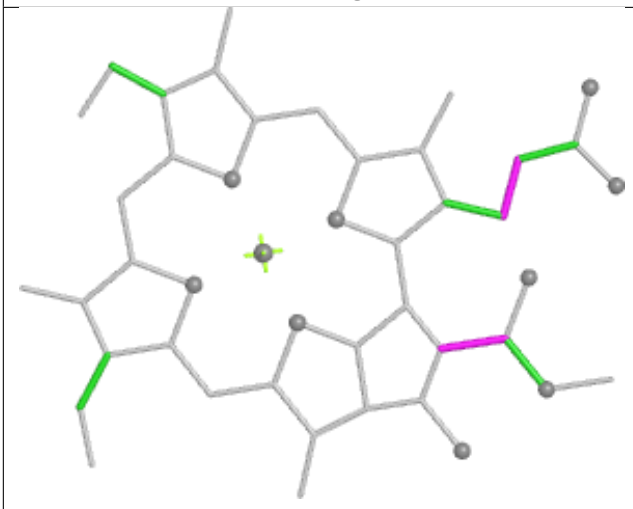
Ligand CLA bA 816



Bond lengths



Bond angles

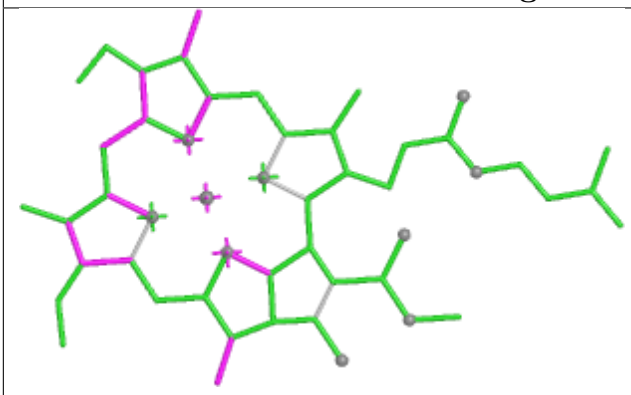


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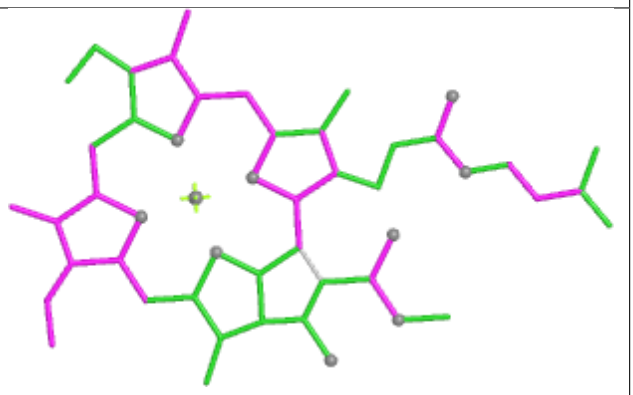


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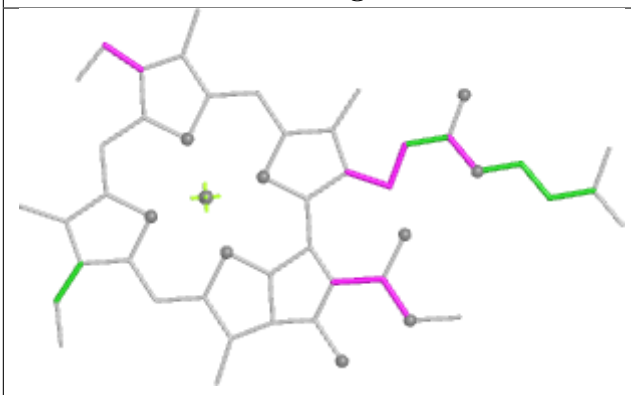
Ligand CLA a1 415



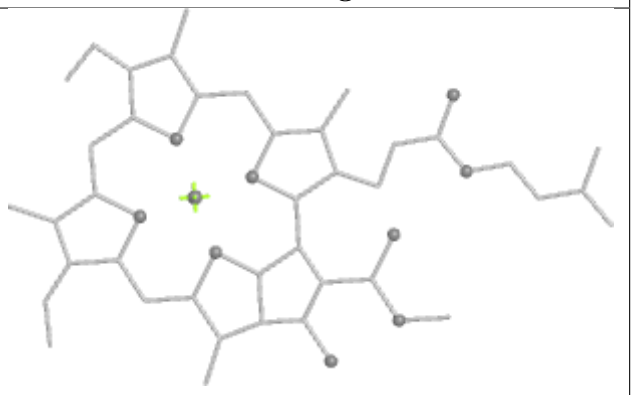
Bond lengths



Bond angles



Torsions

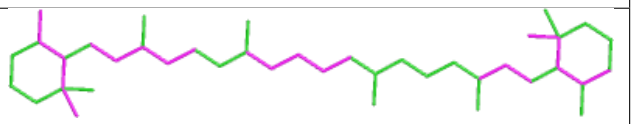


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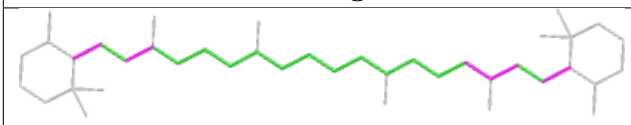
Ligand BCR bL 205



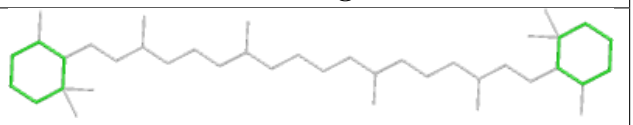
Bond lengths



Bond angles

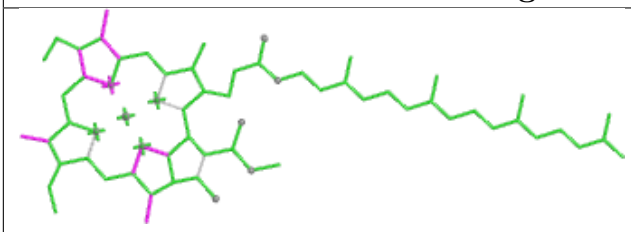


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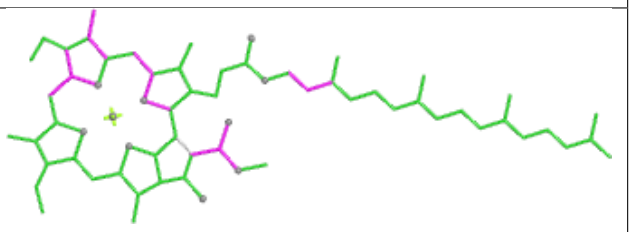


Rings

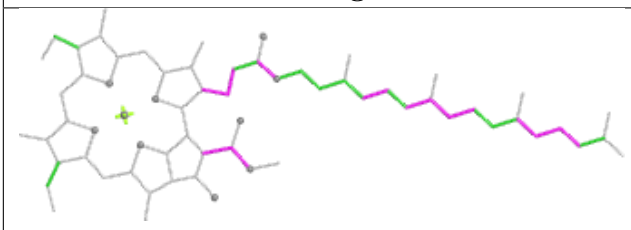
Ligand CLA b4 402



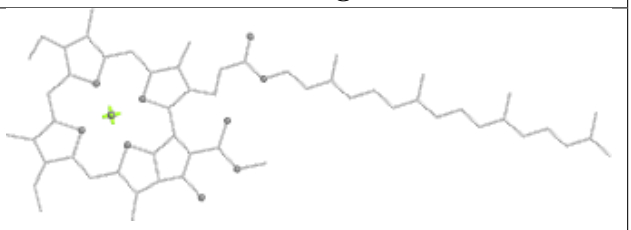
Bond lengths



Bond angles

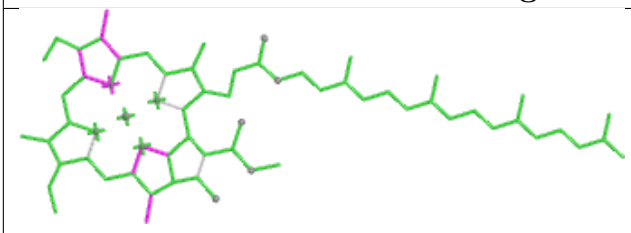


Torsions

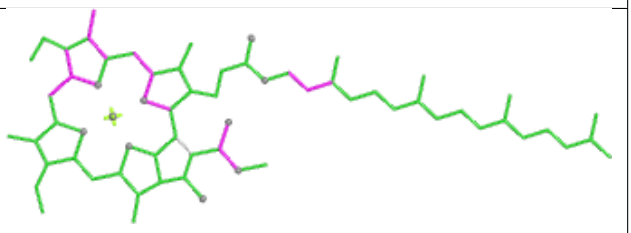


Rings

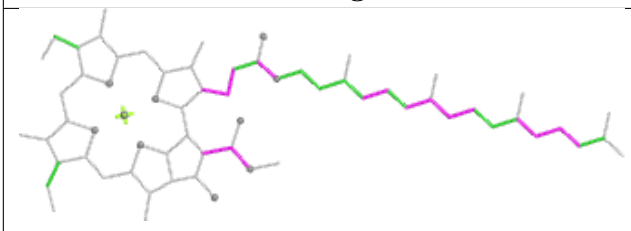
Ligand CLA a6 403



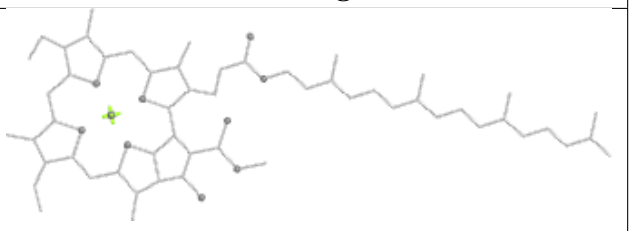
Bond lengths



Bond angles

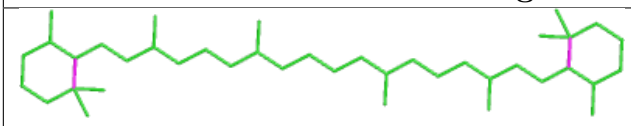


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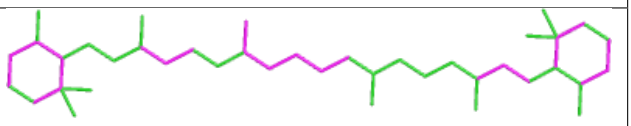


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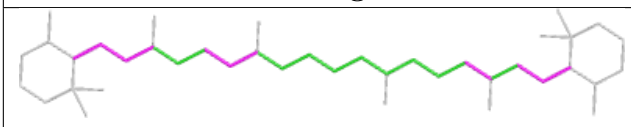
Ligand BCR b5 419



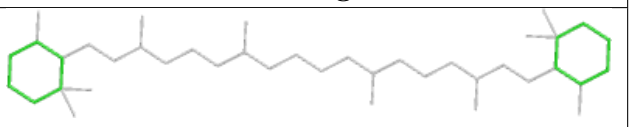
Bond lengths



Bond angles

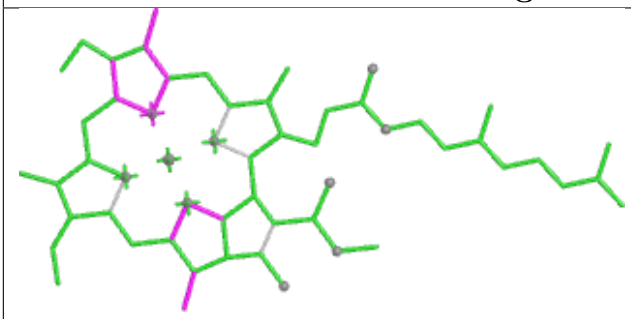


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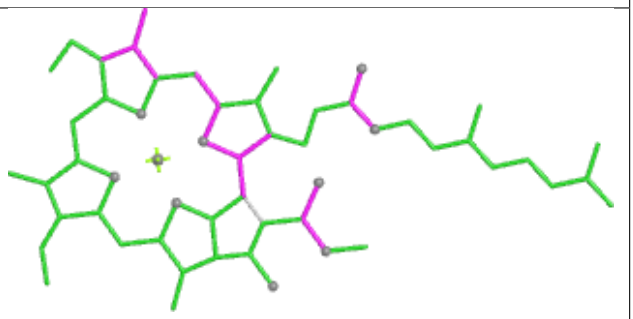


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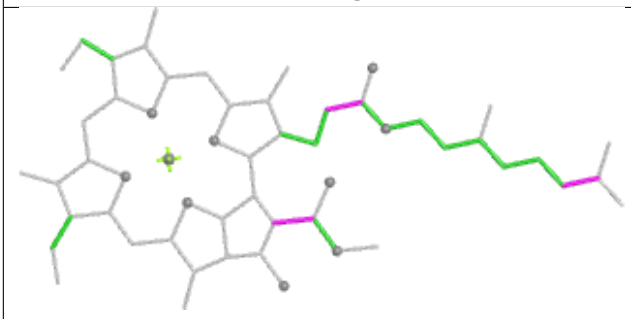
Ligand CLA aB 823



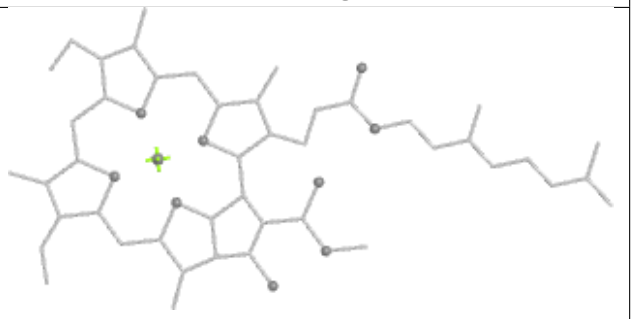
Bond lengths



Bond angles

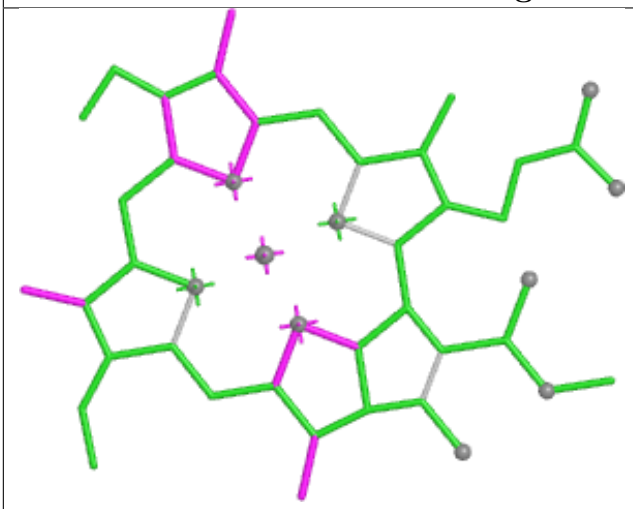


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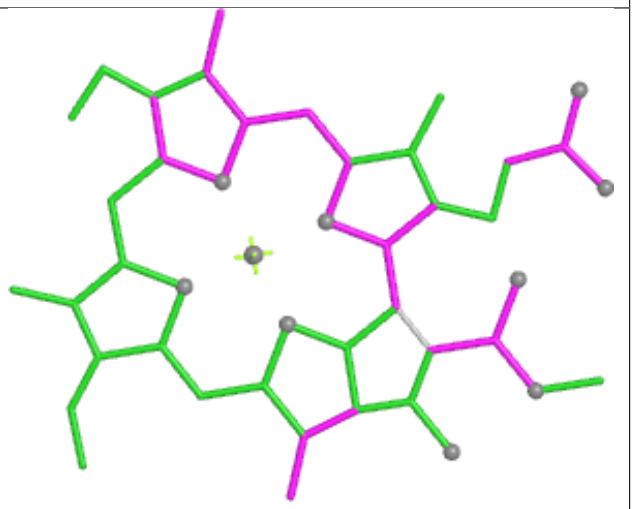


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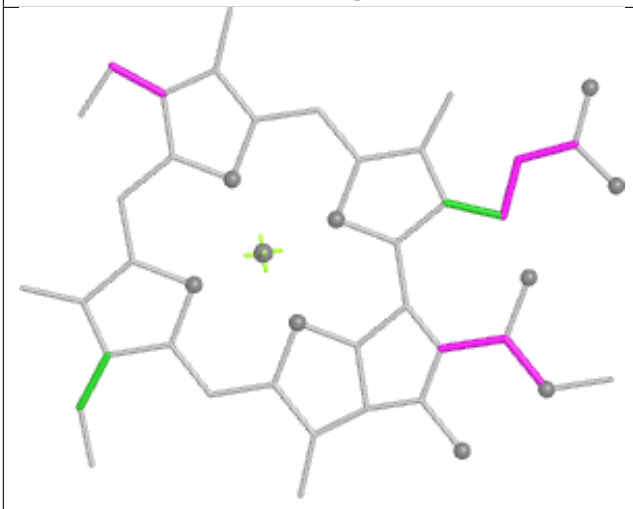
Ligand CLA aX 102



Bond lengths



Bond angles

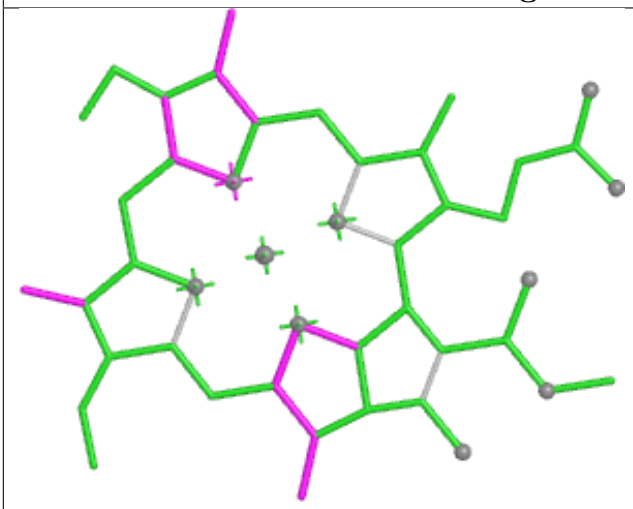


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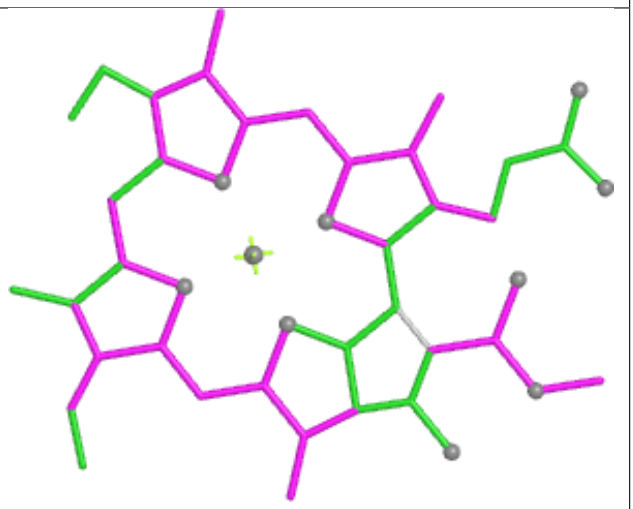


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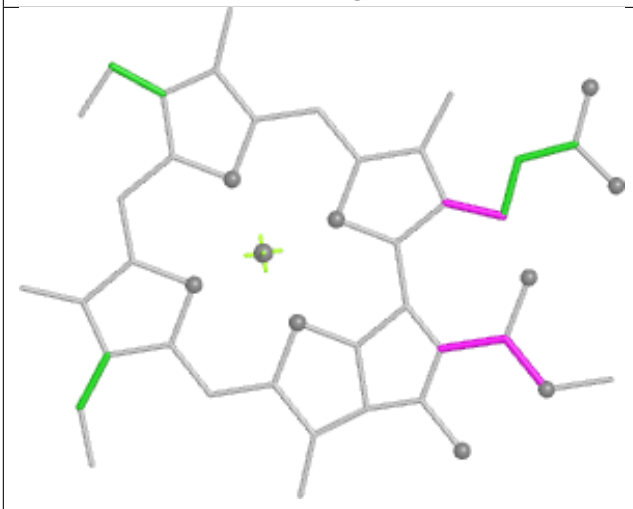
Ligand CLA a5 405



Bond lengths



Bond angles

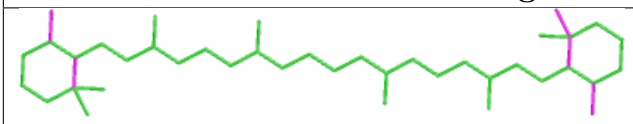


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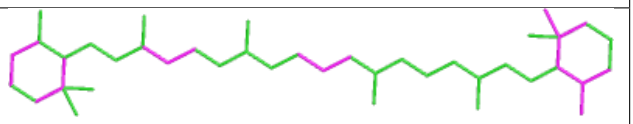


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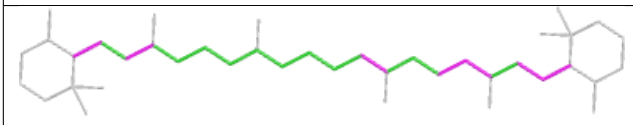
Ligand BCR c2 419



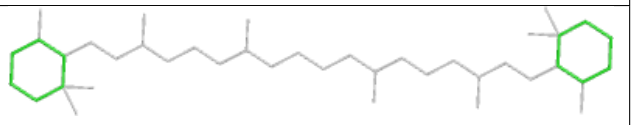
Bond lengths



Bond angles

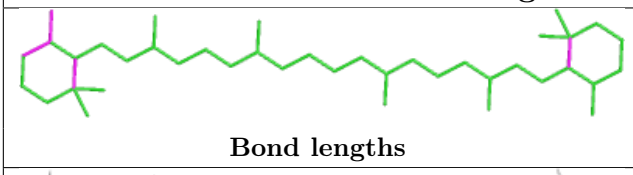


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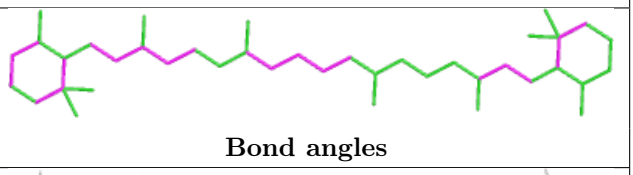


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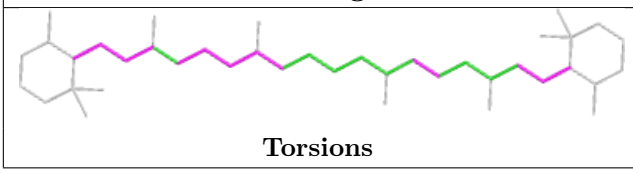
Ligand BCR c3 401



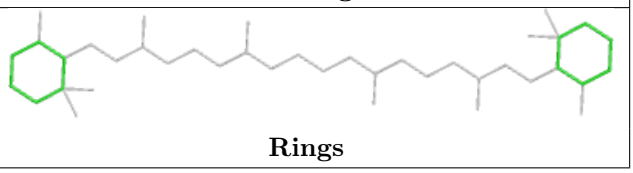
Bond lengths



Bond angles

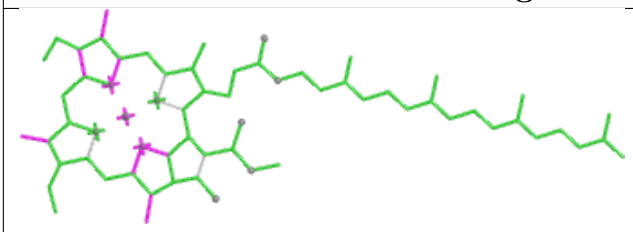


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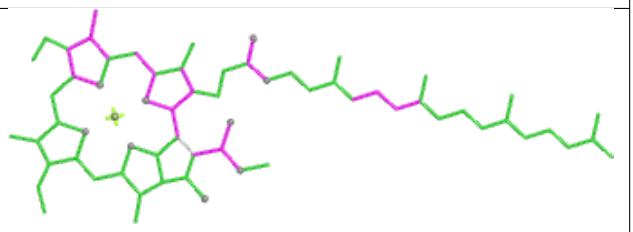


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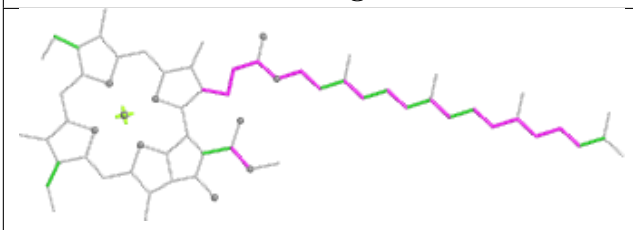
Ligand CLA cA 829



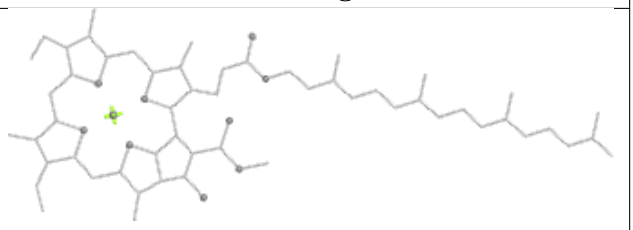
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Bond angles

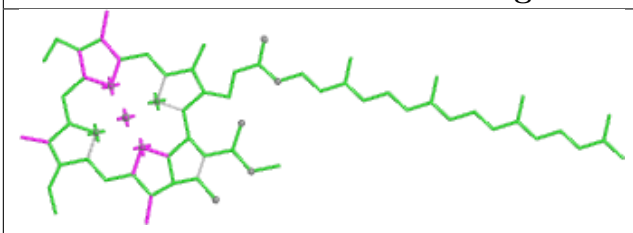


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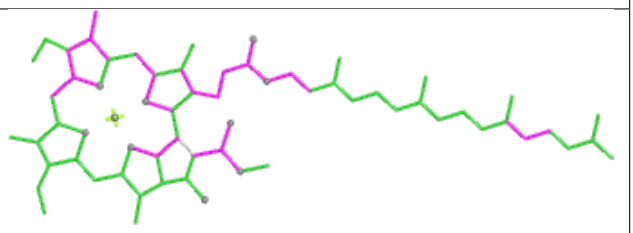


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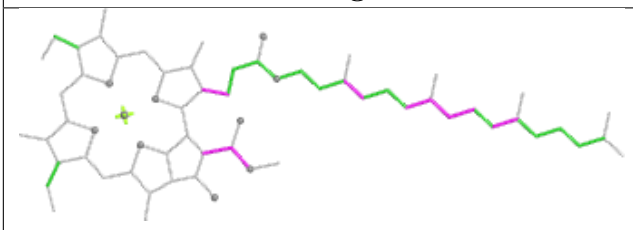
Ligand CLA bB 827



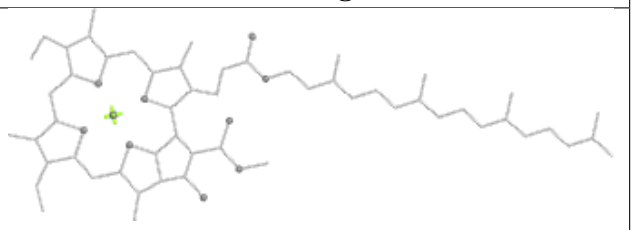
Bond lengths



Bond angles

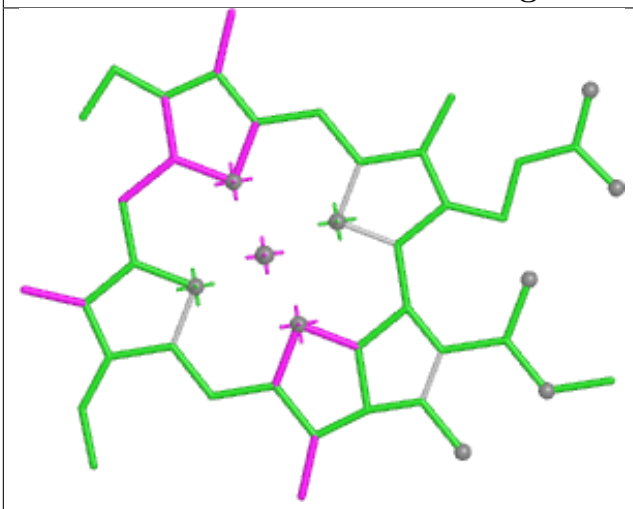


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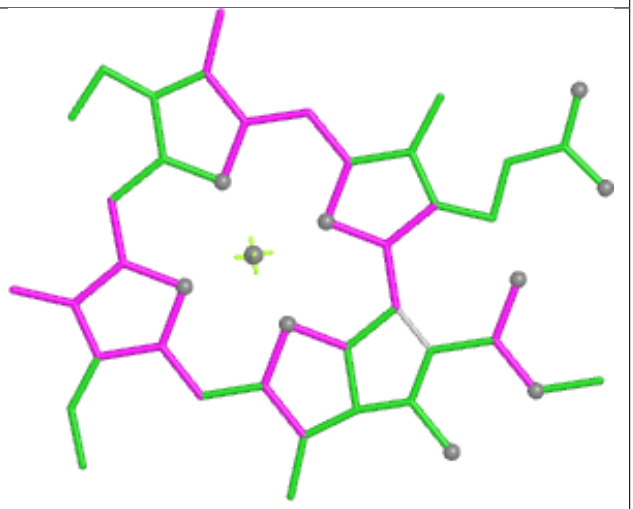


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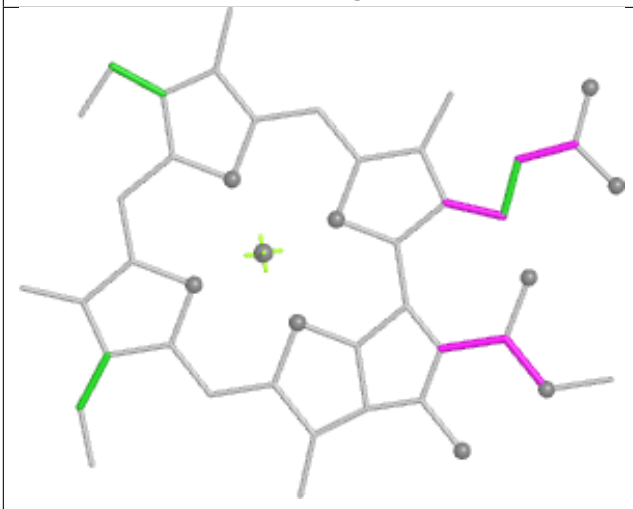
Ligand CLA a1 411



Bond lengths



Bond angles

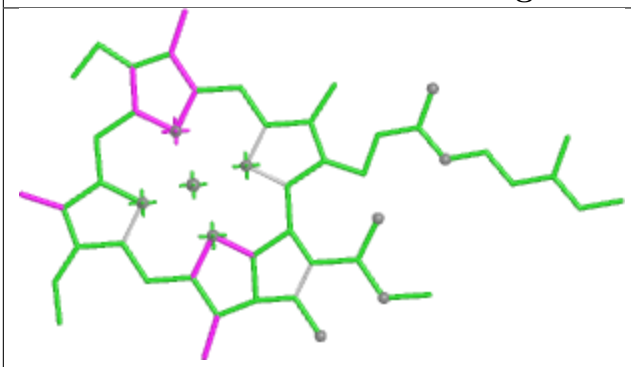


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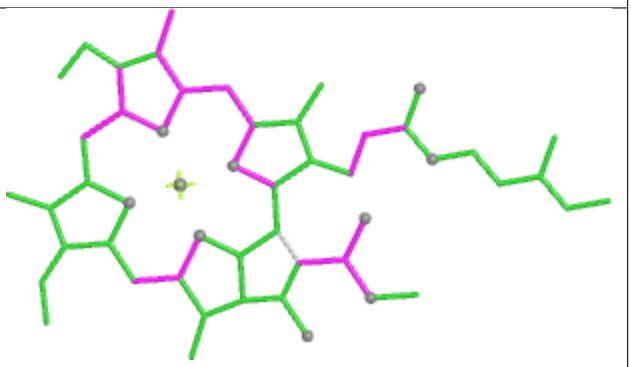


Rings

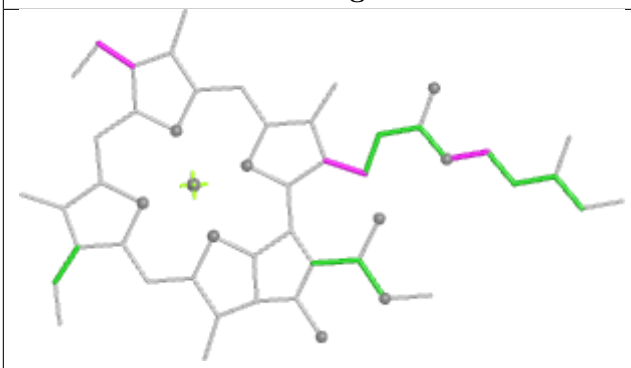
Ligand CLA cA 808



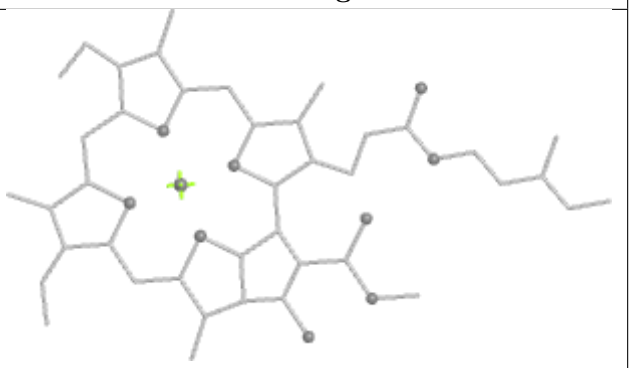
Bond lengths



Bond angles

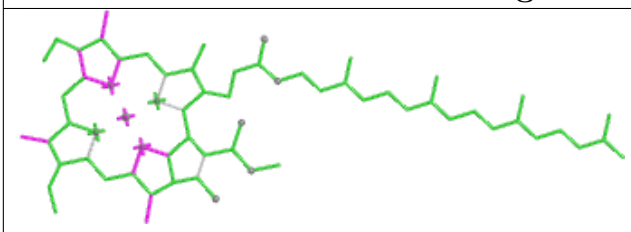


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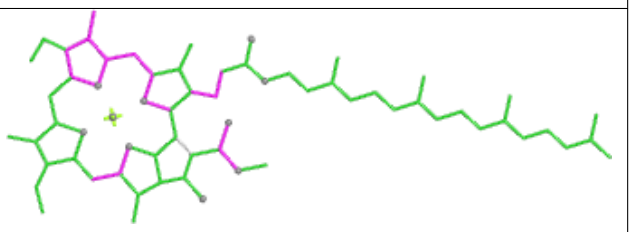


Rings

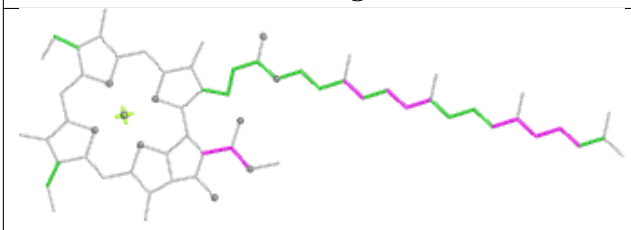
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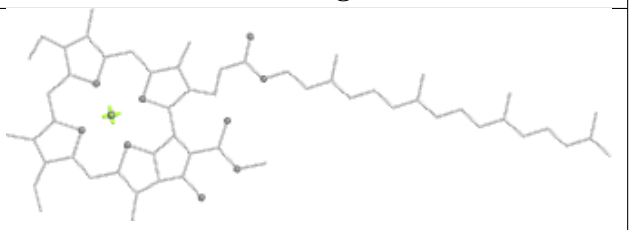
Bond lengths



Bond angles

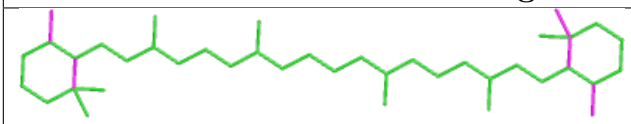


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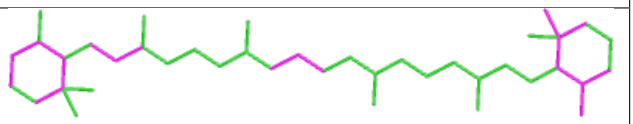


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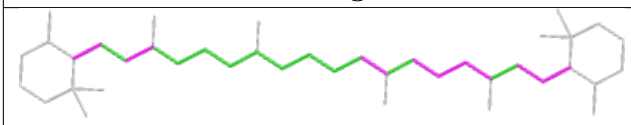
Ligand BCR a3 418



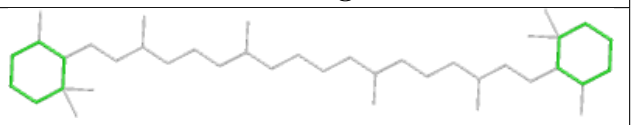
Bond lengths



Bond angles

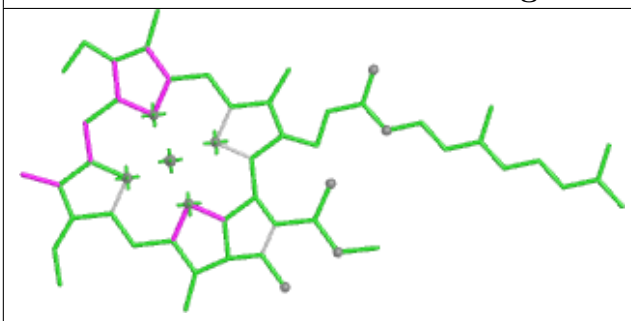


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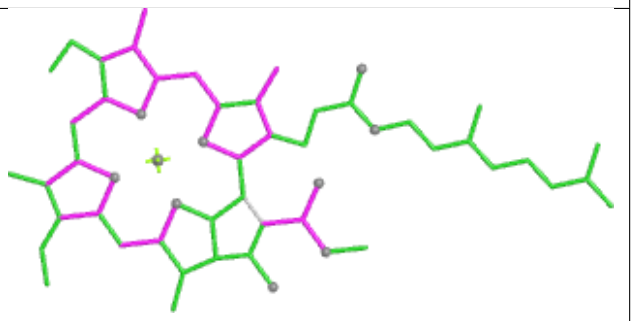


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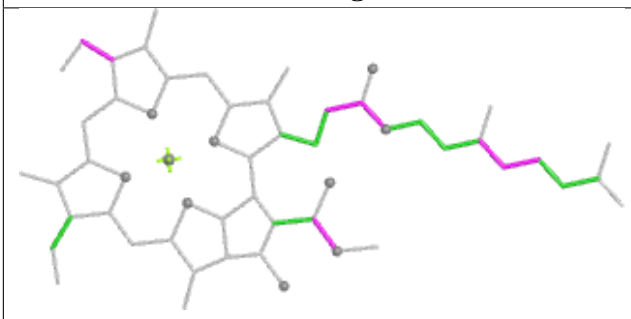
Ligand CLA c5 417



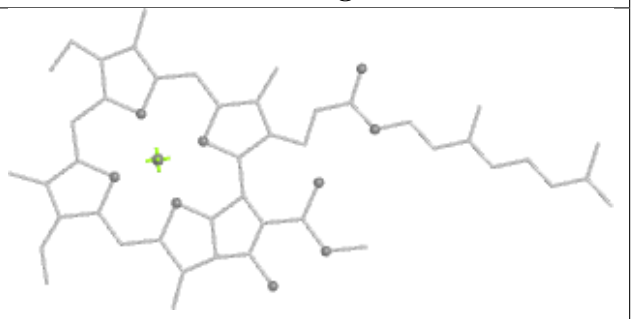
Bond lengths



Bond angles

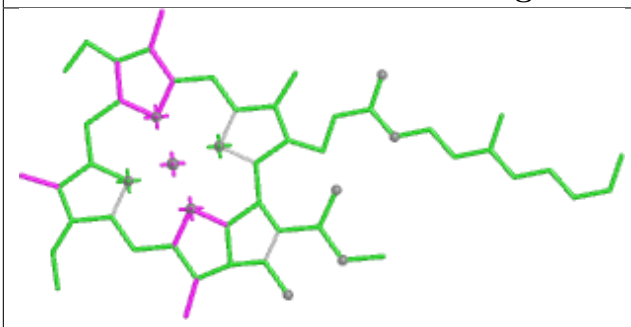


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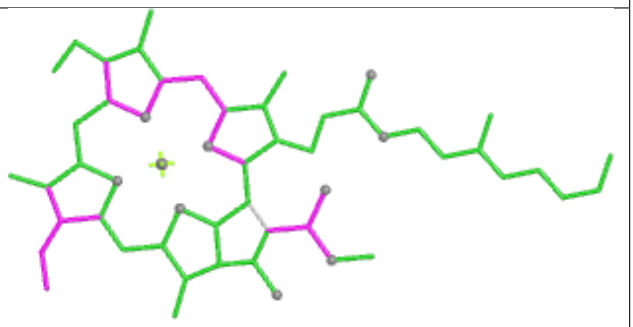


Rings

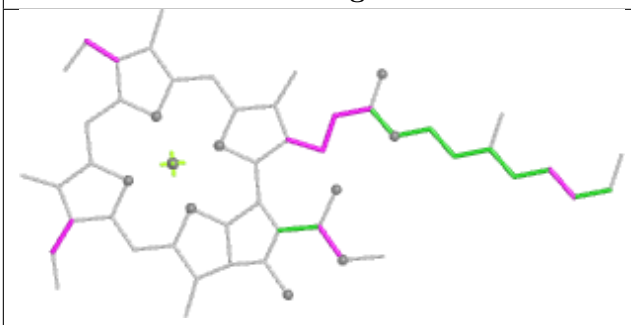
Ligand CLA aA 819



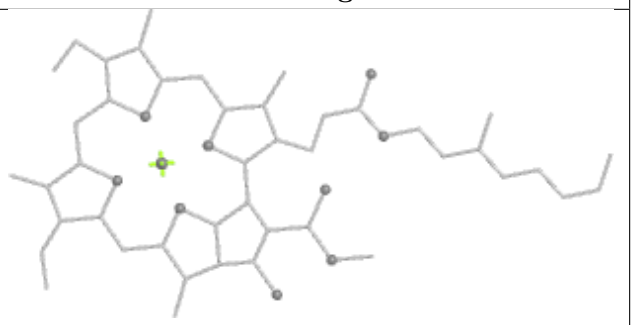
Bond lengths



Bond angles

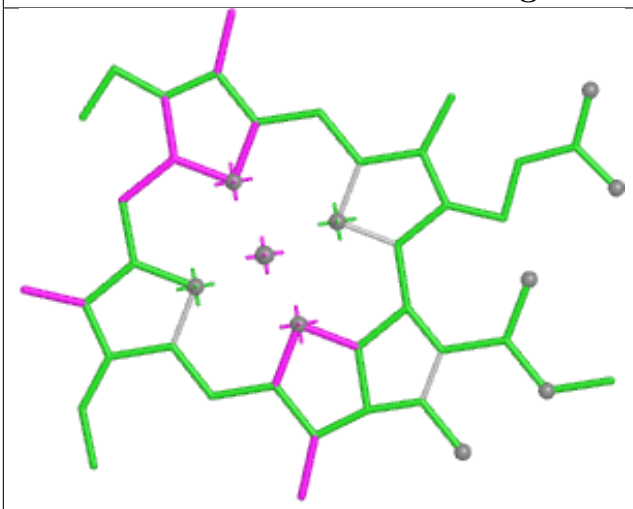


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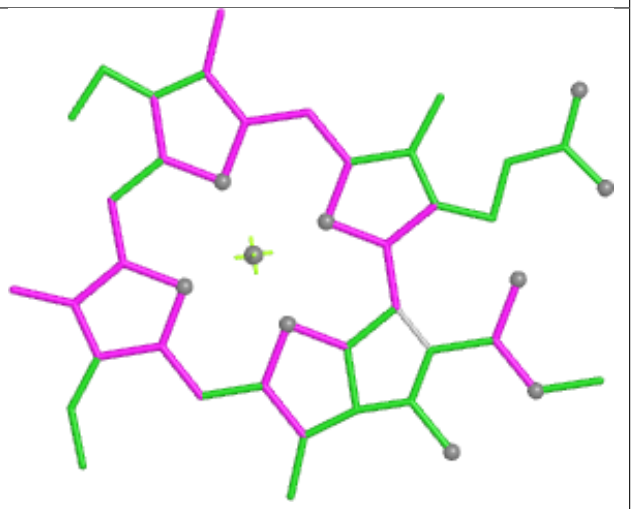


Rings

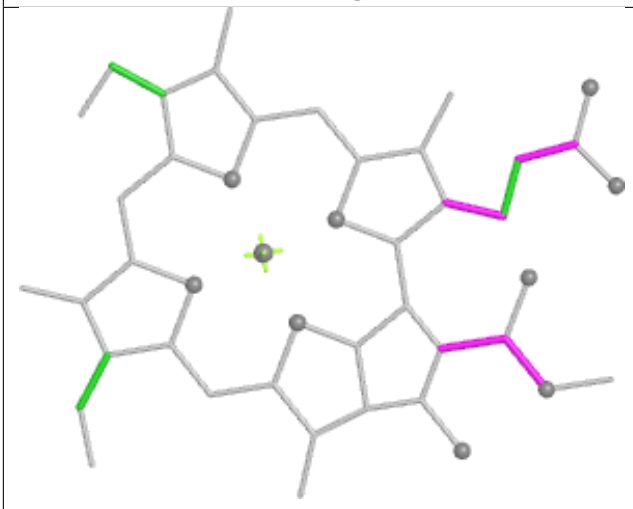
Ligand CLA a2 413



Bond lengths



Bond angles

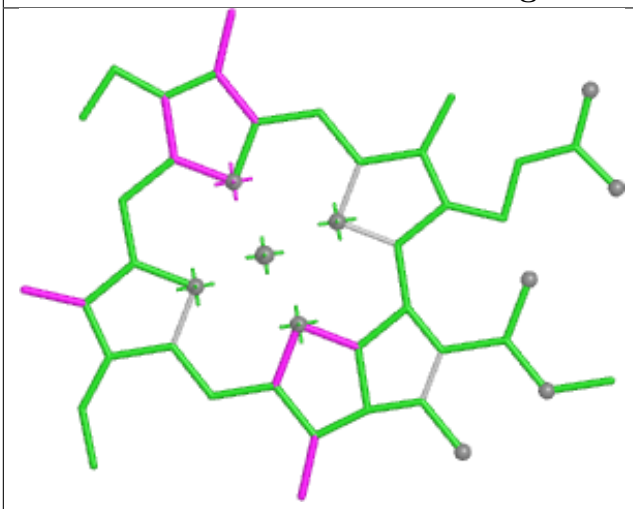


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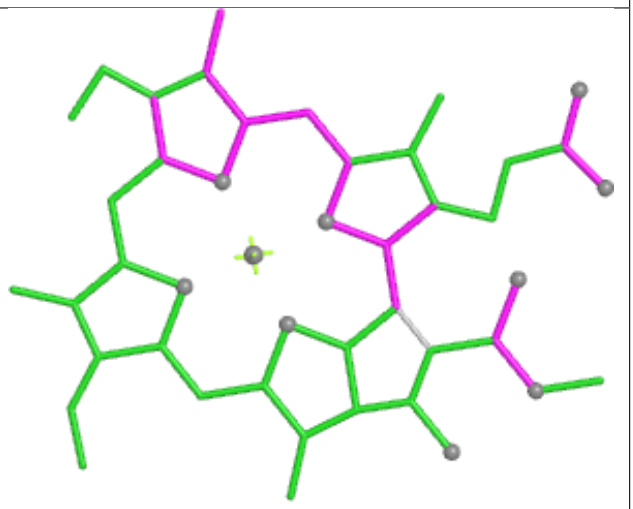


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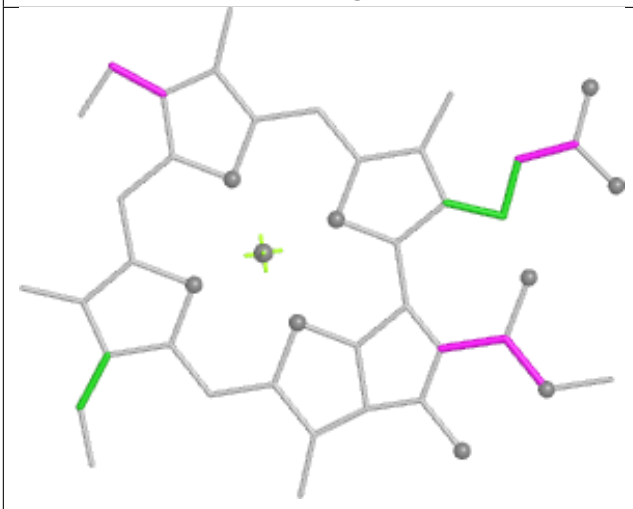
Ligand CLA a1 406



Bond lengths



Bond angles

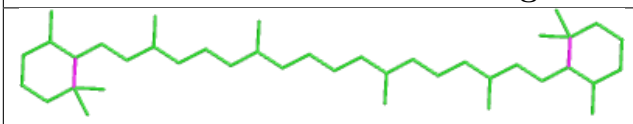


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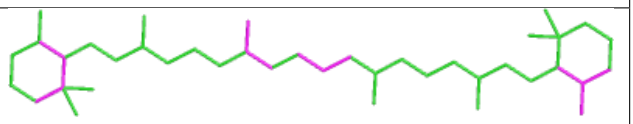


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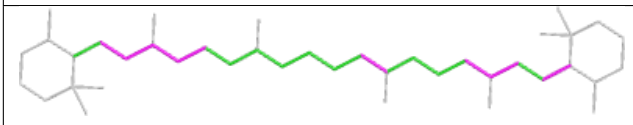
Ligand BCR aI 101



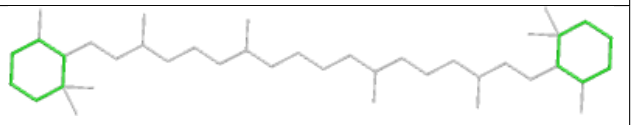
Bond lengths



Bond angles

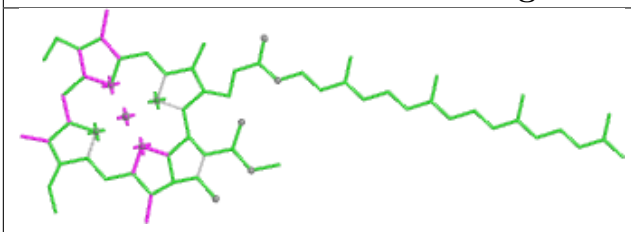


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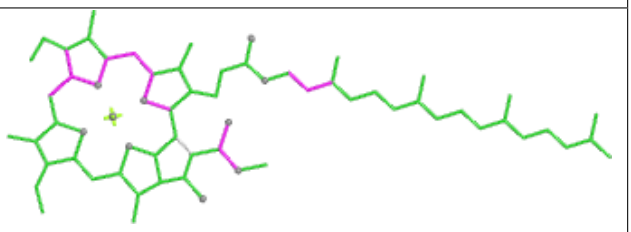


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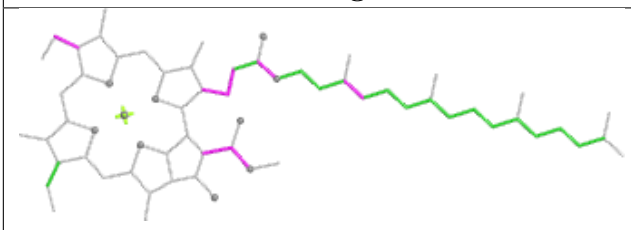
Ligand CLA b4 404



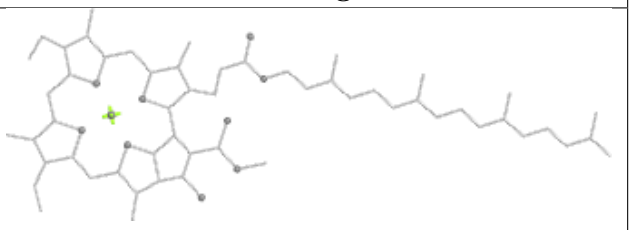
Bond lengths



Bond angles

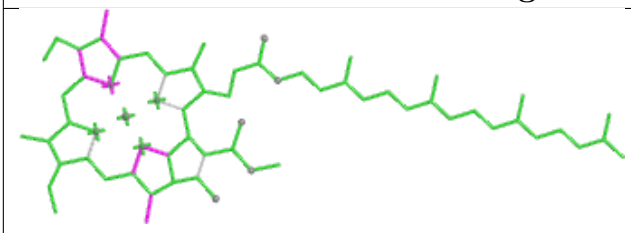


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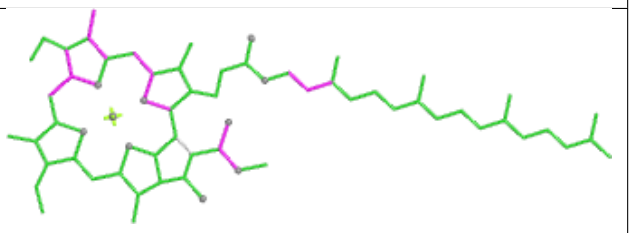


Rings

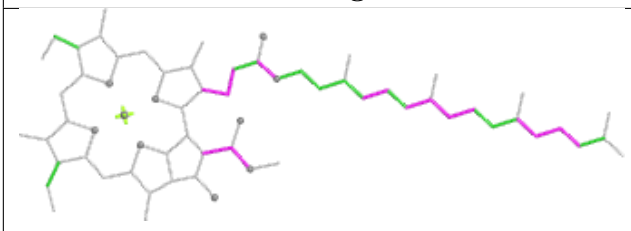
Ligand CLA b3 402



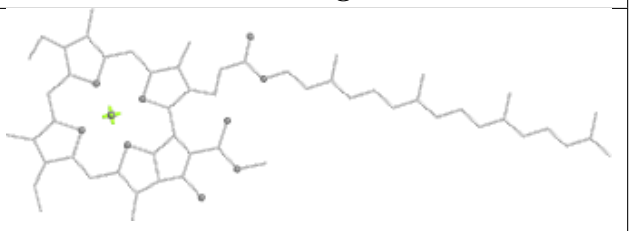
Bond lengths



Bond angles

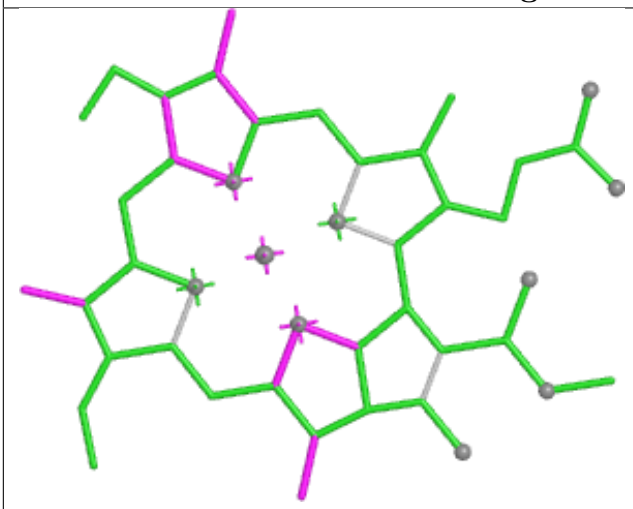


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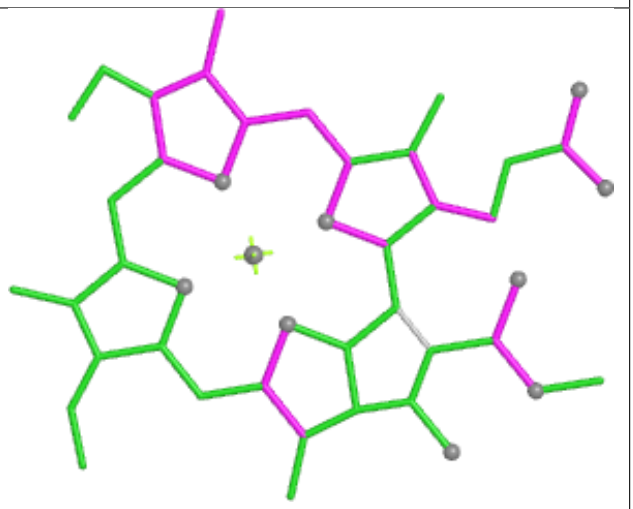


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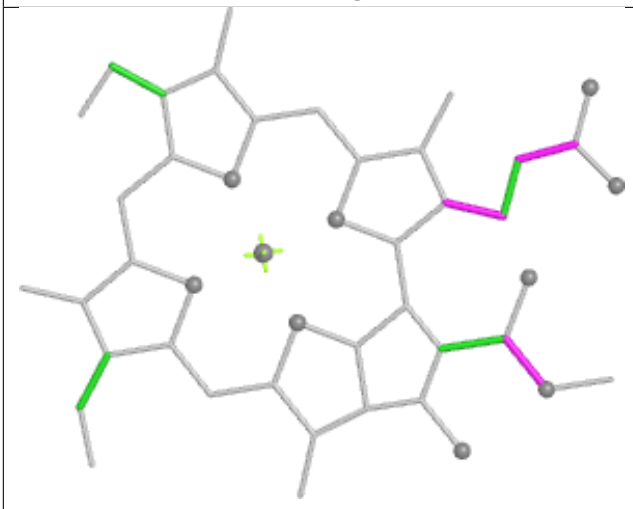
Ligand CLA c3 408



Bond lengths



Bond angles

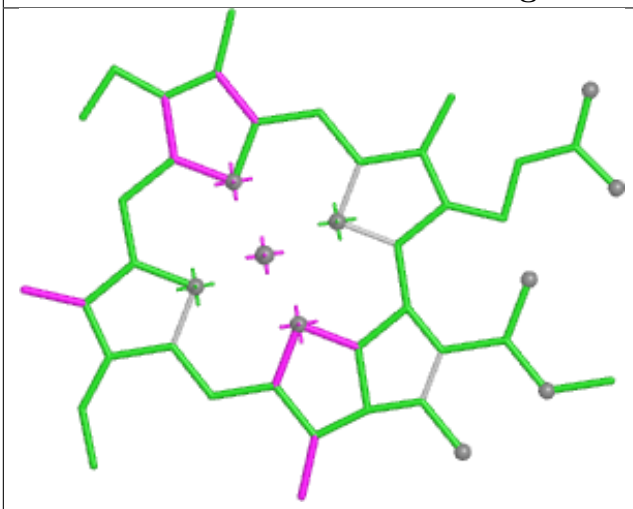


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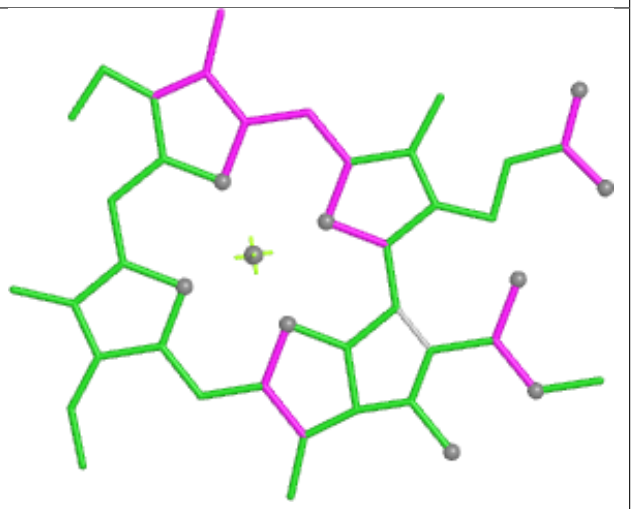


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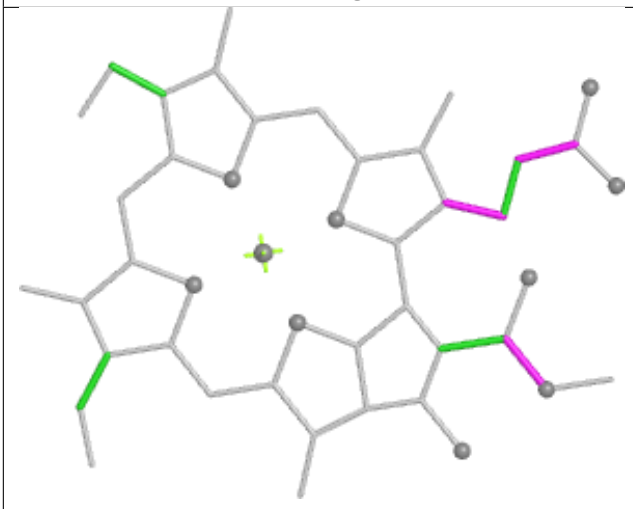
Ligand CLA a2 409



Bond lengths



Bond angles

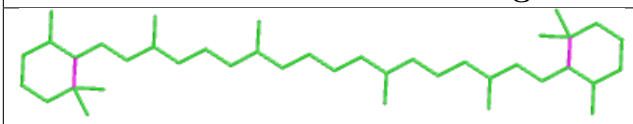


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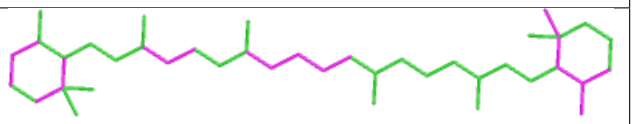


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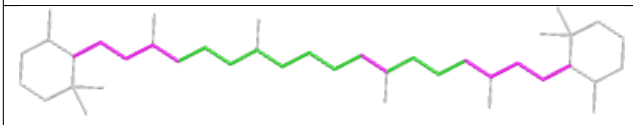
Ligand BCR aA 849



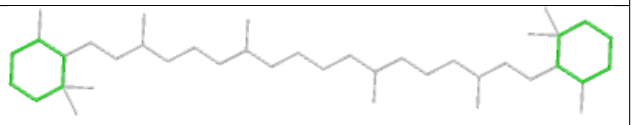
Bond lengths



Bond angles

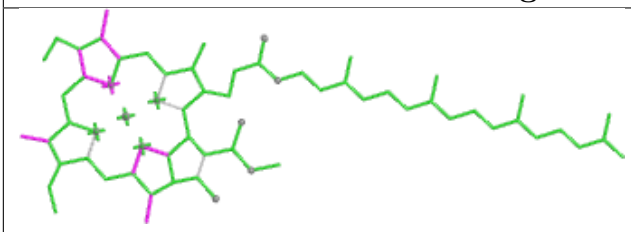


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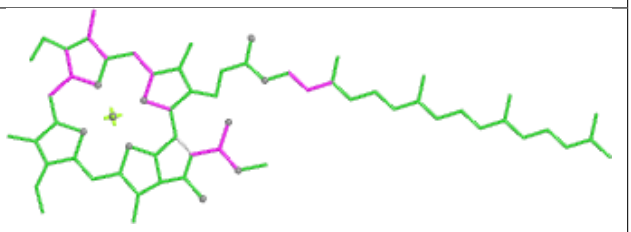


Rings

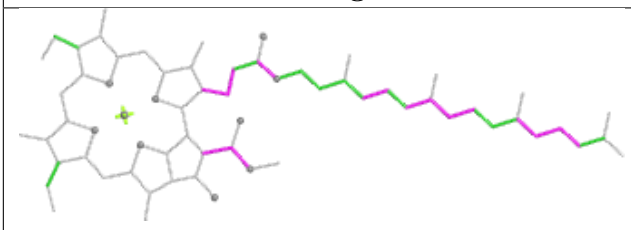
Ligand CLA a4 402



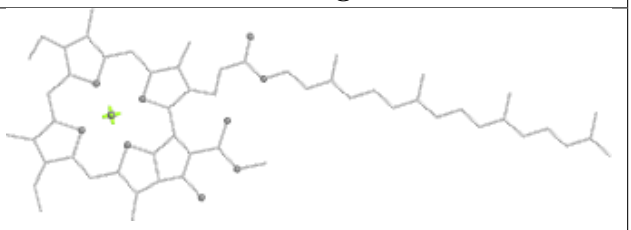
Bond lengths



Bond angles

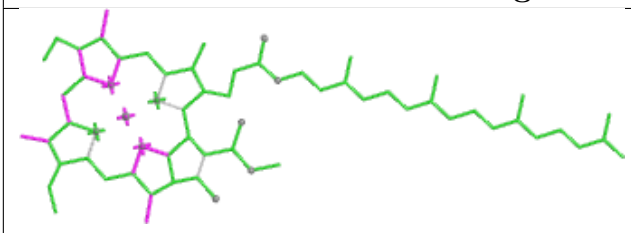


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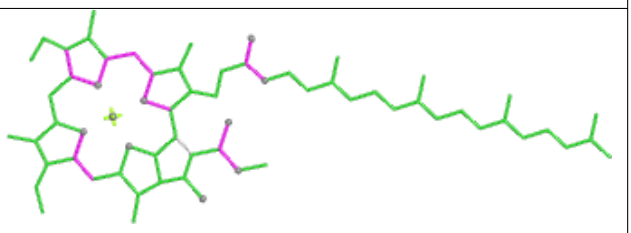


Rings

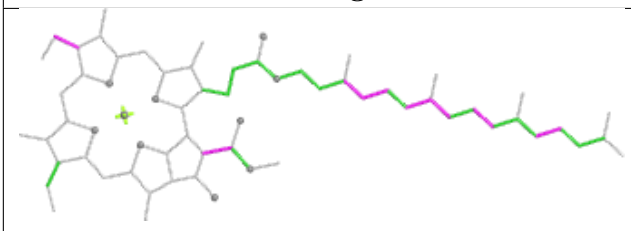
Ligand CLA bA 828



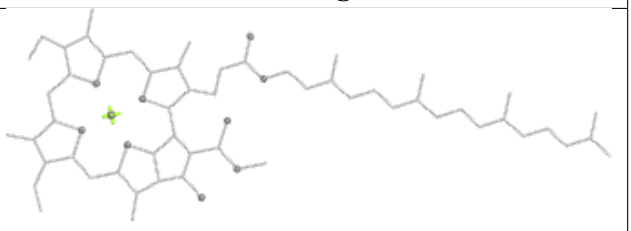
Bond lengths



Bond angles

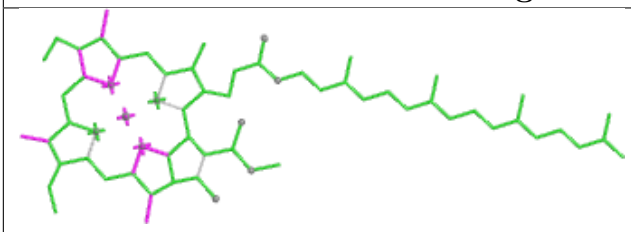


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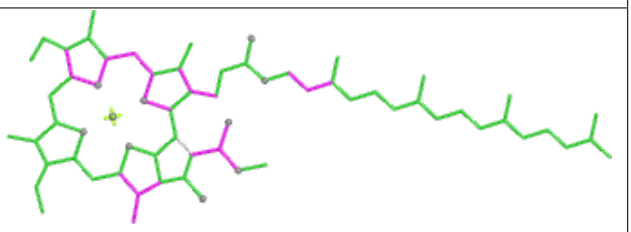


Rings

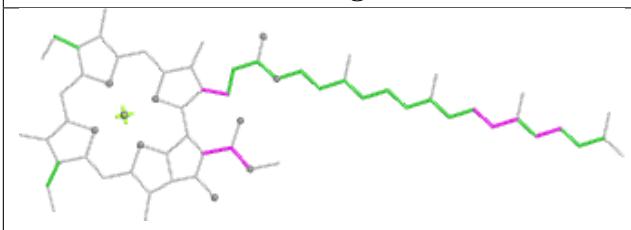
Ligand CLA cA 804



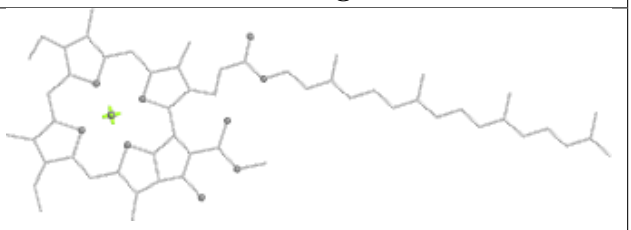
Bond lengths



Bond angles

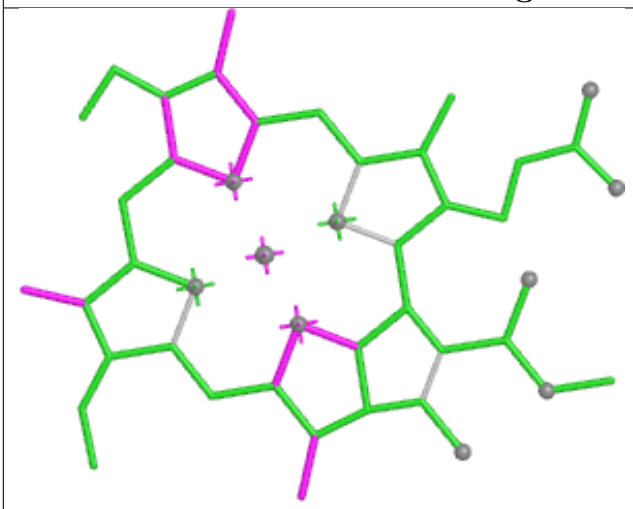


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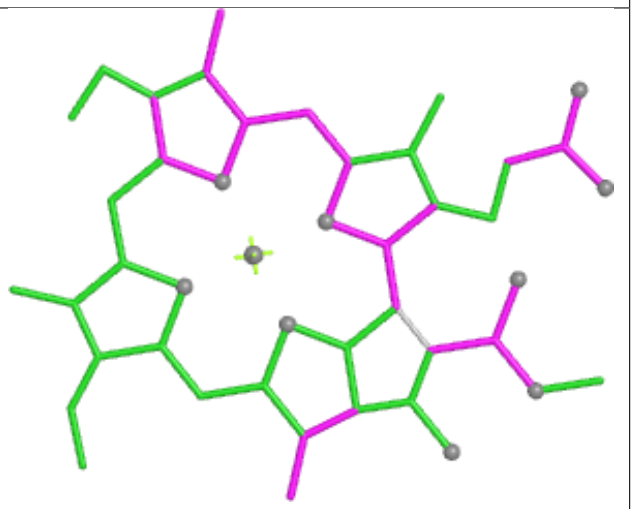


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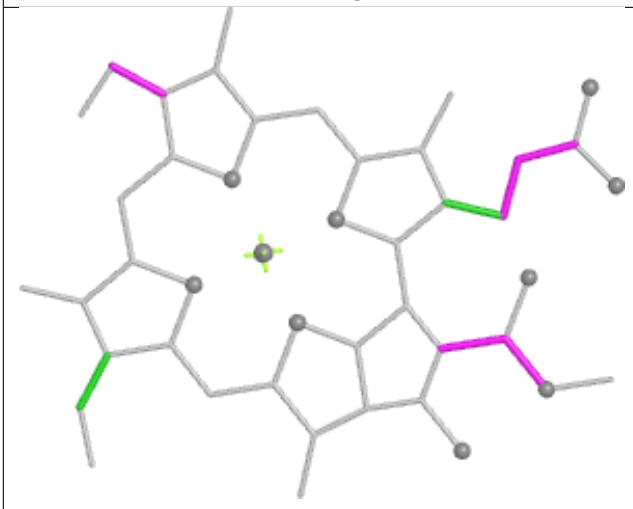
Ligand CLA cX 102



Bond lengths



Bond angles

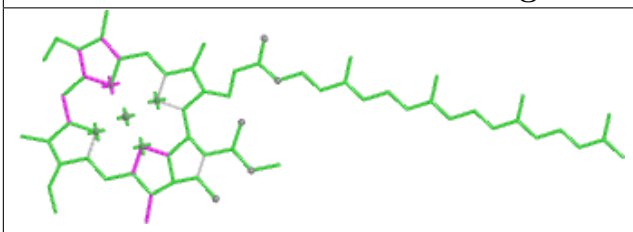


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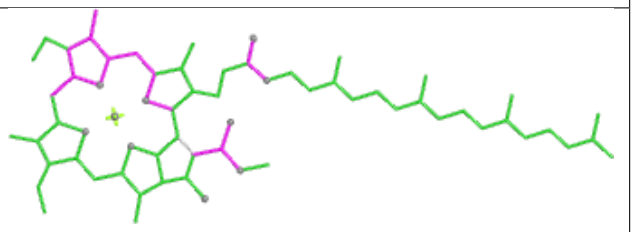


Rings

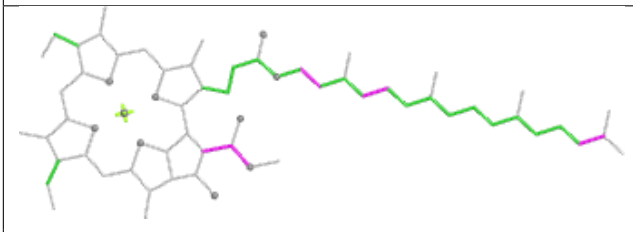
Ligand CLA a2 410



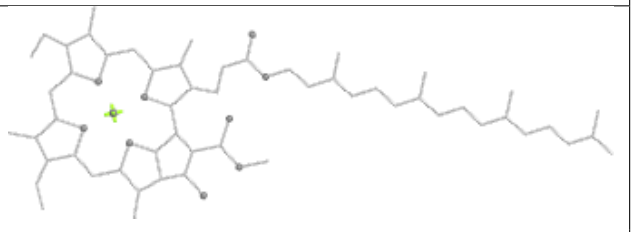
Bond lengths



Bond angles

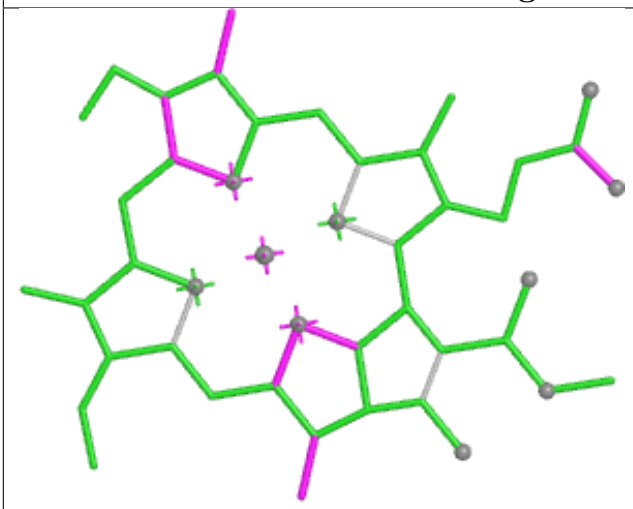


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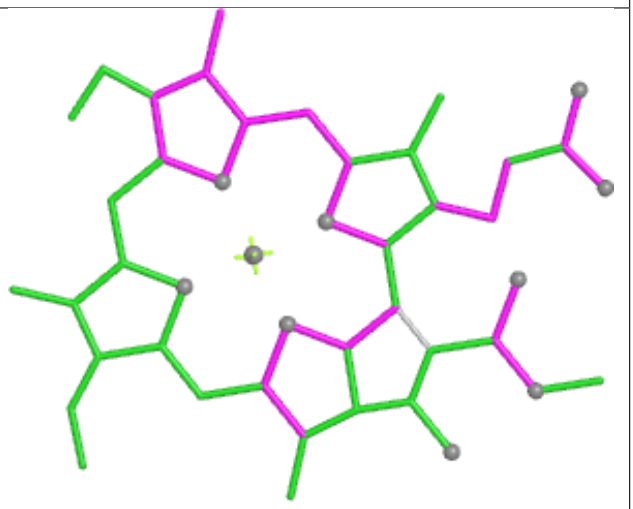


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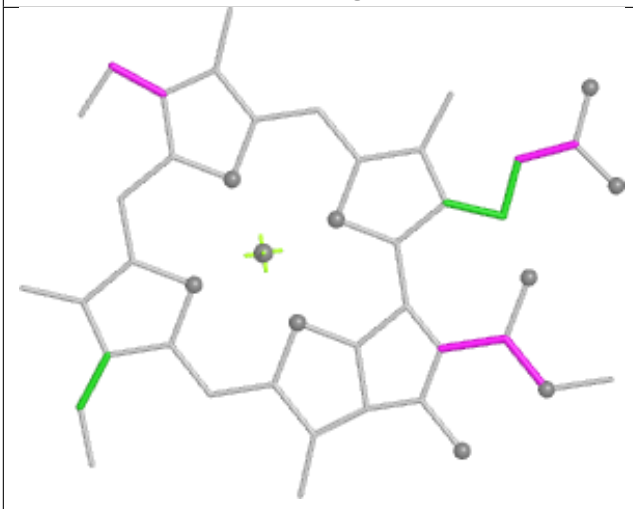
Ligand CLA b3 415



Bond lengths



Bond angles

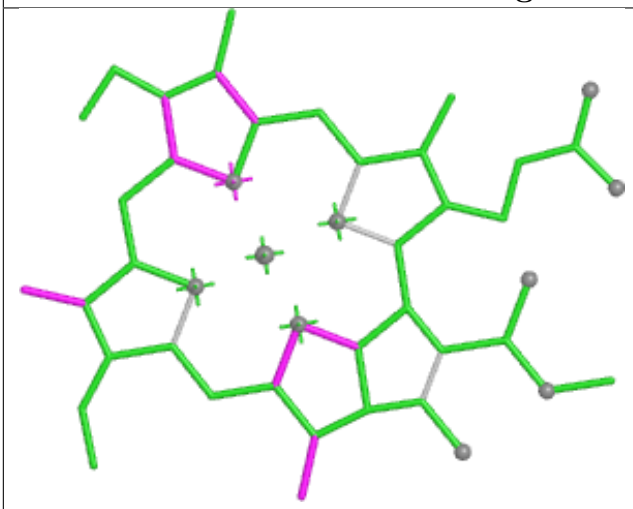


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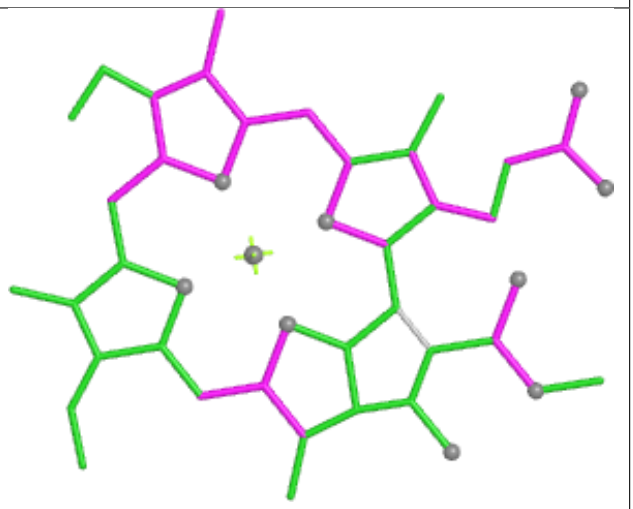


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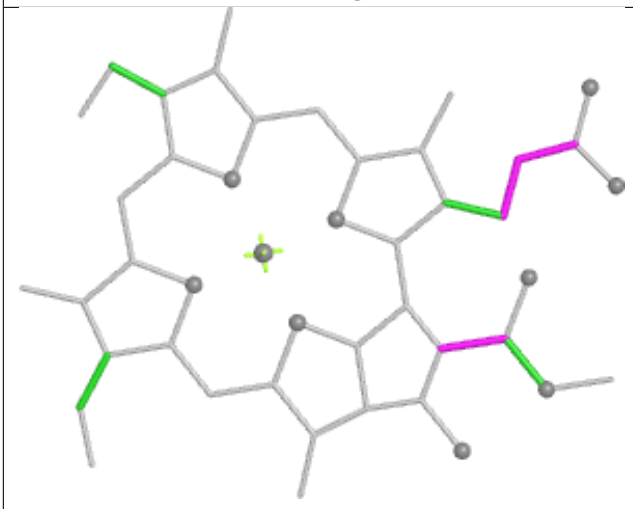
Ligand CLA aB 824



Bond lengths



Bond angles

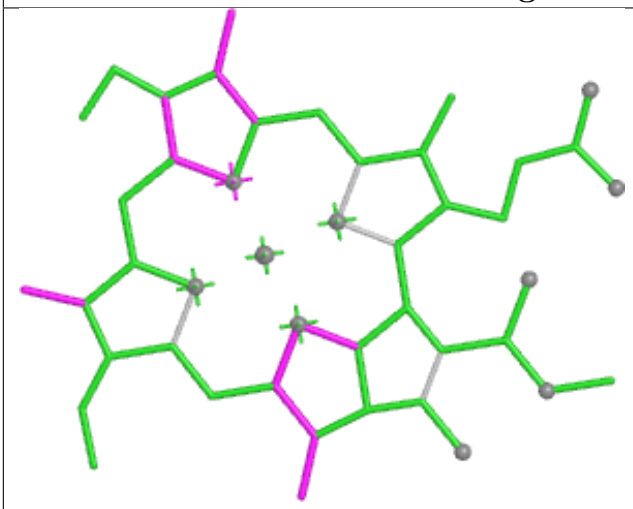


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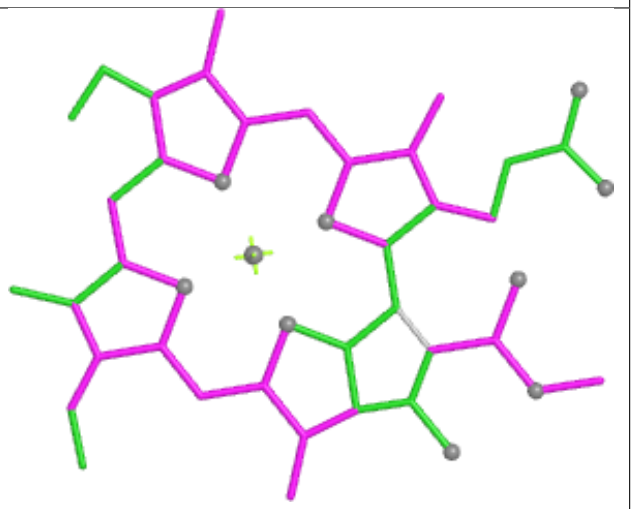


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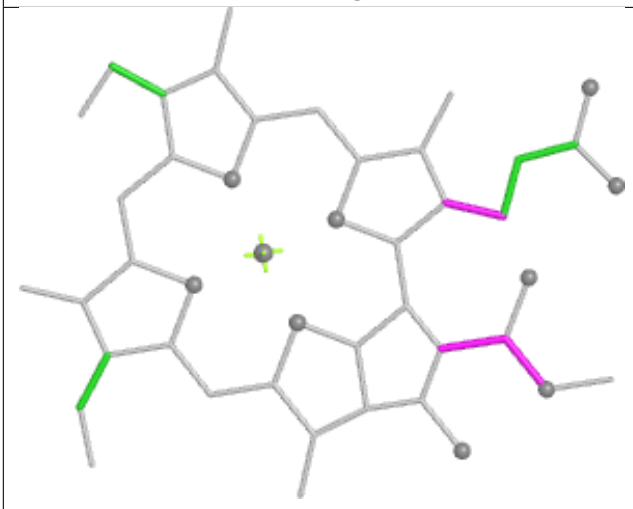
Ligand CLA b5 405



Bond lengths



Bond angles

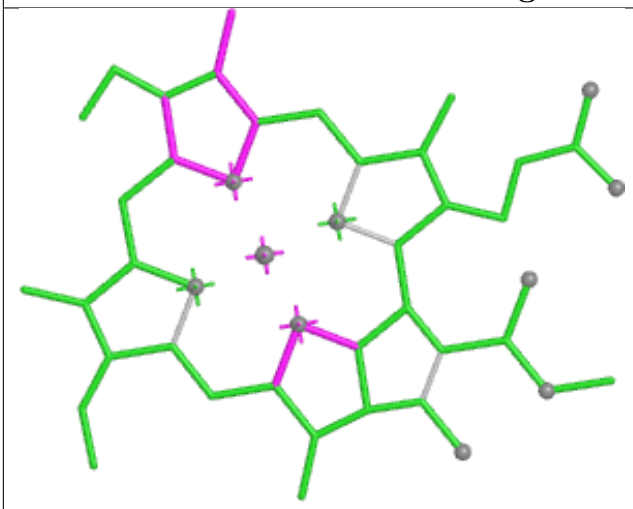


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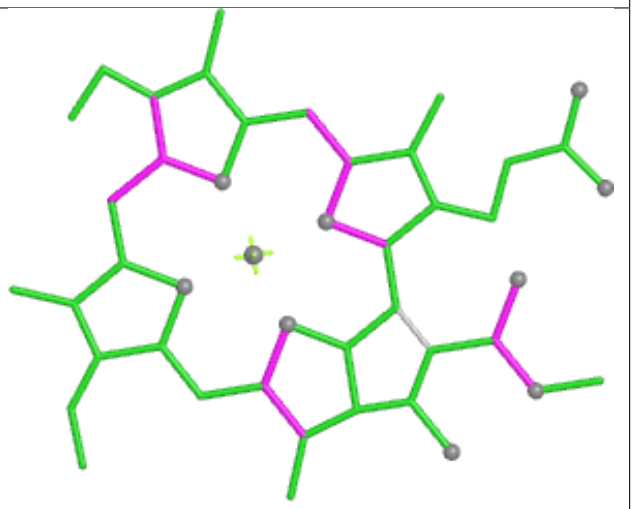


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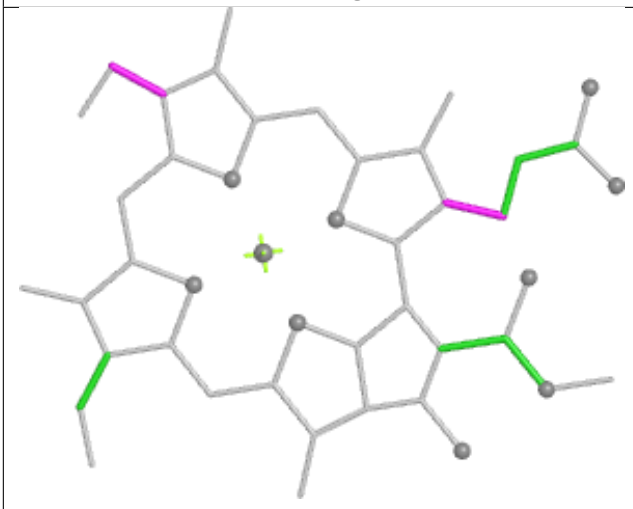
Ligand CLA b2 414



Bond lengths



Bond angles

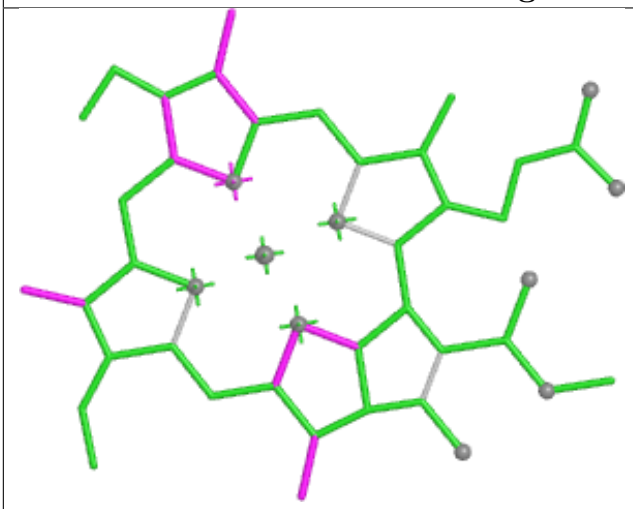


Torsions

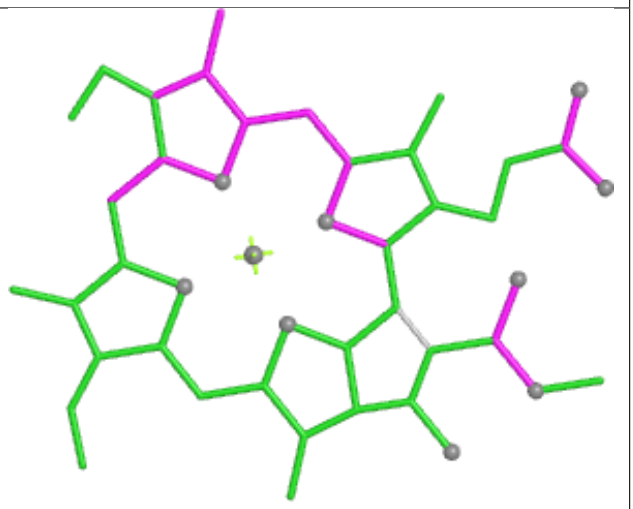


Rings

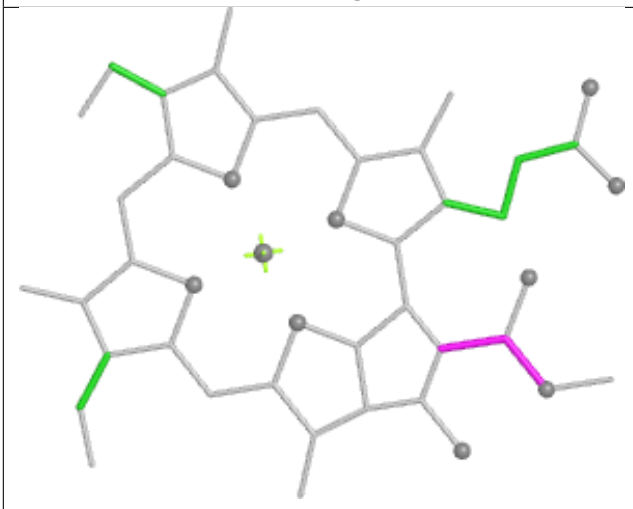
Ligand CLA b1 406



Bond lengths



Bond angles

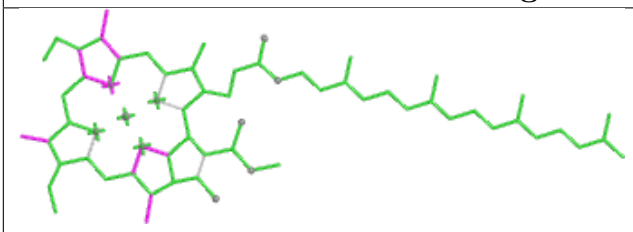


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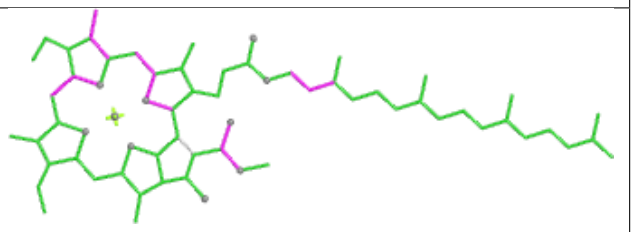


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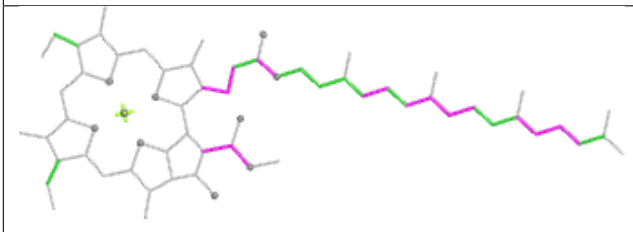
Ligand CLA c5 402



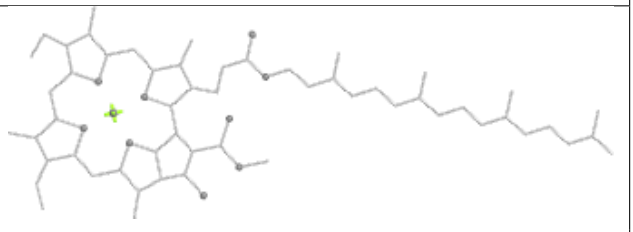
Bond lengths



Bond angles

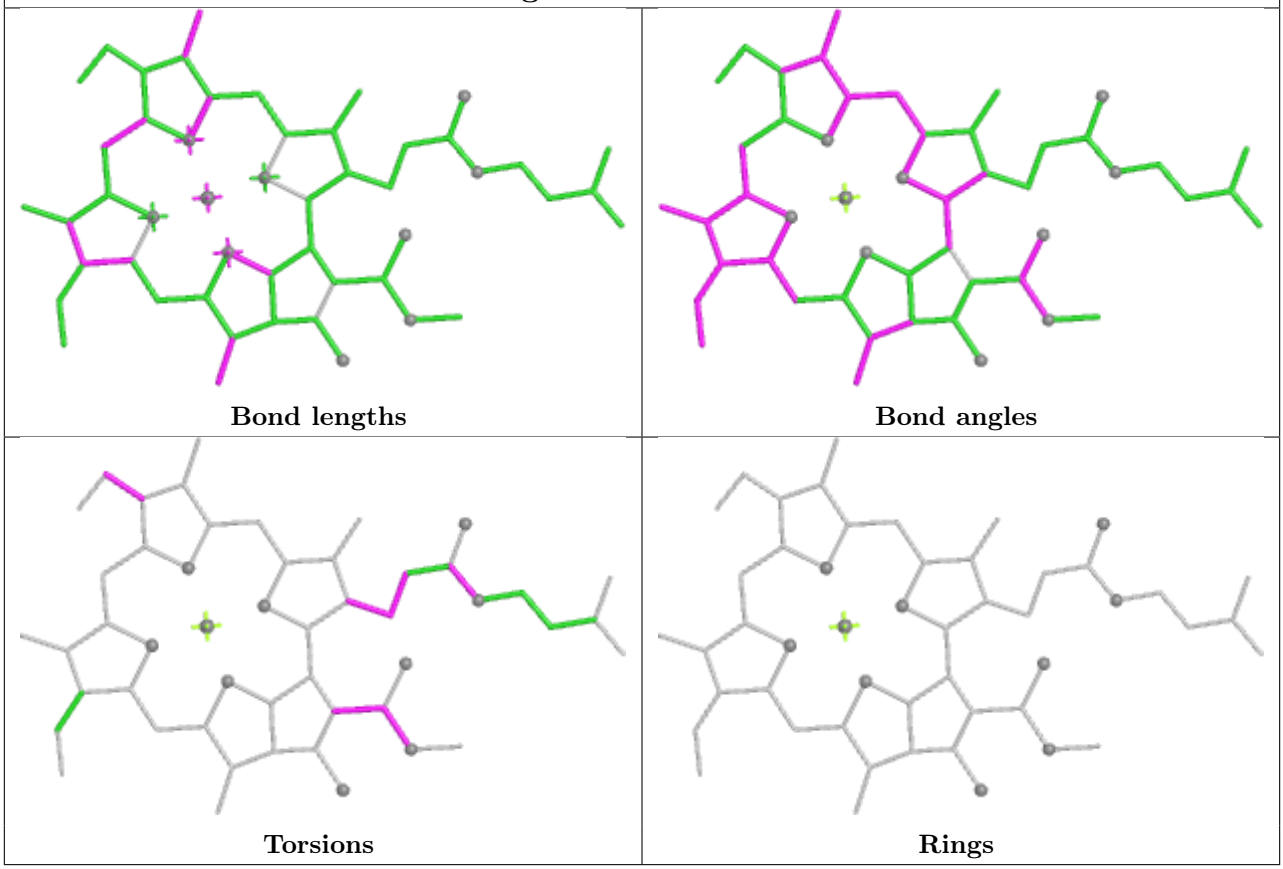


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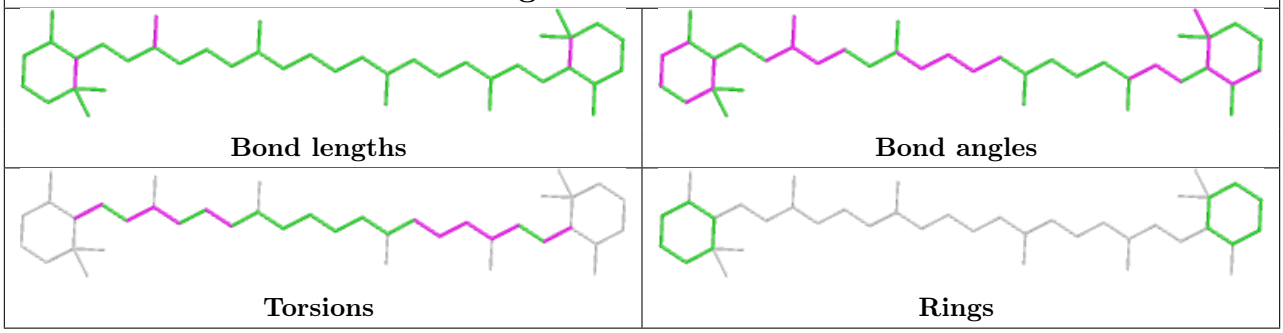


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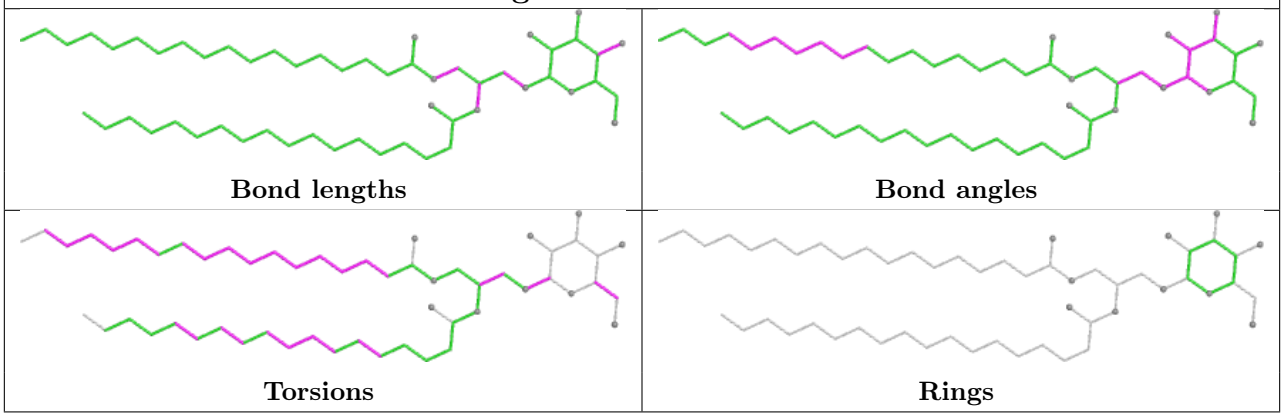
Ligand CLA c5 416

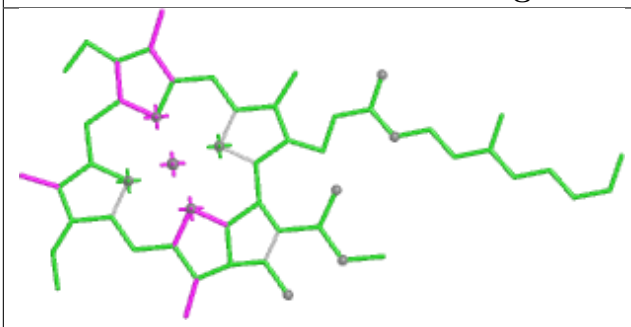
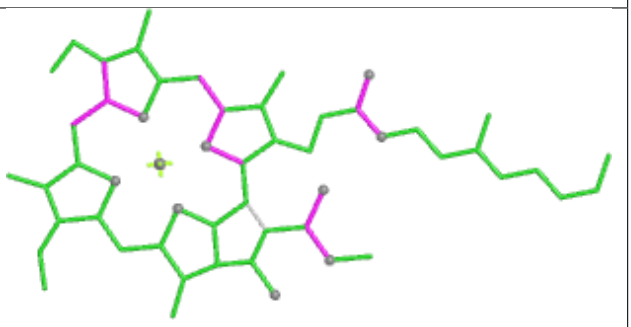
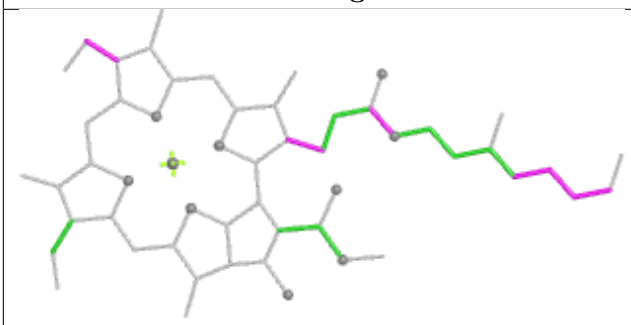
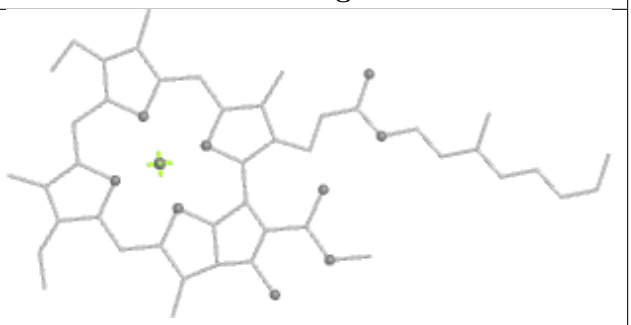


Ligand BCR a1 420

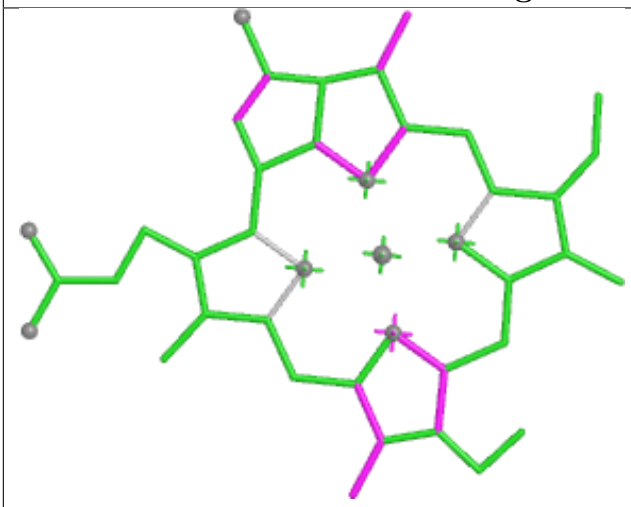


Ligand LMG aB 850

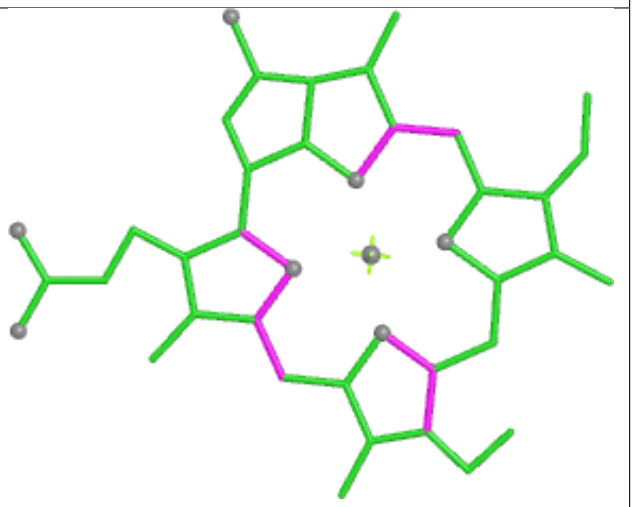


Ligand CLA bA 836	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

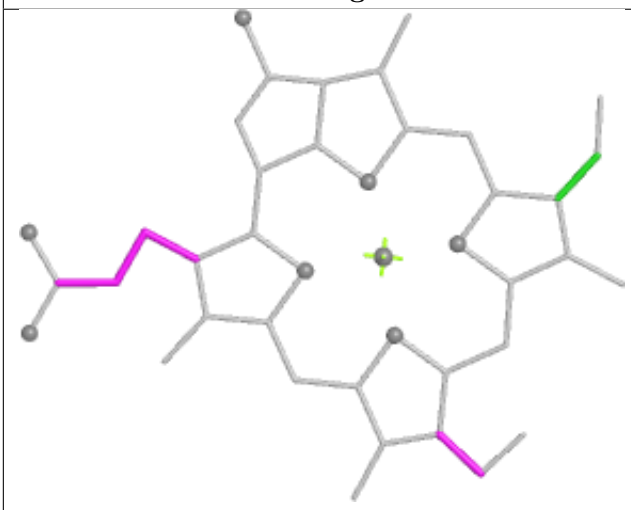
Ligand CLA aA 844



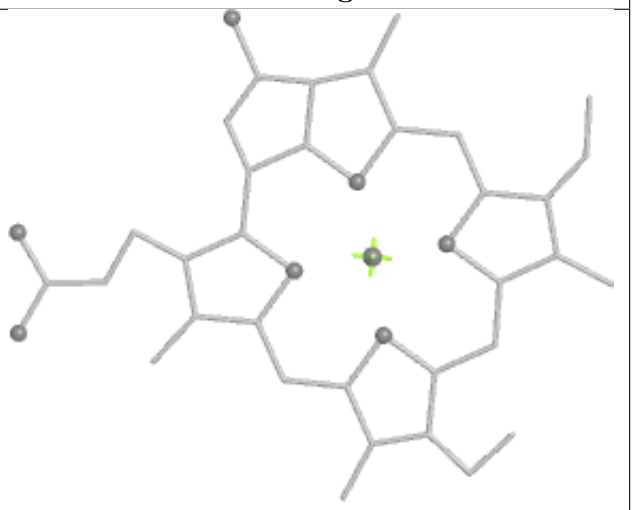
Bond lengths



Bond angles

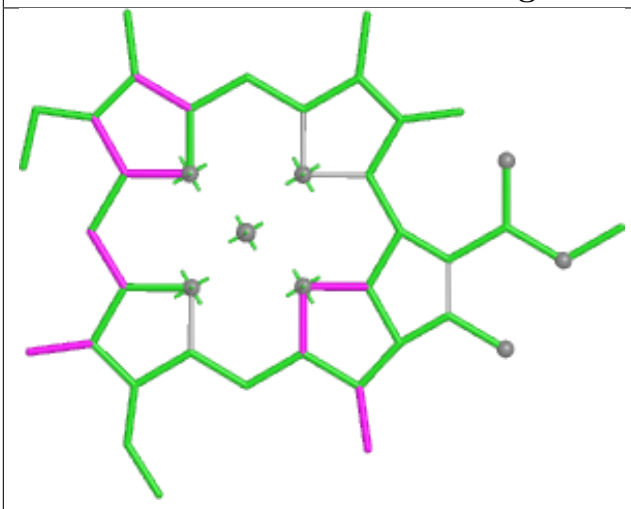


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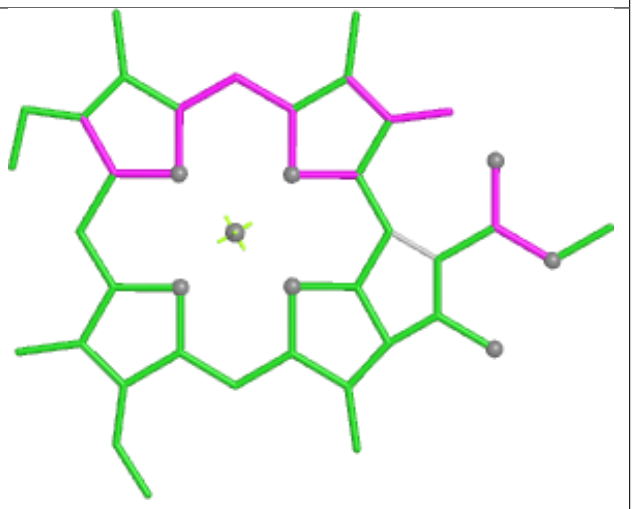


Rings

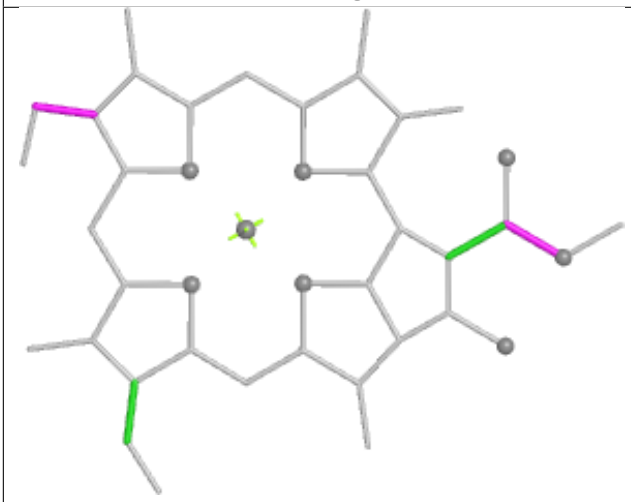
Ligand CLA b6 415



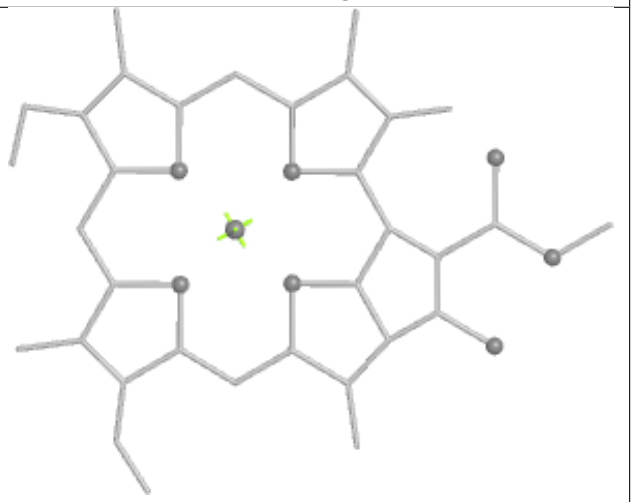
Bond lengths



Bond angles

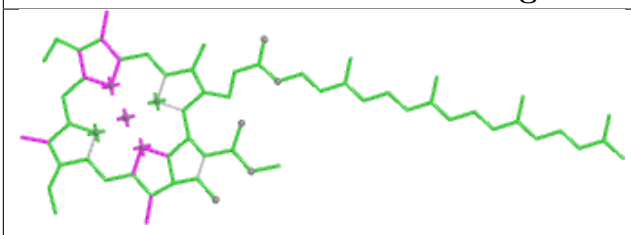


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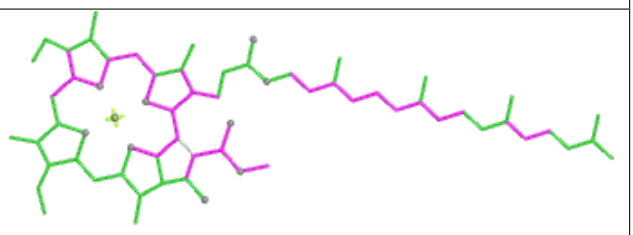


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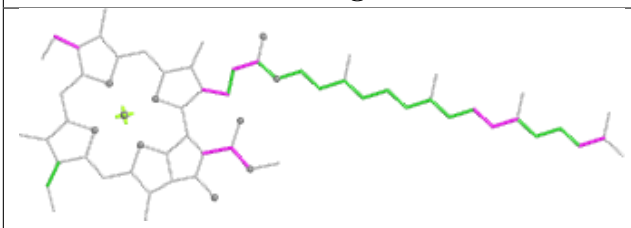
Ligand CLA a2 422



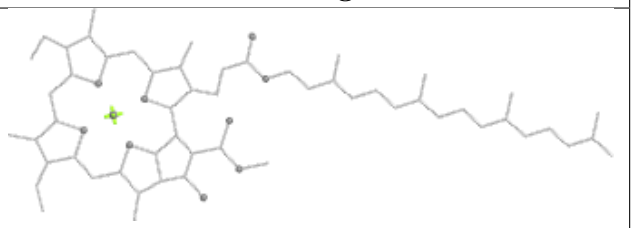
Bond lengths



Bond angles

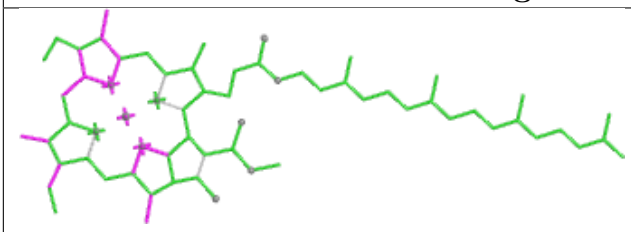


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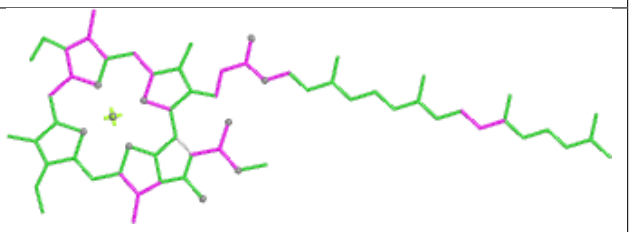


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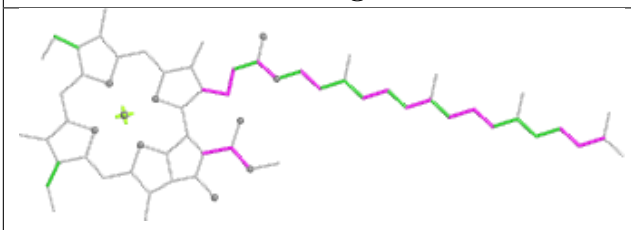
Ligand CLA bA 803



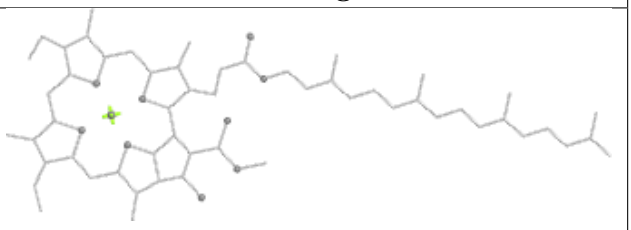
Bond lengths



Bond angles

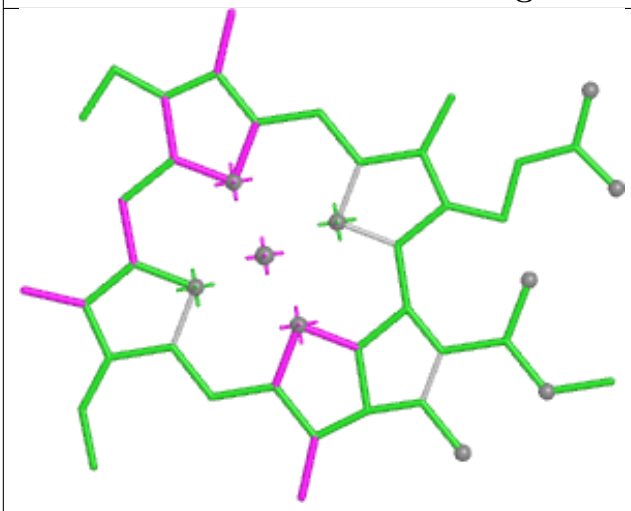


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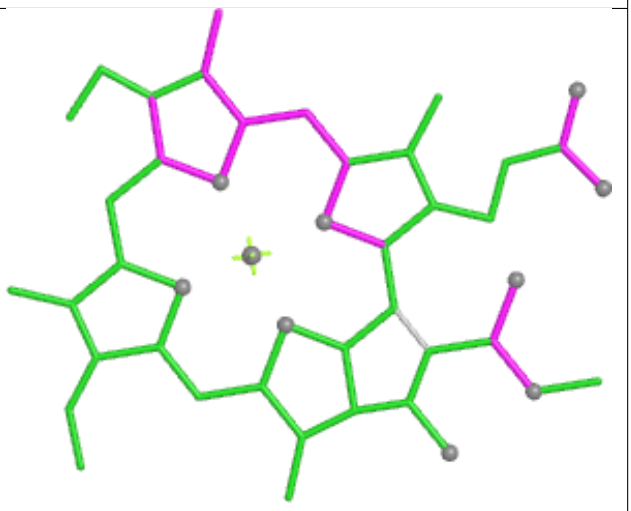


Rings

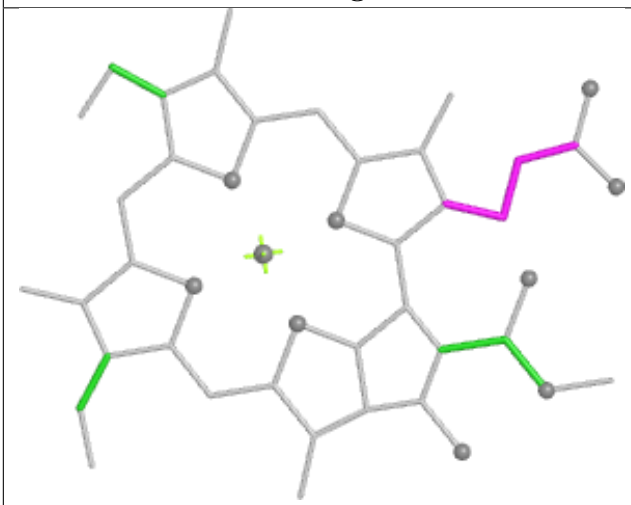
Ligand CLA aB 813



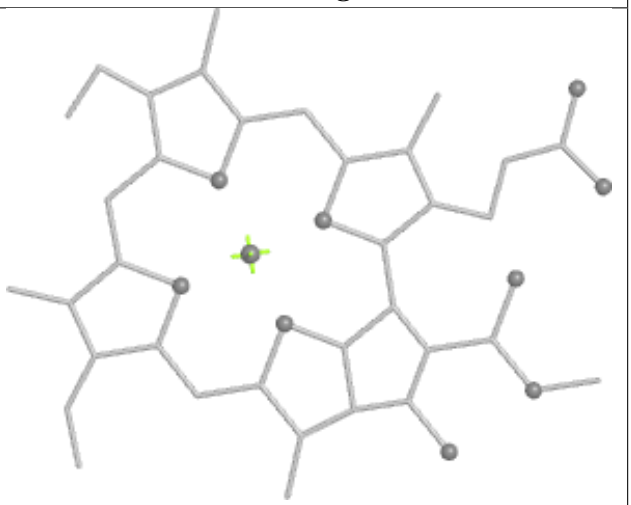
Bond lengths



Bond angles

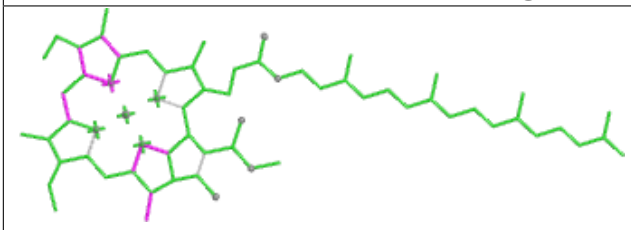


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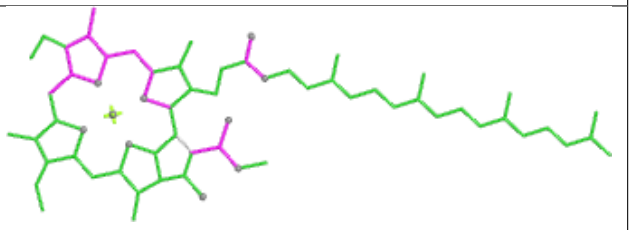


Rings

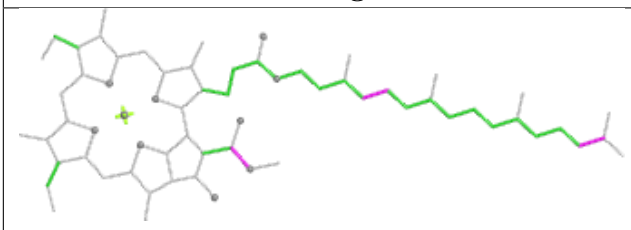
Ligand CLA a4 409



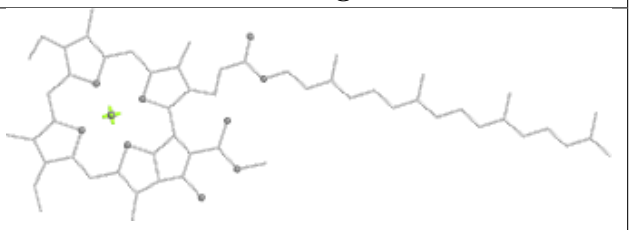
Bond lengths



Bond angles

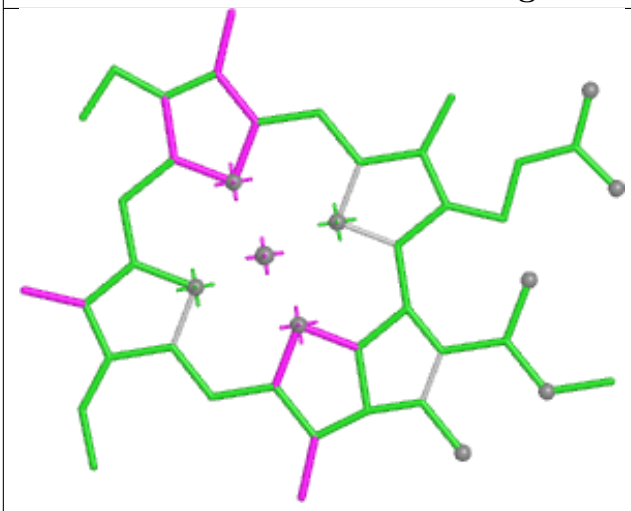


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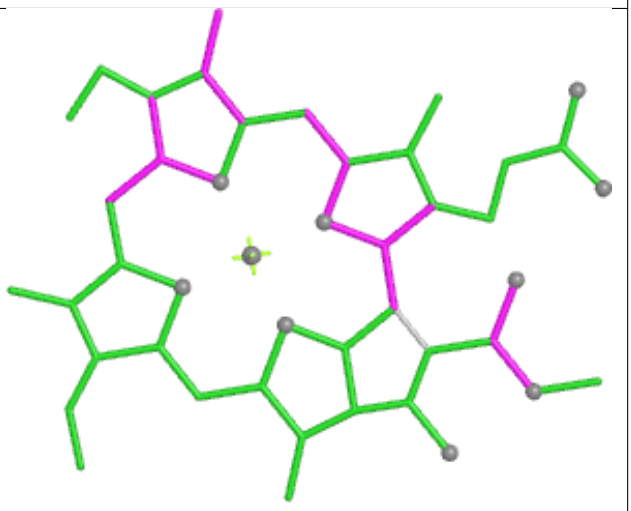


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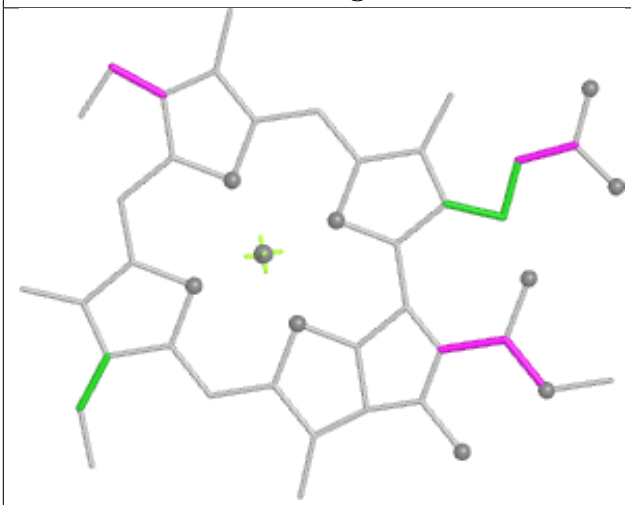
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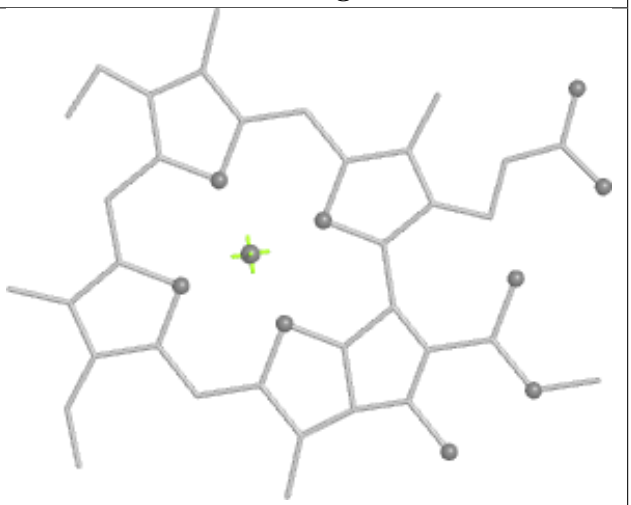
Bond lengths



Bond angles

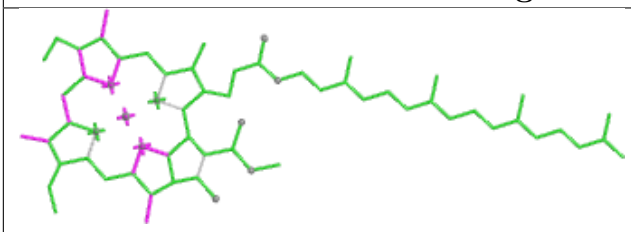


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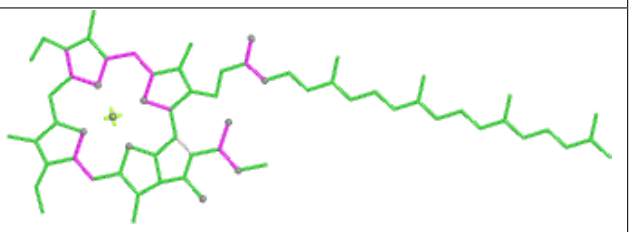


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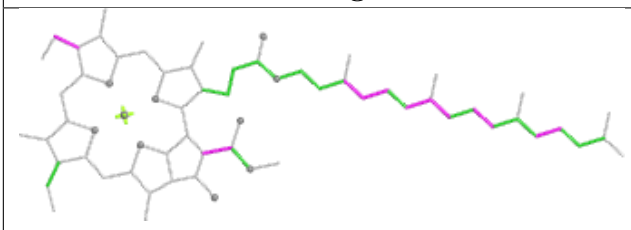
Ligand CLA cA 828



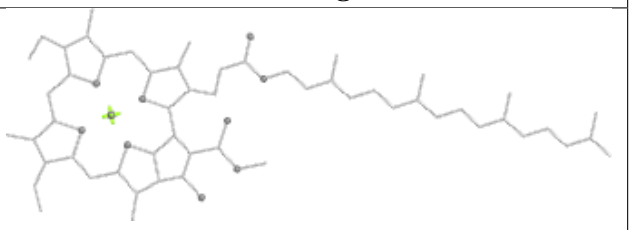
Bond lengths



Bond angles

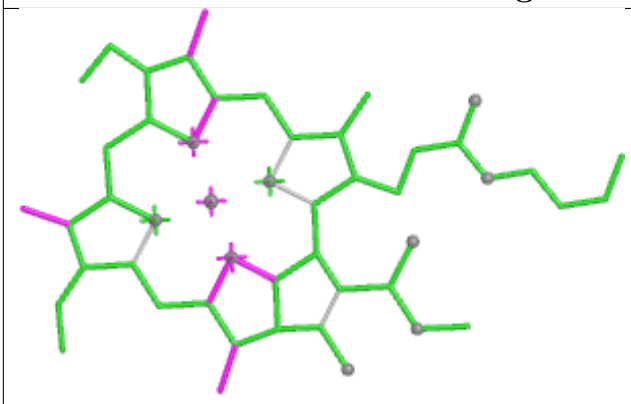


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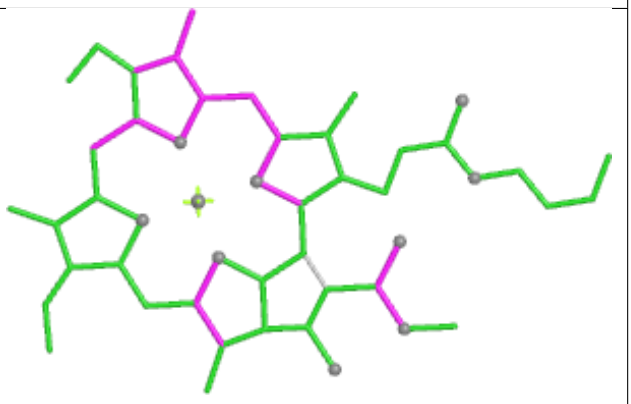


Rings

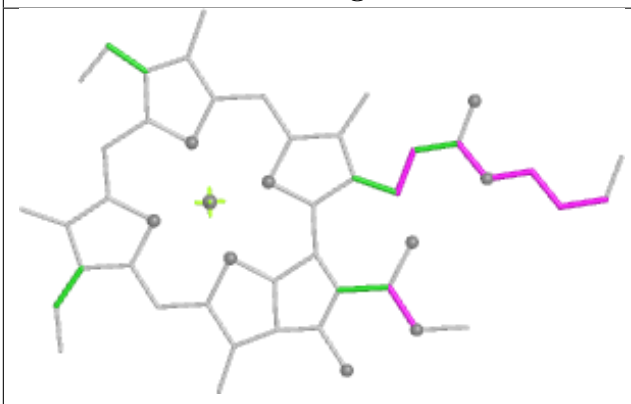
Ligand CLA aB 832



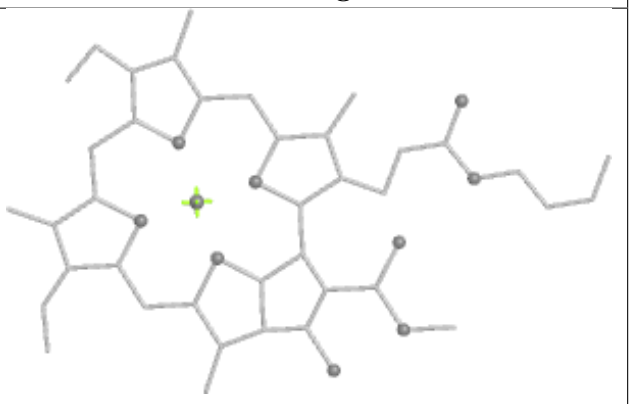
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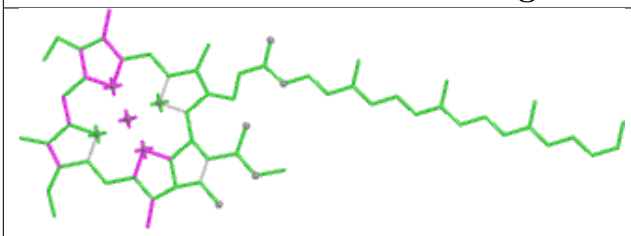
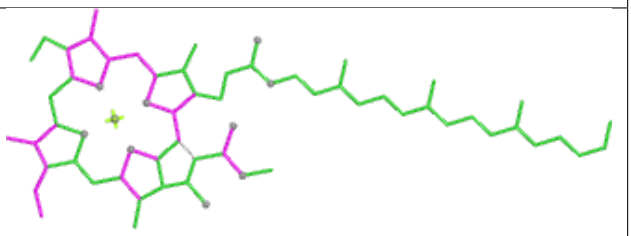
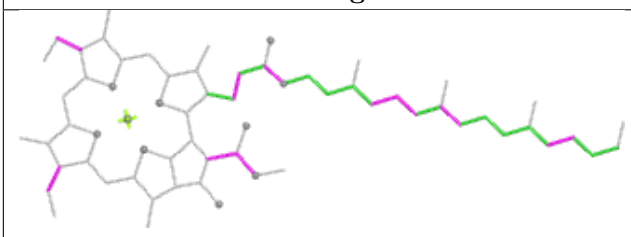
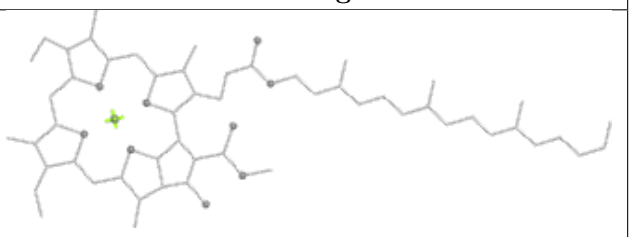
Bond angles

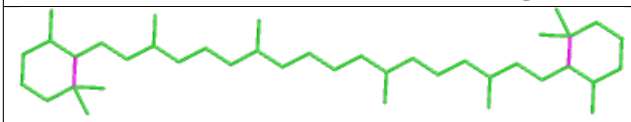
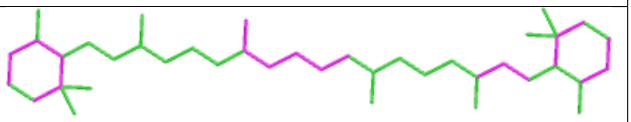
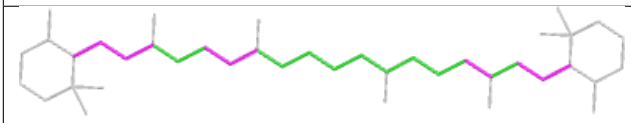
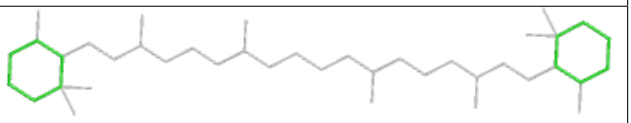


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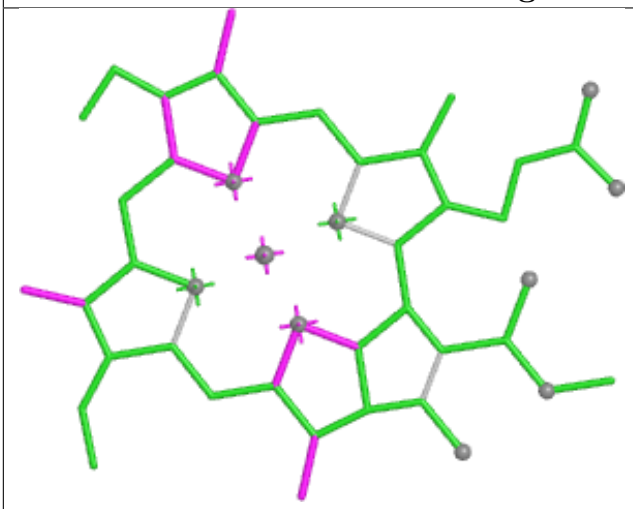


Rings

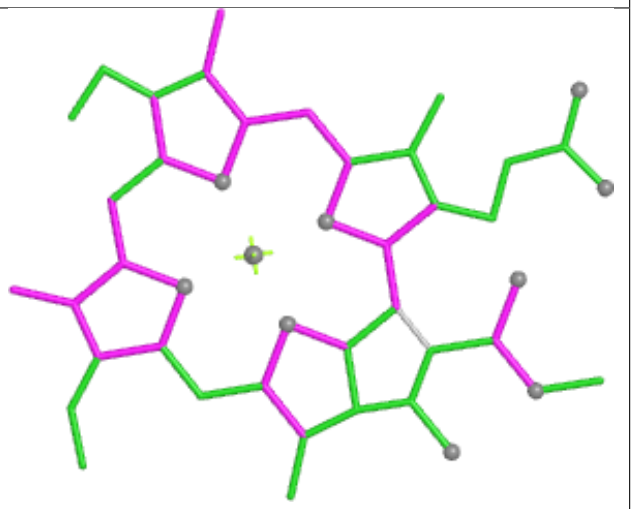
Ligand CLA b6 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a2 421	
	
Bond lengths	Bond angles
	
Torsions	Rings

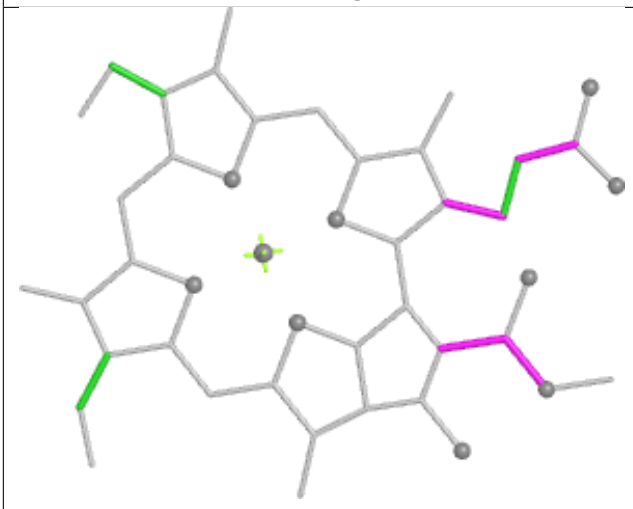
Ligand CLA b3 412



Bond lengths



Bond angles

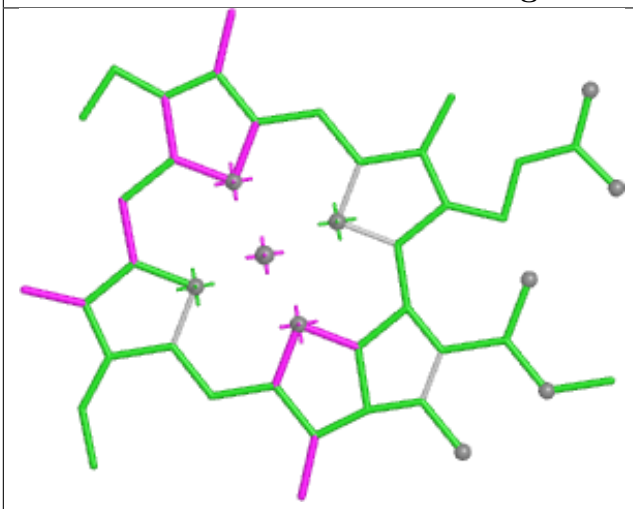


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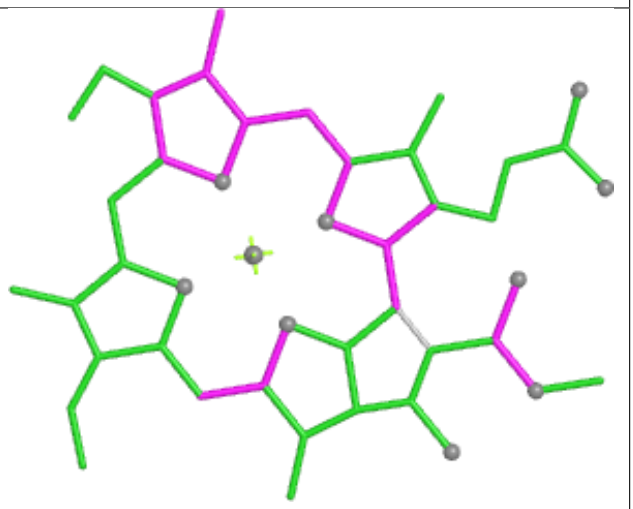


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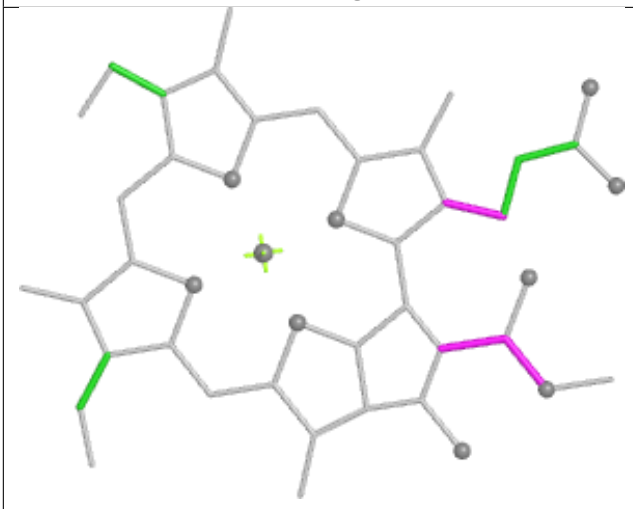
Ligand CLA c1 411



Bond lengths



Bond angles

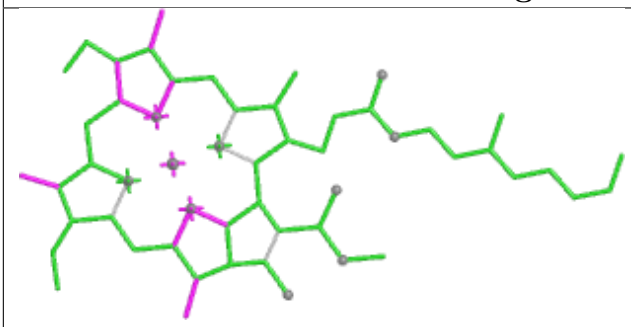


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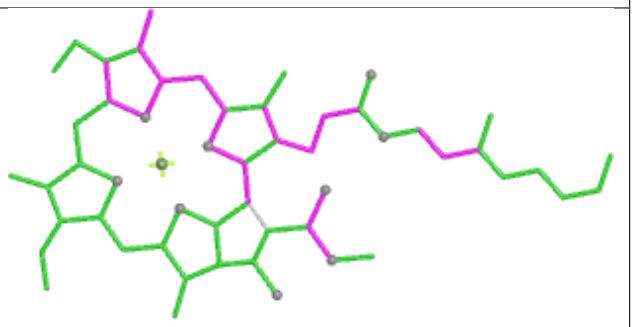


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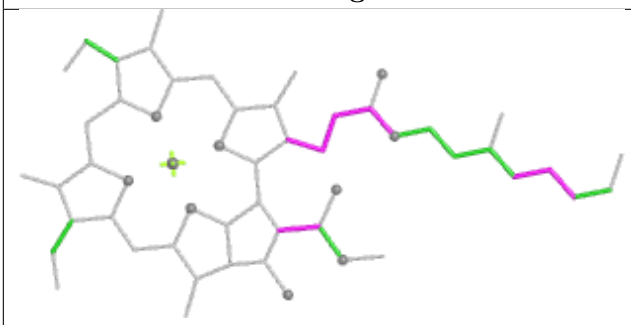
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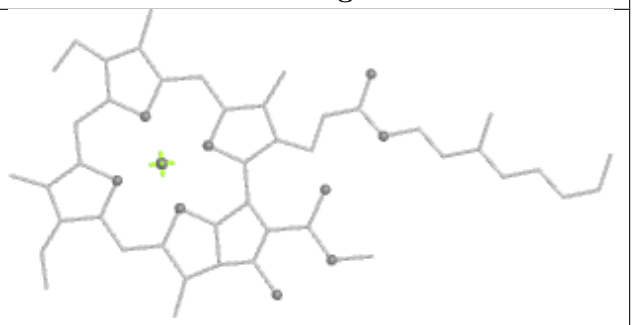
Bond lengths



Bond angles

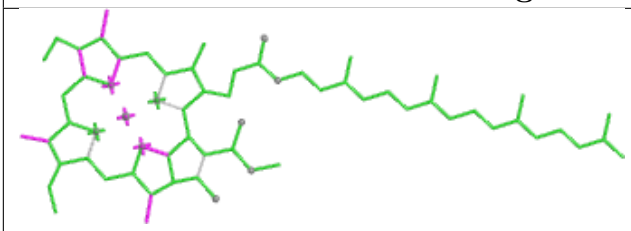


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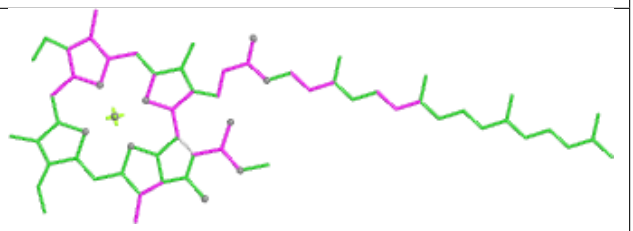


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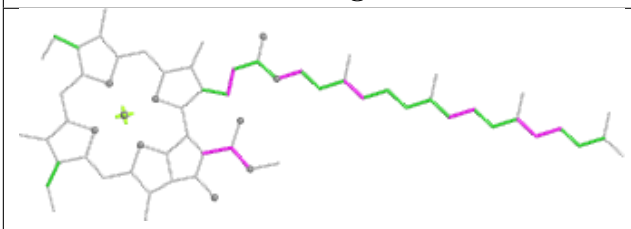
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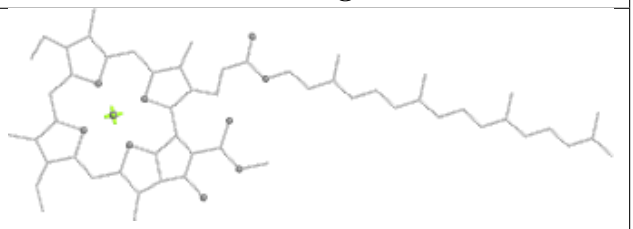
Bond lengths



Bond angles

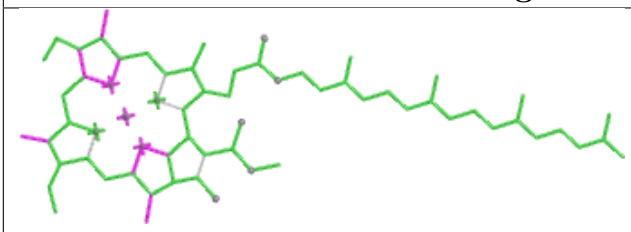


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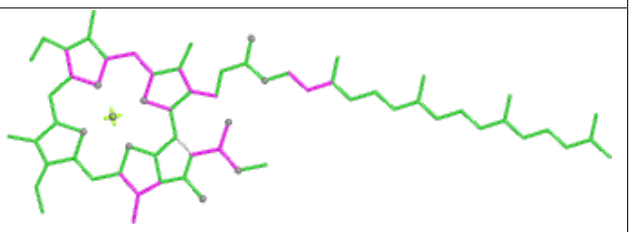


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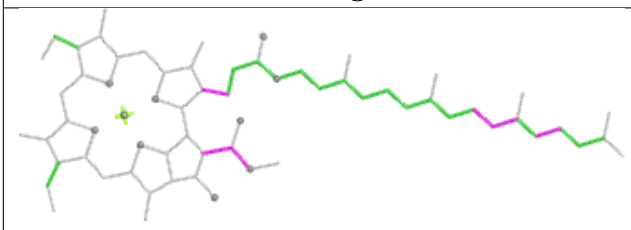
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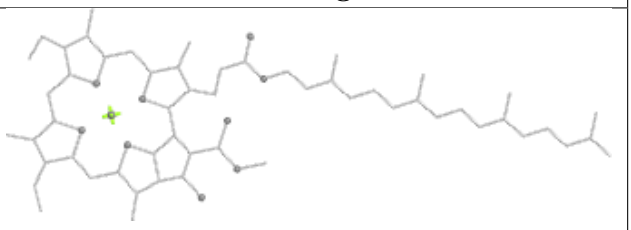
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Bond angles

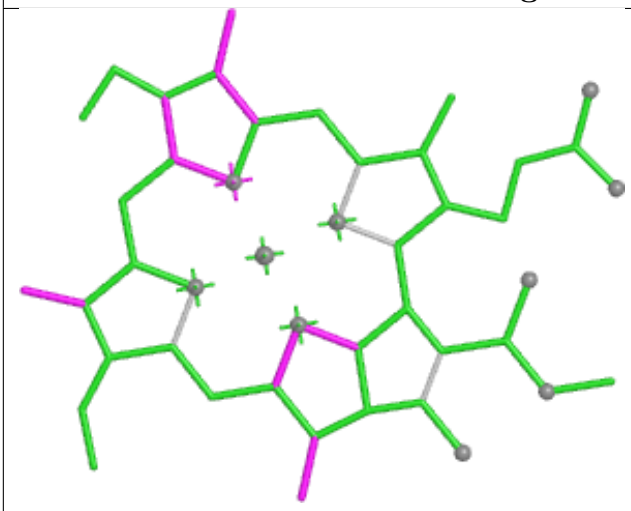


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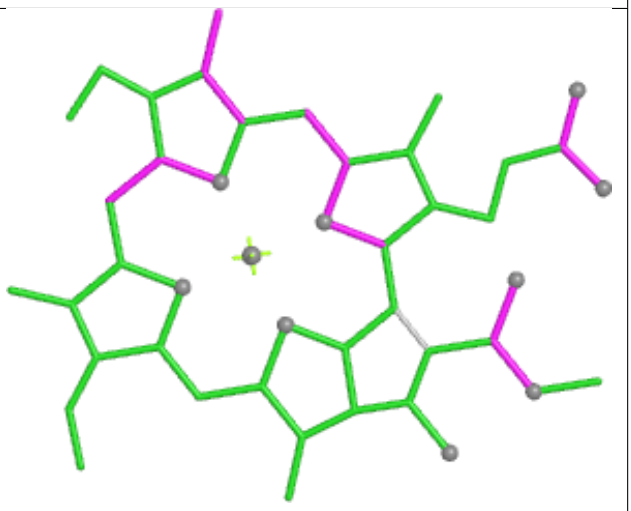


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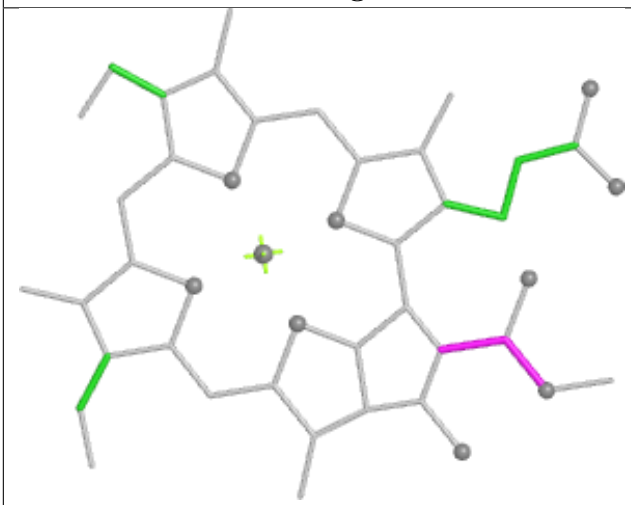
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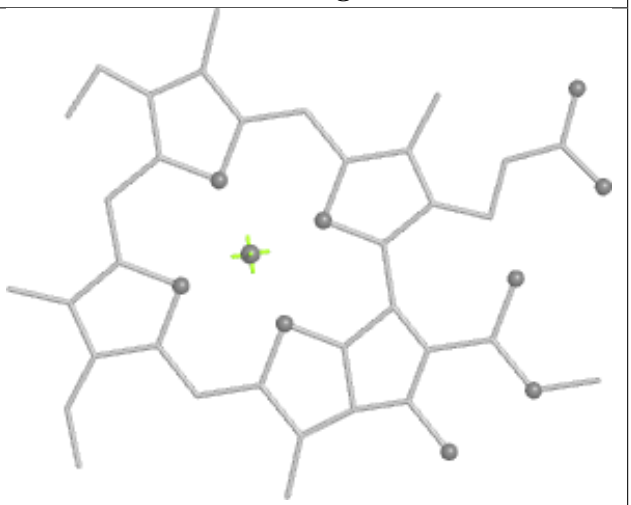
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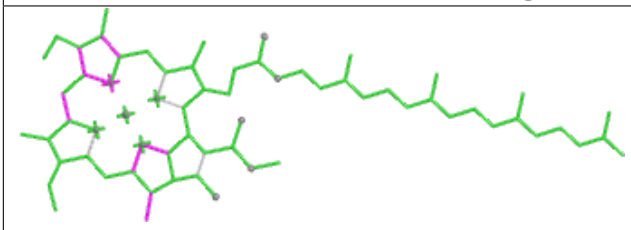


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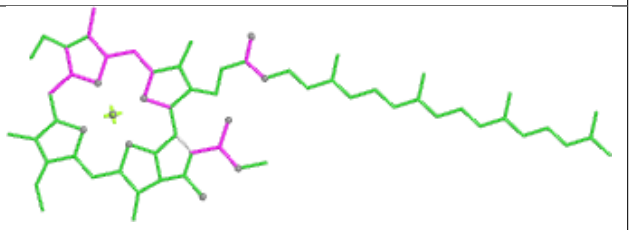


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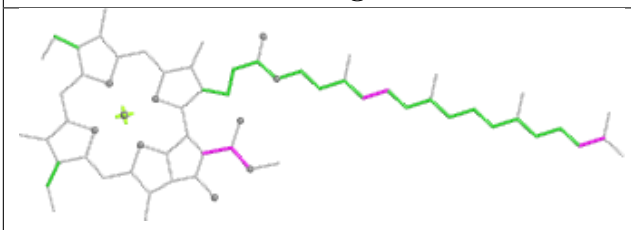
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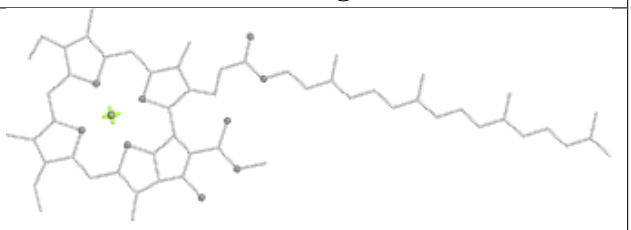
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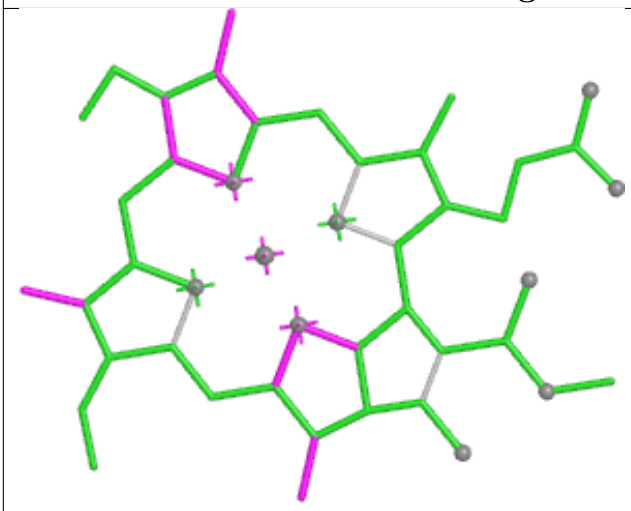


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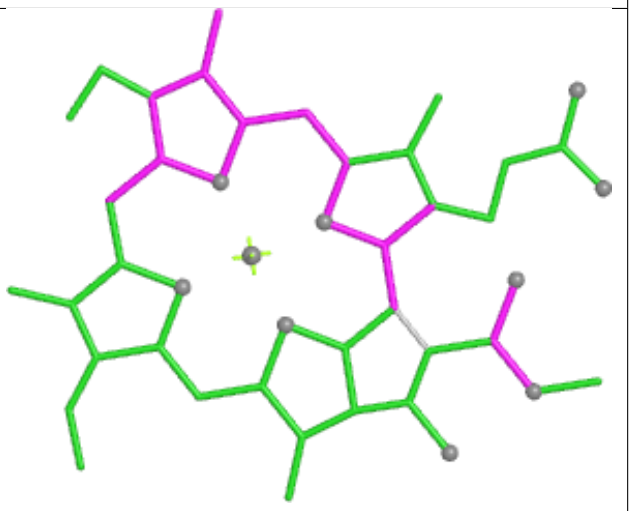


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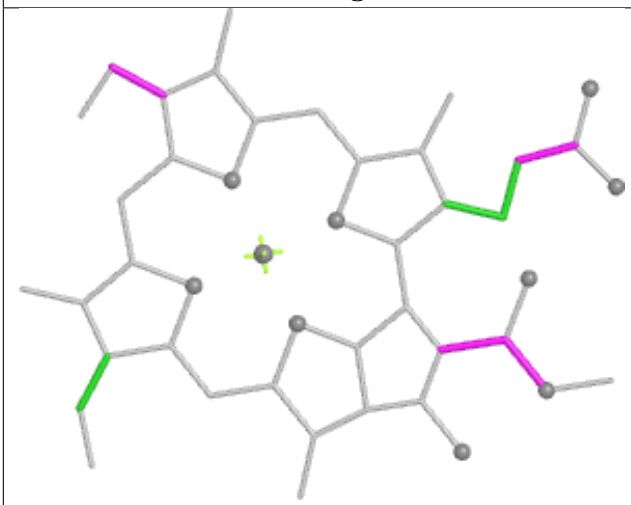
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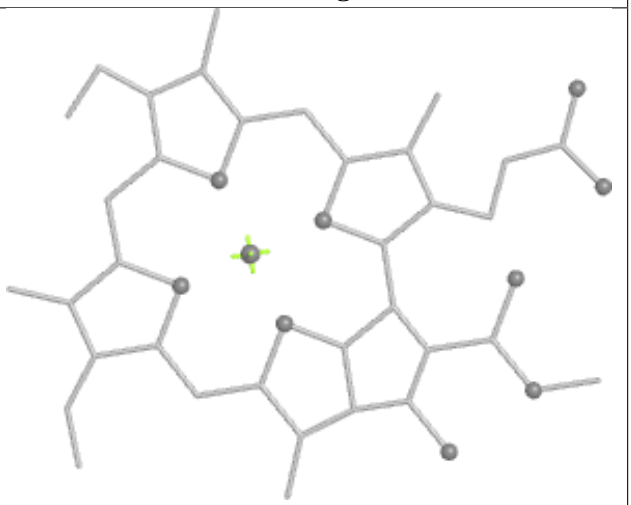
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Bond angles

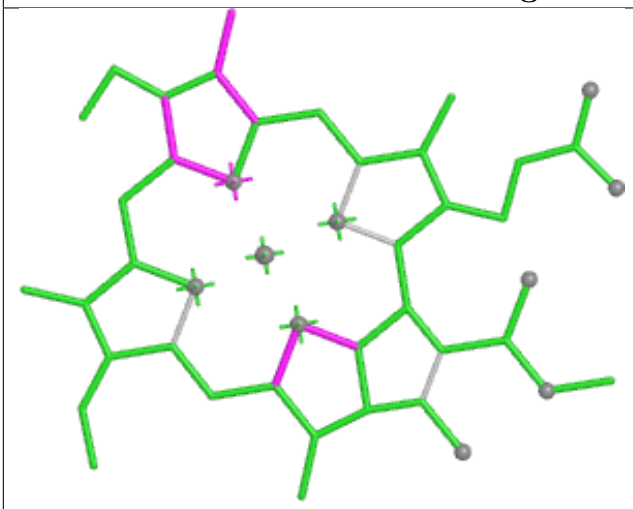


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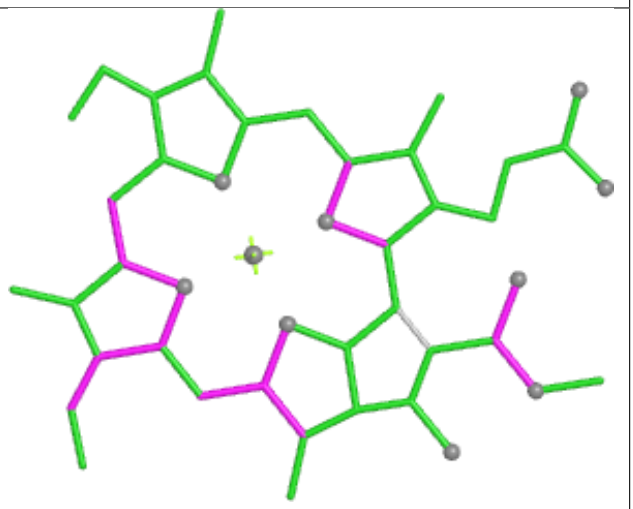


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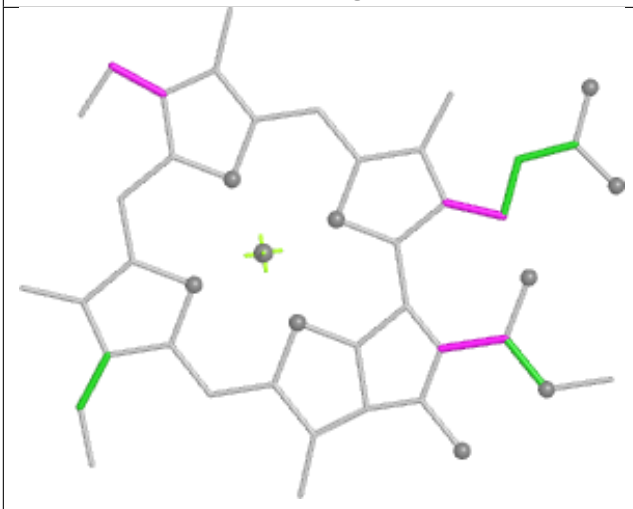
Ligand CLA c6 415



Bond lengths



Bond angles

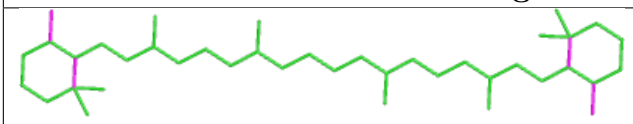


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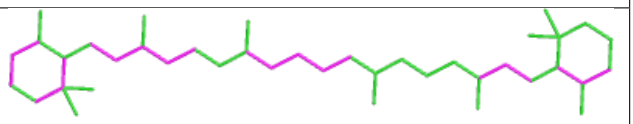


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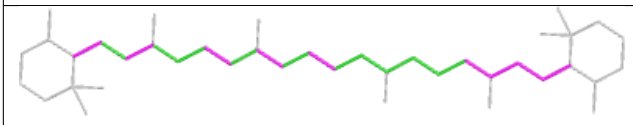
Ligand BCR bB 848



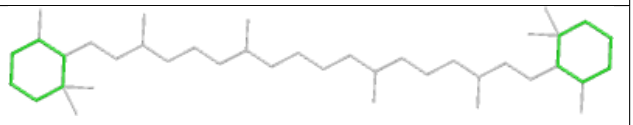
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Bond angles

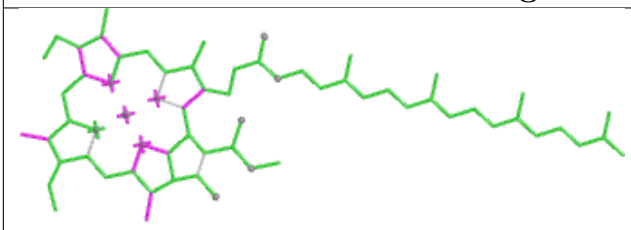


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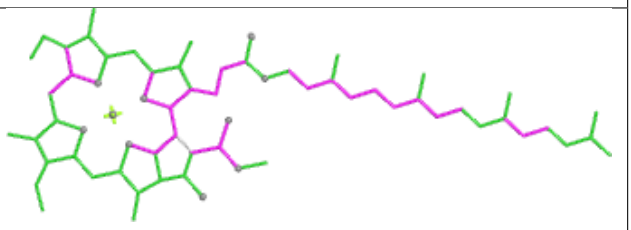


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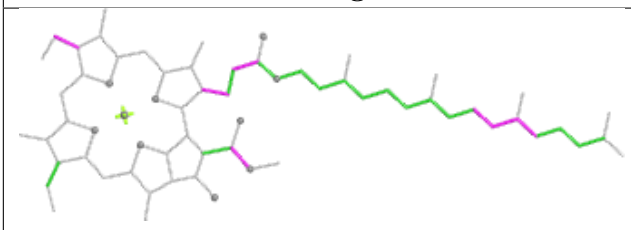
Ligand CLA a3 421



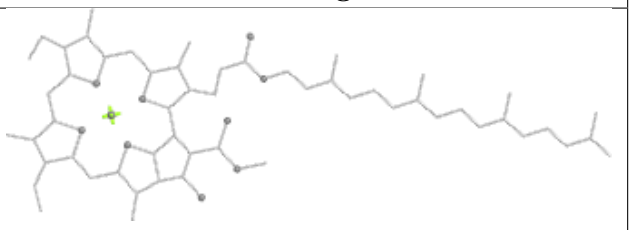
Bond lengths



Bond angles

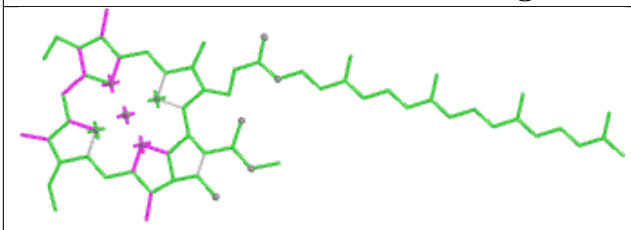


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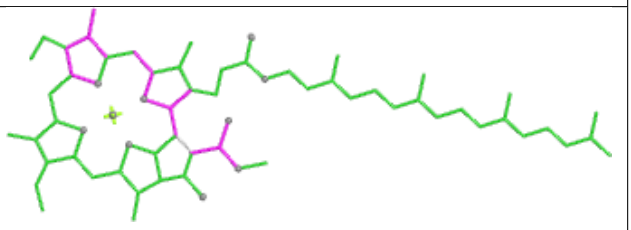


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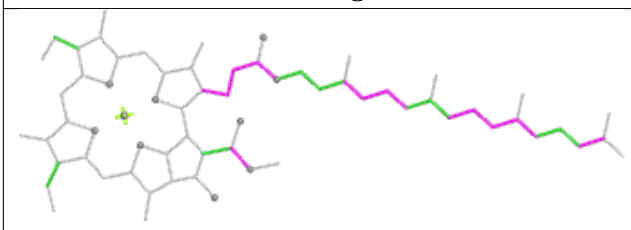
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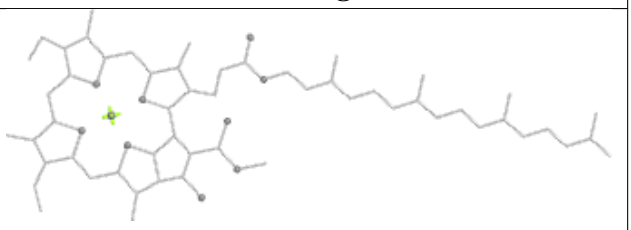
Bond lengths



Bond angles

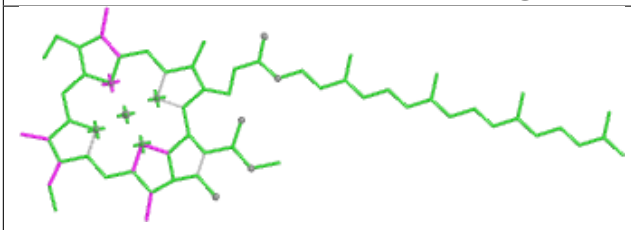


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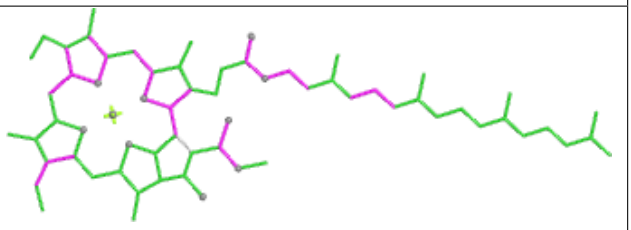


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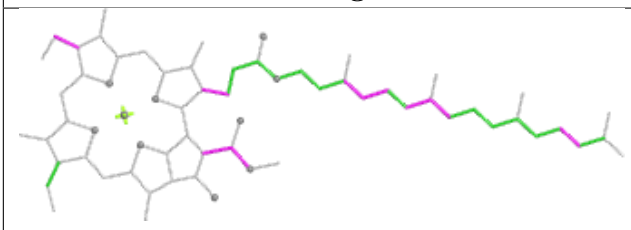
Ligand CLA cB 811



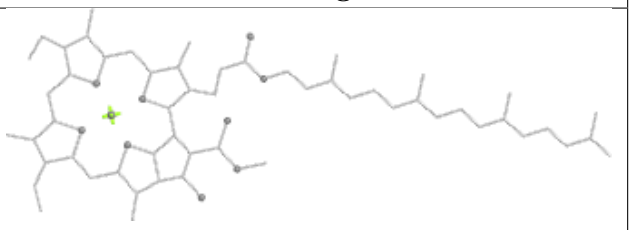
Bond lengths



Bond angles

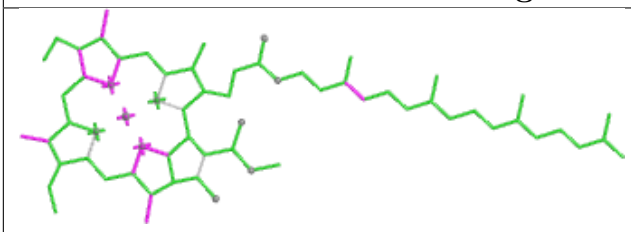


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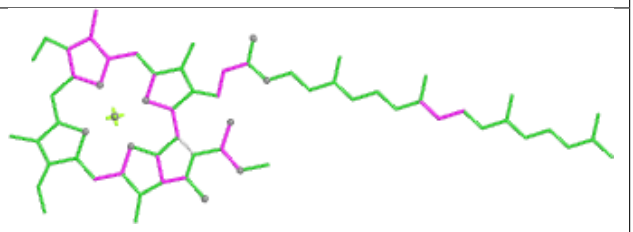


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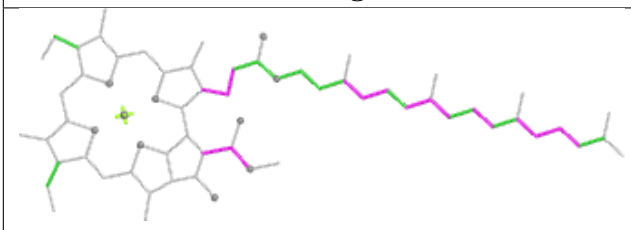
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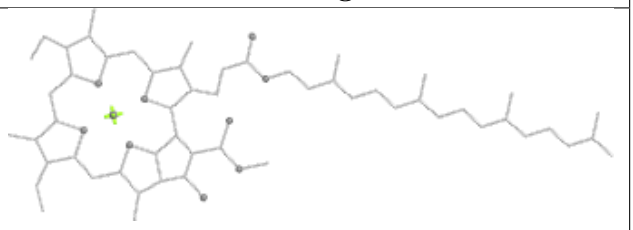
Bond lengths



Bond angles

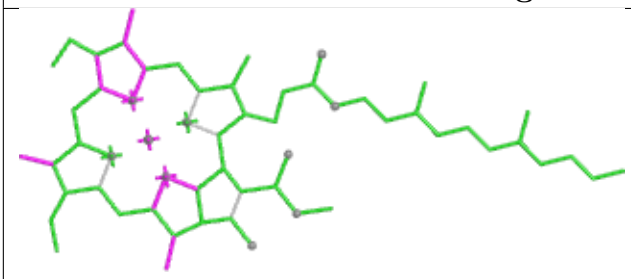


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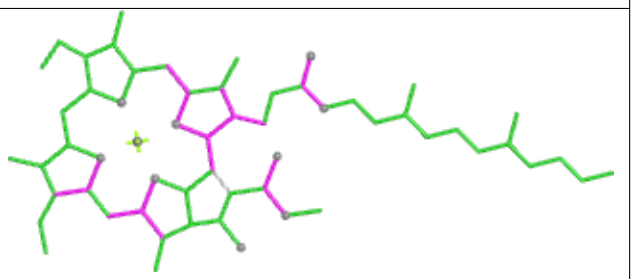


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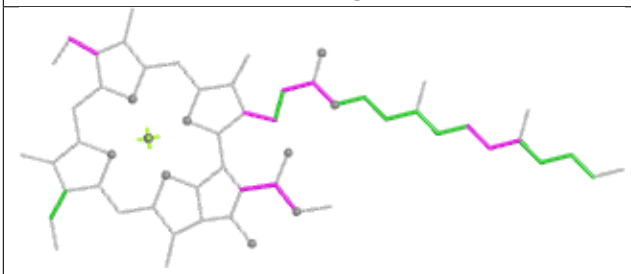
Ligand CLA aB 834



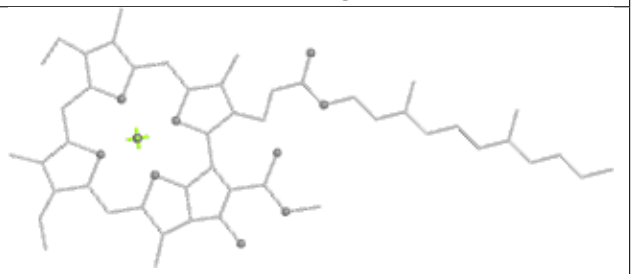
Bond lengths



Bond angles

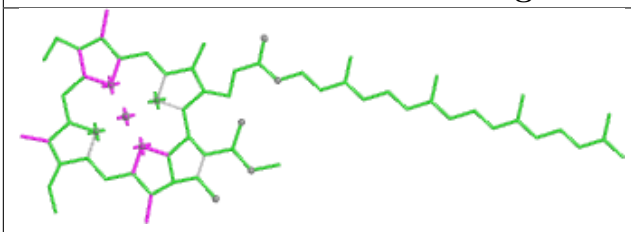


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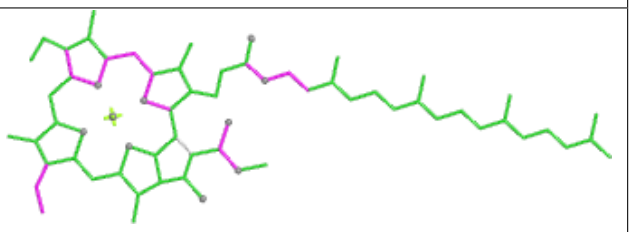


Rings

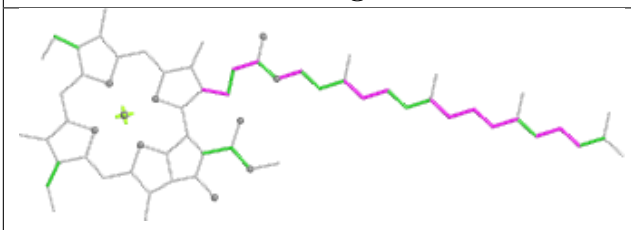
Ligand CLA aA 843



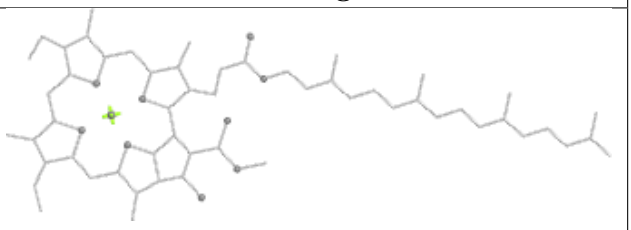
Bond lengths



Bond angles

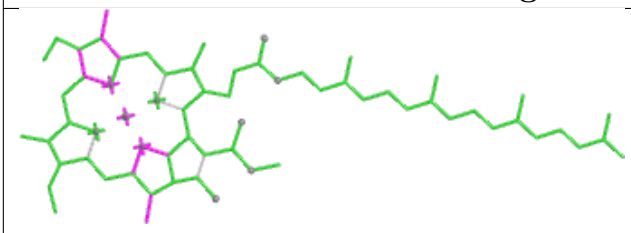


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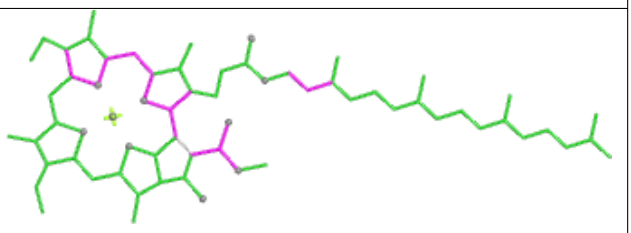


Rings

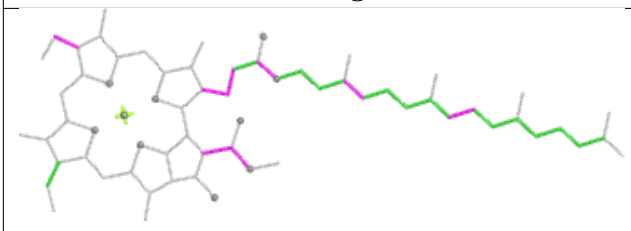
Ligand CLA a1 403



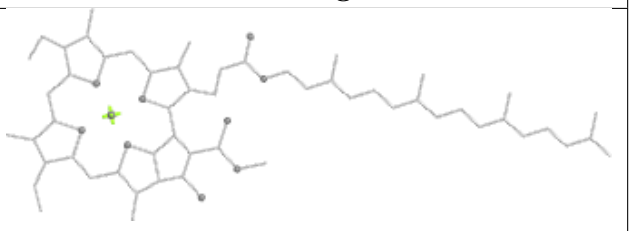
Bond lengths



Bond angles

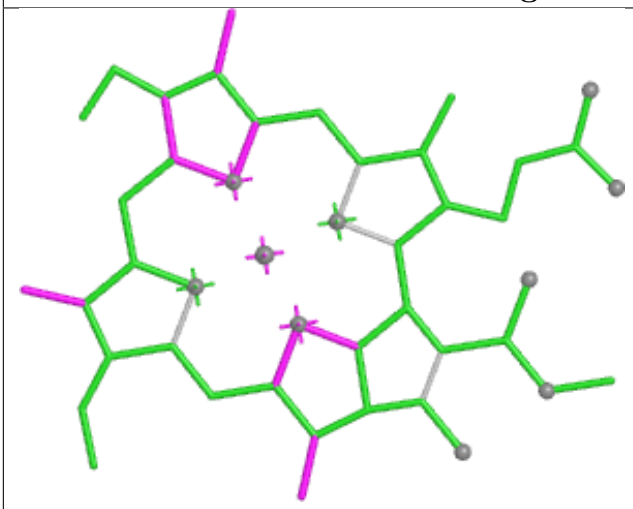


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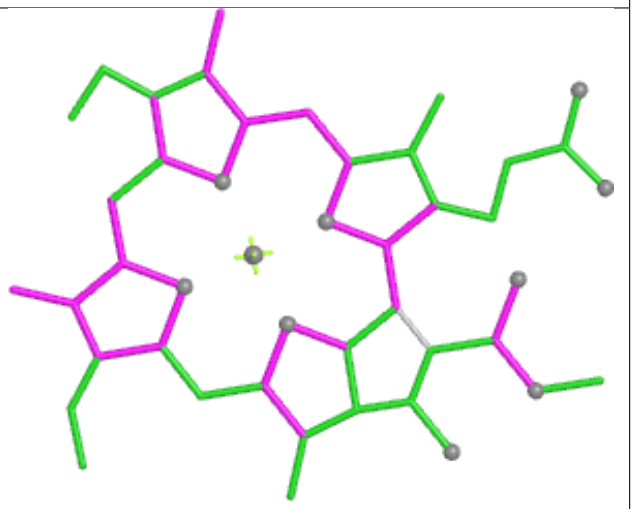


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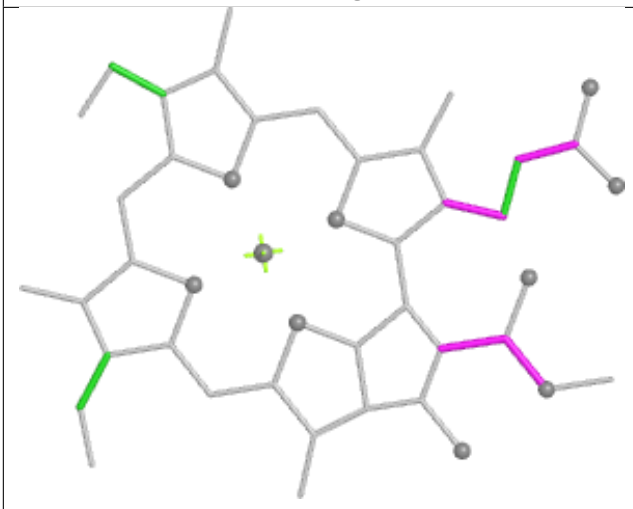
Ligand CLA c4 412



Bond lengths



Bond angles

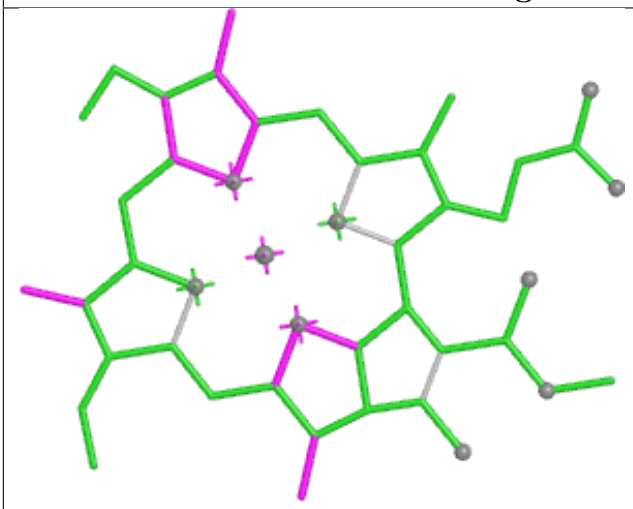


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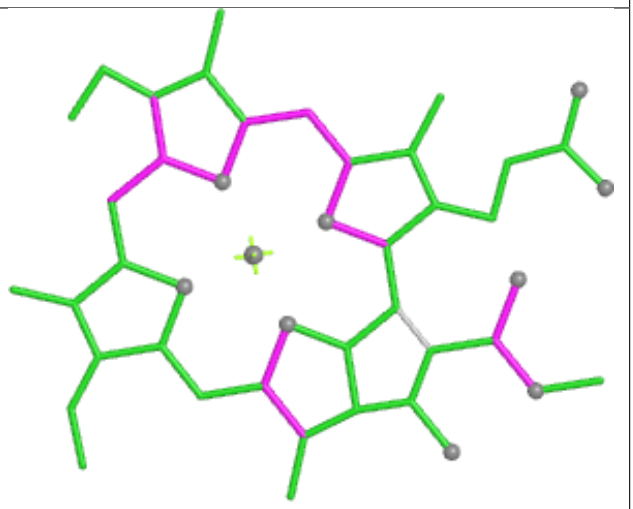


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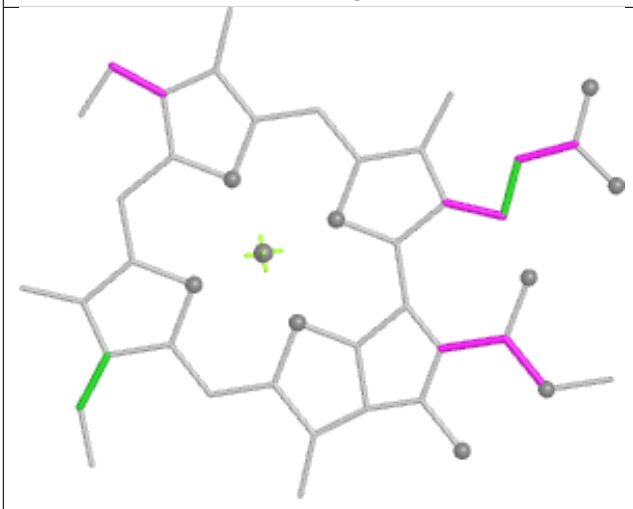
Ligand CLA aA 811



Bond lengths



Bond angles

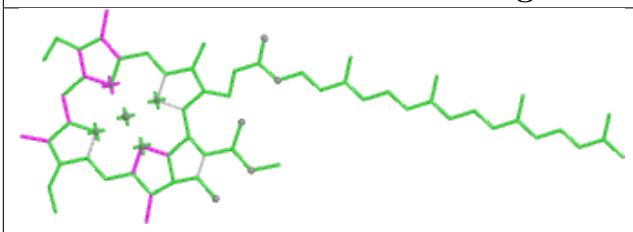


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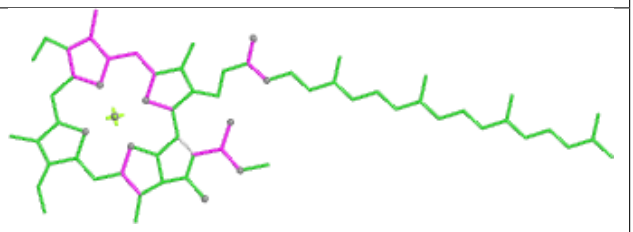


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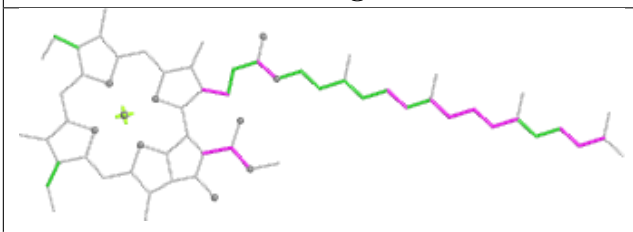
Ligand CLA cB 815



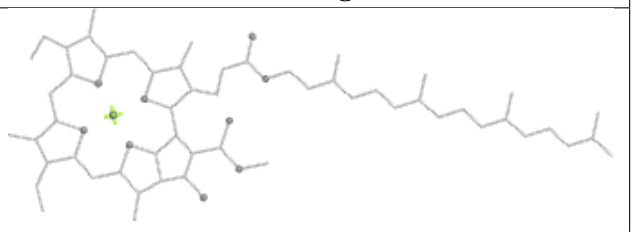
Bond lengths



Bond angles

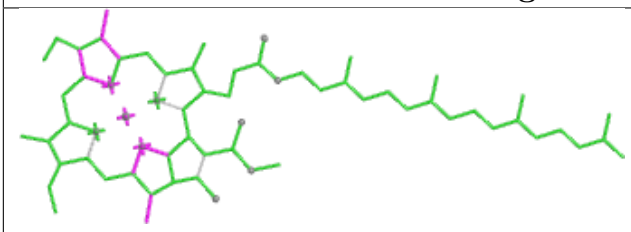


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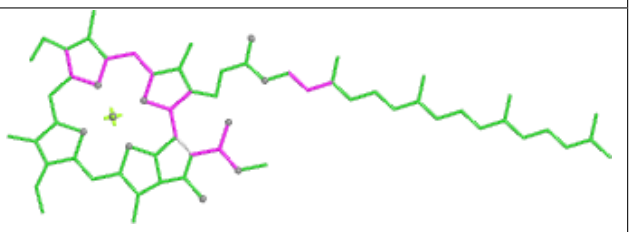


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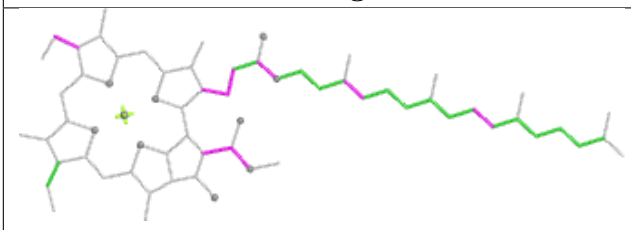
Ligand CLA b1 404



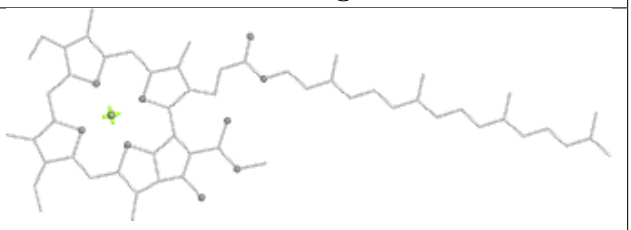
Bond lengths



Bond angles

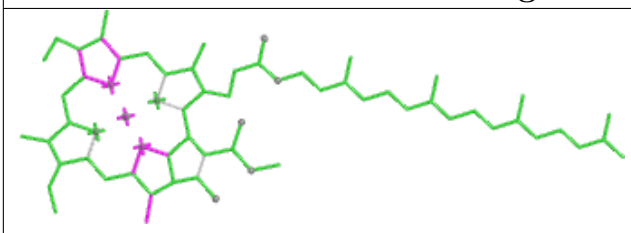


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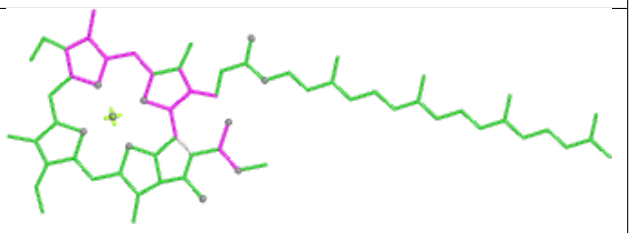


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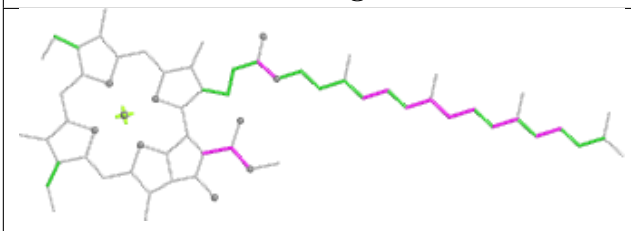
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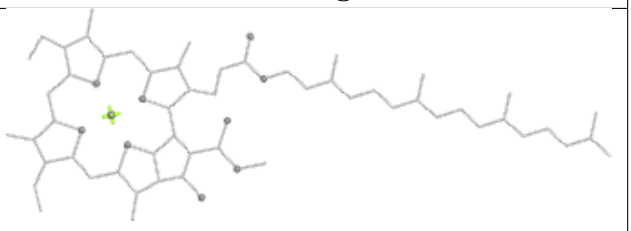
Bond lengths



Bond angles

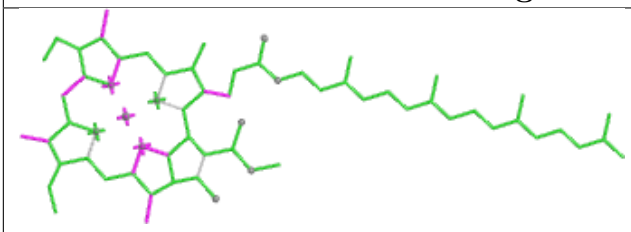


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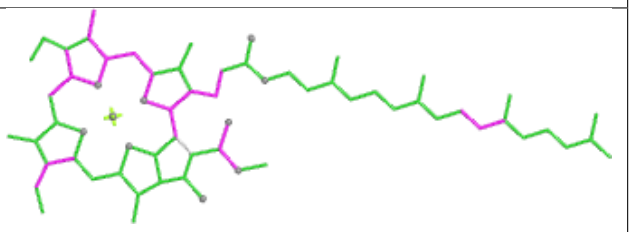


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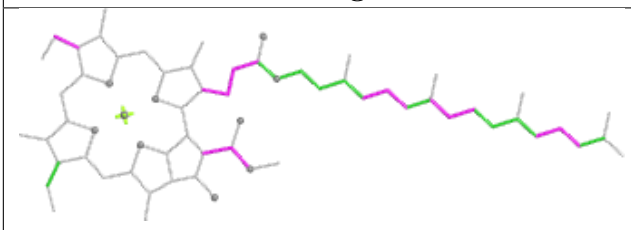
Ligand CLA aB 810



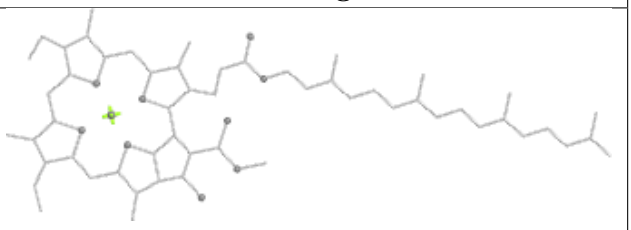
Bond lengths



Bond angles

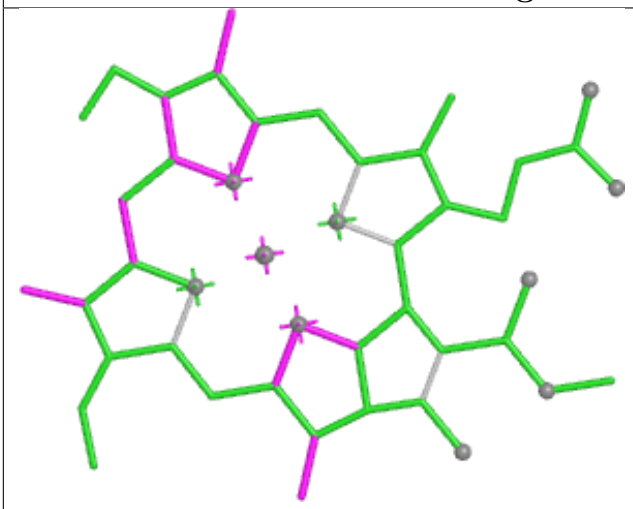


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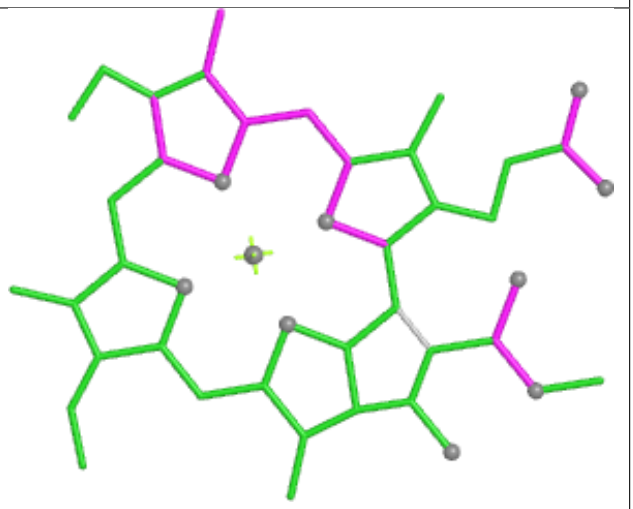


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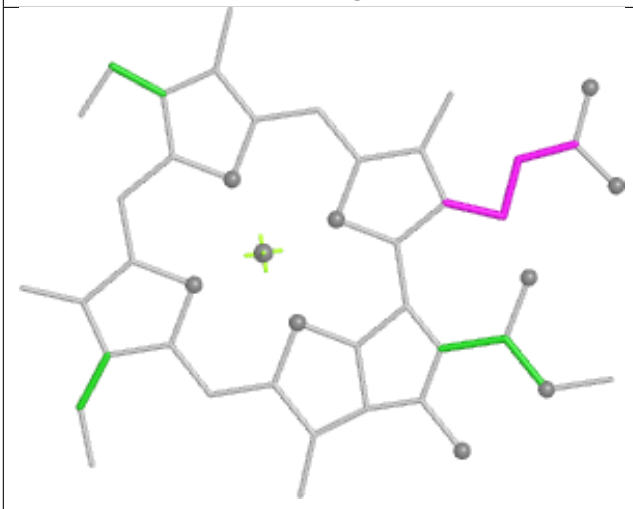
Ligand CLA cB 813



Bond lengths



Bond angles

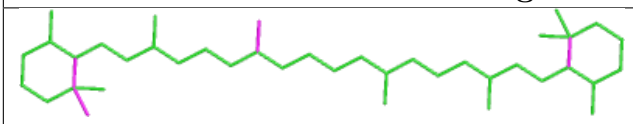


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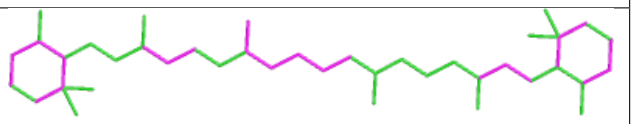


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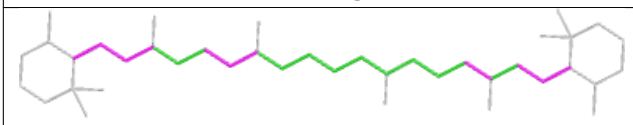
Ligand BCR b1 420



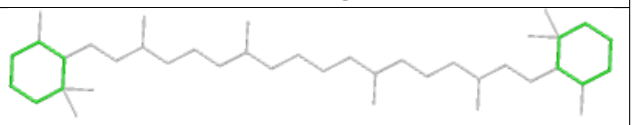
Bond lengths



Bond angles

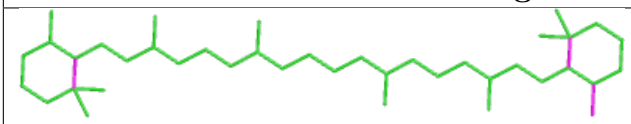


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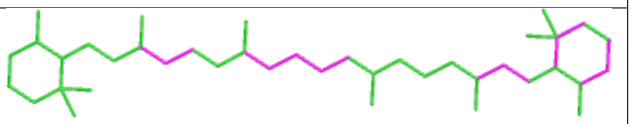


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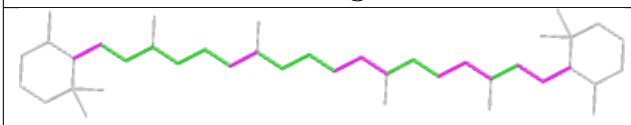
Ligand BCR cA 847



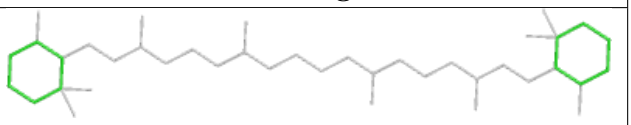
Bond lengths



Bond angles

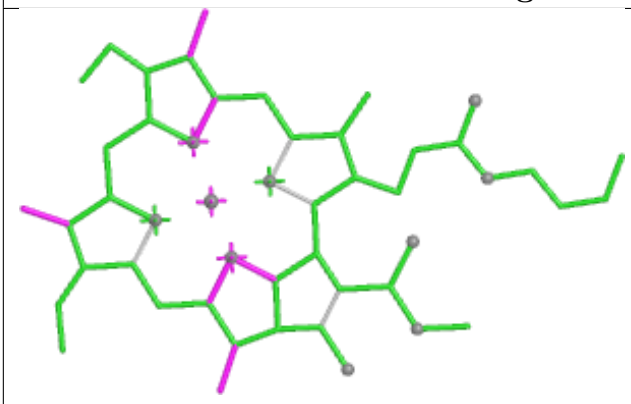


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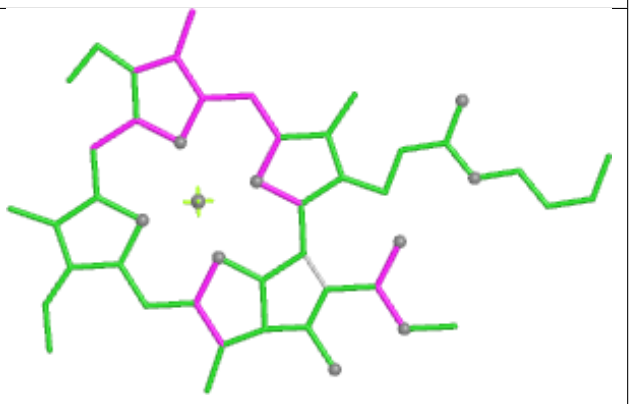


Rings

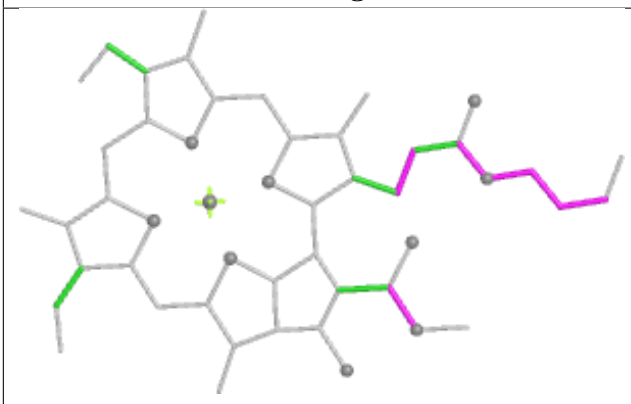
Ligand CLA cB 832



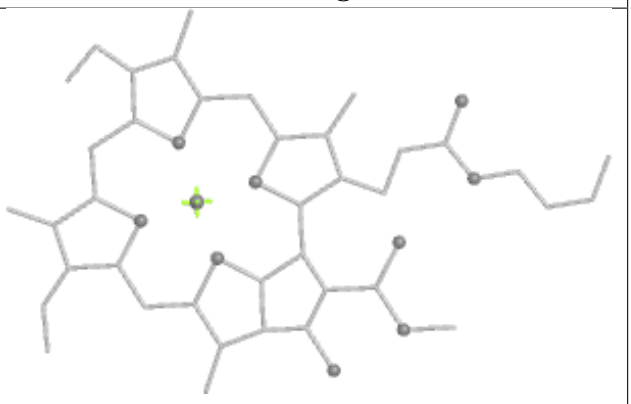
Bond lengths



Bond angles

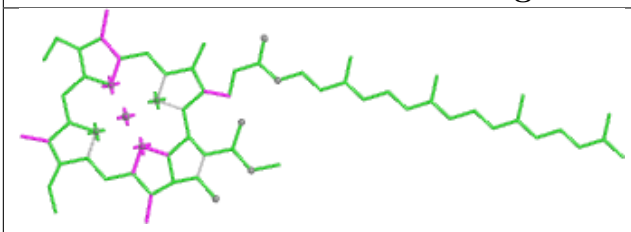


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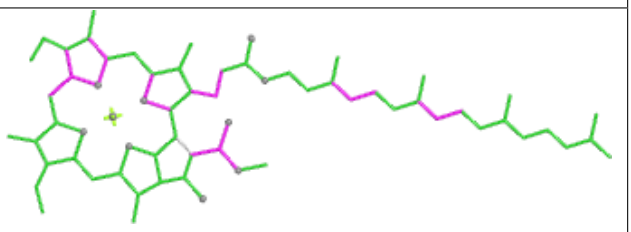


Rings

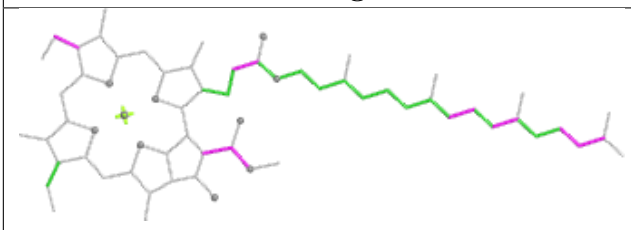
Ligand CLA bB 802



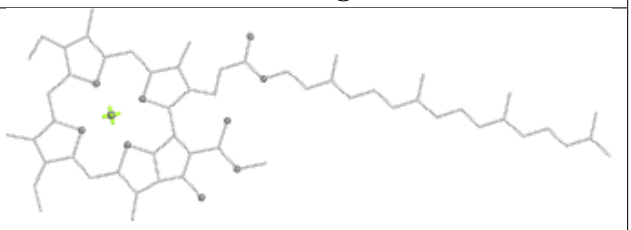
Bond lengths



Bond angles

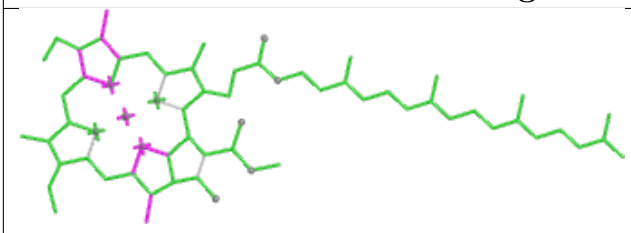


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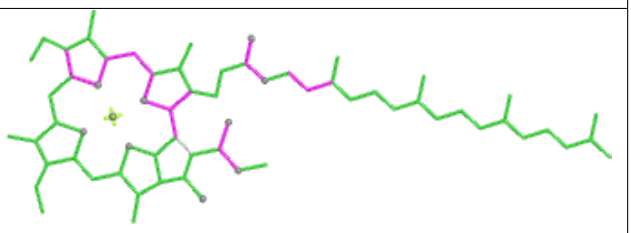


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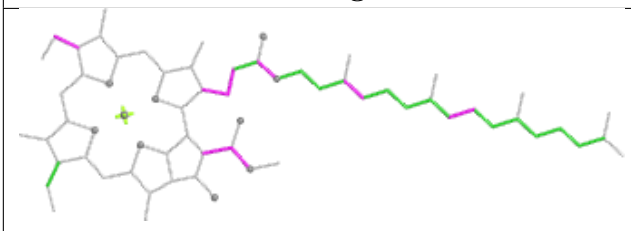
Ligand CLA b3 404



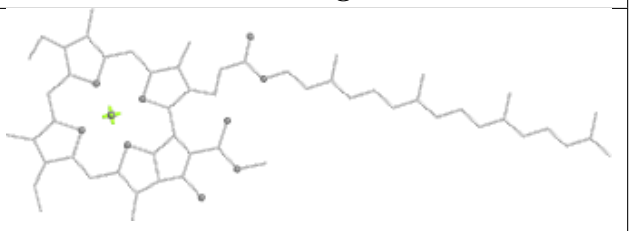
Bond lengths



Bond angles

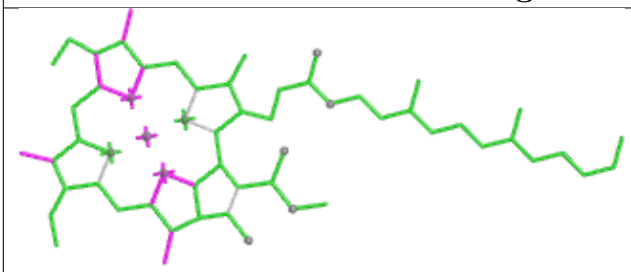


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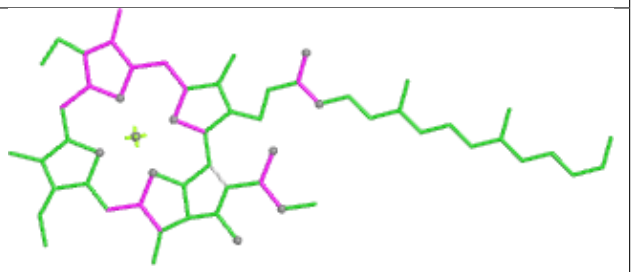


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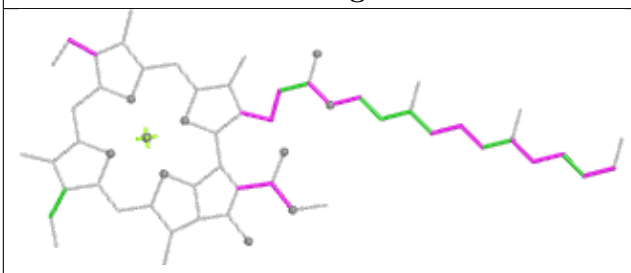
Ligand CLA cA 825



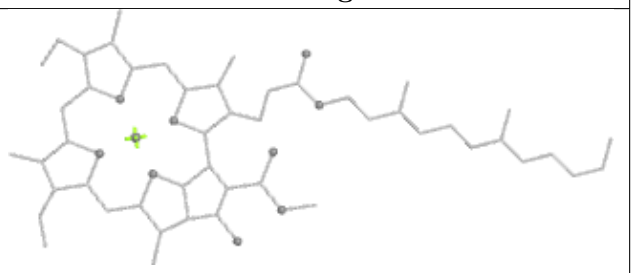
Bond lengths



Bond angles

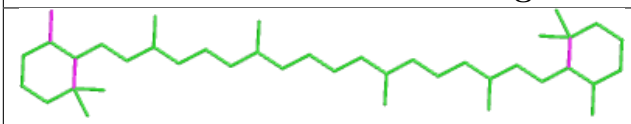


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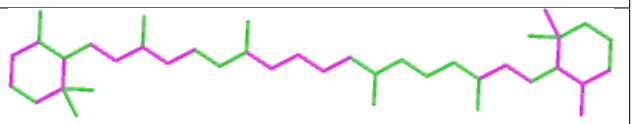


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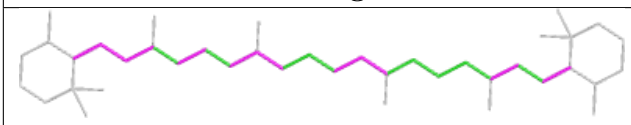
Ligand BCR bL 206



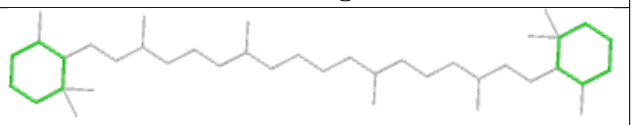
Bond lengths



Bond angles

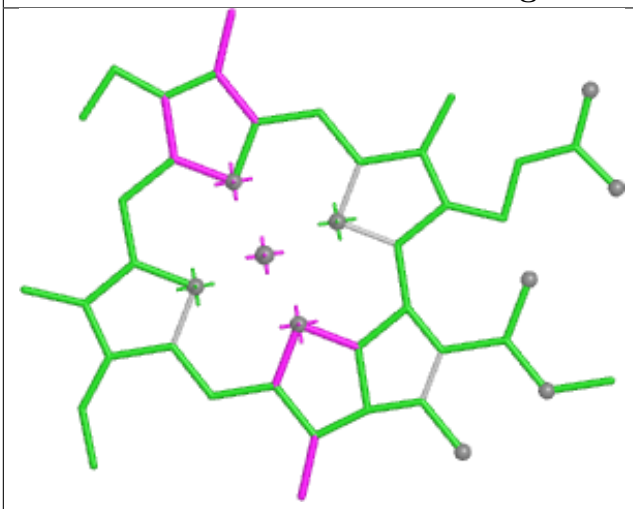


Torsions

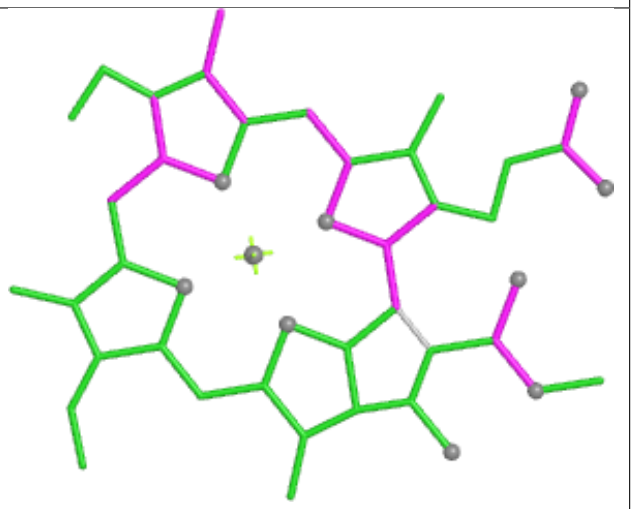


Rings

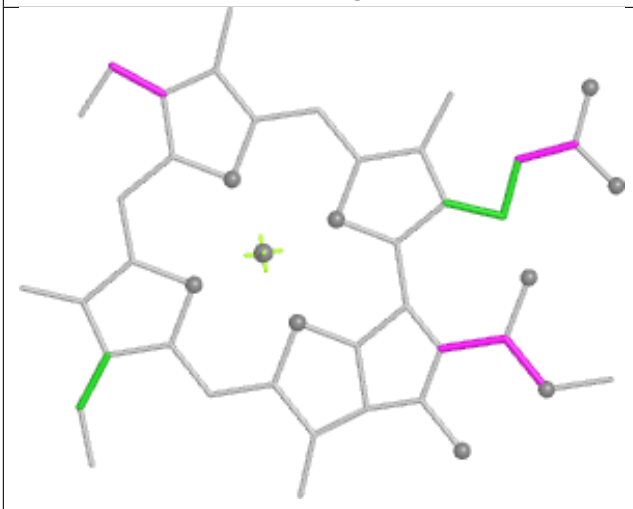
Ligand CLA a6 408



Bond lengths



Bond angles

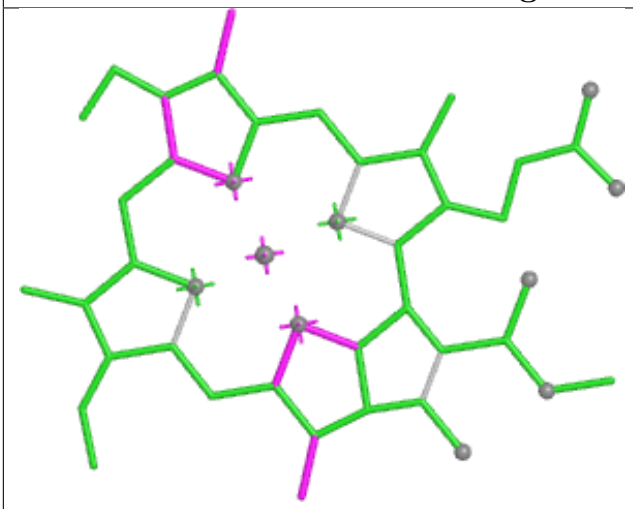


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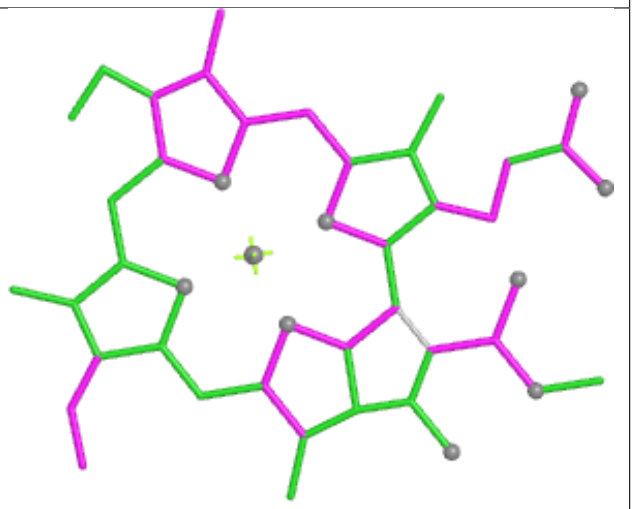


Rings

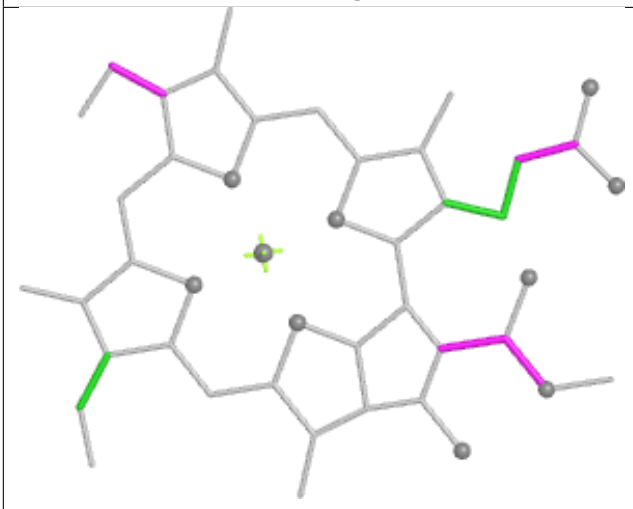
Ligand CLA a4 415



Bond lengths



Bond angles

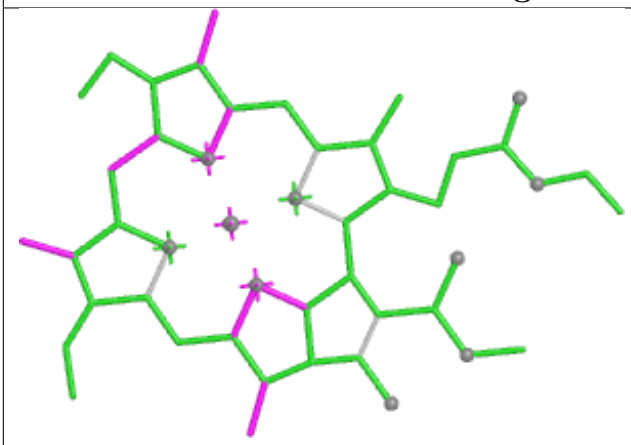


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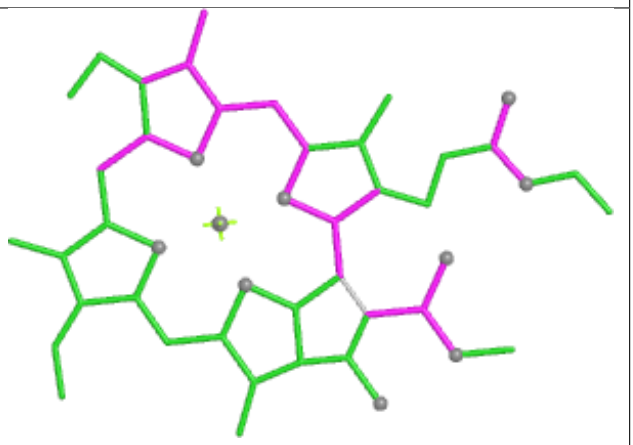


Rings

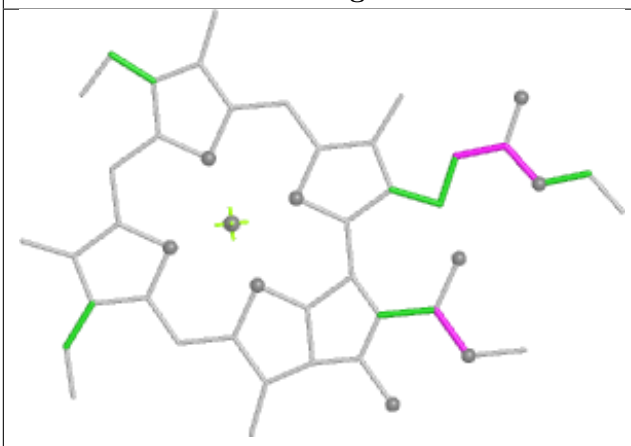
Ligand CLA bA 840



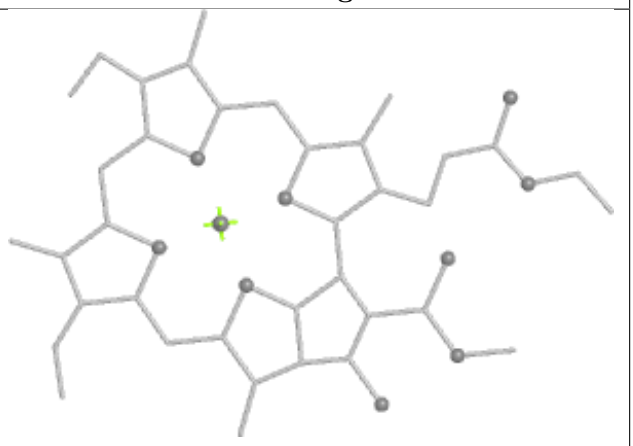
Bond lengths



Bond angles

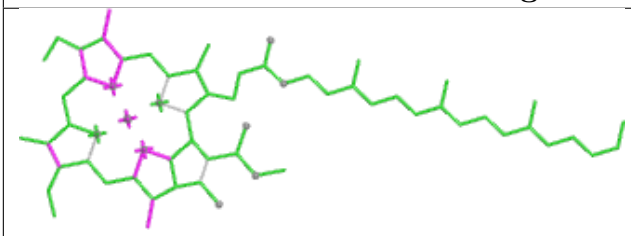


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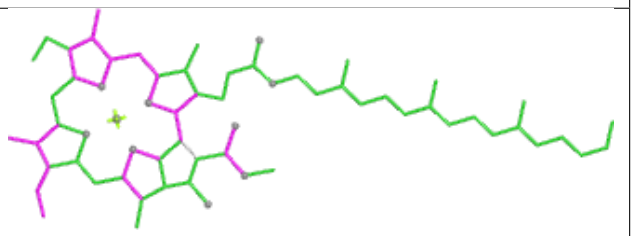


Rings

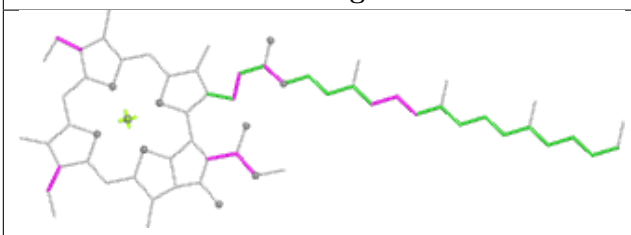
Ligand CLA c6 412



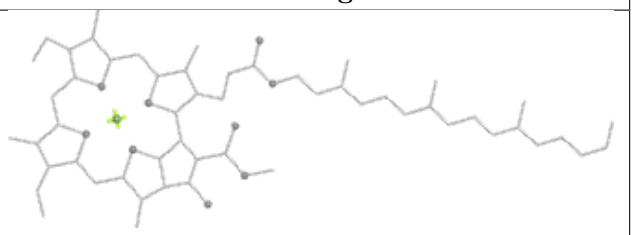
Bond lengths



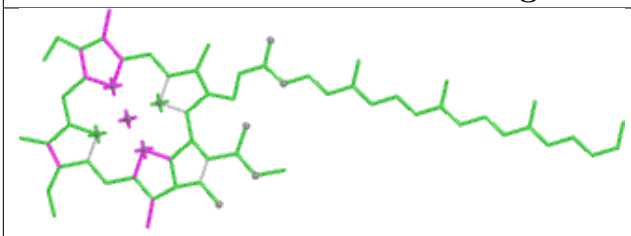
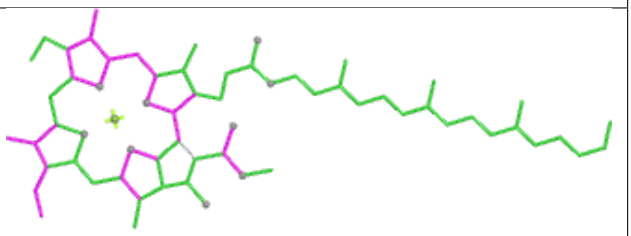
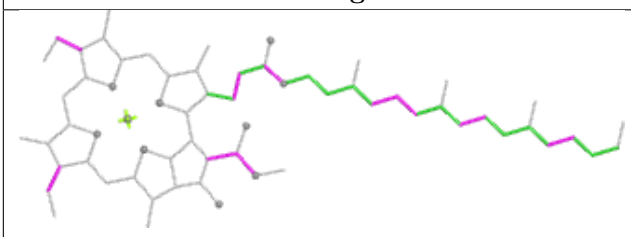
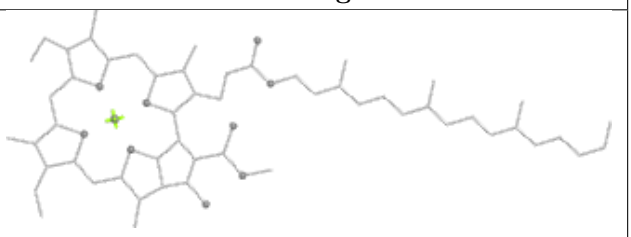
Bond angles

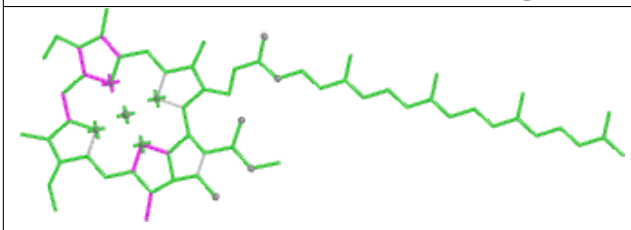
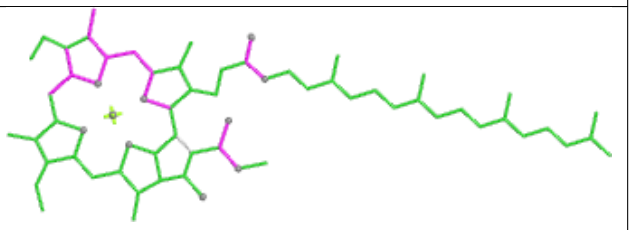
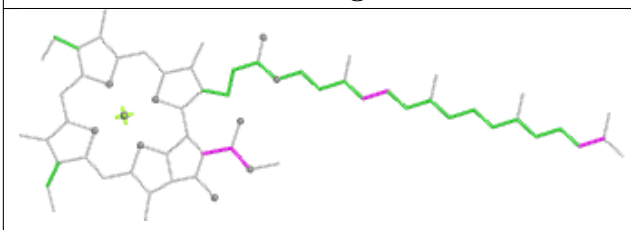
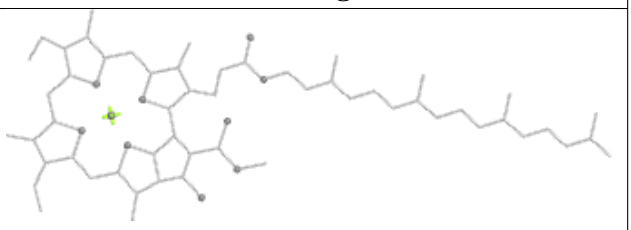


Torsions

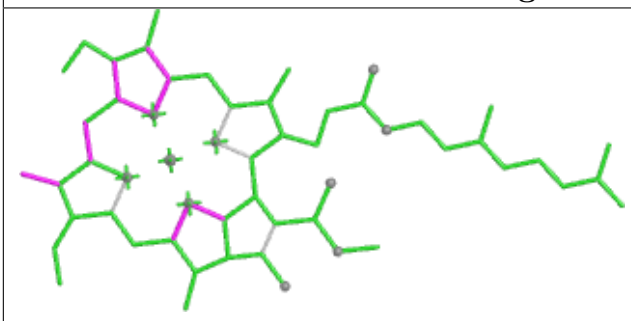


Rings

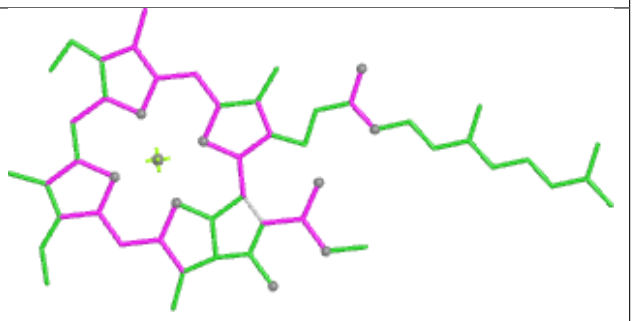
Ligand CLA a5 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b1 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

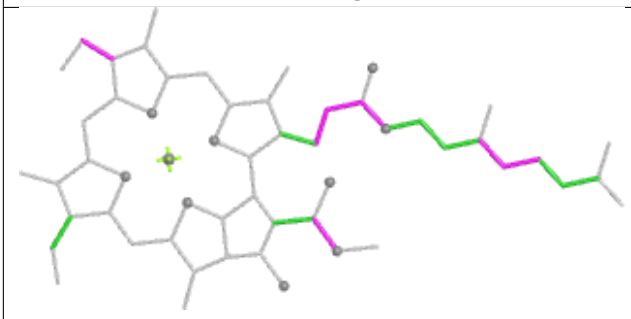
Ligand CLA b3 417



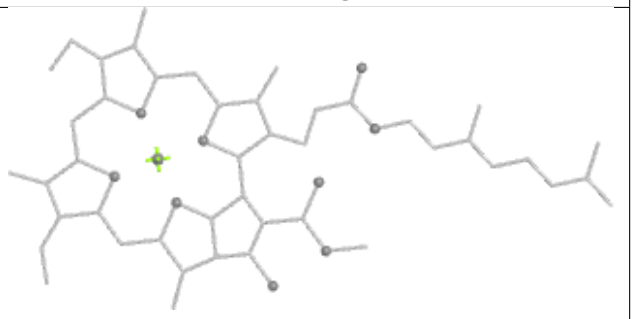
Bond lengths



Bond angles

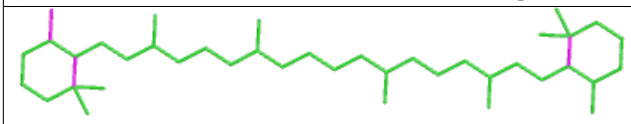


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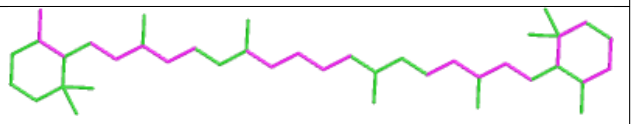


Rings

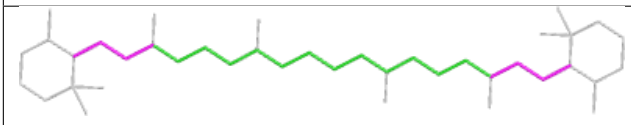
Ligand BCR bA 848



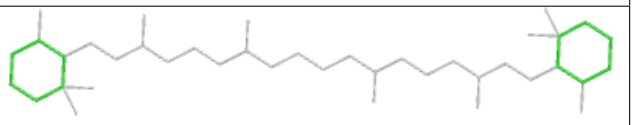
Bond lengths



Bond angles

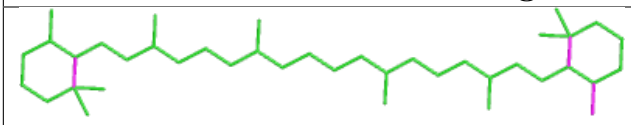


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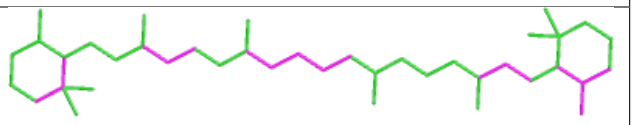


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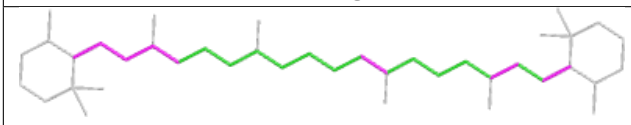
Ligand BCR cJ 104



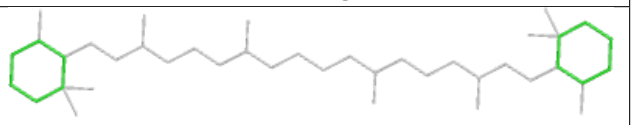
Bond lengths



Bond angles

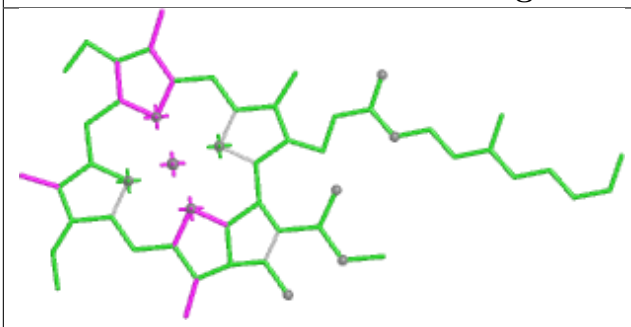


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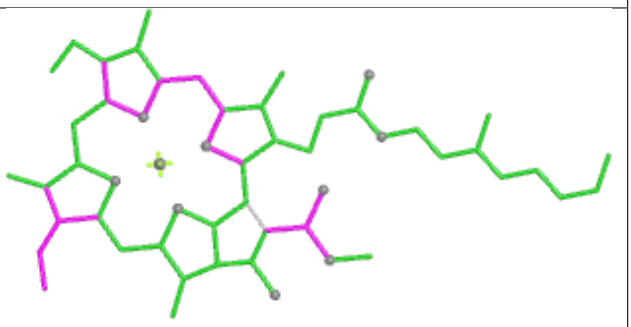


Rings

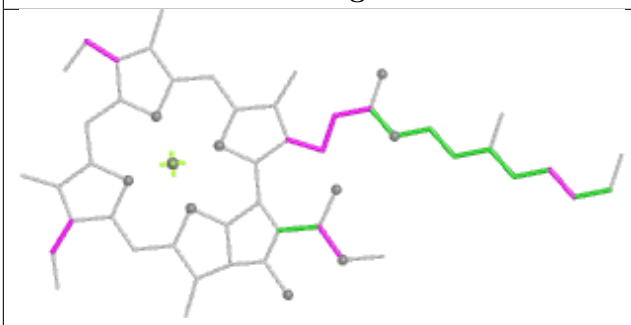
Ligand CLA cA 819



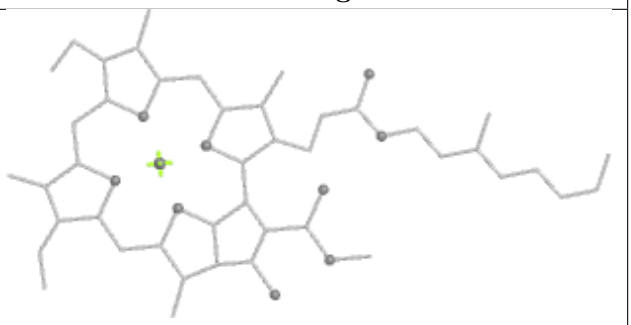
Bond lengths



Bond angles

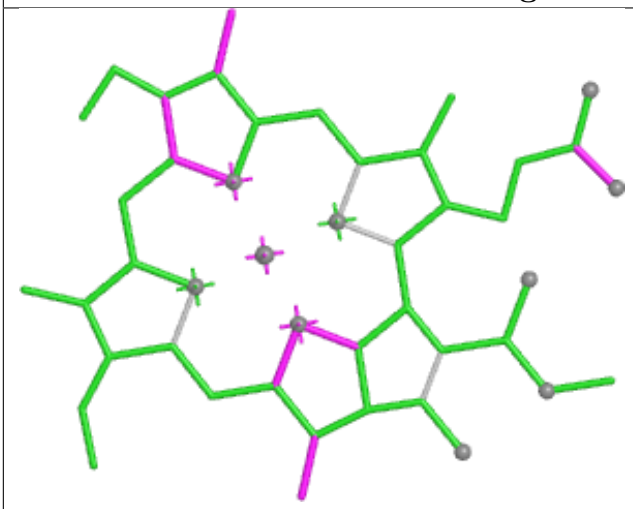


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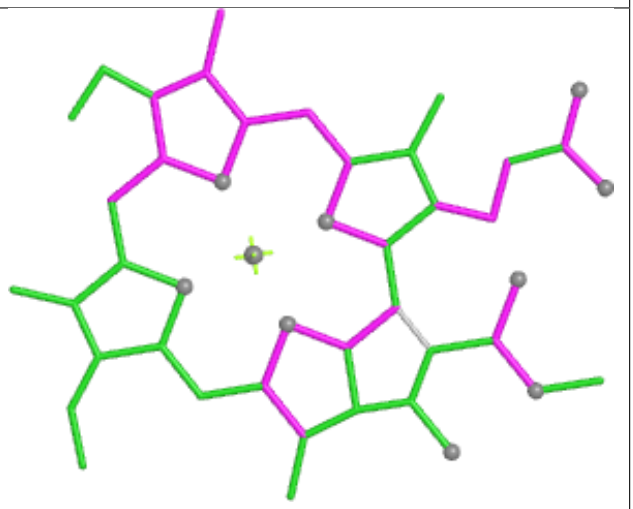


Rings

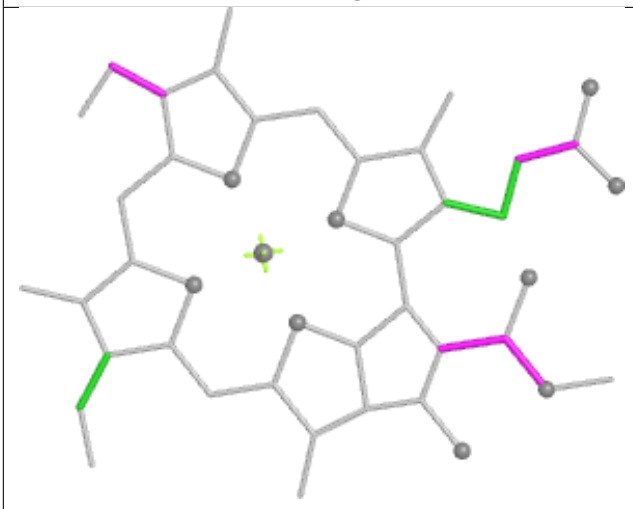
Ligand CLA a3 415



Bond lengths



Bond angles

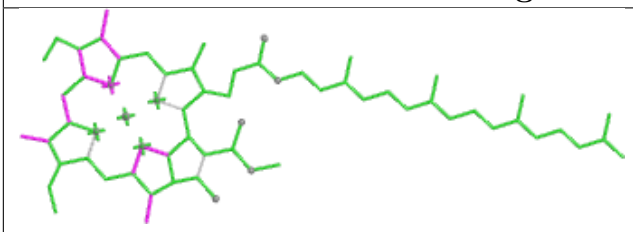


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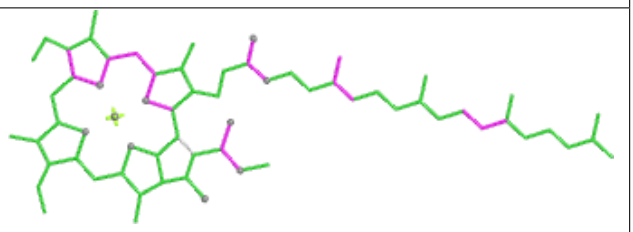


Rings

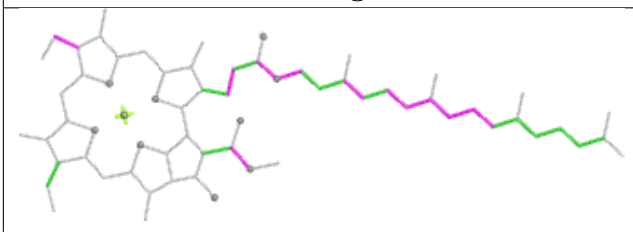
Ligand CLA cA 841



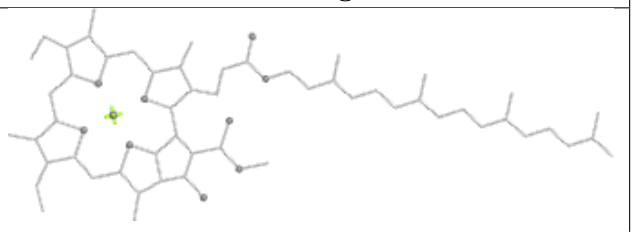
Bond lengths



Bond angles

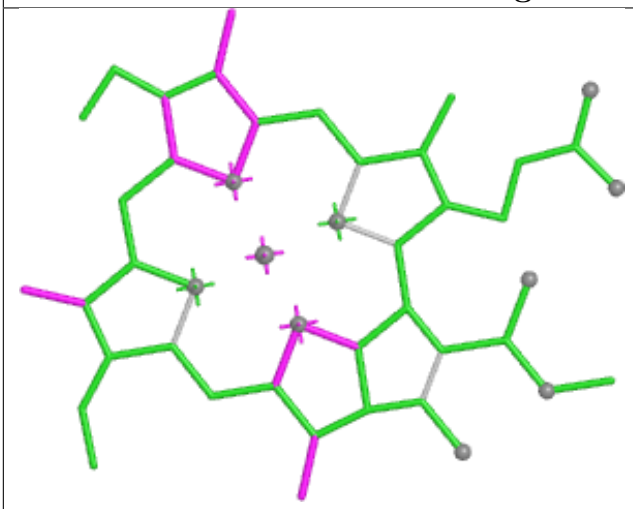


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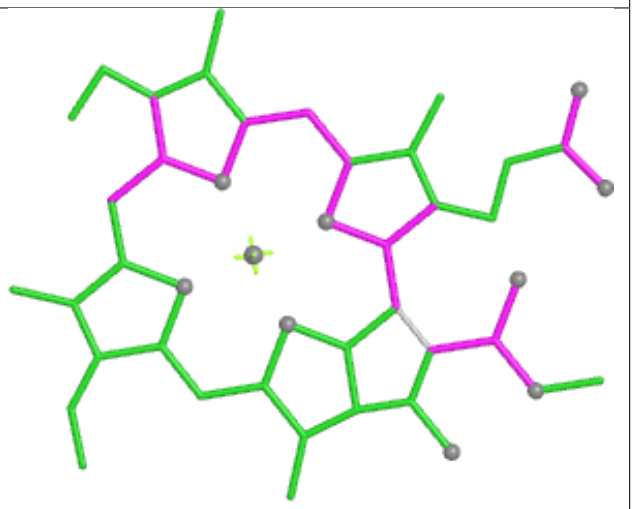


Rings

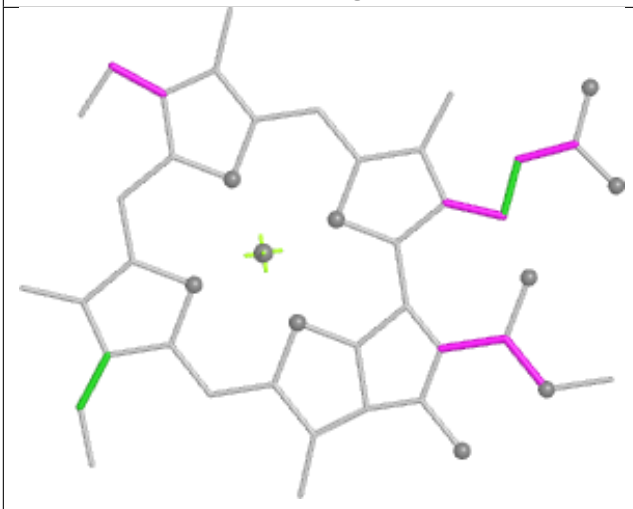
Ligand CLA aK 102



Bond lengths



Bond angles

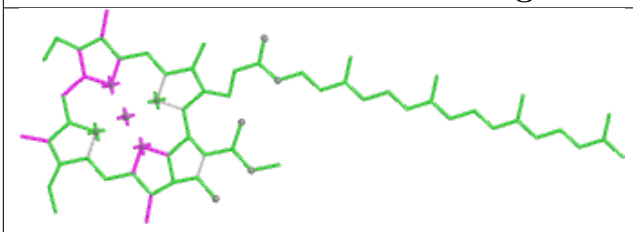


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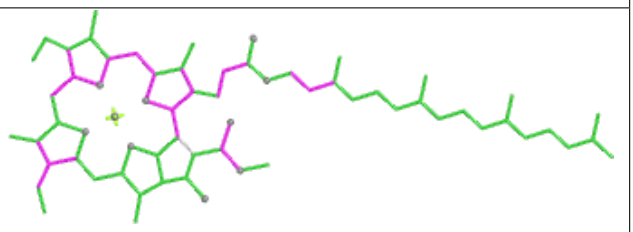


Rings

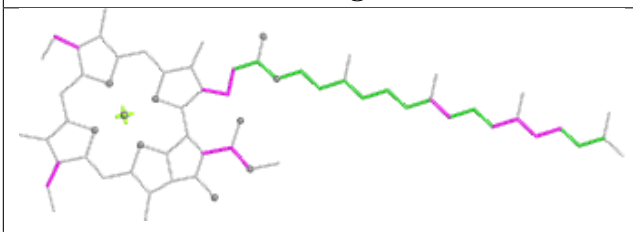
Ligand CLA aB 840



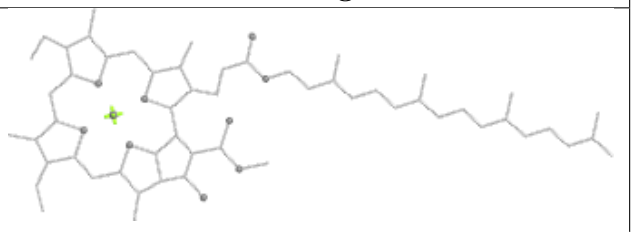
Bond lengths



Bond angles

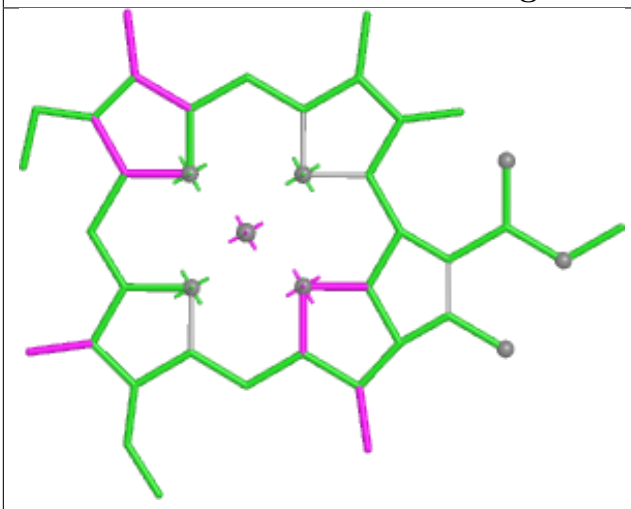


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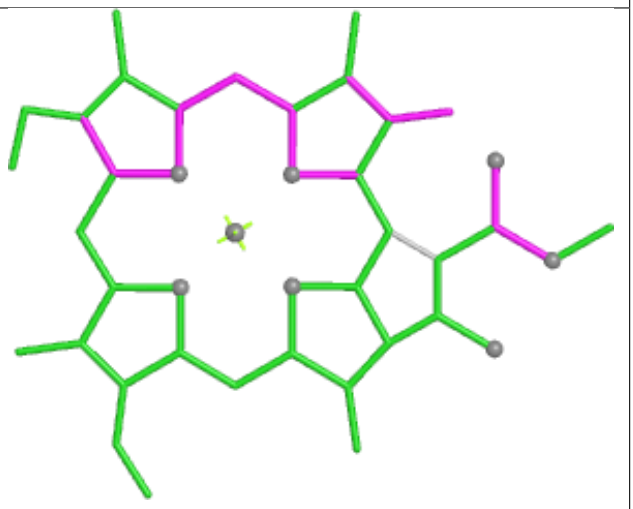


Rings

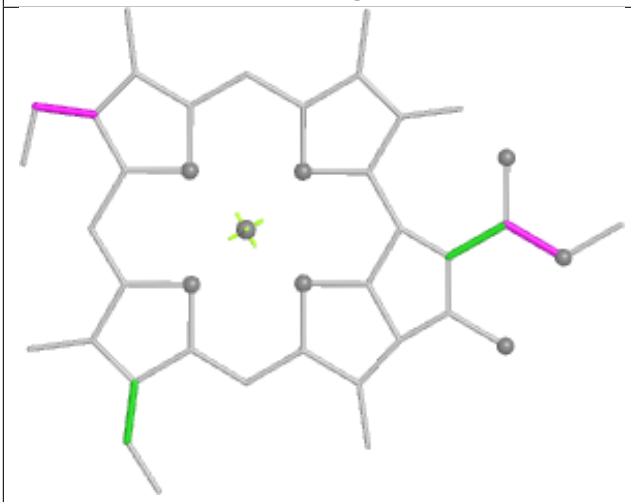
Ligand CLA a4 414



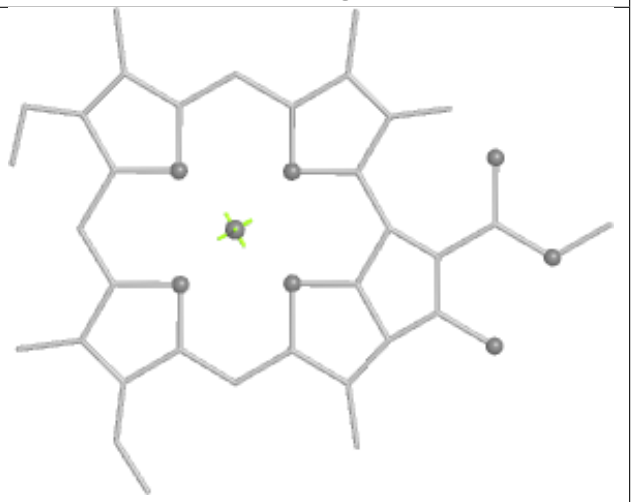
Bond lengths



Bond angles



Torsions

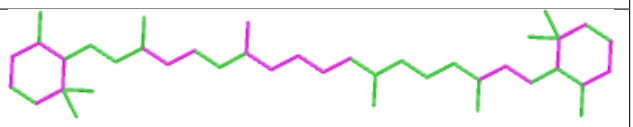


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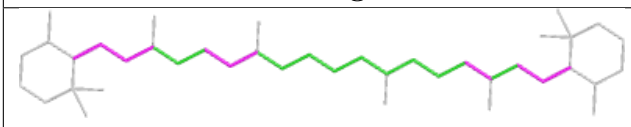
Ligand BCR c4 420



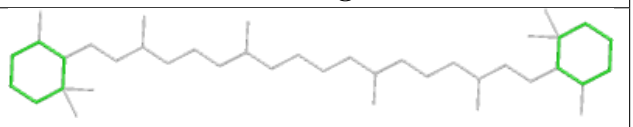
Bond lengths



Bond angles

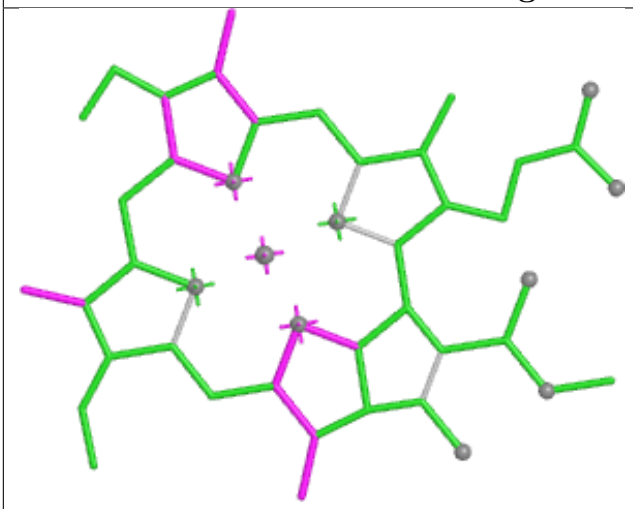


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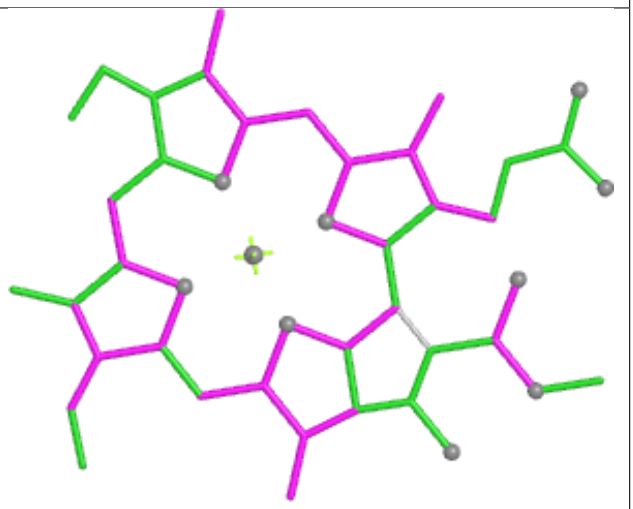


Rings

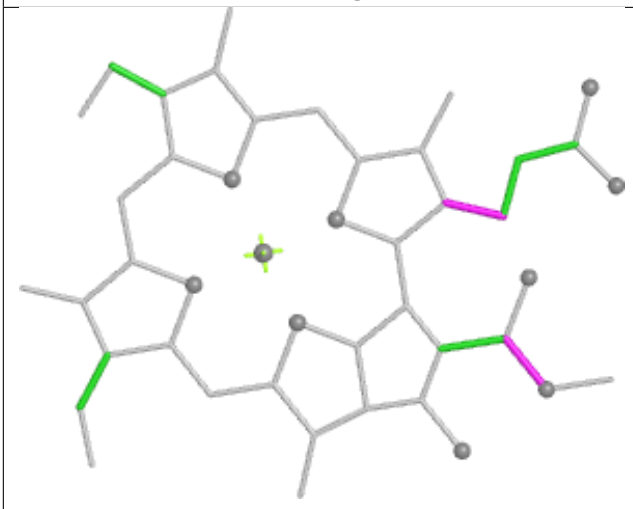
Ligand CLA b3 405



Bond lengths



Bond angles

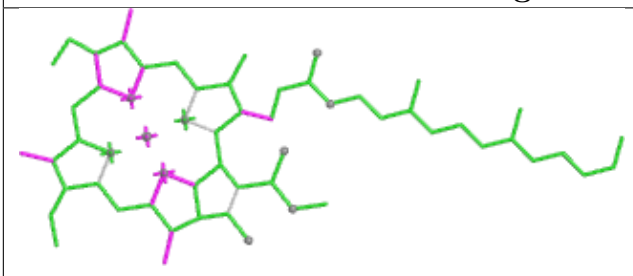


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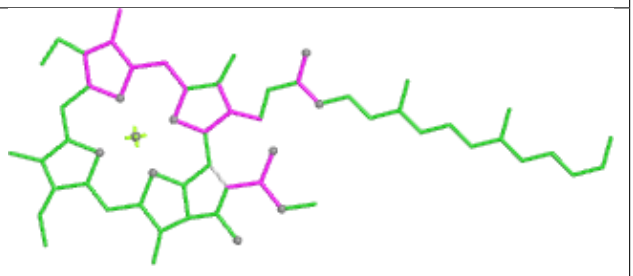


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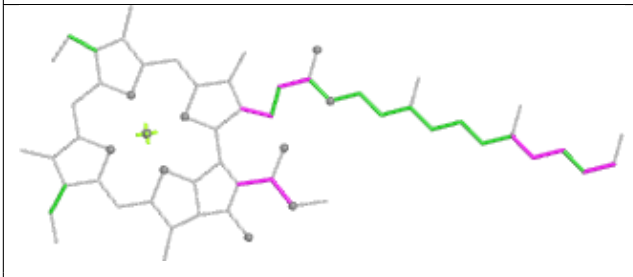
Ligand CLA bA 805



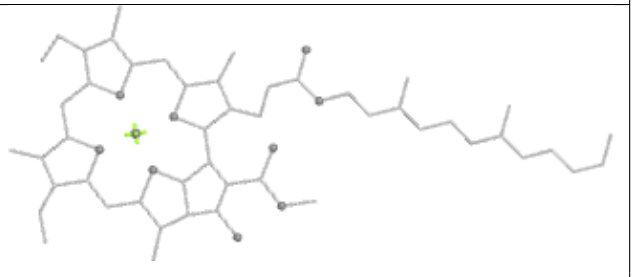
Bond lengths



Bond angles

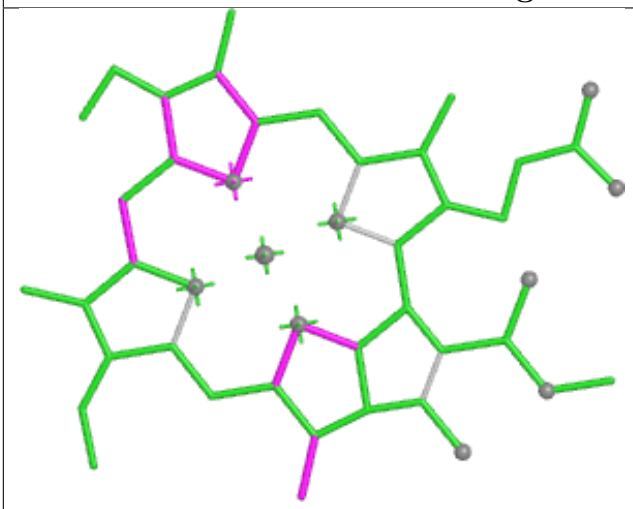


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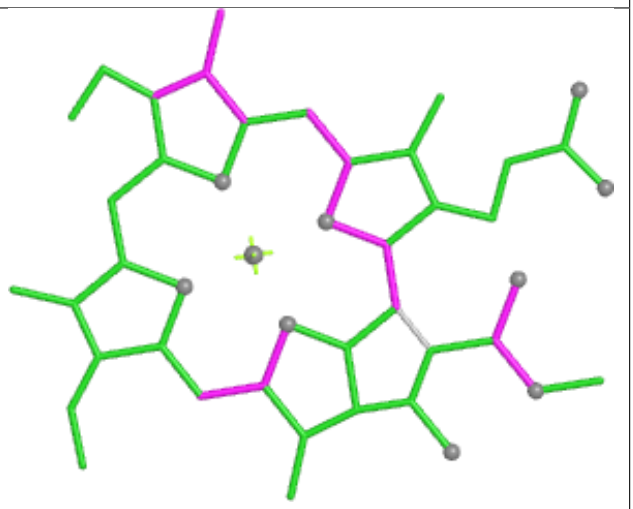


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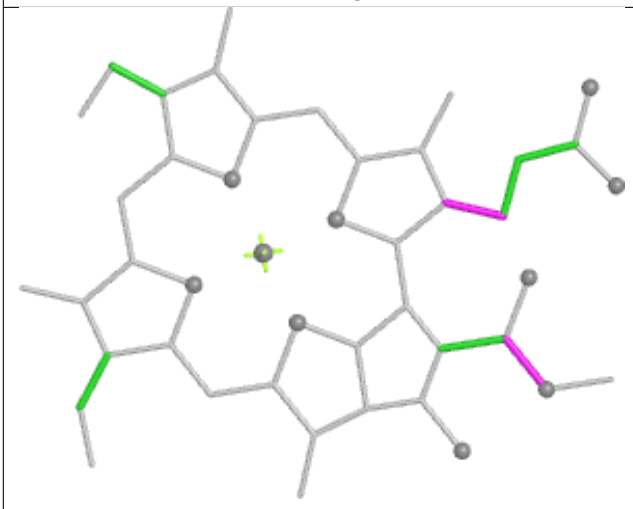
Ligand CLA cB 812



Bond lengths



Bond angles

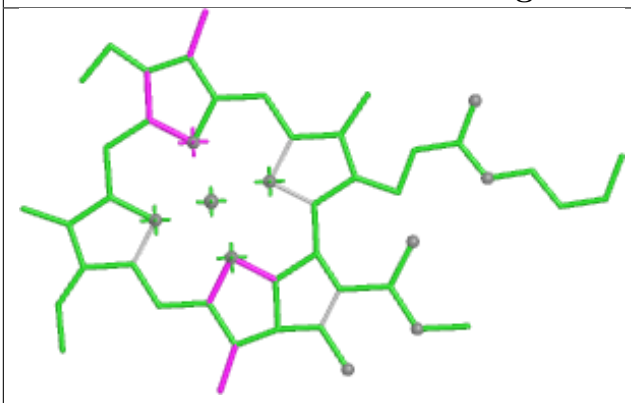


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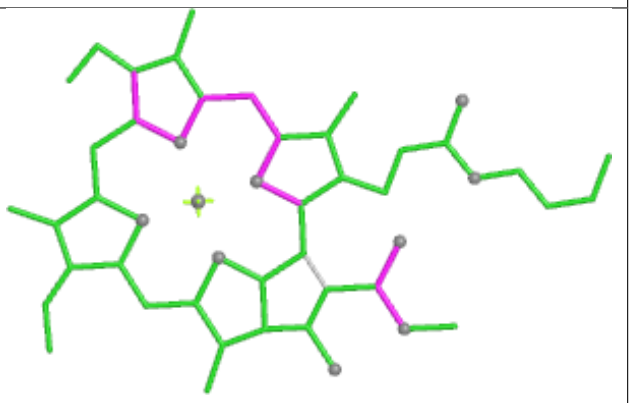


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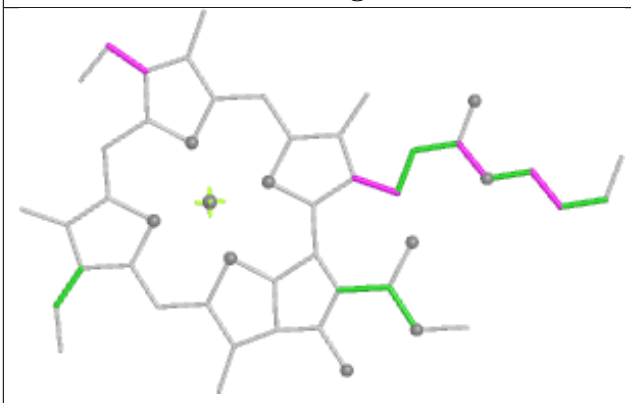
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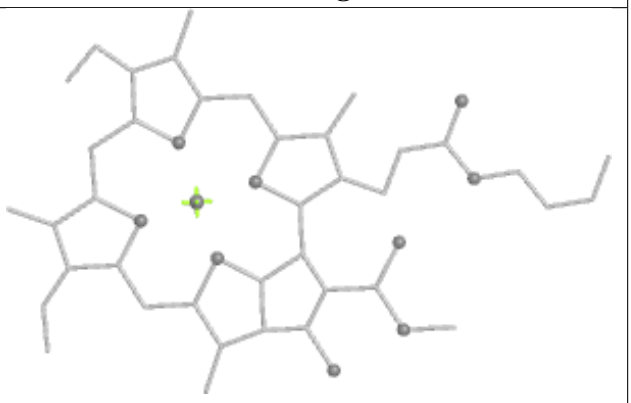
Bond lengths



Bond angles

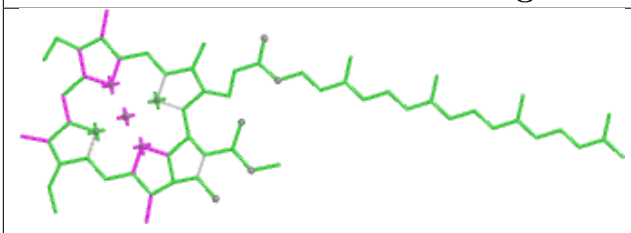


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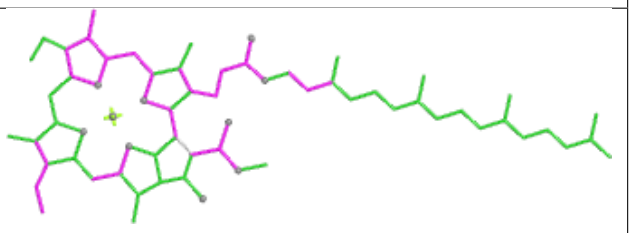


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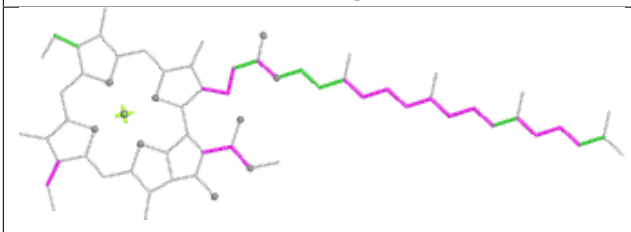
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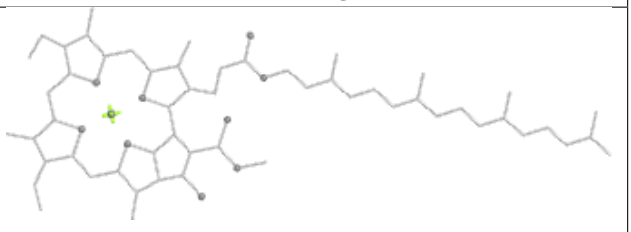
Bond lengths



Bond angles

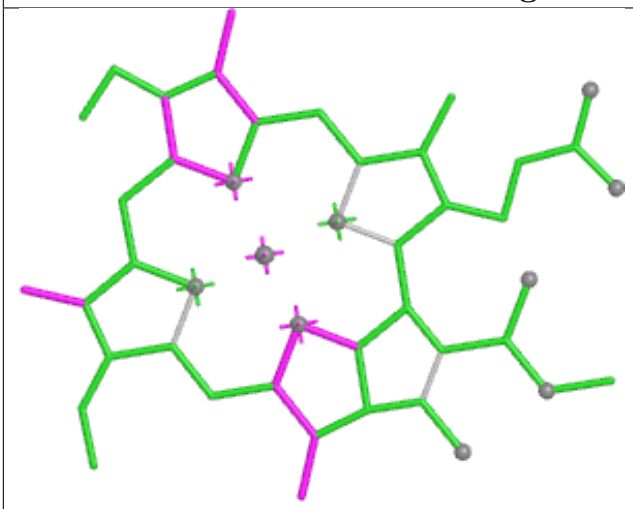


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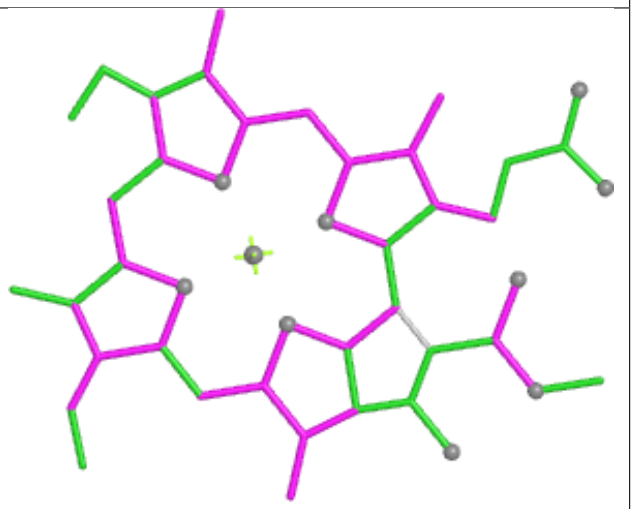


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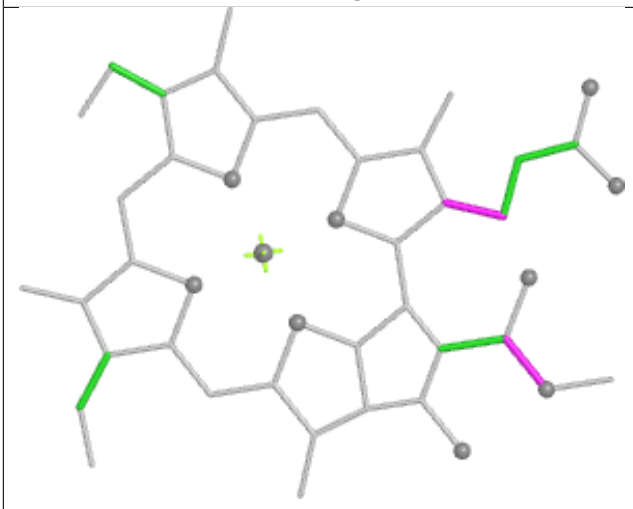
Ligand CLA a3 405



Bond lengths



Bond angles

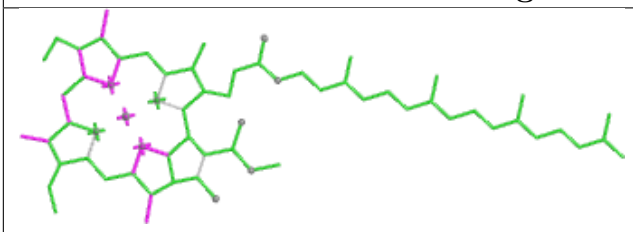


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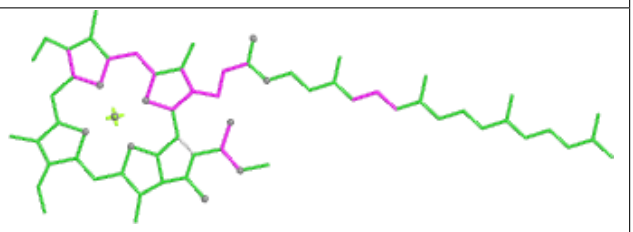


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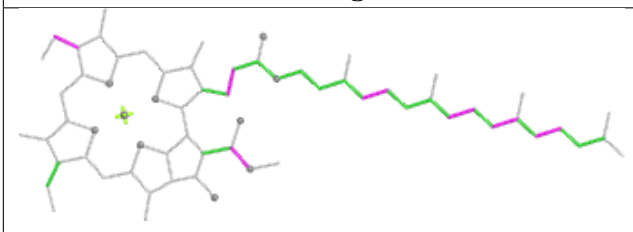
Ligand CLA cB 839



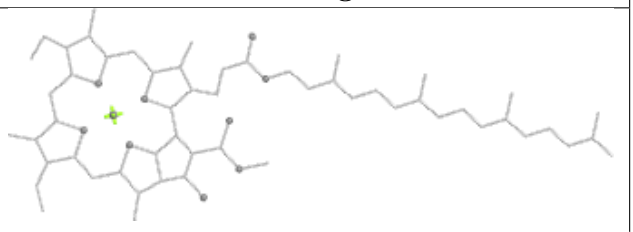
Bond lengths



Bond angles

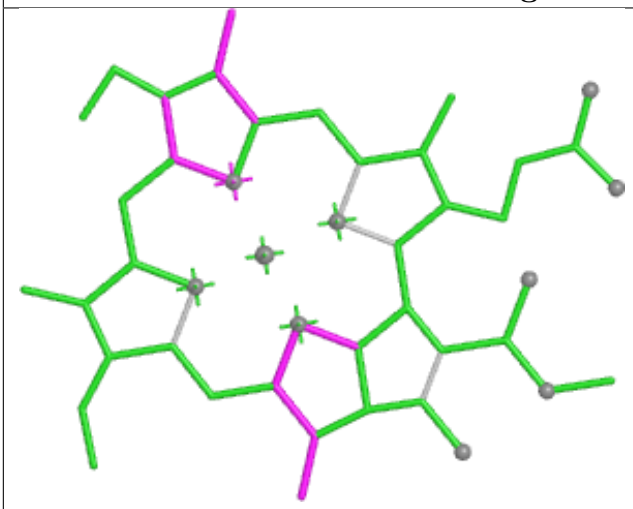


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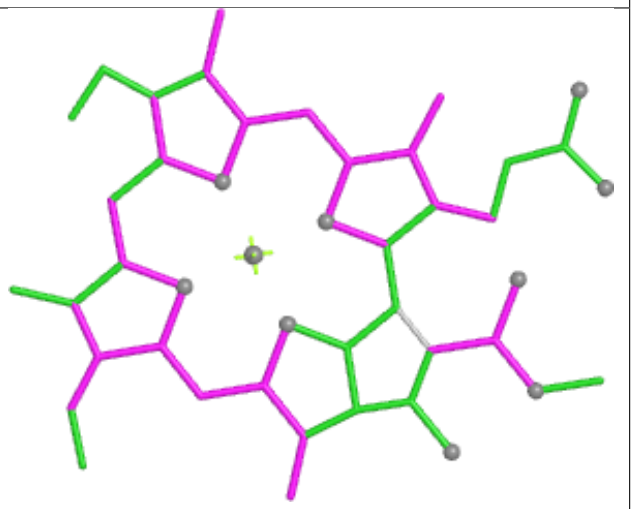


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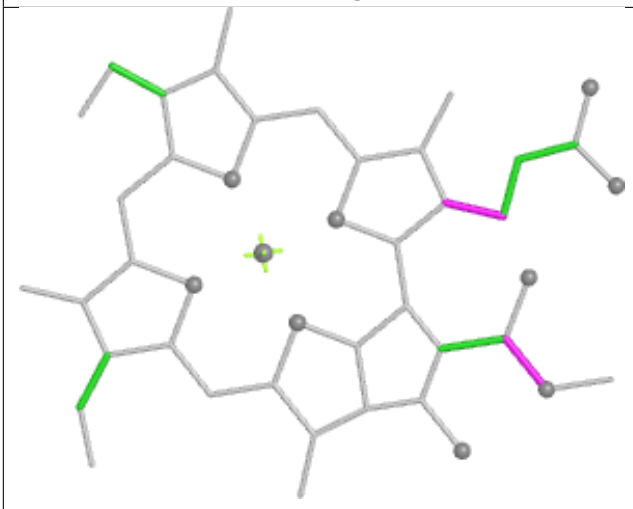
Ligand CLA c6 407



Bond lengths



Bond angles

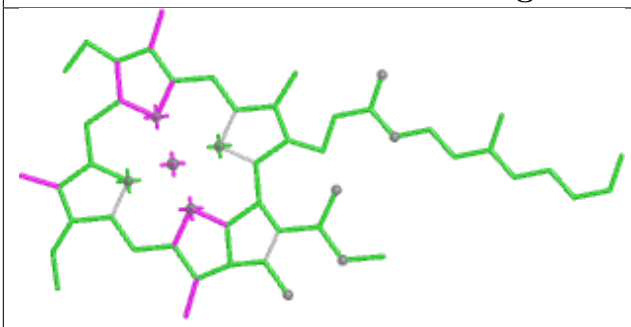


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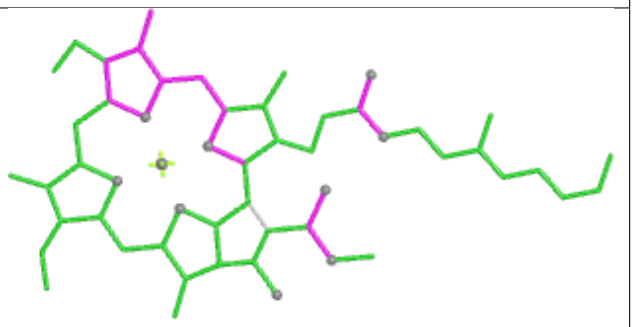


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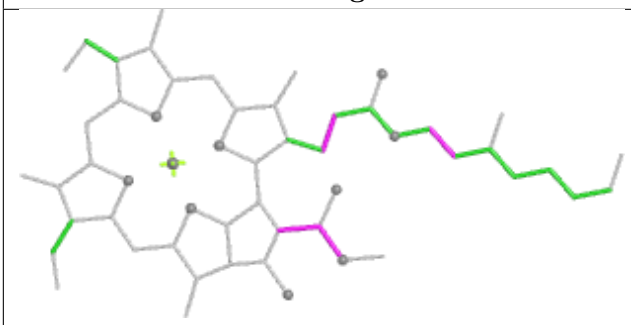
Ligand CLA cB 805



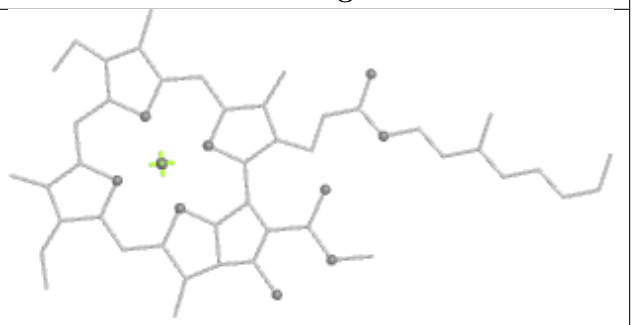
Bond lengths



Bond angles

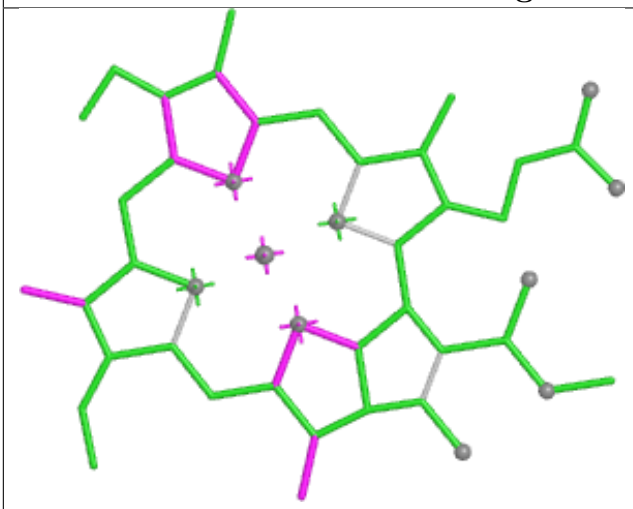


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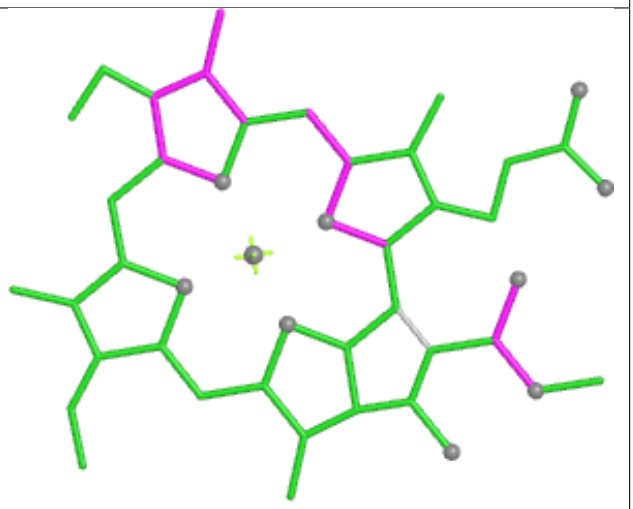


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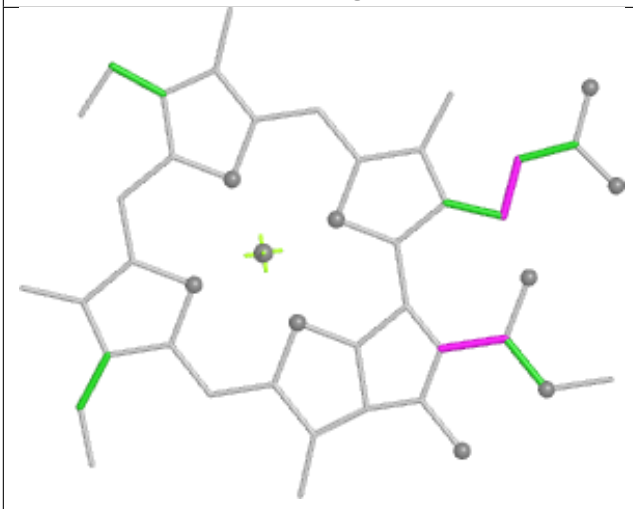
Ligand CLA cA 816



Bond lengths



Bond angles

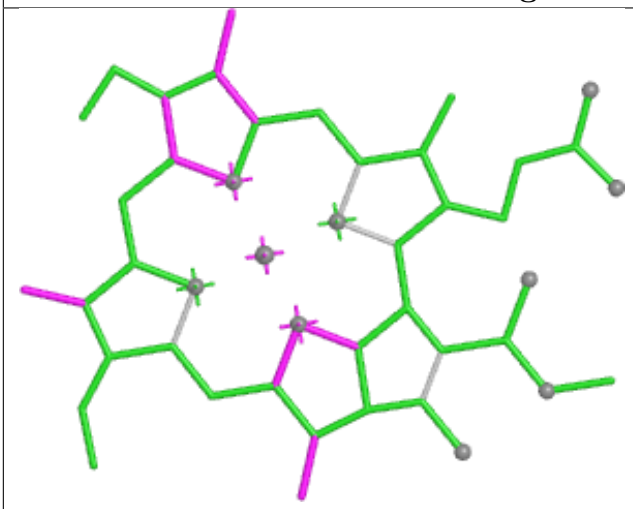


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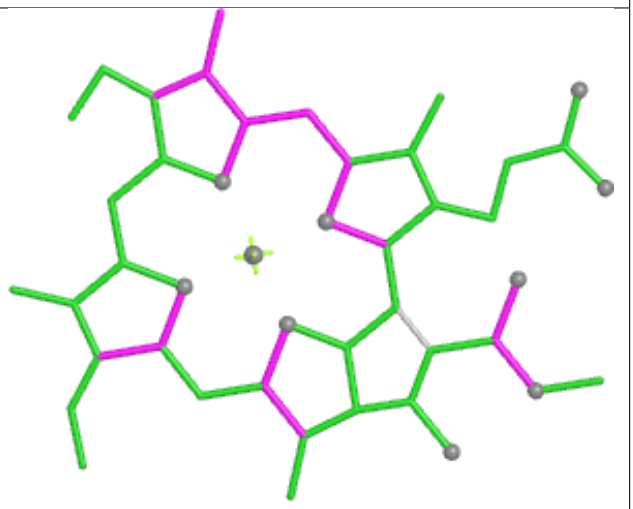


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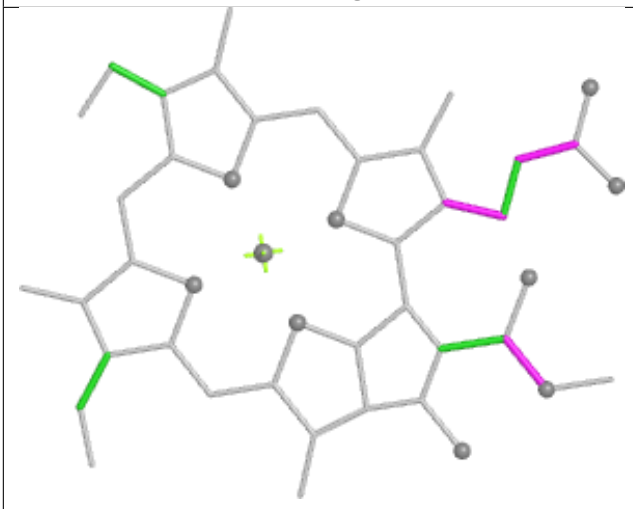
Ligand CLA a1 407



Bond lengths



Bond angles

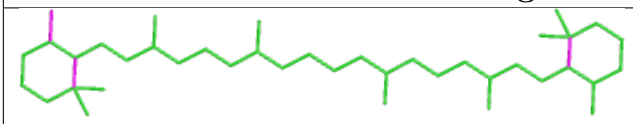


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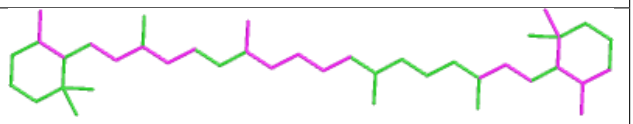


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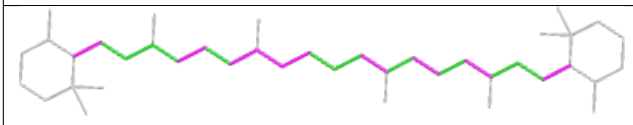
Ligand BCR aJ 204



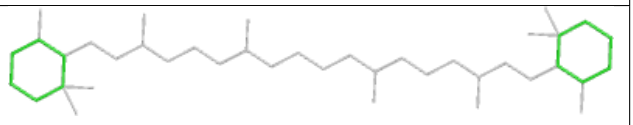
Bond lengths



Bond angles

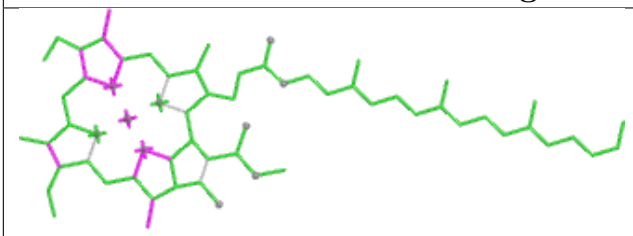


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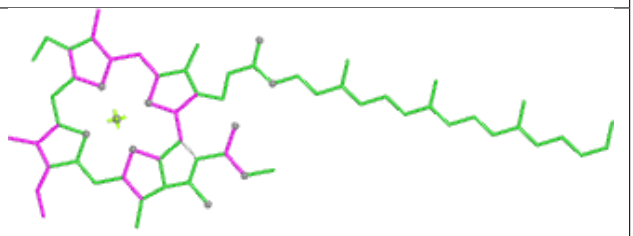


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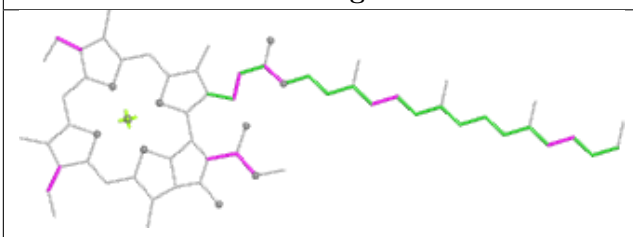
Ligand CLA a3 410



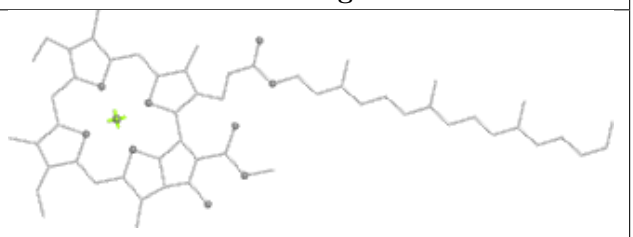
Bond lengths



Bond angles

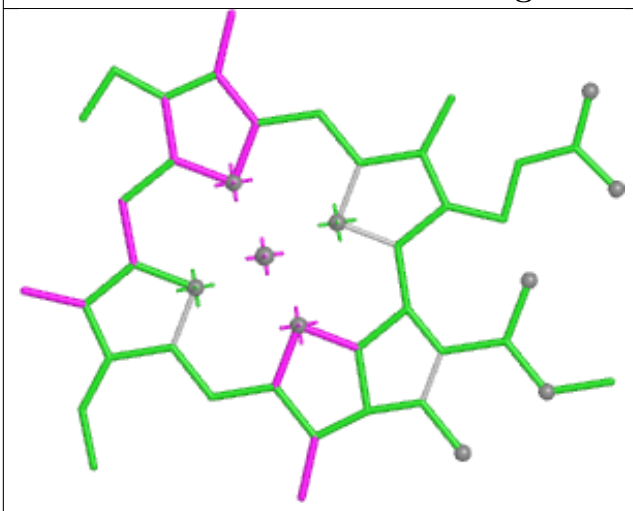


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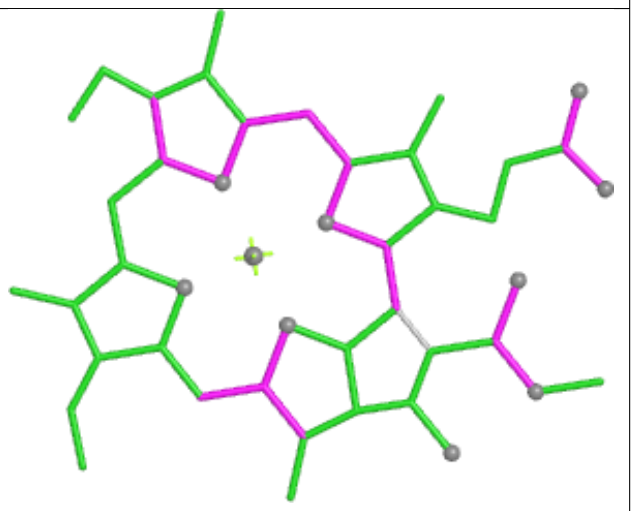


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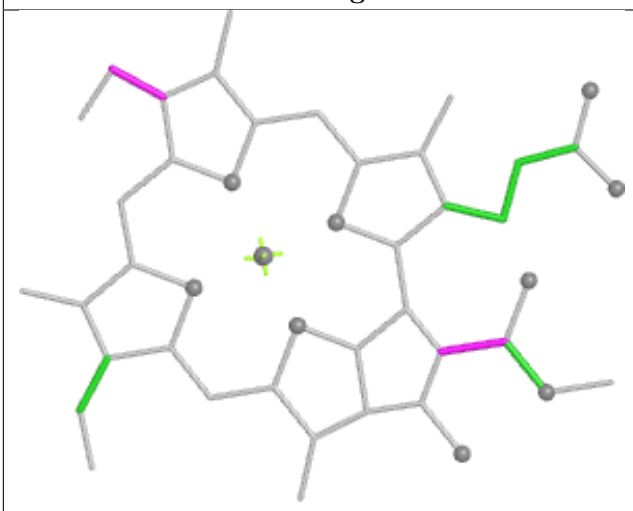
Ligand CLA aA 815



Bond lengths



Bond angles

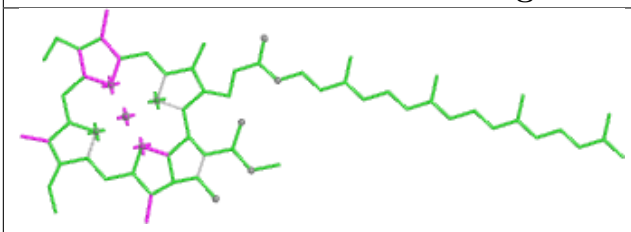


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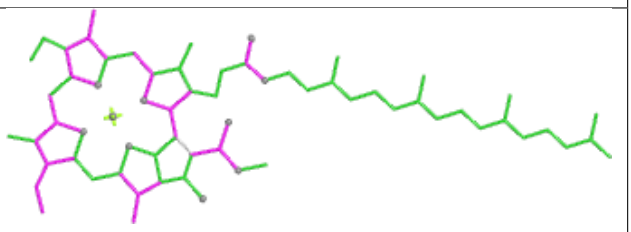


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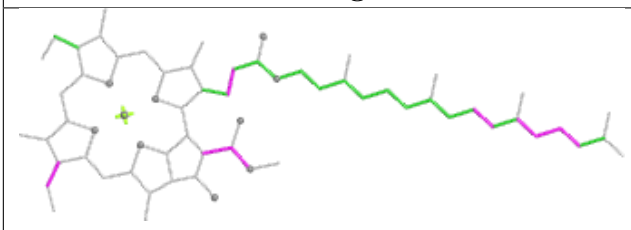
Ligand CLA cB 804



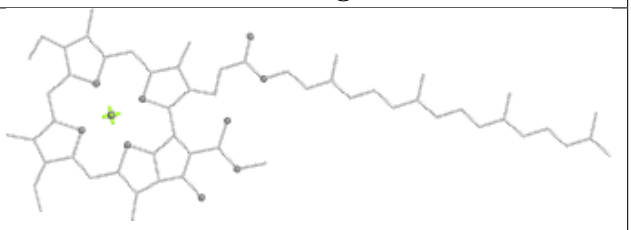
Bond lengths



Bond angles

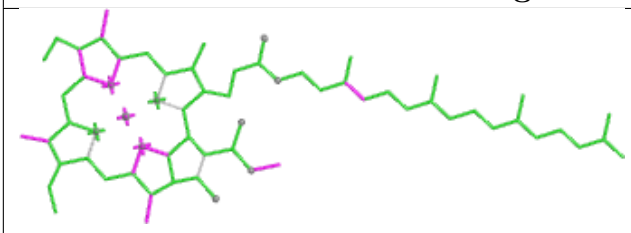


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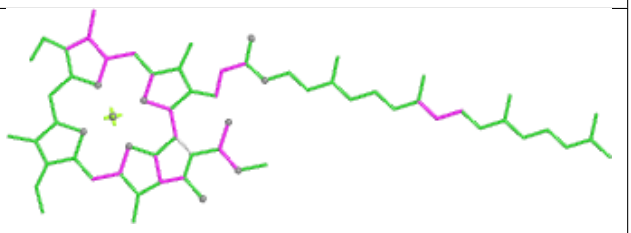


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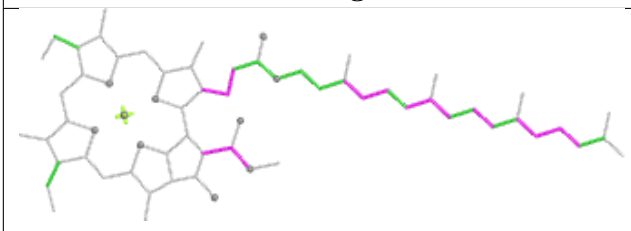
Ligand CLA bA 802



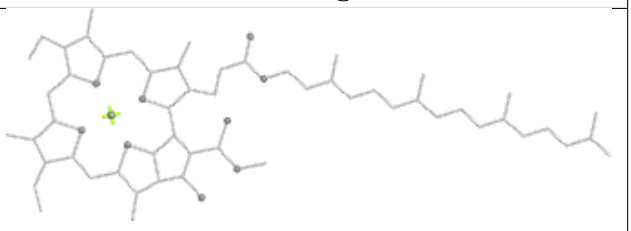
Bond lengths



Bond angles

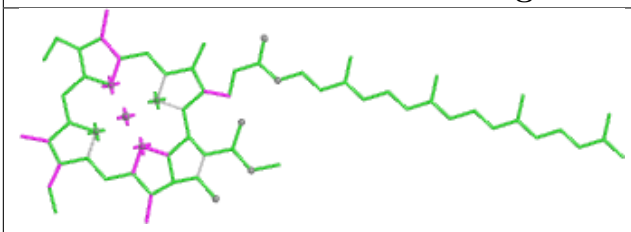


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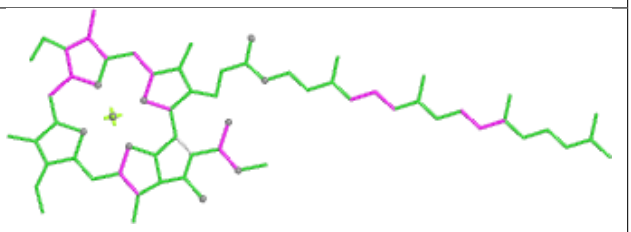


Rings

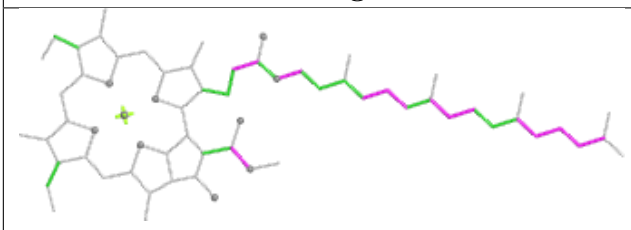
Ligand CLA aB 807



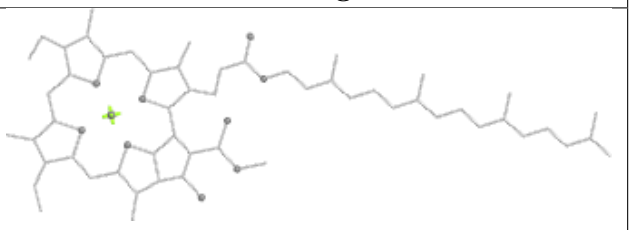
Bond lengths



Bond angles

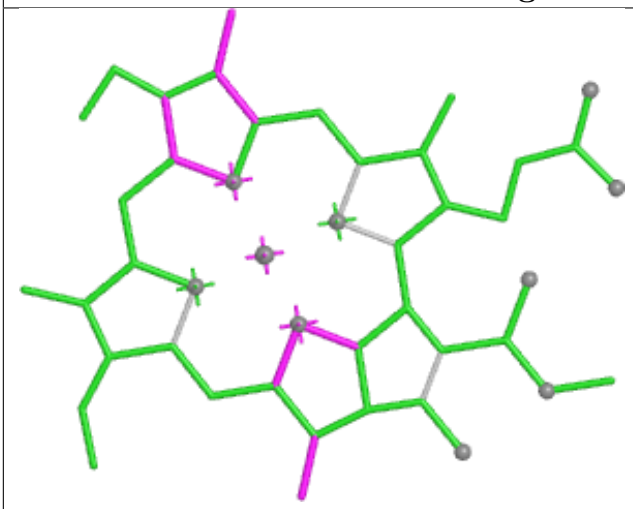


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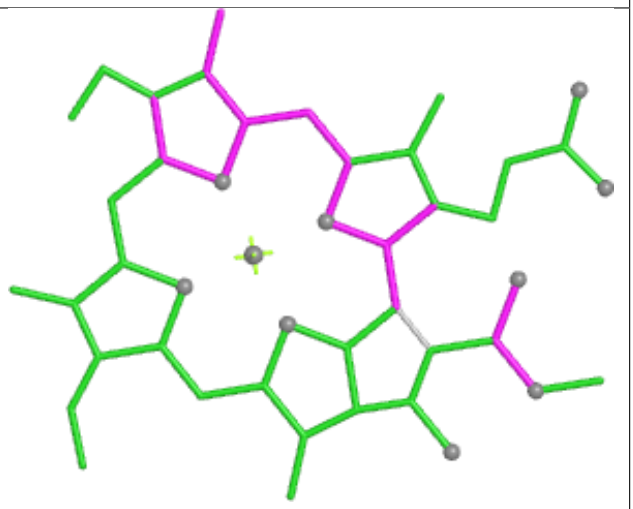


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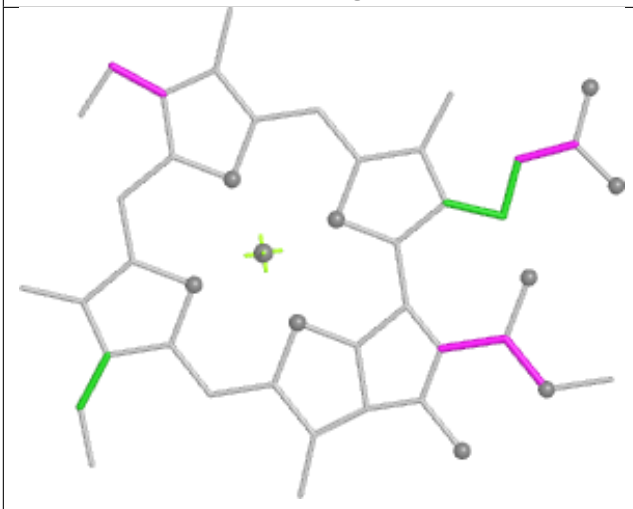
Ligand CLA b1 407



Bond lengths



Bond angles

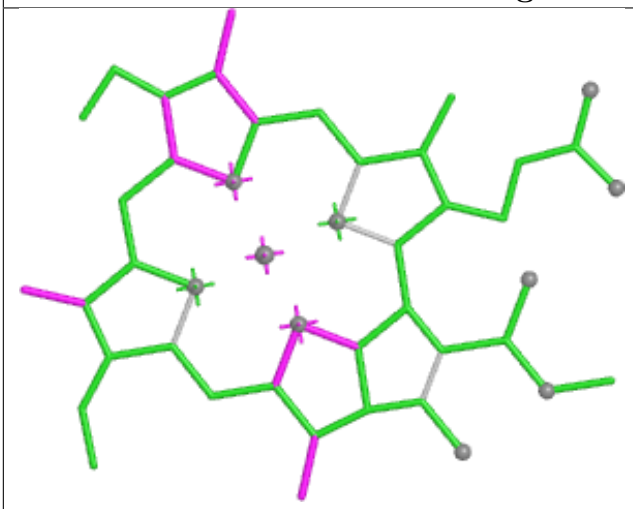


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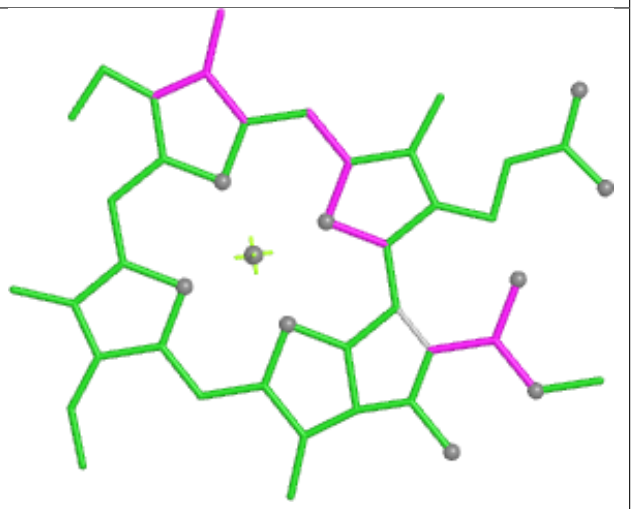


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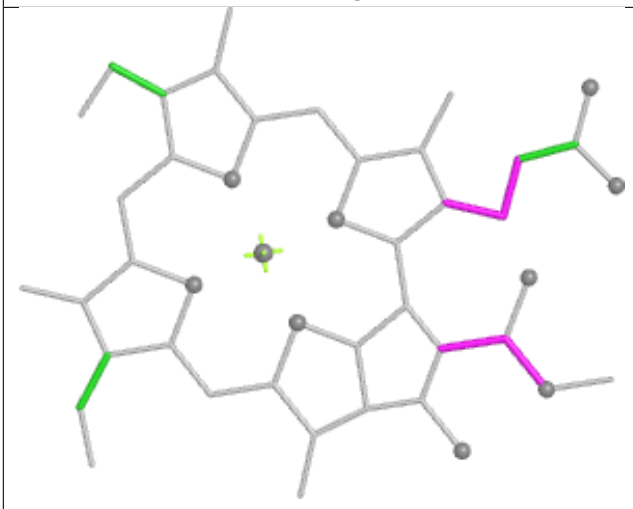
Ligand CLA cB 816



Bond lengths



Bond angles

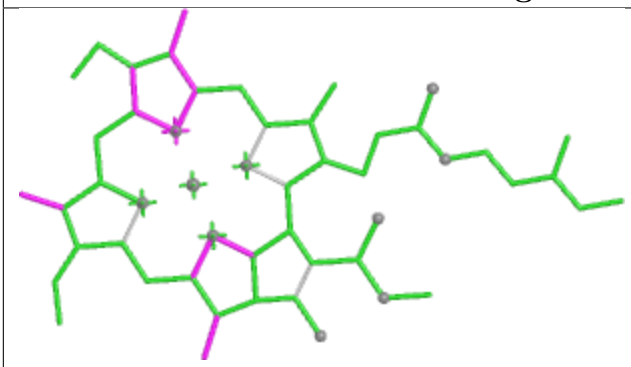


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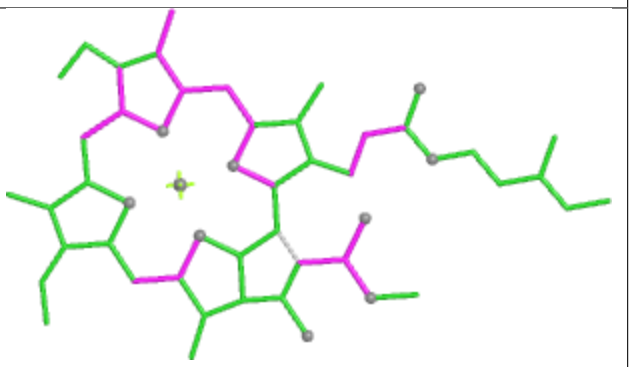


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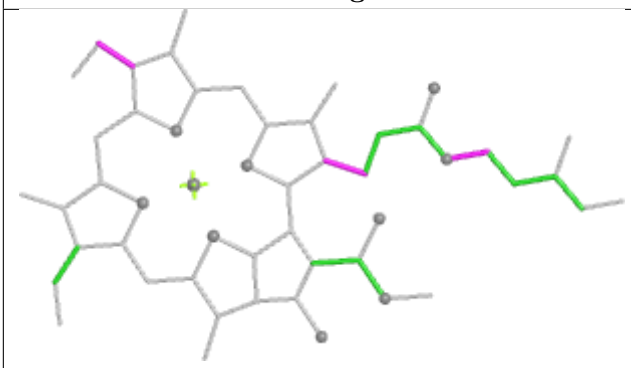
Ligand CLA aA 808



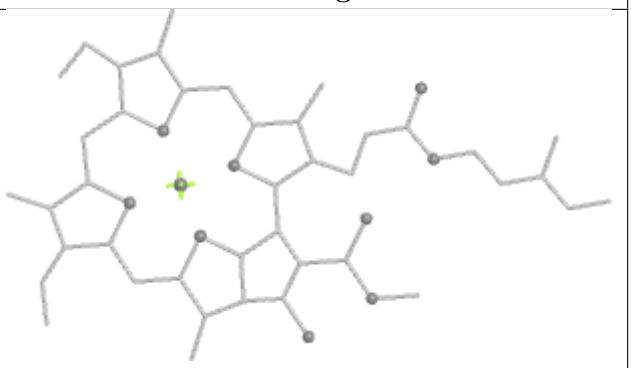
Bond lengths



Bond angles

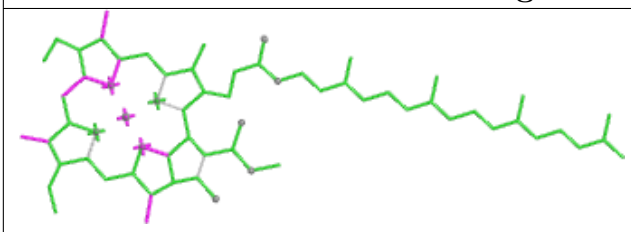


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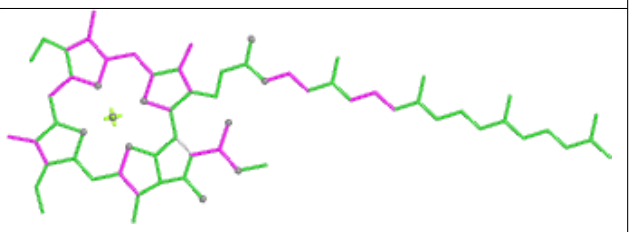


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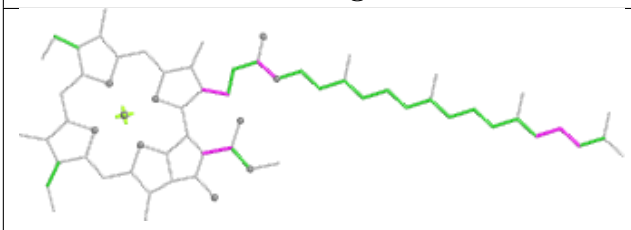
Ligand CLA cB 830



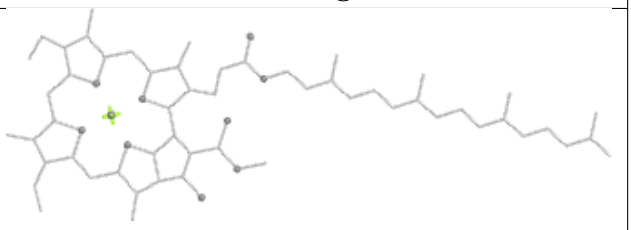
Bond lengths



Bond angles

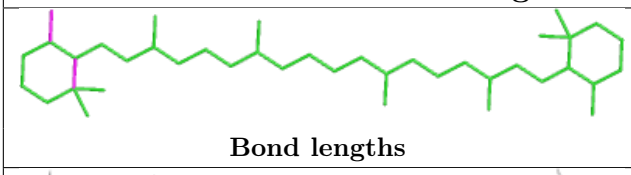


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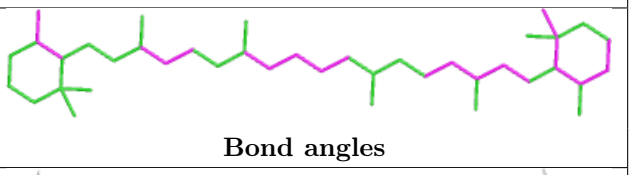


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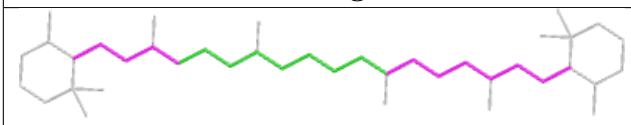
Ligand BCR bA 851



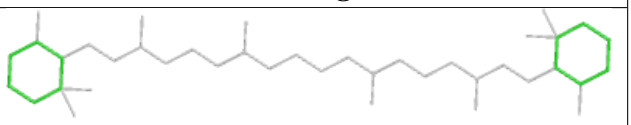
Bond lengths



Bond angles

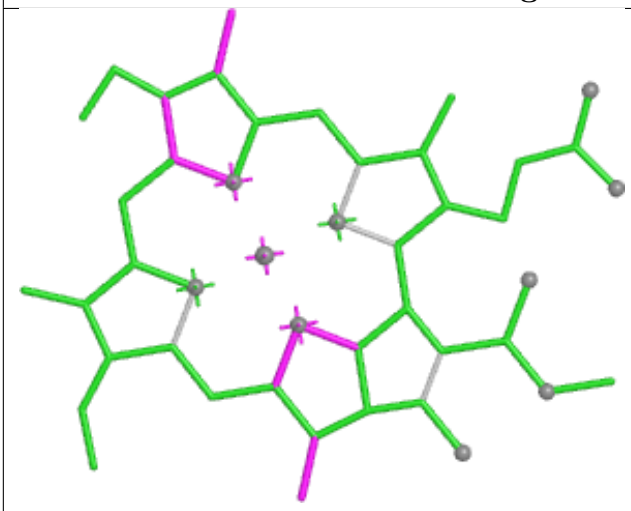


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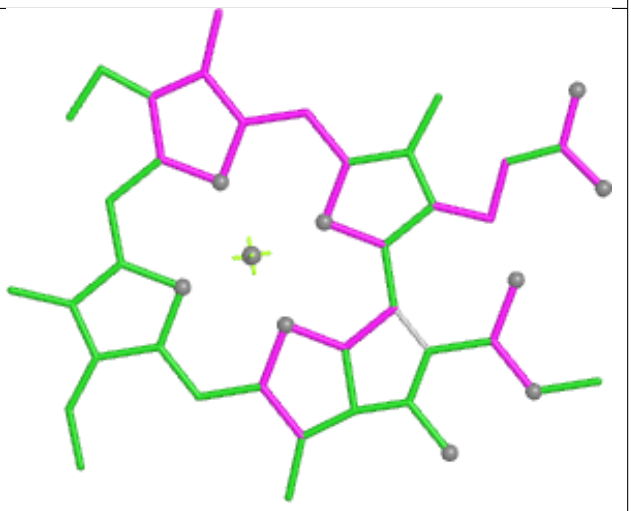


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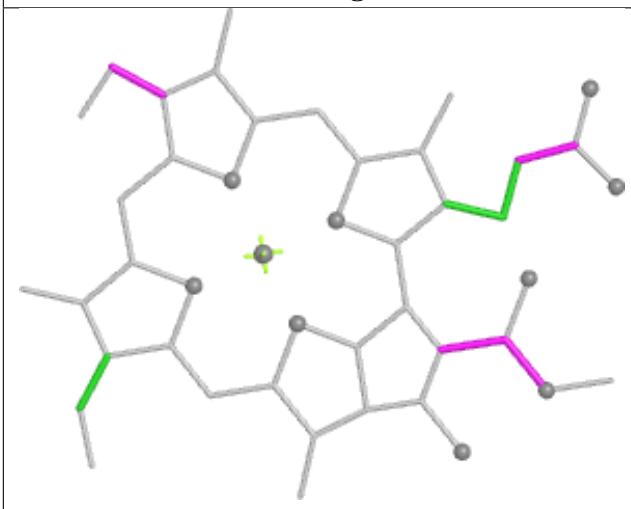
Ligand CLA c6 417



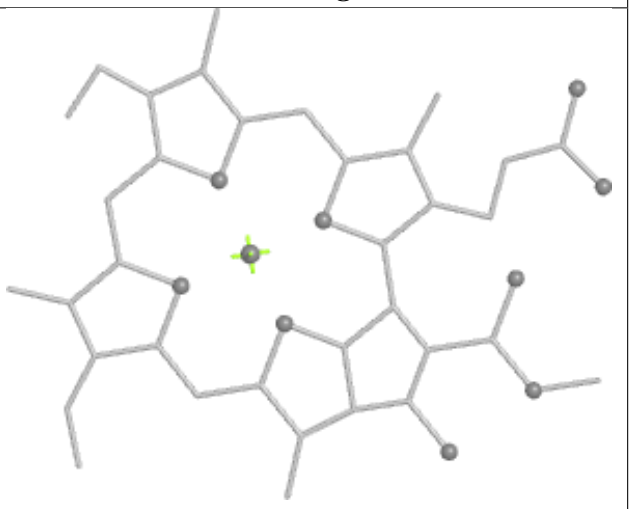
Bond lengths



Bond angles

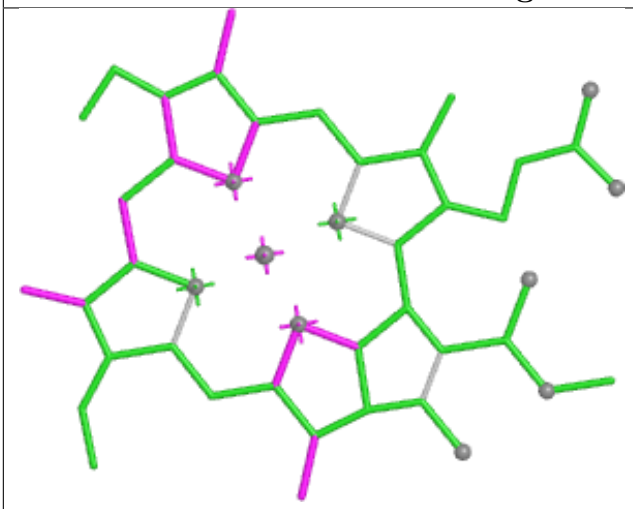


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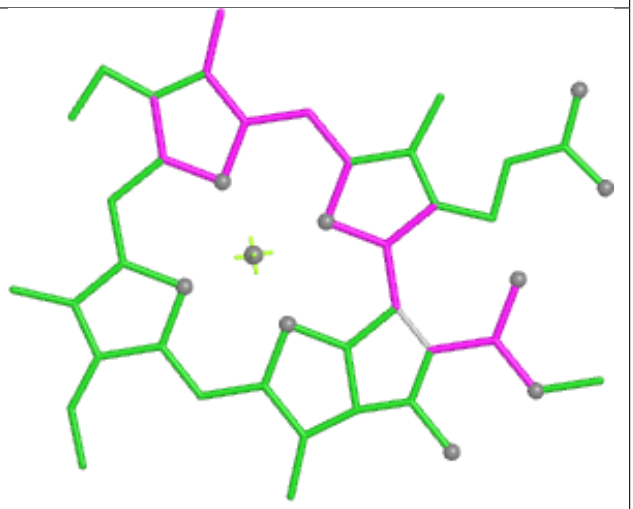


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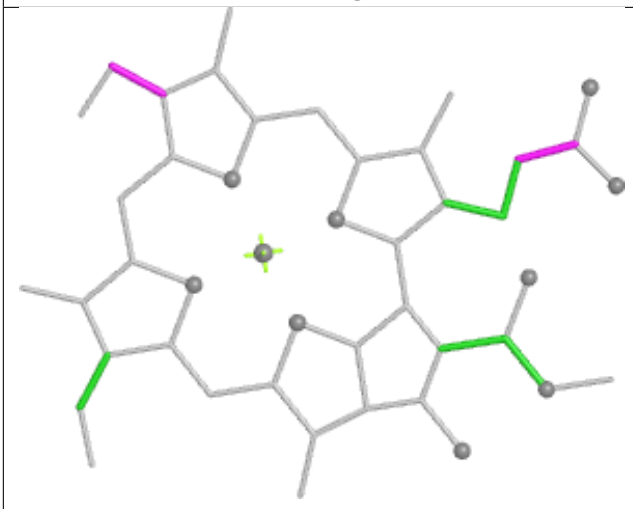
Ligand CLA cB 841



Bond lengths



Bond angles

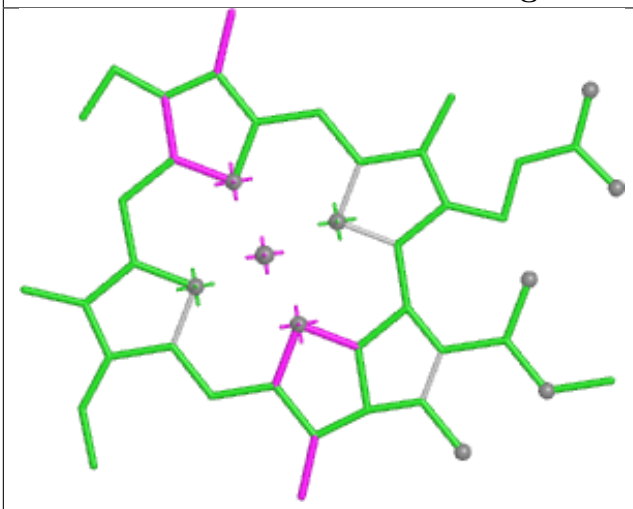


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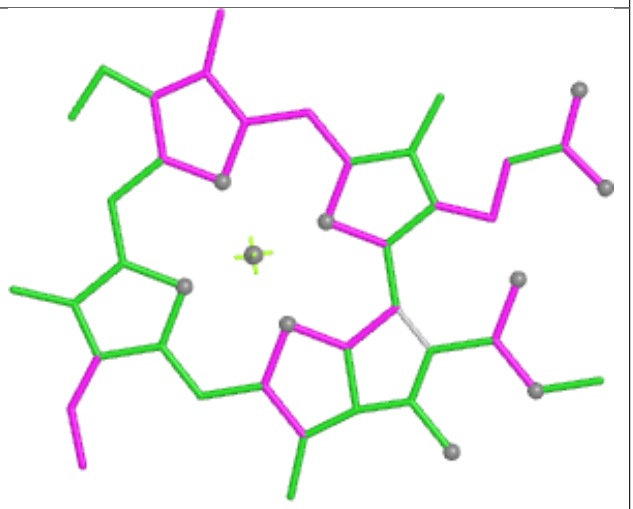


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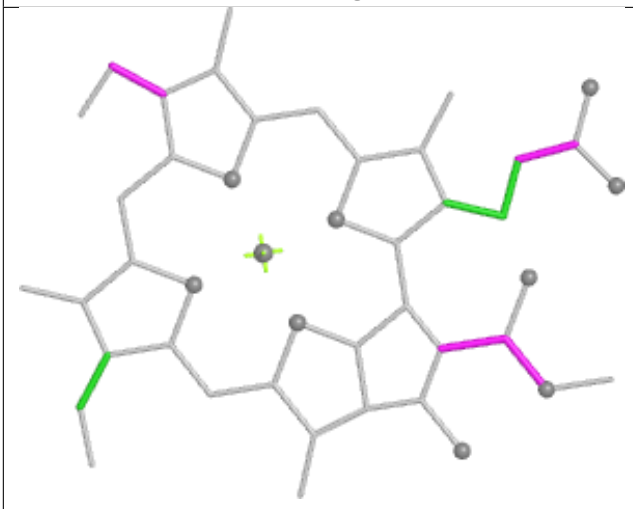
Ligand CLA c4 415



Bond lengths



Bond angles

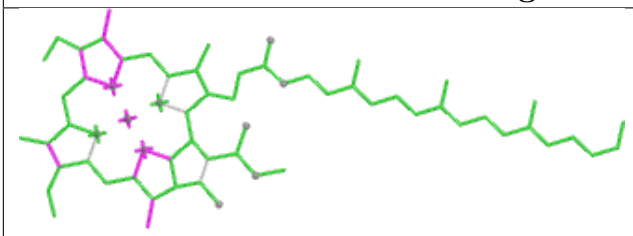


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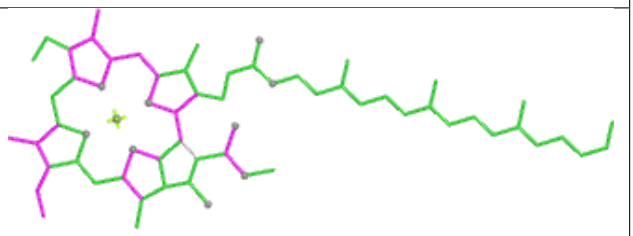


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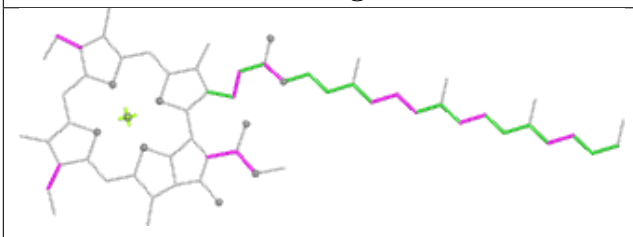
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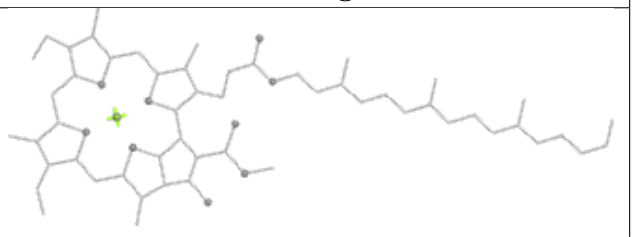
Bond lengths



Bond angles

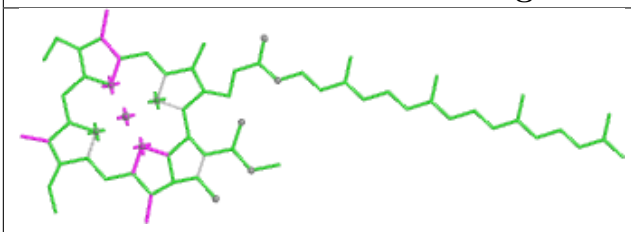


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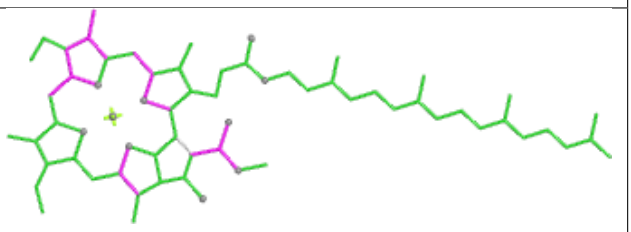


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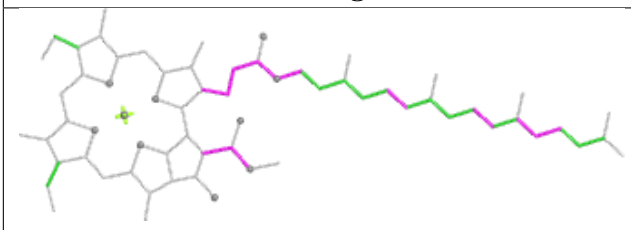
Ligand CLA aB 829



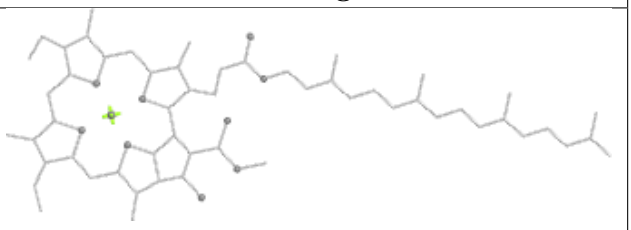
Bond lengths



Bond angles

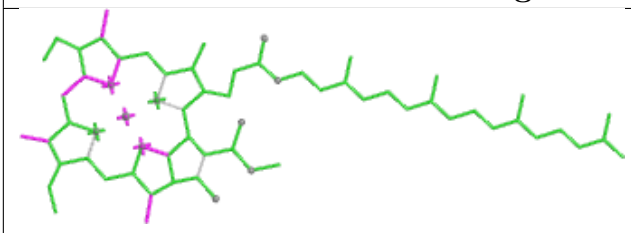


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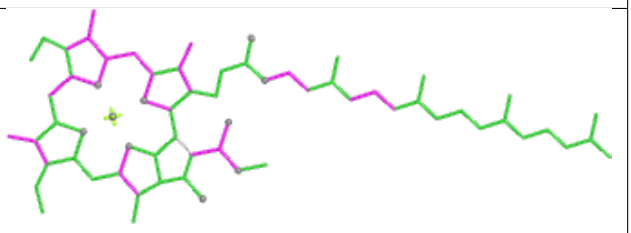


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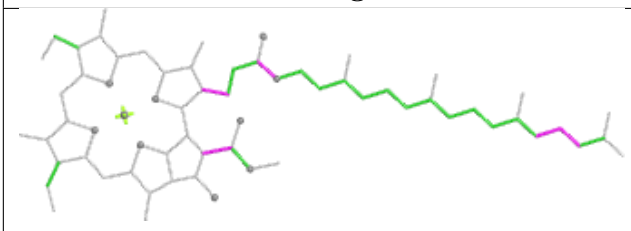
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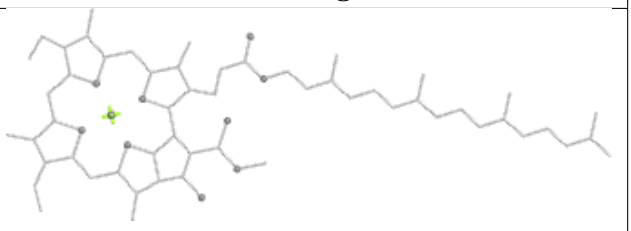
Bond lengths



Bond angles

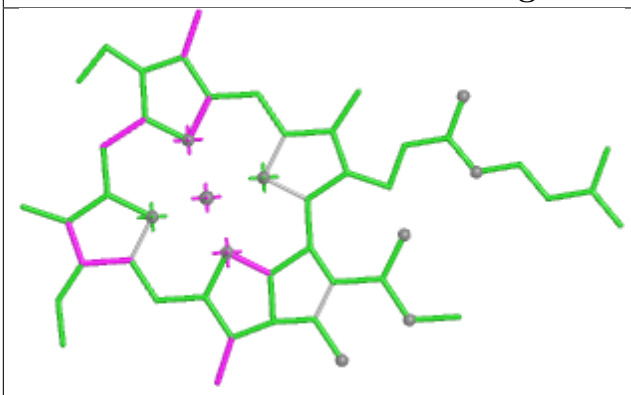


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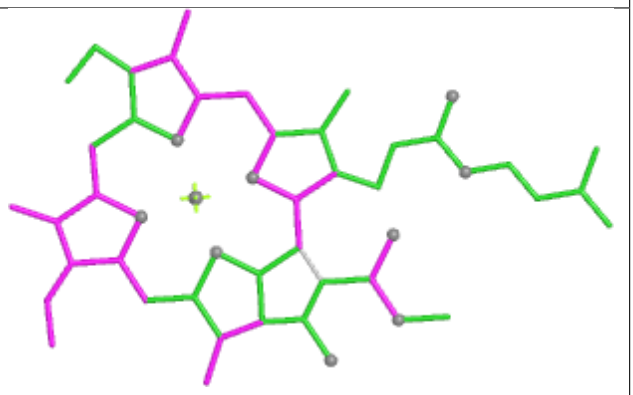


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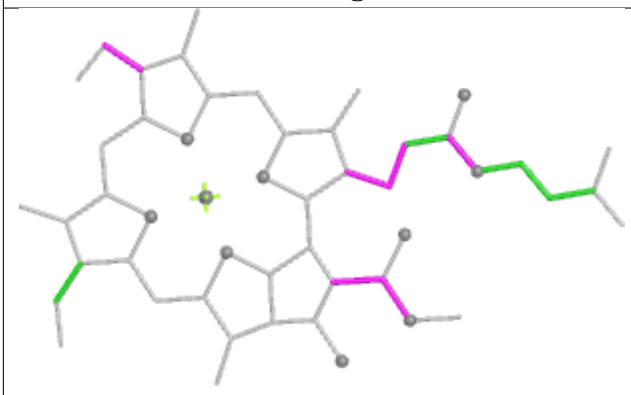
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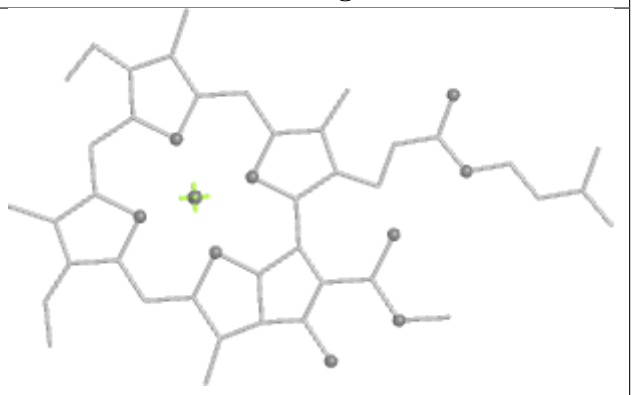
Bond lengths



Bond angles

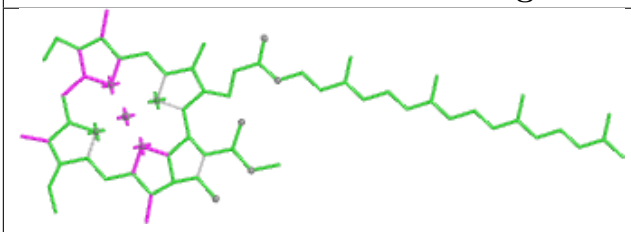


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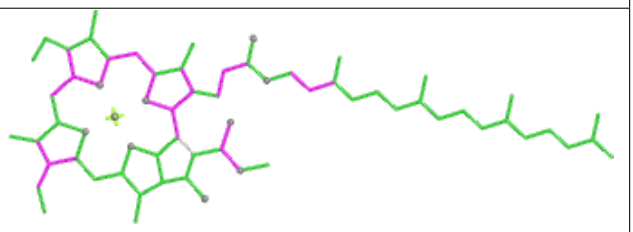


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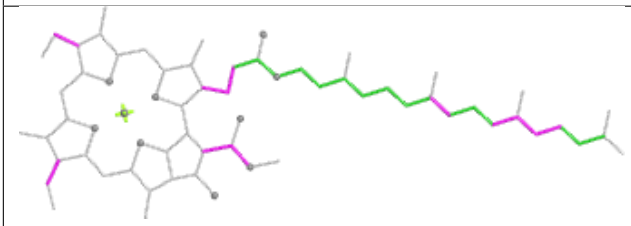
Ligand CLA cB 840



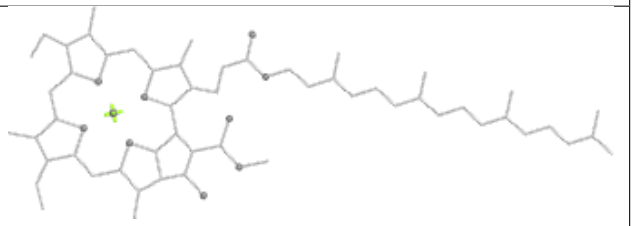
Bond lengths



Bond angles

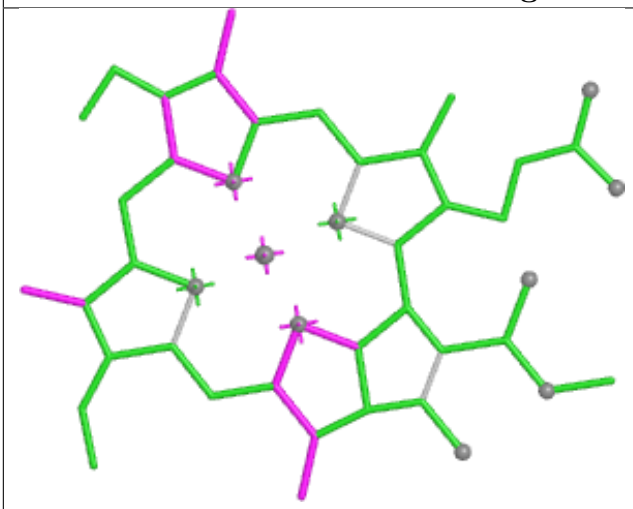


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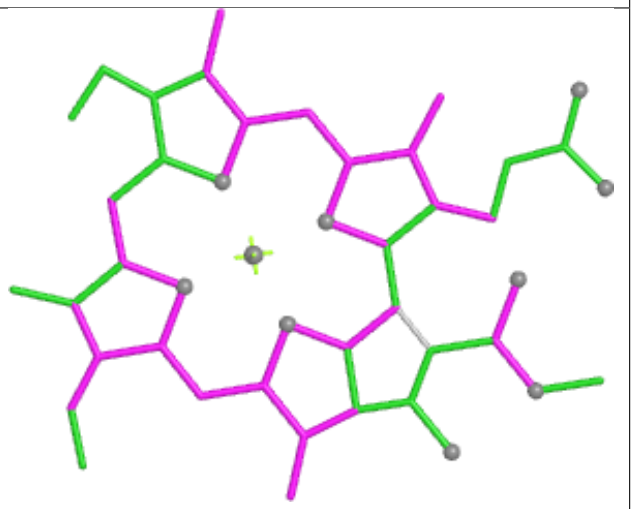


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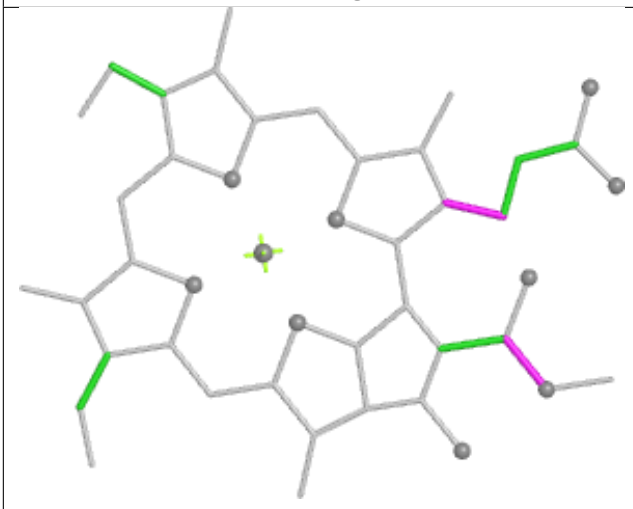
Ligand CLA c3 405



Bond lengths



Bond angles

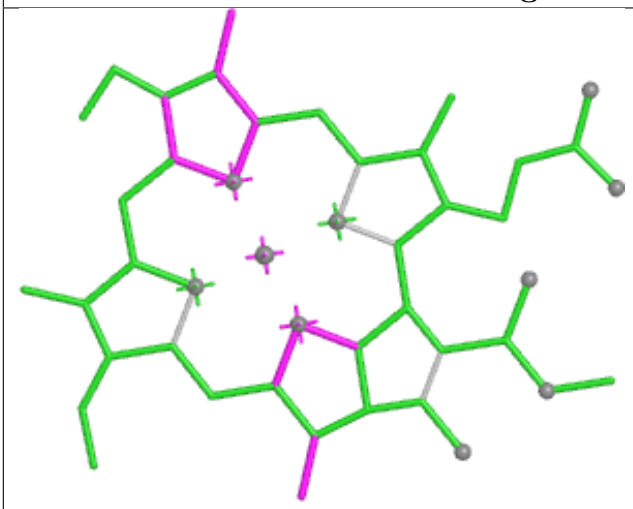


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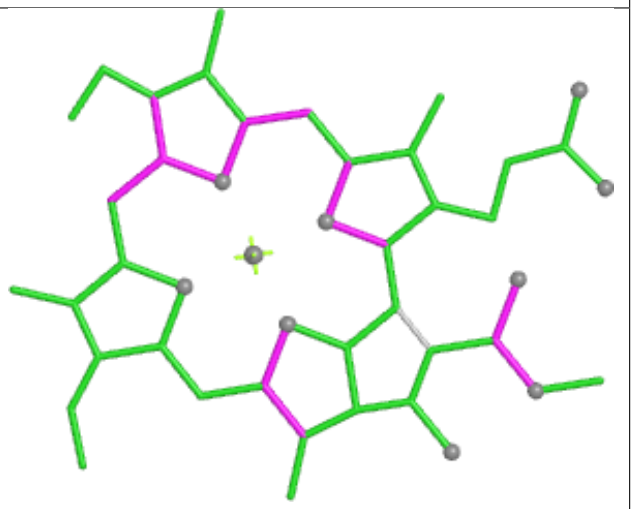


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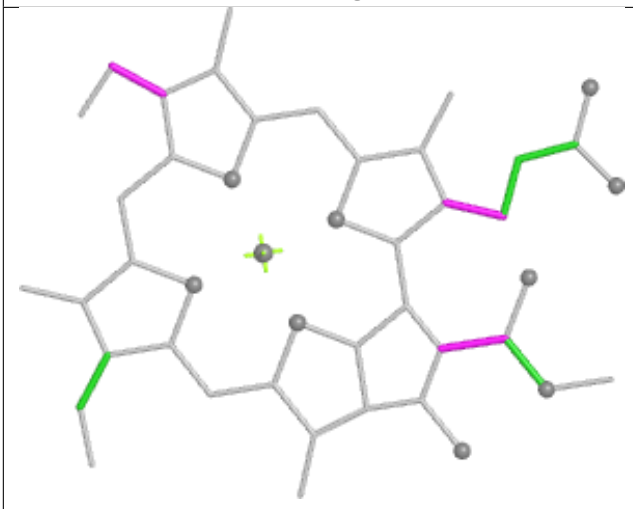
Ligand CLA c4 413



Bond lengths



Bond angles

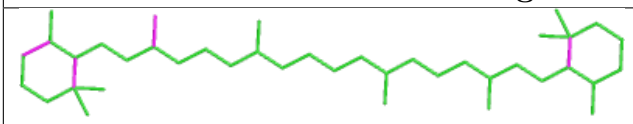


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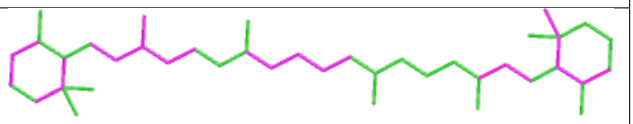


Rings

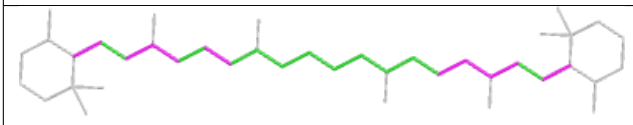
Ligand BCR b6 401



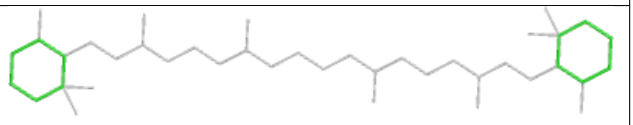
Bond lengths



Bond angles

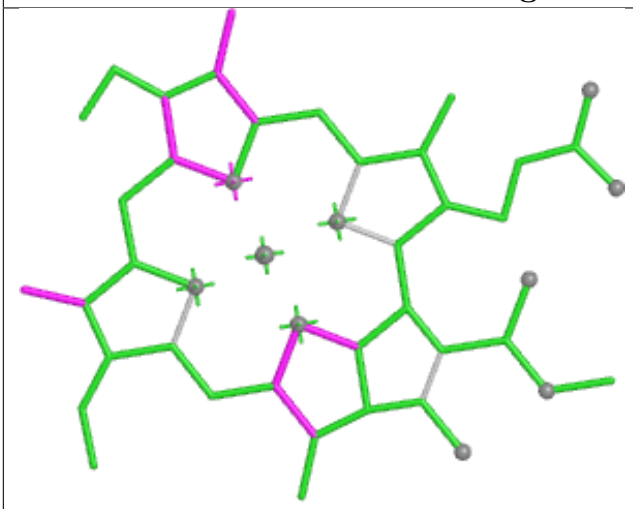


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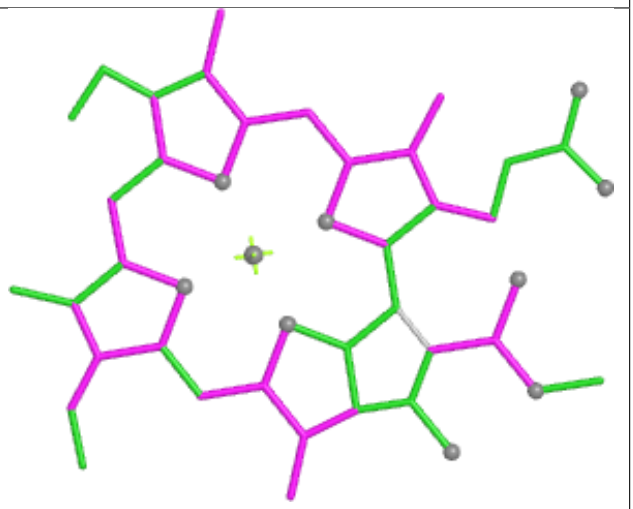


Rings

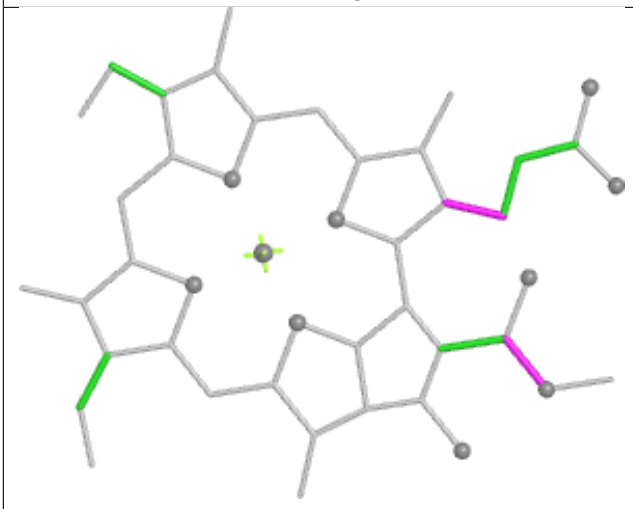
Ligand CLA a1 404



Bond lengths



Bond angles

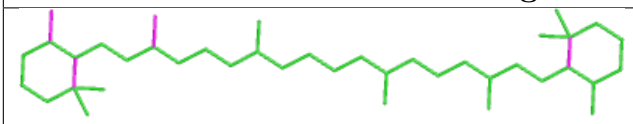


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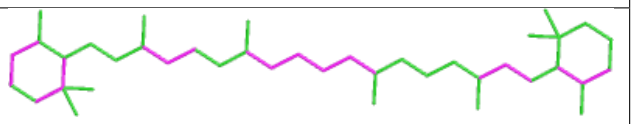


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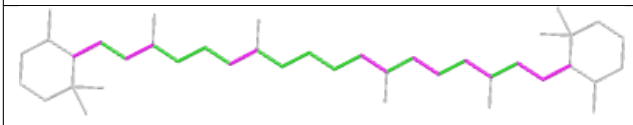
Ligand BCR aI 102



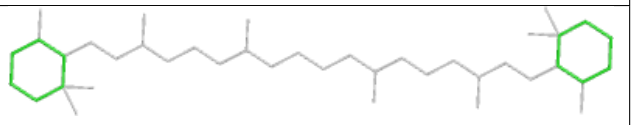
Bond lengths



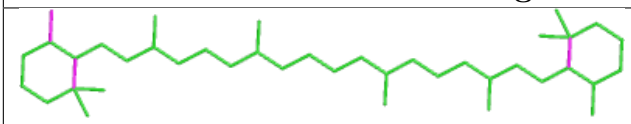
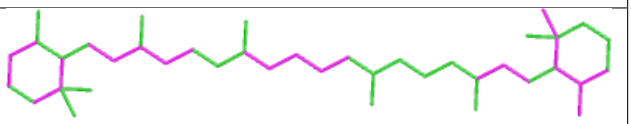
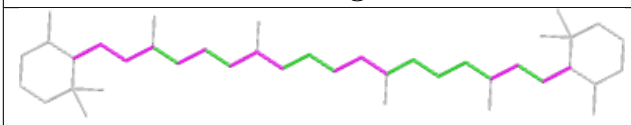
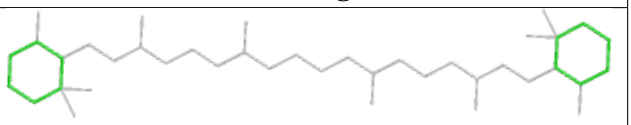
Bond angles

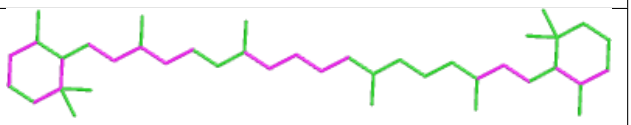
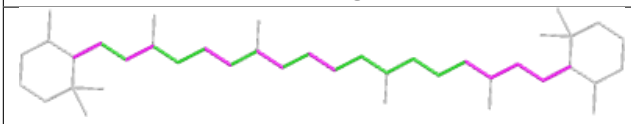
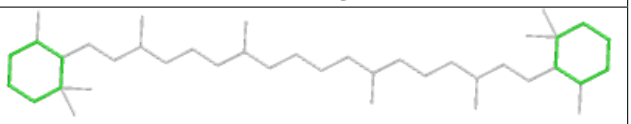


Torsions

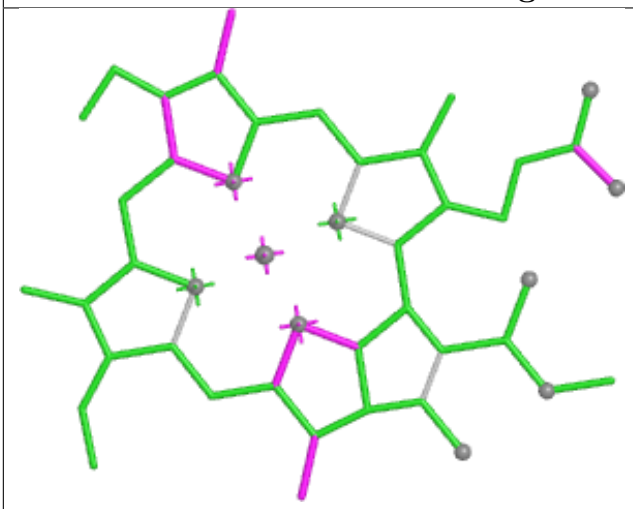


Rings

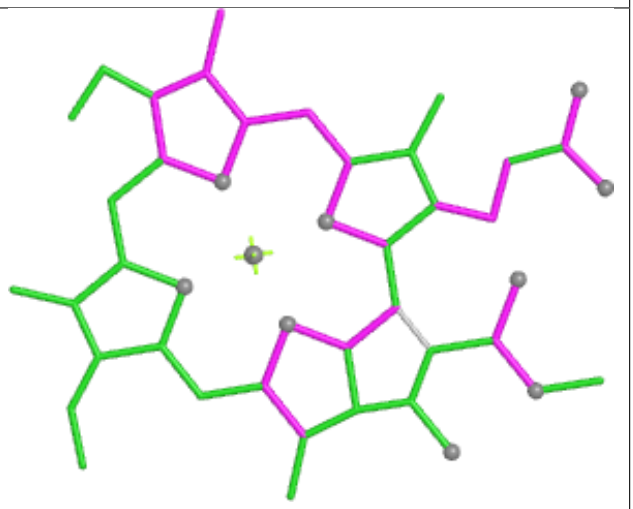
Ligand BCR bL 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCR cB 848	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

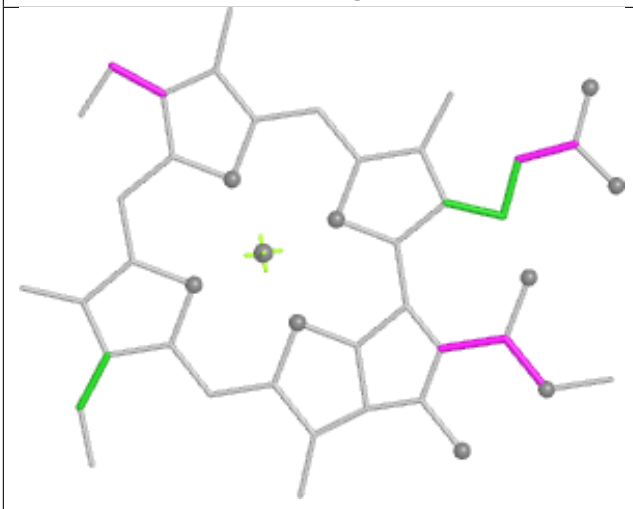
Ligand CLA b2 416



Bond lengths



Bond angles

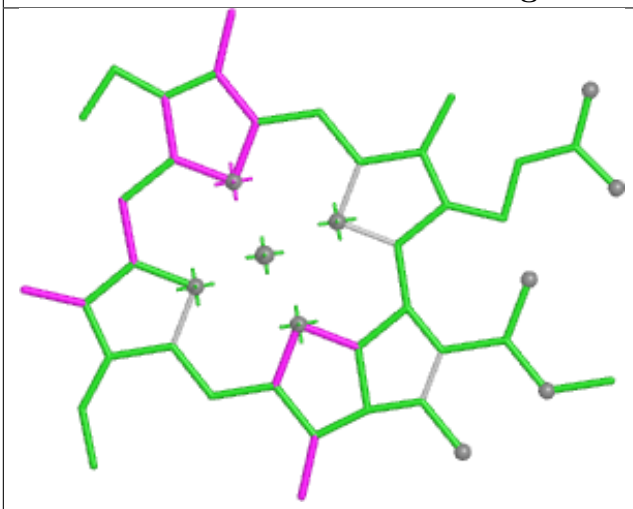


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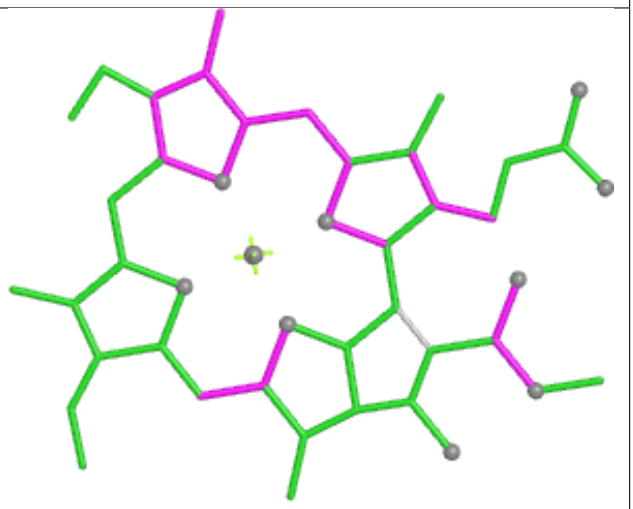


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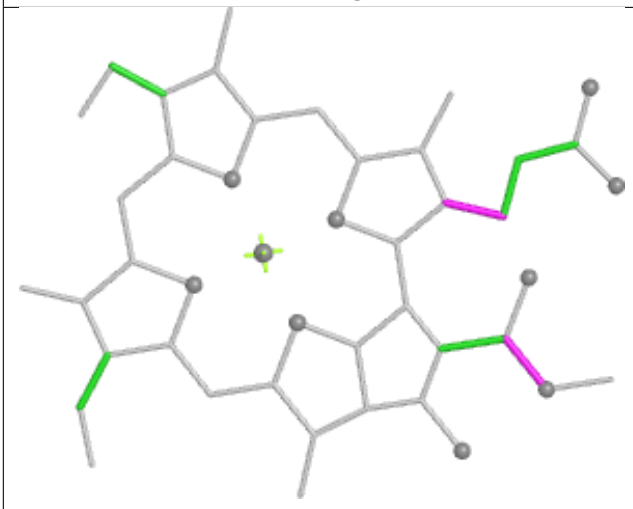
Ligand CLA c4 411



Bond lengths



Bond angles

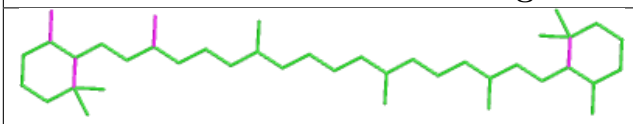


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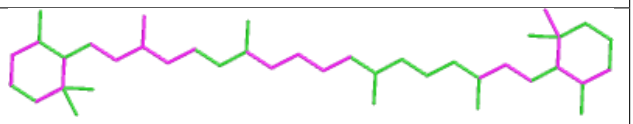


Rings

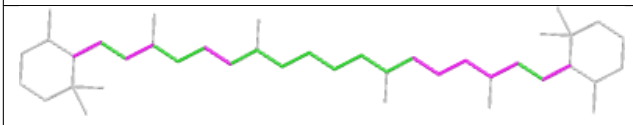
Ligand BCR b1 419



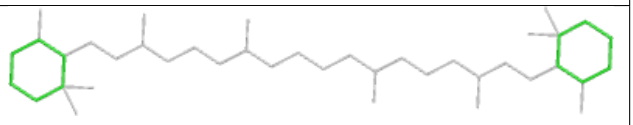
Bond lengths



Bond angles

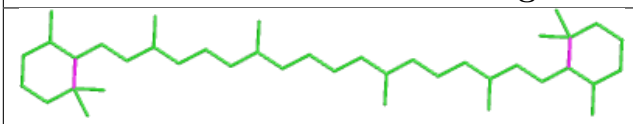


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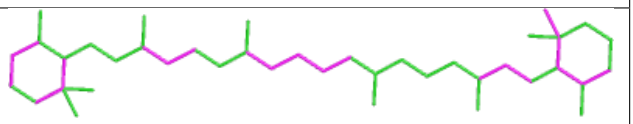


Rings

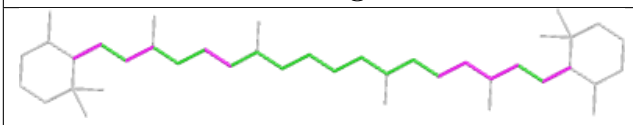
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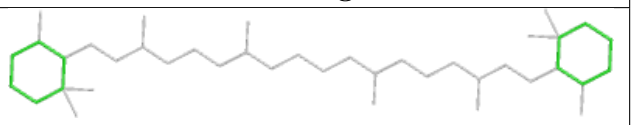
Bond lengths



Bond angles

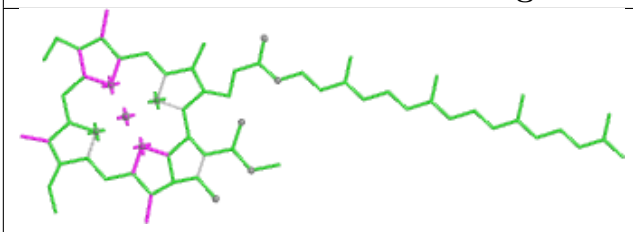


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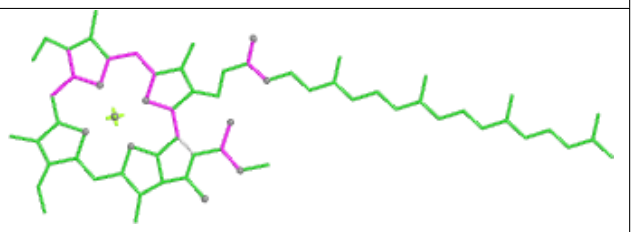


Rings

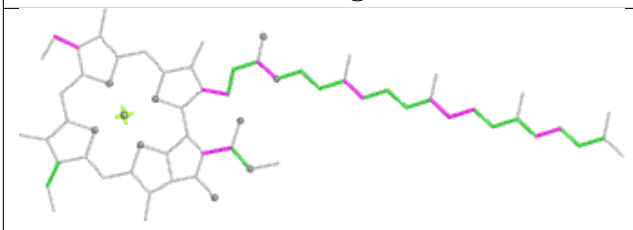
Ligand CLA bL 202



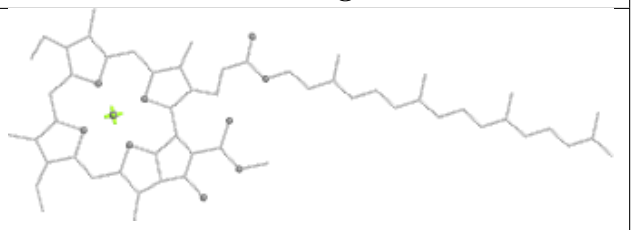
Bond lengths



Bond angles

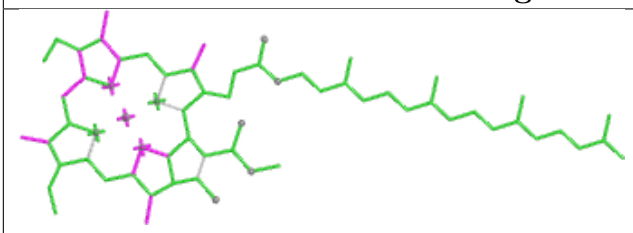


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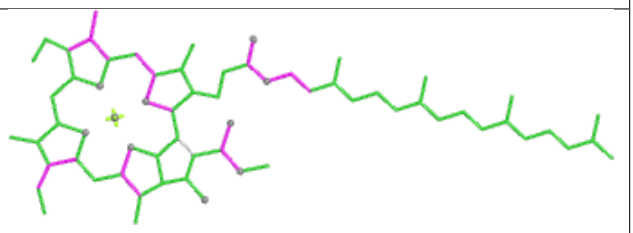


Rings

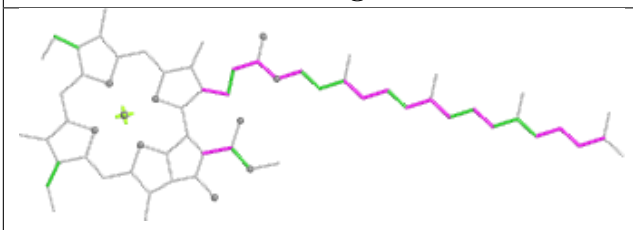
Ligand CLA bB 806



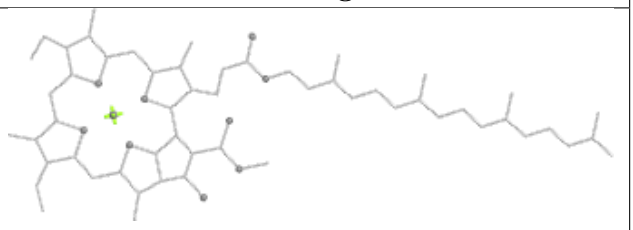
Bond lengths



Bond angles

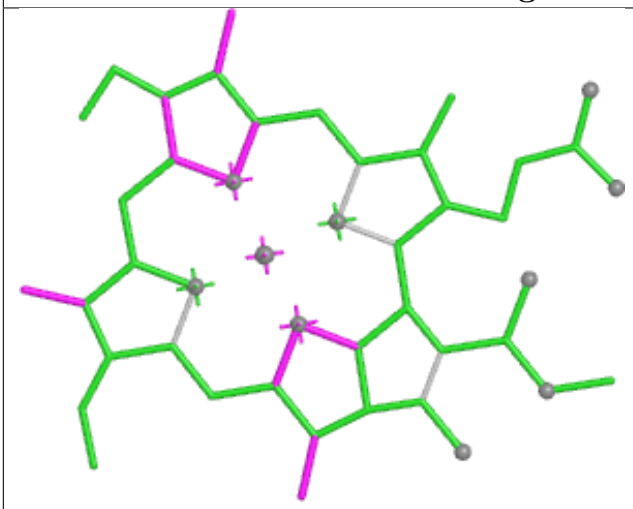


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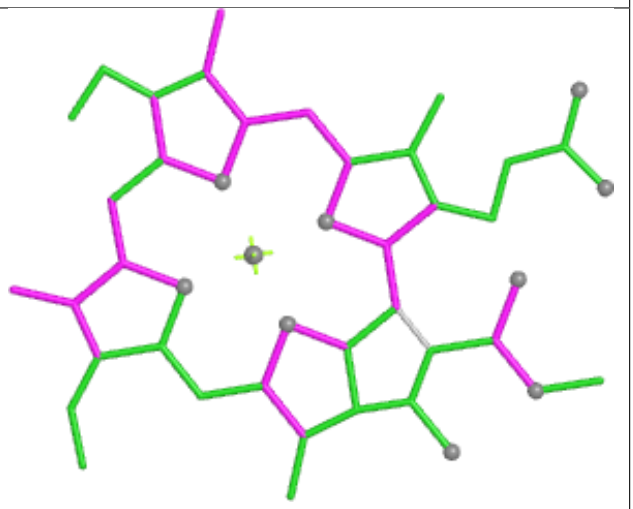


Rings

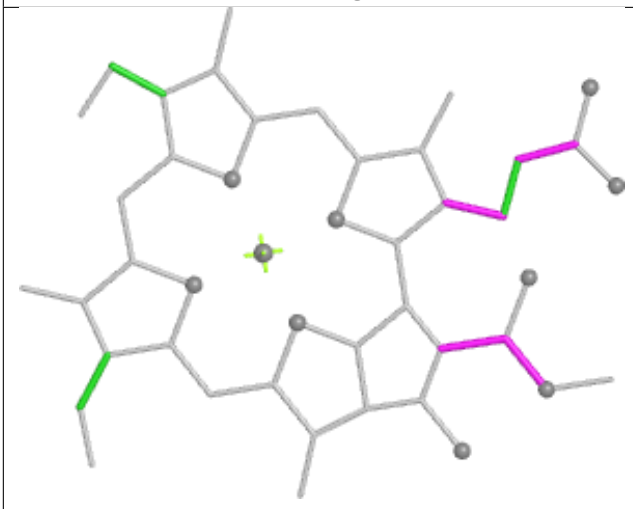
Ligand CLA b5 412



Bond lengths



Bond angles

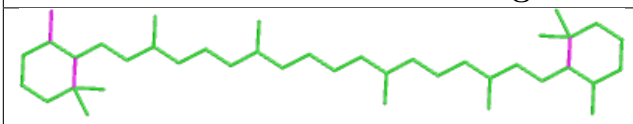


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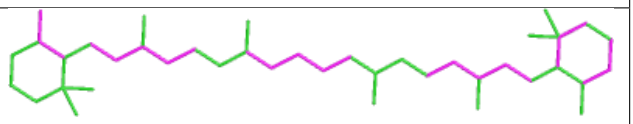


Rings

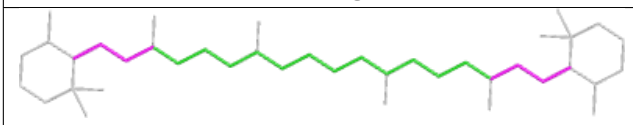
Ligand BCR aK 101



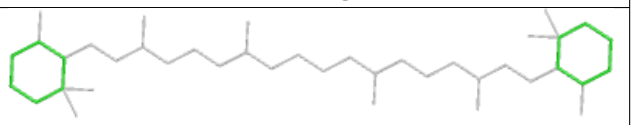
Bond lengths



Bond angles

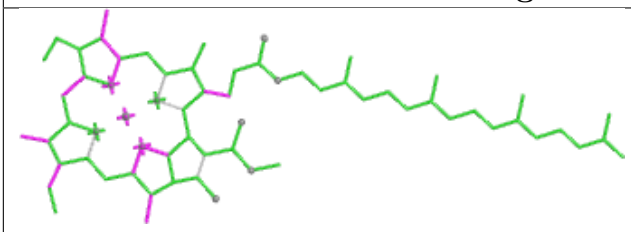


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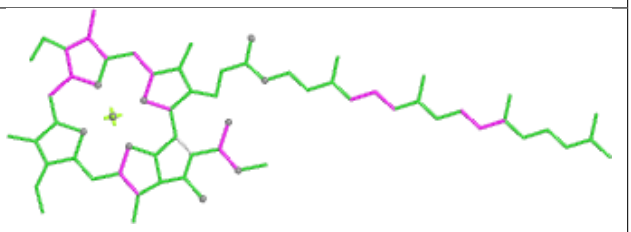


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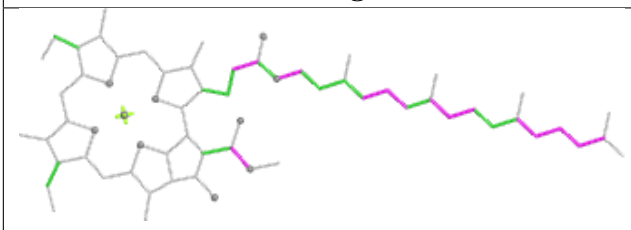
Ligand CLA cB 807



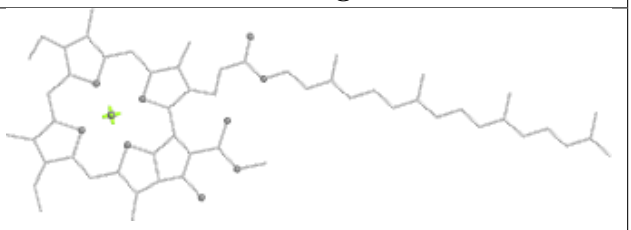
Bond lengths



Bond angles



Torsions

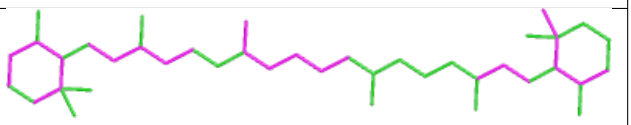


Rings

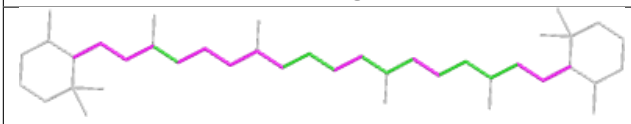
Ligand BCR b5 401



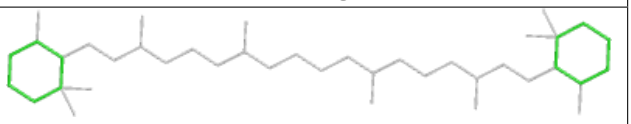
Bond lengths



Bond angles

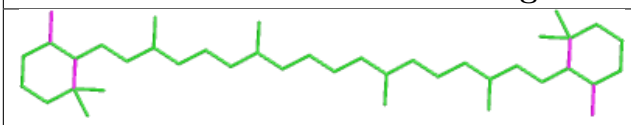


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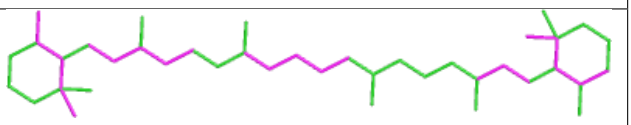


Rings

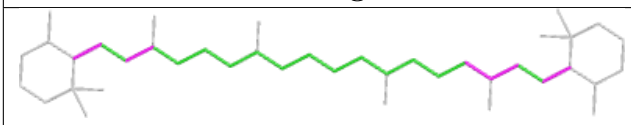
Ligand BCR aI 103



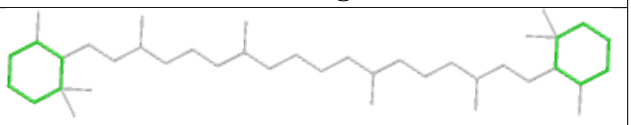
Bond lengths



Bond angles

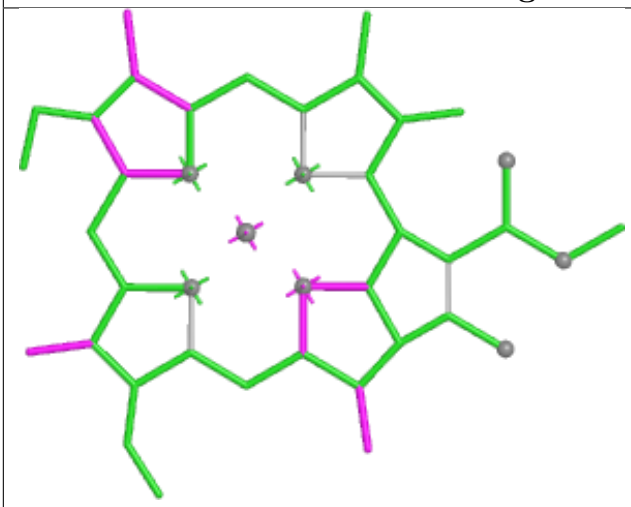


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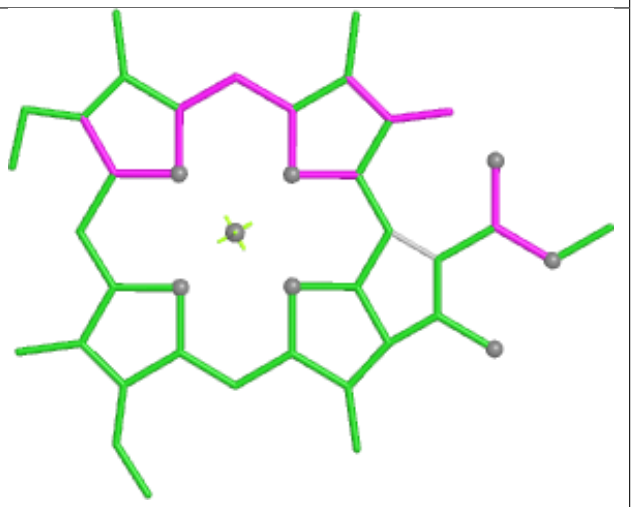


Rings

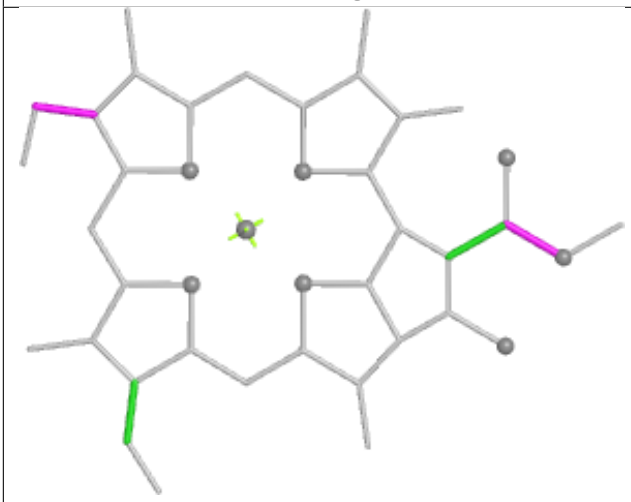
Ligand CLA b4 414



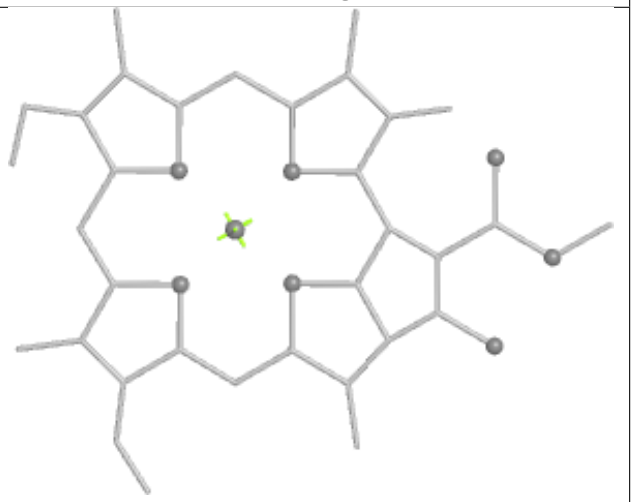
Bond lengths



Bond angles

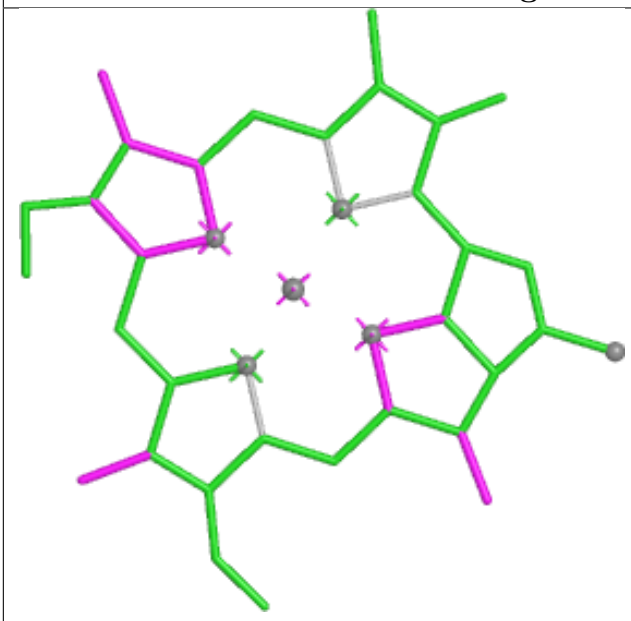


Torsions



Rings

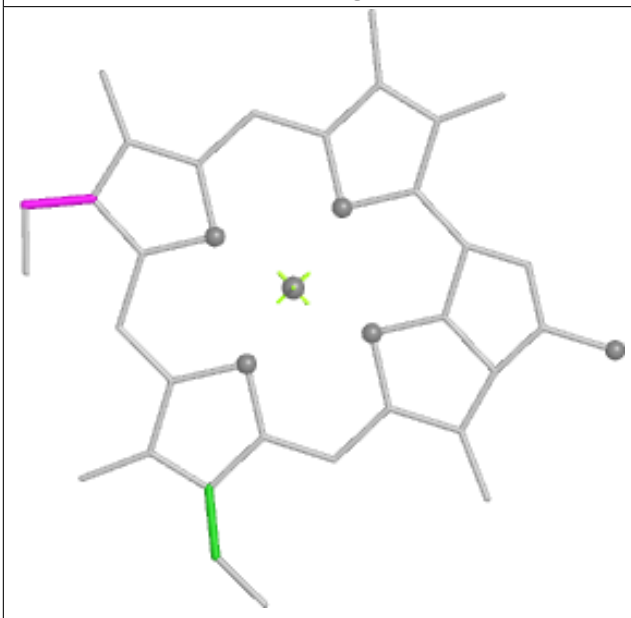
Ligand CLA cJ 102



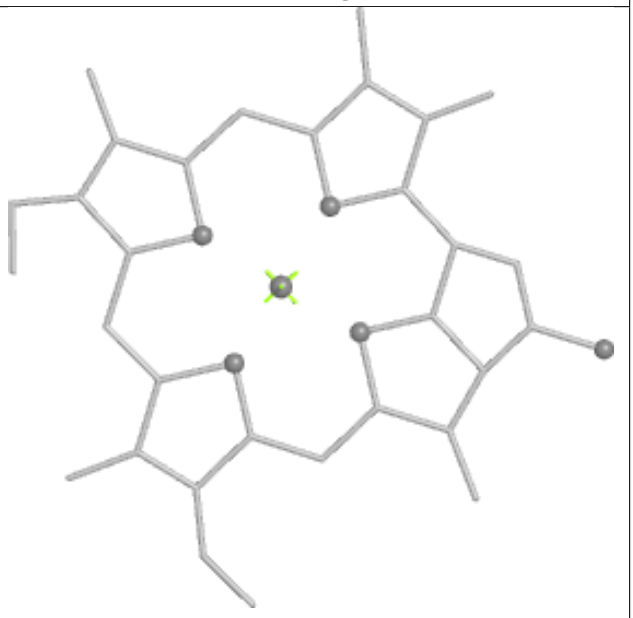
Bond lengths



Bond angles

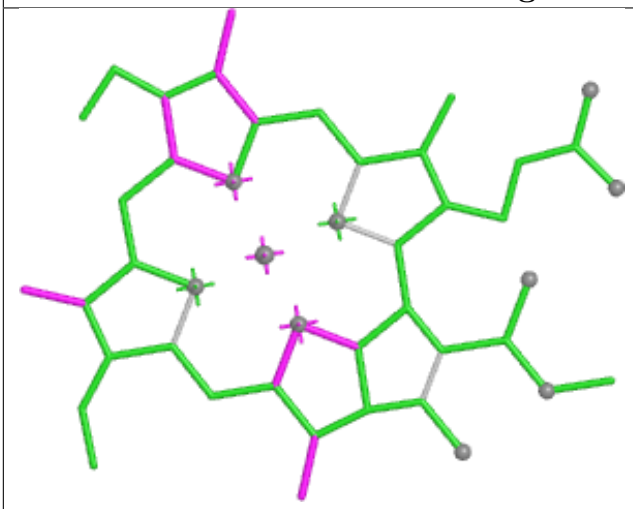


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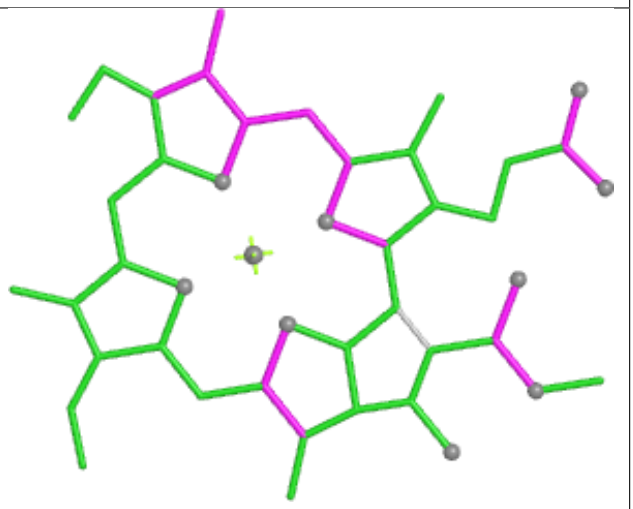


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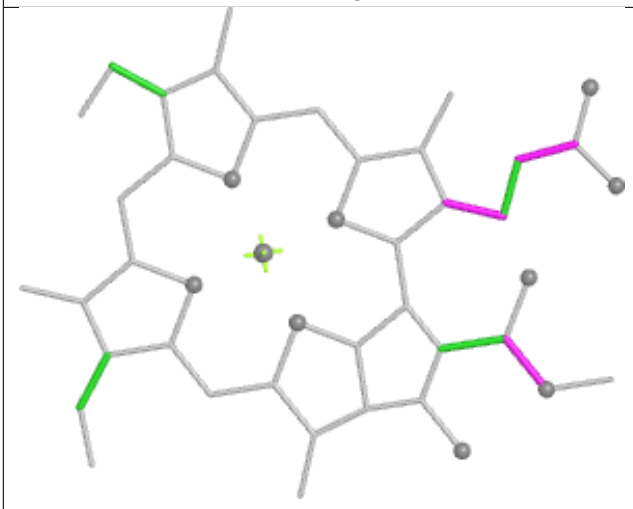
Ligand CLA b4 408



Bond lengths



Bond angles

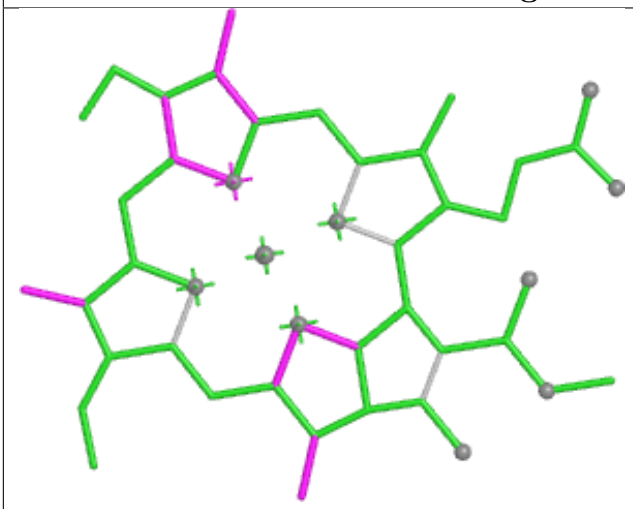


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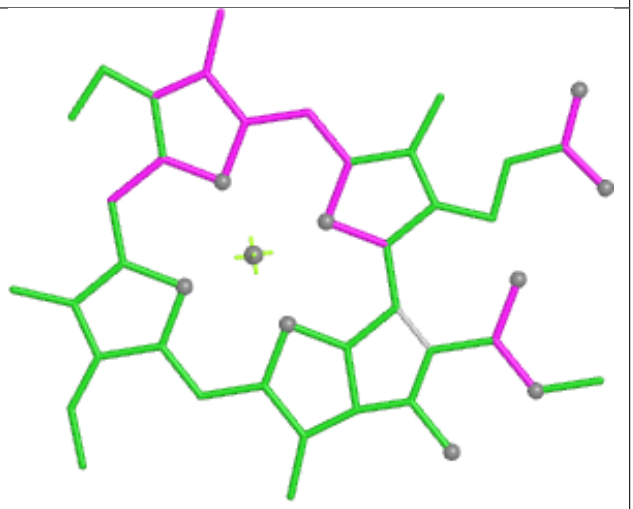


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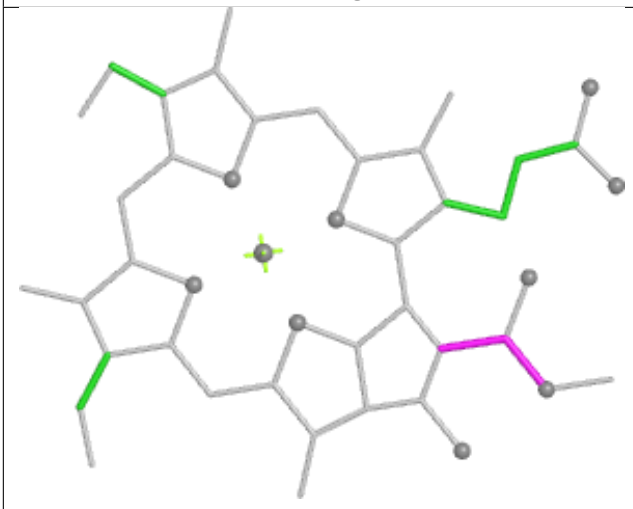
Ligand CLA c1 406



Bond lengths



Bond angles

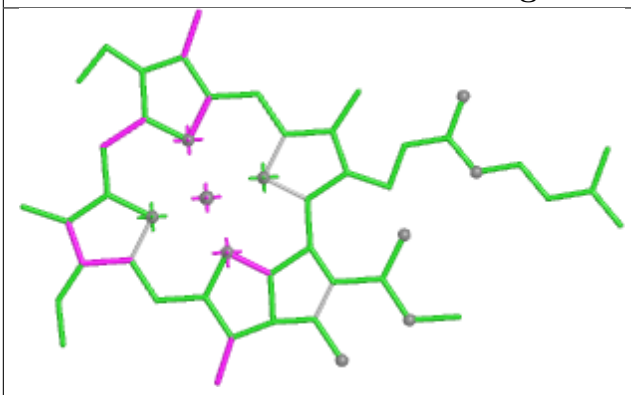


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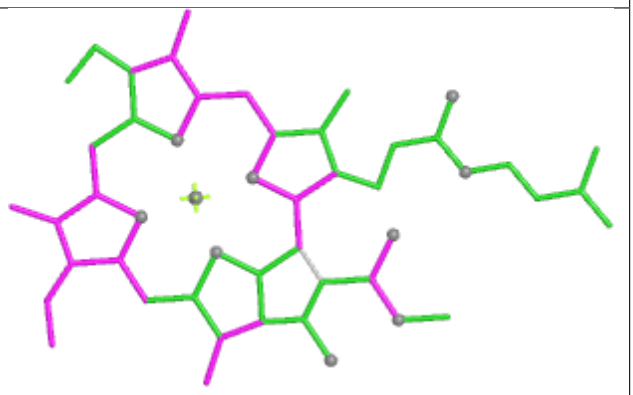


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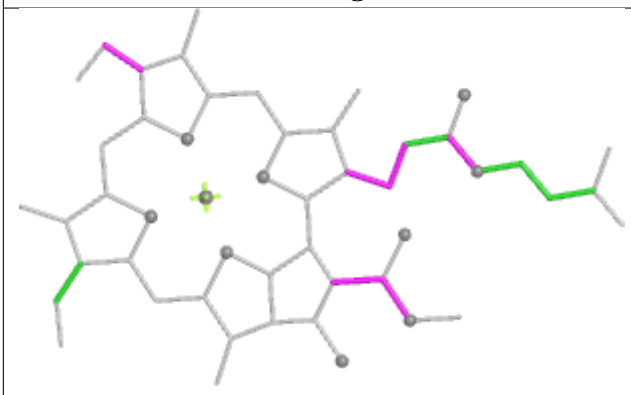
Ligand CLA a5 416



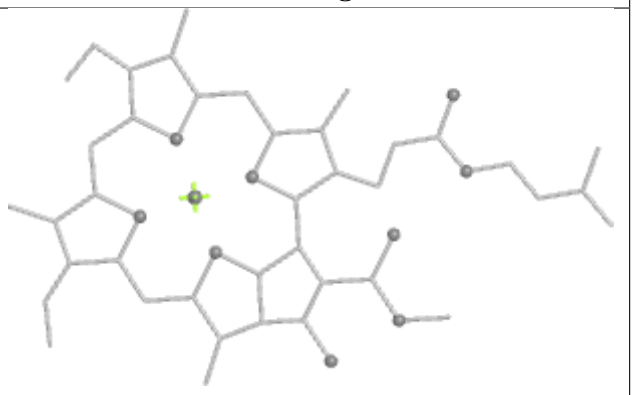
Bond lengths



Bond angles

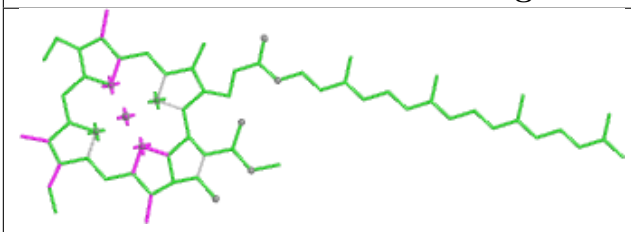


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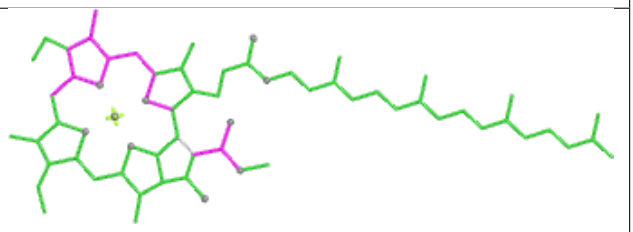


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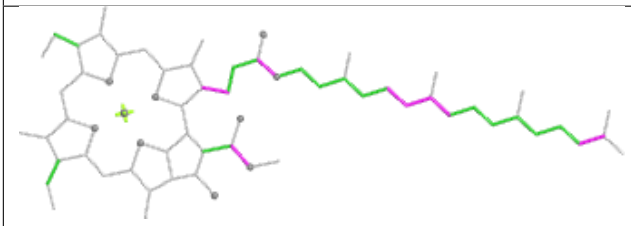
Ligand CLA aA 833



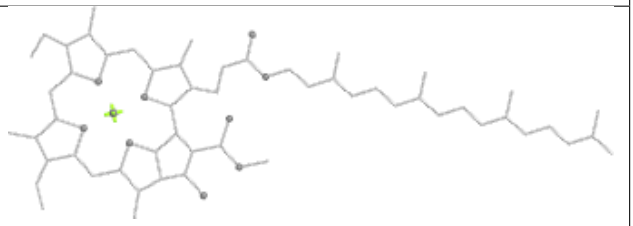
Bond lengths



Bond angles

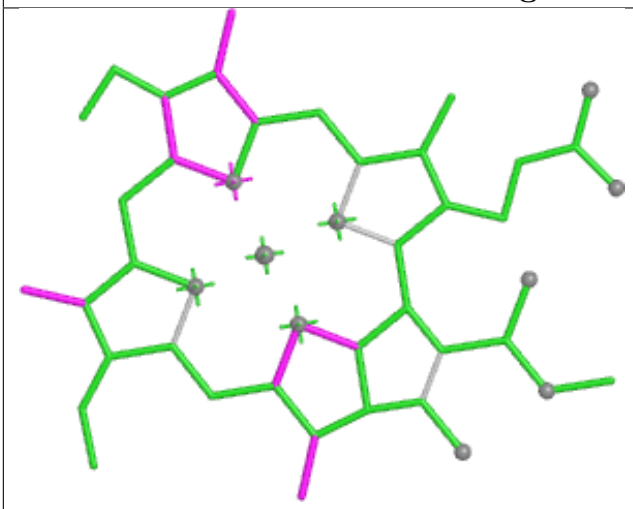


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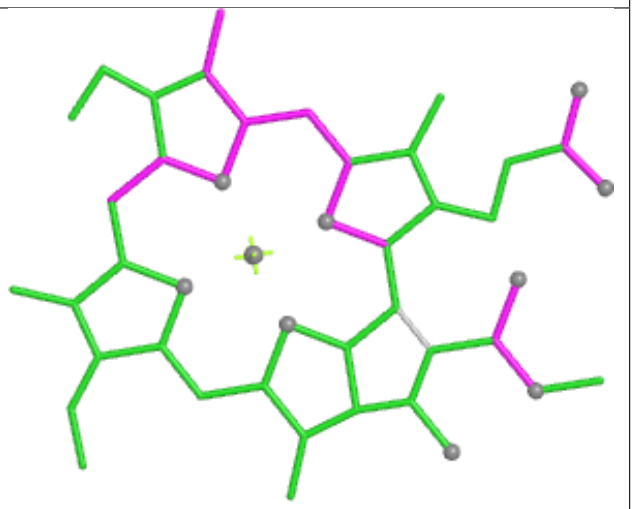


Rings

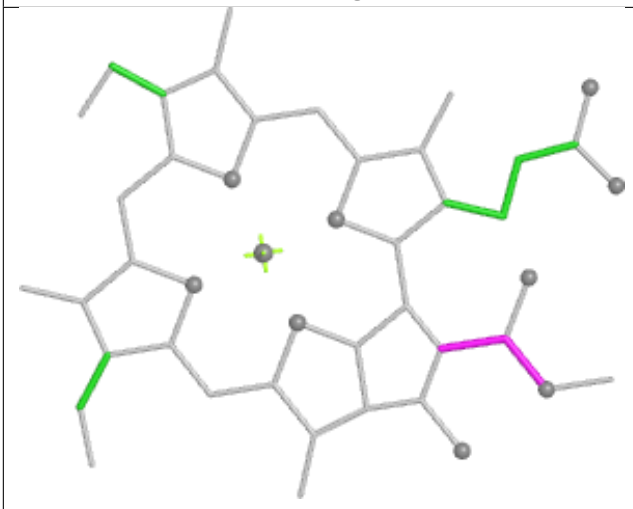
Ligand CLA a3 406



Bond lengths



Bond angles

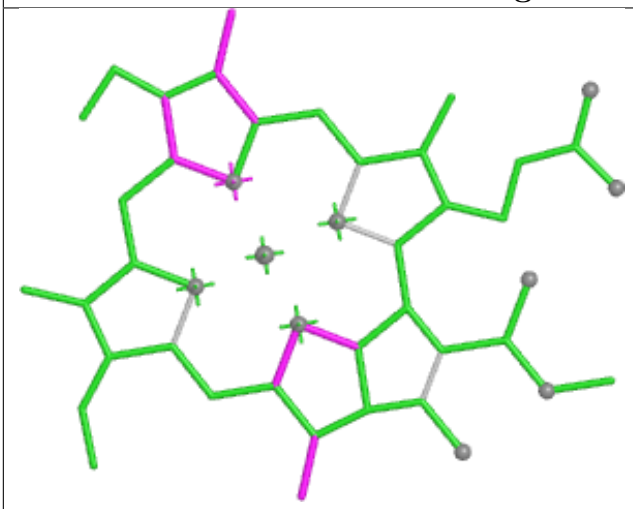


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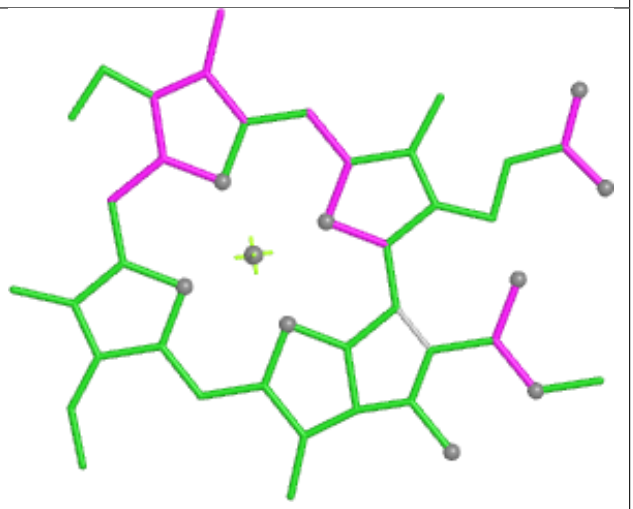


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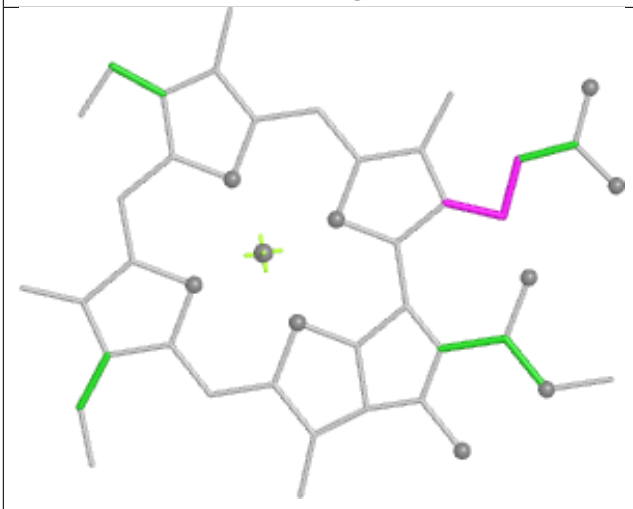
Ligand CLA bB 822



Bond lengths



Bond angles

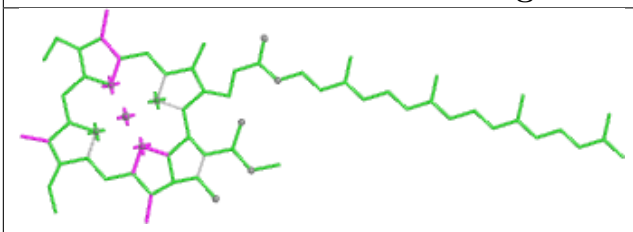


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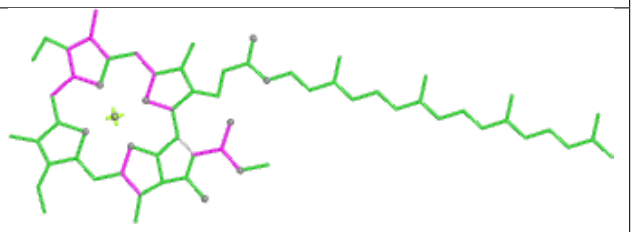


Rings

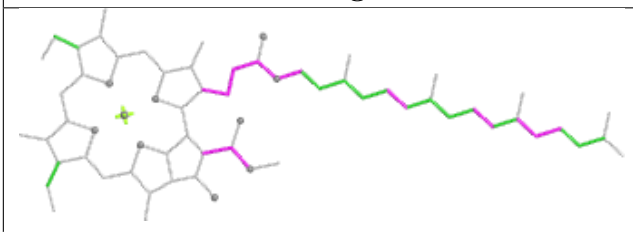
Ligand CLA cB 829



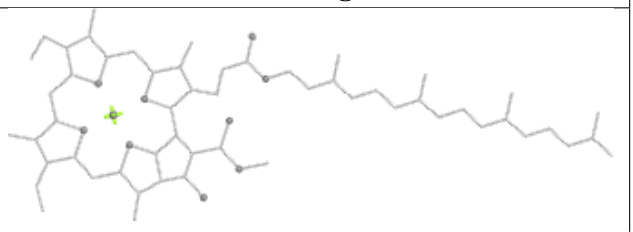
Bond lengths



Bond angles

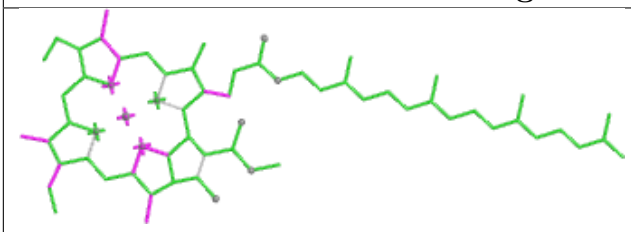


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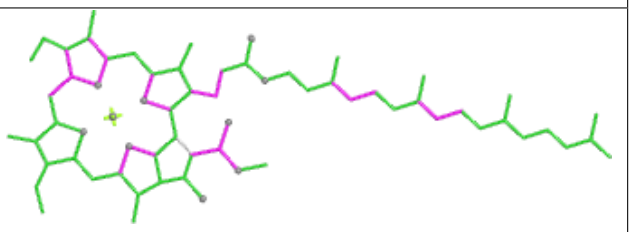


Rings

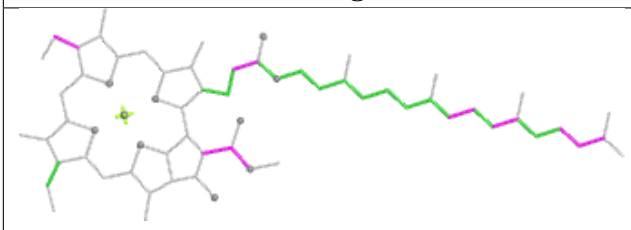
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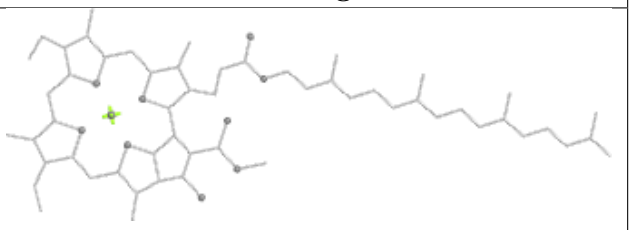
Bond lengths



Bond angles

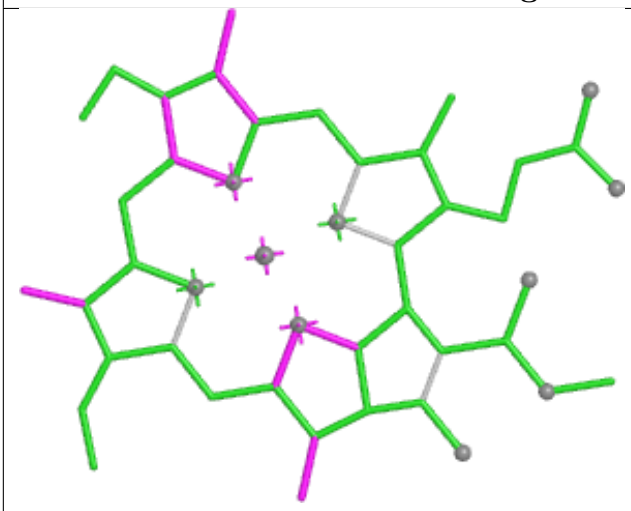


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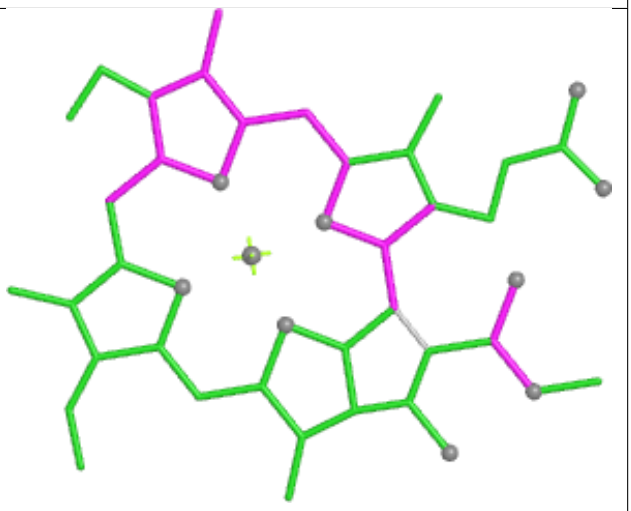


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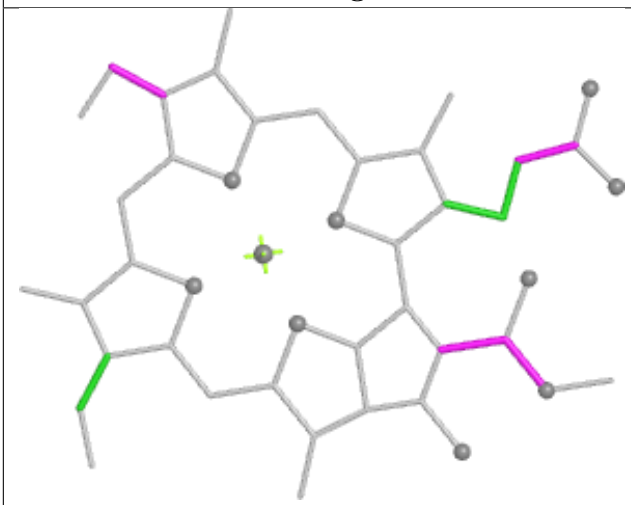
Ligand CLA c3 407



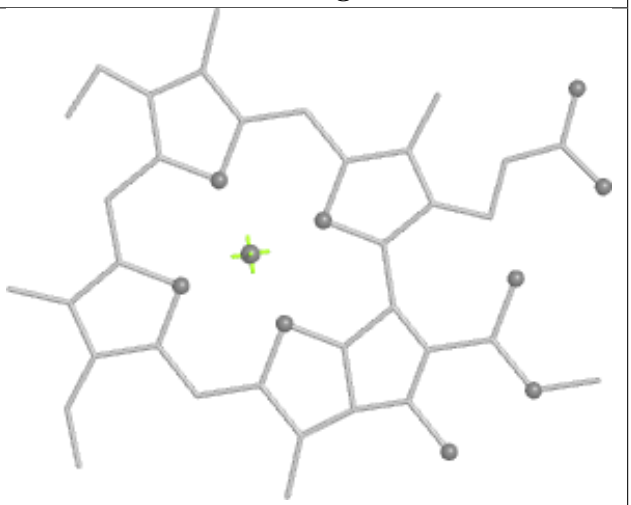
Bond lengths



Bond angles

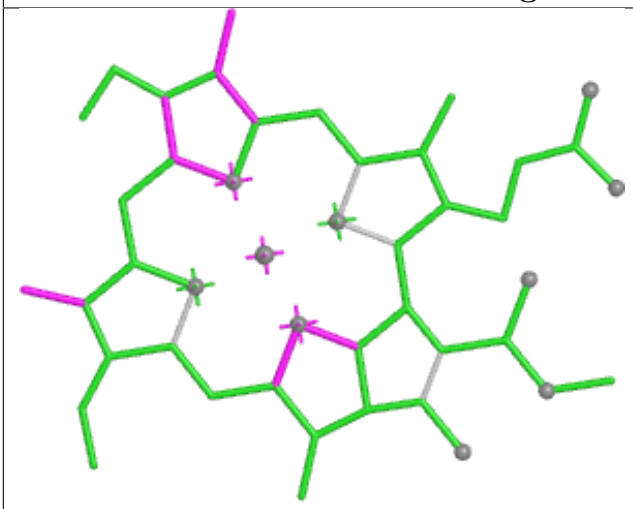


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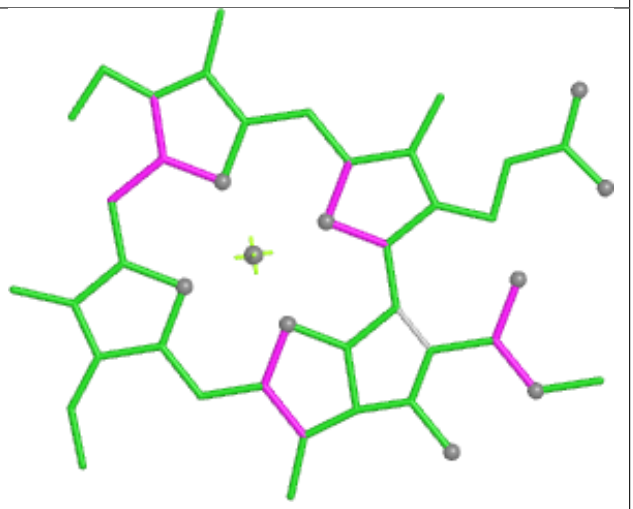


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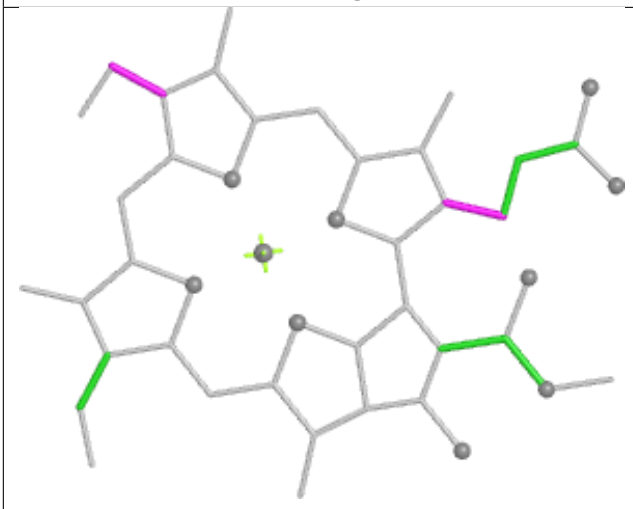
Ligand CLA a5 413



Bond lengths



Bond angles

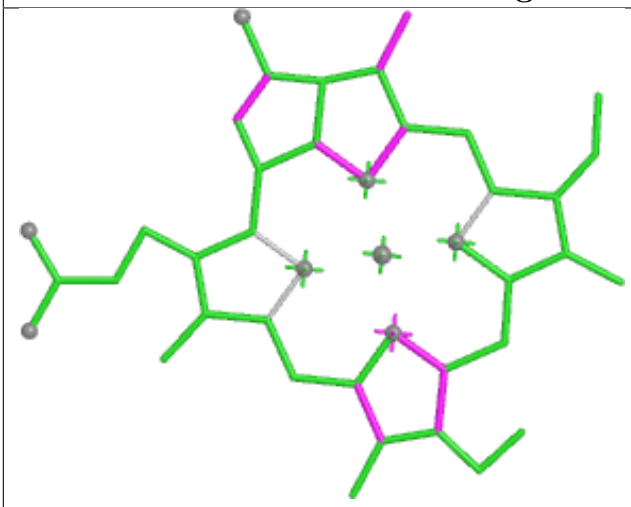


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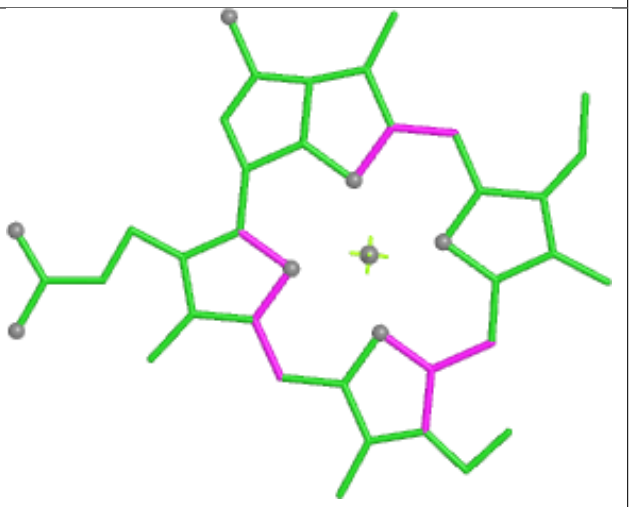


Rings

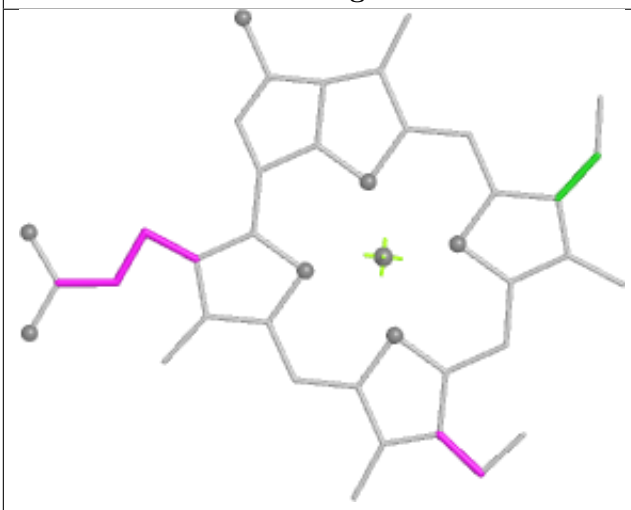
Ligand CLA cA 843



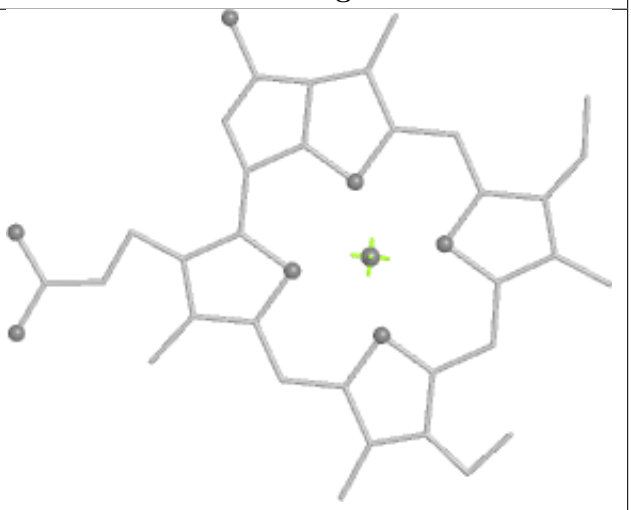
Bond lengths



Bond angles

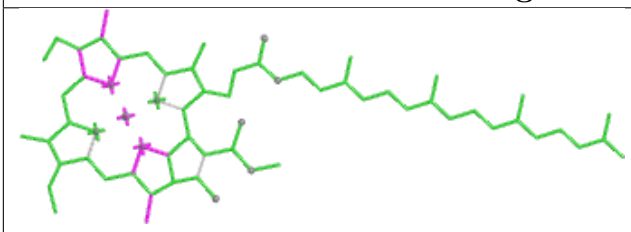


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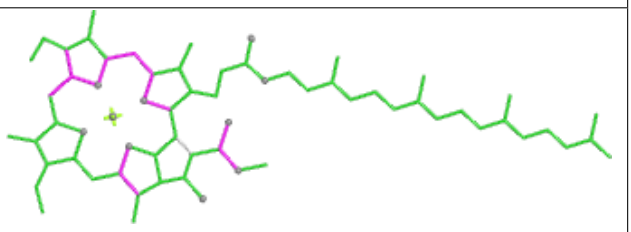


Rings

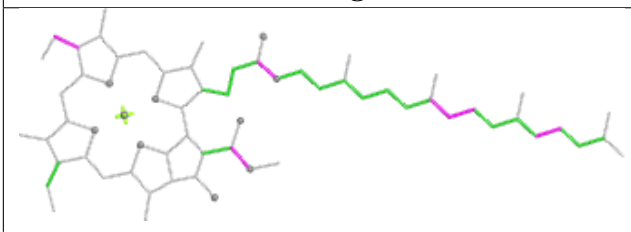
Ligand CLA aB 820



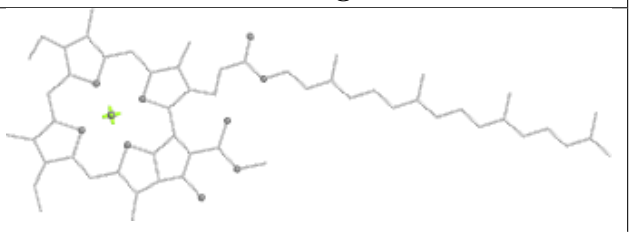
Bond lengths



Bond angles

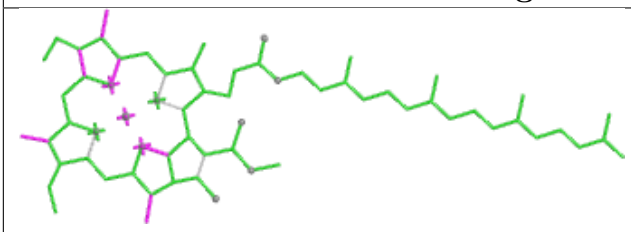


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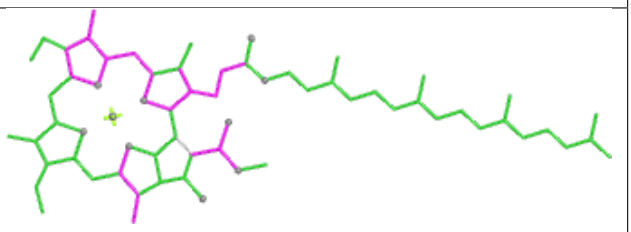


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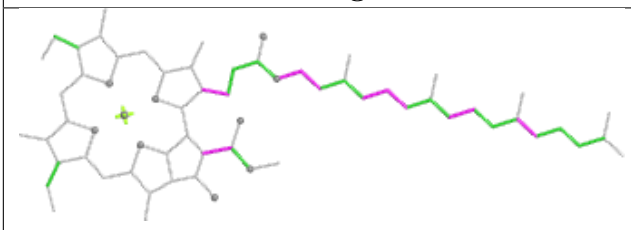
Ligand CLA cA 827



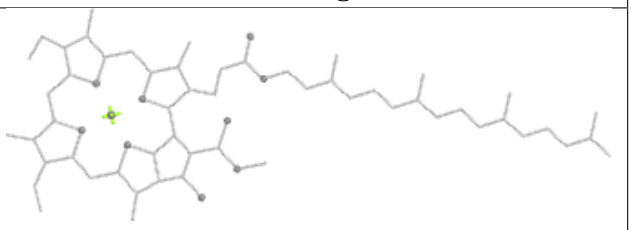
Bond lengths



Bond angles

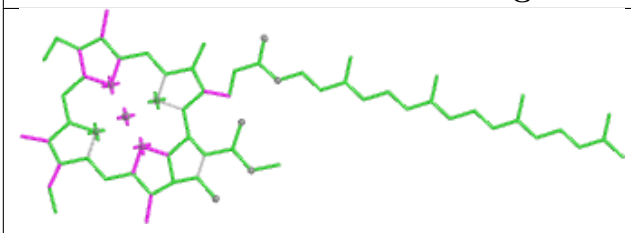


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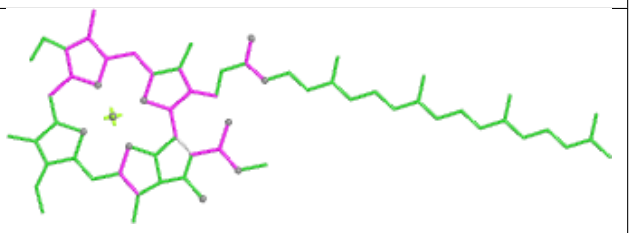


Rings

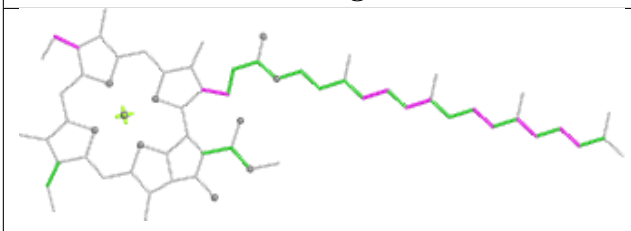
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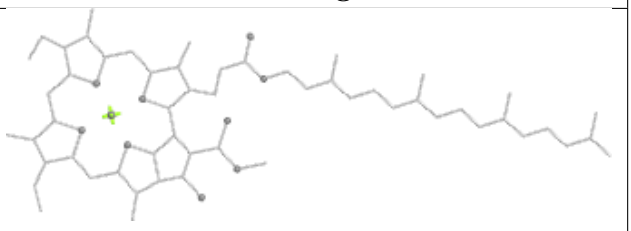
Bond lengths



Bond angles

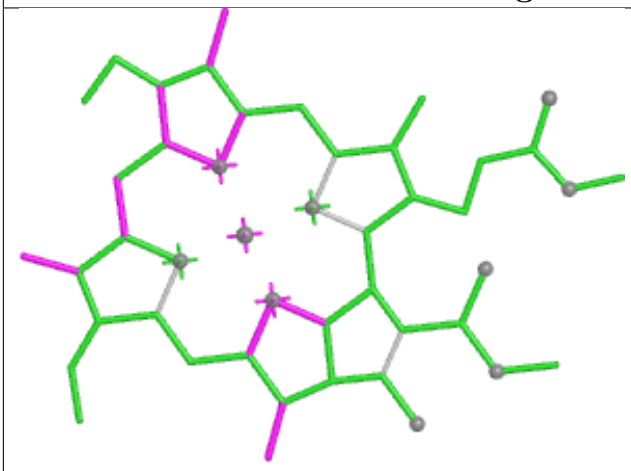


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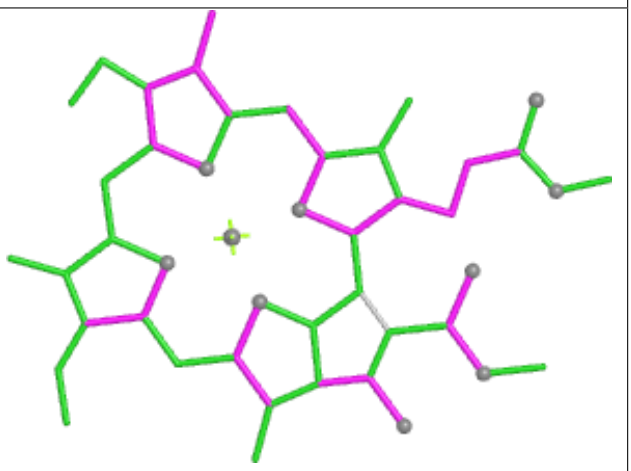


Rings

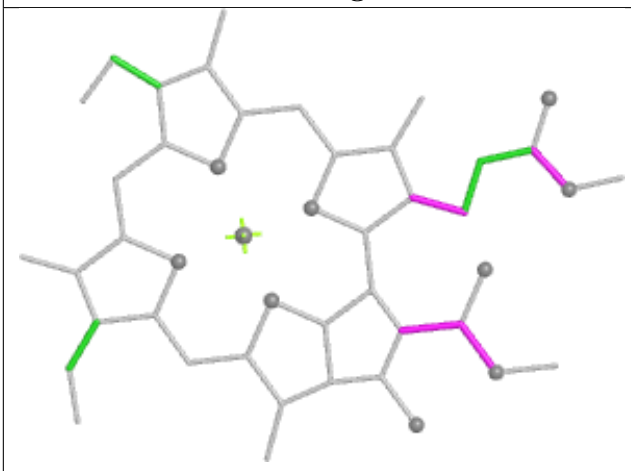
Ligand CLA aB 826



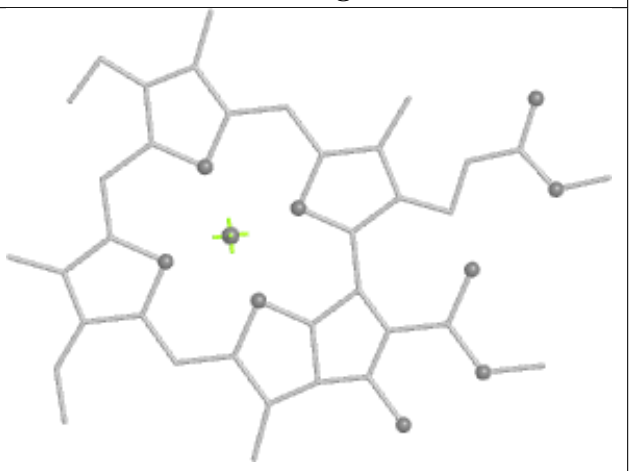
Bond lengths



Bond angles

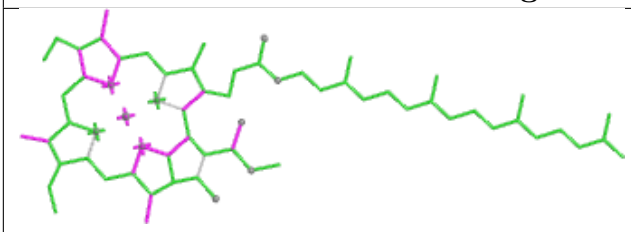


Torsions

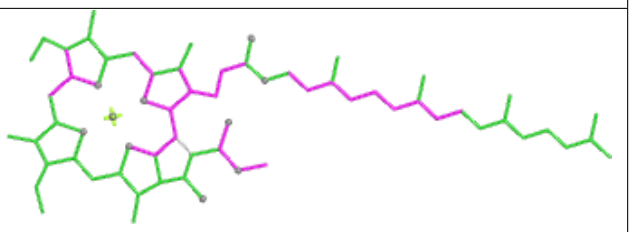


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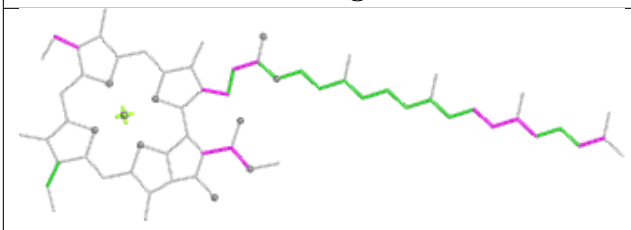
Ligand CLA c4 421



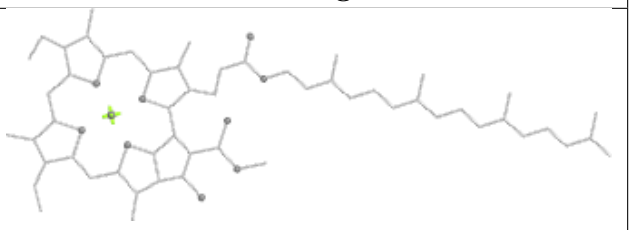
Bond lengths



Bond angles

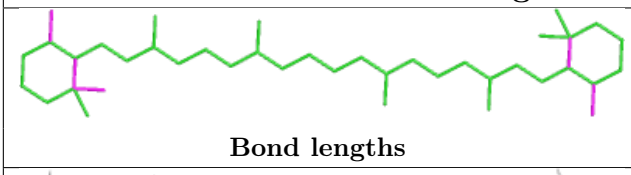


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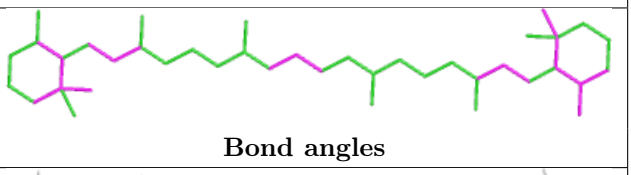


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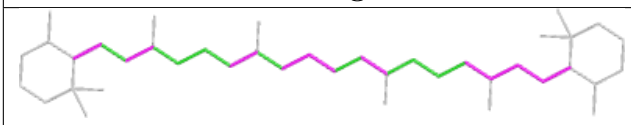
Ligand BCR bB 849



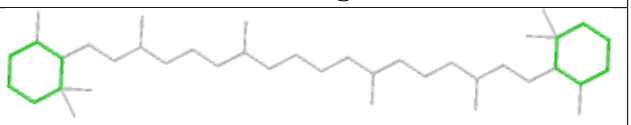
Bond lengths



Bond angles

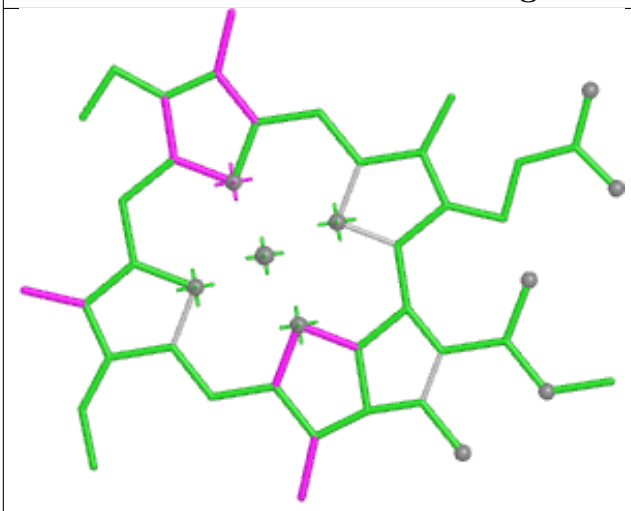


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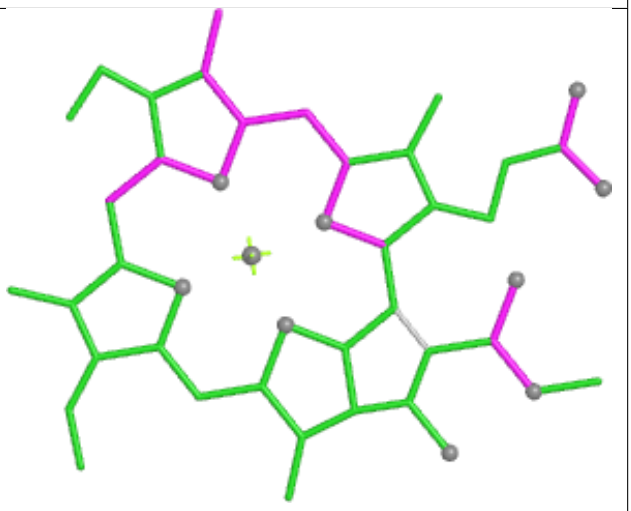


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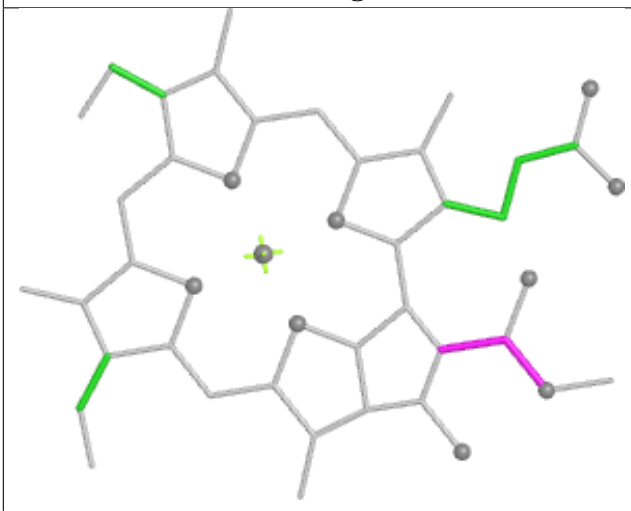
Ligand CLA a4 406



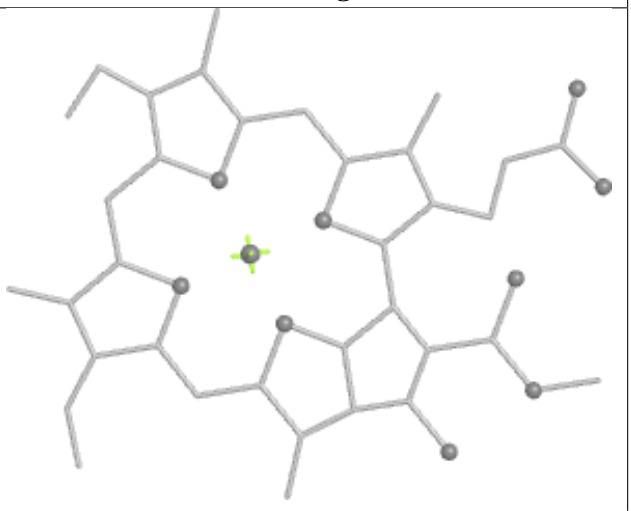
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Bond angles

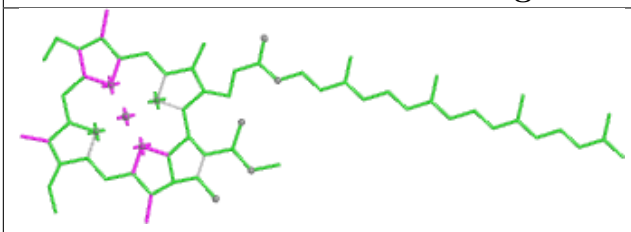


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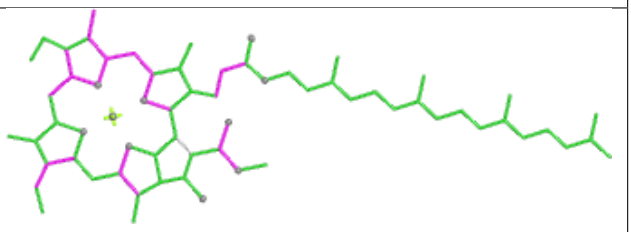


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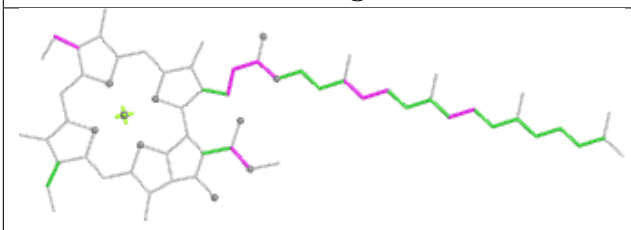
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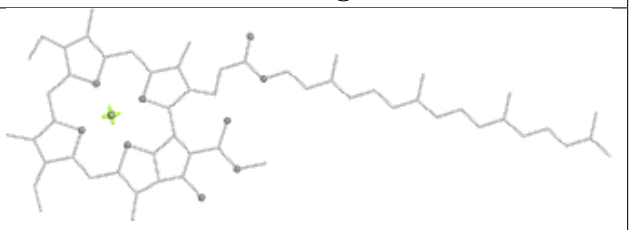
Bond lengths



Bond angles

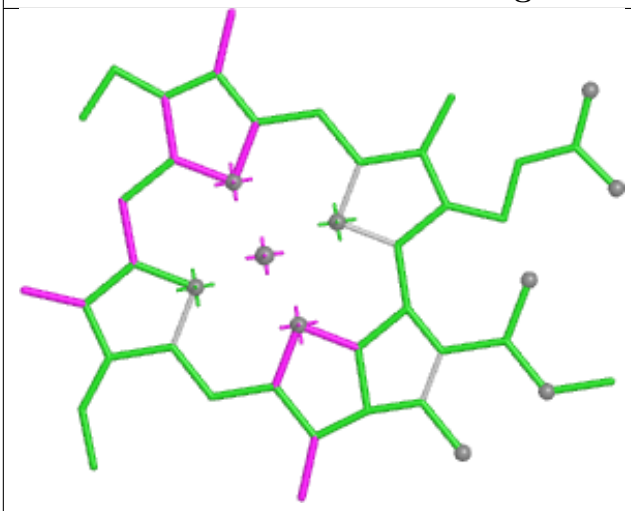


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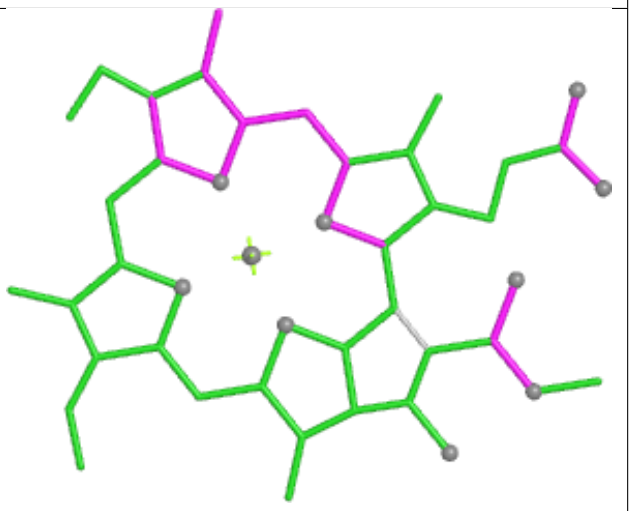


Rings

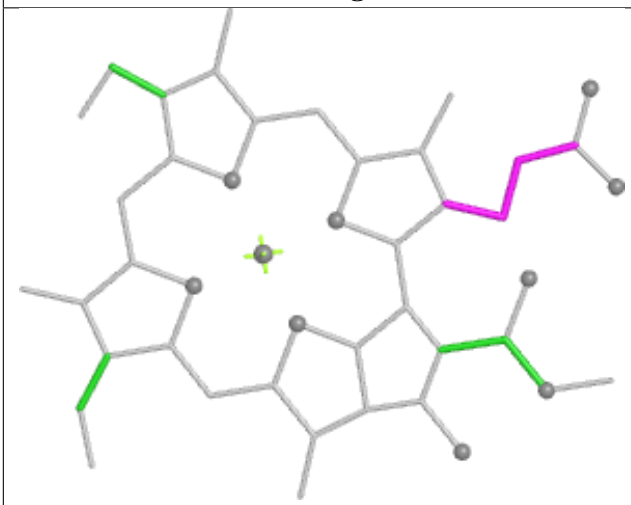
Ligand CLA bB 813



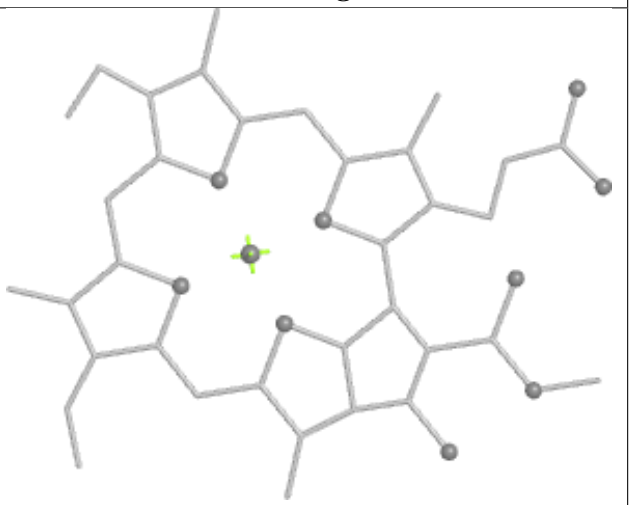
Bond lengths



Bond angles

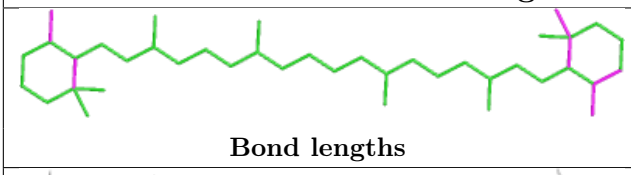


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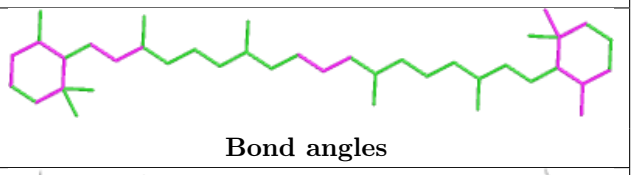


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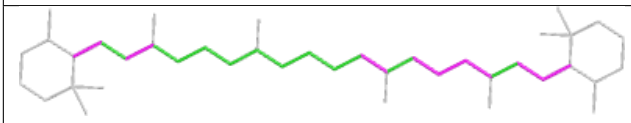
Ligand BCR a5 418



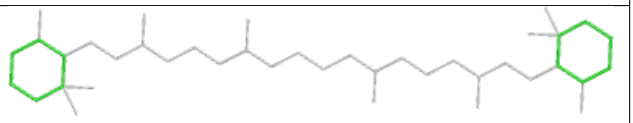
Bond lengths



Bond angles



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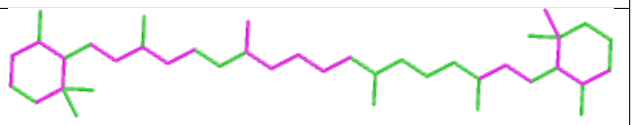


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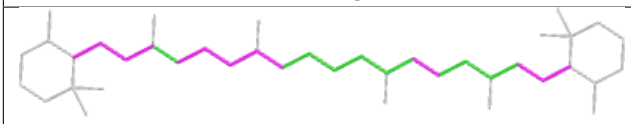
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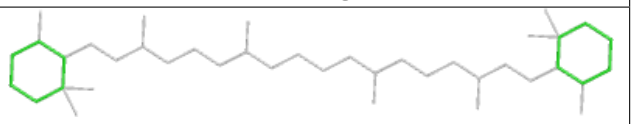
Bond lengths



Bond angles

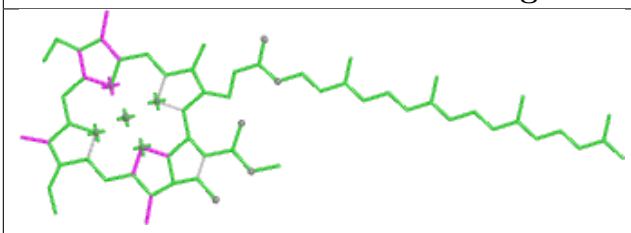


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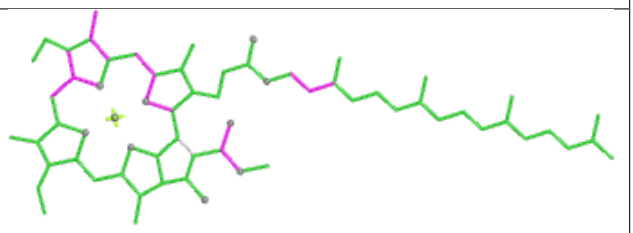


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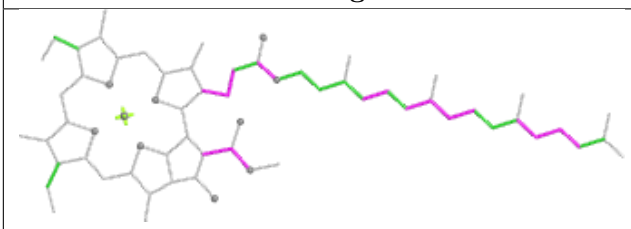
Ligand CLA c1 402



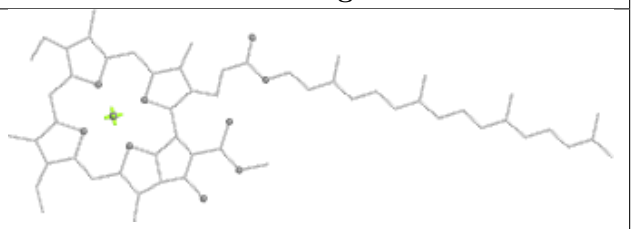
Bond lengths



Bond angles

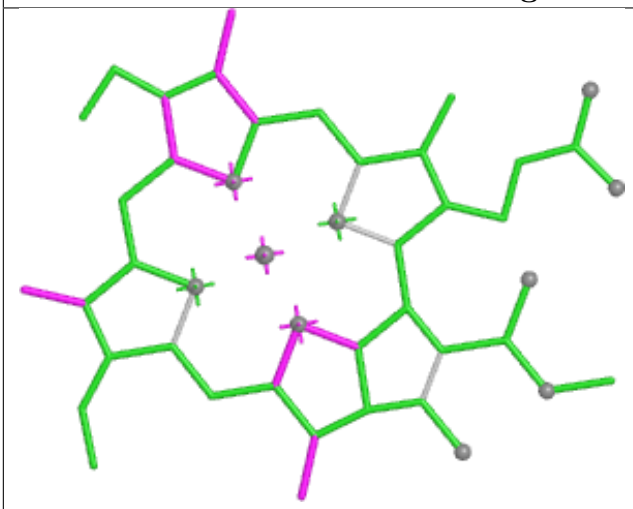


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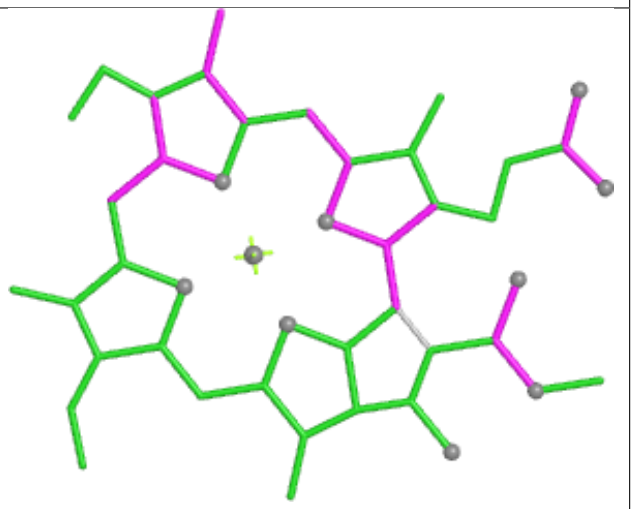


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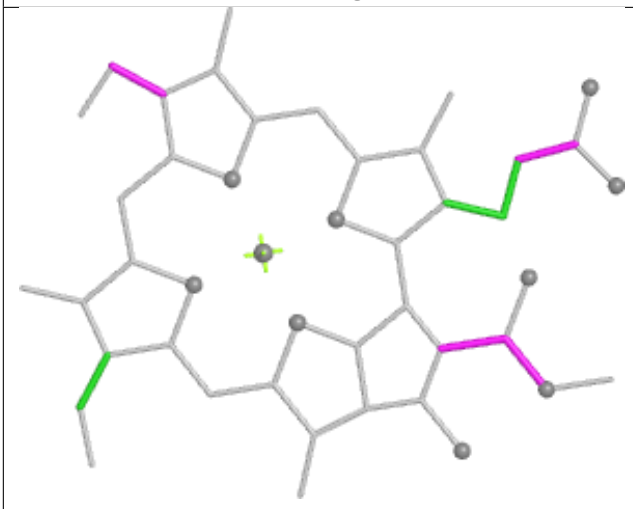
Ligand CLA c1 407



Bond lengths



Bond angles

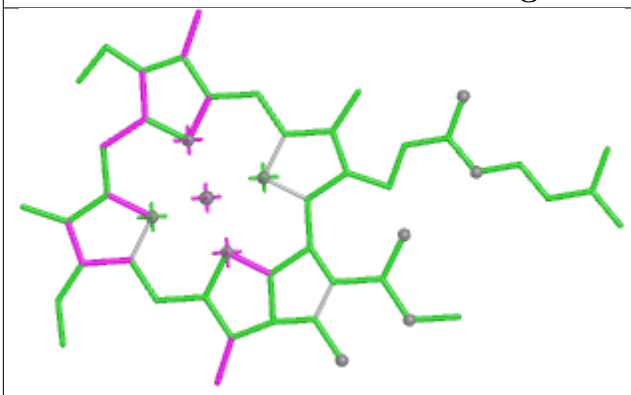


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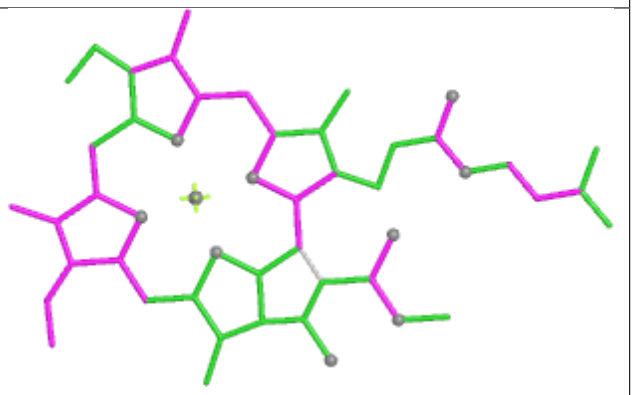


Rings

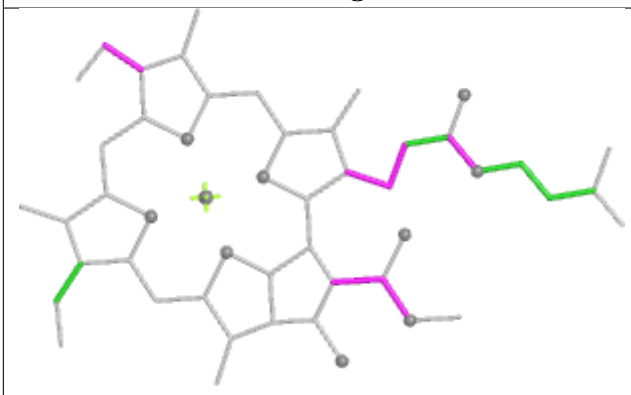
Ligand CLA c1 416



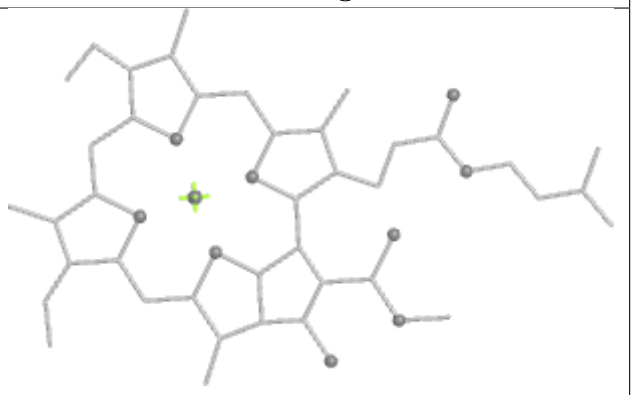
Bond lengths



Bond angles

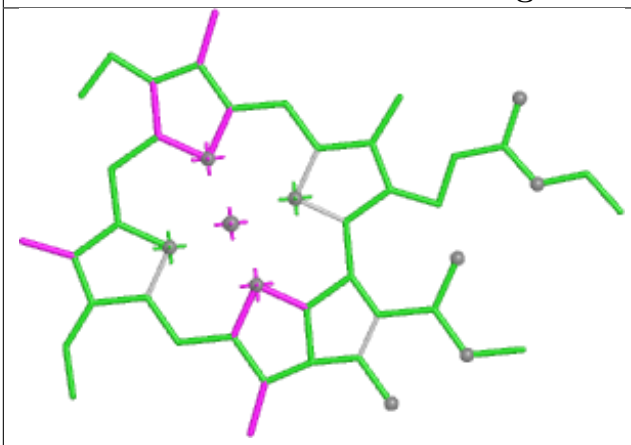


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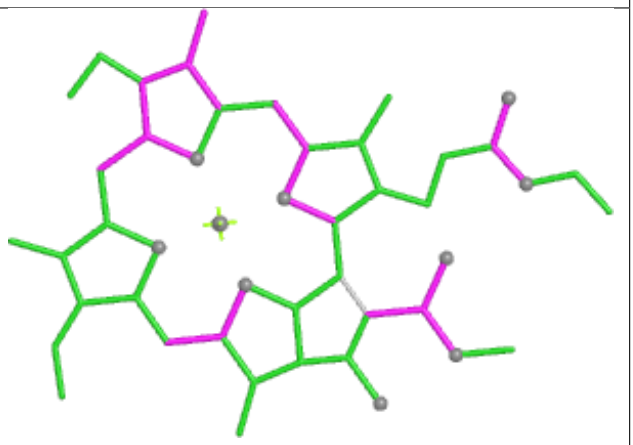


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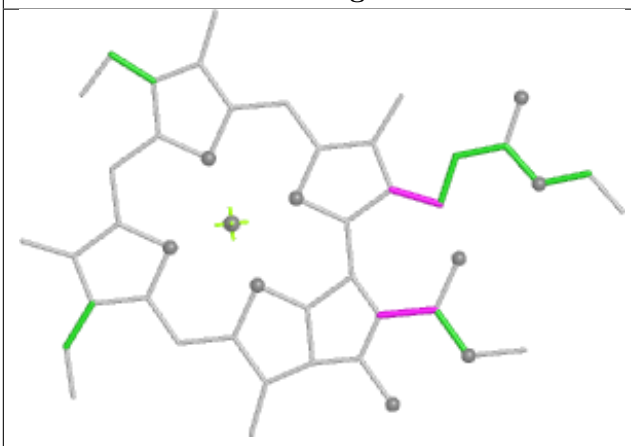
Ligand CLA cB 838



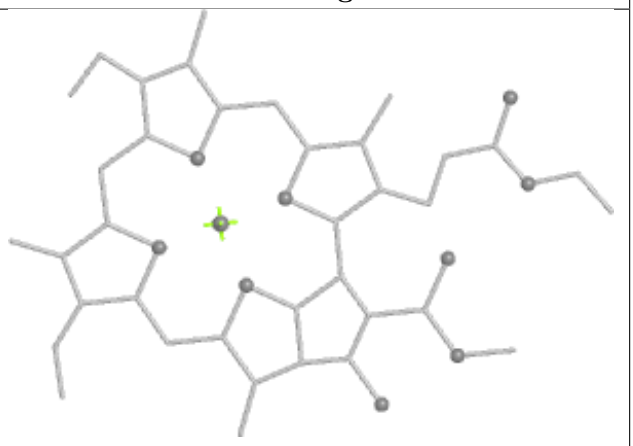
Bond lengths



Bond angles

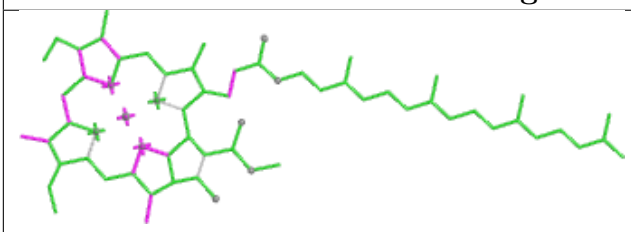


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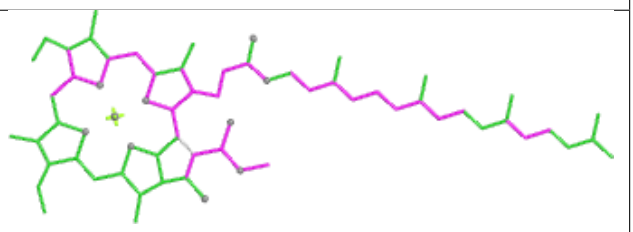


Rings

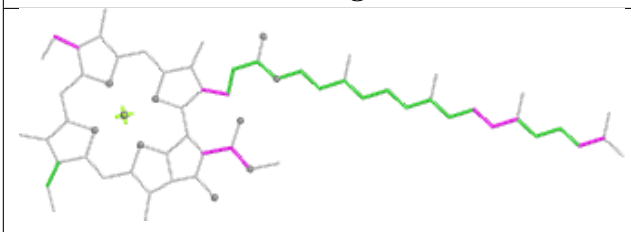
Ligand CLA c2 406



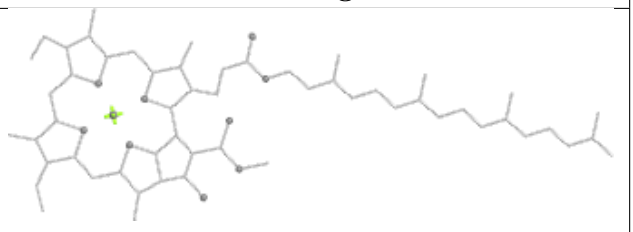
Bond lengths



Bond angles

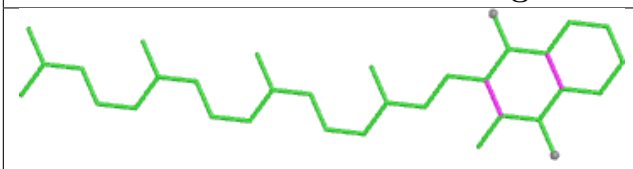


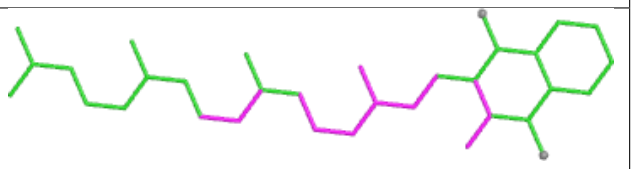
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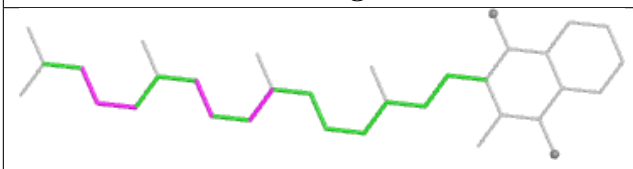


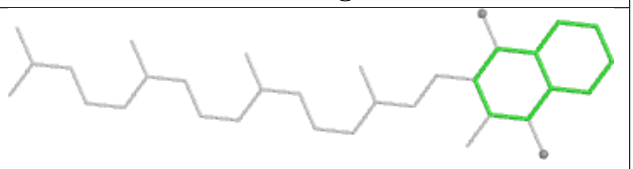
Rings

Ligand PQN bA 846

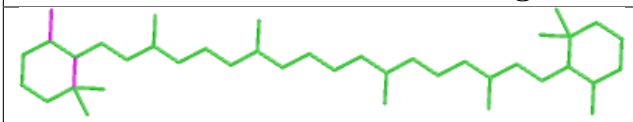

Bond lengths

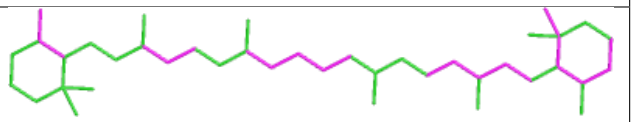

Bond angles

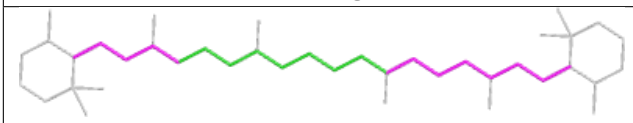

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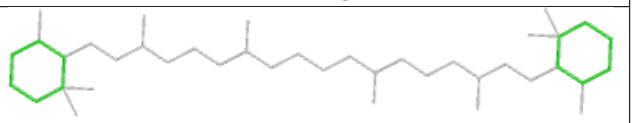

Rings

Ligand BCR cA 849

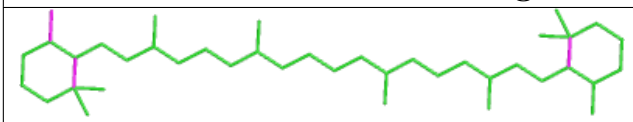

Bond lengths

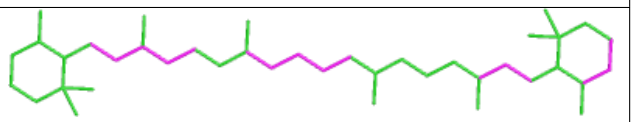

Bond angles

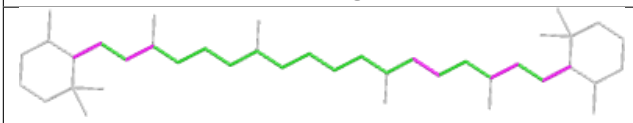

Torsions

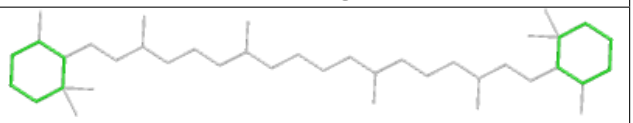

Rings

Ligand BCR cB 844

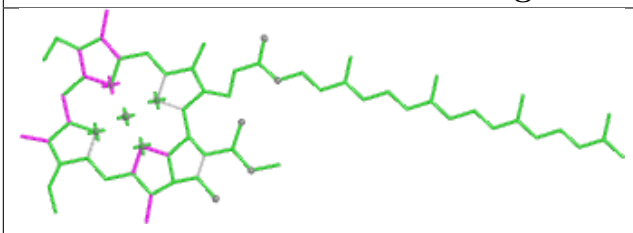

Bond lengths

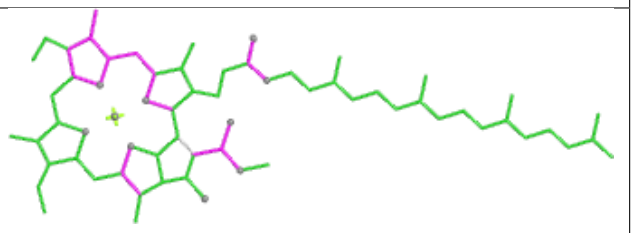

Bond angles

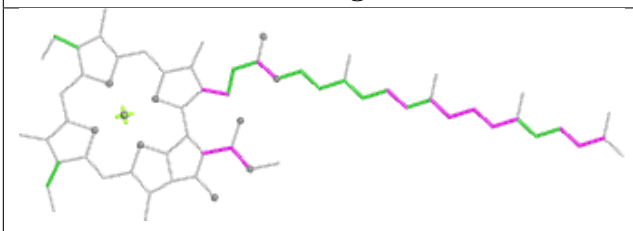

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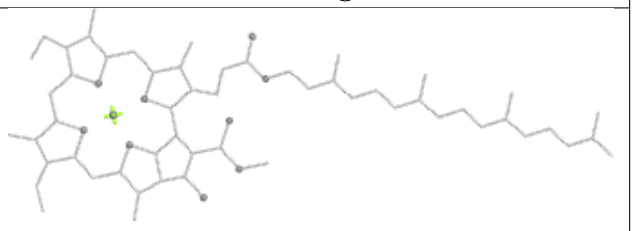

Rings

Ligand CLA bB 815

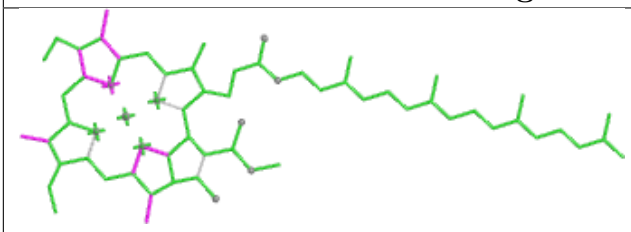

Bond lengths


Bond angles

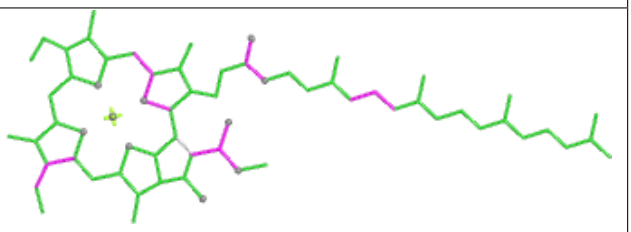

Torsions


Rings

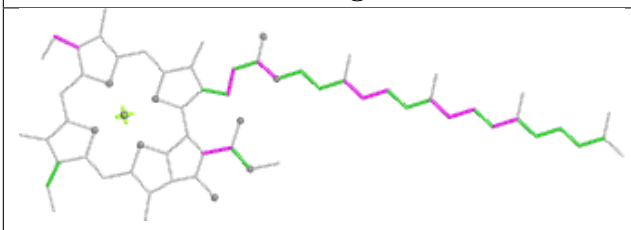
Ligand CLA cB 808



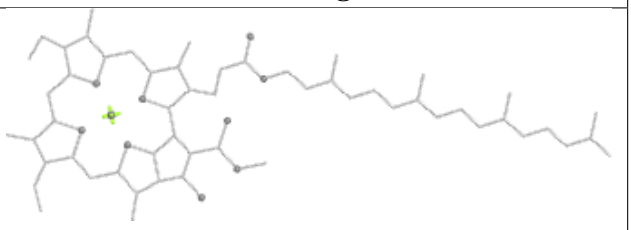
Bond lengths



Bond angles

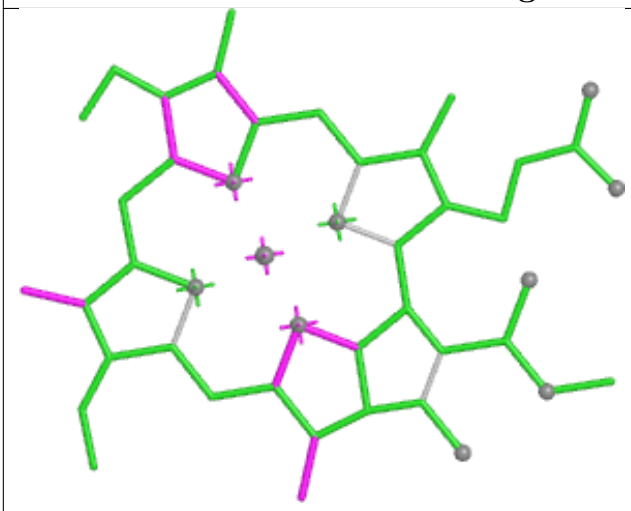


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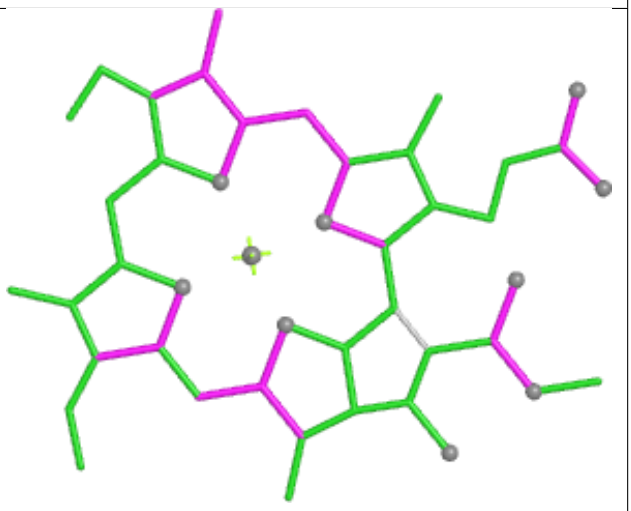


Rings

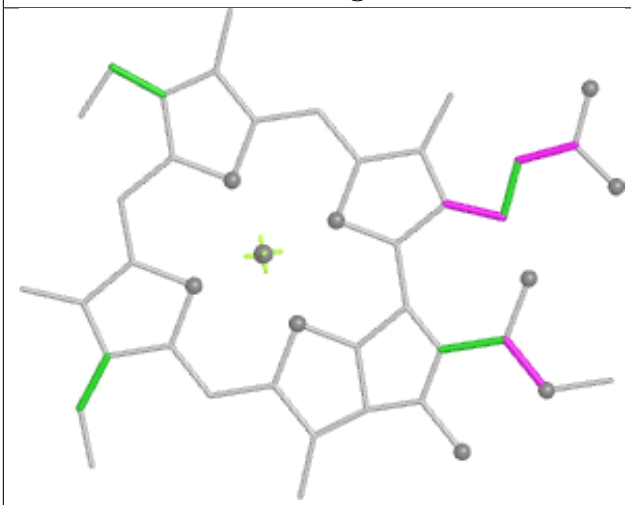
Ligand CLA b2 409



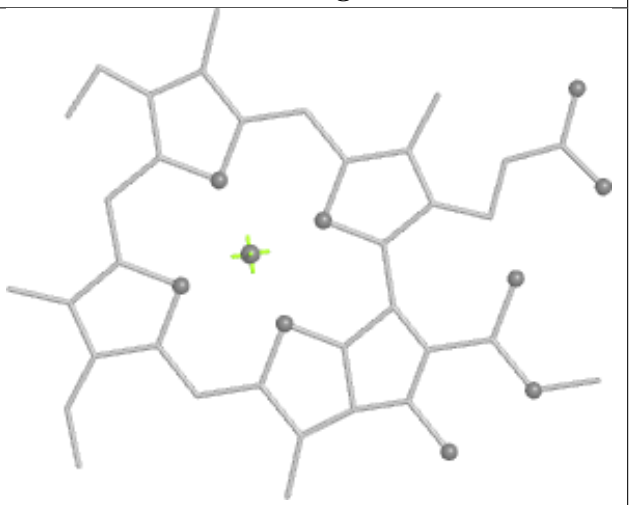
Bond lengths



Bond angles

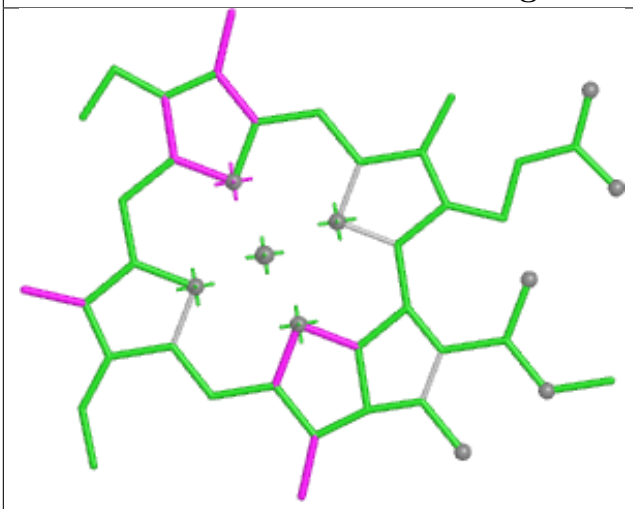


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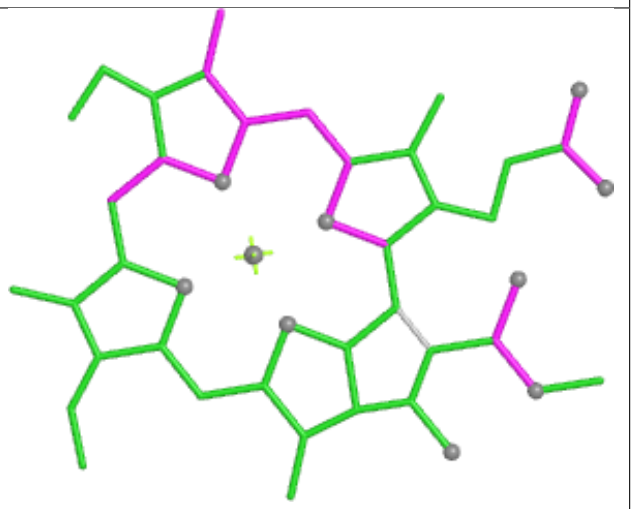


Rings

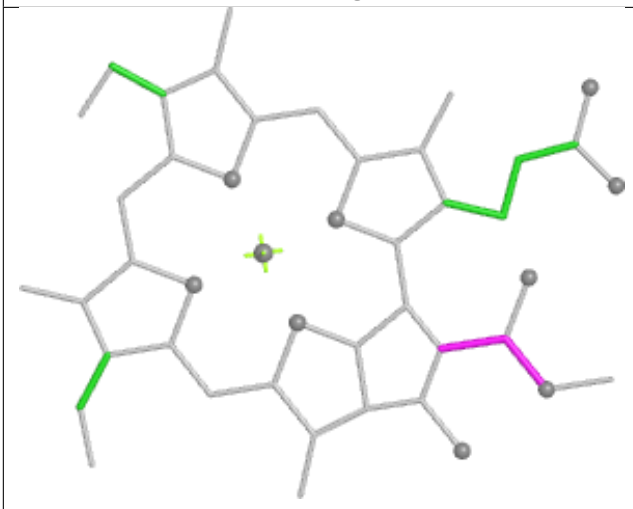
Ligand CLA a6 407



Bond lengths



Bond angles

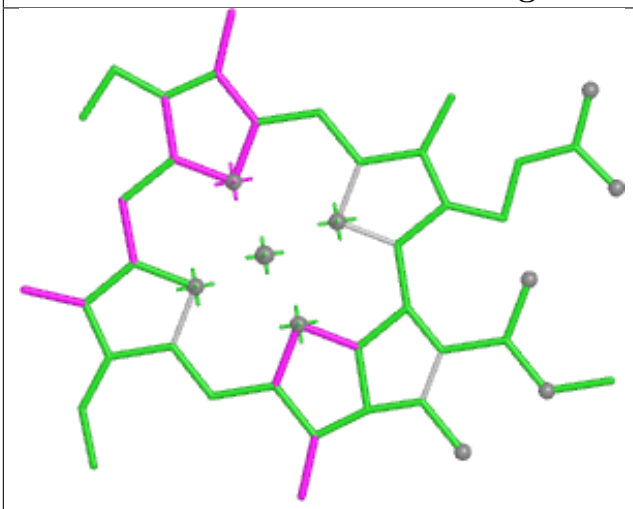


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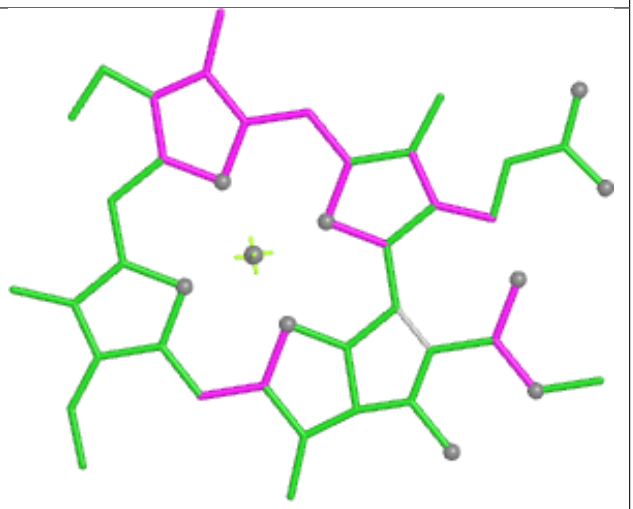


Rings

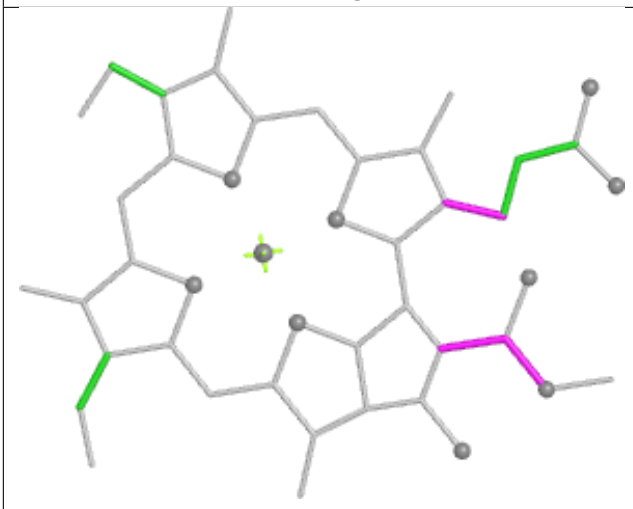
Ligand CLA b4 411



Bond lengths



Bond angles

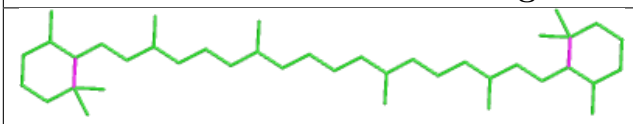


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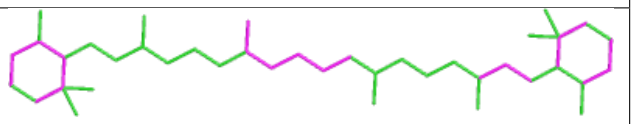


Rings

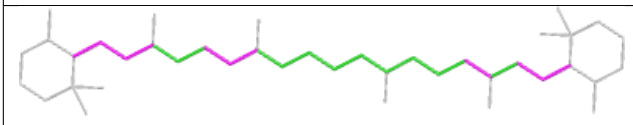
Ligand BCR c3 420



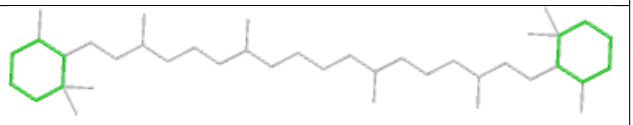
Bond lengths



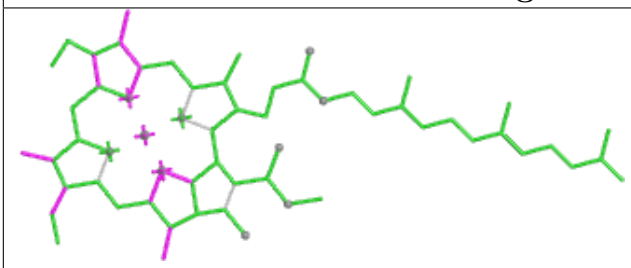
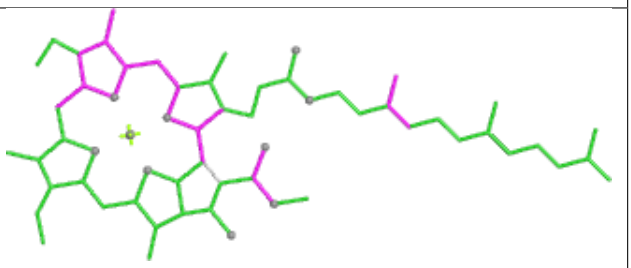
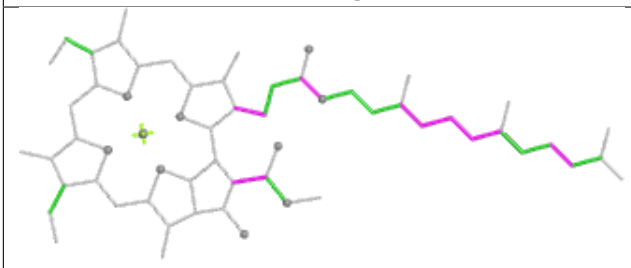
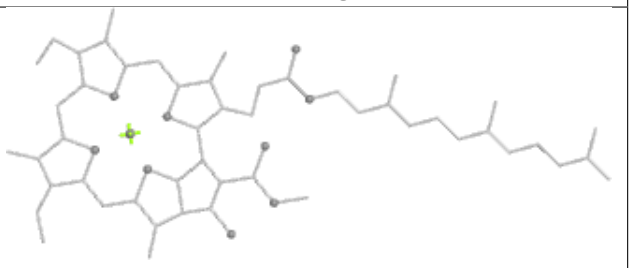
Bond angles

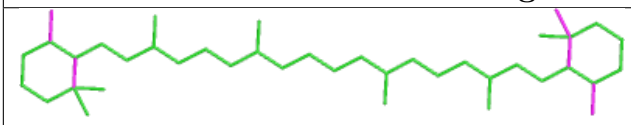
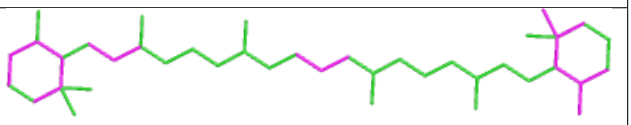
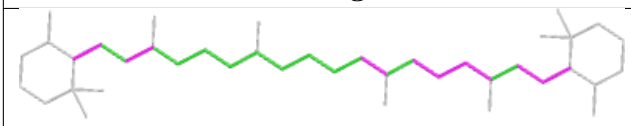
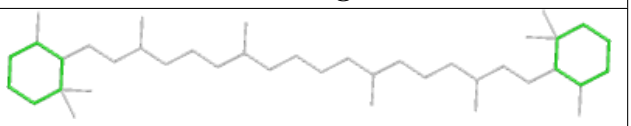


Torsions

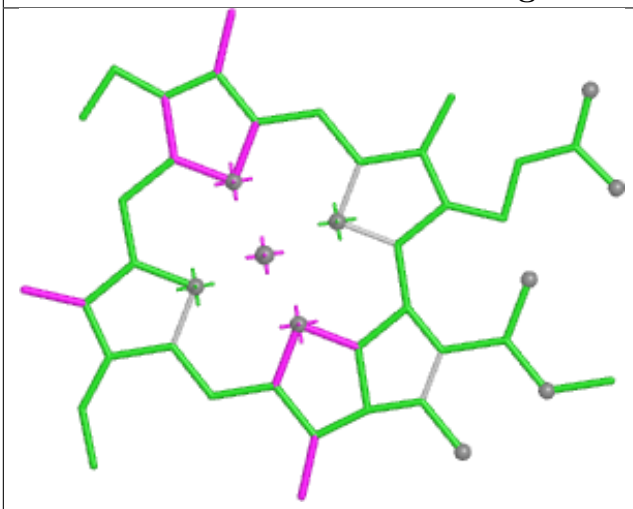


Rings

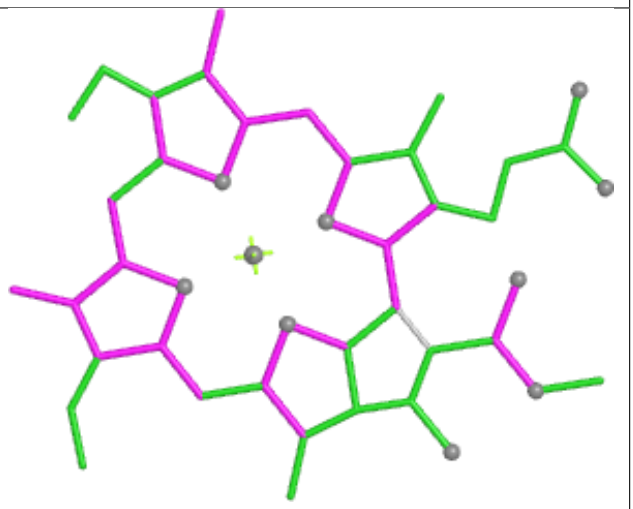
Ligand CLA cB 819	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCR c5 418	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

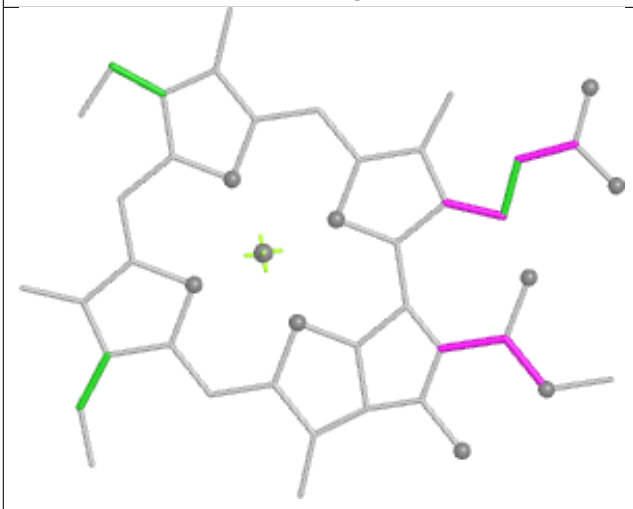
Ligand CLA b2 413



Bond lengths



Bond angles

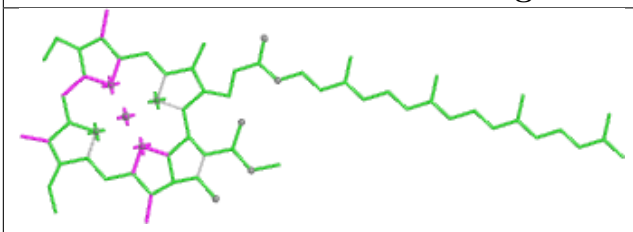


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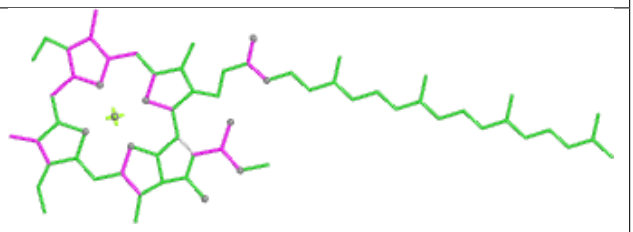


Rings

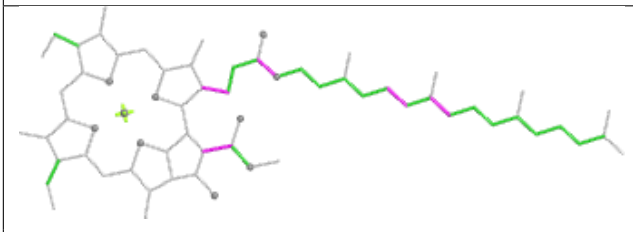
Ligand CLA aA 831



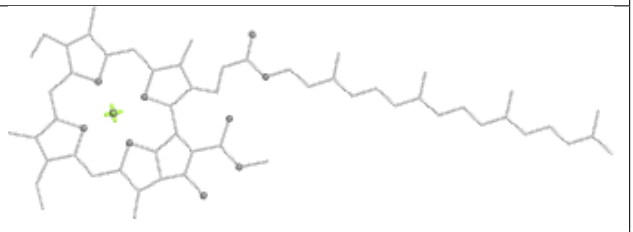
Bond lengths



Bond angles

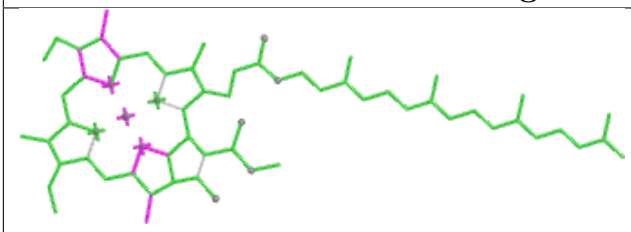


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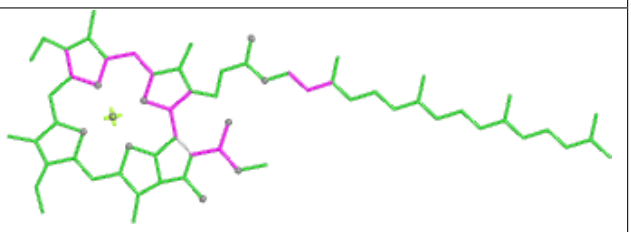


Rings

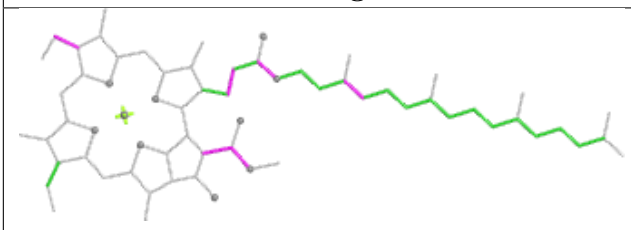
Ligand CLA a5 404



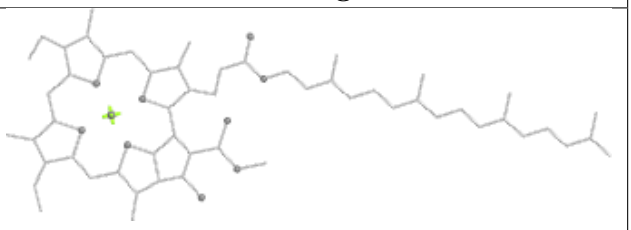
Bond lengths



Bond angles

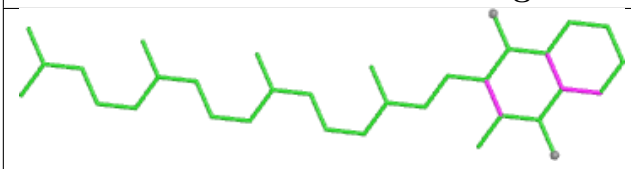


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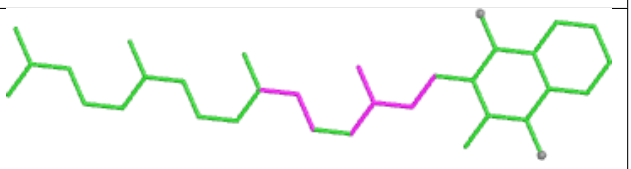


Rings

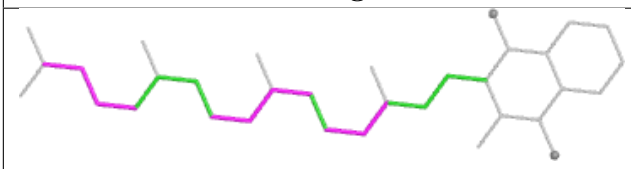
Ligand PQN aB 843



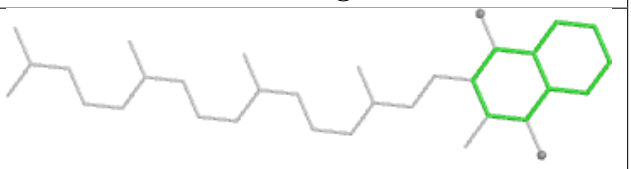
Bond lengths



Bond angles

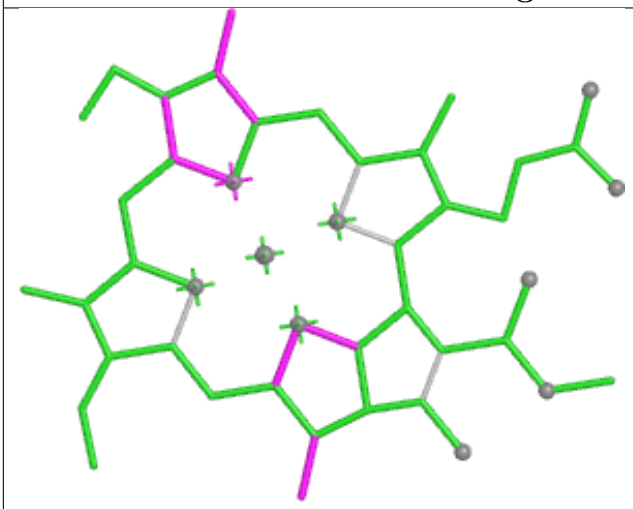


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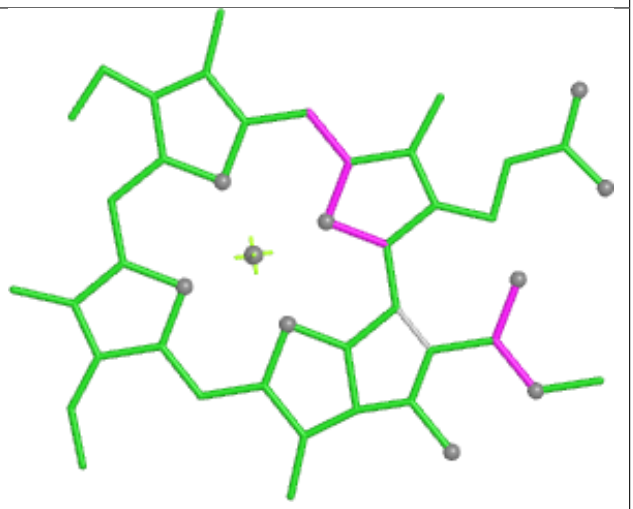


Rings

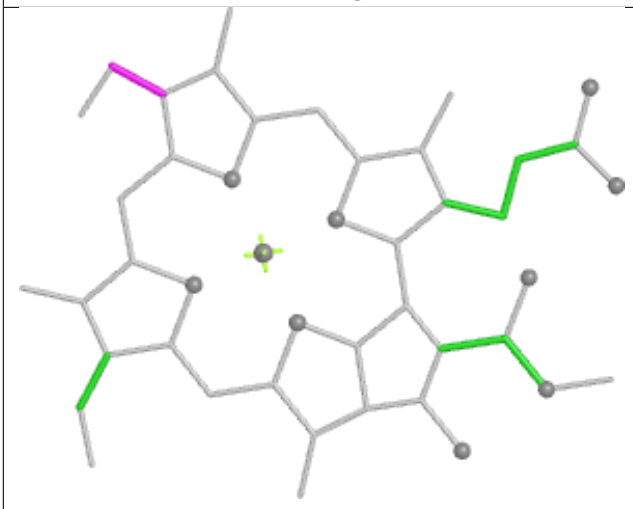
Ligand CLA cB 842



Bond lengths



Bond angles

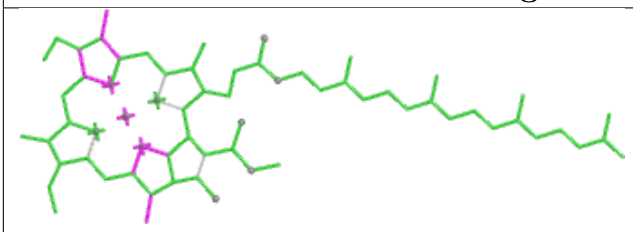


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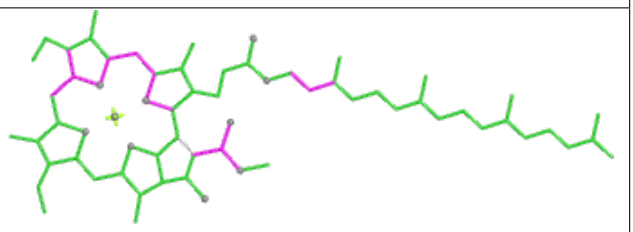


Rings

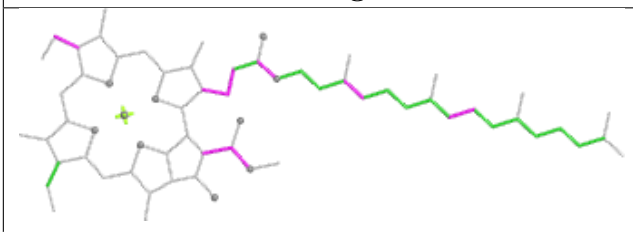
Ligand CLA c1 404



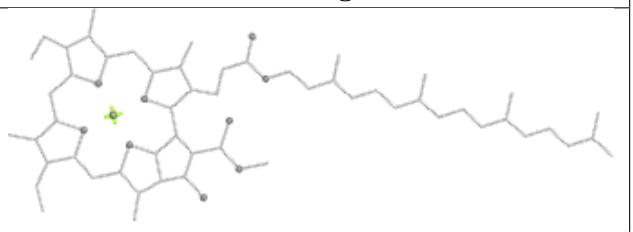
Bond lengths



Bond angles

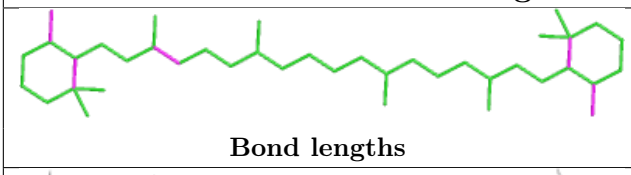


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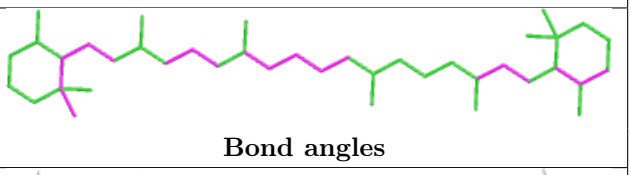


Rings

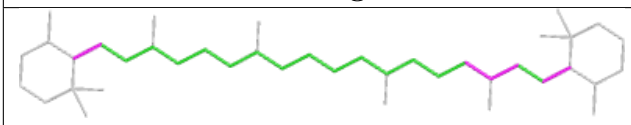
Ligand BCR cA 850



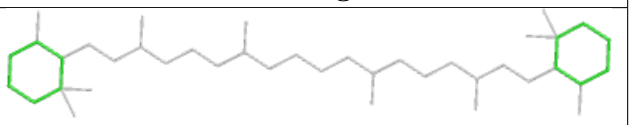
Bond lengths



Bond angles

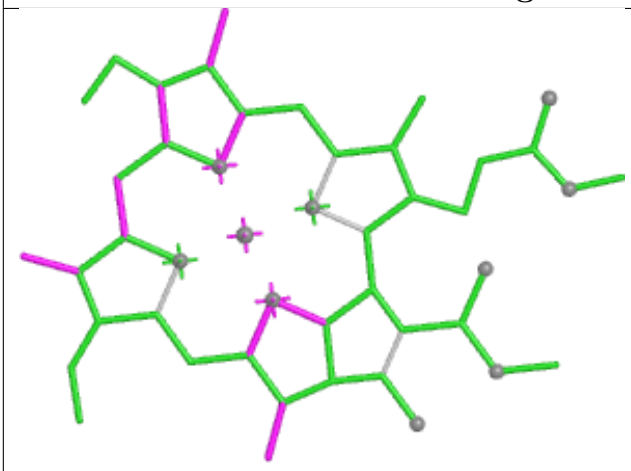


Torsions

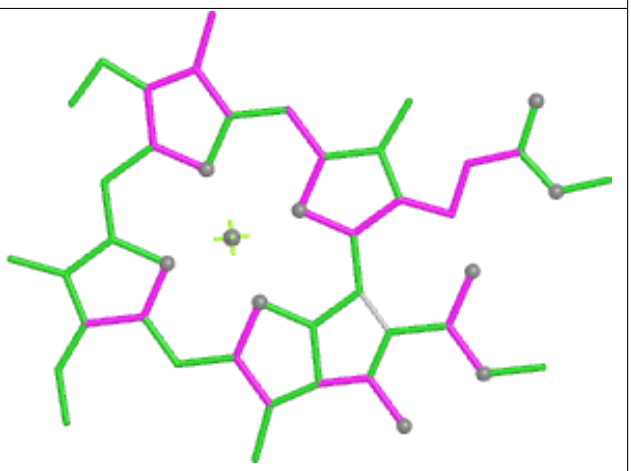


Rings

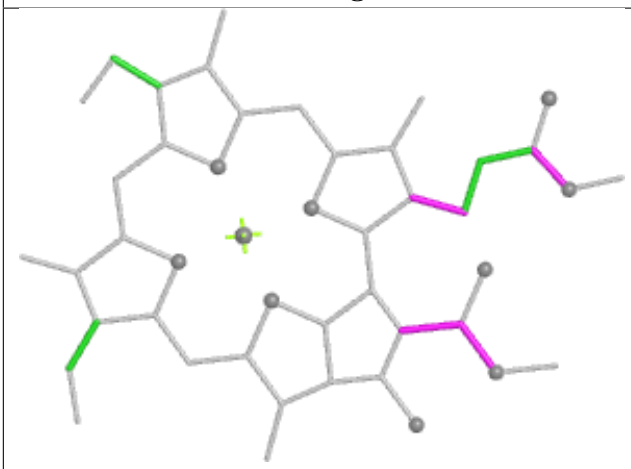
Ligand CLA cB 826



Bond lengths



Bond angles

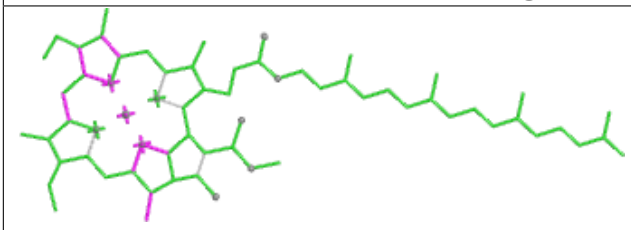


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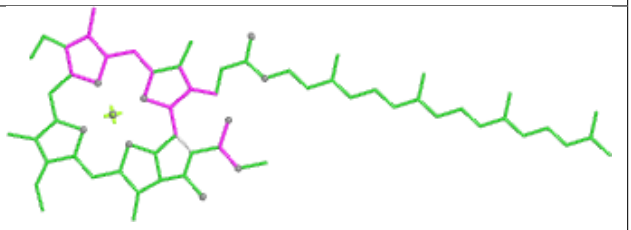


Rings

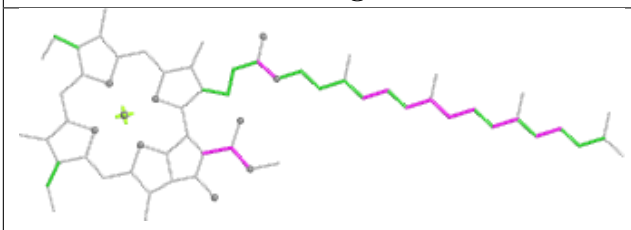
Ligand CLA c2 403



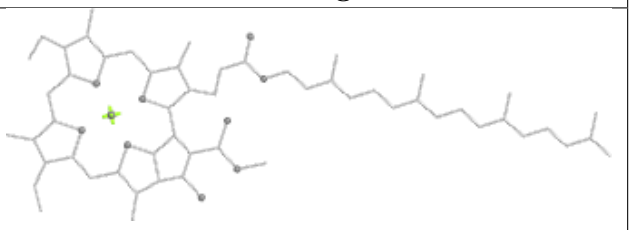
Bond lengths



Bond angles

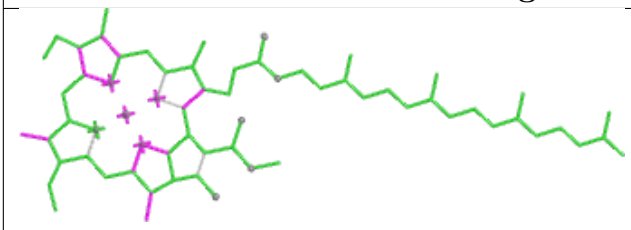


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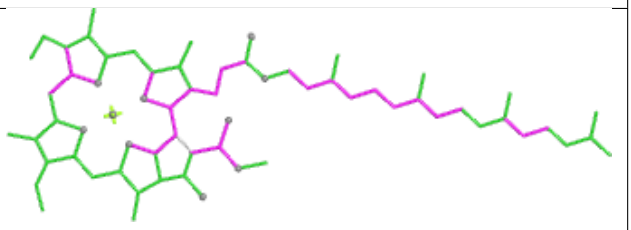


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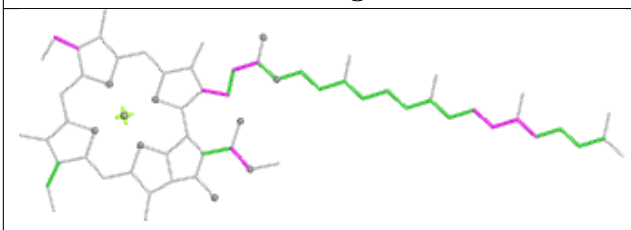
Ligand CLA b3 421



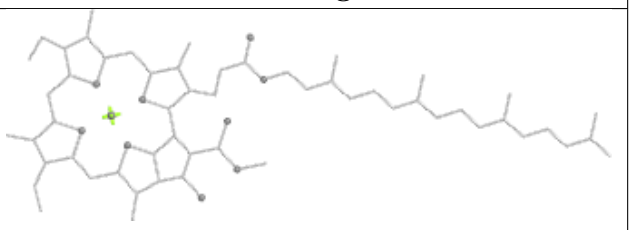
Bond lengths



Bond angles

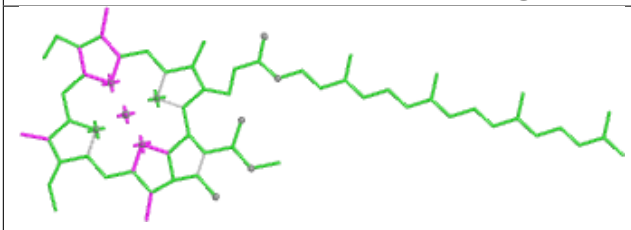


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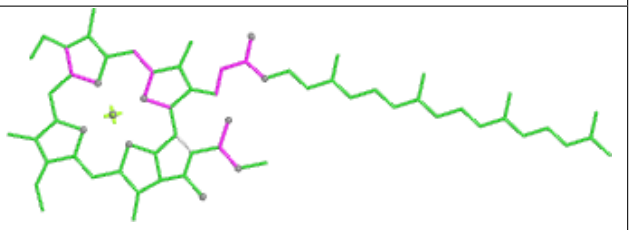


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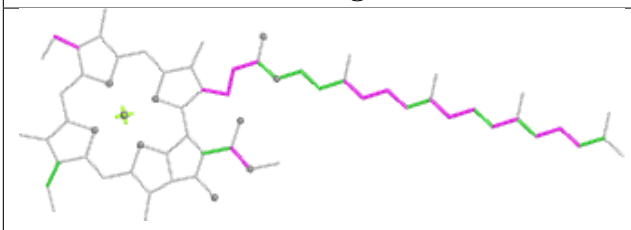
Ligand CLA aA 810



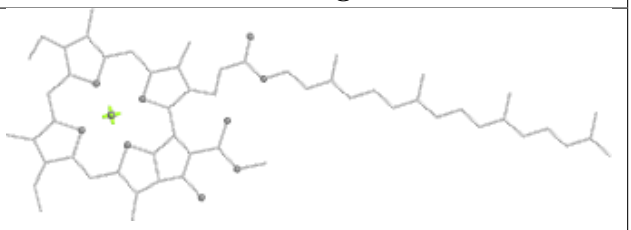
Bond lengths



Bond angles

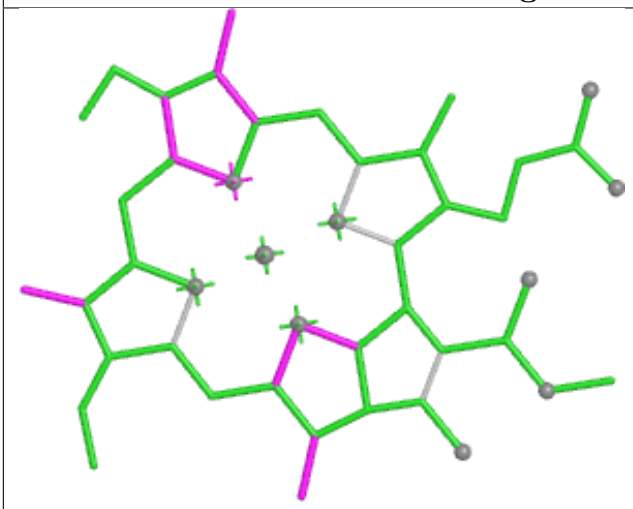


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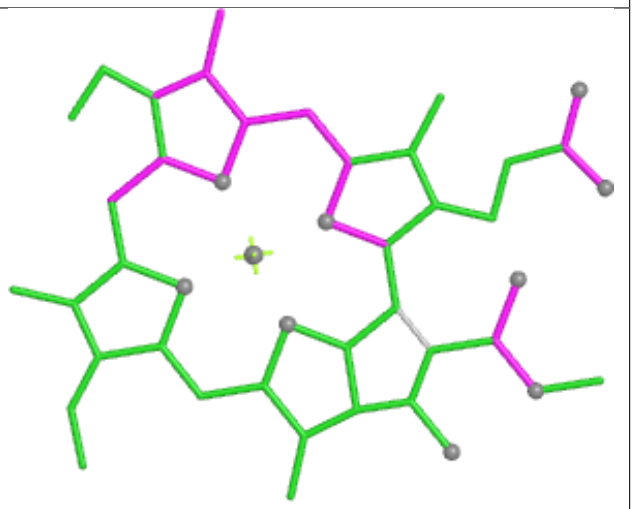


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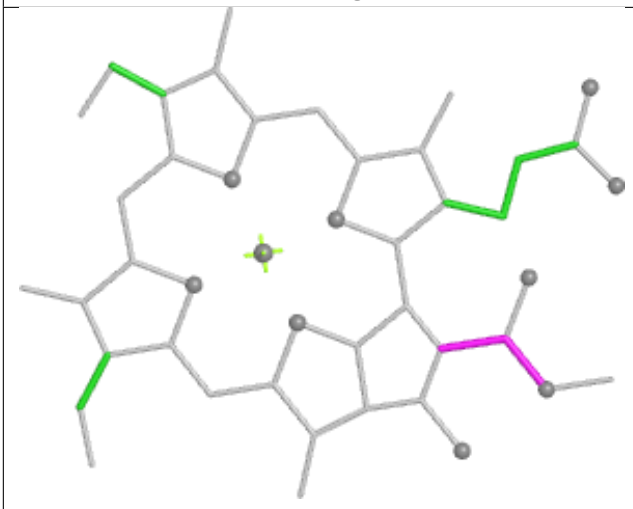
Ligand CLA a1 405



Bond lengths



Bond angles

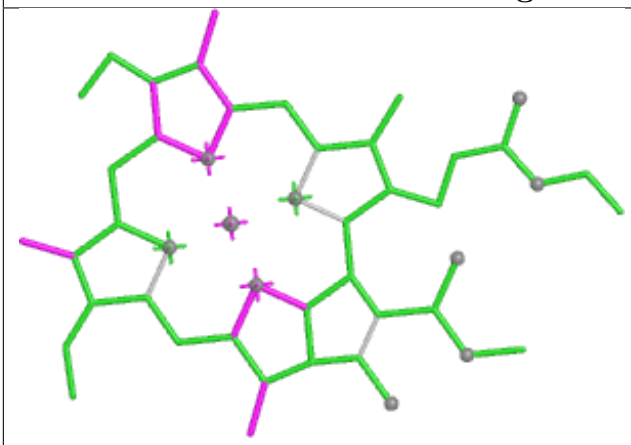


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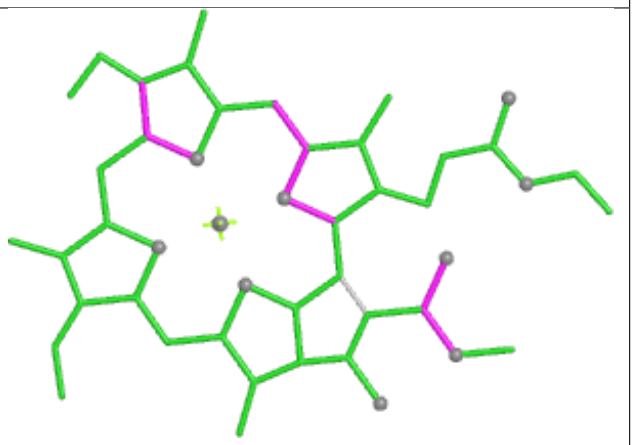


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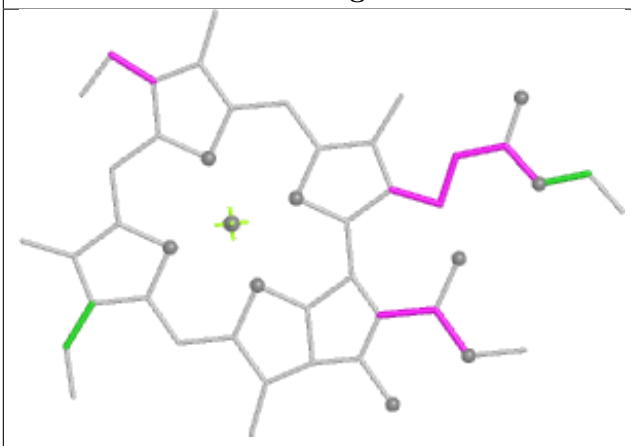
Ligand CLA cB 821



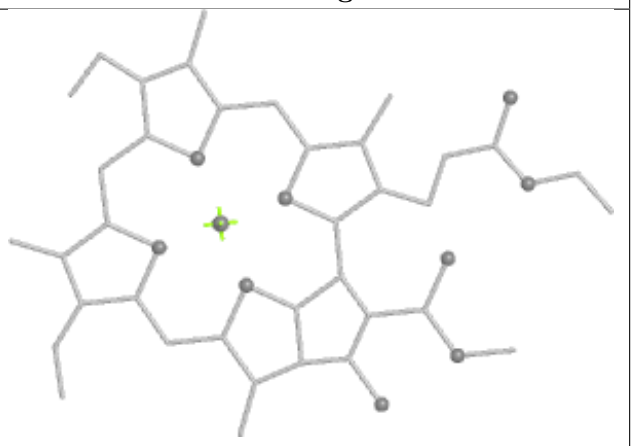
Bond lengths



Bond angles

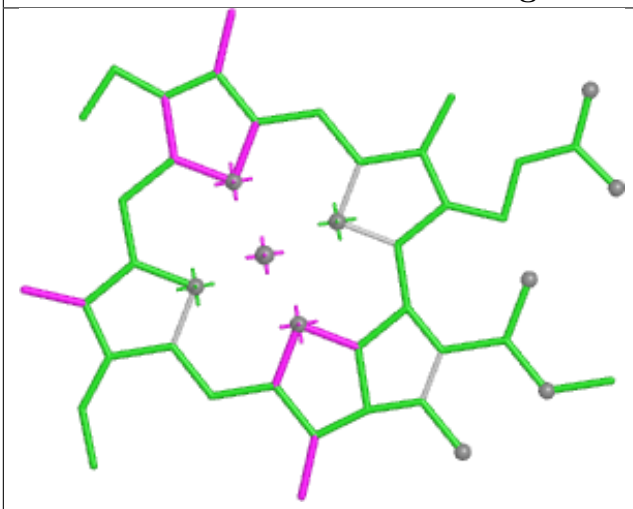


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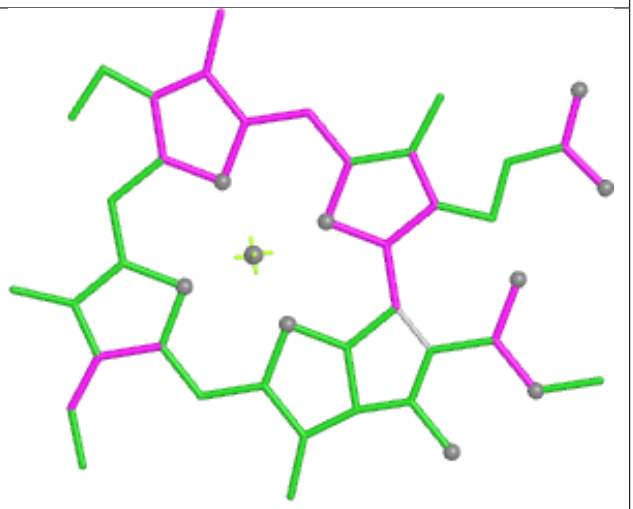


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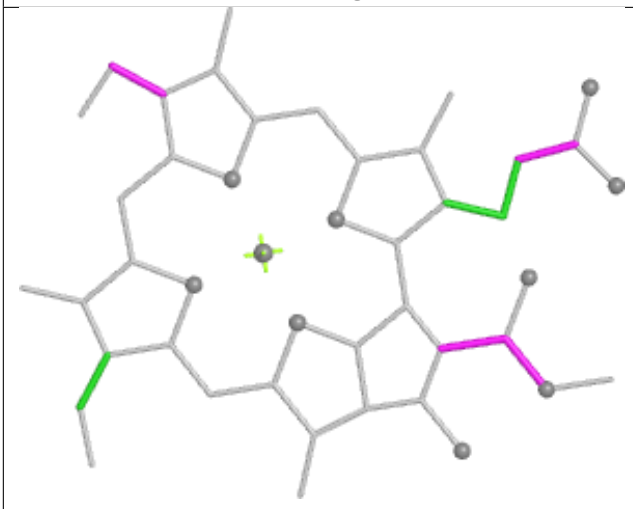
Ligand CLA aJ 201



Bond lengths



Bond angles

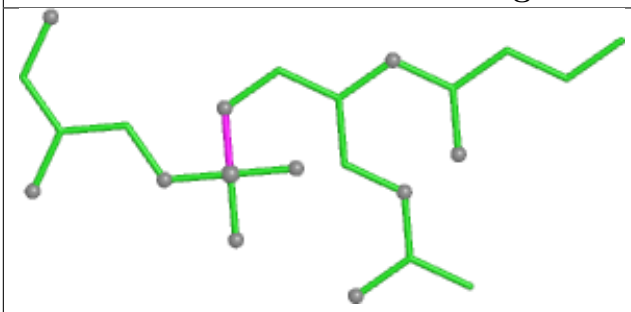


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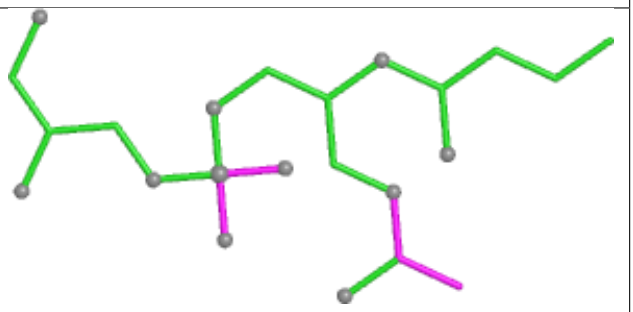


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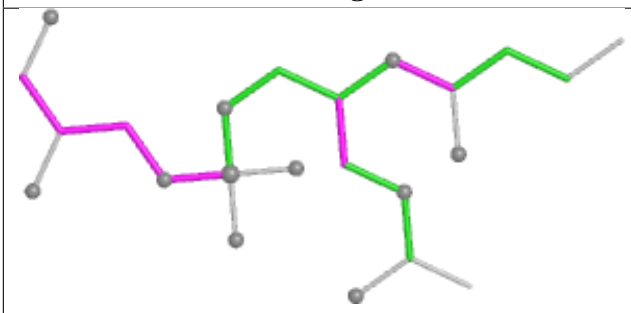
Ligand LHG aX 101



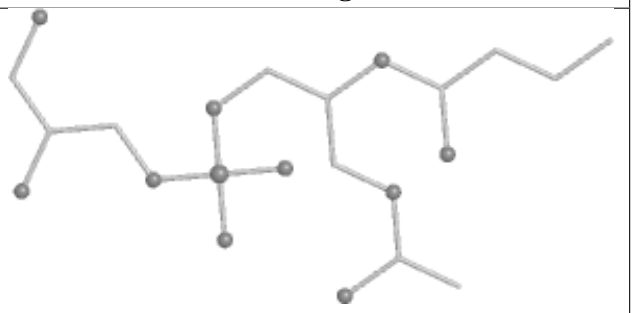
Bond lengths



Bond angles

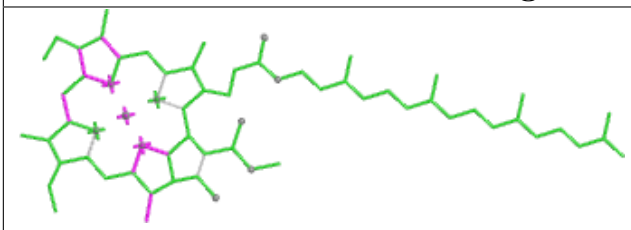


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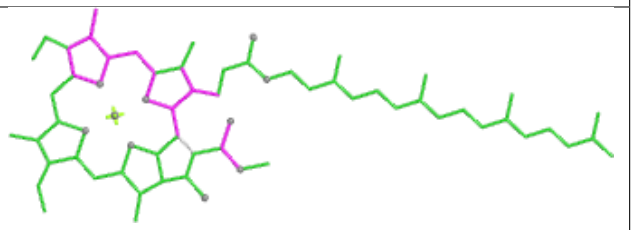


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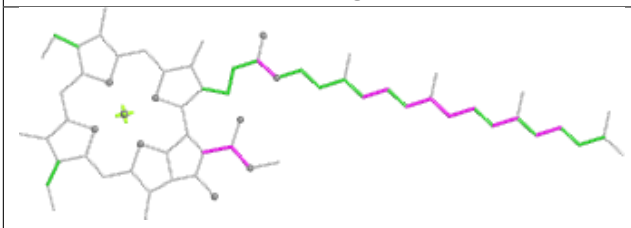
Ligand CLA a6 404



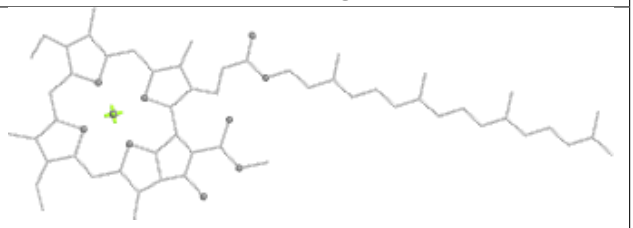
Bond lengths



Bond angles

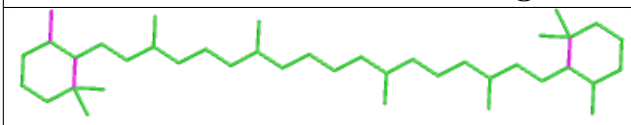


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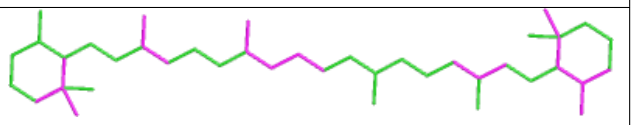


Rings

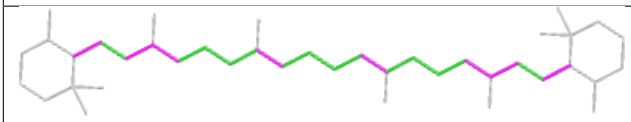
Ligand BCR aF 202



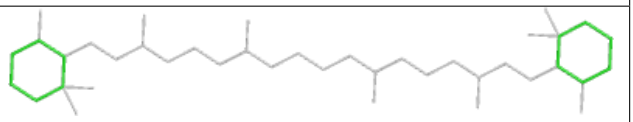
Bond lengths



Bond angles

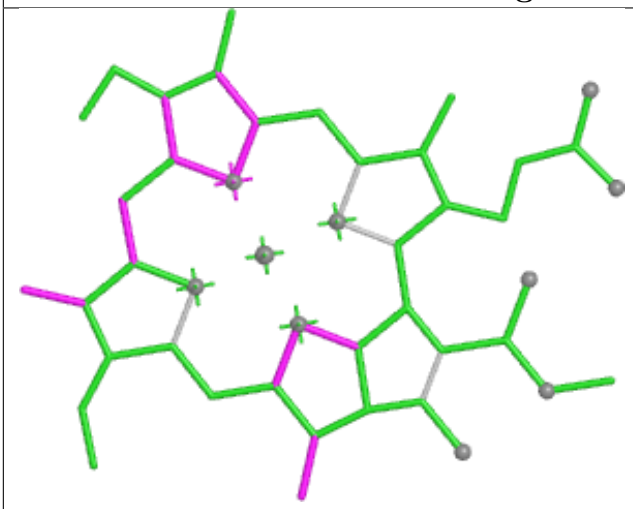


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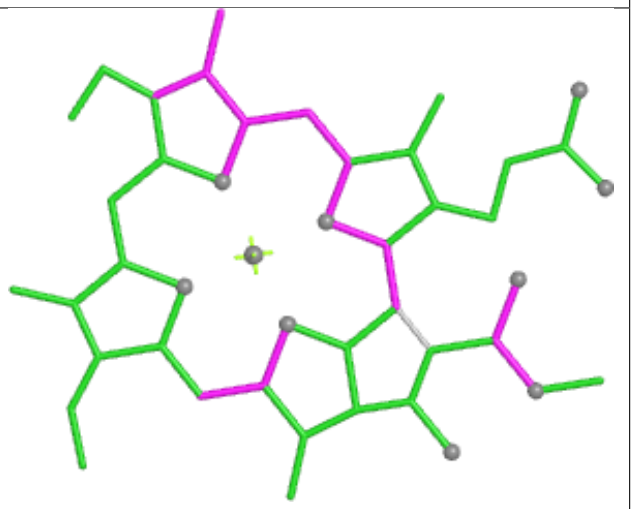


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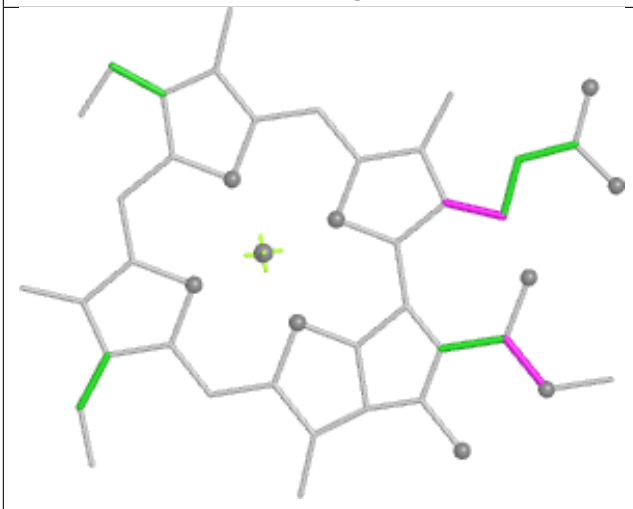
Ligand CLA aB 812



Bond lengths



Bond angles

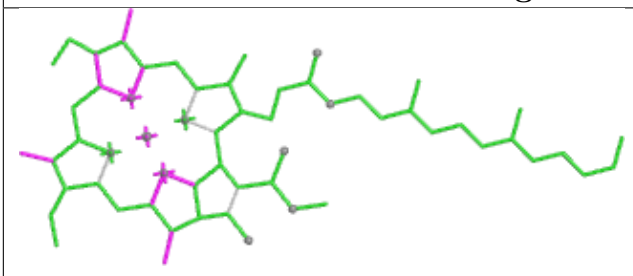


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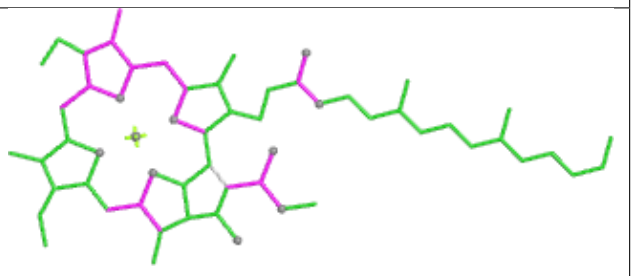


Rings

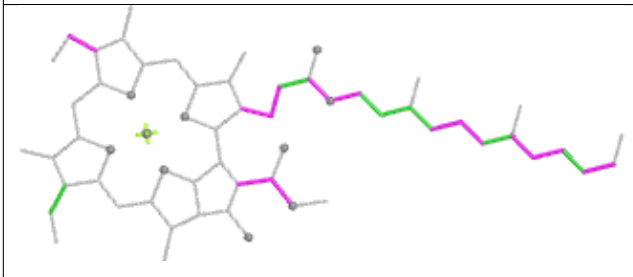
Ligand CLA aA 825



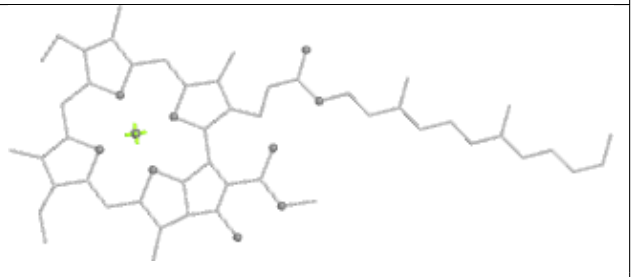
Bond lengths



Bond angles

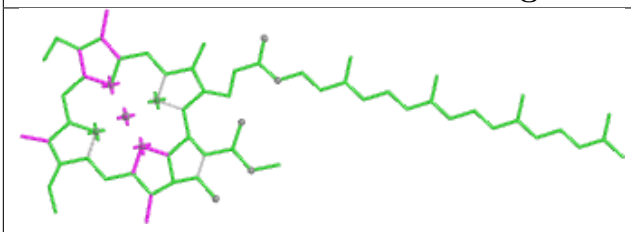


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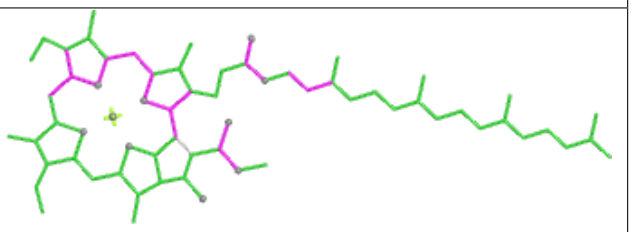


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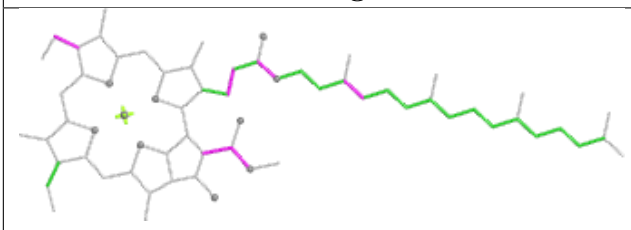
Ligand CLA c6 406



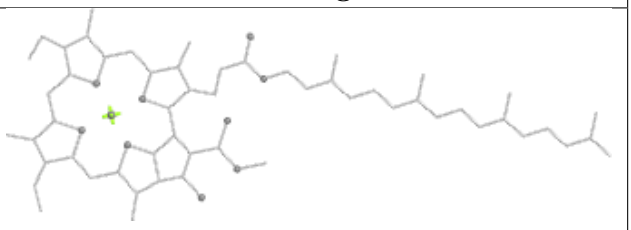
Bond lengths



Bond angles

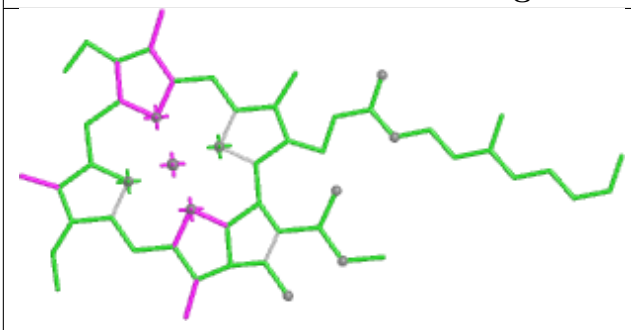


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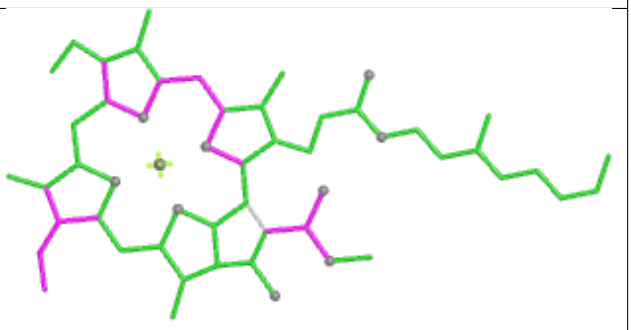


Rings

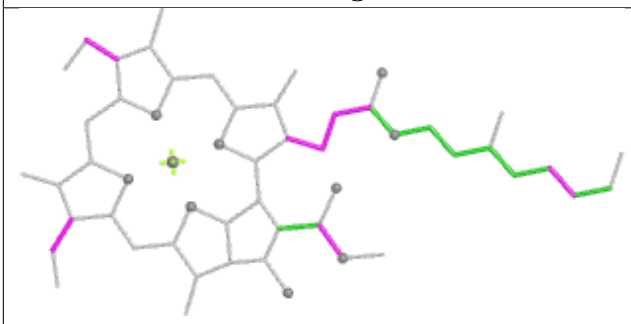
Ligand CLA bA 819



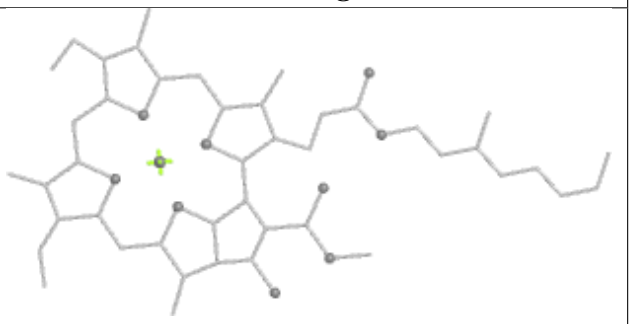
Bond lengths



Bond angles

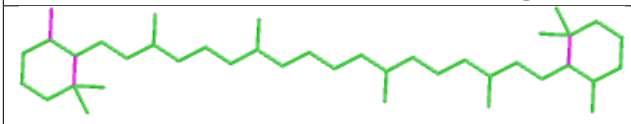


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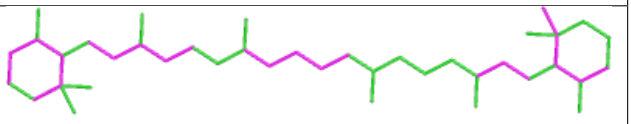


Rings

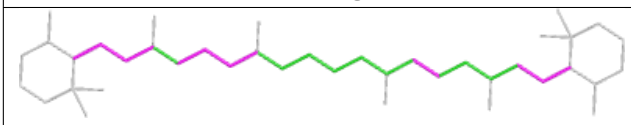
Ligand BCR a4 401



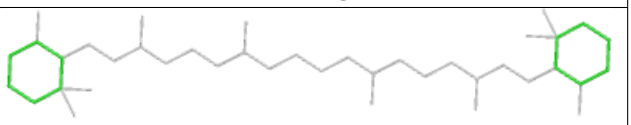
Bond lengths



Bond angles

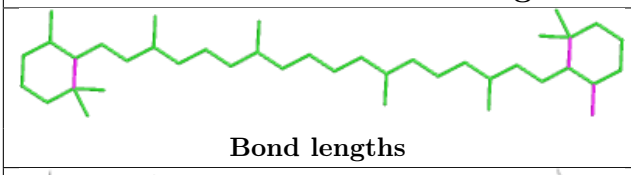


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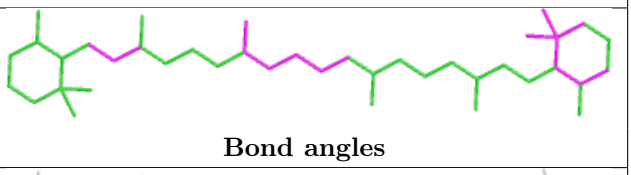


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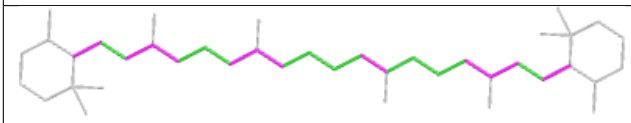
Ligand BCR aB 846



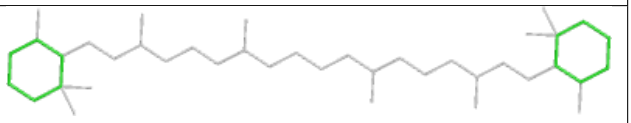
Bond lengths



Bond angles

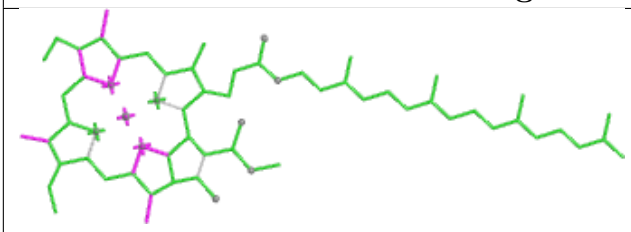


Torsions

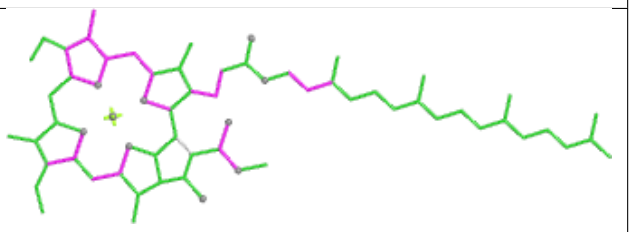


Rings

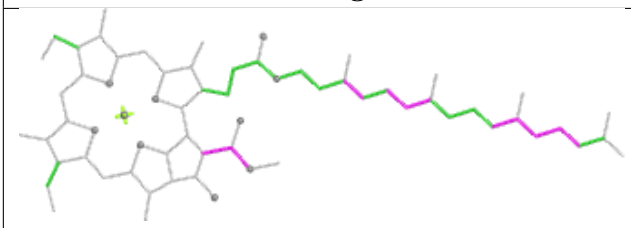
Ligand CLA aB 837



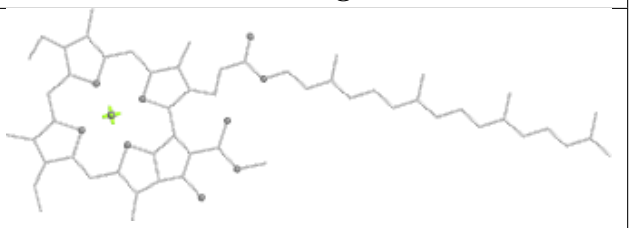
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Bond angles

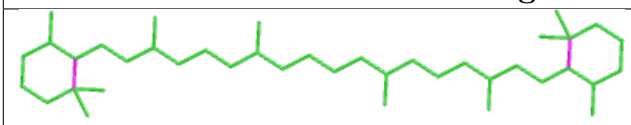


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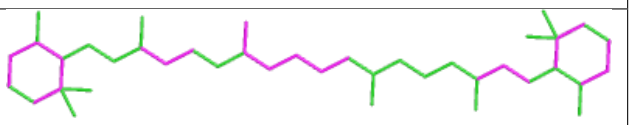


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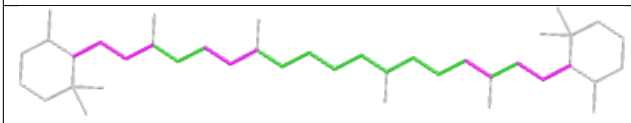
Ligand BCR c5 419



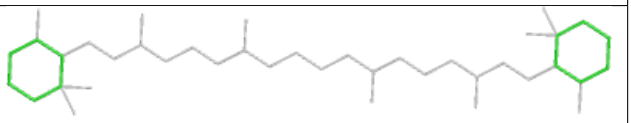
Bond lengths



Bond angles

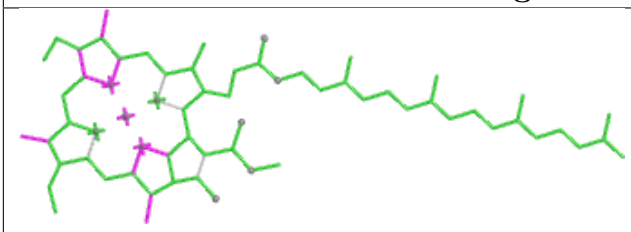


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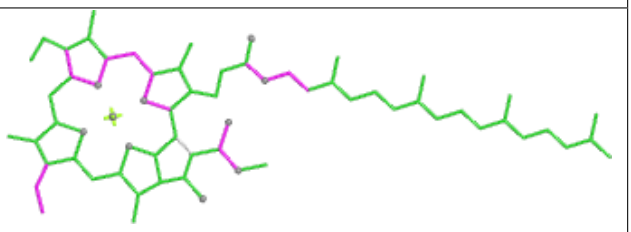


Rings

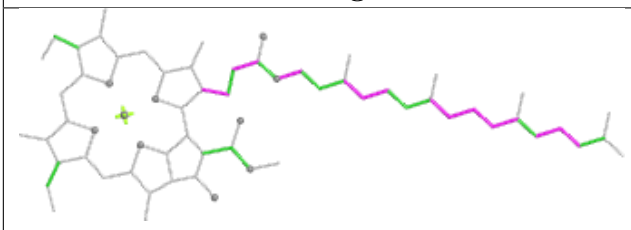
Ligand CLA bA 843



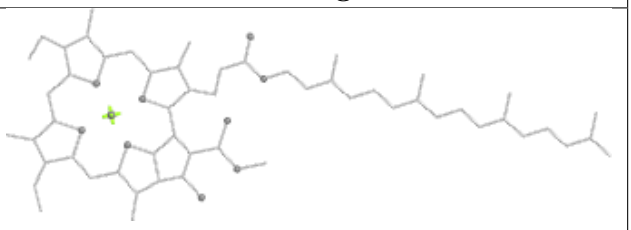
Bond lengths



Bond angles

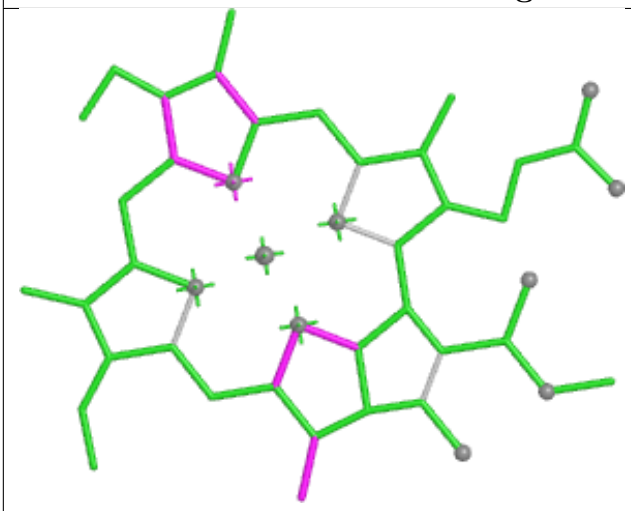


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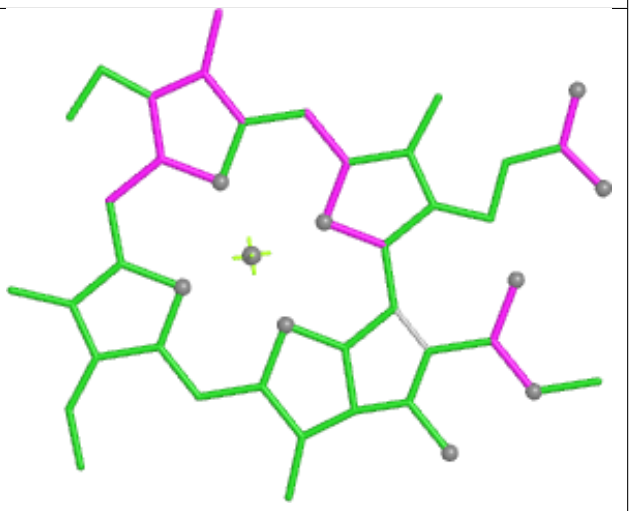


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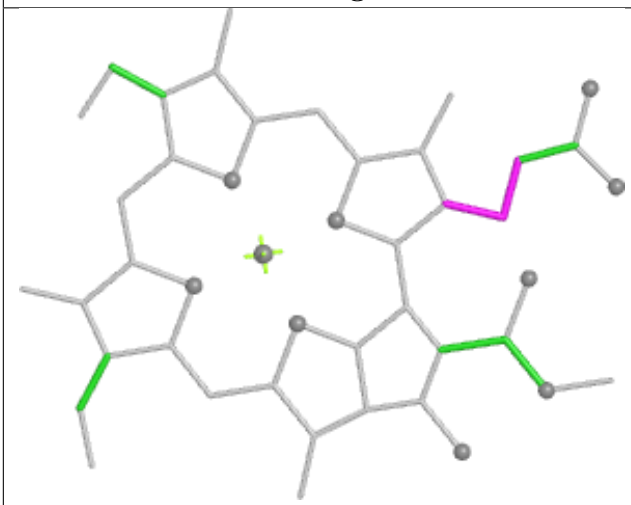
Ligand CLA aB 822



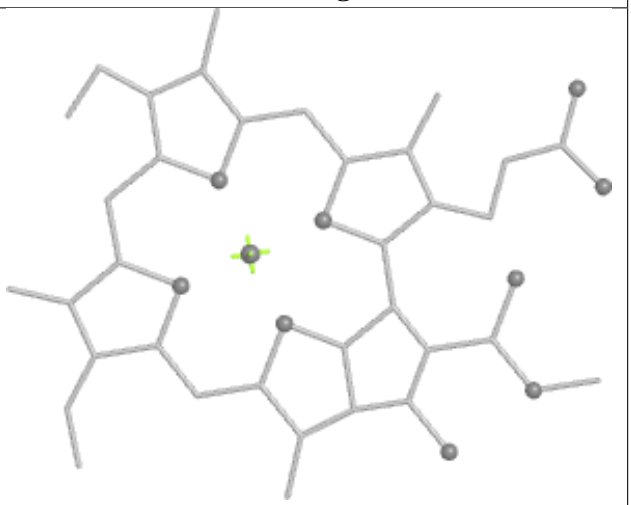
Bond lengths



Bond angles

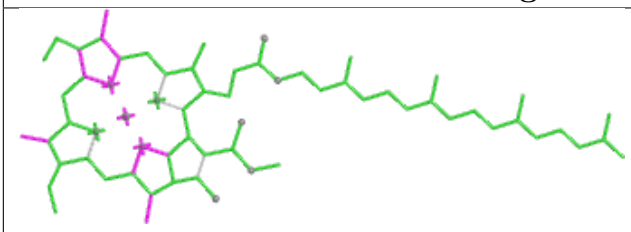


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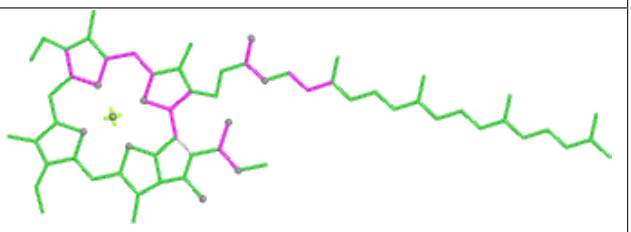


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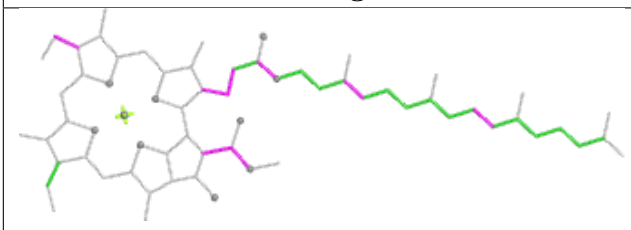
Ligand CLA a3 404



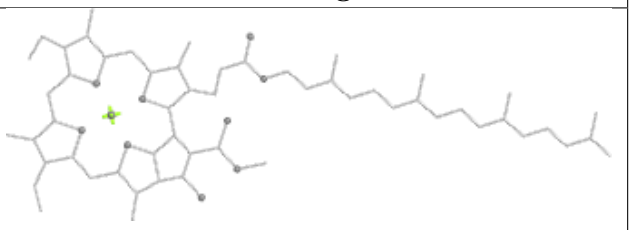
Bond lengths



Bond angles

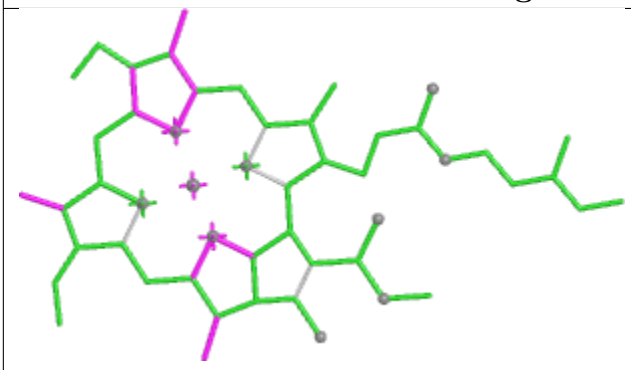


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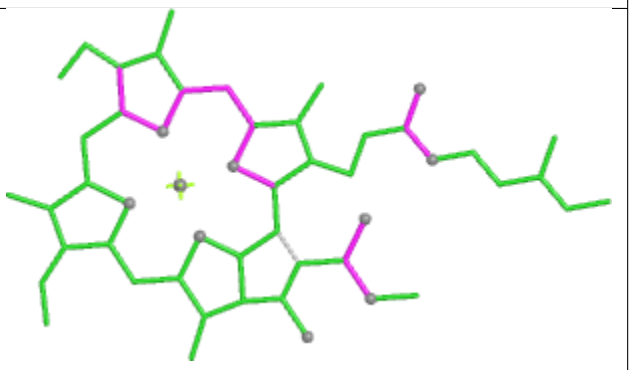


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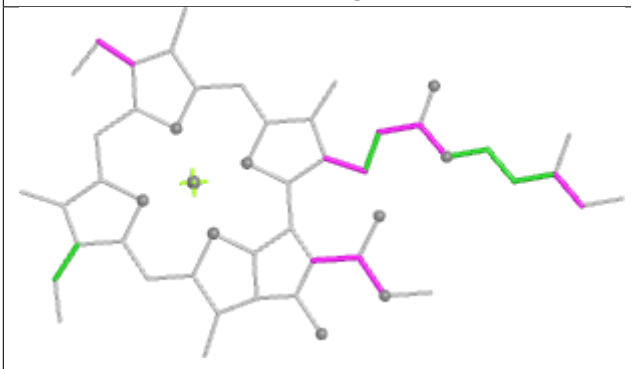
Ligand CLA aA 824



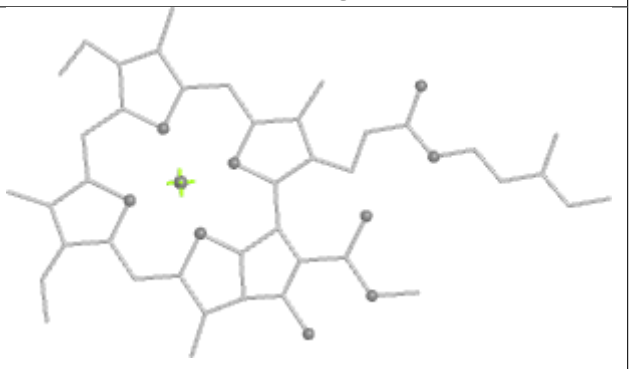
Bond lengths



Bond angles

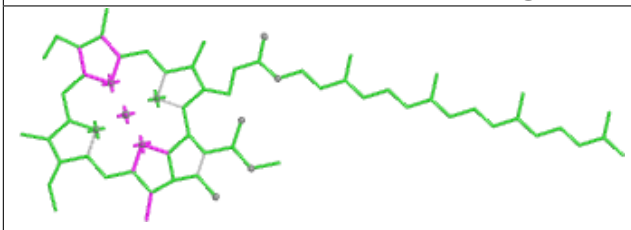


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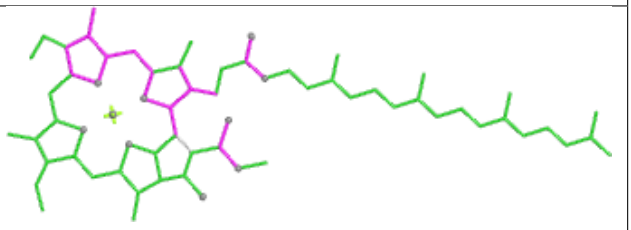


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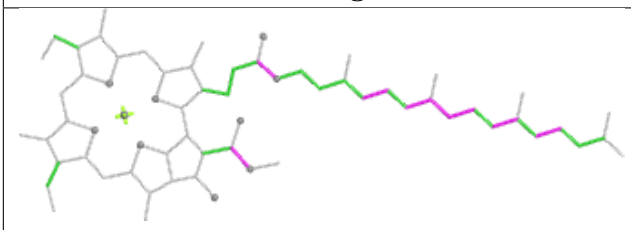
Ligand CLA a3 403



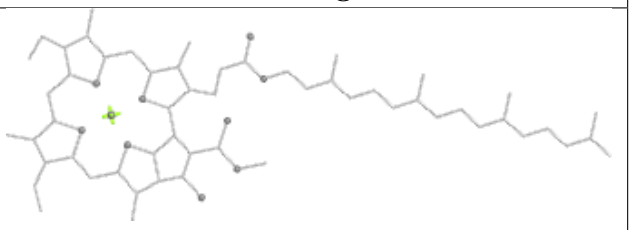
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Bond angles

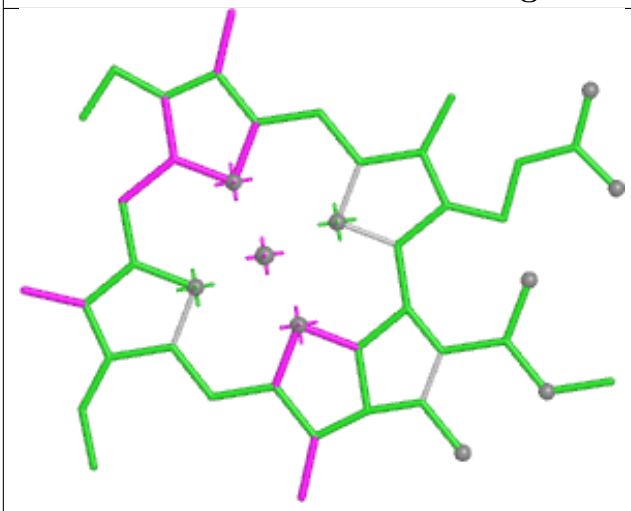


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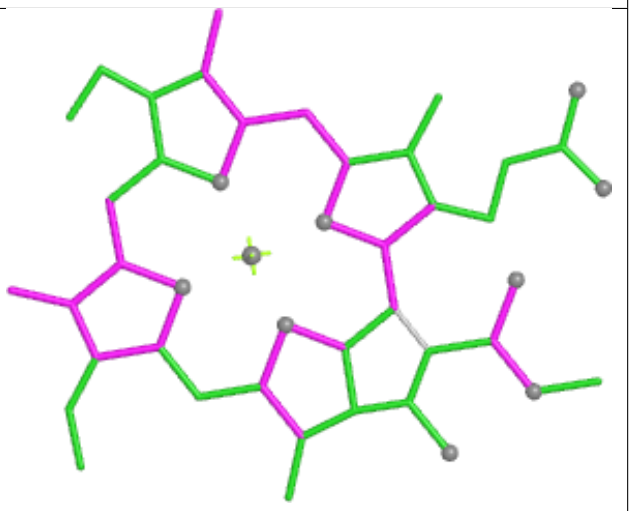


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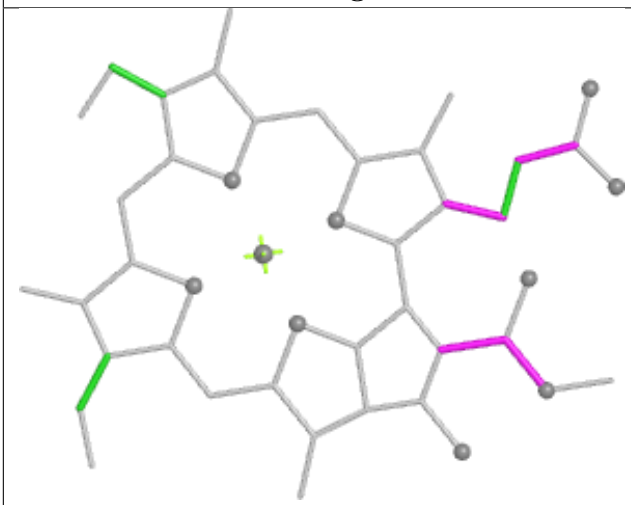
Ligand CLA c1 412



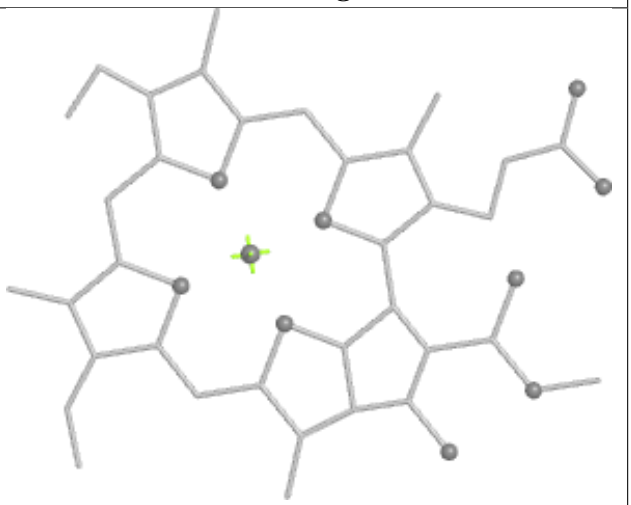
Bond lengths



Bond angles

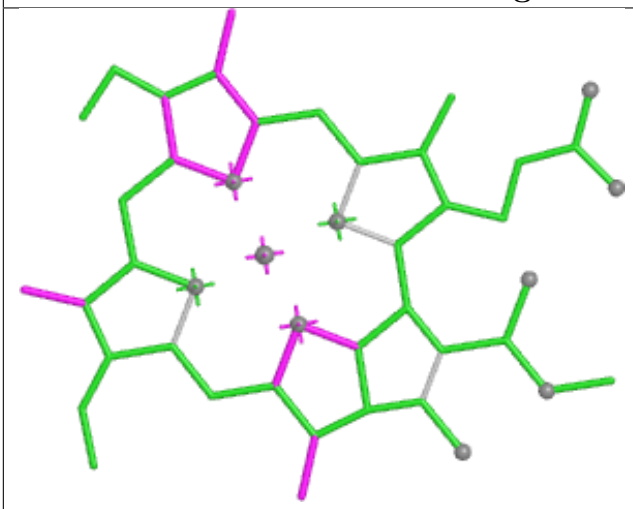


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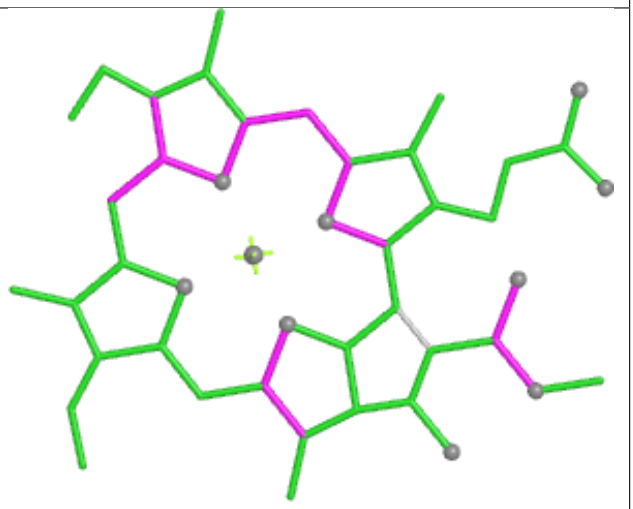


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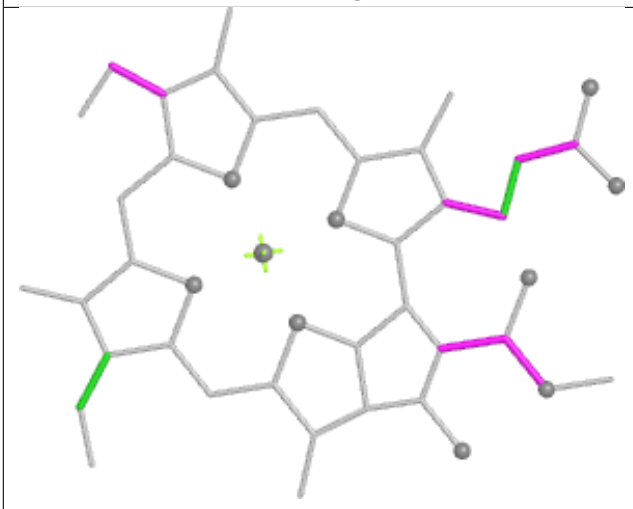
Ligand CLA bA 811



Bond lengths



Bond angles

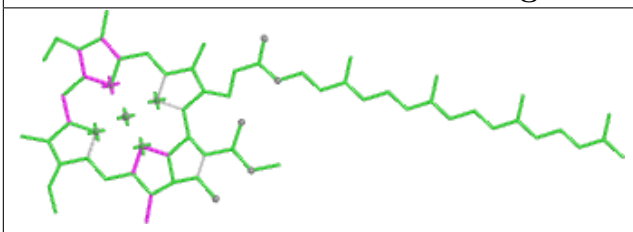


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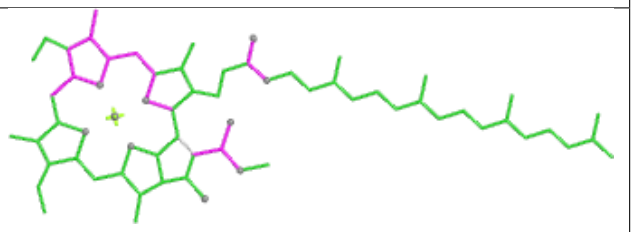


Rings

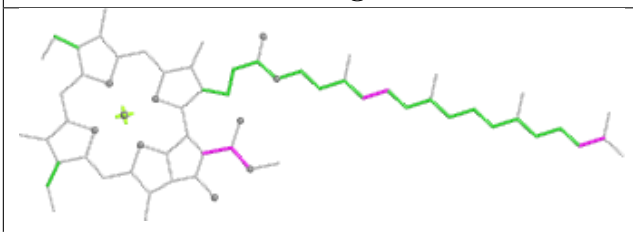
Ligand CLA c2 410



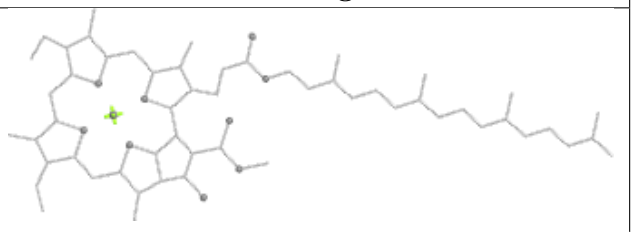
Bond lengths



Bond angles

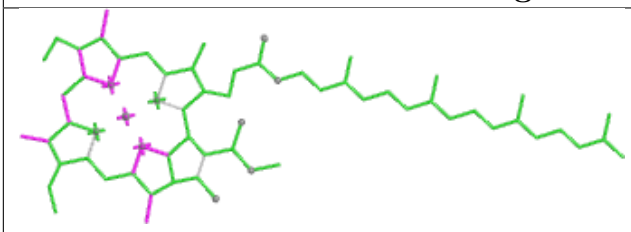


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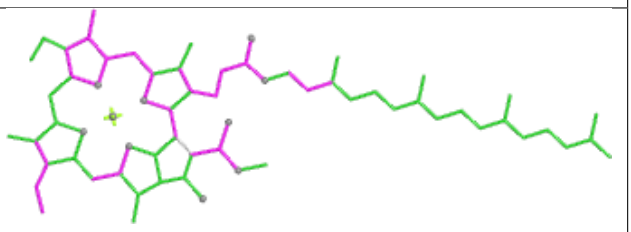


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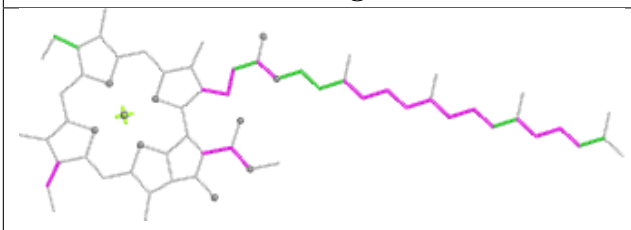
Ligand CLA bB 814



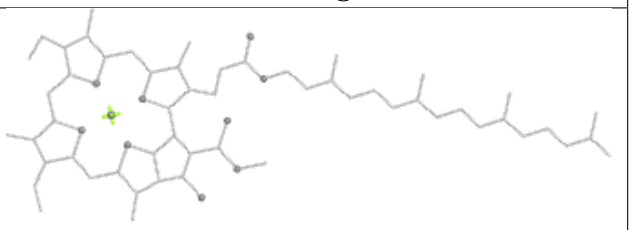
Bond lengths



Bond angles



Torsions

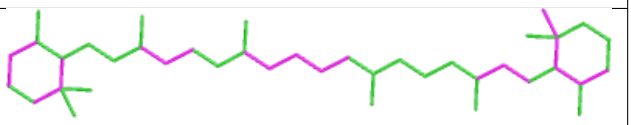


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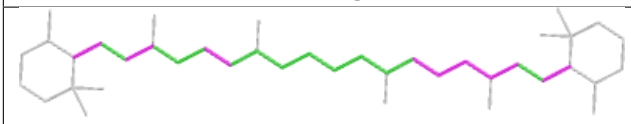
Ligand BCR b2 420



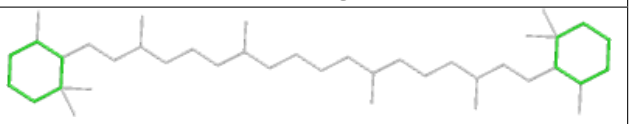
Bond lengths



Bond angles

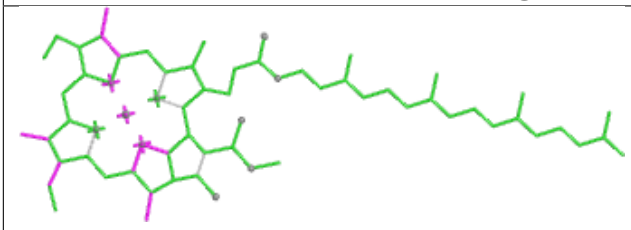


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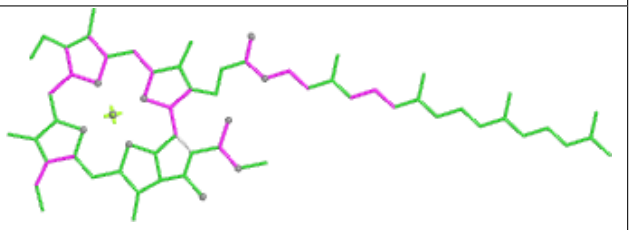


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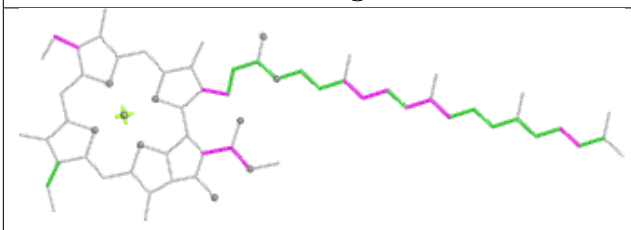
Ligand CLA aB 811



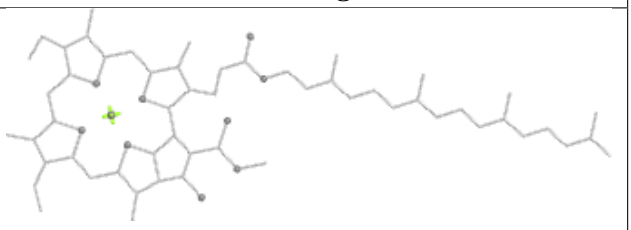
Bond lengths



Bond angles

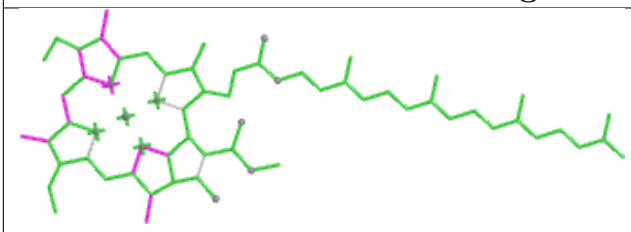


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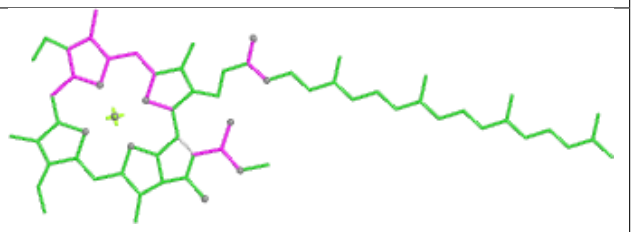


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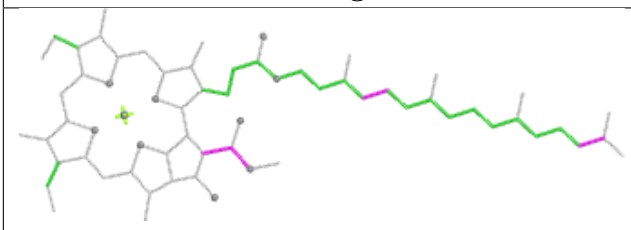
Ligand CLA a3 409



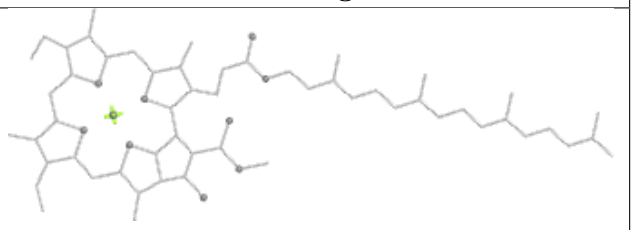
Bond lengths



Bond angles

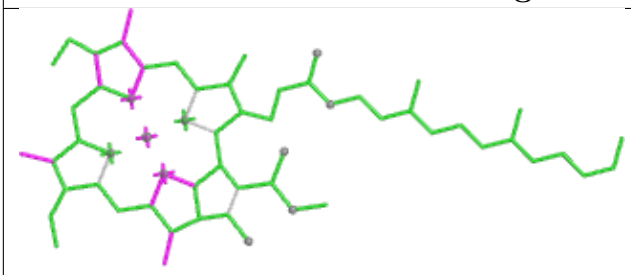


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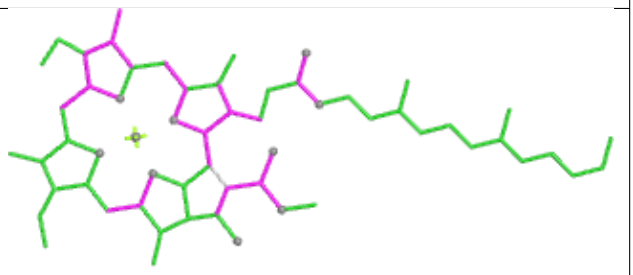


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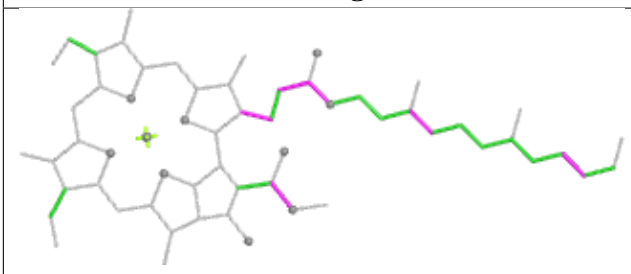
Ligand CLA bB 818



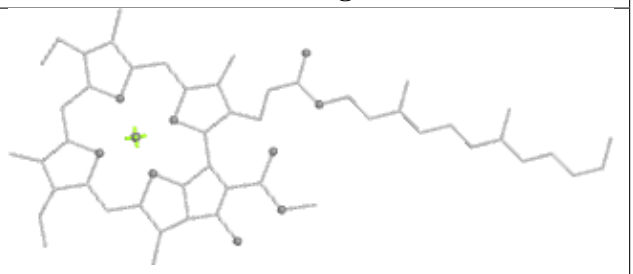
Bond lengths



Bond angles

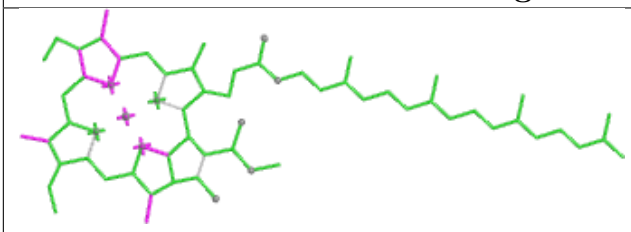


Torsions

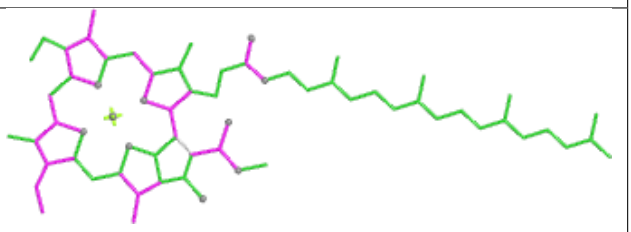


Rings

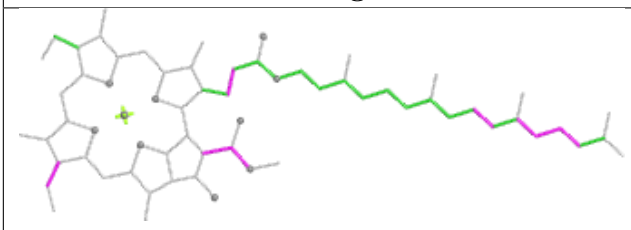
Ligand CLA bB 804



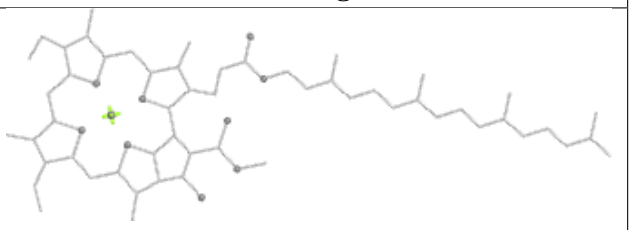
Bond lengths



Bond angles

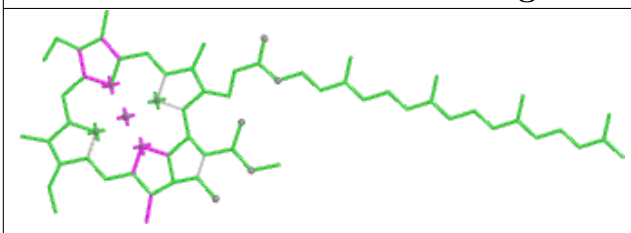


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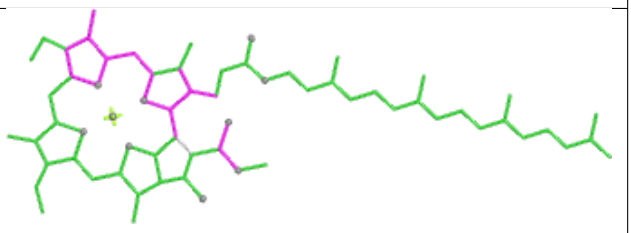


Rings

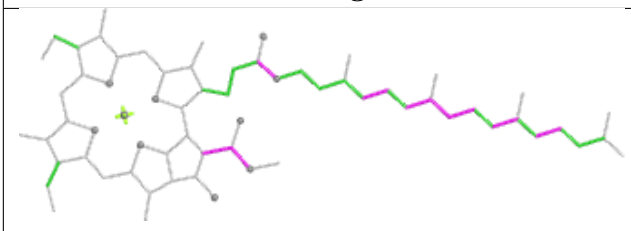
Ligand CLA b6 404



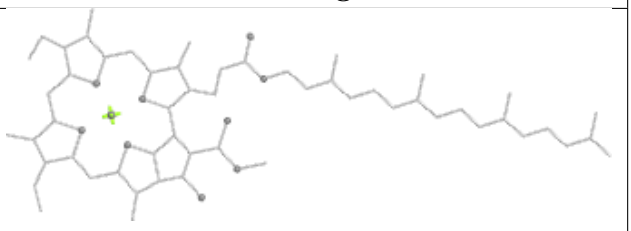
Bond lengths



Bond angles

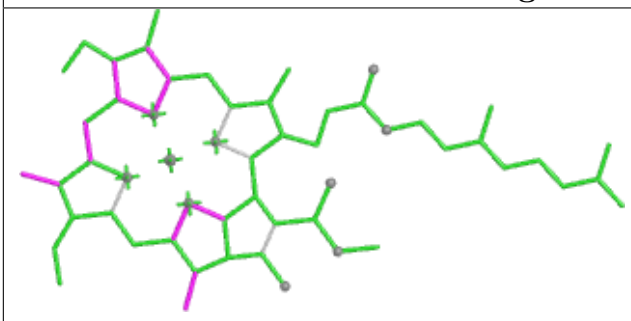


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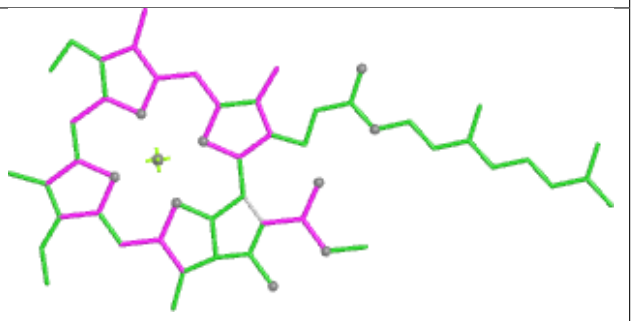


Rings

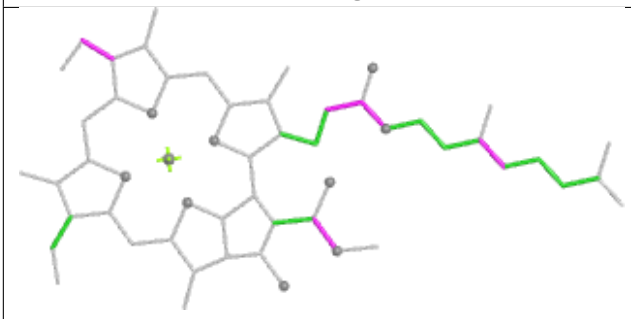
Ligand CLA b4 417



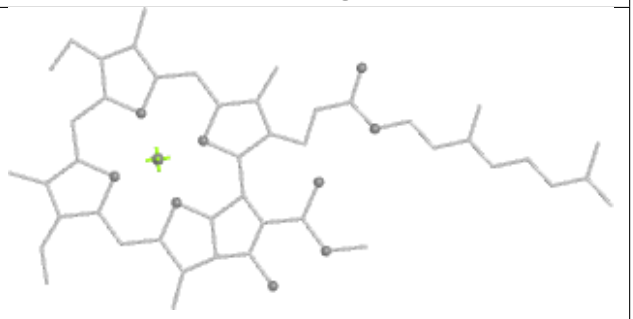
Bond lengths



Bond angles

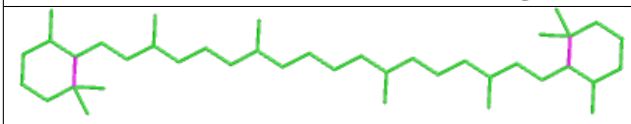


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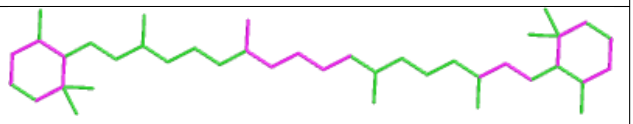


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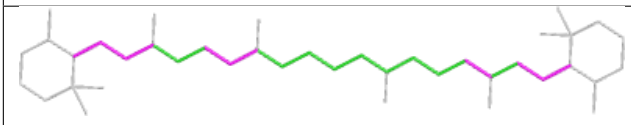
Ligand BCR b2 421



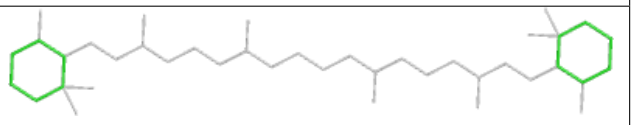
Bond lengths



Bond angles

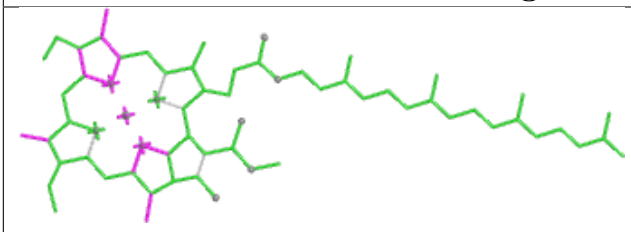


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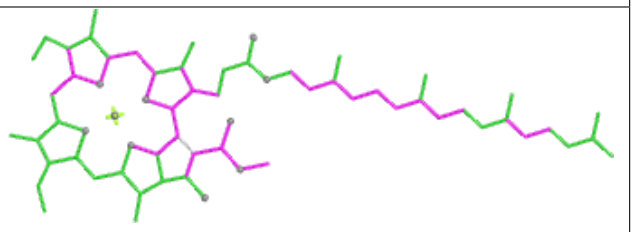


Rings

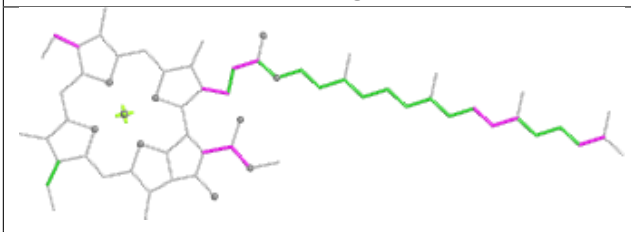
Ligand CLA c2 422



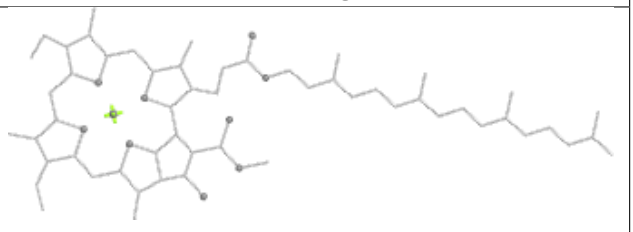
Bond lengths



Bond angles

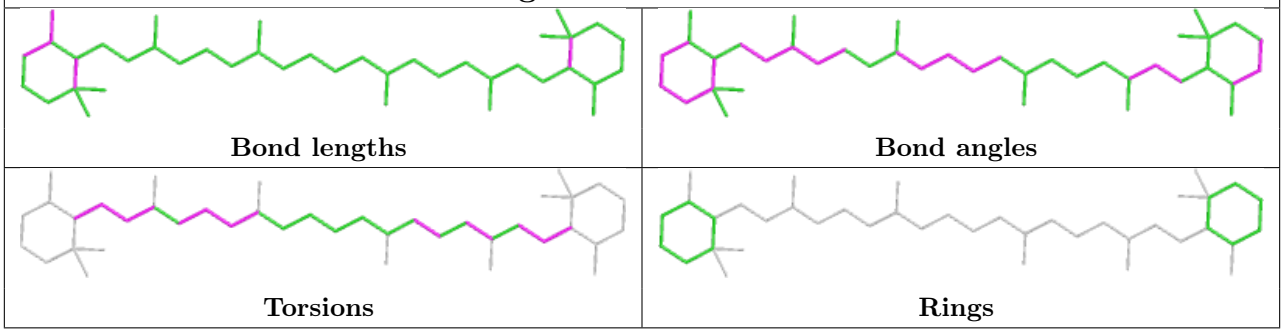


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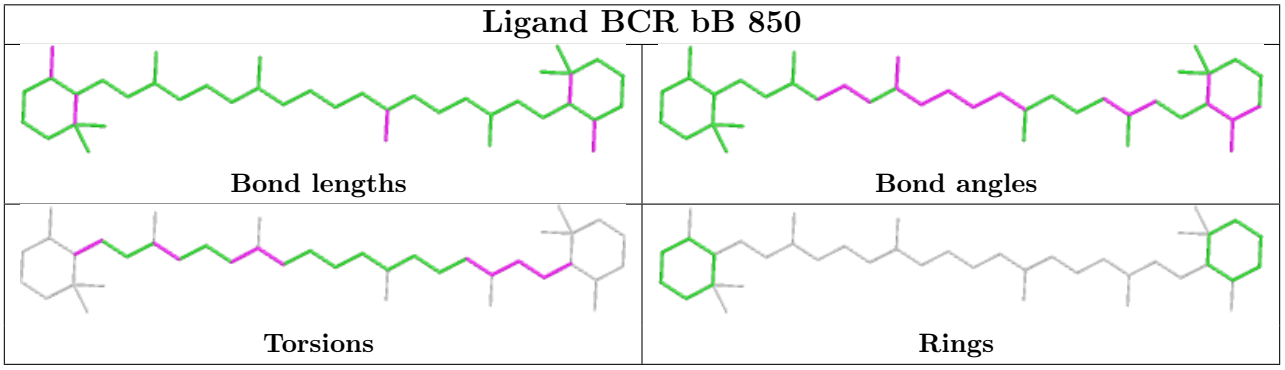


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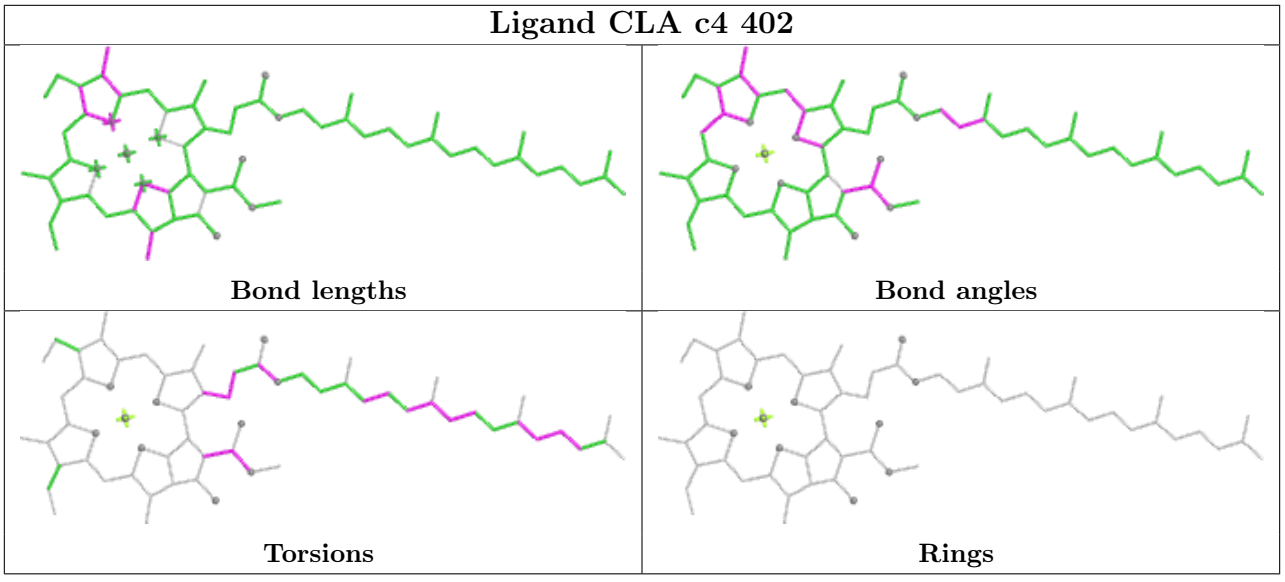
Ligand BCR a6 421



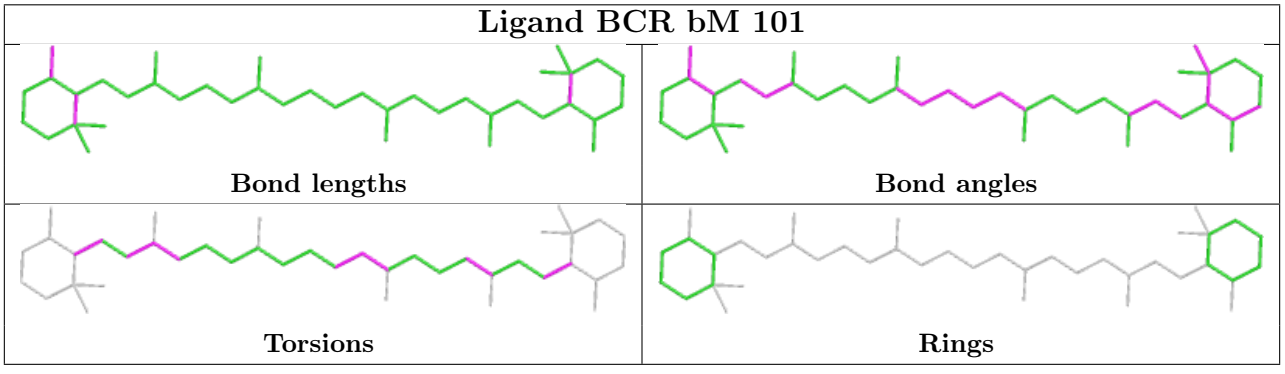
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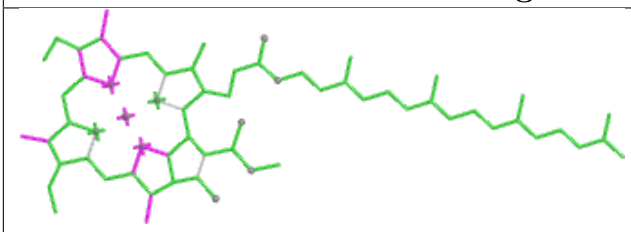
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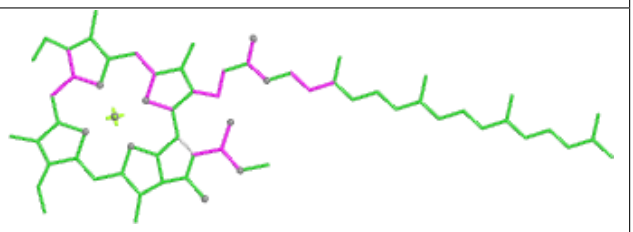
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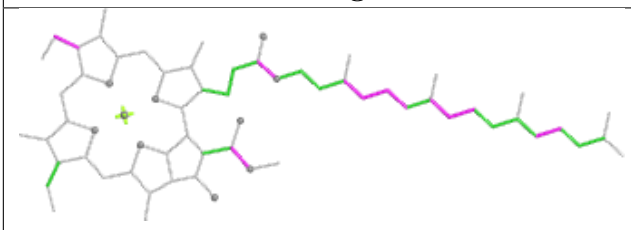
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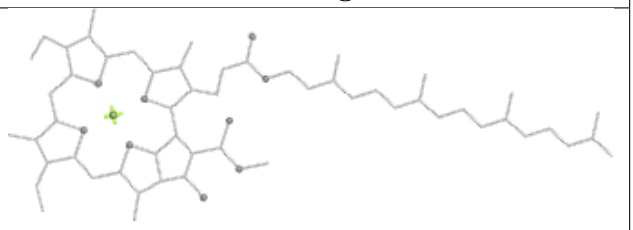
Bond lengths



Bond angles



Torsions

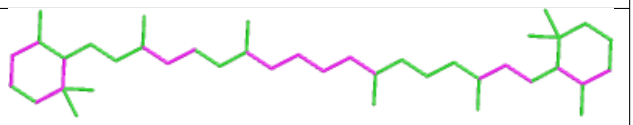


Rings

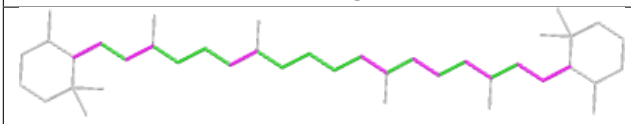
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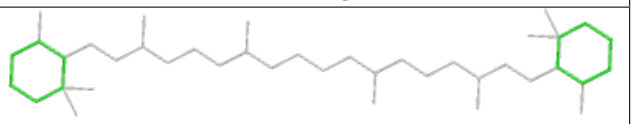
Bond lengths



Bond angles

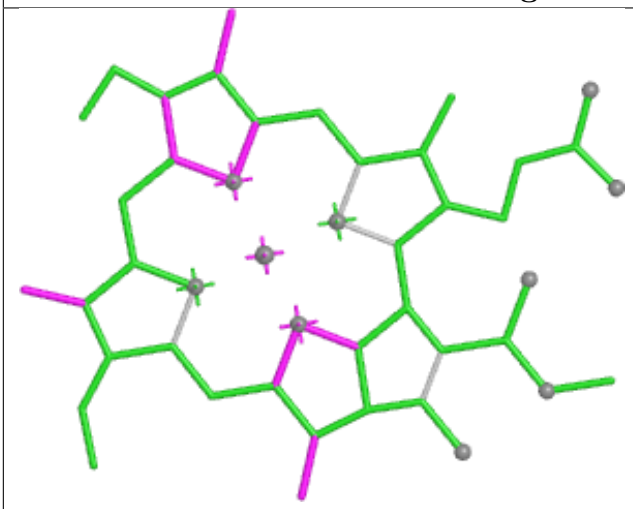


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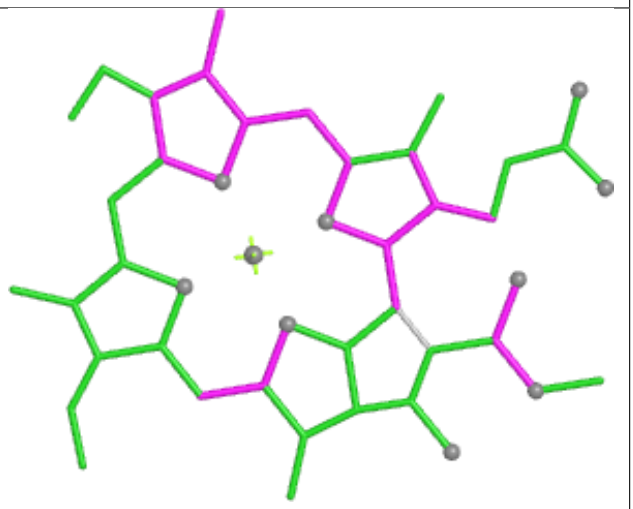


Rings

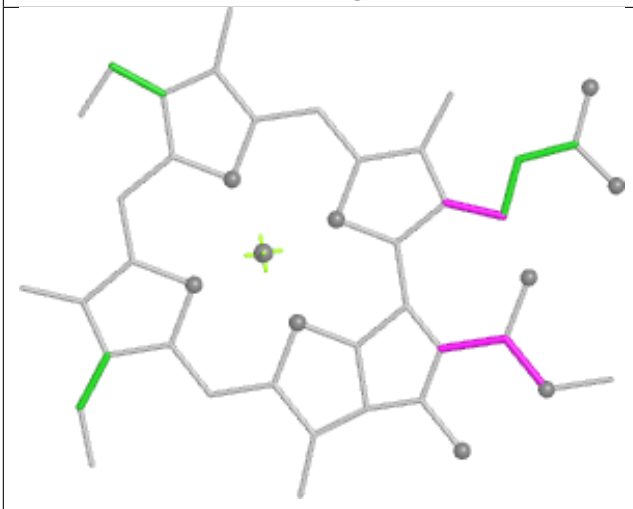
Ligand CLA c3 411



Bond lengths



Bond angles

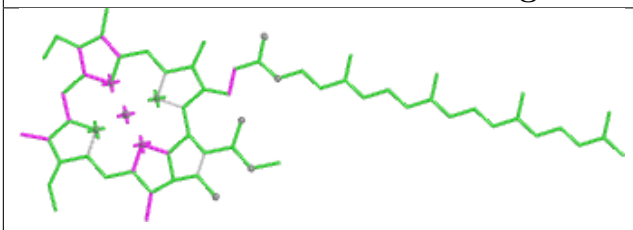


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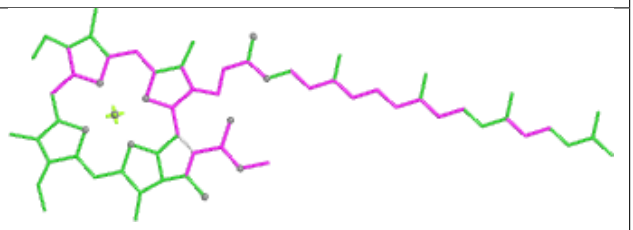


Rings

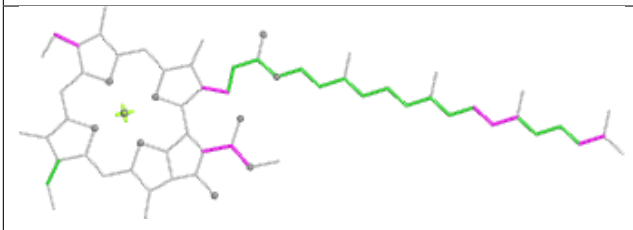
Ligand CLA a2 406



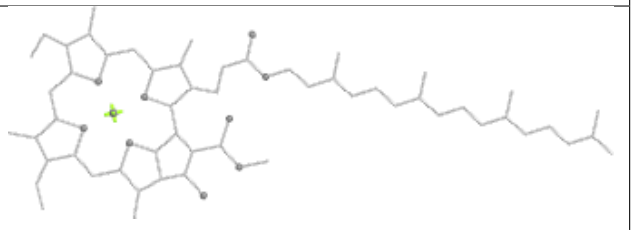
Bond lengths



Bond angles

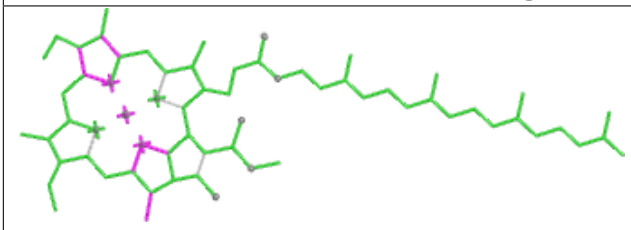


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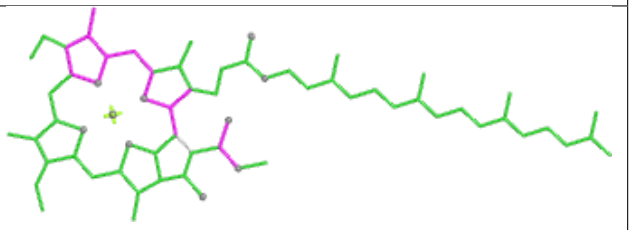


Rings

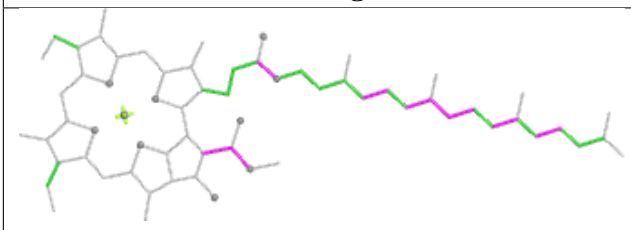
Ligand CLA c4 403



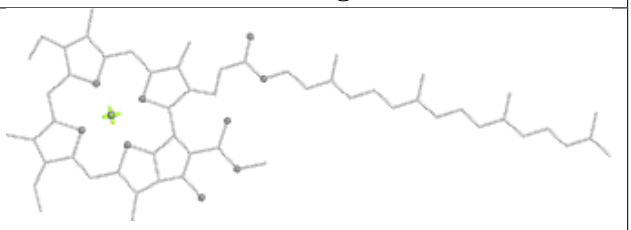
Bond lengths



Bond angles

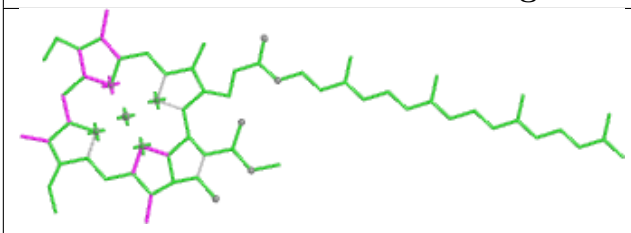


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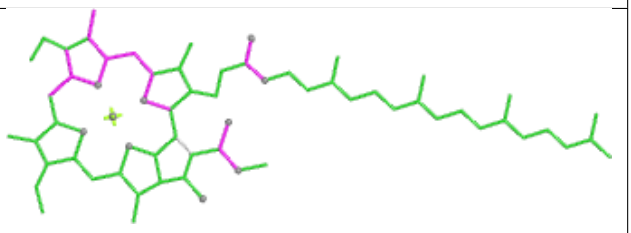


Rings

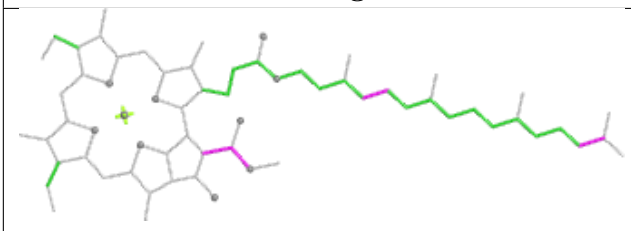
Ligand CLA a5 409



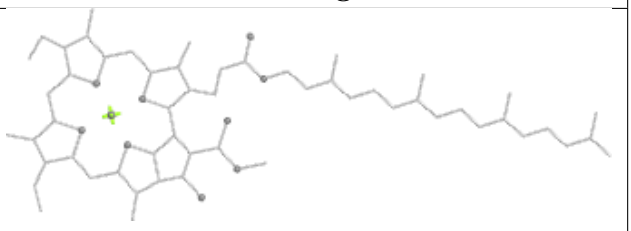
Bond lengths



Bond angles

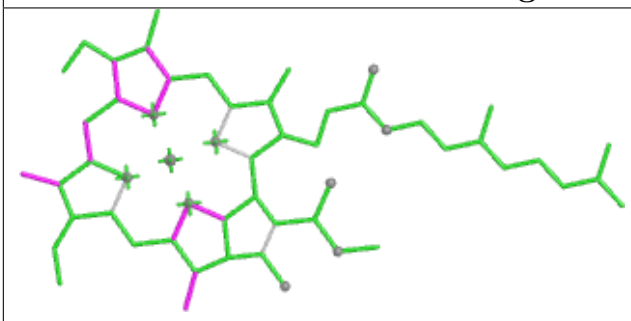


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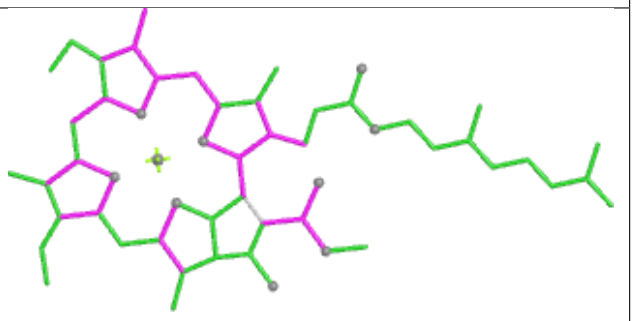


Rings

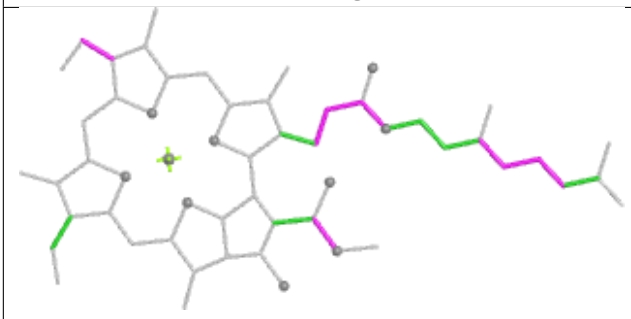
Ligand CLA b1 417



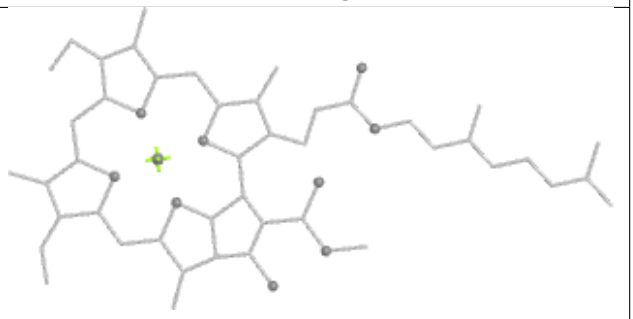
Bond lengths



Bond angles

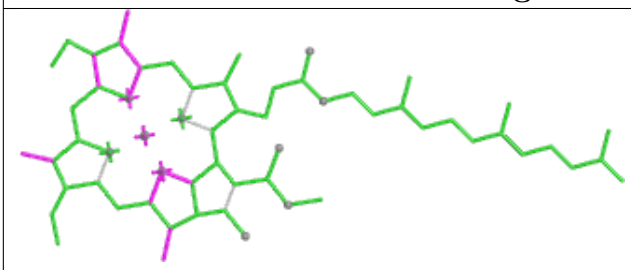


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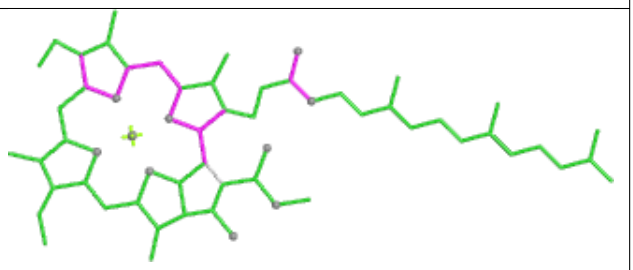


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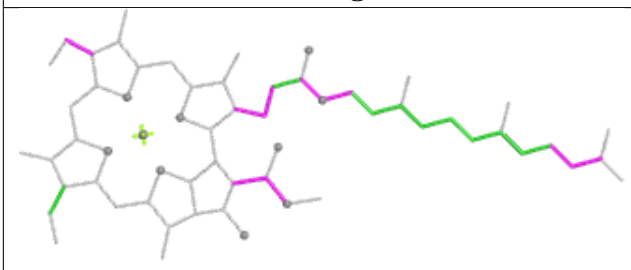
Ligand CLA bA 814



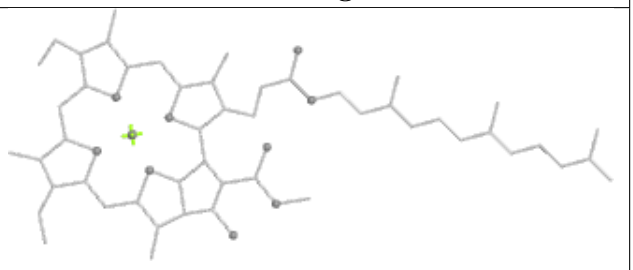
Bond lengths



Bond angles



Torsions

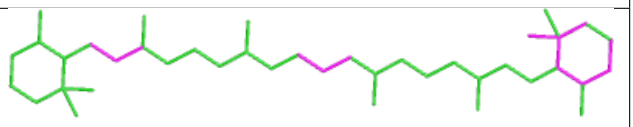


Rings

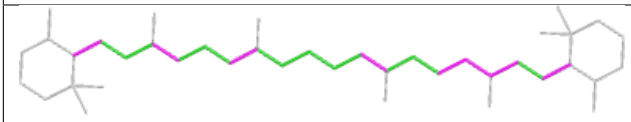
Ligand BCR aB 845



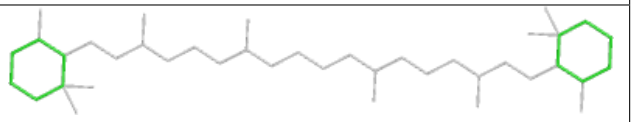
Bond lengths



Bond angles

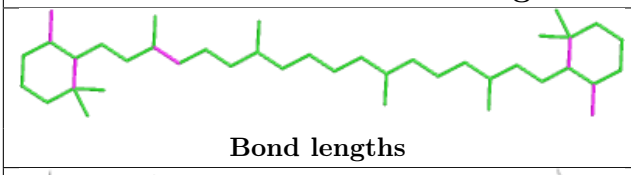


Torsions

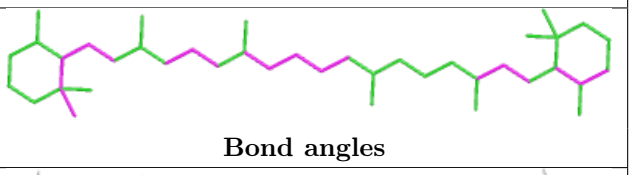


Rings

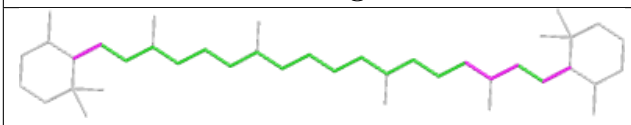
Ligand BCR aA 851



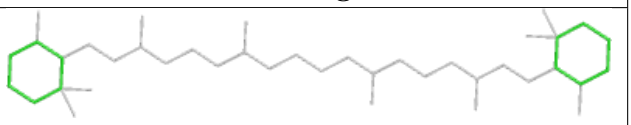
Bond lengths



Bond angles

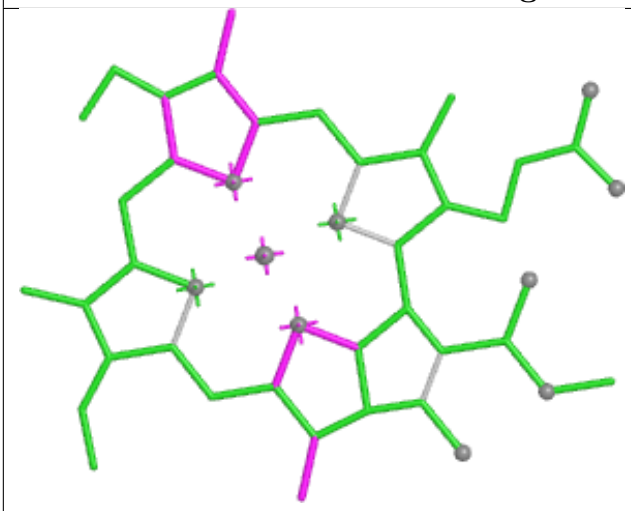


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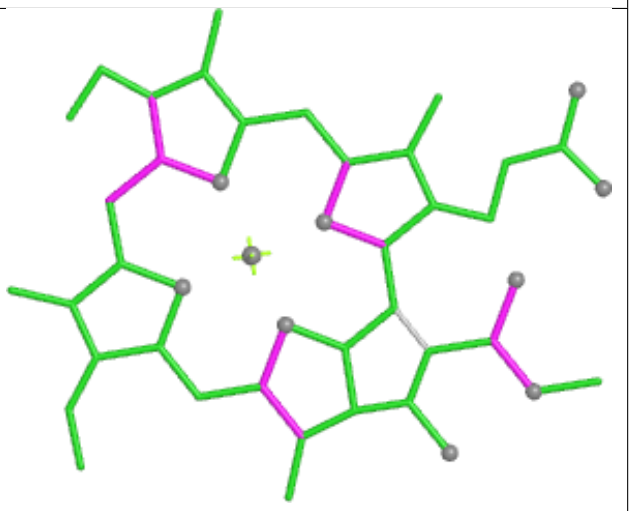


Rings

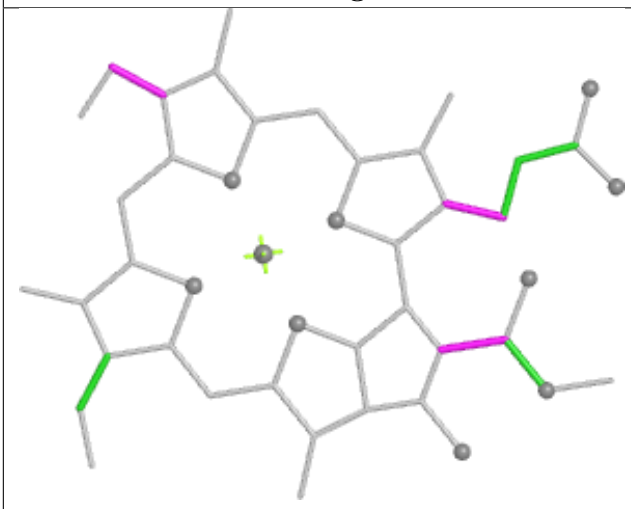
Ligand CLA a4 413



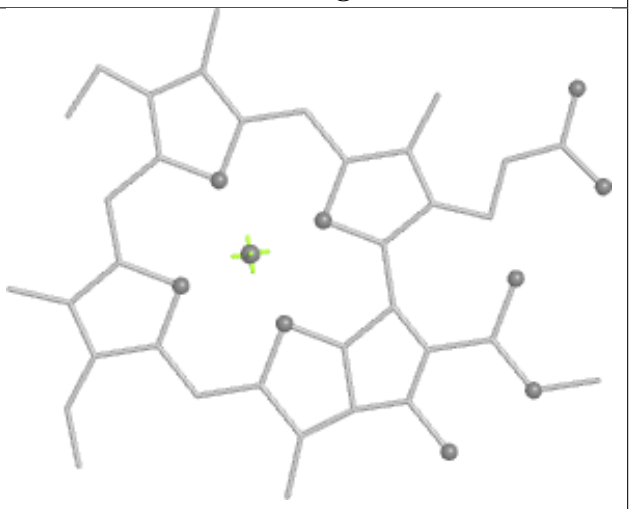
Bond lengths



Bond angles

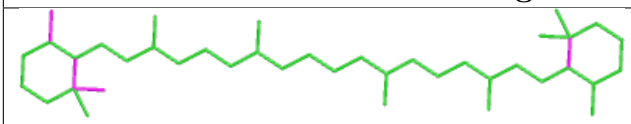


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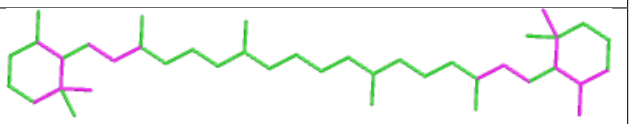


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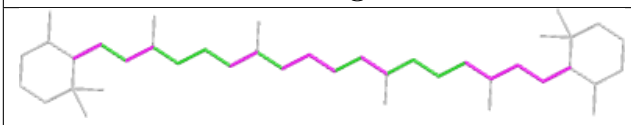
Ligand BCR aF 201



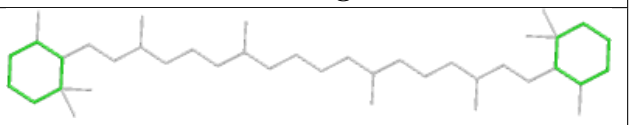
Bond lengths



Bond angles

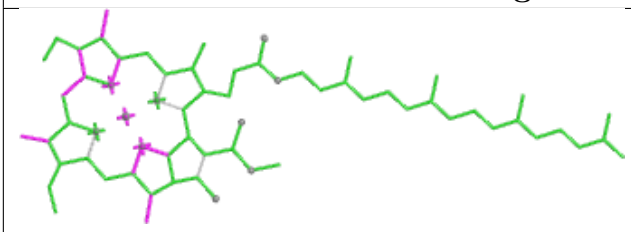


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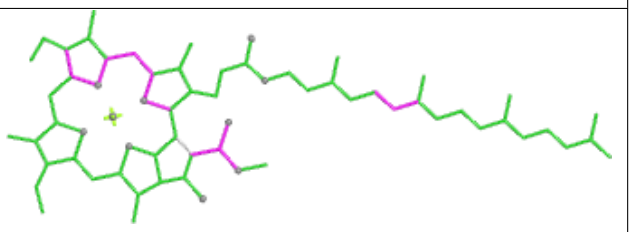


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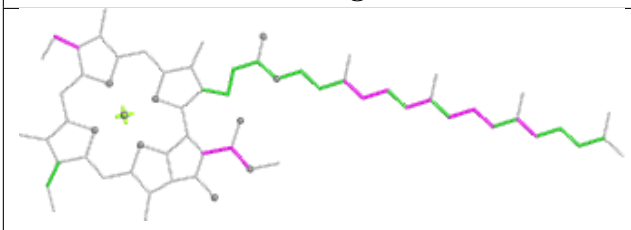
Ligand CLA bA 839



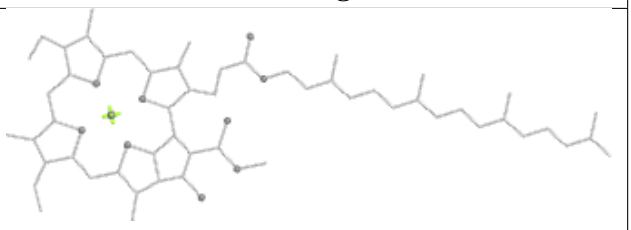
Bond lengths



Bond angles

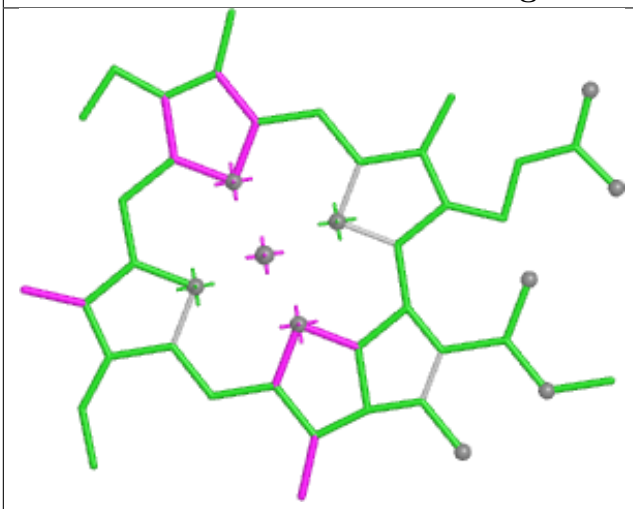


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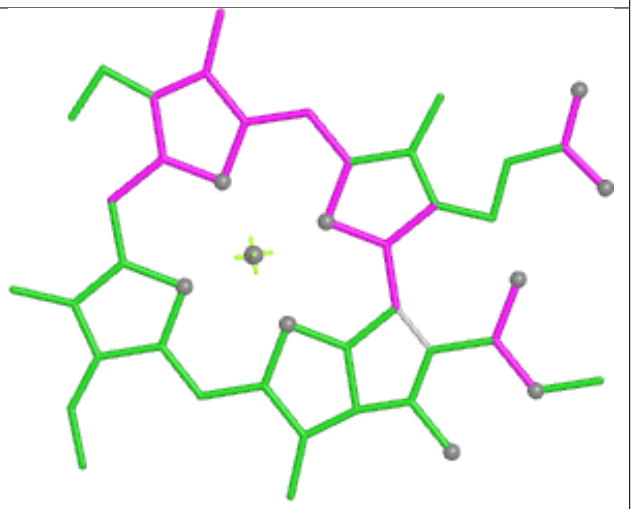


Rings

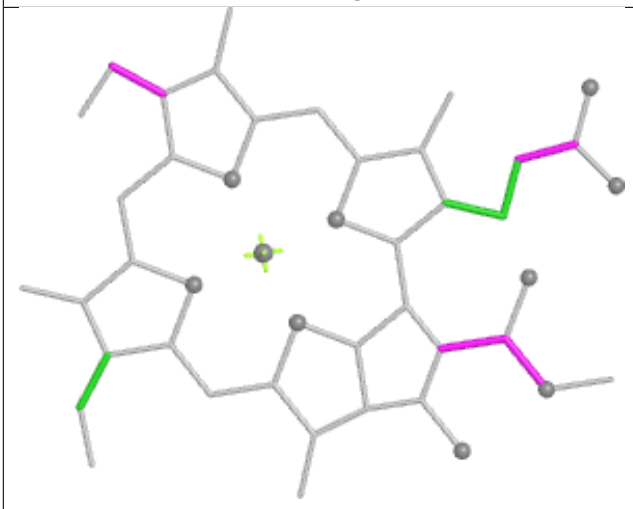
Ligand CLA a2 408



Bond lengths



Bond angles

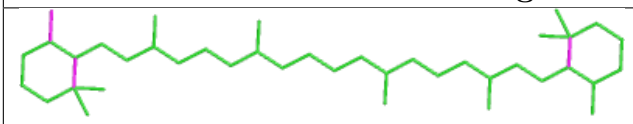


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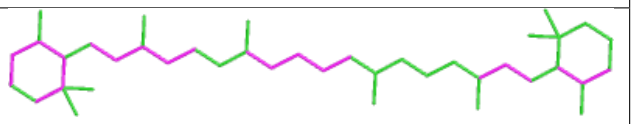


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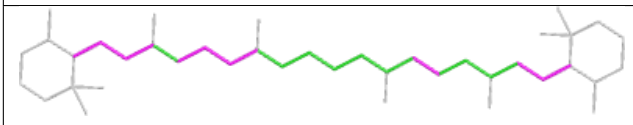
Ligand BCR b4 401



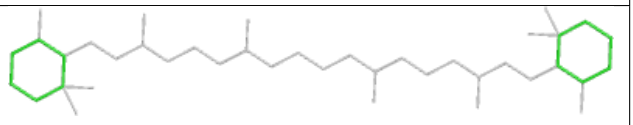
Bond lengths



Bond angles

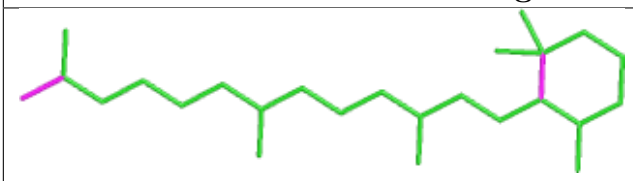


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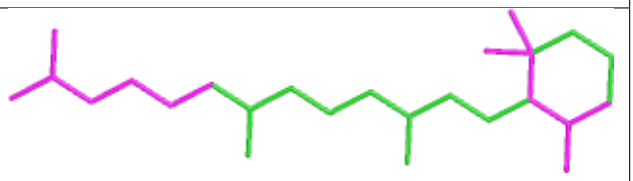


Rings

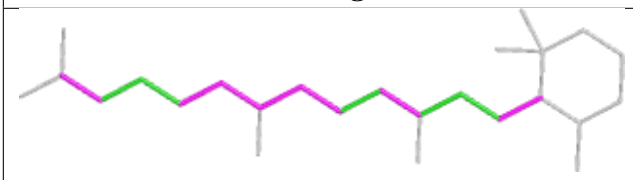
Ligand BCR cB 847



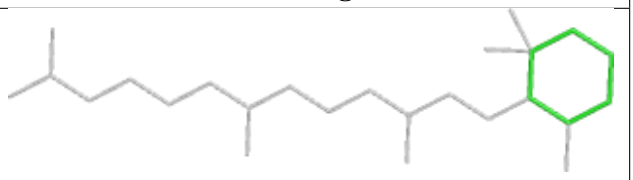
Bond lengths



Bond angles

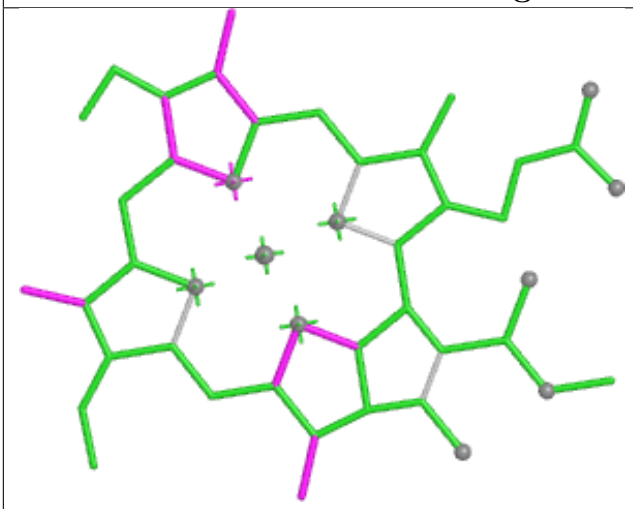


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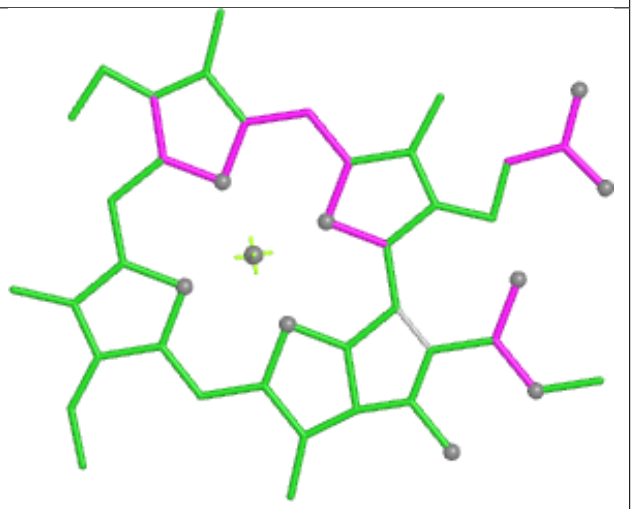


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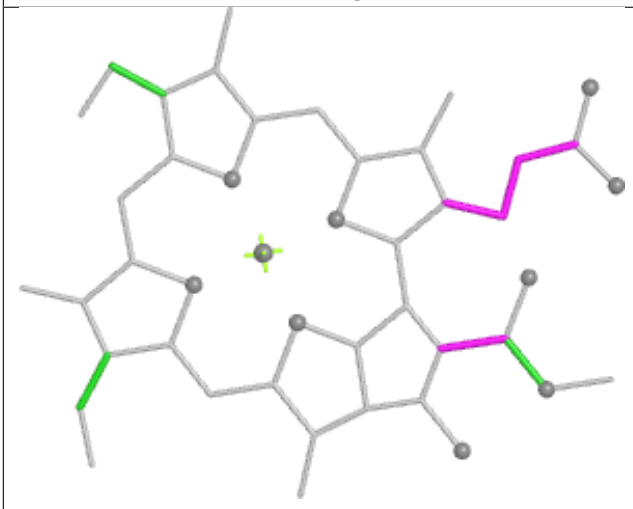
Ligand CLA bA 837



Bond lengths



Bond angles

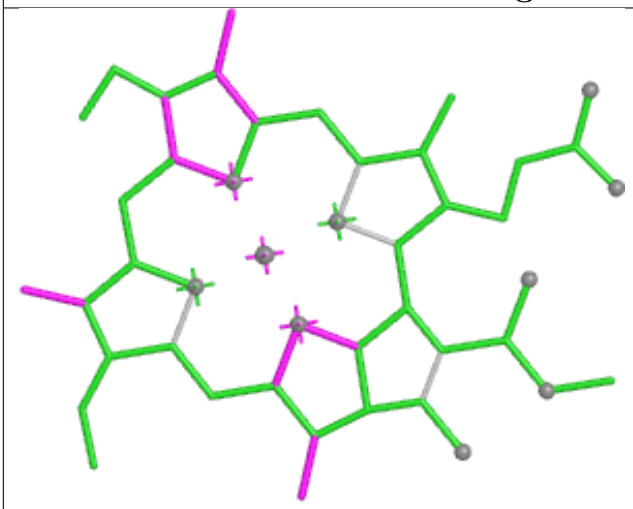


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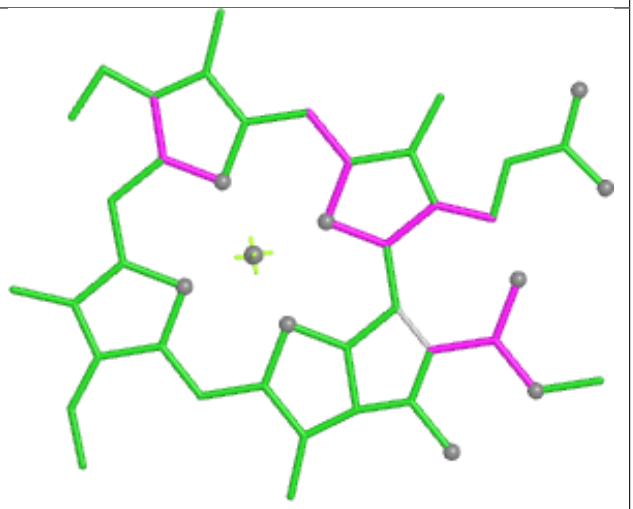


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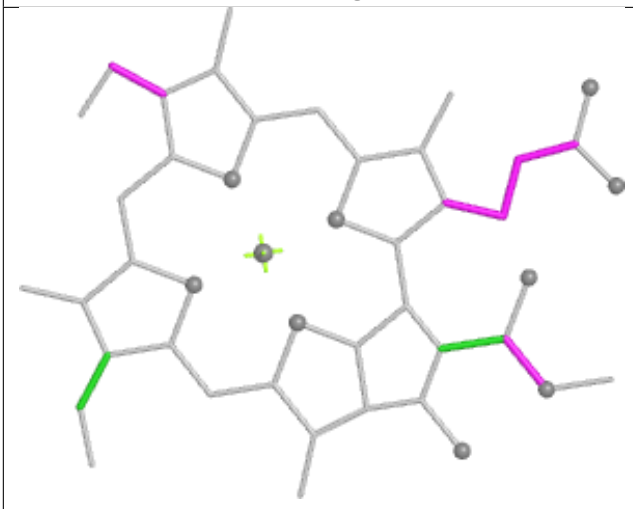
Ligand CLA aB 835



Bond lengths



Bond angles

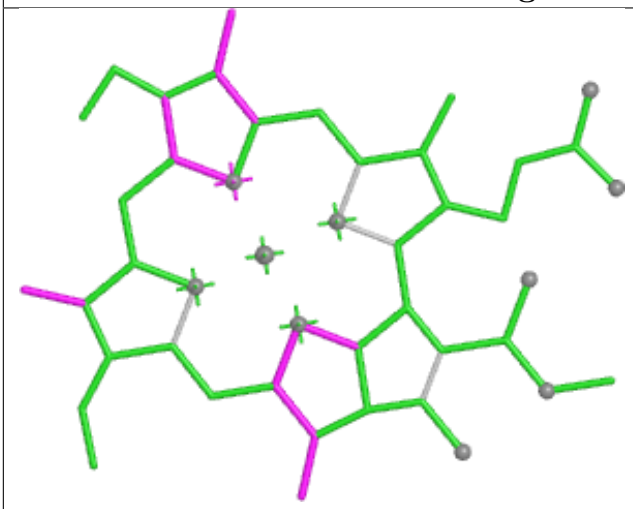


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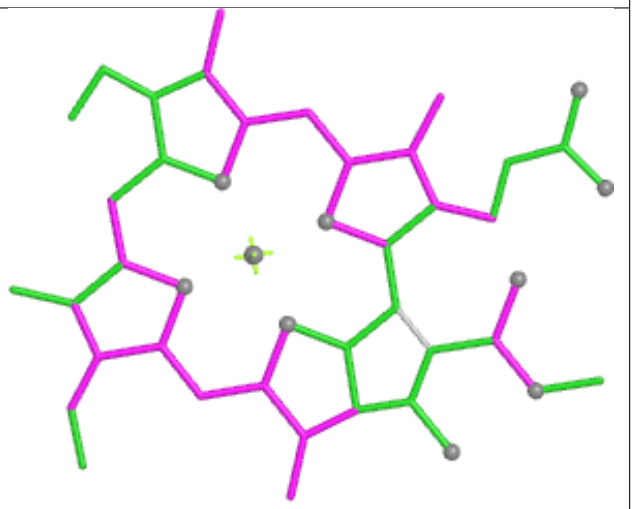


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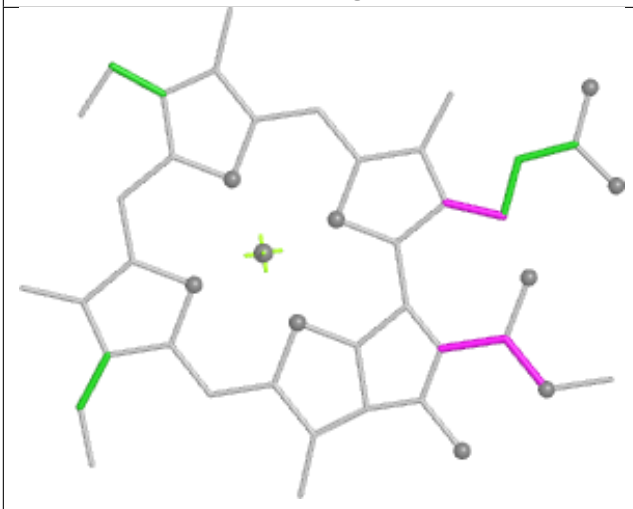
Ligand CLA b4 405



Bond lengths



Bond angles

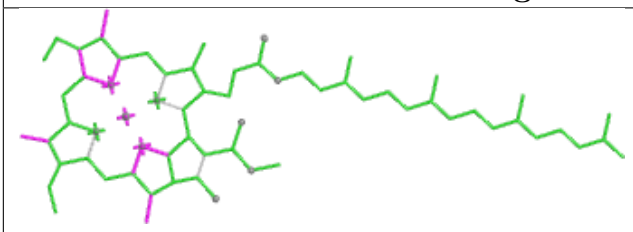


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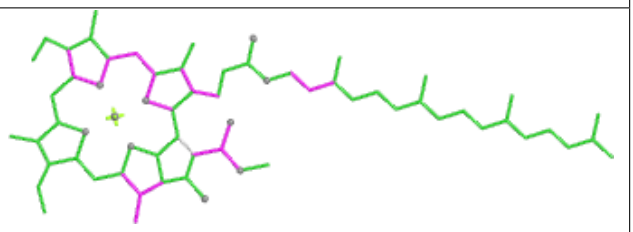


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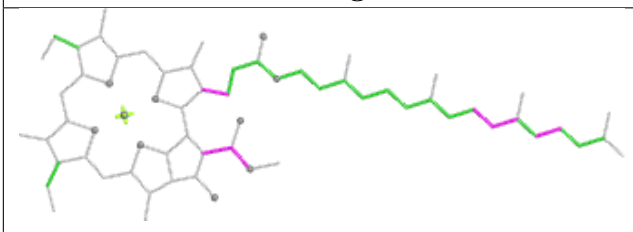
Ligand CLA bA 804



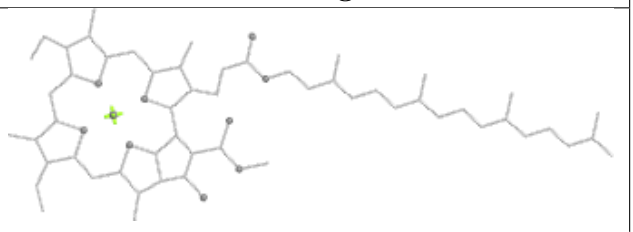
Bond lengths



Bond angles

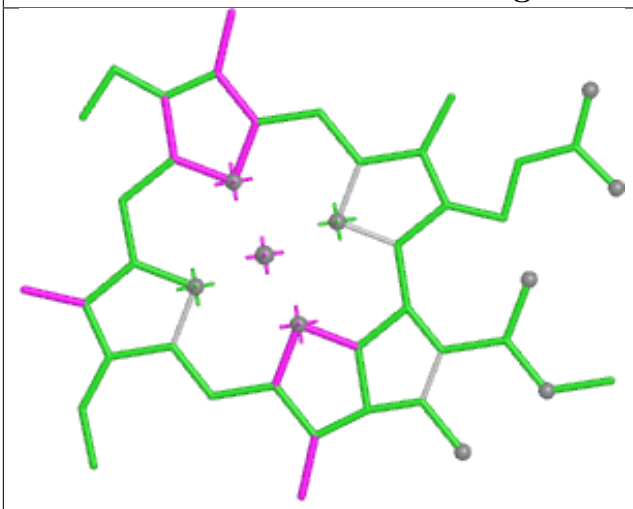


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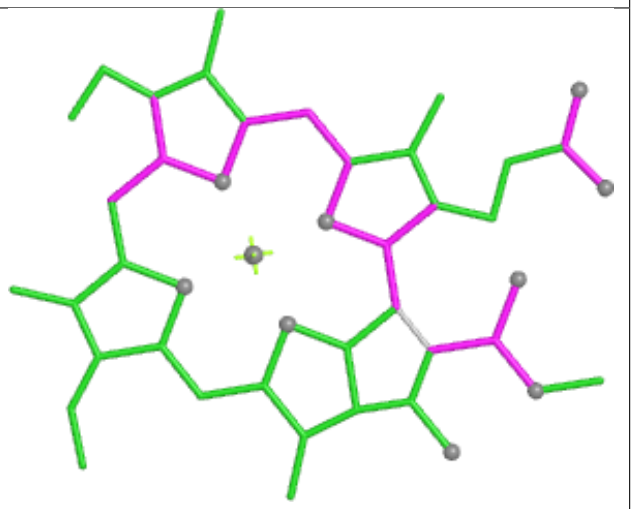


Rings

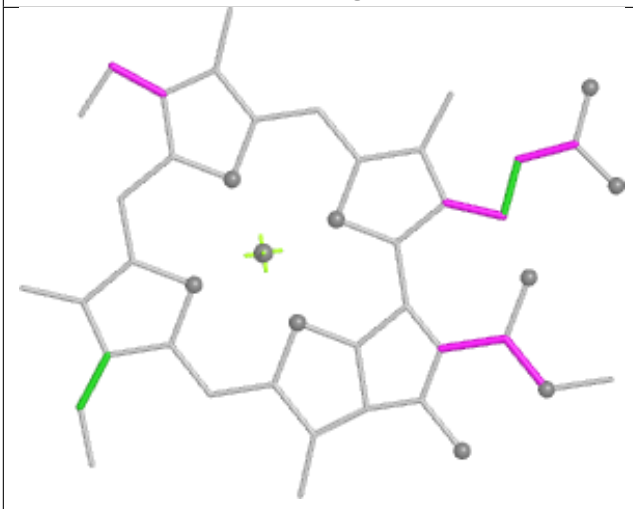
Ligand CLA bK 101



Bond lengths



Bond angles

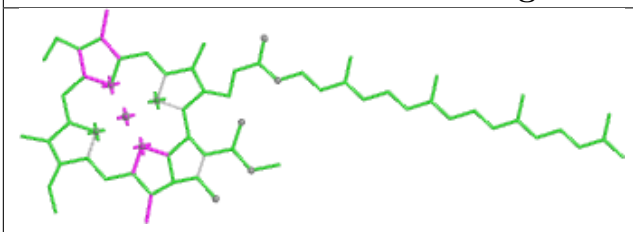


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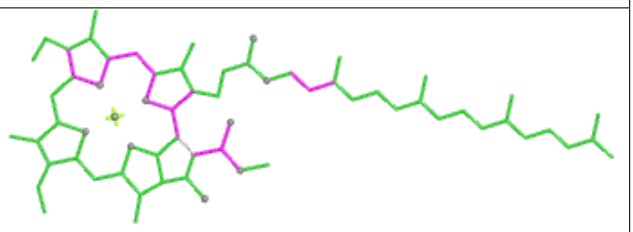


Rings

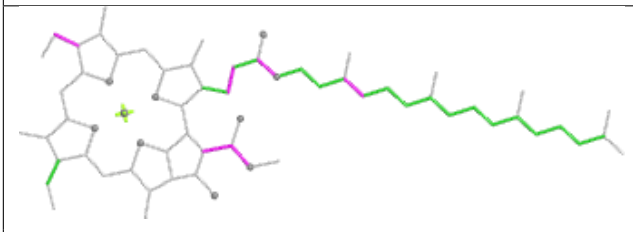
Ligand CLA b5 404



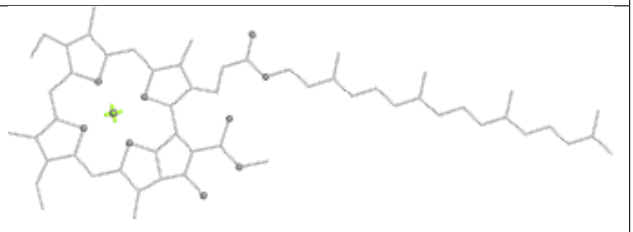
Bond lengths



Bond angles

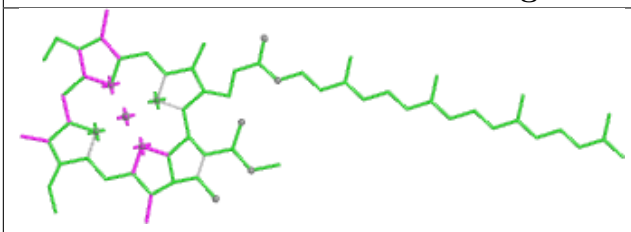


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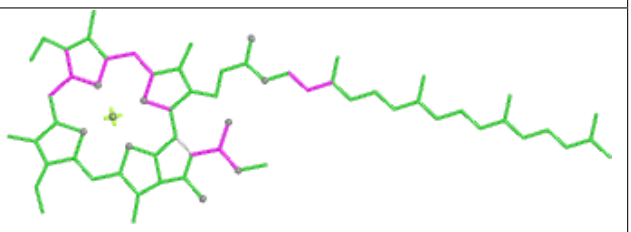


Rings

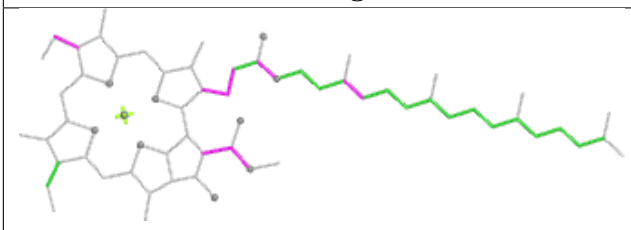
Ligand CLA c4 404



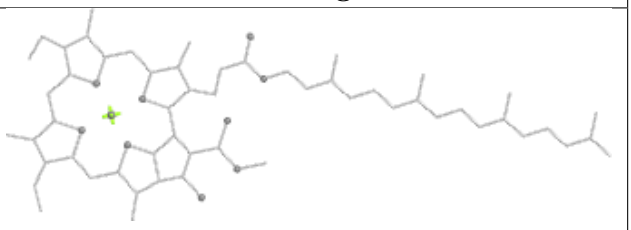
Bond lengths



Bond angles

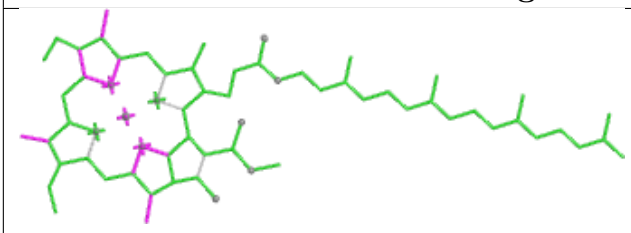


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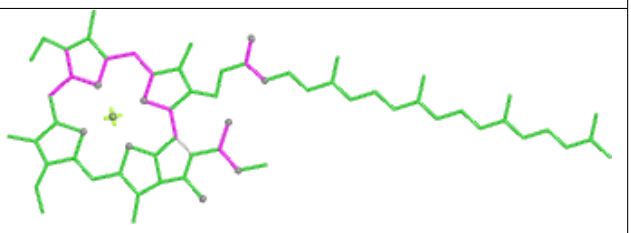


Rings

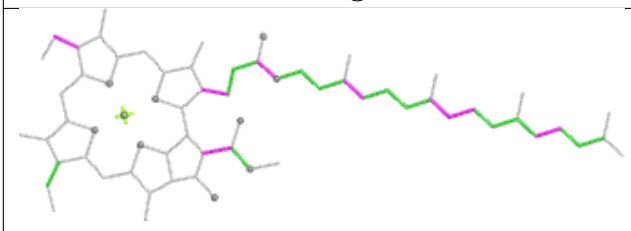
Ligand CLA aL 201



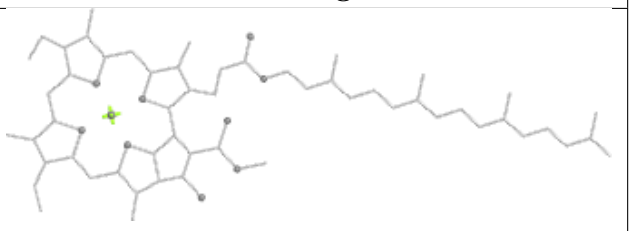
Bond lengths



Bond angles

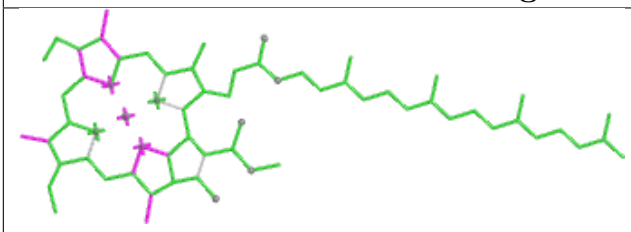


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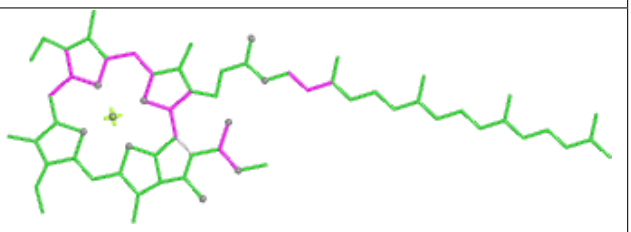


Rings

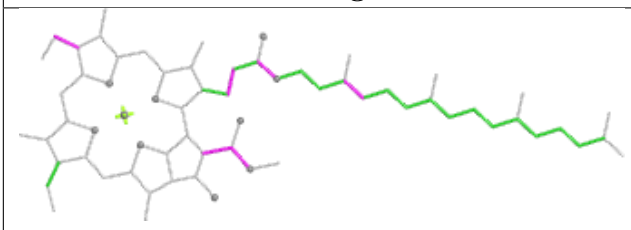
Ligand CLA a6 405



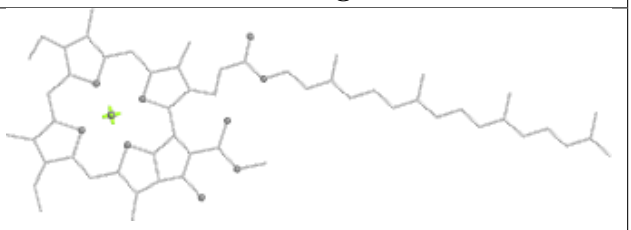
Bond lengths



Bond angles

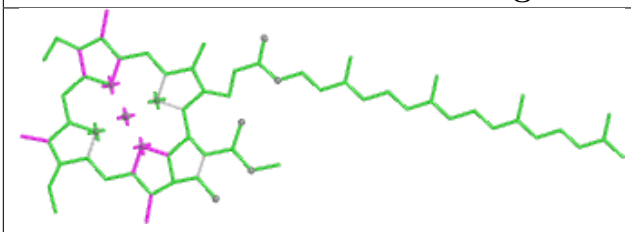


Torsions

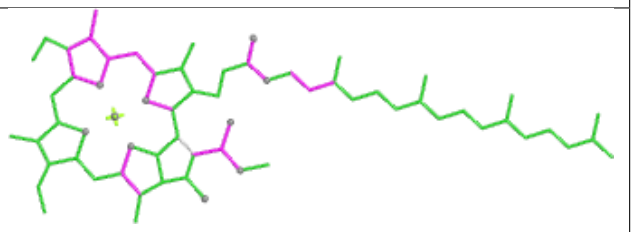


Rings

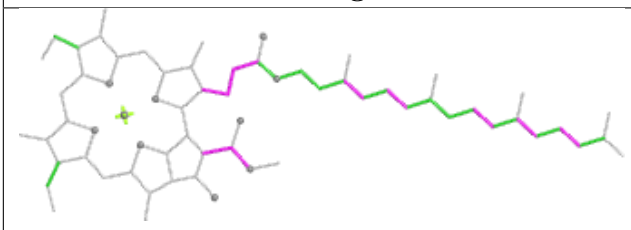
Ligand CLA bA 830



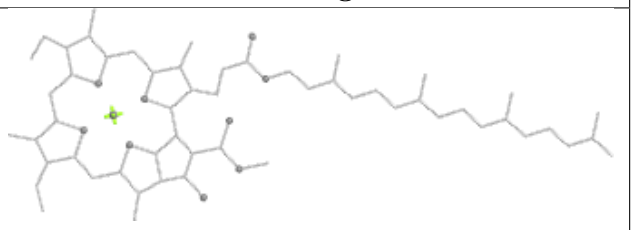
Bond lengths



Bond angles

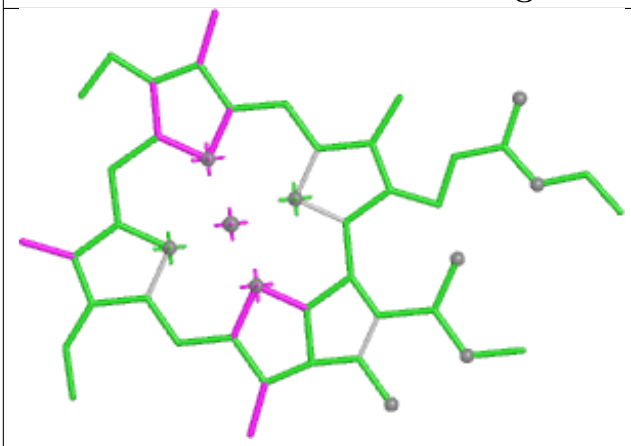


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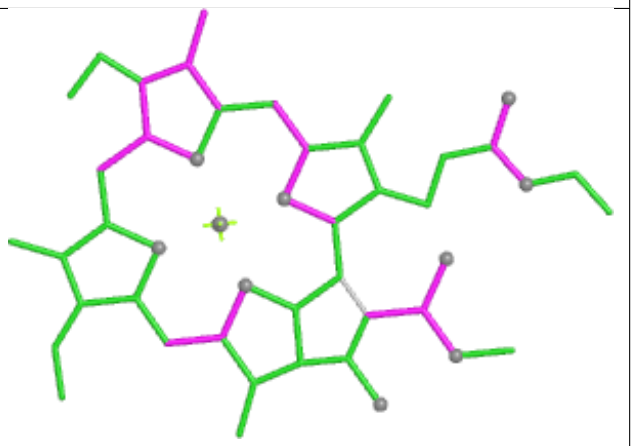


Rings

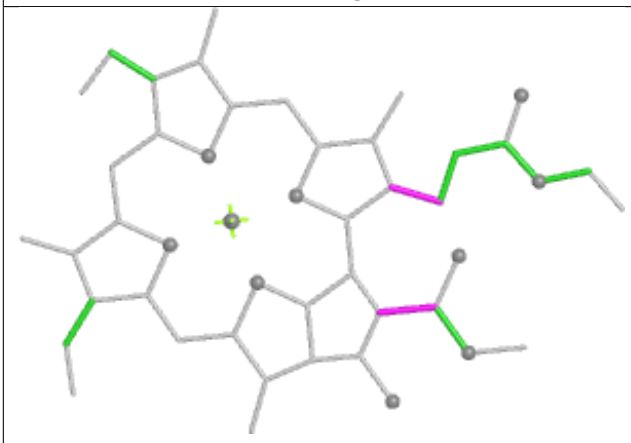
Ligand CLA aB 838



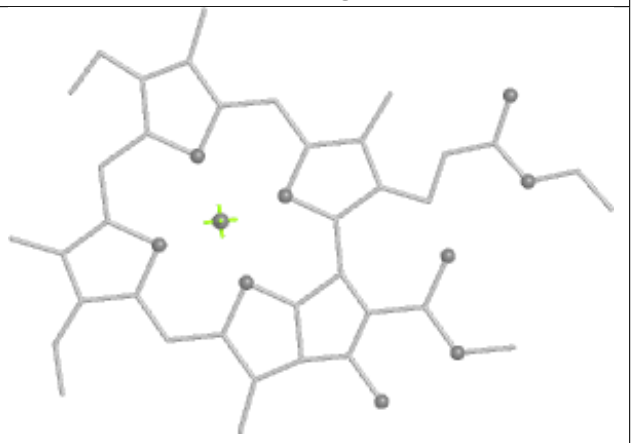
Bond lengths



Bond angles

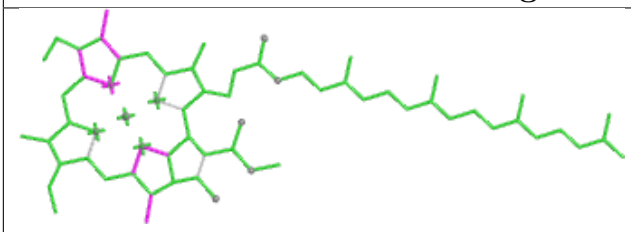


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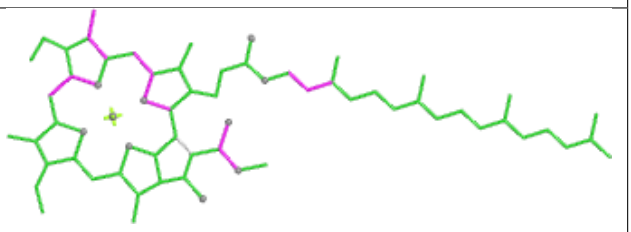


Rings

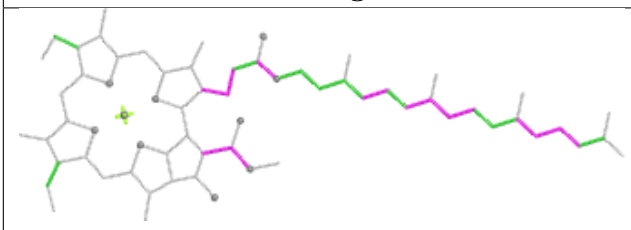
Ligand CLA a2 402



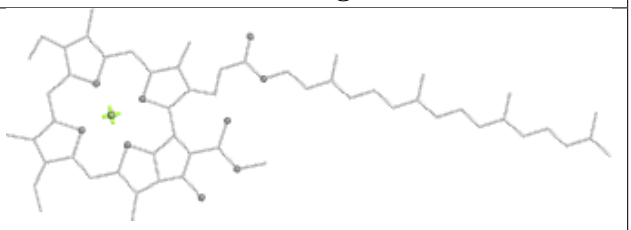
Bond lengths



Bond angles

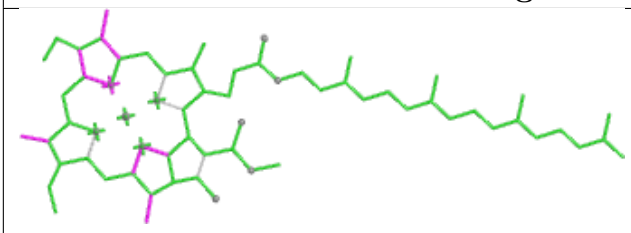


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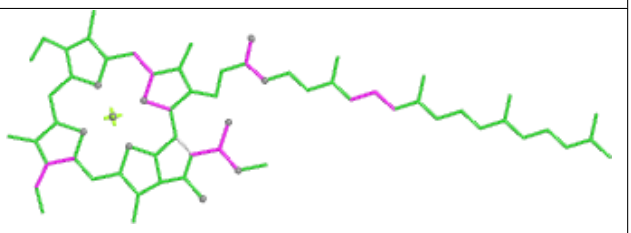


Rings

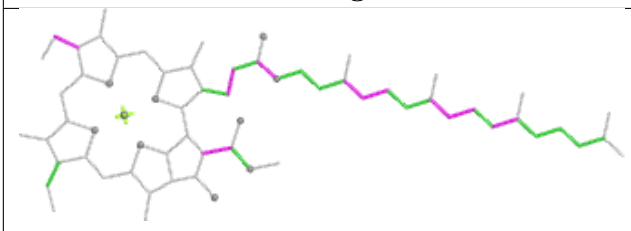
Ligand CLA aB 808



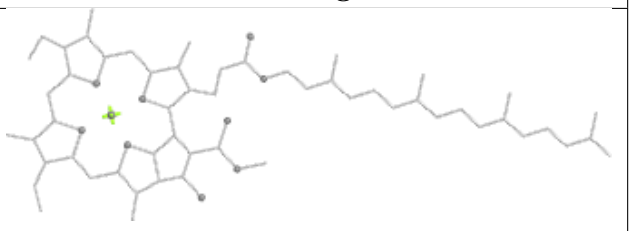
Bond lengths



Bond angles

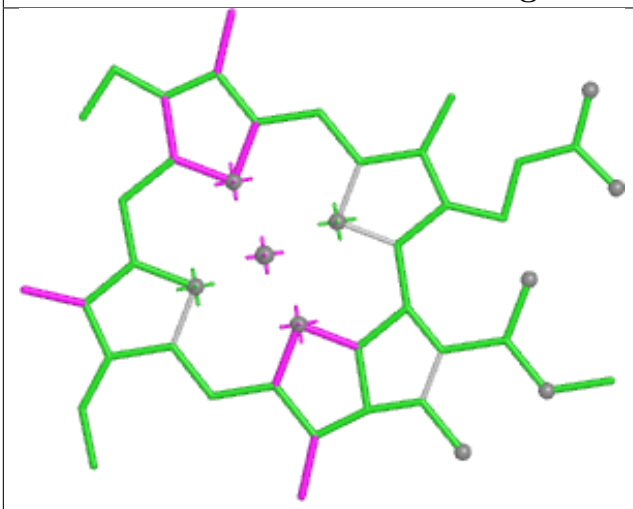


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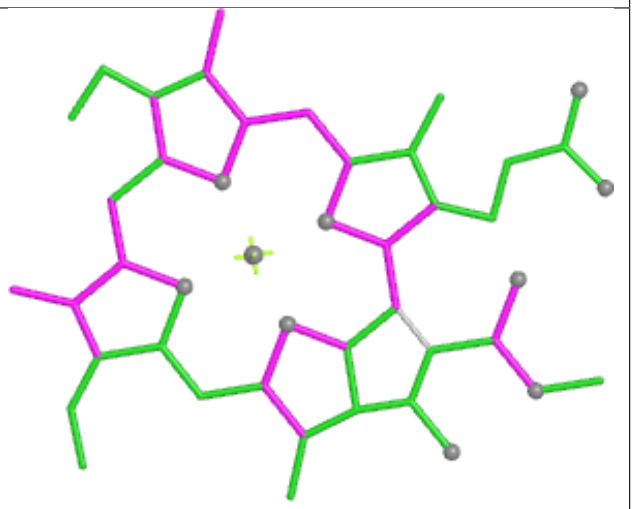


Rings

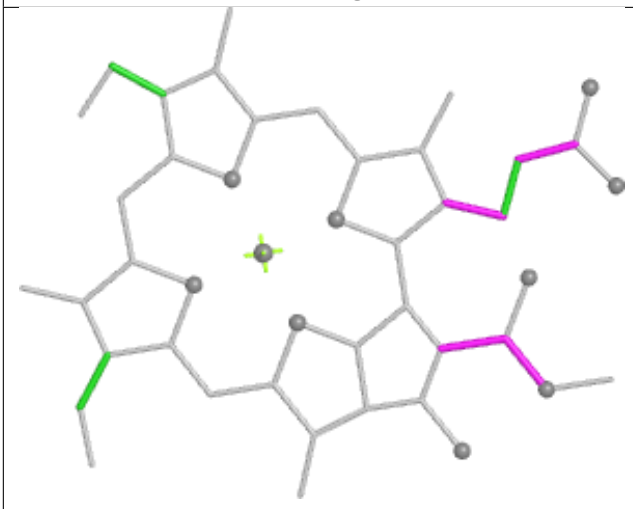
Ligand CLA a5 412



Bond lengths



Bond angles

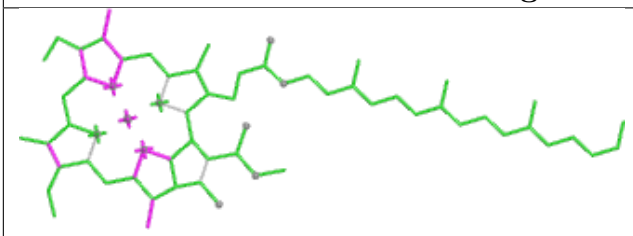


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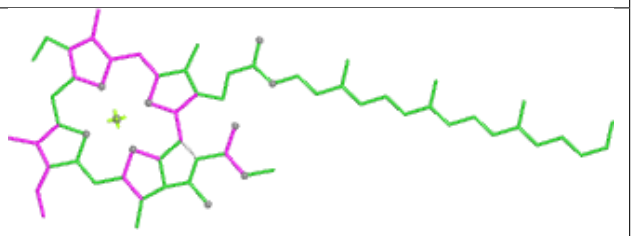


Rings

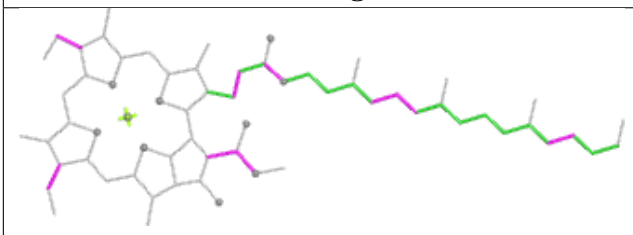
Ligand CLA c4 410



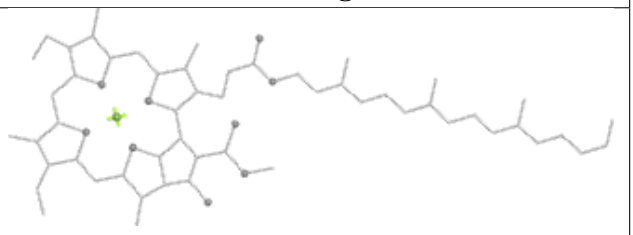
Bond lengths



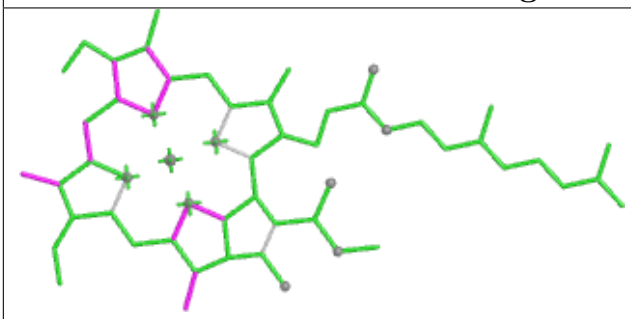
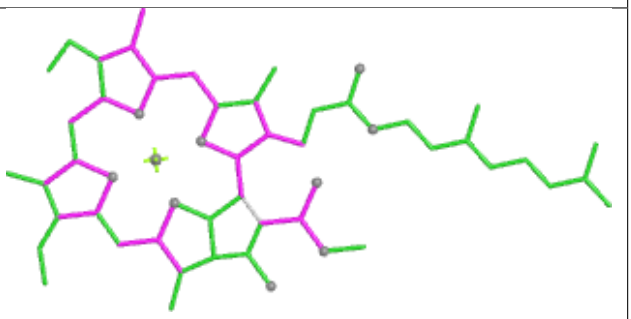
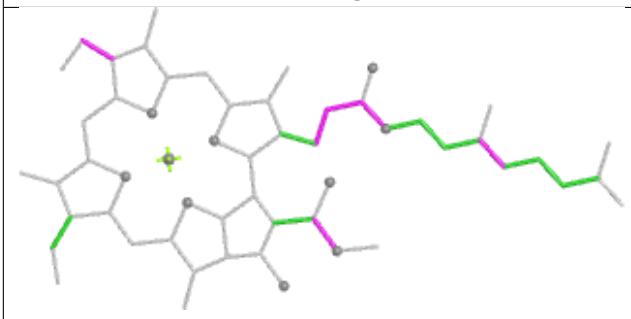
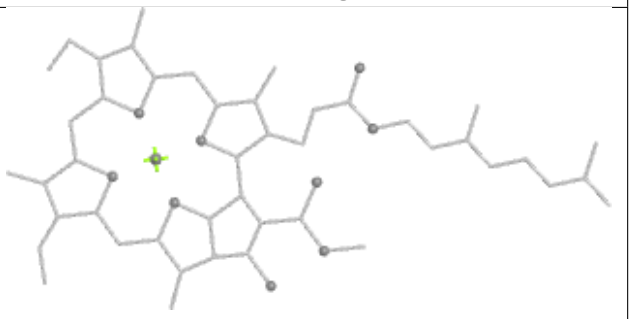
Bond angles

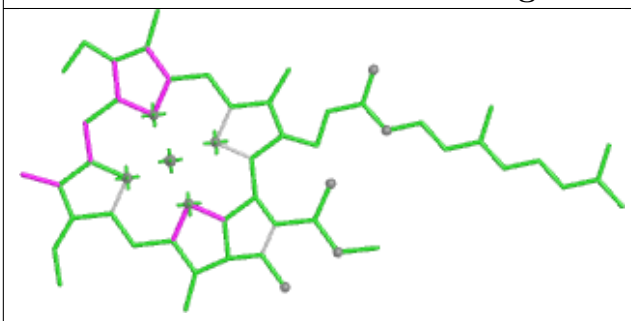
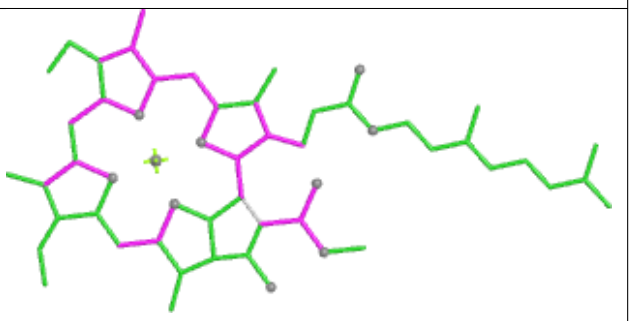
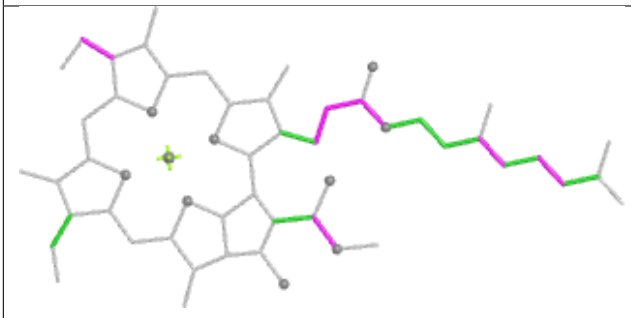
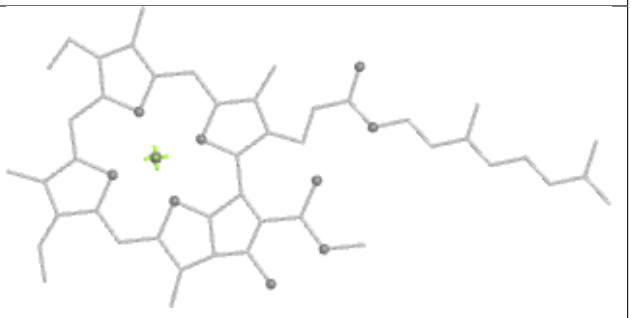


Torsions

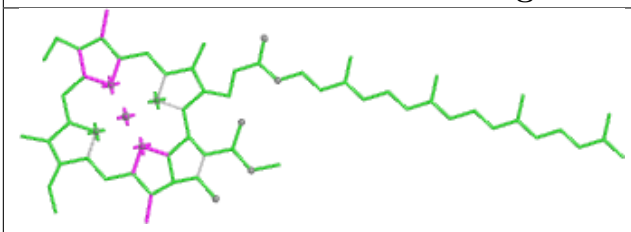


Rings

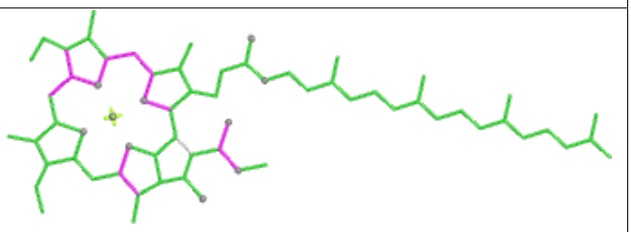
Ligand CLA a1 416	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b2 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

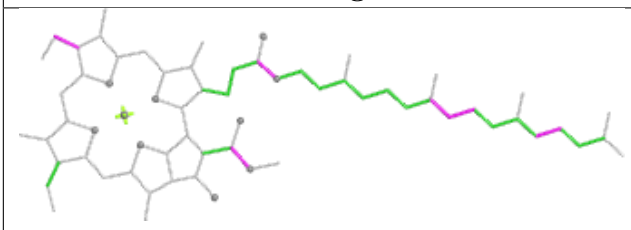
Ligand CLA cB 820



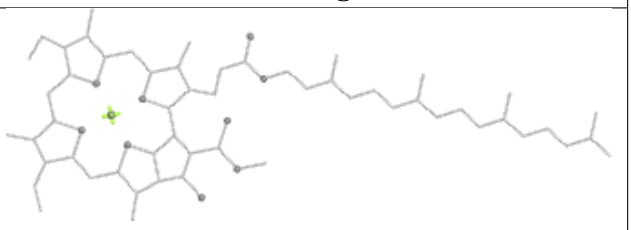
Bond lengths



Bond angles

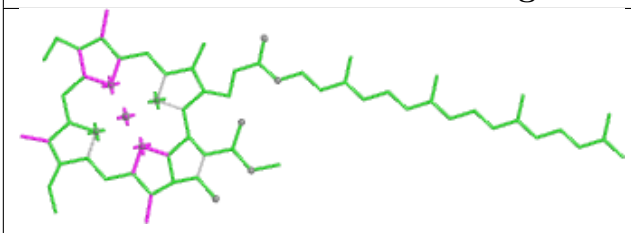


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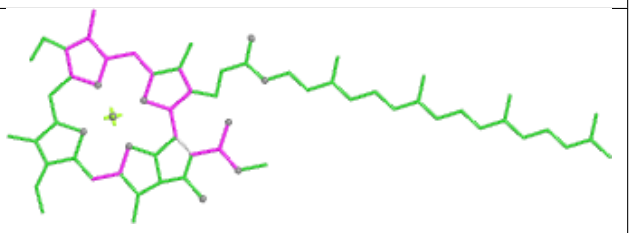


Rings

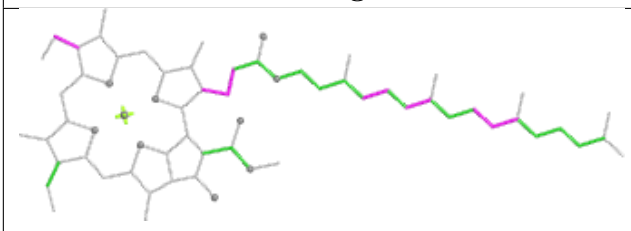
Ligand CLA cL 203



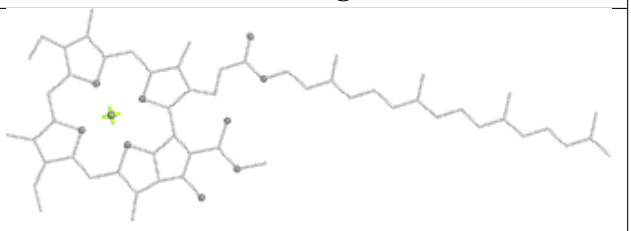
Bond lengths



Bond angles

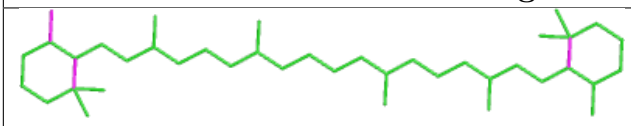


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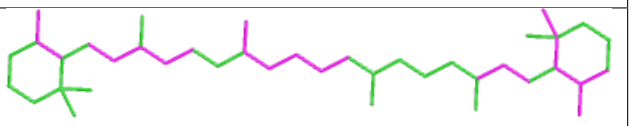


Rings

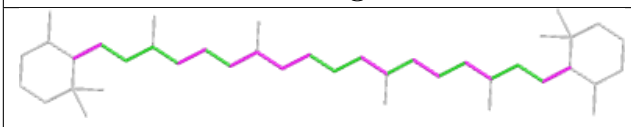
Ligand BCR cJ 103



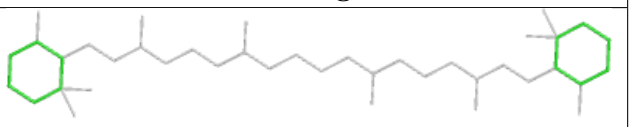
Bond lengths



Bond angles

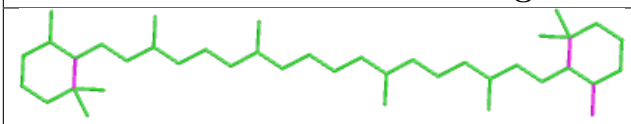


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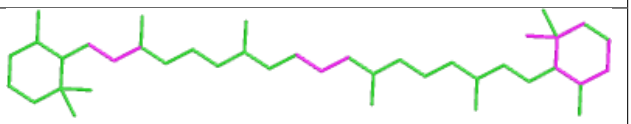


Rings

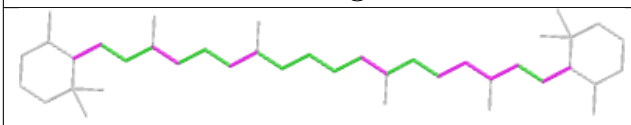
Ligand BCR cB 845



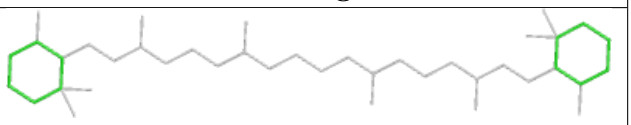
Bond lengths



Bond angles

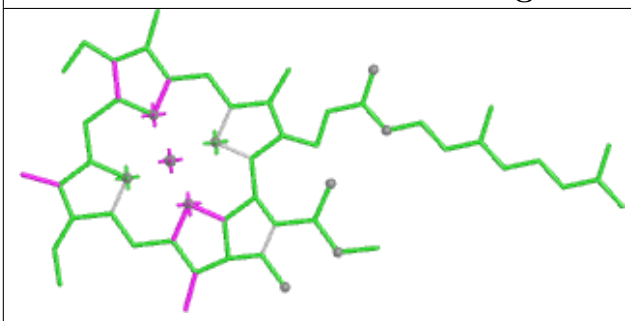


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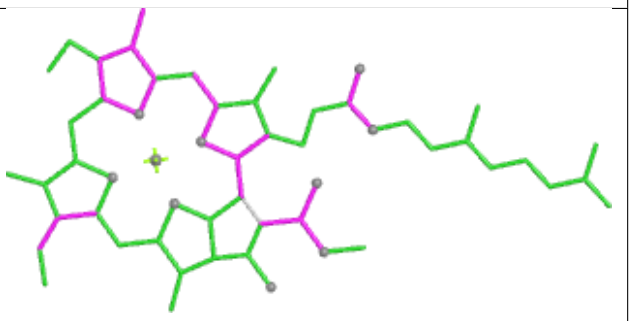


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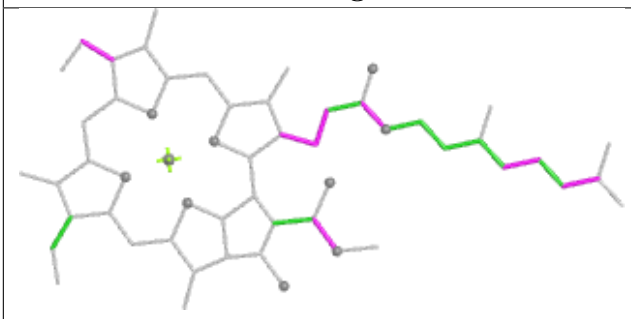
Ligand CLA aB 817



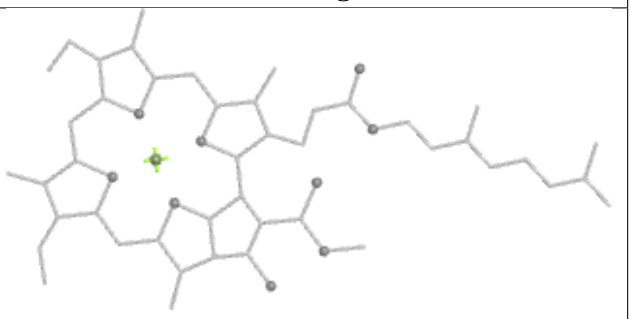
Bond lengths



Bond angles

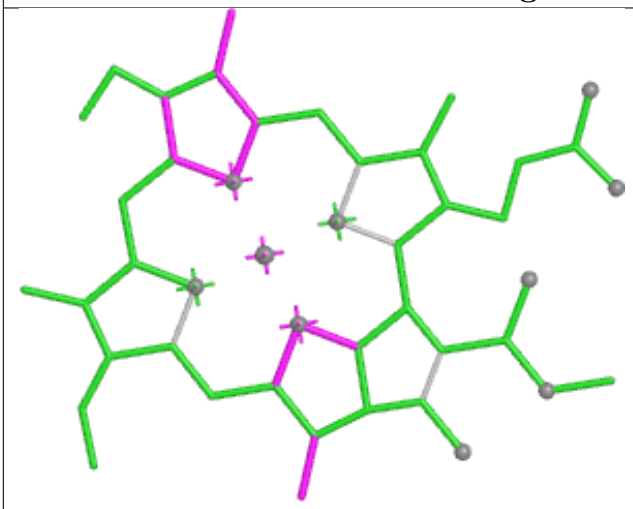


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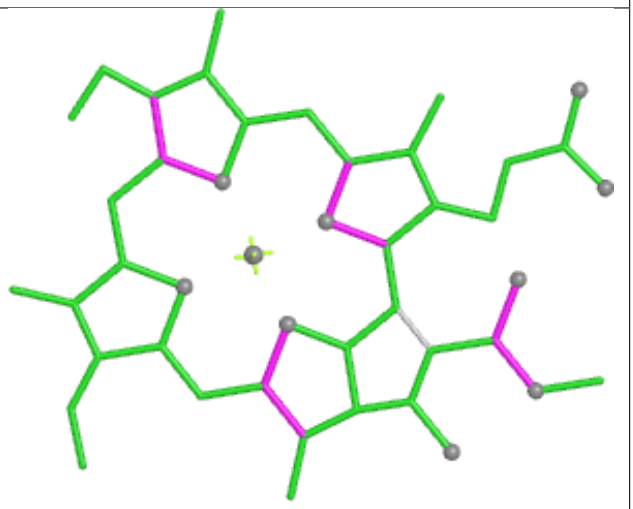


Rings

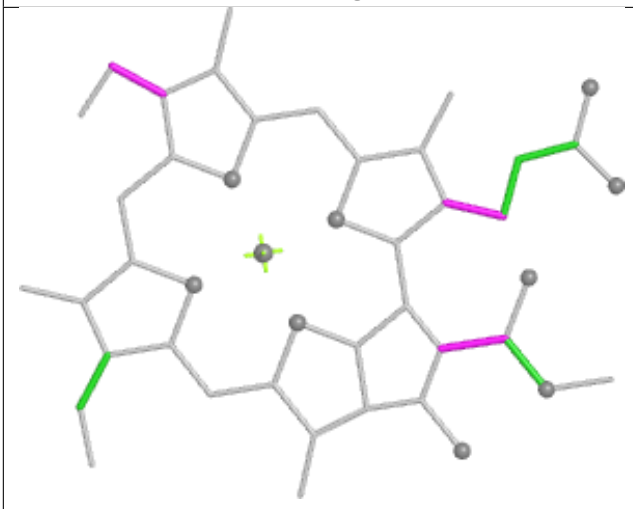
Ligand CLA a1 412



Bond lengths



Bond angles

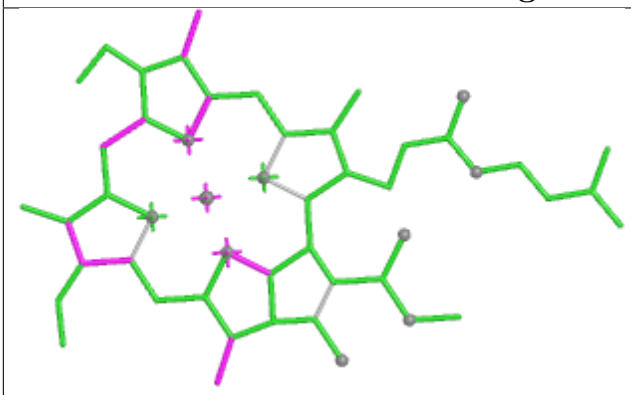


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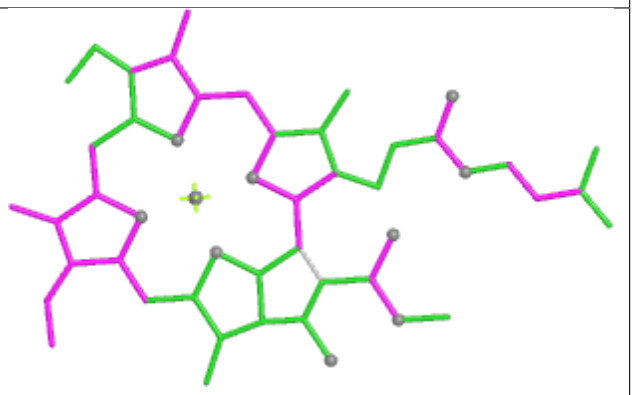


Rings

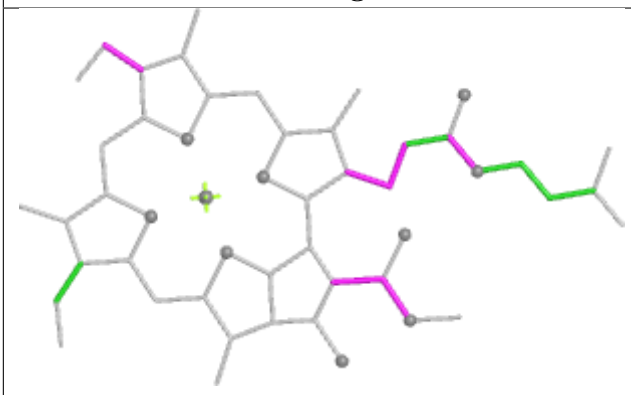
Ligand CLA b1 416



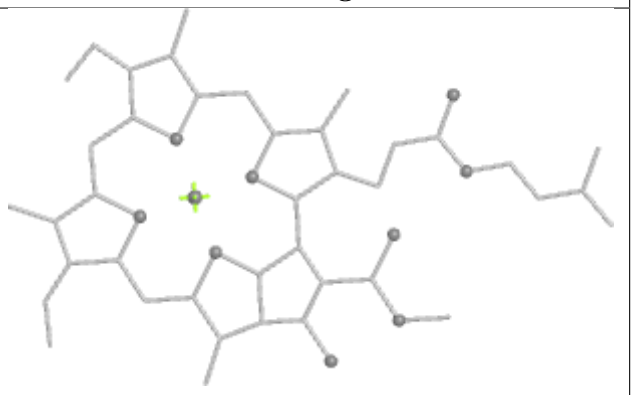
Bond lengths



Bond angles



Torsions

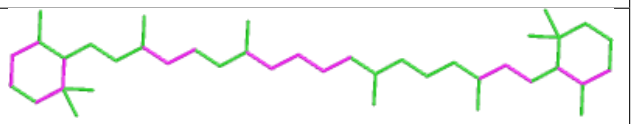


Rings

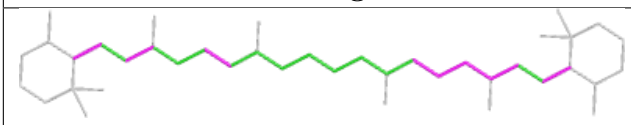
Ligand BCR a4 419



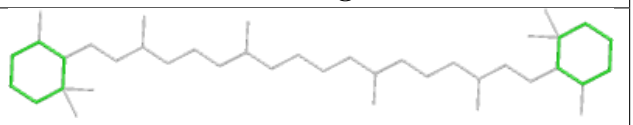
Bond lengths



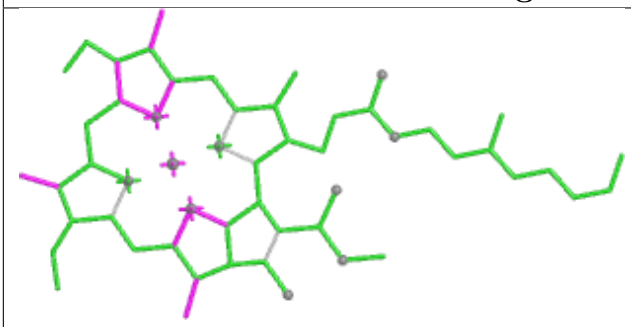
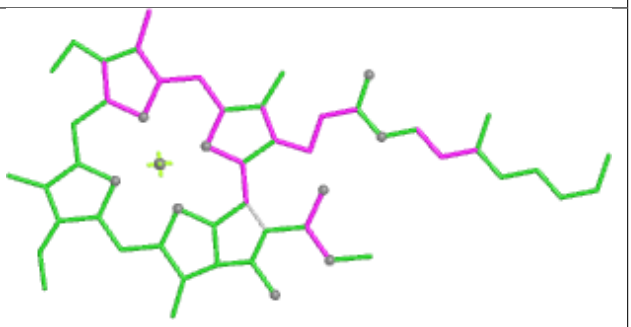
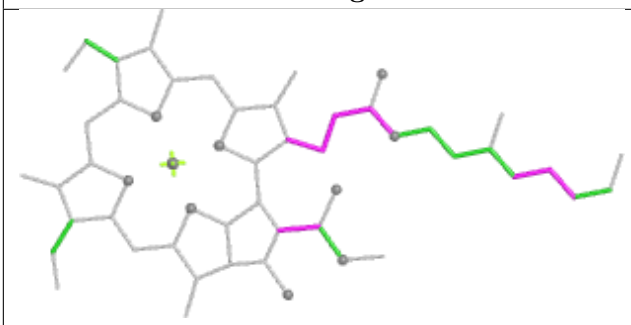
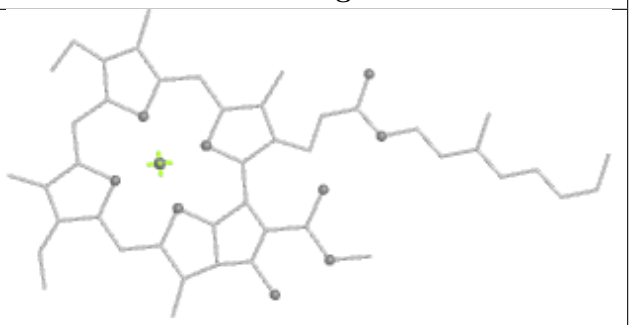
Bond angles

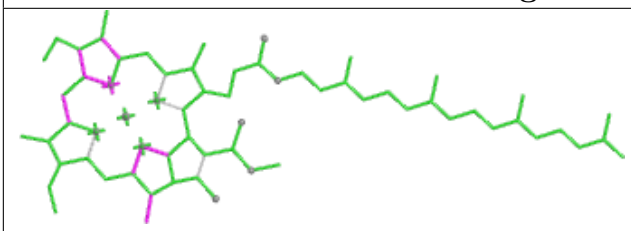
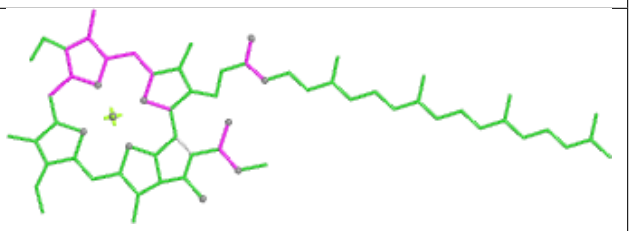
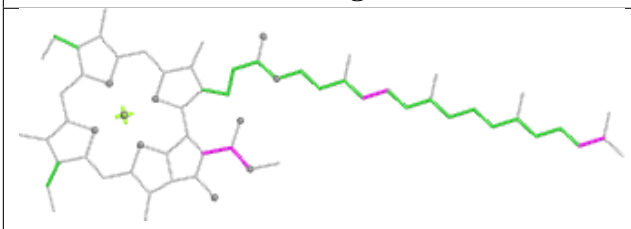
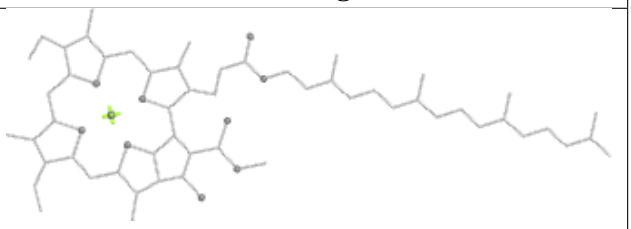


Torsions

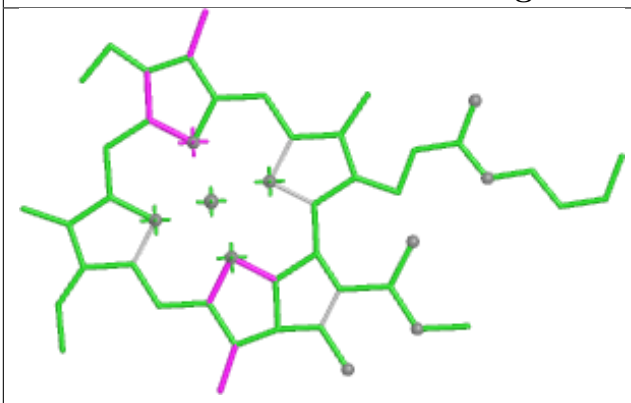


Rings

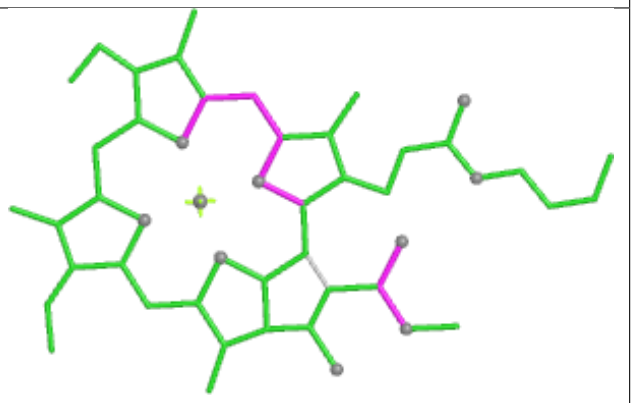
Ligand CLA cA 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a1 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

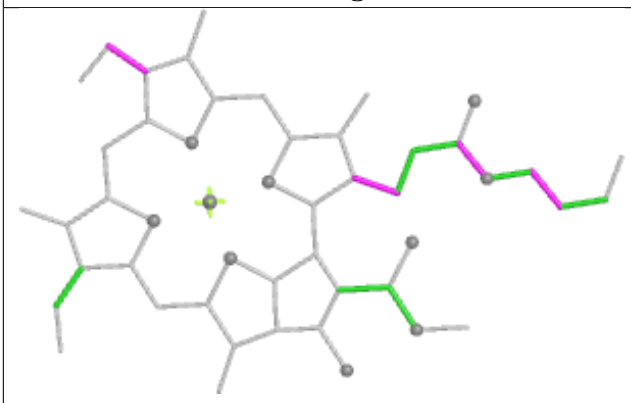
Ligand CLA aA 817



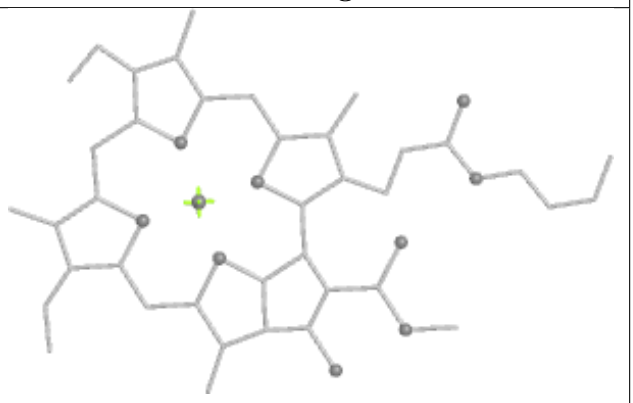
Bond lengths



Bond angles

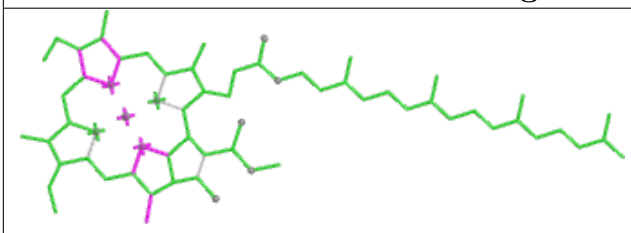


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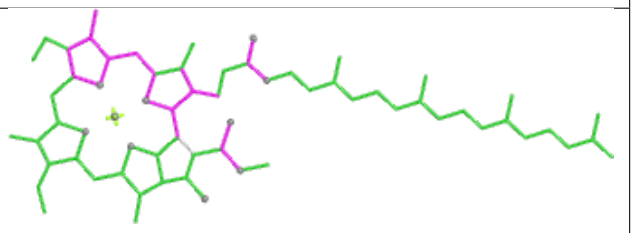


Rings

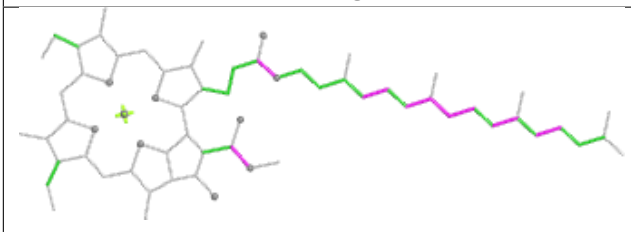
Ligand CLA c3 403



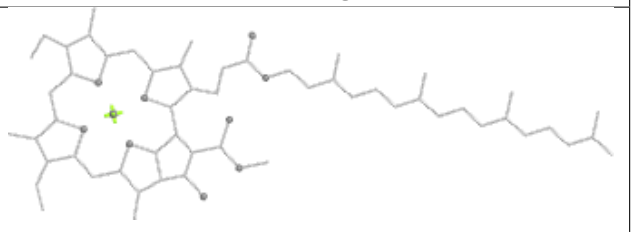
Bond lengths



Bond angles

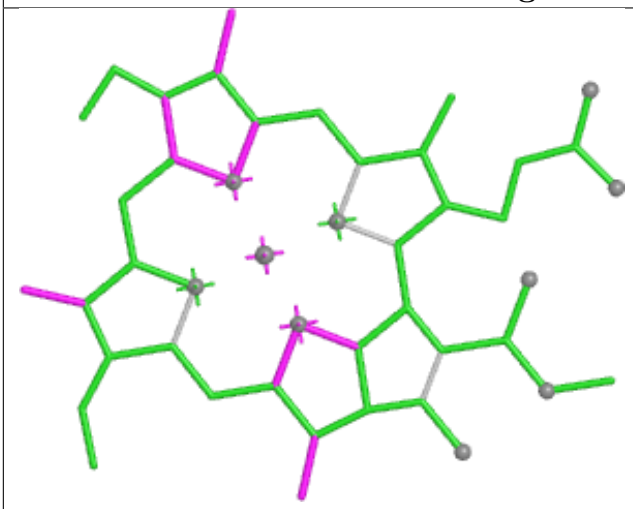


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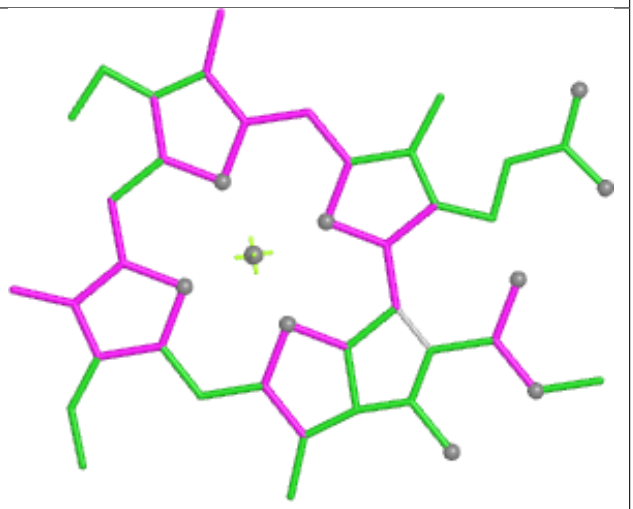


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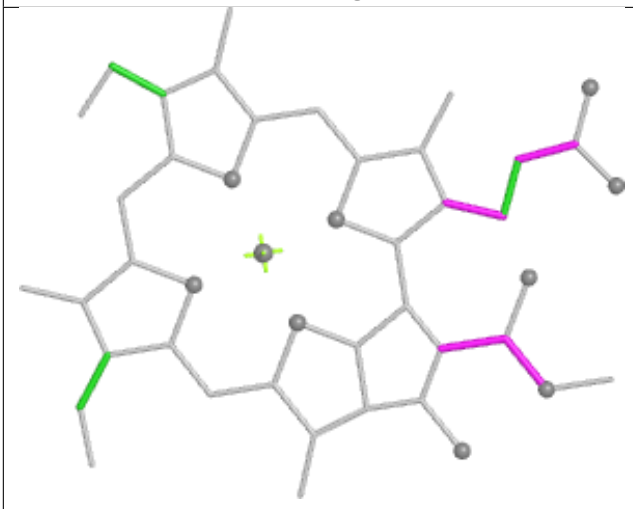
Ligand CLA b1 412



Bond lengths



Bond angles

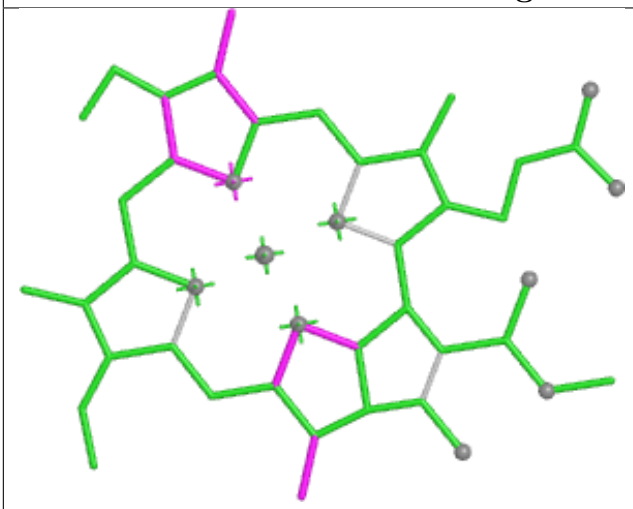


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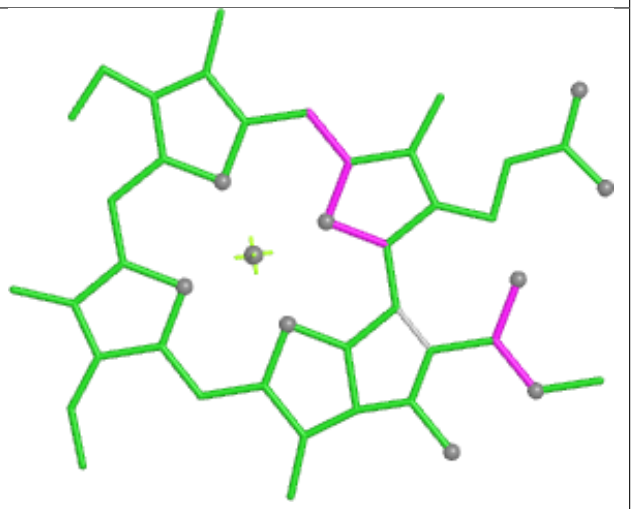


Rings

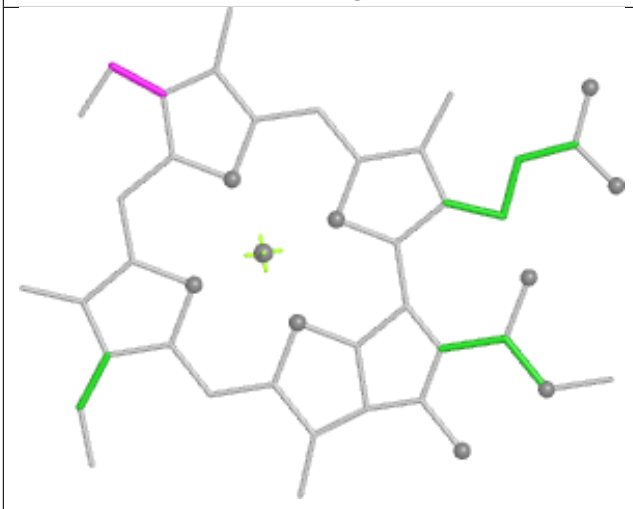
Ligand CLA aB 842



Bond lengths



Bond angles

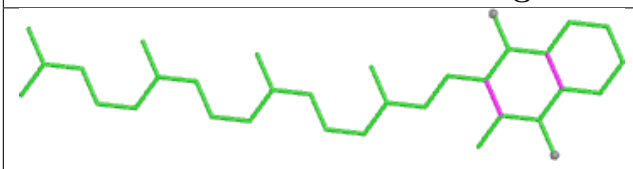


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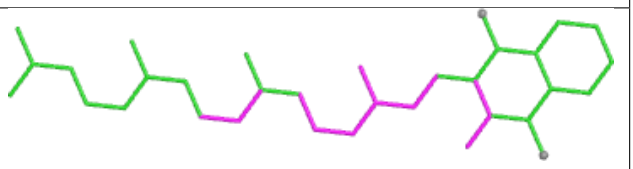


Rings

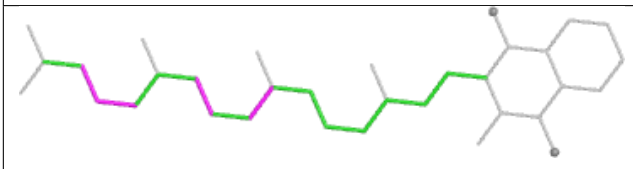
Ligand PQN cA 845



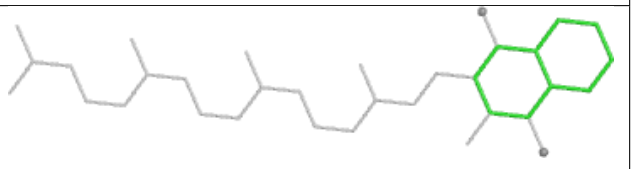
Bond lengths



Bond angles

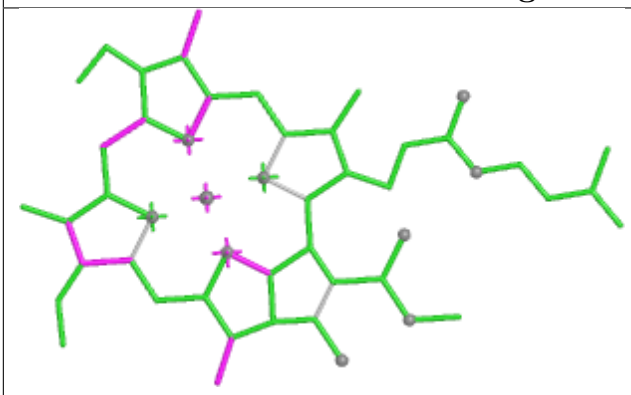


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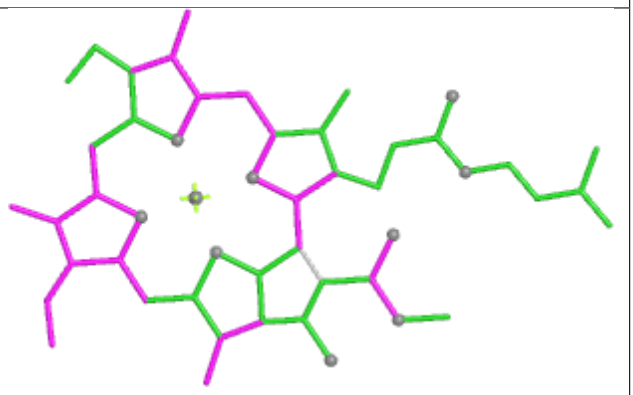


Rings

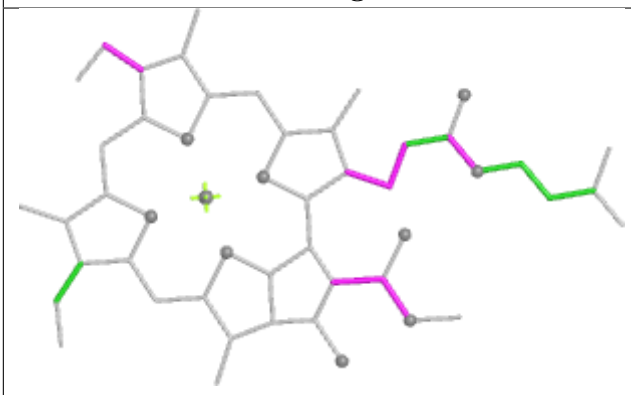
Ligand CLA b4 416



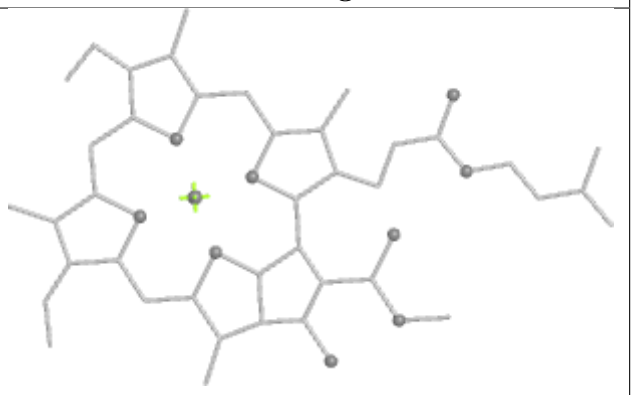
Bond lengths



Bond angles

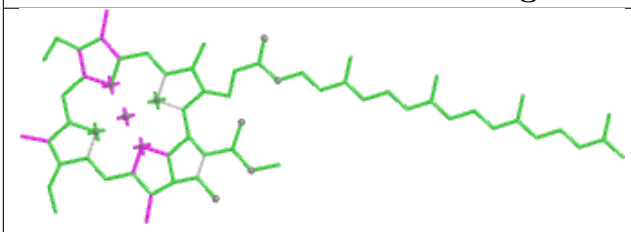


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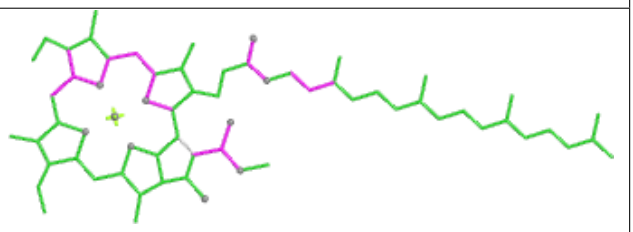


Rings

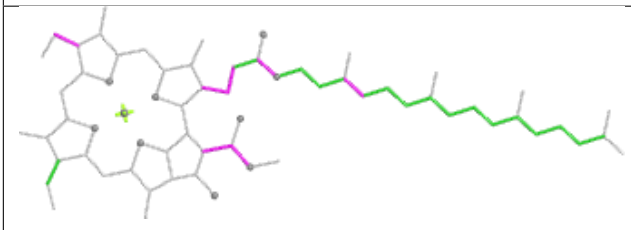
Ligand CLA a2 404



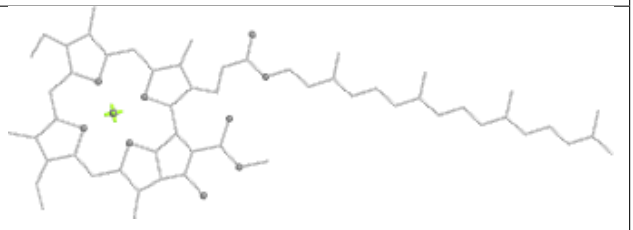
Bond lengths



Bond angles

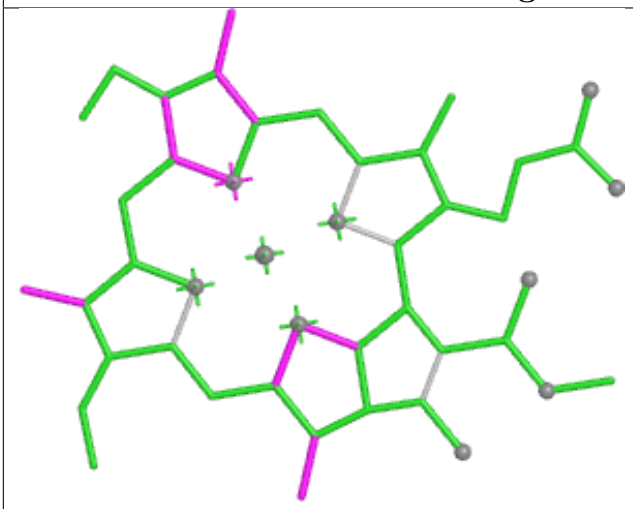


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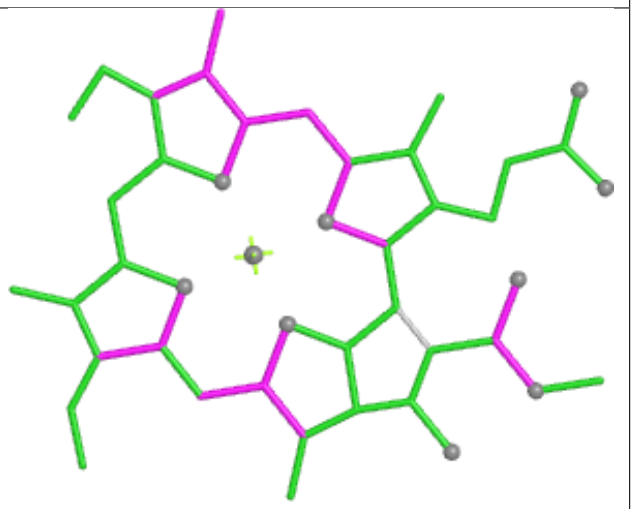


Rings

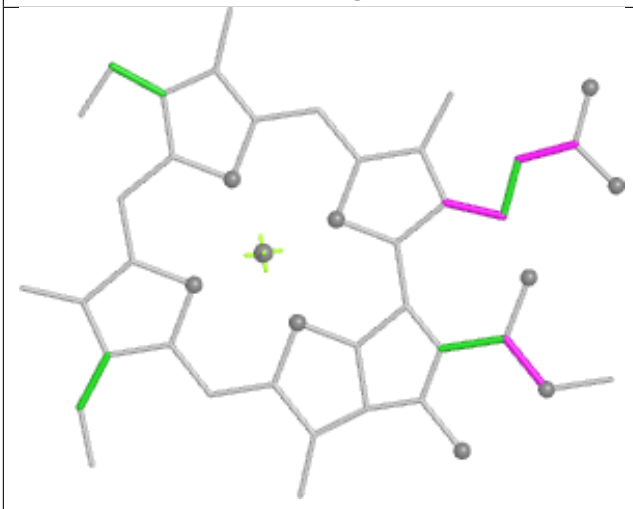
Ligand CLA b1 408



Bond lengths



Bond angles

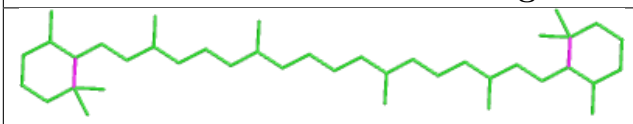


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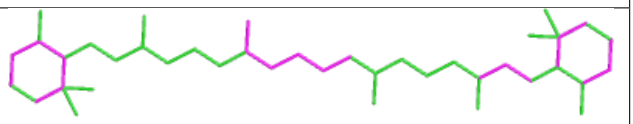


Rings

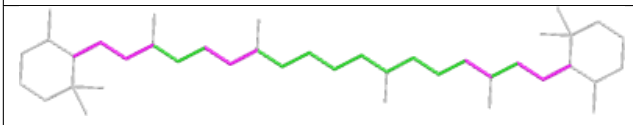
Ligand BCR c2 421



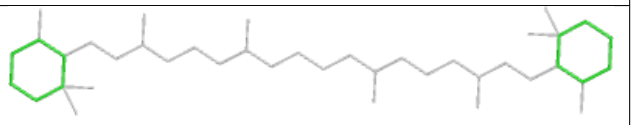
Bond lengths



Bond angles

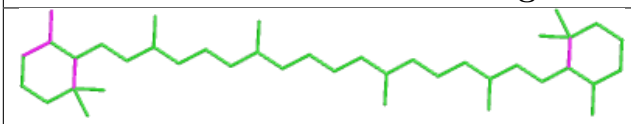


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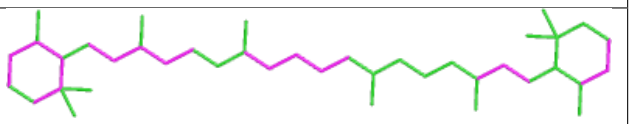


Rings

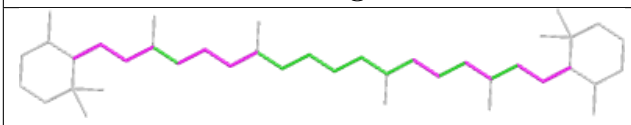
Ligand BCR c6 403



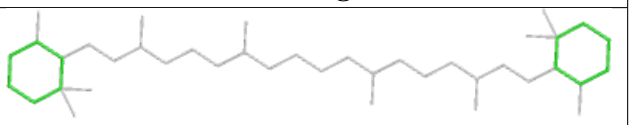
Bond lengths



Bond angles



Torsions

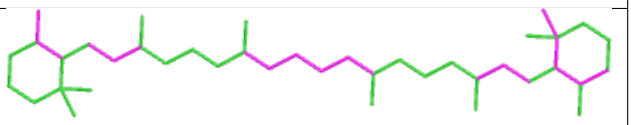


Rings

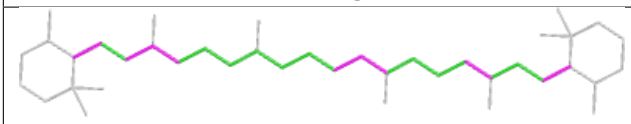
Ligand BCR aM 101



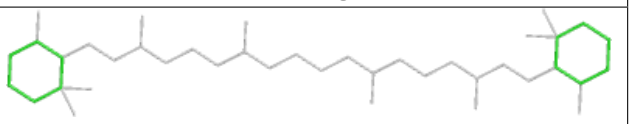
Bond lengths



Bond angles

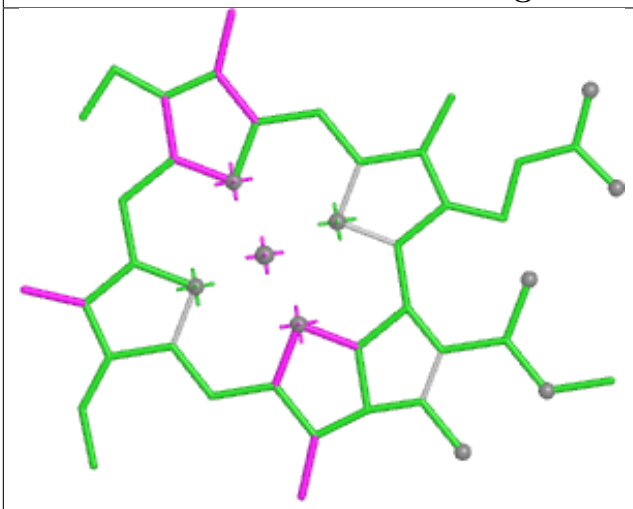


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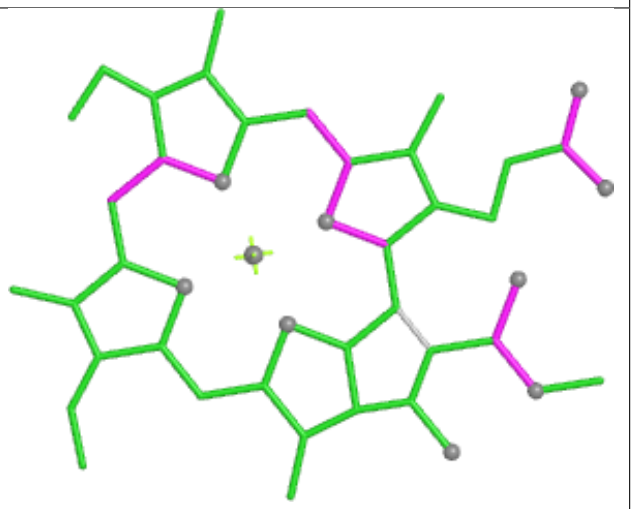


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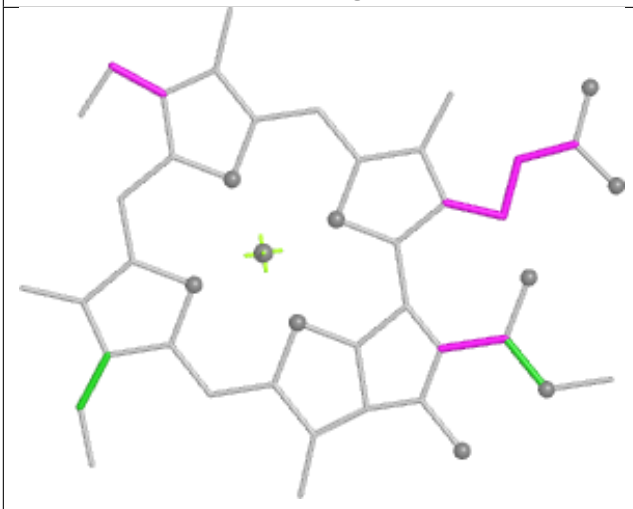
Ligand CLA bB 831



Bond lengths



Bond angles

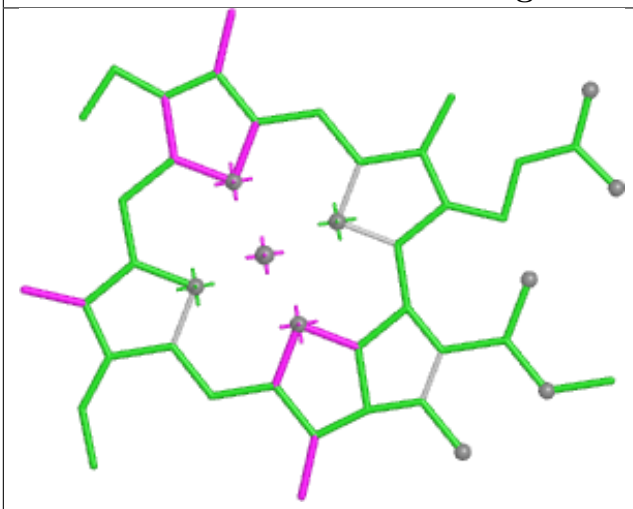


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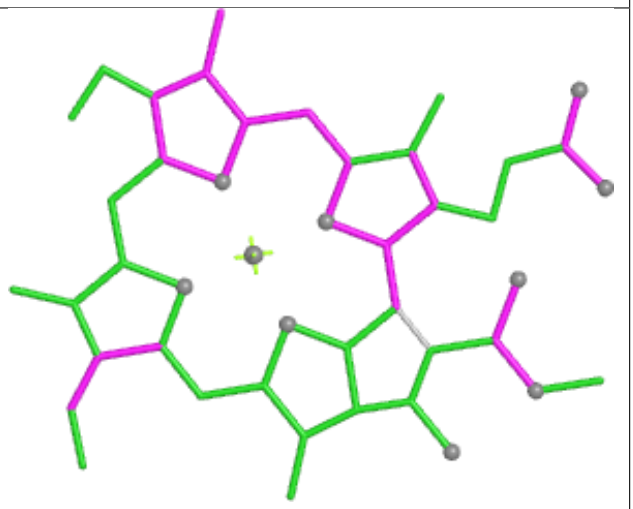


Rings

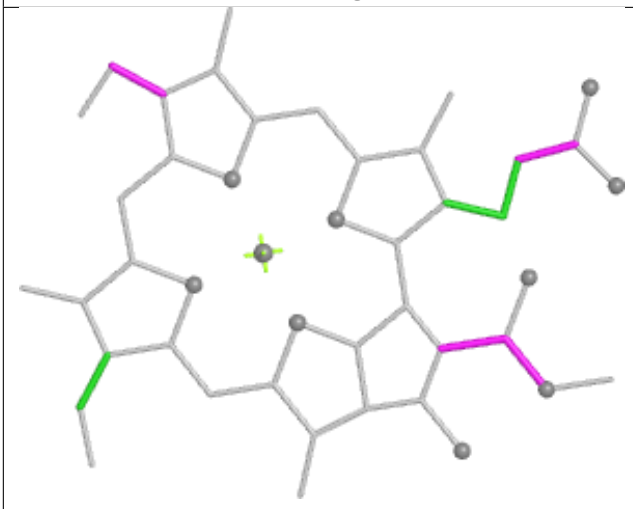
Ligand CLA bF 201



Bond lengths



Bond angles

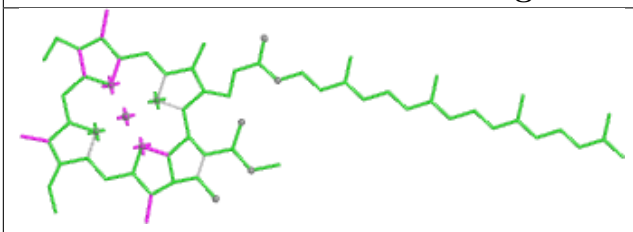


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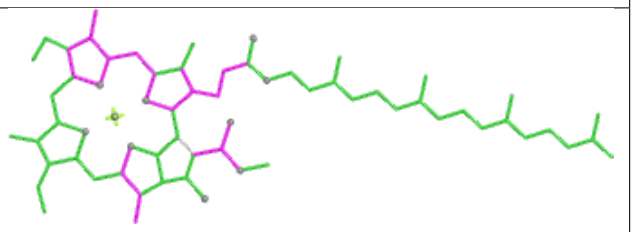


Rings

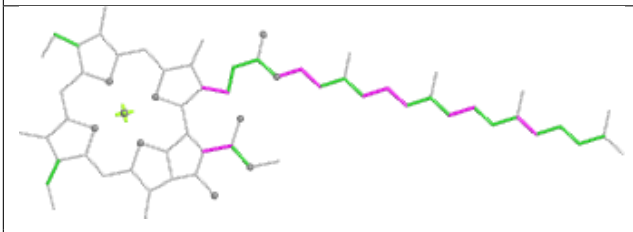
Ligand CLA aA 827



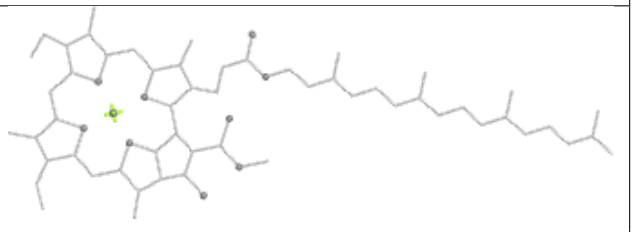
Bond lengths



Bond angles

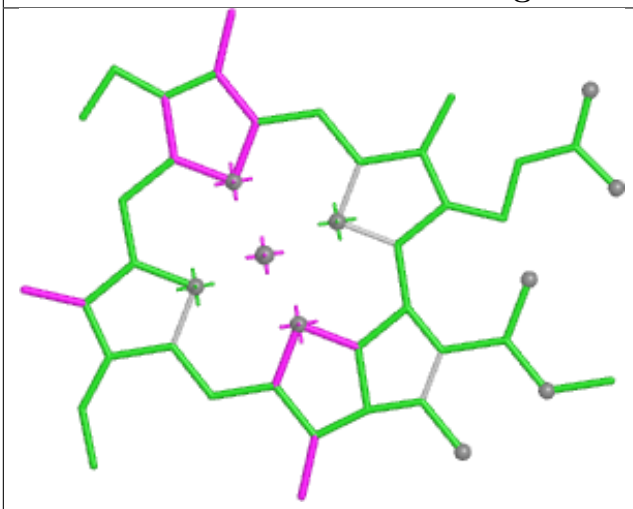


Torsions

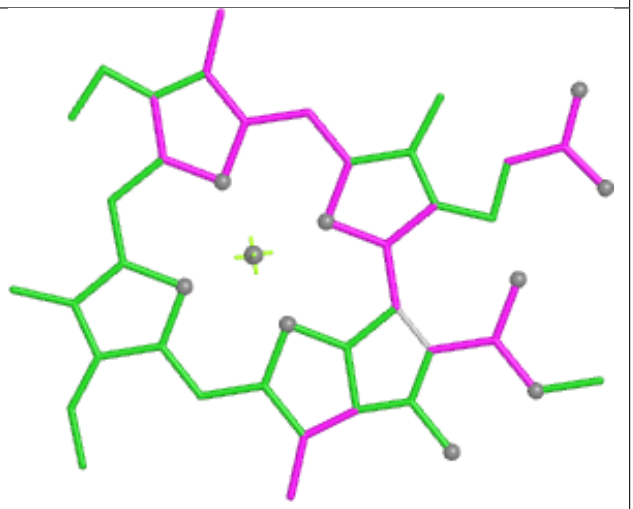


Rings

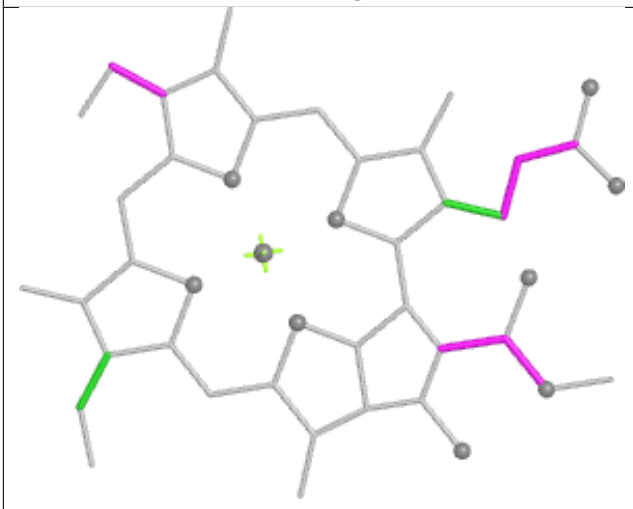
Ligand CLA bX 102



Bond lengths



Bond angles

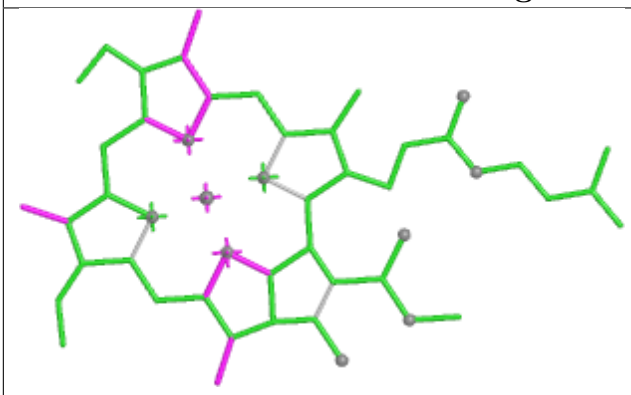


Torsions

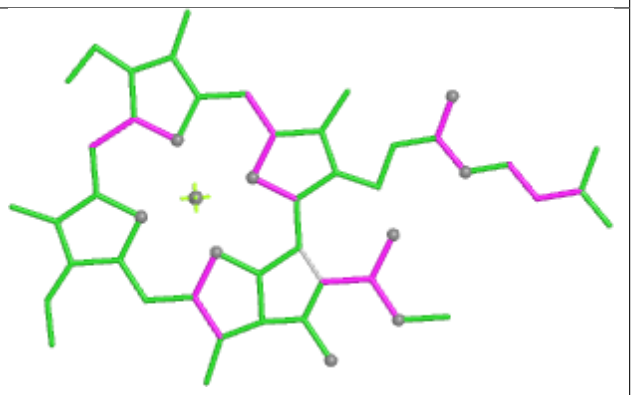


Rings

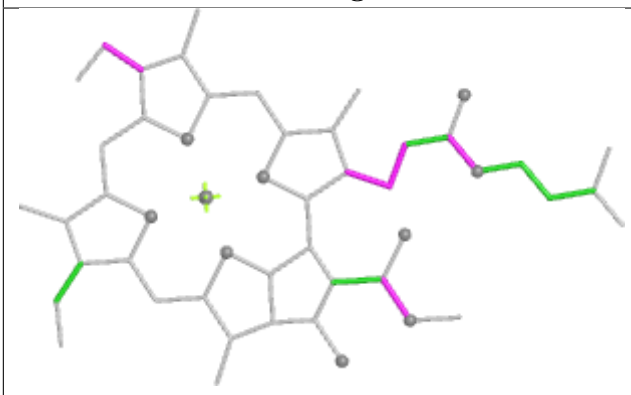
Ligand CLA aA 832



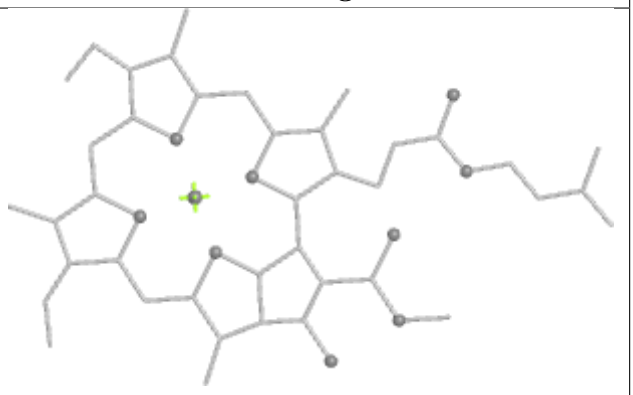
Bond lengths



Bond angles

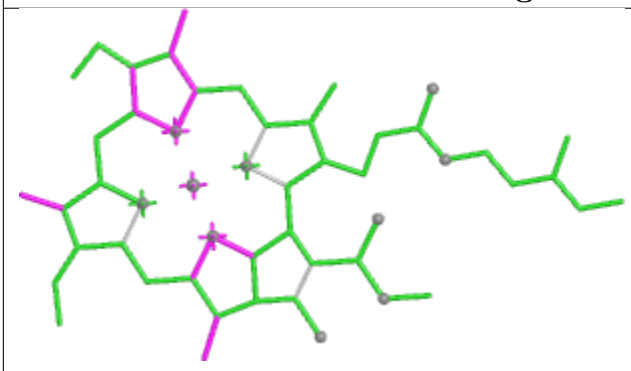


Torsions

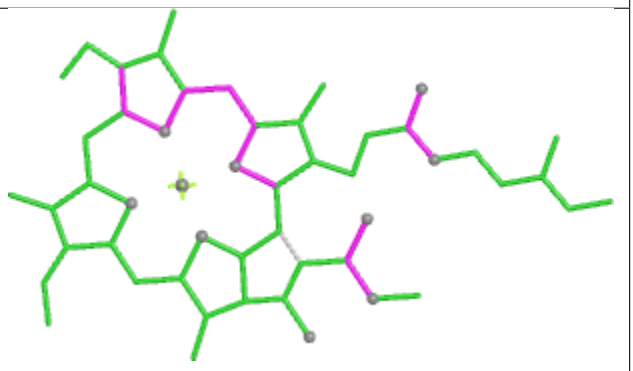


Rings

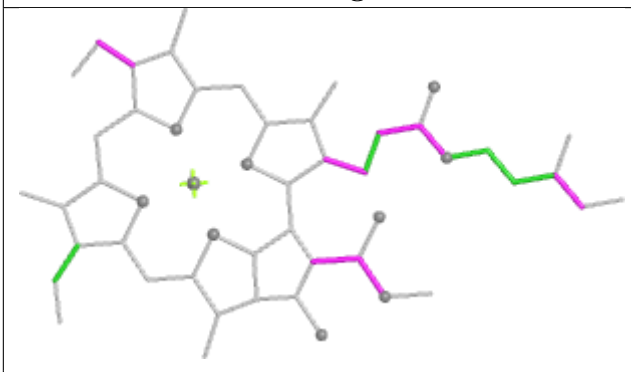
Ligand CLA cA 824



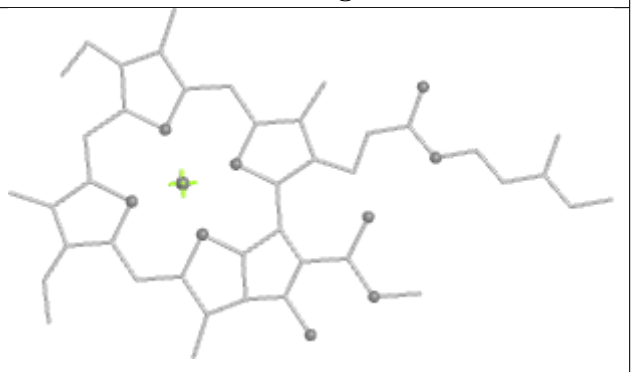
Bond lengths



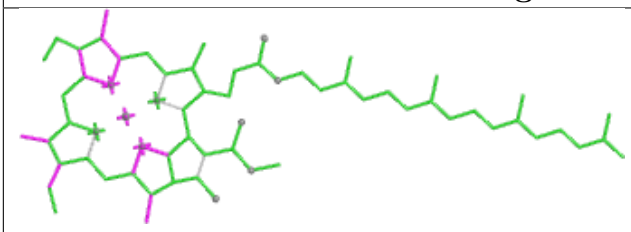
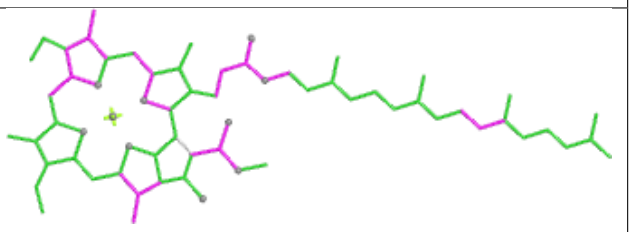
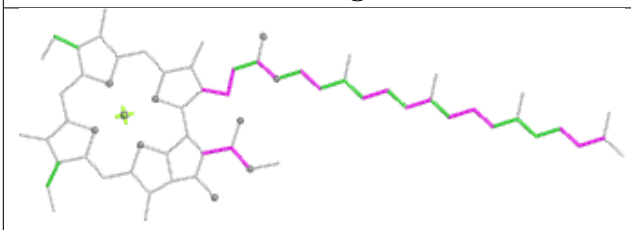
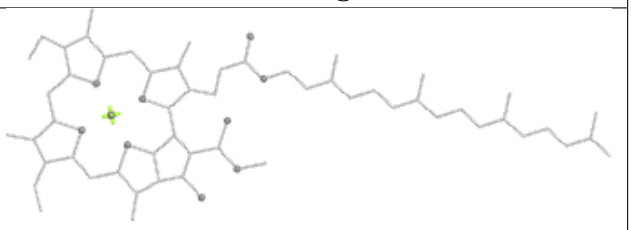
Bond angles



Torsions



Rings

Ligand CLA aA 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

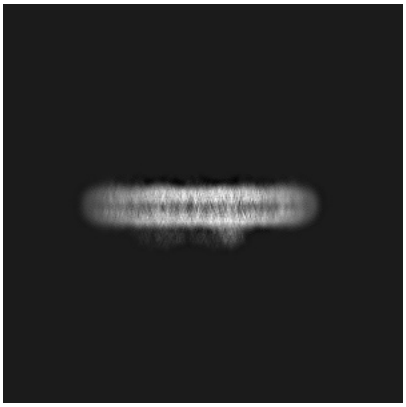
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9908. These allow visual inspection of the internal detail of the map and identification of artifacts.

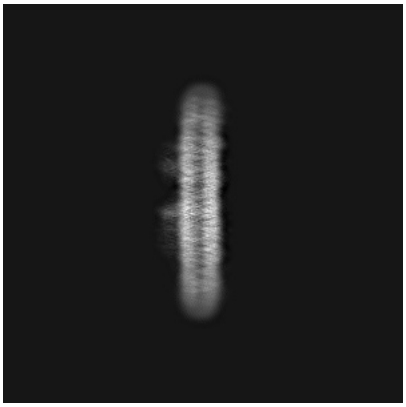
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

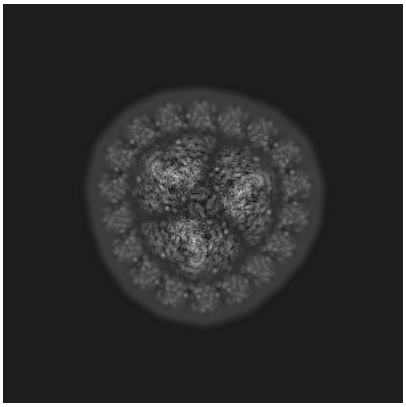
6.1.1 Primary map



X



Y

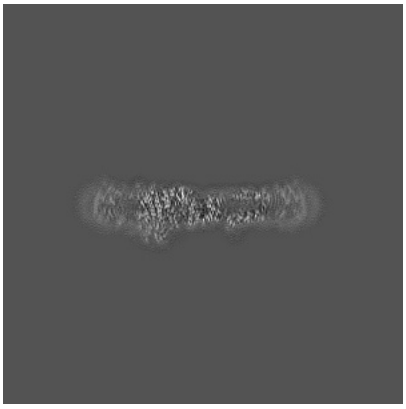


Z

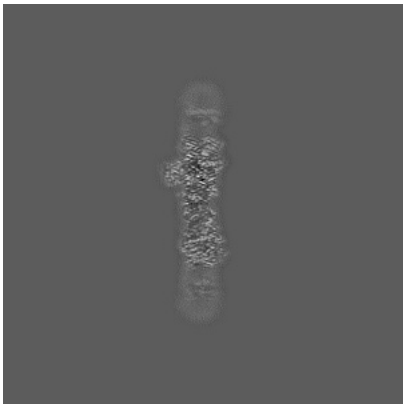
The images above show the map projected in three orthogonal directions.

6.2 Central slices

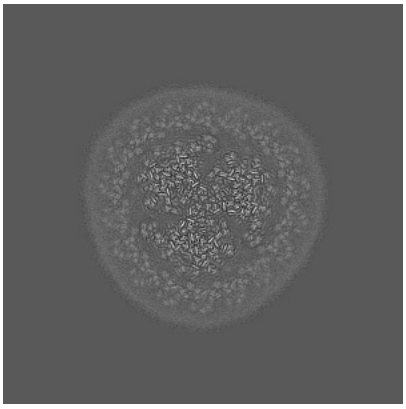
6.2.1 Primary map



X Index: 240



Y Index: 240

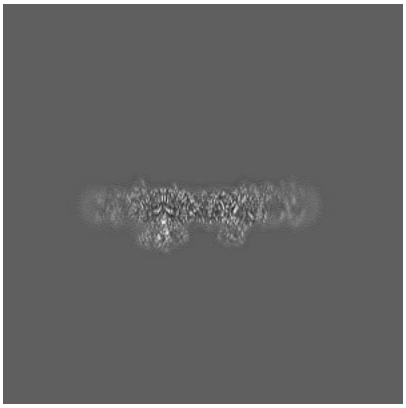


Z Index: 240

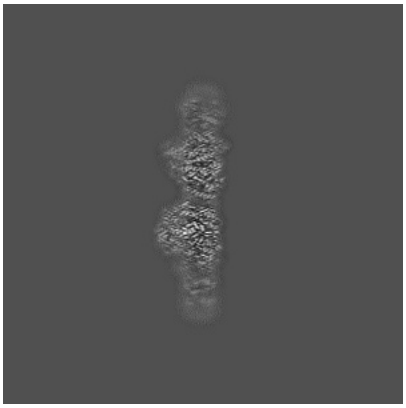
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

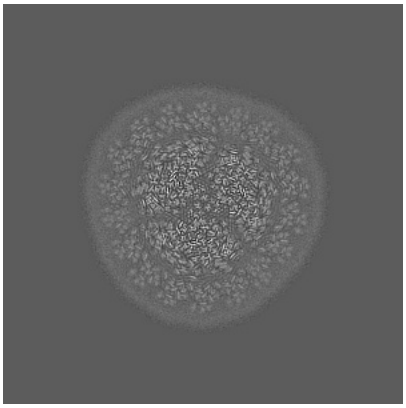
6.3.1 Primary map



X Index: 229



Y Index: 273

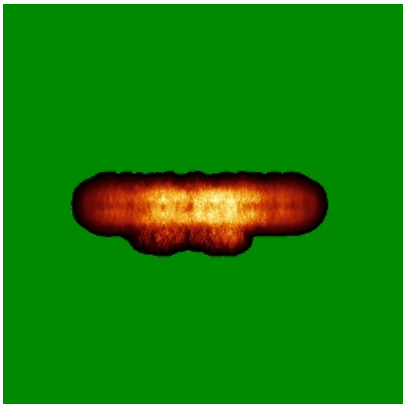


Z Index: 245

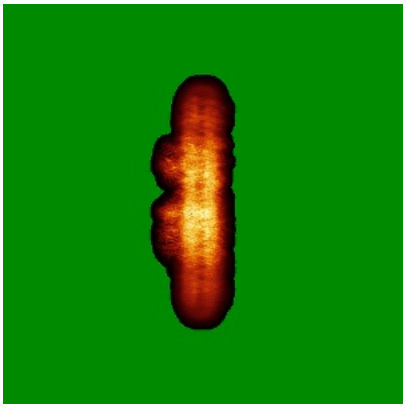
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

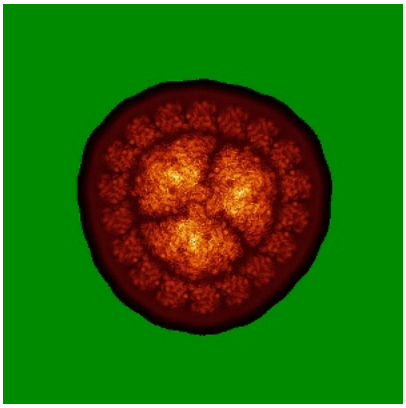
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

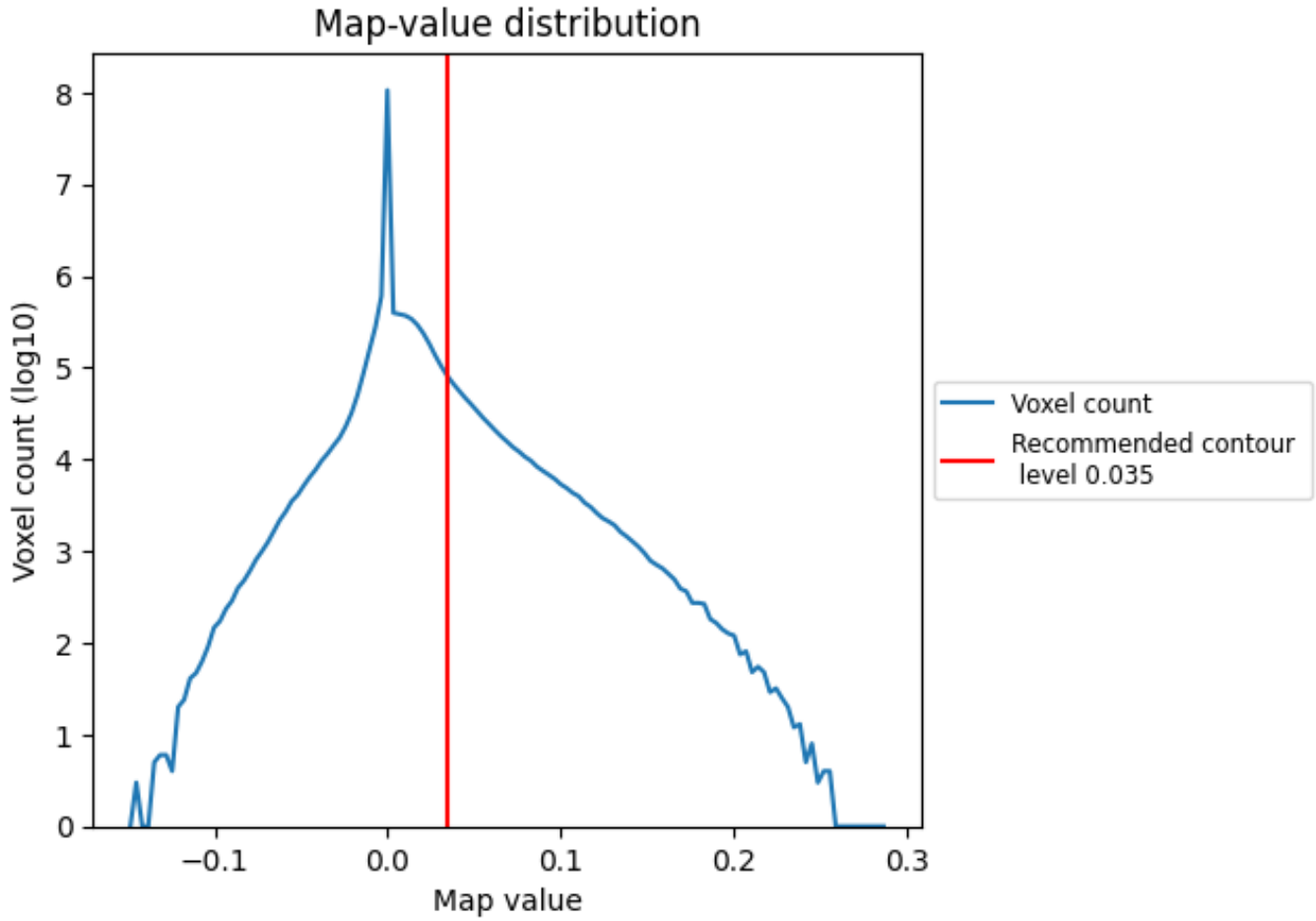
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

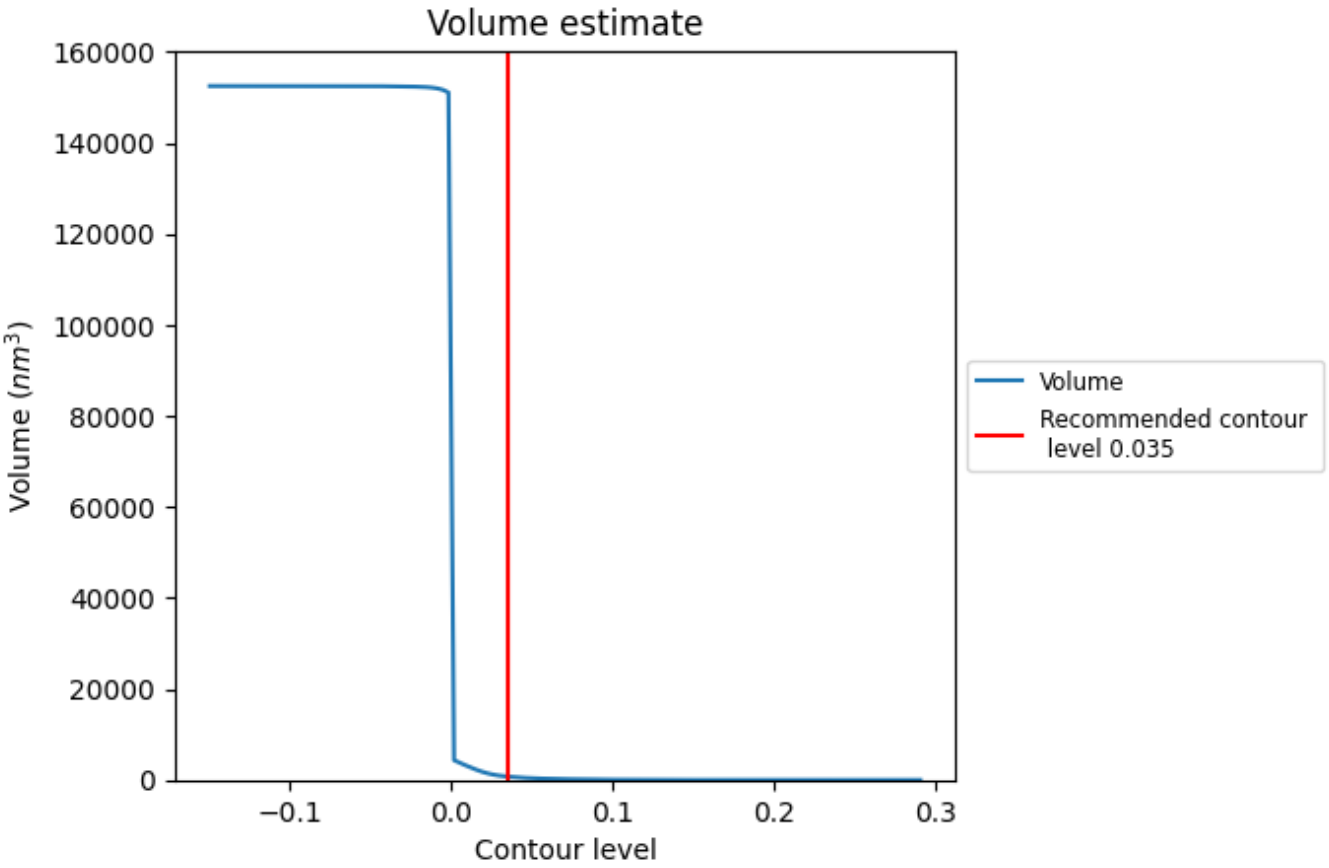
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

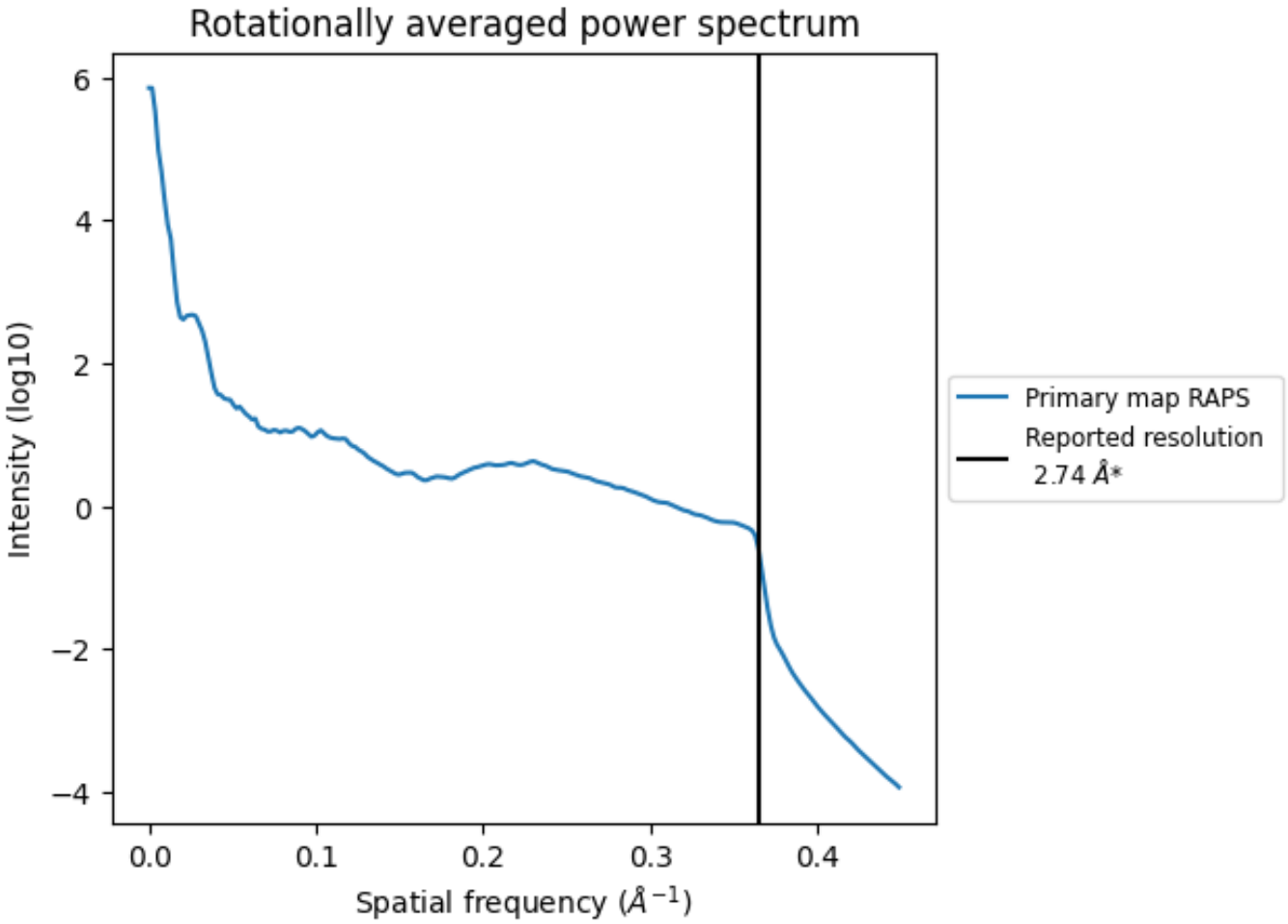
7.2 Volume estimate



The volume at the recommended contour level is 747 nm^3; this corresponds to an approximate mass of 675 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

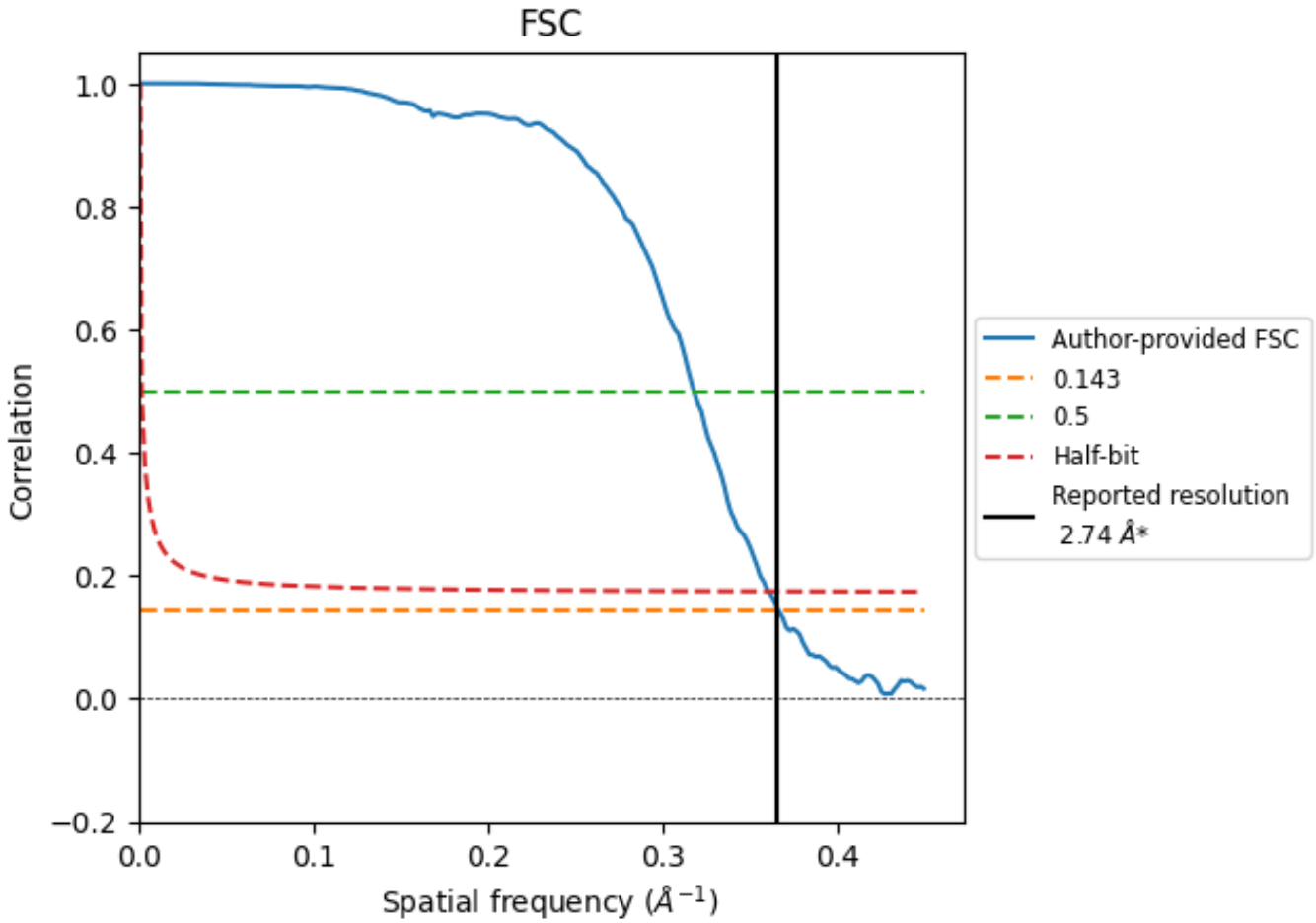


*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8.2 Resolution estimates (i)

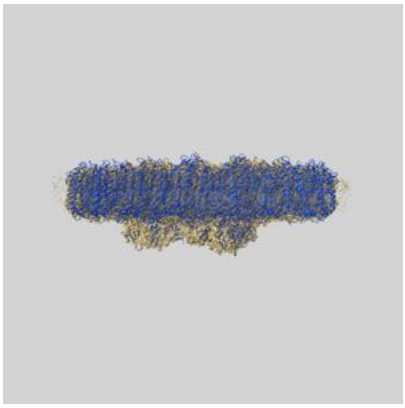
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.15	2.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

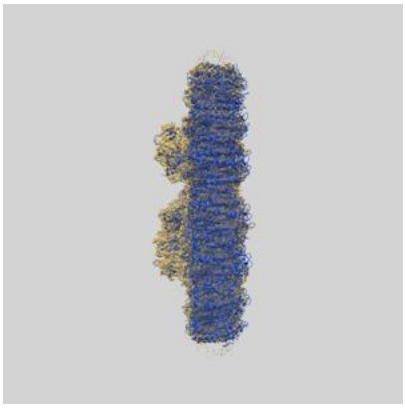
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9908 and PDB model 6K33. Per-residue inclusion information can be found in section 3 on page 50.

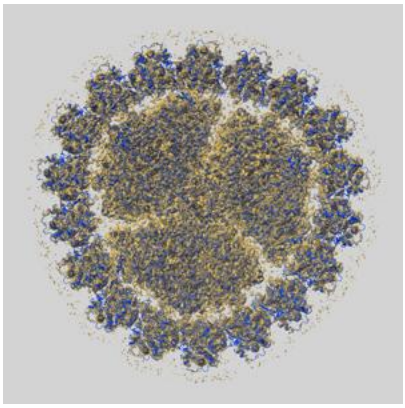
9.1 Map-model overlay



X



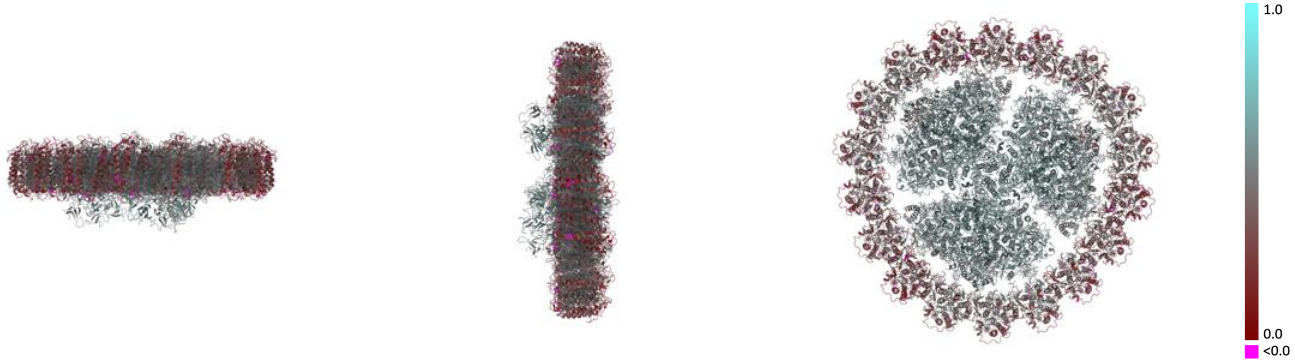
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

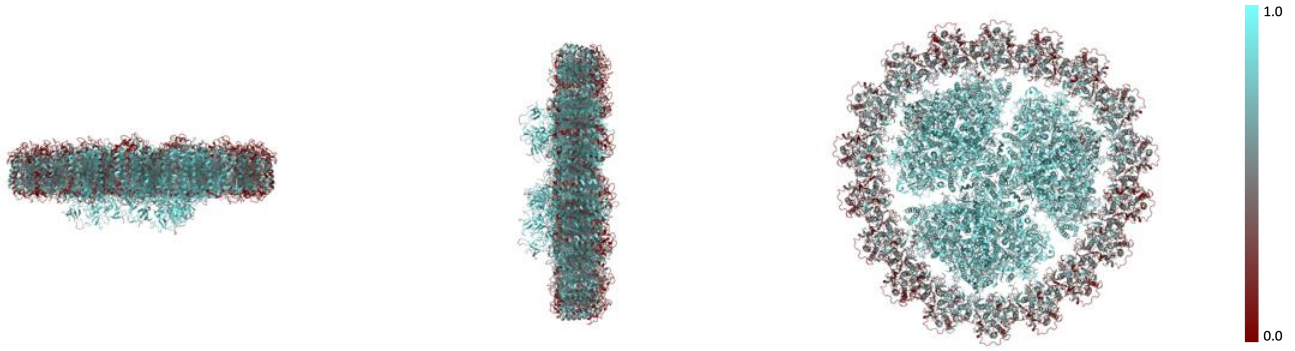
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

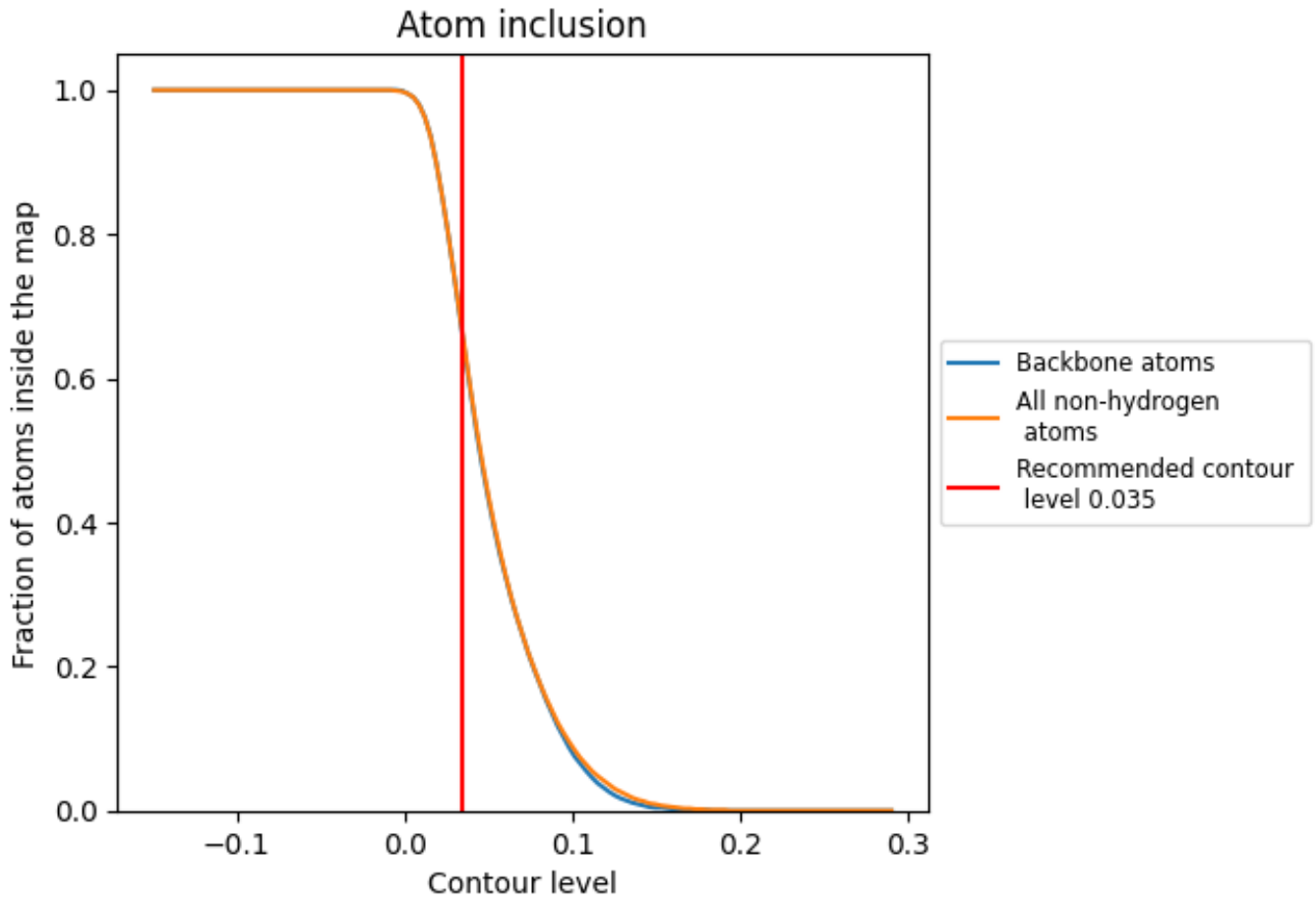
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.4450
a1	0.4050	0.2890
a2	0.3810	0.2690
a3	0.5040	0.3620
a4	0.4840	0.3610
a5	0.4290	0.3390
a6	0.3750	0.2970
aA	0.8720	0.5710
aB	0.8890	0.5690
aC	0.9200	0.5550
aD	0.8210	0.5560
aE	0.7720	0.5160
aF	0.7100	0.4700
aI	0.8900	0.5860
aJ	0.8030	0.5310
aK	0.8060	0.4710
aL	0.8830	0.5860
aM	0.8010	0.5490
aX	0.8250	0.5250
b1	0.4030	0.2870
b2	0.3720	0.2590
b3	0.4950	0.3600
b4	0.4810	0.3600
b5	0.4320	0.3380
b6	0.3710	0.2950
bA	0.8710	0.5680
bB	0.8900	0.5680
bC	0.9150	0.5500
bD	0.8220	0.5470
bE	0.7650	0.5100
bF	0.7370	0.5110
bI	0.9020	0.5940
bJ	0.8310	0.5420
bK	0.8190	0.4930
bL	0.8760	0.5850



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
bM	0.7910	0.5420
bX	0.8250	0.5140
c1	0.4120	0.2890
c2	0.3680	0.2650
c3	0.4980	0.3590
c4	0.4880	0.3590
c5	0.4310	0.3390
c6	0.3710	0.2990
cA	0.8720	0.5700
cB	0.8870	0.5670
cC	0.9170	0.5510
cD	0.8250	0.5510
cE	0.7820	0.5150
cF	0.6930	0.4520
cI	0.8940	0.5930
cJ	0.8190	0.5400
cK	0.8300	0.4940
cL	0.8880	0.5900
cM	0.8090	0.5490
cX	0.8350	0.5280