wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 12:01 PM EDT

PDB ID	:	10EG / pdb_000010eg
EMDB ID	:	EMD-75106
Title	:	Thermosynechococcus vestitus (BP-1) Photosystem I Complexed with Platinum Nanoparticles
Authors	:	Emerson, M.D.; Gisriel, C.J.
Deposited on	:	2026-01-15
Resolution	:	3.40 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

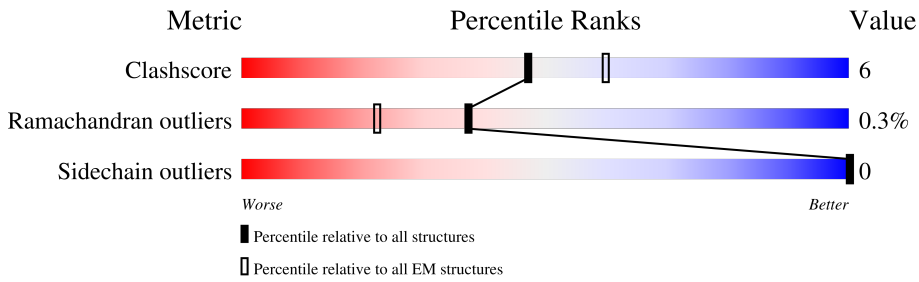
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

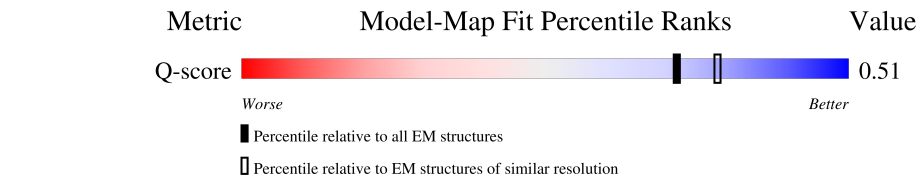
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	A	755	85% 12%
1	G	755	84% 14%
1	a	755	85% 13%
2	B	741	86% 13%

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Mol	Chain	Length	Quality of chain
2	H	741	85% 14%
2	b	741	87% 12%
3	C	81	85% 14%
3	N	81	85% 12%
3	c	81	85% 12%
4	D	139	91% 8%
4	O	139	89% 9%
4	d	139	84% 14%
5	E	76	83% 8% 9%
5	P	76	83% 8% 9%
5	e	76	75% 16% 9%
6	F	164	10% 73% 13% 14%
6	Q	164	9% 76% 10% 14%
6	f	164	10% 77% 9% 14%
7	I	38	84% 13%
7	R	38	87% 11%
7	i	38	79% 21%
8	J	41	95% 5%
8	S	41	93% 7%
8	j	41	93% 7%
9	K	83	12% 52% 45%
9	T	83	10% 52% 45%
9	k	83	11% 52% 45%
10	L	155	88% 10%
10	U	155	87% 10%

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Mol	Chain	Length	Quality of chain
10	l	155	92% 6% •
11	M	31	90% 10%
11	V	31	87% 10% •
11	m	31	90% 6% •
12	W	39	8% 69% 5% 26%
12	X	39	5% 67% 8% 26%
12	x	39	8% 67% 8% 26%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 71748 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
			Total	C	N	O	S		
1	A	740	5784	3794	988	976	26	0	0
1	G	740	5784	3794	988	976	26	0	0
1	a	740	5784	3794	988	976	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	739	5883	3870	987	1005	21	0	0
2	H	739	5883	3870	987	1005	21	0	0
2	b	739	5883	3870	987	1005	21	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	137	1068	678	185	202	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	137	1068	678	185	202	3	0	0
4	d	137	1068	678	185	202	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	69	539	342	93	104	0	0
5	P	69	539	342	93	104	0	0
5	e	69	539	342	93	104	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	141	1065	680	184	197	4	0	0
6	Q	141	1065	680	184	197	4	0	0
6	f	141	1065	680	184	197	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	38	301	208	40	48	5	0	0
7	R	38	301	208	40	48	5	0	0
7	i	38	301	208	40	48	5	0	0

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	K	46	222	130	46	46	0	0
			Total	C	N	O		
9	T	46	222	130	46	46	0	0
			Total	C	N	O		
9	k	46	222	130	46	46	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	151	1119	735	179	201	4	0	0
			Total	C	N	O	S		
10	U	151	1119	735	179	201	4	0	0
			Total	C	N	O	S		
10	l	151	1119	735	179	201	4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
U	143	LEU	SER	conflict	UNP Q8DGB4
l	143	LEU	SER	conflict	UNP Q8DGB4

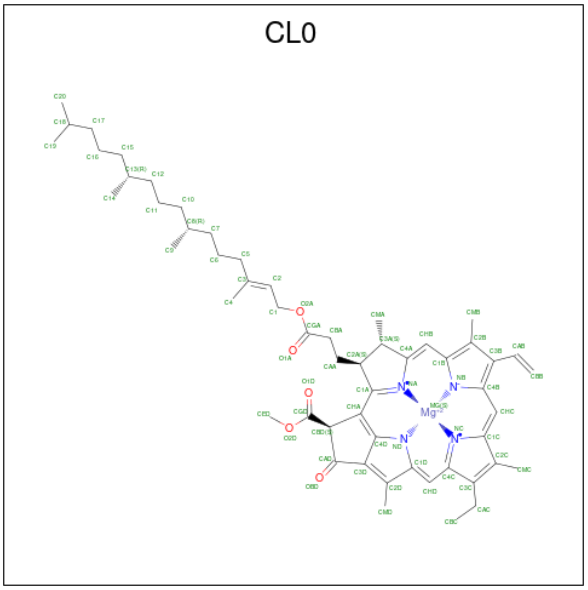
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	31	237	158	35	43	1	0	0
			Total	C	N	O	S		
11	V	31	237	158	35	43	1	0	0
			Total	C	N	O	S		
11	m	31	237	158	35	43	1	0	0

- Molecule 12 is a protein called Photosystem I 4.8K protein.

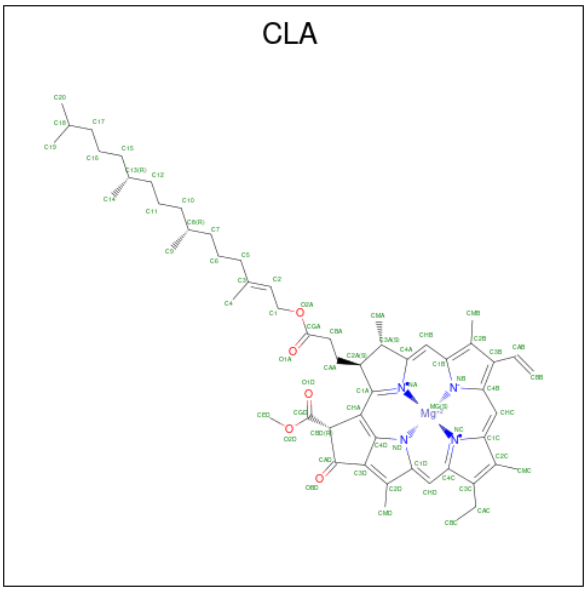
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	29	Total 232	C 163	N 34	O 35	0	0
12	X	29	Total 232	C 163	N 34	O 35	0	0
12	x	29	Total 232	C 163	N 34	O 35	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
14	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	b	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	Q	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	J	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	J	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	J	1	37	31	1	4	1	0
			Total	C	Mg	N	O	
14	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	S	1	37	31	1	4	1	0
			Total	C	Mg	N	O	
14	j	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	j	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	j	1	37	31	1	4	1	0
			Total	C	Mg	N	O	
14	K	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	T	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
14	T	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
14	k	1	41	33	1	4	3	0

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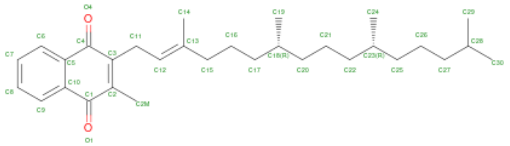
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	k	1	45	35	1	4	5	0
14	L	1	65	55	1	4	5	0
14	L	1	65	55	1	4	5	0
14	L	1	65	55	1	4	5	0
14	L	1	65	55	1	4	5	0
14	U	1	65	55	1	4	5	0
14	U	1	65	55	1	4	5	0
14	U	1	65	55	1	4	5	0
14	U	1	65	55	1	4	5	0
14	l	1	65	55	1	4	5	0
14	l	1	65	55	1	4	5	0
14	l	1	65	55	1	4	5	0
14	M	1	45	35	1	4	5	0
14	V	1	45	35	1	4	5	0
14	m	1	50	40	1	4	5	0
14	m	1	45	35	1	4	5	0
14	W	1	45	35	1	4	5	0
14	X	1	45	35	1	4	5	0
14	x	1	45	35	1	4	5	0

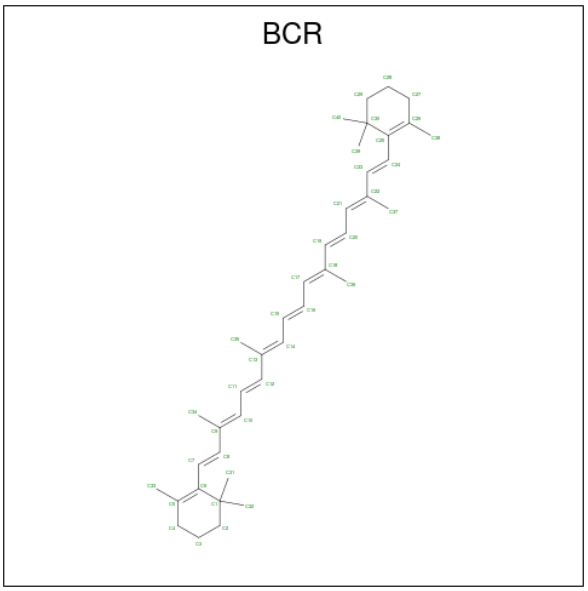
- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).

PQN



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	A	1	33	31	2	0
15	G	1	33	31	2	0
15	a	1	33	31	2	0
15	B	1	33	31	2	0
15	H	1	33	31	2	0
15	b	1	33	31	2	0

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	A	1	40	40	0
			Total	C	
16	A	1	40	40	0
			Total	C	
16	A	1	40	40	0
			Total	C	
16	A	1	40	40	0
			Total	C	
16	A	1	40	40	0
			Total	C	
16	A	1	40	40	0
			Total	C	
16	G	1	40	40	0
			Total	C	
16	G	1	40	40	0
			Total	C	
16	G	1	40	40	0
			Total	C	
16	G	1	40	40	0
			Total	C	
16	G	1	40	40	0
			Total	C	
16	G	1	40	40	0
			Total	C	
16	a	1	40	40	0
			Total	C	
16	a	1	40	40	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	a	1	40	40	0
			Total	C	
16	a	1	40	40	0
			Total	C	
16	a	1	40	40	0
			Total	C	
16	a	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	B	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	H	1	40	40	0
			Total	C	
16	b	1	40	40	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	b	1	40	40	0
			Total	C	
16	b	1	40	40	0
			Total	C	
16	b	1	40	40	0
			Total	C	
16	b	1	40	40	0
			Total	C	
16	b	1	40	40	0
			Total	C	
16	b	1	40	40	0
			Total	C	
16	b	1	40	40	0
			Total	C	
16	F	1	40	40	0
			Total	C	
16	Q	1	40	40	0
			Total	C	
16	f	1	40	40	0
			Total	C	
16	I	1	40	40	0
			Total	C	
16	R	1	40	40	0
			Total	C	
16	i	1	40	40	0
			Total	C	
16	J	1	40	40	0
			Total	C	
16	J	1	40	40	0
			Total	C	
16	S	1	40	40	0
			Total	C	
16	S	1	40	40	0
			Total	C	
16	j	1	40	40	0
			Total	C	
16	j	1	40	40	0
			Total	C	
16	L	1	40	40	0
			Total	C	
16	L	1	40	40	0

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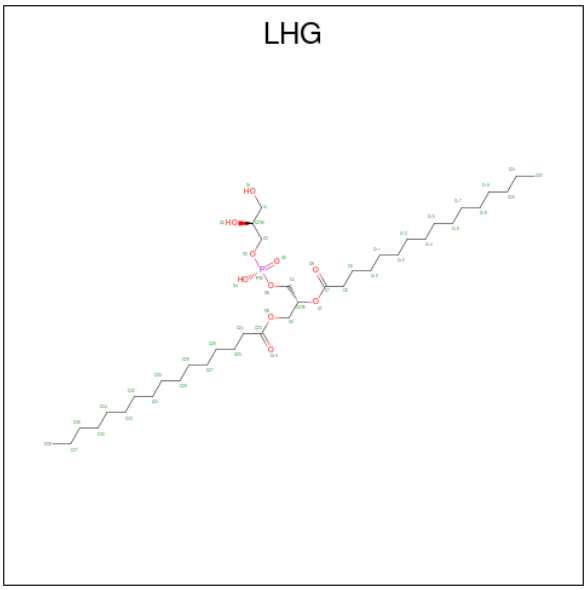
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	L	1	40	40	0
16	U	1	40	40	0
16	U	1	40	40	0
16	U	1	40	40	0
16	l	1	40	40	0
16	l	1	40	40	0
16	l	1	40	40	0
16	M	1	40	40	0
16	V	1	40	40	0
16	m	1	40	40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	A	1	49	38	10	1	0

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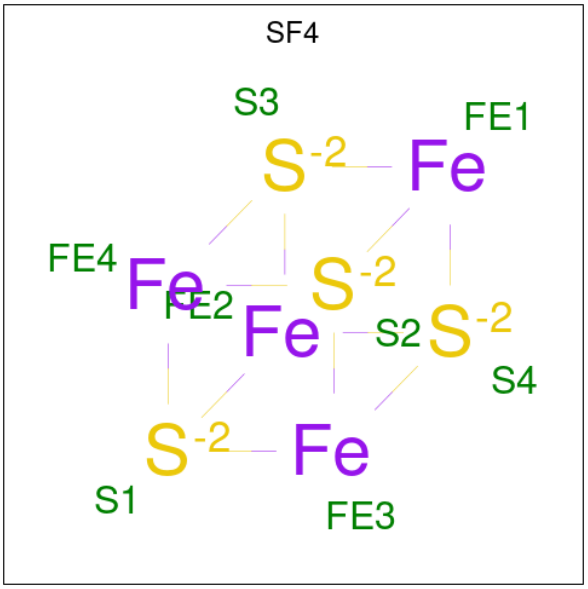
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	A	1	27	16	10	1	0
17	G	1	49	38	10	1	0
17	G	1	27	16	10	1	0
17	a	1	49	38	10	1	0
17	a	1	27	16	10	1	0

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	A	1	8	4	4	0
18	G	1	8	4	4	0
18	a	1	8	4	4	0
18	C	1	8	4	4	0
18	C	1	8	4	4	0
18	N	1	8	4	4	0

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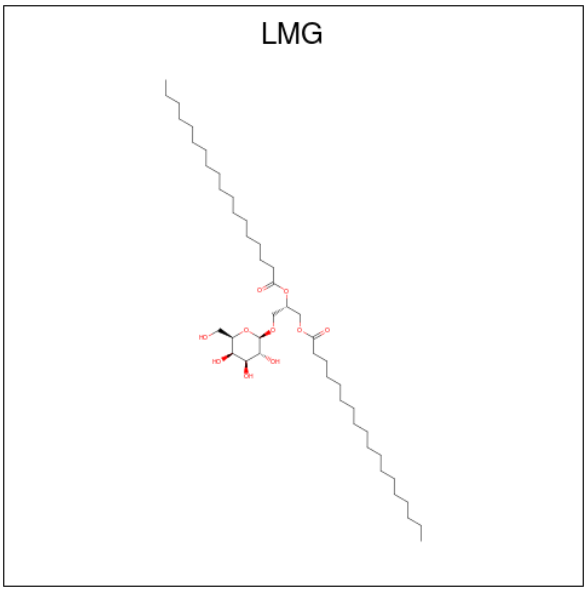
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	N	1	8	4	4	0
			Total	Fe	S	
18	c	1	8	4	4	0
			Total	Fe	S	
18	c	1	8	4	4	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
19	B	1	51	41	10	0
			Total	C	O	
19	H	1	51	41	10	0
			Total	C	O	
19	b	1	51	41	10	0

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

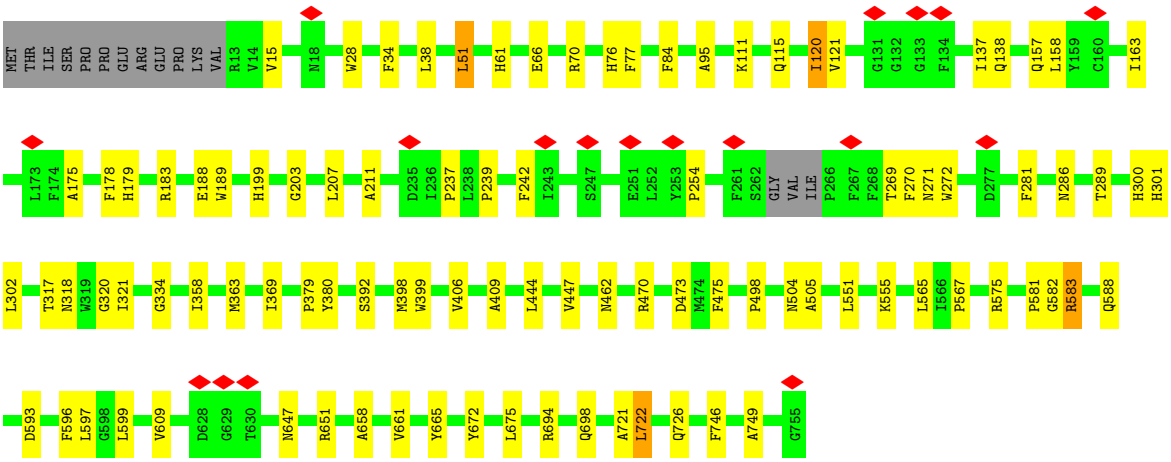
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
20	L	2	2	2	0
			Total	Ca	
20	U	1	1	1	0

3 Residue-property plots (i)

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

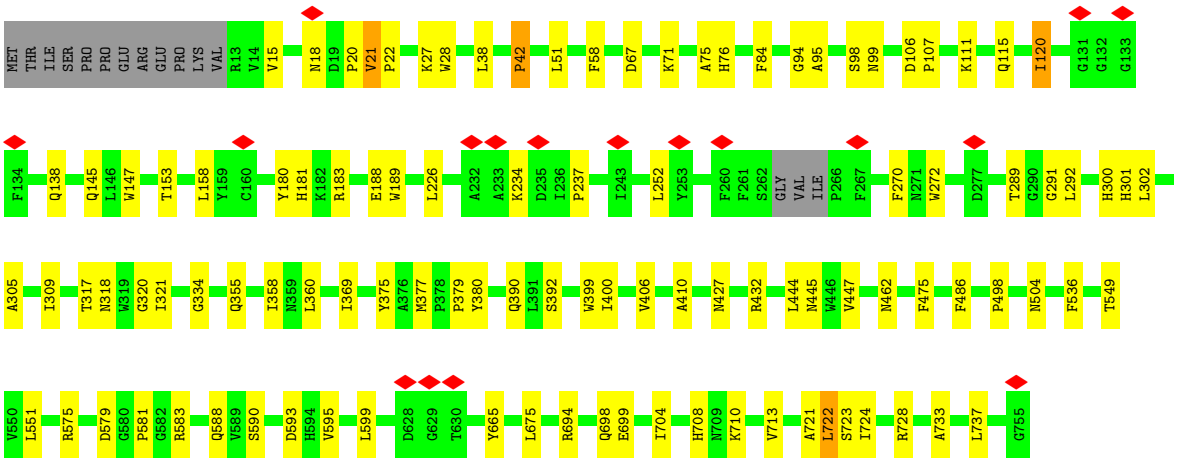
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



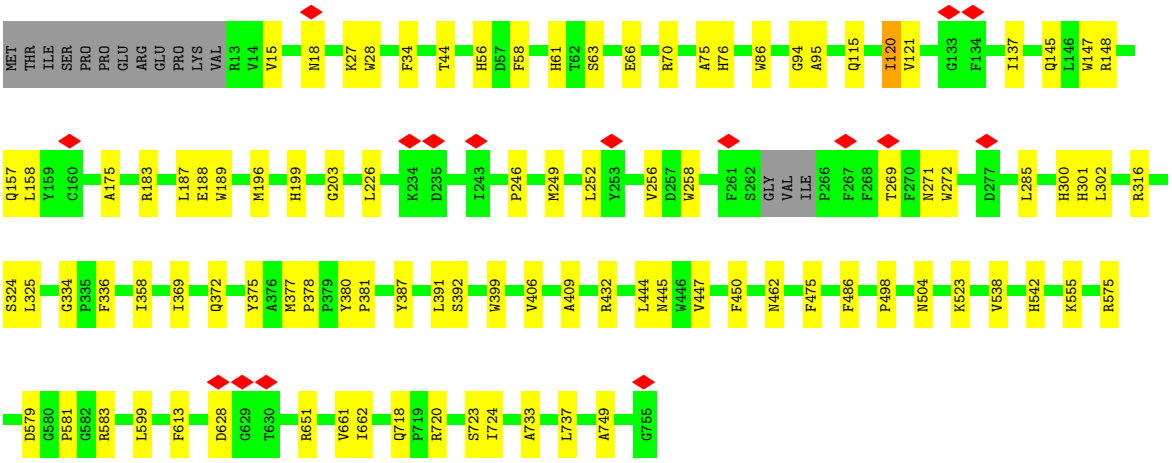
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain G:



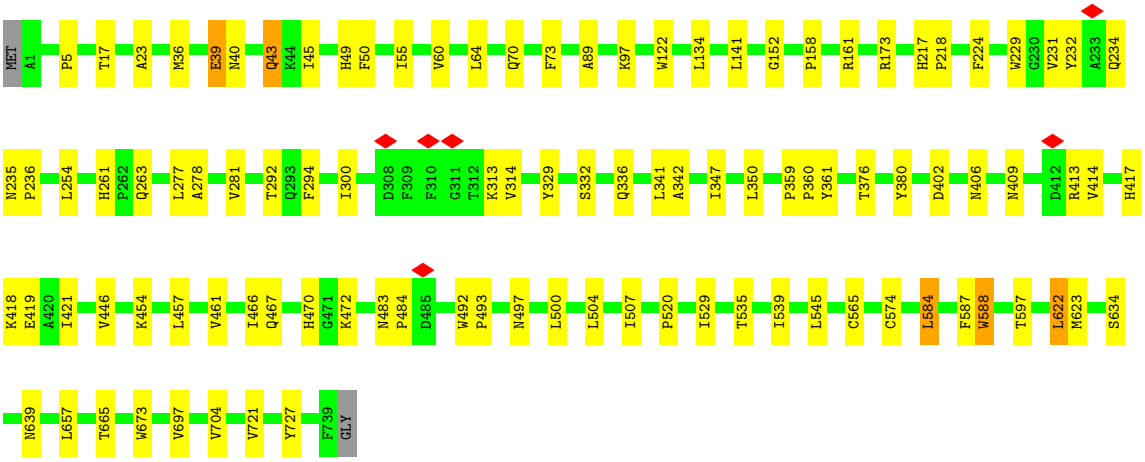
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:



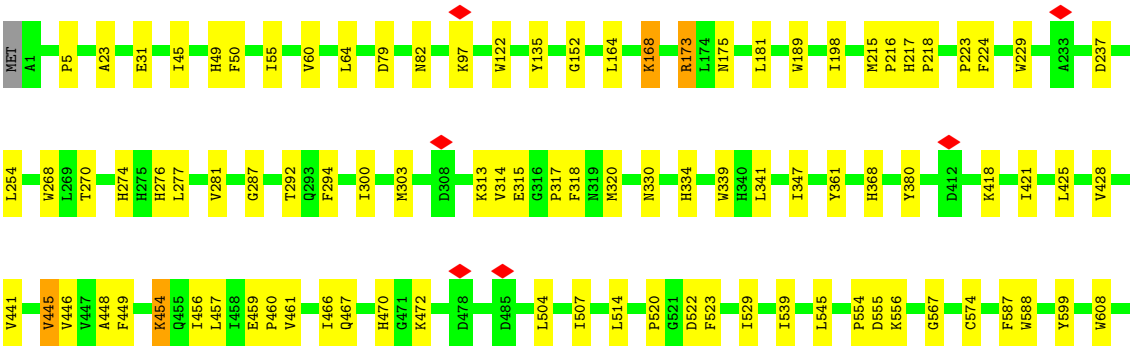
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



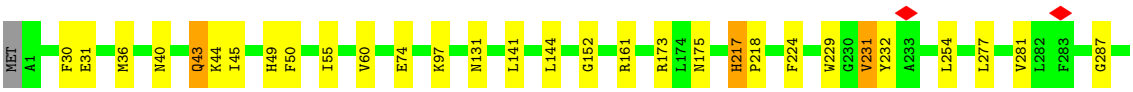
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

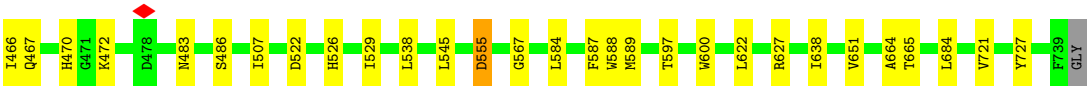
Chain H:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

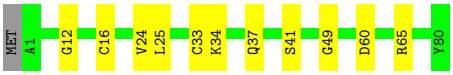
Chain b:





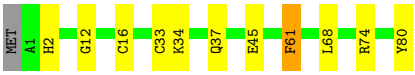
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



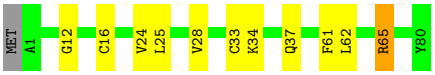
• Molecule 3: Photosystem I iron-sulfur center

Chain N:



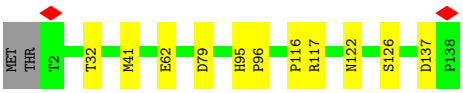
• Molecule 3: Photosystem I iron-sulfur center

Chain c:



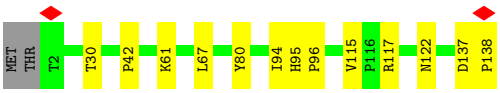
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



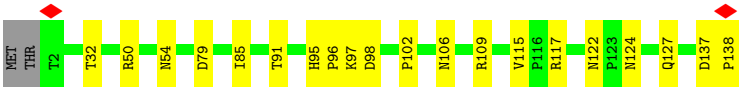
• Molecule 4: Photosystem I reaction center subunit II

Chain O:



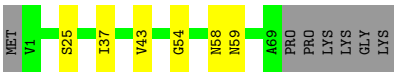
• Molecule 4: Photosystem I reaction center subunit II

Chain d:



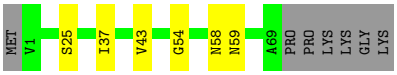
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



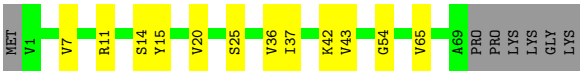
• Molecule 5: Photosystem I reaction center subunit IV

Chain P:



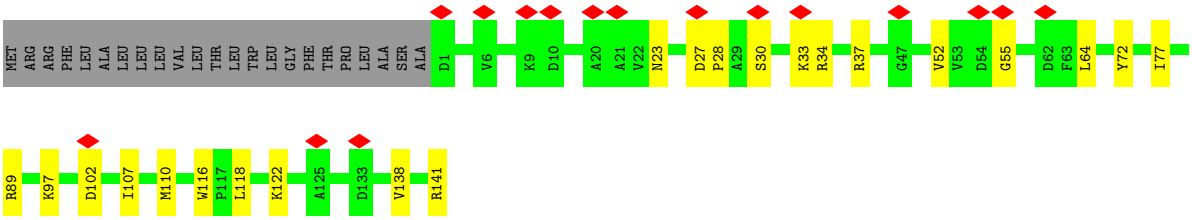
• Molecule 5: Photosystem I reaction center subunit IV

Chain e:



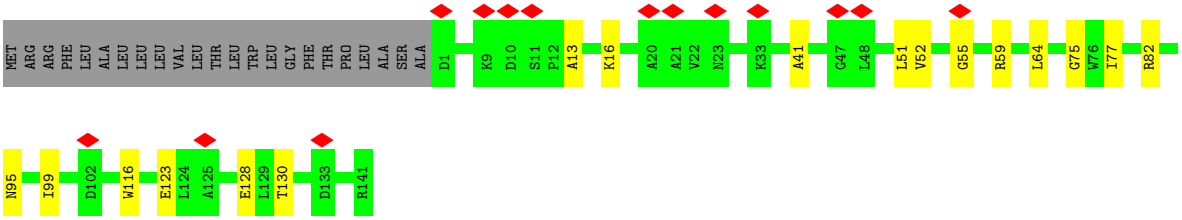
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



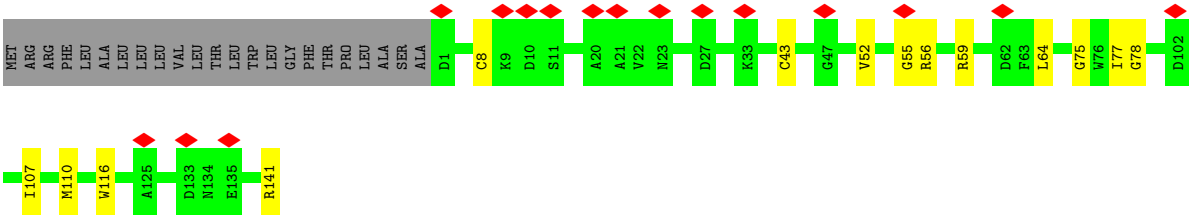
• Molecule 6: Photosystem I reaction center subunit III

Chain Q:



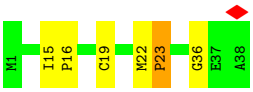
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



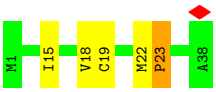
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain R:

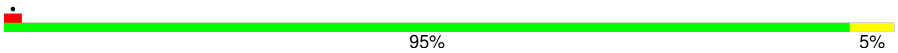


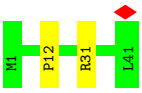
• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:

• Molecule 8: Photosystem I reaction center subunit IX

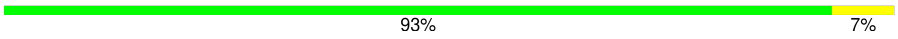
Chain J:

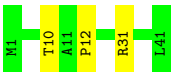




• Molecule 8: Photosystem I reaction center subunit IX

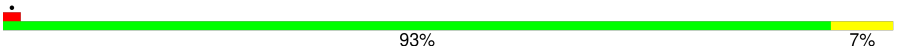
Chain S:





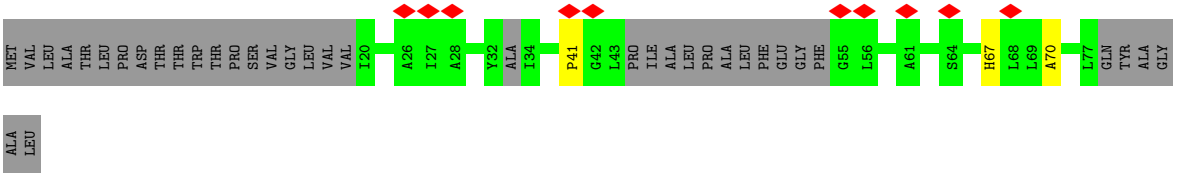
• Molecule 8: Photosystem I reaction center subunit IX

Chain j:



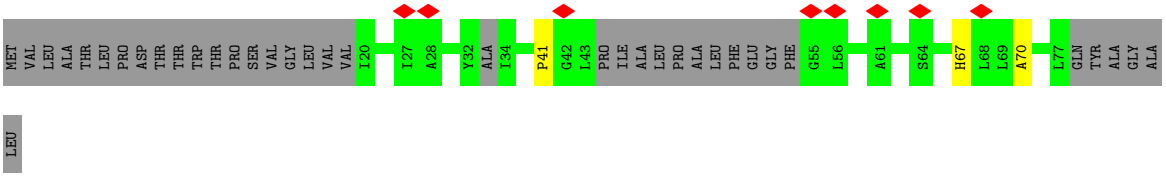
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



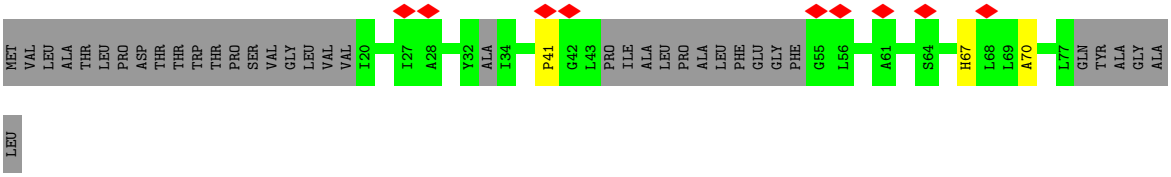
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain T:



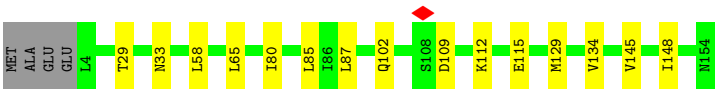
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain k:



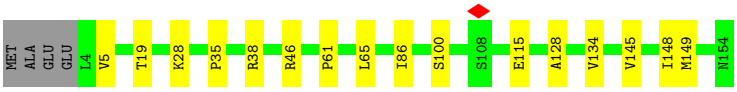
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



• Molecule 10: Photosystem I reaction center subunit XI

Chain U:

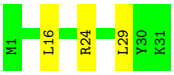


• Molecule 10: Photosystem I reaction center subunit XI

Chain l:

• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



• Molecule 11: Photosystem I reaction center subunit XII

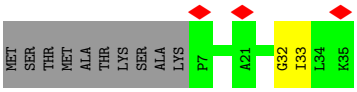
Chain V:

• Molecule 11: Photosystem I reaction center subunit XII

Chain m:

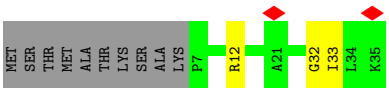
• Molecule 12: Photosystem I 4.8K protein

Chain W:



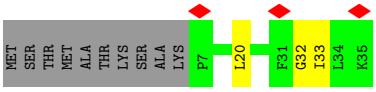
• Molecule 12: Photosystem I 4.8K protein

Chain X:



• Molecule 12: Photosystem I 4.8K protein

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19151	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.968	Depositor
Minimum map value	-0.994	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.302	Depositor
Map size (Å)	383.04, 383.04, 383.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	A	0.54	7/5983 (0.1%)	0.80	11/8158 (0.1%)
1	G	0.73	17/5983 (0.3%)	1.07	31/8158 (0.4%)
1	a	0.44	2/5983 (0.0%)	0.77	6/8158 (0.1%)
2	B	0.56	6/6100 (0.1%)	0.82	11/8336 (0.1%)
2	H	0.53	3/6100 (0.0%)	0.86	19/8336 (0.2%)
2	b	0.59	12/6100 (0.2%)	0.85	11/8336 (0.1%)
3	C	0.43	0/608	0.91	0/824
3	N	0.45	0/608	0.97	2/824 (0.2%)
3	c	0.48	0/608	0.88	3/824 (0.4%)
4	D	0.34	0/1094	0.64	1/1482 (0.1%)
4	O	0.28	0/1094	0.65	0/1482
4	d	0.37	0/1094	0.70	1/1482 (0.1%)
5	E	0.40	0/551	0.72	0/750
5	P	0.33	0/551	0.67	0/750
5	e	0.37	0/551	0.71	0/750
6	F	0.41	0/1087	0.74	0/1476
6	Q	0.44	1/1087 (0.1%)	0.79	2/1476 (0.1%)
6	f	0.40	0/1087	0.74	0/1476
7	I	0.46	0/312	0.92	2/425 (0.5%)
7	R	0.49	0/312	0.94	1/425 (0.2%)
7	i	0.38	0/312	0.79	1/425 (0.2%)
8	J	0.45	0/350	0.92	0/477
8	S	0.47	0/350	0.89	0/477
8	j	0.44	0/350	0.92	1/477 (0.2%)
9	K	0.24	0/219	0.54	0/297
9	T	0.25	0/219	0.55	0/297
9	k	0.26	0/219	0.58	0/297
10	L	0.35	0/1148	0.67	0/1558
10	U	0.39	0/1148	0.72	1/1558 (0.1%)
10	l	0.37	0/1148	0.73	1/1558 (0.1%)
11	M	0.44	0/240	0.78	0/328
11	V	0.44	0/240	0.92	2/328 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	m	0.48	0/240	0.98	3/328 (0.9%)
12	W	0.40	0/241	0.70	0/330
12	X	0.39	0/241	0.72	0/330
12	x	0.40	0/241	0.72	0/330
All	All	0.52	48/53799 (0.1%)	0.83	110/73323 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	H	0	1
2	b	0	1
4	D	0	1
4	O	0	1
4	d	0	1
6	F	0	2
6	Q	0	1
6	f	0	1
11	M	0	1
11	V	0	1
11	m	0	1
All	All	0	13

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	22	PRO	CG-CD	-26.43	0.60	1.50
1	A	498	PRO	CG-CD	-13.60	1.04	1.50
1	G	107	PRO	CG-CD	-13.28	1.05	1.50
1	G	237	PRO	N-CA	11.03	1.61	1.47
1	G	107	PRO	CB-CG	-9.96	0.99	1.49

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	237	PRO	N-CD-CG	-29.91	58.34	103.20
1	G	22	PRO	N-CD-CG	-27.69	61.66	103.20
1	G	237	PRO	CA-CB-CG	-25.88	55.32	104.50
1	G	107	PRO	CB-CG-CD	23.08	179.95	106.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	498	PRO	N-CD-CG	-18.82	74.97	103.20

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	39	GLU	Mainchain
4	D	95	HIS	Peptide
2	H	315	GLU	Sidechain
4	O	95	HIS	Peptide
2	b	161	ARG	Sidechain

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	A	5784	0	5639	65	0
1	G	5784	0	5639	71	0
1	a	5784	0	5639	69	0
2	B	5883	0	5643	78	0
2	H	5883	0	5643	76	0
2	b	5883	0	5643	65	0
3	C	598	0	580	8	0
3	N	598	0	580	8	0
3	c	598	0	580	7	0
4	D	1068	0	1067	6	0
4	O	1068	0	1067	6	0
4	d	1068	0	1067	10	0
5	E	539	0	528	4	0
5	P	539	0	528	3	0
5	e	539	0	528	7	0
6	F	1065	0	1077	12	0
6	Q	1065	0	1077	10	0
6	f	1065	0	1077	9	0
7	I	301	0	306	3	0
7	R	301	0	306	3	0
7	i	301	0	306	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	338	0	347	3	0
8	S	338	0	347	3	0
8	j	338	0	347	3	0
9	K	222	0	110	1	0
9	T	222	0	110	1	0
9	k	222	0	110	1	0
10	L	1119	0	1125	11	0
10	U	1119	0	1125	11	0
10	l	1119	0	1125	6	0
11	M	237	0	253	3	0
11	V	237	0	253	4	0
11	m	237	0	253	1	0
12	W	232	0	220	0	0
12	X	232	0	220	1	0
12	x	232	0	220	1	0
13	A	65	0	72	0	0
13	G	65	0	72	0	0
13	a	65	0	72	1	0
14	A	2382	0	2287	56	0
14	B	2398	0	2338	57	0
14	F	65	0	71	1	0
14	G	2341	0	2258	58	0
14	H	2398	0	2336	57	0
14	J	127	0	89	0	0
14	K	45	0	32	0	0
14	L	260	0	286	2	0
14	M	45	0	32	3	0
14	Q	110	0	104	2	0
14	R	65	0	71	1	0
14	S	82	0	56	0	0
14	T	86	0	61	0	0
14	U	260	0	286	4	0
14	V	45	0	32	3	0
14	W	45	0	32	1	0
14	X	45	0	32	1	0
14	a	2471	0	2402	61	0
14	b	2283	0	2229	52	0
14	j	127	0	89	0	0
14	k	86	0	61	0	0
14	l	195	0	215	2	0
14	m	95	0	71	2	0
14	x	45	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	33	0	46	3	0
15	B	33	0	46	3	0
15	G	33	0	46	2	0
15	H	33	0	46	3	0
15	a	33	0	46	3	0
15	b	33	0	46	3	0
16	A	240	0	293	13	0
16	B	320	0	392	17	0
16	F	40	0	49	2	0
16	G	240	0	294	15	0
16	H	320	0	392	16	0
16	I	40	0	49	4	0
16	J	80	0	98	6	0
16	L	120	0	147	6	0
16	M	40	0	49	3	0
16	Q	40	0	49	2	0
16	R	40	0	49	4	0
16	S	80	0	98	6	0
16	U	120	0	147	8	0
16	V	40	0	49	3	0
16	a	240	0	293	17	0
16	b	320	0	393	19	0
16	f	40	0	49	3	0
16	i	40	0	49	3	0
16	j	80	0	98	6	0
16	l	120	0	147	7	0
16	m	40	0	49	3	0
17	A	76	0	98	1	0
17	G	76	0	98	2	0
17	a	76	0	98	3	0
18	A	8	0	0	0	0
18	C	16	0	0	1	0
18	G	8	0	0	0	0
18	N	16	0	0	1	0
18	a	8	0	0	0	0
18	c	16	0	0	1	0
19	B	51	0	75	4	0
19	H	51	0	75	3	0
19	b	51	0	75	4	0
20	L	2	0	0	0	0
20	U	1	0	0	0	0
All	All	71748	0	70431	854	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 6.

The worst 5 of 854 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)
6:F:33:LYS:O	6:F:37:ARG:HB2	1.73	0.88
1:a:66:GLU:OE1	1:a:70:ARG:NH1	2.13	0.81
2:B:43:GLN:HE21	2:B:161:ARG:HH22	1.28	0.78
2:b:40:ASN:HA	2:b:43:GLN:HE21	1.52	0.74
2:b:555:ASP:OD1	3:c:65:ARG:NH1	2.21	0.72

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	A	736/755 (98%)	700 (95%)	35 (5%)	1 (0%)	48	78
1	G	736/755 (98%)	691 (94%)	44 (6%)	1 (0%)	48	78
1	a	736/755 (98%)	695 (94%)	41 (6%)	0	100	100
2	B	737/741 (100%)	690 (94%)	45 (6%)	2 (0%)	36	65
2	H	737/741 (100%)	675 (92%)	59 (8%)	3 (0%)	30	59
2	b	737/741 (100%)	686 (93%)	49 (7%)	2 (0%)	36	65
3	C	78/81 (96%)	70 (90%)	8 (10%)	0	100	100
3	N	78/81 (96%)	70 (90%)	8 (10%)	0	100	100
3	c	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	9	33
4	D	135/139 (97%)	124 (92%)	10 (7%)	1 (1%)	18	47
4	O	135/139 (97%)	121 (90%)	13 (10%)	1 (1%)	18	47
4	d	135/139 (97%)	121 (90%)	13 (10%)	1 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	67/76 (88%)	62 (92%)	5 (8%)	0	100	100
5	P	67/76 (88%)	62 (92%)	5 (8%)	0	100	100
5	e	67/76 (88%)	61 (91%)	6 (9%)	0	100	100
6	F	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
6	Q	139/164 (85%)	130 (94%)	9 (6%)	0	100	100
6	f	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
7	I	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
7	R	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
7	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	J	39/41 (95%)	35 (90%)	4 (10%)	0	100	100
8	S	39/41 (95%)	35 (90%)	4 (10%)	0	100	100
8	j	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
9	K	40/83 (48%)	37 (92%)	2 (5%)	1 (2%)	4	21
9	T	40/83 (48%)	37 (92%)	2 (5%)	1 (2%)	4	21
9	k	40/83 (48%)	36 (90%)	3 (8%)	1 (2%)	4	21
10	L	149/155 (96%)	143 (96%)	6 (4%)	0	100	100
10	U	149/155 (96%)	141 (95%)	8 (5%)	0	100	100
10	l	149/155 (96%)	144 (97%)	5 (3%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	W	27/39 (69%)	23 (85%)	2 (7%)	2 (7%)	1	5
12	X	27/39 (69%)	23 (85%)	2 (7%)	2 (7%)	1	5
12	x	27/39 (69%)	23 (85%)	2 (7%)	2 (7%)	1	5
All	All	6636/7029 (94%)	6183 (93%)	431 (6%)	22 (0%)	37	65

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ILE
1	G	321	ILE
2	B	97	LYS
2	B	314	VAL
2	H	97	LYS

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	A	589/603 (98%)	589 (100%)	0	100	100
1	G	589/603 (98%)	589 (100%)	0	100	100
1	a	589/603 (98%)	589 (100%)	0	100	100
2	B	596/598 (100%)	596 (100%)	0	100	100
2	H	596/598 (100%)	596 (100%)	0	100	100
2	b	596/598 (100%)	596 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	c	67/68 (98%)	67 (100%)	0	100	100
4	D	114/116 (98%)	114 (100%)	0	100	100
4	O	114/116 (98%)	114 (100%)	0	100	100
4	d	114/116 (98%)	114 (100%)	0	100	100
5	E	59/65 (91%)	59 (100%)	0	100	100
5	P	59/65 (91%)	59 (100%)	0	100	100
5	e	59/65 (91%)	59 (100%)	0	100	100
6	F	109/128 (85%)	109 (100%)	0	100	100
6	Q	109/128 (85%)	109 (100%)	0	100	100
6	f	109/128 (85%)	109 (100%)	0	100	100
7	I	32/32 (100%)	32 (100%)	0	100	100
7	R	32/32 (100%)	32 (100%)	0	100	100
7	i	32/32 (100%)	32 (100%)	0	100	100
8	J	36/36 (100%)	36 (100%)	0	100	100
8	S	36/36 (100%)	36 (100%)	0	100	100
8	j	36/36 (100%)	36 (100%)	0	100	100
10	L	117/120 (98%)	117 (100%)	0	100	100
10	U	117/120 (98%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	l	117/120 (98%)	117 (100%)	0	100	100
11	M	25/26 (96%)	25 (100%)	0	100	100
11	V	25/26 (96%)	25 (100%)	0	100	100
11	m	25/26 (96%)	25 (100%)	0	100	100
12	W	20/31 (64%)	20 (100%)	0	100	100
12	X	20/31 (64%)	20 (100%)	0	100	100
12	x	20/31 (64%)	20 (100%)	0	100	100
All	All	5292/5469 (97%)	5292 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
4	O	121	GLN
4	d	127	GLN
10	L	9	ASN
1	a	301	HIS
1	a	240	HIS

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 381 ligands modelled in this entry, 3 are monoatomic - leaving 378 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	$\#\|Z\| > 2$
16	BCR	a	848	-	41,41,41	2.66	6 (14%)	56,56,56	6.53	19 (33%)
14	CLA	b	805	-	69,73,73	2.20	22 (31%)	82,113,113	2.52	24 (29%)
14	CLA	H	828	-	69,73,73	2.23	23 (33%)	82,113,113	2.54	27 (32%)
16	BCR	b	842	-	41,41,41	2.58	6 (14%)	56,56,56	6.73	20 (35%)
14	CLA	G	837	1	49,53,73	2.53	22 (44%)	58,89,113	2.82	23 (39%)
14	CLA	b	827	-	69,73,73	2.26	22 (31%)	82,113,113	2.40	27 (32%)
14	CLA	H	822	-	49,53,73	2.61	22 (44%)	58,89,113	2.57	23 (39%)
14	CLA	G	827	1	69,73,73	2.26	24 (34%)	82,113,113	2.47	27 (32%)
14	CLA	J	1301	-	49,53,73	2.56	23 (46%)	58,89,113	2.57	23 (39%)
16	BCR	G	845	-	41,41,41	2.61	6 (14%)	56,56,56	6.56	23 (41%)
16	BCR	U	208	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	18 (32%)
14	CLA	a	827	-	69,73,73	2.26	24 (34%)	82,113,113	2.46	28 (34%)
14	CLA	b	815	-	59,63,73	2.45	23 (38%)	70,101,113	2.67	25 (35%)
14	CLA	B	833	-	49,53,73	2.54	22 (44%)	58,89,113	2.74	24 (41%)
14	CLA	a	809	1	49,53,73	2.51	21 (42%)	58,89,113	2.82	24 (41%)
14	CLA	A	805	-	69,73,73	2.23	22 (31%)	82,113,113	2.48	24 (29%)
16	BCR	B	849	-	41,41,41	2.68	6 (14%)	56,56,56	6.71	26 (46%)
19	LMG	H	851	-	51,51,55	1.44	7 (13%)	59,59,63	1.10	2 (3%)
14	CLA	A	812	-	64,68,73	2.26	23 (35%)	76,107,113	2.90	31 (40%)
14	CLA	G	828	-	69,73,73	2.21	21 (30%)	82,113,113	2.43	26 (31%)
14	CLA	U	206	10	69,73,73	2.21	23 (33%)	82,113,113	2.49	26 (31%)
14	CLA	G	822	-	55,59,73	2.50	23 (41%)	64,96,113	2.83	27 (42%)
16	BCR	M	1602	-	41,41,41	2.63	6 (14%)	56,56,56	6.73	26 (46%)
14	CLA	a	816	-	54,58,73	2.53	24 (44%)	64,95,113	2.75	27 (42%)
14	CLA	B	803	-	69,73,73	2.26	23 (33%)	82,113,113	2.43	27 (32%)
14	CLA	B	807	2	54,58,73	2.54	23 (42%)	64,95,113	2.83	25 (39%)
14	CLA	G	836	-	69,73,73	2.21	23 (33%)	82,113,113	2.45	28 (34%)
16	BCR	G	848	-	41,41,41	2.68	6 (14%)	56,56,56	7.04	27 (48%)
16	BCR	H	852	-	41,41,41	2.64	6 (14%)	56,56,56	6.50	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	A	831	1	69,73,73	2.22	23 (33%)	82,113,113	2.46	27 (32%)
14	CLA	a	819	-	59,63,73	2.45	24 (40%)	70,101,113	2.72	29 (41%)
14	CLA	b	819	-	49,53,73	2.58	21 (42%)	58,89,113	2.60	23 (39%)
18	SF4	c	102	3	0,12,12	-	-	-		
16	BCR	F	202	-	41,41,41	2.59	6 (14%)	56,56,56	6.45	25 (44%)
14	CLA	H	826	2	58,62,73	2.71	23 (39%)	68,99,113	2.51	33 (48%)
16	BCR	B	848	-	41,41,41	2.64	7 (17%)	56,56,56	6.69	30 (53%)
16	BCR	H	846	-	41,41,41	2.62	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	b	808	-	69,73,73	2.20	21 (30%)	82,113,113	2.63	27 (32%)
14	CLA	b	829	2	49,53,73	2.55	20 (40%)	58,89,113	2.76	29 (50%)
14	CLA	V	1601	-	49,53,73	2.57	21 (42%)	58,89,113	2.80	25 (43%)
14	CLA	B	842	2	69,73,73	2.20	22 (31%)	82,113,113	2.50	29 (35%)
17	LHG	G	850	-	26,26,48	1.27	2 (7%)	29,32,54	1.26	3 (10%)
14	CLA	a	832	1	69,73,73	2.23	21 (30%)	82,113,113	2.45	27 (32%)
14	CLA	m	1202	-	49,53,73	2.57	22 (44%)	58,89,113	2.82	24 (41%)
14	CLA	b	811	2	49,53,73	2.56	23 (46%)	58,89,113	2.76	26 (44%)
14	CLA	L	201	-	69,73,73	2.20	23 (33%)	82,113,113	2.52	26 (31%)
18	SF4	c	101	3	0,12,12	-	-	-		
14	CLA	G	815	1	49,53,73	2.57	20 (40%)	58,89,113	2.83	23 (39%)
16	BCR	A	844	-	41,41,41	2.60	6 (14%)	56,56,56	6.73	21 (37%)
17	LHG	a	851	-	26,26,48	1.26	2 (7%)	29,32,54	1.28	3 (10%)
14	CLA	G	838	-	54,58,73	2.51	22 (40%)	64,95,113	2.81	27 (42%)
14	CLA	a	813	-	49,53,73	2.54	23 (46%)	58,89,113	2.98	26 (44%)
14	CLA	U	207	-	69,73,73	2.24	24 (34%)	82,113,113	2.41	25 (30%)
16	BCR	G	844	-	41,41,41	2.60	6 (14%)	56,56,56	6.58	24 (42%)
14	CLA	A	820	-	69,73,73	2.23	24 (34%)	82,113,113	2.44	26 (31%)
14	CLA	B	805	-	69,73,73	2.35	21 (30%)	82,113,113	2.20	23 (28%)
14	CLA	B	801	-	69,73,73	2.29	20 (28%)	82,113,113	2.08	23 (28%)
14	CLA	G	808	1	69,73,73	2.27	23 (33%)	82,113,113	2.46	27 (32%)
14	CLA	G	821	-	49,53,73	2.51	22 (44%)	58,89,113	2.93	27 (46%)
14	CLA	A	834	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	22 (37%)
14	CLA	H	812	2	69,73,73	2.23	22 (31%)	82,113,113	2.38	29 (35%)
14	CLA	b	825	-	69,73,73	2.23	23 (33%)	82,113,113	2.50	27 (32%)
16	BCR	l	206	-	41,41,41	2.59	6 (14%)	56,56,56	6.56	19 (33%)
14	CLA	a	824	-	69,73,73	2.22	22 (31%)	82,113,113	2.35	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	A	807	1	69,73,73	2.23	21 (30%)	82,113,113	2.54	29 (35%)
14	CLA	H	833	-	49,53,73	2.54	22 (44%)	58,89,113	2.75	24 (41%)
16	BCR	H	849	-	41,41,41	2.67	6 (14%)	56,56,56	6.68	27 (48%)
14	CLA	G	824	-	69,73,73	2.22	23 (33%)	82,113,113	2.41	26 (31%)
13	CL0	G	801	-	69,73,73	2.25	20 (28%)	82,113,113	2.36	23 (28%)
14	CLA	b	818	-	69,73,73	2.21	24 (34%)	82,113,113	2.43	27 (32%)
14	CLA	A	837	1	49,53,73	2.54	22 (44%)	58,89,113	2.82	23 (39%)
14	CLA	a	839	-	54,58,73	2.51	24 (44%)	64,95,113	2.80	25 (39%)
14	CLA	H	809	2	69,73,73	2.21	23 (33%)	82,113,113	2.43	24 (29%)
14	CLA	H	838	2	64,68,73	2.30	21 (32%)	76,107,113	2.52	26 (34%)
14	CLA	G	834	-	49,53,73	2.53	22 (44%)	58,89,113	2.82	23 (39%)
14	CLA	B	830	2	69,73,73	2.27	23 (33%)	82,113,113	2.45	27 (32%)
14	CLA	B	821	-	69,73,73	2.22	24 (34%)	82,113,113	2.42	28 (34%)
14	CLA	A	803	1,14	59,63,73	2.41	22 (37%)	70,101,113	2.64	30 (42%)
14	CLA	G	825	-	69,73,73	2.23	23 (33%)	82,113,113	2.49	27 (32%)
14	CLA	a	812	-	64,68,73	2.29	22 (34%)	76,107,113	2.80	30 (39%)
14	CLA	H	831	-	69,73,73	2.24	23 (33%)	82,113,113	2.56	29 (35%)
14	CLA	B	838	-	64,68,73	2.32	23 (35%)	76,107,113	2.52	28 (36%)
14	CLA	b	823	-	58,62,73	2.43	23 (39%)	68,99,113	2.61	28 (41%)
14	CLA	j	1302	8	49,53,73	2.57	23 (46%)	58,89,113	2.82	24 (41%)
14	CLA	a	805	-	69,73,73	2.22	21 (30%)	82,113,113	2.50	24 (29%)
14	CLA	H	832	2	49,53,73	2.50	20 (40%)	58,89,113	2.79	26 (44%)
14	CLA	G	830	1	54,58,73	2.51	23 (42%)	64,95,113	2.79	25 (39%)
14	CLA	a	840	1	69,73,73	2.24	24 (34%)	82,113,113	2.52	27 (32%)
14	CLA	a	831	1	69,73,73	2.22	23 (33%)	82,113,113	2.46	27 (32%)
16	BCR	i	101	-	41,41,41	2.62	6 (14%)	56,56,56	6.71	21 (37%)
16	BCR	S	103	-	41,41,41	2.61	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	a	820	-	69,73,73	2.24	24 (34%)	82,113,113	2.43	25 (30%)
18	SF4	A	853	1,2	0,12,12	-	-	-		
14	CLA	B	808	-	69,73,73	2.20	22 (31%)	82,113,113	2.48	24 (29%)
14	CLA	a	802	-	69,73,73	2.24	22 (31%)	82,113,113	2.45	25 (30%)
14	CLA	J	1302	8	49,53,73	2.58	22 (44%)	58,89,113	2.79	22 (37%)
14	CLA	H	805	-	69,73,73	2.24	22 (31%)	82,113,113	2.53	27 (32%)
14	CLA	G	818	-	69,73,73	2.25	23 (33%)	82,113,113	2.42	26 (31%)
14	CLA	G	802	1	69,73,73	2.24	23 (33%)	82,113,113	2.50	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	BCR	b	845	-	41,41,41	2.36	7 (17%)	56,56,56	6.15	29 (51%)
14	CLA	B	841	-	69,73,73	2.23	24 (34%)	82,113,113	2.48	26 (31%)
14	CLA	A	813	-	49,53,73	2.54	23 (46%)	58,89,113	2.89	26 (44%)
16	BCR	L	207	-	41,41,41	2.58	6 (14%)	56,56,56	6.57	19 (33%)
16	BCR	L	202	-	41,41,41	2.65	6 (14%)	56,56,56	6.57	23 (41%)
15	PQN	b	841	-	34,34,34	1.60	2 (5%)	43,45,45	1.01	3 (6%)
18	SF4	G	852	1,2	0,12,12	-	-	-		
14	CLA	H	835	-	49,53,73	2.54	23 (46%)	58,89,113	2.73	22 (37%)
14	CLA	b	826	-	69,73,73	2.23	21 (30%)	82,113,113	2.47	28 (34%)
14	CLA	b	813	2	69,73,73	2.18	22 (31%)	82,113,113	2.59	26 (31%)
14	CLA	l	205	-	69,73,73	2.24	23 (33%)	82,113,113	2.41	24 (29%)
14	CLA	a	829	1	69,73,73	2.22	22 (31%)	82,113,113	2.45	26 (31%)
14	CLA	A	833	1	54,58,73	2.55	22 (40%)	64,95,113	2.71	27 (42%)
14	CLA	A	836	-	69,73,73	2.21	22 (31%)	82,113,113	2.48	27 (32%)
14	CLA	a	818	-	69,73,73	2.25	23 (33%)	82,113,113	2.44	27 (32%)
14	CLA	a	807	1	69,73,73	2.21	22 (31%)	82,113,113	2.57	29 (35%)
14	CLA	a	806	-	54,58,73	2.53	22 (40%)	64,95,113	2.82	27 (42%)
14	CLA	b	816	2	59,63,73	2.42	23 (38%)	70,101,113	2.64	29 (41%)
14	CLA	a	837	1	49,53,73	2.54	22 (44%)	58,89,113	2.81	23 (39%)
16	BCR	l	202	-	41,41,41	2.57	6 (14%)	56,56,56	6.63	26 (46%)
14	CLA	A	839	1	69,73,73	2.24	23 (33%)	82,113,113	2.50	26 (31%)
14	CLA	G	831	1	69,73,73	2.22	23 (33%)	82,113,113	2.45	27 (32%)
14	CLA	G	816	-	54,58,73	2.53	24 (44%)	64,95,113	2.74	26 (40%)
16	BCR	G	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.53	19 (33%)
14	CLA	B	823	2	49,53,73	2.57	22 (44%)	58,89,113	2.93	25 (43%)
14	CLA	j	1303	-	41,45,73	2.64	21 (51%)	50,78,113	2.81	20 (40%)
14	CLA	L	206	-	69,73,73	2.24	23 (33%)	82,113,113	2.43	25 (30%)
14	CLA	B	814	-	49,53,73	2.55	22 (44%)	58,89,113	2.79	23 (39%)
16	BCR	B	852	-	41,41,41	2.64	6 (14%)	56,56,56	6.55	24 (42%)
14	CLA	B	829	2	69,73,73	2.23	22 (31%)	82,113,113	2.48	27 (32%)
14	CLA	G	805	1	69,73,73	2.23	22 (31%)	82,113,113	2.54	26 (31%)
14	CLA	G	820	-	69,73,73	2.24	24 (34%)	82,113,113	2.44	25 (30%)
14	CLA	b	822	-	49,53,73	2.57	23 (46%)	58,89,113	2.76	24 (41%)
14	CLA	A	840	-	69,73,73	2.21	22 (31%)	82,113,113	2.43	27 (32%)
14	CLA	A	828	-	69,73,73	2.22	21 (30%)	82,113,113	2.45	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	F	201	2	69,73,73	2.24	23 (33%)	82,113,113	2.45	30 (36%)
16	BCR	H	844	-	41,41,41	2.57	6 (14%)	56,56,56	6.70	20 (35%)
14	CLA	b	839	-	69,73,73	2.24	23 (33%)	82,113,113	2.48	28 (34%)
14	CLA	B	811	-	69,73,73	2.22	22 (31%)	82,113,113	2.60	26 (31%)
14	CLA	x	1701	12	49,53,73	2.54	23 (46%)	58,89,113	2.80	23 (39%)
14	CLA	A	832	-	69,73,73	2.22	22 (31%)	82,113,113	2.48	27 (32%)
17	LHG	G	849	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
16	BCR	m	1203	-	41,41,41	2.63	6 (14%)	56,56,56	6.73	27 (48%)
14	CLA	A	804	1	69,73,73	2.18	21 (30%)	82,113,113	2.51	29 (35%)
14	CLA	A	824	-	69,73,73	2.25	21 (30%)	82,113,113	2.23	27 (32%)
14	CLA	H	811	2	69,73,73	2.19	21 (30%)	82,113,113	2.64	27 (32%)
14	CLA	b	809	2	69,73,73	2.23	22 (31%)	82,113,113	2.40	28 (34%)
14	CLA	b	838	2	49,53,73	2.51	21 (42%)	58,89,113	2.84	25 (43%)
14	CLA	b	812	-	69,73,73	2.27	23 (33%)	82,113,113	2.53	28 (34%)
14	CLA	G	833	-	54,58,73	2.54	23 (42%)	64,95,113	2.76	28 (43%)
16	BCR	a	844	-	41,41,41	2.60	6 (14%)	56,56,56	6.70	22 (39%)
14	CLA	B	827	-	50,54,73	2.72	23 (46%)	59,90,113	2.75	25 (42%)
14	CLA	T	102	-	49,53,73	2.56	22 (44%)	58,89,113	2.82	26 (44%)
14	CLA	H	820	-	64,68,73	2.33	24 (37%)	76,107,113	2.61	27 (35%)
16	BCR	l	201	-	41,41,41	2.65	6 (14%)	56,56,56	6.57	23 (41%)
14	CLA	A	830	1	54,58,73	2.52	23 (42%)	64,95,113	2.78	26 (40%)
14	CLA	B	818	-	59,63,73	2.45	23 (38%)	70,101,113	2.67	26 (37%)
16	BCR	b	843	-	41,41,41	2.56	6 (14%)	56,56,56	6.70	23 (41%)
14	CLA	b	831	-	69,73,73	2.22	23 (33%)	82,113,113	2.51	27 (32%)
15	PQN	A	843	-	34,34,34	1.69	2 (5%)	43,45,45	1.67	7 (16%)
14	CLA	G	819	1	59,63,73	2.46	24 (40%)	70,101,113	2.70	27 (38%)
16	BCR	A	848	-	41,41,41	2.66	6 (14%)	56,56,56	6.53	19 (33%)
14	CLA	H	836	-	49,53,73	2.54	22 (44%)	58,89,113	2.76	25 (43%)
14	CLA	b	840	-	69,73,73	2.22	22 (31%)	82,113,113	2.52	29 (35%)
16	BCR	H	845	-	41,41,41	2.56	6 (14%)	56,56,56	6.69	23 (41%)
15	PQN	a	843	-	34,34,34	1.67	2 (5%)	43,45,45	1.15	2 (4%)
16	BCR	f	201	-	41,41,41	2.60	6 (14%)	56,56,56	6.48	25 (44%)
16	BCR	L	209	-	41,41,41	2.58	6 (14%)	56,56,56	6.62	26 (46%)
14	CLA	B	819	2	59,63,73	2.42	23 (38%)	70,101,113	2.65	29 (41%)
14	CLA	A	810	14	69,73,73	2.22	22 (31%)	82,113,113	2.54	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	G	803	14	59,63,73	2.40	23 (38%)	70,101,113	2.70	31 (44%)
16	BCR	A	849	-	41,41,41	2.66	6 (14%)	56,56,56	7.04	24 (42%)
16	BCR	G	846	-	41,41,41	2.62	6 (14%)	56,56,56	6.72	28 (50%)
14	CLA	H	840	2	49,53,73	2.52	21 (42%)	58,89,113	2.85	26 (44%)
14	CLA	G	812	-	64,68,73	2.26	24 (37%)	76,107,113	2.73	28 (36%)
14	CLA	H	813	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	25 (43%)
14	CLA	B	832	2	49,53,73	2.57	18 (36%)	58,89,113	2.75	27 (46%)
14	CLA	W	1701	12	49,53,73	2.54	23 (46%)	58,89,113	2.80	23 (39%)
14	CLA	A	835	-	54,58,73	2.52	22 (40%)	64,95,113	2.73	25 (39%)
14	CLA	L	205	10	69,73,73	2.22	23 (33%)	82,113,113	2.50	27 (32%)
14	CLA	U	201	-	69,73,73	2.20	22 (31%)	82,113,113	2.51	27 (32%)
14	CLA	G	840	-	69,73,73	2.21	22 (31%)	82,113,113	2.41	27 (32%)
14	CLA	A	818	-	69,73,73	2.25	23 (33%)	82,113,113	2.44	29 (35%)
17	LHG	A	850	-	48,48,48	0.92	2 (4%)	51,54,54	1.12	4 (7%)
14	CLA	A	806	-	54,58,73	2.52	22 (40%)	64,95,113	2.79	26 (40%)
14	CLA	B	813	-	49,53,73	2.53	23 (46%)	58,89,113	2.81	24 (41%)
14	CLA	A	825	-	69,73,73	2.22	23 (33%)	82,113,113	2.50	27 (32%)
14	CLA	H	839	2	69,73,73	2.25	23 (33%)	82,113,113	2.49	26 (31%)
16	BCR	b	844	-	41,41,41	2.62	6 (14%)	56,56,56	6.61	23 (41%)
14	CLA	A	814	-	49,53,73	2.53	21 (42%)	58,89,113	2.84	26 (44%)
14	CLA	a	830	-	54,58,73	2.51	22 (40%)	64,95,113	2.85	26 (40%)
14	CLA	H	827	-	50,54,73	2.75	22 (44%)	59,90,113	2.77	26 (44%)
14	CLA	a	828	-	69,73,73	2.23	21 (30%)	82,113,113	2.43	25 (30%)
14	CLA	b	806	-	69,73,73	2.21	22 (31%)	82,113,113	2.46	25 (30%)
14	CLA	H	815	-	69,73,73	2.24	23 (33%)	82,113,113	2.54	30 (36%)
14	CLA	a	836	1	69,73,73	2.21	23 (33%)	82,113,113	2.48	27 (32%)
14	CLA	B	835	-	49,53,73	2.54	23 (46%)	58,89,113	2.70	22 (37%)
14	CLA	a	835	-	54,58,73	2.54	23 (42%)	64,95,113	2.73	24 (37%)
14	CLA	H	837	-	49,53,73	2.56	22 (44%)	58,89,113	2.80	26 (44%)
14	CLA	a	817	1	54,58,73	2.56	24 (44%)	64,95,113	2.99	31 (48%)
14	CLA	A	802	1	69,73,73	2.24	23 (33%)	82,113,113	2.52	26 (31%)
14	CLA	B	815	-	69,73,73	2.24	23 (33%)	82,113,113	2.53	28 (34%)
16	BCR	H	848	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	24 (42%)
14	CLA	H	824	-	59,63,73	2.42	24 (40%)	70,101,113	2.66	26 (37%)
14	CLA	B	839	2	69,73,73	2.25	22 (31%)	82,113,113	2.49	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	B	834	-	62,66,73	2.37	22 (35%)	73,104,113	2.58	31 (42%)
14	CLA	L	204	10	69,73,73	2.24	22 (31%)	82,113,113	2.48	28 (34%)
14	CLA	b	802	-	69,73,73	2.24	22 (31%)	82,113,113	2.47	29 (35%)
16	BCR	j	1304	-	41,41,41	2.61	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	B	812	2	69,73,73	2.22	21 (30%)	82,113,113	2.39	28 (34%)
16	BCR	A	845	-	41,41,41	2.59	6 (14%)	56,56,56	6.59	24 (42%)
14	CLA	a	814	-	49,53,73	2.54	22 (44%)	58,89,113	2.82	25 (43%)
14	CLA	a	804	1	69,73,73	2.22	21 (30%)	82,113,113	2.52	26 (31%)
14	CLA	T	101	-	45,49,73	2.50	21 (46%)	54,83,113	2.74	22 (40%)
14	CLA	A	823	-	59,63,73	2.44	23 (38%)	70,101,113	2.64	27 (38%)
14	CLA	A	842	-	54,58,73	2.55	23 (42%)	64,95,113	2.75	29 (45%)
14	CLA	G	841	-	54,58,73	2.54	23 (42%)	64,95,113	2.73	28 (43%)
14	CLA	A	808	1	69,73,73	2.24	22 (31%)	82,113,113	2.46	27 (32%)
14	CLA	B	822	-	49,53,73	2.55	22 (44%)	58,89,113	2.75	24 (41%)
18	SF4	N	101	3	0,12,12	-	-	-		
14	CLA	a	810	14	69,73,73	2.22	22 (31%)	82,113,113	2.51	26 (31%)
15	PQN	H	843	-	34,34,34	1.50	2 (5%)	43,45,45	1.07	2 (4%)
14	CLA	a	826	1	69,73,73	2.23	22 (31%)	82,113,113	2.54	30 (36%)
14	CLA	R	101	-	69,73,73	2.19	22 (31%)	82,113,113	2.51	27 (32%)
14	CLA	a	853	-	69,73,73	2.19	21 (30%)	82,113,113	2.42	25 (30%)
14	CLA	J	1303	-	41,45,73	2.63	21 (51%)	50,78,113	2.83	20 (40%)
14	CLA	G	829	1	69,73,73	2.22	22 (31%)	82,113,113	2.49	27 (32%)
14	CLA	b	807	2	69,73,73	2.23	22 (31%)	82,113,113	2.50	27 (32%)
16	BCR	A	847	-	41,41,41	2.61	6 (14%)	56,56,56	6.73	28 (50%)
14	CLA	H	806	-	69,73,73	2.20	20 (28%)	82,113,113	2.44	26 (31%)
14	CLA	B	840	2	49,53,73	2.51	21 (42%)	58,89,113	2.85	26 (44%)
14	CLA	b	837	2	69,73,73	2.25	22 (31%)	82,113,113	2.51	29 (35%)
16	BCR	B	850	-	41,41,41	2.59	6 (14%)	56,56,56	6.84	20 (35%)
14	CLA	G	826	1	69,73,73	2.25	22 (31%)	82,113,113	2.55	30 (36%)
14	CLA	A	852	-	69,73,73	2.18	21 (30%)	82,113,113	2.56	28 (34%)
16	BCR	V	1602	-	41,41,41	2.61	6 (14%)	56,56,56	6.73	26 (46%)
16	BCR	a	849	-	41,41,41	2.67	6 (14%)	56,56,56	6.99	26 (46%)
14	CLA	b	824	-	50,54,73	2.71	23 (46%)	59,90,113	2.78	26 (44%)
14	CLA	A	838	-	54,58,73	2.53	23 (42%)	64,95,113	2.80	26 (40%)
14	CLA	b	828	2	69,73,73	2.24	23 (33%)	82,113,113	2.55	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	k	101	-	45,49,73	2.50	21 (46%)	54,83,113	2.74	22 (40%)
14	CLA	a	852	-	69,73,73	2.21	21 (30%)	82,113,113	2.52	28 (34%)
14	CLA	a	834	-	49,53,73	2.54	22 (44%)	58,89,113	2.81	23 (39%)
16	BCR	Q	203	-	41,41,41	2.59	6 (14%)	56,56,56	6.40	25 (44%)
14	CLA	G	809	1	49,53,73	2.52	21 (42%)	58,89,113	2.85	28 (48%)
14	CLA	A	821	-	49,53,73	2.50	22 (44%)	58,89,113	2.96	28 (48%)
14	CLA	B	816	2	69,73,73	2.23	20 (28%)	82,113,113	2.65	31 (37%)
14	CLA	B	831	-	69,73,73	2.24	23 (33%)	82,113,113	2.54	28 (34%)
14	CLA	H	802	-	69,73,73	2.22	21 (30%)	82,113,113	2.48	33 (40%)
14	CLA	H	829	-	69,73,73	2.25	22 (31%)	82,113,113	2.47	29 (35%)
14	CLA	b	817	-	64,68,73	2.33	24 (37%)	76,107,113	2.59	28 (36%)
16	BCR	B	847	-	41,41,41	2.52	6 (14%)	56,56,56	6.44	30 (53%)
14	CLA	b	833	-	49,53,73	2.53	23 (46%)	58,89,113	2.69	22 (37%)
14	CLA	b	836	-	64,68,73	2.32	22 (34%)	76,107,113	2.56	29 (38%)
14	CLA	A	816	-	54,58,73	2.53	24 (44%)	64,95,113	2.72	27 (42%)
14	CLA	A	841	-	45,49,73	2.49	20 (44%)	54,83,113	2.64	22 (40%)
14	CLA	a	825	-	69,73,73	2.22	23 (33%)	82,113,113	2.51	26 (31%)
14	CLA	S	101	8	49,53,73	2.59	23 (46%)	58,89,113	2.81	24 (41%)
14	CLA	a	833	1	54,58,73	2.54	22 (40%)	64,95,113	2.77	26 (40%)
16	BCR	B	845	-	41,41,41	2.57	6 (14%)	56,56,56	6.70	23 (41%)
14	CLA	H	818	2	59,63,73	2.45	23 (38%)	70,101,113	2.69	27 (38%)
14	CLA	A	827	1	69,73,73	2.27	24 (34%)	82,113,113	2.49	30 (36%)
15	PQN	G	842	-	34,34,34	1.64	2 (5%)	43,45,45	1.62	5 (11%)
14	CLA	B	826	-	58,62,73	2.44	22 (37%)	68,99,113	2.50	26 (38%)
14	CLA	a	803	1,14	59,63,73	2.41	22 (37%)	70,101,113	2.73	28 (40%)
16	BCR	H	850	-	41,41,41	2.63	6 (14%)	56,56,56	6.82	20 (35%)
14	CLA	G	851	-	69,73,73	2.20	21 (30%)	82,113,113	2.33	22 (26%)
14	CLA	B	809	-	69,73,73	2.20	22 (31%)	82,113,113	2.44	26 (31%)
14	CLA	H	817	2	49,53,73	2.51	22 (44%)	58,89,113	2.78	25 (43%)
14	CLA	H	823	2	49,53,73	2.55	22 (44%)	58,89,113	2.88	25 (43%)
14	CLA	A	815	1	49,53,73	2.56	23 (46%)	58,89,113	2.75	22 (37%)
14	CLA	A	819	-	59,63,73	2.44	23 (38%)	70,101,113	2.74	27 (38%)
14	CLA	j	1301	-	49,53,73	2.56	23 (46%)	58,89,113	2.60	24 (41%)
14	CLA	M	1601	-	49,53,73	2.57	22 (44%)	58,89,113	2.83	25 (43%)
14	CLA	H	814	-	49,53,73	2.57	23 (46%)	58,89,113	2.74	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	B	837	-	49,53,73	2.55	22 (44%)	58,89,113	2.78	26 (44%)
14	CLA	b	804	-	69,73,73	2.22	21 (30%)	82,113,113	2.41	28 (34%)
16	BCR	B	844	-	41,41,41	2.58	6 (14%)	56,56,56	6.70	20 (35%)
16	BCR	a	846	-	41,41,41	2.63	6 (14%)	56,56,56	6.49	23 (41%)
14	CLA	a	841	-	69,73,73	2.21	22 (31%)	82,113,113	2.43	27 (32%)
19	LMG	b	849	-	51,51,55	1.44	7 (13%)	59,59,63	1.10	2 (3%)
16	BCR	R	102	-	41,41,41	2.62	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	B	806	-	69,73,73	2.21	21 (30%)	82,113,113	2.33	26 (31%)
19	LMG	B	851	-	51,51,55	1.43	7 (13%)	59,59,63	1.05	2 (3%)
14	CLA	G	817	1	54,58,73	2.58	22 (40%)	64,95,113	2.87	29 (45%)
14	CLA	G	823	1	59,63,73	2.42	23 (38%)	70,101,113	2.63	26 (37%)
16	BCR	b	848	-	41,41,41	2.59	6 (14%)	56,56,56	6.86	20 (35%)
14	CLA	H	830	-	69,73,73	2.27	23 (33%)	82,113,113	2.43	27 (32%)
14	CLA	b	801	-	69,73,73	2.24	20 (28%)	82,113,113	2.10	22 (26%)
14	CLA	a	842	-	54,58,73	2.56	23 (42%)	64,95,113	2.75	30 (46%)
13	CL0	A	801	-	69,73,73	2.27	22 (31%)	82,113,113	2.40	27 (32%)
14	CLA	A	817	1	54,58,73	2.56	24 (44%)	64,95,113	2.92	29 (45%)
18	SF4	N	102	3	0,12,12	-	-	-		
14	CLA	k	102	-	49,53,73	2.57	23 (46%)	58,89,113	2.82	26 (44%)
16	BCR	j	1305	-	41,41,41	2.65	6 (14%)	56,56,56	6.79	20 (35%)
16	BCR	J	1305	-	41,41,41	2.70	6 (14%)	56,56,56	6.80	20 (35%)
14	CLA	b	820	2	49,53,73	2.55	22 (44%)	58,89,113	2.88	25 (43%)
16	BCR	U	202	-	41,41,41	2.66	6 (14%)	56,56,56	6.58	25 (44%)
16	BCR	S	104	-	41,41,41	2.67	6 (14%)	56,56,56	6.78	19 (33%)
14	CLA	A	829	-	69,73,73	2.22	21 (30%)	82,113,113	2.43	26 (31%)
14	CLA	G	832	1	69,73,73	2.23	22 (31%)	82,113,113	2.46	26 (31%)
16	BCR	J	1304	-	41,41,41	2.61	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	H	816	2	69,73,73	2.21	20 (28%)	82,113,113	2.61	26 (31%)
14	CLA	H	841	-	69,73,73	2.23	24 (34%)	82,113,113	2.47	26 (31%)
14	CLA	K	1401	-	49,53,73	2.56	22 (44%)	58,89,113	2.82	25 (43%)
16	BCR	G	843	-	41,41,41	2.59	6 (14%)	56,56,56	6.70	22 (39%)
14	CLA	A	811	-	54,58,73	2.53	22 (40%)	64,95,113	2.75	28 (43%)
16	BCR	B	846	-	41,41,41	2.62	6 (14%)	56,56,56	6.61	22 (39%)
16	BCR	U	203	-	41,41,41	2.58	6 (14%)	56,56,56	6.61	25 (44%)
14	CLA	a	815	1	49,53,73	2.56	22 (44%)	58,89,113	2.76	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	X	1701	12	49,53,73	2.54	23 (46%)	58,89,113	2.81	23 (39%)
14	CLA	A	822	-	55,59,73	2.50	23 (41%)	64,96,113	2.85	27 (42%)
14	CLA	a	838	1	69,73,73	2.25	24 (34%)	82,113,113	2.48	28 (34%)
16	BCR	H	847	-	41,41,41	2.51	6 (14%)	56,56,56	6.36	31 (55%)
14	CLA	b	810	-	49,53,73	2.54	23 (46%)	58,89,113	2.79	26 (44%)
14	CLA	b	834	-	49,53,73	2.55	22 (44%)	58,89,113	2.76	25 (43%)
14	CLA	l	203	10	69,73,73	2.24	22 (31%)	82,113,113	2.49	28 (34%)
14	CLA	G	804	1	69,73,73	2.19	21 (30%)	82,113,113	2.49	26 (31%)
14	CLA	U	205	10	69,73,73	2.24	22 (31%)	82,113,113	2.48	26 (31%)
14	CLA	H	825	-	49,53,73	2.57	22 (44%)	58,89,113	2.84	25 (43%)
14	CLA	H	834	-	62,66,73	2.37	22 (35%)	73,104,113	2.56	31 (42%)
14	CLA	A	809	1	49,53,73	2.50	21 (42%)	58,89,113	2.85	25 (43%)
14	CLA	a	821	-	49,53,73	2.50	22 (44%)	58,89,113	2.96	28 (48%)
14	CLA	b	830	-	49,53,73	2.55	22 (44%)	58,89,113	2.73	25 (43%)
14	CLA	l	204	10	69,73,73	2.21	22 (31%)	82,113,113	2.51	26 (31%)
14	CLA	H	819	2	59,63,73	2.41	23 (38%)	70,101,113	2.66	29 (41%)
14	CLA	a	808	1	69,73,73	2.25	22 (31%)	82,113,113	2.50	27 (32%)
14	CLA	a	822	-	55,59,73	2.49	23 (41%)	64,96,113	2.83	26 (40%)
18	SF4	C	102	3	0,12,12	-	-	-		
16	BCR	a	847	-	41,41,41	2.60	6 (14%)	56,56,56	6.70	28 (50%)
14	CLA	H	807	2	54,58,73	2.54	23 (42%)	64,95,113	2.90	27 (42%)
14	CLA	b	835	-	49,53,73	2.55	22 (44%)	58,89,113	2.78	26 (44%)
14	CLA	B	824	-	59,63,73	2.43	24 (40%)	70,101,113	2.65	26 (37%)
14	CLA	G	835	-	54,58,73	2.52	22 (40%)	64,95,113	2.75	26 (40%)
18	SF4	a	854	1,2	0,12,12	-	-	-		
14	CLA	G	839	1	69,73,73	2.24	24 (34%)	82,113,113	2.50	28 (34%)
17	LHG	a	850	-	48,48,48	0.92	2 (4%)	51,54,54	1.11	4 (7%)
14	CLA	B	828	-	69,73,73	2.24	23 (33%)	82,113,113	2.51	27 (32%)
14	CLA	H	821	-	69,73,73	2.22	24 (34%)	82,113,113	2.37	27 (32%)
15	PQN	B	843	-	34,34,34	1.66	2 (5%)	43,45,45	1.03	2 (4%)
14	CLA	S	102	-	41,45,73	2.64	21 (51%)	50,78,113	2.81	20 (40%)
14	CLA	G	807	1	69,73,73	2.22	22 (31%)	82,113,113	2.55	31 (37%)
14	CLA	H	803	-	69,73,73	2.24	23 (33%)	82,113,113	2.44	27 (32%)
14	CLA	B	817	2	49,53,73	2.50	22 (44%)	58,89,113	2.81	25 (43%)
16	BCR	b	850	-	41,41,41	2.65	6 (14%)	56,56,56	6.54	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CL0	a	801	-	69,73,73	2.24	20 (28%)	82,113,113	2.38	25 (30%)
14	CLA	B	836	-	49,53,73	2.55	22 (44%)	58,89,113	2.76	25 (43%)
14	CLA	B	825	-	49,53,73	2.59	23 (46%)	58,89,113	2.92	26 (44%)
14	CLA	H	804	-	69,73,73	2.25	24 (34%)	82,113,113	2.49	28 (34%)
14	CLA	A	826	1	69,73,73	2.16	22 (31%)	82,113,113	2.49	31 (37%)
14	CLA	B	810	2	69,73,73	2.23	22 (31%)	82,113,113	2.51	27 (32%)
14	CLA	b	803	1	69,73,73	2.25	24 (34%)	82,113,113	2.46	27 (32%)
14	CLA	b	814	2	49,53,73	2.50	22 (44%)	58,89,113	2.80	25 (43%)
14	CLA	G	814	-	49,53,73	2.52	22 (44%)	58,89,113	2.81	26 (44%)
14	CLA	G	806	-	54,58,73	2.54	23 (42%)	64,95,113	2.82	27 (42%)
17	LHG	A	851	-	26,26,48	1.27	2 (7%)	29,32,54	1.27	3 (10%)
18	SF4	C	101	3	0,12,12	-	-	-		
14	CLA	G	810	14	69,73,73	2.22	23 (33%)	82,113,113	2.58	27 (32%)
14	CLA	B	802	-	69,73,73	2.23	21 (30%)	82,113,113	2.45	30 (36%)
14	CLA	B	804	1	69,73,73	2.26	24 (34%)	82,113,113	2.49	29 (35%)
14	CLA	H	842	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	30 (36%)
16	BCR	a	845	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	25 (44%)
14	CLA	H	808	-	69,73,73	2.18	22 (31%)	82,113,113	2.47	26 (31%)
16	BCR	b	846	-	41,41,41	2.62	6 (14%)	56,56,56	6.63	23 (41%)
14	CLA	a	823	-	59,63,73	2.43	23 (38%)	70,101,113	2.66	27 (38%)
16	BCR	I	101	-	41,41,41	2.62	6 (14%)	56,56,56	6.70	22 (39%)
14	CLA	Q	202	-	49,53,73	2.54	22 (44%)	58,89,113	2.71	22 (37%)
14	CLA	G	813	1	49,53,73	2.53	23 (46%)	58,89,113	2.90	25 (43%)
14	CLA	m	1201	2	54,58,73	2.53	23 (42%)	64,95,113	2.85	25 (39%)
14	CLA	Q	201	2	69,73,73	2.31	23 (33%)	82,113,113	2.30	27 (32%)
14	CLA	H	810	2	69,73,73	2.23	22 (31%)	82,113,113	2.50	27 (32%)
16	BCR	A	846	-	41,41,41	2.61	6 (14%)	56,56,56	6.56	22 (39%)
14	CLA	a	811	-	54,58,73	2.54	22 (40%)	64,95,113	2.77	27 (42%)
14	CLA	H	801	-	69,73,73	2.29	23 (33%)	82,113,113	2.38	27 (32%)
14	CLA	b	832	2	62,66,73	2.37	22 (35%)	73,104,113	2.58	29 (39%)
14	CLA	G	811	-	54,58,73	2.53	22 (40%)	64,95,113	2.77	29 (45%)
14	CLA	b	821	-	59,63,73	2.44	24 (40%)	70,101,113	2.63	26 (37%)
16	BCR	b	847	-	41,41,41	2.67	6 (14%)	56,56,56	6.70	26 (46%)
14	CLA	B	820	-	64,68,73	2.33	24 (37%)	76,107,113	2.61	27 (35%)

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
16	BCR	a	848	-	-	9/29/63/63	0/2/2/2
14	CLA	b	805	-	-	15/39/115/115	-
14	CLA	H	828	-	-	12/39/115/115	-
16	BCR	b	842	-	-	11/29/63/63	0/2/2/2
14	CLA	G	837	1	-	3/15/91/115	-
14	CLA	b	827	-	-	18/39/115/115	-
14	CLA	H	822	-	-	10/15/91/115	-
14	CLA	G	827	1	-	15/39/115/115	-
14	CLA	J	1301	-	-	6/15/91/115	-
16	BCR	G	845	-	-	8/29/63/63	0/2/2/2
16	BCR	U	208	-	-	12/29/63/63	0/2/2/2
14	CLA	a	827	-	-	15/39/115/115	-
14	CLA	b	815	-	-	9/27/103/115	-
14	CLA	B	833	-	-	8/15/91/115	-
14	CLA	a	809	1	-	9/15/91/115	-
14	CLA	A	805	-	-	17/39/115/115	-
16	BCR	B	849	-	-	10/29/63/63	0/2/2/2
19	LMG	H	851	-	-	7/46/66/70	0/1/1/1
14	CLA	A	812	-	-	18/33/109/115	-
14	CLA	G	828	-	-	16/39/115/115	-
14	CLA	U	206	10	-	17/39/115/115	-
14	CLA	G	822	-	-	11/23/99/115	-
16	BCR	M	1602	-	-	7/29/63/63	0/2/2/2
14	CLA	a	816	-	-	5/21/97/115	-
14	CLA	B	803	-	-	15/39/115/115	-
14	CLA	B	807	2	-	8/21/97/115	-
14	CLA	G	836	-	-	16/39/115/115	-
16	BCR	G	848	-	-	15/29/63/63	0/2/2/2
16	BCR	H	852	-	-	10/29/63/63	0/2/2/2
14	CLA	A	831	1	-	13/39/115/115	-
14	CLA	a	819	-	-	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	819	-	-	10/15/91/115	-
18	SF4	c	102	3	-	-	0/6/5/5
16	BCR	F	202	-	-	4/29/63/63	0/2/2/2
14	CLA	H	826	2	-	13/26/102/115	-
16	BCR	B	848	-	-	4/29/63/63	0/2/2/2
16	BCR	H	846	-	-	13/29/63/63	0/2/2/2
14	CLA	b	808	-	-	14/39/115/115	-
14	CLA	b	829	2	-	10/15/91/115	-
14	CLA	V	1601	-	-	9/15/91/115	-
14	CLA	B	842	2	-	12/39/115/115	-
17	LHG	G	850	-	-	16/31/31/53	-
14	CLA	a	832	1	-	19/39/115/115	-
14	CLA	m	1202	-	-	9/15/91/115	-
14	CLA	b	811	2	-	6/15/91/115	-
14	CLA	L	201	-	-	14/39/115/115	-
18	SF4	c	101	3	-	-	0/6/5/5
14	CLA	G	815	1	-	5/15/91/115	-
16	BCR	A	844	-	-	9/29/63/63	0/2/2/2
17	LHG	a	851	-	-	15/31/31/53	-
14	CLA	G	838	-	-	5/21/97/115	-
14	CLA	a	813	-	-	7/15/91/115	-
14	CLA	U	207	-	-	11/39/115/115	-
16	BCR	G	844	-	-	12/29/63/63	0/2/2/2
14	CLA	A	820	-	-	14/39/115/115	-
14	CLA	B	805	-	-	16/39/115/115	-
14	CLA	B	801	-	-	13/39/115/115	-
14	CLA	G	808	1	-	9/39/115/115	-
14	CLA	G	821	-	-	10/15/91/115	-
14	CLA	A	834	-	-	7/15/91/115	-
14	CLA	H	812	2	-	18/39/115/115	-
14	CLA	b	825	-	-	11/39/115/115	-
16	BCR	l	206	-	-	12/29/63/63	0/2/2/2
14	CLA	a	824	-	-	18/39/115/115	-
14	CLA	A	807	1	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	833	-	-	8/15/91/115	-
16	BCR	H	849	-	-	10/29/63/63	0/2/2/2
14	CLA	G	824	-	-	18/39/115/115	-
13	CL0	G	801	-	-	10/39/115/115	-
14	CLA	b	818	-	-	10/39/115/115	-
14	CLA	A	837	1	-	3/15/91/115	-
14	CLA	a	839	-	-	4/21/97/115	-
14	CLA	H	809	2	-	15/39/115/115	-
14	CLA	H	838	2	-	15/33/109/115	-
14	CLA	G	834	-	-	5/15/91/115	-
14	CLA	B	830	2	-	18/39/115/115	-
14	CLA	B	821	-	-	12/39/115/115	-
14	CLA	A	803	1,14	-	9/27/103/115	-
14	CLA	G	825	-	-	14/39/115/115	-
14	CLA	a	812	-	-	17/33/109/115	-
14	CLA	H	831	-	-	11/39/115/115	-
14	CLA	B	838	-	-	18/33/109/115	-
14	CLA	b	823	-	-	13/26/102/115	-
14	CLA	j	1302	8	-	7/15/91/115	-
14	CLA	a	805	-	-	15/39/115/115	-
14	CLA	H	832	2	-	9/15/91/115	-
14	CLA	G	830	1	-	10/21/97/115	-
14	CLA	a	840	1	-	17/39/115/115	-
14	CLA	a	831	1	-	13/39/115/115	-
16	BCR	i	101	-	-	8/29/63/63	0/2/2/2
16	BCR	S	103	-	-	12/29/63/63	0/2/2/2
14	CLA	a	820	-	-	13/39/115/115	-
18	SF4	A	853	1,2	-	-	0/6/5/5
14	CLA	B	808	-	-	15/39/115/115	-
14	CLA	a	802	-	-	16/39/115/115	-
14	CLA	J	1302	8	-	8/15/91/115	-
14	CLA	H	805	-	-	15/39/115/115	-
14	CLA	G	818	-	-	13/39/115/115	-
14	CLA	G	802	1	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	b	845	-	-	9/29/63/63	0/2/2/2
14	CLA	B	841	-	-	12/39/115/115	-
14	CLA	A	813	-	-	7/15/91/115	-
16	BCR	L	207	-	-	12/29/63/63	0/2/2/2
16	BCR	L	202	-	-	13/29/63/63	0/2/2/2
15	PQN	b	841	-	-	5/23/43/43	0/2/2/2
18	SF4	G	852	1,2	-	-	0/6/5/5
14	CLA	H	835	-	-	6/15/91/115	-
14	CLA	b	826	-	-	18/39/115/115	-
14	CLA	b	813	2	-	13/39/115/115	-
14	CLA	l	205	-	-	11/39/115/115	-
14	CLA	a	829	1	-	12/39/115/115	-
14	CLA	A	833	1	-	4/21/97/115	-
14	CLA	A	836	-	-	17/39/115/115	-
14	CLA	a	818	-	-	13/39/115/115	-
14	CLA	a	807	1	-	20/39/115/115	-
14	CLA	a	806	-	-	9/21/97/115	-
14	CLA	b	816	2	-	12/27/103/115	-
14	CLA	a	837	1	-	3/15/91/115	-
16	BCR	l	202	-	-	4/29/63/63	0/2/2/2
14	CLA	A	839	1	-	18/39/115/115	-
14	CLA	G	831	1	-	13/39/115/115	-
14	CLA	G	816	-	-	4/21/97/115	-
16	BCR	G	847	-	-	10/29/63/63	0/2/2/2
14	CLA	B	823	2	-	7/15/91/115	-
14	CLA	j	1303	-	-	2/4/76/115	-
14	CLA	L	206	-	-	11/39/115/115	-
14	CLA	B	814	-	-	6/15/91/115	-
16	BCR	B	852	-	-	9/29/63/63	0/2/2/2
14	CLA	B	829	2	-	17/39/115/115	-
14	CLA	G	805	1	-	15/39/115/115	-
14	CLA	G	820	-	-	14/39/115/115	-
14	CLA	b	822	-	-	4/15/91/115	-
14	CLA	A	840	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	828	-	-	16/39/115/115	-
14	CLA	F	201	2	-	22/39/115/115	-
16	BCR	H	844	-	-	13/29/63/63	0/2/2/2
14	CLA	b	839	-	-	12/39/115/115	-
14	CLA	B	811	-	-	13/39/115/115	-
14	CLA	x	1701	12	-	9/15/91/115	-
14	CLA	A	832	-	-	19/39/115/115	-
17	LHG	G	849	-	-	26/53/53/53	-
16	BCR	m	1203	-	-	7/29/63/63	0/2/2/2
14	CLA	A	804	1	-	19/39/115/115	-
14	CLA	A	824	-	-	18/39/115/115	-
14	CLA	H	811	2	-	13/39/115/115	-
14	CLA	b	809	2	-	17/39/115/115	-
14	CLA	b	838	2	-	7/15/91/115	-
14	CLA	b	812	-	-	22/39/115/115	-
14	CLA	G	833	-	-	4/21/97/115	-
16	BCR	a	844	-	-	9/29/63/63	0/2/2/2
14	CLA	B	827	-	-	4/17/93/115	-
14	CLA	T	102	-	-	7/15/91/115	-
14	CLA	H	820	-	-	10/33/109/115	-
16	BCR	l	201	-	-	13/29/63/63	0/2/2/2
14	CLA	A	830	1	-	10/21/97/115	-
14	CLA	B	818	-	-	10/27/103/115	-
16	BCR	b	843	-	-	8/29/63/63	0/2/2/2
14	CLA	b	831	-	-	20/39/115/115	-
15	PQN	A	843	-	-	5/23/43/43	0/2/2/2
14	CLA	G	819	1	-	13/27/103/115	-
16	BCR	A	848	-	-	8/29/63/63	0/2/2/2
14	CLA	H	836	-	-	5/15/91/115	-
14	CLA	b	840	-	-	12/39/115/115	-
16	BCR	H	845	-	-	8/29/63/63	0/2/2/2
15	PQN	a	843	-	-	5/23/43/43	0/2/2/2
16	BCR	f	201	-	-	4/29/63/63	0/2/2/2
16	BCR	L	209	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	819	2	-	13/27/103/115	-
14	CLA	A	810	14	-	12/39/115/115	-
14	CLA	G	803	14	-	8/27/103/115	-
16	BCR	A	849	-	-	15/29/63/63	0/2/2/2
16	BCR	G	846	-	-	8/29/63/63	0/2/2/2
14	CLA	H	840	2	-	5/15/91/115	-
14	CLA	G	812	-	-	18/33/109/115	-
14	CLA	H	813	-	-	5/15/91/115	-
14	CLA	B	832	2	-	10/15/91/115	-
14	CLA	W	1701	12	-	7/15/91/115	-
14	CLA	A	835	-	-	8/21/97/115	-
14	CLA	L	205	10	-	17/39/115/115	-
14	CLA	U	201	-	-	14/39/115/115	-
14	CLA	G	840	-	-	13/39/115/115	-
14	CLA	A	818	-	-	13/39/115/115	-
17	LHG	A	850	-	-	27/53/53/53	-
14	CLA	A	806	-	-	9/21/97/115	-
14	CLA	B	813	-	-	5/15/91/115	-
14	CLA	A	825	-	-	14/39/115/115	-
14	CLA	H	839	2	-	10/39/115/115	-
16	BCR	b	844	-	-	13/29/63/63	0/2/2/2
14	CLA	A	814	-	-	9/15/91/115	-
14	CLA	a	830	-	-	10/21/97/115	-
14	CLA	H	827	-	-	4/17/93/115	-
14	CLA	a	828	-	-	16/39/115/115	-
14	CLA	b	806	-	-	16/39/115/115	-
14	CLA	H	815	-	-	21/39/115/115	-
14	CLA	a	836	1	-	16/39/115/115	-
14	CLA	B	835	-	-	7/15/91/115	-
14	CLA	a	835	-	-	8/21/97/115	-
14	CLA	H	837	-	-	6/15/91/115	-
14	CLA	a	817	1	-	12/21/97/115	-
14	CLA	A	802	1	-	16/39/115/115	-
14	CLA	B	815	-	-	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	H	848	-	-	5/29/63/63	0/2/2/2
14	CLA	H	824	-	-	15/27/103/115	-
14	CLA	B	839	2	-	10/39/115/115	-
14	CLA	B	834	-	-	13/31/107/115	-
14	CLA	L	204	10	-	12/39/115/115	-
14	CLA	b	802	-	-	12/39/115/115	-
16	BCR	j	1304	-	-	12/29/63/63	0/2/2/2
14	CLA	B	812	2	-	16/39/115/115	-
16	BCR	A	845	-	-	12/29/63/63	0/2/2/2
14	CLA	a	814	-	-	9/15/91/115	-
14	CLA	a	804	1	-	20/39/115/115	-
14	CLA	T	101	-	-	5/9/81/115	-
14	CLA	A	823	-	-	9/27/103/115	-
14	CLA	A	842	-	-	11/21/97/115	-
14	CLA	G	841	-	-	11/21/97/115	-
14	CLA	A	808	1	-	9/39/115/115	-
14	CLA	B	822	-	-	10/15/91/115	-
18	SF4	N	101	3	-	-	0/6/5/5
14	CLA	a	810	14	-	11/39/115/115	-
15	PQN	H	843	-	-	6/23/43/43	0/2/2/2
14	CLA	a	826	1	-	12/39/115/115	-
14	CLA	R	101	-	-	15/39/115/115	-
14	CLA	a	853	-	-	13/39/115/115	-
14	CLA	J	1303	-	-	2/4/76/115	-
14	CLA	G	829	1	-	11/39/115/115	-
14	CLA	b	807	2	-	11/39/115/115	-
16	BCR	A	847	-	-	8/29/63/63	0/2/2/2
14	CLA	H	806	-	-	16/39/115/115	-
14	CLA	B	840	2	-	7/15/91/115	-
14	CLA	b	837	2	-	11/39/115/115	-
16	BCR	B	850	-	-	7/29/63/63	0/2/2/2
14	CLA	G	826	1	-	12/39/115/115	-
14	CLA	A	852	-	-	15/39/115/115	-
16	BCR	V	1602	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	a	849	-	-	15/29/63/63	0/2/2/2
14	CLA	b	824	-	-	4/17/93/115	-
14	CLA	A	838	-	-	4/21/97/115	-
14	CLA	b	828	2	-	11/39/115/115	-
14	CLA	k	101	-	-	5/9/81/115	-
14	CLA	a	852	-	-	16/39/115/115	-
14	CLA	a	834	-	-	7/15/91/115	-
16	BCR	Q	203	-	-	3/29/63/63	0/2/2/2
14	CLA	G	809	1	-	9/15/91/115	-
14	CLA	A	821	-	-	10/15/91/115	-
14	CLA	B	816	2	-	17/39/115/115	-
14	CLA	B	831	-	-	10/39/115/115	-
14	CLA	H	802	-	-	12/39/115/115	-
14	CLA	H	829	-	-	17/39/115/115	-
14	CLA	b	817	-	-	11/33/109/115	-
16	BCR	B	847	-	-	7/29/63/63	0/2/2/2
14	CLA	b	833	-	-	7/15/91/115	-
14	CLA	b	836	-	-	17/33/109/115	-
14	CLA	A	816	-	-	4/21/97/115	-
14	CLA	A	841	-	-	5/9/81/115	-
14	CLA	a	825	-	-	14/39/115/115	-
14	CLA	S	101	8	-	5/15/91/115	-
14	CLA	a	833	1	-	4/21/97/115	-
16	BCR	B	845	-	-	8/29/63/63	0/2/2/2
14	CLA	H	818	2	-	8/27/103/115	-
14	CLA	A	827	1	-	16/39/115/115	-
15	PQN	G	842	-	-	5/23/43/43	0/2/2/2
14	CLA	B	826	-	-	13/26/102/115	-
14	CLA	a	803	1,14	-	11/27/103/115	-
16	BCR	H	850	-	-	8/29/63/63	0/2/2/2
14	CLA	G	851	-	-	13/39/115/115	-
14	CLA	B	809	-	-	15/39/115/115	-
14	CLA	H	817	2	-	8/15/91/115	-
14	CLA	H	823	2	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	815	1	-	5/15/91/115	-
14	CLA	A	819	-	-	12/27/103/115	-
14	CLA	j	1301	-	-	6/15/91/115	-
14	CLA	M	1601	-	-	9/15/91/115	-
14	CLA	H	814	-	-	6/15/91/115	-
14	CLA	B	837	-	-	6/15/91/115	-
14	CLA	b	804	-	-	15/39/115/115	-
16	BCR	B	844	-	-	10/29/63/63	0/2/2/2
16	BCR	a	846	-	-	7/29/63/63	0/2/2/2
14	CLA	a	841	-	-	13/39/115/115	-
19	LMG	b	849	-	-	8/46/66/70	0/1/1/1
16	BCR	R	102	-	-	8/29/63/63	0/2/2/2
14	CLA	B	806	-	-	13/39/115/115	-
19	LMG	B	851	-	-	10/46/66/70	0/1/1/1
14	CLA	G	817	1	-	12/21/97/115	-
14	CLA	G	823	1	-	9/27/103/115	-
16	BCR	b	848	-	-	8/29/63/63	0/2/2/2
14	CLA	H	830	-	-	18/39/115/115	-
14	CLA	b	801	-	-	13/39/115/115	-
14	CLA	a	842	-	-	10/21/97/115	-
13	CL0	A	801	-	-	10/39/115/115	-
14	CLA	A	817	1	-	11/21/97/115	-
18	SF4	N	102	3	-	-	0/6/5/5
14	CLA	k	102	-	-	7/15/91/115	-
16	BCR	j	1305	-	-	12/29/63/63	0/2/2/2
16	BCR	J	1305	-	-	12/29/63/63	0/2/2/2
14	CLA	b	820	2	-	7/15/91/115	-
16	BCR	U	202	-	-	13/29/63/63	0/2/2/2
16	BCR	S	104	-	-	12/29/63/63	0/2/2/2
14	CLA	A	829	-	-	12/39/115/115	-
14	CLA	G	832	1	-	19/39/115/115	-
16	BCR	J	1304	-	-	12/29/63/63	0/2/2/2
14	CLA	H	816	2	-	14/39/115/115	-
14	CLA	H	841	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	K	1401	-	-	7/15/91/115	-
16	BCR	G	843	-	-	9/29/63/63	0/2/2/2
14	CLA	A	811	-	-	11/21/97/115	-
16	BCR	B	846	-	-	13/29/63/63	0/2/2/2
16	BCR	U	203	-	-	3/29/63/63	0/2/2/2
14	CLA	a	815	1	-	6/15/91/115	-
14	CLA	X	1701	12	-	7/15/91/115	-
14	CLA	A	822	-	-	11/23/99/115	-
14	CLA	a	838	1	-	10/39/115/115	-
16	BCR	H	847	-	-	13/29/63/63	0/2/2/2
14	CLA	b	810	-	-	5/15/91/115	-
14	CLA	b	834	-	-	5/15/91/115	-
14	CLA	l	203	10	-	12/39/115/115	-
14	CLA	G	804	1	-	21/39/115/115	-
14	CLA	U	205	10	-	12/39/115/115	-
14	CLA	H	825	-	-	3/15/91/115	-
14	CLA	H	834	-	-	13/31/107/115	-
14	CLA	A	809	1	-	9/15/91/115	-
14	CLA	a	821	-	-	10/15/91/115	-
14	CLA	b	830	-	-	8/15/91/115	-
14	CLA	l	204	10	-	17/39/115/115	-
14	CLA	H	819	2	-	13/27/103/115	-
14	CLA	a	808	1	-	9/39/115/115	-
14	CLA	a	822	-	-	11/23/99/115	-
18	SF4	C	102	3	-	-	0/6/5/5
16	BCR	a	847	-	-	7/29/63/63	0/2/2/2
14	CLA	H	807	2	-	7/21/97/115	-
14	CLA	b	835	-	-	6/15/91/115	-
14	CLA	B	824	-	-	15/27/103/115	-
14	CLA	G	835	-	-	8/21/97/115	-
18	SF4	a	854	1,2	-	-	0/6/5/5
14	CLA	G	839	1	-	20/39/115/115	-
17	LHG	a	850	-	-	26/53/53/53	-
14	CLA	B	828	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	821	-	-	12/39/115/115	-
15	PQN	B	843	-	-	6/23/43/43	0/2/2/2
14	CLA	S	102	-	-	2/4/76/115	-
14	CLA	G	807	1	-	20/39/115/115	-
14	CLA	H	803	-	-	13/39/115/115	-
14	CLA	B	817	2	-	7/15/91/115	-
16	BCR	b	850	-	-	6/29/63/63	0/2/2/2
13	CL0	a	801	-	-	13/39/115/115	-
14	CLA	B	836	-	-	5/15/91/115	-
14	CLA	B	825	-	-	3/15/91/115	-
14	CLA	H	804	-	-	10/39/115/115	-
14	CLA	A	826	1	-	14/39/115/115	-
14	CLA	B	810	2	-	11/39/115/115	-
14	CLA	b	803	1	-	14/39/115/115	-
14	CLA	b	814	2	-	7/15/91/115	-
14	CLA	G	814	-	-	9/15/91/115	-
14	CLA	G	806	-	-	9/21/97/115	-
17	LHG	A	851	-	-	16/31/31/53	-
18	SF4	C	101	3	-	-	0/6/5/5
14	CLA	G	810	14	-	12/39/115/115	-
14	CLA	B	802	-	-	13/39/115/115	-
14	CLA	B	804	1	-	8/39/115/115	-
14	CLA	H	842	-	-	13/39/115/115	-
16	BCR	a	845	-	-	12/29/63/63	0/2/2/2
14	CLA	H	808	-	-	15/39/115/115	-
16	BCR	b	846	-	-	5/29/63/63	0/2/2/2
14	CLA	a	823	-	-	9/27/103/115	-
16	BCR	I	101	-	-	7/29/63/63	0/2/2/2
14	CLA	Q	202	-	-	6/15/91/115	-
14	CLA	G	813	1	-	7/15/91/115	-
14	CLA	m	1201	2	-	9/21/97/115	-
14	CLA	Q	201	2	-	20/39/115/115	-
14	CLA	H	810	2	-	11/39/115/115	-
16	BCR	A	846	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	811	-	-	11/21/97/115	-
14	CLA	H	801	-	-	11/39/115/115	-
14	CLA	b	832	2	-	13/31/107/115	-
14	CLA	G	811	-	-	11/21/97/115	-
14	CLA	b	821	-	-	15/27/103/115	-
16	BCR	b	847	-	-	11/29/63/63	0/2/2/2
14	CLA	B	820	-	-	11/33/109/115	-

The worst 5 of 6875 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	848	BCR	C8-C9	-8.66	1.27	1.46
16	B	849	BCR	C8-C9	-8.61	1.27	1.46
16	a	849	BCR	C8-C9	-8.60	1.27	1.46
16	J	1305	BCR	C8-C9	-8.59	1.27	1.46
16	A	849	BCR	C8-C9	-8.56	1.27	1.46

The worst 5 of 9188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	848	BCR	C20-C21-C22	23.64	160.43	127.28
16	A	849	BCR	C20-C21-C22	23.62	160.41	127.28
16	G	848	BCR	C16-C17-C18	23.54	160.29	127.28
16	A	849	BCR	C16-C17-C18	23.43	160.14	127.28
16	a	849	BCR	C20-C21-C22	23.41	160.11	127.28

There are no chirality outliers.

5 of 4046 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	CLA	C2-C1-O2A-CGA
14	A	802	CLA	CHA-CBD-CGD-O1D
14	A	802	CLA	CHA-CBD-CGD-O2D
14	A	803	CLA	CHA-CBD-CGD-O1D
14	A	803	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

266 monomers are involved in 497 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	848	BCR	3	0
14	b	805	CLA	1	0
14	H	828	CLA	1	0
16	b	842	BCR	3	0
14	b	827	CLA	5	0
14	G	827	CLA	10	0
16	G	845	BCR	2	0
16	U	208	BCR	1	0
14	a	827	CLA	7	0
14	b	815	CLA	1	0
14	a	809	CLA	2	0
14	A	805	CLA	3	0
16	B	849	BCR	1	0
19	H	851	LMG	3	0
14	A	812	CLA	4	0
14	G	828	CLA	1	0
14	U	206	CLA	1	0
16	M	1602	BCR	3	0
14	a	816	CLA	3	0
14	B	803	CLA	2	0
14	G	836	CLA	2	0
16	G	848	BCR	3	0
16	H	852	BCR	2	0
14	A	831	CLA	3	0
14	a	819	CLA	1	0
14	b	819	CLA	1	0
18	c	102	SF4	1	0
16	F	202	BCR	2	0
14	H	826	CLA	8	0
16	B	848	BCR	2	0
16	H	846	BCR	2	0
14	b	808	CLA	1	0
14	b	829	CLA	3	0
14	V	1601	CLA	3	0
17	G	850	LHG	1	0
14	a	832	CLA	1	0
14	m	1202	CLA	2	0
14	L	201	CLA	1	0
16	A	844	BCR	1	0
17	a	851	LHG	1	0
14	a	813	CLA	1	0
14	U	207	CLA	1	0
16	G	844	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	820	CLA	2	0
14	B	805	CLA	4	0
14	B	801	CLA	3	0
14	G	808	CLA	3	0
14	H	812	CLA	1	0
16	l	206	BCR	1	0
14	a	824	CLA	2	0
14	A	807	CLA	3	0
16	H	849	BCR	1	0
14	G	824	CLA	2	0
14	b	818	CLA	2	0
14	H	809	CLA	4	0
14	H	838	CLA	1	0
14	B	830	CLA	7	0
14	B	821	CLA	2	0
14	A	803	CLA	2	0
14	G	825	CLA	4	0
14	a	812	CLA	2	0
14	B	838	CLA	2	0
14	b	823	CLA	8	0
14	a	805	CLA	2	0
14	H	832	CLA	3	0
14	a	840	CLA	2	0
14	a	831	CLA	2	0
16	i	101	BCR	3	0
16	S	103	BCR	3	0
14	a	820	CLA	2	0
14	B	808	CLA	1	0
14	a	802	CLA	3	0
14	H	805	CLA	3	0
14	G	818	CLA	1	0
14	G	802	CLA	1	0
16	b	845	BCR	2	0
14	B	841	CLA	4	0
14	A	813	CLA	1	0
16	L	202	BCR	1	0
15	b	841	PQN	3	0
14	b	826	CLA	4	0
14	b	813	CLA	3	0
14	l	205	CLA	1	0
14	a	829	CLA	2	0
14	A	833	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	836	CLA	1	0
14	a	818	CLA	1	0
14	a	807	CLA	3	0
16	l	202	BCR	5	0
14	A	839	CLA	2	0
14	G	831	CLA	4	0
14	G	816	CLA	2	0
16	G	847	BCR	1	0
16	B	852	BCR	2	0
14	B	829	CLA	4	0
14	G	805	CLA	2	0
14	G	820	CLA	2	0
14	A	840	CLA	3	0
14	A	828	CLA	1	0
14	F	201	CLA	1	0
16	H	844	BCR	3	0
14	b	839	CLA	2	0
14	B	811	CLA	1	0
14	x	1701	CLA	2	0
14	A	832	CLA	1	0
17	G	849	LHG	1	0
16	m	1203	BCR	3	0
14	A	804	CLA	2	0
14	A	824	CLA	1	0
14	H	811	CLA	1	0
14	b	809	CLA	1	0
14	b	838	CLA	1	0
14	b	812	CLA	1	0
16	a	844	BCR	1	0
14	H	820	CLA	2	0
16	l	201	BCR	1	0
14	B	818	CLA	1	0
16	b	843	BCR	1	0
14	b	831	CLA	2	0
15	A	843	PQN	3	0
14	G	819	CLA	1	0
16	A	848	BCR	3	0
14	H	836	CLA	1	0
14	b	840	CLA	1	0
15	a	843	PQN	3	0
16	f	201	BCR	3	0
16	L	209	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	819	CLA	1	0
14	G	803	CLA	4	0
16	A	849	BCR	2	0
16	G	846	BCR	6	0
14	H	840	CLA	1	0
14	G	812	CLA	3	0
14	B	832	CLA	4	0
14	W	1701	CLA	1	0
14	L	205	CLA	1	0
14	U	201	CLA	2	0
14	G	840	CLA	4	0
14	A	825	CLA	2	0
14	H	839	CLA	4	0
16	b	844	BCR	3	0
14	b	806	CLA	4	0
14	H	815	CLA	2	0
14	a	836	CLA	4	0
14	H	837	CLA	1	0
14	a	817	CLA	2	0
14	A	802	CLA	2	0
16	H	848	BCR	2	0
14	H	824	CLA	2	0
14	B	839	CLA	3	0
14	B	834	CLA	1	0
16	j	1304	BCR	3	0
16	A	845	BCR	2	0
14	a	804	CLA	3	0
14	A	842	CLA	1	0
14	G	841	CLA	1	0
14	A	808	CLA	3	0
14	B	822	CLA	1	0
14	a	810	CLA	1	0
15	H	843	PQN	3	0
14	R	101	CLA	1	0
14	a	853	CLA	6	0
14	G	829	CLA	3	0
14	b	807	CLA	1	0
16	A	847	BCR	4	0
14	H	806	CLA	4	0
14	B	840	CLA	1	0
14	b	837	CLA	3	0
16	B	850	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	826	CLA	1	0
14	A	852	CLA	2	0
16	V	1602	BCR	3	0
16	a	849	BCR	3	0
14	a	852	CLA	2	0
16	Q	203	BCR	2	0
14	B	816	CLA	1	0
14	H	829	CLA	3	0
14	b	817	CLA	2	0
16	B	847	BCR	2	0
14	b	836	CLA	3	0
14	A	816	CLA	2	0
14	a	825	CLA	2	0
16	B	845	BCR	1	0
14	A	827	CLA	10	0
15	G	842	PQN	2	0
14	B	826	CLA	4	0
14	a	803	CLA	3	0
16	H	850	BCR	4	0
14	G	851	CLA	3	0
14	B	809	CLA	5	0
14	H	817	CLA	1	0
14	A	819	CLA	1	0
14	M	1601	CLA	3	0
14	B	837	CLA	1	0
14	b	804	CLA	3	0
16	B	844	BCR	3	0
16	a	846	BCR	3	0
14	a	841	CLA	2	0
19	b	849	LMG	4	0
16	R	102	BCR	4	0
14	B	806	CLA	3	0
19	B	851	LMG	4	0
14	G	817	CLA	1	0
16	b	848	BCR	4	0
14	H	830	CLA	6	0
14	b	801	CLA	2	0
14	a	842	CLA	1	0
14	A	817	CLA	1	0
18	N	102	SF4	1	0
16	j	1305	BCR	3	0
16	J	1305	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	U	202	BCR	1	0
16	S	104	BCR	3	0
14	A	829	CLA	4	0
14	G	832	CLA	1	0
16	J	1304	BCR	2	0
14	H	841	CLA	1	0
16	G	843	BCR	2	0
14	A	811	CLA	1	0
16	B	846	BCR	2	0
16	U	203	BCR	6	0
14	X	1701	CLA	1	0
14	a	838	CLA	1	0
16	H	847	BCR	2	0
14	b	834	CLA	1	0
14	G	804	CLA	4	0
14	H	825	CLA	1	0
14	H	834	CLA	1	0
14	A	809	CLA	3	0
14	l	204	CLA	1	0
14	a	808	CLA	3	0
18	C	102	SF4	1	0
16	a	847	BCR	6	0
14	b	835	CLA	1	0
14	G	835	CLA	1	0
14	G	839	CLA	1	0
17	a	850	LHG	2	0
14	H	821	CLA	3	0
15	B	843	PQN	3	0
14	G	807	CLA	2	0
14	H	803	CLA	1	0
14	B	817	CLA	1	0
16	b	850	BCR	2	0
13	a	801	CL0	1	0
14	B	836	CLA	1	0
14	H	804	CLA	1	0
14	A	826	CLA	2	0
14	b	803	CLA	2	0
14	b	814	CLA	1	0
17	A	851	LHG	1	0
14	G	810	CLA	2	0
14	B	802	CLA	1	0
14	B	804	CLA	1	0

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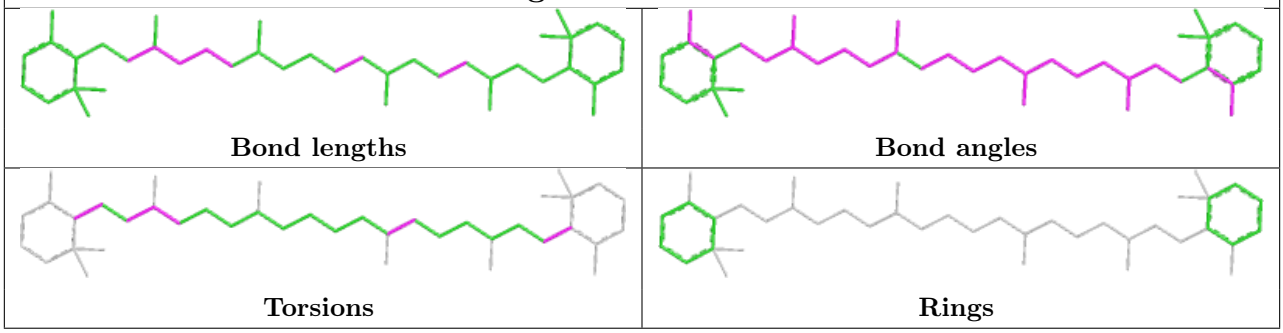
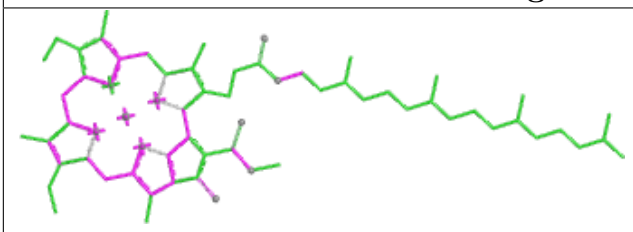
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	842	CLA	1	0
16	a	845	BCR	1	0
14	H	808	CLA	3	0
16	b	846	BCR	3	0
16	I	101	BCR	4	0
14	Q	201	CLA	2	0
14	H	810	CLA	1	0
16	A	846	BCR	1	0
14	a	811	CLA	1	0
14	H	801	CLA	1	0
14	G	811	CLA	1	0
16	b	847	BCR	1	0
14	B	820	CLA	3	0

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.

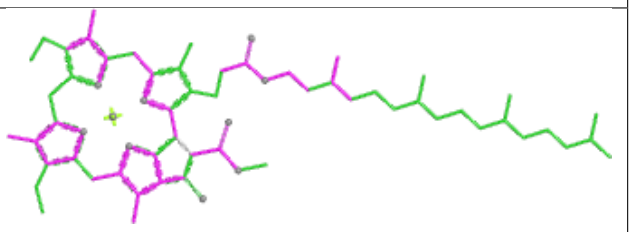
Ligand BCR a 848



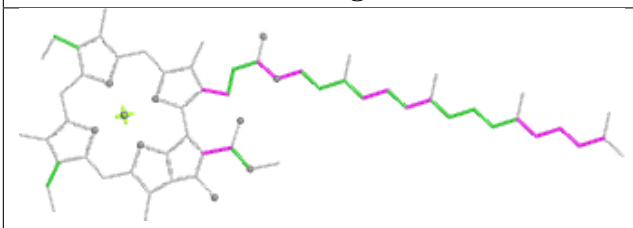
Ligand CLA b 805



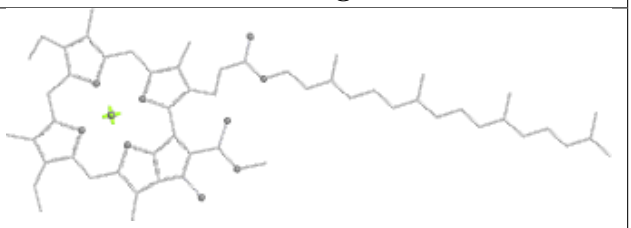
Bond lengths



Bond angles

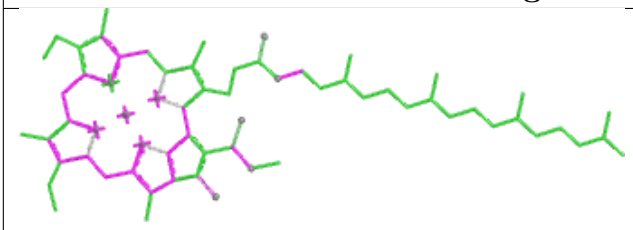


Torsions

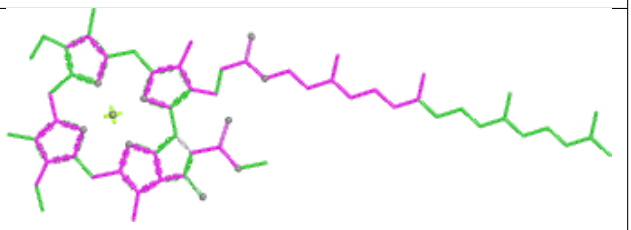


Rings

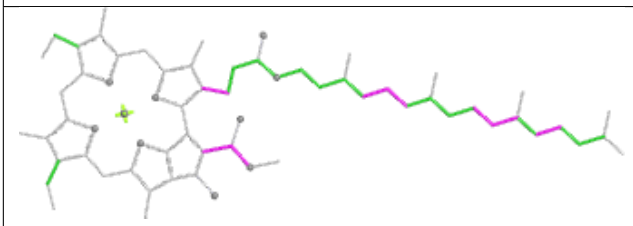
Ligand CLA H 828



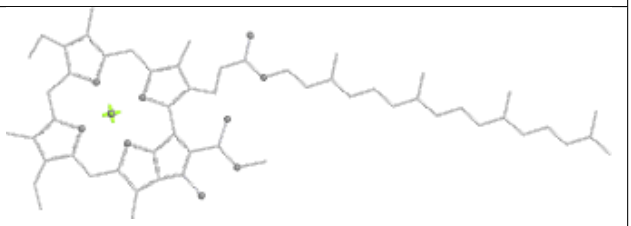
Bond lengths



Bond angles

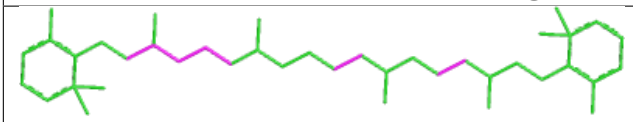


Torsions

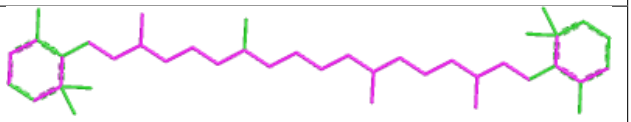


Rings

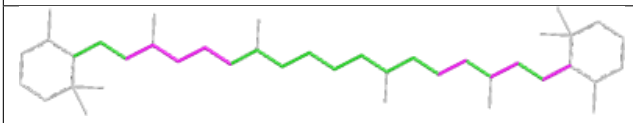
Ligand BCR b 842



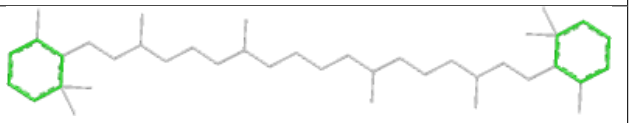
Bond lengths



Bond angles

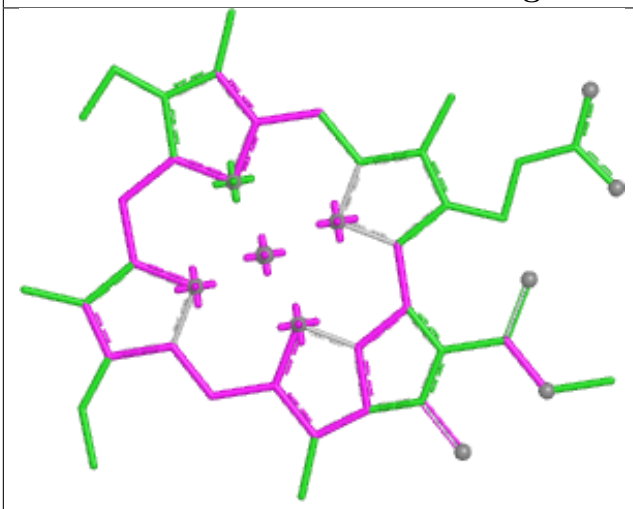


Torsions

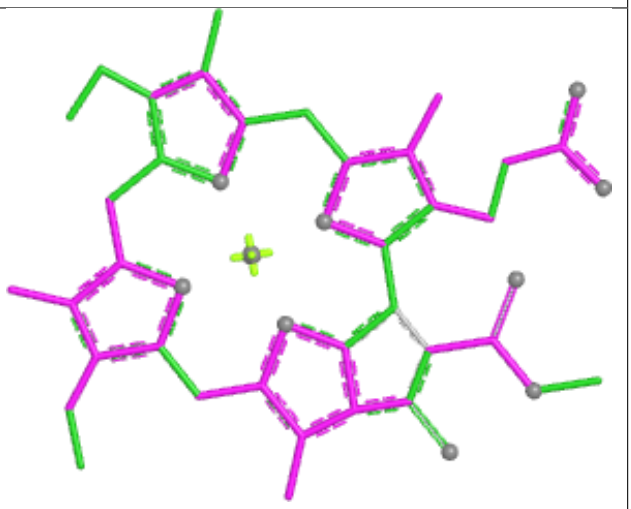


Rings

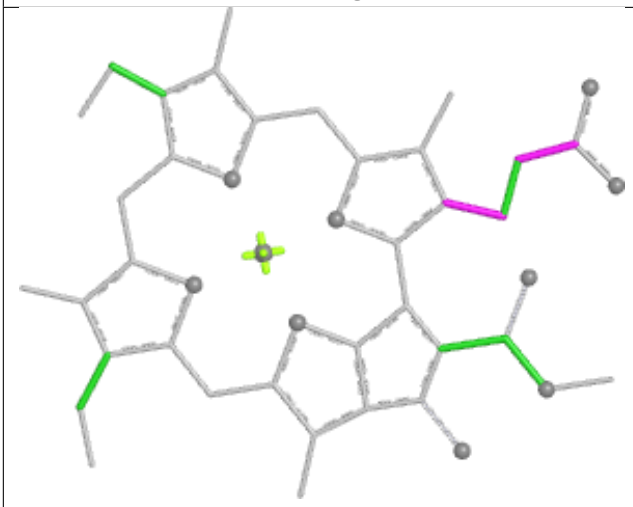
Ligand CLA G 837



Bond lengths



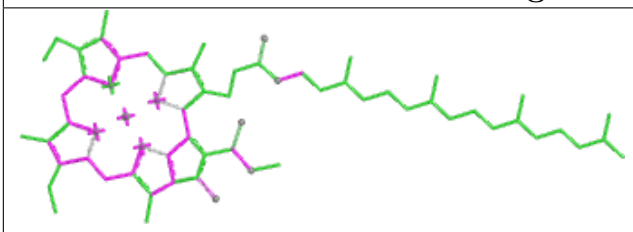
Bond angles



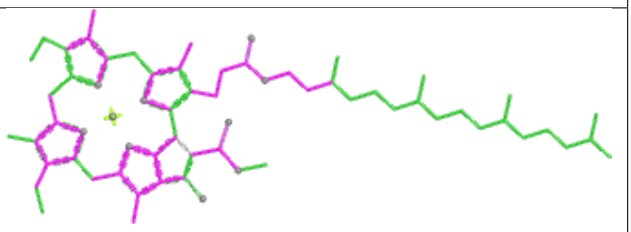
Torsions

Rings

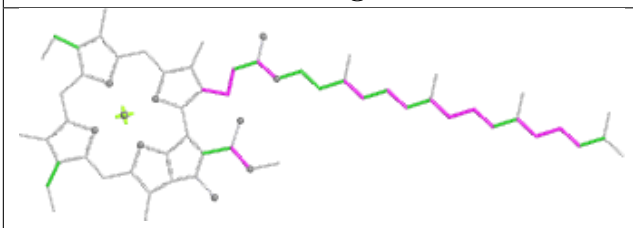
Ligand CLA b 827



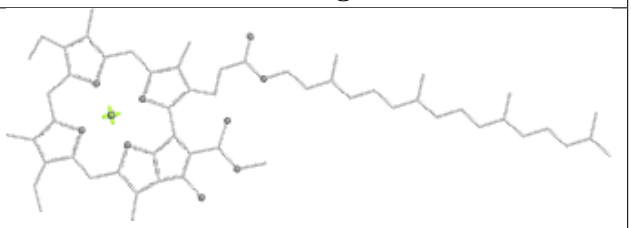
Bond lengths



Bond angles

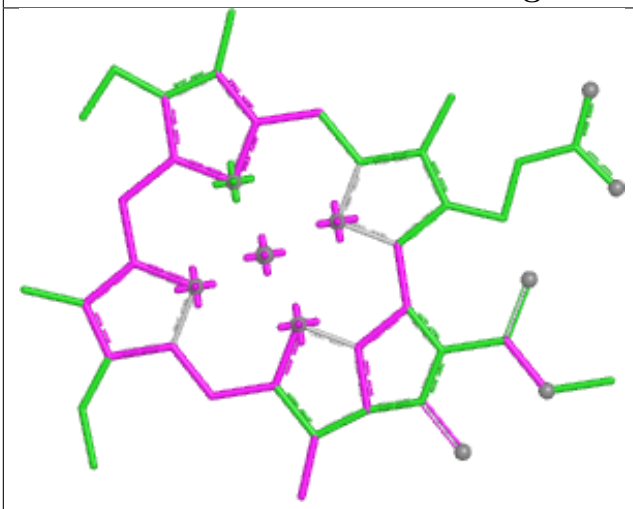


Torsions



Rings

Ligand CLA H 822



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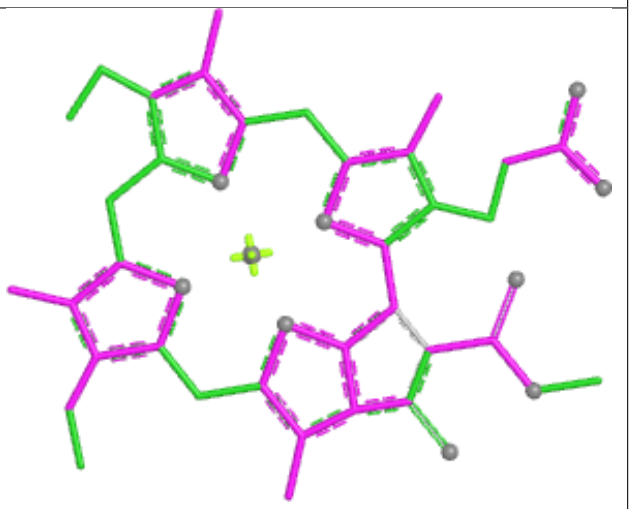
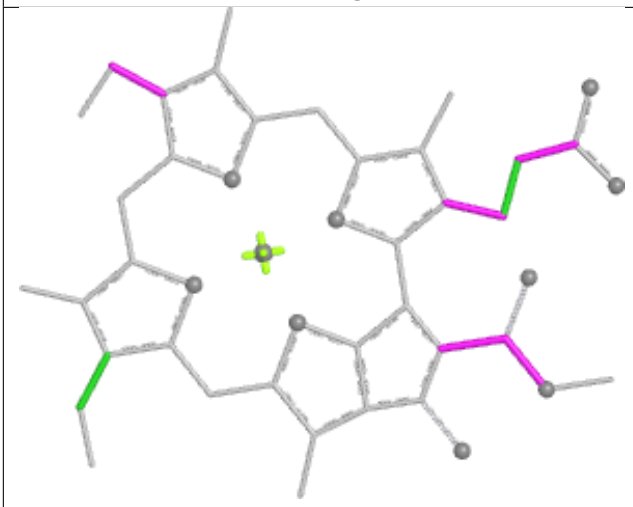


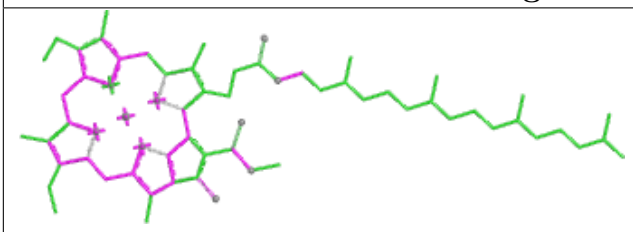
Bond angles



Torsions

Rings

Ligand CLA G 827



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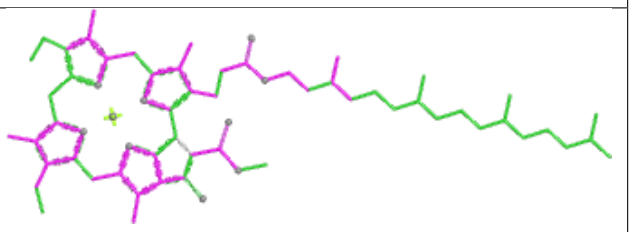
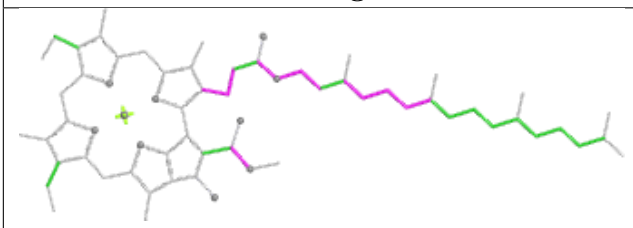
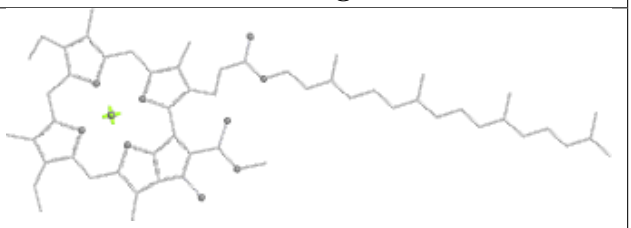


Bond angles

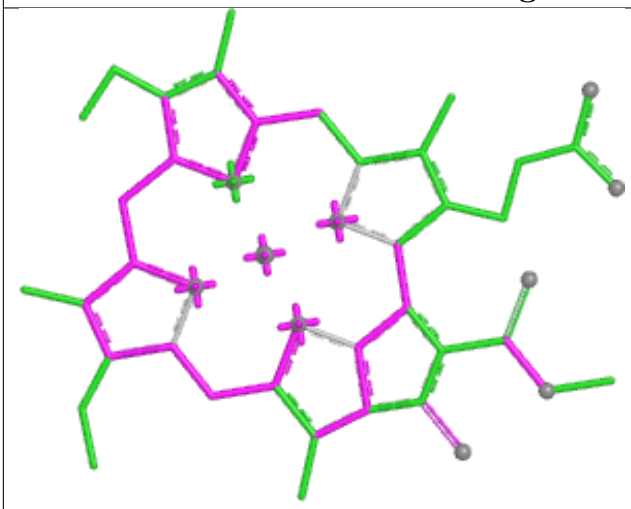


Torsions



Rings

Ligand CLA J 1301



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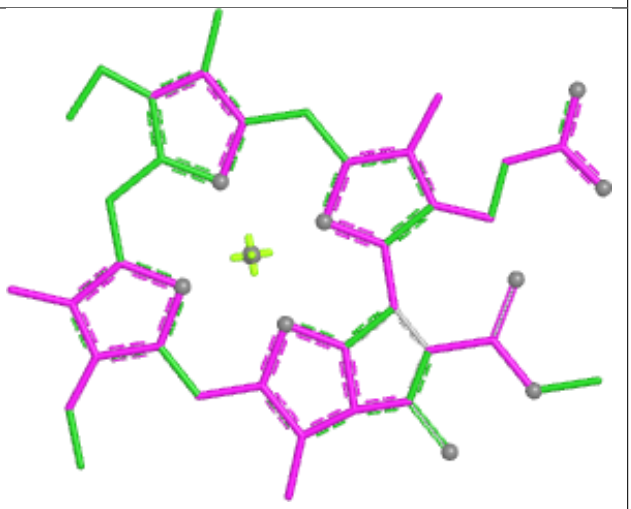
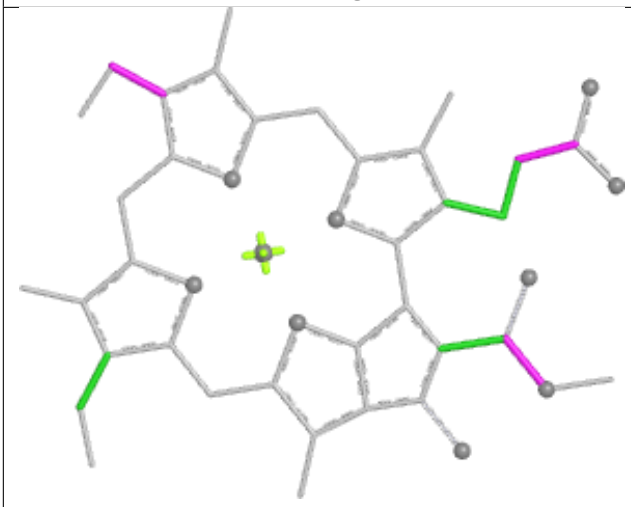


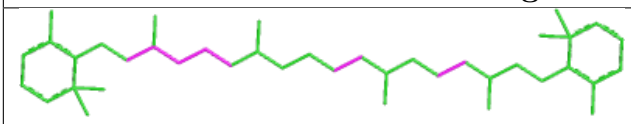
Bond angles



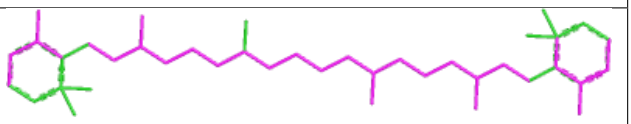
Torsions

Rings

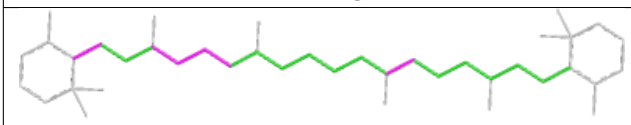
Ligand BCR G 845



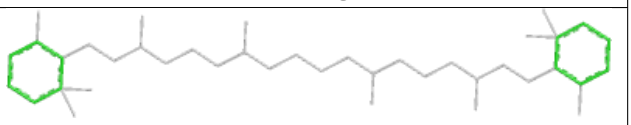
Bond lengths



Bond angles

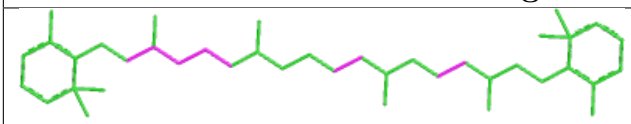


Torsions

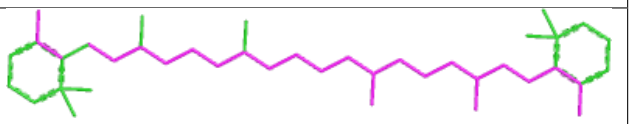


Rings

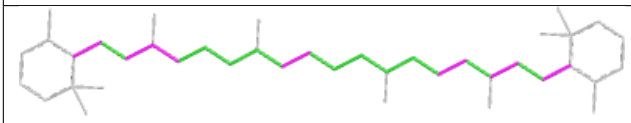
Ligand BCR U 208



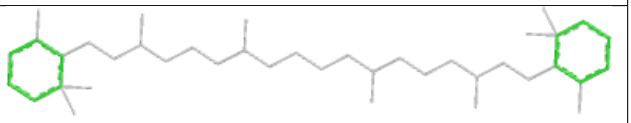
Bond lengths



Bond angles

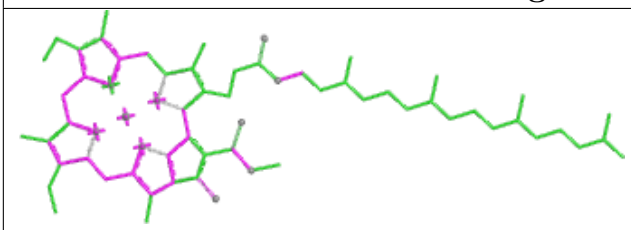


Torsions



Rings

Ligand CLA a 827



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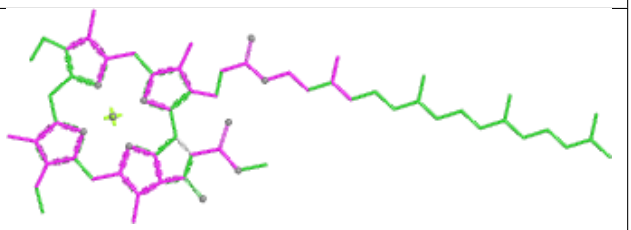
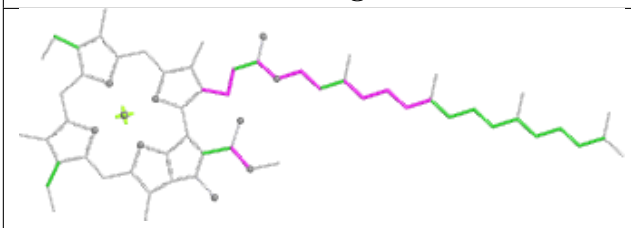


Bond angles



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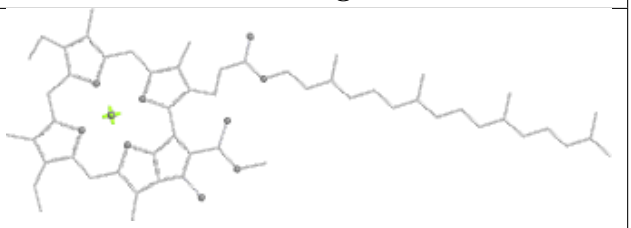
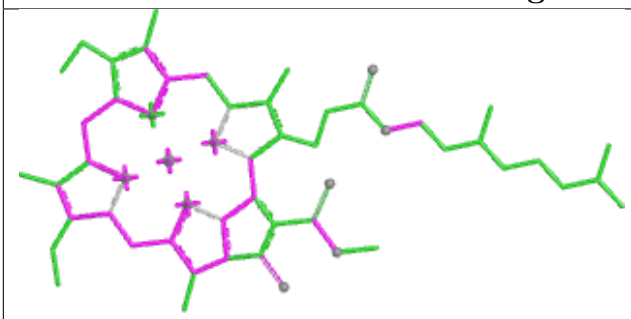


Rings

Ligand CLA b 815



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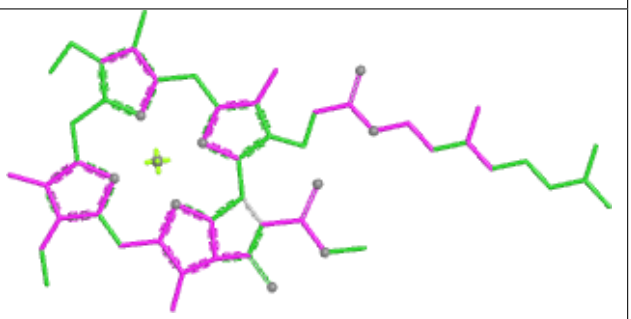

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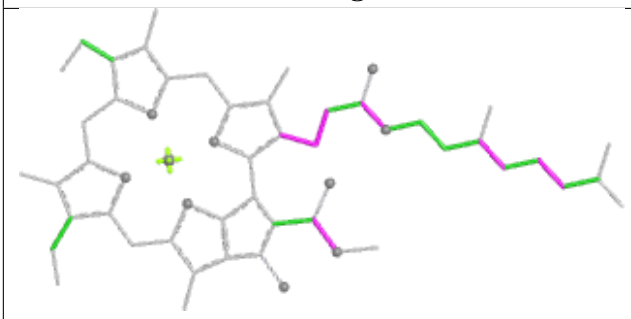

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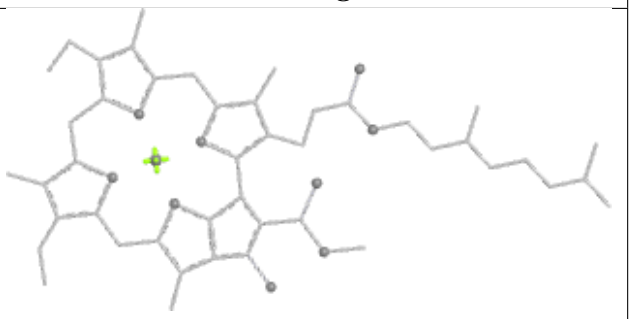
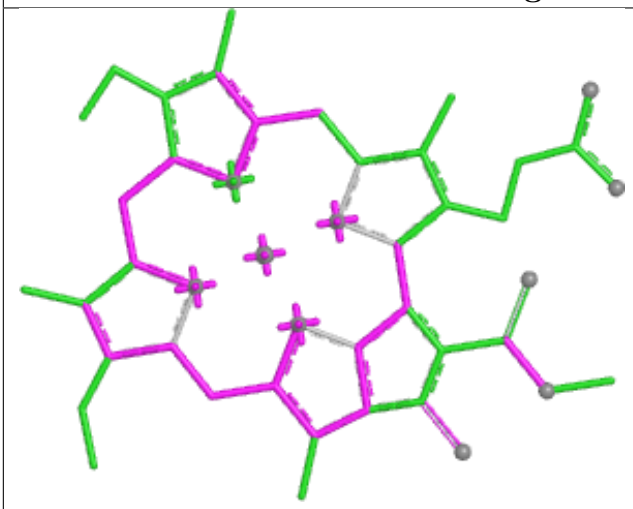


Rings

Ligand CLA B 833



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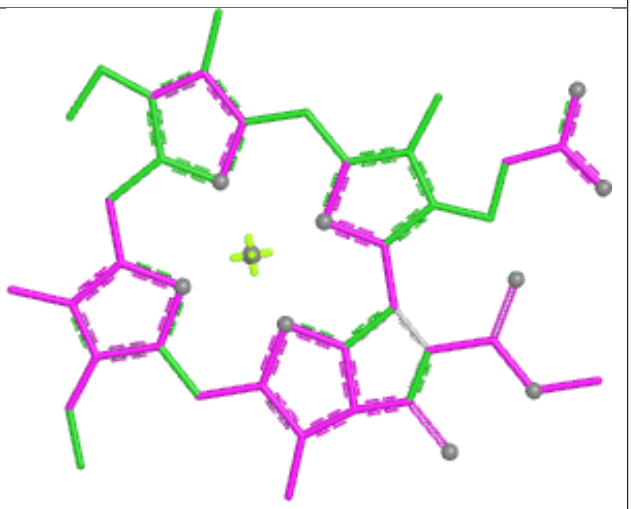

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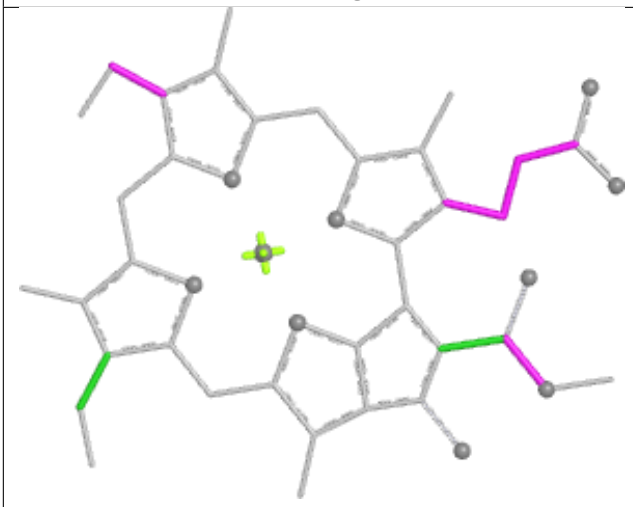
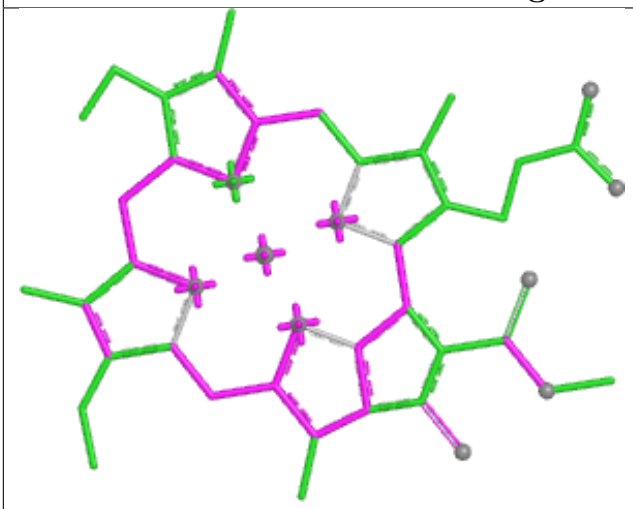


Torsions

Rings

Ligand CLA a 809



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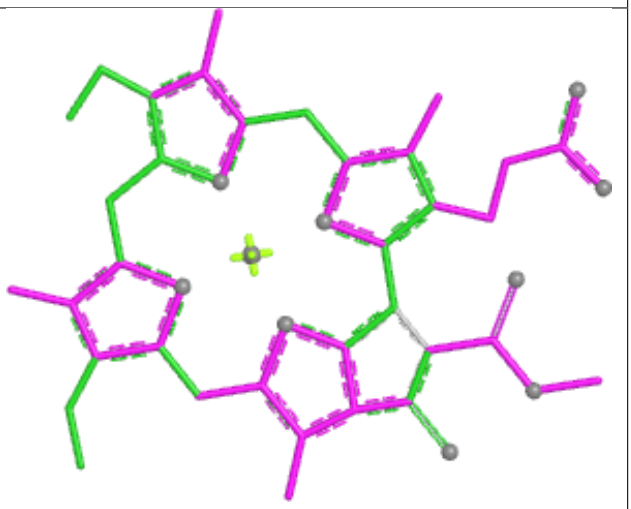

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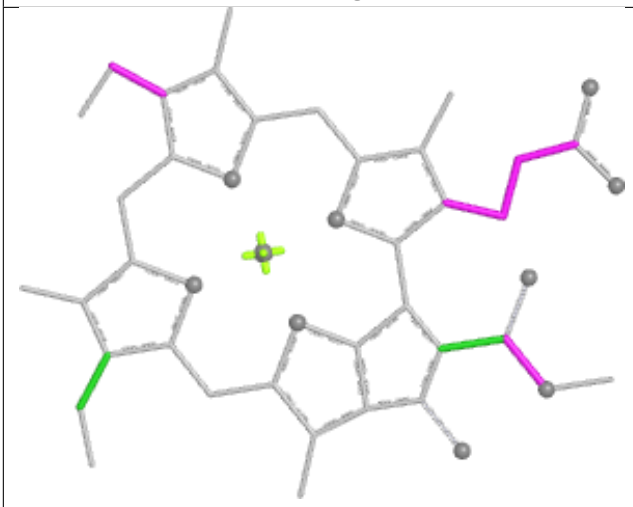
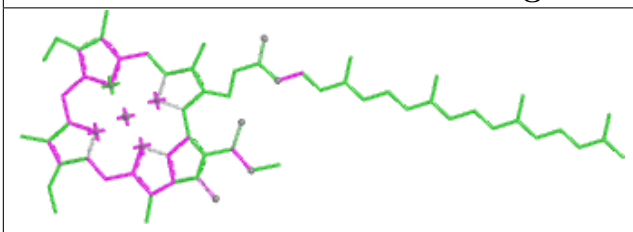


Torsions

Rings

Ligand CLA A 805



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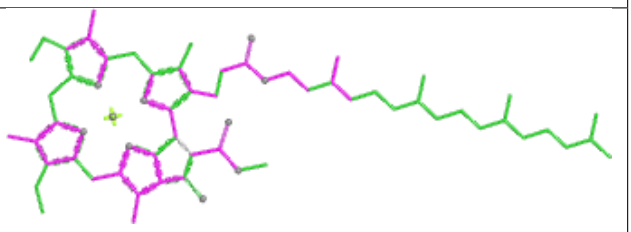

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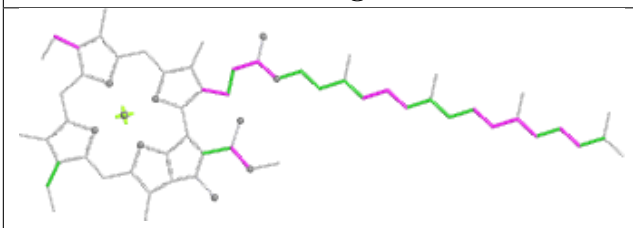

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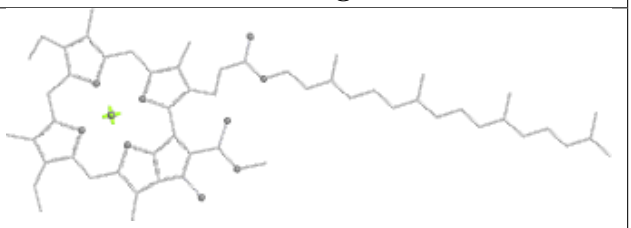
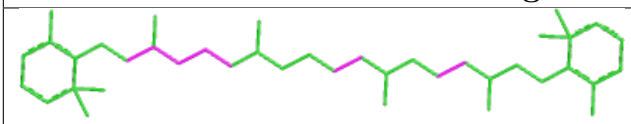


Rings

Ligand BCR B 849



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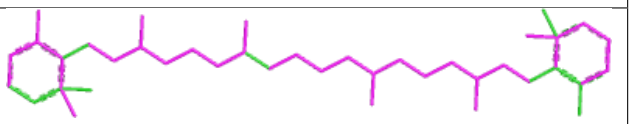

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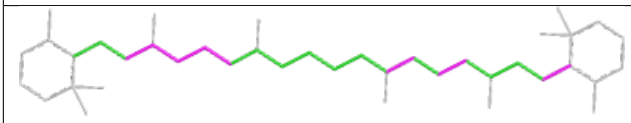

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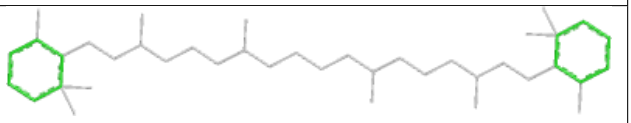
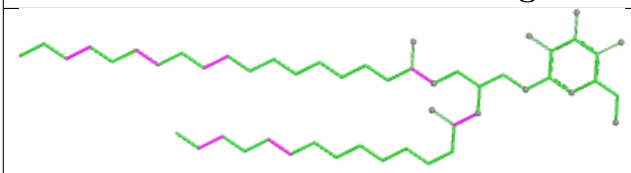


Rings

Ligand LMG H 851



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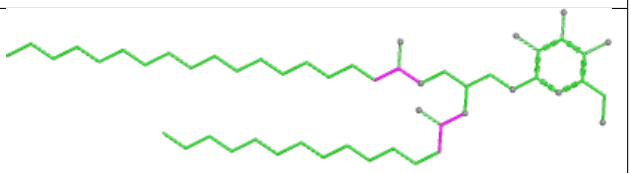
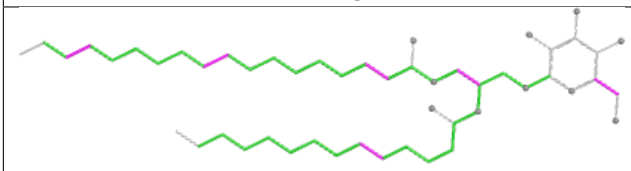


Bond angles



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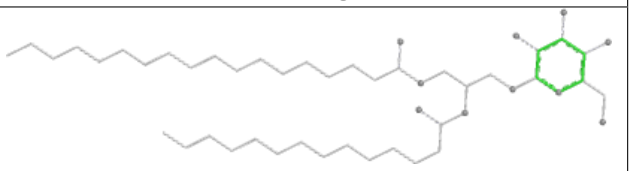
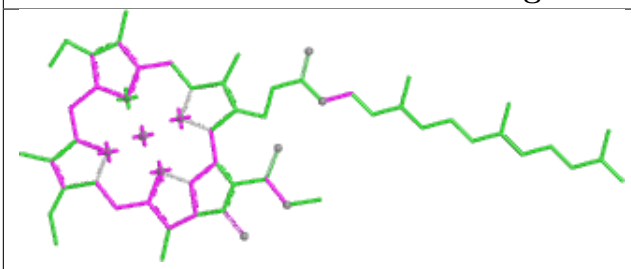


Rings

Ligand CLA A 812



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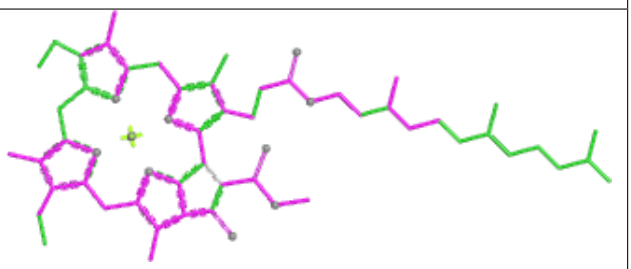
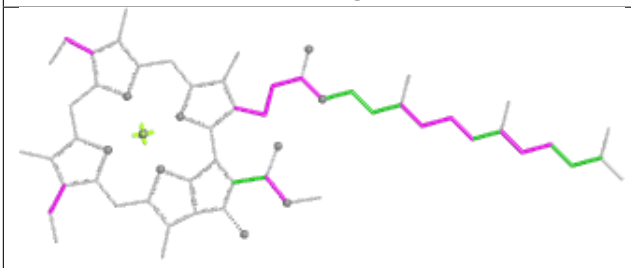
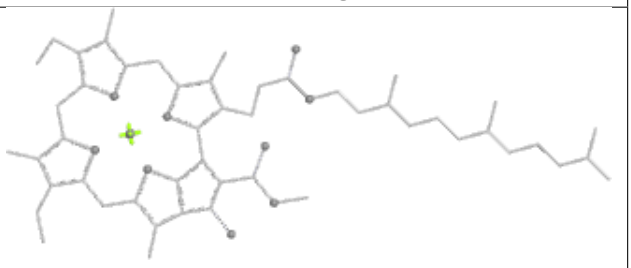


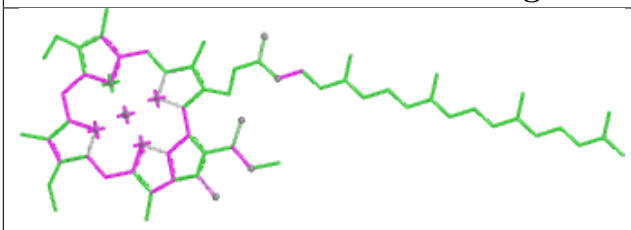
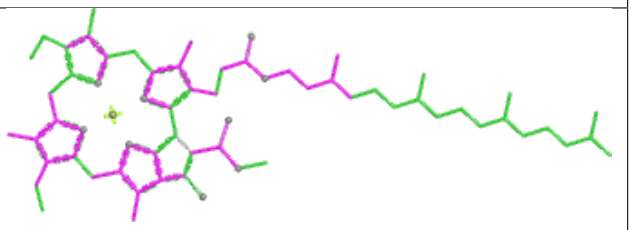
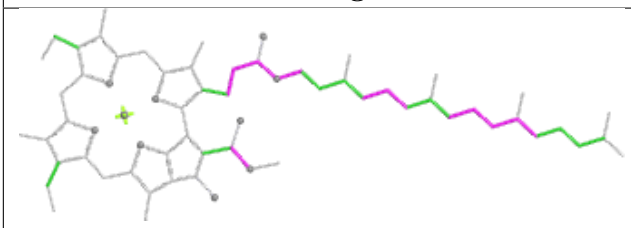
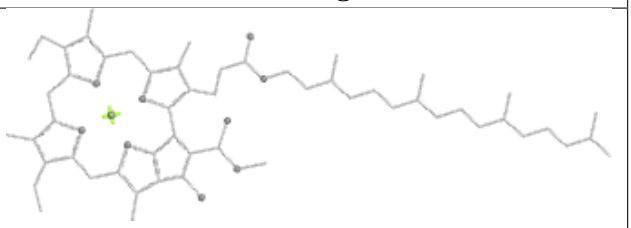
Bond angles

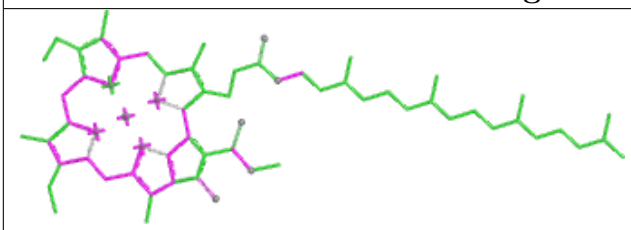
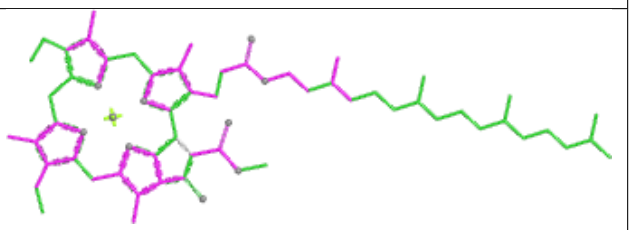
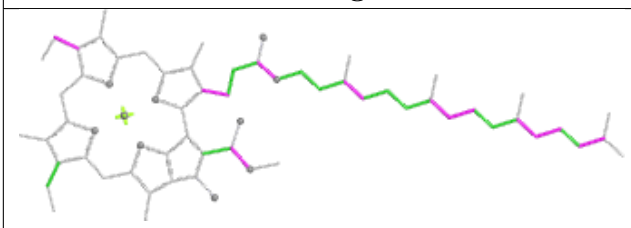
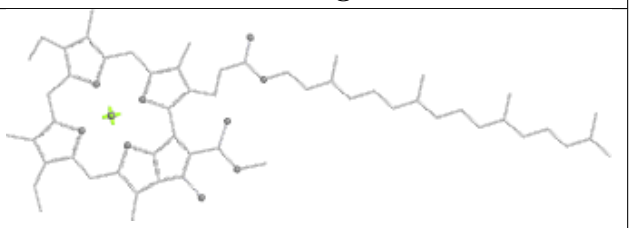


Torsions

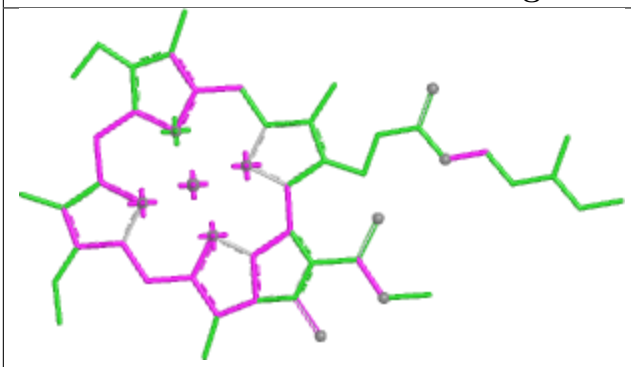


Rings

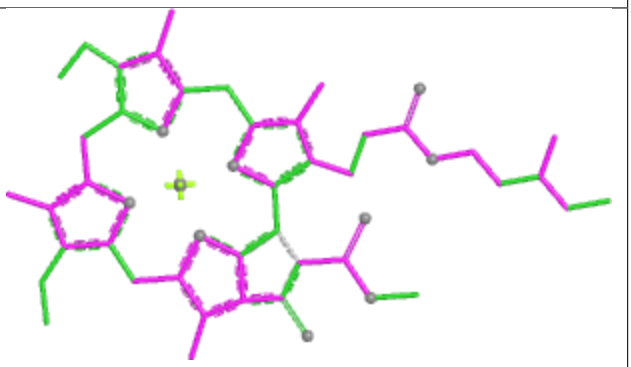
Ligand CLA G 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

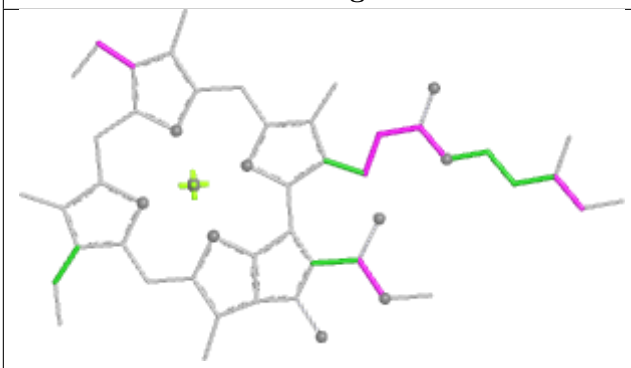
Ligand CLA G 822



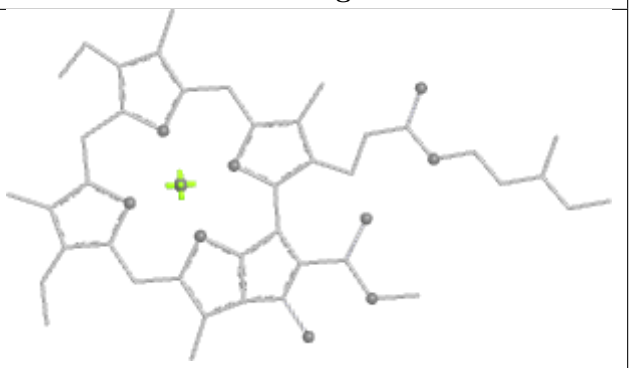
Bond lengths



Bond angles

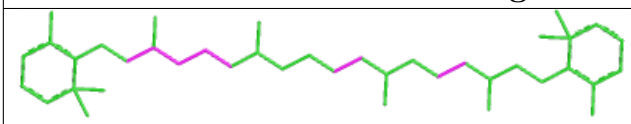


Torsions

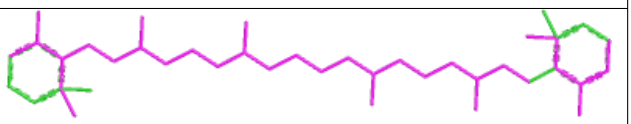


Rings

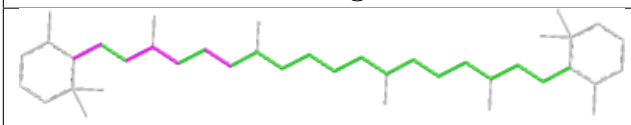
Ligand BCR M 1602



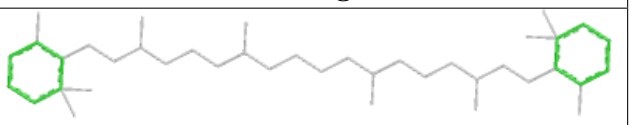
Bond lengths



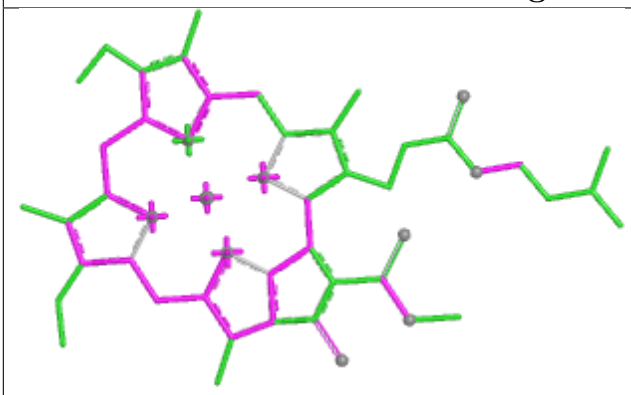
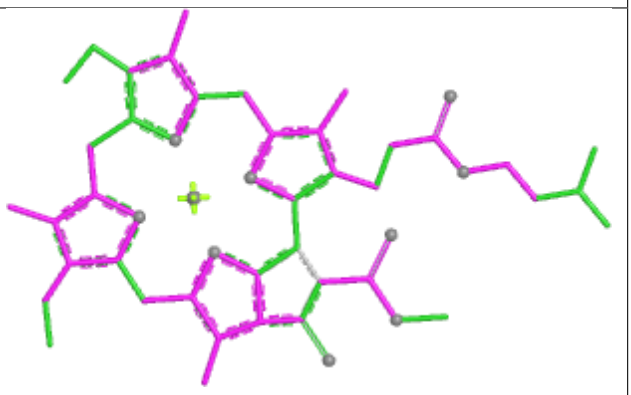
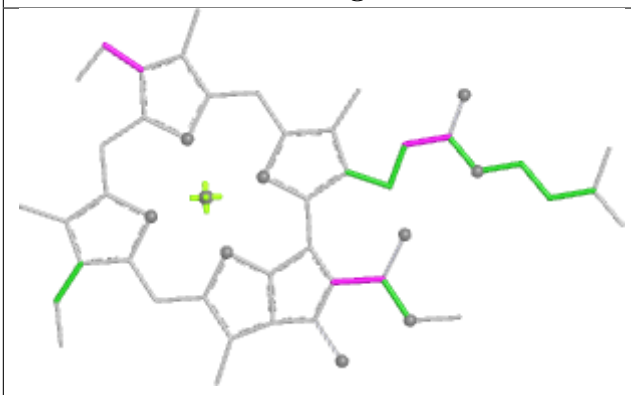
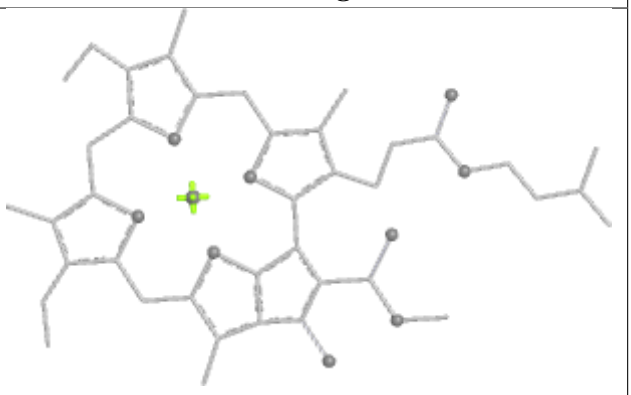
Bond angles

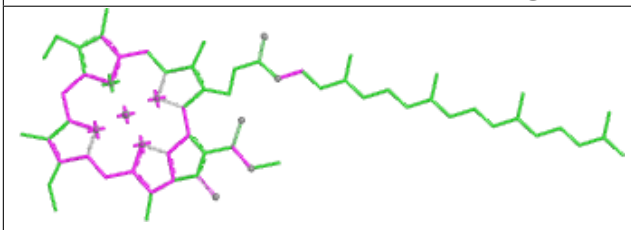
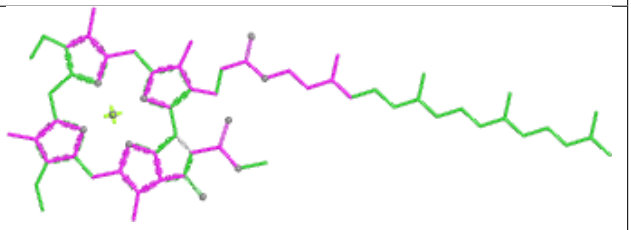
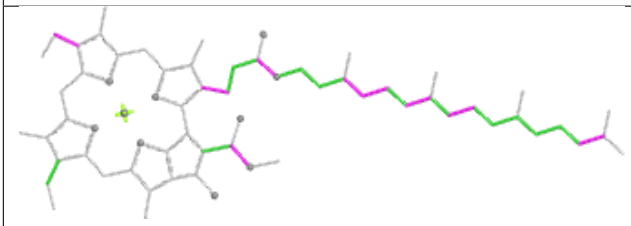
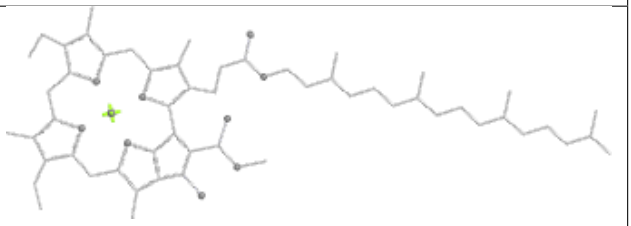


Torsions



Rings

Ligand CLA a 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

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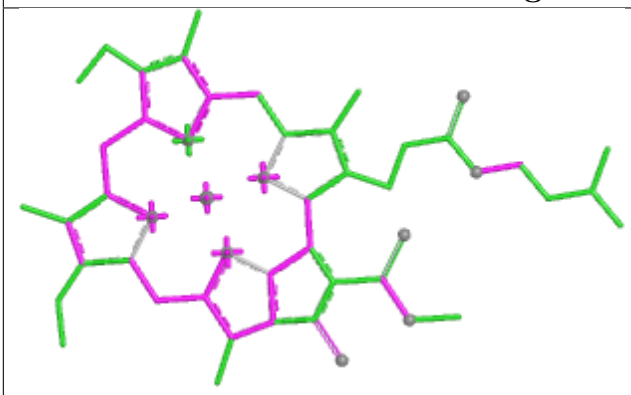
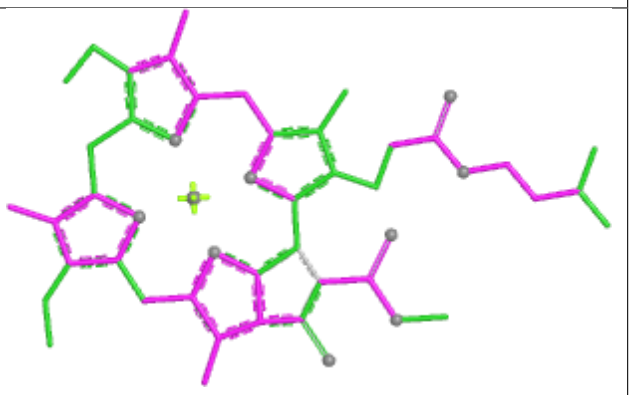
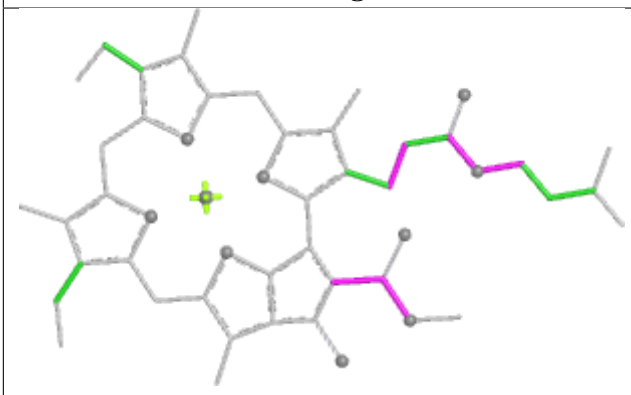
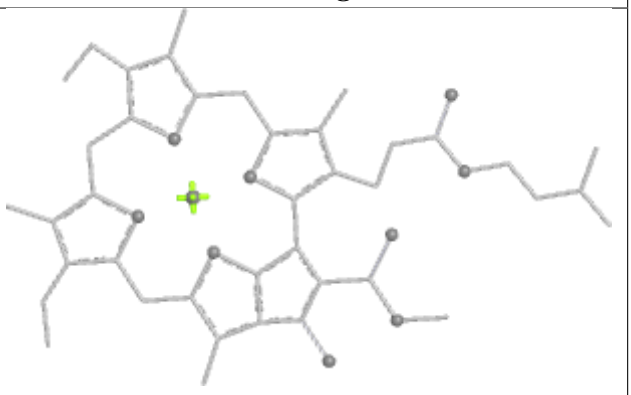
 Bond lengths	 Bond angles
 Torsions	 Rings

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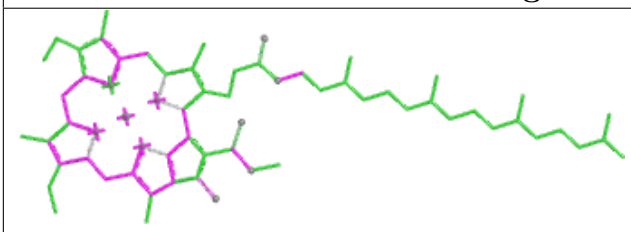
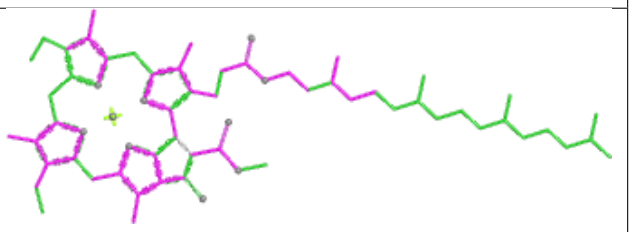
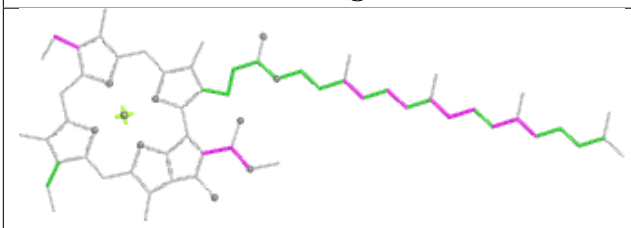
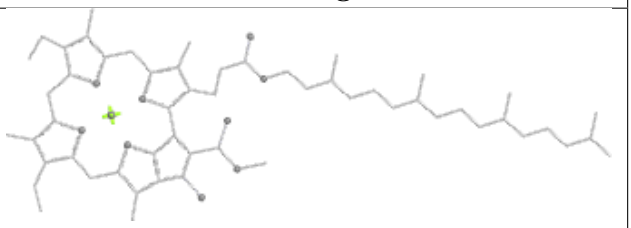
 Bond lengths	 Bond angles
 Torsions	 Rings

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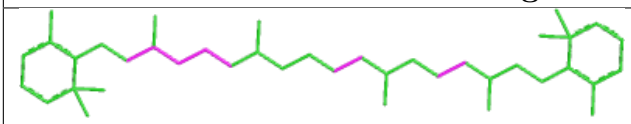
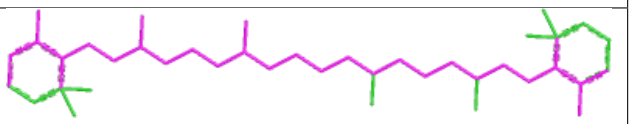
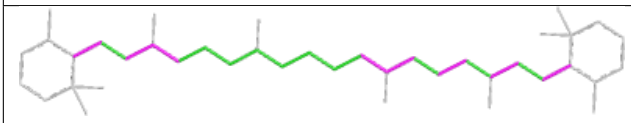
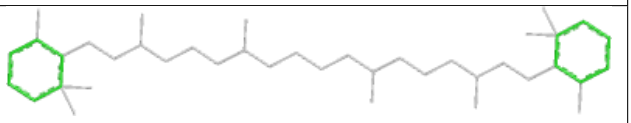
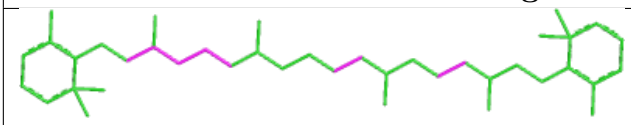
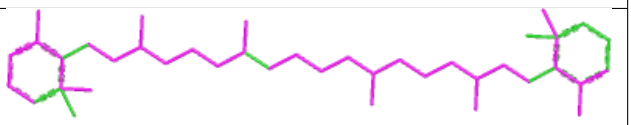
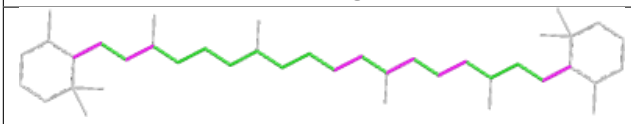
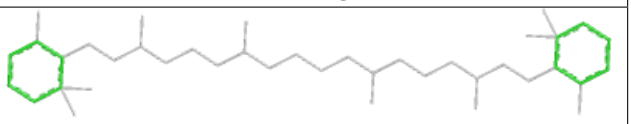
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR H 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

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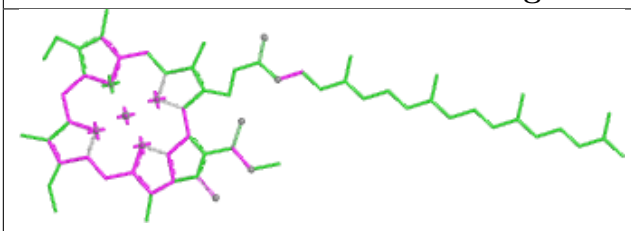
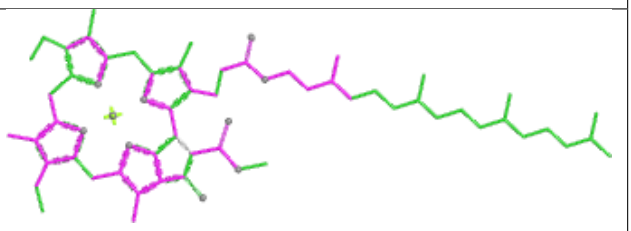
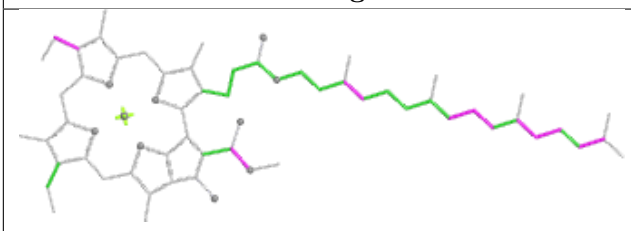
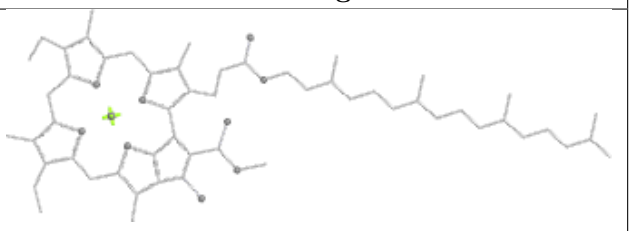
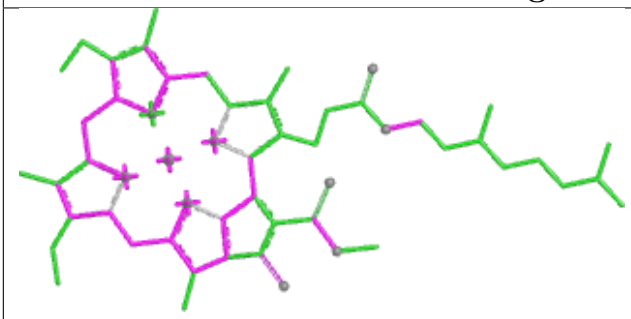
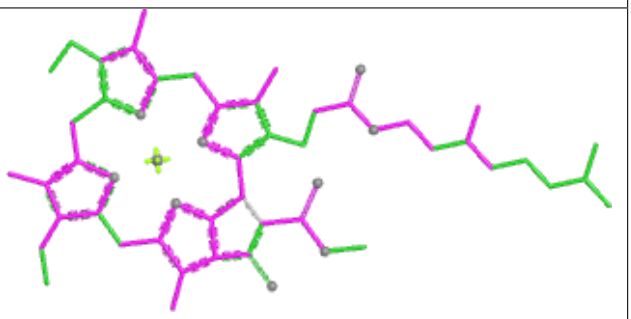
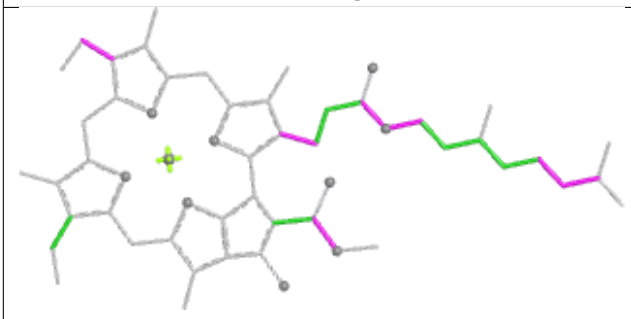
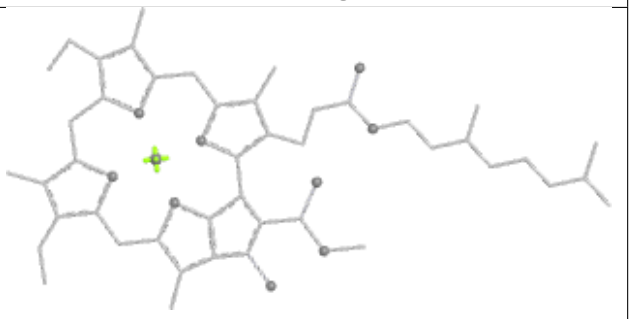
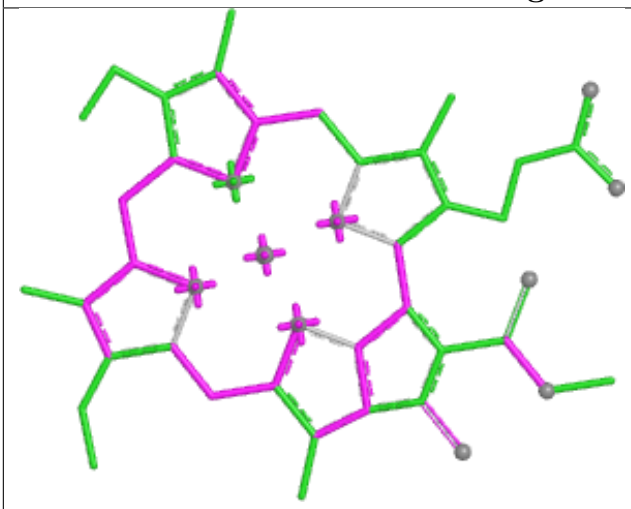
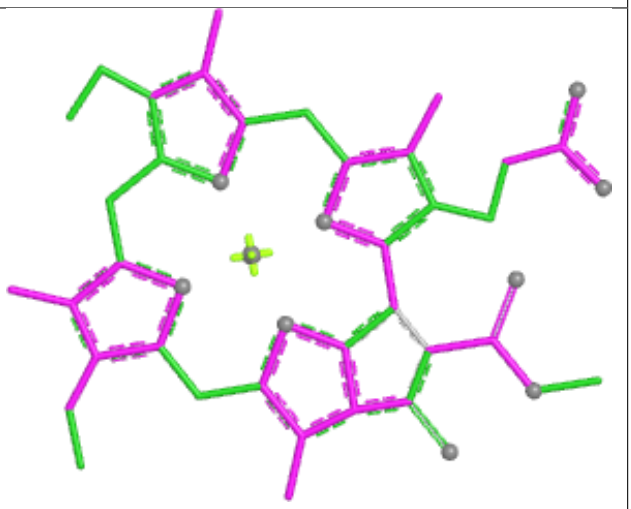
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

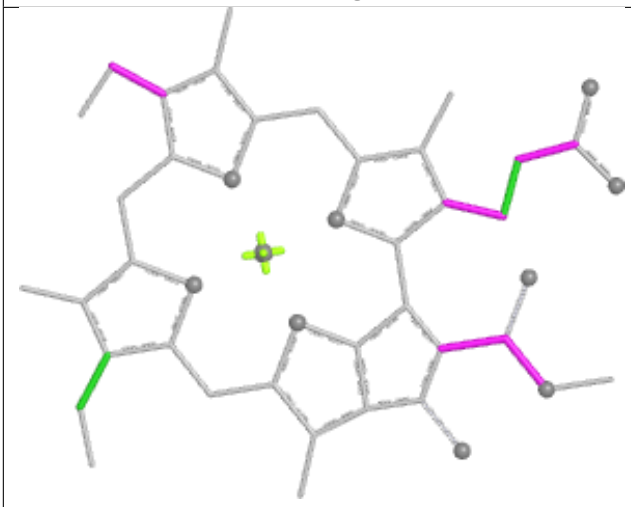
Ligand CLA b 819



Bond lengths



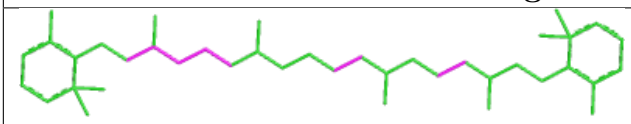
Bond angles



Torsions

Rings

Ligand BCR F 202



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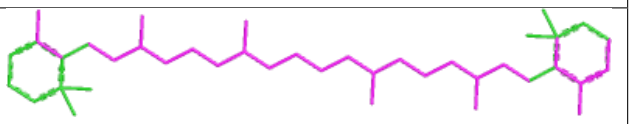
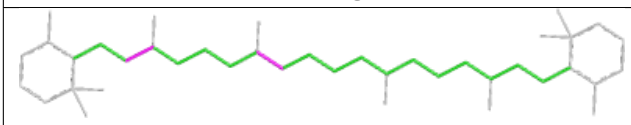
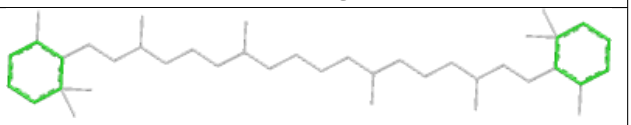


Bond angles

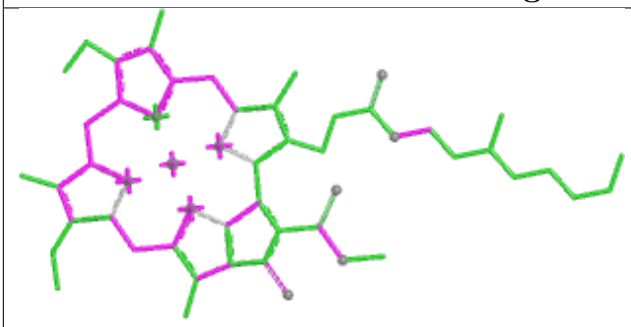


Torsions



Rings

Ligand CLA H 826



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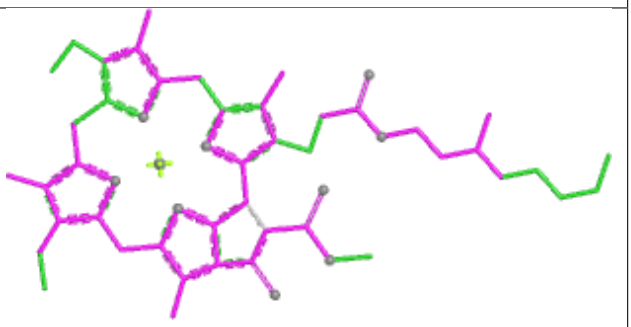
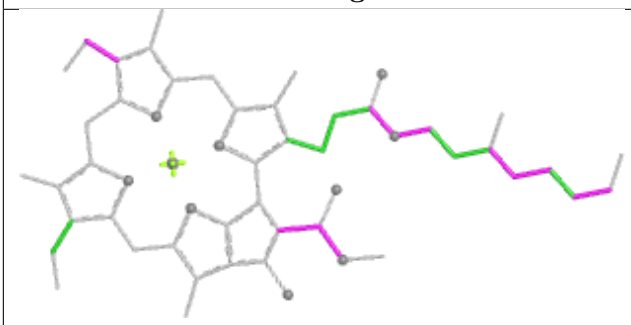


Bond angles



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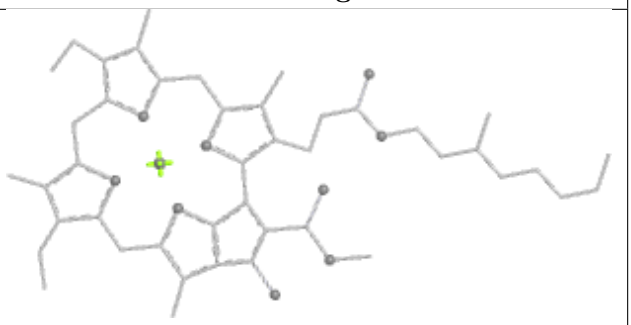
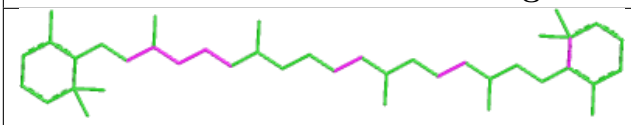


Rings

Ligand BCR B 848



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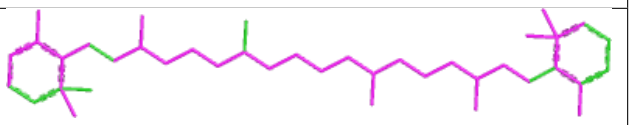
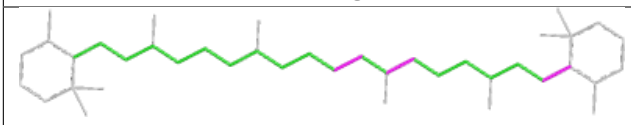


Bond angles



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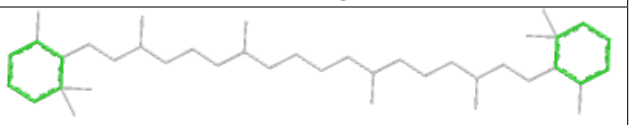
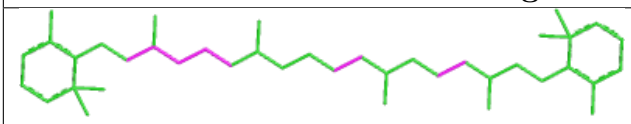


Rings

Ligand BCR H 846



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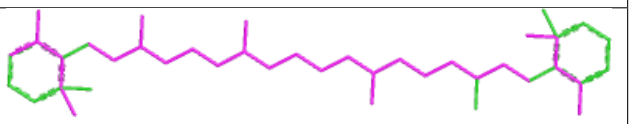
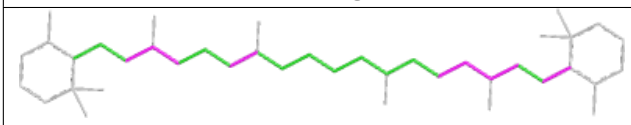
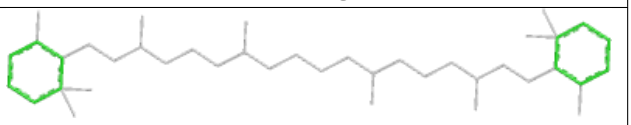


Bond angles

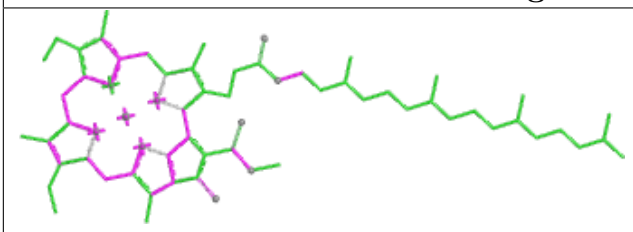


Torsions



Rings

Ligand CLA b 808



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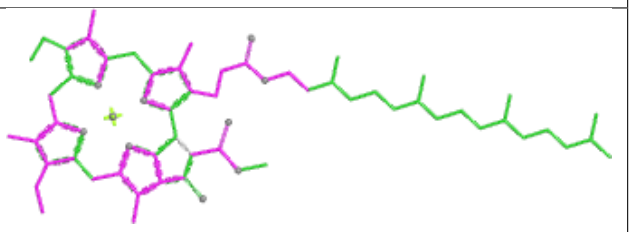
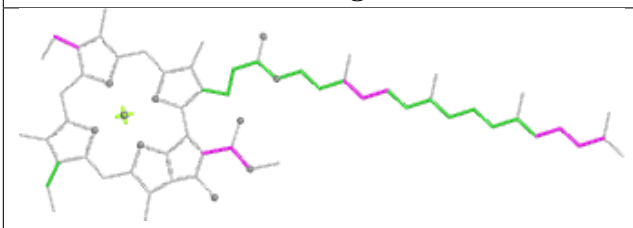
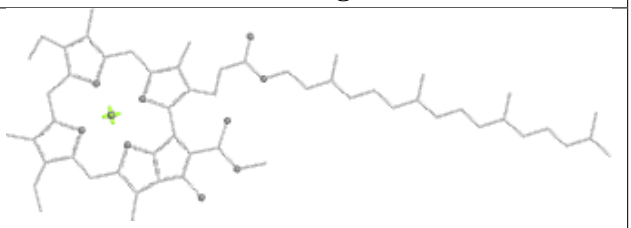


Bond angles

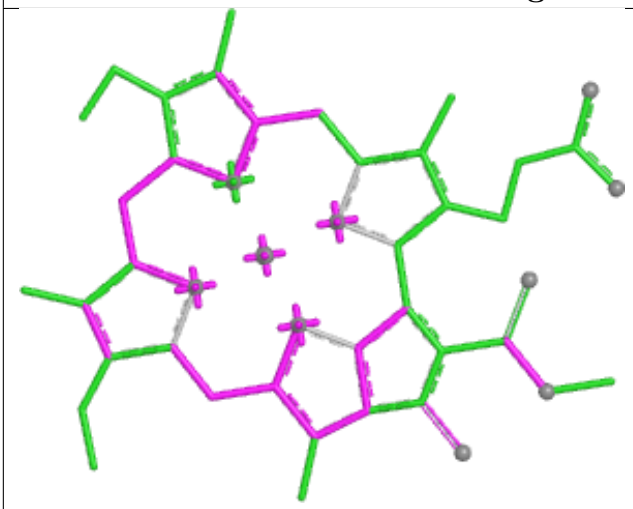


Torsions

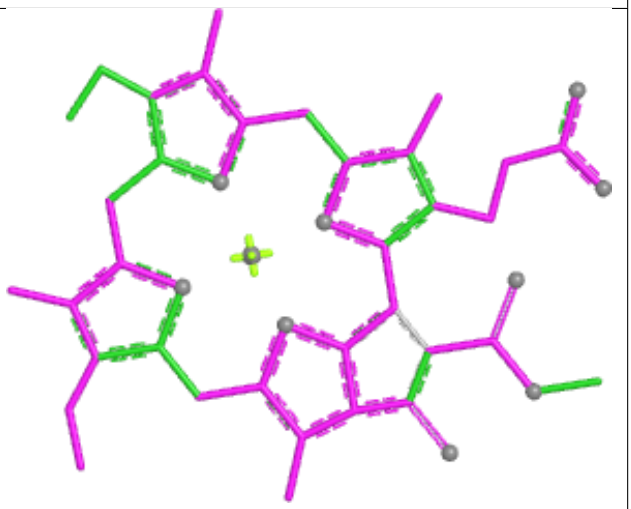


Rings

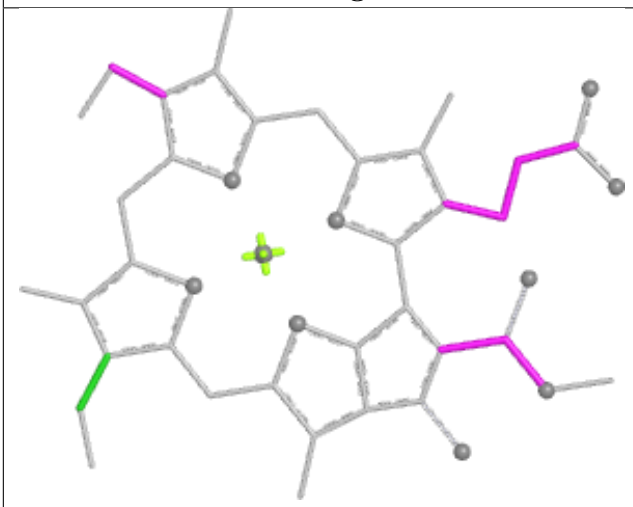
Ligand CLA b 829



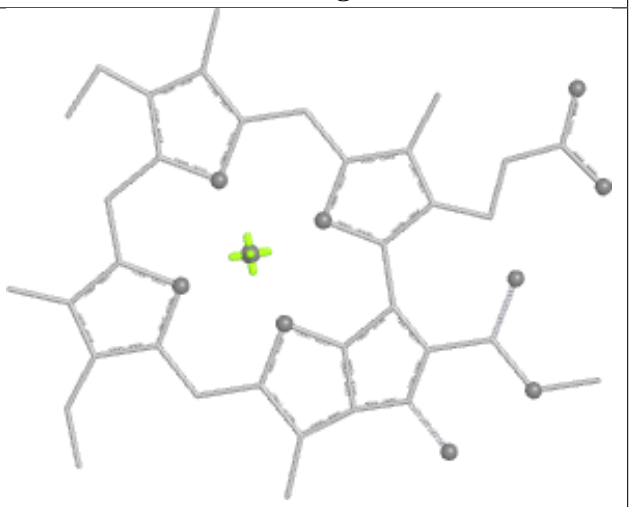
Bond lengths



Bond angles

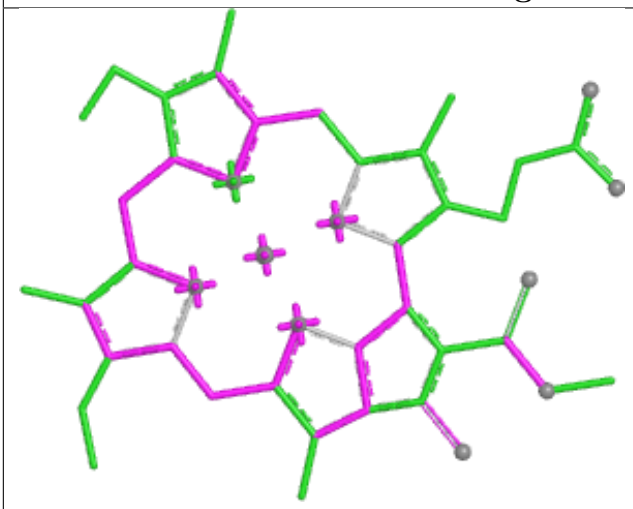


Torsions

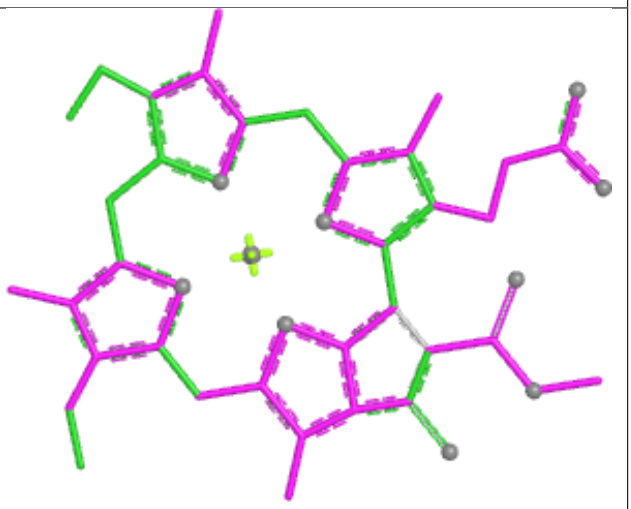


Rings

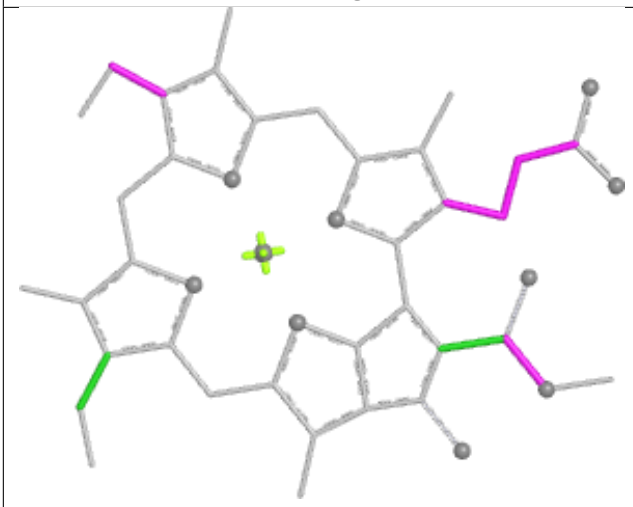
Ligand CLA V 1601



Bond lengths



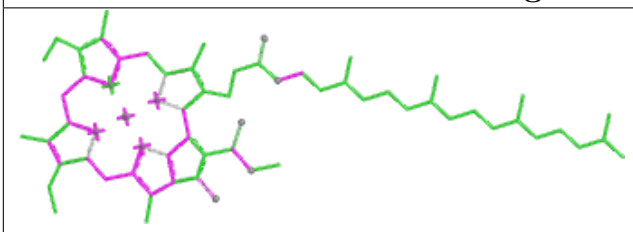
Bond angles



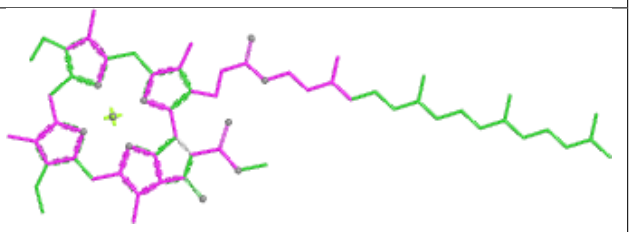
Torsions

Rings

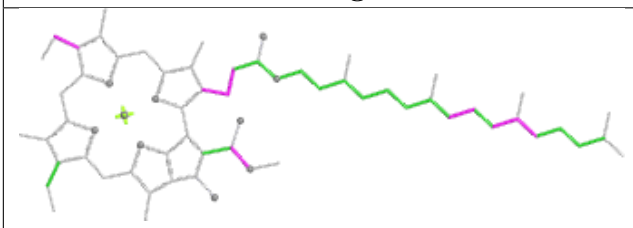
Ligand CLA B 842



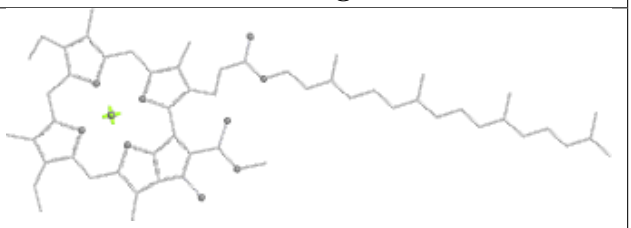
Bond lengths



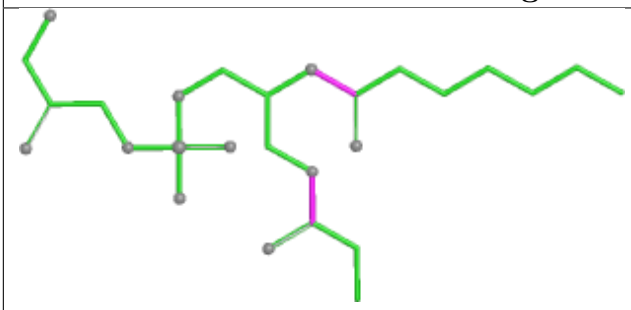
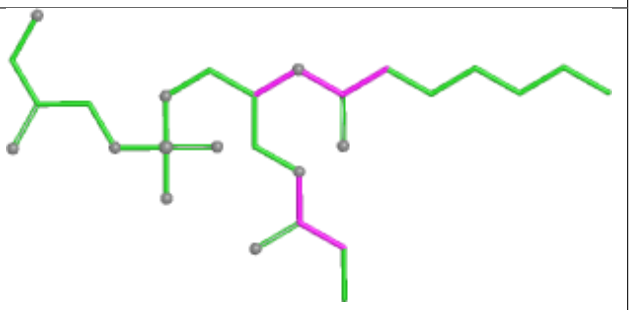
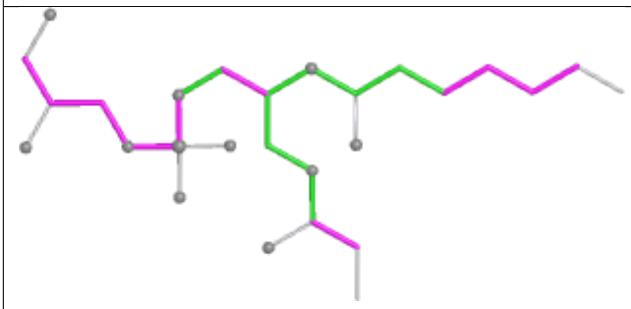
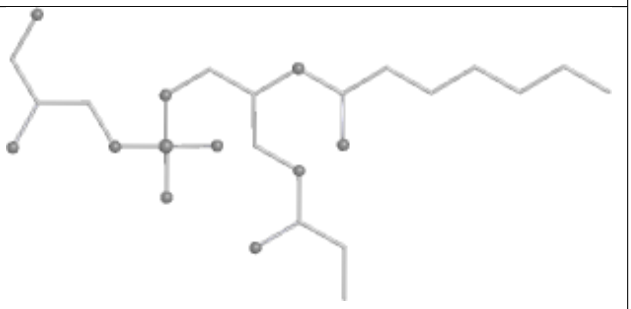
Bond angles

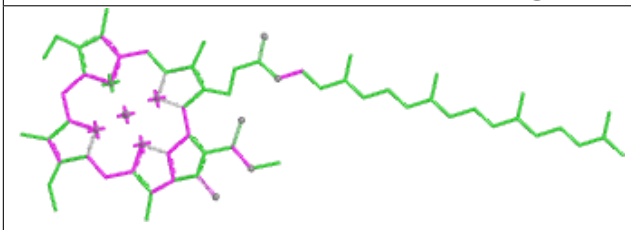
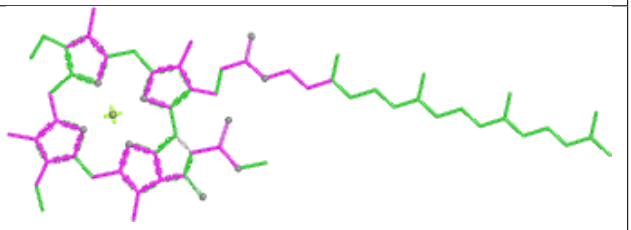
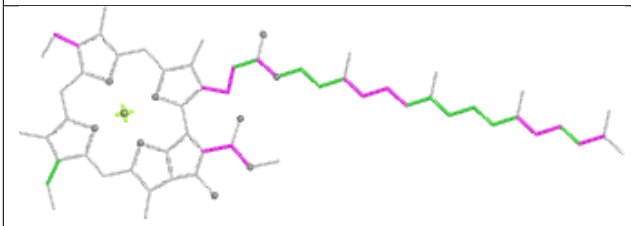
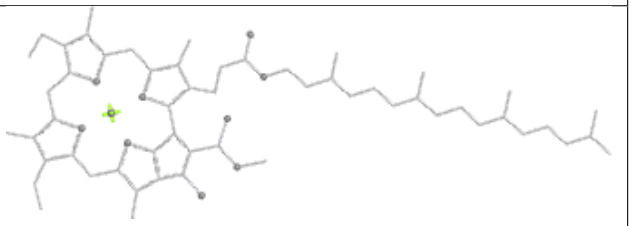


Torsions

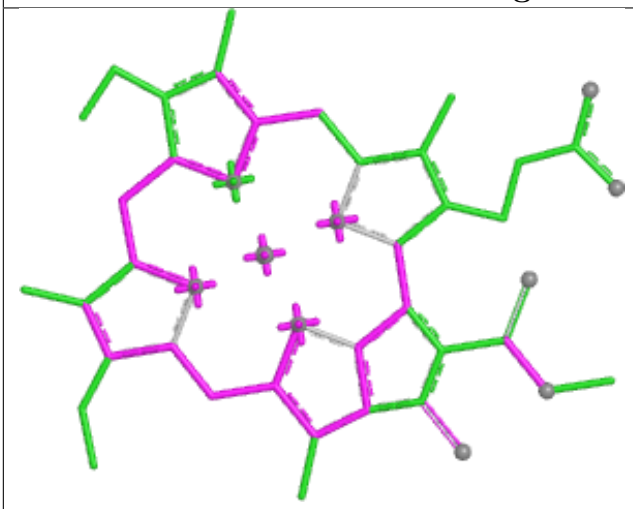


Rings

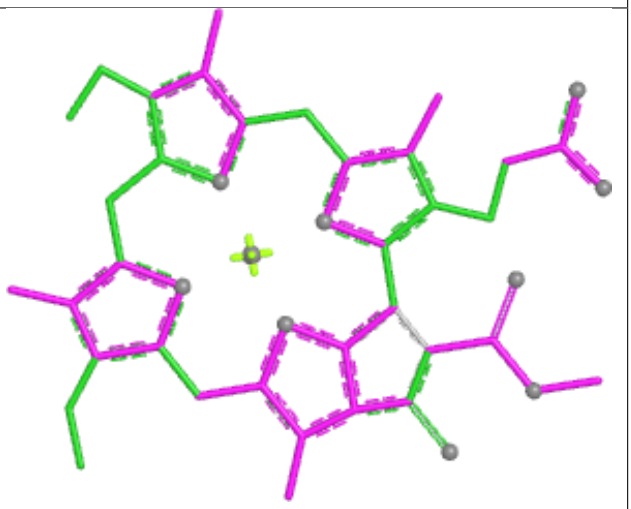
Ligand LHG G 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

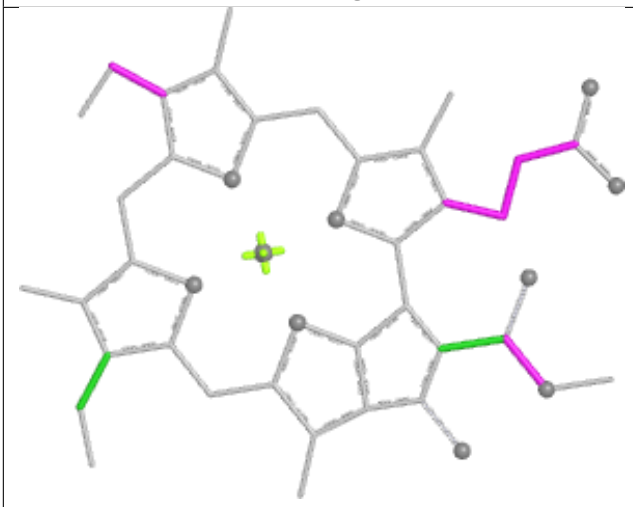
Ligand CLA m 1202



Bond lengths



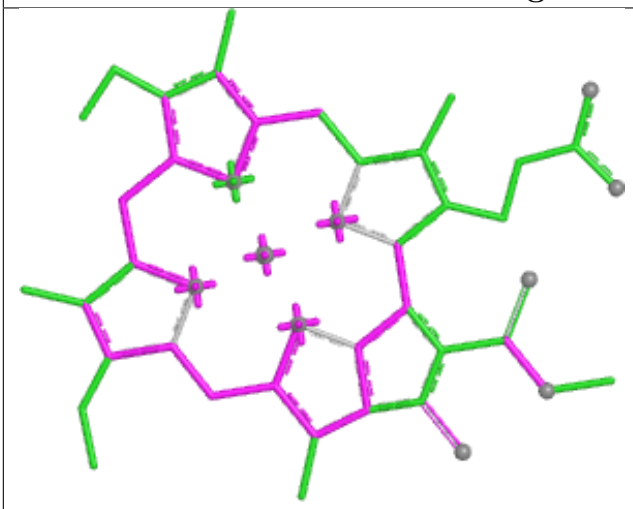
Bond angles



Torsions

Rings

Ligand CLA b 811



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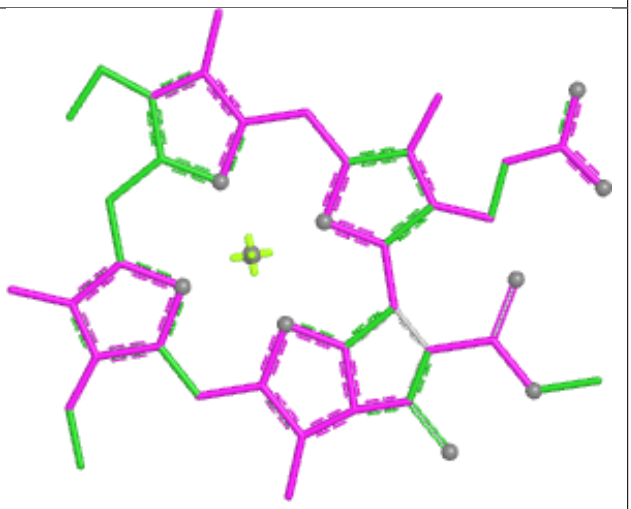

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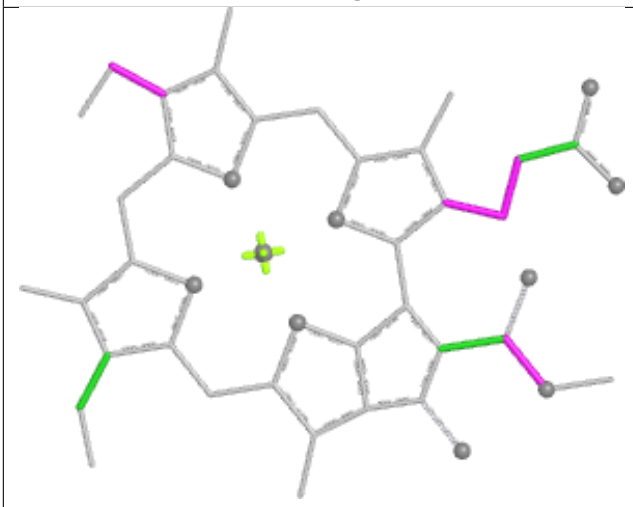
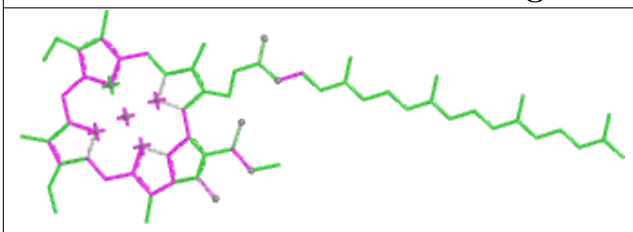


Torsions

Rings

Ligand CLA L 201



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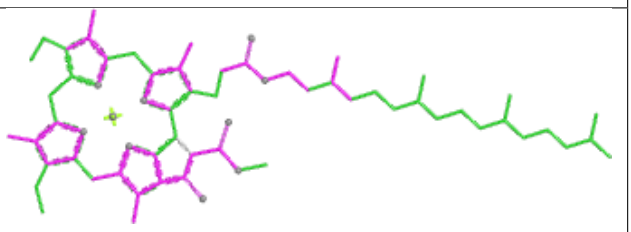
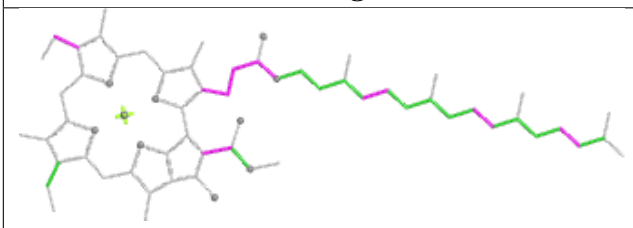
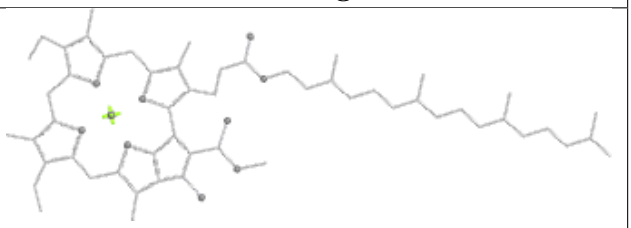


Bond angles

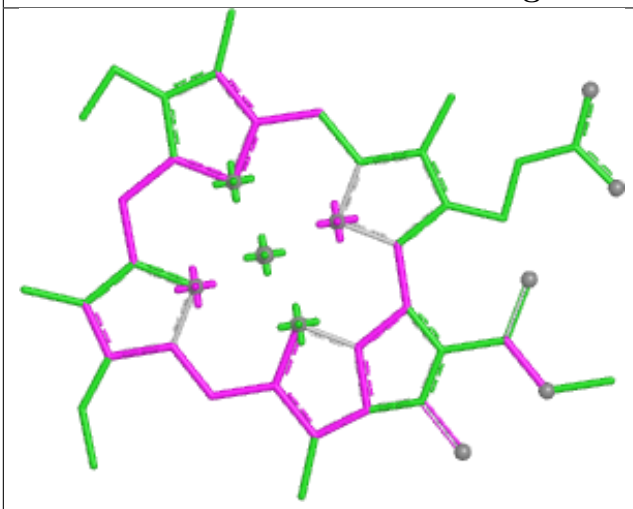


Torsions



Rings

Ligand CLA G 815



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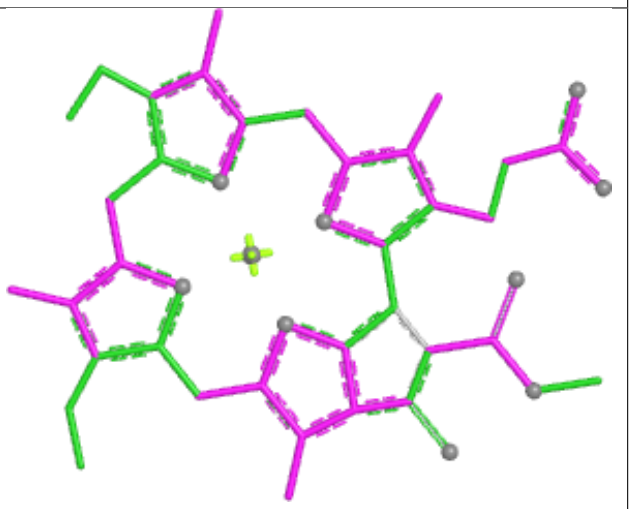
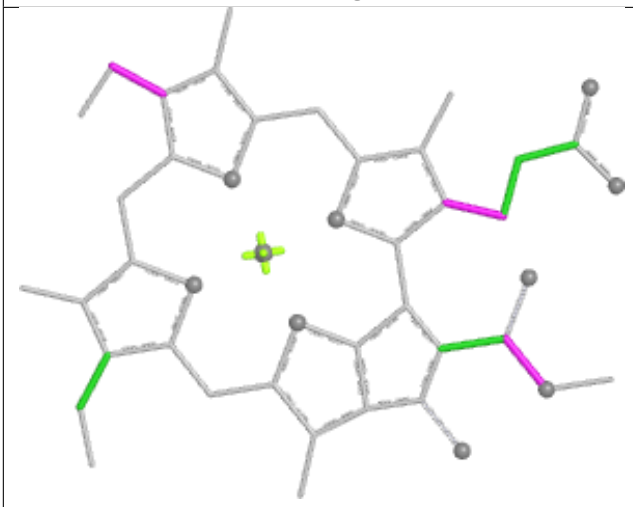


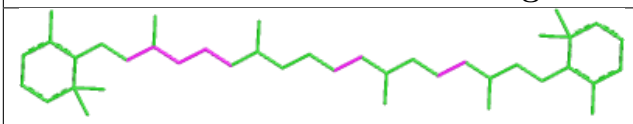
Bond angles



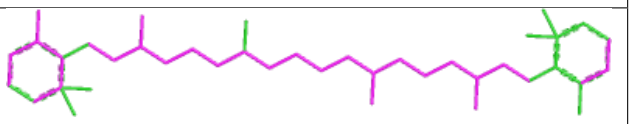
Torsions

Rings

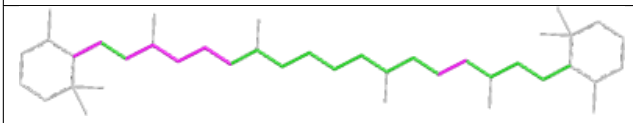
Ligand BCR A 844



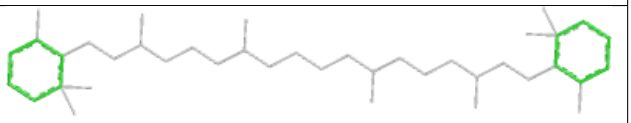
Bond lengths



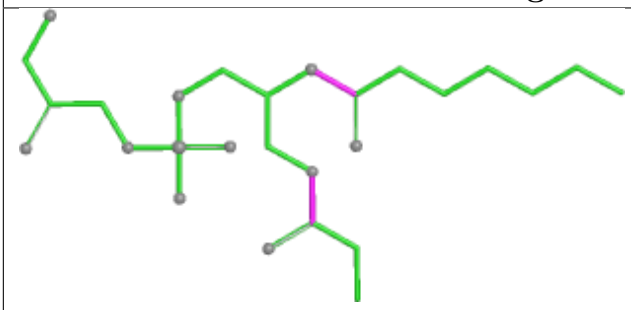
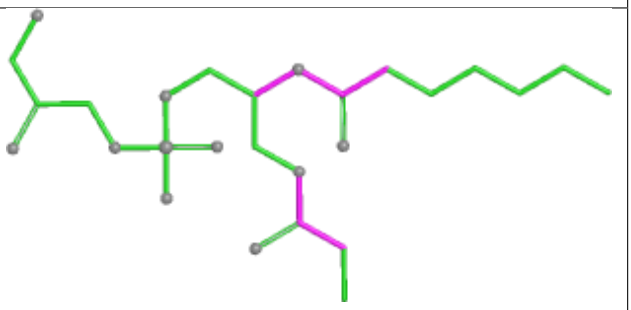
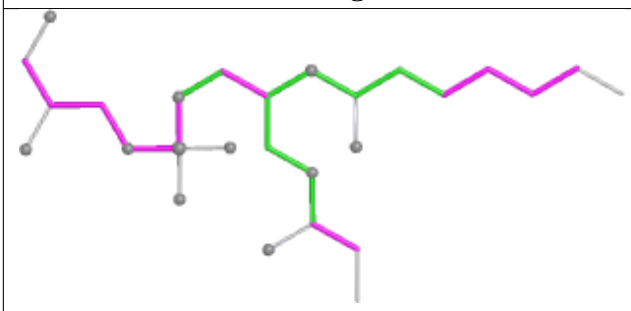
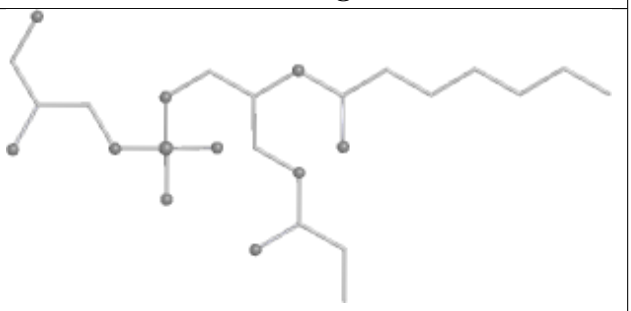
Bond angles

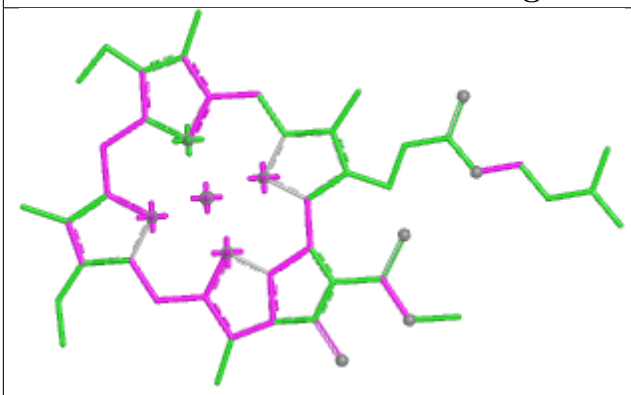
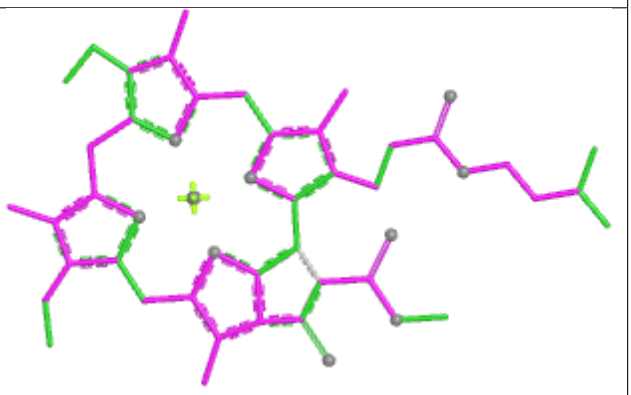
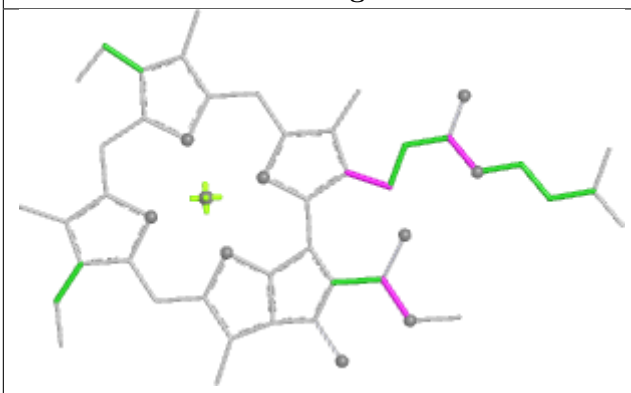
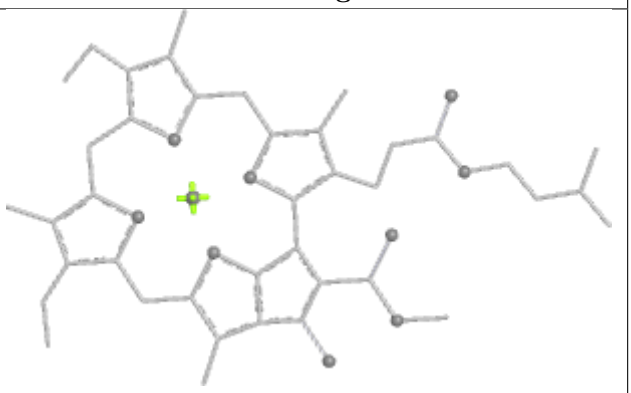


Torsions

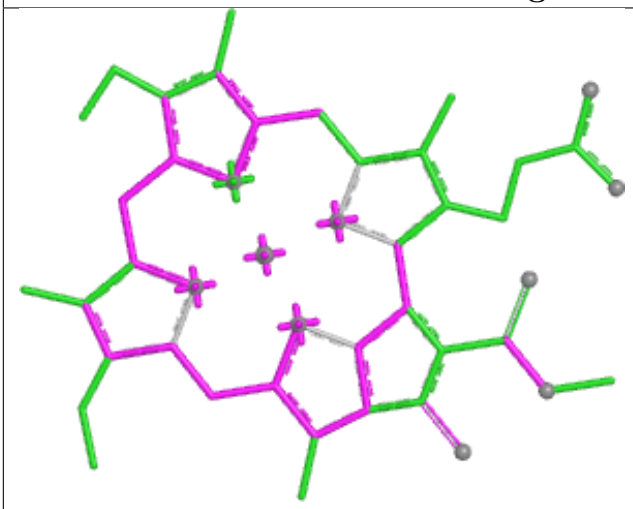


Rings

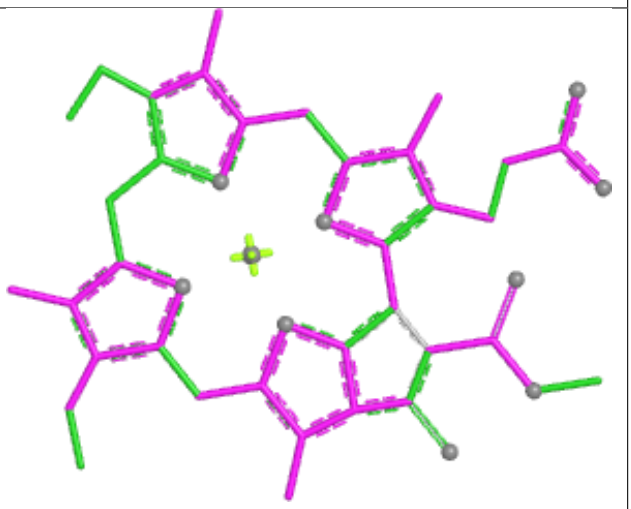
Ligand LHG a 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

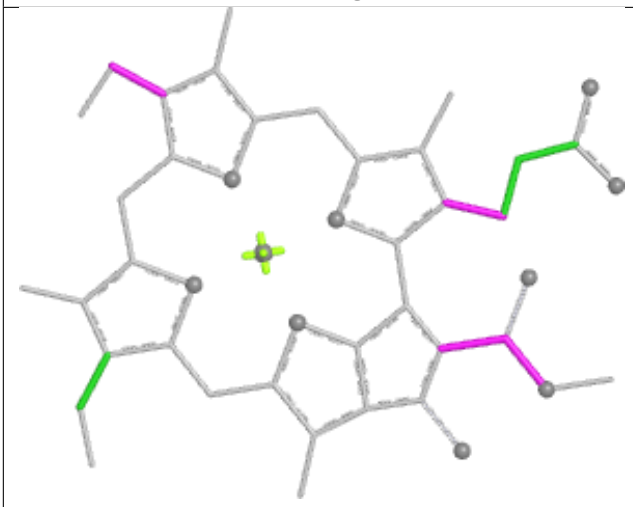
Ligand CLA a 813



Bond lengths



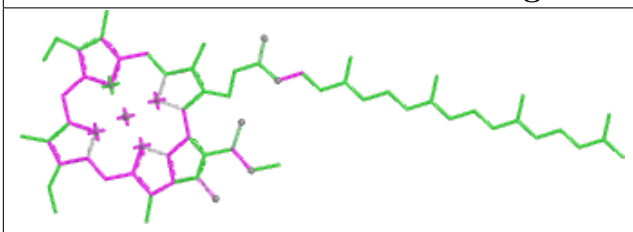
Bond angles



Torsions

Rings

Ligand CLA U 207



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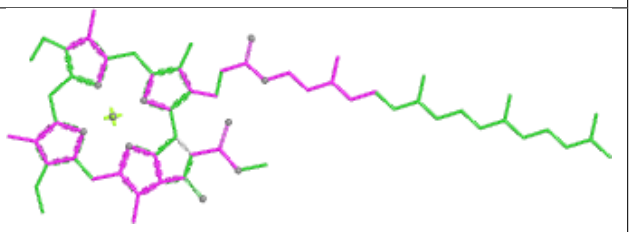
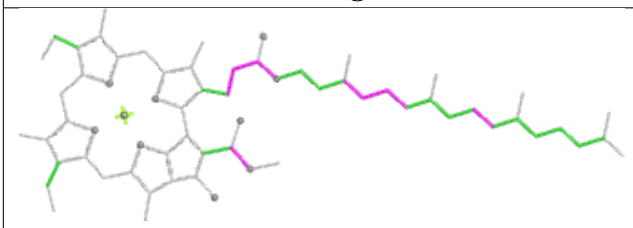
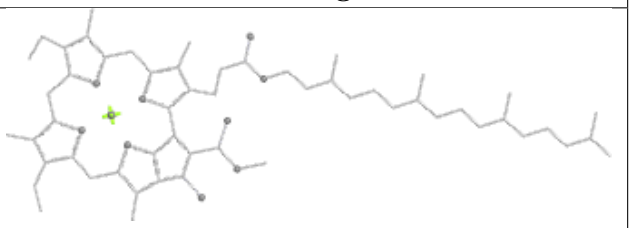


Bond angles

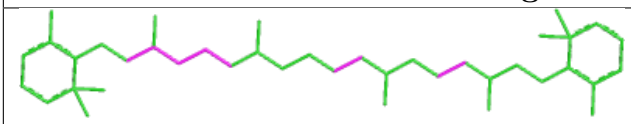


Torsions

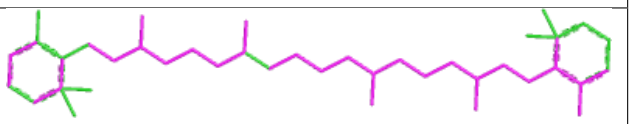


Rings

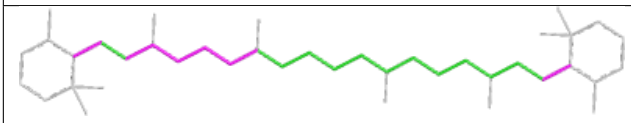
Ligand BCR G 844



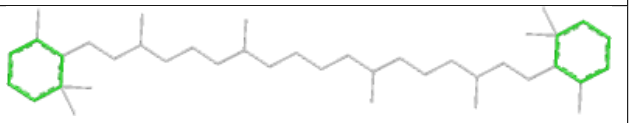
Bond lengths



Bond angles

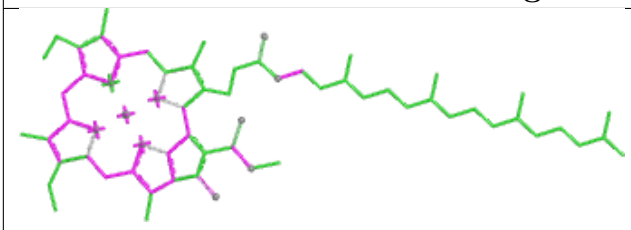


Torsions

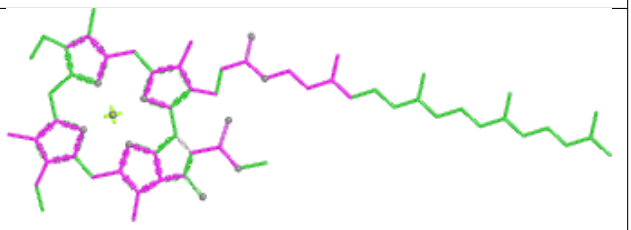


Rings

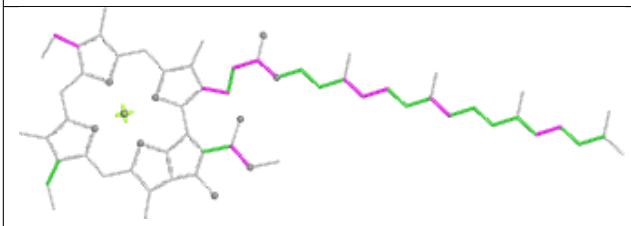
Ligand CLA A 820



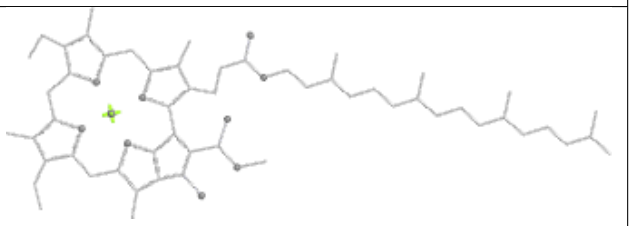
Bond lengths



Bond angles

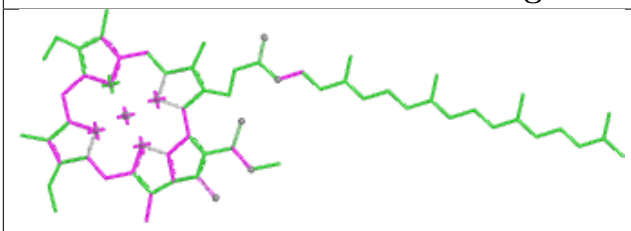


Torsions



Rings

Ligand CLA B 805



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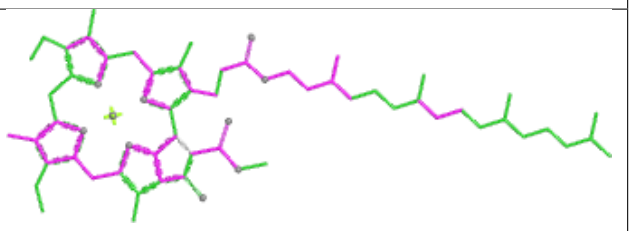
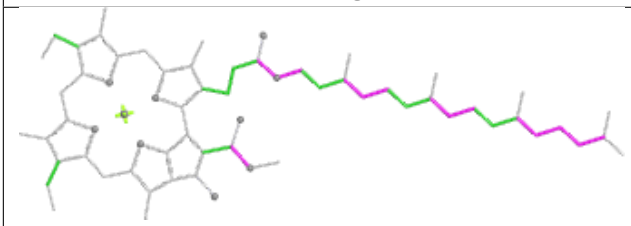
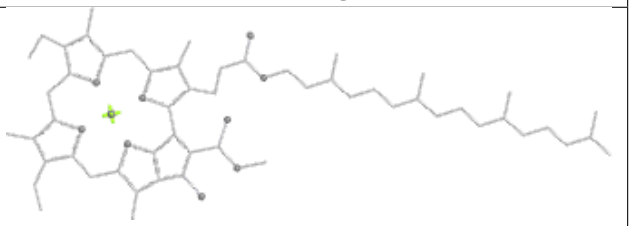


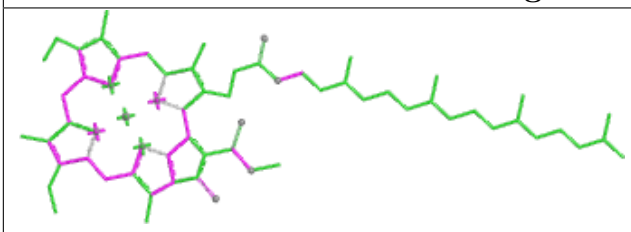
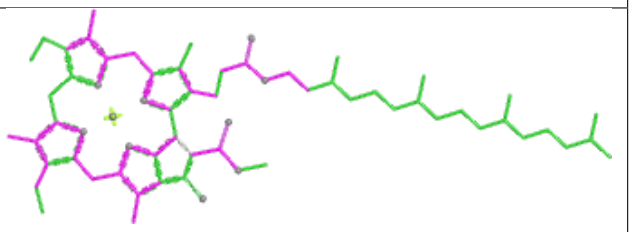
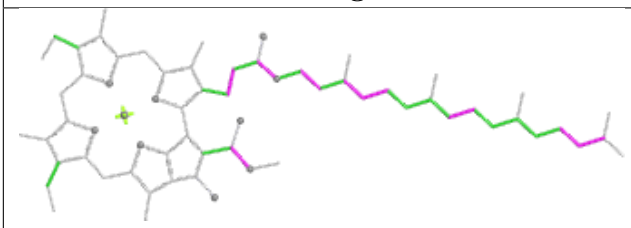
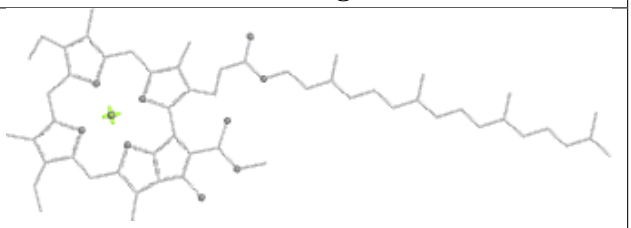
Bond angles



Torsions



Rings

Ligand CLA B 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

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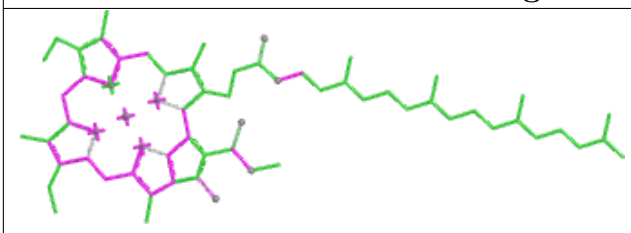
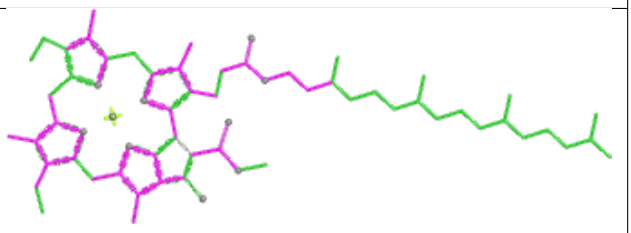
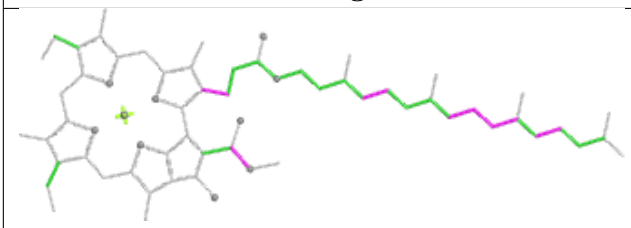
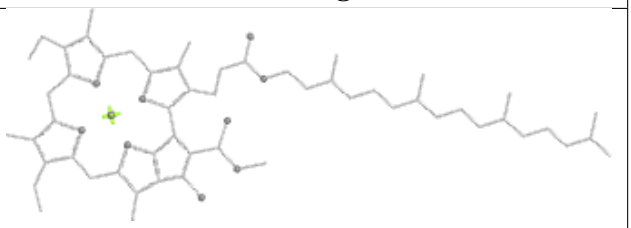
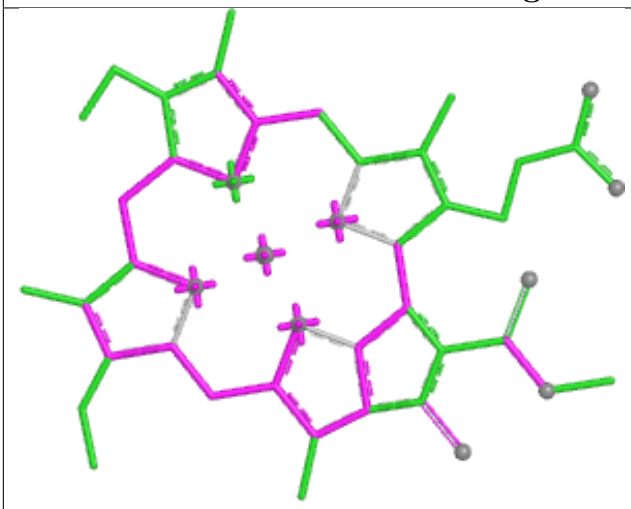
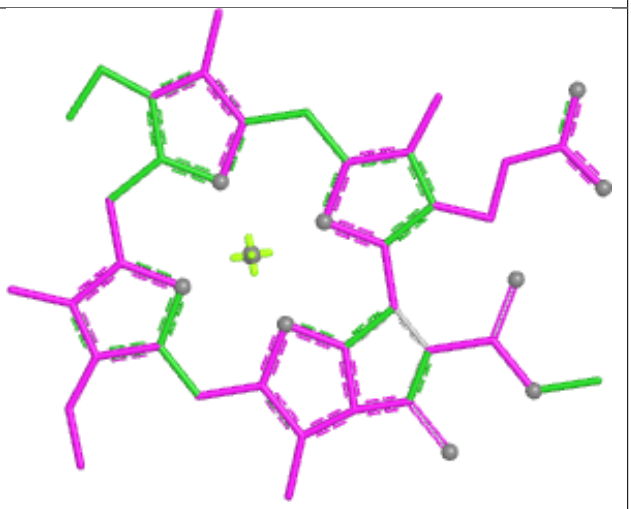
 Bond lengths	 Bond angles
 Torsions	 Rings

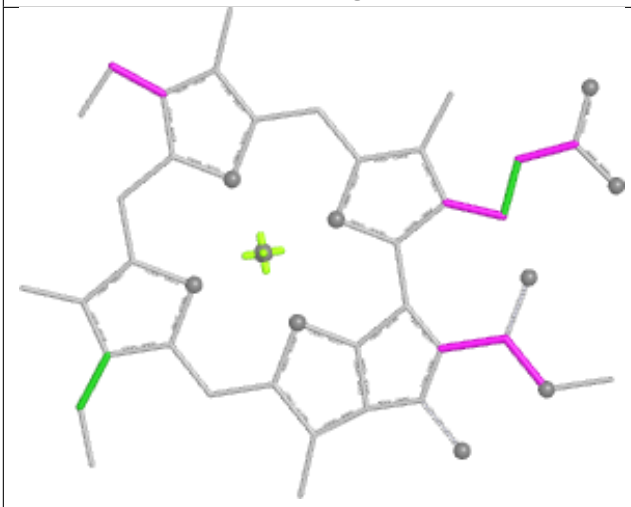
Ligand CLA G 821



Bond lengths



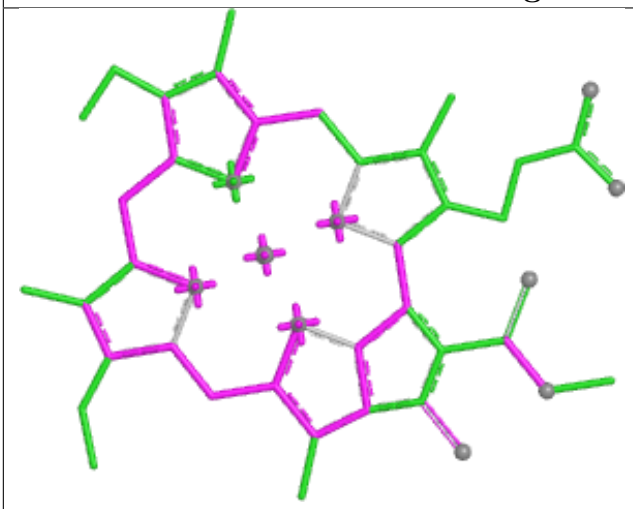
Bond angles



Torsions

Rings

Ligand CLA A 834



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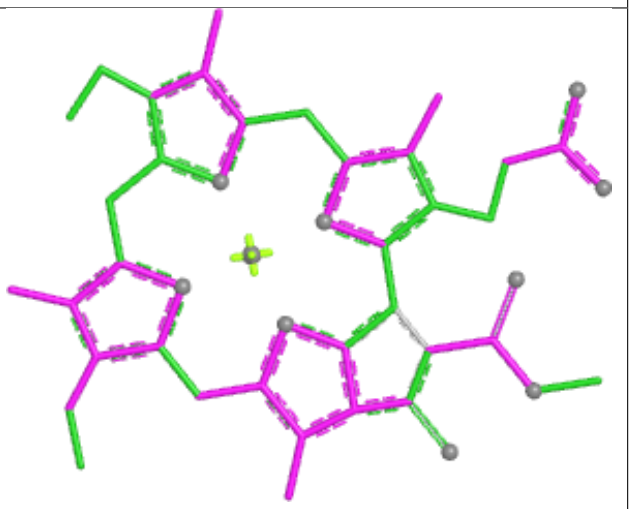
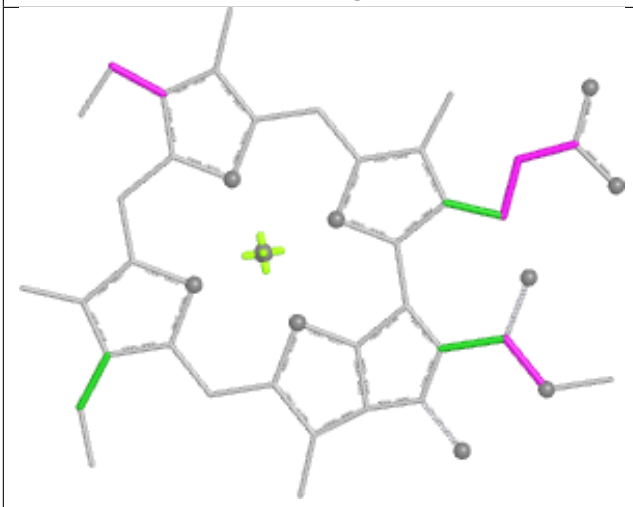


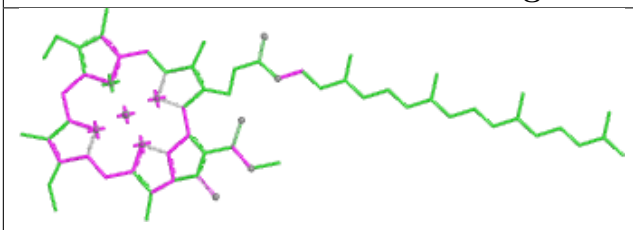
Bond angles



Torsions

Rings

Ligand CLA H 812



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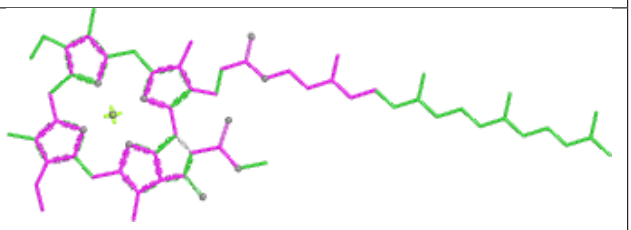
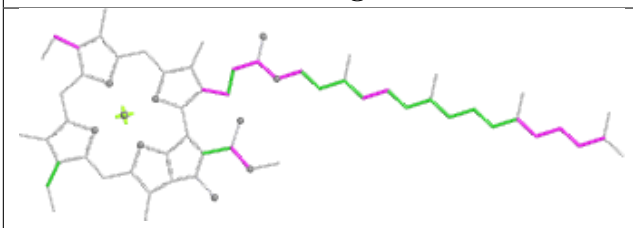
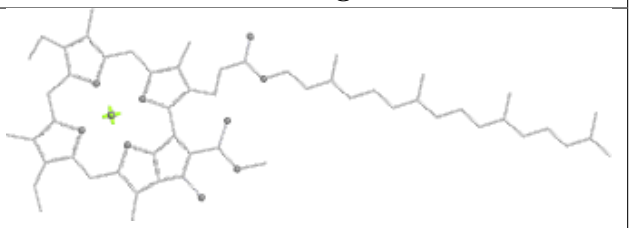


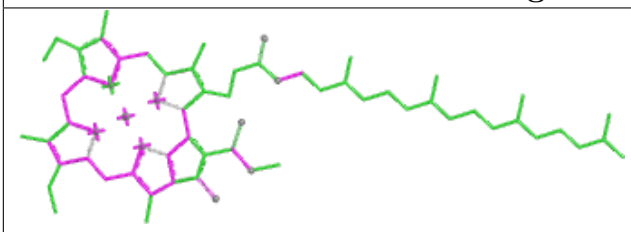
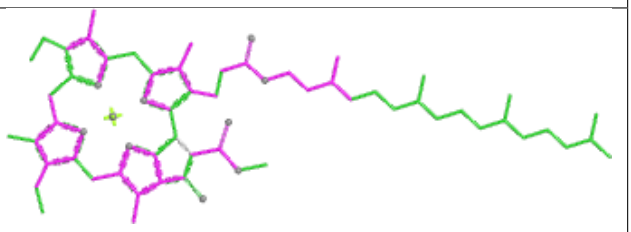
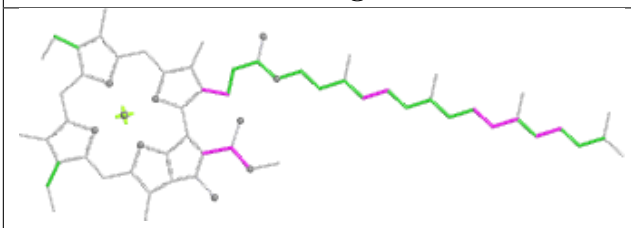
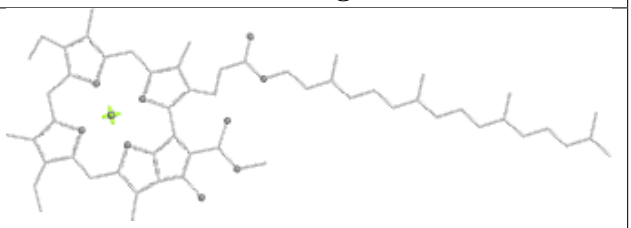
Bond angles

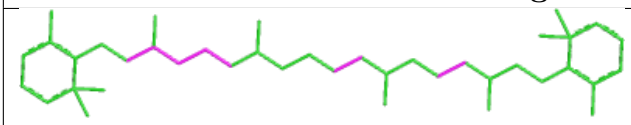
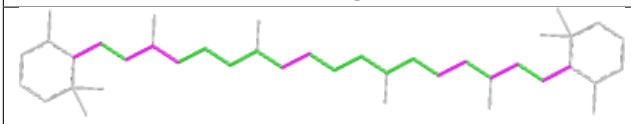
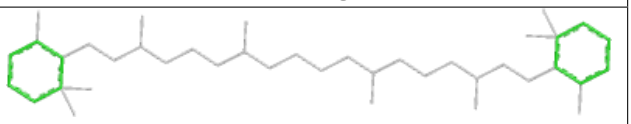


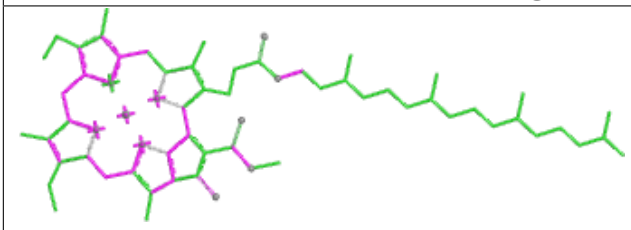
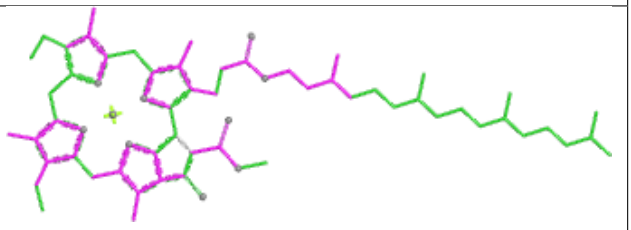
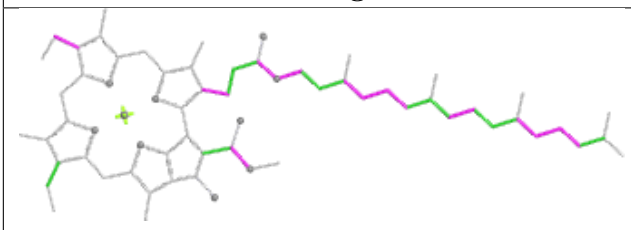
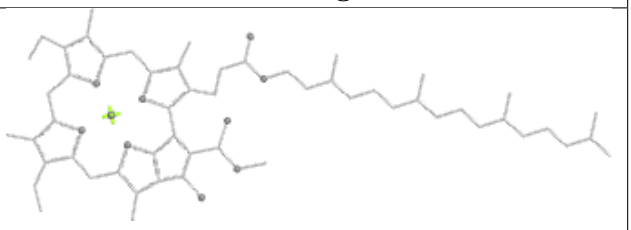
Torsions



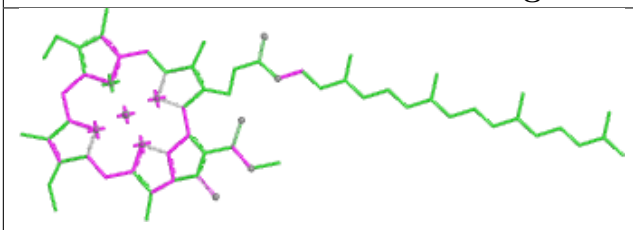
Rings

Ligand CLA b 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

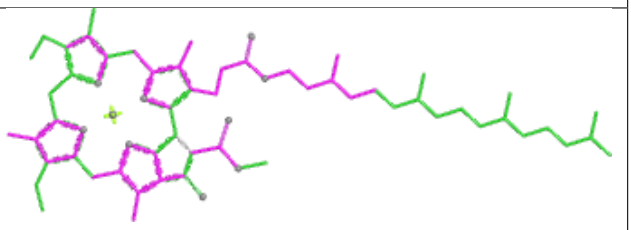
Ligand BCR l 206	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA a 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

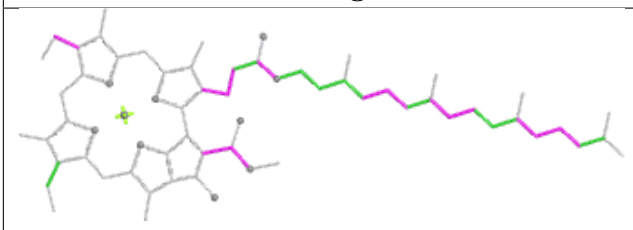
Ligand CLA A 807



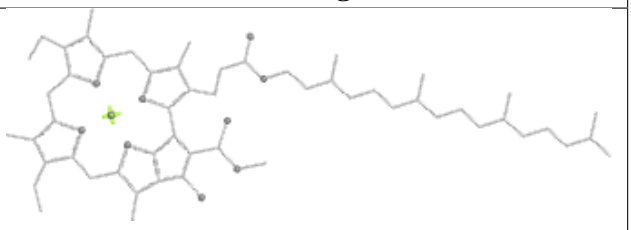
Bond lengths



Bond angles

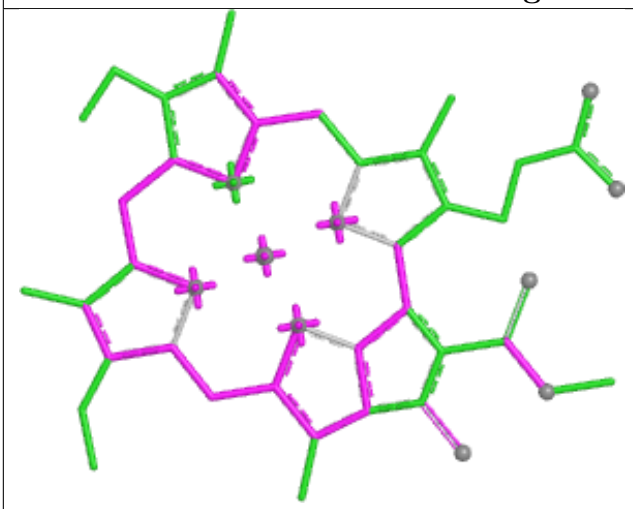


Torsions



Rings

Ligand CLA H 833



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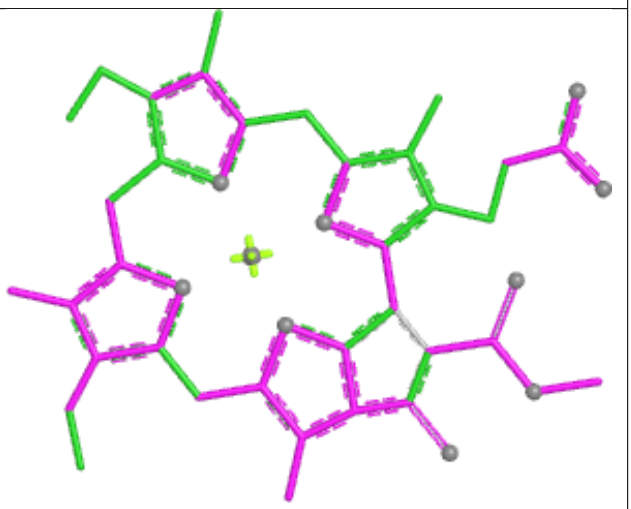
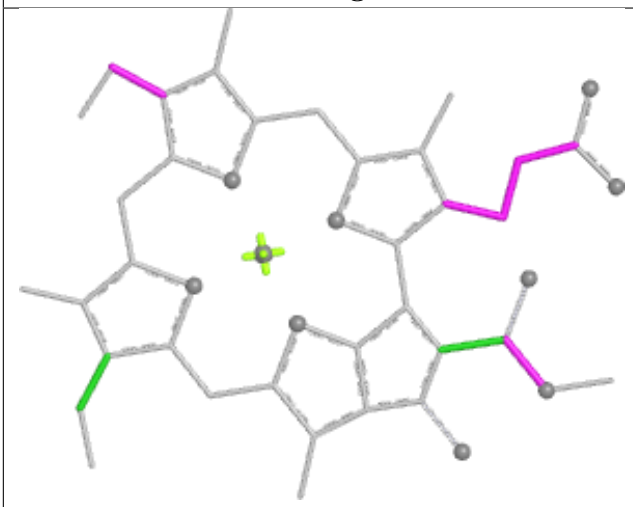


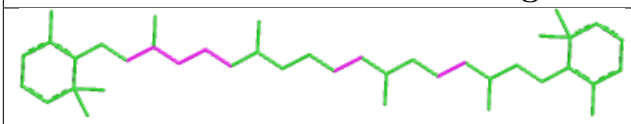
Bond angles



Torsions

Rings

Ligand BCR H 849



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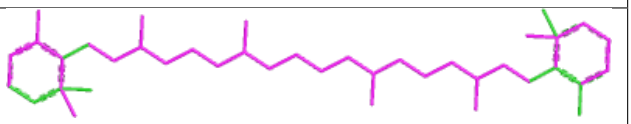
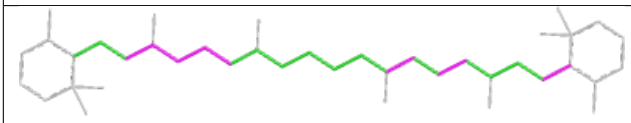
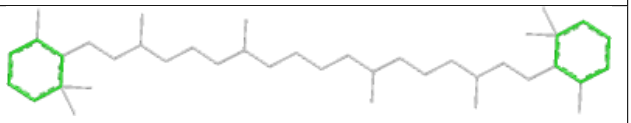


Bond angles

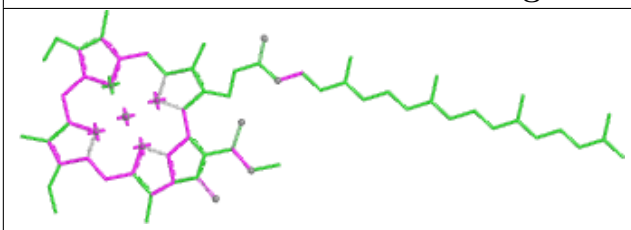


Torsions



Rings

Ligand CLA G 824



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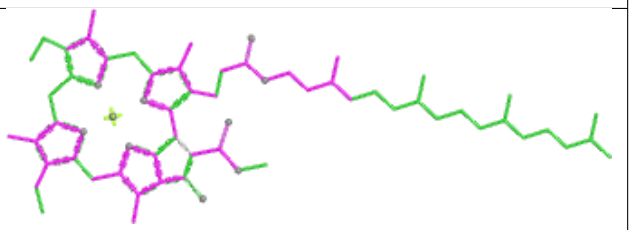
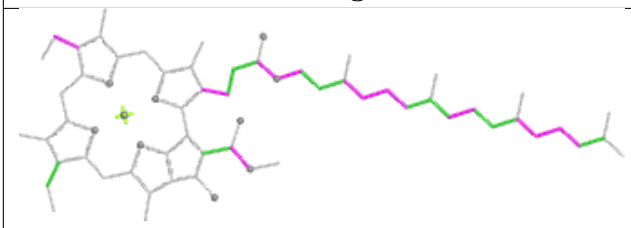
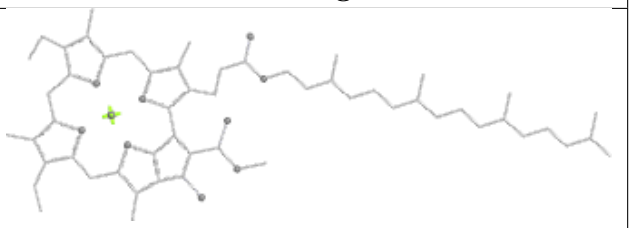


Bond angles

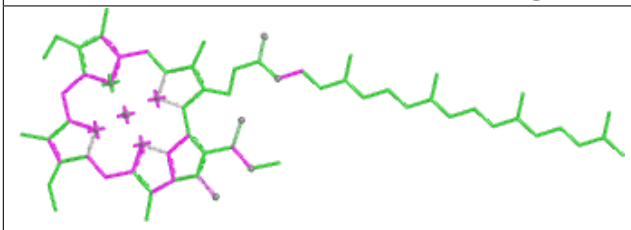


Torsions



Rings

Ligand CL0 G 801



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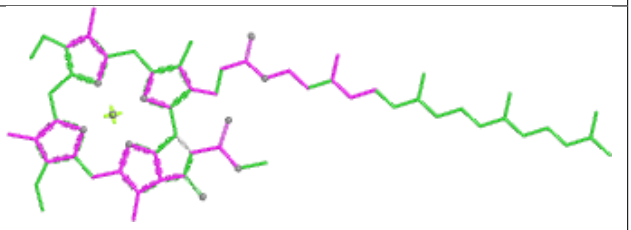
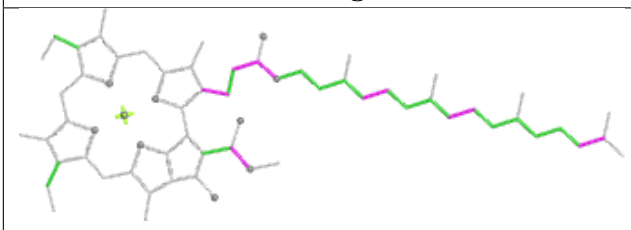
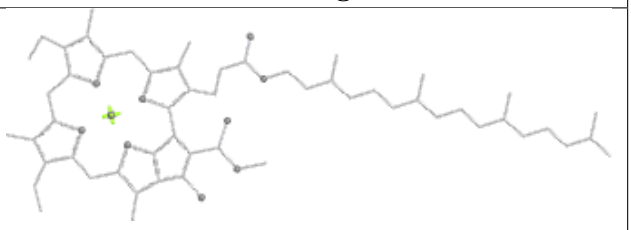


Bond angles

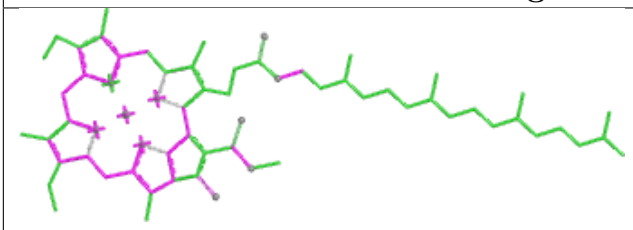


Torsions

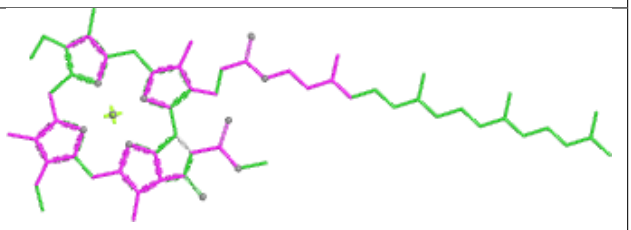


Rings

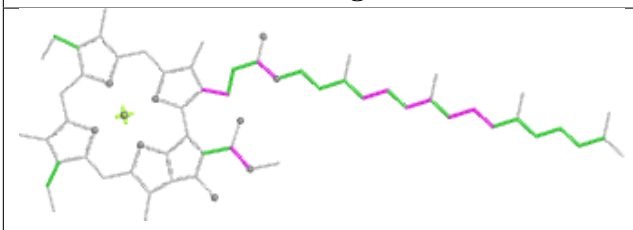
Ligand CLA b 818



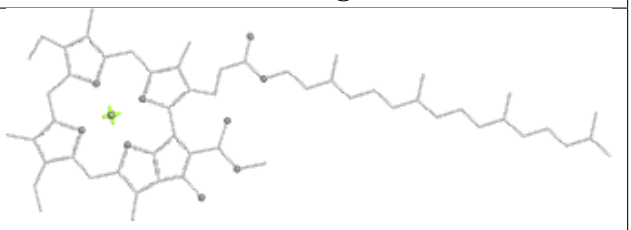
Bond lengths



Bond angles

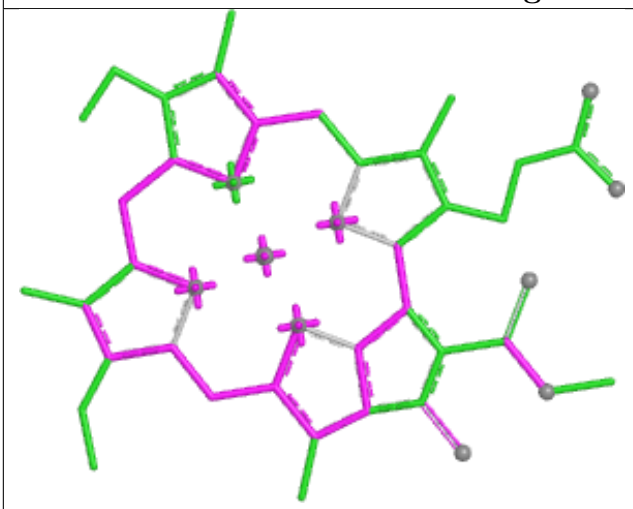


Torsions



Rings

Ligand CLA A 837



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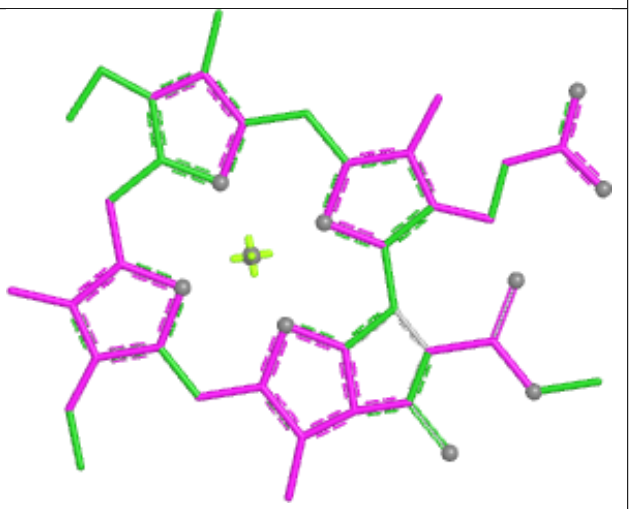
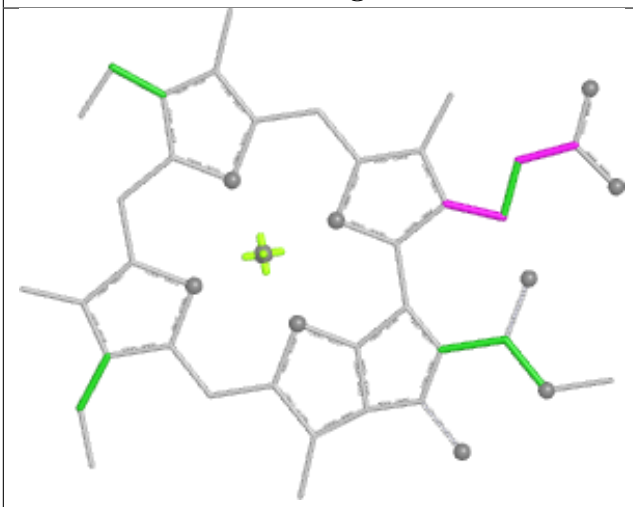
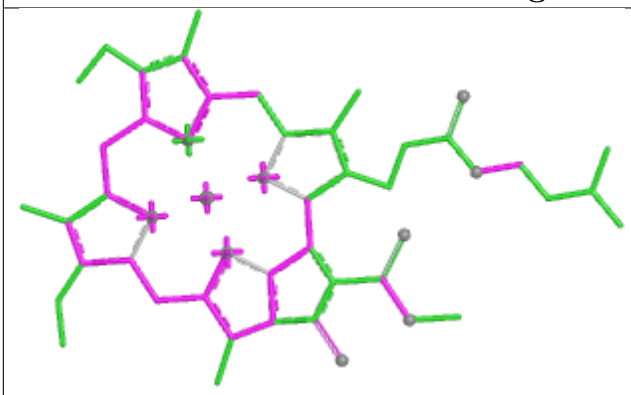
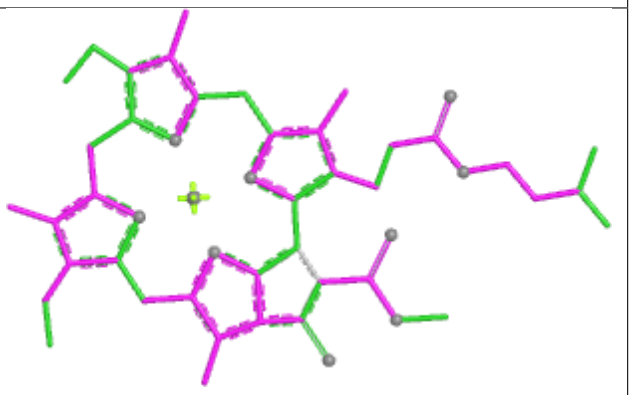
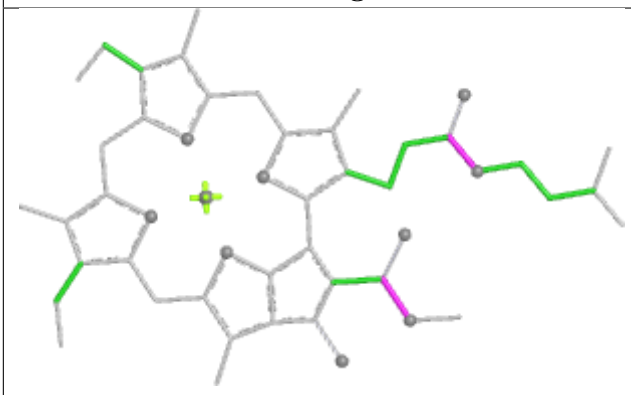
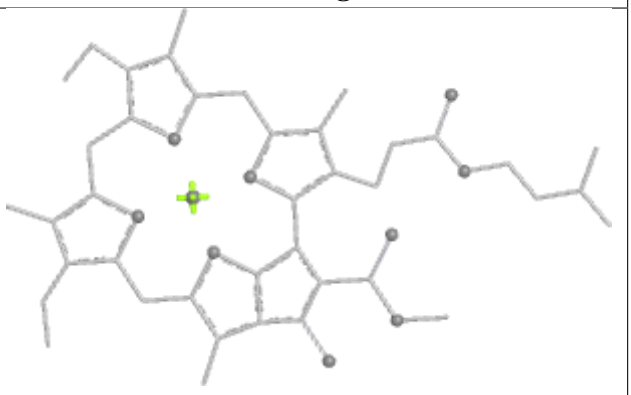


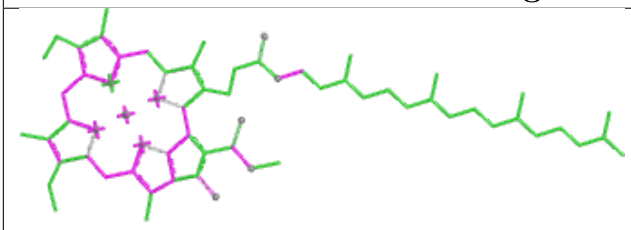
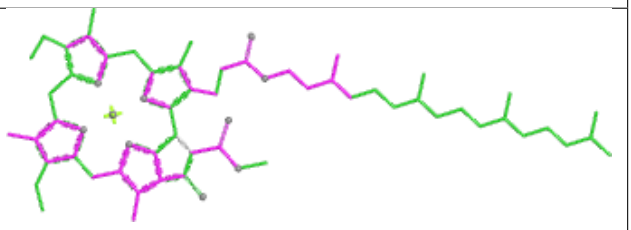
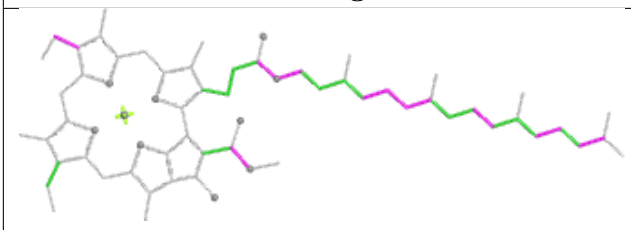
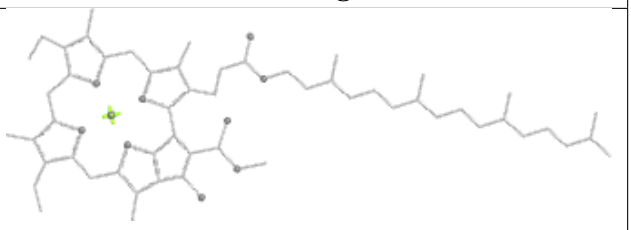
Bond angles



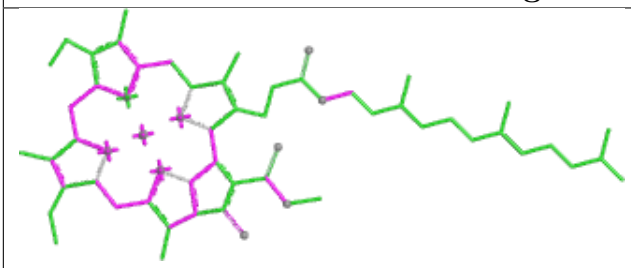
Torsions

Rings

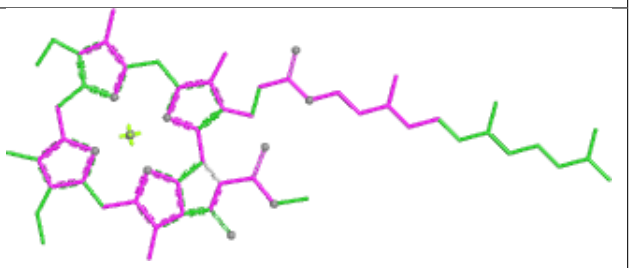
Ligand CLA a 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

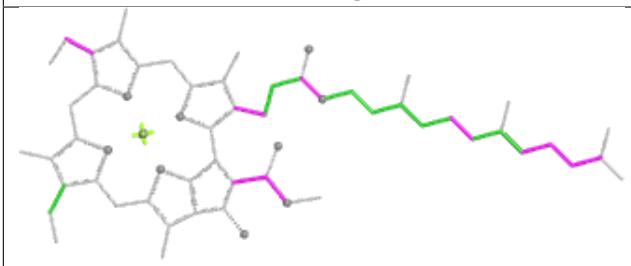
Ligand CLA H 838



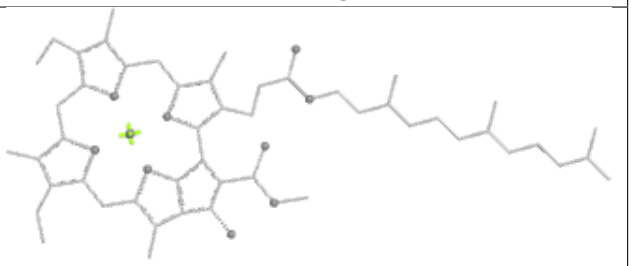
Bond lengths



Bond angles

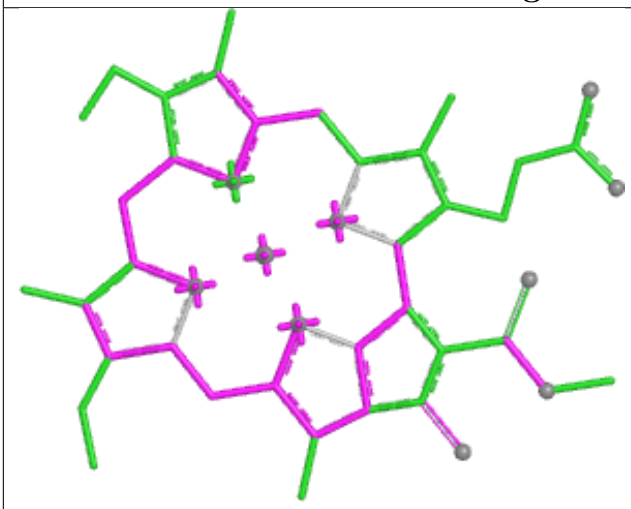


Torsions

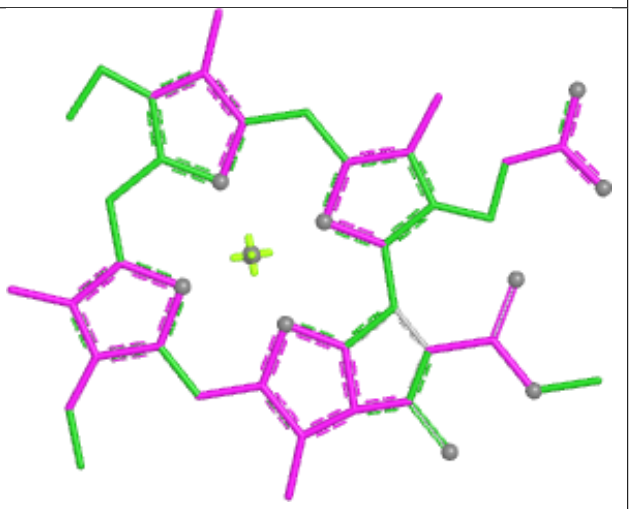


Rings

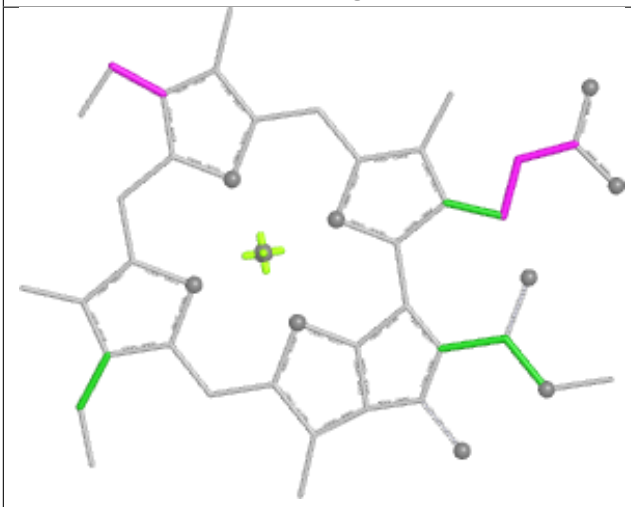
Ligand CLA G 834



Bond lengths

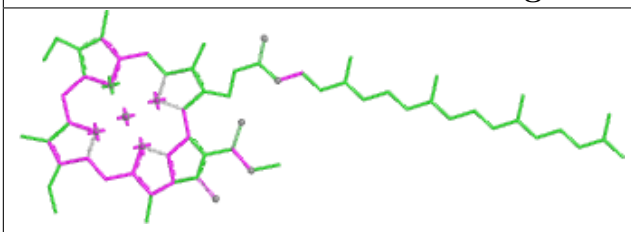
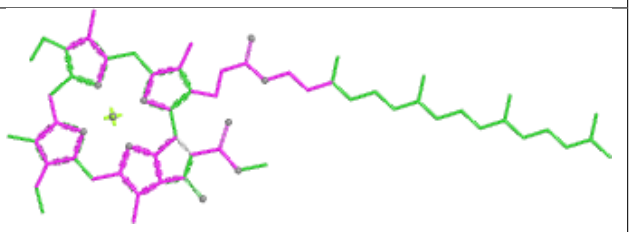
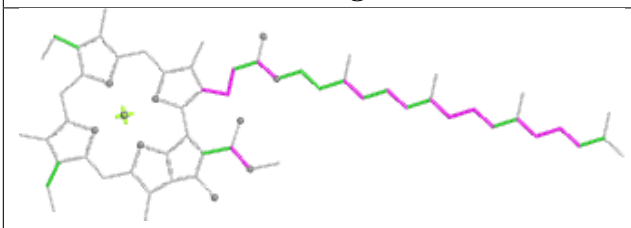
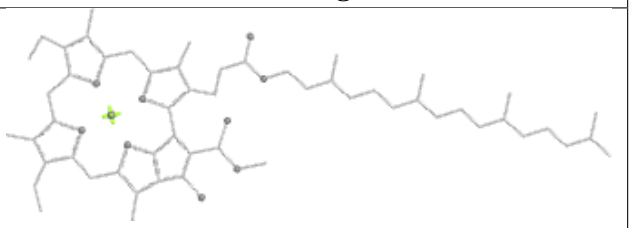


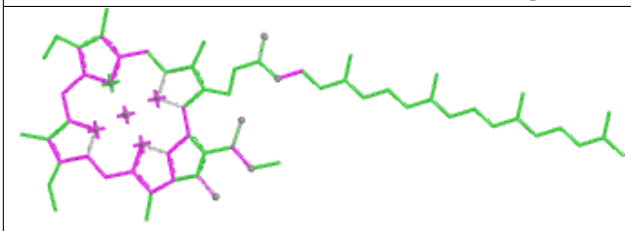
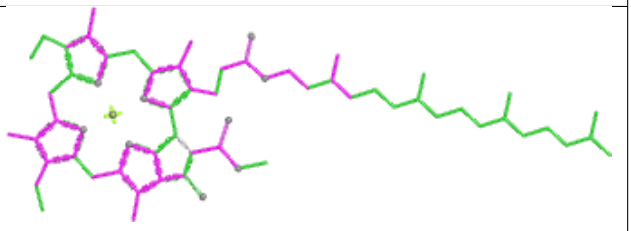
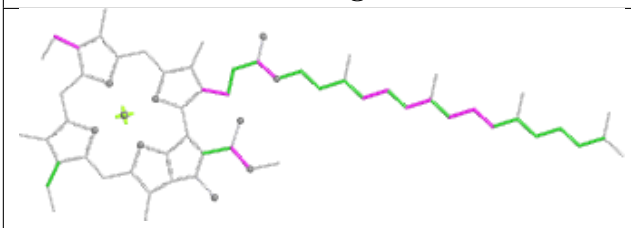
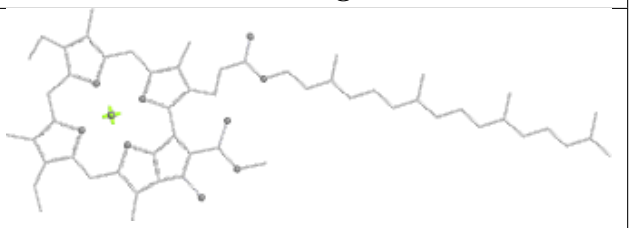
Bond angles



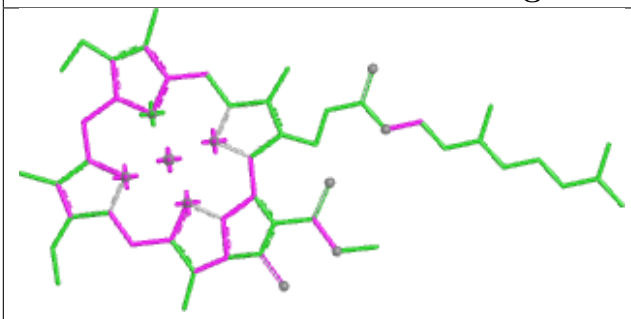
Torsions

Rings

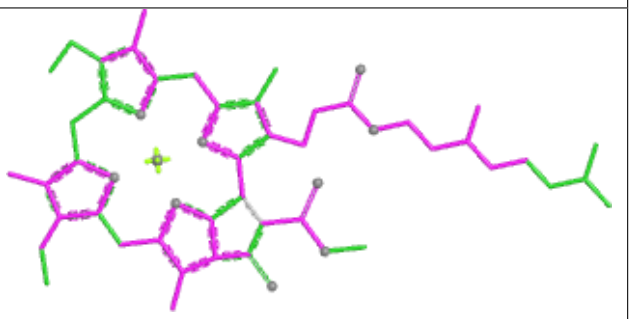
Ligand CLA B 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

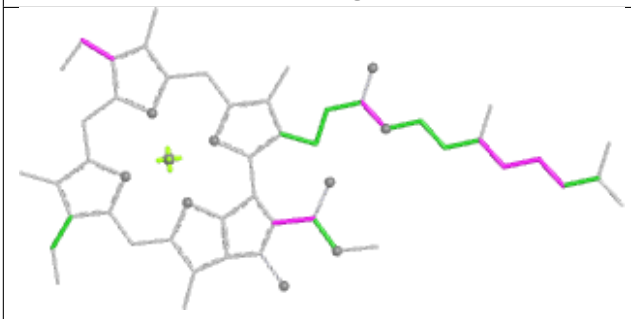
Ligand CLA A 803



Bond lengths



Bond angles



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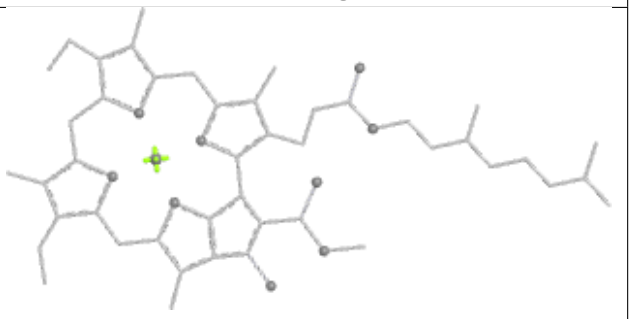
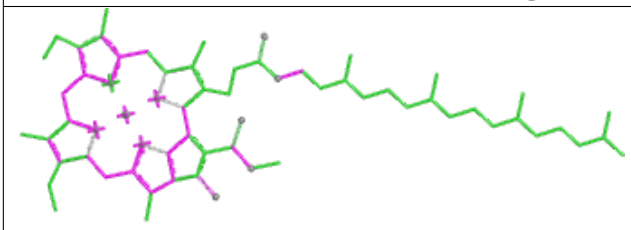


Rings

Ligand CLA G 825



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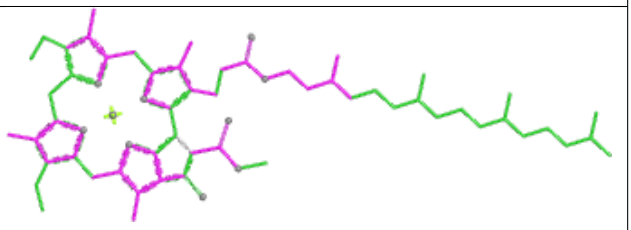
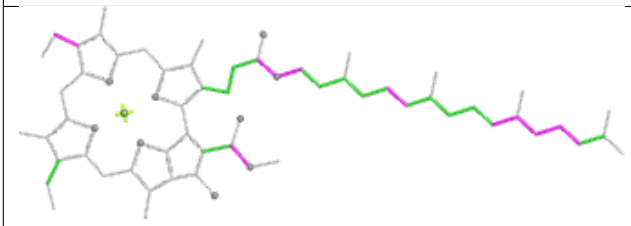


Bond angles



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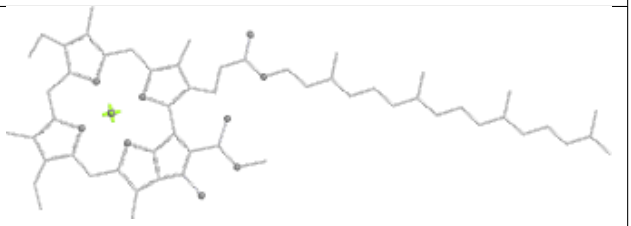
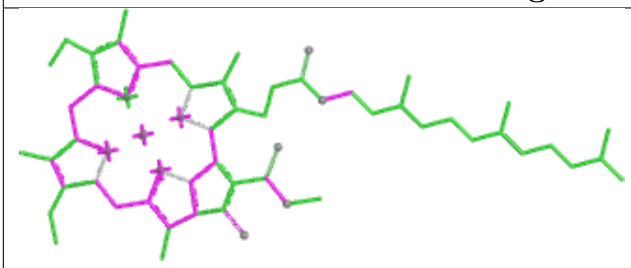
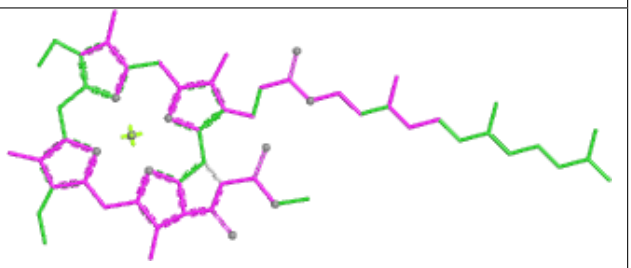
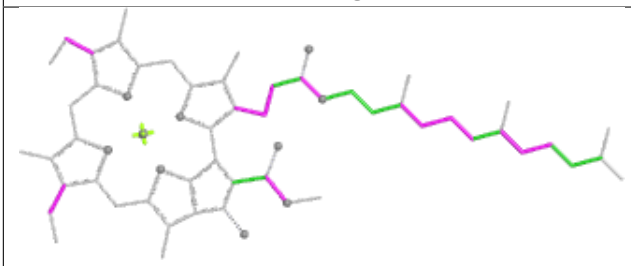
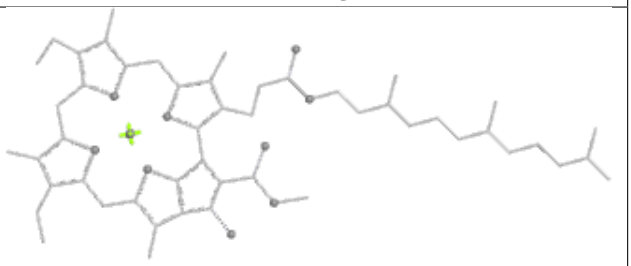
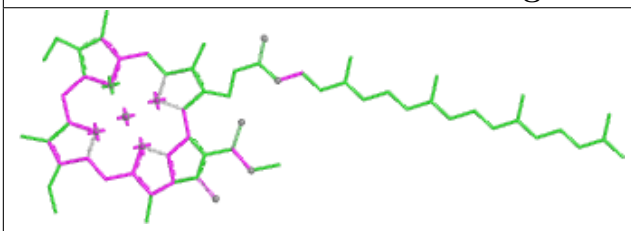
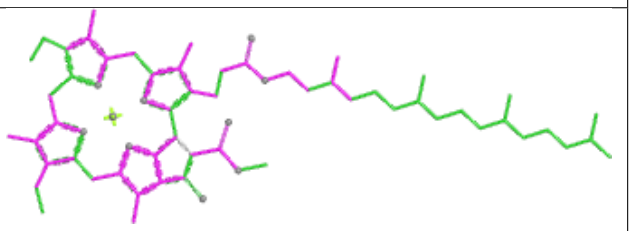
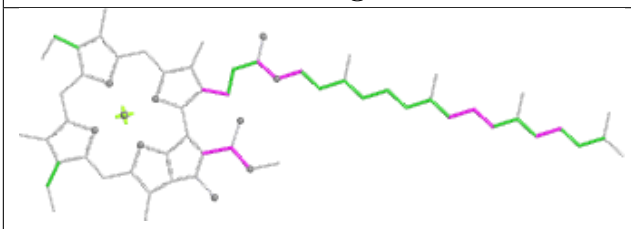
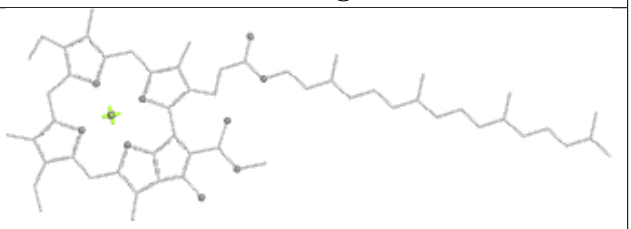
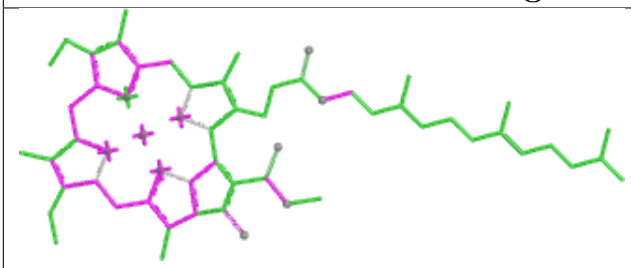
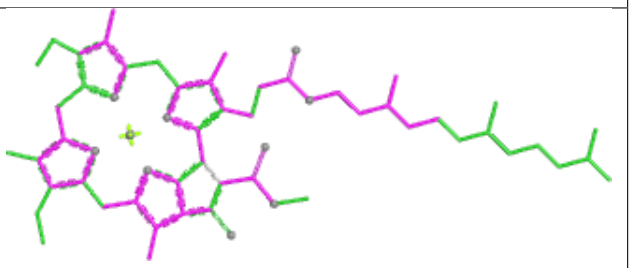
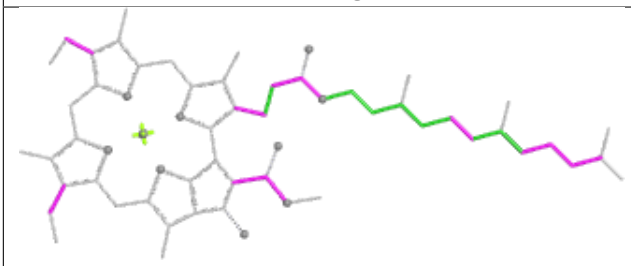
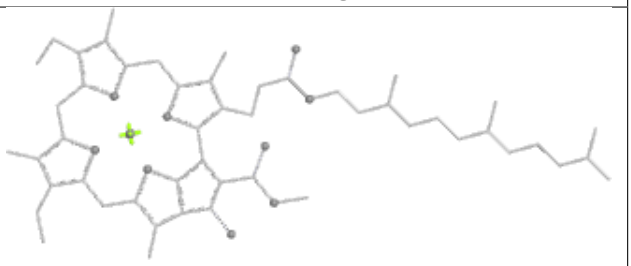
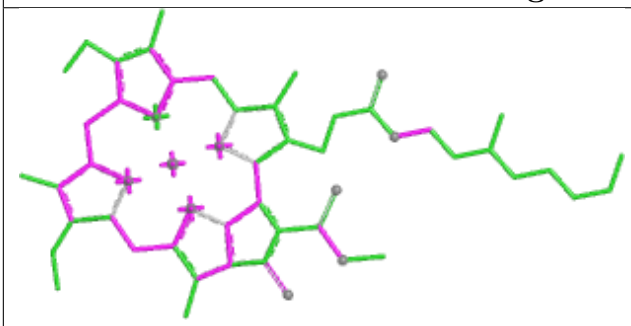
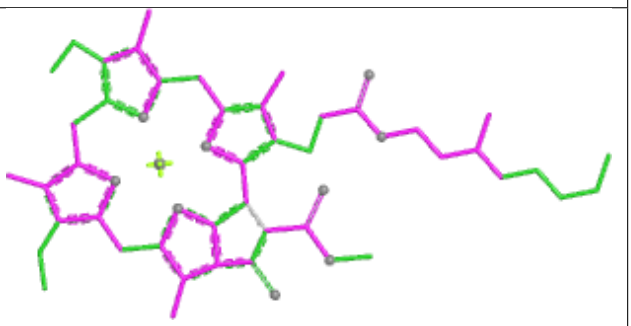
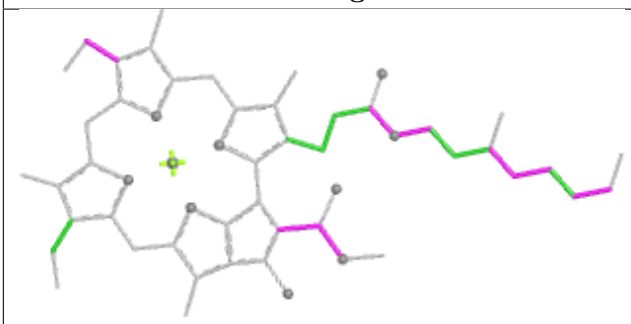
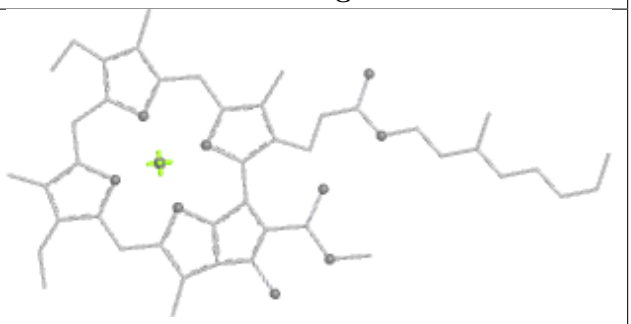


Rings

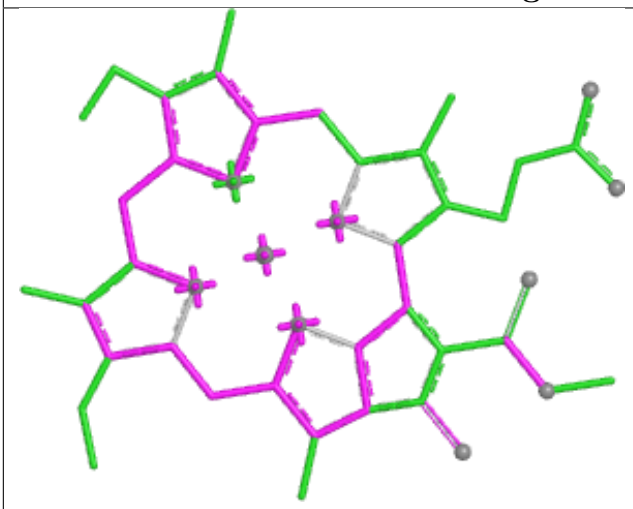
Ligand CLA a 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

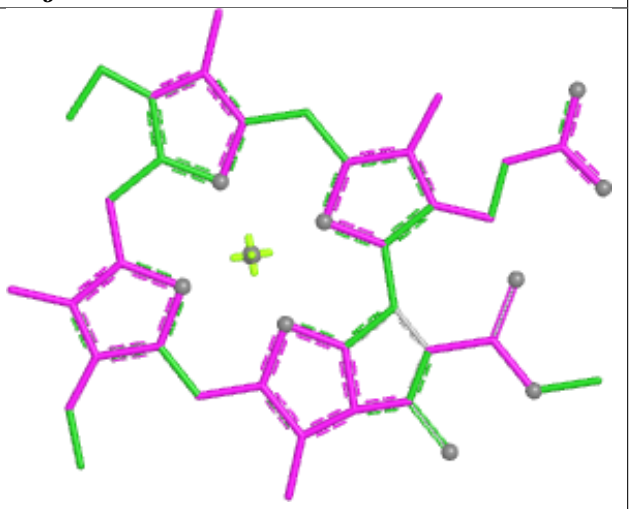
Ligand CLA B 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

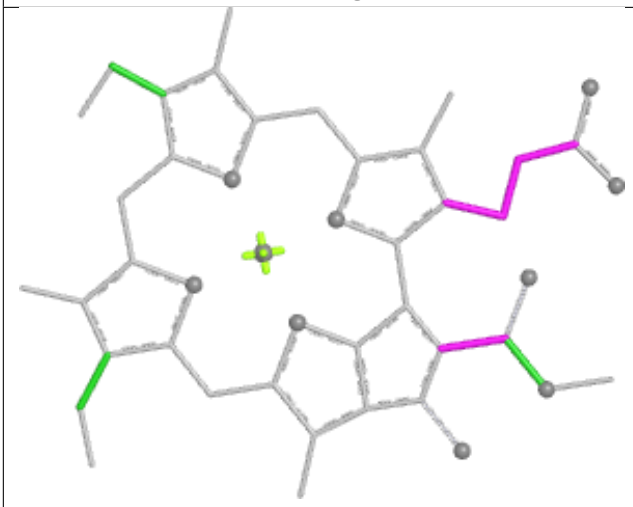
Ligand CLA j 1302



Bond lengths



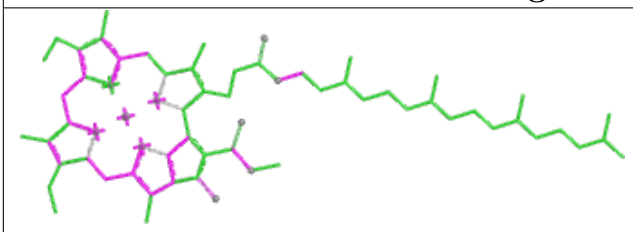
Bond angles



Torsions

Rings

Ligand CLA a 805



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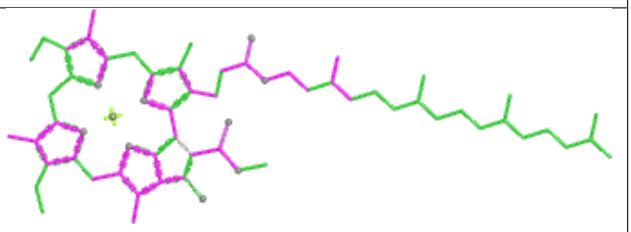
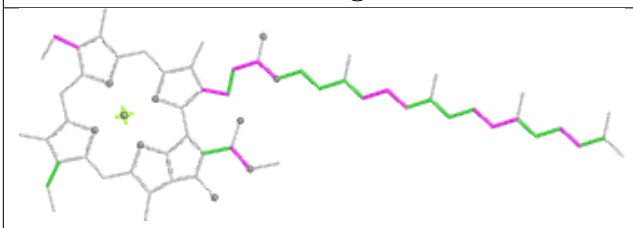
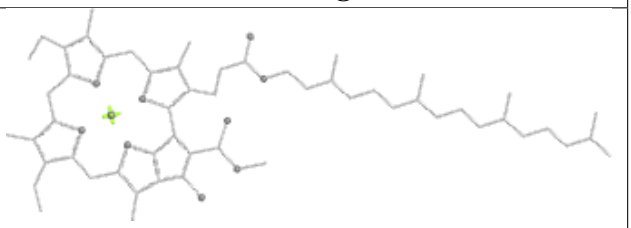


Bond angles

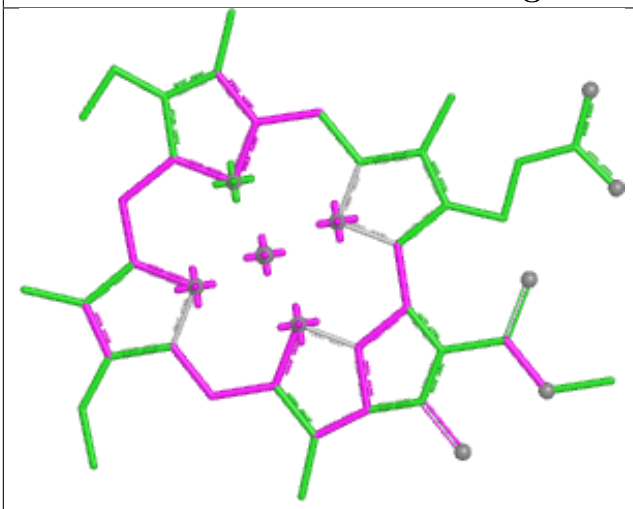


Torsions



Rings

Ligand CLA H 832



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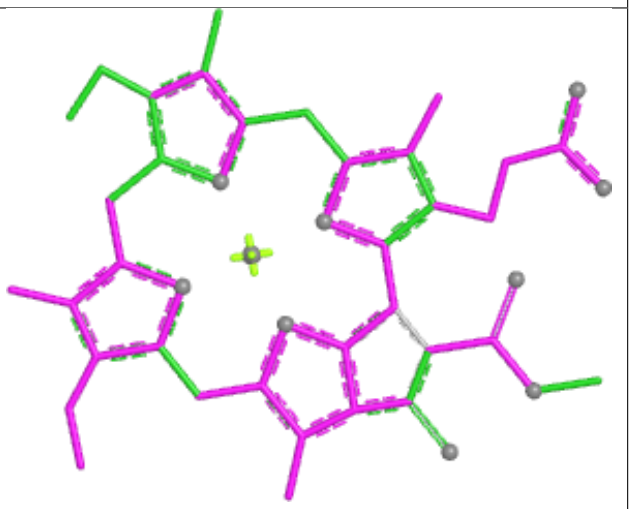
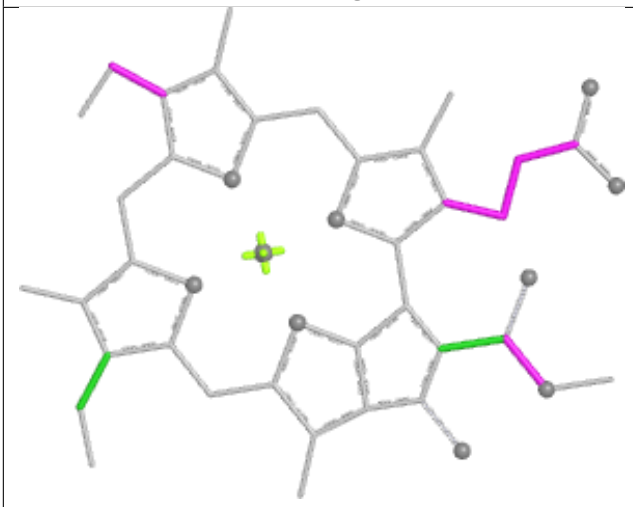
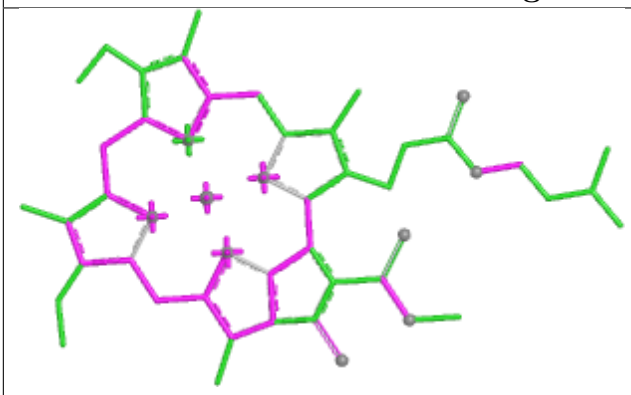
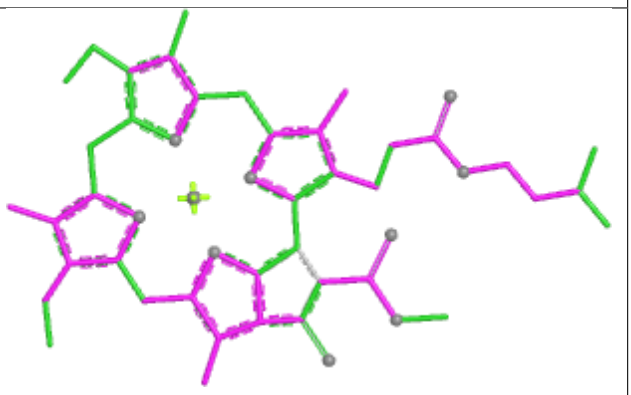
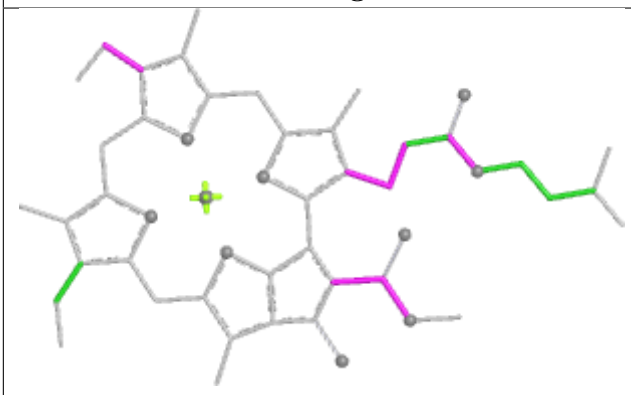
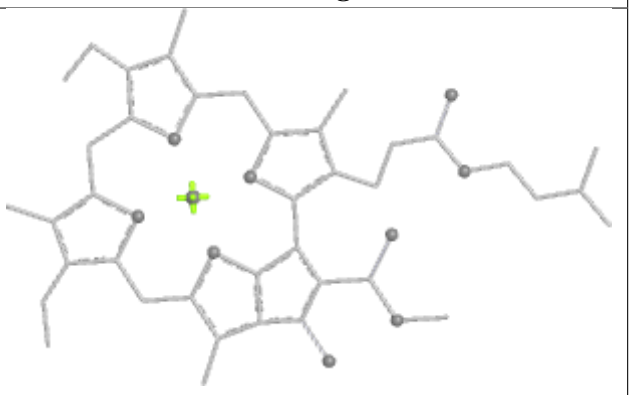


Bond angles



Torsions

Rings

Ligand CLA G 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

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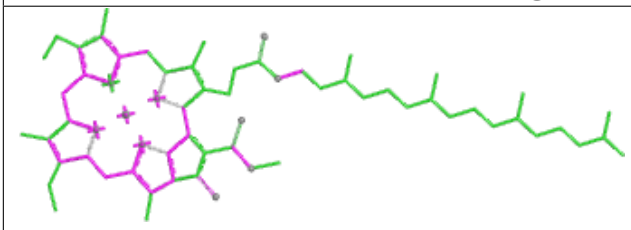
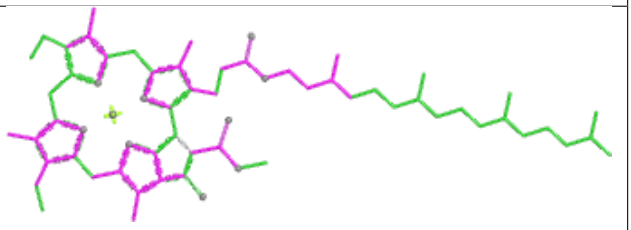
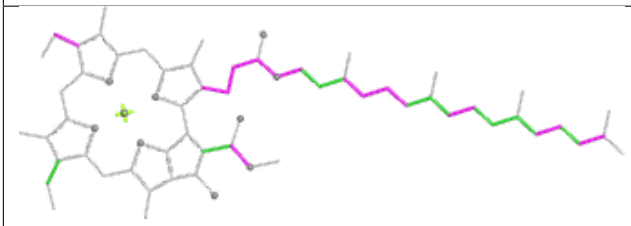
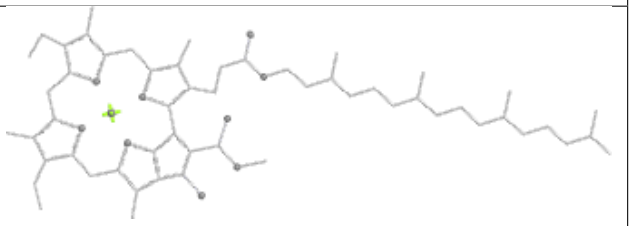
 Bond lengths	 Bond angles
 Torsions	 Rings

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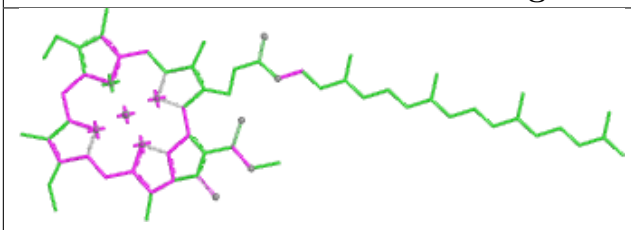
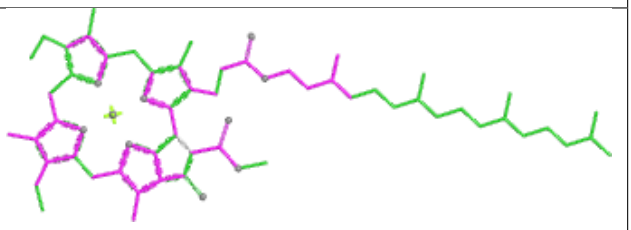
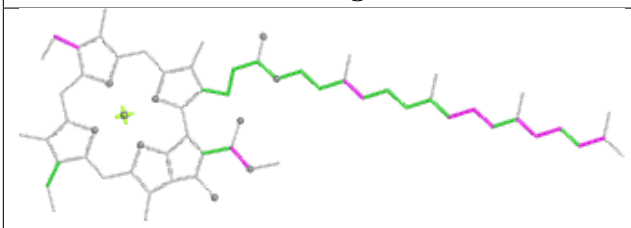
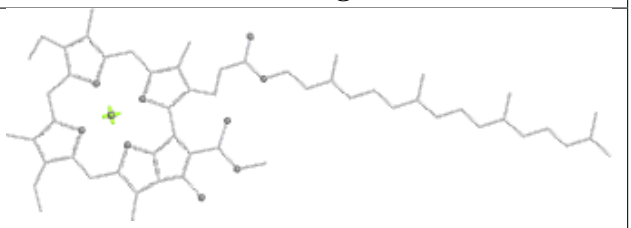
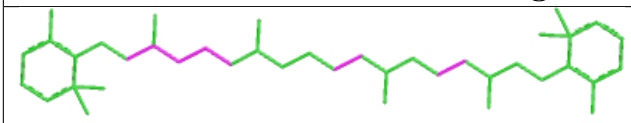
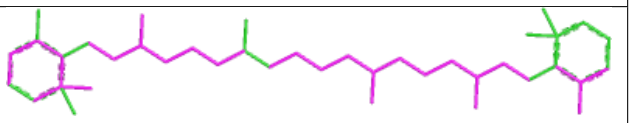
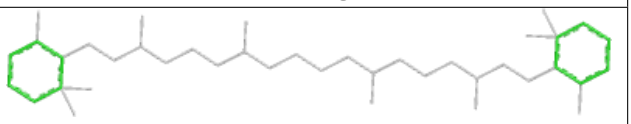
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR i 101	
 Bond lengths	 Bond angles
Torsions	 Rings

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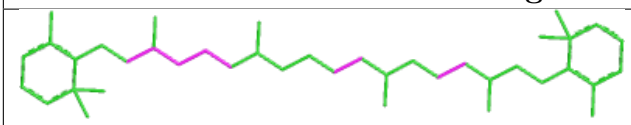
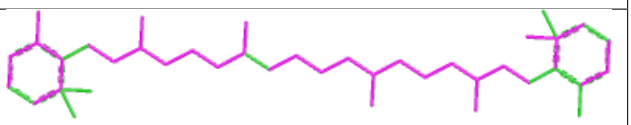
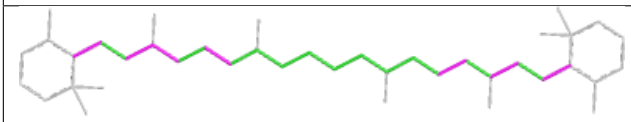
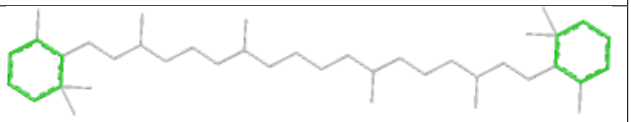
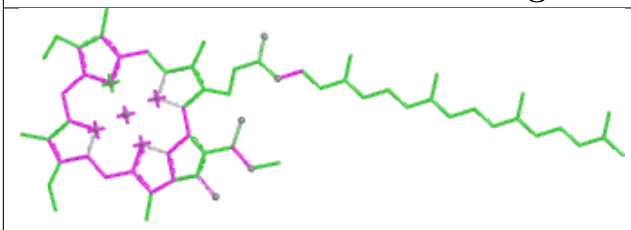
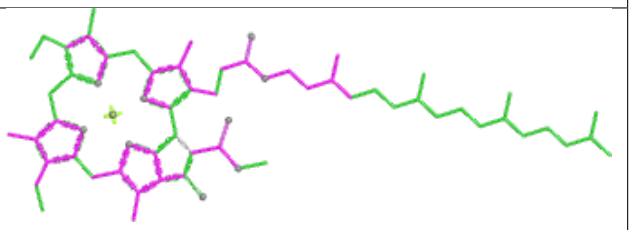
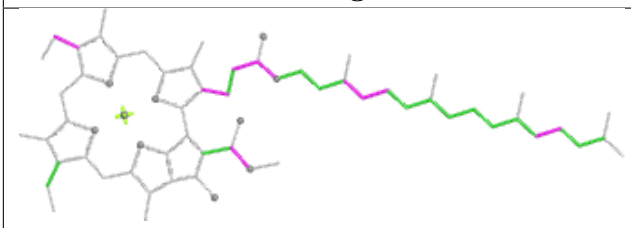
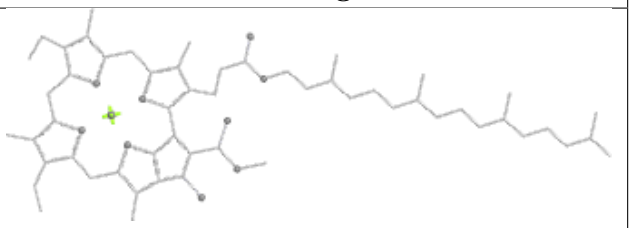
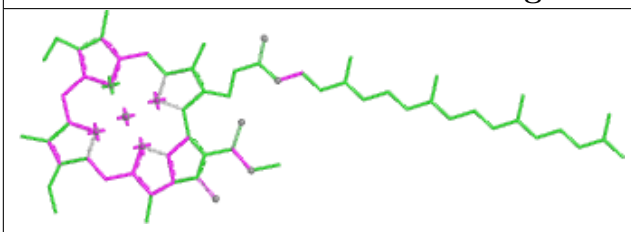
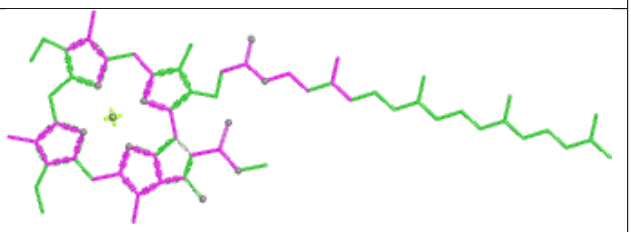
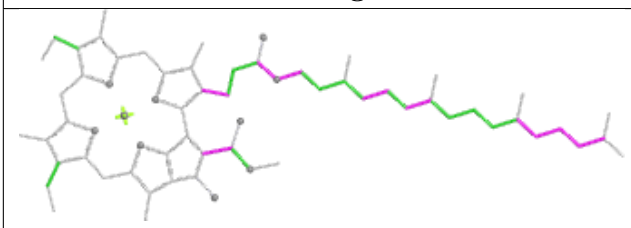
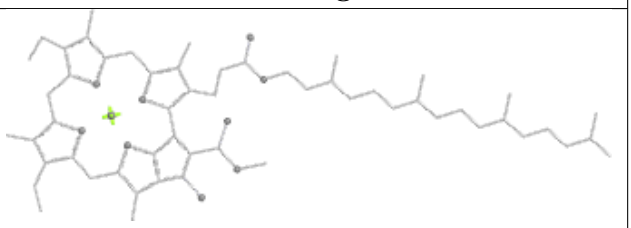
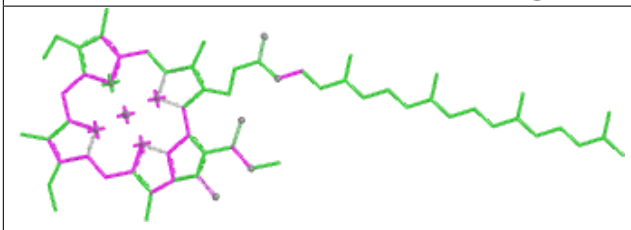
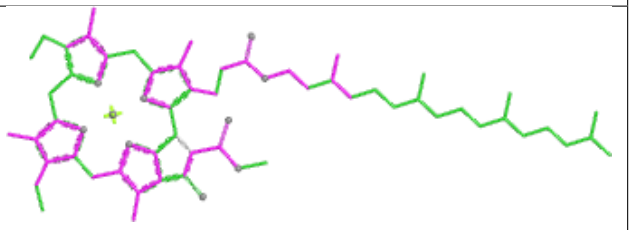
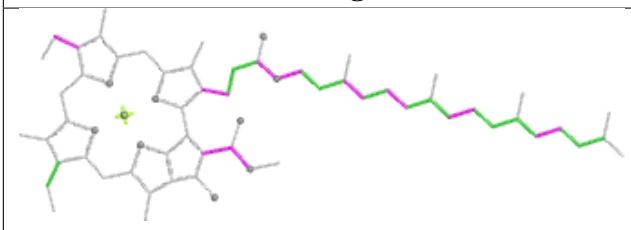
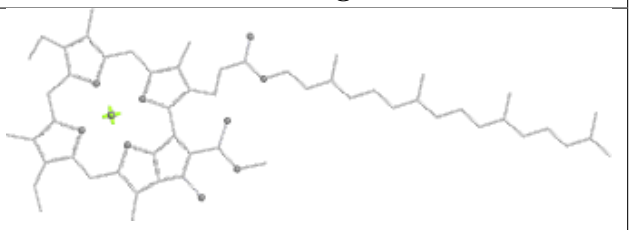
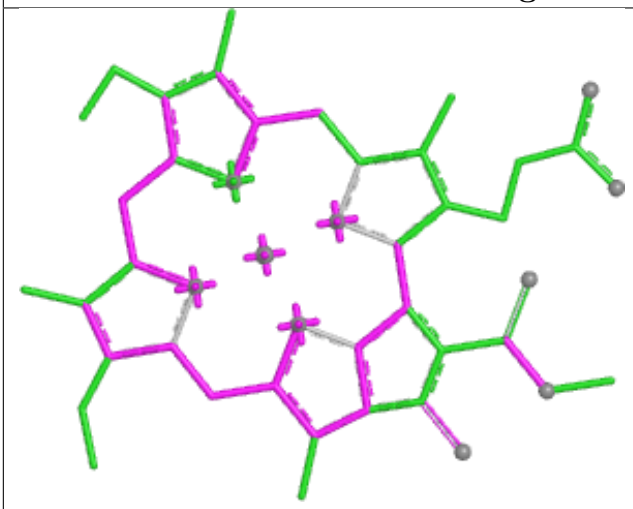
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

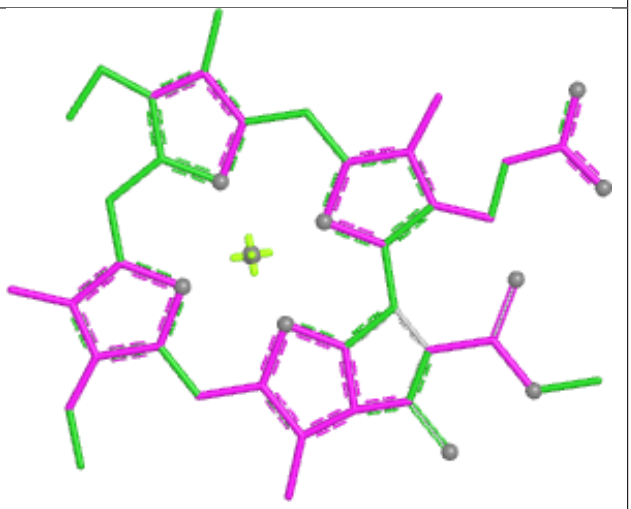
Ligand CLA B 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

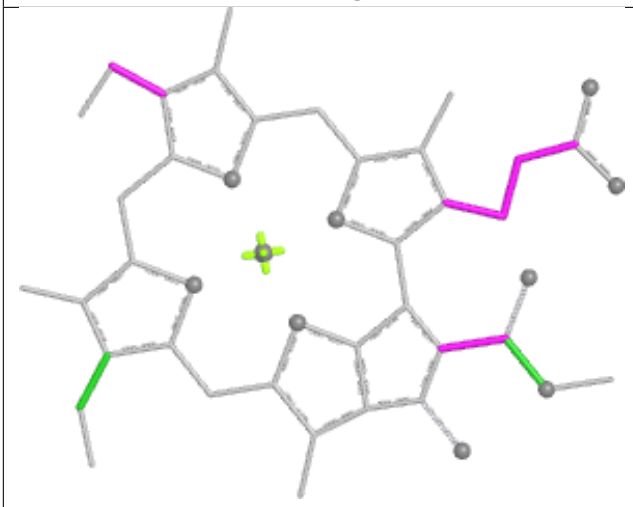
Ligand CLA J 1302



Bond lengths



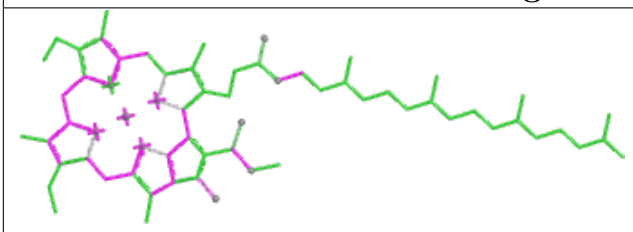
Bond angles



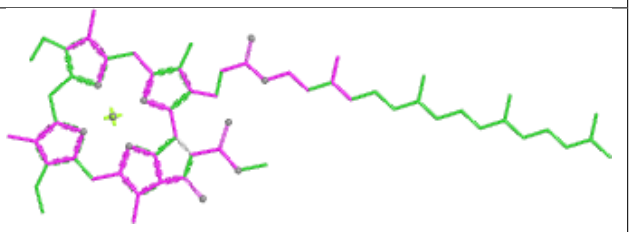
Torsions

Rings

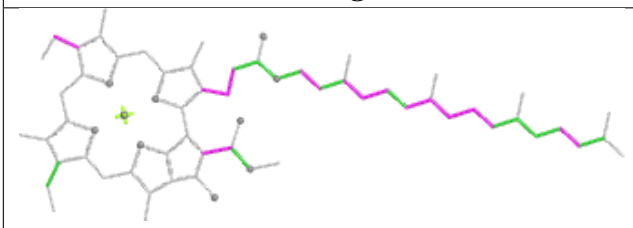
Ligand CLA H 805



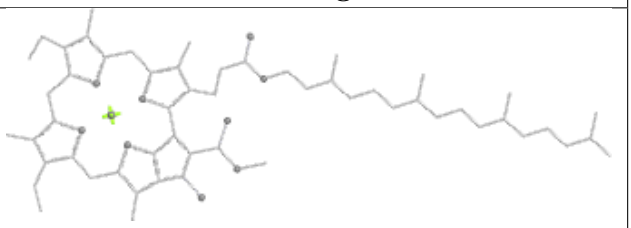
Bond lengths



Bond angles

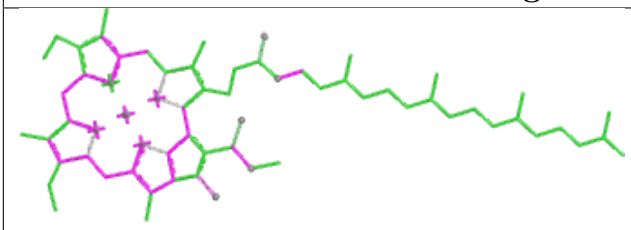


Torsions

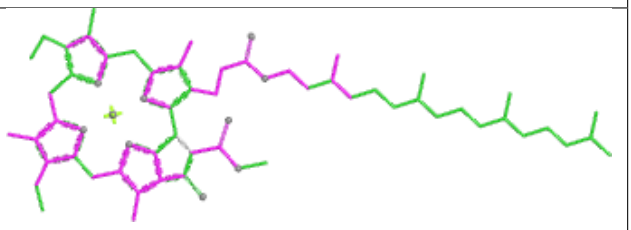


Rings

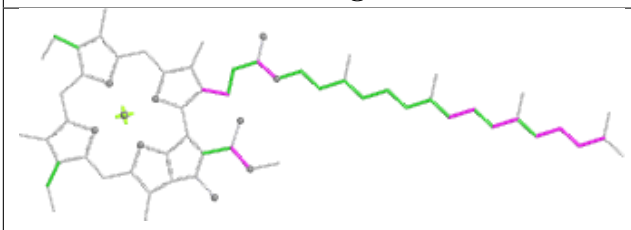
Ligand CLA G 818



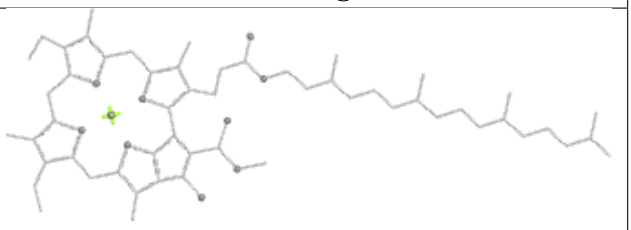
Bond lengths



Bond angles

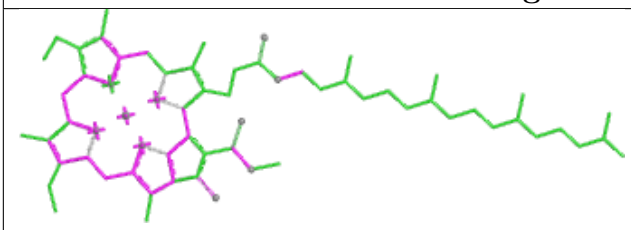


Torsions

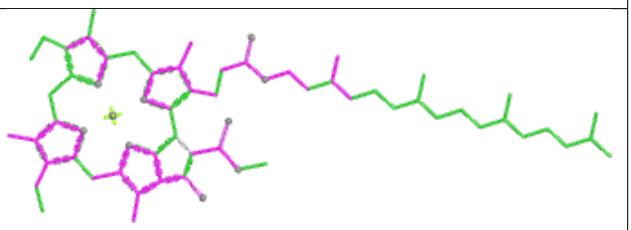


Rings

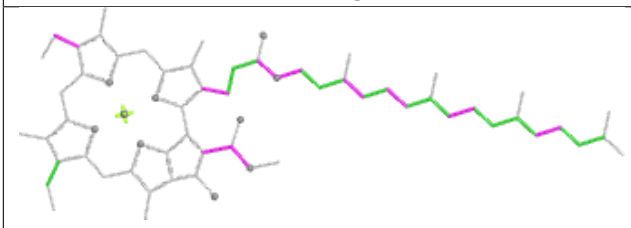
Ligand CLA G 802



Bond lengths



Bond angles



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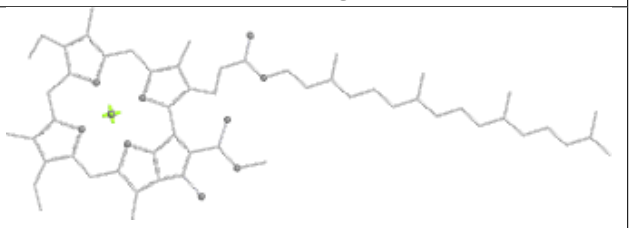
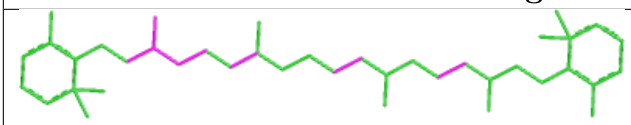


Rings

Ligand BCR b 845



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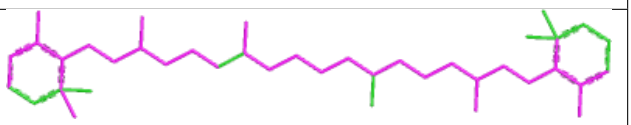
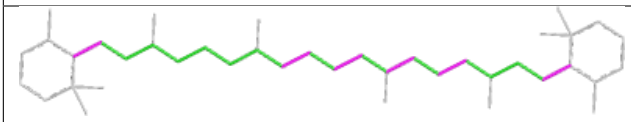


Bond angles



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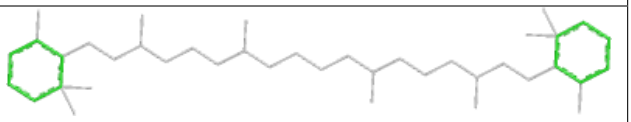
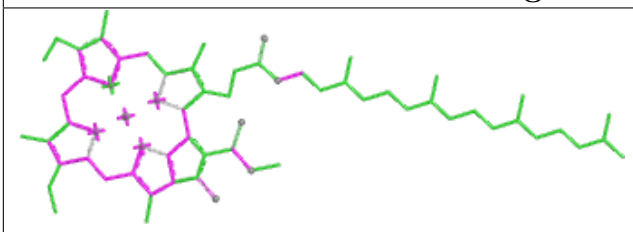


Rings

Ligand CLA B 841



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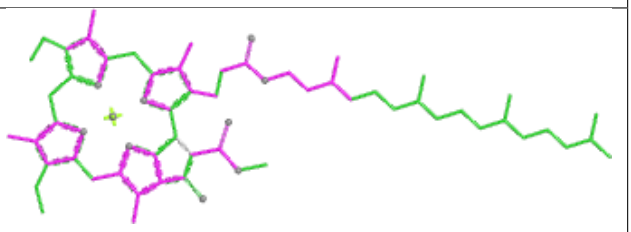
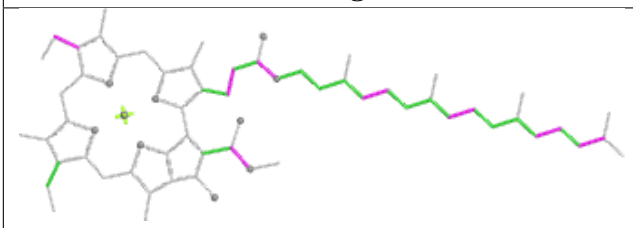


Bond angles



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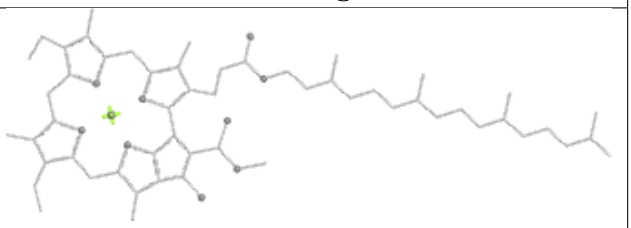
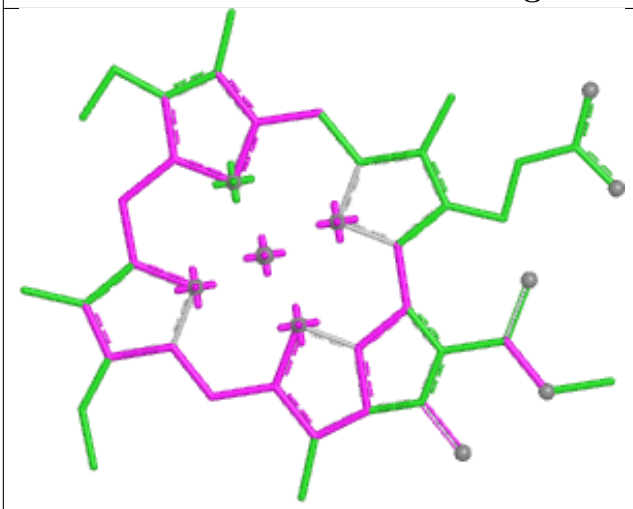


Rings

Ligand CLA A 813



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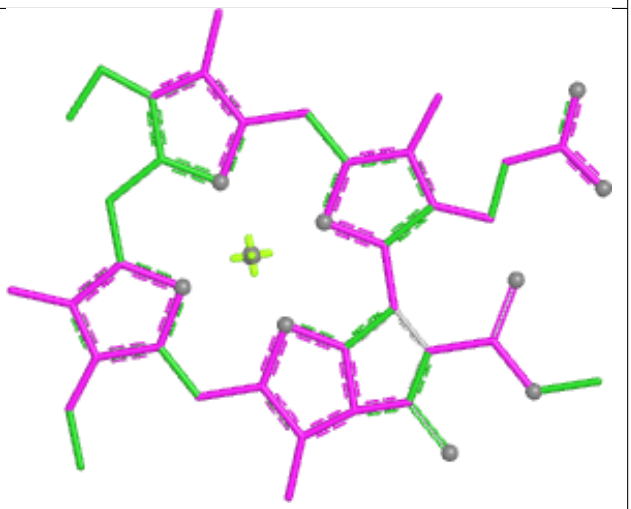
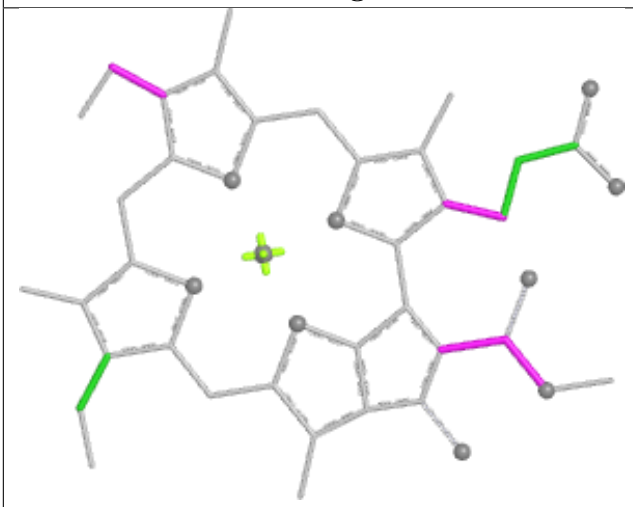
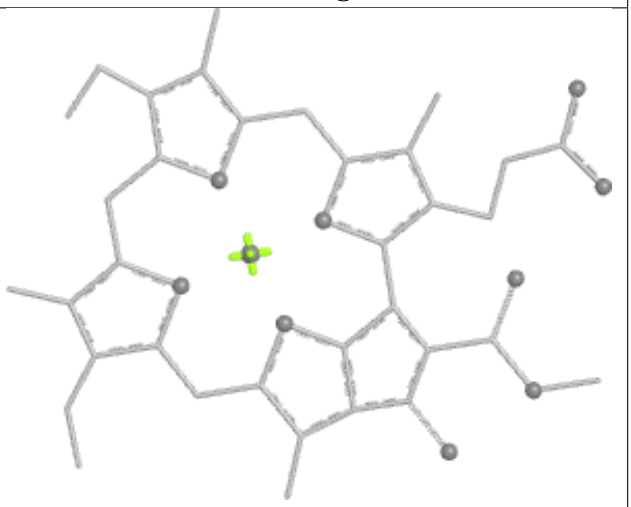


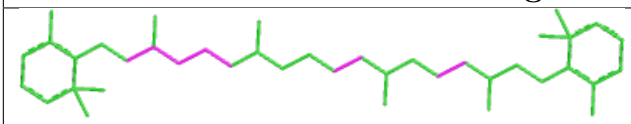
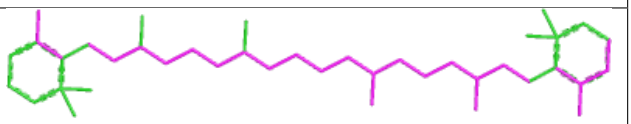
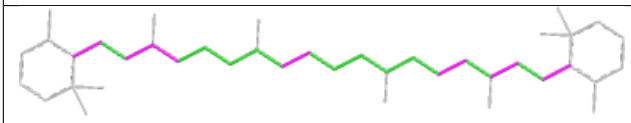
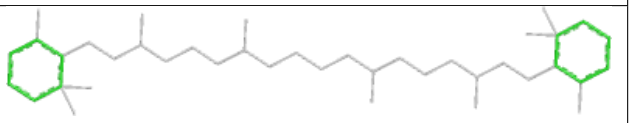
Bond angles



Torsions



Rings

Ligand BCR L 207	
 Bond lengths	 Bond angles
 Torsions	 Rings

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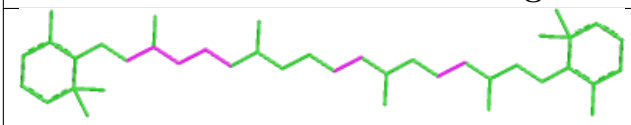
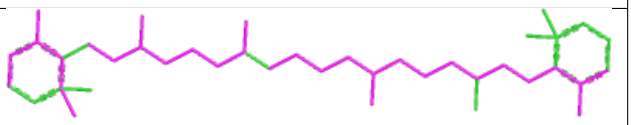
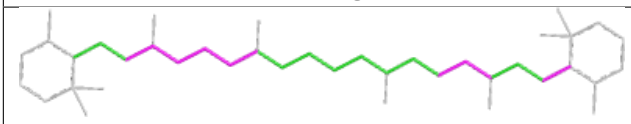
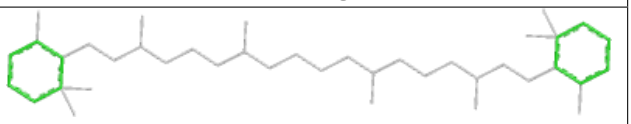
 Bond lengths	 Bond angles
 Torsions	 Rings

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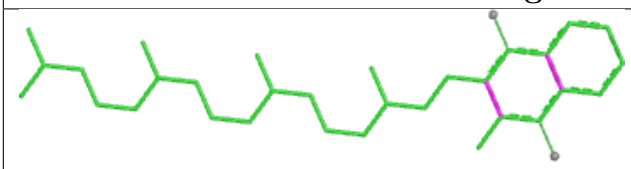
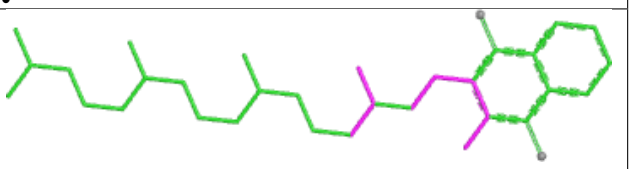
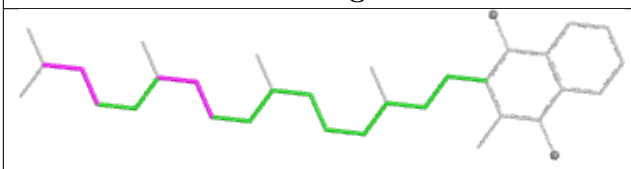
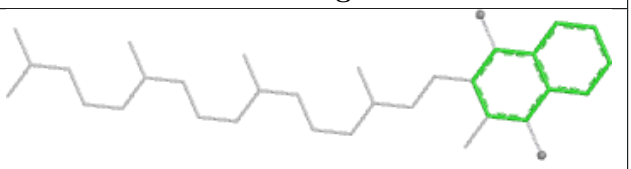
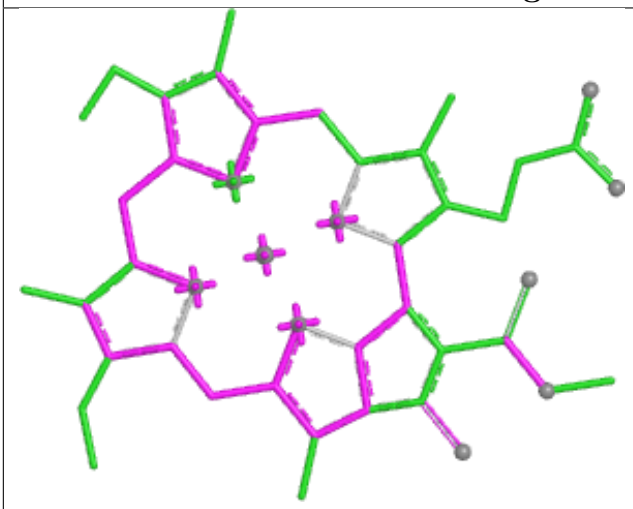
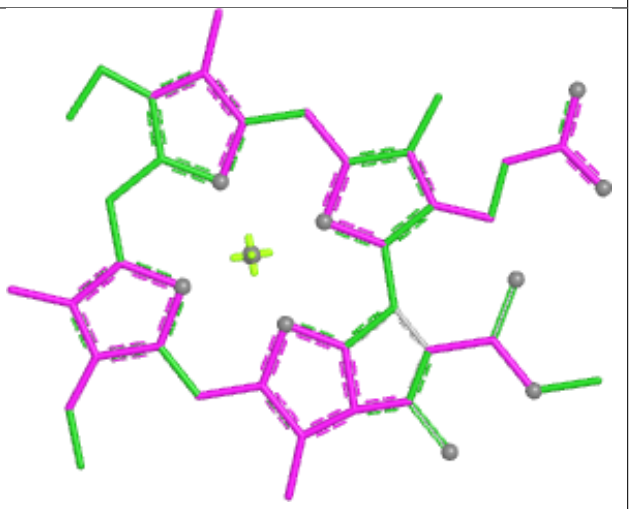
 Bond lengths	 Bond angles
 Torsions	 Rings

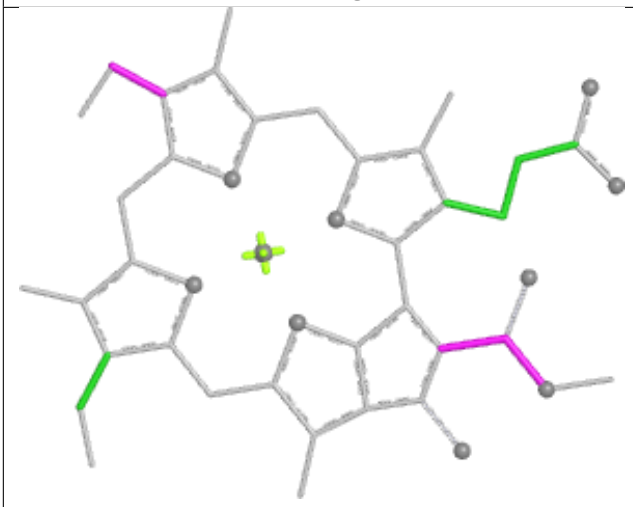
Ligand CLA H 835



Bond lengths



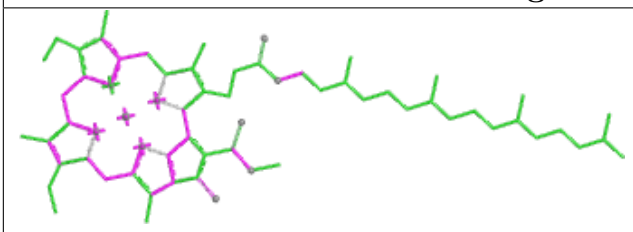
Bond angles



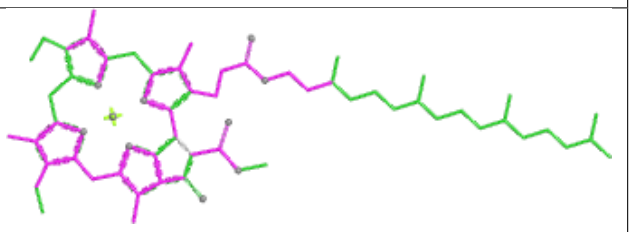
Torsions

Rings

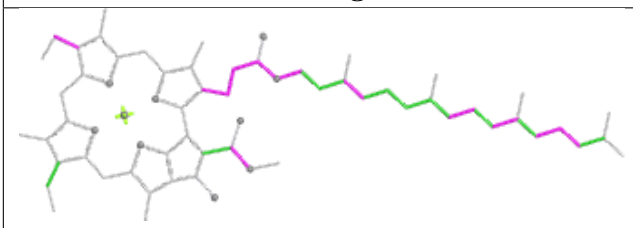
Ligand CLA b 826



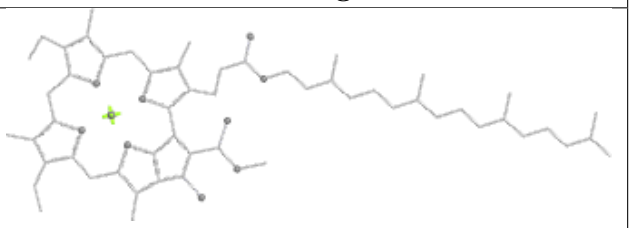
Bond lengths



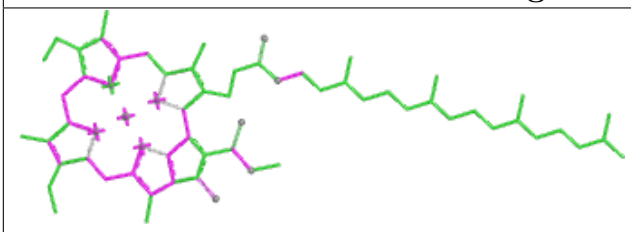
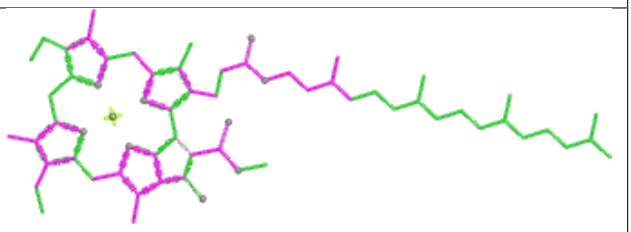
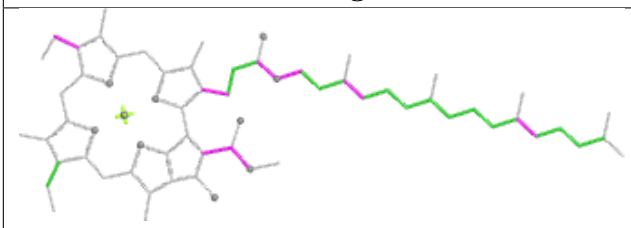
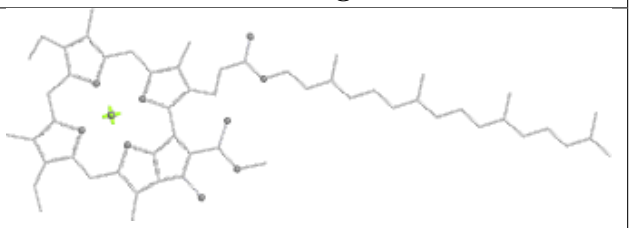
Bond angles

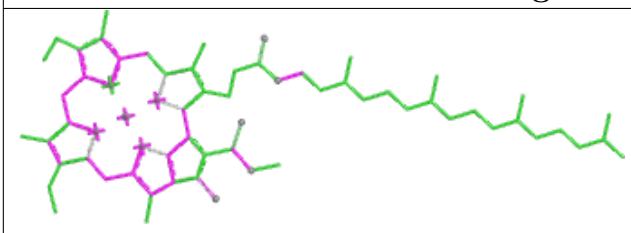
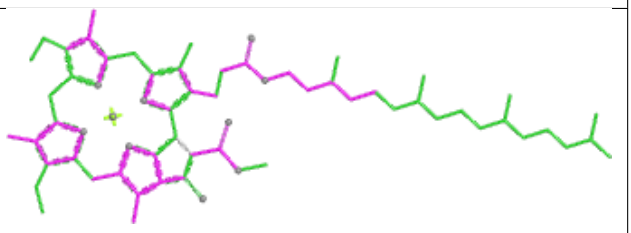
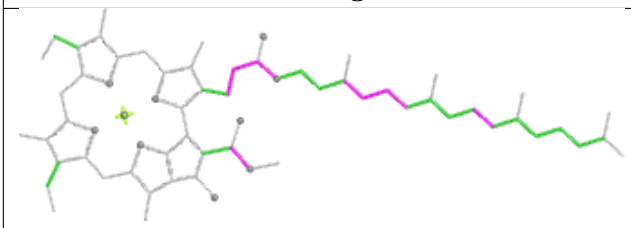
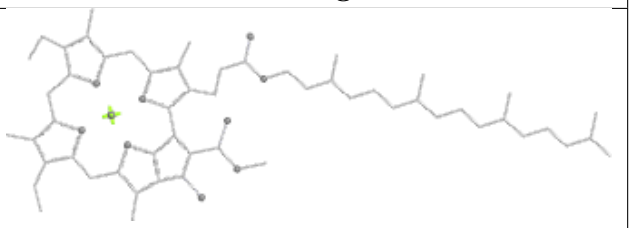


Torsions



Rings

Ligand CLA b 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA l 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

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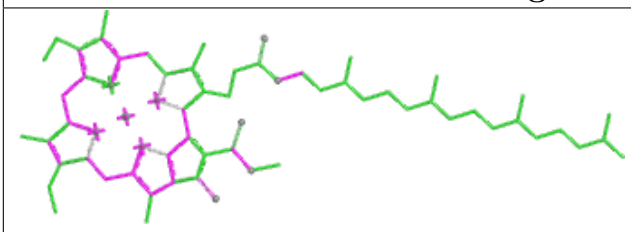
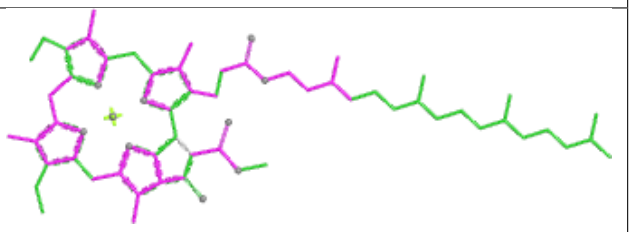
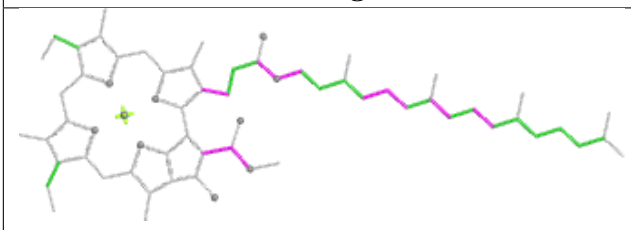
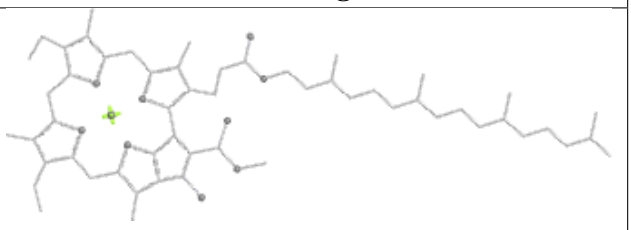
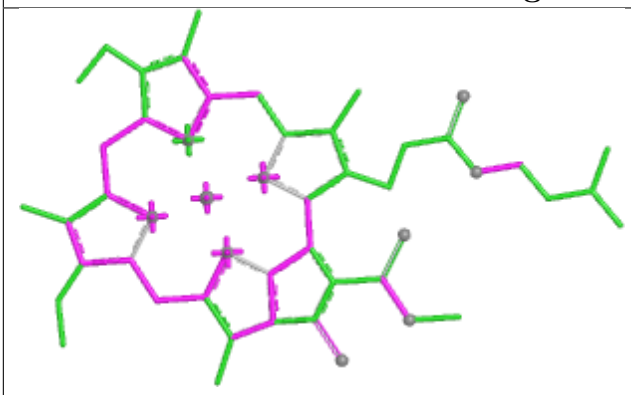
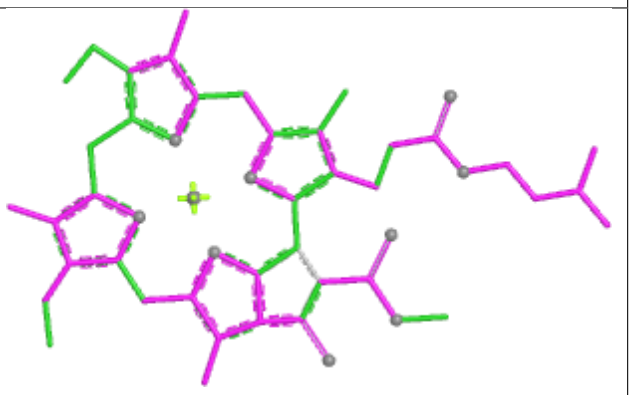
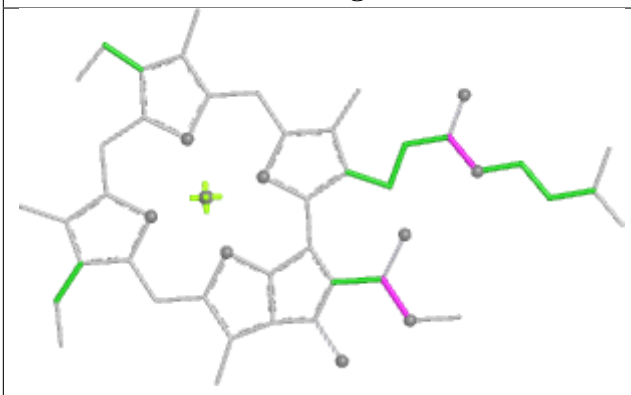
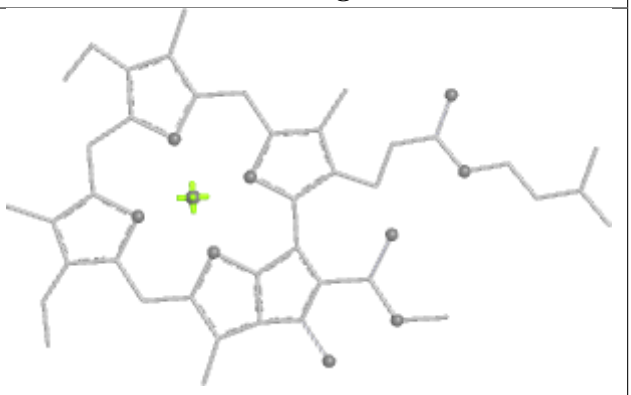
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

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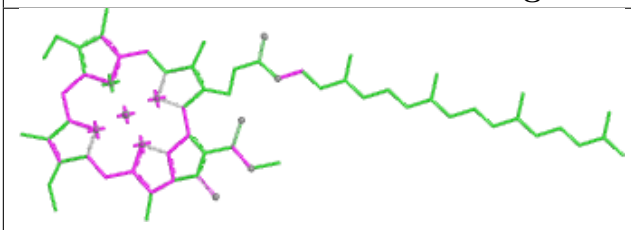
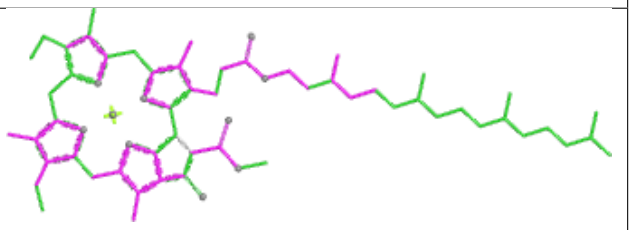
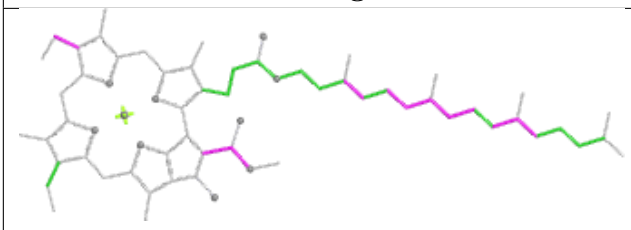
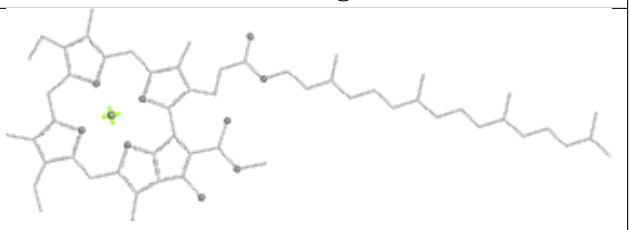
 Bond lengths	 Bond angles
 Torsions	 Rings

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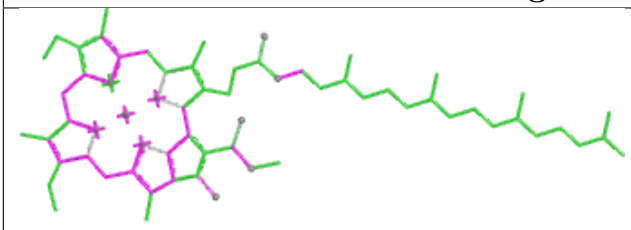
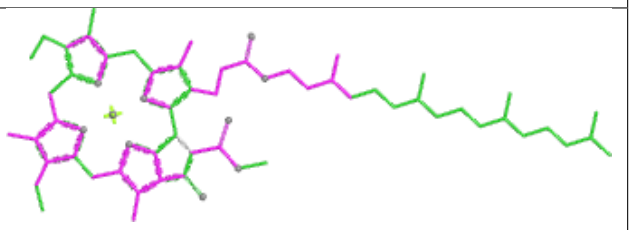
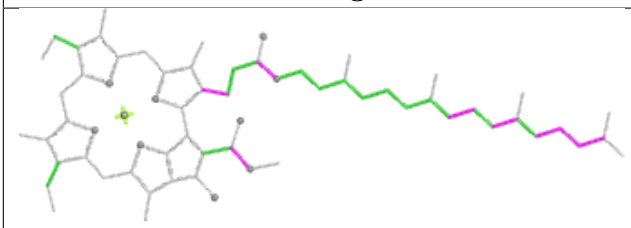
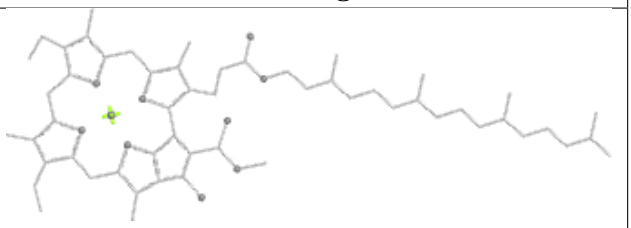
 Bond lengths	 Bond angles
 Torsions	 Rings

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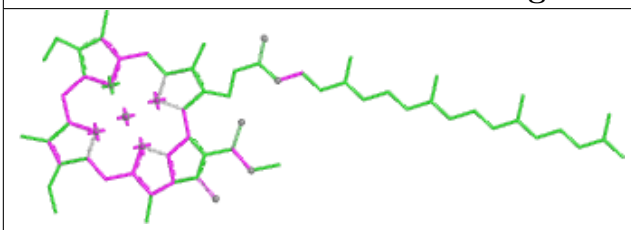
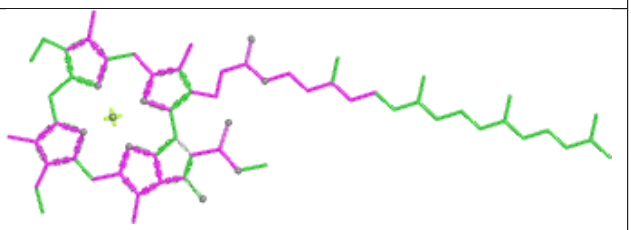
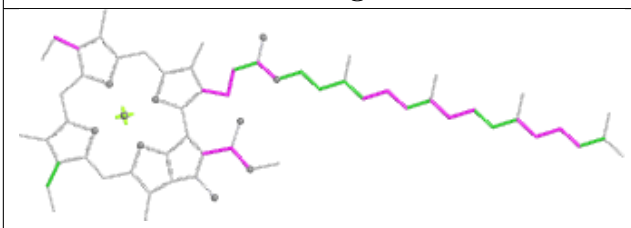
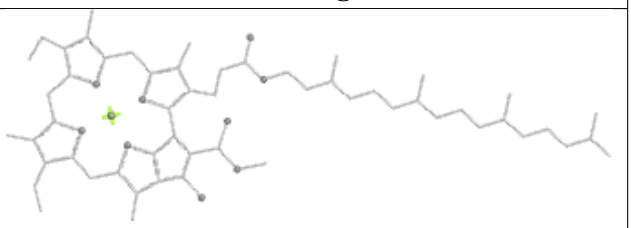
 Bond lengths	 Bond angles
 Torsions	 Rings

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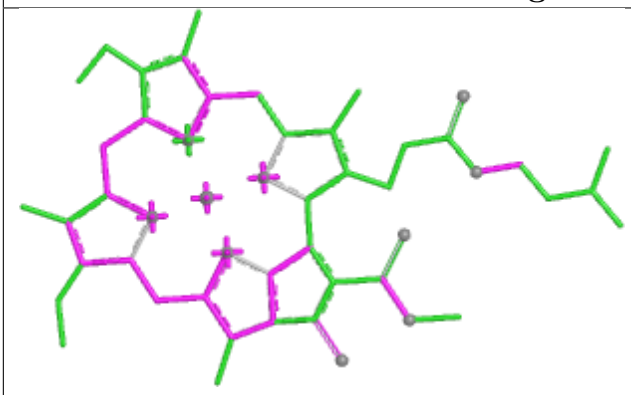

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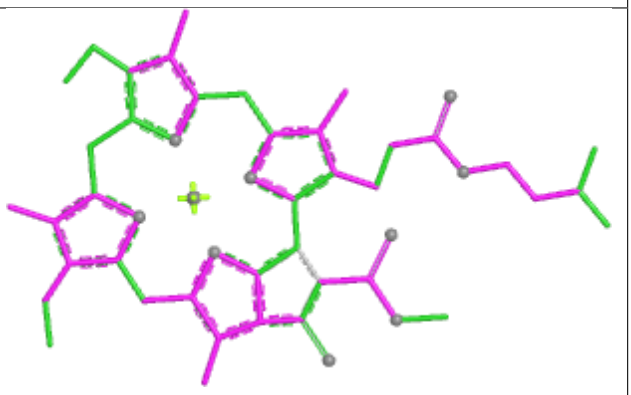
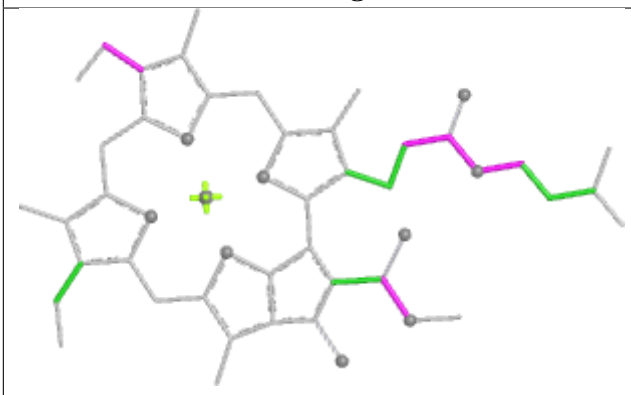


Bond angles



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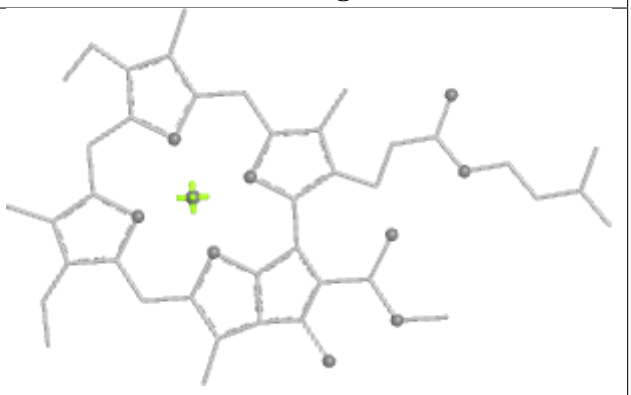
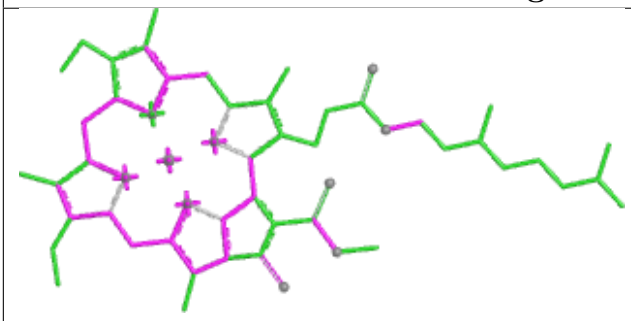


Rings

Ligand CLA b 816



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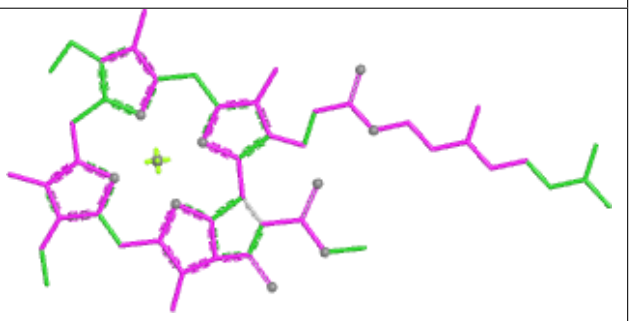
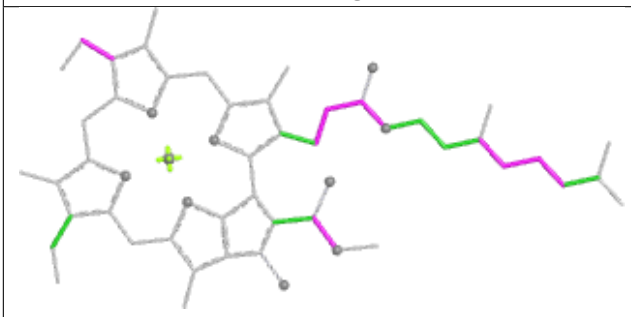


Bond angles



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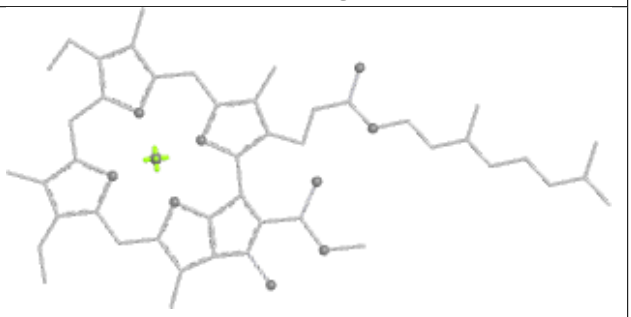
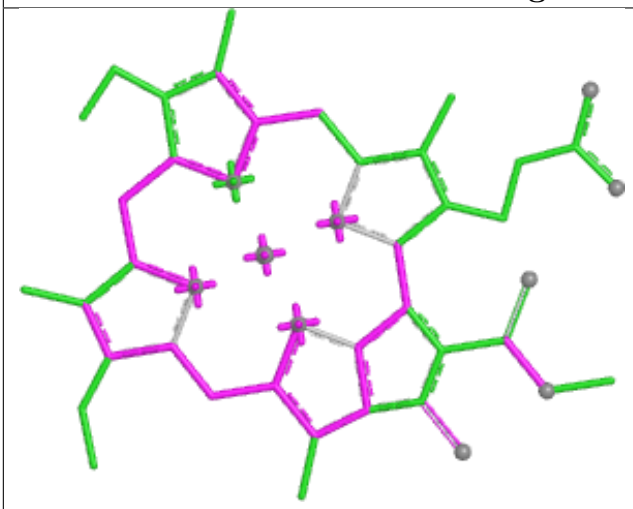


Rings

Ligand CLA a 837



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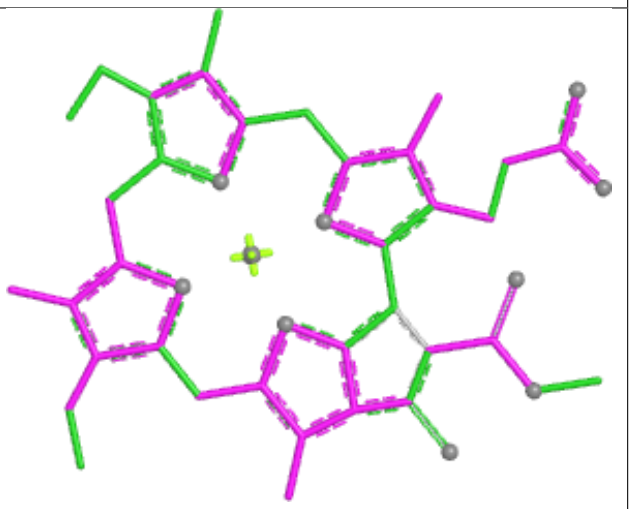
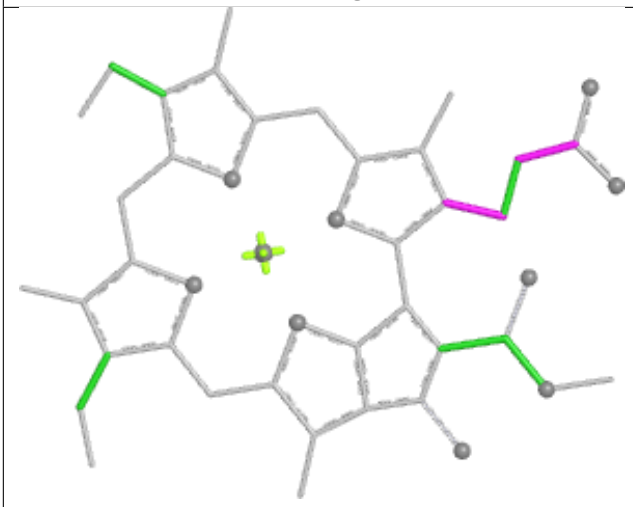


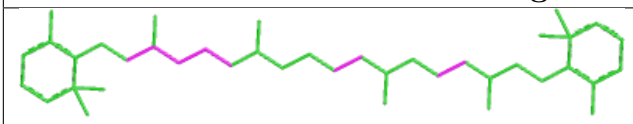
Bond angles



Torsions

Rings

Ligand BCR l 202



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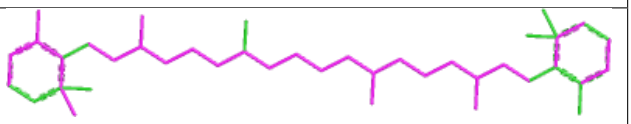
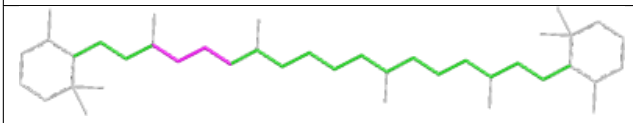


Bond angles



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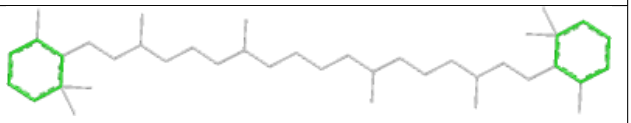
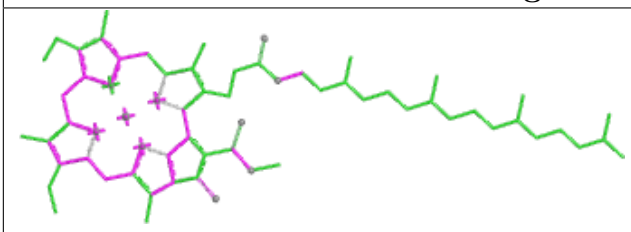
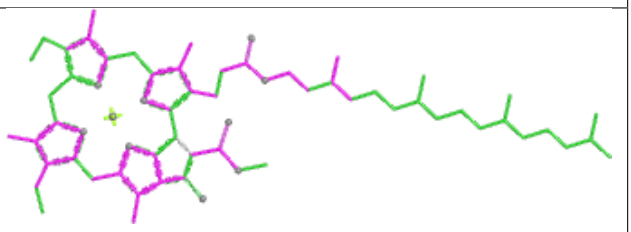
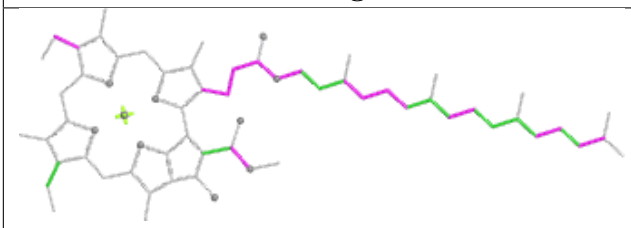
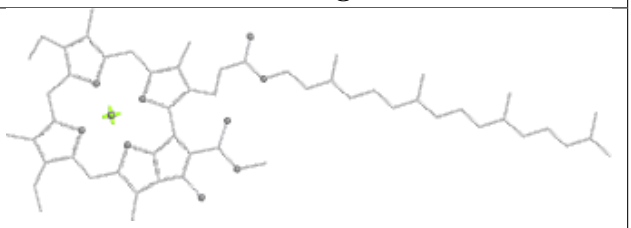


Rings

Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

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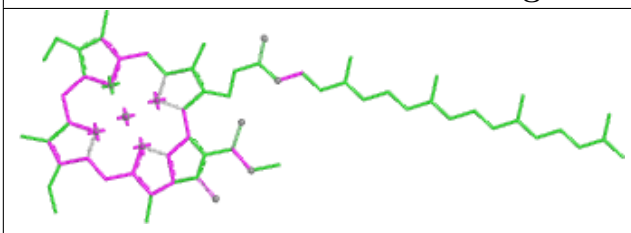
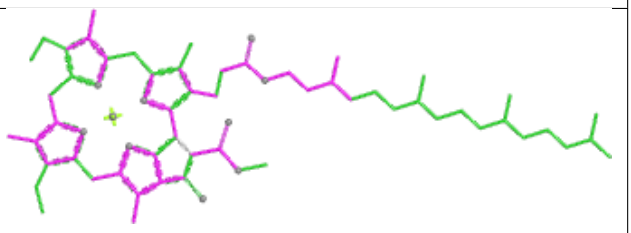
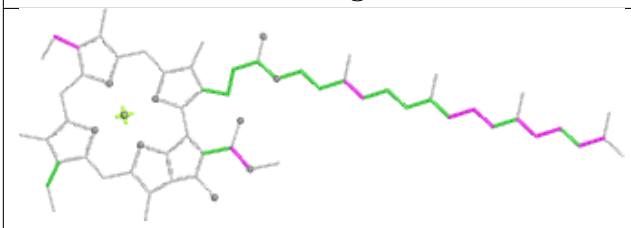
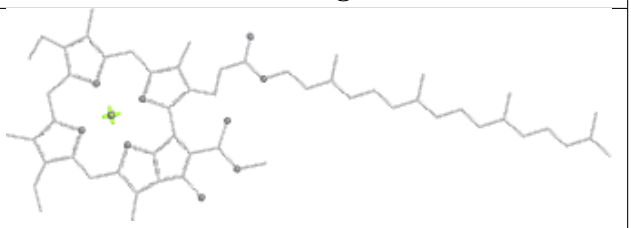
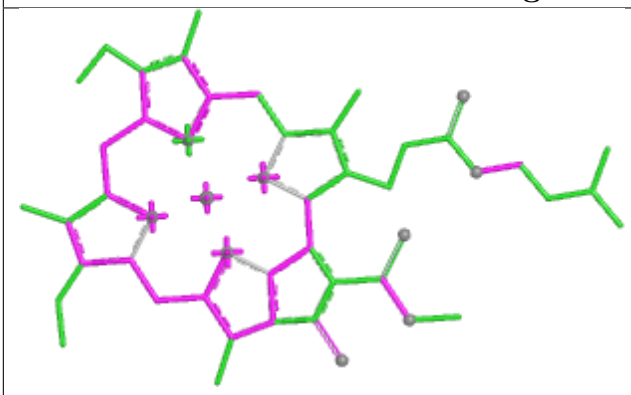
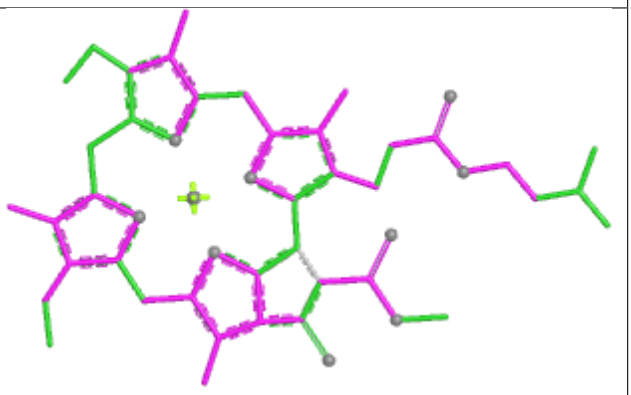
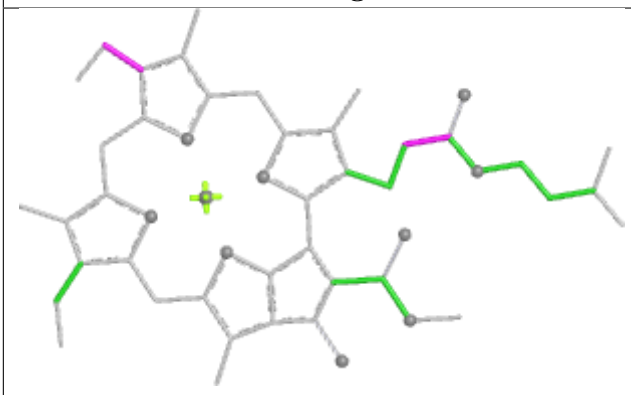
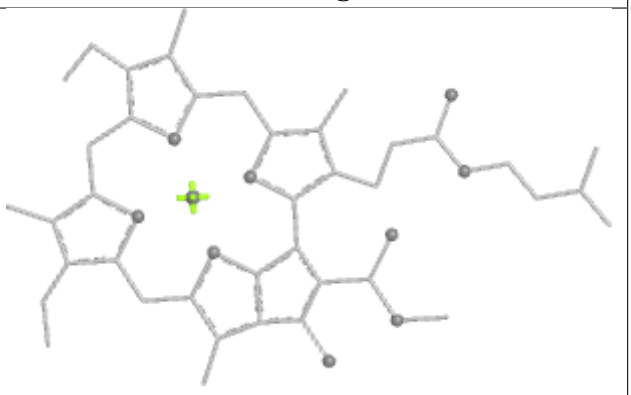
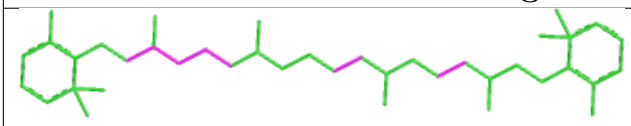
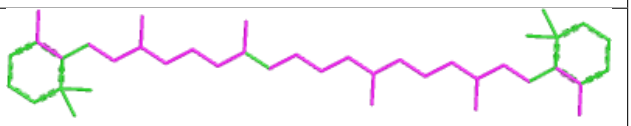
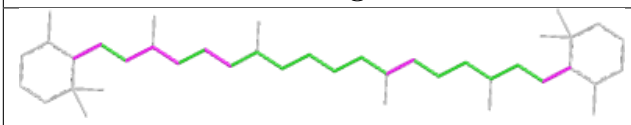
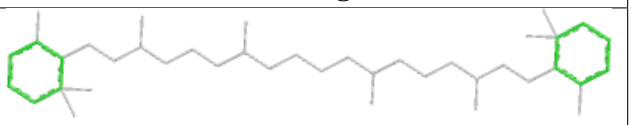
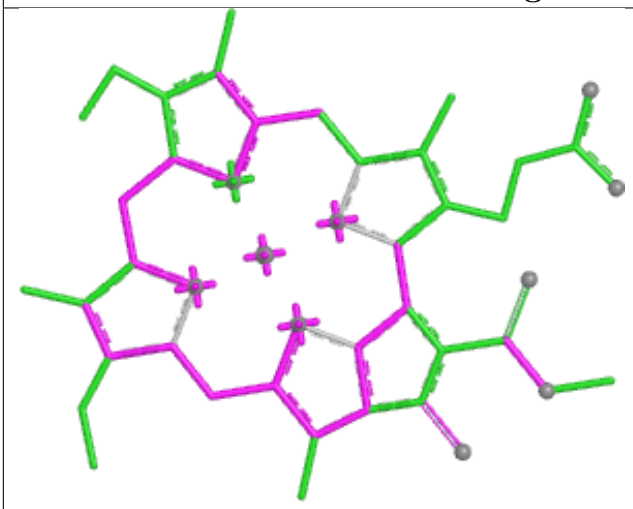
 Bond lengths	 Bond angles
 Torsions	 Rings

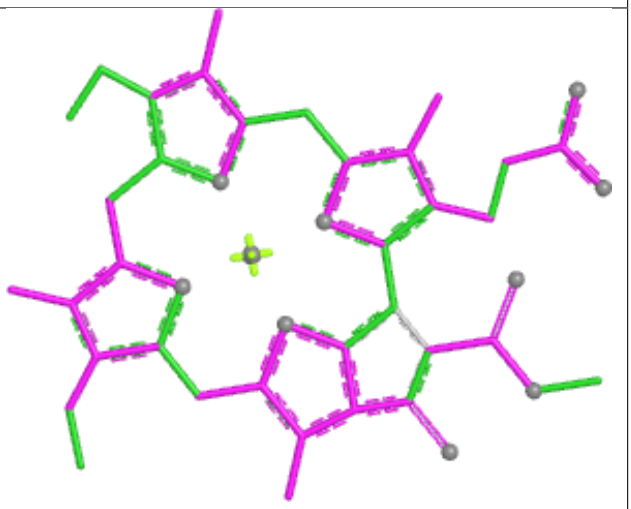
Ligand CLA G 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR G 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

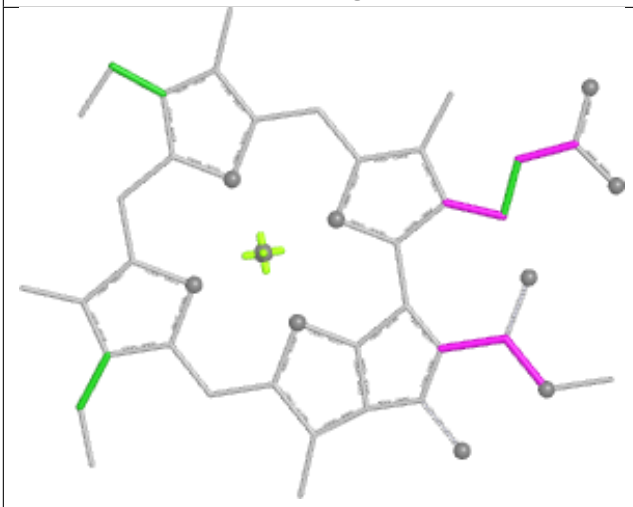
Ligand CLA B 823



Bond lengths



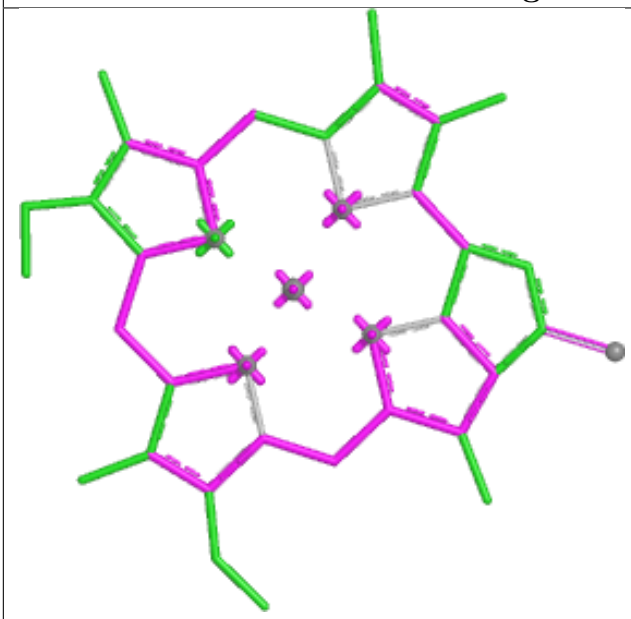
Bond angles



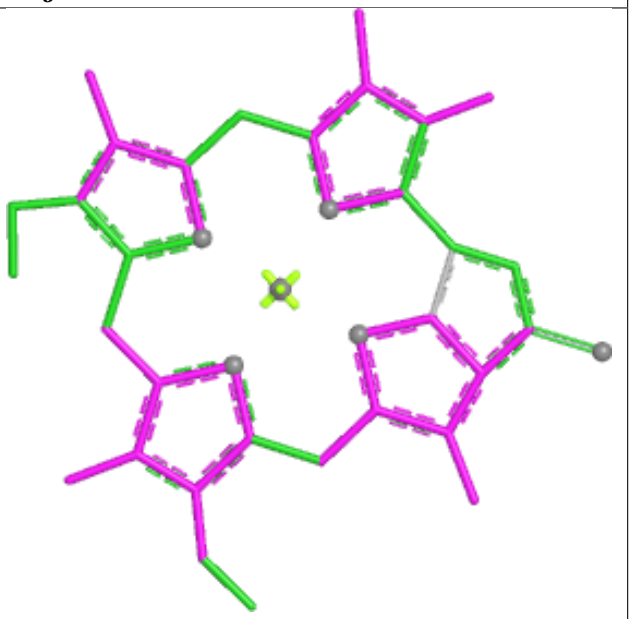
Torsions

Rings

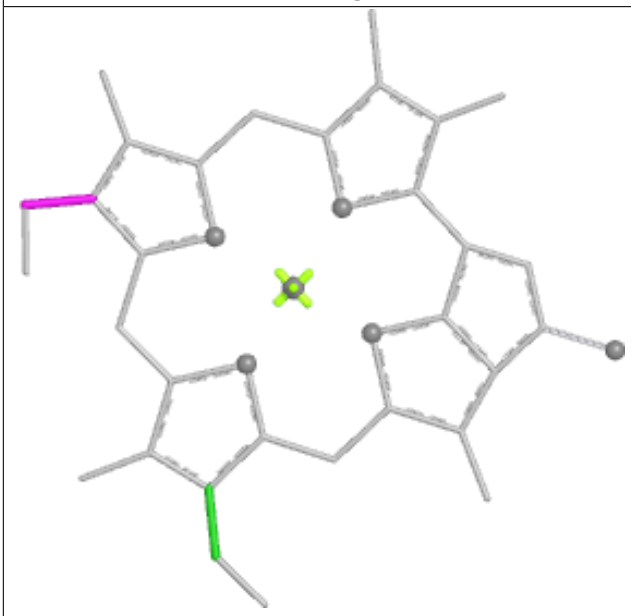
Ligand CLA j 1303



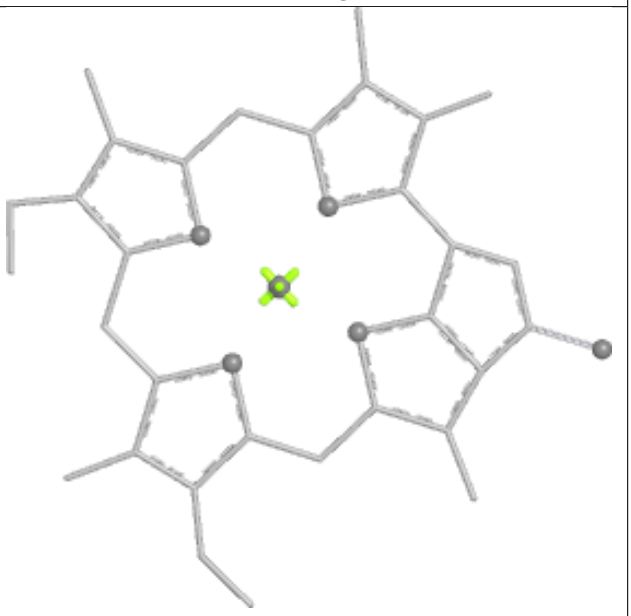
Bond lengths



Bond angles

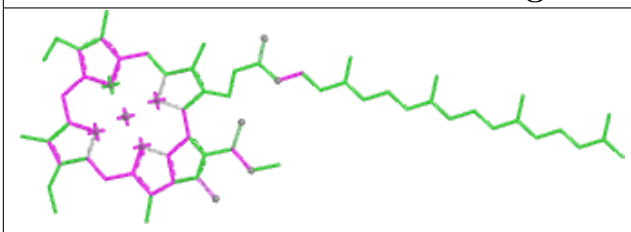


Torsions



Rings

Ligand CLA L 206



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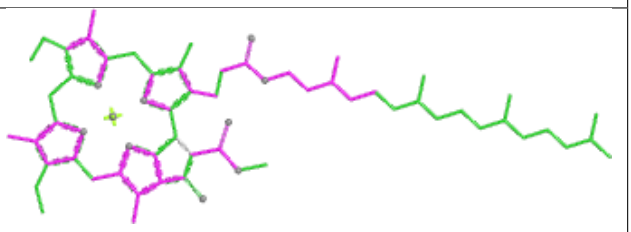
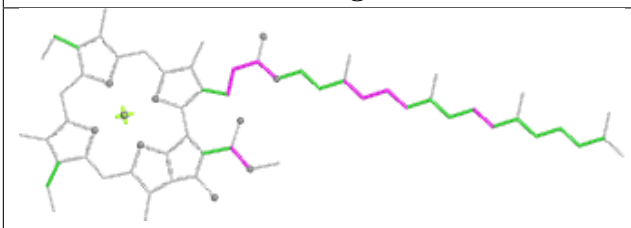


Bond angles



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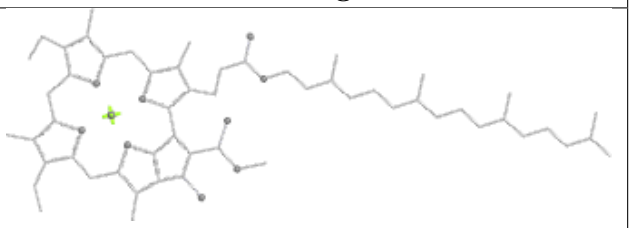
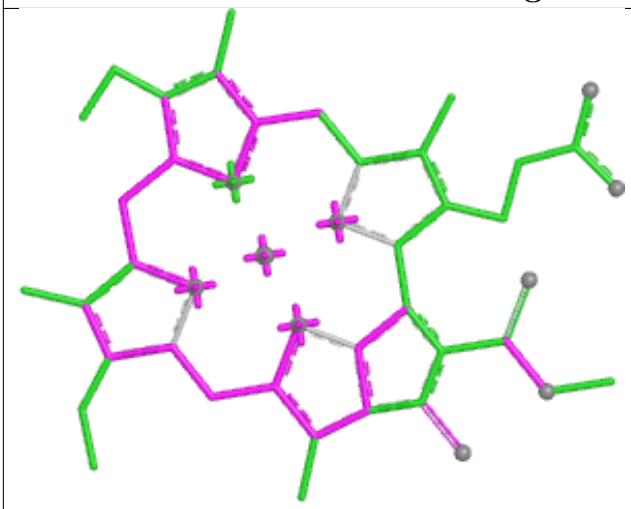
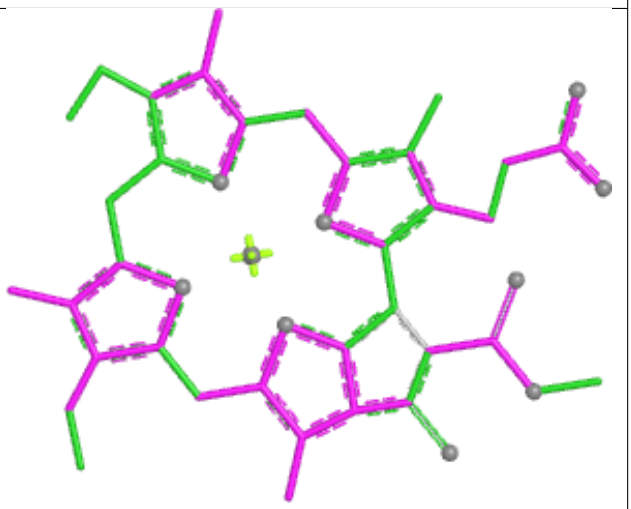


Rings

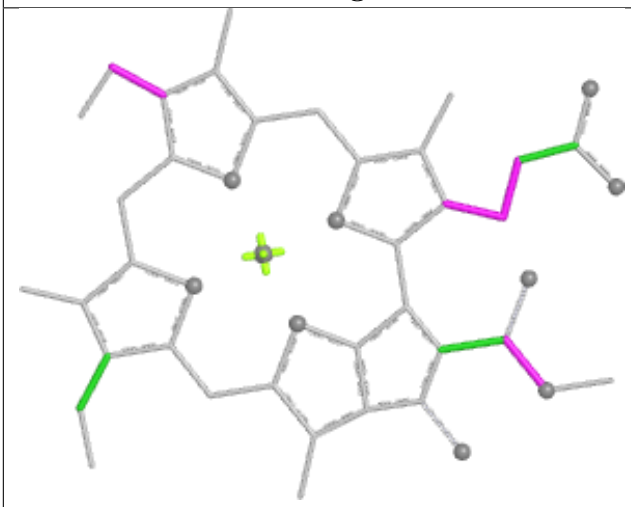
Ligand CLA B 814



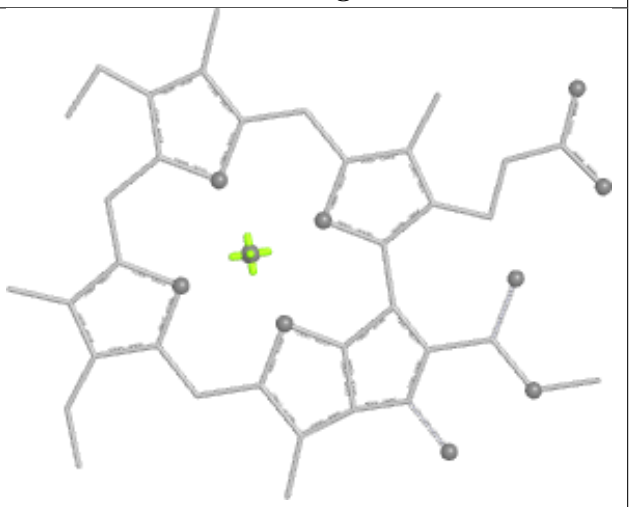
Bond lengths



Bond angles

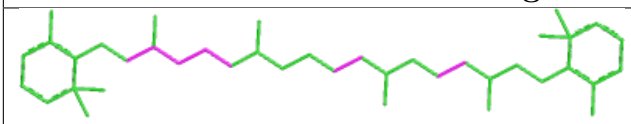


Torsions

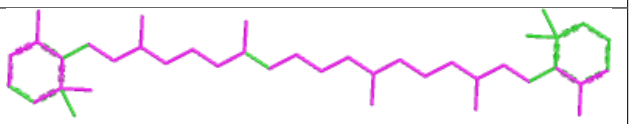


Rings

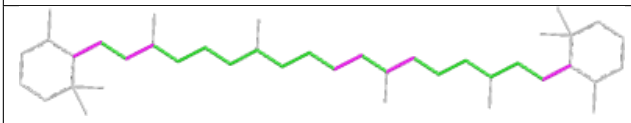
Ligand BCR B 852



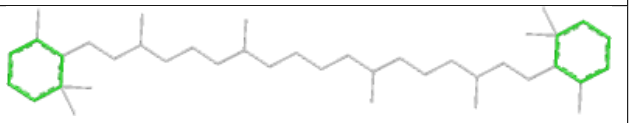
Bond lengths



Bond angles

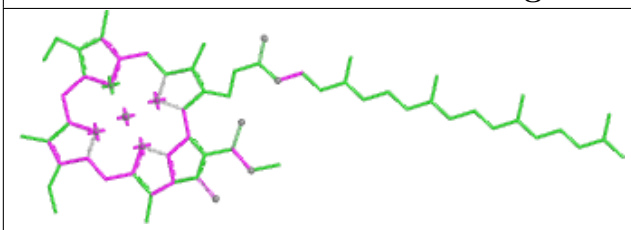


Torsions

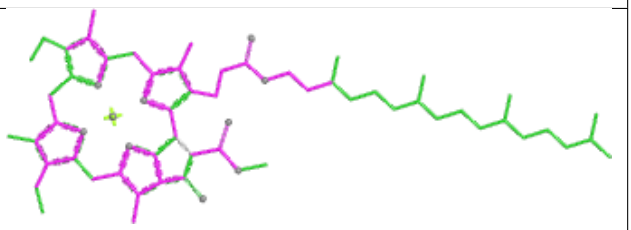


Rings

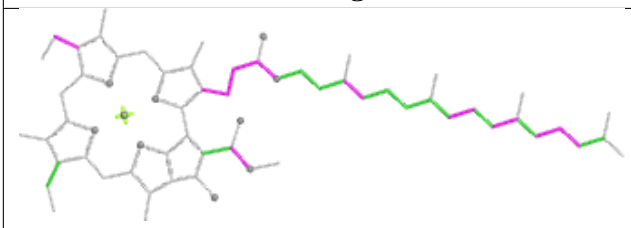
Ligand CLA B 829



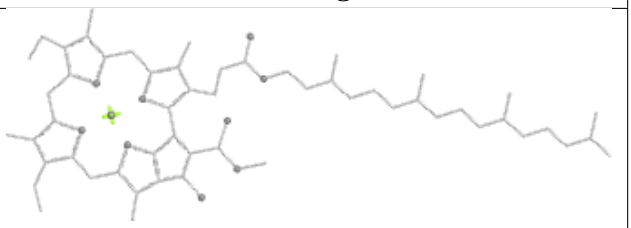
Bond lengths



Bond angles

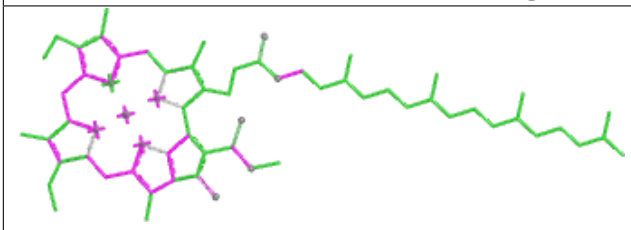


Torsions



Rings

Ligand CLA G 805



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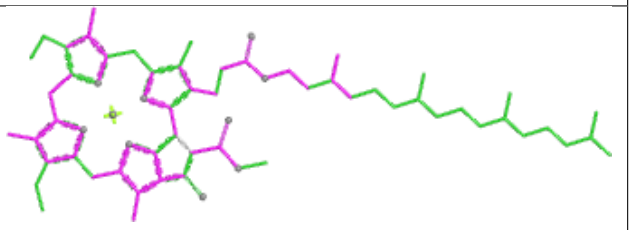
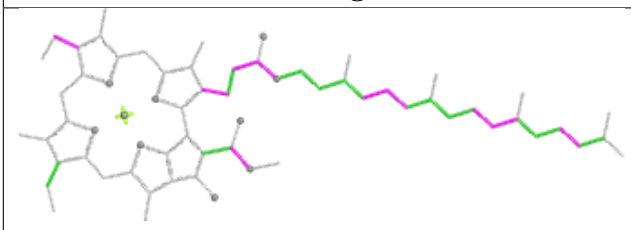
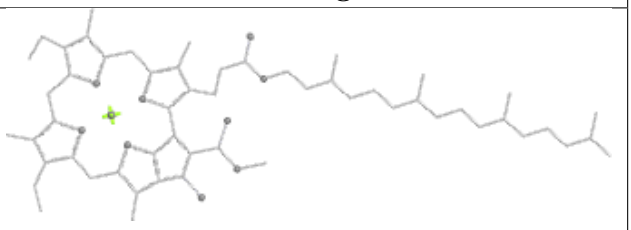


Bond angles

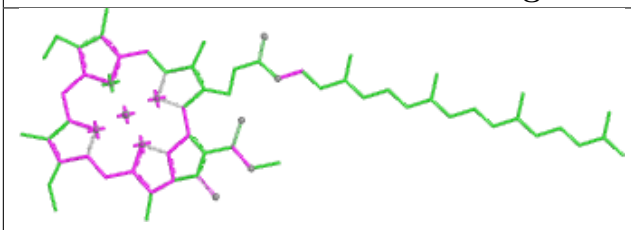


Torsions



Rings

Ligand CLA G 820



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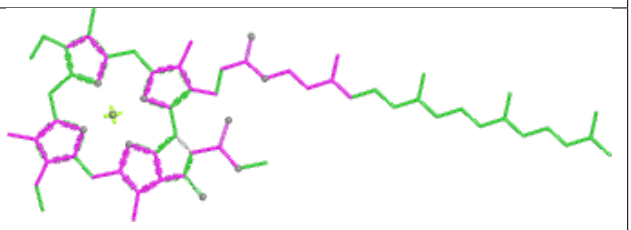
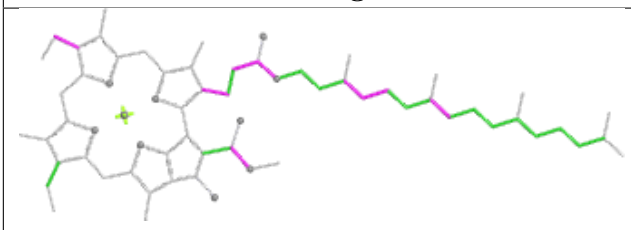


Bond angles



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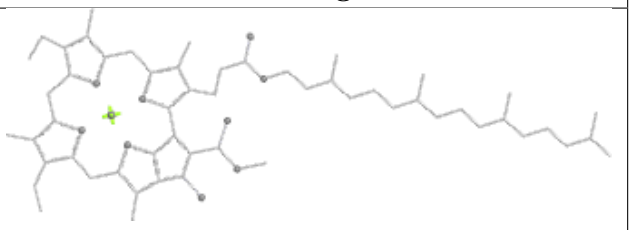
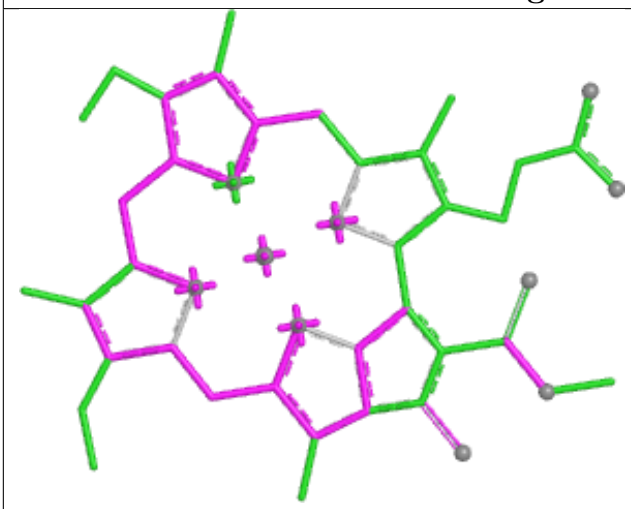
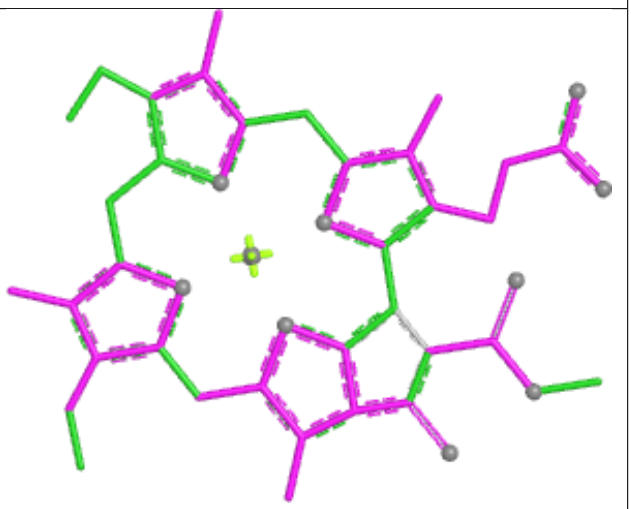


Rings

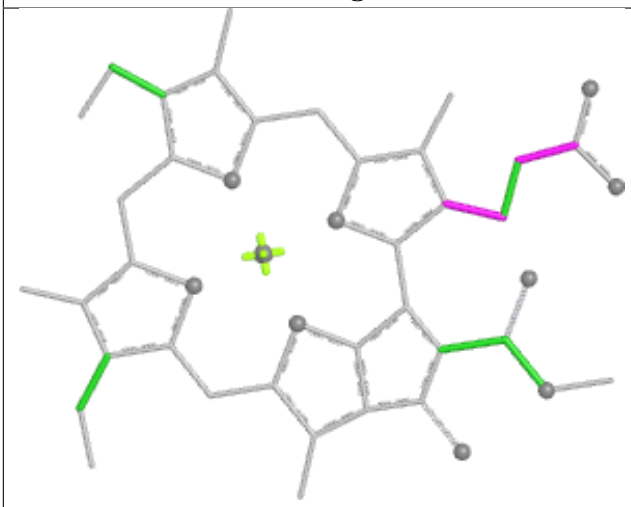
Ligand CLA b 822



Bond lengths

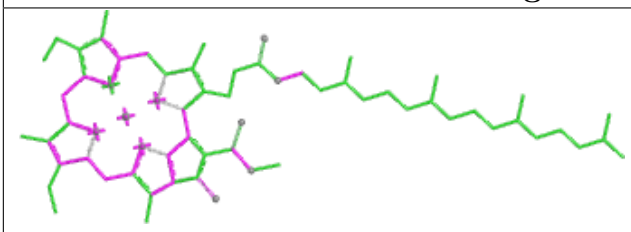
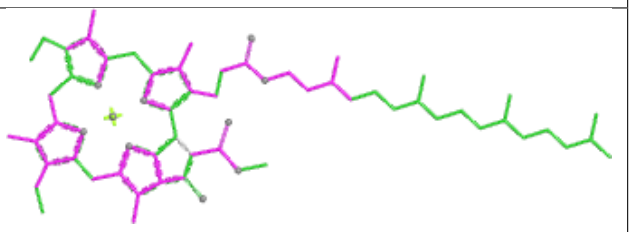
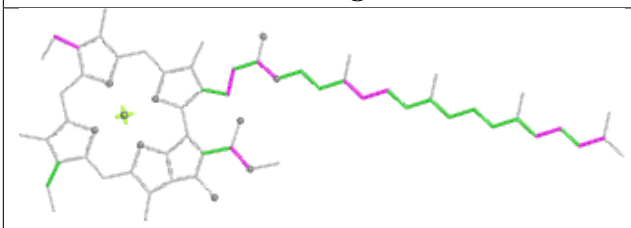
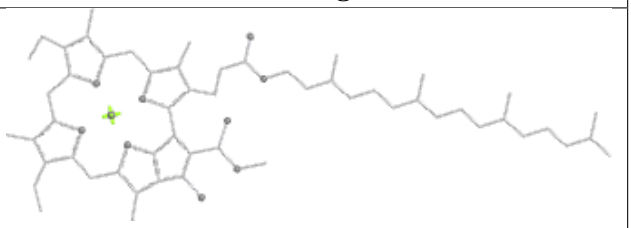


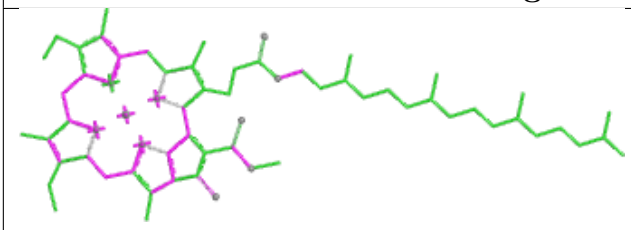
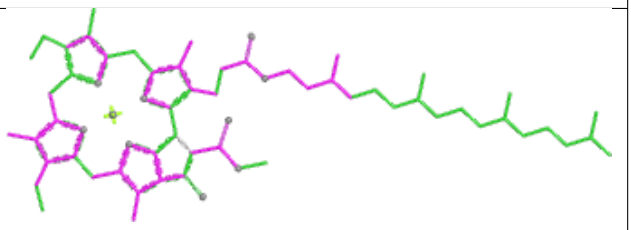
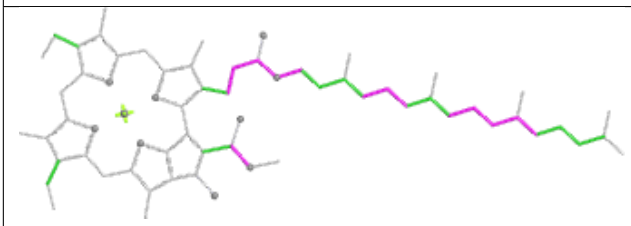
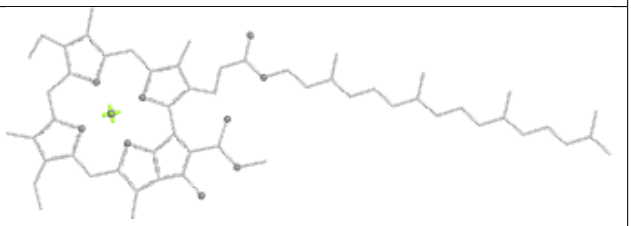
Bond angles

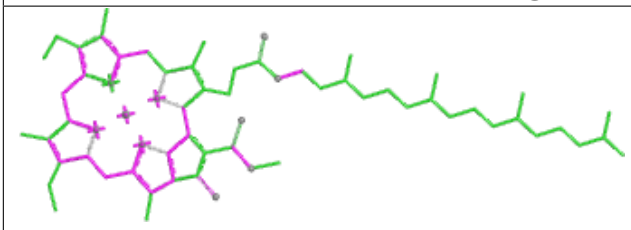
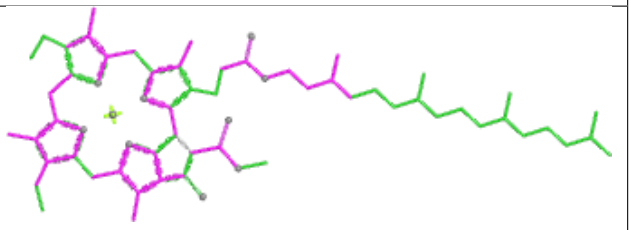
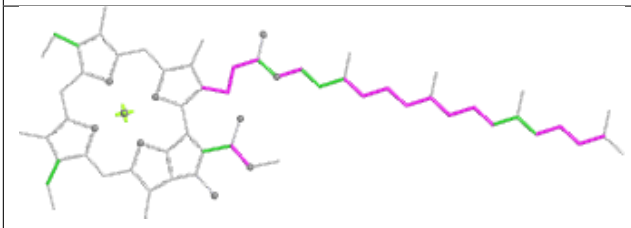
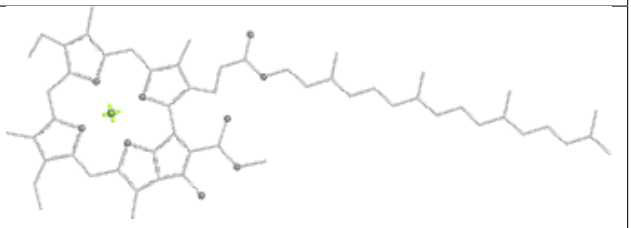


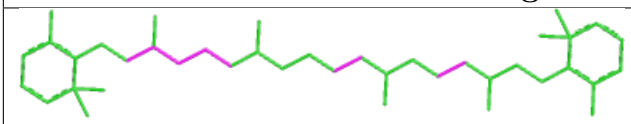
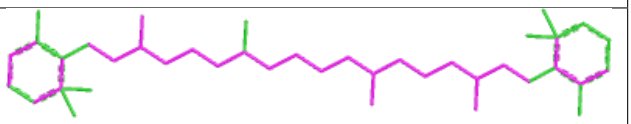
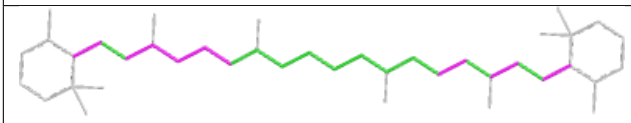
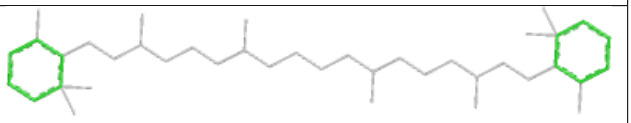
Torsions

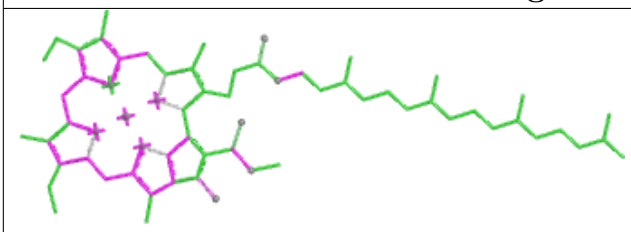
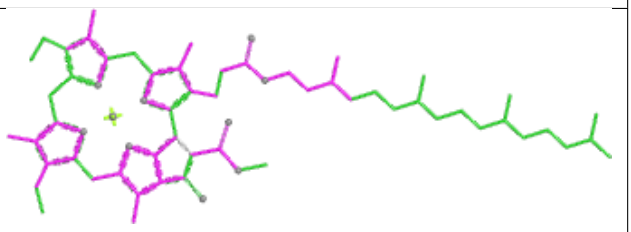
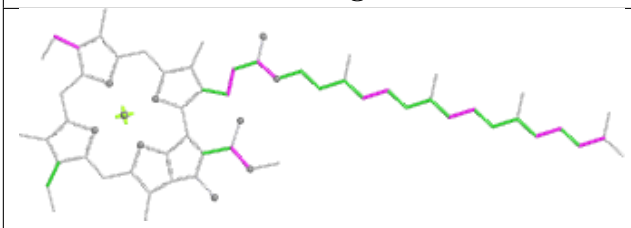
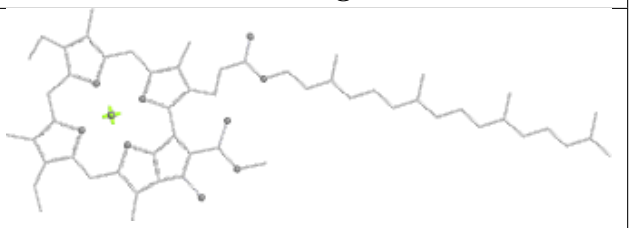
Rings

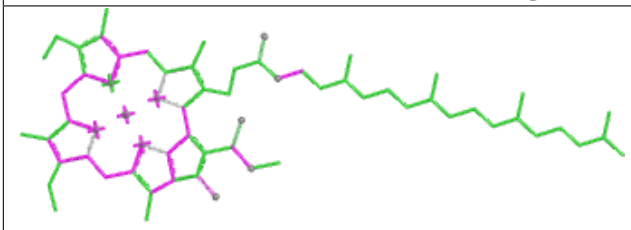
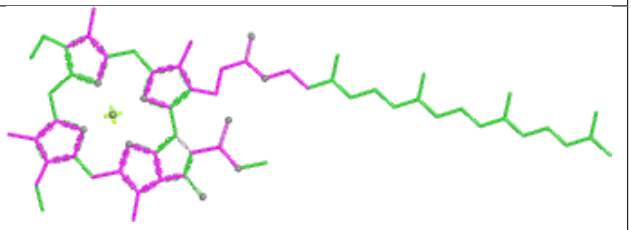
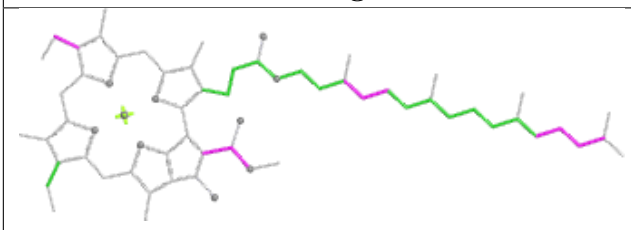
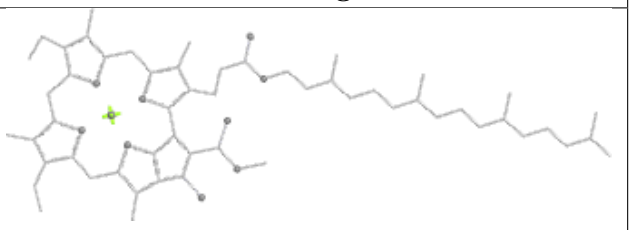
Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

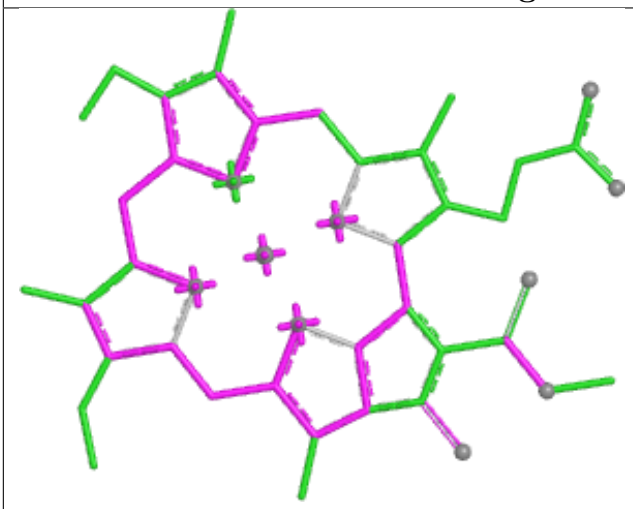
Ligand CLA F 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR H 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

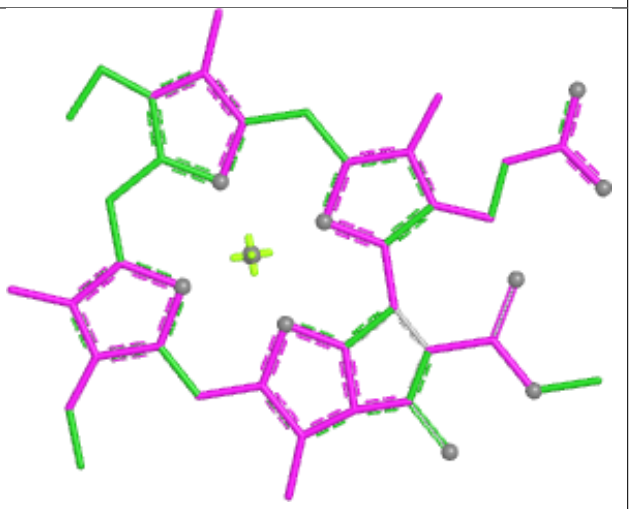
Ligand CLA b 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

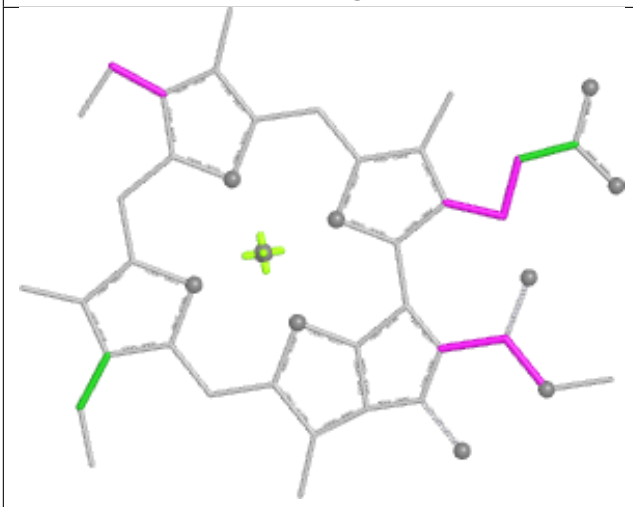
Ligand CLA x 1701



Bond lengths



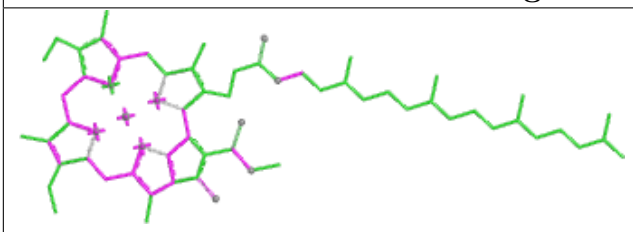
Bond angles



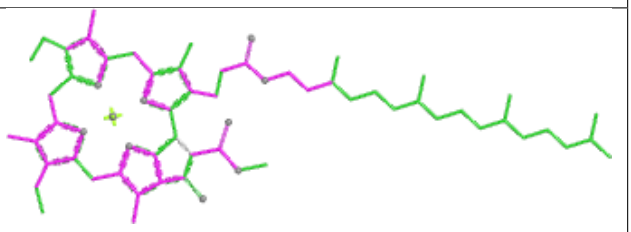
Torsions

Rings

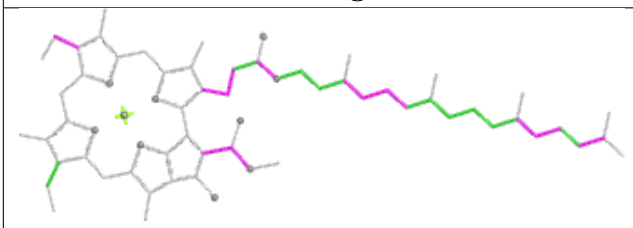
Ligand CLA A 832



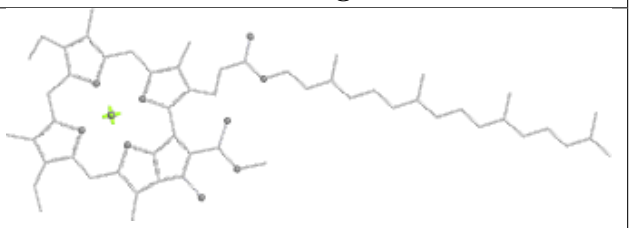
Bond lengths



Bond angles

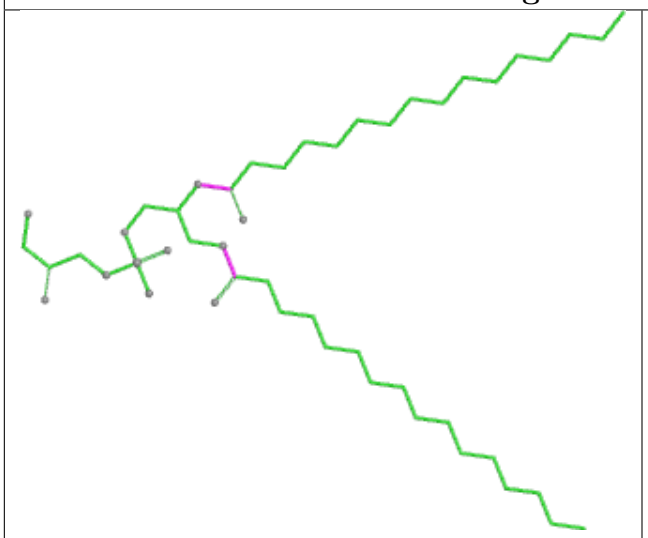


Torsions

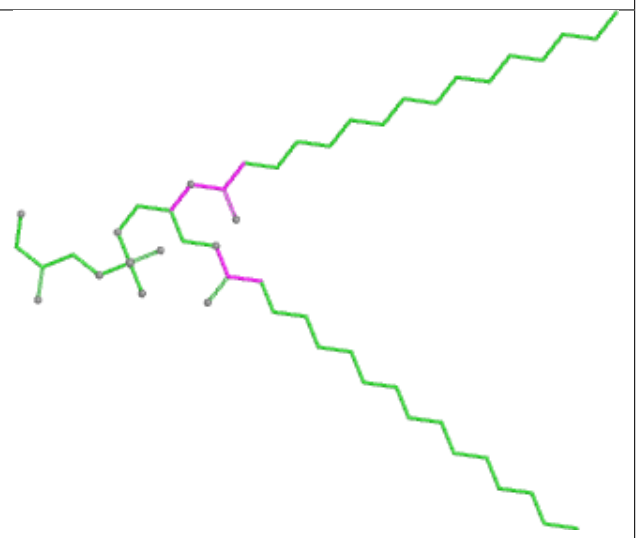


Rings

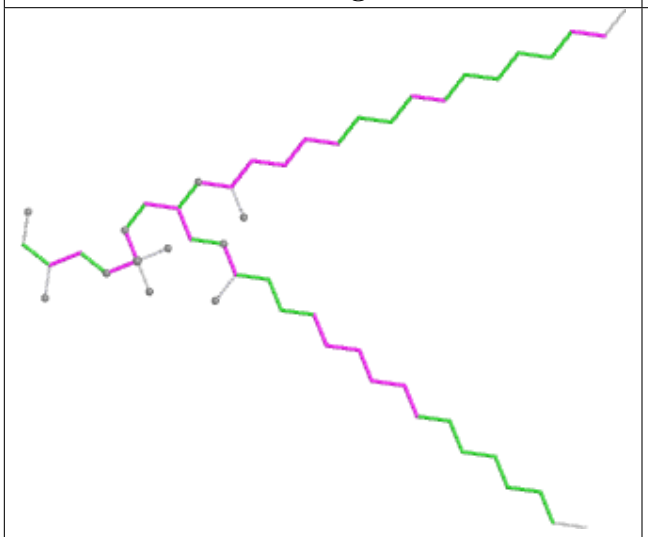
Ligand LHG G 849



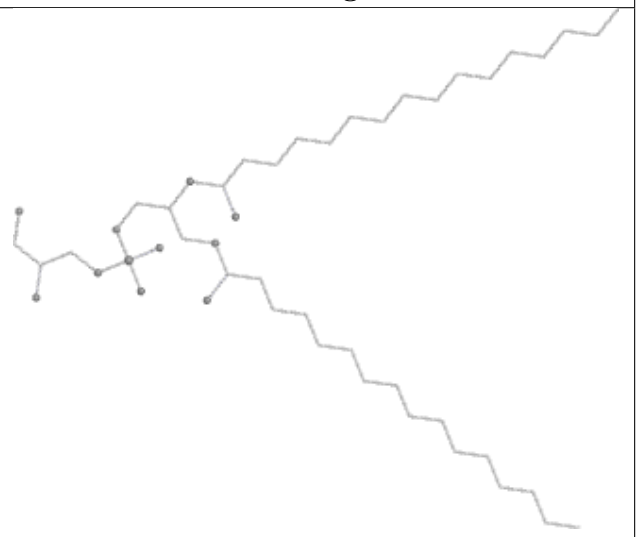
Bond lengths



Bond angles

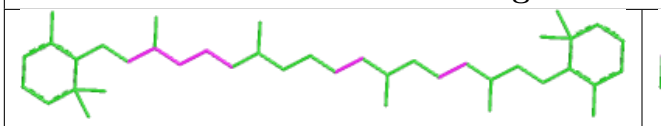


Torsions



Rings

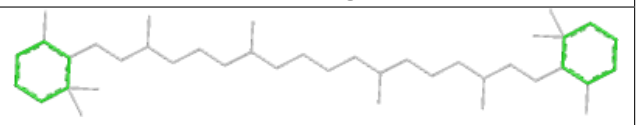
Ligand BCR m 1203



Bond lengths

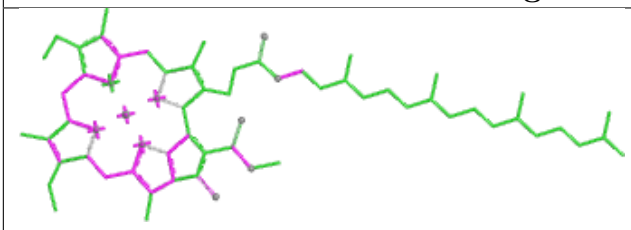
Bond angles

Torsions



Rings

Ligand CLA A 804



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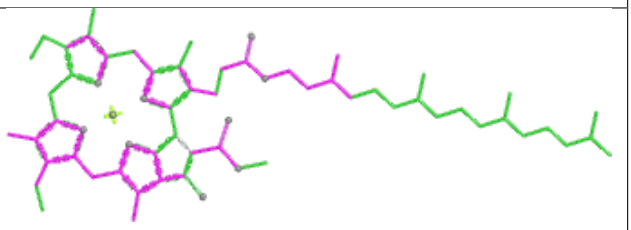
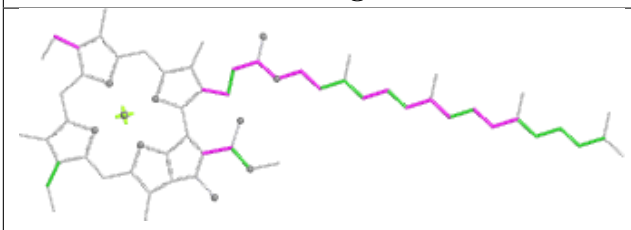
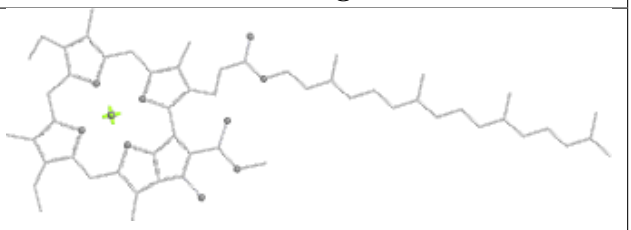


Bond angles

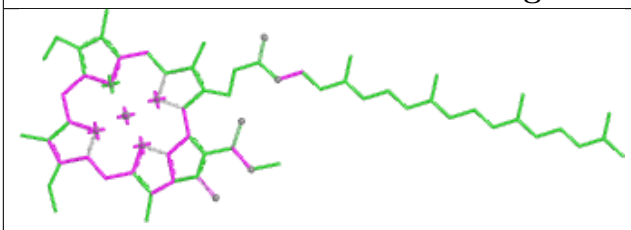


Torsions

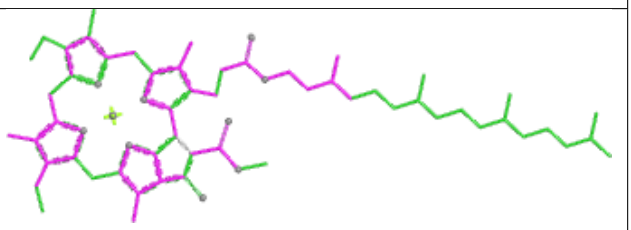


Rings

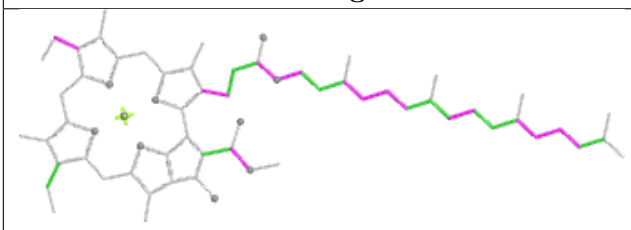
Ligand CLA A 824



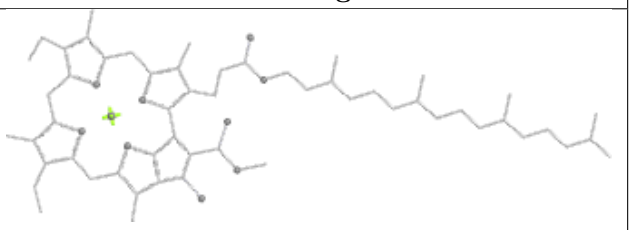
Bond lengths



Bond angles

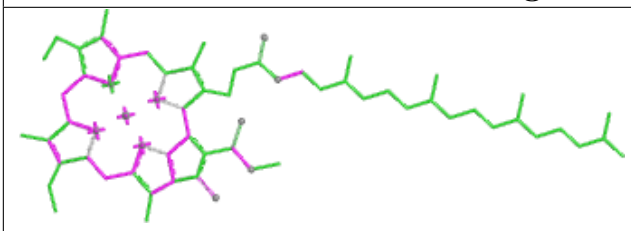


Torsions



Rings

Ligand CLA H 811



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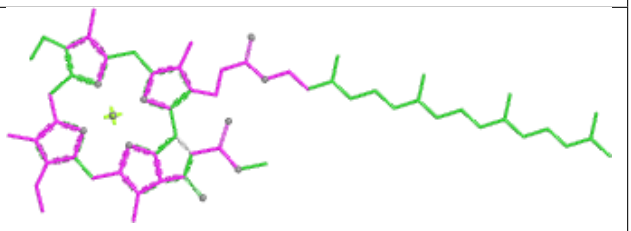
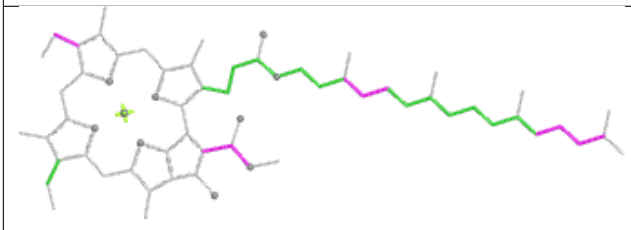


Bond angles



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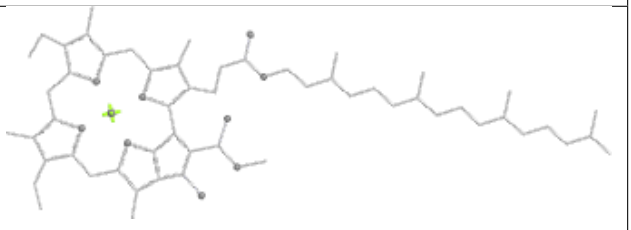
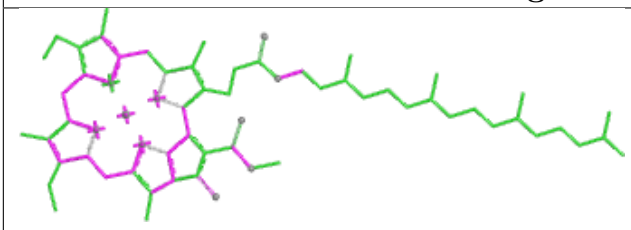


Rings

Ligand CLA b 809



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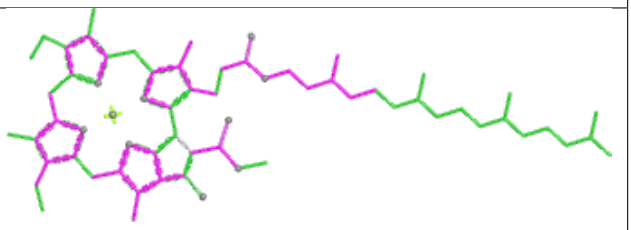
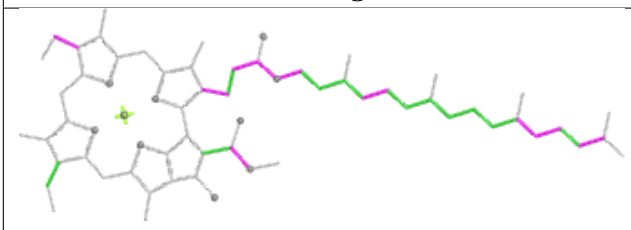
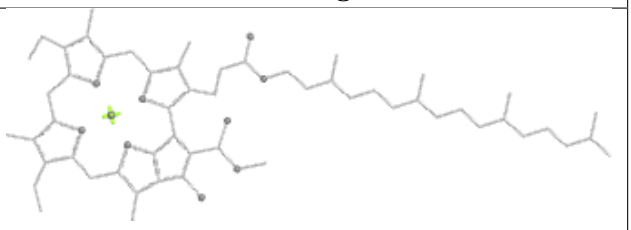


Bond angles

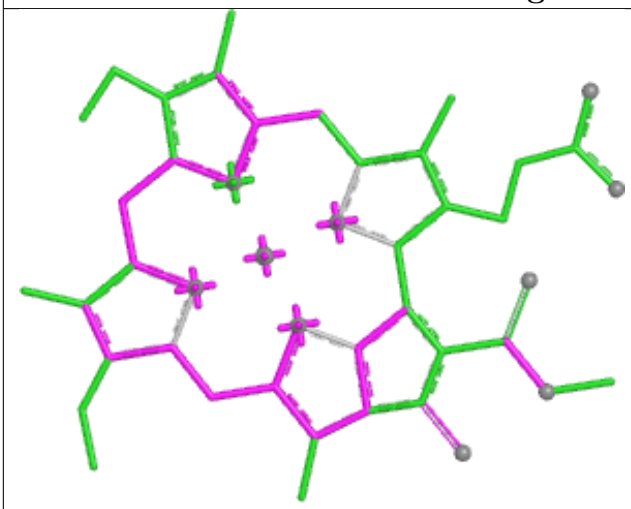


Torsions



Rings

Ligand CLA b 838



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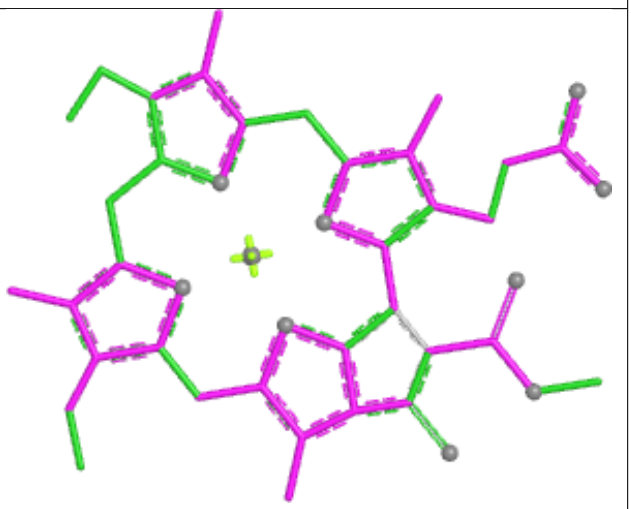
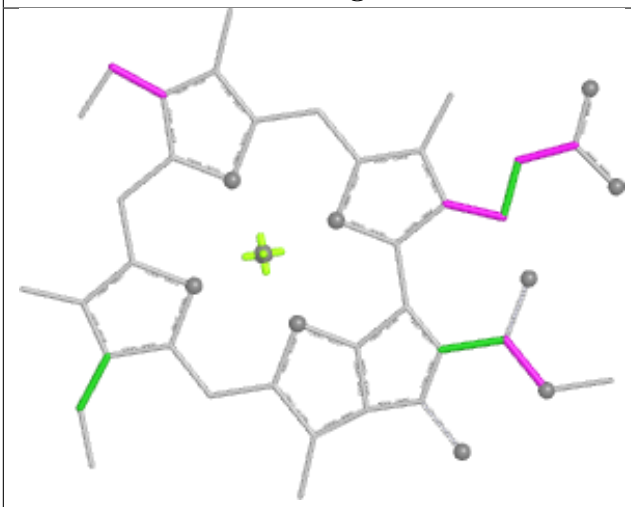
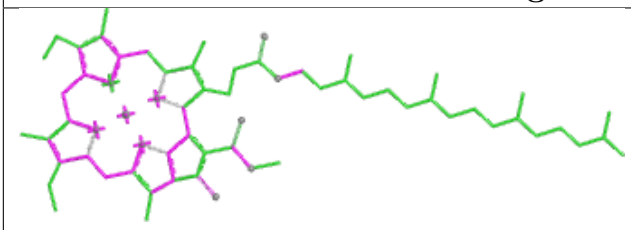
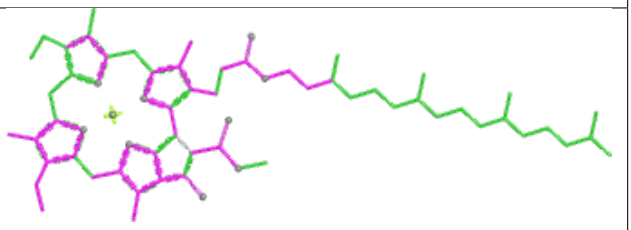
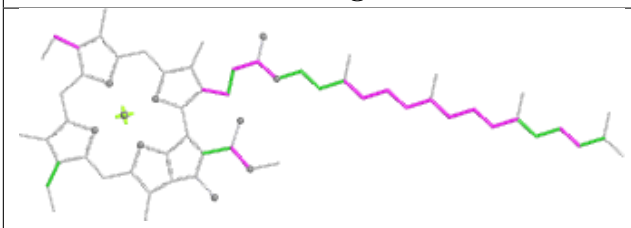
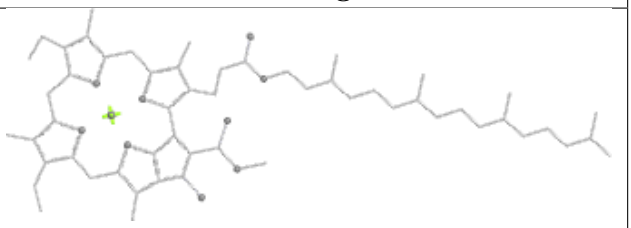


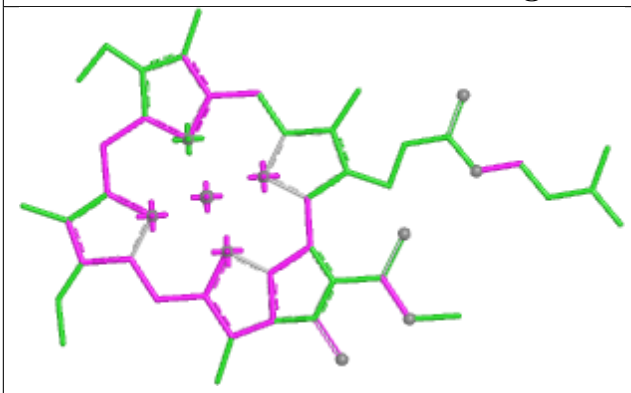
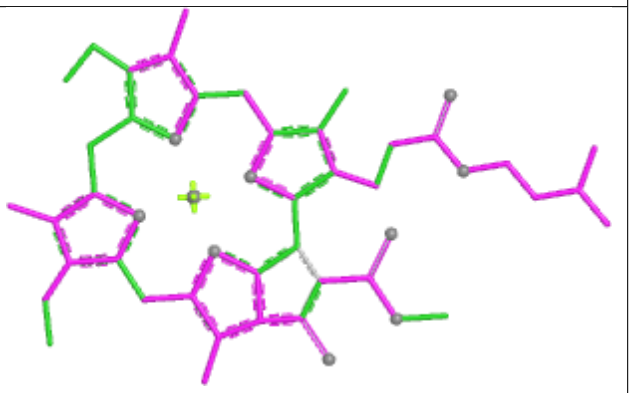
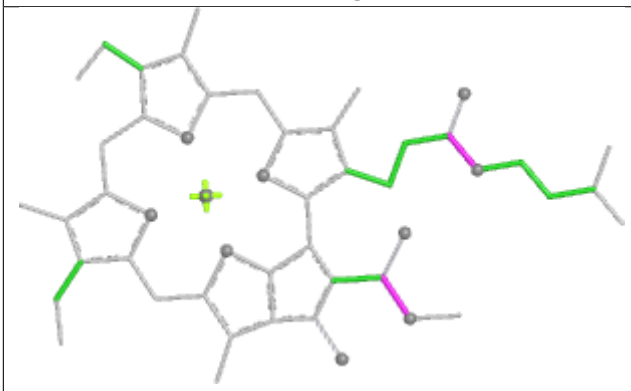
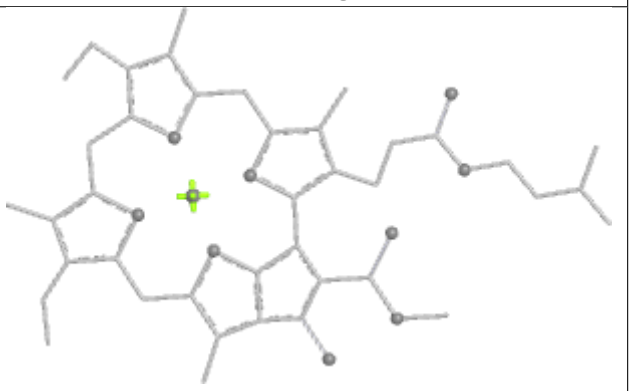
Bond angles

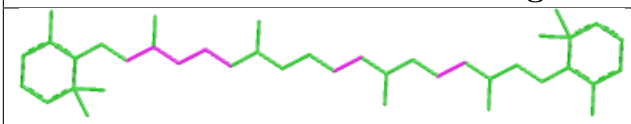
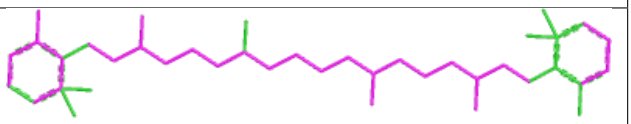
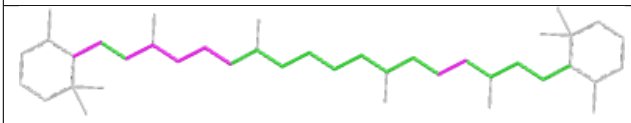
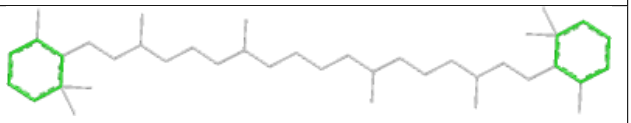


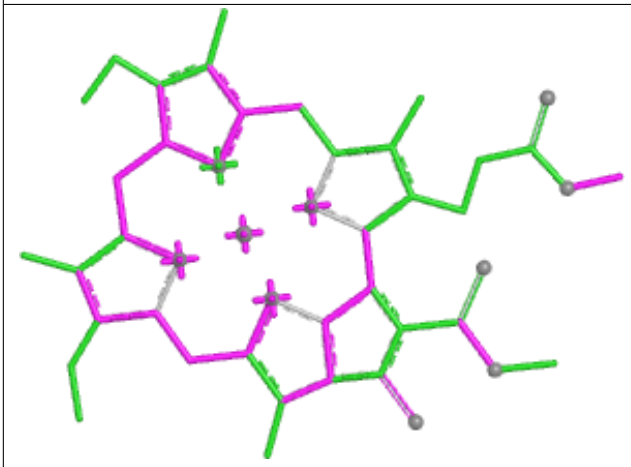
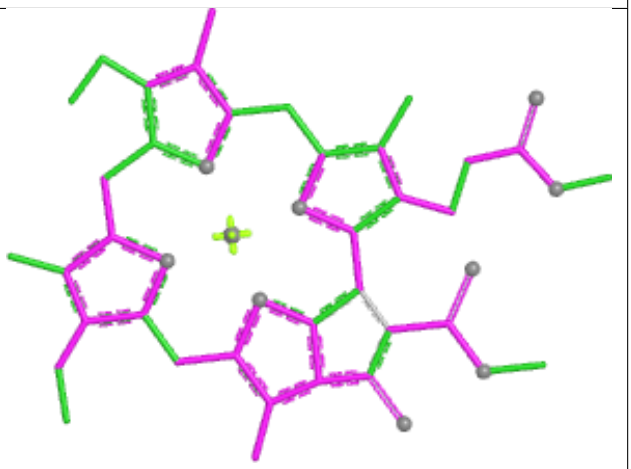
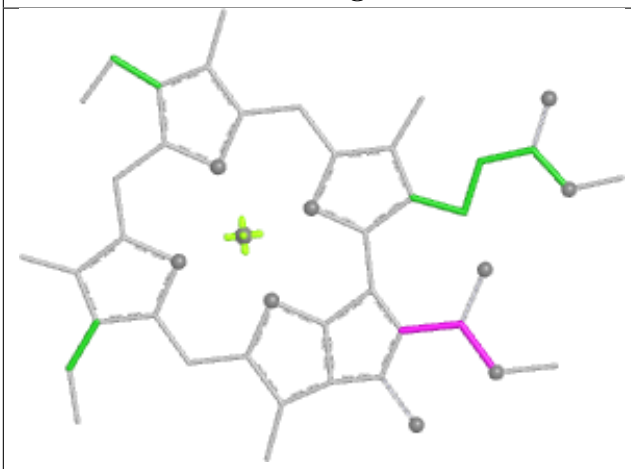
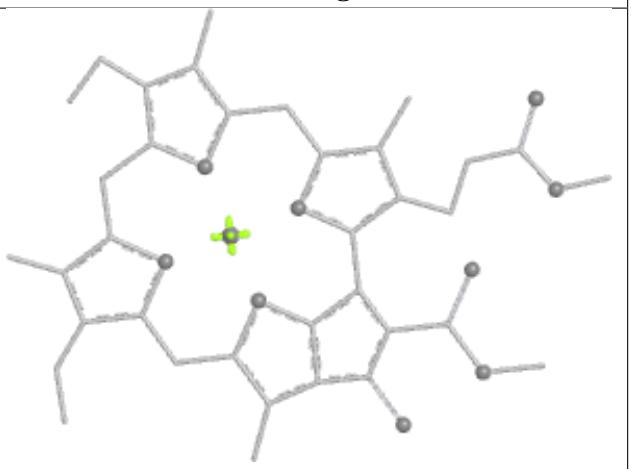
Torsions

Rings

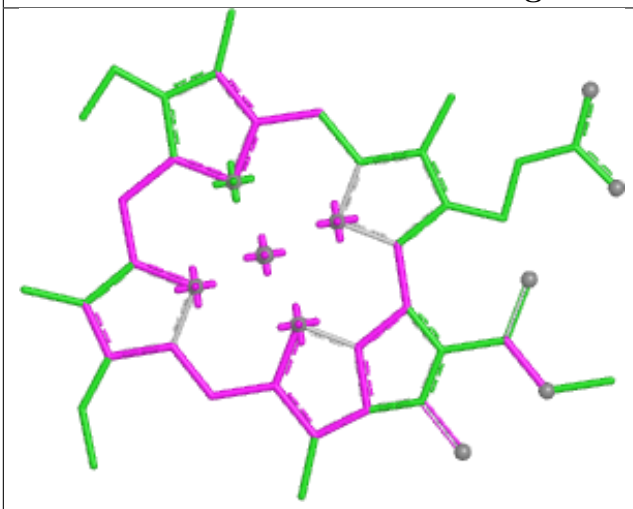
Ligand CLA b 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

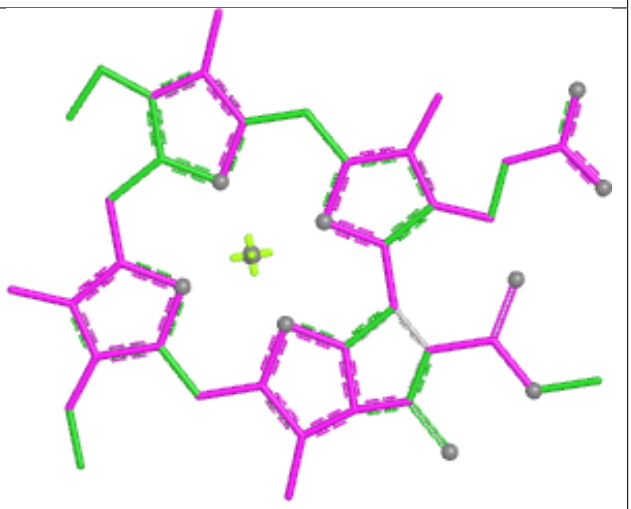
Ligand BCR a 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

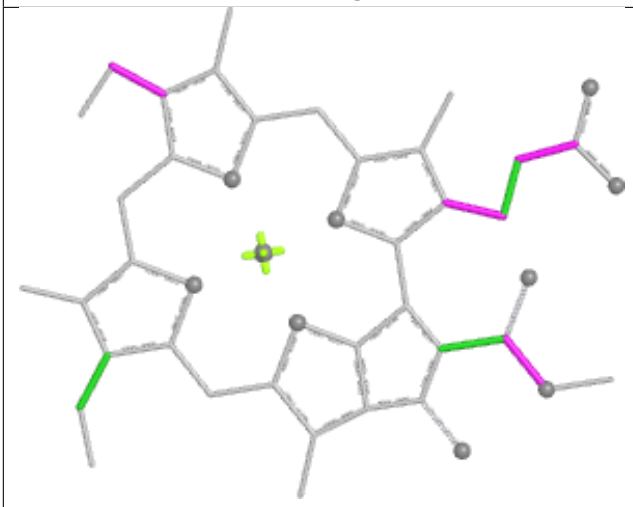
Ligand CLA T 102



Bond lengths



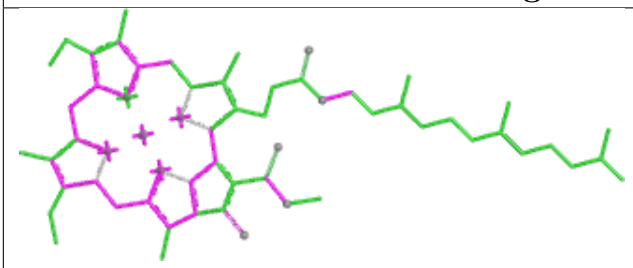
Bond angles



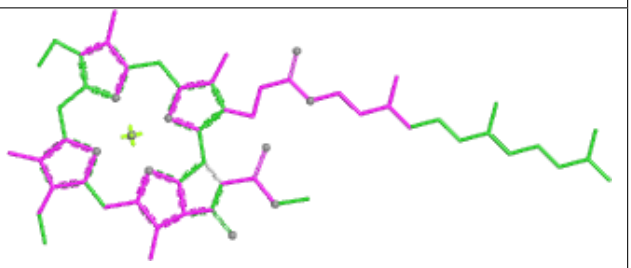
Torsions

Rings

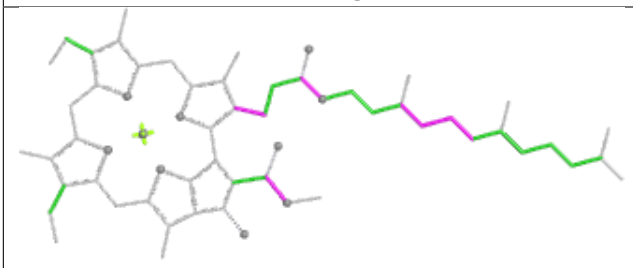
Ligand CLA H 820



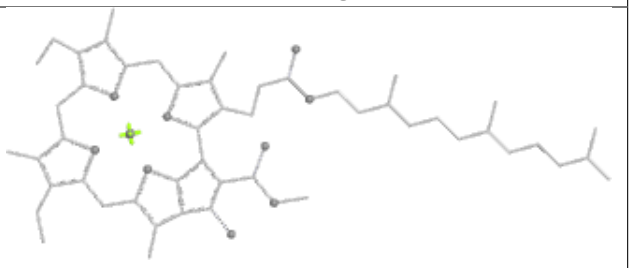
Bond lengths



Bond angles

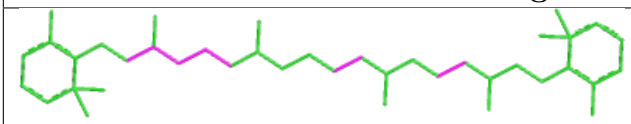


Torsions

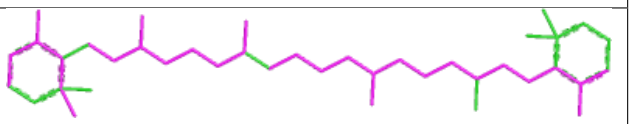


Rings

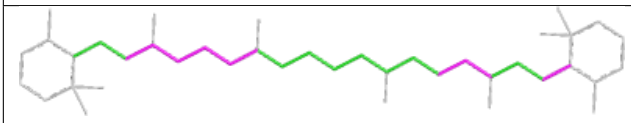
Ligand BCR l 201



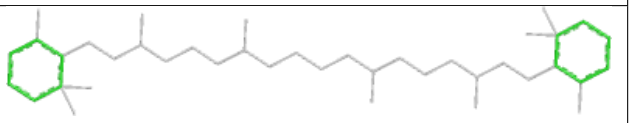
Bond lengths



Bond angles

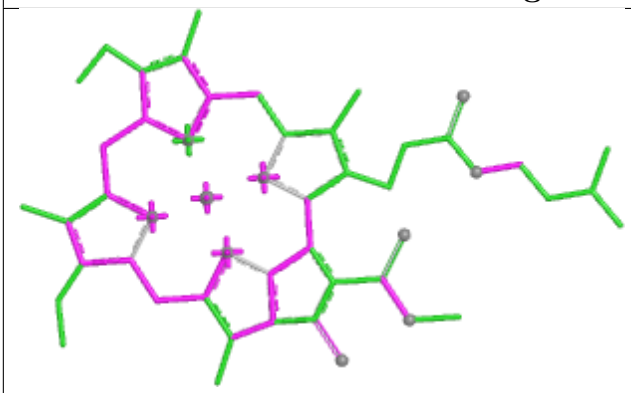


Torsions

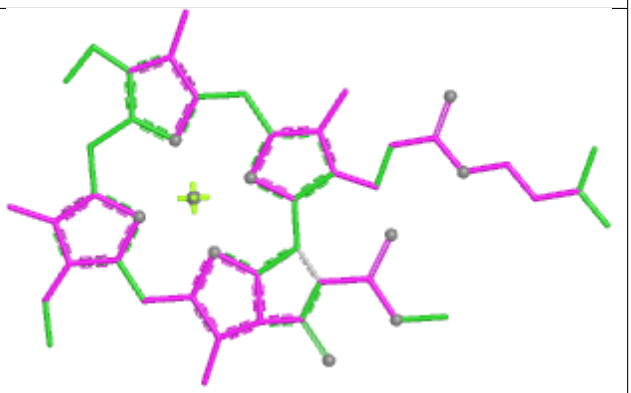


Rings

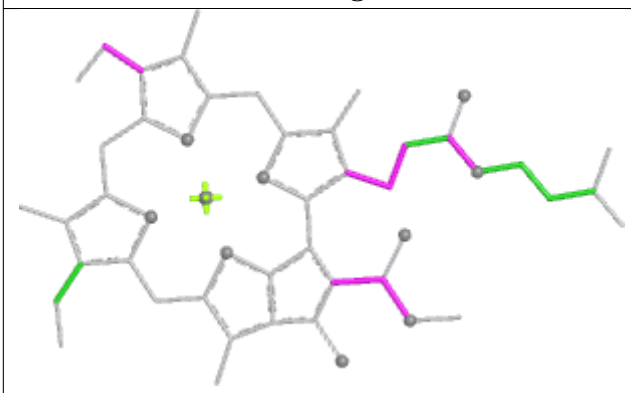
Ligand CLA A 830



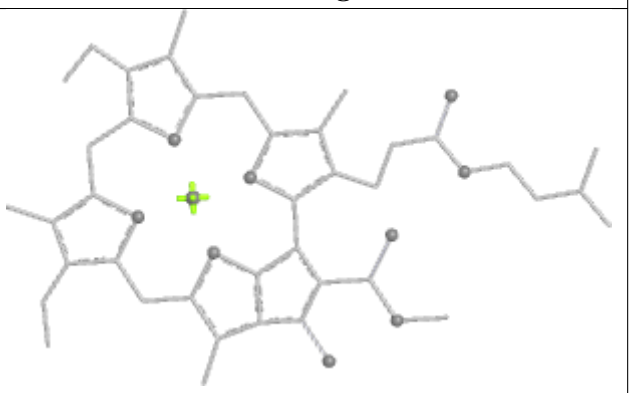
Bond lengths



Bond angles

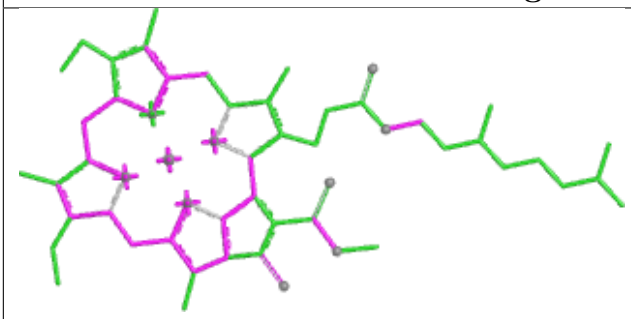


Torsions

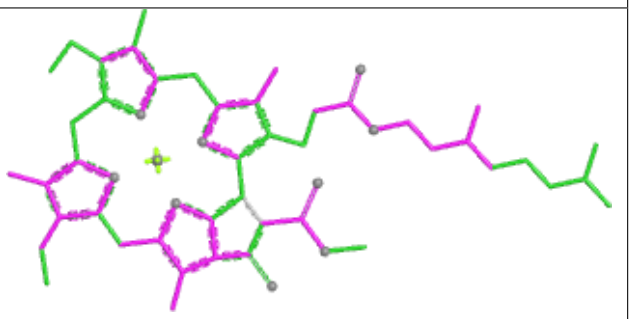


Rings

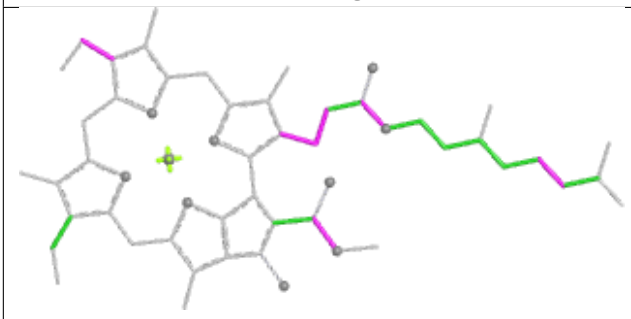
Ligand CLA B 818



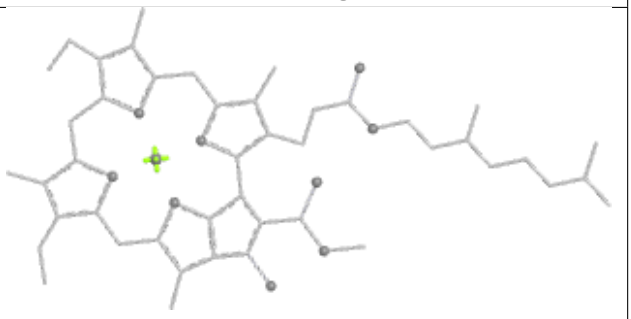
Bond lengths



Bond angles

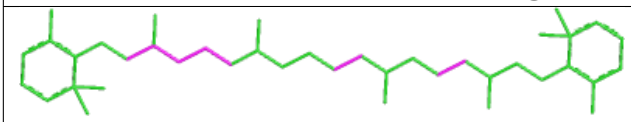


Torsions



Rings

Ligand BCR b 843



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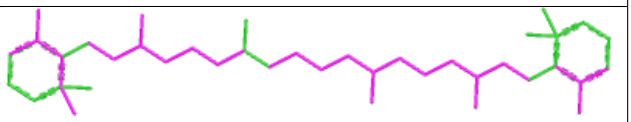
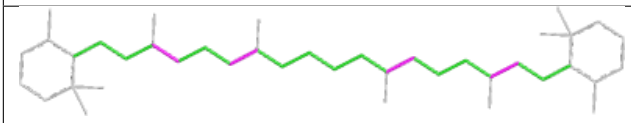
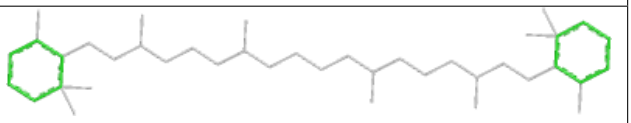


Bond angles

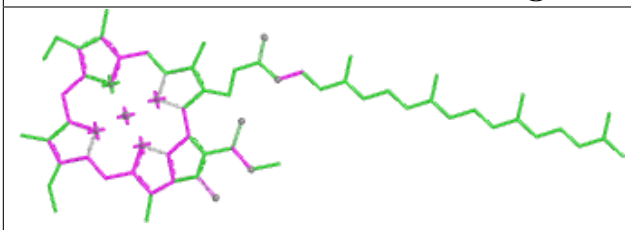


Torsions



Rings

Ligand CLA b 831



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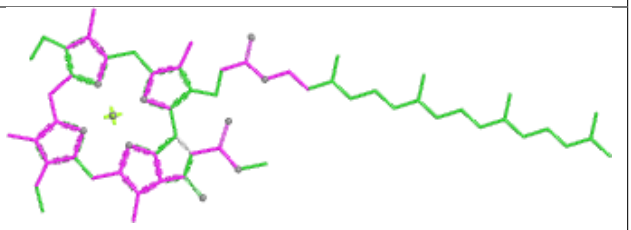
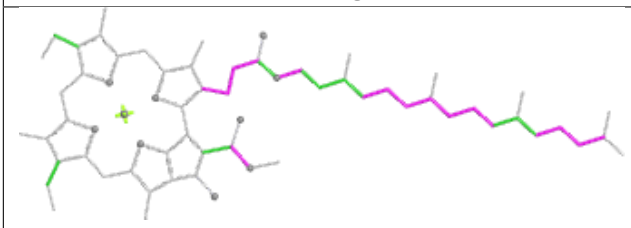


Bond angles



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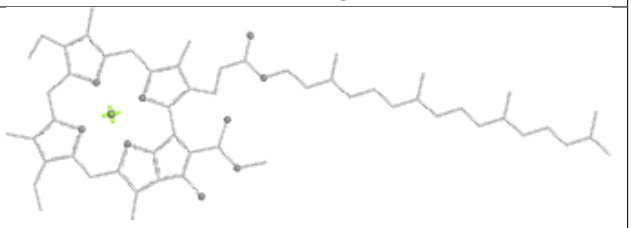
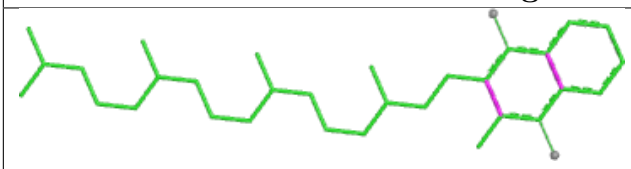


Rings

Ligand PQN A 843



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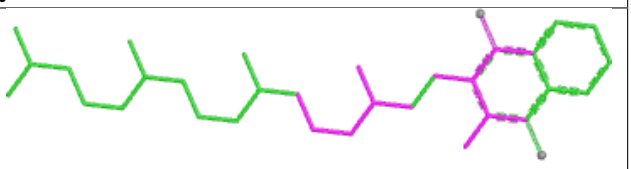
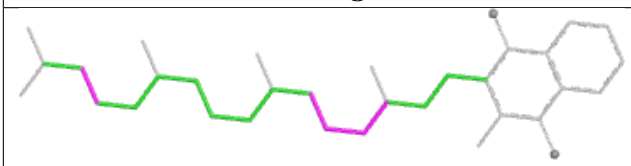


Bond angles



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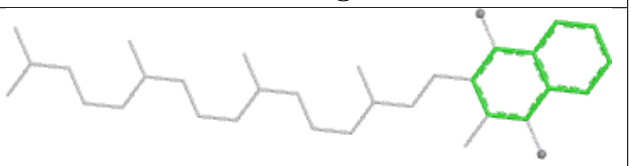
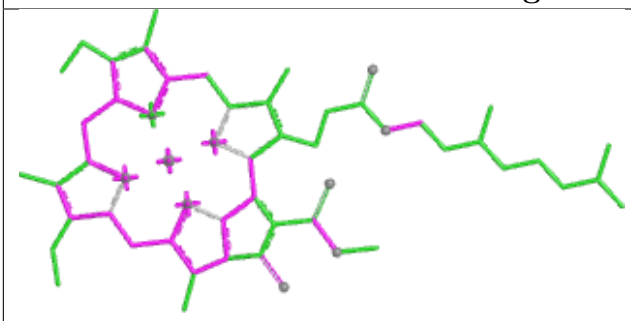


Rings

Ligand CLA G 819



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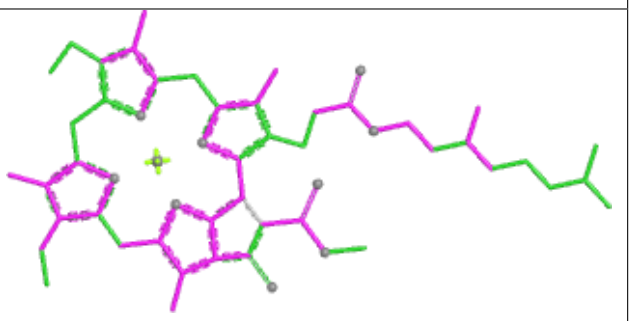
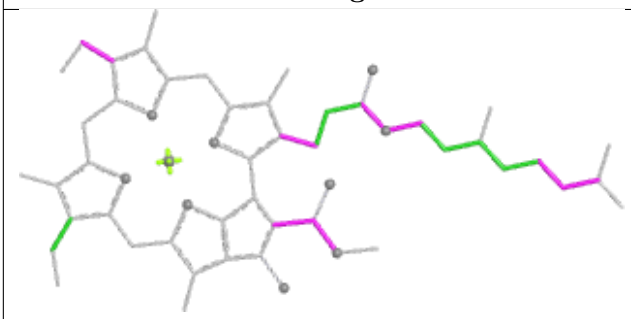


Bond angles



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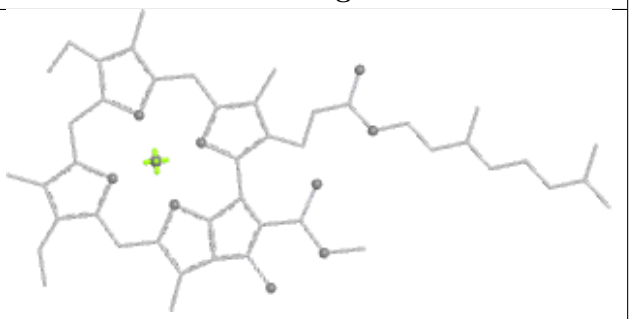
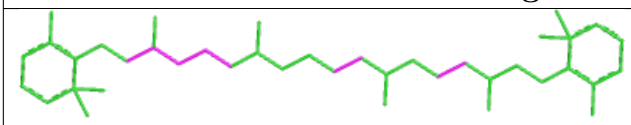
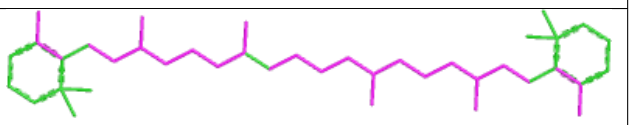


Rings

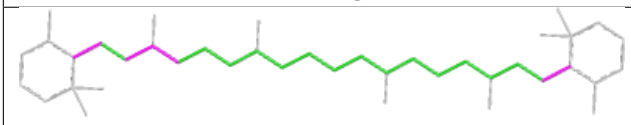
Ligand BCR A 848



Bond lengths



Bond angles



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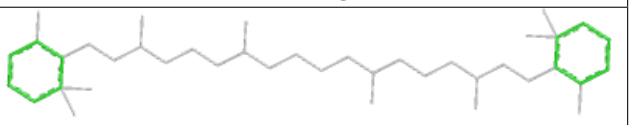
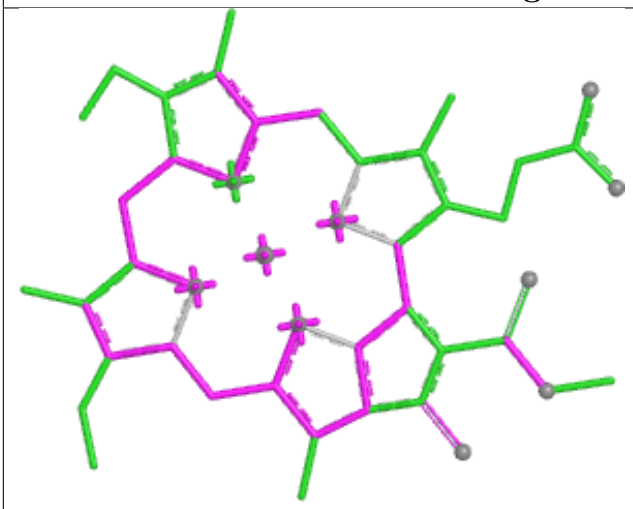


Rings

Ligand CLA H 836



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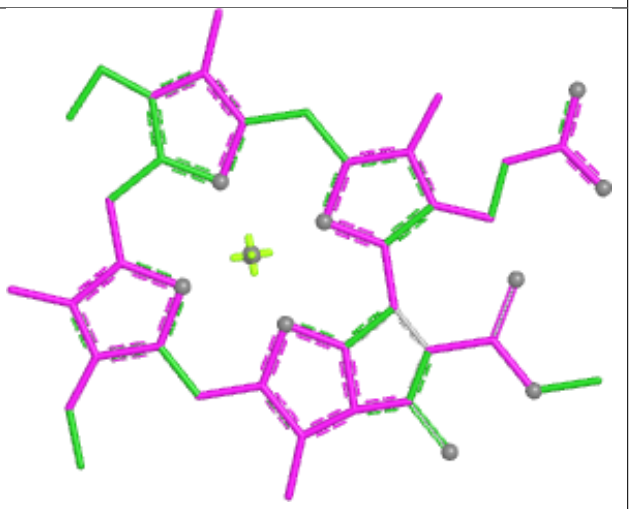
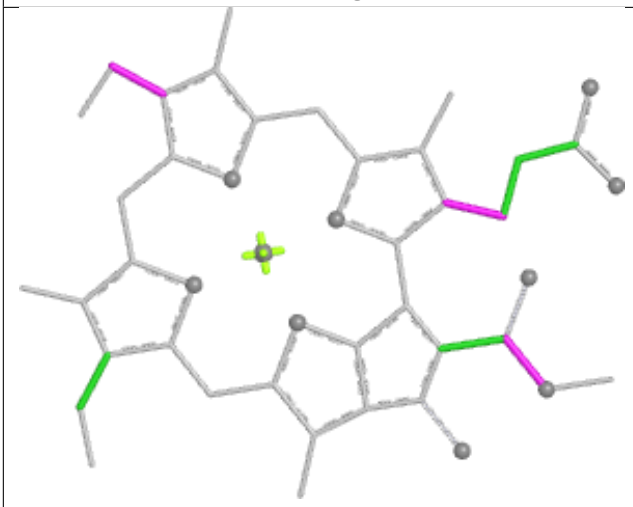


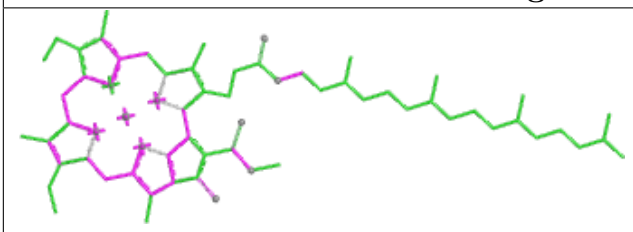
Bond angles



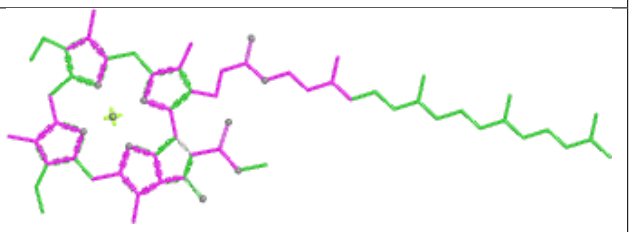
Torsions

Rings

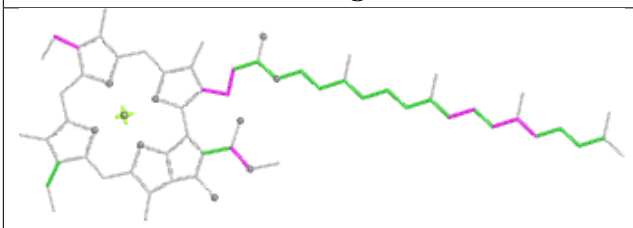
Ligand CLA b 840



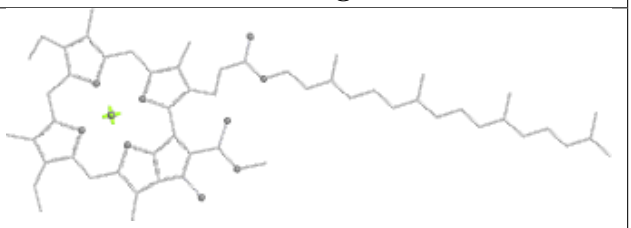
Bond lengths



Bond angles

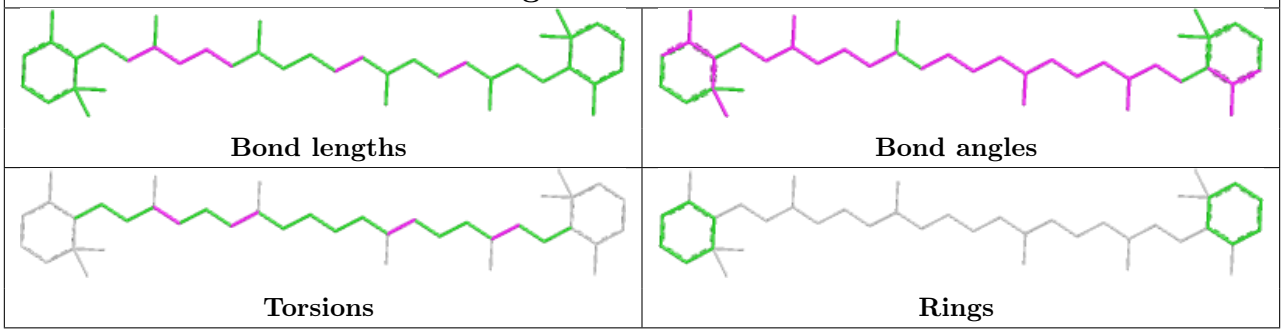


Torsions

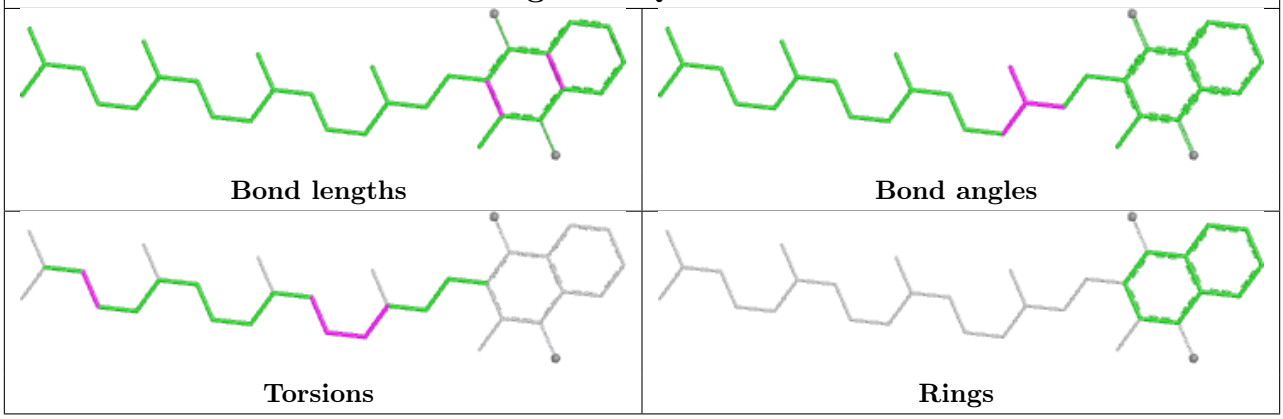


Rings

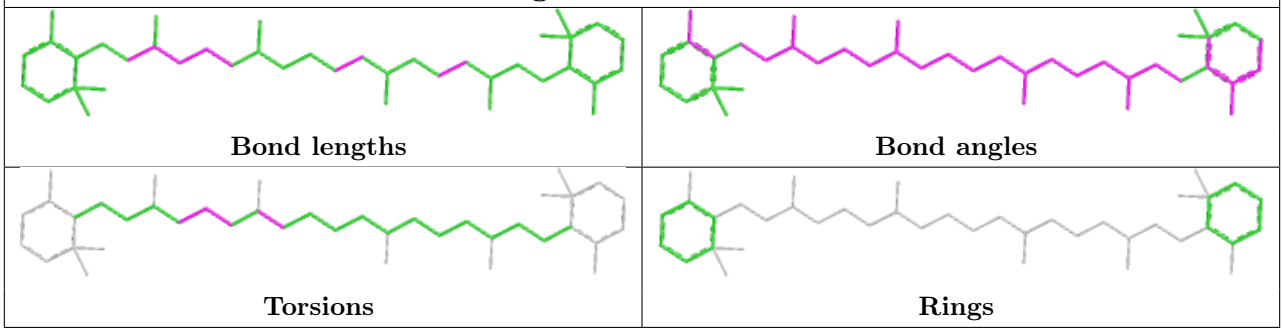
Ligand BCR H 845



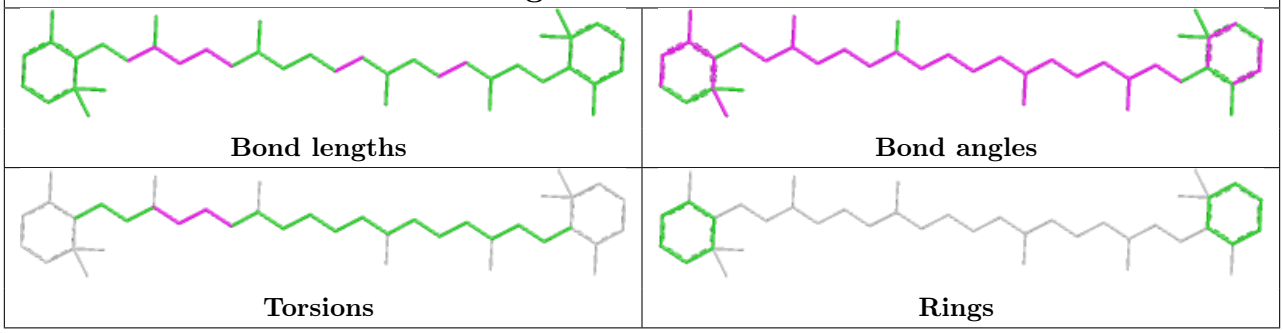
Ligand PQN a 843

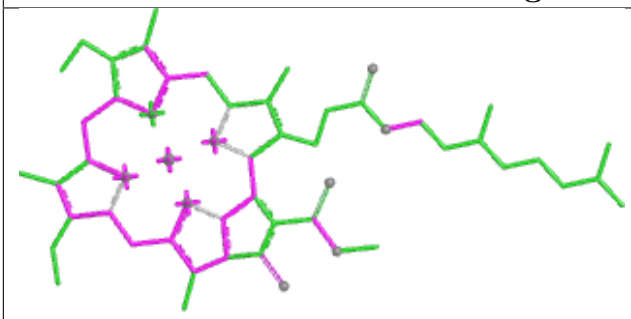
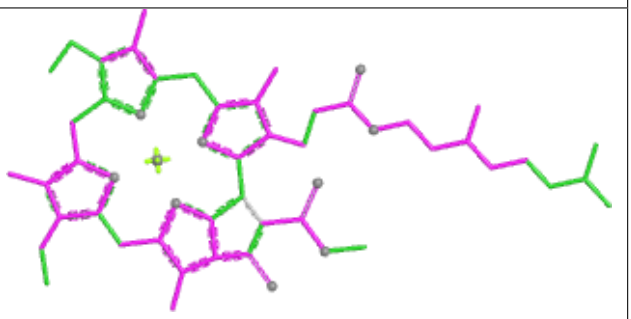
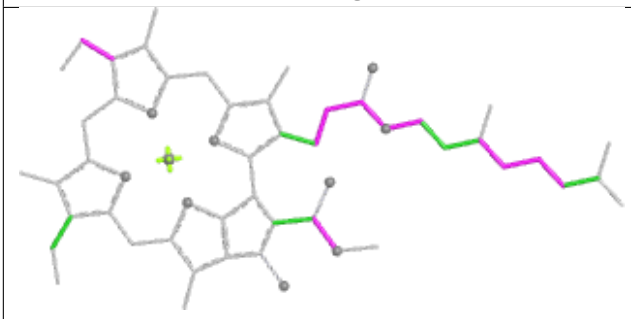
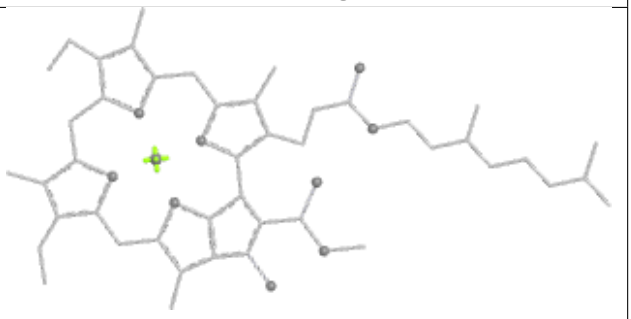


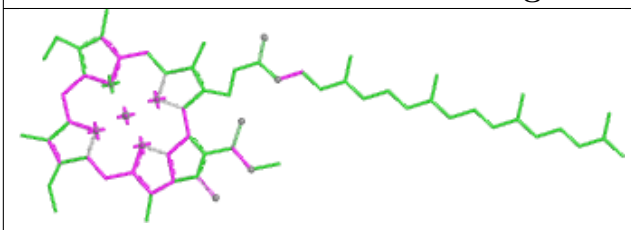
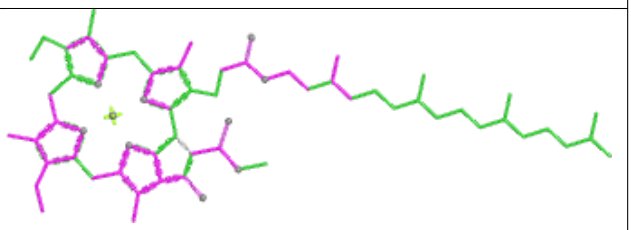
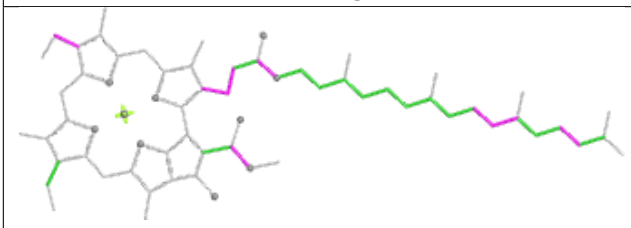
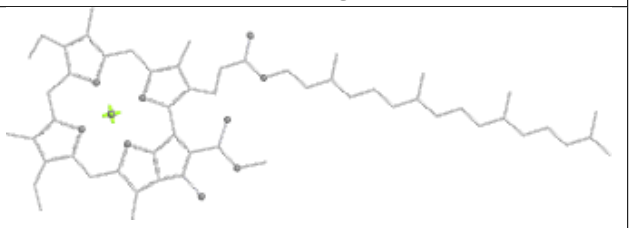
Ligand BCR f 201



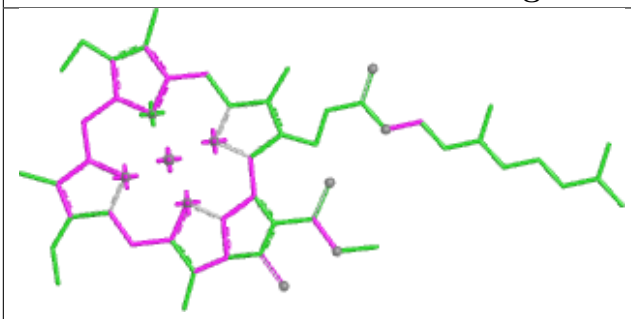
Ligand BCR L 209



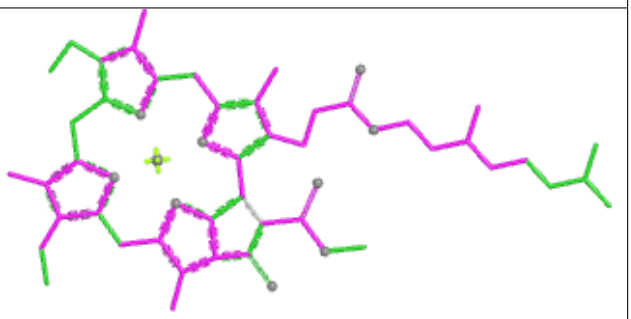
Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

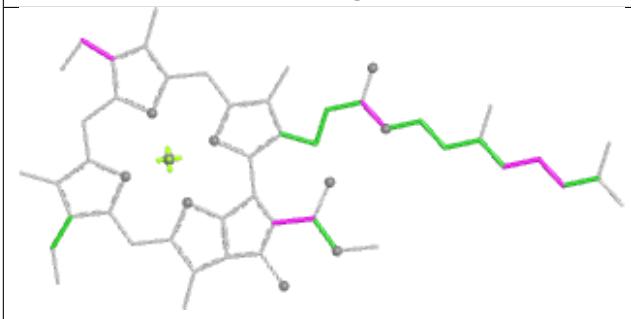
Ligand CLA G 803



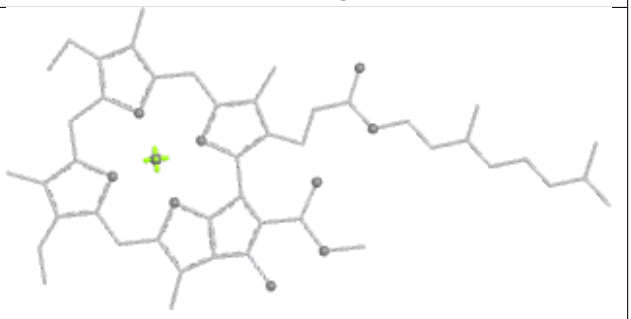
Bond lengths



Bond angles

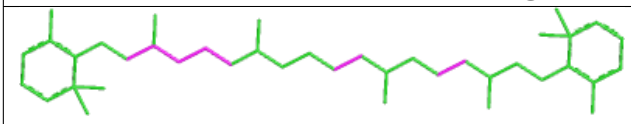


Torsions

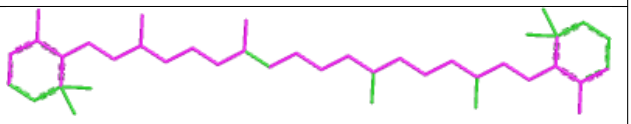


Rings

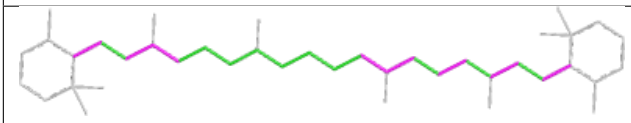
Ligand BCR A 849



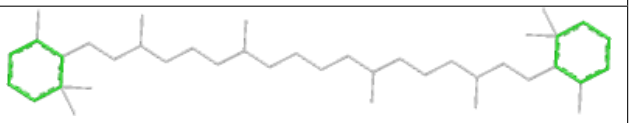
Bond lengths



Bond angles

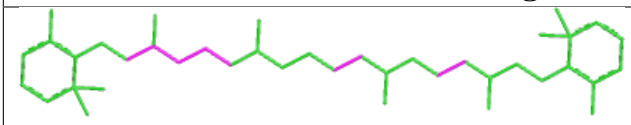


Torsions

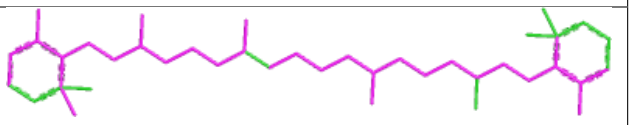


Rings

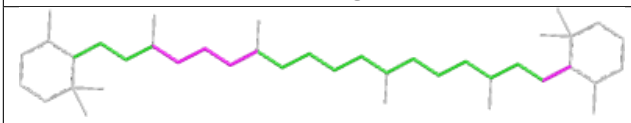
Ligand BCR G 846



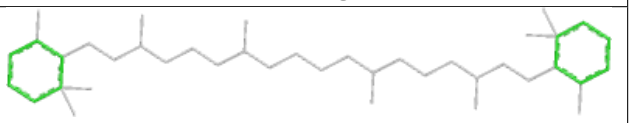
Bond lengths



Bond angles

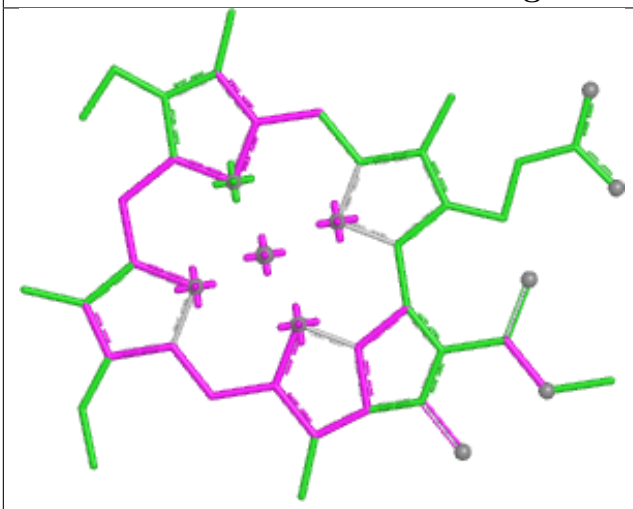


Torsions

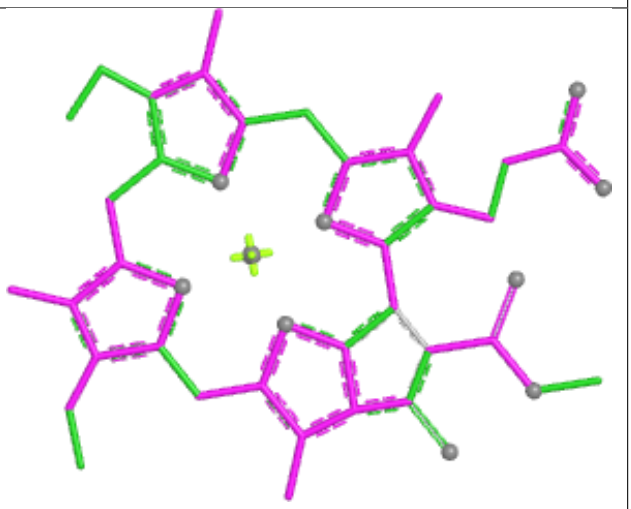


Rings

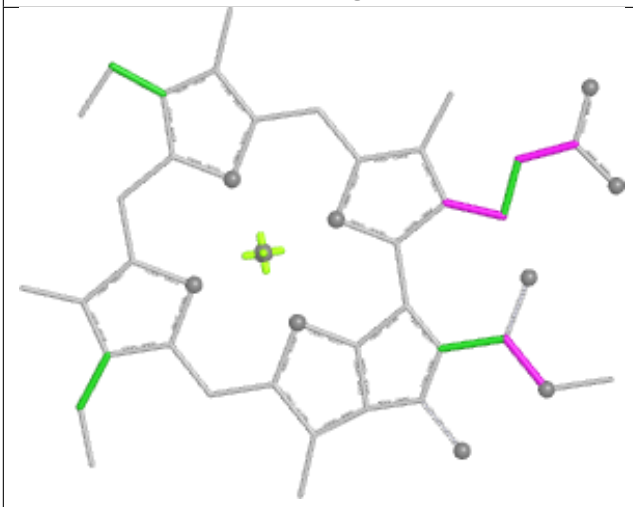
Ligand CLA H 840



Bond lengths



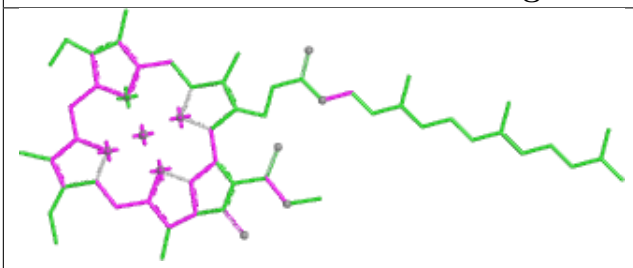
Bond angles



Torsions

Rings

Ligand CLA G 812



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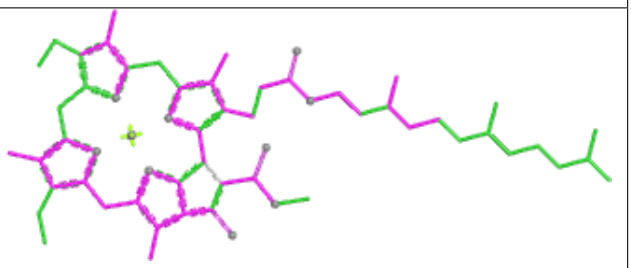
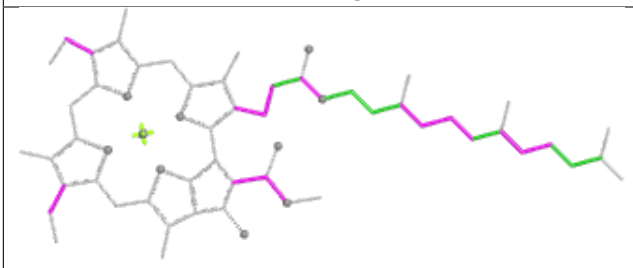
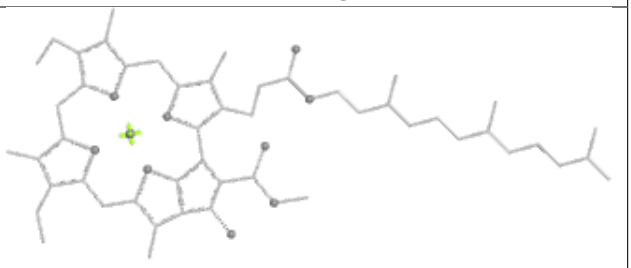


Bond angles

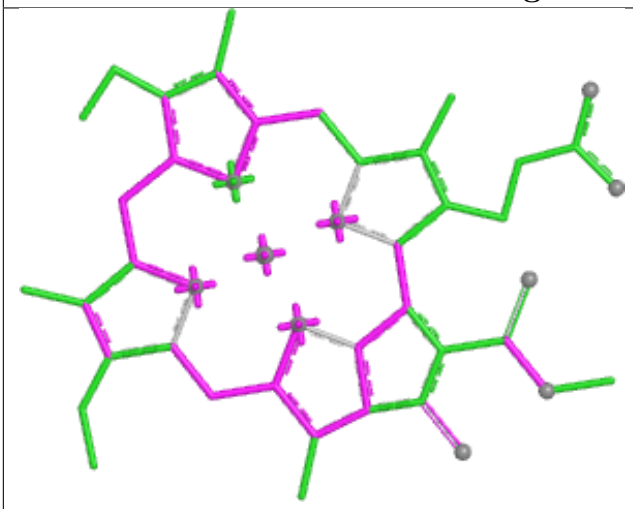


Torsions



Rings

Ligand CLA H 813



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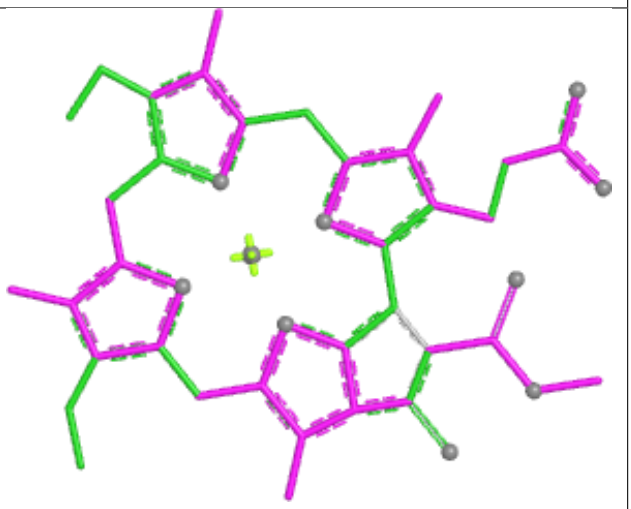
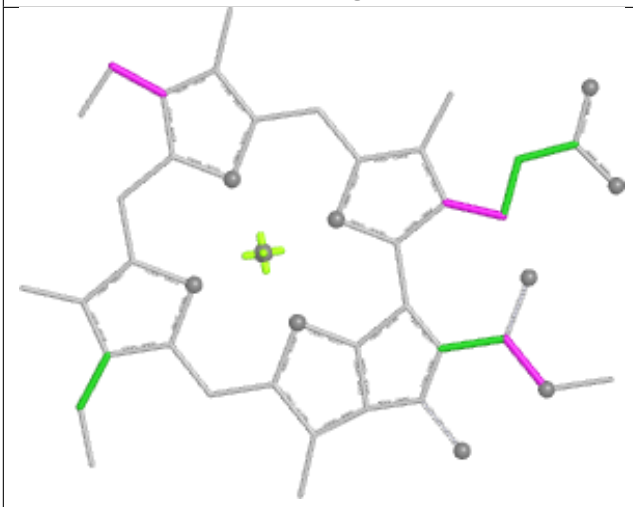


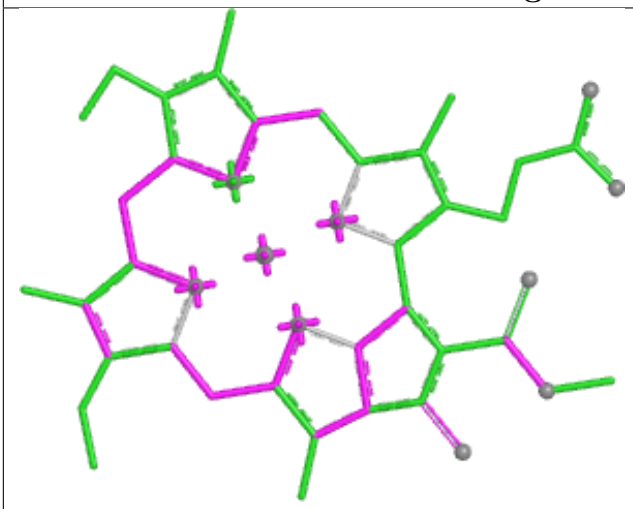
Bond angles



Torsions

Rings

Ligand CLA B 832



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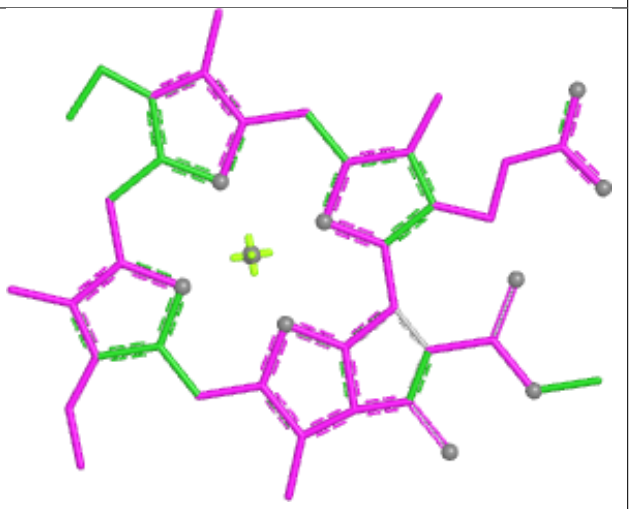
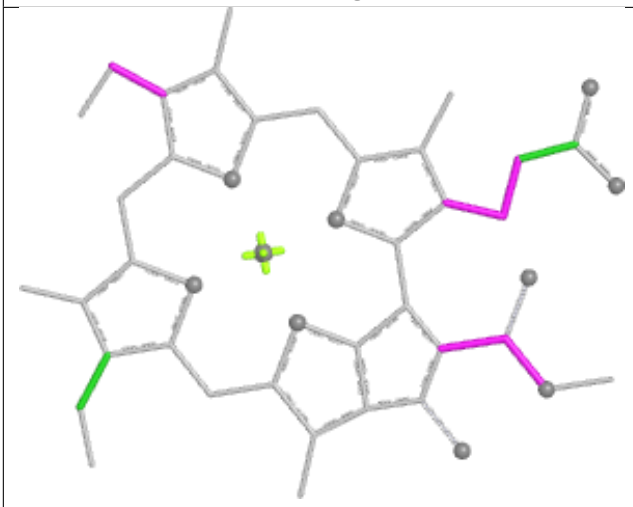


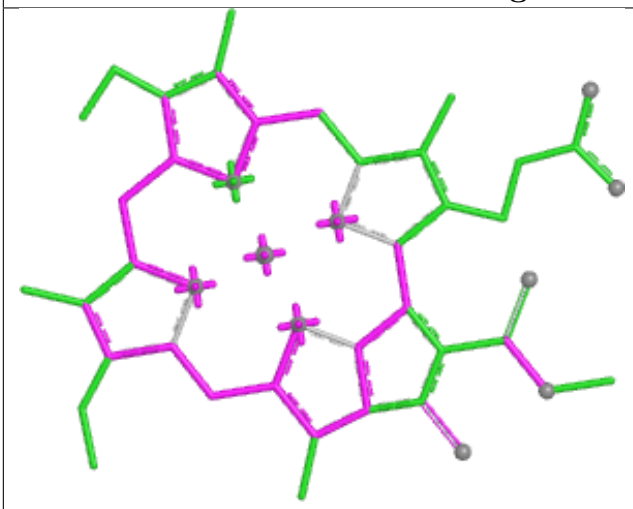
Bond angles



Torsions

Rings

Ligand CLA W 1701



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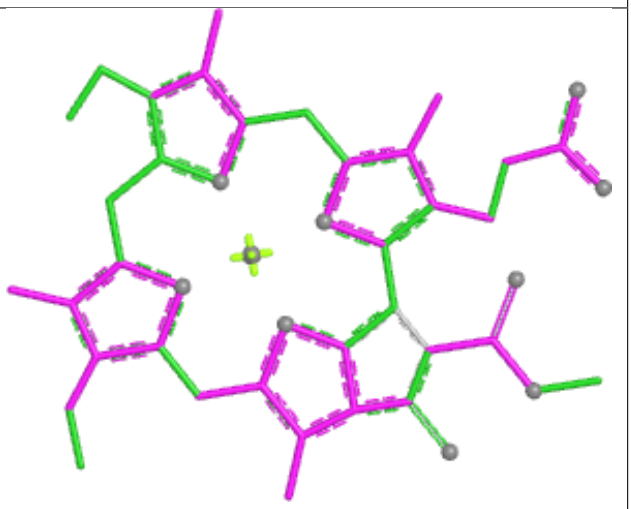
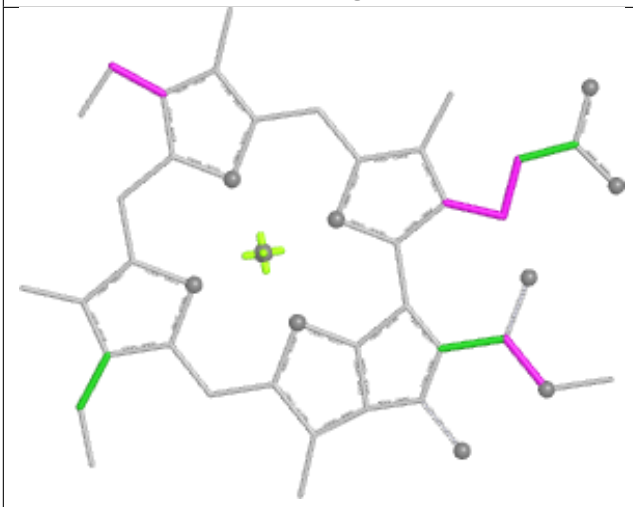
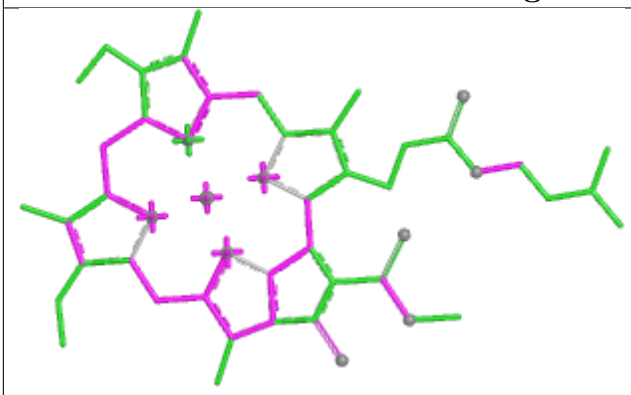
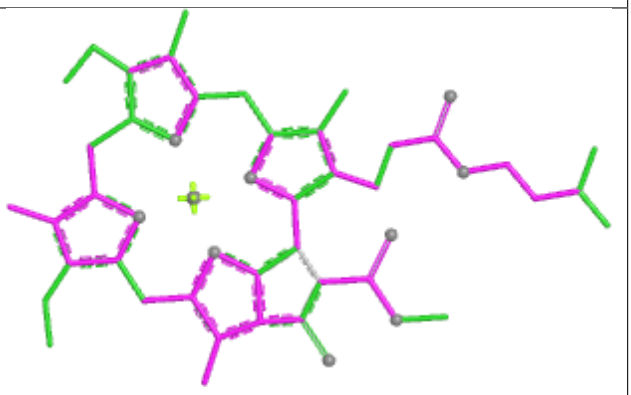
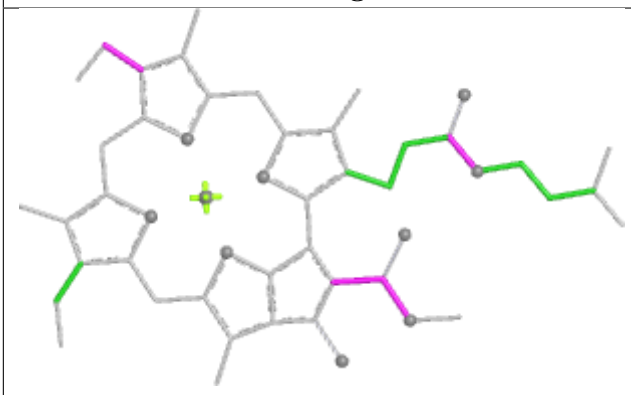
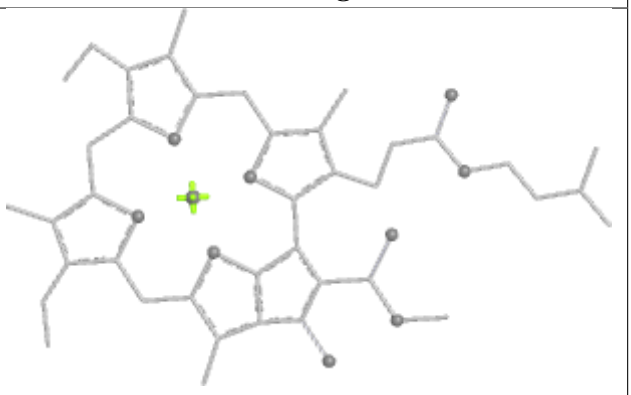


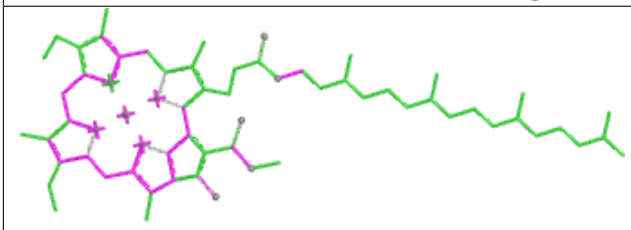
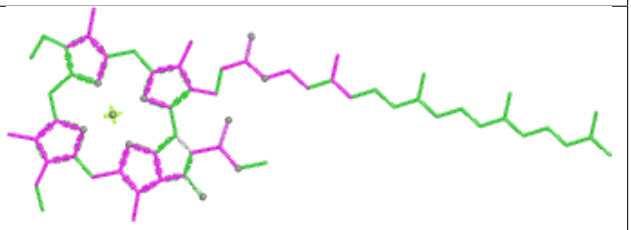
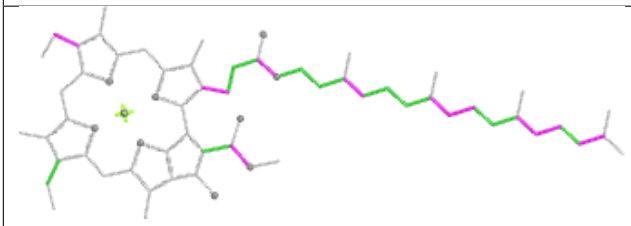
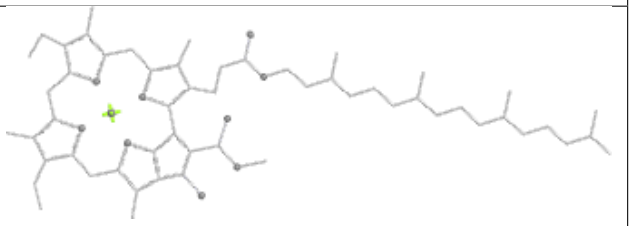
Bond angles

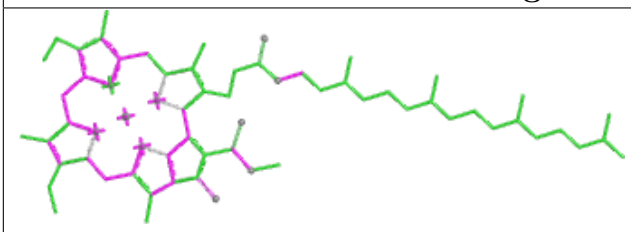
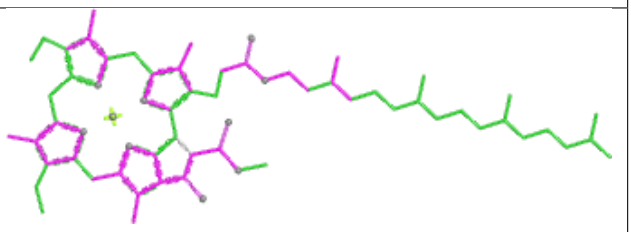
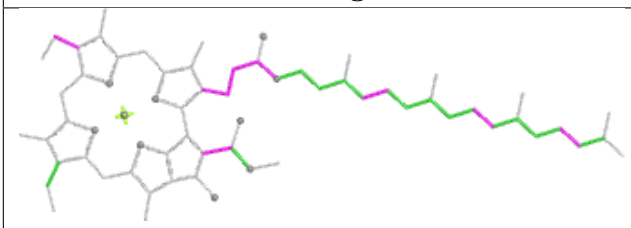
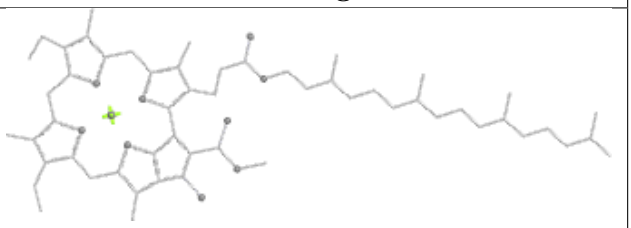


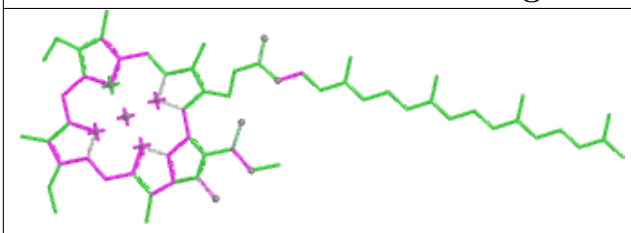
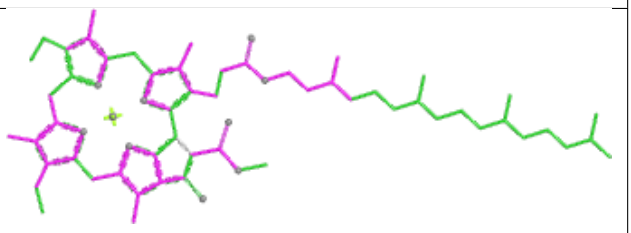
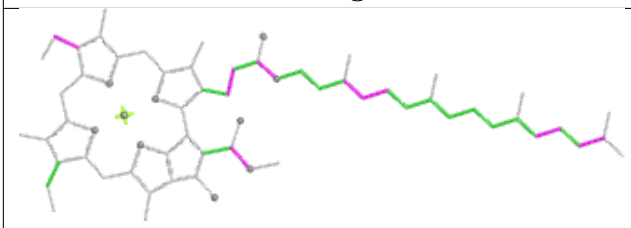
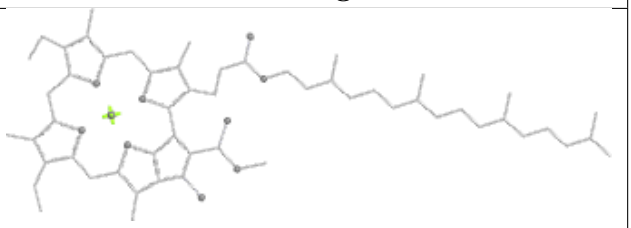
Torsions

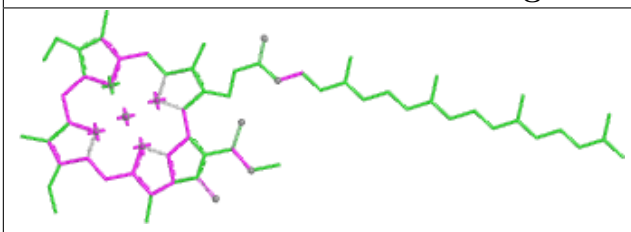
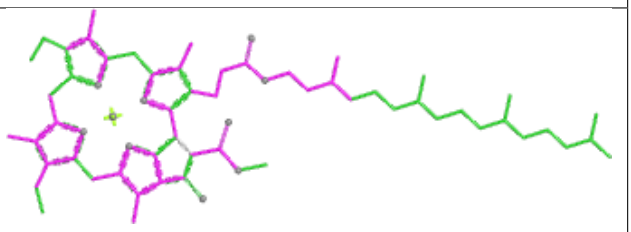
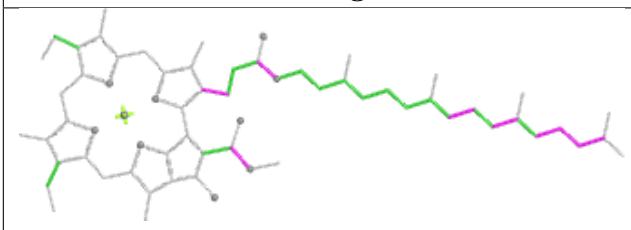
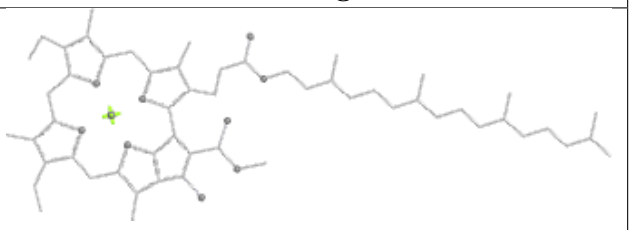
Rings

Ligand CLA A 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

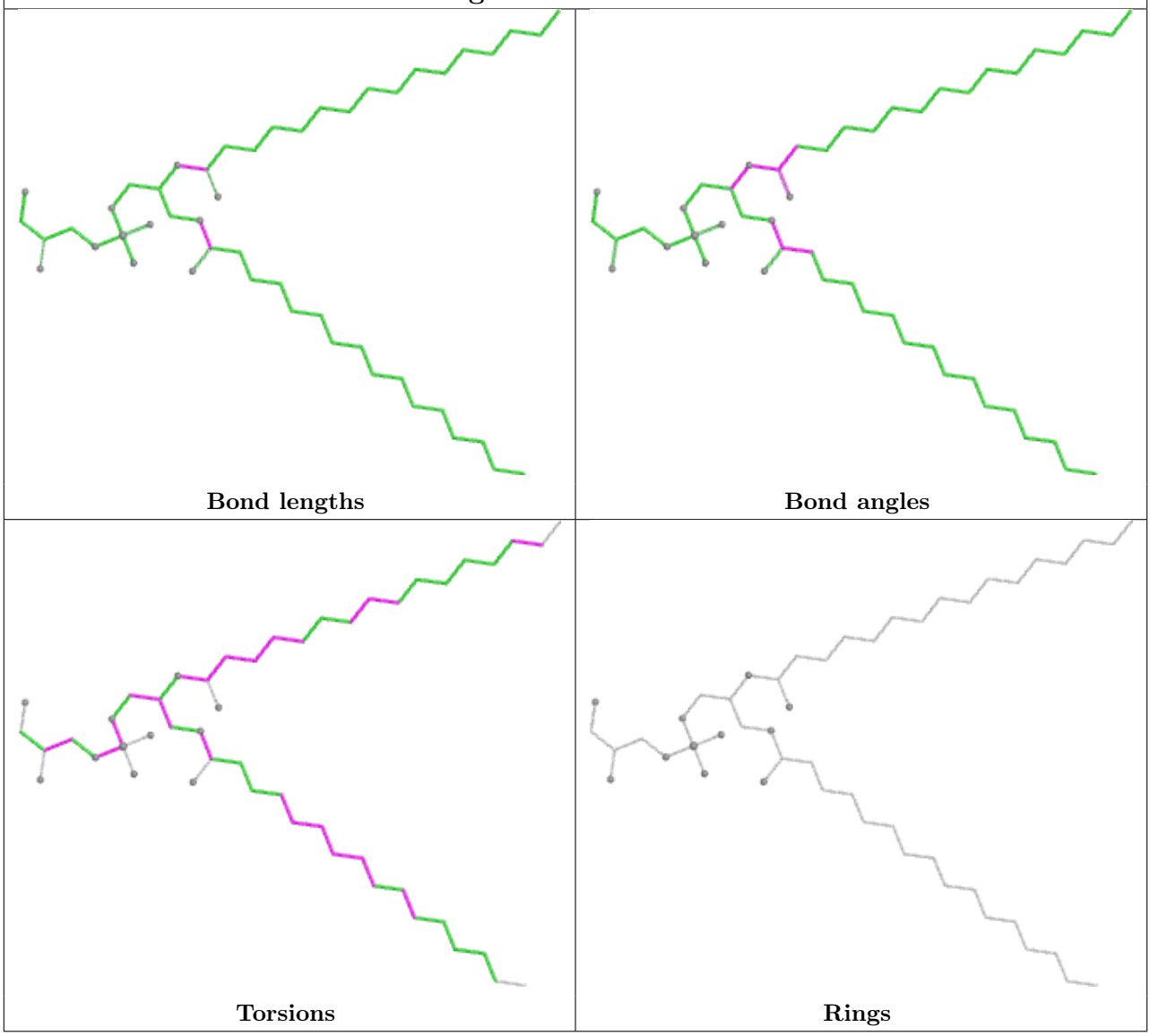
Ligand CLA L 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

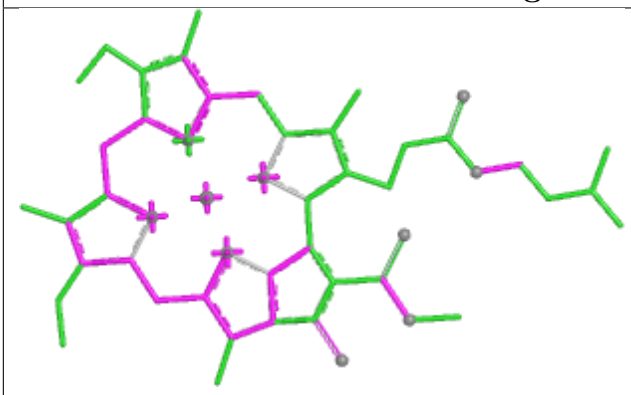
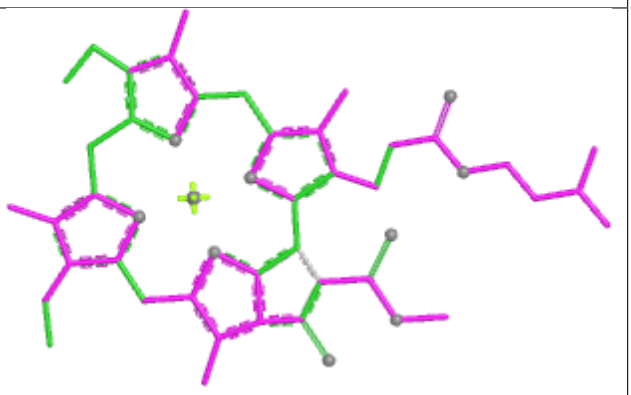
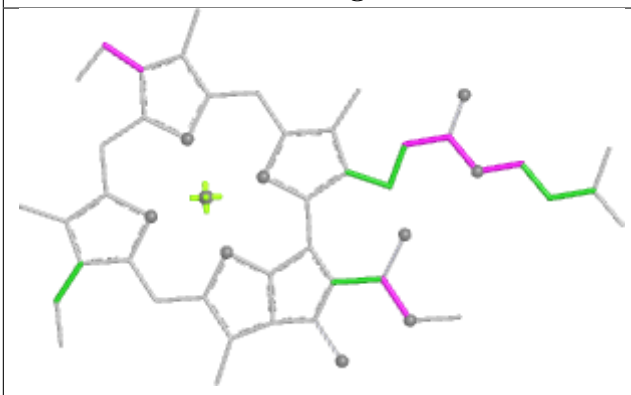
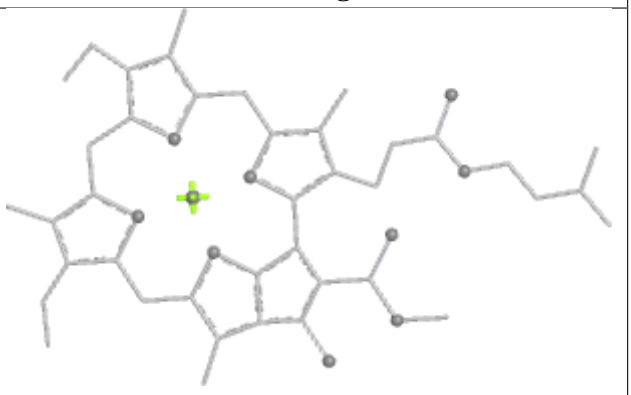
Ligand CLA U 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

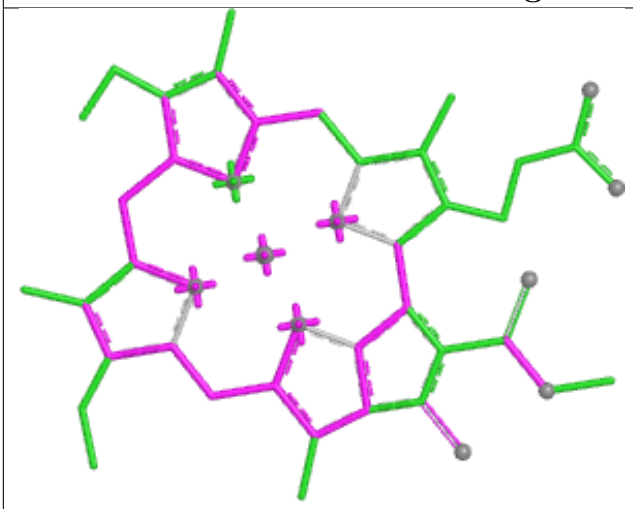
Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 850

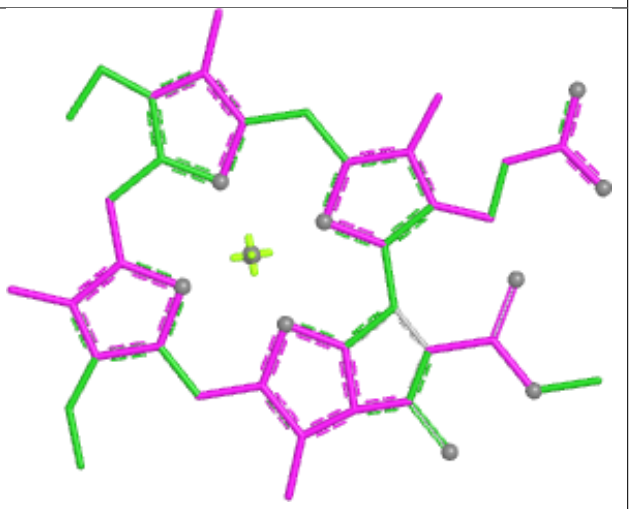


Ligand CLA A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

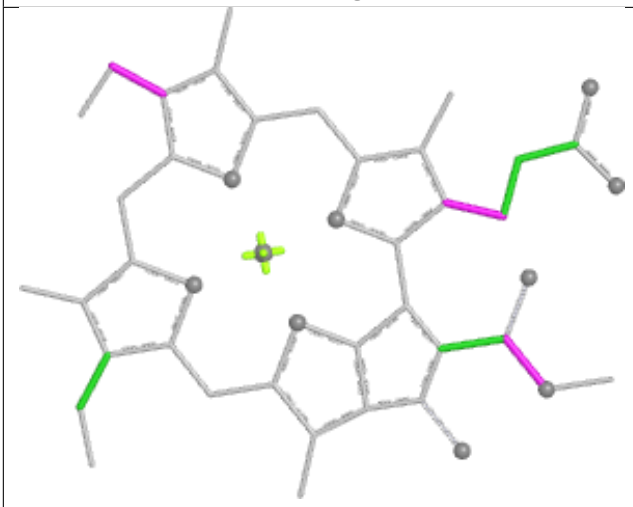
Ligand CLA B 813



Bond lengths



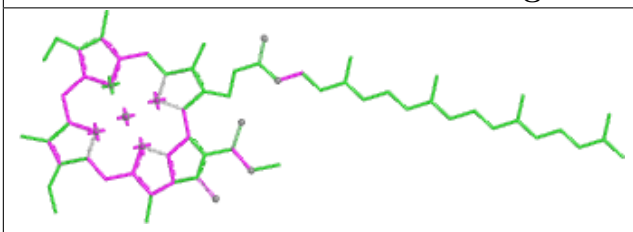
Bond angles



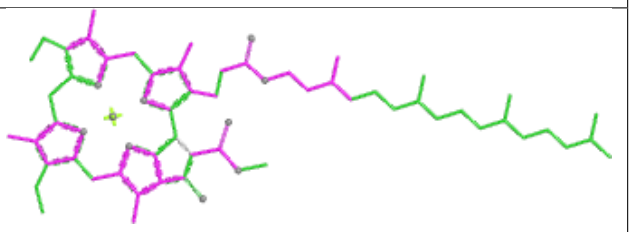
Torsions

Rings

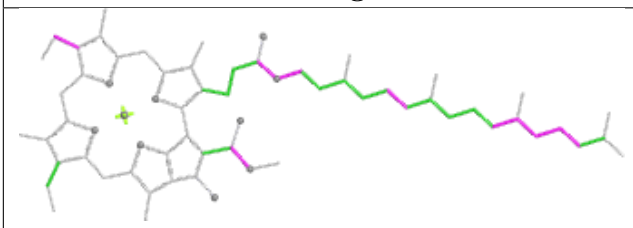
Ligand CLA A 825



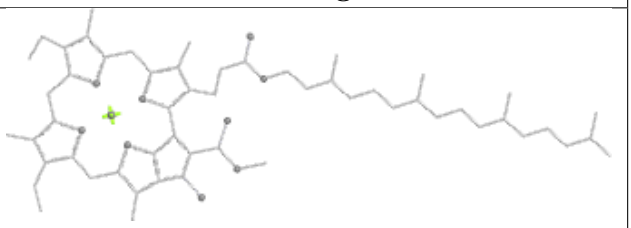
Bond lengths



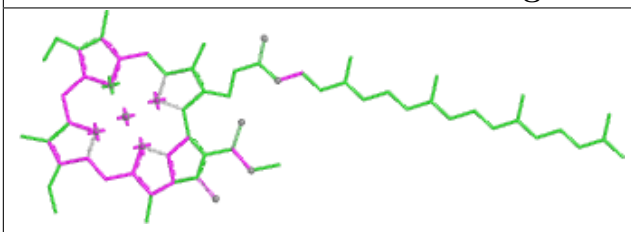
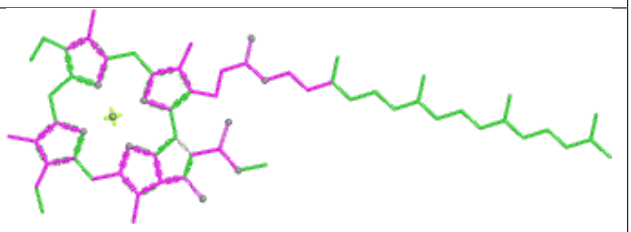
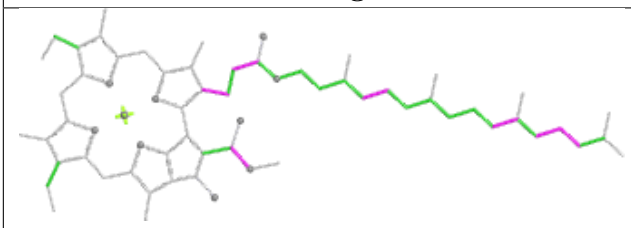
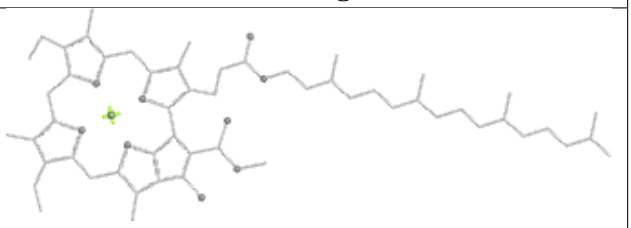
Bond angles

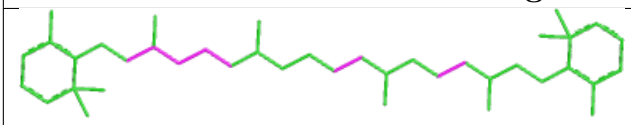
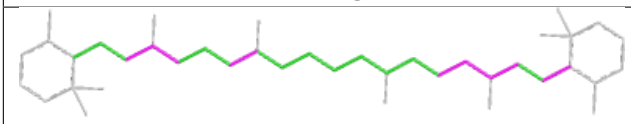
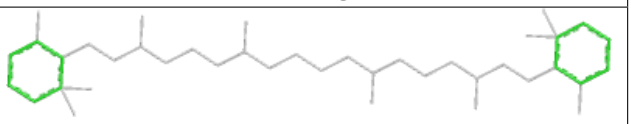


Torsions

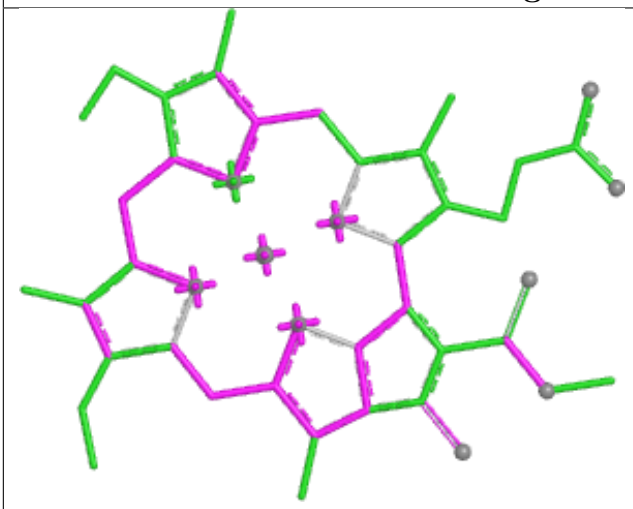


Rings

Ligand CLA H 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 844	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA A 814



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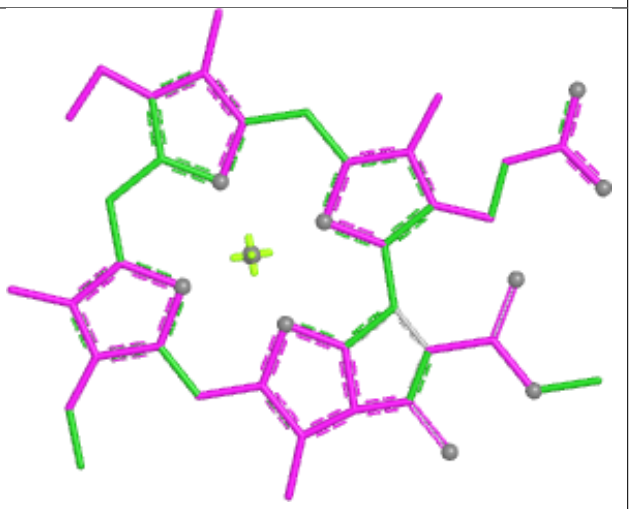

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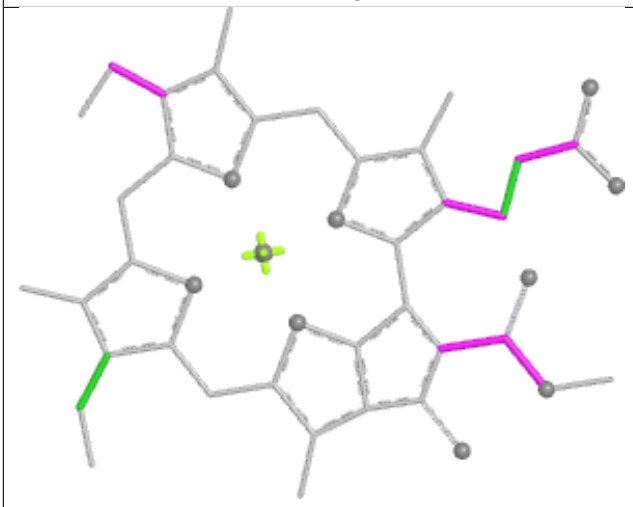
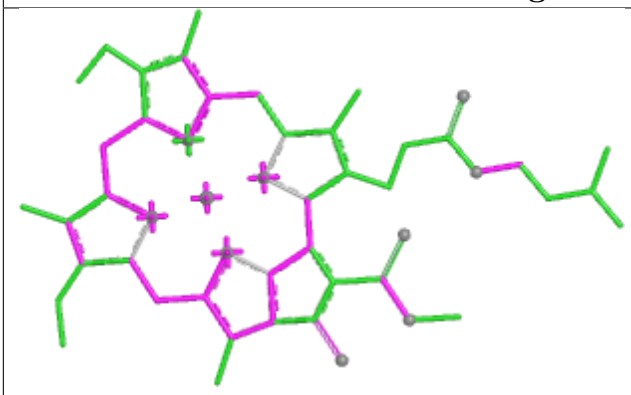
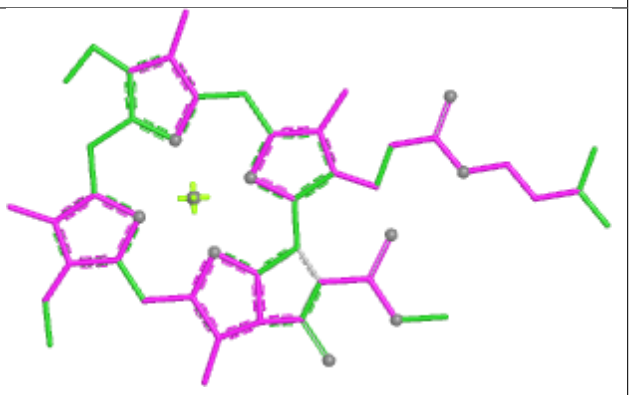
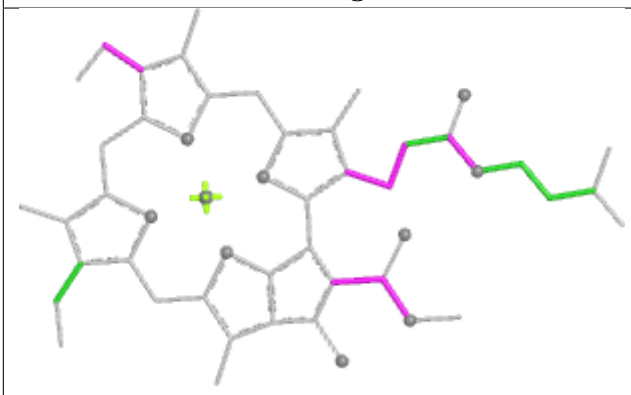
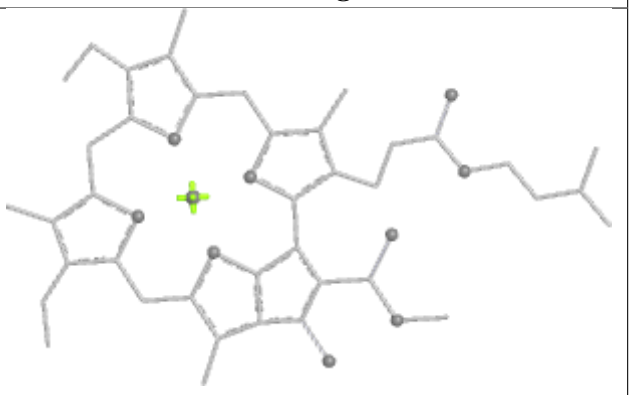
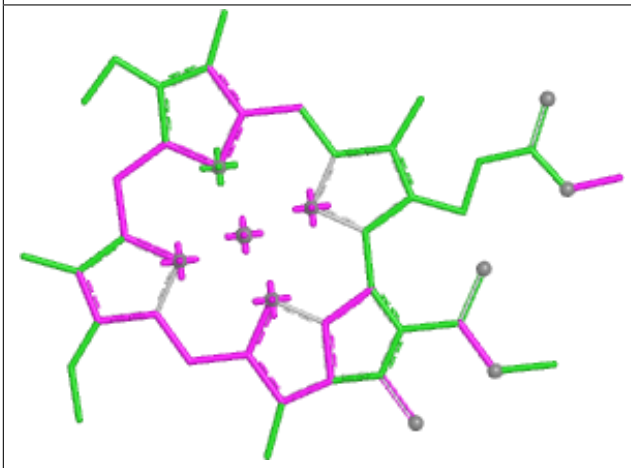


Torsions

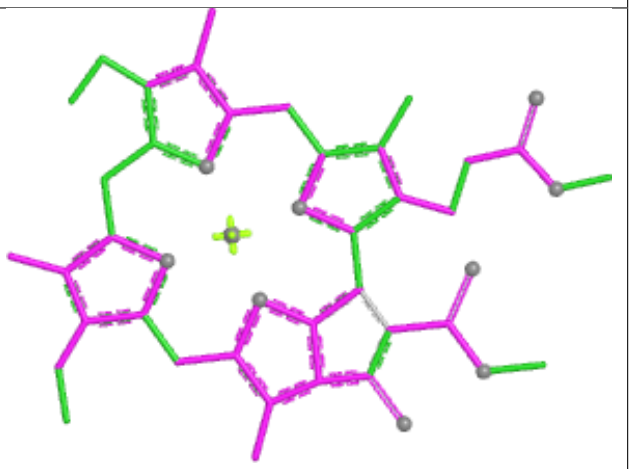
Rings

Ligand CLA a 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 827



Bond lengths



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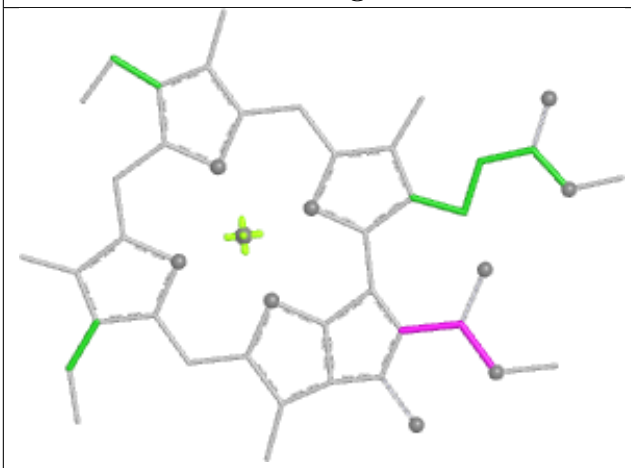

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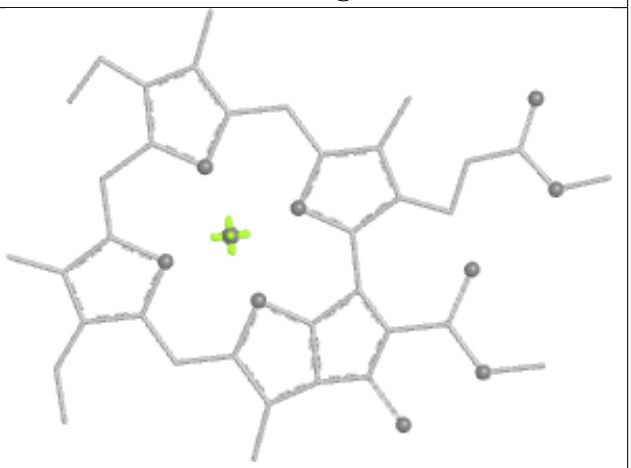
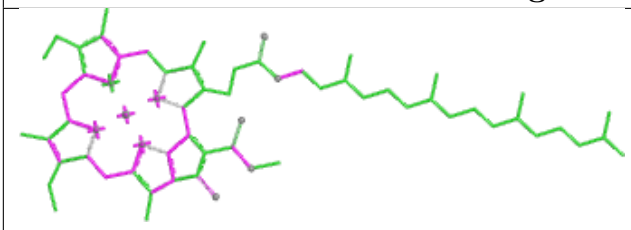
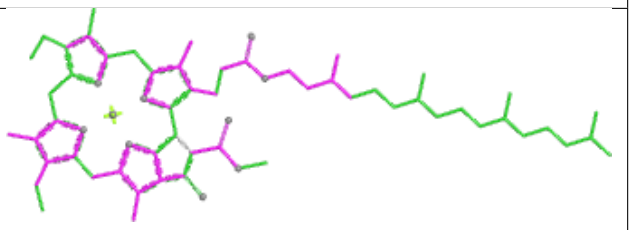


Rings

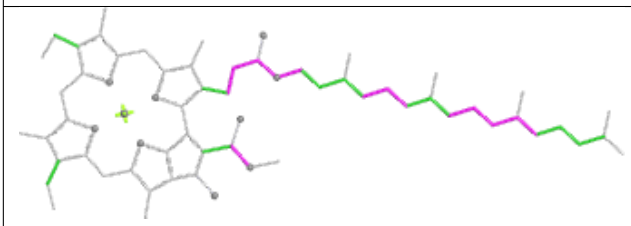
Ligand CLA a 828



Bond lengths



Bond angles



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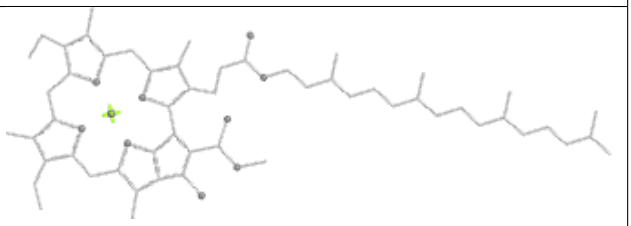
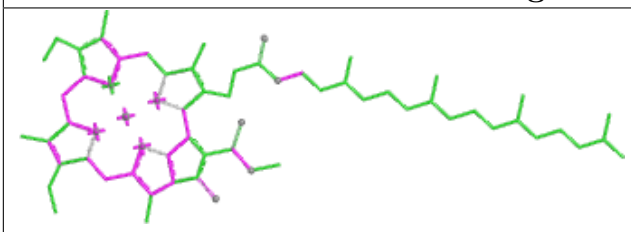
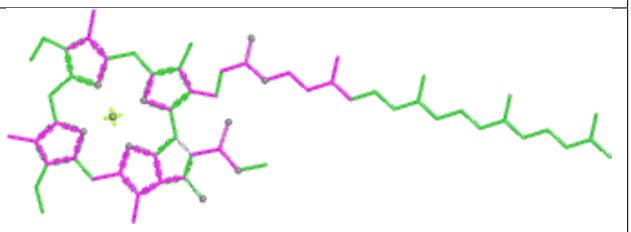
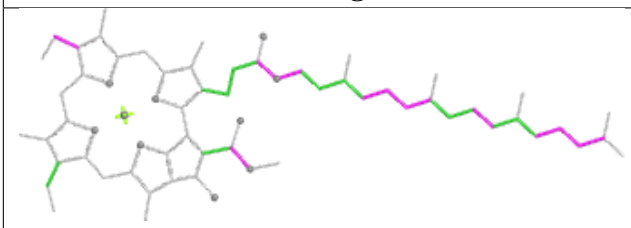
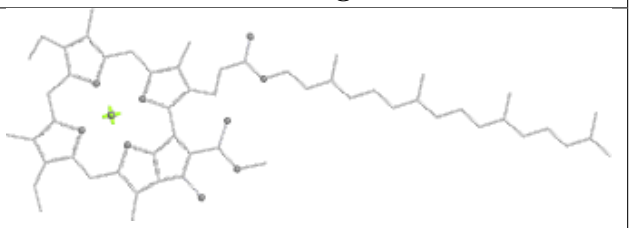
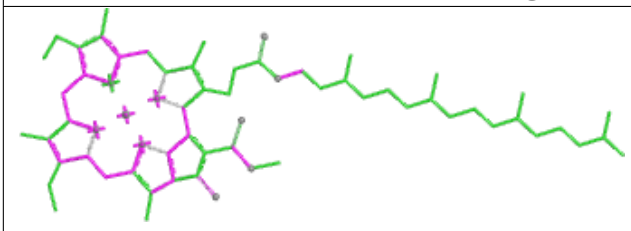
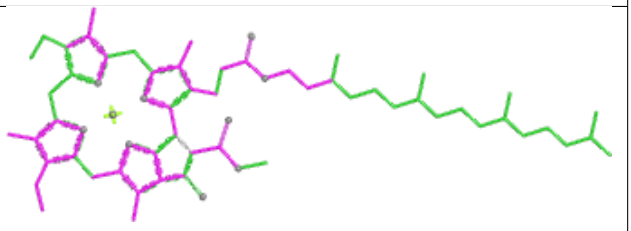
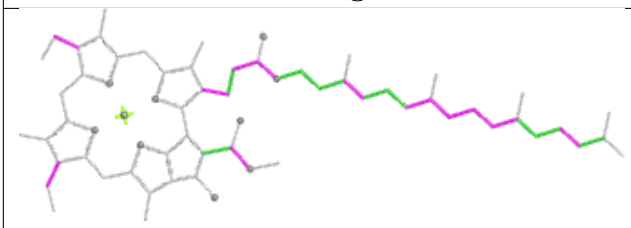
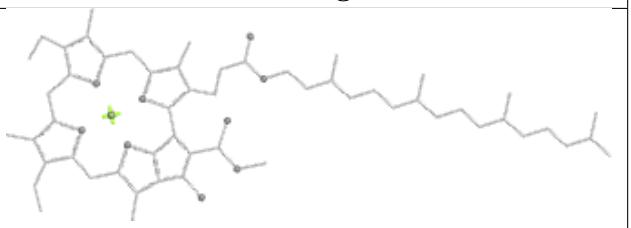
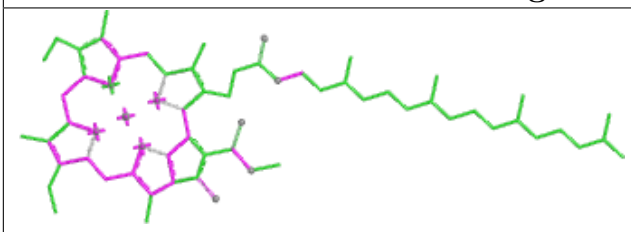
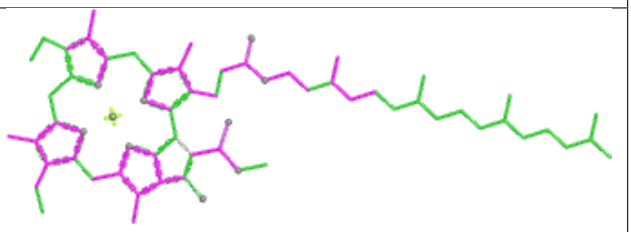
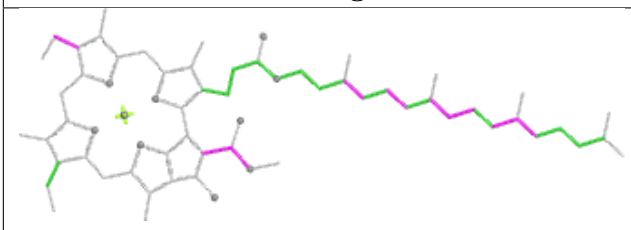
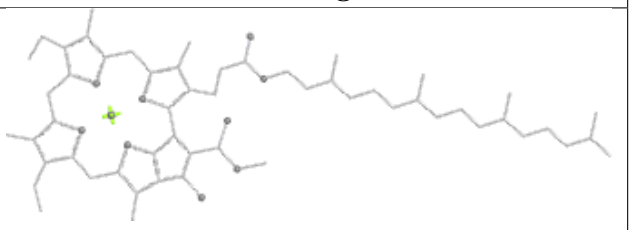


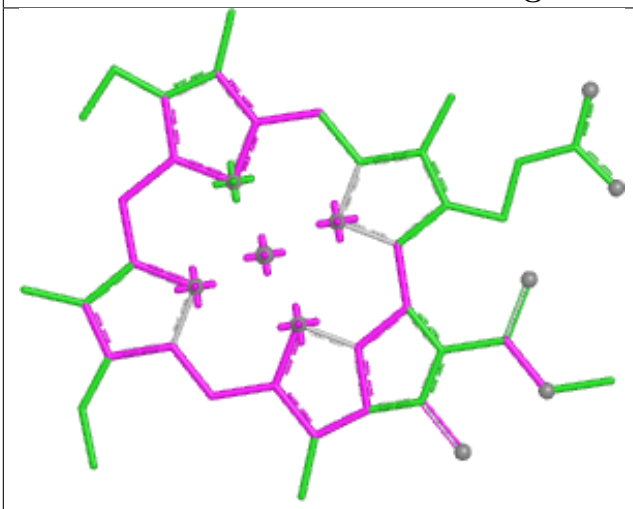
Rings

Ligand CLA b 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

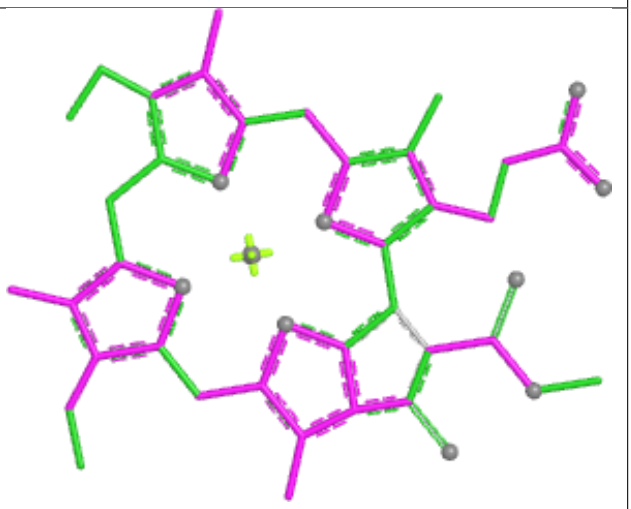
Ligand CLA H 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

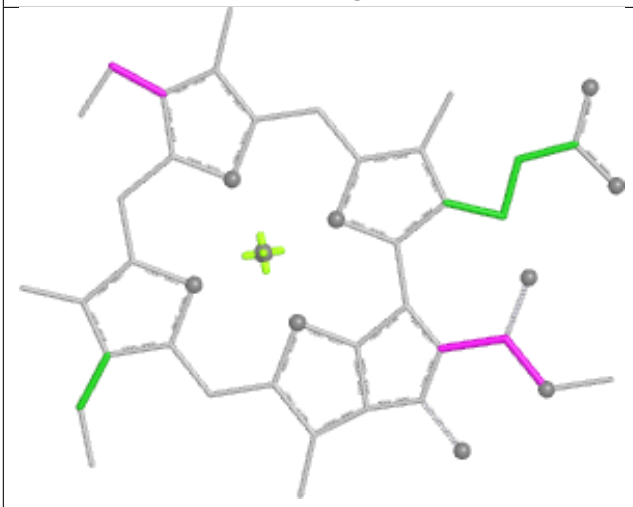
Ligand CLA B 835



Bond lengths

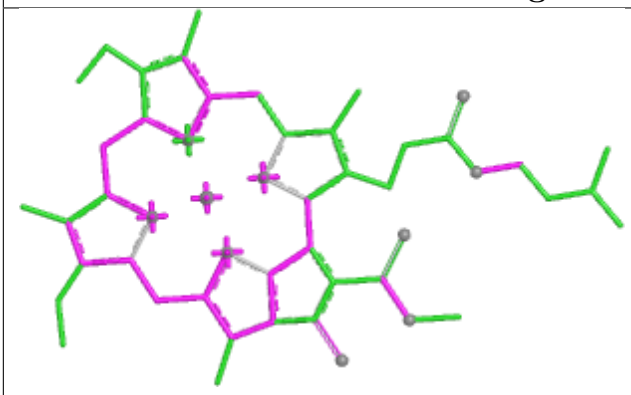
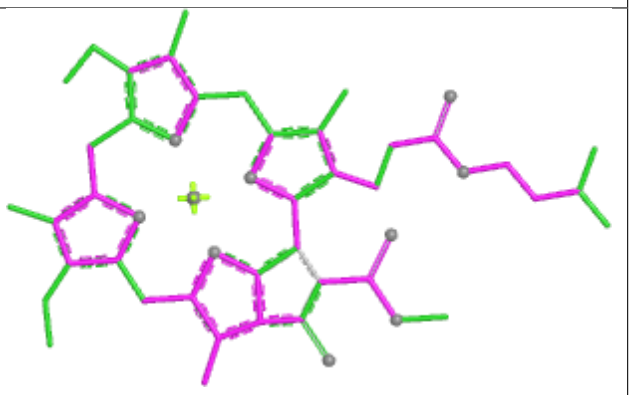
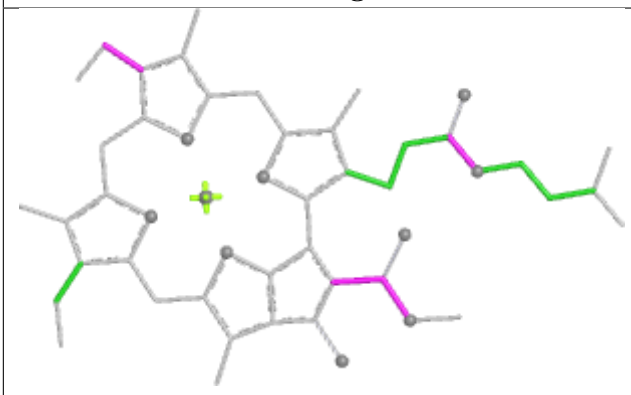
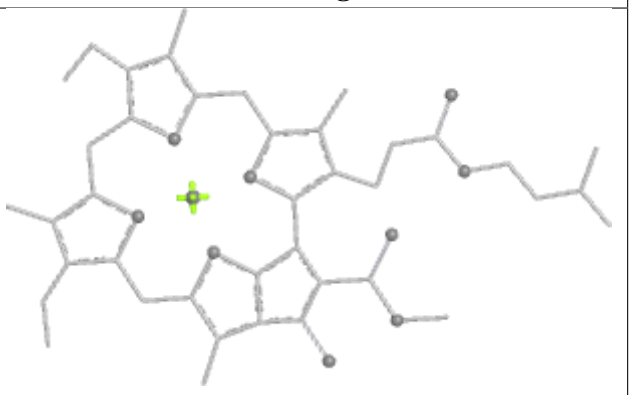


Bond angles

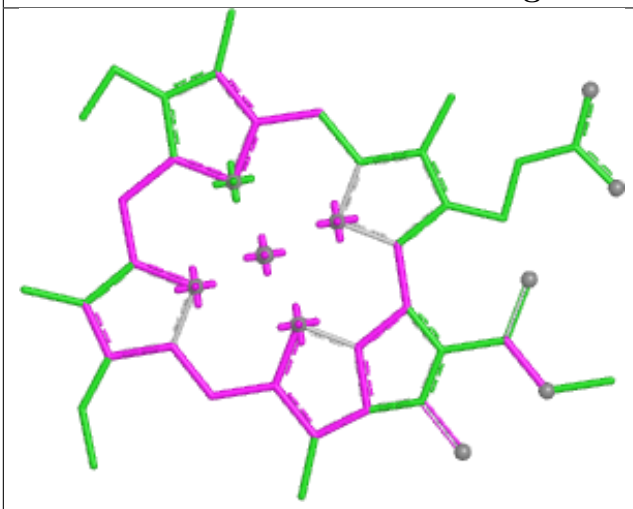


Torsions

Rings

Ligand CLA a 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 837



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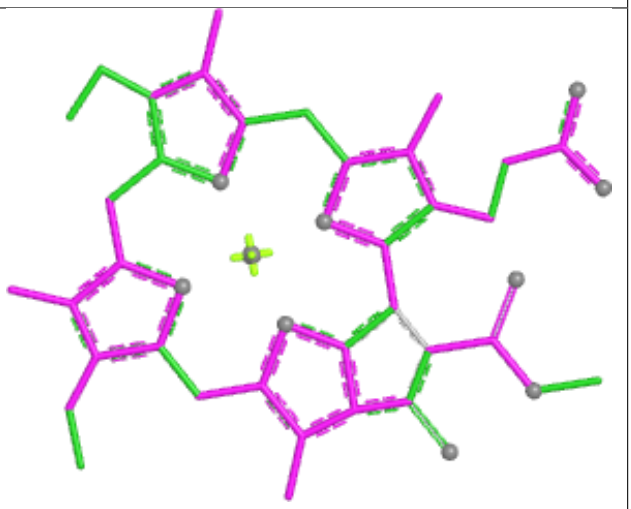
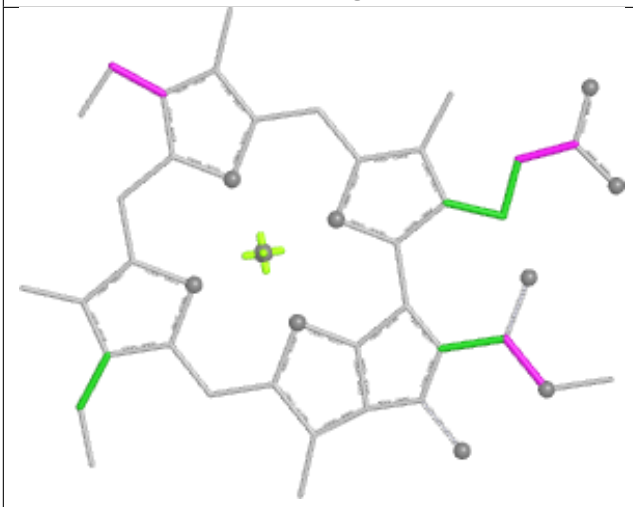
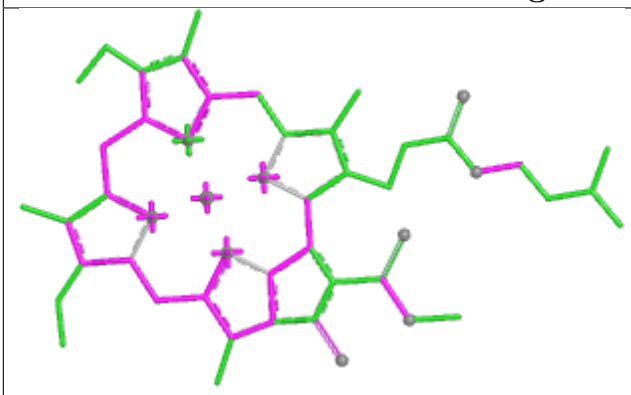
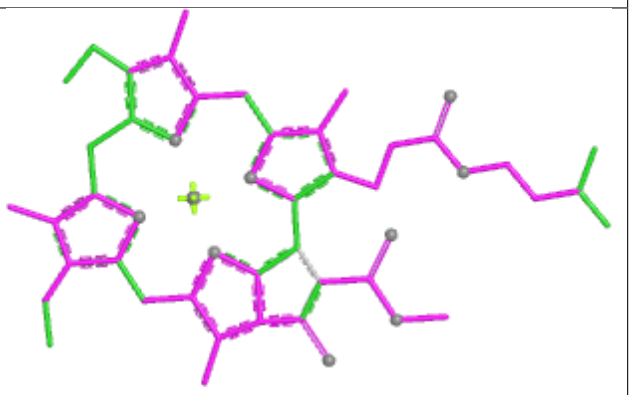
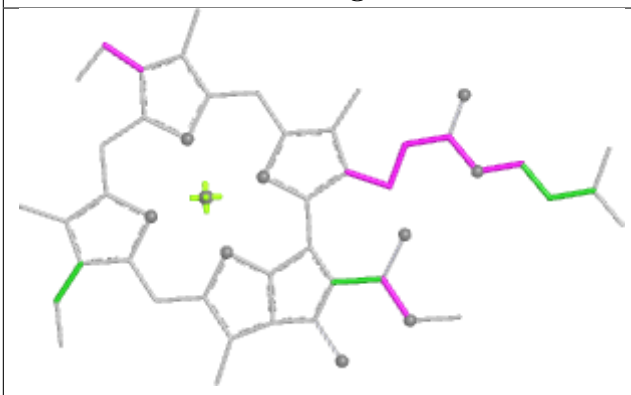
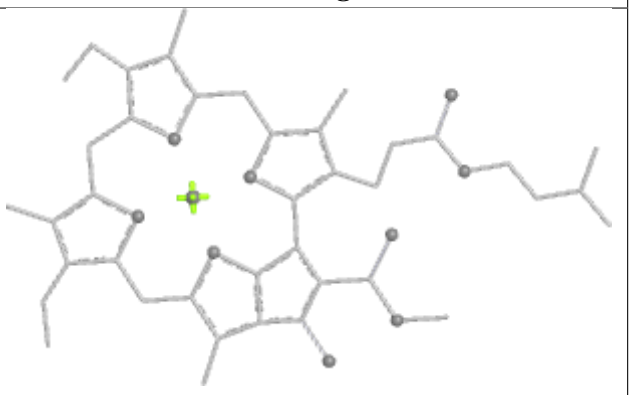


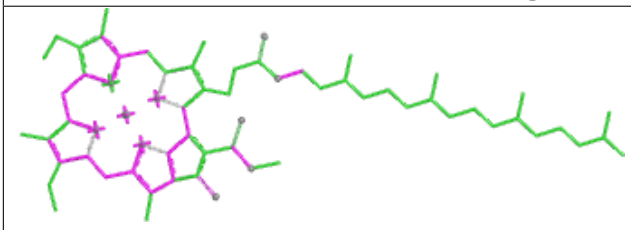
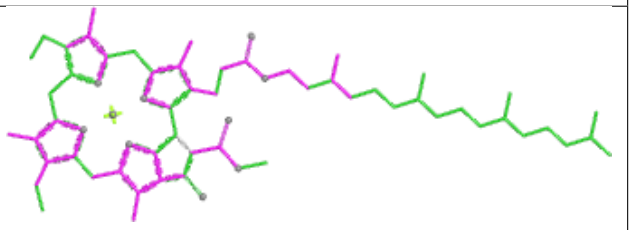
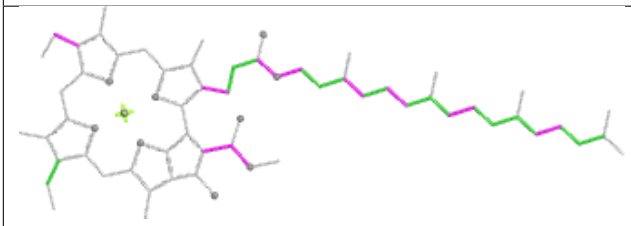
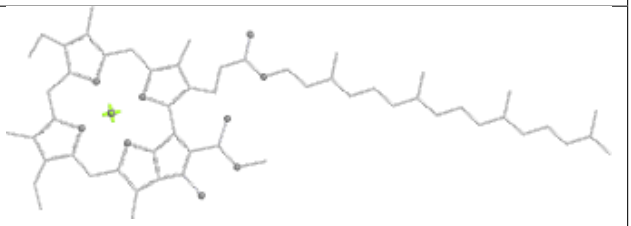
Bond angles



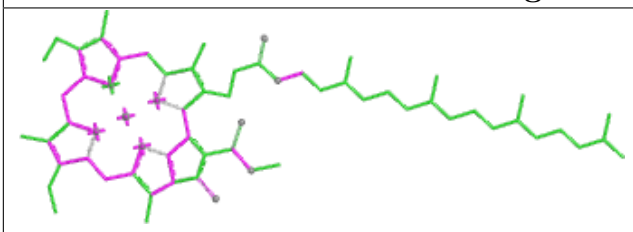
Torsions

Rings

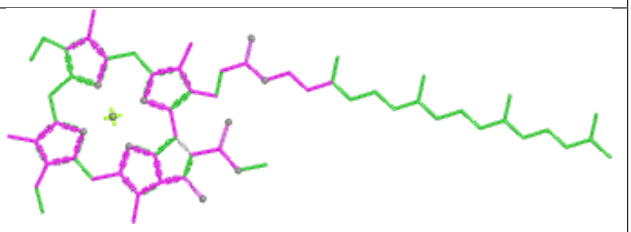
Ligand CLA a 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

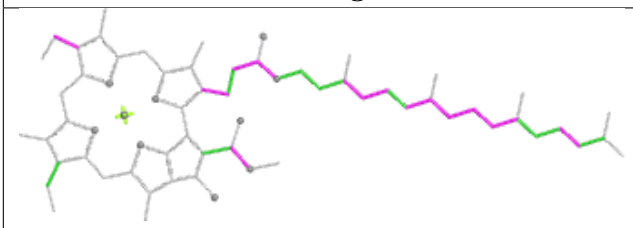
Ligand CLA B 815



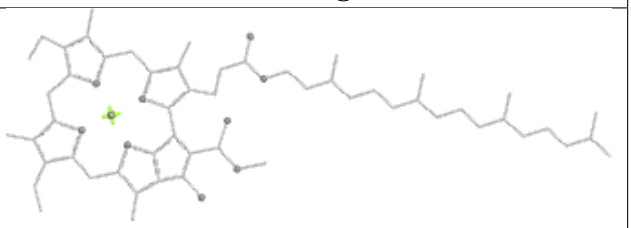
Bond lengths



Bond angles

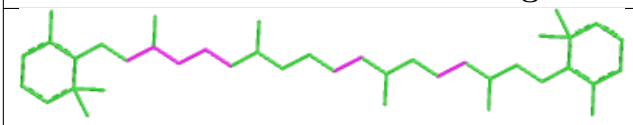


Torsions



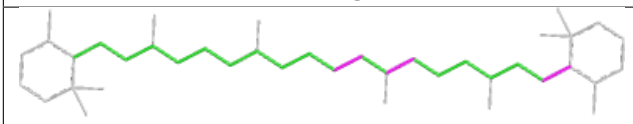
Rings

Ligand BCR H 848

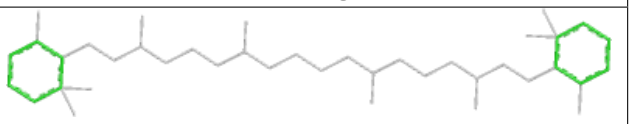


Bond lengths

Bond angles

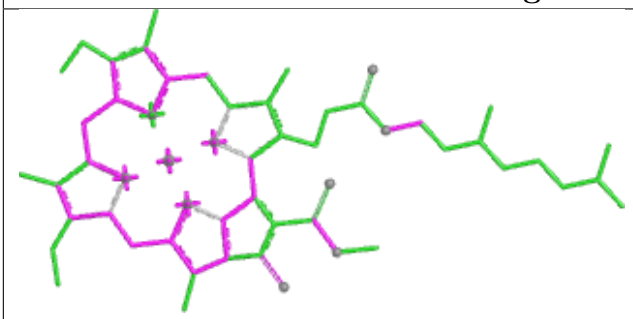


Torsions

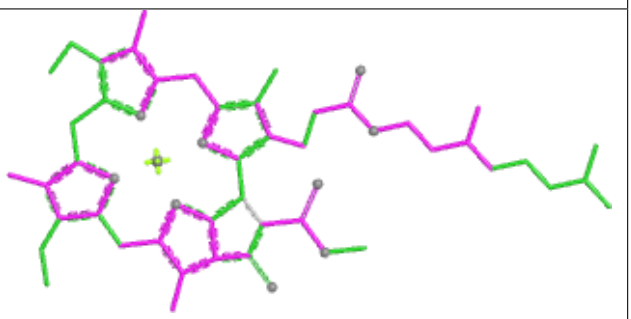


Rings

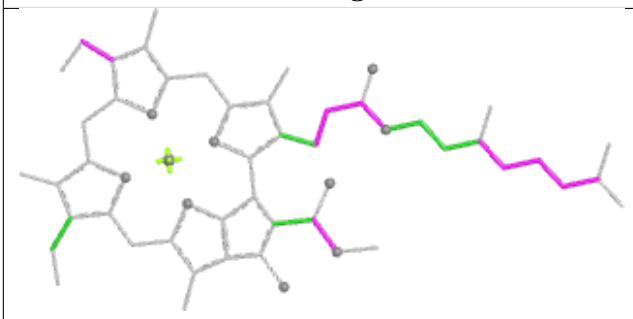
Ligand CLA H 824



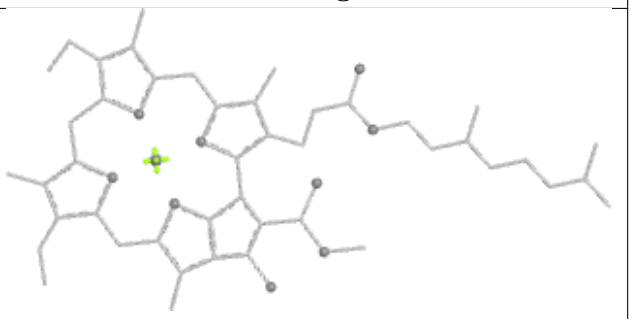
Bond lengths



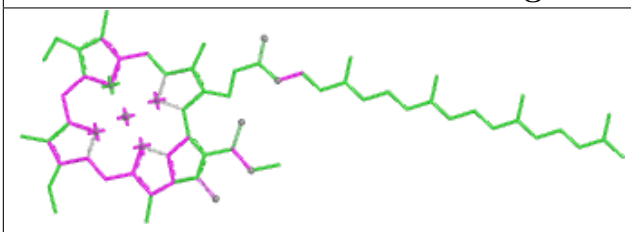
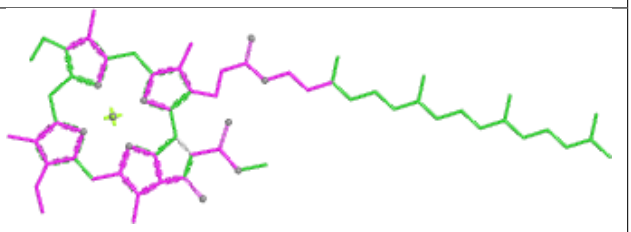
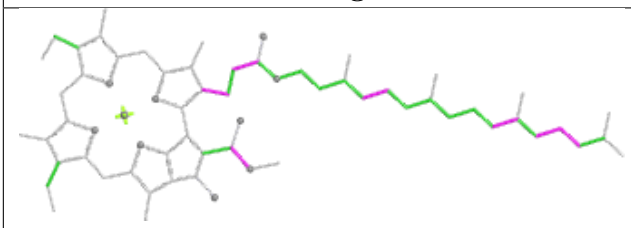
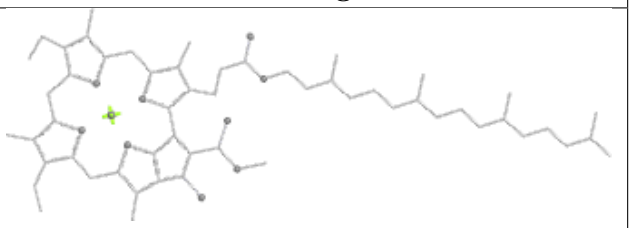
Bond angles



Torsions



Rings

Ligand CLA B 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

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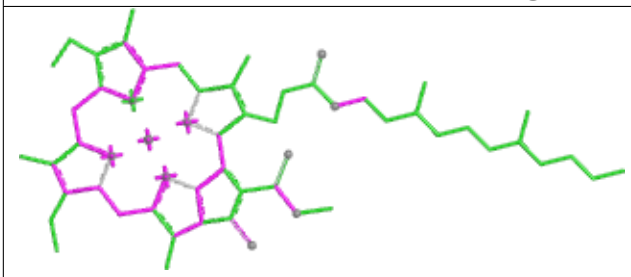
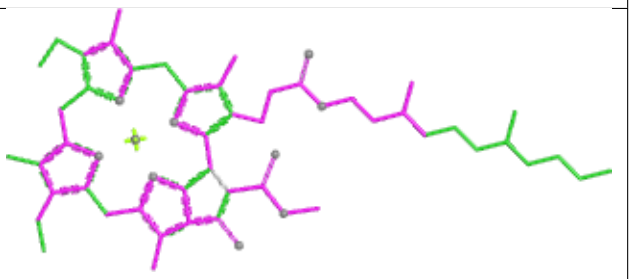
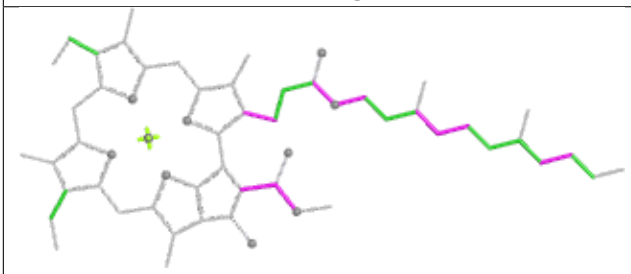
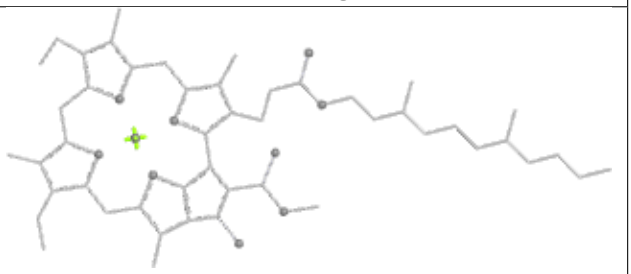
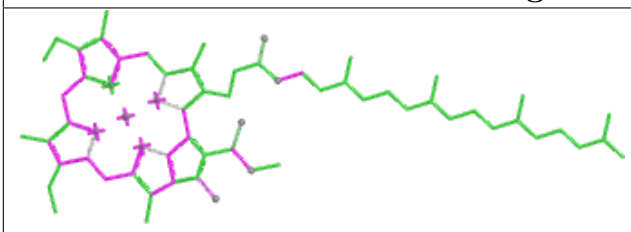
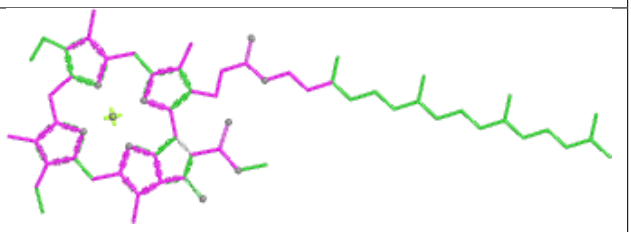
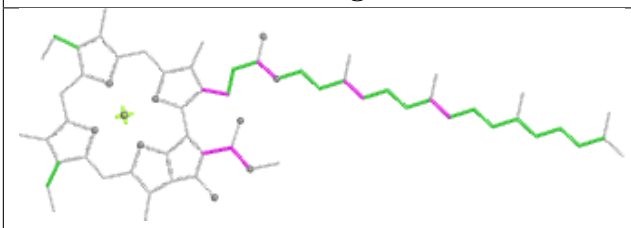
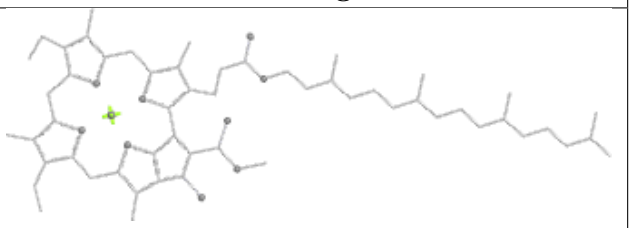
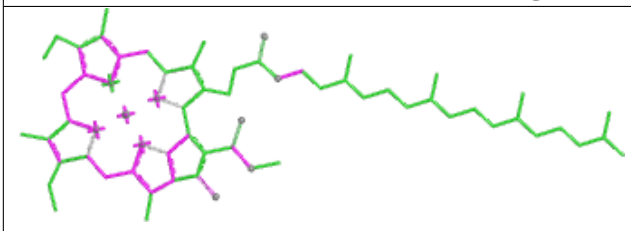
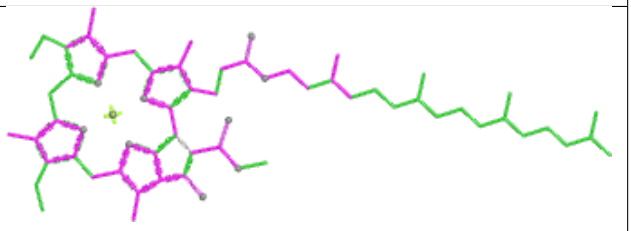
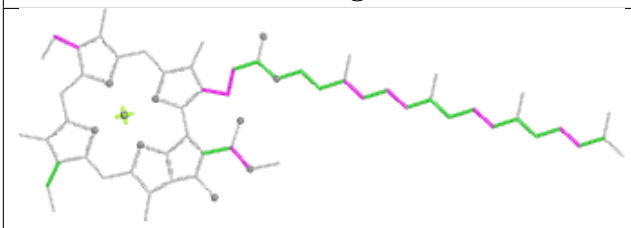
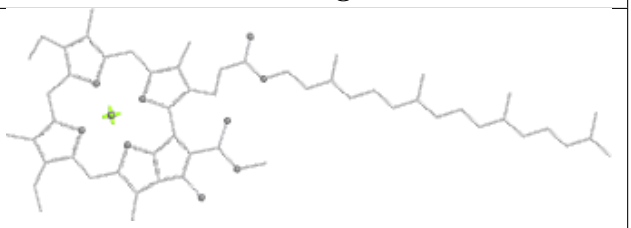
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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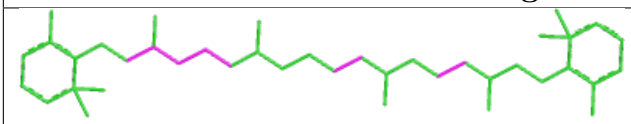
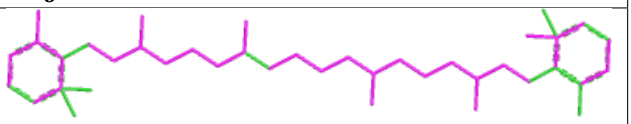
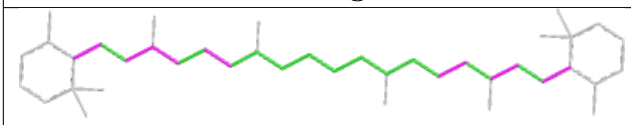
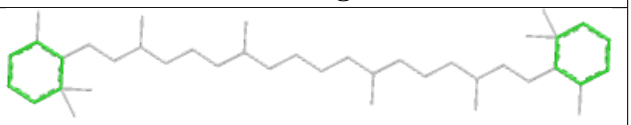
 Bond lengths	 Bond angles
 Torsions	 Rings

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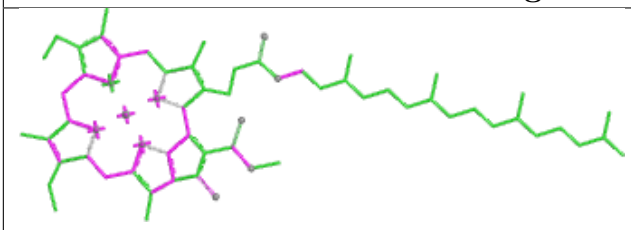
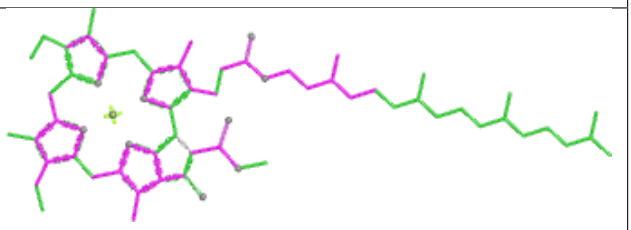
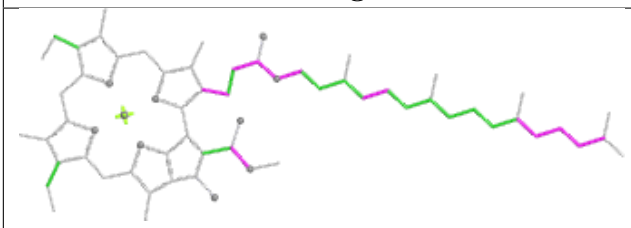
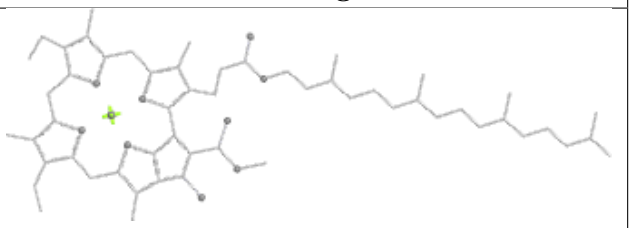
 Bond lengths	 Bond angles
 Torsions	 Rings

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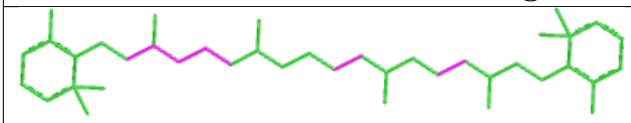
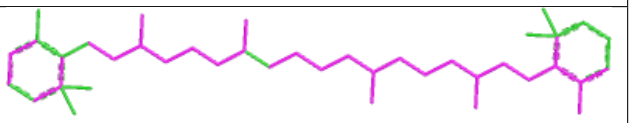
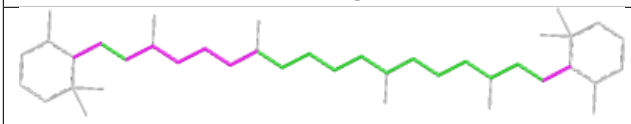
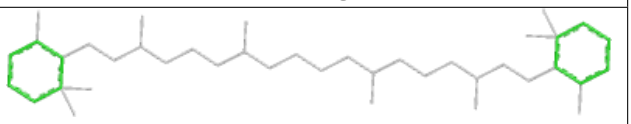
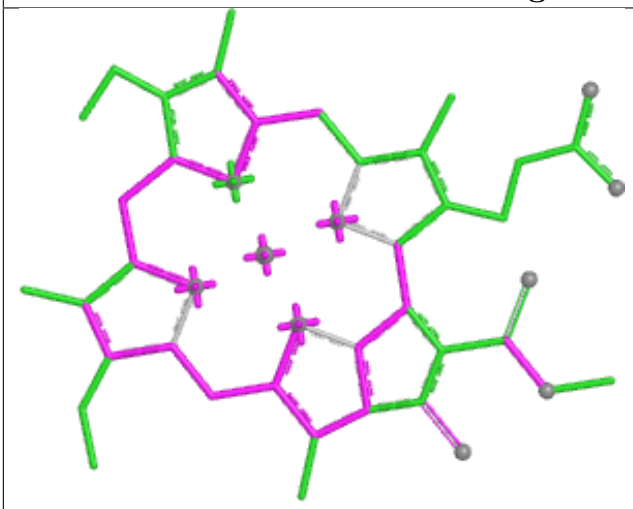
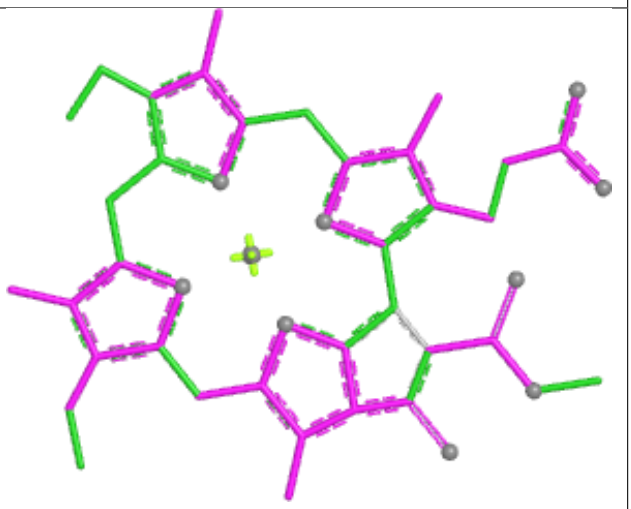
 Bond lengths	 Bond angles
 Torsions	 Rings

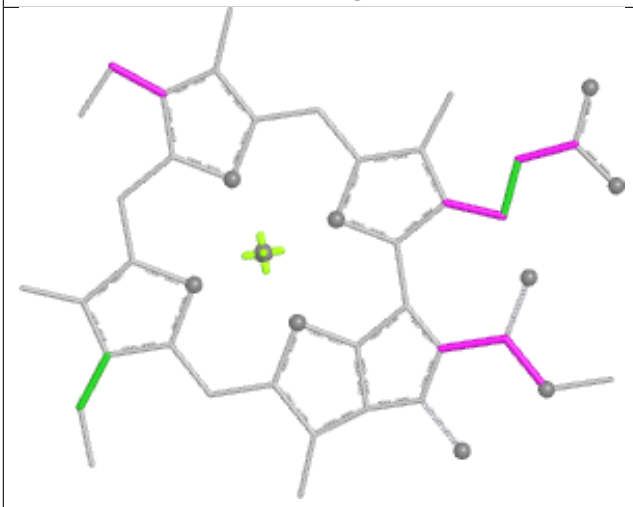
Ligand CLA a 814



Bond lengths



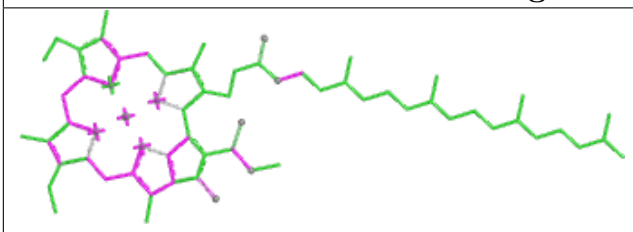
Bond angles



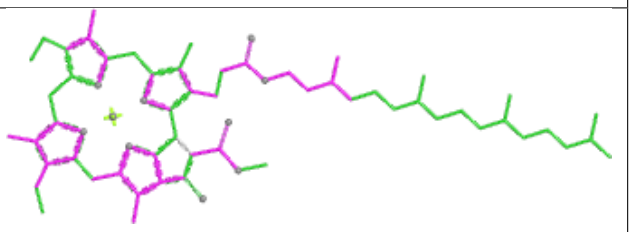
Torsions

Rings

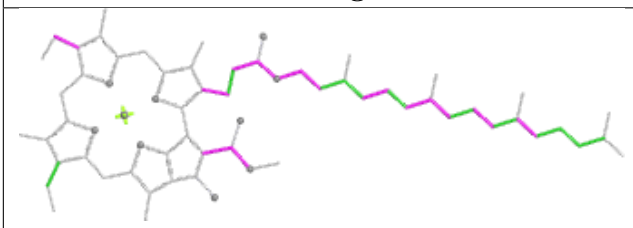
Ligand CLA a 804



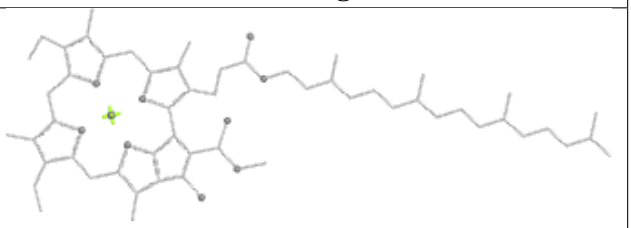
Bond lengths



Bond angles

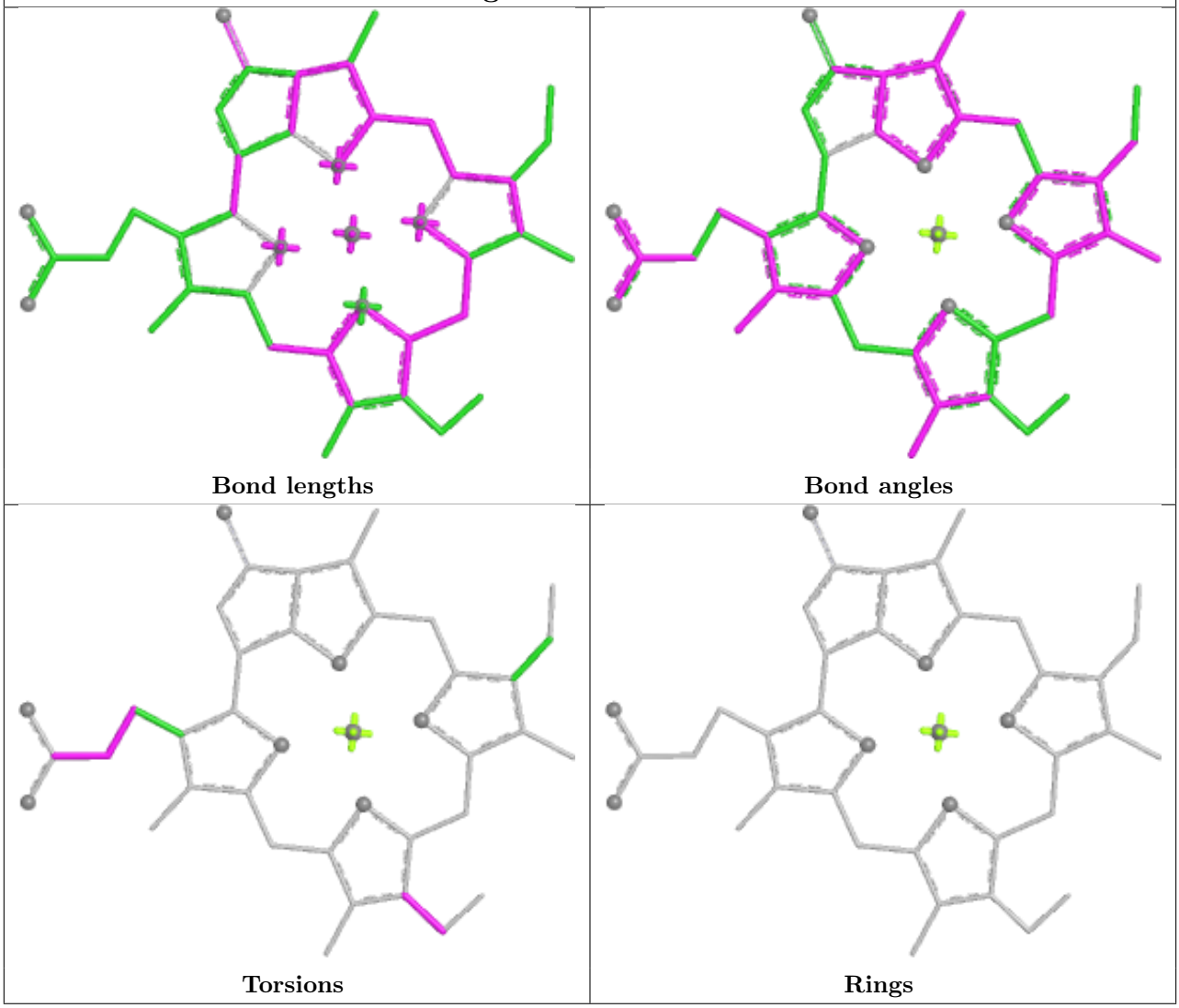


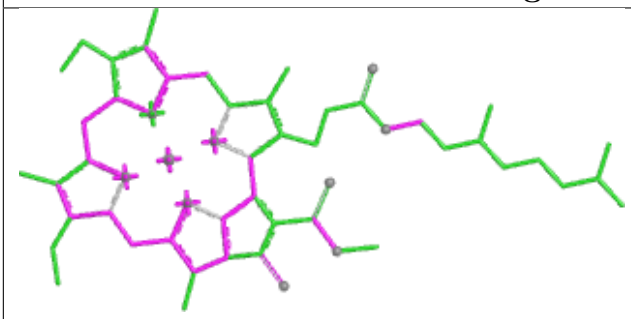
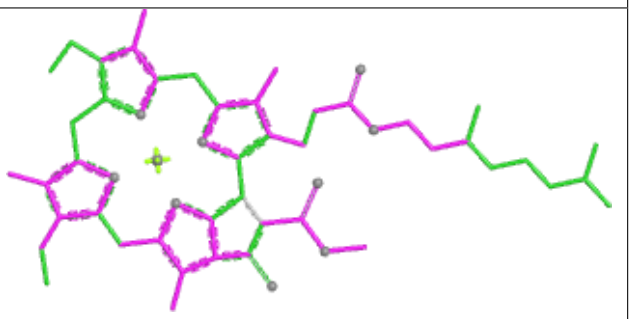
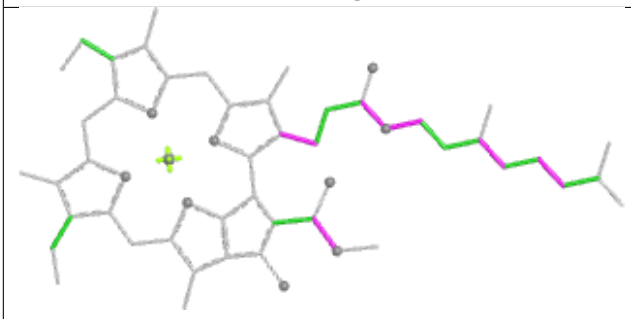
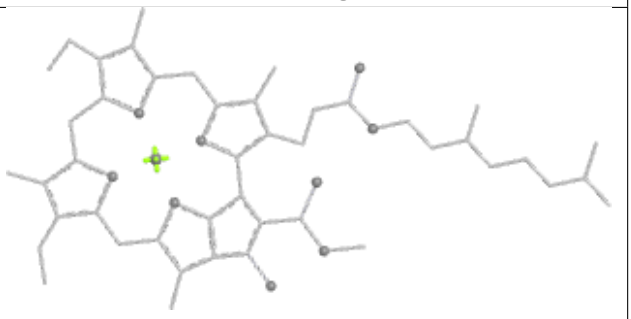
Torsions



Rings

Ligand CLA T 101



Ligand CLA A 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

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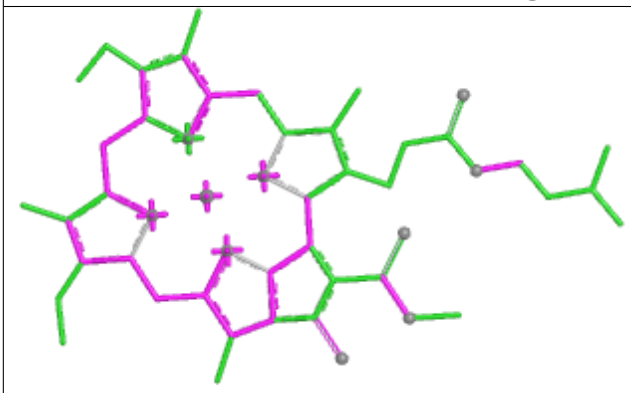
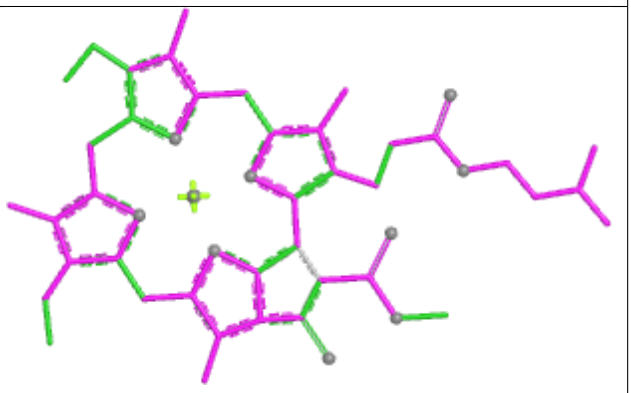
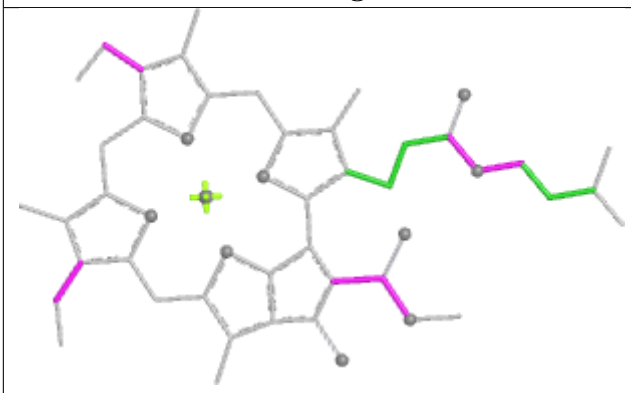
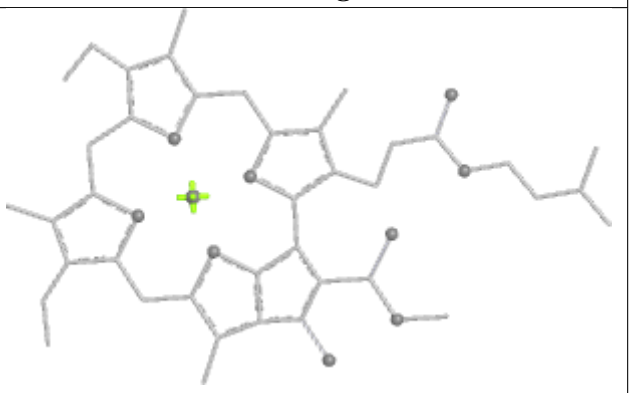
 Bond lengths	 Bond angles
 Torsions	 Rings

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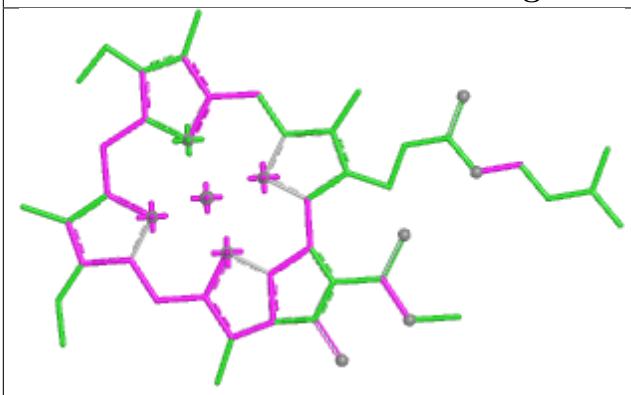
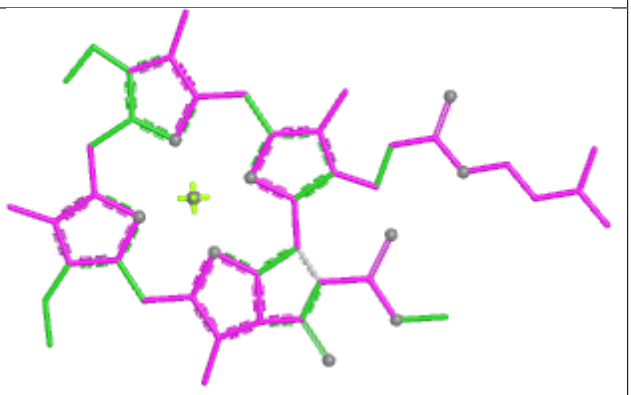
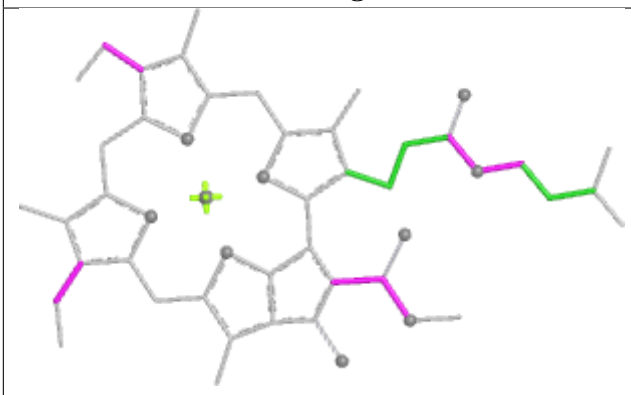
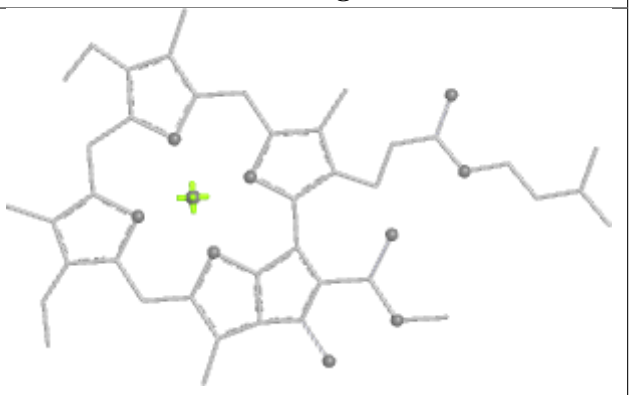
 Bond lengths	 Bond angles
 Torsions	 Rings

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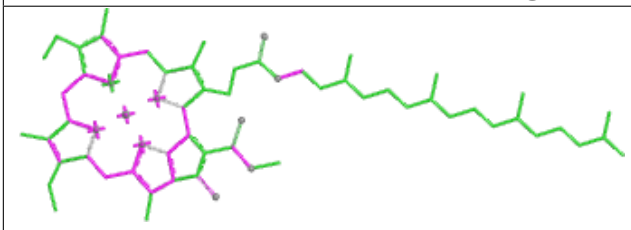
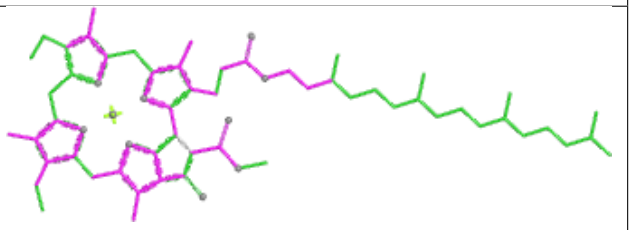
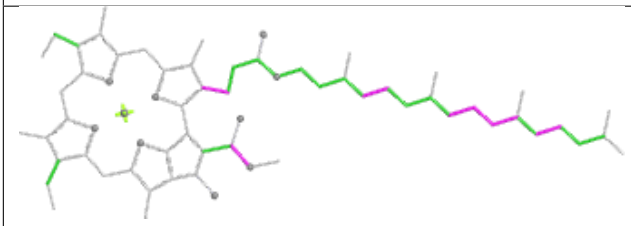
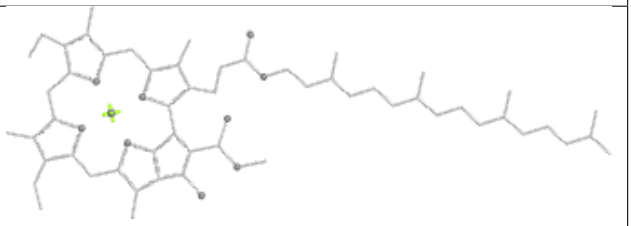
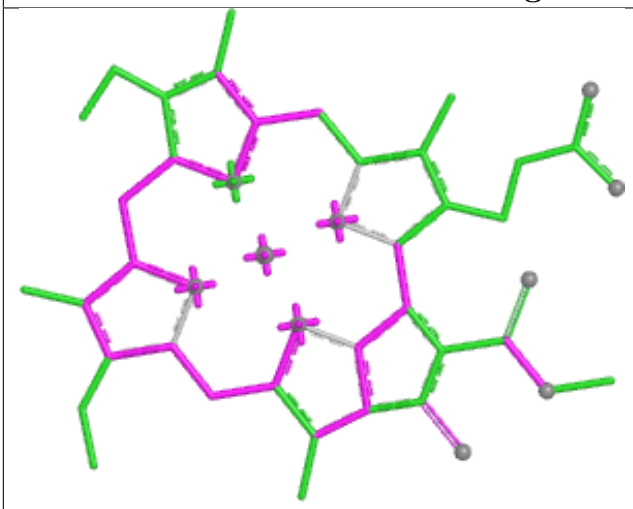
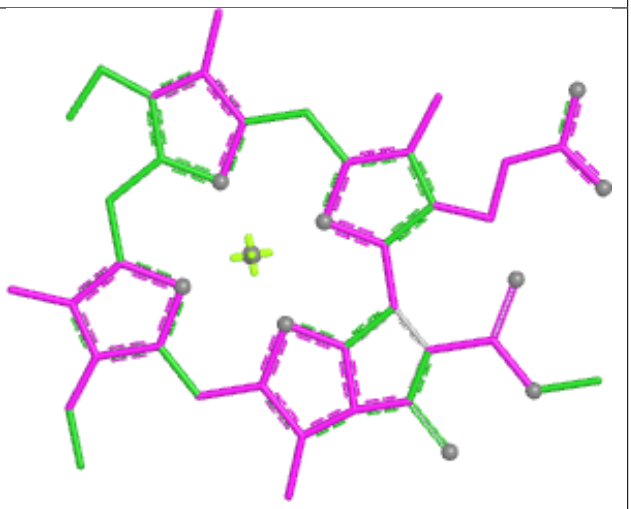
 Bond lengths	 Bond angles
 Torsions	 Rings

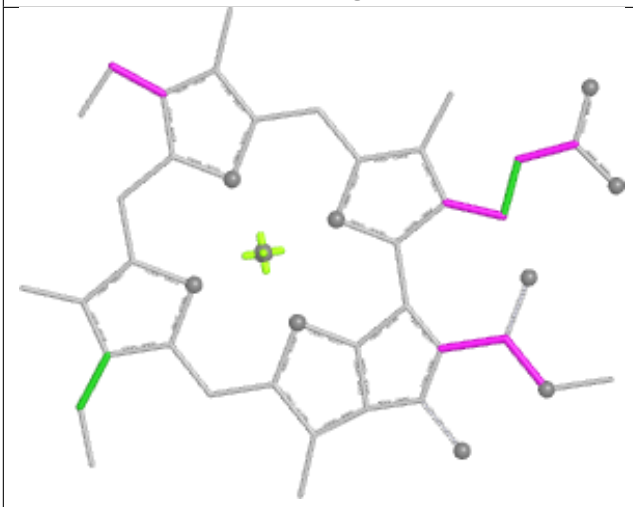
Ligand CLA B 822



Bond lengths



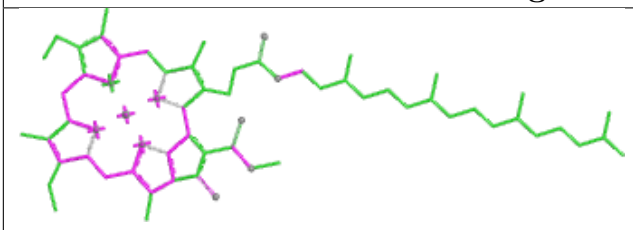
Bond angles



Torsions

Rings

Ligand CLA a 810



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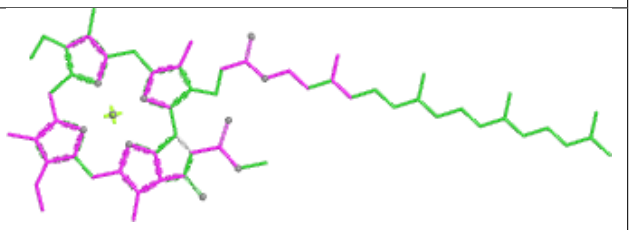

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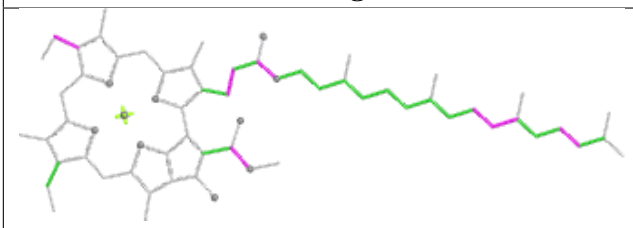

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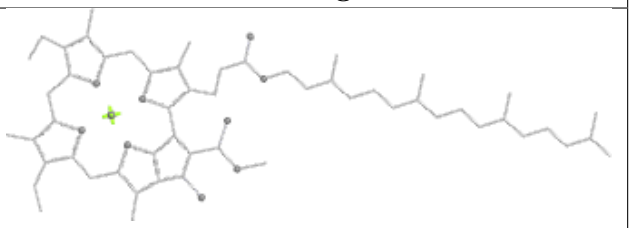
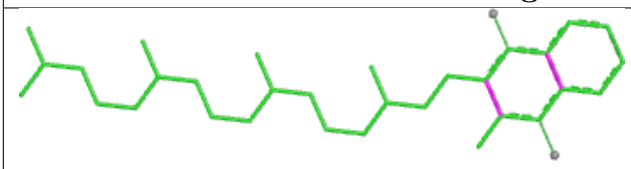


Rings

Ligand PQN H 843



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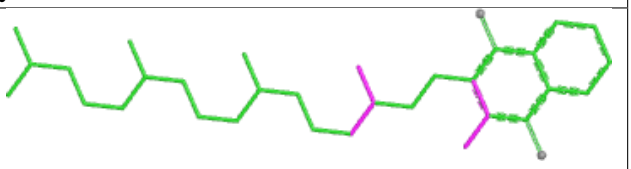

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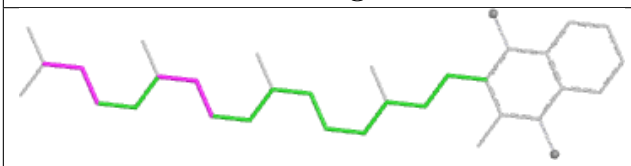

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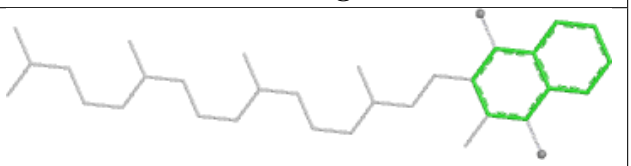
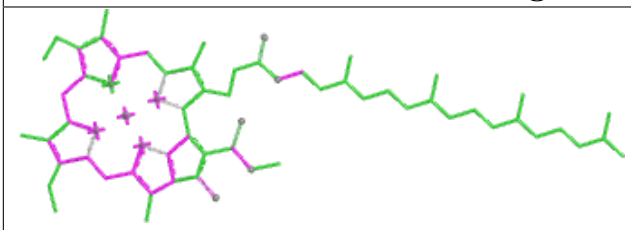


Rings

Ligand CLA a 826



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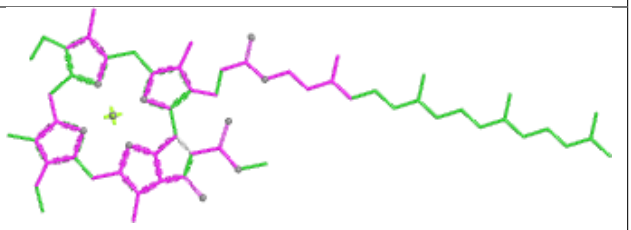

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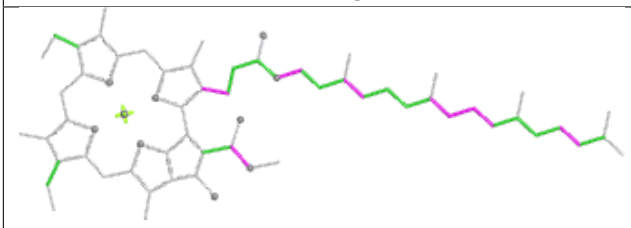

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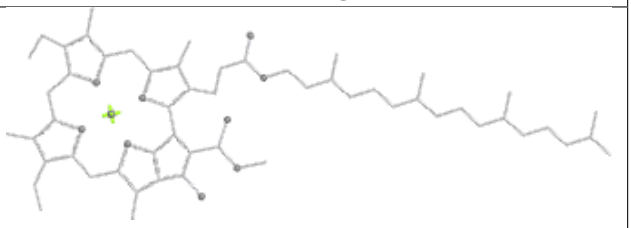
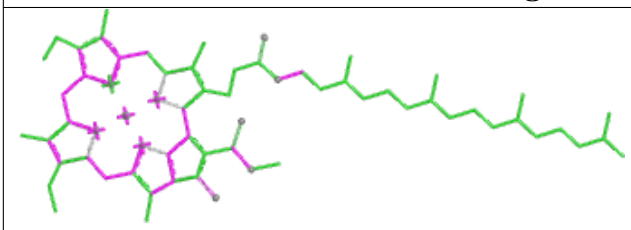


Rings

Ligand CLA R 101



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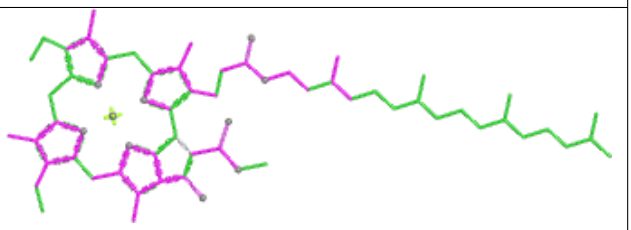

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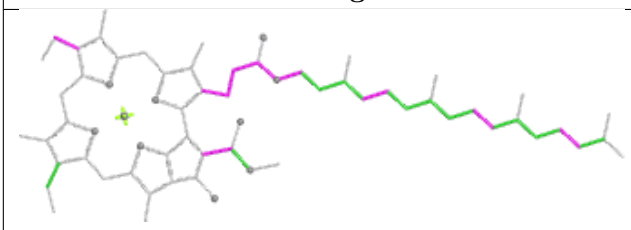

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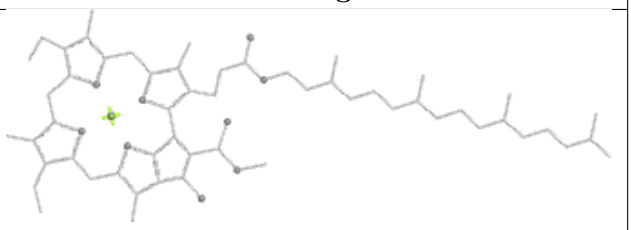
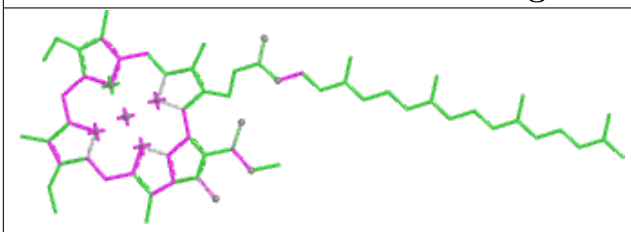
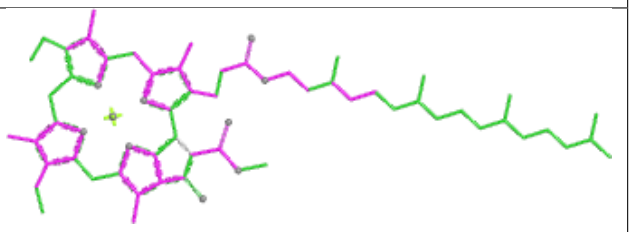
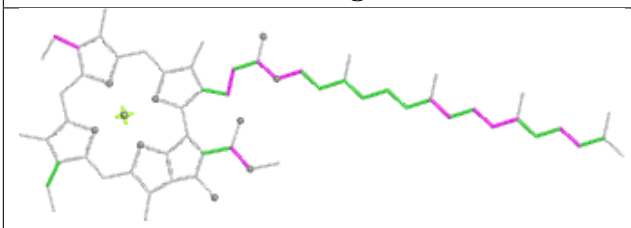
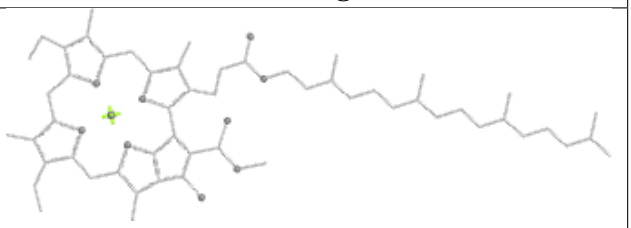
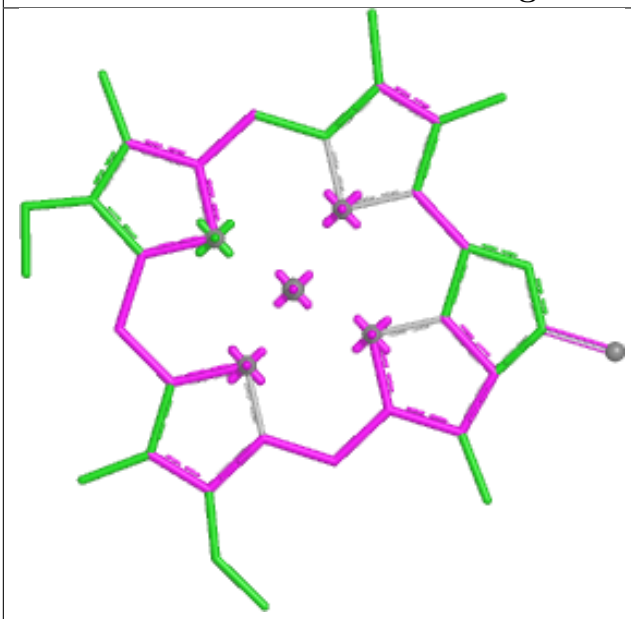


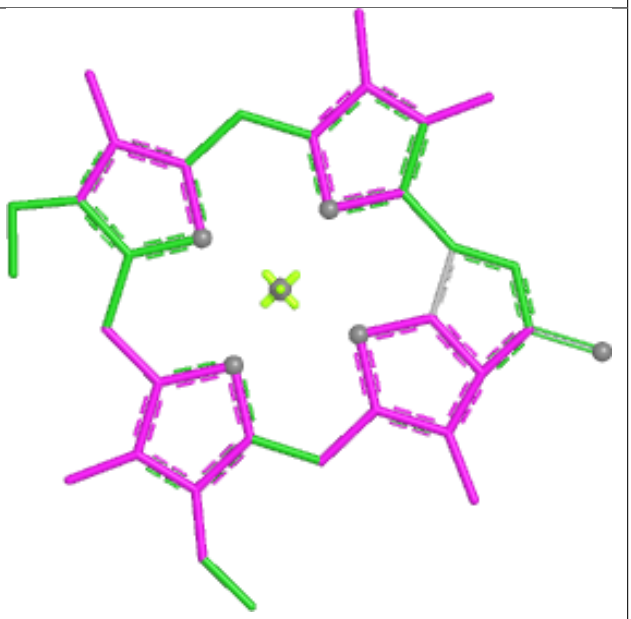
Rings

Ligand CLA a 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

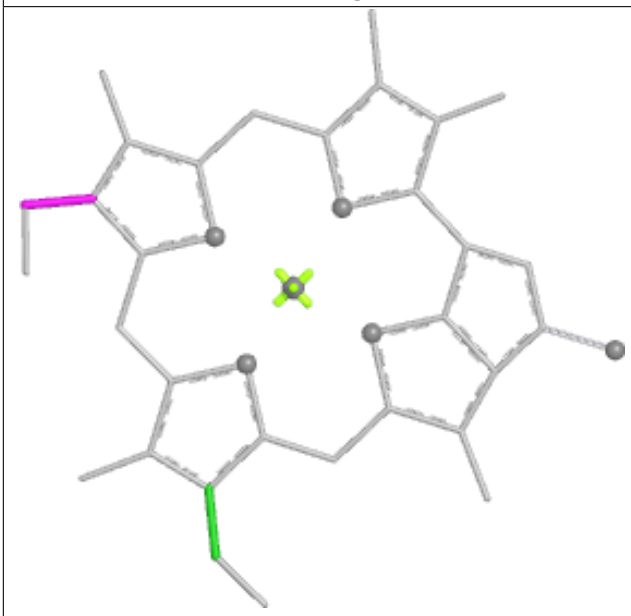
Ligand CLA J 1303



Bond lengths



Bond angles



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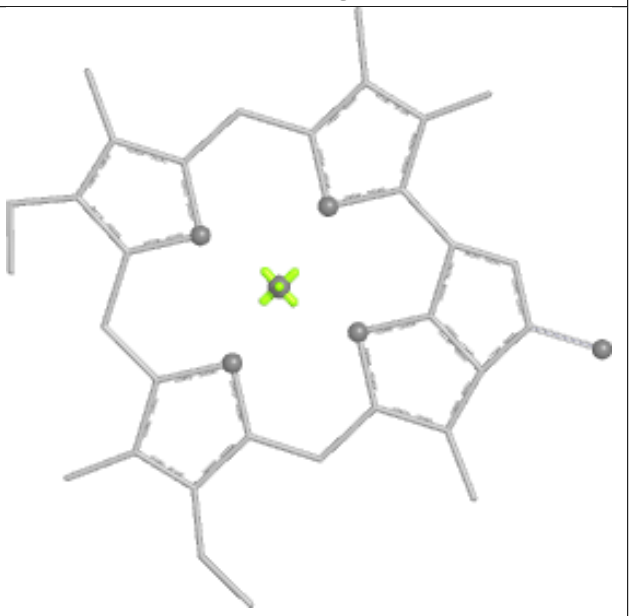
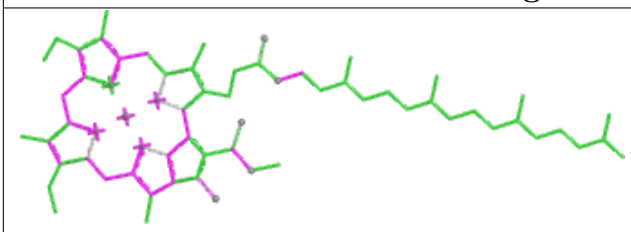
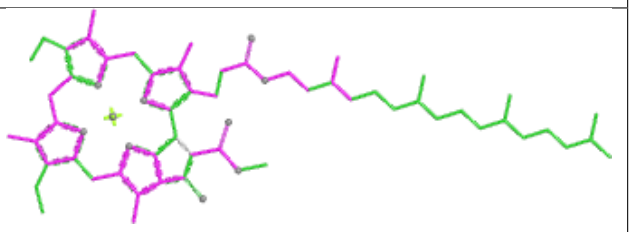
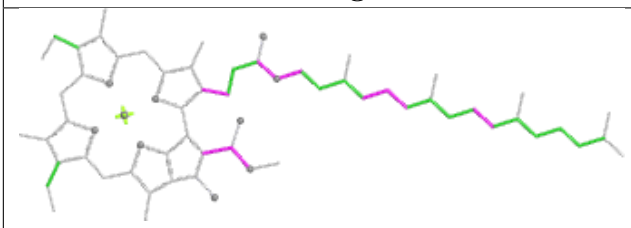
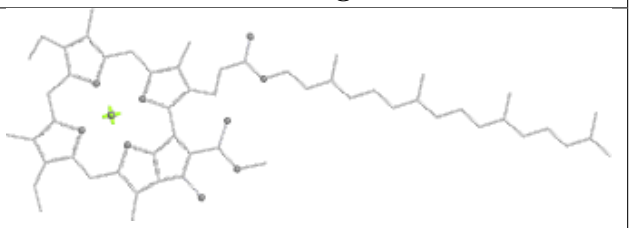
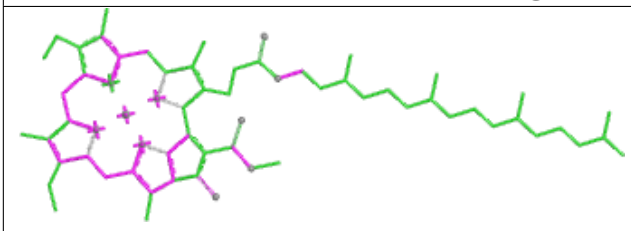
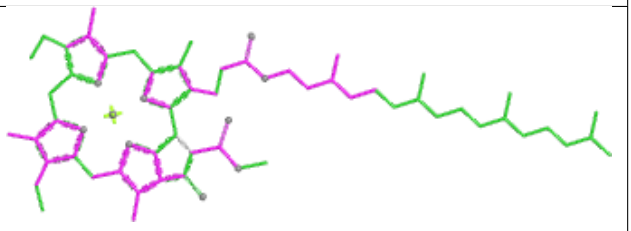
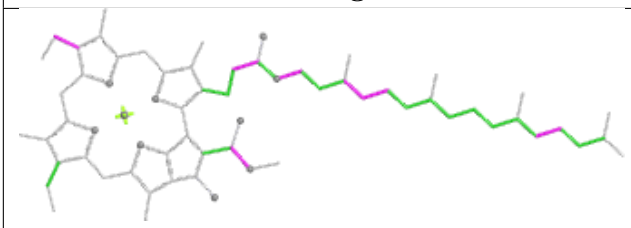
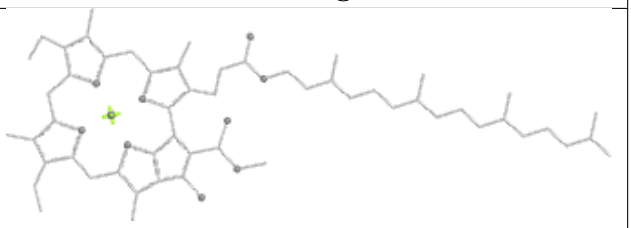
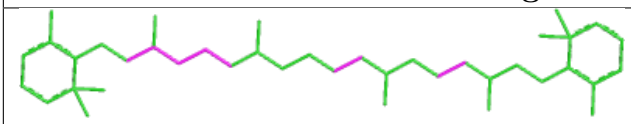
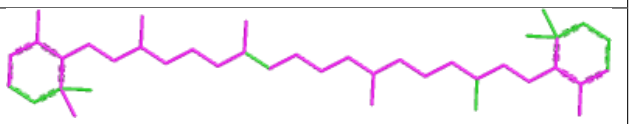
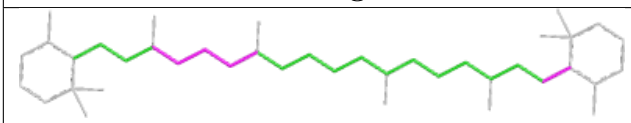
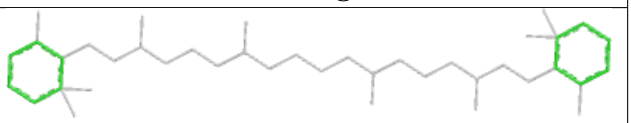


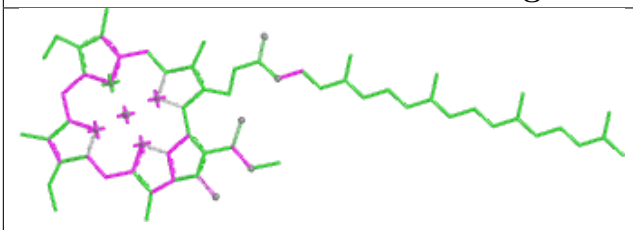
Rings

Ligand CLA G 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

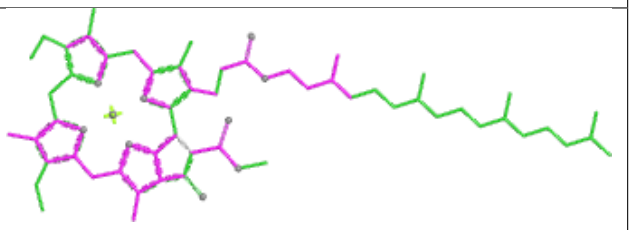
Ligand CLA b 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

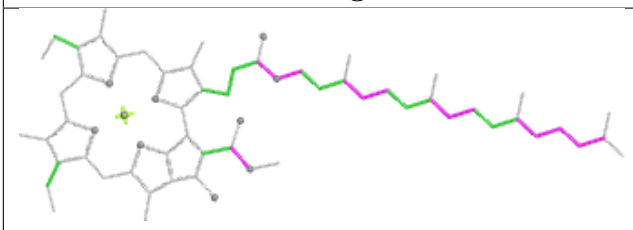
Ligand CLA H 806



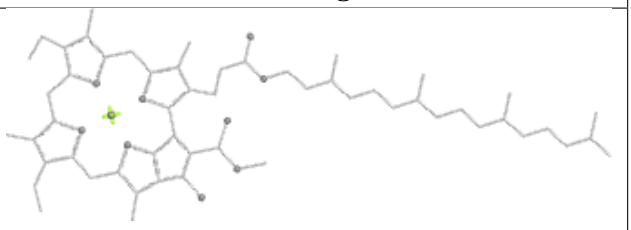
Bond lengths



Bond angles

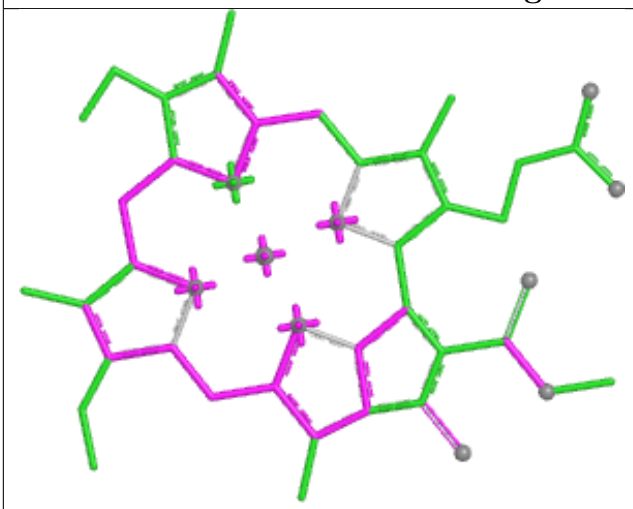


Torsions

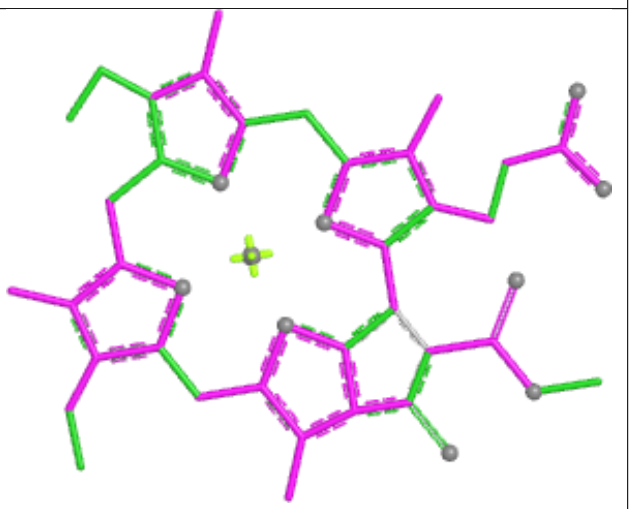


Rings

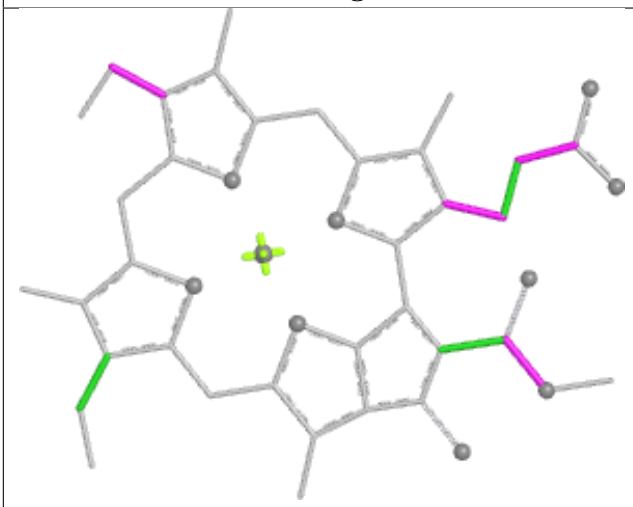
Ligand CLA B 840



Bond lengths

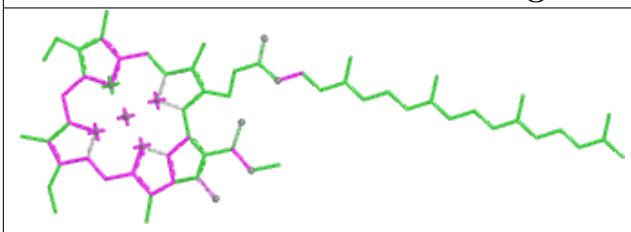
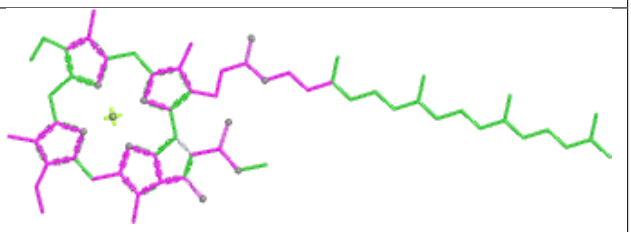
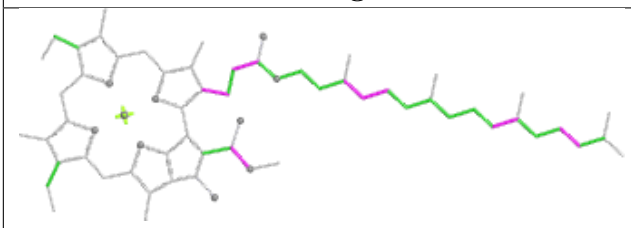
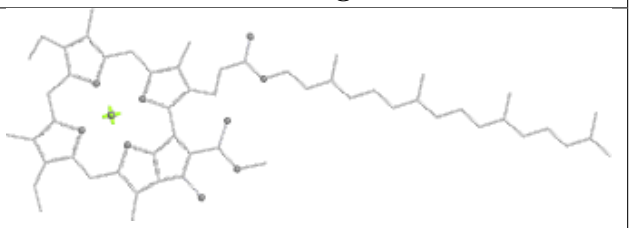


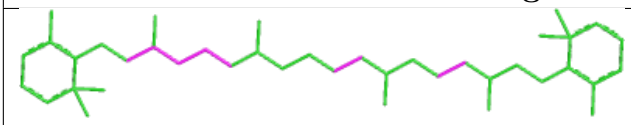
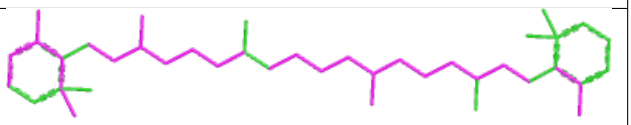
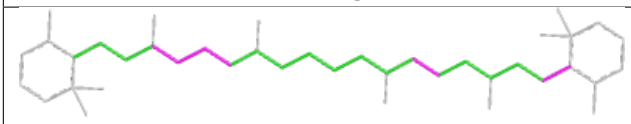
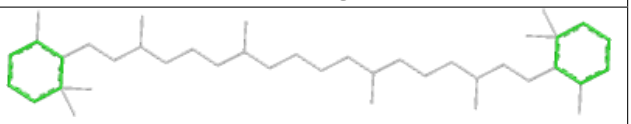
Bond angles

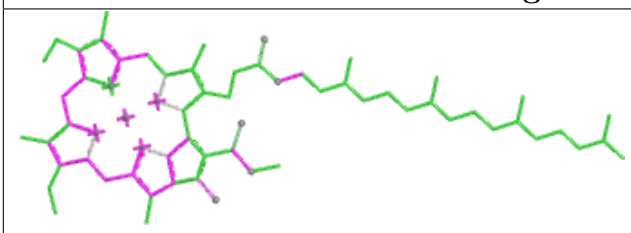
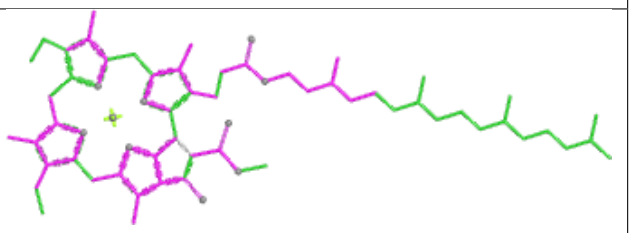
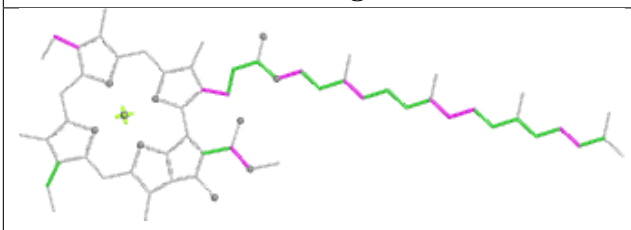
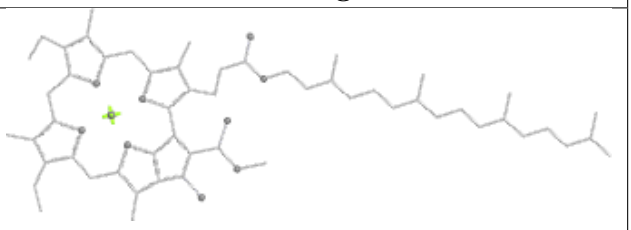


Torsions

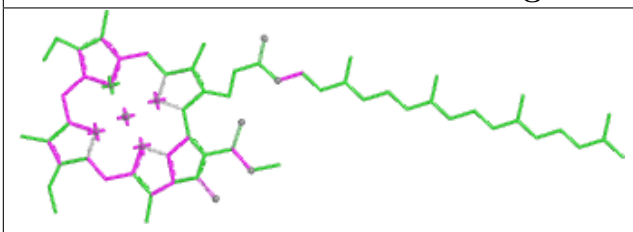
Rings

Ligand CLA b 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 852



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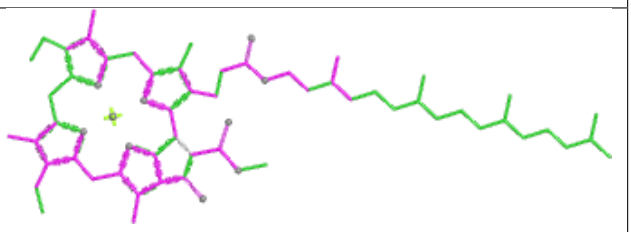
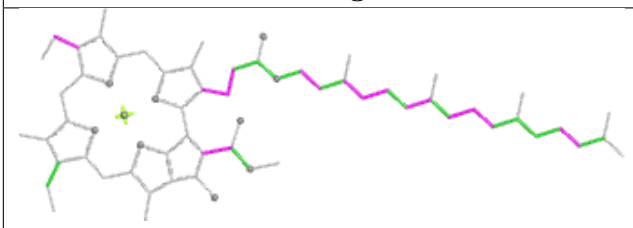


Bond angles



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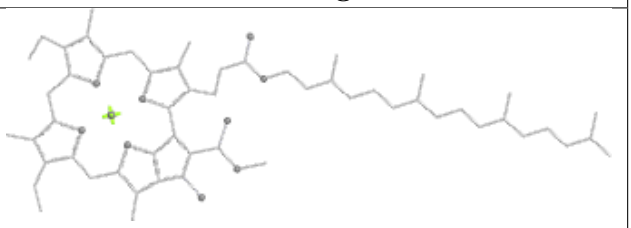
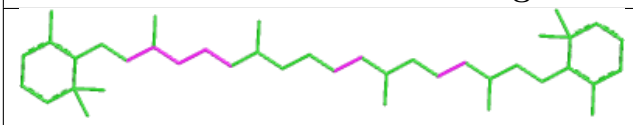


Rings

Ligand BCR V 1602



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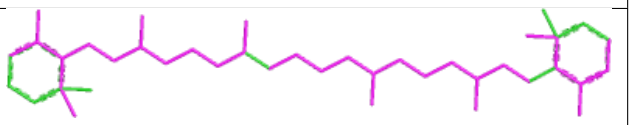
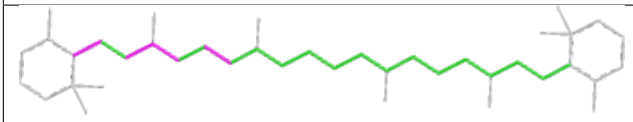


Bond angles



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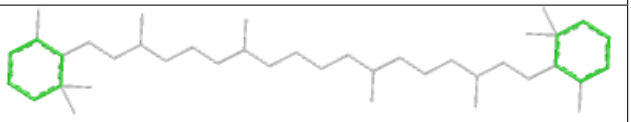
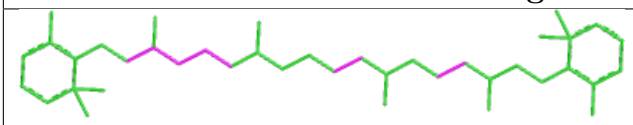


Rings

Ligand BCR a 849



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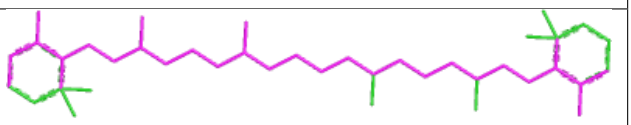

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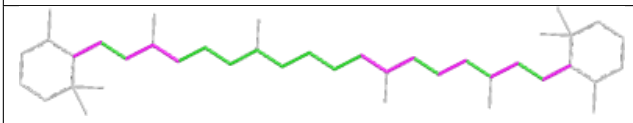

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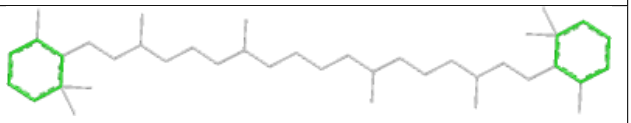
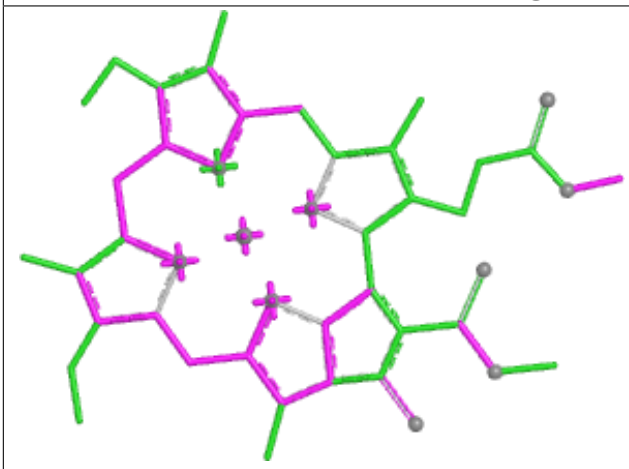
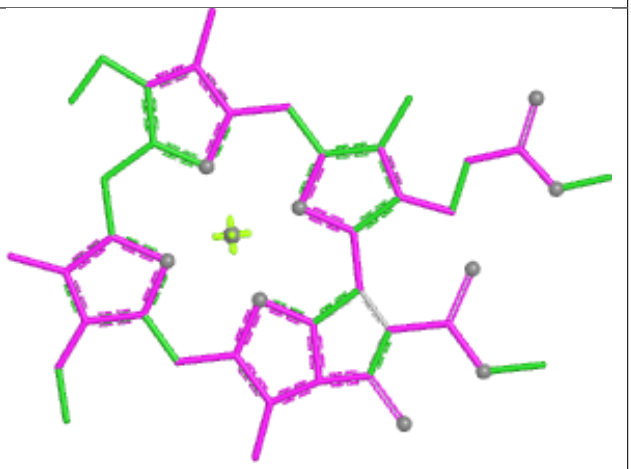
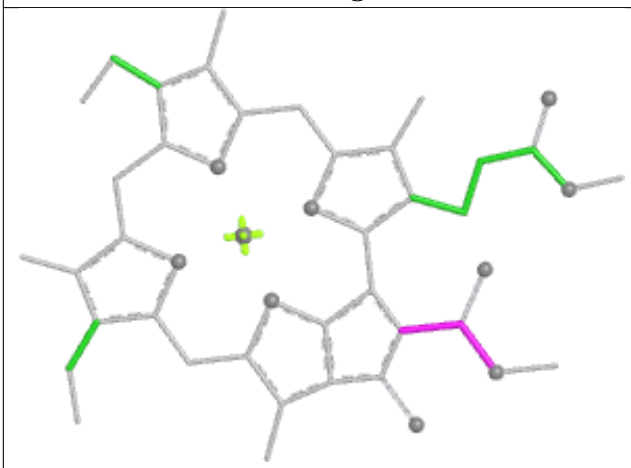
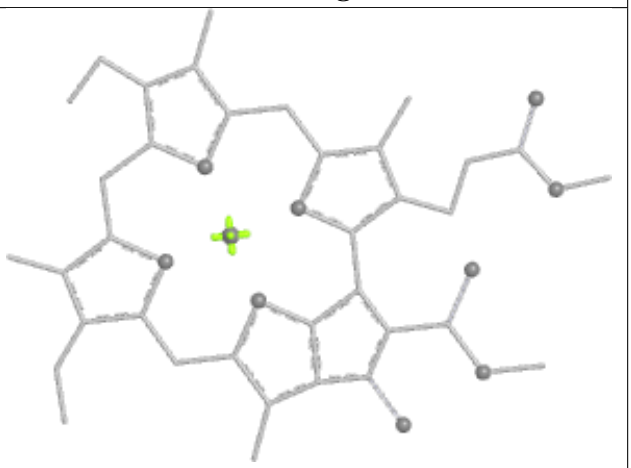
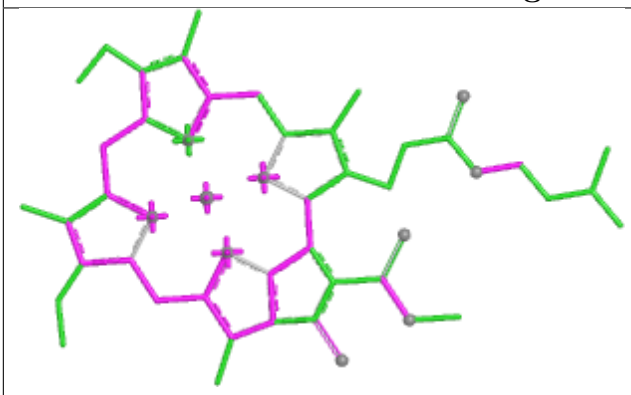
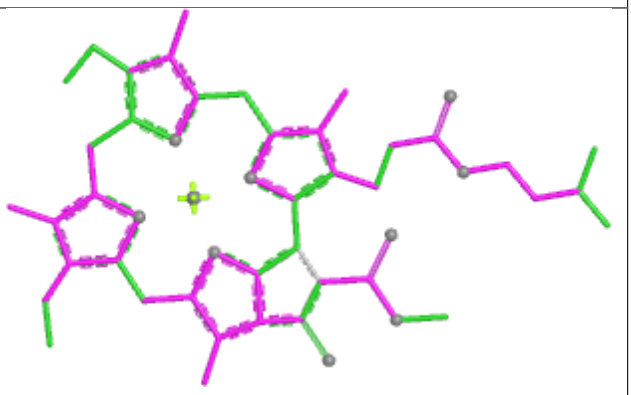
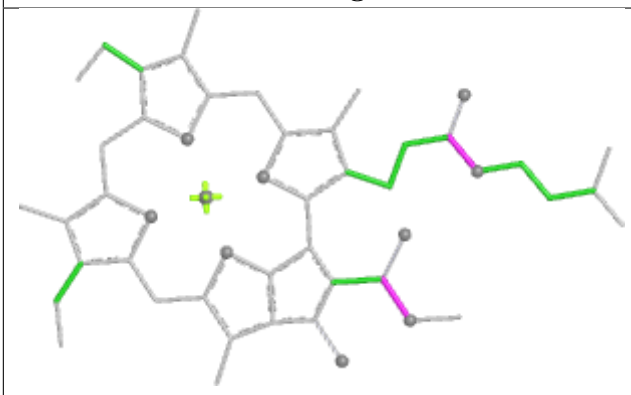
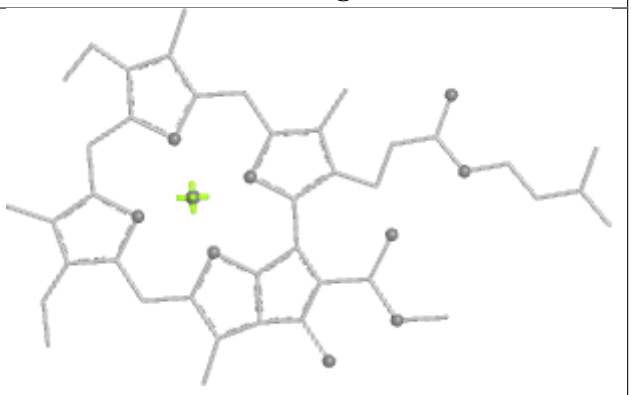
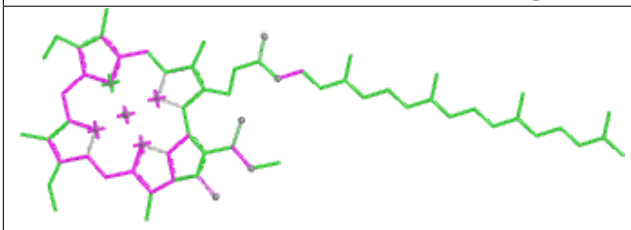
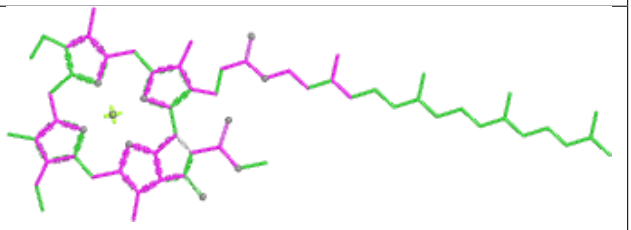
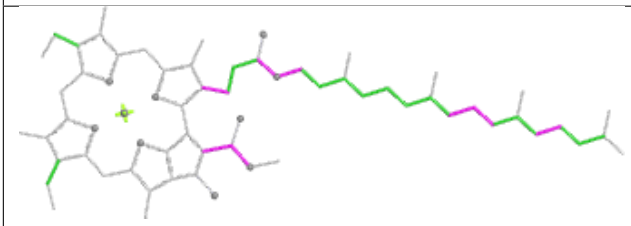
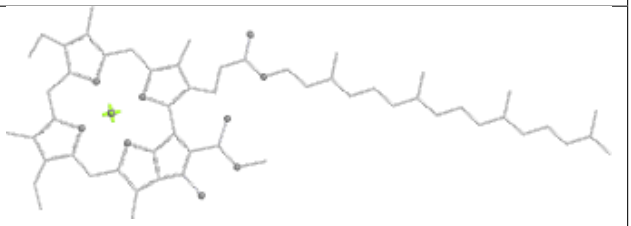


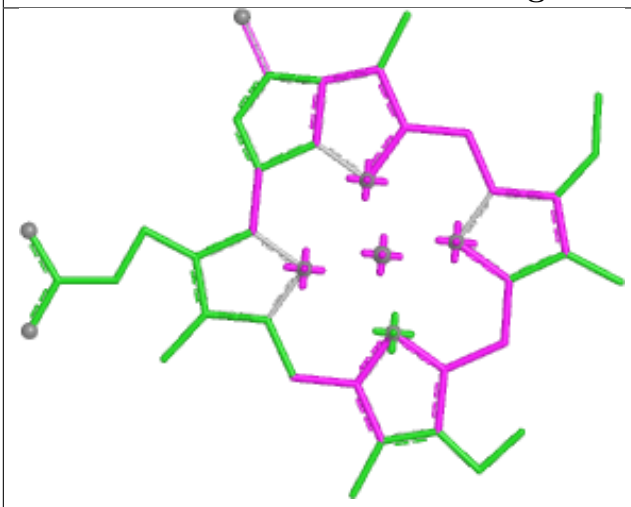
Rings

Ligand CLA b 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 101



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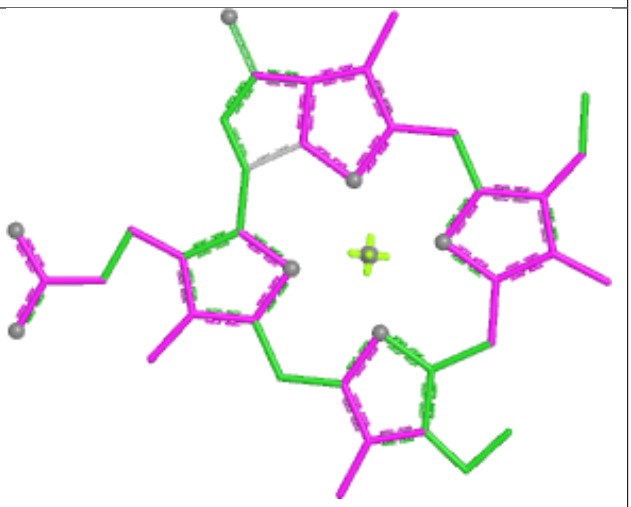

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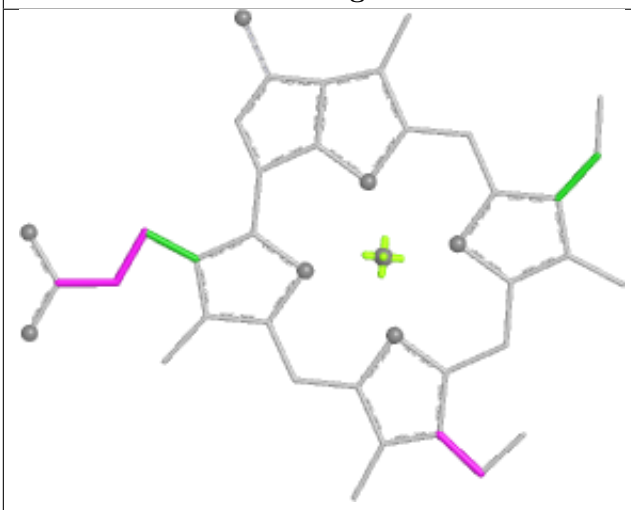

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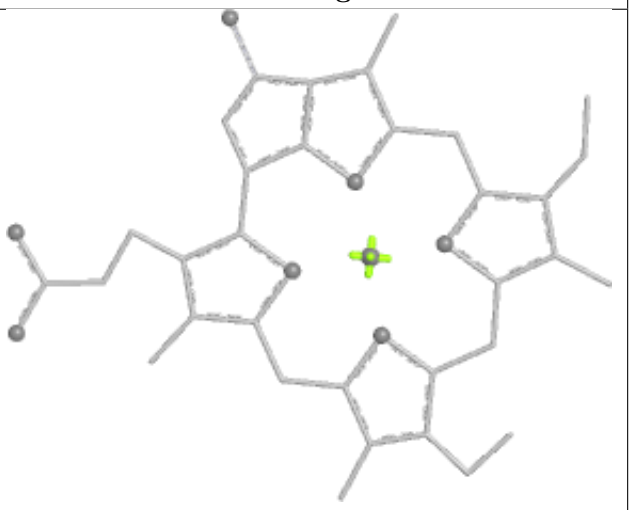
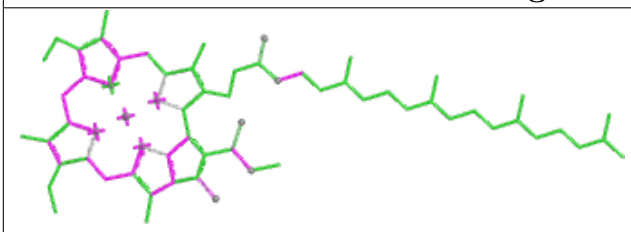


Rings

Ligand CLA a 852



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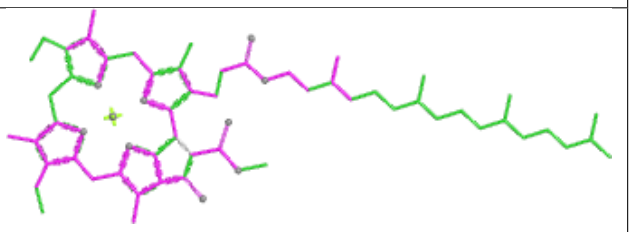
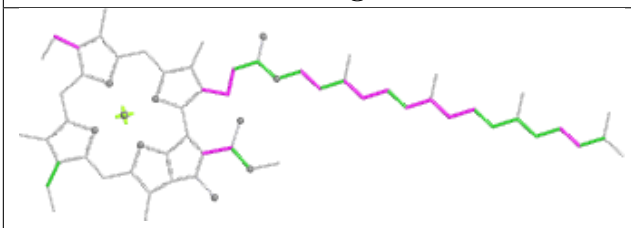


Bond angles



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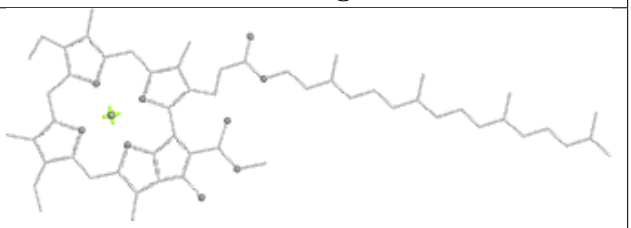
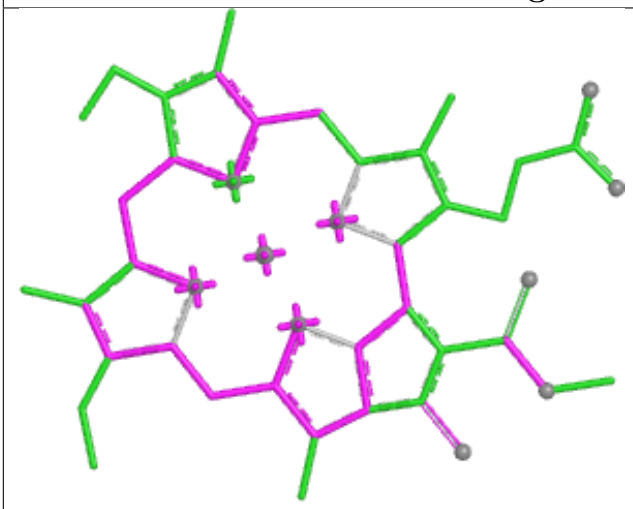


Rings

Ligand CLA a 834



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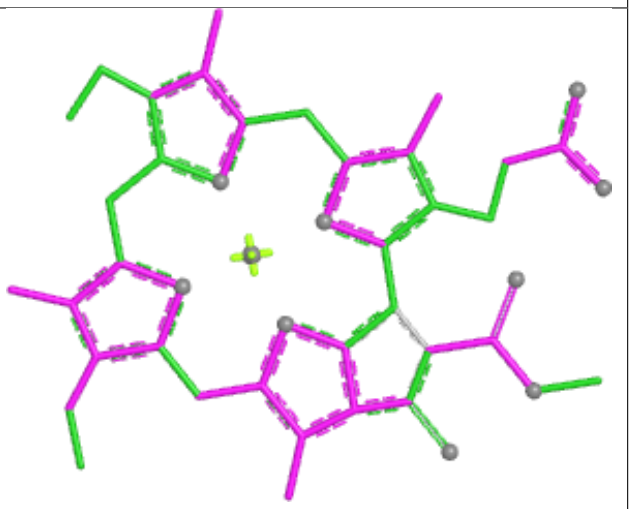
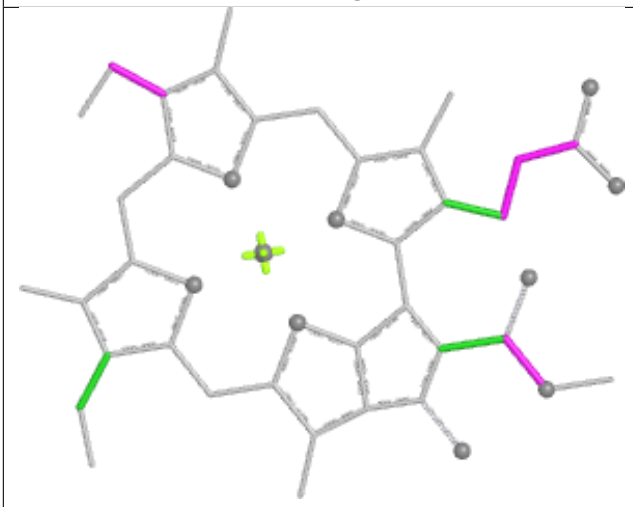


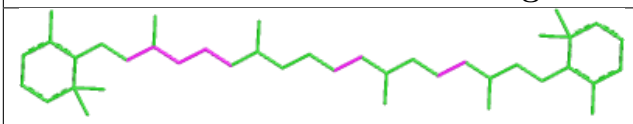
Bond angles



Torsions

Rings

Ligand BCR Q 203



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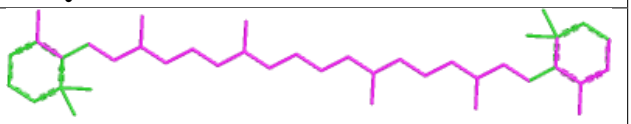

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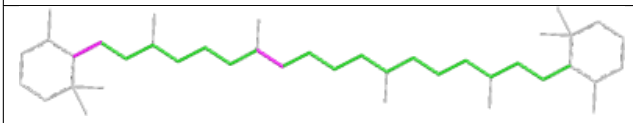
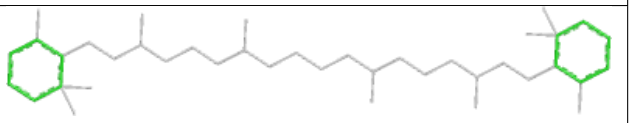
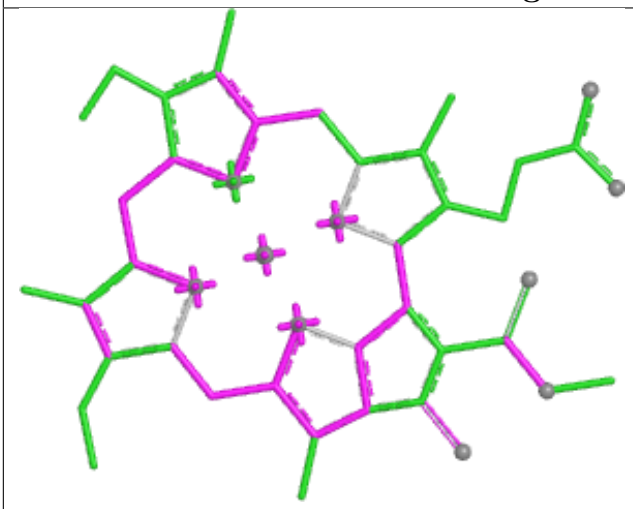


Torsions



Rings

Ligand CLA G 809



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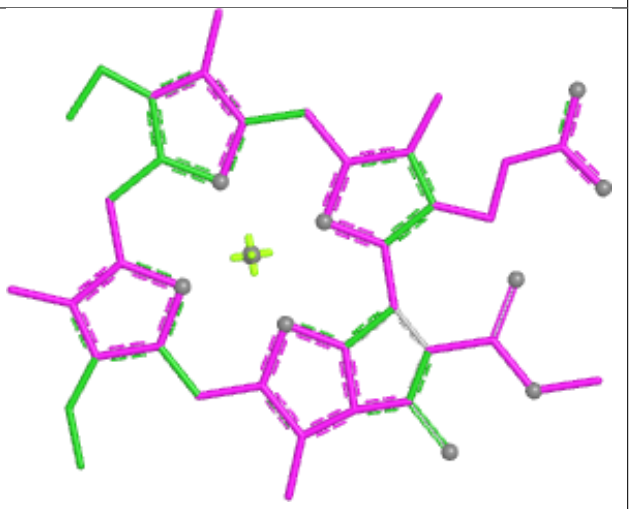
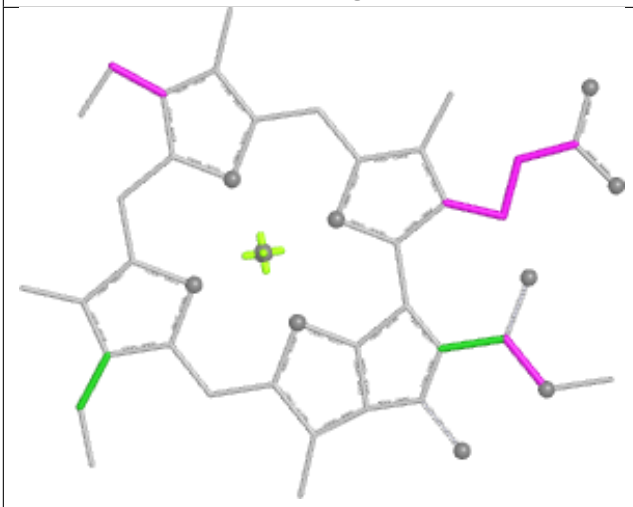


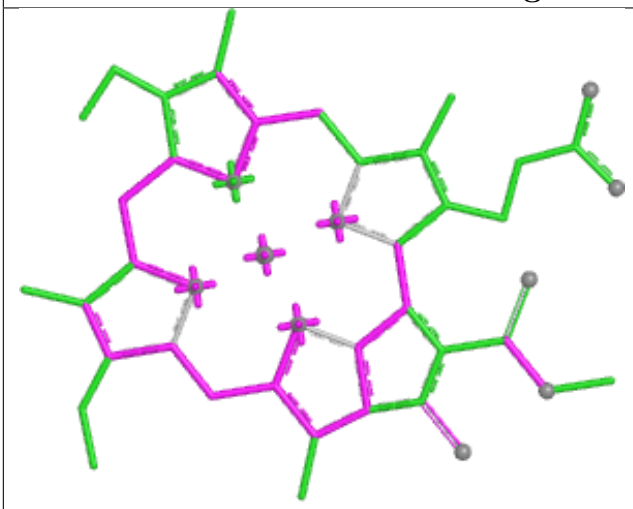
Bond angles



Torsions

Rings

Ligand CLA A 821



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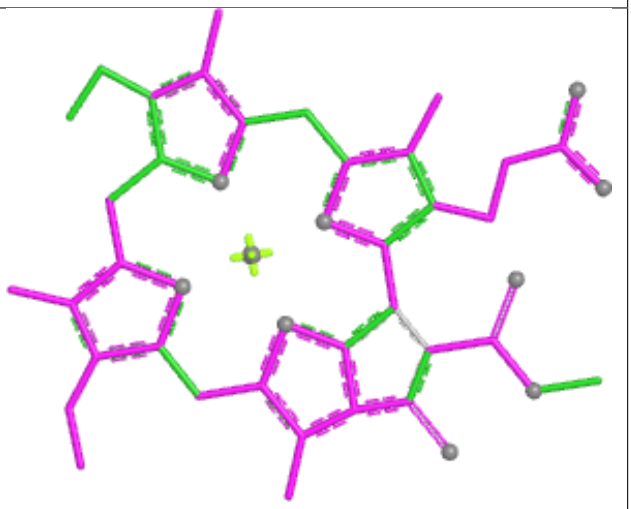
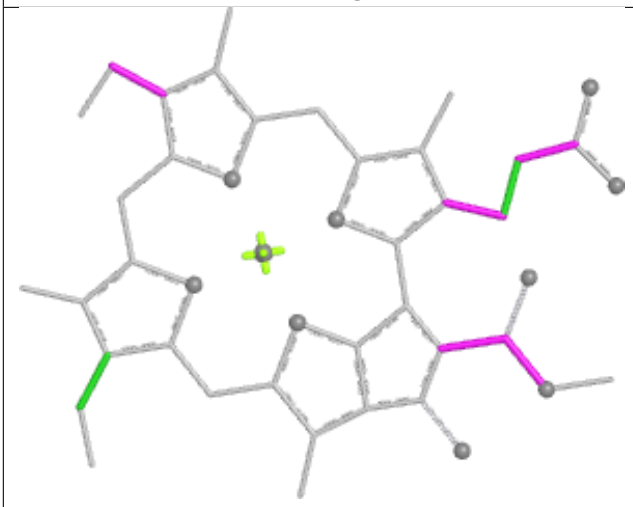


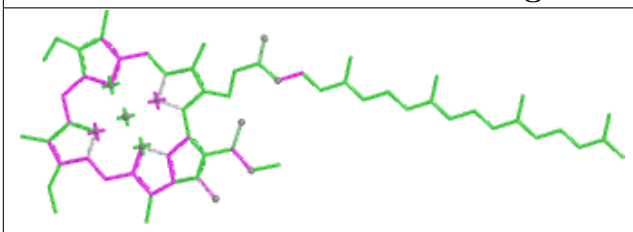
Bond angles



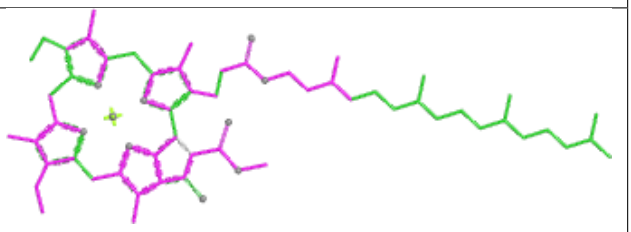
Torsions

Rings

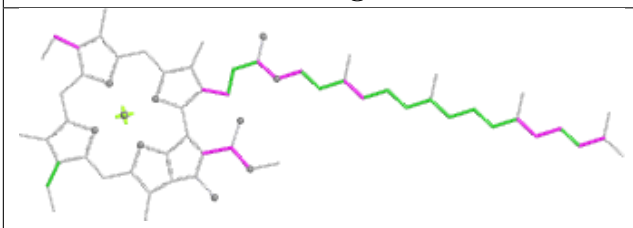
Ligand CLA B 816



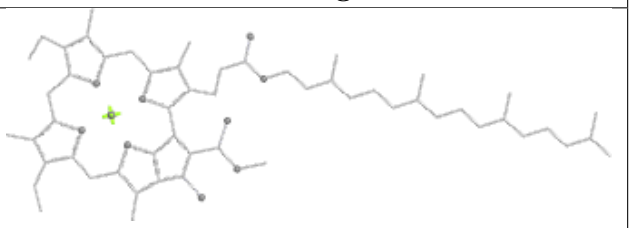
Bond lengths



Bond angles

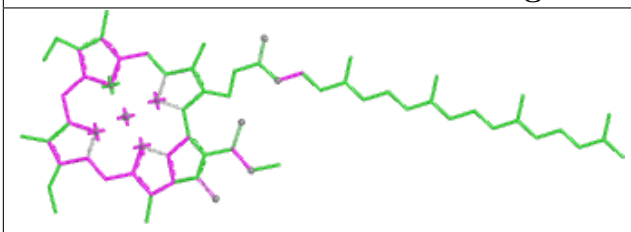


Torsions

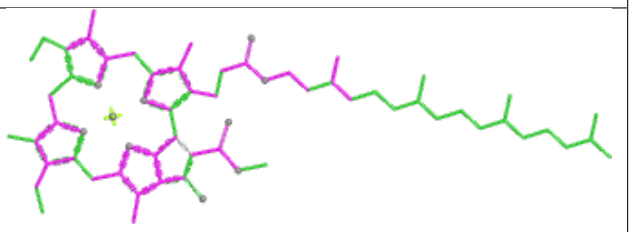


Rings

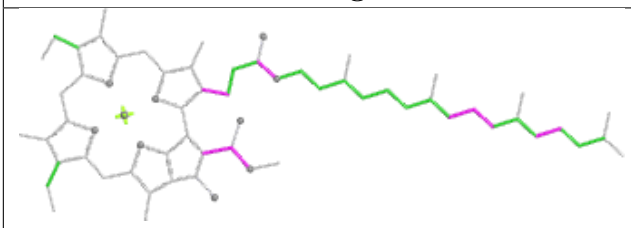
Ligand CLA B 831



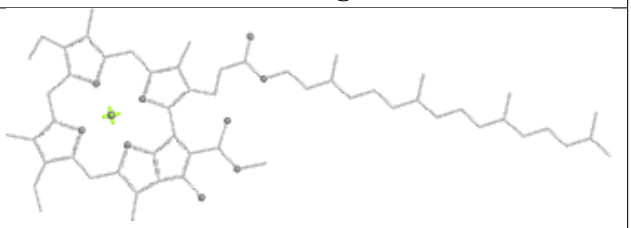
Bond lengths



Bond angles

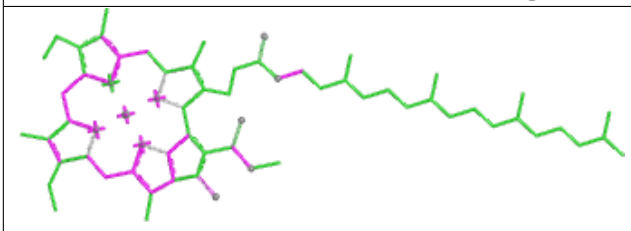


Torsions

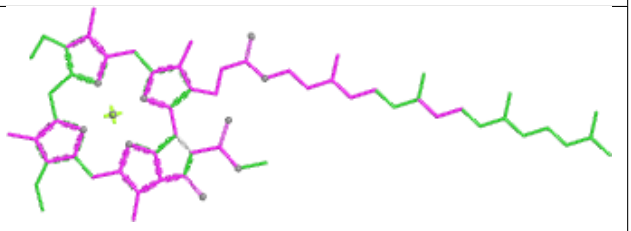


Rings

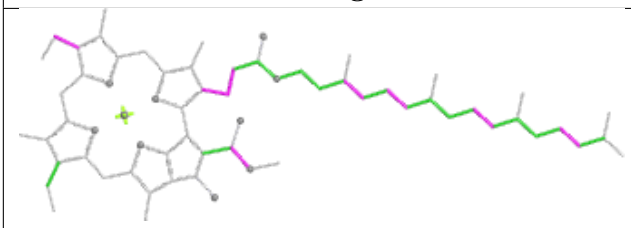
Ligand CLA H 802



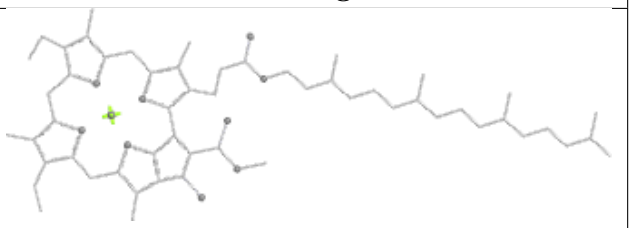
Bond lengths



Bond angles

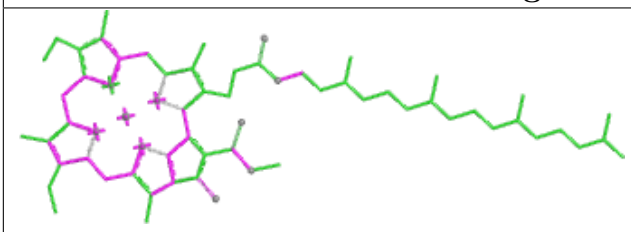


Torsions



Rings

Ligand CLA H 829



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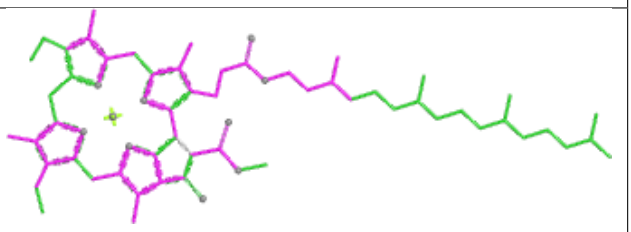
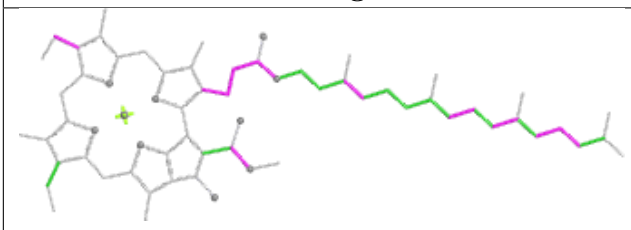
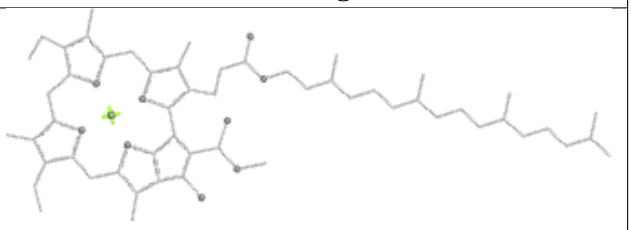


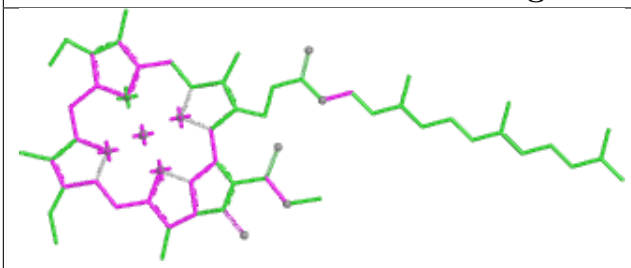
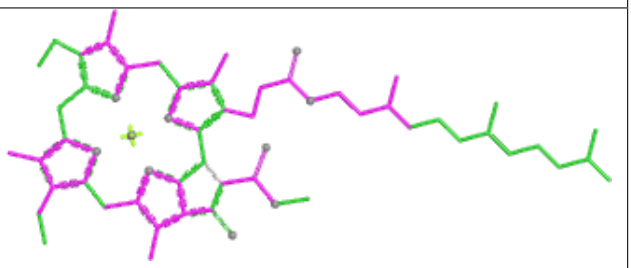
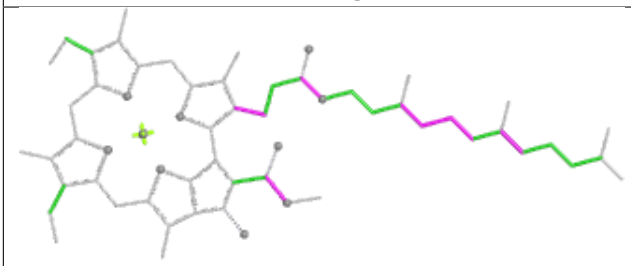
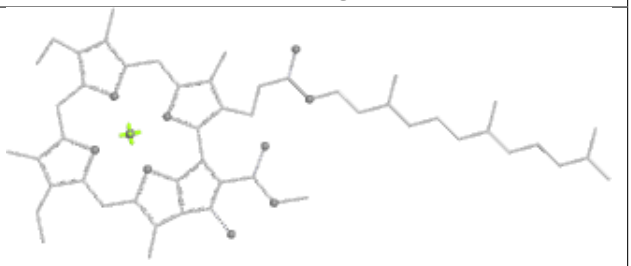
Bond angles

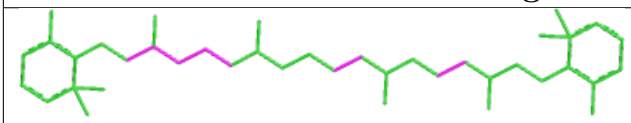
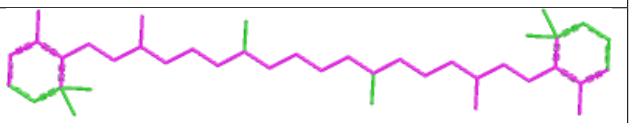
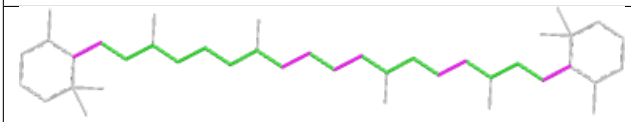
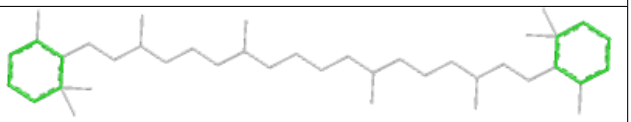


Torsions

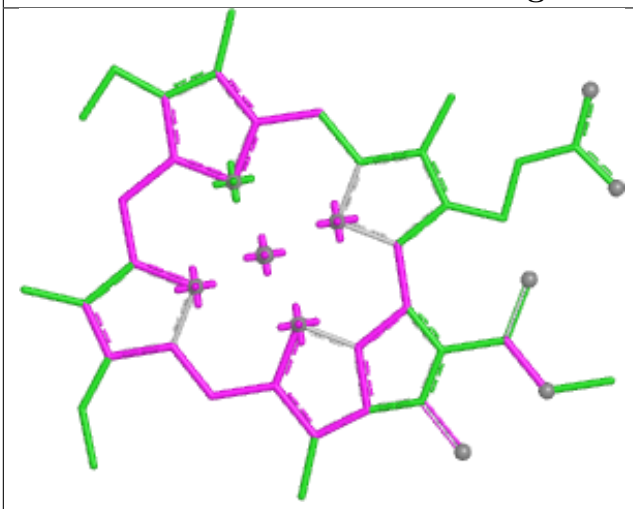


Rings

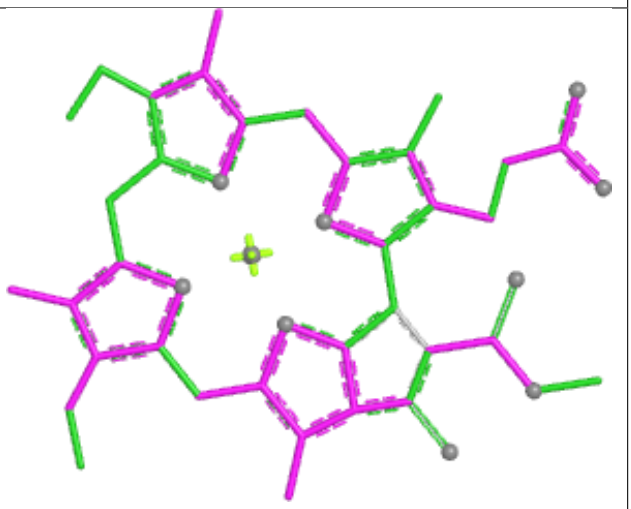
Ligand CLA b 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

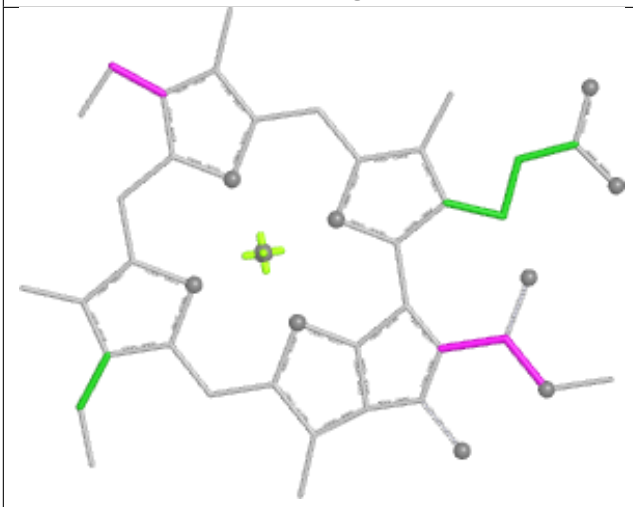
Ligand CLA b 833



Bond lengths



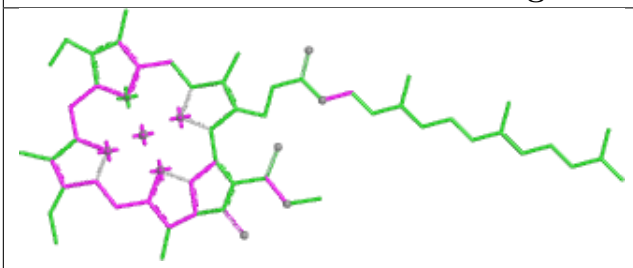
Bond angles



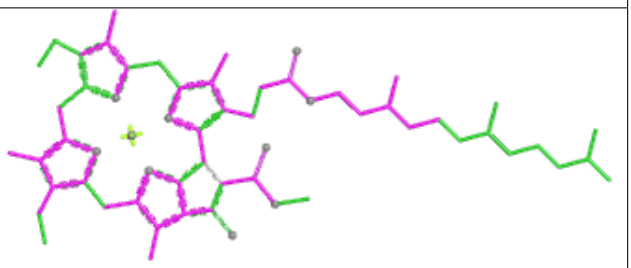
Torsions

Rings

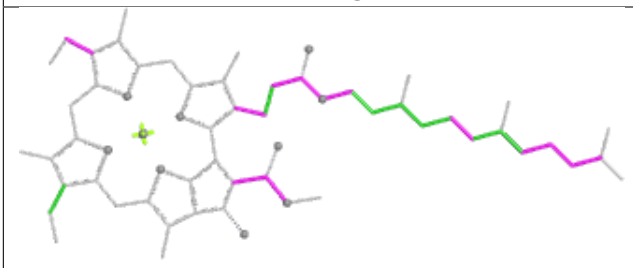
Ligand CLA b 836



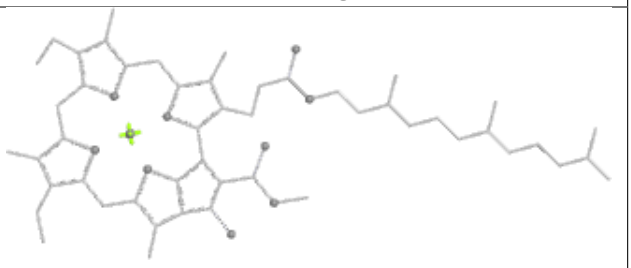
Bond lengths



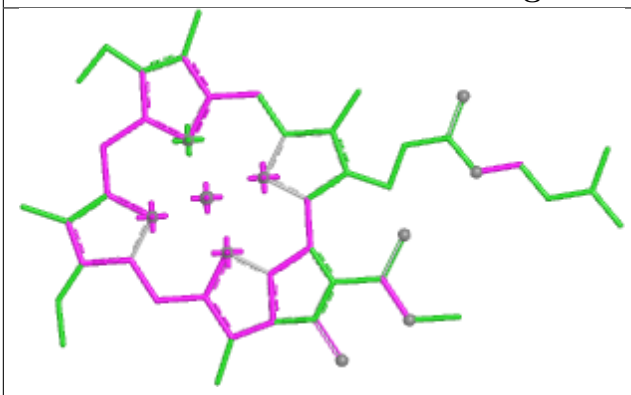
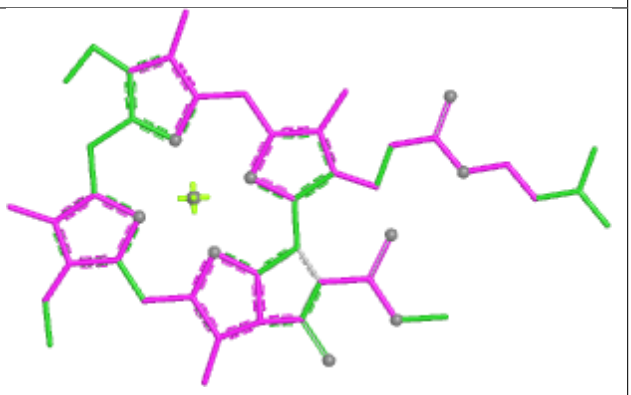
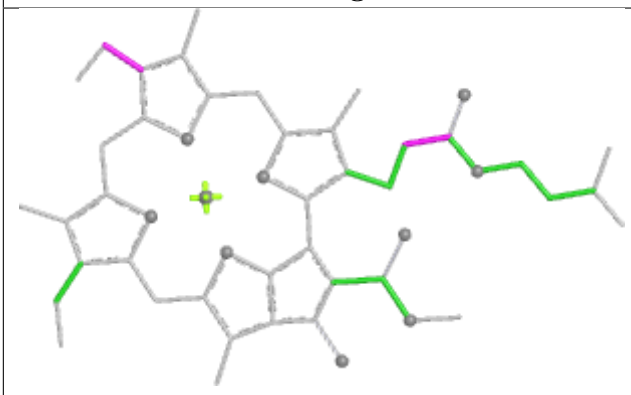
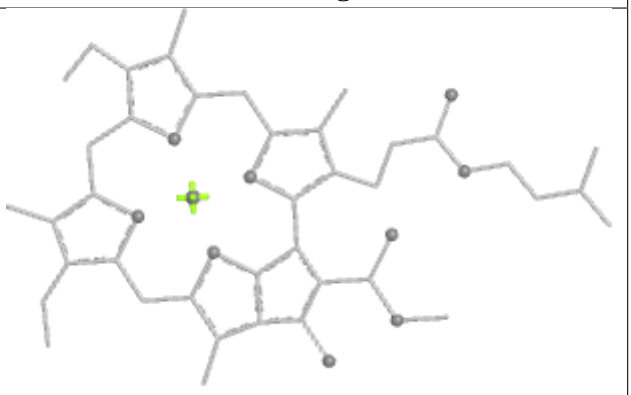
Bond angles



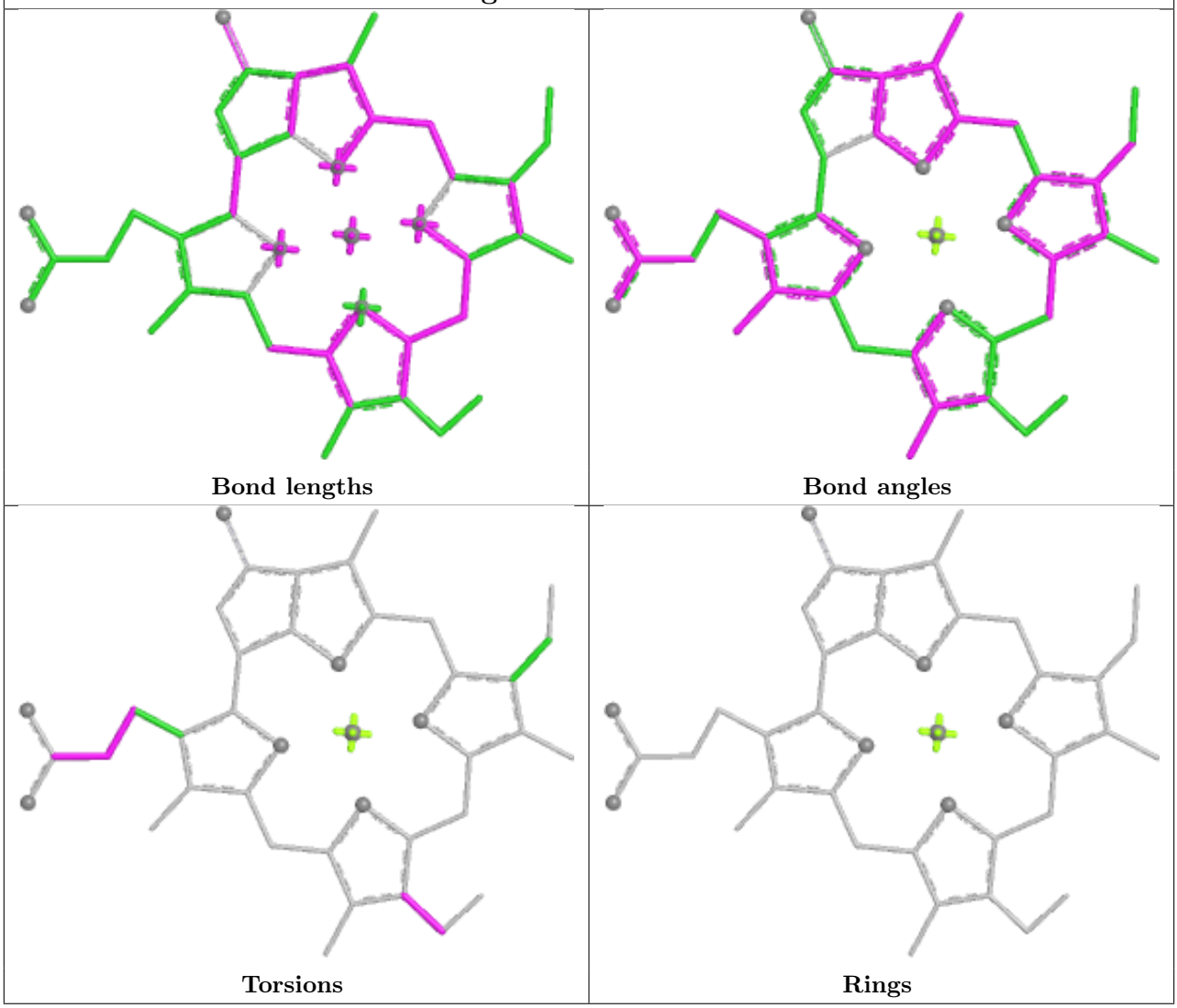
Torsions



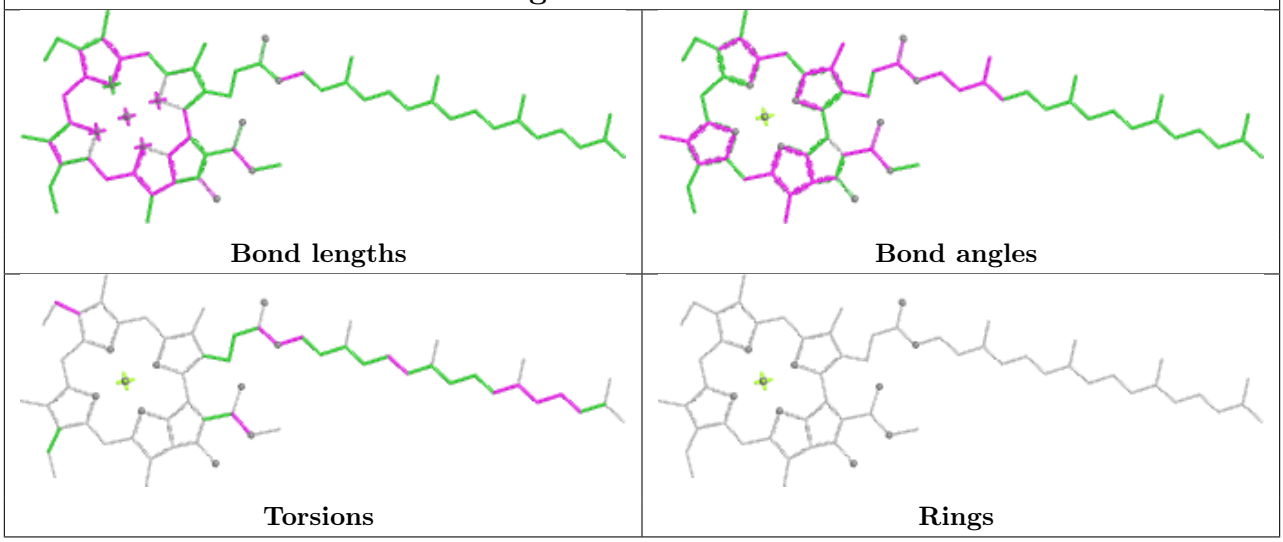
Rings

Ligand CLA A 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

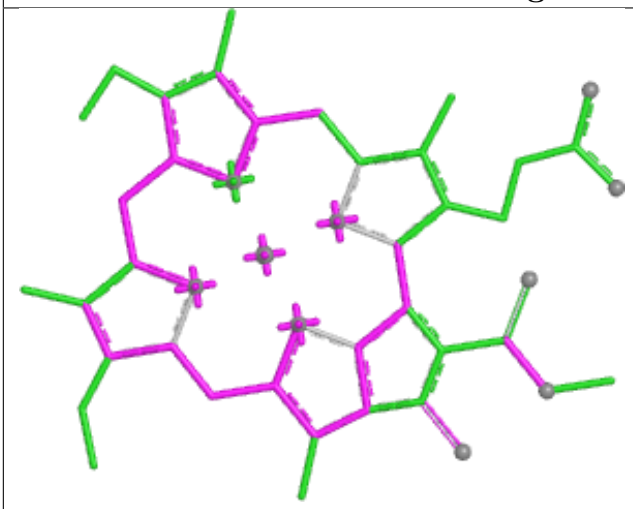
Ligand CLA A 841



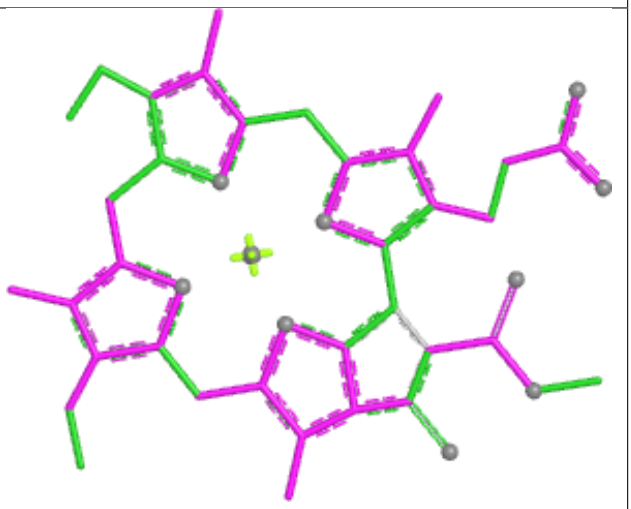
Ligand CLA a 825



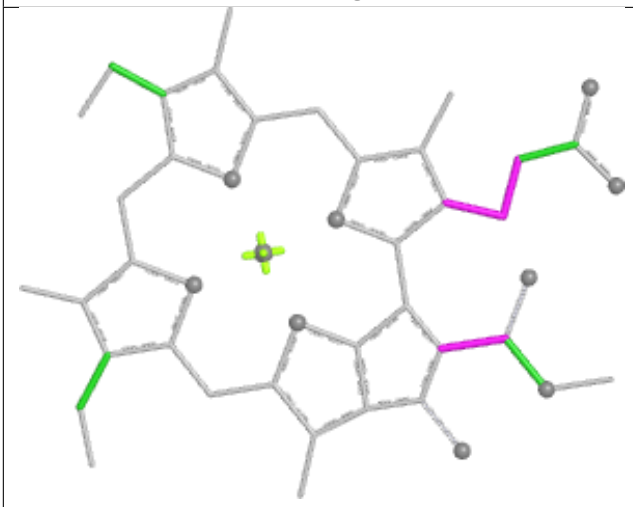
Ligand CLA S 101



Bond lengths



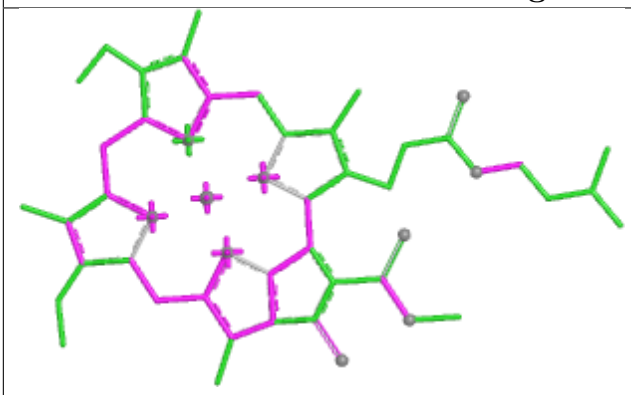
Bond angles



Torsions

Rings

Ligand CLA a 833



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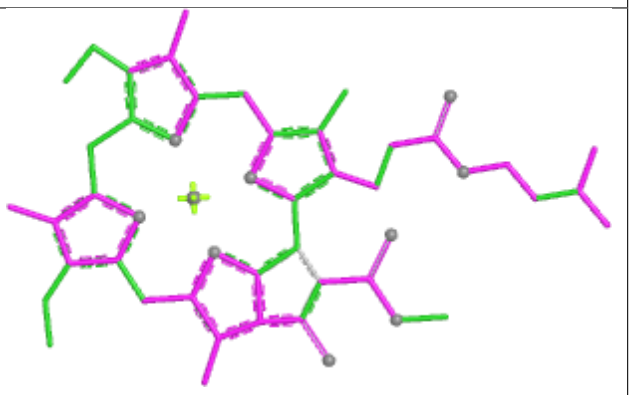
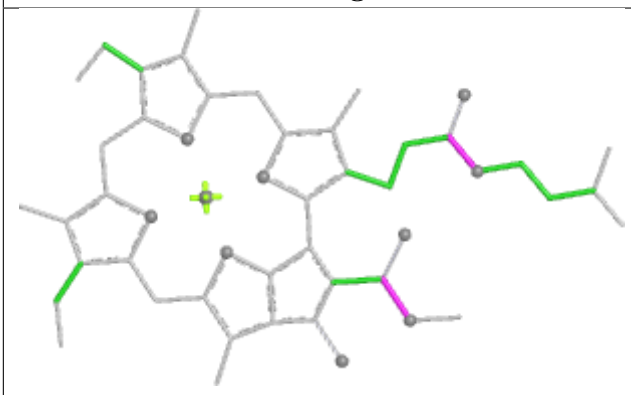
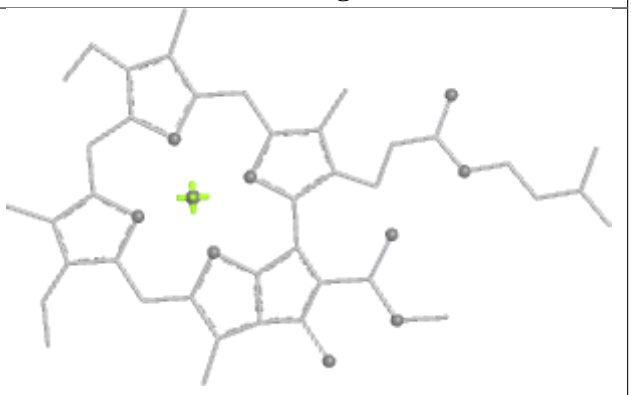


Bond angles

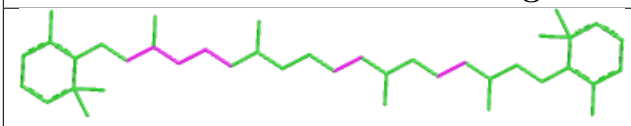


Torsions

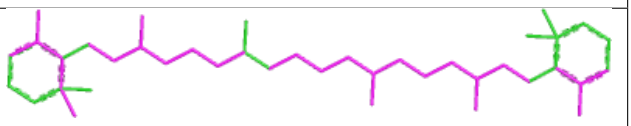


Rings

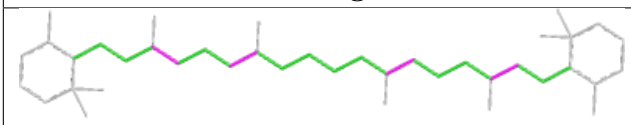
Ligand BCR B 845



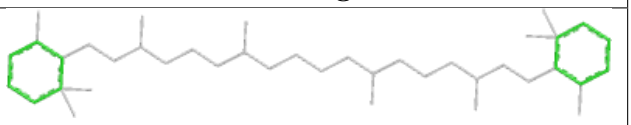
Bond lengths



Bond angles

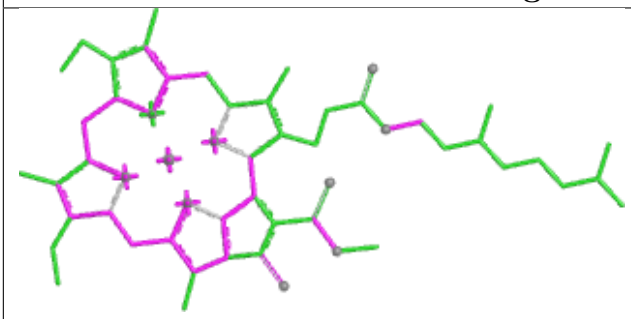


Torsions

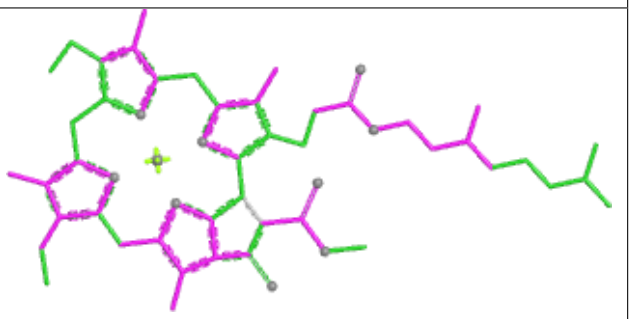


Rings

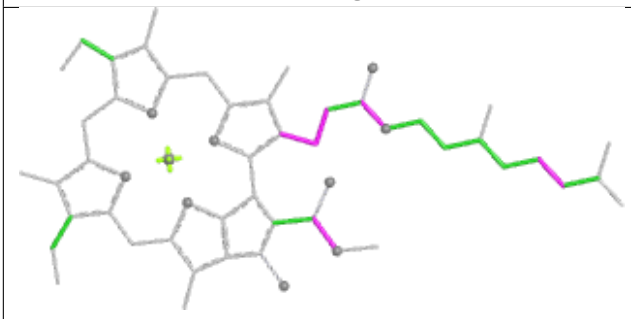
Ligand CLA H 818



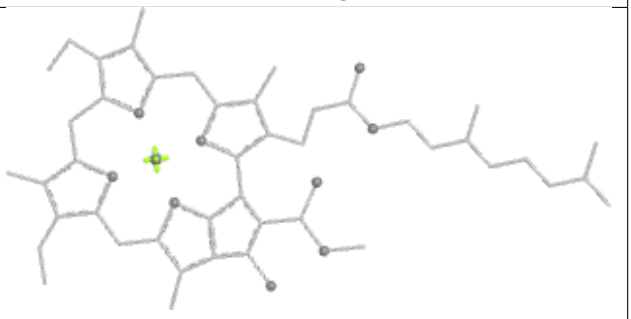
Bond lengths



Bond angles

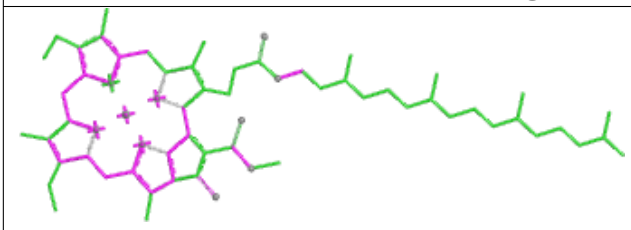


Torsions

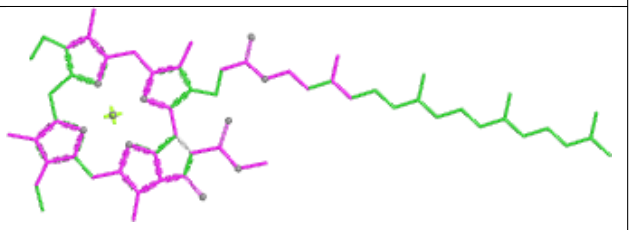


Rings

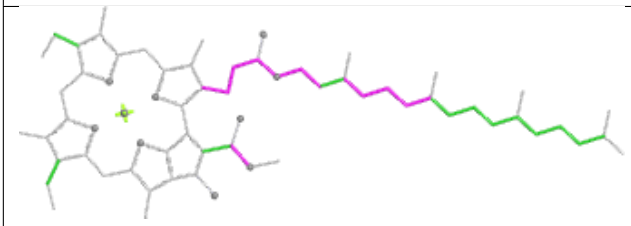
Ligand CLA A 827



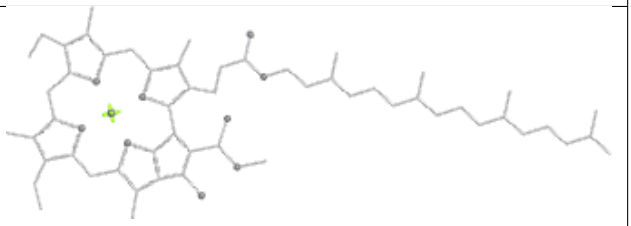
Bond lengths



Bond angles

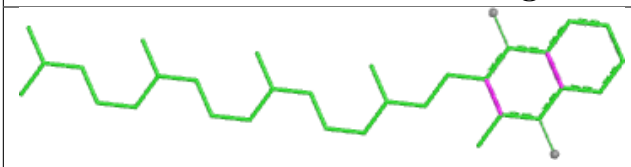


Torsions

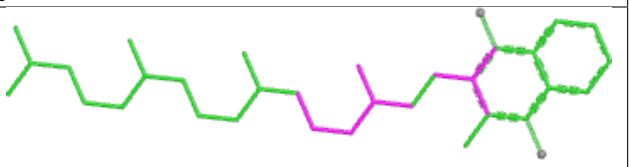


Rings

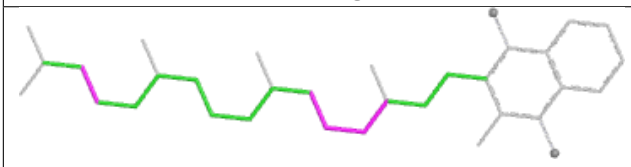
Ligand PQN G 842



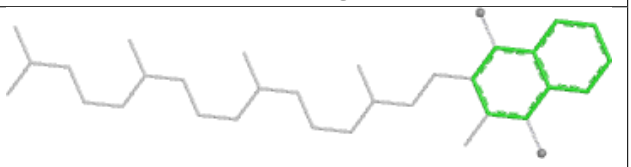
Bond lengths



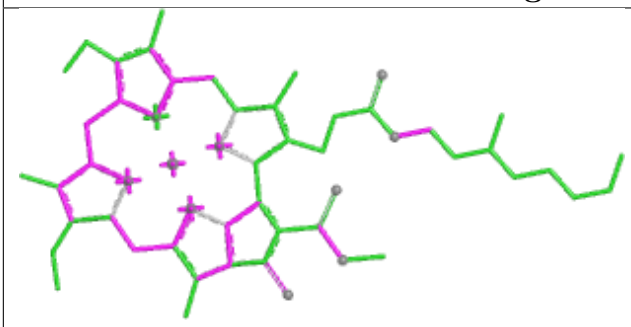
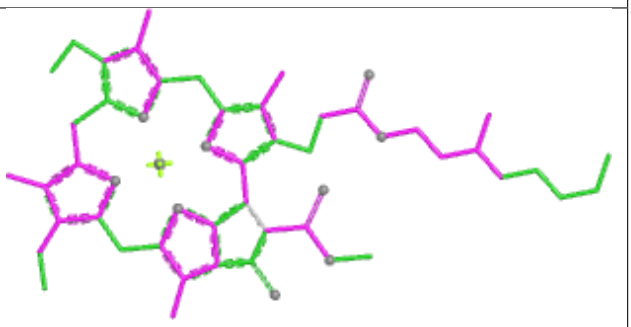
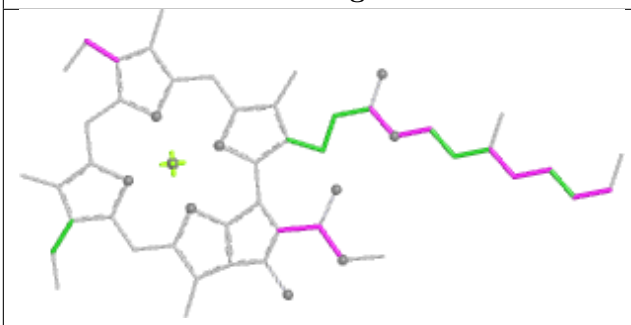
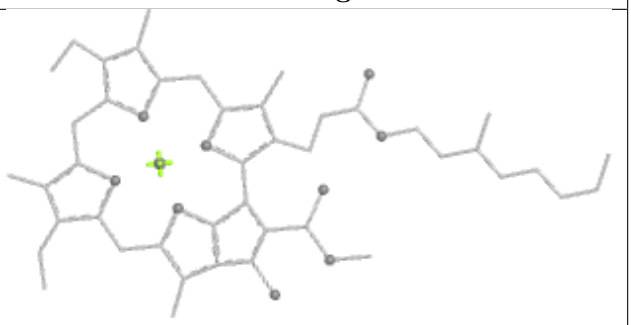
Bond angles



Torsions



Rings

Ligand CLA B 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

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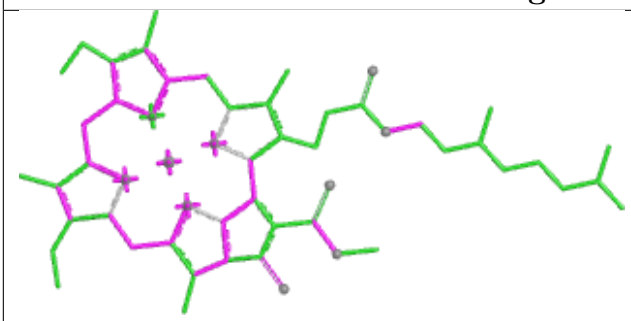
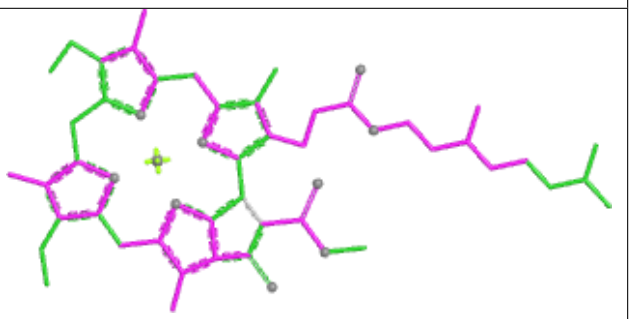
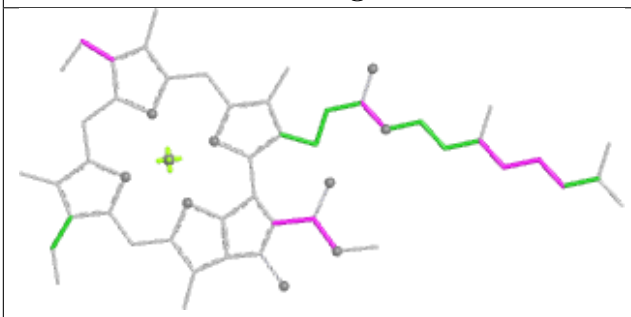
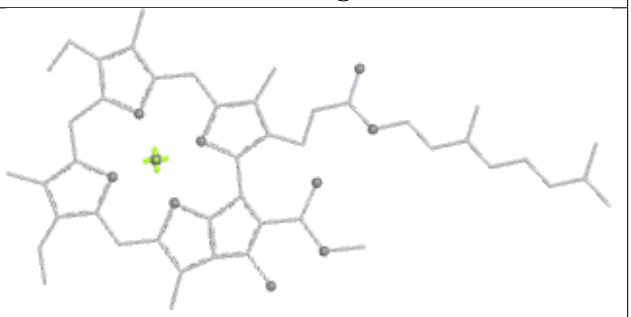
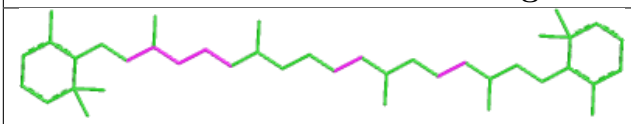
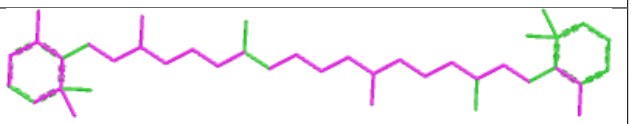
 Bond lengths	 Bond angles
 Torsions	 Rings

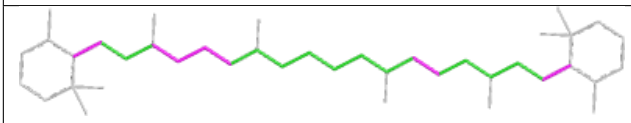
Ligand BCR H 850



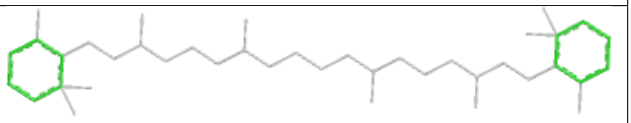
Bond lengths



Bond angles

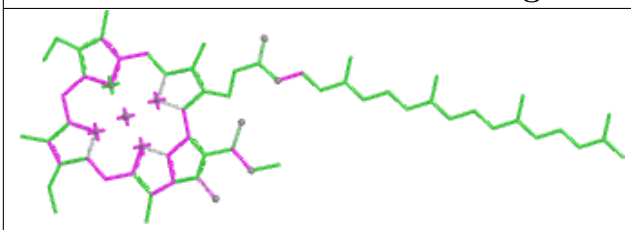


Torsions



Rings

Ligand CLA G 851



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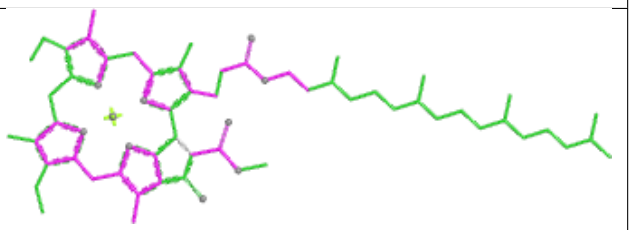
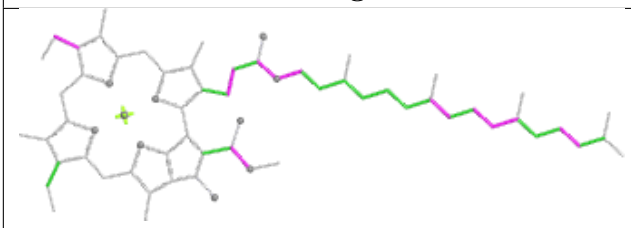


Bond angles



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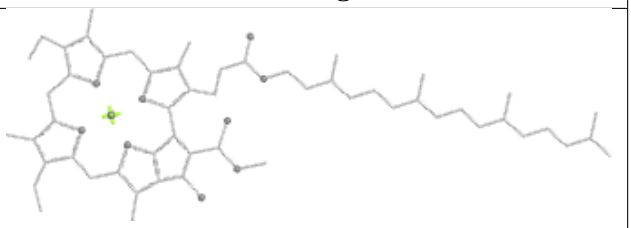
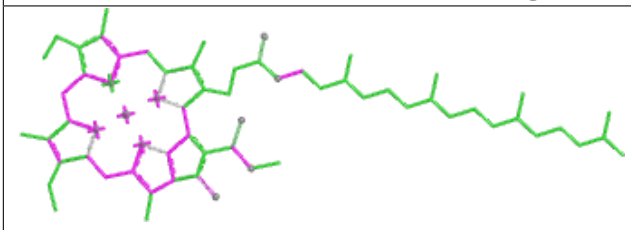
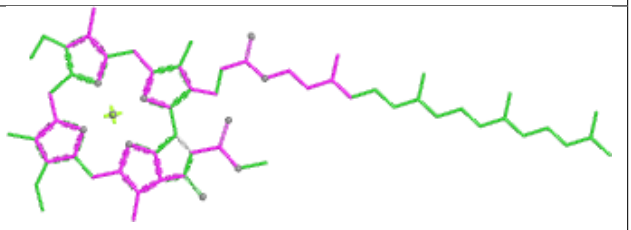


Rings

Ligand CLA B 809



Bond lengths



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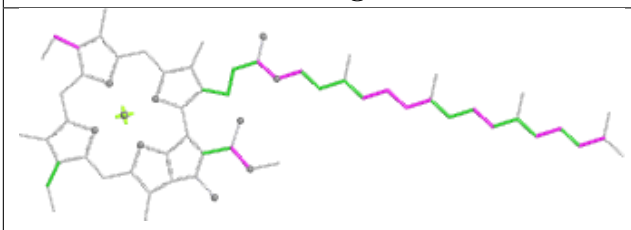

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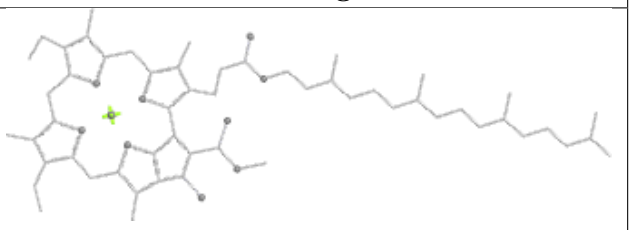
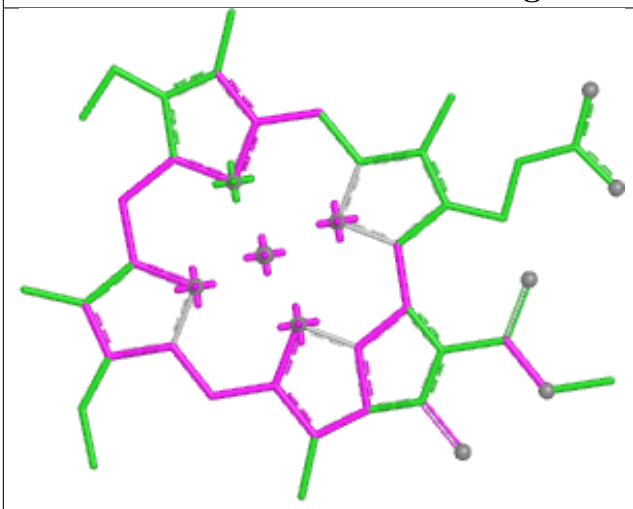


Rings

Ligand CLA H 817



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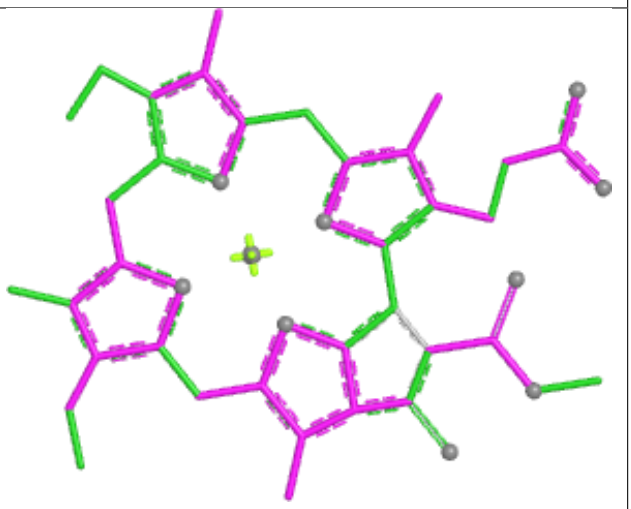
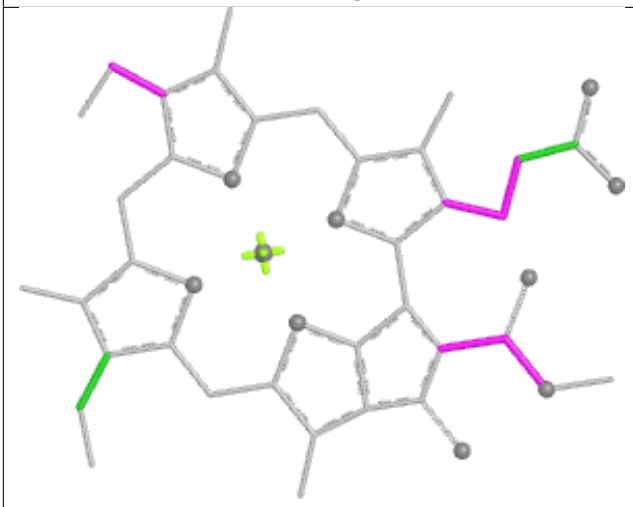


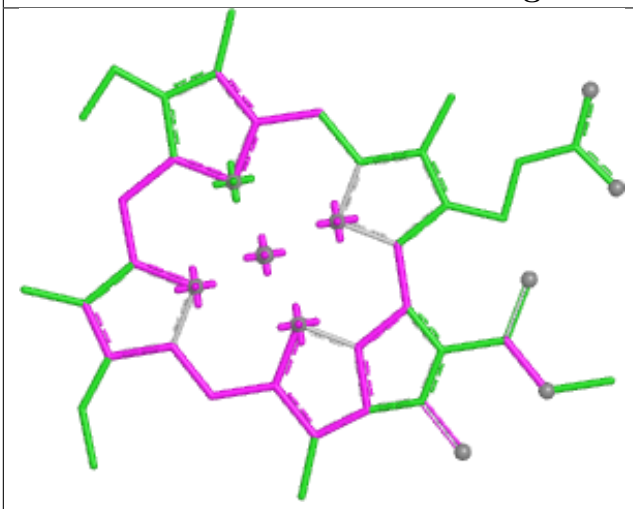
Bond angles



Torsions

Rings

Ligand CLA H 823



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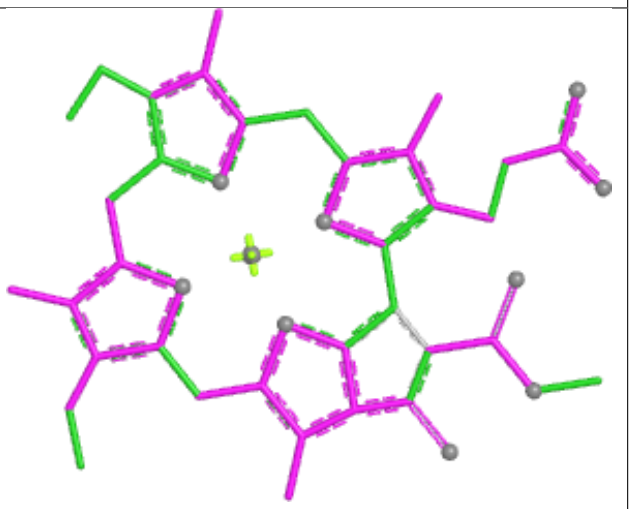
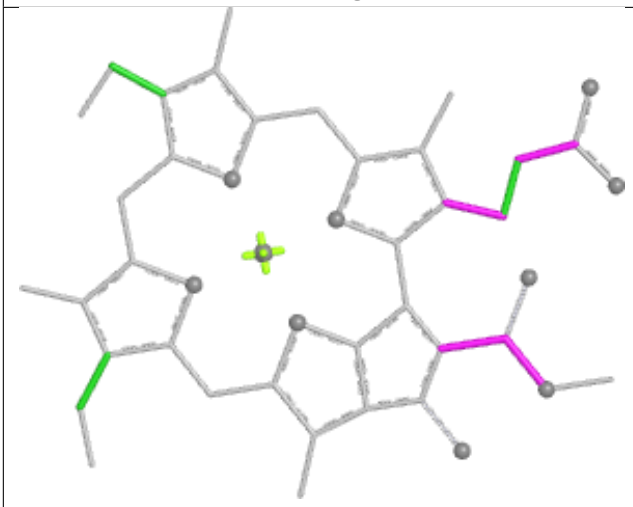


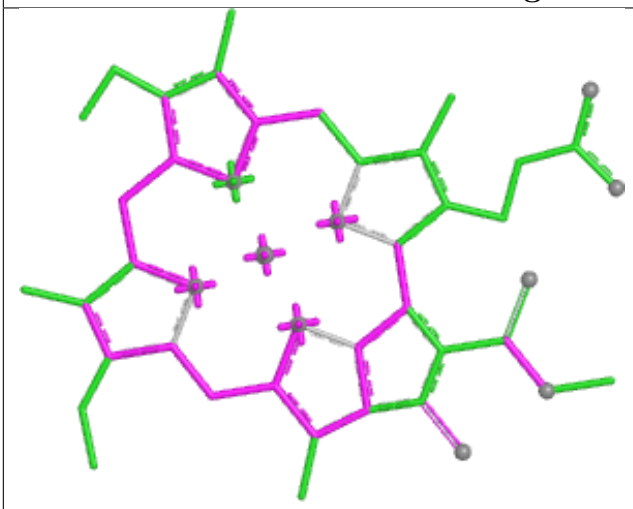
Bond angles



Torsions

Rings

Ligand CLA A 815



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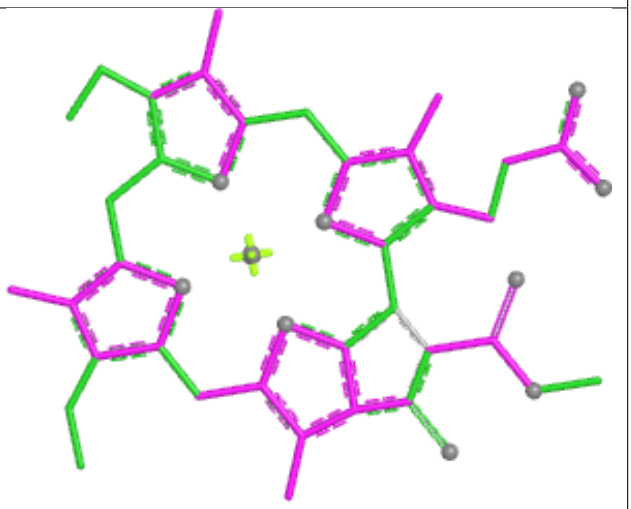
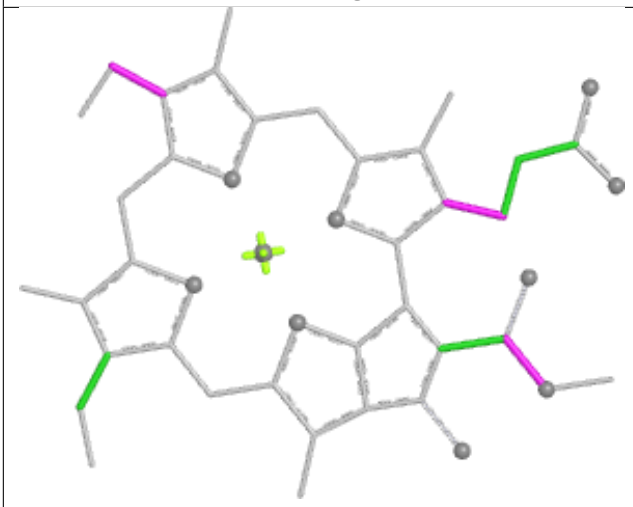
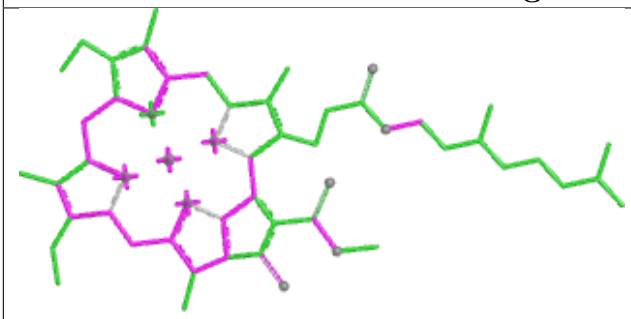
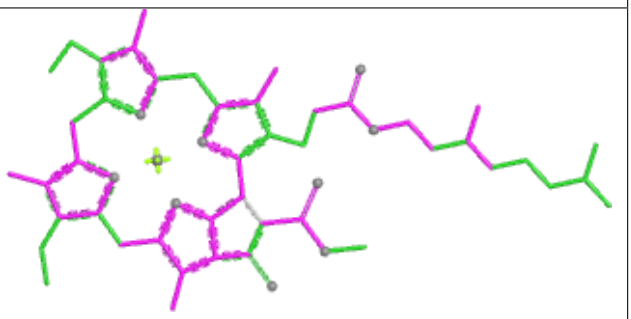
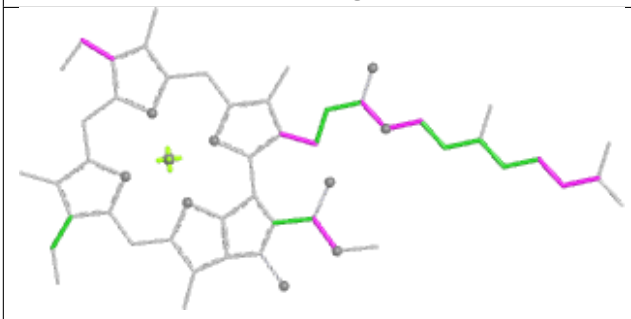
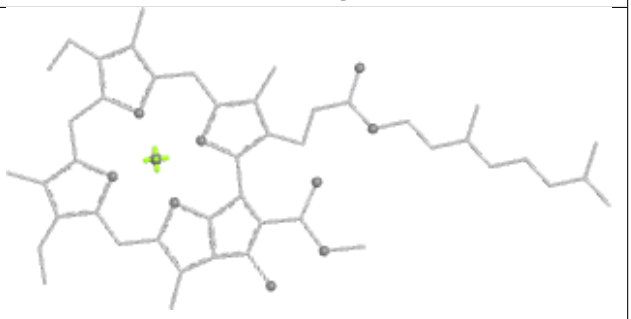


Bond angles

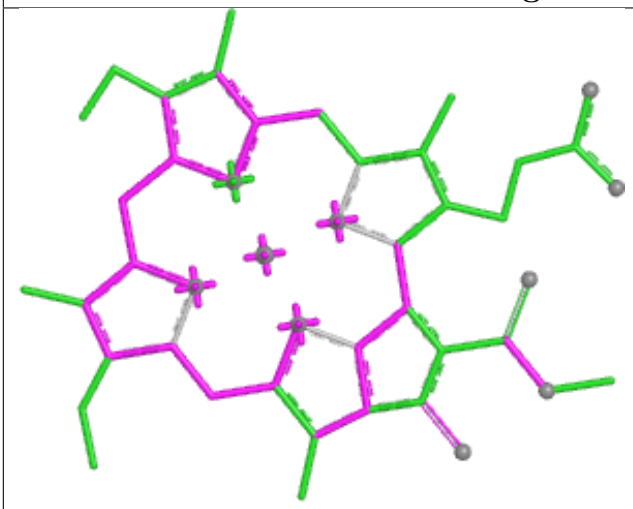


Torsions

Rings

Ligand CLA A 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 1301



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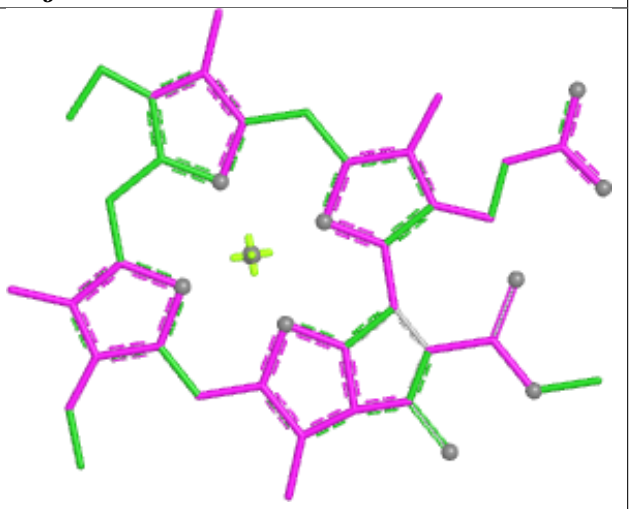
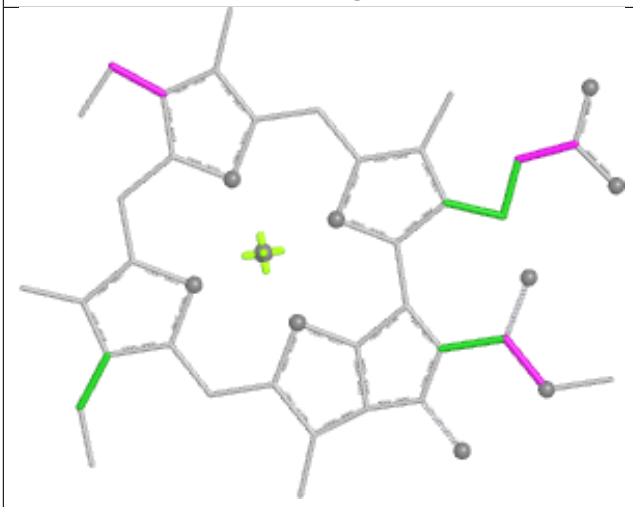


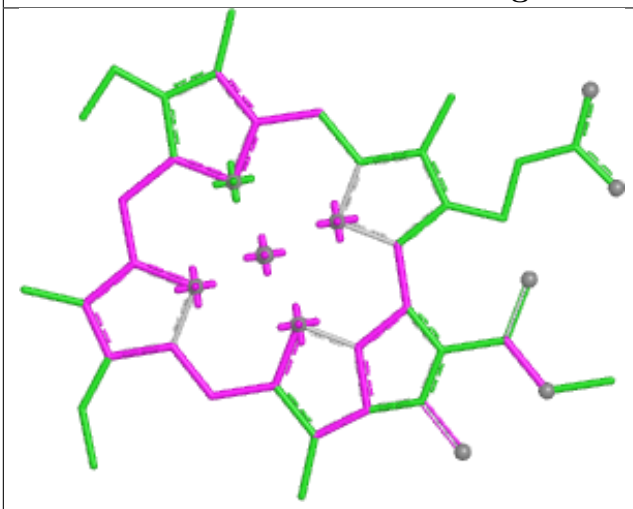
Bond angles



Torsions

Rings

Ligand CLA M 1601



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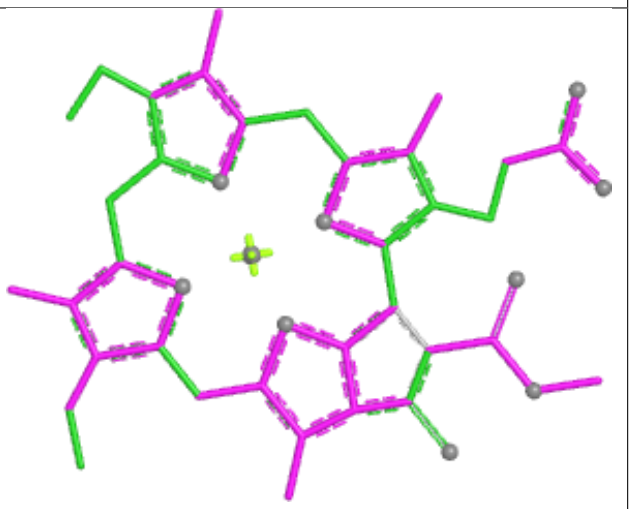
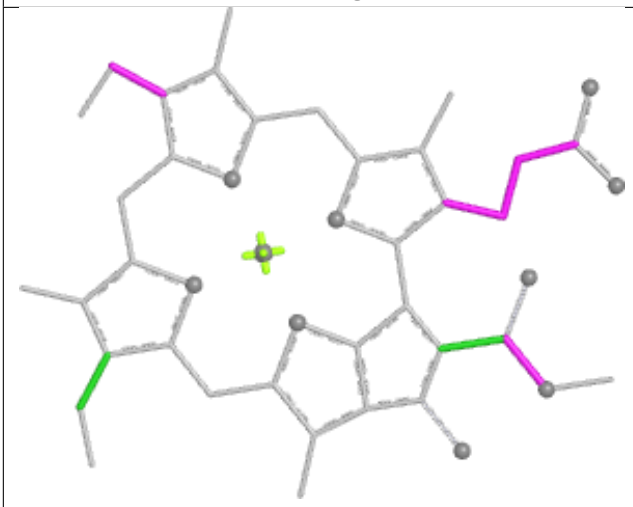


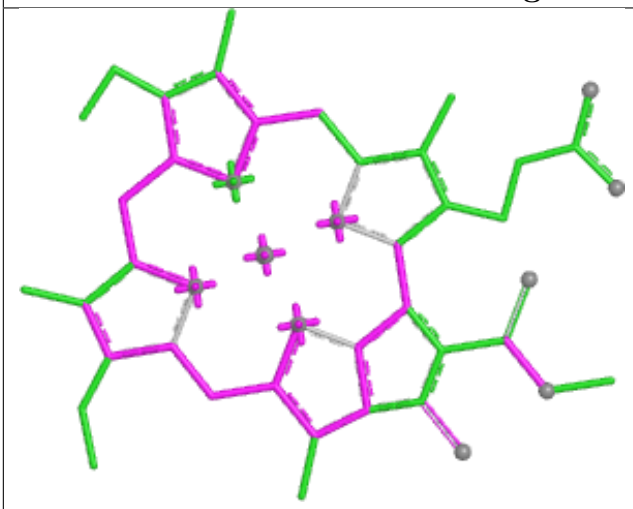
Bond angles



Torsions

Rings

Ligand CLA H 814



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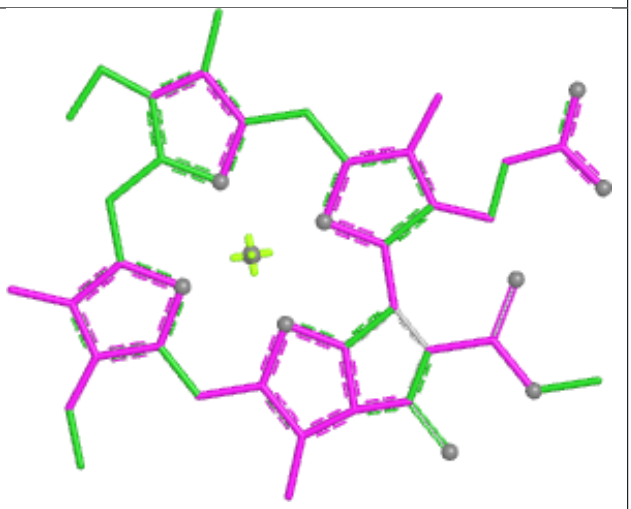
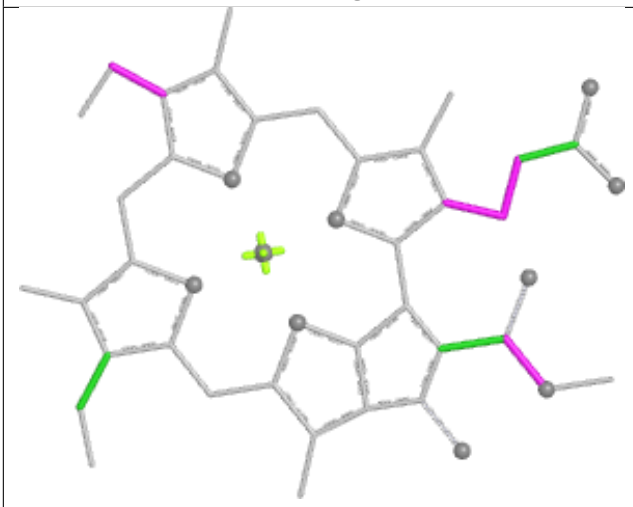


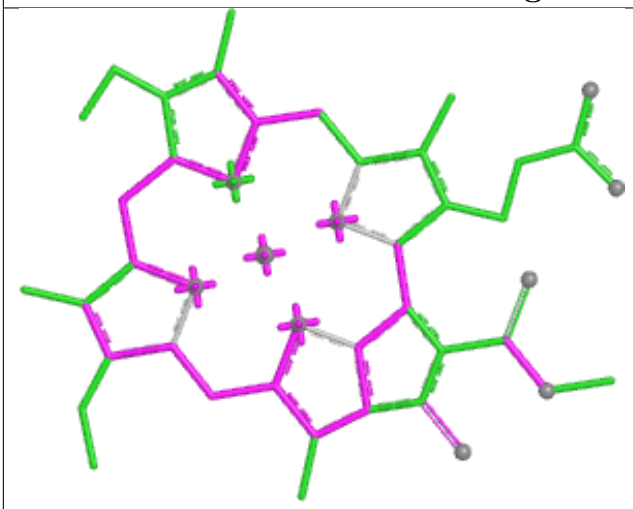
Bond angles



Torsions

Rings

Ligand CLA B 837



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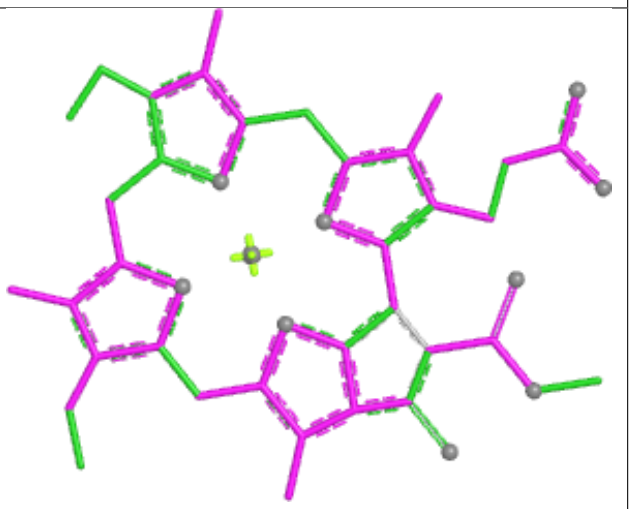
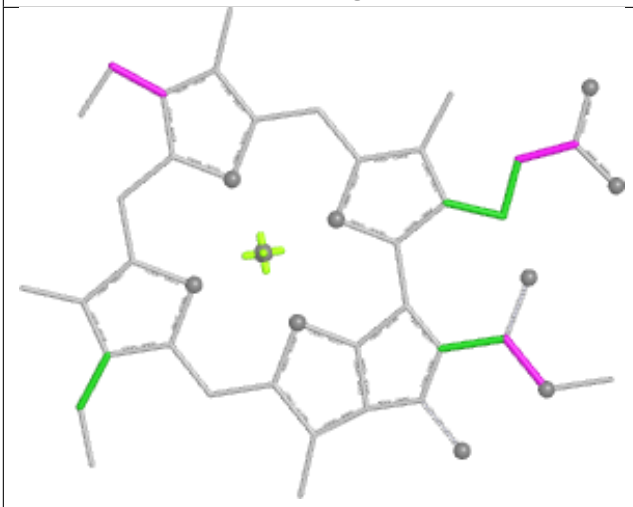


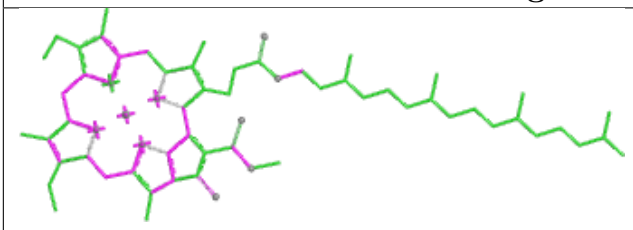
Bond angles



Torsions

Rings

Ligand CLA b 804



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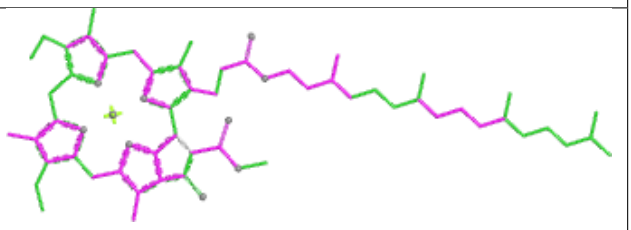
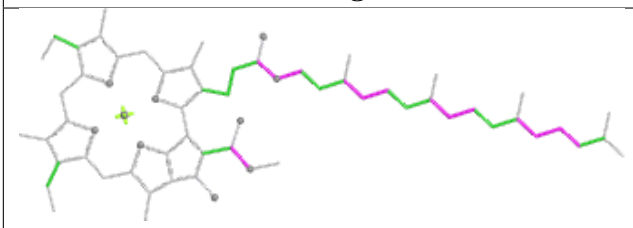
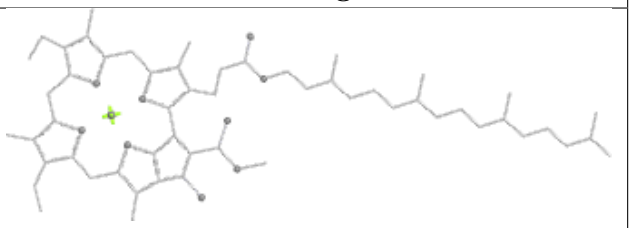


Bond angles

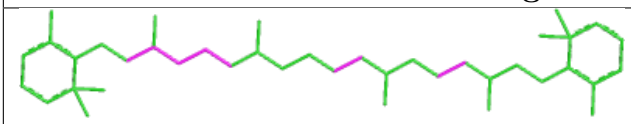


Torsions

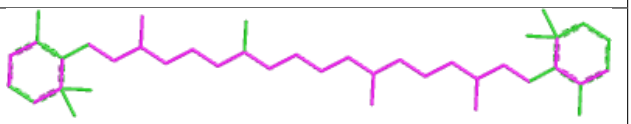


Rings

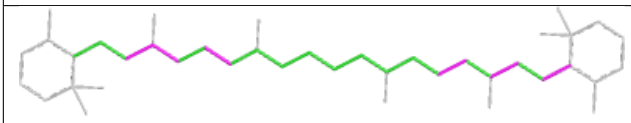
Ligand BCR B 844



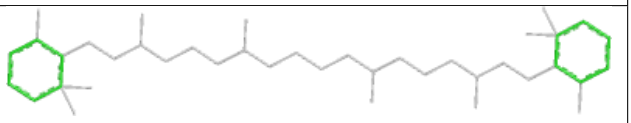
Bond lengths



Bond angles

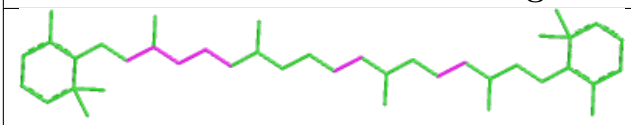


Torsions



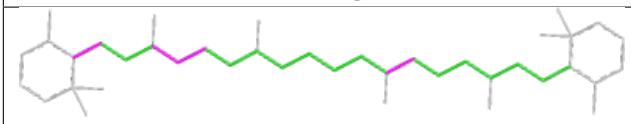
Rings

Ligand BCR a 846



Bond lengths

Bond angles



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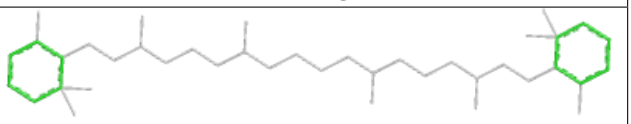
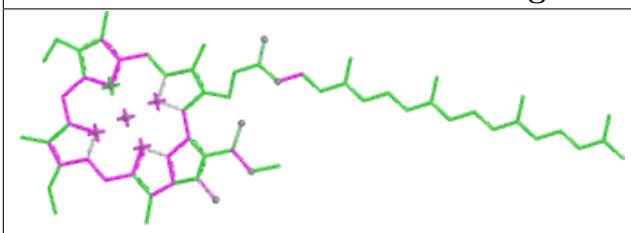


Rings

Ligand CLA a 841



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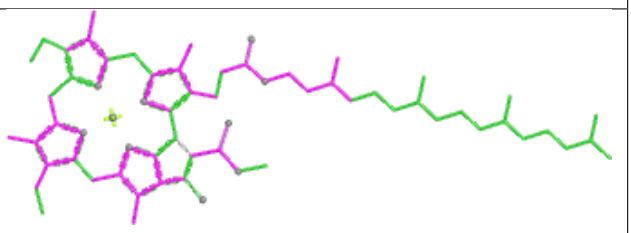
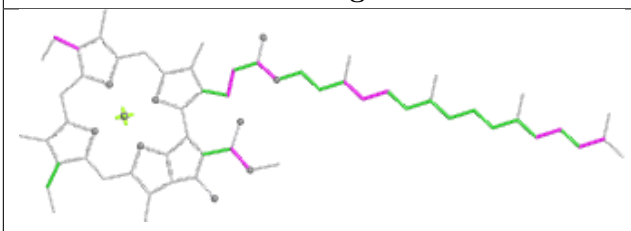


Bond angles



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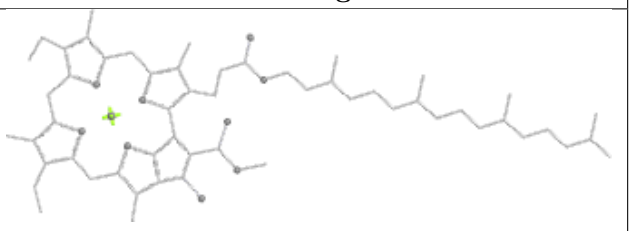
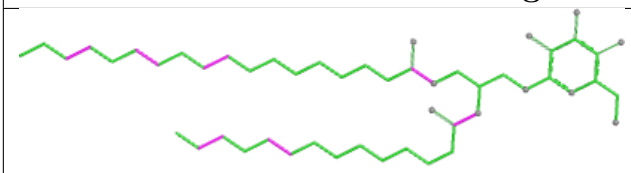


Rings

Ligand LMG b 849



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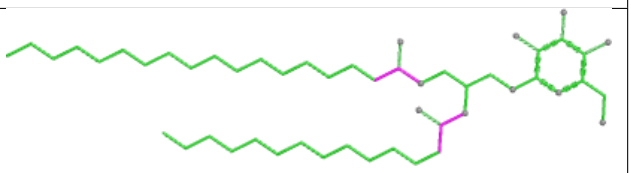
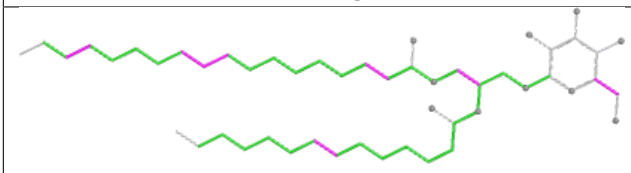


Bond angles



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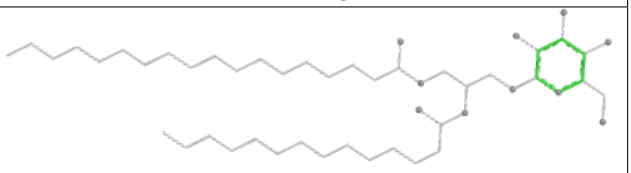
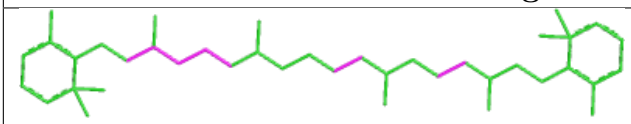


Rings

Ligand BCR R 102



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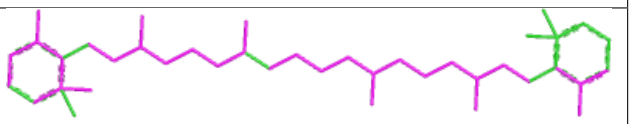
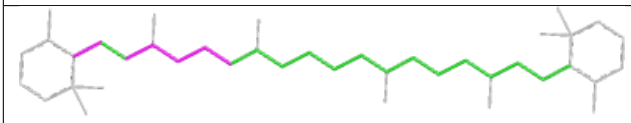


Bond angles



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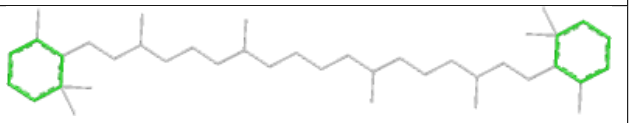
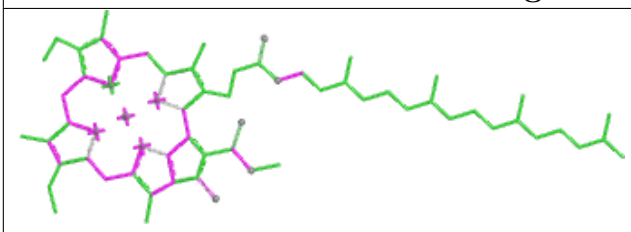


Rings

Ligand CLA B 806



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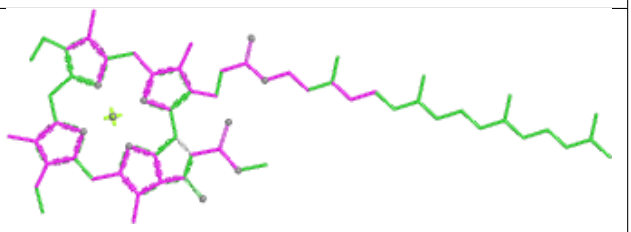
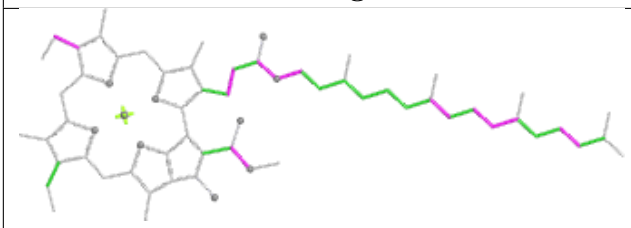


Bond angles



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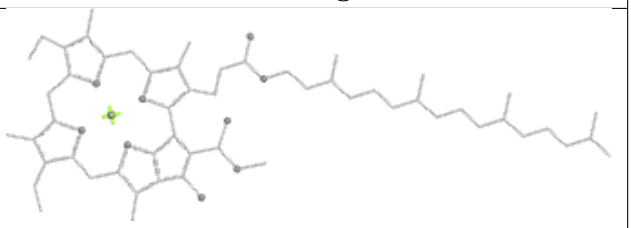
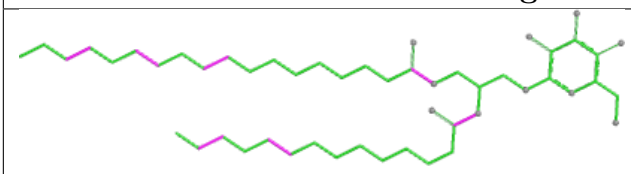
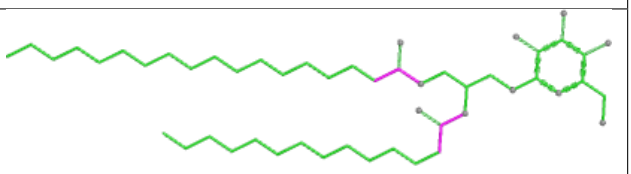


Rings

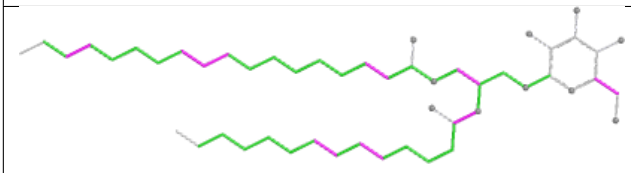
Ligand LMG B 851



Bond lengths



Bond angles



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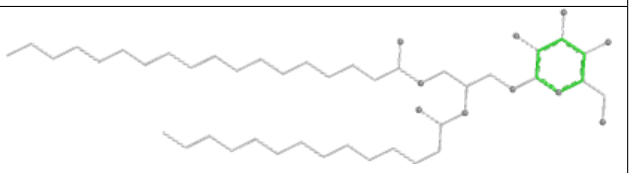
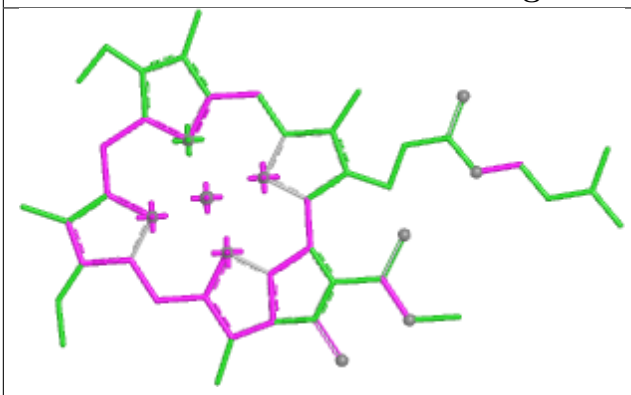


Rings

Ligand CLA G 817



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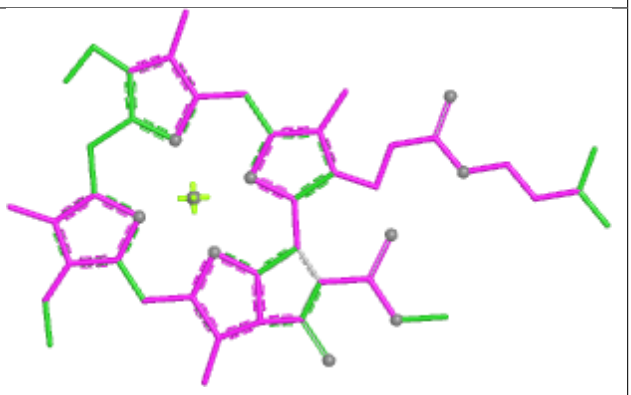
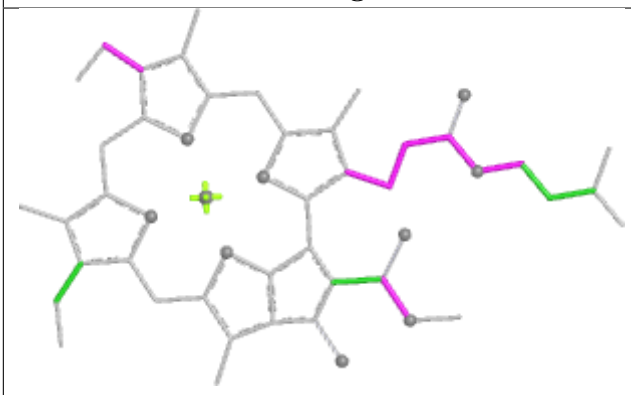


Bond angles



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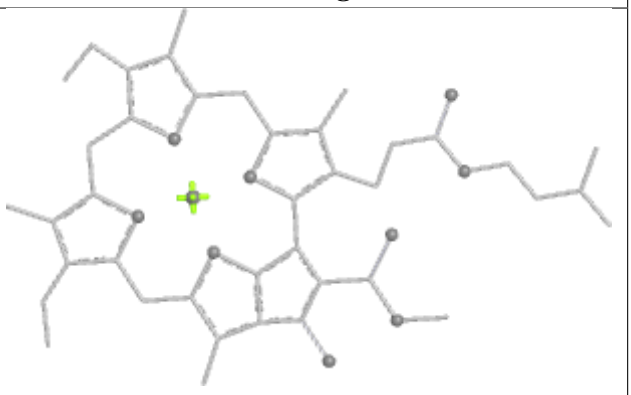
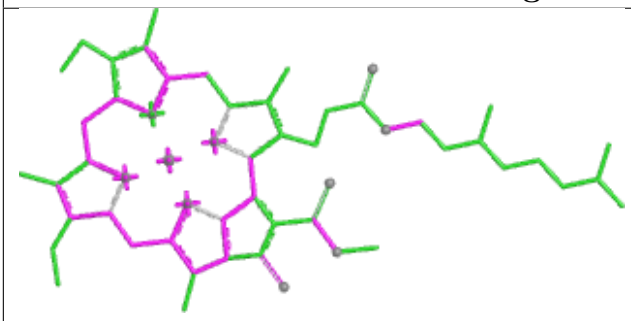
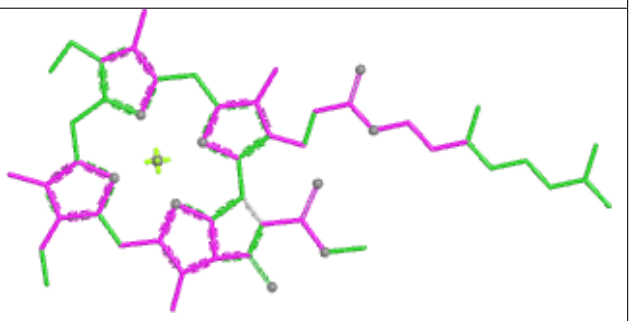


Rings

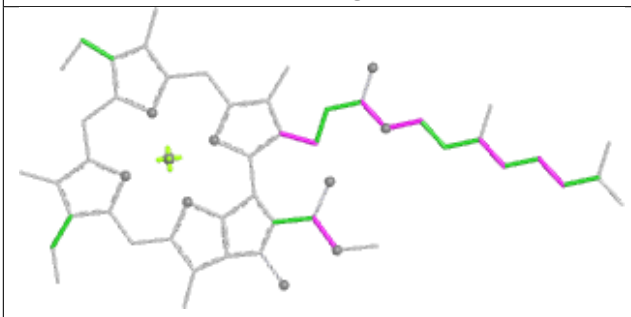
Ligand CLA G 823



Bond lengths



Bond angles



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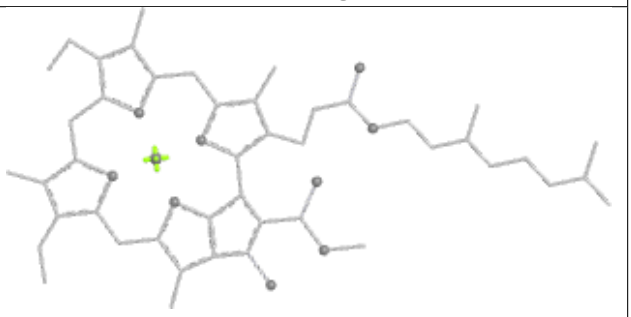
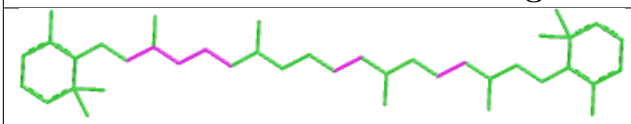
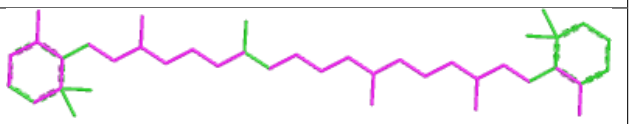


Rings

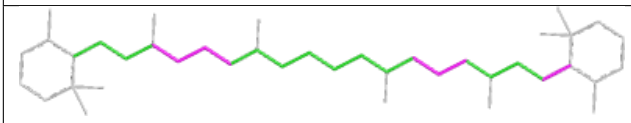
Ligand BCR b 848



Bond lengths



Bond angles



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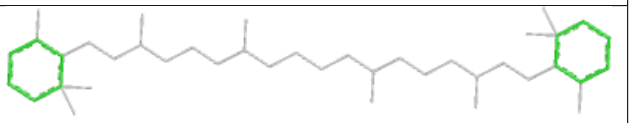
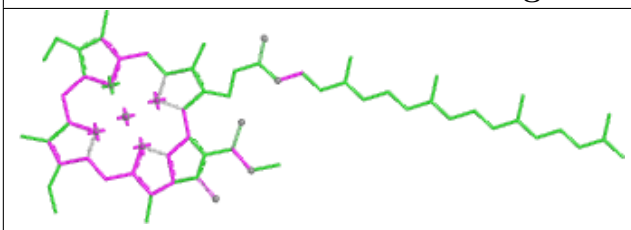


Rings

Ligand CLA H 830



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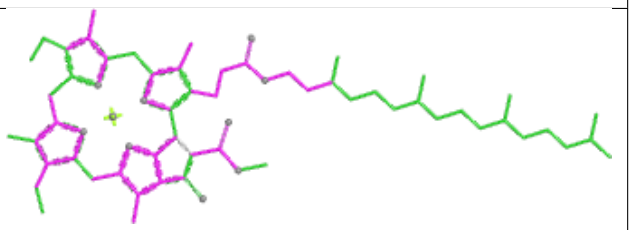
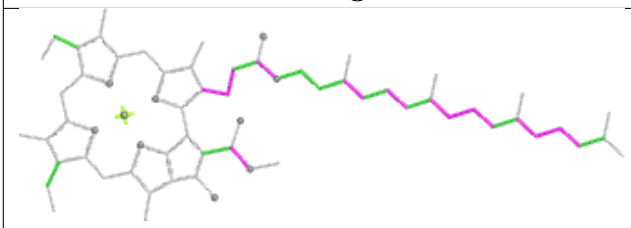


Bond angles



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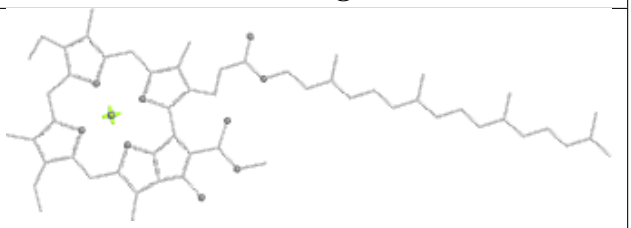
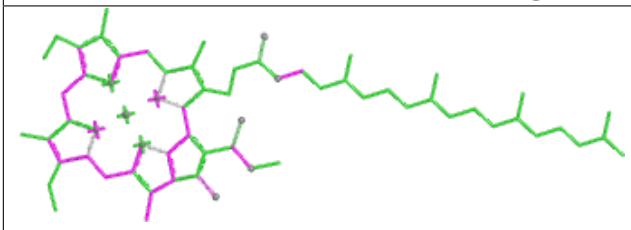


Rings

Ligand CLA b 801



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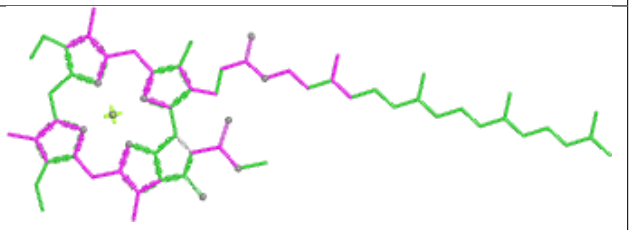
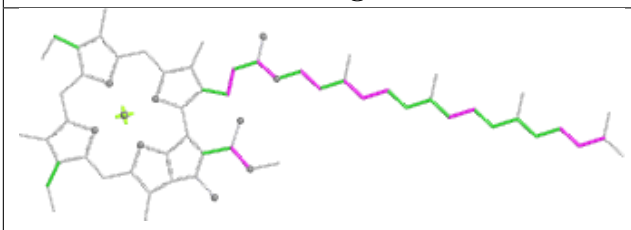
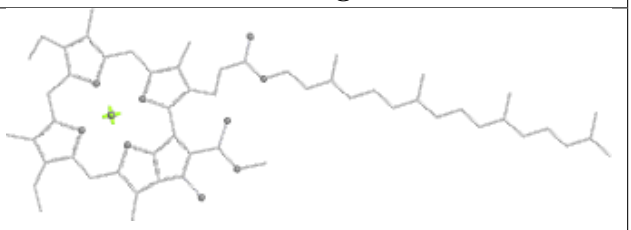


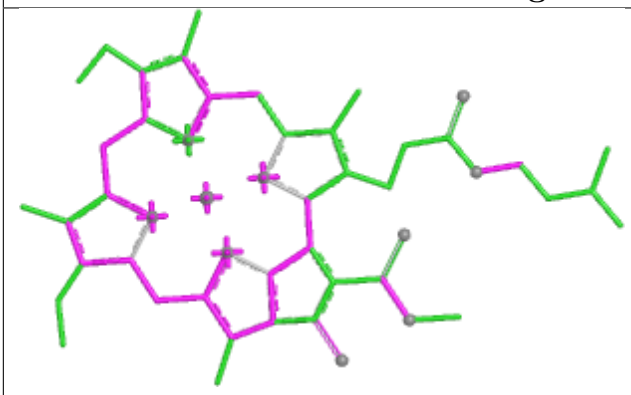
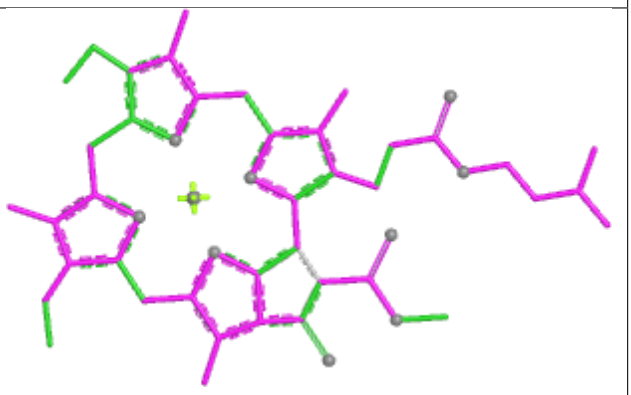
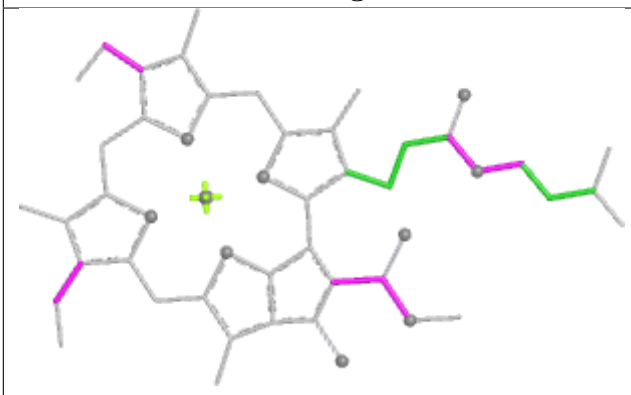
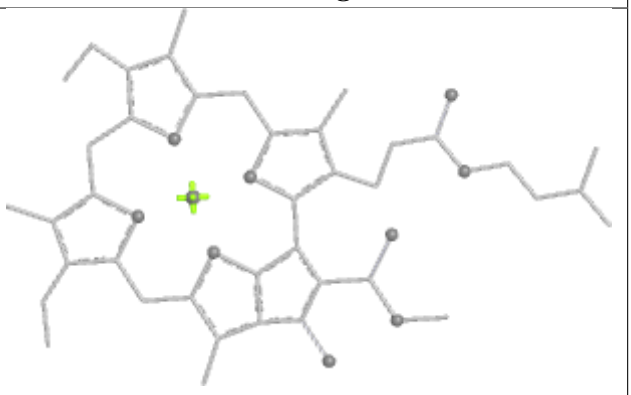
Bond angles

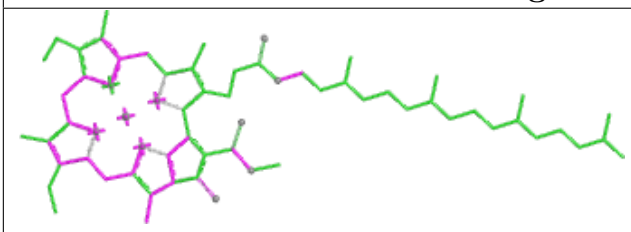
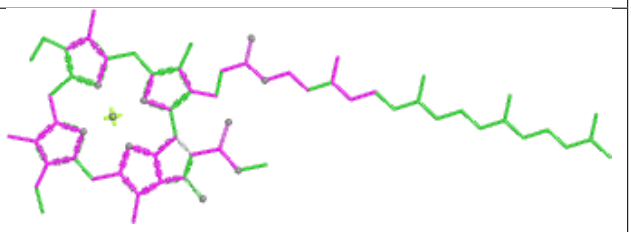
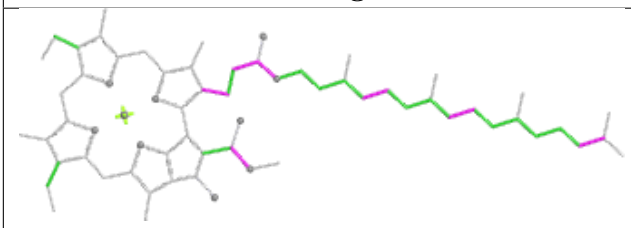
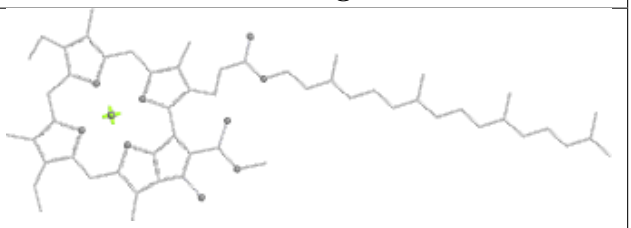


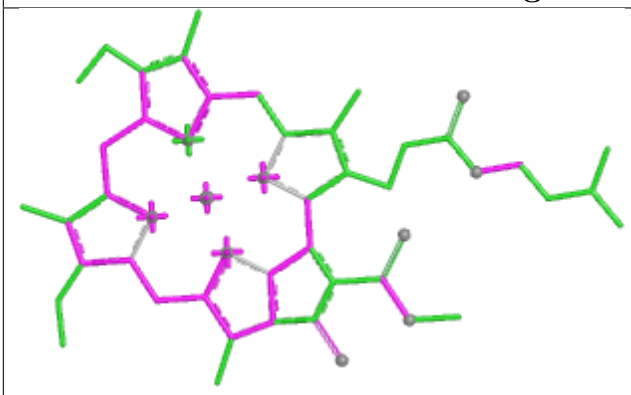
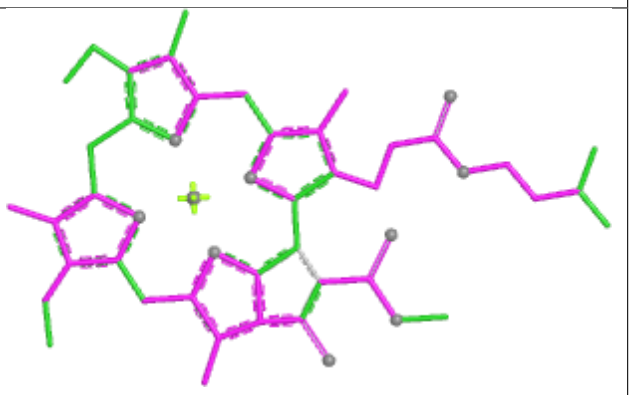
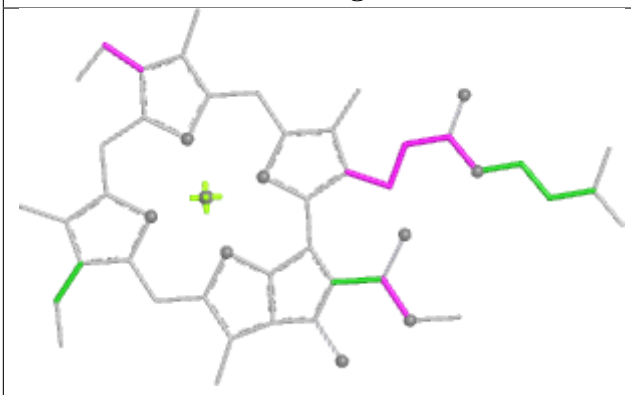
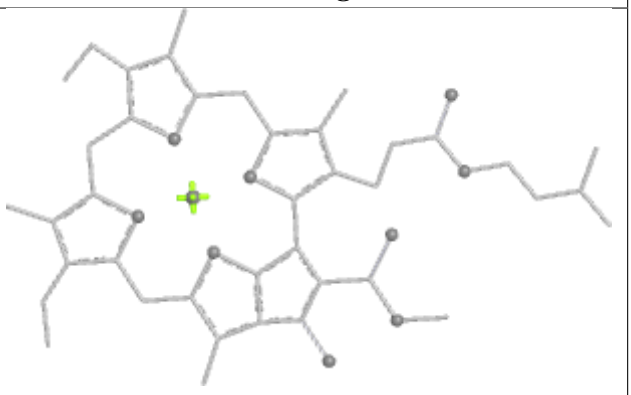
Torsions



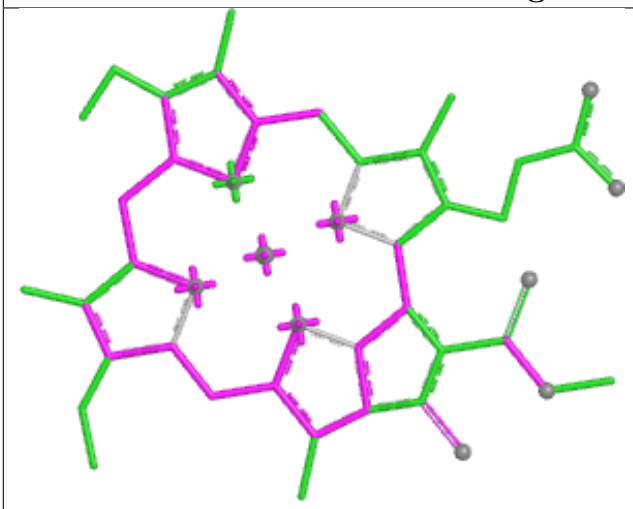
Rings

Ligand CLA a 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 102



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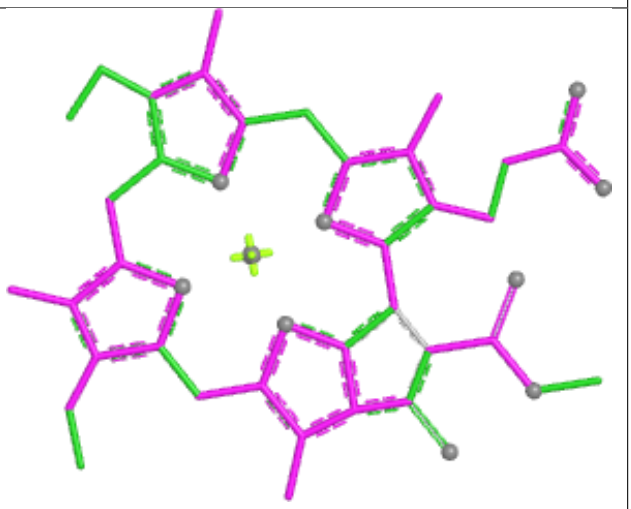

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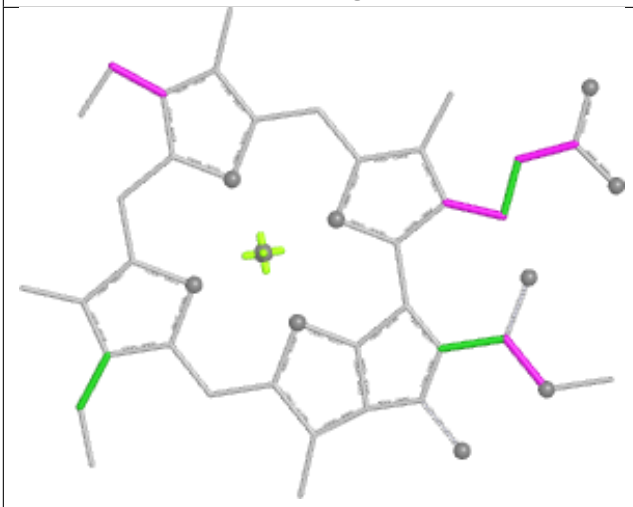
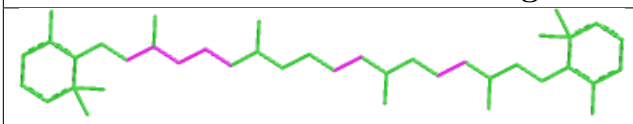


Torsions

Rings

Ligand BCR j 1305



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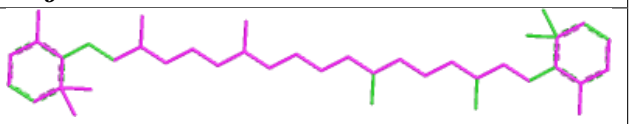

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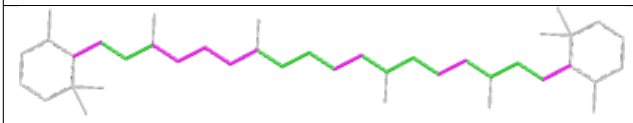

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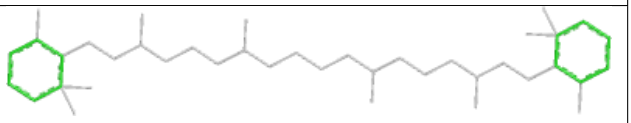
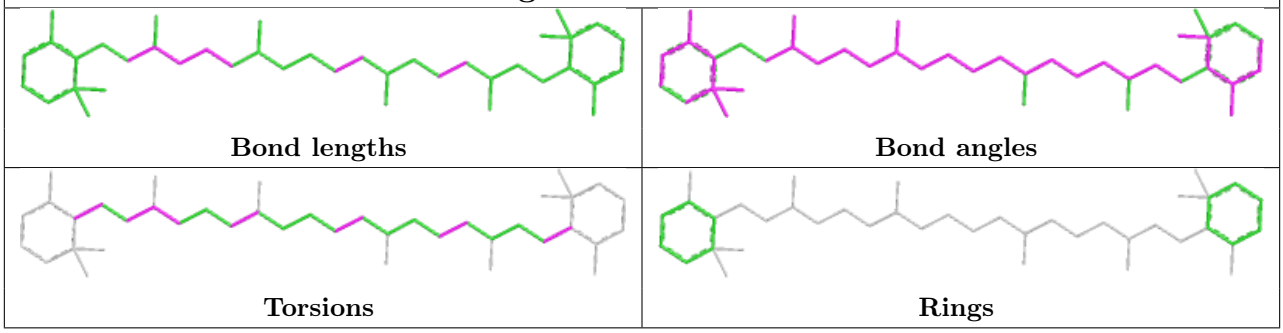
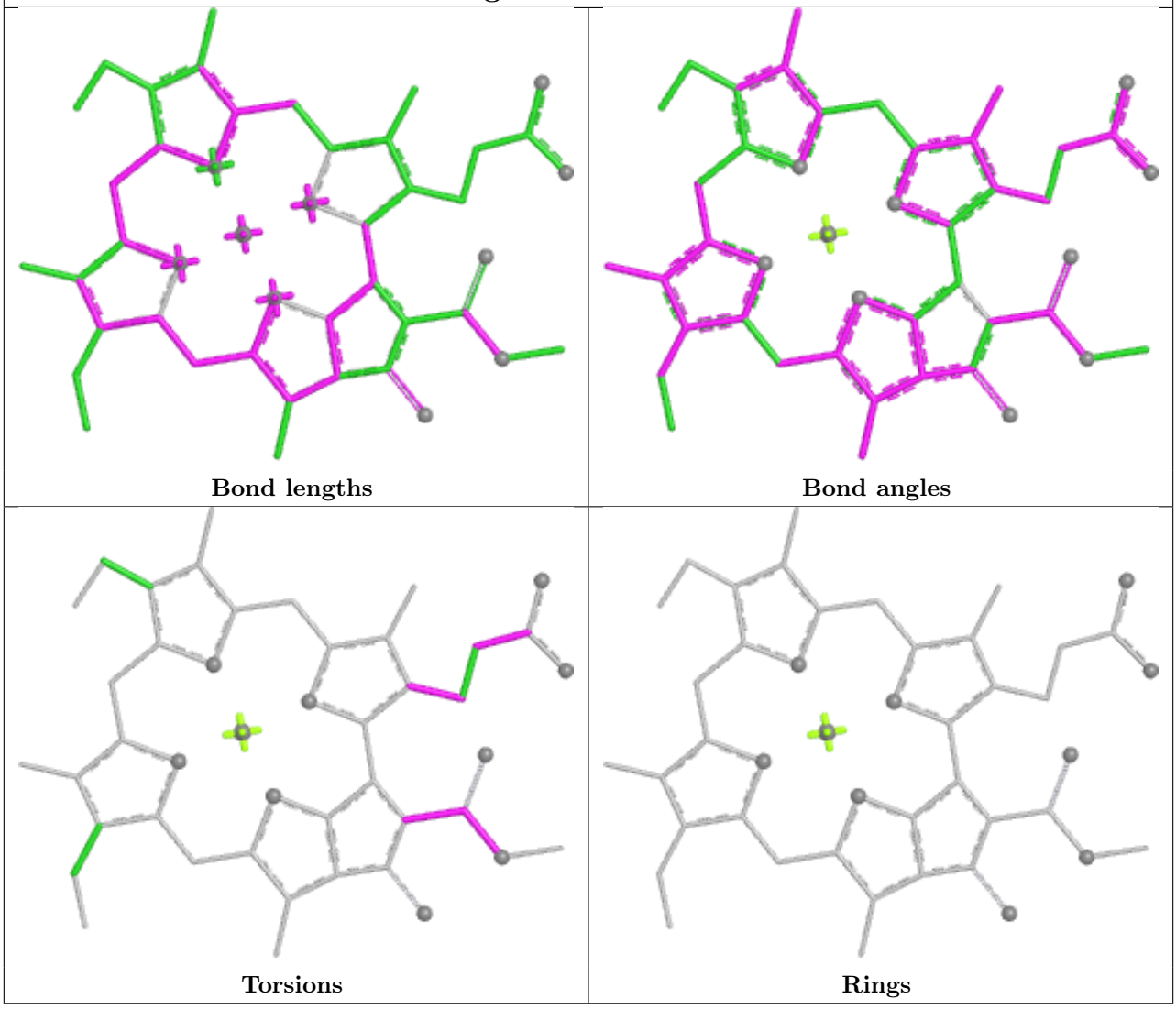


Rings

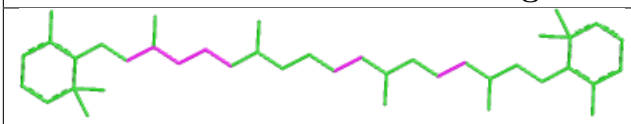
Ligand BCR J 1305



Ligand CLA b 820



Ligand BCR U 202



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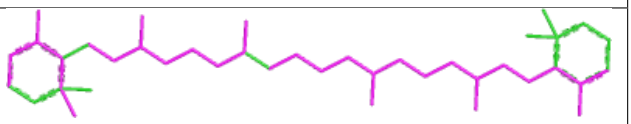
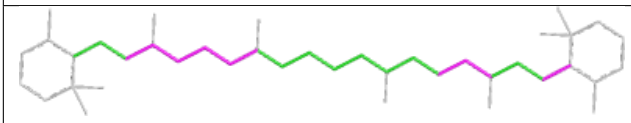


Bond angles



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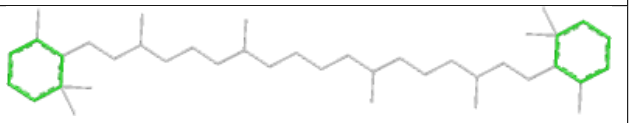
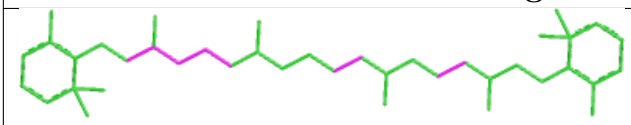


Rings

Ligand BCR S 104



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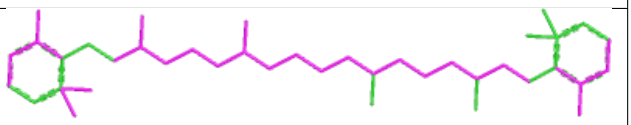

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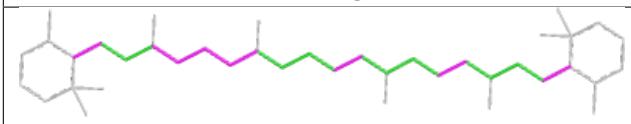

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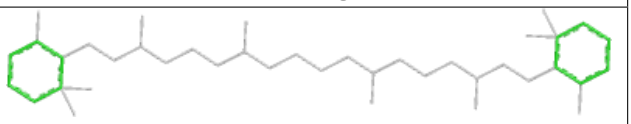
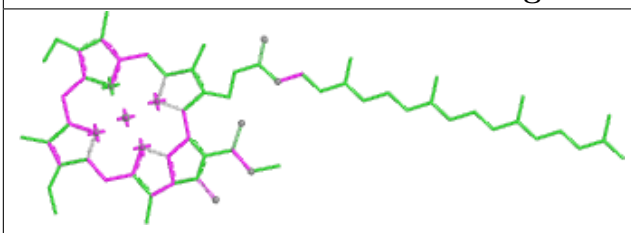


Rings

Ligand CLA A 829



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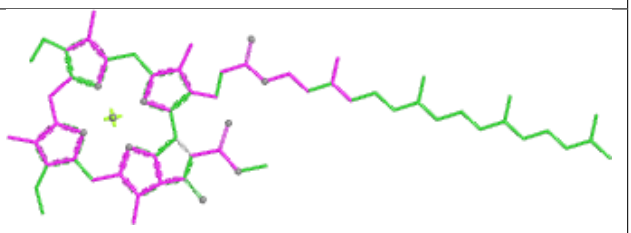
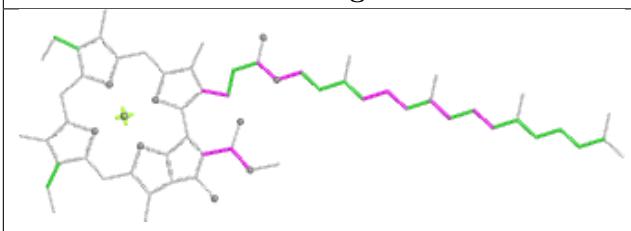


Bond angles



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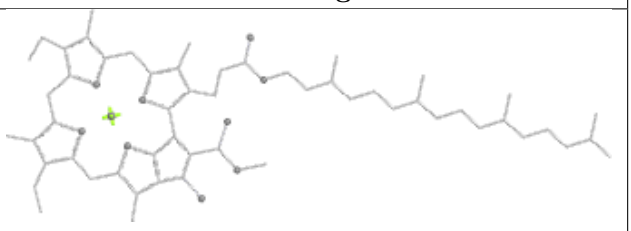
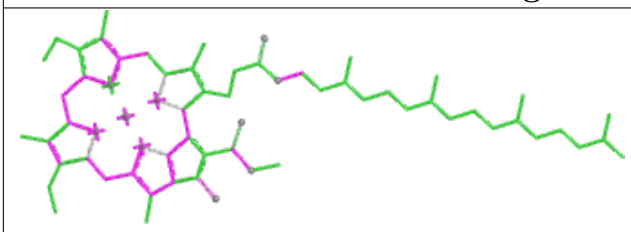


Rings

Ligand CLA G 832



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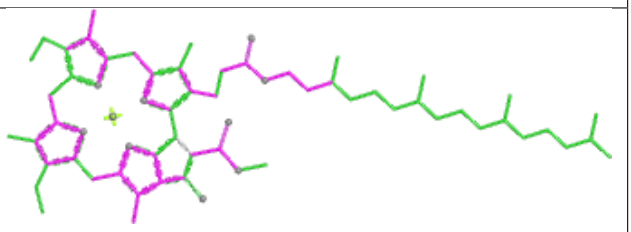

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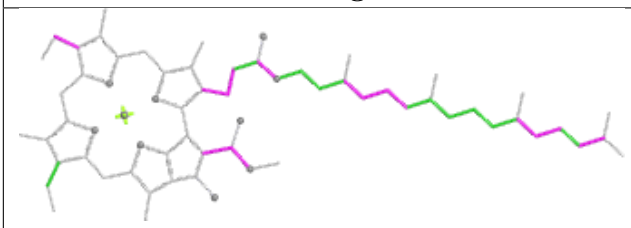

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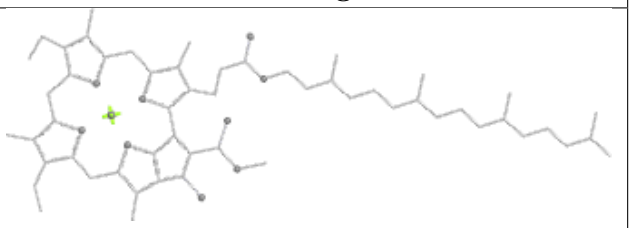
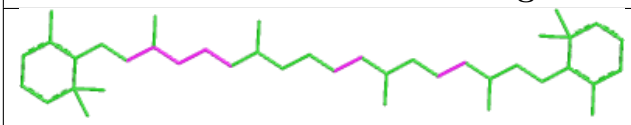


Rings

Ligand BCR J 1304



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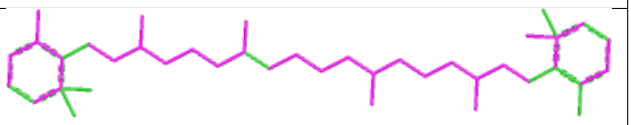

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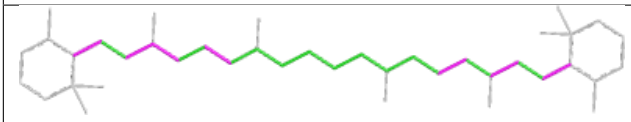

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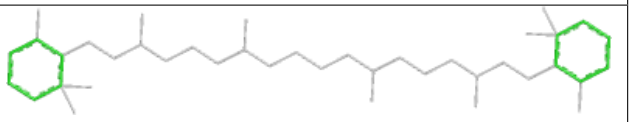
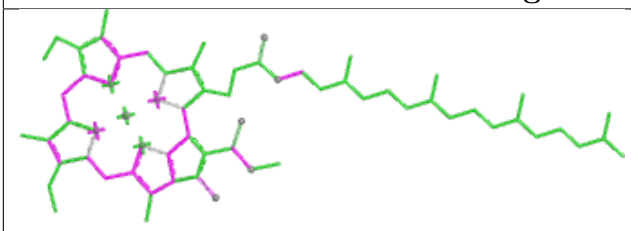


Rings

Ligand CLA H 816



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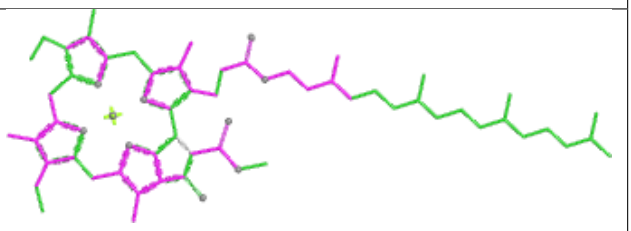

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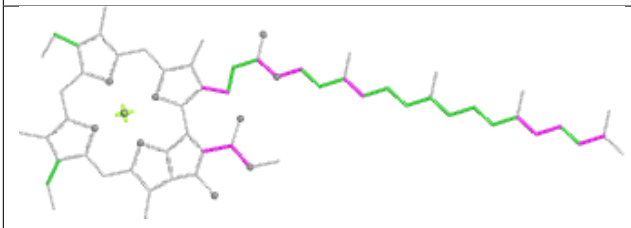

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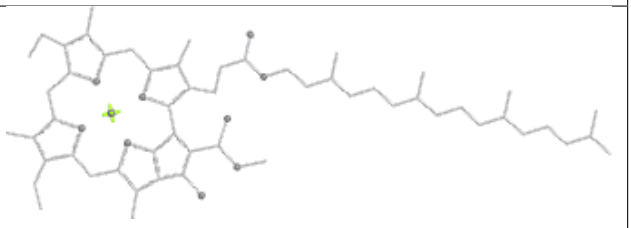
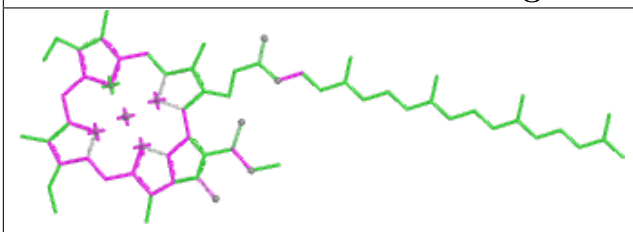


Rings

Ligand CLA H 841



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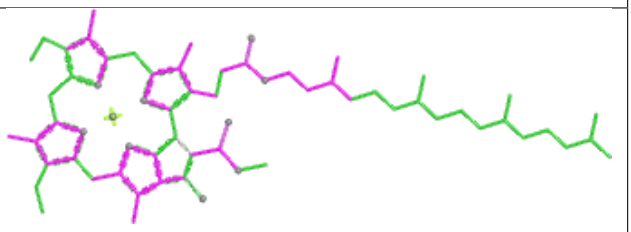
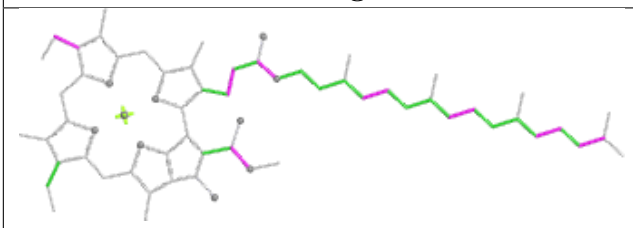


Bond angles



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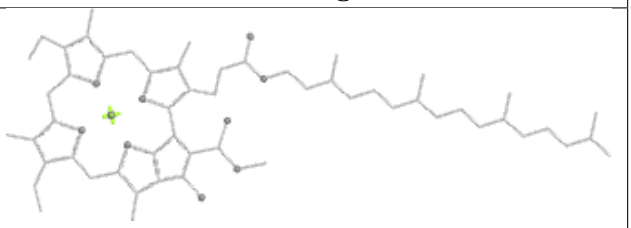
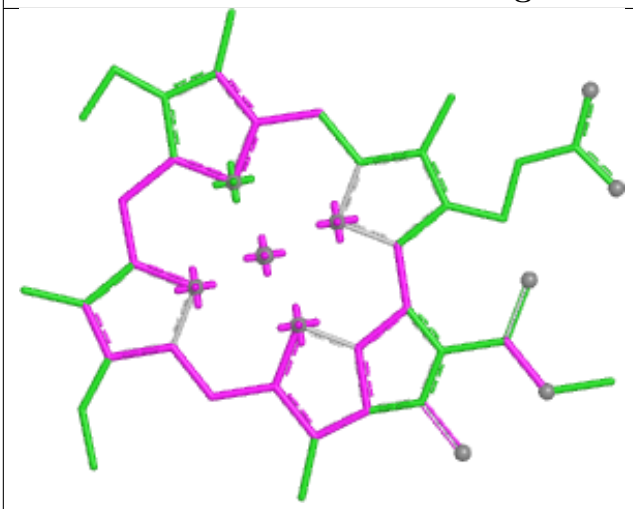


Rings

Ligand CLA K 1401



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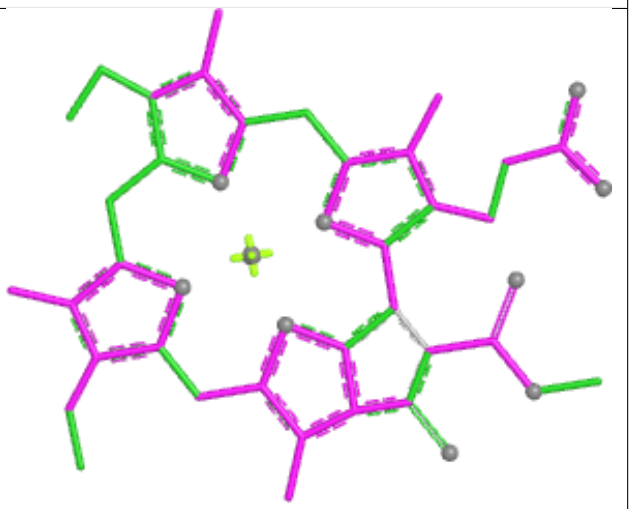
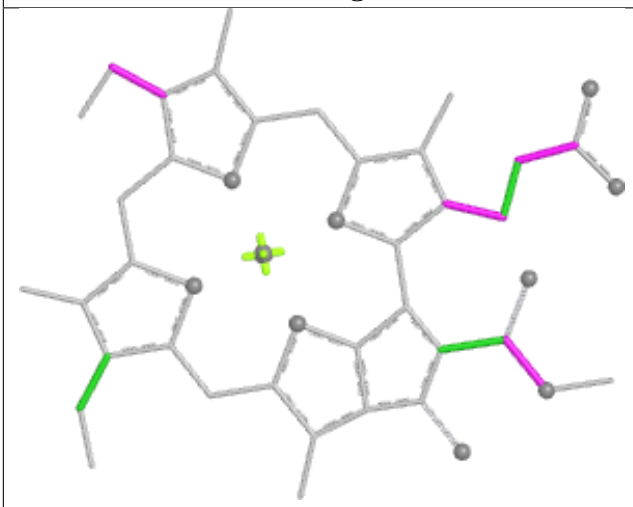


Bond angles



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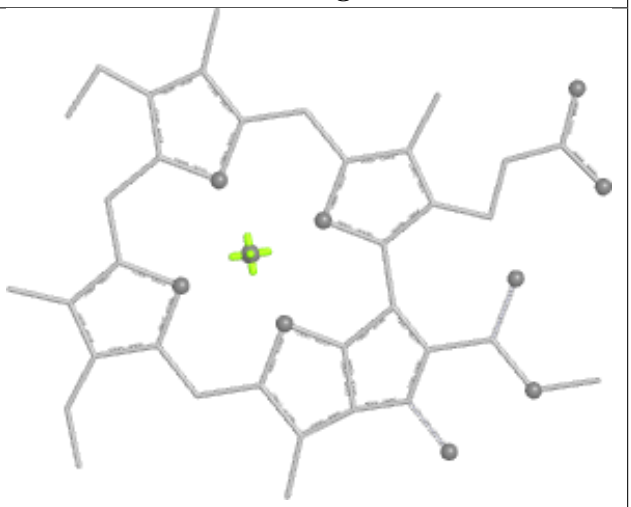
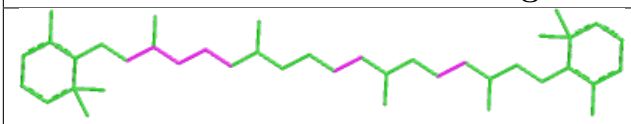


Rings

Ligand BCR G 843



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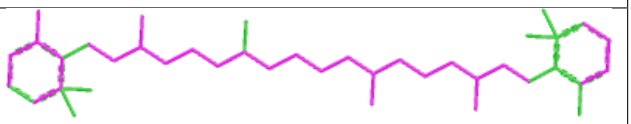
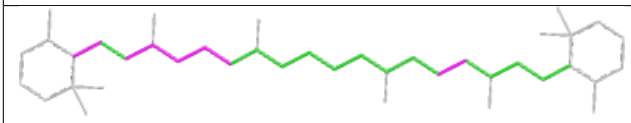


Bond angles



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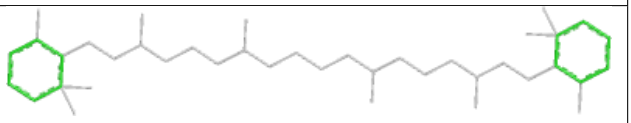
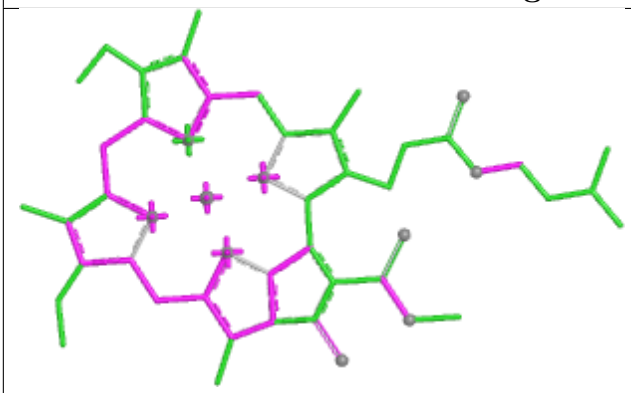


Rings

Ligand CLA A 811



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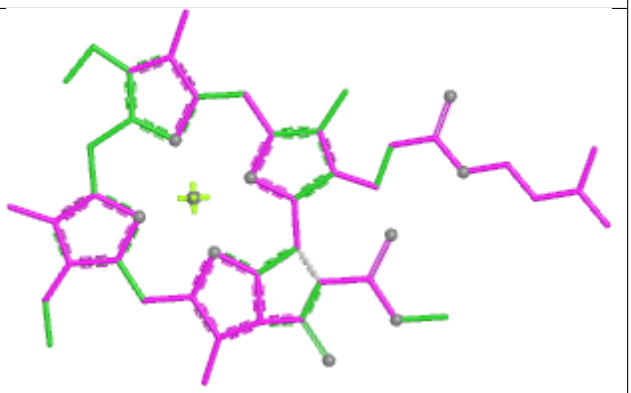
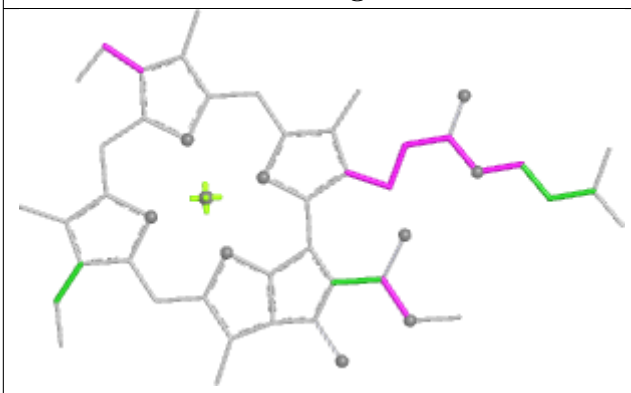
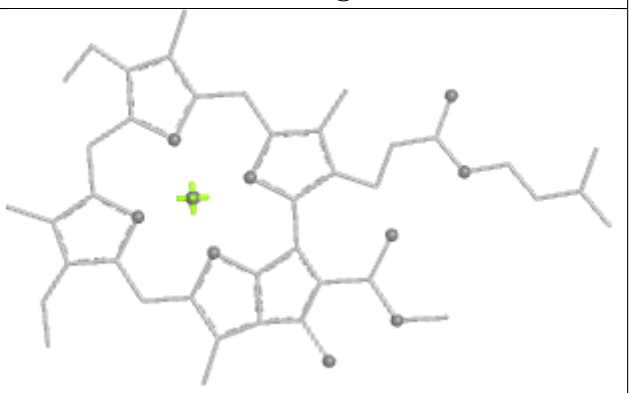


Bond angles

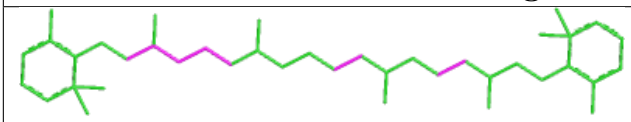


Torsions

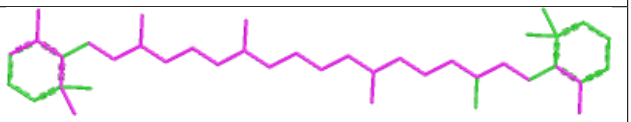


Rings

Ligand BCR B 846

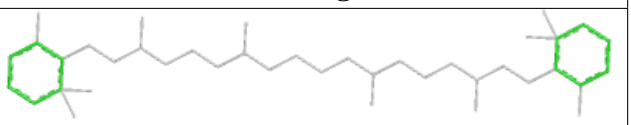


Bond lengths



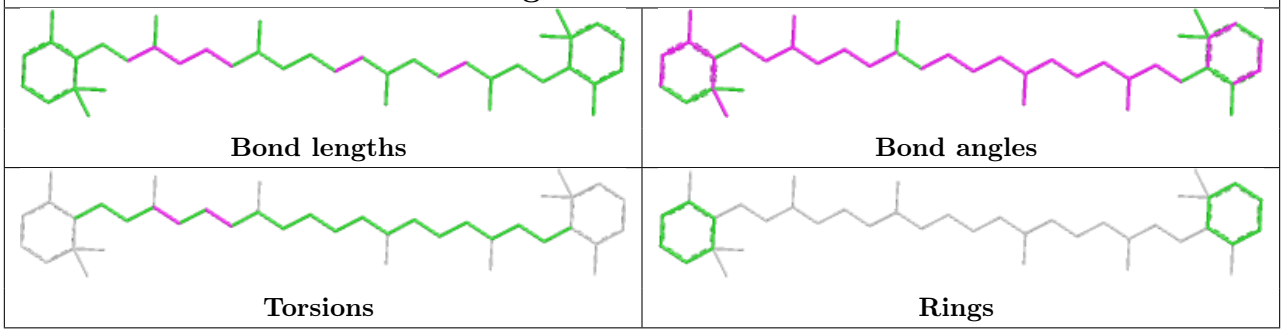
Bond angles

Torsions

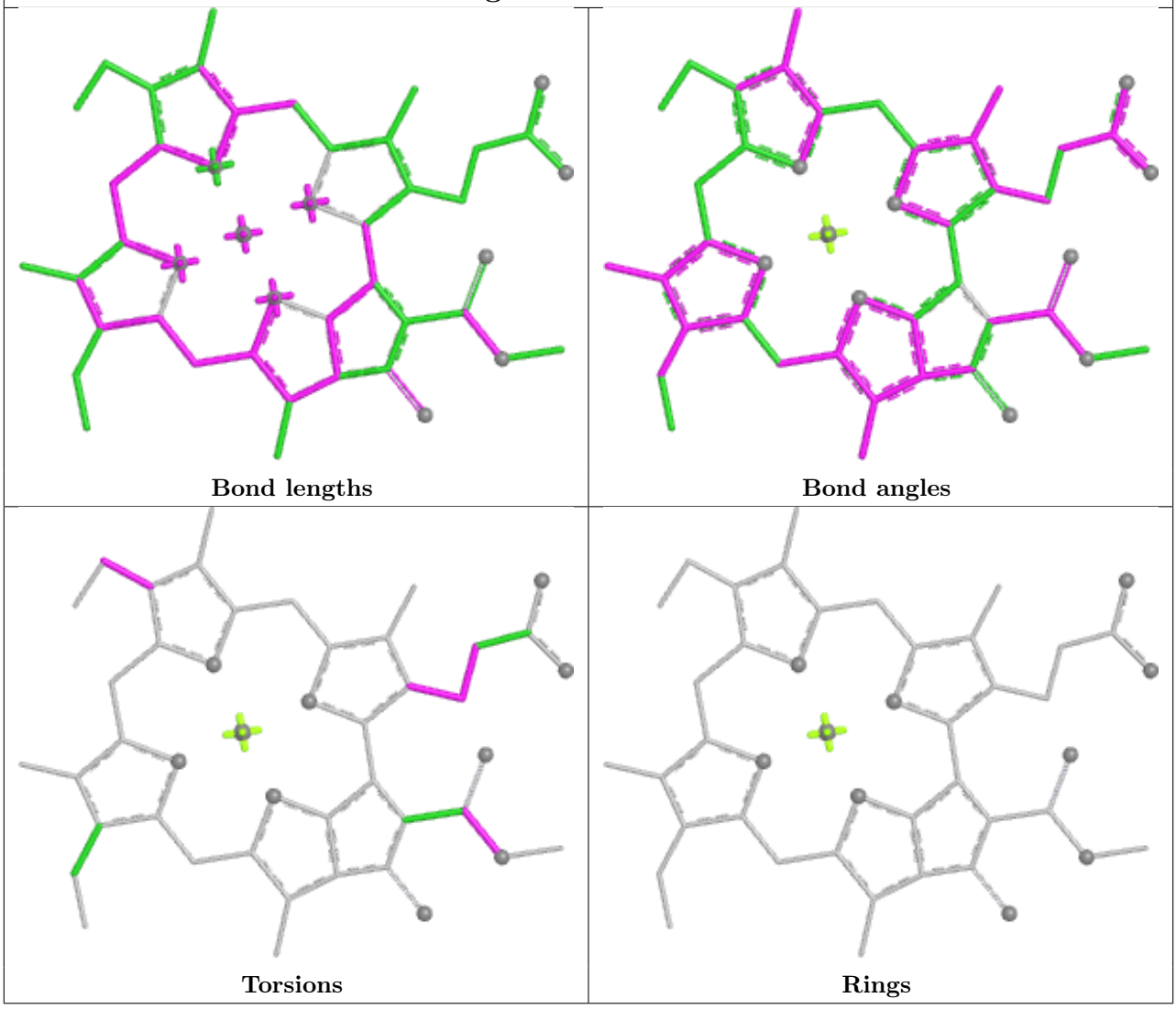


Rings

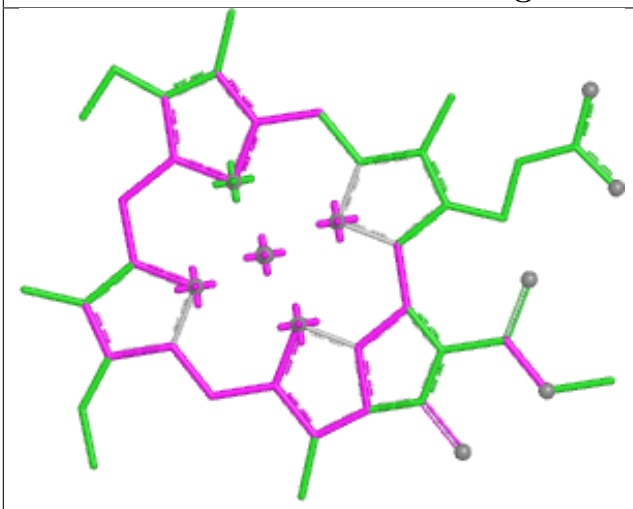
Ligand BCR U 203



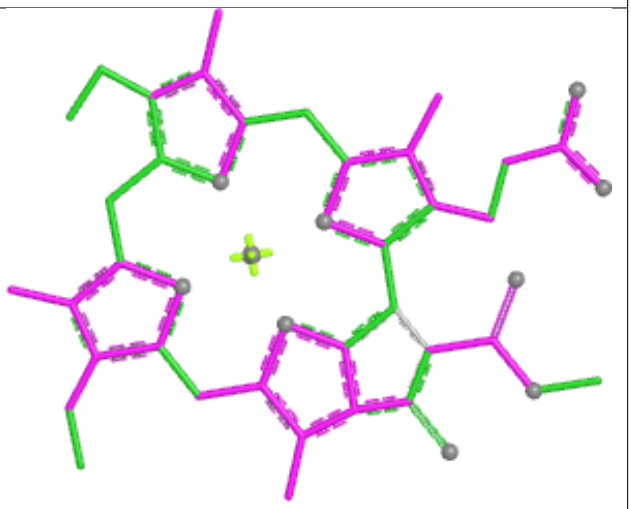
Ligand CLA a 815



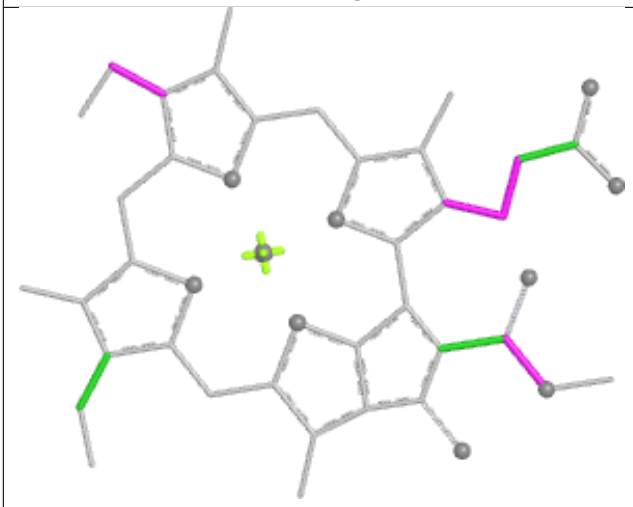
Ligand CLA X 1701



Bond lengths

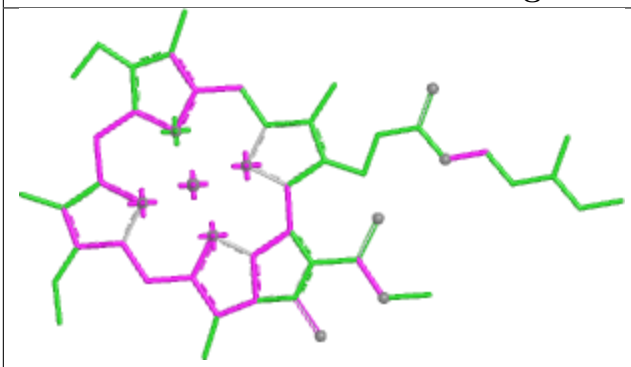
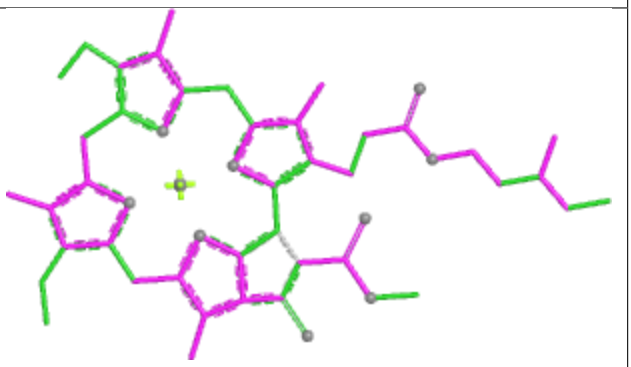
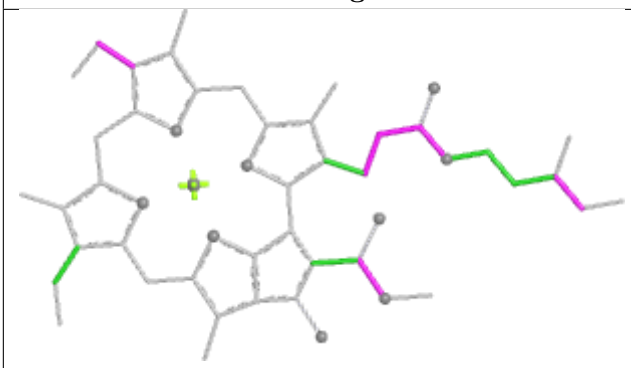
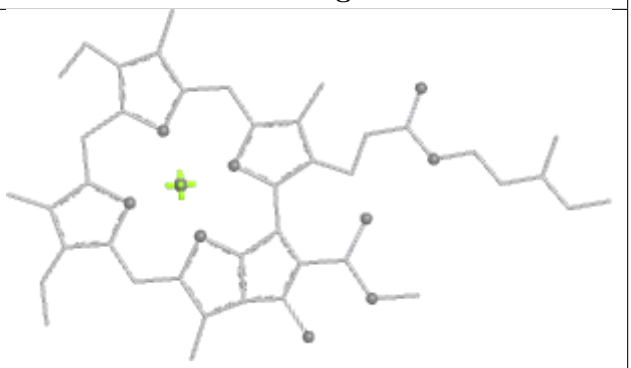


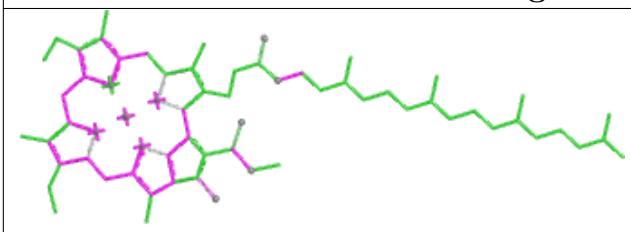
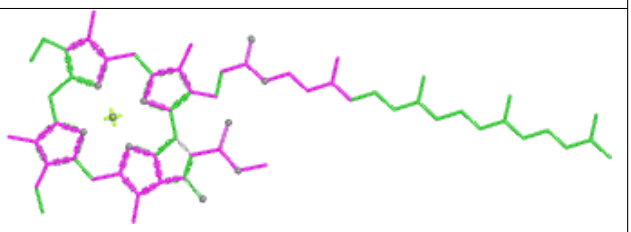
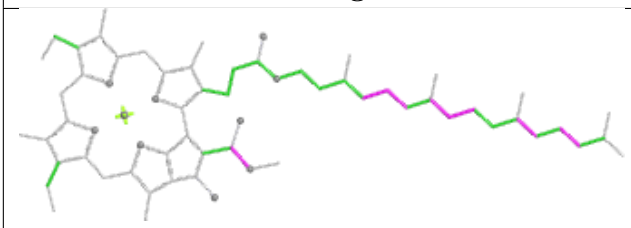
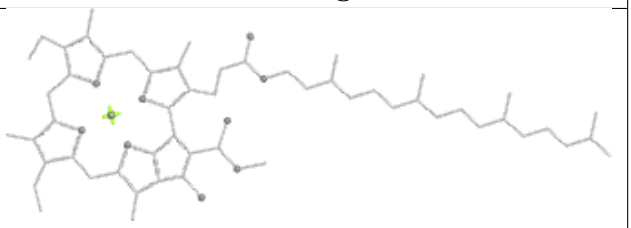
Bond angles



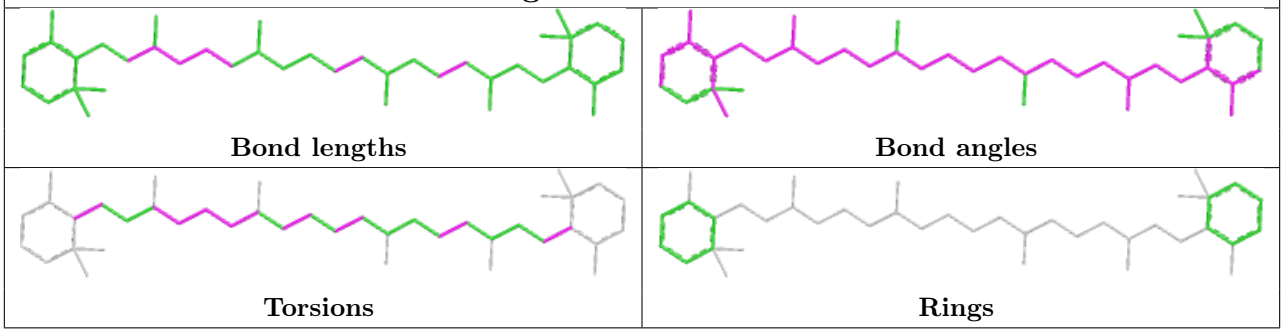
Torsions

Rings

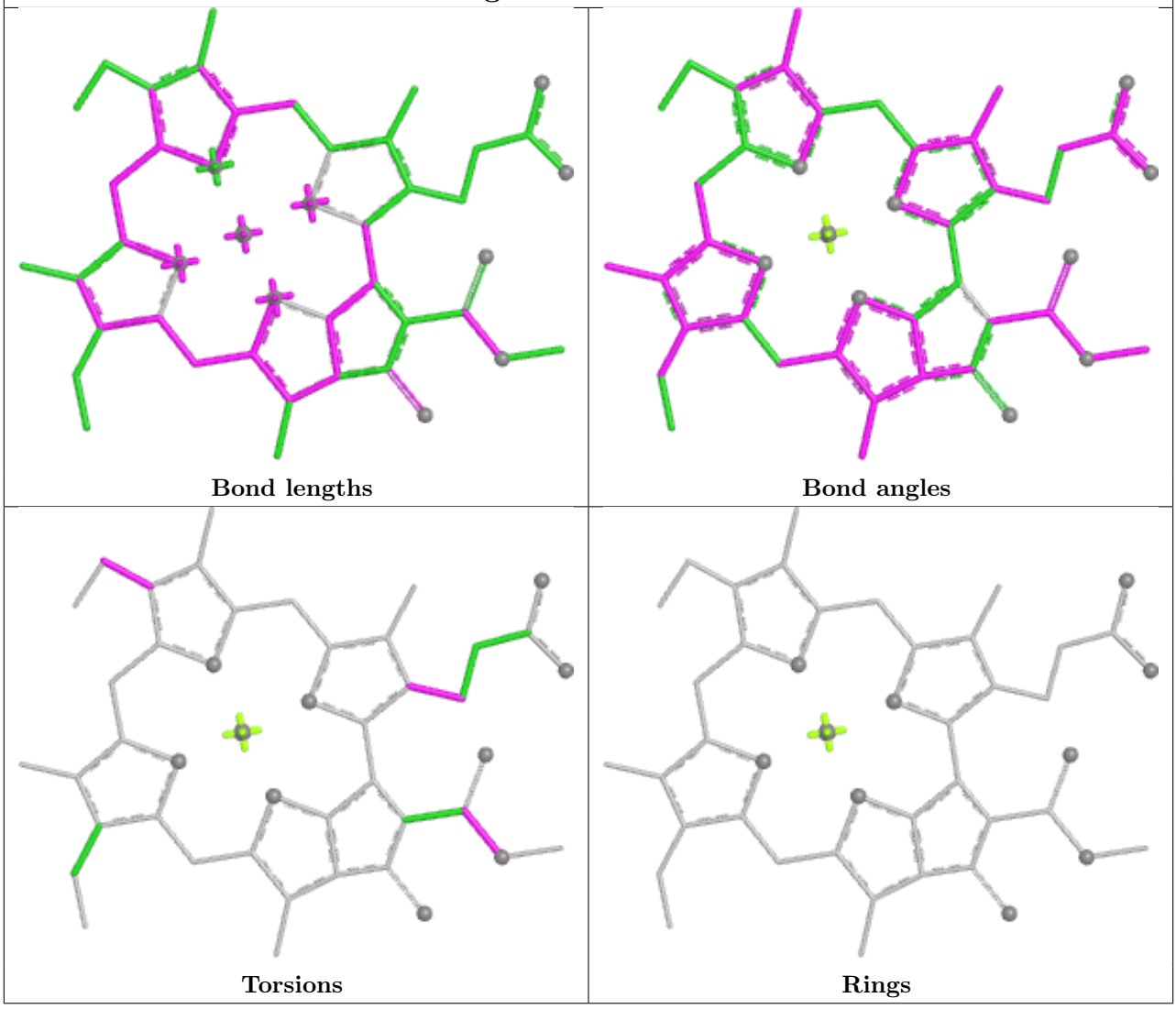
Ligand CLA A 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

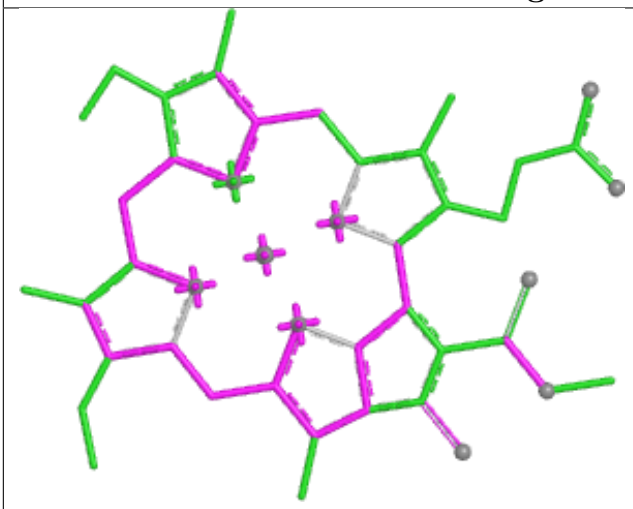
Ligand BCR H 847



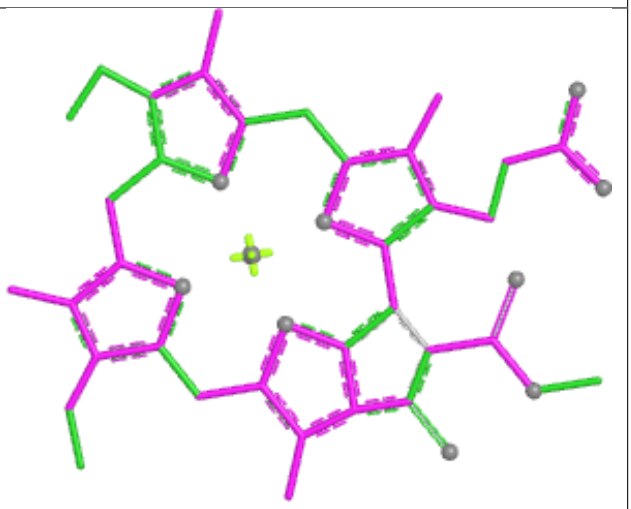
Ligand CLA b 810



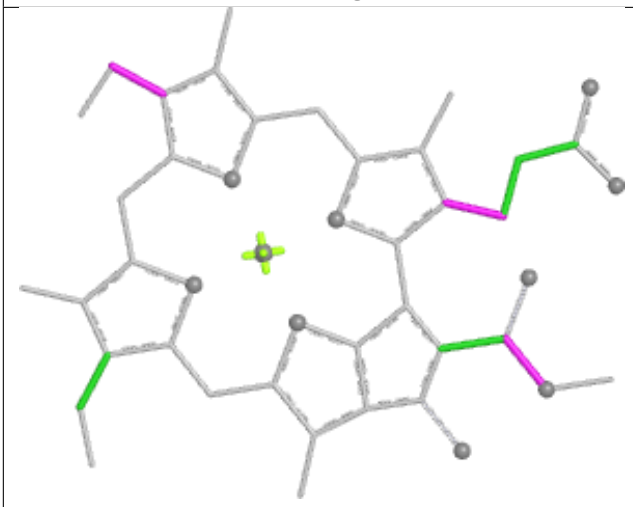
Ligand CLA b 834



Bond lengths



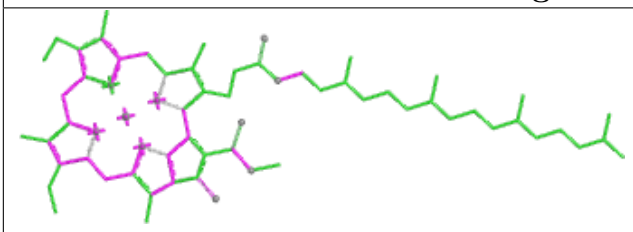
Bond angles



Torsions

Rings

Ligand CLA l 203



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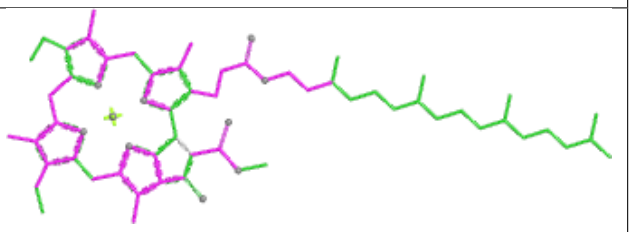
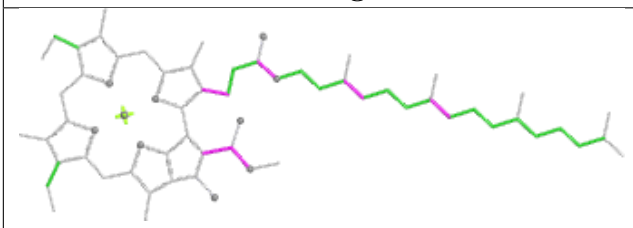
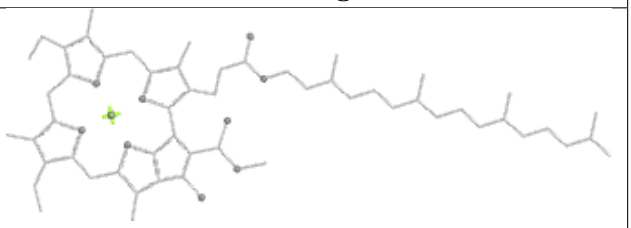


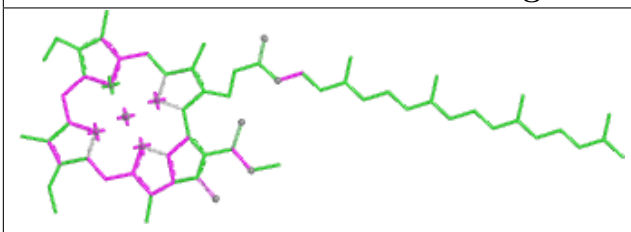
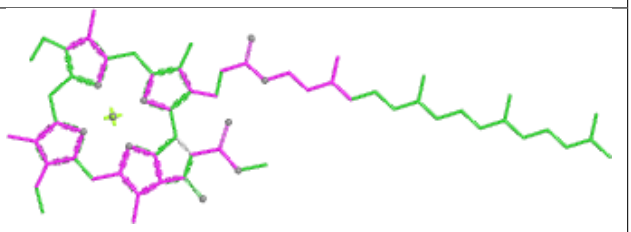
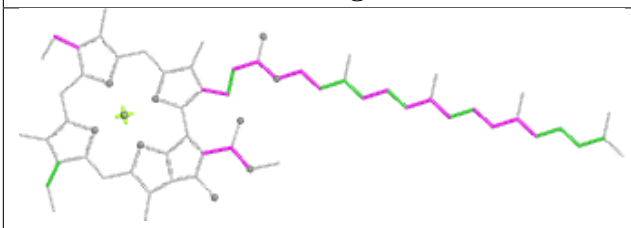
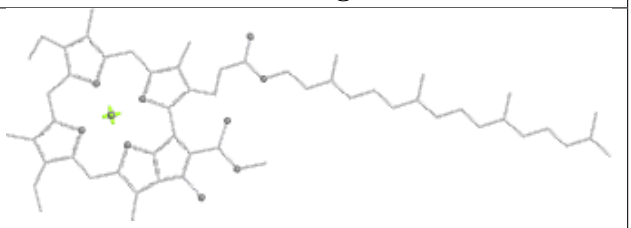
Bond angles

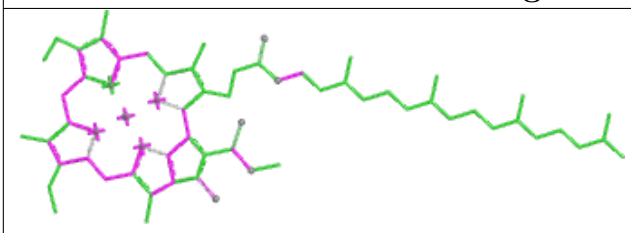
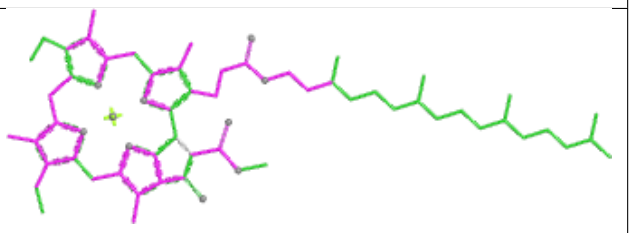
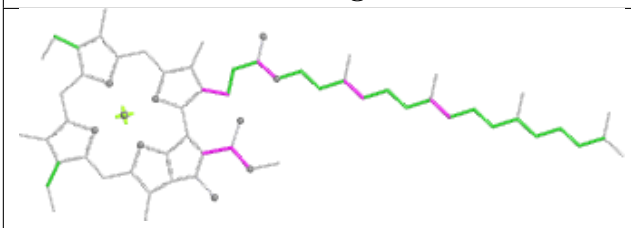
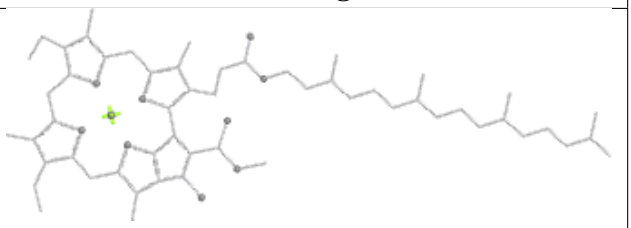


Torsions

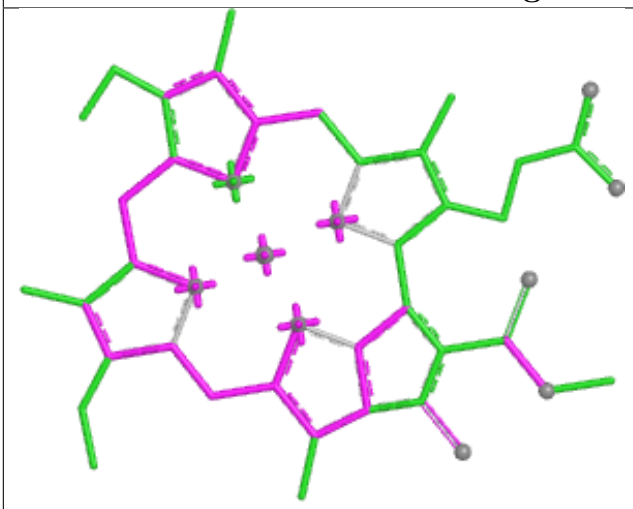


Rings

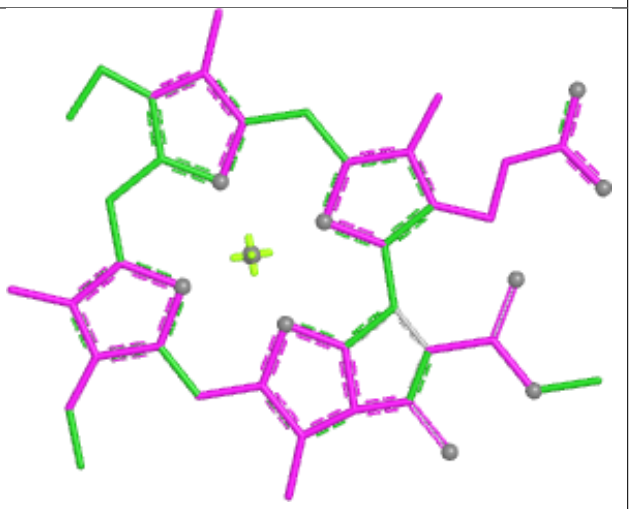
Ligand CLA G 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

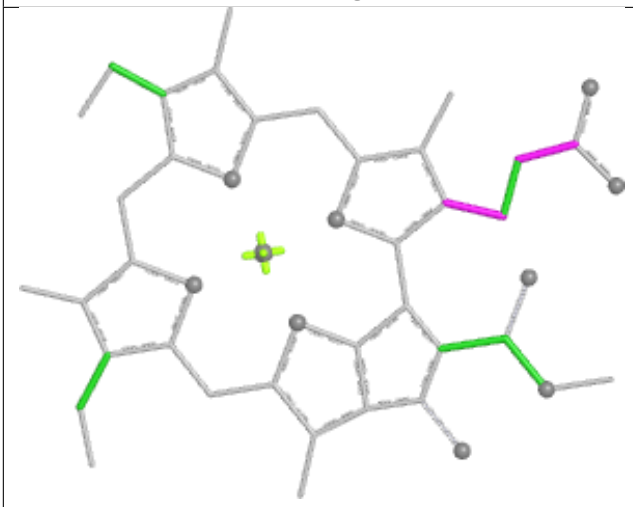
Ligand CLA H 825



Bond lengths



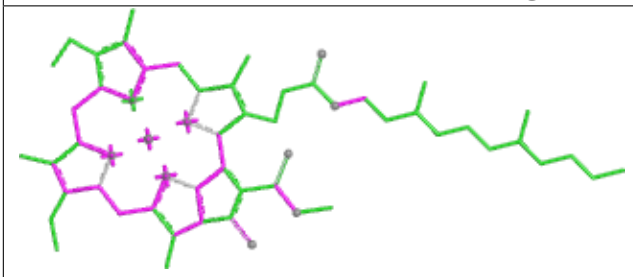
Bond angles



Torsions

Rings

Ligand CLA H 834



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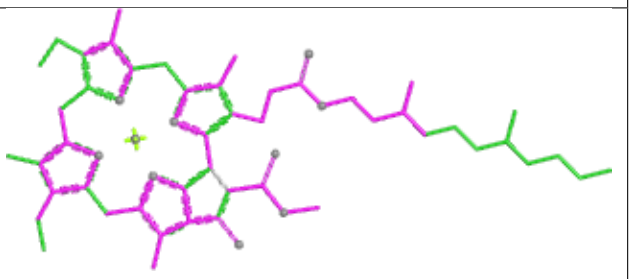
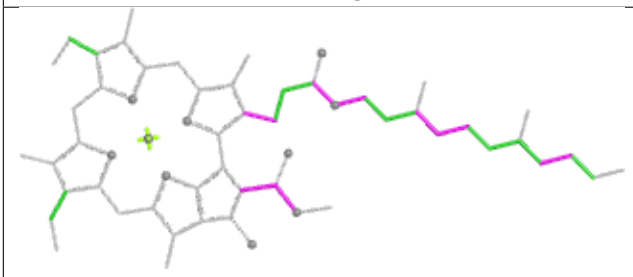
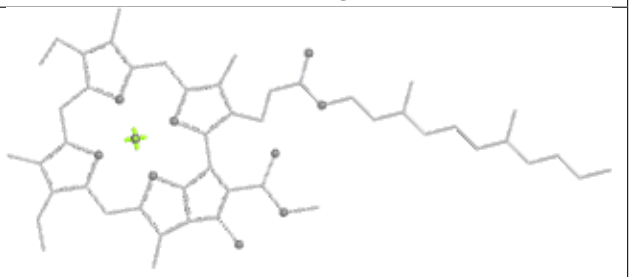


Bond angles

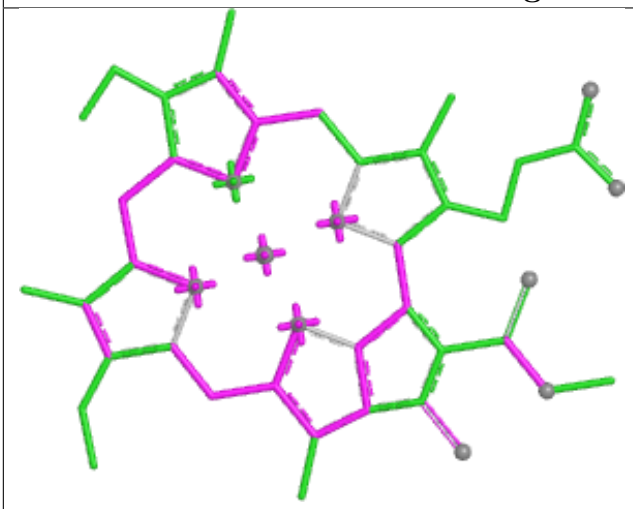


Torsions



Rings

Ligand CLA A 809



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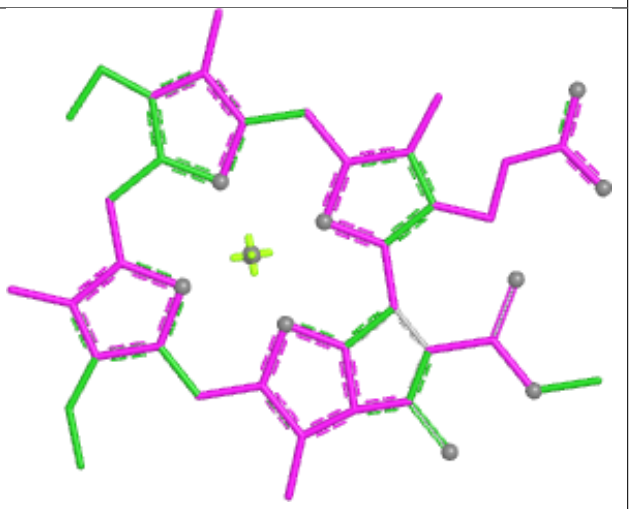
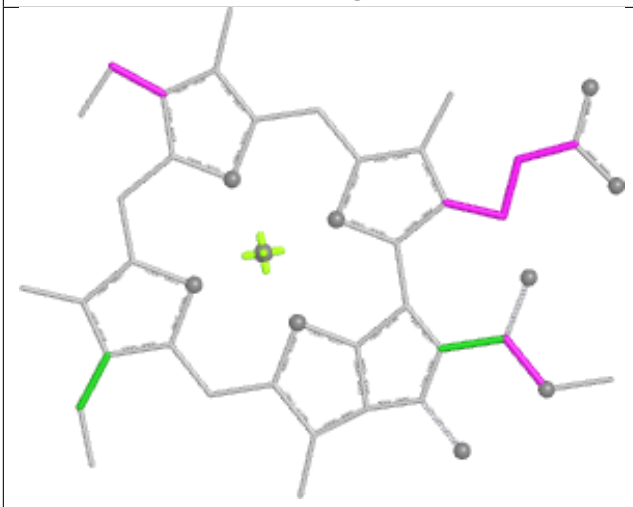


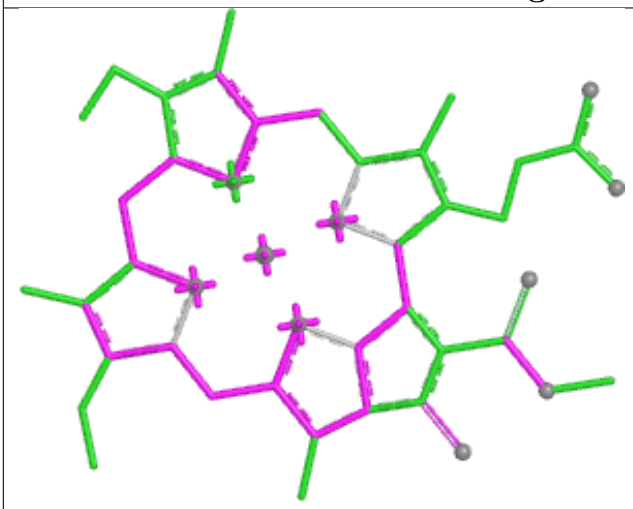
Bond angles



Torsions

Rings

Ligand CLA a 821



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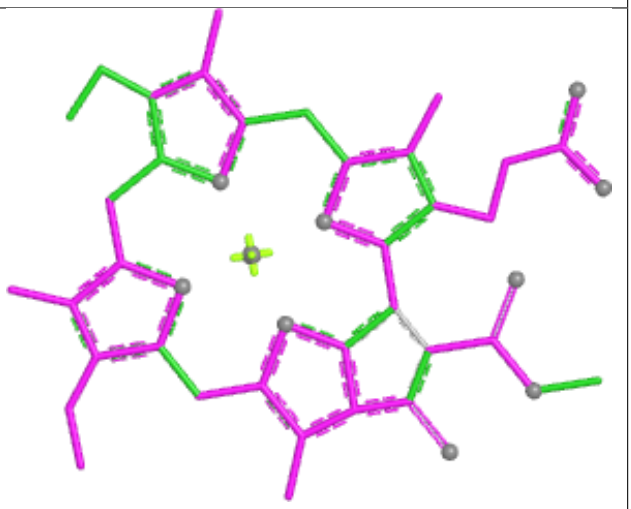
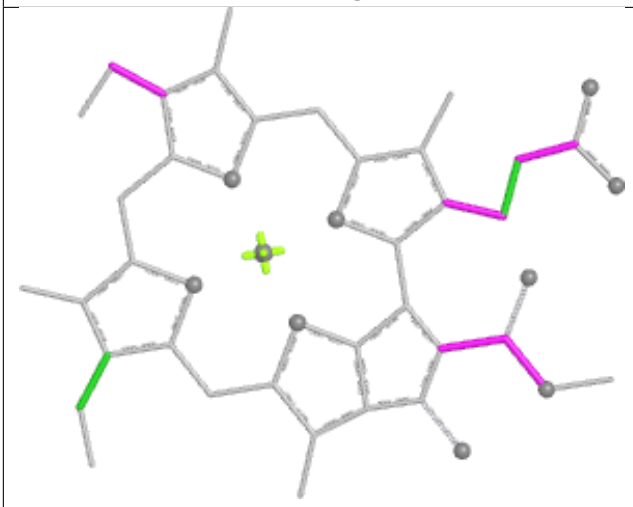


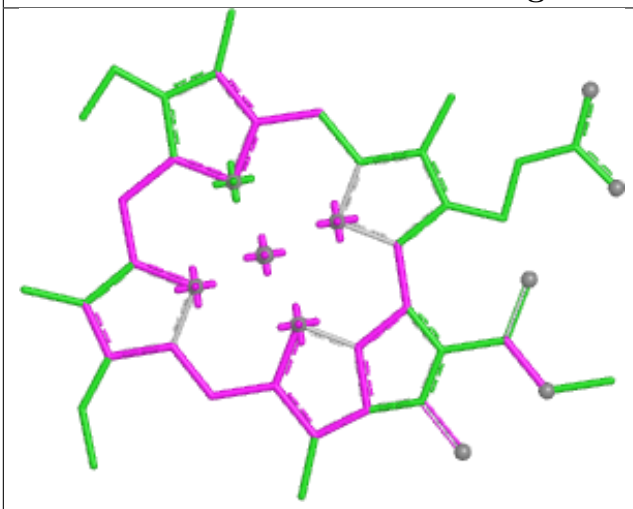
Bond angles



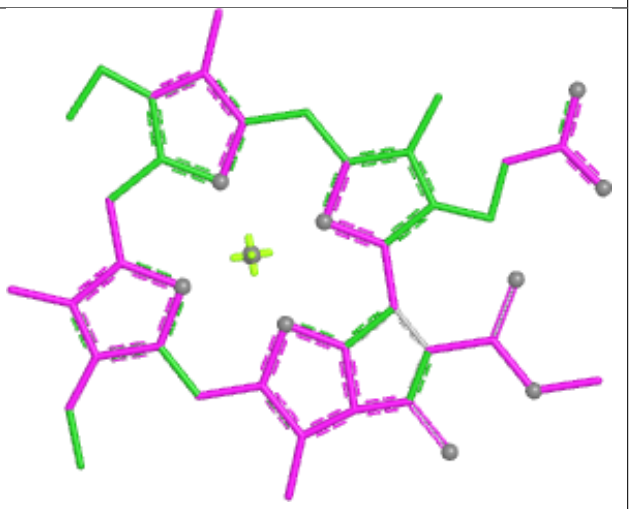
Torsions

Rings

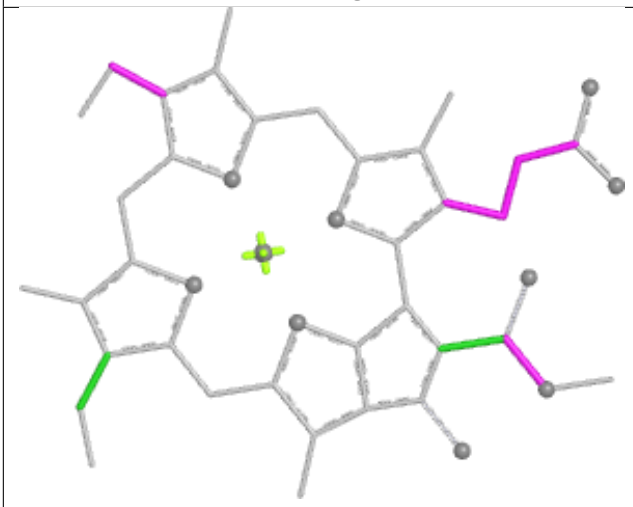
Ligand CLA b 830



Bond lengths



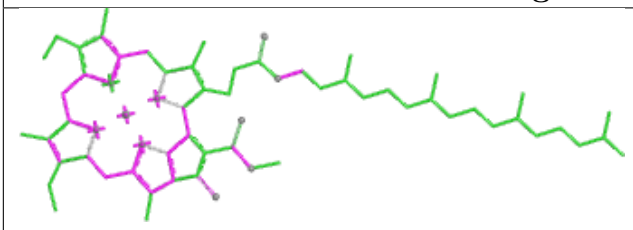
Bond angles



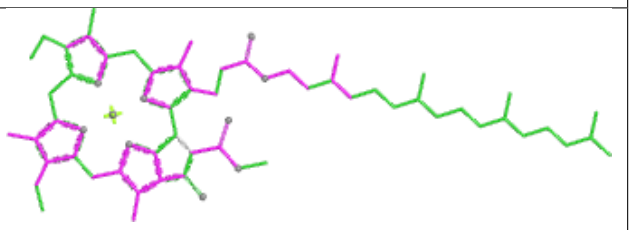
Torsions

Rings

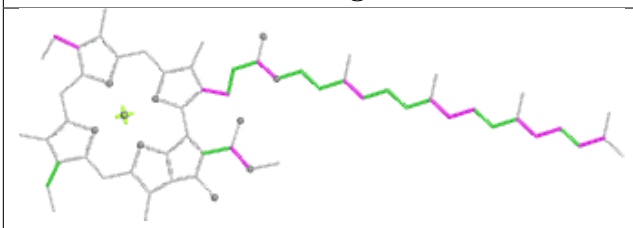
Ligand CLA l 204



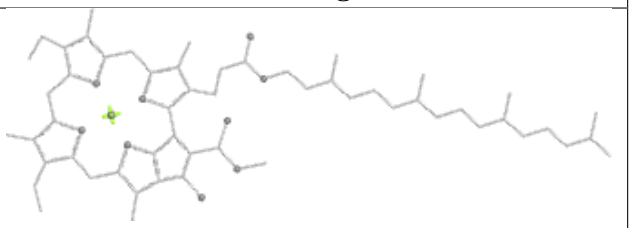
Bond lengths



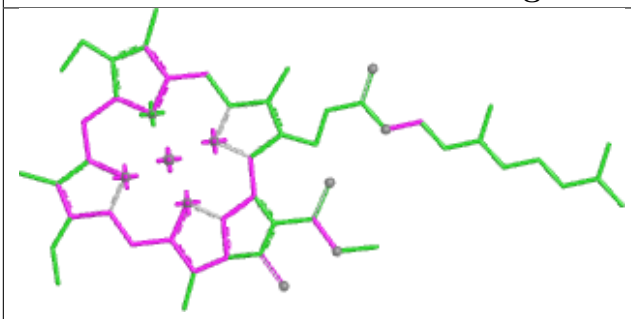
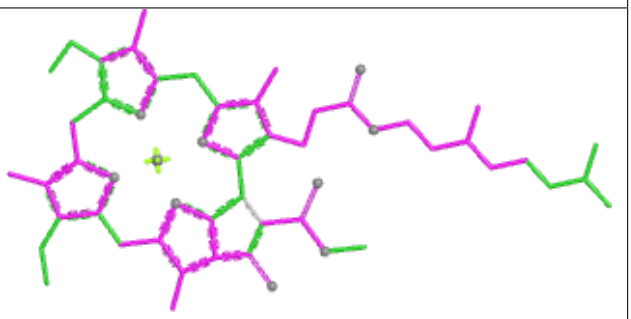
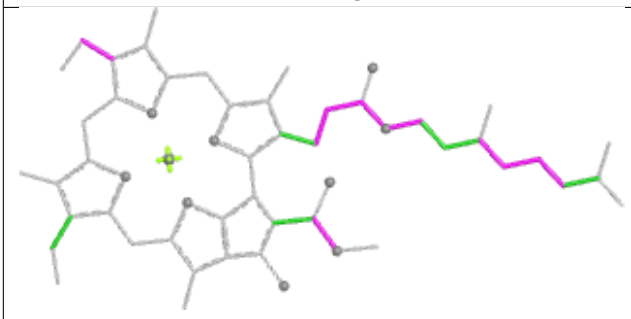
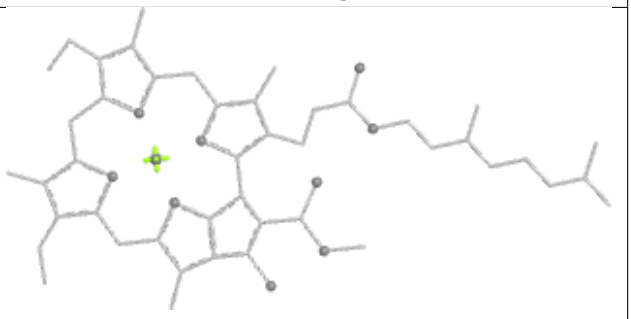
Bond angles

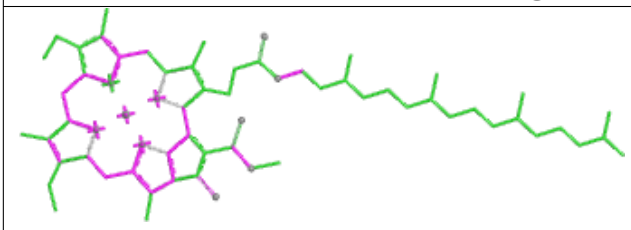
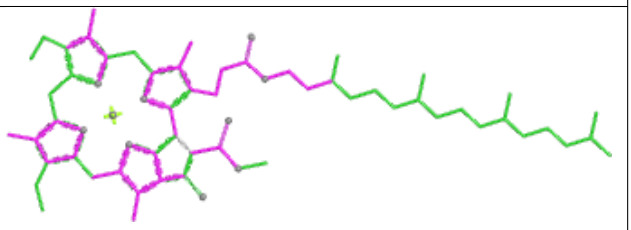
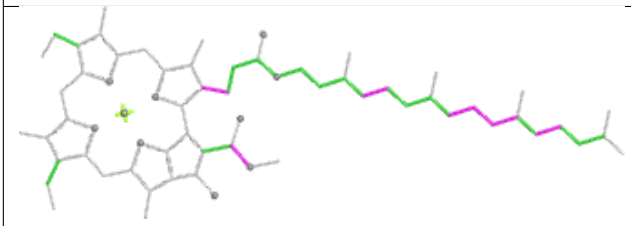
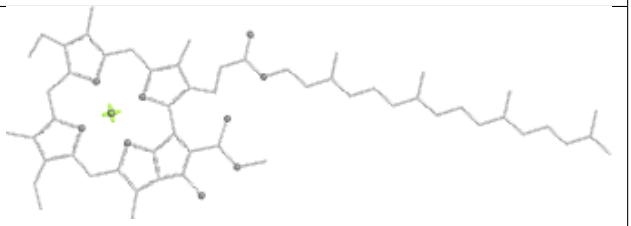


Torsions



Rings

Ligand CLA H 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

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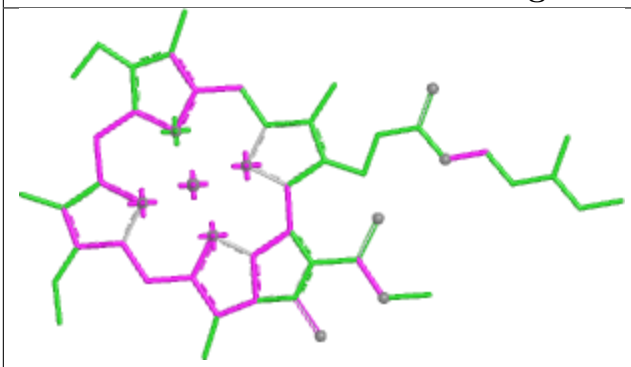

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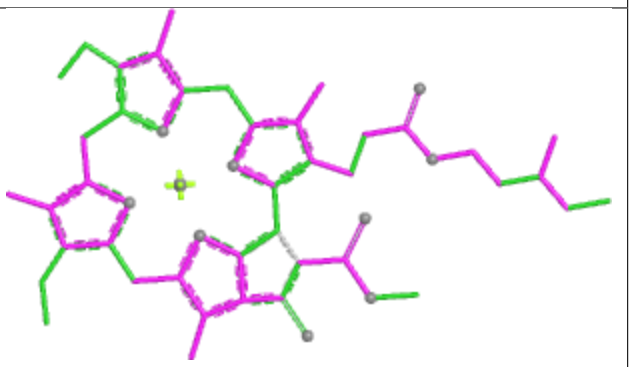

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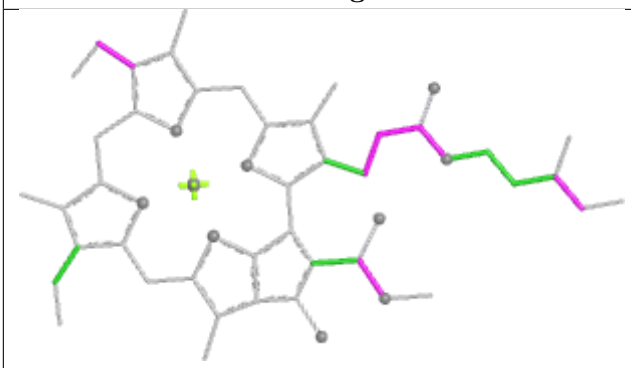

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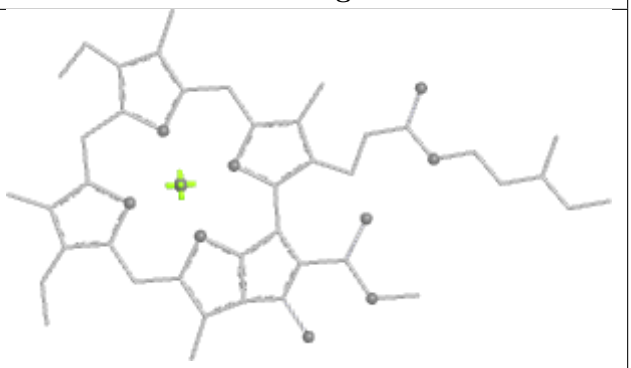
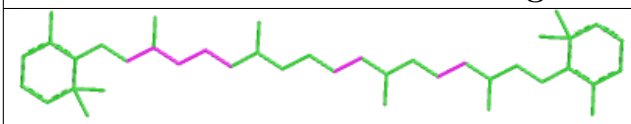


Rings

Ligand BCR a 847



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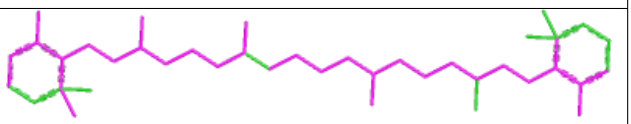

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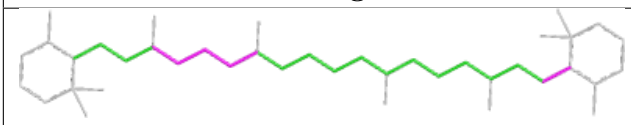

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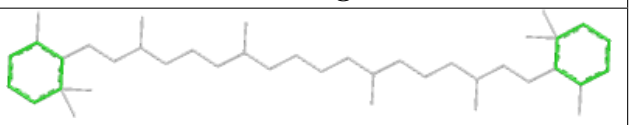
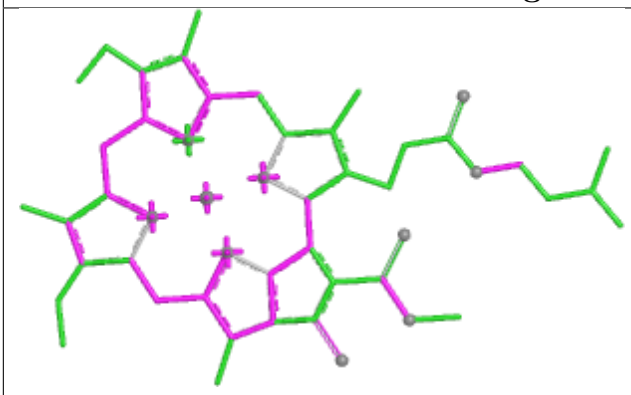
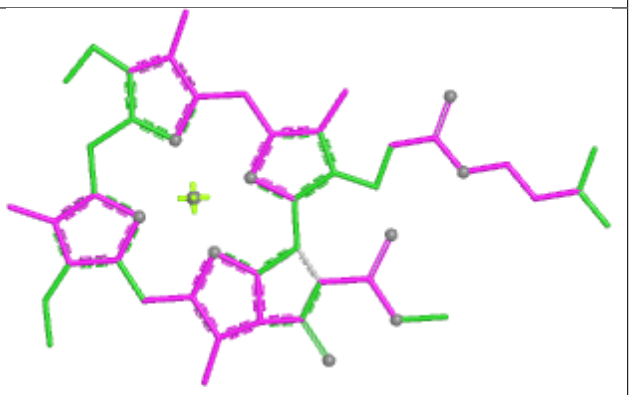
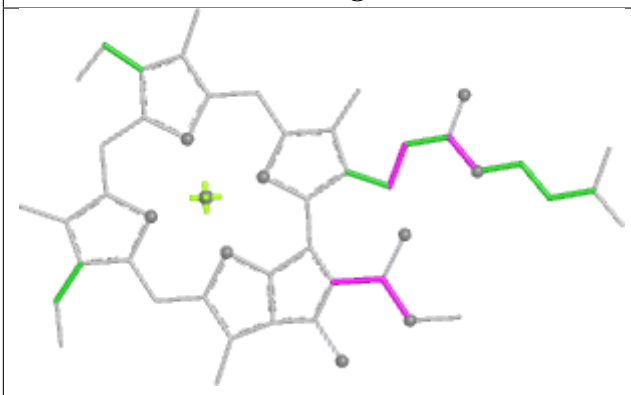
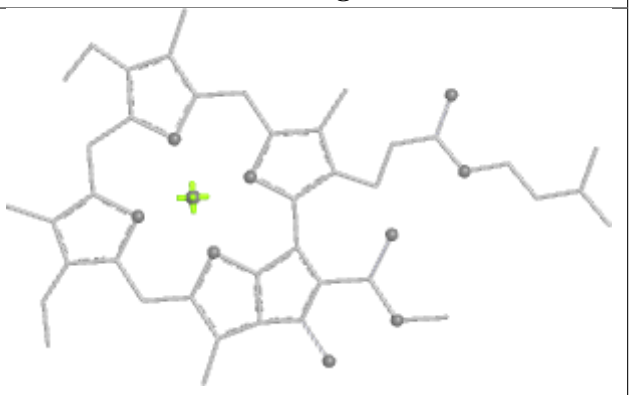
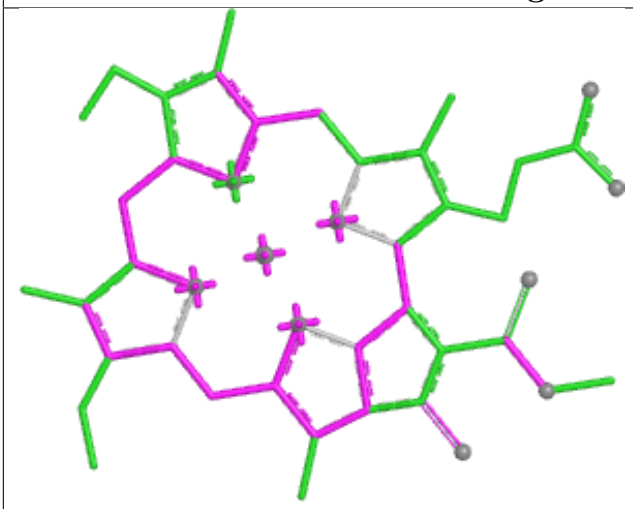


Rings

Ligand CLA H 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 835



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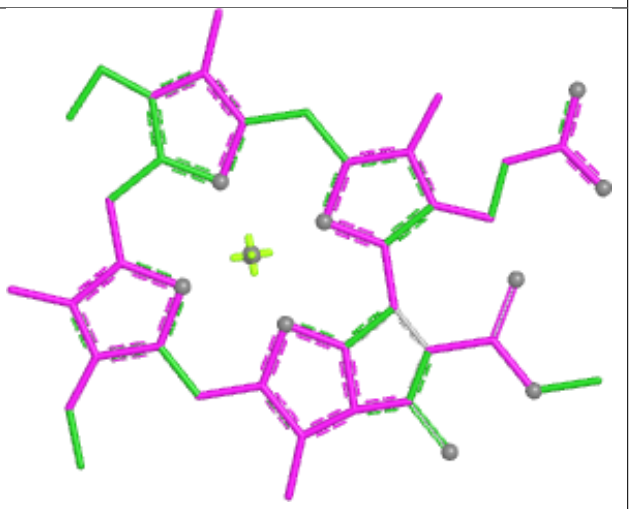
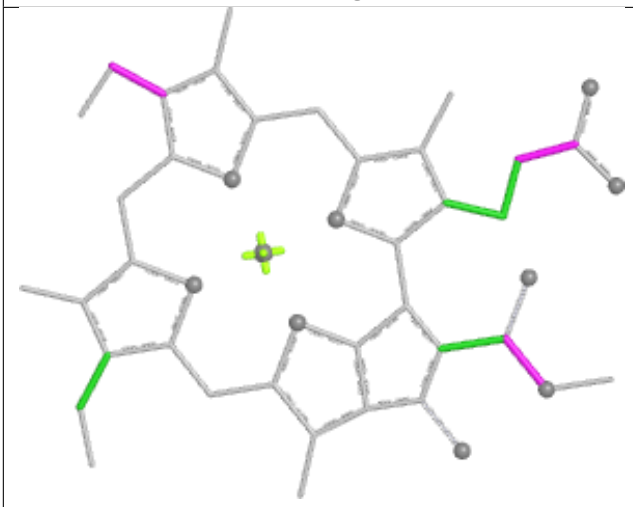


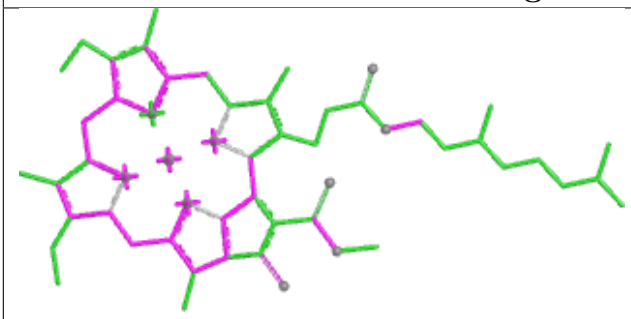
Bond angles



Torsions

Rings

Ligand CLA B 824



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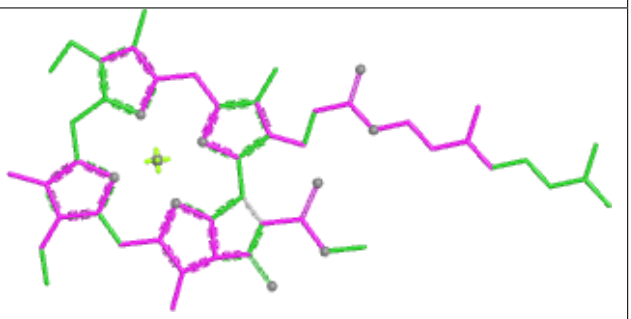
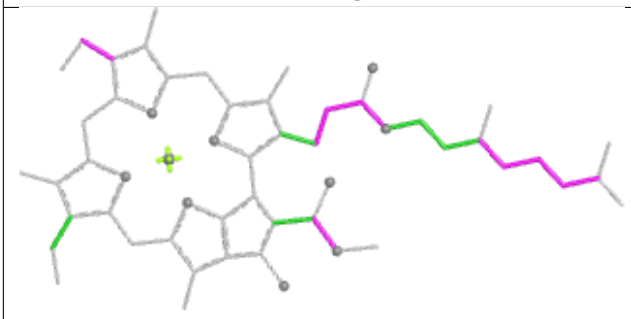


Bond angles



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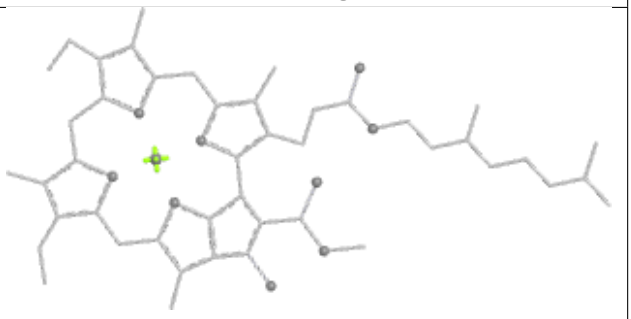
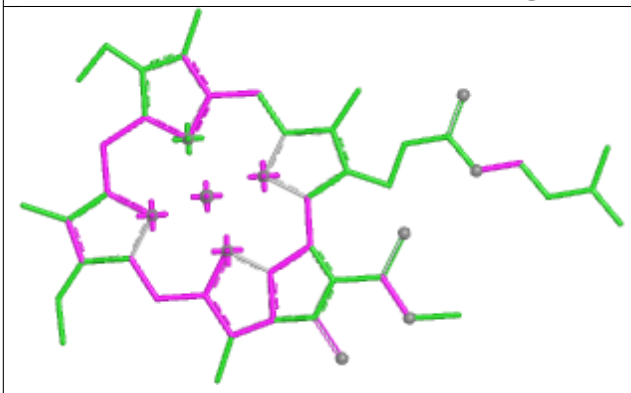


Rings

Ligand CLA G 835



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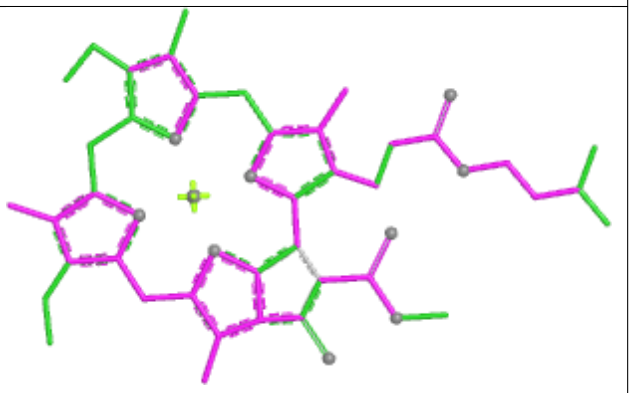
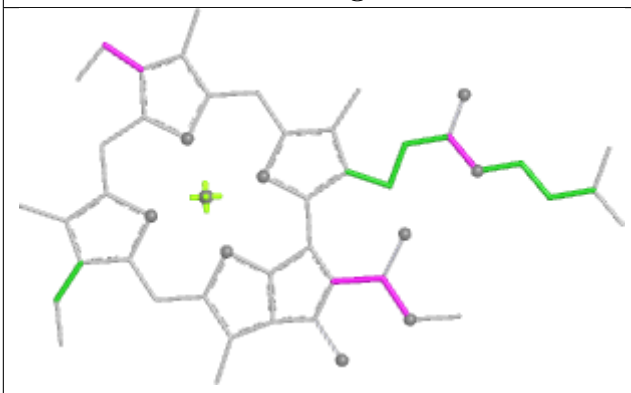


Bond angles



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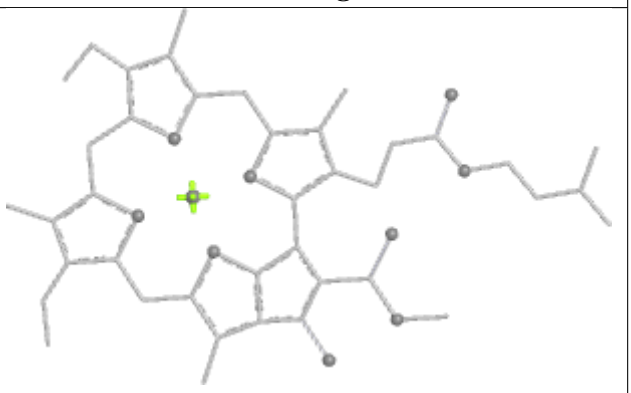
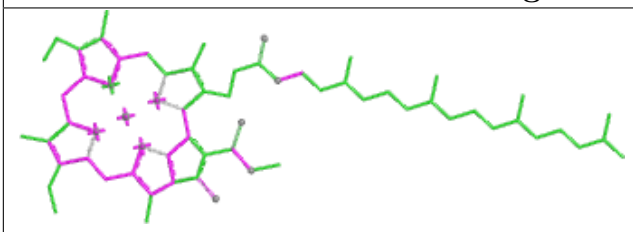


Rings

Ligand CLA G 839



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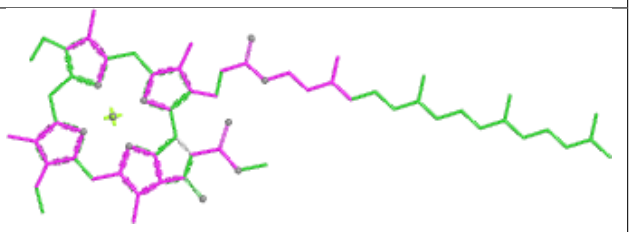
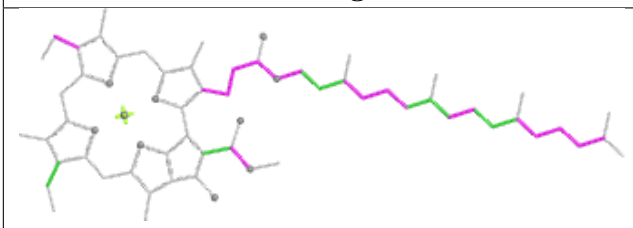


Bond angles



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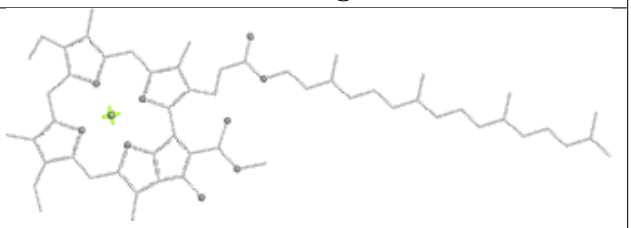
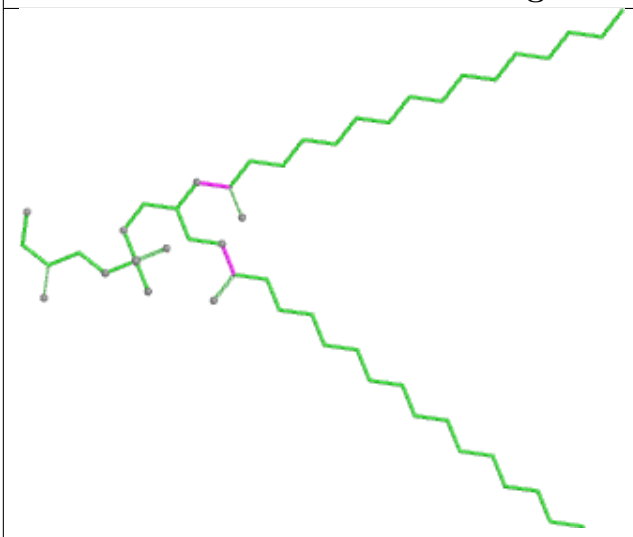


Rings

Ligand LHG a 850



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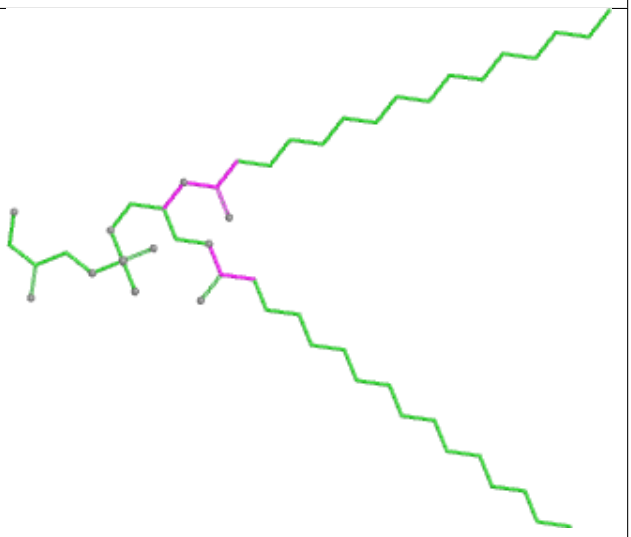
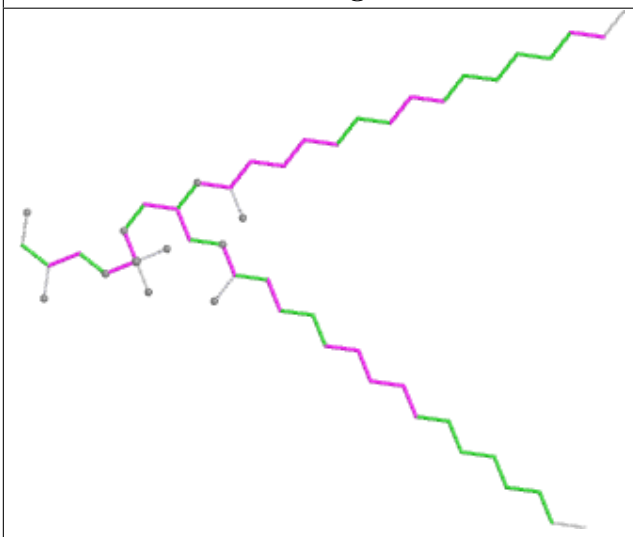


Bond angles



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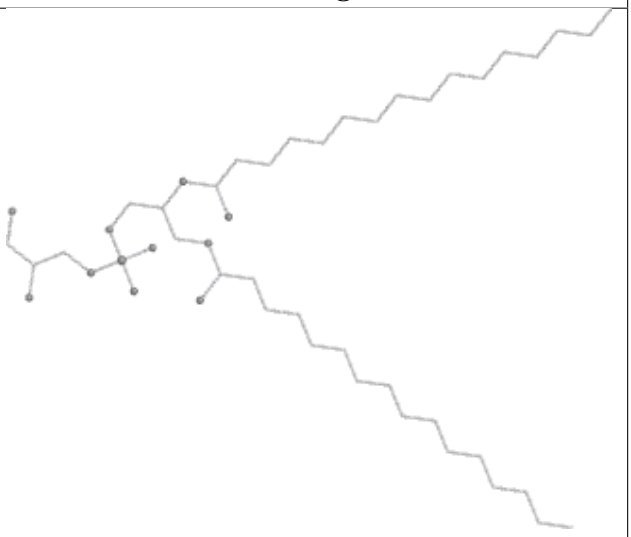
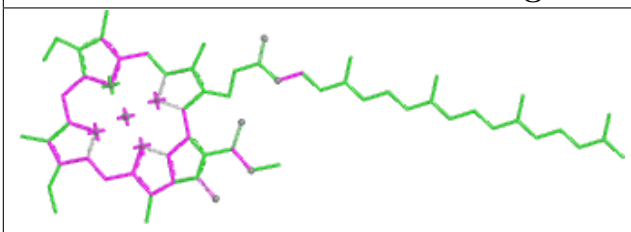


Rings

Ligand CLA B 828



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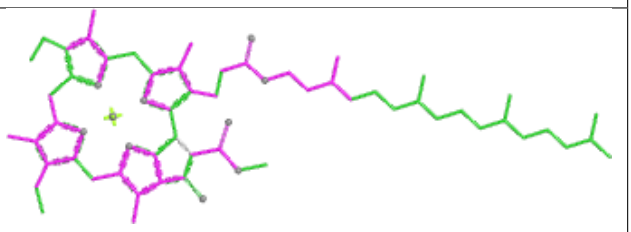
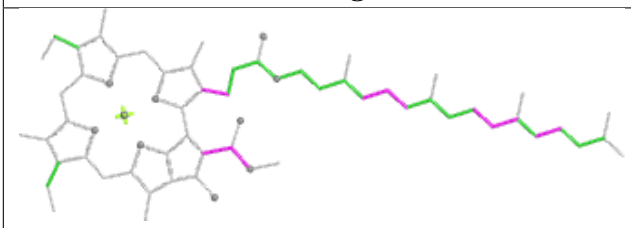


Bond angles



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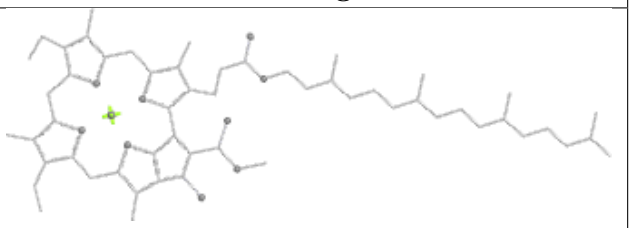
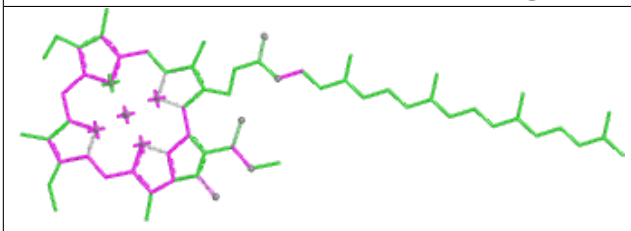


Rings

Ligand CLA H 821



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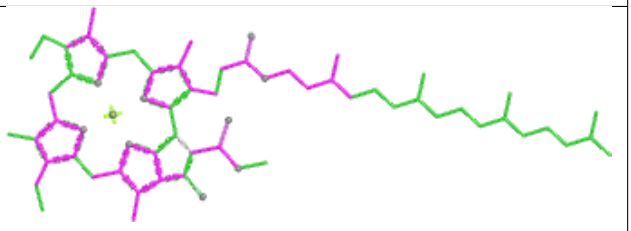
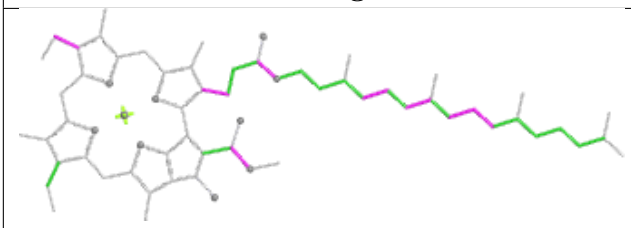


Bond angles



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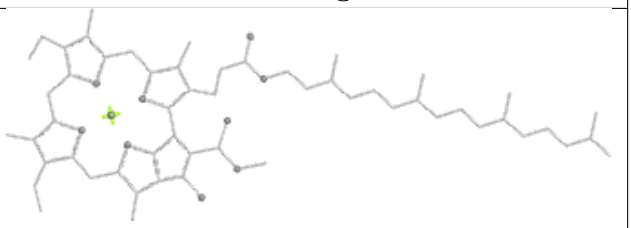
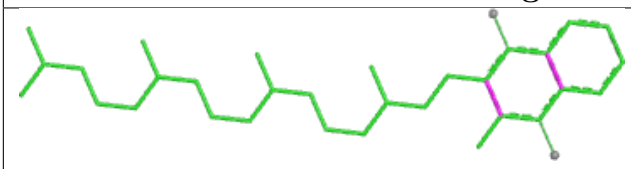


Rings

Ligand PQN B 843



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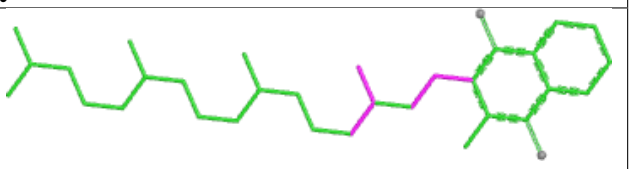
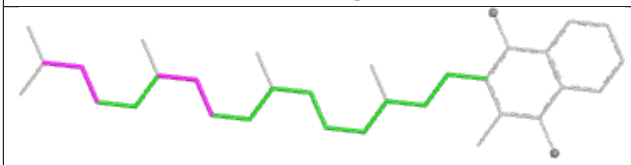


Bond angles



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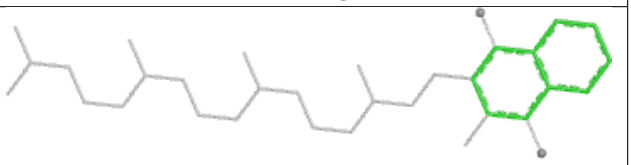
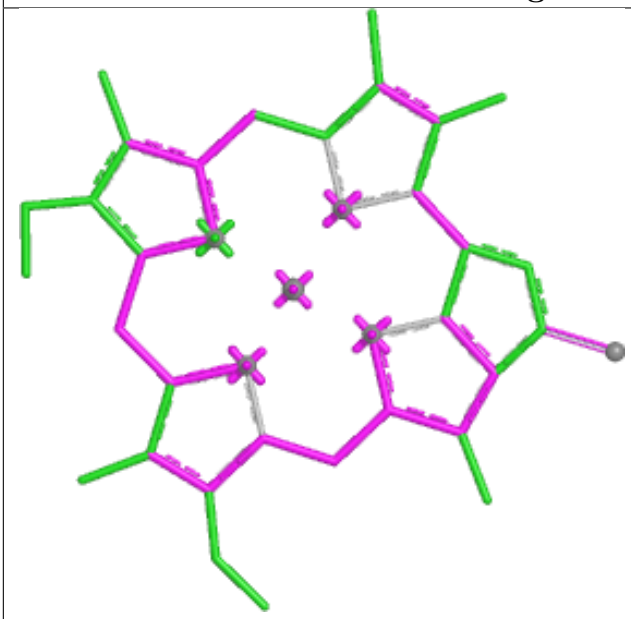


Rings

Ligand CLA S 102



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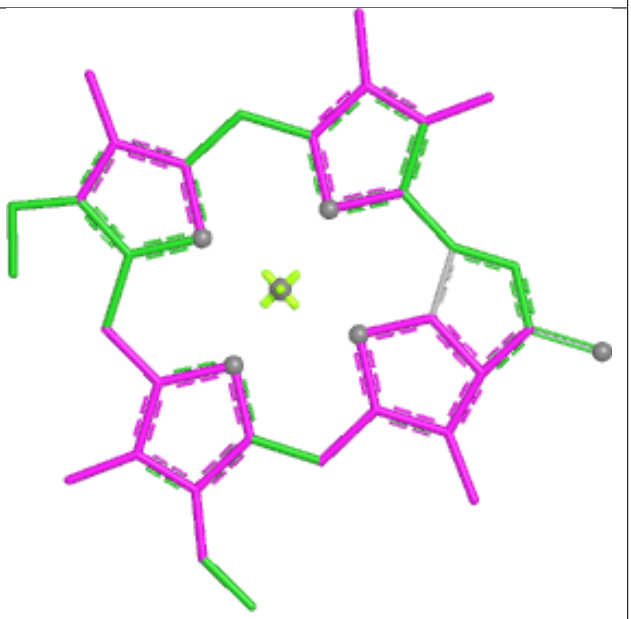
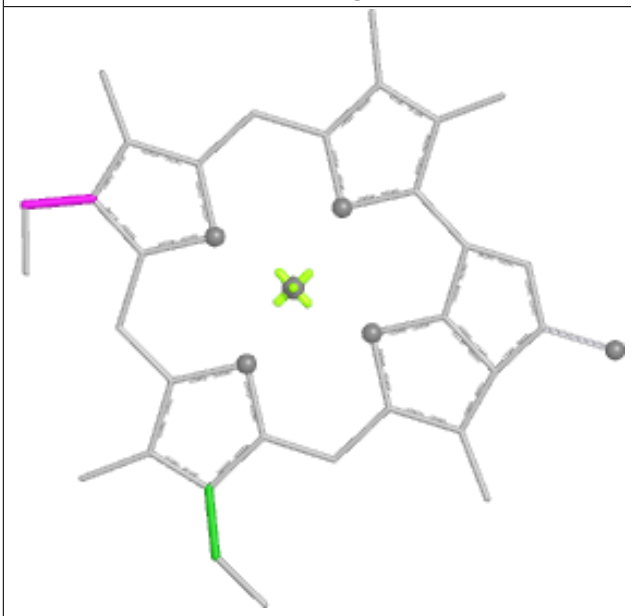


Bond angles



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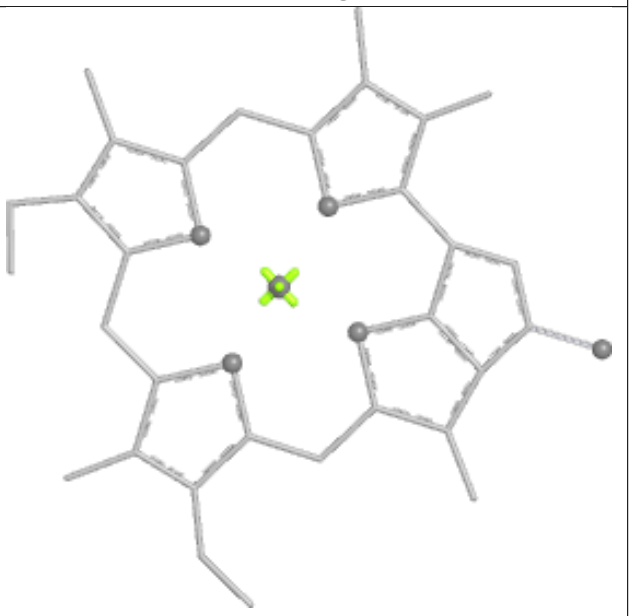
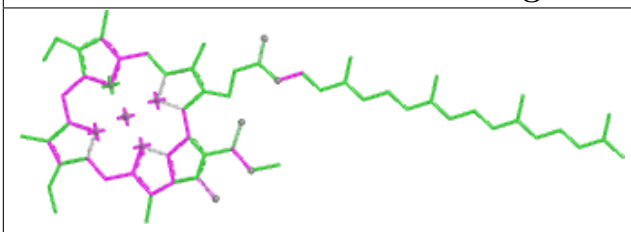
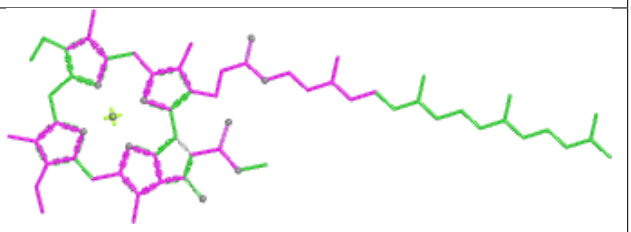
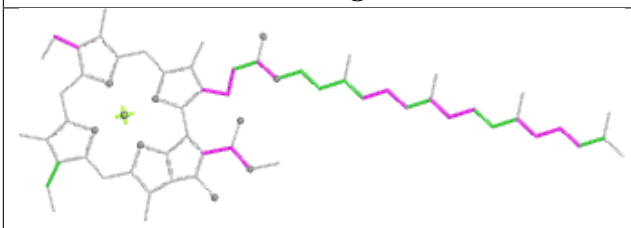
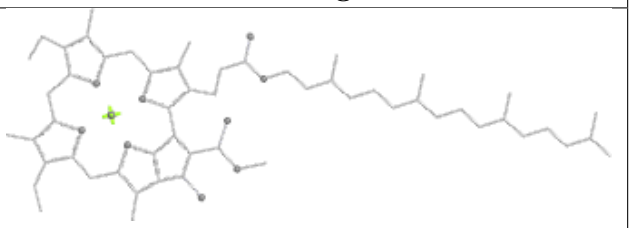
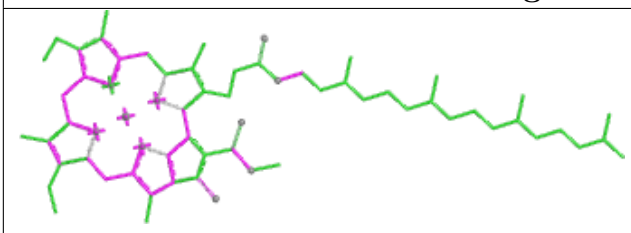
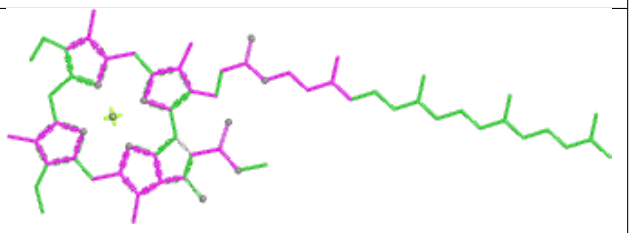
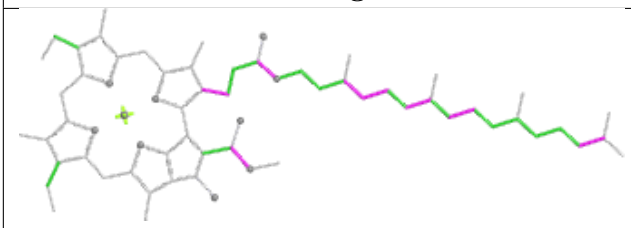
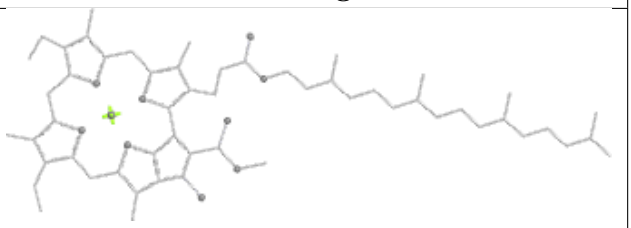
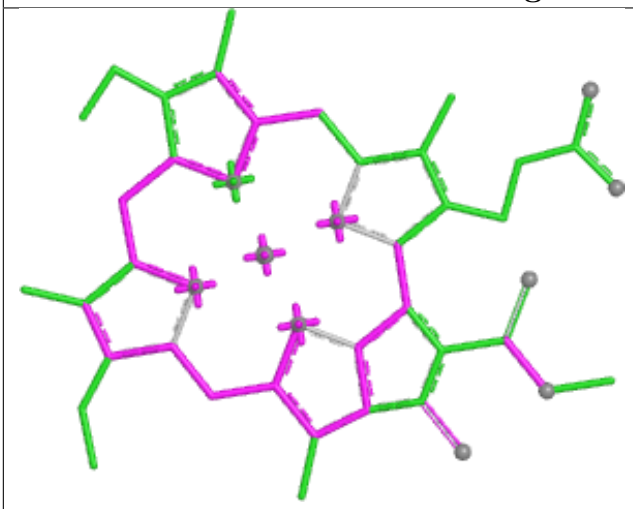


Rings

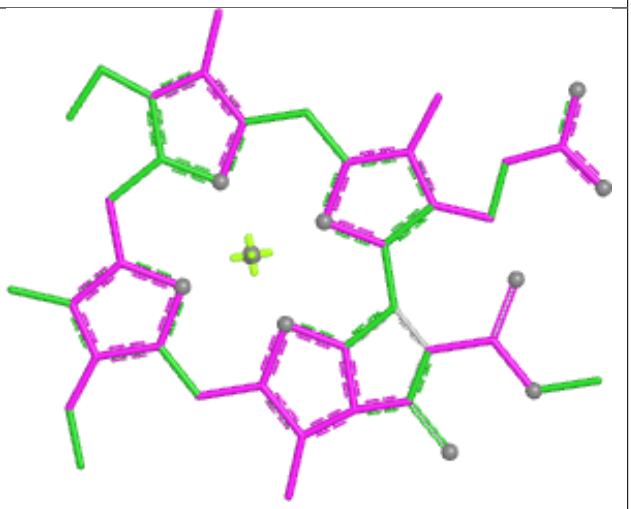
Ligand CLA G 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

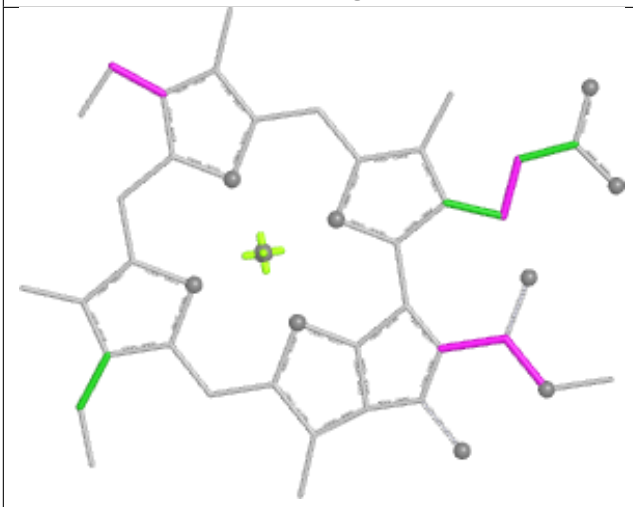
Ligand CLA B 817



Bond lengths



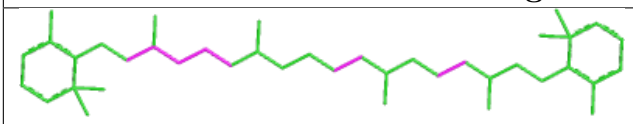
Bond angles



Torsions

Rings

Ligand BCR b 850



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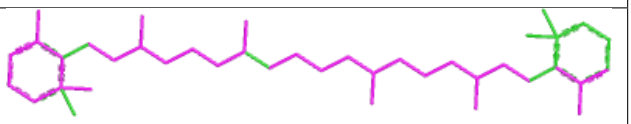
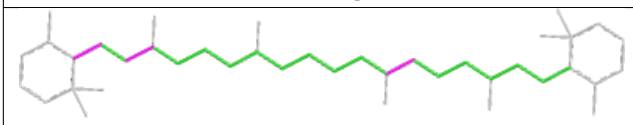


Bond angles



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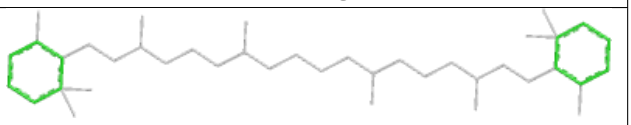
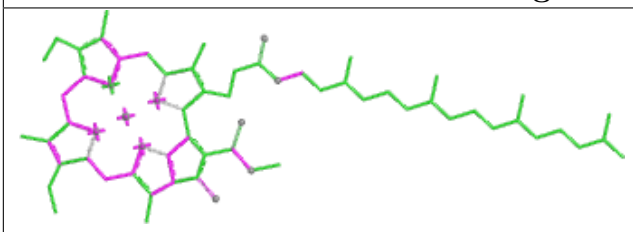


Rings

Ligand CL0 a 801



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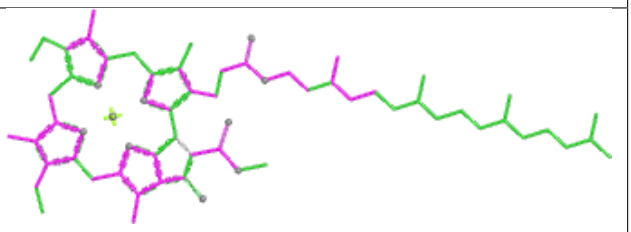
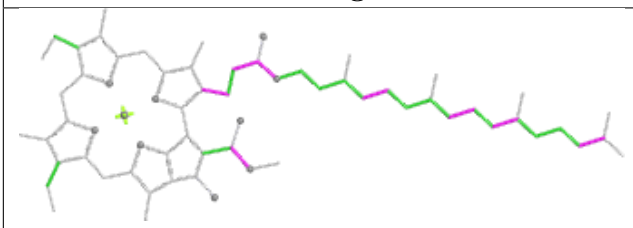


Bond angles



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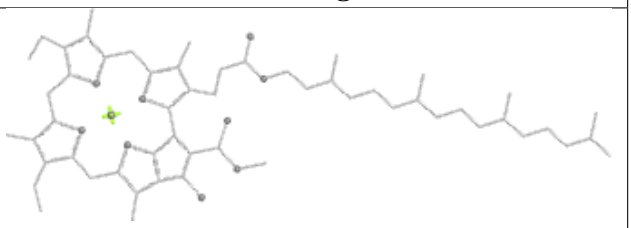
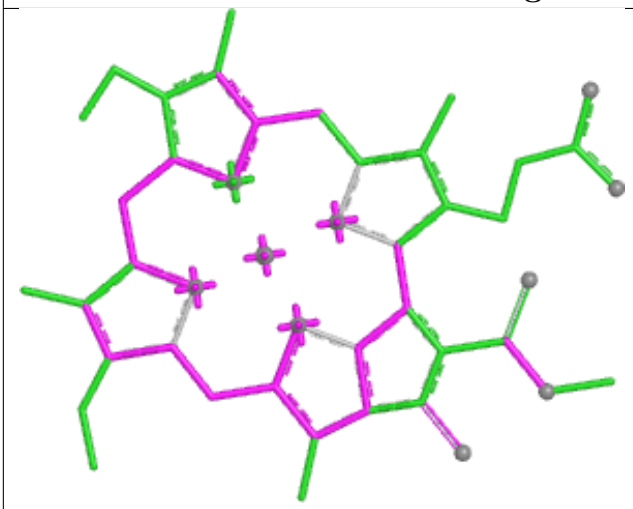


Rings

Ligand CLA B 836



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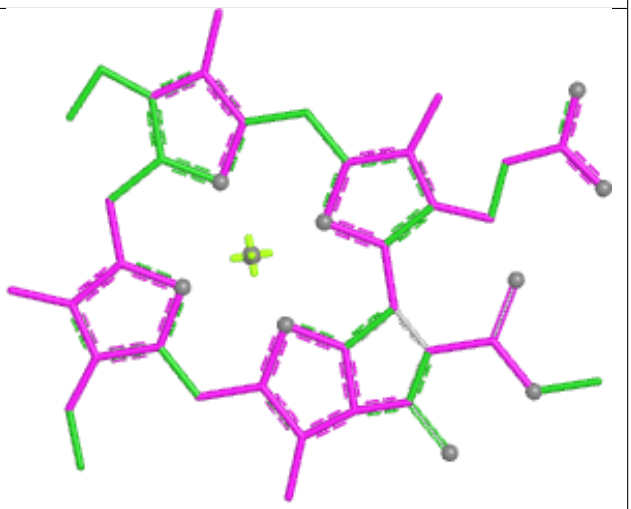
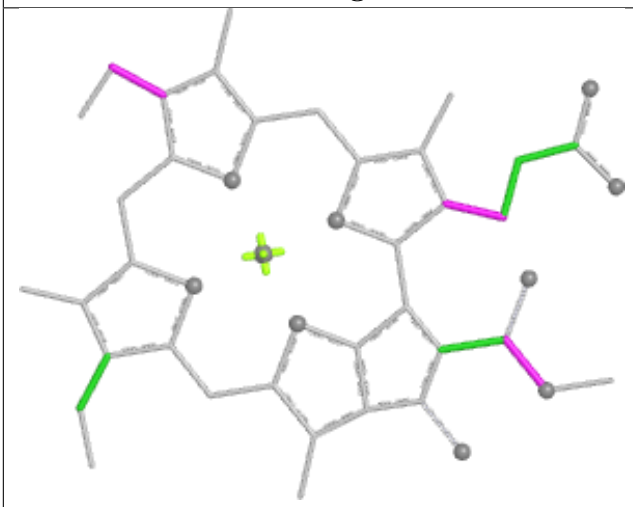


Bond angles



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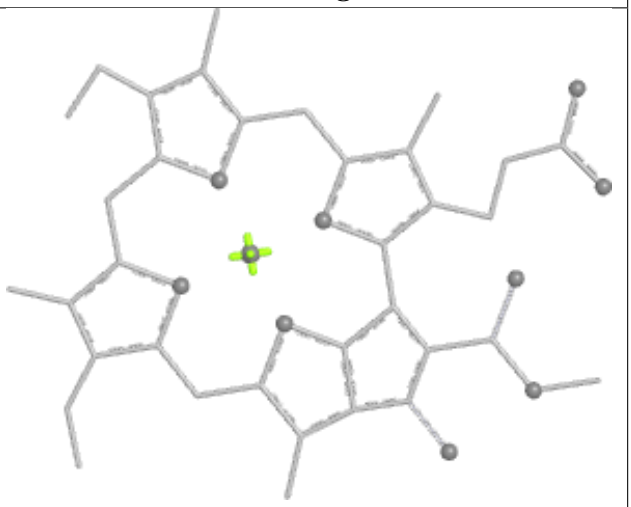
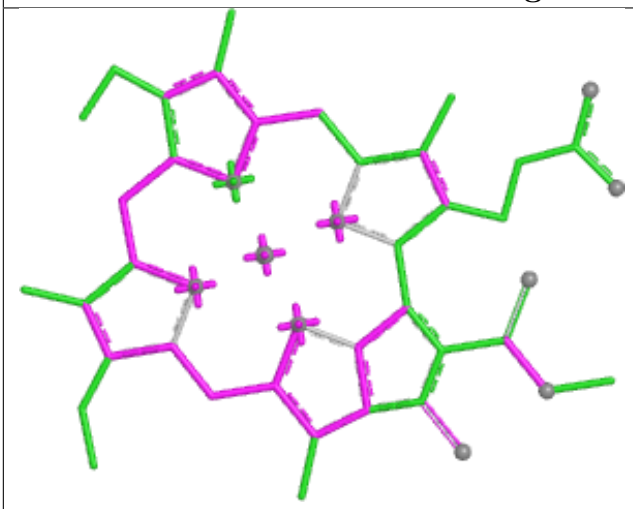


Rings

Ligand CLA B 825



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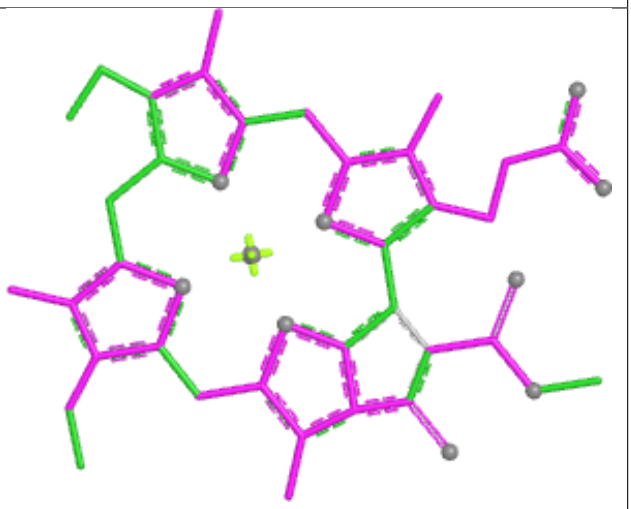

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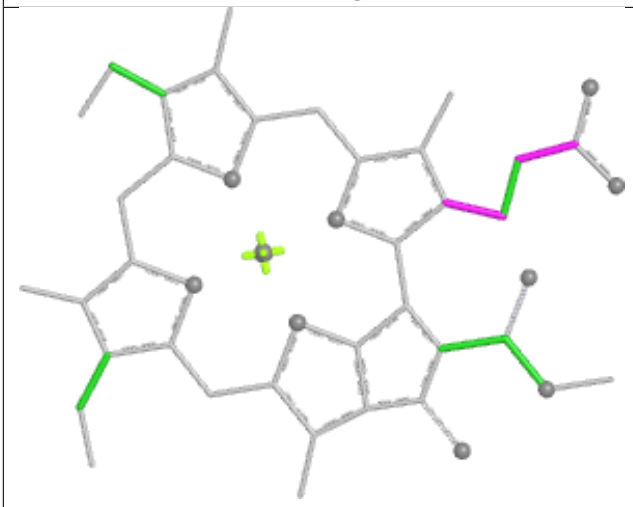
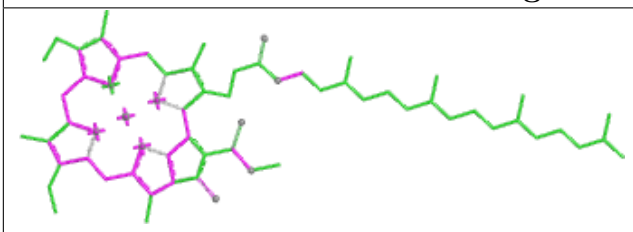


Torsions

Rings

Ligand CLA H 804



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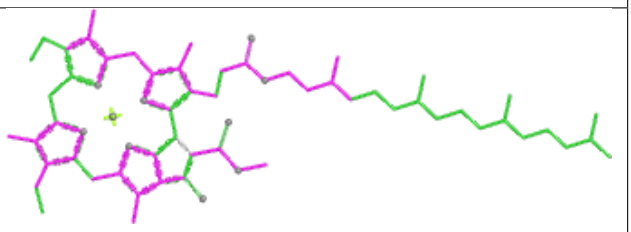
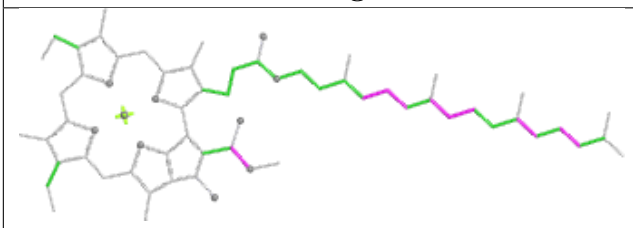


Bond angles



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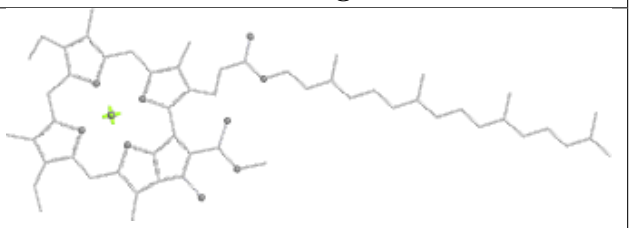
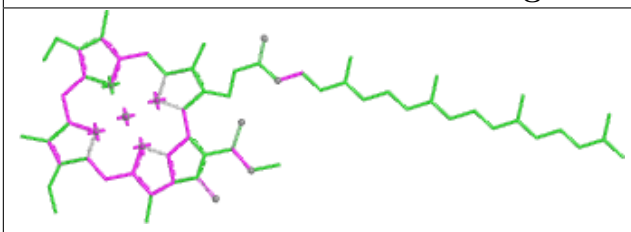


Rings

Ligand CLA A 826



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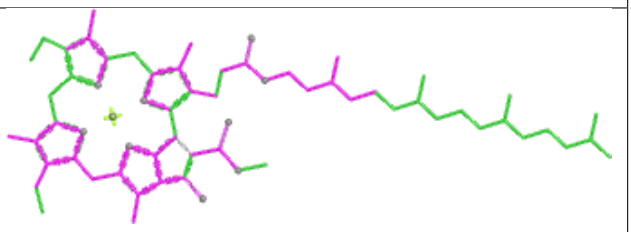

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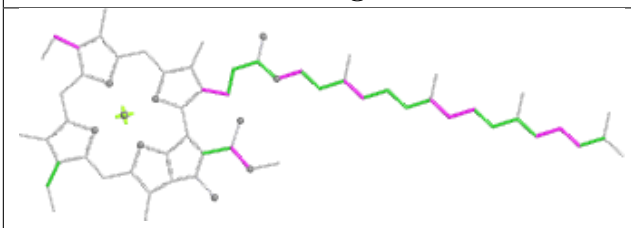

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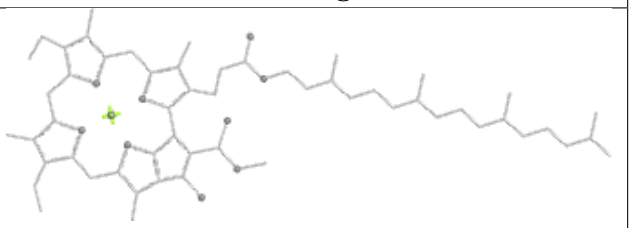
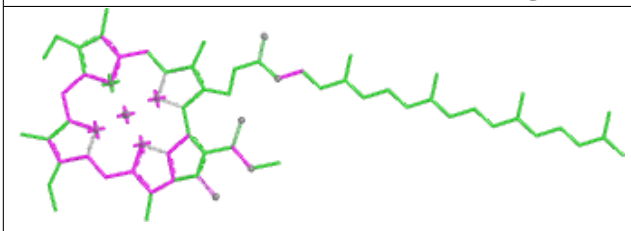


Rings

Ligand CLA B 810



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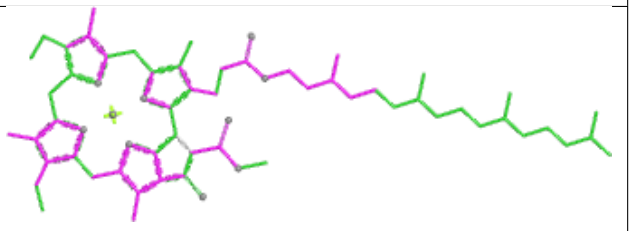

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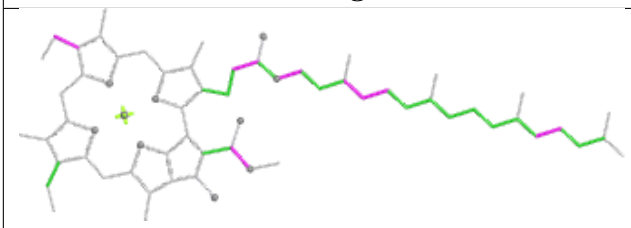

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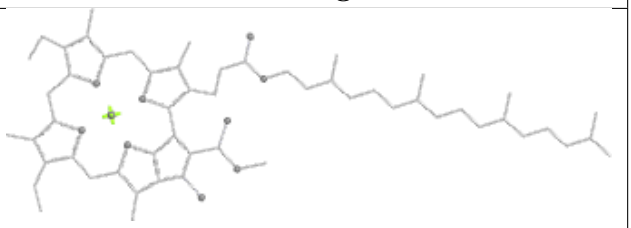
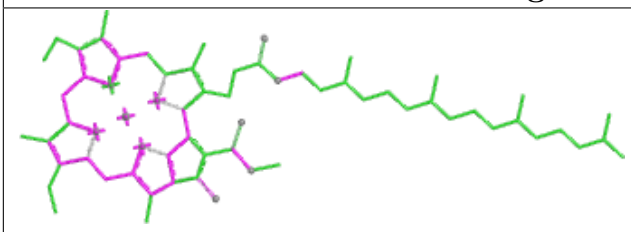


Rings

Ligand CLA b 803



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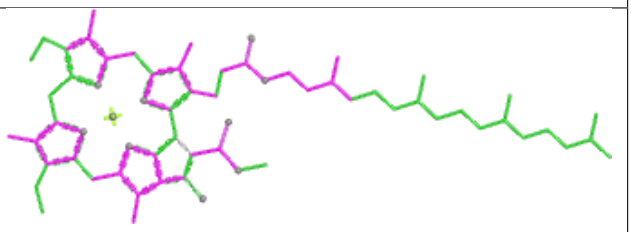
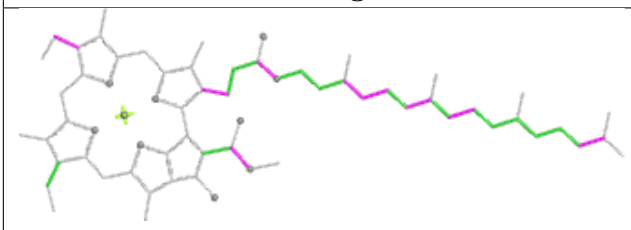


Bond angles



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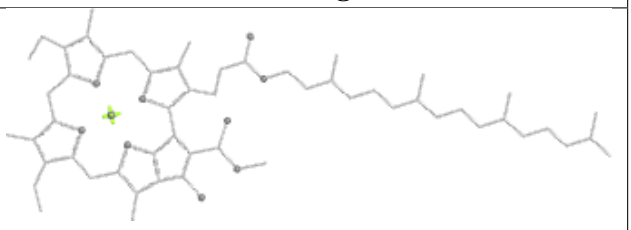
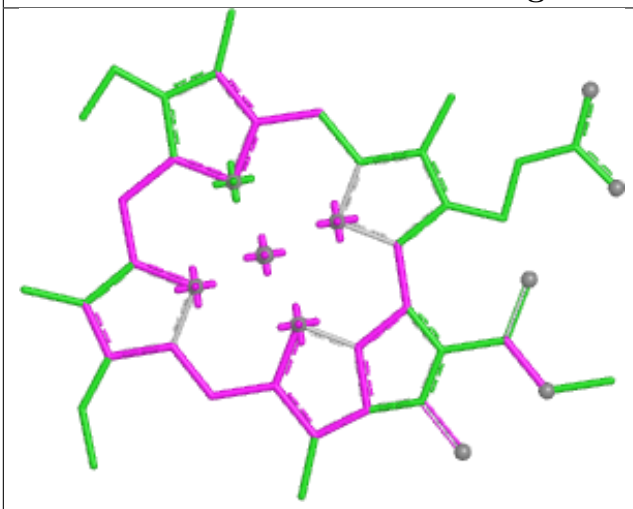


Rings

Ligand CLA b 814



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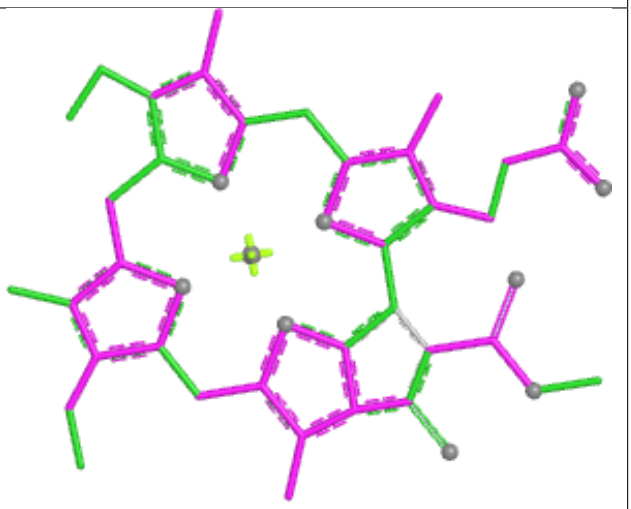
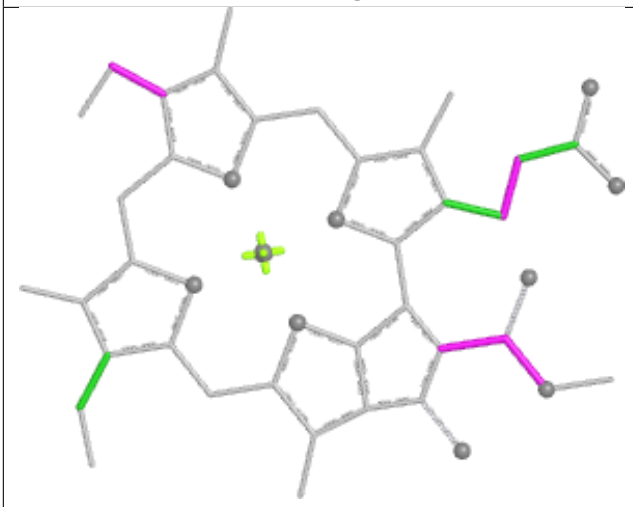


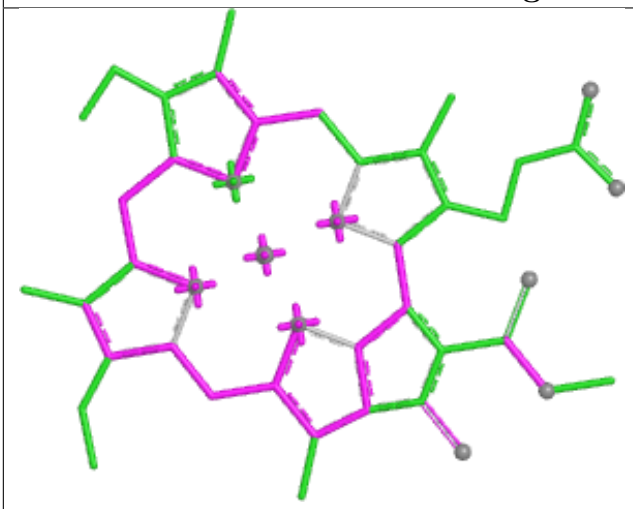
Bond angles



Torsions

Rings

Ligand CLA G 814



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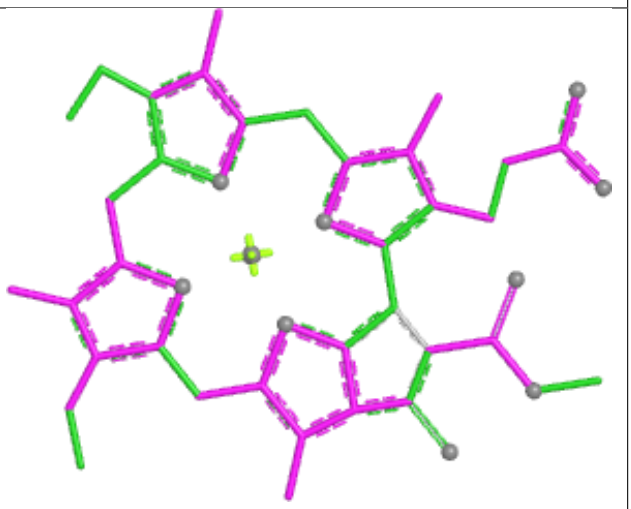
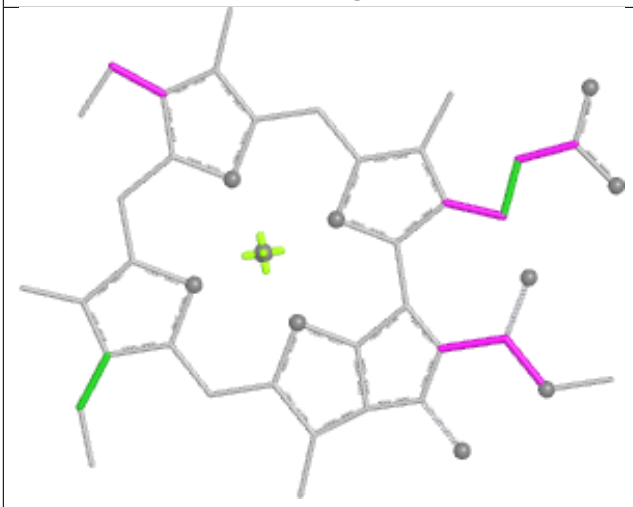


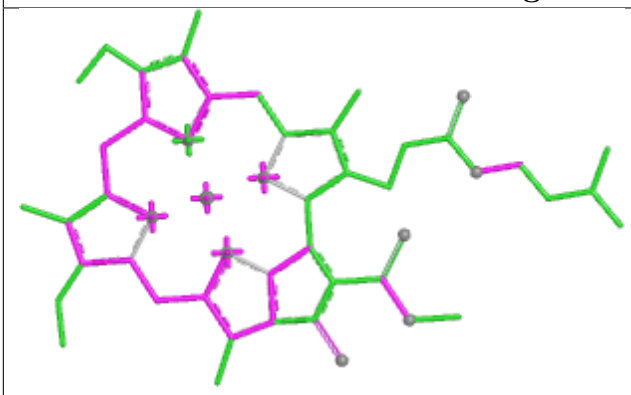
Bond angles



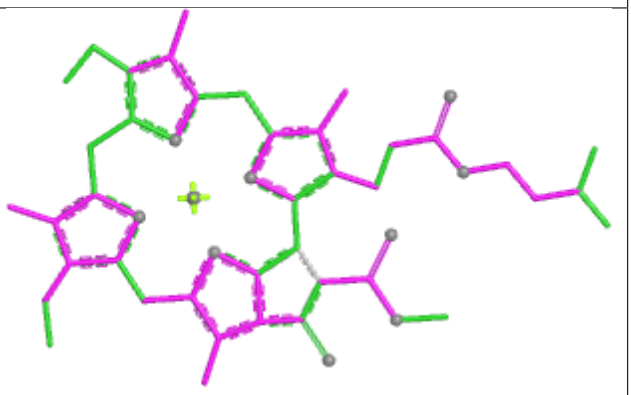
Torsions

Rings

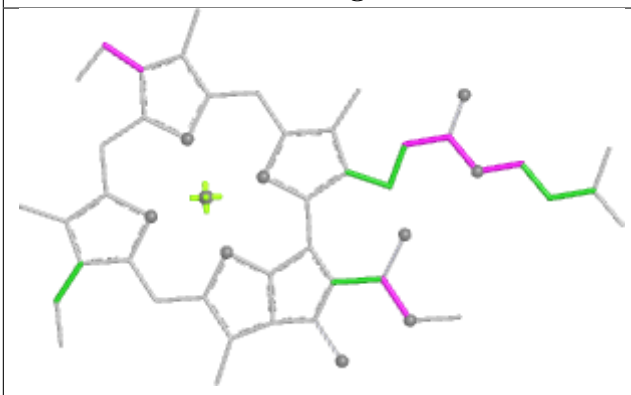
Ligand CLA G 806



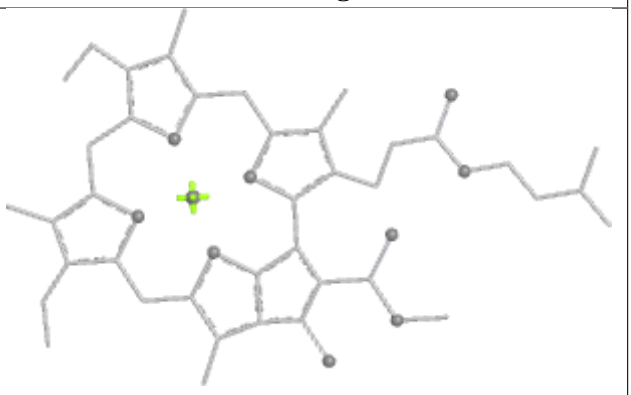
Bond lengths



Bond angles

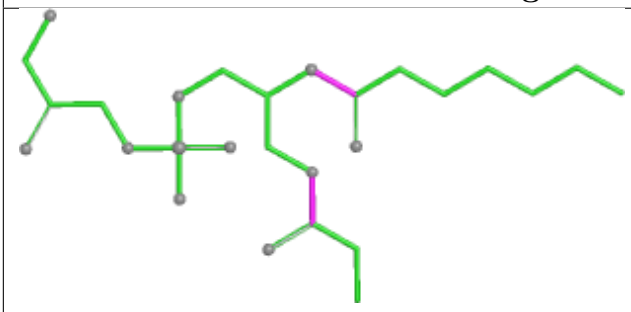


Torsions



Rings

Ligand LHG A 851



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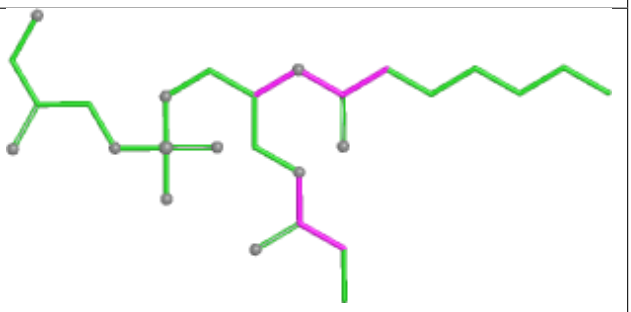
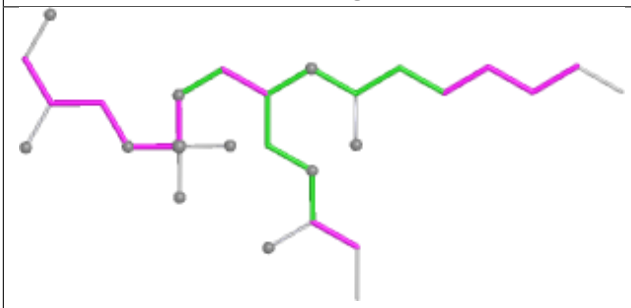
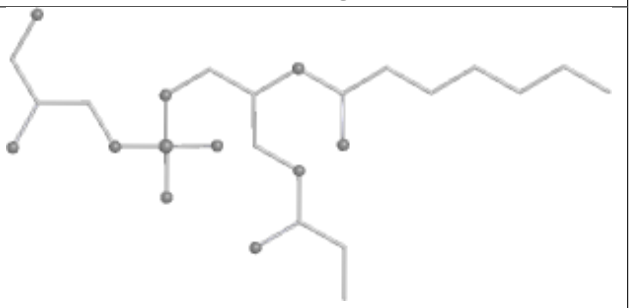


Bond angles

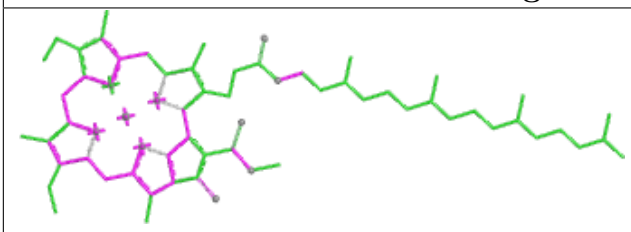


Torsions

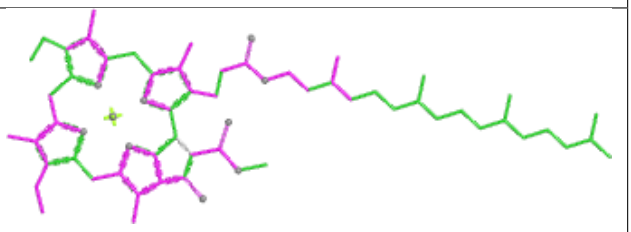


Rings

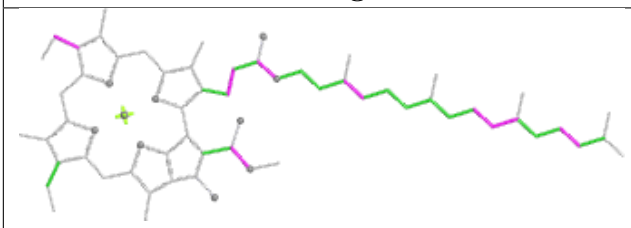
Ligand CLA G 810



Bond lengths



Bond angles



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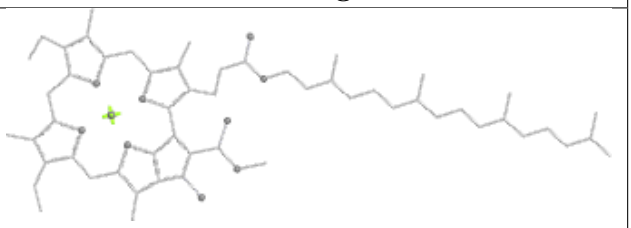
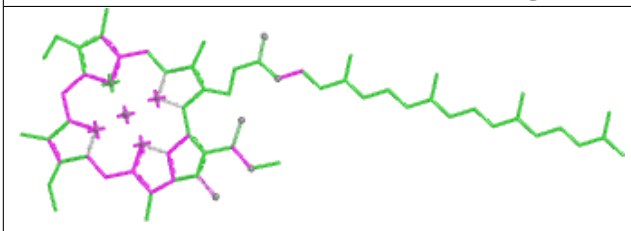


Rings

Ligand CLA B 802



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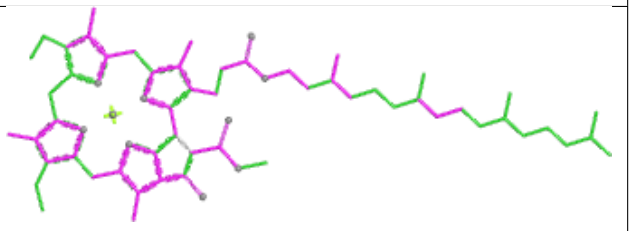
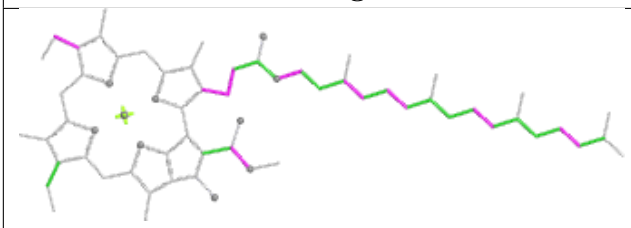
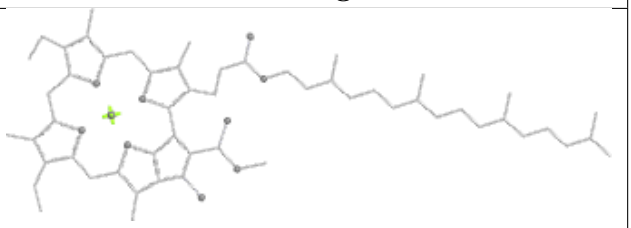


Bond angles

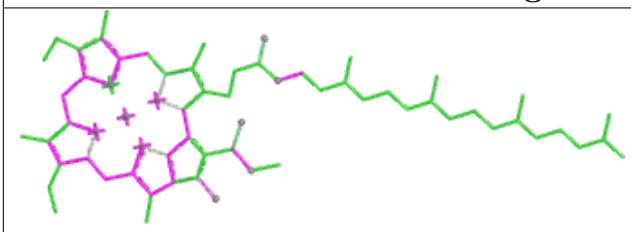


Torsions



Rings

Ligand CLA B 804



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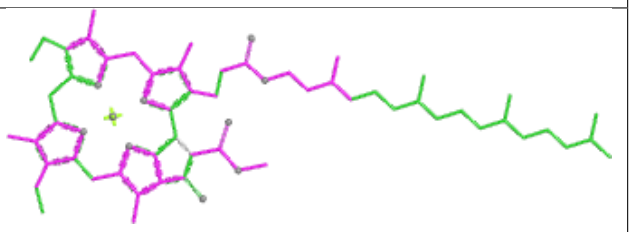
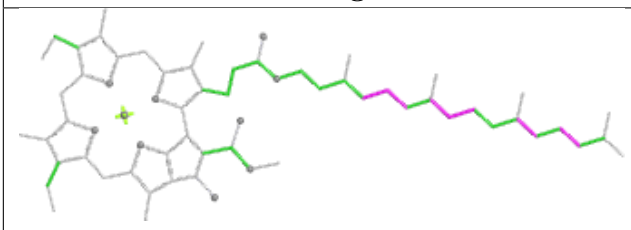


Bond angles



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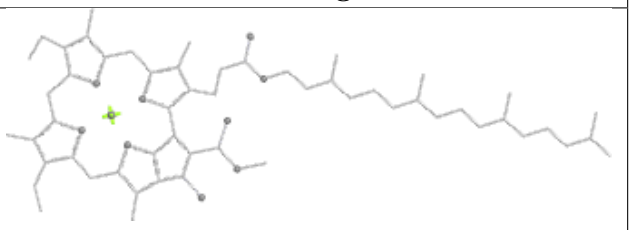
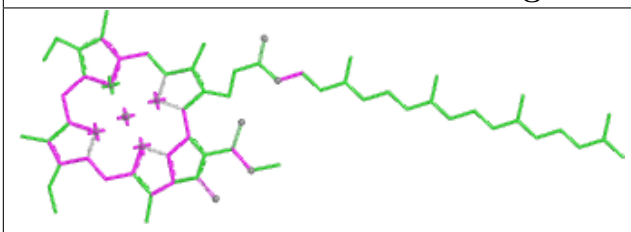


Rings

Ligand CLA H 842



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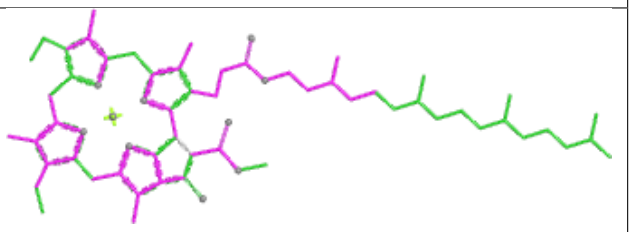
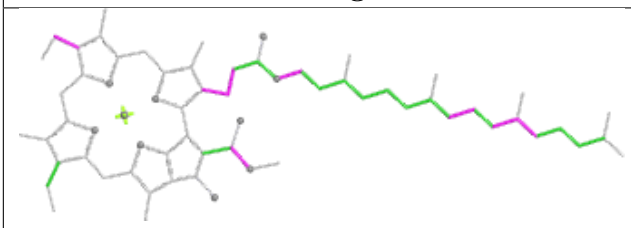


Bond angles



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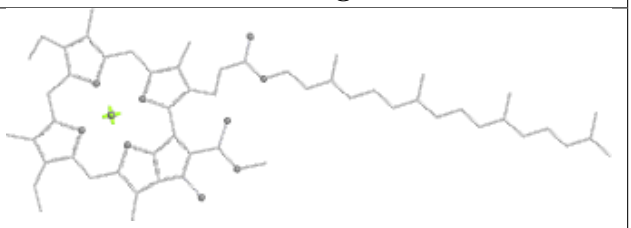
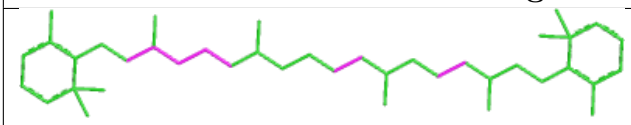


Rings

Ligand BCR a 845



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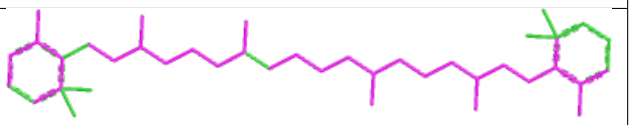

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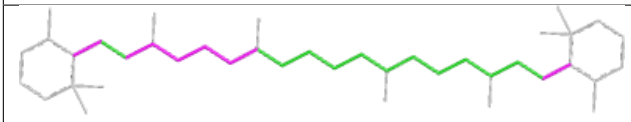

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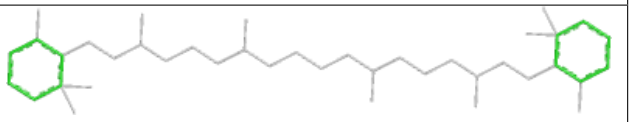
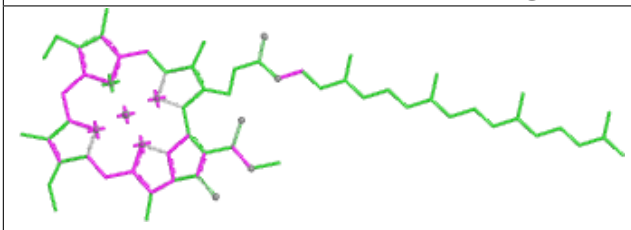


Rings

Ligand CLA H 808



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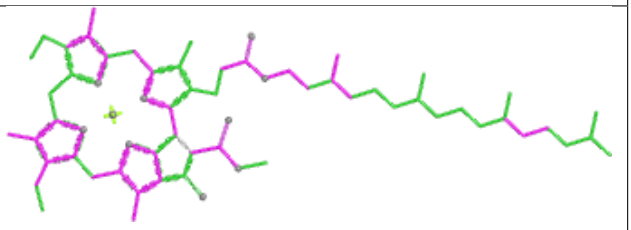

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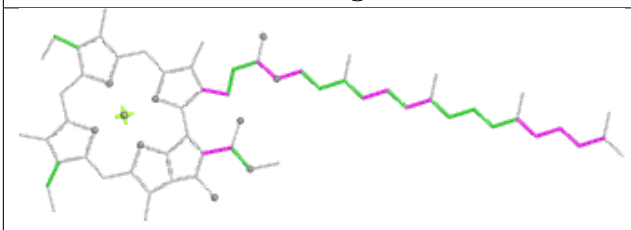

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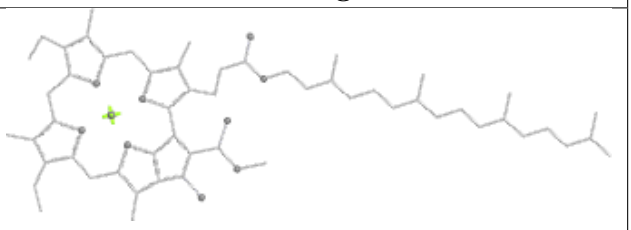
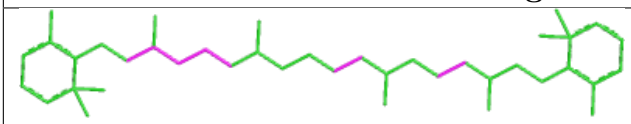


Rings

Ligand BCR b 846



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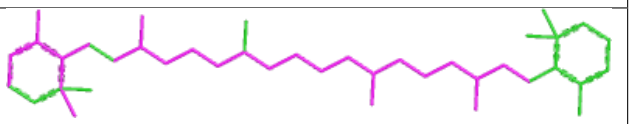

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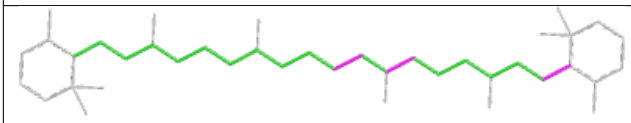

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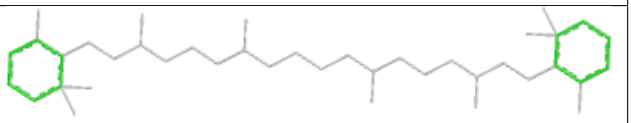
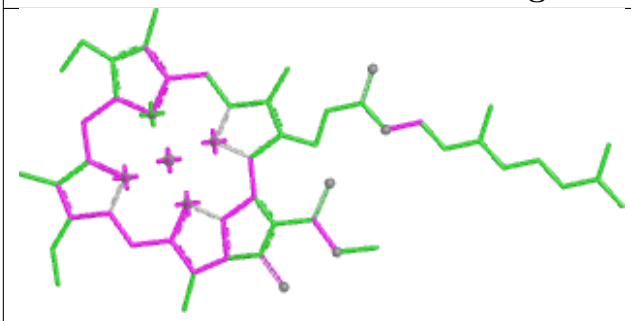


Rings

Ligand CLA a 823



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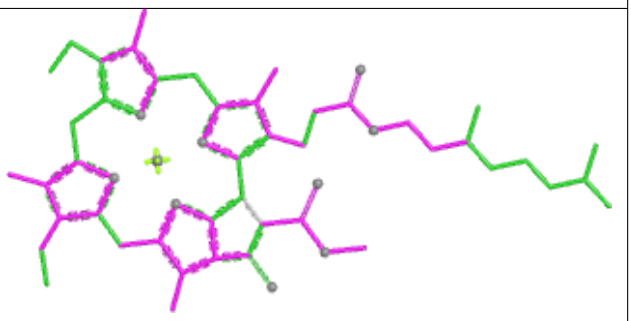
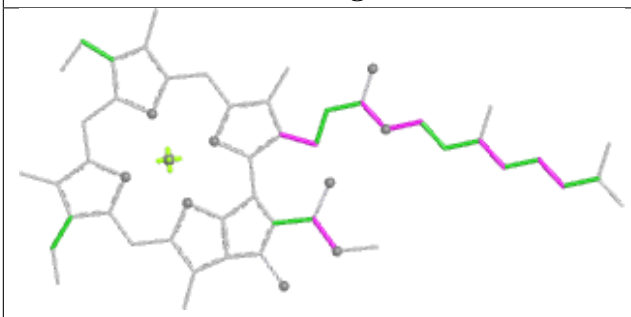


Bond angles



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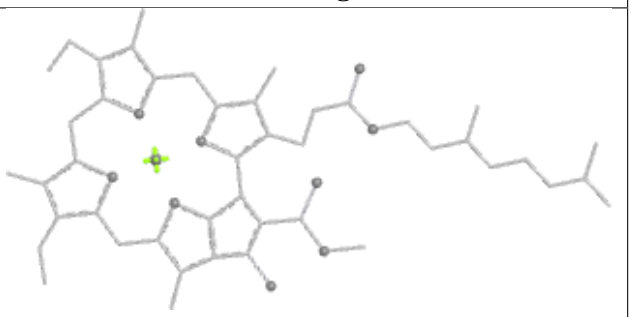
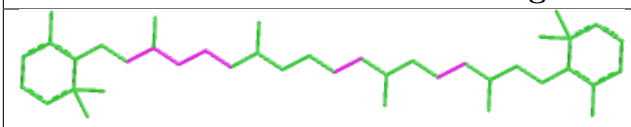


Rings

Ligand BCR I 101



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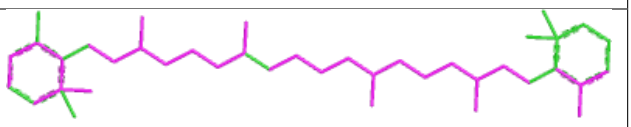

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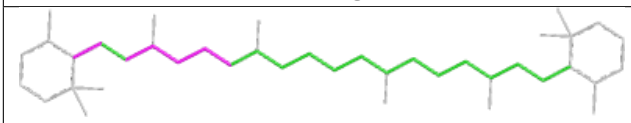

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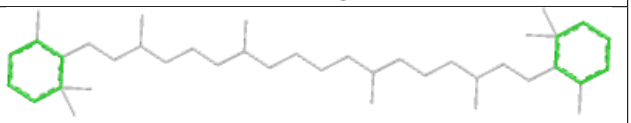
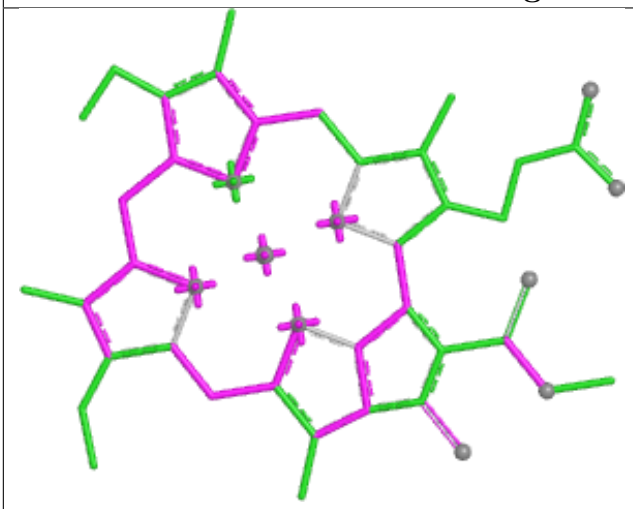


Rings

Ligand CLA Q 202



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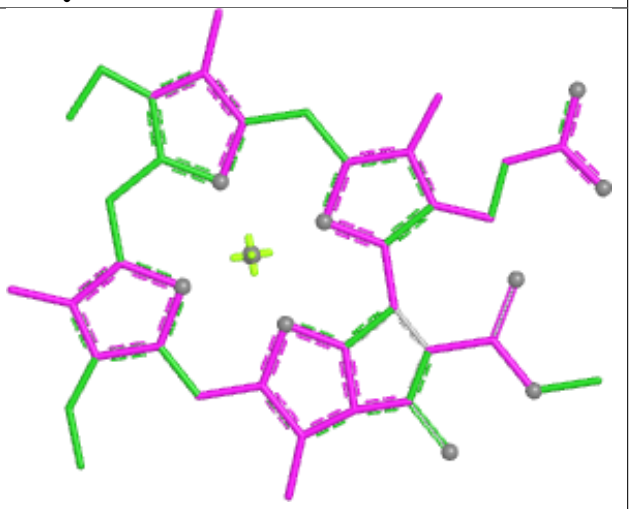
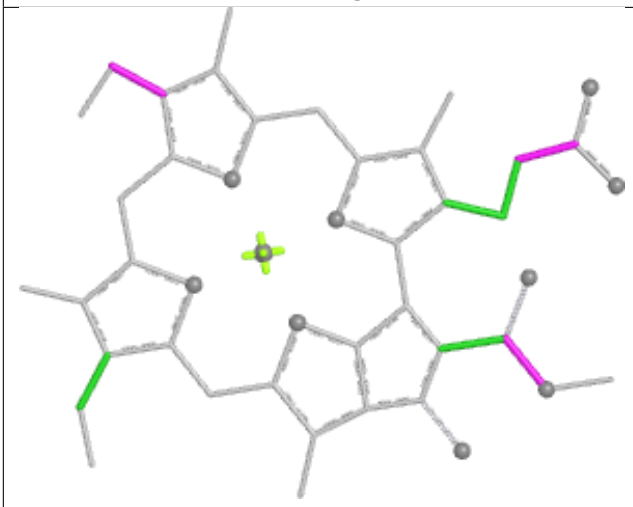


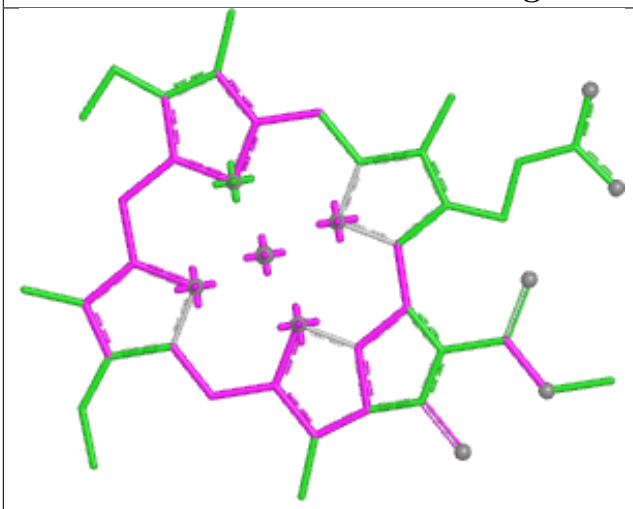
Bond angles



Torsions

Rings

Ligand CLA G 813



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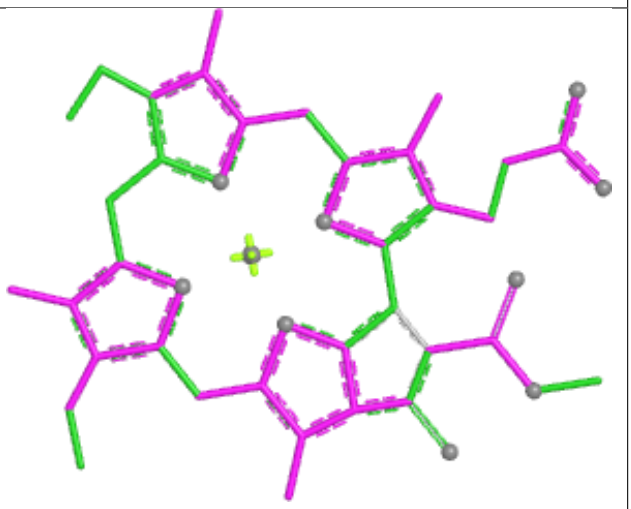
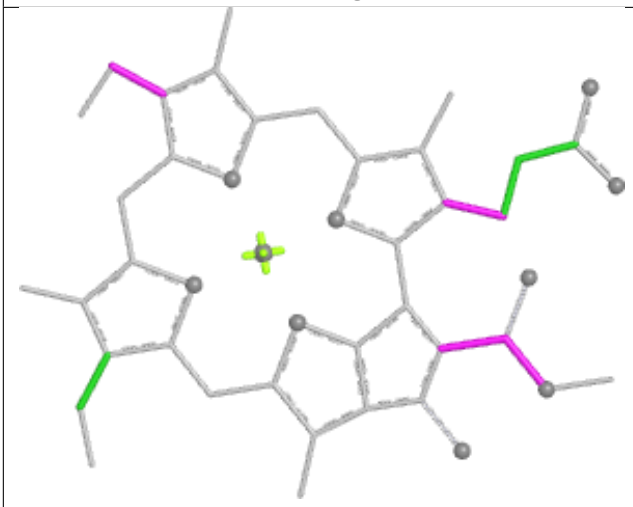
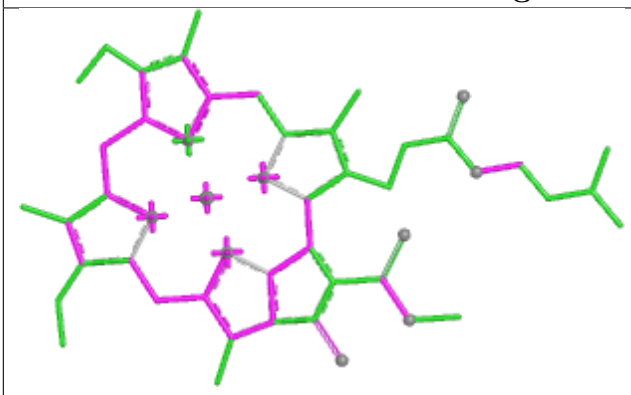
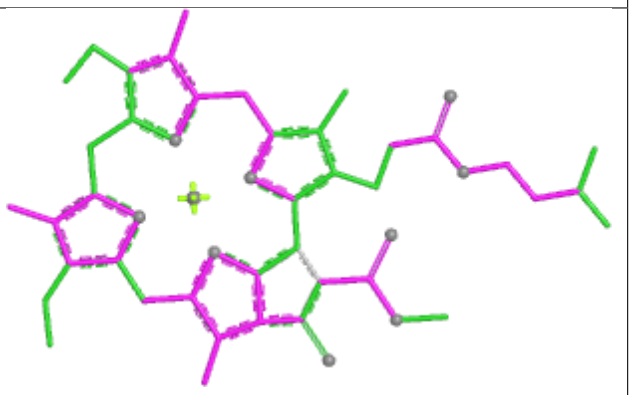
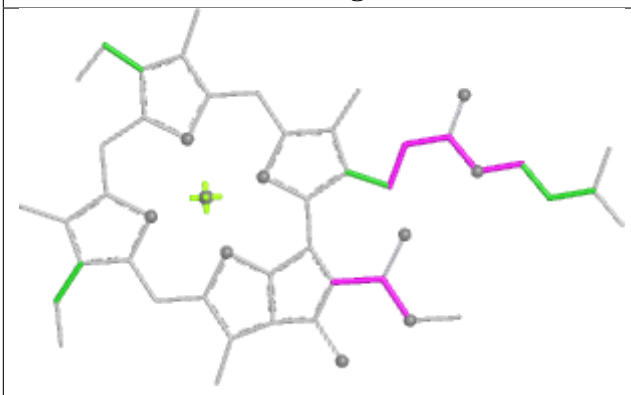
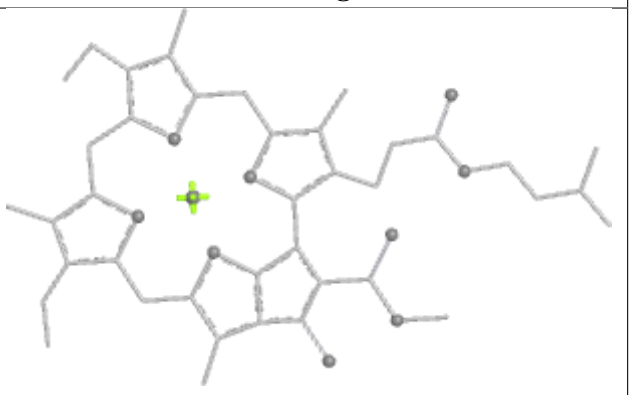


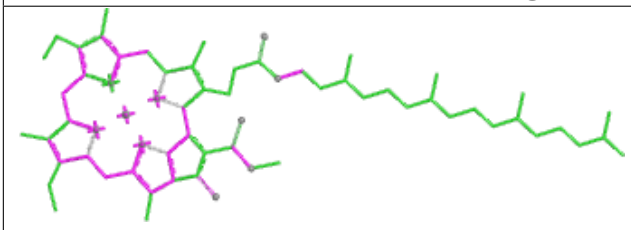
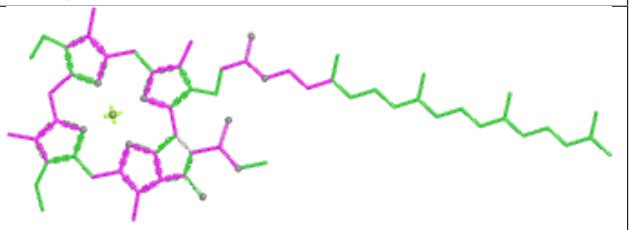
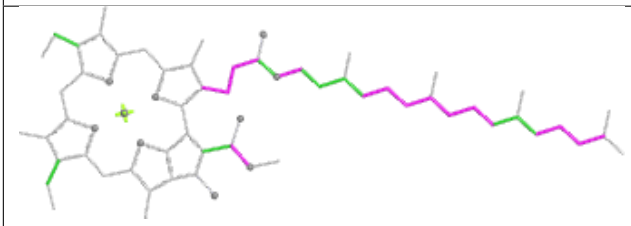
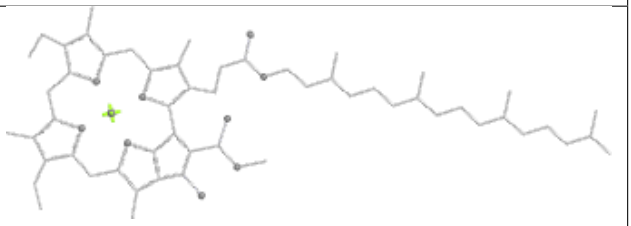
Bond angles

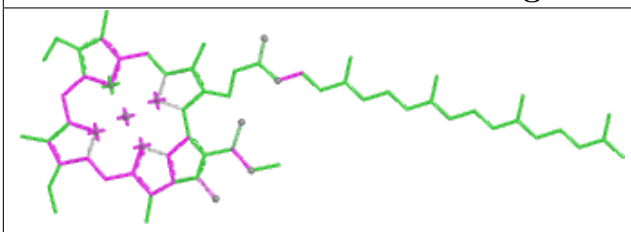
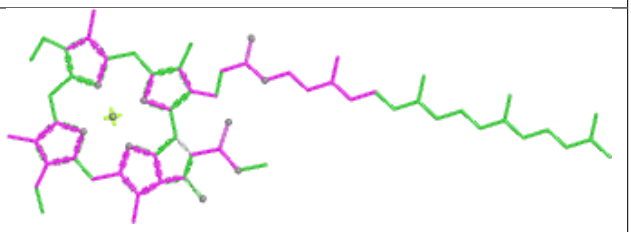
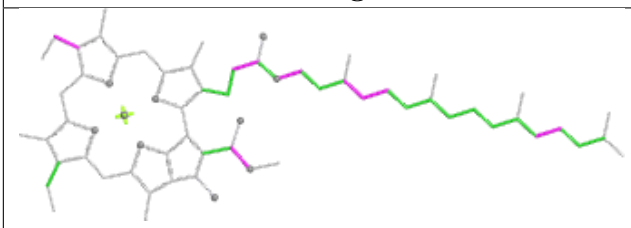
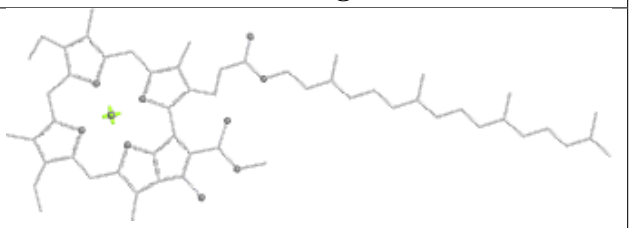


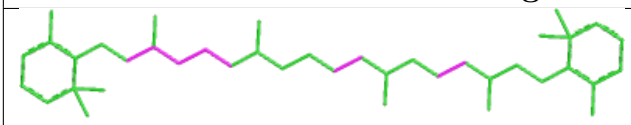
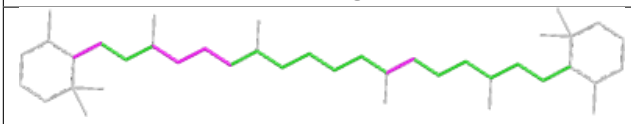
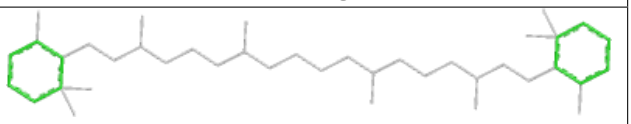
Torsions

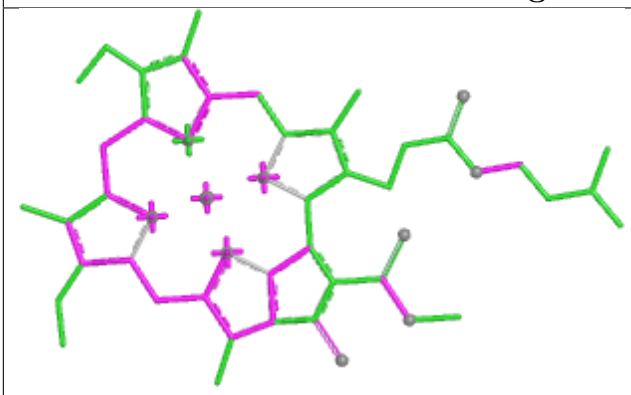
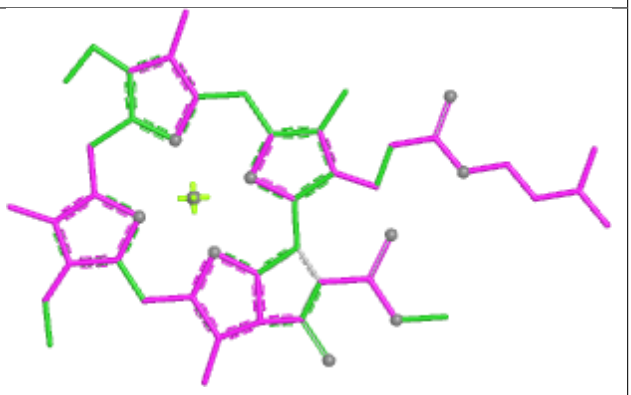
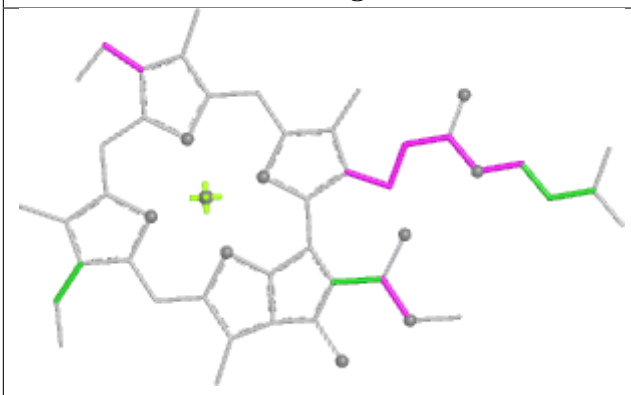
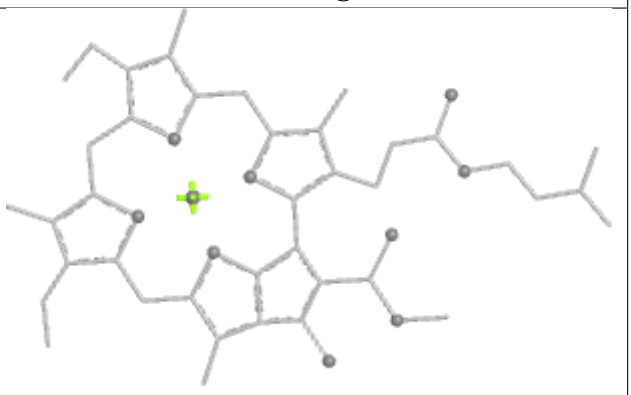
Rings

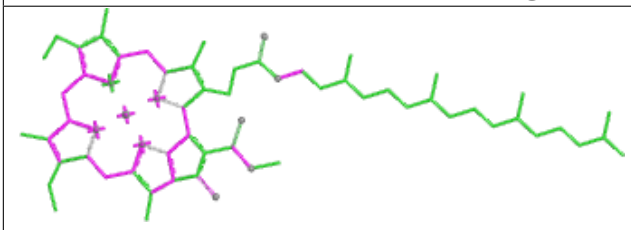
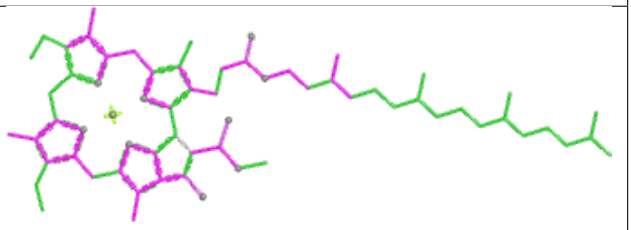
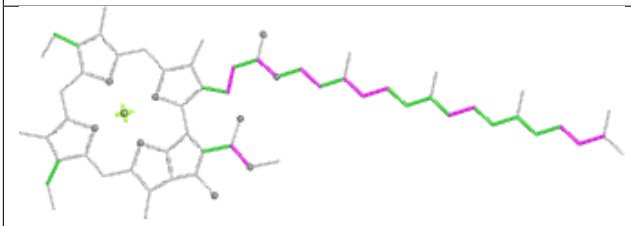
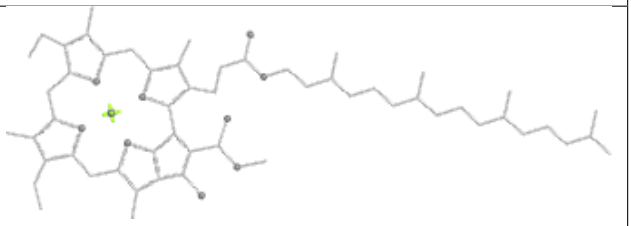
Ligand CLA m 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

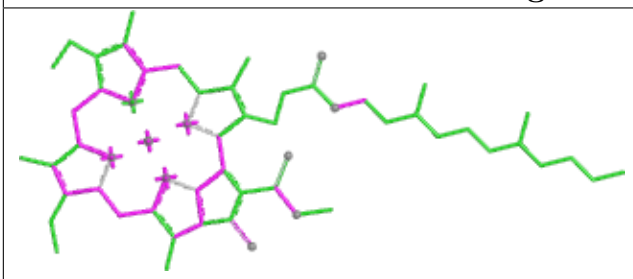
Ligand CLA H 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 846	
 Bond lengths	Bond angles
 Torsions	 Rings

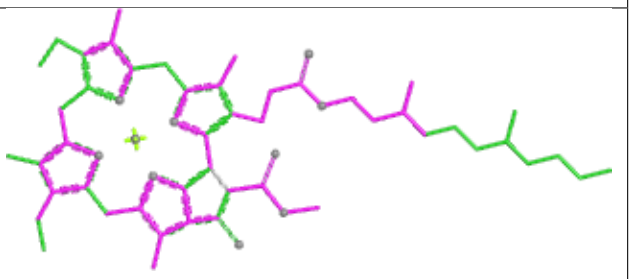
Ligand CLA a 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

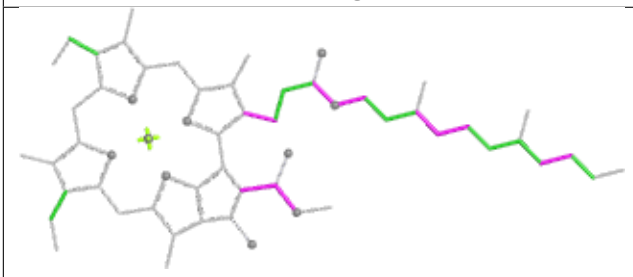
Ligand CLA b 832



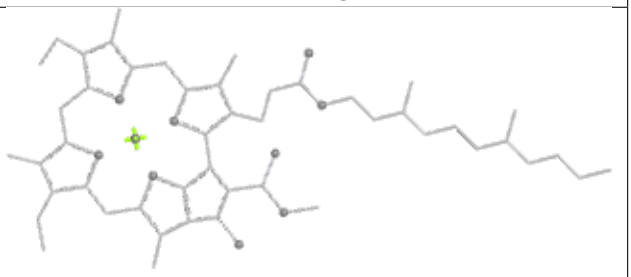
Bond lengths



Bond angles

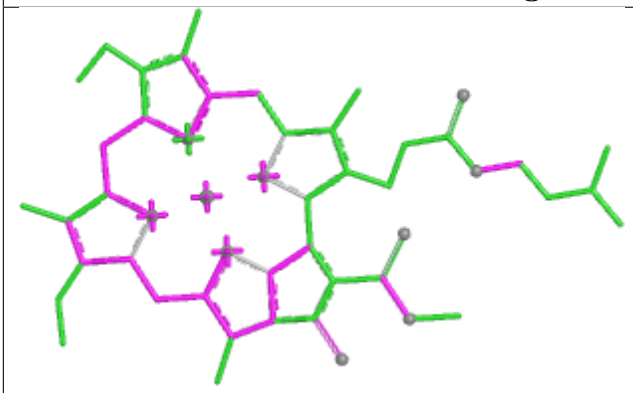


Torsions

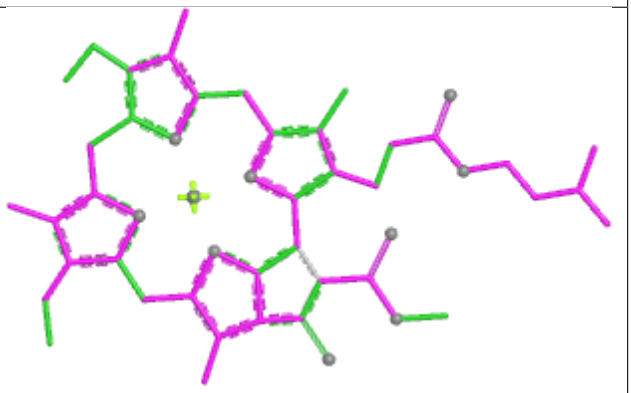


Rings

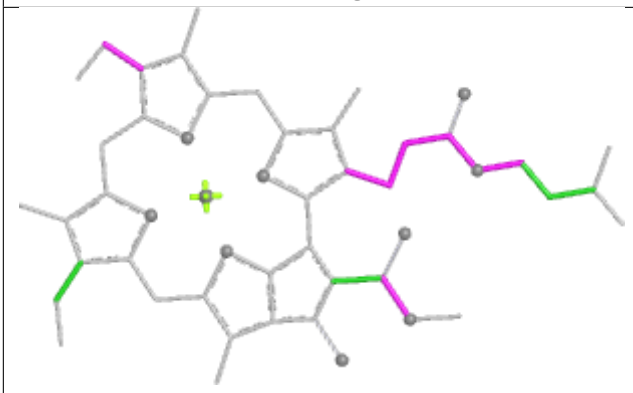
Ligand CLA G 811



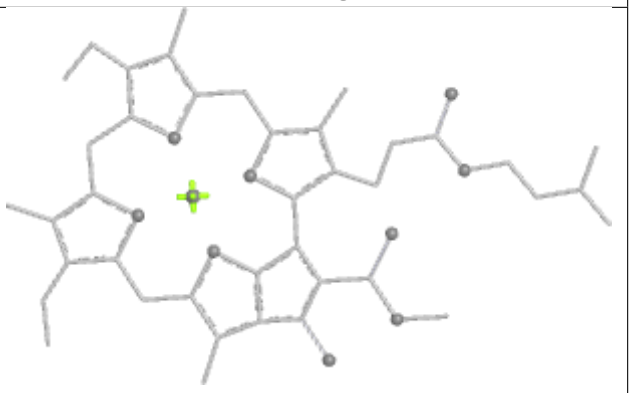
Bond lengths



Bond angles

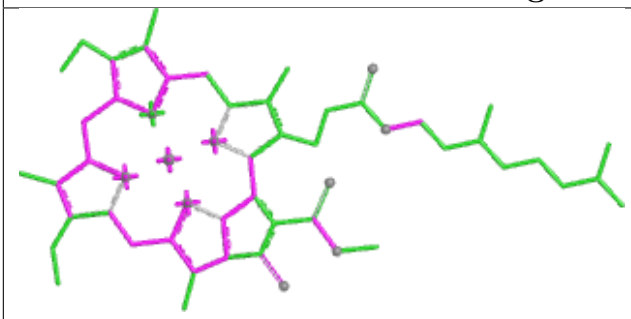


Torsions

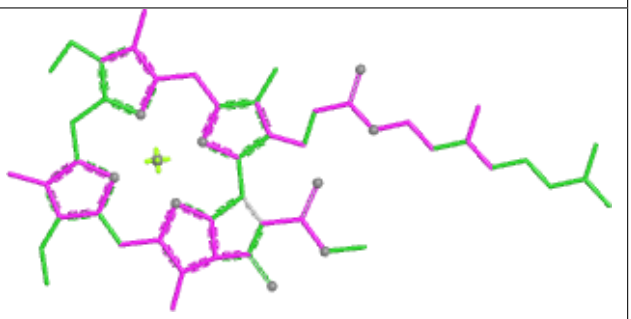


Rings

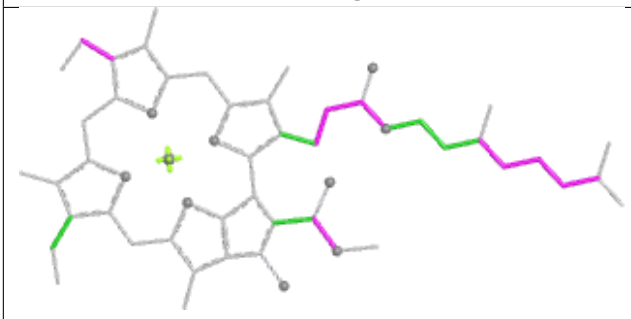
Ligand CLA b 821



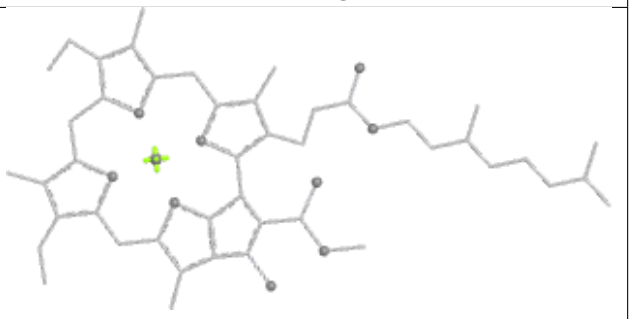
Bond lengths



Bond angles

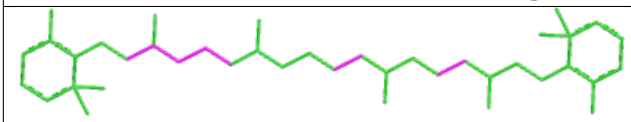


Torsions

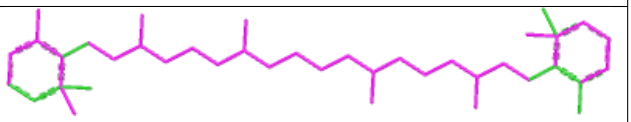


Rings

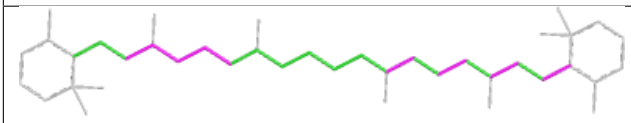
Ligand BCR b 847



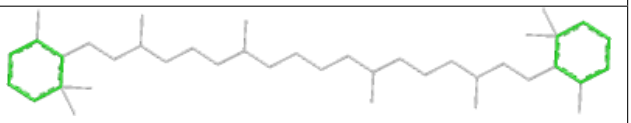
Bond lengths



Bond angles

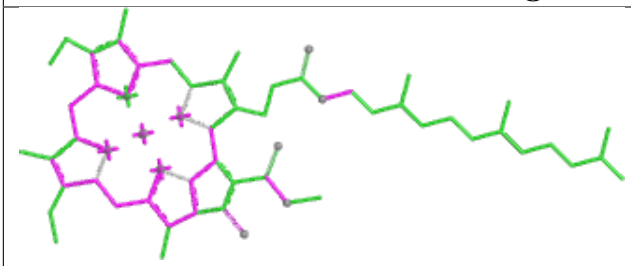


Torsions

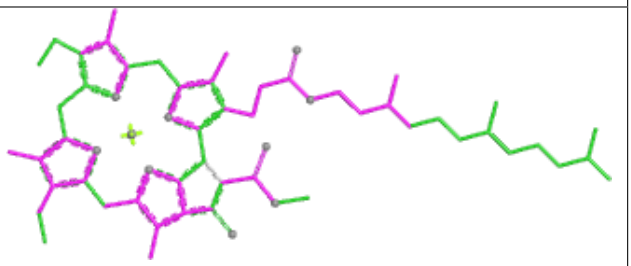


Rings

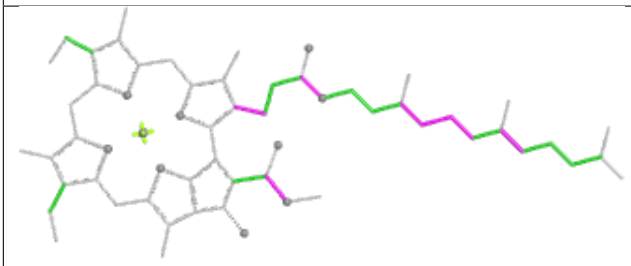
Ligand CLA B 820



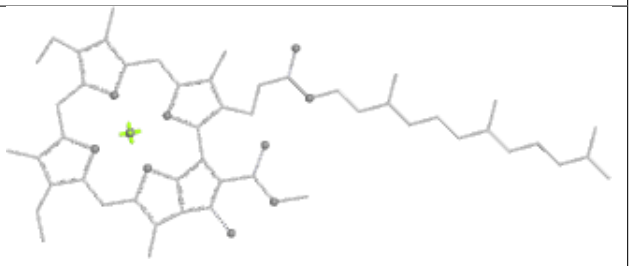
Bond lengths



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.

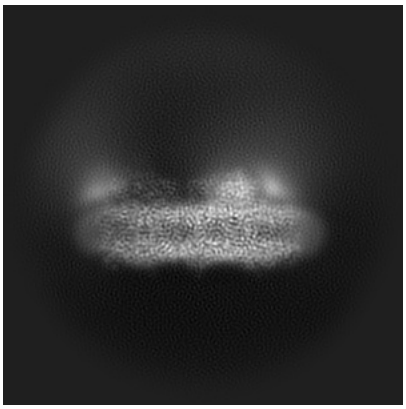
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-75106. These allow visual inspection of the internal detail of the map and identification of artifacts.

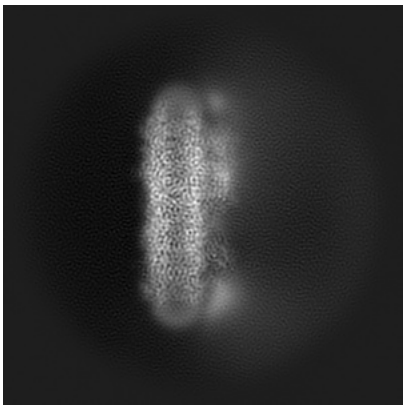
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

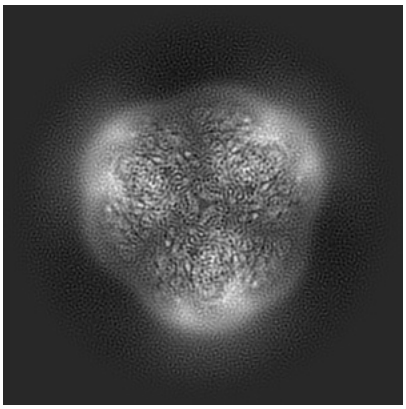
6.1.1 Primary map



X

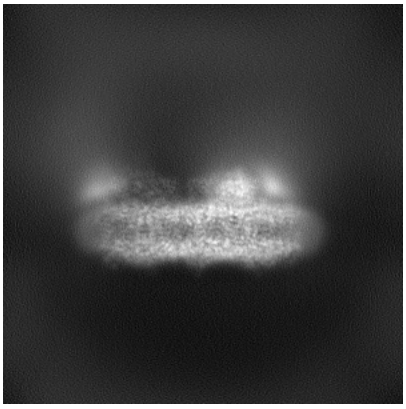


Y

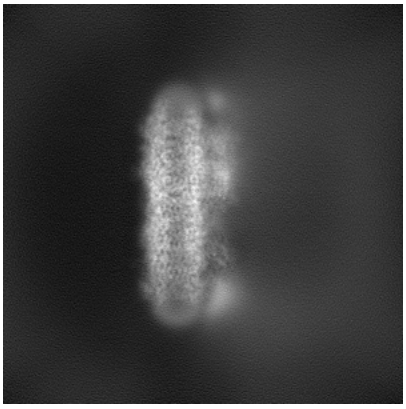


Z

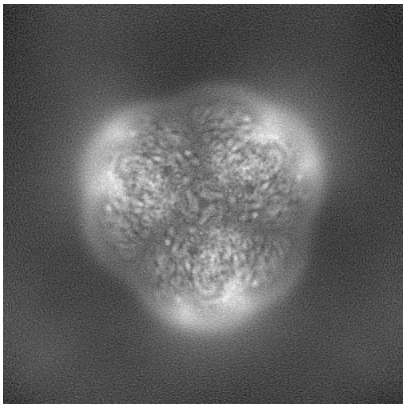
6.1.2 Raw map



X



Y

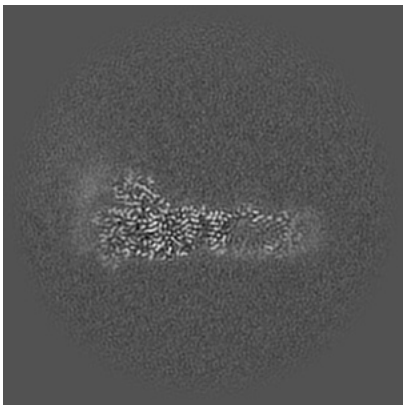


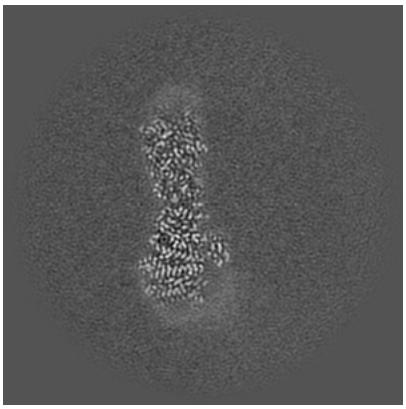
Z

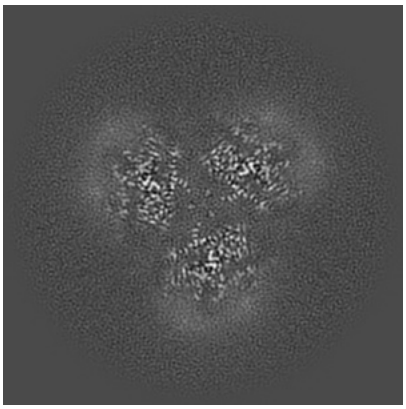
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

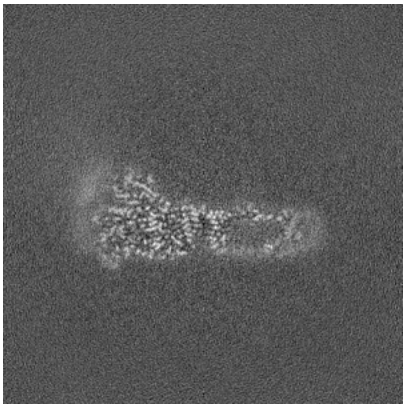
6.2.1 Primary map

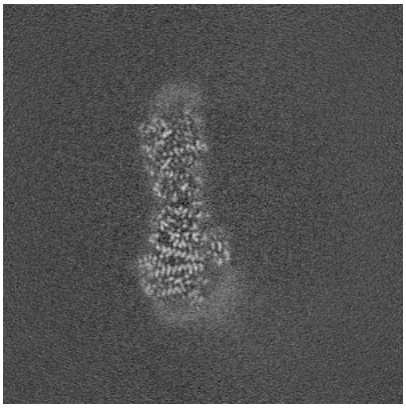

X Index: 180

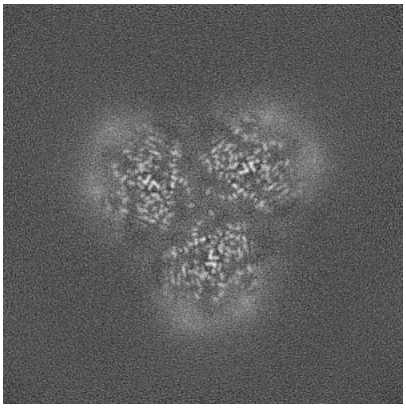

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

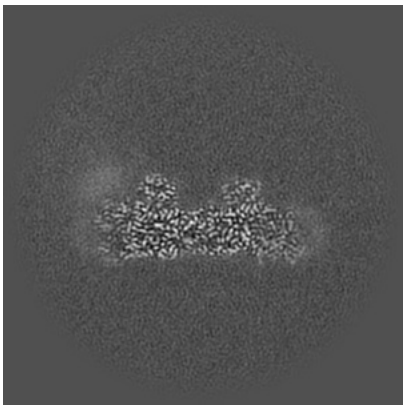

Y Index: 180

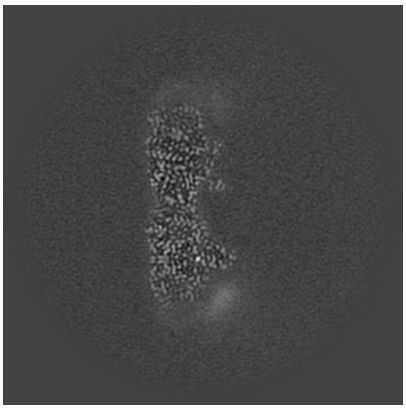

Z Index: 180

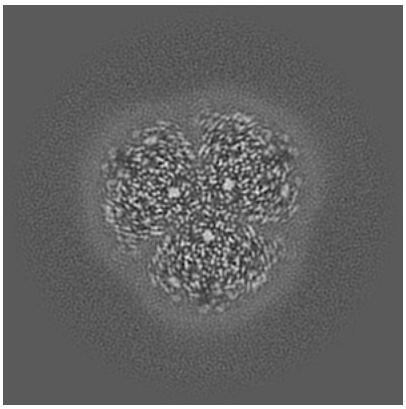
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

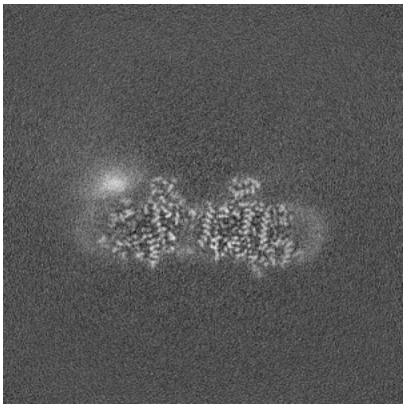
6.3.1 Primary map

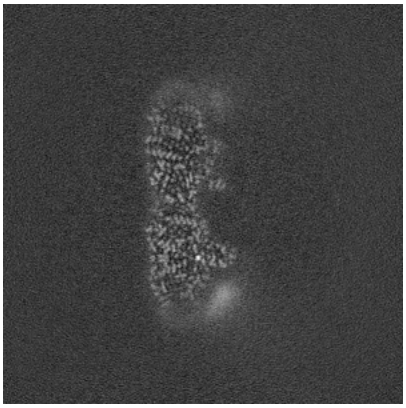

X Index: 194

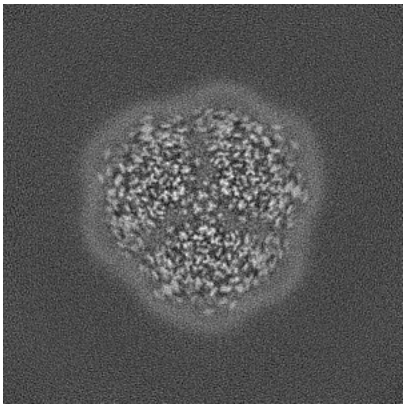

Y Index: 200


Z Index: 169

6.3.2 Raw map


X Index: 204

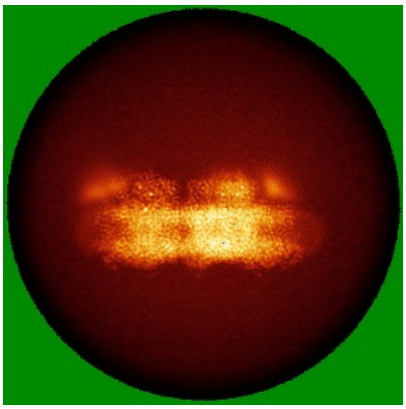

Y Index: 200

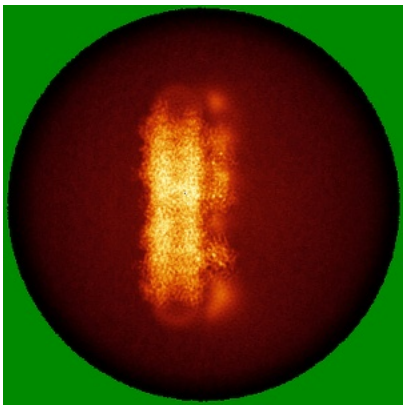

Z Index: 145

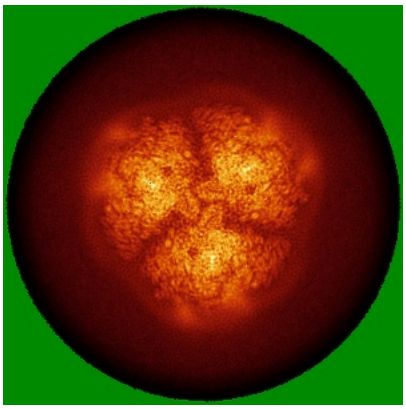
The images above show the largest variance slices of the map in three orthogonal directions.

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

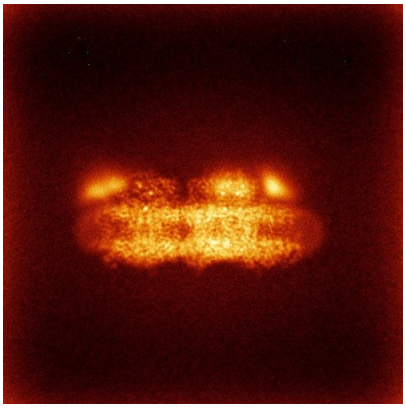
6.4.1 Primary map

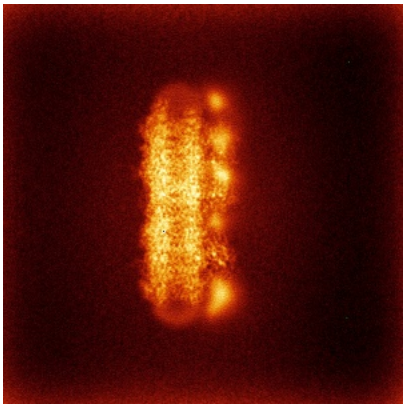

X

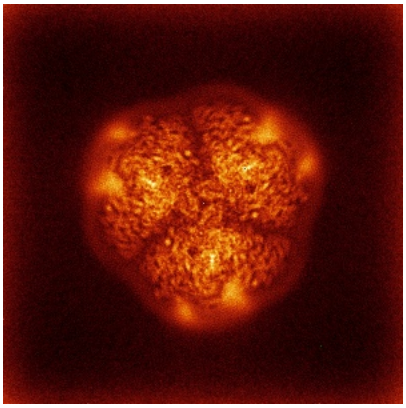

Y


Z

6.4.2 Raw map


X

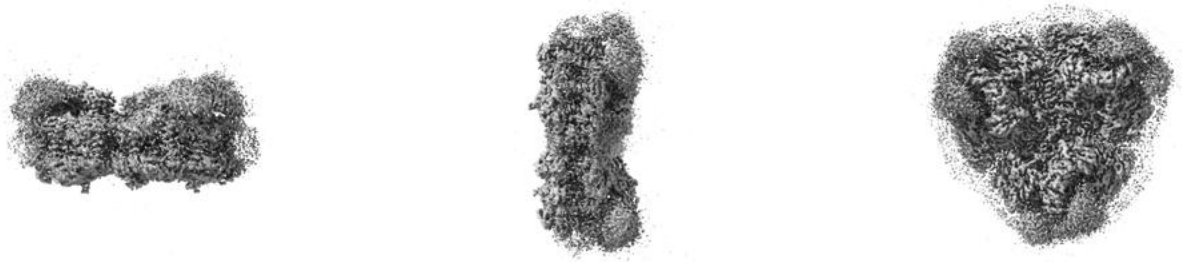

Y


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)

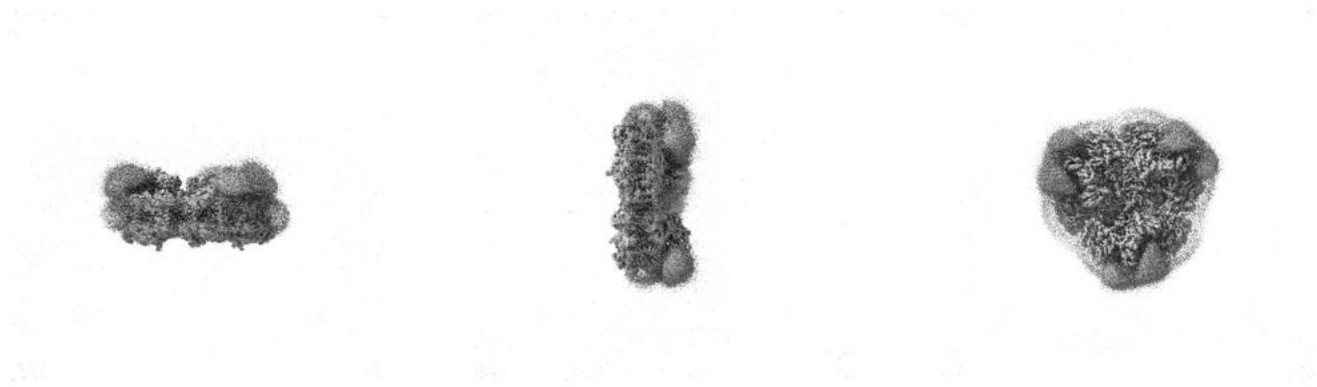
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

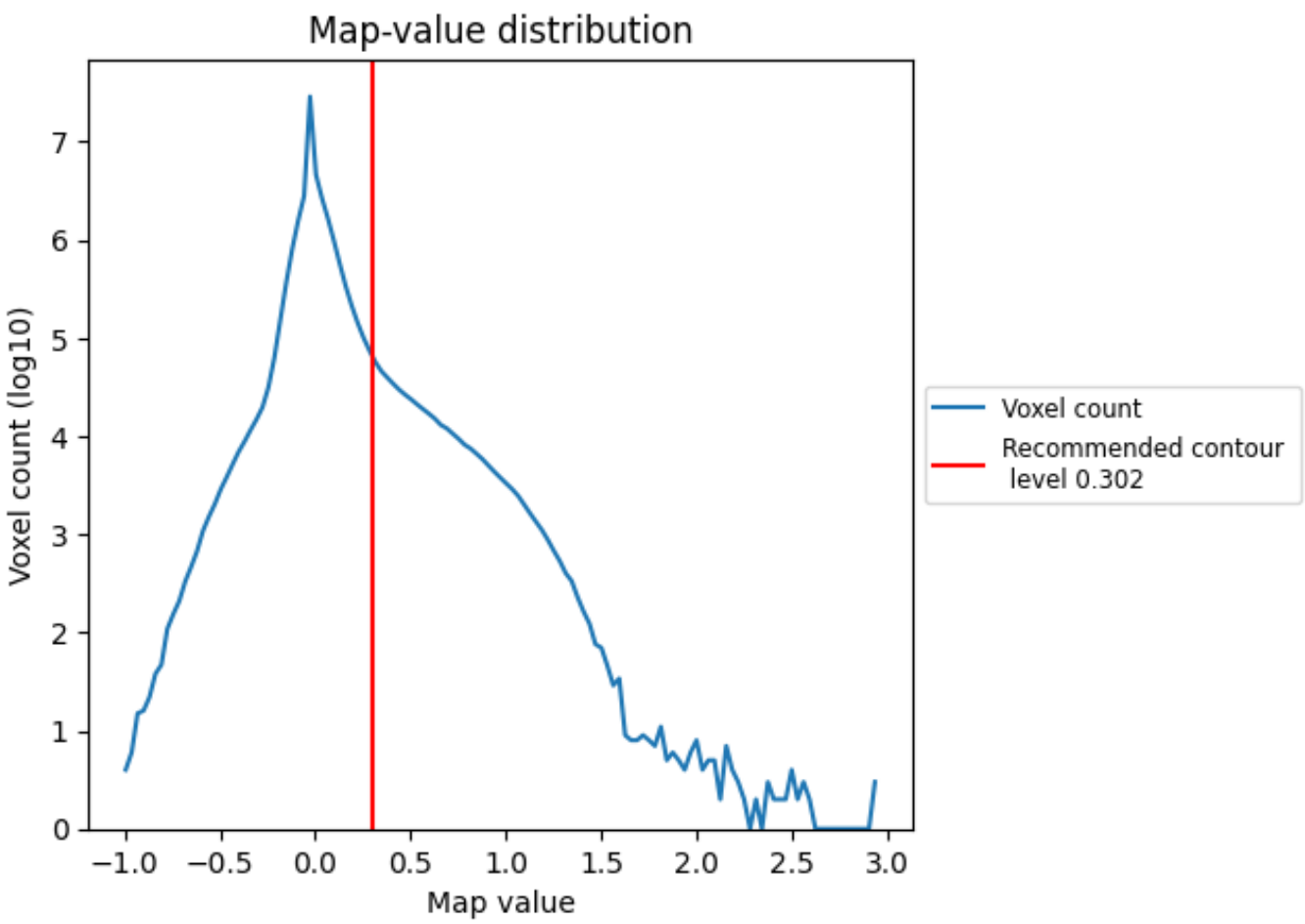
6.6 Mask visualisation (i)

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

7 Map analysis (i)

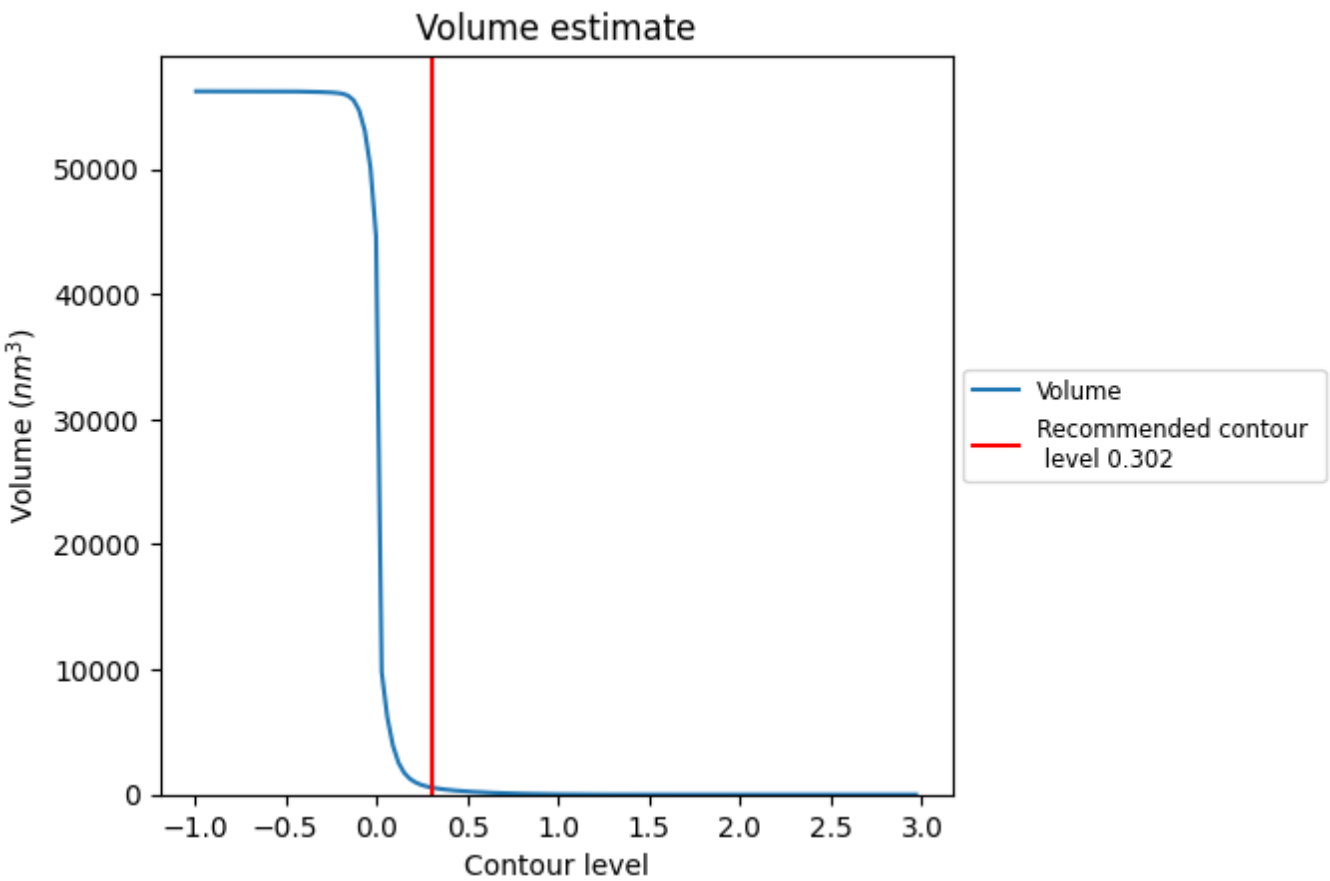
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

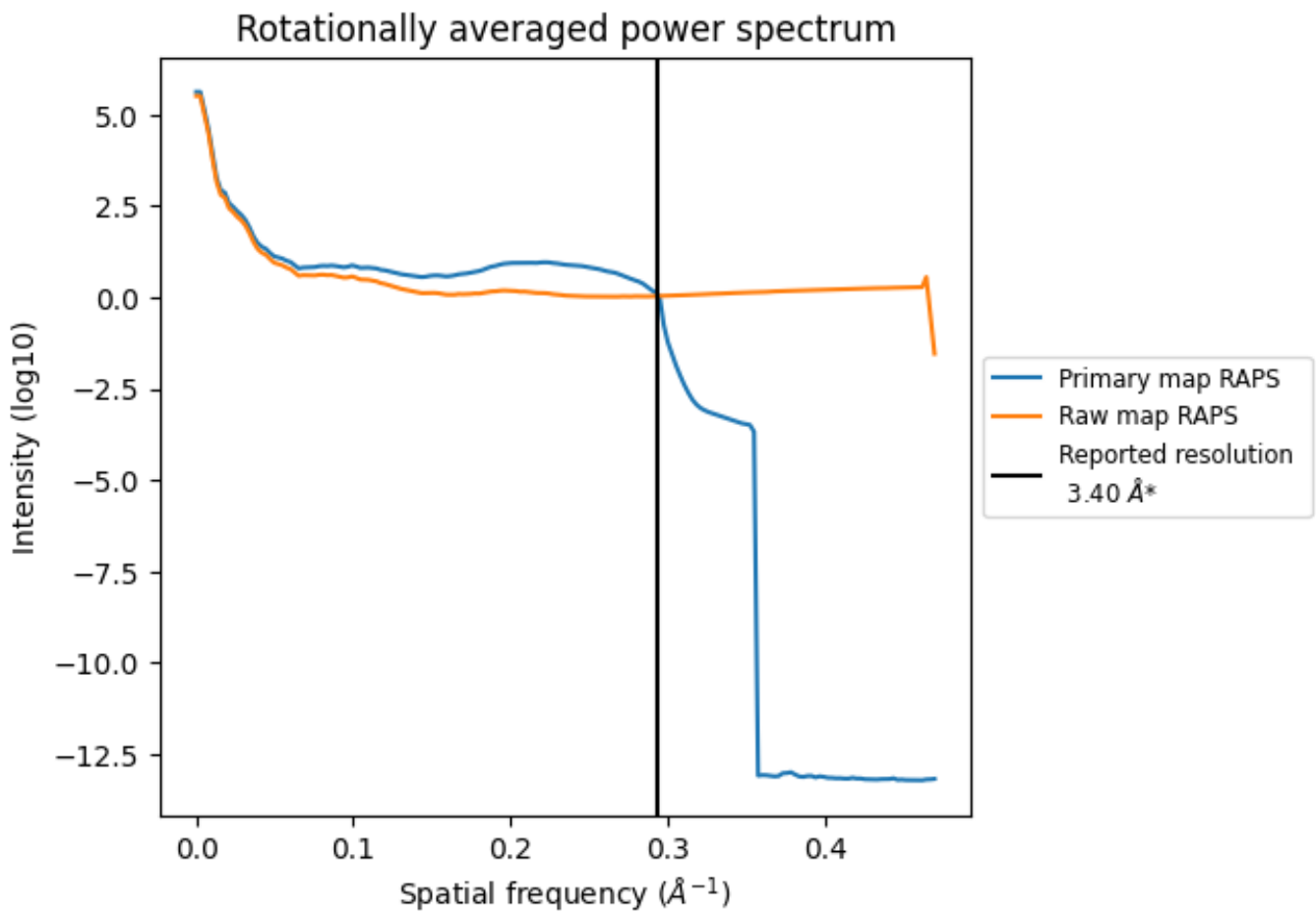
7.2 Volume estimate (i)



The volume at the recommended contour level is 563 nm^3; this corresponds to an approximate mass of 508 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)

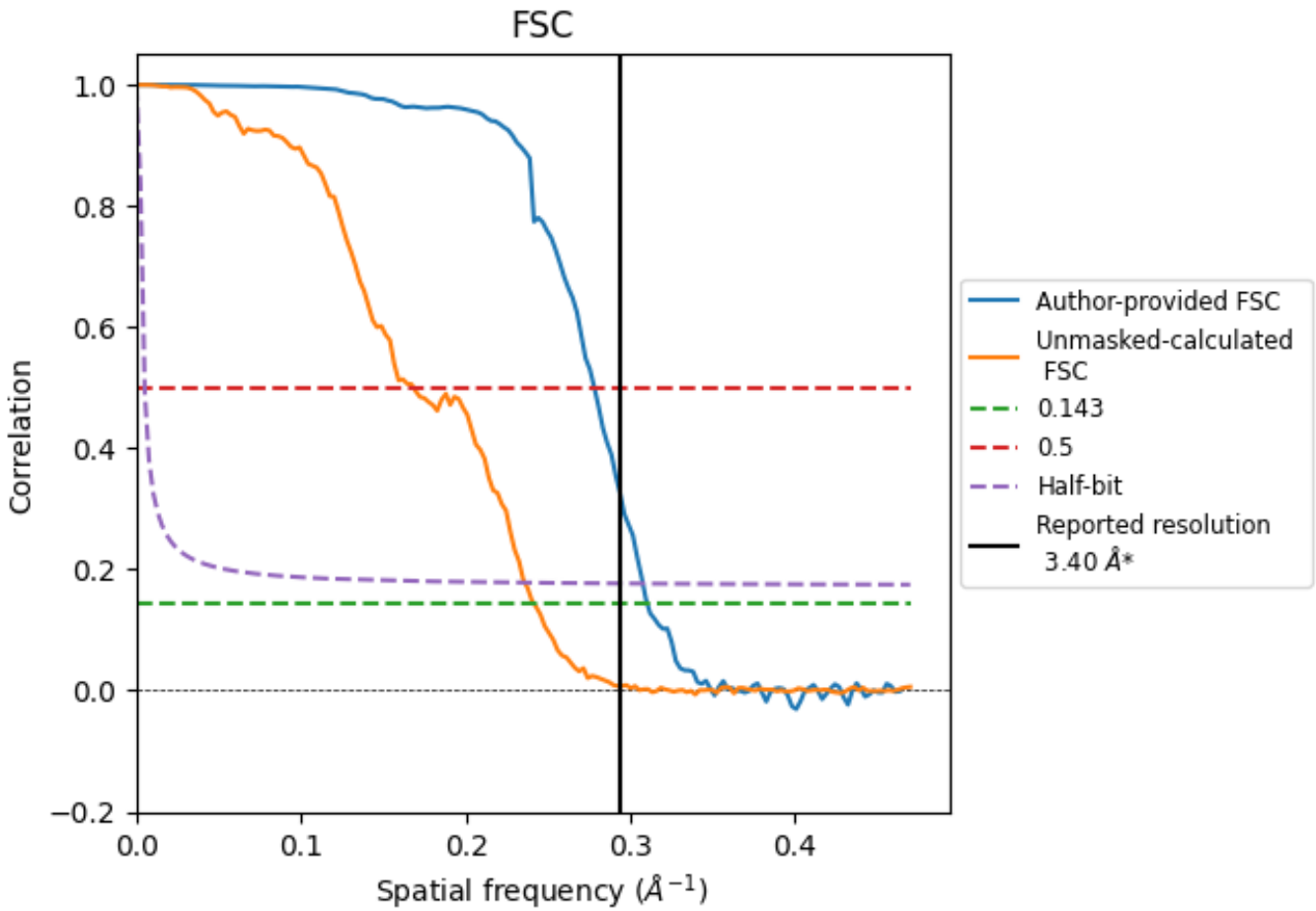


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

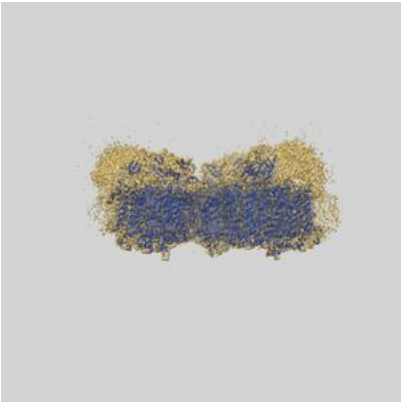
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.22	3.60	3.25
Unmasked-calculated*	4.14	5.94	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.4 by more than 10 %

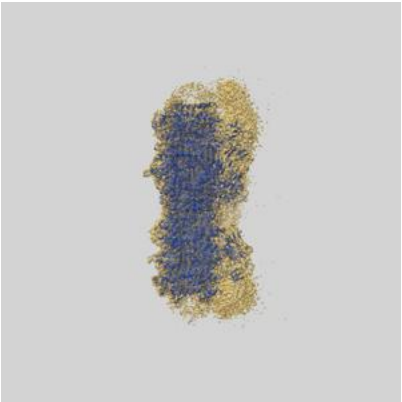
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-75106 and PDB model 10EG. Per-residue inclusion information can be found in section 3 on page 30.

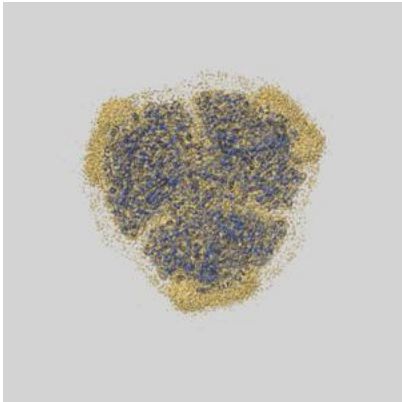
9.1 Map-model overlay (i)



X



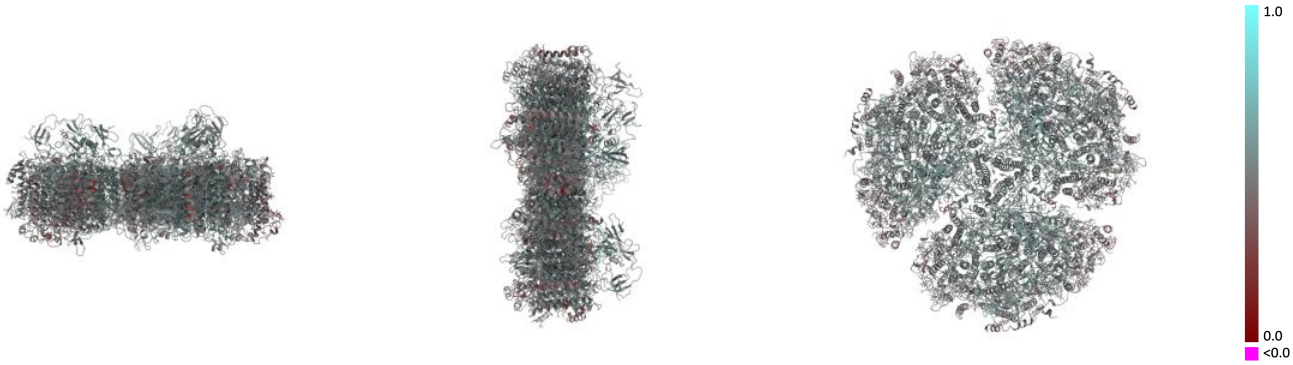
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.302 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.

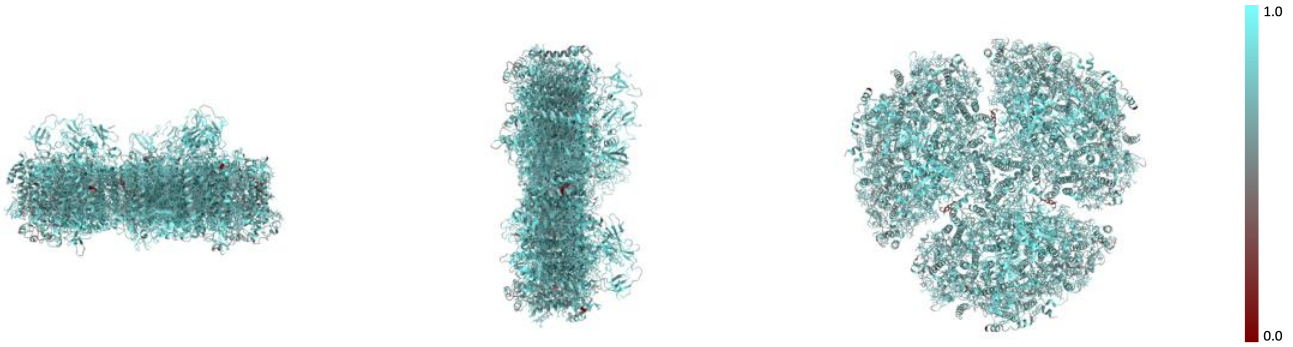
9.2 Q-score mapped to coordinate model (i)



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.

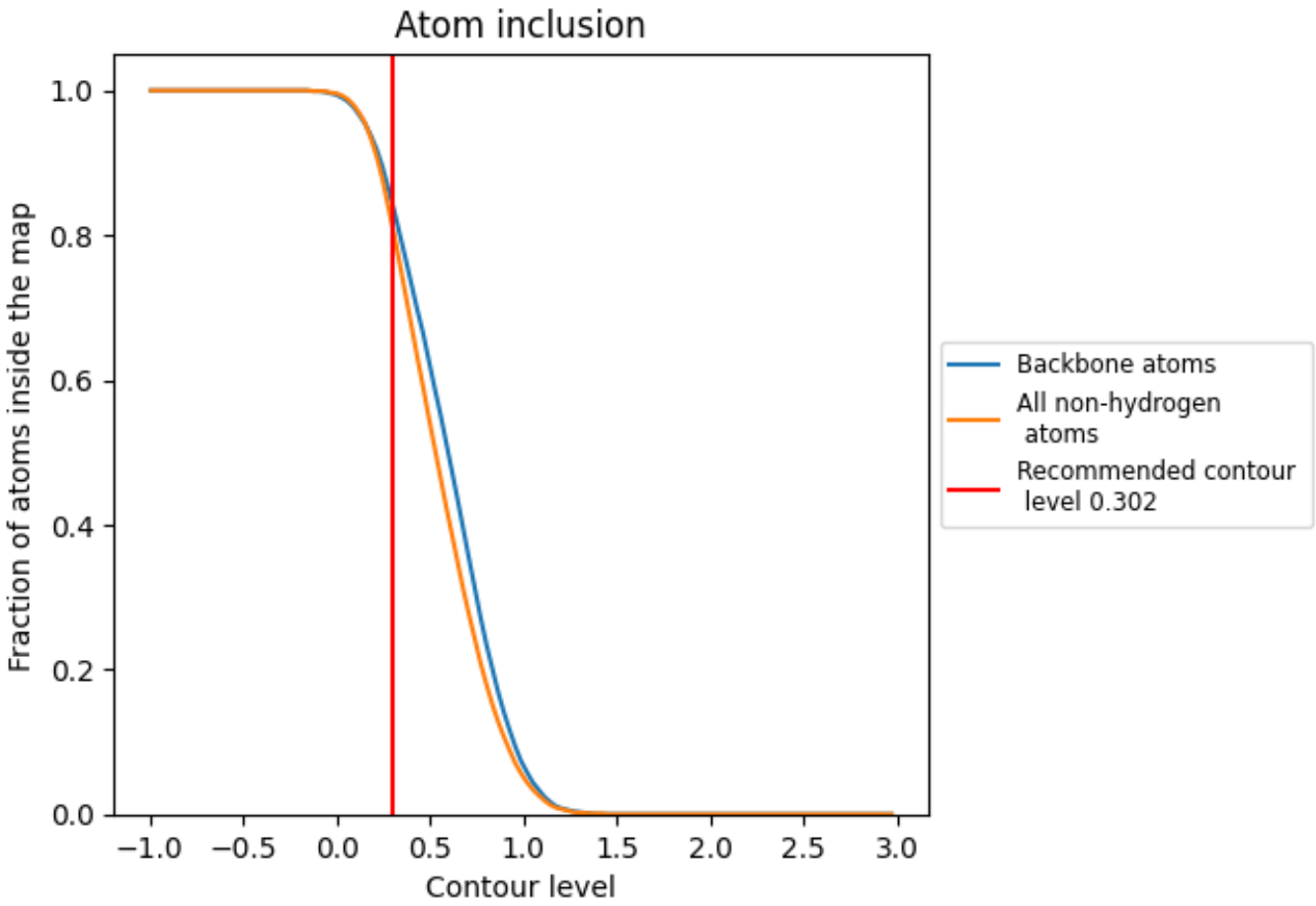
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.302).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.302) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.5100
A	0.8070	0.5070
B	0.8230	0.5160
C	0.8780	0.5320
D	0.8370	0.5340
E	0.7890	0.5190
F	0.6570	0.4680
G	0.8080	0.5080
H	0.8260	0.5150
I	0.8720	0.5510
J	0.7030	0.4820
K	0.6620	0.3960
L	0.8780	0.5490
M	0.7290	0.4810
N	0.8780	0.5320
O	0.8320	0.5280
P	0.8030	0.5170
Q	0.6620	0.4700
R	0.8870	0.5510
S	0.7080	0.4830
T	0.6600	0.3930
U	0.8720	0.5470
V	0.7390	0.4730
W	0.6480	0.4050
X	0.6590	0.4050
a	0.8060	0.5090
b	0.8220	0.5150
c	0.8780	0.5290
d	0.8320	0.5320
e	0.7930	0.5050
f	0.6630	0.4660
i	0.8810	0.5530
j	0.7060	0.4850
k	0.6630	0.3890
l	0.8730	0.5500

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Chain	Atom inclusion	Q-score
m	0.7470	0.4850
x	0.6400	0.4050