wwPDB EM Validation Summary Report

Sep 30, 2026 – 06:42 PM JST

PDB ID	:	6KMX / pdb_00006kmx
EMDB ID	:	EMD-0727
Title	:	Structure of PSI from H. hongdechloris grown under far-red light condition
Authors	:	Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on	:	2019-08-01
Resolution	:	2.41 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:

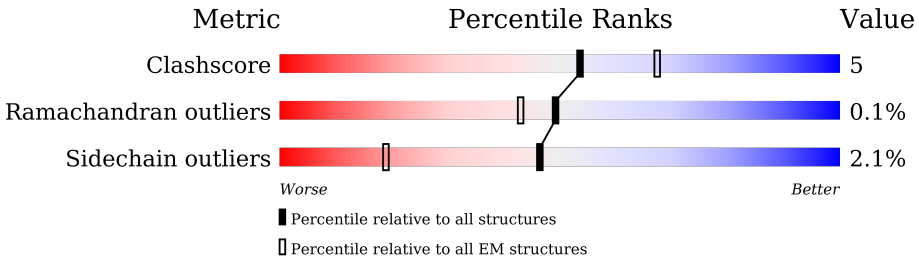
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

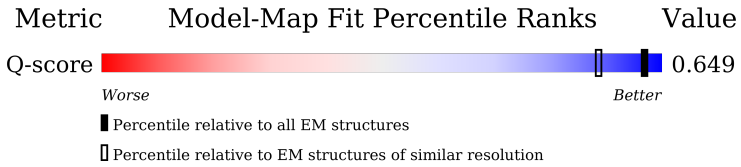
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.41 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.





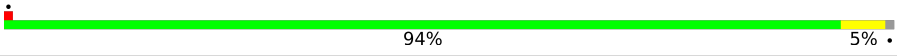
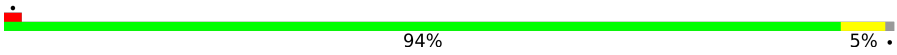
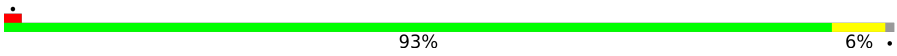
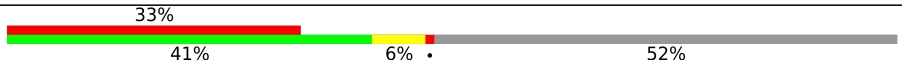
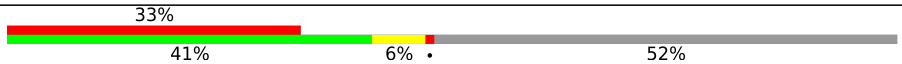
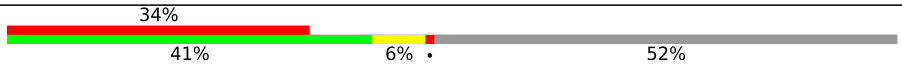
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5662 (1.92 - 2.91)

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	784	8% 81% 10% • 9%
1	bA	784	8% 81% 10% • 9%
1	cA	784	8% 81% 10% • 9%
2	aB	743	13% 86% 11% •

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Mol	Chain	Length	Quality of chain
2	bB	743	
2	cB	743	
3	aC	81	
3	bC	81	
3	cC	81	
4	aD	142	
4	bD	142	
4	cD	142	
5	aE	68	
5	bE	68	
5	cE	68	
6	aI	63	
6	bI	63	
6	cI	63	
7	aK	96	
7	bK	96	
7	cK	96	
8	aL	189	
8	bL	189	
8	cL	189	
9	aM	31	
9	bM	31	
9	cM	31	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	F6C	aA	826	X	-	-	-
12	F6C	aA	827	X	-	-	-
12	F6C	aA	830	X	-	-	-
12	F6C	aA	832	X	-	-	-
12	F6C	aA	844	X	-	-	-
12	F6C	aB	824	X	-	-	-
12	F6C	aL	202	X	-	-	-
12	F6C	bA	826	X	-	-	-
12	F6C	bA	827	X	-	-	-
12	F6C	bA	830	X	-	-	-
12	F6C	bA	832	X	-	-	-
12	F6C	bA	844	X	-	-	-
12	F6C	bB	824	X	-	-	-
12	F6C	bL	202	X	-	-	-
12	F6C	cA	826	X	-	-	-
12	F6C	cA	827	X	-	-	-
12	F6C	cA	830	X	-	-	-
12	F6C	cA	832	X	-	-	-
12	F6C	cA	844	X	-	-	-
12	F6C	cB	824	X	-	-	-
12	F6C	cL	202	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 65112 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	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		
1	bA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		
1	cA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		
2	bB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		
2	cB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		

- 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
			596	366	102	117	11		
3	bC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		
3	cC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		
4	cD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	61	Total	C	N	O	0	0
			499	317	87	95		
5	bE	61	Total	C	N	O	0	0
			499	317	87	95		
5	cE	61	Total	C	N	O	0	0
			499	317	87	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		
6	bI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		
6	cI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		
7	bK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		
7	cK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		
8	bL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		

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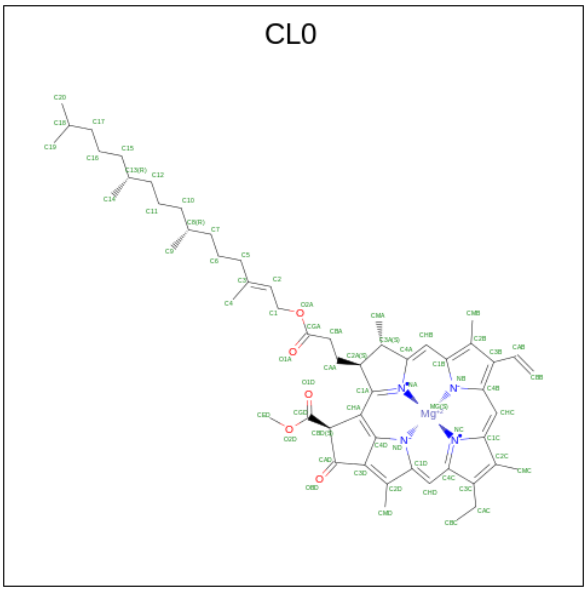
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Mol	Chain	Residues	Atoms					AltConf	Trace
8	cL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		

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

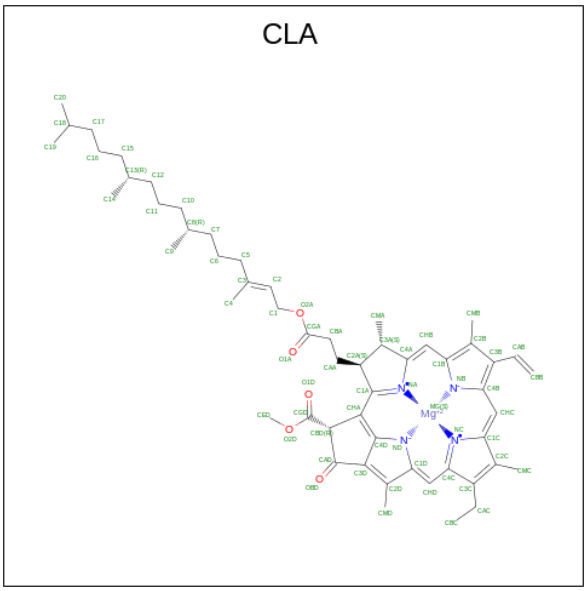
Mol	Chain	Residues	Atoms					AltConf	Trace
9	aM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
9	bM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
9	cM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

- Molecule 10 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	aK	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
11	aK	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bK	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
11	bK	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	cB	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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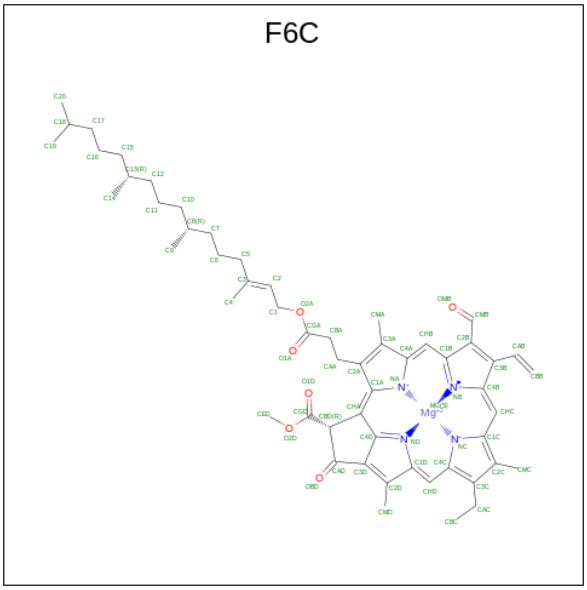
Mol	Chain	Residues	Atoms					AltConf
11	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cK	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
11	cK	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

- Molecule 12 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$).



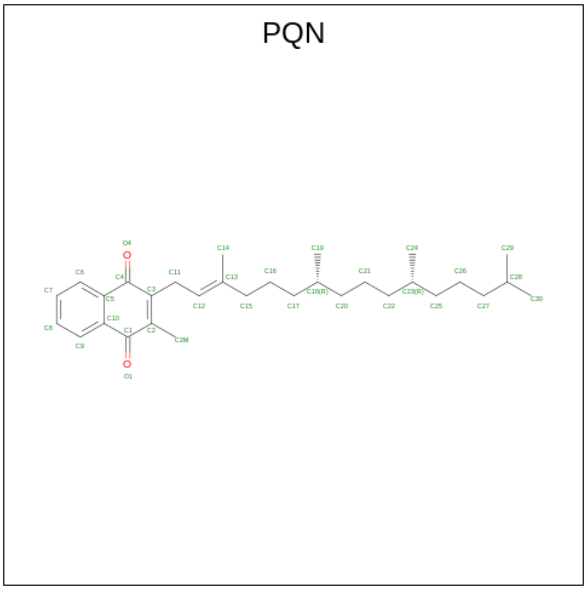
Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	aB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	aL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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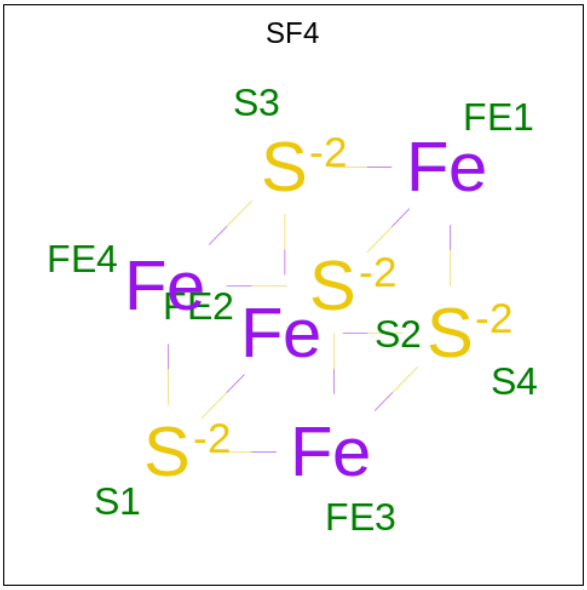
Mol	Chain	Residues	Atoms					AltConf
12	bA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	bB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	bL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	cL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms	AltConf
13	aA	1	Total C O 33 31 2	0
13	aB	1	Total C O 28 26 2	0
13	bA	1	Total C O 33 31 2	0
13	bB	1	Total C O 28 26 2	0
13	cA	1	Total C O 33 31 2	0
13	cB	1	Total C O 28 26 2	0

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



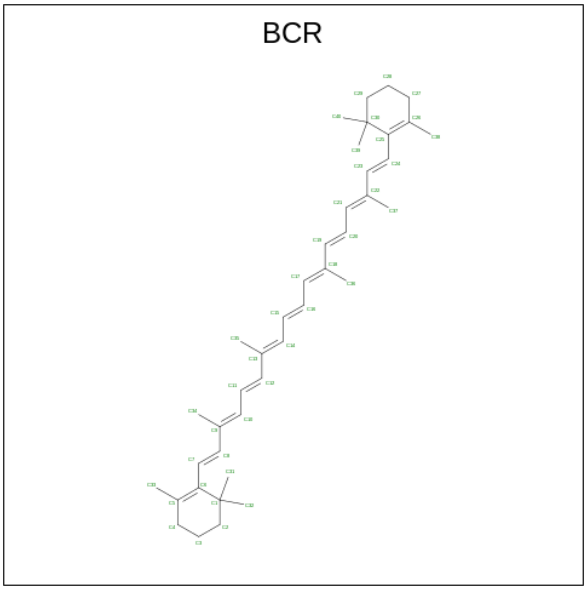
Mol	Chain	Residues	Atoms	AltConf
14	aA	1	Total Fe S 8 4 4	0
14	aC	1	Total Fe S 8 4 4	0
14	aC	1	Total Fe S 8 4 4	0
14	bA	1	Total Fe S 8 4 4	0
14	bC	1	Total Fe S 8 4 4	0
14	bC	1	Total Fe S 8 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
14	cA	1	Total Fe S 8 4 4	0
14	cC	1	Total Fe S 8 4 4	0
14	cC	1	Total Fe S 8 4 4	0

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aI	1	Total C 40 40	0
15	aK	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aM	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bI	1	Total C 40 40	0

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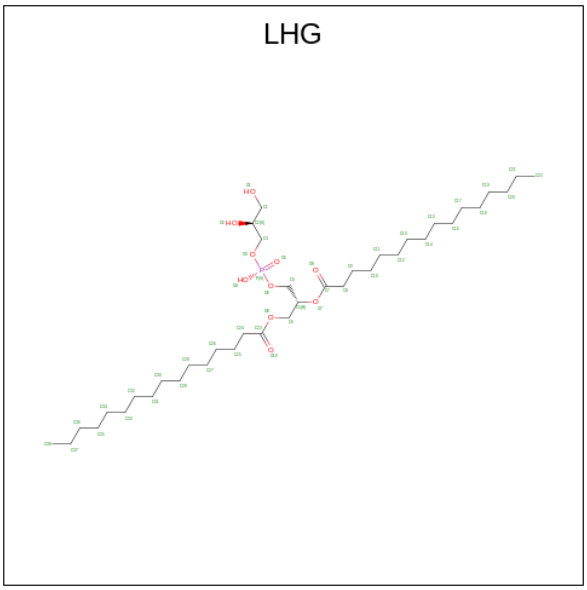
Mol	Chain	Residues	Atoms	AltConf
15	bK	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bM	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cI	1	Total C 40 40	0
15	cK	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0

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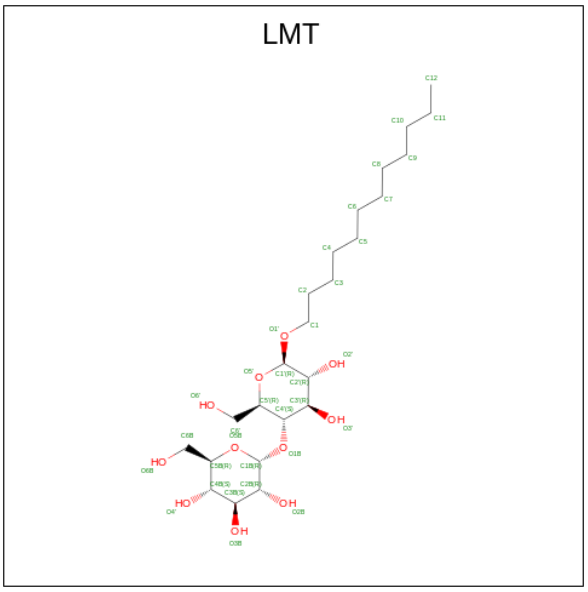
Mol	Chain	Residues	Atoms	AltConf
15	cM	1	Total C 40 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



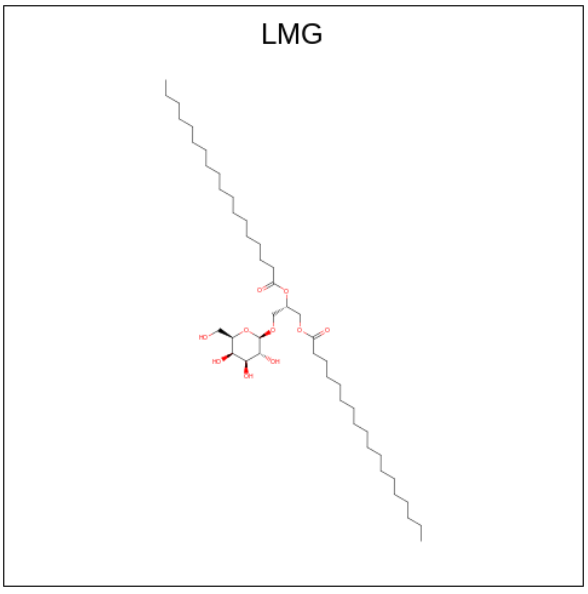
Mol	Chain	Residues	Atoms	AltConf
16	aA	1	Total C O P 49 38 10 1	0
16	bA	1	Total C O P 49 38 10 1	0
16	cA	1	Total C O P 49 38 10 1	0

- Molecule 17 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
17	aA	1	Total	C	O	0
			35	24	11	
17	bA	1	Total	C	O	0
			35	24	11	
17	cA	1	Total	C	O	0
			35	24	11	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
18	aB	1	Total C O 46 36 10	0
18	bB	1	Total C O 46 36 10	0
18	cB	1	Total C O 46 36 10	0

- Molecule 19 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	AltConf
19	aI	1	Total C 9 9	0
19	aL	4	Total C O 56 52 4	0
19	bI	1	Total C 9 9	0
19	bL	4	Total C O 56 52 4	0
19	cI	2	Total C O 25 23 2	0
19	cL	3	Total C O 40 38 2	0

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	AltConf
21	aA	72	Total O 72 72	0
21	aB	72	Total O 72 72	0
21	aC	21	Total O 21 21	0

Continued on next page...

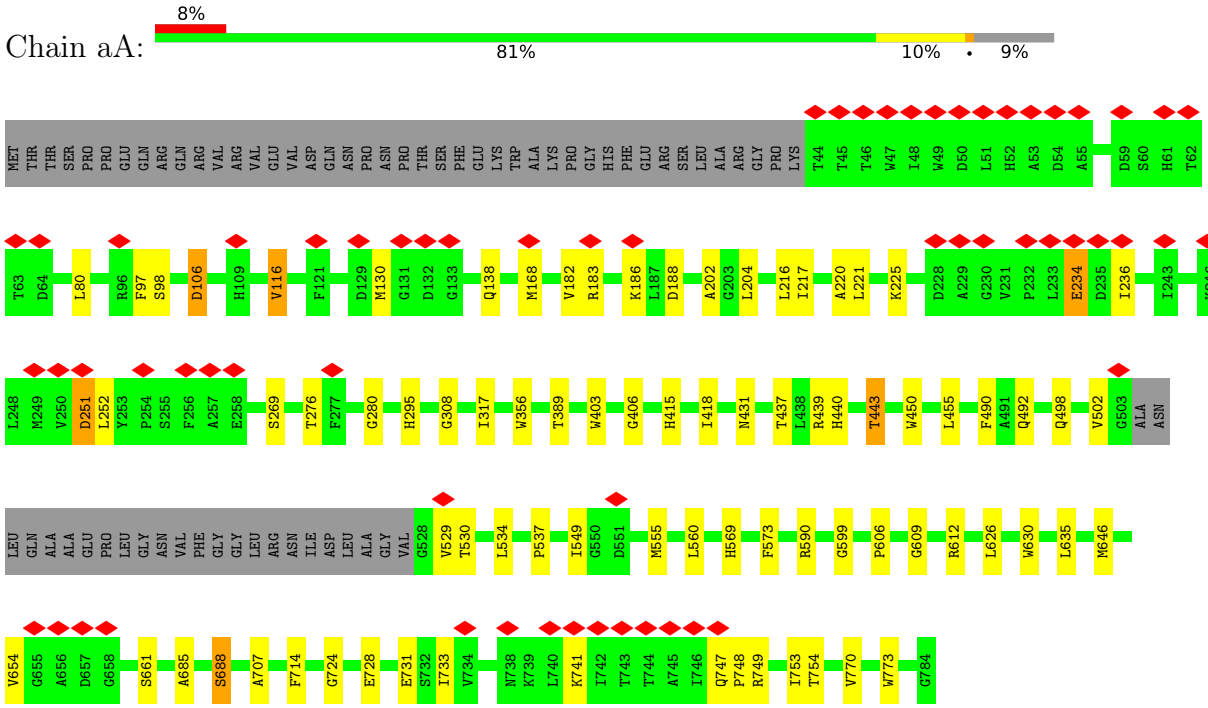
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
21	aD	15	Total O 15 15	0
21	aI	5	Total O 5 5	0
21	aK	1	Total O 1 1	0
21	aL	25	Total O 25 25	0
21	aM	1	Total O 1 1	0
21	bA	72	Total O 72 72	0
21	bB	72	Total O 72 72	0
21	bC	20	Total O 20 20	0
21	bD	16	Total O 16 16	0
21	bI	6	Total O 6 6	0
21	bK	1	Total O 1 1	0
21	bL	24	Total O 24 24	0
21	bM	1	Total O 1 1	0
21	cA	72	Total O 72 72	0
21	cB	72	Total O 72 72	0
21	cC	21	Total O 21 21	0
21	cD	15	Total O 15 15	0
21	cI	6	Total O 6 6	0
21	cK	1	Total O 1 1	0
21	cL	24	Total O 24 24	0
21	cM	1	Total O 1 1	0

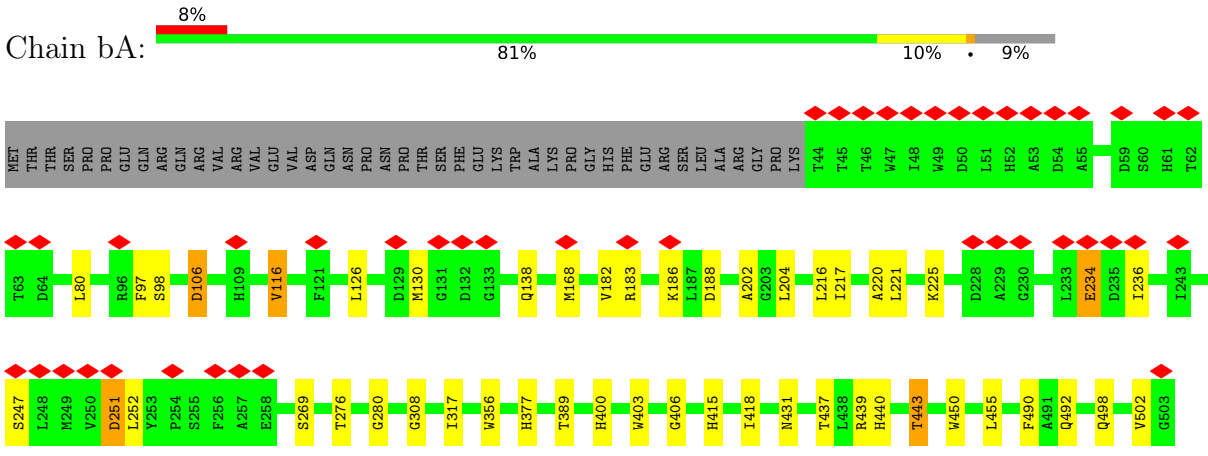
3 Residue-property plots (i)

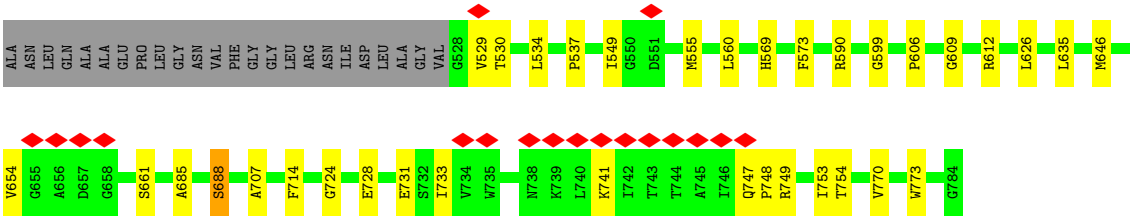
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

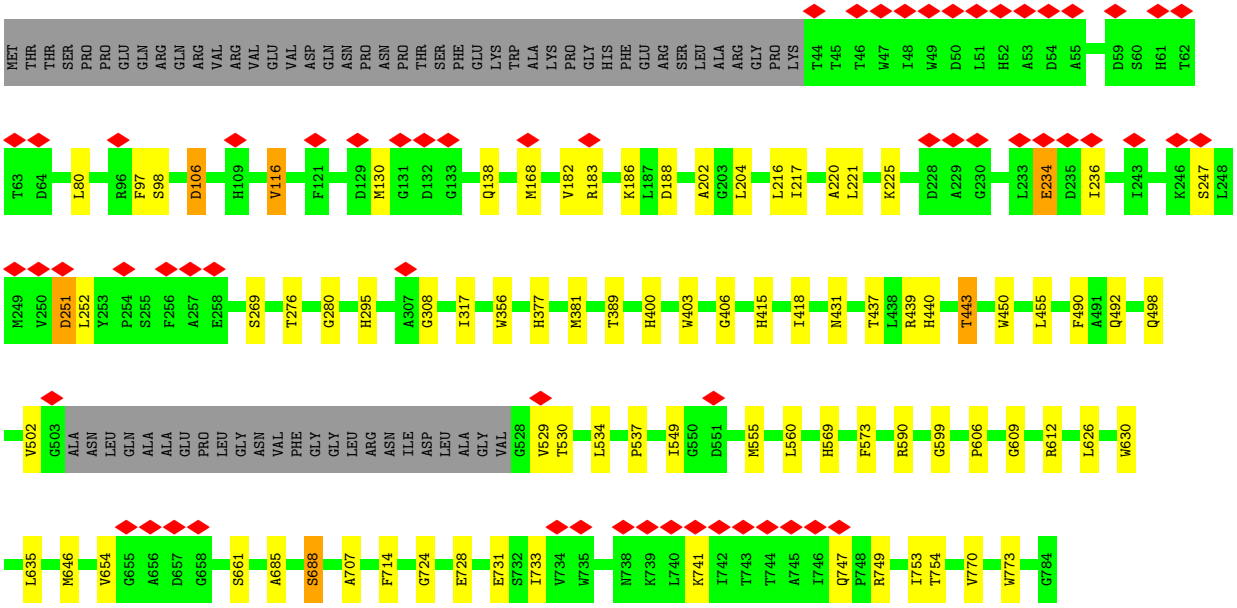




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:

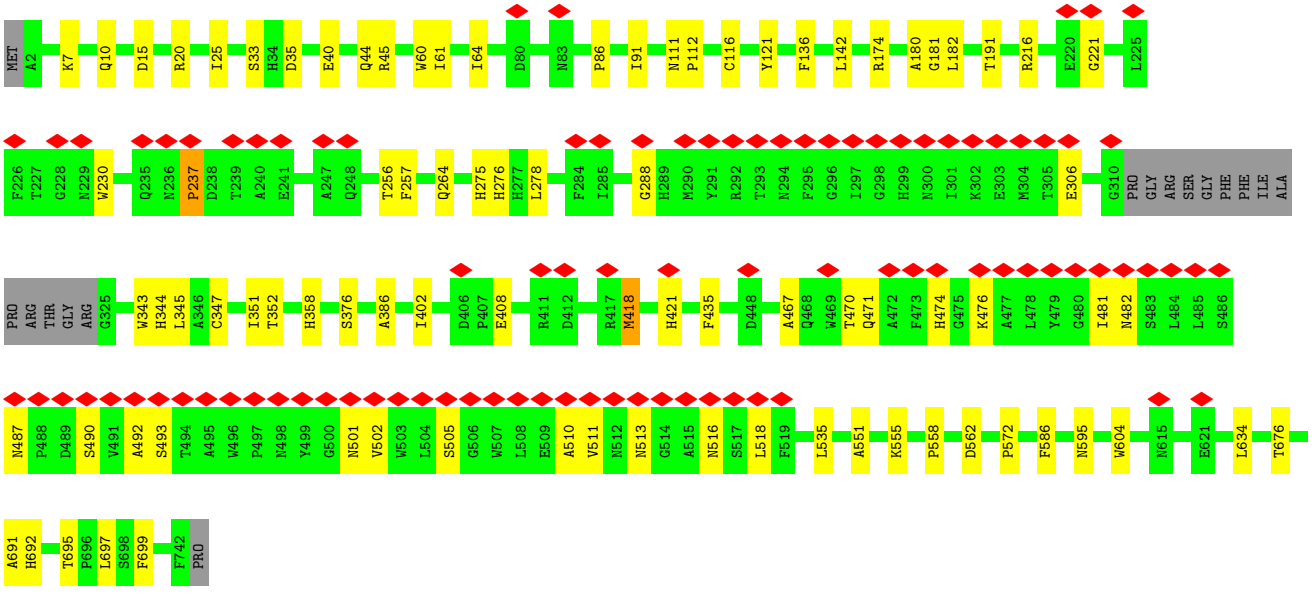




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

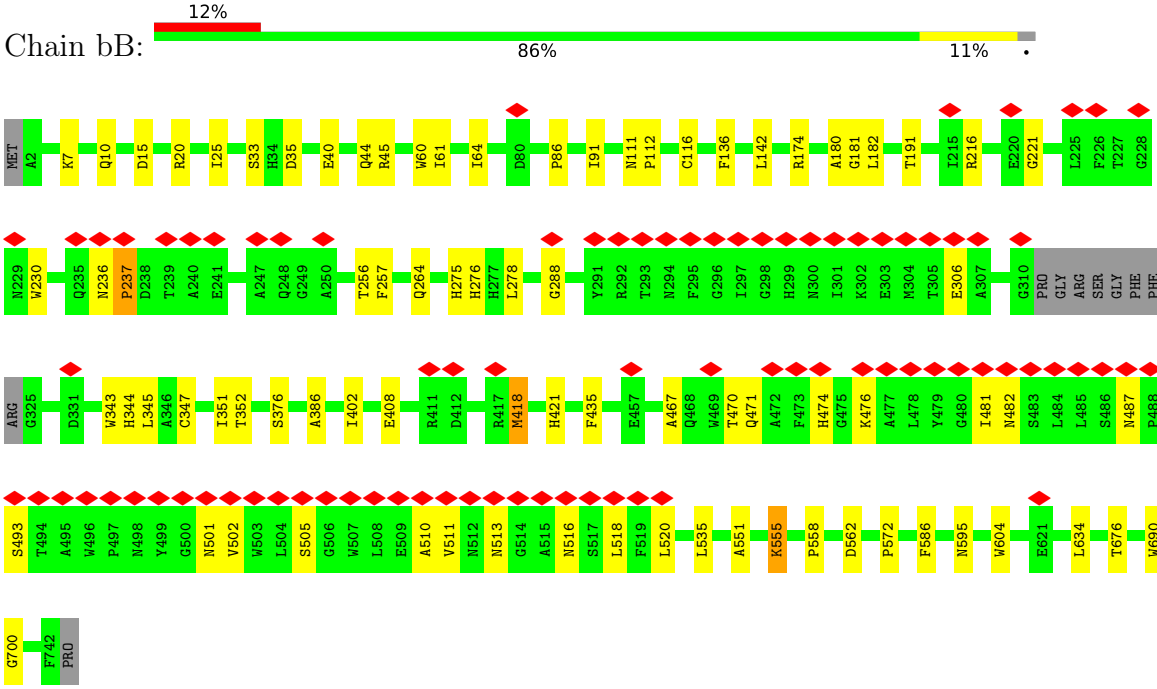
Chain aB:





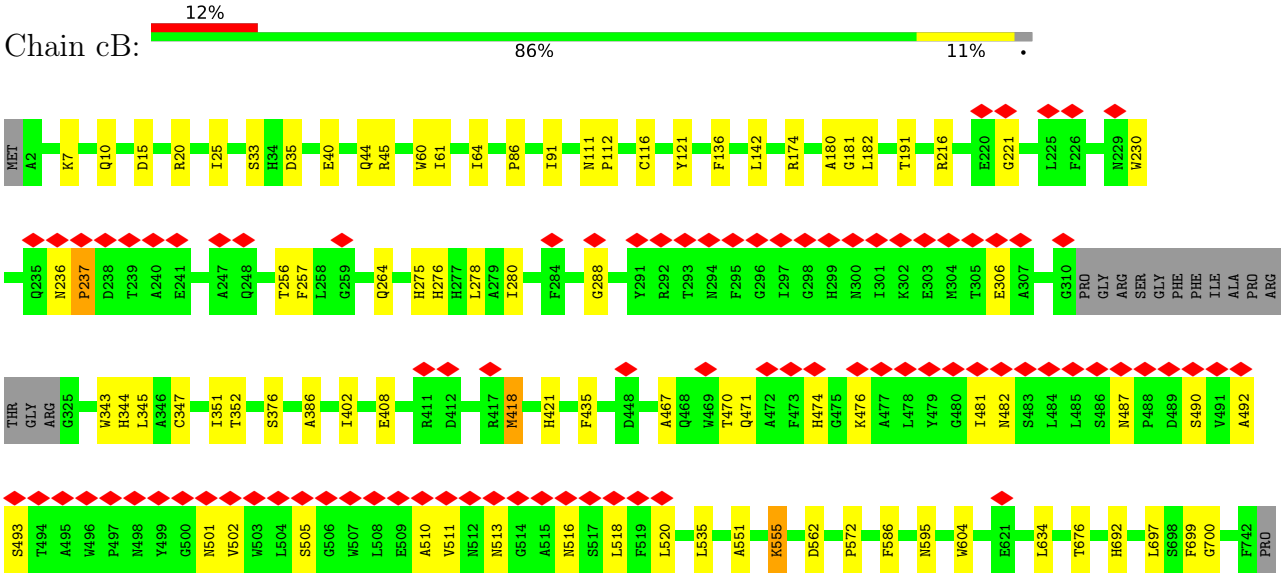
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB:



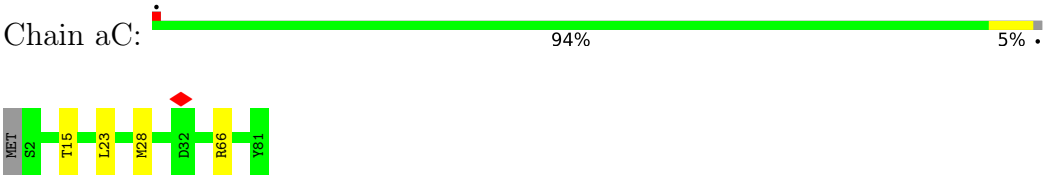
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB:



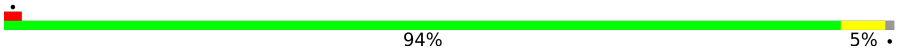
• Molecule 3: Photosystem I iron-sulfur center

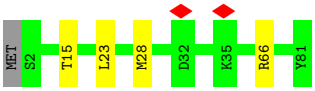
Chain aC:



• Molecule 3: Photosystem I iron-sulfur center

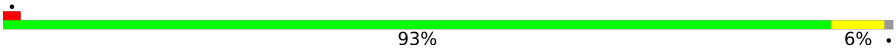
Chain bC:

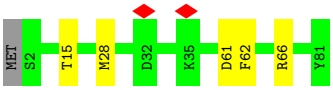




• Molecule 3: Photosystem I iron-sulfur center

Chain cC:

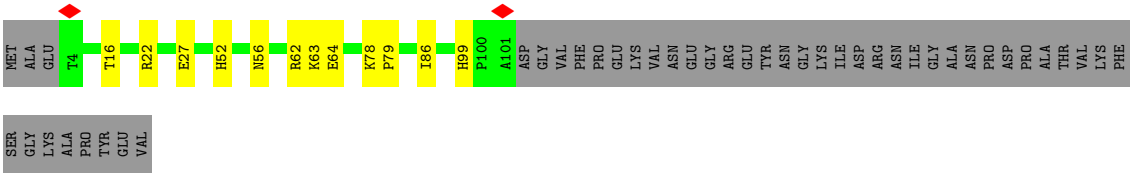




• Molecule 4: Photosystem I reaction center subunit II

Chain aD:

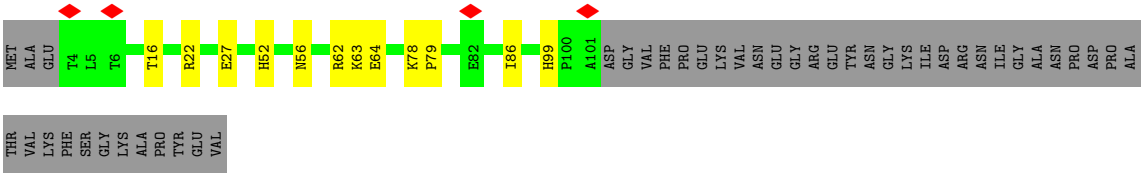




• Molecule 4: Photosystem I reaction center subunit II

Chain bD:

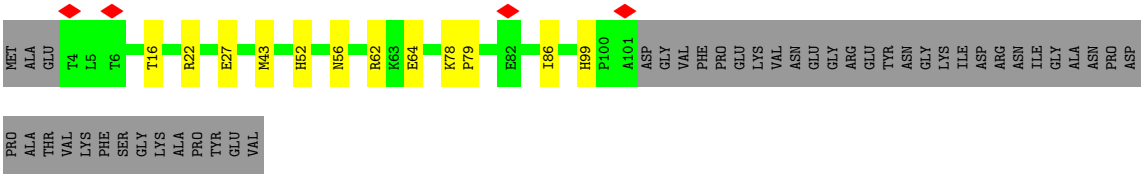




• Molecule 4: Photosystem I reaction center subunit II

Chain cD:

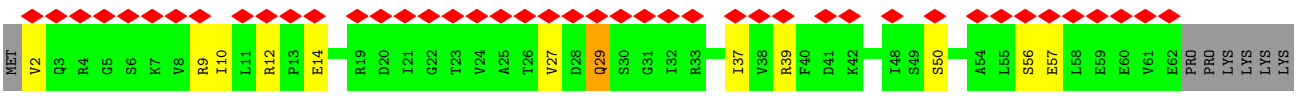




• Molecule 5: Photosystem I reaction center subunit IV

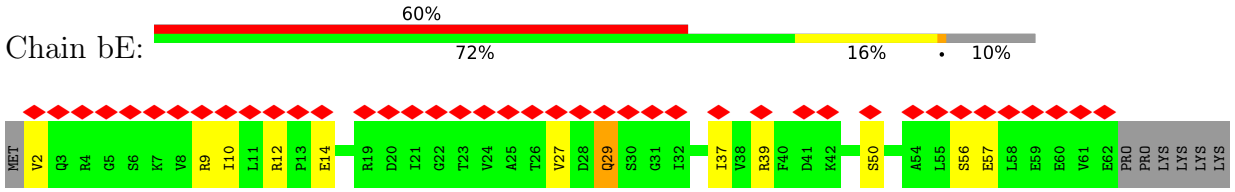
Chain aE:





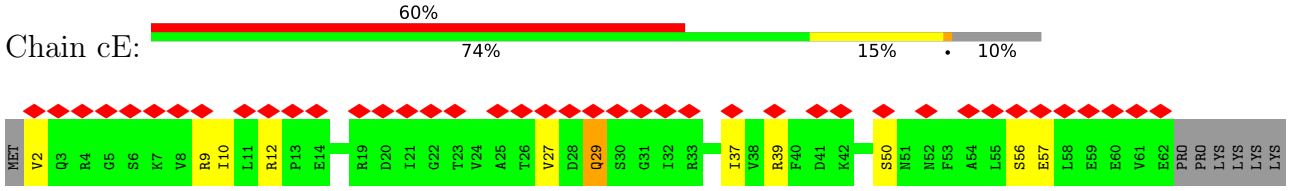
• Molecule 5: Photosystem I reaction center subunit IV

Chain bE:



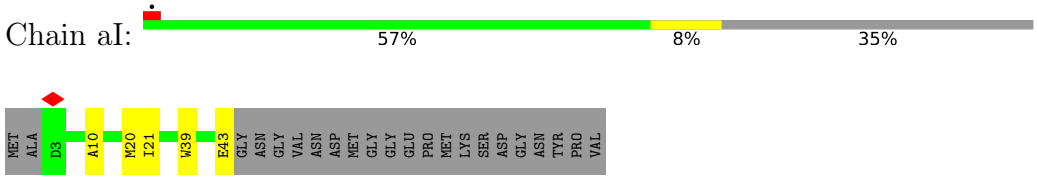
• Molecule 5: Photosystem I reaction center subunit IV

Chain cE:



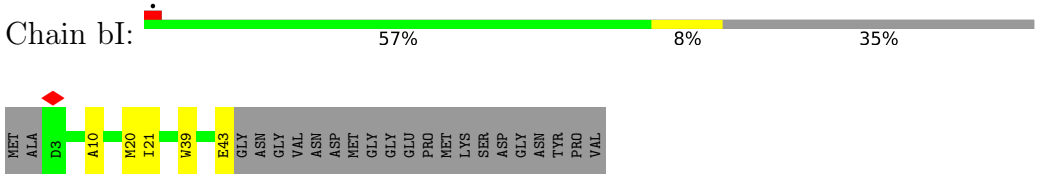
• Molecule 6: Photosystem I reaction center subunit VIII

Chain aI:



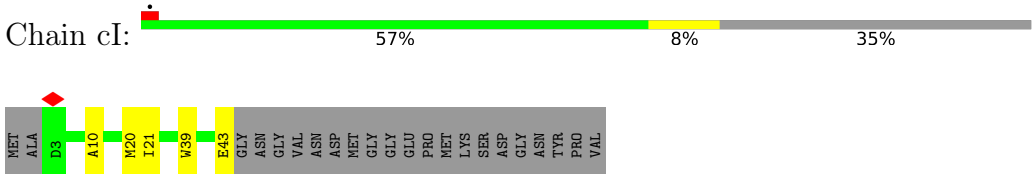
• Molecule 6: Photosystem I reaction center subunit VIII

Chain bI:



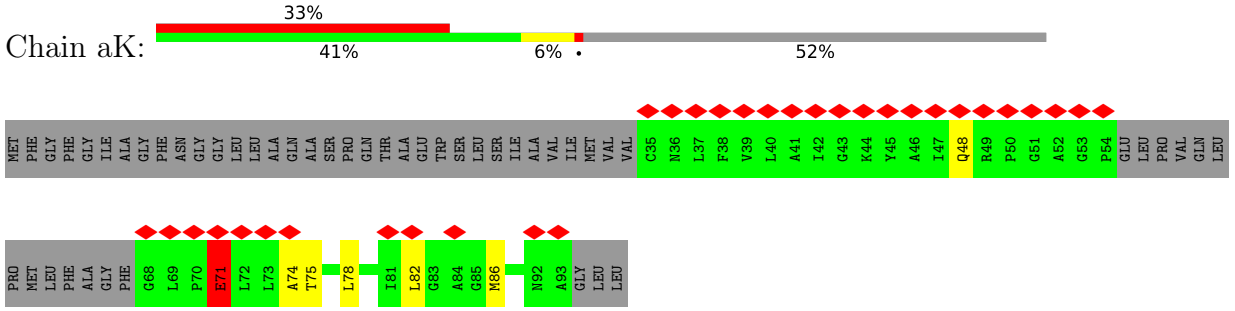
• Molecule 6: Photosystem I reaction center subunit VIII

Chain cI:



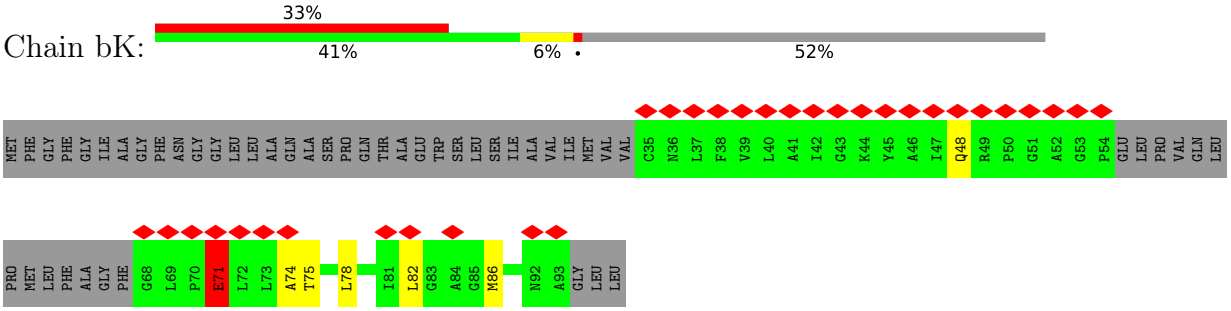
• Molecule 7: Photosystem I reaction center subunit PsaK

Chain aK:



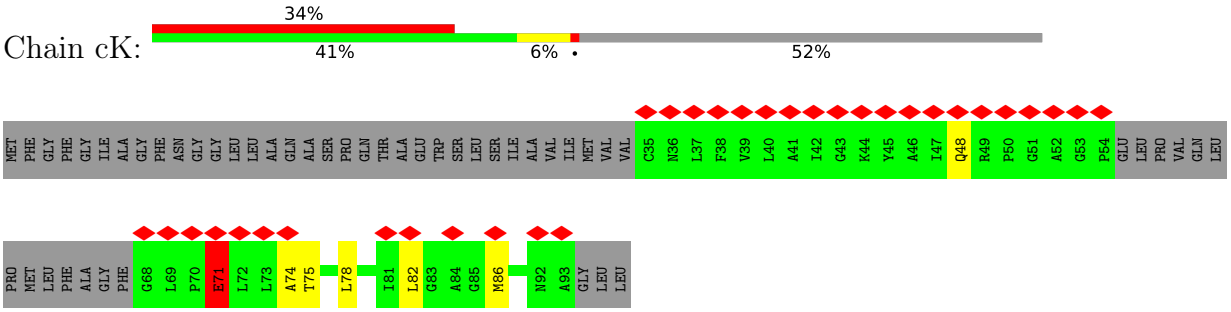
• Molecule 7: Photosystem I reaction center subunit PsaK

Chain bK:



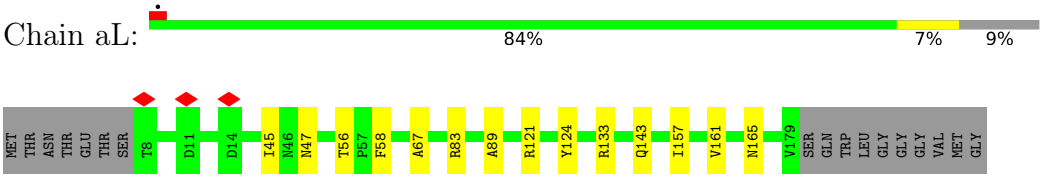
• Molecule 7: Photosystem I reaction center subunit PsaK

Chain cK:



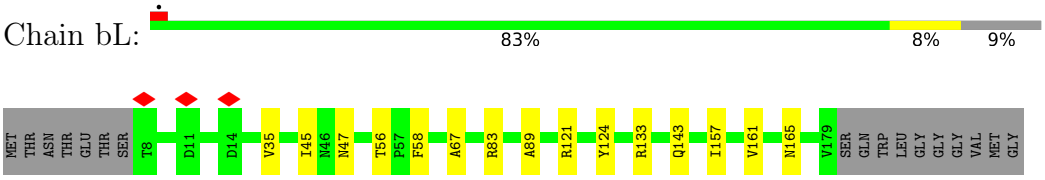
• Molecule 8: Photosystem I reaction center subunit XI

Chain aL:



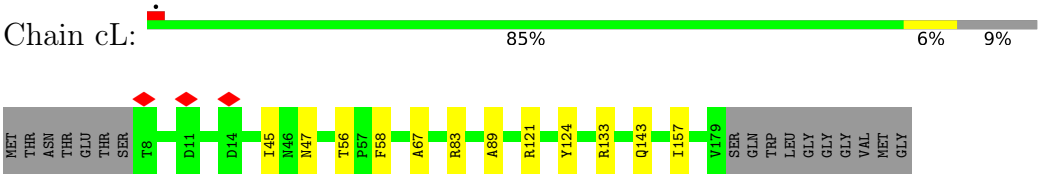
• Molecule 8: Photosystem I reaction center subunit XI

Chain bL:



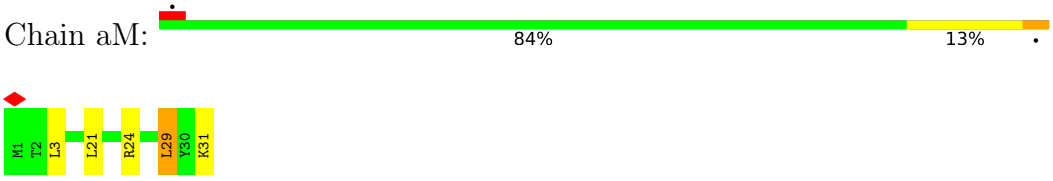
• Molecule 8: Photosystem I reaction center subunit XI

Chain cL:



• Molecule 9: Photosystem I reaction center subunit XII

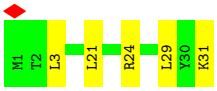
Chain aM:



• Molecule 9: Photosystem I reaction center subunit XII

Chain bM:

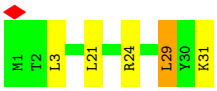




• Molecule 9: Photosystem I reaction center subunit XII

Chain cM:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	311993	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 ($e^-/Å^2$)	47	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	0.915	Depositor
Minimum map value	-0.310	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	313.2, 313.2, 313.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6C, LHG, SF4, LMG, CA, UNL, LMT, CL0, BCR, PQN, CLA

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	0.20	0/5868	0.47	3/7993 (0.0%)
1	bA	0.20	0/5868	0.47	3/7993 (0.0%)
1	cA	0.20	0/5868	0.47	2/7993 (0.0%)
2	aB	0.20	0/5993	0.49	1/8185 (0.0%)
2	bB	0.20	0/5993	0.49	1/8185 (0.0%)
2	cB	0.20	0/5993	0.49	1/8185 (0.0%)
3	aC	0.18	0/606	0.49	0/820
3	bC	0.18	0/606	0.49	0/820
3	cC	0.18	0/606	0.49	0/820
4	aD	0.17	0/785	0.43	0/1061
4	bD	0.17	0/785	0.43	0/1061
4	cD	0.17	0/785	0.43	0/1061
5	aE	0.31	0/509	0.71	1/689 (0.1%)
5	bE	0.31	0/509	0.71	1/689 (0.1%)
5	cE	0.31	0/509	0.71	1/689 (0.1%)
6	aI	0.30	0/365	0.64	0/503
6	bI	0.30	0/365	0.64	0/503
6	cI	0.30	0/365	0.64	0/503
7	aK	0.23	0/321	0.71	1/433 (0.2%)
7	bK	0.24	0/321	0.71	1/433 (0.2%)
7	cK	0.24	0/321	0.71	1/433 (0.2%)
8	aL	0.19	0/1334	0.45	0/1819
8	bL	0.19	0/1334	0.45	0/1819
8	cL	0.20	0/1334	0.45	0/1819
9	aM	0.23	0/244	0.61	0/332
9	bM	0.23	0/244	0.60	0/332
9	cM	0.23	0/244	0.60	0/332
All	All	0.21	0/48075	0.50	17/65505 (0.0%)

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
9	aM	0	1
9	bM	0	1
9	cM	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	cA	234	GLU	CA-CB-CG	7.39	128.89	114.10
1	bA	234	GLU	CA-CB-CG	7.37	128.84	114.10
1	aA	234	GLU	CA-CB-CG	7.35	128.79	114.10
7	aK	71	GLU	CA-CB-CG	6.70	127.49	114.10
7	cK	71	GLU	CA-CB-CG	6.69	127.48	114.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	aB	481	ILE	Peptide
9	aM	29	LEU	Peptide
2	bB	481	ILE	Peptide
9	bM	29	LEU	Peptide
2	cB	481	ILE	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	5669	0	5487	49	0
1	bA	5669	0	5487	50	0
1	cA	5669	0	5487	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	aB	5783	0	5519	59	0
2	bB	5783	0	5519	59	0
2	cB	5783	0	5519	59	0
3	aC	596	0	576	3	0
3	bC	596	0	576	3	0
3	cC	596	0	576	3	0
4	aD	768	0	774	8	0
4	bD	768	0	774	7	0
4	cD	768	0	774	8	0
5	aE	499	0	488	4	0
5	bE	499	0	488	4	0
5	cE	499	0	488	3	0
6	aI	349	0	353	5	0
6	bI	349	0	353	4	0
6	cI	349	0	353	5	0
7	aK	317	0	336	5	0
7	bK	317	0	336	5	0
7	cK	317	0	336	5	0
8	aL	1303	0	1301	14	0
8	bL	1303	0	1301	15	0
8	cL	1303	0	1301	13	0
9	aM	241	0	266	6	0
9	bM	241	0	266	4	0
9	cM	241	0	266	6	0
10	aA	65	0	72	0	0
10	bA	65	0	72	0	0
10	cA	65	0	72	0	0
11	aA	2112	0	1999	48	0
11	aB	2116	0	1932	53	0
11	aK	89	0	68	1	0
11	aL	195	0	216	6	0
11	bA	2112	0	1999	46	0
11	bB	2116	0	1932	48	0
11	bK	89	0	68	1	0
11	bL	195	0	216	8	0
11	cA	2112	0	1999	53	0
11	cB	2116	0	1932	54	0
11	cK	89	0	68	1	0
11	cL	195	0	216	5	0
12	aA	305	0	0	0	0
12	aB	58	0	0	1	0
12	aL	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	bA	305	0	0	0	0
12	bB	58	0	0	0	0
12	bL	66	0	0	0	0
12	cA	305	0	0	0	0
12	cB	58	0	0	1	0
12	cL	66	0	0	0	0
13	aA	33	0	46	0	0
13	aB	28	0	33	3	0
13	bA	33	0	46	1	0
13	bB	28	0	33	2	0
13	cA	33	0	46	1	0
13	cB	28	0	33	1	0
14	aA	8	0	0	0	0
14	aC	16	0	0	0	0
14	bA	8	0	0	0	0
14	bC	16	0	0	0	0
14	cA	8	0	0	0	0
14	cC	16	0	0	0	0
15	aA	200	0	280	16	0
15	aB	240	0	336	9	0
15	aI	40	0	56	2	0
15	aK	40	0	56	2	0
15	aL	120	0	168	7	0
15	aM	40	0	56	0	0
15	bA	200	0	280	18	0
15	bB	240	0	336	7	0
15	bI	40	0	56	0	0
15	bK	40	0	56	2	0
15	bL	120	0	168	7	0
15	bM	40	0	56	2	0
15	cA	200	0	280	15	0
15	cB	240	0	336	10	0
15	cI	40	0	56	0	0
15	cK	40	0	56	2	0
15	cL	120	0	168	9	0
15	cM	40	0	56	0	0
16	aA	49	0	74	1	0
16	bA	49	0	74	1	0
16	cA	49	0	74	1	0
17	aA	35	0	46	2	0
17	bA	35	0	46	2	0
17	cA	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	aB	46	0	65	1	0
18	bB	46	0	65	1	0
18	cB	46	0	65	1	0
19	aI	9	0	0	0	0
19	aL	56	0	0	0	0
19	bI	9	0	0	0	0
19	bL	56	0	0	0	0
19	cI	25	0	0	0	0
19	cL	40	0	0	0	0
20	aL	1	0	0	0	0
20	bL	1	0	0	0	0
20	cL	1	0	0	0	0
21	aA	72	0	0	1	0
21	aB	72	0	0	1	0
21	aC	21	0	0	0	0
21	aD	15	0	0	0	0
21	aI	5	0	0	0	0
21	aK	1	0	0	0	0
21	aL	25	0	0	0	0
21	aM	1	0	0	0	0
21	bA	72	0	0	1	0
21	bB	72	0	0	1	0
21	bC	20	0	0	0	0
21	bD	16	0	0	0	0
21	bI	6	0	0	0	0
21	bK	1	0	0	0	0
21	bL	24	0	0	0	0
21	bM	1	0	0	0	0
21	cA	72	0	0	1	0
21	cB	72	0	0	1	0
21	cC	21	0	0	0	0
21	cD	15	0	0	0	0
21	cI	6	0	0	0	0
21	cK	1	0	0	0	0
21	cL	24	0	0	0	0
21	cM	1	0	0	0	0
All	All	65112	0	61809	653	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 5.

The worst 5 of 653 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)
4:aD:52:HIS:H	4:aD:56:ASN:HD21	1.33	0.76
4:cD:52:HIS:H	4:cD:56:ASN:HD21	1.34	0.76
4:bD:52:HIS:H	4:bD:56:ASN:HD21	1.34	0.75
11:aB:840:CLA:HAC2	15:aB:846:BCR:H21C	1.69	0.73
11:cB:840:CLA:HAC2	15:cB:846:BCR:H21C	1.69	0.73

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	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
1	bA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
1	cA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
2	aB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	48	63
2	bB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	48	63
2	cB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	48	63
3	aC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	bC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	cC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	aD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
4	bD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
4	cD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
5	aE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
5	bE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
5	cE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
6	aI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	bI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
6	cI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
7	aK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
7	bK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
7	cK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
8	aL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
8	bL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
8	cL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
9	aM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
9	bM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
9	cM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	5847/6591 (89%)	5661 (97%)	183 (3%)	3 (0%)	49	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	aB	237	PRO
2	bB	237	PRO
2	cB	237	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	578/633 (91%)	562 (97%)	16 (3%)	38	58
1	bA	578/633 (91%)	562 (97%)	16 (3%)	38	58
1	cA	578/633 (91%)	562 (97%)	16 (3%)	38	58
2	aB	586/598 (98%)	576 (98%)	10 (2%)	53	73
2	bB	586/598 (98%)	576 (98%)	10 (2%)	53	73
2	cB	586/598 (98%)	576 (98%)	10 (2%)	53	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	aD	80/115 (70%)	80 (100%)	0	100	100
4	bD	80/115 (70%)	80 (100%)	0	100	100
4	cD	80/115 (70%)	80 (100%)	0	100	100
5	aE	54/61 (88%)	49 (91%)	5 (9%)	8	13
5	bE	54/61 (88%)	49 (91%)	5 (9%)	8	13
5	cE	54/61 (88%)	49 (91%)	5 (9%)	8	13
6	aI	36/52 (69%)	35 (97%)	1 (3%)	38	58
6	bI	36/52 (69%)	35 (97%)	1 (3%)	38	58
6	cI	36/52 (69%)	35 (97%)	1 (3%)	38	58
7	aK	30/67 (45%)	28 (93%)	2 (7%)	15	24
7	bK	30/67 (45%)	28 (93%)	2 (7%)	15	24
7	cK	30/67 (45%)	28 (93%)	2 (7%)	15	24
8	aL	136/149 (91%)	136 (100%)	0	100	100
8	bL	136/149 (91%)	136 (100%)	0	100	100
8	cL	136/149 (91%)	136 (100%)	0	100	100
9	aM	27/27 (100%)	27 (100%)	0	100	100
9	bM	27/27 (100%)	27 (100%)	0	100	100
9	cM	27/27 (100%)	27 (100%)	0	100	100
All	All	4785/5313 (90%)	4683 (98%)	102 (2%)	46	67

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	bB	513	ASN
1	cA	168	MET
6	cI	21	ILE
2	bB	562	ASP
6	bI	21	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
8	bL	143	GLN
2	cB	300	ASN
1	cA	138	GLN
1	cA	755	GLN
2	cB	620	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 363 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 345 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	$\#\|Z\| > 2$
14	SF4	aA	846	2,1	0,12,12	-	-	-		
10	CL0	bA	801	1	69,73,73	1.98	20 (28%)	83,113,113	2.81	32 (38%)
14	SF4	cC	101	3	0,12,12	-	-	-		
11	CLA	cA	834	1	69,73,73	1.99	20 (28%)	83,113,113	2.72	32 (38%)
11	CLA	aB	811	2	49,53,73	2.44	21 (42%)	59,89,113	3.08	24 (40%)
11	CLA	cB	823	2	58,62,73	2.18	21 (36%)	69,99,113	2.97	29 (42%)
11	CLA	cA	835	1	69,73,73	2.00	19 (27%)	83,113,113	2.75	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	bL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	6 (10%)
11	CLA	aB	823	2	58,62,73	2.18	21 (36%)	69,99,113	2.97	29 (42%)
17	LMT	aA	853	-	36,36,36	0.40	0	47,47,47	1.37	5 (10%)
11	CLA	bB	817	2	64,68,73	2.09	19 (29%)	77,107,113	2.91	29 (37%)
11	CLA	bB	833	2	49,53,73	2.44	20 (40%)	59,89,113	3.20	27 (45%)
11	CLA	bB	808	2	69,73,73	1.97	20 (28%)	83,113,113	2.70	29 (34%)
11	CLA	cA	840	1	69,73,73	2.02	20 (28%)	83,113,113	2.93	33 (39%)
11	CLA	bA	816	1	49,53,73	2.42	20 (40%)	59,89,113	3.10	24 (40%)
11	CLA	cA	842	-	49,53,73	2.42	21 (42%)	59,89,113	3.18	26 (44%)
14	SF4	cC	102	3	0,12,12	-	-	-		
11	CLA	aB	819	2	51,55,73	2.35	21 (41%)	61,91,113	3.00	28 (45%)
15	BCR	cB	848	-	41,41,41	1.00	2 (4%)	56,56,56	1.42	8 (14%)
15	BCR	cB	843	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
11	CLA	bA	837	1	49,53,73	2.41	21 (42%)	59,89,113	3.21	26 (44%)
11	CLA	cA	805	1	49,53,73	2.44	21 (42%)	59,89,113	3.19	25 (42%)
11	CLA	aB	838	2	51,55,73	2.33	20 (39%)	61,91,113	3.18	27 (44%)
13	PQN	bB	841	-	29,29,34	1.69	2 (6%)	36,39,45	1.17	4 (11%)
11	CLA	cB	813	2	60,64,73	2.15	21 (35%)	72,102,113	2.85	30 (41%)
14	SF4	aC	102	3	0,12,12	-	-	-		
15	BCR	aB	848	-	41,41,41	0.99	2 (4%)	56,56,56	1.42	8 (14%)
11	CLA	bA	802	21	69,73,73	1.98	20 (28%)	83,113,113	2.89	35 (42%)
16	LHG	cA	852	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
12	F6C	cA	827	21	62,64,74	2.66	26 (41%)	69,102,114	4.10	35 (50%)
11	CLA	bA	813	11,1	58,62,73	2.22	20 (34%)	69,99,113	2.90	27 (39%)
11	CLA	bA	805	1	49,53,73	2.45	21 (42%)	59,89,113	3.20	25 (42%)
11	CLA	cB	816	2	63,67,73	2.15	20 (31%)	75,105,113	2.86	30 (40%)
11	CLA	cA	815	1	49,53,73	2.41	20 (40%)	59,89,113	3.09	26 (44%)
11	CLA	cB	839	21	69,73,73	2.00	19 (27%)	83,113,113	2.61	27 (32%)
11	CLA	bB	813	2	60,64,73	2.15	21 (35%)	72,102,113	2.84	30 (41%)
11	CLA	cA	813	11,1	58,62,73	2.22	20 (34%)	69,99,113	2.90	27 (39%)
14	SF4	aC	101	3	0,12,12	-	-	-		
11	CLA	cA	804	1	49,53,73	2.43	20 (40%)	59,89,113	3.14	26 (44%)
11	CLA	cL	205	8	69,73,73	2.00	20 (28%)	83,113,113	2.70	27 (32%)
11	CLA	bA	812	1	69,73,73	2.06	20 (28%)	83,113,113	2.70	28 (33%)
15	BCR	aI	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	F6C	bL	202	2	72,74,74	2.49	28 (38%)	81,114,114	3.51	36 (44%)
11	CLA	cB	837	2	59,63,73	2.19	20 (33%)	71,101,113	2.90	28 (39%)
11	CLA	cA	803	-	60,64,73	2.12	19 (31%)	72,102,113	2.96	30 (41%)
11	CLA	cA	822	21	69,73,73	2.02	19 (27%)	83,113,113	2.59	28 (33%)
15	BCR	bL	207	-	41,41,41	1.05	2 (4%)	56,56,56	1.41	9 (16%)
11	CLA	cA	811	11,1	49,53,73	2.44	20 (40%)	59,89,113	3.13	25 (42%)
11	CLA	cB	805	2	69,73,73	2.01	20 (28%)	83,113,113	2.78	30 (36%)
11	CLA	cA	809	1	49,53,73	2.40	21 (42%)	59,89,113	3.20	27 (45%)
11	CLA	cB	838	2	51,55,73	2.33	20 (39%)	61,91,113	3.19	27 (44%)
11	CLA	aA	840	1	69,73,73	2.02	20 (28%)	83,113,113	2.93	32 (38%)
11	CLA	bA	840	1	69,73,73	2.02	20 (28%)	83,113,113	2.93	33 (39%)
11	CLA	aA	821	1	65,69,73	2.06	21 (32%)	78,108,113	2.72	30 (38%)
11	CLA	aB	817	2	64,68,73	2.08	19 (29%)	77,107,113	2.90	29 (37%)
11	CLA	aA	831	1	69,73,73	1.99	19 (27%)	83,113,113	2.68	29 (34%)
15	BCR	bA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.35	7 (12%)
11	CLA	bA	838	1	55,59,73	2.24	20 (36%)	66,96,113	3.06	33 (50%)
11	CLA	cA	807	1	69,73,73	2.00	20 (28%)	83,113,113	2.79	32 (38%)
11	CLA	cA	838	1	55,59,73	2.24	20 (36%)	66,96,113	3.05	32 (48%)
15	BCR	bB	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	5 (8%)
11	CLA	bB	814	2	49,53,73	2.41	21 (42%)	59,89,113	3.17	27 (45%)
11	CLA	aB	802	21	61,65,73	2.13	20 (32%)	73,103,113	3.05	30 (41%)
11	CLA	aB	815	2	59,63,73	2.18	21 (35%)	71,101,113	2.93	28 (39%)
11	CLA	aL	206	21	69,73,73	2.01	20 (28%)	83,113,113	2.72	30 (36%)
11	CLA	aA	808	1	55,59,73	2.27	21 (38%)	66,96,113	3.10	27 (40%)
11	CLA	cA	810	1	49,53,73	2.38	20 (40%)	59,89,113	3.07	27 (45%)
15	BCR	cM	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)
11	CLA	cB	825	2	69,73,73	2.02	20 (28%)	83,113,113	2.78	29 (34%)
11	CLA	aA	842	-	49,53,73	2.42	21 (42%)	59,89,113	3.18	26 (44%)
11	CLA	cA	814	1	69,73,73	2.03	20 (28%)	83,113,113	2.76	30 (36%)
11	CLA	cA	833	1	69,73,73	2.03	20 (28%)	83,113,113	2.71	27 (32%)
11	CLA	bA	829	1	69,73,73	2.03	21 (30%)	83,113,113	4.59	31 (37%)
12	F6C	aA	844	21	72,74,74	2.47	27 (37%)	81,114,114	3.71	37 (45%)
11	CLA	bB	826	2	65,69,73	2.03	21 (32%)	78,108,113	2.86	30 (38%)
17	LMT	cA	853	-	36,36,36	0.39	0	47,47,47	1.37	5 (10%)
15	BCR	bI	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	cA	802	21	69,73,73	1.99	20 (28%)	83,113,113	2.90	35 (42%)
15	BCR	aB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
15	BCR	aB	843	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
11	CLA	cB	834	-	49,53,73	2.44	20 (40%)	59,89,113	3.03	25 (42%)
11	CLA	bB	831	2	60,64,73	2.19	20 (33%)	72,102,113	3.08	31 (43%)
11	CLA	bB	811	2	49,53,73	2.45	20 (40%)	59,89,113	3.09	24 (40%)
11	CLA	cB	840	2	49,53,73	2.37	19 (38%)	59,89,113	3.09	24 (40%)
11	CLA	bA	804	1	49,53,73	2.44	20 (40%)	59,89,113	3.15	25 (42%)
15	BCR	bB	843	-	41,41,41	1.04	2 (4%)	56,56,56	1.15	3 (5%)
11	CLA	cB	804	2	54,58,73	2.29	21 (38%)	65,95,113	3.15	32 (49%)
11	CLA	cB	807	2	65,69,73	2.04	20 (30%)	78,108,113	2.82	29 (37%)
11	CLA	aB	835	-	49,53,73	2.43	21 (42%)	59,89,113	3.14	26 (44%)
11	CLA	cA	828	1	64,68,73	2.06	19 (29%)	77,107,113	2.93	31 (40%)
12	F6C	cA	830	1	72,74,74	2.44	26 (36%)	81,114,114	3.64	35 (43%)
11	CLA	bA	821	1	65,69,73	2.07	21 (32%)	78,108,113	2.72	30 (38%)
14	SF4	cA	846	2,1	0,12,12	-	-	-		
11	CLA	aA	818	1	58,62,73	2.15	20 (34%)	69,99,113	3.07	27 (39%)
11	CLA	aA	823	1	49,53,73	2.36	20 (40%)	59,89,113	3.26	24 (40%)
11	CLA	cA	806	1	69,73,73	2.01	20 (28%)	83,113,113	2.82	31 (37%)
11	CLA	aA	815	1	49,53,73	2.41	20 (40%)	59,89,113	3.09	26 (44%)
11	CLA	aB	804	2	54,58,73	2.28	21 (38%)	65,95,113	3.16	32 (49%)
12	F6C	aL	202	2	72,74,74	2.49	28 (38%)	81,114,114	3.51	36 (44%)
11	CLA	aA	822	21	69,73,73	2.02	19 (27%)	83,113,113	2.60	27 (32%)
11	CLA	cA	836	1	49,53,73	2.31	19 (38%)	59,89,113	2.99	25 (42%)
11	CLA	bA	803	-	60,64,73	2.12	18 (30%)	72,102,113	2.95	30 (41%)
11	CLA	cB	808	2	69,73,73	1.97	20 (28%)	83,113,113	2.70	29 (34%)
11	CLA	aA	810	1	49,53,73	2.38	21 (42%)	59,89,113	3.08	27 (45%)
11	CLA	aB	829	2	49,53,73	2.38	19 (38%)	59,89,113	3.12	27 (45%)
15	BCR	aB	842	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	4 (7%)
11	CLA	bA	809	1	49,53,73	2.40	21 (42%)	59,89,113	3.20	27 (45%)
11	CLA	bA	835	1	69,73,73	2.00	19 (27%)	83,113,113	2.75	28 (33%)
15	BCR	cL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.24	6 (10%)
11	CLA	aB	813	2	60,64,73	2.15	21 (35%)	72,102,113	2.85	30 (41%)
15	BCR	aA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
11	CLA	cB	836	2	55,59,73	2.26	20 (36%)	66,96,113	3.04	29 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	bB	848	-	41,41,41	1.00	2 (4%)	56,56,56	1.42	8 (14%)
11	CLA	cB	802	21	61,65,73	2.13	20 (32%)	73,103,113	3.04	30 (41%)
11	CLA	cB	815	2	59,63,73	2.19	21 (35%)	71,101,113	2.93	28 (39%)
11	CLA	cA	825	1	69,73,73	2.00	20 (28%)	83,113,113	2.66	31 (37%)
15	BCR	cB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	5 (8%)
11	CLA	cL	204	8	69,73,73	2.01	21 (30%)	83,113,113	2.73	26 (31%)
10	CL0	aA	801	1	69,73,73	1.99	20 (28%)	83,113,113	2.82	32 (38%)
11	CLA	bA	823	1	49,53,73	2.36	20 (40%)	59,89,113	3.26	24 (40%)
11	CLA	aB	808	2	69,73,73	1.97	20 (28%)	83,113,113	2.71	29 (34%)
15	BCR	aL	207	-	41,41,41	1.05	2 (4%)	56,56,56	1.41	9 (16%)
11	CLA	bB	838	2	51,55,73	2.33	20 (39%)	61,91,113	3.18	27 (44%)
11	CLA	cB	803	-	65,69,73	2.01	20 (30%)	78,108,113	2.80	26 (33%)
11	CLA	aB	801	2	69,73,73	1.94	20 (28%)	83,113,113	2.85	34 (40%)
12	F6C	cB	824	21	64,66,74	2.58	27 (42%)	71,104,114	4.08	36 (50%)
11	CLA	cB	835	-	49,53,73	2.43	21 (42%)	59,89,113	3.15	26 (44%)
11	CLA	cB	811	2	49,53,73	2.44	20 (40%)	59,89,113	3.09	24 (40%)
11	CLA	aA	839	1	69,73,73	1.99	19 (27%)	83,113,113	2.70	29 (34%)
15	BCR	aB	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	5 (8%)
13	PQN	cA	845	-	34,34,34	1.60	2 (5%)	42,45,45	1.11	4 (9%)
11	CLA	aB	812	2	69,73,73	2.04	21 (30%)	83,113,113	2.69	31 (37%)
11	CLA	cA	816	1	49,53,73	2.43	21 (42%)	59,89,113	3.11	24 (40%)
11	CLA	aA	824	-	55,59,73	2.26	19 (34%)	66,96,113	3.02	29 (43%)
11	CLA	aA	820	1	69,73,73	2.01	19 (27%)	83,113,113	2.70	31 (37%)
11	CLA	aB	810	2	49,53,73	2.40	20 (40%)	59,89,113	3.14	27 (45%)
11	CLA	bB	820	2	49,53,73	2.39	20 (40%)	59,89,113	3.19	25 (42%)
15	BCR	bK	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	7 (12%)
14	SF4	bA	846	2,1	0,12,12	-	-	-		
12	F6C	cA	826	21	72,74,74	2.51	24 (33%)	81,114,114	3.53	33 (40%)
15	BCR	cB	842	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	4 (7%)
11	CLA	aB	832	2	49,53,73	2.44	21 (42%)	59,89,113	3.17	26 (44%)
11	CLA	cB	819	2	51,55,73	2.35	21 (41%)	61,91,113	3.00	27 (44%)
11	CLA	aB	809	2	51,55,73	2.28	19 (37%)	61,91,113	3.05	26 (42%)
11	CLA	aA	829	1	69,73,73	2.03	21 (30%)	83,113,113	4.59	31 (37%)
17	LMT	bA	853	-	36,36,36	0.40	0	47,47,47	1.37	5 (10%)
11	CLA	bK	101	7	43,46,73	2.33	17 (39%)	51,79,113	3.30	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aA	802	21	69,73,73	1.99	20 (28%)	83,113,113	2.89	35 (42%)
11	CLA	cA	818	1	58,62,73	2.15	20 (34%)	69,99,113	3.08	27 (39%)
18	LMG	bB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.37	8 (14%)
11	CLA	bB	819	2	51,55,73	2.35	21 (41%)	61,91,113	3.00	27 (44%)
11	CLA	bB	822	2	49,53,73	2.38	18 (36%)	59,89,113	3.32	25 (42%)
11	CLA	bA	819	1	58,62,73	2.21	19 (32%)	69,99,113	3.00	27 (39%)
12	F6C	bA	832	1	57,59,74	2.74	27 (47%)	63,96,114	4.21	36 (57%)
11	CLA	aA	841	1	54,58,73	2.30	21 (38%)	65,95,113	3.07	29 (44%)
11	CLA	aB	807	2	65,69,73	2.04	20 (30%)	78,108,113	2.83	29 (37%)
11	CLA	cK	103	21	55,59,73	2.27	21 (38%)	66,96,113	3.07	28 (42%)
11	CLA	bB	809	2	51,55,73	2.29	20 (39%)	61,91,113	3.06	26 (42%)
11	CLA	cA	821	1	65,69,73	2.07	21 (32%)	78,108,113	2.72	30 (38%)
11	CLA	cB	832	2	49,53,73	2.45	21 (42%)	59,89,113	3.16	26 (44%)
15	BCR	cB	846	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	5 (8%)
11	CLA	aB	822	2	49,53,73	2.38	18 (36%)	59,89,113	3.32	25 (42%)
11	CLA	aB	814	2	49,53,73	2.40	20 (40%)	59,89,113	3.18	27 (45%)
15	BCR	cA	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	8 (14%)
11	CLA	cB	812	2	69,73,73	2.03	21 (30%)	83,113,113	2.67	30 (36%)
11	CLA	bA	807	1	69,73,73	2.00	20 (28%)	83,113,113	2.79	32 (38%)
11	CLA	bB	829	2	49,53,73	2.39	19 (38%)	59,89,113	3.13	27 (45%)
11	CLA	aB	837	2	59,63,73	2.18	20 (33%)	71,101,113	2.89	28 (39%)
11	CLA	bA	831	1	69,73,73	2.00	19 (27%)	83,113,113	2.68	29 (34%)
11	CLA	bB	804	2	54,58,73	2.29	21 (38%)	65,95,113	3.15	32 (49%)
12	F6C	aA	832	1	57,59,74	2.74	27 (47%)	63,96,114	4.21	36 (57%)
13	PQN	cB	841	-	29,29,34	1.70	2 (6%)	36,39,45	1.18	4 (11%)
15	BCR	aL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	8 (14%)
11	CLA	cA	817	21	53,57,73	2.33	21 (39%)	62,93,113	3.01	26 (41%)
11	CLA	bA	839	1	69,73,73	1.99	19 (27%)	83,113,113	2.71	29 (34%)
11	CLA	aB	827	2	69,73,73	1.98	20 (28%)	83,113,113	2.57	27 (32%)
11	CLA	aA	825	1	69,73,73	2.00	20 (28%)	83,113,113	2.66	31 (37%)
11	CLA	cB	828	2	59,63,73	2.19	18 (30%)	71,101,113	2.78	29 (40%)
11	CLA	aB	826	2	65,69,73	2.03	21 (32%)	78,108,113	2.84	30 (38%)
11	CLA	cA	820	1	69,73,73	2.02	19 (27%)	83,113,113	2.70	31 (37%)
12	F6C	aB	824	21	64,66,74	2.59	27 (42%)	71,104,114	4.08	36 (50%)
15	BCR	cI	103	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aA	833	1	69,73,73	2.03	20 (28%)	83,113,113	2.71	27 (32%)
11	CLA	cB	831	2	60,64,73	2.19	20 (33%)	72,102,113	3.09	30 (41%)
11	CLA	bB	828	2	59,63,73	2.19	18 (30%)	71,101,113	2.78	28 (39%)
12	F6C	bA	844	21	72,74,74	2.47	27 (37%)	81,114,114	3.72	37 (45%)
11	CLA	aA	807	1	69,73,73	2.00	20 (28%)	83,113,113	2.78	32 (38%)
11	CLA	bB	836	2	55,59,73	2.27	20 (36%)	66,96,113	3.04	29 (43%)
15	BCR	bA	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	6 (10%)
11	CLA	cB	809	2	51,55,73	2.28	20 (39%)	61,91,113	3.05	26 (42%)
11	CLA	bB	815	2	59,63,73	2.18	21 (35%)	71,101,113	2.94	28 (39%)
11	CLA	cB	827	2	69,73,73	1.98	20 (28%)	83,113,113	2.58	27 (32%)
15	BCR	cL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.40	9 (16%)
11	CLA	cA	824	-	55,59,73	2.25	19 (34%)	66,96,113	3.02	30 (45%)
18	LMG	aB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.37	8 (14%)
15	BCR	aA	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	5 (8%)
11	CLA	cB	822	2	49,53,73	2.37	18 (36%)	59,89,113	3.31	25 (42%)
15	BCR	cA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	3 (5%)
11	CLA	bB	803	-	65,69,73	2.01	20 (30%)	78,108,113	2.80	26 (33%)
11	CLA	bB	805	2	69,73,73	2.01	20 (28%)	83,113,113	2.79	30 (36%)
12	F6C	bB	824	21	64,66,74	2.59	27 (42%)	71,104,114	4.08	36 (50%)
11	CLA	bB	835	-	49,53,73	2.43	21 (42%)	59,89,113	3.15	26 (44%)
11	CLA	cA	812	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
11	CLA	bB	825	2	69,73,73	2.03	20 (28%)	83,113,113	2.78	29 (34%)
11	CLA	cB	801	2	69,73,73	1.94	20 (28%)	83,113,113	2.84	34 (40%)
11	CLA	aB	803	-	65,69,73	2.01	20 (30%)	78,108,113	2.80	26 (33%)
11	CLA	bA	818	1	58,62,73	2.15	20 (34%)	69,99,113	3.07	27 (39%)
15	BCR	bA	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	8 (14%)
11	CLA	bA	815	1	49,53,73	2.41	20 (40%)	59,89,113	3.09	26 (44%)
14	SF4	bC	102	3	0,12,12	-	-	-		
15	BCR	aL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.25	6 (10%)
11	CLA	cB	829	2	49,53,73	2.38	19 (38%)	59,89,113	3.14	27 (45%)
11	CLA	bL	206	21	69,73,73	2.00	20 (28%)	83,113,113	2.72	29 (34%)
11	CLA	bB	834	-	49,53,73	2.44	20 (40%)	59,89,113	3.03	25 (42%)
11	CLA	aA	806	1	69,73,73	2.01	20 (28%)	83,113,113	2.82	31 (37%)
12	F6C	bA	826	21	72,74,74	2.51	24 (33%)	81,114,114	3.53	33 (40%)
11	CLA	bB	801	2	69,73,73	1.94	19 (27%)	83,113,113	2.84	34 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	bB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
15	BCR	bB	844	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	5 (8%)
11	CLA	cB	814	2	49,53,73	2.40	20 (40%)	59,89,113	3.17	27 (45%)
15	BCR	bA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
11	CLA	aB	833	2	49,53,73	2.44	20 (40%)	59,89,113	3.21	27 (45%)
11	CLA	aA	803	-	60,64,73	2.13	18 (30%)	72,102,113	2.96	30 (41%)
11	CLA	bA	814	1	69,73,73	2.03	21 (30%)	83,113,113	2.77	29 (34%)
11	CLA	bA	843	1	55,59,73	2.27	20 (36%)	66,96,113	2.98	28 (42%)
11	CLA	aA	835	1	69,73,73	2.00	19 (27%)	83,113,113	2.75	28 (33%)
11	CLA	cL	206	21	69,73,73	2.00	20 (28%)	83,113,113	2.72	29 (34%)
15	BCR	aA	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	8 (14%)
11	CLA	cA	839	1	69,73,73	1.99	19 (27%)	83,113,113	2.70	29 (34%)
18	LMG	cB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.37	8 (14%)
11	CLA	aB	840	2	49,53,73	2.37	19 (38%)	59,89,113	3.08	24 (40%)
12	F6C	bA	830	1	72,74,74	2.43	25 (34%)	81,114,114	3.64	35 (43%)
12	F6C	cA	844	21	72,74,74	2.47	27 (37%)	81,114,114	3.73	37 (45%)
11	CLA	cB	818	-	69,73,73	2.01	19 (27%)	83,113,113	2.65	25 (30%)
11	CLA	bB	832	2	49,53,73	2.45	21 (42%)	59,89,113	3.17	26 (44%)
12	F6C	aA	830	1	72,74,74	2.43	26 (36%)	81,114,114	3.65	35 (43%)
11	CLA	bA	833	1	69,73,73	2.03	20 (28%)	83,113,113	2.71	27 (32%)
11	CLA	bL	205	8	69,73,73	2.01	20 (28%)	83,113,113	2.70	27 (32%)
11	CLA	cB	830	2	53,57,73	2.33	21 (39%)	62,93,113	3.04	27 (43%)
11	CLA	aB	818	-	69,73,73	2.01	19 (27%)	83,113,113	2.65	24 (28%)
14	SF4	bC	101	3	0,12,12	-	-	-		
11	CLA	aA	819	1	58,62,73	2.21	20 (34%)	69,99,113	3.01	28 (40%)
11	CLA	bL	204	8	69,73,73	2.01	21 (30%)	83,113,113	2.74	26 (31%)
11	CLA	aA	813	11,1	58,62,73	2.22	20 (34%)	69,99,113	2.90	27 (39%)
11	CLA	bA	820	1	69,73,73	2.01	19 (27%)	83,113,113	2.71	31 (37%)
11	CLA	cB	821	-	59,63,73	2.23	21 (35%)	71,101,113	2.89	27 (38%)
10	CL0	cA	801	1	69,73,73	1.99	20 (28%)	83,113,113	2.82	32 (38%)
11	CLA	cB	810	2	49,53,73	2.39	20 (40%)	59,89,113	3.13	27 (45%)
11	CLA	aB	830	2	53,57,73	2.33	21 (39%)	62,93,113	3.04	26 (41%)
15	BCR	bB	842	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	4 (7%)
11	CLA	bB	810	2	49,53,73	2.39	20 (40%)	59,89,113	3.13	27 (45%)
11	CLA	aK	103	21	55,59,73	2.27	21 (38%)	66,96,113	3.05	28 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aB	820	2	49,53,73	2.39	20 (40%)	59,89,113	3.21	25 (42%)
16	LHG	aA	852	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
11	CLA	cB	833	2	49,53,73	2.44	20 (40%)	59,89,113	3.21	27 (45%)
15	BCR	aA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	4 (7%)
15	BCR	bA	850	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	4 (7%)
11	CLA	aL	205	8	69,73,73	2.01	21 (30%)	83,113,113	2.69	27 (32%)
11	CLA	bB	806	2	69,73,73	1.99	19 (27%)	83,113,113	2.72	28 (33%)
11	CLA	bA	817	21	53,57,73	2.33	21 (39%)	62,93,113	3.02	26 (41%)
11	CLA	cB	817	2	64,68,73	2.08	19 (29%)	77,107,113	2.91	30 (38%)
11	CLA	aA	837	1	49,53,73	2.41	21 (42%)	59,89,113	3.21	26 (44%)
11	CLA	bK	103	21	55,59,73	2.27	21 (38%)	66,96,113	3.07	28 (42%)
11	CLA	bB	802	21	61,65,73	2.13	20 (32%)	73,103,113	3.04	30 (41%)
13	PQN	aB	841	-	29,29,34	1.68	2 (6%)	36,39,45	1.17	4 (11%)
15	BCR	aB	844	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	5 (8%)
11	CLA	aA	805	1	49,53,73	2.44	21 (42%)	59,89,113	3.19	25 (42%)
11	CLA	cB	820	2	49,53,73	2.40	20 (40%)	59,89,113	3.20	25 (42%)
15	BCR	aA	847	-	41,41,41	1.04	2 (4%)	56,56,56	1.34	7 (12%)
11	CLA	aA	838	1	55,59,73	2.25	20 (36%)	66,96,113	3.06	31 (46%)
11	CLA	aB	805	2	69,73,73	2.01	20 (28%)	83,113,113	2.79	30 (36%)
11	CLA	bB	812	2	69,73,73	2.04	20 (28%)	83,113,113	2.68	30 (36%)
16	LHG	bA	852	-	48,48,48	0.60	1 (2%)	51,54,54	1.25	6 (11%)
11	CLA	bB	823	2	58,62,73	2.19	21 (36%)	69,99,113	2.98	29 (42%)
11	CLA	cA	841	1	54,58,73	2.30	21 (38%)	65,95,113	3.07	29 (44%)
11	CLA	cA	843	1	55,59,73	2.27	20 (36%)	66,96,113	2.99	28 (42%)
15	BCR	cA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	7 (12%)
11	CLA	aA	828	1	64,68,73	2.06	19 (29%)	77,107,113	2.92	31 (40%)
11	CLA	bA	828	1	64,68,73	2.06	19 (29%)	77,107,113	2.93	31 (40%)
15	BCR	cA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
13	PQN	bA	845	-	34,34,34	1.60	2 (5%)	42,45,45	1.10	4 (9%)
11	CLA	bA	825	1	69,73,73	2.00	20 (28%)	83,113,113	2.67	31 (37%)
11	CLA	bB	837	2	59,63,73	2.19	20 (33%)	71,101,113	2.90	28 (39%)
15	BCR	aK	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	8 (14%)
12	F6C	cL	202	2	72,74,74	2.49	28 (38%)	81,114,114	3.51	35 (43%)
11	CLA	bA	806	1	69,73,73	2.01	20 (28%)	83,113,113	2.82	31 (37%)
13	PQN	aA	845	-	34,34,34	1.60	2 (5%)	42,45,45	1.11	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	cA	823	1	49,53,73	2.36	20 (40%)	59,89,113	3.26	24 (40%)
11	CLA	aB	806	2	69,73,73	2.00	19 (27%)	83,113,113	2.72	28 (33%)
11	CLA	bA	841	1	54,58,73	2.30	21 (38%)	65,95,113	3.07	29 (44%)
11	CLA	bB	840	2	49,53,73	2.37	19 (38%)	59,89,113	3.08	24 (40%)
11	CLA	bB	807	2	65,69,73	2.04	20 (30%)	78,108,113	2.83	29 (37%)
15	BCR	bM	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	8 (14%)
11	CLA	aB	836	2	55,59,73	2.26	19 (34%)	66,96,113	3.05	29 (43%)
15	BCR	cB	844	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	5 (8%)
11	CLA	bB	816	2	63,67,73	2.14	20 (31%)	75,105,113	2.85	30 (40%)
11	CLA	bA	834	1	69,73,73	2.00	20 (28%)	83,113,113	2.72	32 (38%)
11	CLA	bA	824	-	55,59,73	2.26	19 (34%)	66,96,113	3.02	30 (45%)
11	CLA	aA	809	1	49,53,73	2.40	21 (42%)	59,89,113	3.21	27 (45%)
11	CLA	aB	821	-	59,63,73	2.23	21 (35%)	71,101,113	2.90	27 (38%)
11	CLA	aA	834	1	69,73,73	2.00	20 (28%)	83,113,113	2.72	32 (38%)
11	CLA	aL	204	8	69,73,73	2.00	21 (30%)	83,113,113	2.73	25 (30%)
11	CLA	cB	806	2	69,73,73	1.99	19 (27%)	83,113,113	2.71	29 (34%)
11	CLA	aB	828	2	59,63,73	2.19	18 (30%)	71,101,113	2.77	30 (42%)
11	CLA	cA	808	1	55,59,73	2.27	21 (38%)	66,96,113	3.10	27 (40%)
12	F6C	bA	827	21	62,64,74	2.66	26 (41%)	69,102,114	4.11	36 (52%)
11	CLA	cA	837	1	49,53,73	2.42	21 (42%)	59,89,113	3.22	26 (44%)
11	CLA	cB	826	2	65,69,73	2.03	21 (32%)	78,108,113	2.85	30 (38%)
11	CLA	aB	834	-	49,53,73	2.45	20 (40%)	59,89,113	3.03	25 (42%)
11	CLA	bB	818	-	69,73,73	2.01	19 (27%)	83,113,113	2.65	25 (30%)
15	BCR	aM	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	7 (12%)
11	CLA	aA	804	1	49,53,73	2.43	20 (40%)	59,89,113	3.13	26 (44%)
11	CLA	aA	812	1	69,73,73	2.06	21 (30%)	83,113,113	2.69	28 (33%)
11	CLA	aA	814	1	69,73,73	2.03	20 (28%)	83,113,113	2.77	30 (36%)
11	CLA	bB	839	21	69,73,73	2.00	19 (27%)	83,113,113	2.61	27 (32%)
11	CLA	aA	843	1	55,59,73	2.28	20 (36%)	66,96,113	2.98	28 (42%)
11	CLA	bB	821	-	59,63,73	2.23	21 (35%)	71,101,113	2.90	27 (38%)
11	CLA	aB	825	2	69,73,73	2.03	20 (28%)	83,113,113	2.77	29 (34%)
15	BCR	bL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
15	BCR	cA	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.28	5 (8%)
11	CLA	bB	827	2	69,73,73	1.98	20 (28%)	83,113,113	2.58	26 (31%)
11	CLA	bA	842	-	49,53,73	2.41	21 (42%)	59,89,113	3.17	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aB	831	2	60,64,73	2.19	20 (33%)	72,102,113	3.08	31 (43%)
11	CLA	bA	836	1	49,53,73	2.32	19 (38%)	59,89,113	2.99	25 (42%)
11	CLA	bA	808	1	55,59,73	2.27	21 (38%)	66,96,113	3.10	27 (40%)
12	F6C	aA	827	21	62,64,74	2.66	26 (41%)	69,102,114	4.11	36 (52%)
11	CLA	aA	836	1	49,53,73	2.32	19 (38%)	59,89,113	3.00	25 (42%)
11	CLA	aA	817	21	53,57,73	2.33	21 (39%)	62,93,113	3.02	26 (41%)
11	CLA	aB	839	21	69,73,73	1.99	19 (27%)	83,113,113	2.61	27 (32%)
15	BCR	cK	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	8 (14%)
15	BCR	cL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
12	F6C	aA	826	21	72,74,74	2.51	24 (33%)	81,114,114	3.53	33 (40%)
11	CLA	bB	830	2	53,57,73	2.33	21 (39%)	62,93,113	3.04	26 (41%)
11	CLA	cA	829	1	69,73,73	2.03	21 (30%)	83,113,113	4.59	31 (37%)
11	CLA	bA	810	1	49,53,73	2.38	21 (42%)	59,89,113	3.08	27 (45%)
11	CLA	cK	101	7	43,46,73	2.33	17 (39%)	51,79,113	3.30	25 (49%)
11	CLA	aK	101	7	43,46,73	2.34	17 (39%)	51,79,113	3.30	25 (49%)
11	CLA	bA	822	21	69,73,73	2.02	19 (27%)	83,113,113	2.60	27 (32%)
11	CLA	cA	819	1	58,62,73	2.21	20 (34%)	69,99,113	3.00	28 (40%)
11	CLA	aA	816	1	49,53,73	2.42	21 (42%)	59,89,113	3.11	24 (40%)
12	F6C	cA	832	1	57,59,74	2.74	27 (47%)	63,96,114	4.20	36 (57%)
11	CLA	bA	811	11,1	49,53,73	2.43	20 (40%)	59,89,113	3.12	24 (40%)
11	CLA	cA	831	1	69,73,73	1.99	18 (26%)	83,113,113	2.67	29 (34%)
11	CLA	aA	811	11,1	49,53,73	2.43	20 (40%)	59,89,113	3.11	24 (40%)
11	CLA	aB	816	2	63,67,73	2.15	20 (31%)	75,105,113	2.86	30 (40%)

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
14	SF4	aA	846	2,1	-	-	0/6/5/5
10	CL0	bA	801	1	-	5/39/115/115	-
14	SF4	cC	101	3	-	-	0/6/5/5
11	CLA	cA	834	1	-	9/39/115/115	-
11	CLA	aB	811	2	-	5/15/91/115	-
11	CLA	cB	823	2	-	9/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cA	835	1	-	13/39/115/115	-
15	BCR	bL	203	-	-	8/29/63/63	0/2/2/2
11	CLA	aB	823	2	-	9/26/102/115	-
17	LMT	aA	853	-	-	12/21/61/61	0/2/2/2
11	CLA	bB	817	2	-	14/33/109/115	-
11	CLA	bB	833	2	-	5/15/91/115	-
11	CLA	bB	808	2	-	11/39/115/115	-
11	CLA	cA	840	1	-	19/39/115/115	-
11	CLA	bA	816	1	-	5/15/91/115	-
11	CLA	cA	842	-	-	8/15/91/115	-
14	SF4	cC	102	3	-	-	0/6/5/5
11	CLA	aB	819	2	-	9/18/94/115	-
15	BCR	cB	848	-	-	18/29/63/63	0/2/2/2
15	BCR	cB	843	-	-	9/29/63/63	0/2/2/2
11	CLA	bA	837	1	-	6/15/91/115	-
11	CLA	cA	805	1	-	8/15/91/115	-
11	CLA	aB	838	2	-	5/18/94/115	-
13	PQN	bB	841	-	-	2/17/37/43	0/2/2/2
11	CLA	cB	813	2	-	10/29/105/115	-
14	SF4	aC	102	3	-	-	0/6/5/5
15	BCR	aB	848	-	-	18/29/63/63	0/2/2/2
11	CLA	bA	802	21	-	6/39/115/115	-
16	LHG	cA	852	-	-	27/53/53/53	-
12	F6C	cA	827	21	2/2/8/16	11/29/85/97	-
11	CLA	bA	813	11,1	-	8/26/102/115	-
11	CLA	bA	805	1	-	8/15/91/115	-
11	CLA	cB	816	2	-	12/32/108/115	-
11	CLA	cA	815	1	-	5/15/91/115	-
11	CLA	cB	839	21	-	10/39/115/115	-
11	CLA	bB	813	2	-	10/29/105/115	-
11	CLA	cA	813	11,1	-	8/26/102/115	-
14	SF4	aC	101	3	-	-	0/6/5/5
11	CLA	cA	804	1	-	11/15/91/115	-
11	CLA	cL	205	8	-	15/39/115/115	-
11	CLA	bA	812	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	aI	101	-	-	11/29/63/63	0/2/2/2
12	F6C	bL	202	2	1/1/10/16	16/41/97/97	-
11	CLA	cB	837	2	-	8/27/103/115	-
11	CLA	cA	803	-	-	7/29/105/115	-
11	CLA	cA	822	21	-	19/39/115/115	-
15	BCR	bL	207	-	-	9/29/63/63	0/2/2/2
11	CLA	cA	811	11,1	-	5/15/91/115	-
11	CLA	cB	805	2	-	13/39/115/115	-
11	CLA	cA	809	1	-	8/15/91/115	-
11	CLA	cB	838	2	-	5/18/94/115	-
11	CLA	aA	840	1	-	19/39/115/115	-
11	CLA	bA	840	1	-	19/39/115/115	-
11	CLA	aA	821	1	-	16/35/111/115	-
11	CLA	aB	817	2	-	14/33/109/115	-
11	CLA	aA	831	1	-	12/39/115/115	-
15	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
11	CLA	bA	838	1	-	9/23/99/115	-
11	CLA	cA	807	1	-	18/39/115/115	-
11	CLA	cA	838	1	-	9/23/99/115	-
15	BCR	bB	846	-	-	13/29/63/63	0/2/2/2
11	CLA	bB	814	2	-	6/15/91/115	-
11	CLA	aB	802	21	-	10/30/106/115	-
11	CLA	aB	815	2	-	13/27/103/115	-
11	CLA	aL	206	21	-	15/39/115/115	-
11	CLA	aA	808	1	-	5/23/99/115	-
11	CLA	cA	810	1	-	4/15/91/115	-
15	BCR	cM	101	-	-	7/29/63/63	0/2/2/2
11	CLA	cB	825	2	-	10/39/115/115	-
11	CLA	aA	842	-	-	8/15/91/115	-
11	CLA	cA	814	1	-	14/39/115/115	-
11	CLA	cA	833	1	-	14/39/115/115	-
11	CLA	bA	829	1	-	12/39/115/115	-
12	F6C	aA	844	21	1/1/10/16	13/41/97/97	-
11	CLA	bB	826	2	-	12/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LMT	cA	853	-	-	12/21/61/61	0/2/2/2
15	BCR	bI	101	-	-	11/29/63/63	0/2/2/2
11	CLA	cA	802	21	-	6/39/115/115	-
15	BCR	aB	845	-	-	9/29/63/63	0/2/2/2
15	BCR	aB	843	-	-	9/29/63/63	0/2/2/2
11	CLA	cB	834	-	-	6/15/91/115	-
11	CLA	bB	831	2	-	7/29/105/115	-
11	CLA	bB	811	2	-	5/15/91/115	-
11	CLA	cB	840	2	-	5/15/91/115	-
11	CLA	bA	804	1	-	11/15/91/115	-
15	BCR	bB	843	-	-	9/29/63/63	0/2/2/2
11	CLA	cB	804	2	-	8/21/97/115	-
11	CLA	cB	807	2	-	3/35/111/115	-
12	F6C	cA	830	1	1/1/10/16	7/41/97/97	-
11	CLA	aB	835	-	-	4/15/91/115	-
11	CLA	cA	828	1	-	12/33/109/115	-
11	CLA	bA	821	1	-	16/35/111/115	-
14	SF4	cA	846	2,1	-	-	0/6/5/5
11	CLA	aA	818	1	-	10/26/102/115	-
11	CLA	aA	823	1	-	9/15/91/115	-
11	CLA	cA	806	1	-	16/39/115/115	-
11	CLA	aA	815	1	-	5/15/91/115	-
11	CLA	aB	804	2	-	8/21/97/115	-
12	F6C	aL	202	2	1/1/10/16	16/41/97/97	-
11	CLA	aA	822	21	-	19/39/115/115	-
11	CLA	cA	836	1	-	6/15/91/115	-
11	CLA	bA	803	-	-	7/29/105/115	-
11	CLA	cB	808	2	-	10/39/115/115	-
11	CLA	aA	810	1	-	4/15/91/115	-
11	CLA	aB	829	2	-	6/15/91/115	-
15	BCR	aB	842	-	-	15/29/63/63	0/2/2/2
11	CLA	bA	809	1	-	8/15/91/115	-
11	CLA	bA	835	1	-	13/39/115/115	-
15	BCR	cL	203	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aB	813	2	-	10/29/105/115	-
15	BCR	aA	848	-	-	13/29/63/63	0/2/2/2
11	CLA	cB	836	2	-	10/23/99/115	-
15	BCR	bB	848	-	-	18/29/63/63	0/2/2/2
11	CLA	cB	802	21	-	10/30/106/115	-
11	CLA	cB	815	2	-	13/27/103/115	-
11	CLA	cA	825	1	-	14/39/115/115	-
15	BCR	cB	845	-	-	9/29/63/63	0/2/2/2
11	CLA	cL	204	8	-	5/39/115/115	-
10	CL0	aA	801	1	-	5/39/115/115	-
11	CLA	bA	823	1	-	9/15/91/115	-
11	CLA	aB	808	2	-	11/39/115/115	-
15	BCR	aL	207	-	-	9/29/63/63	0/2/2/2
11	CLA	bB	838	2	-	5/18/94/115	-
11	CLA	cB	803	-	-	7/35/111/115	-
11	CLA	aB	801	2	-	11/39/115/115	-
12	F6C	cB	824	21	1/1/8/16	9/32/88/97	-
11	CLA	cB	835	-	-	4/15/91/115	-
11	CLA	cB	811	2	-	5/15/91/115	-
11	CLA	aA	839	1	-	7/39/115/115	-
15	BCR	aB	846	-	-	13/29/63/63	0/2/2/2
13	PQN	cA	845	-	-	3/23/43/43	0/2/2/2
11	CLA	aB	812	2	-	18/39/115/115	-
11	CLA	cA	816	1	-	5/15/91/115	-
11	CLA	aA	824	-	-	12/23/99/115	-
11	CLA	aA	820	1	-	12/39/115/115	-
11	CLA	aB	810	2	-	7/15/91/115	-
11	CLA	bB	820	2	-	8/15/91/115	-
15	BCR	bK	102	-	-	8/29/63/63	0/2/2/2
14	SF4	bA	846	2,1	-	-	0/6/5/5
12	F6C	cA	826	21	1/1/10/16	11/41/97/97	-
15	BCR	cB	842	-	-	15/29/63/63	0/2/2/2
11	CLA	aB	832	2	-	9/15/91/115	-
11	CLA	cB	819	2	-	9/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aB	809	2	-	11/18/94/115	-
11	CLA	aA	829	1	-	12/39/115/115	-
17	LMT	bA	853	-	-	12/21/61/61	0/2/2/2
11	CLA	bK	101	7	-	2/6/78/115	-
11	CLA	aA	802	21	-	6/39/115/115	-
11	CLA	cA	818	1	-	10/26/102/115	-
18	LMG	bB	847	-	-	17/41/61/70	0/1/1/1
11	CLA	bB	819	2	-	9/18/94/115	-
11	CLA	bB	822	2	-	8/15/91/115	-
11	CLA	bA	819	1	-	12/26/102/115	-
12	F6C	bA	832	1	1/1/7/16	11/23/79/97	-
11	CLA	aA	841	1	-	6/21/97/115	-
11	CLA	aB	807	2	-	3/35/111/115	-
11	CLA	cK	103	21	-	6/23/99/115	-
11	CLA	bB	809	2	-	11/18/94/115	-
11	CLA	cA	821	1	-	16/35/111/115	-
11	CLA	cB	832	2	-	9/15/91/115	-
15	BCR	cB	846	-	-	13/29/63/63	0/2/2/2
11	CLA	aB	822	2	-	8/15/91/115	-
11	CLA	aB	814	2	-	6/15/91/115	-
15	BCR	cA	851	-	-	20/29/63/63	0/2/2/2
11	CLA	cB	812	2	-	18/39/115/115	-
11	CLA	bA	807	1	-	18/39/115/115	-
11	CLA	bB	829	2	-	6/15/91/115	-
11	CLA	aB	837	2	-	8/27/103/115	-
11	CLA	bA	831	1	-	12/39/115/115	-
11	CLA	bB	804	2	-	8/21/97/115	-
12	F6C	aA	832	1	1/1/7/16	11/23/79/97	-
13	PQN	cB	841	-	-	2/17/37/43	0/2/2/2
15	BCR	aL	208	-	-	7/29/63/63	0/2/2/2
11	CLA	cA	817	21	-	7/20/96/115	-
11	CLA	bA	839	1	-	7/39/115/115	-
11	CLA	aB	827	2	-	10/39/115/115	-
11	CLA	aA	825	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cB	828	2	-	7/27/103/115	-
11	CLA	aB	826	2	-	12/35/111/115	-
11	CLA	cA	820	1	-	12/39/115/115	-
12	F6C	aB	824	21	1/1/8/16	9/32/88/97	-
15	BCR	cI	103	-	-	11/29/63/63	0/2/2/2
11	CLA	aA	833	1	-	14/39/115/115	-
11	CLA	cB	831	2	-	7/29/105/115	-
11	CLA	bB	828	2	-	7/27/103/115	-
12	F6C	bA	844	21	1/1/10/16	13/41/97/97	-
11	CLA	aA	807	1	-	18/39/115/115	-
11	CLA	bB	836	2	-	10/23/99/115	-
15	BCR	bA	849	-	-	12/29/63/63	0/2/2/2
11	CLA	cB	809	2	-	11/18/94/115	-
11	CLA	bB	815	2	-	13/27/103/115	-
11	CLA	cB	827	2	-	10/39/115/115	-
15	BCR	cL	207	-	-	9/29/63/63	0/2/2/2
11	CLA	cA	824	-	-	12/23/99/115	-
18	LMG	aB	847	-	-	17/41/61/70	0/1/1/1
15	BCR	aA	849	-	-	12/29/63/63	0/2/2/2
11	CLA	cB	822	2	-	8/15/91/115	-
15	BCR	cA	850	-	-	6/29/63/63	0/2/2/2
11	CLA	bB	803	-	-	7/35/111/115	-
11	CLA	bB	805	2	-	13/39/115/115	-
12	F6C	bB	824	21	1/1/8/16	9/32/88/97	-
11	CLA	bB	835	-	-	4/15/91/115	-
11	CLA	cA	812	1	-	13/39/115/115	-
11	CLA	bB	825	2	-	10/39/115/115	-
11	CLA	cB	801	2	-	11/39/115/115	-
11	CLA	aB	803	-	-	7/35/111/115	-
11	CLA	bA	818	1	-	10/26/102/115	-
15	BCR	bA	851	-	-	20/29/63/63	0/2/2/2
11	CLA	bA	815	1	-	5/15/91/115	-
14	SF4	bC	102	3	-	-	0/6/5/5
15	BCR	aL	203	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cB	829	2	-	6/15/91/115	-
11	CLA	bL	206	21	-	15/39/115/115	-
11	CLA	bB	834	-	-	7/15/91/115	-
11	CLA	aA	806	1	-	16/39/115/115	-
12	F6C	bA	826	21	1/1/10/16	11/41/97/97	-
11	CLA	bB	801	2	-	11/39/115/115	-
15	BCR	bB	845	-	-	9/29/63/63	0/2/2/2
15	BCR	bB	844	-	-	11/29/63/63	0/2/2/2
11	CLA	cB	814	2	-	6/15/91/115	-
15	BCR	bA	848	-	-	13/29/63/63	0/2/2/2
11	CLA	aB	833	2	-	5/15/91/115	-
11	CLA	aA	803	-	-	7/29/105/115	-
11	CLA	bA	814	1	-	14/39/115/115	-
11	CLA	bA	843	1	-	9/23/99/115	-
11	CLA	aA	835	1	-	13/39/115/115	-
11	CLA	cL	206	21	-	15/39/115/115	-
15	BCR	aA	851	-	-	20/29/63/63	0/2/2/2
11	CLA	cA	839	1	-	7/39/115/115	-
18	LMG	cB	847	-	-	17/41/61/70	0/1/1/1
12	F6C	bA	830	1	1/1/10/16	7/41/97/97	-
11	CLA	aB	840	2	-	5/15/91/115	-
12	F6C	cA	844	21	1/1/10/16	13/41/97/97	-
11	CLA	cB	818	-	-	8/39/115/115	-
11	CLA	bB	832	2	-	9/15/91/115	-
12	F6C	aA	830	1	1/1/10/16	7/41/97/97	-
11	CLA	bA	833	1	-	14/39/115/115	-
11	CLA	bL	205	8	-	15/39/115/115	-
11	CLA	cB	830	2	-	9/20/96/115	-
11	CLA	aB	818	-	-	8/39/115/115	-
14	SF4	bC	101	3	-	-	0/6/5/5
11	CLA	aA	819	1	-	12/26/102/115	-
11	CLA	bL	204	8	-	5/39/115/115	-
11	CLA	aA	813	11,1	-	8/26/102/115	-
11	CLA	bA	820	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cB	821	-	-	10/27/103/115	-
10	CL0	cA	801	1	-	5/39/115/115	-
11	CLA	cB	810	2	-	7/15/91/115	-
11	CLA	aB	830	2	-	9/20/96/115	-
15	BCR	bB	842	-	-	15/29/63/63	0/2/2/2
11	CLA	bB	810	2	-	7/15/91/115	-
11	CLA	aK	103	21	-	6/23/99/115	-
11	CLA	aB	820	2	-	8/15/91/115	-
16	LHG	aA	852	-	-	27/53/53/53	-
11	CLA	cB	833	2	-	5/15/91/115	-
15	BCR	aA	850	-	-	6/29/63/63	0/2/2/2
15	BCR	bA	850	-	-	6/29/63/63	0/2/2/2
11	CLA	aL	205	8	-	15/39/115/115	-
11	CLA	bB	806	2	-	20/39/115/115	-
11	CLA	bA	817	21	-	7/20/96/115	-
11	CLA	cB	817	2	-	14/33/109/115	-
11	CLA	aA	837	1	-	6/15/91/115	-
11	CLA	bK	103	21	-	6/23/99/115	-
11	CLA	bB	802	21	-	10/30/106/115	-
13	PQN	aB	841	-	-	2/17/37/43	0/2/2/2
15	BCR	aB	844	-	-	11/29/63/63	0/2/2/2
11	CLA	aA	805	1	-	8/15/91/115	-
11	CLA	cB	820	2	-	8/15/91/115	-
15	BCR	aA	847	-	-	9/29/63/63	0/2/2/2
11	CLA	aA	838	1	-	9/23/99/115	-
11	CLA	aB	805	2	-	13/39/115/115	-
11	CLA	bB	812	2	-	18/39/115/115	-
16	LHG	bA	852	-	-	27/53/53/53	-
11	CLA	bB	823	2	-	9/26/102/115	-
11	CLA	cA	841	1	-	6/21/97/115	-
11	CLA	cA	843	1	-	9/23/99/115	-
15	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
11	CLA	aA	828	1	-	12/33/109/115	-
11	CLA	bA	828	1	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	cA	848	-	-	13/29/63/63	0/2/2/2
13	PQN	bA	845	-	-	3/23/43/43	0/2/2/2
11	CLA	bA	825	1	-	14/39/115/115	-
11	CLA	bB	837	2	-	8/27/103/115	-
15	BCR	aK	102	-	-	8/29/63/63	0/2/2/2
12	F6C	cL	202	2	1/1/10/16	16/41/97/97	-
11	CLA	bA	806	1	-	16/39/115/115	-
13	PQN	aA	845	-	-	3/23/43/43	0/2/2/2
11	CLA	cA	823	1	-	9/15/91/115	-
11	CLA	aB	806	2	-	20/39/115/115	-
11	CLA	bA	841	1	-	6/21/97/115	-
11	CLA	bB	840	2	-	5/15/91/115	-
11	CLA	bB	807	2	-	3/35/111/115	-
15	BCR	bM	101	-	-	7/29/63/63	0/2/2/2
11	CLA	aB	836	2	-	10/23/99/115	-
15	BCR	cB	844	-	-	11/29/63/63	0/2/2/2
11	CLA	bB	816	2	-	12/32/108/115	-
11	CLA	bA	834	1	-	9/39/115/115	-
11	CLA	bA	824	-	-	12/23/99/115	-
11	CLA	aA	809	1	-	8/15/91/115	-
11	CLA	aB	821	-	-	10/27/103/115	-
11	CLA	aA	834	1	-	9/39/115/115	-
11	CLA	aL	204	8	-	5/39/115/115	-
11	CLA	cB	806	2	-	20/39/115/115	-
11	CLA	aB	828	2	-	7/27/103/115	-
11	CLA	cA	808	1	-	5/23/99/115	-
12	F6C	bA	827	21	2/2/8/16	11/29/85/97	-
11	CLA	cA	837	1	-	6/15/91/115	-
11	CLA	cB	826	2	-	12/35/111/115	-
11	CLA	aB	834	-	-	7/15/91/115	-
11	CLA	bB	818	-	-	8/39/115/115	-
15	BCR	aM	101	-	-	7/29/63/63	0/2/2/2
11	CLA	aA	804	1	-	11/15/91/115	-
11	CLA	aA	812	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aA	814	1	-	14/39/115/115	-
11	CLA	bB	839	21	-	10/39/115/115	-
11	CLA	aA	843	1	-	9/23/99/115	-
11	CLA	bB	821	-	-	10/27/103/115	-
11	CLA	aB	825	2	-	10/39/115/115	-
15	BCR	bL	208	-	-	7/29/63/63	0/2/2/2
15	BCR	cA	849	-	-	12/29/63/63	0/2/2/2
11	CLA	bB	827	2	-	10/39/115/115	-
11	CLA	bA	842	-	-	8/15/91/115	-
11	CLA	aB	831	2	-	7/29/105/115	-
11	CLA	bA	836	1	-	6/15/91/115	-
11	CLA	bA	808	1	-	5/23/99/115	-
12	F6C	aA	827	21	2/2/8/16	11/29/85/97	-
11	CLA	aA	836	1	-	6/15/91/115	-
11	CLA	aA	817	21	-	7/20/96/115	-
11	CLA	aB	839	21	-	10/39/115/115	-
15	BCR	cK	102	-	-	8/29/63/63	0/2/2/2
15	BCR	cL	208	-	-	7/29/63/63	0/2/2/2
12	F6C	aA	826	21	1/1/10/16	11/41/97/97	-
11	CLA	bB	830	2	-	9/20/96/115	-
11	CLA	cA	829	1	-	12/39/115/115	-
11	CLA	bA	810	1	-	4/15/91/115	-
11	CLA	cK	101	7	-	2/6/78/115	-
11	CLA	aK	101	7	-	2/6/78/115	-
11	CLA	bA	822	21	-	19/39/115/115	-
11	CLA	cA	819	1	-	12/26/102/115	-
11	CLA	aA	816	1	-	5/15/91/115	-
12	F6C	cA	832	1	1/1/7/16	11/23/79/97	-
11	CLA	bA	811	11,1	-	5/15/91/115	-
11	CLA	cA	831	1	-	12/39/115/115	-
11	CLA	aA	811	11,1	-	5/15/91/115	-
11	CLA	aB	816	2	-	12/32/108/115	-

The worst 5 of 5655 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	826	F6C	C2A-C3A	8.12	1.54	1.36
12	bA	826	F6C	C2A-C3A	8.11	1.54	1.36
12	cA	826	F6C	C1A-CHA	8.11	1.50	1.35
12	aA	826	F6C	C2A-C3A	8.09	1.53	1.36
12	bA	826	F6C	C1A-CHA	8.08	1.50	1.35

The worst 5 of 8126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	829	CLA	C4-C3-C5	-21.94	78.37	115.27
11	cA	829	CLA	C4-C3-C5	-21.93	78.38	115.27
11	bA	829	CLA	C4-C3-C5	-21.91	78.42	115.27
11	bA	829	CLA	C5-C3-C2	19.02	159.62	121.12
11	aA	829	CLA	C5-C3-C2	19.00	159.57	121.12

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	aA	826	F6C	NA
12	aA	827	F6C	C8
12	aA	827	F6C	NA
12	aA	830	F6C	NA
12	aA	832	F6C	NA

5 of 3337 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	aA	804	CLA	C2B-C3B-CAB-CBB
11	aA	804	CLA	C4B-C3B-CAB-CBB
11	aA	804	CLA	CBD-CGD-O2D-CED
11	aA	805	CLA	CHA-CBD-CGD-O1D
11	aA	805	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

240 monomers are involved in 402 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	cA	834	CLA	1	0
11	cB	823	CLA	5	0
11	cA	835	CLA	1	0
15	bL	203	BCR	3	0
11	aB	823	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	aA	853	LMT	2	0
11	bB	817	CLA	1	0
11	bB	833	CLA	1	0
11	bB	808	CLA	4	0
11	cA	840	CLA	2	0
15	cB	848	BCR	3	0
11	aB	838	CLA	2	0
13	bB	841	PQN	2	0
11	cB	813	CLA	1	0
15	aB	848	BCR	2	0
16	cA	852	LHG	1	0
11	bA	813	CLA	1	0
11	cB	816	CLA	3	0
11	cB	839	CLA	1	0
11	bB	813	CLA	1	0
11	cA	813	CLA	2	0
11	cA	804	CLA	1	0
11	cL	205	CLA	3	0
11	bA	812	CLA	1	0
15	aI	101	BCR	2	0
11	cB	837	CLA	3	0
11	cA	803	CLA	2	0
11	cA	822	CLA	5	0
15	bL	207	BCR	2	0
11	cB	805	CLA	3	0
11	cA	809	CLA	2	0
11	cB	838	CLA	2	0
11	aA	840	CLA	3	0
11	bA	840	CLA	2	0
11	aA	821	CLA	2	0
11	aB	817	CLA	2	0
11	aA	831	CLA	1	0
15	bA	847	BCR	4	0
11	bA	838	CLA	2	0
11	cA	807	CLA	1	0
11	cA	838	CLA	2	0
15	bB	846	BCR	1	0
11	aB	802	CLA	4	0
11	aB	815	CLA	3	0
11	aL	206	CLA	2	0
11	cB	825	CLA	1	0
11	cA	814	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	cA	833	CLA	2	0
11	bA	829	CLA	4	0
11	bB	826	CLA	1	0
17	cA	853	LMT	2	0
11	cA	802	CLA	1	0
15	aB	845	BCR	2	0
15	aB	843	BCR	1	0
11	cB	834	CLA	1	0
11	cB	840	CLA	1	0
11	bA	804	CLA	1	0
15	bB	843	BCR	1	0
11	cB	804	CLA	4	0
11	cB	807	CLA	1	0
11	cA	828	CLA	1	0
11	bA	821	CLA	2	0
11	aA	818	CLA	2	0
11	aA	823	CLA	1	0
11	cA	806	CLA	5	0
11	aB	804	CLA	4	0
11	aA	822	CLA	4	0
11	cA	836	CLA	2	0
11	bA	803	CLA	1	0
11	cB	808	CLA	3	0
15	aB	842	BCR	1	0
11	bA	809	CLA	2	0
15	cL	203	BCR	2	0
11	aB	813	CLA	1	0
15	aA	848	BCR	3	0
11	cB	836	CLA	2	0
15	bB	848	BCR	2	0
11	cB	802	CLA	3	0
11	cB	815	CLA	2	0
11	cA	825	CLA	2	0
15	cB	845	BCR	2	0
11	cL	204	CLA	1	0
11	bA	823	CLA	2	0
11	aB	808	CLA	4	0
15	aL	207	BCR	2	0
11	bB	838	CLA	1	0
11	cB	803	CLA	1	0
11	aB	801	CLA	3	0
12	cB	824	F6C	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	aA	839	CLA	3	0
15	aB	846	BCR	2	0
13	cA	845	PQN	1	0
11	aB	812	CLA	3	0
11	aA	824	CLA	2	0
11	aA	820	CLA	3	0
11	aB	810	CLA	1	0
15	bK	102	BCR	2	0
15	cB	842	BCR	1	0
11	aB	832	CLA	1	0
11	aA	829	CLA	3	0
17	bA	853	LMT	2	0
11	aA	802	CLA	1	0
11	cA	818	CLA	2	0
18	bB	847	LMG	1	0
11	bB	819	CLA	1	0
11	bA	819	CLA	2	0
11	aB	807	CLA	1	0
11	cK	103	CLA	1	0
11	cA	821	CLA	2	0
11	cB	832	CLA	1	0
15	cB	846	BCR	2	0
15	cA	851	BCR	7	0
11	cB	812	CLA	5	0
11	bB	829	CLA	1	0
11	aB	837	CLA	2	0
11	bA	831	CLA	1	0
11	bB	804	CLA	3	0
13	cB	841	PQN	1	0
15	aL	208	BCR	3	0
11	bA	839	CLA	3	0
11	aB	827	CLA	3	0
11	aA	825	CLA	3	0
11	cB	828	CLA	3	0
11	aB	826	CLA	1	0
11	cA	820	CLA	4	0
12	aB	824	F6C	1	0
11	aA	833	CLA	2	0
11	bB	828	CLA	2	0
11	bB	836	CLA	2	0
15	bA	849	BCR	3	0
11	bB	815	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	cB	827	CLA	3	0
15	cL	207	BCR	2	0
11	cA	824	CLA	2	0
18	aB	847	LMG	1	0
15	aA	849	BCR	2	0
15	cA	850	BCR	1	0
11	bB	805	CLA	3	0
11	cA	812	CLA	1	0
11	bB	825	CLA	1	0
11	cB	801	CLA	2	0
11	aB	803	CLA	1	0
11	bA	818	CLA	2	0
15	bA	851	BCR	7	0
15	aL	203	BCR	2	0
11	cB	829	CLA	1	0
11	bL	206	CLA	3	0
11	bB	834	CLA	1	0
11	aA	806	CLA	4	0
11	bB	801	CLA	2	0
15	bB	845	BCR	1	0
15	bB	844	BCR	1	0
15	bA	848	BCR	3	0
11	aB	833	CLA	1	0
11	aA	803	CLA	3	0
11	bA	814	CLA	3	0
11	bA	843	CLA	2	0
11	cL	206	CLA	1	0
15	aA	851	BCR	7	0
11	cA	839	CLA	3	0
18	cB	847	LMG	1	0
11	aB	840	CLA	1	0
11	cB	818	CLA	1	0
11	bB	832	CLA	1	0
11	bA	833	CLA	3	0
11	bL	205	CLA	3	0
11	aB	818	CLA	1	0
11	aA	819	CLA	1	0
11	bL	204	CLA	2	0
11	aA	813	CLA	3	0
11	bA	820	CLA	3	0
11	cB	821	CLA	1	0
11	cB	810	CLA	1	0

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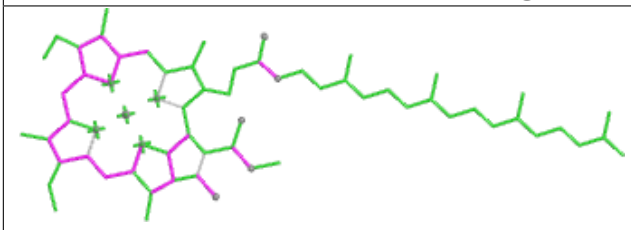
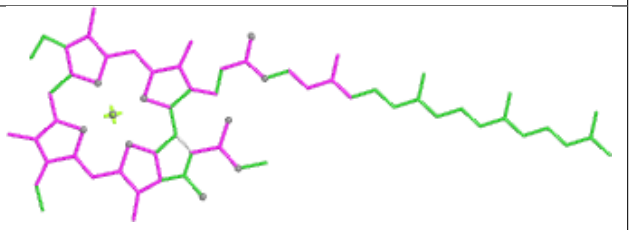
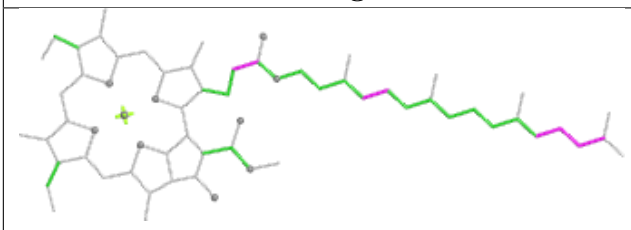
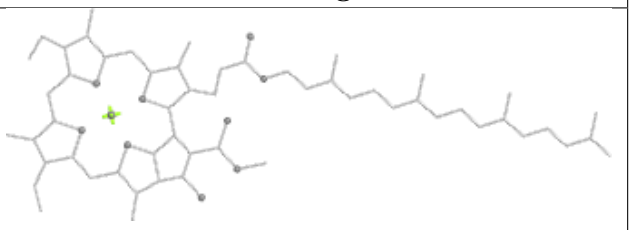
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bB	842	BCR	1	0
11	bB	810	CLA	1	0
11	aK	103	CLA	1	0
16	aA	852	LHG	1	0
11	cB	833	CLA	1	0
15	aA	850	BCR	1	0
15	bA	850	BCR	1	0
11	aL	205	CLA	3	0
11	bB	806	CLA	3	0
11	cB	817	CLA	1	0
11	bK	103	CLA	1	0
11	bB	802	CLA	4	0
13	aB	841	PQN	3	0
15	aB	844	BCR	1	0
15	aA	847	BCR	3	0
11	aA	838	CLA	2	0
11	aB	805	CLA	2	0
11	bB	812	CLA	3	0
16	bA	852	LHG	1	0
11	bB	823	CLA	4	0
11	cA	843	CLA	2	0
15	cA	847	BCR	2	0
11	aA	828	CLA	2	0
11	bA	828	CLA	1	0
15	cA	848	BCR	3	0
13	bA	845	PQN	1	0
11	bA	825	CLA	2	0
11	bB	837	CLA	2	0
15	aK	102	BCR	2	0
11	bA	806	CLA	5	0
11	cA	823	CLA	1	0
11	aB	806	CLA	3	0
11	bB	840	CLA	1	0
11	bB	807	CLA	1	0
15	bM	101	BCR	2	0
11	aB	836	CLA	2	0
15	cB	844	BCR	2	0
11	bB	816	CLA	4	0
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11	cB	806	CLA	3	0

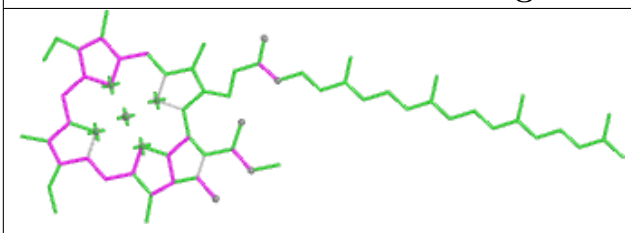
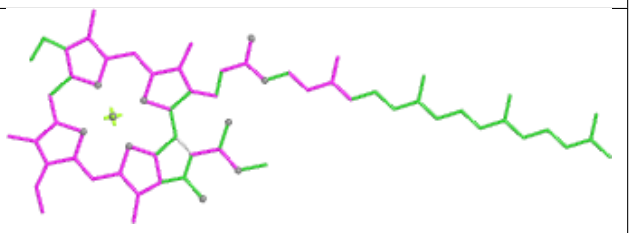
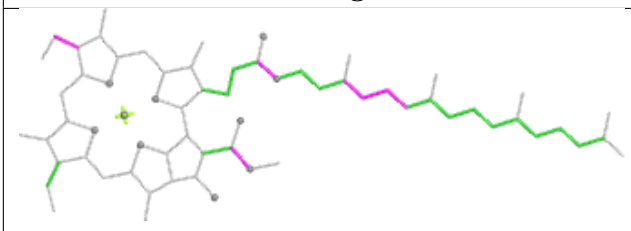
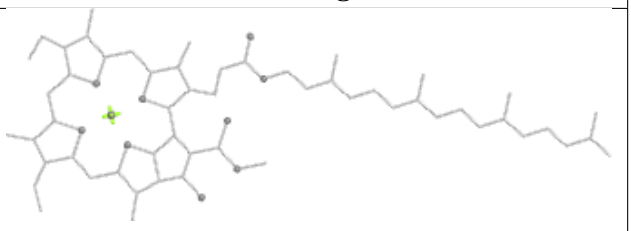
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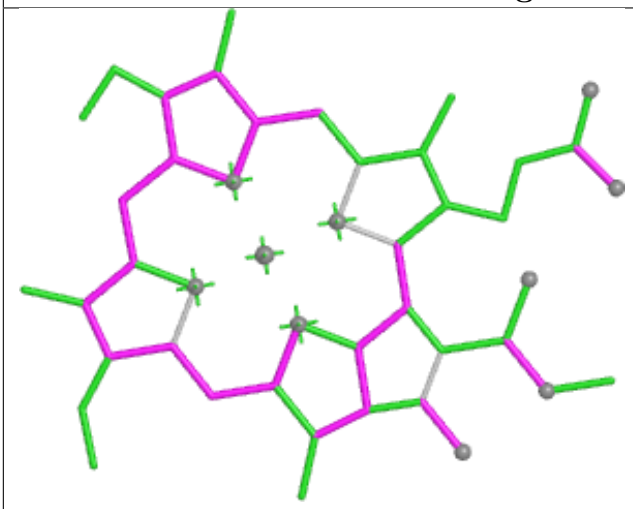
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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11	cB	826	CLA	1	0
11	aB	834	CLA	1	0
11	bB	818	CLA	1	0
11	aA	804	CLA	1	0
11	aA	812	CLA	1	0
11	aA	814	CLA	3	0
11	bB	839	CLA	1	0
11	aA	843	CLA	2	0
11	bB	821	CLA	1	0
11	aB	825	CLA	1	0
15	bL	208	BCR	2	0
15	cA	849	BCR	2	0
11	bB	827	CLA	3	0
11	bA	836	CLA	2	0
11	aA	836	CLA	2	0
11	aB	839	CLA	1	0
15	cK	102	BCR	2	0
15	cL	208	BCR	5	0
11	cA	829	CLA	5	0
11	bA	810	CLA	1	0
11	bA	822	CLA	4	0
11	cA	819	CLA	3	0
11	cA	831	CLA	1	0
11	aB	816	CLA	4	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.

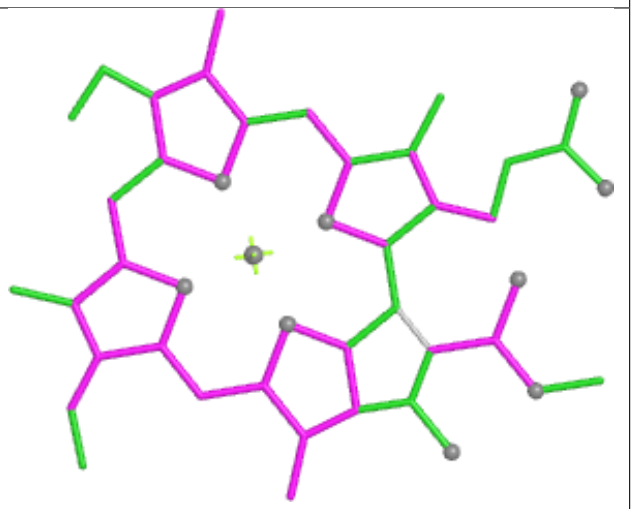
Ligand CL0 bA 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

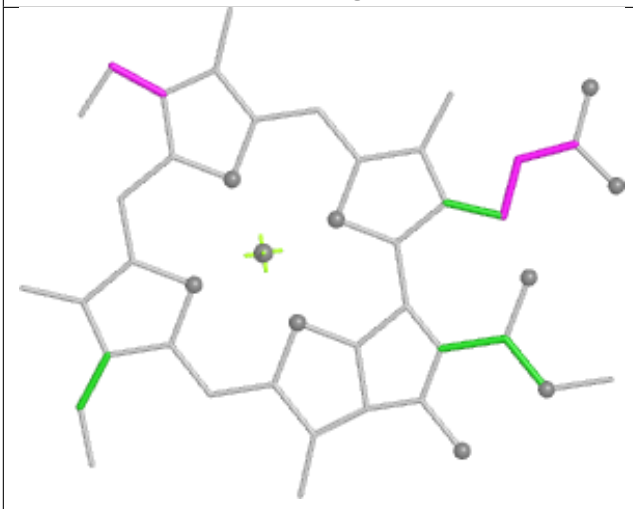
Ligand CLA aB 811



Bond lengths



Bond angles

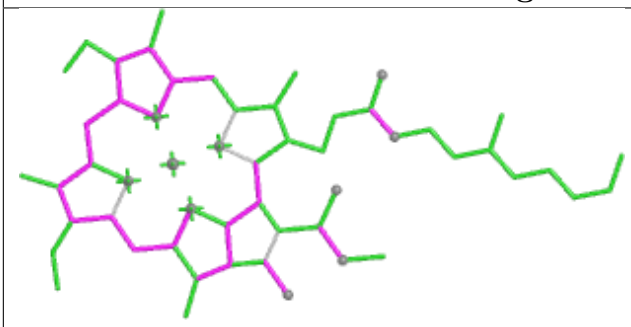


Torsions

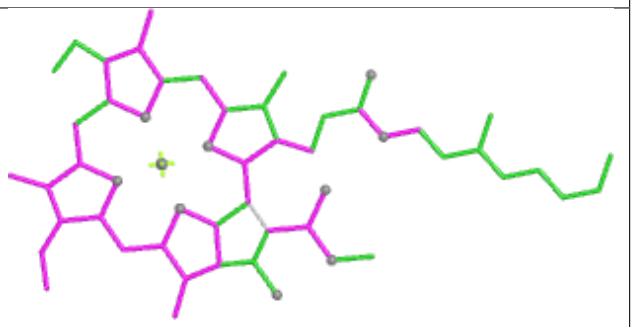


Rings

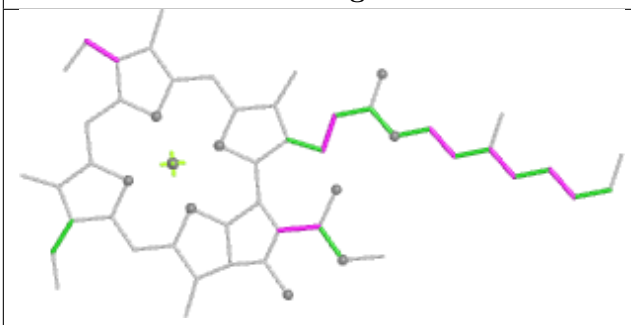
Ligand CLA cB 823



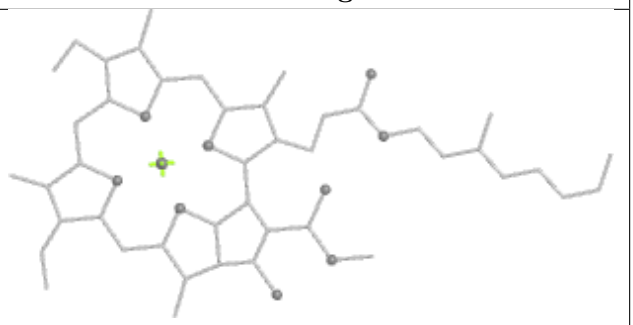
Bond lengths



Bond angles

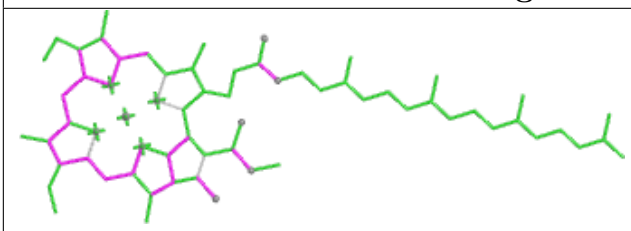


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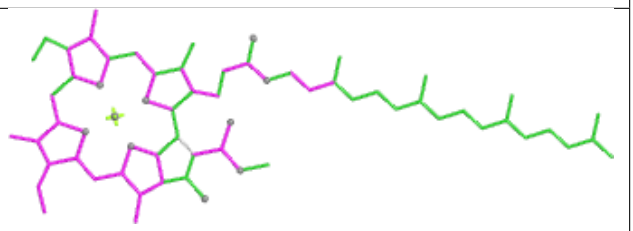


Rings

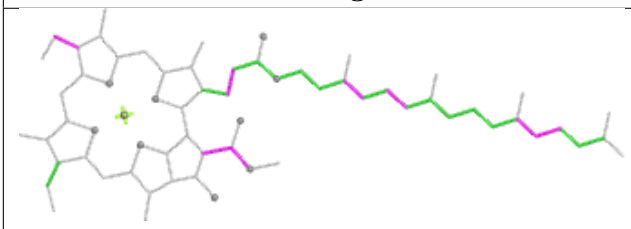
Ligand CLA cA 835



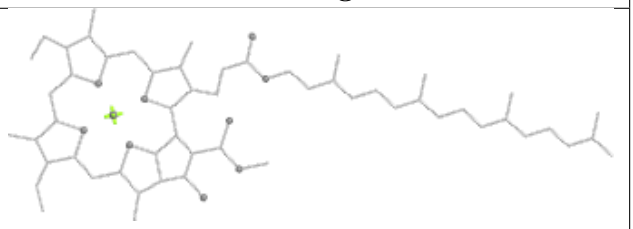
Bond lengths



Bond angles

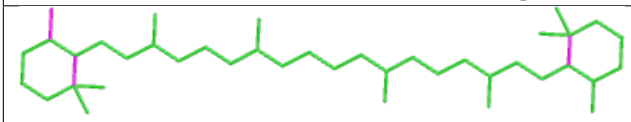


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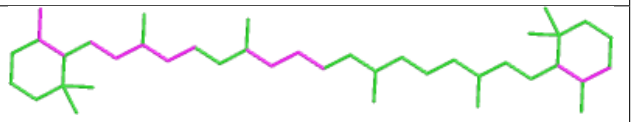


Rings

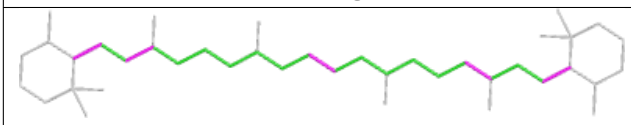
Ligand BCR bL 203



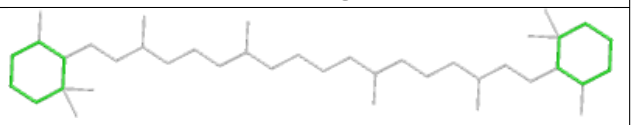
Bond lengths



Bond angles

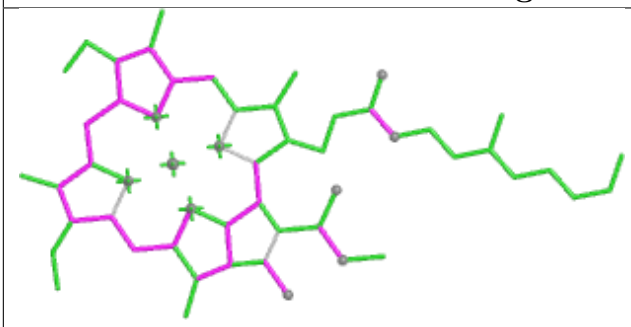


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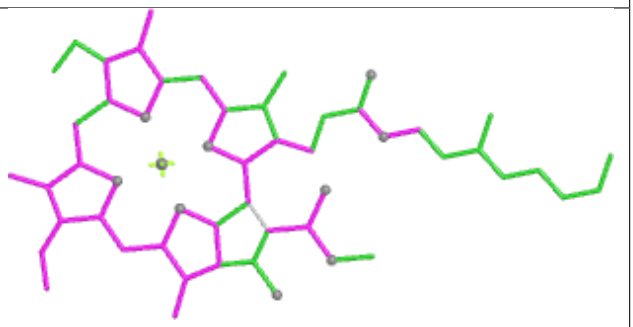


Rings

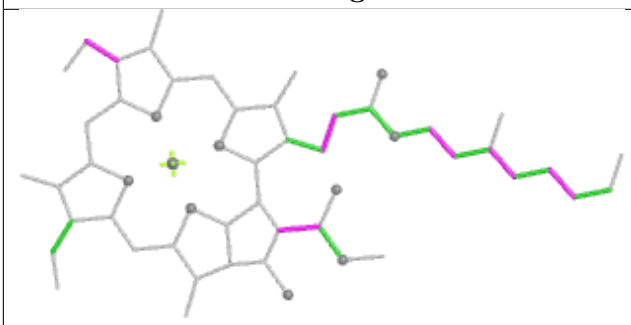
Ligand CLA aB 823



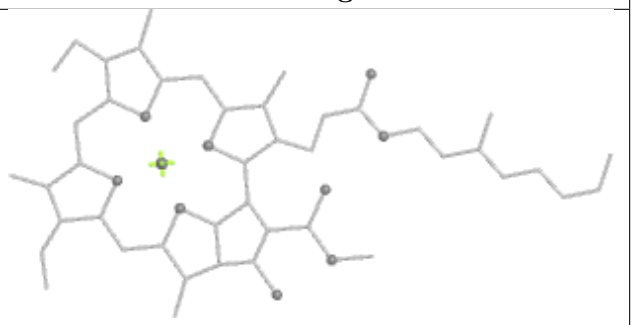
Bond lengths



Bond angles

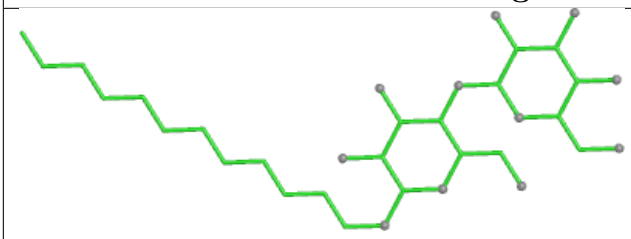


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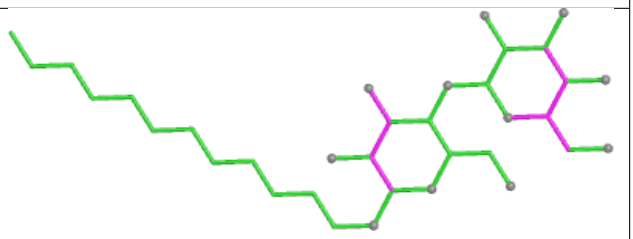


Rings

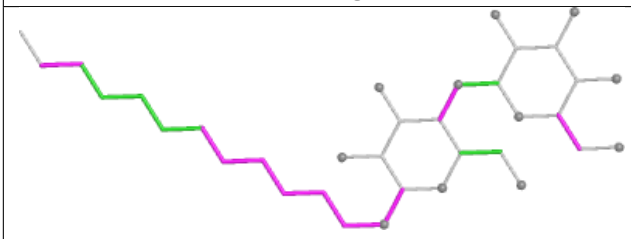
Ligand LMT aA 853



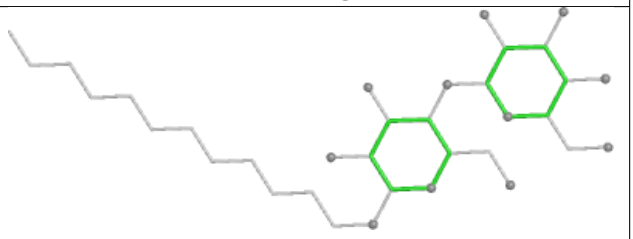
Bond lengths



Bond angles

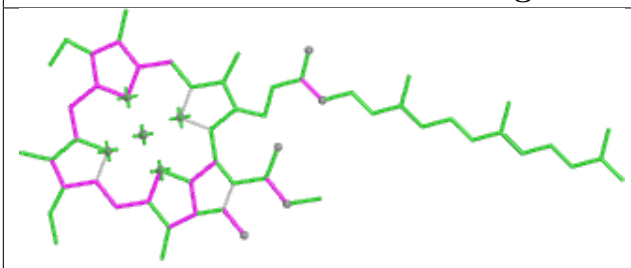


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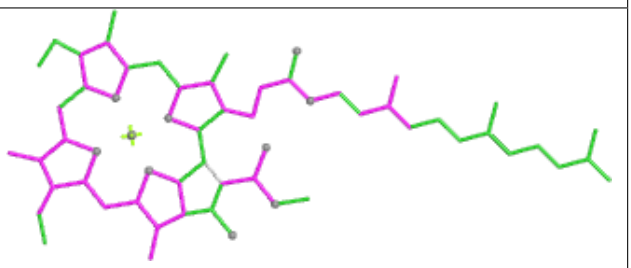


Rings

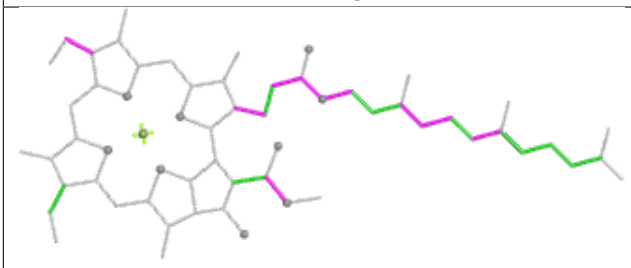
Ligand CLA bB 817



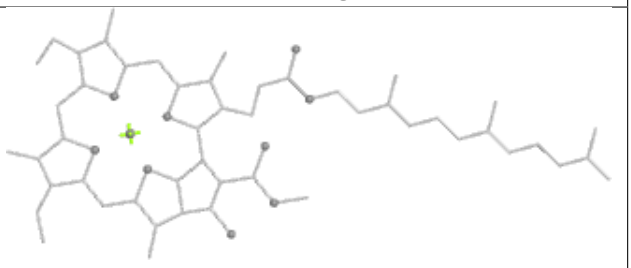
Bond lengths



Bond angles

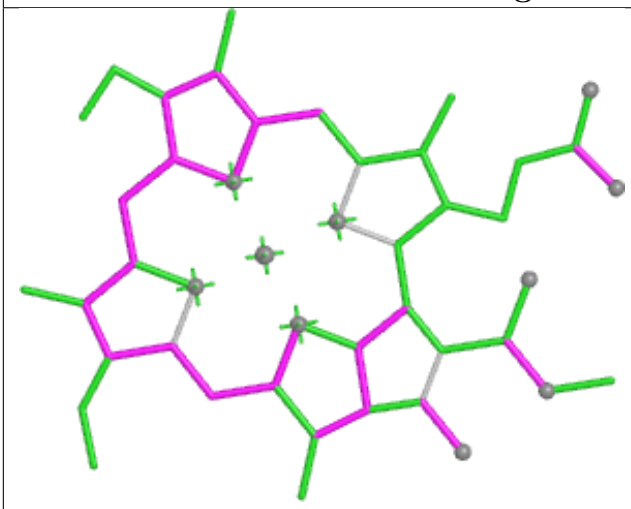


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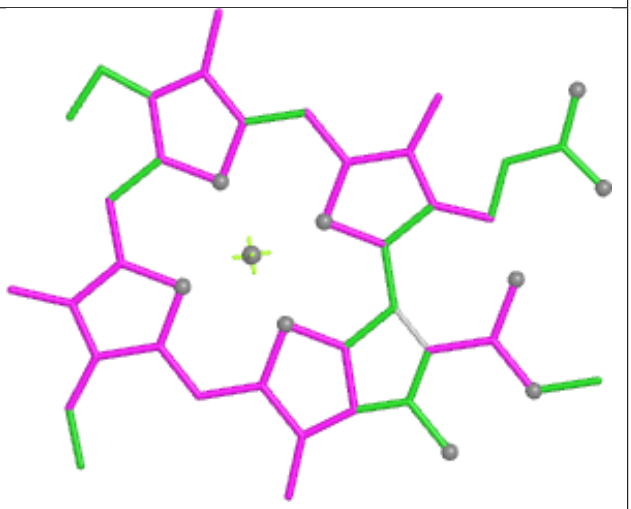


Rings

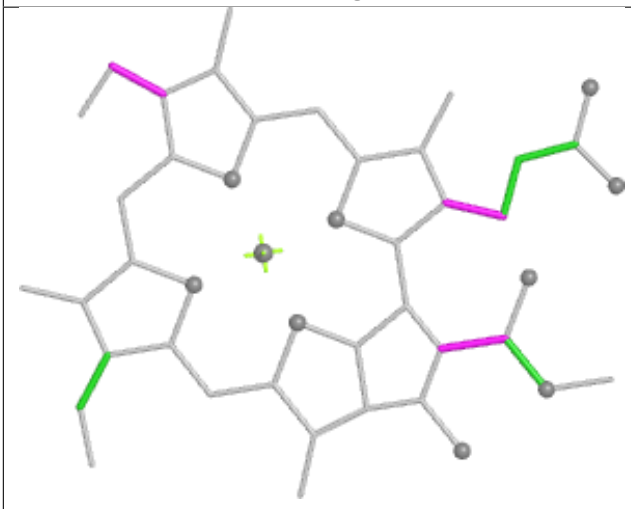
Ligand CLA bB 833



Bond lengths



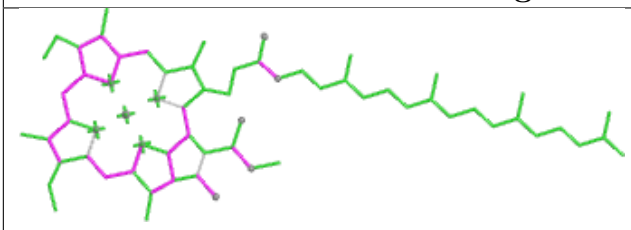
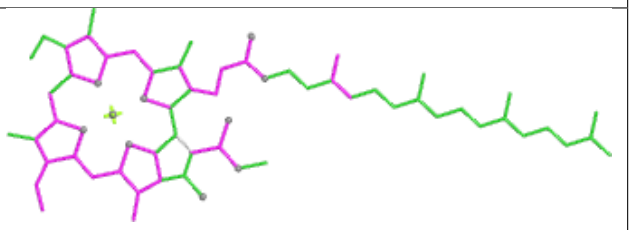
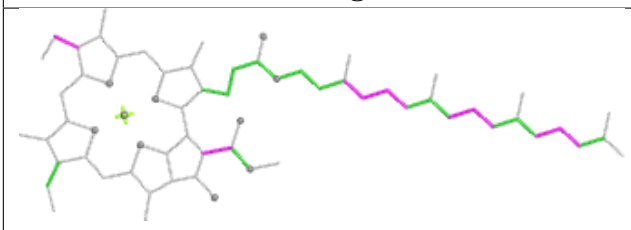
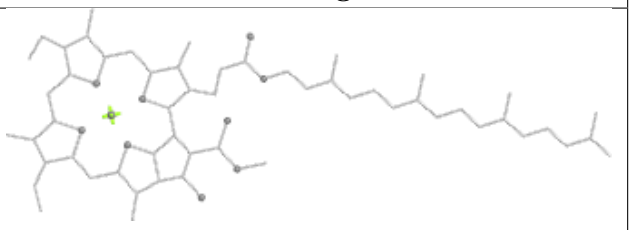
Bond angles

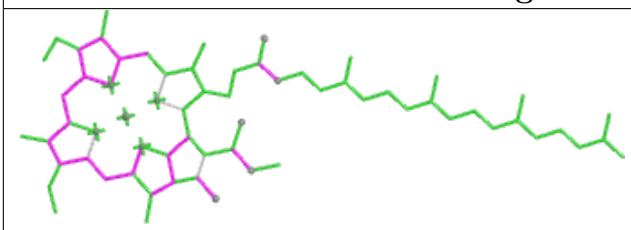
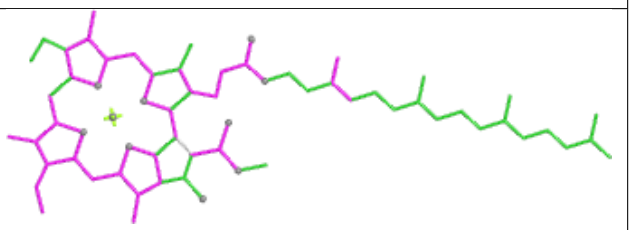
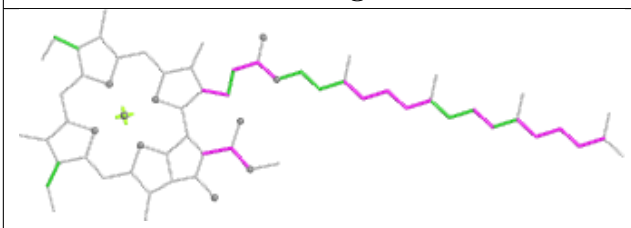
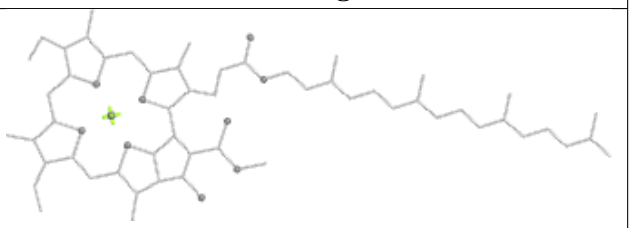


Torsions

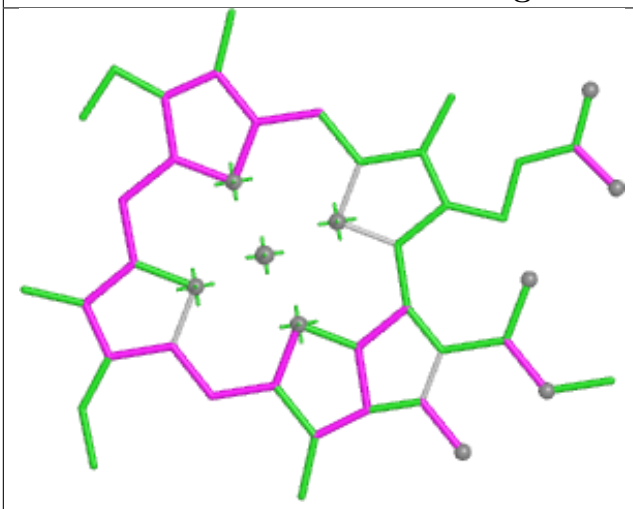


Rings

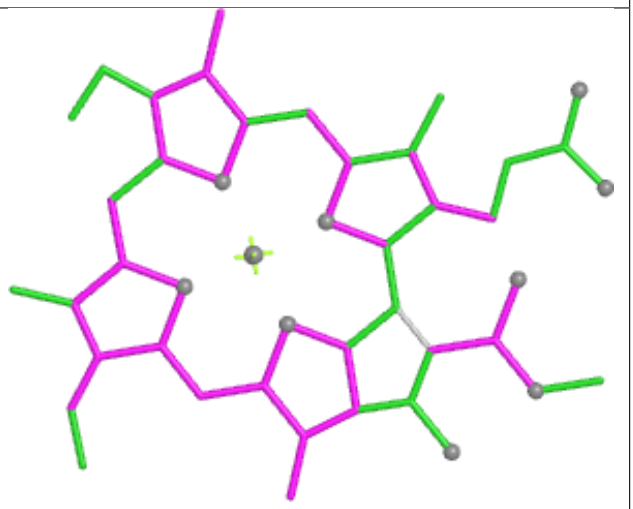
Ligand CLA bB 808	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA cA 840	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

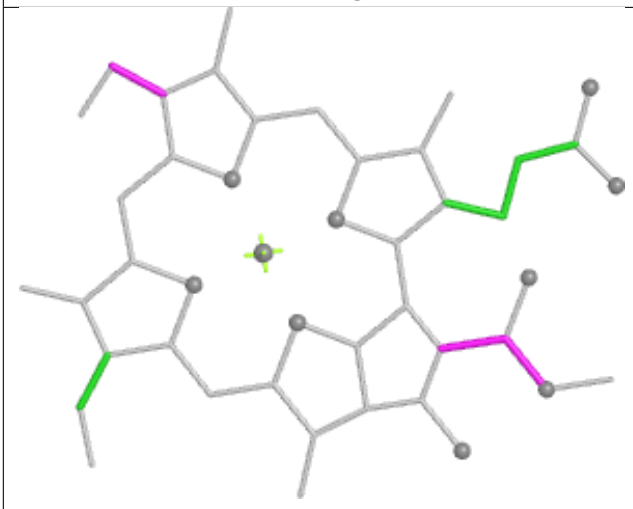
Ligand CLA bA 816



Bond lengths



Bond angles

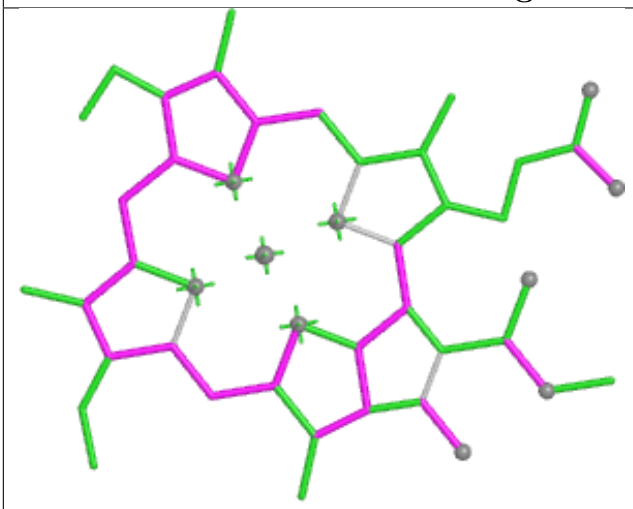


Torsions

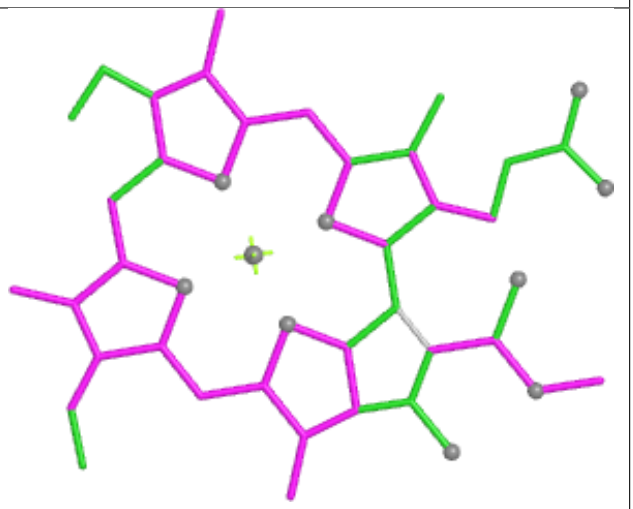


Rings

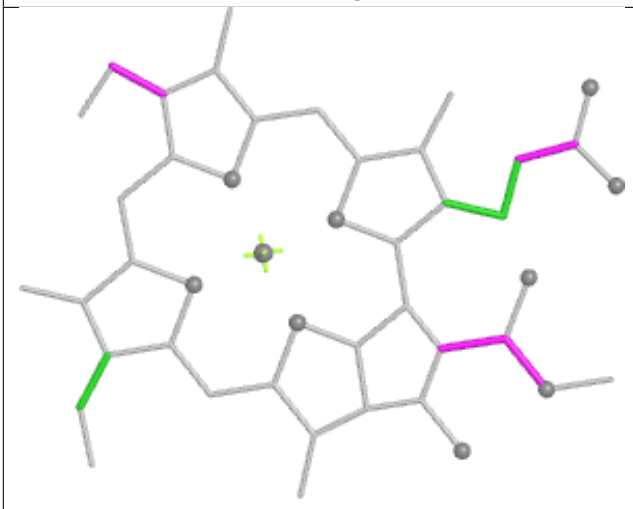
Ligand CLA cA 842



Bond lengths



Bond angles

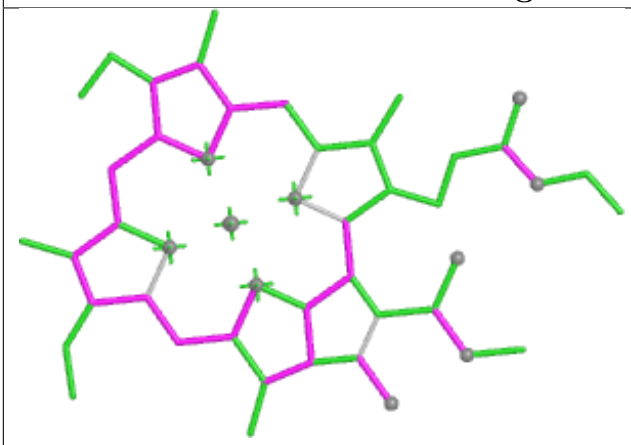


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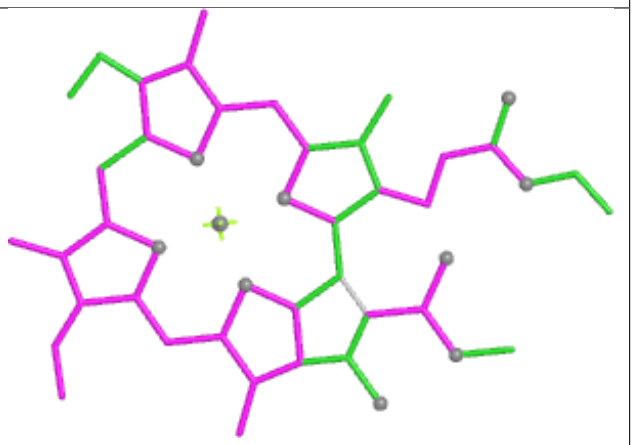


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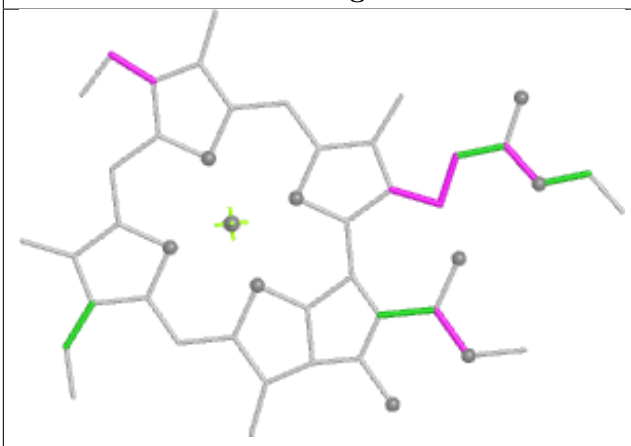
Ligand CLA aB 819



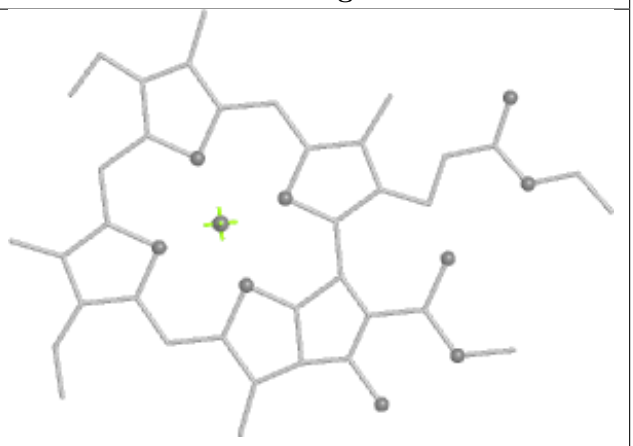
Bond lengths



Bond angles



Torsions

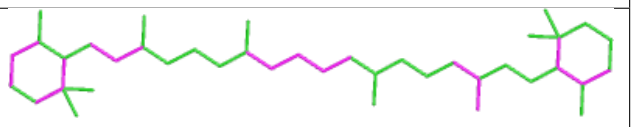


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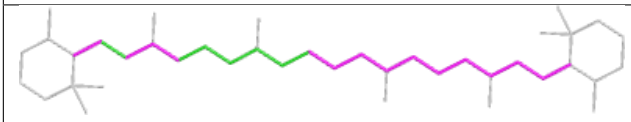
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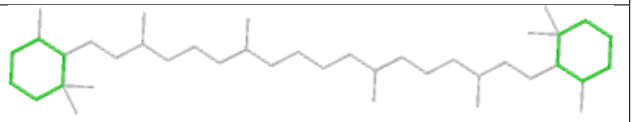
Bond lengths



Bond angles

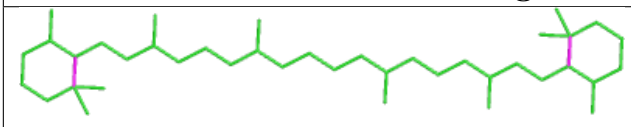


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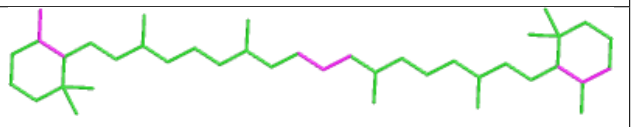


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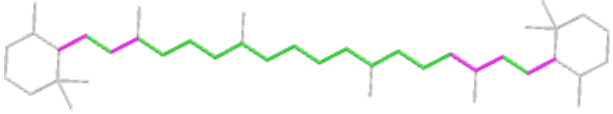
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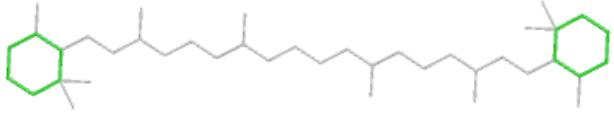
Bond lengths



Bond angles

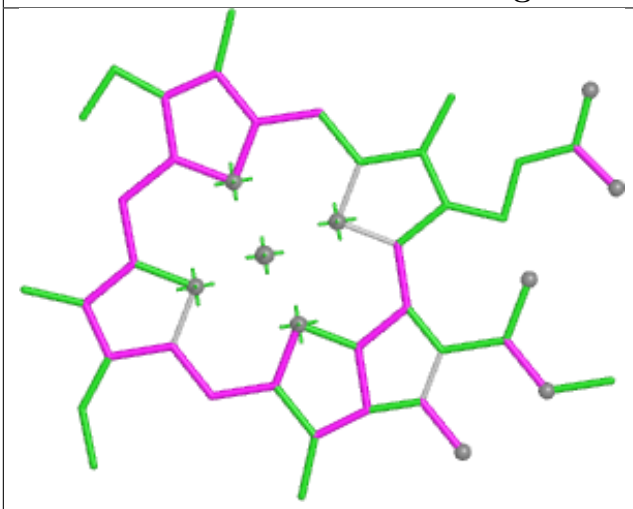


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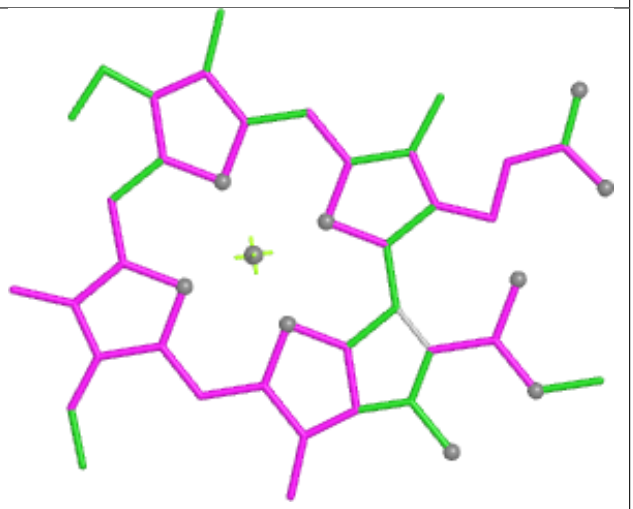


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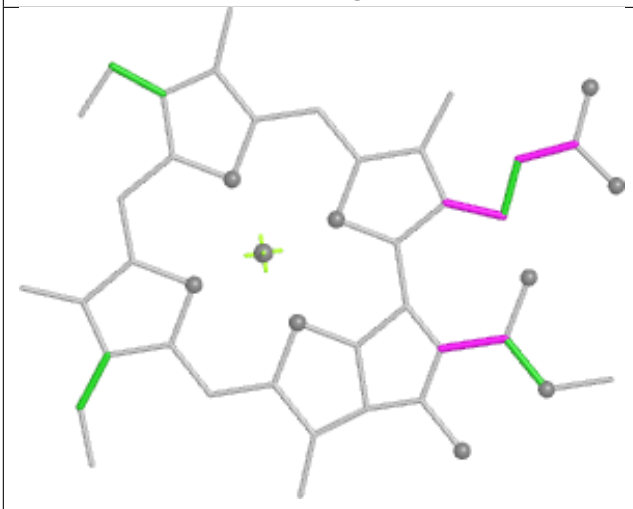
Ligand CLA bA 837



Bond lengths



Bond angles

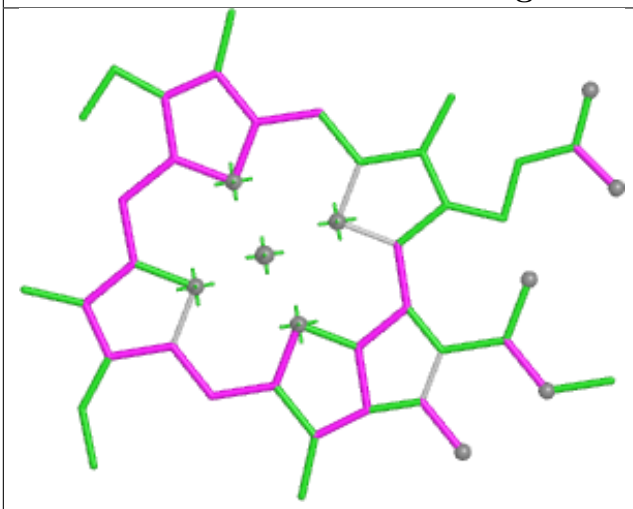


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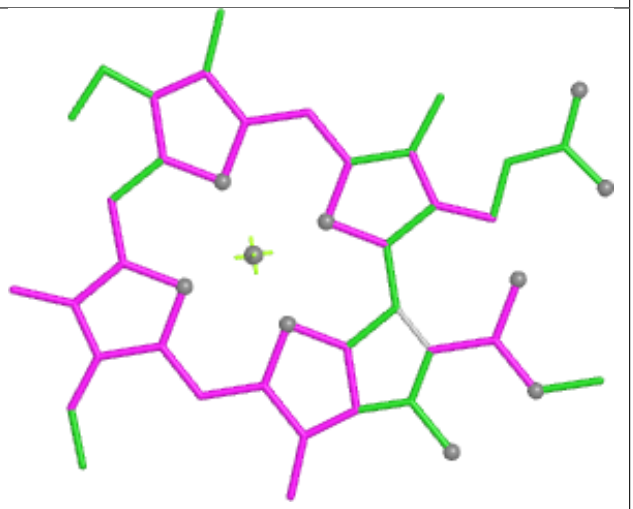


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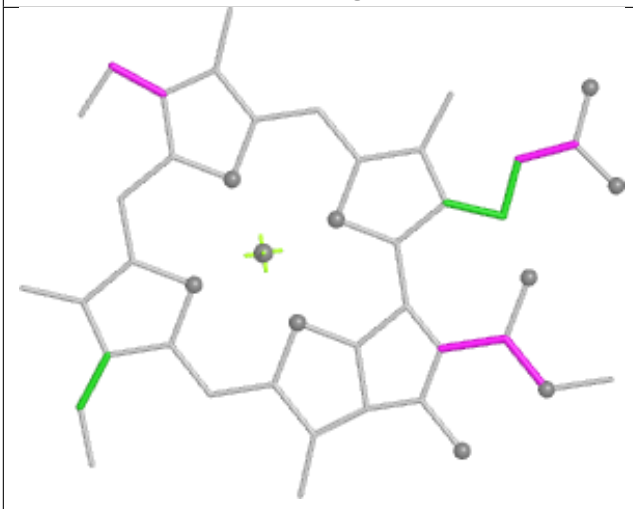
Ligand CLA cA 805



Bond lengths



Bond angles

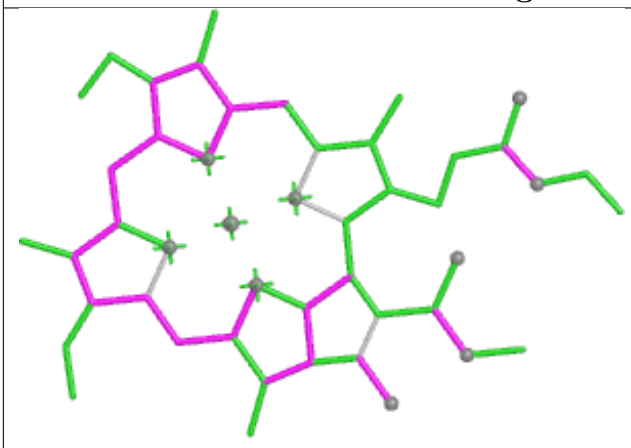


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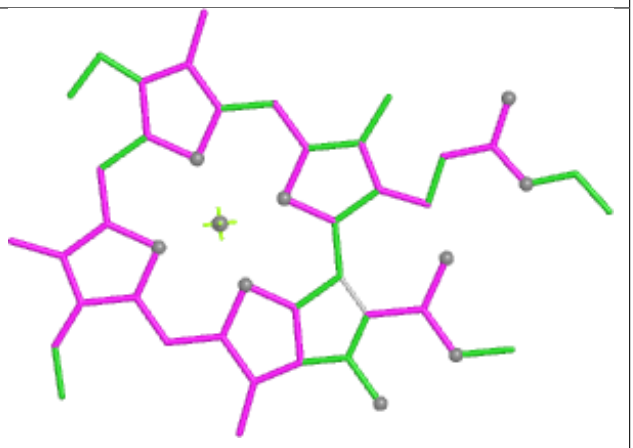


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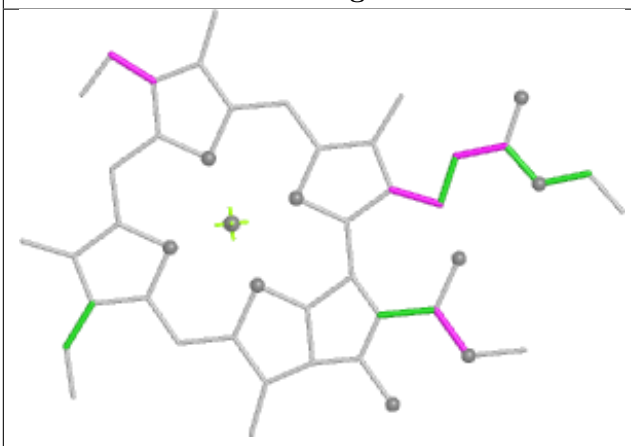
Ligand CLA aB 838



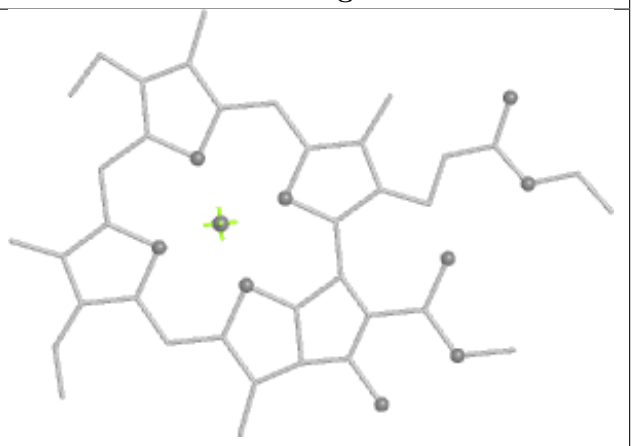
Bond lengths



Bond angles

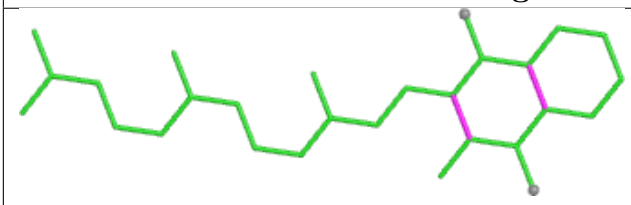


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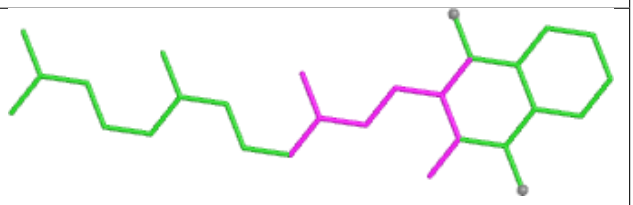


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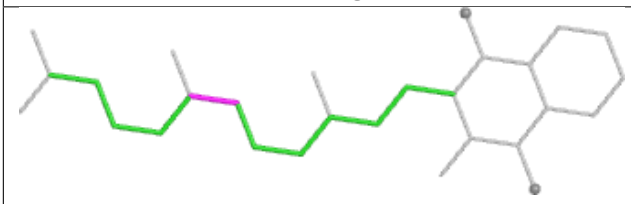
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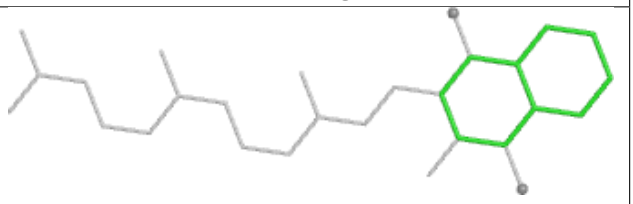
Bond lengths



Bond angles

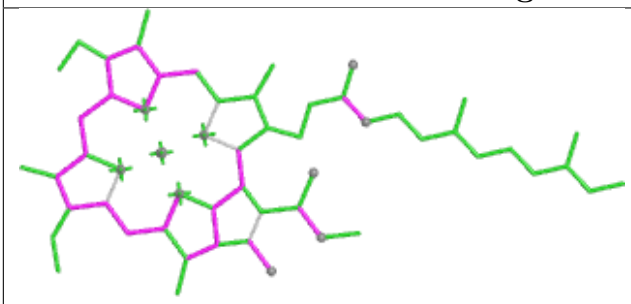


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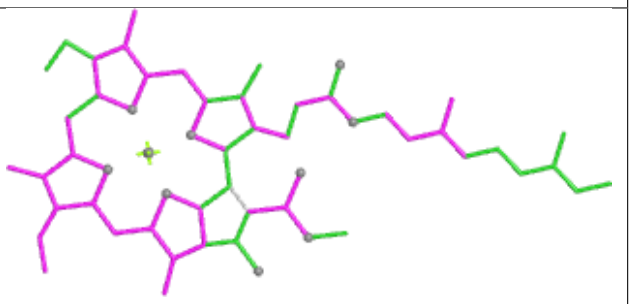


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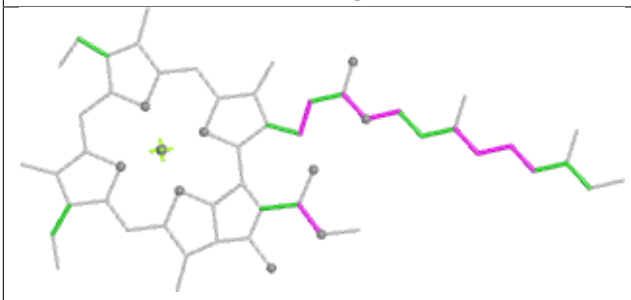
Ligand CLA cB 813



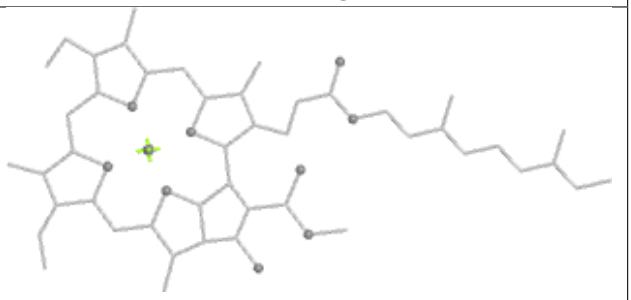
Bond lengths



Bond angles

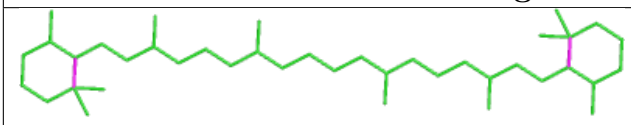


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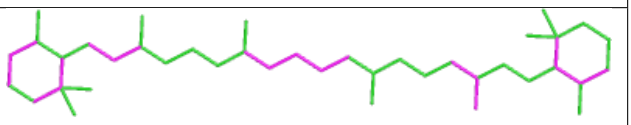


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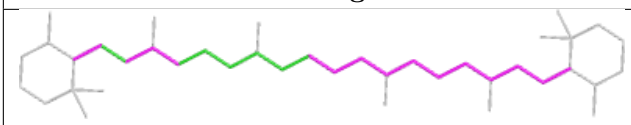
Ligand BCR aB 848



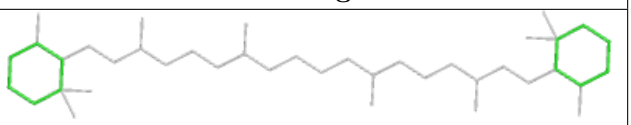
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Bond angles

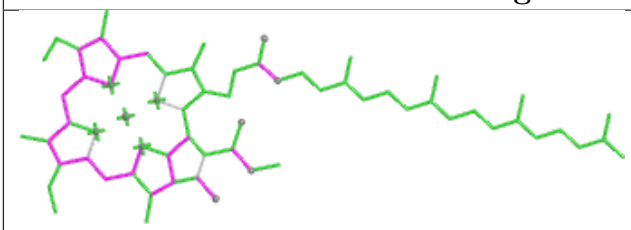


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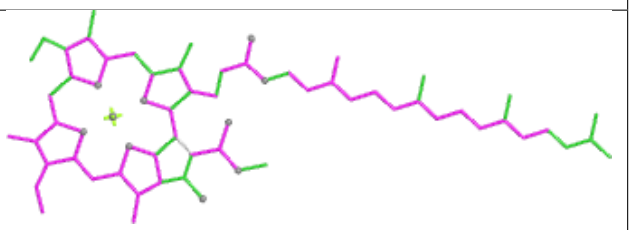


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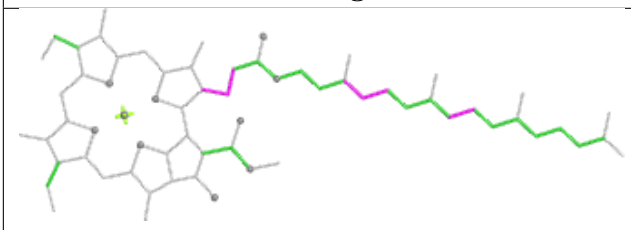
Ligand CLA bA 802



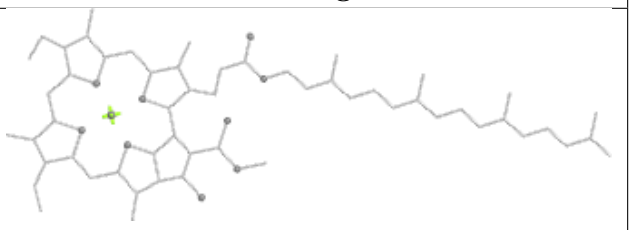
Bond lengths



Bond angles

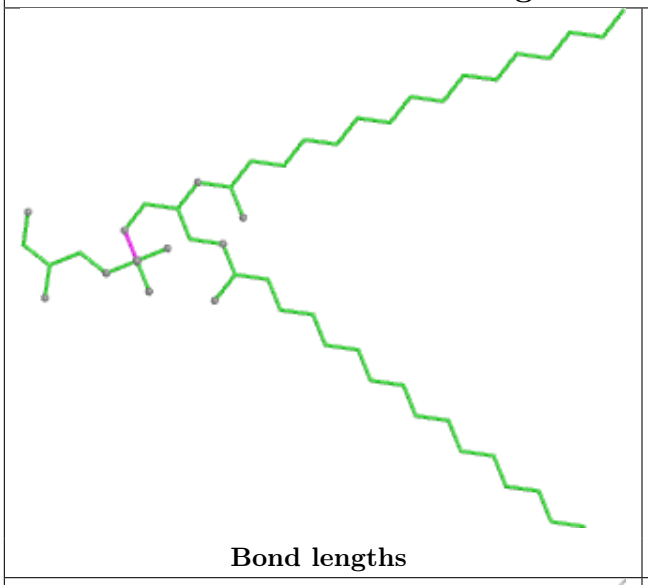


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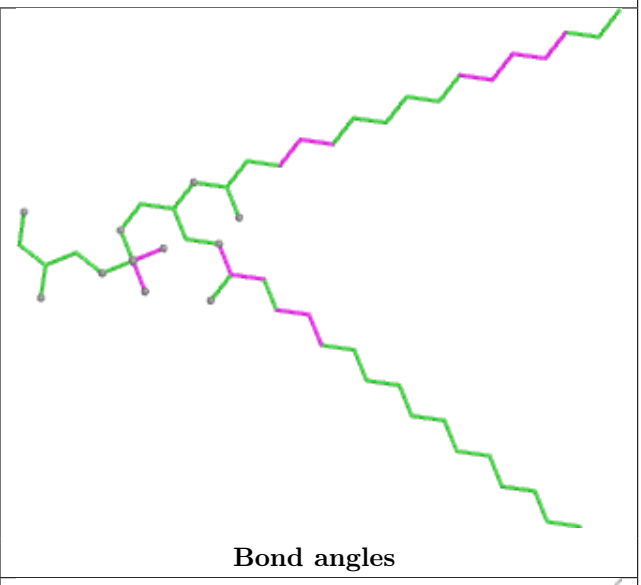


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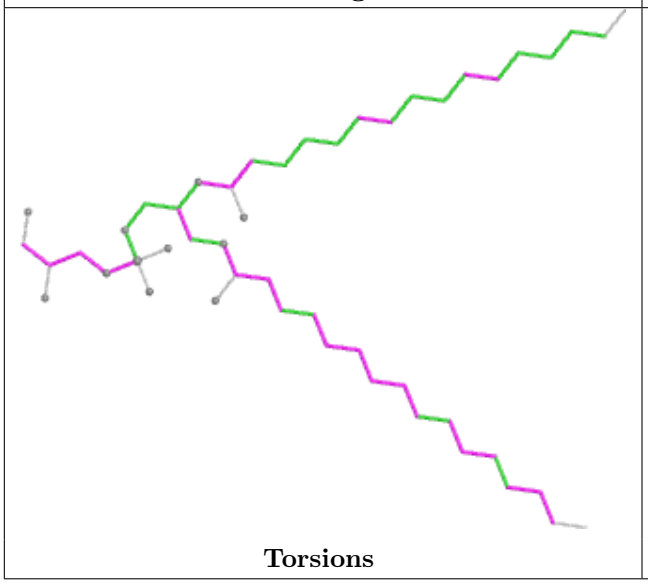
Ligand LHG cA 852



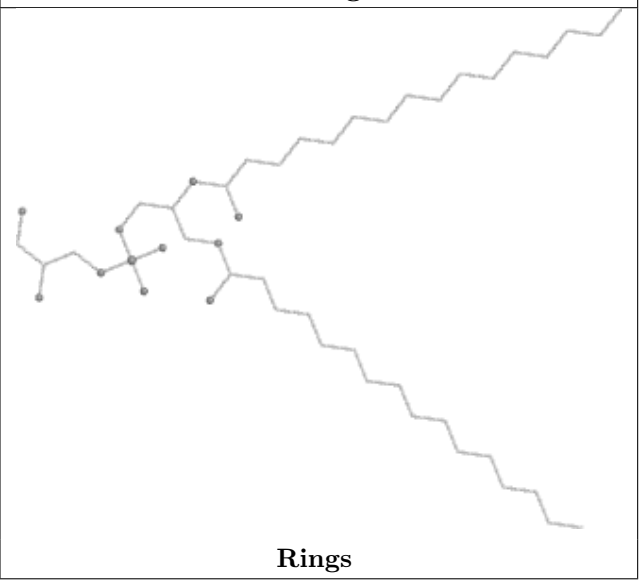
Bond lengths



Bond angles

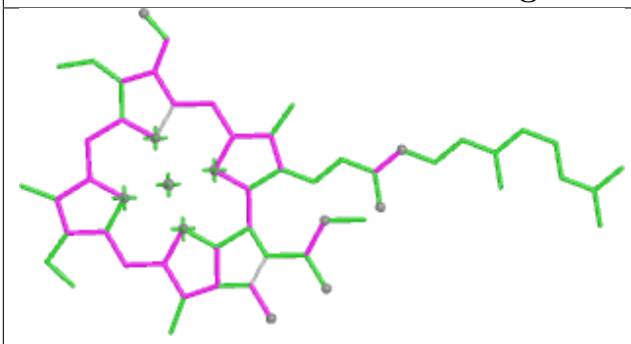


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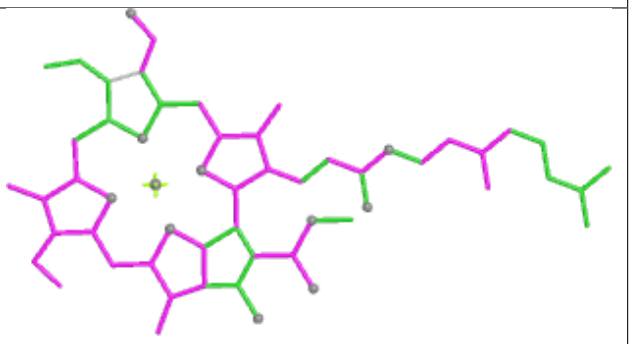


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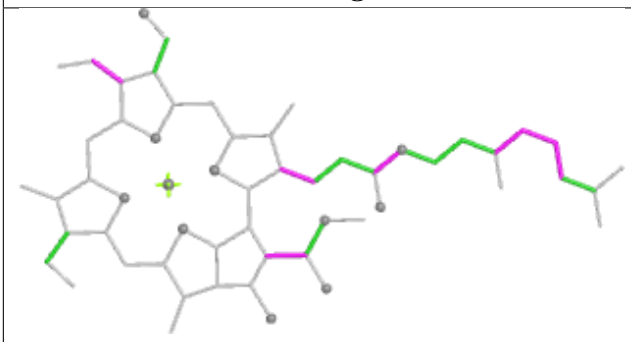
Ligand F6C cA 827



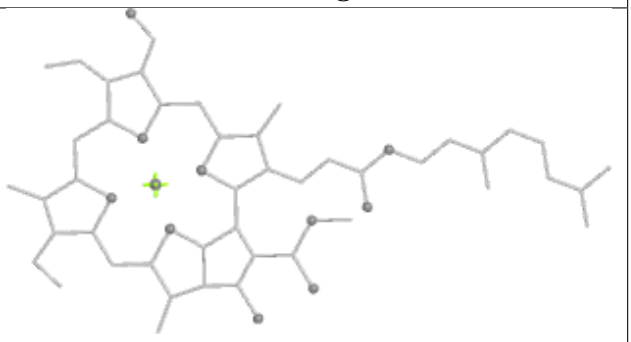
Bond lengths



Bond angles

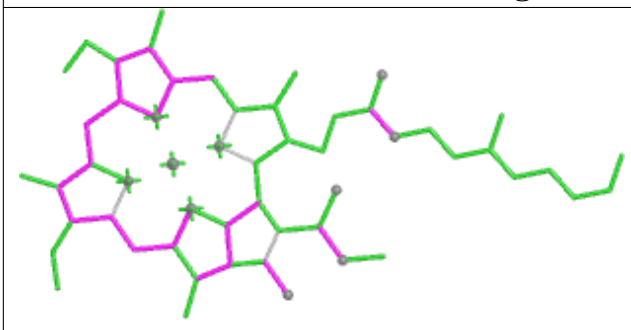


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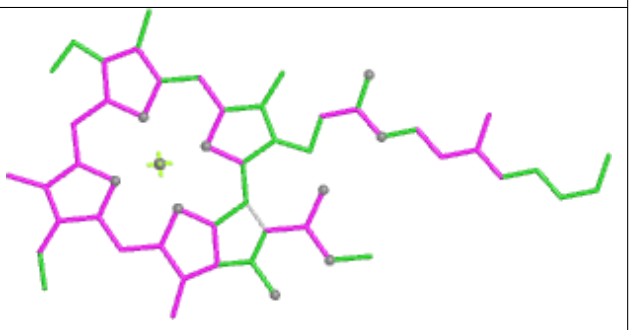


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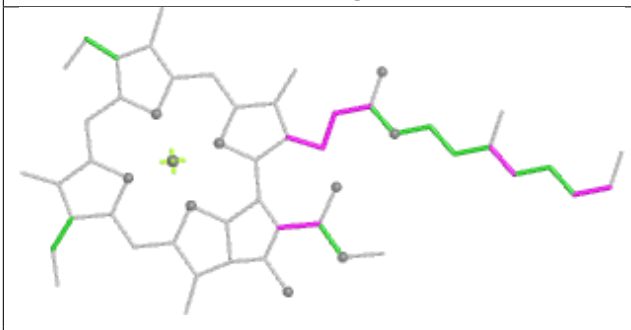
Ligand CLA bA 813



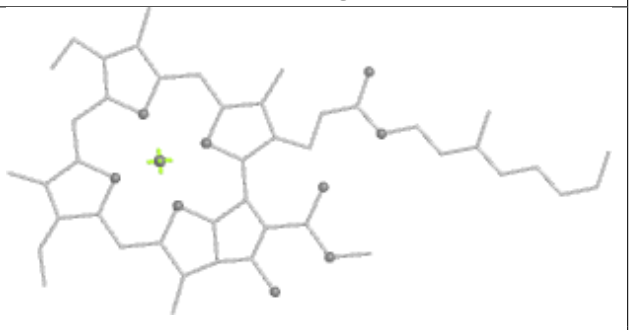
Bond lengths



Bond angles

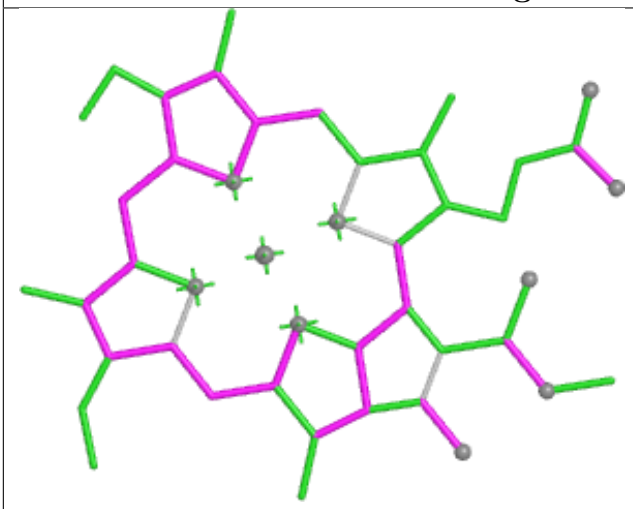


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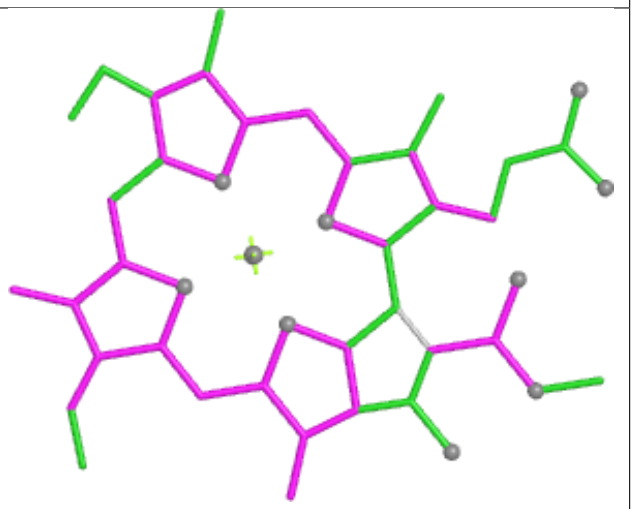


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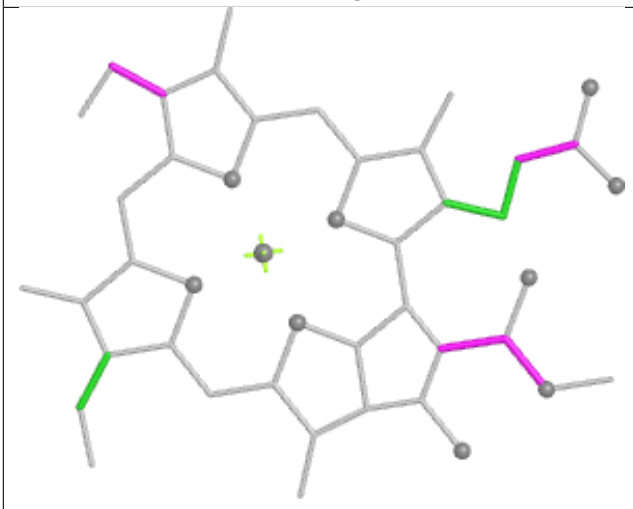
Ligand CLA bA 805



Bond lengths



Bond angles

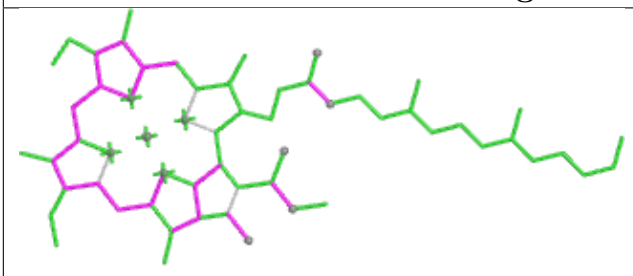


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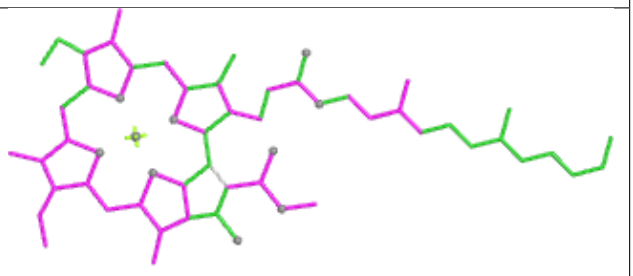


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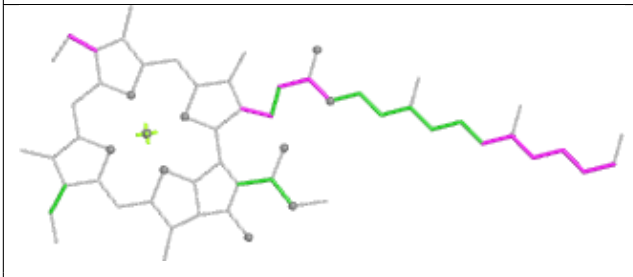
Ligand CLA cB 816



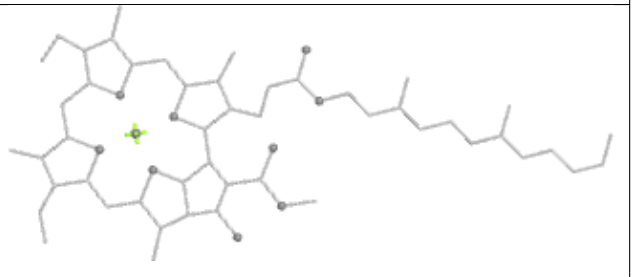
Bond lengths



Bond angles

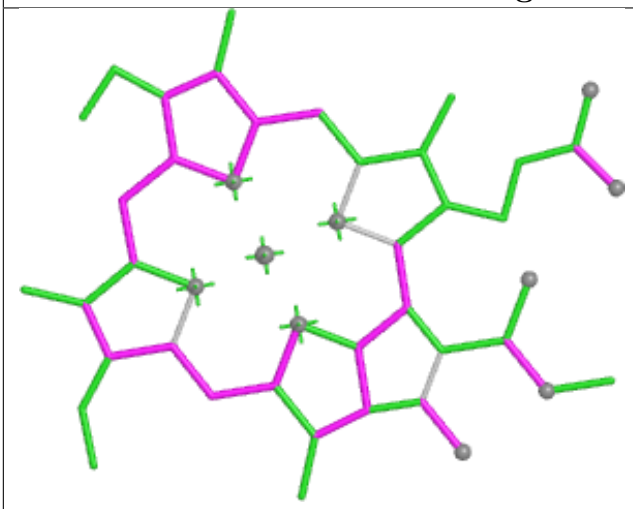


Torsions

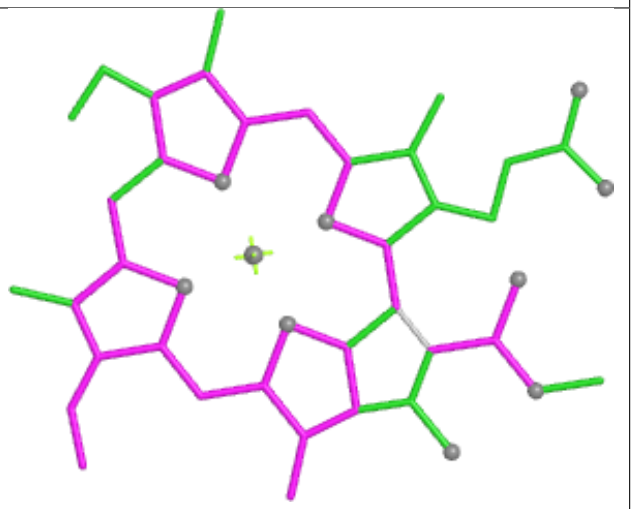


Rings

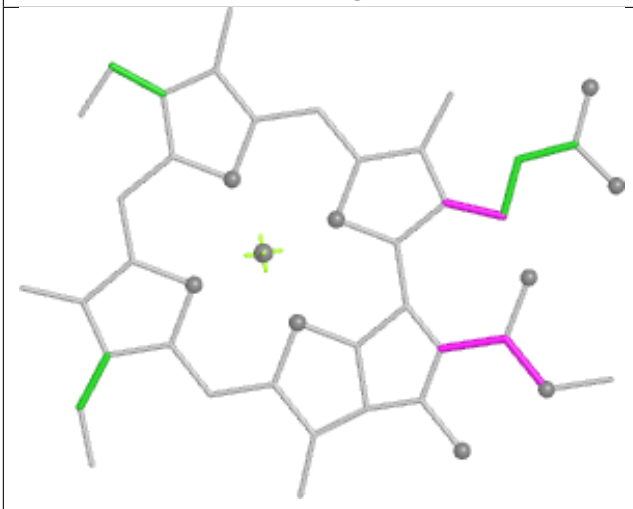
Ligand CLA cA 815



Bond lengths



Bond angles

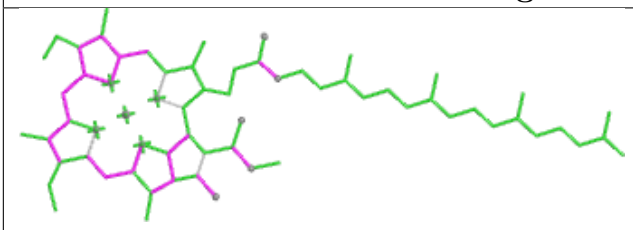


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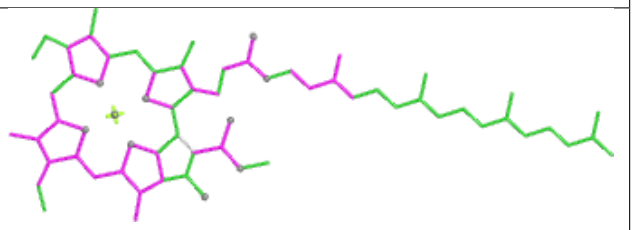


Rings

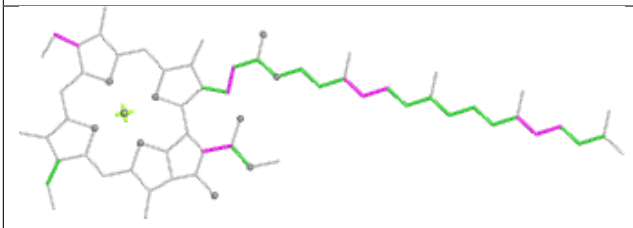
Ligand CLA cB 839



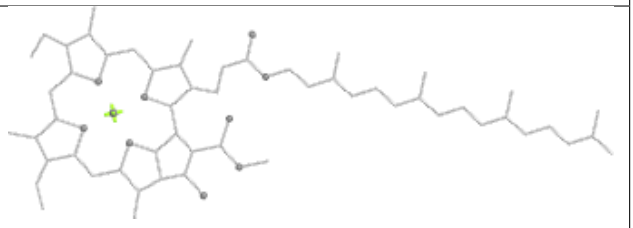
Bond lengths



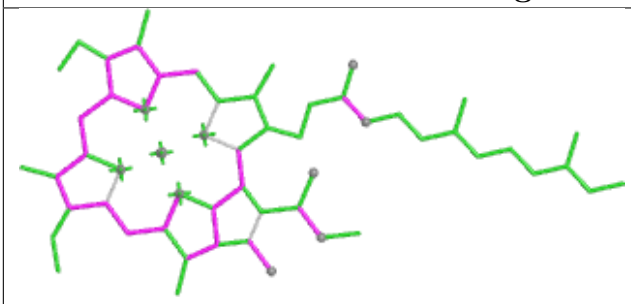
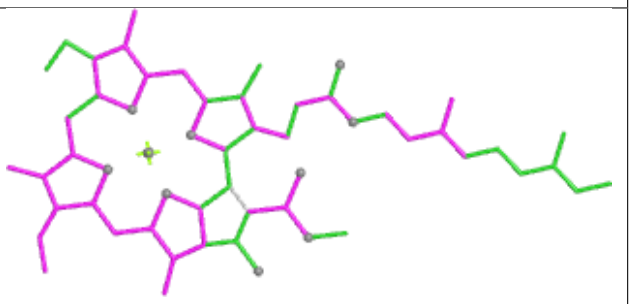
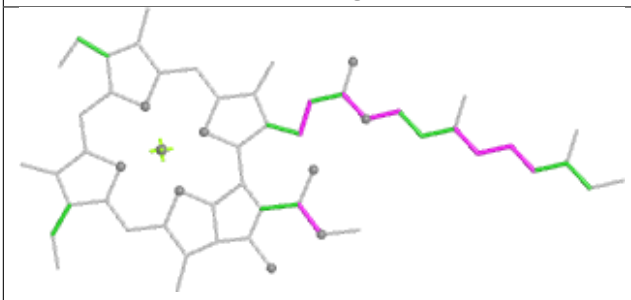
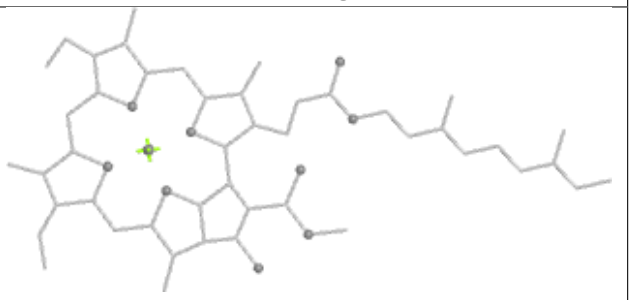
Bond angles

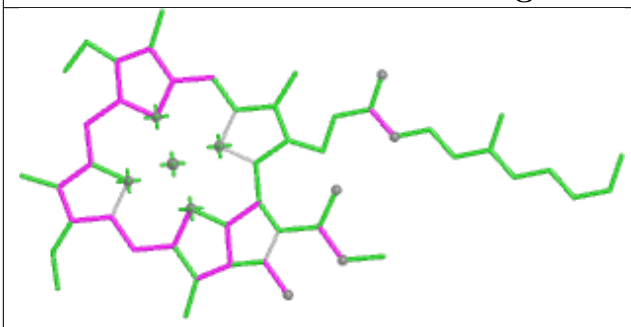
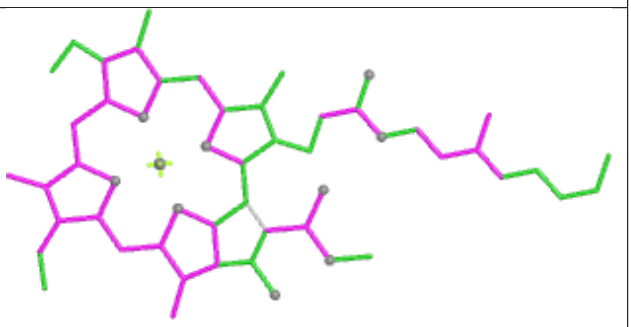
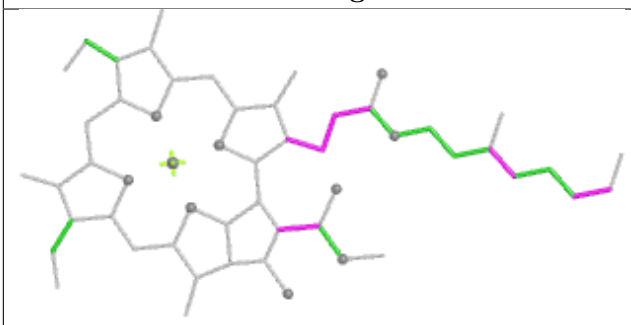
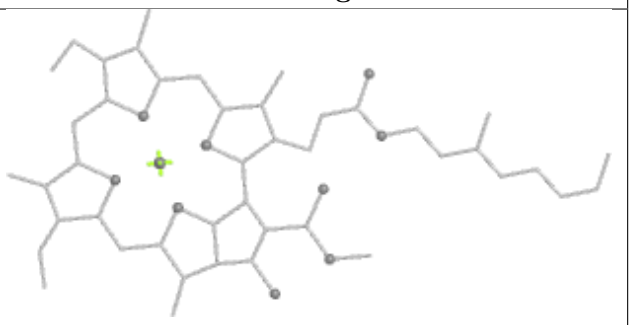


Torsions

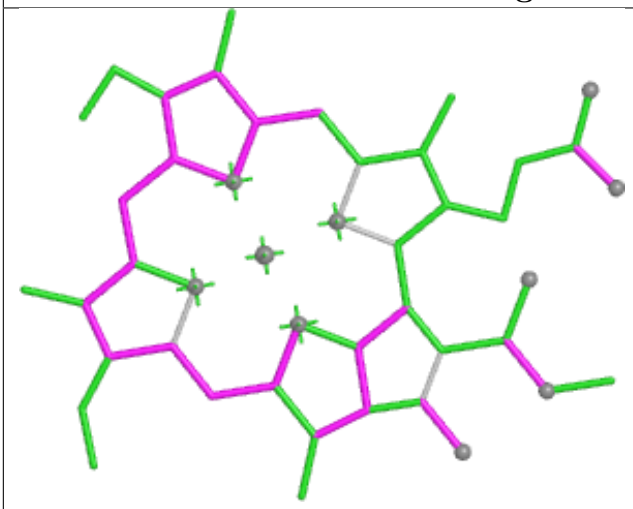


Rings

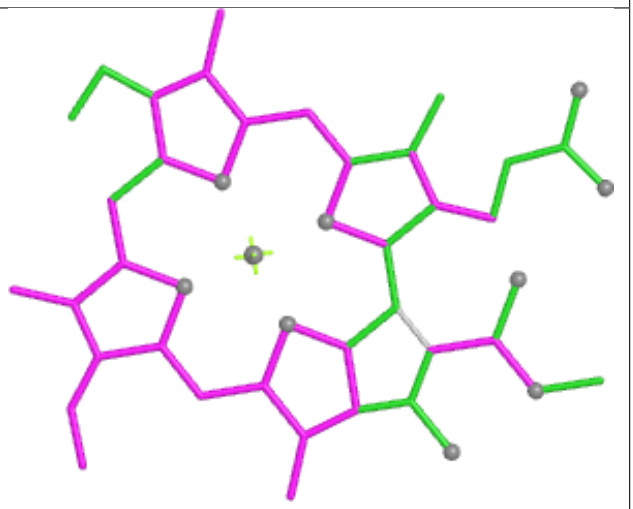
Ligand CLA bB 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

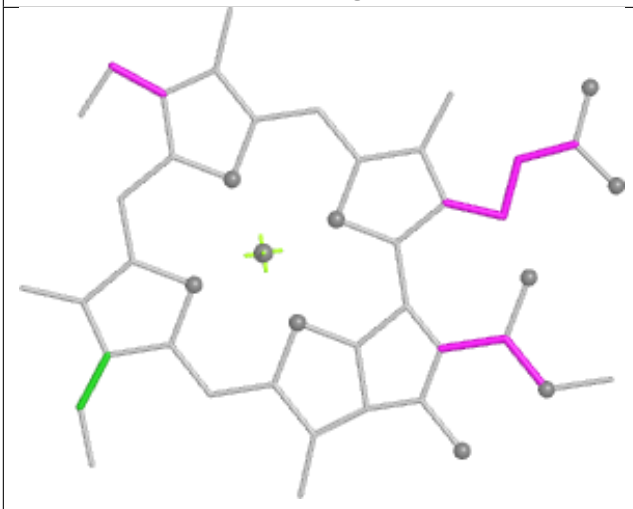
Ligand CLA cA 804



Bond lengths



Bond angles

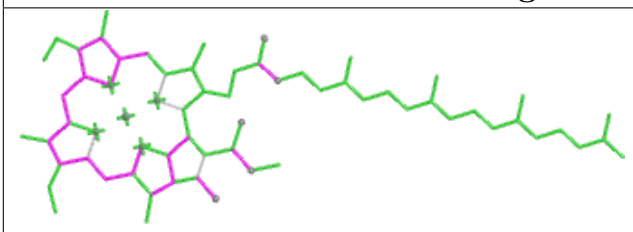


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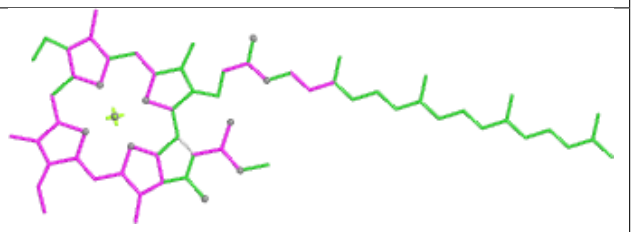


Rings

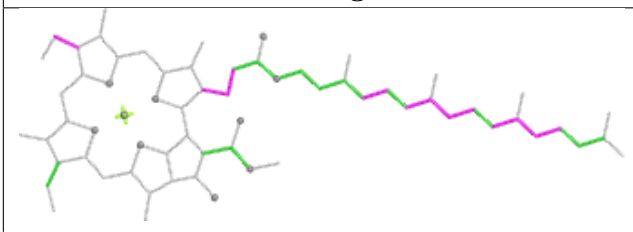
Ligand CLA cL 205



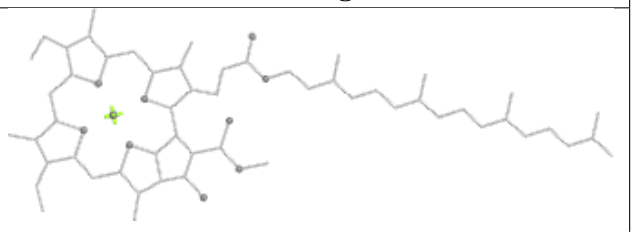
Bond lengths



Bond angles

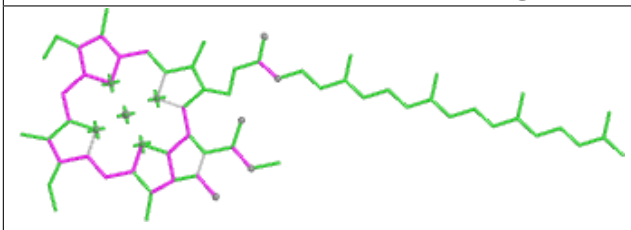


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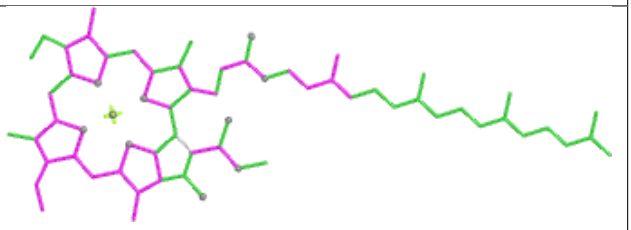


Rings

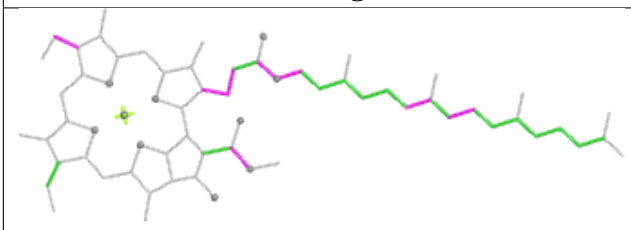
Ligand CLA bA 812



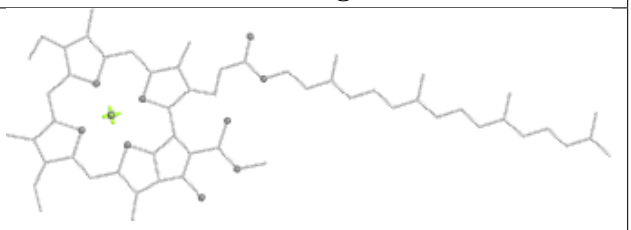
Bond lengths



Bond angles



Torsions

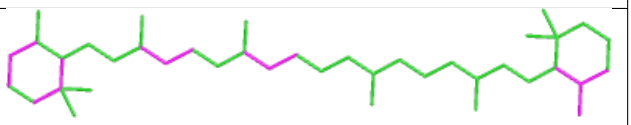


Rings

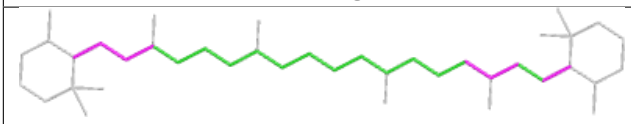
Ligand BCR aI 101



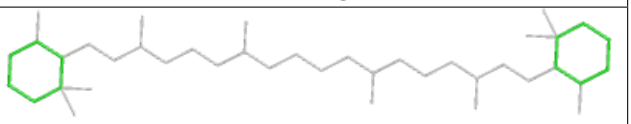
Bond lengths



Bond angles

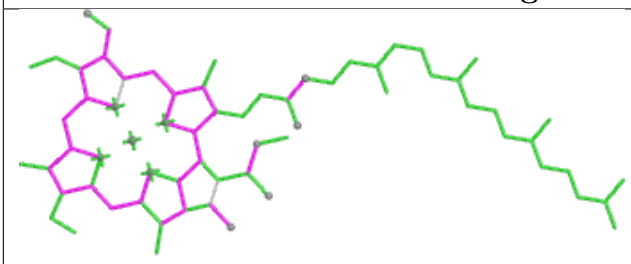


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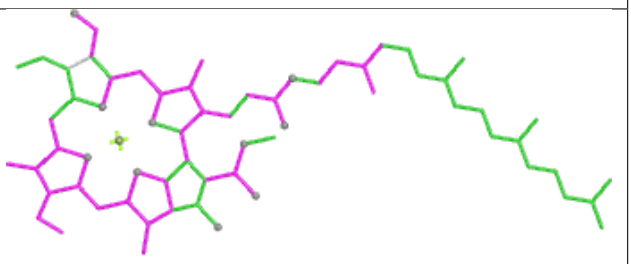


Rings

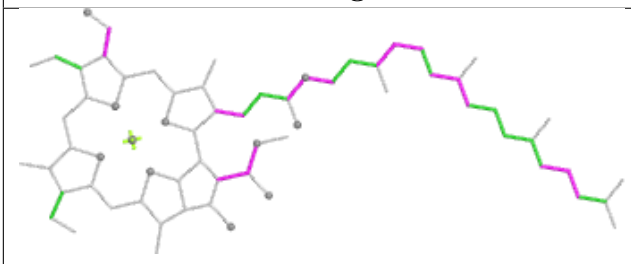
Ligand F6C bL 202



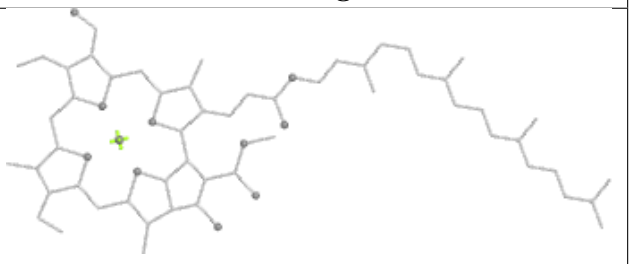
Bond lengths



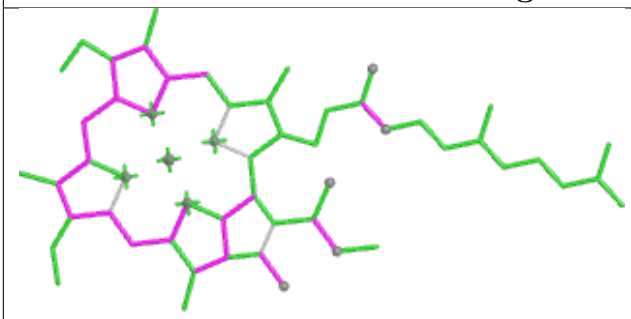
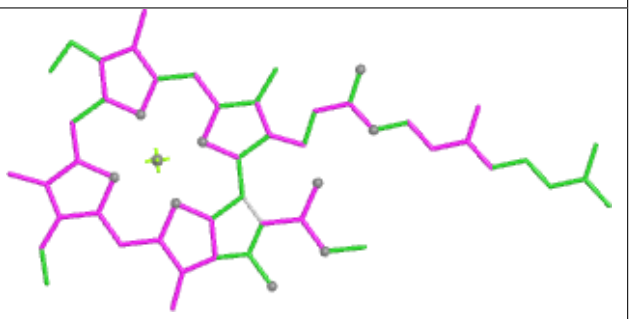
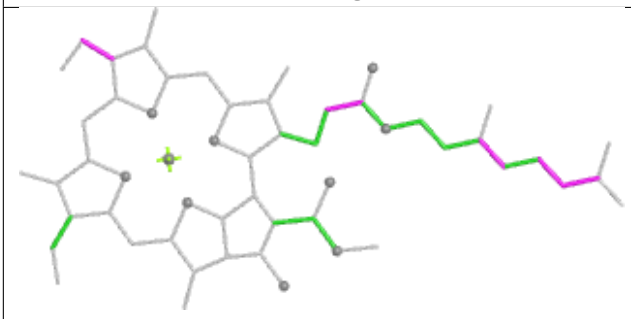
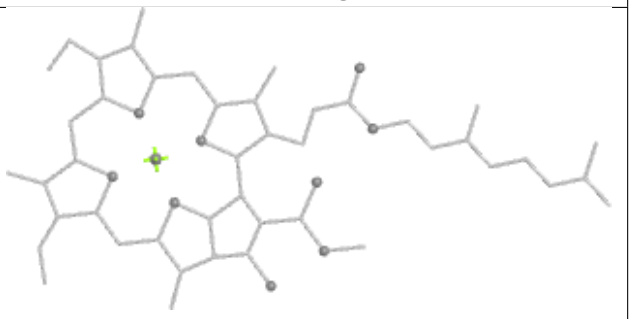
Bond angles

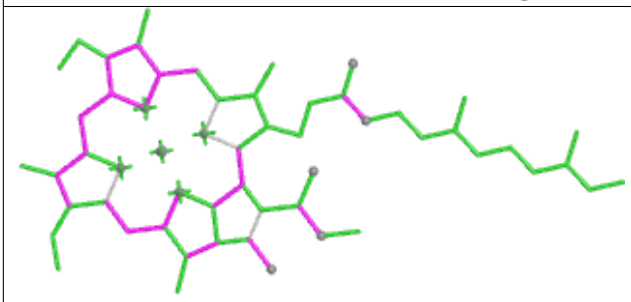
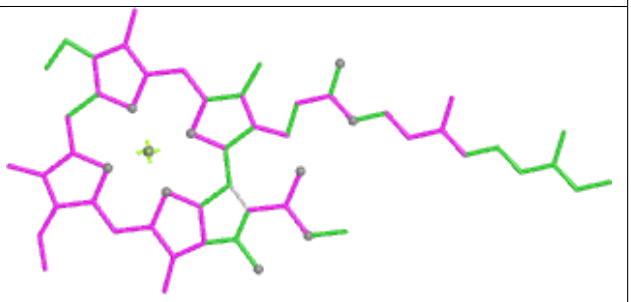
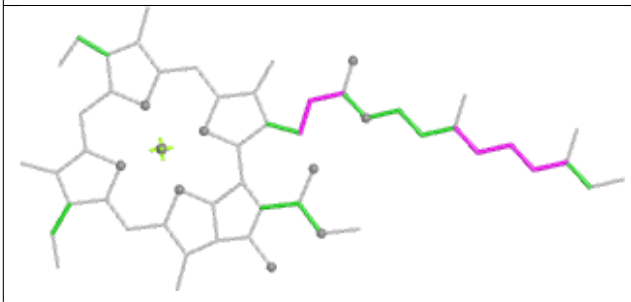
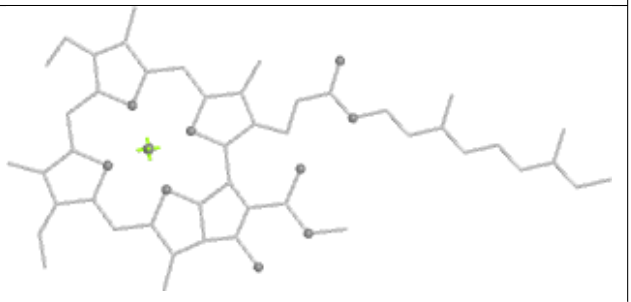


Torsions

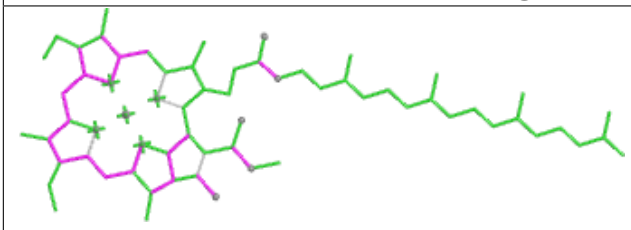


Rings

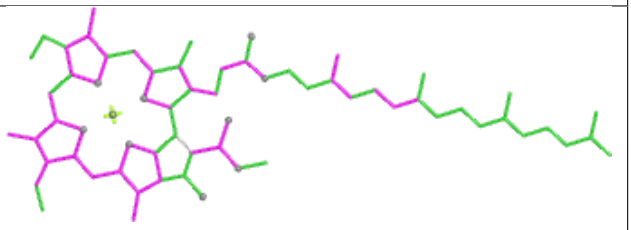
Ligand CLA cB 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

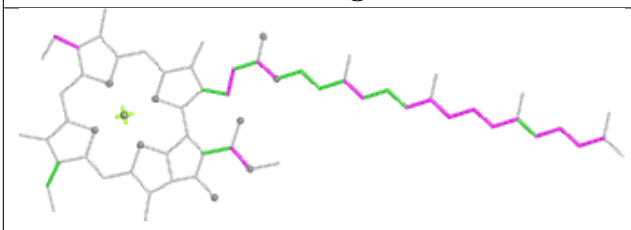
Ligand CLA cA 822



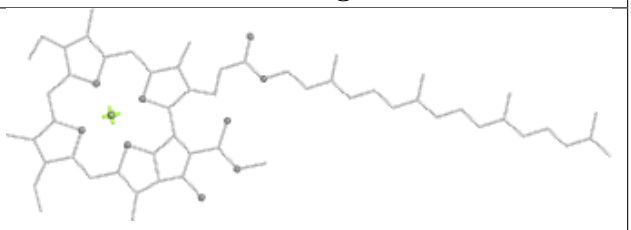
Bond lengths



Bond angles



Torsions

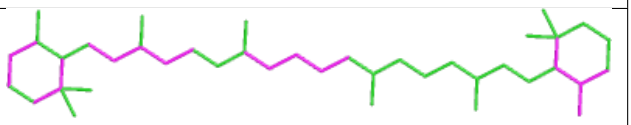


Rings

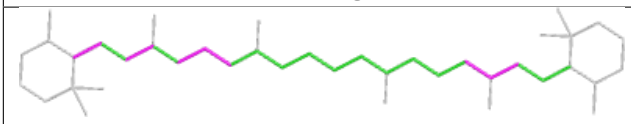
Ligand BCR bL 207



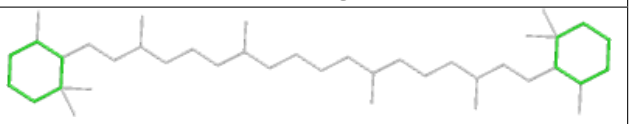
Bond lengths



Bond angles

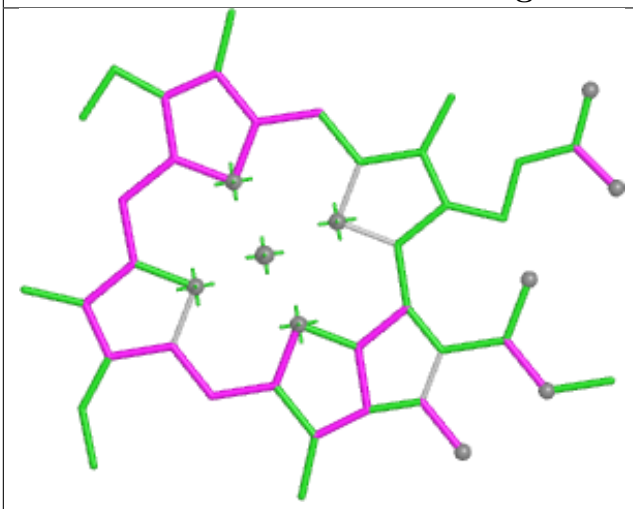


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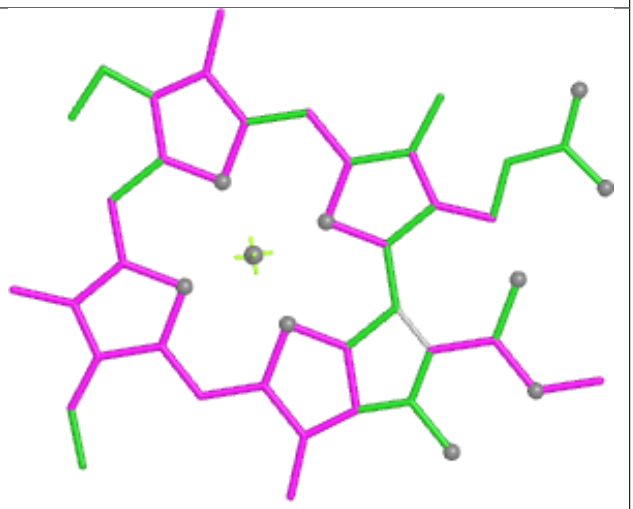


Rings

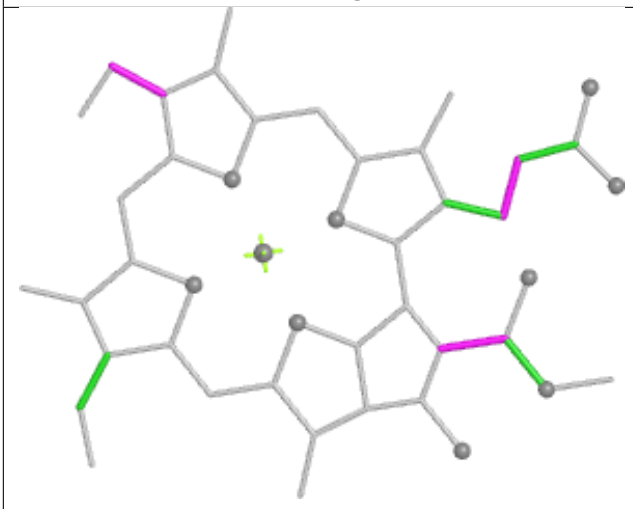
Ligand CLA cA 811



Bond lengths



Bond angles

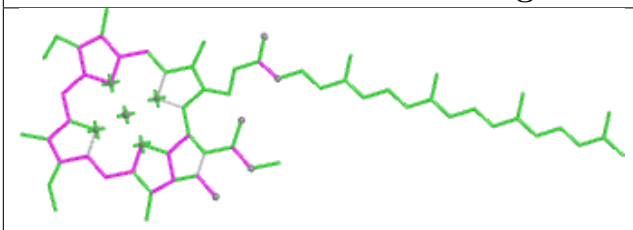


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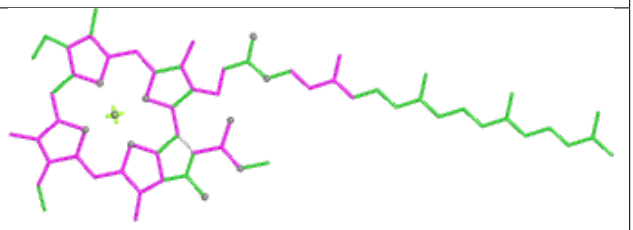


Rings

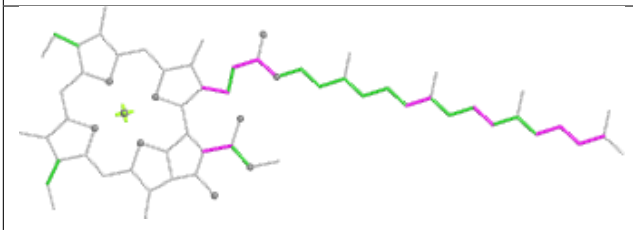
Ligand CLA cB 805



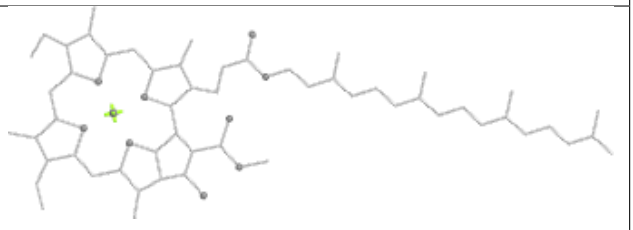
Bond lengths



Bond angles

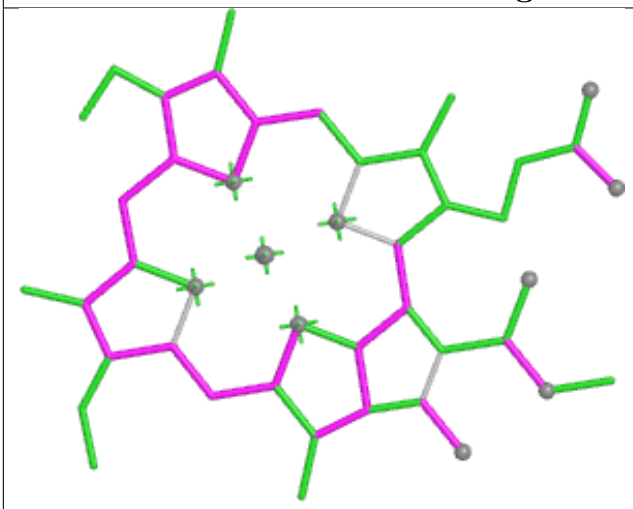


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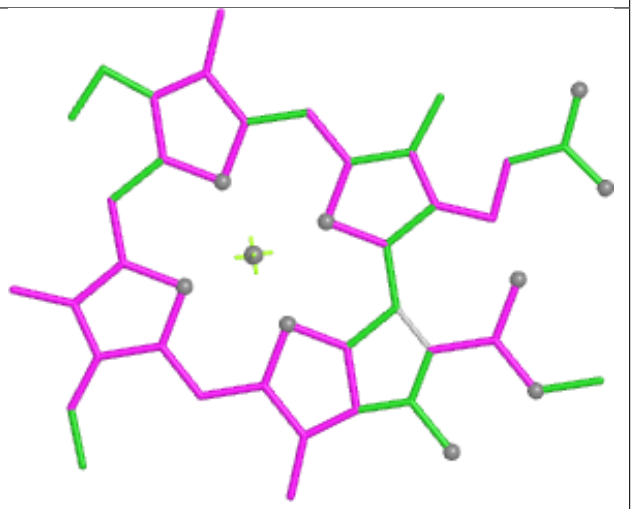


Rings

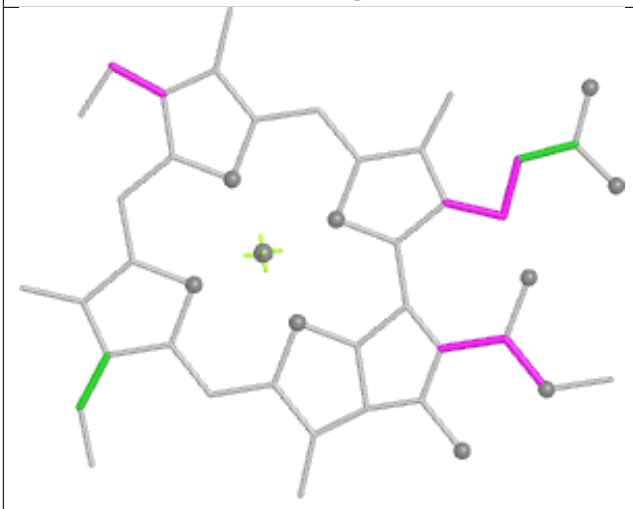
Ligand CLA cA 809



Bond lengths



Bond angles

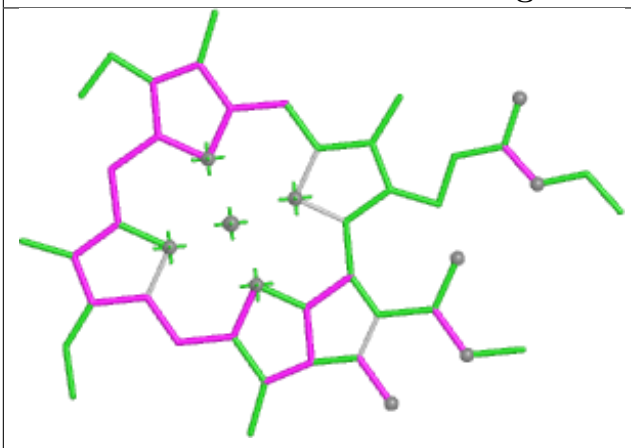


Torsions

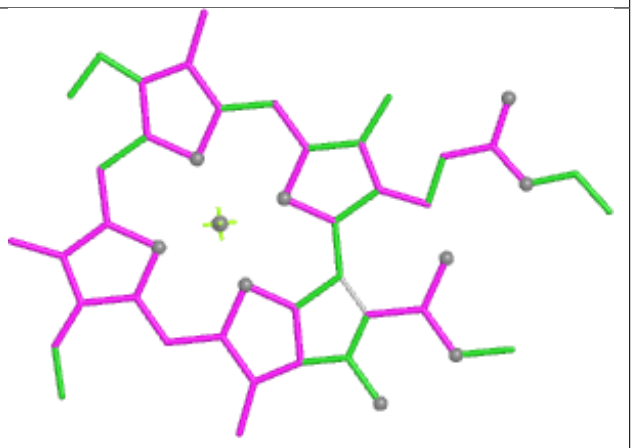


Rings

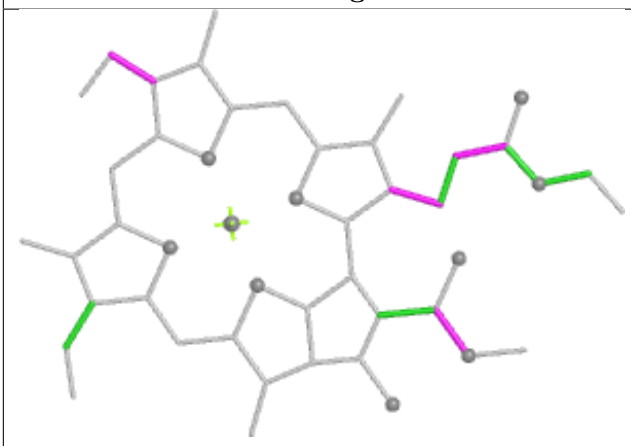
Ligand CLA cB 838



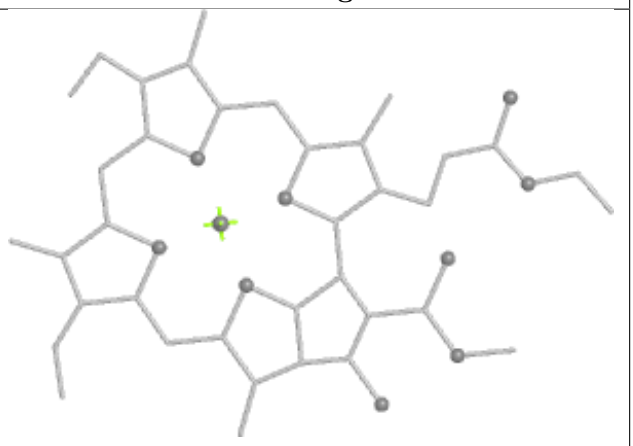
Bond lengths



Bond angles

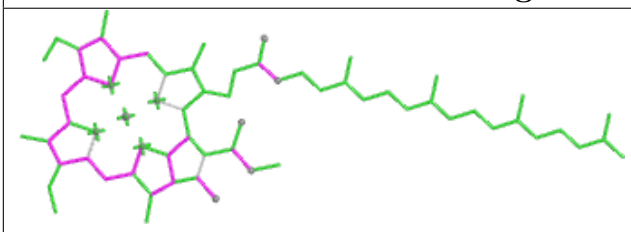


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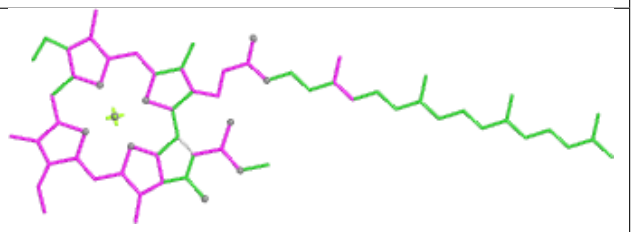


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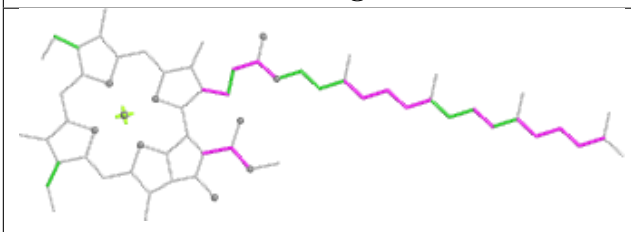
Ligand CLA aA 840



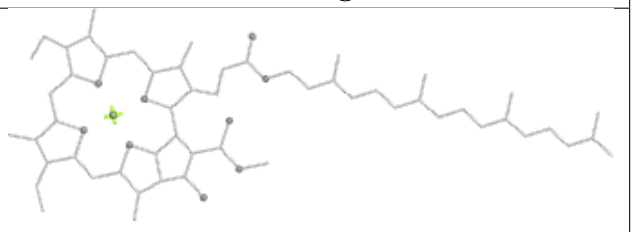
Bond lengths



Bond angles

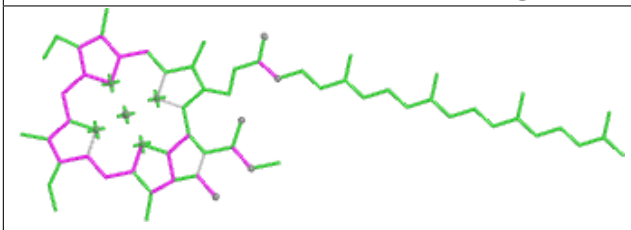


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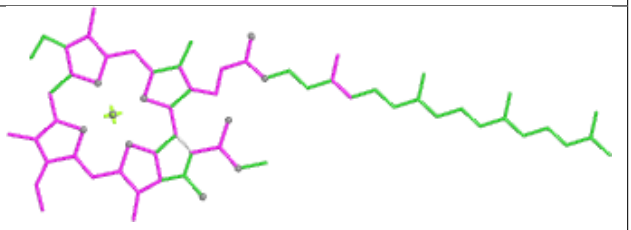


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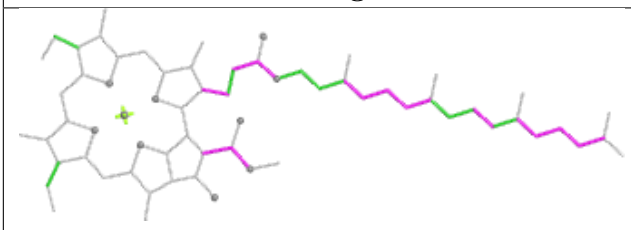
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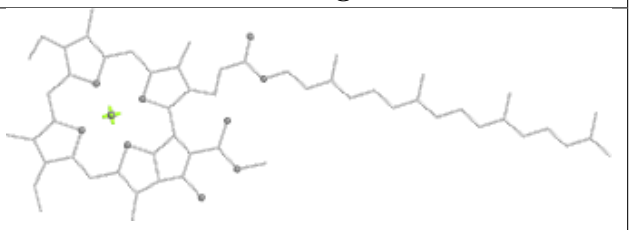
Bond lengths



Bond angles

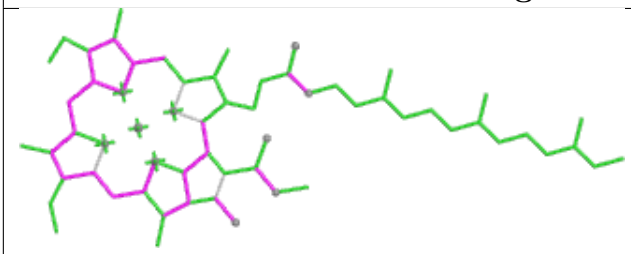


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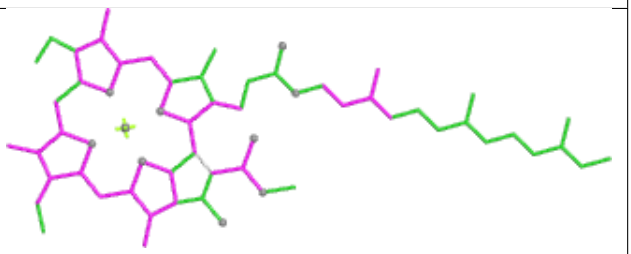


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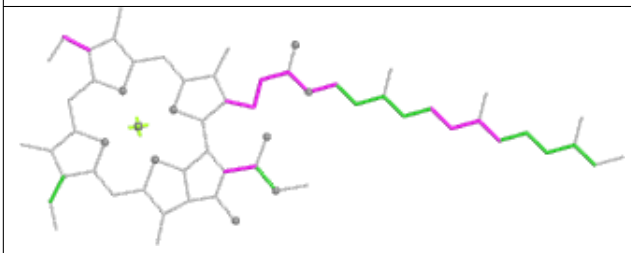
Ligand CLA aA 821



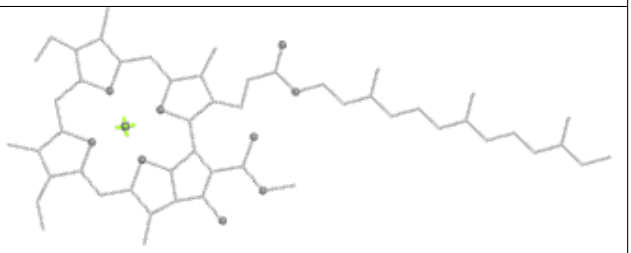
Bond lengths



Bond angles

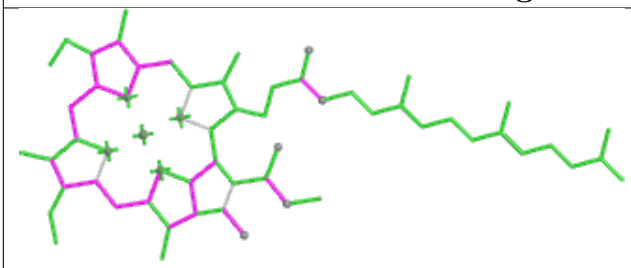


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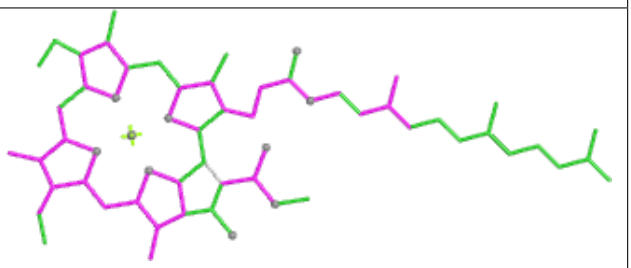


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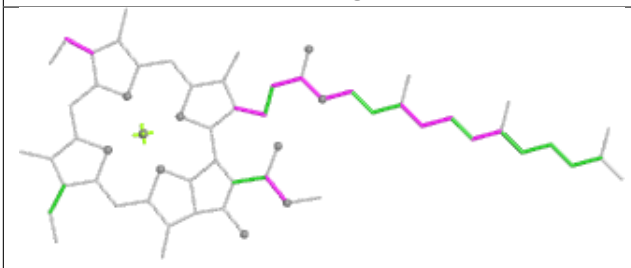
Ligand CLA aB 817



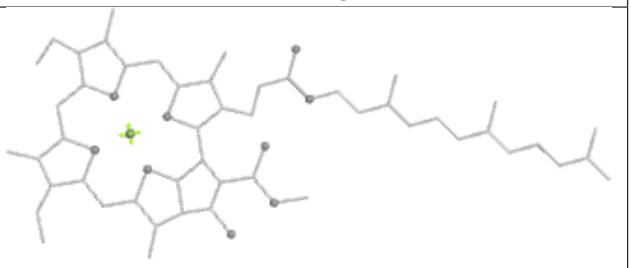
Bond lengths



Bond angles

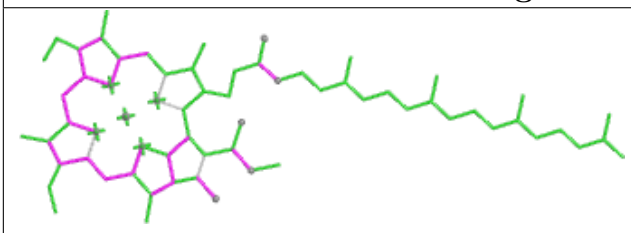


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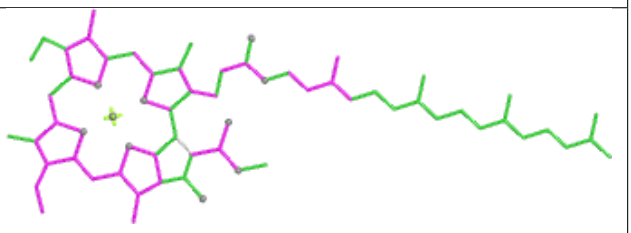


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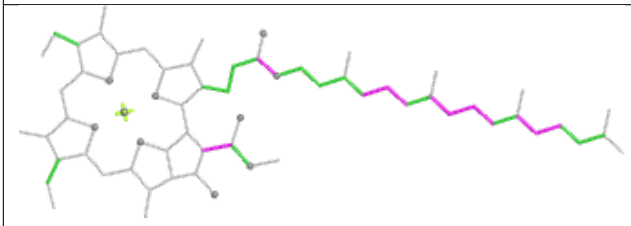
Ligand CLA aA 831



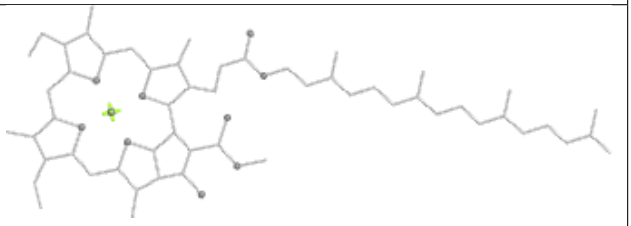
Bond lengths



Bond angles



Torsions

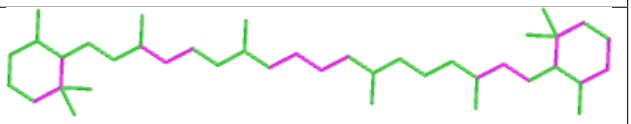


Rings

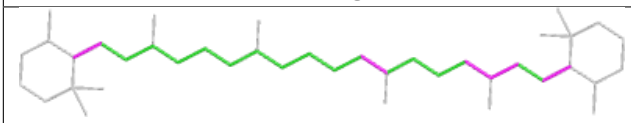
Ligand BCR bA 847



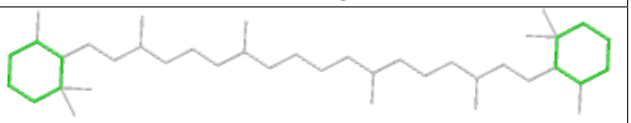
Bond lengths



Bond angles

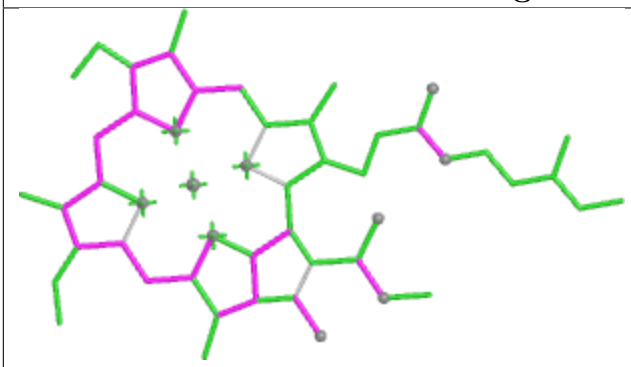


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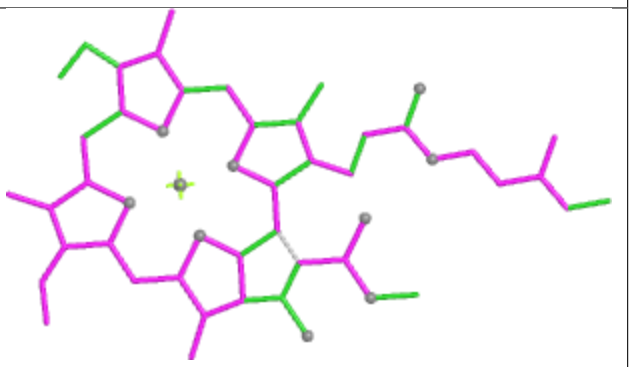


Rings

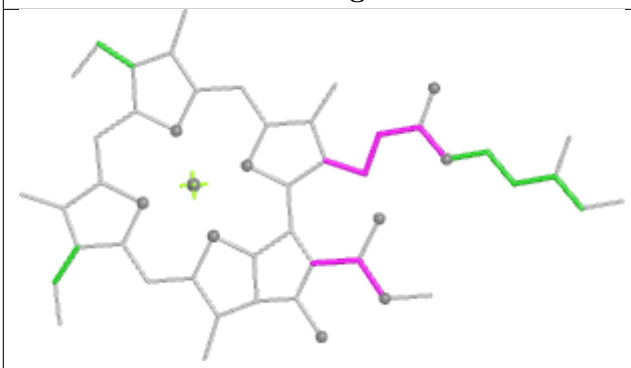
Ligand CLA bA 838



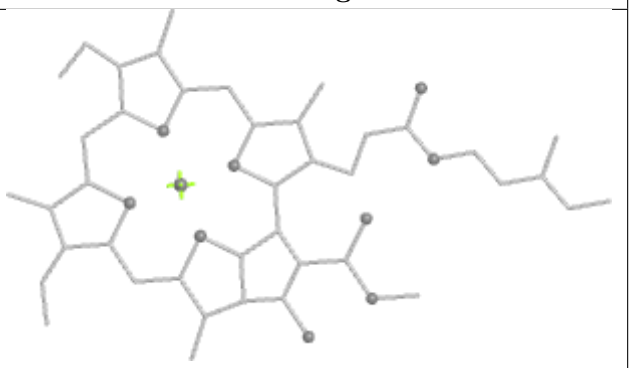
Bond lengths



Bond angles

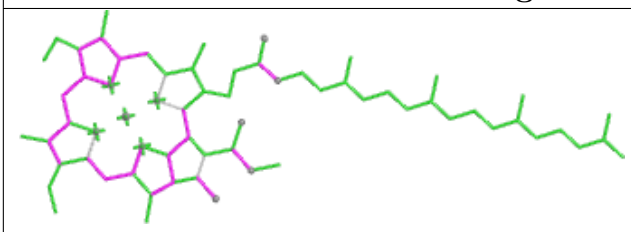


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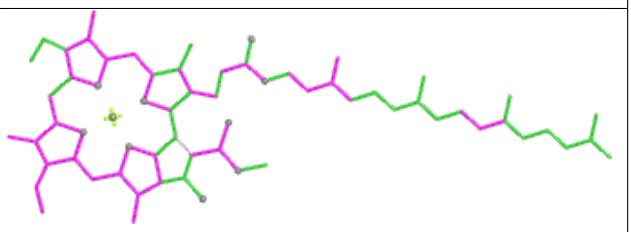


Rings

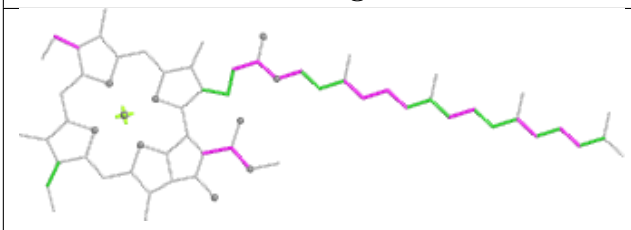
Ligand CLA cA 807



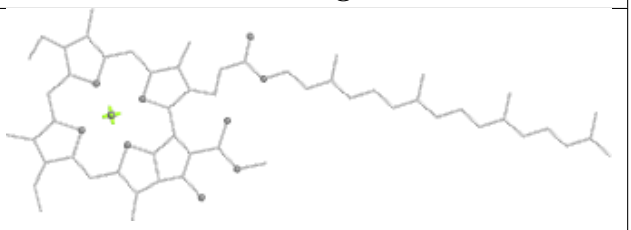
Bond lengths



Bond angles

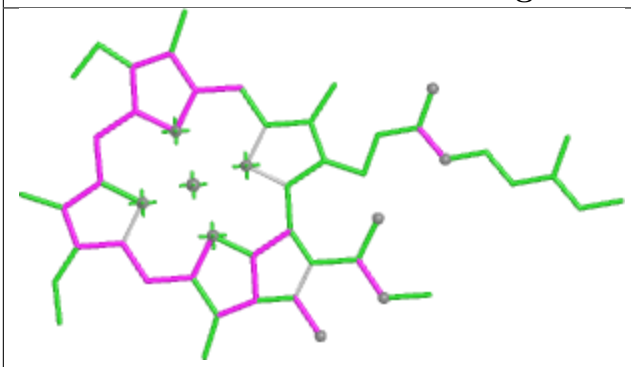


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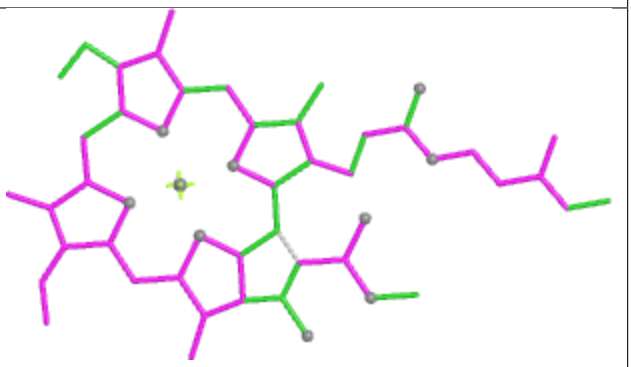


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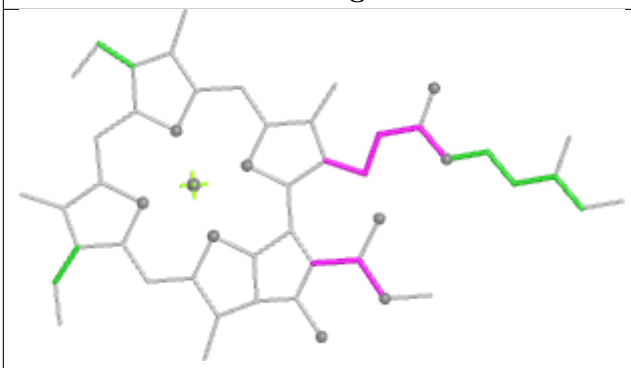
Ligand CLA cA 838



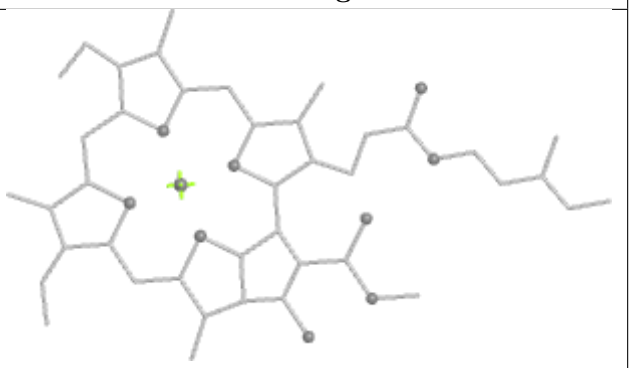
Bond lengths



Bond angles

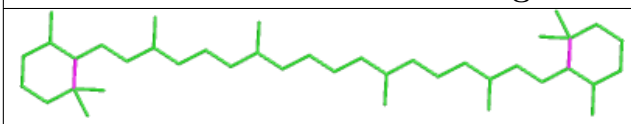


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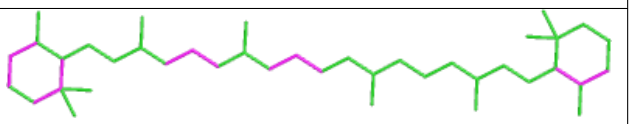


Rings

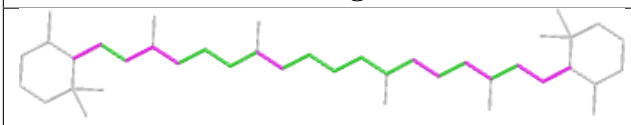
Ligand BCR bB 846



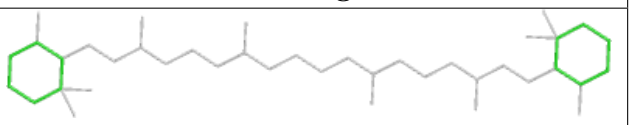
Bond lengths



Bond angles

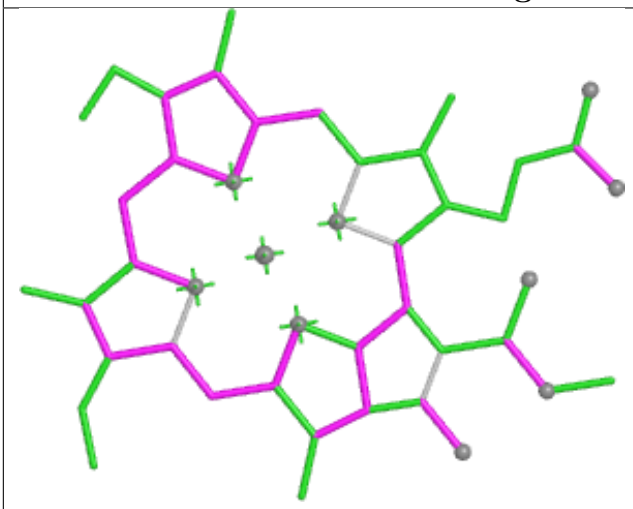


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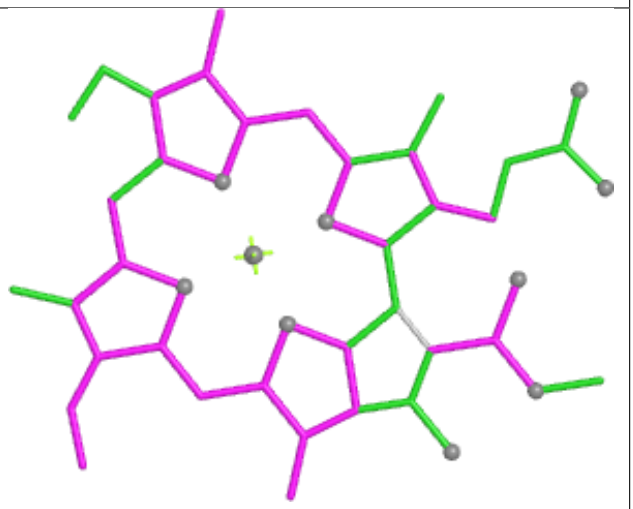


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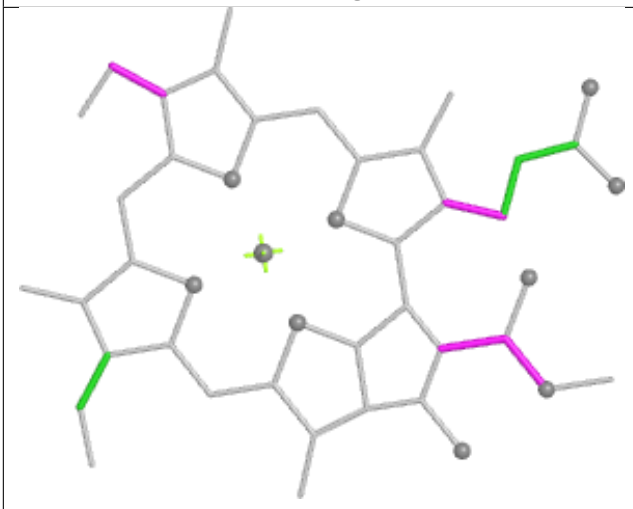
Ligand CLA bB 814



Bond lengths



Bond angles

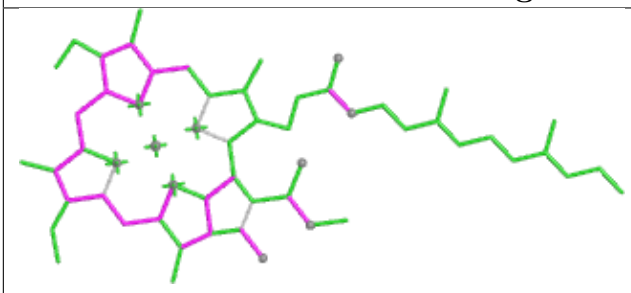


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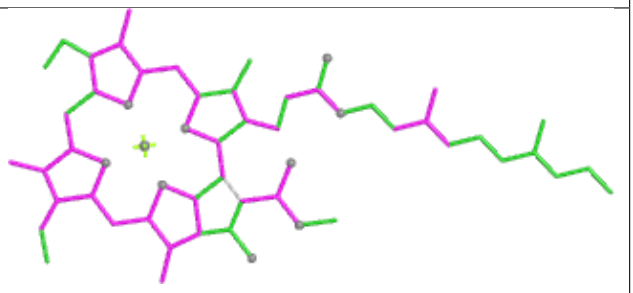


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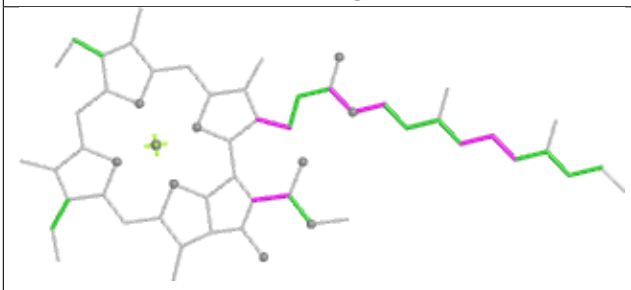
Ligand CLA aB 802



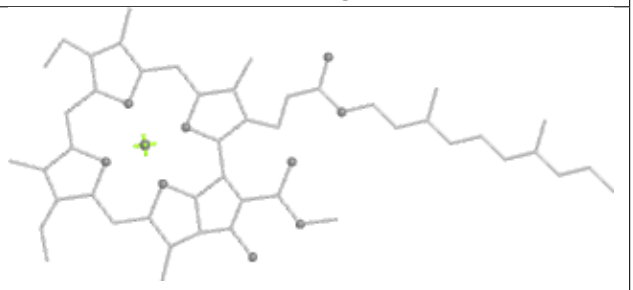
Bond lengths



Bond angles

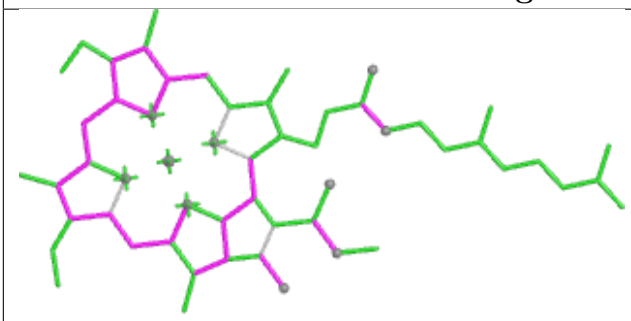


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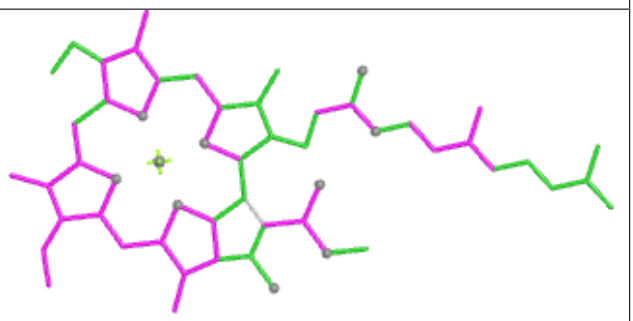


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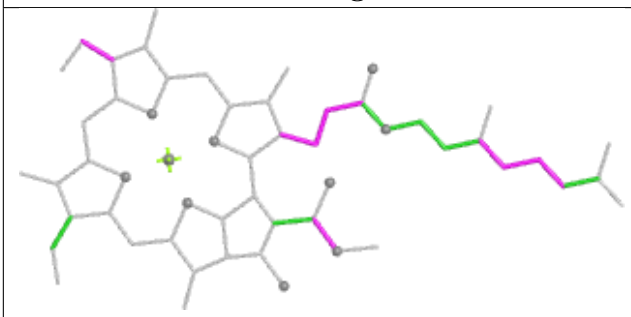
Ligand CLA aB 815



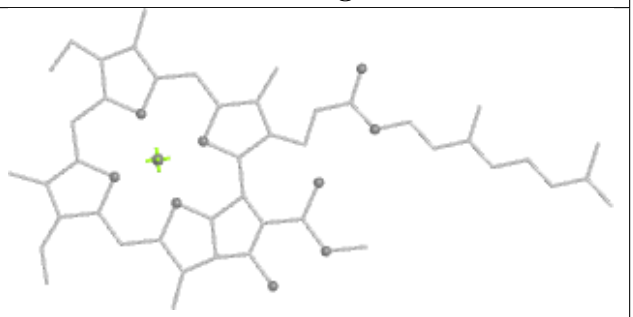
Bond lengths



Bond angles

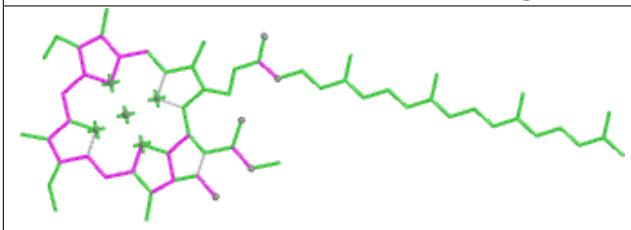


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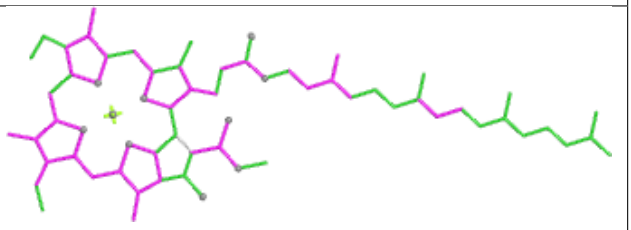


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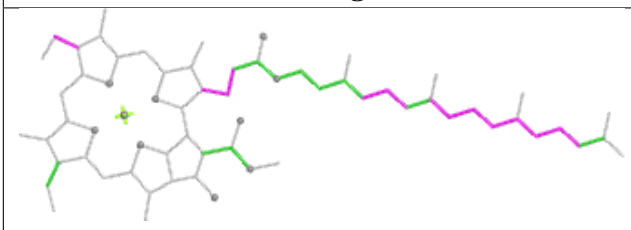
Ligand CLA aL 206



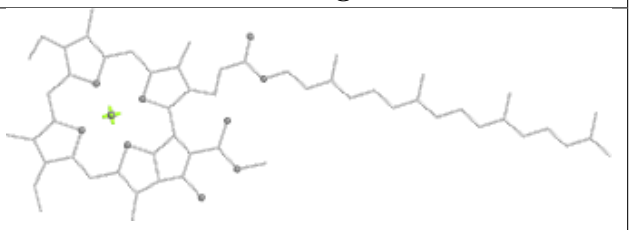
Bond lengths



Bond angles

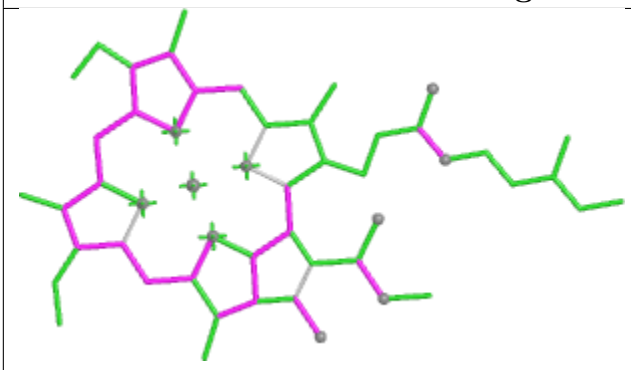


Torsions

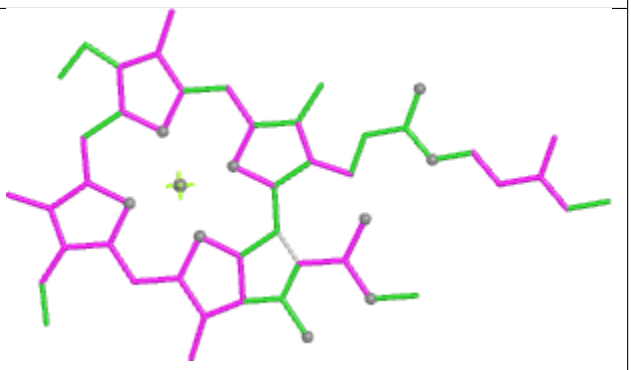


Rings

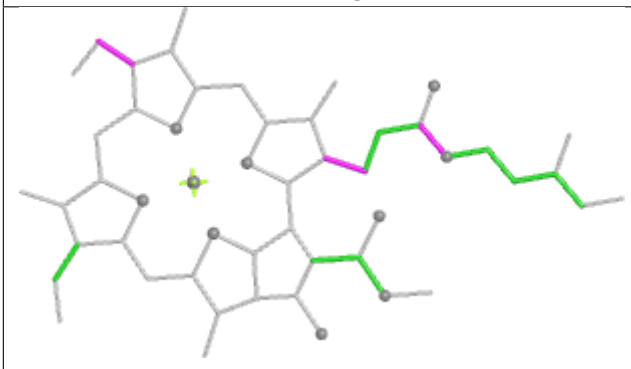
Ligand CLA aA 808



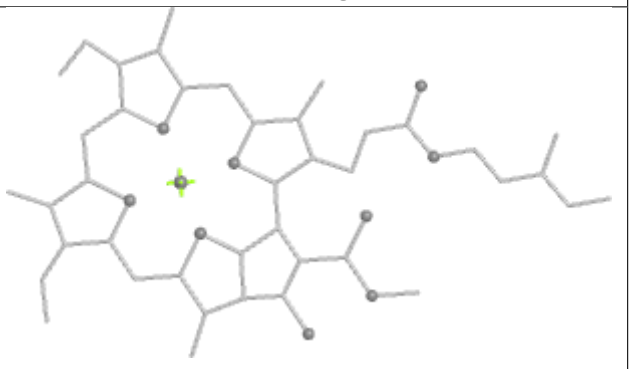
Bond lengths



Bond angles

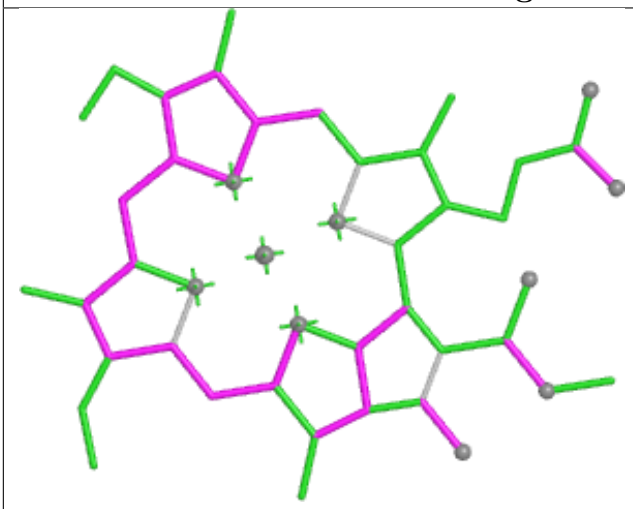


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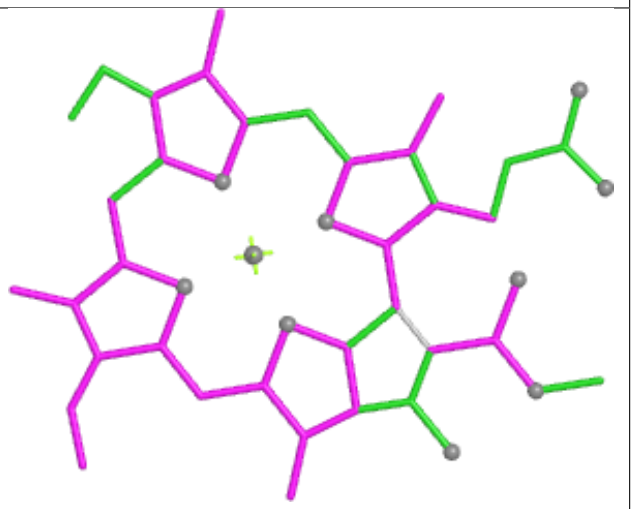


Rings

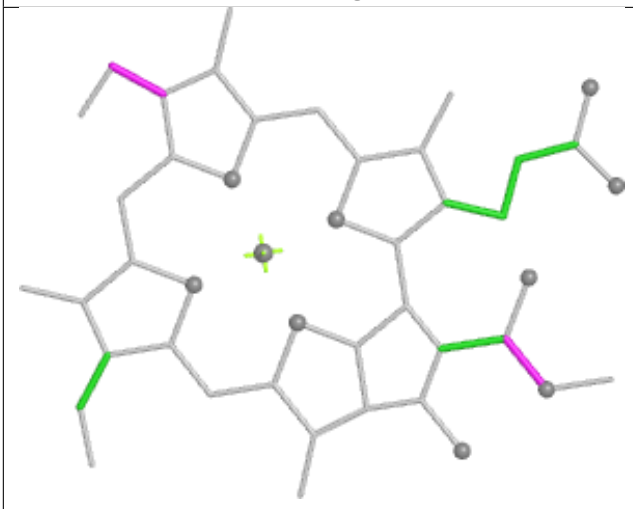
Ligand CLA cA 810



Bond lengths



Bond angles

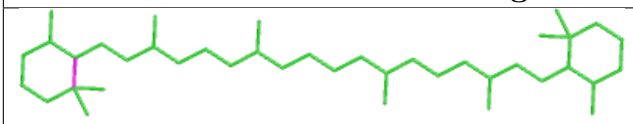


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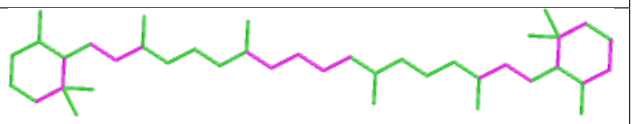


Rings

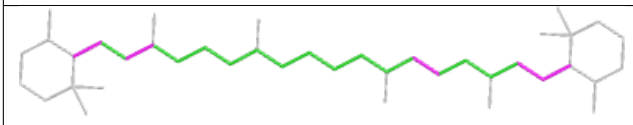
Ligand BCR cM 101



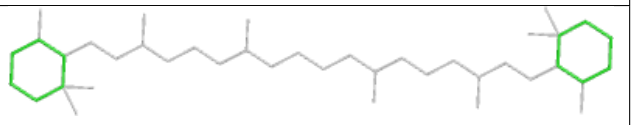
Bond lengths



Bond angles

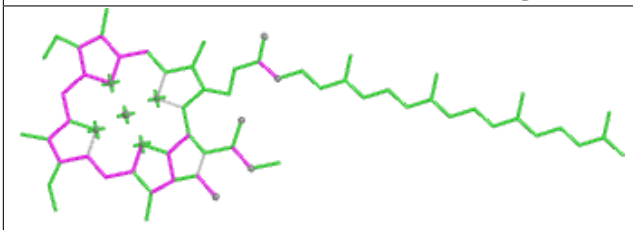


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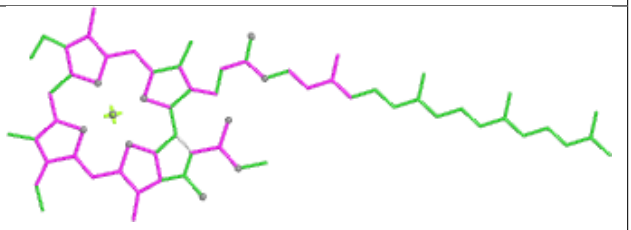


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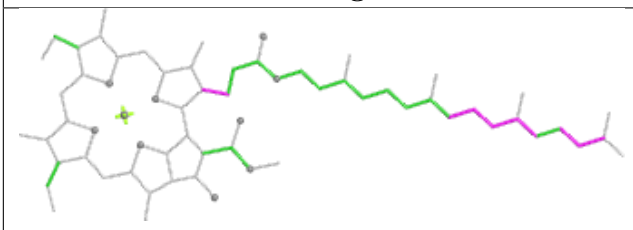
Ligand CLA cB 825



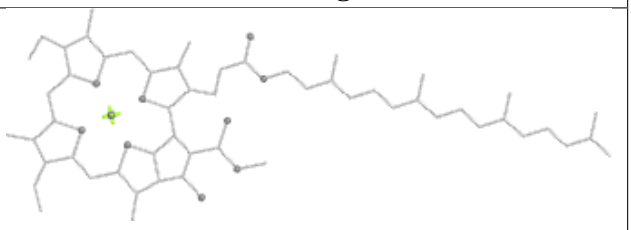
Bond lengths



Bond angles

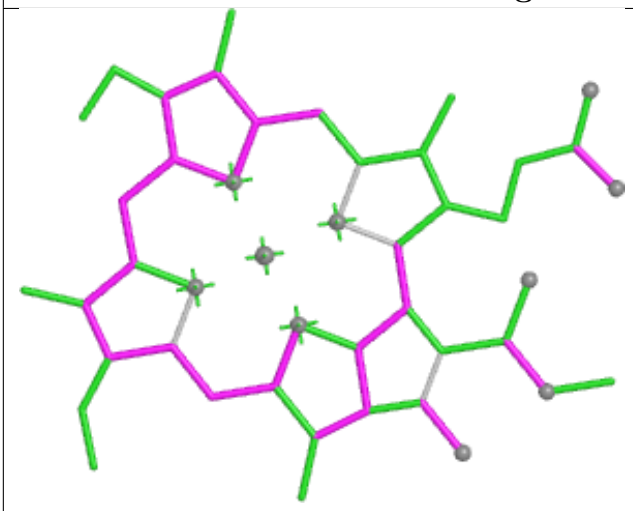


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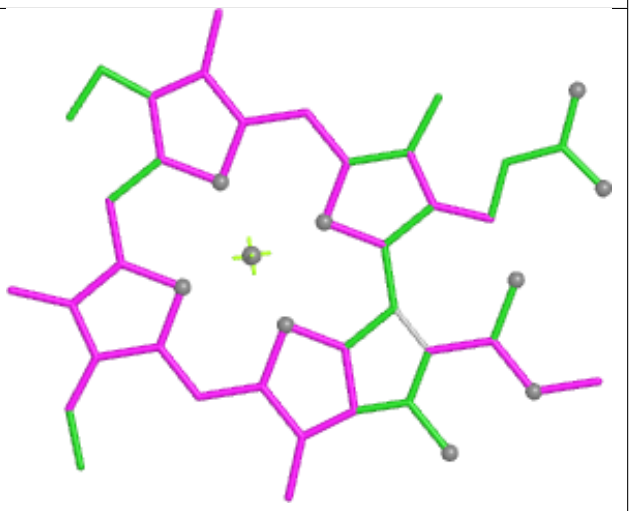


Rings

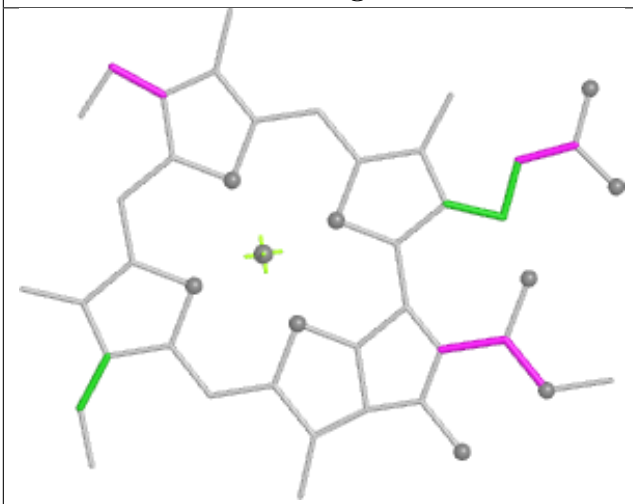
Ligand CLA aA 842



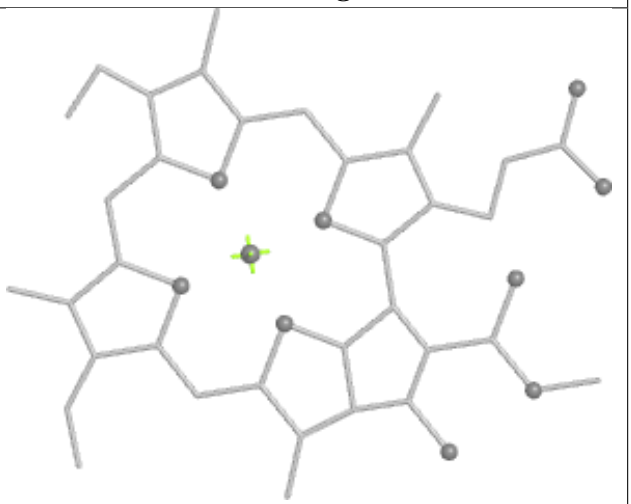
Bond lengths



Bond angles

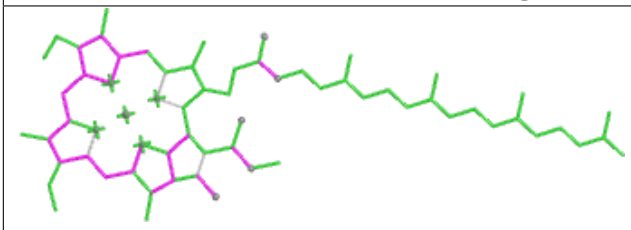


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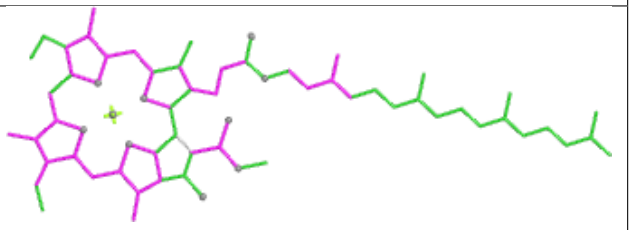


Rings

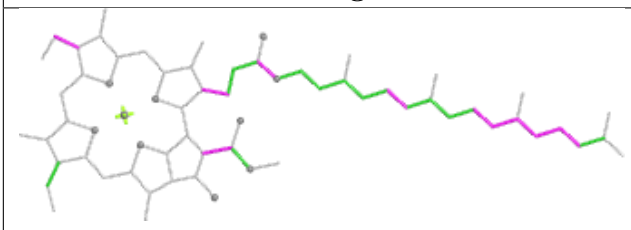
Ligand CLA cA 814



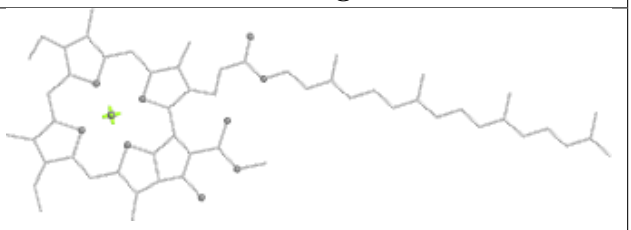
Bond lengths



Bond angles

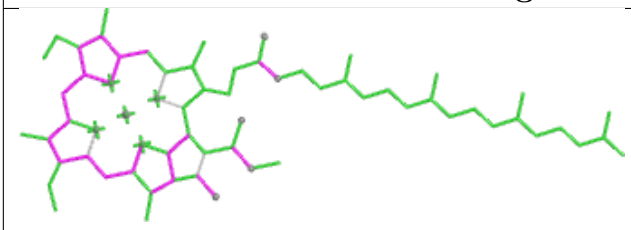


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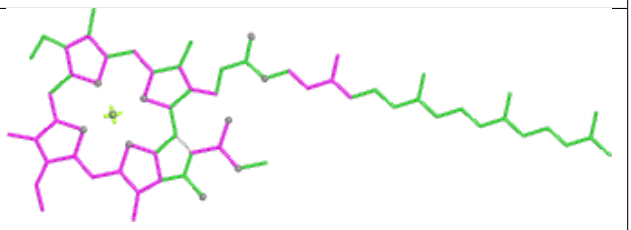


Rings

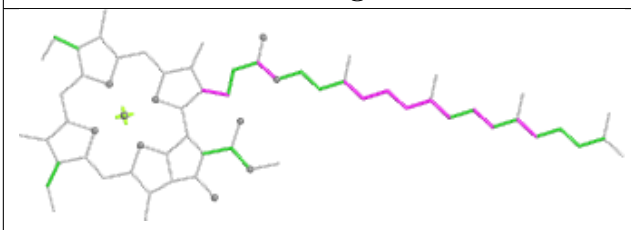
Ligand CLA cA 833



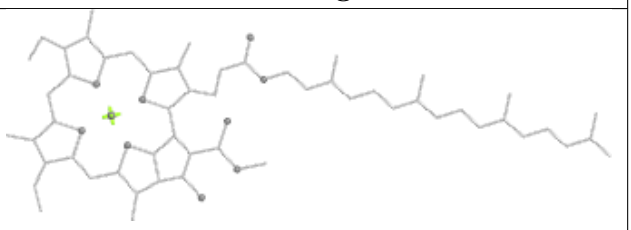
Bond lengths



Bond angles

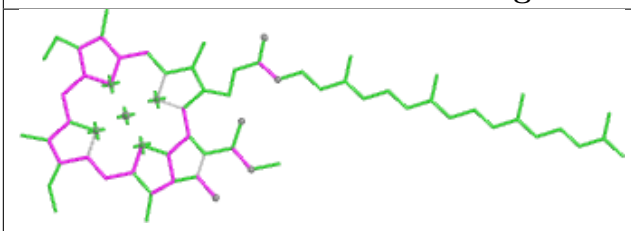


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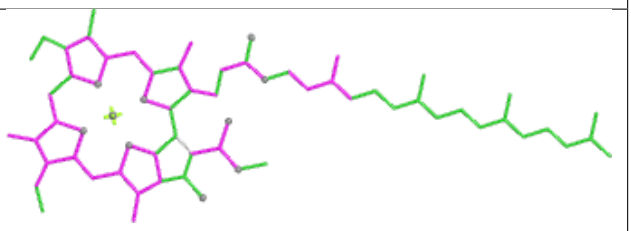


Rings

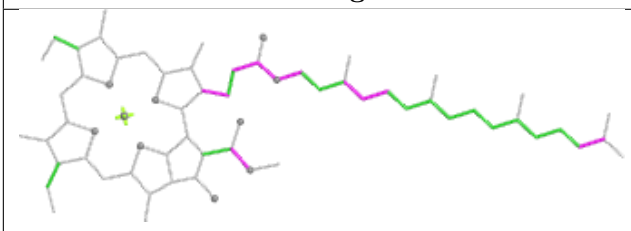
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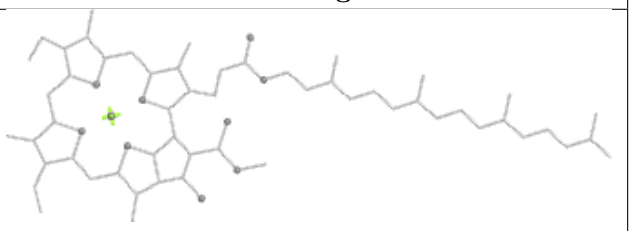
Bond lengths



Bond angles

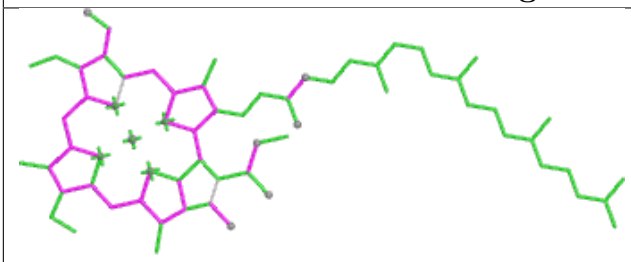


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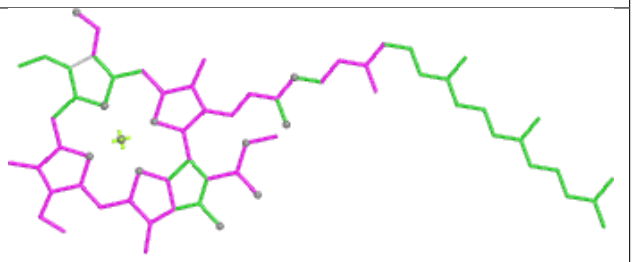


Rings

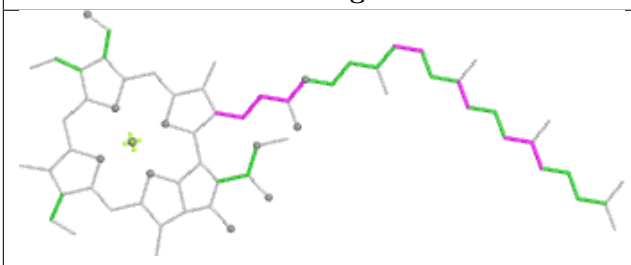
Ligand F6C aA 844



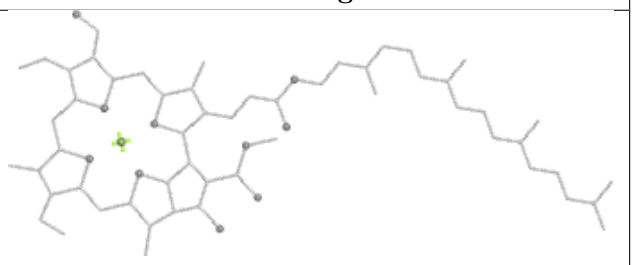
Bond lengths



Bond angles

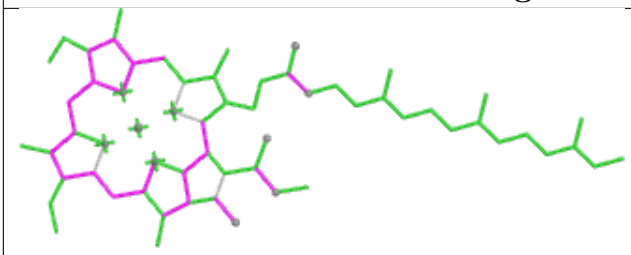


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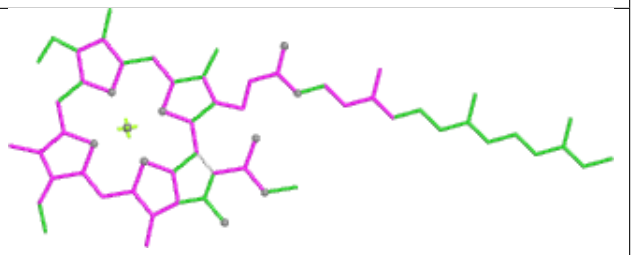


Rings

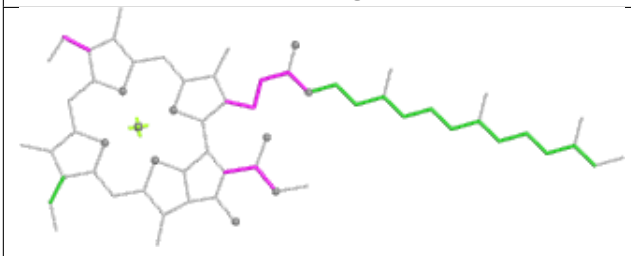
Ligand CLA bB 826



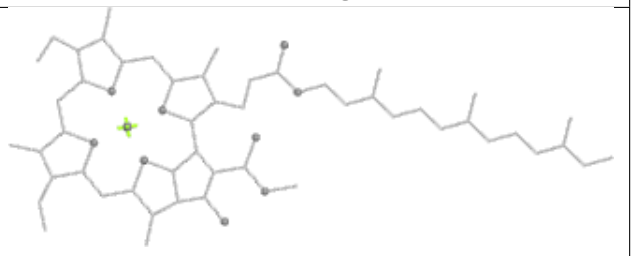
Bond lengths



Bond angles

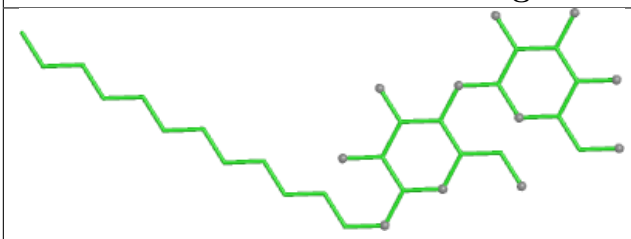


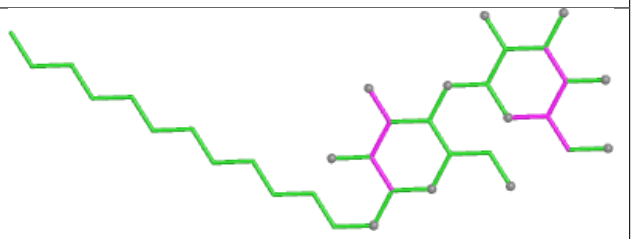
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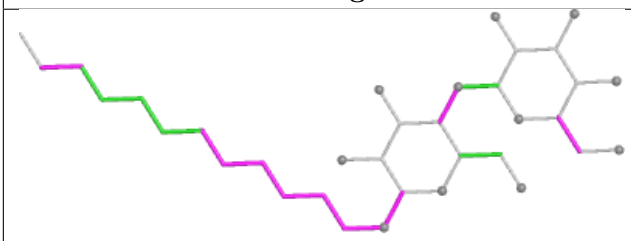


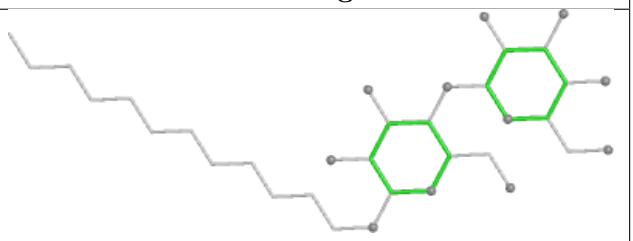
Rings

Ligand LMT cA 853

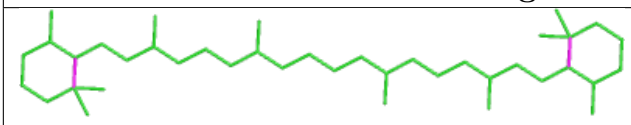

Bond lengths

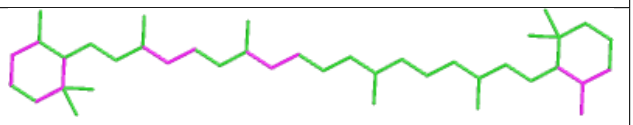

Bond angles

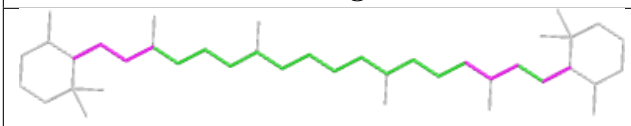

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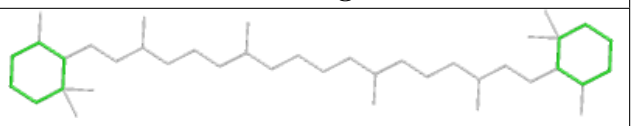

Rings

Ligand BCR bI 101

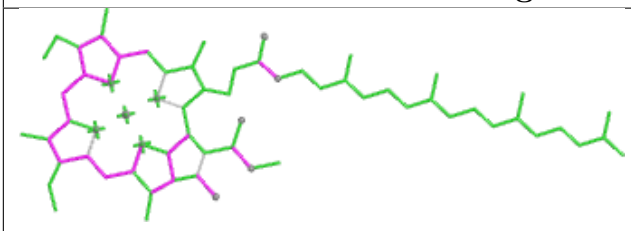

Bond lengths

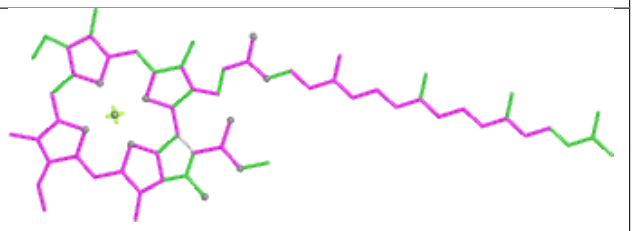

Bond angles

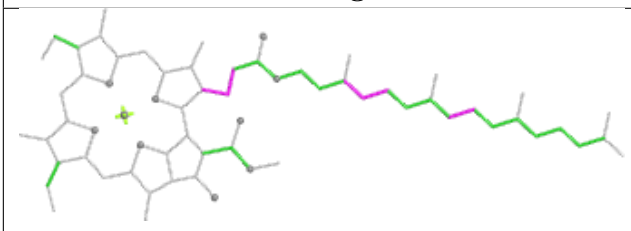

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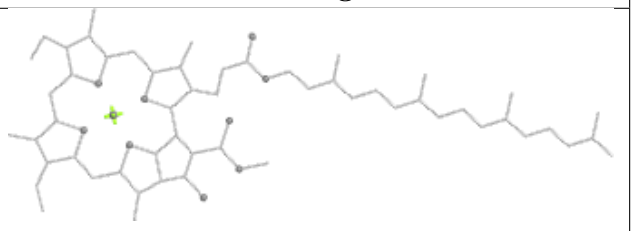

Rings

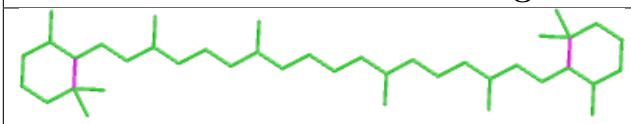
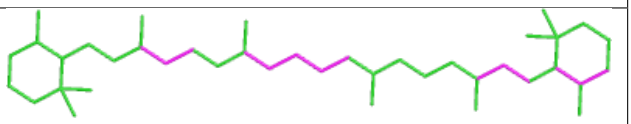
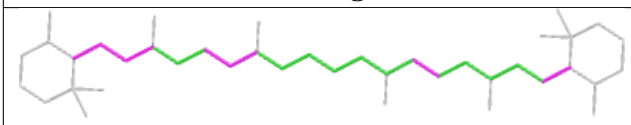
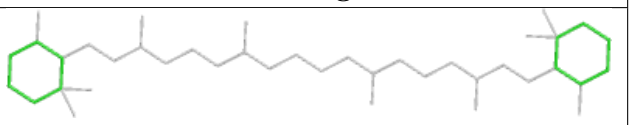
Ligand CLA cA 802

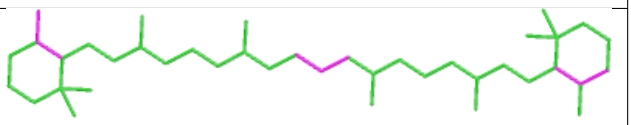
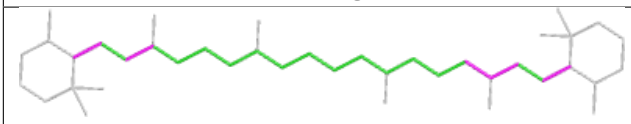
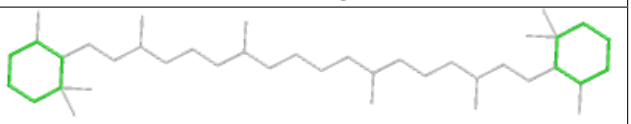

Bond lengths


Bond angles

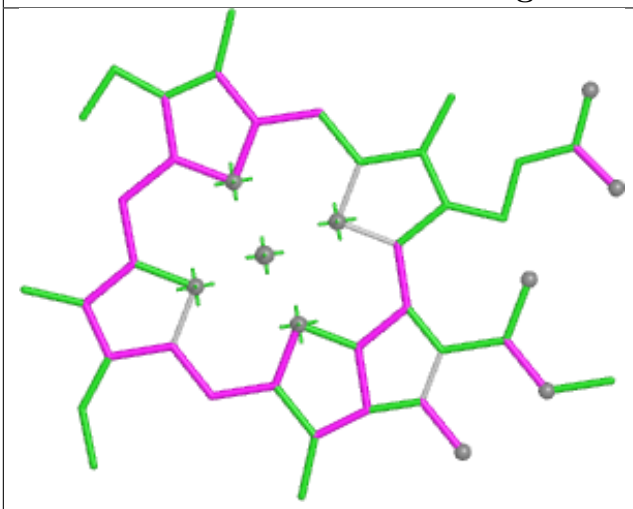

Torsions


Rings

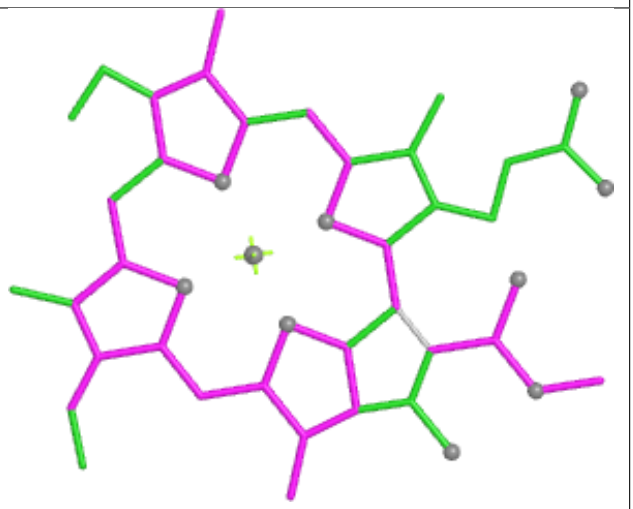
Ligand BCR aB 845	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCR aB 843	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

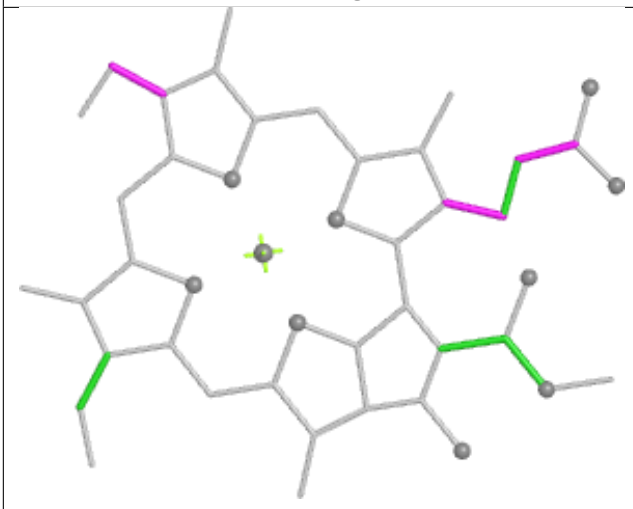
Ligand CLA cB 834



Bond lengths



Bond angles

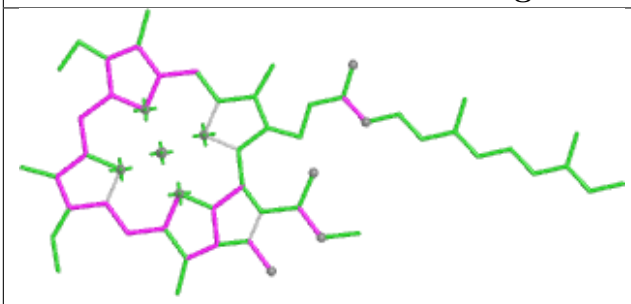


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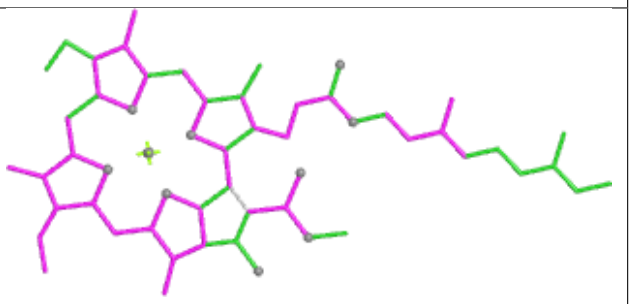


Rings

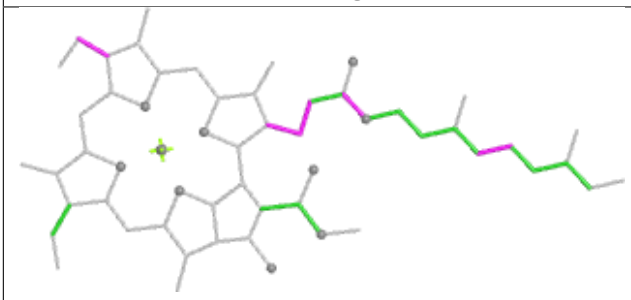
Ligand CLA bB 831



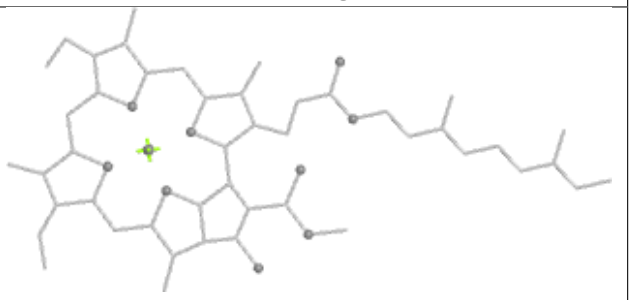
Bond lengths



Bond angles

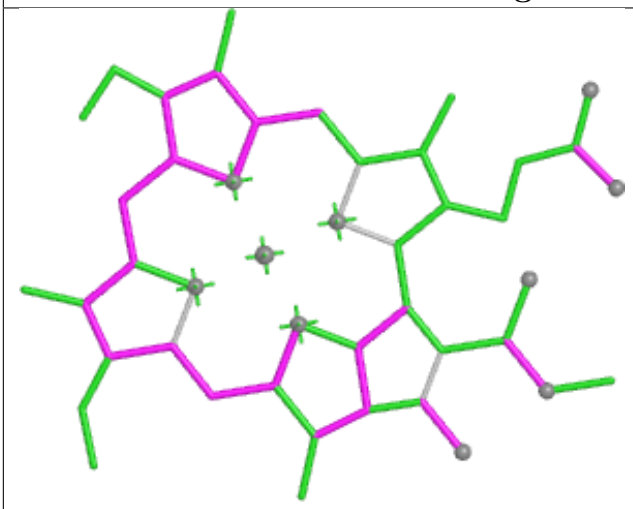


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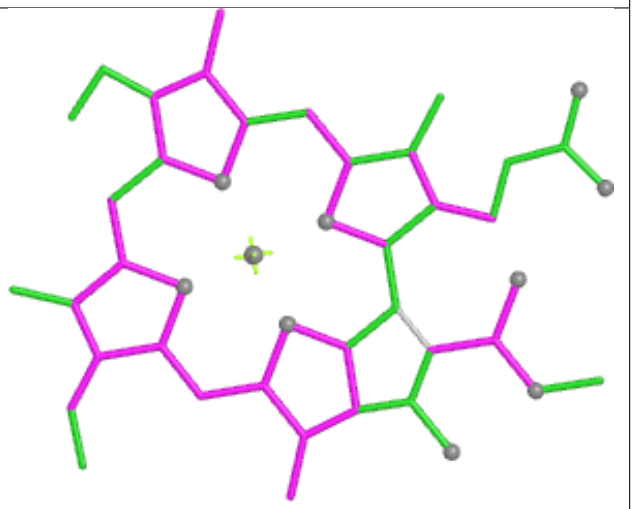


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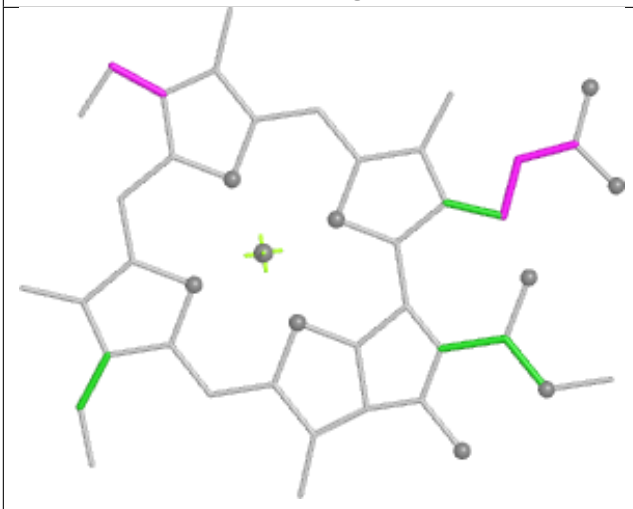
Ligand CLA bB 811



Bond lengths



Bond angles

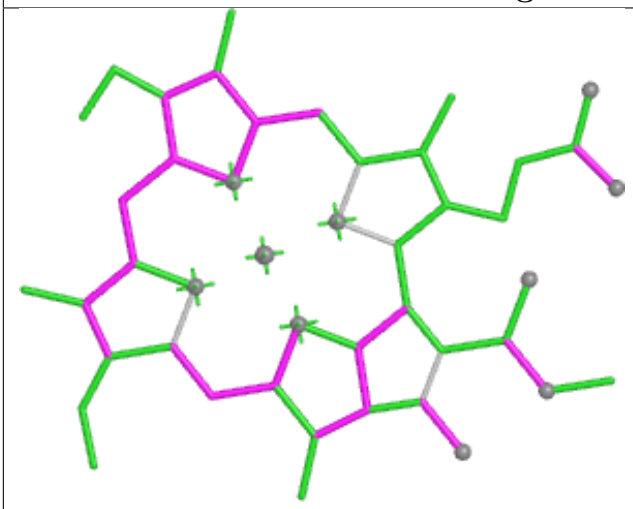


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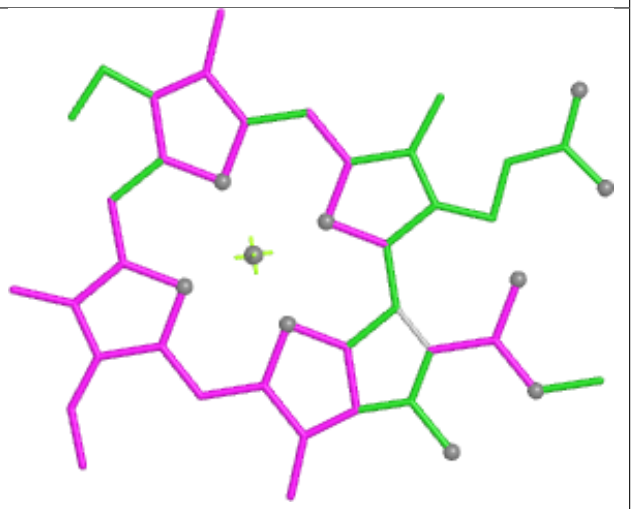


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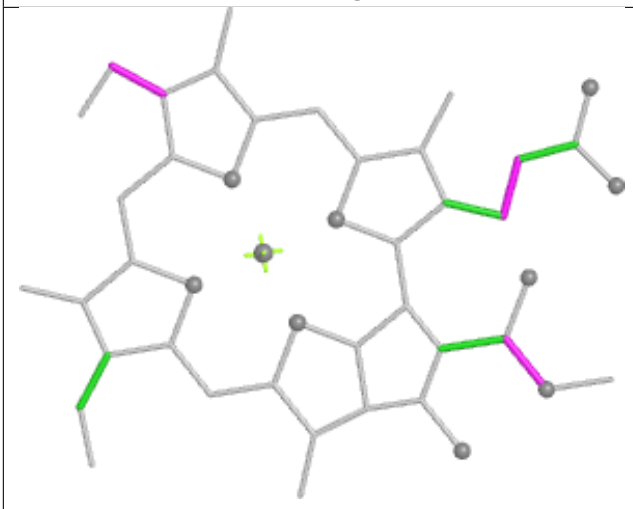
Ligand CLA cB 840



Bond lengths



Bond angles

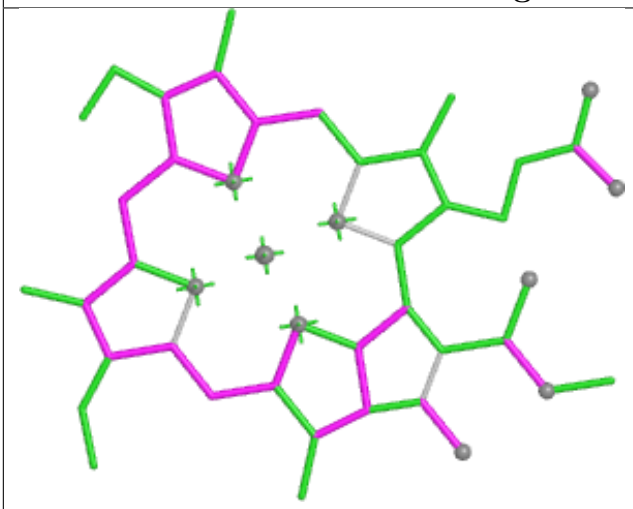


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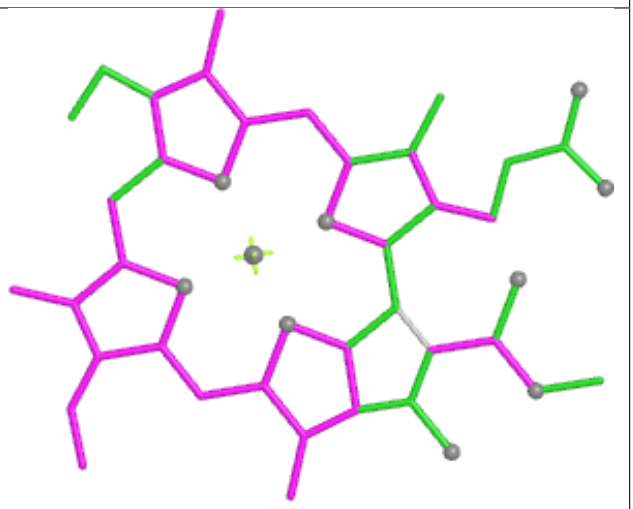


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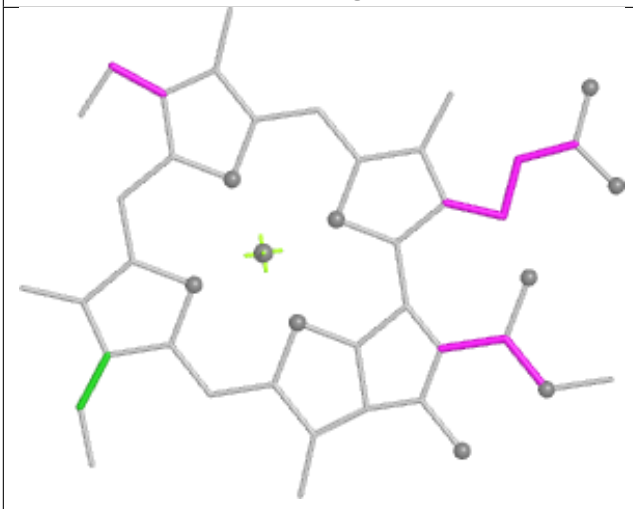
Ligand CLA bA 804



Bond lengths



Bond angles

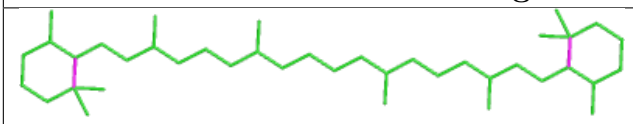


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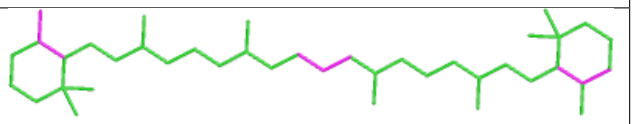


Rings

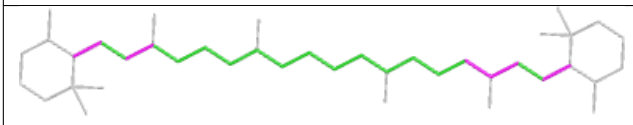
Ligand BCR bB 843



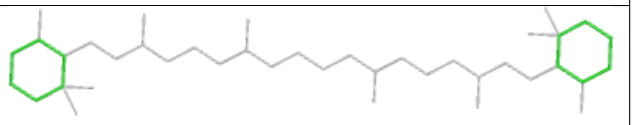
Bond lengths



Bond angles

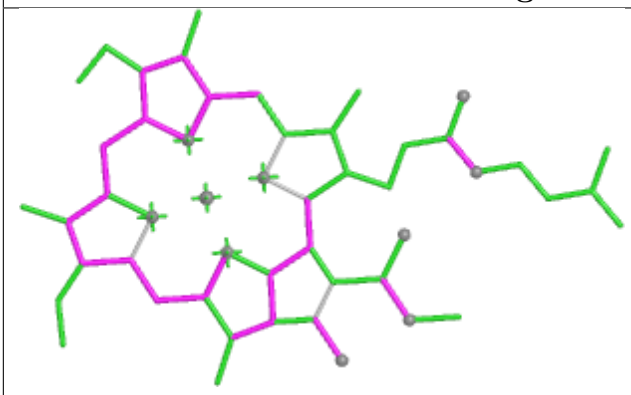


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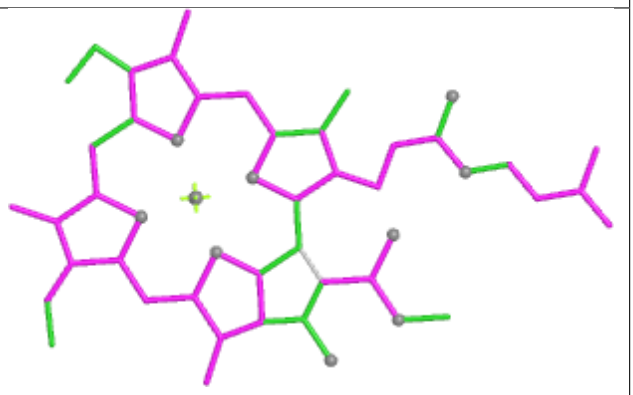


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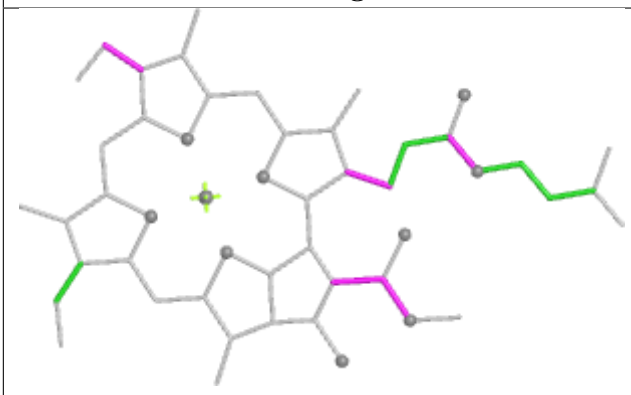
Ligand CLA cB 804



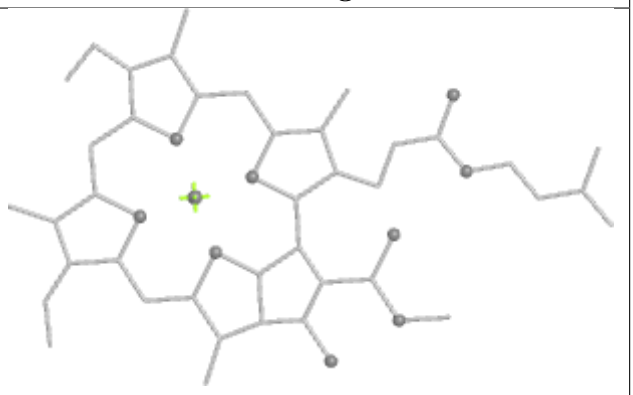
Bond lengths



Bond angles

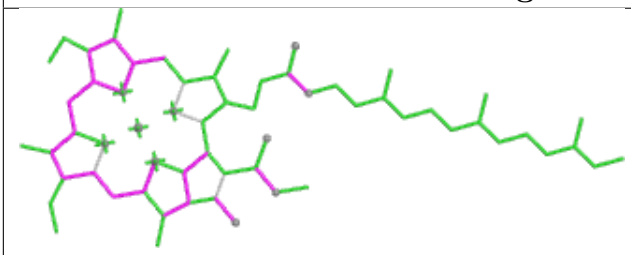


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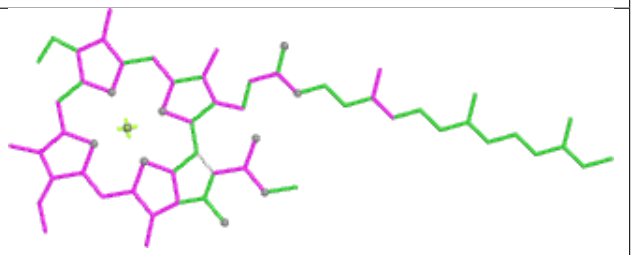


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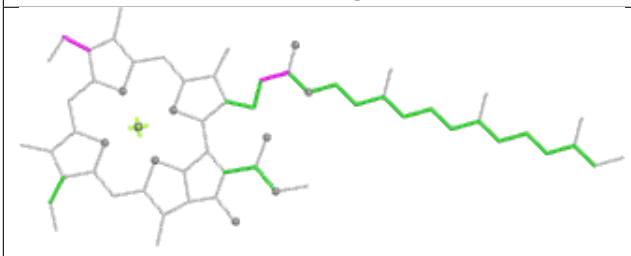
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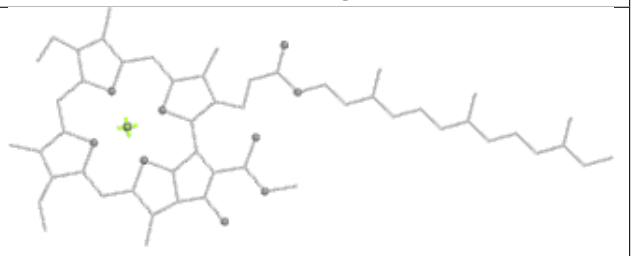
Bond lengths



Bond angles

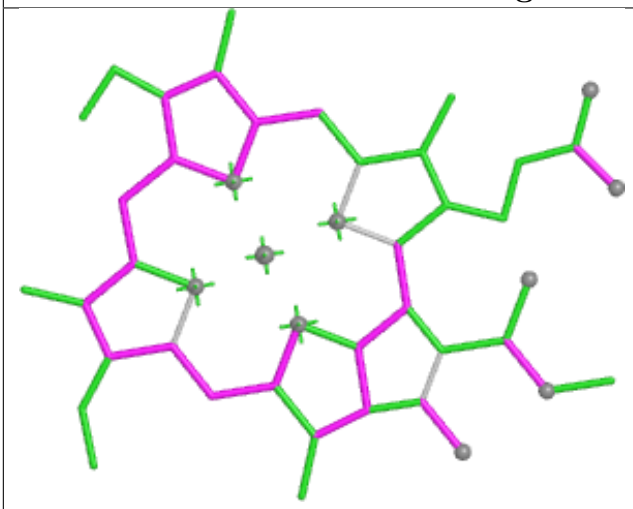


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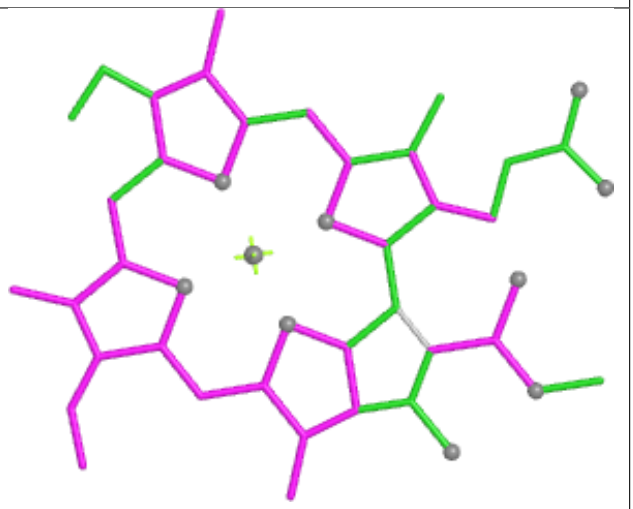


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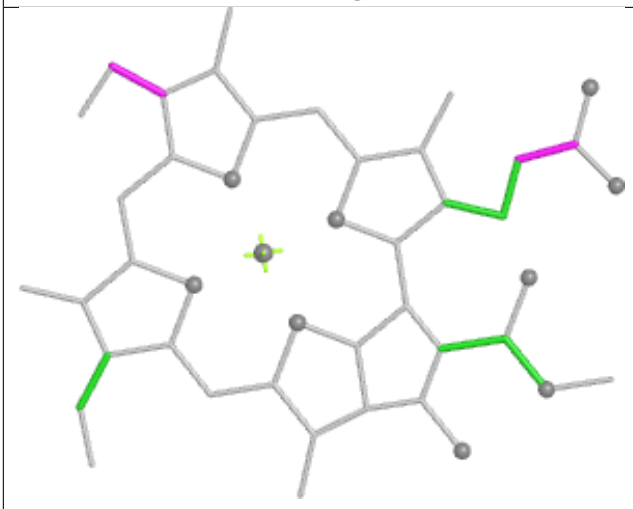
Ligand CLA aB 835



Bond lengths



Bond angles

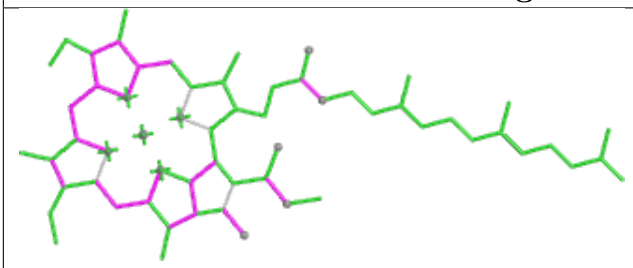


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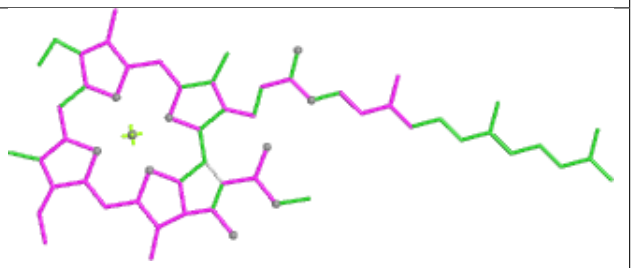


Rings

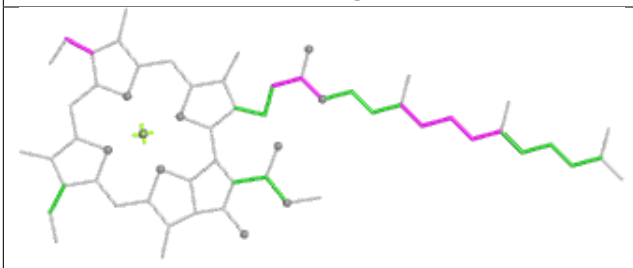
Ligand CLA cA 828



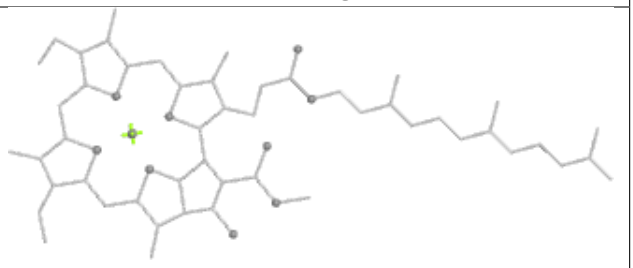
Bond lengths



Bond angles

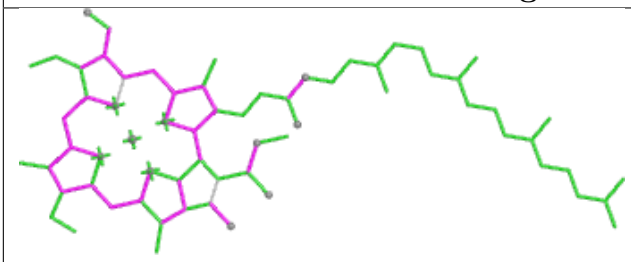


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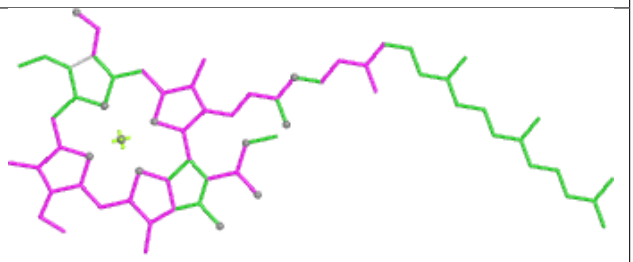


Rings

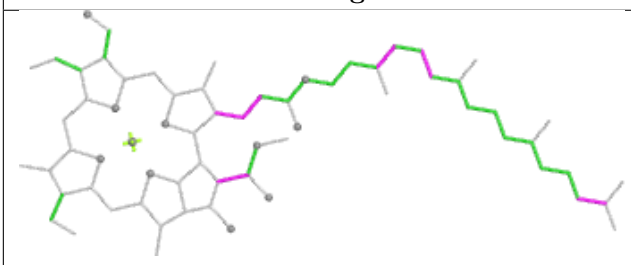
Ligand F6C cA 830



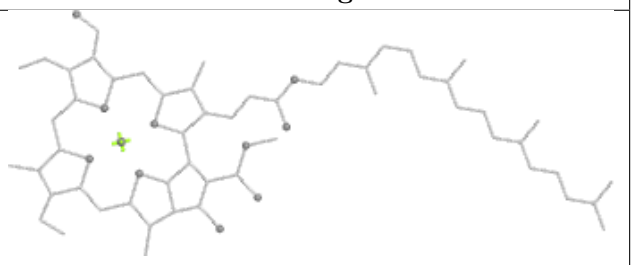
Bond lengths



Bond angles

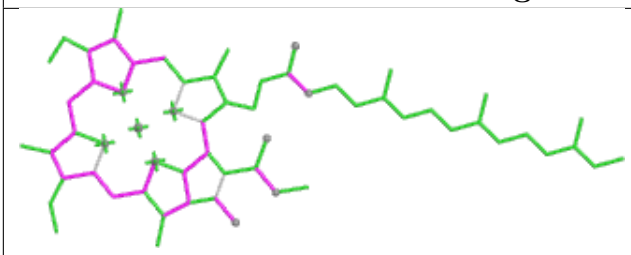


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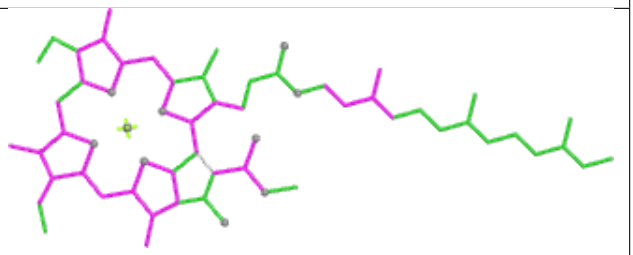


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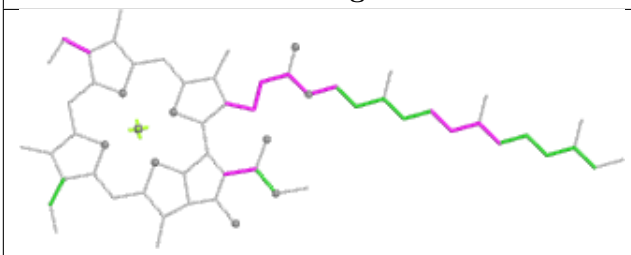
Ligand CLA bA 821



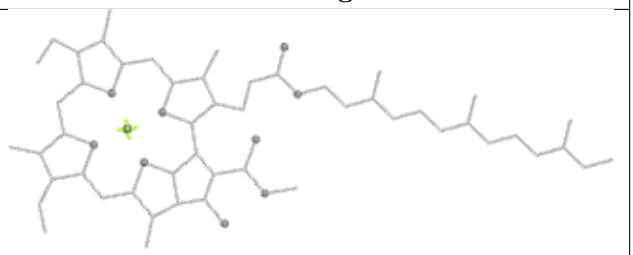
Bond lengths



Bond angles

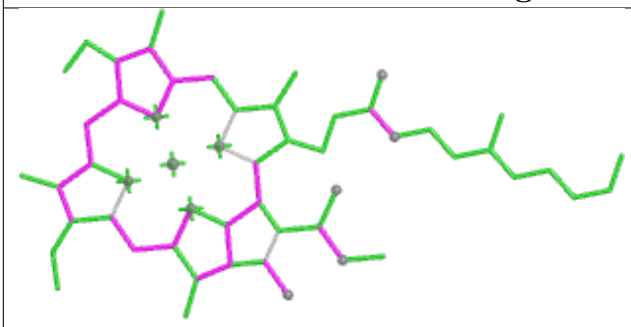


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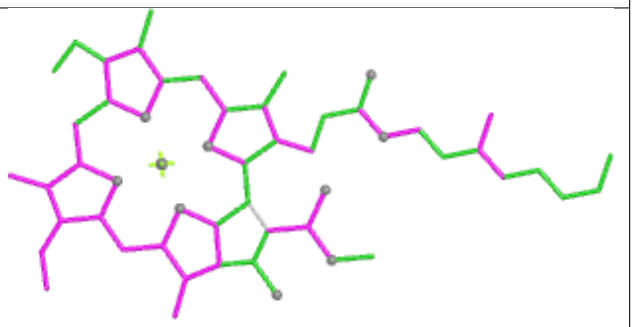


Rings

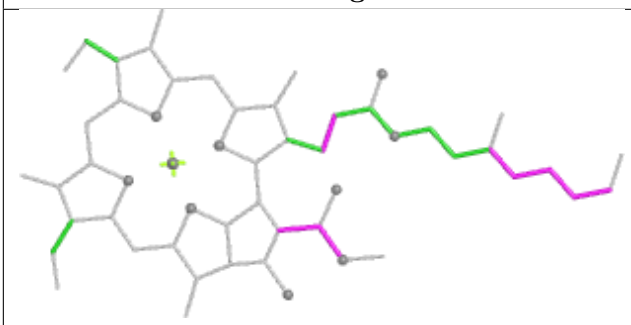
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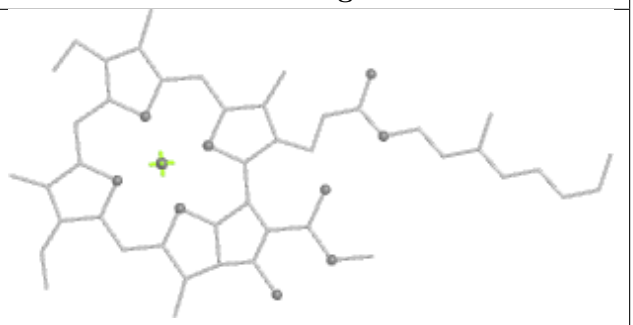
Bond lengths



Bond angles

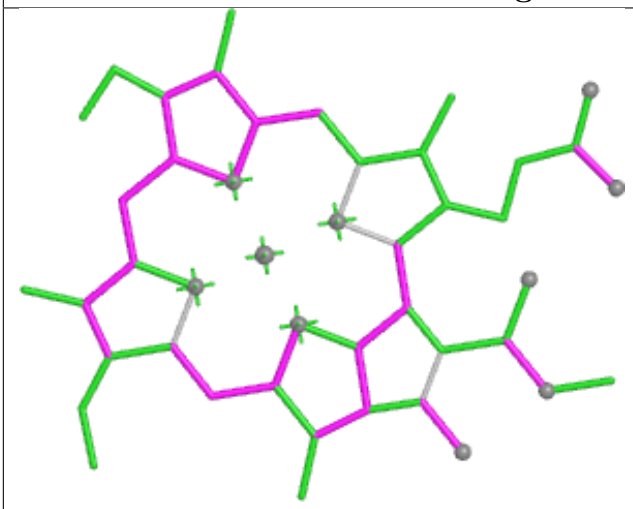


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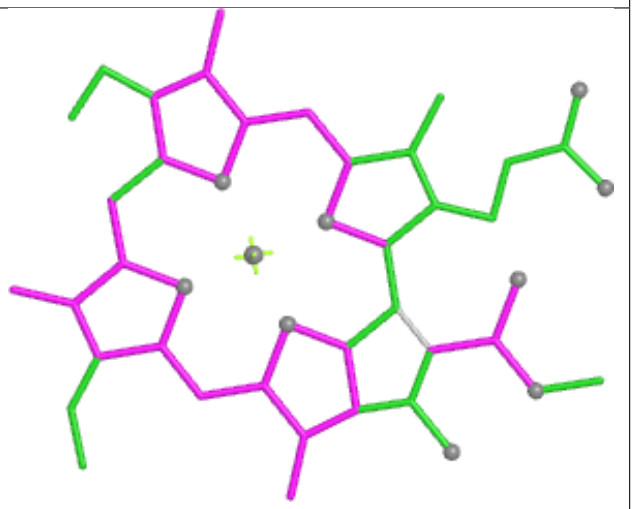


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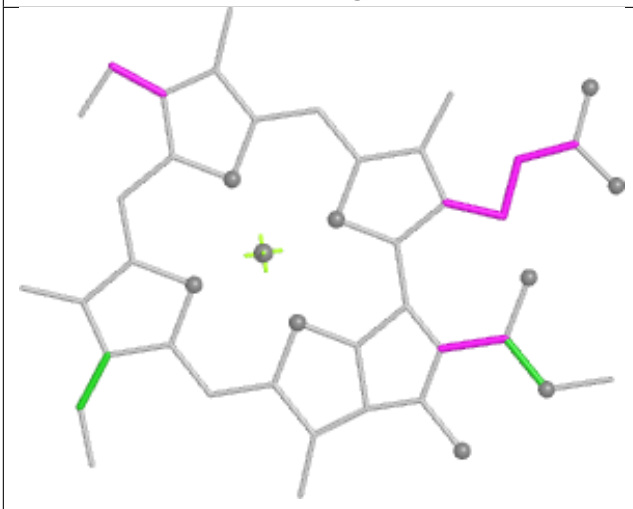
Ligand CLA aA 823



Bond lengths



Bond angles

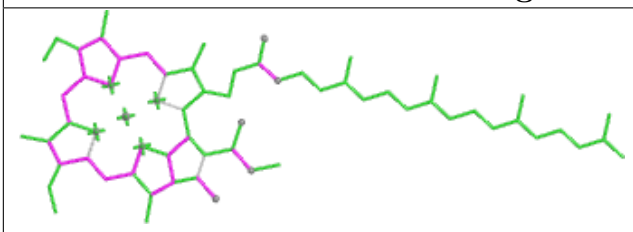


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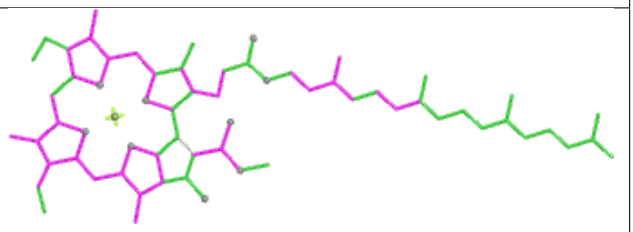


Rings

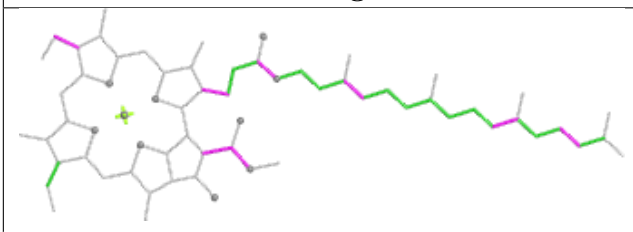
Ligand CLA cA 806



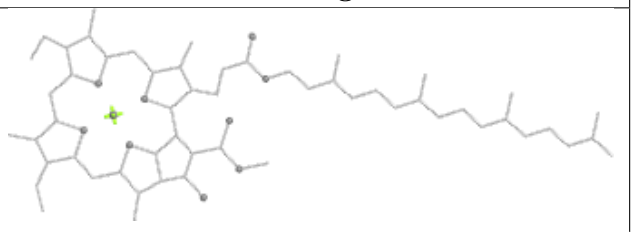
Bond lengths



Bond angles

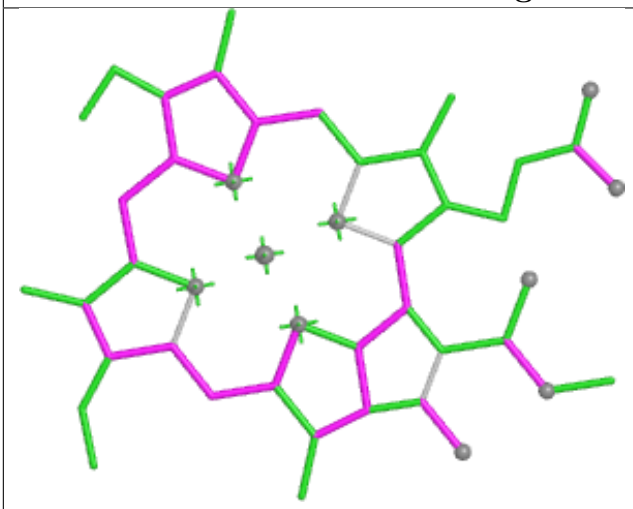


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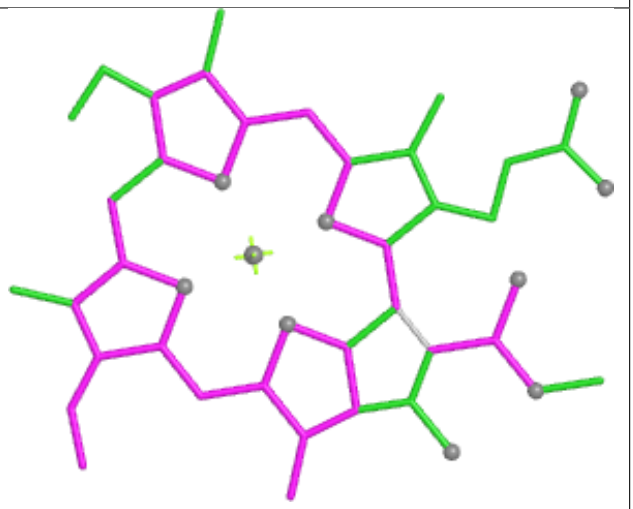


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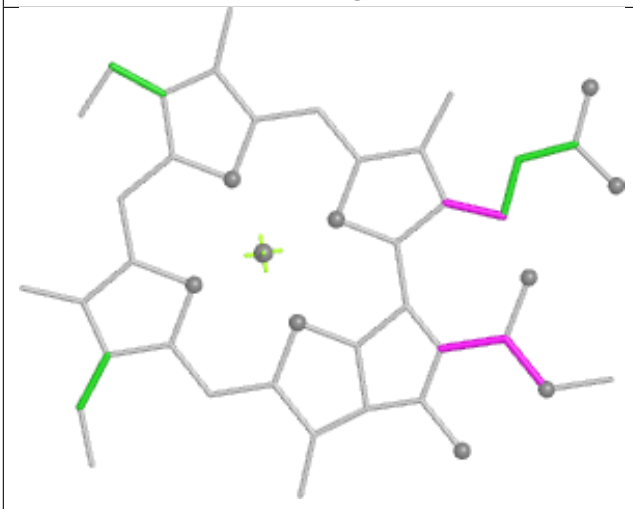
Ligand CLA aA 815



Bond lengths



Bond angles

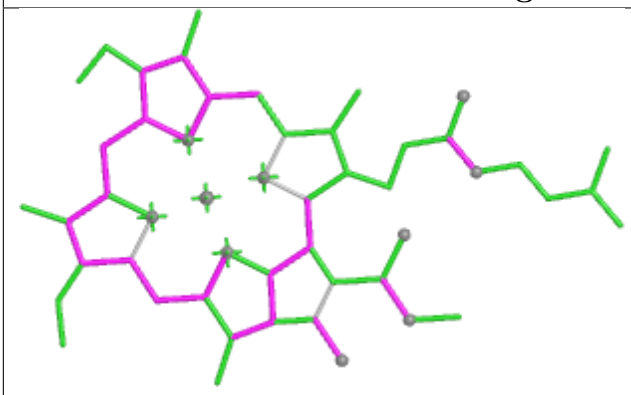


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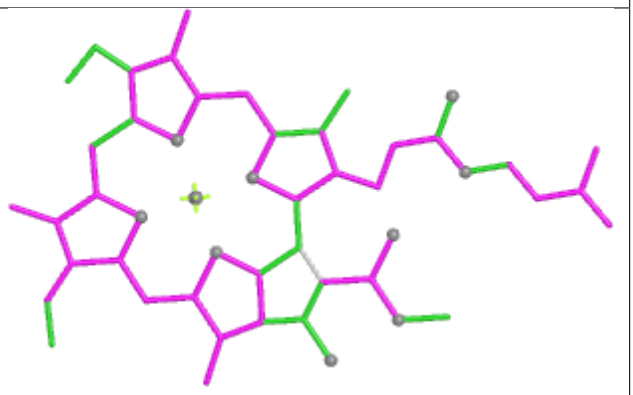


Rings

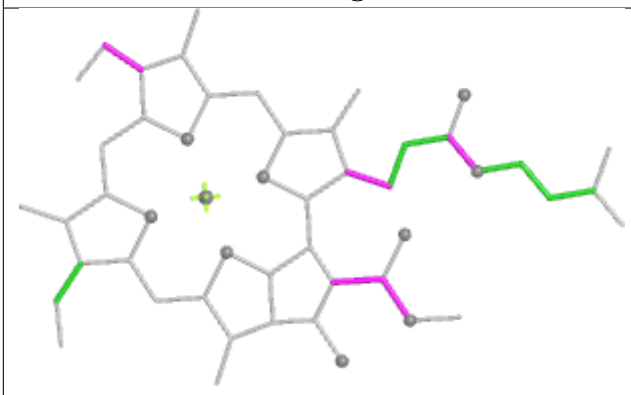
Ligand CLA aB 804



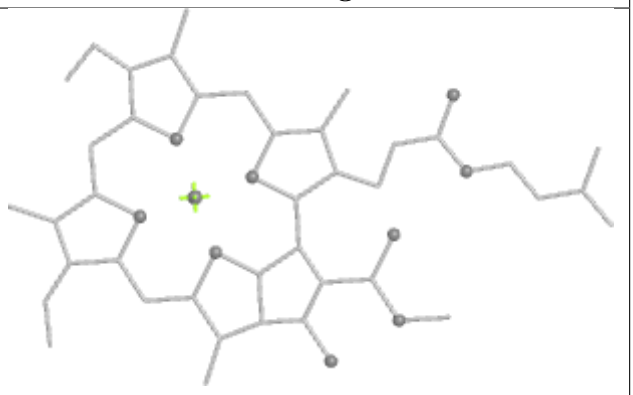
Bond lengths



Bond angles

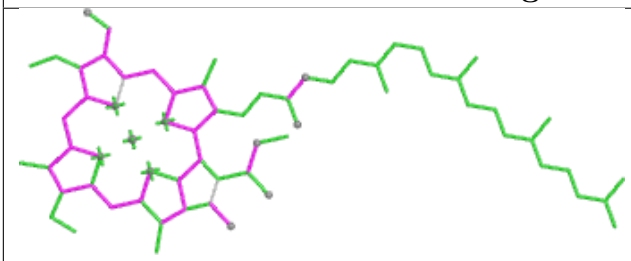


Torsions

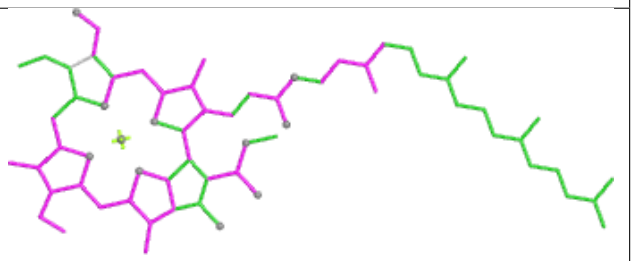


Rings

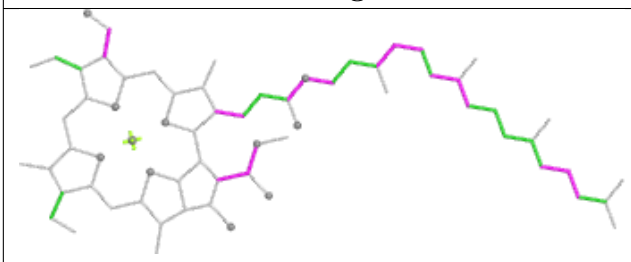
Ligand F6C aL 202



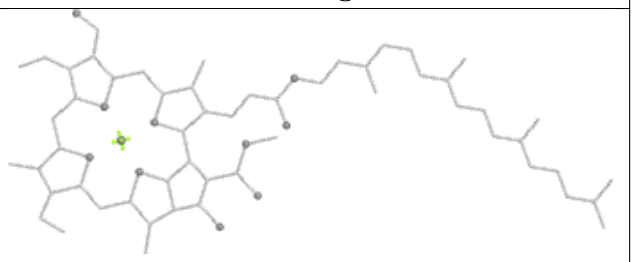
Bond lengths



Bond angles

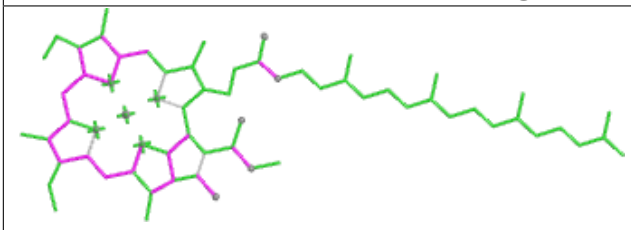


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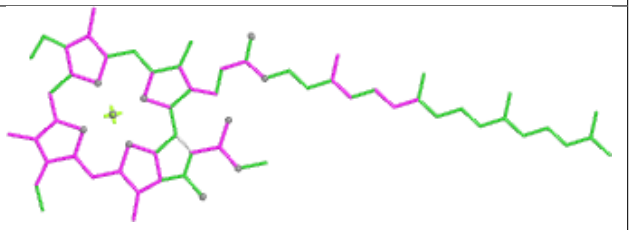


Rings

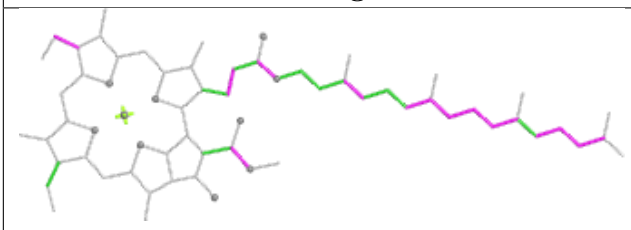
Ligand CLA aA 822



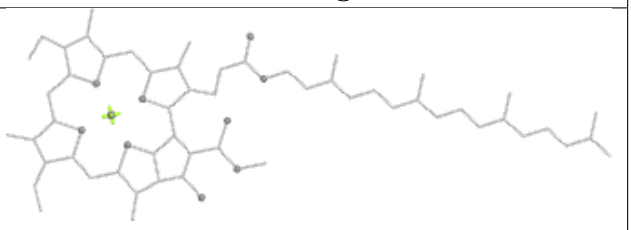
Bond lengths



Bond angles

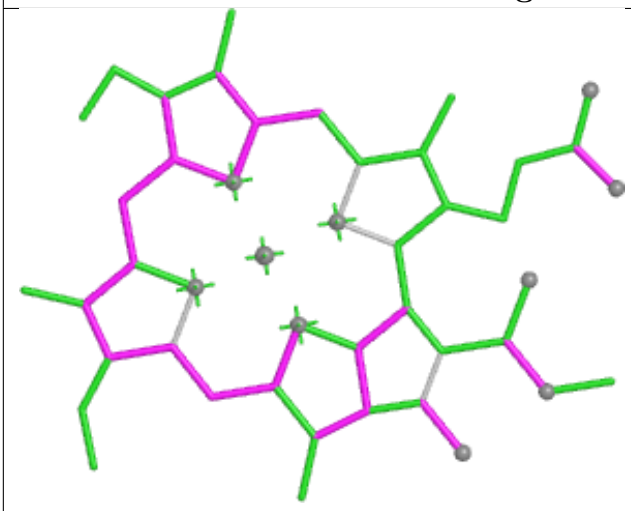


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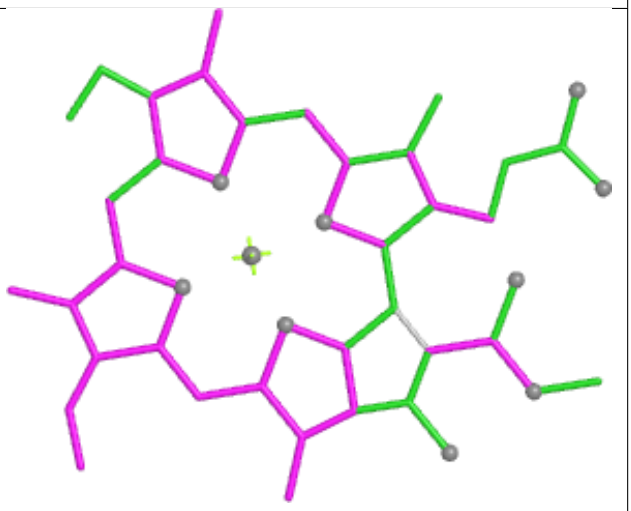


Rings

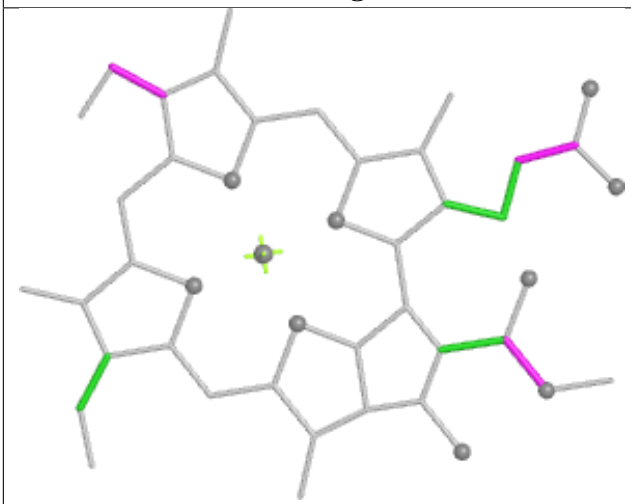
Ligand CLA cA 836



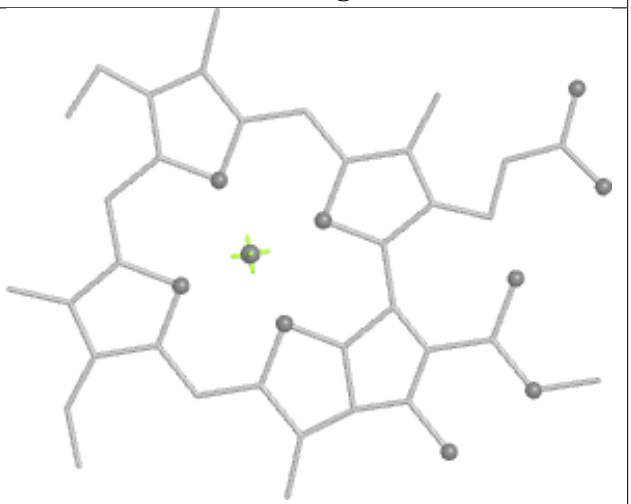
Bond lengths



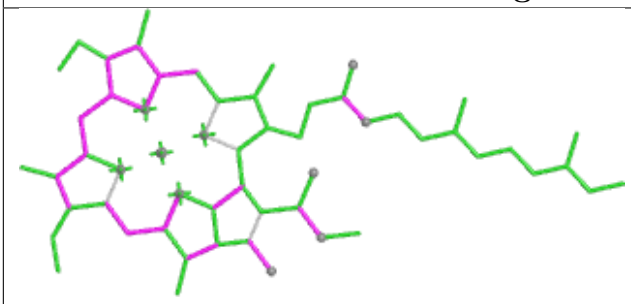
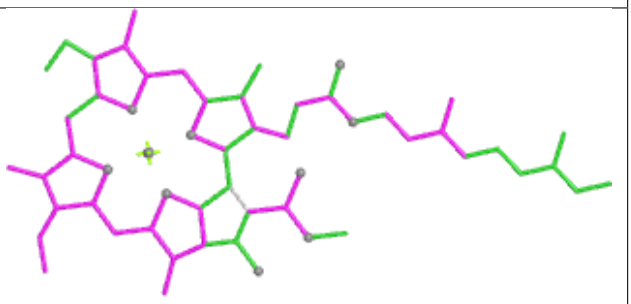
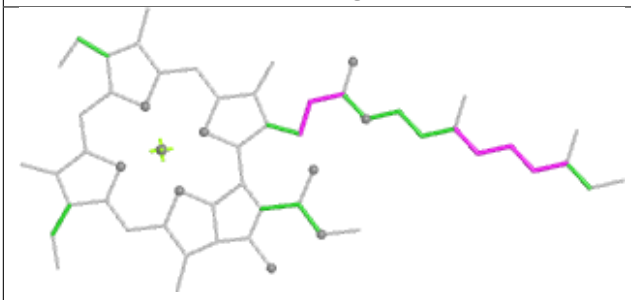
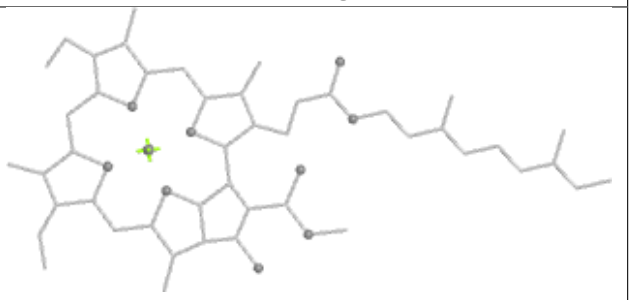
Bond angles

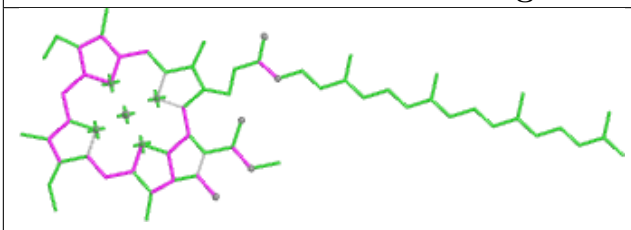
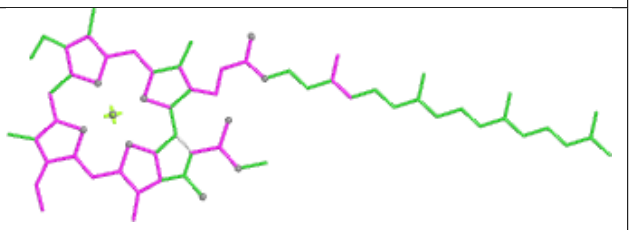
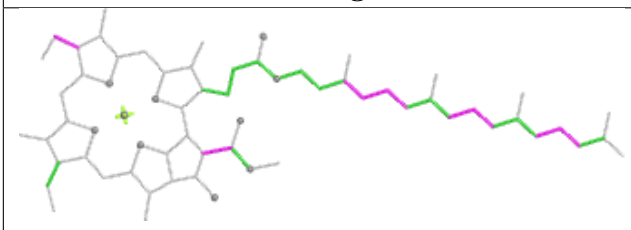
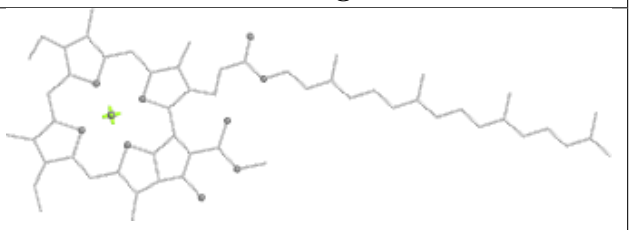


Torsions

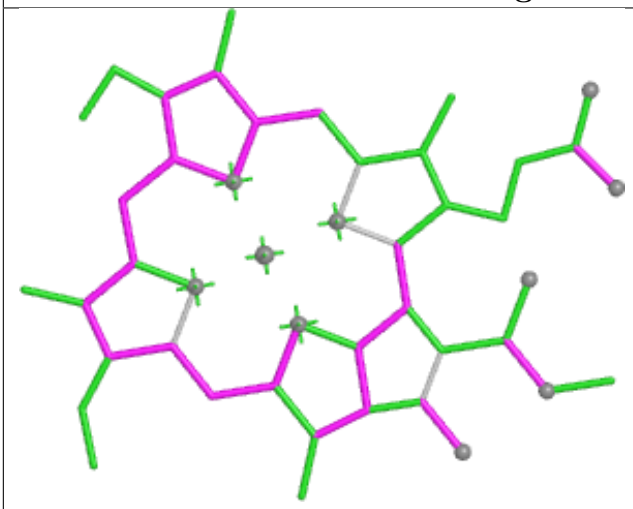


Rings

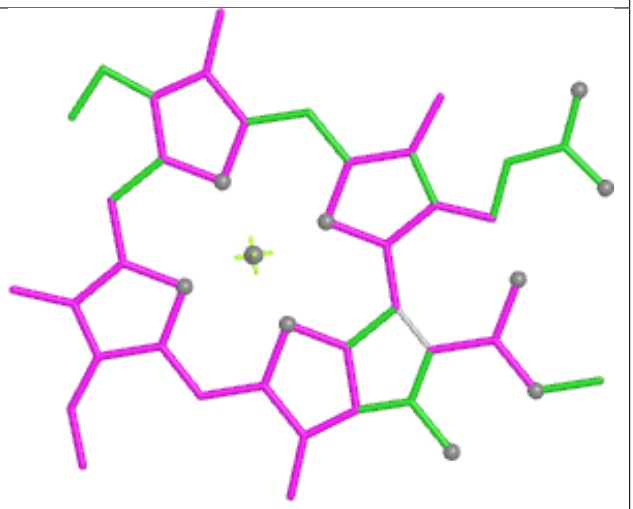
Ligand CLA bA 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

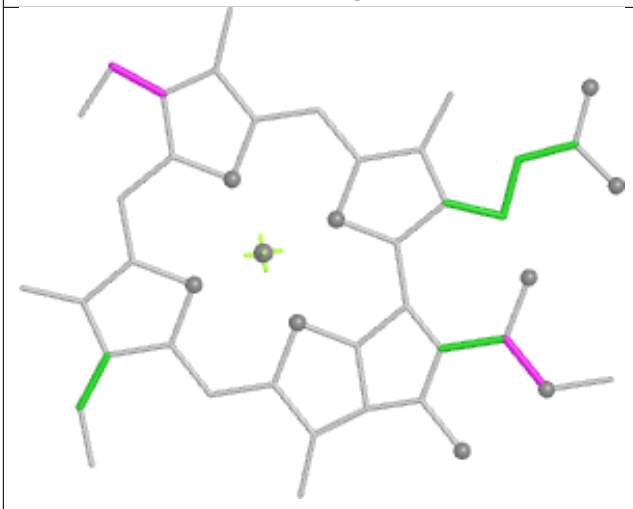
Ligand CLA aA 810



Bond lengths



Bond angles

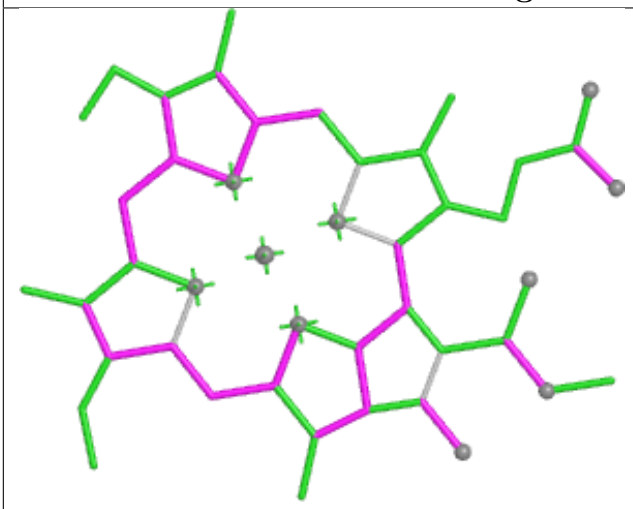


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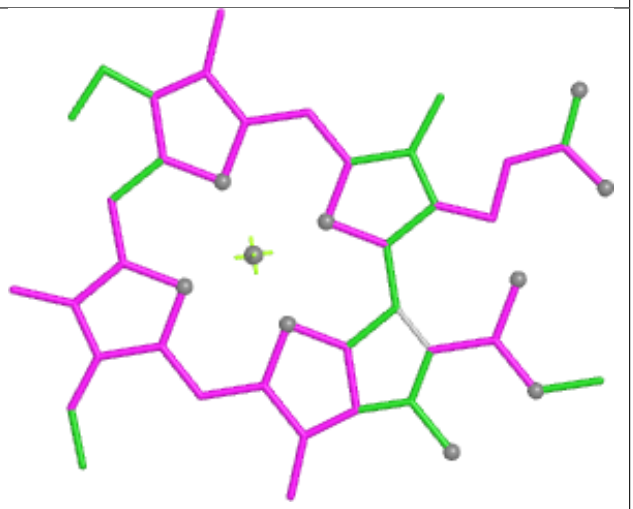


Rings

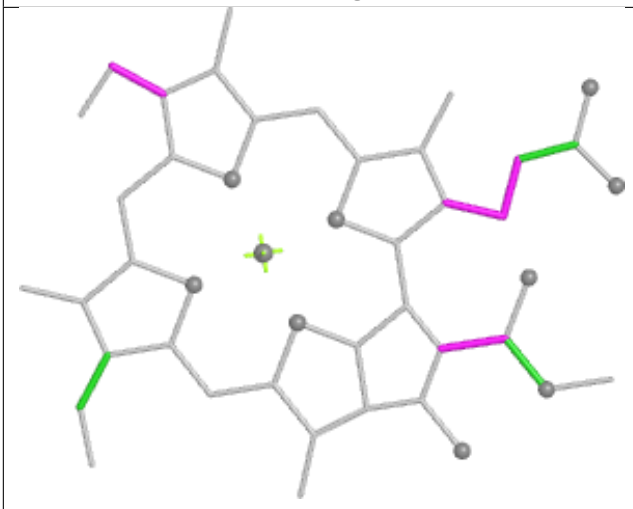
Ligand CLA aB 829



Bond lengths



Bond angles

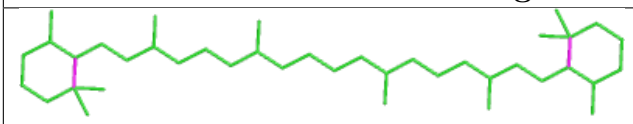


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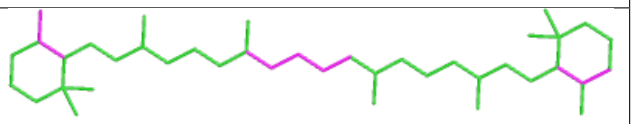


Rings

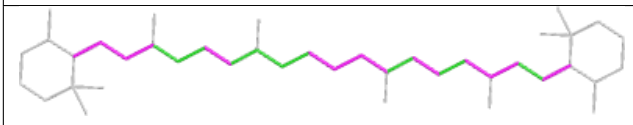
Ligand BCR aB 842



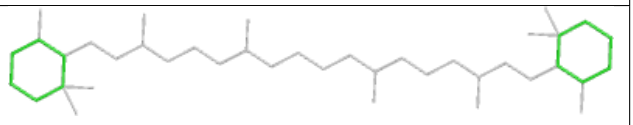
Bond lengths



Bond angles

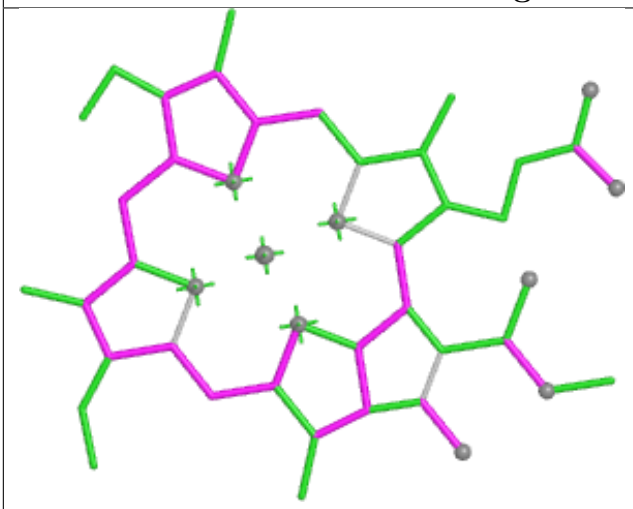


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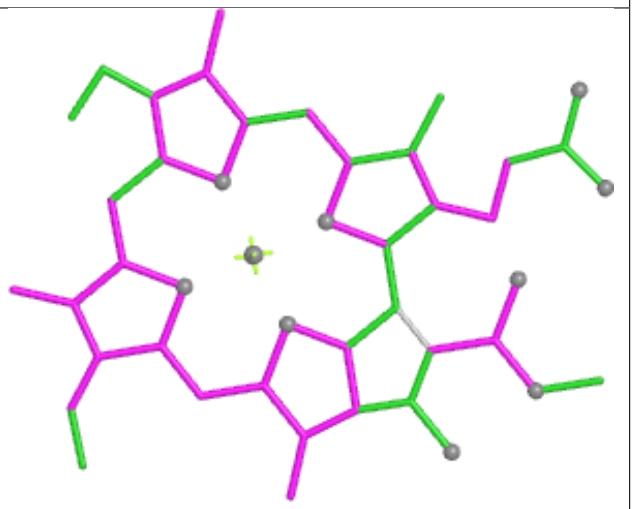


Rings

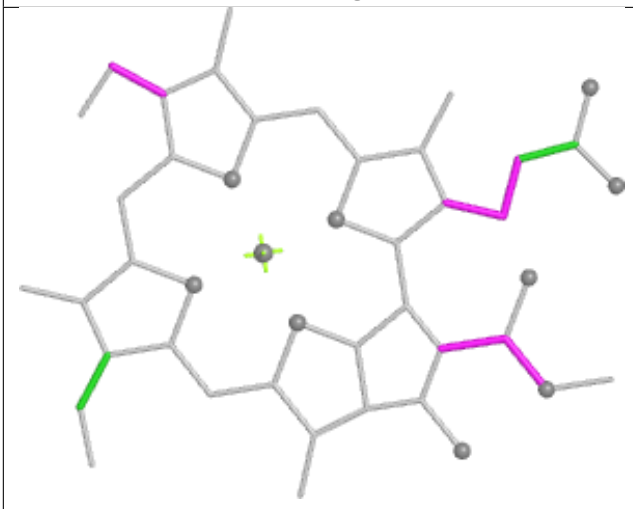
Ligand CLA bA 809



Bond lengths



Bond angles

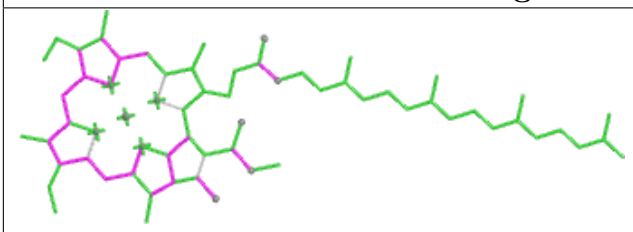


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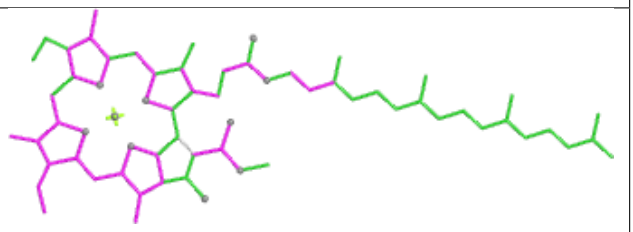


Rings

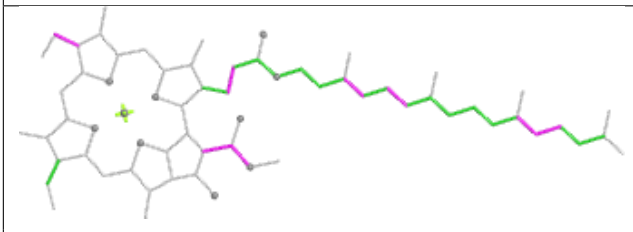
Ligand CLA bA 835



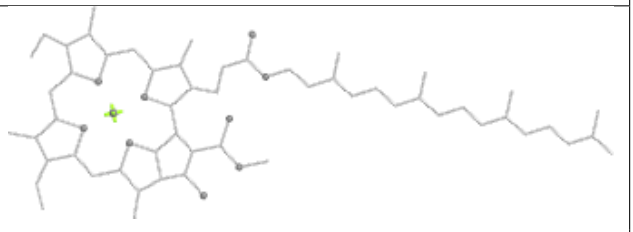
Bond lengths



Bond angles

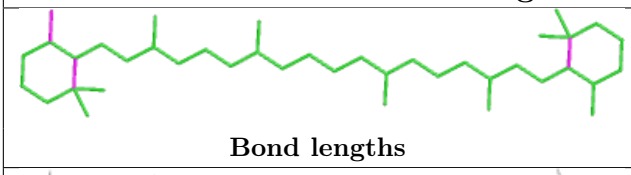


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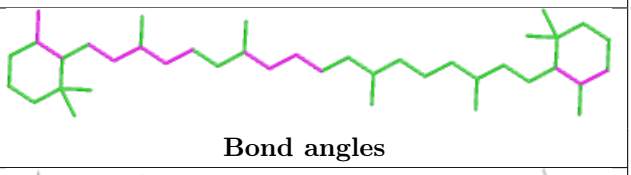


Rings

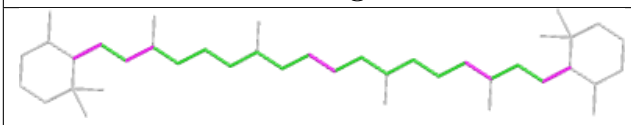
Ligand BCR cL 203



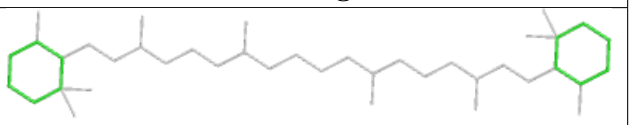
Bond lengths



Bond angles

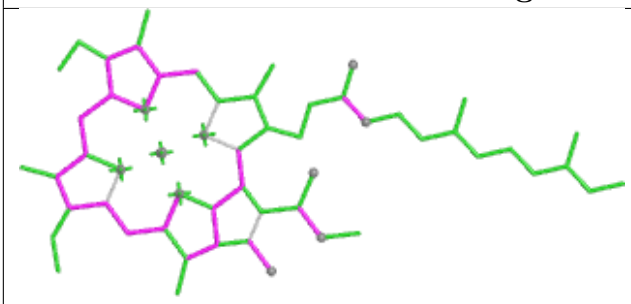


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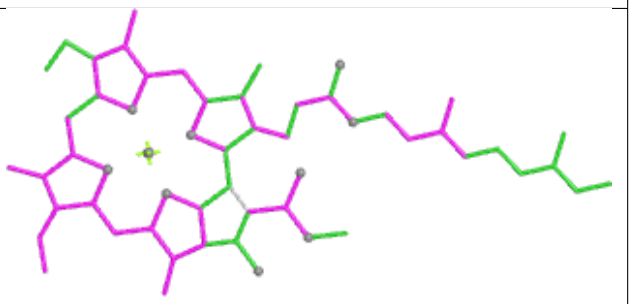


Rings

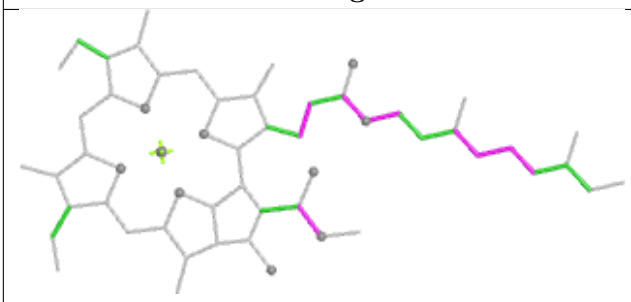
Ligand CLA aB 813



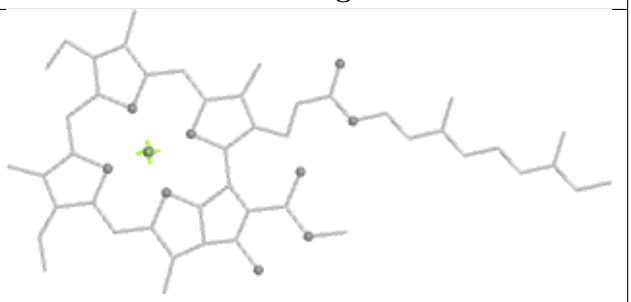
Bond lengths



Bond angles



Torsions

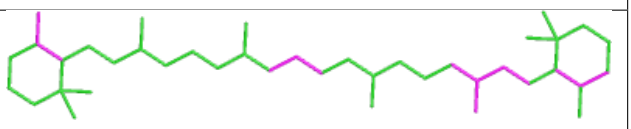


Rings

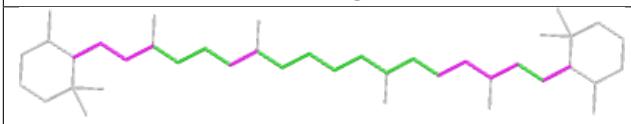
Ligand BCR aA 848



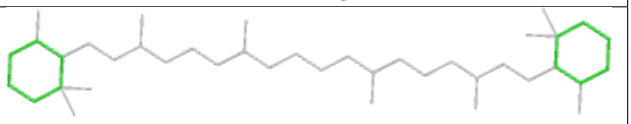
Bond lengths



Bond angles

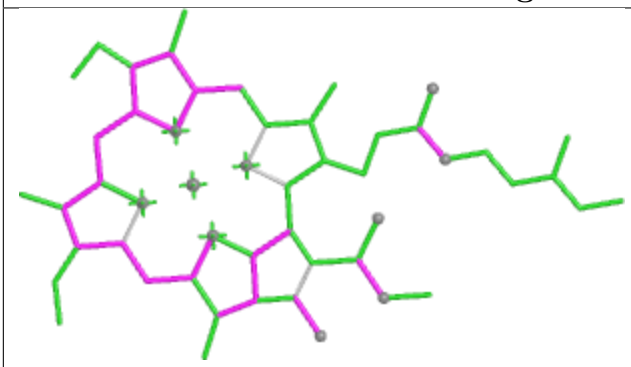


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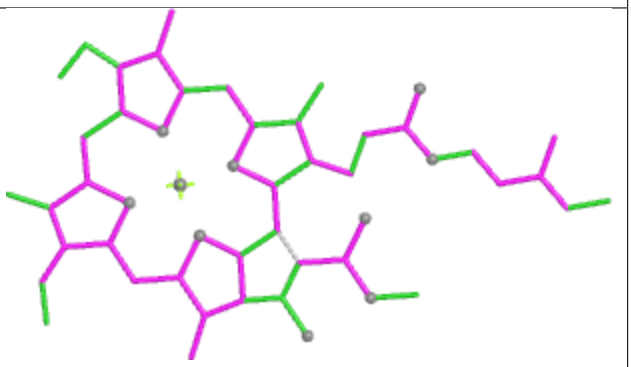


Rings

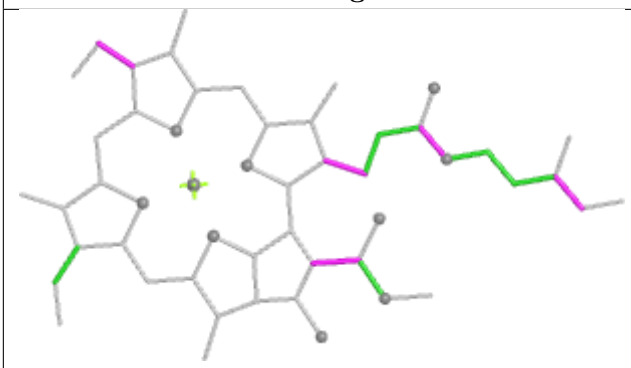
Ligand CLA cB 836



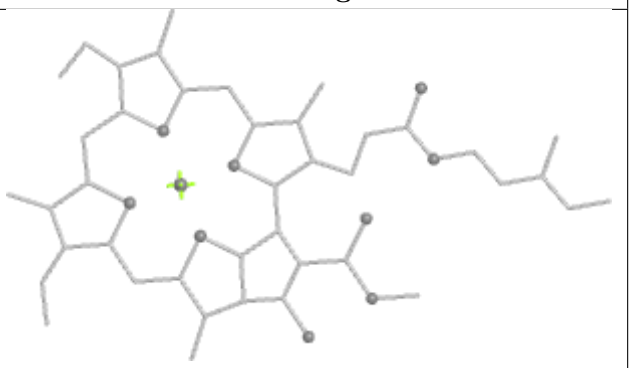
Bond lengths



Bond angles

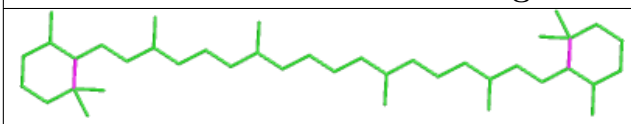


Torsions

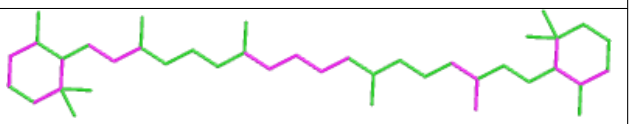


Rings

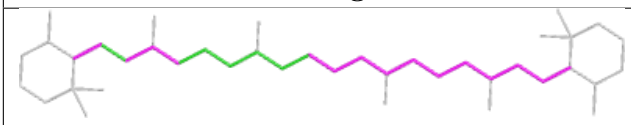
Ligand BCR bB 848



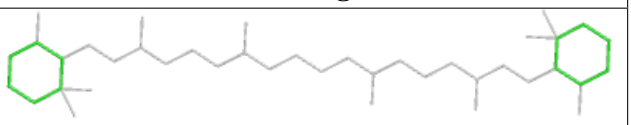
Bond lengths



Bond angles

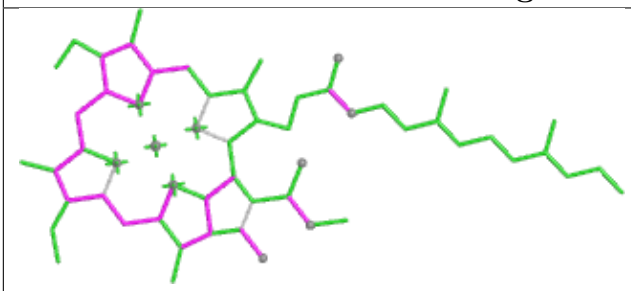


Torsions

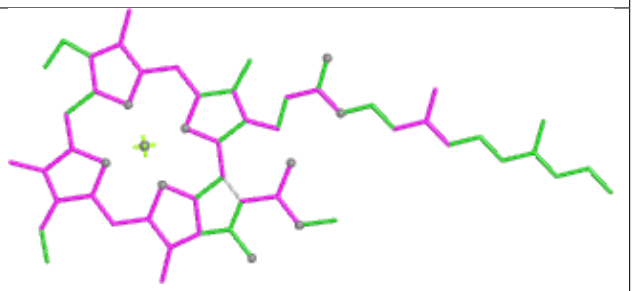


Rings

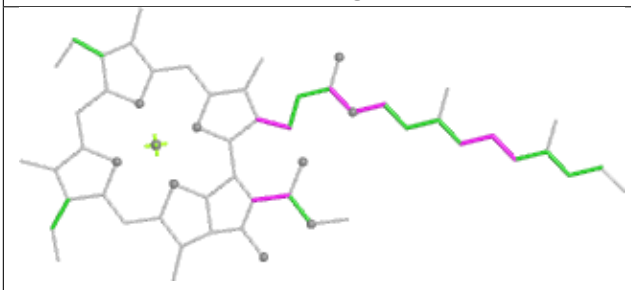
Ligand CLA cB 802



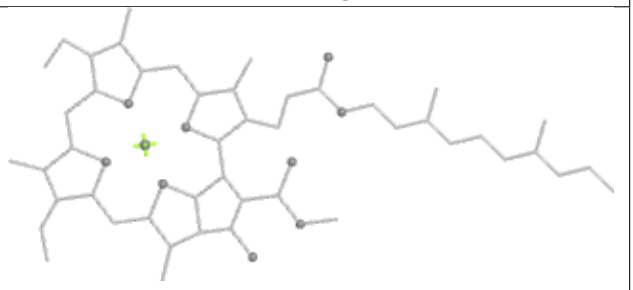
Bond lengths



Bond angles

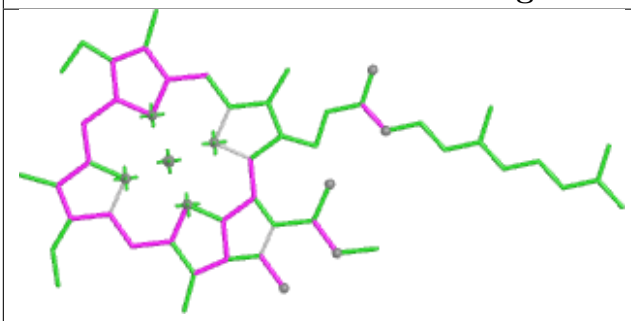


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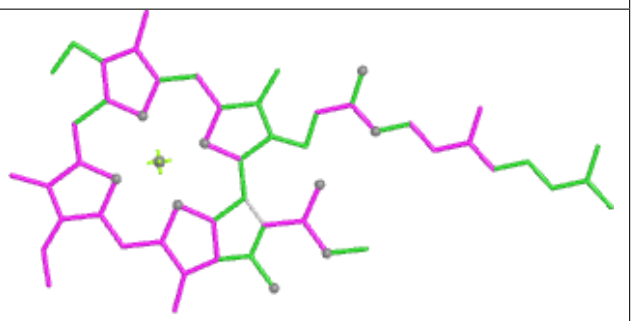


Rings

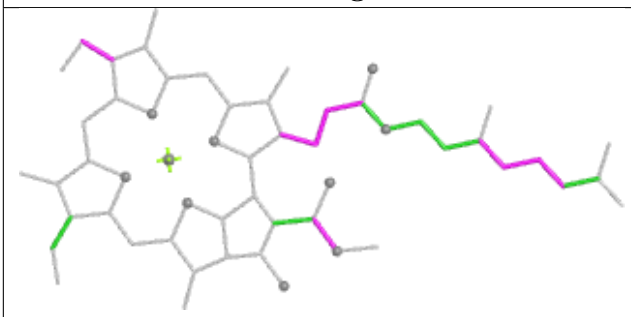
Ligand CLA cB 815



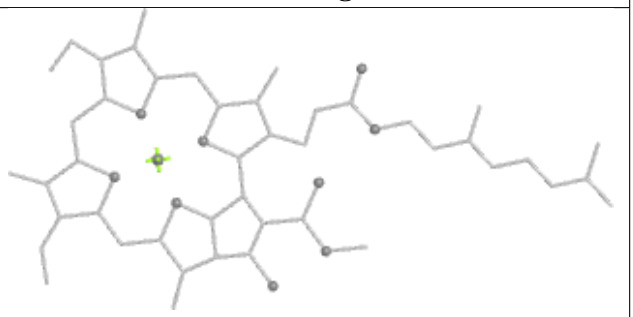
Bond lengths



Bond angles

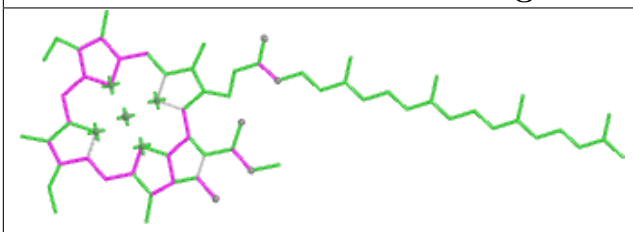


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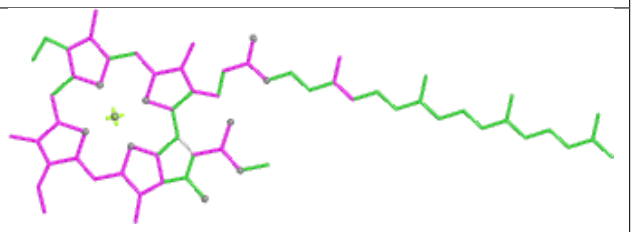


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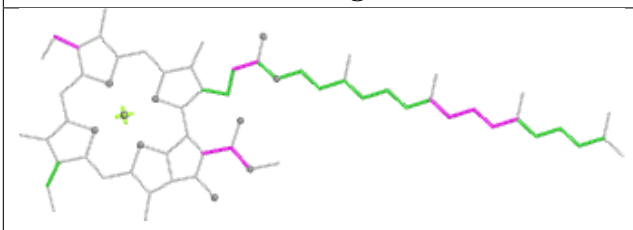
Ligand CLA cA 825



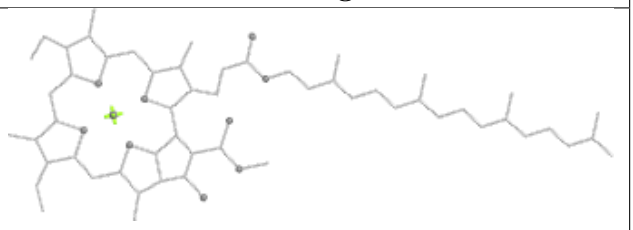
Bond lengths



Bond angles



Torsions

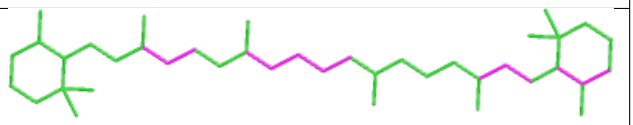


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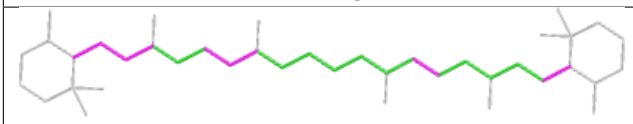
Ligand BCR cB 845



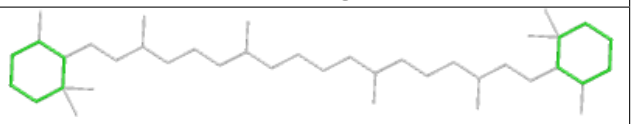
Bond lengths



Bond angles

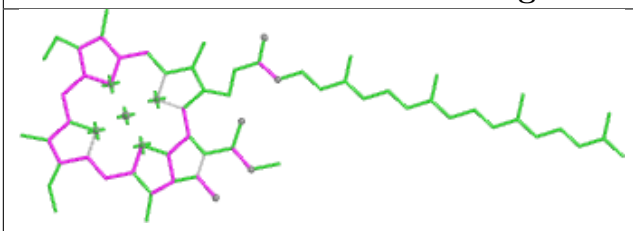


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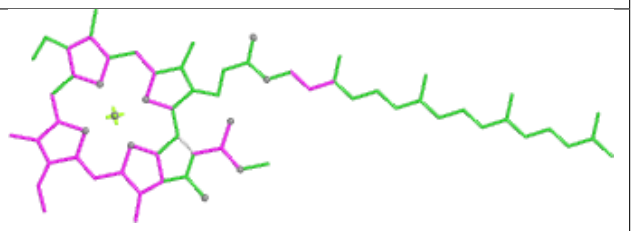


Rings

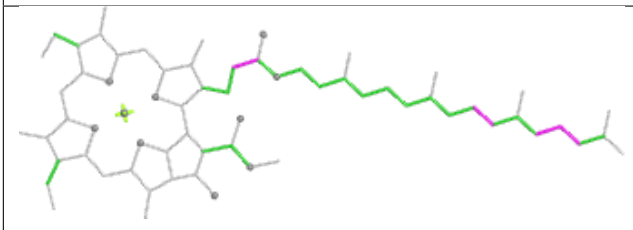
Ligand CLA cL 204



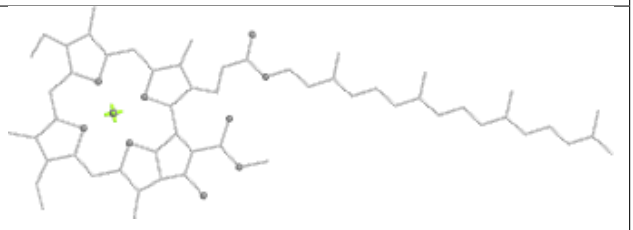
Bond lengths



Bond angles

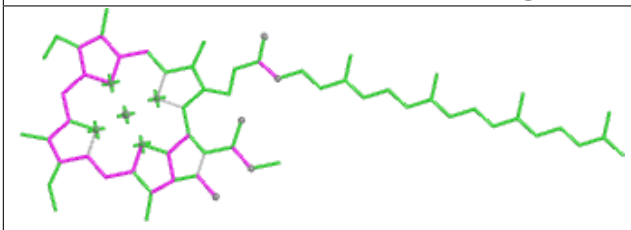


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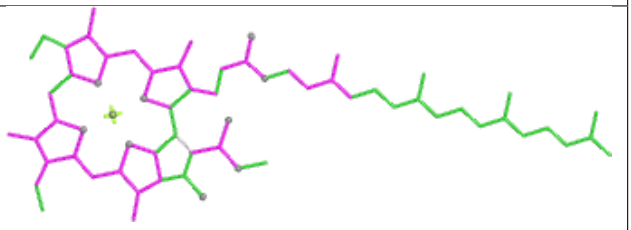


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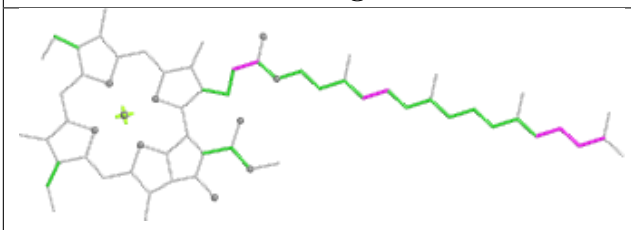
Ligand CL0 aA 801



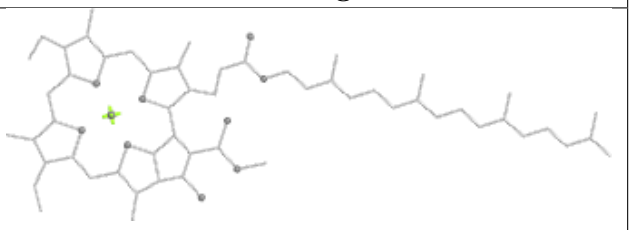
Bond lengths



Bond angles

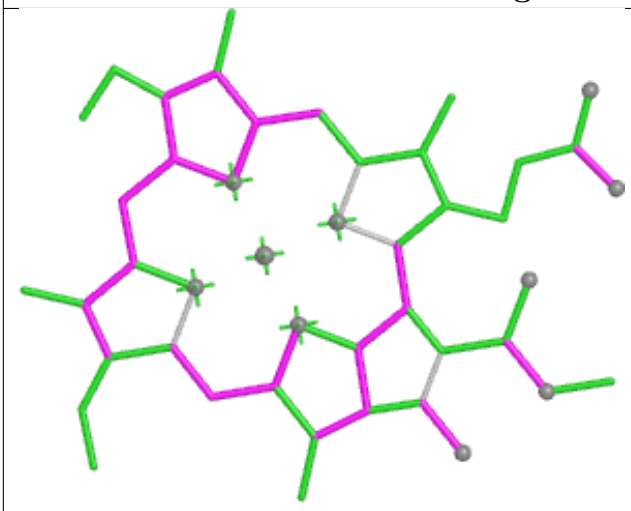


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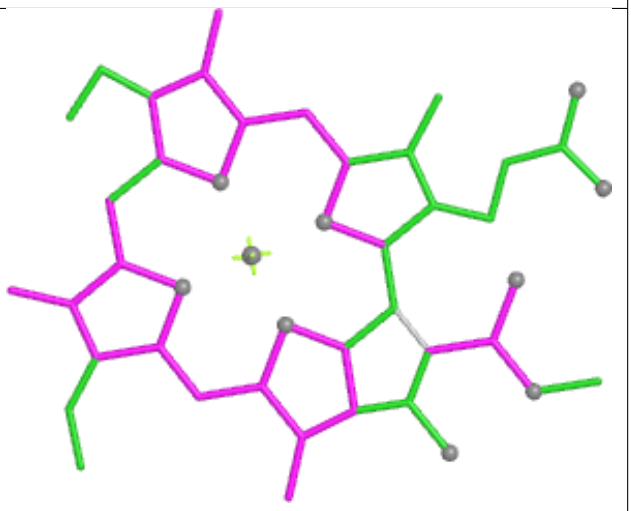


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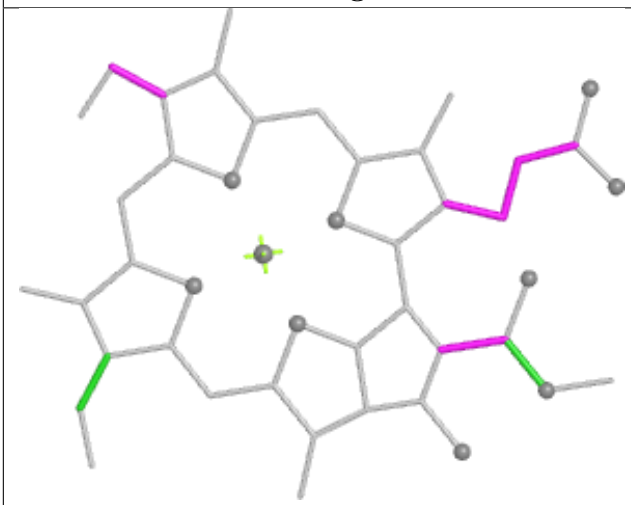
Ligand CLA bA 823



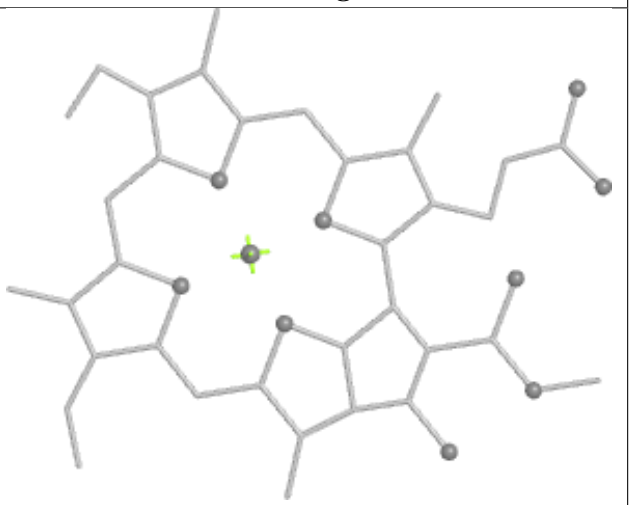
Bond lengths



Bond angles

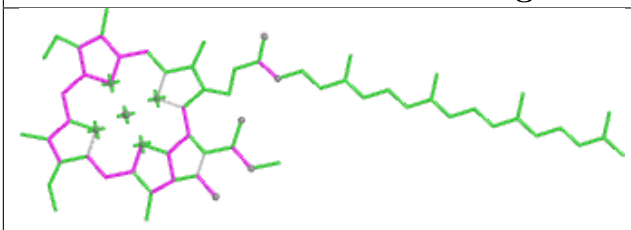


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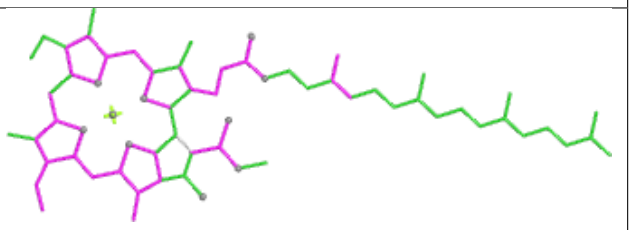


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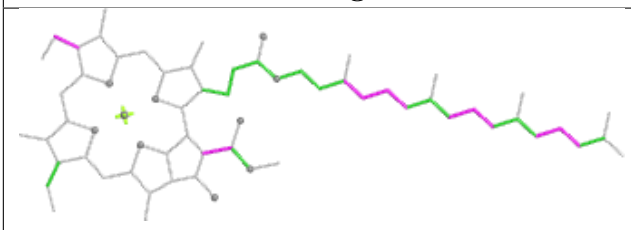
Ligand CLA aB 808



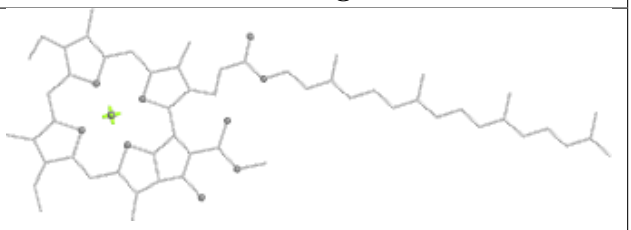
Bond lengths



Bond angles

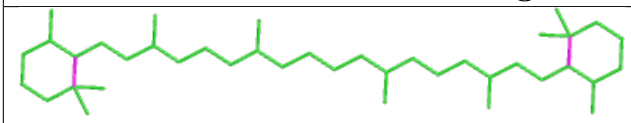


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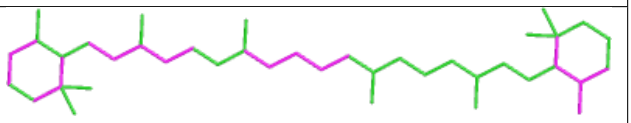


Rings

Ligand BCR aL 207



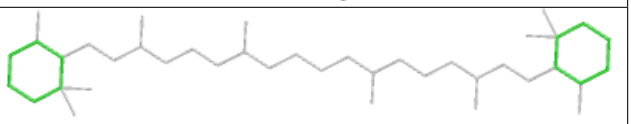
Bond lengths



Bond angles

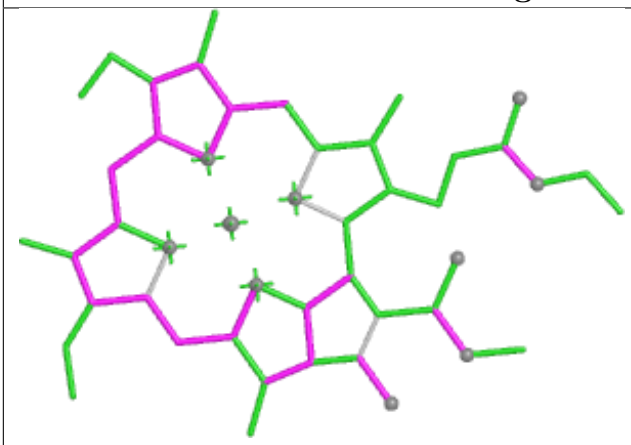


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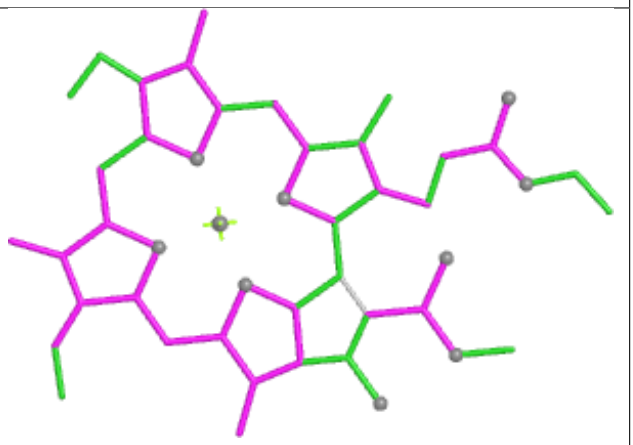


Rings

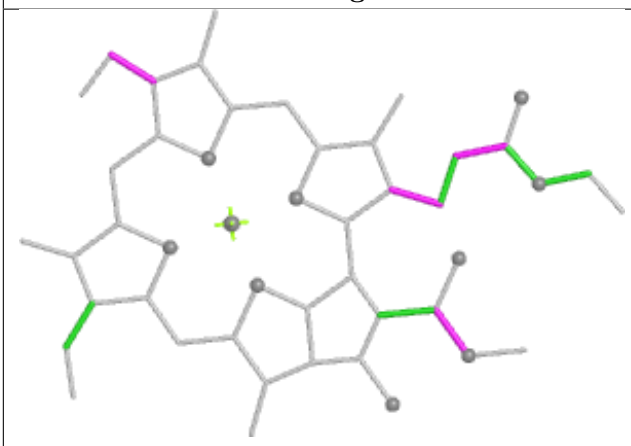
Ligand CLA bB 838



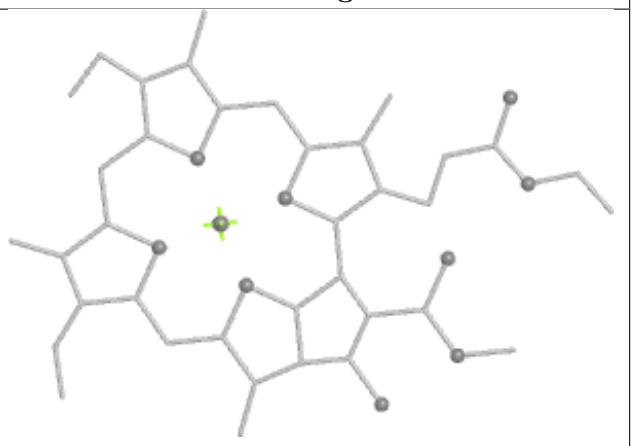
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Bond angles

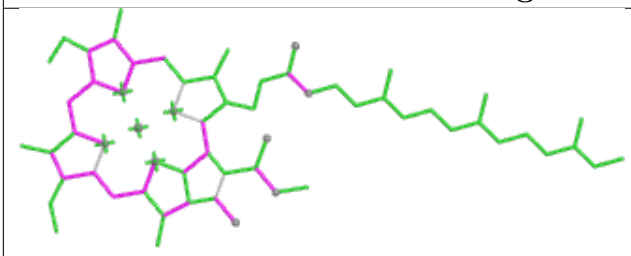


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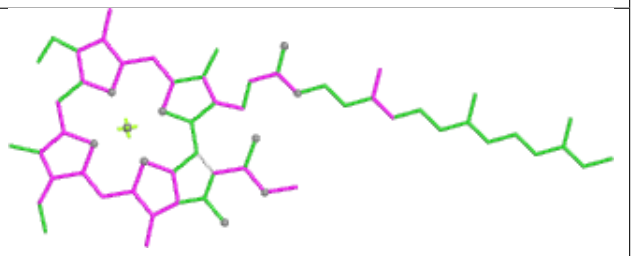


Rings

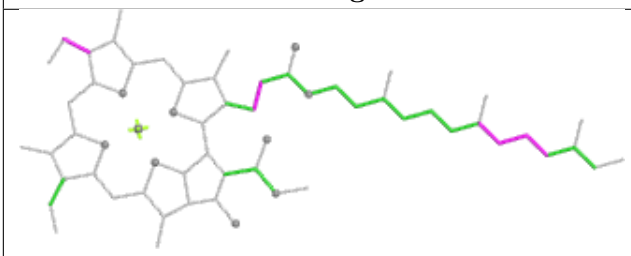
Ligand CLA cB 803



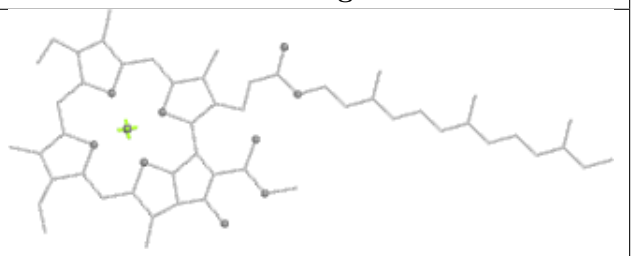
Bond lengths



Bond angles

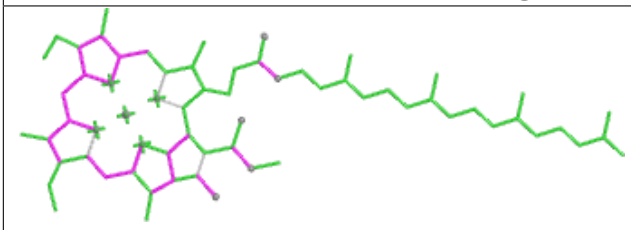


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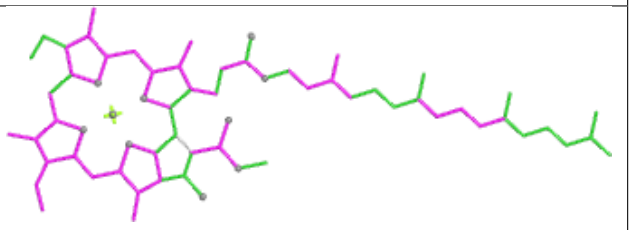


Rings

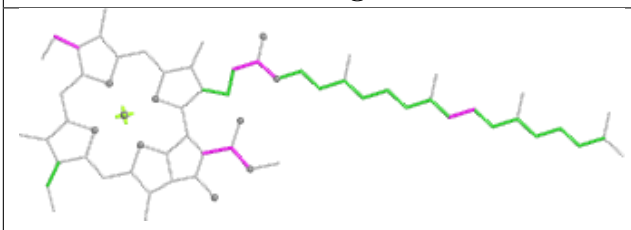
Ligand CLA aB 801



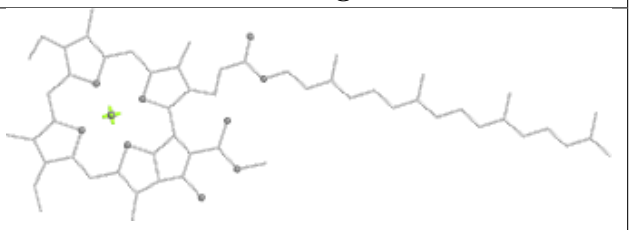
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Bond angles

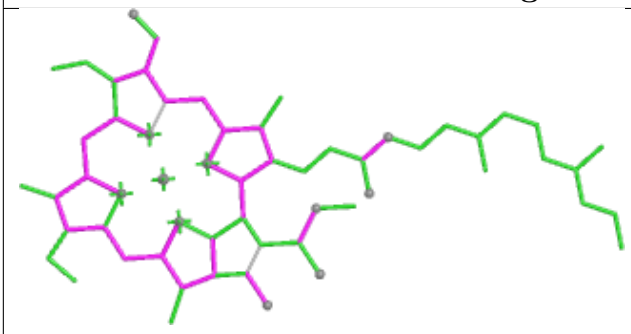


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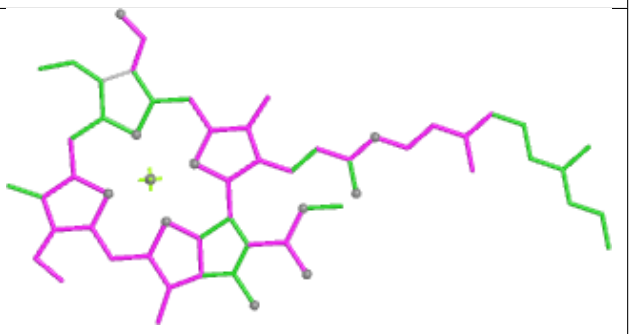


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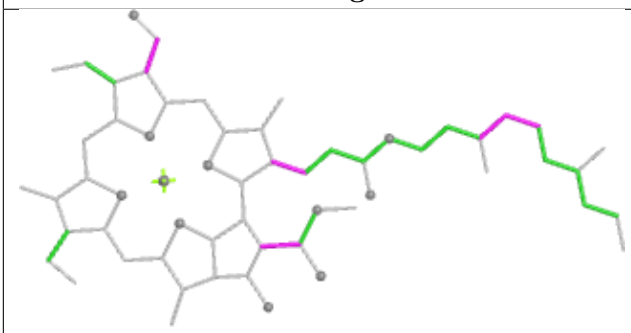
Ligand F6C cB 824



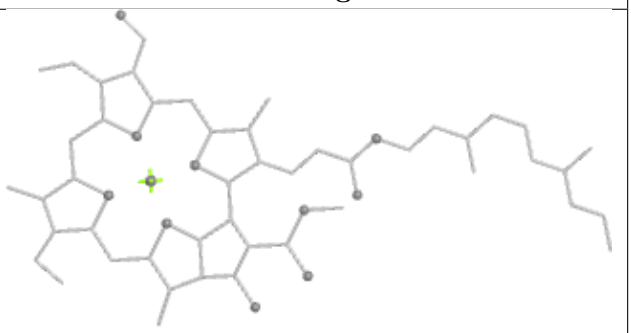
Bond lengths



Bond angles

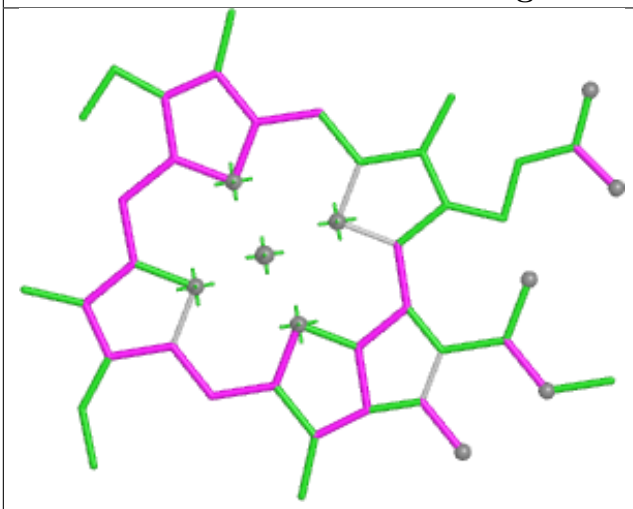


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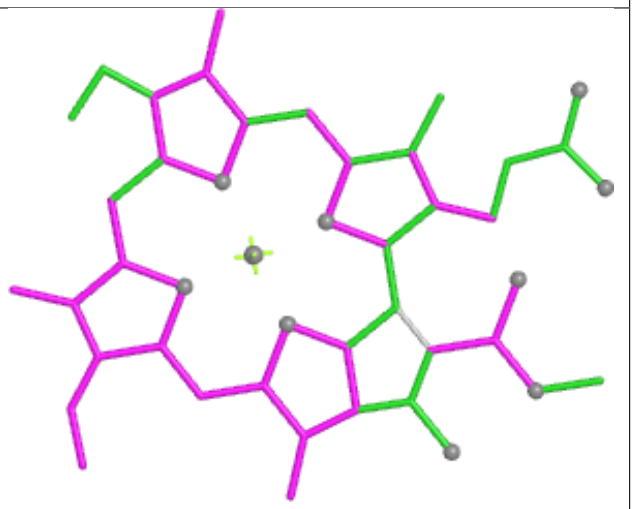


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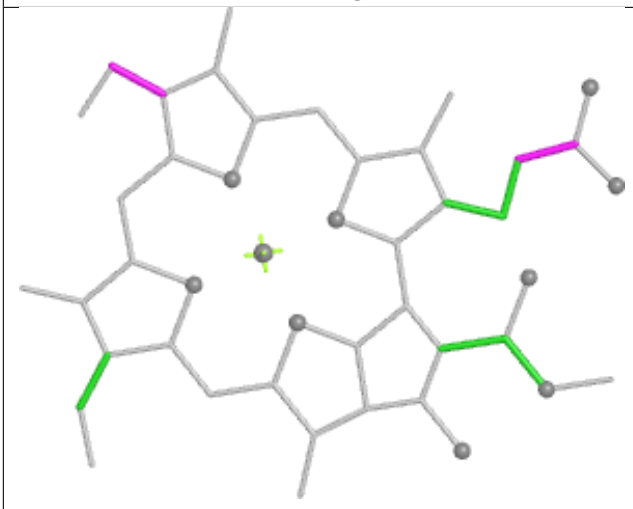
Ligand CLA cB 835



Bond lengths



Bond angles

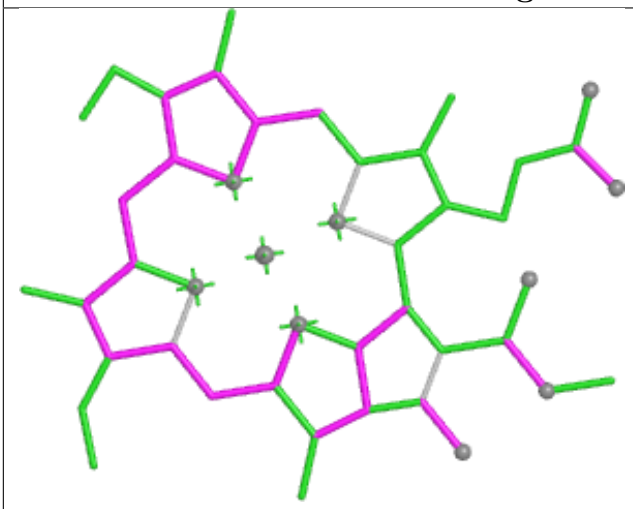


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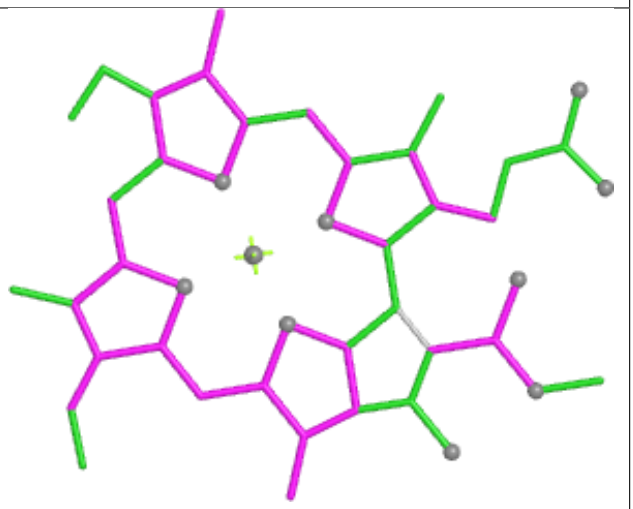


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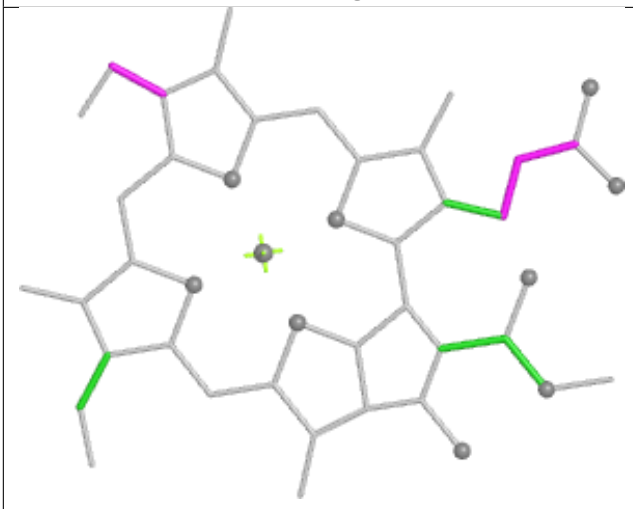
Ligand CLA cB 811



Bond lengths



Bond angles

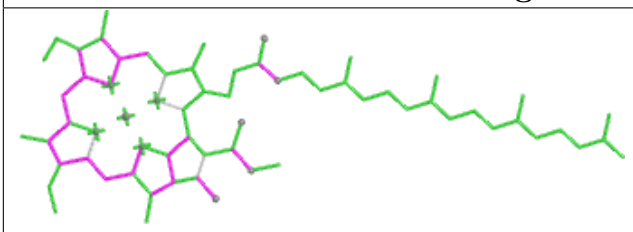


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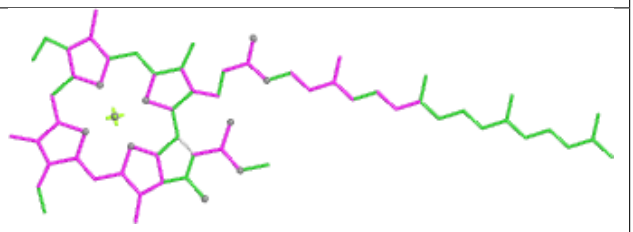


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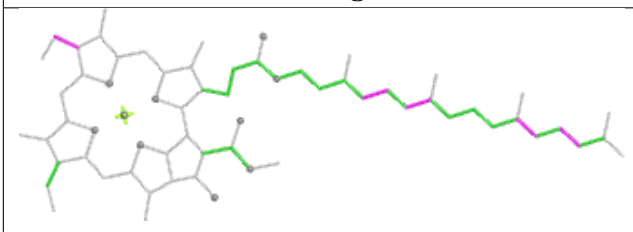
Ligand CLA aA 839



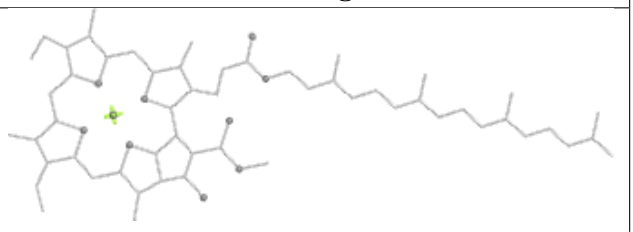
Bond lengths



Bond angles

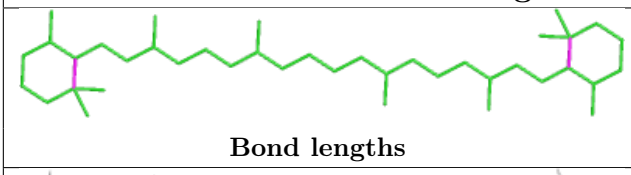


Torsions

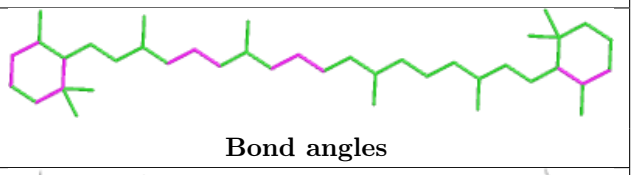


Rings

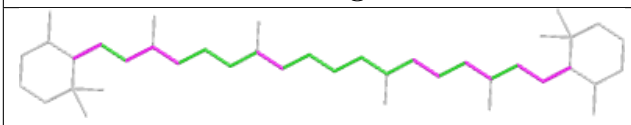
Ligand BCR aB 846



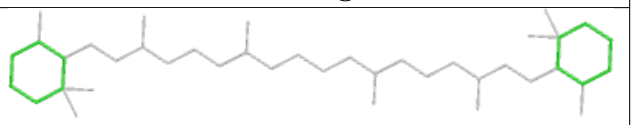
Bond lengths



Bond angles

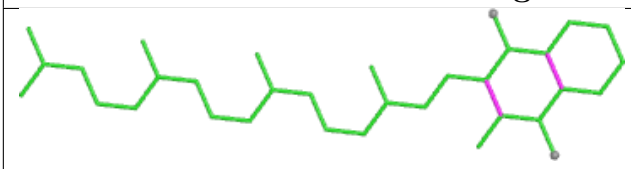


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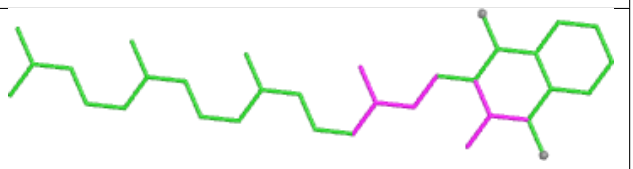


Rings

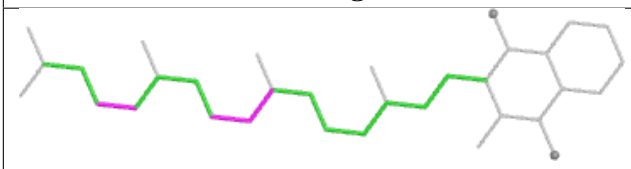
Ligand PQN cA 845



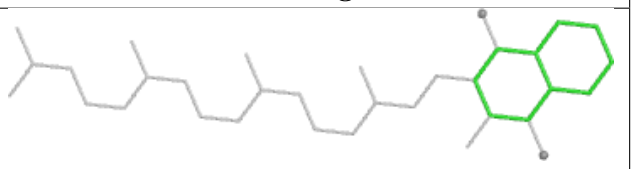
Bond lengths



Bond angles

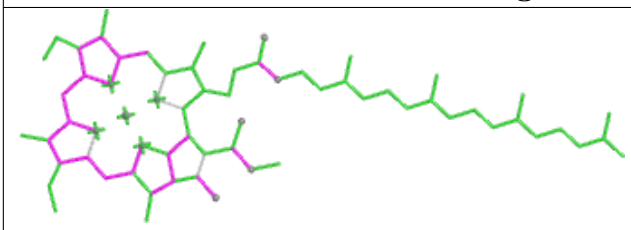


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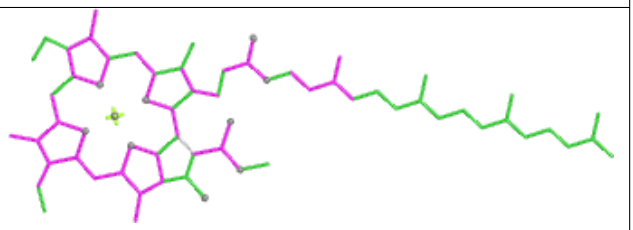


Rings

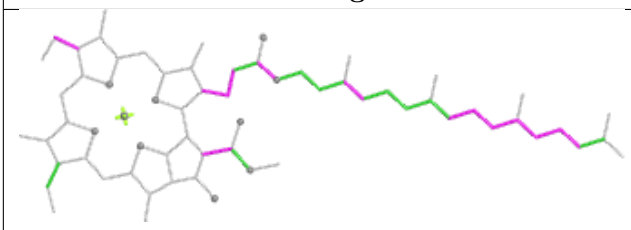
Ligand CLA aB 812



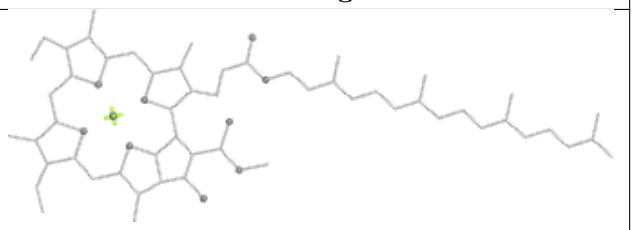
Bond lengths



Bond angles

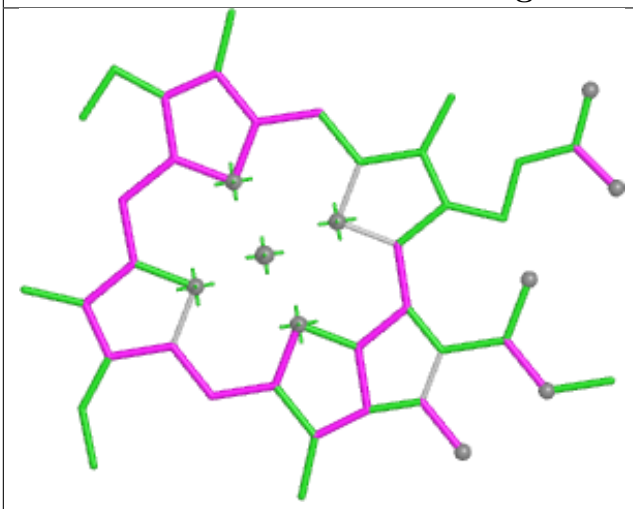


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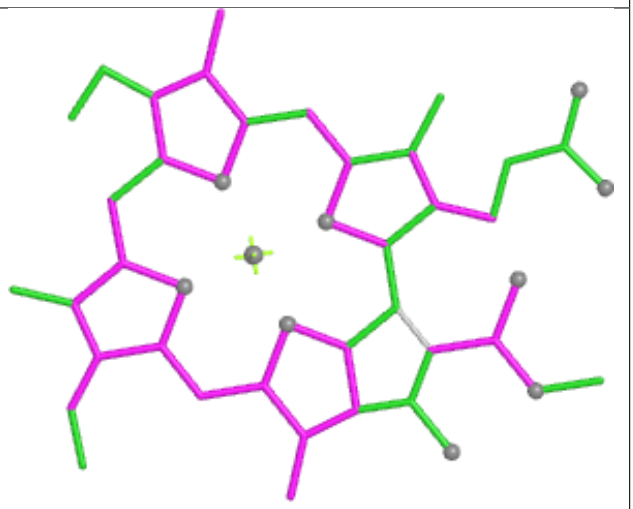


Rings

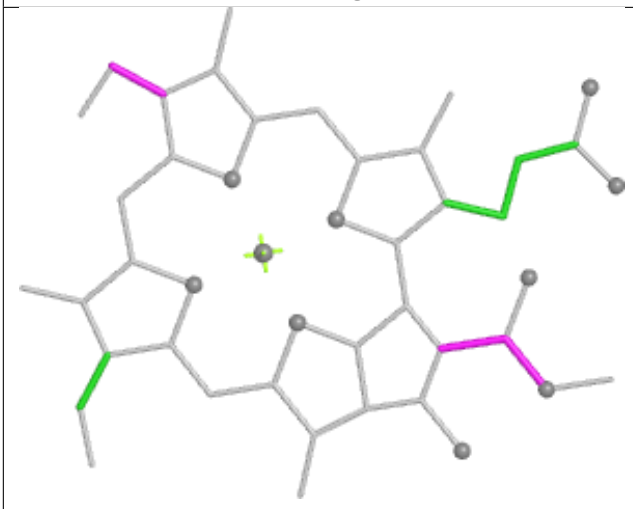
Ligand CLA cA 816



Bond lengths



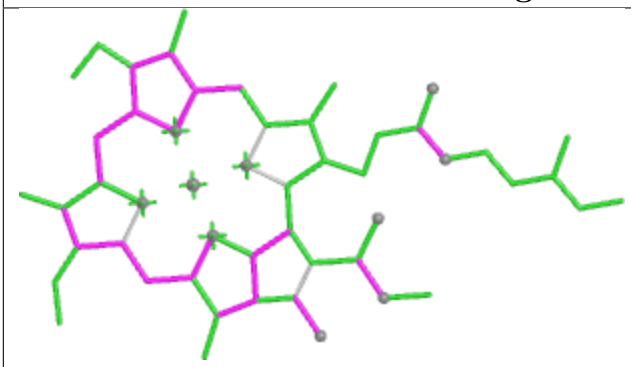
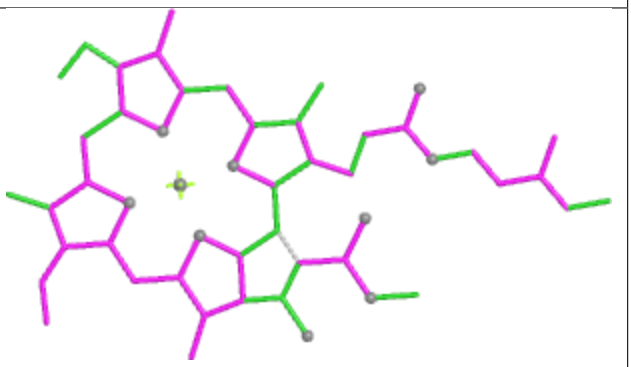
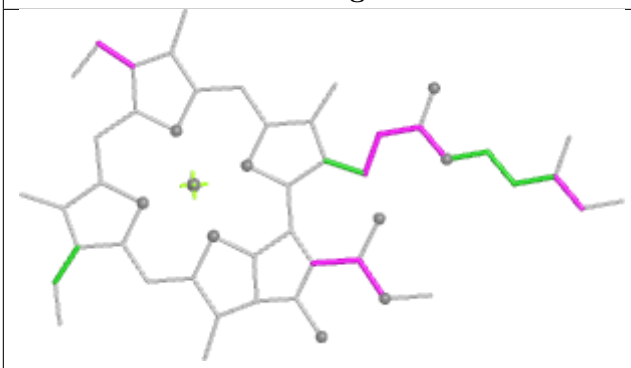
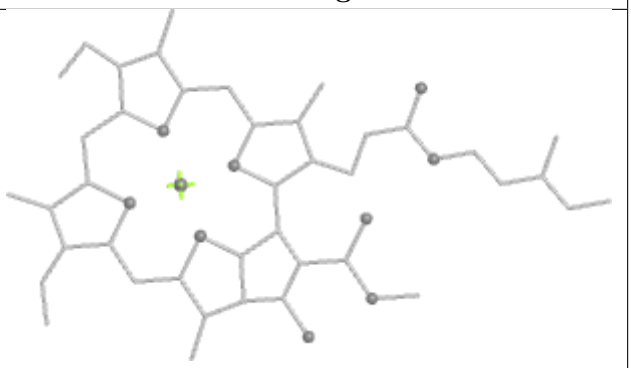
Bond angles

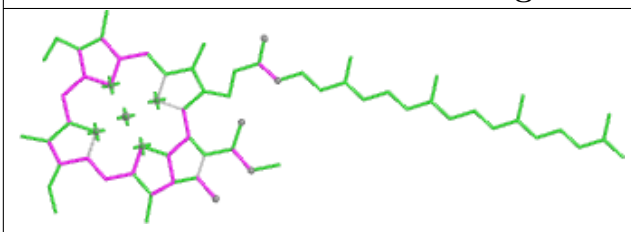
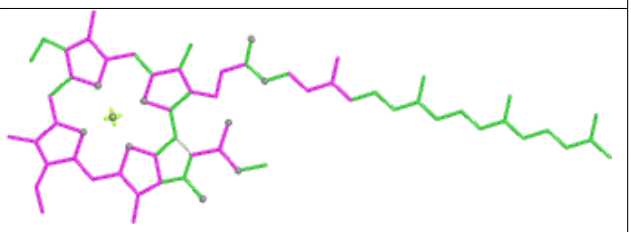
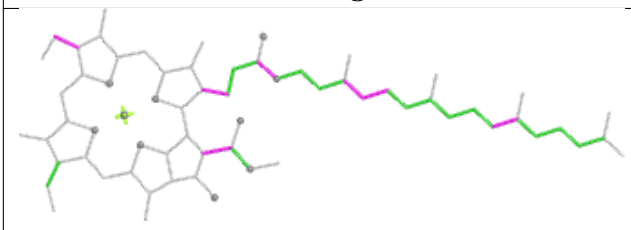
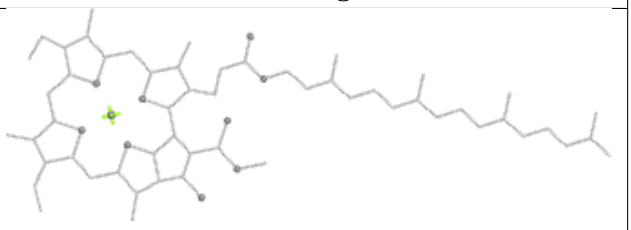


Torsions

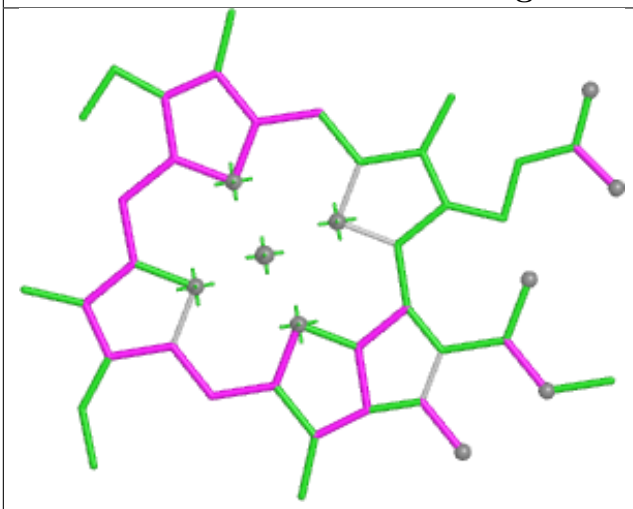


Rings

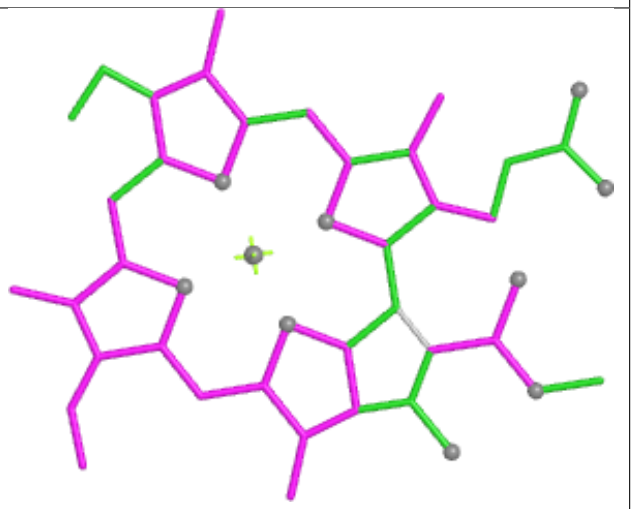
Ligand CLA aA 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aA 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

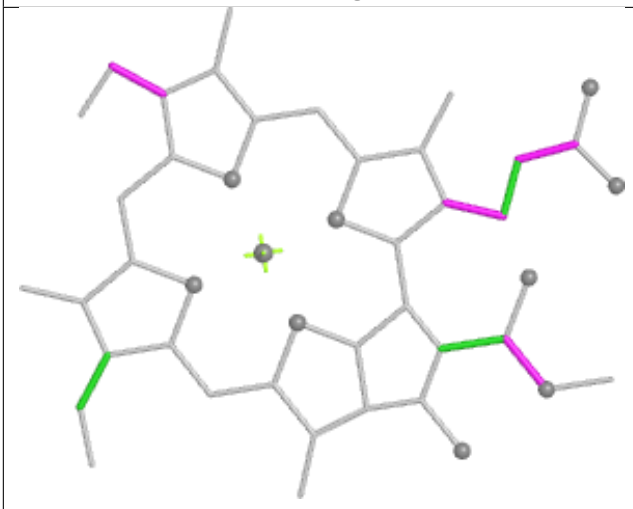
Ligand CLA aB 810



Bond lengths



Bond angles

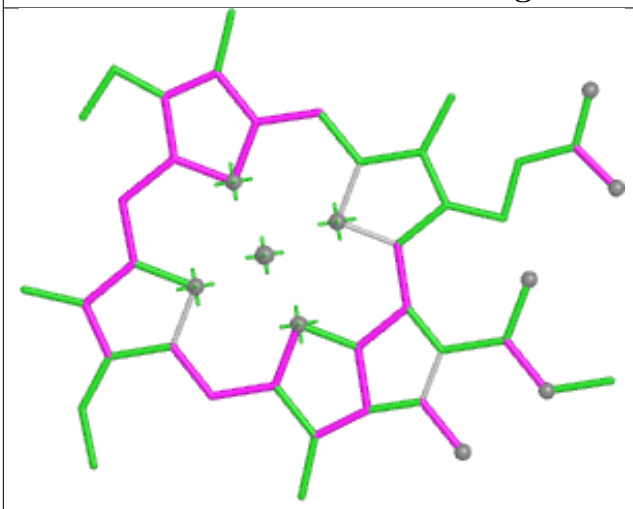


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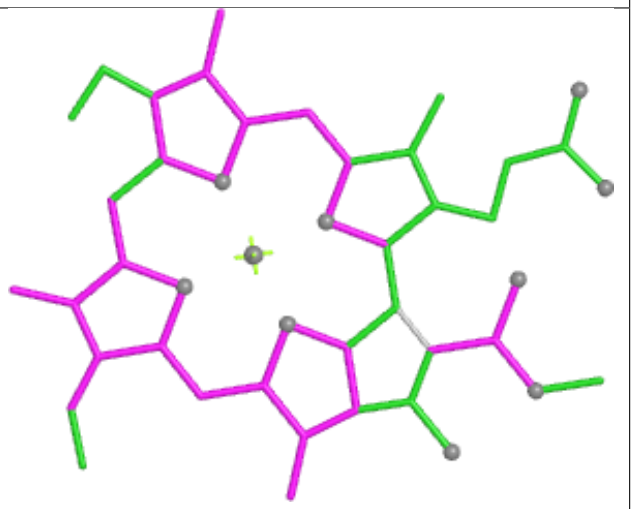


Rings

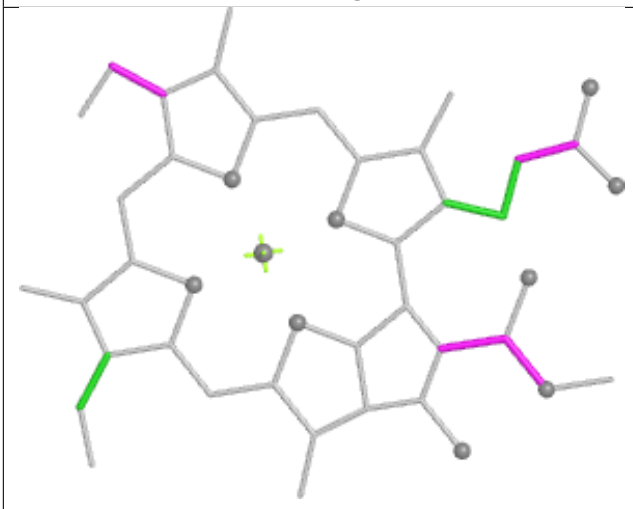
Ligand CLA bB 820



Bond lengths



Bond angles

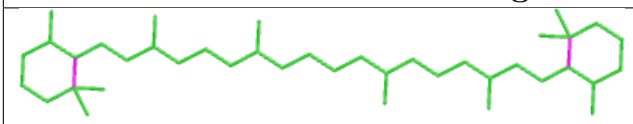


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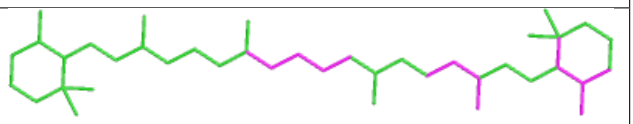


Rings

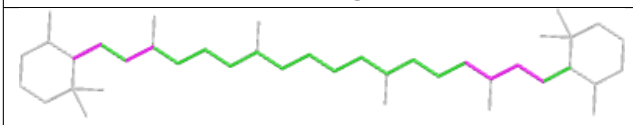
Ligand BCR bK 102



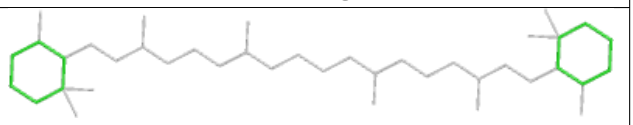
Bond lengths



Bond angles

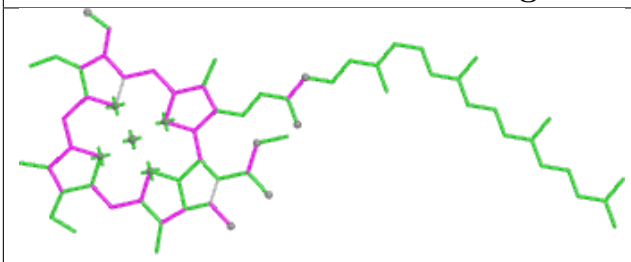


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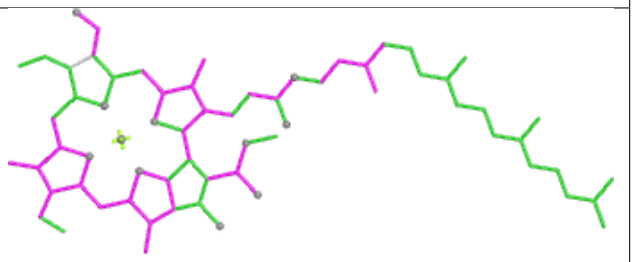


Rings

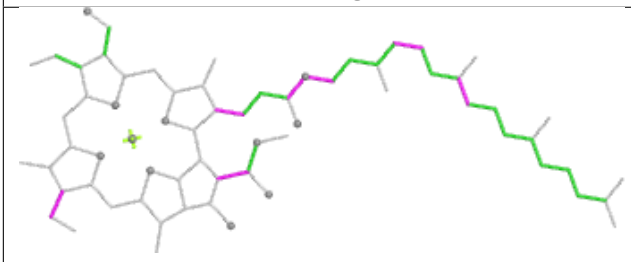
Ligand F6C cA 826



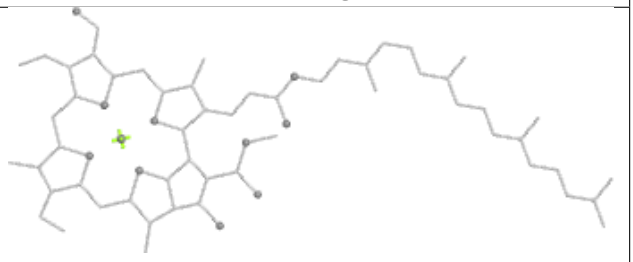
Bond lengths



Bond angles



Torsions

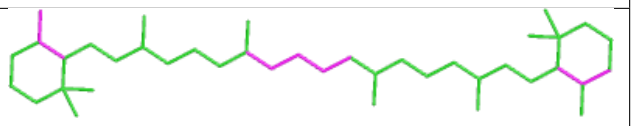


Rings

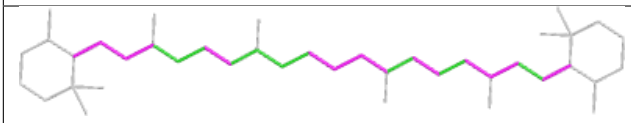
Ligand BCR cB 842



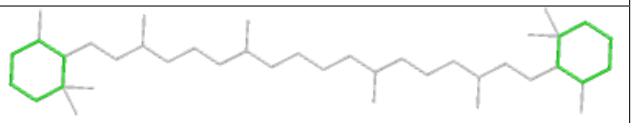
Bond lengths



Bond angles

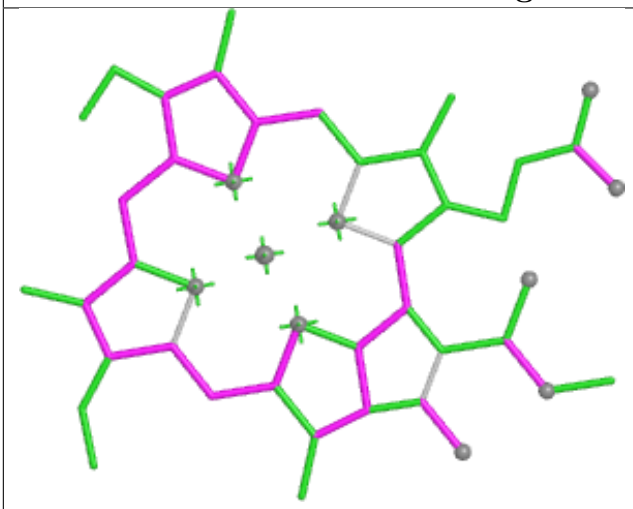


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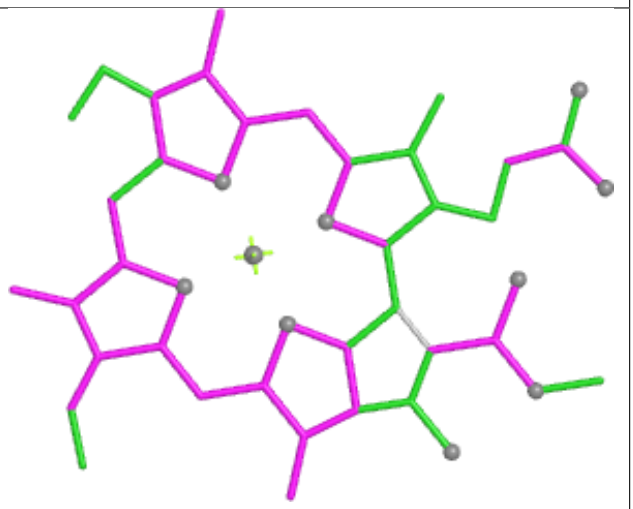


Rings

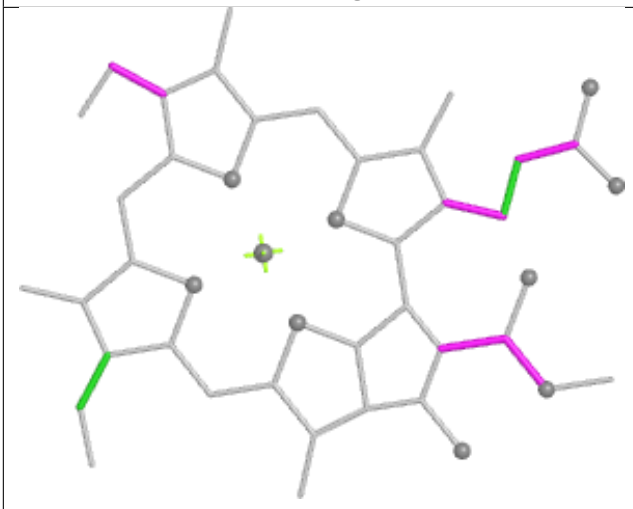
Ligand CLA aB 832



Bond lengths



Bond angles

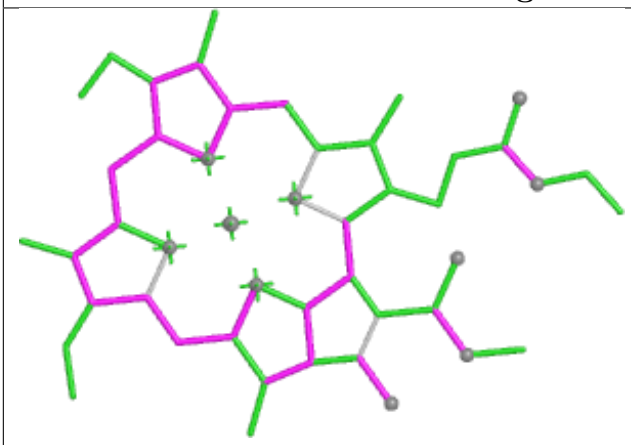


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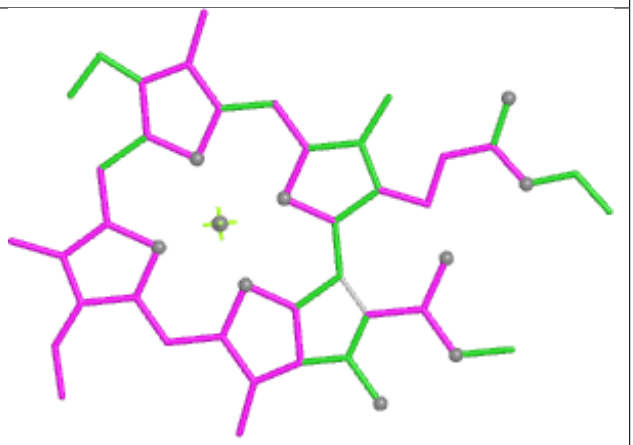


Rings

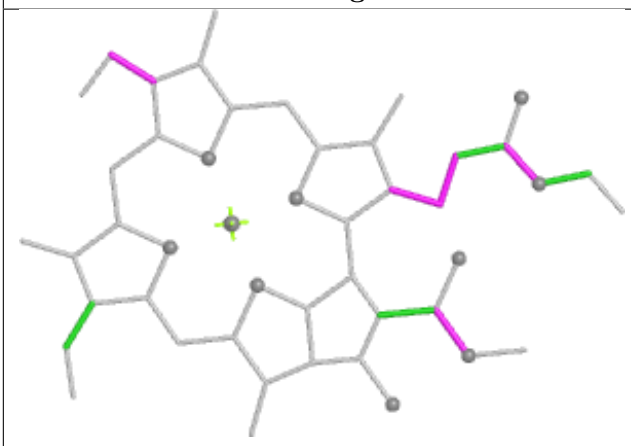
Ligand CLA cB 819



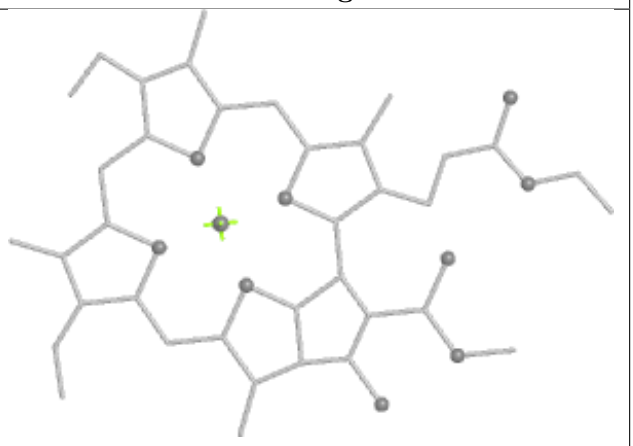
Bond lengths



Bond angles

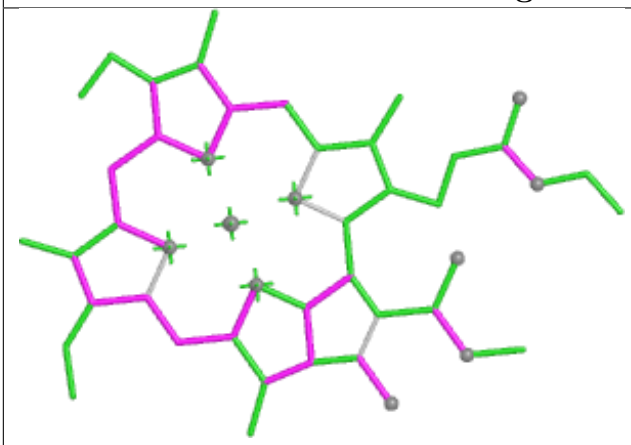


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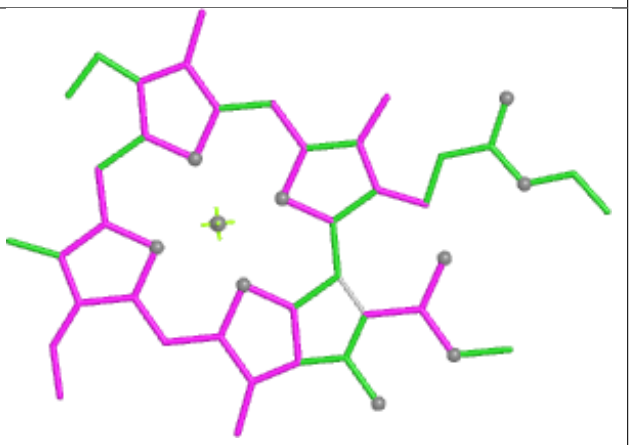


Rings

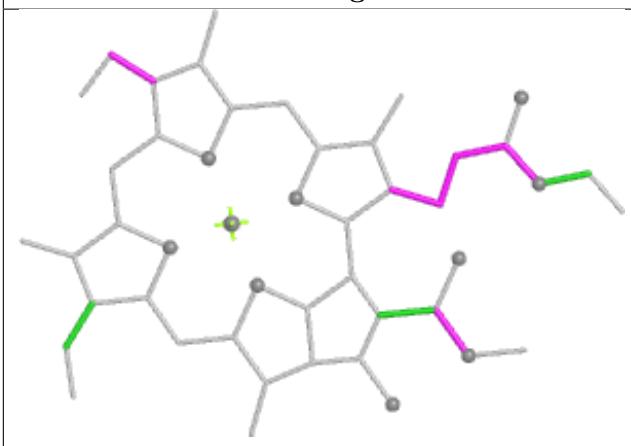
Ligand CLA aB 809



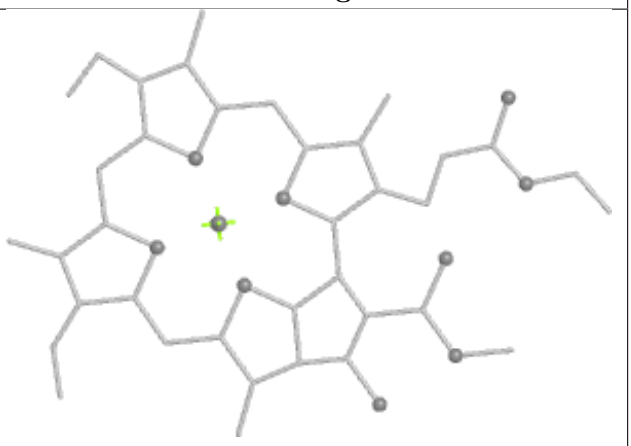
Bond lengths



Bond angles

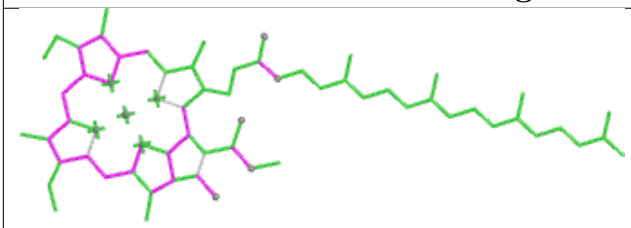


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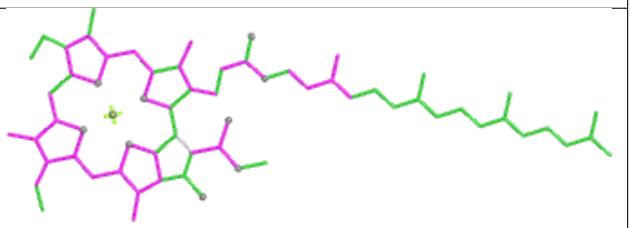


Rings

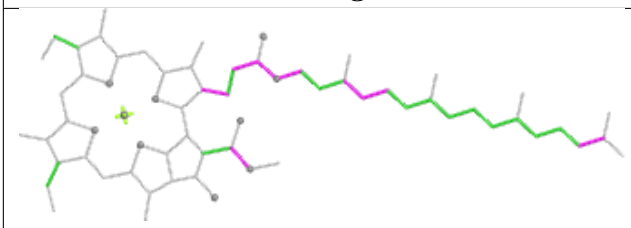
Ligand CLA aA 829



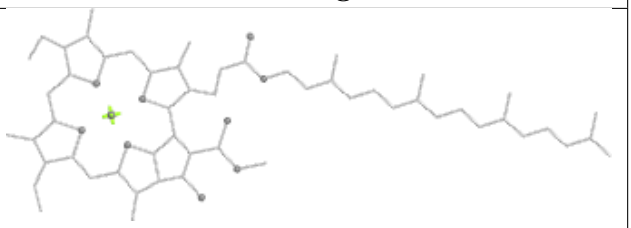
Bond lengths



Bond angles

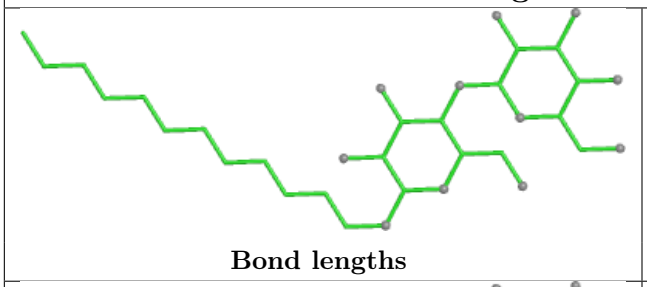


Torsions

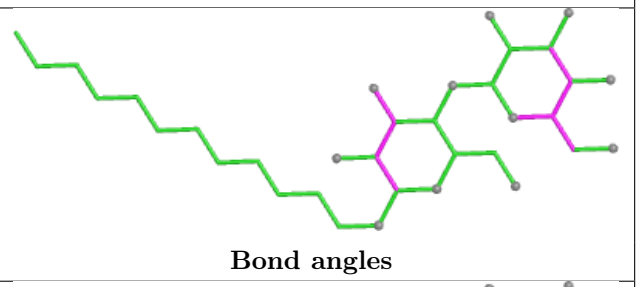


Rings

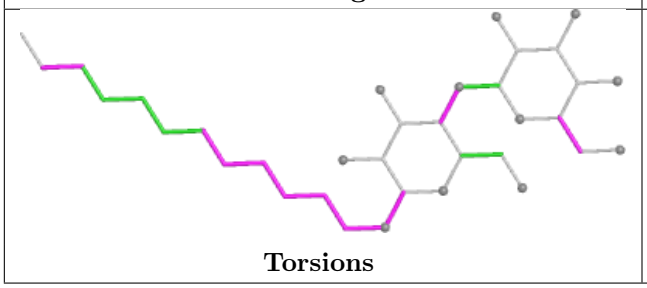
Ligand LMT bA 853



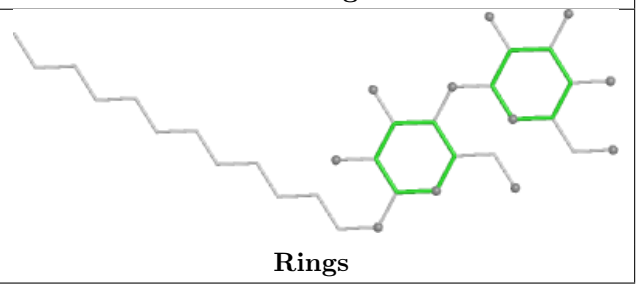
Bond lengths



Bond angles

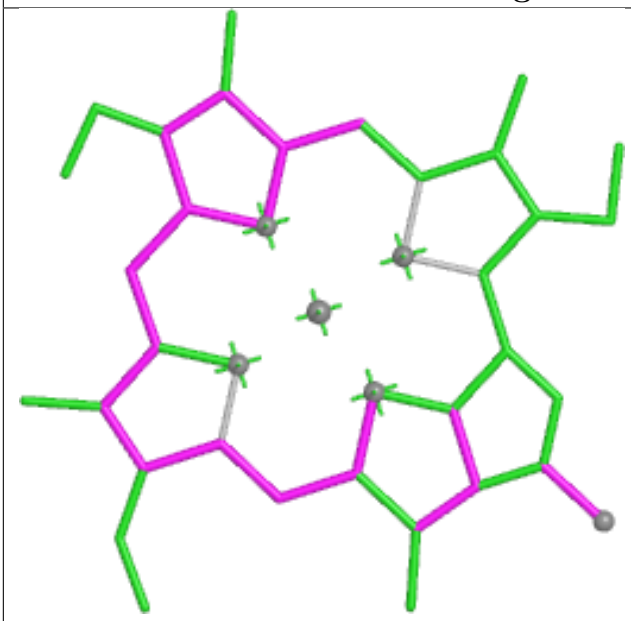


Torsions



Rings

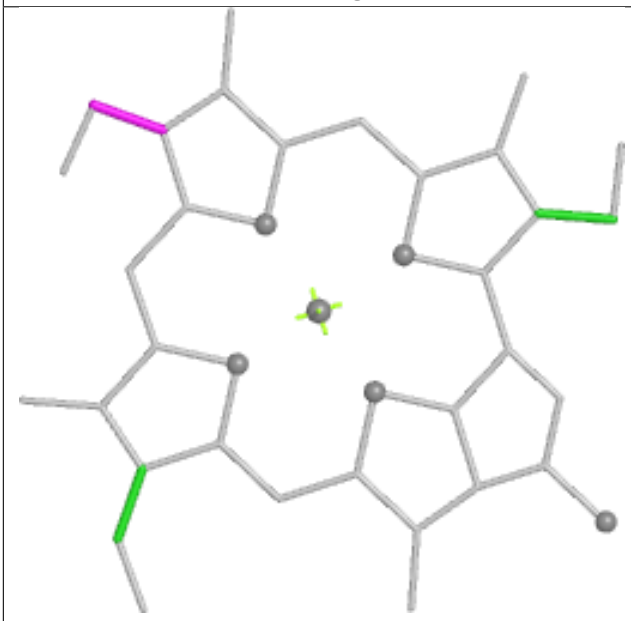
Ligand CLA bK 101



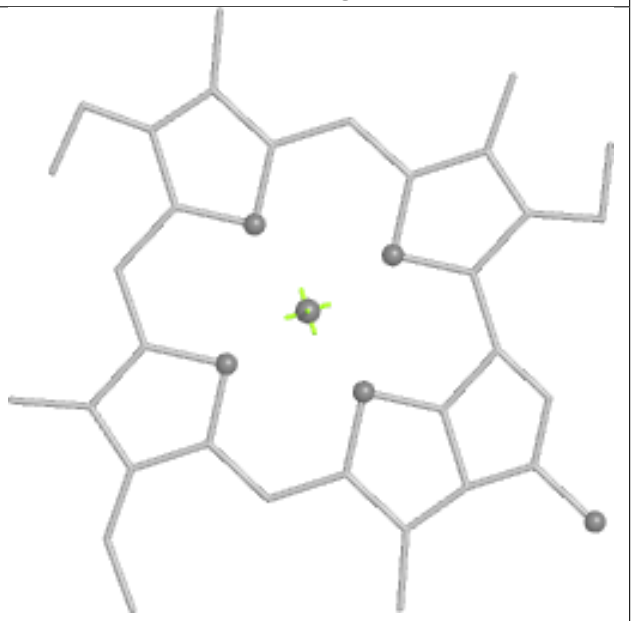
Bond lengths



Bond angles

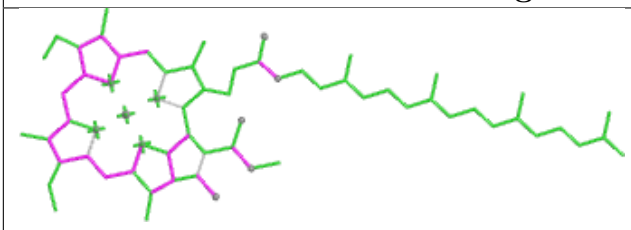


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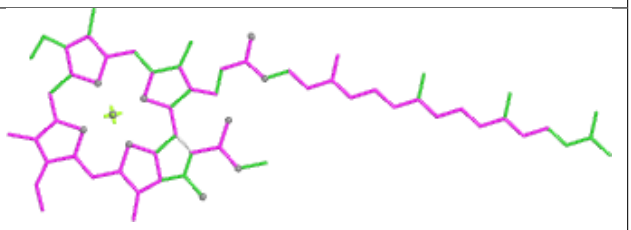


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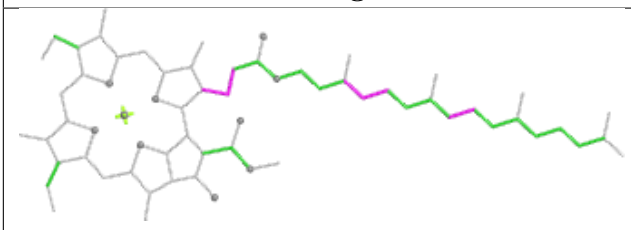
Ligand CLA aA 802



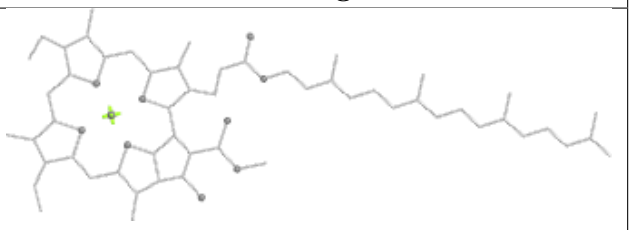
Bond lengths



Bond angles

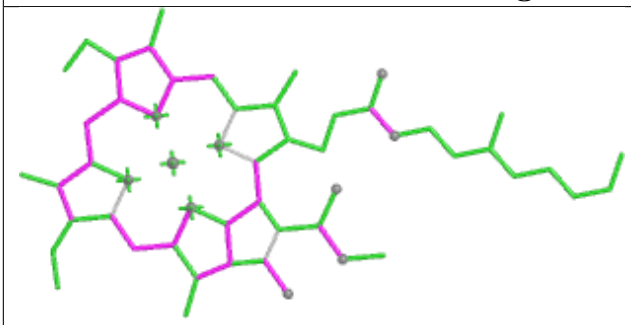


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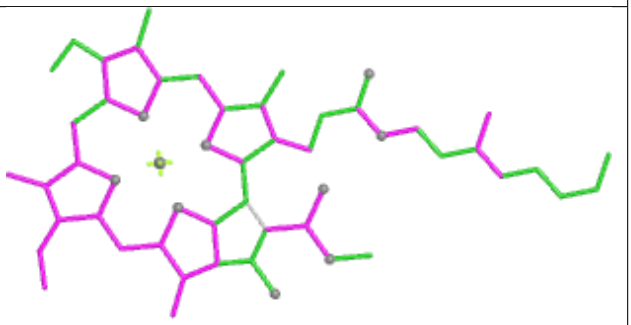


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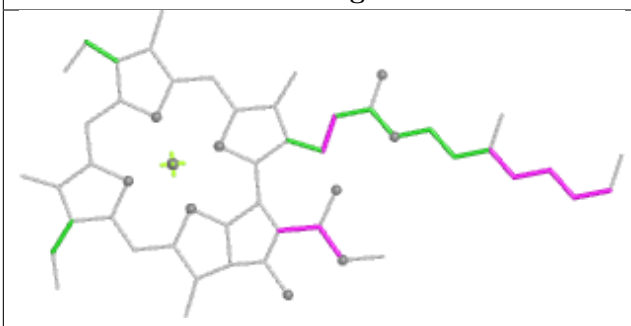
Ligand CLA cA 818



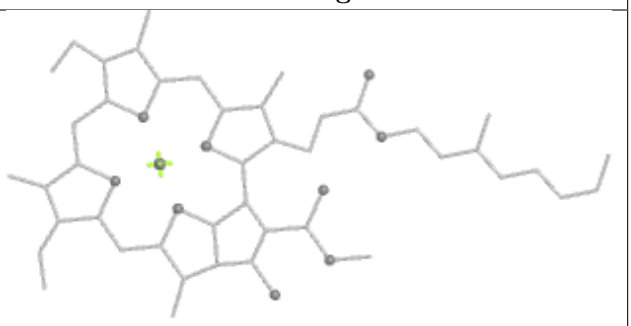
Bond lengths



Bond angles

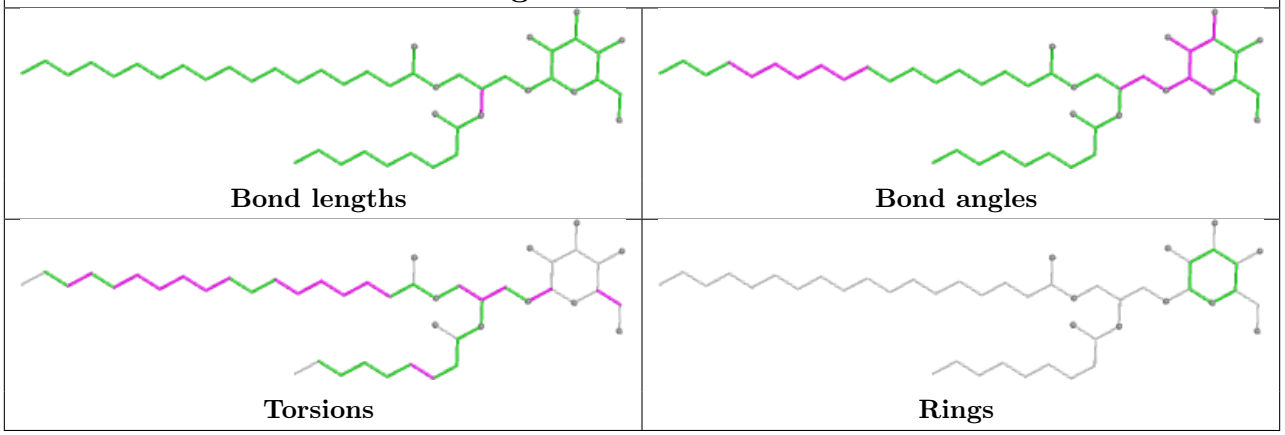


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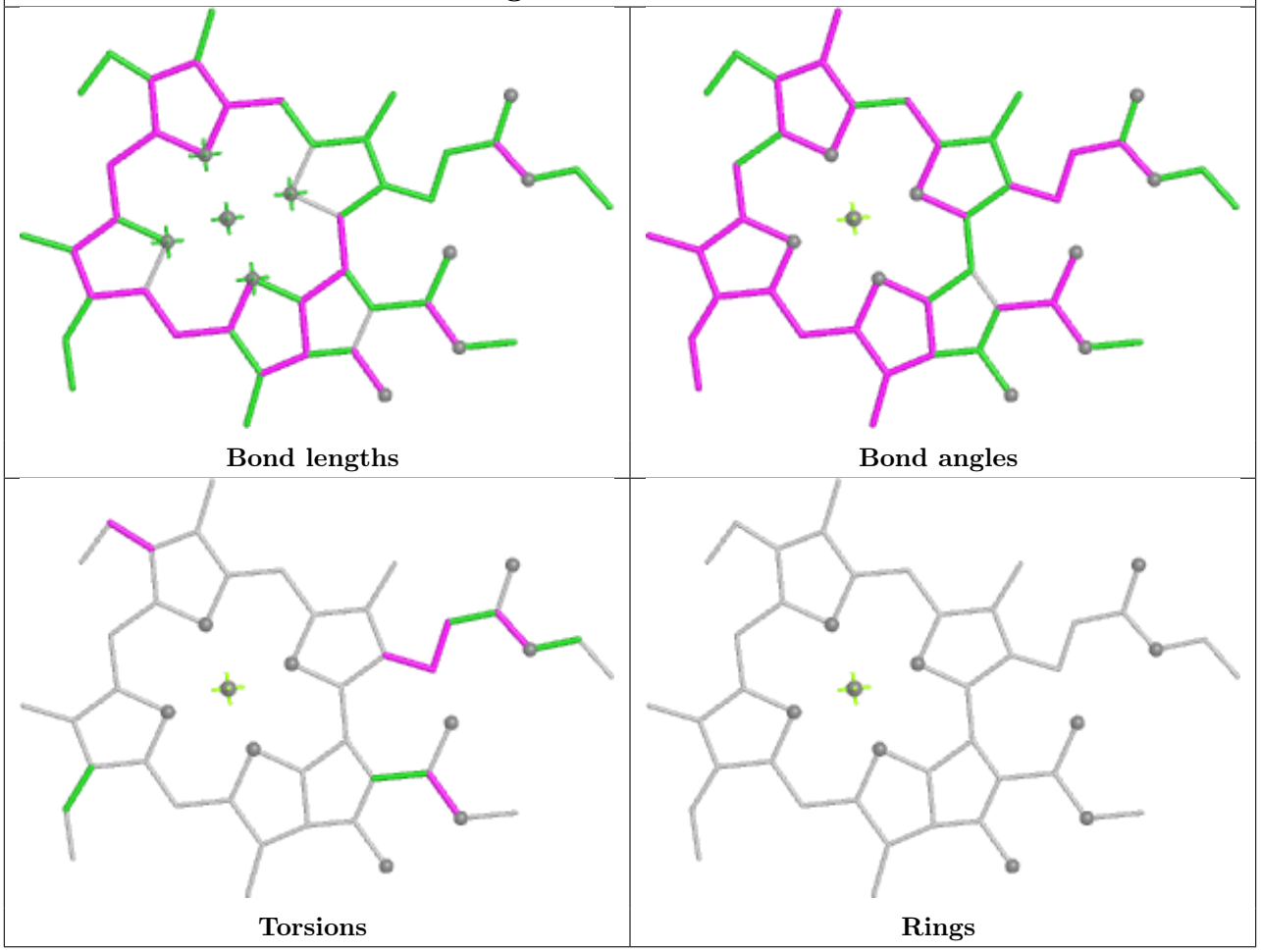


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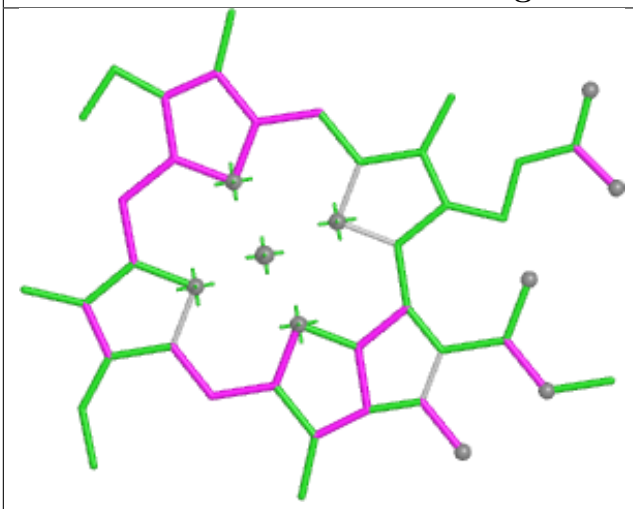
Ligand LMG bB 847



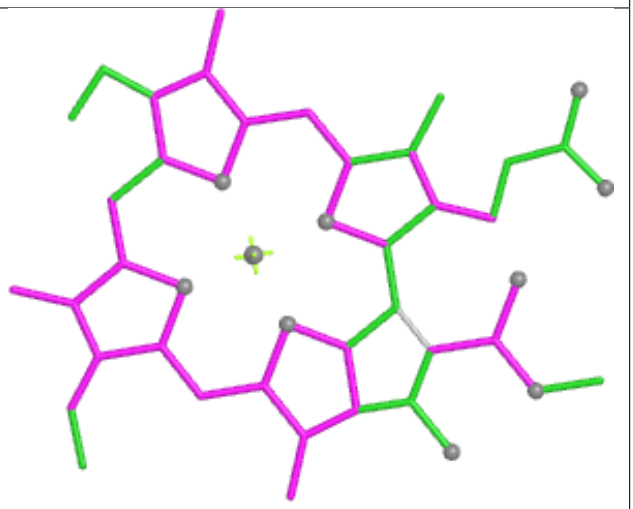
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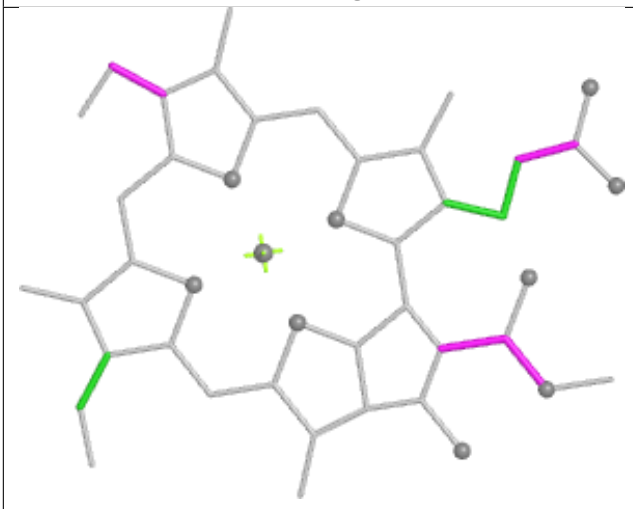
Ligand CLA bB 822



Bond lengths



Bond angles

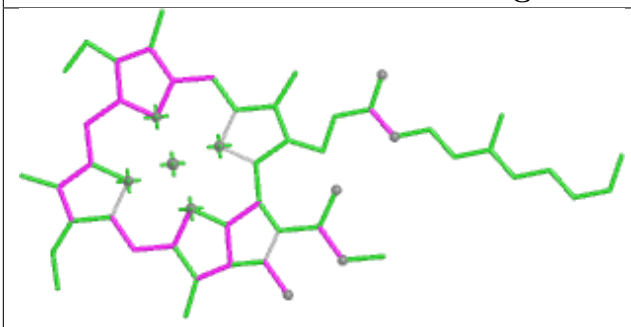


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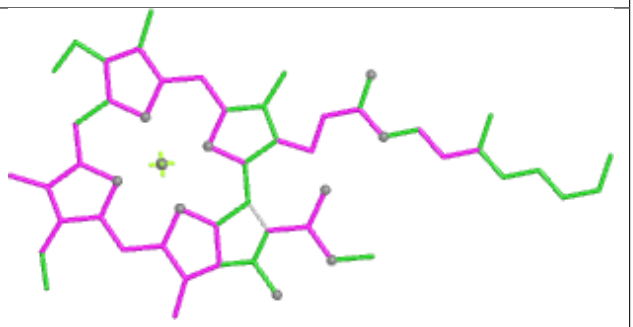


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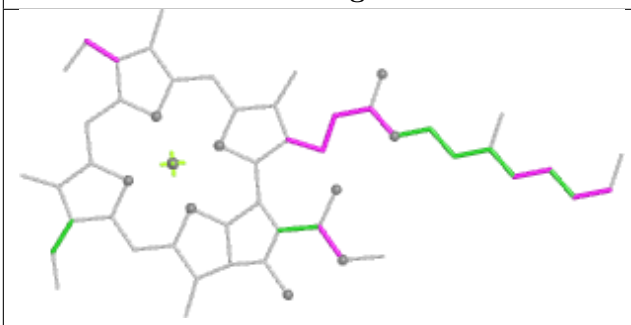
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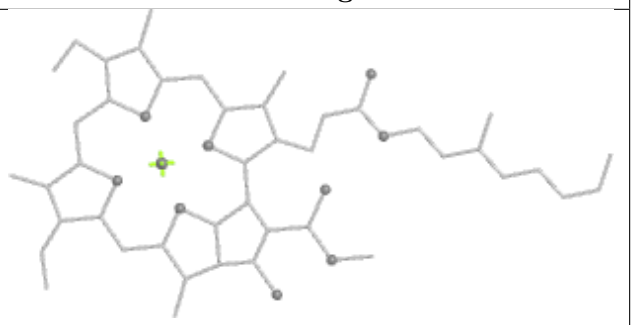
Bond lengths



Bond angles

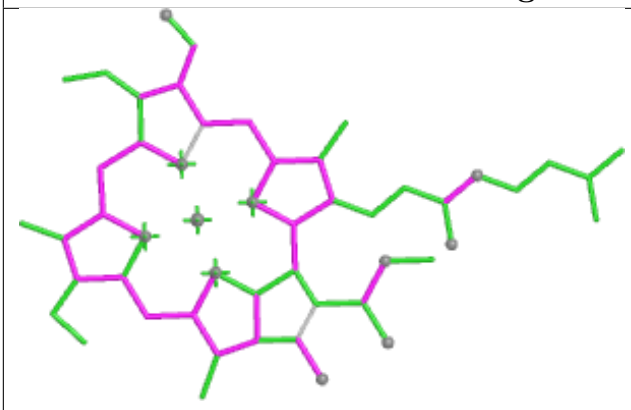


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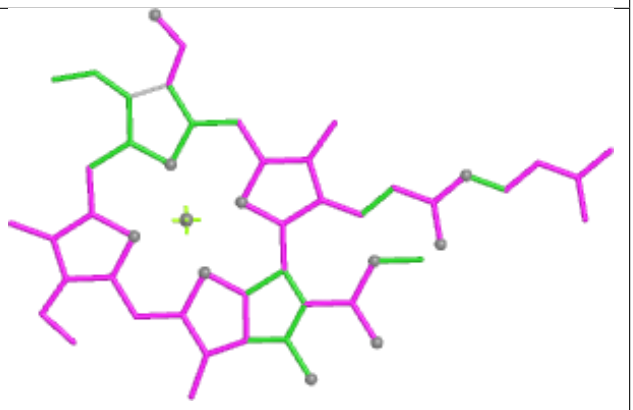


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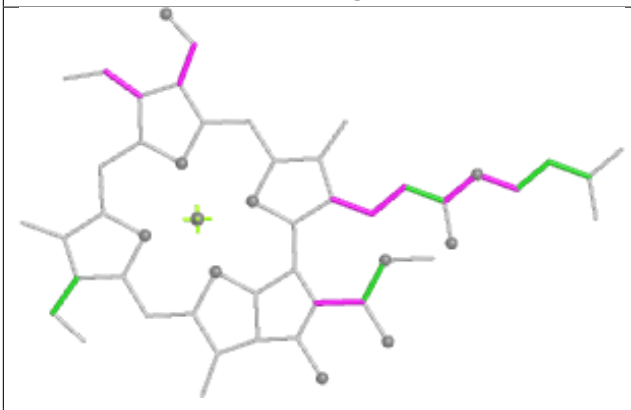
Ligand F6C bA 832



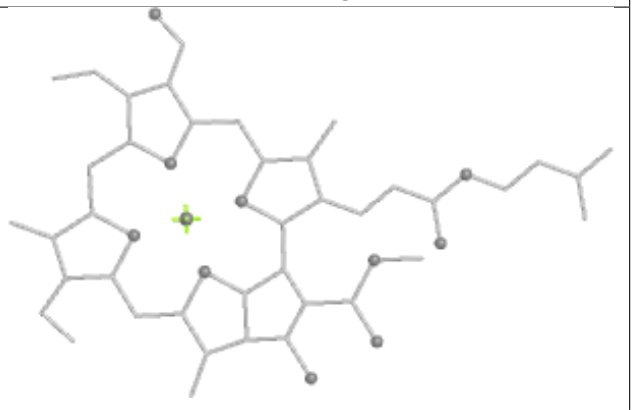
Bond lengths



Bond angles

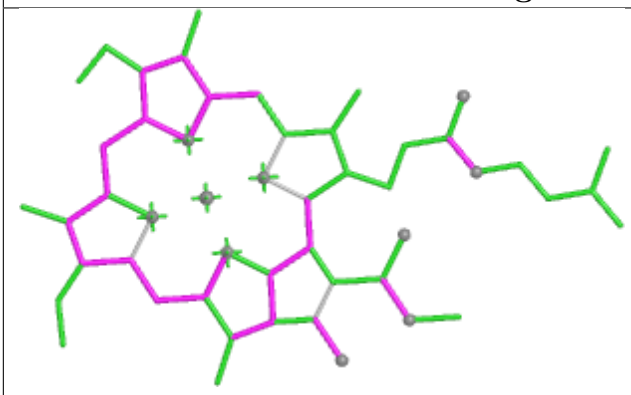


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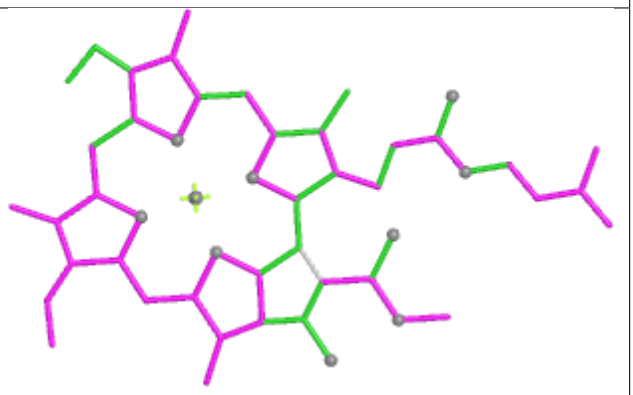


Rings

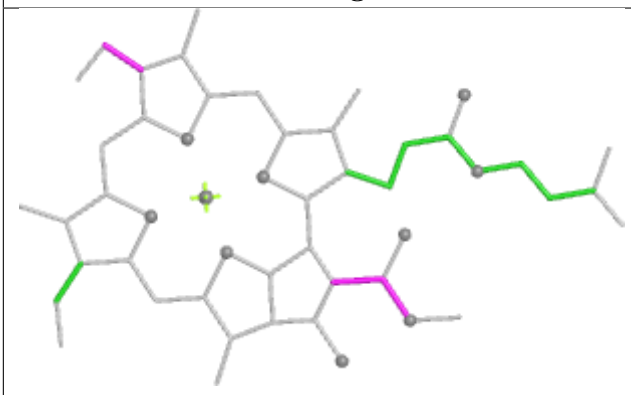
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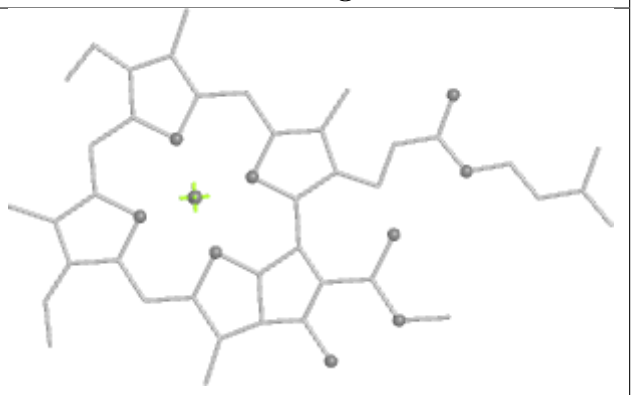
Bond lengths



Bond angles

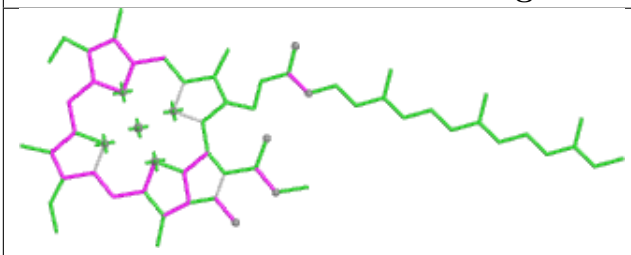


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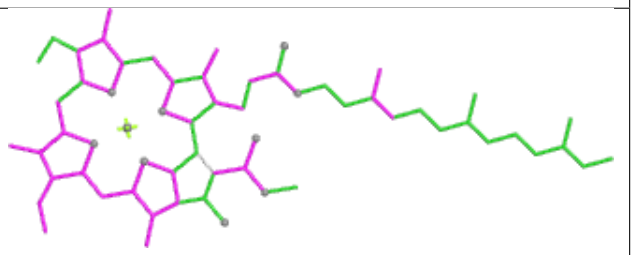


Rings

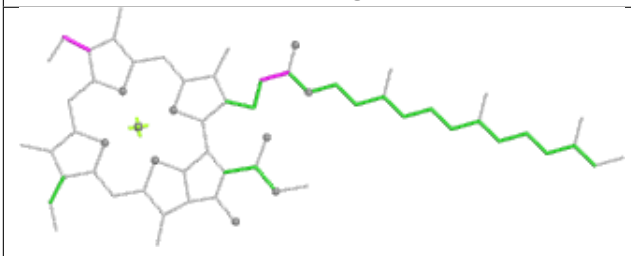
Ligand CLA aB 807



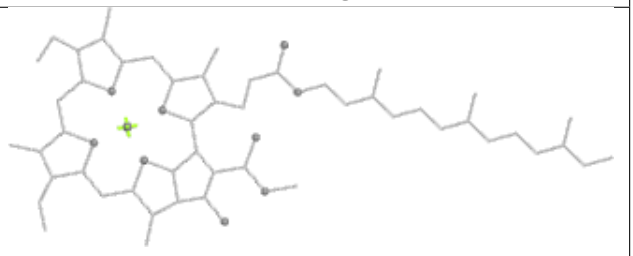
Bond lengths



Bond angles

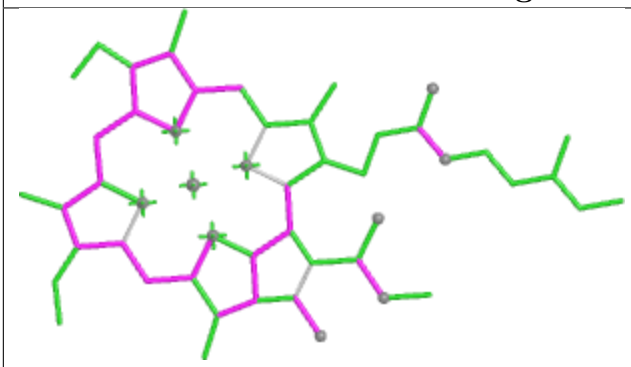


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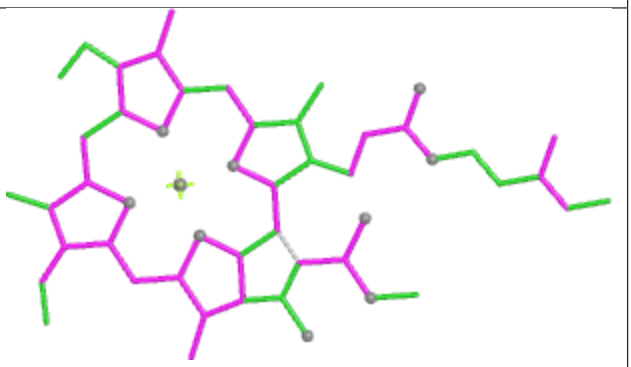


Rings

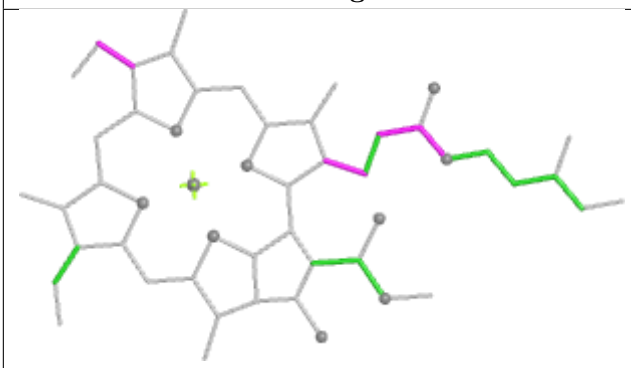
Ligand CLA cK 103



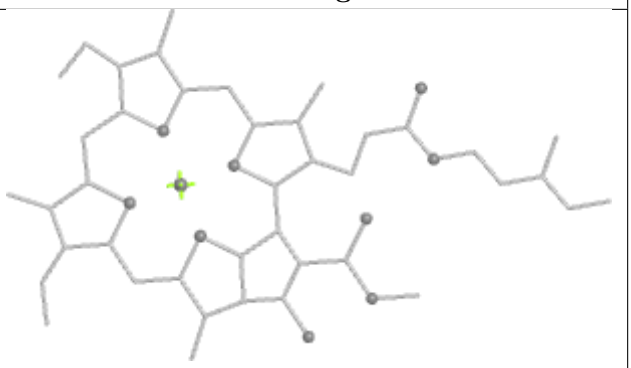
Bond lengths



Bond angles

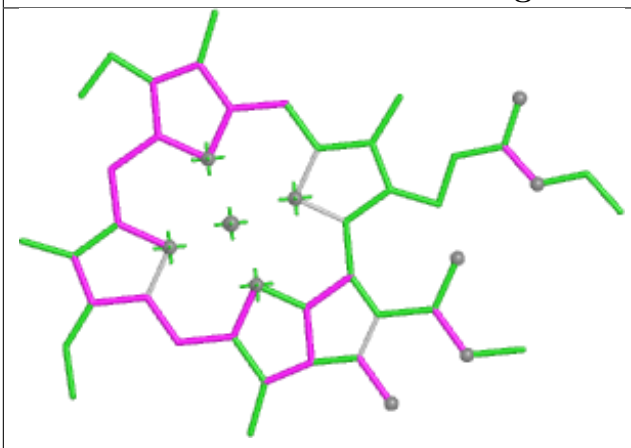


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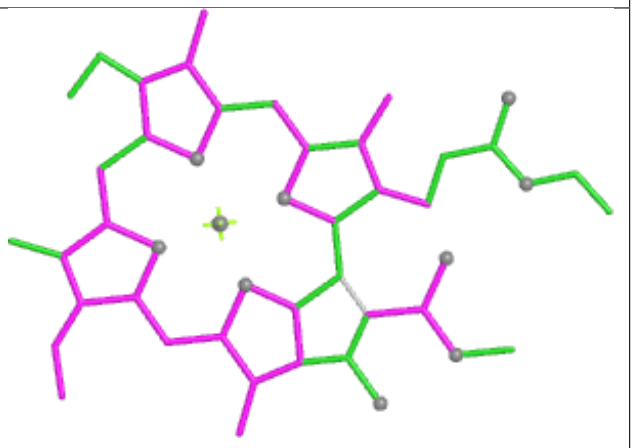


Rings

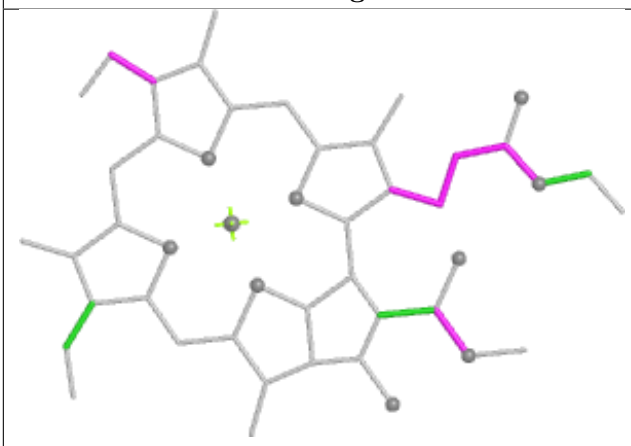
Ligand CLA bB 809



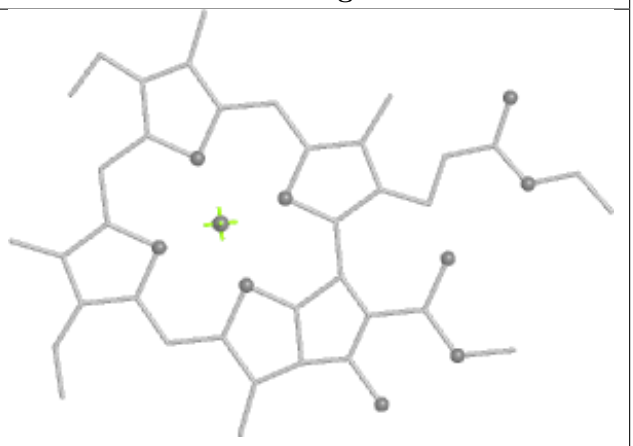
Bond lengths



Bond angles

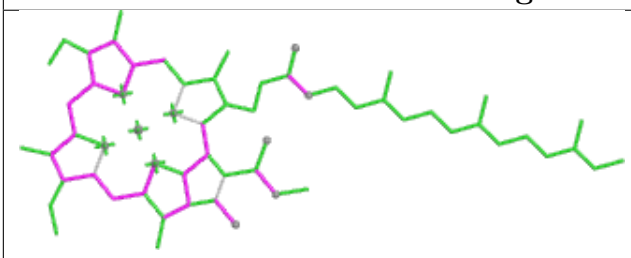


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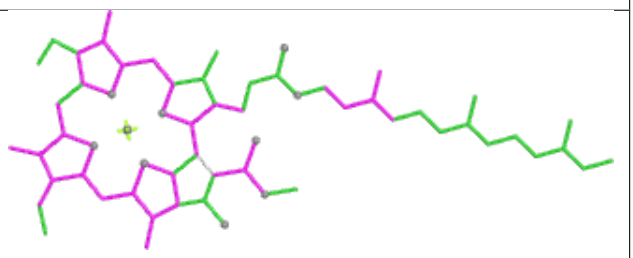


Rings

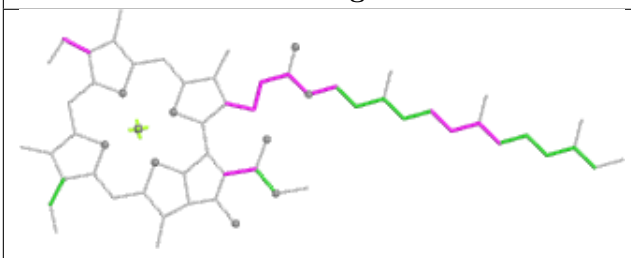
Ligand CLA cA 821



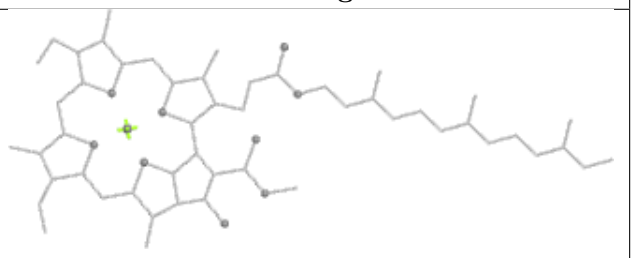
Bond lengths



Bond angles

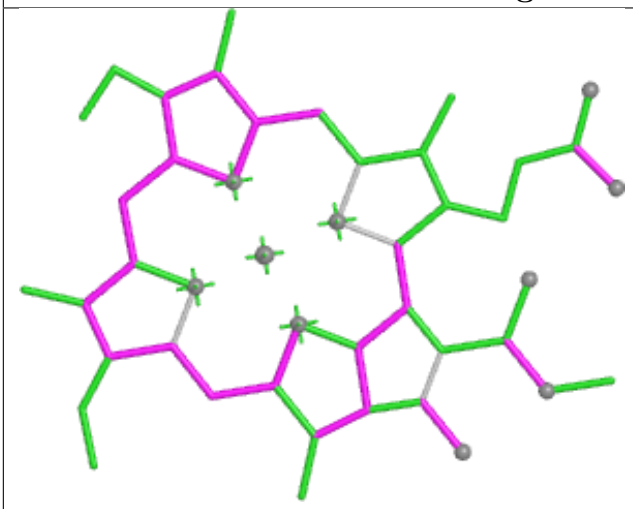


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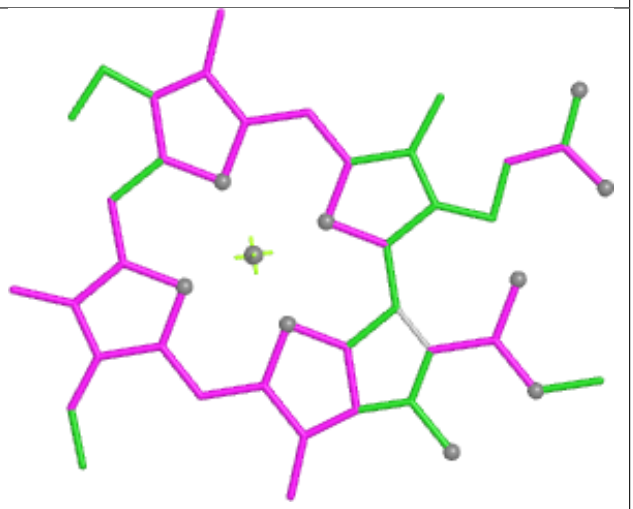


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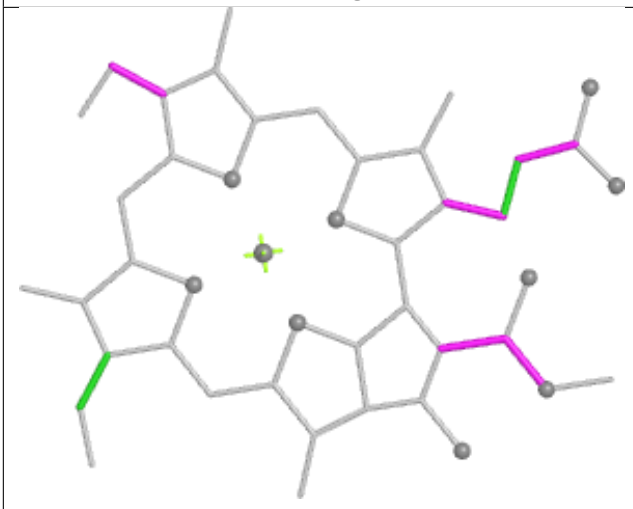
Ligand CLA cB 832



Bond lengths



Bond angles

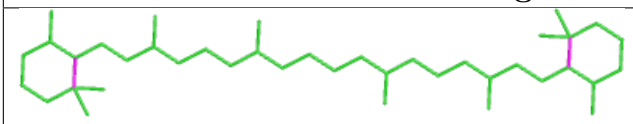


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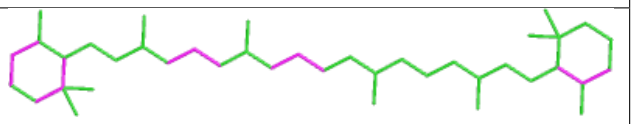


Rings

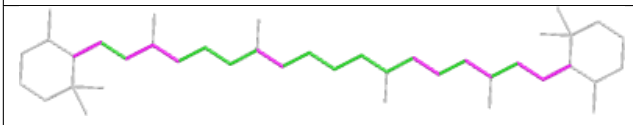
Ligand BCR cB 846



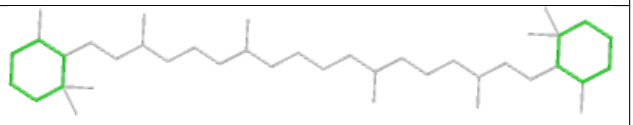
Bond lengths



Bond angles

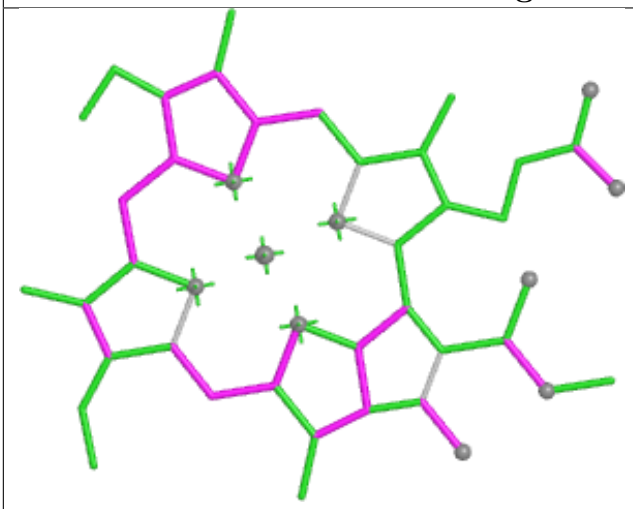


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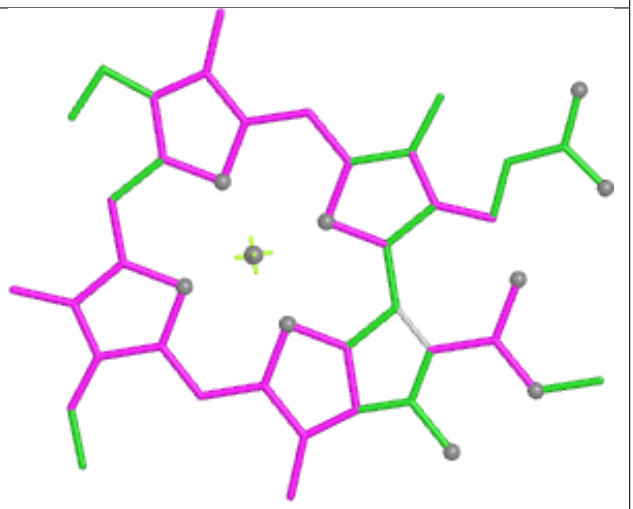


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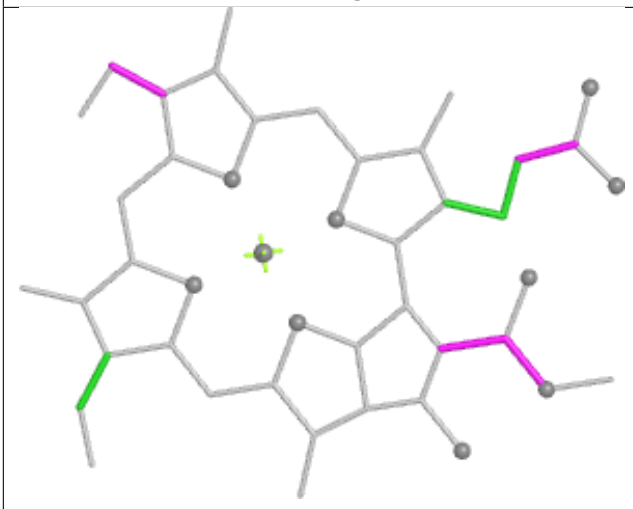
Ligand CLA aB 822



Bond lengths



Bond angles

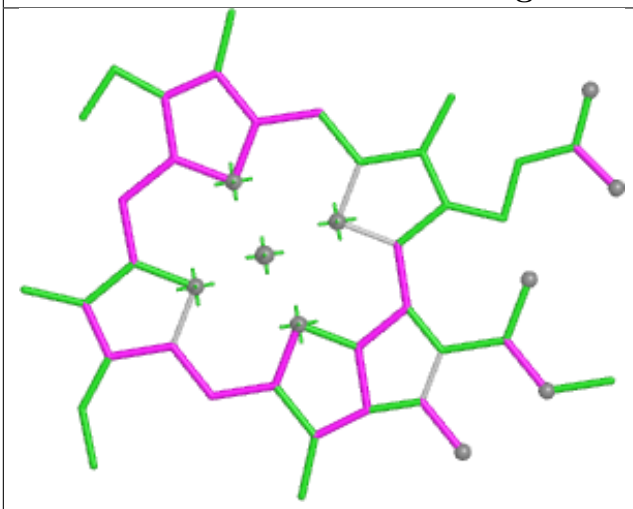


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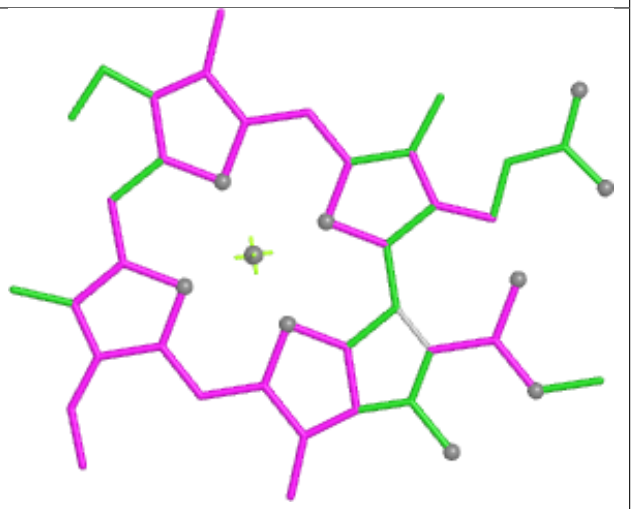


Rings

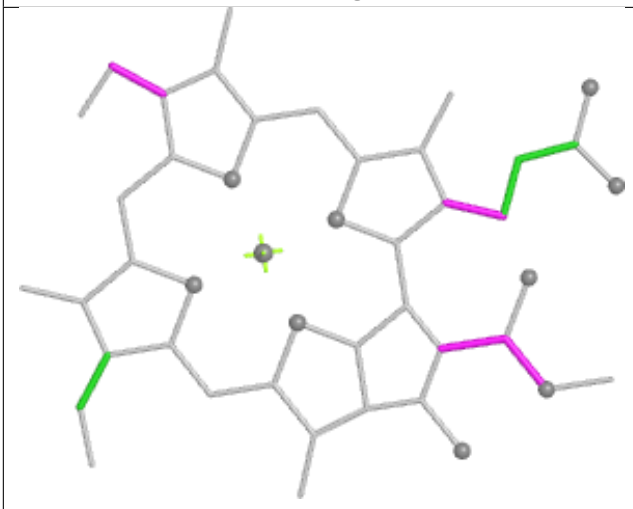
Ligand CLA aB 814



Bond lengths



Bond angles

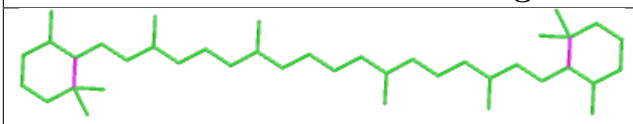


Torsions

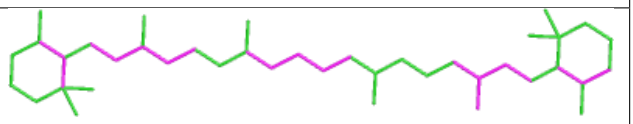


Rings

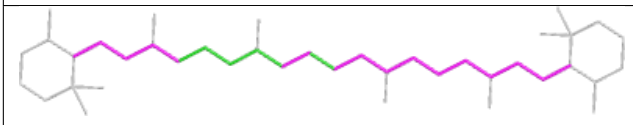
Ligand BCR cA 851



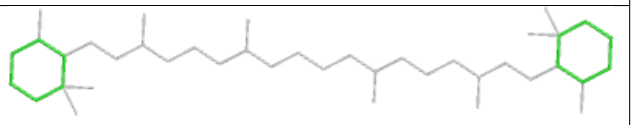
Bond lengths



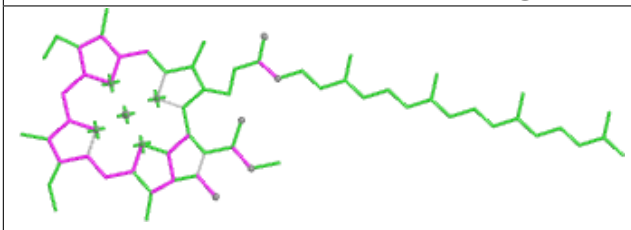
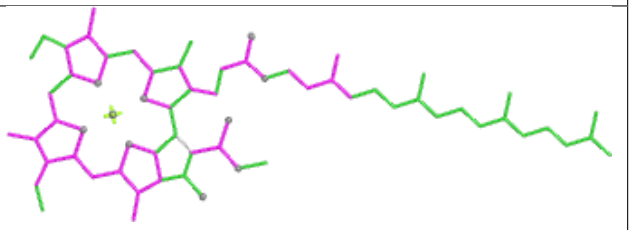
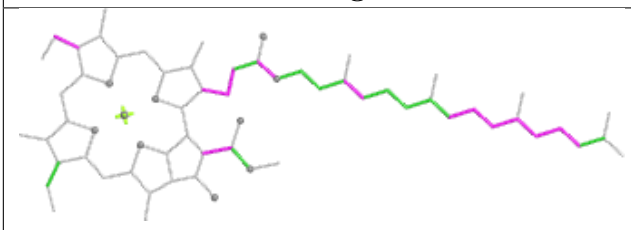
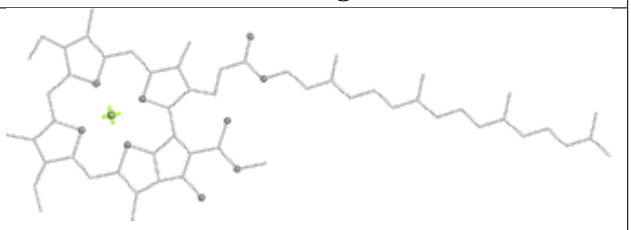
Bond angles

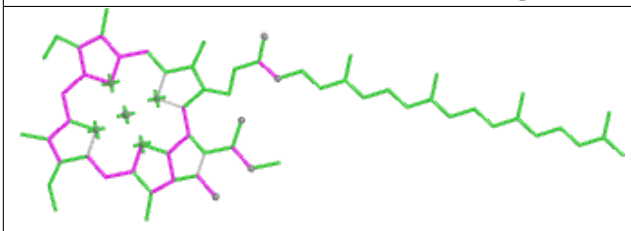
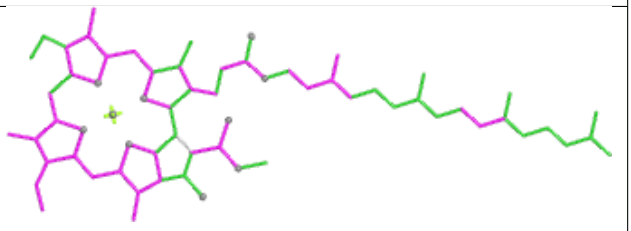
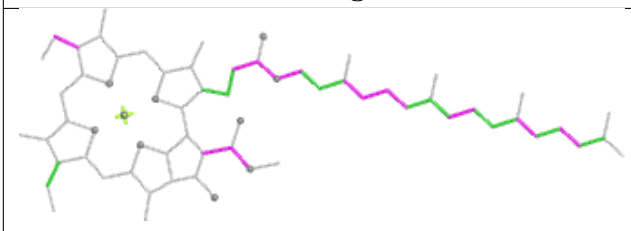
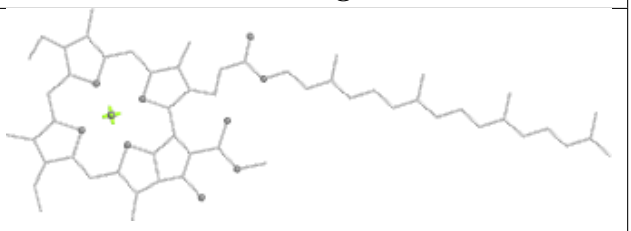


Torsions

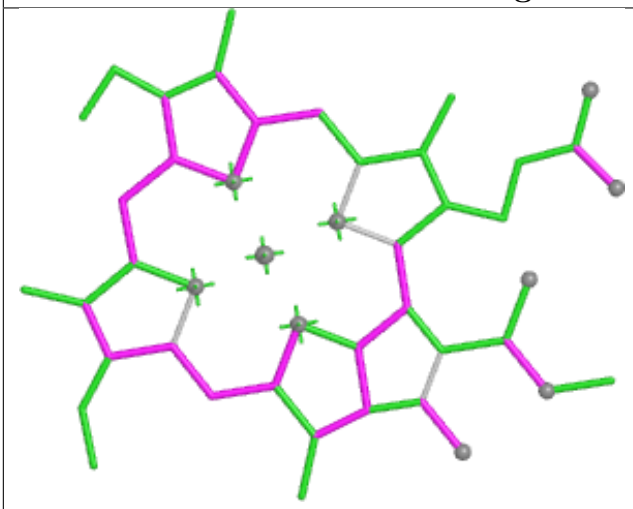


Rings

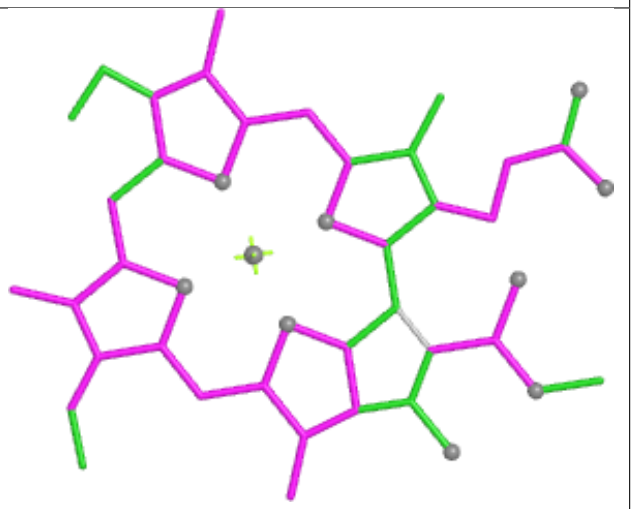
Ligand CLA cB 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bA 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

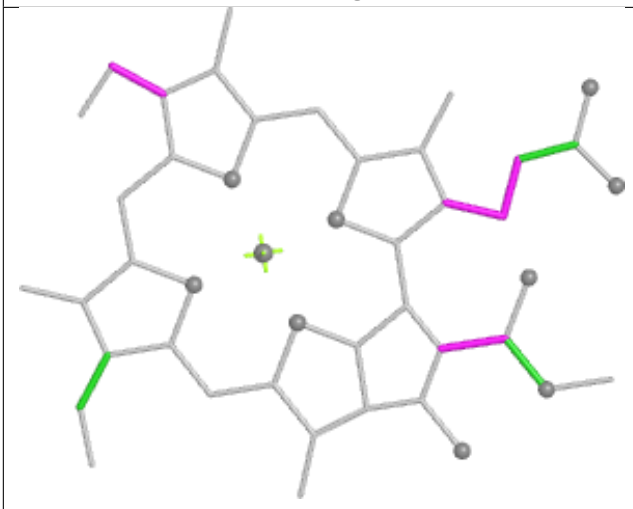
Ligand CLA bB 829



Bond lengths



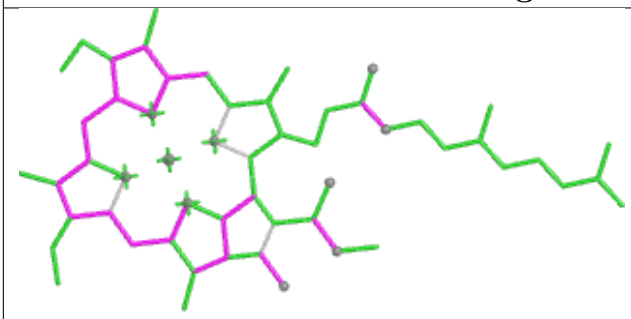
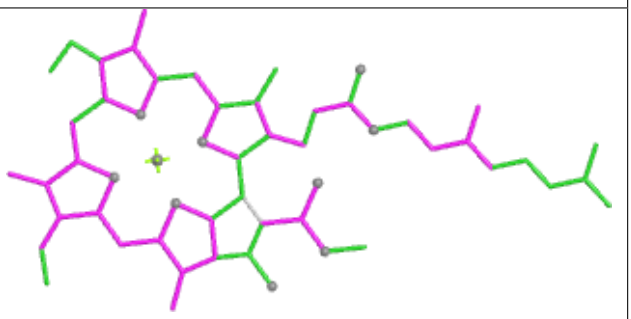
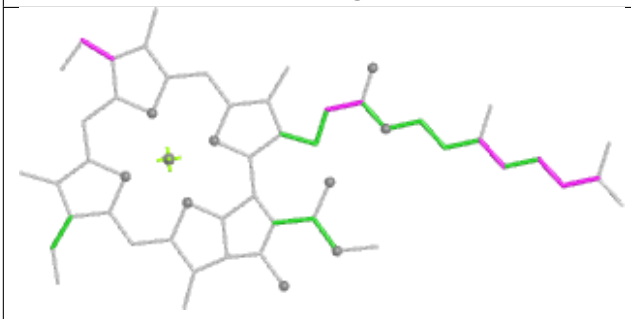
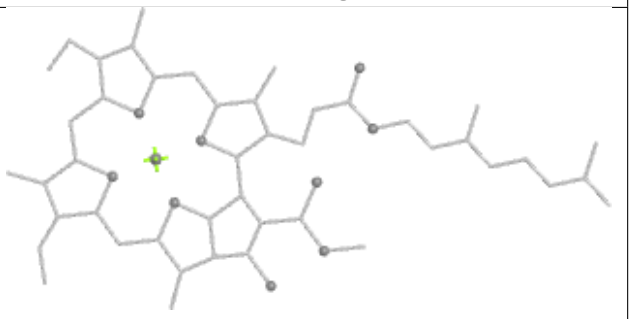
Bond angles

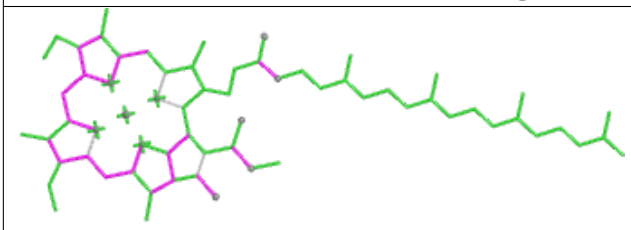
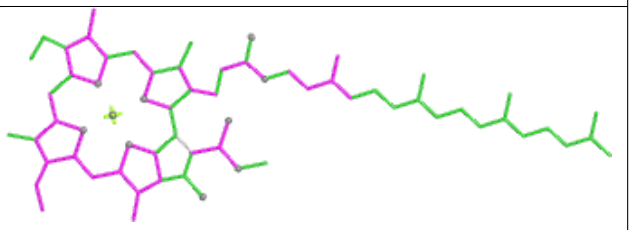
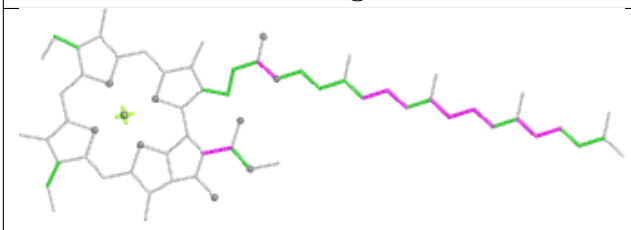
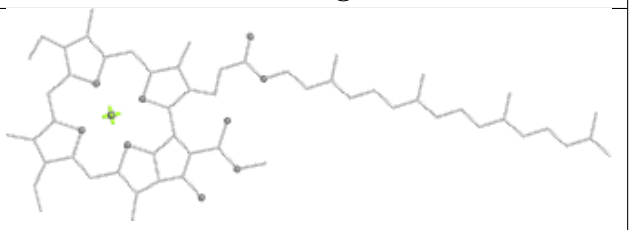


Torsions

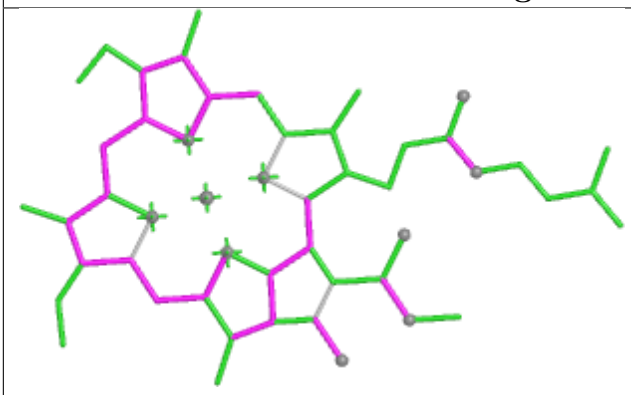


Rings

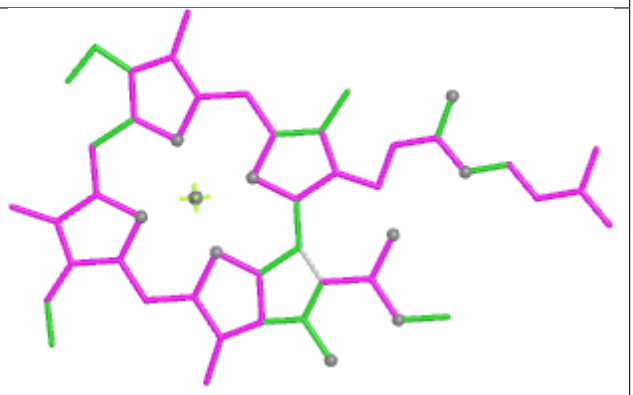
Ligand CLA aB 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

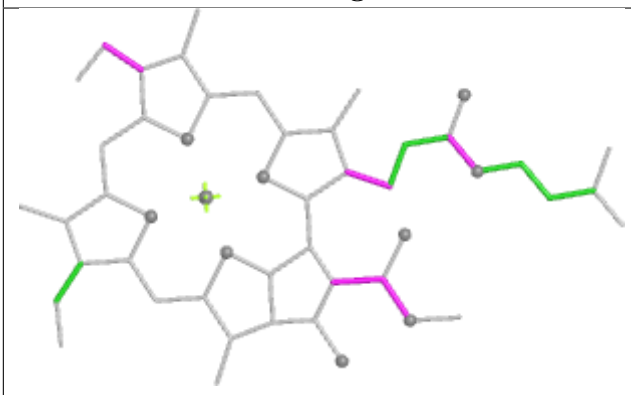
Ligand CLA bB 804



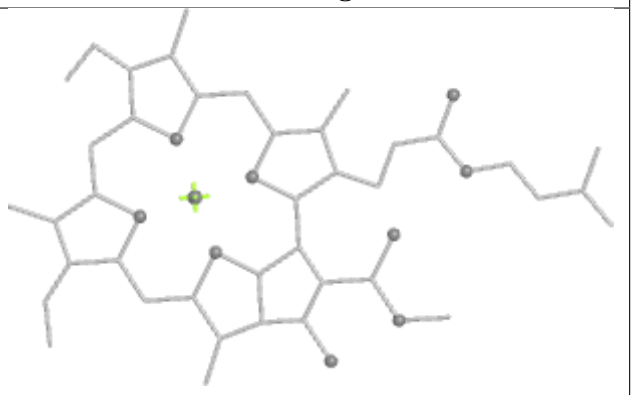
Bond lengths



Bond angles

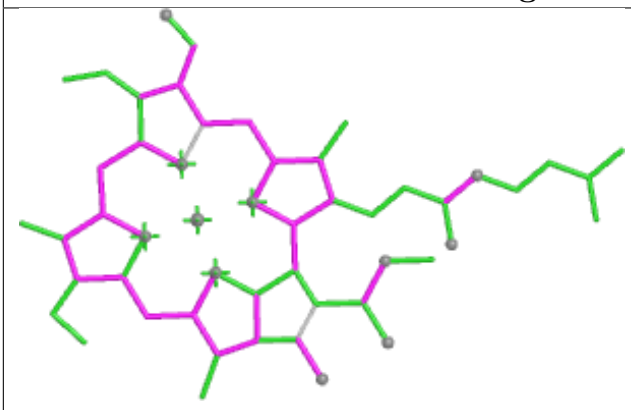


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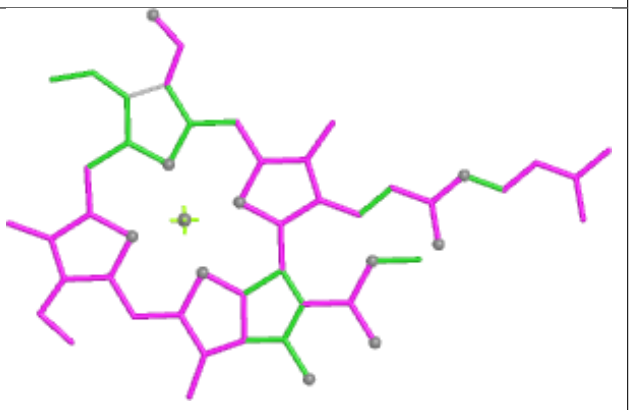


Rings

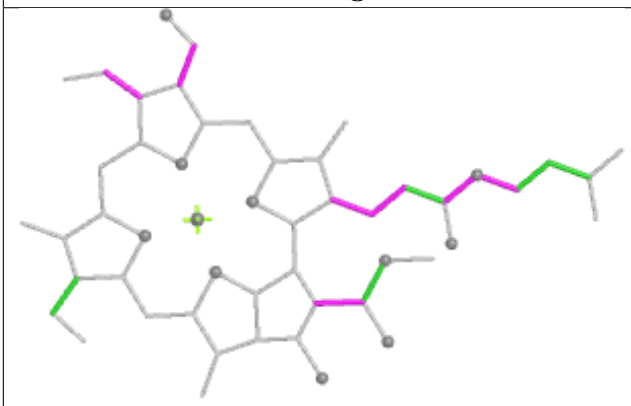
Ligand F6C aA 832



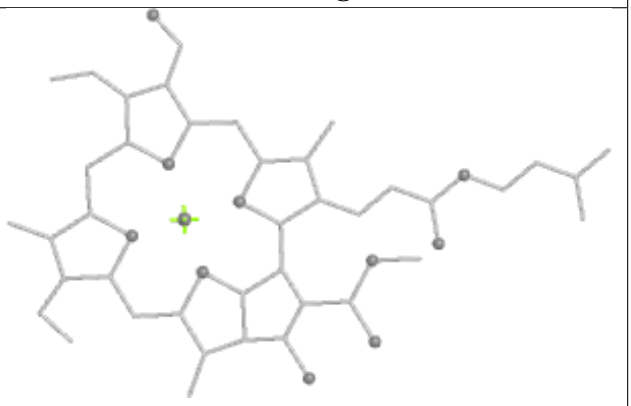
Bond lengths



Bond angles

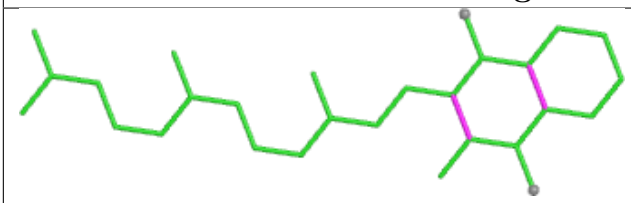


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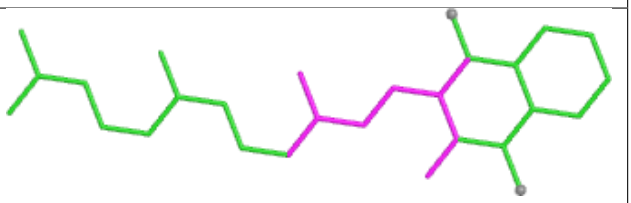


Rings

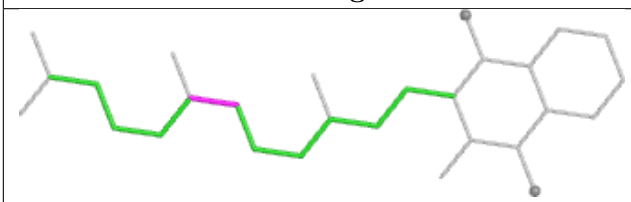
Ligand PQN cB 841



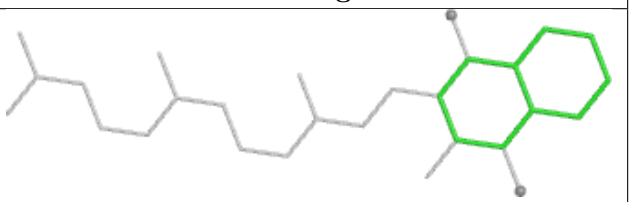
Bond lengths



Bond angles

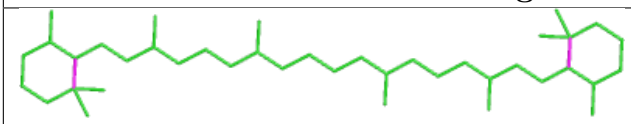


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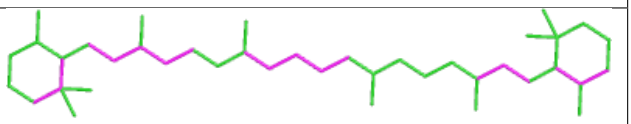


Rings

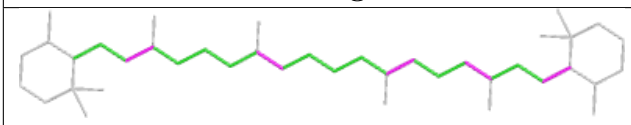
Ligand BCR aL 208



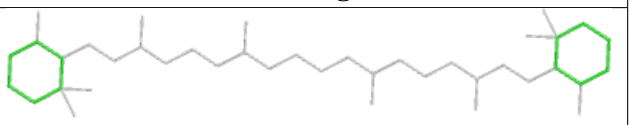
Bond lengths



Bond angles

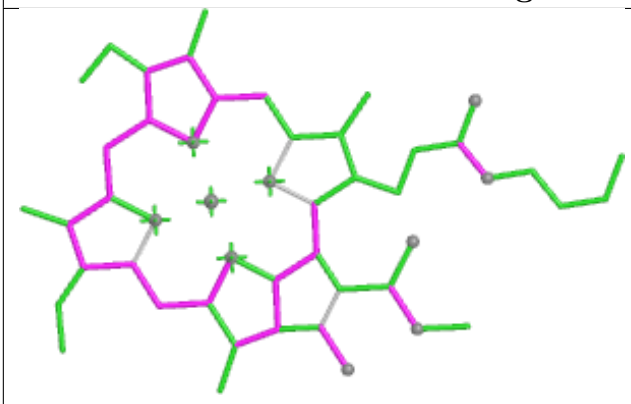


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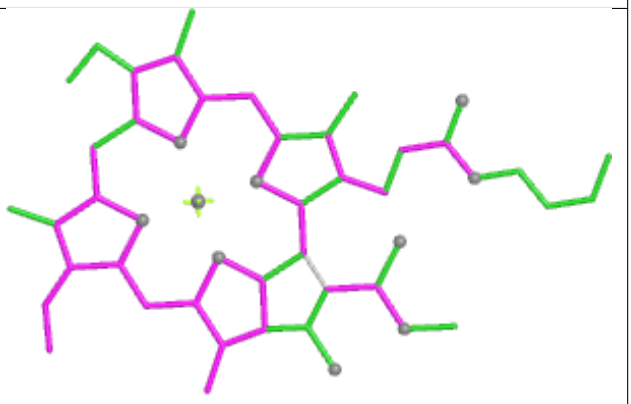


Rings

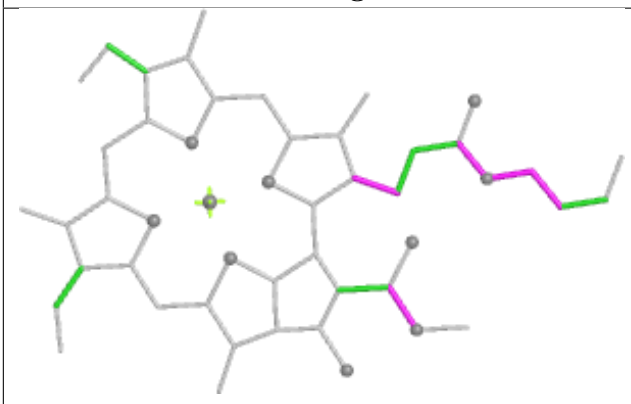
Ligand CLA cA 817



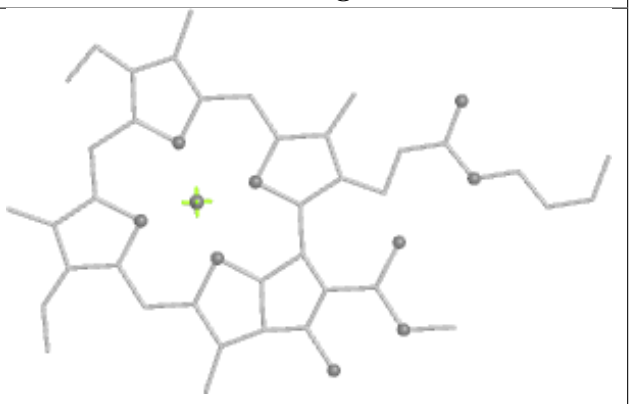
Bond lengths



Bond angles

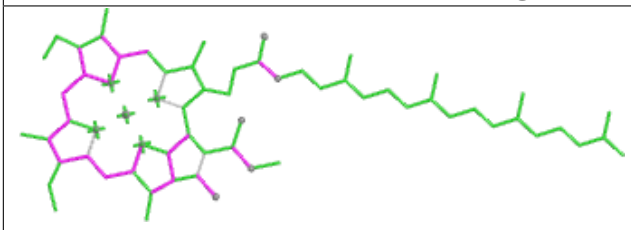


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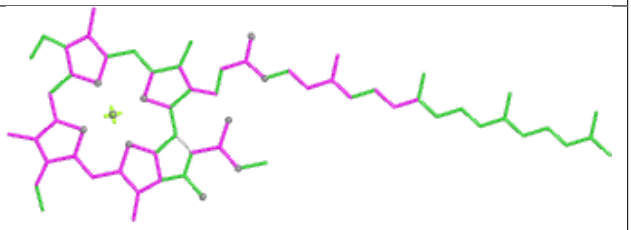


Rings

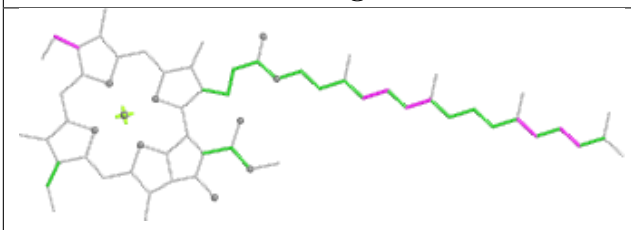
Ligand CLA bA 839



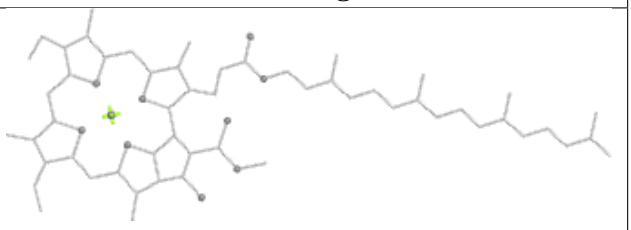
Bond lengths



Bond angles

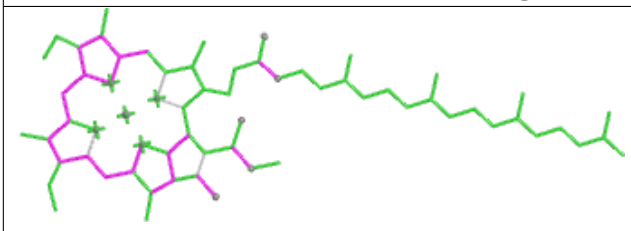


Torsions

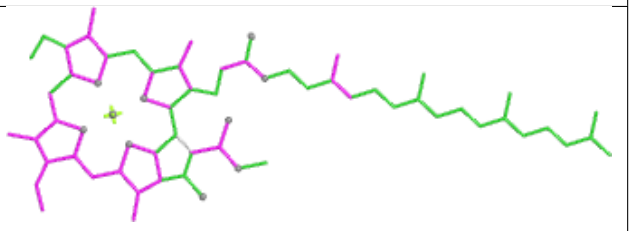


Rings

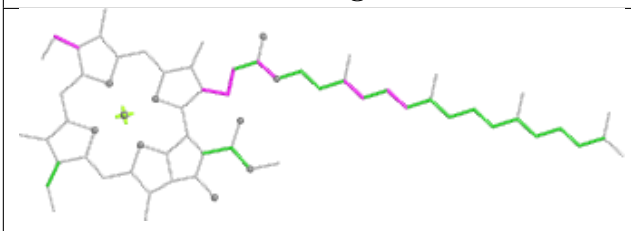
Ligand CLA aB 827



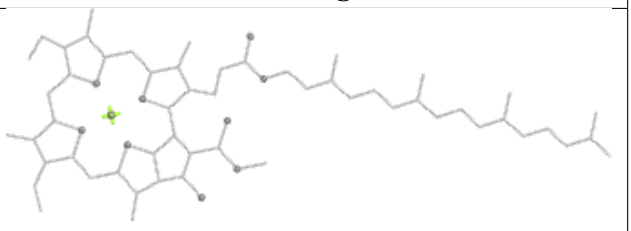
Bond lengths



Bond angles

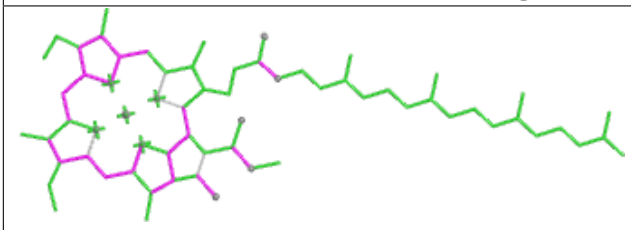


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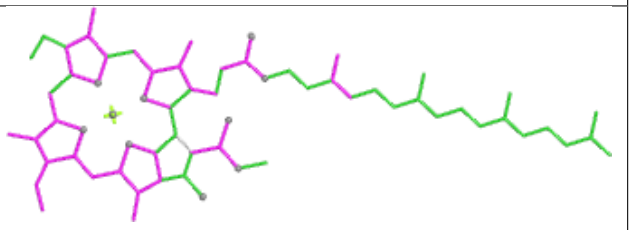


Rings

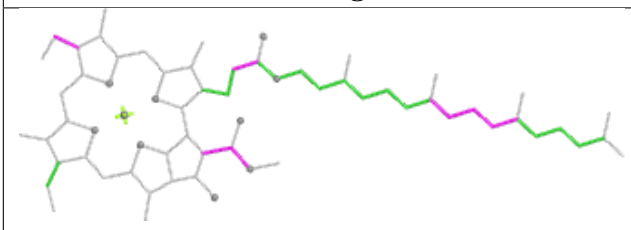
Ligand CLA aA 825



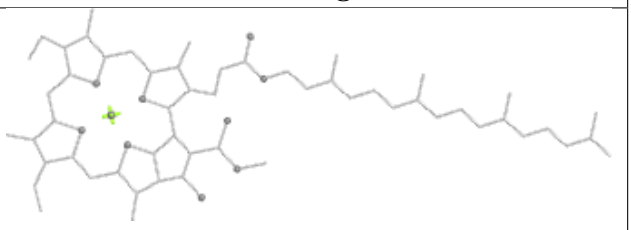
Bond lengths



Bond angles

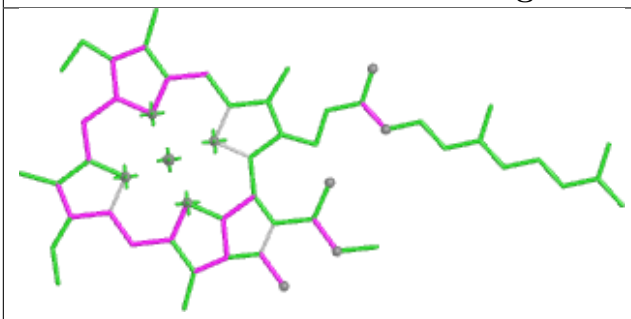


Torsions

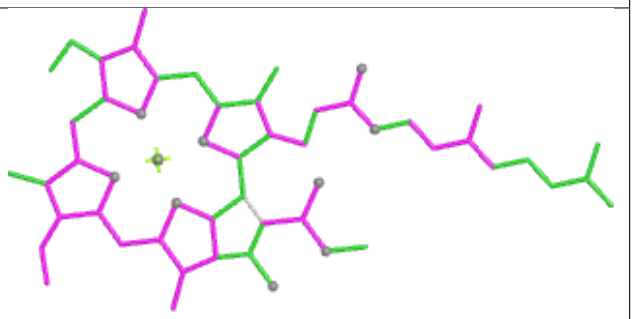


Rings

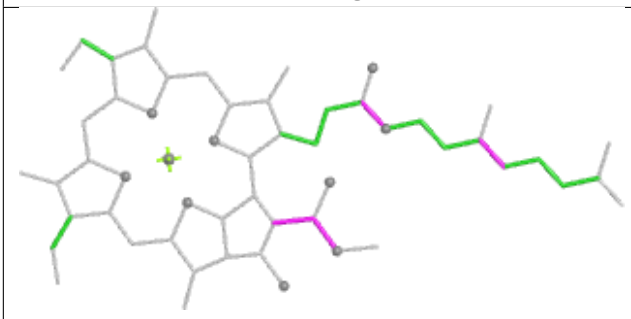
Ligand CLA cB 828



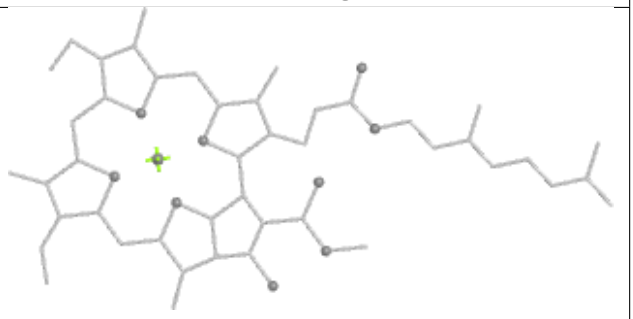
Bond lengths



Bond angles

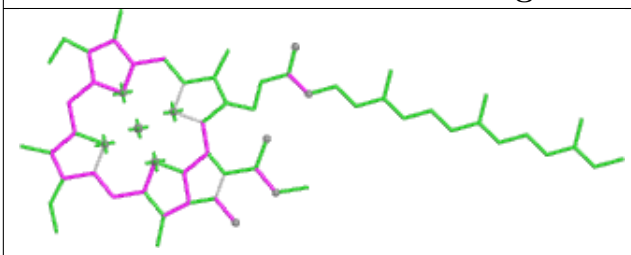


Torsions

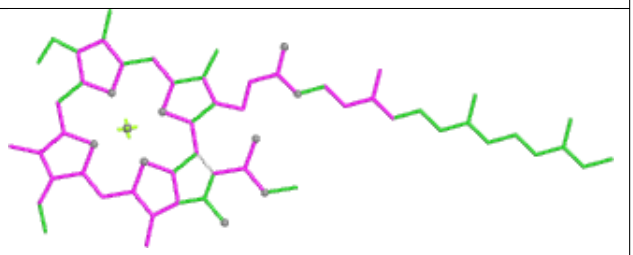


Rings

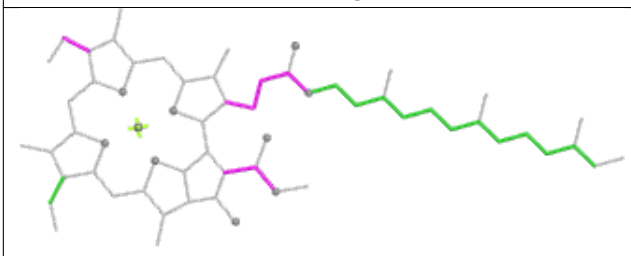
Ligand CLA aB 826



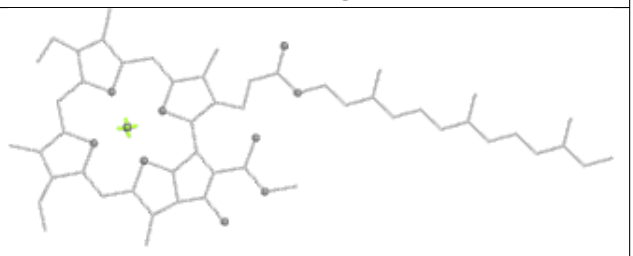
Bond lengths



Bond angles

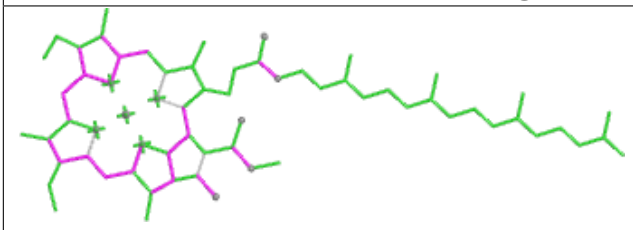


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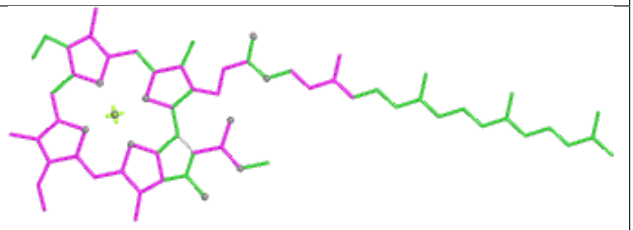


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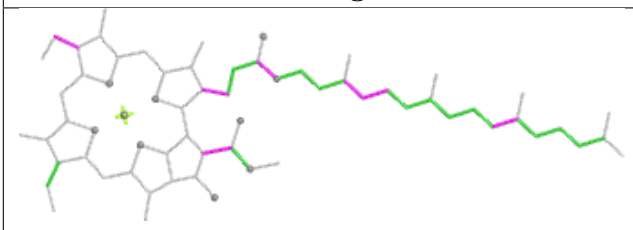
Ligand CLA cA 820



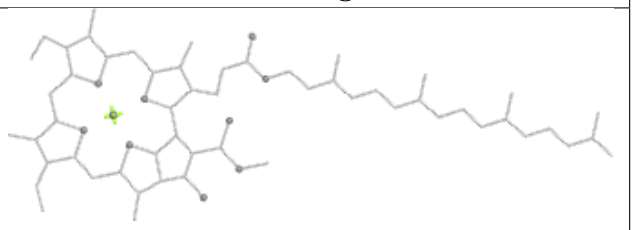
Bond lengths



Bond angles

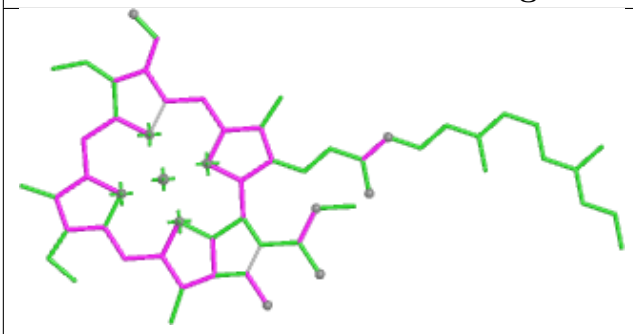


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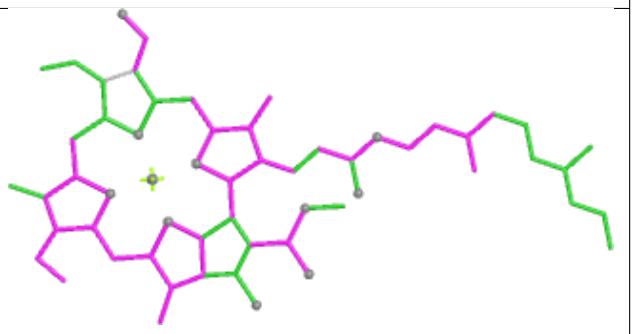


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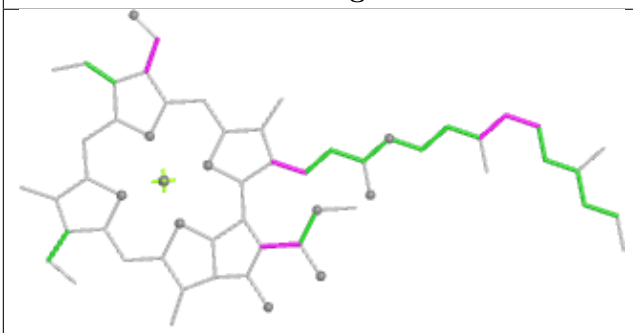
Ligand F6C aB 824



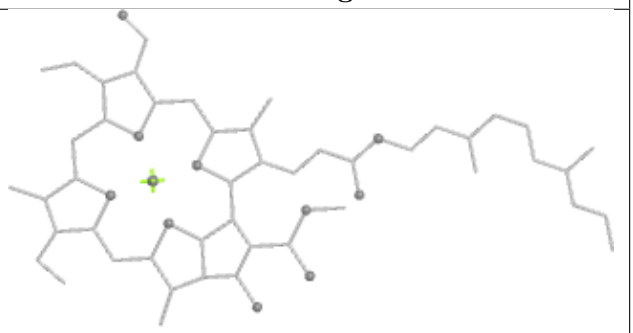
Bond lengths



Bond angles

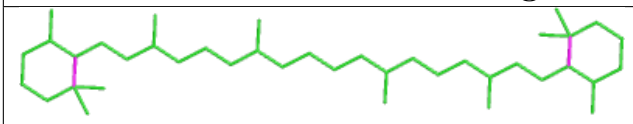


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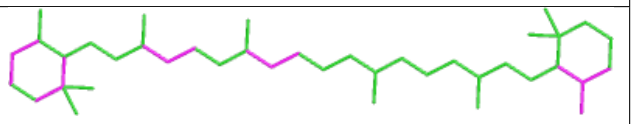


Rings

Ligand BCR cI 103



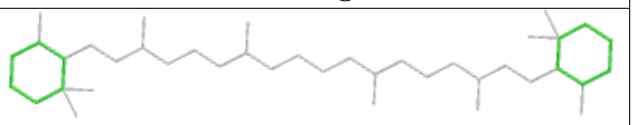
Bond lengths



Bond angles

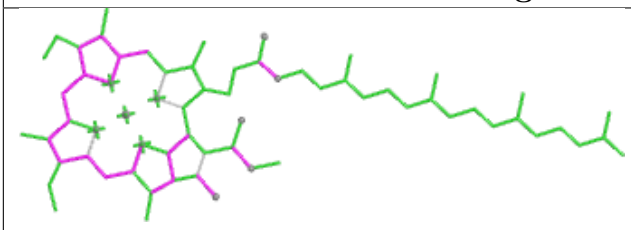


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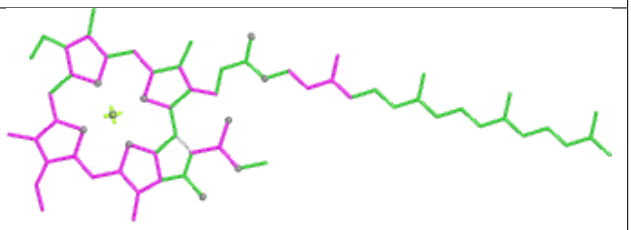


Rings

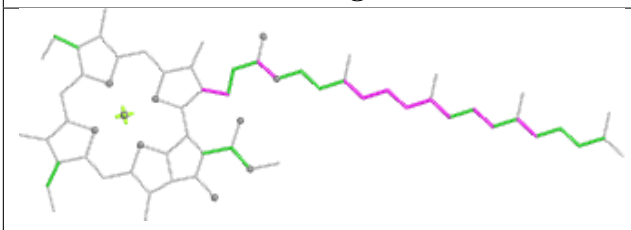
Ligand CLA aA 833



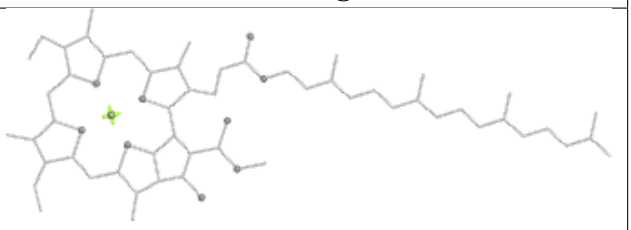
Bond lengths



Bond angles

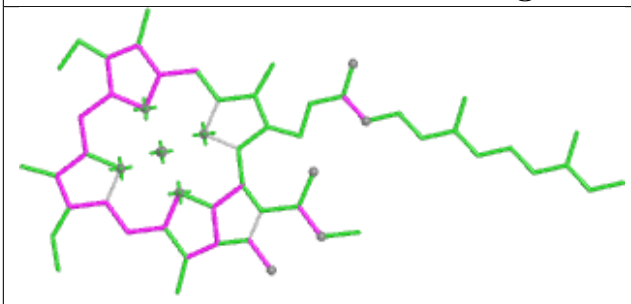


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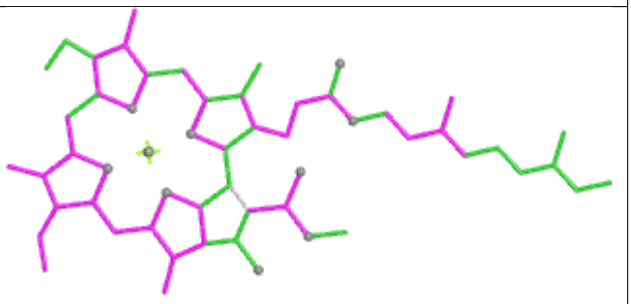


Rings

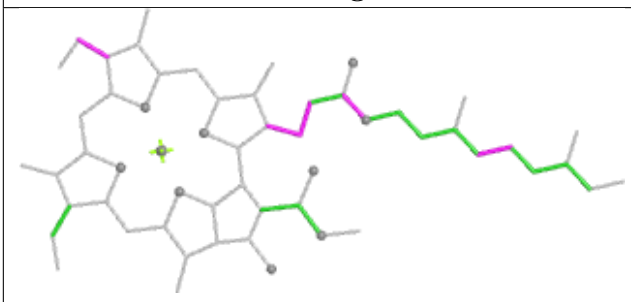
Ligand CLA cB 831



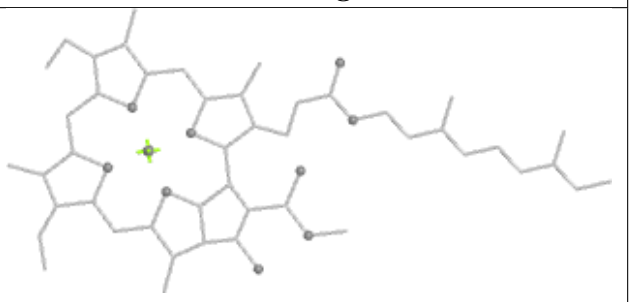
Bond lengths



Bond angles

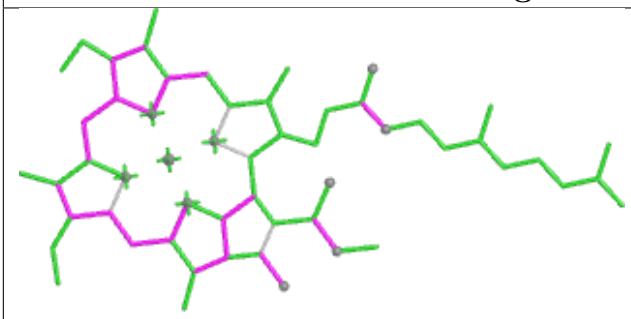


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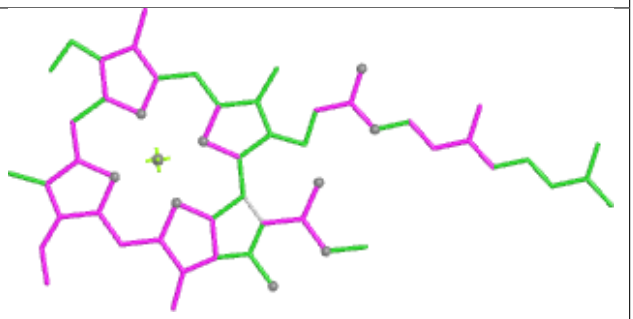


Rings

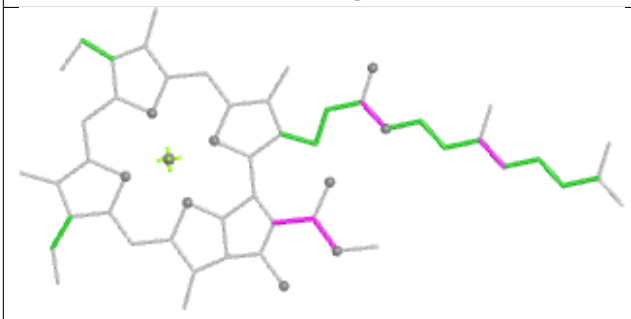
Ligand CLA bB 828



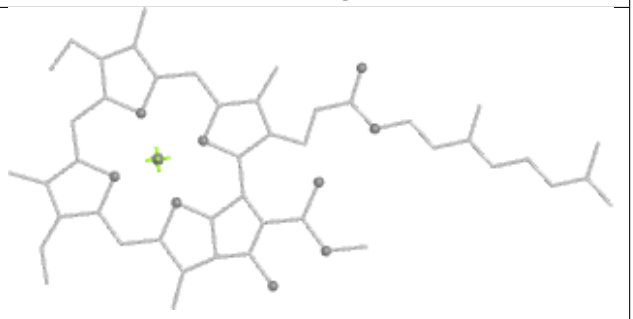
Bond lengths



Bond angles

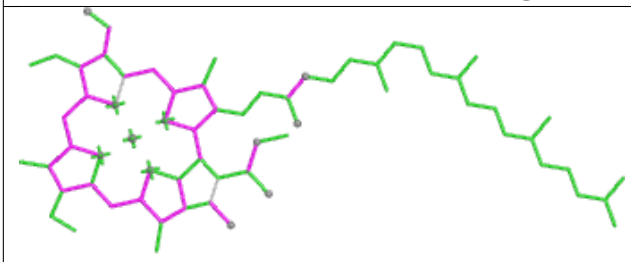


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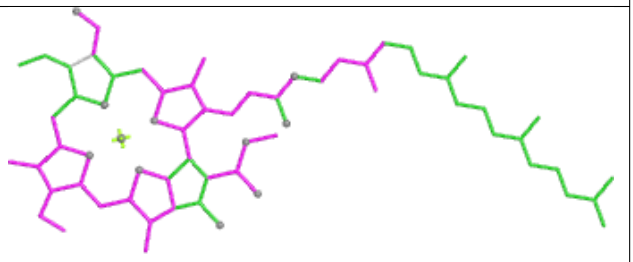


Rings

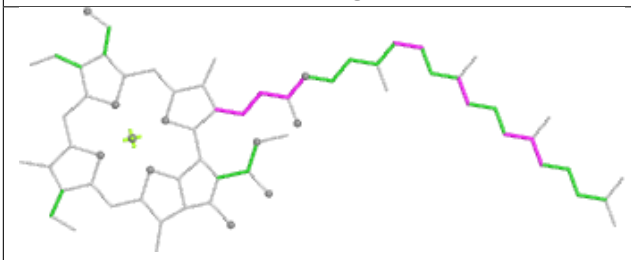
Ligand F6C bA 844



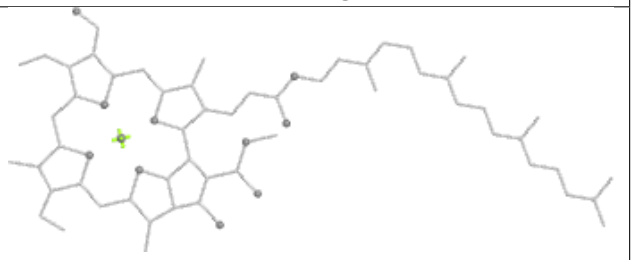
Bond lengths



Bond angles

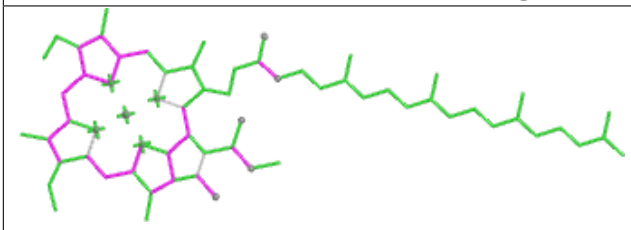


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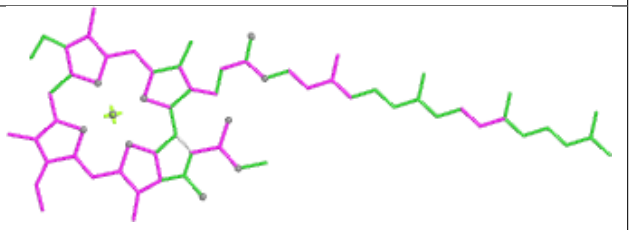


Rings

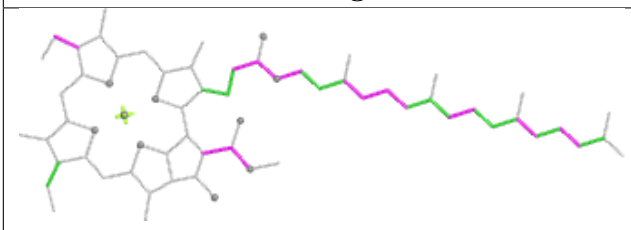
Ligand CLA aA 807



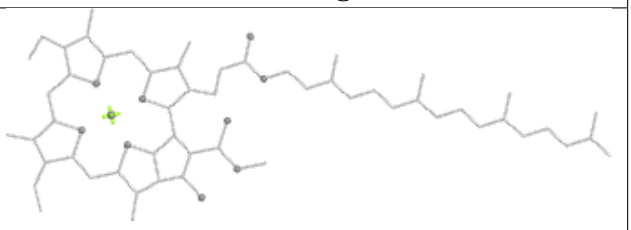
Bond lengths



Bond angles

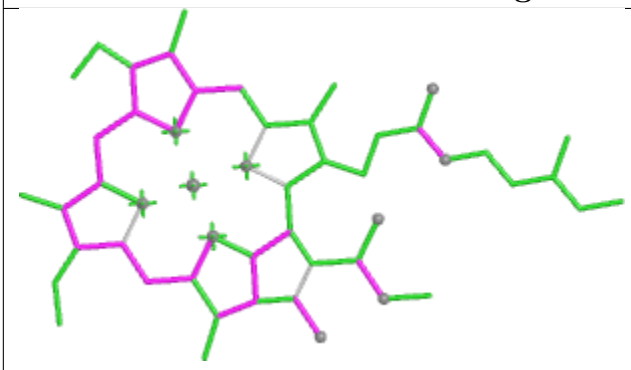


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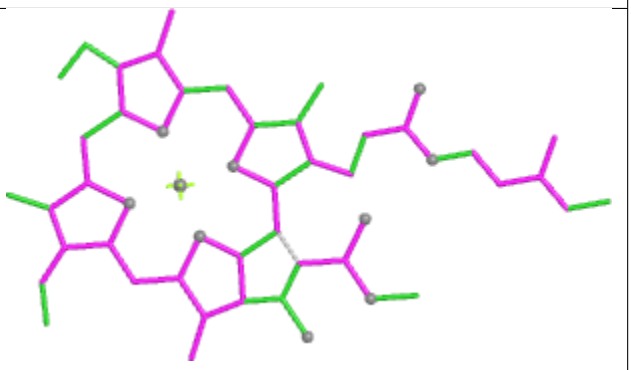


Rings

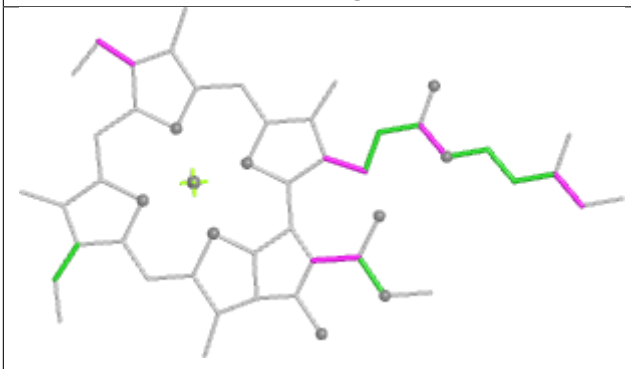
Ligand CLA bB 836



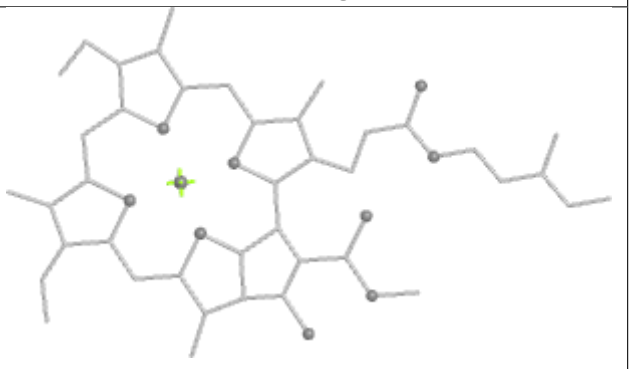
Bond lengths



Bond angles

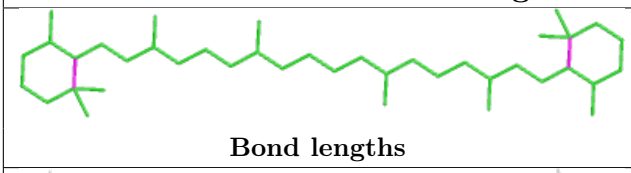


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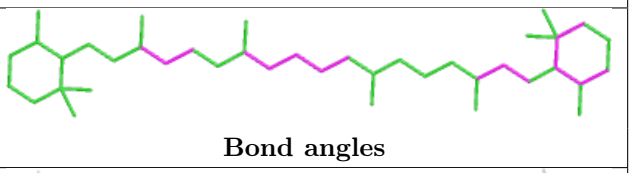


Rings

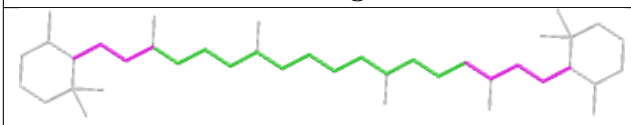
Ligand BCR bA 849



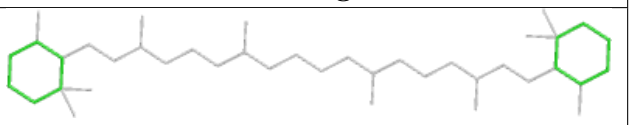
Bond lengths



Bond angles

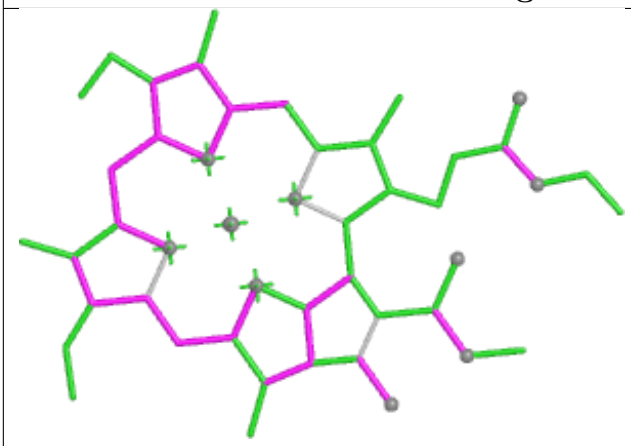


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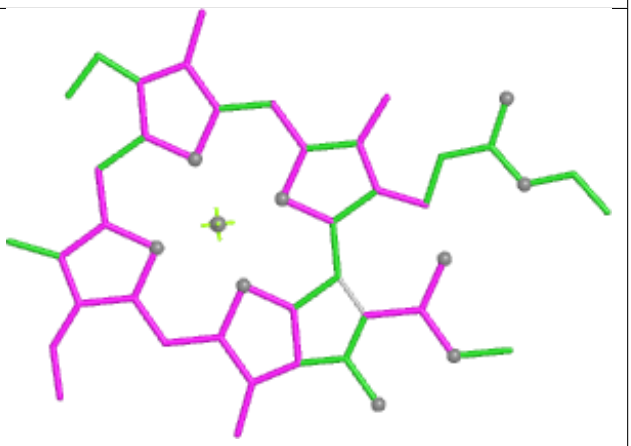


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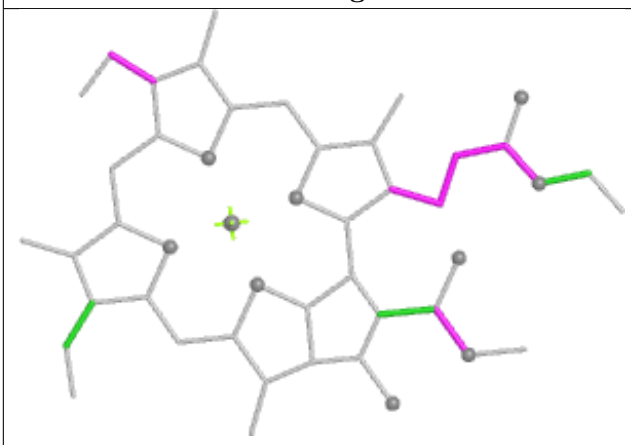
Ligand CLA cB 809



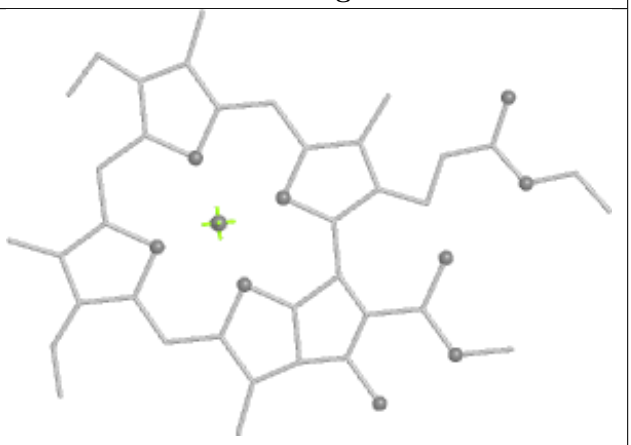
Bond lengths



Bond angles

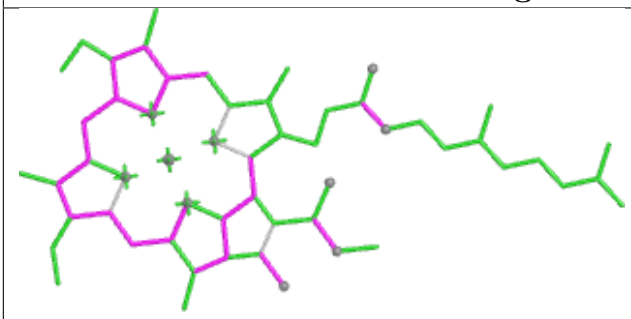


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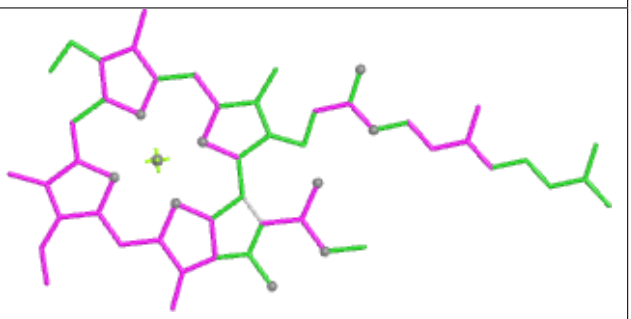


Rings

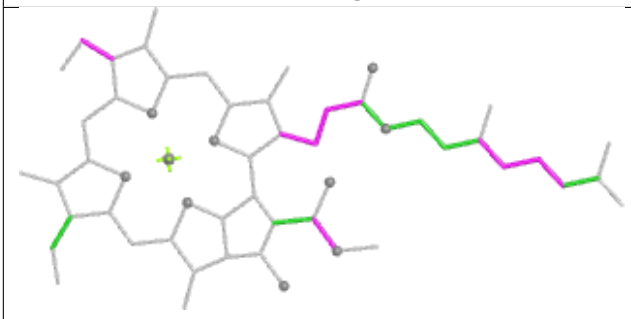
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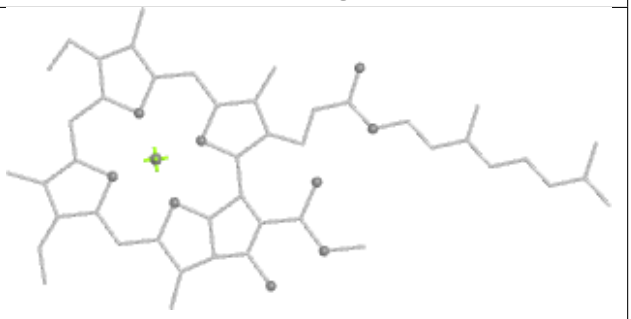
Bond lengths



Bond angles

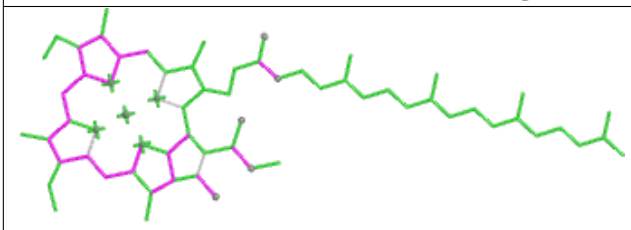


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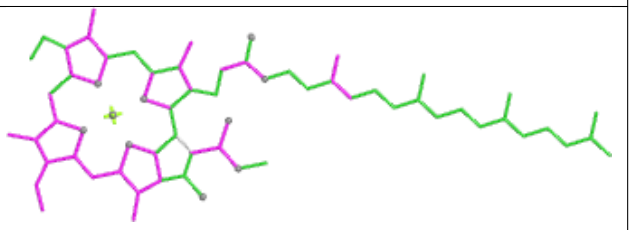


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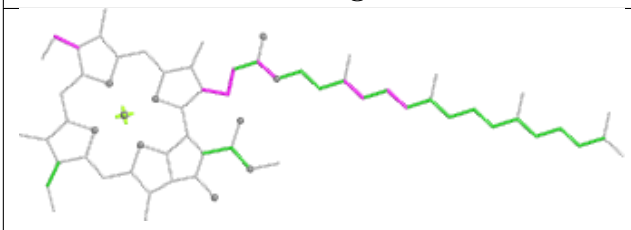
Ligand CLA cB 827



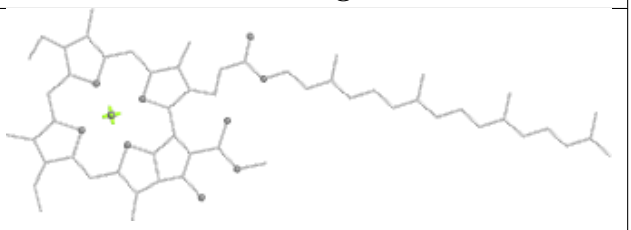
Bond lengths



Bond angles

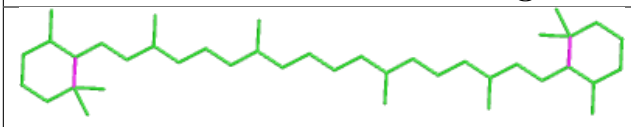


Torsions

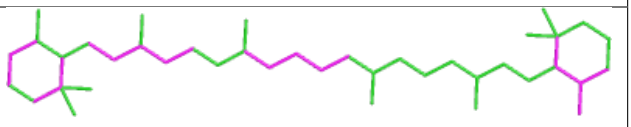


Rings

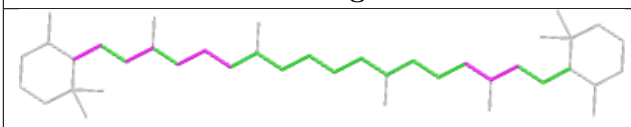
Ligand BCR cL 207



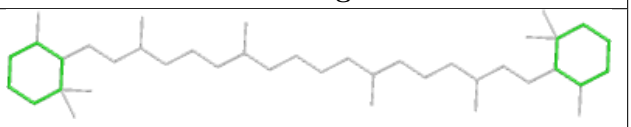
Bond lengths



Bond angles

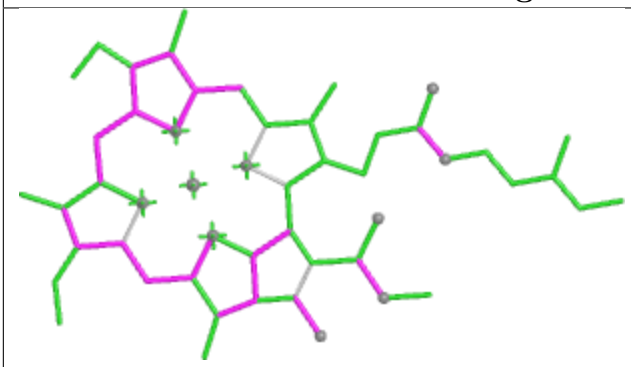


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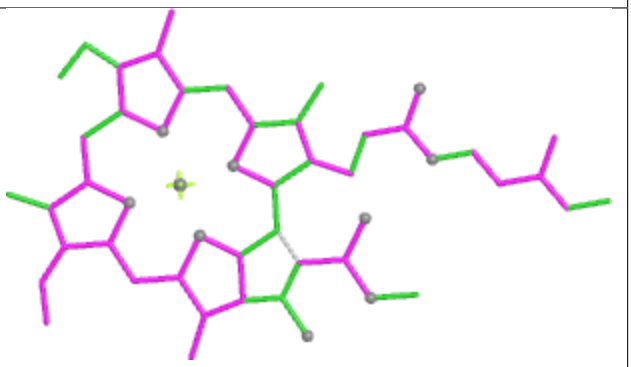


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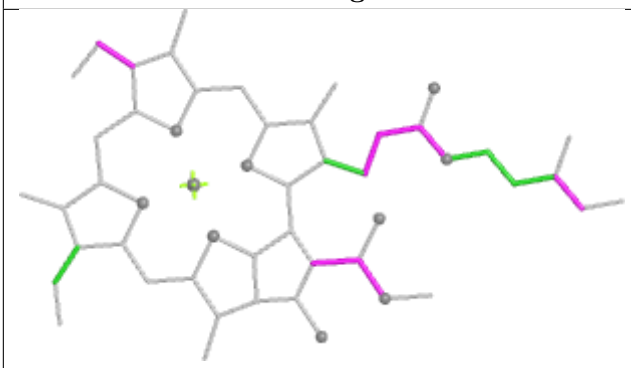
Ligand CLA cA 824



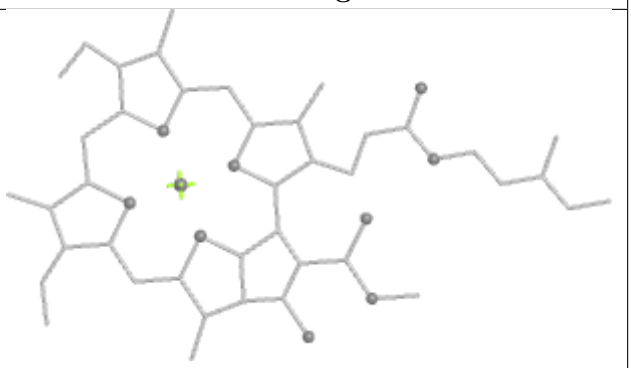
Bond lengths



Bond angles

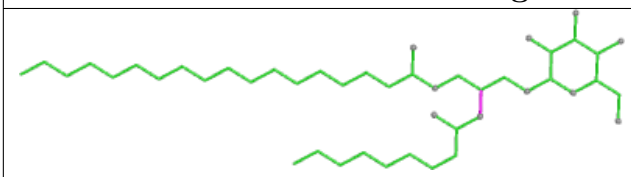


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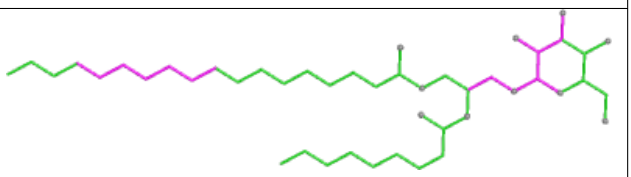


Rings

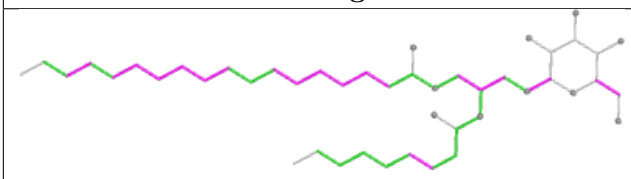
Ligand LMG aB 847



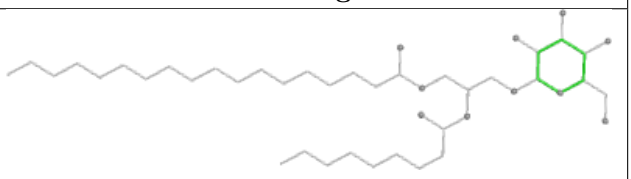
Bond lengths



Bond angles

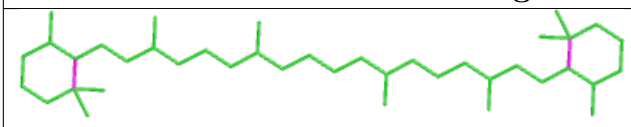


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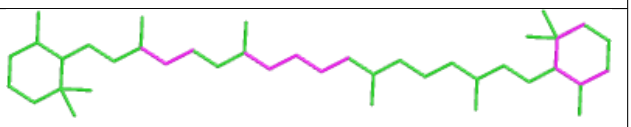


Rings

Ligand BCR aA 849



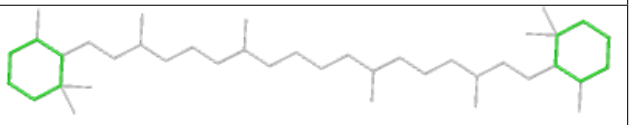
Bond lengths



Bond angles

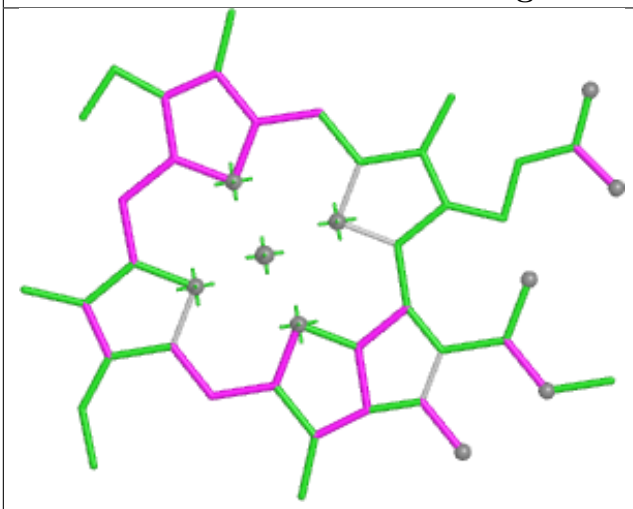


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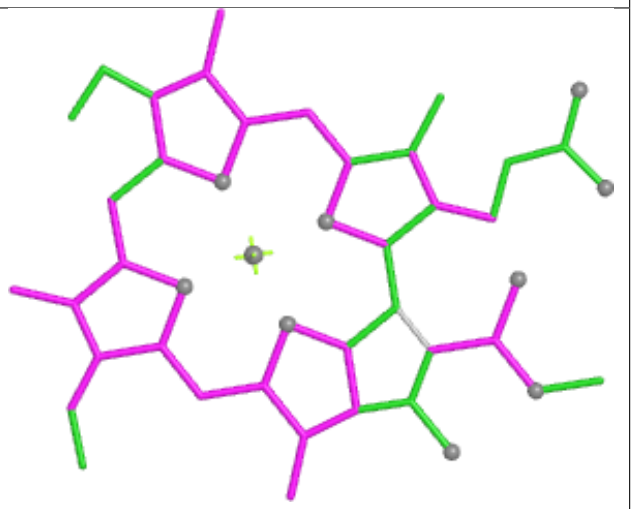


Rings

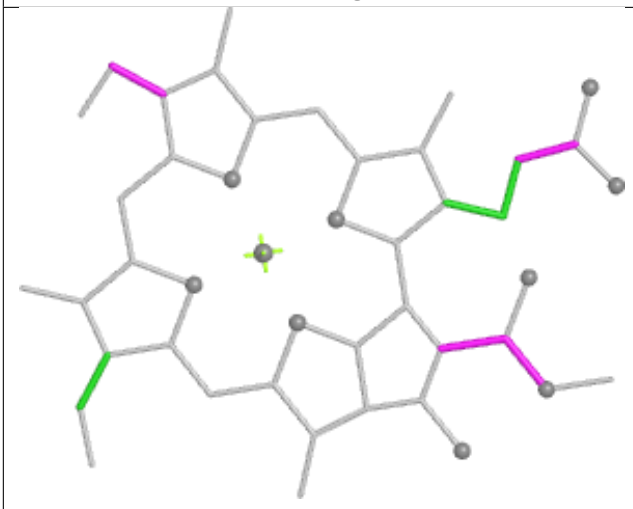
Ligand CLA cB 822



Bond lengths



Bond angles

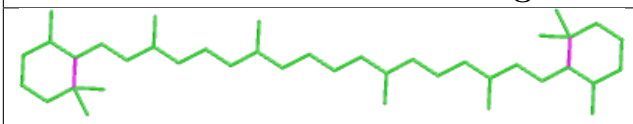


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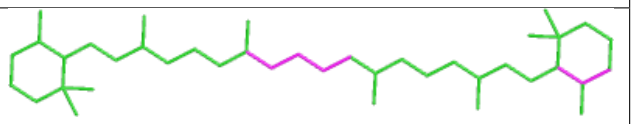


Rings

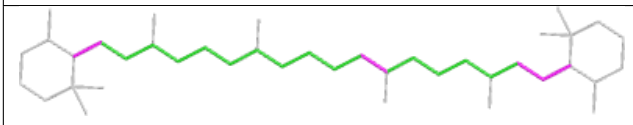
Ligand BCR cA 850



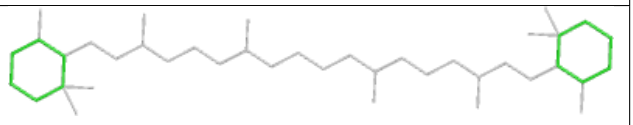
Bond lengths



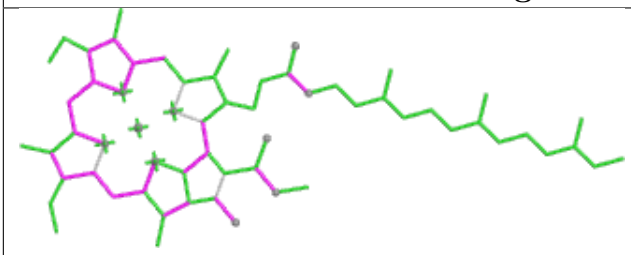
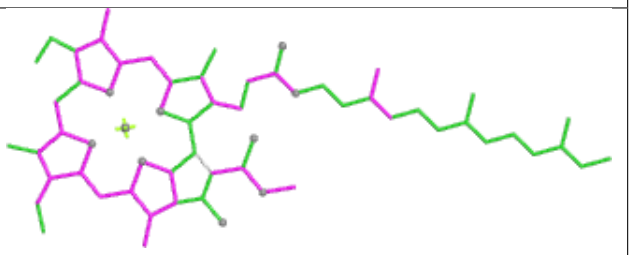
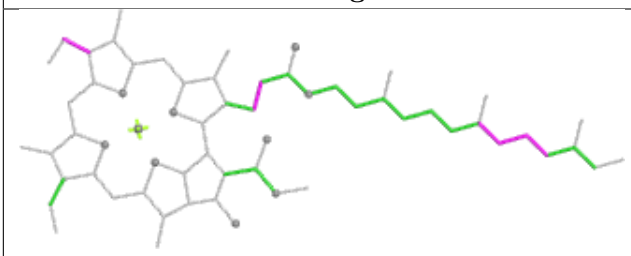
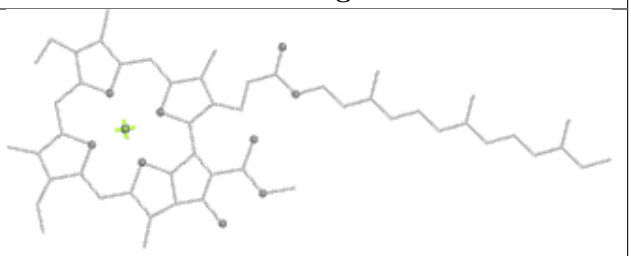
Bond angles

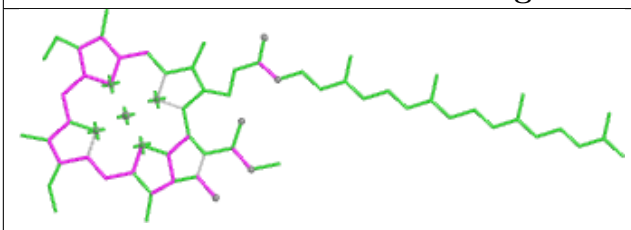
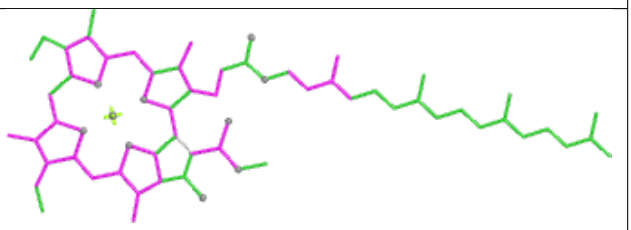
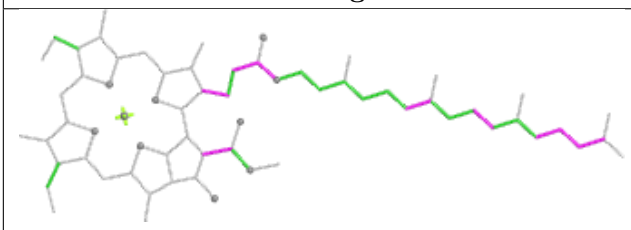
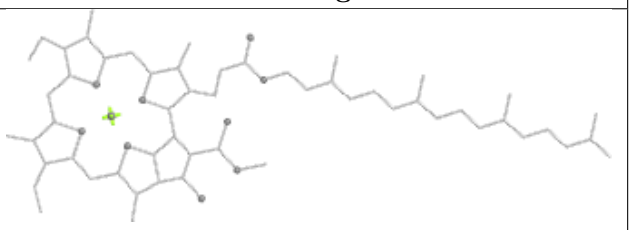


Torsions

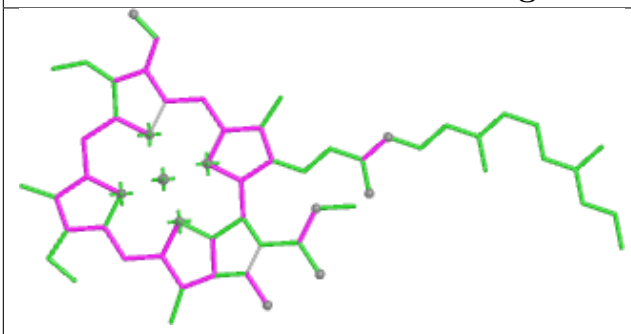


Rings

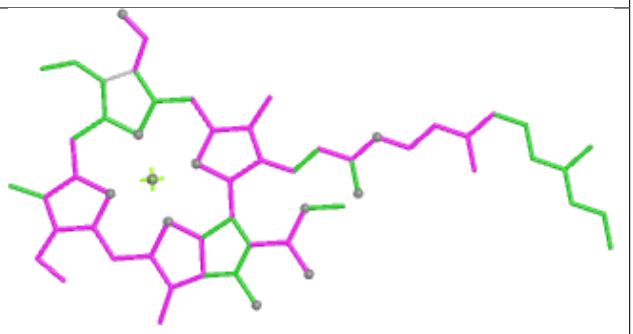
Ligand CLA bB 803	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA bB 805	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

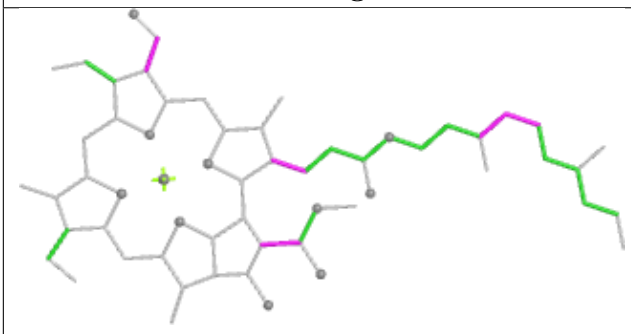
Ligand F6C bB 824



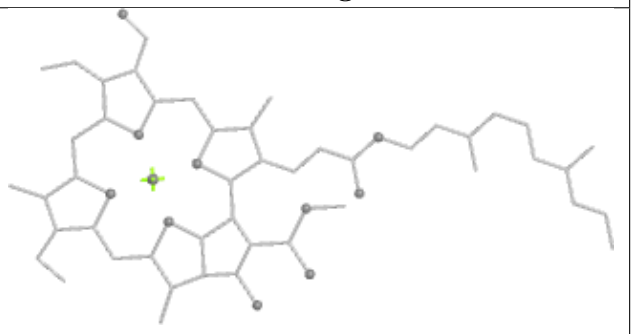
Bond lengths



Bond angles

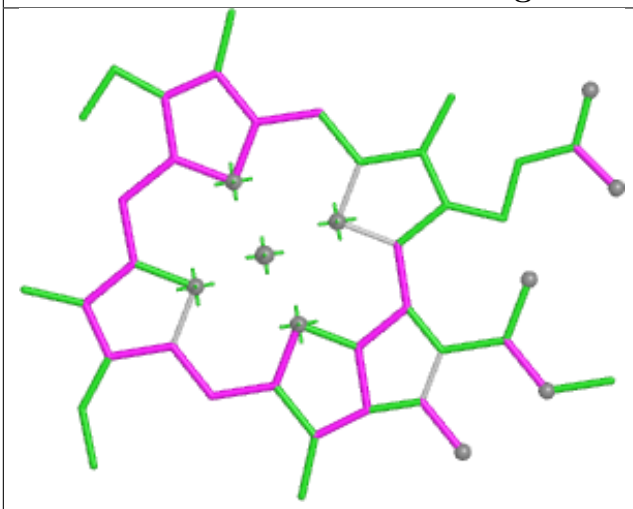


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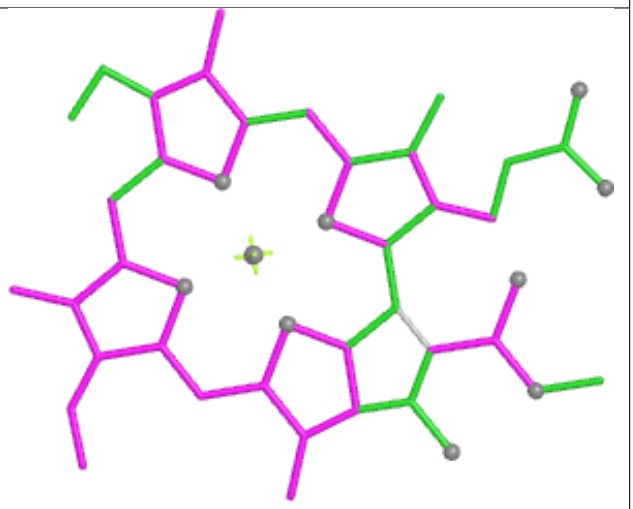


Rings

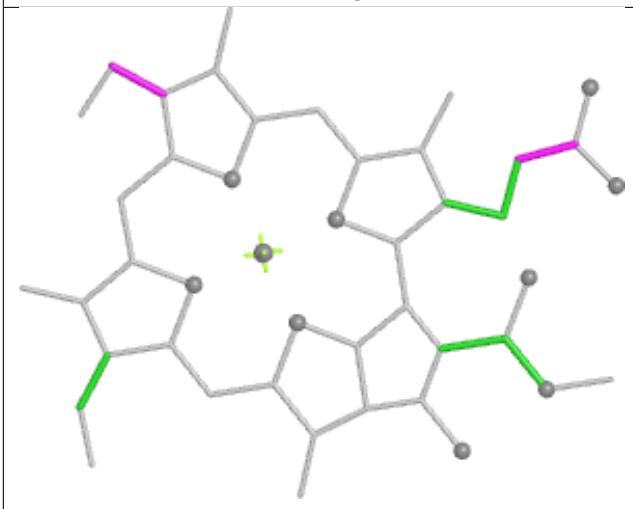
Ligand CLA bB 835



Bond lengths



Bond angles

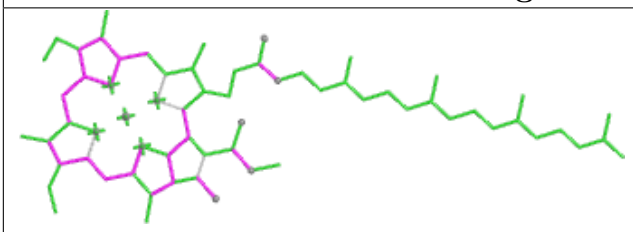


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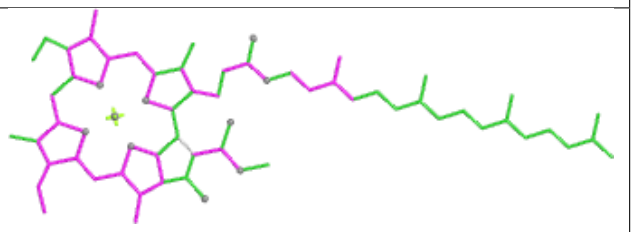


Rings

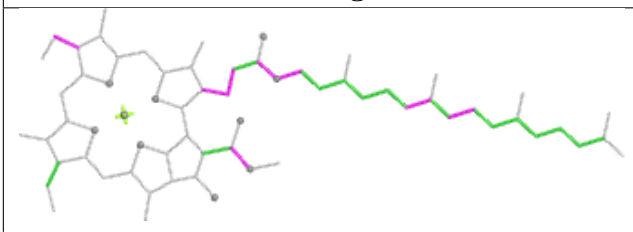
Ligand CLA cA 812



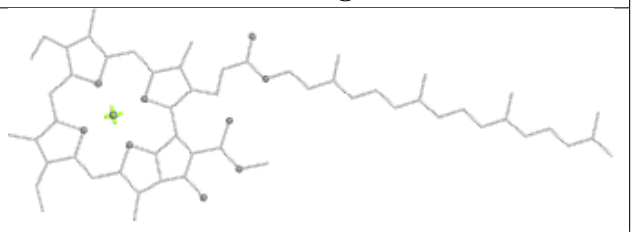
Bond lengths



Bond angles

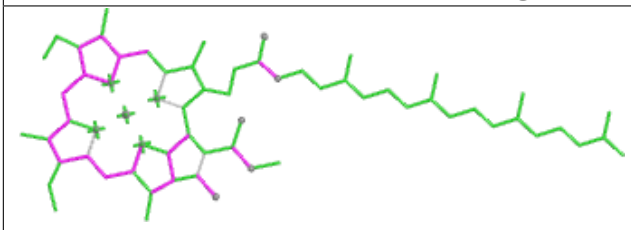


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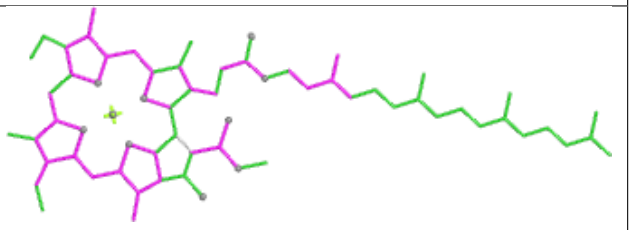


Rings

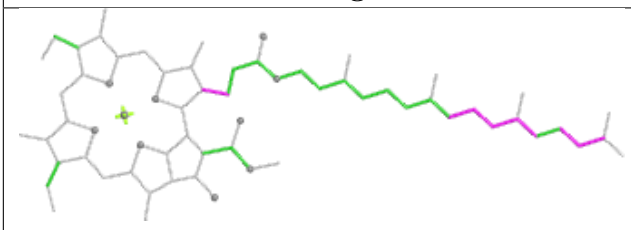
Ligand CLA bB 825



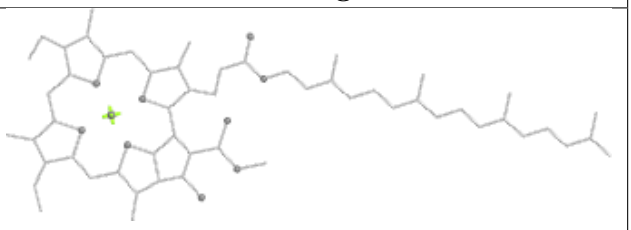
Bond lengths



Bond angles

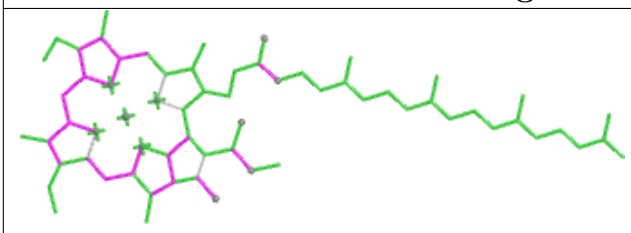


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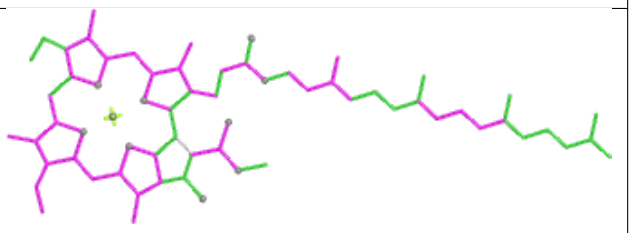


Rings

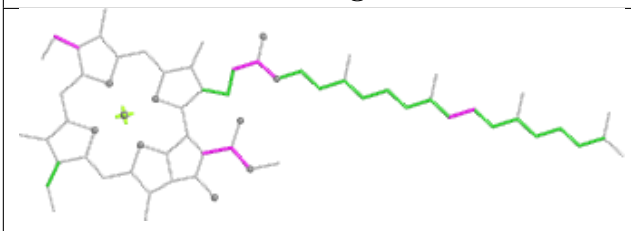
Ligand CLA cB 801



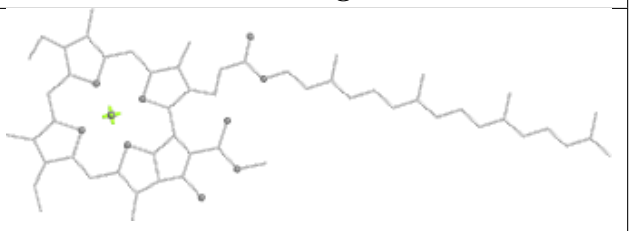
Bond lengths



Bond angles

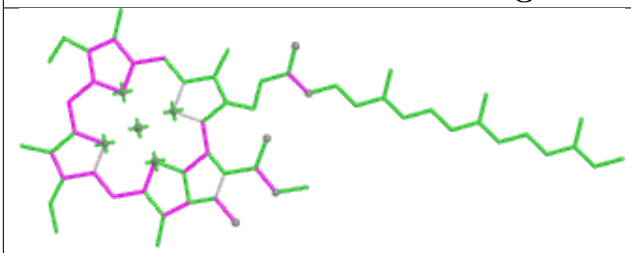


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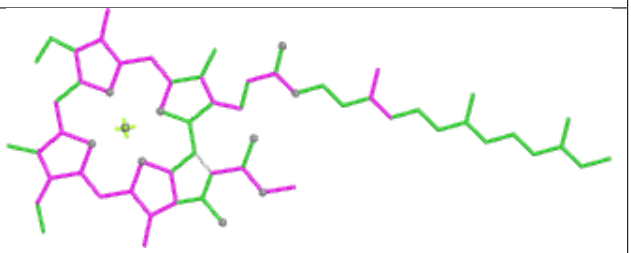


Rings

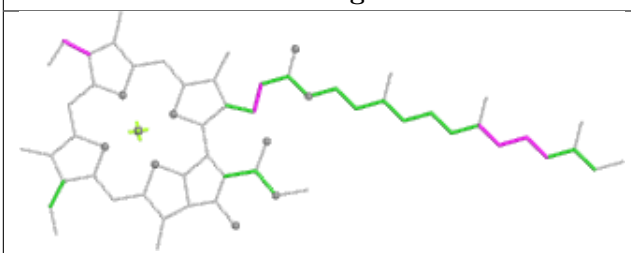
Ligand CLA aB 803



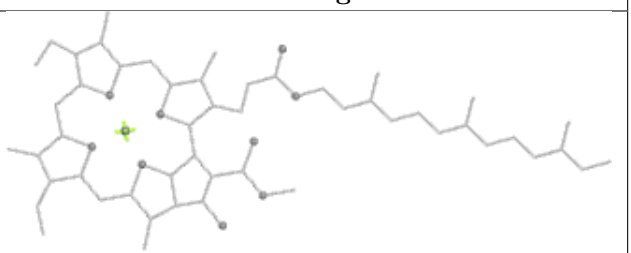
Bond lengths



Bond angles

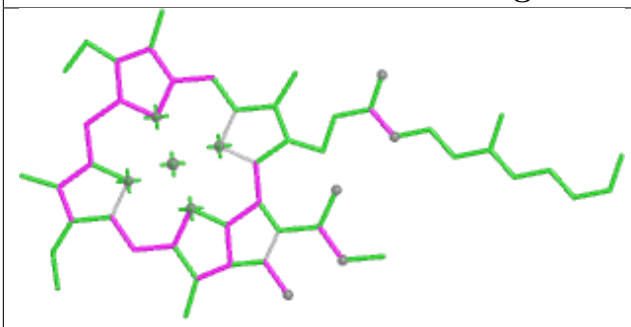


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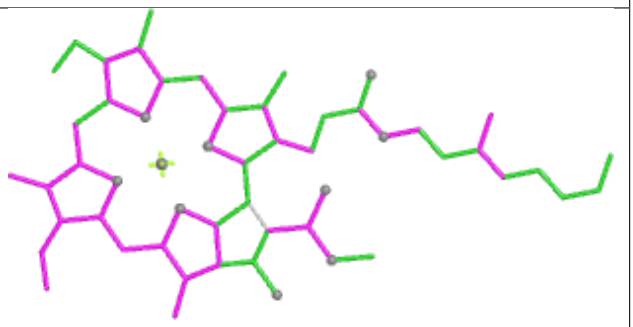


Rings

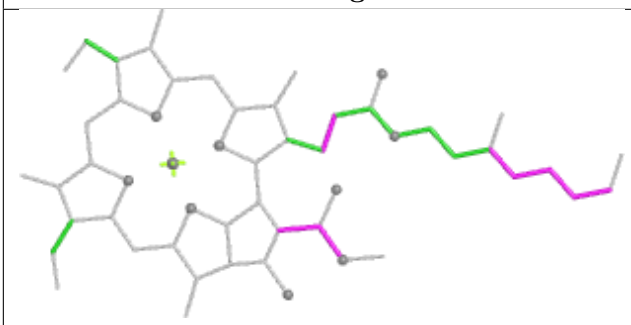
Ligand CLA bA 818



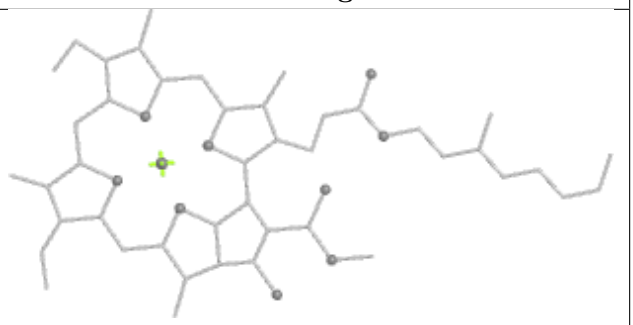
Bond lengths



Bond angles



Torsions

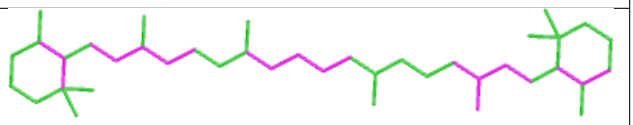


Rings

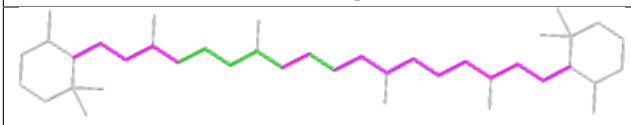
Ligand BCR bA 851



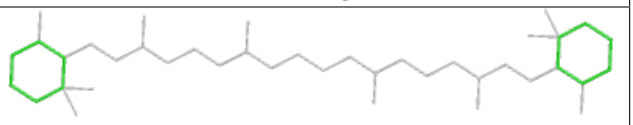
Bond lengths



Bond angles

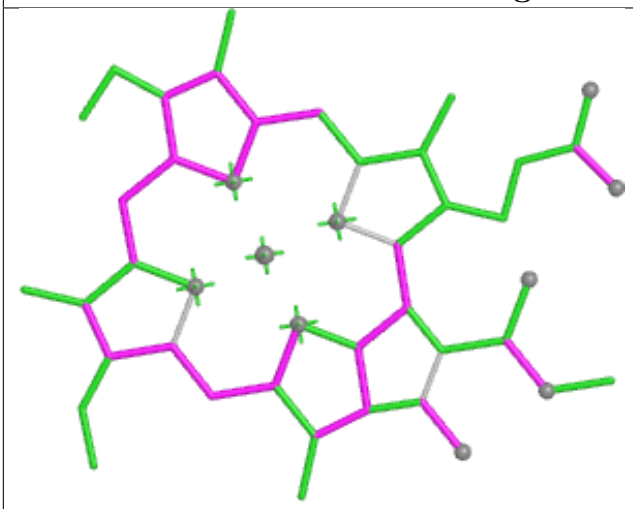


Torsions

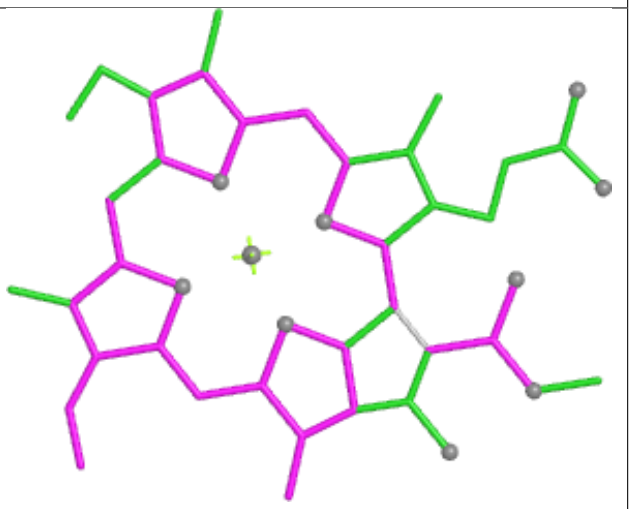


Rings

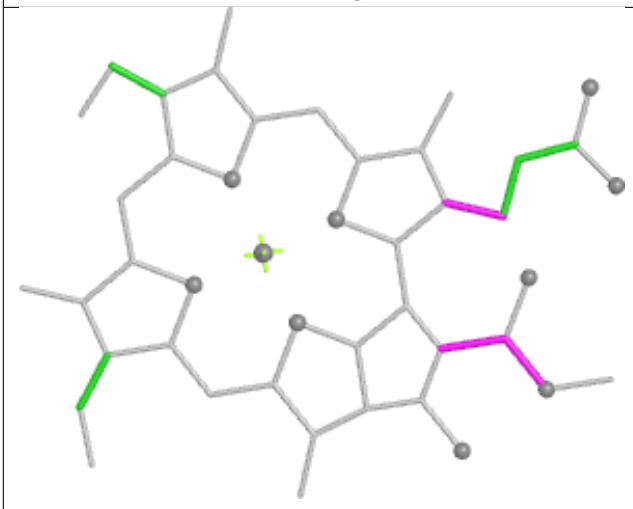
Ligand CLA bA 815



Bond lengths



Bond angles

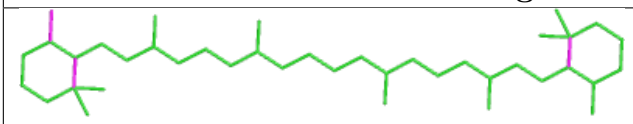


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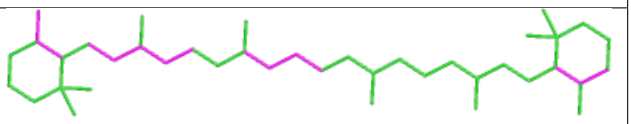


Rings

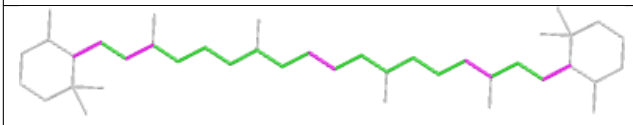
Ligand BCR aL 203



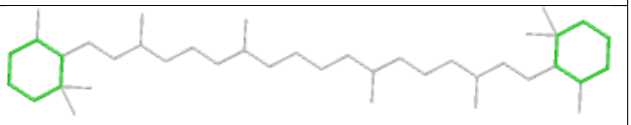
Bond lengths



Bond angles

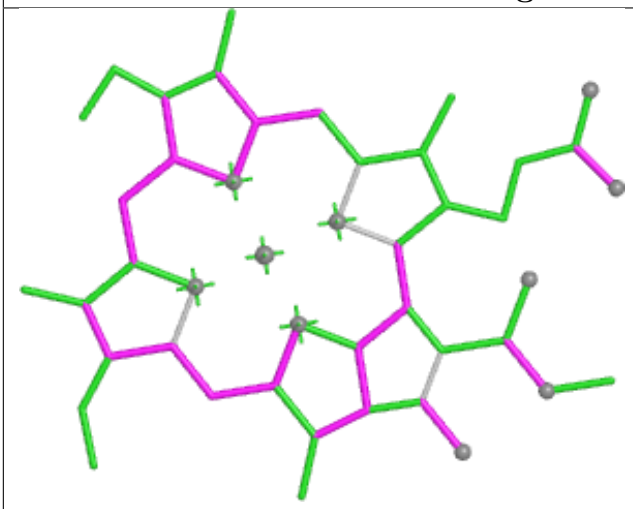


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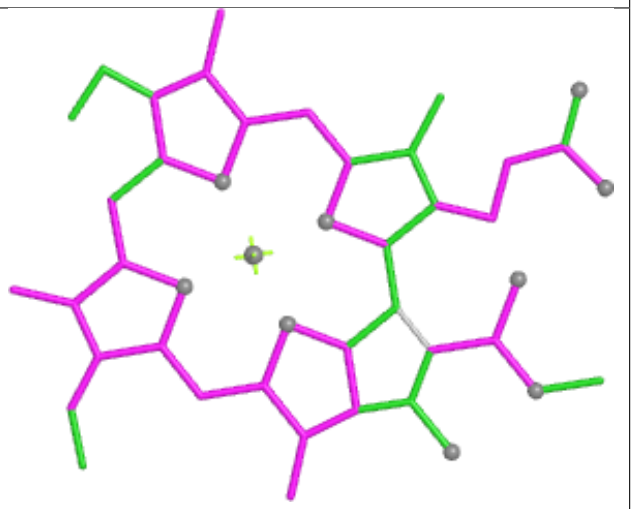


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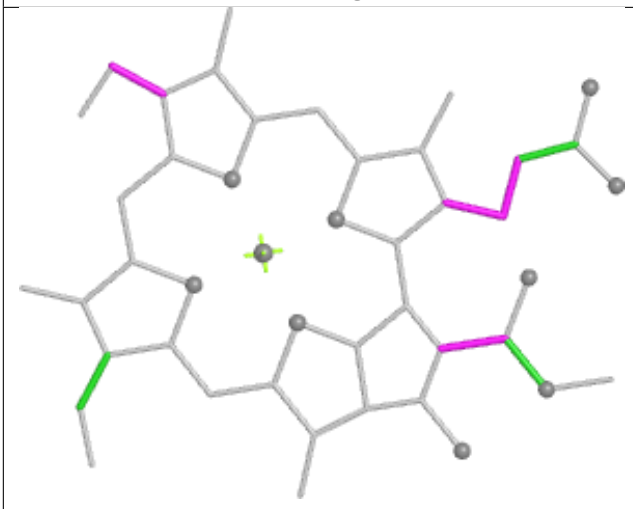
Ligand CLA cB 829



Bond lengths



Bond angles

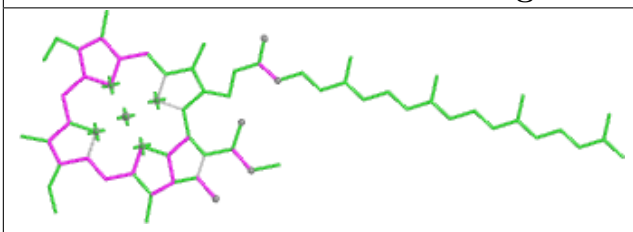


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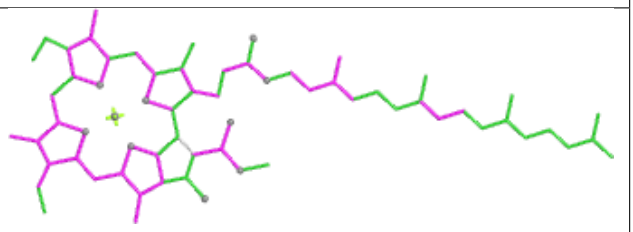


Rings

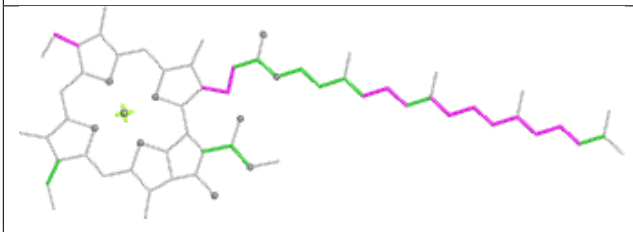
Ligand CLA bL 206



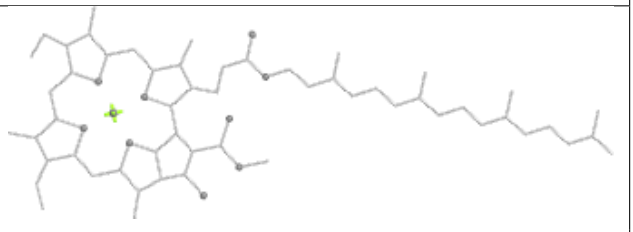
Bond lengths



Bond angles

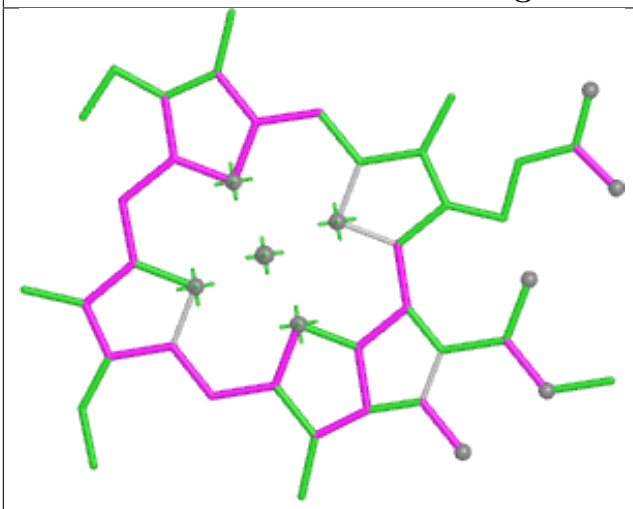


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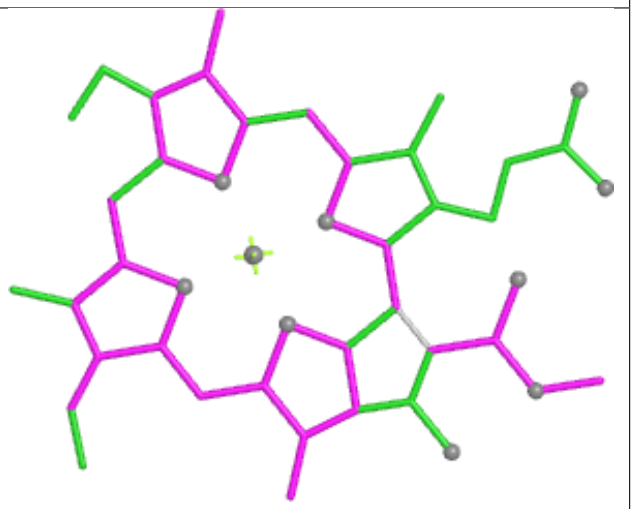


Rings

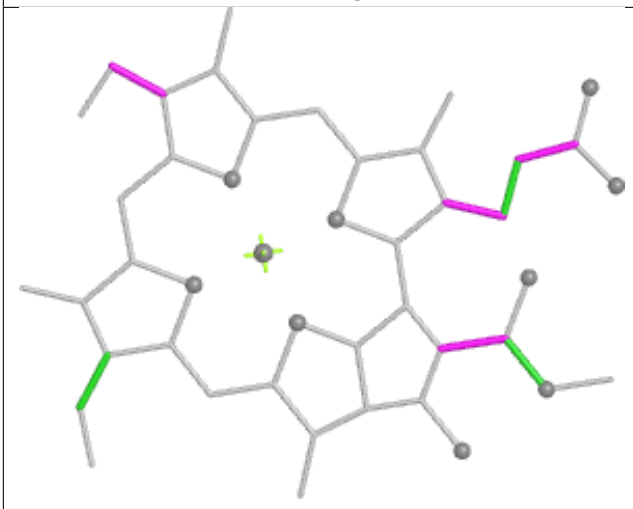
Ligand CLA bB 834



Bond lengths



Bond angles

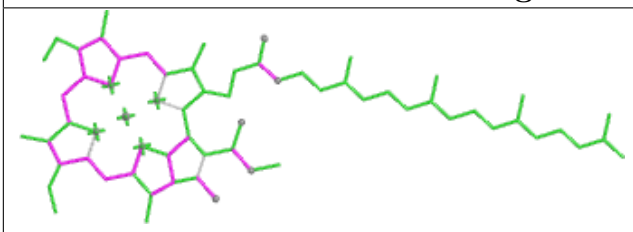


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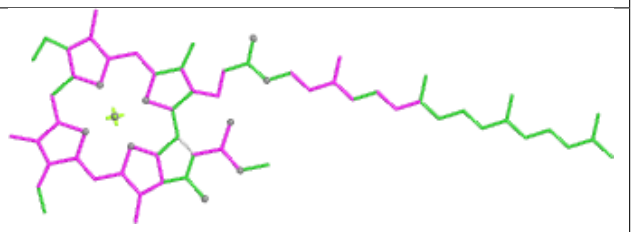


Rings

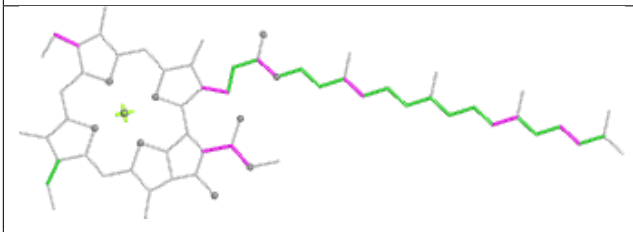
Ligand CLA aA 806



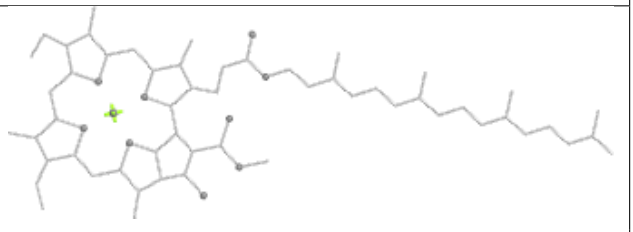
Bond lengths



Bond angles

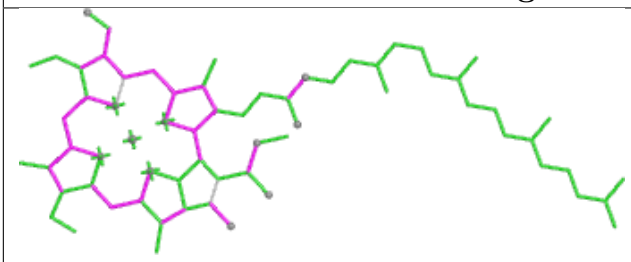


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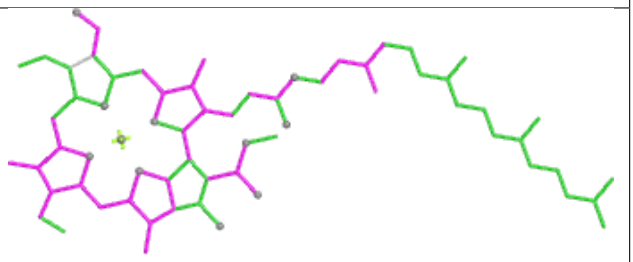


Rings

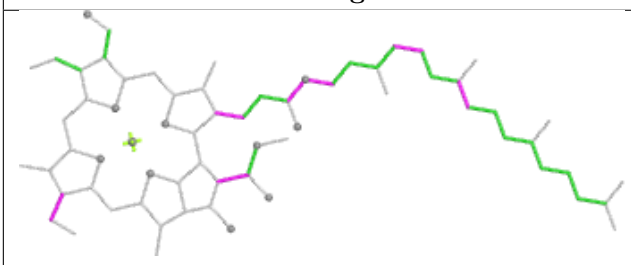
Ligand F6C bA 826



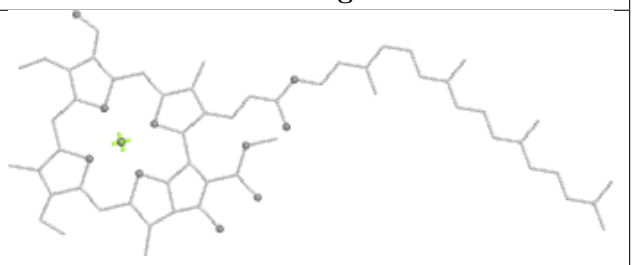
Bond lengths



Bond angles

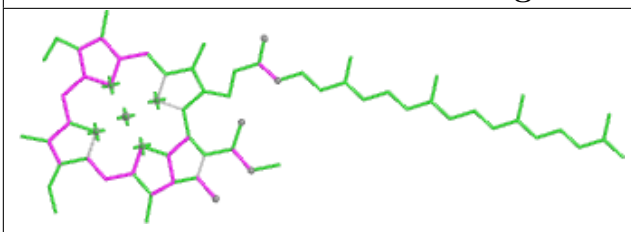


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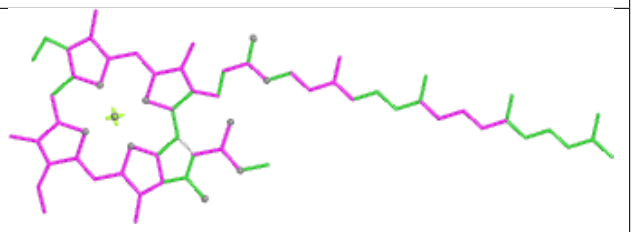


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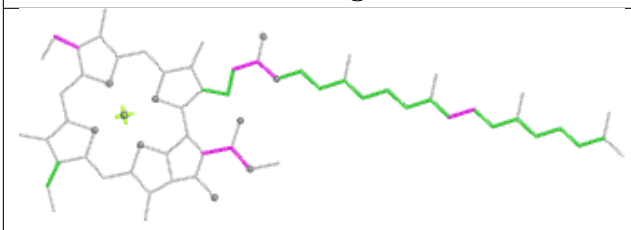
Ligand CLA bB 801



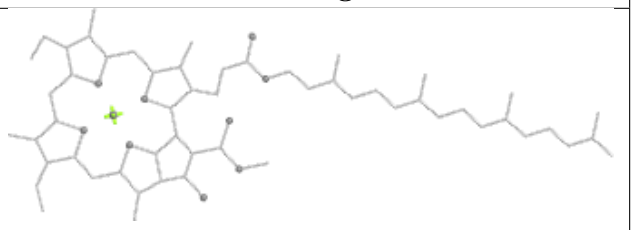
Bond lengths



Bond angles

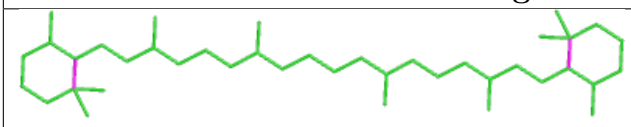


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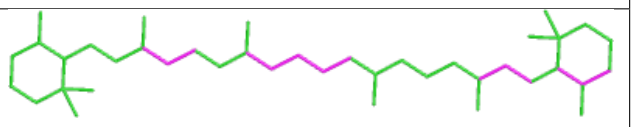


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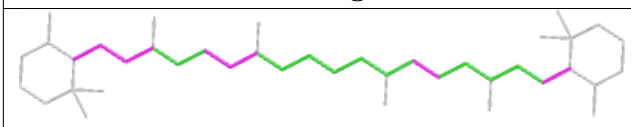
Ligand BCR bB 845



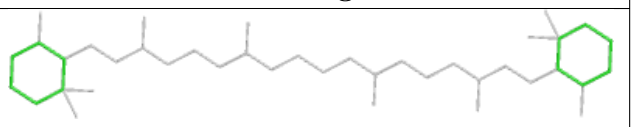
Bond lengths



Bond angles

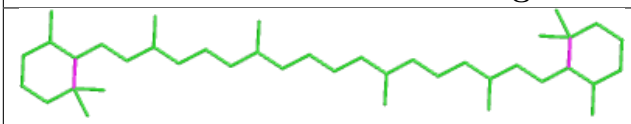


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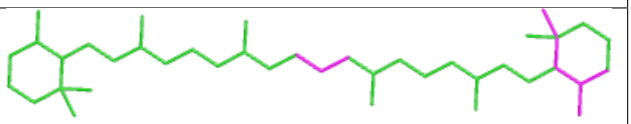


Rings

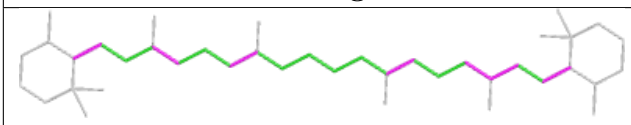
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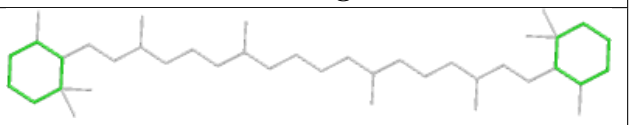
Bond lengths



Bond angles

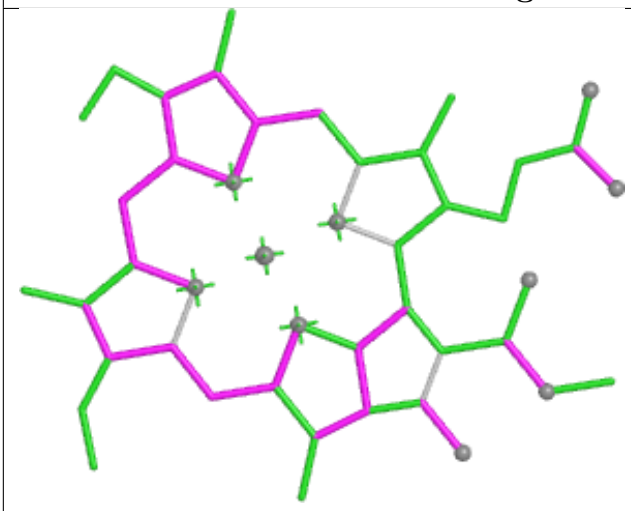


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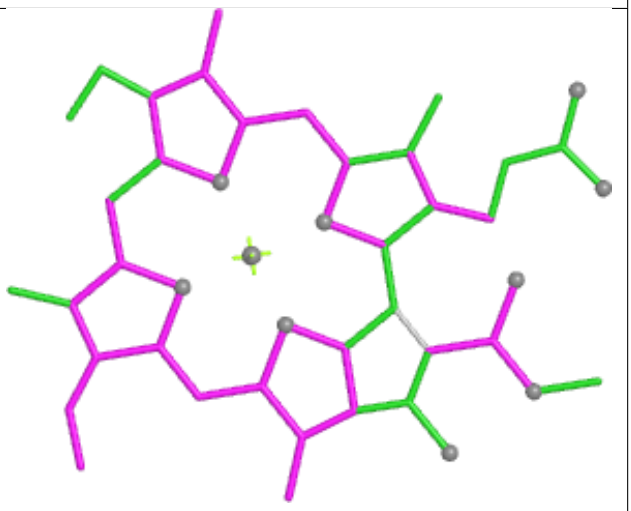


Rings

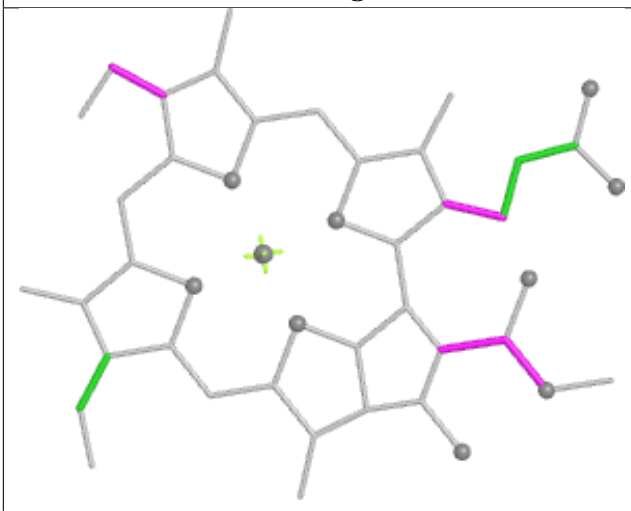
Ligand CLA cB 814



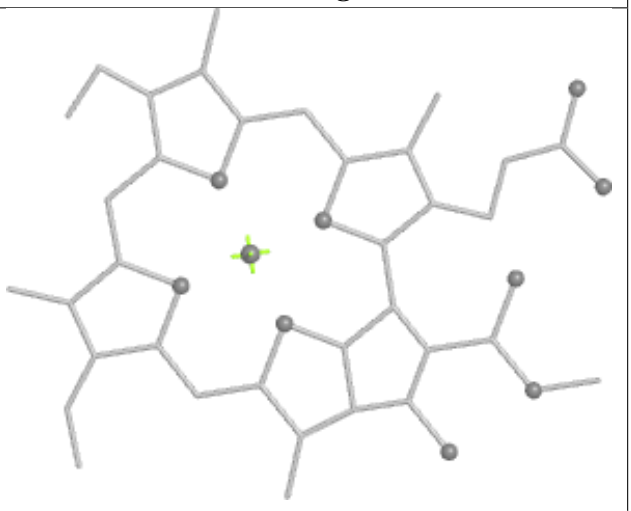
Bond lengths



Bond angles

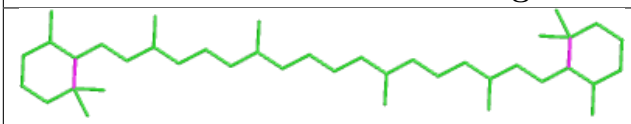


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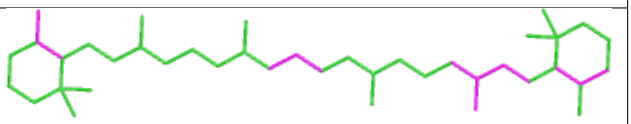


Rings

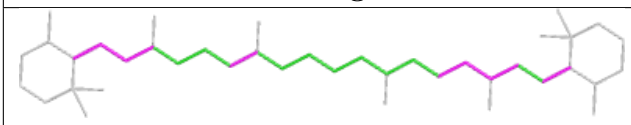
Ligand BCR bA 848



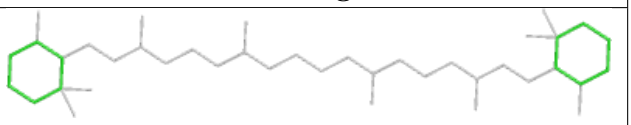
Bond lengths



Bond angles

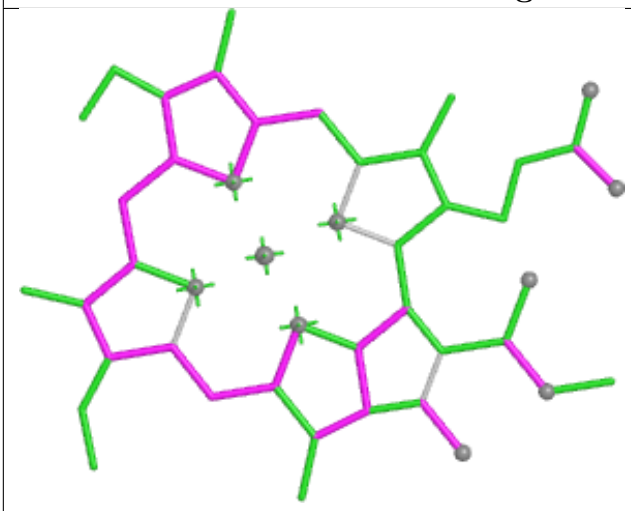


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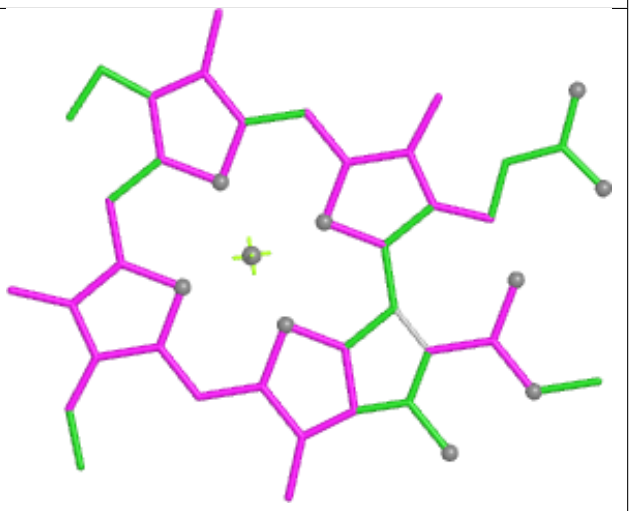


Rings

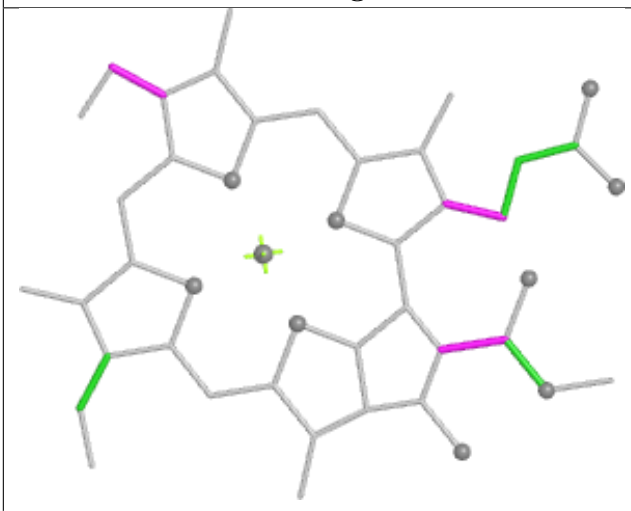
Ligand CLA aB 833



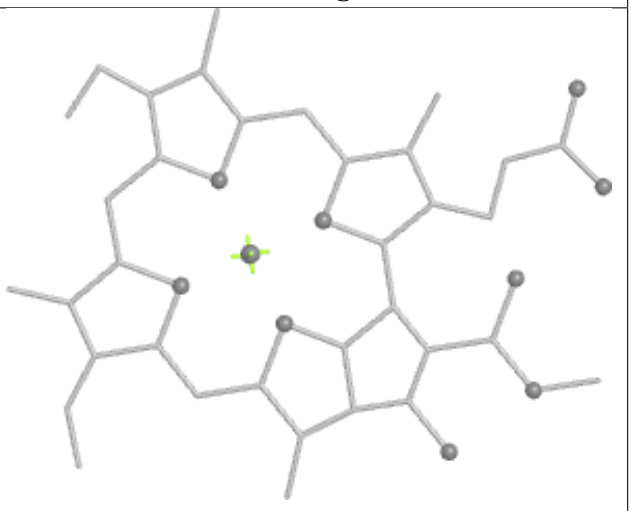
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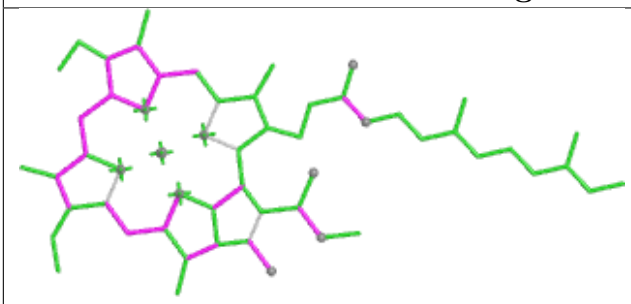
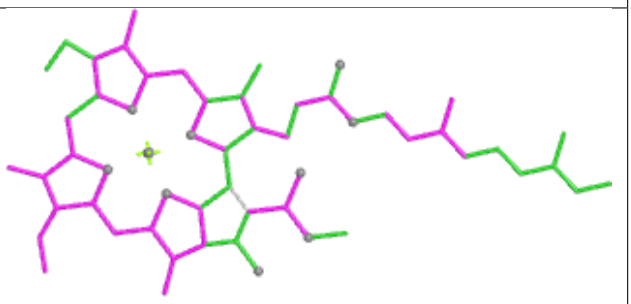
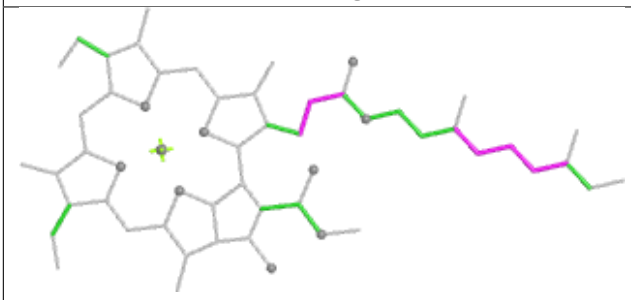
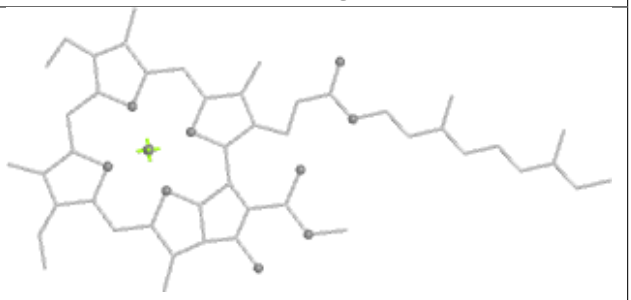
Bond angles

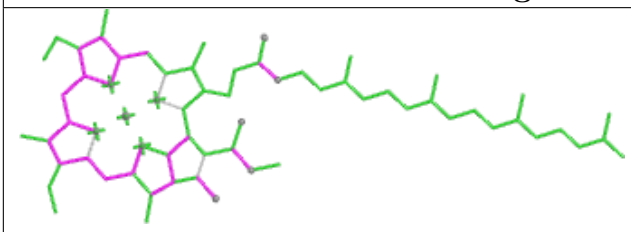
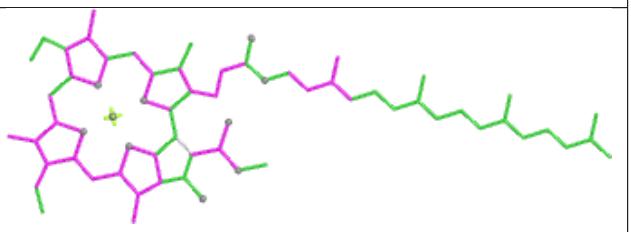
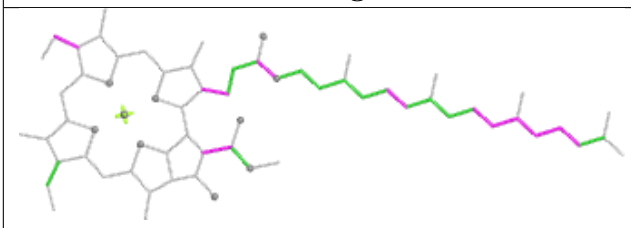
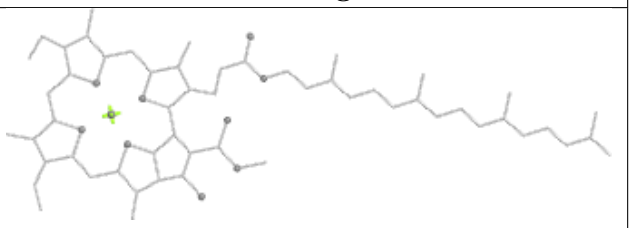


Torsions

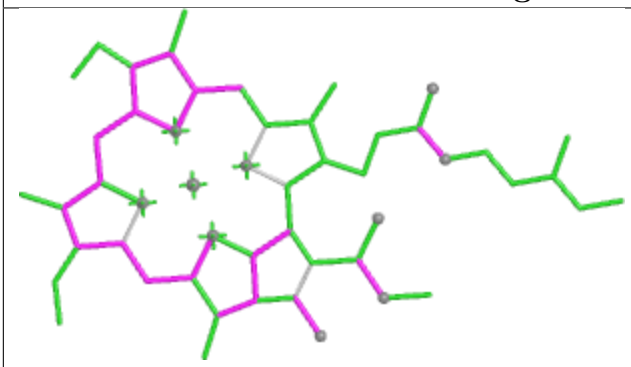


Rings

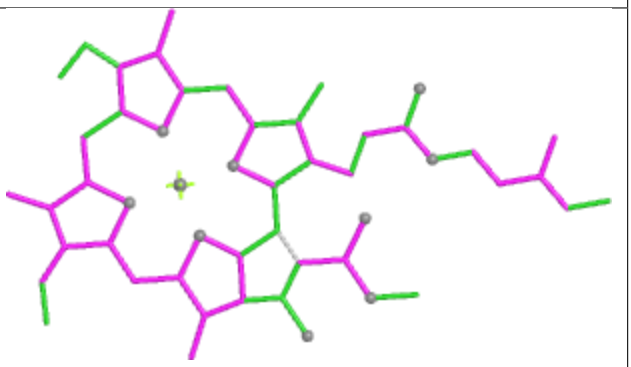
Ligand CLA aA 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

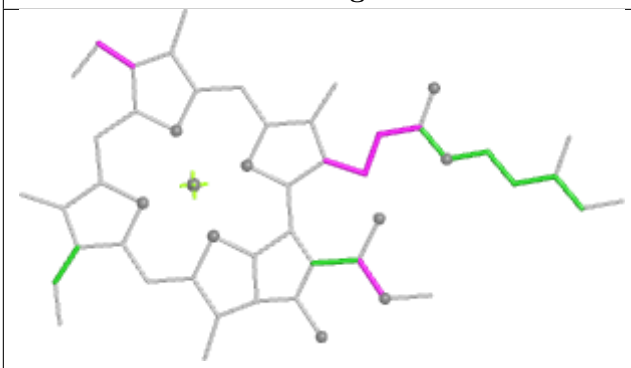
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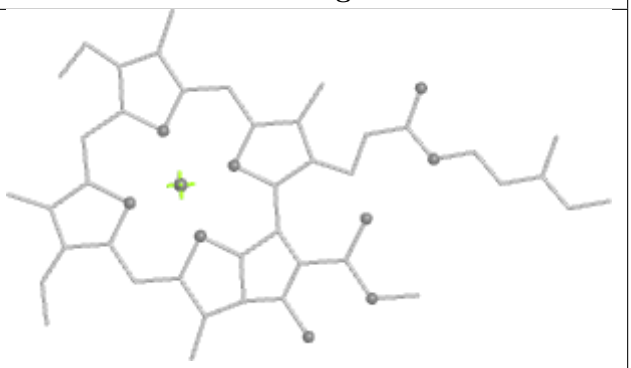
Bond lengths



Bond angles

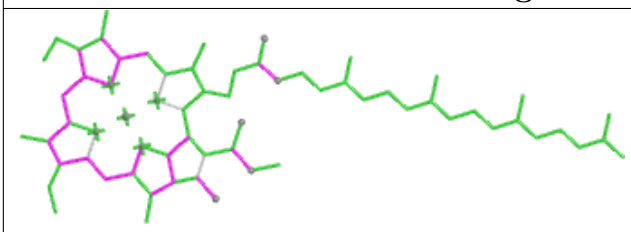


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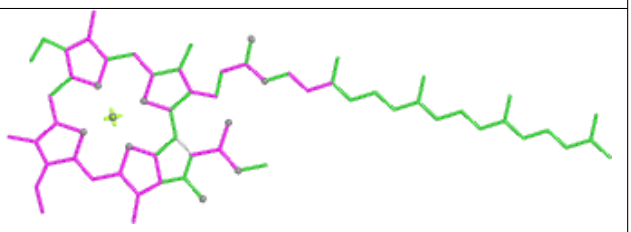


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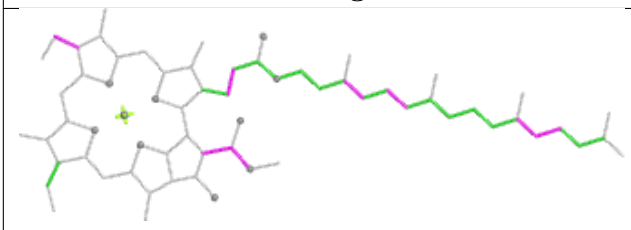
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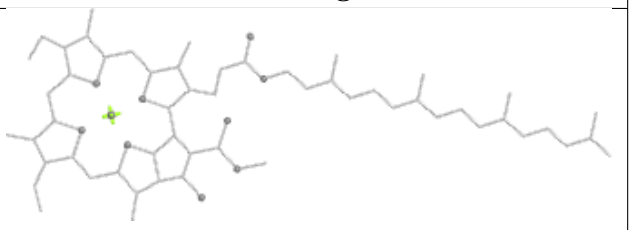
Bond lengths



Bond angles

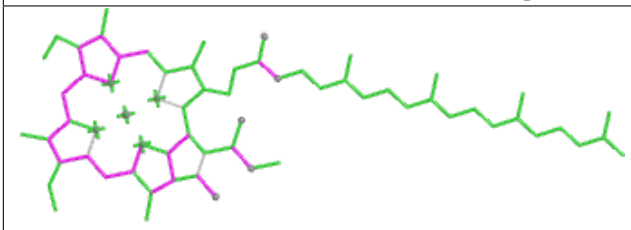


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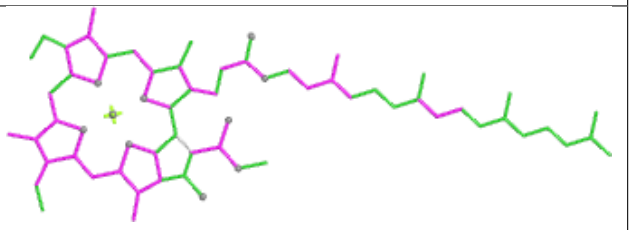


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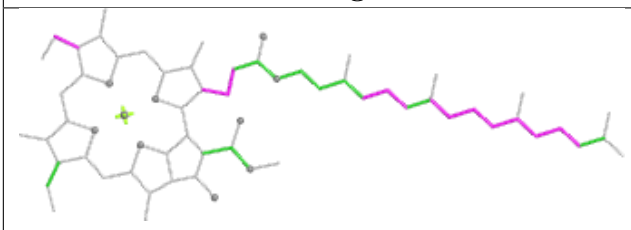
Ligand CLA cL 206



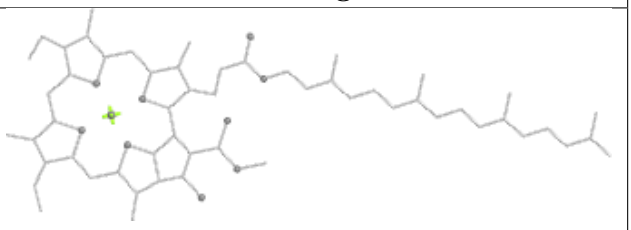
Bond lengths



Bond angles



Torsions

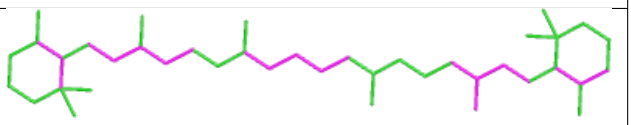


Rings

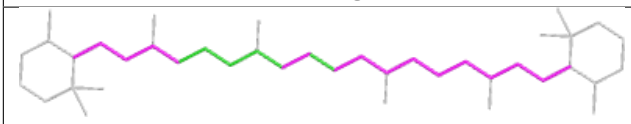
Ligand BCR aA 851



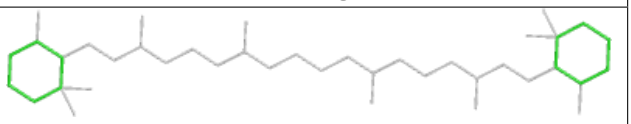
Bond lengths



Bond angles

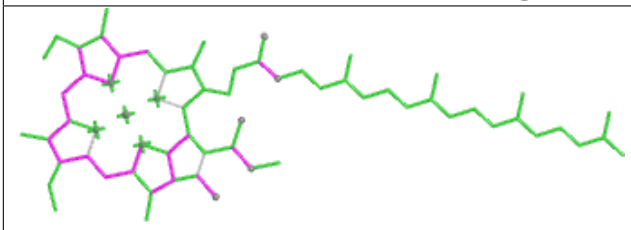


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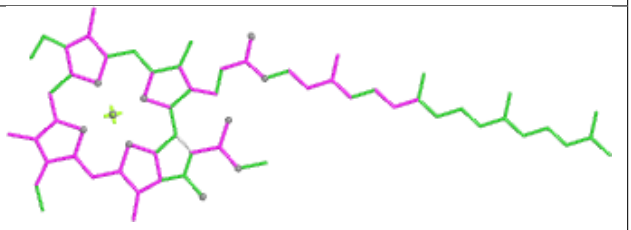


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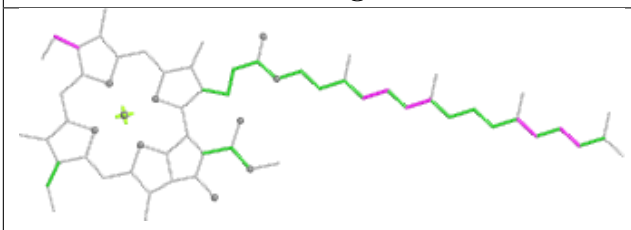
Ligand CLA cA 839



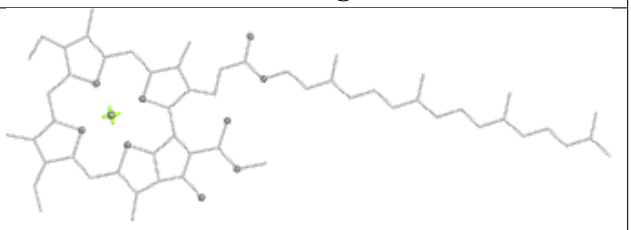
Bond lengths



Bond angles

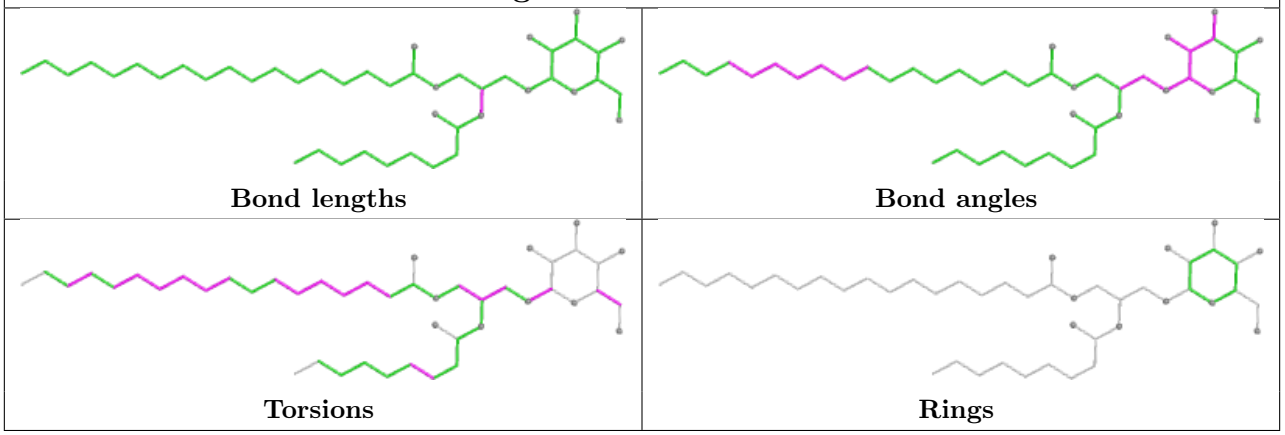


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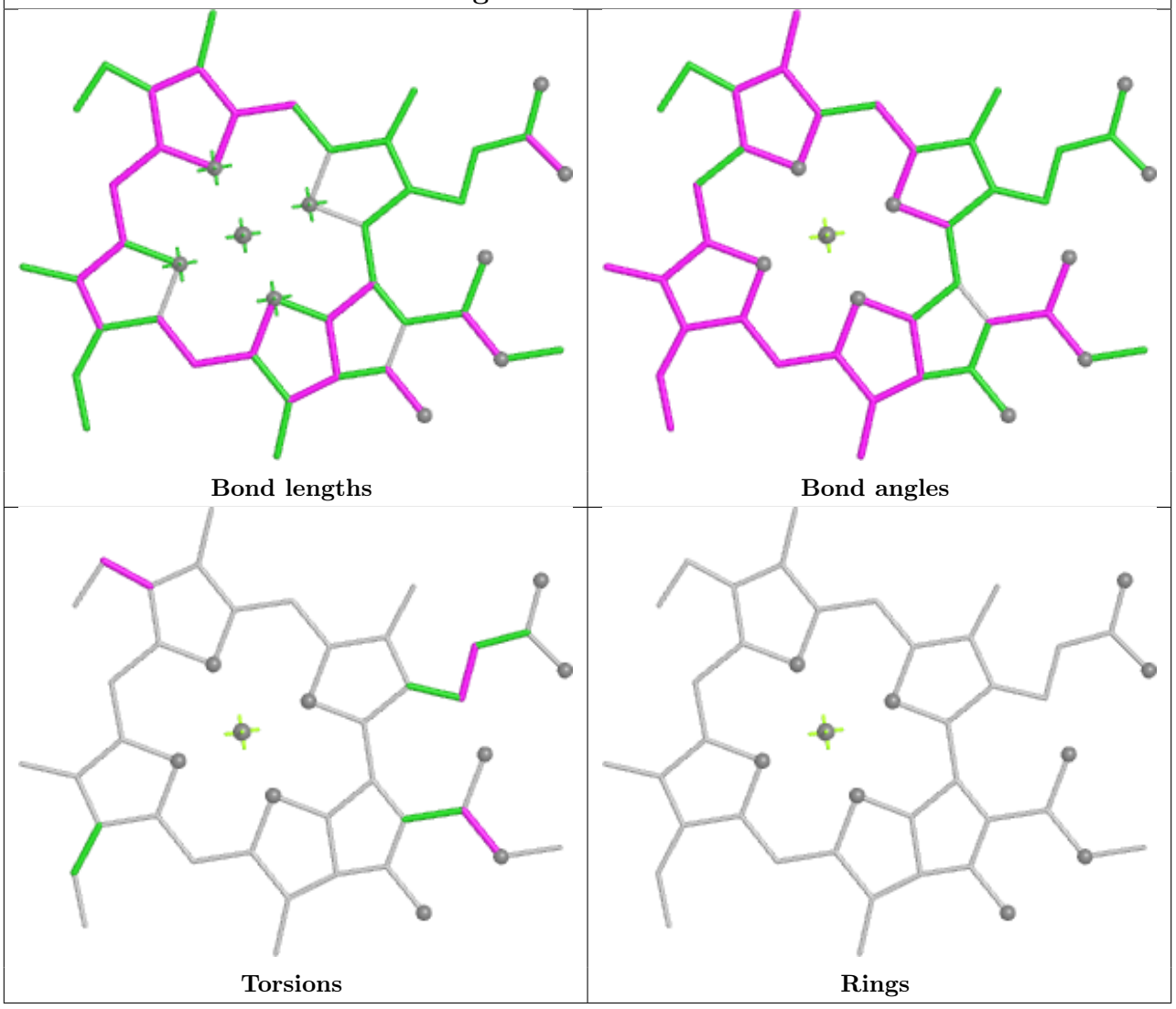


Rings

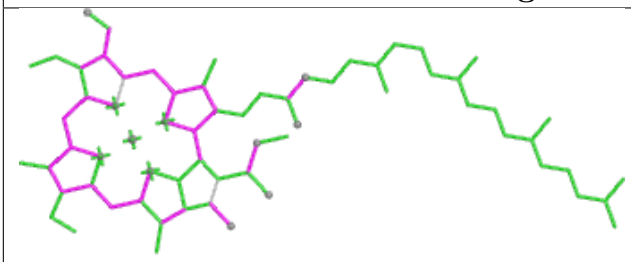
Ligand LMG cB 847



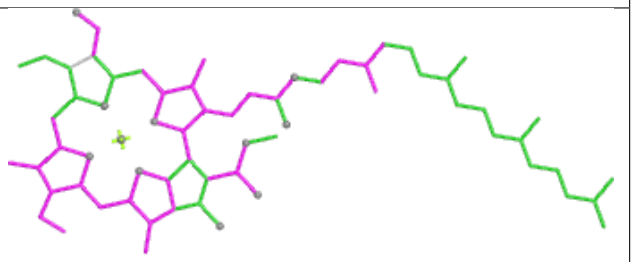
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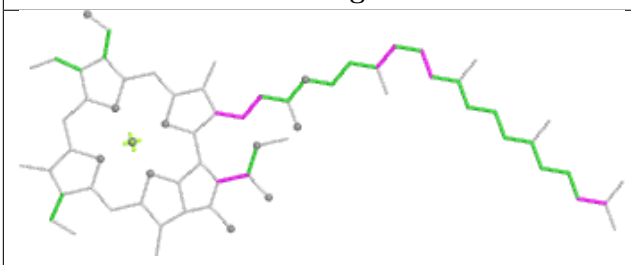
Ligand F6C bA 830



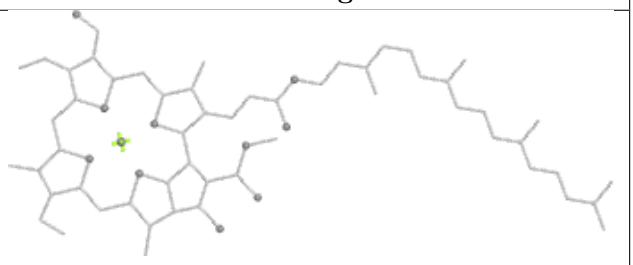
Bond lengths



Bond angles

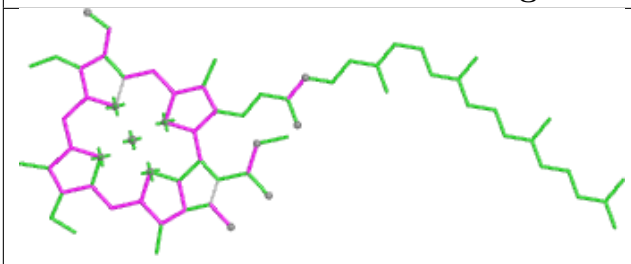


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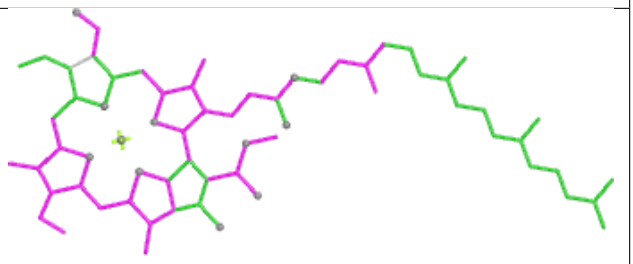


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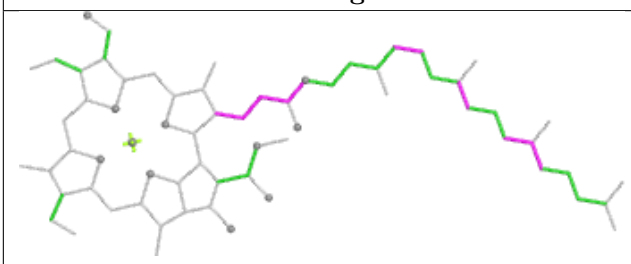
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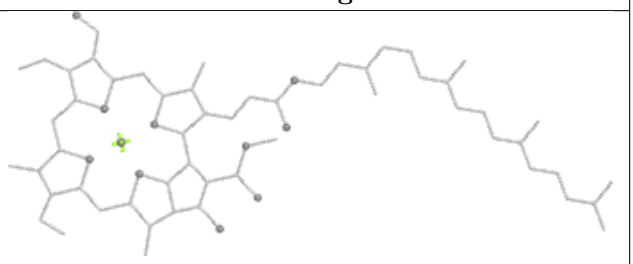
Bond lengths



Bond angles

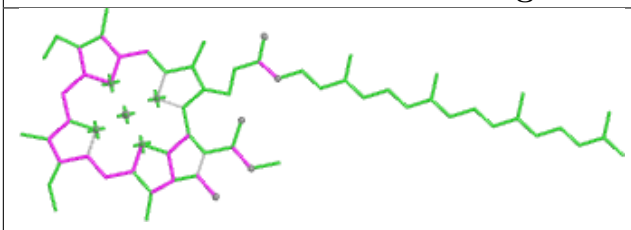


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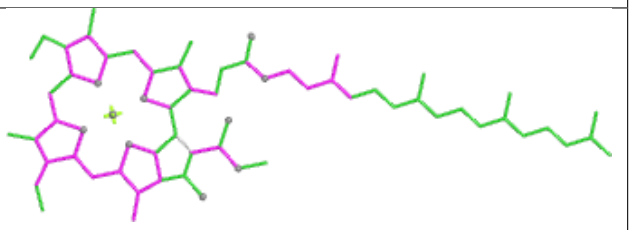


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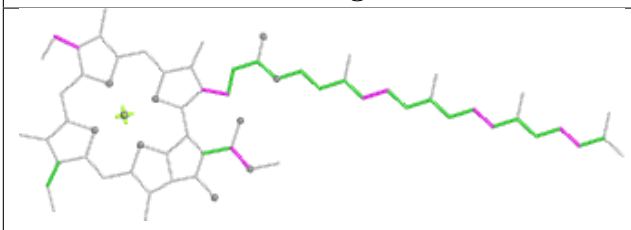
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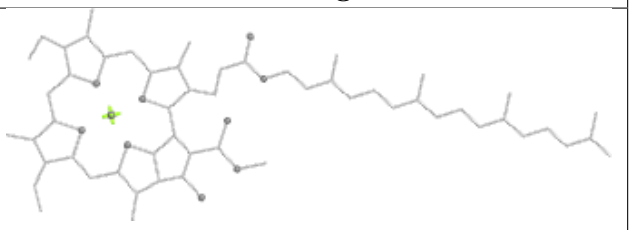
Bond lengths



Bond angles

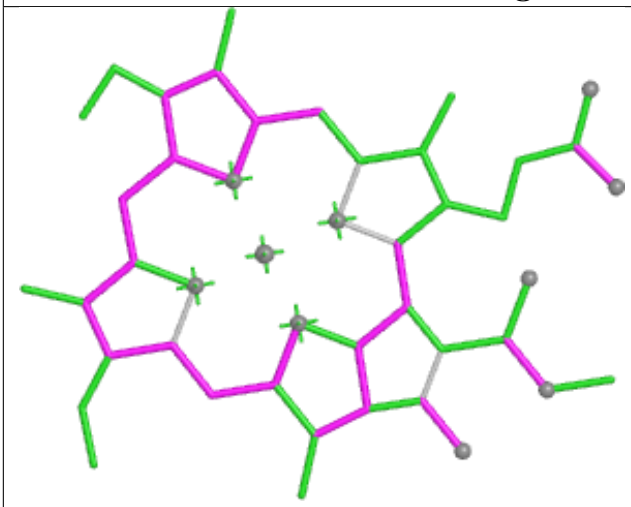


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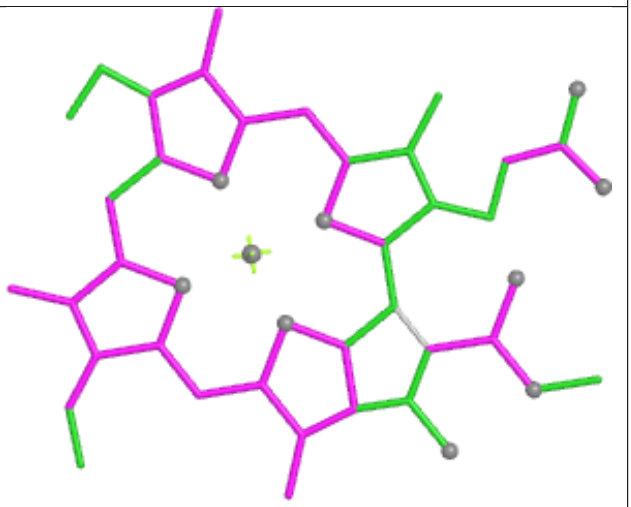


Rings

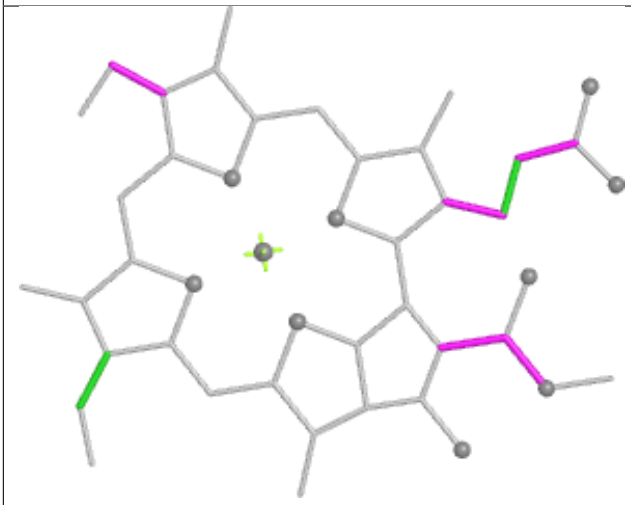
Ligand CLA bB 832



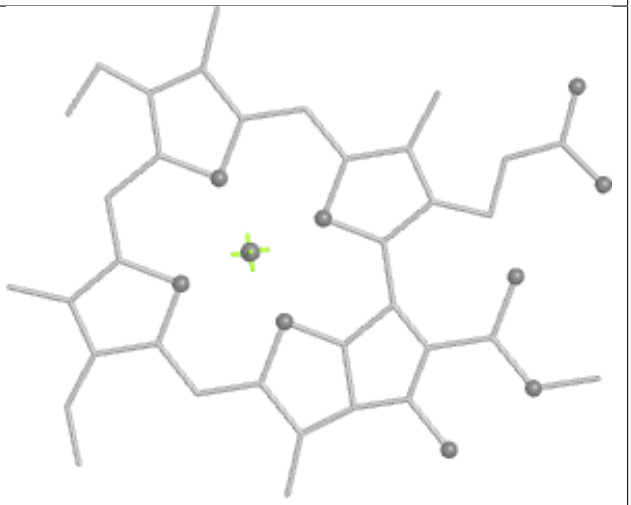
Bond lengths



Bond angles

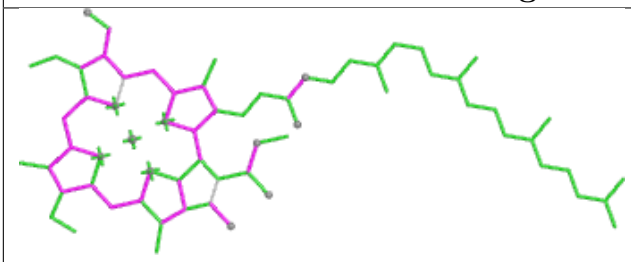


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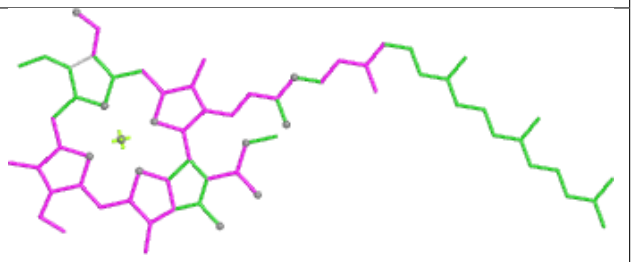


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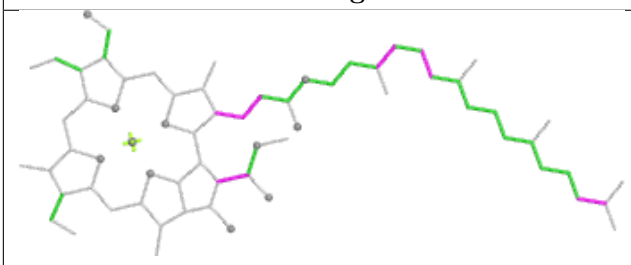
Ligand F6C aA 830



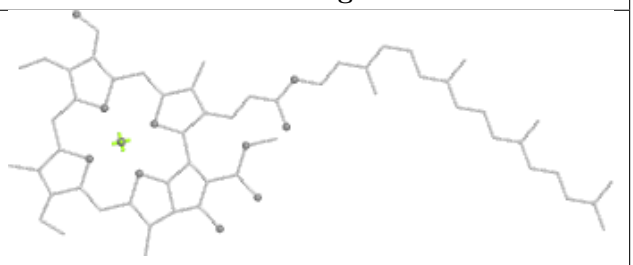
Bond lengths



Bond angles

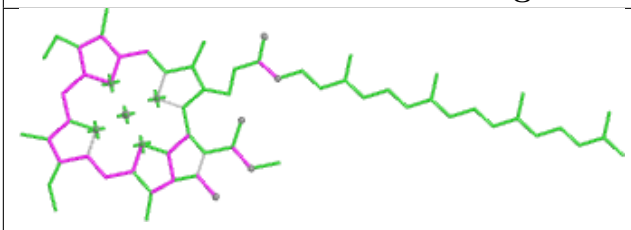


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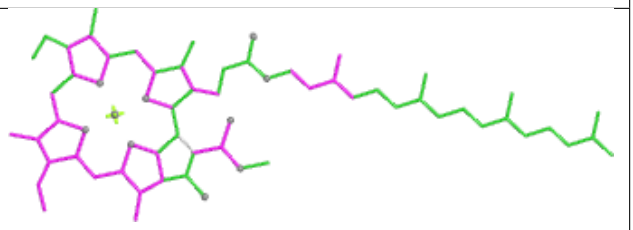


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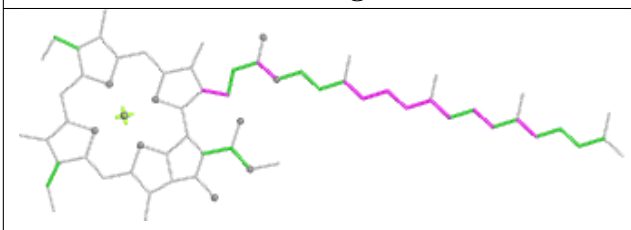
Ligand CLA bA 833



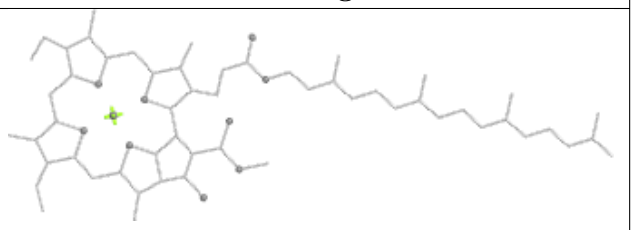
Bond lengths



Bond angles

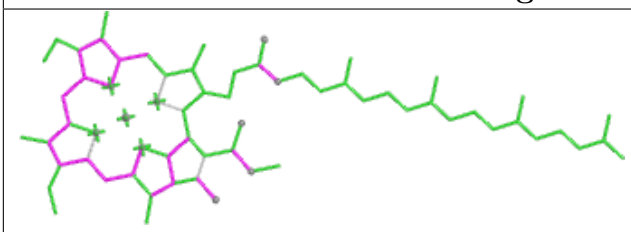


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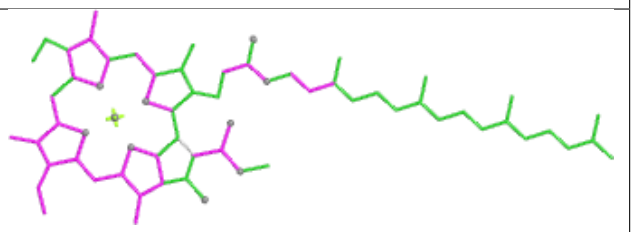


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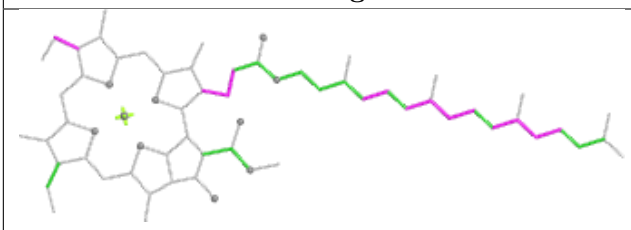
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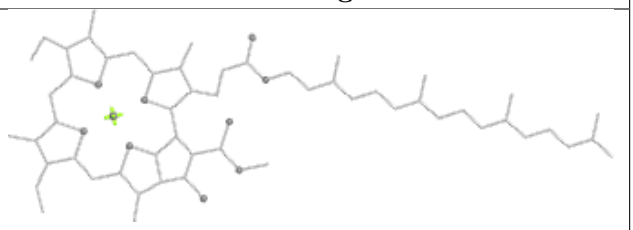
Bond lengths



Bond angles

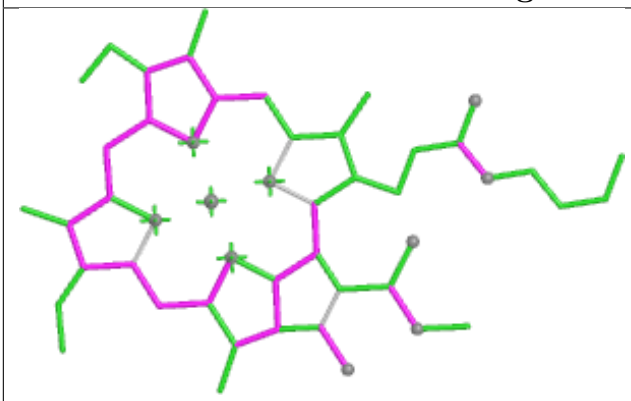


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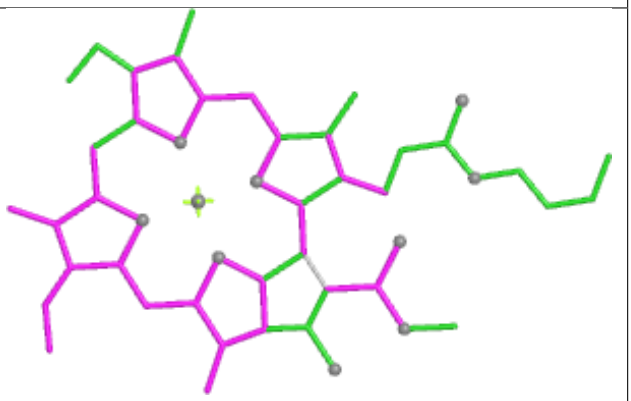


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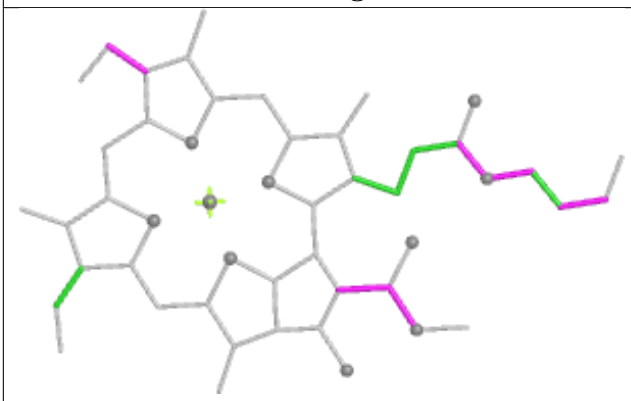
Ligand CLA cB 830



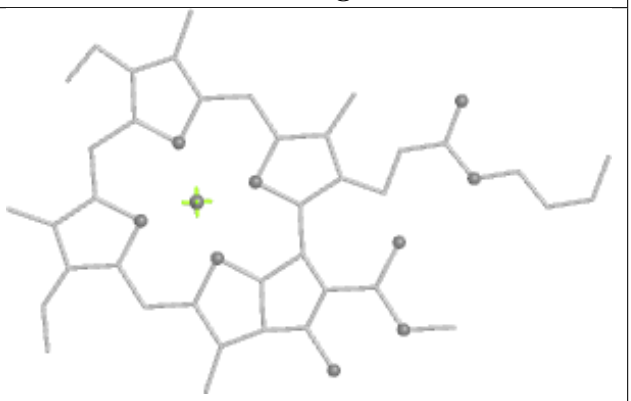
Bond lengths



Bond angles

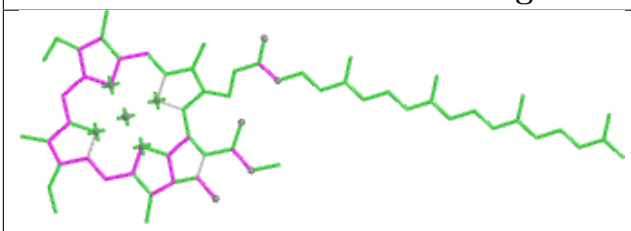


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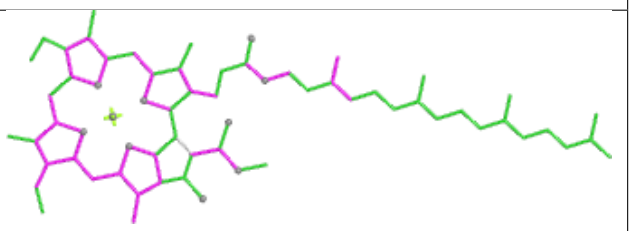


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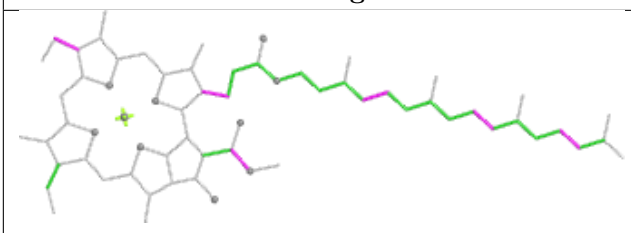
Ligand CLA aB 818



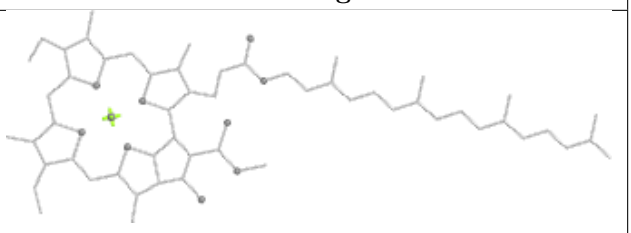
Bond lengths



Bond angles

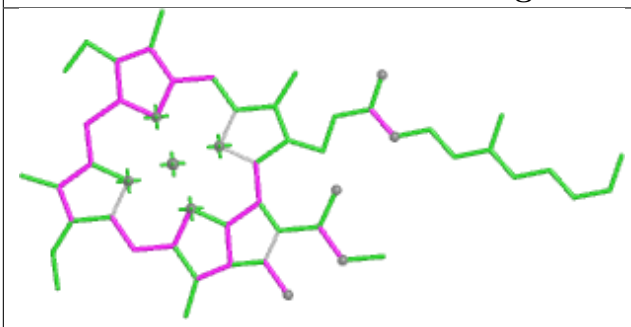


Torsions

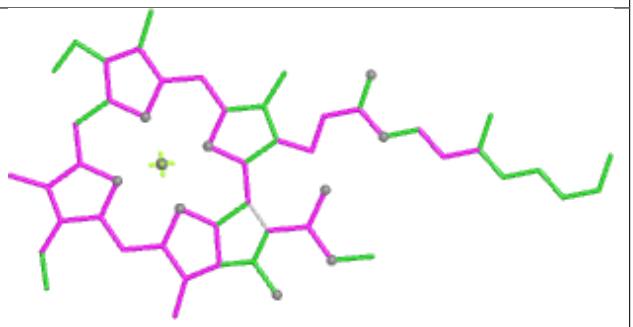


Rings

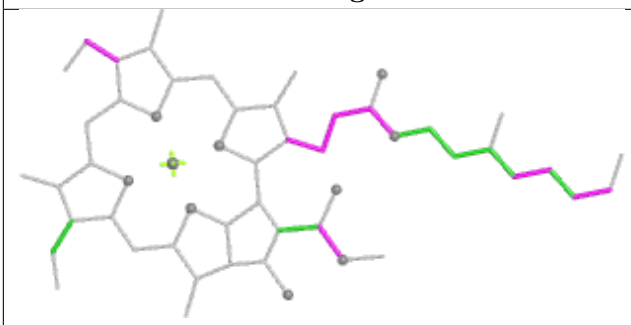
Ligand CLA aA 819



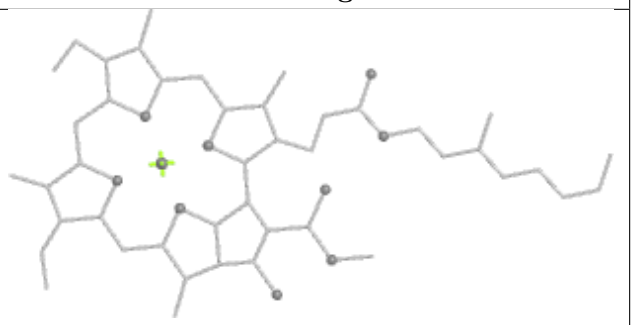
Bond lengths



Bond angles

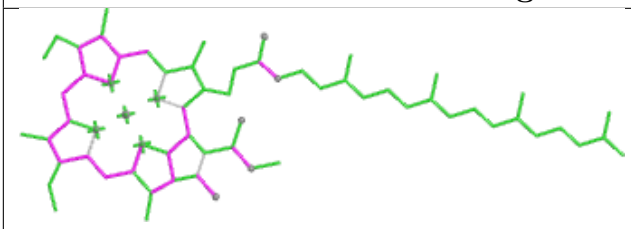


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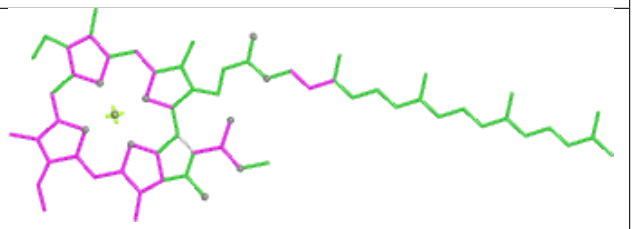


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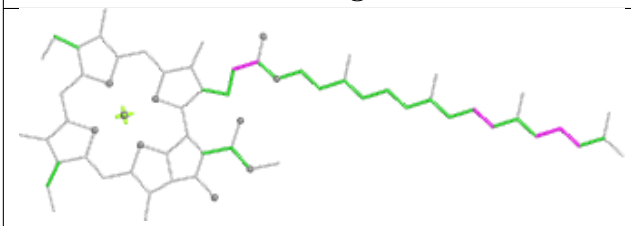
Ligand CLA bL 204



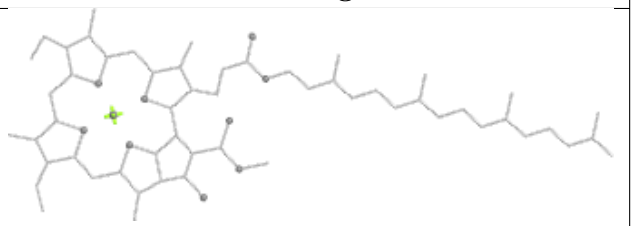
Bond lengths



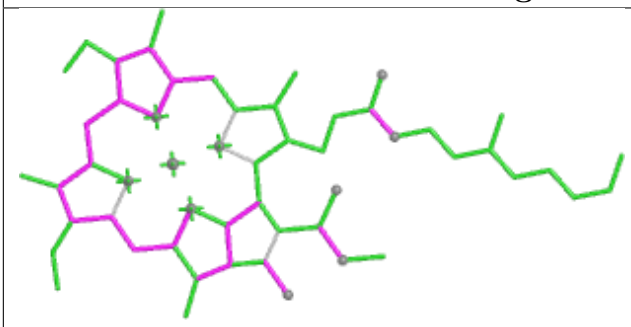
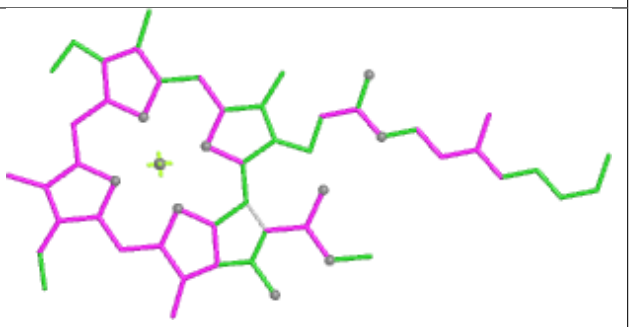
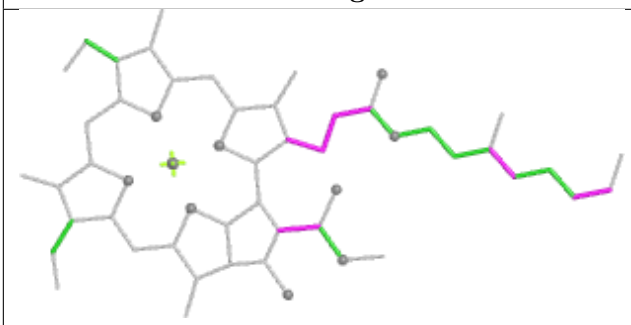
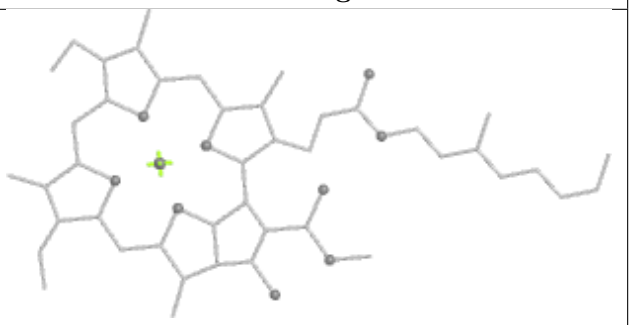
Bond angles

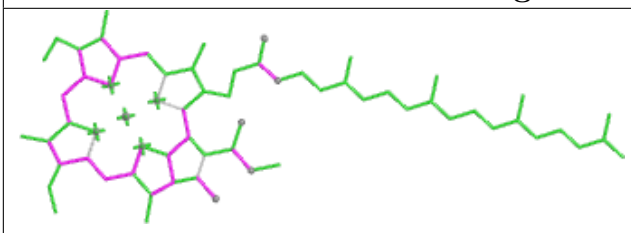
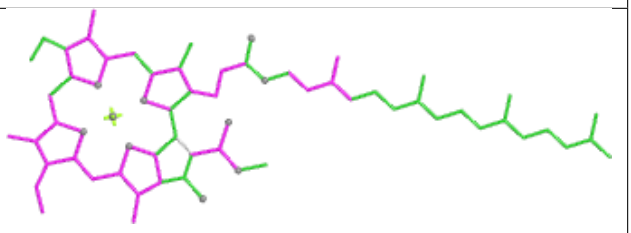
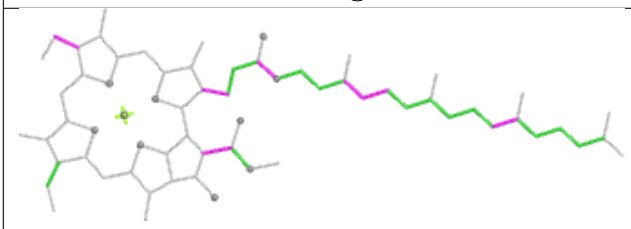
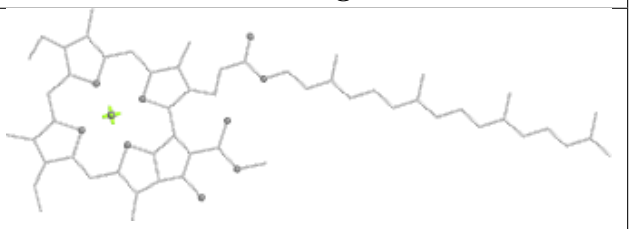


Torsions

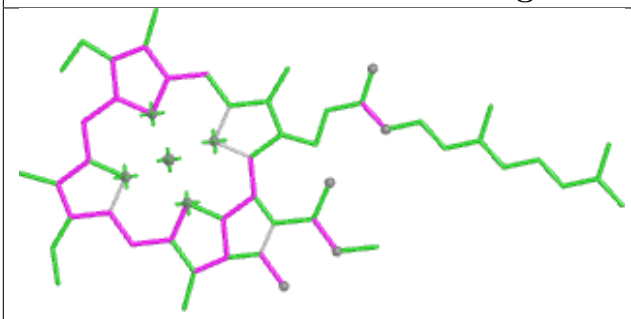


Rings

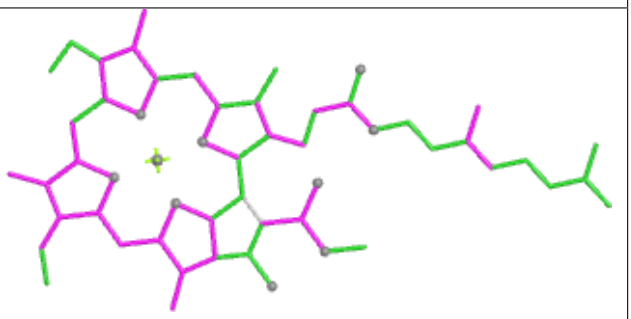
Ligand CLA aA 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

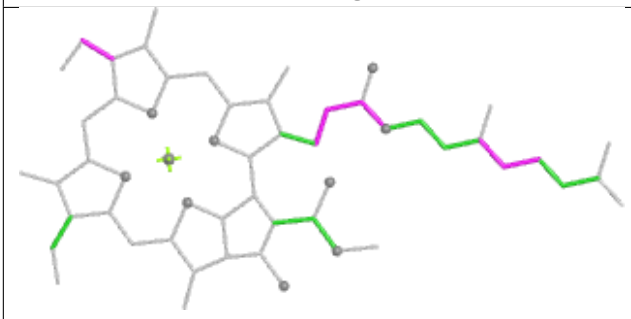
Ligand CLA cB 821



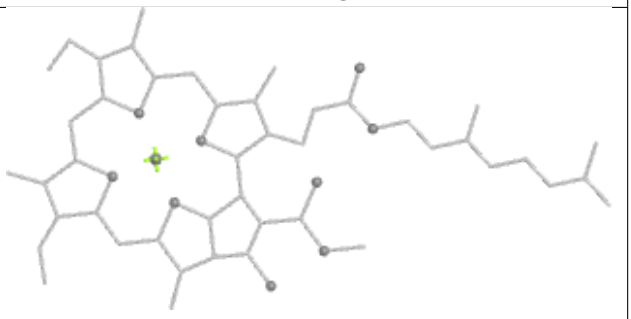
Bond lengths



Bond angles

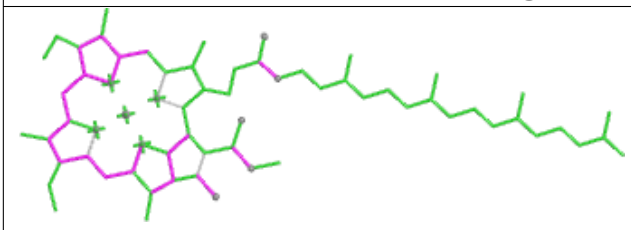


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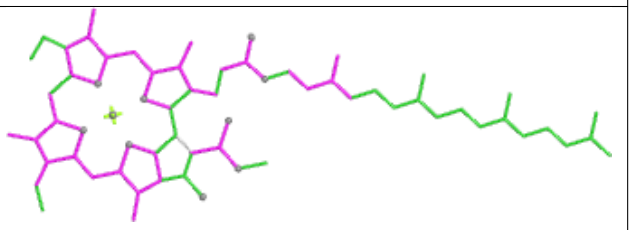


Rings

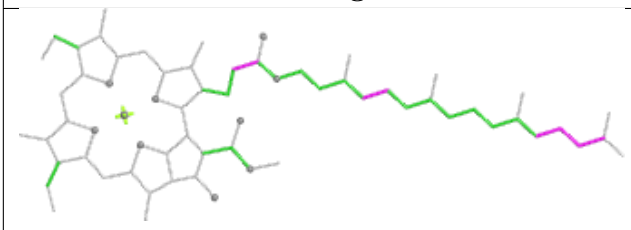
Ligand CL0 cA 801



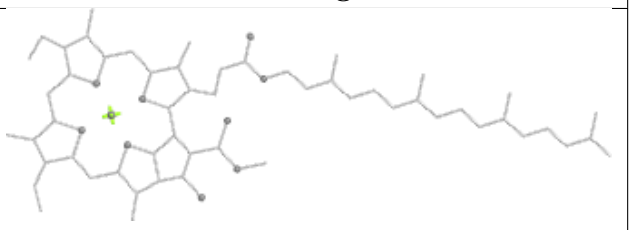
Bond lengths



Bond angles

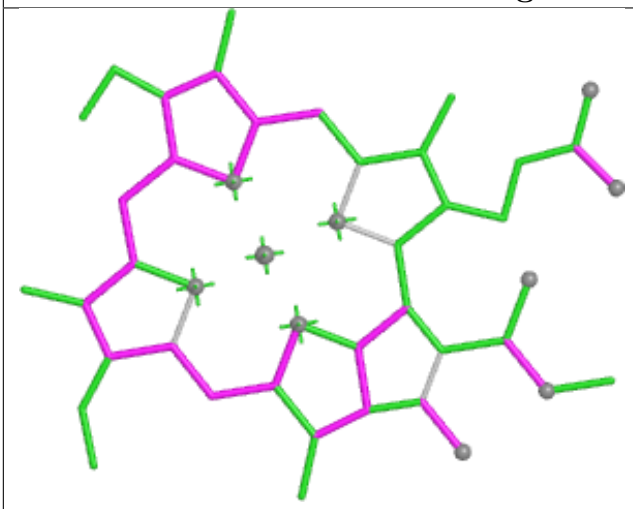


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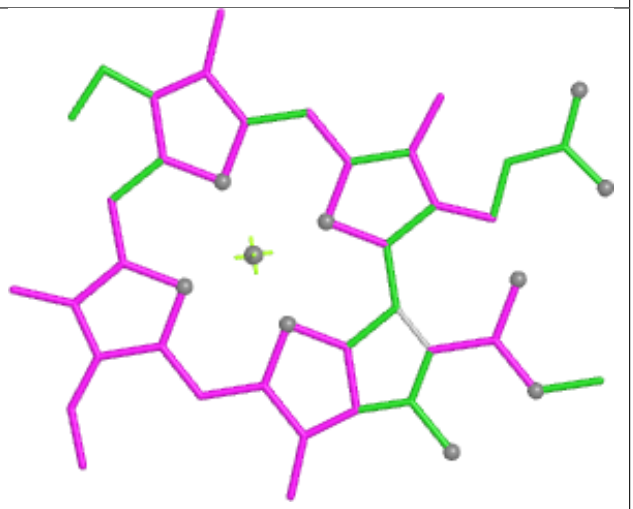


Rings

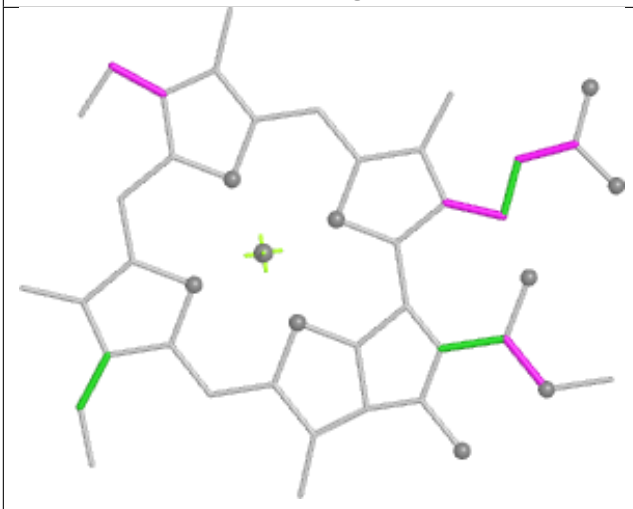
Ligand CLA cB 810



Bond lengths



Bond angles

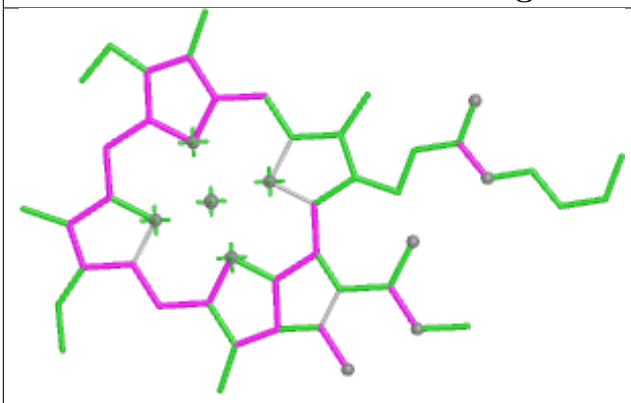


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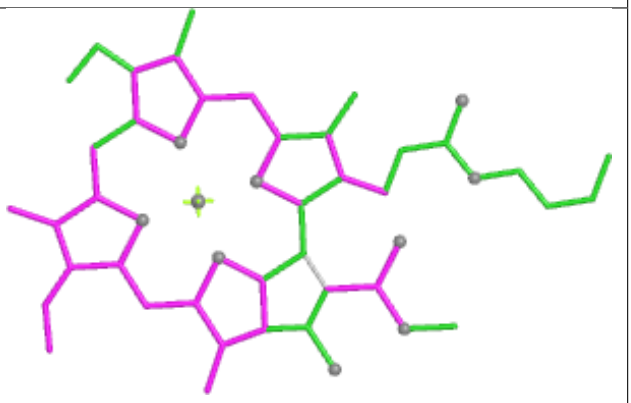


Rings

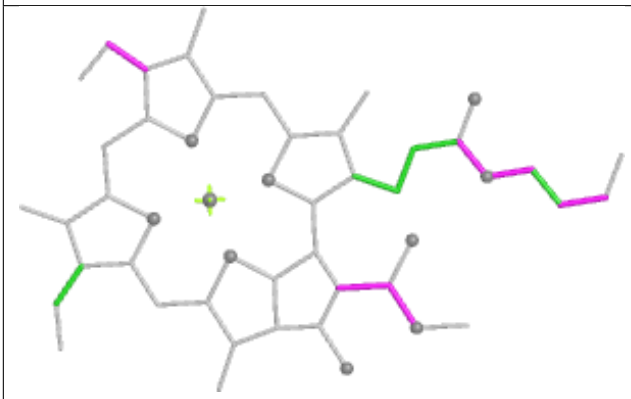
Ligand CLA aB 830



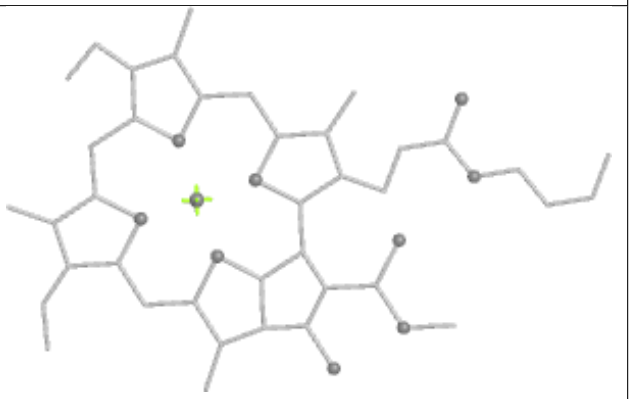
Bond lengths



Bond angles



Torsions

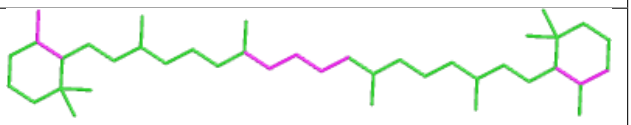


Rings

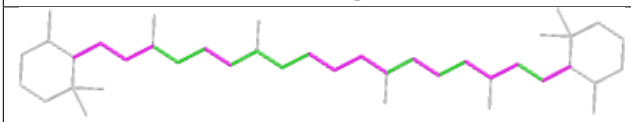
Ligand BCR bB 842



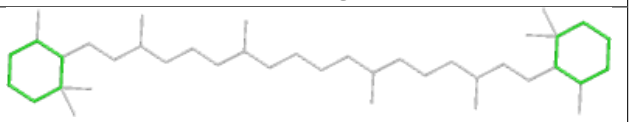
Bond lengths



Bond angles

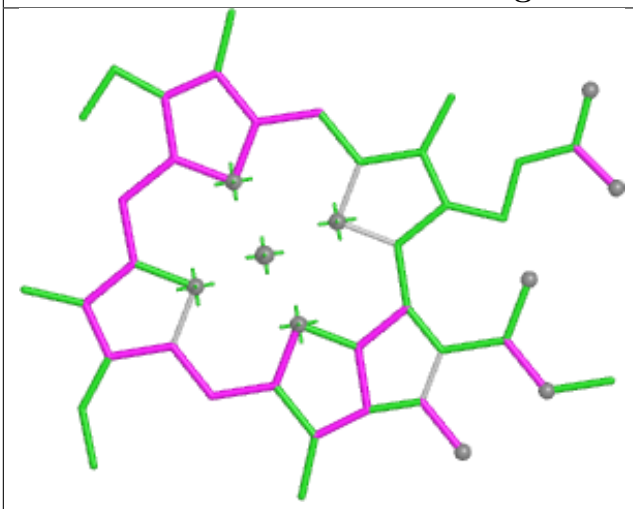


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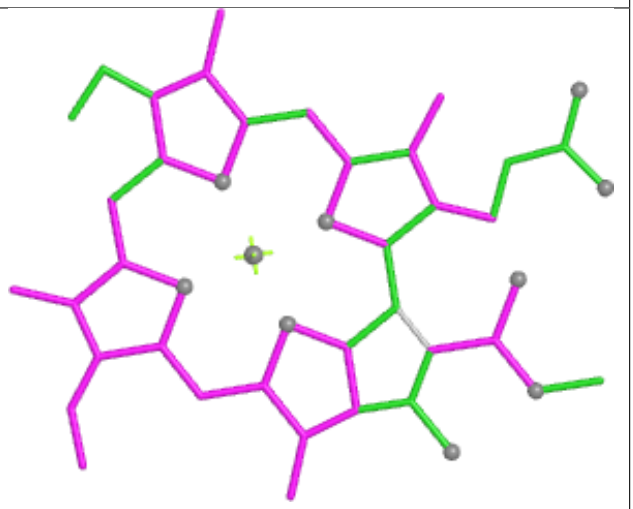


Rings

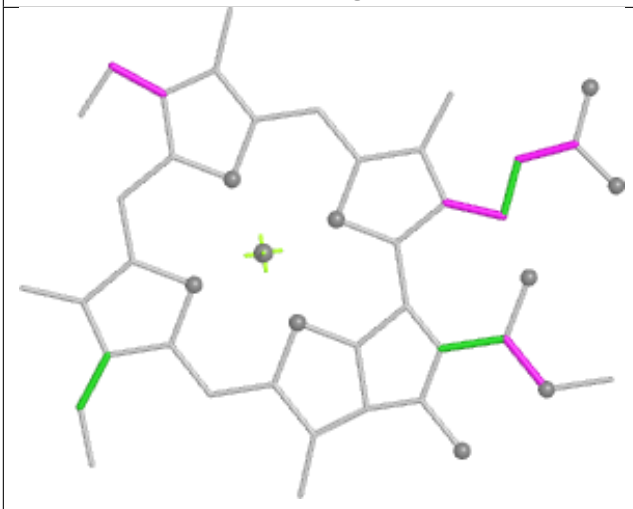
Ligand CLA bB 810



Bond lengths



Bond angles

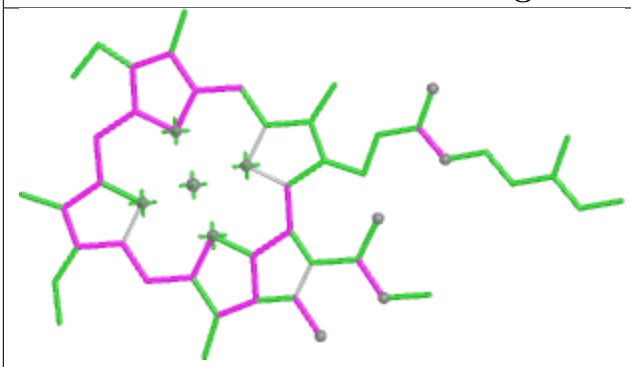


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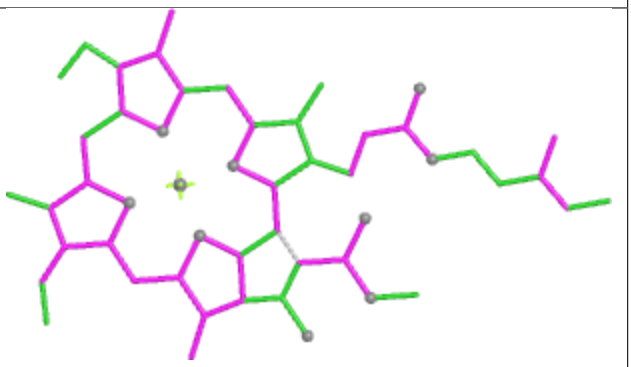


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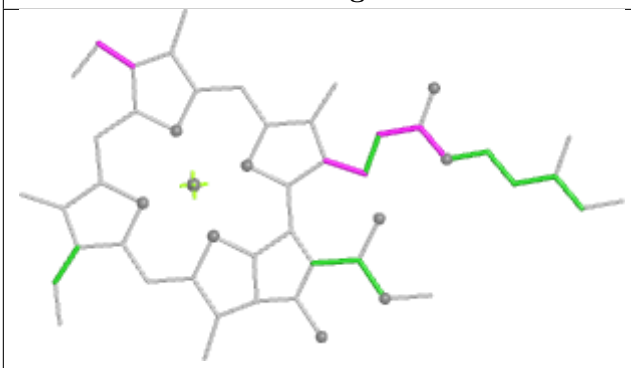
Ligand CLA aK 103



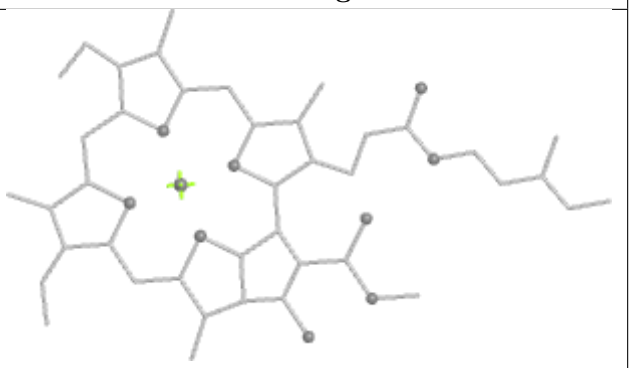
Bond lengths



Bond angles

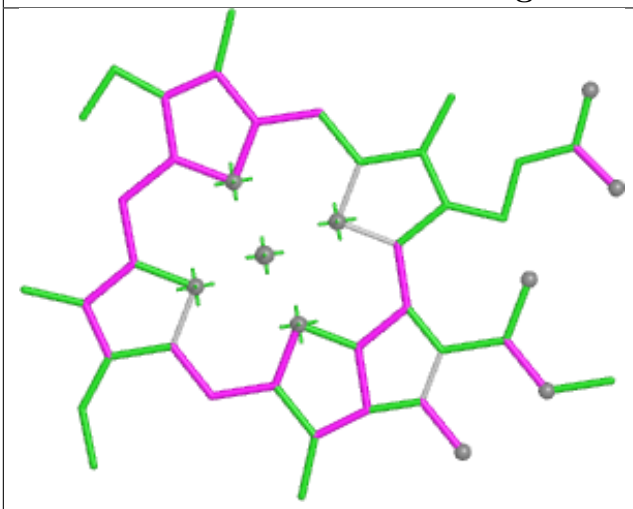


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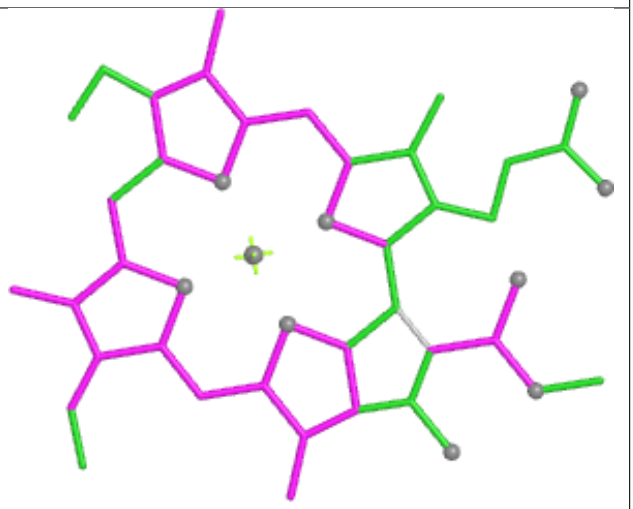


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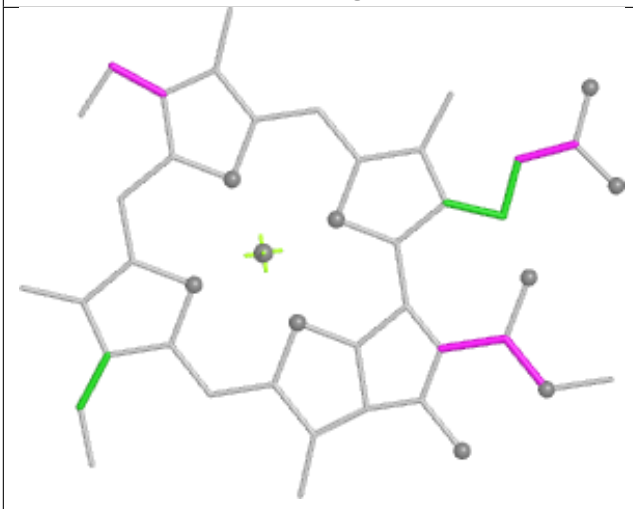
Ligand CLA aB 820



Bond lengths



Bond angles

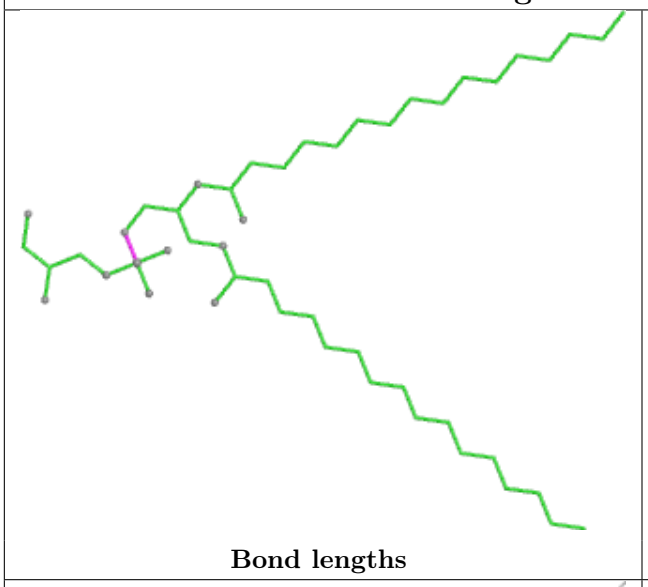


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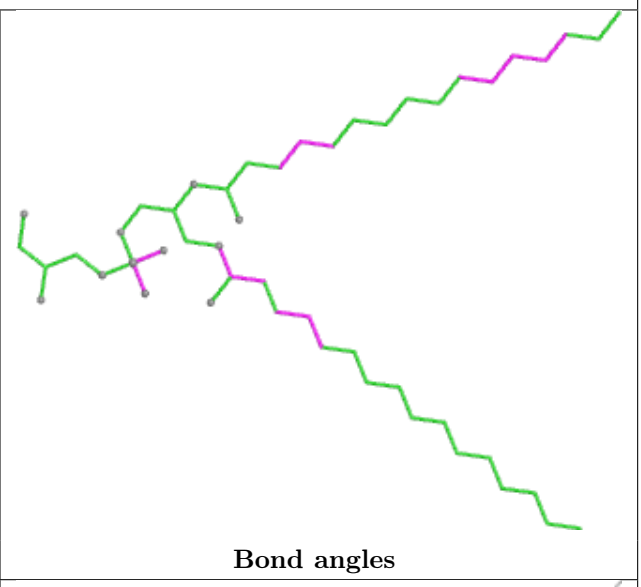


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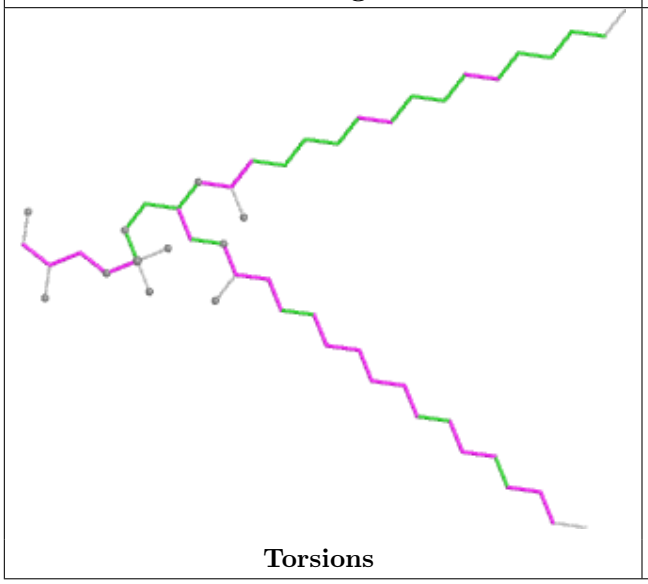
Ligand LHG aA 852



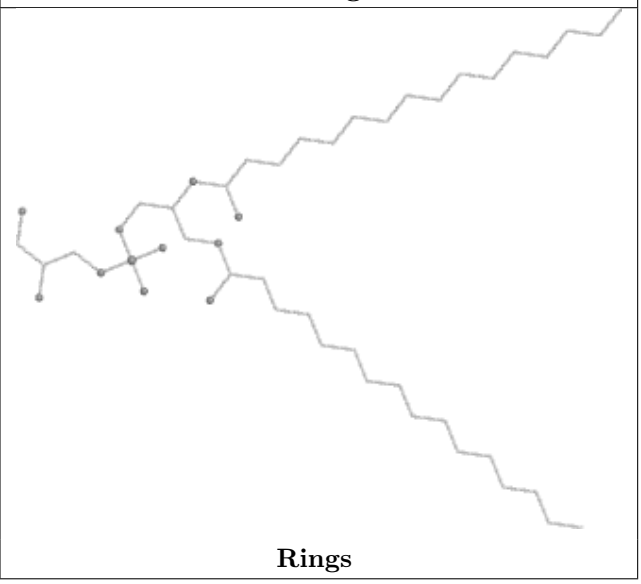
Bond lengths



Bond angles

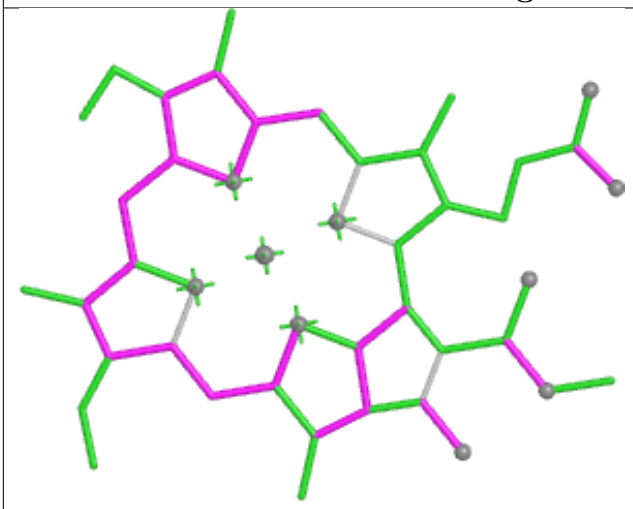


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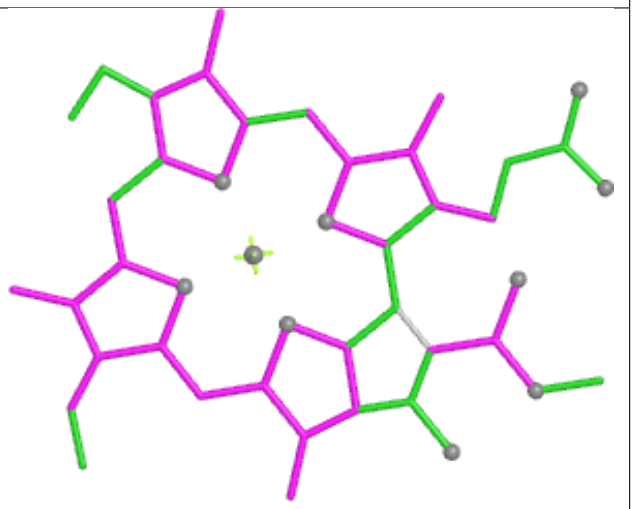


Rings

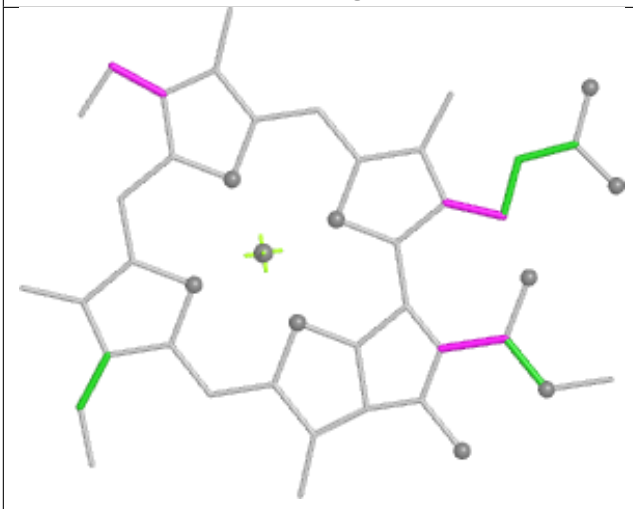
Ligand CLA cB 833



Bond lengths



Bond angles

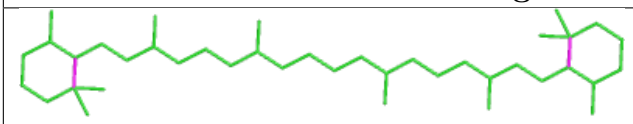


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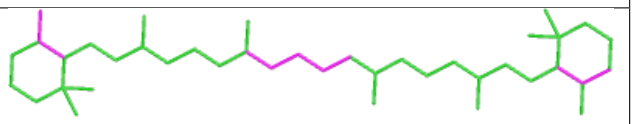


Rings

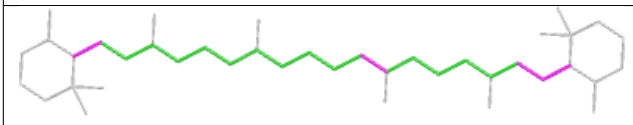
Ligand BCR aA 850



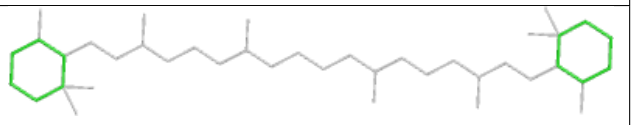
Bond lengths



Bond angles

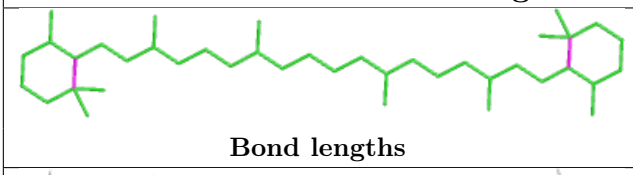


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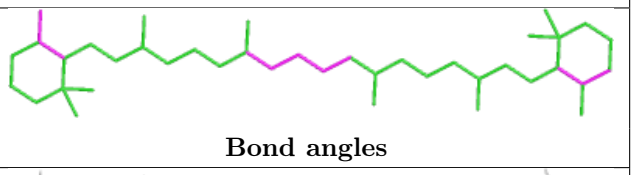


Rings

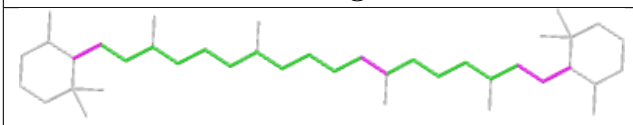
Ligand BCR bA 850



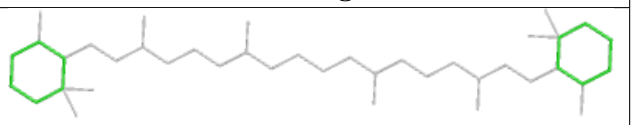
Bond lengths



Bond angles

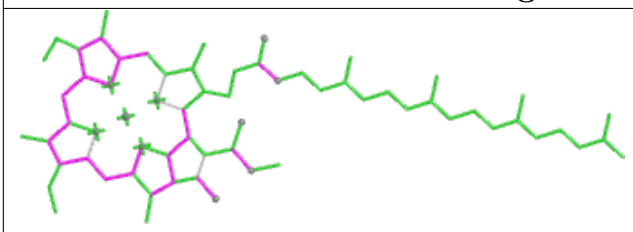


Torsions

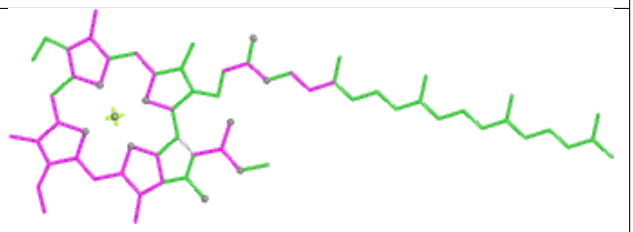


Rings

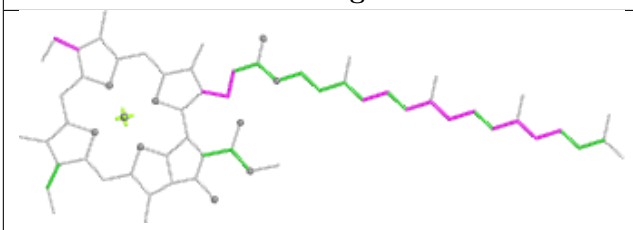
Ligand CLA aL 205



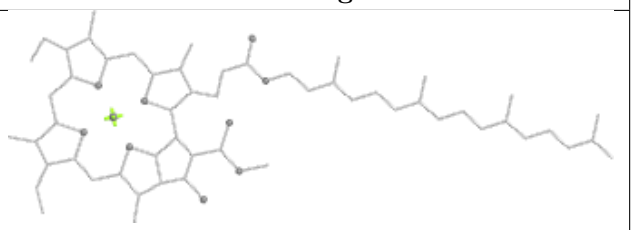
Bond lengths



Bond angles

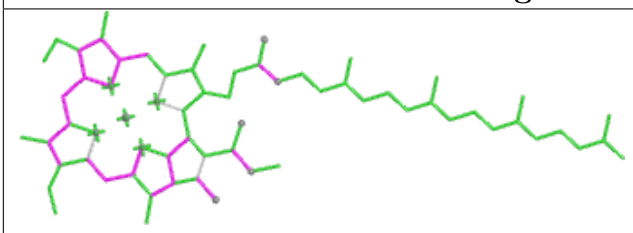


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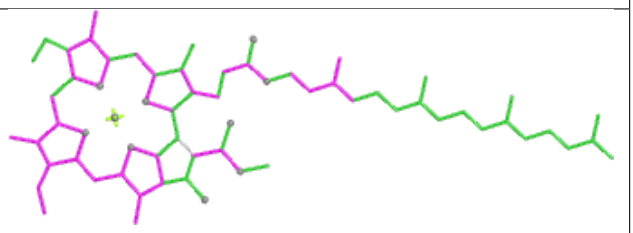


Rings

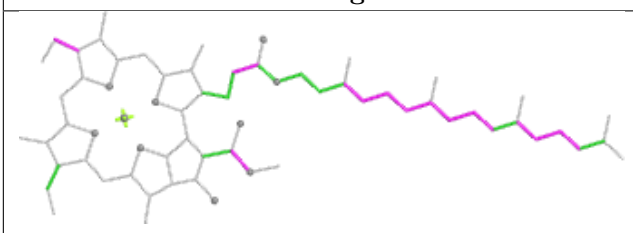
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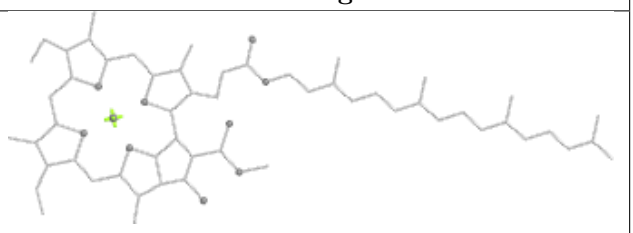
Bond lengths



Bond angles

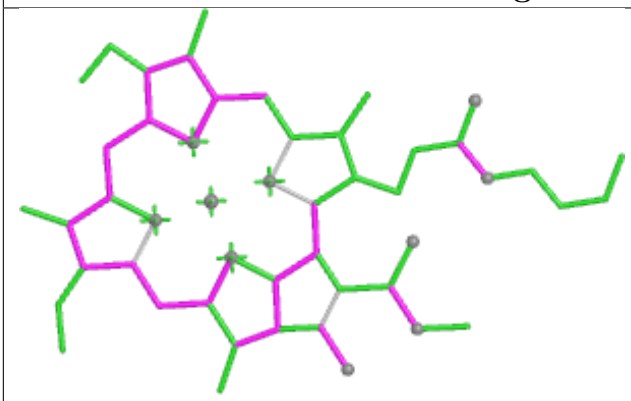


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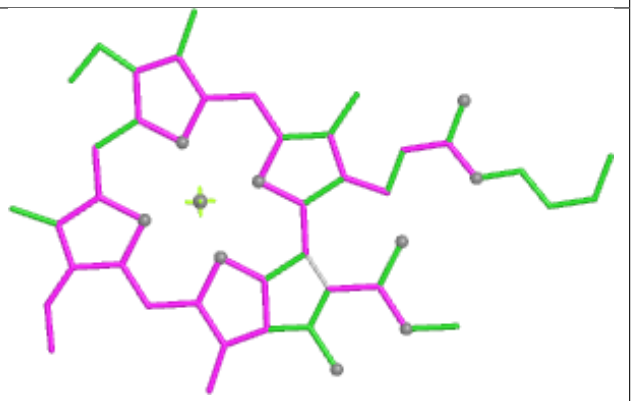


Rings

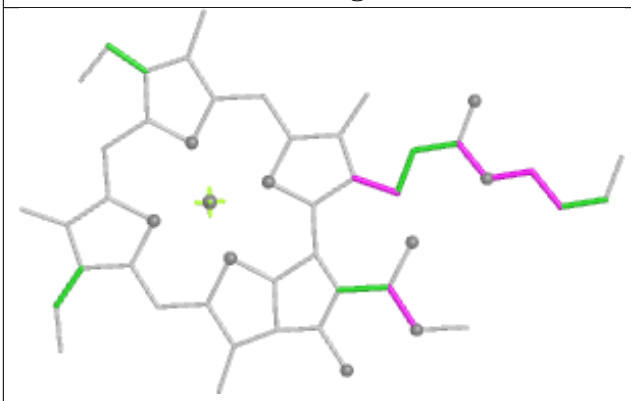
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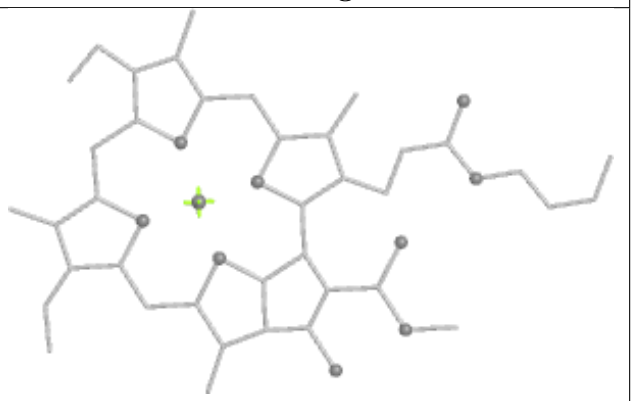
Bond lengths



Bond angles

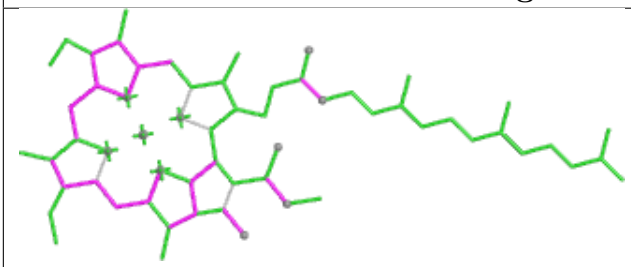


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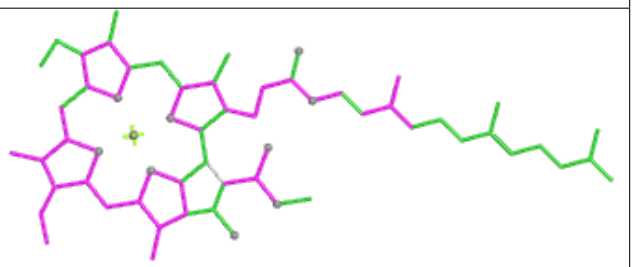


Rings

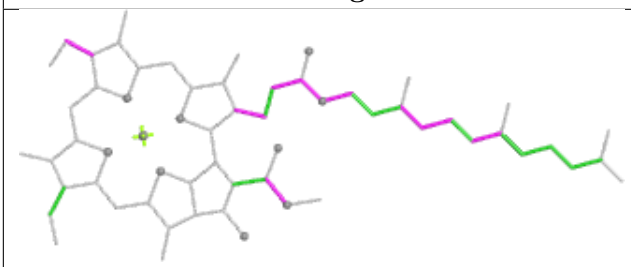
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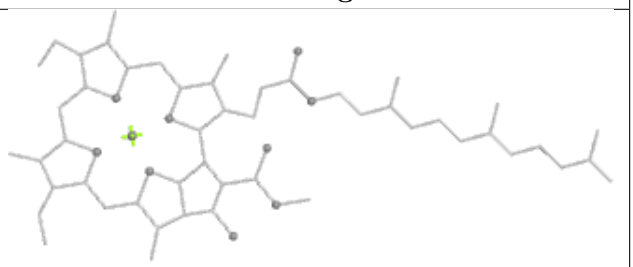
Bond lengths



Bond angles

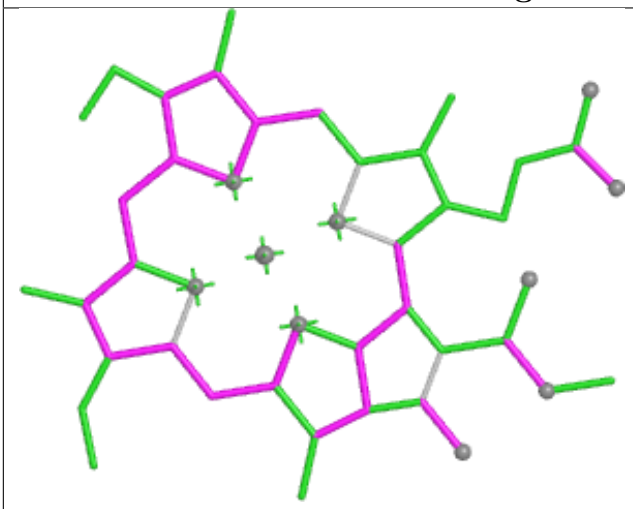


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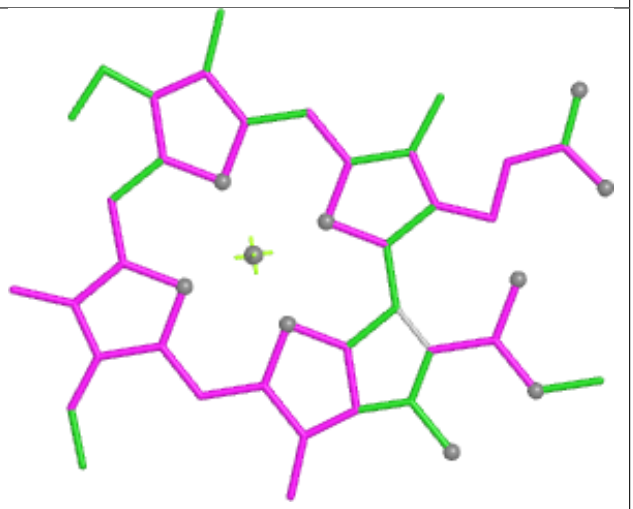


Rings

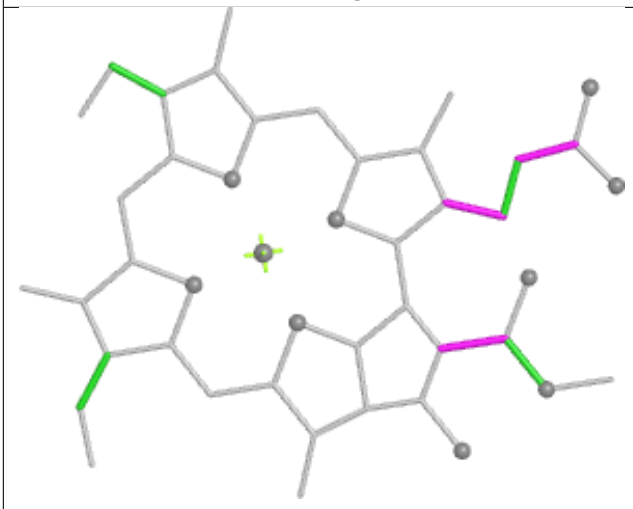
Ligand CLA aA 837



Bond lengths



Bond angles

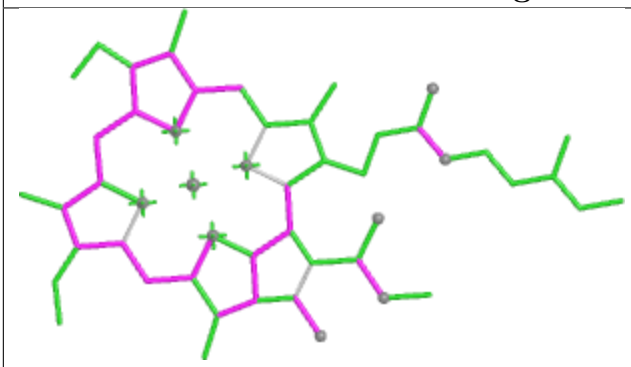


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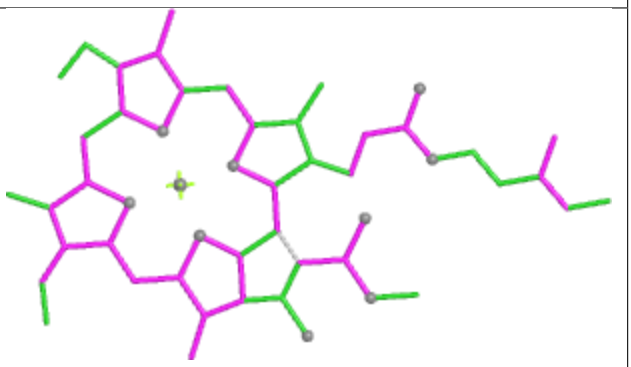


Rings

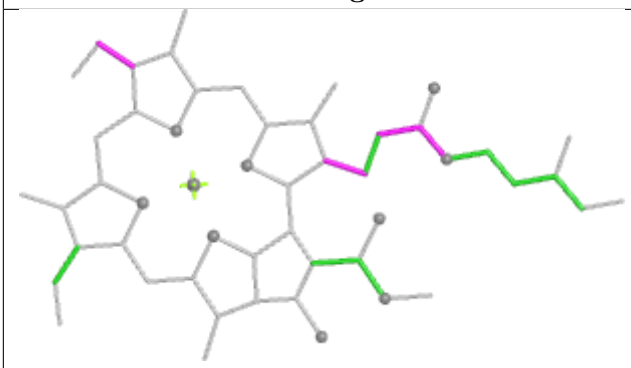
Ligand CLA bK 103



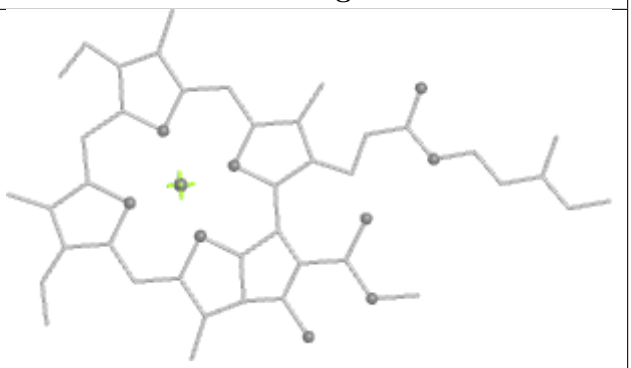
Bond lengths



Bond angles

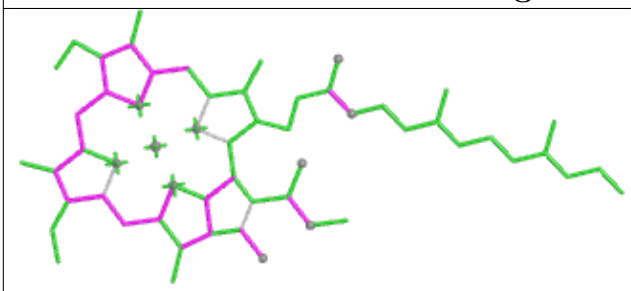


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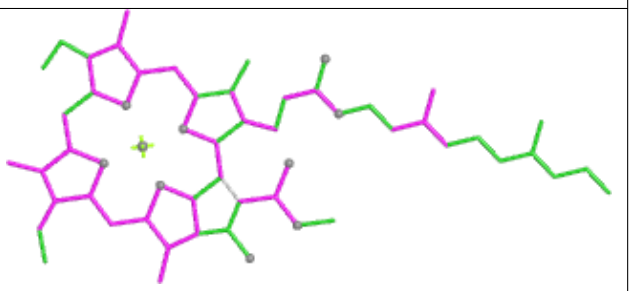


Rings

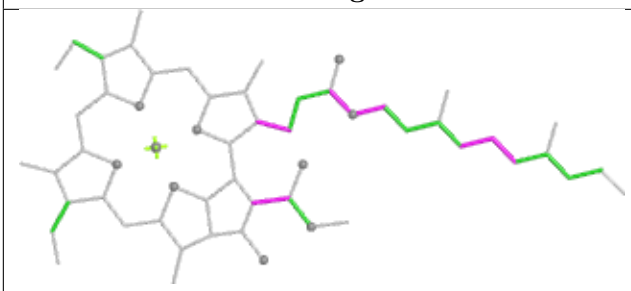
Ligand CLA bB 802



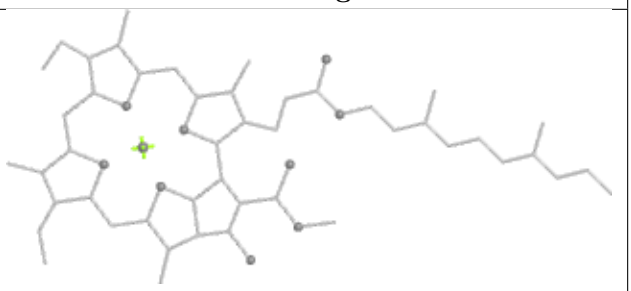
Bond lengths



Bond angles

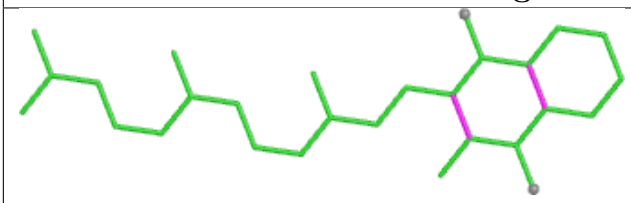


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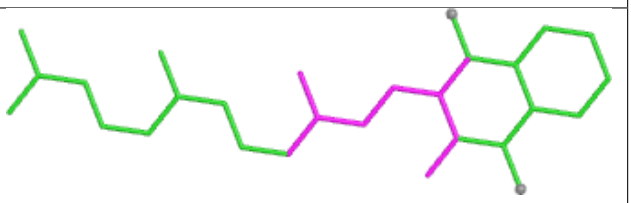


Rings

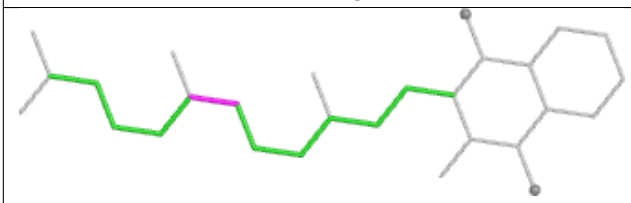
Ligand PQN aB 841



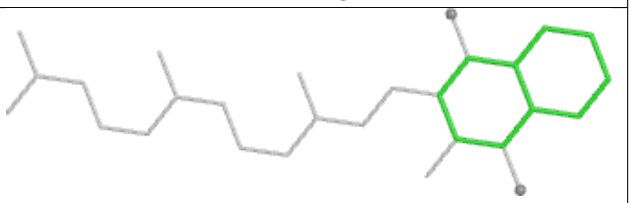
Bond lengths



Bond angles

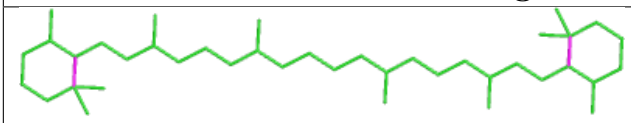


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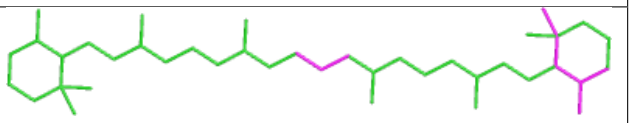


Rings

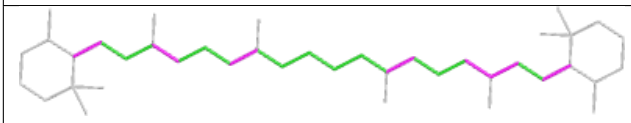
Ligand BCR aB 844



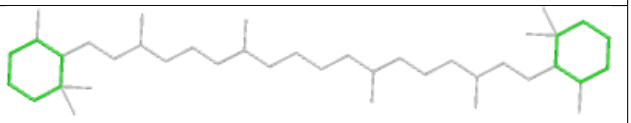
Bond lengths



Bond angles

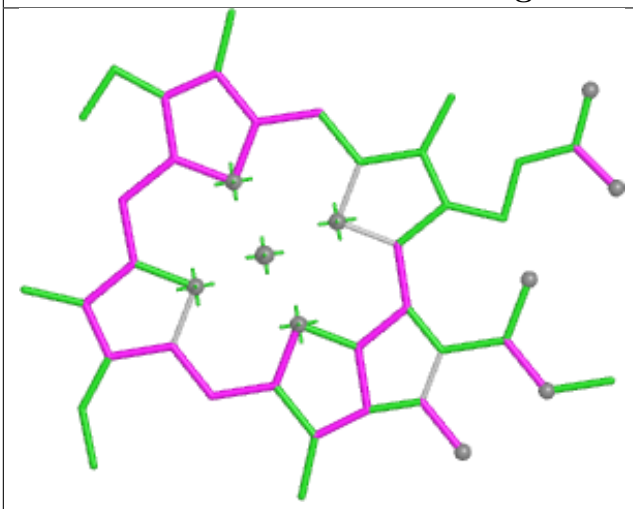


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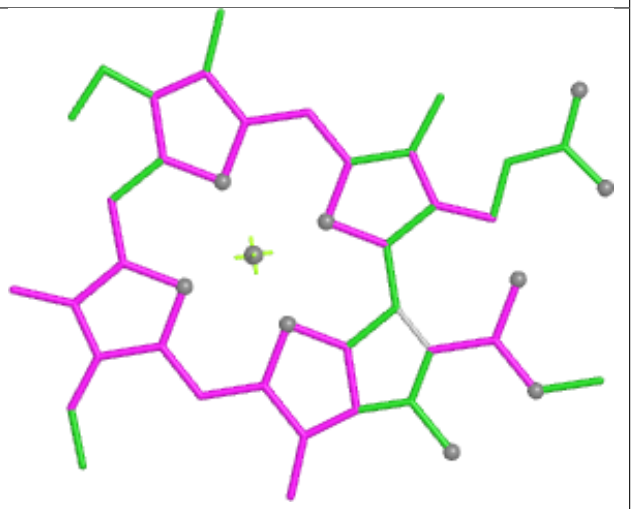


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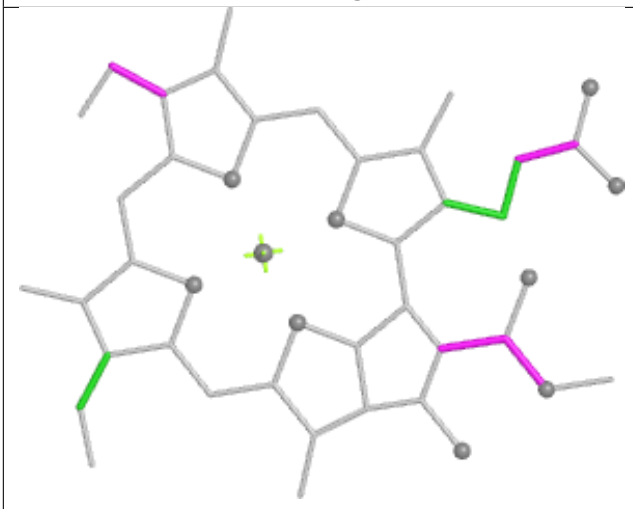
Ligand CLA aA 805



Bond lengths



Bond angles

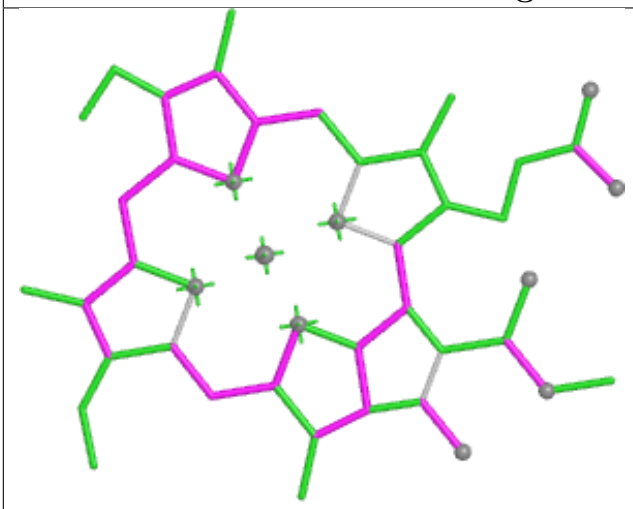


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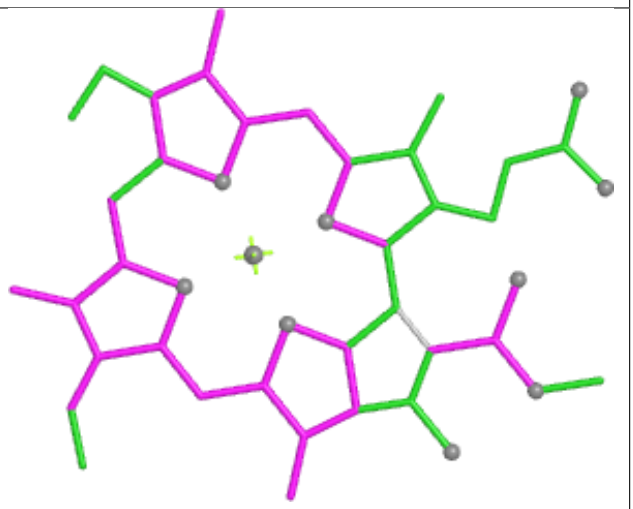


Rings

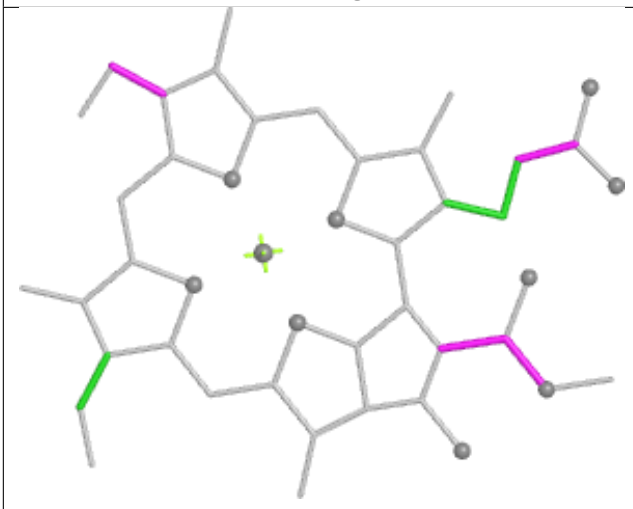
Ligand CLA cB 820



Bond lengths



Bond angles

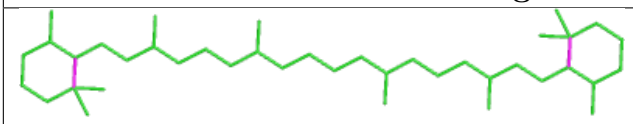


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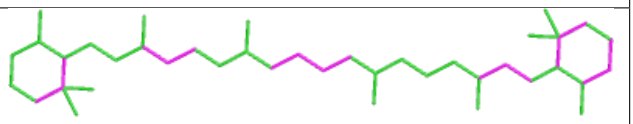


Rings

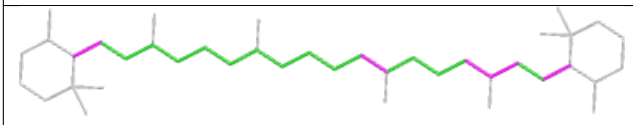
Ligand BCR aA 847



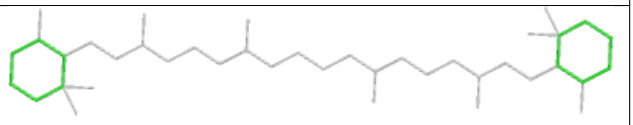
Bond lengths



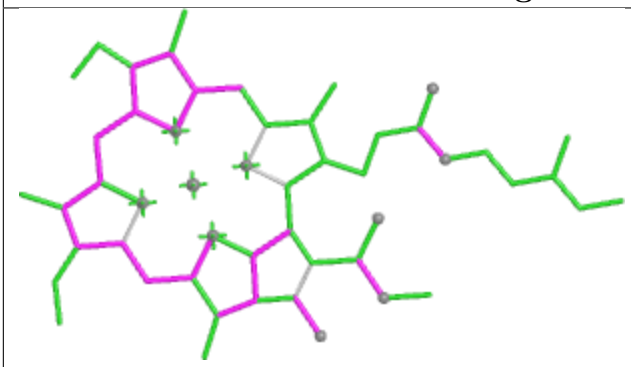
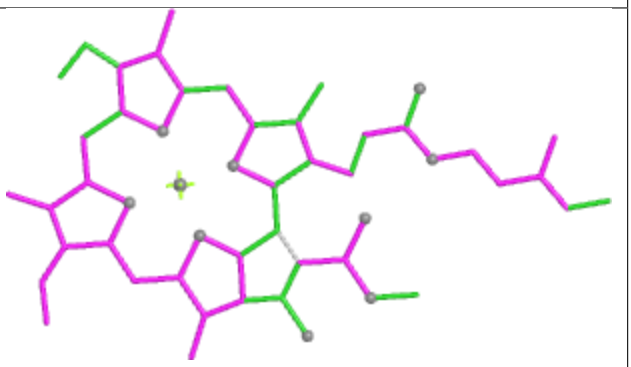
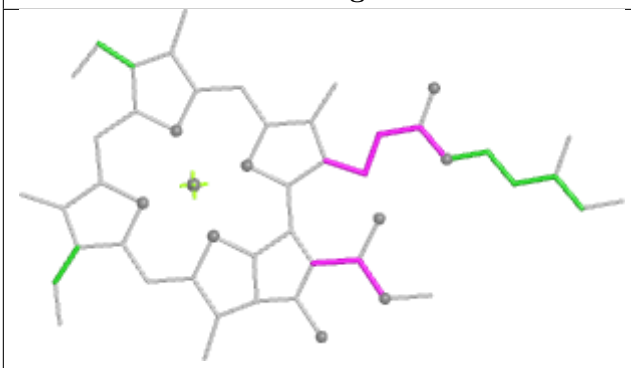
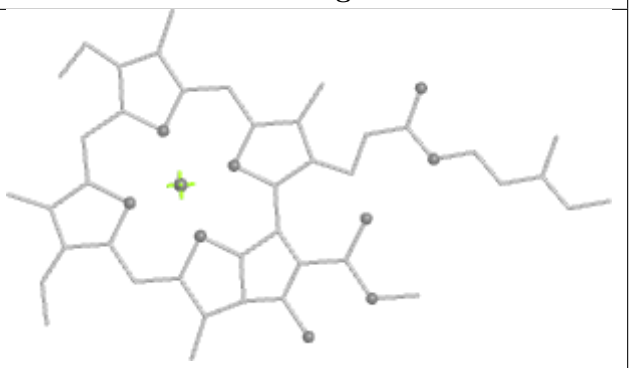
Bond angles

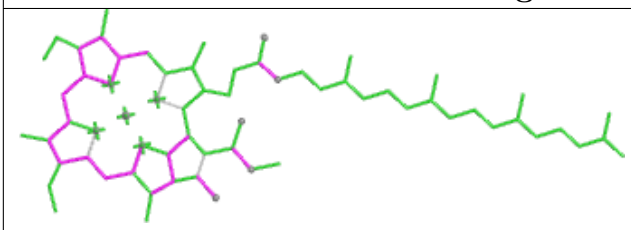
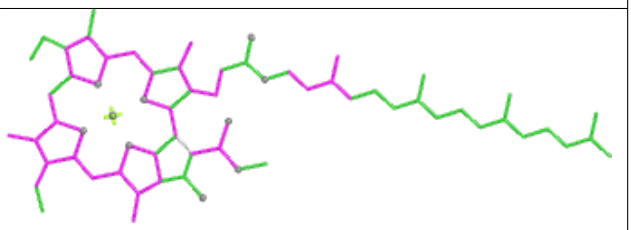
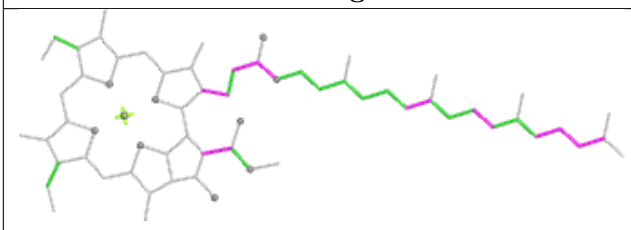
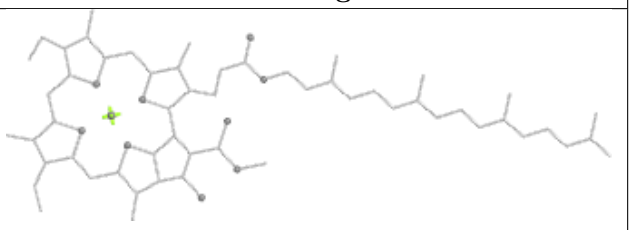


Torsions

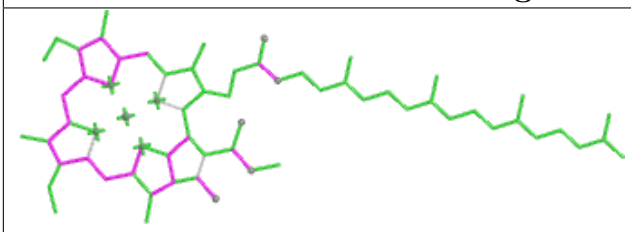


Rings

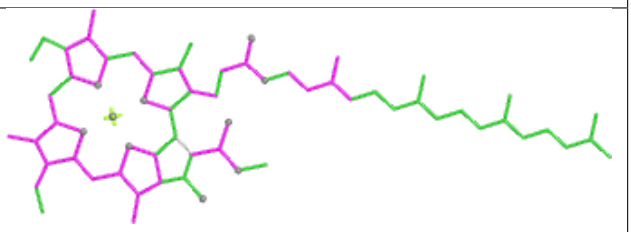
Ligand CLA aA 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

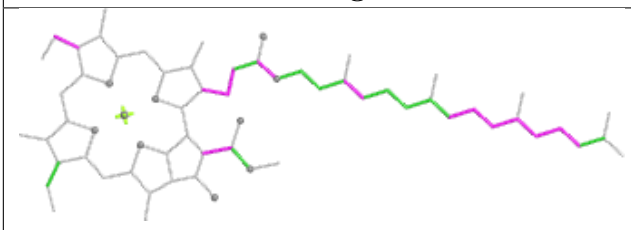
Ligand CLA bB 812



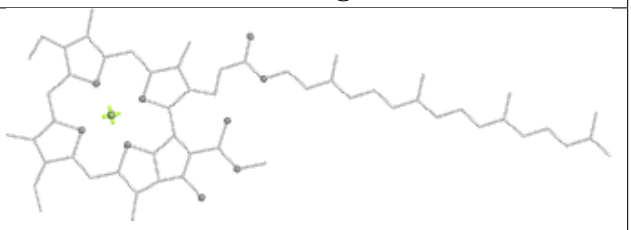
Bond lengths



Bond angles

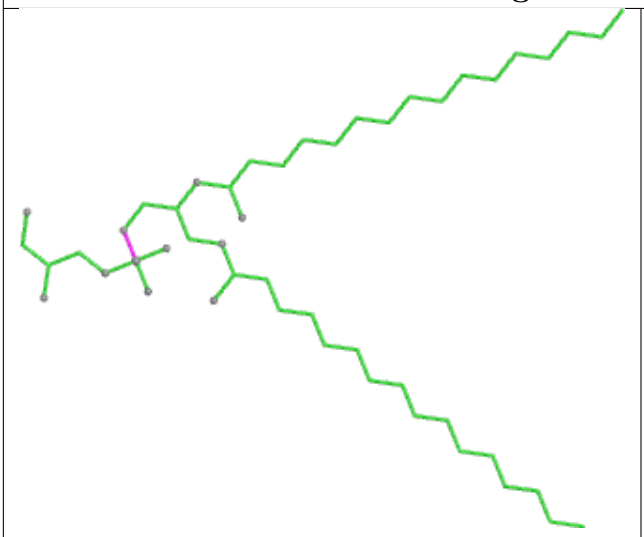


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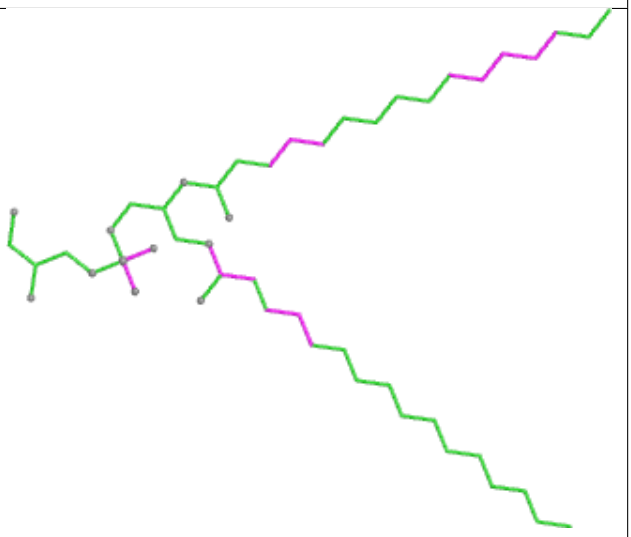


Rings

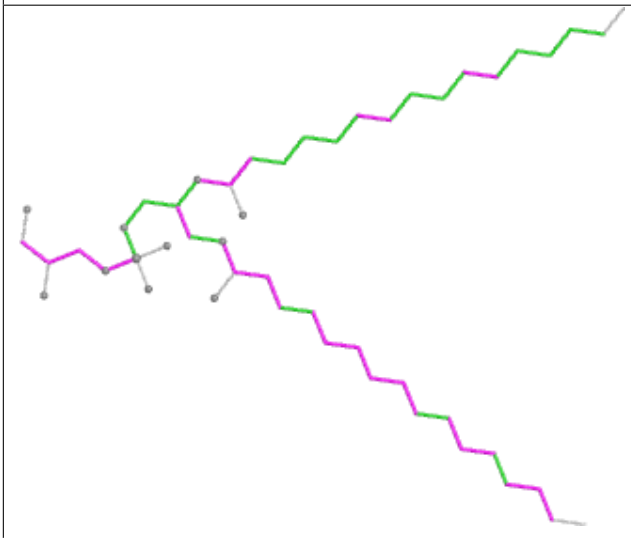
Ligand LHG bA 852



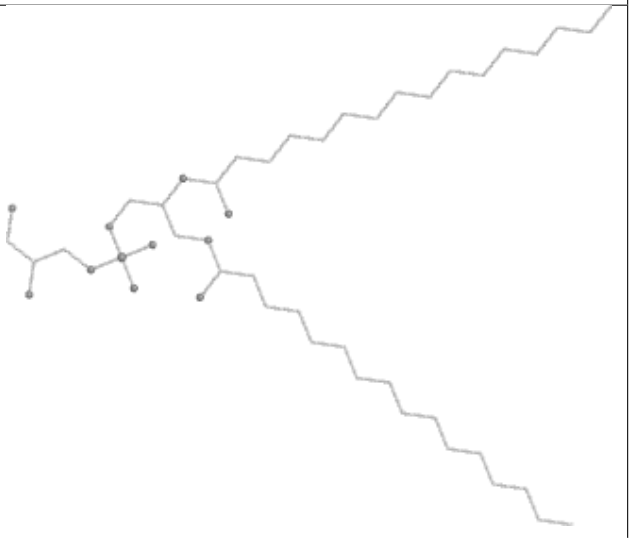
Bond lengths



Bond angles

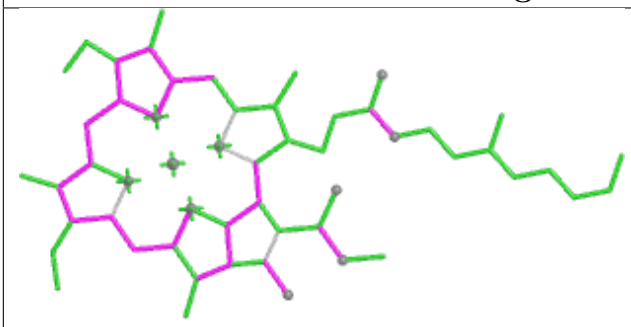


Torsions

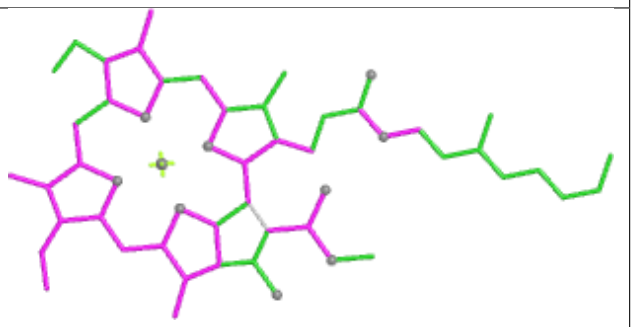


Rings

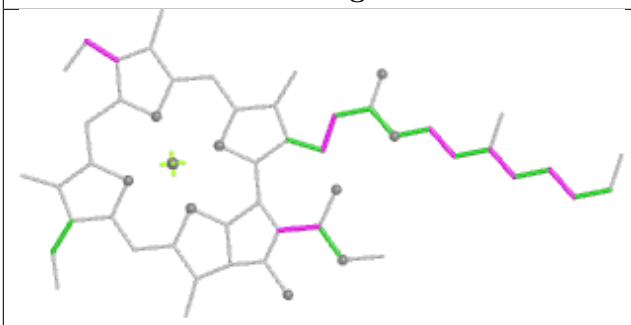
Ligand CLA bB 823



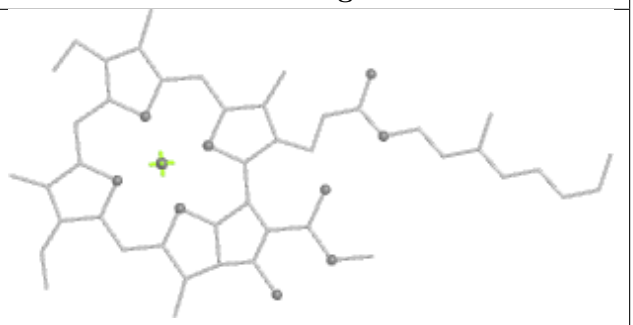
Bond lengths



Bond angles

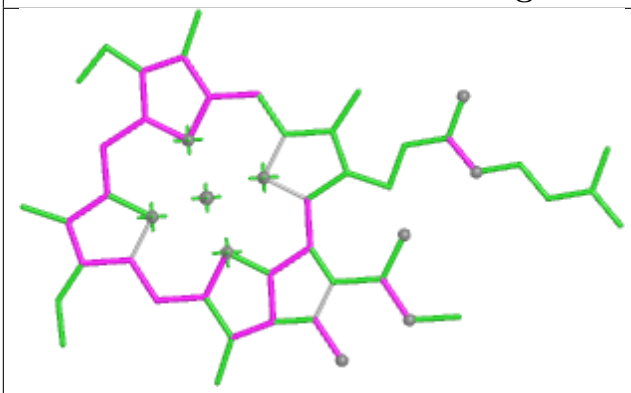


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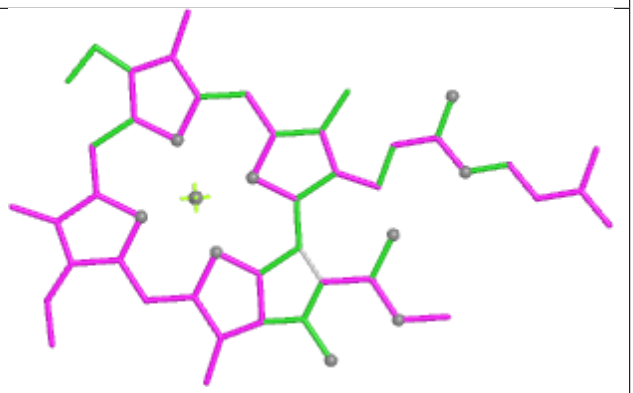


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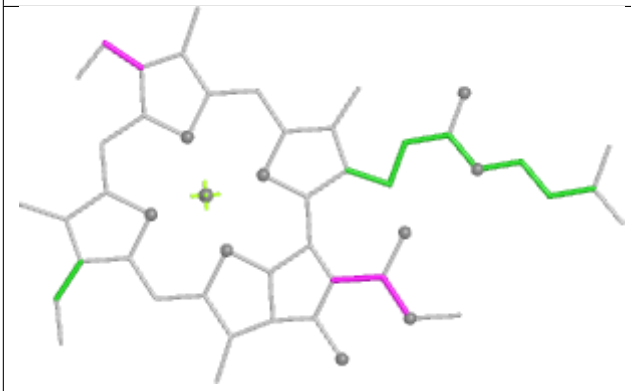
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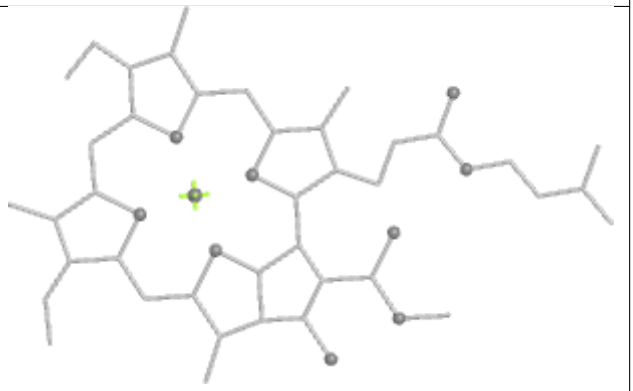
Bond lengths



Bond angles

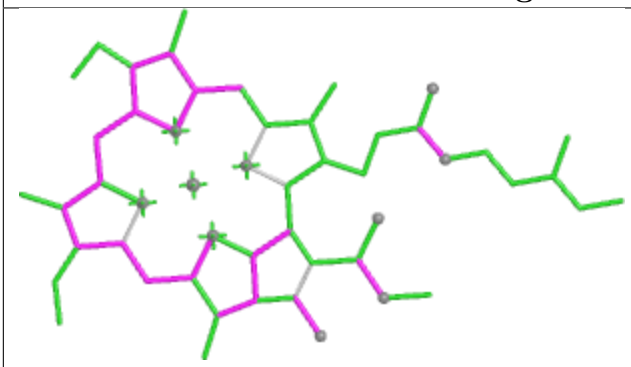


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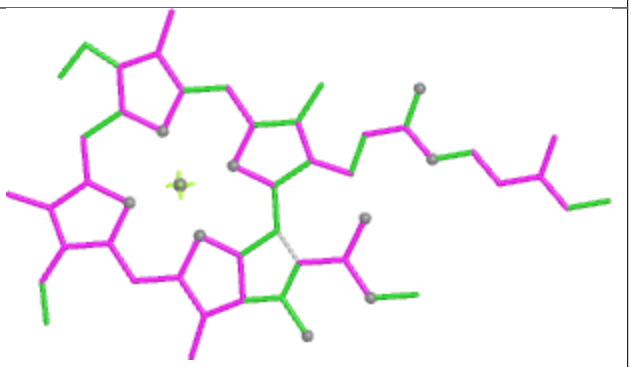


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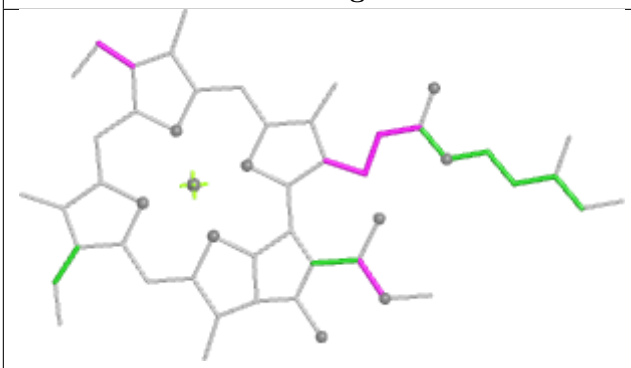
Ligand CLA cA 843



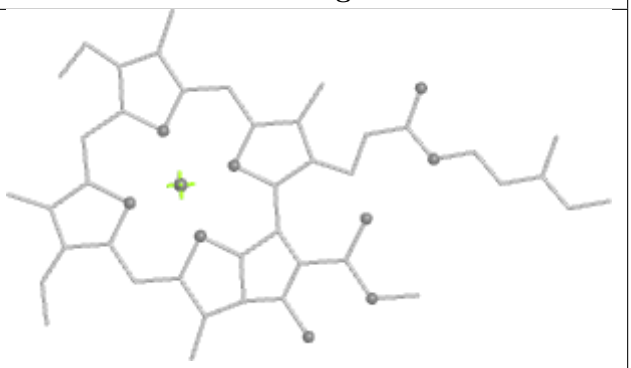
Bond lengths



Bond angles

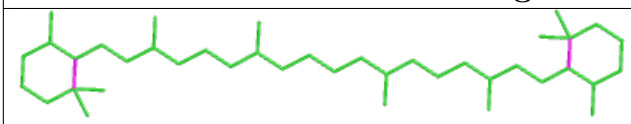


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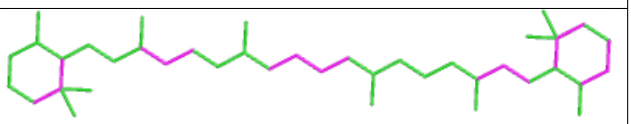


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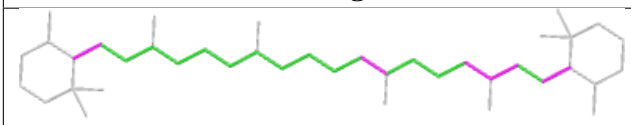
Ligand BCR cA 847



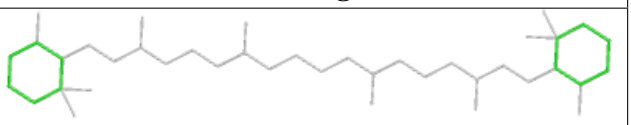
Bond lengths



Bond angles

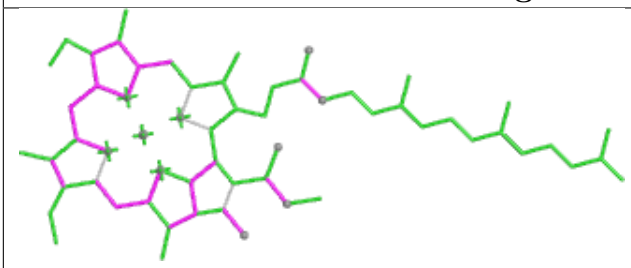


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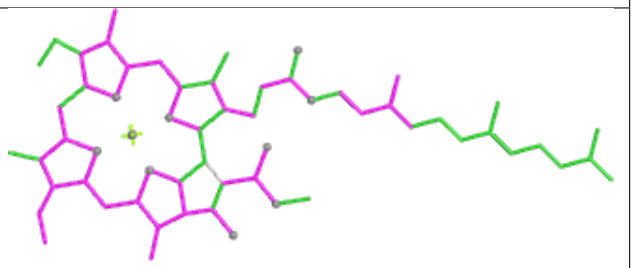


Rings

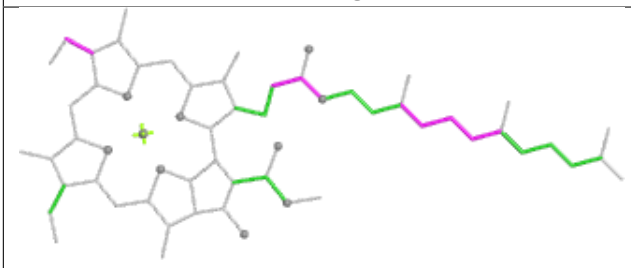
Ligand CLA aA 828



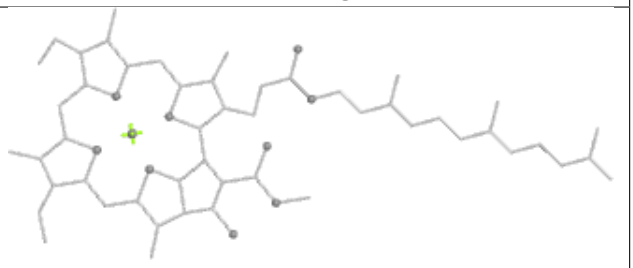
Bond lengths



Bond angles

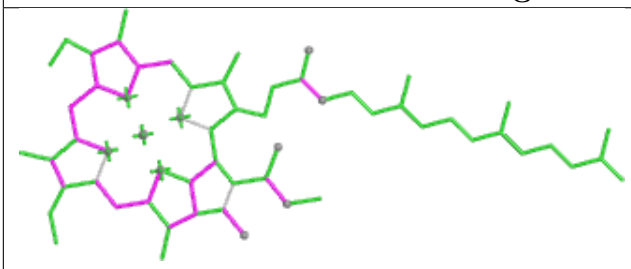


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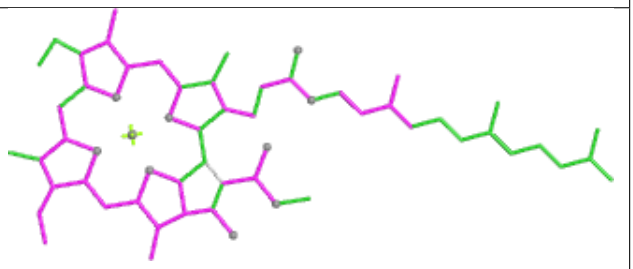


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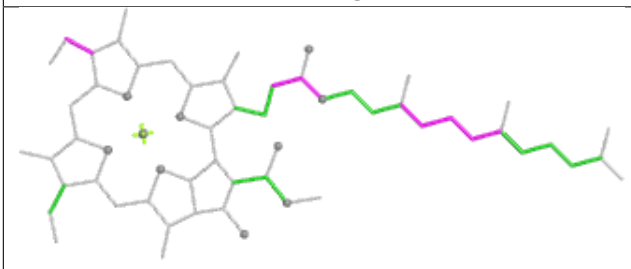
Ligand CLA bA 828



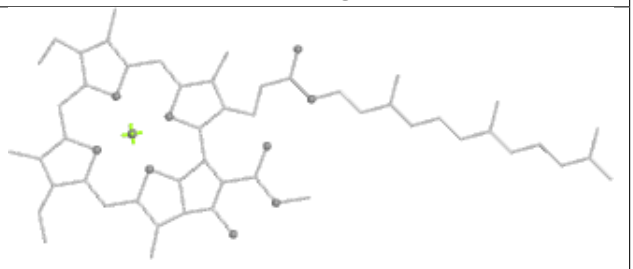
Bond lengths



Bond angles

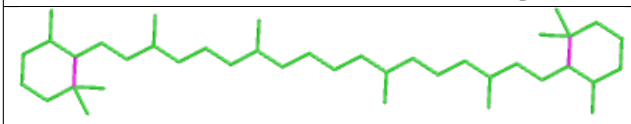


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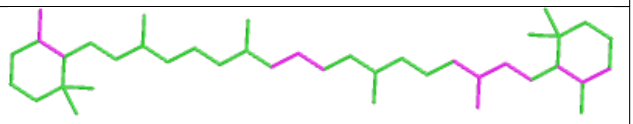


Rings

Ligand BCR cA 848



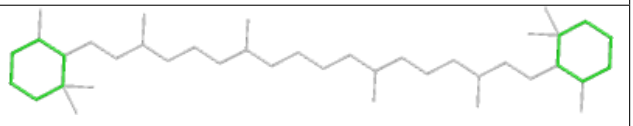
Bond lengths



Bond angles

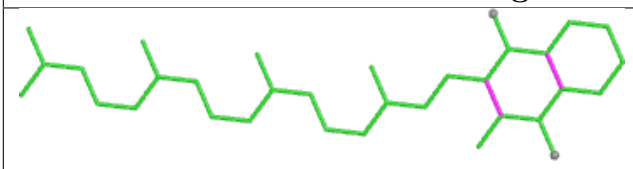


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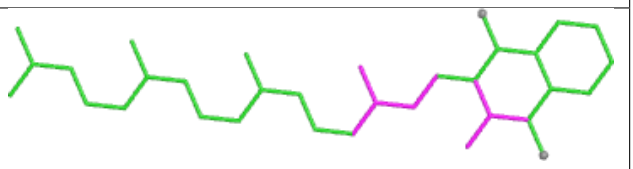


Rings

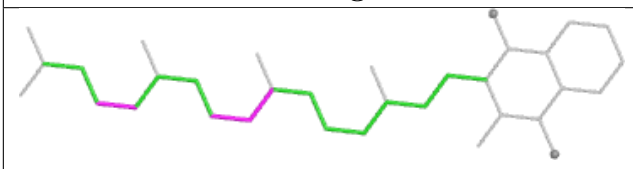
Ligand PQN bA 845



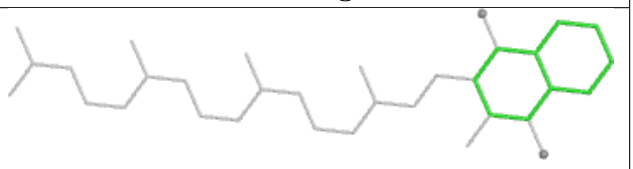
Bond lengths



Bond angles

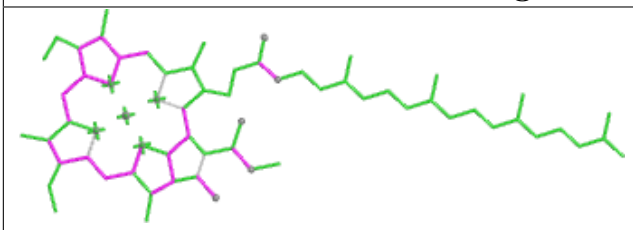


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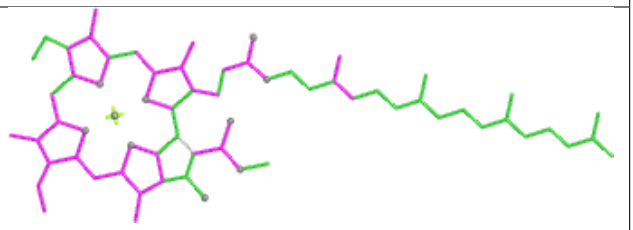


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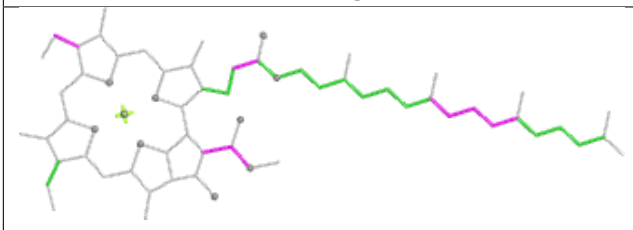
Ligand CLA bA 825



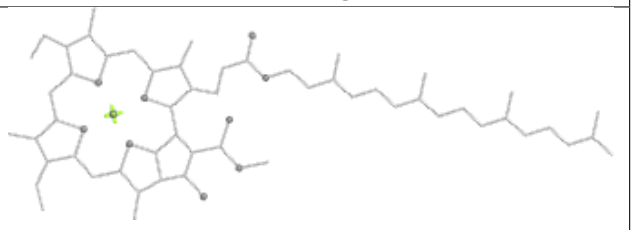
Bond lengths



Bond angles

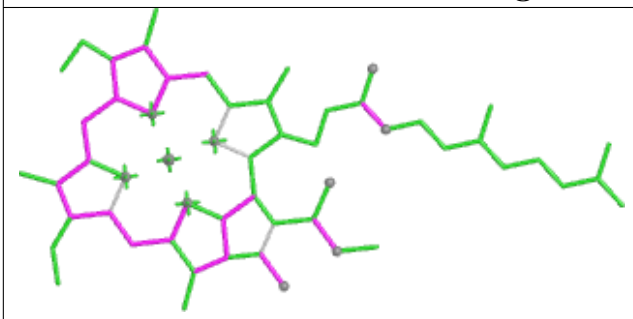


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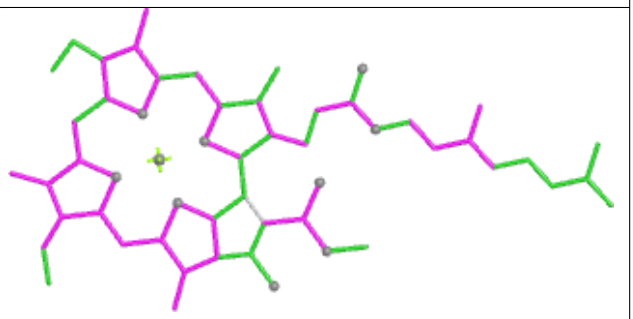


Rings

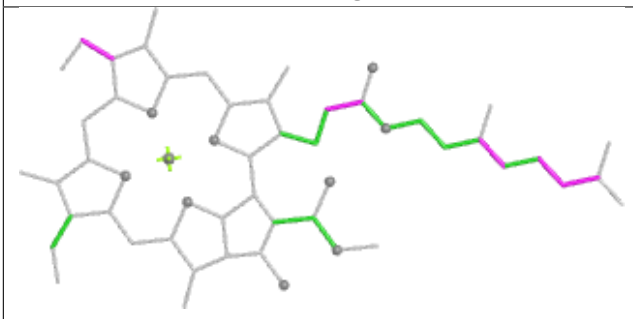
Ligand CLA bB 837



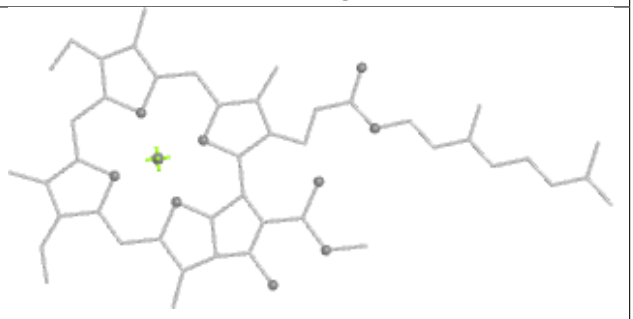
Bond lengths



Bond angles

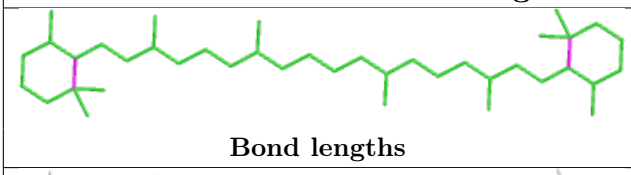


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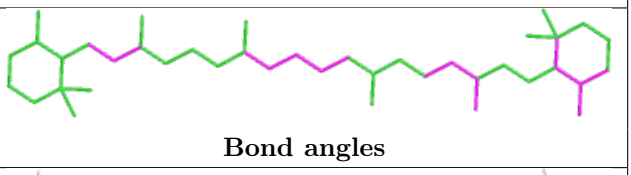


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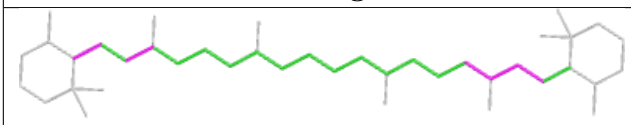
Ligand BCR aK 102



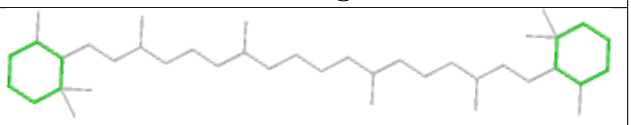
Bond lengths



Bond angles

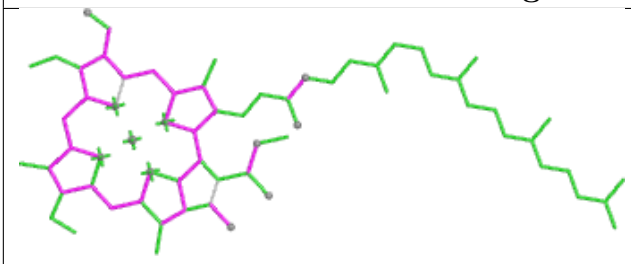


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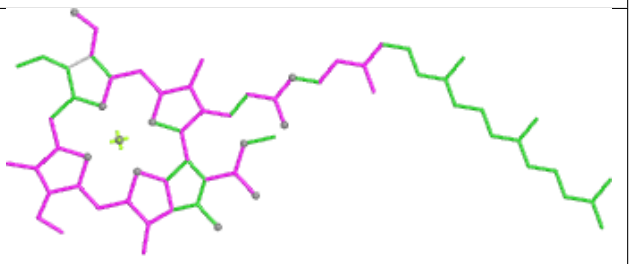


Rings

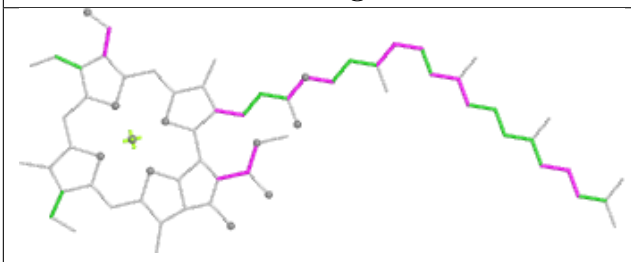
Ligand F6C cL 202



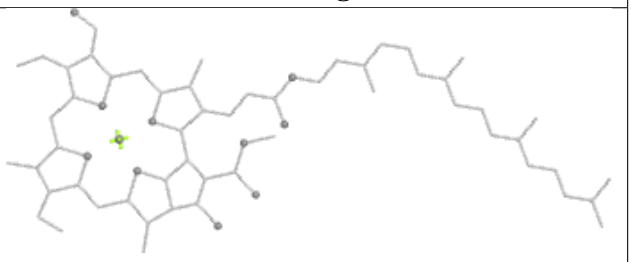
Bond lengths



Bond angles

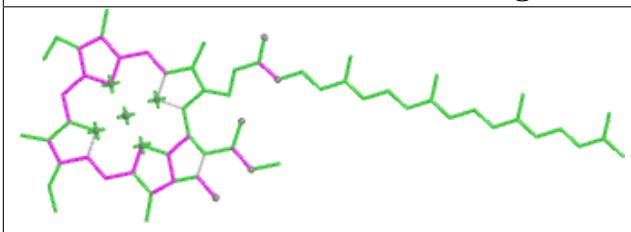


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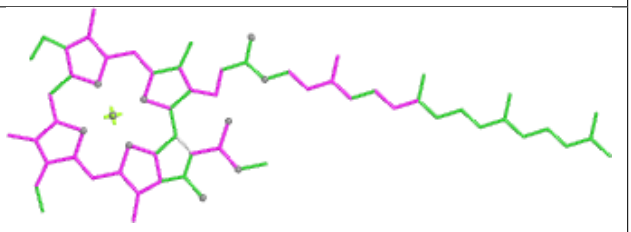


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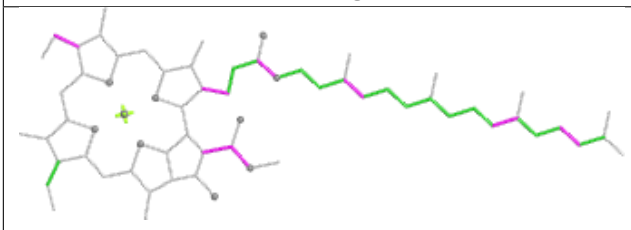
Ligand CLA bA 806



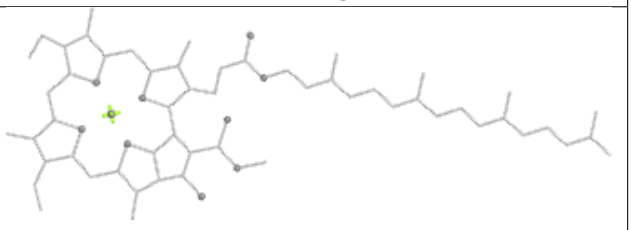
Bond lengths



Bond angles

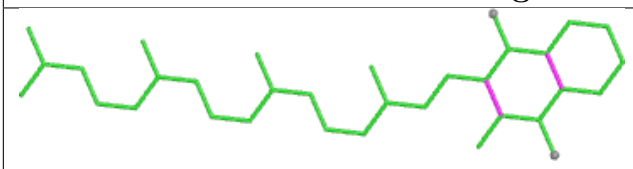


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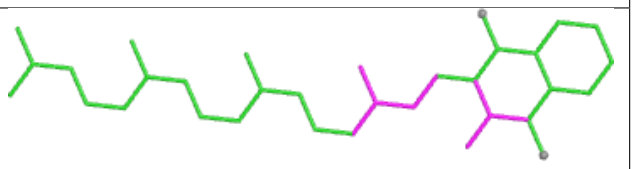


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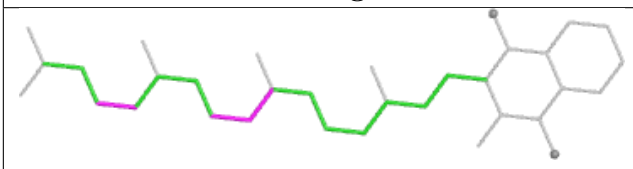
Ligand PQN aA 845



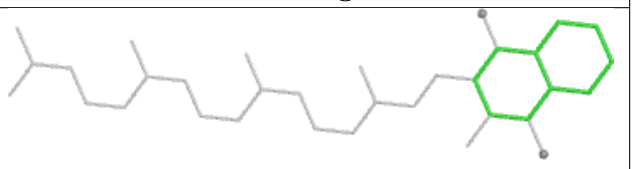
Bond lengths



Bond angles

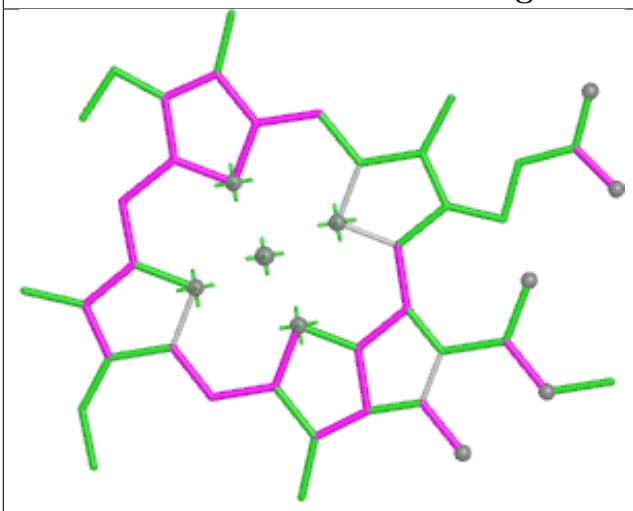


Torsions

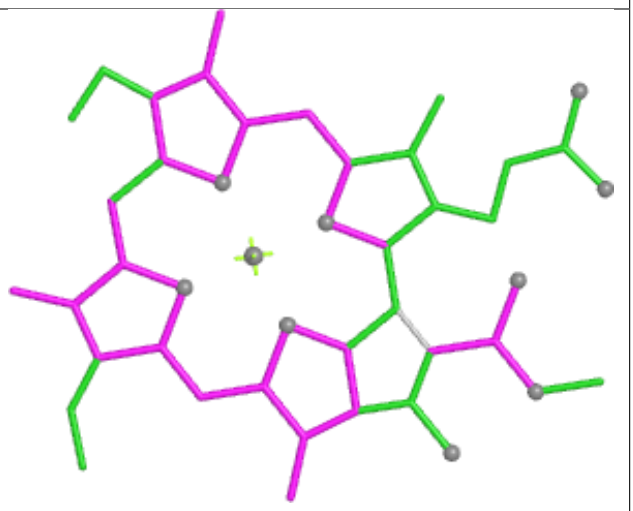


Rings

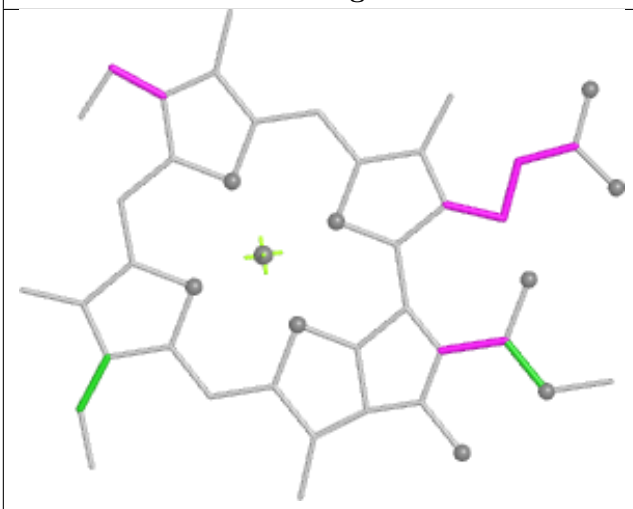
Ligand CLA cA 823



Bond lengths



Bond angles

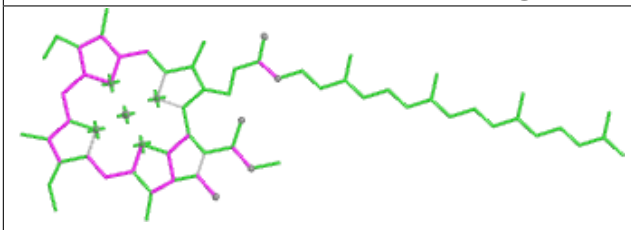


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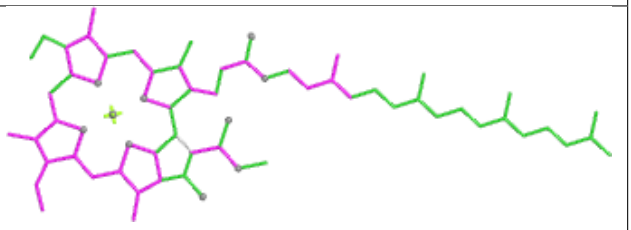


Rings

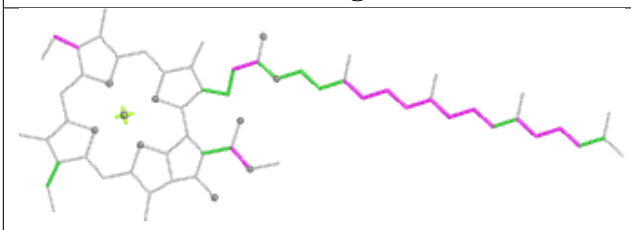
Ligand CLA aB 806



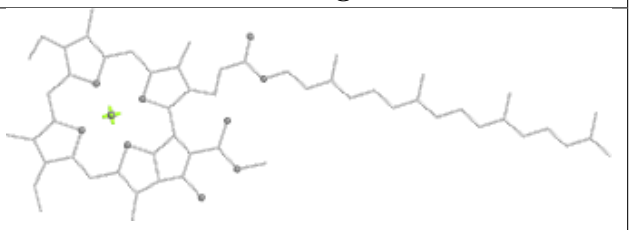
Bond lengths



Bond angles

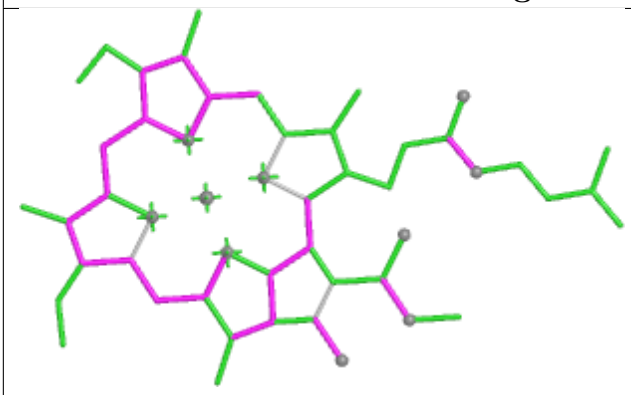


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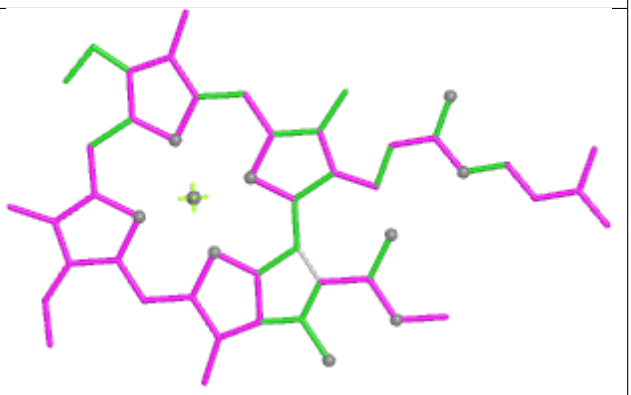


Rings

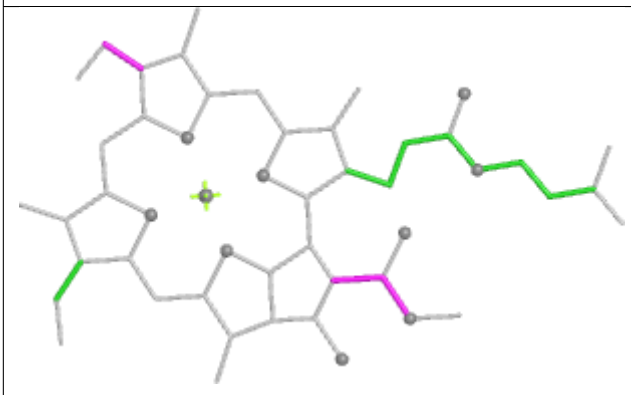
Ligand CLA bA 841



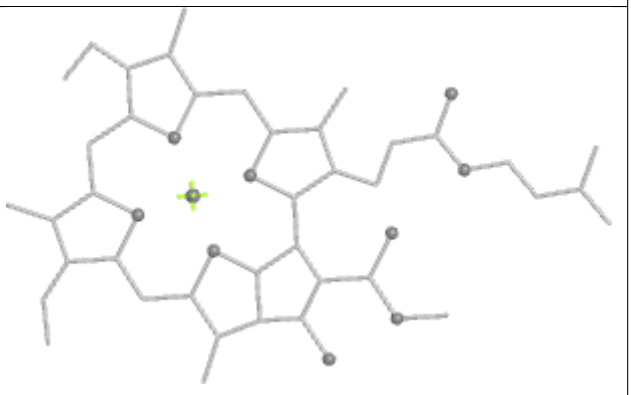
Bond lengths



Bond angles

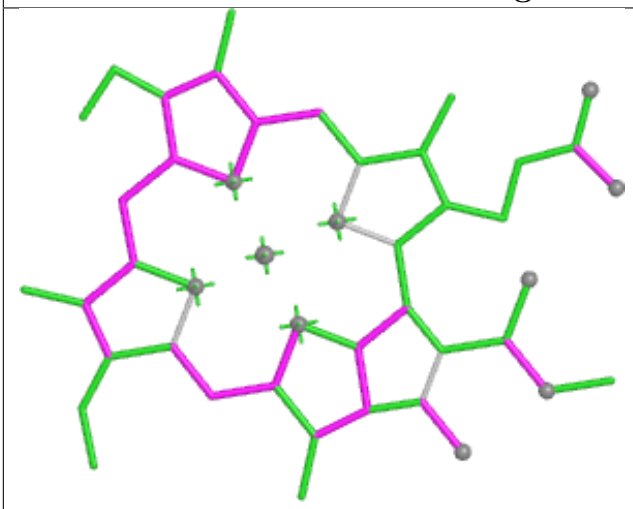


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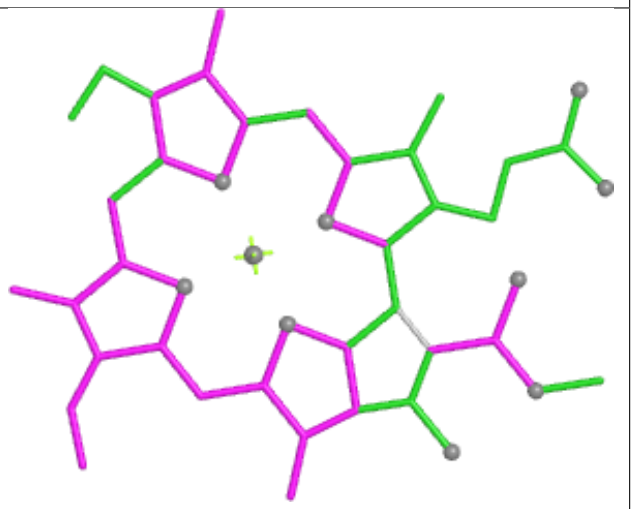


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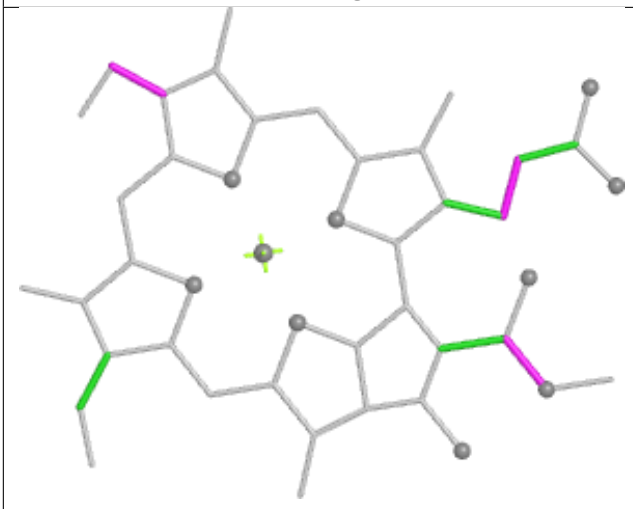
Ligand CLA bB 840



Bond lengths



Bond angles

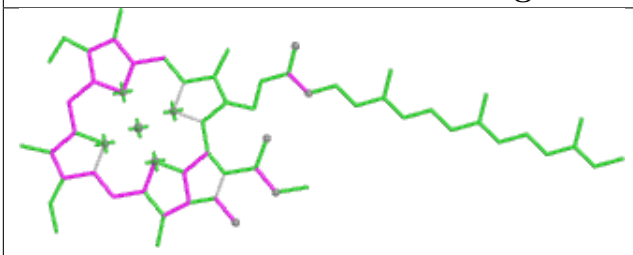


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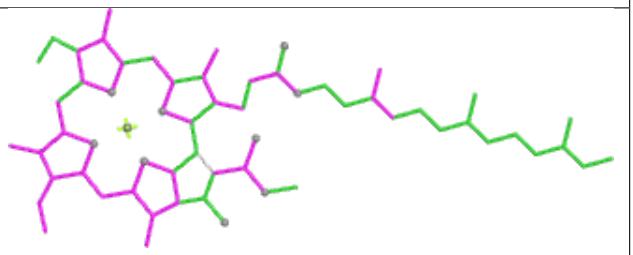


Rings

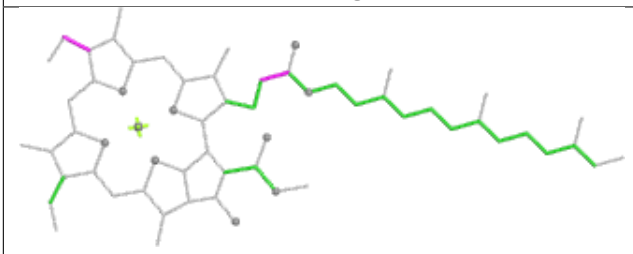
Ligand CLA bB 807



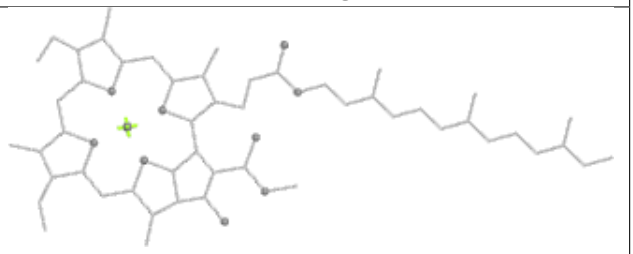
Bond lengths



Bond angles

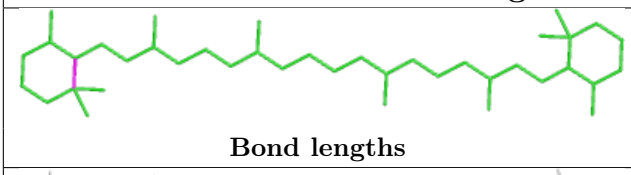


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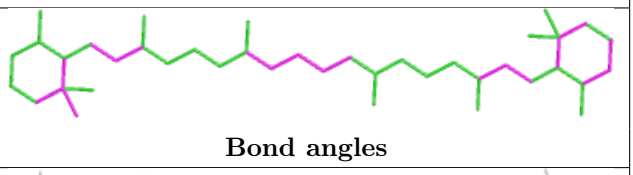


Rings

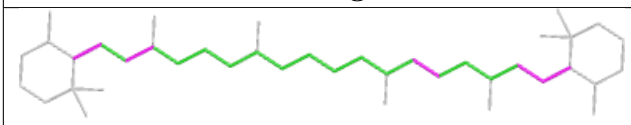
Ligand BCR bM 101



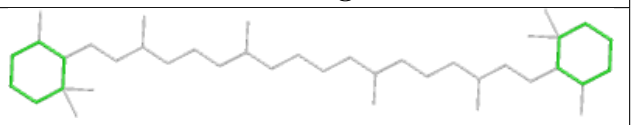
Bond lengths



Bond angles

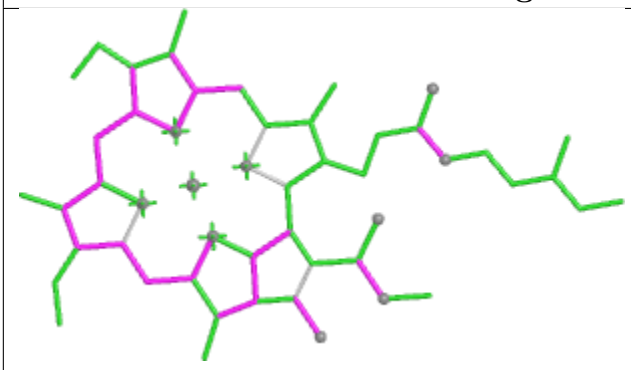


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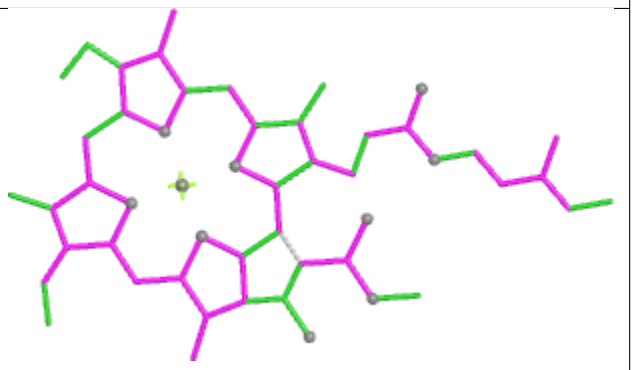


Rings

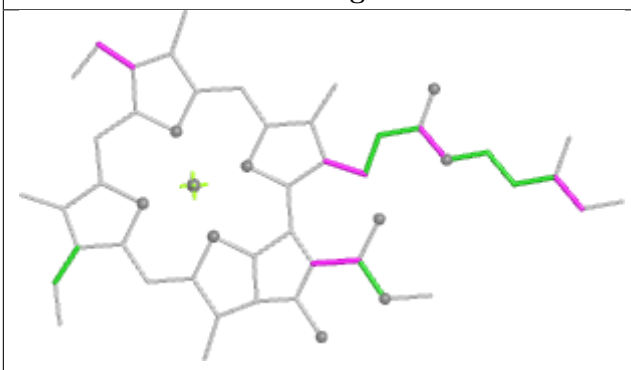
Ligand CLA aB 836



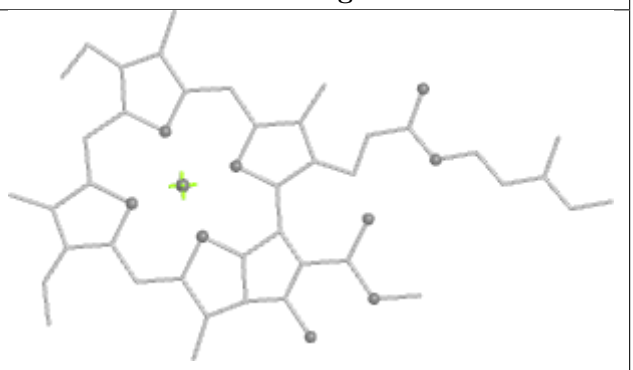
Bond lengths



Bond angles

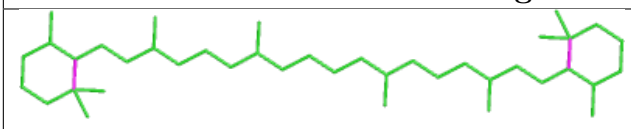


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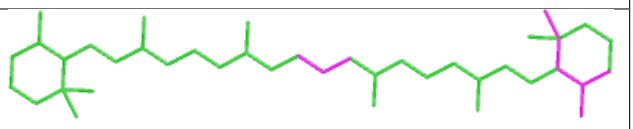


Rings

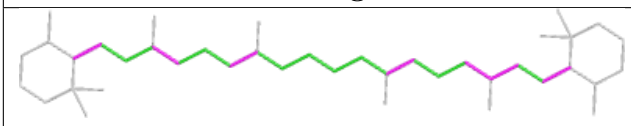
Ligand BCR cB 844



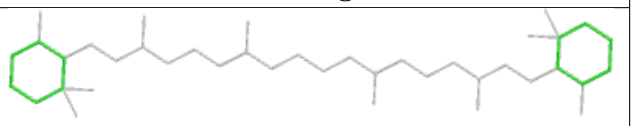
Bond lengths



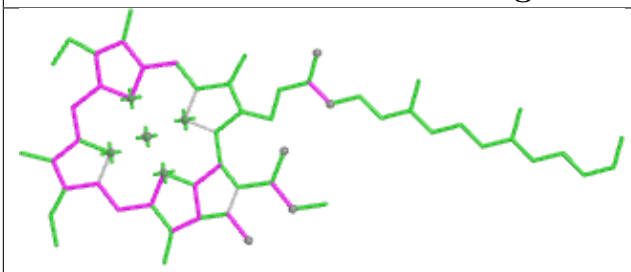
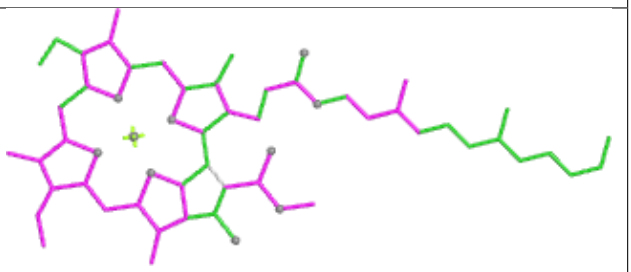
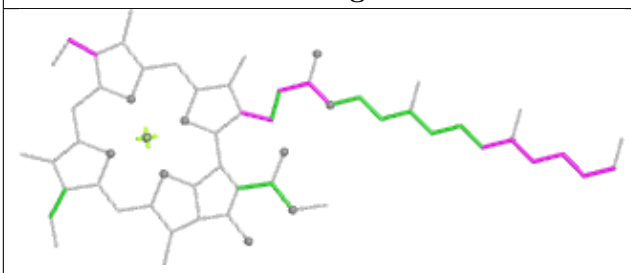
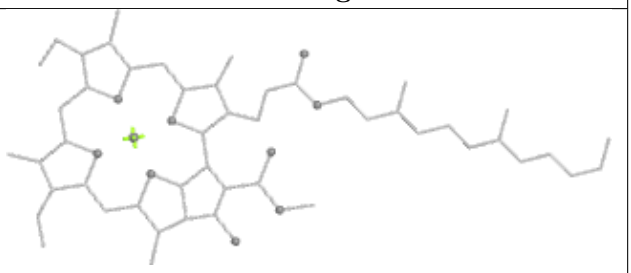
Bond angles

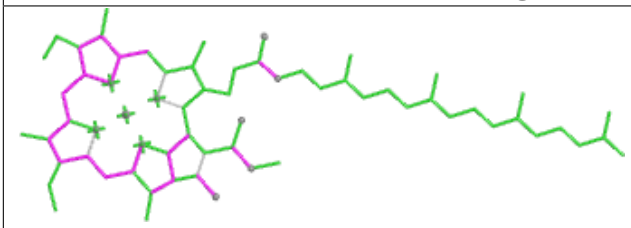
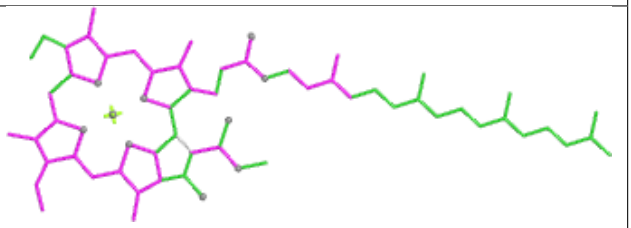
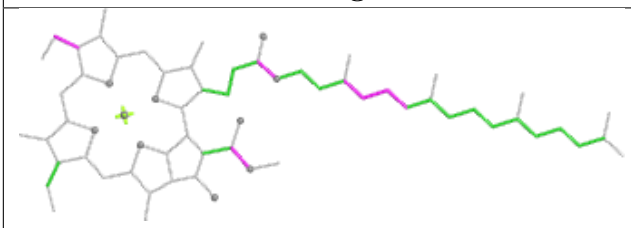
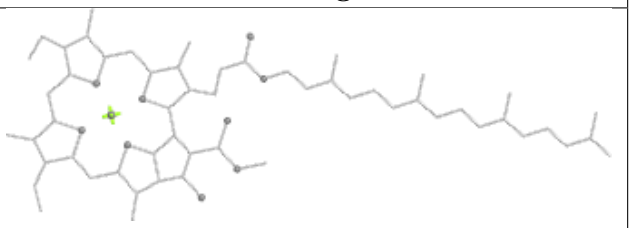


Torsions

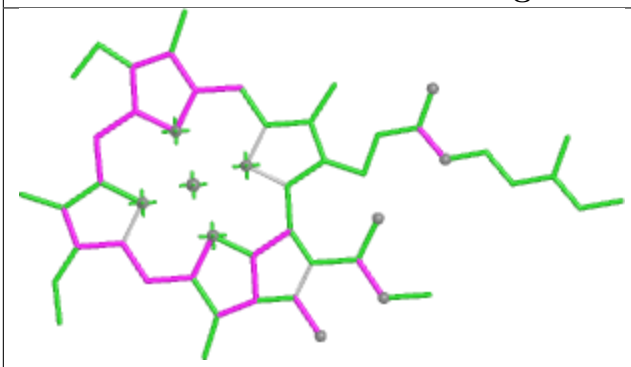


Rings

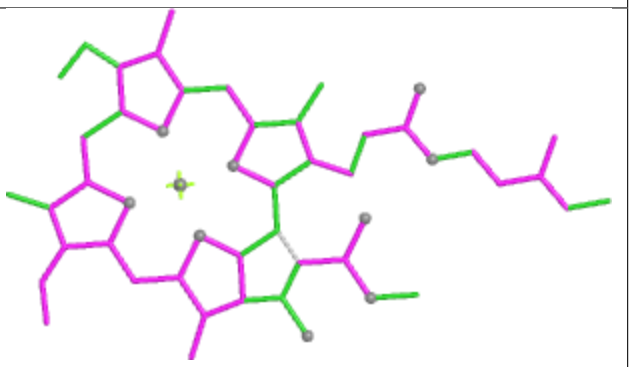
Ligand CLA bB 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

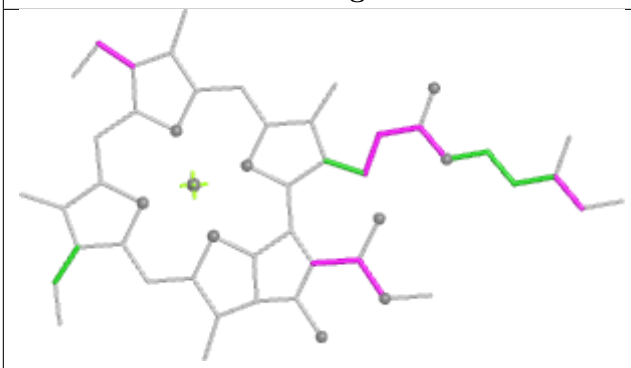
Ligand CLA bA 824



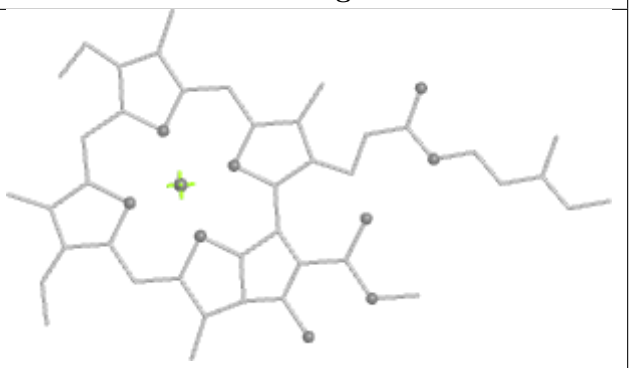
Bond lengths



Bond angles

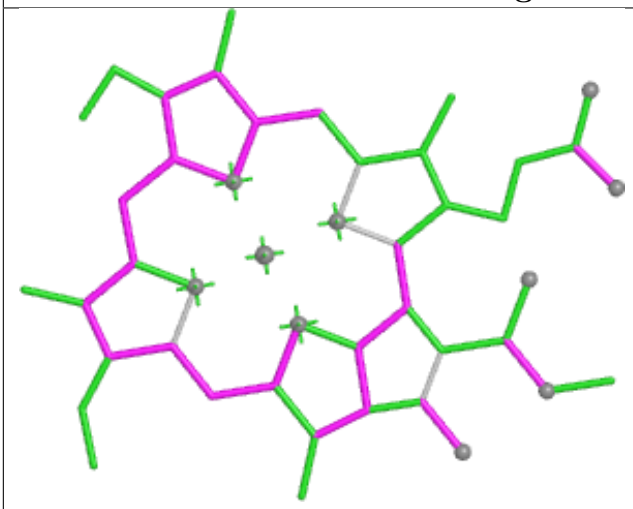


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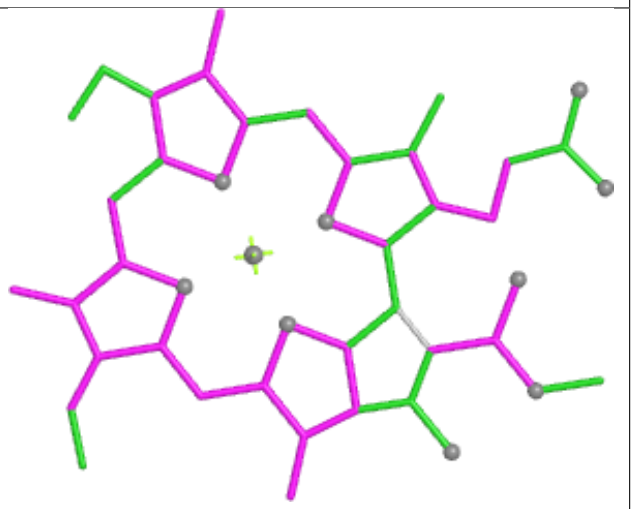


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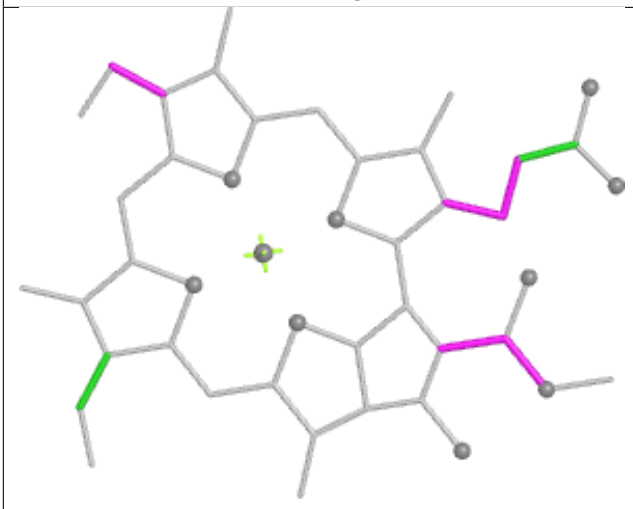
Ligand CLA aA 809



Bond lengths



Bond angles

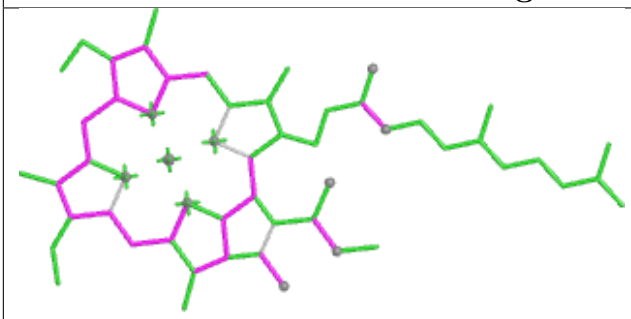


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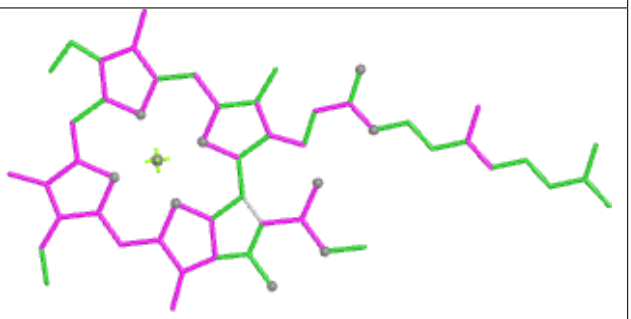


Rings

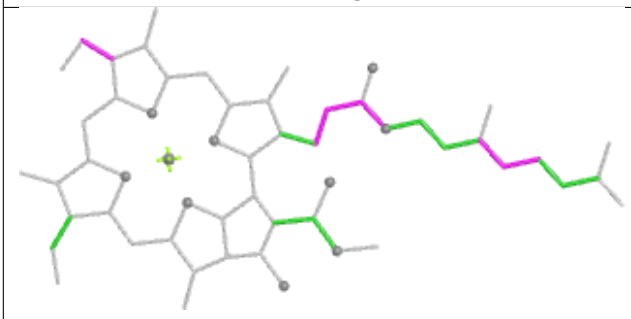
Ligand CLA aB 821



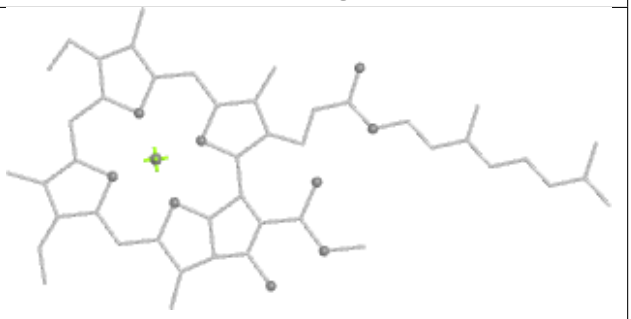
Bond lengths



Bond angles

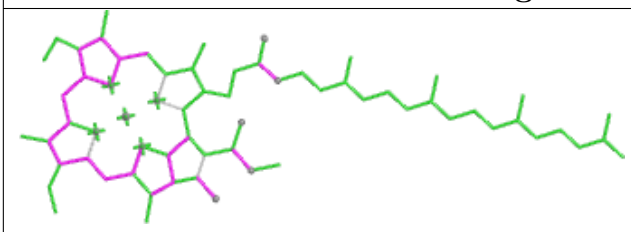


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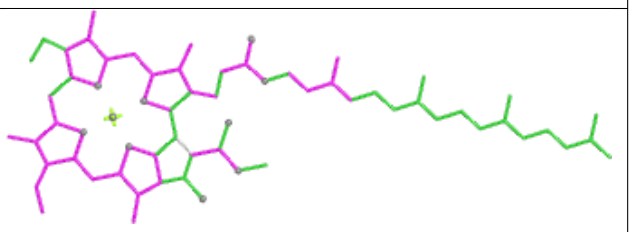


Rings

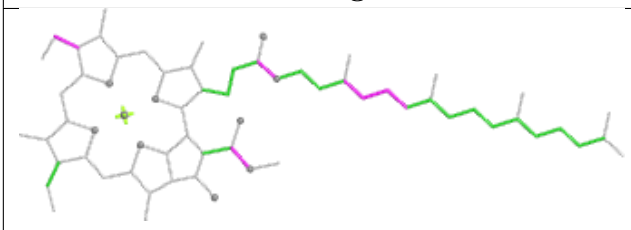
Ligand CLA aA 834



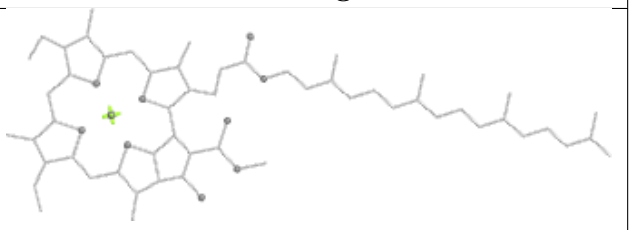
Bond lengths



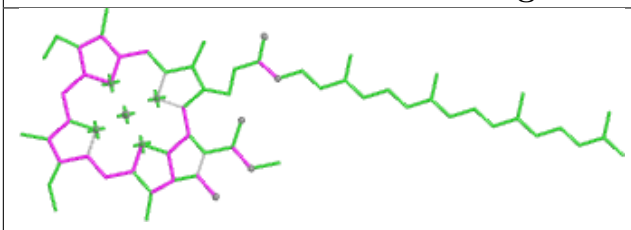
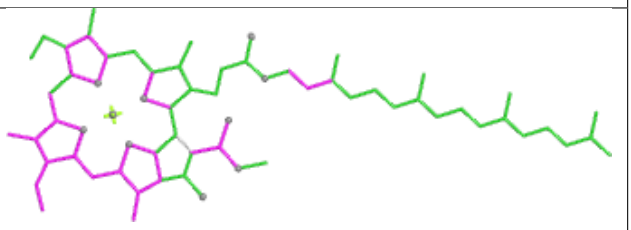
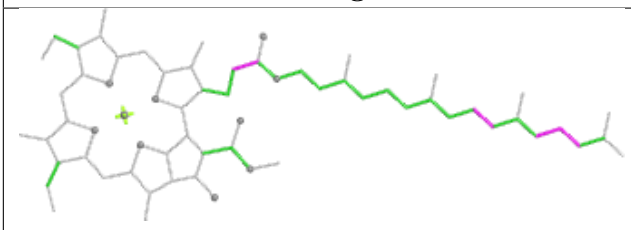
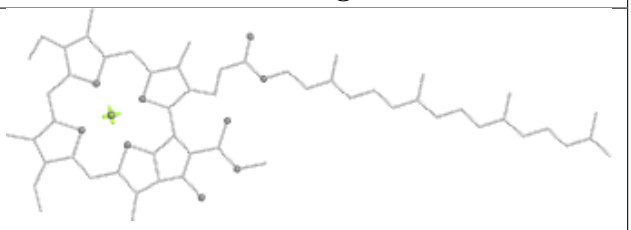
Bond angles

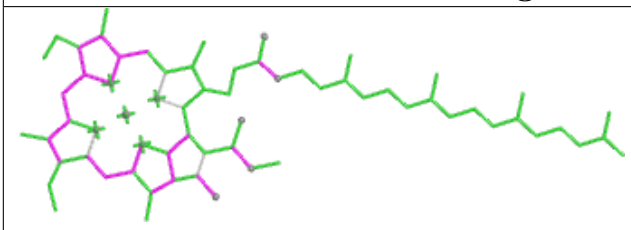
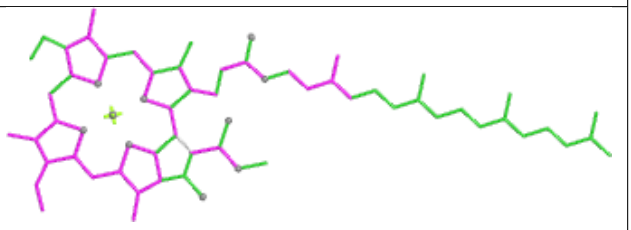
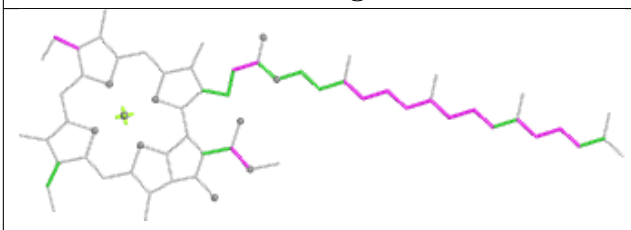
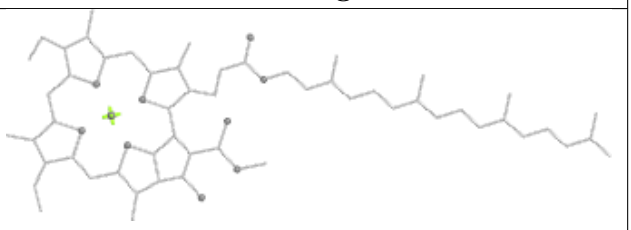


Torsions

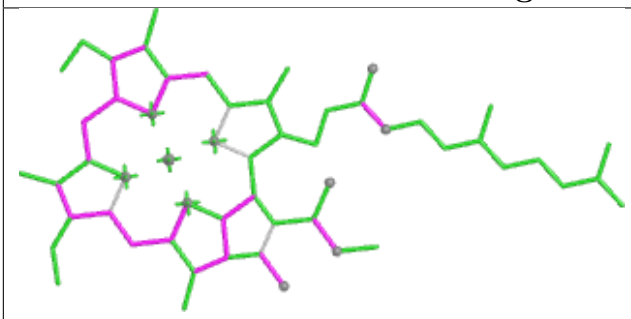


Rings

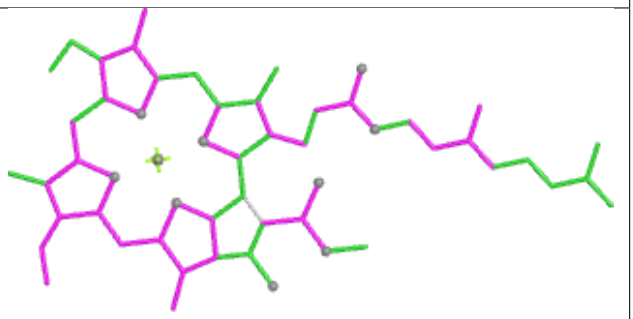
Ligand CLA aL 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

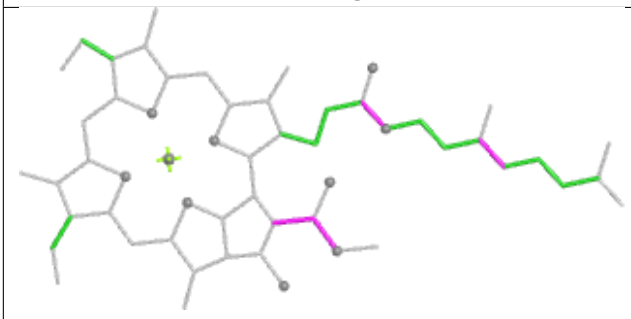
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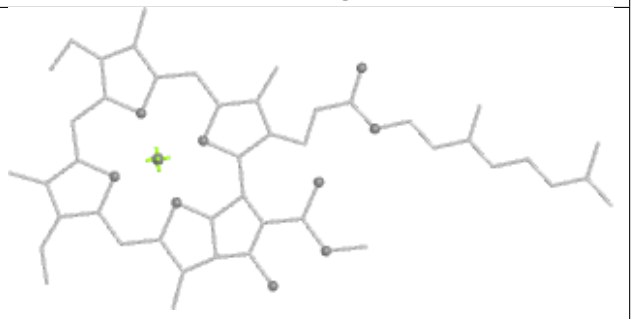
Bond lengths



Bond angles

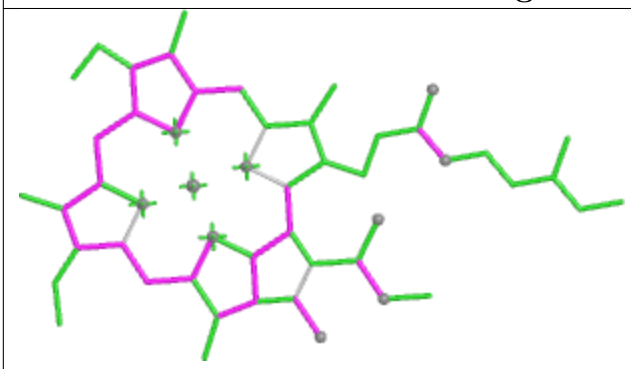


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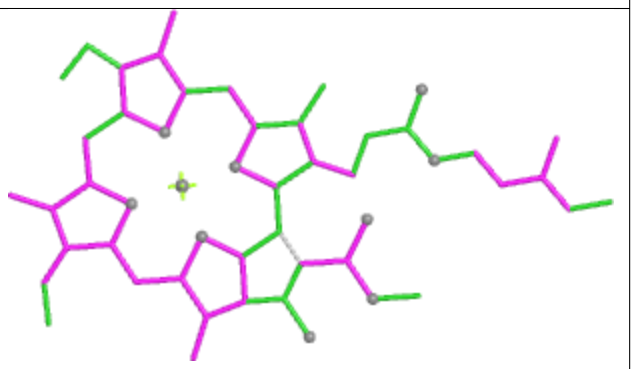


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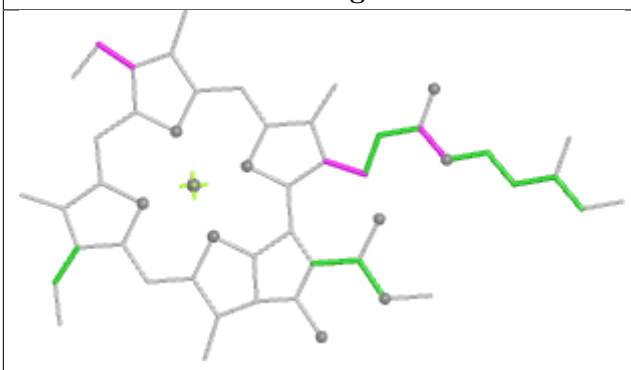
Ligand CLA cA 808



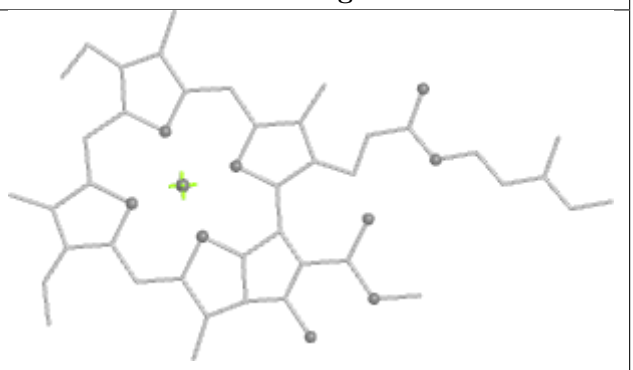
Bond lengths



Bond angles

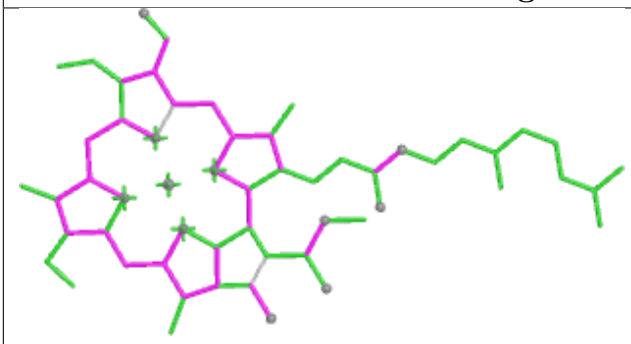


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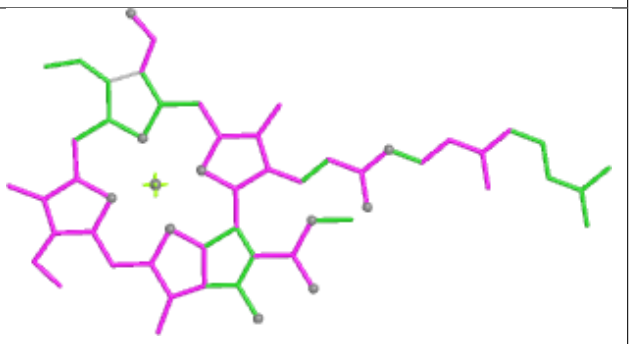


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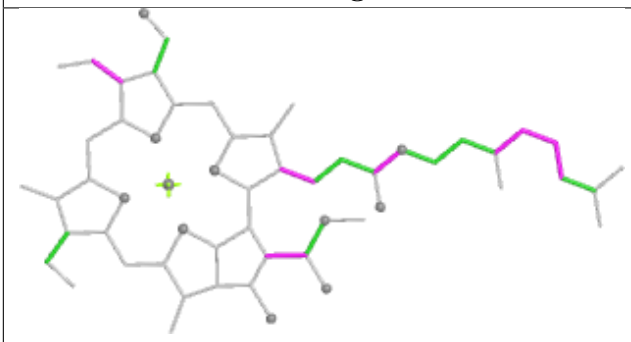
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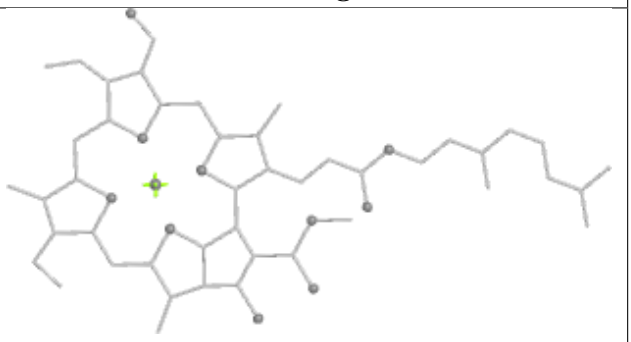
Bond lengths



Bond angles

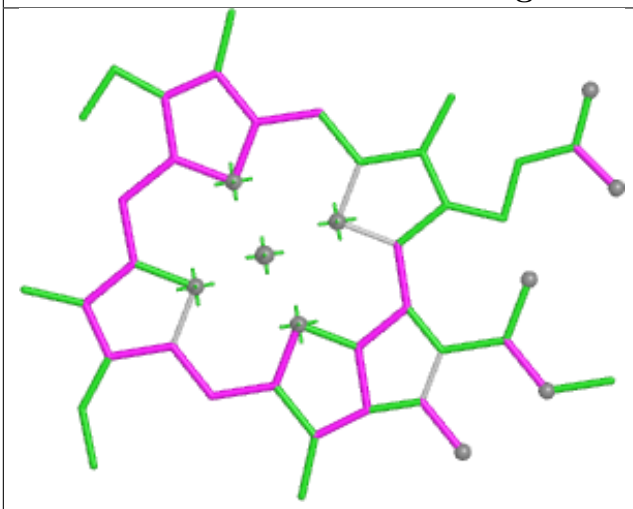


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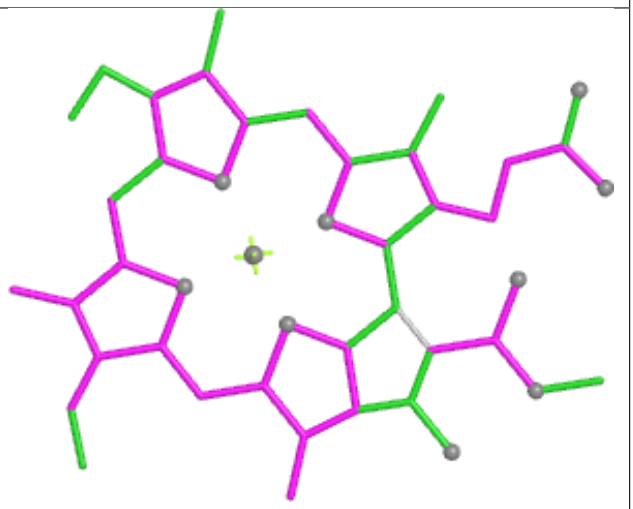


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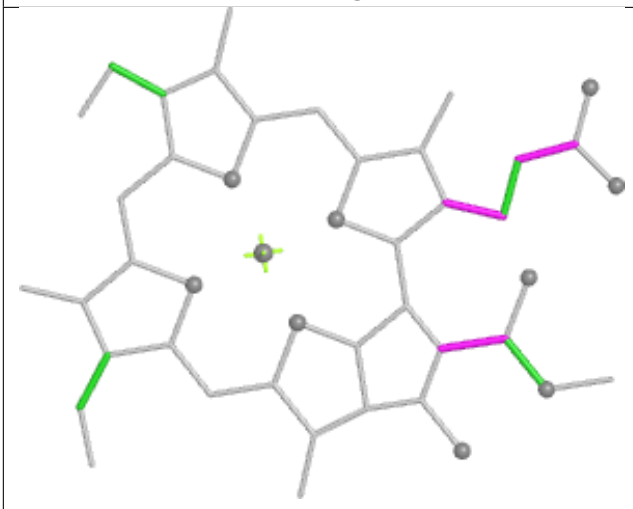
Ligand CLA cA 837



Bond lengths



Bond angles

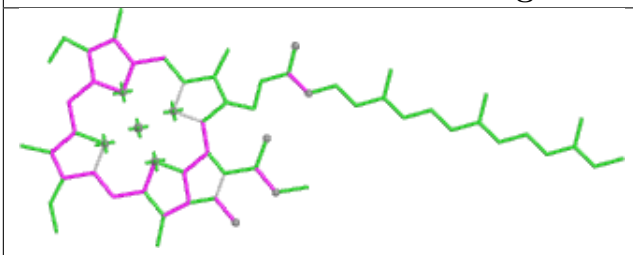


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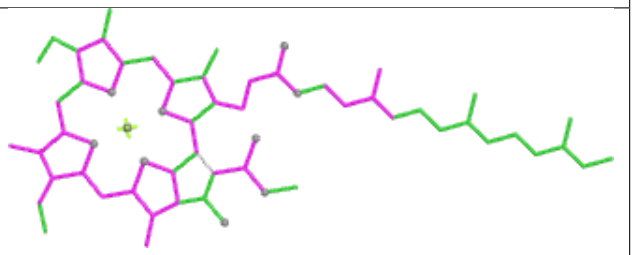


Rings

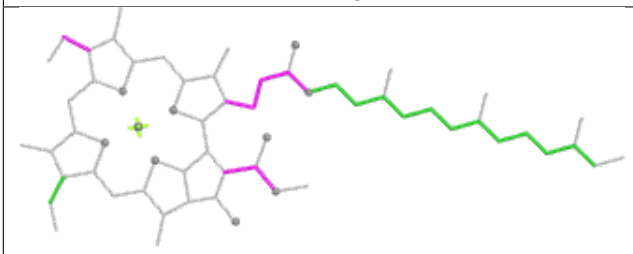
Ligand CLA cB 826



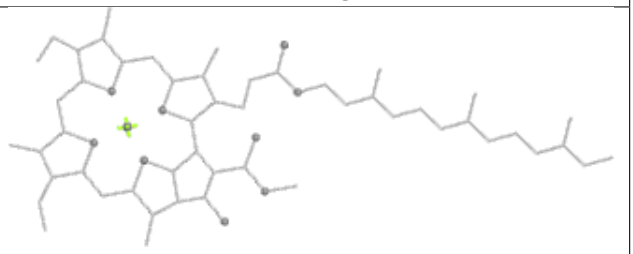
Bond lengths



Bond angles

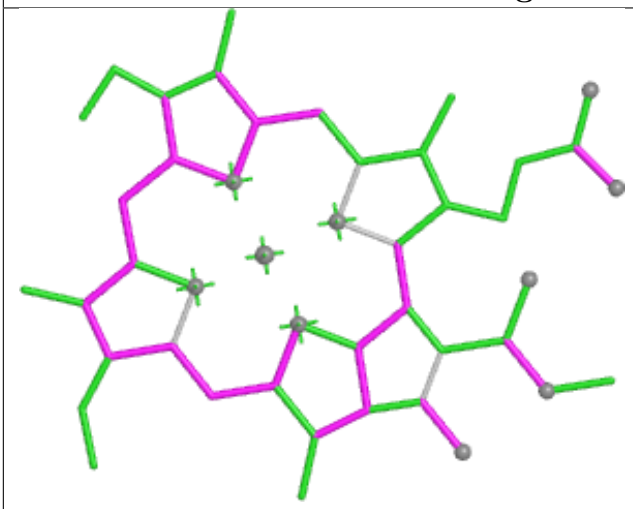


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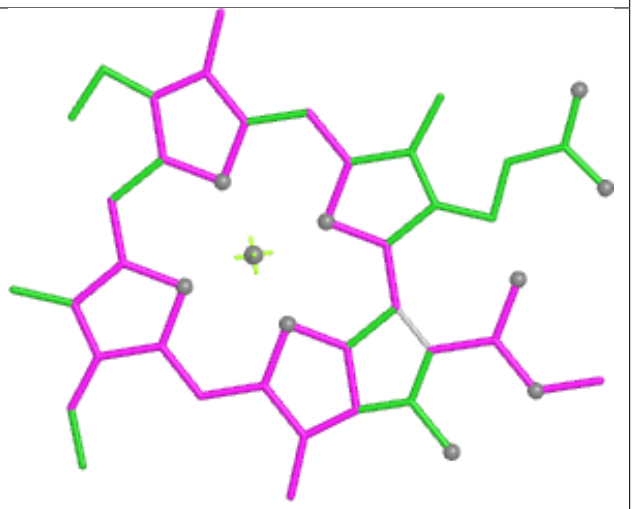


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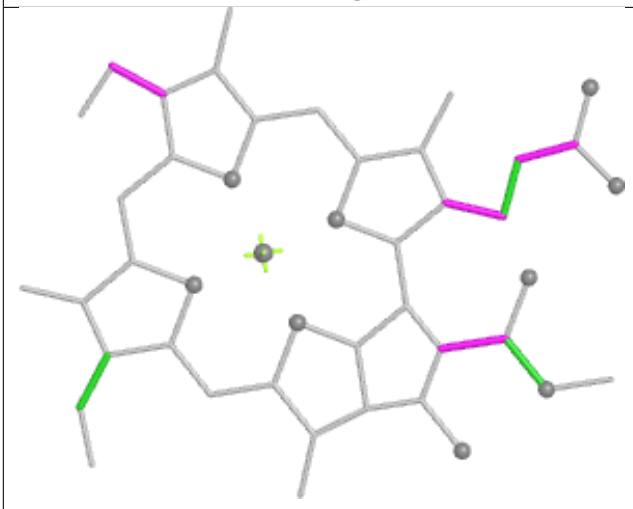
Ligand CLA aB 834



Bond lengths



Bond angles

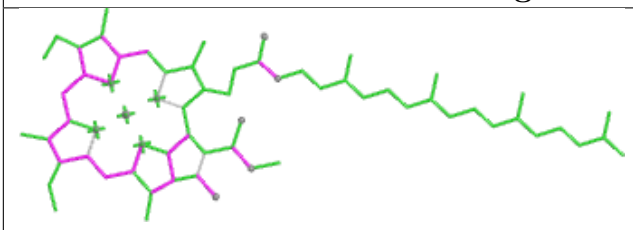


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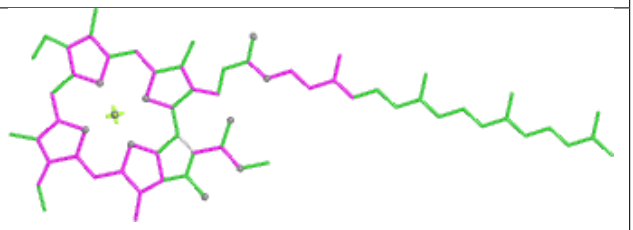


Rings

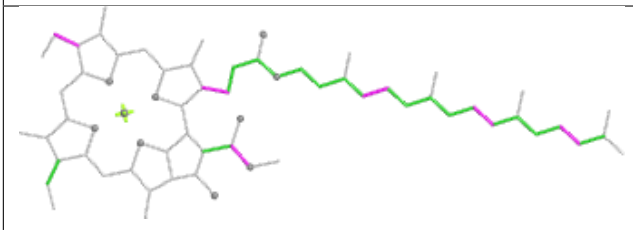
Ligand CLA bB 818



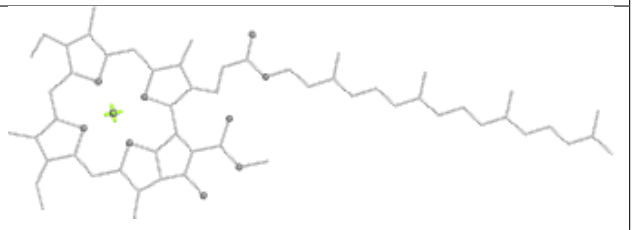
Bond lengths



Bond angles

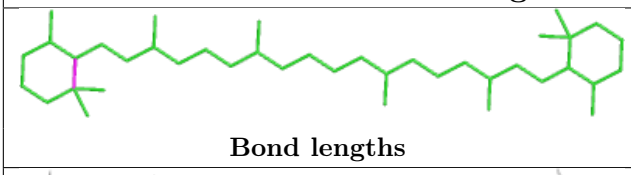


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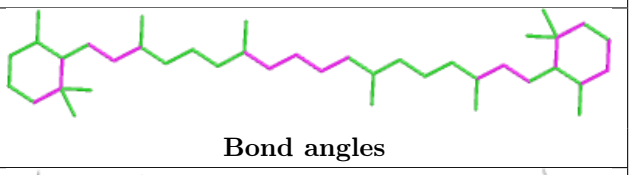


Rings

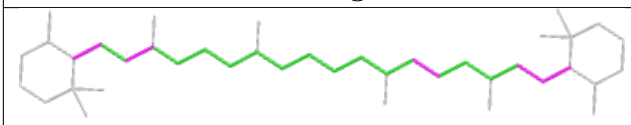
Ligand BCR aM 101



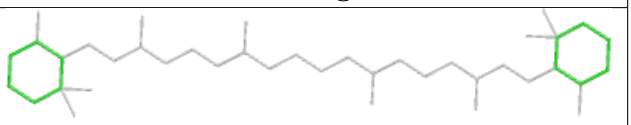
Bond lengths



Bond angles

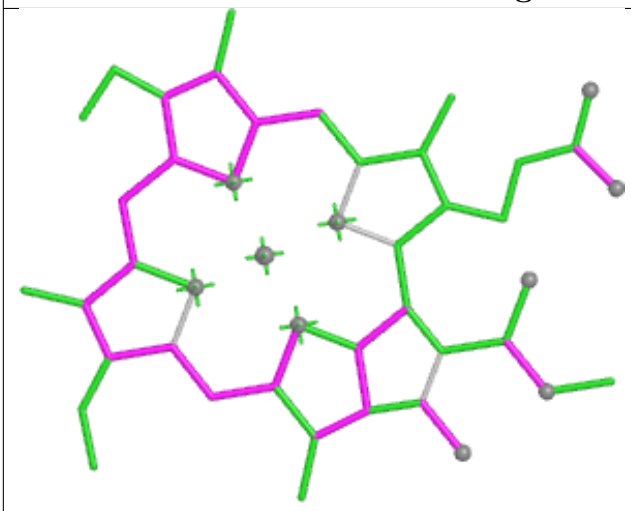


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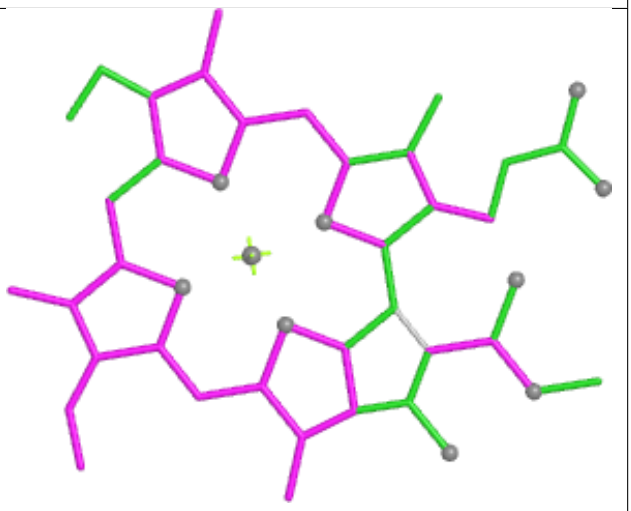


Rings

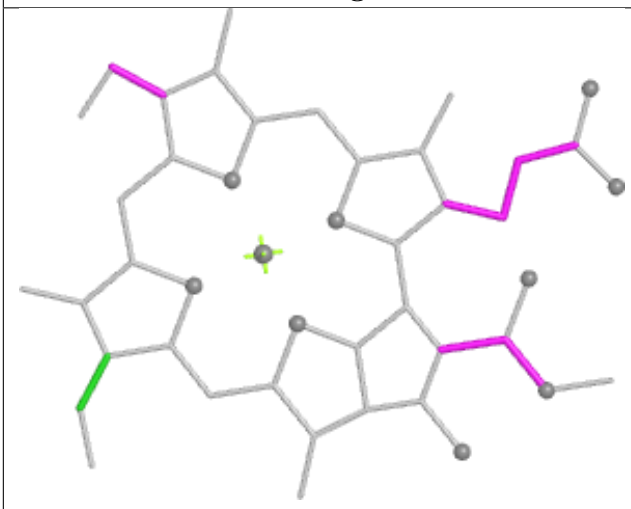
Ligand CLA aA 804



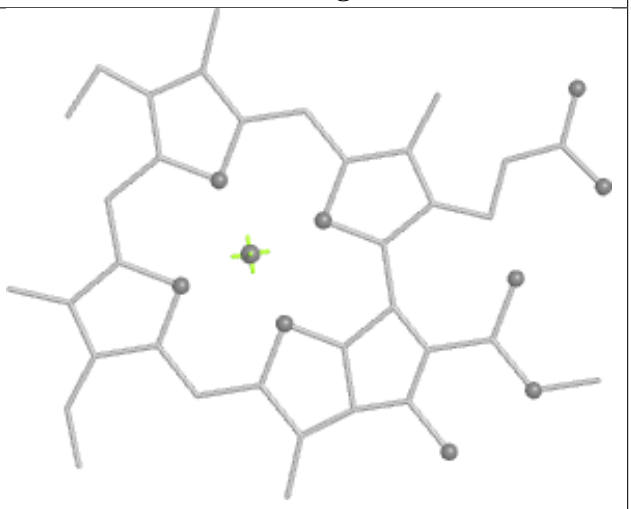
Bond lengths



Bond angles

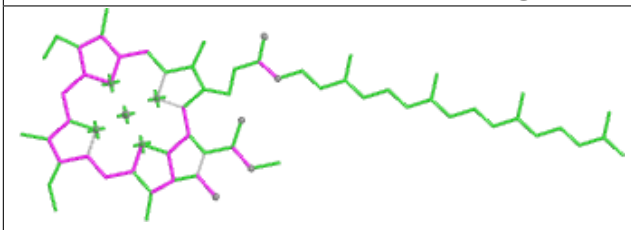


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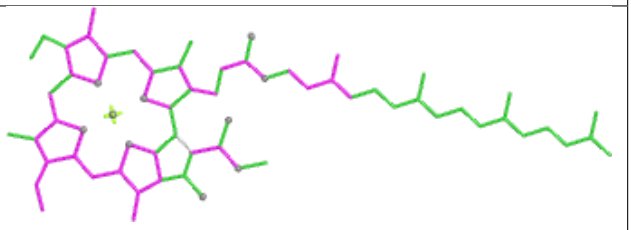


Rings

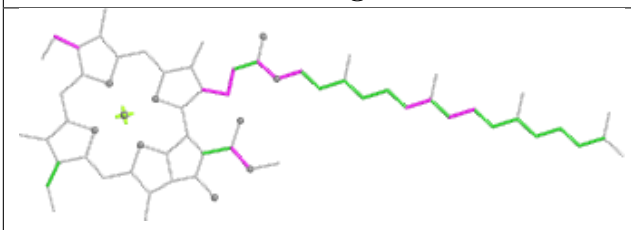
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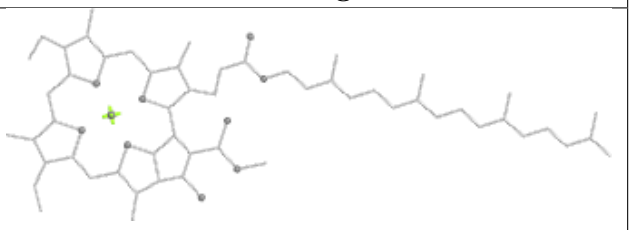
Bond lengths



Bond angles

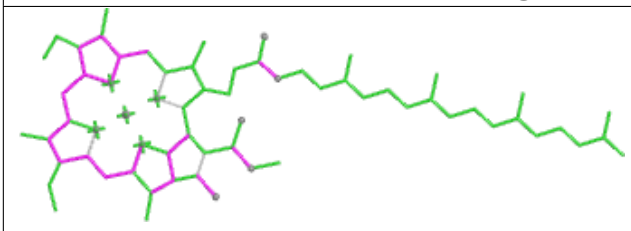


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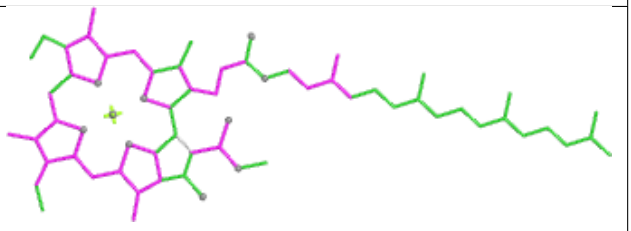


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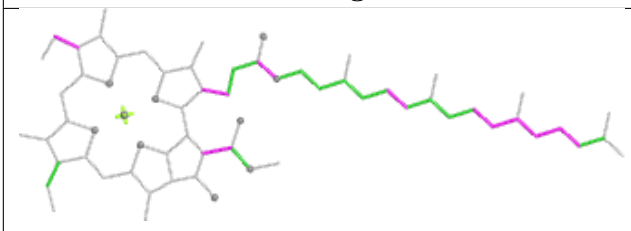
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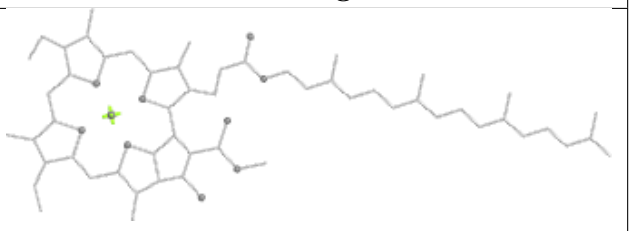
Bond lengths



Bond angles

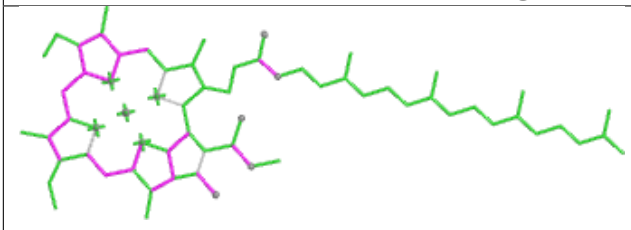


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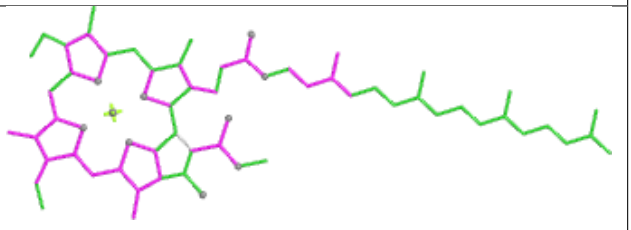


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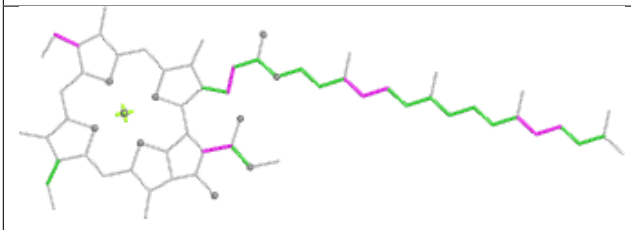
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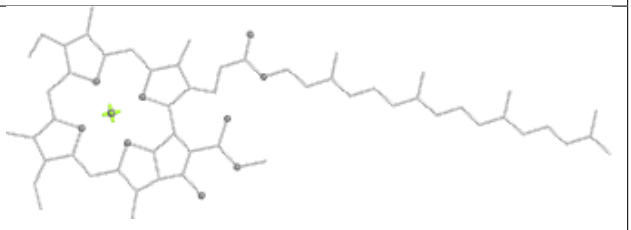
Bond lengths



Bond angles

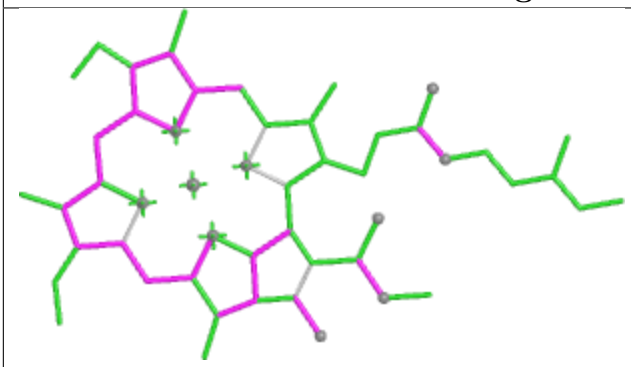


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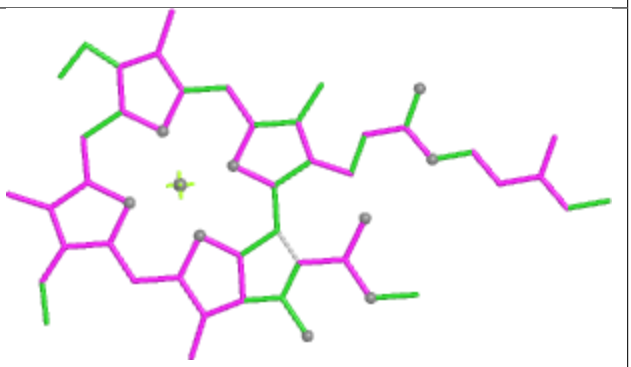


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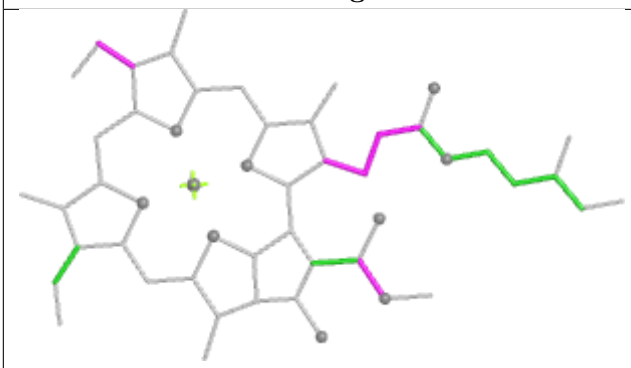
Ligand CLA aA 843



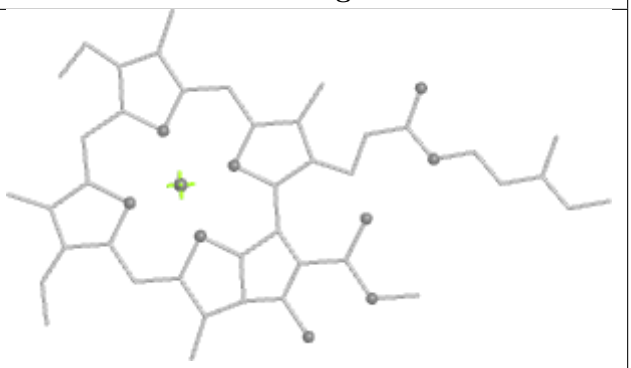
Bond lengths



Bond angles

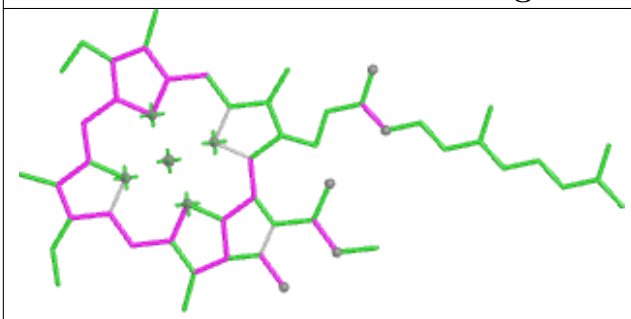


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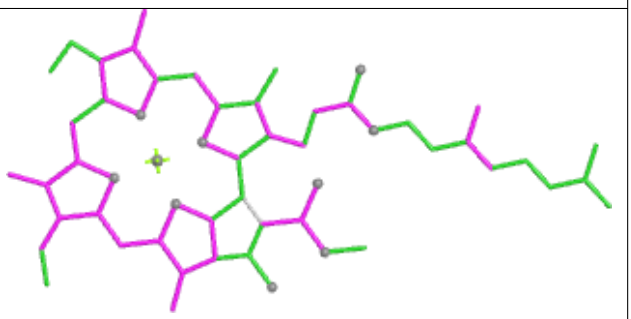


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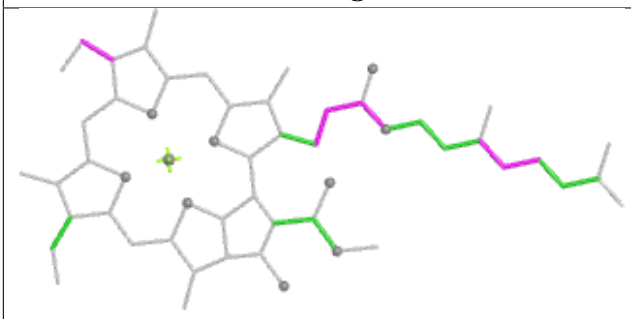
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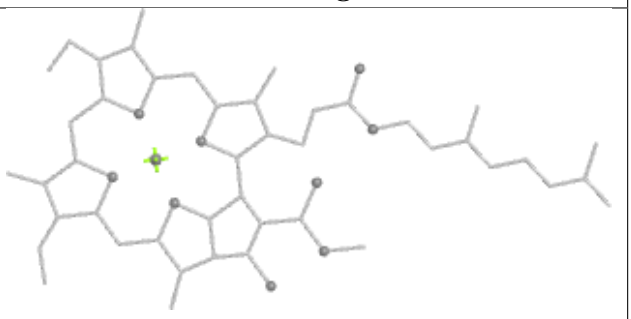
Bond lengths



Bond angles

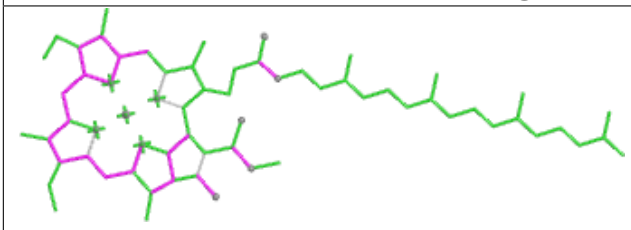


Torsions

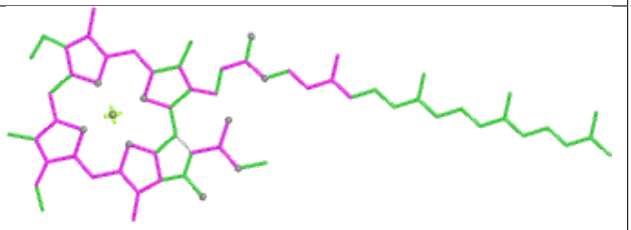


Rings

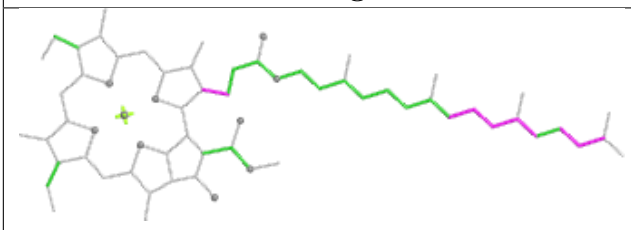
Ligand CLA aB 825



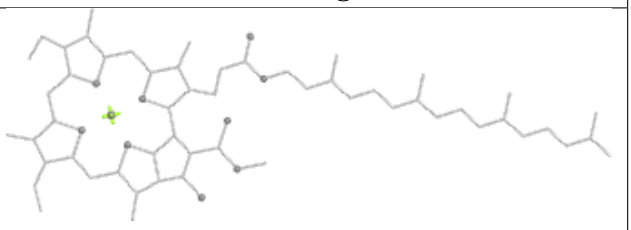
Bond lengths



Bond angles



Torsions

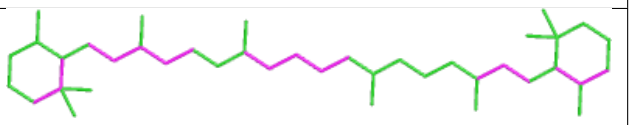


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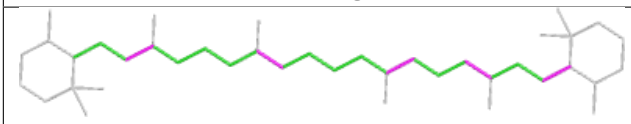
Ligand BCR bL 208



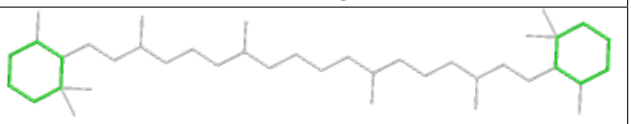
Bond lengths



Bond angles

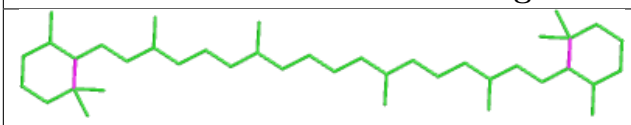


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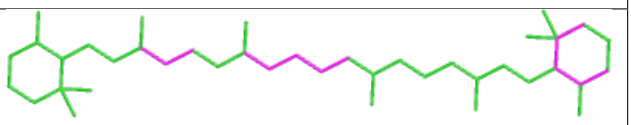


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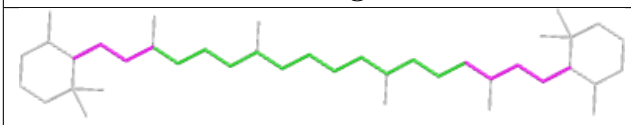
Ligand BCR cA 849



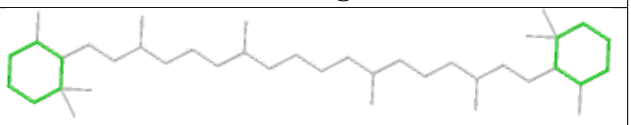
Bond lengths



Bond angles

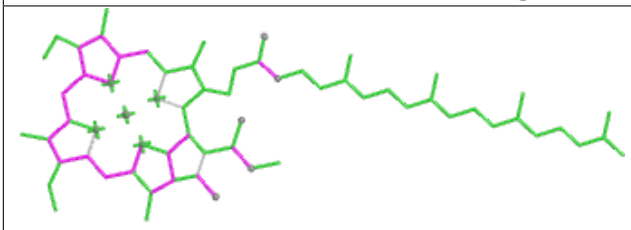


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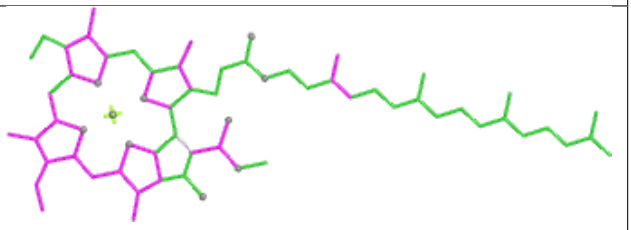


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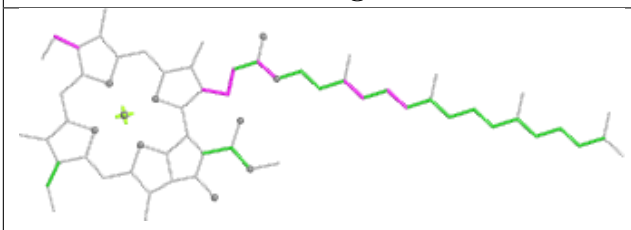
Ligand CLA bB 827



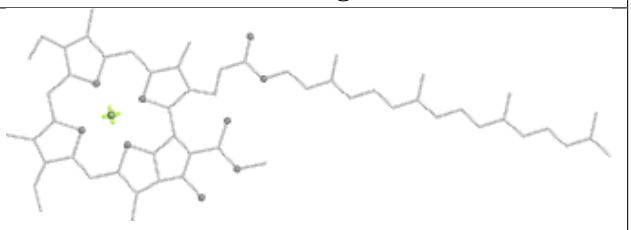
Bond lengths



Bond angles

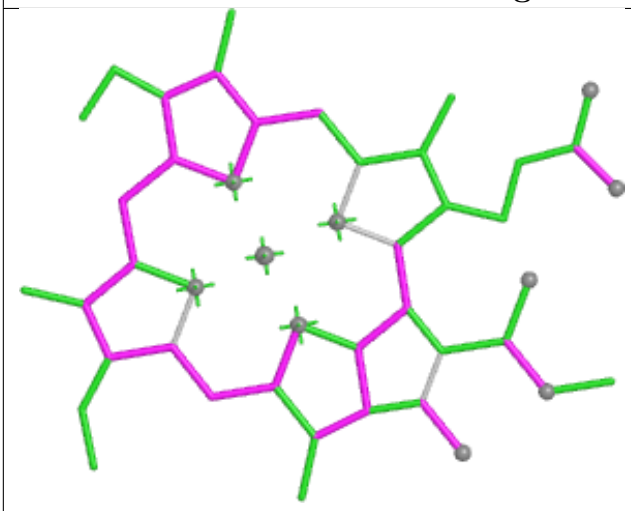


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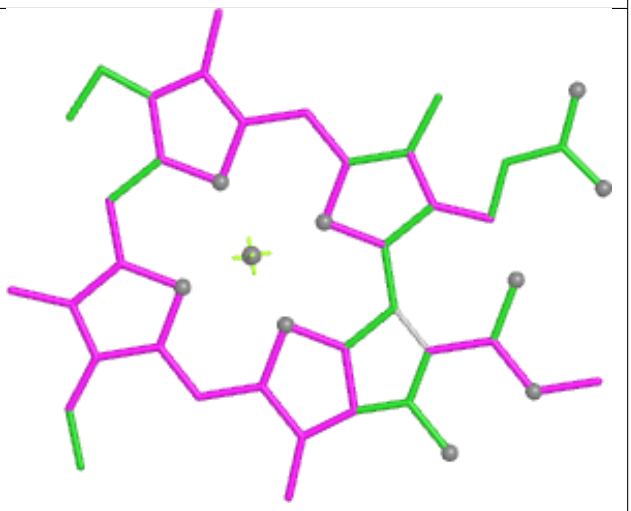


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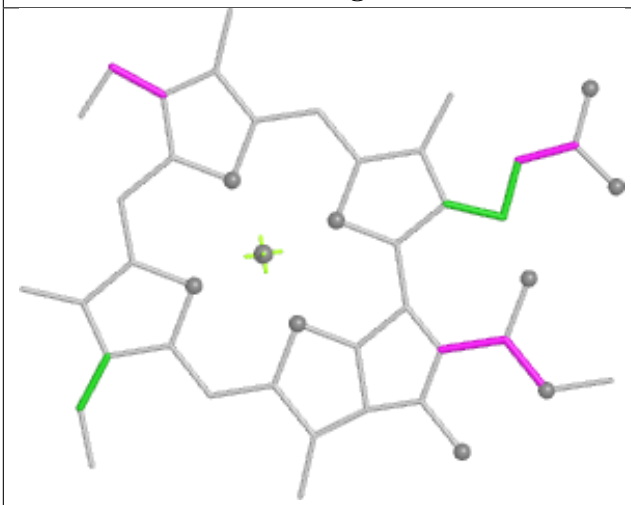
Ligand CLA bA 842



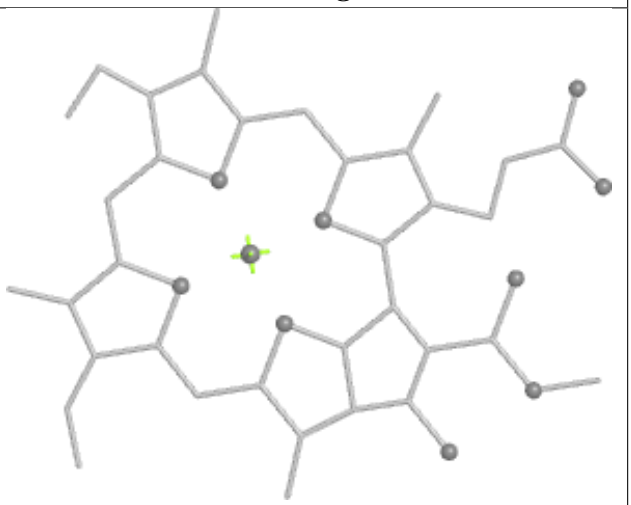
Bond lengths



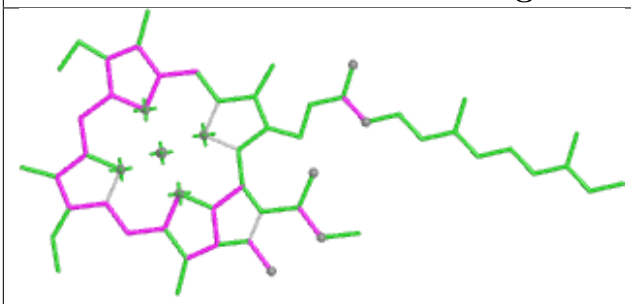
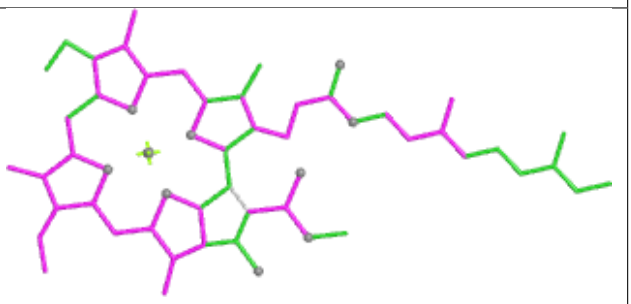
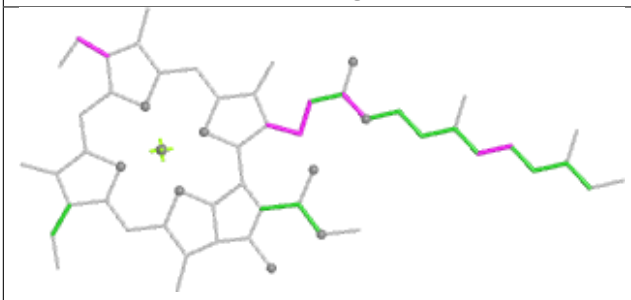
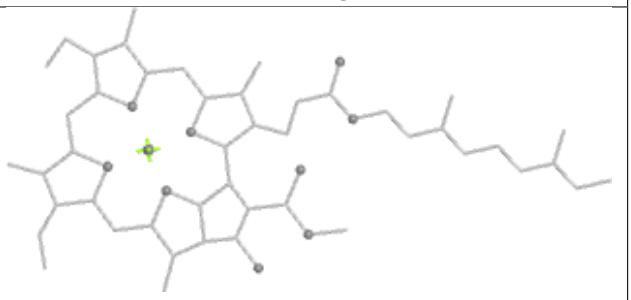
Bond angles



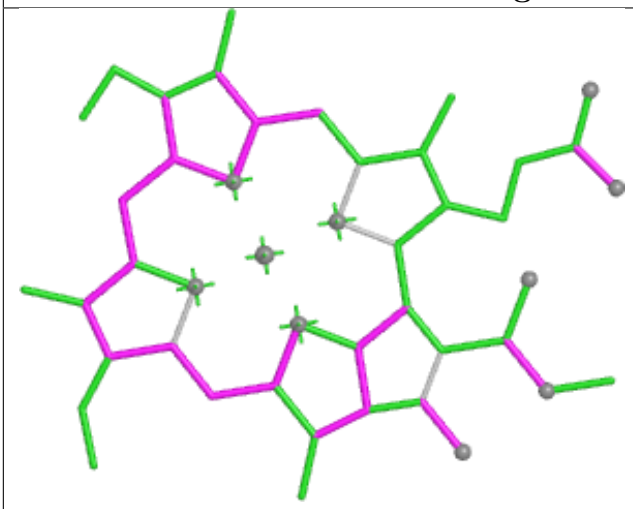
Torsions



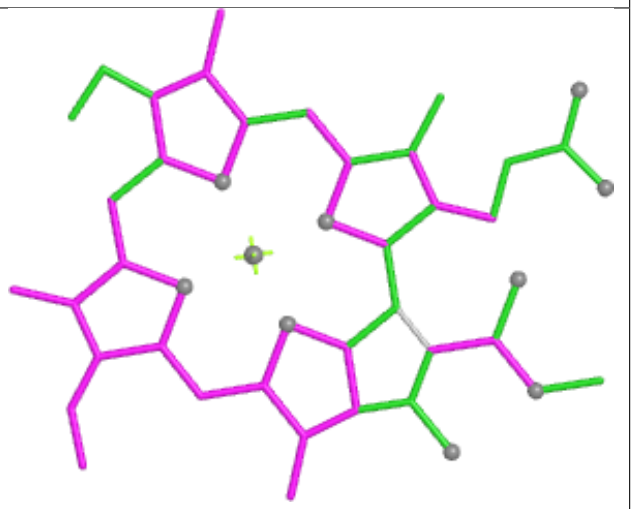
Rings

Ligand CLA aB 831	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

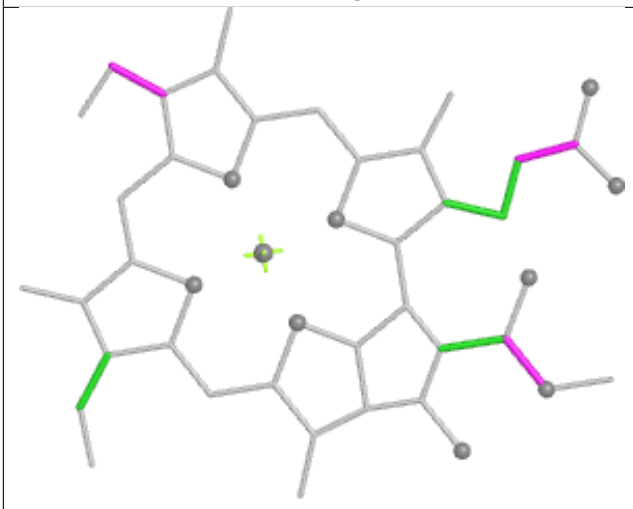
Ligand CLA bA 836



Bond lengths



Bond angles

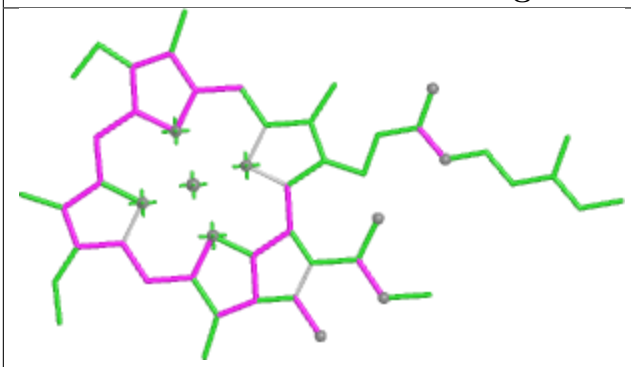


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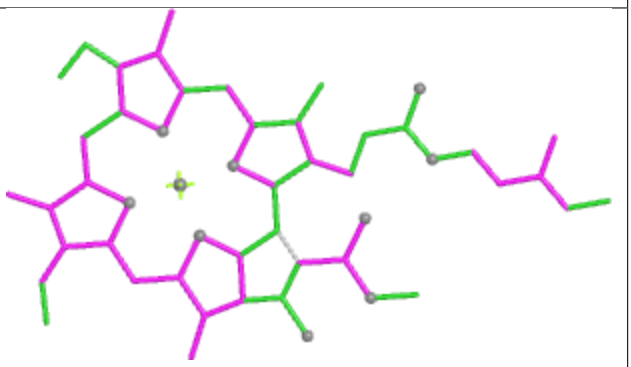


Rings

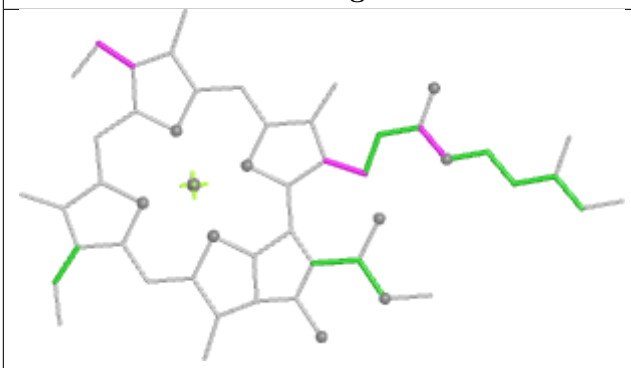
Ligand CLA bA 808



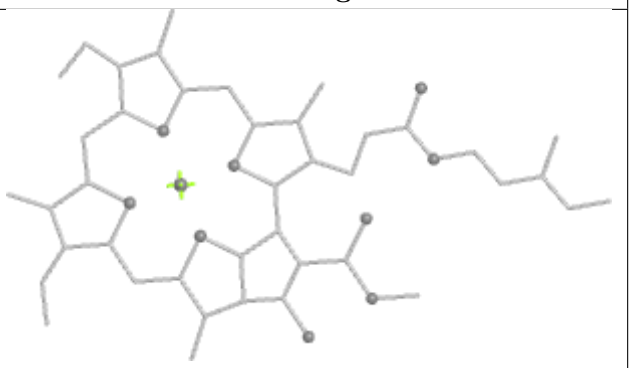
Bond lengths



Bond angles

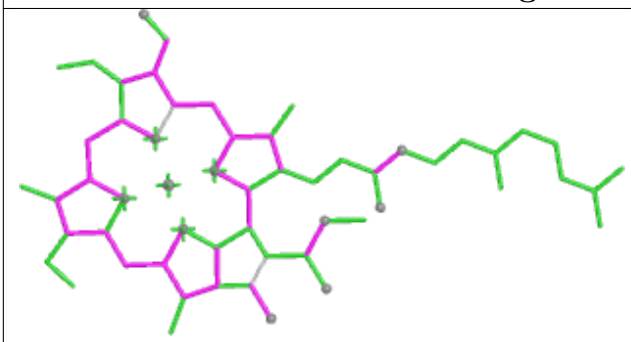


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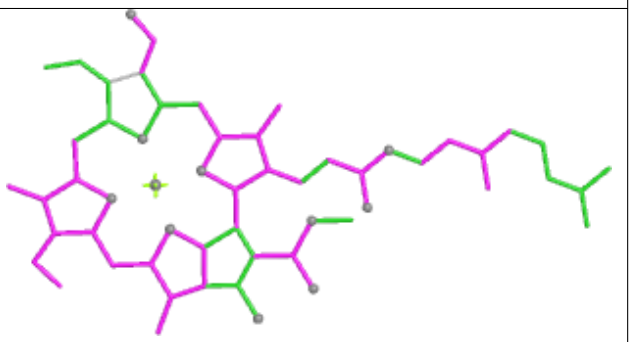


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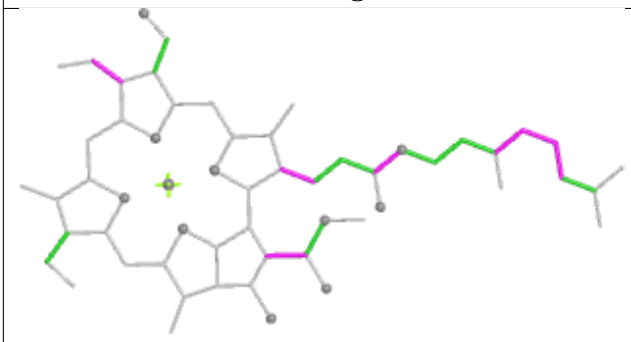
Ligand F6C aA 827



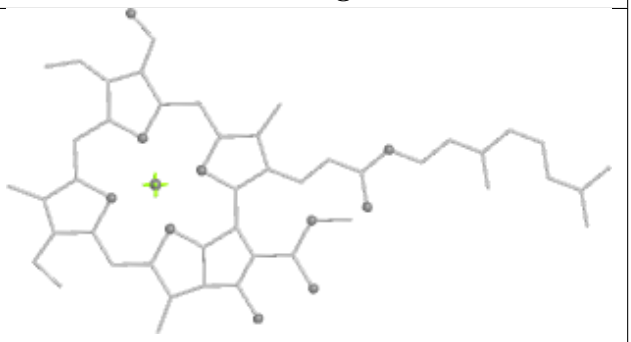
Bond lengths



Bond angles

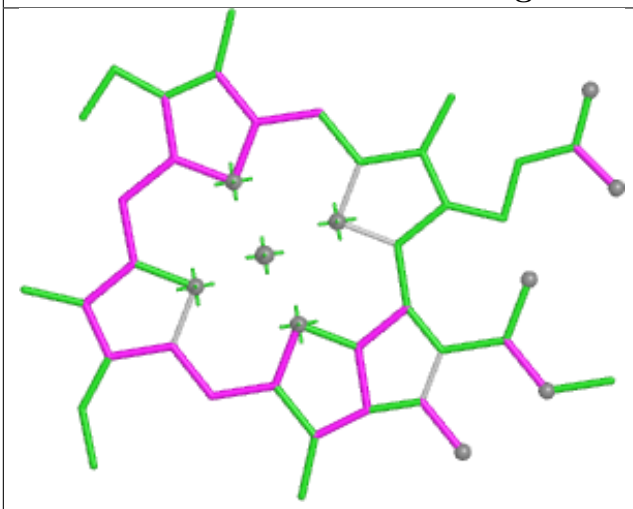


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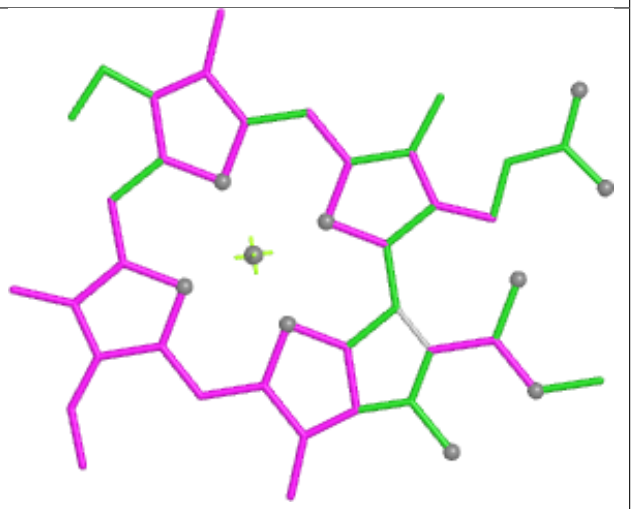


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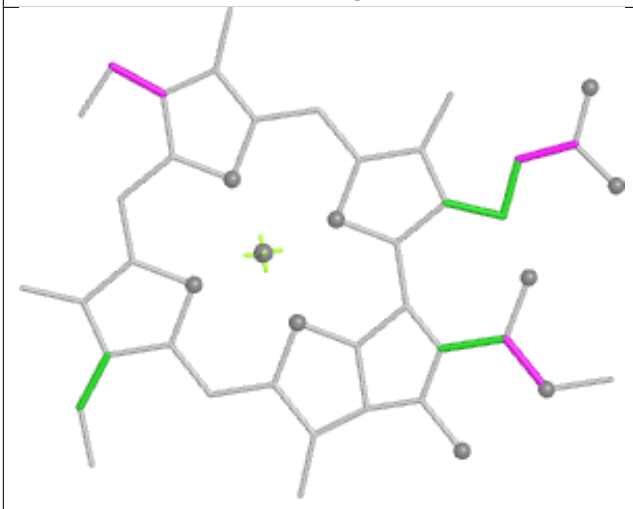
Ligand CLA aA 836



Bond lengths



Bond angles

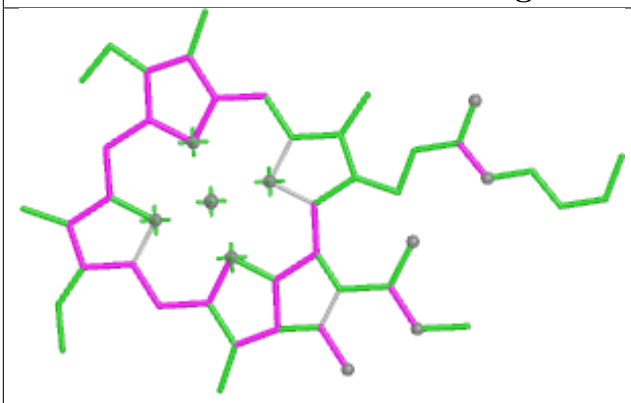


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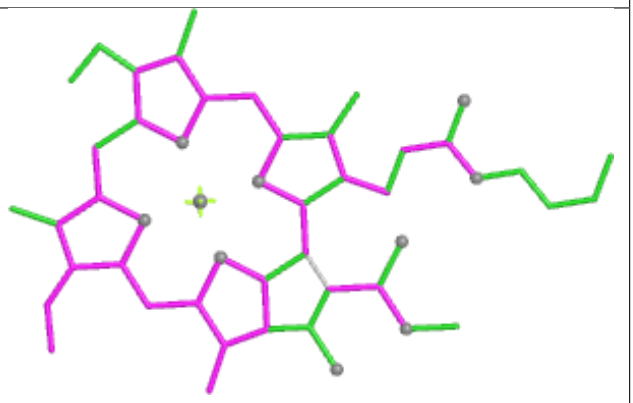


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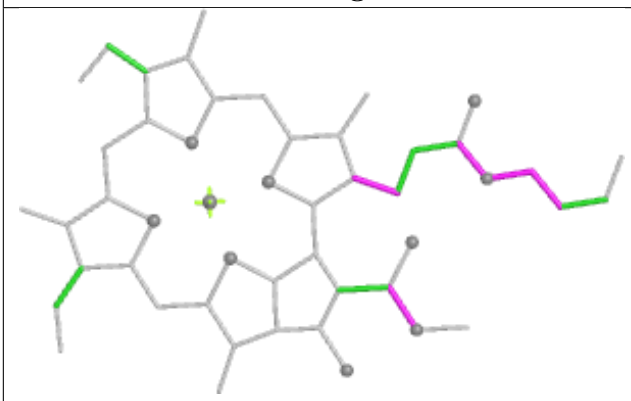
Ligand CLA aA 817



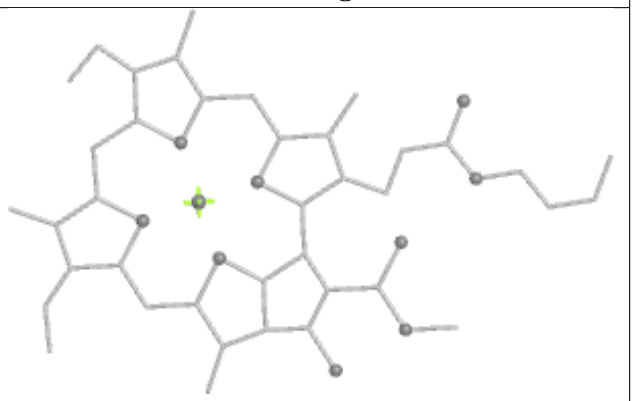
Bond lengths



Bond angles

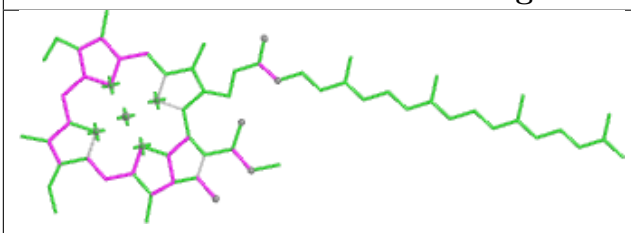


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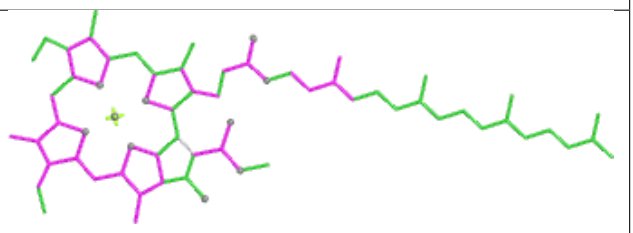


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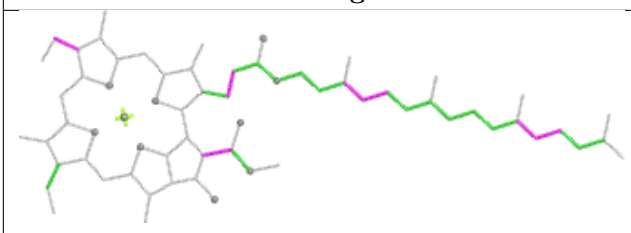
Ligand CLA aB 839



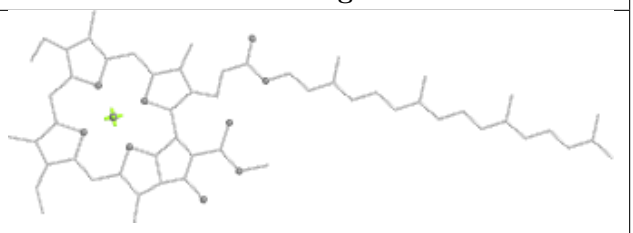
Bond lengths



Bond angles

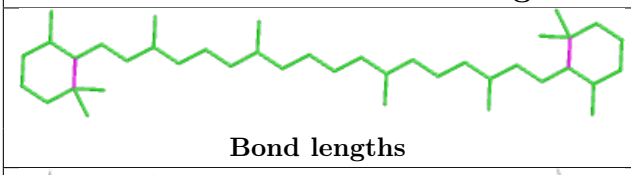


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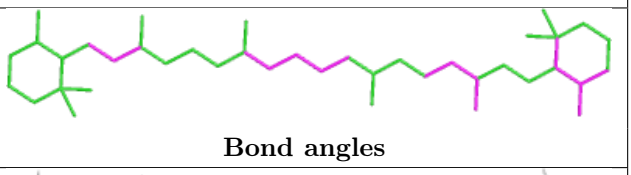


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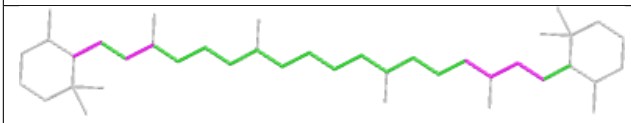
Ligand BCR cK 102



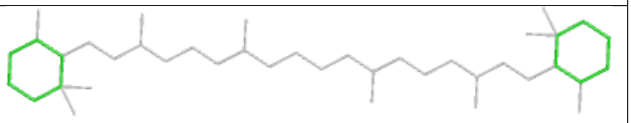
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Bond angles



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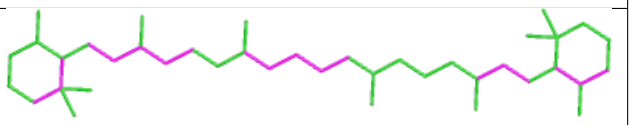


Rings

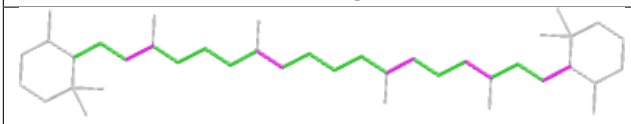
Ligand BCR cL 208



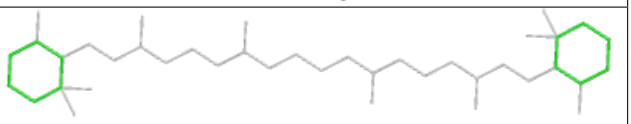
Bond lengths



Bond angles

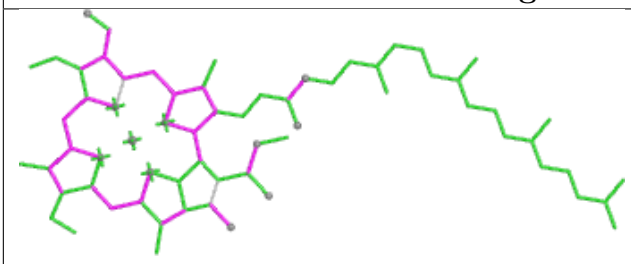


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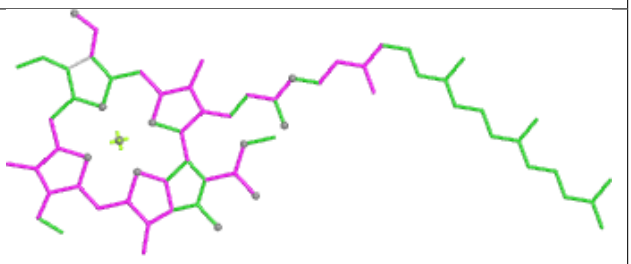


Rings

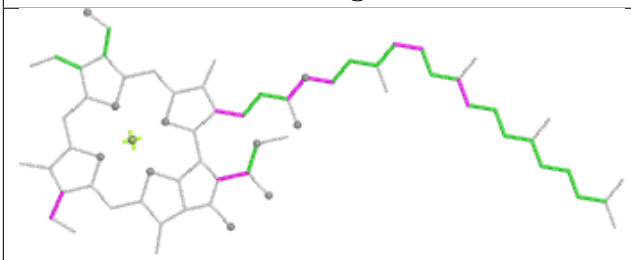
Ligand F6C aA 826



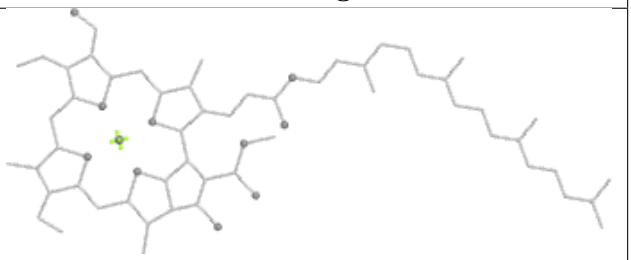
Bond lengths



Bond angles

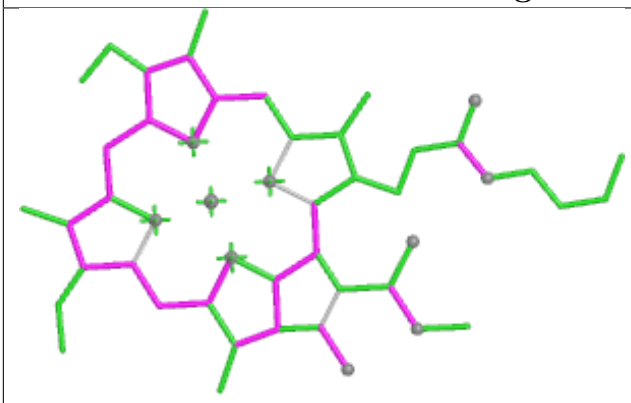


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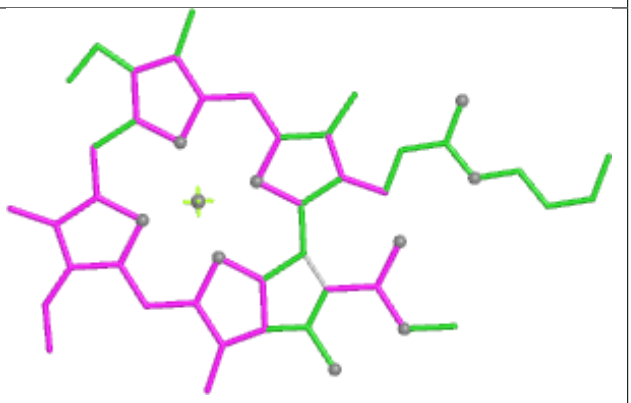


Rings

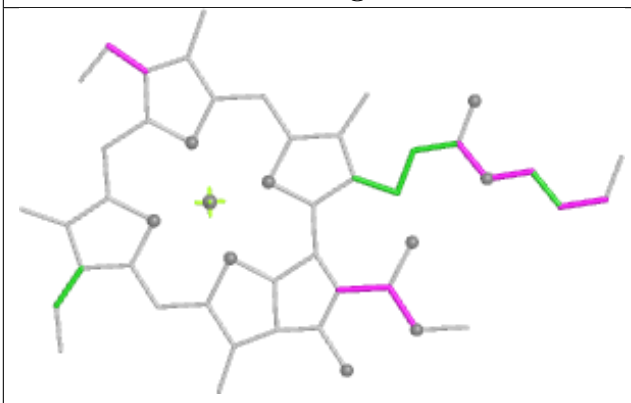
Ligand CLA bB 830



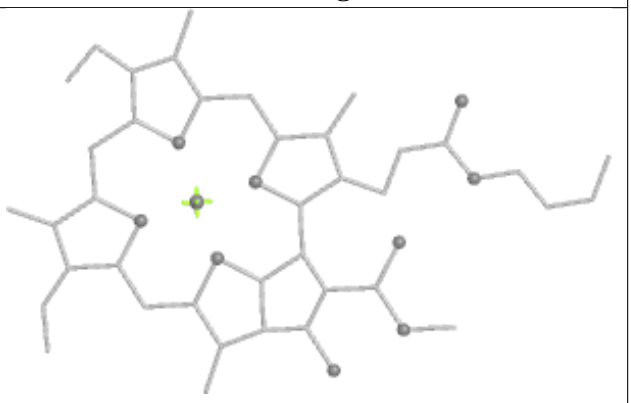
Bond lengths



Bond angles

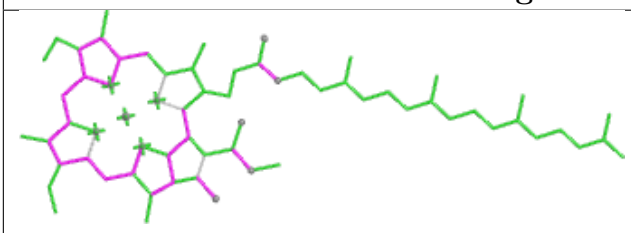


Torsions

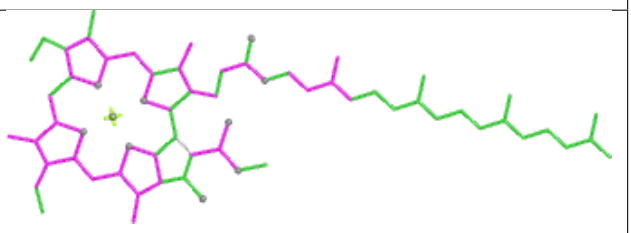


Rings

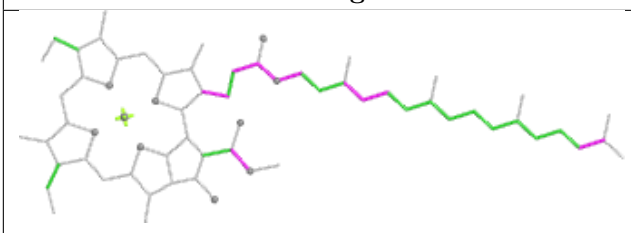
Ligand CLA cA 829



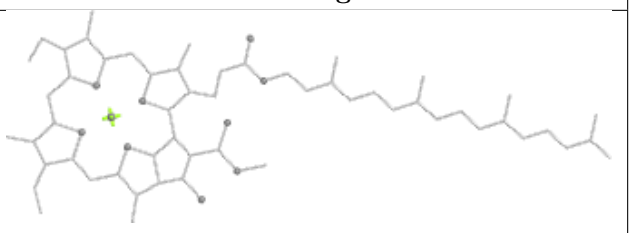
Bond lengths



Bond angles

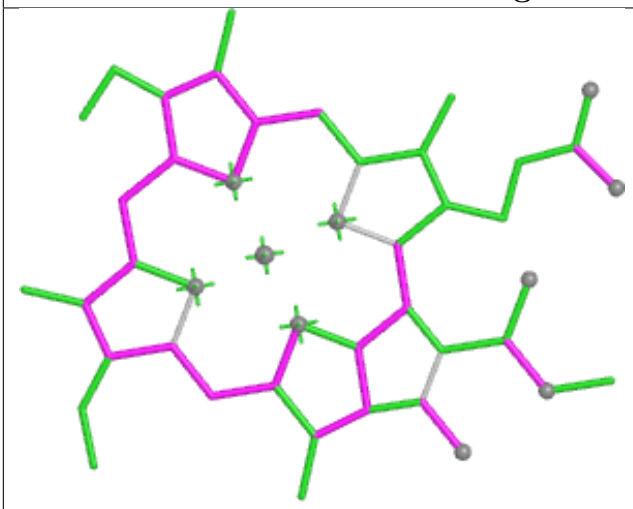


Torsions

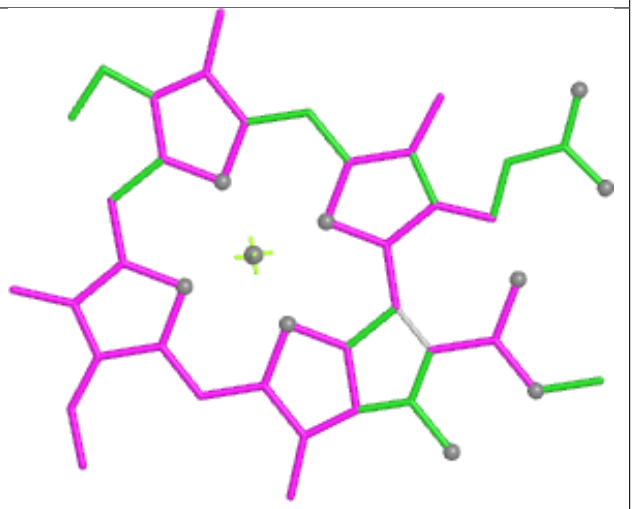


Rings

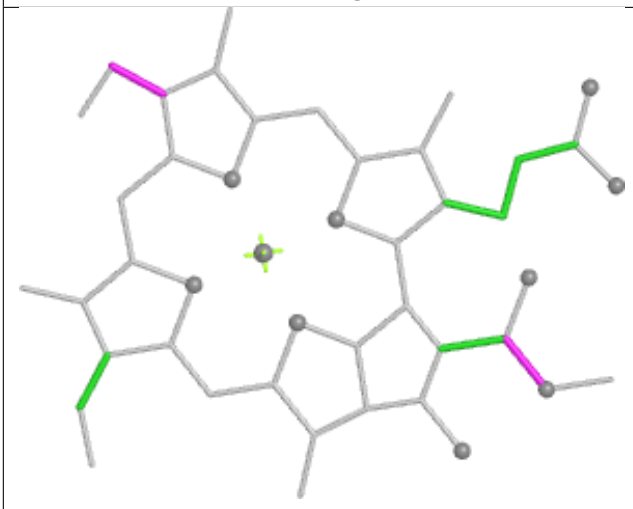
Ligand CLA bA 810



Bond lengths



Bond angles

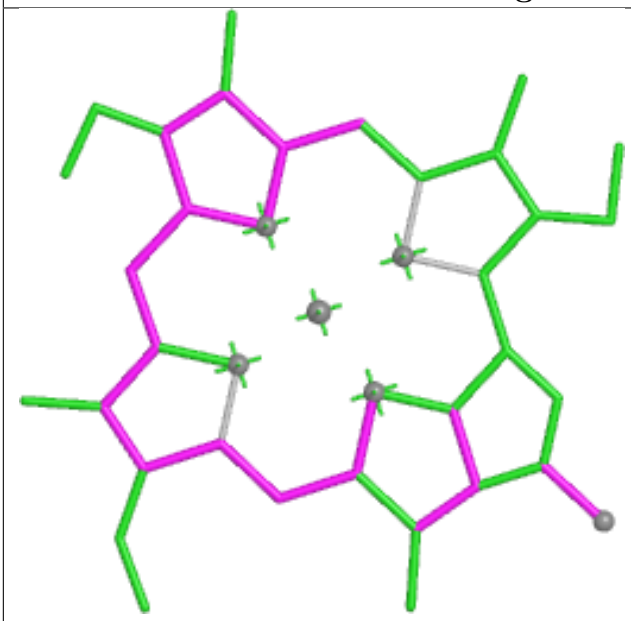


Torsions



Rings

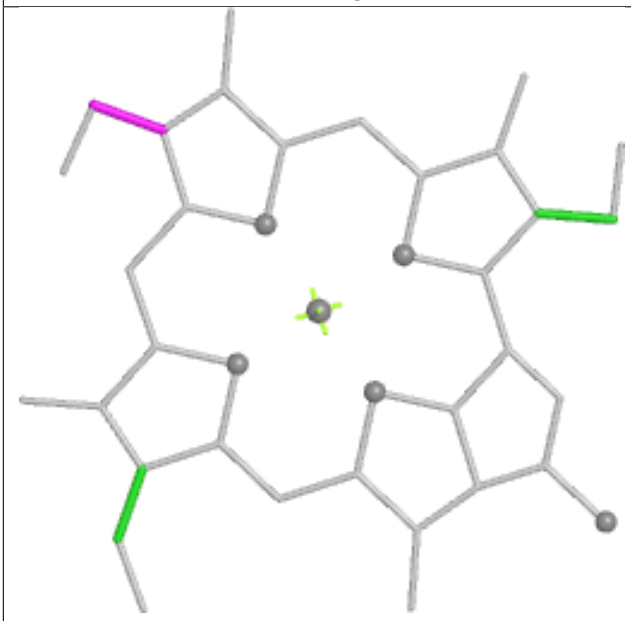
Ligand CLA cK 101



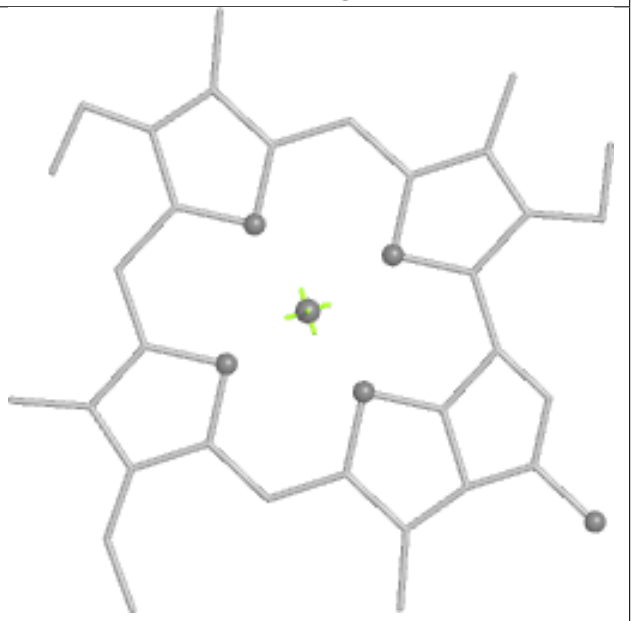
Bond lengths



Bond angles

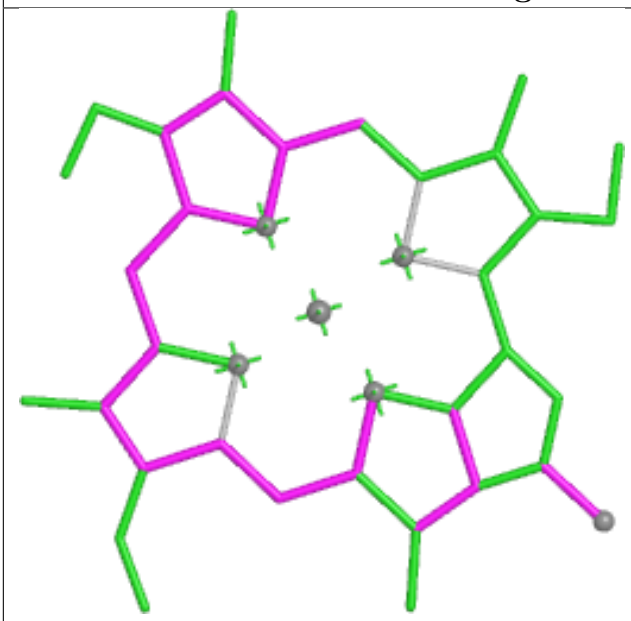


Torsions



Rings

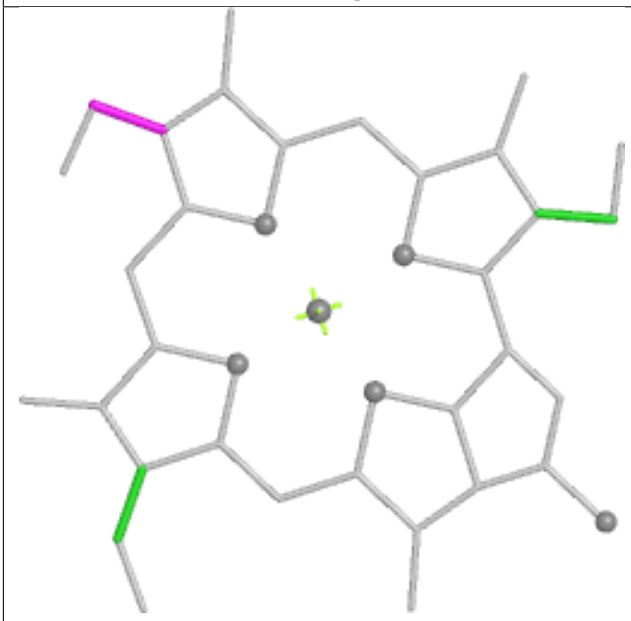
Ligand CLA aK 101



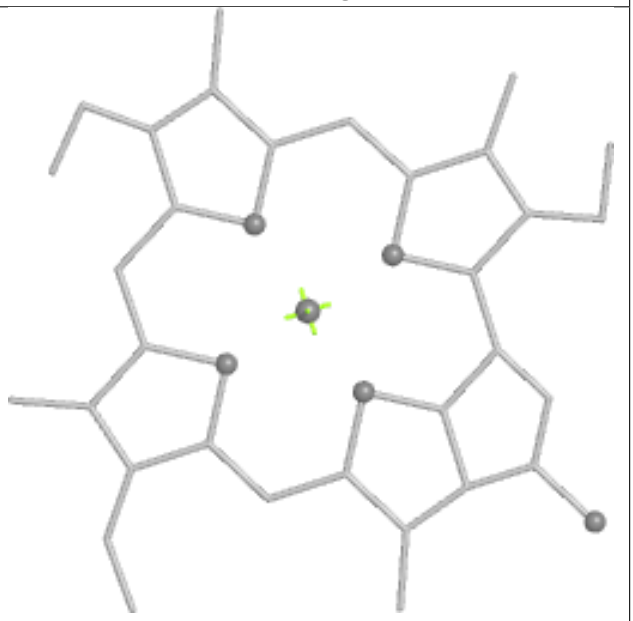
Bond lengths



Bond angles

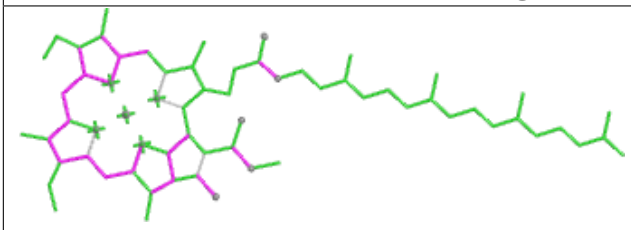


Torsions

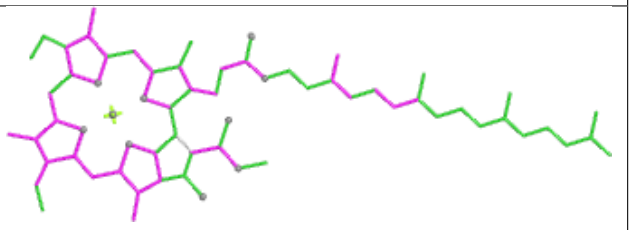


Rings

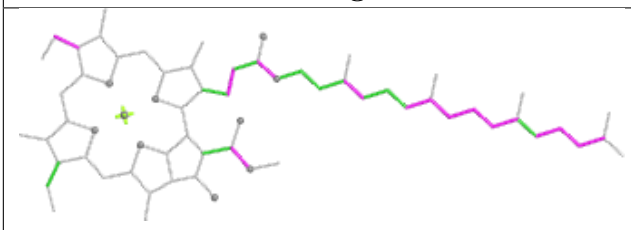
Ligand CLA bA 822



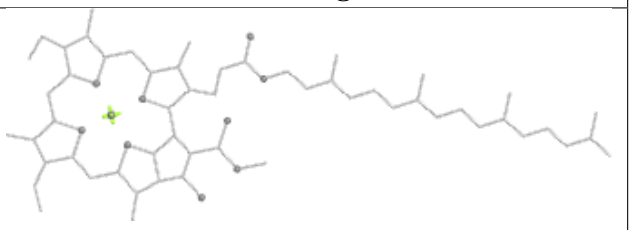
Bond lengths



Bond angles

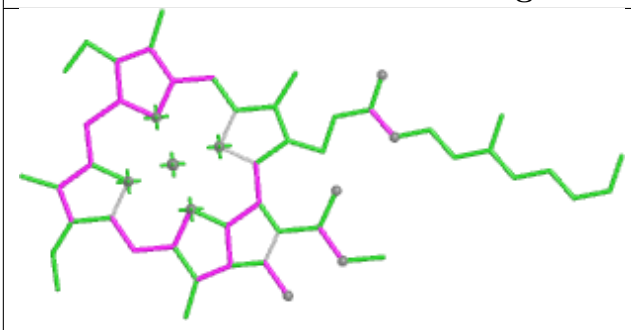


Torsions

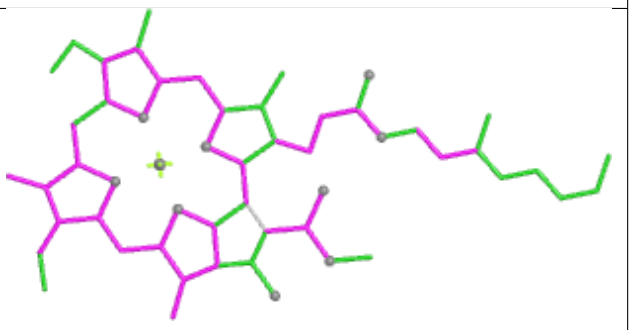


Rings

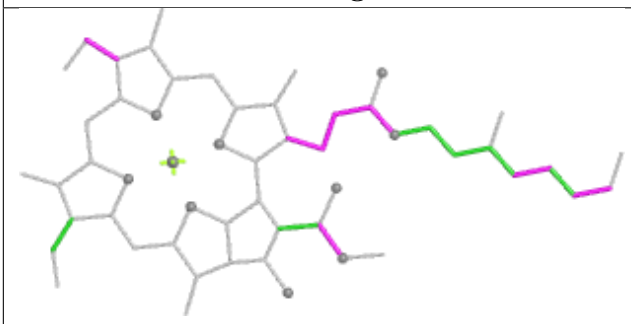
Ligand CLA cA 819



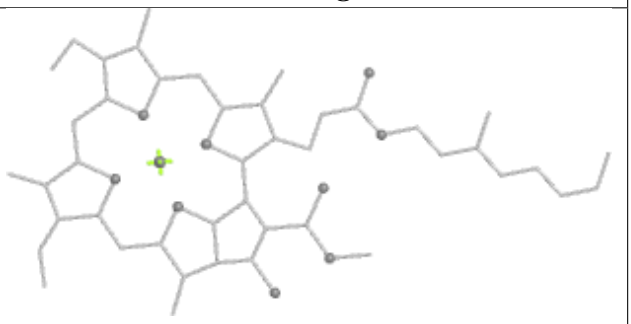
Bond lengths



Bond angles

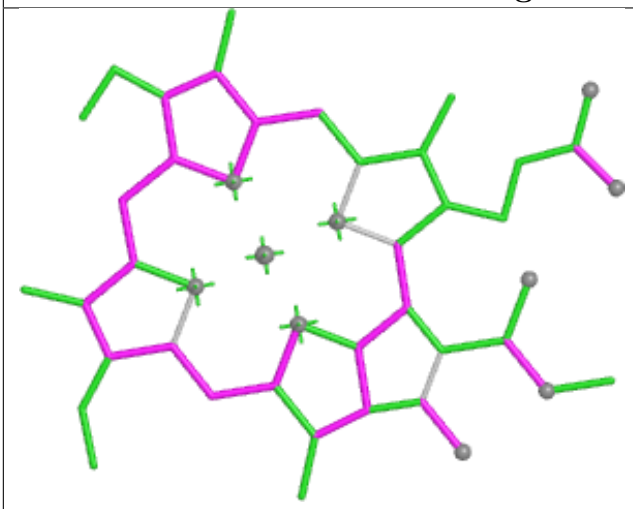


Torsions

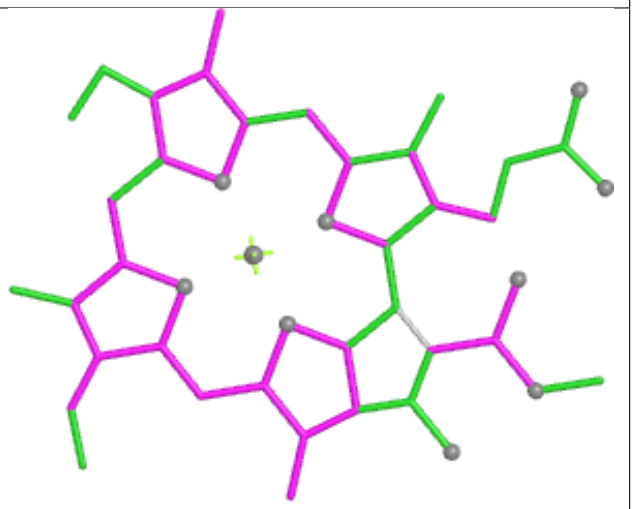


Rings

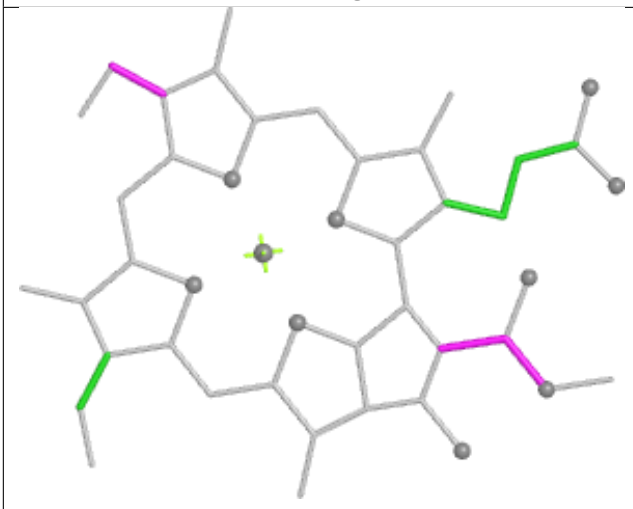
Ligand CLA aA 816



Bond lengths



Bond angles

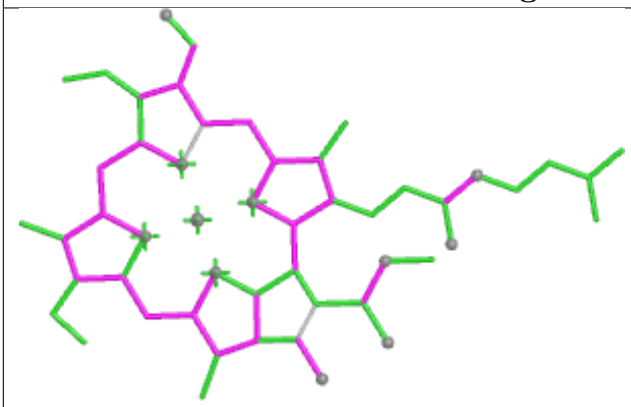


Torsions

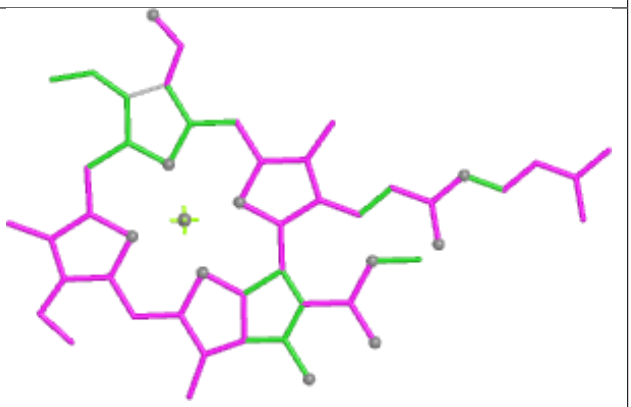


Rings

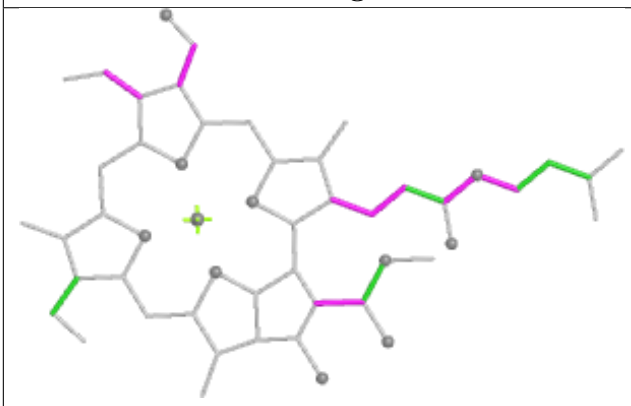
Ligand F6C cA 832



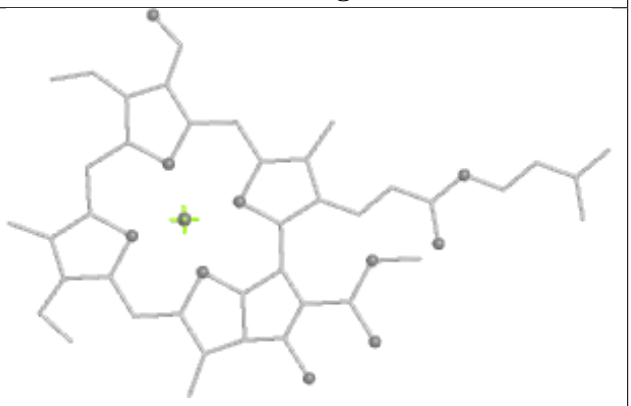
Bond lengths



Bond angles

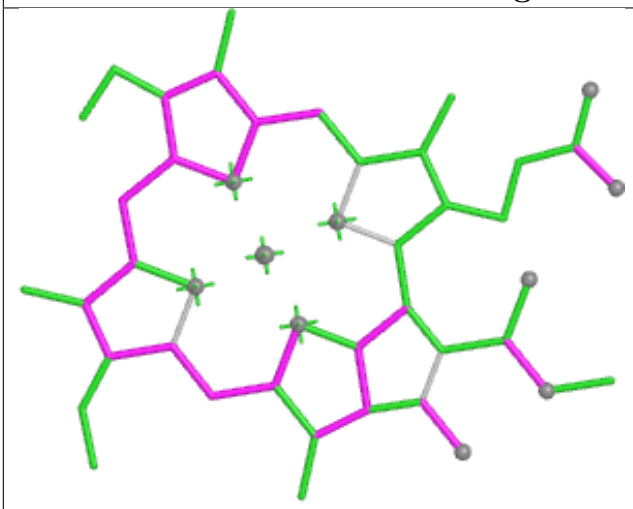


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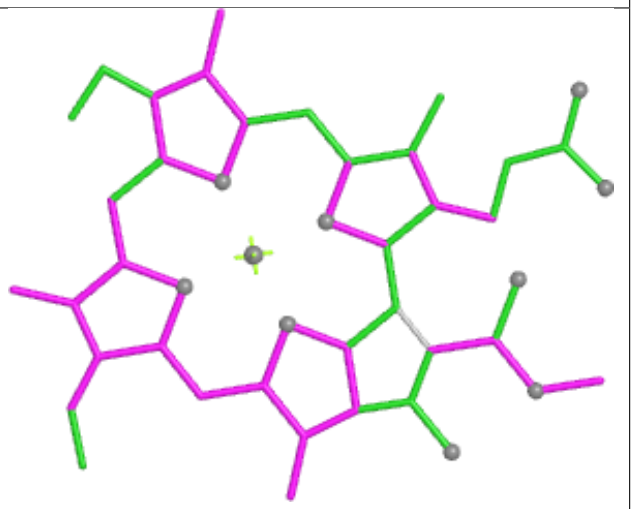


Rings

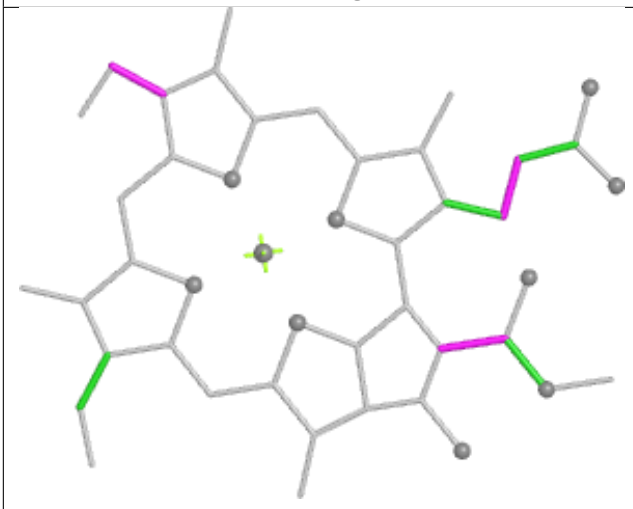
Ligand CLA bA 811



Bond lengths



Bond angles

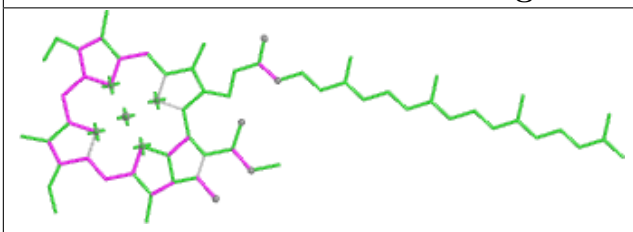


Torsions

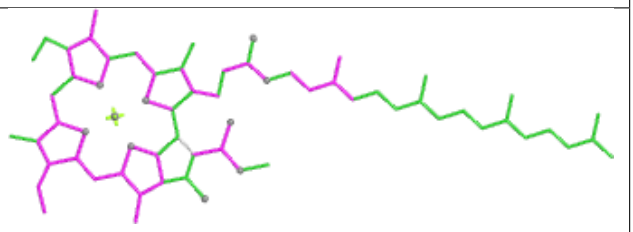


Rings

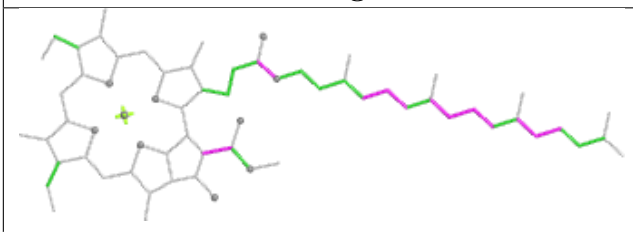
Ligand CLA cA 831



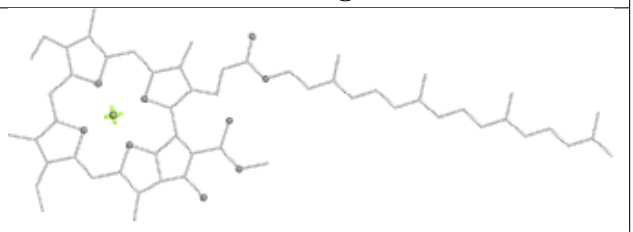
Bond lengths



Bond angles

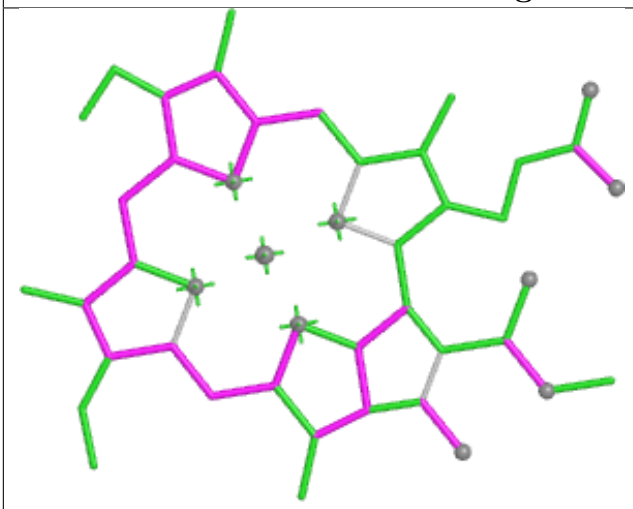


Torsions

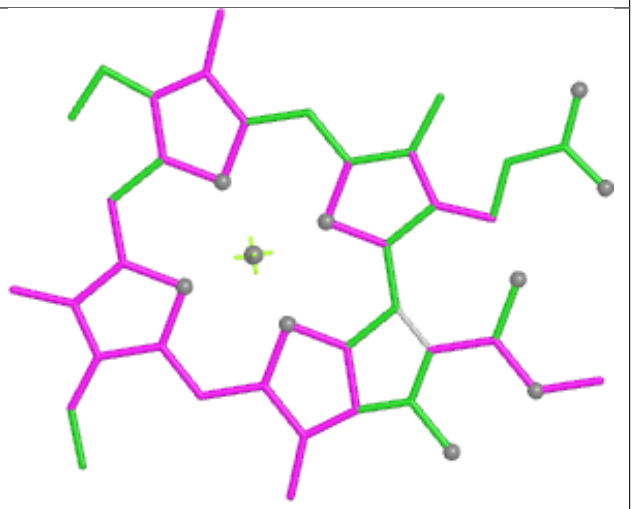


Rings

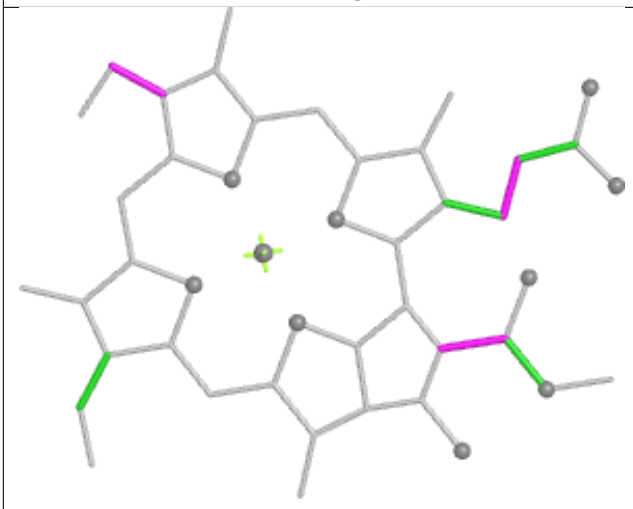
Ligand CLA aA 811



Bond lengths



Bond angles

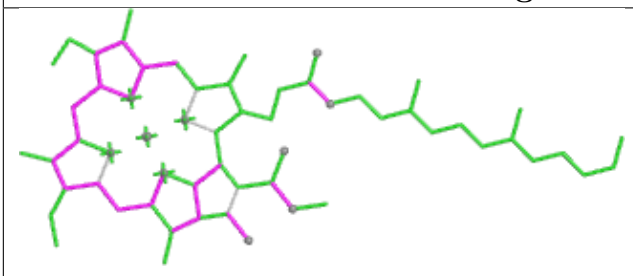


Torsions

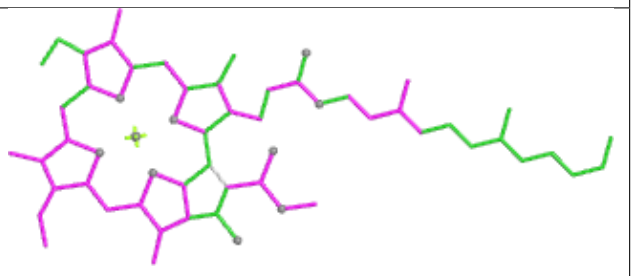


Rings

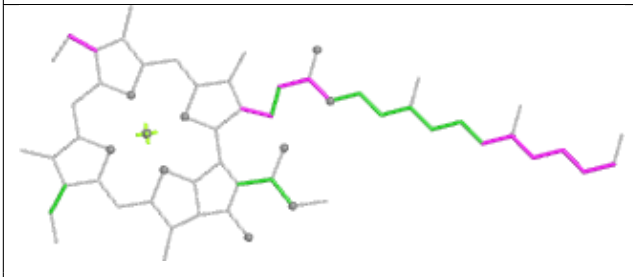
Ligand CLA aB 816



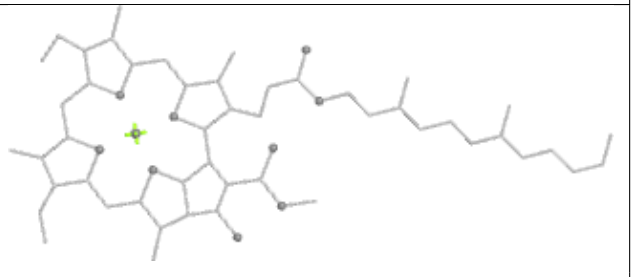
Bond lengths



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.

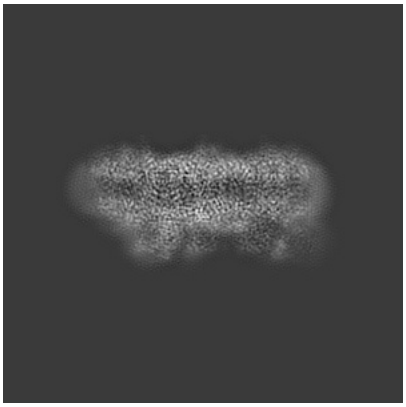
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0727. These allow visual inspection of the internal detail of the map and identification of artifacts.

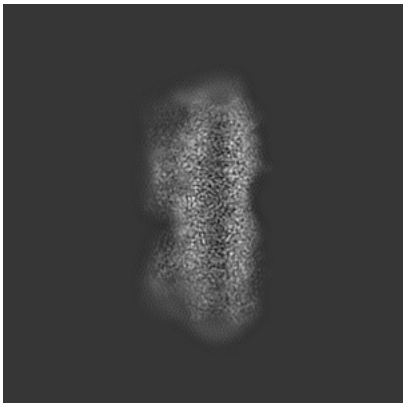
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

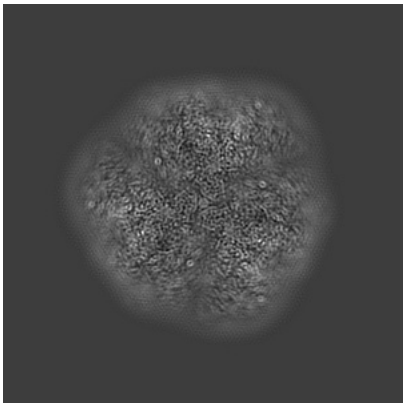
6.1.1 Primary map



X



Y



Z

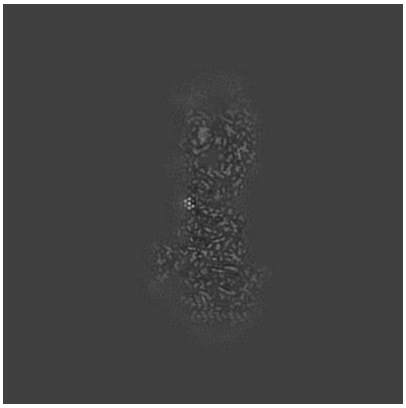
The images above show the map projected in three orthogonal directions.

6.2 Central slices

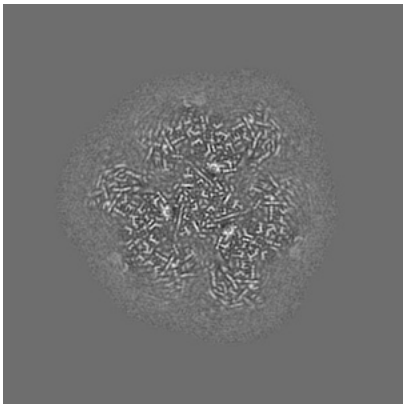
6.2.1 Primary map



X Index: 180



Y Index: 180

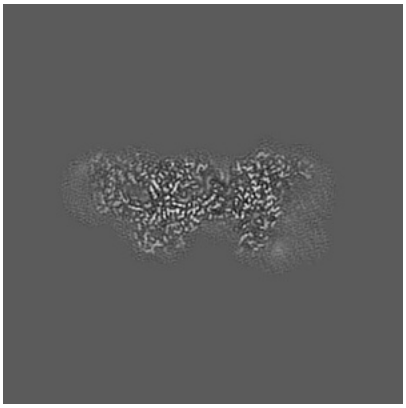


Z Index: 180

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

6.3 Largest variance slices (i)

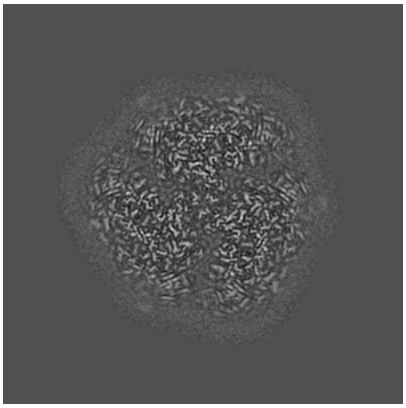
6.3.1 Primary map



X Index: 200



Y Index: 176

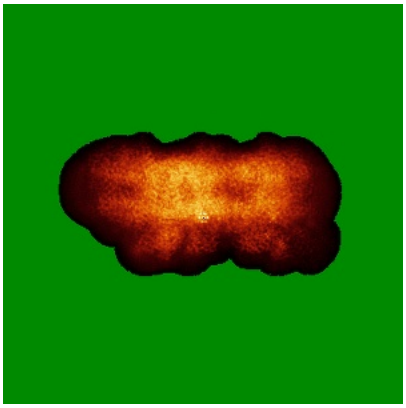


Z Index: 204

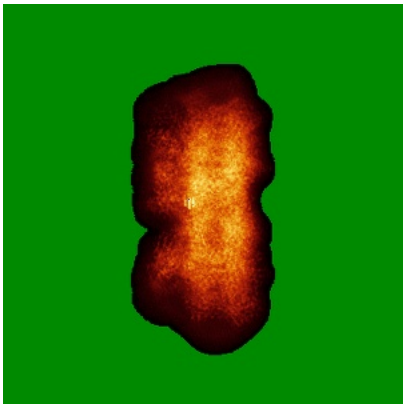
The images above show the largest variance slices of the map in three orthogonal directions.

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

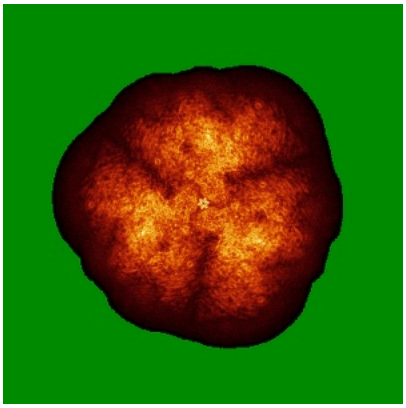
6.4.1 Primary map



X



Y

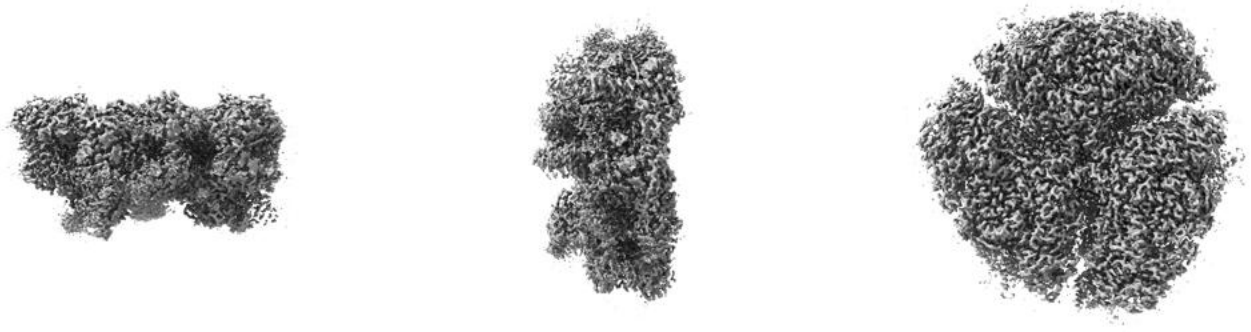


Z

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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

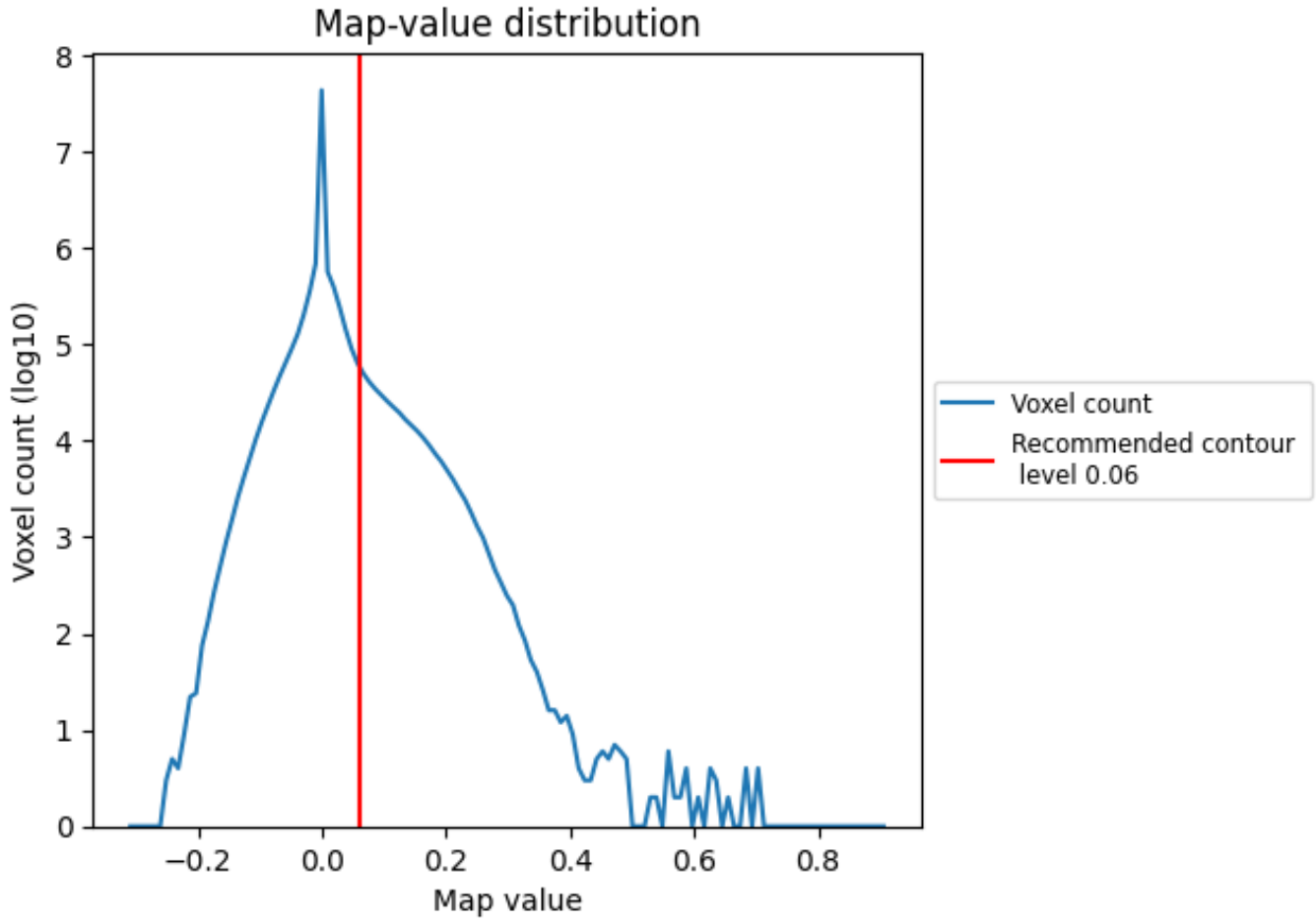
6.6 Mask visualisation (i)

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

7 Map analysis

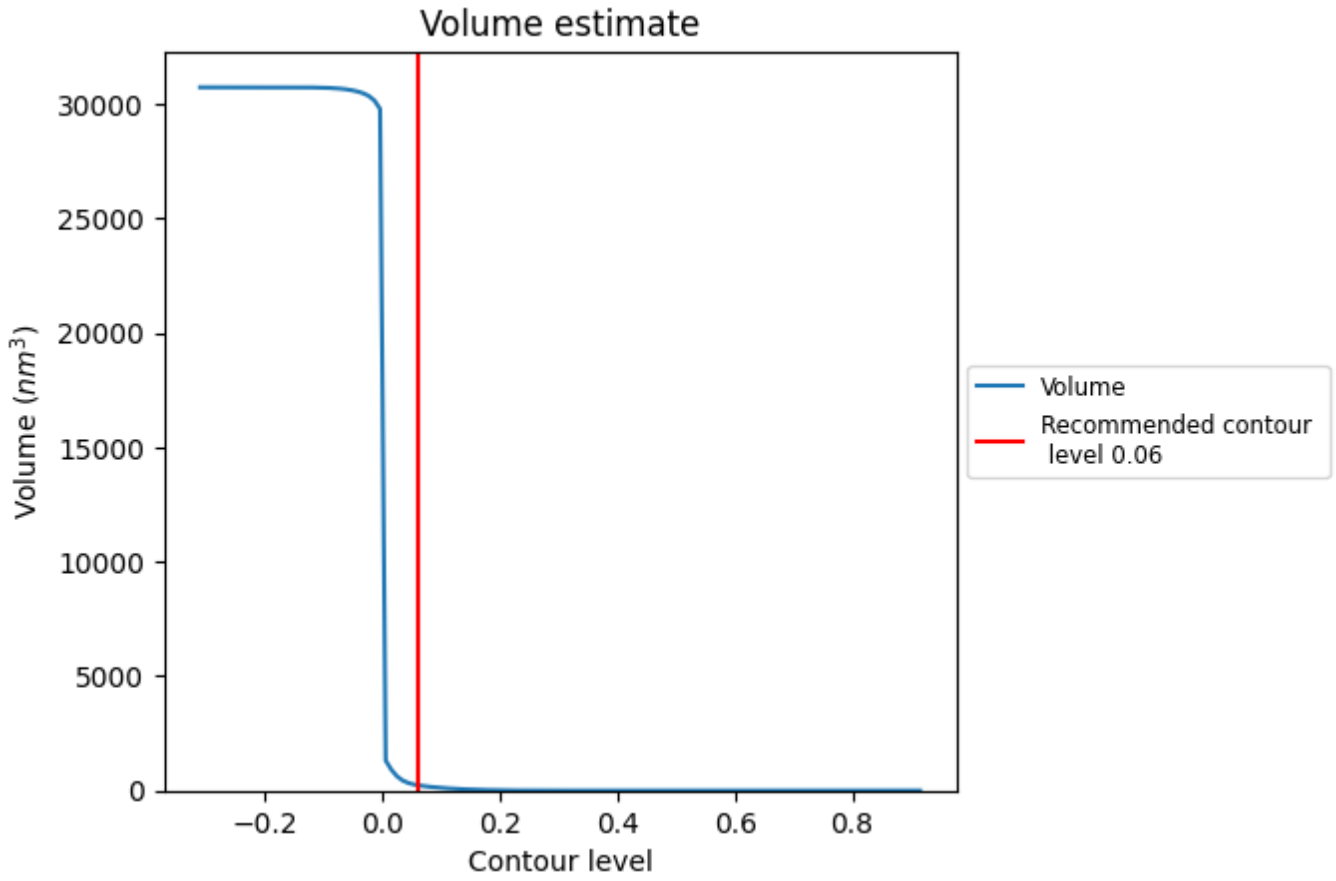
This section contains the results of statistical analysis of the map.

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.

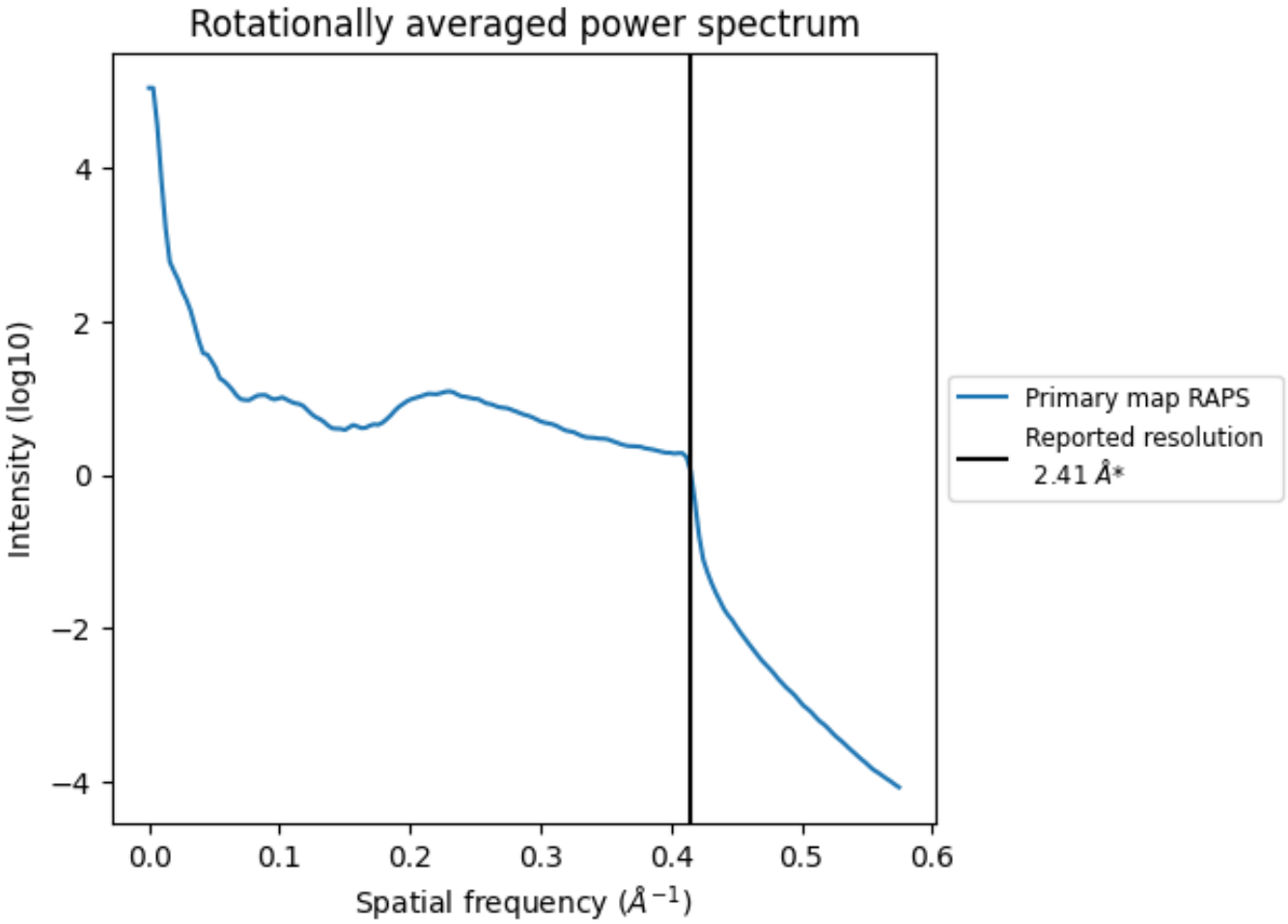
7.2 Volume estimate (i)



The volume at the recommended contour level is 239 nm^3; this corresponds to an approximate mass of 215 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)

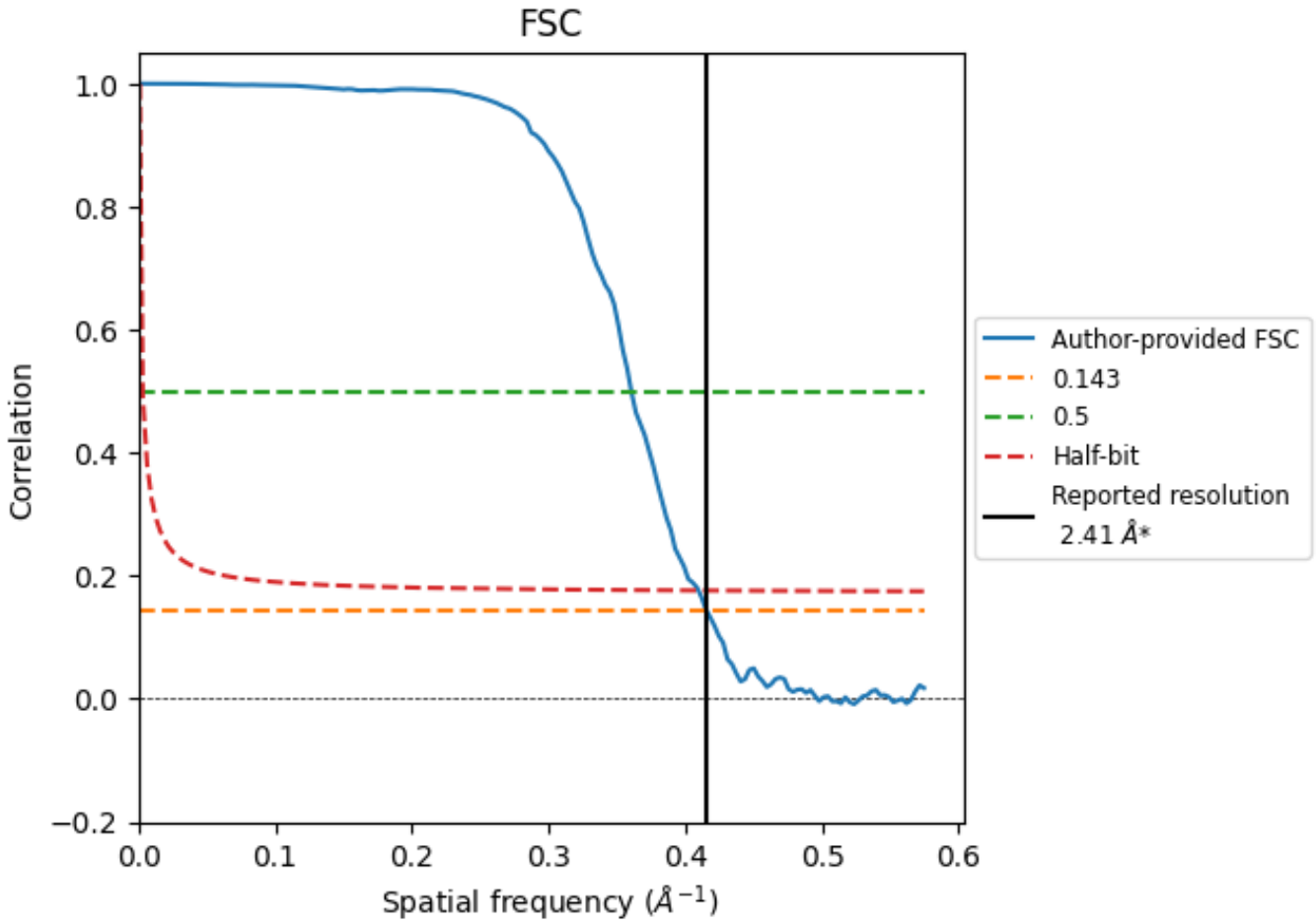


*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

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 0.415 $Å^{-1}$

8.2 Resolution estimates (i)

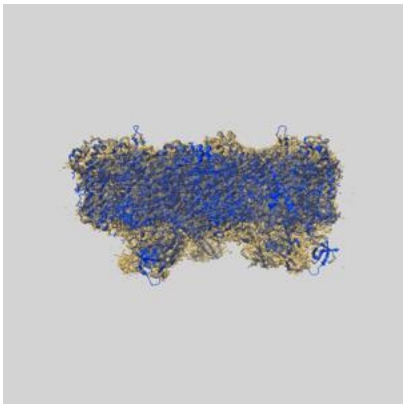
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.77	2.44
Unmasked-calculated*	-	-	-

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

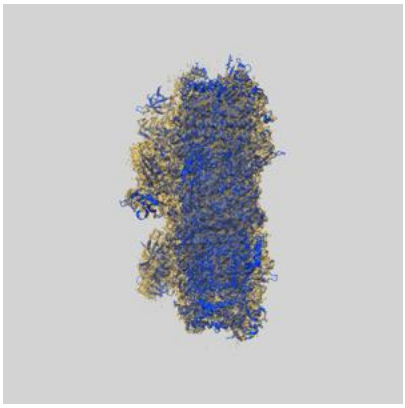
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0727 and PDB model 6KMX. Per-residue inclusion information can be found in section 3 on page 30.

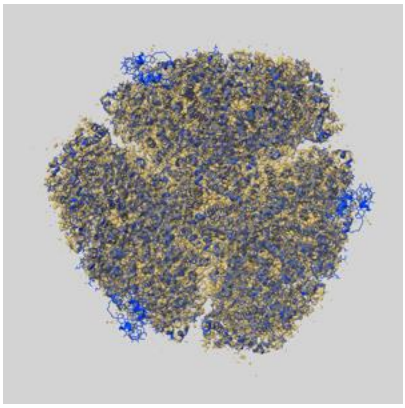
9.1 Map-model overlay



X



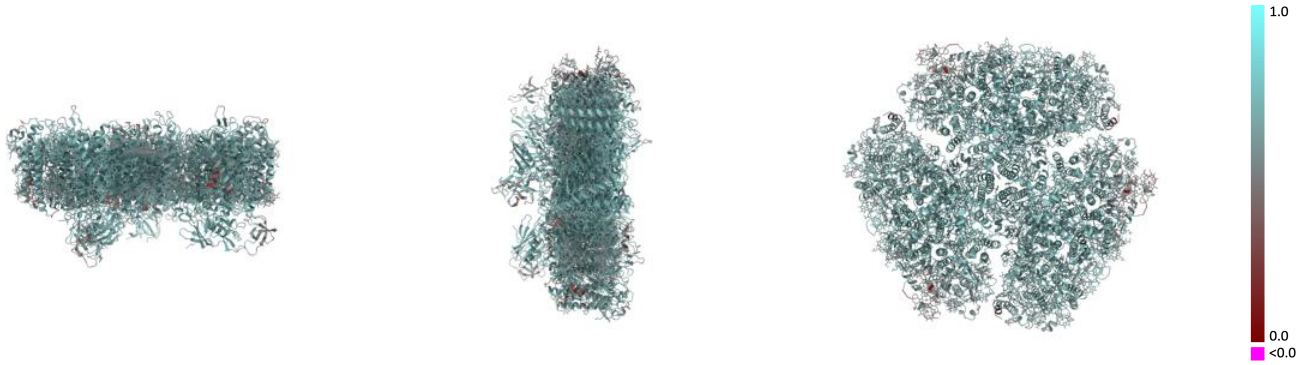
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

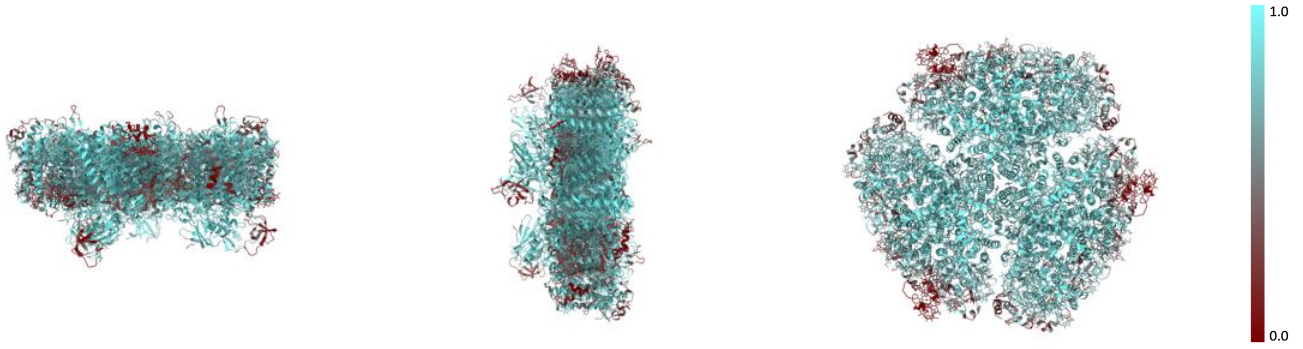
9.2 Q-score mapped to coordinate model



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.

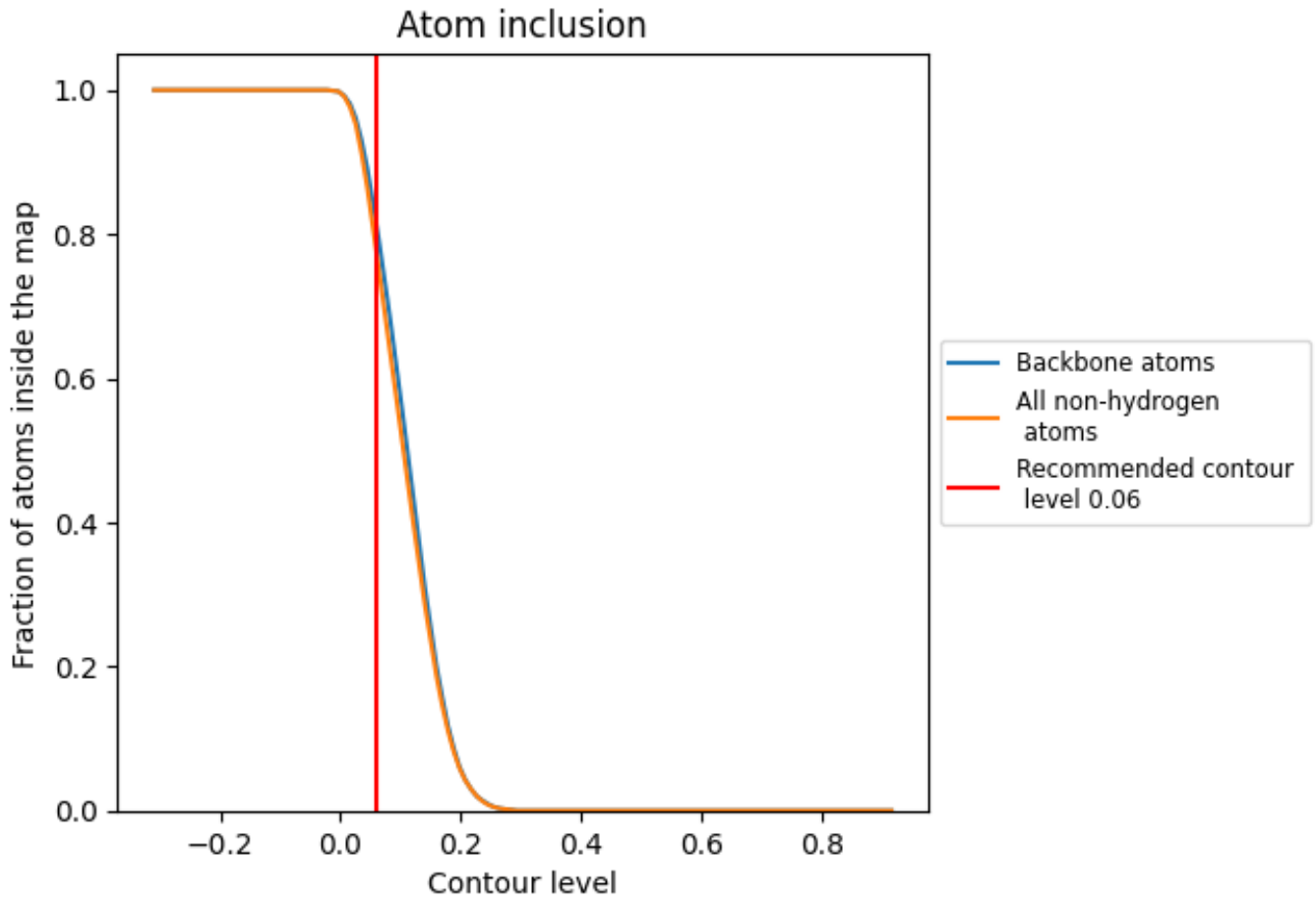
9.3 Atom inclusion mapped to coordinate model



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7730	0.6490
aA	0.7920	0.6560
aB	0.7450	0.6400
aC	0.9000	0.6780
aD	0.8630	0.6760
aE	0.3350	0.5280
aI	0.8930	0.6970
aK	0.3490	0.5080
aL	0.9090	0.6980
aM	0.7880	0.6400
bA	0.7920	0.6570
bB	0.7500	0.6400
bC	0.9010	0.6780
bD	0.8730	0.6760
bE	0.3310	0.5280
bI	0.8930	0.6980
bK	0.3430	0.5070
bL	0.9130	0.6970
bM	0.7840	0.6440
cA	0.7920	0.6560
cB	0.7490	0.6410
cC	0.8960	0.6800
cD	0.8700	0.6740
cE	0.3240	0.5240
cI	0.8800	0.6940
cK	0.3330	0.5040
cL	0.9140	0.6970
cM	0.7880	0.6400

