wwPDB EM Validation Summary Report (i)

Oct 27, 2024 – 05:55 PM JST

PDB ID	:	7FIX
EMDB ID	:	EMD-31605
Title	:	Cryo-EM structure of cyanobacterial photosystem I in the presence of ferredoxin and cytochrome c6
Authors	:	Li, J.; Kurisu, G.
Deposited on	:	2021-08-01
Resolution	:	1.97 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 (1)) were used in the production of this report:

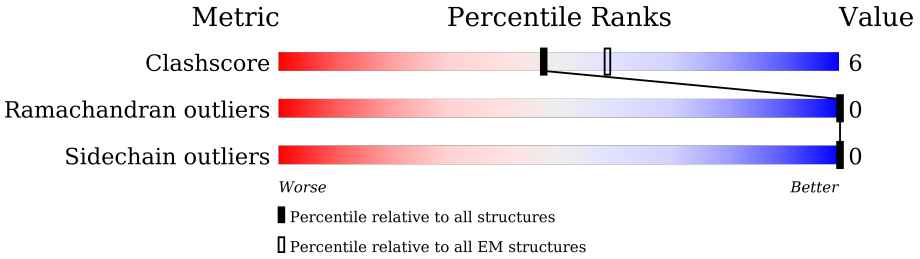
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.97 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A1	755	89% 10% •
1	A2	755	89% 10% •
1	A3	755	89% 9% •
2	B1	741	89% 11%
2	B2	741	88% 12%
2	B3	741	89% 11%
3	C1	81	93% 6% •
3	C2	81	91% 7% •

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Mol	Chain	Length	Quality of chain
3	C3	81	91% 7%
4	D1	139	94% 6%
4	D2	139	92% 7%
4	D3	139	94% 6%
5	E1	76	87% 9%
5	E2	76	87% 9%
5	E3	76	87% 9%
6	F1	174	74% 7% 19%
6	F2	174	74% 7% 19%
6	F3	174	74% 7% 19%
7	I1	38	84% 16%
7	I2	38	82% 18%
7	I3	38	84% 16%
8	J1	41	83% 17%
8	J2	41	78% 22%
8	J3	41	78% 22%
9	K1	83	90% 5% 5%
9	K2	83	90% 5% 5%
9	K3	83	90% 5% 5%
10	L1	155	90% 8%
10	L2	155	91% 7%
10	L3	155	90% 8%
11	M1	31	100%
11	M2	31	100%
11	M3	31	100%

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Mol	Chain	Length	Quality of chain
12	R1	98	56% 74% 24%
12	R2	98	50% 76% 23%
12	R3	98	51% 74% 24%
13	X1	39	67% 5% 28%
13	X2	39	67% 5% 28%
13	X3	39	67% 5% 28%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL0	A1	801	X	-	-	-
14	CL0	A2	801	X	-	-	-
14	CL0	A3	801	X	-	-	-
15	CLA	A1	802	X	-	-	-
15	CLA	A1	803	X	-	-	-
15	CLA	A1	804	X	-	-	-
15	CLA	A1	805	X	-	-	-
15	CLA	A1	806	X	-	-	-
15	CLA	A1	807	X	-	-	-
15	CLA	A1	808	X	-	-	-
15	CLA	A1	809	X	-	-	-
15	CLA	A1	810	X	-	-	-
15	CLA	A1	811	X	-	-	-
15	CLA	A1	812	X	-	-	-
15	CLA	A1	813	X	-	-	-
15	CLA	A1	814	X	-	-	-
15	CLA	A1	815	X	-	-	-
15	CLA	A1	816	X	-	-	-
15	CLA	A1	817	X	-	-	-
15	CLA	A1	818	X	-	-	-
15	CLA	A1	819	X	-	-	-
15	CLA	A1	820	X	-	-	-
15	CLA	A1	821	X	-	-	-
15	CLA	A1	822	X	-	-	-
15	CLA	A1	823	X	-	-	-
15	CLA	A1	824	X	-	-	-
15	CLA	A1	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A1	826	X	-	-	-
15	CLA	A1	827	X	-	-	-
15	CLA	A1	828	X	-	-	-
15	CLA	A1	829	X	-	-	-
15	CLA	A1	830	X	-	-	-
15	CLA	A1	831	X	-	-	-
15	CLA	A1	832	X	-	-	-
15	CLA	A1	833	X	-	-	-
15	CLA	A1	834	X	-	-	-
15	CLA	A1	835	X	-	-	-
15	CLA	A1	836	X	-	-	-
15	CLA	A1	837	X	-	-	-
15	CLA	A1	838	X	-	-	-
15	CLA	A1	839	X	-	-	-
15	CLA	A1	840	X	-	-	-
15	CLA	A1	841	X	-	-	-
15	CLA	A1	842	X	-	-	-
15	CLA	A1	843	X	-	-	-
15	CLA	A1	844	X	-	-	-
15	CLA	A1	856	X	-	-	-
15	CLA	A2	802	X	-	-	-
15	CLA	A2	803	X	-	-	-
15	CLA	A2	804	X	-	-	-
15	CLA	A2	805	X	-	-	-
15	CLA	A2	806	X	-	-	-
15	CLA	A2	807	X	-	-	-
15	CLA	A2	808	X	-	-	-
15	CLA	A2	809	X	-	-	-
15	CLA	A2	810	X	-	-	-
15	CLA	A2	811	X	-	-	-
15	CLA	A2	812	X	-	-	-
15	CLA	A2	813	X	-	-	-
15	CLA	A2	814	X	-	-	-
15	CLA	A2	815	X	-	-	-
15	CLA	A2	816	X	-	-	-
15	CLA	A2	817	X	-	-	-
15	CLA	A2	818	X	-	-	-
15	CLA	A2	819	X	-	-	-
15	CLA	A2	820	X	-	-	-
15	CLA	A2	821	X	-	-	-
15	CLA	A2	822	X	-	-	-
15	CLA	A2	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A2	824	X	-	-	-
15	CLA	A2	825	X	-	-	-
15	CLA	A2	826	X	-	-	-
15	CLA	A2	827	X	-	-	-
15	CLA	A2	828	X	-	-	-
15	CLA	A2	829	X	-	-	-
15	CLA	A2	830	X	-	-	-
15	CLA	A2	831	X	-	-	-
15	CLA	A2	832	X	-	-	-
15	CLA	A2	833	X	-	-	-
15	CLA	A2	834	X	-	-	-
15	CLA	A2	835	X	-	-	-
15	CLA	A2	836	X	-	-	-
15	CLA	A2	837	X	-	-	-
15	CLA	A2	838	X	-	-	-
15	CLA	A2	839	X	-	-	-
15	CLA	A2	840	X	-	-	-
15	CLA	A2	841	X	-	-	-
15	CLA	A2	842	X	-	-	-
15	CLA	A2	843	X	-	-	-
15	CLA	A2	844	X	-	-	-
15	CLA	A2	856	X	-	-	-
15	CLA	A3	802	X	-	-	-
15	CLA	A3	803	X	-	-	-
15	CLA	A3	804	X	-	-	-
15	CLA	A3	805	X	-	-	-
15	CLA	A3	806	X	-	-	-
15	CLA	A3	807	X	-	-	-
15	CLA	A3	808	X	-	-	-
15	CLA	A3	809	X	-	-	-
15	CLA	A3	810	X	-	-	-
15	CLA	A3	811	X	-	-	-
15	CLA	A3	812	X	-	-	-
15	CLA	A3	813	X	-	-	-
15	CLA	A3	814	X	-	-	-
15	CLA	A3	815	X	-	-	-
15	CLA	A3	816	X	-	-	-
15	CLA	A3	817	X	-	-	-
15	CLA	A3	818	X	-	-	-
15	CLA	A3	819	X	-	-	-
15	CLA	A3	820	X	-	-	-
15	CLA	A3	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A3	822	X	-	-	-
15	CLA	A3	823	X	-	-	-
15	CLA	A3	824	X	-	-	-
15	CLA	A3	825	X	-	-	-
15	CLA	A3	826	X	-	-	-
15	CLA	A3	827	X	-	-	-
15	CLA	A3	828	X	-	-	-
15	CLA	A3	829	X	-	-	-
15	CLA	A3	830	X	-	-	-
15	CLA	A3	831	X	-	-	-
15	CLA	A3	832	X	-	-	-
15	CLA	A3	833	X	-	-	-
15	CLA	A3	834	X	-	-	-
15	CLA	A3	835	X	-	-	-
15	CLA	A3	836	X	-	-	-
15	CLA	A3	837	X	-	-	-
15	CLA	A3	838	X	-	-	-
15	CLA	A3	839	X	-	-	-
15	CLA	A3	840	X	-	-	-
15	CLA	A3	841	X	-	-	-
15	CLA	A3	842	X	-	-	-
15	CLA	A3	843	X	-	-	-
15	CLA	A3	844	X	-	-	-
15	CLA	A3	856	X	-	-	-
15	CLA	B1	801	X	-	-	-
15	CLA	B1	802	X	-	-	-
15	CLA	B1	803	X	-	-	-
15	CLA	B1	804	X	-	-	-
15	CLA	B1	805	X	-	-	-
15	CLA	B1	806	X	-	-	-
15	CLA	B1	807	X	-	-	-
15	CLA	B1	808	X	-	-	-
15	CLA	B1	809	X	-	-	-
15	CLA	B1	810	X	-	-	-
15	CLA	B1	811	X	-	-	-
15	CLA	B1	812	X	-	-	-
15	CLA	B1	813	X	-	-	-
15	CLA	B1	814	X	-	-	-
15	CLA	B1	815	X	-	-	-
15	CLA	B1	816	X	-	-	-
15	CLA	B1	817	X	-	-	-
15	CLA	B1	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B1	819	X	-	-	-
15	CLA	B1	820	X	-	-	-
15	CLA	B1	821	X	-	-	-
15	CLA	B1	822	X	-	-	-
15	CLA	B1	823	X	-	-	-
15	CLA	B1	824	X	-	-	-
15	CLA	B1	825	X	-	-	-
15	CLA	B1	826	X	-	-	-
15	CLA	B1	827	X	-	-	-
15	CLA	B1	828	X	-	-	-
15	CLA	B1	829	X	-	-	-
15	CLA	B1	830	X	-	-	-
15	CLA	B1	831	X	-	-	-
15	CLA	B1	832	X	-	-	-
15	CLA	B1	833	X	-	-	-
15	CLA	B1	834	X	-	-	-
15	CLA	B1	835	X	-	-	-
15	CLA	B1	836	X	-	-	-
15	CLA	B1	837	X	-	-	-
15	CLA	B1	838	X	-	-	-
15	CLA	B1	839	X	-	-	-
15	CLA	B1	849	X	-	-	-
15	CLA	B2	801	X	-	-	-
15	CLA	B2	802	X	-	-	-
15	CLA	B2	803	X	-	-	-
15	CLA	B2	804	X	-	-	-
15	CLA	B2	805	X	-	-	-
15	CLA	B2	806	X	-	-	-
15	CLA	B2	807	X	-	-	-
15	CLA	B2	808	X	-	-	-
15	CLA	B2	809	X	-	-	-
15	CLA	B2	810	X	-	-	-
15	CLA	B2	811	X	-	-	-
15	CLA	B2	812	X	-	-	-
15	CLA	B2	813	X	-	-	-
15	CLA	B2	814	X	-	-	-
15	CLA	B2	815	X	-	-	-
15	CLA	B2	816	X	-	-	-
15	CLA	B2	817	X	-	-	-
15	CLA	B2	818	X	-	-	-
15	CLA	B2	819	X	-	-	-
15	CLA	B2	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B2	821	X	-	-	-
15	CLA	B2	822	X	-	-	-
15	CLA	B2	823	X	-	-	-
15	CLA	B2	824	X	-	-	-
15	CLA	B2	825	X	-	-	-
15	CLA	B2	826	X	-	-	-
15	CLA	B2	827	X	-	-	-
15	CLA	B2	828	X	-	-	-
15	CLA	B2	829	X	-	-	-
15	CLA	B2	830	X	-	-	-
15	CLA	B2	831	X	-	-	-
15	CLA	B2	832	X	-	-	-
15	CLA	B2	833	X	-	-	-
15	CLA	B2	834	X	-	-	-
15	CLA	B2	835	X	-	-	-
15	CLA	B2	836	X	-	-	-
15	CLA	B2	837	X	-	-	-
15	CLA	B2	838	X	-	-	-
15	CLA	B2	839	X	-	-	-
15	CLA	B2	849	X	-	-	-
15	CLA	B3	801	X	-	-	-
15	CLA	B3	802	X	-	-	-
15	CLA	B3	803	X	-	-	-
15	CLA	B3	804	X	-	-	-
15	CLA	B3	805	X	-	-	-
15	CLA	B3	806	X	-	-	-
15	CLA	B3	807	X	-	-	-
15	CLA	B3	808	X	-	-	-
15	CLA	B3	809	X	-	-	-
15	CLA	B3	810	X	-	-	-
15	CLA	B3	811	X	-	-	-
15	CLA	B3	812	X	-	-	-
15	CLA	B3	813	X	-	-	-
15	CLA	B3	814	X	-	-	-
15	CLA	B3	815	X	-	-	-
15	CLA	B3	816	X	-	-	-
15	CLA	B3	817	X	-	-	-
15	CLA	B3	818	X	-	-	-
15	CLA	B3	819	X	-	-	-
15	CLA	B3	820	X	-	-	-
15	CLA	B3	821	X	-	-	-
15	CLA	B3	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B3	823	X	-	-	-
15	CLA	B3	824	X	-	-	-
15	CLA	B3	825	X	-	-	-
15	CLA	B3	826	X	-	-	-
15	CLA	B3	827	X	-	-	-
15	CLA	B3	828	X	-	-	-
15	CLA	B3	829	X	-	-	-
15	CLA	B3	830	X	-	-	-
15	CLA	B3	831	X	-	-	-
15	CLA	B3	832	X	-	-	-
15	CLA	B3	833	X	-	-	-
15	CLA	B3	834	X	-	-	-
15	CLA	B3	835	X	-	-	-
15	CLA	B3	836	X	-	-	-
15	CLA	B3	837	X	-	-	-
15	CLA	B3	838	X	-	-	-
15	CLA	B3	839	X	-	-	-
15	CLA	B3	849	X	-	-	-
15	CLA	I1	101	X	-	-	-
15	CLA	I2	101	X	-	-	-
15	CLA	I3	101	X	-	-	-
15	CLA	J1	1301	X	-	-	-
15	CLA	J1	1302	X	-	-	-
15	CLA	J1	1303	X	-	-	-
15	CLA	J1	1307	X	-	-	-
15	CLA	J2	1301	X	-	-	-
15	CLA	J2	1302	X	-	-	-
15	CLA	J2	1303	X	-	-	-
15	CLA	J2	1307	X	-	-	-
15	CLA	J3	1301	X	-	-	-
15	CLA	J3	1302	X	-	-	-
15	CLA	J3	1303	X	-	-	-
15	CLA	J3	1307	X	-	-	-
15	CLA	K1	101	X	-	-	-
15	CLA	K1	103	X	-	-	-
15	CLA	K2	101	X	-	-	-
15	CLA	K2	103	X	-	-	-
15	CLA	K3	101	X	-	-	-
15	CLA	K3	103	X	-	-	-
15	CLA	L1	1002	X	-	-	-
15	CLA	L1	1003	X	-	-	-
15	CLA	L1	1004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	L2	1002	X	-	-	-
15	CLA	L2	1003	X	-	-	-
15	CLA	L2	1004	X	-	-	-
15	CLA	L3	1002	X	-	-	-
15	CLA	L3	1003	X	-	-	-
15	CLA	L3	1004	X	-	-	-
15	CLA	X1	102	X	-	-	-
15	CLA	X2	102	X	-	-	-
15	CLA	X3	102	X	-	-	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 73929 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	A1	745	5676	3708	990	952	26	0	0
1	A2	745	5676	3708	990	952	26	0	0
1	A3	745	5676	3708	990	952	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	B1	740	5853	3853	984	995	21	0	0
2	B2	740	5853	3853	984	995	21	0	0
2	B3	740	5853	3853	984	995	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	C1	80	598	367	103	117	11	0	0
3	C2	80	598	367	103	117	11	0	0
3	C3	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	D1	138	1067	677	185	202	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D2	138	1067	677	185	202	3	0	0
4	D3	138	1067	677	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	E1	69	532	339	93	100	0	0
5	E2	69	532	339	93	100	0	0
5	E3	69	532	339	93	100	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	F1	141	1038	667	183	184	4	0	0
6	F2	141	1038	667	183	184	4	0	0
6	F3	141	1038	667	183	184	4	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	-9	HIS	-	expression tag	UNP P0A401
F1	-8	HIS	-	expression tag	UNP P0A401
F1	-7	HIS	-	expression tag	UNP P0A401
F1	-6	HIS	-	expression tag	UNP P0A401
F1	-5	HIS	-	expression tag	UNP P0A401
F1	-4	HIS	-	expression tag	UNP P0A401
F1	-3	HIS	-	expression tag	UNP P0A401
F1	-2	HIS	-	expression tag	UNP P0A401
F1	-1	HIS	-	expression tag	UNP P0A401
F1	0	HIS	-	expression tag	UNP P0A401
F2	-9	HIS	-	expression tag	UNP P0A401
F2	-8	HIS	-	expression tag	UNP P0A401
F2	-7	HIS	-	expression tag	UNP P0A401
F2	-6	HIS	-	expression tag	UNP P0A401

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Chain	Residue	Modelled	Actual	Comment	Reference
F2	-5	HIS	-	expression tag	UNP P0A401
F2	-4	HIS	-	expression tag	UNP P0A401
F2	-3	HIS	-	expression tag	UNP P0A401
F2	-2	HIS	-	expression tag	UNP P0A401
F2	-1	HIS	-	expression tag	UNP P0A401
F2	0	HIS	-	expression tag	UNP P0A401
F3	-9	HIS	-	expression tag	UNP P0A401
F3	-8	HIS	-	expression tag	UNP P0A401
F3	-7	HIS	-	expression tag	UNP P0A401
F3	-6	HIS	-	expression tag	UNP P0A401
F3	-5	HIS	-	expression tag	UNP P0A401
F3	-4	HIS	-	expression tag	UNP P0A401
F3	-3	HIS	-	expression tag	UNP P0A401
F3	-2	HIS	-	expression tag	UNP P0A401
F3	-1	HIS	-	expression tag	UNP P0A401
F3	0	HIS	-	expression tag	UNP P0A401

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I1	38	301	208	40	48	5	0	0
7	I2	38	301	208	40	48	5	0	0
7	I3	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	J1	41	337	231	51	53	2	0	0
8	J2	41	337	231	51	53	2	0	0
8	J3	41	337	231	51	53	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	S		
9	K1	79	483	306	84	92	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K2	79	483	306	84	92	1	0	0
9	K3	79	483	306	84	92	1	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	L1	152	1121	736	180	201	4	0	0
10	L2	152	1121	736	180	201	4	0	0
10	L3	152	1121	736	180	201	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M1	31	241	161	36	43	1	0	0
11	M2	31	241	161	36	43	1	0	0
11	M3	31	241	161	36	43	1	0	0

- Molecule 12 is a protein called Ferredoxin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R1	97	748	463	116	164	5	0	0
12	R2	97	748	463	116	164	5	0	0
12	R3	97	748	463	116	164	5	0	0

- Molecule 13 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	X1	28	225	159	33	33	0	0
13	X2	28	225	159	33	33	0	0

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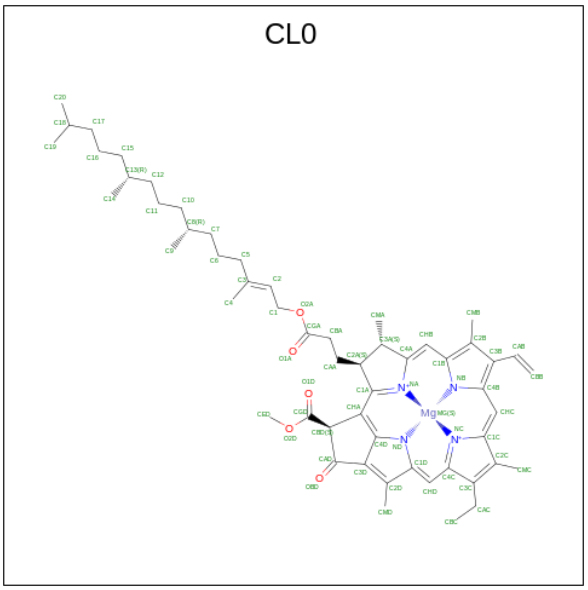
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	X3	28	225	159	33	33	0	0

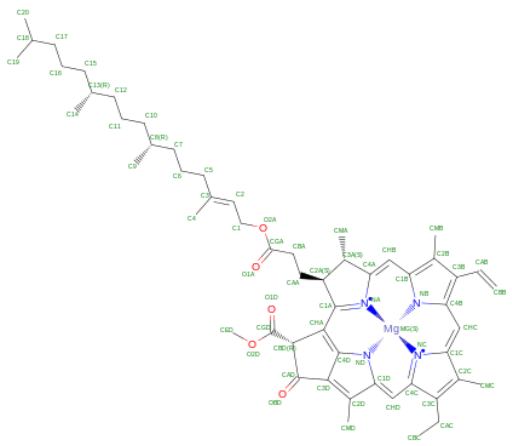
- Molecule 14 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
14	A3	1	65	55	1	4	5	0

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).

CLA



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A1	1	65	55	1	4	5	0
15	A1	1	64	54	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	A1	1	44	34	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	A1	1	38	30	1	4	3	0
15	A1	1	65	55	1	4	5	0
15	A1	1	40	32	1	4	3	0
15	A1	1	44	34	1	4	5	0
15	A1	1	33	27	1	4	1	0
15	A1	1	36	28	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A1	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A1	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
15	A1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A1	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A1	1	50	40	1	4	5	0
15	A1	1	55	45	1	4	5	0
15	A1	1	55	45	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	A1	1	40	32	1	4	3	0
15	A1	1	65	55	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	A1	1	45	35	1	4	5	0
15	A1	1	65	55	1	4	5	0
15	B1	1	65	55	1	4	5	0
15	B1	1	65	55	1	4	5	0
15	B1	1	54	44	1	4	5	0
15	B1	1	55	45	1	4	5	0
15	B1	1	65	55	1	4	5	0
15	B1	1	50	40	1	4	5	0
15	B1	1	60	50	1	4	5	0
15	B1	1	65	55	1	4	5	0
15	B1	1	65	55	1	4	5	0
15	B1	1	44	34	1	4	5	0
15	B1	1	45	35	1	4	5	0
15	B1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	B1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	B1	1	38	31	1	4	2	0
			Total	C	Mg	N	O	
15	B1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	B1	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	35	29	1	4	1	0
			Total	C	Mg	N	O	
15	B1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	37	31	1	4	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	B1	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	I1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	J1	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	J1	1	35	29	1	4	1	0
			Total	C	Mg	N	O	
15	J1	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	J1	1	34	28	1	4	1	0
			Total	C	Mg	N	O	
15	K1	1	34	28	1	4	1	0
			Total	C	Mg	N	O	
15	K1	1	32	26	1	4	1	0
			Total	C	Mg	N	O	
15	L1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	L1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	L1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	X1	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	33	27	1	4	1	0
			Total	C	Mg	N	O	
15	A2	1	36	28	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	B2	1	38	31	1	4	2	0
			Total	C	Mg	N	O	
15	B2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	B2	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	40	32	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	B2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	35	29	1	4	1	0
			Total	C	Mg	N	O	
15	B2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	37	31	1	4	1	0
			Total	C	Mg	N	O	
15	B2	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	I2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	J2	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	J2	1	35	29	1	4	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	J2	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	J2	1	34	28	1	4	1	0
			Total	C	Mg	N	O	
15	K2	1	34	28	1	4	1	0
			Total	C	Mg	N	O	
15	K2	1	32	26	1	4	1	0
			Total	C	Mg	N	O	
15	L2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	L2	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	L2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	X2	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	33	27	1	4	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A3	1	36	28	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	A3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B3	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	B3	1	38	31	1	4	2	0
			Total	C	Mg	N	O	
15	B3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
15	B3	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
15	B3	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
15	B3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B3	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
15	B3	1	35	29	1	4	1	0
			Total	C	Mg	N	O	
15	B3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
15	B3	1	40	32	1	4	3	0

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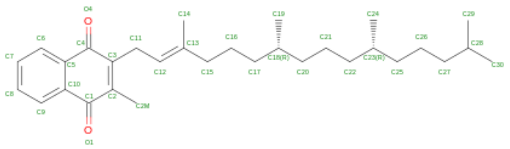
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	B3	1	37	31	1	4	1	0
15	B3	1	39	31	1	4	3	0
15	B3	1	46	36	1	4	5	0
15	B3	1	45	35	1	4	5	0
15	B3	1	41	33	1	4	3	0
15	B3	1	65	55	1	4	5	0
15	B3	1	65	55	1	4	5	0
15	B3	1	45	35	1	4	5	0
15	I3	1	65	55	1	4	5	0
15	J3	1	38	30	1	4	3	0
15	J3	1	35	29	1	4	1	0
15	J3	1	36	30	1	4	1	0
15	J3	1	34	28	1	4	1	0
15	K3	1	34	28	1	4	1	0
15	K3	1	32	26	1	4	1	0
15	L3	1	65	55	1	4	5	0
15	L3	1	60	50	1	4	5	0
15	L3	1	65	55	1	4	5	0
15	X3	1	40	32	1	4	3	0

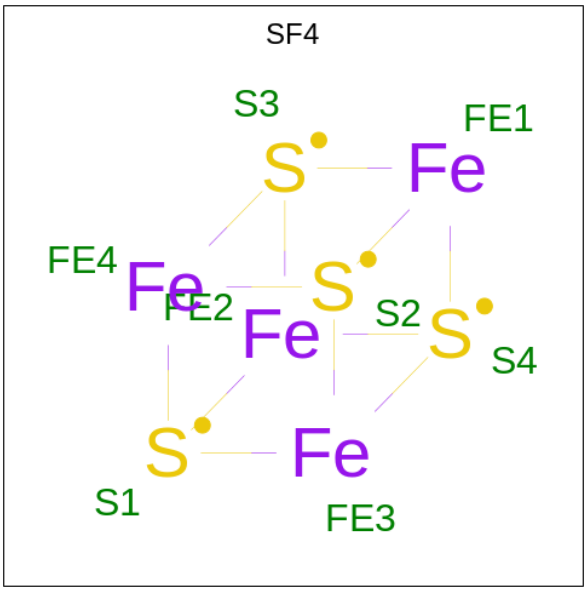
- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).

PQN



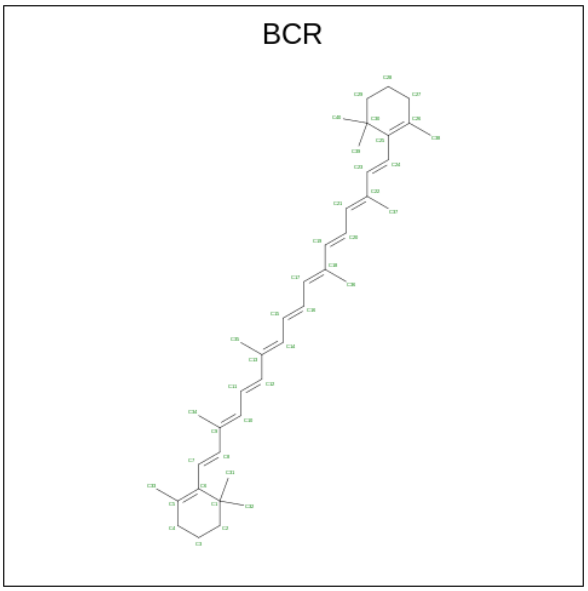
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	A1	1	33	31	2	0
16	B1	1	33	31	2	0
16	A2	1	33	31	2	0
16	B2	1	33	31	2	0
16	A3	1	33	31	2	0
16	B3	1	33	31	2	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	A1	1	8	4	4	0
17	C1	1	8	4	4	0
17	C1	1	8	4	4	0
17	A2	1	8	4	4	0
17	C2	1	8	4	4	0
17	C2	1	8	4	4	0
17	A3	1	8	4	4	0
17	C3	1	8	4	4	0
17	C3	1	8	4	4	0

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
18	A1	1	40	40	0
			Total	C	
18	A1	1	40	40	0
			Total	C	
18	A1	1	40	40	0
			Total	C	
18	A1	1	40	40	0
			Total	C	
18	A1	1	40	40	0
			Total	C	
18	A1	1	40	40	0
			Total	C	
18	A1	1	30	30	0
			Total	C	
18	B1	1	40	40	0
			Total	C	
18	B1	1	30	30	0
			Total	C	
18	B1	1	25	25	0
			Total	C	
18	B1	1	40	40	0
			Total	C	
18	B1	1	40	40	0
			Total	C	
18	B1	1	40	40	0
			Total	C	
18	B1	1	40	40	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
18	F1	1	40	40	0
			Total	C	
18	I1	1	40	40	0
			Total	C	
18	I1	1	40	40	0
			Total	C	
18	J1	1	40	40	0
			Total	C	
18	J1	1	40	40	0
			Total	C	
18	J1	1	40	40	0
			Total	C	
18	K1	1	25	25	0
			Total	C	
18	L1	1	40	40	0
			Total	C	
18	L1	1	40	40	0
			Total	C	
18	L1	1	40	40	0
			Total	C	
18	M1	1	40	40	0
			Total	C	
18	A2	1	40	40	0
			Total	C	
18	A2	1	40	40	0
			Total	C	
18	A2	1	40	40	0
			Total	C	
18	A2	1	40	40	0
			Total	C	
18	A2	1	40	40	0
			Total	C	
18	A2	1	40	40	0
			Total	C	
18	A2	1	30	30	0
			Total	C	
18	B2	1	40	40	0
			Total	C	
18	B2	1	30	30	0
			Total	C	
18	B2	1	25	25	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
18	B2	1	40	40	0
			Total	C	
18	B2	1	40	40	0
			Total	C	
18	B2	1	40	40	0
			Total	C	
18	B2	1	40	40	0
			Total	C	
18	F2	1	40	40	0
			Total	C	
18	I2	1	40	40	0
			Total	C	
18	I2	1	40	40	0
			Total	C	
18	J2	1	40	40	0
			Total	C	
18	J2	1	40	40	0
			Total	C	
18	J2	1	40	40	0
			Total	C	
18	K2	1	25	25	0
			Total	C	
18	L2	1	40	40	0
			Total	C	
18	L2	1	40	40	0
			Total	C	
18	M2	1	40	40	0
			Total	C	
18	A3	1	40	40	0
			Total	C	
18	A3	1	40	40	0
			Total	C	
18	A3	1	40	40	0
			Total	C	
18	A3	1	40	40	0
			Total	C	
18	A3	1	40	40	0
			Total	C	
18	A3	1	40	40	0
			Total	C	
18	A3	1	30	30	0

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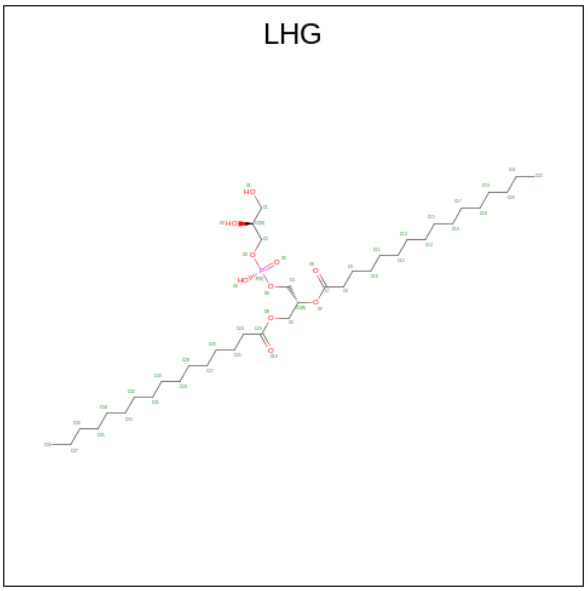
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
18	B3	1	40	40	0
			Total	C	
18	B3	1	30	30	0
			Total	C	
18	B3	1	25	25	0
			Total	C	
18	B3	1	40	40	0
			Total	C	
18	B3	1	40	40	0
			Total	C	
18	B3	1	40	40	0
			Total	C	
18	B3	1	40	40	0
			Total	C	
18	F3	1	40	40	0
			Total	C	
18	I3	1	40	40	0
			Total	C	
18	I3	1	40	40	0
			Total	C	
18	J3	1	40	40	0
			Total	C	
18	J3	1	40	40	0
			Total	C	
18	J3	1	40	40	0
			Total	C	
18	K3	1	25	25	0
			Total	C	
18	L3	1	40	40	0
			Total	C	
18	M3	1	40	40	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	A1	1	47	36	10	1	0
19	A1	1	35	24	10	1	0
19	X1	1	42	31	10	1	0
19	A2	1	47	36	10	1	0
19	A2	1	35	24	10	1	0
19	X2	1	42	31	10	1	0
19	A3	1	47	36	10	1	0
19	A3	1	35	24	10	1	0
19	X3	1	42	31	10	1	0

- Molecule 20 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	A1	7	97	97	0
20	I1	4	61	61	0

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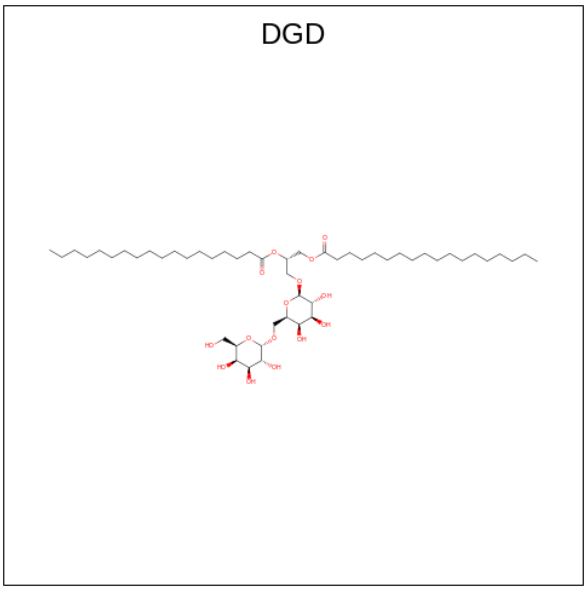
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	L1	4	64	64	0
			Total	C	
20	M1	2	32	32	0
			Total	C	
20	A2	7	97	97	0
			Total	C	
20	I2	4	61	61	0
			Total	C	
20	L2	4	64	64	0
			Total	C	
20	M2	2	32	32	0
			Total	C	
20	A3	7	97	97	0
			Total	C	
20	I3	4	61	61	0
			Total	C	
20	L3	4	64	64	0
			Total	C	
20	M3	2	32	32	0

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	B1	1	66	51	15	0

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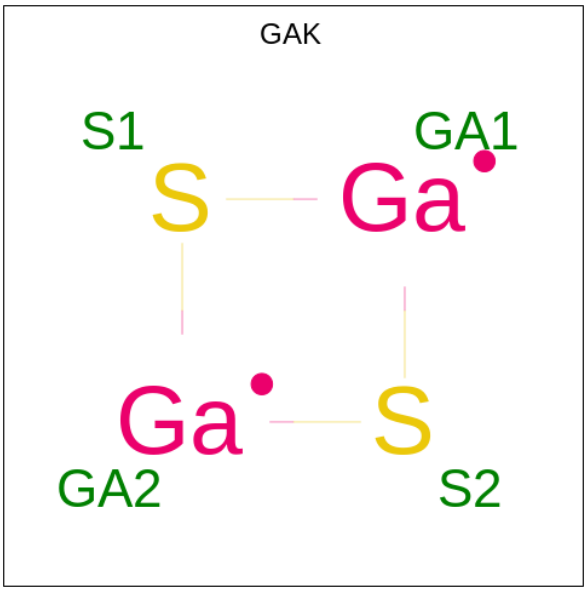
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	B2	1	66	51	15	0
21	B3	1	66	51	15	0

- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
22	L1	1	1	1	0
22	L2	1	1	1	0
22	L3	1	1	1	0

- Molecule 23 is [2Ga-2S] cluster (three-letter code: GAK) (formula: Ga_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Ga	S	
23	R1	1	4	2	2	0
23	R2	1	4	2	2	0
23	R3	1	4	2	2	0

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
24	A1	26	26	26	0
24	B1	42	42	42	0
24	C1	13	13	13	0
24	D1	7	7	7	0
24	E1	1	1	1	0
24	I1	1	1	1	0
24	L1	22	22	22	0
24	R1	4	4	4	0
24	A2	26	26	26	0
24	B2	42	42	42	0
24	C2	13	13	13	0
24	D2	7	7	7	0
24	E2	1	1	1	0
24	I2	1	1	1	0
24	L2	22	22	22	0
24	R2	4	4	4	0
24	A3	26	26	26	0
24	B3	42	42	42	0
24	C3	13	13	13	0
24	D3	7	7	7	0
24	E3	1	1	1	0

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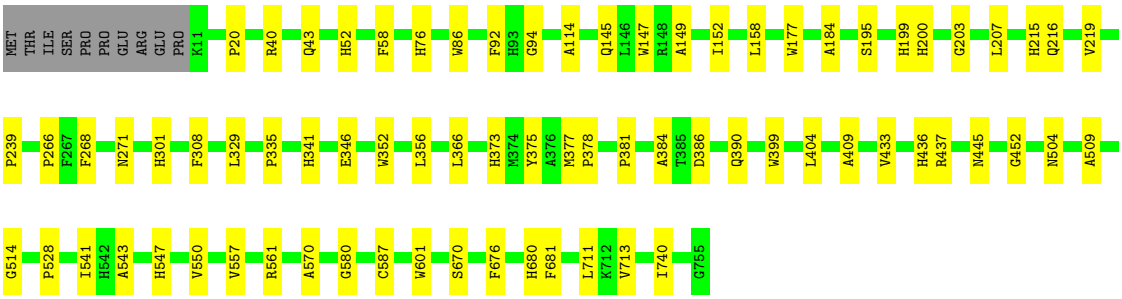
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
24	I3	1	1	1	0
			Total	O	
24	L3	22	22	22	0
			Total	O	
24	R3	4	4	4	0

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.

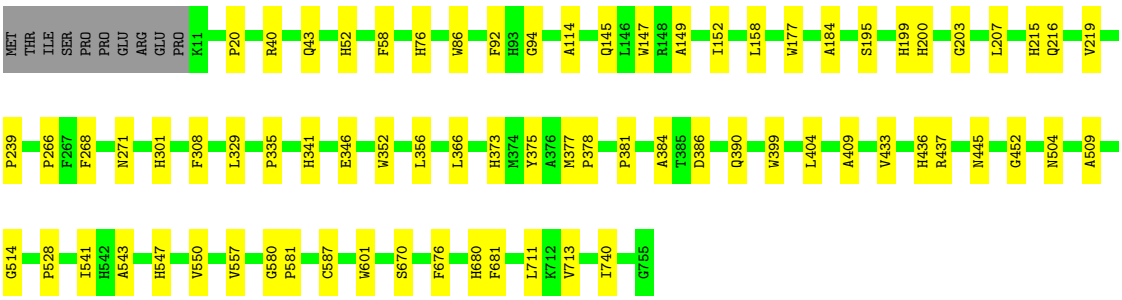
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A1:



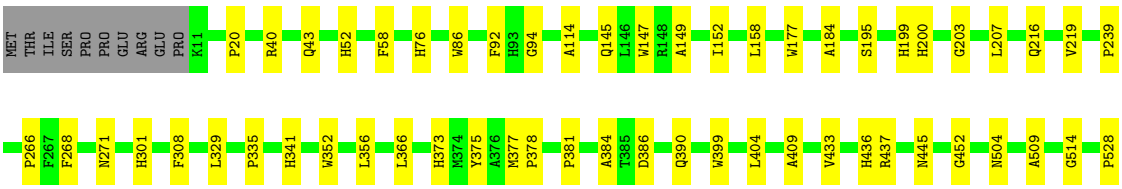
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A2:



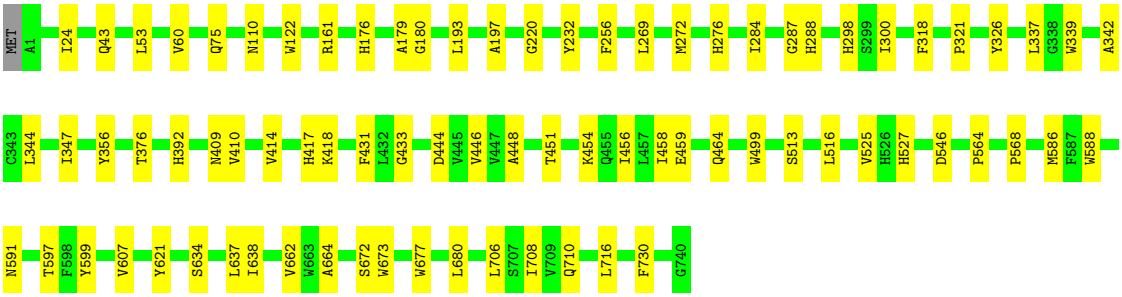
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A3:



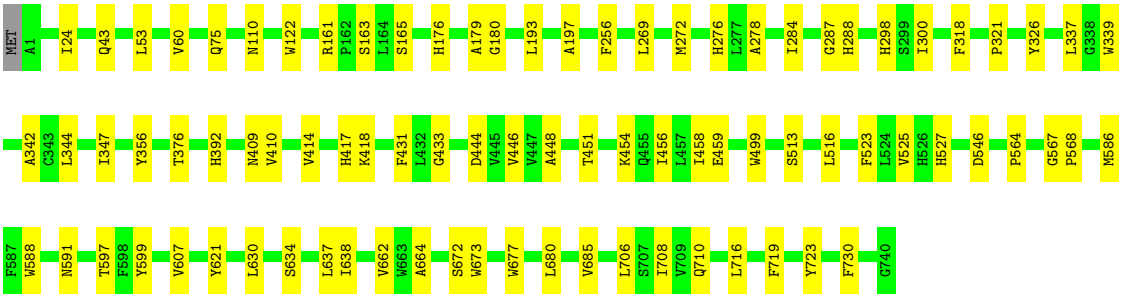
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B1: 89% 11%



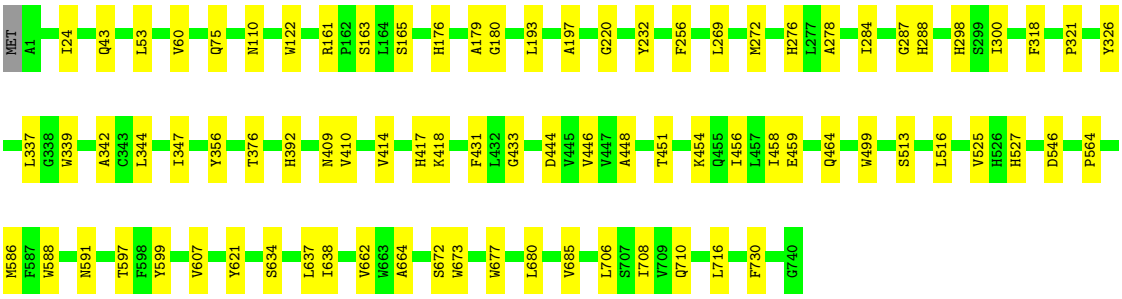
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B2: 88% 12%



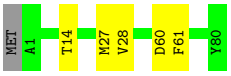
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B3: 89% 11%



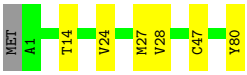
• Molecule 3: Photosystem I iron-sulfur center

Chain C1: 93% 6%



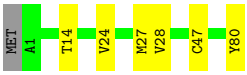
• Molecule 3: Photosystem I iron-sulfur center

Chain C2:



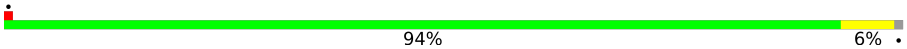
• Molecule 3: Photosystem I iron-sulfur center

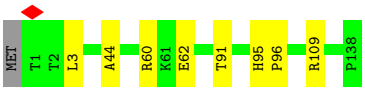
Chain C3:



• Molecule 4: Photosystem I reaction center subunit II

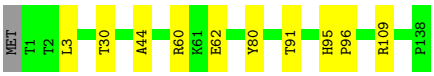
Chain D1:





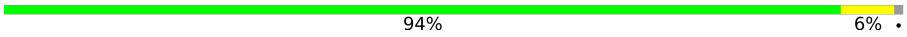
• Molecule 4: Photosystem I reaction center subunit II

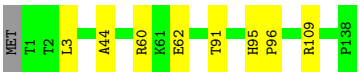
Chain D2:



• Molecule 4: Photosystem I reaction center subunit II

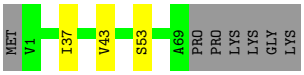
Chain D3:





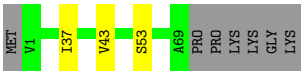
• Molecule 5: Photosystem I reaction center subunit IV

Chain E1:



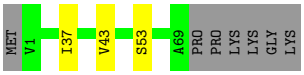
• Molecule 5: Photosystem I reaction center subunit IV

Chain E2:



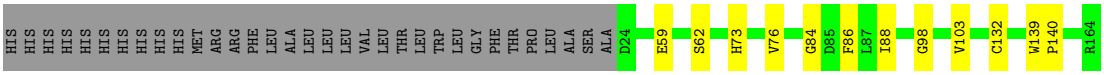
• Molecule 5: Photosystem I reaction center subunit IV

Chain E3:



• Molecule 6: Photosystem I reaction center subunit III

Chain F1:



• Molecule 6: Photosystem I reaction center subunit III

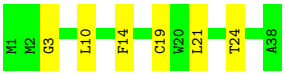
Chain F2:

• Molecule 6: Photosystem I reaction center subunit III

Chain F3:

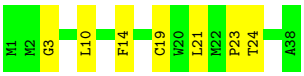
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain I2:

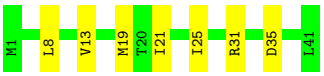


• Molecule 7: Photosystem I reaction center subunit VIII

Chain I3:

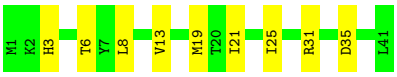
• Molecule 8: Photosystem I reaction center subunit IX

Chain J1:



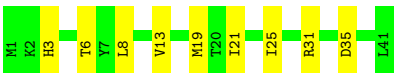
• Molecule 8: Photosystem I reaction center subunit IX

Chain J2:



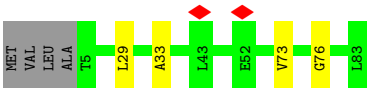
• Molecule 8: Photosystem I reaction center subunit IX

Chain J3:



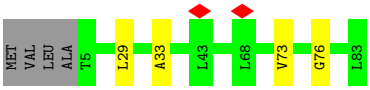
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K1:



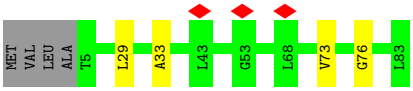
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K2:



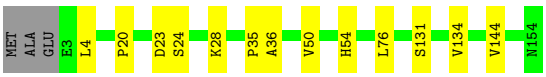
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K3:



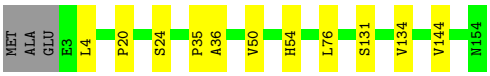
• Molecule 10: Photosystem I reaction center subunit XI

Chain L1:



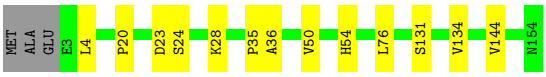
• Molecule 10: Photosystem I reaction center subunit XI

Chain L2: 91% 7%



• Molecule 10: Photosystem I reaction center subunit XI

Chain L3: 90% 8%



• Molecule 11: Photosystem I reaction center subunit XII

Chain M1: 100%

There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem I reaction center subunit XII

Chain M2: 100%

There are no outlier residues recorded for this chain.

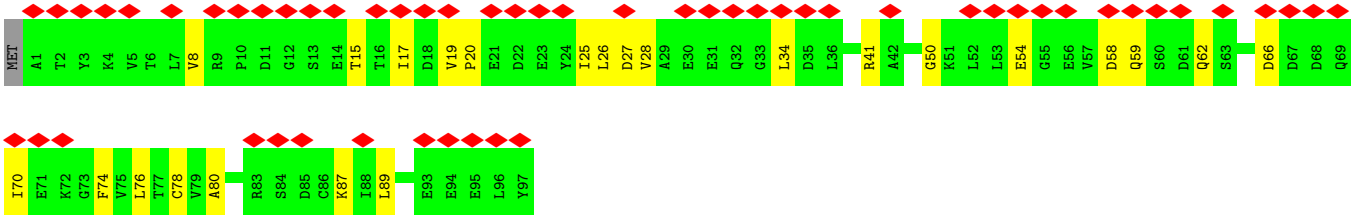
• Molecule 11: Photosystem I reaction center subunit XII

Chain M3: 100%

There are no outlier residues recorded for this chain.

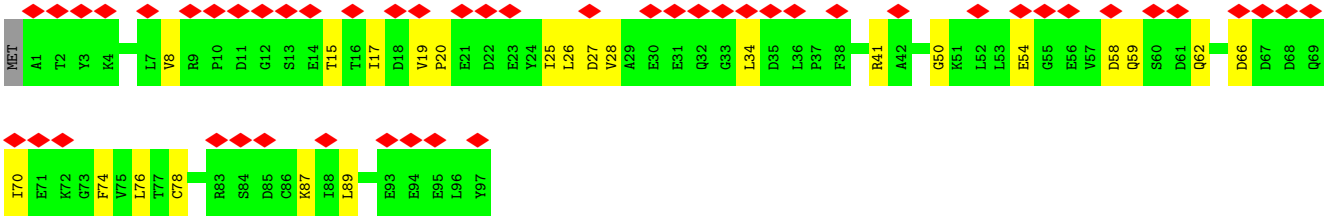
• Molecule 12: Ferredoxin-1

Chain R1: 56% 74% 24%



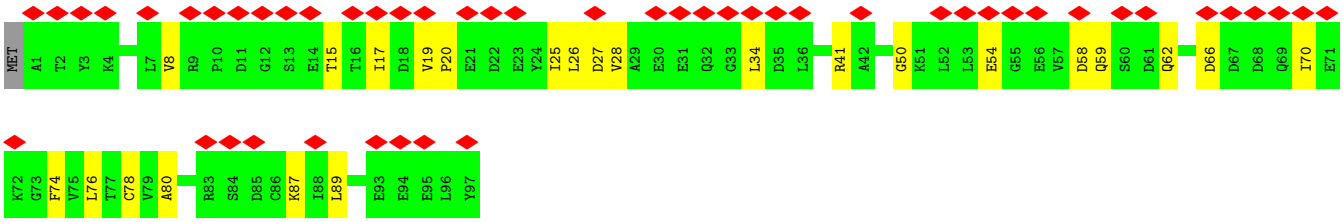
• Molecule 12: Ferredoxin-1

Chain R2: 50% 76% 23%



• Molecule 12: Ferredoxin-1

Chain R3:



• Molecule 13: Photosystem I 4.8K protein

Chain X1:

• Molecule 13: Photosystem I 4.8K protein

Chain X2:

• Molecule 13: Photosystem I 4.8K protein

Chain X3:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	207142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	322.4, 322.4, 322.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.806, 0.806, 0.806	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	A1	0.26	0/5862	0.43	0/8000
1	A2	0.26	0/5862	0.43	0/8000
1	A3	0.26	0/5862	0.43	0/8000
2	B1	0.26	0/6071	0.42	0/8302
2	B2	0.26	0/6071	0.42	0/8302
2	B3	0.26	0/6071	0.42	0/8302
3	C1	0.25	0/608	0.51	0/824
3	C2	0.25	0/608	0.51	0/824
3	C3	0.25	0/608	0.51	0/824
4	D1	0.26	0/1093	0.49	0/1483
4	D2	0.26	0/1093	0.49	0/1483
4	D3	0.26	0/1093	0.49	0/1483
5	E1	0.26	0/544	0.47	0/741
5	E2	0.26	0/544	0.47	0/741
5	E3	0.26	0/544	0.47	0/741
6	F1	0.24	0/1060	0.46	0/1443
6	F2	0.24	0/1060	0.46	0/1443
6	F3	0.24	0/1060	0.46	0/1443
7	I1	0.26	0/312	0.41	0/425
7	I2	0.26	0/312	0.41	0/425
7	I3	0.26	0/312	0.41	0/425
8	J1	0.27	0/349	0.45	0/476
8	J2	0.27	0/349	0.45	0/476
8	J3	0.27	0/349	0.45	0/476
9	K1	0.25	0/490	0.40	0/674
9	K2	0.25	0/490	0.40	0/674
9	K3	0.25	0/490	0.40	0/674
10	L1	0.26	0/1150	0.40	0/1561
10	L2	0.26	0/1150	0.40	0/1561
10	L3	0.26	0/1150	0.40	0/1561
11	M1	0.24	0/244	0.41	0/332
11	M2	0.24	0/244	0.41	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	M3	0.24	0/244	0.41	0/332
12	R1	0.26	0/758	0.48	0/1029
12	R2	0.26	0/758	0.48	0/1029
12	R3	0.26	0/758	0.48	0/1029
13	X1	0.35	0/234	0.47	0/320
13	X2	0.35	0/234	0.47	0/320
13	X3	0.35	0/234	0.47	0/320
All	All	0.26	0/56325	0.44	0/76830

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A1	5676	0	5476	67	0
1	A2	5676	0	5476	67	0
1	A3	5676	0	5476	64	0
2	B1	5853	0	5580	64	0
2	B2	5853	0	5580	69	0
2	B3	5853	0	5580	68	0
3	C1	598	0	580	3	0
3	C2	598	0	580	4	0
3	C3	598	0	580	4	0
4	D1	1067	0	1062	5	0
4	D2	1067	0	1062	6	0
4	D3	1067	0	1062	5	0
5	E1	532	0	522	4	0
5	E2	532	0	522	4	0
5	E3	532	0	522	4	0
6	F1	1038	0	1040	7	0
6	F2	1038	0	1040	8	0
6	F3	1038	0	1040	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I1	301	0	306	5	0
7	I2	301	0	306	6	0
7	I3	301	0	306	5	0
8	J1	337	0	344	7	0
8	J2	337	0	344	8	0
8	J3	337	0	344	8	0
9	K1	483	0	409	3	0
9	K2	483	0	409	3	0
9	K3	483	0	409	3	0
10	L1	1121	0	1117	9	0
10	L2	1121	0	1117	8	0
10	L3	1121	0	1117	9	0
11	M1	241	0	264	0	0
11	M2	241	0	264	0	0
11	M3	241	0	264	0	0
12	R1	748	0	705	16	0
12	R2	748	0	705	15	0
12	R3	748	0	705	16	0
13	X1	225	0	213	3	0
13	X2	225	0	213	3	0
13	X3	225	0	213	2	0
14	A1	65	0	72	4	0
14	A2	65	0	72	2	0
14	A3	65	0	72	2	0
15	A1	2328	0	2111	66	0
15	A2	2328	0	2111	67	0
15	A3	2328	0	2111	65	0
15	B1	1961	0	1678	44	0
15	B2	1961	0	1678	50	0
15	B3	1961	0	1678	49	0
15	I1	65	0	72	3	0
15	I2	65	0	72	3	0
15	I3	65	0	72	3	0
15	J1	143	0	75	0	0
15	J2	143	0	75	1	0
15	J3	143	0	75	1	0
15	K1	66	0	30	2	0
15	K2	66	0	30	2	0
15	K3	66	0	30	2	0
15	L1	190	0	203	9	0
15	L2	190	0	203	7	0
15	L3	190	0	203	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	X1	40	0	24	1	0
15	X2	40	0	24	1	0
15	X3	40	0	24	1	0
16	A1	33	0	46	0	0
16	A2	33	0	46	0	0
16	A3	33	0	46	0	0
16	B1	33	0	46	4	0
16	B2	33	0	46	4	0
16	B3	33	0	46	5	0
17	A1	8	0	0	0	0
17	A2	8	0	0	0	0
17	A3	8	0	0	0	0
17	C1	16	0	0	0	0
17	C2	16	0	0	0	0
17	C3	16	0	0	0	0
18	A1	270	0	375	22	0
18	A2	270	0	375	18	0
18	A3	270	0	375	19	0
18	B1	255	0	352	15	0
18	B2	255	0	352	12	0
18	B3	255	0	352	14	0
18	F1	40	0	56	3	0
18	F2	40	0	56	4	0
18	F3	40	0	56	3	0
18	I1	80	0	112	2	0
18	I2	80	0	112	2	0
18	I3	80	0	112	4	0
18	J1	120	0	168	11	0
18	J2	120	0	168	8	0
18	J3	120	0	168	11	0
18	K1	25	0	33	0	0
18	K2	25	0	33	0	0
18	K3	25	0	33	0	0
18	L1	120	0	168	8	0
18	L2	80	0	112	5	0
18	L3	40	0	56	4	0
18	M1	40	0	56	2	0
18	M2	40	0	56	2	0
18	M3	40	0	56	3	0
19	A1	82	0	110	0	0
19	A2	82	0	110	0	0
19	A3	82	0	110	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	X1	42	0	57	5	0
19	X2	42	0	57	5	0
19	X3	42	0	57	4	0
20	A1	97	0	0	0	0
20	A2	97	0	0	0	0
20	A3	97	0	0	0	0
20	I1	61	0	0	0	0
20	I2	61	0	0	0	0
20	I3	61	0	0	0	0
20	L1	64	0	0	0	0
20	L2	64	0	0	0	0
20	L3	64	0	0	0	0
20	M1	32	0	0	0	0
20	M2	32	0	0	0	0
20	M3	32	0	0	0	0
21	B1	66	0	96	0	0
21	B2	66	0	96	0	0
21	B3	66	0	96	0	0
22	L1	1	0	0	0	0
22	L2	1	0	0	0	0
22	L3	1	0	0	0	0
23	R1	4	0	0	0	0
23	R2	4	0	0	0	0
23	R3	4	0	0	0	0
24	A1	26	0	0	1	0
24	A2	26	0	0	1	0
24	A3	26	0	0	1	0
24	B1	42	0	0	1	0
24	B2	42	0	0	1	0
24	B3	42	0	0	1	0
24	C1	13	0	0	0	0
24	C2	13	0	0	0	0
24	C3	13	0	0	0	0
24	D1	7	0	0	0	0
24	D2	7	0	0	0	0
24	D3	7	0	0	0	0
24	E1	1	0	0	0	0
24	E2	1	0	0	0	0
24	E3	1	0	0	0	0
24	I1	1	0	0	0	0
24	I2	1	0	0	0	0
24	I3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	L1	22	0	0	0	0
24	L2	22	0	0	0	0
24	L3	22	0	0	0	0
24	R1	4	0	0	0	0
24	R2	4	0	0	0	0
24	R3	4	0	0	0	0
All	All	73929	0	70506	829	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 829 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)
1:A2:207:LEU:HD11	15:A2:820:CLA:HMC1	1.72	0.72
8:J2:31:ARG:HE	18:J2:1305:BCR:H312	1.55	0.72
1:A1:207:LEU:HD11	15:A1:820:CLA:HMC1	1.72	0.71
1:A3:207:LEU:HD11	15:A3:820:CLA:HMC1	1.72	0.71
8:J3:31:ARG:HE	18:J3:1305:BCR:H312	1.55	0.70

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	A1	743/755 (98%)	729 (98%)	14 (2%)	0	100	100
1	A2	743/755 (98%)	729 (98%)	14 (2%)	0	100	100
1	A3	743/755 (98%)	729 (98%)	14 (2%)	0	100	100
2	B1	738/741 (100%)	724 (98%)	14 (2%)	0	100	100
2	B2	738/741 (100%)	724 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B3	738/741 (100%)	724 (98%)	14 (2%)	0	100	100
3	C1	78/81 (96%)	78 (100%)	0	0	100	100
3	C2	78/81 (96%)	78 (100%)	0	0	100	100
3	C3	78/81 (96%)	78 (100%)	0	0	100	100
4	D1	136/139 (98%)	129 (95%)	7 (5%)	0	100	100
4	D2	136/139 (98%)	129 (95%)	7 (5%)	0	100	100
4	D3	136/139 (98%)	129 (95%)	7 (5%)	0	100	100
5	E1	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
5	E2	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
5	E3	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
6	F1	139/174 (80%)	138 (99%)	1 (1%)	0	100	100
6	F2	139/174 (80%)	138 (99%)	1 (1%)	0	100	100
6	F3	139/174 (80%)	138 (99%)	1 (1%)	0	100	100
7	I1	36/38 (95%)	36 (100%)	0	0	100	100
7	I2	36/38 (95%)	36 (100%)	0	0	100	100
7	I3	36/38 (95%)	36 (100%)	0	0	100	100
8	J1	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	J2	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	J3	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
9	K1	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
9	K2	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
9	K3	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
10	L1	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
10	L2	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
10	L3	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
11	M1	29/31 (94%)	29 (100%)	0	0	100	100
11	M2	29/31 (94%)	29 (100%)	0	0	100	100
11	M3	29/31 (94%)	29 (100%)	0	0	100	100
12	R1	95/98 (97%)	89 (94%)	6 (6%)	0	100	100
12	R2	95/98 (97%)	89 (94%)	6 (6%)	0	100	100
12	R3	95/98 (97%)	89 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	X1	26/39 (67%)	26 (100%)	0	0	100	100
13	X2	26/39 (67%)	26 (100%)	0	0	100	100
13	X3	26/39 (67%)	26 (100%)	0	0	100	100
All	All	7059/7353 (96%)	6912 (98%)	147 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A1	557/603 (92%)	557 (100%)	0	100	100
1	A2	557/603 (92%)	557 (100%)	0	100	100
1	A3	557/603 (92%)	557 (100%)	0	100	100
2	B1	586/598 (98%)	586 (100%)	0	100	100
2	B2	586/598 (98%)	586 (100%)	0	100	100
2	B3	586/598 (98%)	586 (100%)	0	100	100
3	C1	67/68 (98%)	67 (100%)	0	100	100
3	C2	67/68 (98%)	67 (100%)	0	100	100
3	C3	67/68 (98%)	67 (100%)	0	100	100
4	D1	113/116 (97%)	113 (100%)	0	100	100
4	D2	113/116 (97%)	113 (100%)	0	100	100
4	D3	113/116 (97%)	113 (100%)	0	100	100
5	E1	57/65 (88%)	57 (100%)	0	100	100
5	E2	57/65 (88%)	57 (100%)	0	100	100
5	E3	57/65 (88%)	57 (100%)	0	100	100
6	F1	101/138 (73%)	101 (100%)	0	100	100
6	F2	101/138 (73%)	101 (100%)	0	100	100
6	F3	101/138 (73%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I1	32/32 (100%)	32 (100%)	0	100	100
7	I2	32/32 (100%)	32 (100%)	0	100	100
7	I3	32/32 (100%)	32 (100%)	0	100	100
8	J1	35/36 (97%)	35 (100%)	0	100	100
8	J2	35/36 (97%)	35 (100%)	0	100	100
8	J3	35/36 (97%)	35 (100%)	0	100	100
9	K1	33/61 (54%)	33 (100%)	0	100	100
9	K2	33/61 (54%)	33 (100%)	0	100	100
9	K3	33/61 (54%)	33 (100%)	0	100	100
10	L1	115/120 (96%)	115 (100%)	0	100	100
10	L2	115/120 (96%)	115 (100%)	0	100	100
10	L3	115/120 (96%)	115 (100%)	0	100	100
11	M1	26/26 (100%)	26 (100%)	0	100	100
11	M2	26/26 (100%)	26 (100%)	0	100	100
11	M3	26/26 (100%)	26 (100%)	0	100	100
12	R1	85/86 (99%)	85 (100%)	0	100	100
12	R2	85/86 (99%)	85 (100%)	0	100	100
12	R3	85/86 (99%)	85 (100%)	0	100	100
13	X1	19/31 (61%)	19 (100%)	0	100	100
13	X2	19/31 (61%)	19 (100%)	0	100	100
13	X3	19/31 (61%)	19 (100%)	0	100	100
All	All	5478/5940 (92%)	5478 (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 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B2	105	GLN
1	A3	445	ASN
2	B3	105	GLN
2	B1	105	GLN
1	A1	445	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 444 ligands modelled in this entry, 51 are unknown and 3 are monoatomic - leaving 390 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	A3	843	24	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	B1	829	-	35,43,73	1.79	8 (22%)	41,74,113	2.09	13 (31%)
15	CLA	L3	1004	24	65,73,73	1.28	7 (10%)	76,113,113	1.38	10 (13%)
15	CLA	A1	817	-	39,46,73	1.73	10 (25%)	46,80,113	1.76	11 (23%)
18	BCR	B1	845	-	41,41,41	0.14	0	56,56,56	0.38	0
15	CLA	B3	805	-	65,73,73	1.26	7 (10%)	76,113,113	1.31	9 (11%)
15	CLA	A2	824	-	45,53,73	1.51	7 (15%)	52,89,113	1.53	9 (17%)
15	CLA	A3	838	-	55,63,73	1.40	7 (12%)	64,101,113	1.40	9 (14%)
15	CLA	B3	812	-	65,73,73	1.29	7 (10%)	76,113,113	1.38	12 (15%)
15	CLA	B1	817	-	50,58,73	1.44	7 (14%)	58,95,113	1.55	10 (17%)
18	BCR	M2	101	-	41,41,41	0.16	0	56,56,56	0.30	0
15	CLA	A2	808	1	65,73,73	1.29	7 (10%)	76,113,113	1.32	9 (11%)
15	CLA	B1	820	-	36,44,73	1.76	7 (19%)	40,76,113	1.89	10 (25%)
18	BCR	A2	850	-	41,41,41	0.11	0	56,56,56	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	BCR	B2	843	-	25,25,41	0.36	0	33,33,56	0.46	0
18	BCR	J3	1305	-	41,41,41	0.18	0	56,56,56	0.29	0
15	CLA	A2	802	24	65,73,73	1.32	7 (10%)	76,113,113	1.36	7 (9%)
15	CLA	B2	835	-	46,54,73	1.48	7 (15%)	53,90,113	1.61	10 (18%)
18	BCR	A3	848	-	41,41,41	0.13	0	56,56,56	0.31	0
15	CLA	B3	832	-	41,48,73	1.63	6 (14%)	45,82,113	1.97	9 (20%)
15	CLA	B3	811	-	45,53,73	1.48	6 (13%)	52,89,113	1.49	9 (17%)
15	CLA	A3	813	-	44,52,73	1.47	8 (18%)	55,88,113	1.53	11 (20%)
15	CLA	B2	829	-	35,43,73	1.79	8 (22%)	41,74,113	2.08	13 (31%)
15	CLA	B3	823	2	41,49,73	1.70	8 (19%)	47,84,113	1.64	10 (21%)
15	CLA	A1	831	-	50,58,73	1.48	7 (14%)	58,95,113	1.63	10 (17%)
15	CLA	B2	815	-	36,44,73	1.73	7 (19%)	40,76,113	1.82	9 (22%)
15	CLA	A2	806	-	65,73,73	1.26	7 (10%)	76,113,113	1.28	9 (11%)
15	CLA	A3	836	1	41,49,73	1.69	7 (17%)	47,84,113	1.67	8 (17%)
18	BCR	I3	103	-	41,41,41	0.18	0	56,56,56	0.35	0
15	CLA	A1	835	-	45,53,73	1.56	6 (13%)	52,89,113	1.50	8 (15%)
15	CLA	A2	835	-	45,53,73	1.56	6 (13%)	52,89,113	1.50	8 (15%)
15	CLA	B2	818	-	50,58,73	1.43	7 (14%)	58,95,113	1.49	9 (15%)
15	CLA	A2	837	-	50,58,73	1.41	7 (14%)	58,95,113	1.53	12 (20%)
15	CLA	J3	1302	8	33,43,73	1.69	8 (24%)	43,76,113	1.77	9 (20%)
15	CLA	B3	838	24	65,73,73	1.27	7 (10%)	76,113,113	1.30	9 (11%)
15	CLA	K3	101	-	33,42,73	1.72	5 (15%)	35,73,113	2.01	11 (31%)
15	CLA	B1	809	2	65,73,73	1.34	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	L2	1002	10	65,73,73	1.24	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	B3	834	-	37,47,73	1.65	7 (18%)	42,81,113	1.79	10 (23%)
15	CLA	B2	809	2	65,73,73	1.34	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	A3	817	-	39,46,73	1.73	10 (25%)	46,80,113	1.76	11 (23%)
15	CLA	A1	829	-	55,63,73	1.34	7 (12%)	64,101,113	1.45	10 (15%)
15	CLA	A2	842	-	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	A2	833	-	65,73,73	1.32	7 (10%)	76,113,113	1.34	10 (13%)
18	BCR	B3	842	-	30,30,41	0.34	0	39,39,56	0.51	0
15	CLA	B3	820	-	36,44,73	1.76	7 (19%)	40,76,113	1.89	10 (25%)
15	CLA	A3	820	-	36,46,73	1.59	8 (22%)	45,80,113	1.76	10 (22%)
15	CLA	B3	803	-	54,62,73	1.45	7 (12%)	62,99,113	1.37	8 (12%)
15	CLA	A1	840	-	65,73,73	1.29	7 (10%)	76,113,113	1.43	9 (11%)
15	CLA	A1	804	-	65,73,73	1.30	7 (10%)	76,113,113	1.37	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	BCR	A2	852	-	41,41,41	0.16	0	56,56,56	0.38	0
15	CLA	A2	839	-	55,63,73	1.43	7 (12%)	64,101,113	1.39	9 (14%)
15	CLA	B2	826	-	45,53,73	1.56	7 (15%)	52,89,113	1.45	8 (15%)
18	BCR	L2	1010	-	41,41,41	0.16	0	56,56,56	0.33	0
15	CLA	J1	1302	8	33,43,73	1.68	8 (24%)	43,76,113	1.77	10 (23%)
18	BCR	B1	841	-	41,41,41	0.19	0	56,56,56	0.35	0
15	CLA	L2	1004	24	65,73,73	1.28	7 (10%)	76,113,113	1.38	10 (13%)
18	BCR	A1	855	-	30,30,41	0.33	0	39,39,56	0.36	0
15	CLA	B1	837	-	41,49,73	1.73	8 (19%)	47,84,113	1.67	9 (19%)
15	CLA	B3	809	2	65,73,73	1.35	7 (10%)	76,113,113	1.28	10 (13%)
15	CLA	A3	826	24	55,63,73	1.38	6 (10%)	64,101,113	1.50	9 (14%)
15	CLA	B1	830	-	41,49,73	1.72	8 (19%)	47,84,113	1.71	8 (17%)
15	CLA	A2	816	-	41,49,73	1.66	8 (19%)	47,84,113	1.71	9 (19%)
15	CLA	B2	831	-	41,49,73	1.73	8 (19%)	47,84,113	1.74	12 (25%)
15	CLA	B1	816	-	38,46,73	1.84	9 (23%)	40,79,113	1.87	10 (25%)
15	CLA	A3	822	-	45,53,73	1.52	7 (15%)	52,89,113	1.64	9 (17%)
15	CLA	A3	830	-	65,73,73	1.29	6 (9%)	76,113,113	1.28	11 (14%)
19	LHG	A2	853	-	46,46,48	0.24	0	49,52,54	0.24	0
15	CLA	K1	101	-	33,42,73	1.72	5 (15%)	35,73,113	2.00	11 (31%)
18	BCR	J2	1304	-	41,41,41	0.16	0	56,56,56	0.29	0
17	SF4	A1	846	1,2	0,12,12	-	-	-		
18	BCR	A1	849	-	41,41,41	0.12	0	56,56,56	0.29	0
15	CLA	B1	819	-	45,53,73	1.54	7 (15%)	52,89,113	1.70	9 (17%)
15	CLA	A1	834	-	65,73,73	1.27	7 (10%)	76,113,113	1.34	10 (13%)
15	CLA	A2	827	-	60,68,73	1.33	7 (11%)	70,107,113	1.38	6 (8%)
15	CLA	A2	813	-	44,52,73	1.47	8 (18%)	55,88,113	1.53	11 (20%)
15	CLA	A1	842	-	65,73,73	1.30	7 (10%)	76,113,113	1.30	9 (11%)
15	CLA	I1	101	2	65,73,73	1.28	7 (10%)	76,113,113	1.27	11 (14%)
15	CLA	A1	856	-	65,73,73	1.30	6 (9%)	76,113,113	1.20	8 (10%)
15	CLA	A3	819	-	58,67,73	1.40	7 (12%)	67,106,113	1.64	11 (16%)
15	CLA	B3	806	-	50,58,73	1.43	7 (14%)	58,95,113	1.46	11 (18%)
15	CLA	L3	1003	-	60,68,73	1.31	6 (10%)	70,107,113	1.40	11 (15%)
21	DGD	B3	848	-	67,67,67	0.17	0	81,81,81	0.16	0
15	CLA	B1	802	24	65,73,73	1.34	6 (9%)	76,113,113	1.35	7 (9%)
18	BCR	J1	1304	-	41,41,41	0.15	0	56,56,56	0.29	0
15	CLA	B3	817	-	50,58,73	1.44	7 (14%)	58,95,113	1.55	10 (17%)
15	CLA	J1	1307	-	34,42,73	1.97	11 (32%)	41,73,113	2.14	12 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	BCR	B1	847	-	41,41,41	0.16	0	56,56,56	0.51	0
17	SF4	C3	102	3	0,12,12	-	-	-		
15	CLA	B3	822	-	39,48,73	1.60	7 (17%)	45,82,113	1.67	7 (15%)
15	CLA	B3	807	-	60,68,73	1.41	6 (10%)	70,107,113	1.64	10 (14%)
15	CLA	B2	823	2	41,49,73	1.71	8 (19%)	47,84,113	1.65	10 (21%)
15	CLA	B3	802	24	65,73,73	1.34	6 (9%)	76,113,113	1.35	7 (9%)
15	CLA	B1	810	-	43,52,73	1.55	7 (16%)	49,88,113	1.59	9 (18%)
16	PQN	B1	840	-	34,34,34	0.22	0	42,45,45	0.53	1 (2%)
15	CLA	A3	821	-	64,72,73	1.28	7 (10%)	75,112,113	1.33	11 (14%)
15	CLA	B3	833	-	37,45,73	1.74	9 (24%)	44,78,113	1.79	10 (22%)
15	CLA	A1	824	-	45,53,73	1.51	7 (15%)	52,89,113	1.53	10 (19%)
15	CLA	K3	103	-	32,40,73	1.80	7 (21%)	38,70,113	2.24	13 (34%)
15	CLA	L1	1004	24	65,73,73	1.28	7 (10%)	76,113,113	1.37	10 (13%)
15	CLA	J2	1302	8	33,43,73	1.69	8 (24%)	43,76,113	1.78	10 (23%)
15	CLA	A2	841	24	39,48,73	1.72	8 (20%)	44,83,113	1.66	11 (25%)
14	CL0	A2	801	-	65,73,73	2.41	7 (10%)	76,113,113	1.18	8 (10%)
15	CLA	B3	849	-	45,53,73	1.61	6 (13%)	52,89,113	1.47	8 (15%)
15	CLA	B1	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.31	9 (11%)
15	CLA	J3	1303	-	35,44,73	1.73	9 (25%)	46,78,113	1.79	11 (23%)
15	CLA	A2	830	-	65,73,73	1.29	6 (9%)	76,113,113	1.28	11 (14%)
15	CLA	A3	834	-	65,73,73	1.27	7 (10%)	76,113,113	1.33	10 (13%)
15	CLA	B1	834	-	37,47,73	1.65	7 (18%)	42,81,113	1.79	10 (23%)
15	CLA	B1	812	-	65,73,73	1.29	7 (10%)	76,113,113	1.38	12 (15%)
15	CLA	A2	832	-	45,53,73	1.59	6 (13%)	52,89,113	1.62	12 (23%)
15	CLA	B2	811	-	45,53,73	1.47	6 (13%)	52,89,113	1.48	9 (17%)
15	CLA	B3	819	-	45,53,73	1.54	7 (15%)	52,89,113	1.70	9 (17%)
18	BCR	J2	1306	-	41,41,41	0.20	0	56,56,56	0.54	0
23	GAK	R2	101	12	0,4,4	-	-	-		
19	LHG	X1	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	2 (4%)
18	BCR	B3	847	-	41,41,41	0.16	0	56,56,56	0.51	0
15	CLA	I3	101	2	65,73,73	1.28	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	J3	1307	-	34,42,73	1.96	11 (32%)	41,73,113	2.15	12 (29%)
18	BCR	B2	842	-	30,30,41	0.34	0	39,39,56	0.51	0
19	LHG	A3	854	-	34,34,48	0.22	0	37,40,54	0.31	0
15	CLA	B2	838	24	65,73,73	1.26	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	I2	101	2	65,73,73	1.28	7 (10%)	76,113,113	1.27	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	A3	835	-	45,53,73	1.57	6 (13%)	52,89,113	1.51	8 (15%)
15	CLA	A1	809	-	65,73,73	1.27	7 (10%)	76,113,113	1.42	10 (13%)
15	CLA	B1	801	-	65,73,73	1.30	6 (9%)	76,113,113	1.27	8 (10%)
15	CLA	B3	828	-	41,50,73	1.65	6 (14%)	49,85,113	1.66	8 (16%)
15	CLA	K1	103	-	32,40,73	1.80	7 (21%)	38,70,113	2.23	13 (34%)
15	CLA	B1	839	-	65,73,73	1.31	7 (10%)	76,113,113	1.27	9 (11%)
17	SF4	C2	101	3	0,12,12	-	-	-		
15	CLA	A3	829	-	55,63,73	1.35	7 (12%)	64,101,113	1.45	10 (15%)
18	BCR	A1	850	-	41,41,41	0.11	0	56,56,56	0.30	0
15	CLA	A1	828	-	42,50,73	1.54	7 (16%)	48,85,113	1.72	9 (18%)
15	CLA	B3	810	-	43,52,73	1.55	7 (16%)	49,88,113	1.59	9 (18%)
15	CLA	B1	835	-	46,54,73	1.48	7 (15%)	53,90,113	1.60	9 (16%)
15	CLA	B2	803	-	54,62,73	1.45	7 (12%)	62,99,113	1.36	8 (12%)
23	GAK	R1	101	12	0,4,4	-	-	-		
14	CL0	A3	801	-	65,73,73	2.41	7 (10%)	76,113,113	1.19	8 (10%)
15	CLA	B2	801	-	65,73,73	1.30	6 (9%)	76,113,113	1.27	8 (10%)
15	CLA	J3	1301	-	40,46,73	1.71	9 (22%)	48,79,113	1.72	12 (25%)
15	CLA	A3	840	-	65,73,73	1.29	7 (10%)	76,113,113	1.43	9 (11%)
15	CLA	X2	102	-	40,48,73	1.73	8 (20%)	46,83,113	1.72	13 (28%)
18	BCR	A3	850	-	41,41,41	0.12	0	56,56,56	0.30	0
15	CLA	A1	815	-	37,44,73	1.90	10 (27%)	43,76,113	1.98	10 (23%)
15	CLA	B3	821	-	38,47,73	1.72	6 (15%)	46,80,113	2.31	12 (26%)
15	CLA	B2	817	-	50,58,73	1.44	7 (14%)	58,95,113	1.55	10 (17%)
15	CLA	B2	808	-	65,73,73	1.34	7 (10%)	76,113,113	1.68	14 (18%)
18	BCR	I2	103	-	41,41,41	0.18	0	56,56,56	0.35	0
15	CLA	A1	837	-	50,58,73	1.41	7 (14%)	58,95,113	1.53	12 (20%)
15	CLA	A2	818	-	50,58,73	1.48	7 (14%)	58,95,113	1.54	9 (15%)
15	CLA	J2	1303	-	35,44,73	1.73	9 (25%)	46,78,113	1.78	12 (26%)
15	CLA	B2	833	-	37,45,73	1.73	9 (24%)	44,78,113	1.79	10 (22%)
15	CLA	A2	820	-	36,46,73	1.59	8 (22%)	45,80,113	1.76	10 (22%)
15	CLA	A1	839	-	55,63,73	1.43	7 (12%)	64,101,113	1.39	9 (14%)
15	CLA	L2	1003	-	60,68,73	1.30	6 (10%)	70,107,113	1.40	11 (15%)
15	CLA	A1	813	-	44,52,73	1.47	8 (18%)	55,88,113	1.53	10 (18%)
15	CLA	A1	803	-	63,72,73	1.31	7 (11%)	73,112,113	1.39	9 (12%)
21	DGD	B2	848	-	67,67,67	0.18	0	81,81,81	0.16	0
18	BCR	J3	1306	-	41,41,41	0.20	0	56,56,56	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	BCR	A2	851	-	41,41,41	0.14	0	56,56,56	0.43	0
15	CLA	A1	816	-	41,49,73	1.66	8 (19%)	47,84,113	1.70	9 (19%)
15	CLA	B1	806	-	50,58,73	1.43	7 (14%)	58,95,113	1.46	10 (17%)
18	BCR	L1	1011	-	41,41,41	0.16	0	56,56,56	0.33	0
15	CLA	A1	838	-	55,63,73	1.40	7 (12%)	64,101,113	1.40	9 (14%)
15	CLA	A1	821	-	64,72,73	1.28	7 (10%)	75,112,113	1.33	11 (14%)
15	CLA	A2	822	-	45,53,73	1.52	7 (15%)	52,89,113	1.65	9 (17%)
15	CLA	A2	814	-	33,41,73	1.75	9 (27%)	43,72,113	2.06	15 (34%)
15	CLA	B3	839	-	65,73,73	1.31	7 (10%)	76,113,113	1.27	9 (11%)
15	CLA	B2	802	24	65,73,73	1.35	6 (9%)	76,113,113	1.35	7 (9%)
15	CLA	B3	827	-	65,73,73	1.25	7 (10%)	76,113,113	1.27	8 (10%)
18	BCR	A1	852	-	41,41,41	0.16	0	56,56,56	0.38	0
17	SF4	A3	846	1,2	0,12,12	-	-	-		
18	BCR	A3	849	-	41,41,41	0.13	0	56,56,56	0.29	0
15	CLA	B1	833	-	37,45,73	1.74	9 (24%)	44,78,113	1.80	10 (22%)
18	BCR	I2	102	-	41,41,41	0.19	0	56,56,56	0.45	0
19	LHG	A1	853	-	46,46,48	0.24	0	49,52,54	0.24	0
15	CLA	A2	826	24	55,63,73	1.38	7 (12%)	64,101,113	1.50	9 (14%)
15	CLA	A2	840	-	65,73,73	1.29	7 (10%)	76,113,113	1.44	10 (13%)
15	CLA	A2	838	-	55,63,73	1.40	7 (12%)	64,101,113	1.41	9 (14%)
15	CLA	B1	826	-	45,53,73	1.55	7 (15%)	52,89,113	1.46	8 (15%)
15	CLA	B1	815	-	36,44,73	1.73	7 (19%)	40,76,113	1.83	9 (22%)
15	CLA	A3	842	-	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	A3	806	-	65,73,73	1.26	7 (10%)	76,113,113	1.29	10 (13%)
15	CLA	A1	832	-	45,53,73	1.58	6 (13%)	52,89,113	1.61	11 (21%)
15	CLA	B3	829	-	35,43,73	1.79	8 (22%)	41,74,113	2.09	13 (31%)
18	BCR	K3	102	-	25,25,41	0.37	0	33,33,56	0.41	0
15	CLA	A2	843	24	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	A1	823	-	41,49,73	1.68	8 (19%)	47,84,113	1.70	8 (17%)
15	CLA	A3	837	-	50,58,73	1.41	7 (14%)	58,95,113	1.53	12 (20%)
15	CLA	A1	810	-	37,46,73	1.92	9 (24%)	42,80,113	2.08	10 (23%)
15	CLA	A2	803	-	63,72,73	1.31	7 (11%)	73,112,113	1.39	9 (12%)
18	BCR	I1	103	-	41,41,41	0.18	0	56,56,56	0.35	0
15	CLA	A2	807	-	43,52,73	1.56	7 (16%)	49,88,113	1.73	10 (20%)
15	CLA	B2	837	-	41,49,73	1.72	8 (19%)	47,84,113	1.67	9 (19%)
15	CLA	A2	809	-	65,73,73	1.27	7 (10%)	76,113,113	1.42	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	A3	844	-	45,53,73	1.49	7 (15%)	52,89,113	1.50	9 (17%)
15	CLA	A3	816	-	41,49,73	1.66	8 (19%)	47,84,113	1.71	9 (19%)
15	CLA	A2	812	-	40,48,73	1.69	8 (20%)	46,83,113	1.71	9 (19%)
15	CLA	B3	831	-	41,49,73	1.73	8 (19%)	47,84,113	1.74	12 (25%)
15	CLA	A2	819	-	58,67,73	1.40	7 (12%)	67,106,113	1.64	11 (16%)
15	CLA	B3	836	-	45,53,73	1.55	7 (15%)	52,89,113	1.59	9 (17%)
16	PQN	A3	845	-	34,34,34	0.24	0	42,45,45	0.46	1 (2%)
18	BCR	B3	846	-	41,41,41	0.19	0	56,56,56	0.47	0
15	CLA	A1	811	-	65,73,73	1.29	7 (10%)	76,113,113	1.34	9 (11%)
15	CLA	J1	1303	-	35,44,73	1.72	9 (25%)	46,78,113	1.78	12 (26%)
18	BCR	K1	102	-	25,25,41	0.37	0	33,33,56	0.41	0
18	BCR	A2	849	-	41,41,41	0.12	0	56,56,56	0.29	0
15	CLA	A3	810	-	37,46,73	1.92	9 (24%)	42,80,113	2.07	10 (23%)
15	CLA	A1	820	-	36,46,73	1.59	8 (22%)	45,80,113	1.76	10 (22%)
18	BCR	K2	102	-	25,25,41	0.37	0	33,33,56	0.41	0
15	CLA	A1	844	-	45,53,73	1.49	7 (15%)	52,89,113	1.51	9 (17%)
15	CLA	B2	827	-	65,73,73	1.25	7 (10%)	76,113,113	1.27	8 (10%)
15	CLA	B2	804	-	55,63,73	1.37	7 (12%)	64,101,113	1.38	11 (17%)
18	BCR	B2	841	-	41,41,41	0.19	0	56,56,56	0.35	0
15	CLA	B1	832	-	41,48,73	1.64	6 (14%)	45,82,113	1.97	9 (20%)
18	BCR	A3	852	-	41,41,41	0.15	0	56,56,56	0.38	0
15	CLA	A2	828	-	42,50,73	1.54	7 (16%)	48,85,113	1.72	9 (18%)
15	CLA	B1	823	2	41,49,73	1.71	8 (19%)	47,84,113	1.65	10 (21%)
15	CLA	A3	809	-	65,73,73	1.27	7 (10%)	76,113,113	1.42	10 (13%)
15	CLA	B2	836	-	45,53,73	1.55	7 (15%)	52,89,113	1.59	9 (17%)
15	CLA	A3	832	-	45,53,73	1.58	6 (13%)	52,89,113	1.61	11 (21%)
15	CLA	J2	1301	-	40,46,73	1.71	9 (22%)	48,79,113	1.73	12 (25%)
15	CLA	A3	814	-	33,41,73	1.74	9 (27%)	43,72,113	2.07	14 (32%)
15	CLA	B2	849	-	45,53,73	1.60	6 (13%)	52,89,113	1.47	8 (15%)
18	BCR	A1	847	-	41,41,41	0.15	0	56,56,56	0.33	0
15	CLA	A3	823	-	41,49,73	1.67	8 (19%)	47,84,113	1.69	8 (17%)
15	CLA	B2	825	-	65,73,73	1.24	7 (10%)	76,113,113	1.28	11 (14%)
15	CLA	B2	813	-	45,53,73	1.52	7 (15%)	52,89,113	1.64	10 (19%)
15	CLA	X1	102	-	40,48,73	1.72	8 (20%)	46,83,113	1.72	13 (28%)
18	BCR	A3	855	-	30,30,41	0.33	0	39,39,56	0.36	0
15	CLA	K2	101	-	33,42,73	1.73	5 (15%)	35,73,113	2.00	11 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	BCR	A1	851	-	41,41,41	0.13	0	56,56,56	0.43	0
15	CLA	B2	839	-	65,73,73	1.30	7 (10%)	76,113,113	1.28	9 (11%)
15	CLA	B2	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.31	9 (11%)
15	CLA	A1	814	-	33,41,73	1.74	9 (27%)	43,72,113	2.06	14 (32%)
18	BCR	B2	844	-	41,41,41	0.13	0	56,56,56	0.28	0
15	CLA	B1	811	-	45,53,73	1.48	6 (13%)	52,89,113	1.49	9 (17%)
15	CLA	A3	818	-	50,58,73	1.48	7 (14%)	58,95,113	1.54	9 (15%)
15	CLA	J1	1301	-	40,46,73	1.71	9 (22%)	48,79,113	1.73	12 (25%)
15	CLA	A1	825	24	60,68,73	1.28	6 (10%)	70,107,113	1.36	12 (17%)
18	BCR	F1	201	-	41,41,41	0.11	0	56,56,56	0.27	0
15	CLA	B2	821	-	38,47,73	1.72	6 (15%)	46,80,113	2.30	12 (26%)
15	CLA	L1	1002	10	65,73,73	1.24	7 (10%)	76,113,113	1.28	10 (13%)
15	CLA	B3	837	-	41,49,73	1.72	8 (19%)	47,84,113	1.68	9 (19%)
15	CLA	B1	813	-	45,53,73	1.52	7 (15%)	52,89,113	1.65	10 (19%)
15	CLA	K2	103	-	32,40,73	1.80	7 (21%)	38,70,113	2.24	13 (34%)
15	CLA	B3	814	-	41,49,73	1.69	8 (19%)	47,84,113	1.62	9 (19%)
15	CLA	X3	102	-	40,48,73	1.72	8 (20%)	46,83,113	1.72	13 (28%)
15	CLA	A3	827	-	60,68,73	1.33	7 (11%)	70,107,113	1.38	6 (8%)
19	LHG	X3	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	2 (4%)
19	LHG	X2	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	2 (4%)
15	CLA	B3	816	-	38,46,73	1.83	9 (23%)	40,79,113	1.87	10 (25%)
15	CLA	B2	806	-	50,58,73	1.43	7 (14%)	58,95,113	1.46	10 (17%)
15	CLA	A3	808	1	65,73,73	1.29	7 (10%)	76,113,113	1.32	9 (11%)
18	BCR	B2	845	-	41,41,41	0.14	0	56,56,56	0.38	0
15	CLA	L1	1003	-	60,68,73	1.30	6 (10%)	70,107,113	1.40	11 (15%)
15	CLA	A3	839	-	55,63,73	1.43	7 (12%)	64,101,113	1.39	9 (14%)
18	BCR	A3	847	-	41,41,41	0.15	0	56,56,56	0.33	0
15	CLA	A1	833	-	65,73,73	1.31	7 (10%)	76,113,113	1.33	10 (13%)
15	CLA	A1	807	-	43,52,73	1.56	7 (16%)	49,88,113	1.73	10 (20%)
15	CLA	A1	808	1	65,73,73	1.29	7 (10%)	76,113,113	1.31	9 (11%)
16	PQN	B3	840	-	34,34,34	0.23	0	42,45,45	0.52	1 (2%)
18	BCR	B3	841	-	41,41,41	0.19	0	56,56,56	0.35	0
15	CLA	A1	802	24	65,73,73	1.32	7 (10%)	76,113,113	1.36	7 (9%)
18	BCR	I1	102	-	41,41,41	0.19	0	56,56,56	0.45	0
18	BCR	B2	846	-	41,41,41	0.19	0	56,56,56	0.48	0
15	CLA	A1	826	24	55,63,73	1.38	7 (12%)	64,101,113	1.50	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	B1	822	-	39,48,73	1.60	7 (17%)	45,82,113	1.66	7 (15%)
15	CLA	B1	803	-	54,62,73	1.45	7 (12%)	62,99,113	1.36	8 (12%)
15	CLA	B1	804	-	55,63,73	1.38	7 (12%)	64,101,113	1.38	11 (17%)
15	CLA	B2	822	-	39,48,73	1.61	7 (17%)	45,82,113	1.67	7 (15%)
15	CLA	B2	807	-	60,68,73	1.41	6 (10%)	70,107,113	1.64	10 (14%)
15	CLA	B2	824	24	45,53,73	1.54	7 (15%)	52,89,113	1.58	8 (15%)
15	CLA	A3	803	-	63,72,73	1.31	7 (11%)	73,112,113	1.38	10 (13%)
18	BCR	A3	851	-	41,41,41	0.13	0	56,56,56	0.43	0
15	CLA	A1	818	-	50,58,73	1.48	7 (14%)	58,95,113	1.54	9 (15%)
18	BCR	F2	201	-	41,41,41	0.11	0	56,56,56	0.28	0
15	CLA	A3	804	-	65,73,73	1.30	7 (10%)	76,113,113	1.38	11 (14%)
15	CLA	B1	838	24	65,73,73	1.27	7 (10%)	76,113,113	1.30	9 (11%)
15	CLA	A3	856	-	65,73,73	1.30	6 (9%)	76,113,113	1.20	8 (10%)
15	CLA	A2	825	24	60,68,73	1.28	6 (10%)	70,107,113	1.36	12 (17%)
15	CLA	A1	819	-	58,67,73	1.40	7 (12%)	67,106,113	1.64	11 (16%)
15	CLA	A2	815	-	37,44,73	1.89	10 (27%)	43,76,113	1.98	9 (20%)
15	CLA	A1	806	-	65,73,73	1.26	7 (10%)	76,113,113	1.28	10 (13%)
15	CLA	B3	813	-	45,53,73	1.53	7 (15%)	52,89,113	1.65	10 (19%)
15	CLA	B3	830	-	41,49,73	1.72	8 (19%)	47,84,113	1.70	8 (17%)
15	CLA	A3	825	24	60,68,73	1.29	7 (11%)	70,107,113	1.36	12 (17%)
15	CLA	A2	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.32	8 (10%)
15	CLA	B2	819	-	45,53,73	1.54	7 (15%)	52,89,113	1.69	9 (17%)
15	CLA	A1	841	24	39,48,73	1.72	8 (20%)	44,83,113	1.66	10 (22%)
15	CLA	B3	808	-	65,73,73	1.35	7 (10%)	76,113,113	1.68	14 (18%)
15	CLA	B3	818	-	50,58,73	1.43	7 (14%)	58,95,113	1.48	9 (15%)
21	DGD	B1	848	-	67,67,67	0.17	0	81,81,81	0.15	0
15	CLA	A1	822	-	45,53,73	1.52	7 (15%)	52,89,113	1.64	9 (17%)
17	SF4	C1	101	3	0,12,12	-	-	-		
17	SF4	C3	101	3	0,12,12	-	-	-		
15	CLA	A1	843	24	65,73,73	1.29	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	B1	824	24	45,53,73	1.54	7 (15%)	52,89,113	1.58	8 (15%)
15	CLA	B3	826	-	45,53,73	1.56	7 (15%)	52,89,113	1.46	8 (15%)
15	CLA	A2	856	-	65,73,73	1.30	6 (9%)	76,113,113	1.20	8 (10%)
17	SF4	C2	102	3	0,12,12	-	-	-		
15	CLA	A2	821	-	64,72,73	1.28	7 (10%)	75,112,113	1.33	11 (14%)
15	CLA	A1	812	-	40,48,73	1.70	8 (20%)	46,83,113	1.72	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	B1	828	-	41,50,73	1.65	6 (14%)	49,85,113	1.67	8 (16%)
16	PQN	A1	845	-	34,34,34	0.24	0	42,45,45	0.46	1 (2%)
15	CLA	A2	829	-	55,63,73	1.35	7 (12%)	64,101,113	1.45	10 (15%)
15	CLA	B1	814	-	41,49,73	1.68	8 (19%)	47,84,113	1.62	9 (19%)
15	CLA	B2	828	-	41,50,73	1.66	6 (14%)	49,85,113	1.67	8 (16%)
18	BCR	J2	1305	-	41,41,41	0.17	0	56,56,56	0.29	0
15	CLA	A2	836	1	41,49,73	1.69	7 (17%)	47,84,113	1.67	8 (17%)
15	CLA	B3	835	-	46,54,73	1.48	7 (15%)	53,90,113	1.60	9 (16%)
15	CLA	A3	833	-	65,73,73	1.31	7 (10%)	76,113,113	1.33	10 (13%)
18	BCR	A2	848	-	41,41,41	0.14	0	56,56,56	0.31	0
15	CLA	A3	807	-	43,52,73	1.56	7 (16%)	49,88,113	1.73	10 (20%)
15	CLA	B1	808	-	65,73,73	1.35	7 (10%)	76,113,113	1.68	14 (18%)
15	CLA	B1	818	-	50,58,73	1.43	7 (14%)	58,95,113	1.48	9 (15%)
15	CLA	A3	802	24	65,73,73	1.32	7 (10%)	76,113,113	1.36	7 (9%)
15	CLA	B1	849	-	45,53,73	1.60	6 (13%)	52,89,113	1.47	8 (15%)
15	CLA	A3	815	-	37,44,73	1.90	10 (27%)	43,76,113	1.97	10 (23%)
15	CLA	A2	804	-	65,73,73	1.30	7 (10%)	76,113,113	1.37	10 (13%)
18	BCR	B3	845	-	41,41,41	0.14	0	56,56,56	0.38	0
15	CLA	A2	831	-	50,58,73	1.48	7 (14%)	58,95,113	1.62	9 (15%)
18	BCR	B1	843	-	25,25,41	0.36	0	33,33,56	0.46	0
23	GAK	R3	101	12	0,4,4	-	-	-		
15	CLA	J2	1307	-	34,42,73	1.97	11 (32%)	41,73,113	2.14	12 (29%)
18	BCR	L3	1005	-	41,41,41	0.22	0	56,56,56	0.47	0
15	CLA	A2	810	-	37,46,73	1.92	9 (24%)	42,80,113	2.09	10 (23%)
15	CLA	B3	804	-	55,63,73	1.37	7 (12%)	64,101,113	1.38	11 (17%)
15	CLA	A3	841	24	39,48,73	1.72	8 (20%)	44,83,113	1.65	10 (22%)
15	CLA	B3	824	24	45,53,73	1.54	7 (15%)	52,89,113	1.58	8 (15%)
15	CLA	A1	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.32	8 (10%)
18	BCR	B2	847	-	41,41,41	0.15	0	56,56,56	0.51	0
15	CLA	A3	831	-	50,58,73	1.48	7 (14%)	58,95,113	1.62	10 (17%)
18	BCR	B3	843	-	25,25,41	0.36	0	33,33,56	0.46	0
15	CLA	B2	816	-	38,46,73	1.84	9 (23%)	40,79,113	1.88	10 (25%)
15	CLA	A2	834	-	65,73,73	1.27	7 (10%)	76,113,113	1.34	11 (14%)
17	SF4	C1	102	3	0,12,12	-	-	-		
16	PQN	A2	845	-	34,34,34	0.25	0	42,45,45	0.46	1 (2%)
18	BCR	M1	101	-	41,41,41	0.16	0	56,56,56	0.30	0
15	CLA	A1	827	-	60,68,73	1.33	7 (11%)	70,107,113	1.38	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	A2	811	-	65,73,73	1.29	7 (10%)	76,113,113	1.35	9 (11%)
15	CLA	B3	825	-	65,73,73	1.24	7 (10%)	76,113,113	1.27	11 (14%)
15	CLA	B2	814	-	41,49,73	1.68	8 (19%)	47,84,113	1.62	8 (17%)
15	CLA	B2	812	-	65,73,73	1.29	7 (10%)	76,113,113	1.38	12 (15%)
18	BCR	A2	855	-	30,30,41	0.33	0	39,39,56	0.36	0
18	BCR	J1	1306	-	41,41,41	0.20	0	56,56,56	0.54	0
15	CLA	A2	844	-	45,53,73	1.49	7 (15%)	52,89,113	1.52	9 (17%)
15	CLA	B3	815	-	36,44,73	1.74	7 (19%)	40,76,113	1.83	9 (22%)
18	BCR	B3	844	-	41,41,41	0.13	0	56,56,56	0.28	0
15	CLA	A2	823	-	41,49,73	1.68	8 (19%)	47,84,113	1.69	8 (17%)
15	CLA	A3	812	-	40,48,73	1.70	8 (20%)	46,83,113	1.72	9 (19%)
18	BCR	L1	1005	-	41,41,41	0.23	0	56,56,56	0.47	0
15	CLA	B2	830	-	41,49,73	1.71	8 (19%)	47,84,113	1.71	8 (17%)
19	LHG	A1	854	-	34,34,48	0.22	0	37,40,54	0.31	0
18	BCR	M3	101	-	41,41,41	0.16	0	56,56,56	0.30	0
15	CLA	A3	828	-	42,50,73	1.54	7 (16%)	48,85,113	1.72	9 (18%)
18	BCR	L1	1006	-	41,41,41	0.16	0	56,56,56	0.33	0
18	BCR	A2	847	-	41,41,41	0.15	0	56,56,56	0.33	0
15	CLA	B1	825	-	65,73,73	1.24	7 (10%)	76,113,113	1.27	11 (14%)
15	CLA	B2	810	-	43,52,73	1.55	7 (16%)	49,88,113	1.58	9 (18%)
16	PQN	B2	840	-	34,34,34	0.22	0	42,45,45	0.53	1 (2%)
15	CLA	A2	817	-	39,46,73	1.73	10 (25%)	46,80,113	1.76	11 (23%)
18	BCR	A1	848	-	41,41,41	0.13	0	56,56,56	0.31	0
18	BCR	F3	201	-	41,41,41	0.12	0	56,56,56	0.27	0
17	SF4	A2	846	1,2	0,12,12	-	-	-		
14	CL0	A1	801	-	65,73,73	2.41	7 (10%)	76,113,113	1.19	8 (10%)
15	CLA	A1	830	-	65,73,73	1.29	6 (9%)	76,113,113	1.28	11 (14%)
15	CLA	A3	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.32	8 (10%)
15	CLA	L3	1002	10	65,73,73	1.24	7 (10%)	76,113,113	1.28	11 (14%)
18	BCR	B1	844	-	41,41,41	0.13	0	56,56,56	0.28	0
15	CLA	A3	811	-	65,73,73	1.29	7 (10%)	76,113,113	1.34	9 (11%)
19	LHG	A3	853	-	46,46,48	0.24	0	49,52,54	0.24	0
15	CLA	B2	834	-	37,47,73	1.65	7 (18%)	42,81,113	1.79	10 (23%)
15	CLA	B1	827	-	65,73,73	1.25	7 (10%)	76,113,113	1.26	8 (10%)
15	CLA	B3	801	-	65,73,73	1.30	6 (9%)	76,113,113	1.27	8 (10%)
19	LHG	A2	854	-	34,34,48	0.23	0	37,40,54	0.31	0
18	BCR	I3	102	-	41,41,41	0.19	0	56,56,56	0.45	0
15	CLA	B1	821	-	38,47,73	1.72	6 (15%)	46,80,113	2.30	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	A1	836	1	41,49,73	1.69	7 (17%)	47,84,113	1.67	8 (17%)
18	BCR	J1	1305	-	41,41,41	0.18	0	56,56,56	0.29	0
18	BCR	L2	1005	-	41,41,41	0.22	0	56,56,56	0.47	0
15	CLA	B1	831	-	41,49,73	1.73	8 (19%)	47,84,113	1.74	12 (25%)
15	CLA	B2	820	-	36,44,73	1.76	7 (19%)	40,76,113	1.89	10 (25%)
15	CLA	B1	836	-	45,53,73	1.55	7 (15%)	52,89,113	1.59	9 (17%)
15	CLA	B2	832	-	41,48,73	1.65	6 (14%)	45,82,113	1.98	9 (20%)
18	BCR	J3	1304	-	41,41,41	0.15	0	56,56,56	0.29	0
15	CLA	B1	807	-	60,68,73	1.41	6 (10%)	70,107,113	1.64	10 (14%)
18	BCR	B1	842	-	30,30,41	0.34	0	39,39,56	0.51	0
18	BCR	B1	846	-	41,41,41	0.19	0	56,56,56	0.48	0
15	CLA	A3	824	-	45,53,73	1.51	7 (15%)	52,89,113	1.54	10 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A3	843	24	1/1/15/20	7/37/115/115	-
15	CLA	B1	829	-	1/1/6/20	0/2/69/115	-
15	CLA	L3	1004	24	1/1/15/20	4/37/115/115	-
15	CLA	A1	817	-	1/1/10/20	0/6/82/115	-
18	BCR	B1	845	-	-	2/29/63/63	0/2/2/2
15	CLA	B3	805	-	1/1/15/20	7/37/115/115	-
15	CLA	A2	824	-	1/1/11/20	6/13/91/115	-
15	CLA	A3	838	-	1/1/13/20	8/25/103/115	-
15	CLA	B3	812	-	1/1/15/20	5/37/115/115	-
15	CLA	B1	817	-	1/1/12/20	2/19/97/115	-
18	BCR	M2	101	-	-	2/29/63/63	0/2/2/2
15	CLA	A2	808	1	1/1/15/20	3/37/115/115	-
15	CLA	B1	820	-	1/1/7/20	0/2/72/115	-
18	BCR	A2	850	-	-	4/29/63/63	0/2/2/2
18	BCR	B2	843	-	-	2/18/35/63	0/1/1/2
18	BCR	J3	1305	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	802	24	1/1/15/20	1/37/115/115	-
15	CLA	B2	835	-	1/1/11/20	4/15/93/115	-
18	BCR	A3	848	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B3	832	-	1/1/9/20	2/8/82/115	-
15	CLA	B3	811	-	1/1/11/20	1/13/91/115	-
15	CLA	A3	813	-	1/1/11/20	5/13/89/115	-
15	CLA	B2	829	-	1/1/6/20	0/2/69/115	-
15	CLA	B3	823	2	1/1/10/20	2/8/86/115	-
15	CLA	A1	831	-	1/1/12/20	2/19/97/115	-
15	CLA	B2	815	-	1/1/7/20	0/2/72/115	-
15	CLA	A2	806	-	1/1/15/20	5/37/115/115	-
15	CLA	A3	836	1	1/1/10/20	2/8/86/115	-
18	BCR	I3	103	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	835	-	1/1/11/20	3/13/91/115	-
15	CLA	A2	835	-	1/1/11/20	3/13/91/115	-
15	CLA	B2	818	-	1/1/12/20	2/19/97/115	-
15	CLA	A2	837	-	1/1/12/20	2/19/97/115	-
15	CLA	J3	1302	8	1/1/8/20	-	-
15	CLA	B3	838	24	1/1/15/20	5/37/115/115	-
15	CLA	K3	101	-	1/1/7/20	0/0/70/115	-
15	CLA	B1	809	2	1/1/15/20	4/37/115/115	-
15	CLA	L2	1002	10	1/1/15/20	8/37/115/115	-
15	CLA	B3	834	-	1/1/9/20	0/6/80/115	-
15	CLA	B2	809	2	1/1/15/20	4/37/115/115	-
15	CLA	A3	817	-	1/1/10/20	0/6/82/115	-
15	CLA	A1	829	-	1/1/13/20	3/25/103/115	-
15	CLA	A2	842	-	1/1/15/20	6/37/115/115	-
15	CLA	A2	833	-	1/1/15/20	6/37/115/115	-
18	BCR	B3	842	-	-	1/24/41/63	0/1/1/2
15	CLA	B3	820	-	1/1/7/20	0/2/72/115	-
15	CLA	A3	820	-	1/1/9/20	1/6/78/115	-
15	CLA	B3	803	-	1/1/12/20	3/24/102/115	-
15	CLA	A1	840	-	1/1/15/20	5/37/115/115	-
15	CLA	A1	804	-	1/1/15/20	4/37/115/115	-
18	BCR	A2	852	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	839	-	1/1/13/20	7/25/103/115	-
15	CLA	B2	826	-	1/1/11/20	2/13/91/115	-
18	BCR	L2	1010	-	-	1/29/63/63	0/2/2/2
15	CLA	J1	1302	8	1/1/8/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	B1	841	-	-	3/29/63/63	0/2/2/2
15	CLA	L2	1004	24	1/1/15/20	4/37/115/115	-
18	BCR	A1	855	-	-	2/24/41/63	0/1/1/2
15	CLA	B1	837	-	1/1/10/20	5/8/86/115	-
15	CLA	B3	809	2	1/1/15/20	4/37/115/115	-
15	CLA	A3	826	24	1/1/13/20	5/25/103/115	-
15	CLA	B1	830	-	1/1/10/20	3/8/86/115	-
15	CLA	A2	816	-	1/1/10/20	0/8/86/115	-
15	CLA	B2	831	-	1/1/10/20	1/8/86/115	-
15	CLA	B1	816	-	1/1/8/20	3/6/76/115	-
15	CLA	A3	822	-	1/1/11/20	2/13/91/115	-
15	CLA	A3	830	-	1/1/15/20	9/37/115/115	-
19	LHG	A2	853	-	-	8/51/51/53	-
15	CLA	K1	101	-	1/1/7/20	0/0/70/115	-
18	BCR	J2	1304	-	-	3/29/63/63	0/2/2/2
17	SF4	A1	846	1,2	-	-	0/6/5/5
18	BCR	A1	849	-	-	0/29/63/63	0/2/2/2
15	CLA	B1	819	-	1/1/11/20	4/13/91/115	-
15	CLA	A1	834	-	1/1/15/20	4/37/115/115	-
15	CLA	A2	827	-	1/1/14/20	9/31/109/115	-
15	CLA	A2	813	-	1/1/11/20	5/13/89/115	-
15	CLA	A1	842	-	1/1/15/20	6/37/115/115	-
15	CLA	I1	101	2	1/1/15/20	4/37/115/115	-
15	CLA	A1	856	-	1/1/15/20	8/37/115/115	-
15	CLA	A3	819	-	1/1/14/20	2/29/107/115	-
15	CLA	B3	806	-	1/1/12/20	2/19/97/115	-
15	CLA	L3	1003	-	1/1/14/20	3/31/109/115	-
21	DGD	B3	848	-	-	8/55/95/95	0/2/2/2
15	CLA	B1	802	24	1/1/15/20	6/37/115/115	-
18	BCR	J1	1304	-	-	3/29/63/63	0/2/2/2
15	CLA	B3	817	-	1/1/12/20	2/19/97/115	-
15	CLA	J1	1307	-	1/1/8/20	0/0/74/115	-
18	BCR	B1	847	-	-	6/29/63/63	0/2/2/2
17	SF4	C3	102	3	-	-	0/6/5/5
15	CLA	B3	822	-	1/1/9/20	0/8/82/115	-
15	CLA	B3	807	-	1/1/14/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B2	823	2	1/1/10/20	2/8/86/115	-
15	CLA	B3	802	24	1/1/15/20	6/37/115/115	-
15	CLA	B1	810	-	1/1/11/20	0/11/89/115	-
16	PQN	B1	840	-	-	0/23/43/43	0/2/2/2
15	CLA	A3	821	-	1/1/15/20	0/35/113/115	-
15	CLA	B3	833	-	1/1/8/20	2/4/76/115	-
15	CLA	A1	824	-	1/1/11/20	6/13/91/115	-
15	CLA	K3	103	-	1/1/8/20	-	-
15	CLA	L1	1004	24	1/1/15/20	4/37/115/115	-
15	CLA	J2	1302	8	1/1/8/20	-	-
15	CLA	A2	841	24	1/1/10/20	1/6/84/115	-
14	CL0	A2	801	-	3/3/20/25	4/37/135/135	-
15	CLA	B3	849	-	1/1/11/20	7/13/91/115	-
15	CLA	B1	805	-	1/1/15/20	7/37/115/115	-
15	CLA	J3	1303	-	1/1/9/20	-	-
15	CLA	A2	830	-	1/1/15/20	9/37/115/115	-
15	CLA	A3	834	-	1/1/15/20	4/37/115/115	-
15	CLA	B1	834	-	1/1/9/20	0/6/80/115	-
15	CLA	B1	812	-	1/1/15/20	5/37/115/115	-
15	CLA	A2	832	-	1/1/11/20	6/13/91/115	-
15	CLA	B2	811	-	1/1/11/20	1/13/91/115	-
15	CLA	B3	819	-	1/1/11/20	4/13/91/115	-
18	BCR	J2	1306	-	-	5/29/63/63	0/2/2/2
23	GAK	R2	101	12	-	-	0/1/1/1
19	LHG	X1	101	-	-	20/46/46/53	-
18	BCR	B3	847	-	-	6/29/63/63	0/2/2/2
15	CLA	I3	101	2	1/1/15/20	4/37/115/115	-
15	CLA	J3	1307	-	1/1/8/20	0/0/74/115	-
18	BCR	B2	842	-	-	1/24/41/63	0/1/1/2
19	LHG	A3	854	-	-	8/38/38/53	-
15	CLA	B2	838	24	1/1/15/20	5/37/115/115	-
15	CLA	I2	101	2	1/1/15/20	4/37/115/115	-
15	CLA	A3	835	-	1/1/11/20	3/13/91/115	-
15	CLA	A1	809	-	1/1/15/20	9/37/115/115	-
15	CLA	B1	801	-	1/1/15/20	8/37/115/115	-
15	CLA	B3	828	-	1/1/10/20	4/7/85/115	-
15	CLA	K1	103	-	1/1/8/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B1	839	-	1/1/15/20	7/37/115/115	-
17	SF4	C2	101	3	-	-	0/6/5/5
15	CLA	A3	829	-	1/1/13/20	3/25/103/115	-
18	BCR	A1	850	-	-	4/29/63/63	0/2/2/2
15	CLA	A1	828	-	1/1/10/20	2/10/88/115	-
15	CLA	B3	810	-	1/1/11/20	0/11/89/115	-
15	CLA	B1	835	-	1/1/11/20	4/15/93/115	-
15	CLA	B2	803	-	1/1/12/20	2/24/102/115	-
23	GAK	R1	101	12	-	-	0/1/1/1
14	CL0	A3	801	-	3/3/20/25	4/37/135/135	-
15	CLA	B2	801	-	1/1/15/20	8/37/115/115	-
15	CLA	J3	1301	-	1/1/10/20	1/8/84/115	-
15	CLA	A3	840	-	1/1/15/20	5/37/115/115	-
15	CLA	X2	102	-	1/1/10/20	2/6/84/115	-
18	BCR	A3	850	-	-	4/29/63/63	0/2/2/2
15	CLA	A1	815	-	1/1/10/20	2/6/82/115	-
15	CLA	B3	821	-	1/1/8/20	3/8/79/115	-
15	CLA	B2	817	-	1/1/12/20	2/19/97/115	-
15	CLA	B2	808	-	1/1/15/20	6/37/115/115	-
18	BCR	I2	103	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	837	-	1/1/12/20	2/19/97/115	-
15	CLA	A2	818	-	1/1/12/20	9/19/97/115	-
15	CLA	J2	1303	-	1/1/9/20	-	-
15	CLA	B2	833	-	1/1/8/20	2/4/76/115	-
15	CLA	A2	820	-	1/1/9/20	1/6/78/115	-
15	CLA	A1	839	-	1/1/13/20	7/25/103/115	-
15	CLA	L2	1003	-	1/1/14/20	3/31/109/115	-
15	CLA	A1	813	-	1/1/11/20	5/13/89/115	-
15	CLA	A1	803	-	1/1/15/20	3/35/113/115	-
21	DGD	B2	848	-	-	8/55/95/95	0/2/2/2
18	BCR	J3	1306	-	-	5/29/63/63	0/2/2/2
18	BCR	A2	851	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	816	-	1/1/10/20	0/8/86/115	-
15	CLA	B1	806	-	1/1/12/20	2/19/97/115	-
18	BCR	L1	1011	-	-	1/29/63/63	0/2/2/2
15	CLA	A1	838	-	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A1	821	-	1/1/15/20	0/35/113/115	-
15	CLA	A2	822	-	1/1/11/20	2/13/91/115	-
15	CLA	A2	814	-	1/1/6/20	-	-
15	CLA	B3	839	-	1/1/15/20	7/37/115/115	-
15	CLA	B2	802	24	1/1/15/20	6/37/115/115	-
15	CLA	B3	827	-	1/1/15/20	12/37/115/115	-
18	BCR	A1	852	-	-	4/29/63/63	0/2/2/2
17	SF4	A3	846	1,2	-	-	0/6/5/5
18	BCR	A3	849	-	-	0/29/63/63	0/2/2/2
15	CLA	B1	833	-	1/1/8/20	2/4/76/115	-
18	BCR	I2	102	-	-	0/29/63/63	0/2/2/2
19	LHG	A1	853	-	-	8/51/51/53	-
15	CLA	A2	826	24	1/1/13/20	5/25/103/115	-
15	CLA	A2	840	-	1/1/15/20	5/37/115/115	-
15	CLA	A2	838	-	1/1/13/20	8/25/103/115	-
15	CLA	B1	826	-	1/1/11/20	2/13/91/115	-
15	CLA	B1	815	-	1/1/7/20	0/2/72/115	-
15	CLA	A3	842	-	1/1/15/20	6/37/115/115	-
15	CLA	A3	806	-	1/1/15/20	5/37/115/115	-
15	CLA	A1	832	-	1/1/11/20	6/13/91/115	-
15	CLA	B3	829	-	1/1/6/20	0/2/69/115	-
18	BCR	K3	102	-	-	2/18/35/63	0/1/1/2
15	CLA	A2	843	24	1/1/15/20	7/37/115/115	-
15	CLA	A1	823	-	1/1/10/20	2/8/86/115	-
15	CLA	A3	837	-	1/1/12/20	2/19/97/115	-
15	CLA	A1	810	-	1/1/10/20	1/4/82/115	-
15	CLA	A2	803	-	1/1/15/20	3/35/113/115	-
18	BCR	I1	103	-	-	5/29/63/63	0/2/2/2
15	CLA	A2	807	-	1/1/11/20	7/11/89/115	-
15	CLA	B2	837	-	1/1/10/20	5/8/86/115	-
15	CLA	A2	809	-	1/1/15/20	9/37/115/115	-
15	CLA	A3	844	-	1/1/11/20	3/13/91/115	-
15	CLA	A3	816	-	1/1/10/20	0/8/86/115	-
15	CLA	A2	812	-	1/1/10/20	0/6/84/115	-
15	CLA	B3	831	-	1/1/10/20	1/8/86/115	-
15	CLA	A2	819	-	1/1/14/20	2/29/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B3	836	-	1/1/11/20	2/13/91/115	-
16	PQN	A3	845	-	-	0/23/43/43	0/2/2/2
18	BCR	B3	846	-	-	0/29/63/63	0/2/2/2
15	CLA	A1	811	-	1/1/15/20	7/37/115/115	-
15	CLA	J1	1303	-	1/1/9/20	-	-
18	BCR	K1	102	-	-	2/18/35/63	0/1/1/2
18	BCR	A2	849	-	-	0/29/63/63	0/2/2/2
15	CLA	A3	810	-	1/1/10/20	1/4/82/115	-
15	CLA	A1	820	-	1/1/9/20	1/6/78/115	-
18	BCR	K2	102	-	-	2/18/35/63	0/1/1/2
15	CLA	A1	844	-	1/1/11/20	3/13/91/115	-
15	CLA	B2	827	-	1/1/15/20	12/37/115/115	-
15	CLA	B2	804	-	1/1/13/20	2/25/103/115	-
18	BCR	B2	841	-	-	3/29/63/63	0/2/2/2
15	CLA	B1	832	-	1/1/9/20	2/8/82/115	-
18	BCR	A3	852	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	828	-	1/1/10/20	2/10/88/115	-
15	CLA	B1	823	2	1/1/10/20	2/8/86/115	-
15	CLA	A3	809	-	1/1/15/20	9/37/115/115	-
15	CLA	B2	836	-	1/1/11/20	2/13/91/115	-
15	CLA	A3	832	-	1/1/11/20	6/13/91/115	-
15	CLA	J2	1301	-	1/1/10/20	1/8/84/115	-
15	CLA	A3	814	-	1/1/6/20	-	-
15	CLA	B2	849	-	1/1/11/20	7/13/91/115	-
18	BCR	A1	847	-	-	1/29/63/63	0/2/2/2
15	CLA	A3	823	-	1/1/10/20	2/8/86/115	-
15	CLA	B2	825	-	1/1/15/20	1/37/115/115	-
15	CLA	B2	813	-	1/1/11/20	7/13/91/115	-
15	CLA	X1	102	-	1/1/10/20	2/6/84/115	-
18	BCR	A3	855	-	-	2/24/41/63	0/1/1/2
15	CLA	K2	101	-	1/1/7/20	0/0/70/115	-
18	BCR	A1	851	-	-	5/29/63/63	0/2/2/2
15	CLA	B2	839	-	1/1/15/20	7/37/115/115	-
15	CLA	B2	805	-	1/1/15/20	7/37/115/115	-
15	CLA	A1	814	-	1/1/6/20	-	-
18	BCR	B2	844	-	-	2/29/63/63	0/2/2/2
15	CLA	B1	811	-	1/1/11/20	1/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A3	818	-	1/1/12/20	9/19/97/115	-
15	CLA	J1	1301	-	1/1/10/20	1/8/84/115	-
15	CLA	A1	825	24	1/1/14/20	9/31/109/115	-
18	BCR	F1	201	-	-	2/29/63/63	0/2/2/2
15	CLA	B2	821	-	1/1/8/20	3/8/79/115	-
15	CLA	L1	1002	10	1/1/15/20	8/37/115/115	-
15	CLA	B3	837	-	1/1/10/20	5/8/86/115	-
15	CLA	B1	813	-	1/1/11/20	7/13/91/115	-
15	CLA	K2	103	-	1/1/8/20	-	-
15	CLA	B3	814	-	1/1/10/20	3/8/86/115	-
15	CLA	X3	102	-	1/1/10/20	2/6/84/115	-
15	CLA	A3	827	-	1/1/14/20	9/31/109/115	-
19	LHG	X3	101	-	-	20/46/46/53	-
19	LHG	X2	101	-	-	20/46/46/53	-
15	CLA	B3	816	-	1/1/8/20	3/6/76/115	-
15	CLA	B2	806	-	1/1/12/20	2/19/97/115	-
15	CLA	A3	808	1	1/1/15/20	3/37/115/115	-
18	BCR	B2	845	-	-	2/29/63/63	0/2/2/2
15	CLA	L1	1003	-	1/1/14/20	3/31/109/115	-
15	CLA	A3	839	-	1/1/13/20	7/25/103/115	-
18	BCR	A3	847	-	-	1/29/63/63	0/2/2/2
15	CLA	A1	833	-	1/1/15/20	6/37/115/115	-
15	CLA	A1	807	-	1/1/11/20	7/11/89/115	-
15	CLA	A1	808	1	1/1/15/20	3/37/115/115	-
16	PQN	B3	840	-	-	0/23/43/43	0/2/2/2
18	BCR	B3	841	-	-	3/29/63/63	0/2/2/2
15	CLA	A1	802	24	1/1/15/20	1/37/115/115	-
18	BCR	I1	102	-	-	0/29/63/63	0/2/2/2
18	BCR	B2	846	-	-	0/29/63/63	0/2/2/2
15	CLA	A1	826	24	1/1/13/20	5/25/103/115	-
15	CLA	B1	822	-	1/1/9/20	0/8/82/115	-
15	CLA	B1	803	-	1/1/12/20	3/24/102/115	-
15	CLA	B1	804	-	1/1/13/20	2/25/103/115	-
15	CLA	B2	822	-	1/1/9/20	0/8/82/115	-
15	CLA	B2	807	-	1/1/14/20	5/31/109/115	-
15	CLA	B2	824	24	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A3	803	-	1/1/15/20	3/35/113/115	-
18	BCR	A3	851	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	818	-	1/1/12/20	9/19/97/115	-
18	BCR	F2	201	-	-	2/29/63/63	0/2/2/2
15	CLA	A3	804	-	1/1/15/20	4/37/115/115	-
15	CLA	B1	838	24	1/1/15/20	5/37/115/115	-
15	CLA	A3	856	-	1/1/15/20	8/37/115/115	-
15	CLA	A2	825	24	1/1/14/20	9/31/109/115	-
15	CLA	A1	819	-	1/1/14/20	2/29/107/115	-
15	CLA	A2	815	-	1/1/10/20	2/6/82/115	-
15	CLA	A1	806	-	1/1/15/20	5/37/115/115	-
15	CLA	B3	813	-	1/1/11/20	7/13/91/115	-
15	CLA	B3	830	-	1/1/10/20	3/8/86/115	-
15	CLA	A3	825	24	1/1/14/20	9/31/109/115	-
15	CLA	A2	805	-	1/1/15/20	4/37/115/115	-
15	CLA	B2	819	-	1/1/11/20	4/13/91/115	-
15	CLA	A1	841	24	1/1/10/20	1/6/84/115	-
15	CLA	B3	808	-	1/1/15/20	6/37/115/115	-
15	CLA	B3	818	-	1/1/12/20	2/19/97/115	-
21	DGD	B1	848	-	-	8/55/95/95	0/2/2/2
15	CLA	A1	822	-	1/1/11/20	2/13/91/115	-
17	SF4	C1	101	3	-	-	0/6/5/5
17	SF4	C3	101	3	-	-	0/6/5/5
15	CLA	A1	843	24	1/1/15/20	7/37/115/115	-
15	CLA	B1	824	24	1/1/11/20	2/13/91/115	-
15	CLA	B3	826	-	1/1/11/20	2/13/91/115	-
15	CLA	A2	856	-	1/1/15/20	8/37/115/115	-
17	SF4	C2	102	3	-	-	0/6/5/5
15	CLA	A2	821	-	1/1/15/20	0/35/113/115	-
15	CLA	A1	812	-	1/1/10/20	0/6/84/115	-
15	CLA	B1	828	-	1/1/10/20	4/7/85/115	-
16	PQN	A1	845	-	-	0/23/43/43	0/2/2/2
15	CLA	A2	829	-	1/1/13/20	3/25/103/115	-
15	CLA	B1	814	-	1/1/10/20	3/8/86/115	-
15	CLA	B2	828	-	1/1/10/20	4/7/85/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	J2	1305	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	836	1	1/1/10/20	2/8/86/115	-
15	CLA	B3	835	-	1/1/11/20	4/15/93/115	-
15	CLA	A3	833	-	1/1/15/20	6/37/115/115	-
18	BCR	A2	848	-	-	4/29/63/63	0/2/2/2
15	CLA	A3	807	-	1/1/11/20	7/11/89/115	-
15	CLA	B1	808	-	1/1/15/20	6/37/115/115	-
15	CLA	B1	818	-	1/1/12/20	2/19/97/115	-
15	CLA	A3	802	24	1/1/15/20	1/37/115/115	-
15	CLA	B1	849	-	1/1/11/20	7/13/91/115	-
15	CLA	A3	815	-	1/1/10/20	2/6/82/115	-
15	CLA	A2	804	-	1/1/15/20	4/37/115/115	-
18	BCR	B3	845	-	-	2/29/63/63	0/2/2/2
15	CLA	A2	831	-	1/1/12/20	2/19/97/115	-
18	BCR	B1	843	-	-	2/18/35/63	0/1/1/2
23	GAK	R3	101	12	-	-	0/1/1/1
15	CLA	J2	1307	-	1/1/8/20	0/0/74/115	-
18	BCR	L3	1005	-	-	2/29/63/63	0/2/2/2
15	CLA	A2	810	-	1/1/10/20	1/4/82/115	-
15	CLA	B3	804	-	1/1/13/20	2/25/103/115	-
15	CLA	A3	841	24	1/1/10/20	1/6/84/115	-
15	CLA	B3	824	24	1/1/11/20	2/13/91/115	-
15	CLA	A1	805	-	1/1/15/20	4/37/115/115	-
18	BCR	B2	847	-	-	6/29/63/63	0/2/2/2
15	CLA	A3	831	-	1/1/12/20	2/19/97/115	-
18	BCR	B3	843	-	-	2/18/35/63	0/1/1/2
15	CLA	B2	816	-	1/1/8/20	3/6/76/115	-
15	CLA	A2	834	-	1/1/15/20	4/37/115/115	-
17	SF4	C1	102	3	-	-	0/6/5/5
16	PQN	A2	845	-	-	0/23/43/43	0/2/2/2
18	BCR	M1	101	-	-	2/29/63/63	0/2/2/2
15	CLA	A1	827	-	1/1/14/20	9/31/109/115	-
15	CLA	A2	811	-	1/1/15/20	7/37/115/115	-
15	CLA	B3	825	-	1/1/15/20	1/37/115/115	-
15	CLA	B2	814	-	1/1/10/20	3/8/86/115	-
15	CLA	B2	812	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	A2	855	-	-	2/24/41/63	0/1/1/2
18	BCR	J1	1306	-	-	5/29/63/63	0/2/2/2
15	CLA	A2	844	-	1/1/11/20	3/13/91/115	-
15	CLA	B3	815	-	1/1/7/20	0/2/72/115	-
18	BCR	B3	844	-	-	2/29/63/63	0/2/2/2
15	CLA	A2	823	-	1/1/10/20	2/8/86/115	-
15	CLA	A3	812	-	1/1/10/20	0/6/84/115	-
18	BCR	L1	1005	-	-	2/29/63/63	0/2/2/2
15	CLA	B2	830	-	1/1/10/20	3/8/86/115	-
19	LHG	A1	854	-	-	8/38/38/53	-
18	BCR	M3	101	-	-	2/29/63/63	0/2/2/2
15	CLA	A3	828	-	1/1/10/20	2/10/88/115	-
18	BCR	L1	1006	-	-	1/29/63/63	0/2/2/2
18	BCR	A2	847	-	-	1/29/63/63	0/2/2/2
15	CLA	B1	825	-	1/1/15/20	2/37/115/115	-
15	CLA	B2	810	-	1/1/11/20	0/11/89/115	-
16	PQN	B2	840	-	-	0/23/43/43	0/2/2/2
15	CLA	A2	817	-	1/1/10/20	0/6/82/115	-
18	BCR	A1	848	-	-	4/29/63/63	0/2/2/2
18	BCR	F3	201	-	-	2/29/63/63	0/2/2/2
17	SF4	A2	846	1,2	-	-	0/6/5/5
14	CL0	A1	801	-	3/3/20/25	4/37/135/135	-
15	CLA	A1	830	-	1/1/15/20	9/37/115/115	-
15	CLA	A3	805	-	1/1/15/20	4/37/115/115	-
15	CLA	L3	1002	10	1/1/15/20	8/37/115/115	-
18	BCR	B1	844	-	-	2/29/63/63	0/2/2/2
15	CLA	A3	811	-	1/1/15/20	7/37/115/115	-
19	LHG	A3	853	-	-	8/51/51/53	-
15	CLA	B2	834	-	1/1/9/20	0/6/80/115	-
15	CLA	B1	827	-	1/1/15/20	12/37/115/115	-
15	CLA	B3	801	-	1/1/15/20	8/37/115/115	-
19	LHG	A2	854	-	-	8/38/38/53	-
18	BCR	I3	102	-	-	0/29/63/63	0/2/2/2
15	CLA	B1	821	-	1/1/8/20	3/8/79/115	-
15	CLA	A1	836	1	1/1/10/20	2/8/86/115	-
18	BCR	J1	1305	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	L2	1005	-	-	2/29/63/63	0/2/2/2
15	CLA	B1	831	-	1/1/10/20	1/8/86/115	-
15	CLA	B2	820	-	1/1/7/20	0/2/72/115	-
15	CLA	B1	836	-	1/1/11/20	2/13/91/115	-
15	CLA	B2	832	-	1/1/9/20	2/8/82/115	-
18	BCR	J3	1304	-	-	3/29/63/63	0/2/2/2
15	CLA	B1	807	-	1/1/14/20	5/31/109/115	-
18	BCR	B1	842	-	-	1/24/41/63	0/1/1/2
18	BCR	B1	846	-	-	0/29/63/63	0/2/2/2
15	CLA	A3	824	-	1/1/11/20	6/13/91/115	-

The worst 5 of 2082 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A3	801	CL0	C4B-NB	13.40	1.47	1.35
14	A1	801	CL0	C4B-NB	13.40	1.47	1.35
14	A2	801	CL0	C4B-NB	13.40	1.47	1.35
14	A1	801	CL0	C1B-NB	9.41	1.43	1.35
14	A3	801	CL0	C1B-NB	9.41	1.43	1.35

The worst 5 of 2818 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B3	821	CLA	C4A-NA-C1A	-8.08	103.07	106.71
15	B1	821	CLA	C4A-NA-C1A	-8.03	103.10	106.71
15	B2	821	CLA	C4A-NA-C1A	-8.02	103.10	106.71
15	B1	808	CLA	C4A-NA-C1A	-7.61	103.28	106.71
15	B2	808	CLA	C4A-NA-C1A	-7.55	103.31	106.71

5 of 294 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A1	801	CL0	NA
14	A1	801	CL0	NC
14	A1	801	CL0	ND
14	A2	801	CL0	NA
14	A2	801	CL0	NC

5 of 1338 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A1	804	CLA	CHA-CBD-CGD-O1D
15	A1	804	CLA	CHA-CBD-CGD-O2D
15	A1	805	CLA	CHA-CBD-CGD-O1D
15	A1	805	CLA	CHA-CBD-CGD-O2D
15	A1	805	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

276 monomers are involved in 522 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A3	843	CLA	1	0
15	L3	1004	CLA	1	0
18	B1	845	BCR	3	0
15	B3	805	CLA	2	0
15	A3	838	CLA	2	0
15	B3	812	CLA	4	0
15	B1	817	CLA	1	0
18	M2	101	BCR	2	0
15	A2	808	CLA	2	0
15	B1	820	CLA	1	0
18	A2	850	BCR	3	0
18	B2	843	BCR	2	0
18	J3	1305	BCR	5	0
15	A2	802	CLA	5	0
15	B2	835	CLA	1	0
18	A3	848	BCR	5	0
15	B3	832	CLA	1	0
15	A3	813	CLA	4	0
15	B3	823	CLA	2	0
15	A1	831	CLA	2	0
15	B2	815	CLA	1	0
15	A2	806	CLA	1	0
15	A3	836	CLA	1	0
18	I3	103	BCR	2	0
15	A1	835	CLA	1	0
15	A2	835	CLA	1	0
15	A2	837	CLA	1	0
15	B3	838	CLA	3	0
15	B1	809	CLA	1	0
15	L2	1002	CLA	3	0
15	B2	809	CLA	2	0
15	A1	829	CLA	4	0
15	A2	842	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A2	833	CLA	3	0
18	B3	842	BCR	3	0
15	B3	820	CLA	1	0
15	A3	820	CLA	1	0
15	B3	803	CLA	2	0
15	A1	840	CLA	1	0
15	A1	804	CLA	2	0
18	A2	852	BCR	3	0
15	A2	839	CLA	2	0
15	B2	826	CLA	1	0
18	L2	1010	BCR	2	0
18	B1	841	BCR	4	0
15	L2	1004	CLA	1	0
18	A1	855	BCR	1	0
15	B3	809	CLA	1	0
15	A3	826	CLA	1	0
15	B2	831	CLA	1	0
15	B1	816	CLA	1	0
15	A3	830	CLA	2	0
18	J2	1304	BCR	2	0
18	A1	849	BCR	3	0
15	A1	834	CLA	1	0
15	A2	827	CLA	1	0
15	A2	813	CLA	4	0
15	A1	842	CLA	4	0
15	I1	101	CLA	3	0
15	A1	856	CLA	4	0
15	A3	819	CLA	5	0
15	L3	1003	CLA	4	0
15	B1	802	CLA	5	0
18	J1	1304	BCR	2	0
15	B3	822	CLA	1	0
15	B3	807	CLA	2	0
15	B2	823	CLA	2	0
15	B3	802	CLA	5	0
15	B1	810	CLA	1	0
16	B1	840	PQN	4	0
15	A3	821	CLA	3	0
15	A1	824	CLA	1	0
15	K3	103	CLA	2	0
15	L1	1004	CLA	1	0
14	A2	801	CL0	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B3	849	CLA	2	0
15	B1	805	CLA	1	0
15	J3	1303	CLA	1	0
15	A2	830	CLA	2	0
15	A3	834	CLA	1	0
15	B1	812	CLA	4	0
18	J2	1306	BCR	2	0
19	X1	101	LHG	5	0
18	B3	847	BCR	1	0
15	I3	101	CLA	3	0
18	B2	842	BCR	2	0
15	B2	838	CLA	3	0
15	I2	101	CLA	3	0
15	A3	835	CLA	1	0
15	A1	809	CLA	1	0
15	B1	801	CLA	4	0
15	K1	103	CLA	2	0
15	B1	839	CLA	3	0
15	A3	829	CLA	3	0
18	A1	850	BCR	3	0
15	A1	828	CLA	4	0
15	B3	810	CLA	1	0
15	B1	835	CLA	1	0
15	B2	803	CLA	2	0
14	A3	801	CL0	2	0
15	B2	801	CLA	4	0
15	A3	840	CLA	1	0
15	X2	102	CLA	1	0
18	A3	850	BCR	3	0
15	A1	815	CLA	1	0
15	B3	821	CLA	1	0
15	B2	808	CLA	5	0
18	I2	103	BCR	1	0
15	A1	837	CLA	1	0
15	A2	818	CLA	3	0
15	J2	1303	CLA	1	0
15	A2	820	CLA	1	0
15	A1	839	CLA	2	0
15	L2	1003	CLA	4	0
15	A1	813	CLA	4	0
15	A1	803	CLA	2	0
18	J3	1306	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A2	851	BCR	5	0
18	L1	1011	BCR	2	0
15	A1	838	CLA	2	0
15	A1	821	CLA	3	0
15	A2	814	CLA	1	0
15	B3	839	CLA	3	0
15	B2	802	CLA	5	0
15	B3	827	CLA	6	0
18	A1	852	BCR	4	0
18	A3	849	BCR	3	0
18	I2	102	BCR	1	0
15	A2	826	CLA	1	0
15	A2	840	CLA	1	0
15	A2	838	CLA	2	0
15	B1	826	CLA	1	0
15	A3	842	CLA	4	0
15	A3	806	CLA	1	0
15	A2	843	CLA	1	0
15	A3	837	CLA	1	0
15	A2	803	CLA	2	0
18	I1	103	BCR	1	0
15	A2	807	CLA	2	0
15	B2	837	CLA	1	0
15	A2	809	CLA	1	0
15	B3	831	CLA	1	0
15	A2	819	CLA	6	0
15	B3	836	CLA	2	0
18	B3	846	BCR	3	0
15	A1	811	CLA	4	0
18	A2	849	BCR	1	0
15	A1	820	CLA	1	0
15	B2	827	CLA	5	0
15	B2	804	CLA	1	0
18	B2	841	BCR	4	0
15	B1	832	CLA	1	0
18	A3	852	BCR	3	0
15	A2	828	CLA	4	0
15	B1	823	CLA	2	0
15	A3	809	CLA	1	0
15	B2	836	CLA	2	0
15	B2	849	CLA	2	0
18	A1	847	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	X1	102	CLA	1	0
18	A3	855	BCR	1	0
18	A1	851	BCR	5	0
15	B2	839	CLA	3	0
15	B2	805	CLA	2	0
15	A1	814	CLA	1	0
15	A3	818	CLA	3	0
15	A1	825	CLA	5	0
18	F1	201	BCR	3	0
15	B2	821	CLA	1	0
15	L1	1002	CLA	5	0
15	B3	837	CLA	1	0
15	K2	103	CLA	2	0
15	X3	102	CLA	1	0
15	A3	827	CLA	1	0
19	X3	101	LHG	4	0
19	X2	101	LHG	5	0
15	B3	816	CLA	1	0
15	A3	808	CLA	2	0
18	B2	845	BCR	1	0
15	L1	1003	CLA	4	0
15	A3	839	CLA	2	0
18	A3	847	BCR	1	0
15	A1	833	CLA	3	0
15	A1	807	CLA	2	0
15	A1	808	CLA	2	0
16	B3	840	PQN	5	0
18	B3	841	BCR	3	0
15	A1	802	CLA	4	0
18	I1	102	BCR	1	0
18	B2	846	BCR	3	0
15	A1	826	CLA	1	0
15	B1	822	CLA	1	0
15	B1	803	CLA	2	0
15	B1	804	CLA	1	0
15	B2	822	CLA	1	0
15	B2	807	CLA	2	0
15	B2	824	CLA	1	0
15	A3	803	CLA	2	0
18	A3	851	BCR	4	0
15	A1	818	CLA	2	0
18	F2	201	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A3	804	CLA	2	0
15	B1	838	CLA	3	0
15	A3	856	CLA	4	0
15	A2	825	CLA	5	0
15	A1	819	CLA	6	0
15	A2	815	CLA	1	0
15	A1	806	CLA	1	0
15	A3	825	CLA	5	0
15	A2	805	CLA	4	0
15	B3	808	CLA	5	0
15	A1	843	CLA	1	0
15	B3	826	CLA	1	0
15	A2	856	CLA	4	0
15	A2	821	CLA	3	0
15	A2	829	CLA	4	0
18	J2	1305	BCR	4	0
15	A2	836	CLA	1	0
15	B3	835	CLA	1	0
15	A3	833	CLA	3	0
18	A2	848	BCR	5	0
15	A3	807	CLA	2	0
15	B1	808	CLA	4	0
15	A3	802	CLA	5	0
15	B1	849	CLA	2	0
15	A3	815	CLA	1	0
15	A2	804	CLA	2	0
18	B3	845	BCR	1	0
15	A2	831	CLA	2	0
18	B1	843	BCR	2	0
18	L3	1005	BCR	4	0
15	B3	804	CLA	1	0
15	B3	824	CLA	1	0
15	A1	805	CLA	4	0
15	A3	831	CLA	2	0
18	B3	843	BCR	2	0
15	B2	816	CLA	1	0
15	A2	834	CLA	1	0
18	M1	101	BCR	2	0
15	A1	827	CLA	1	0
15	A2	811	CLA	4	0
15	B2	812	CLA	4	0
18	A2	855	BCR	1	0

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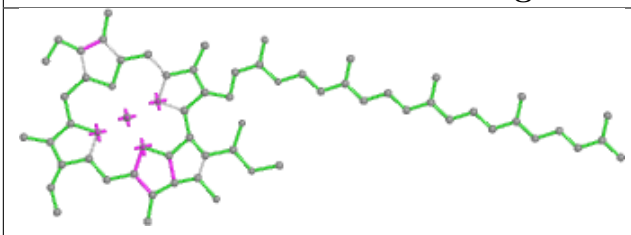
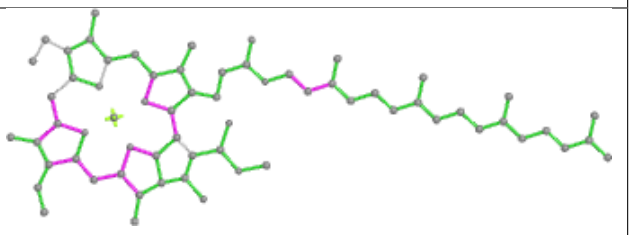
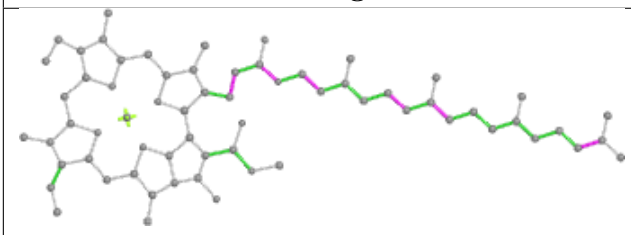
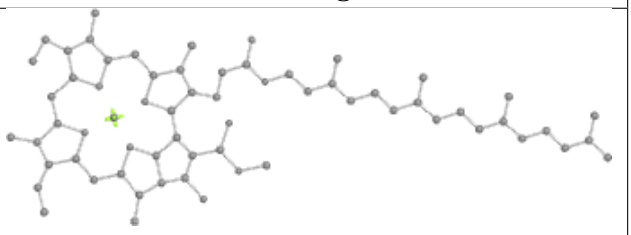
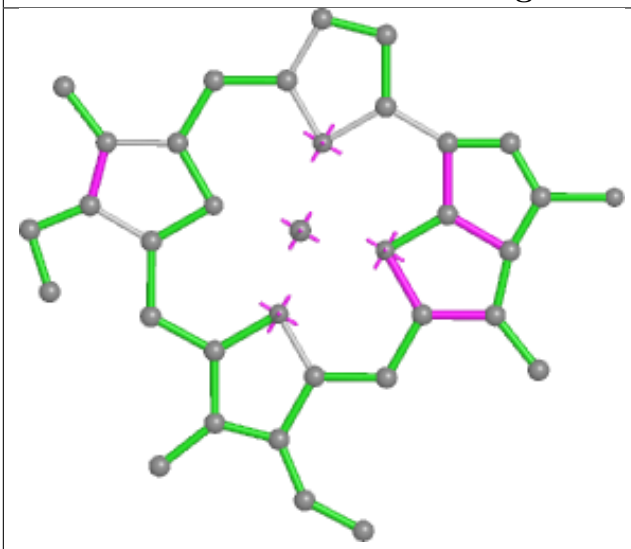
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	J1	1306	BCR	3	0
15	B3	815	CLA	1	0
18	B3	844	BCR	1	0
18	L1	1005	BCR	4	0
18	M3	101	BCR	3	0
15	A3	828	CLA	4	0
18	L1	1006	BCR	2	0
18	A2	847	BCR	1	0
15	B2	810	CLA	1	0
16	B2	840	PQN	4	0
18	A1	848	BCR	5	0
18	F3	201	BCR	3	0
14	A1	801	CL0	4	0
15	A1	830	CLA	2	0
15	A3	805	CLA	4	0
15	L3	1002	CLA	4	0
18	B1	844	BCR	1	0
15	A3	811	CLA	4	0
15	B1	827	CLA	4	0
15	B3	801	CLA	4	0
18	I3	102	BCR	2	0
15	B1	821	CLA	1	0
15	A1	836	CLA	1	0
18	J1	1305	BCR	6	0
18	L2	1005	BCR	3	0
15	B1	831	CLA	1	0
15	B2	820	CLA	2	0
15	B1	836	CLA	2	0
15	B2	832	CLA	1	0
18	J3	1304	BCR	2	0
15	B1	807	CLA	2	0
18	B1	842	BCR	3	0
18	B1	846	BCR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

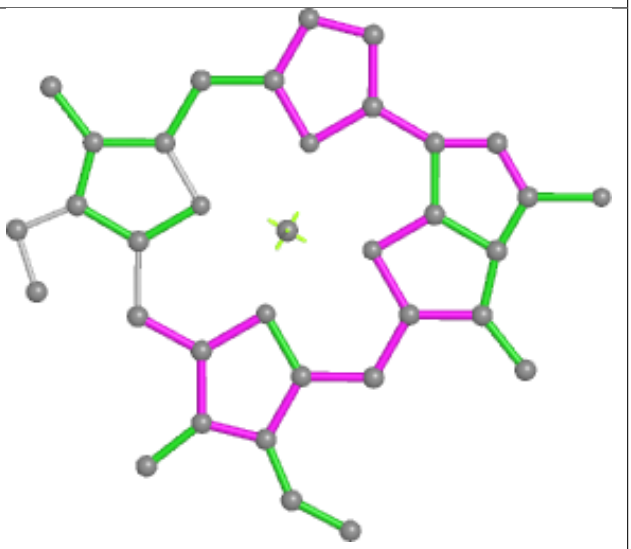
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLA A3 843	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

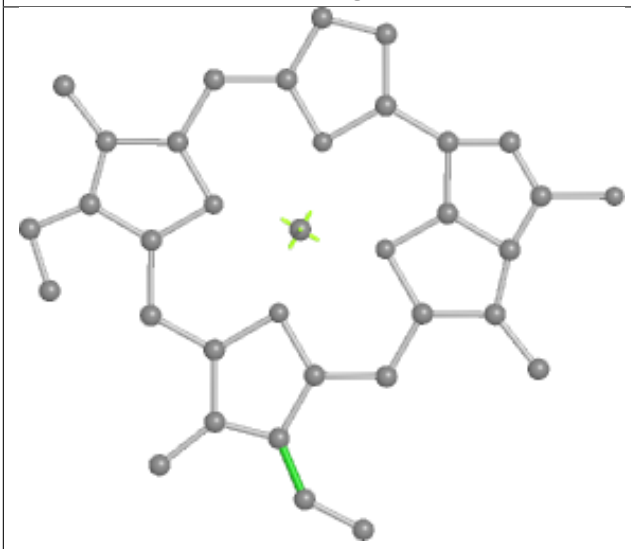
Ligand CLA B1 829



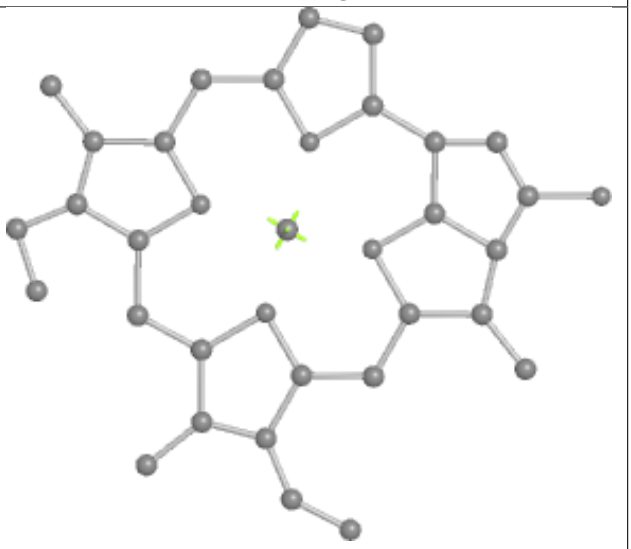
Bond lengths



Bond angles

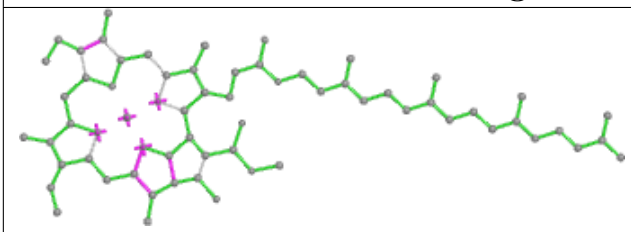


Torsions

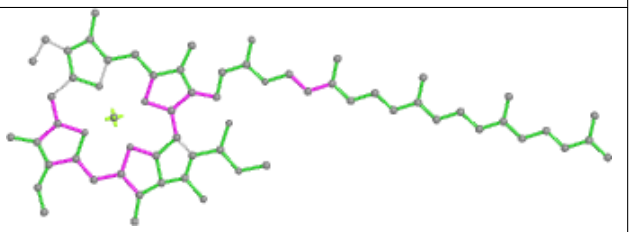


Rings

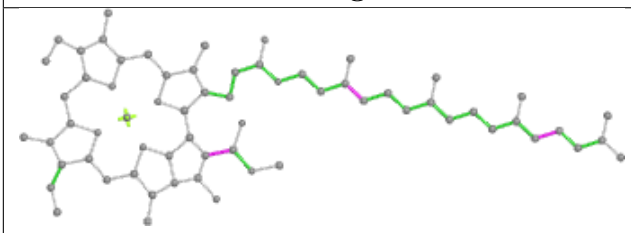
Ligand CLA L3 1004



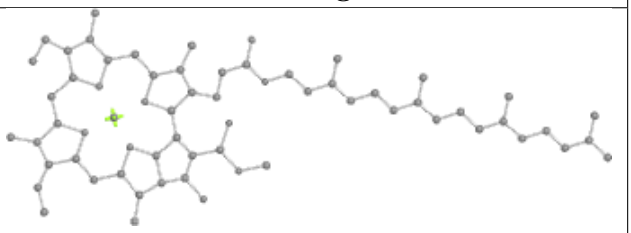
Bond lengths



Bond angles

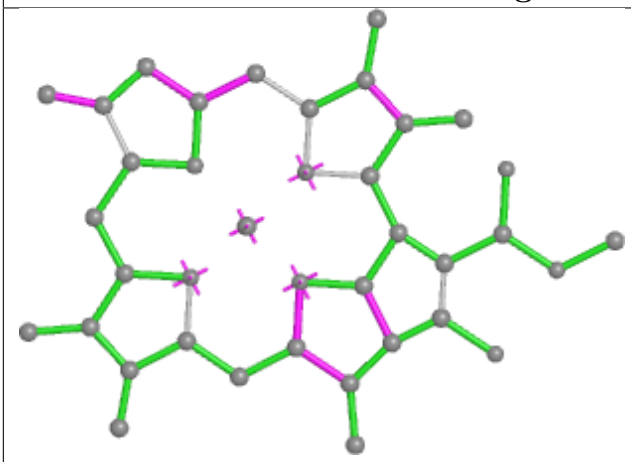


Torsions

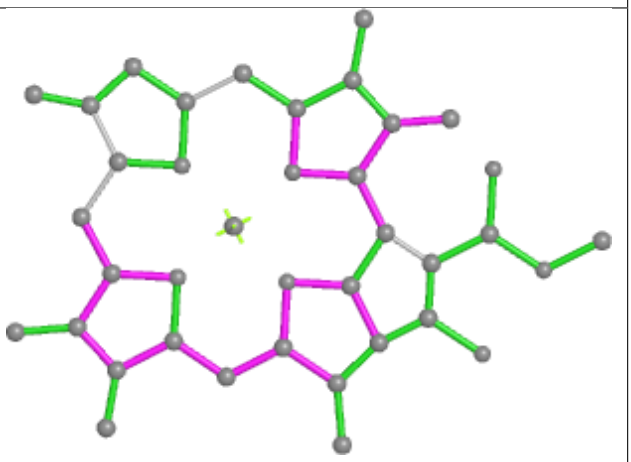


Rings

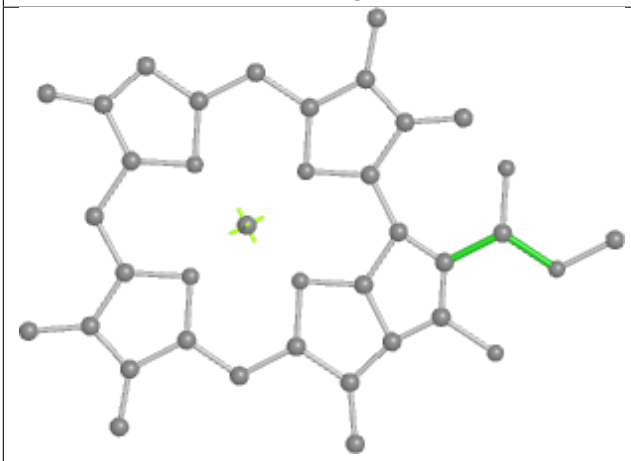
Ligand CLA A1 817



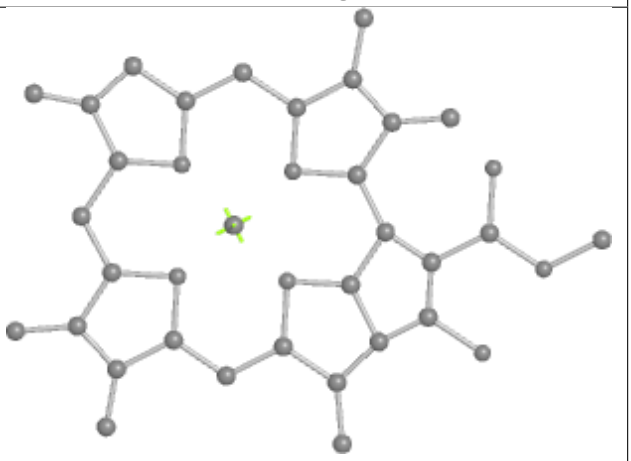
Bond lengths



Bond angles

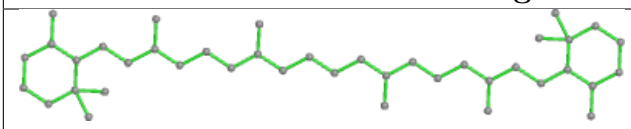


Torsions

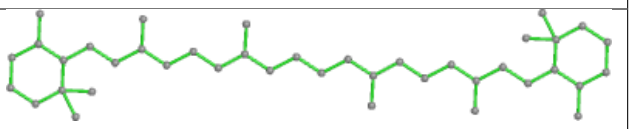


Rings

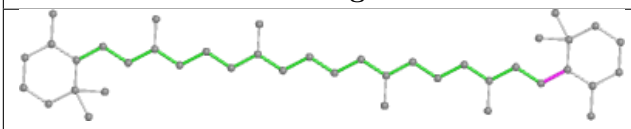
Ligand BCR B1 845



Bond lengths



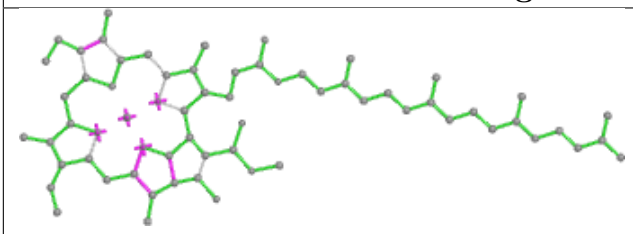
Bond angles



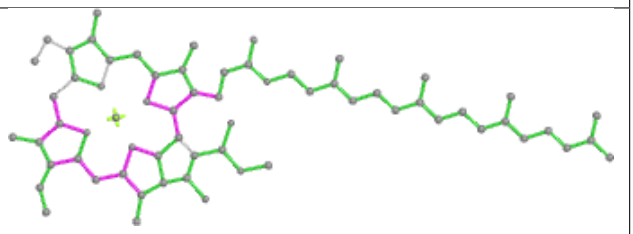
Torsions

Rings

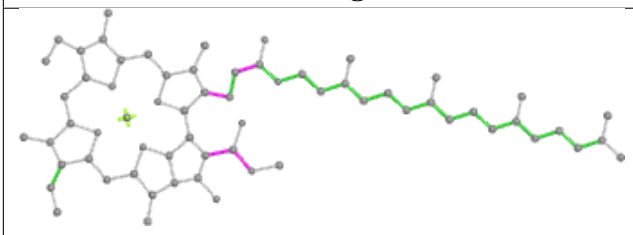
Ligand CLA B3 805



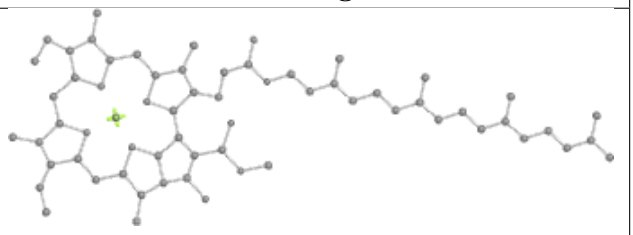
Bond lengths



Bond angles

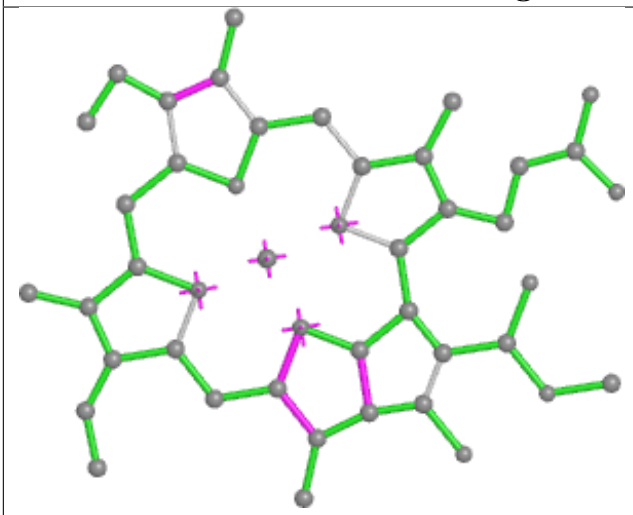


Torsions

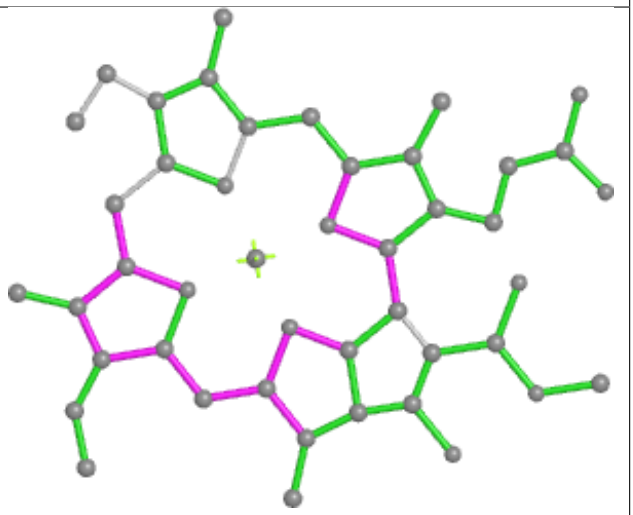


Rings

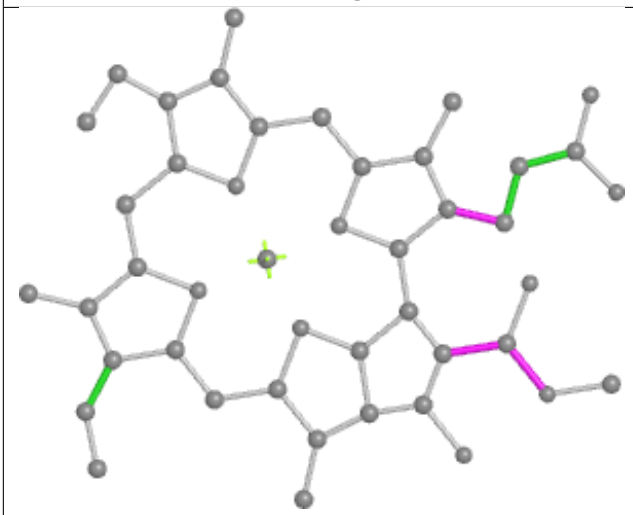
Ligand CLA A2 824



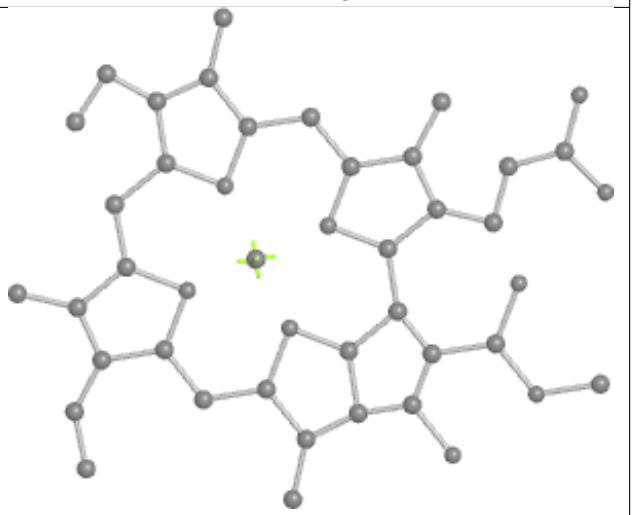
Bond lengths



Bond angles

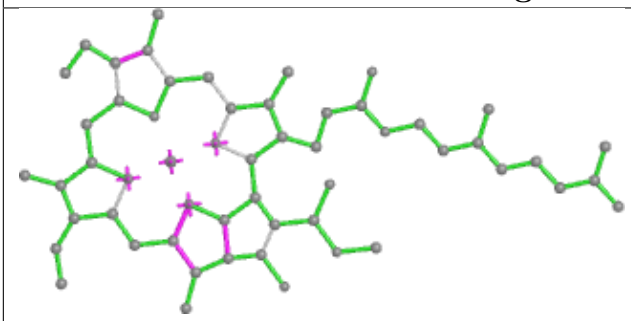


Torsions



Rings

Ligand CLA A3 838



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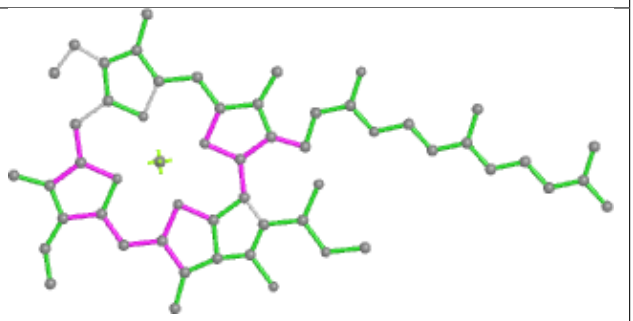
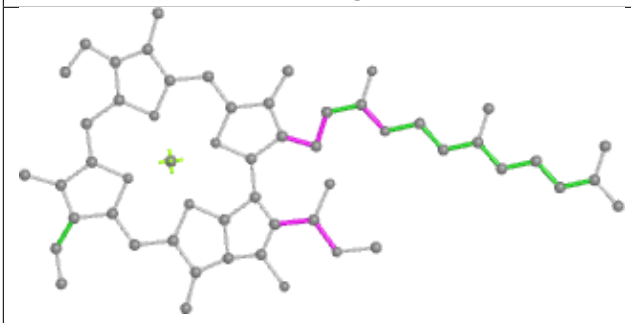
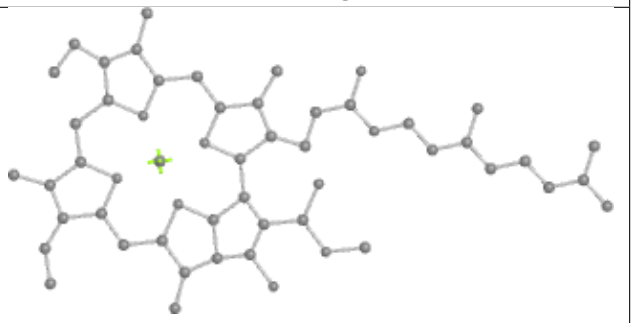


Bond angles

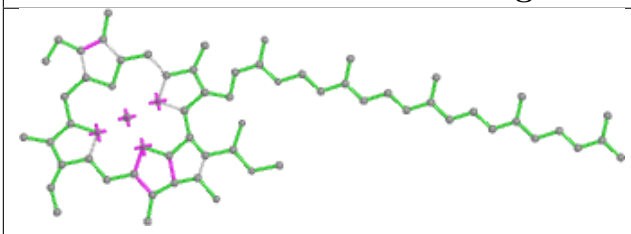


Torsions

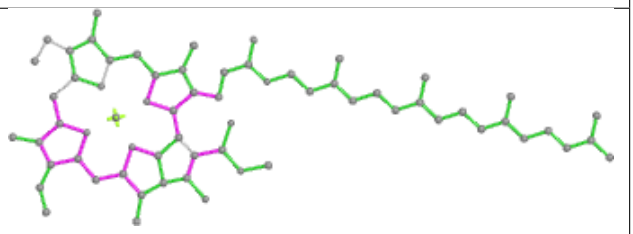


Rings

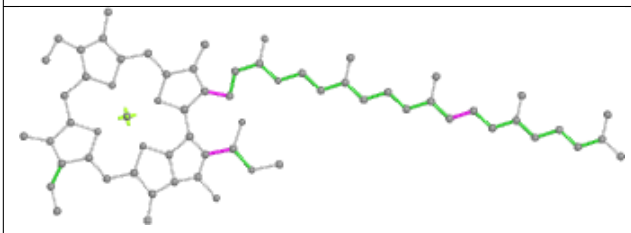
Ligand CLA B3 812



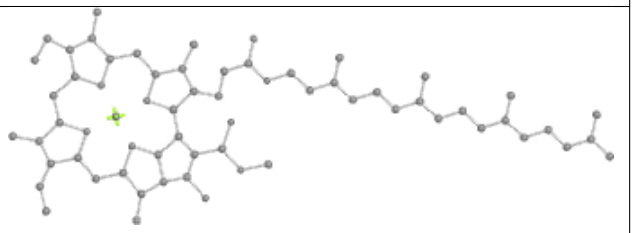
Bond lengths



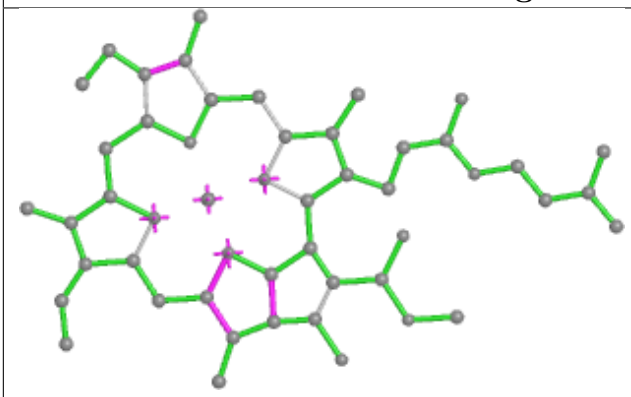
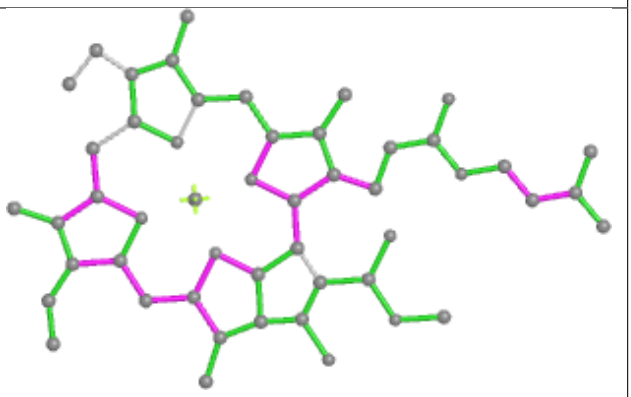
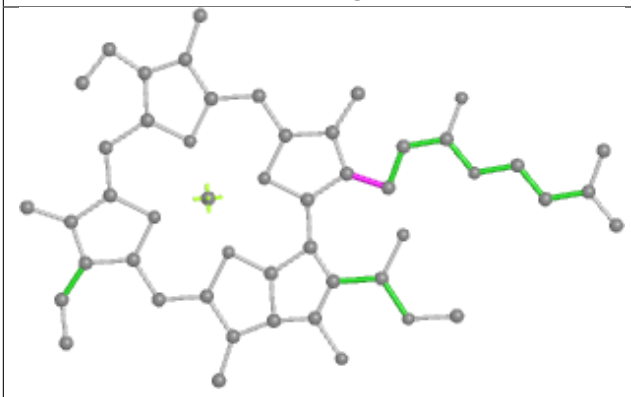
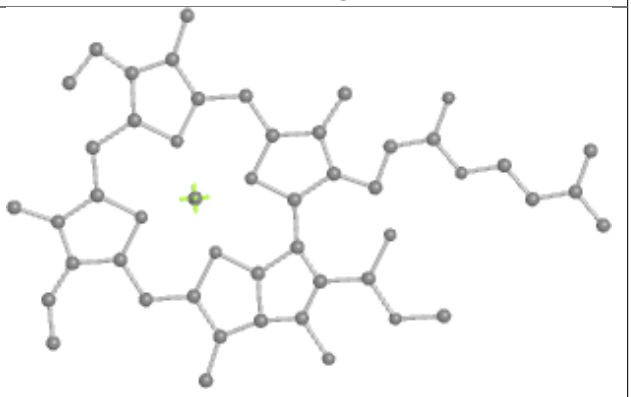
Bond angles

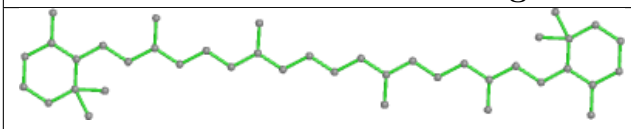
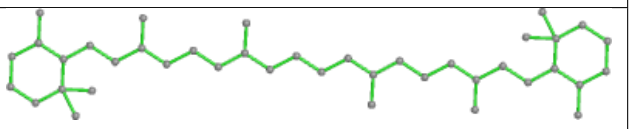
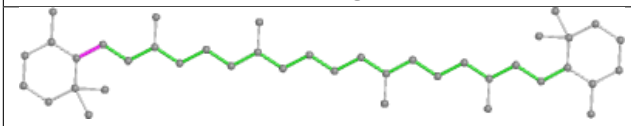
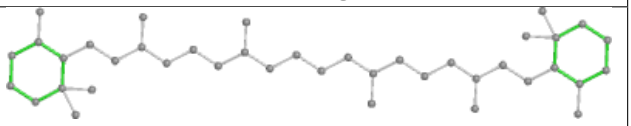


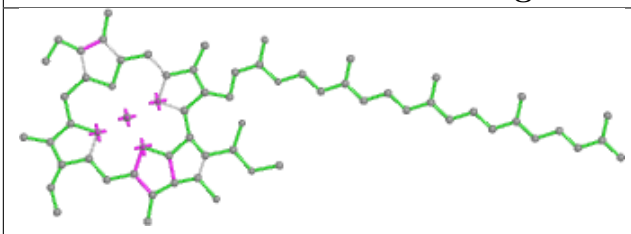
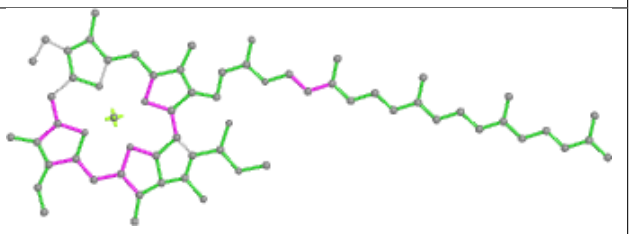
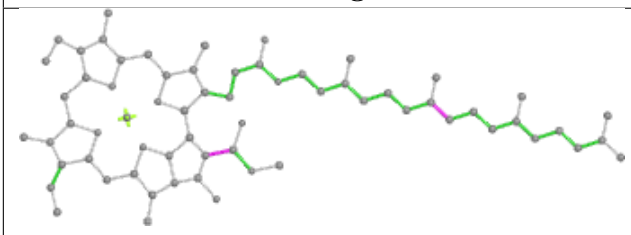
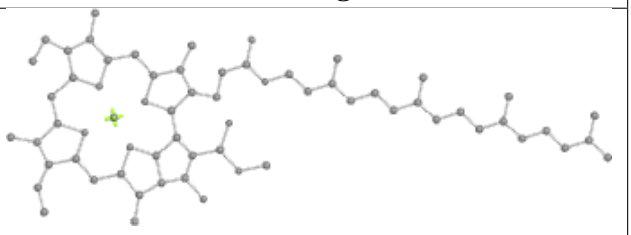
Torsions



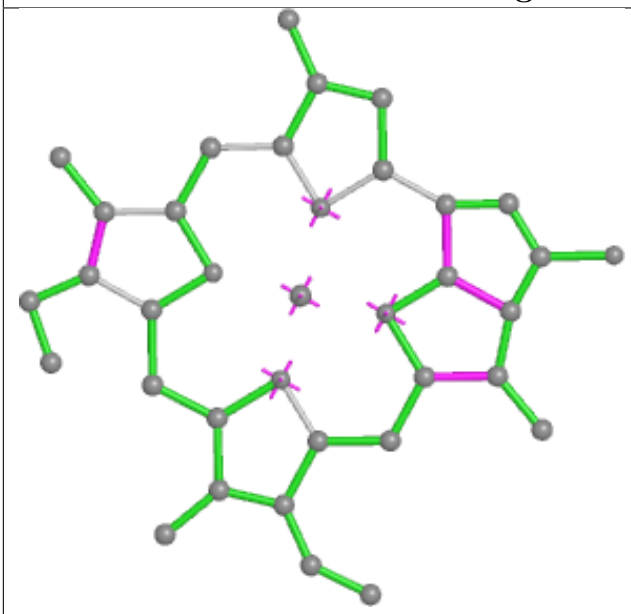
Rings

Ligand CLA B1 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

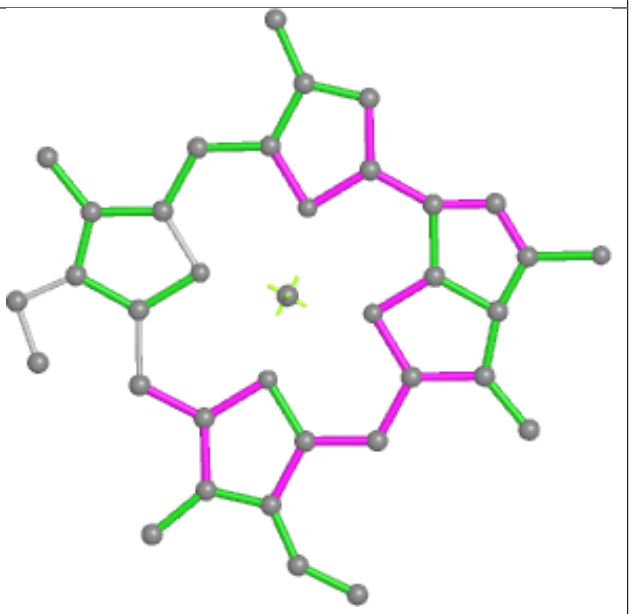
Ligand BCR M2 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

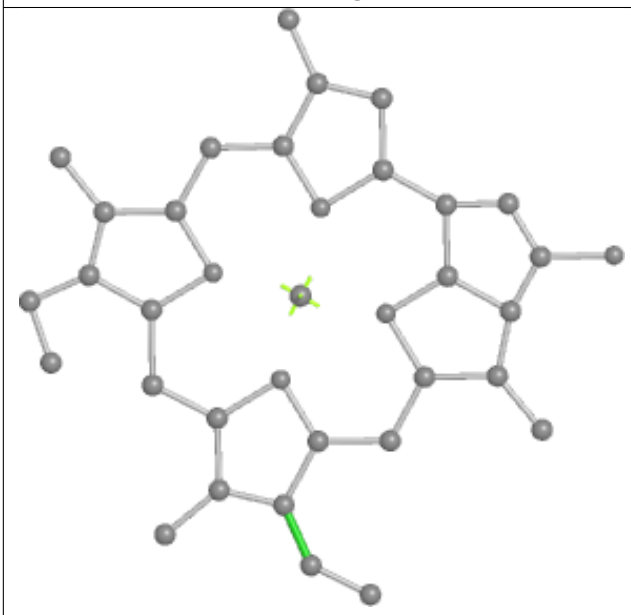
Ligand CLA B1 820



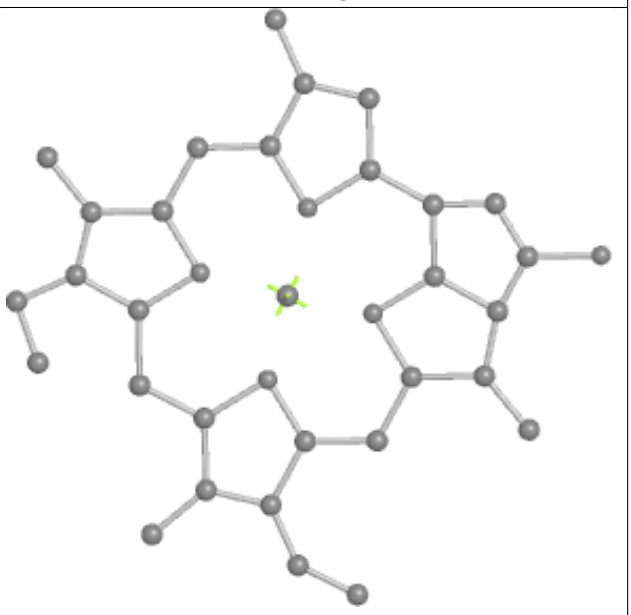
Bond lengths



Bond angles

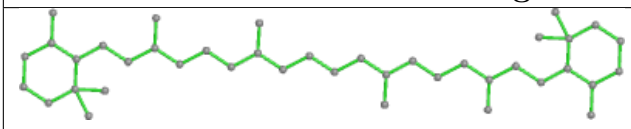


Torsions

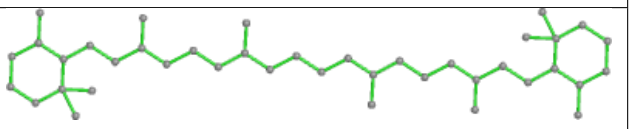


Rings

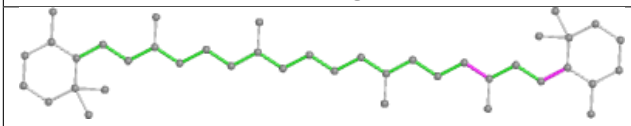
Ligand BCR A2 850



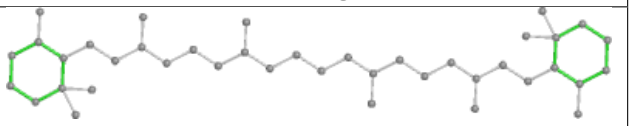
Bond lengths



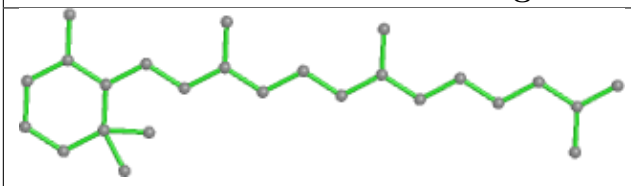
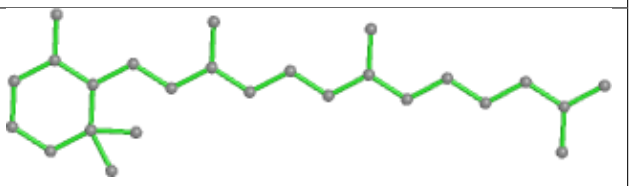
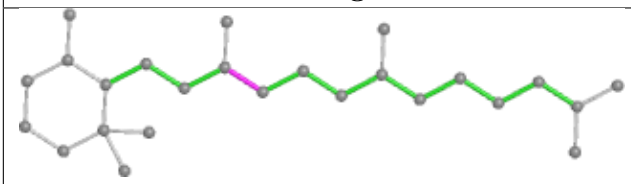
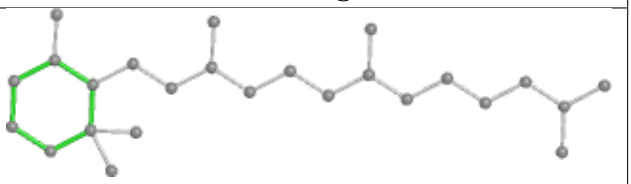
Bond angles

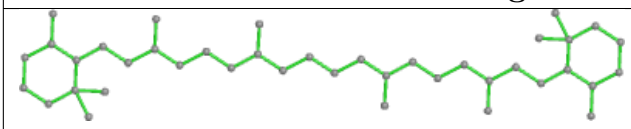
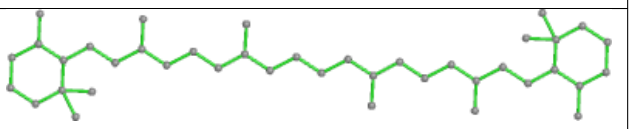
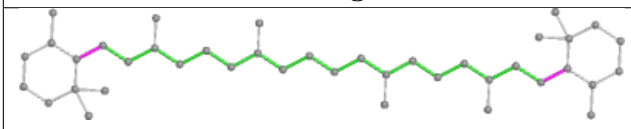
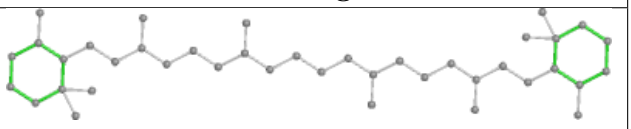


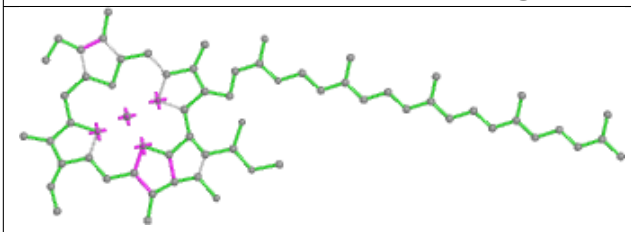
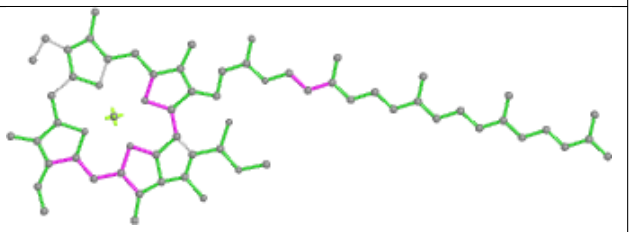
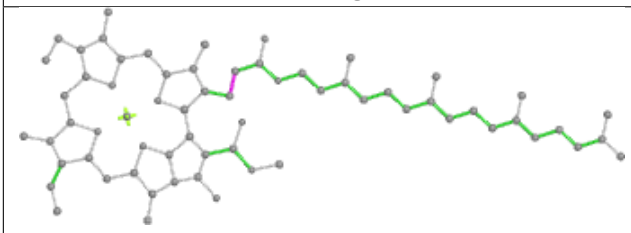
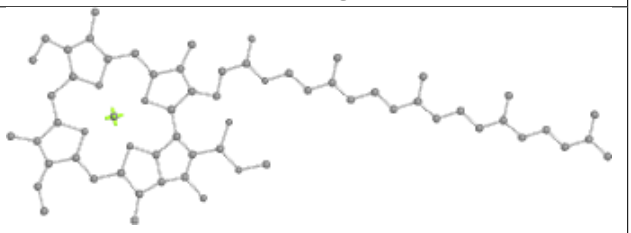
Torsions



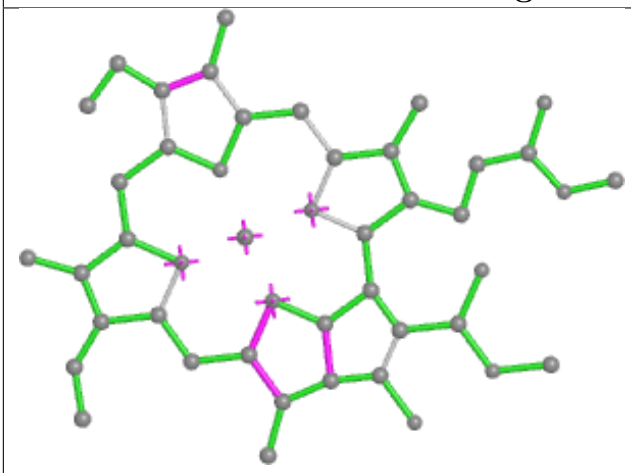
Rings

Ligand BCR B2 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

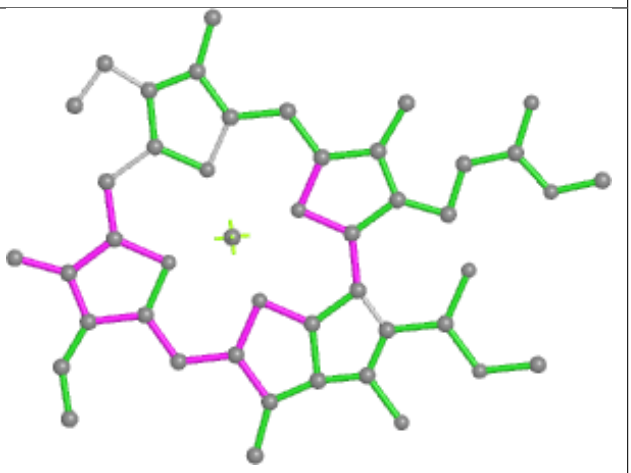
Ligand BCR J3 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

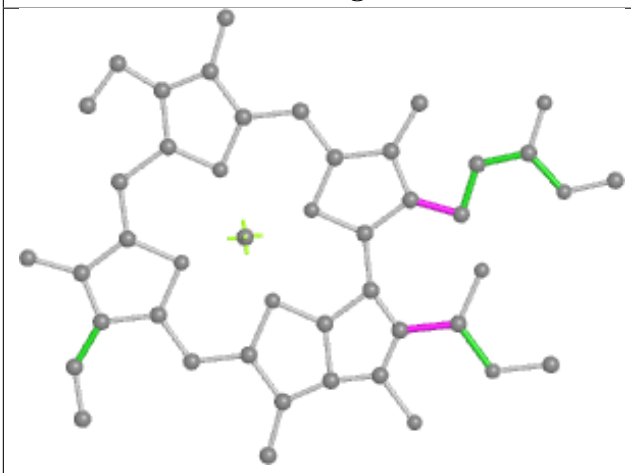
Ligand CLA B2 835



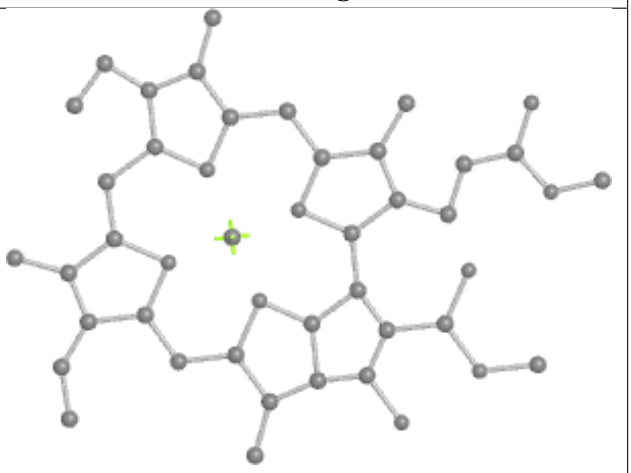
Bond lengths



Bond angles

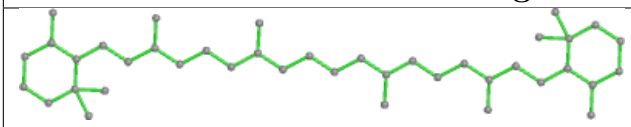


Torsions

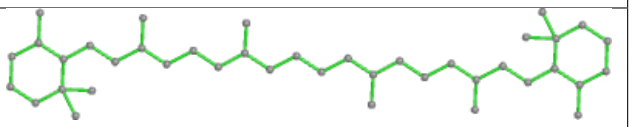


Rings

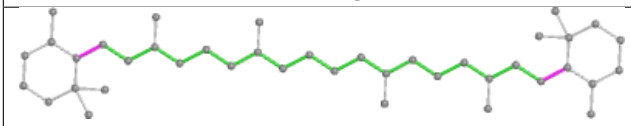
Ligand BCR A3 848



Bond lengths

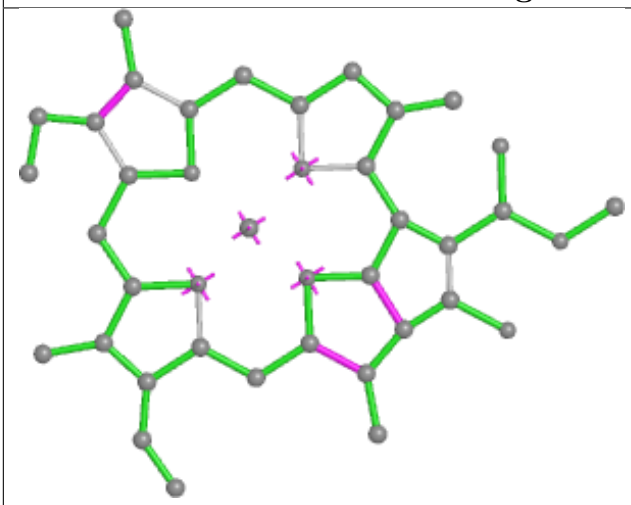
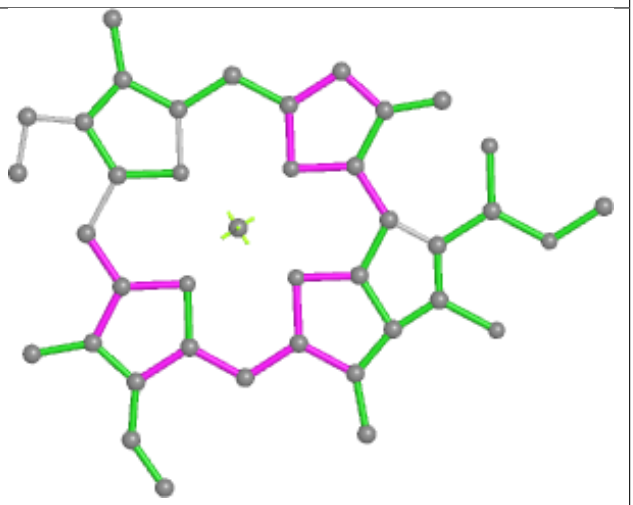
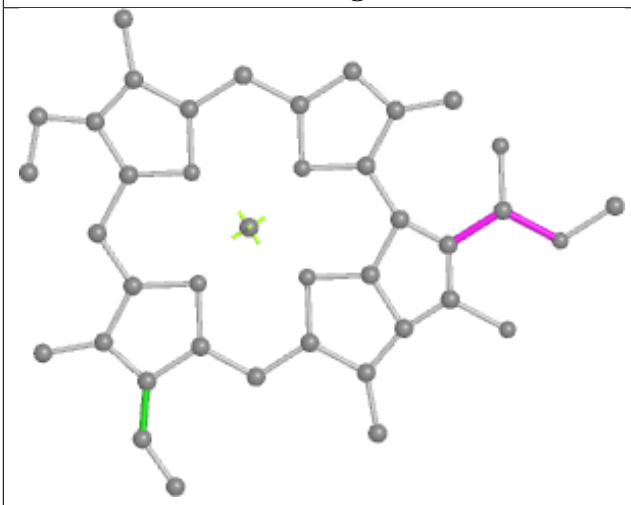
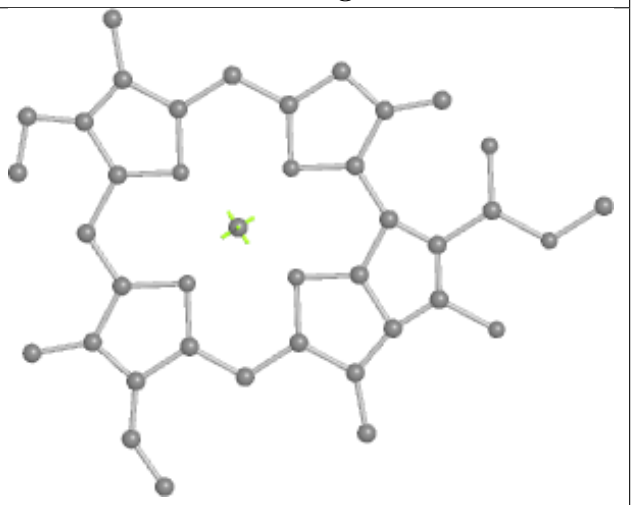


Bond angles

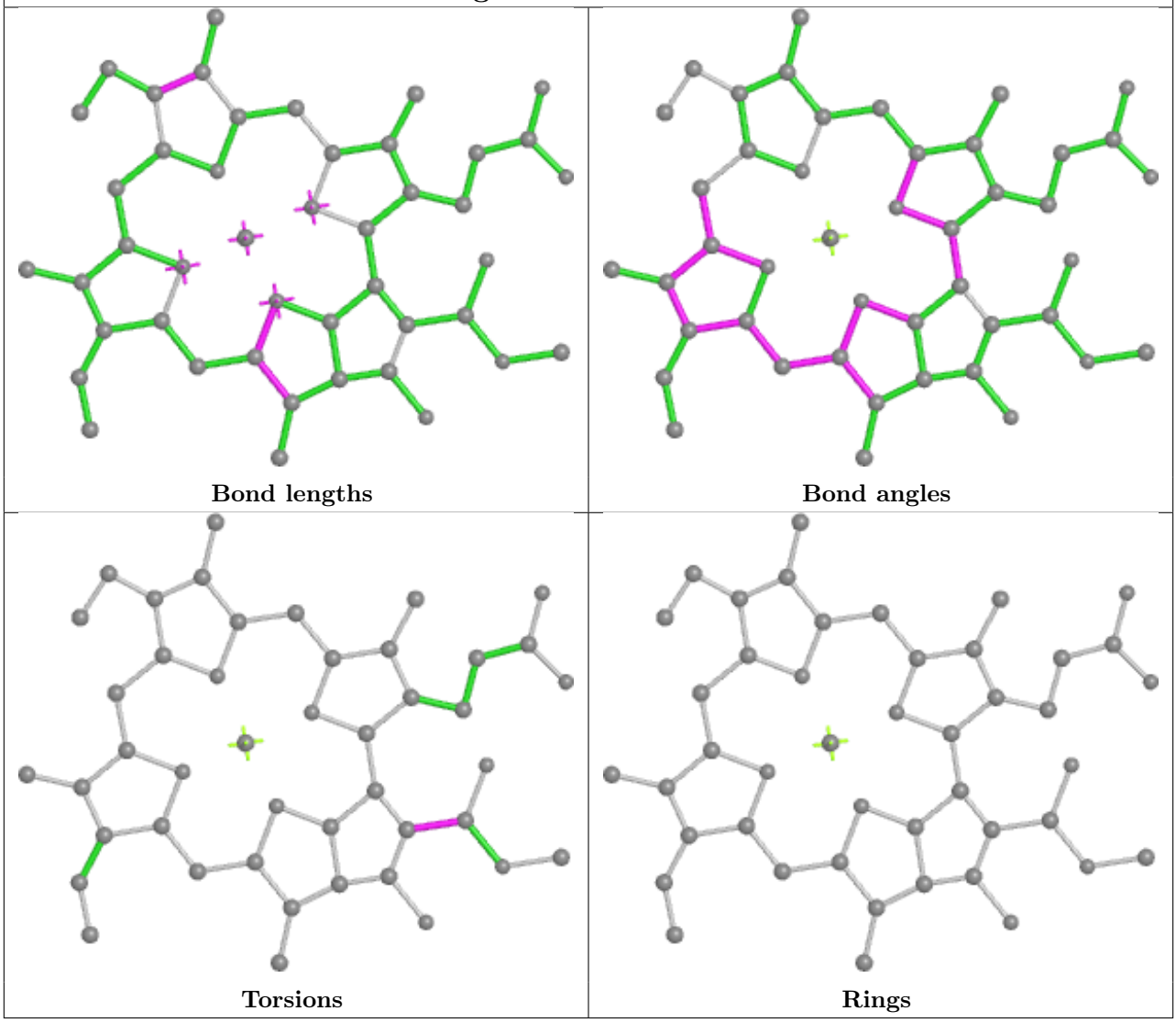


Torsions

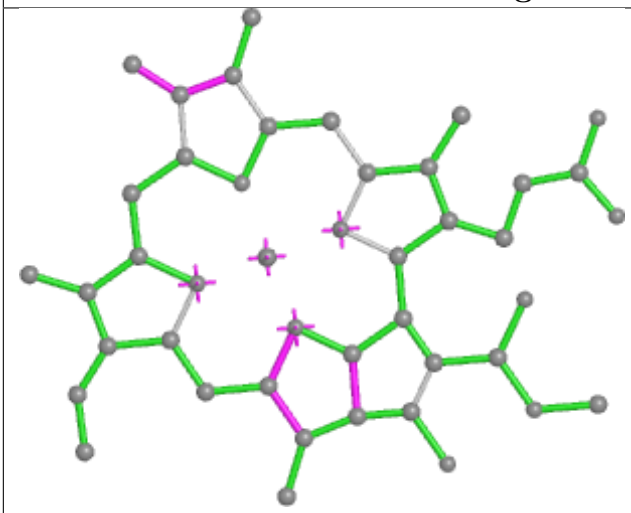
Rings

Ligand CLA B3 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

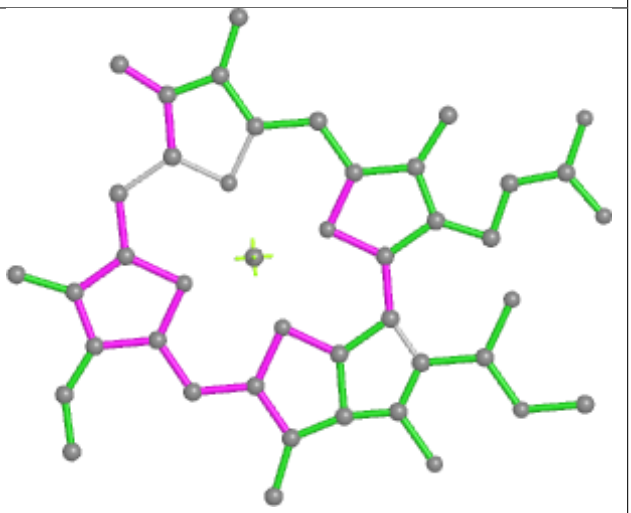
Ligand CLA B3 811



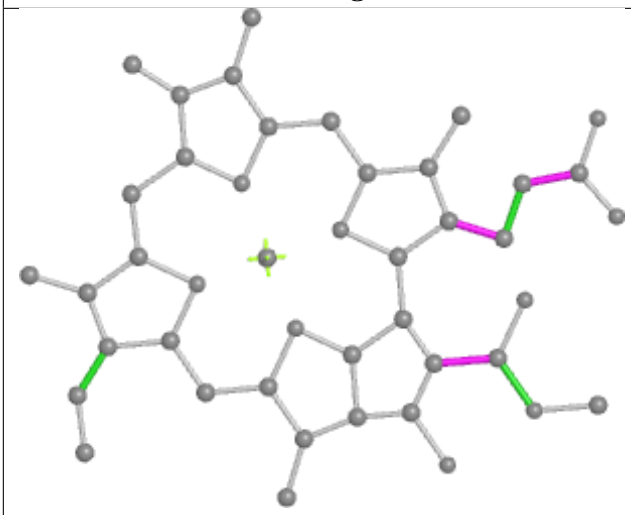
Ligand CLA A3 813



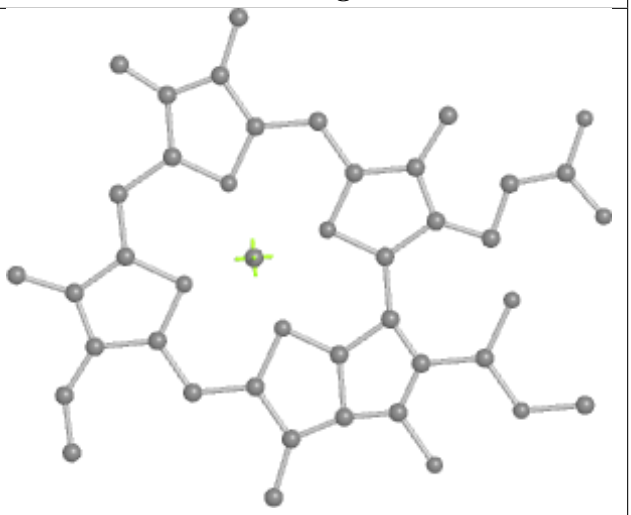
Bond lengths



Bond angles

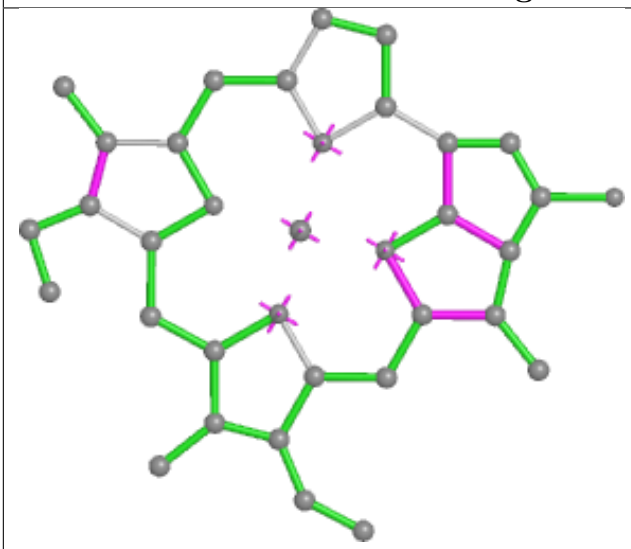


Torsions

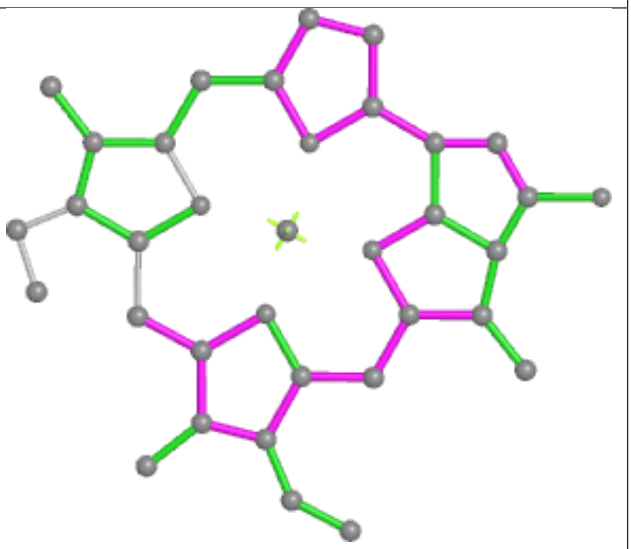


Rings

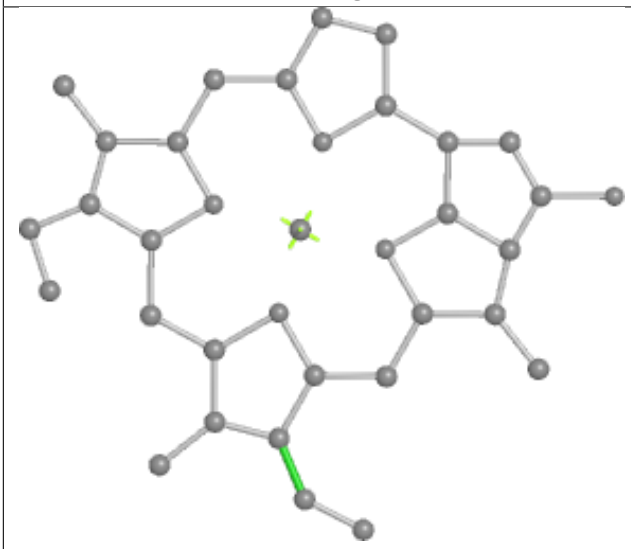
Ligand CLA B2 829



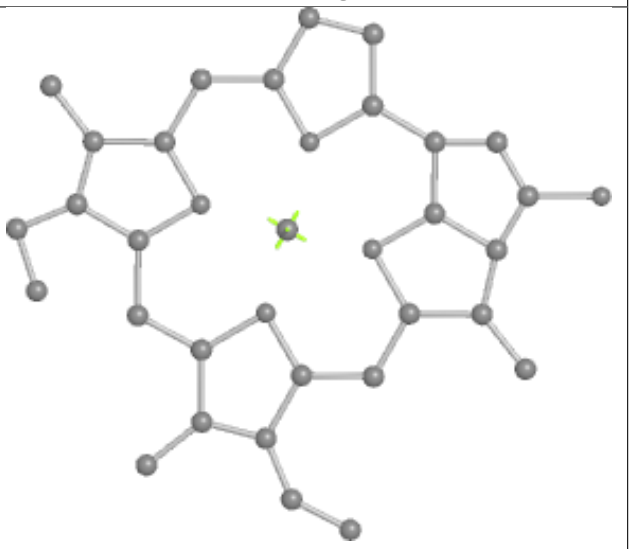
Bond lengths



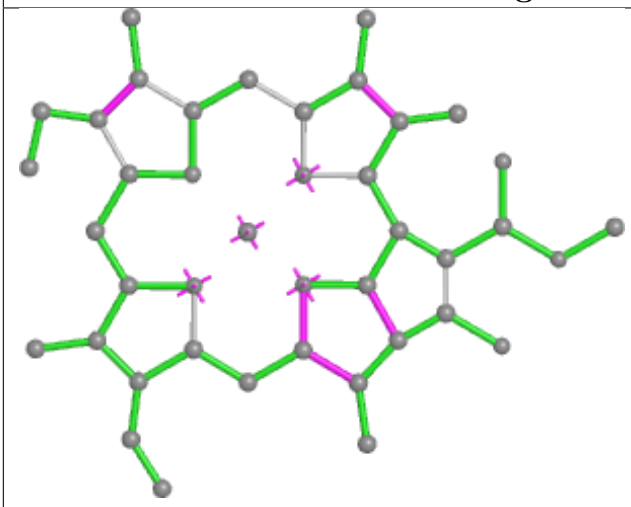
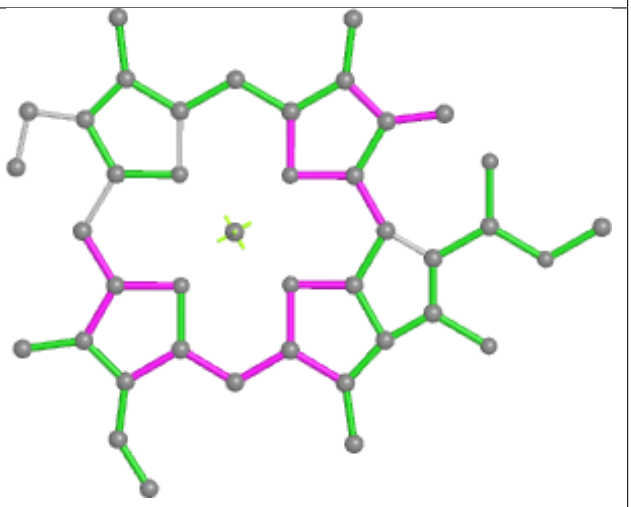
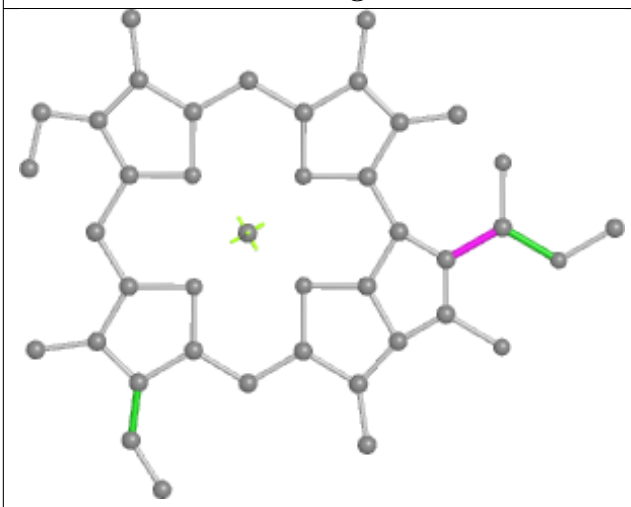
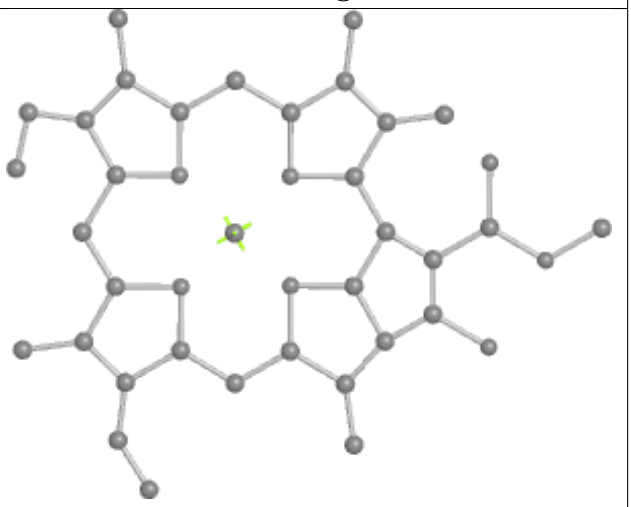
Bond angles

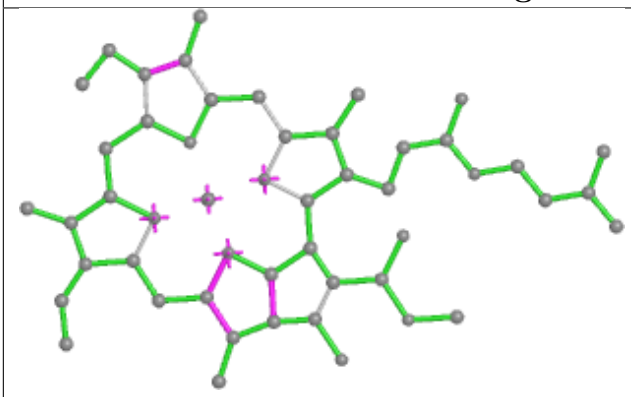
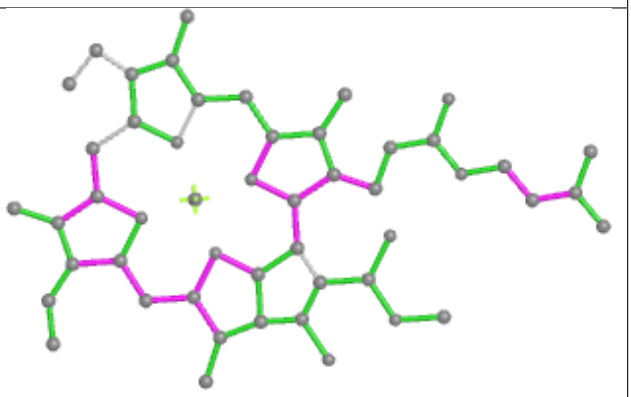
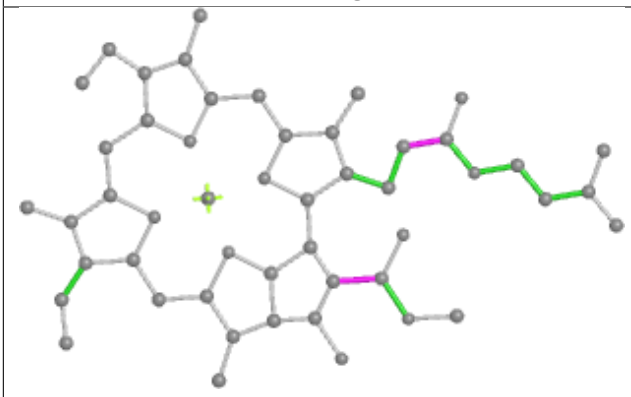
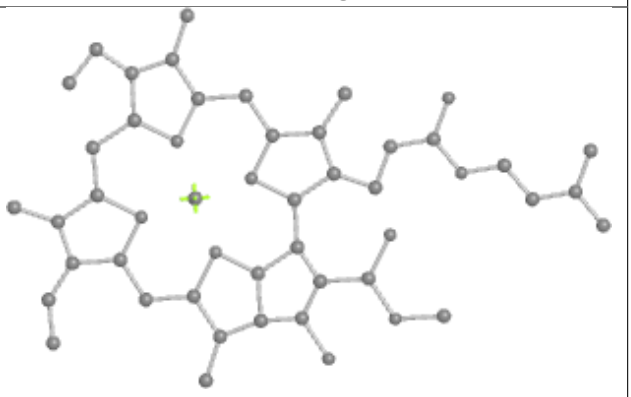


Torsions

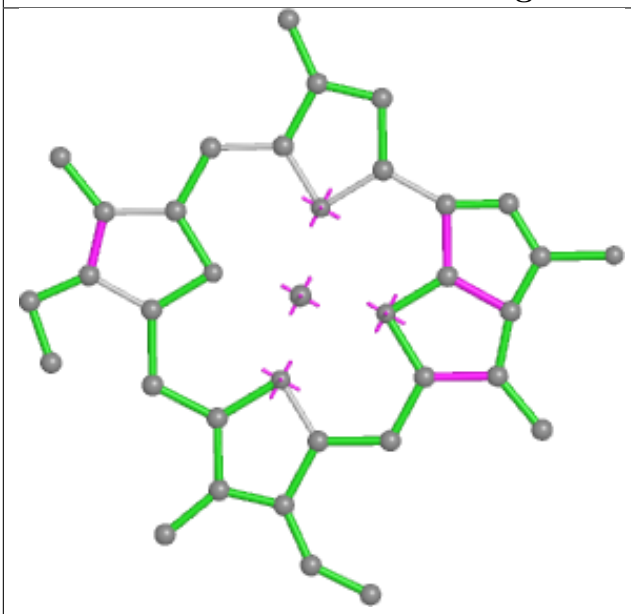


Rings

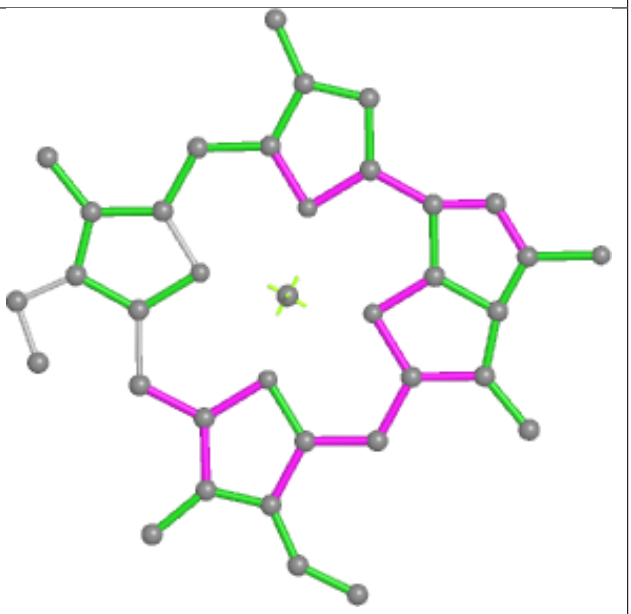
Ligand CLA B3 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

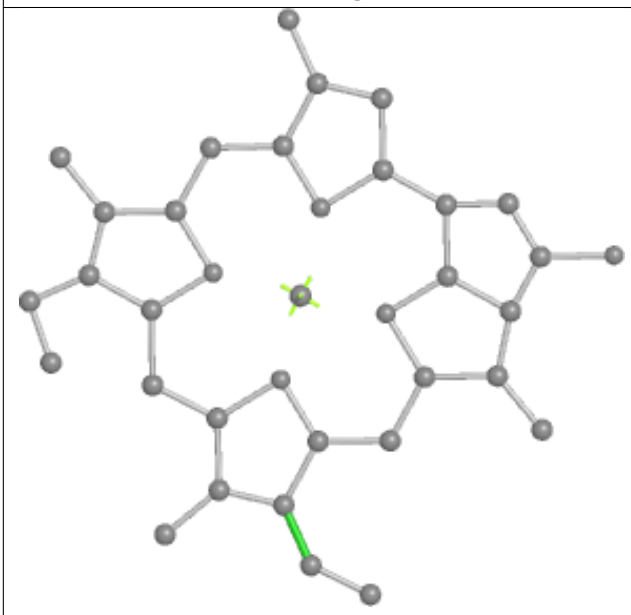
Ligand CLA B2 815



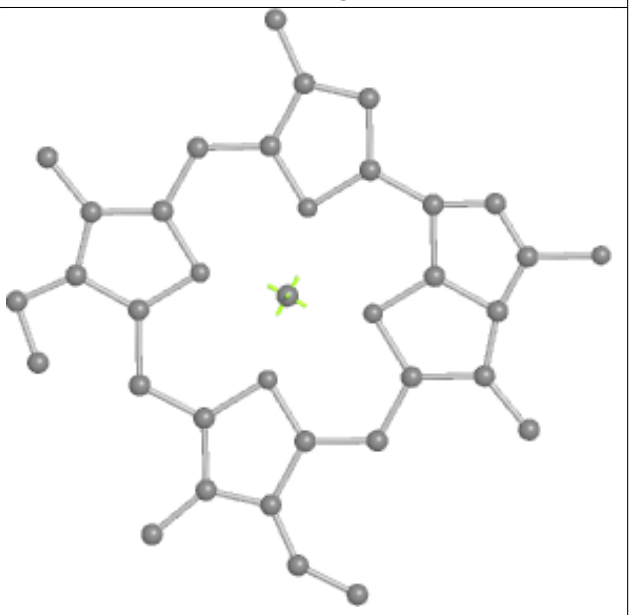
Bond lengths



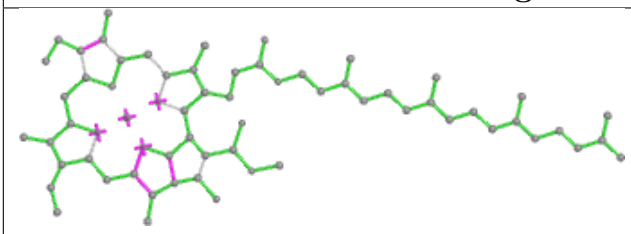
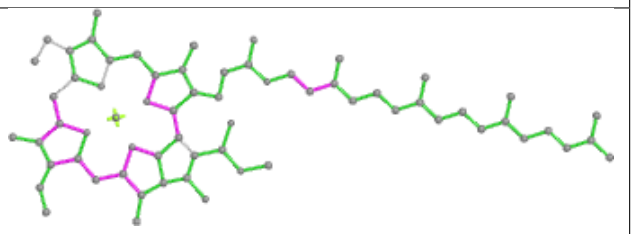
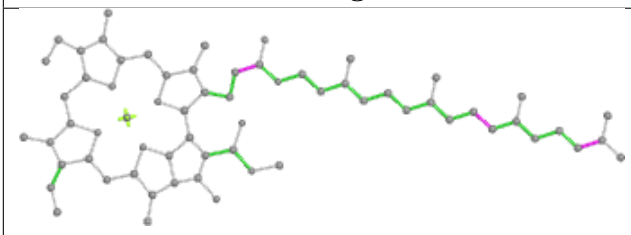
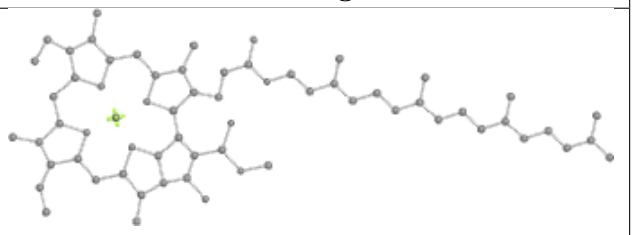
Bond angles

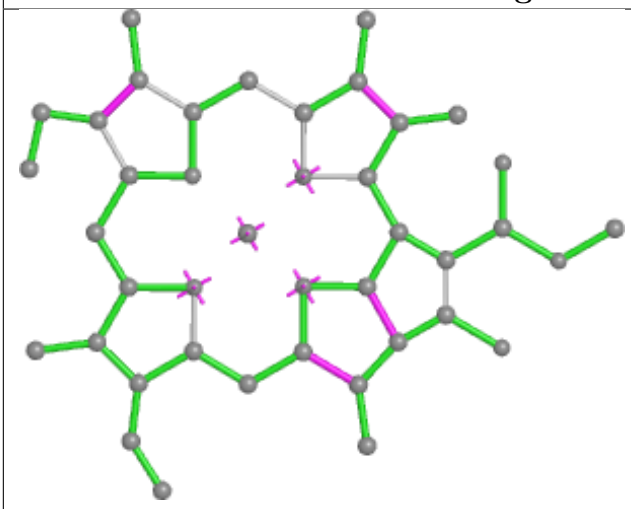
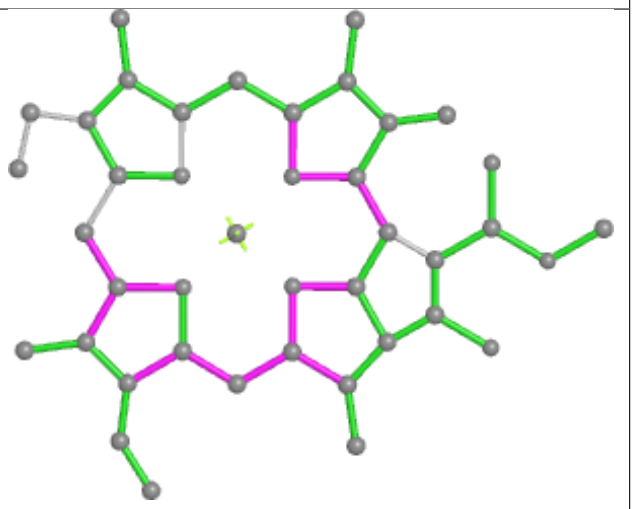
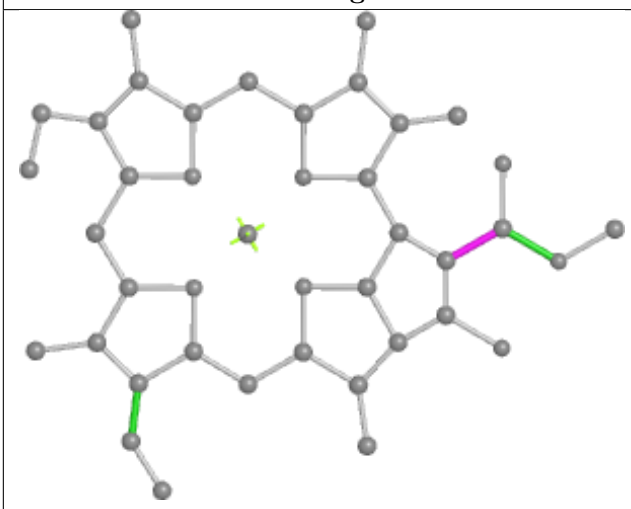
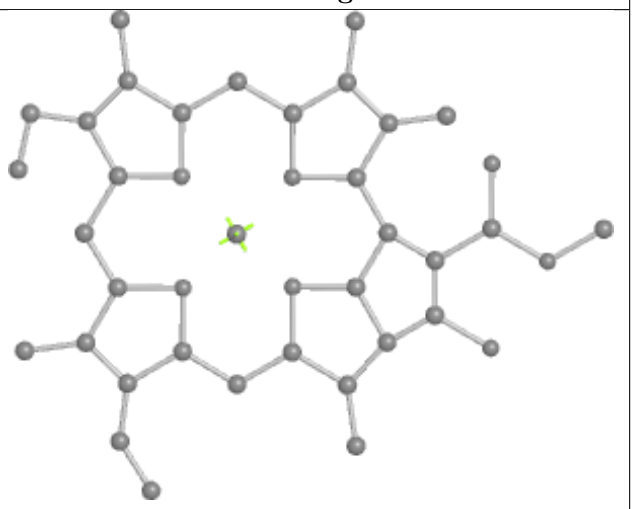


Torsions

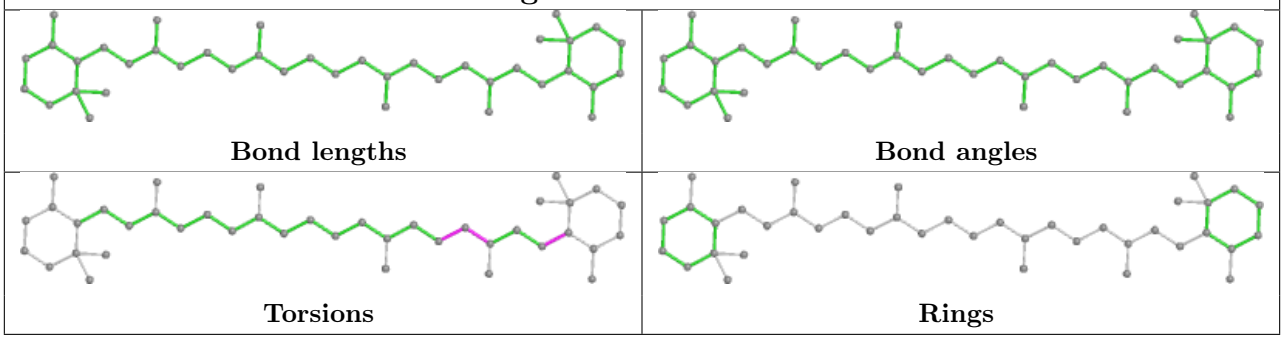


Rings

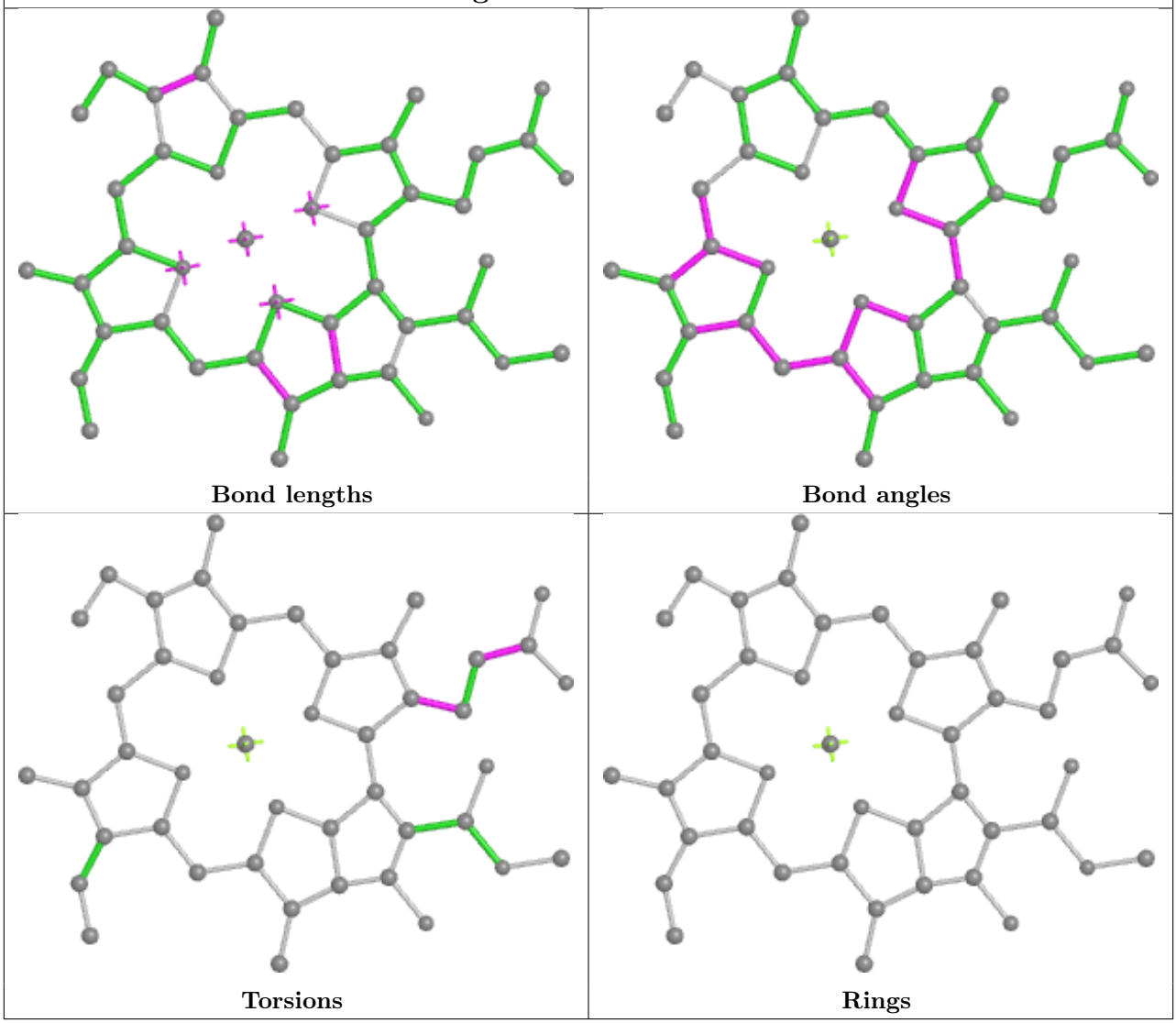
Ligand CLA A2 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A3 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

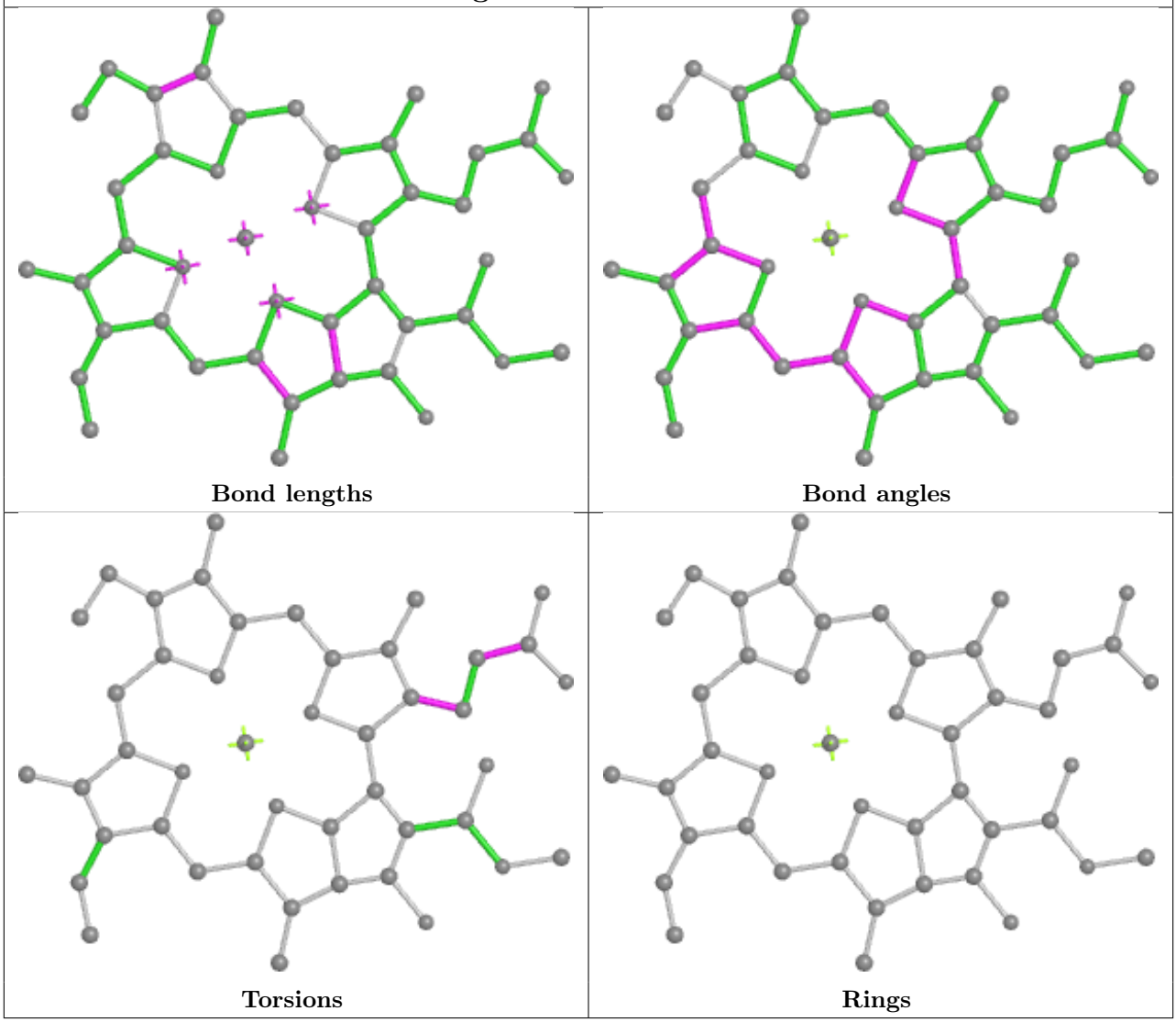
Ligand BCR I3 103

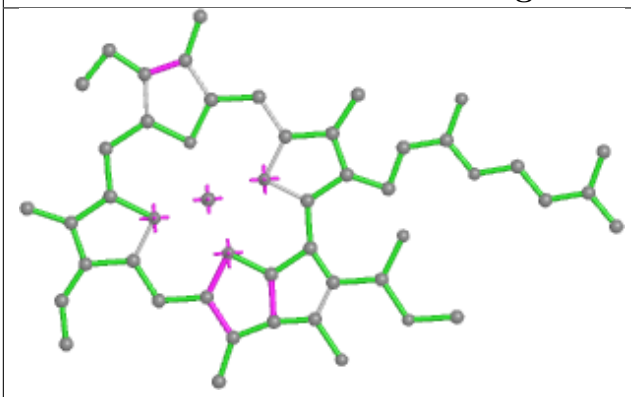
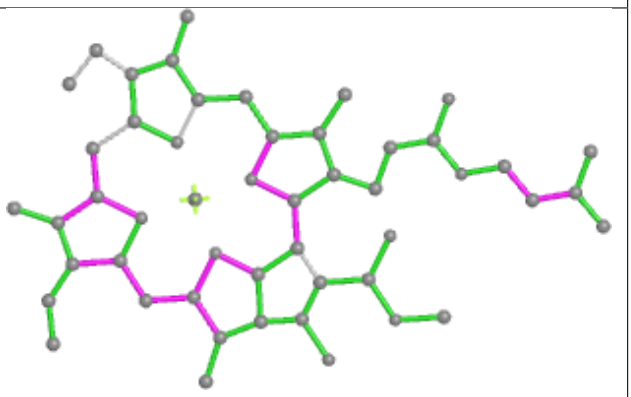
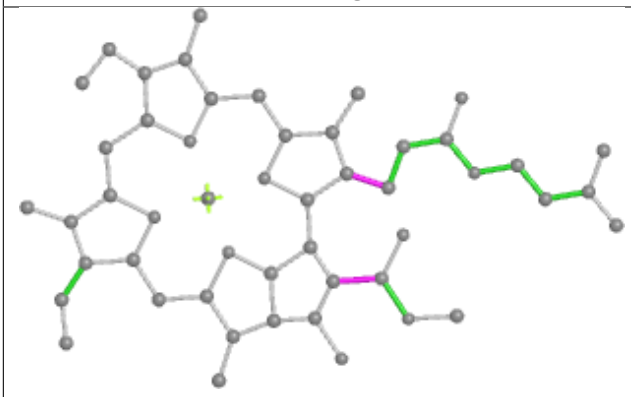
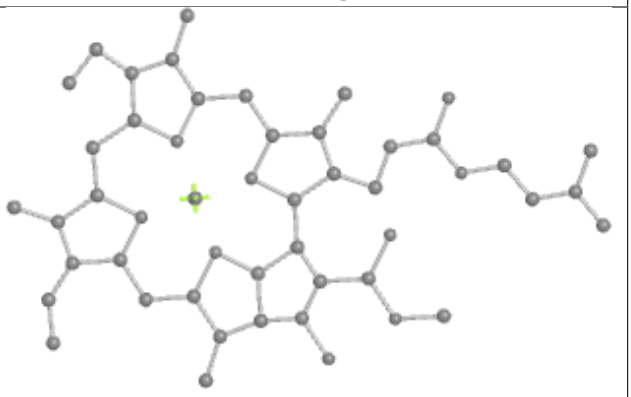


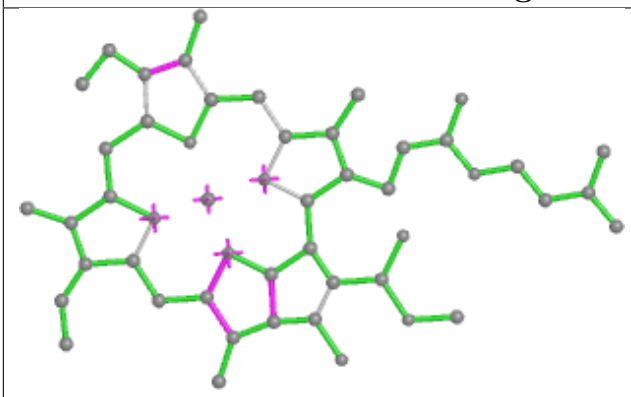
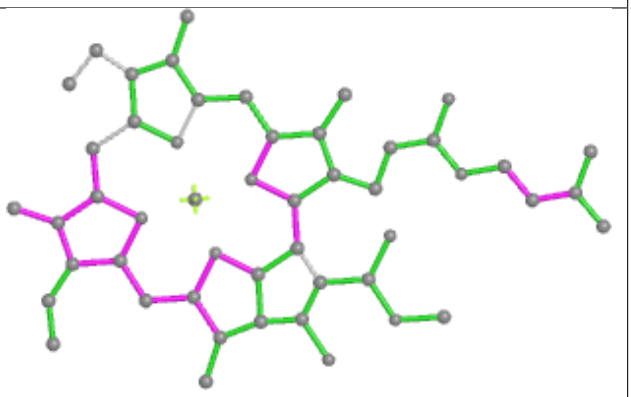
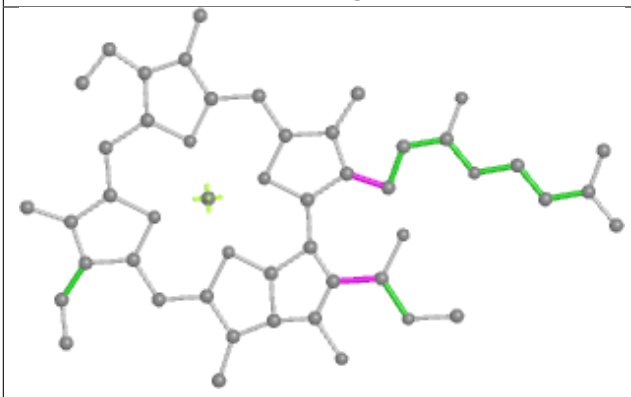
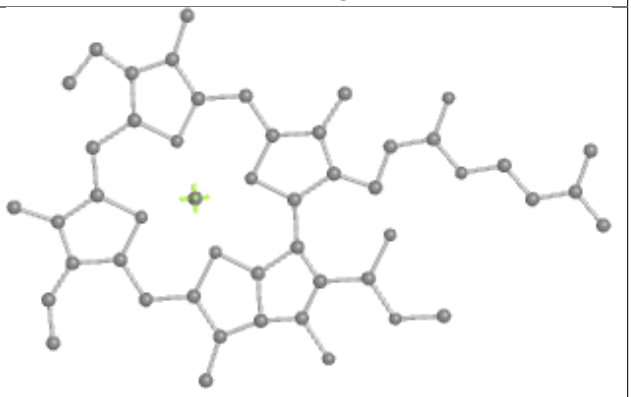
Ligand CLA A1 835



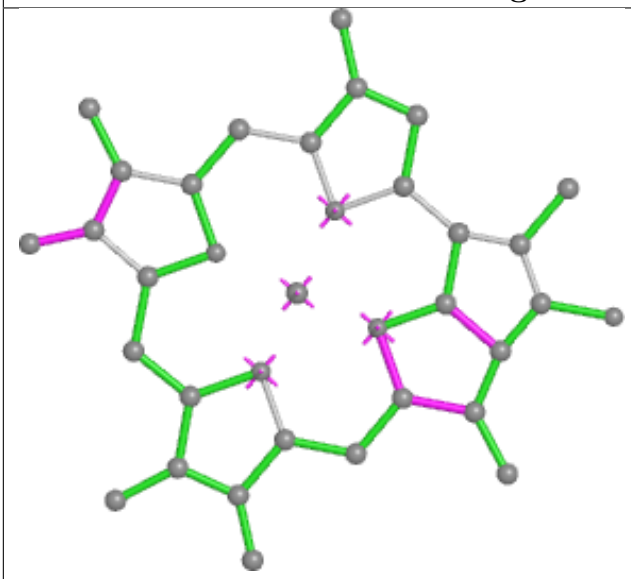
Ligand CLA A2 835



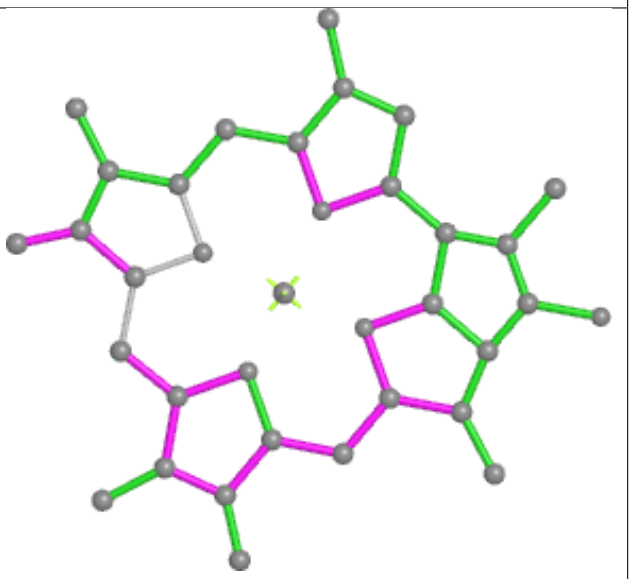
Ligand CLA B2 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

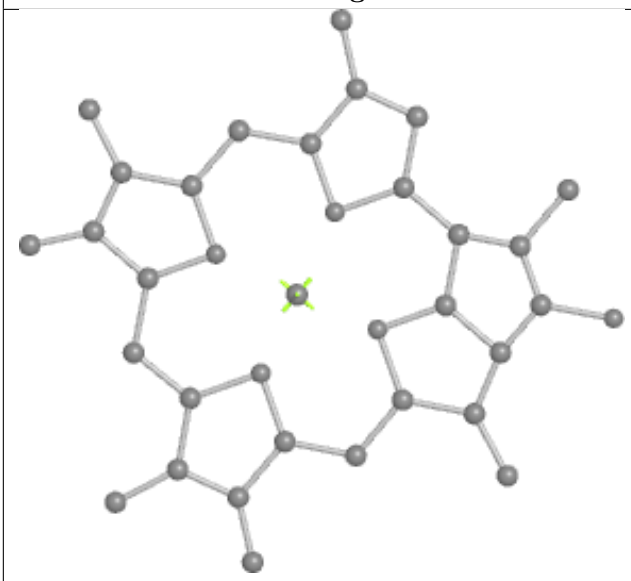
Ligand CLA J3 1302



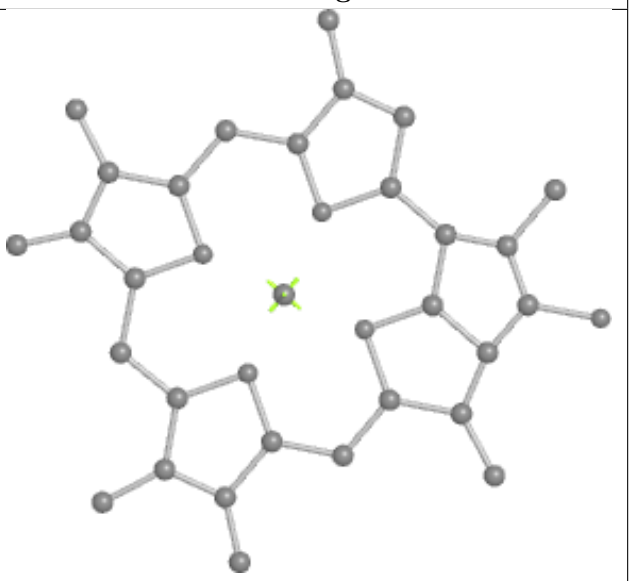
Bond lengths



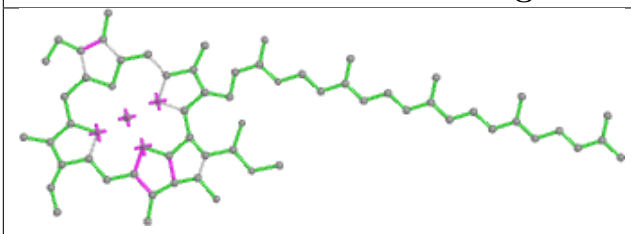
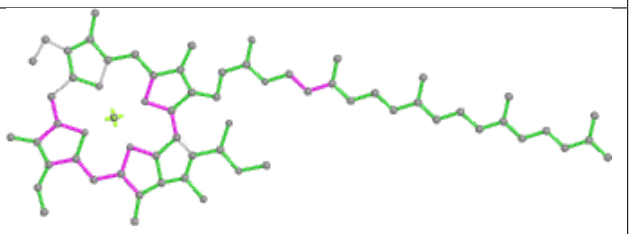
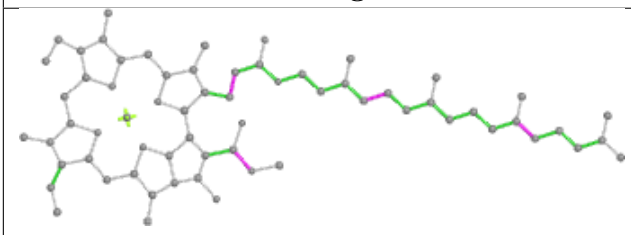
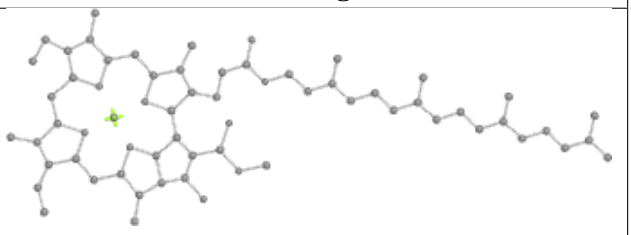
Bond angles



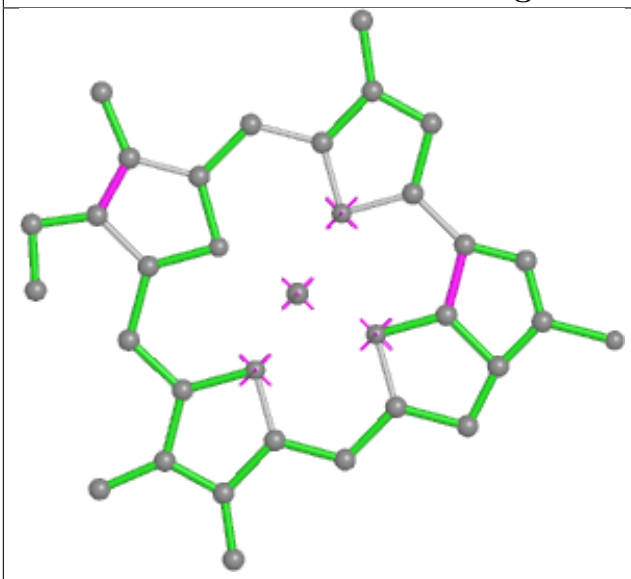
Torsions



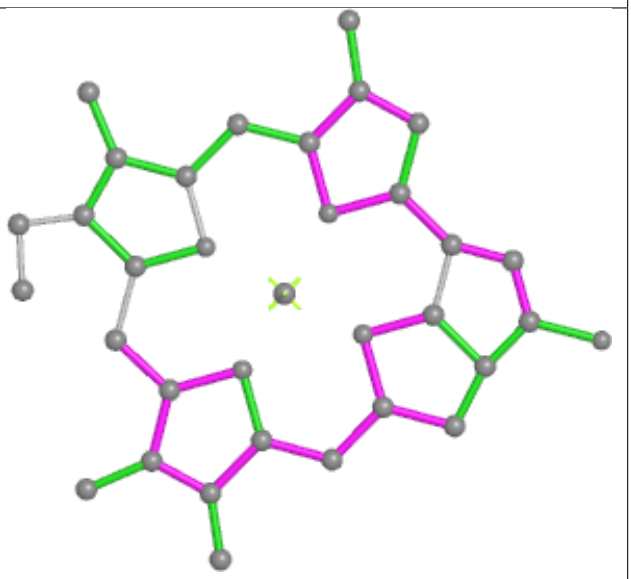
Rings

Ligand CLA B3 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

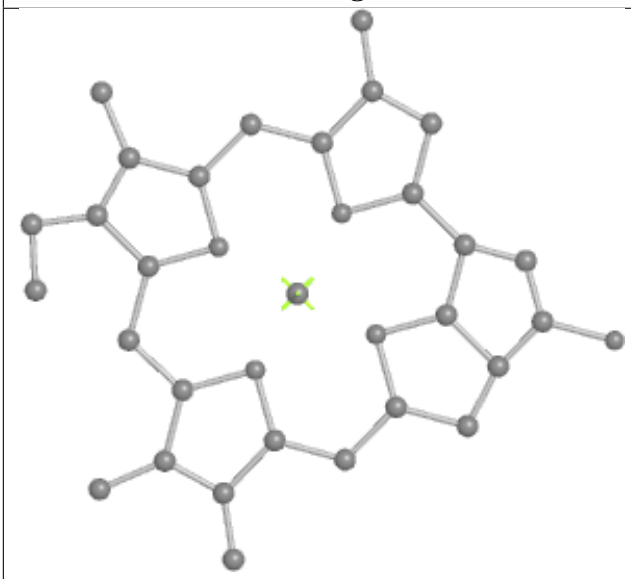
Ligand CLA K3 101



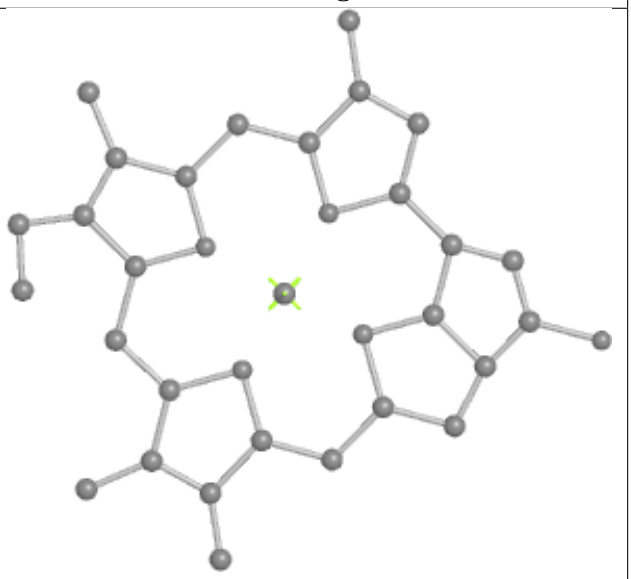
Bond lengths



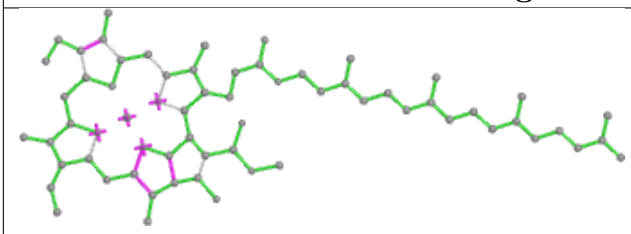
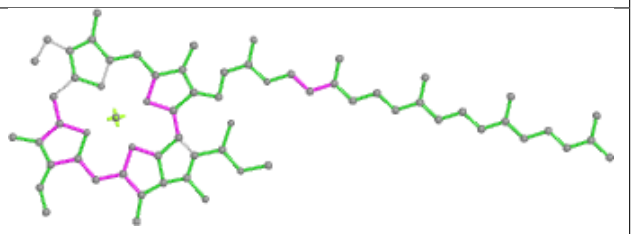
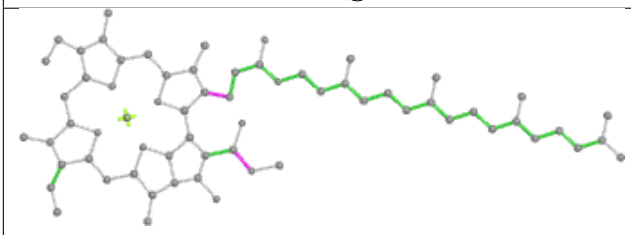
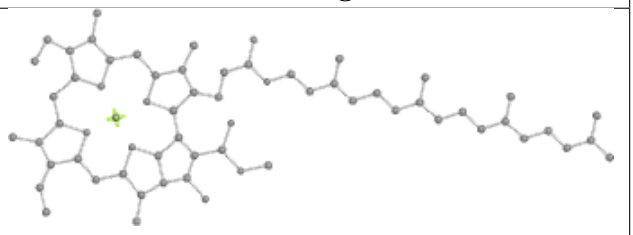
Bond angles

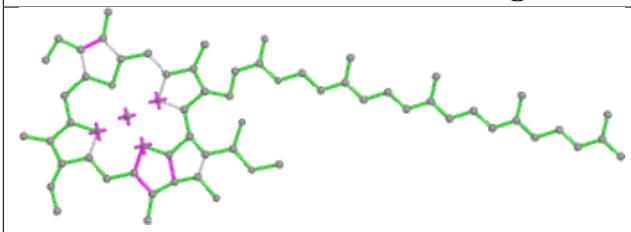
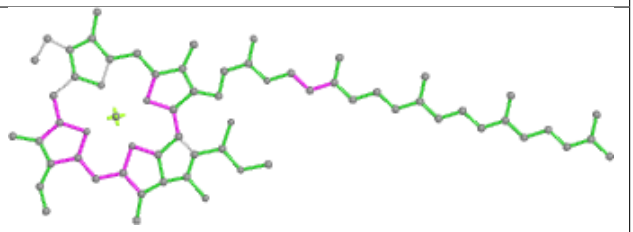
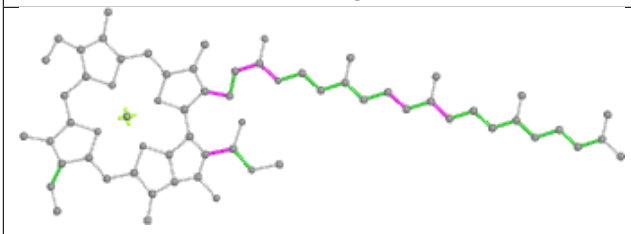
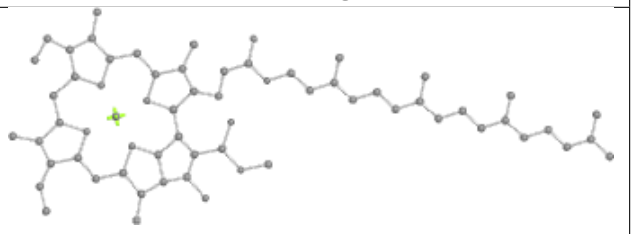


Torsions

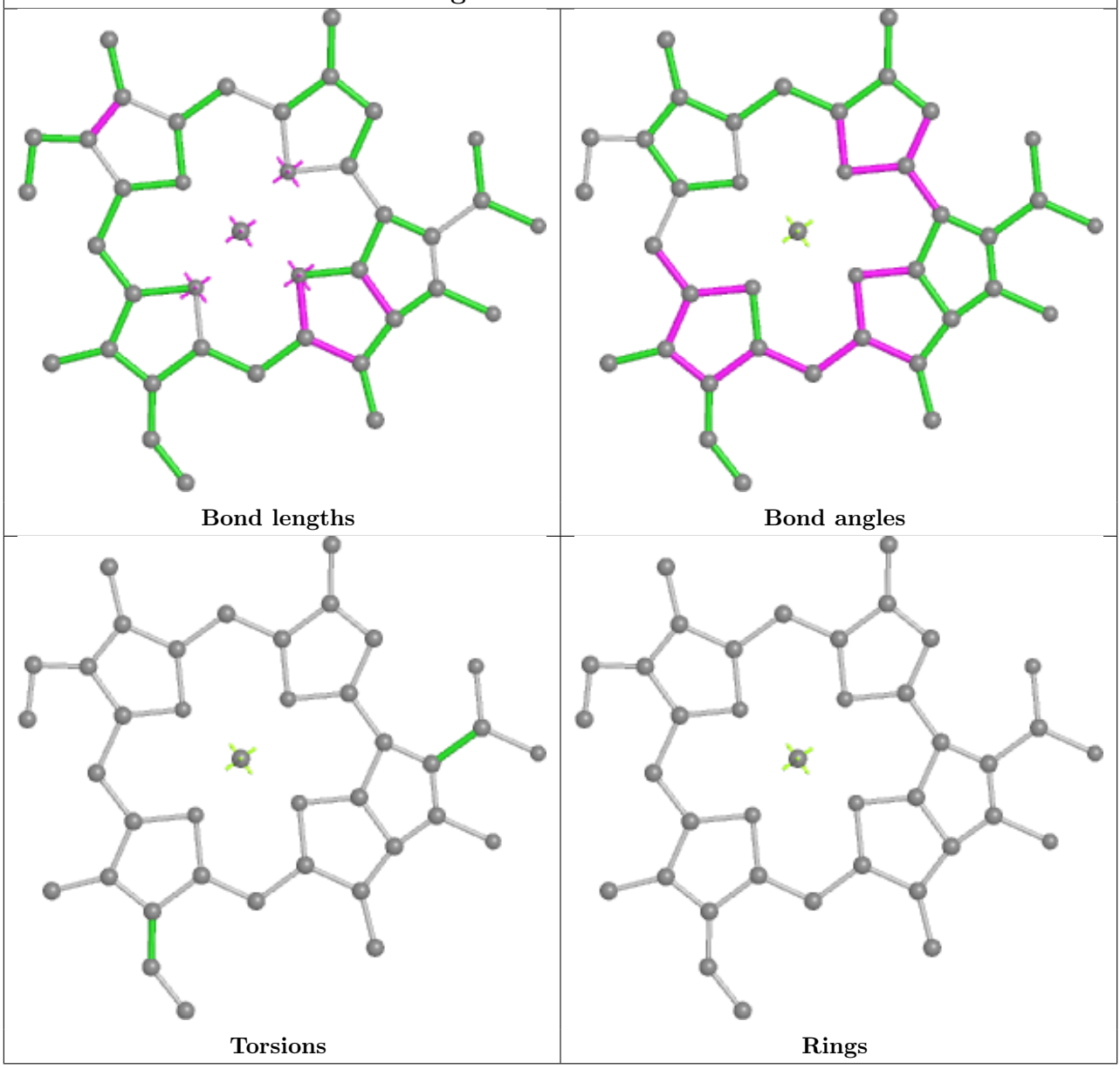


Rings

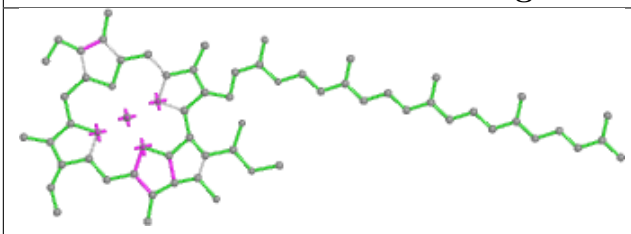
Ligand CLA B1 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L2 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

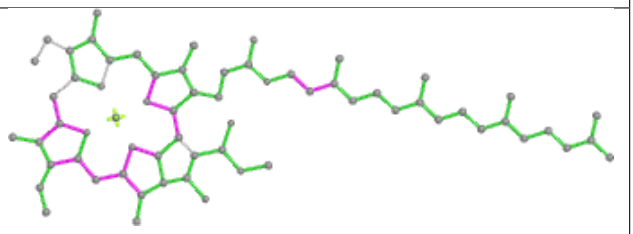
Ligand CLA B3 834



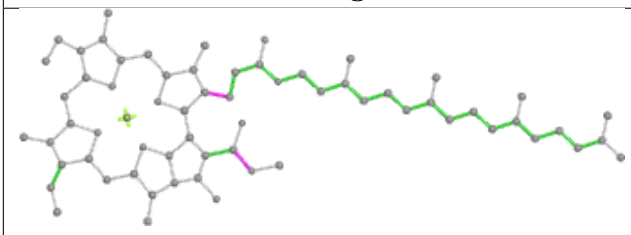
Ligand CLA B2 809



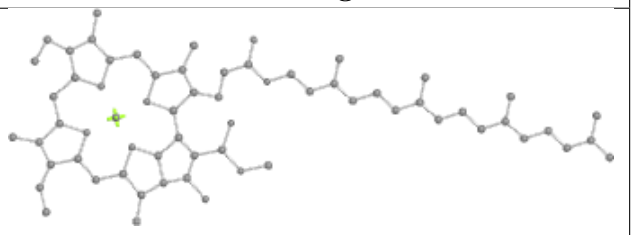
Bond lengths



Bond angles

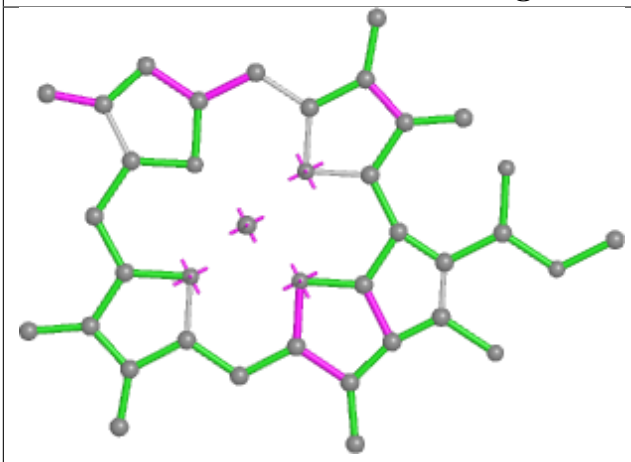


Torsions



Rings

Ligand CLA A3 817



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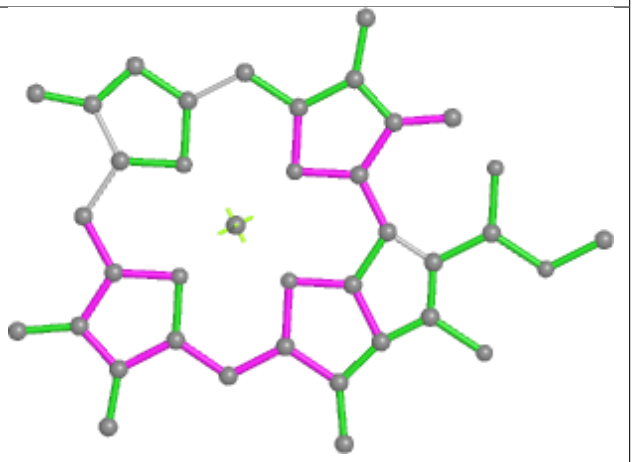
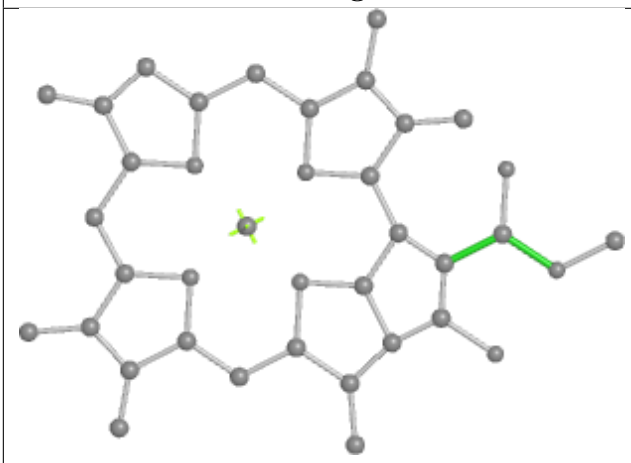
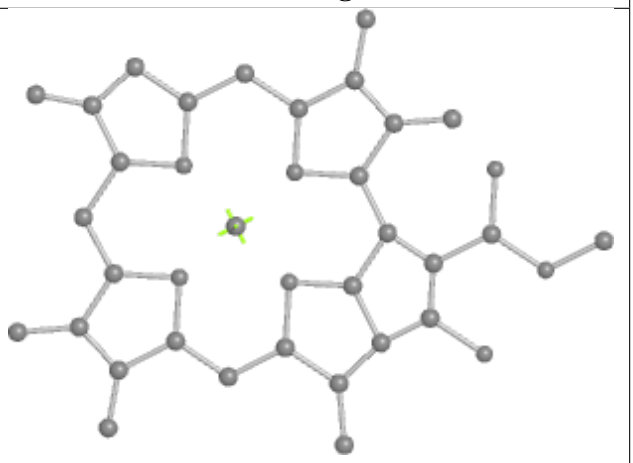


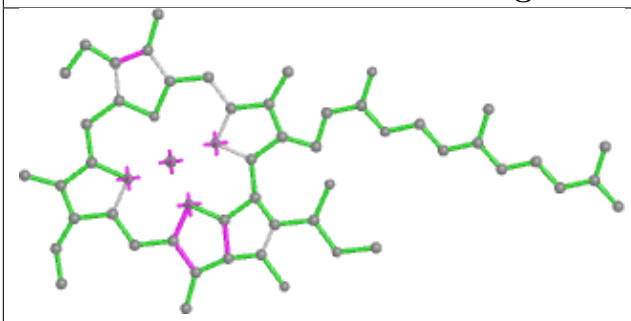
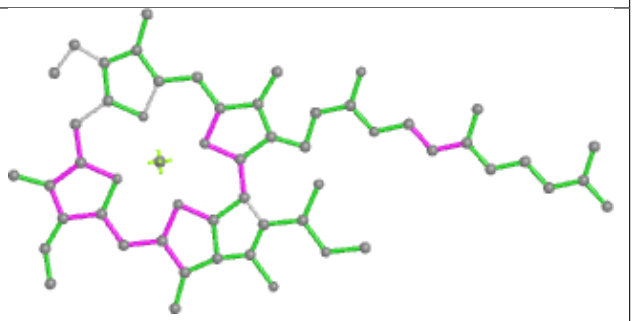
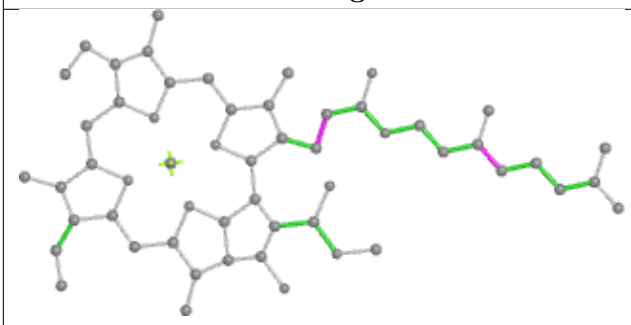
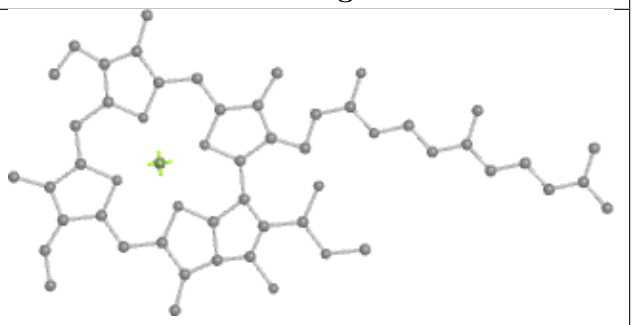
Bond angles

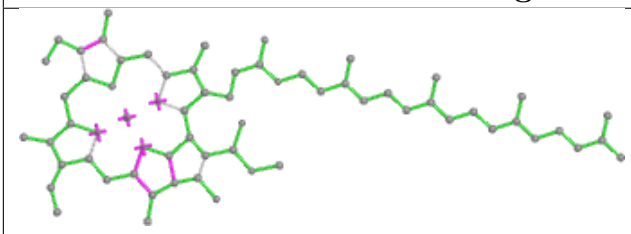
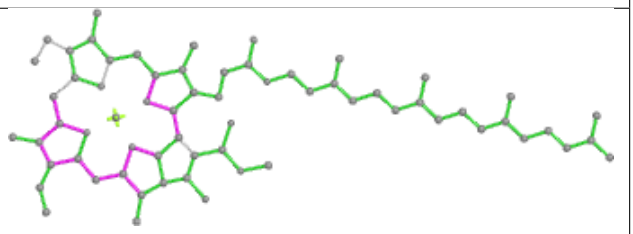
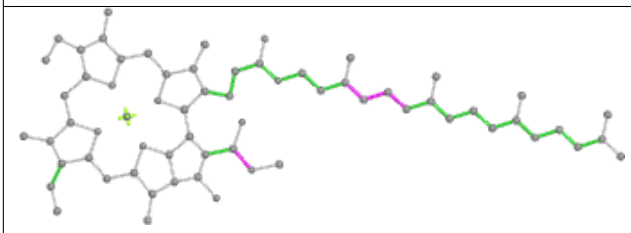
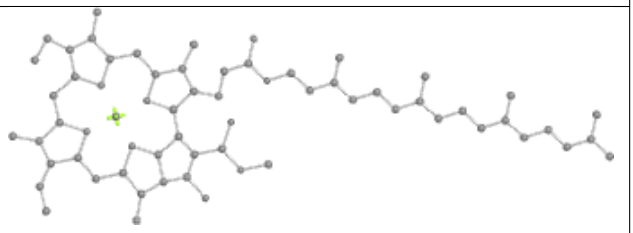


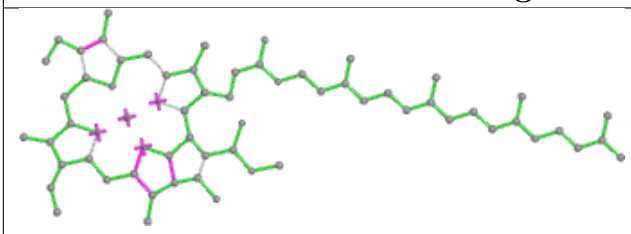
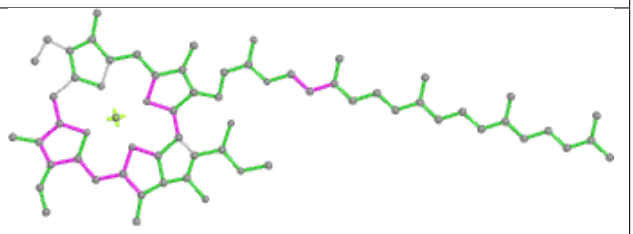
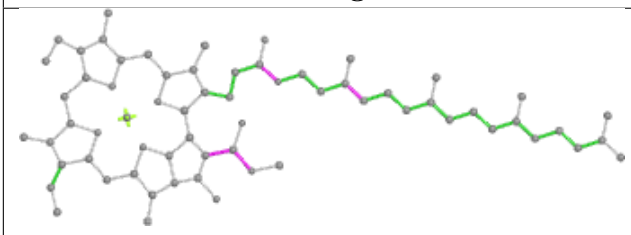
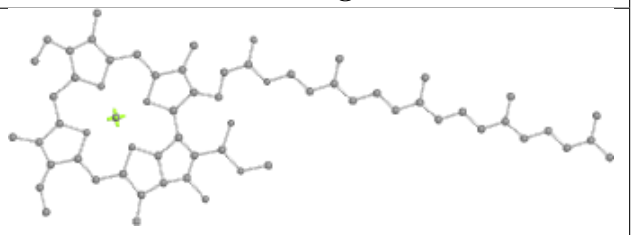
Torsions

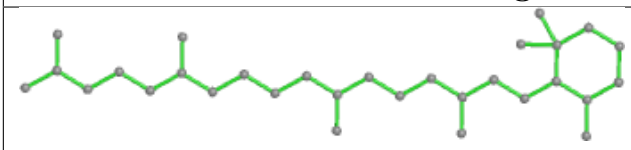
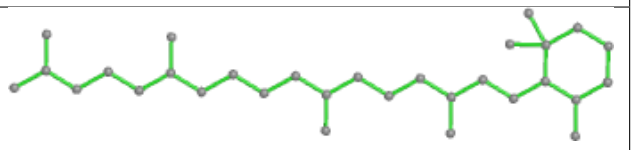
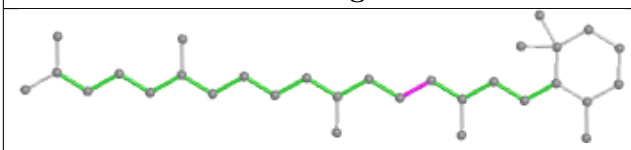
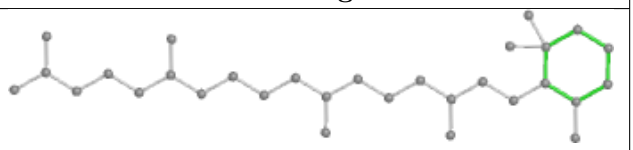


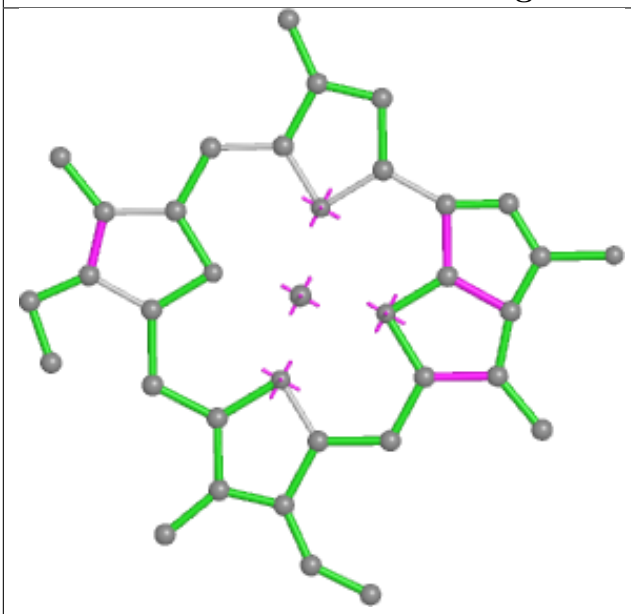
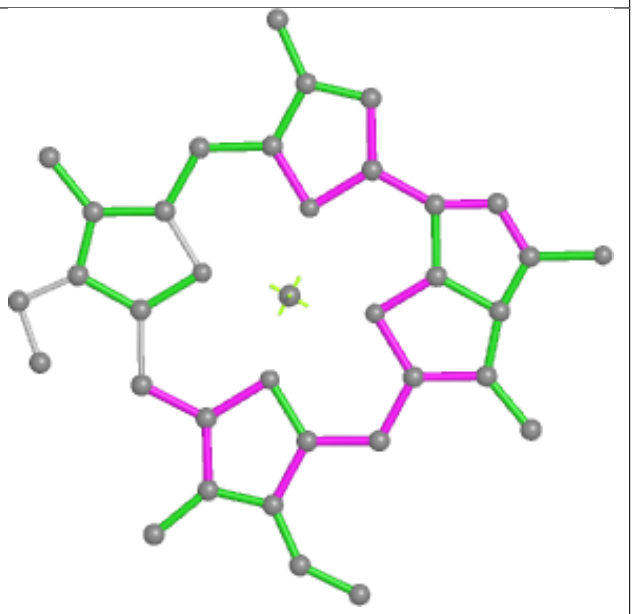
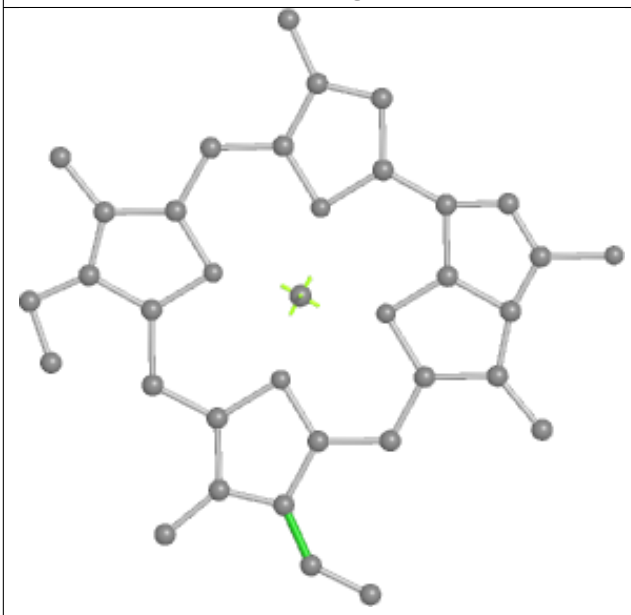
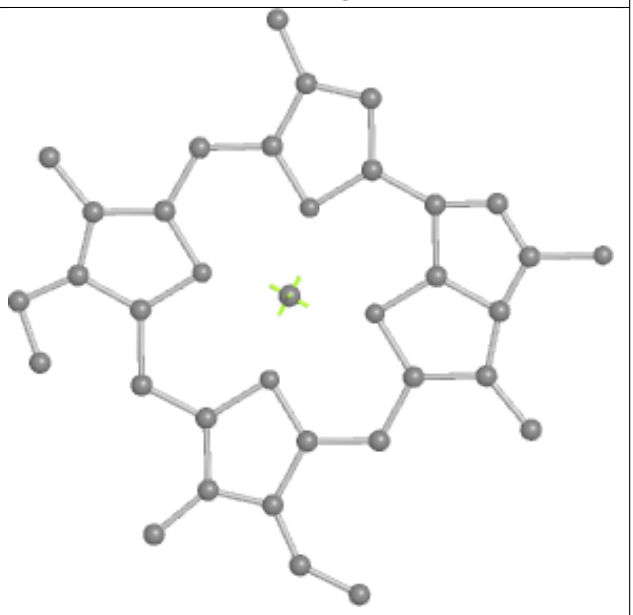
Rings

Ligand CLA A1 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

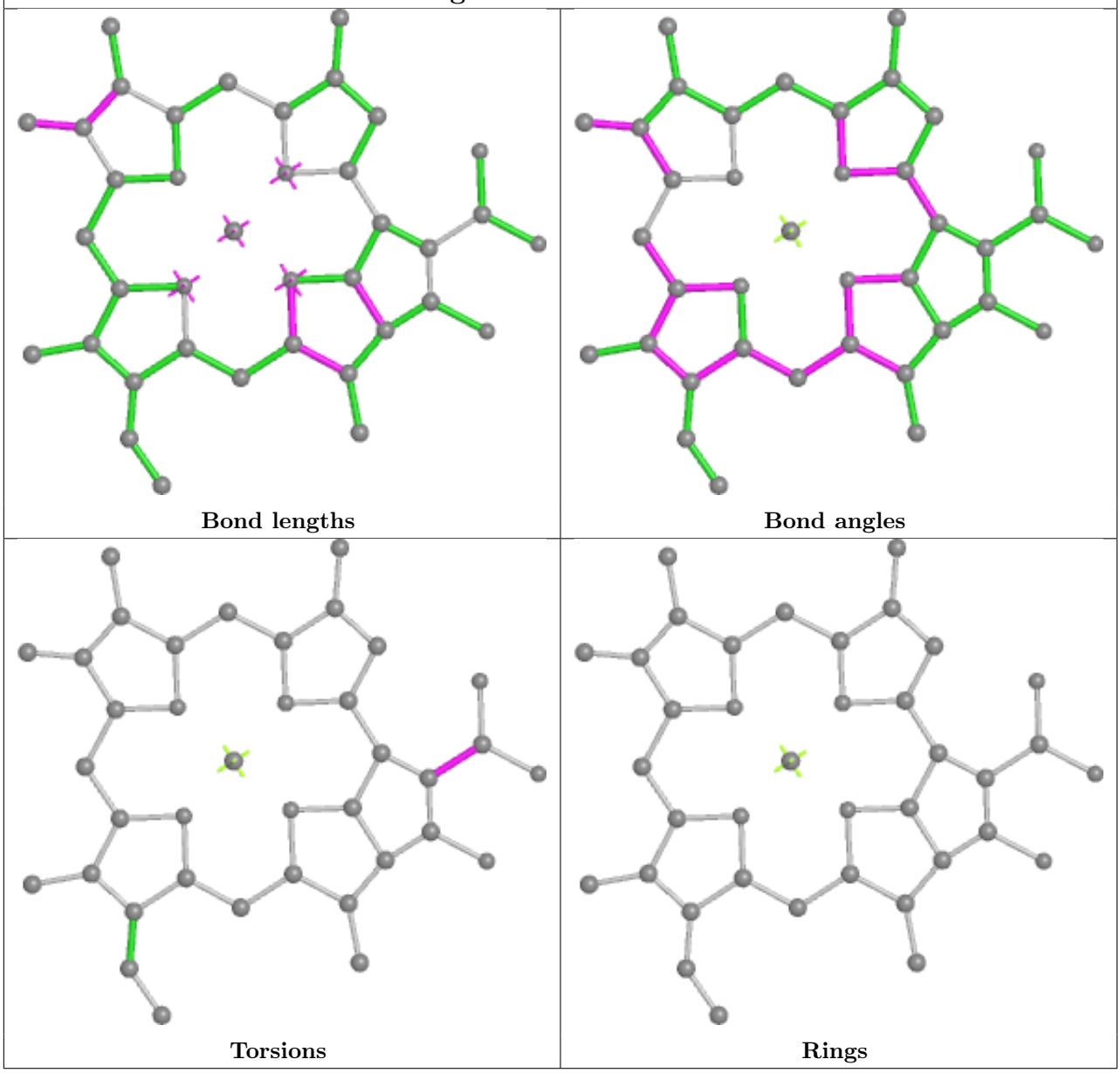
Ligand CLA A2 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

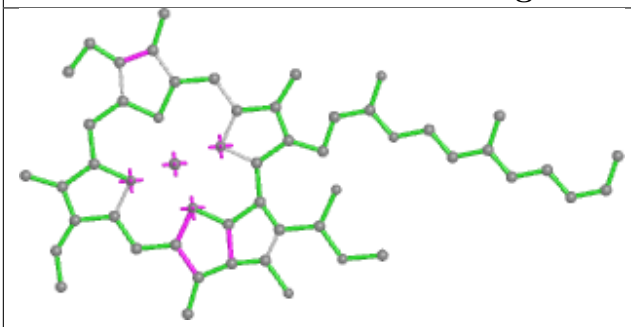
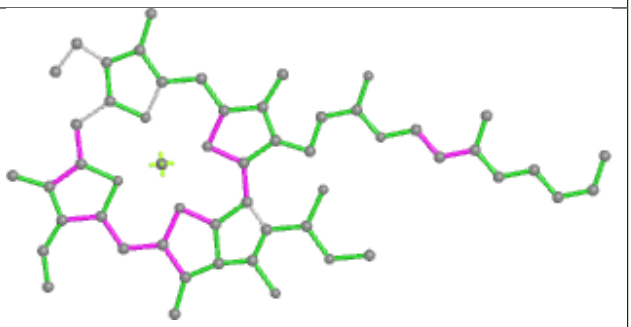
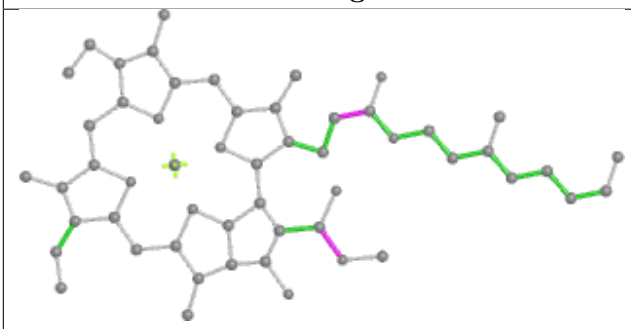
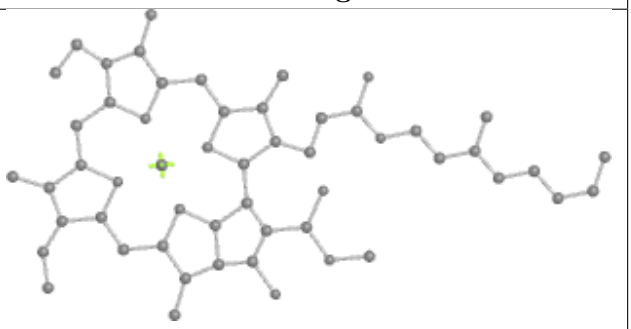
Ligand CLA A2 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

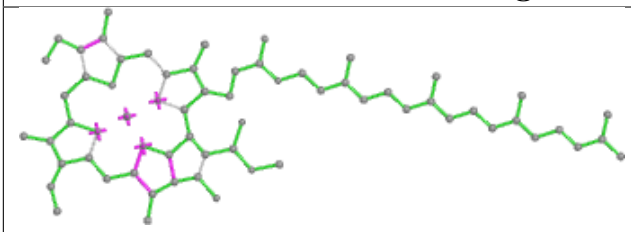
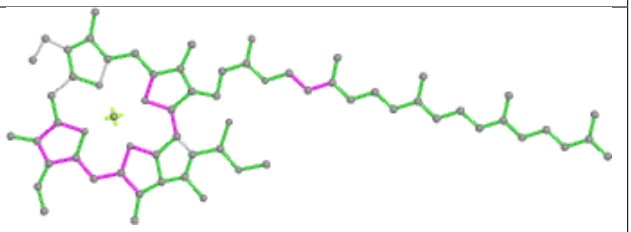
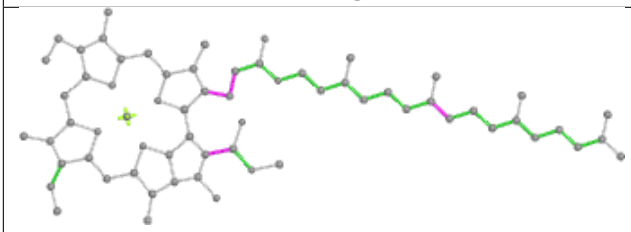
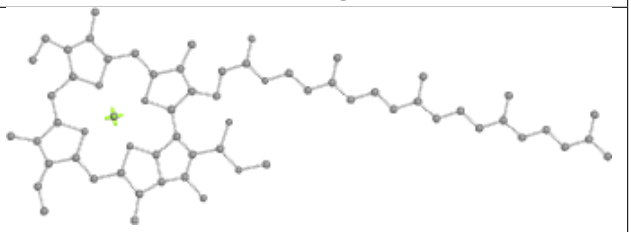
Ligand BCR B3 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B3 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

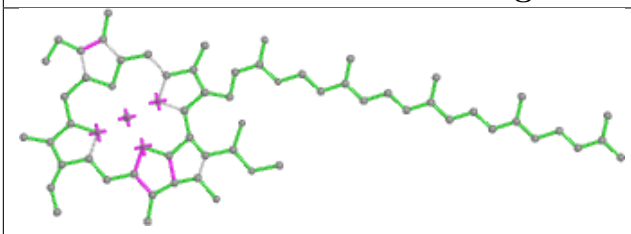
Ligand CLA A3 820



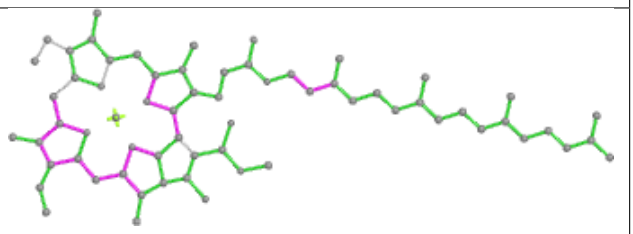
Ligand CLA B3 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

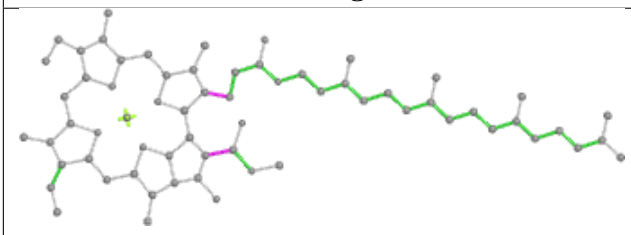
Ligand CLA A1 804



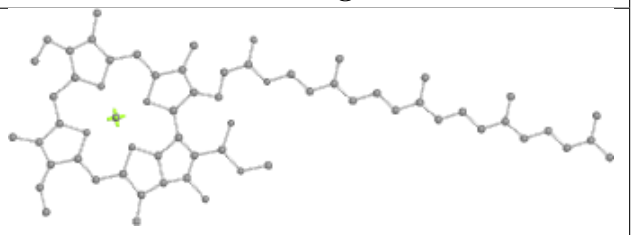
Bond lengths



Bond angles

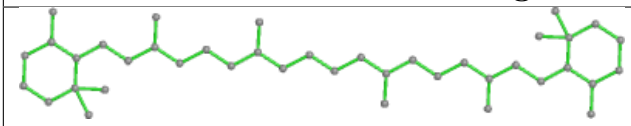


Torsions



Rings

Ligand BCR A2 852



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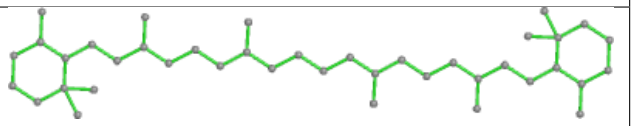
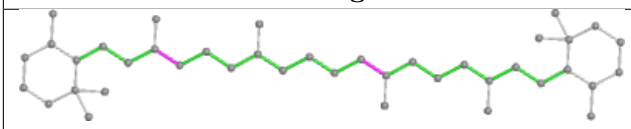


Bond angles



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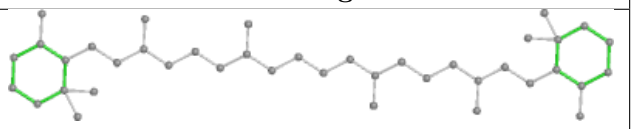
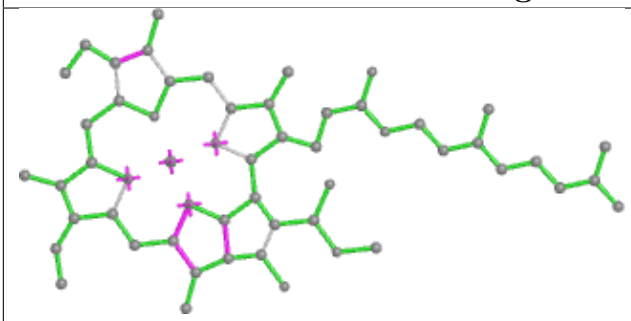
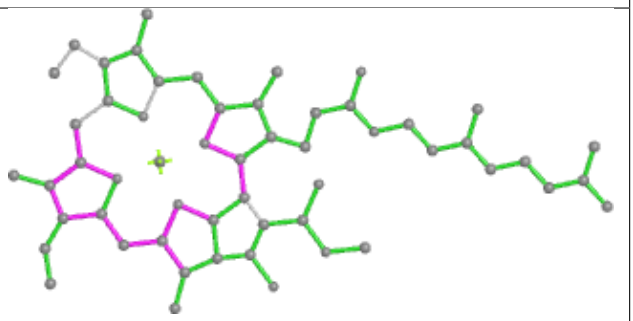


Rings

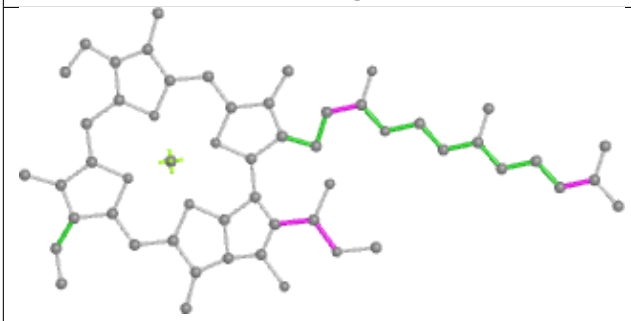
Ligand CLA A2 839



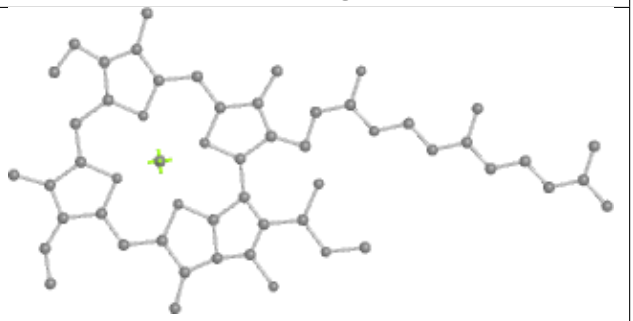
Bond lengths



Bond angles

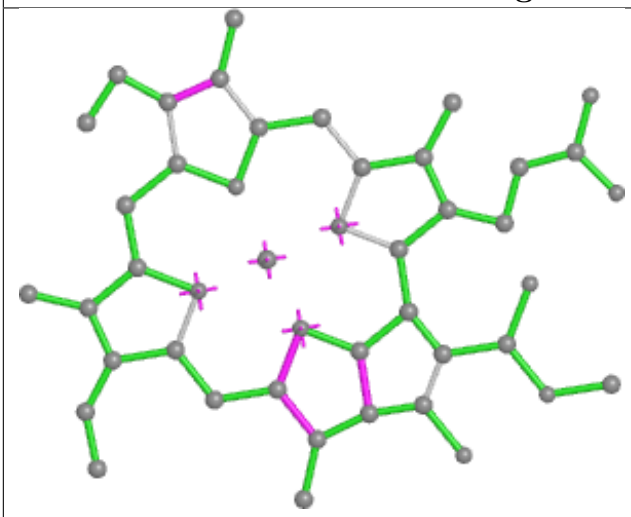


Torsions

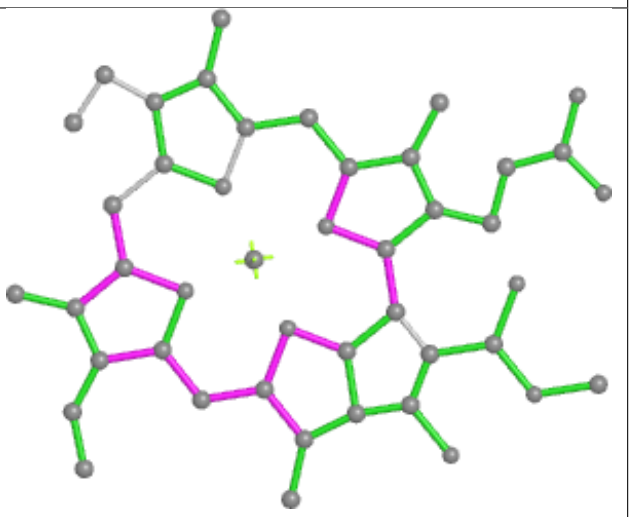


Rings

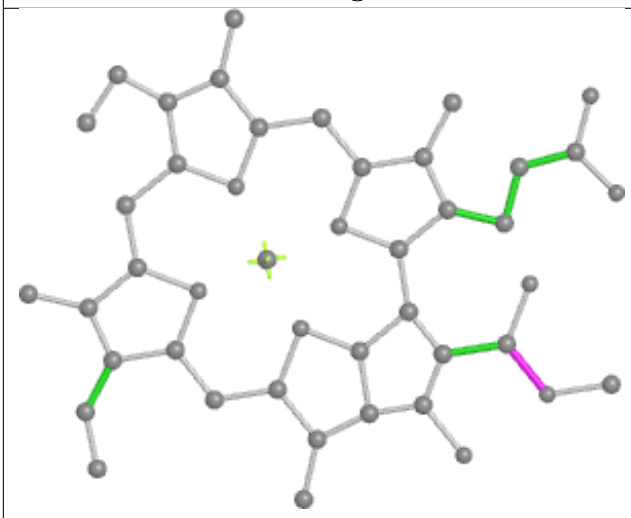
Ligand CLA B2 826



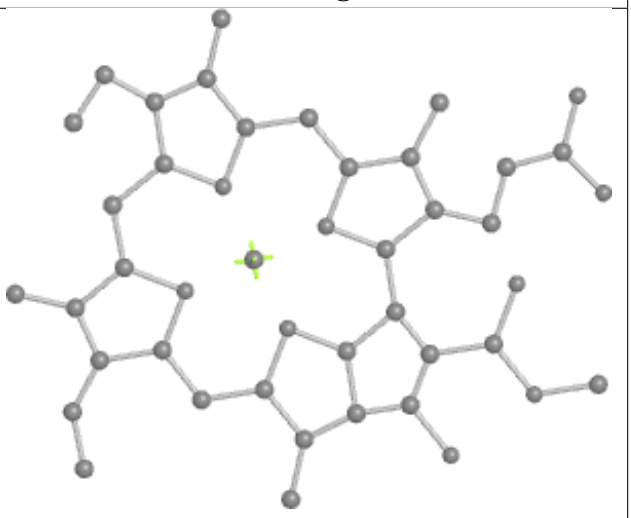
Bond lengths



Bond angles

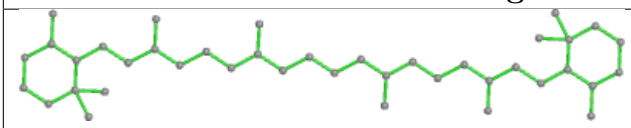


Torsions

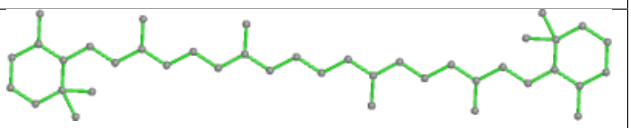


Rings

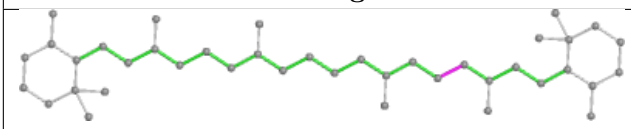
Ligand BCR L2 1010



Bond lengths



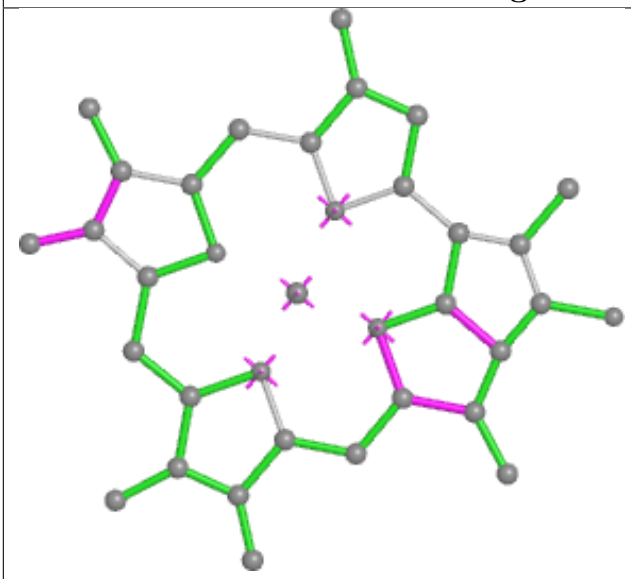
Bond angles



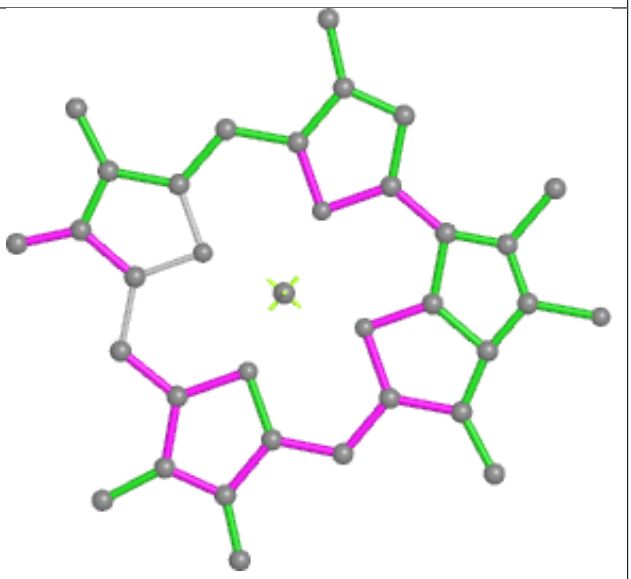
Torsions

Rings

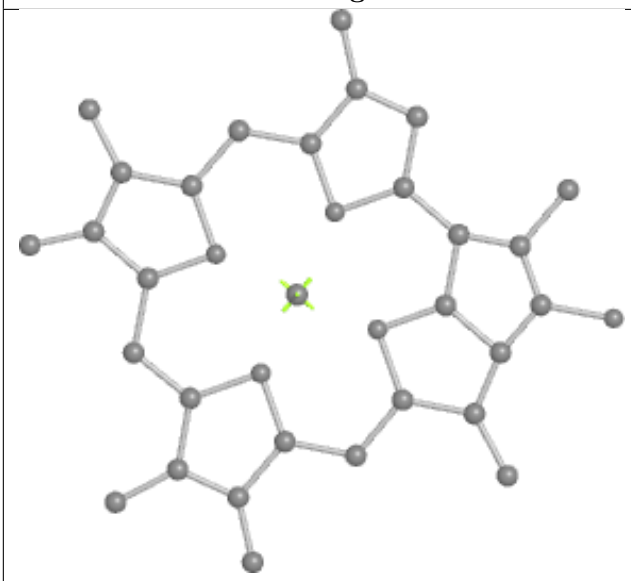
Ligand CLA J1 1302



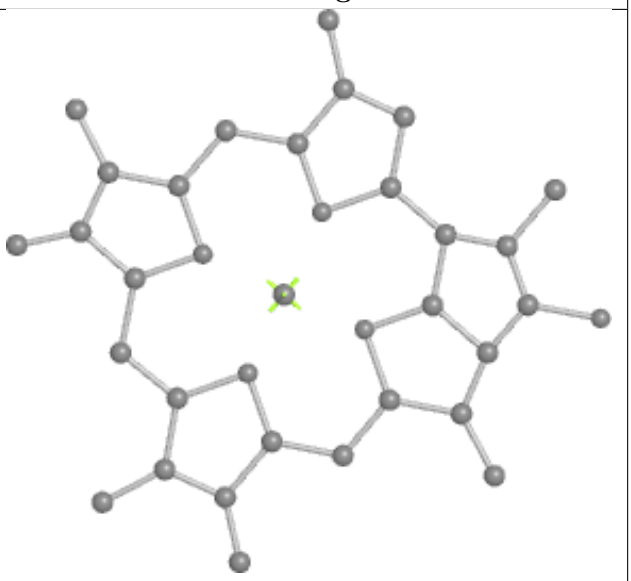
Bond lengths



Bond angles

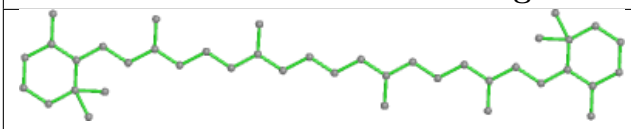


Torsions

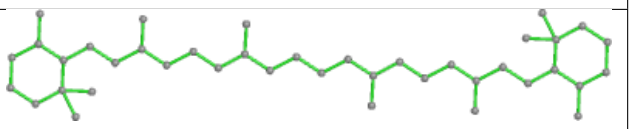


Rings

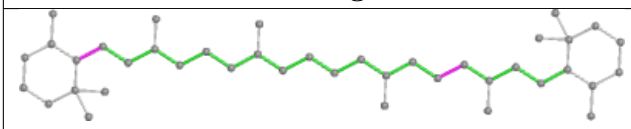
Ligand BCR B1 841



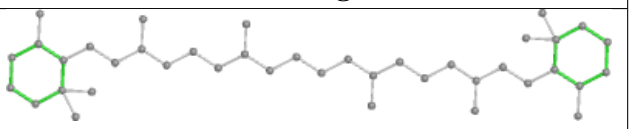
Bond lengths



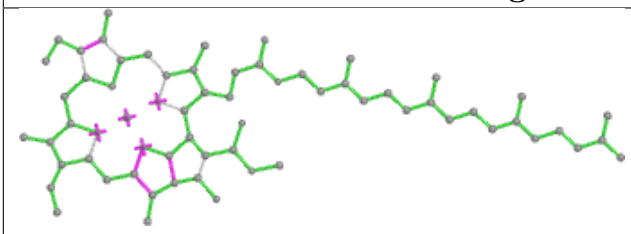
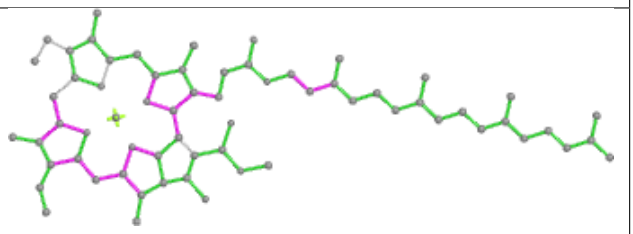
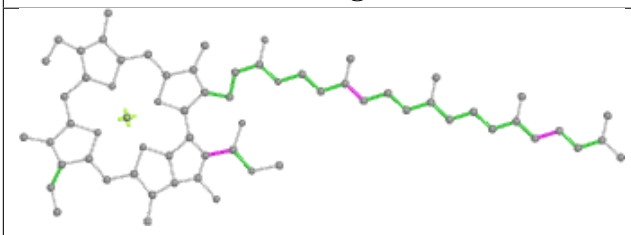
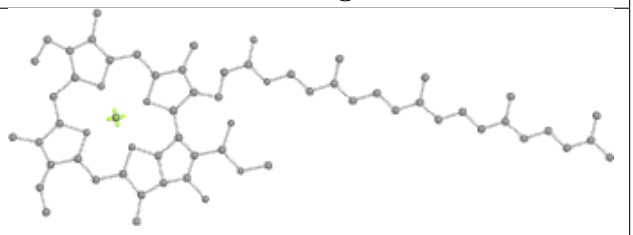
Bond angles

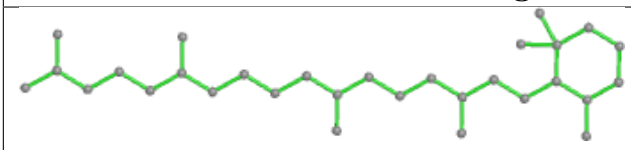
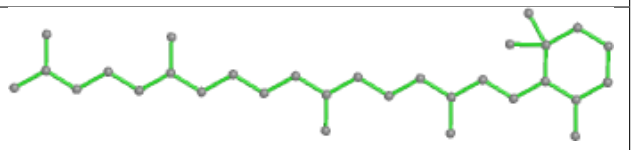
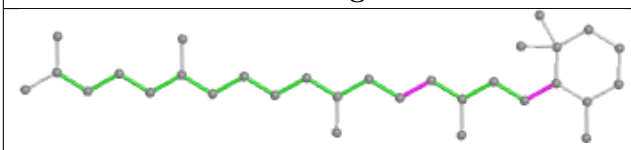
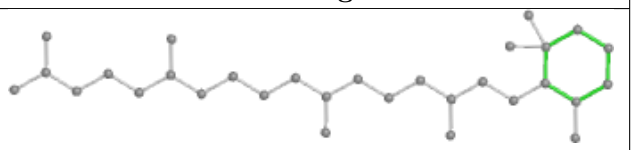


Torsions

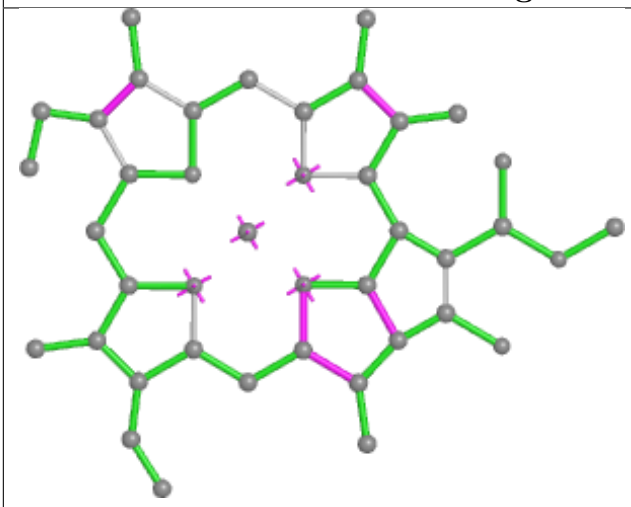


Rings

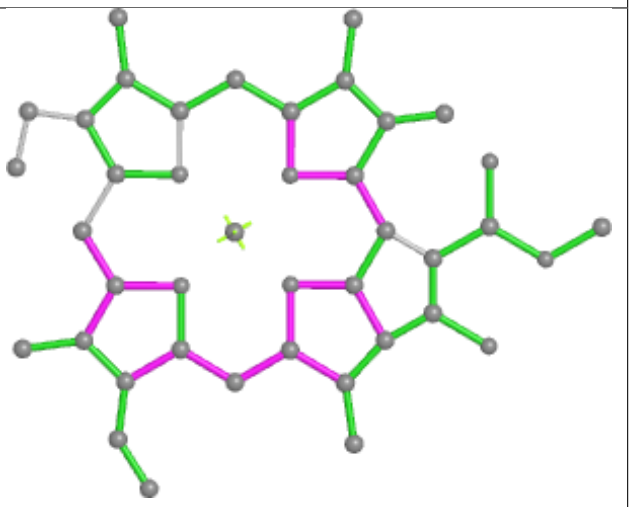
Ligand CLA L2 1004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A1 855	
 Bond lengths	 Bond angles
 Torsions	 Rings

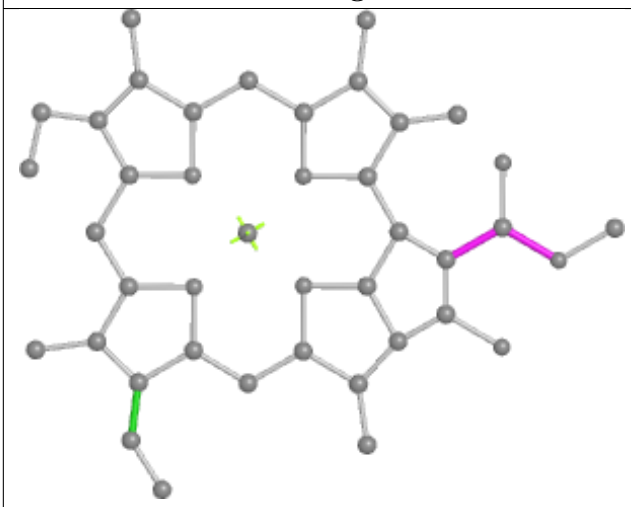
Ligand CLA B1 837



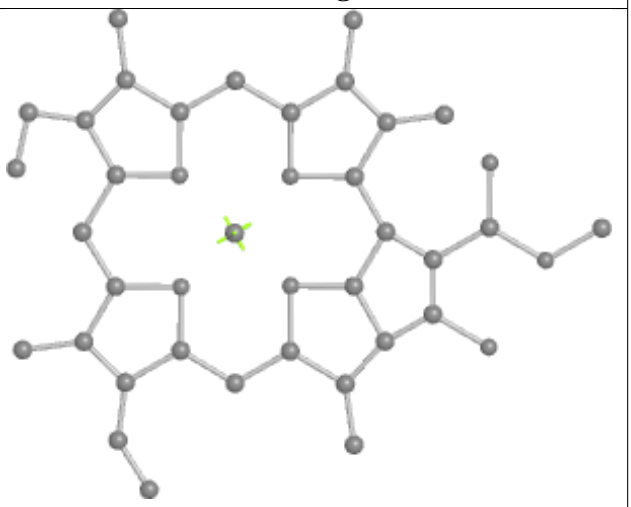
Bond lengths



Bond angles

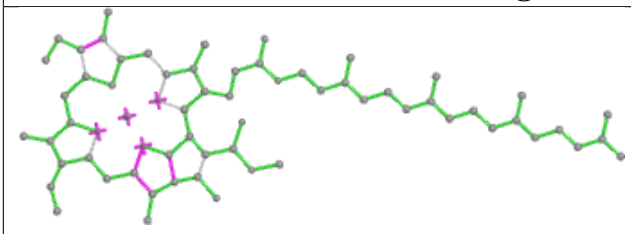


Torsions

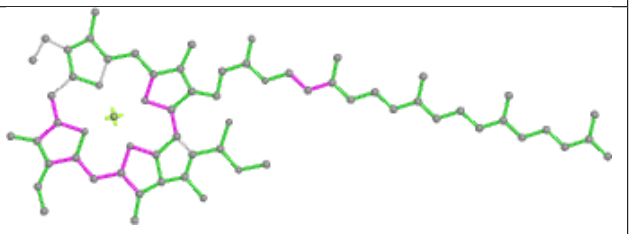


Rings

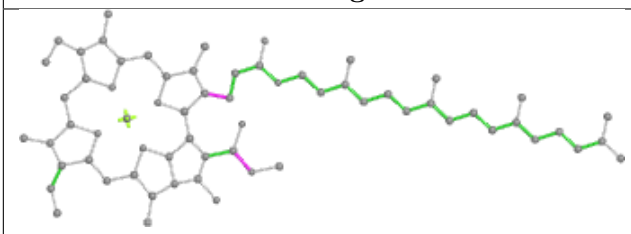
Ligand CLA B3 809



Bond lengths



Bond angles



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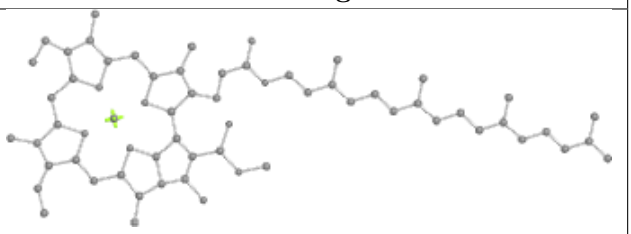
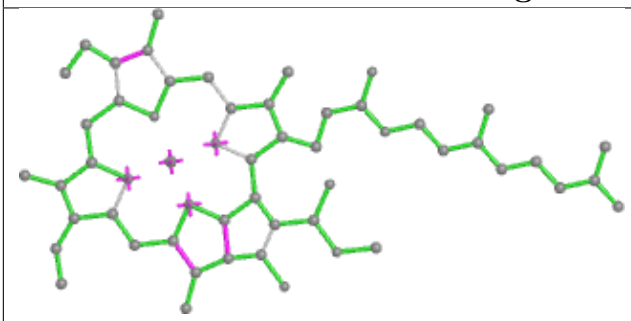
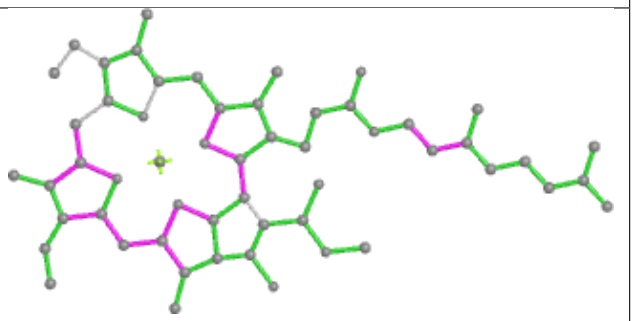
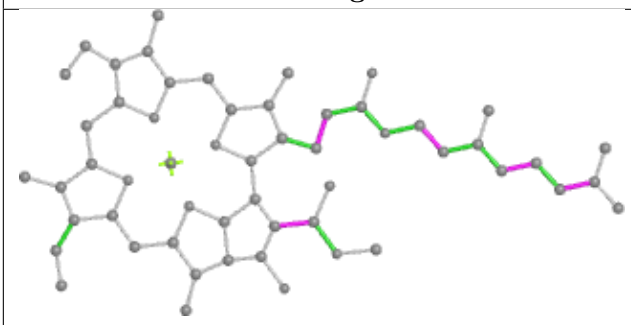
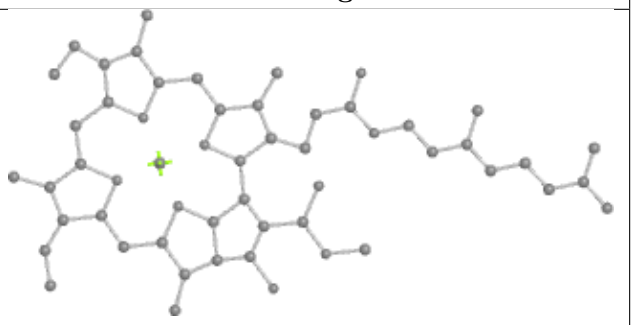
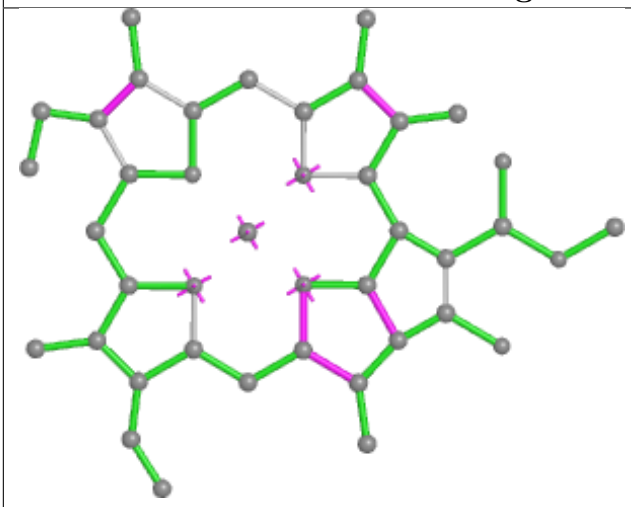


Rings

Ligand CLA A3 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 830



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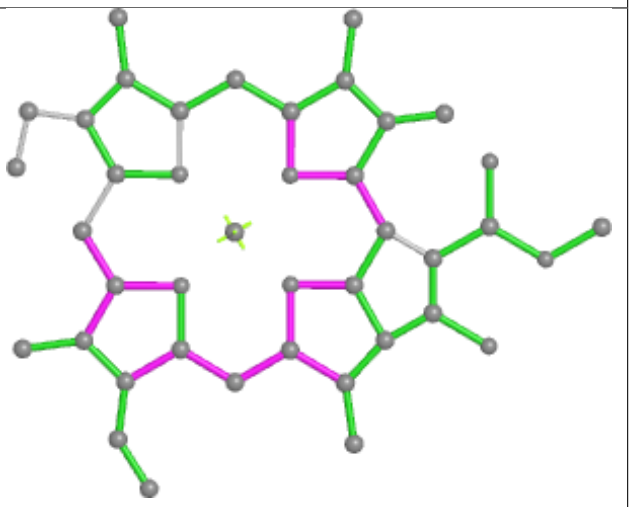
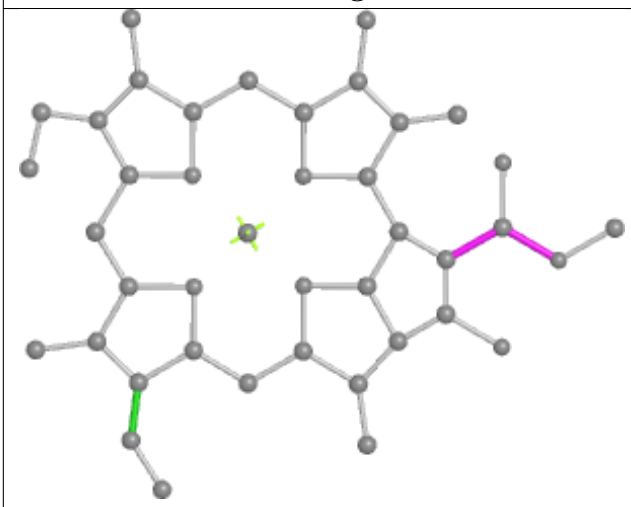


Bond angles



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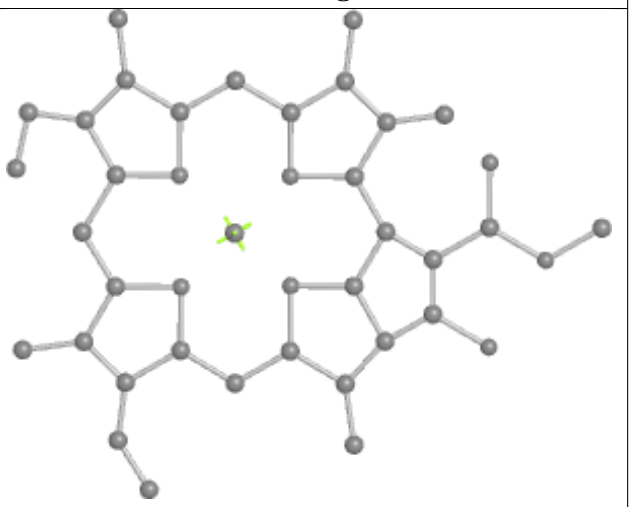
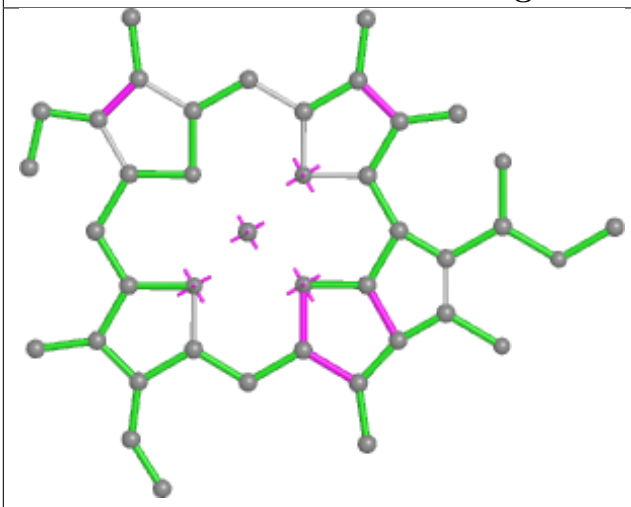
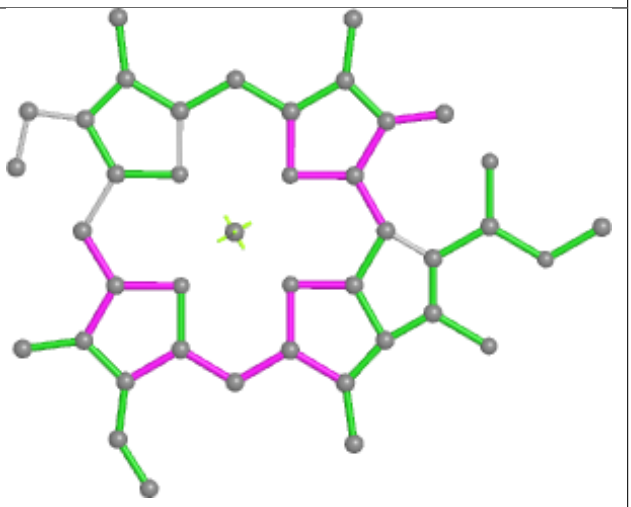
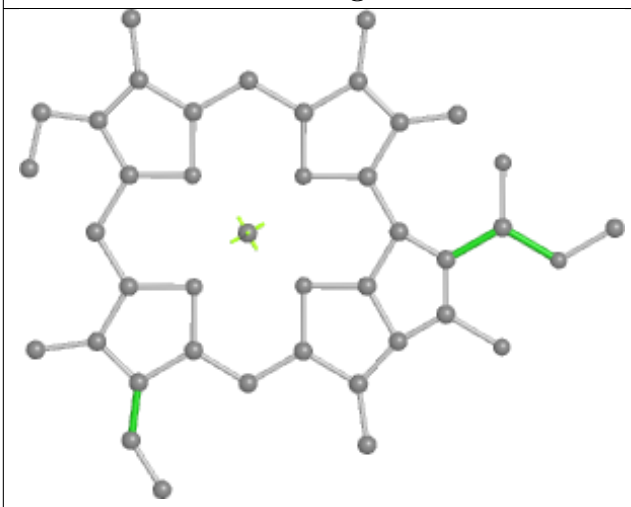
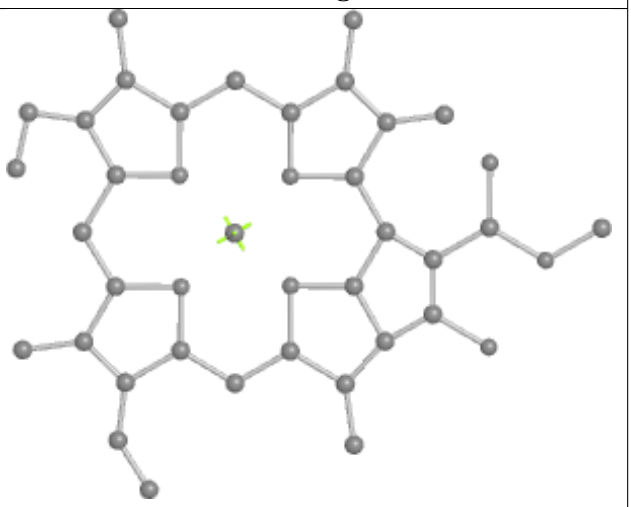
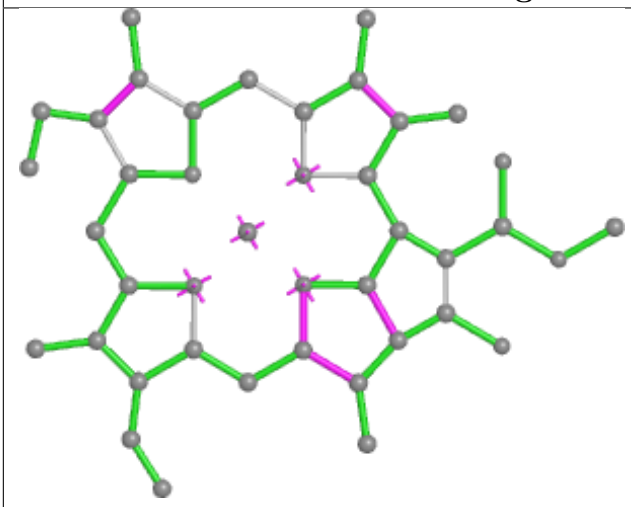


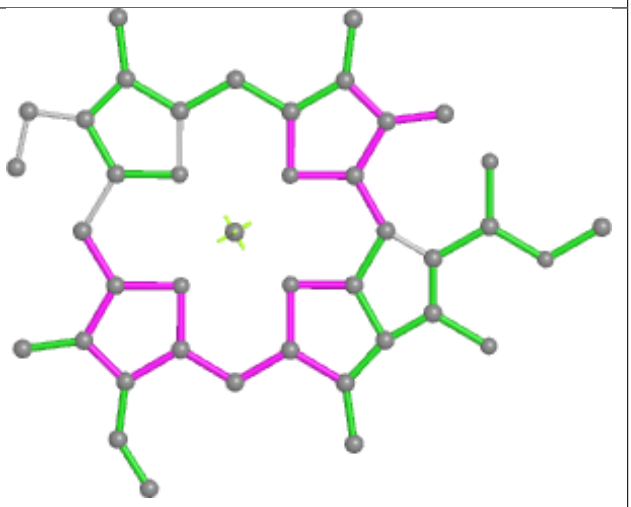
Rings

Ligand CLA A2 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

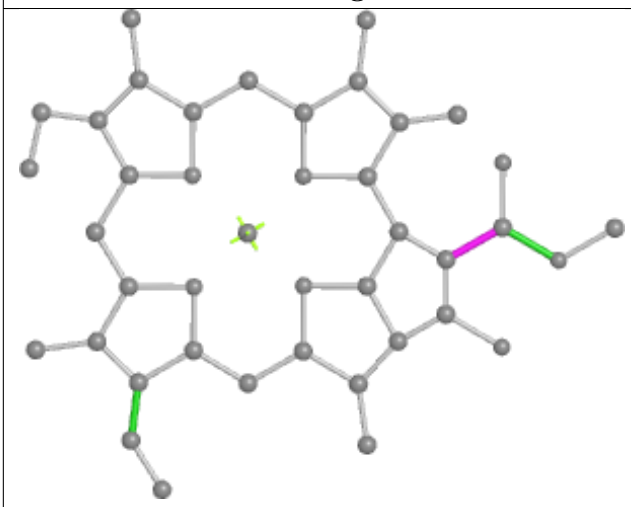
Ligand CLA B2 831



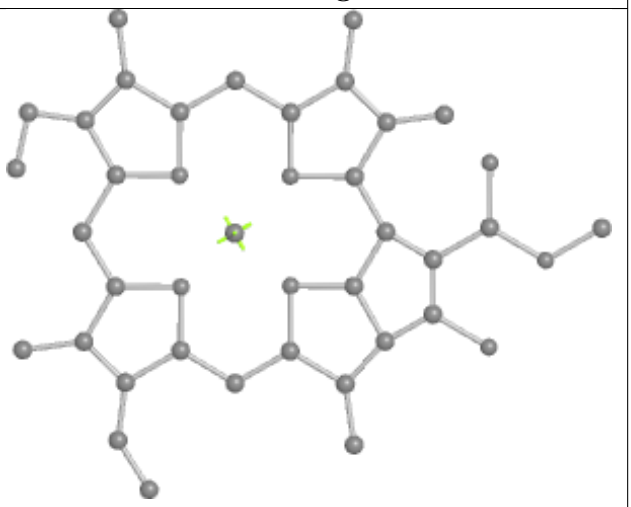
Bond lengths



Bond angles

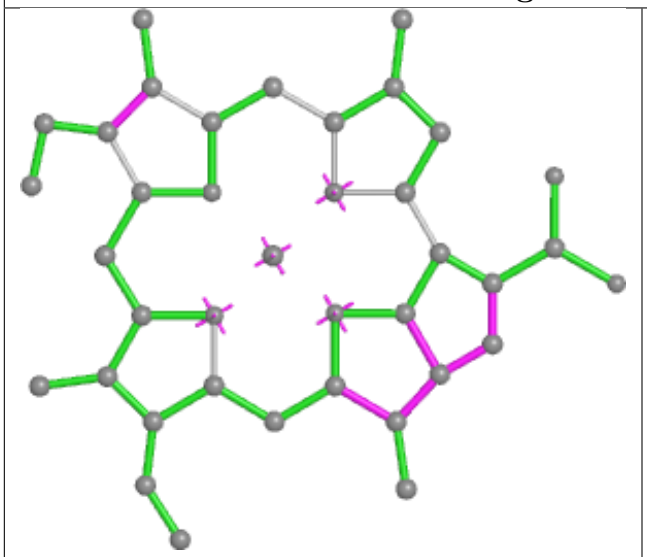


Torsions



Rings

Ligand CLA B1 816



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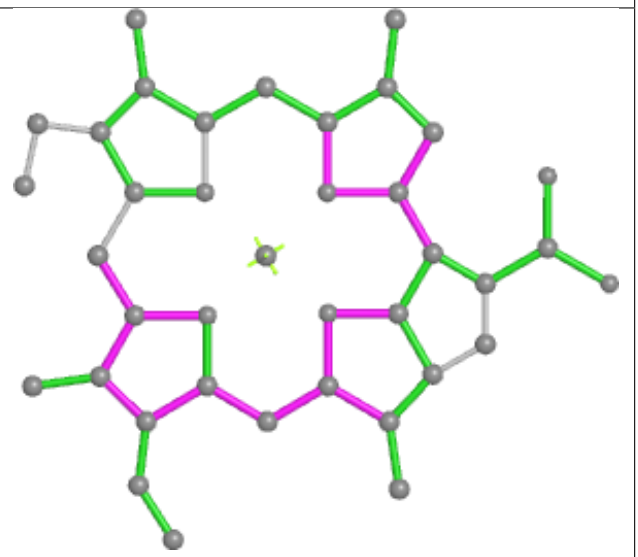
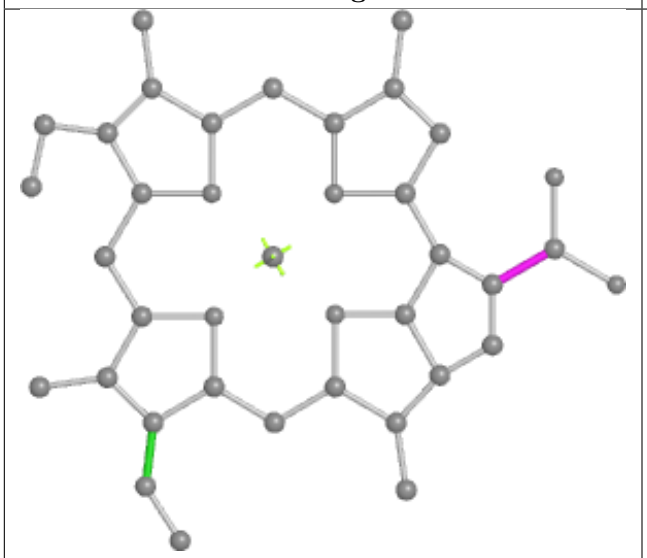


Bond angles



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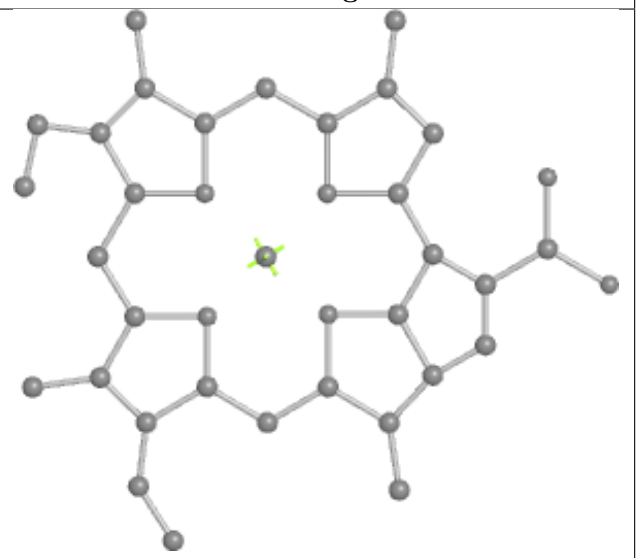
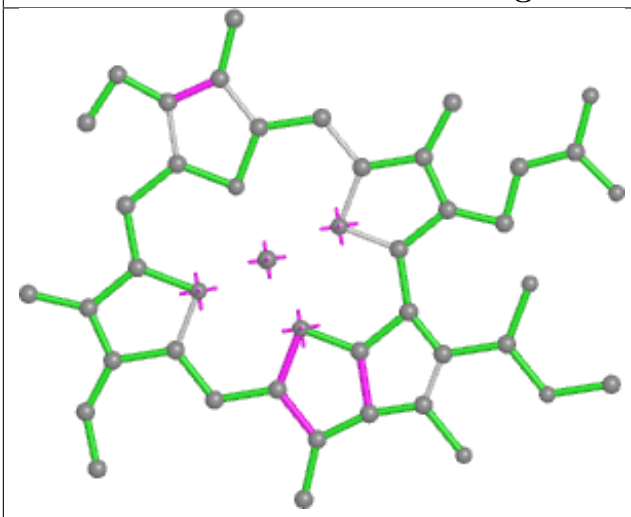


Rings

Ligand CLA A3 822



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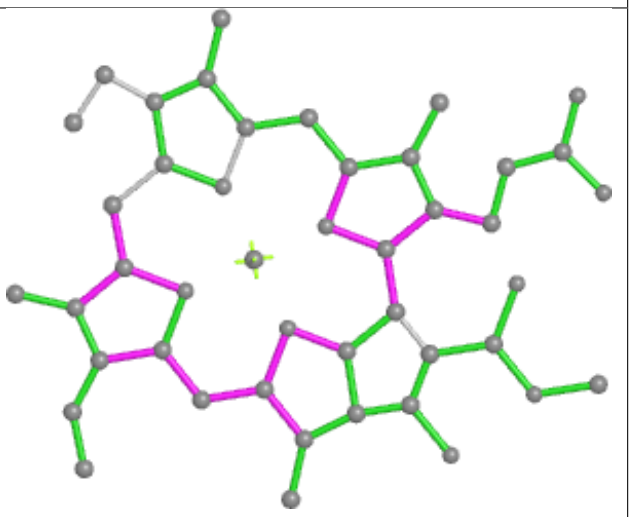
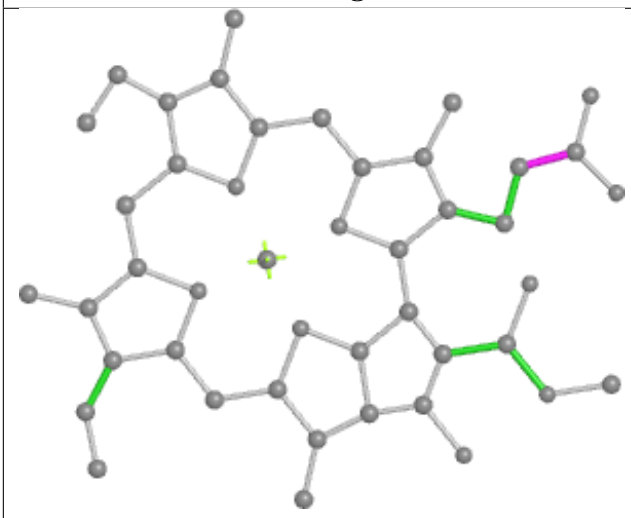


Bond angles



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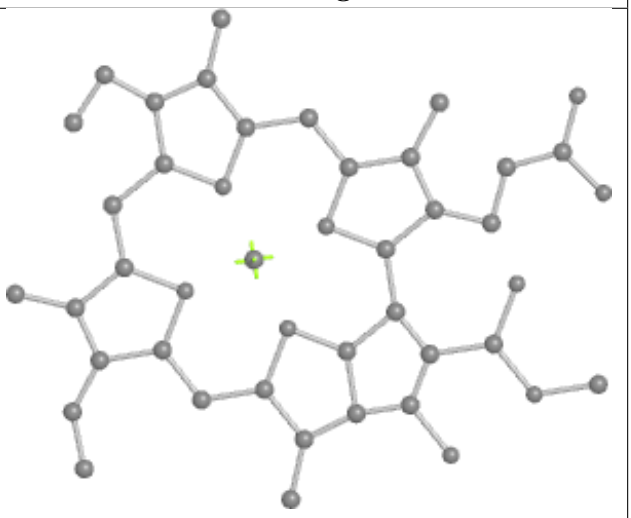
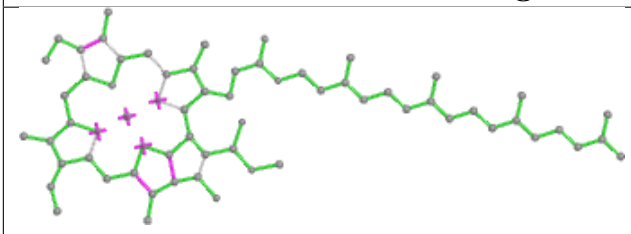
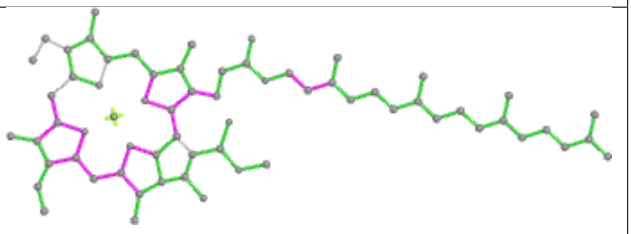


Rings

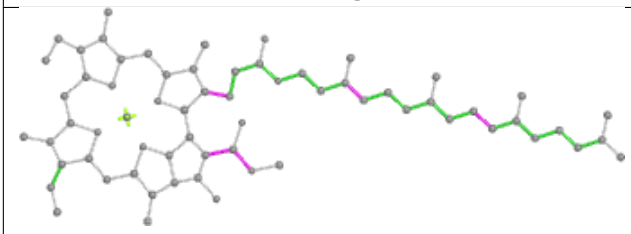
Ligand CLA A3 830



Bond lengths



Bond angles



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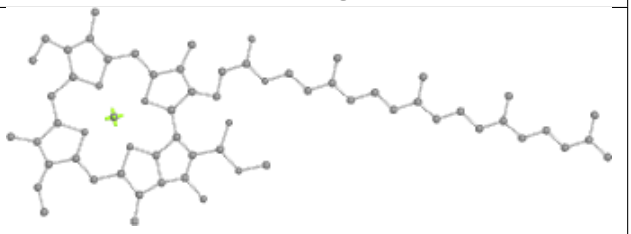
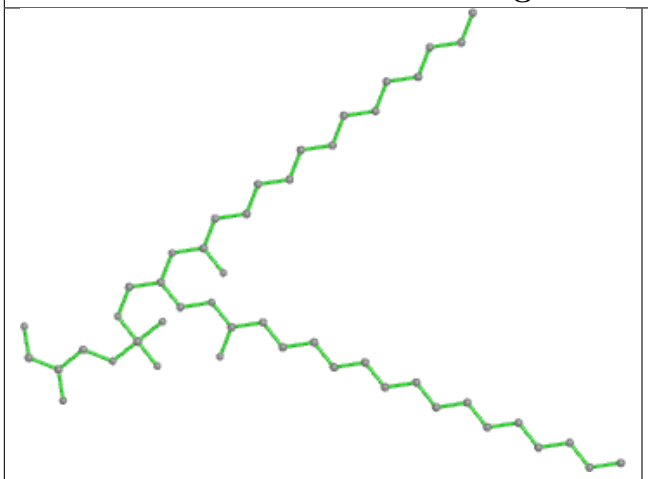
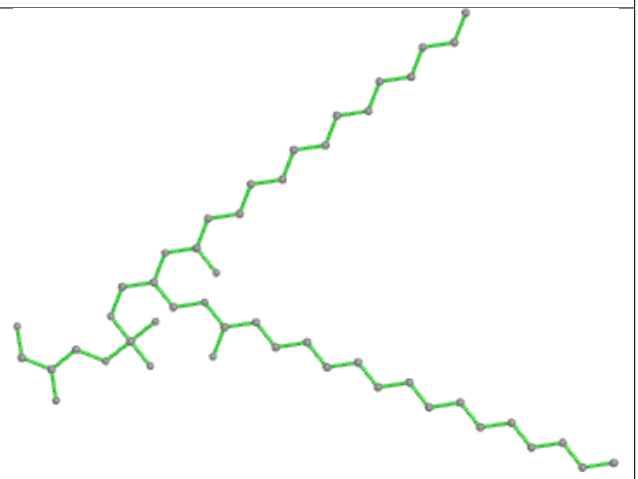


Rings

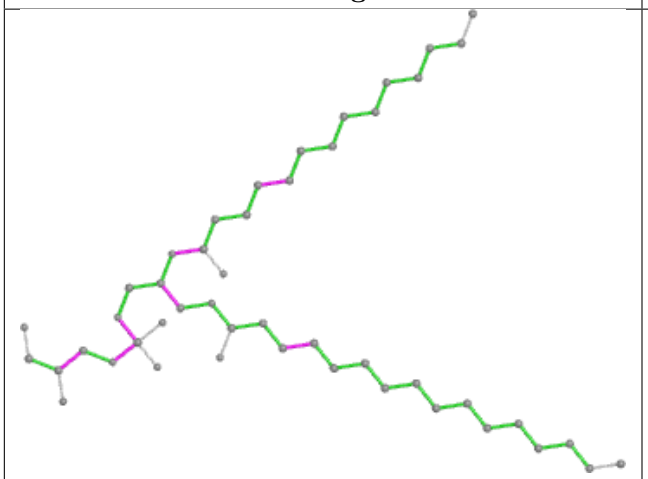
Ligand LHG A2 853



Bond lengths



Bond angles



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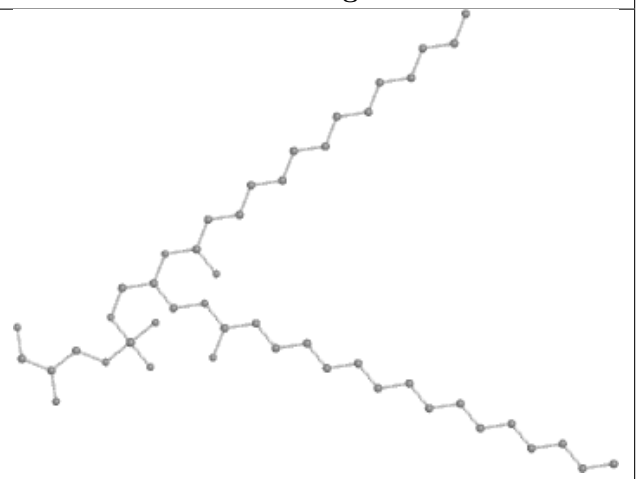
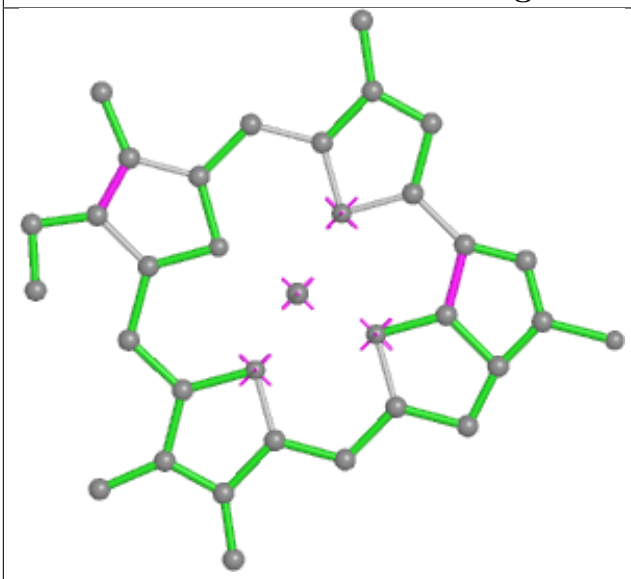


Rings

Ligand CLA K1 101



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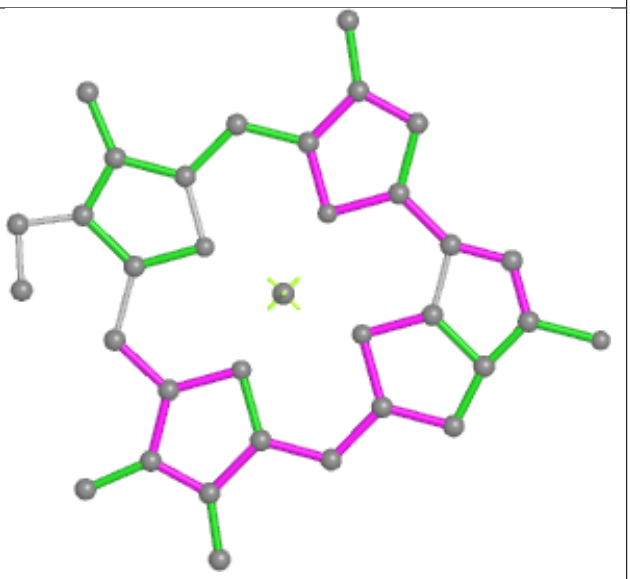
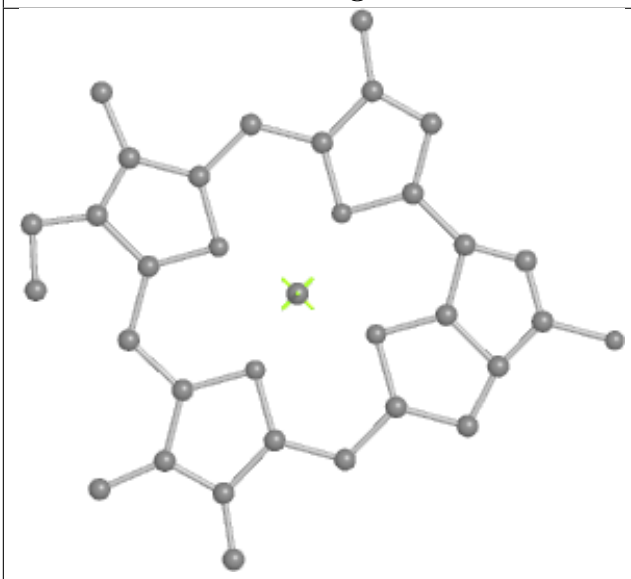


Bond angles



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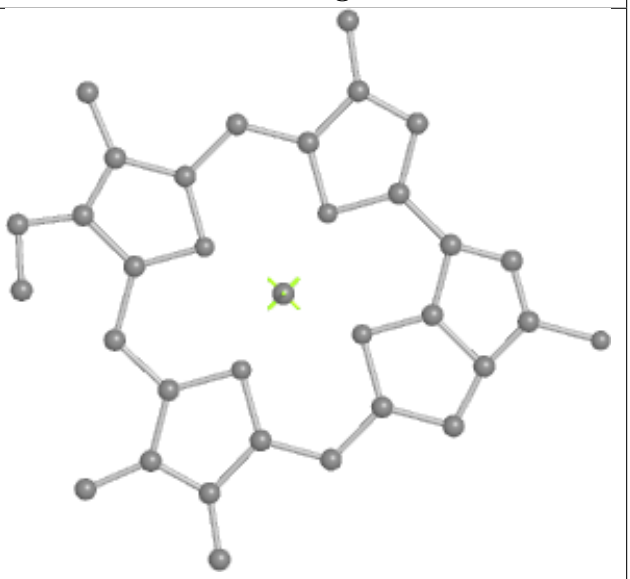
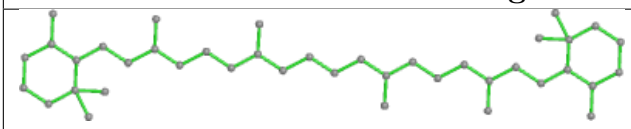
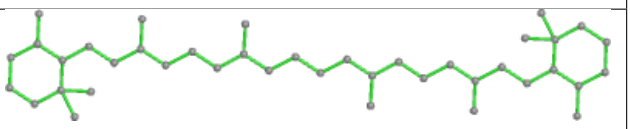


Rings

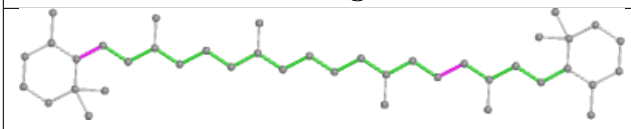
Ligand BCR J2 1304



Bond lengths



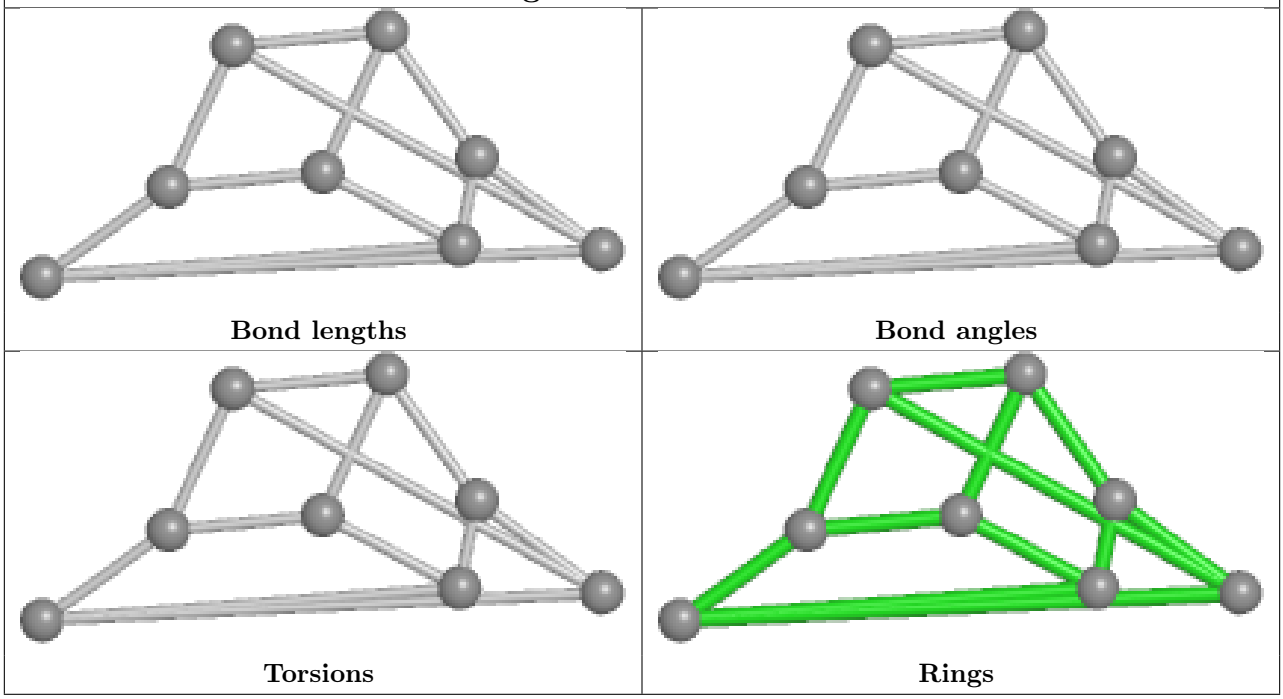
Bond angles



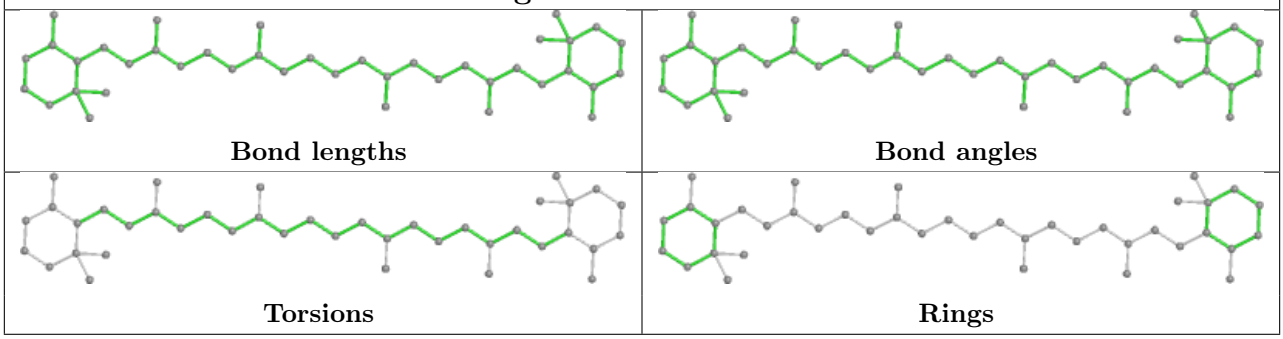
Torsions

Rings

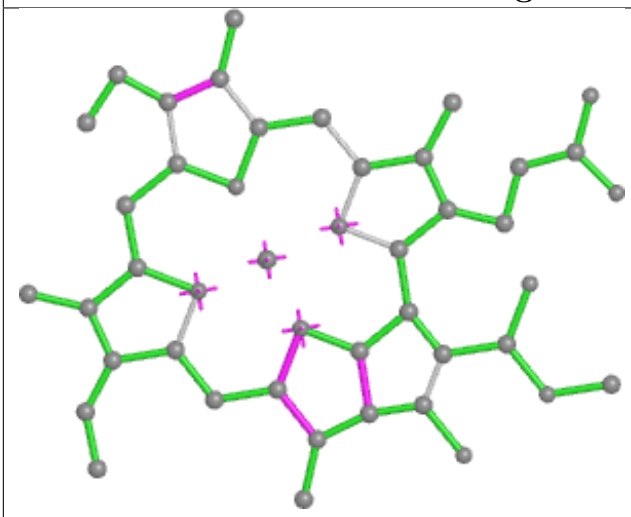
Ligand SF4 A1 846



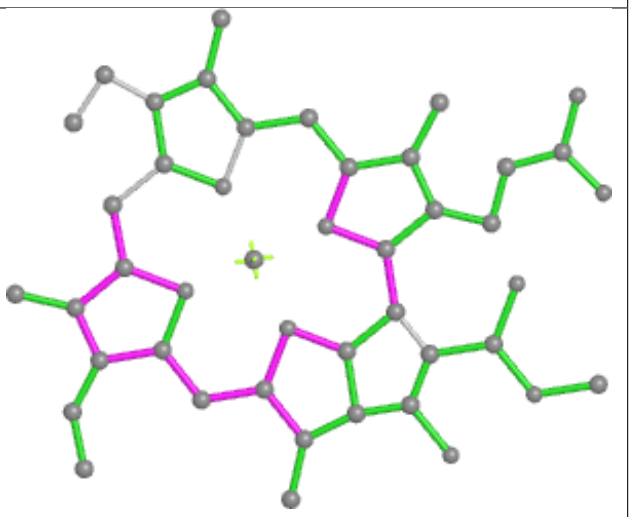
Ligand BCR A1 849



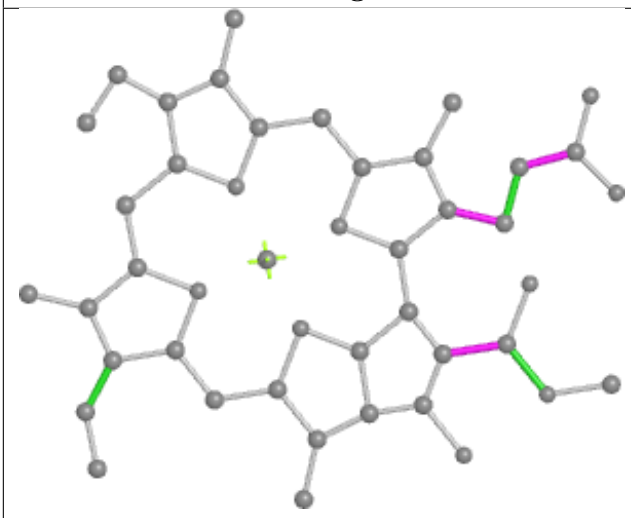
Ligand CLA B1 819



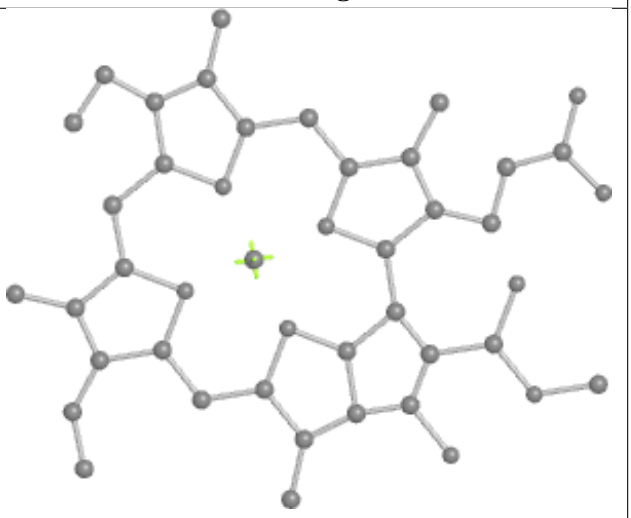
Bond lengths



Bond angles

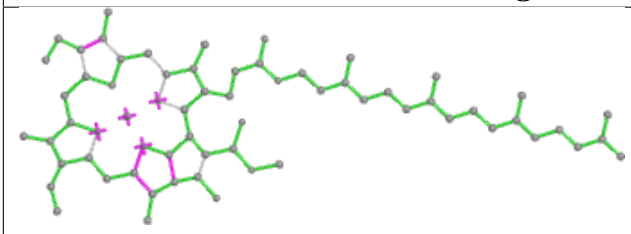


Torsions

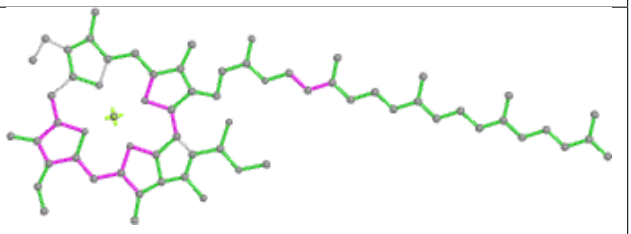


Rings

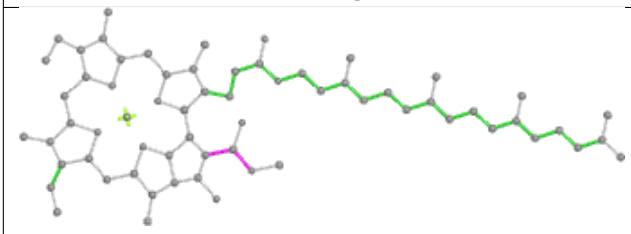
Ligand CLA A1 834



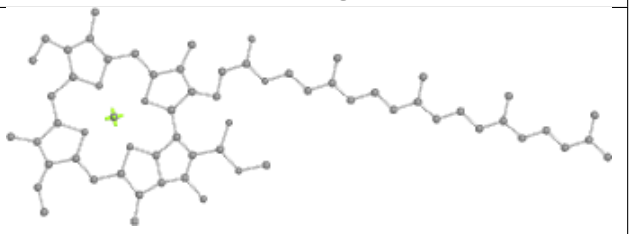
Bond lengths



Bond angles

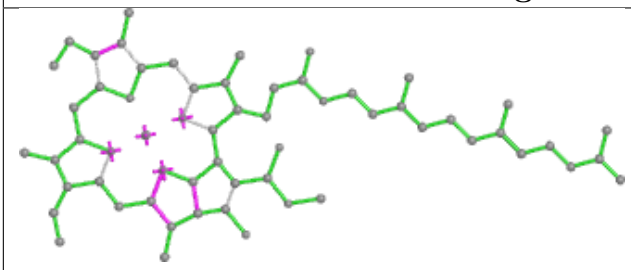


Torsions

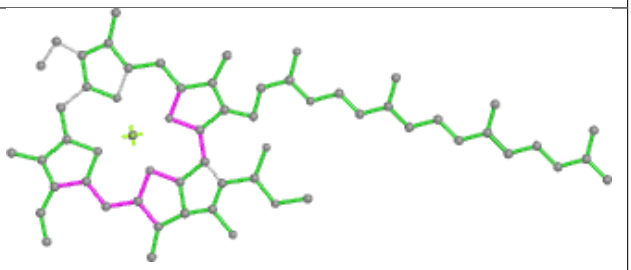


Rings

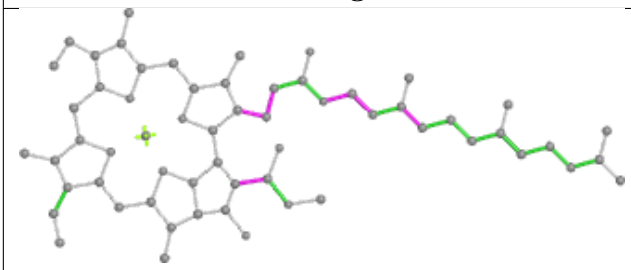
Ligand CLA A2 827



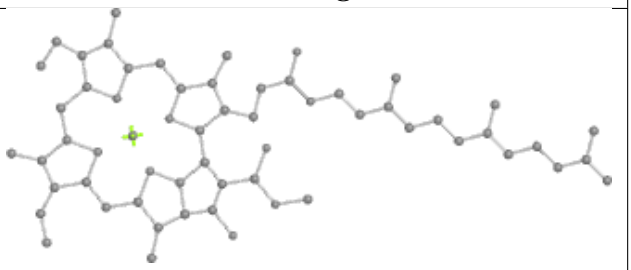
Bond lengths



Bond angles

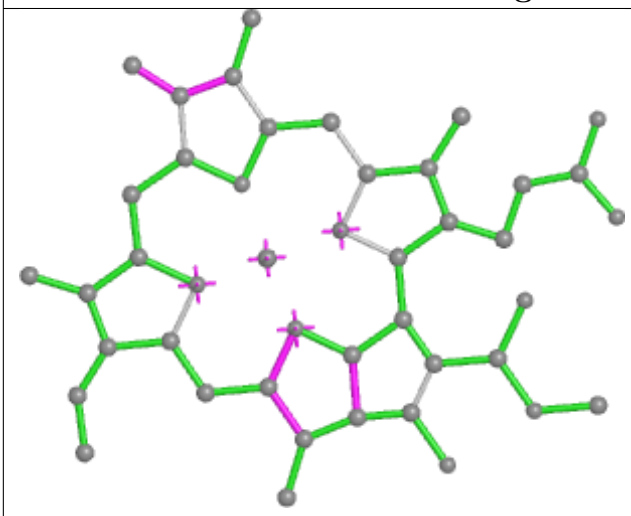


Torsions

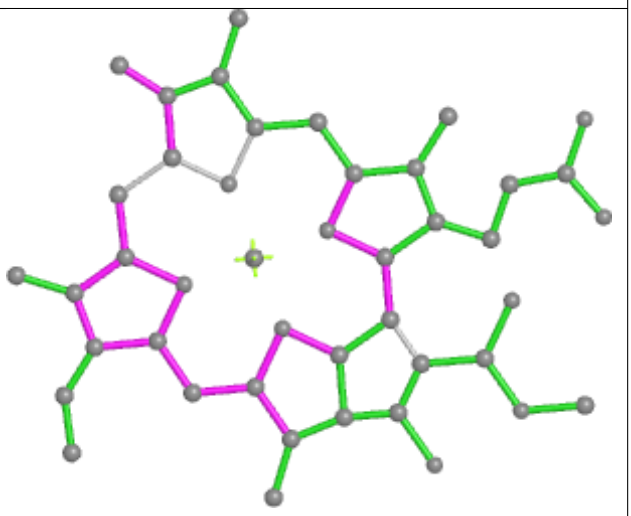


Rings

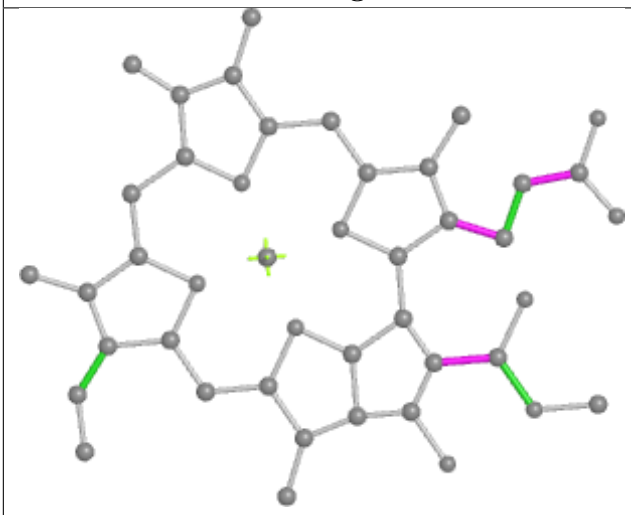
Ligand CLA A2 813



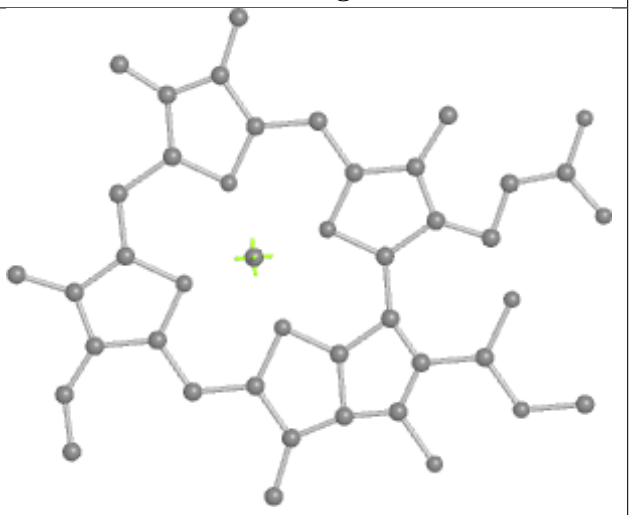
Bond lengths



Bond angles

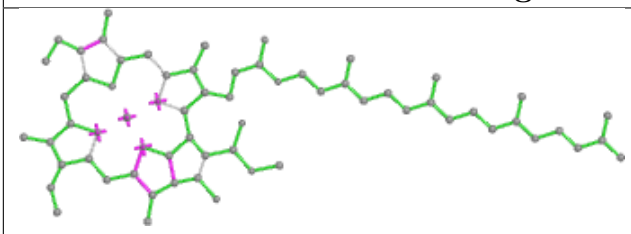


Torsions

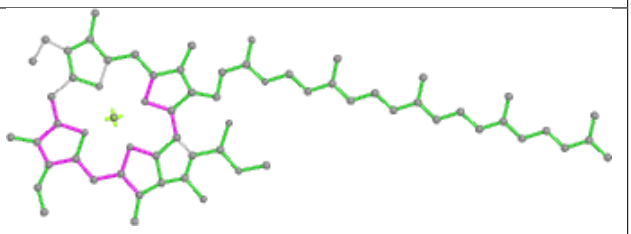


Rings

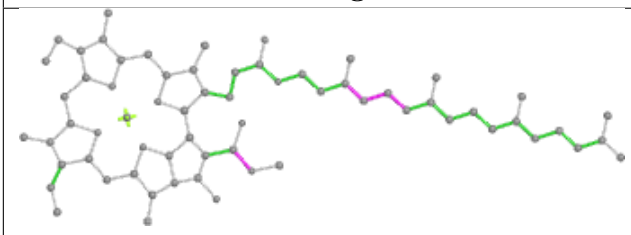
Ligand CLA A1 842



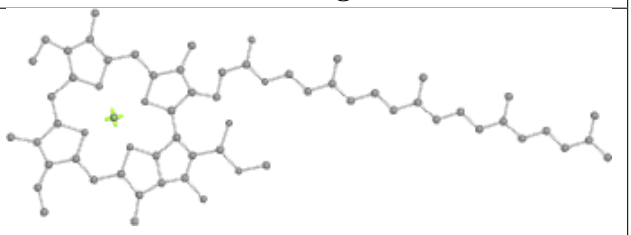
Bond lengths



Bond angles

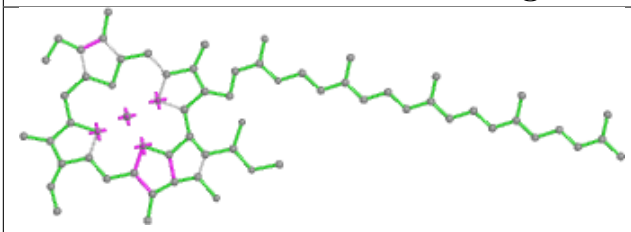


Torsions

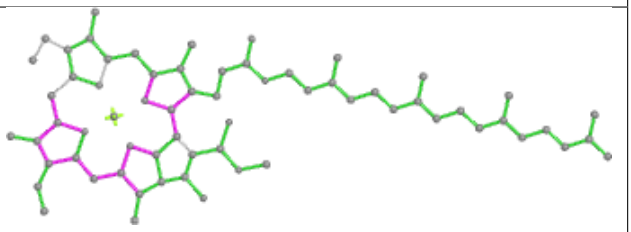


Rings

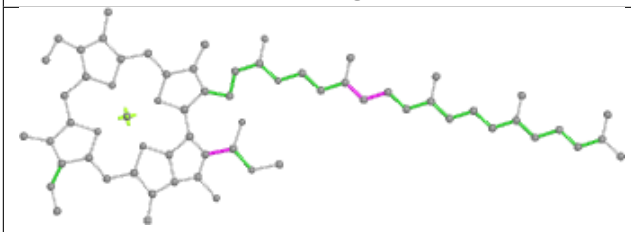
Ligand CLA I1 101



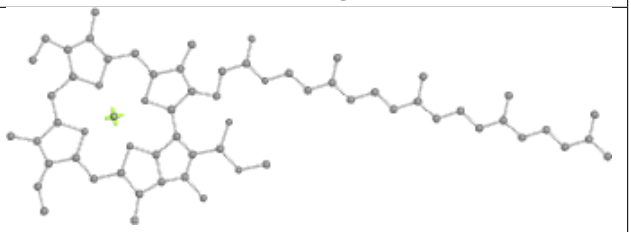
Bond lengths



Bond angles

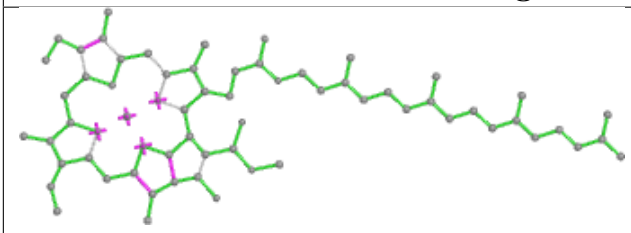


Torsions

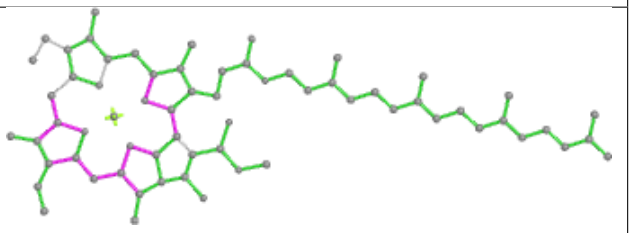


Rings

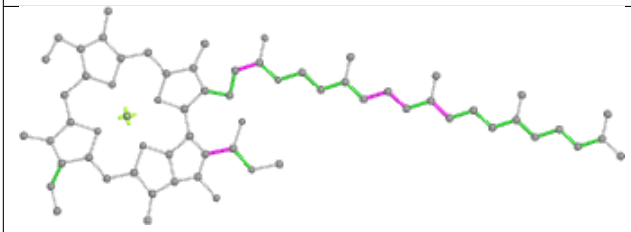
Ligand CLA A1 856



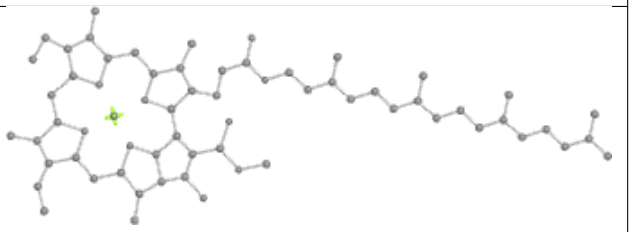
Bond lengths



Bond angles

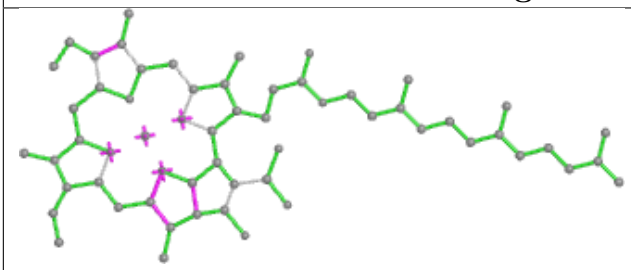


Torsions

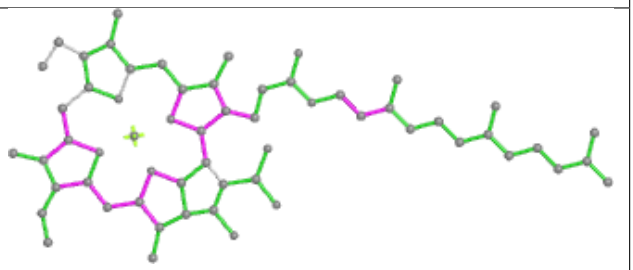


Rings

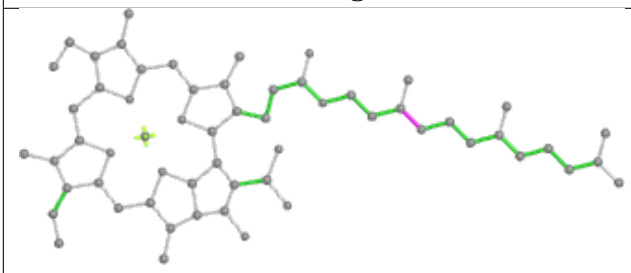
Ligand CLA A3 819



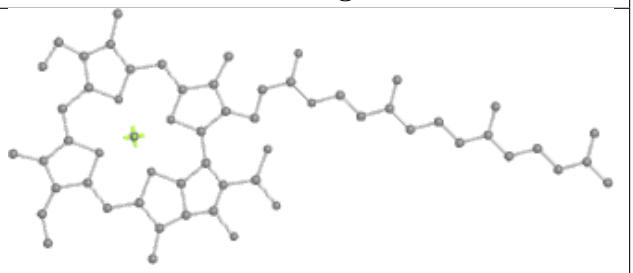
Bond lengths



Bond angles

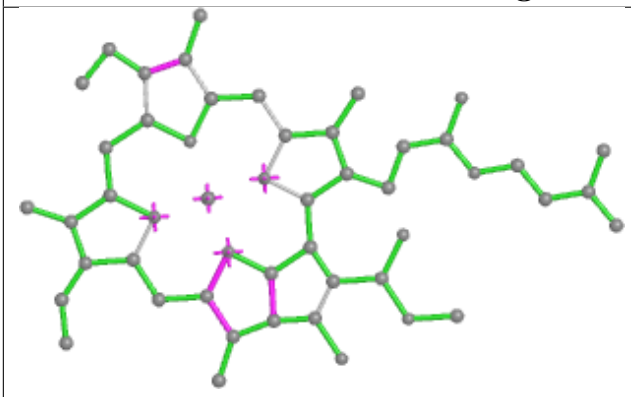


Torsions

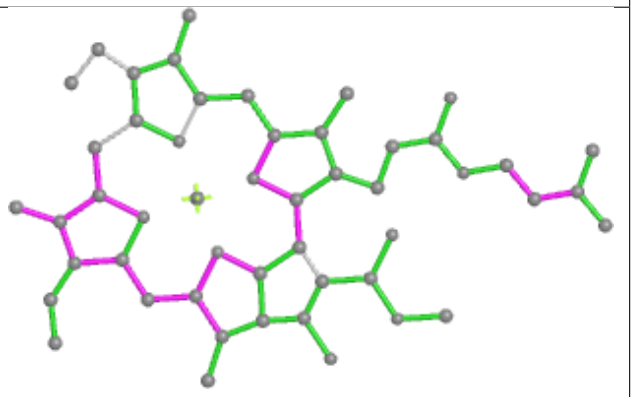


Rings

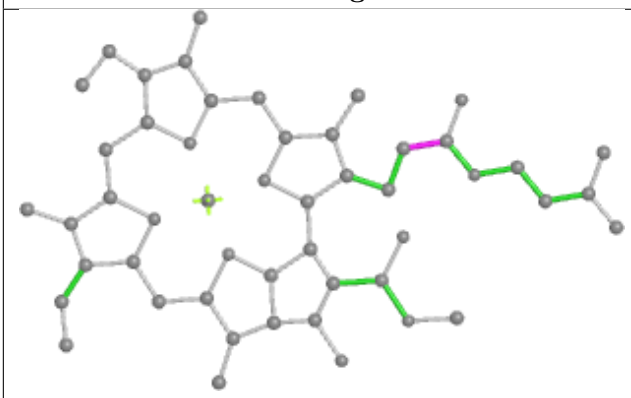
Ligand CLA B3 806



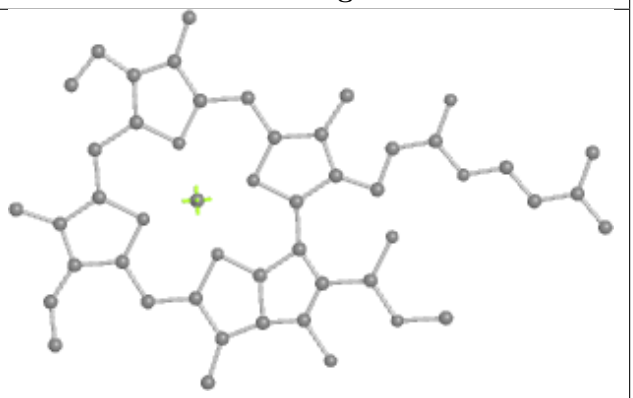
Bond lengths



Bond angles

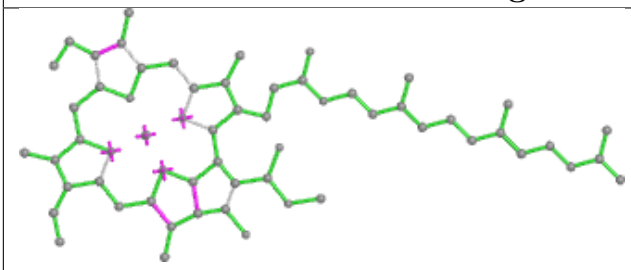


Torsions

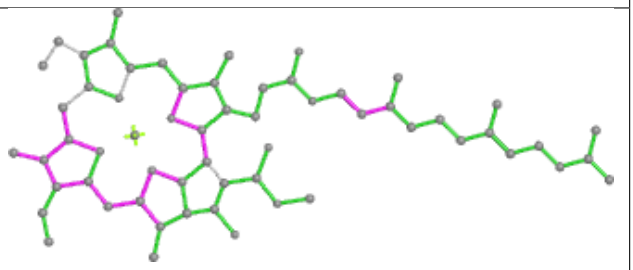


Rings

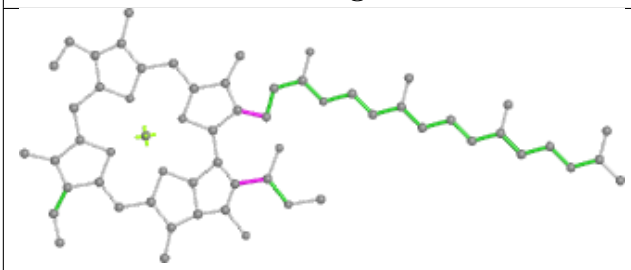
Ligand CLA L3 1003



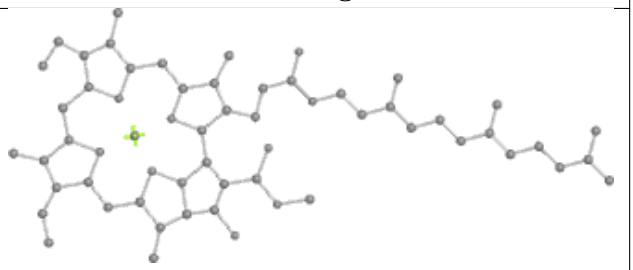
Bond lengths



Bond angles

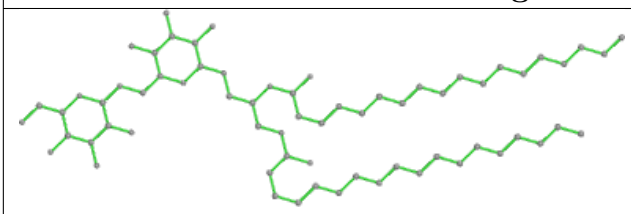


Torsions

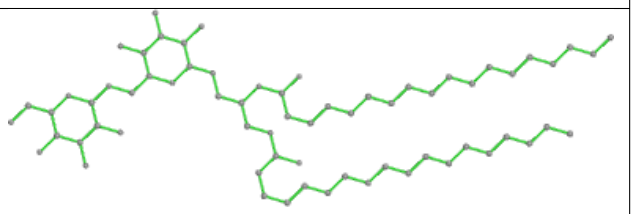


Rings

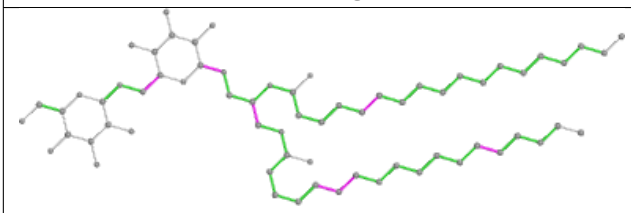
Ligand DGD B3 848



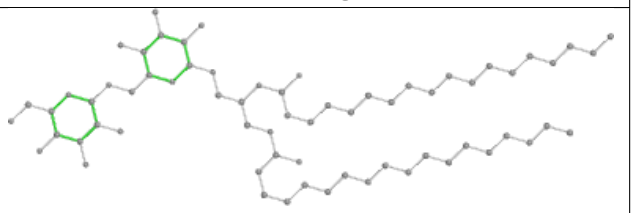
Bond lengths



Bond angles

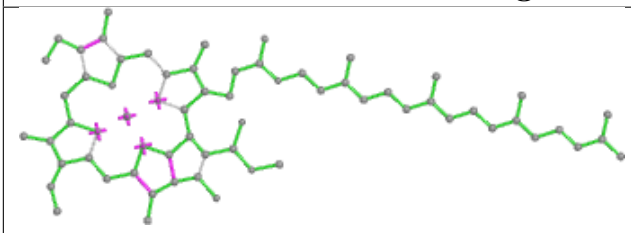


Torsions

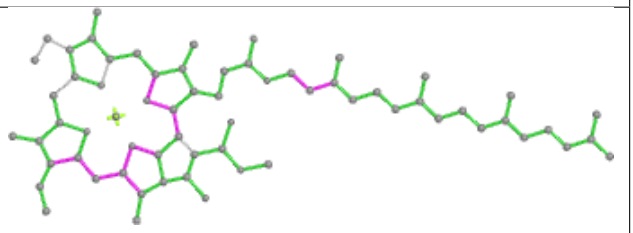


Rings

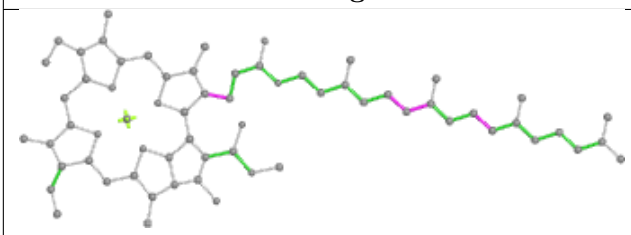
Ligand CLA B1 802



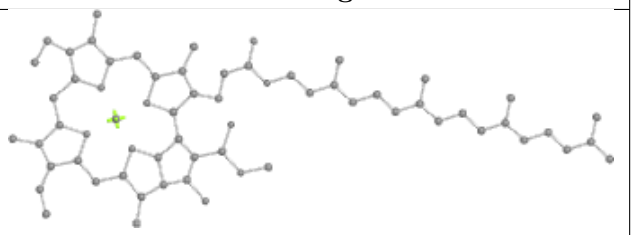
Bond lengths



Bond angles

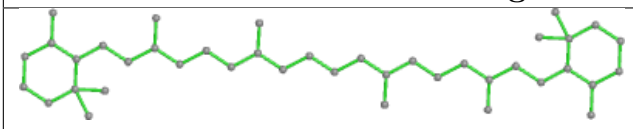


Torsions

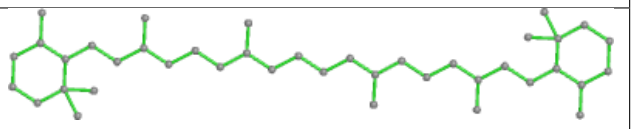


Rings

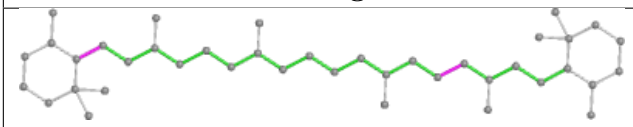
Ligand BCR J1 1304



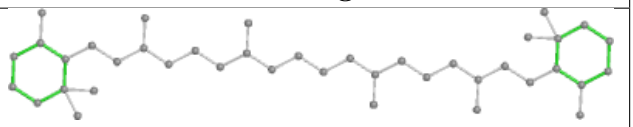
Bond lengths



Bond angles

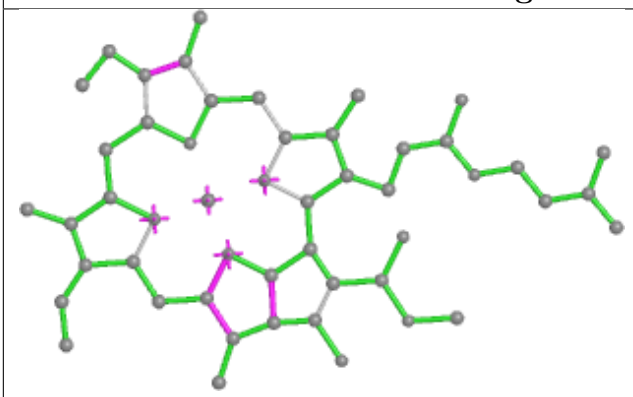


Torsions

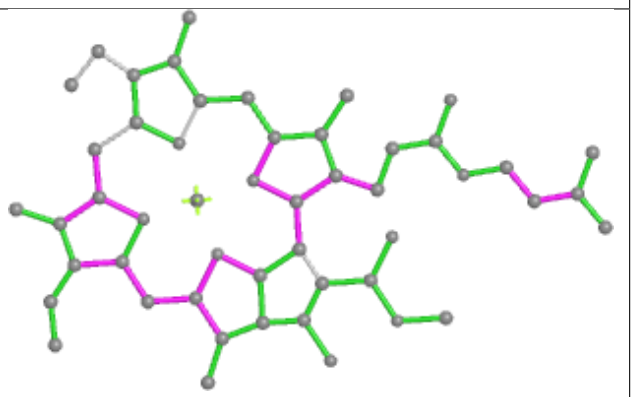


Rings

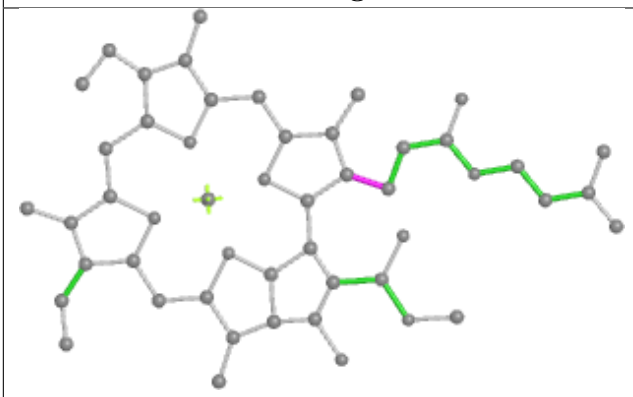
Ligand CLA B3 817



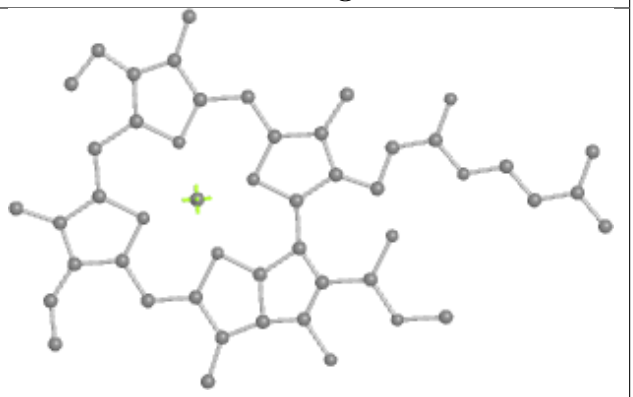
Bond lengths



Bond angles

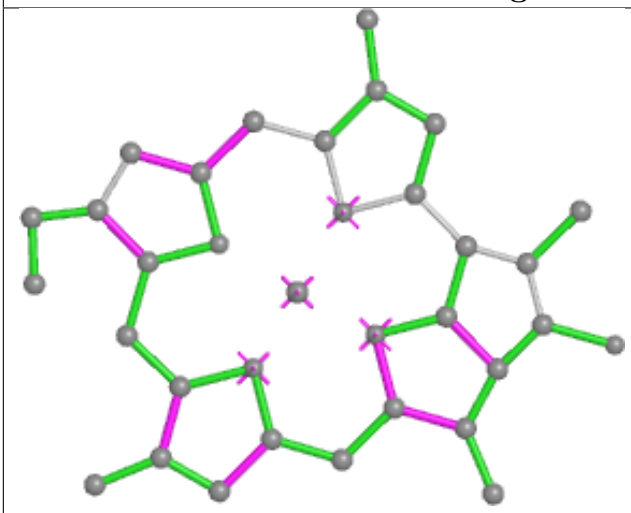


Torsions

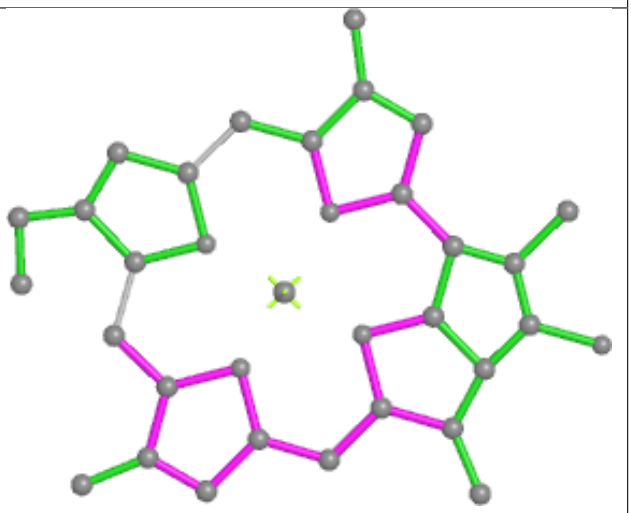


Rings

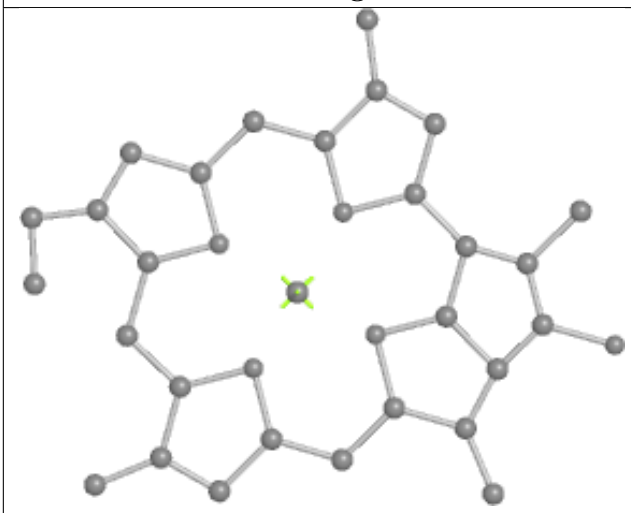
Ligand CLA J1 1307



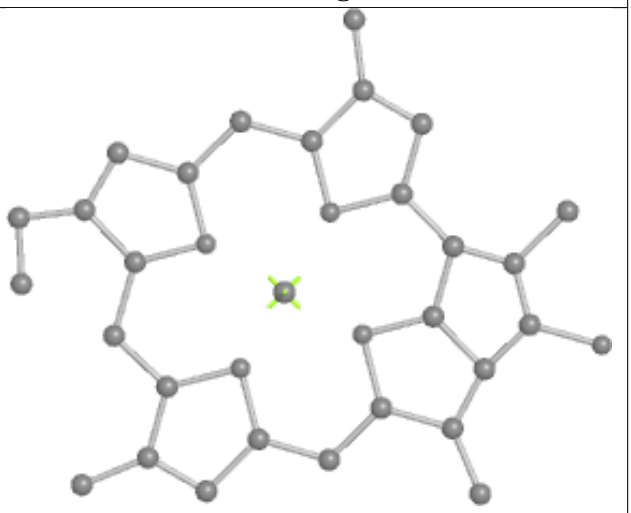
Bond lengths



Bond angles

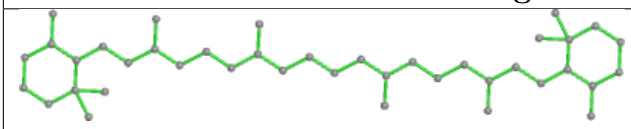


Torsions

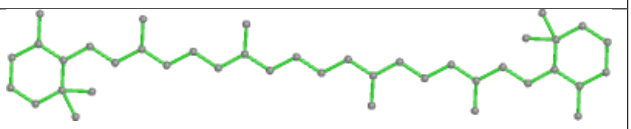


Rings

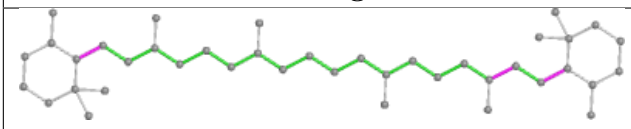
Ligand BCR B1 847



Bond lengths



Bond angles



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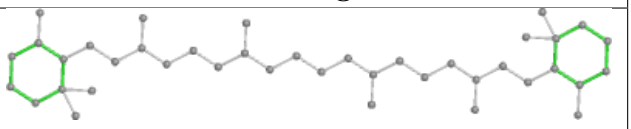
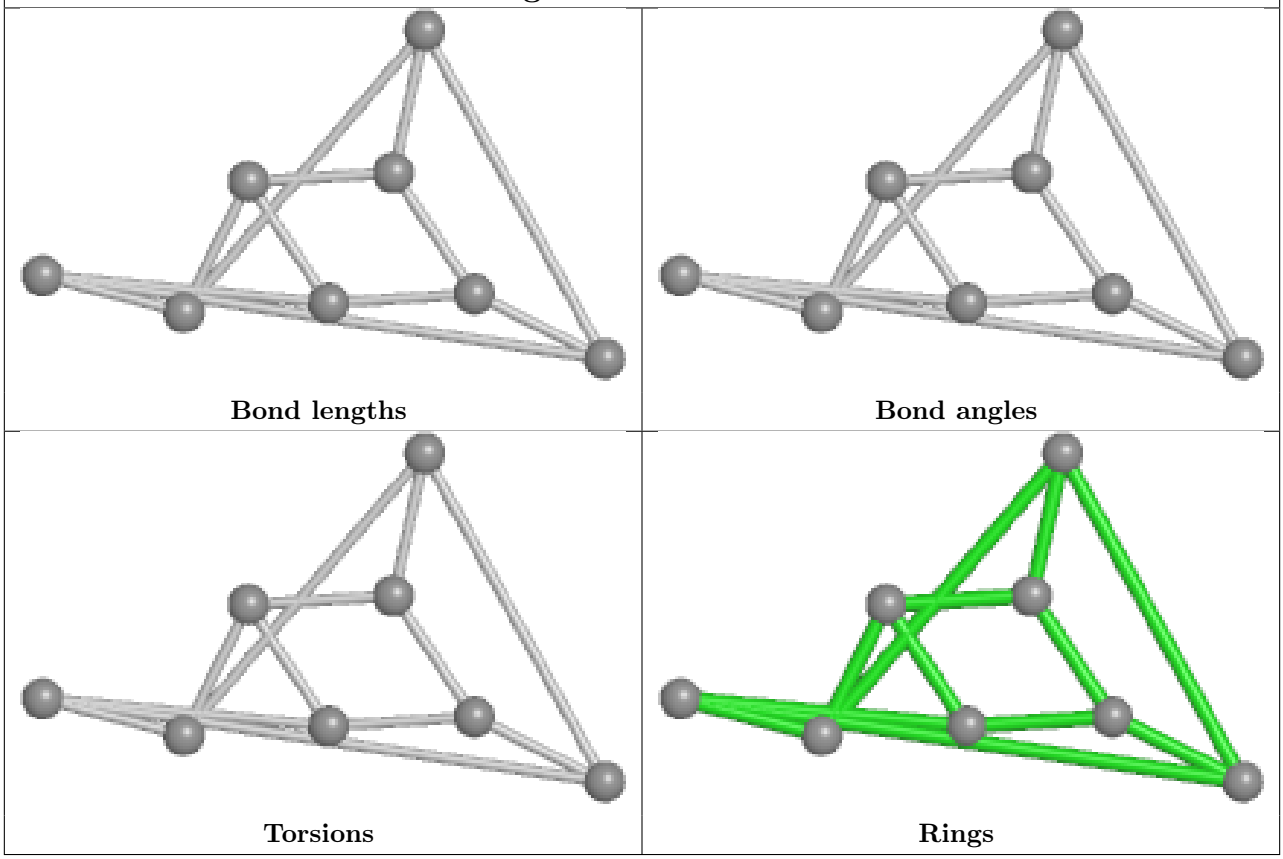
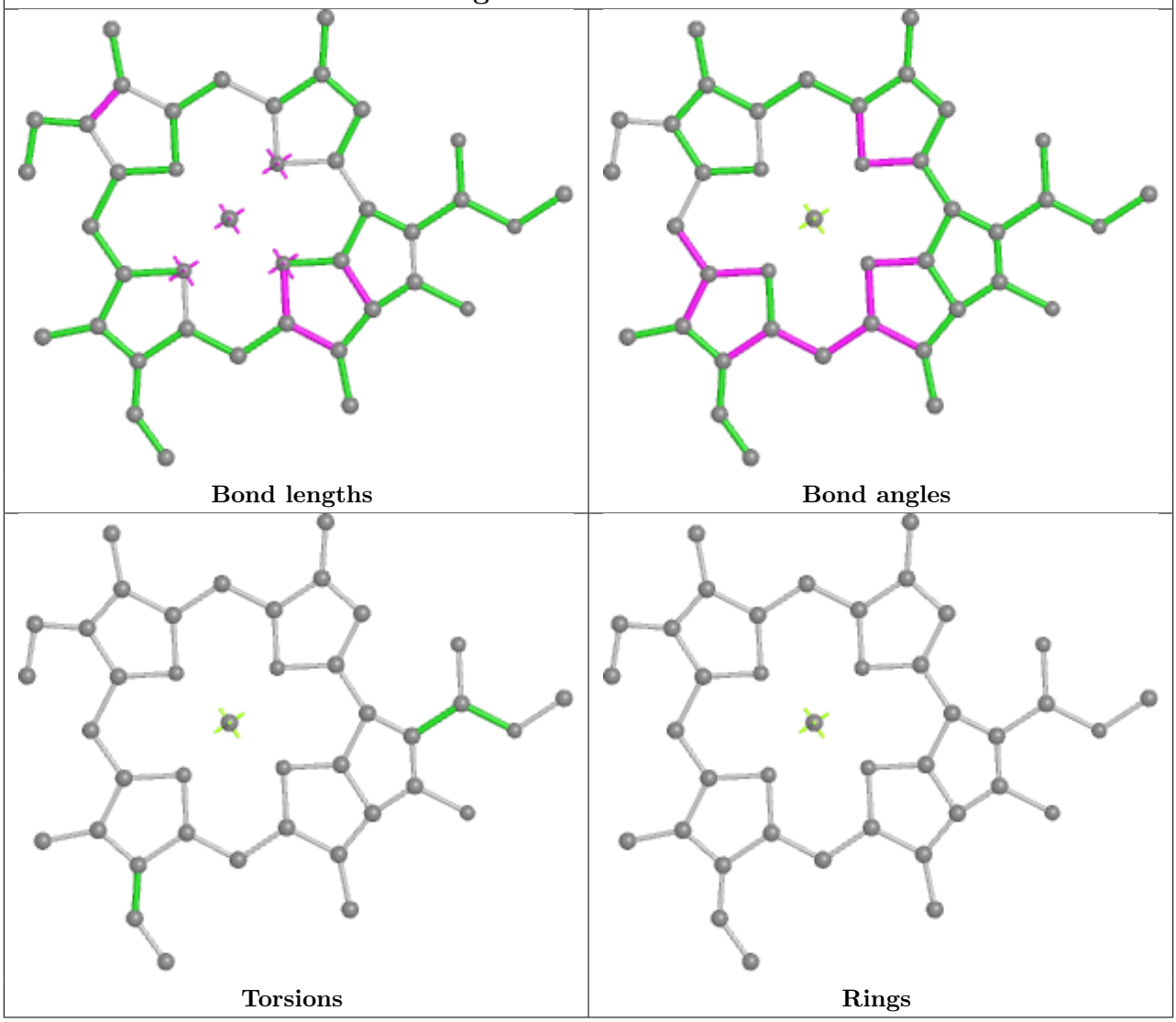


Rings

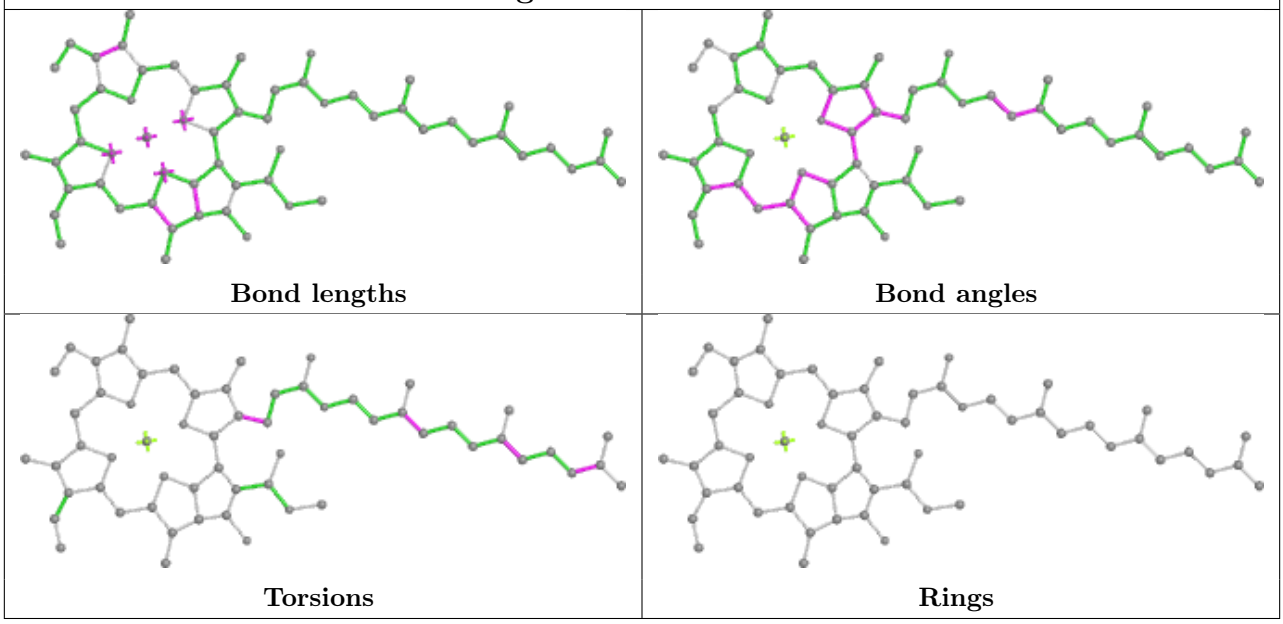
Ligand SF4 C3 102



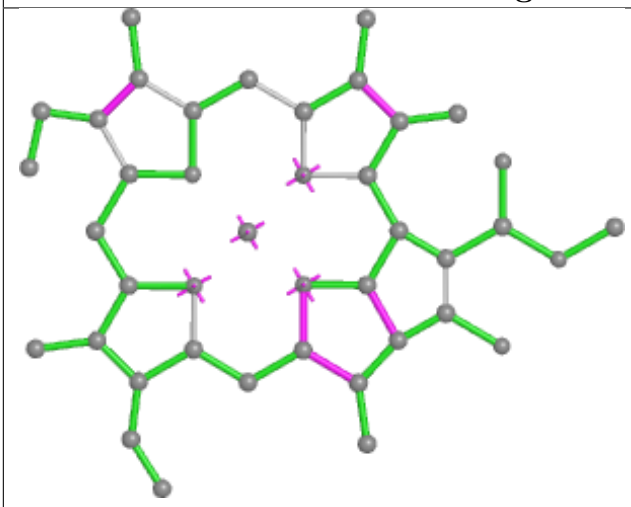
Ligand CLA B3 822



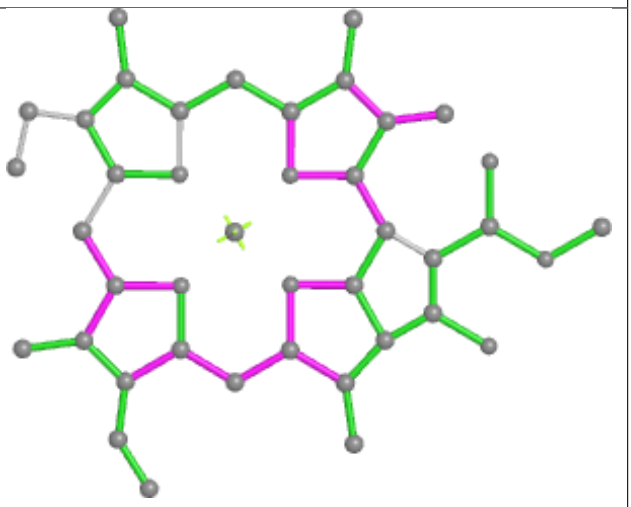
Ligand CLA B3 807



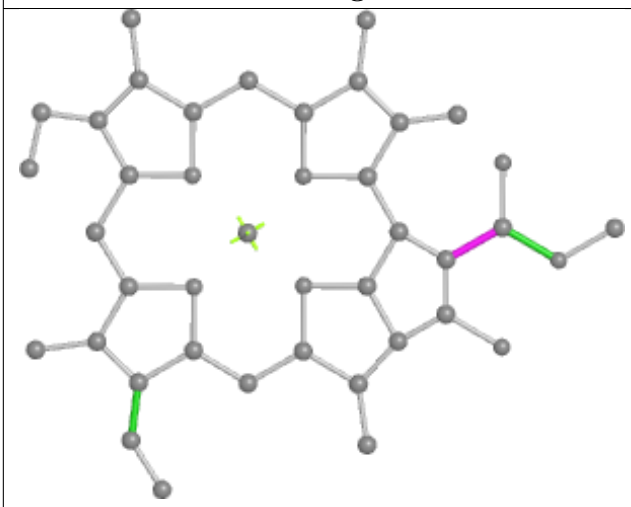
Ligand CLA B2 823



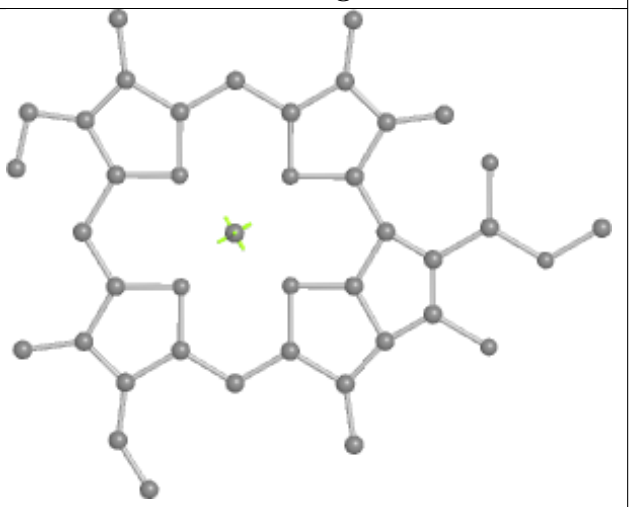
Bond lengths



Bond angles

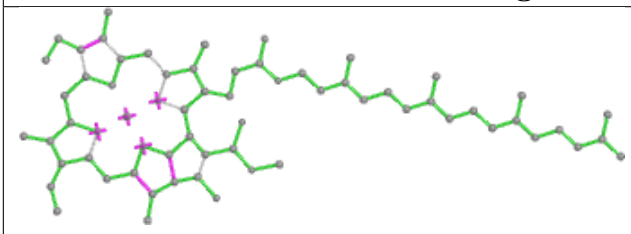


Torsions



Rings

Ligand CLA B3 802



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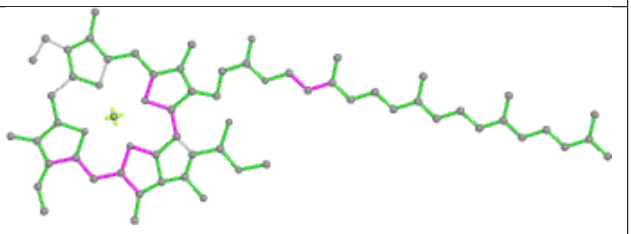
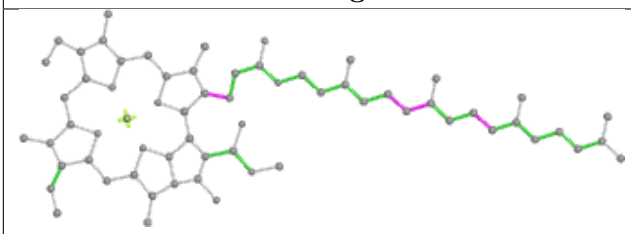
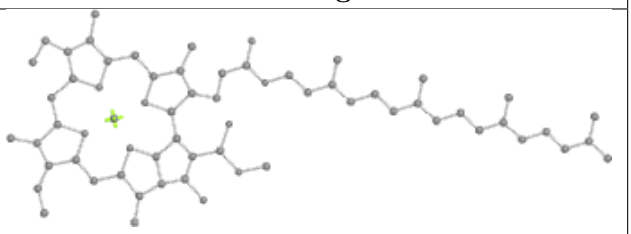


Bond angles

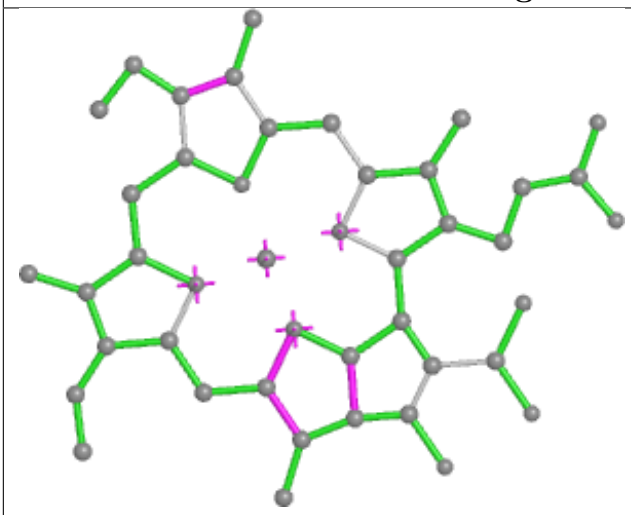


Torsions

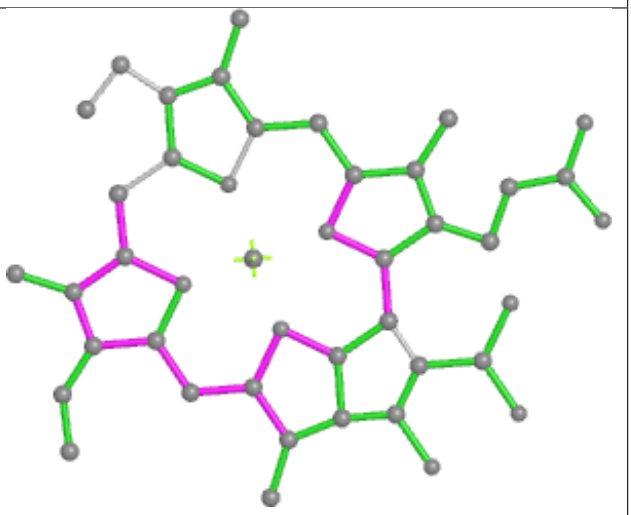


Rings

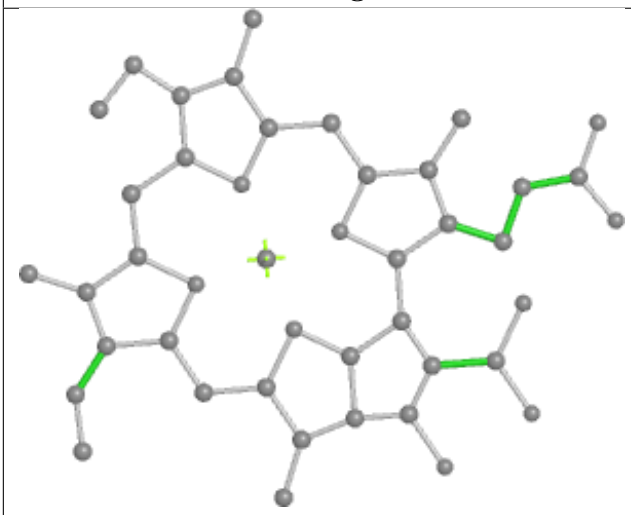
Ligand CLA B1 810



Bond lengths



Bond angles



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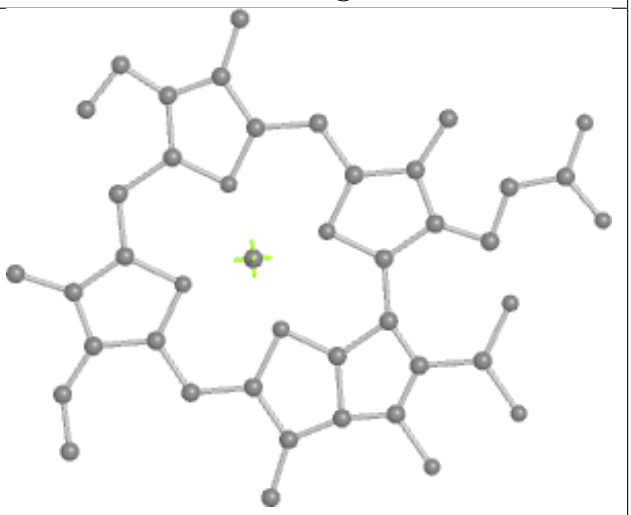
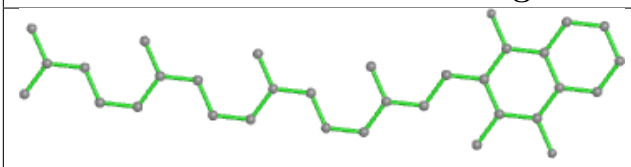
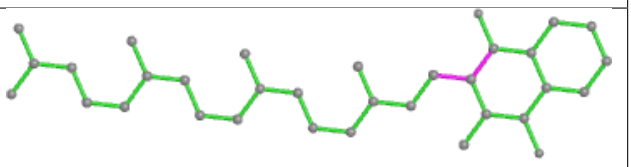


Rings

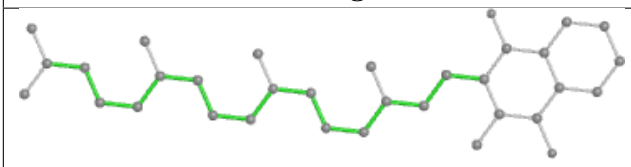
Ligand PQN B1 840



Bond lengths



Bond angles



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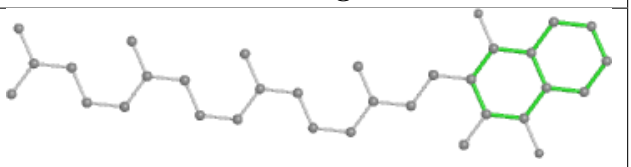
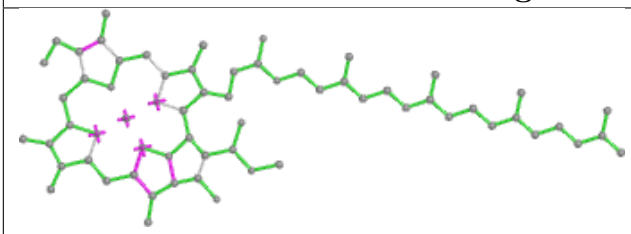
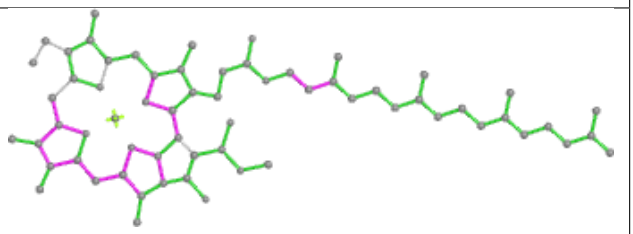
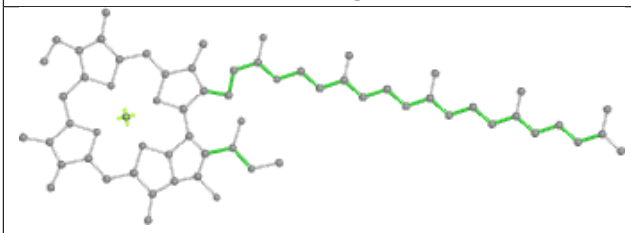
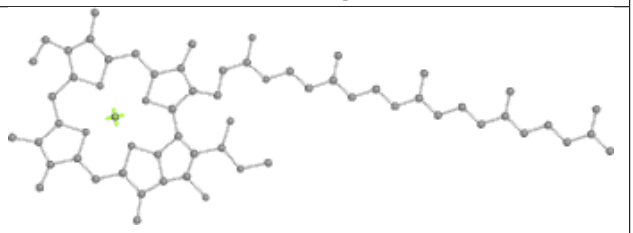
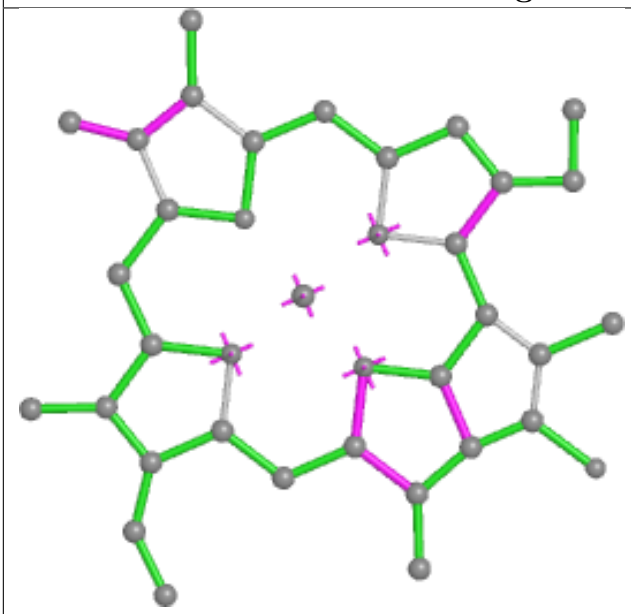


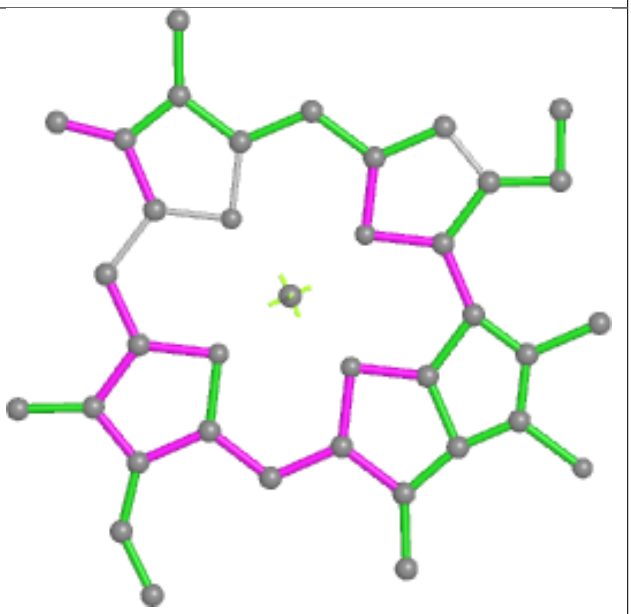
Rings

Ligand CLA A3 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

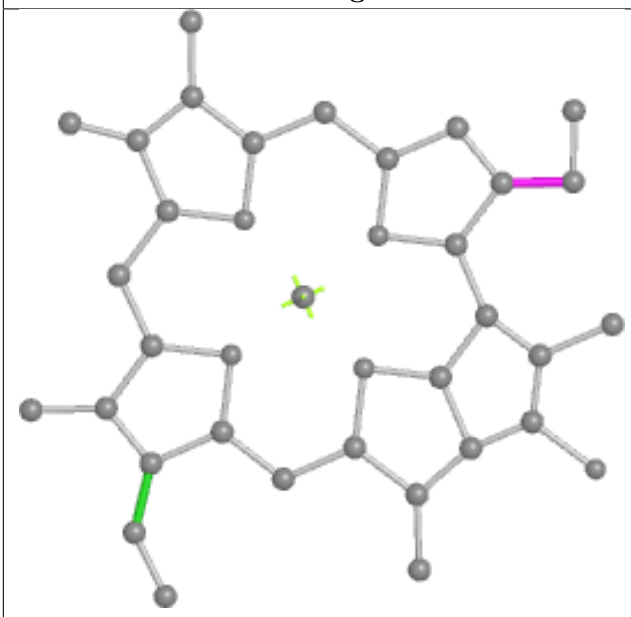
Ligand CLA B3 833



Bond lengths



Bond angles



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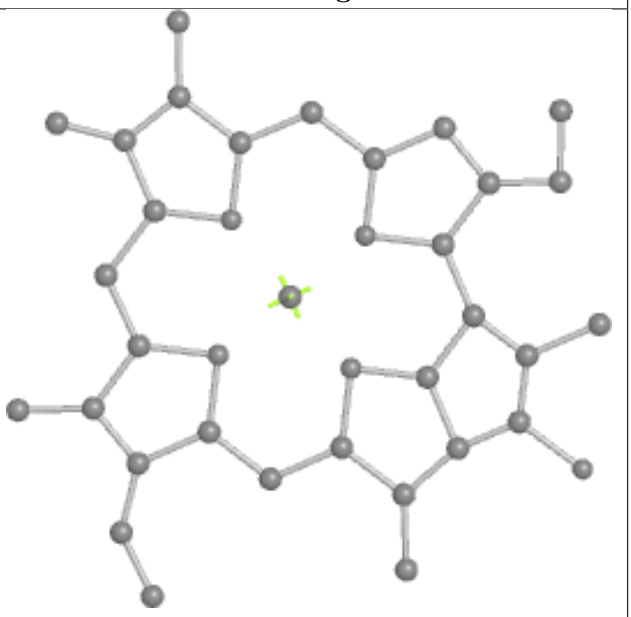
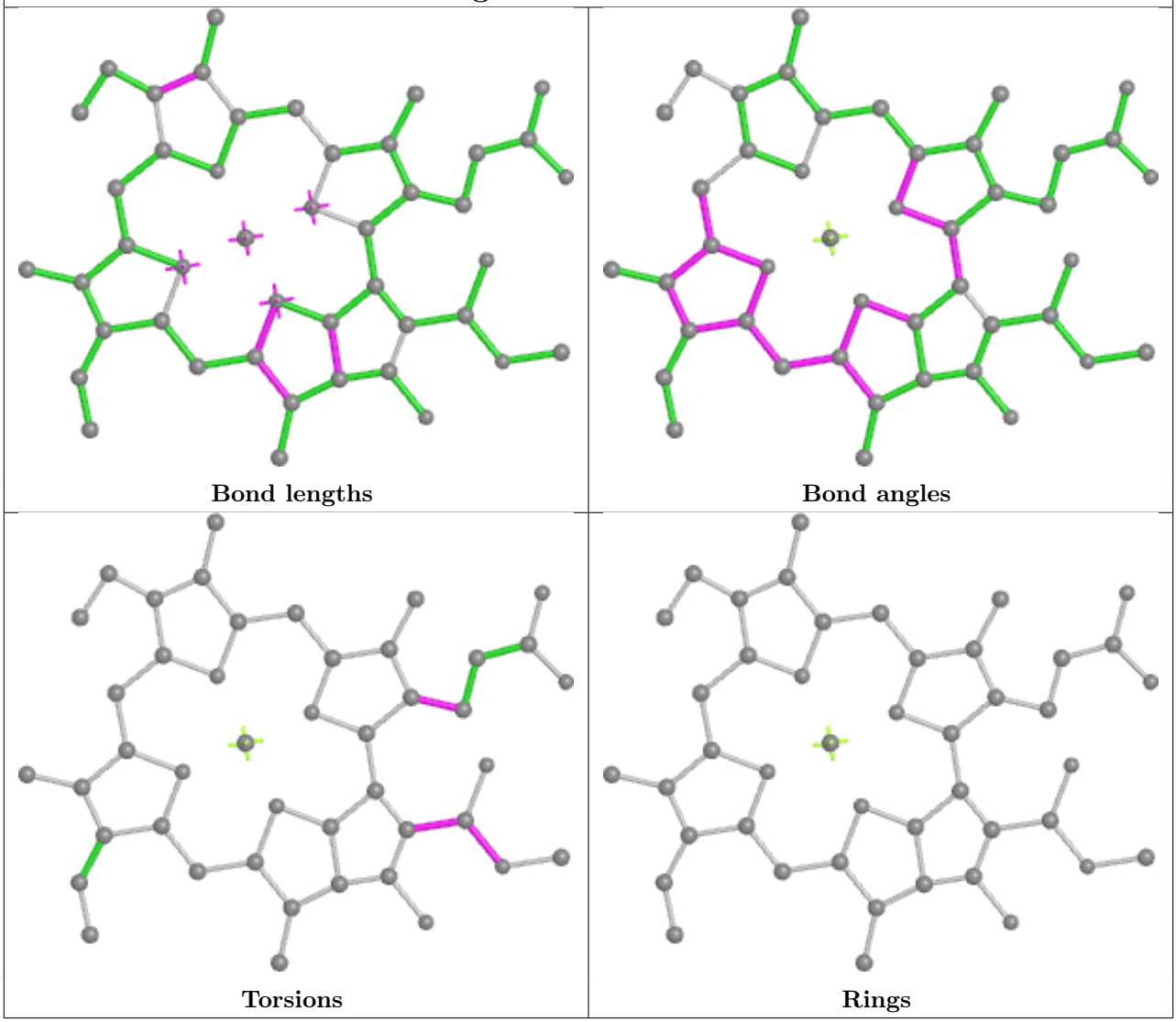
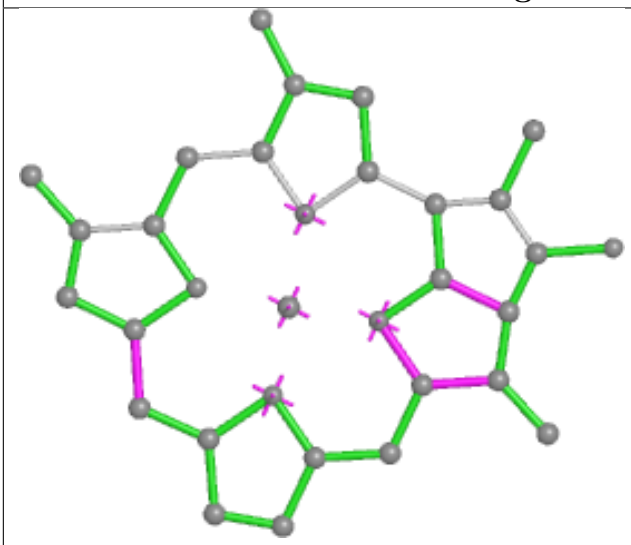


Rings

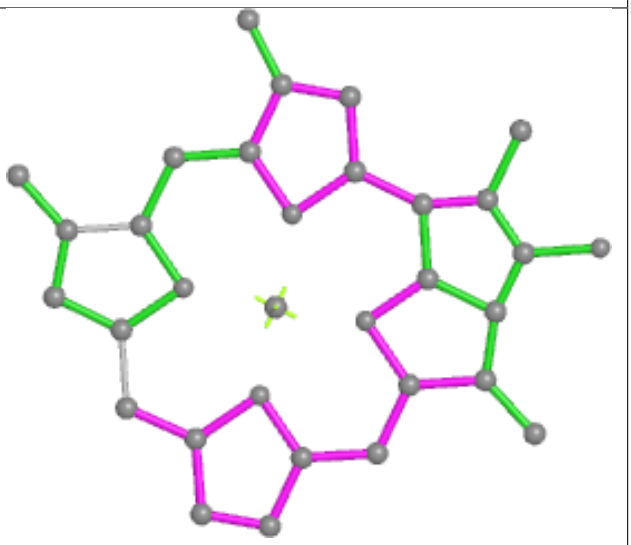
Ligand CLA A1 824



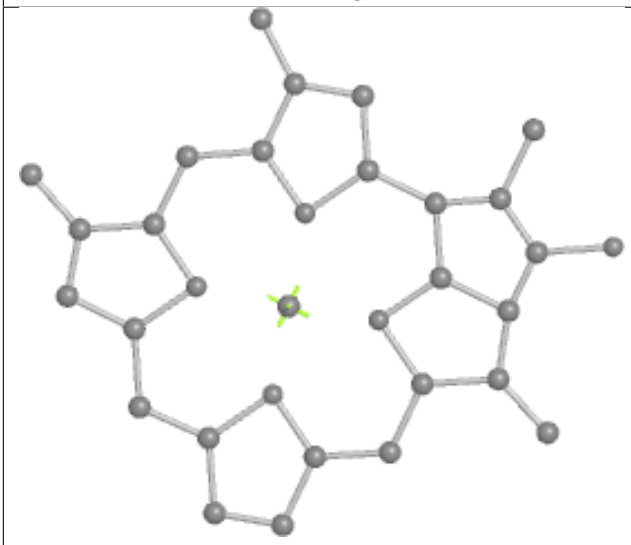
Ligand CLA K3 103



Bond lengths



Bond angles



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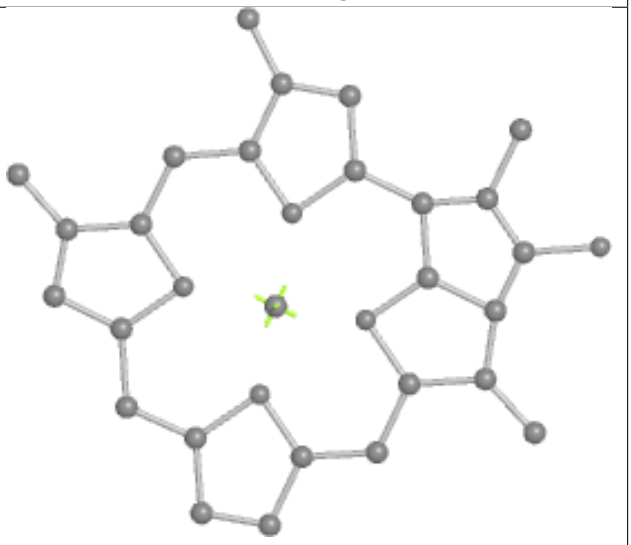
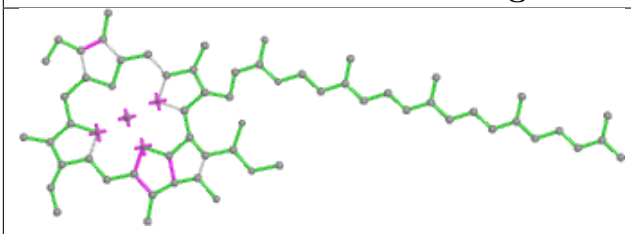
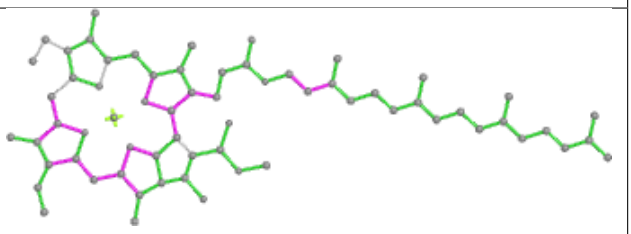


Rings

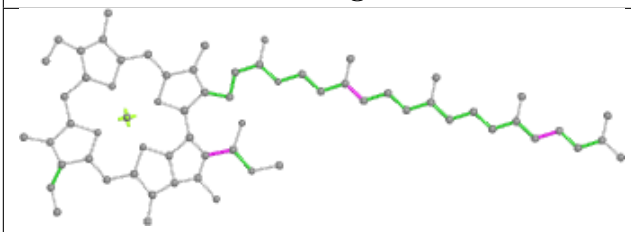
Ligand CLA L1 1004



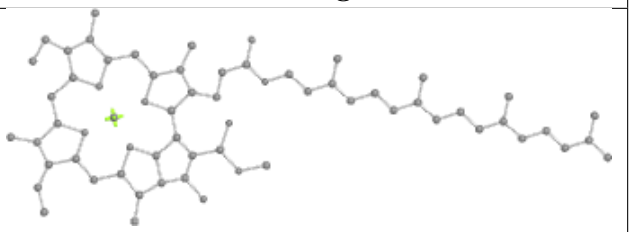
Bond lengths



Bond angles

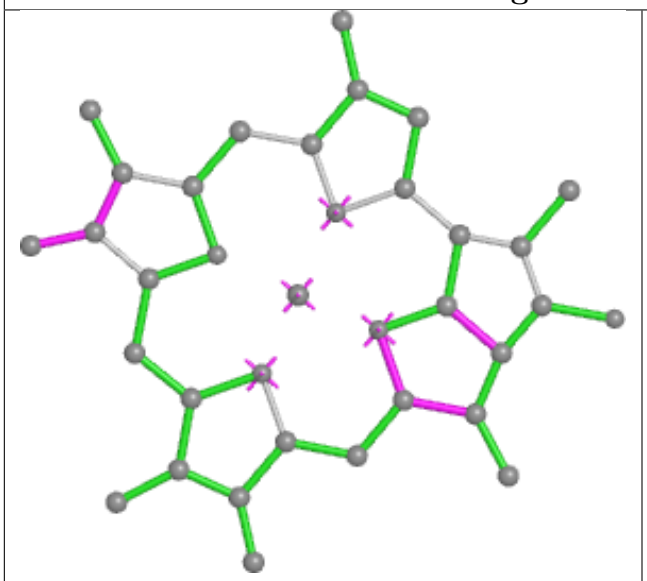


Torsions



Rings

Ligand CLA J2 1302



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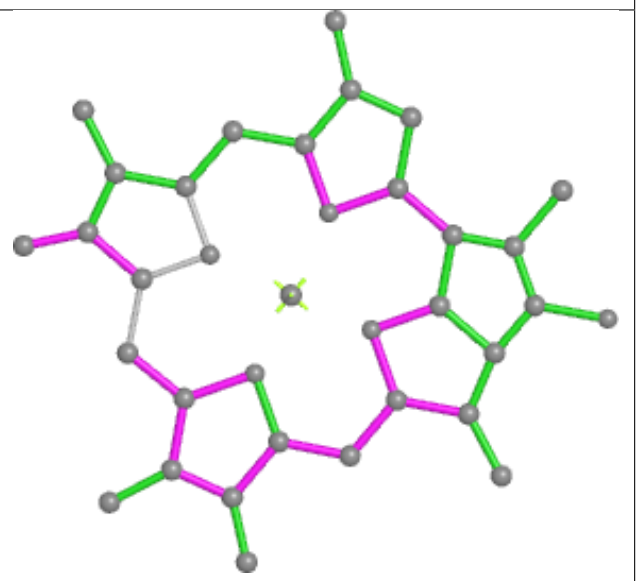
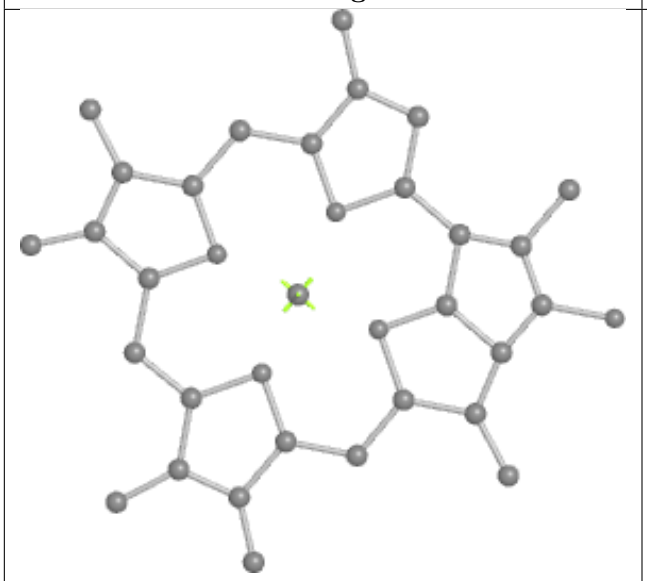


Bond angles



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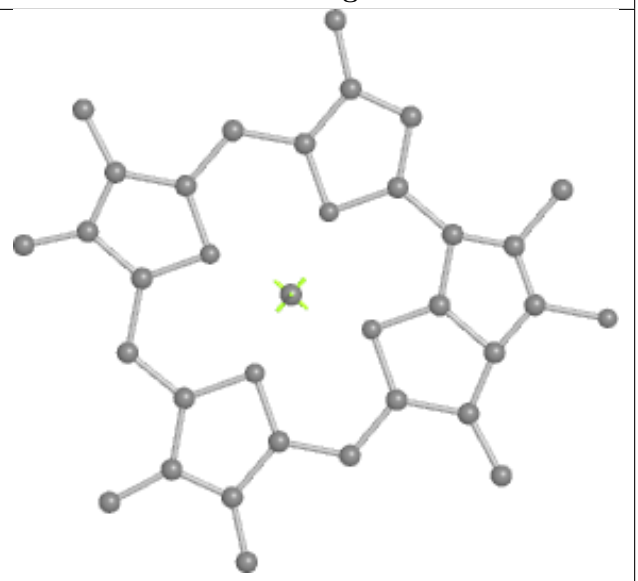
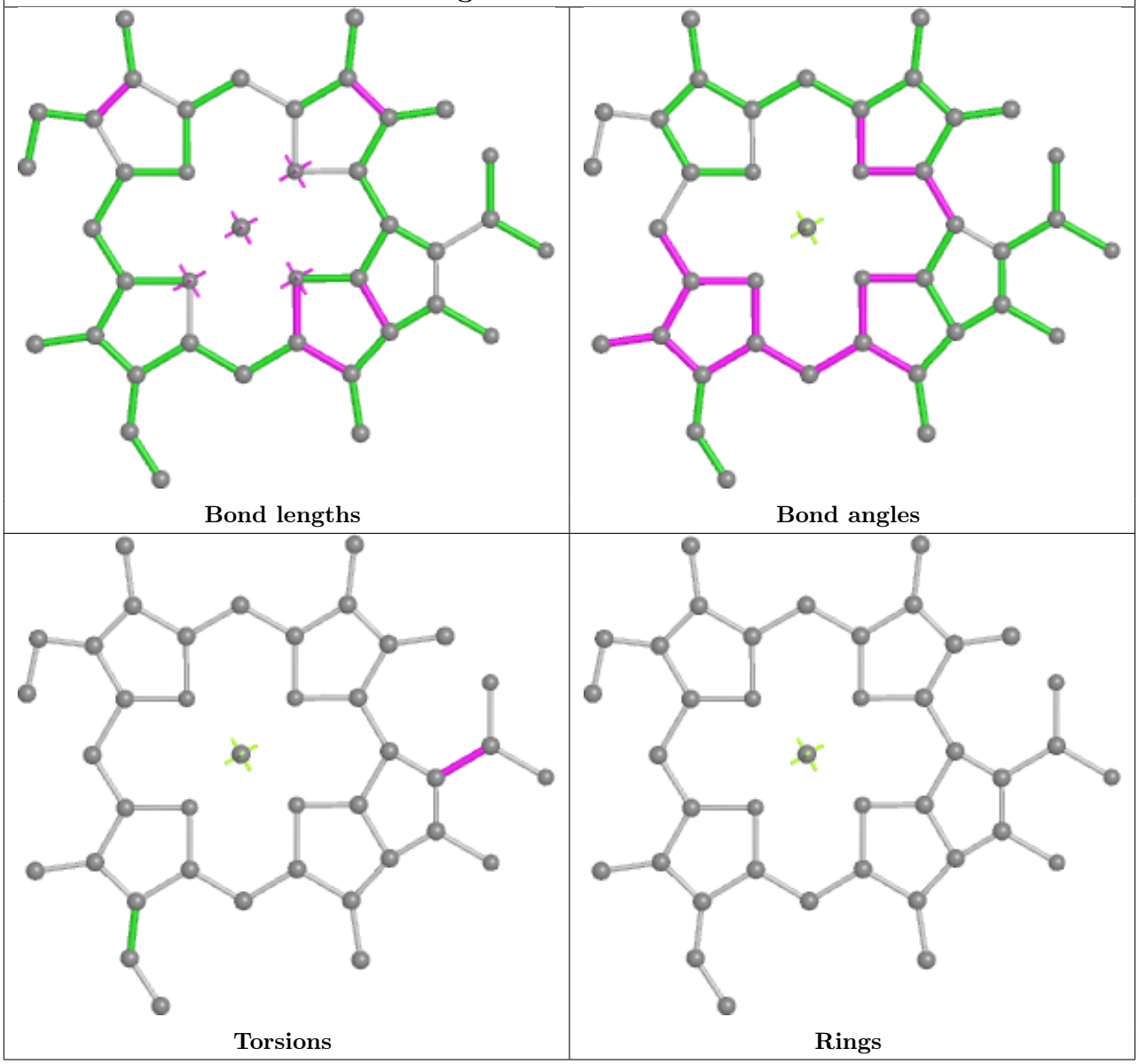
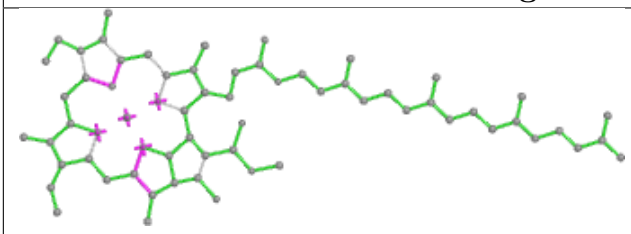


Rings

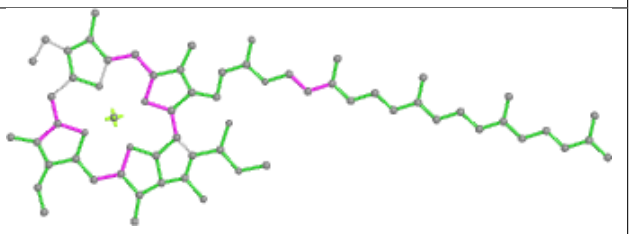
Ligand CLA A2 841



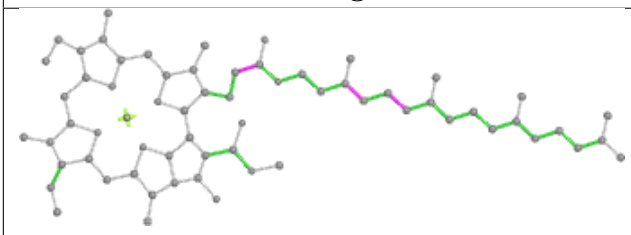
Ligand CL0 A2 801



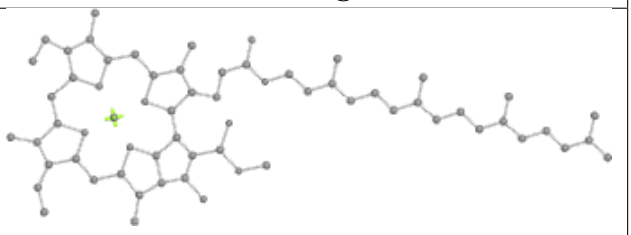
Bond lengths



Bond angles

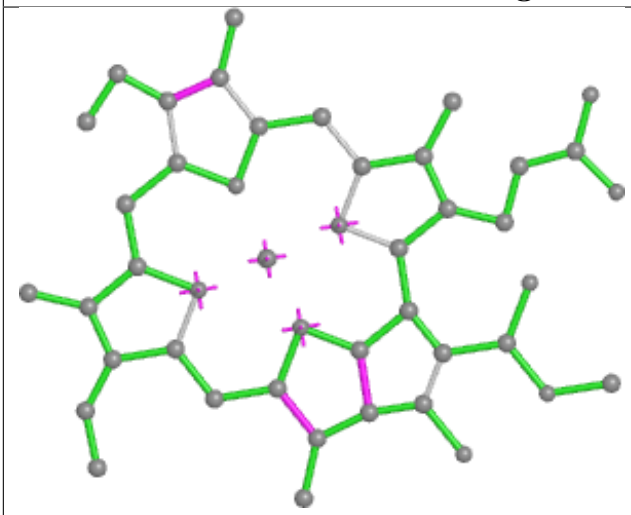


Torsions

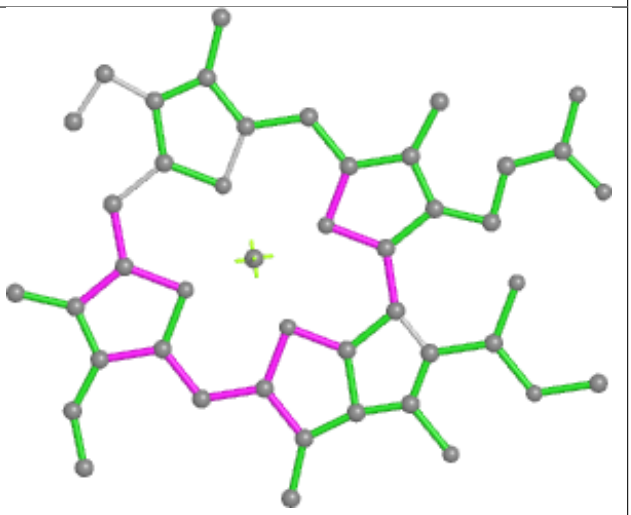


Rings

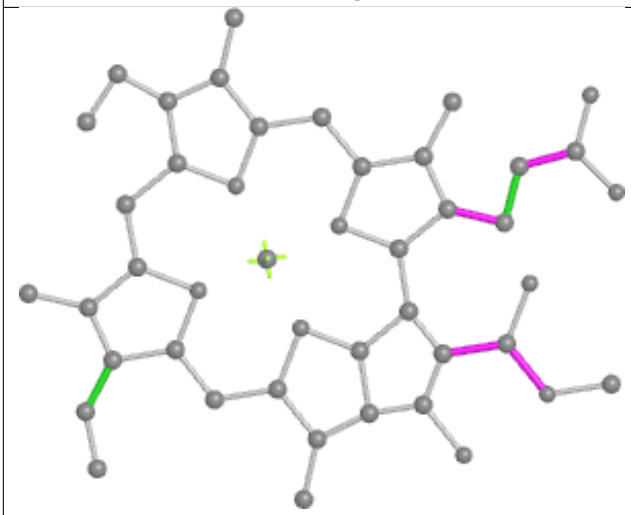
Ligand CLA B3 849



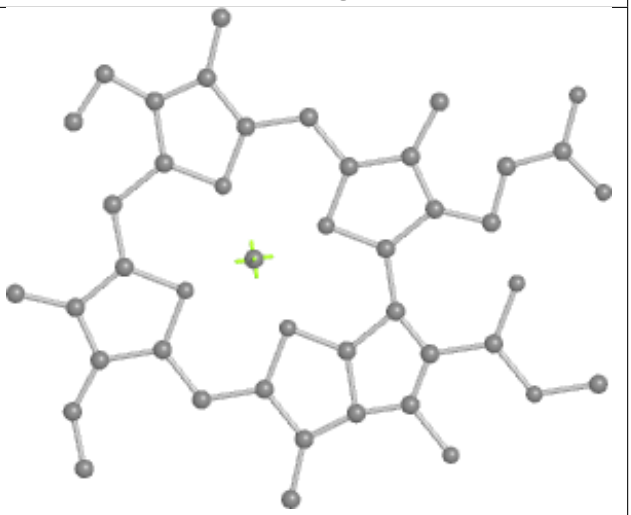
Bond lengths



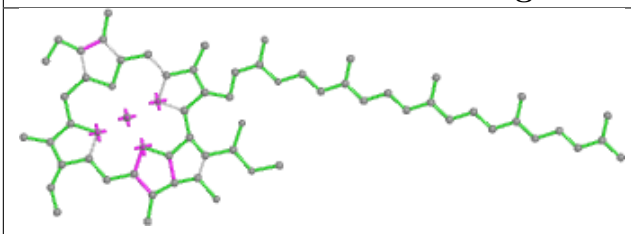
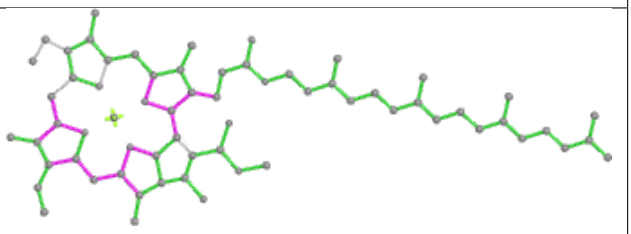
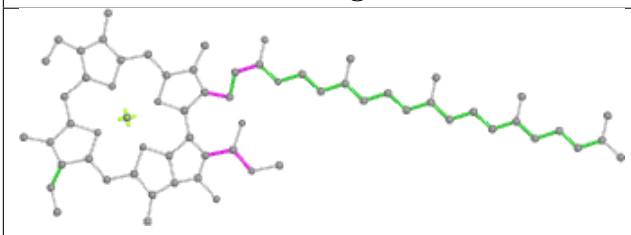
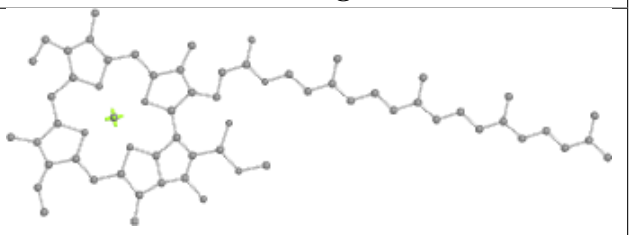
Bond angles



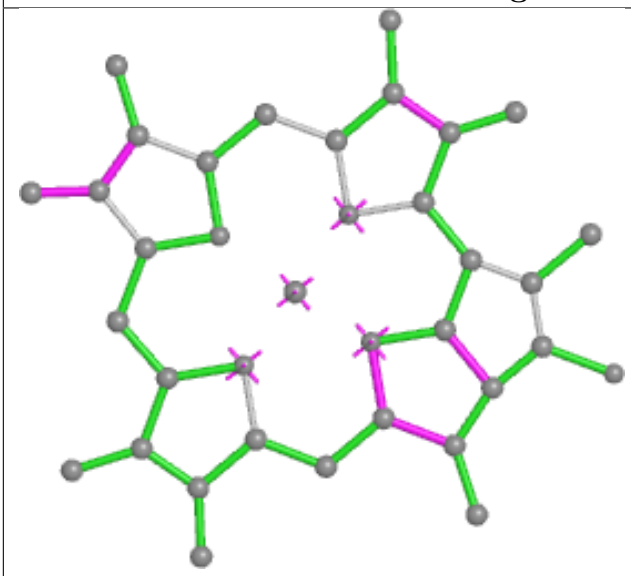
Torsions



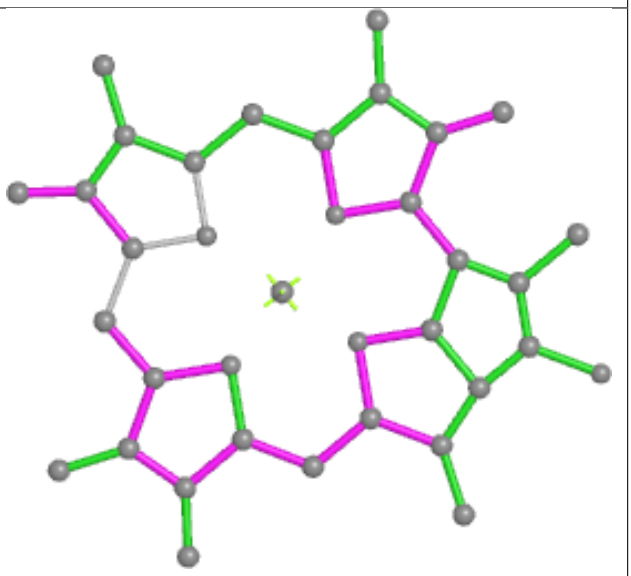
Rings

Ligand CLA B1 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

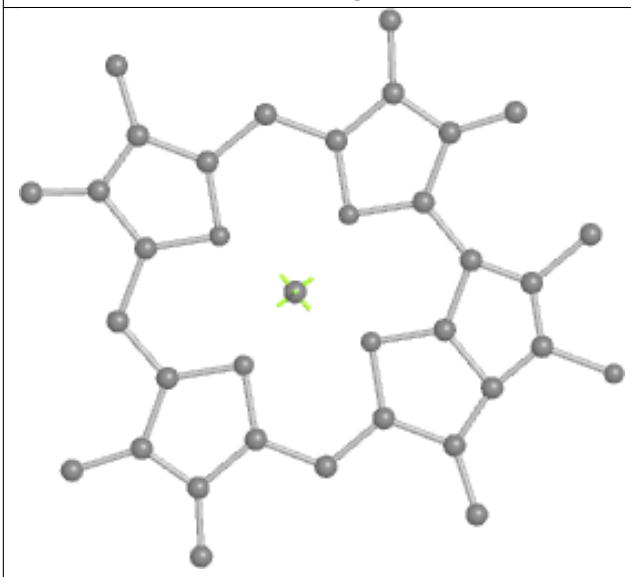
Ligand CLA J3 1303



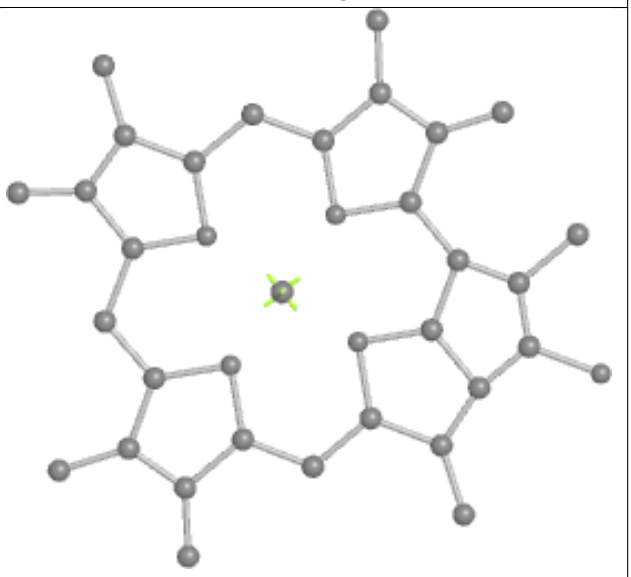
Bond lengths



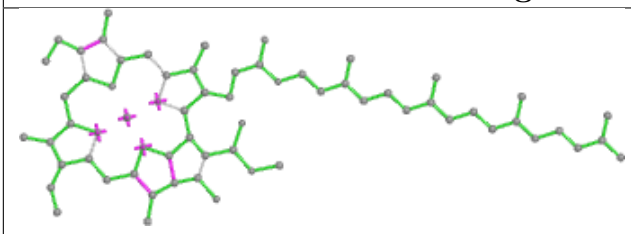
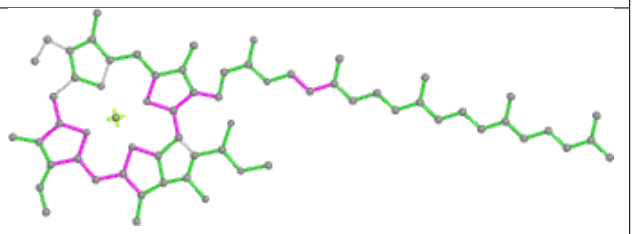
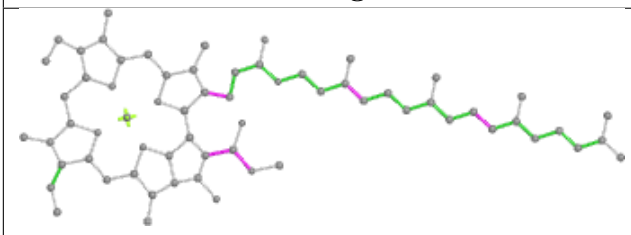
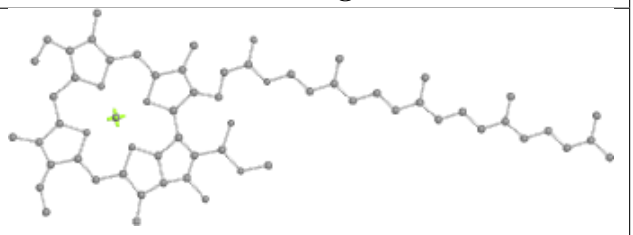
Bond angles

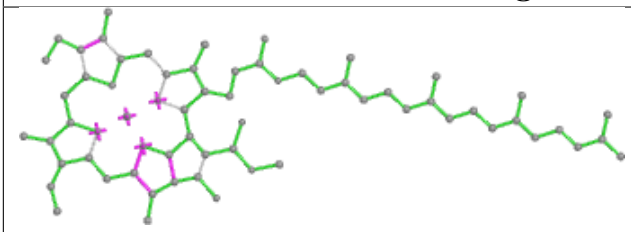
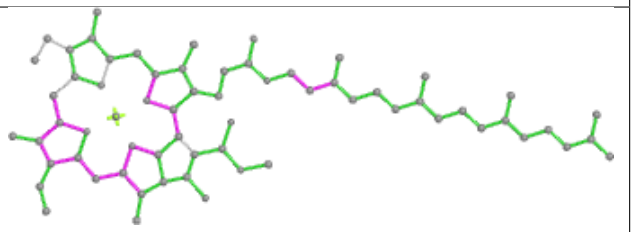
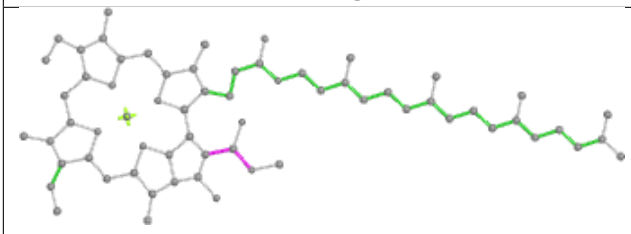
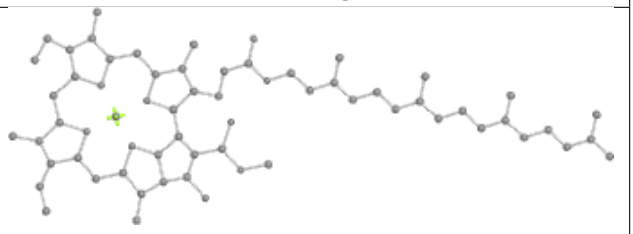


Torsions

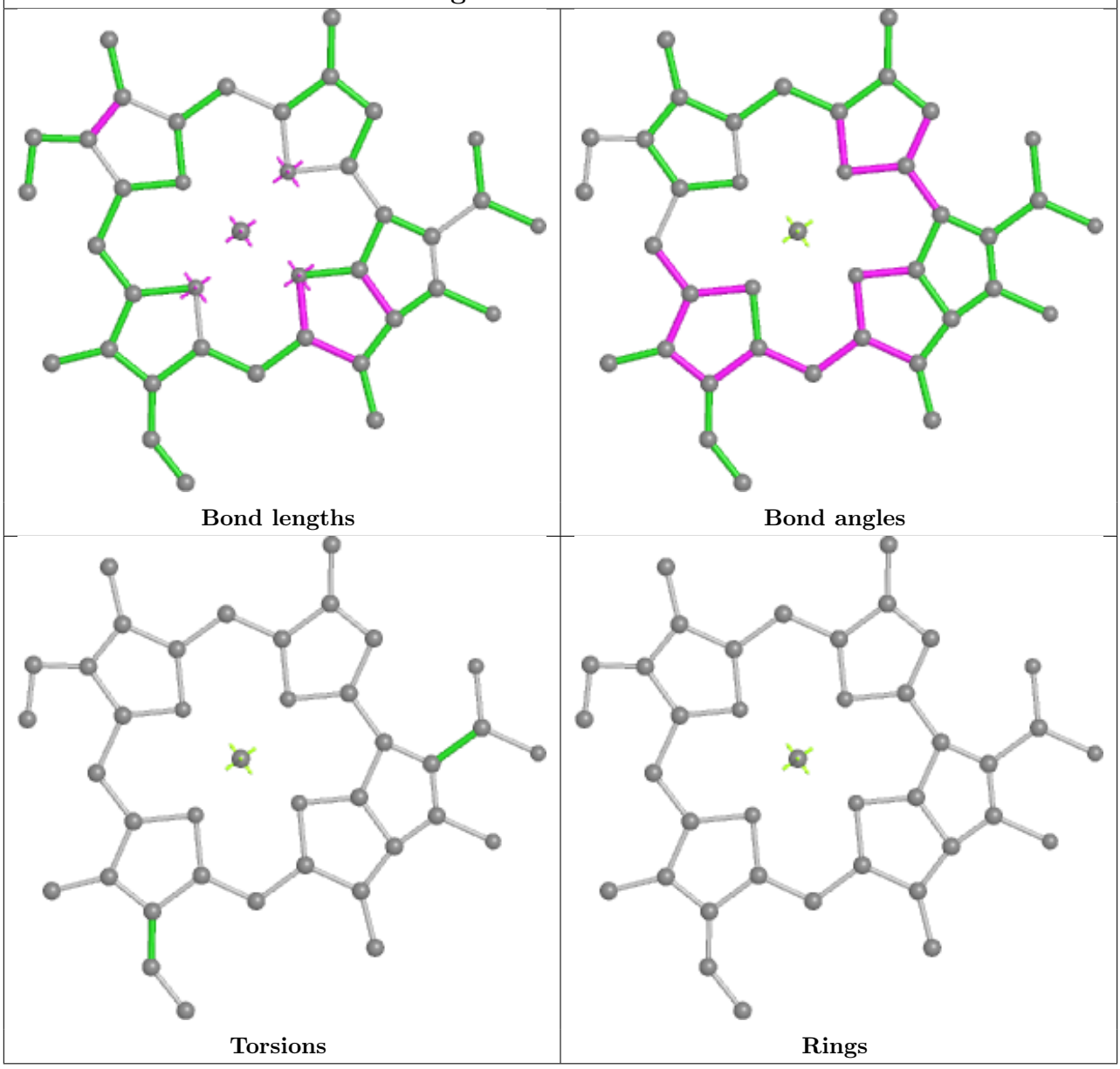


Rings

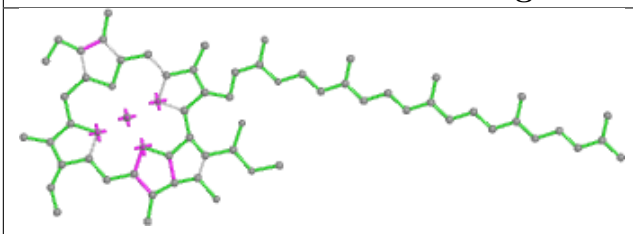
Ligand CLA A2 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A3 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

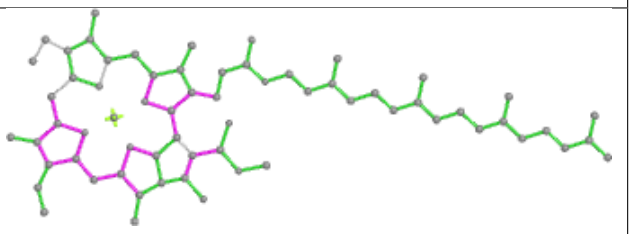
Ligand CLA B1 834



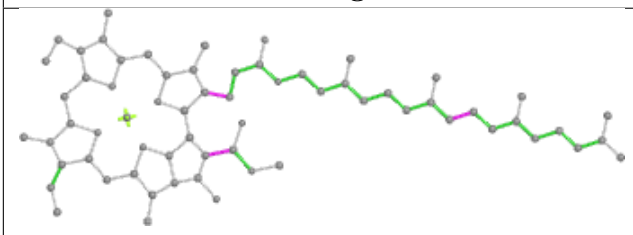
Ligand CLA B1 812



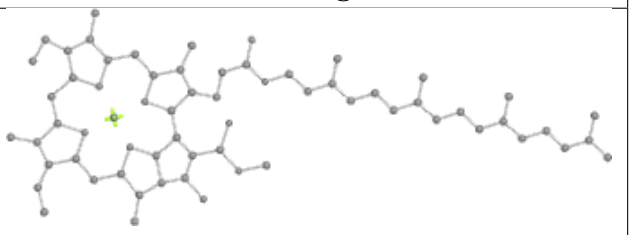
Bond lengths



Bond angles

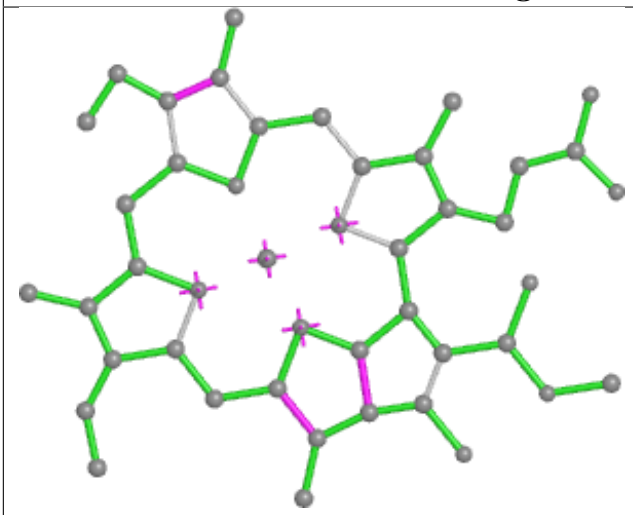


Torsions

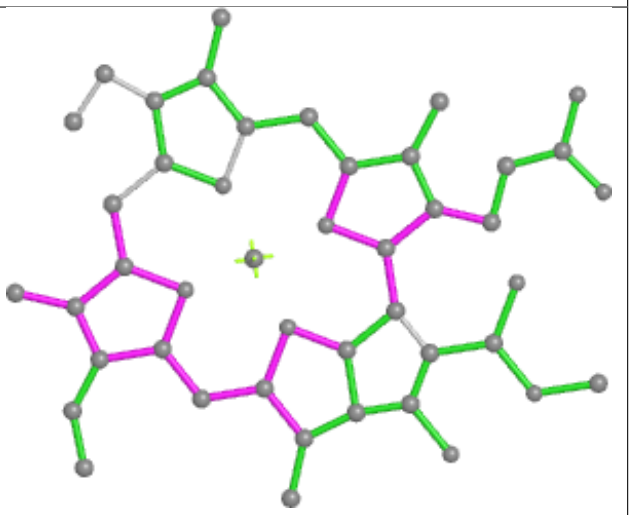


Rings

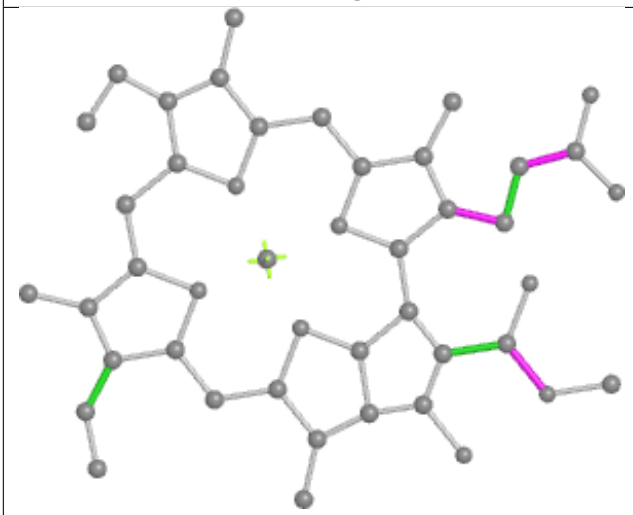
Ligand CLA A2 832



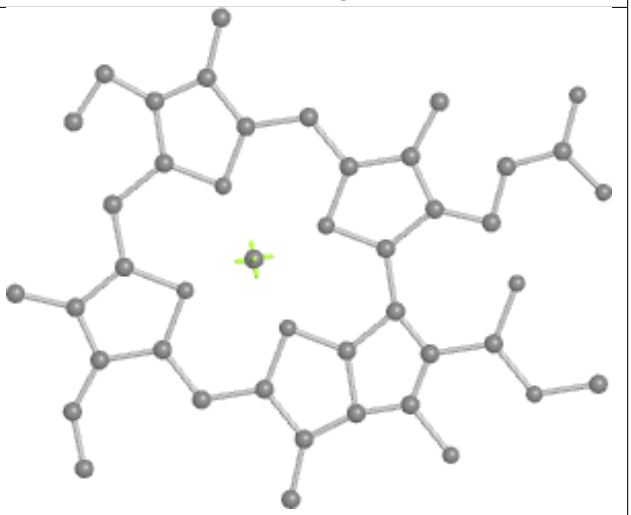
Bond lengths



Bond angles

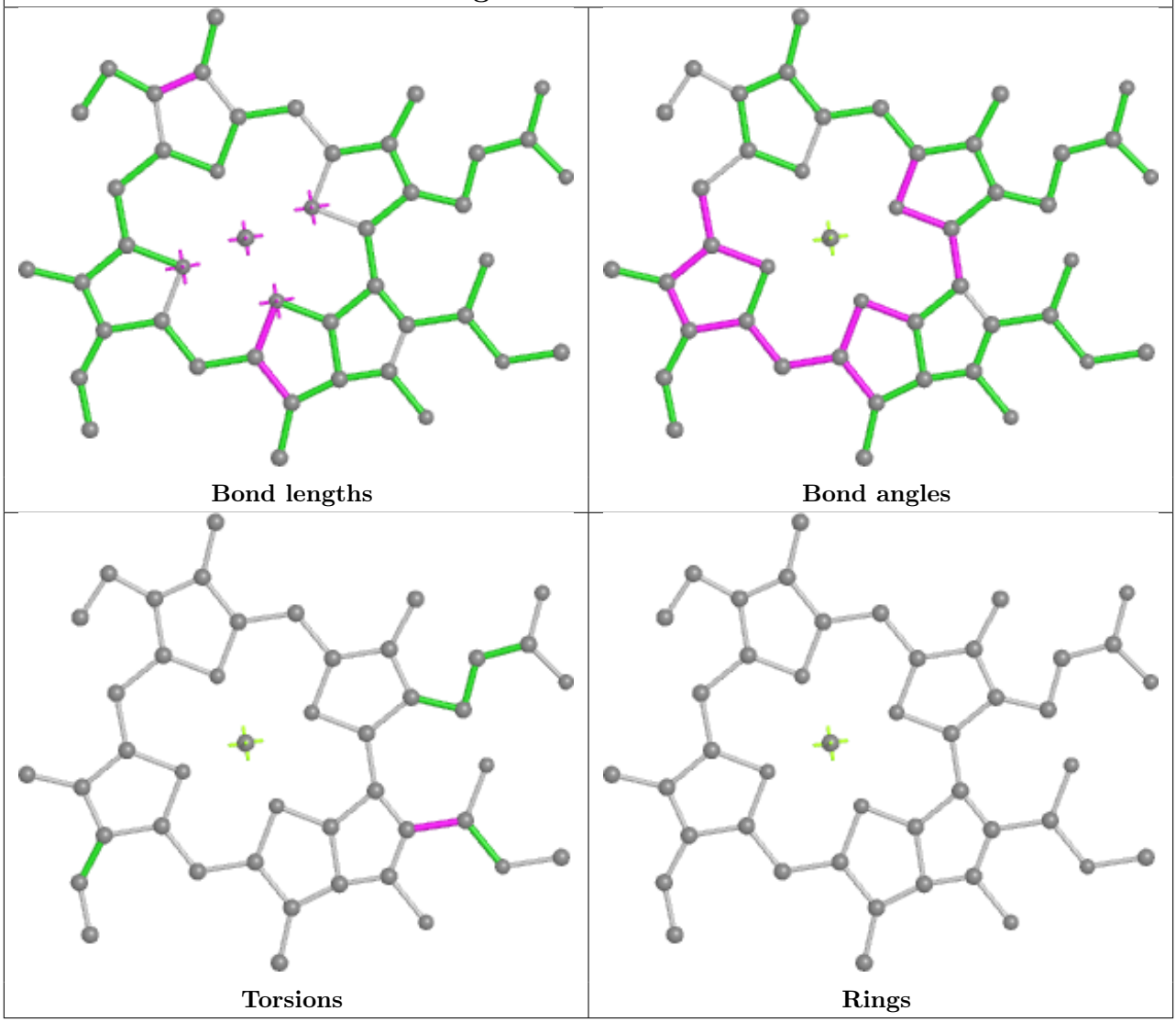


Torsions

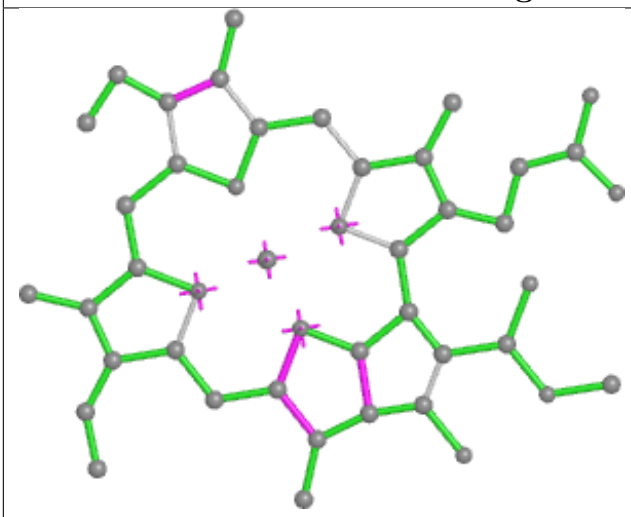


Rings

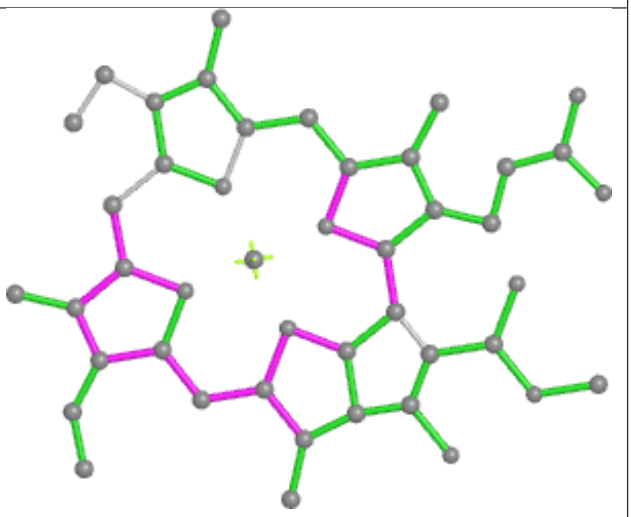
Ligand CLA B2 811



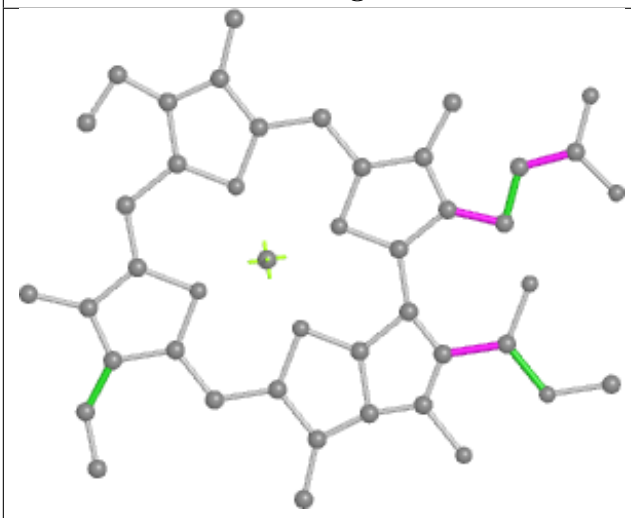
Ligand CLA B3 819



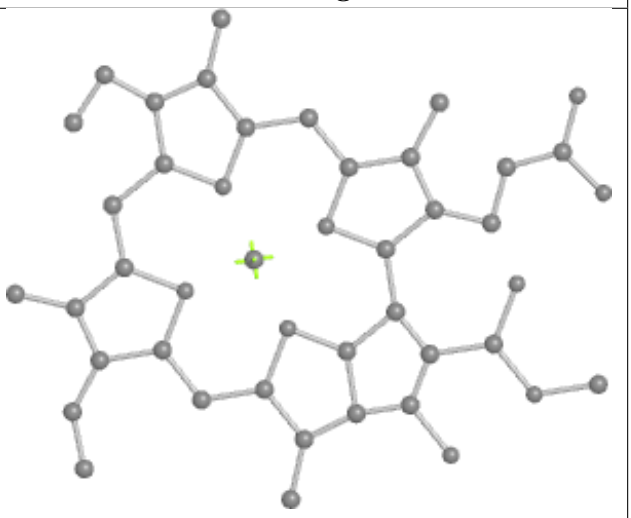
Bond lengths



Bond angles

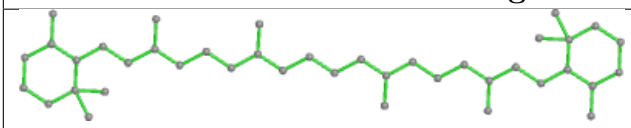


Torsions

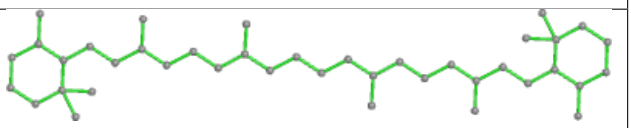


Rings

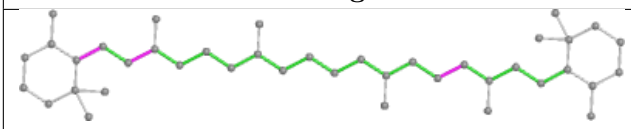
Ligand BCR J2 1306



Bond lengths



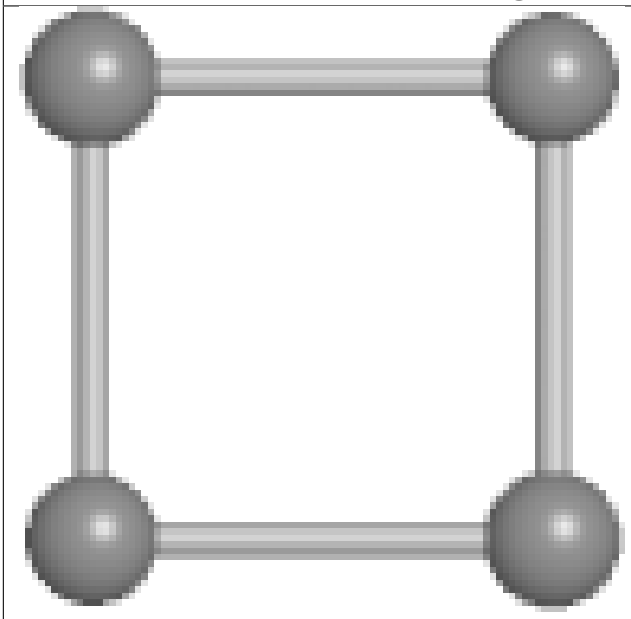
Bond angles



Torsions

Rings

Ligand GAK R2 101



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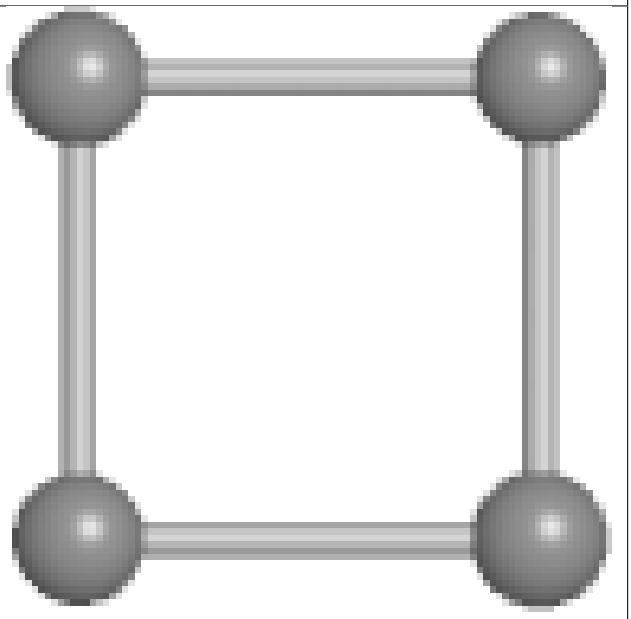
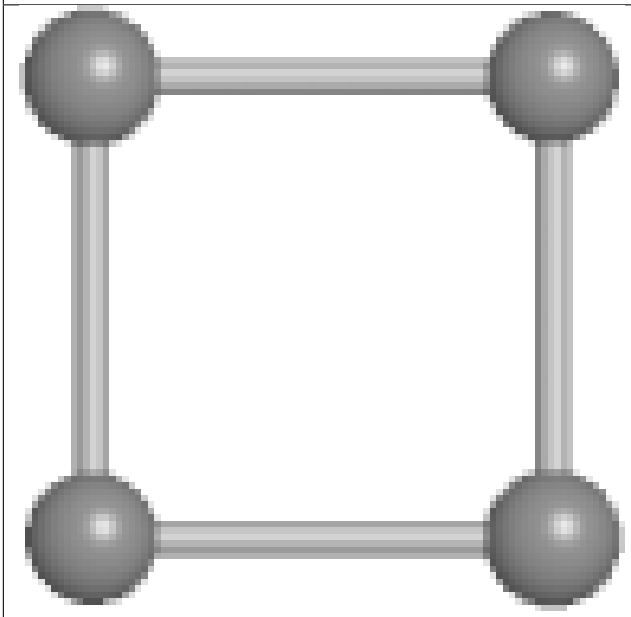
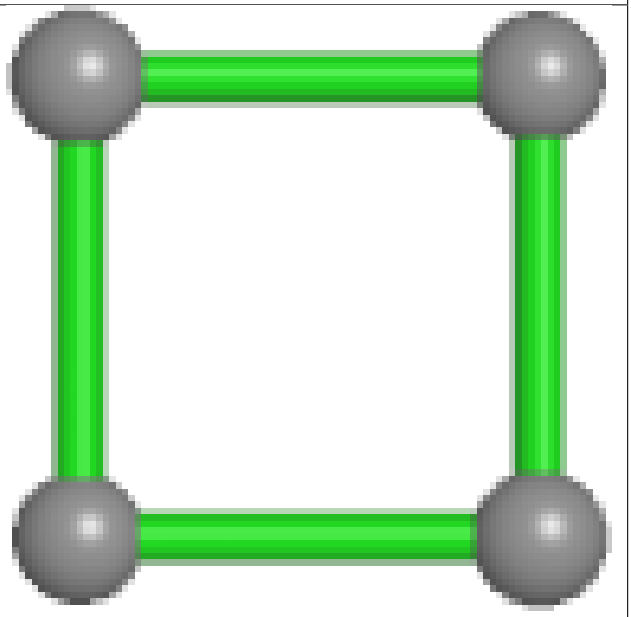


Bond angles

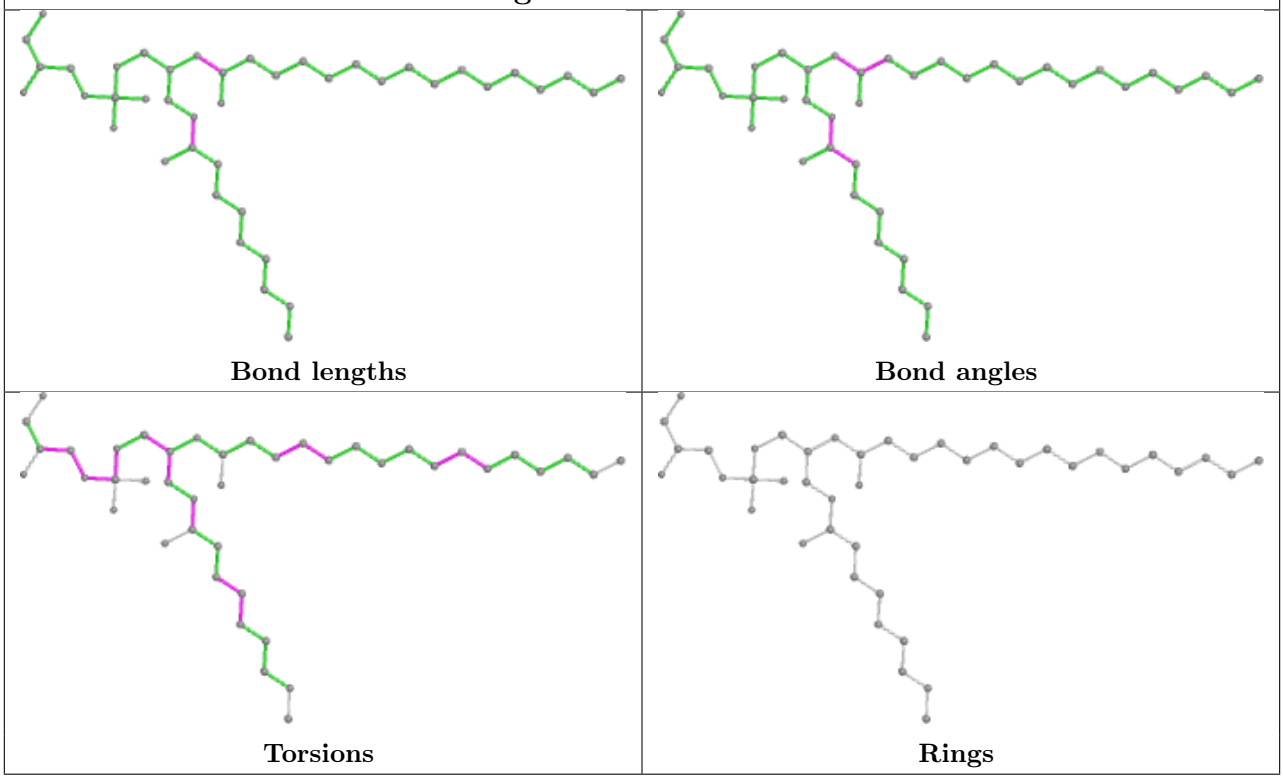


Torsions

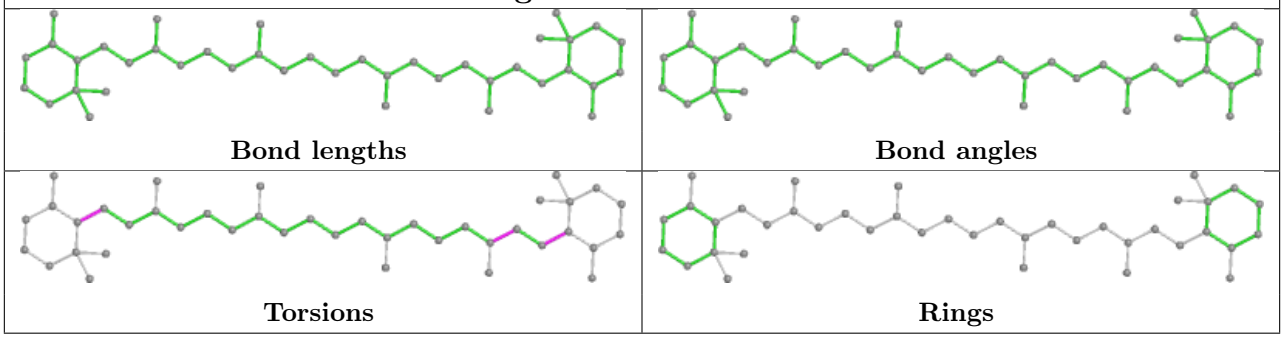


Rings

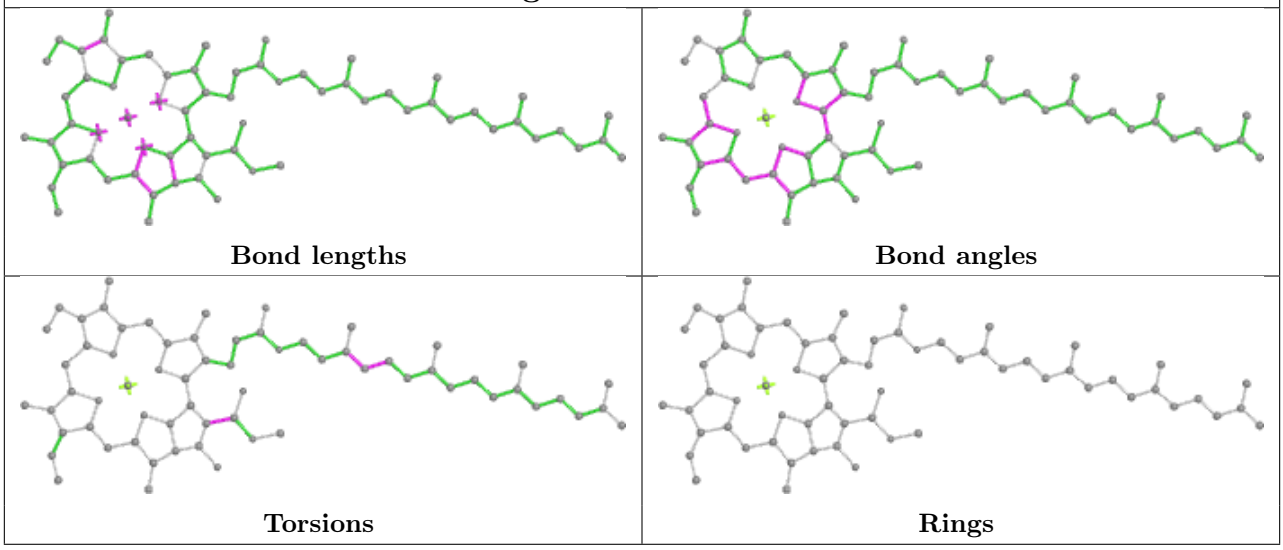
Ligand LHG X1 101



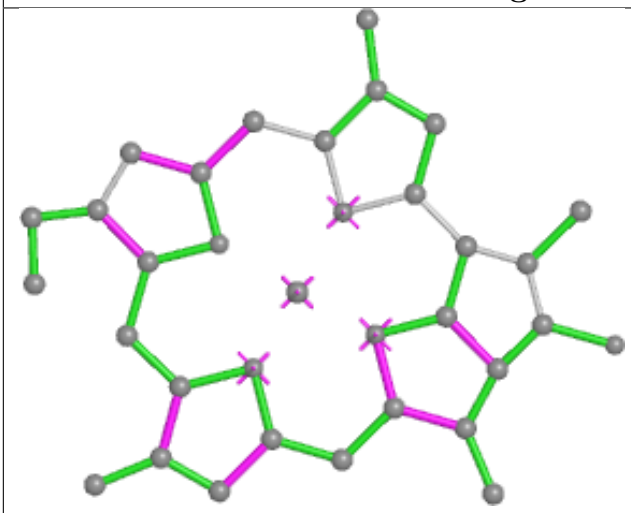
Ligand BCR B3 847



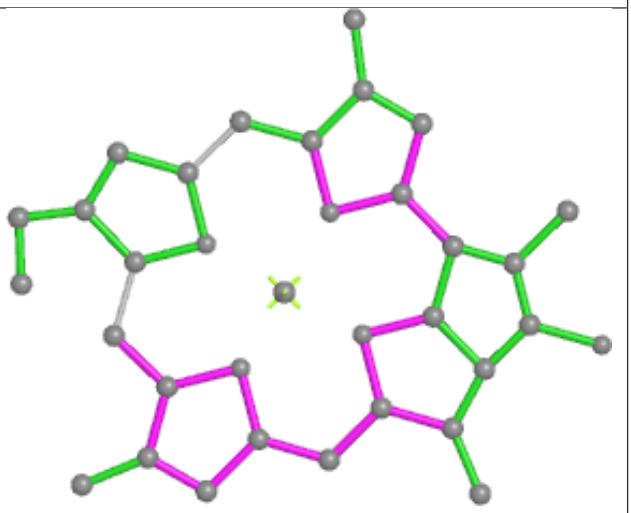
Ligand CLA I3 101



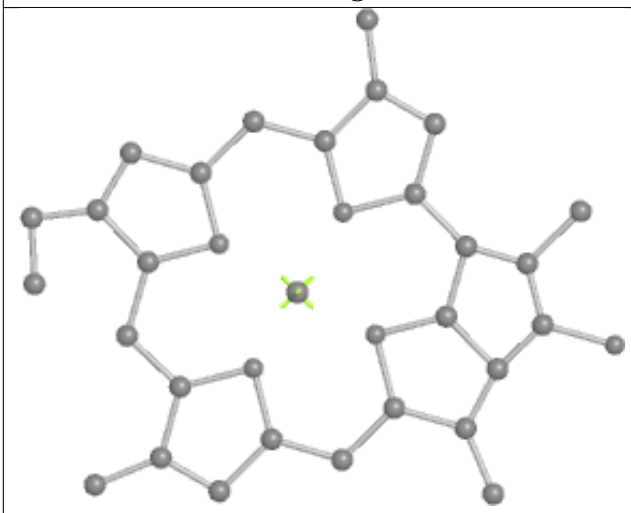
Ligand CLA J3 1307



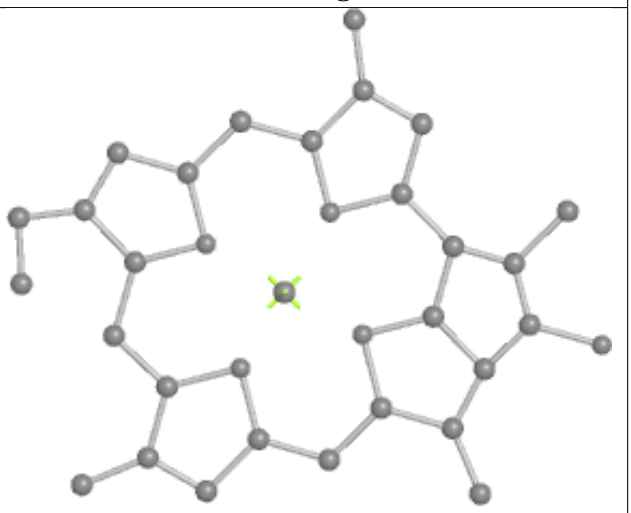
Bond lengths



Bond angles

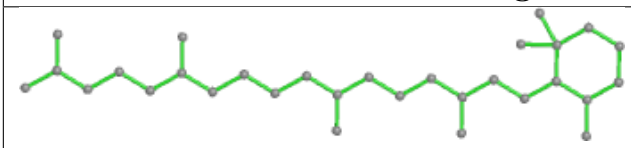


Torsions

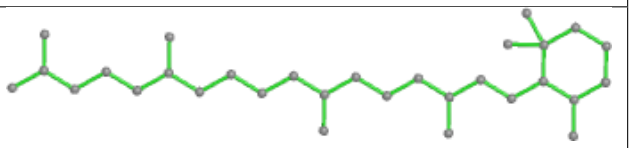


Rings

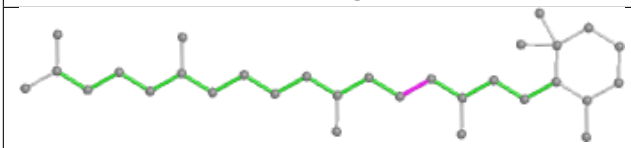
Ligand BCR B2 842



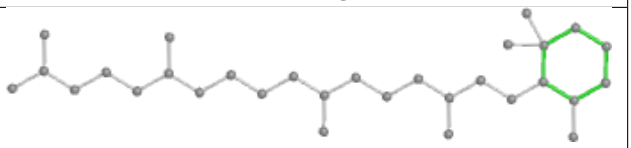
Bond lengths



Bond angles

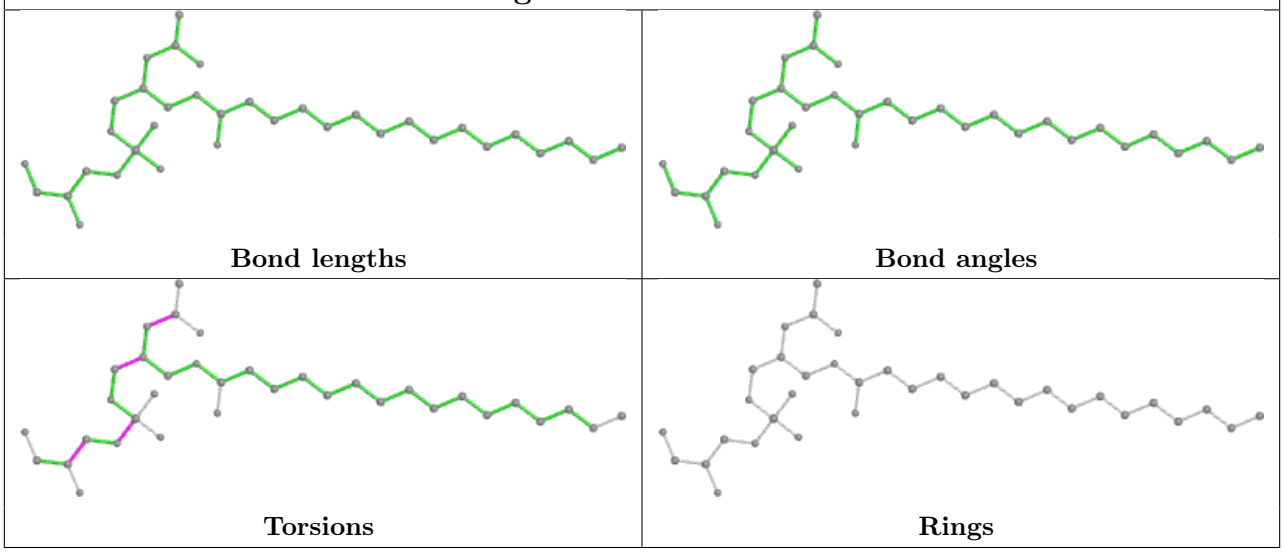


Torsions

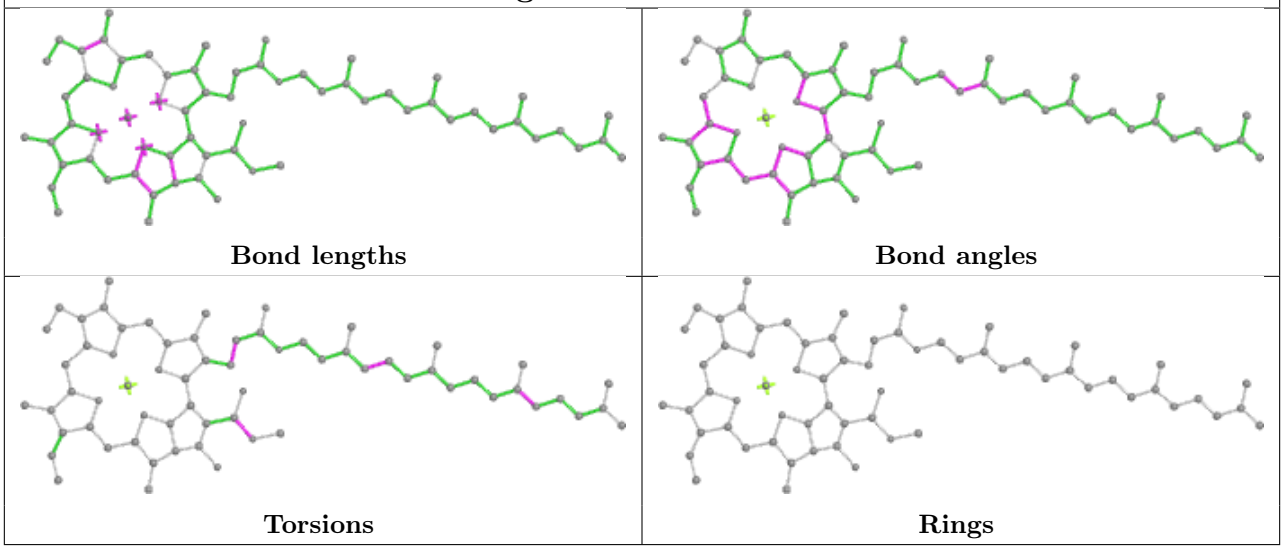


Rings

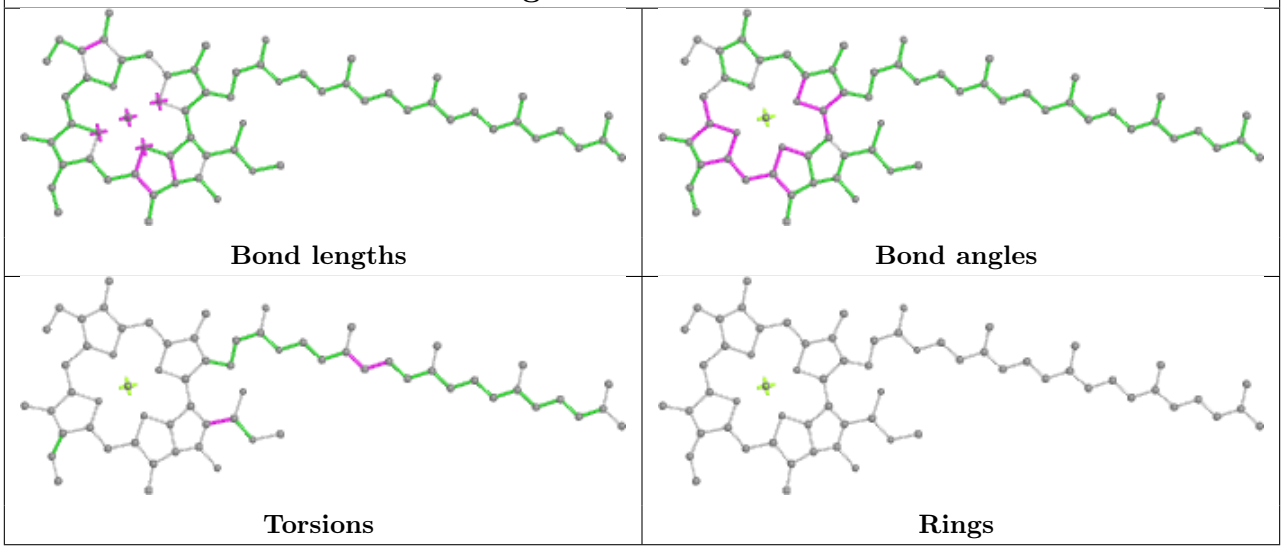
Ligand LHG A3 854



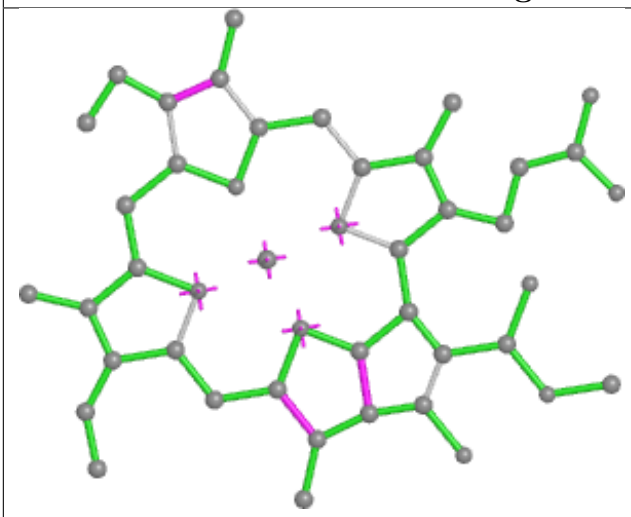
Ligand CLA B2 838



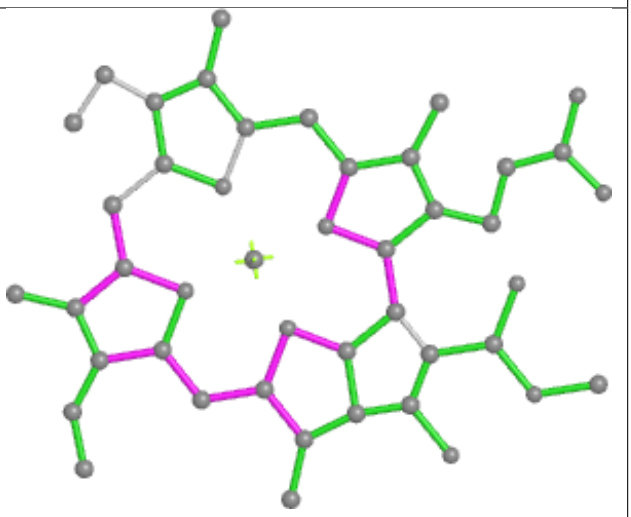
Ligand CLA I2 101



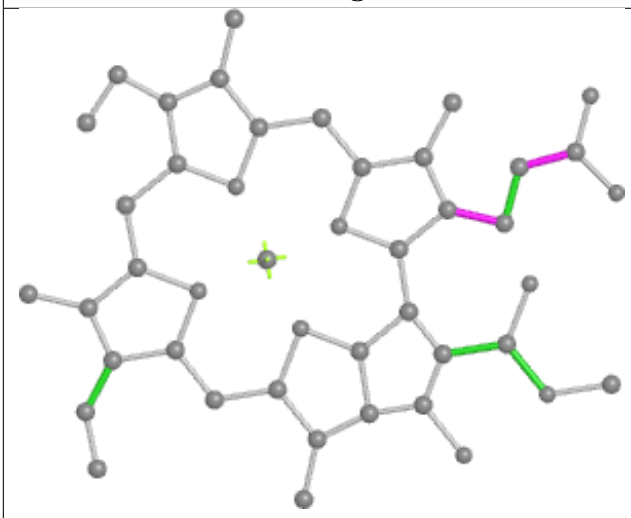
Ligand CLA A3 835



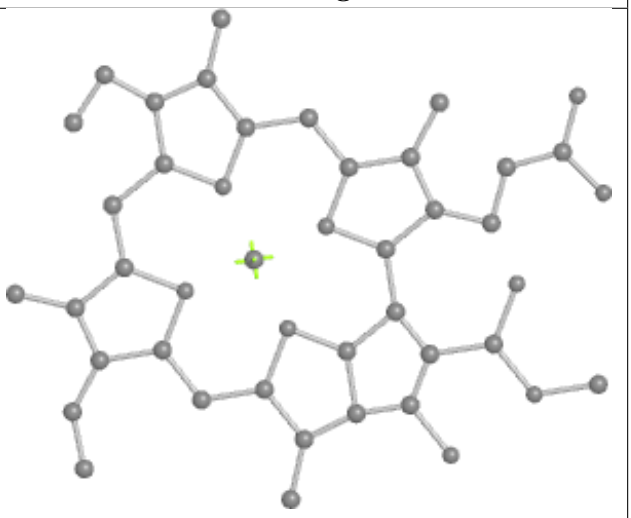
Bond lengths



Bond angles

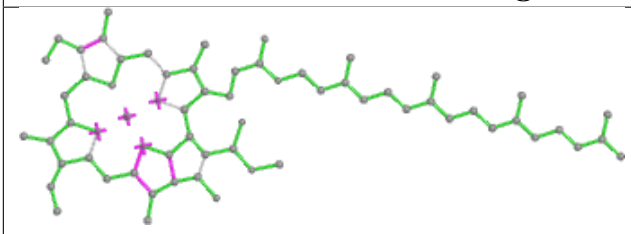


Torsions

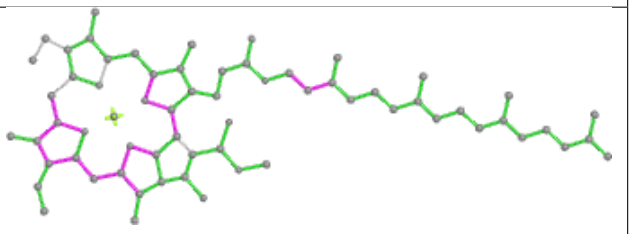


Rings

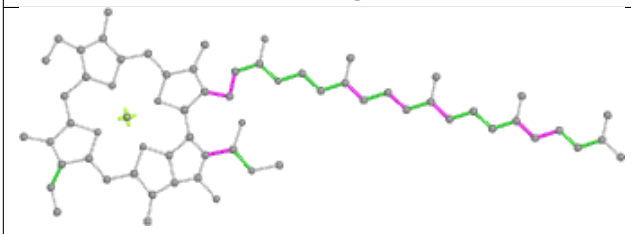
Ligand CLA A1 809



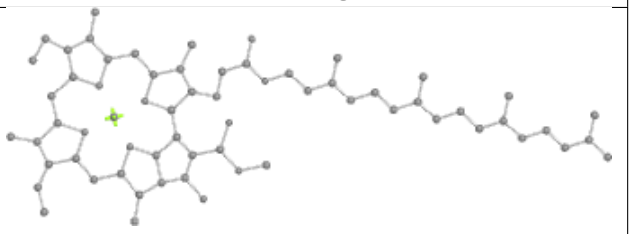
Bond lengths



Bond angles

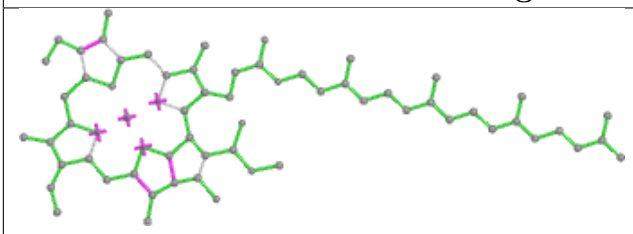


Torsions

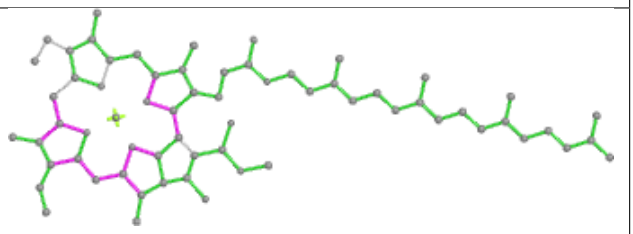


Rings

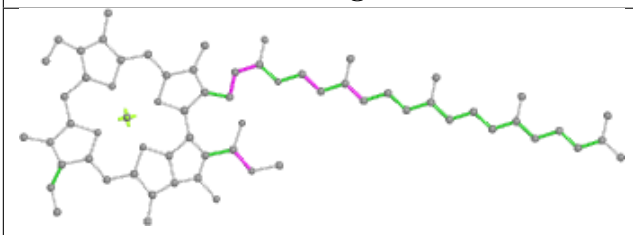
Ligand CLA B1 801



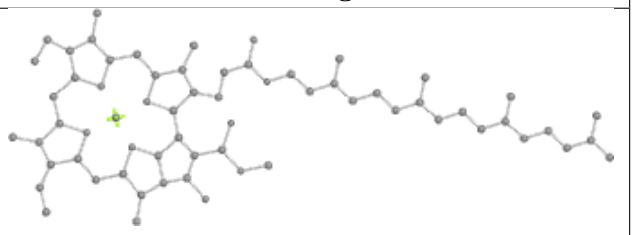
Bond lengths



Bond angles

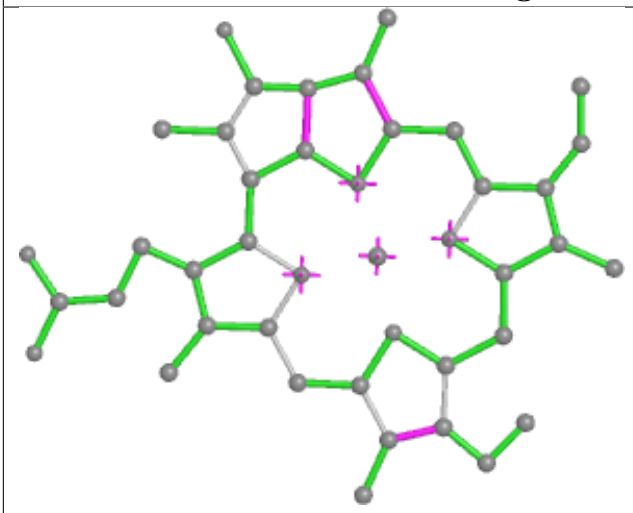


Torsions

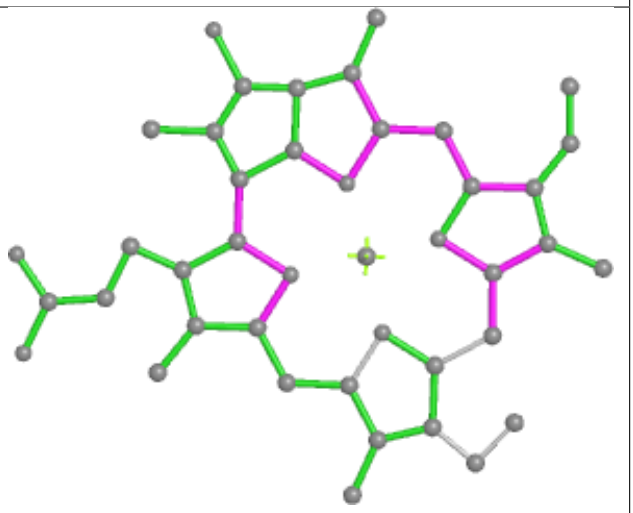


Rings

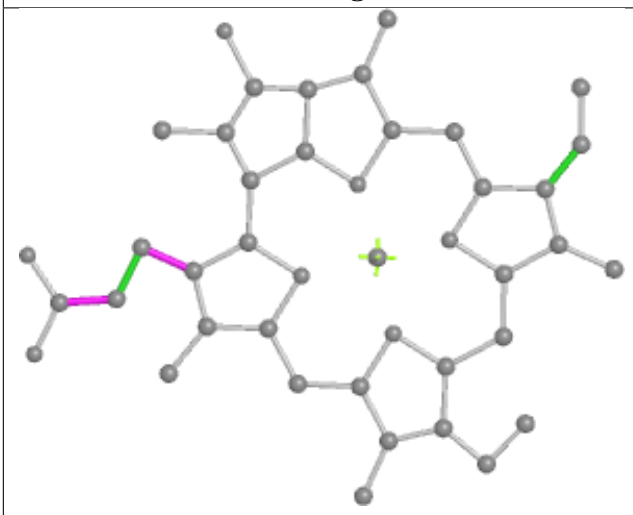
Ligand CLA B3 828



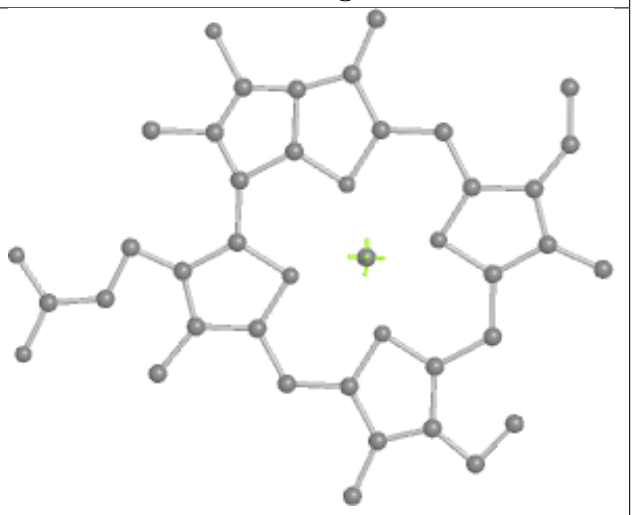
Bond lengths



Bond angles

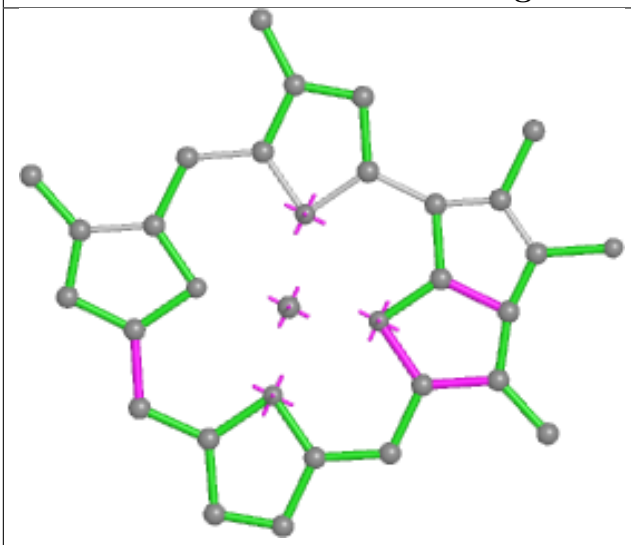


Torsions

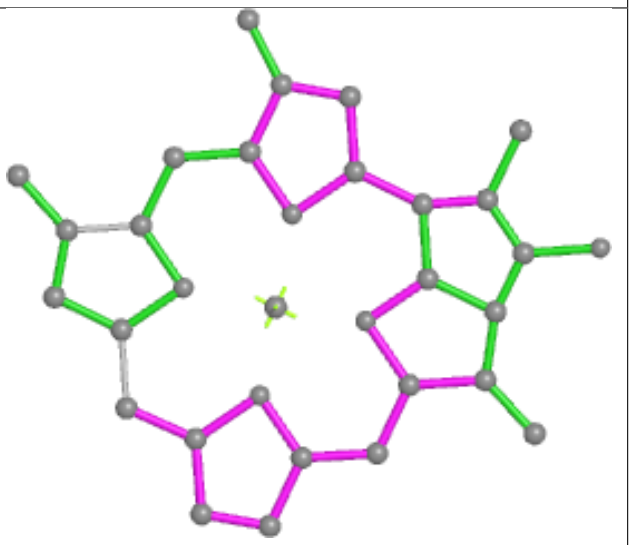


Rings

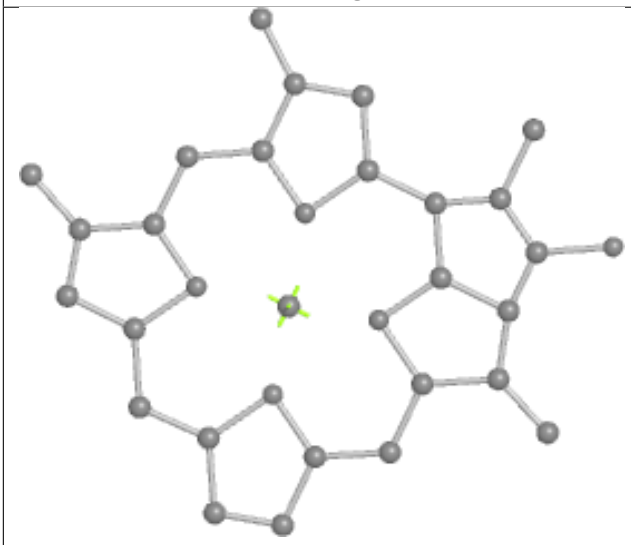
Ligand CLA K1 103



Bond lengths



Bond angles



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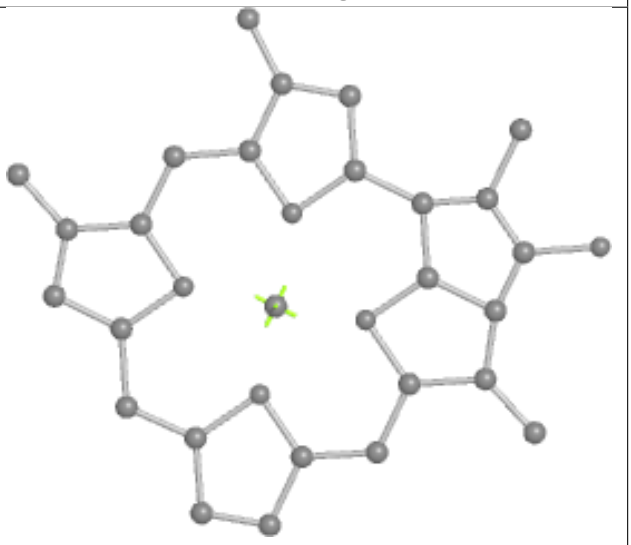
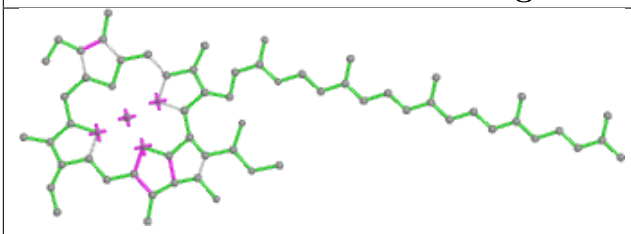


Rings

Ligand CLA B1 839



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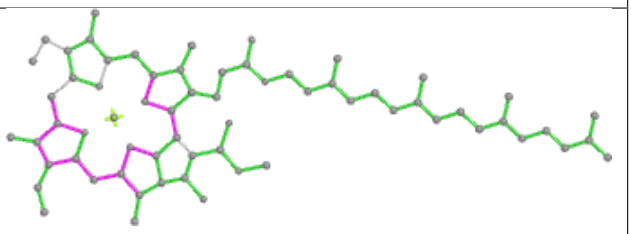
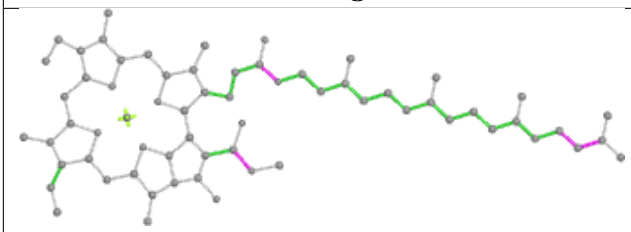
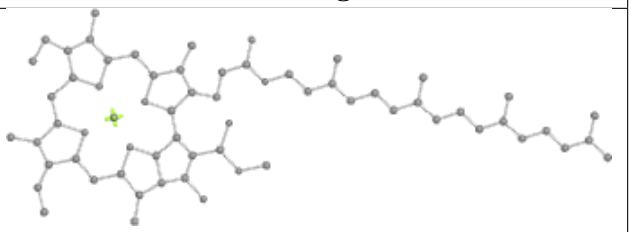


Bond angles

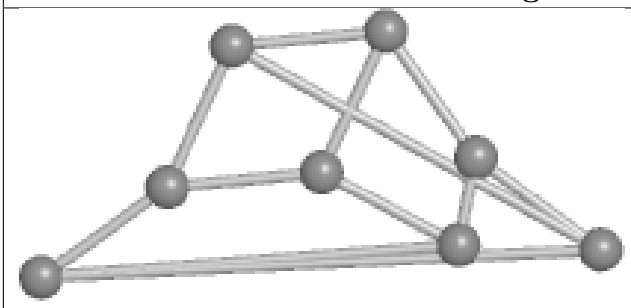


Torsions

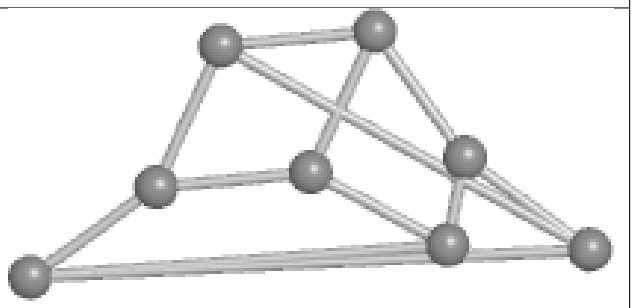


Rings

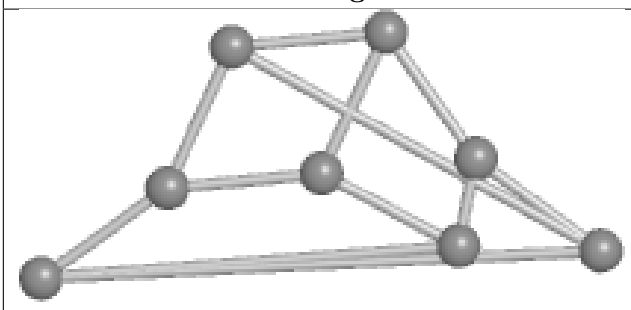
Ligand SF4 C2 101



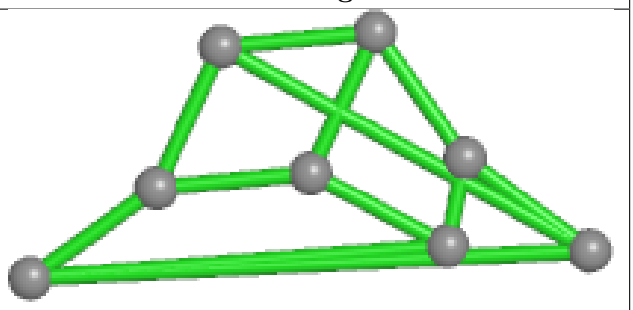
Bond lengths



Bond angles

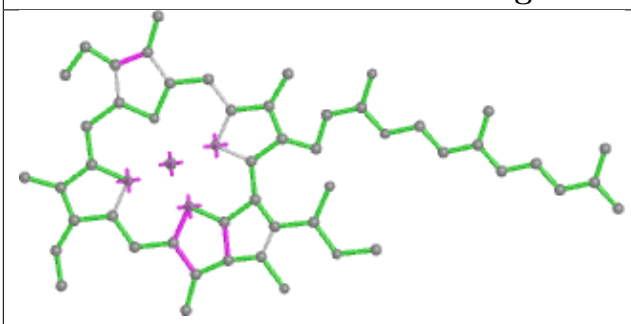


Torsions



Rings

Ligand CLA A3 829



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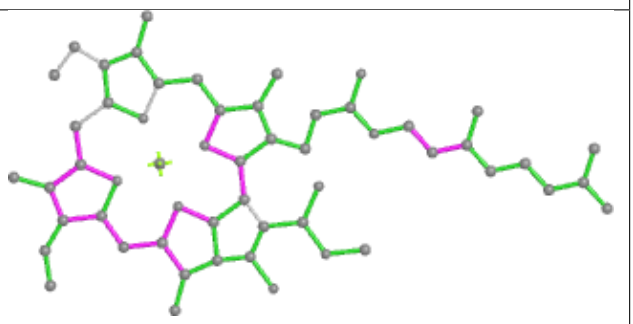
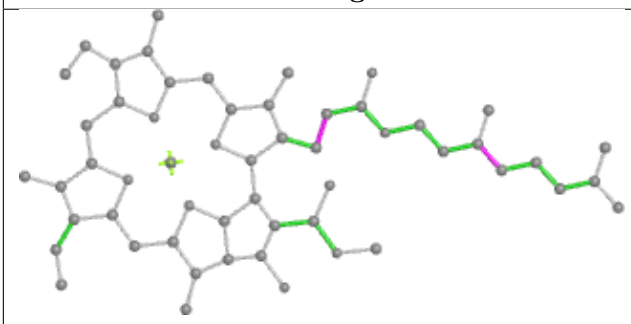


Bond angles



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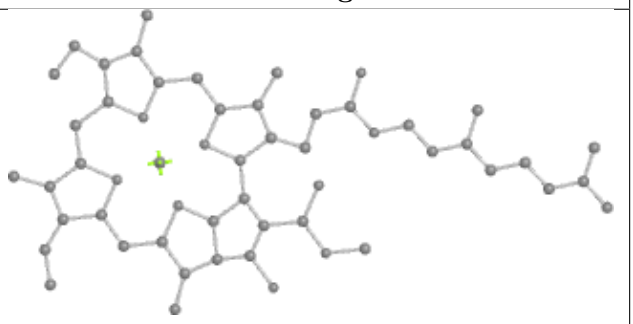
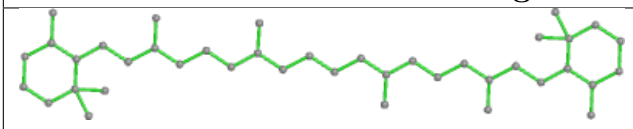
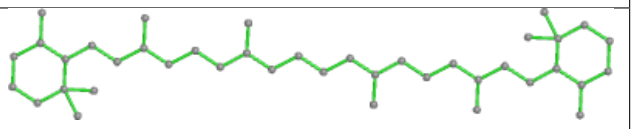


Rings

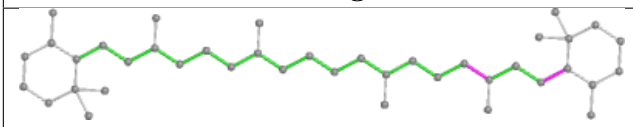
Ligand BCR A1 850



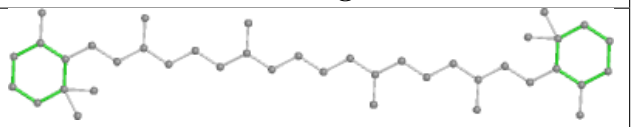
Bond lengths



Bond angles

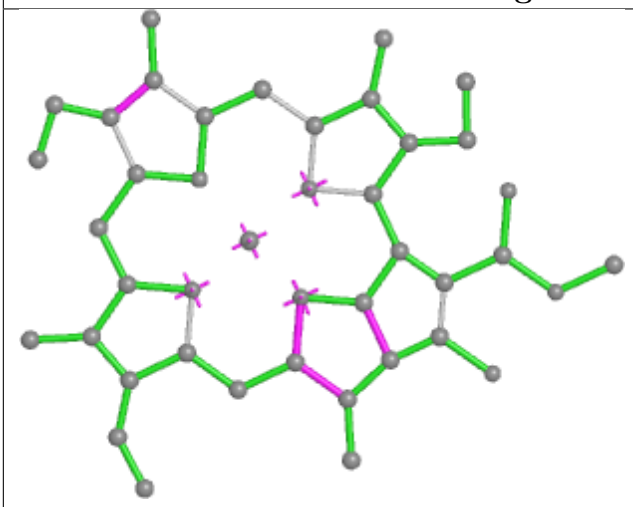


Torsions

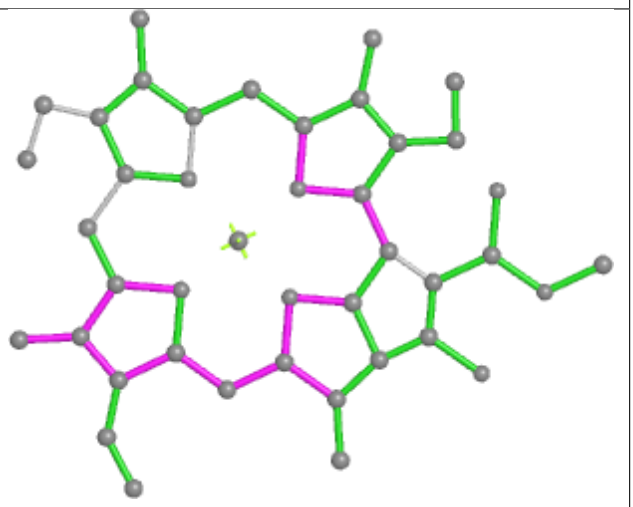


Rings

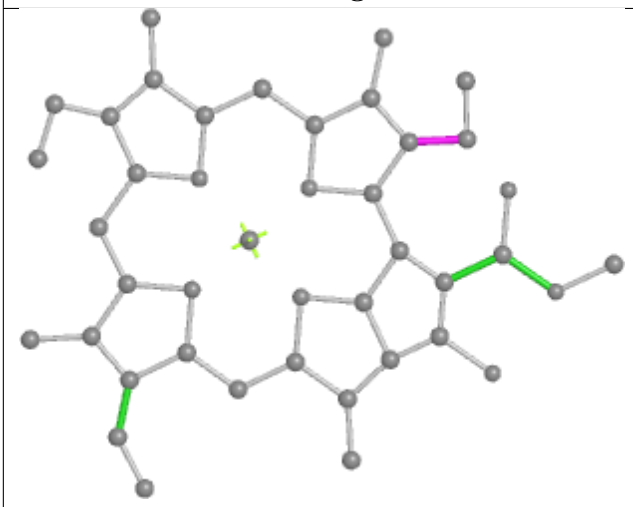
Ligand CLA A1 828



Bond lengths



Bond angles



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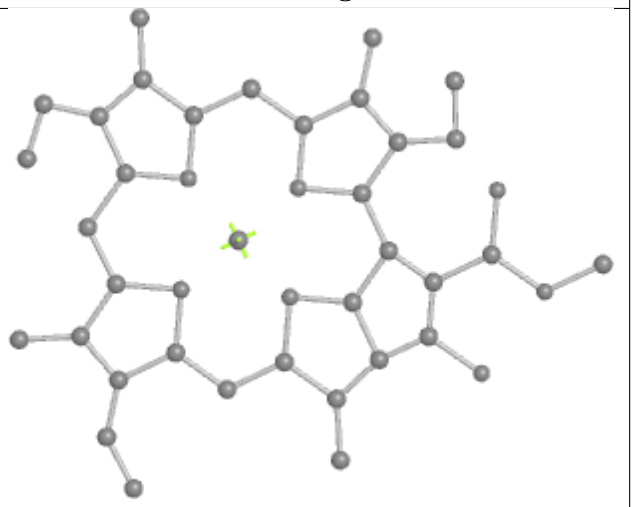
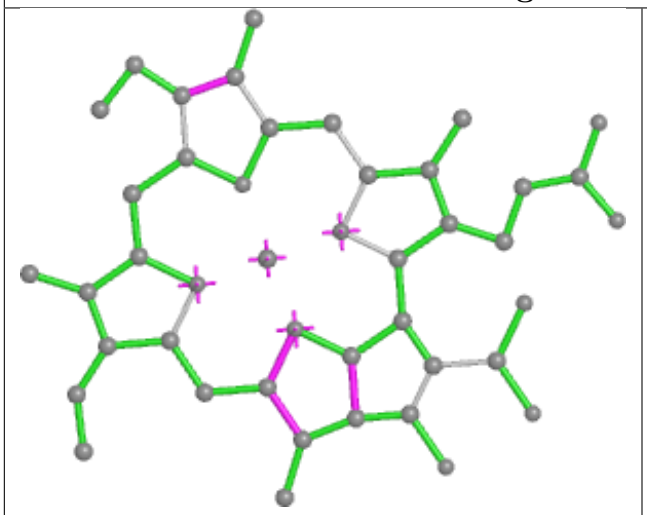
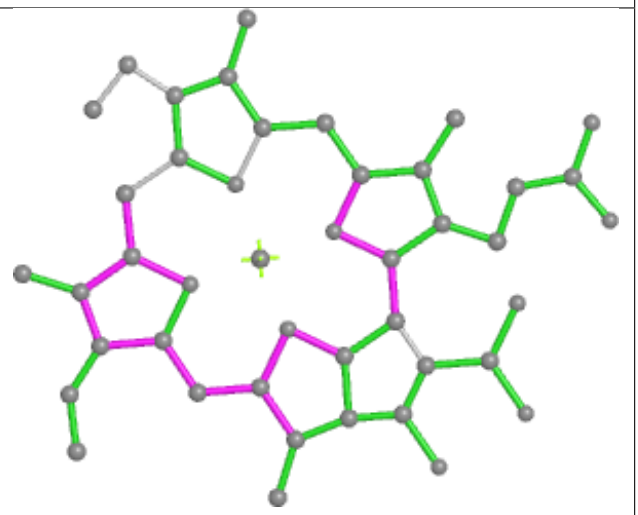


Rings

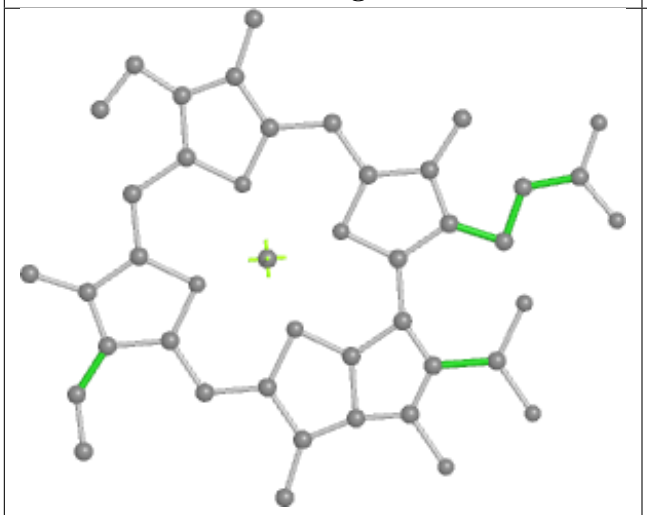
Ligand CLA B3 810



Bond lengths



Bond angles



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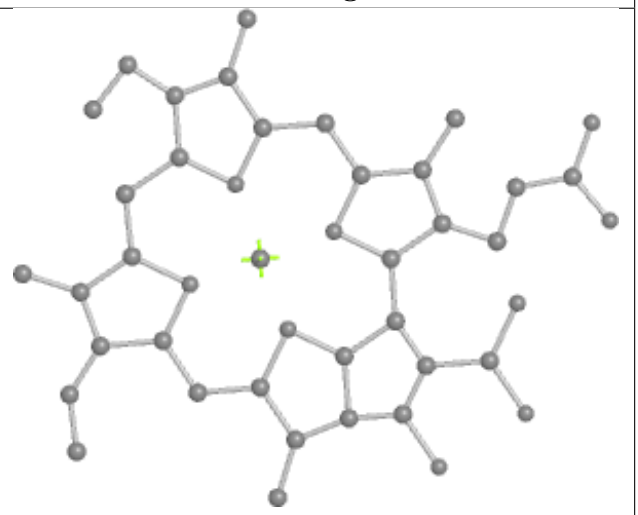
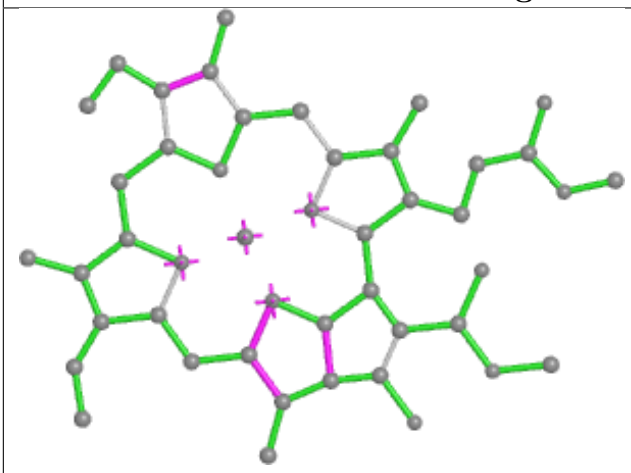
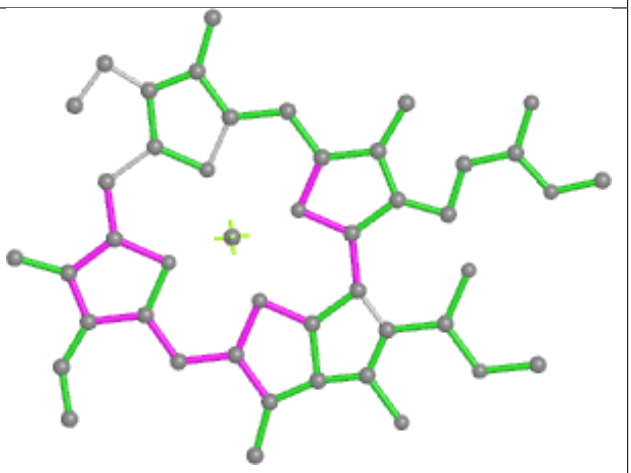


Rings

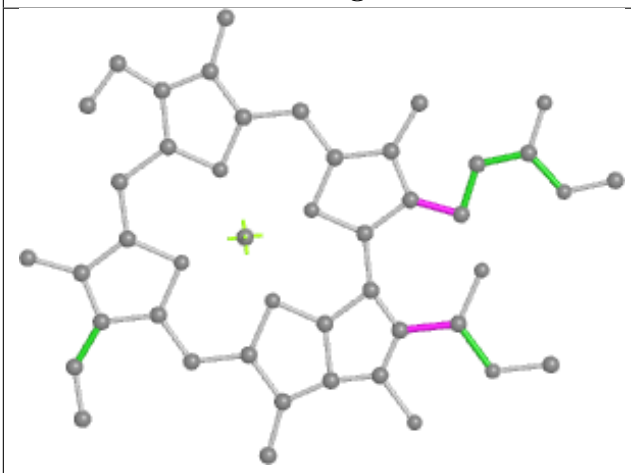
Ligand CLA B1 835



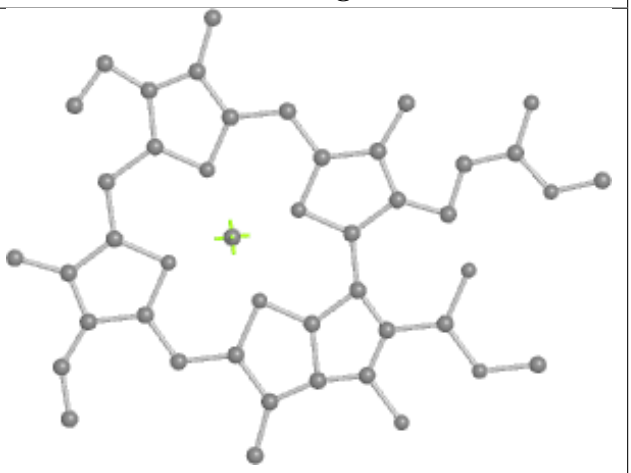
Bond lengths



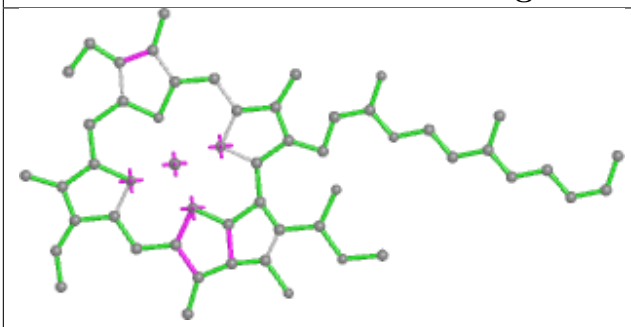
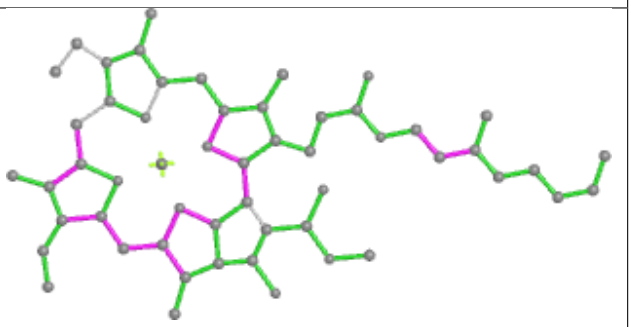
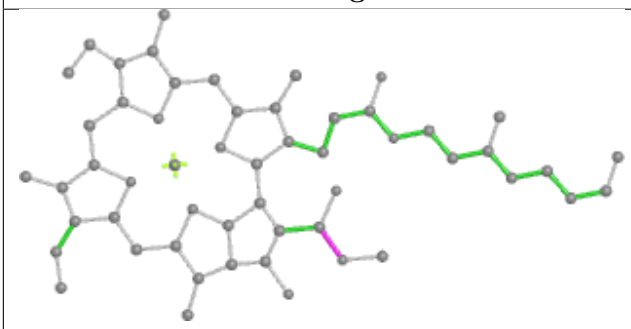
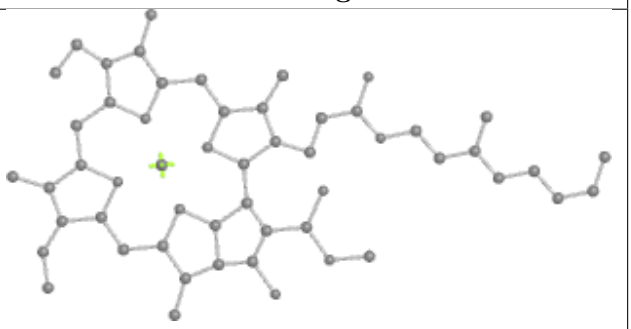
Bond angles



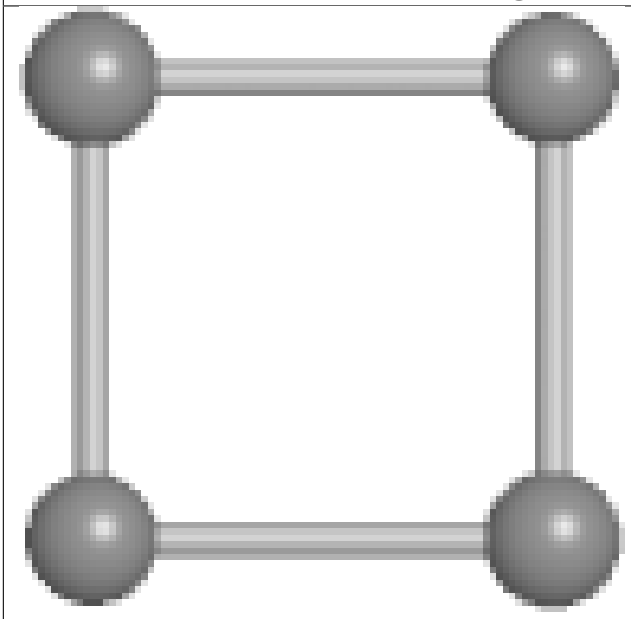
Torsions



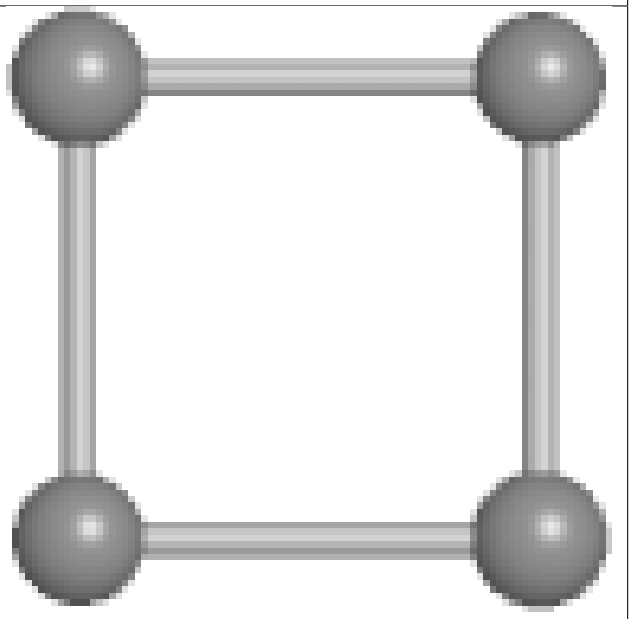
Rings

Ligand CLA B2 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

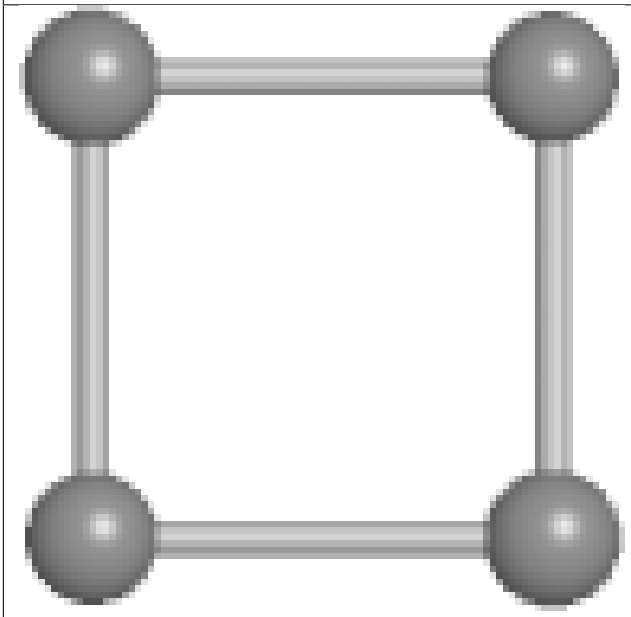
Ligand GAK R1 101



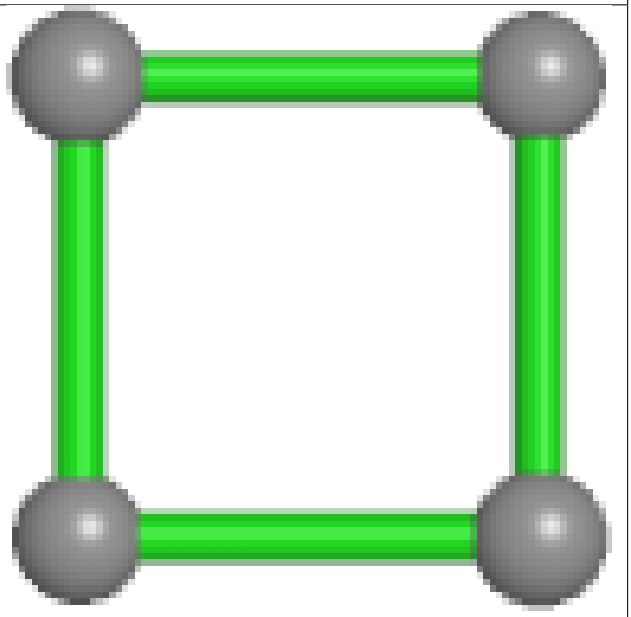
Bond lengths



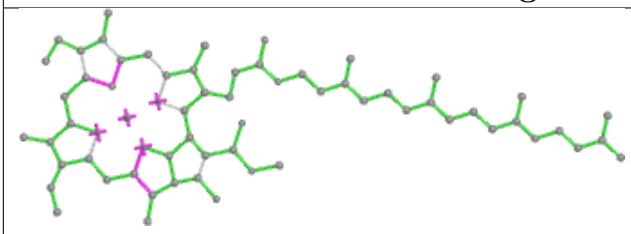
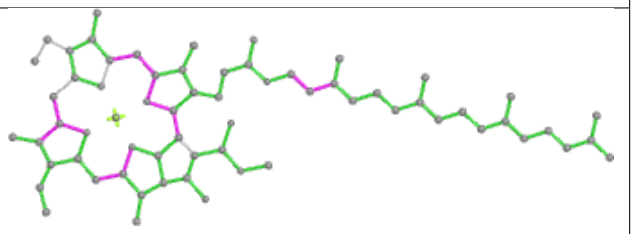
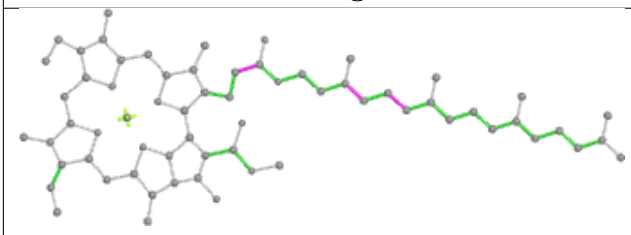
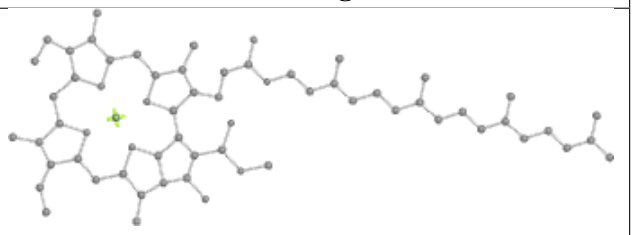
Bond angles

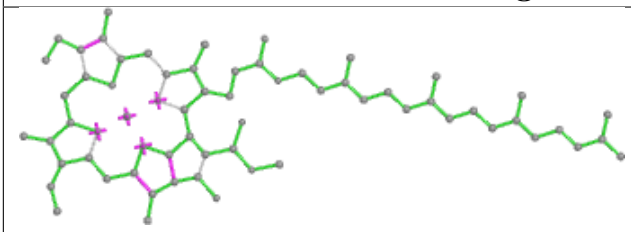
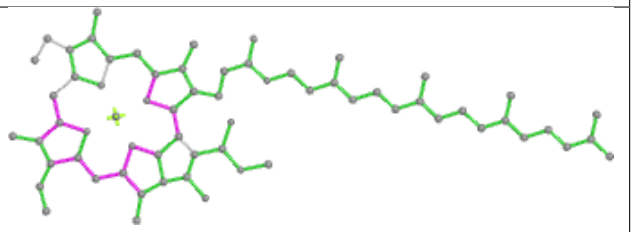
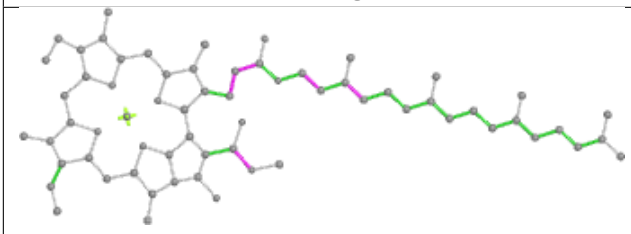
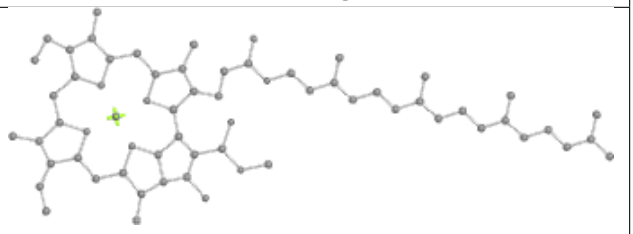


Torsions

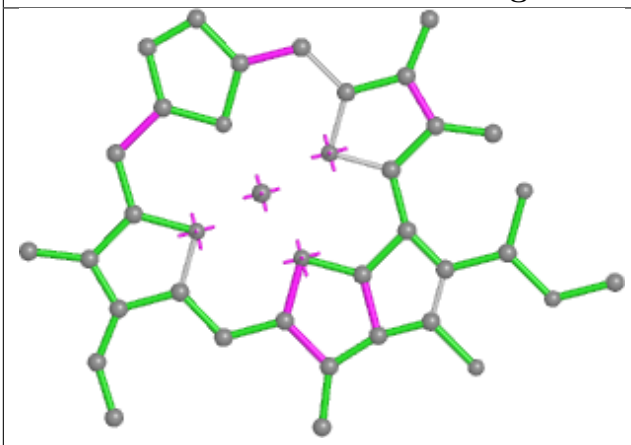


Rings

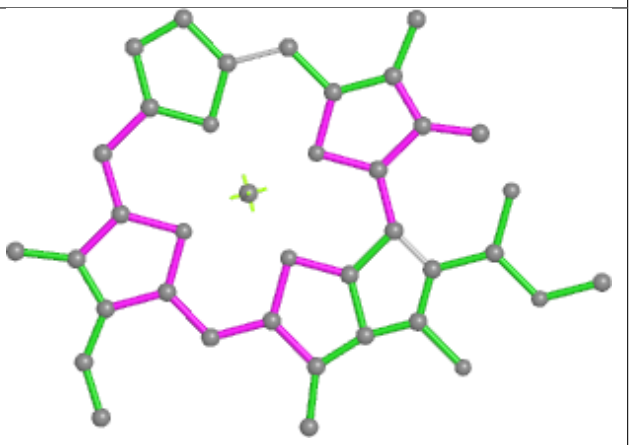
Ligand CL0 A3 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

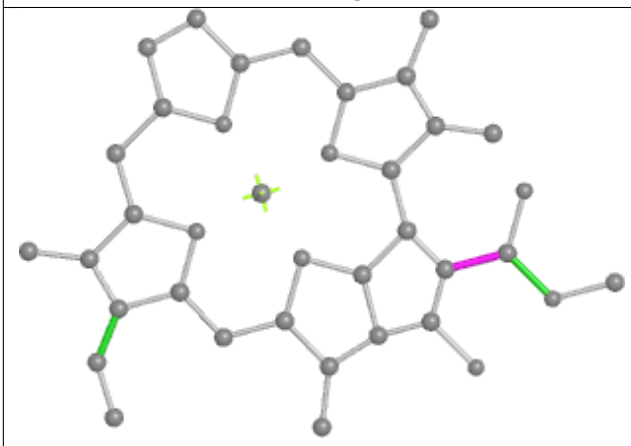
Ligand CLA J3 1301



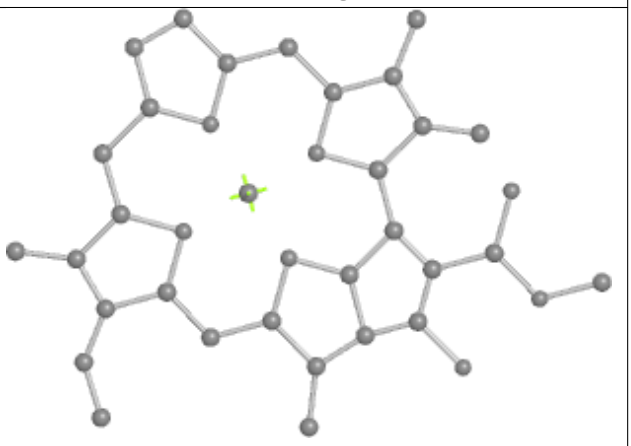
Bond lengths



Bond angles

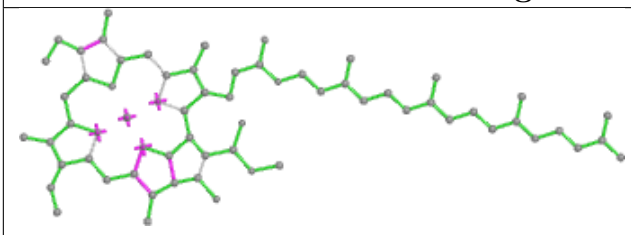


Torsions

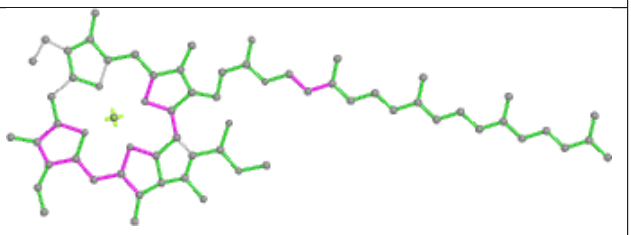


Rings

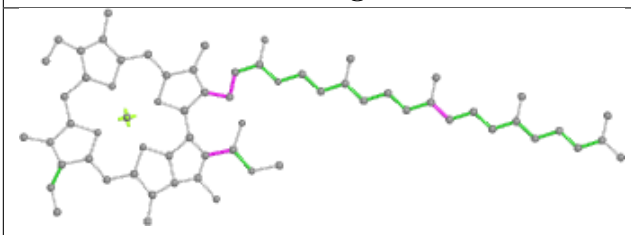
Ligand CLA A3 840



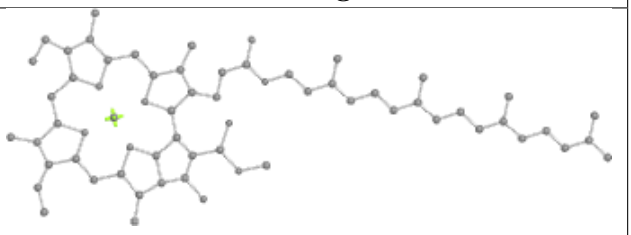
Bond lengths



Bond angles

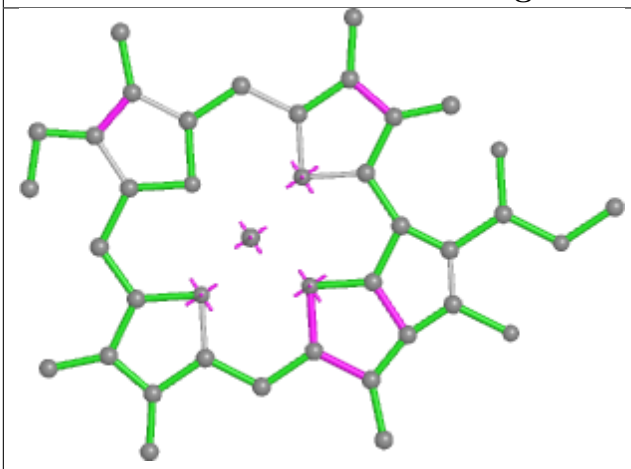


Torsions

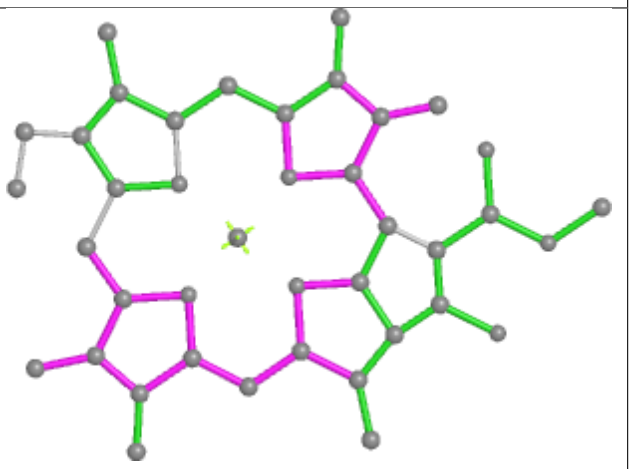


Rings

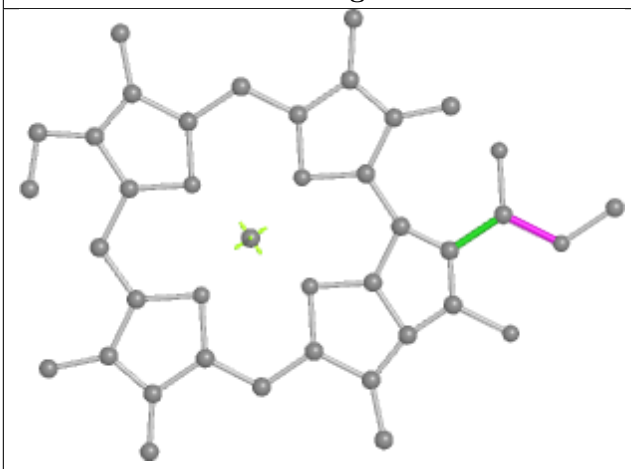
Ligand CLA X2 102



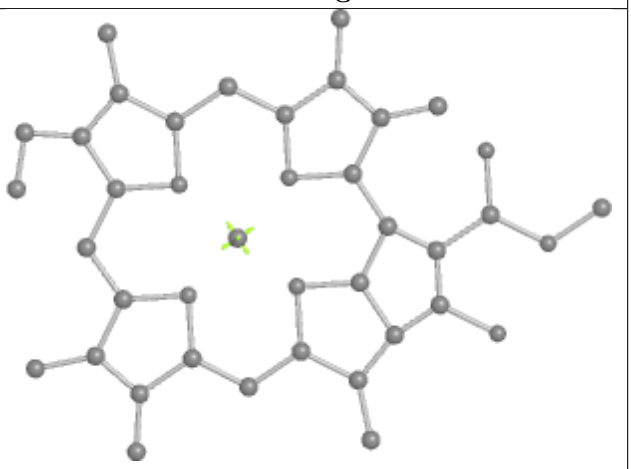
Bond lengths



Bond angles

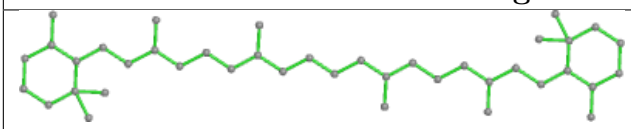


Torsions

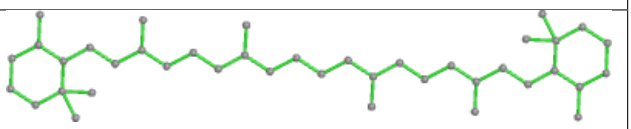


Rings

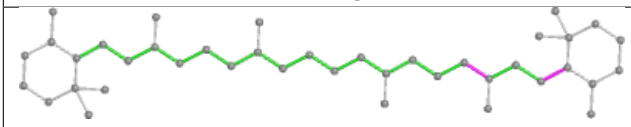
Ligand BCR A3 850



Bond lengths

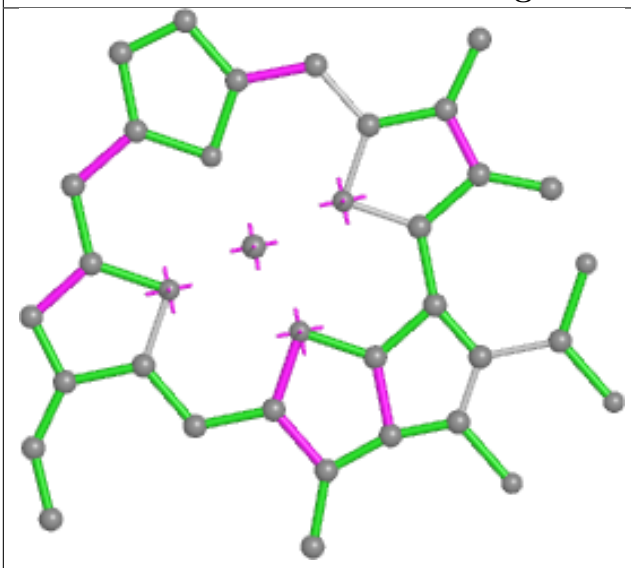
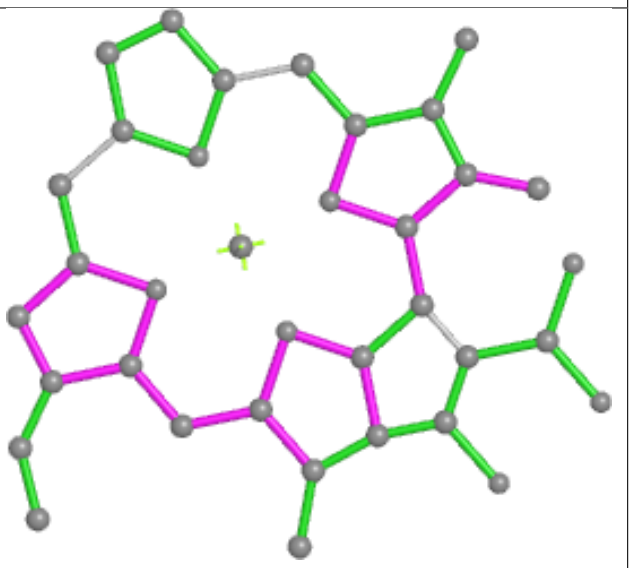
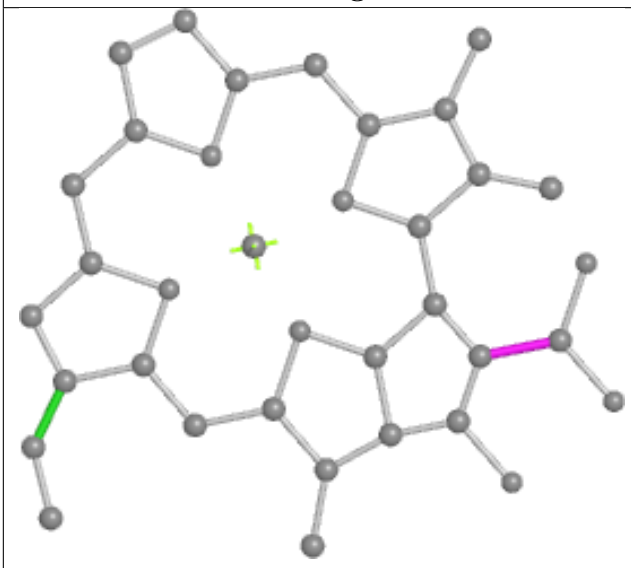
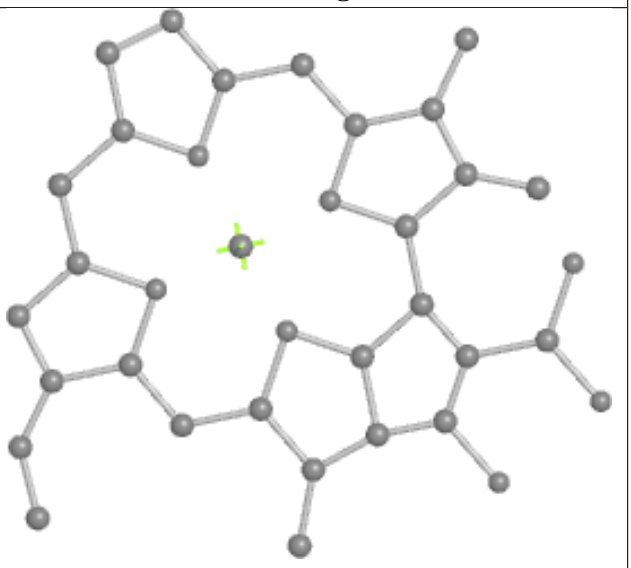


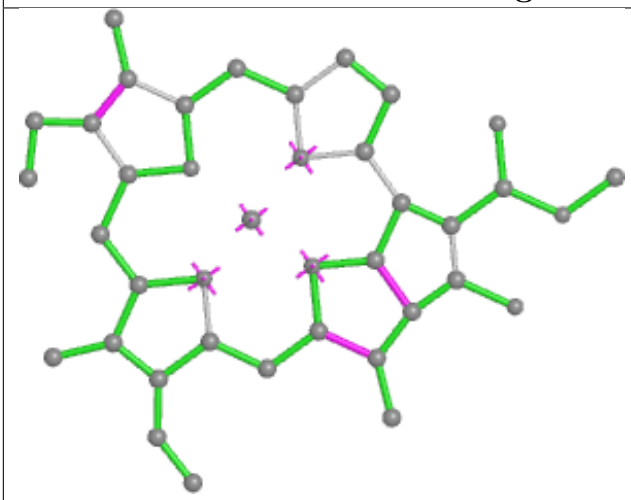
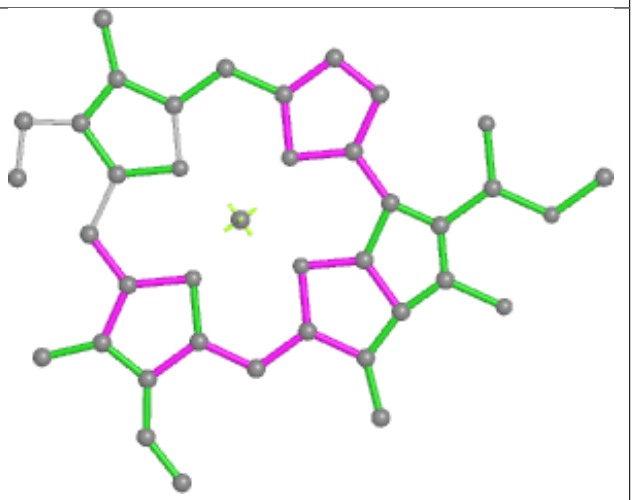
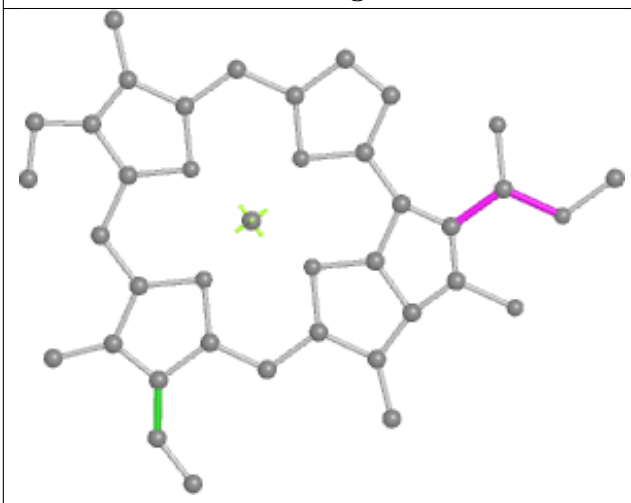
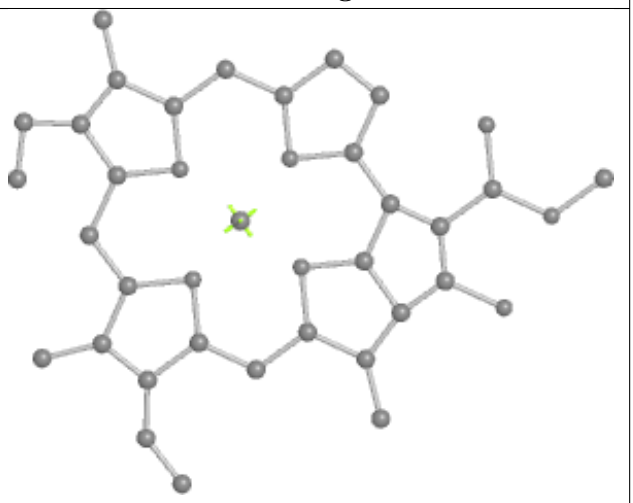
Bond angles

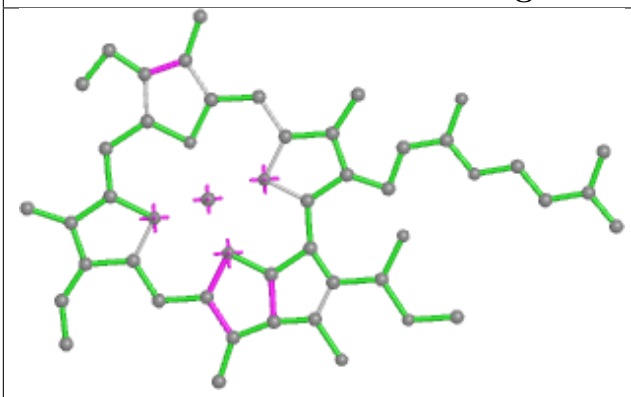
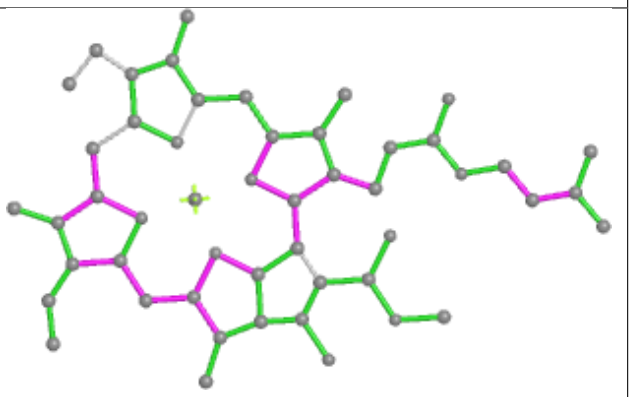
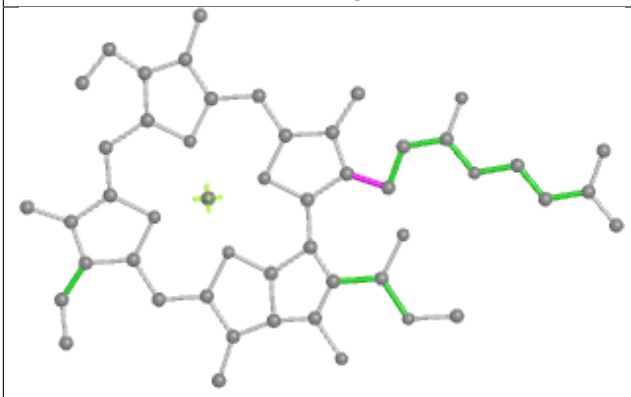
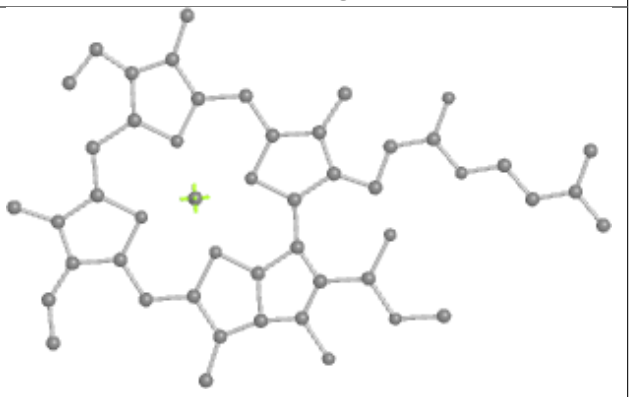


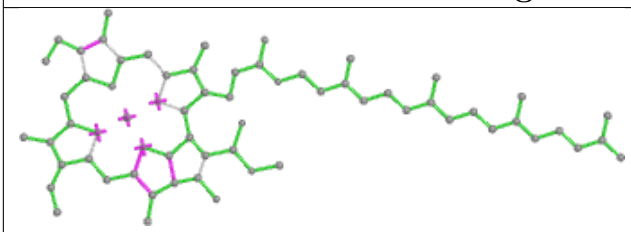
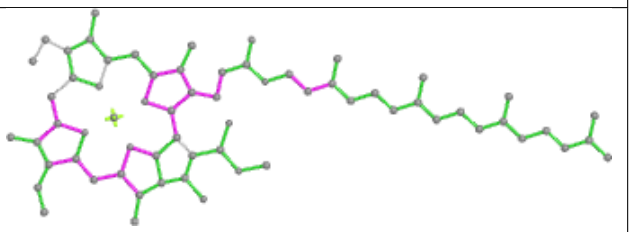
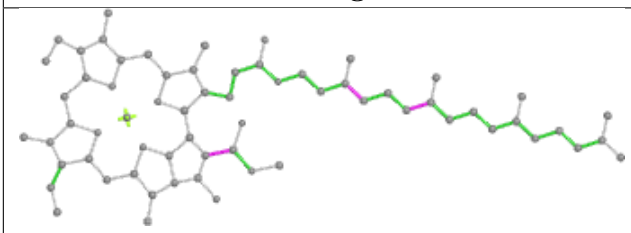
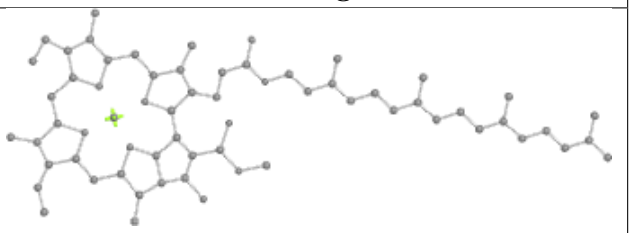
Torsions

Rings

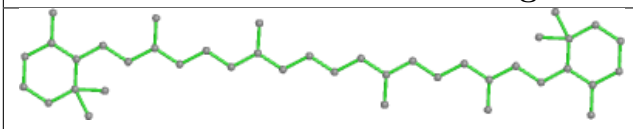
Ligand CLA A1 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B3 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

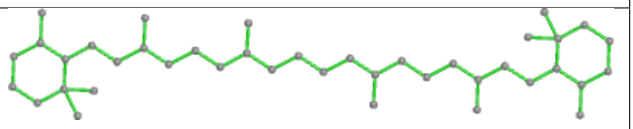
Ligand CLA B2 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

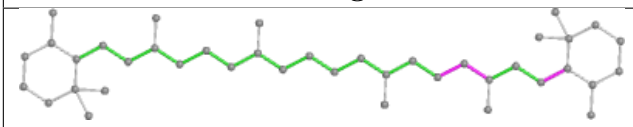
Ligand BCR I2 103



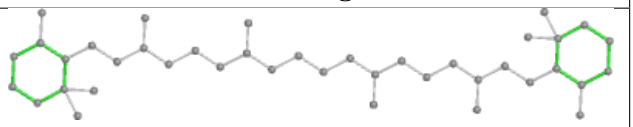
Bond lengths



Bond angles

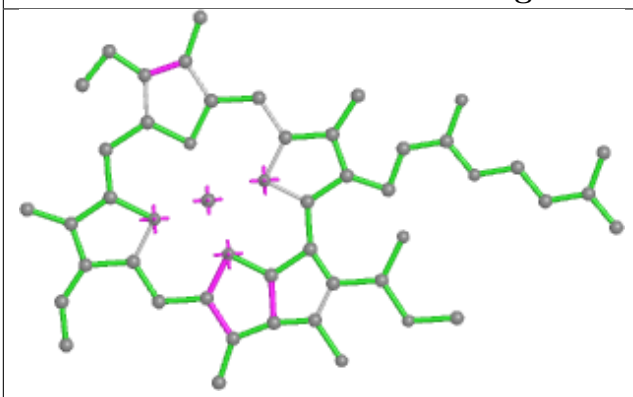


Torsions

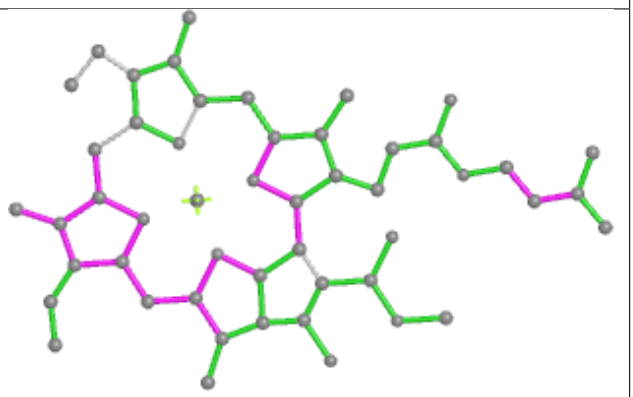


Rings

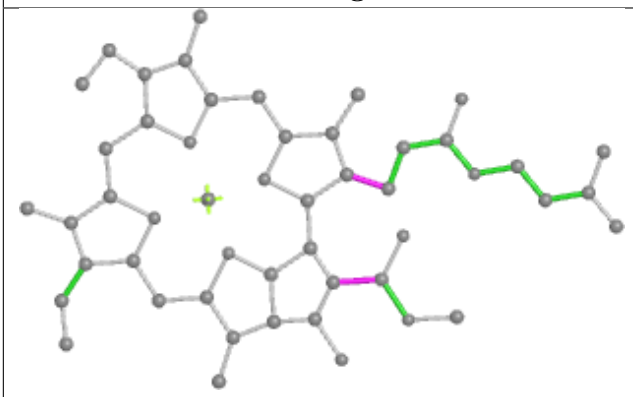
Ligand CLA A1 837



Bond lengths



Bond angles



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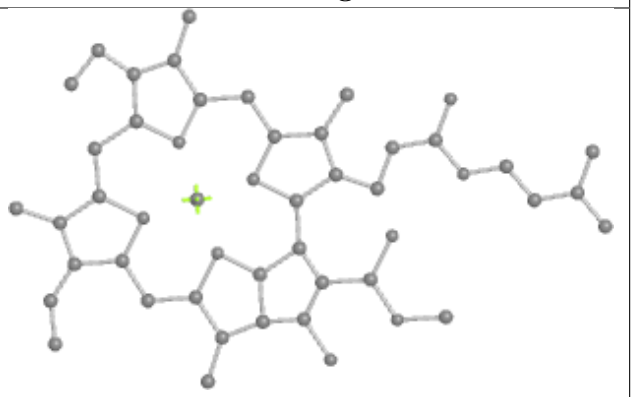
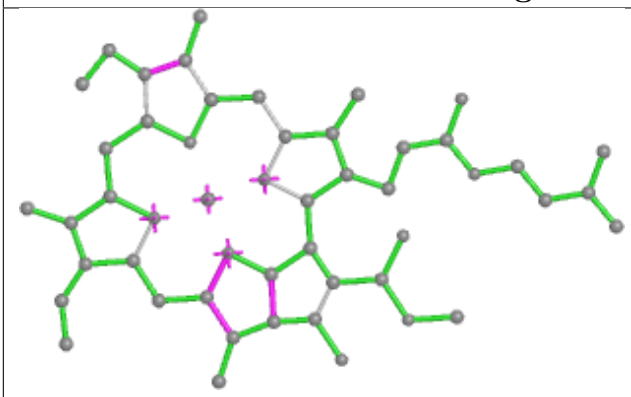
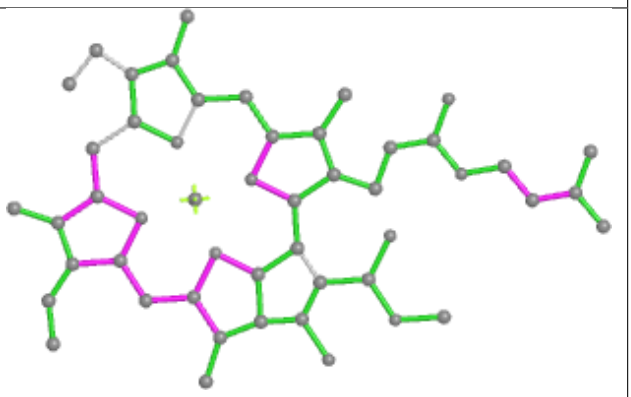
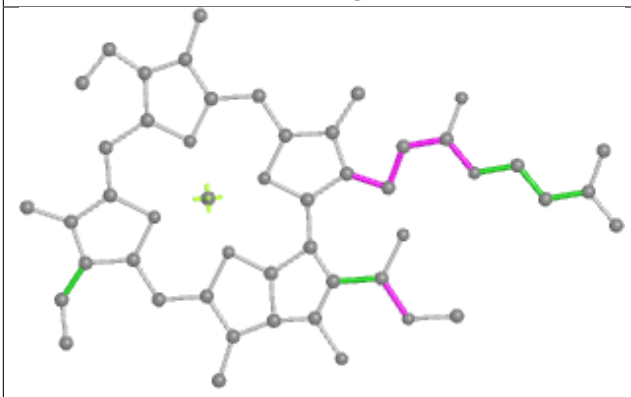
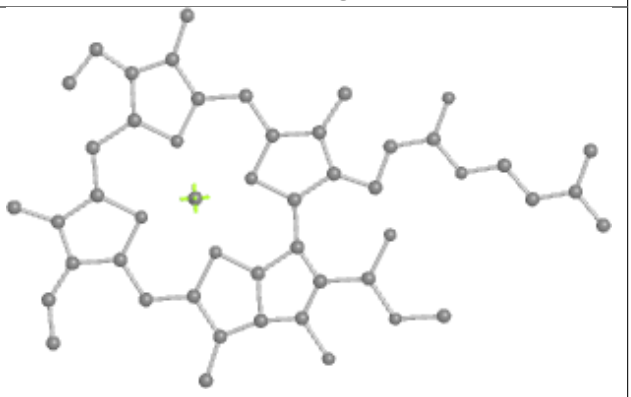
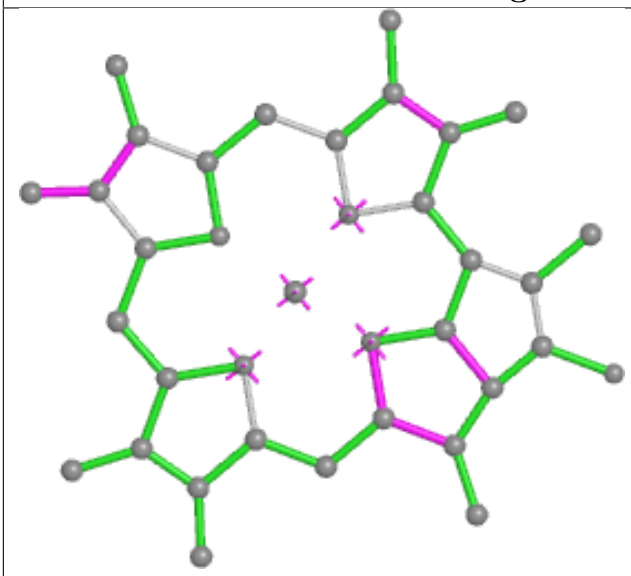
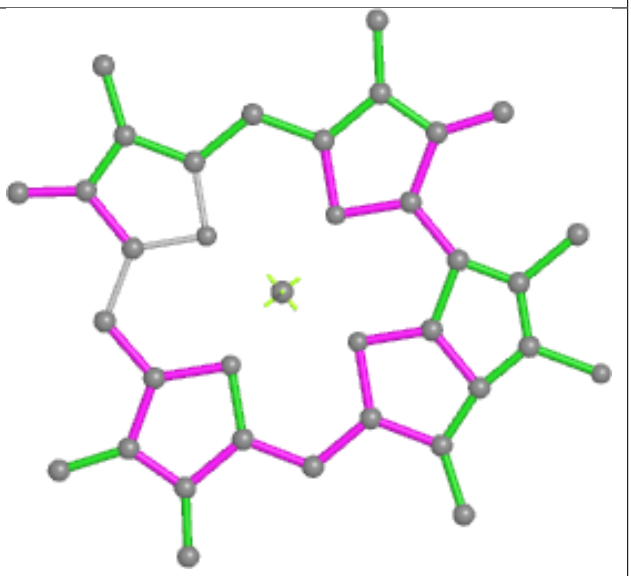
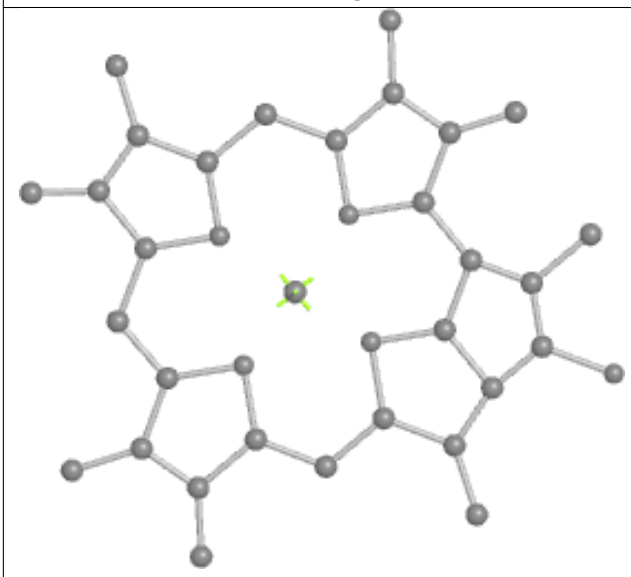
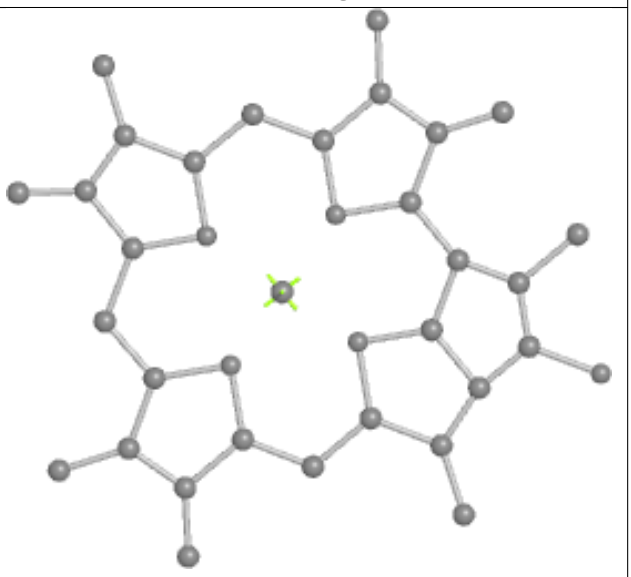
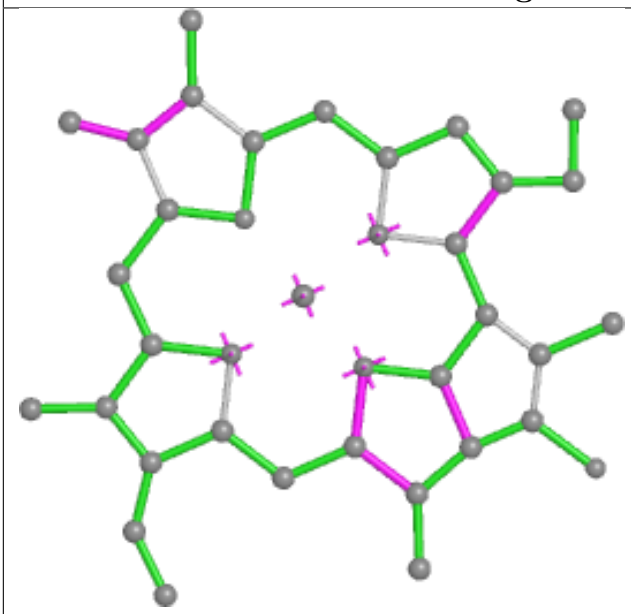
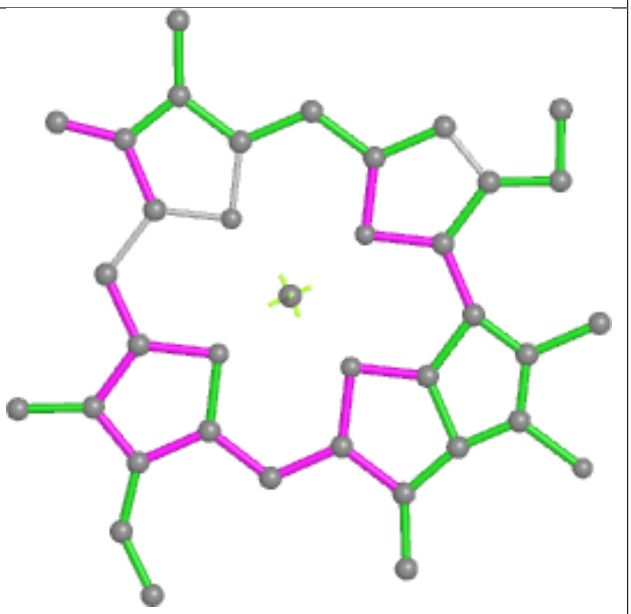
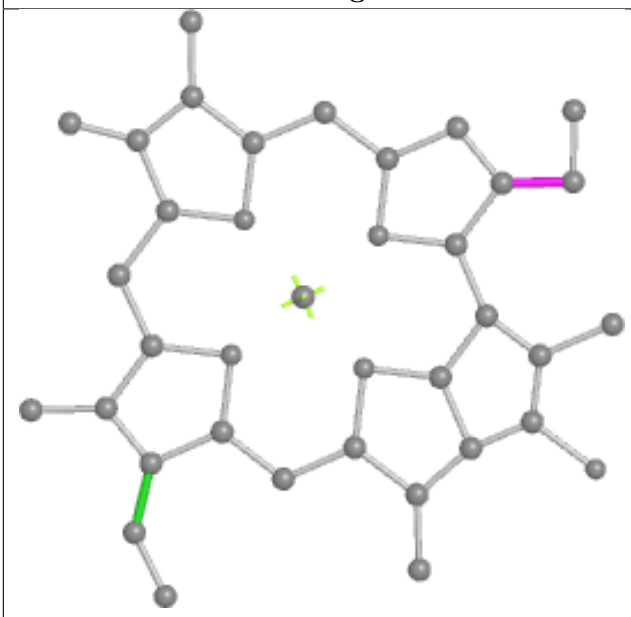
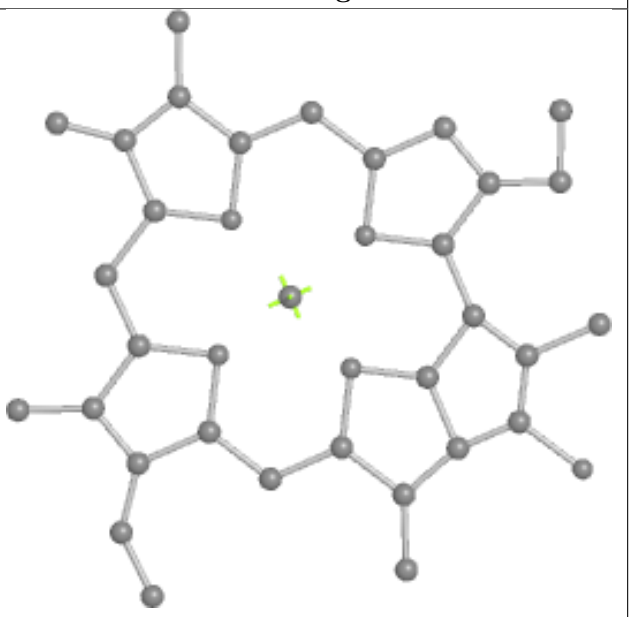


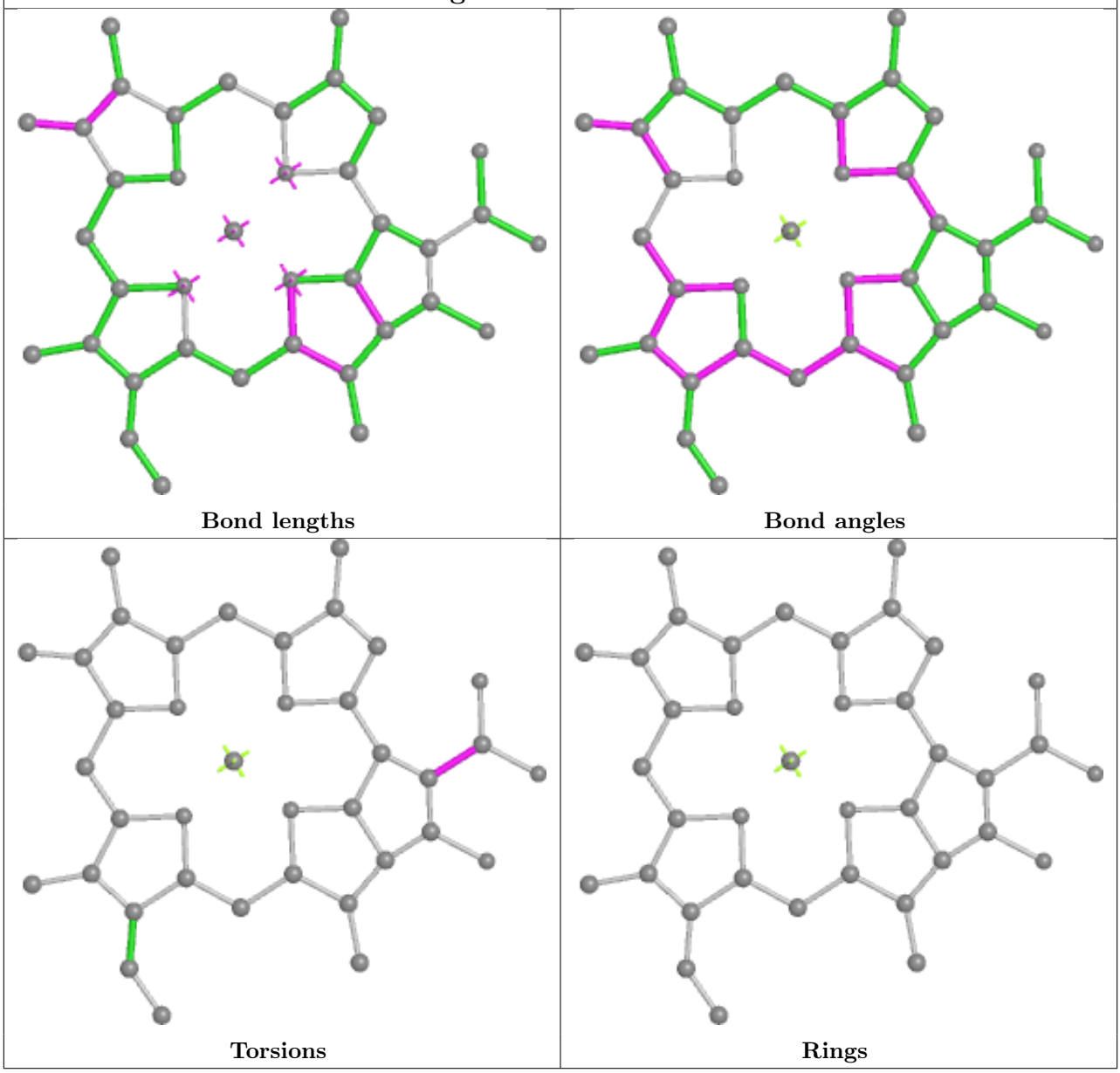
Rings

Ligand CLA A2 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

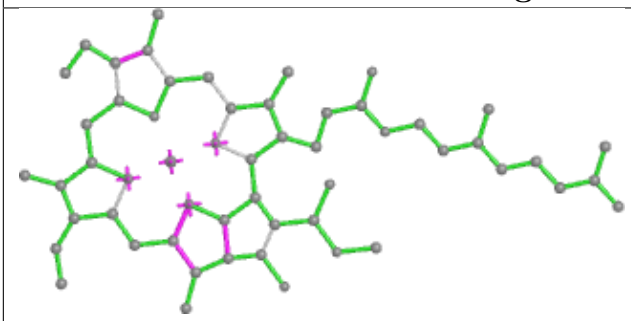
Ligand CLA J2 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

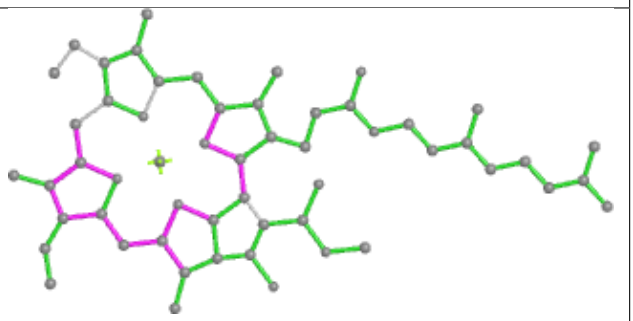
Ligand CLA A2 820



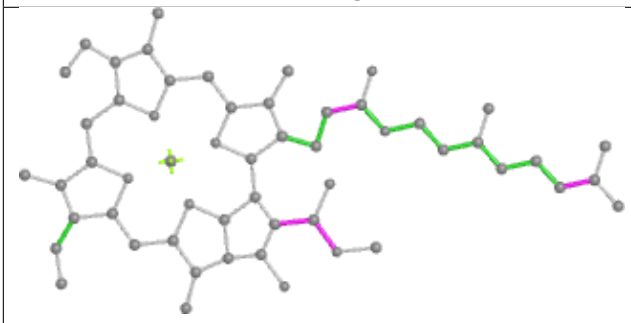
Ligand CLA A1 839



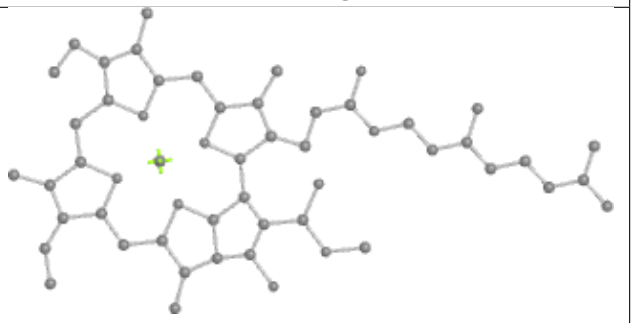
Bond lengths



Bond angles

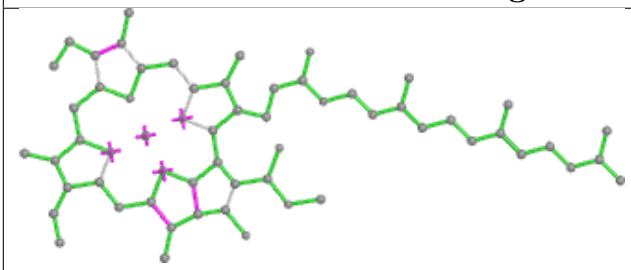


Torsions

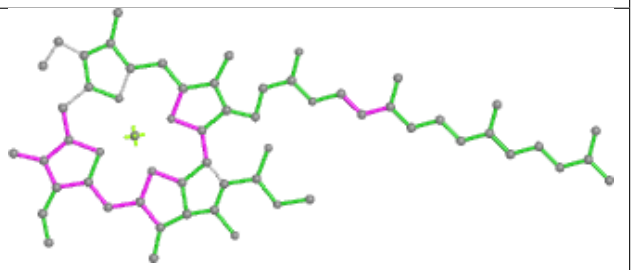


Rings

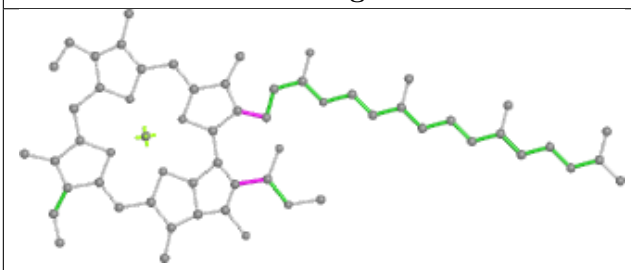
Ligand CLA L2 1003



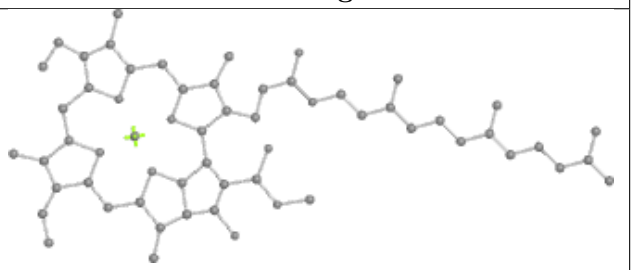
Bond lengths



Bond angles

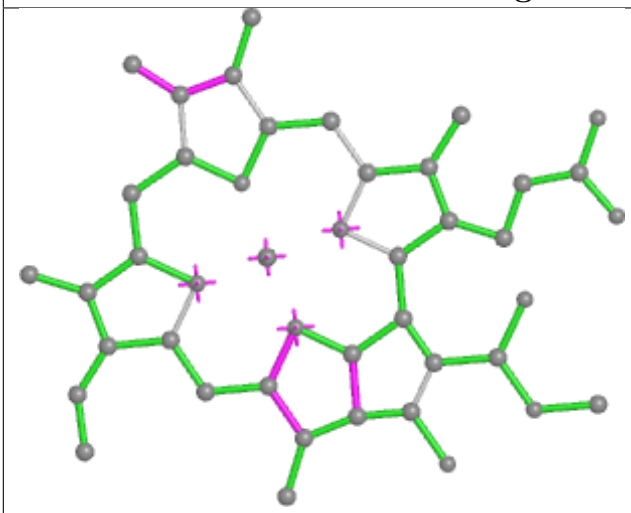


Torsions

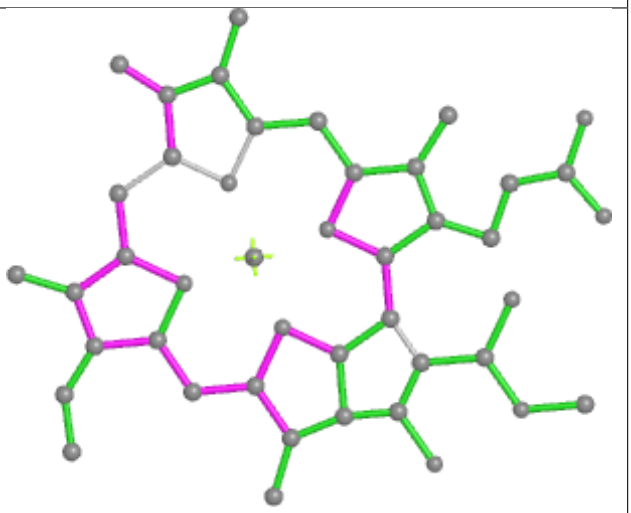


Rings

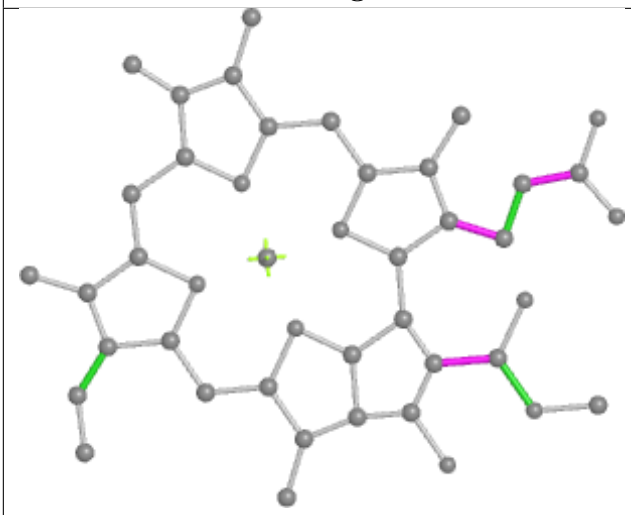
Ligand CLA A1 813



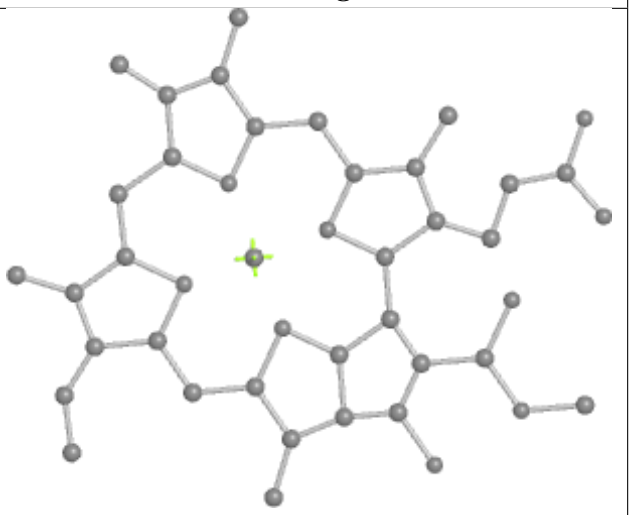
Bond lengths



Bond angles

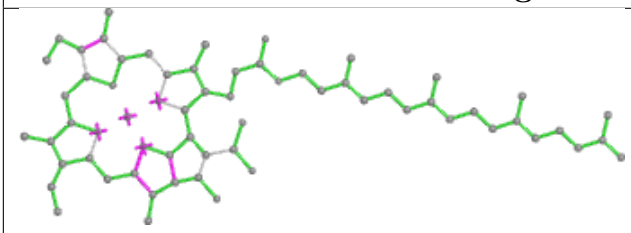


Torsions

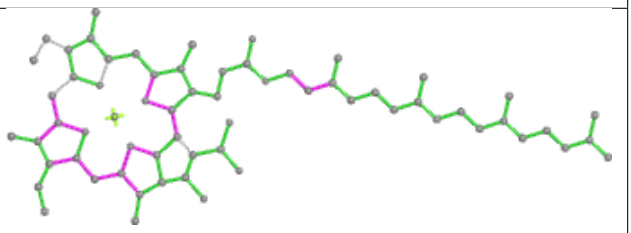


Rings

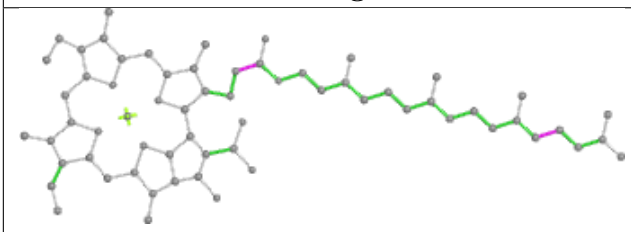
Ligand CLA A1 803



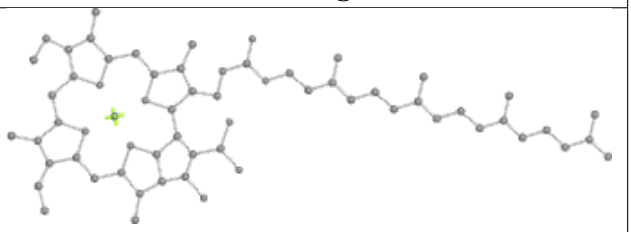
Bond lengths



Bond angles

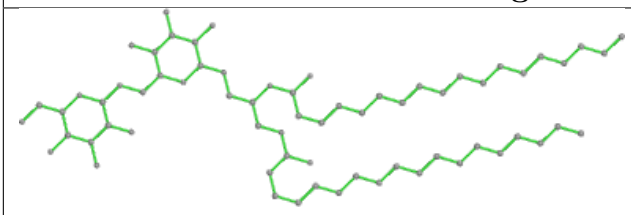


Torsions



Rings

Ligand DGD B2 848



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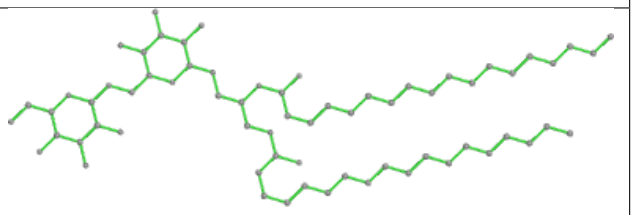
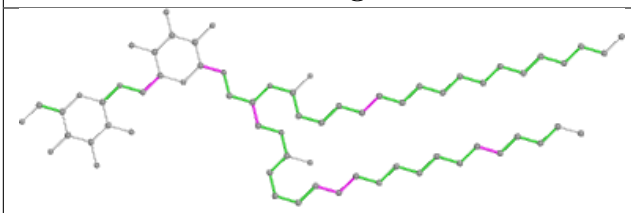
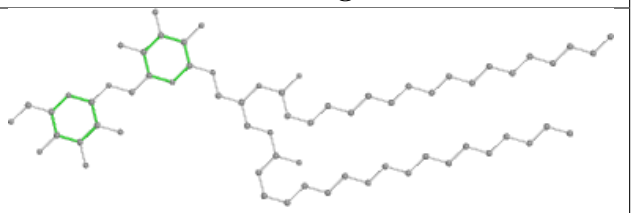


Bond angles

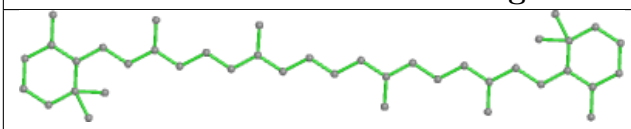


Torsions



Rings

Ligand BCR J3 1306



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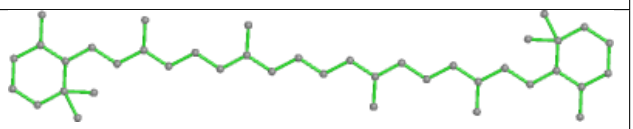
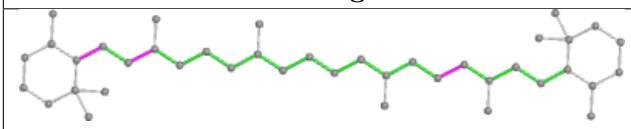
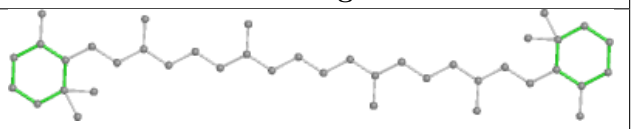


Bond angles

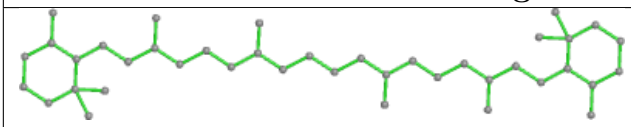


Torsions

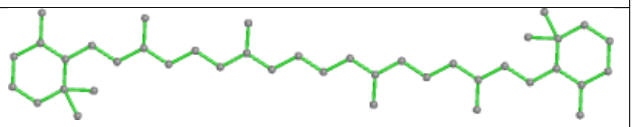


Rings

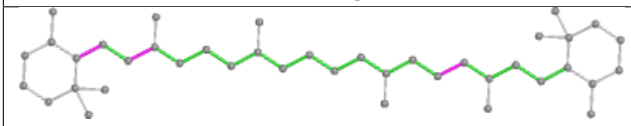
Ligand BCR A2 851



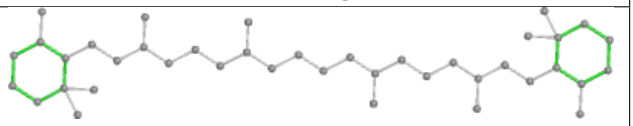
Bond lengths



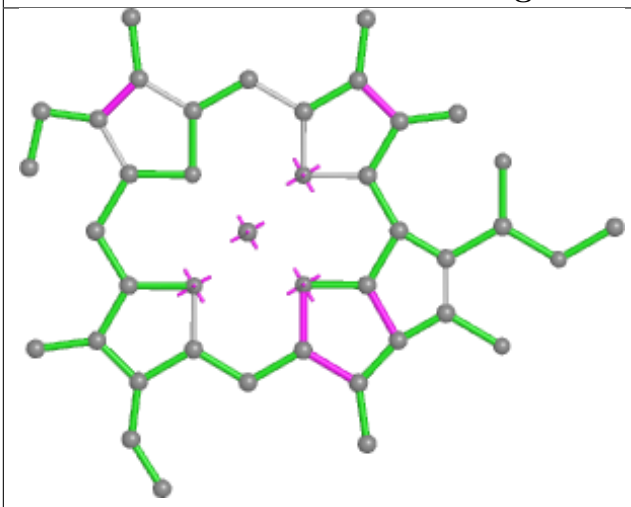
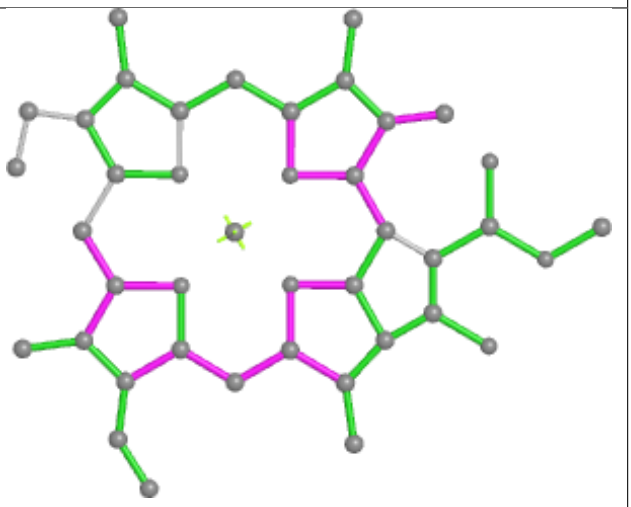
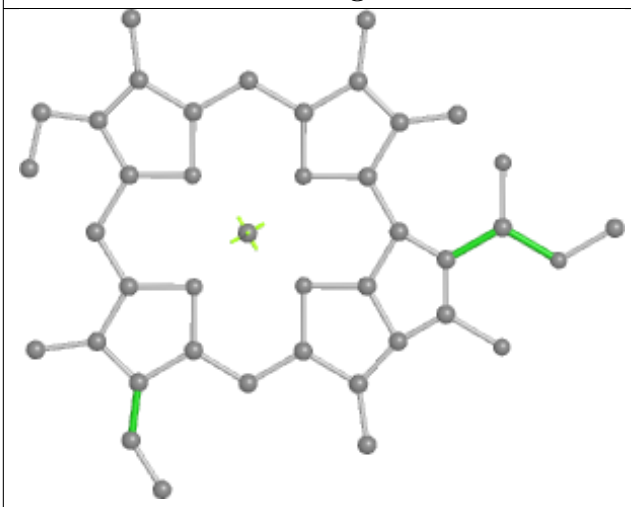
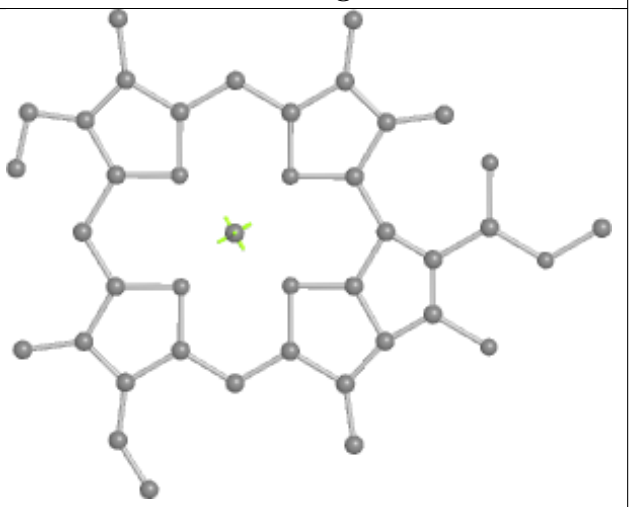
Bond angles



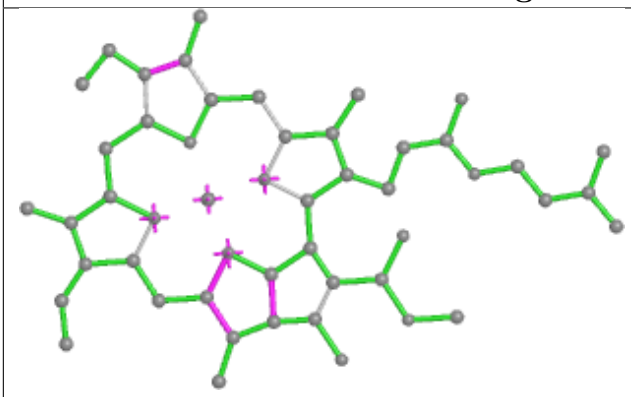
Torsions



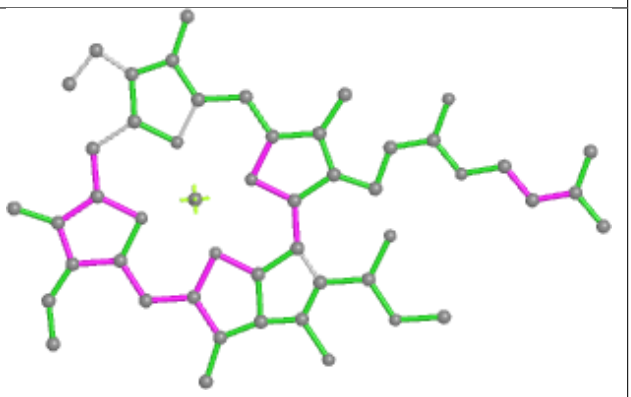
Rings

Ligand CLA A1 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

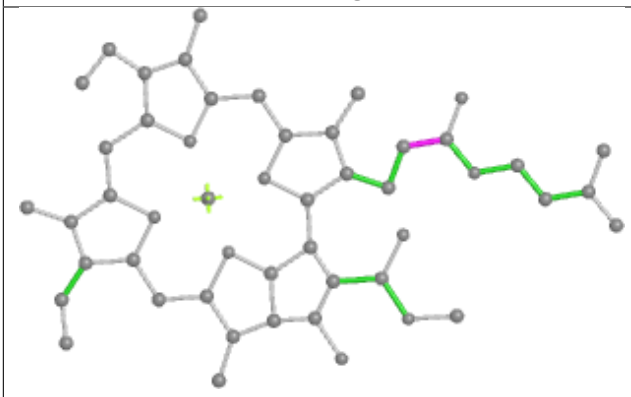
Ligand CLA B1 806



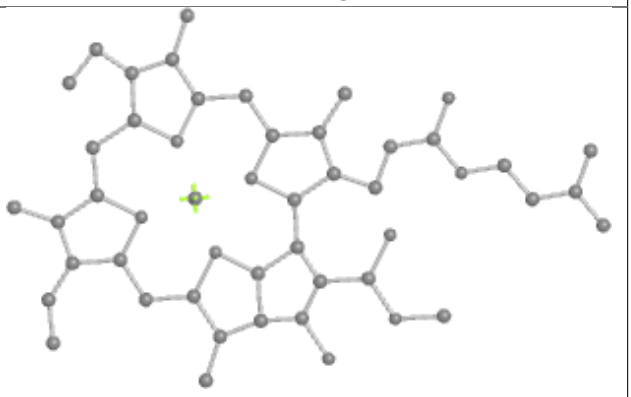
Bond lengths



Bond angles

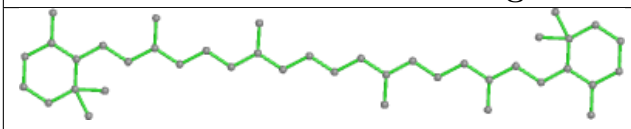


Torsions

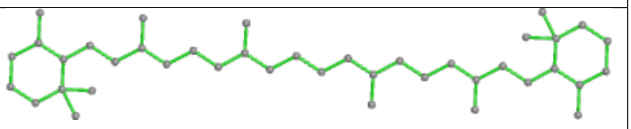


Rings

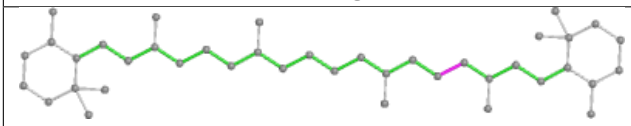
Ligand BCR L1 1011



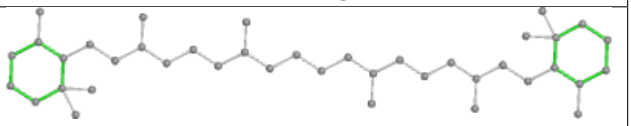
Bond lengths



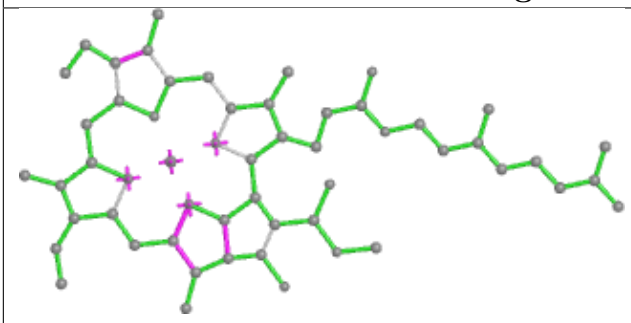
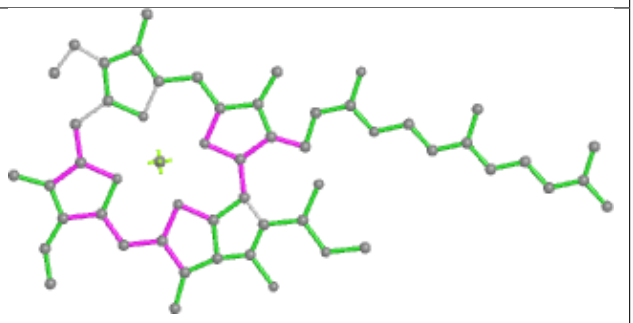
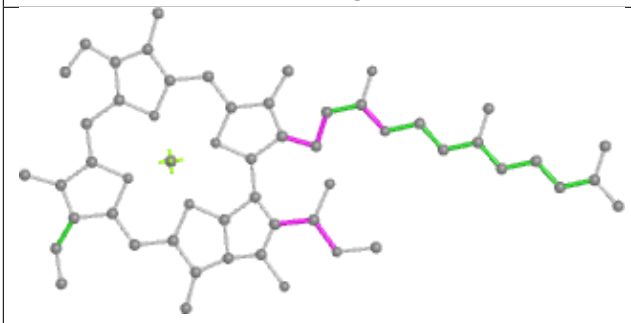
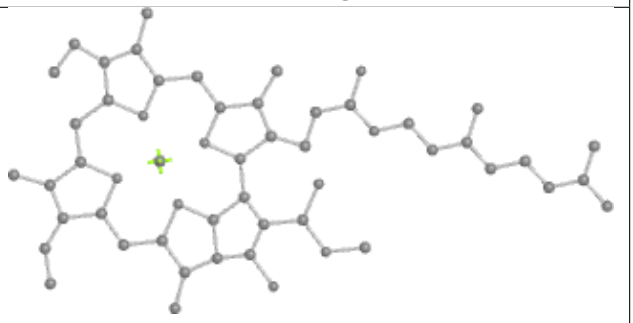
Bond angles

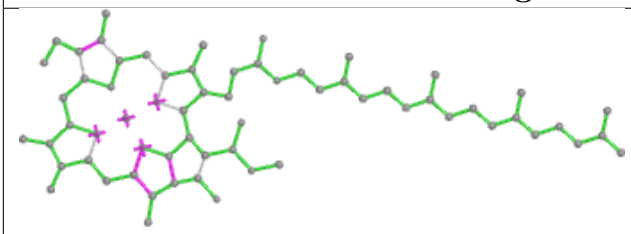
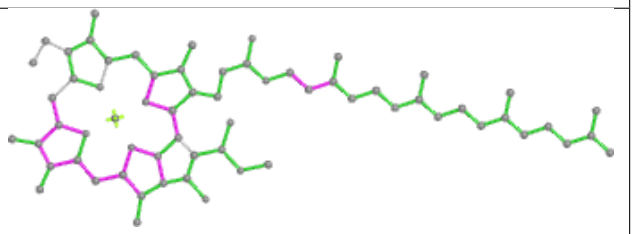
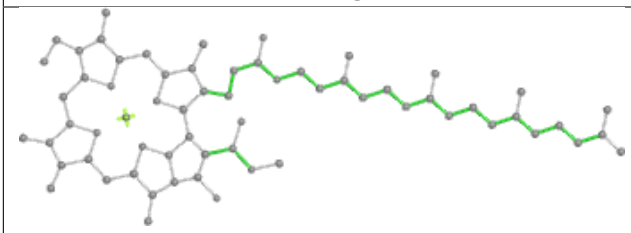
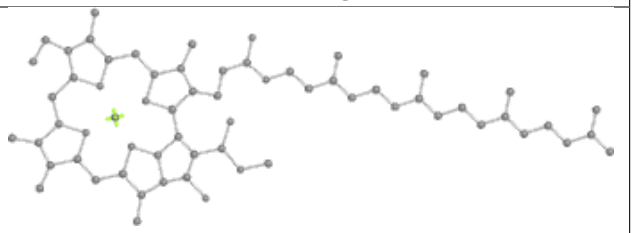


Torsions

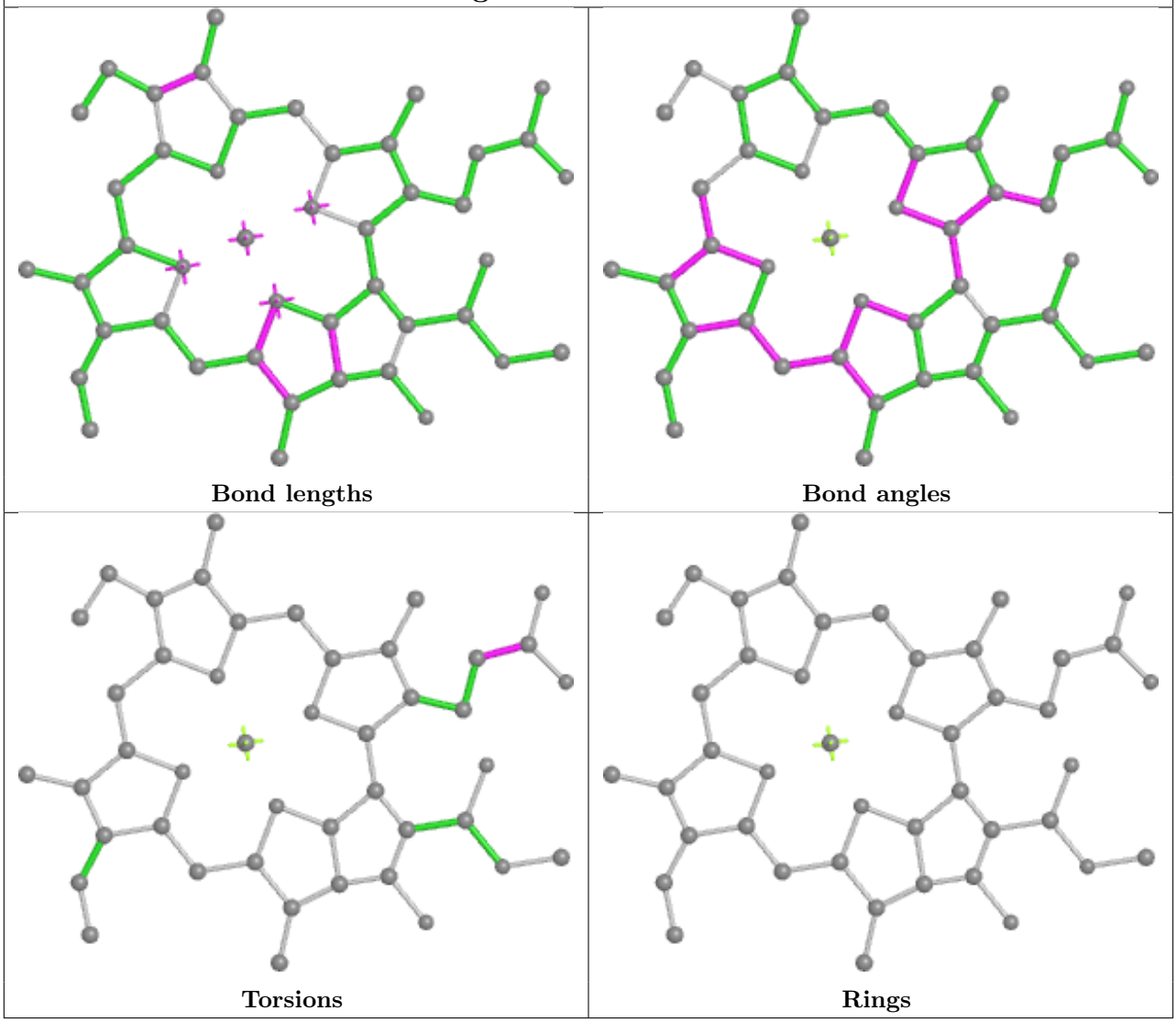


Rings

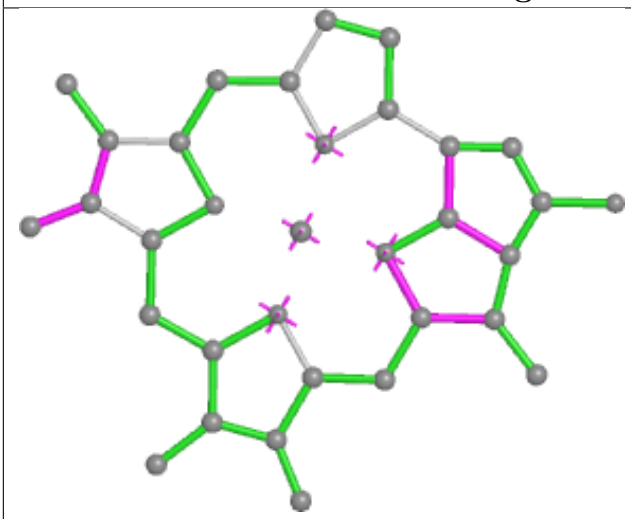
Ligand CLA A1 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

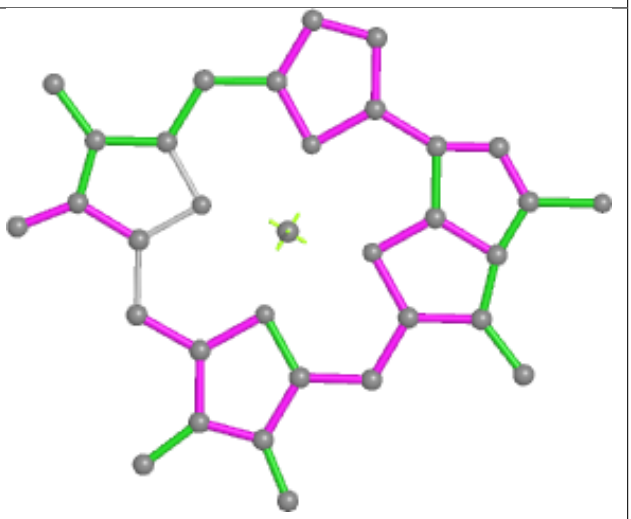
Ligand CLA A2 822



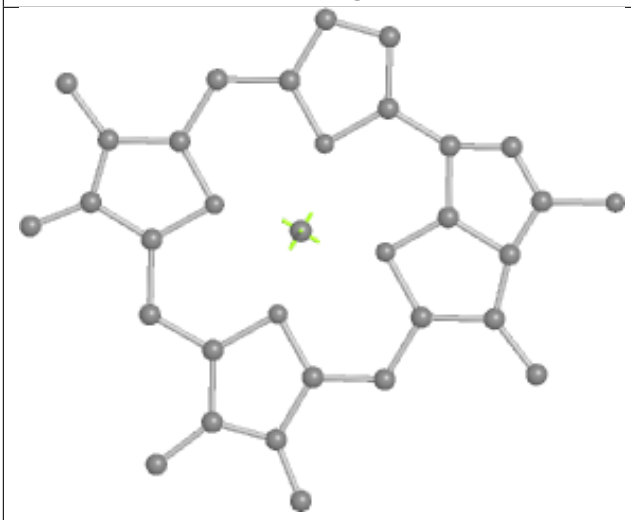
Ligand CLA A2 814



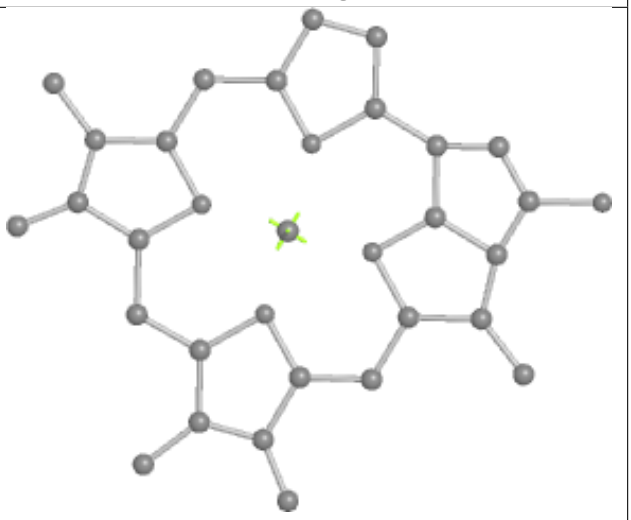
Bond lengths



Bond angles

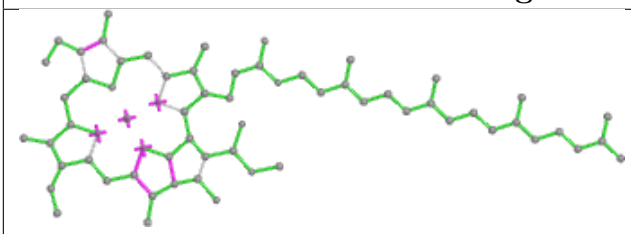


Torsions

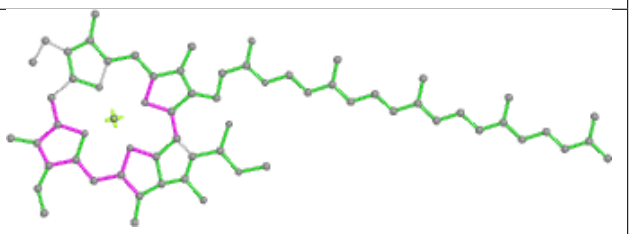


Rings

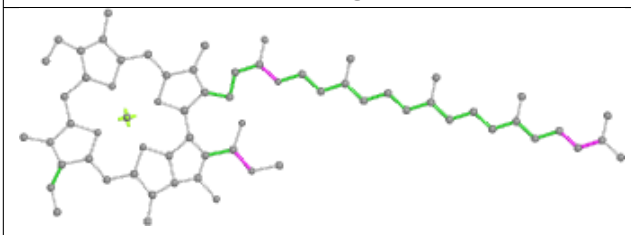
Ligand CLA B3 839



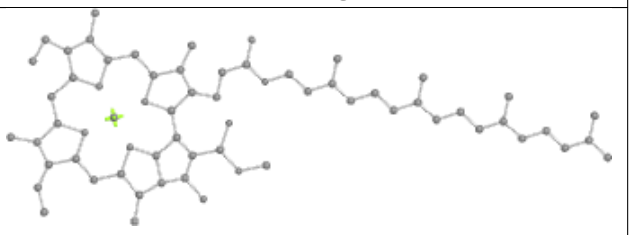
Bond lengths



Bond angles

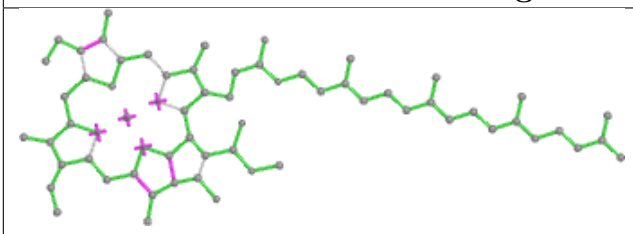


Torsions

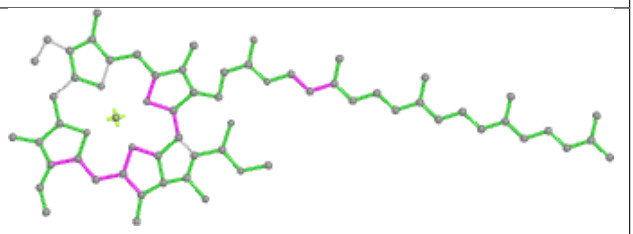


Rings

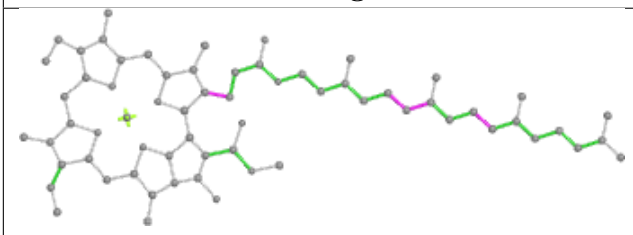
Ligand CLA B2 802



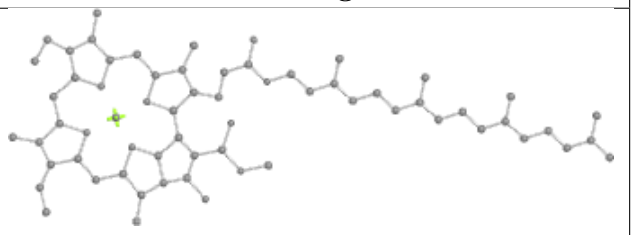
Bond lengths



Bond angles

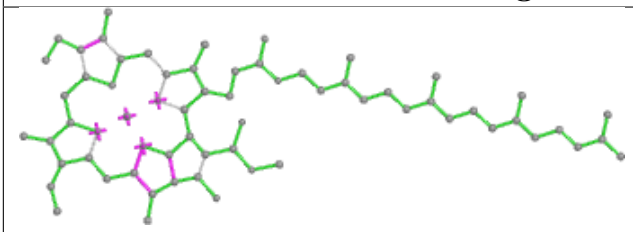


Torsions

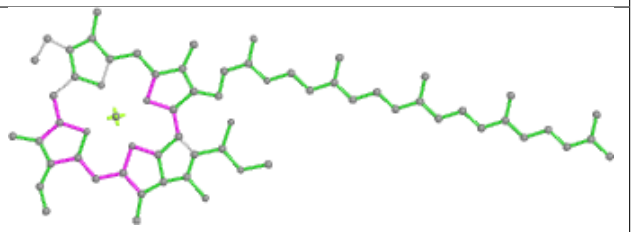


Rings

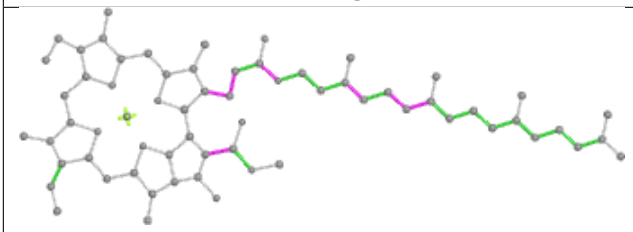
Ligand CLA B3 827



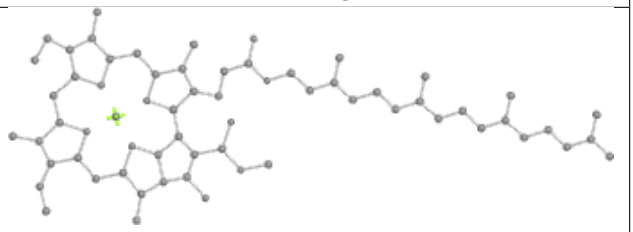
Bond lengths



Bond angles

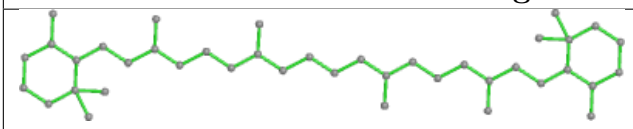


Torsions

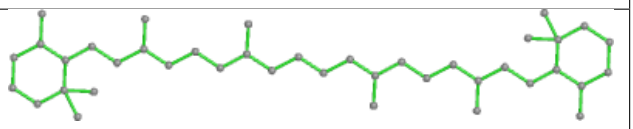


Rings

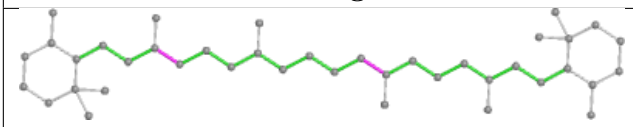
Ligand BCR A1 852



Bond lengths



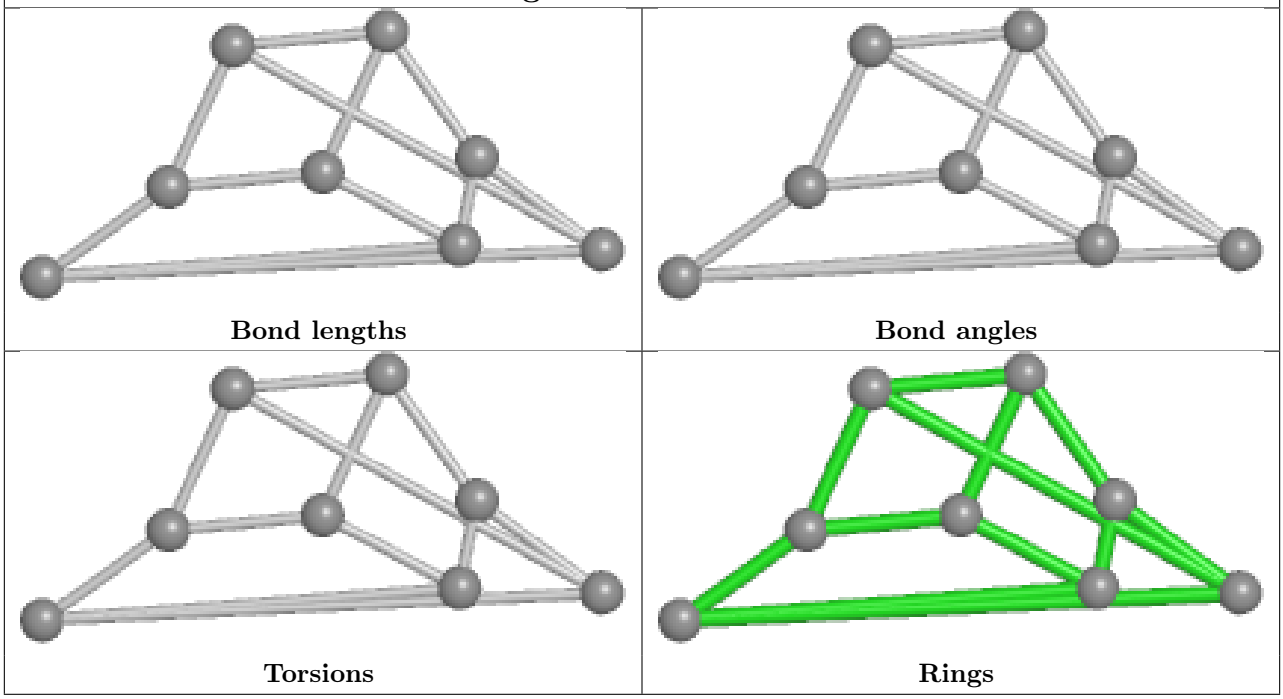
Bond angles



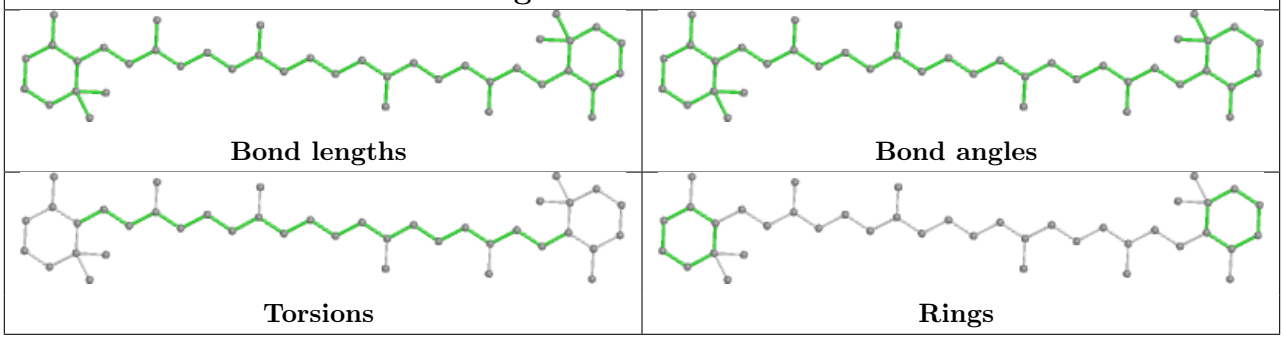
Torsions

Rings

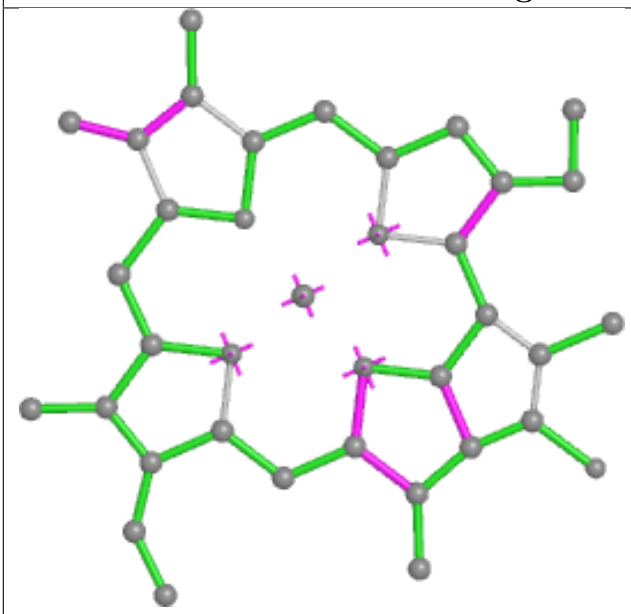
Ligand SF4 A3 846



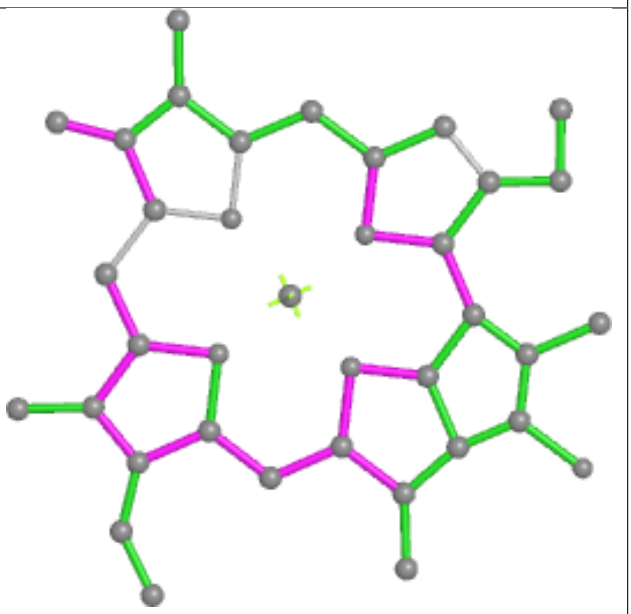
Ligand BCR A3 849



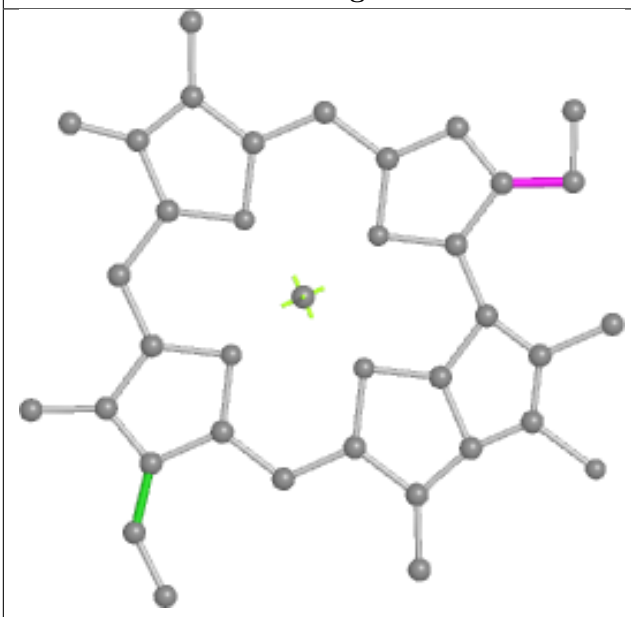
Ligand CLA B1 833



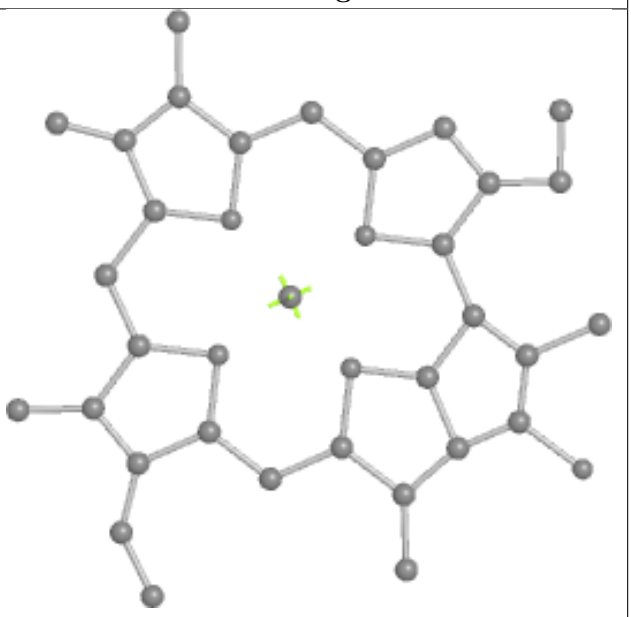
Bond lengths



Bond angles



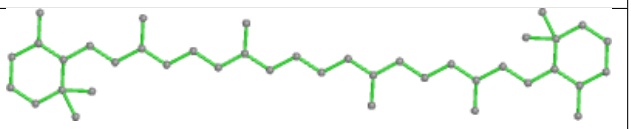
Torsions



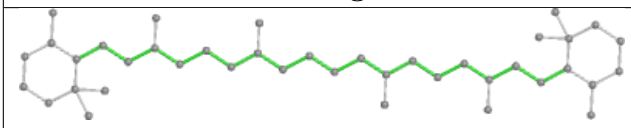
Rings

Ligand BCR I2 102

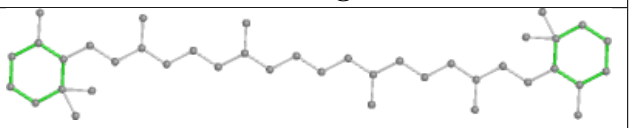
Bond lengths



Bond angles

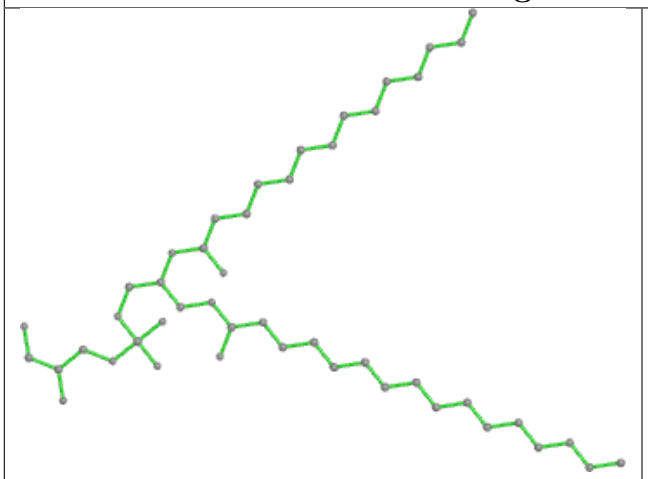


Torsions

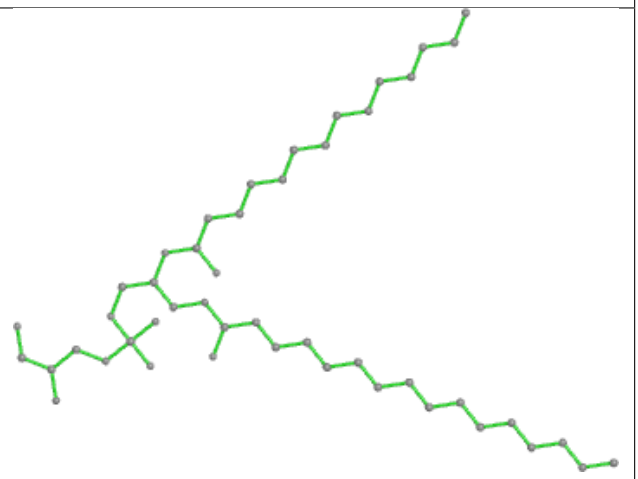


Rings

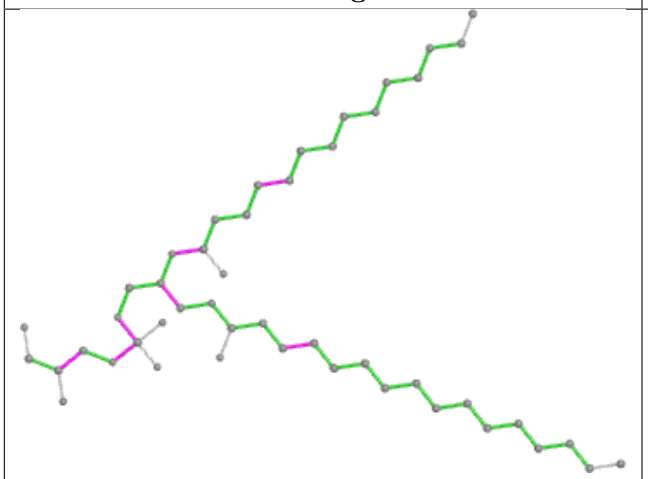
Ligand LHG A1 853



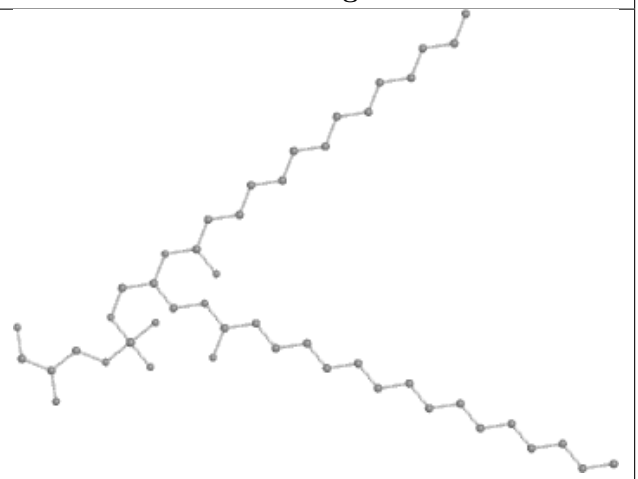
Bond lengths



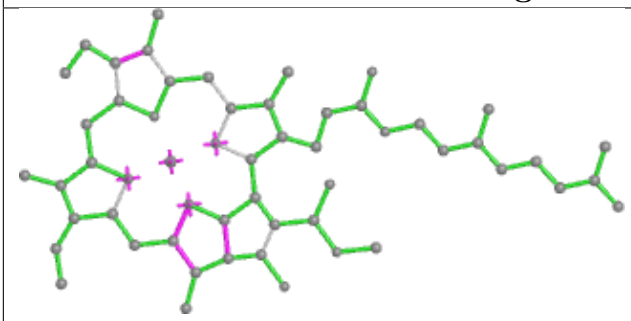
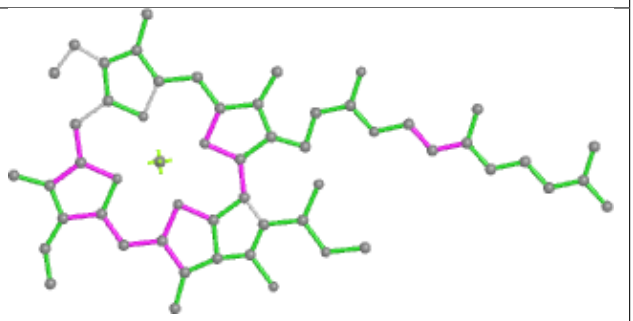
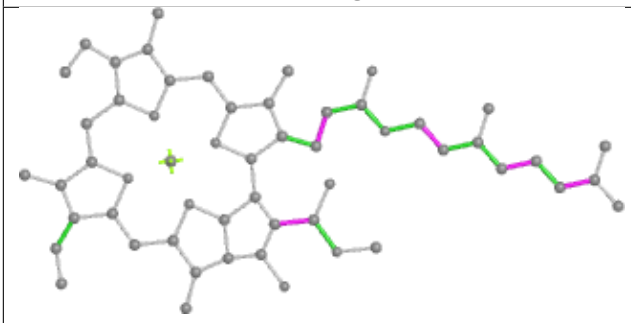
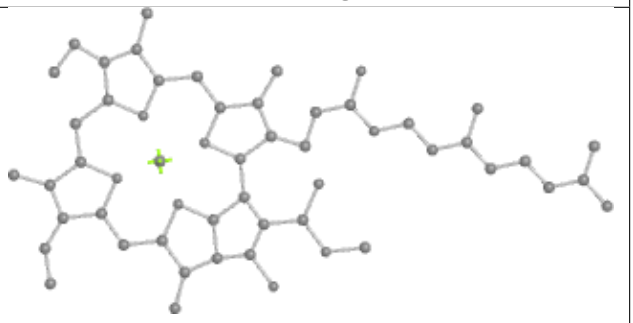
Bond angles

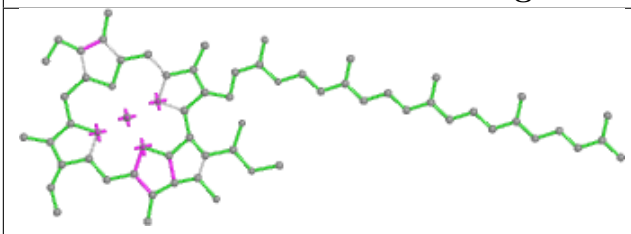
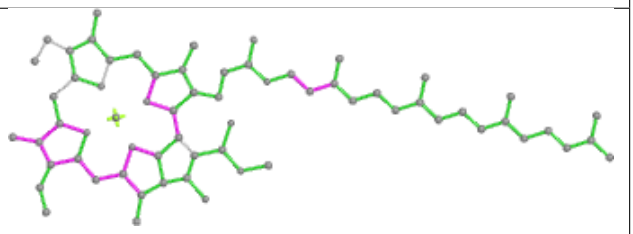
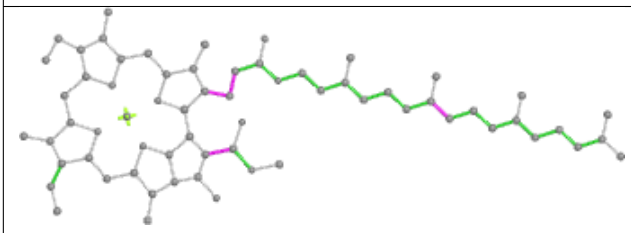
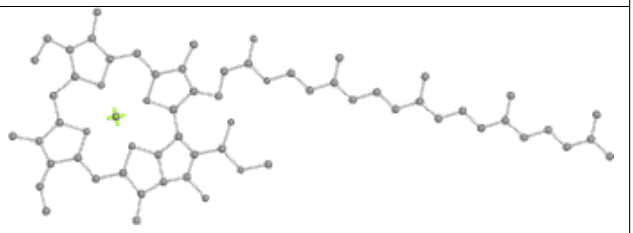


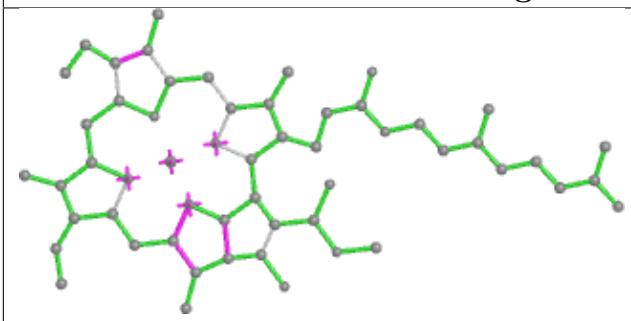
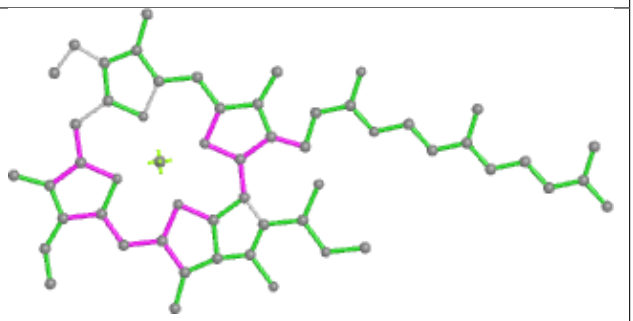
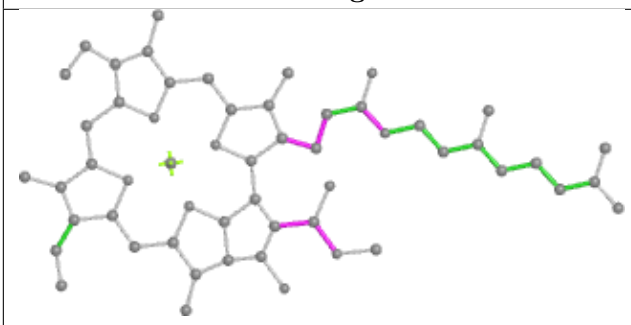
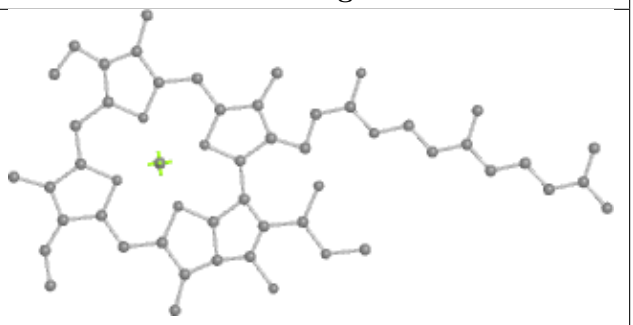
Torsions



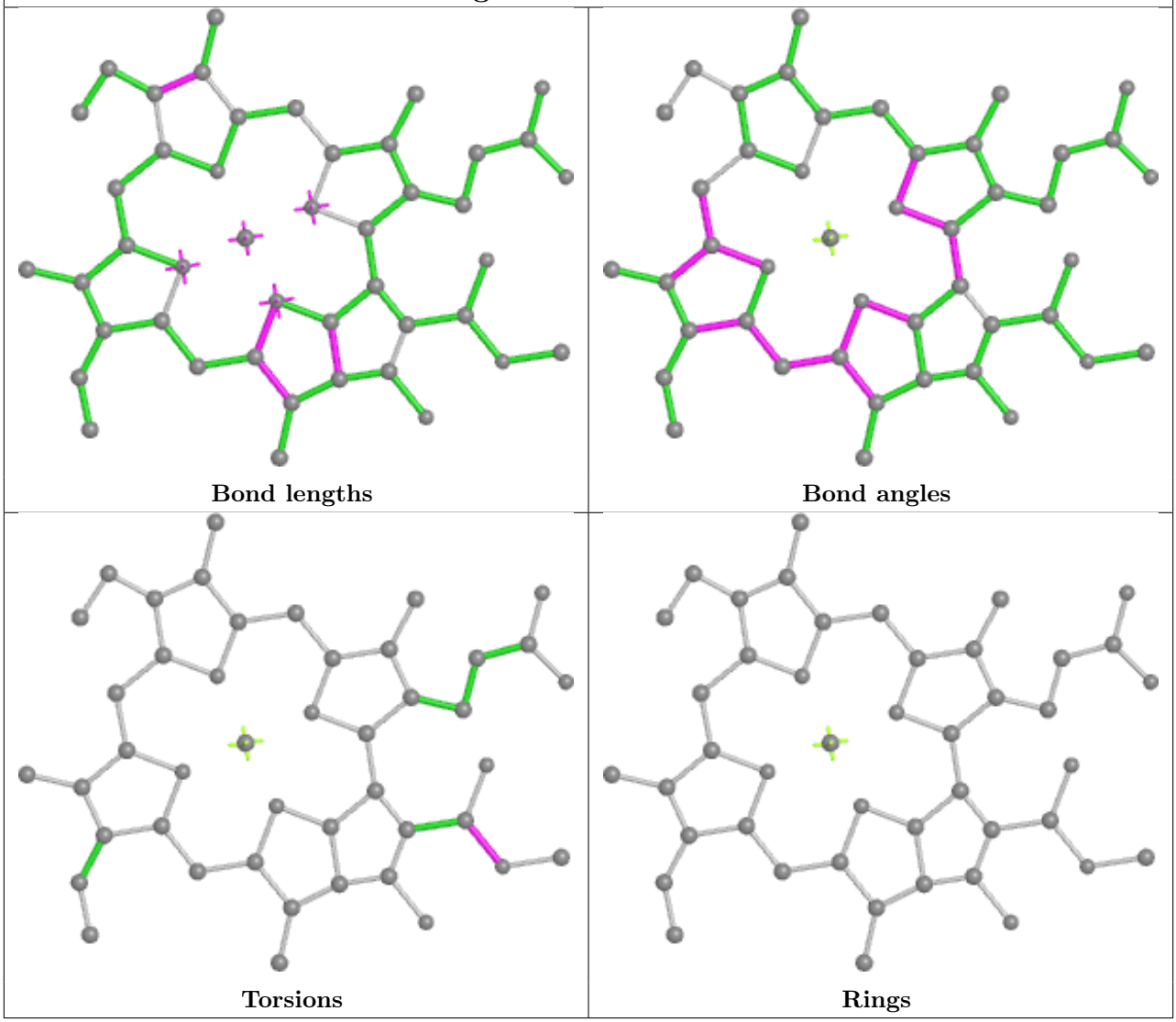
Rings

Ligand CLA A2 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

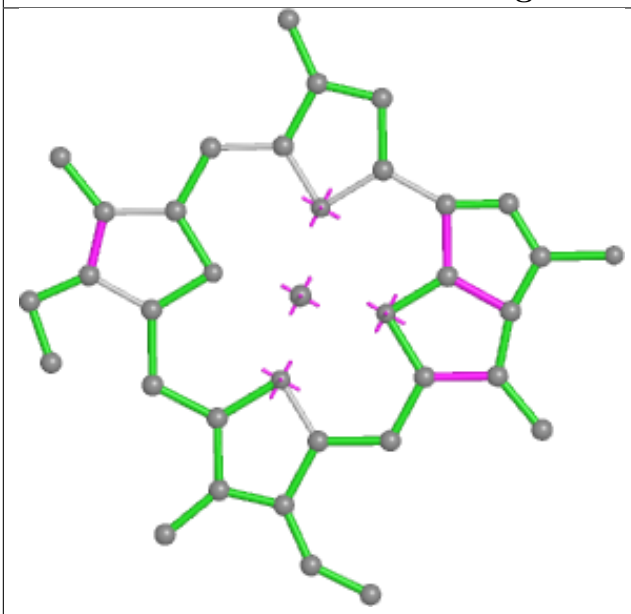
Ligand CLA A2 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

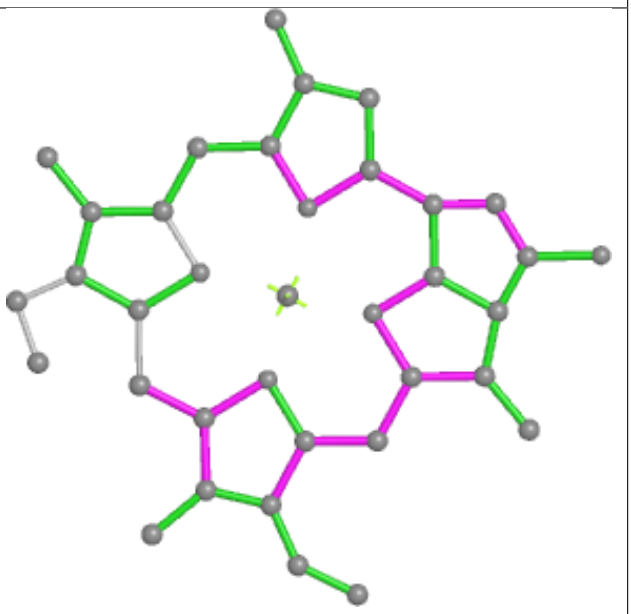
Ligand CLA B1 826



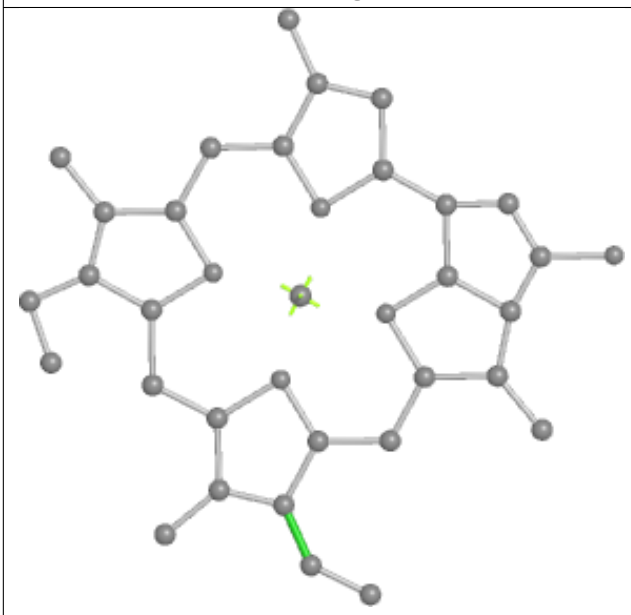
Ligand CLA B1 815



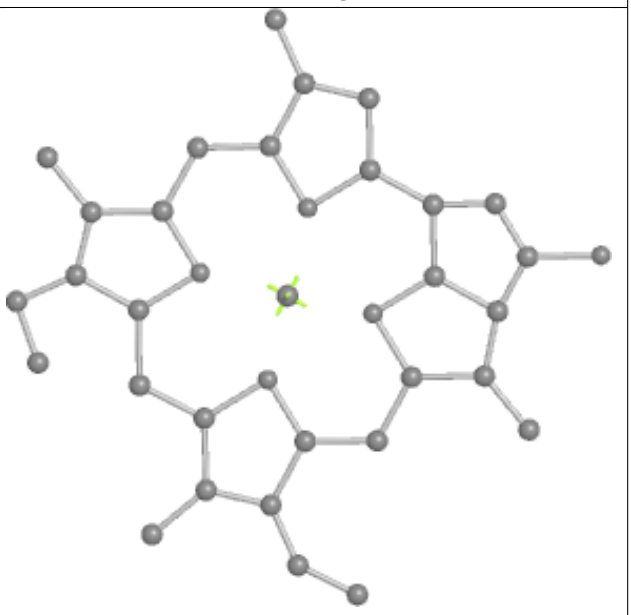
Bond lengths



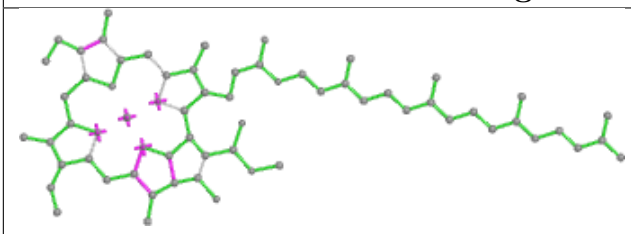
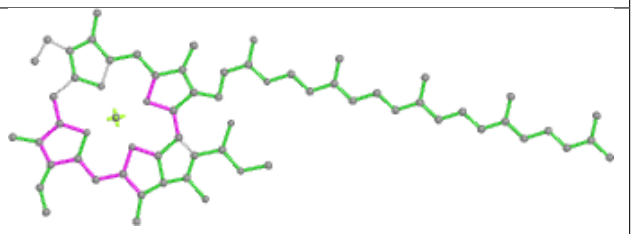
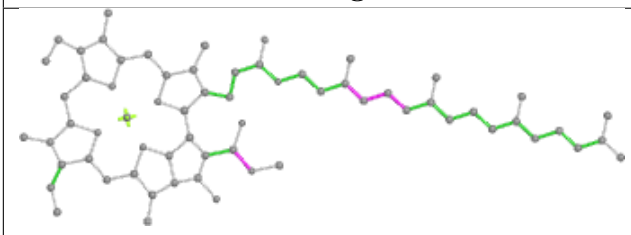
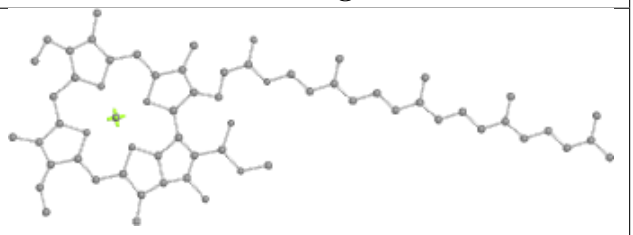
Bond angles

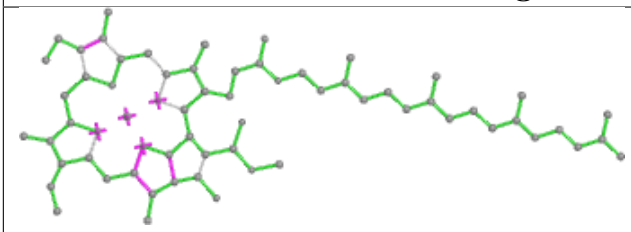
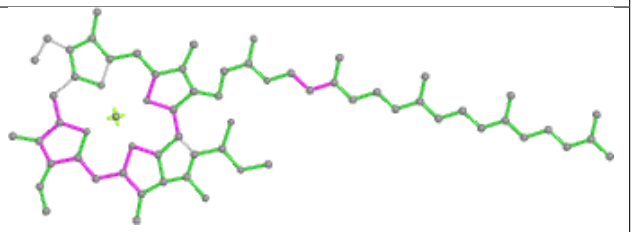
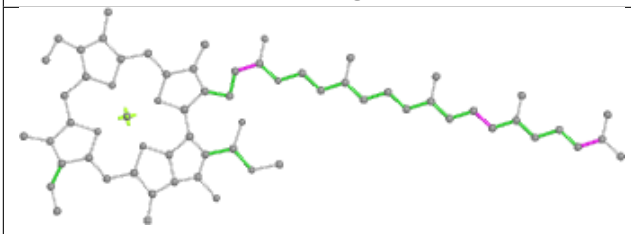
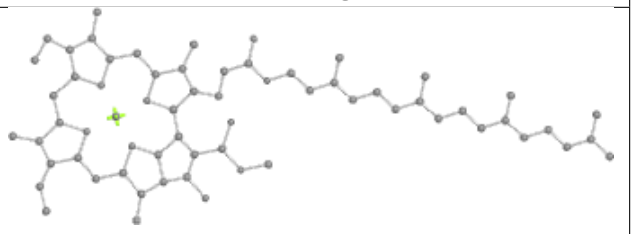


Torsions

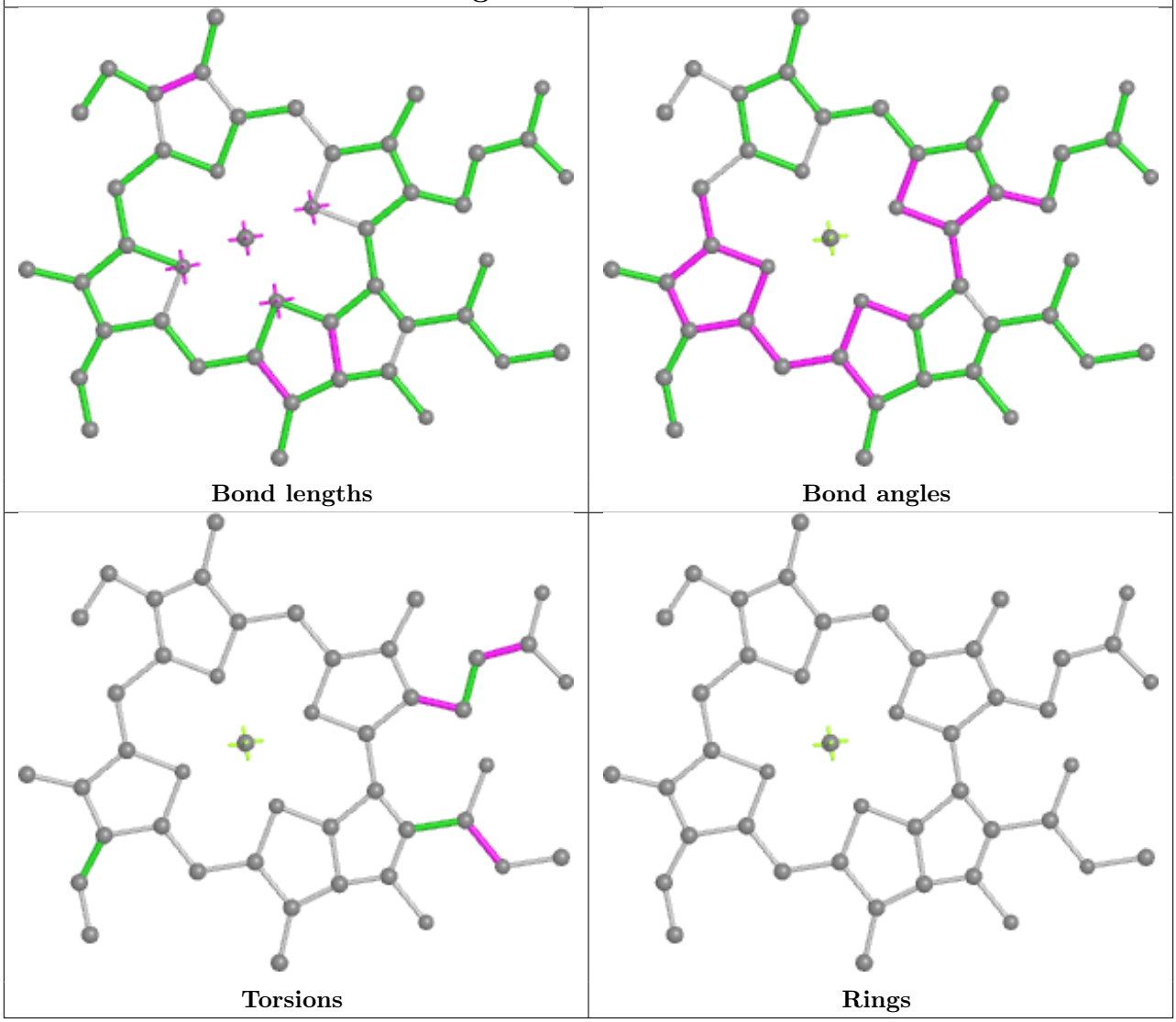


Rings

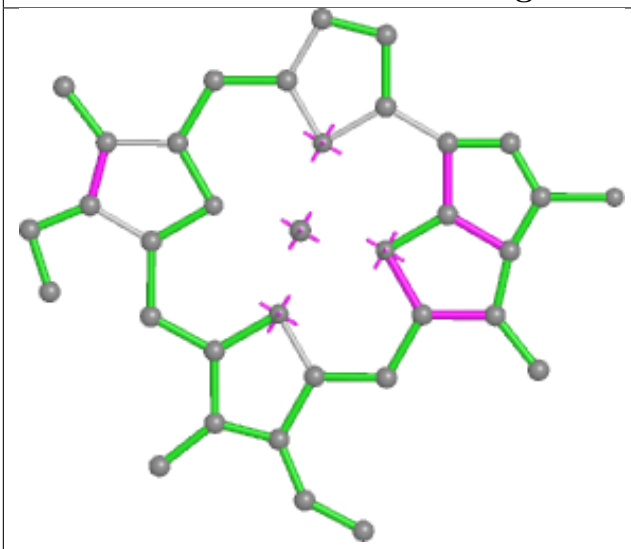
Ligand CLA A3 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A3 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

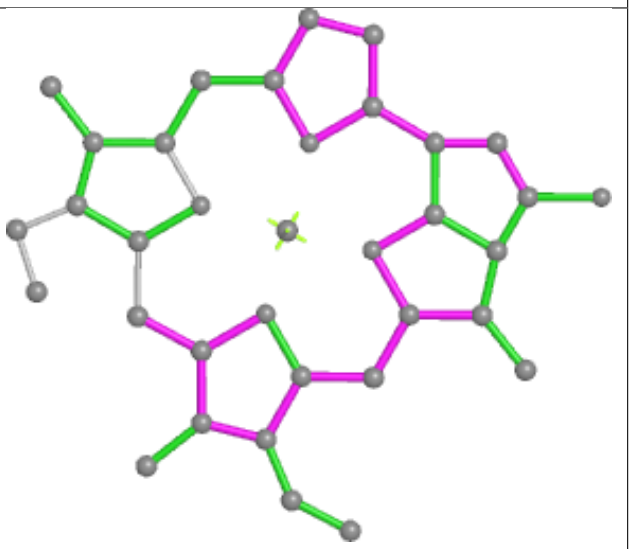
Ligand CLA A1 832



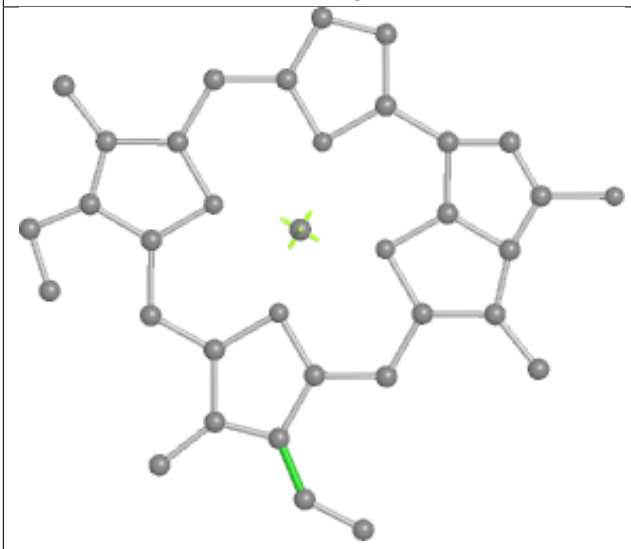
Ligand CLA B3 829



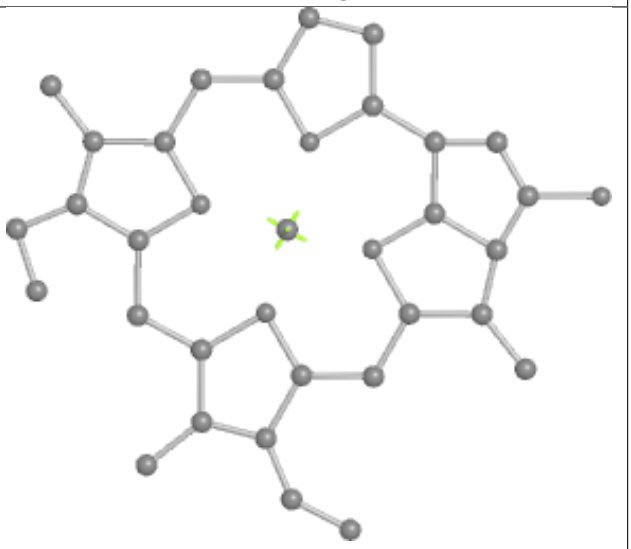
Bond lengths



Bond angles

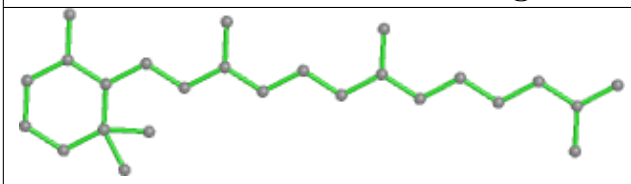


Torsions

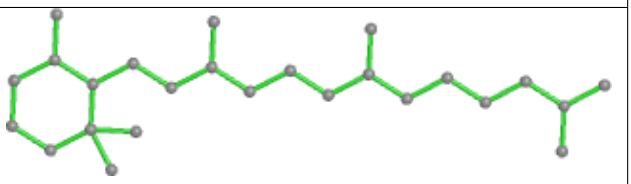


Rings

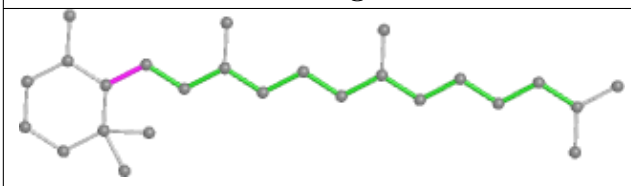
Ligand BCR K3 102



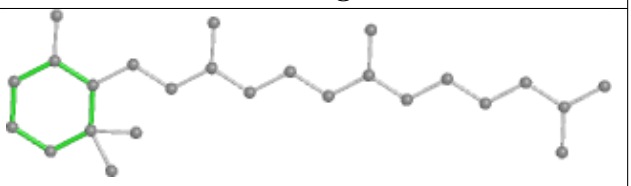
Bond lengths



Bond angles

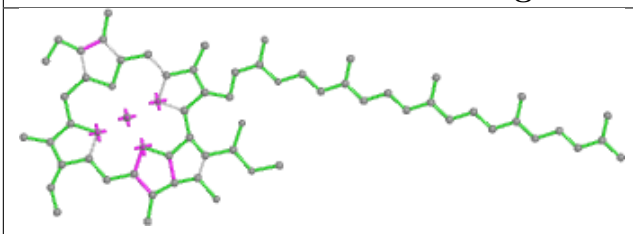


Torsions

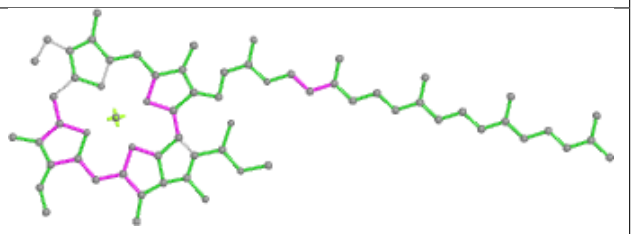


Rings

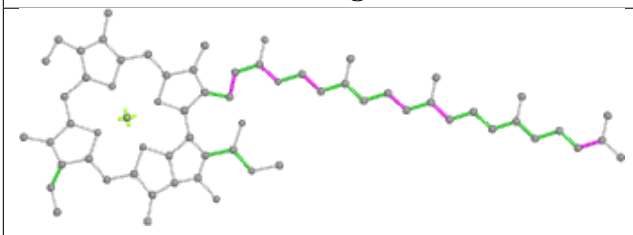
Ligand CLA A2 843



Bond lengths



Bond angles



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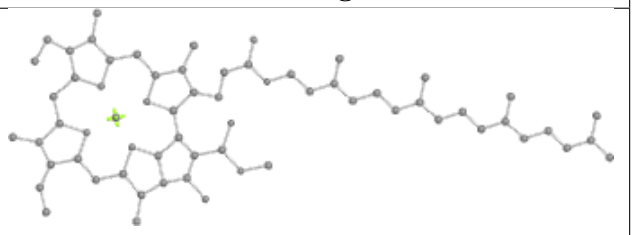
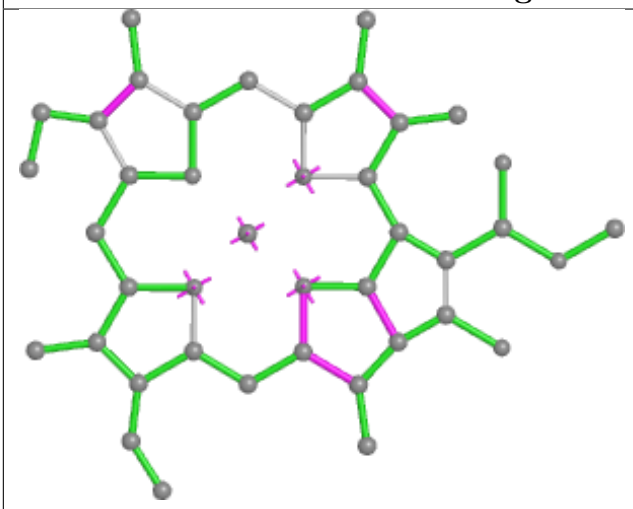
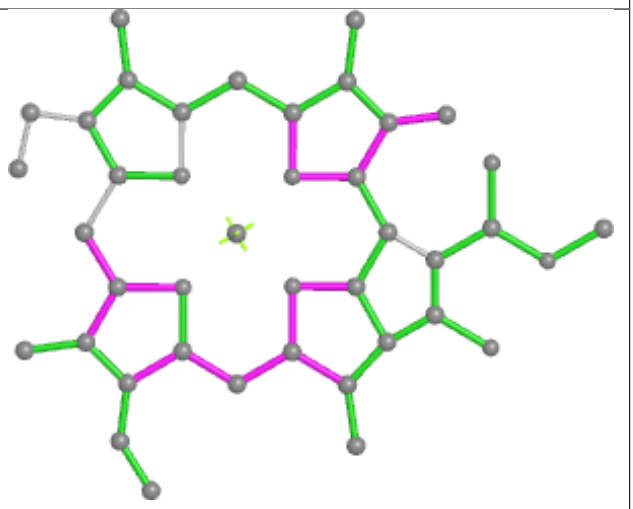


Rings

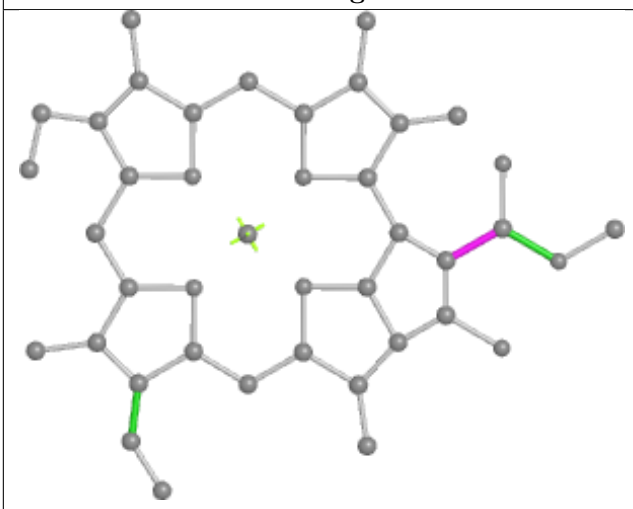
Ligand CLA A1 823



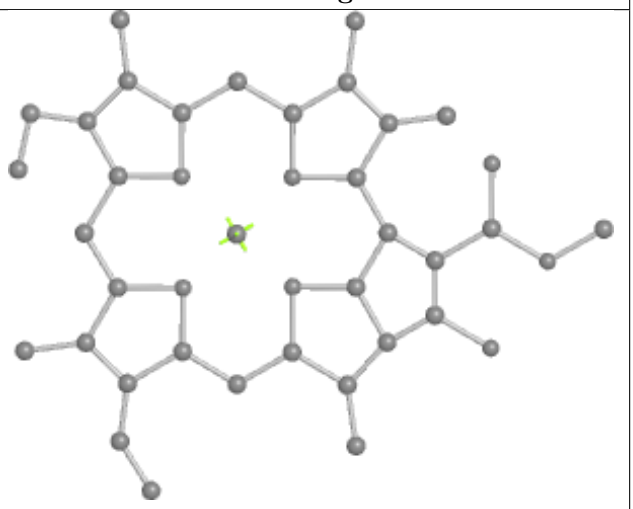
Bond lengths



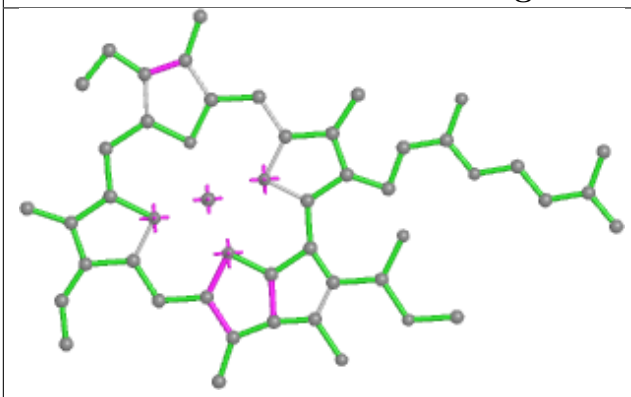
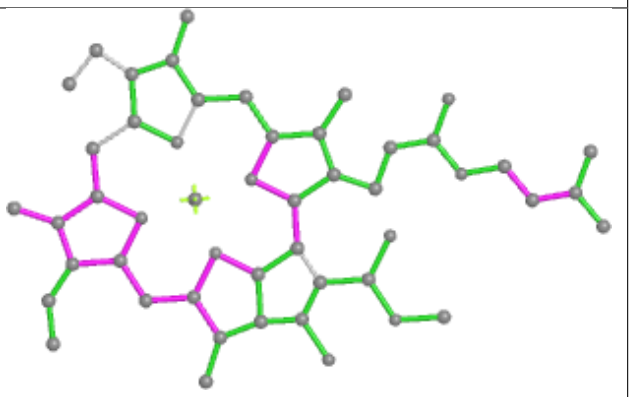
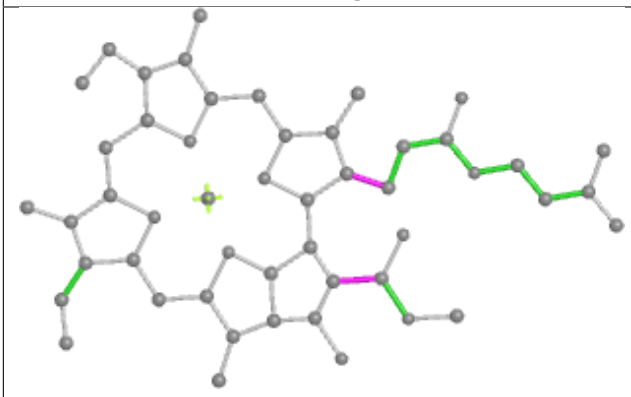
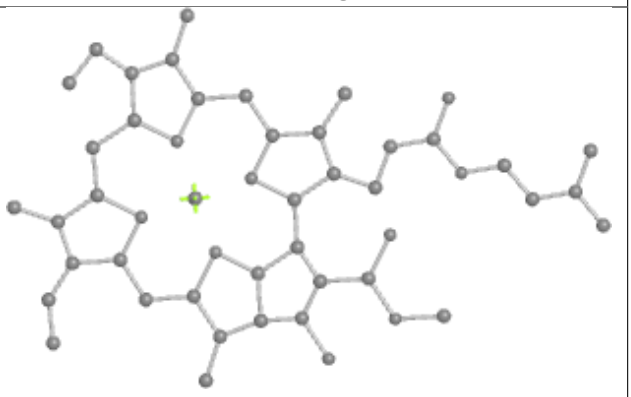
Bond angles



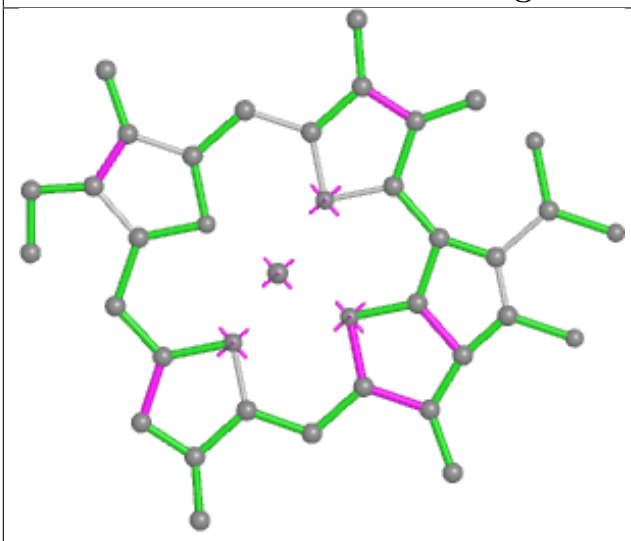
Torsions



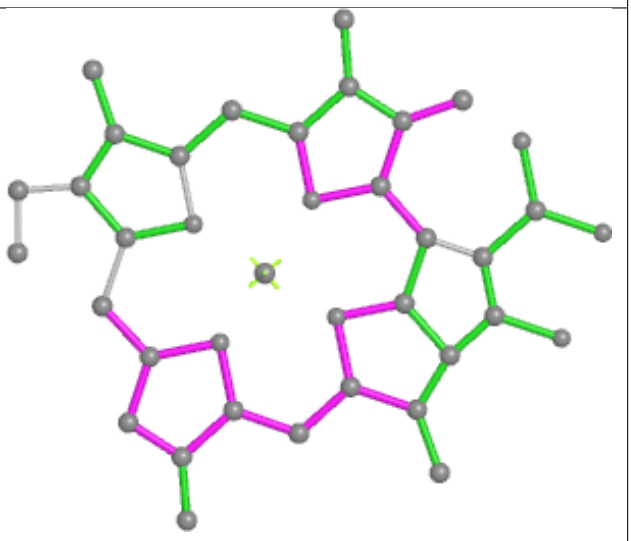
Rings

Ligand CLA A3 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

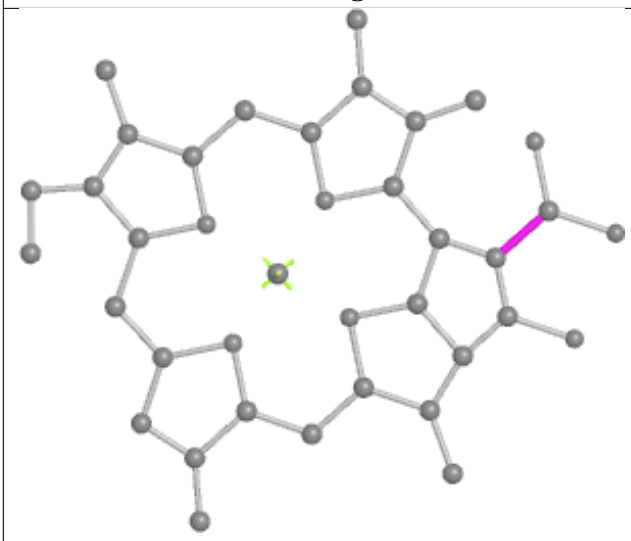
Ligand CLA A1 810



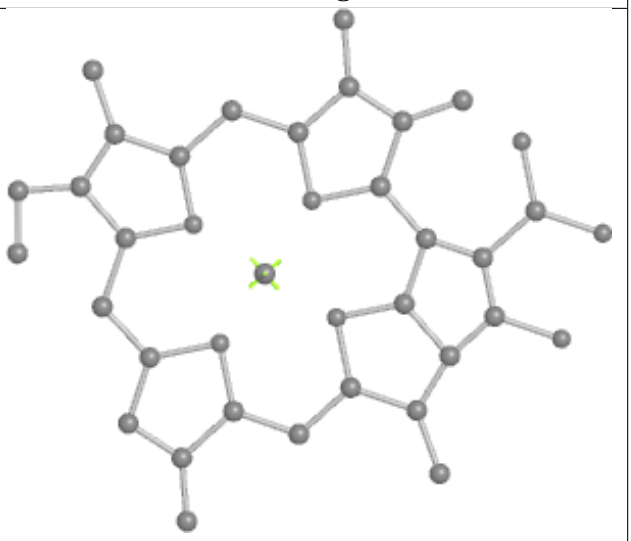
Bond lengths



Bond angles

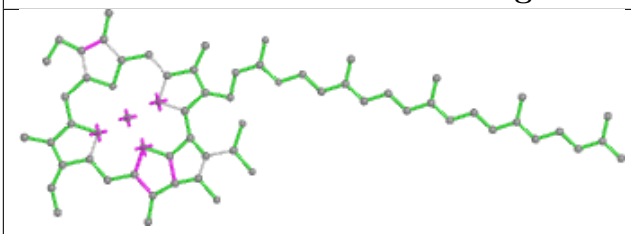


Torsions

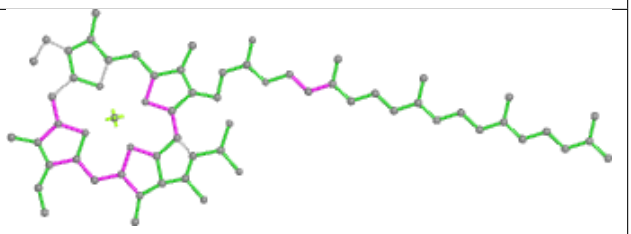


Rings

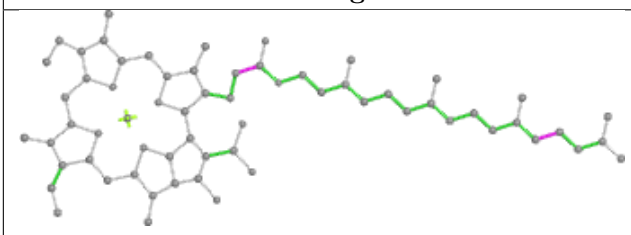
Ligand CLA A2 803



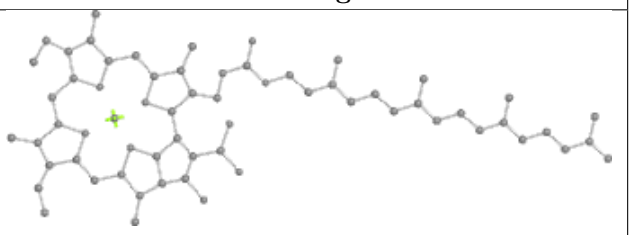
Bond lengths



Bond angles

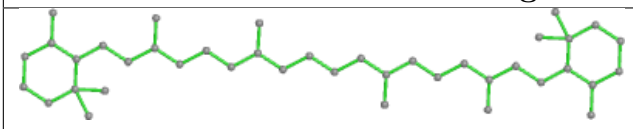


Torsions



Rings

Ligand BCR I1 103



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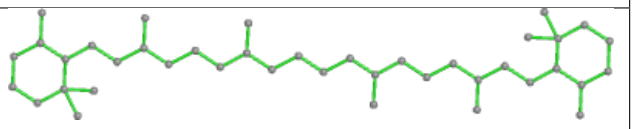
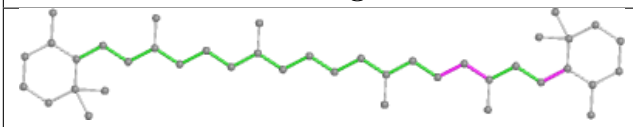
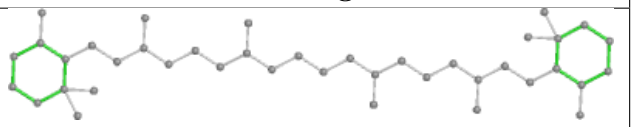


Bond angles

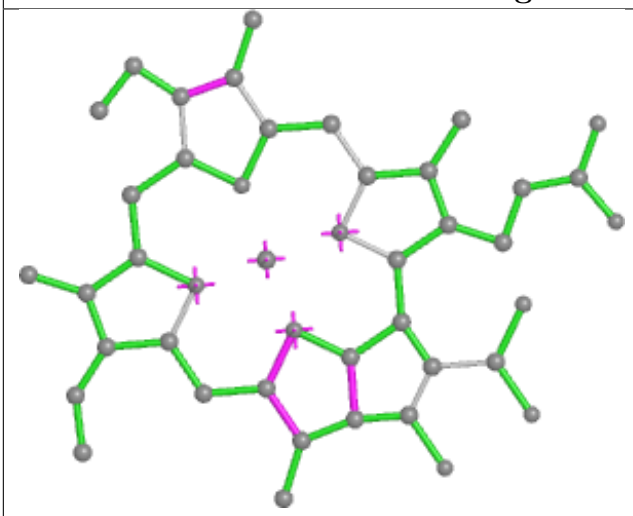


Torsions

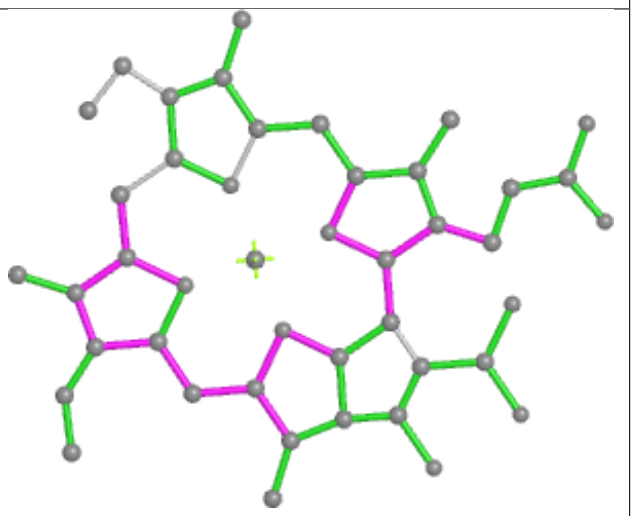


Rings

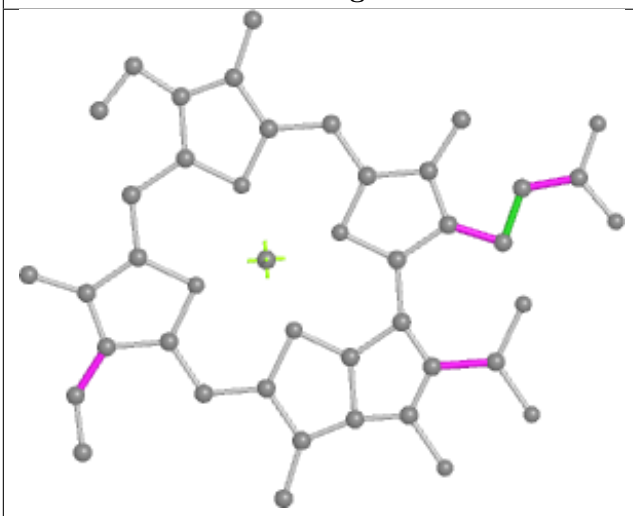
Ligand CLA A2 807



Bond lengths



Bond angles



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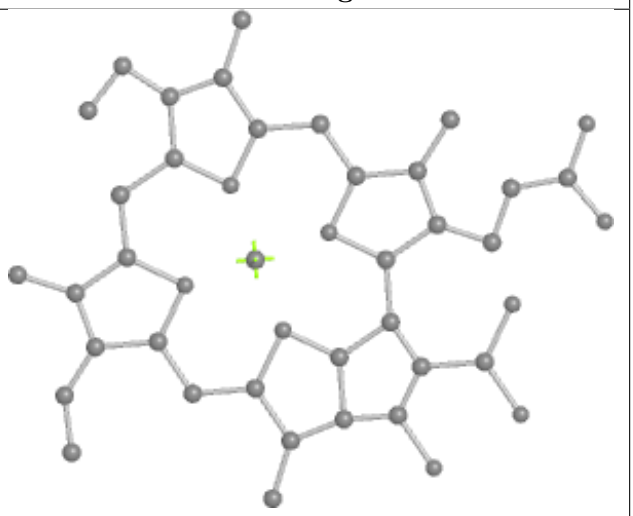
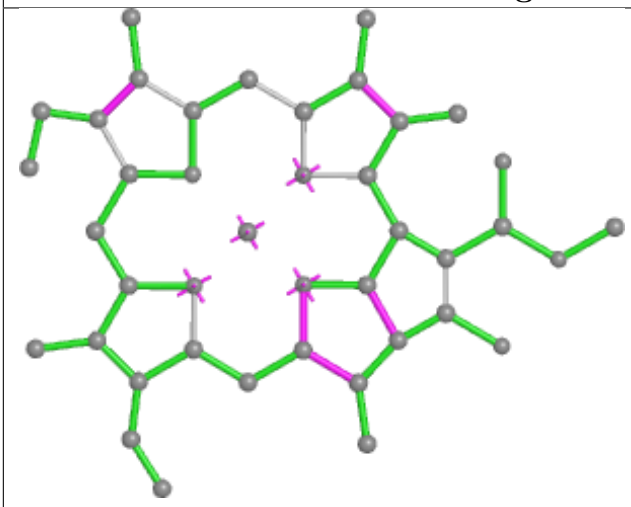


Rings

Ligand CLA B2 837



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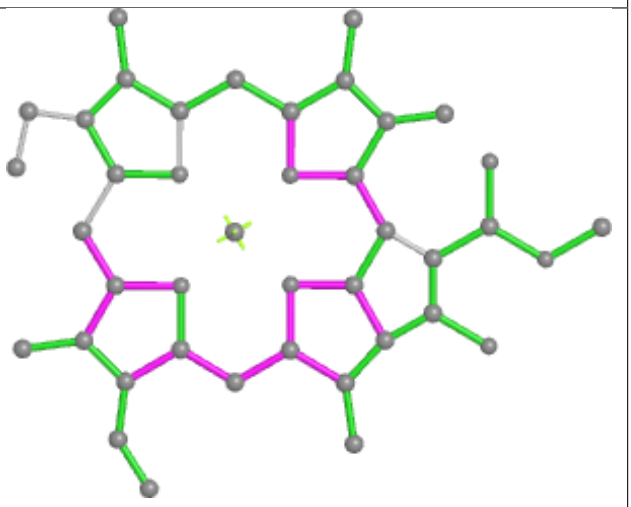
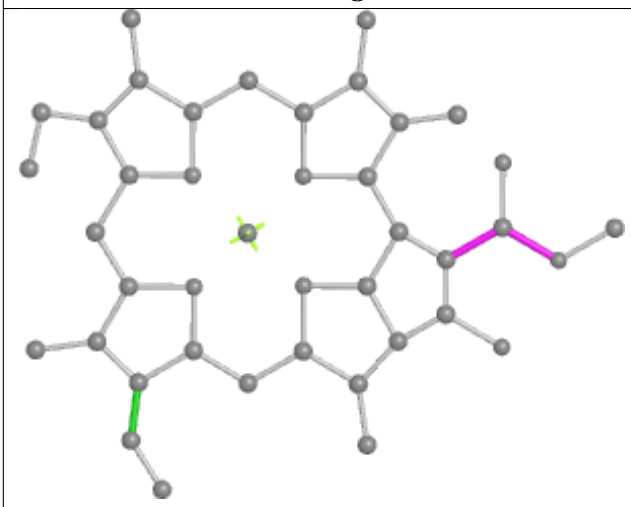


Bond angles



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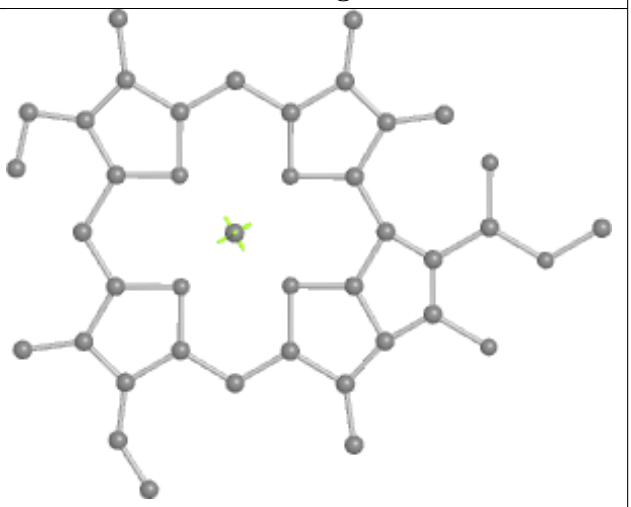
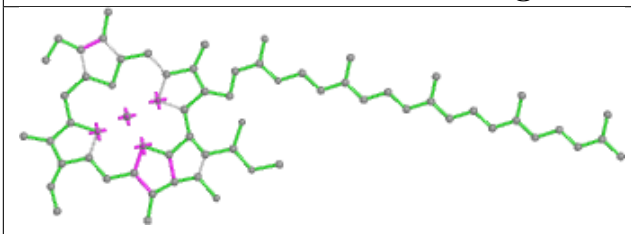
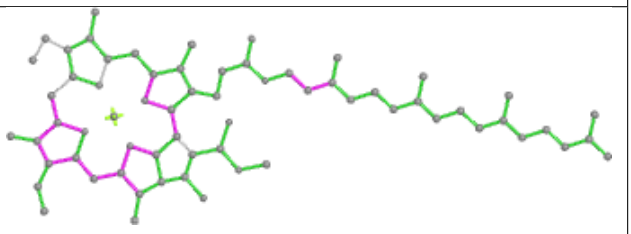


Rings

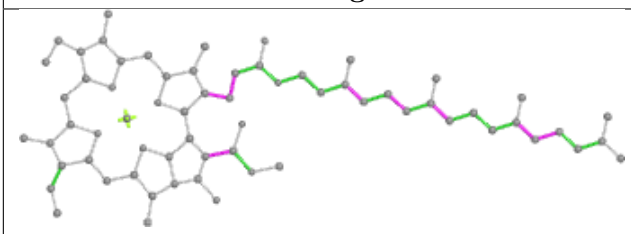
Ligand CLA A2 809



Bond lengths



Bond angles



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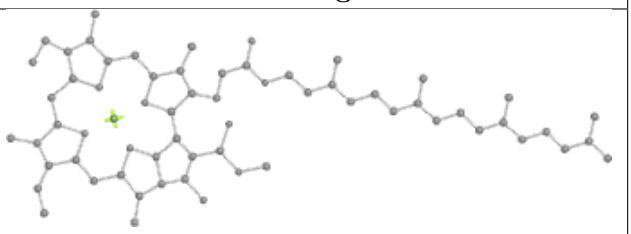
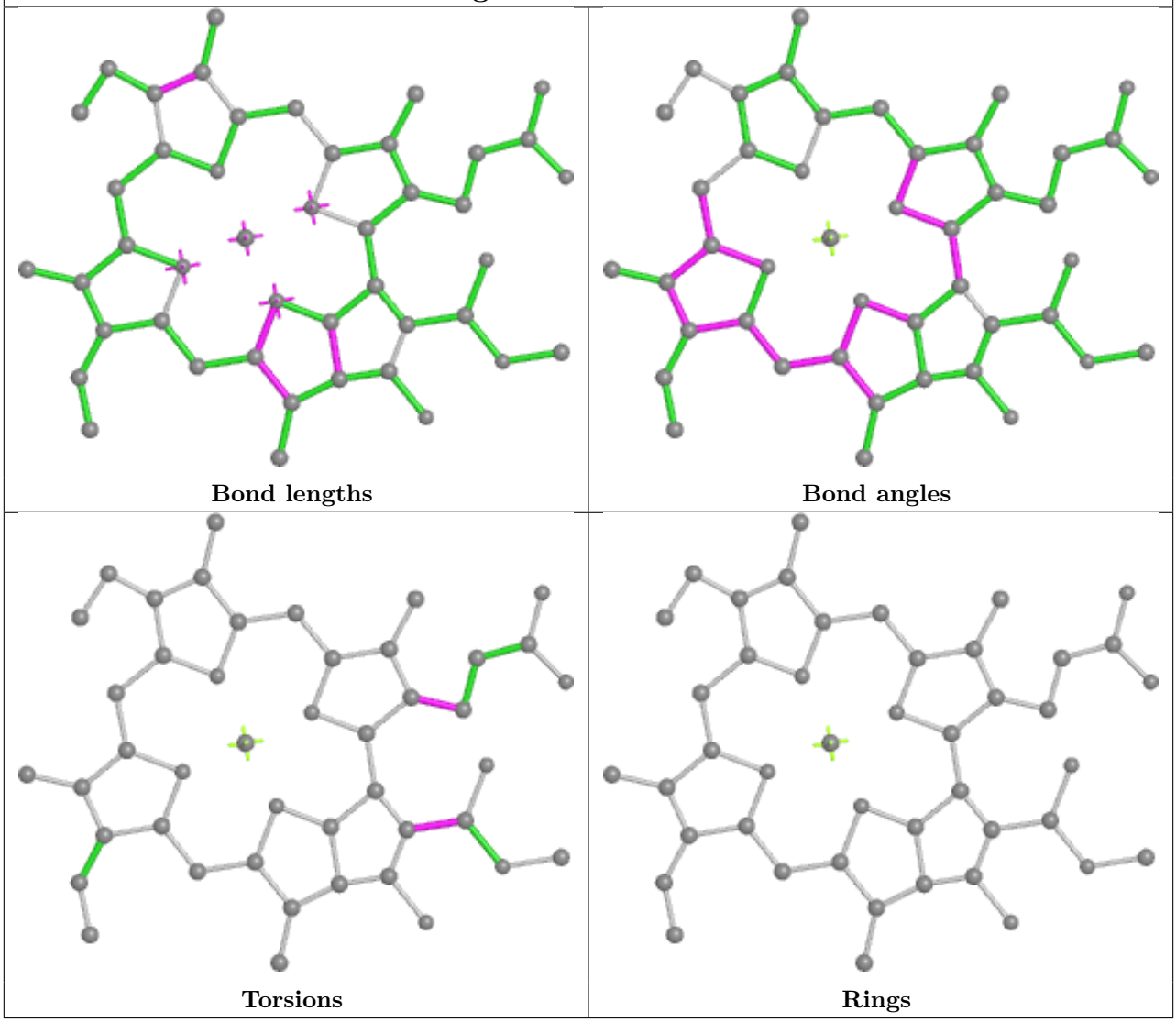
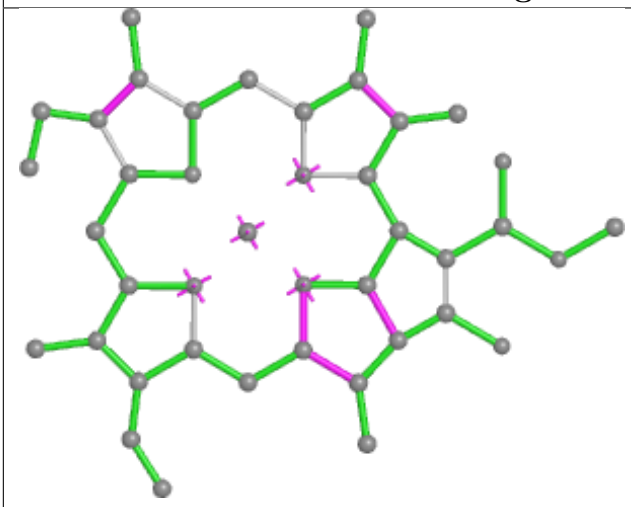
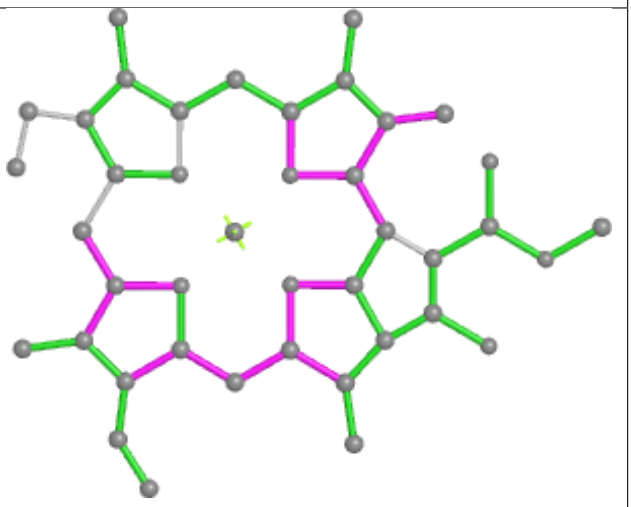
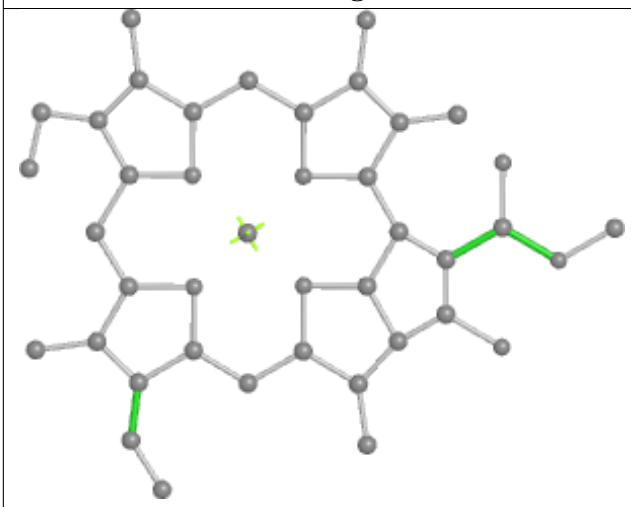
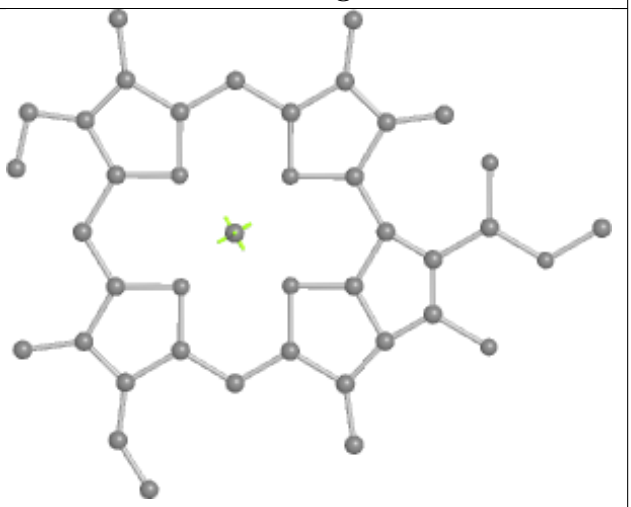
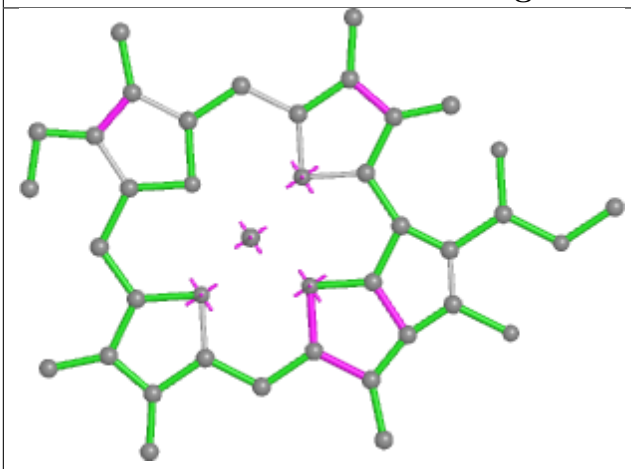
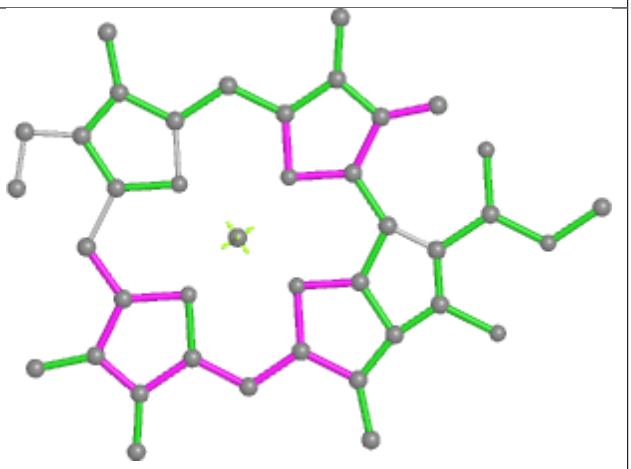
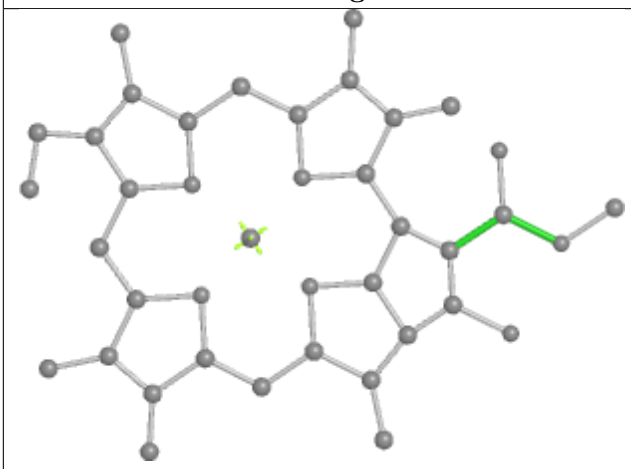
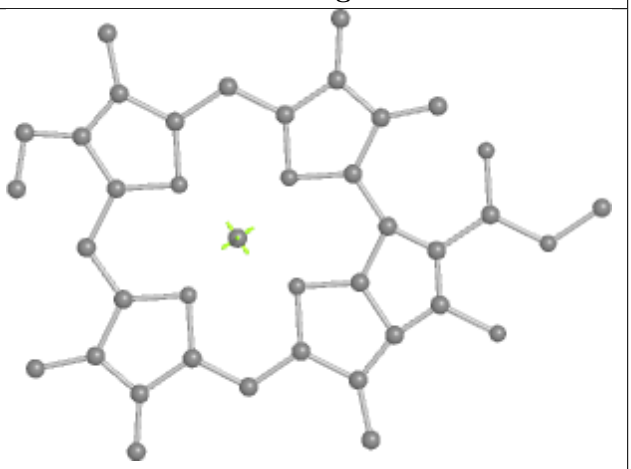


Rings

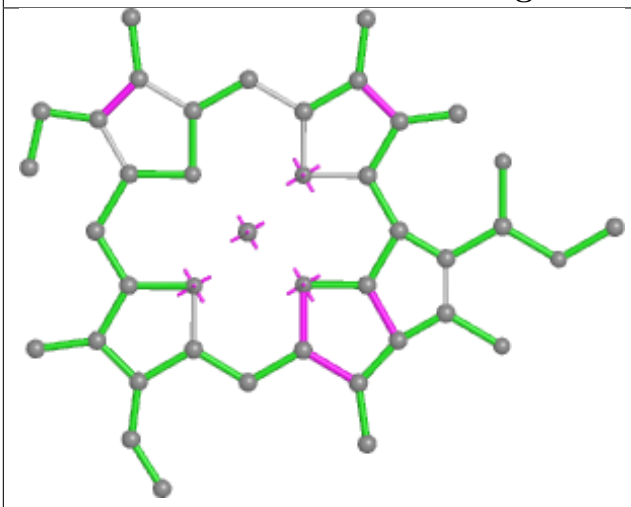
Ligand CLA A3 844



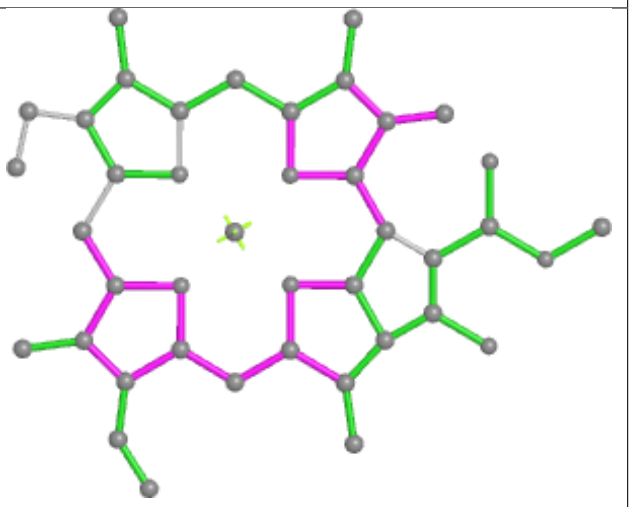
Ligand CLA A3 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

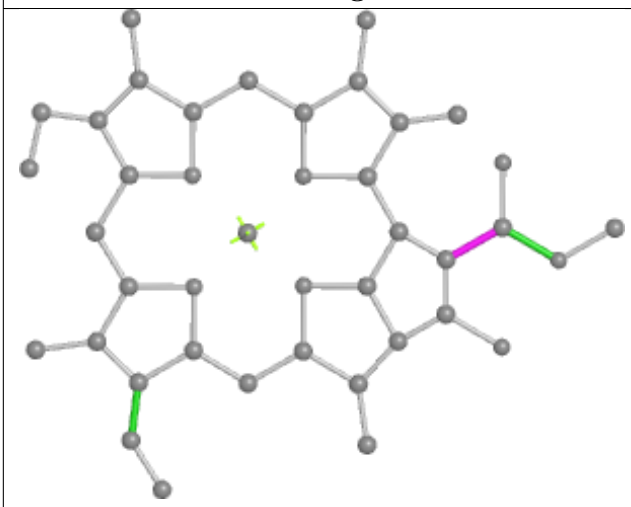
Ligand CLA B3 831



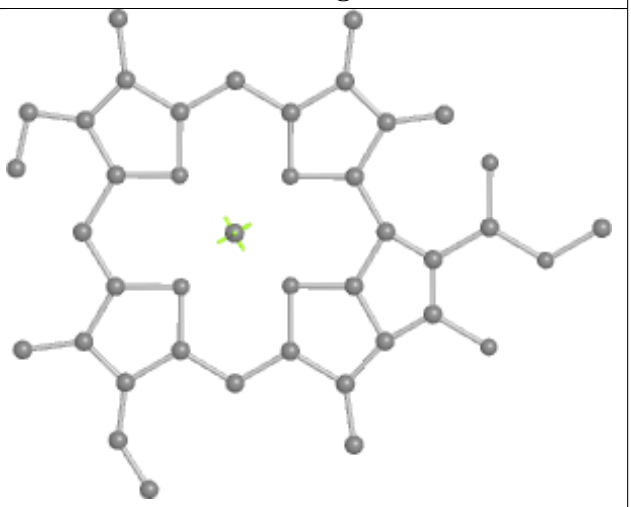
Bond lengths



Bond angles

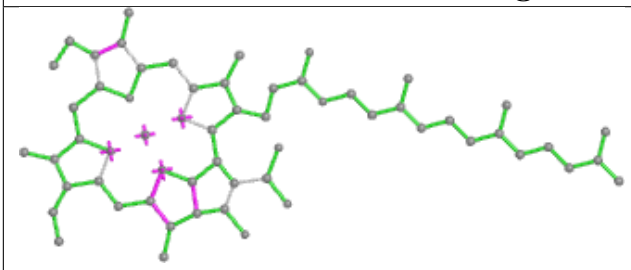


Torsions

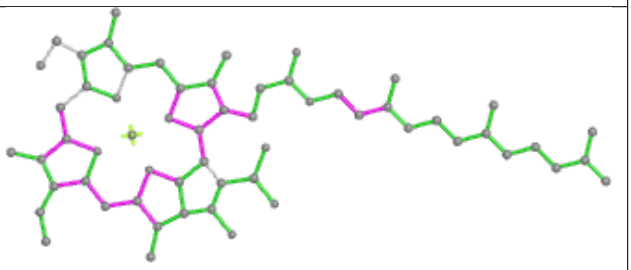


Rings

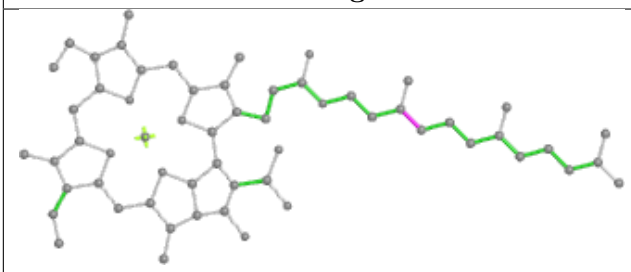
Ligand CLA A2 819



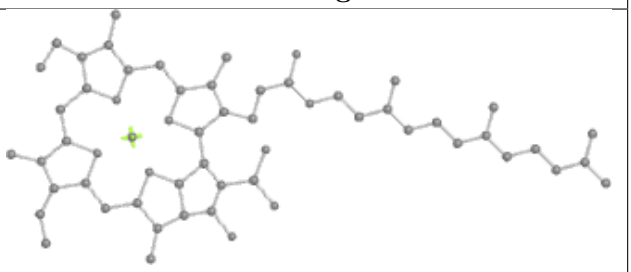
Bond lengths



Bond angles

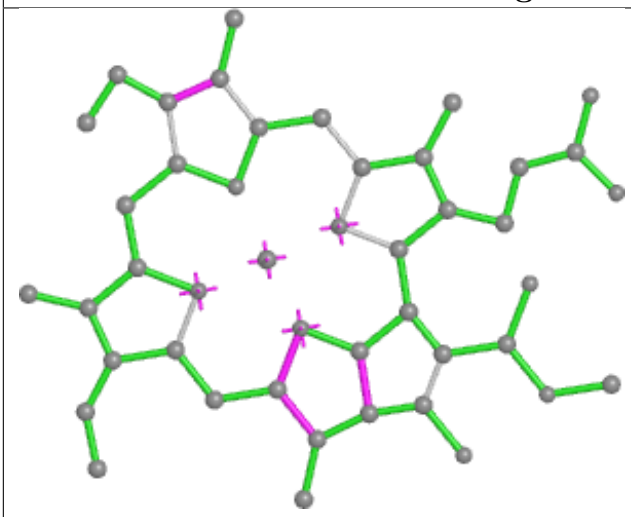


Torsions

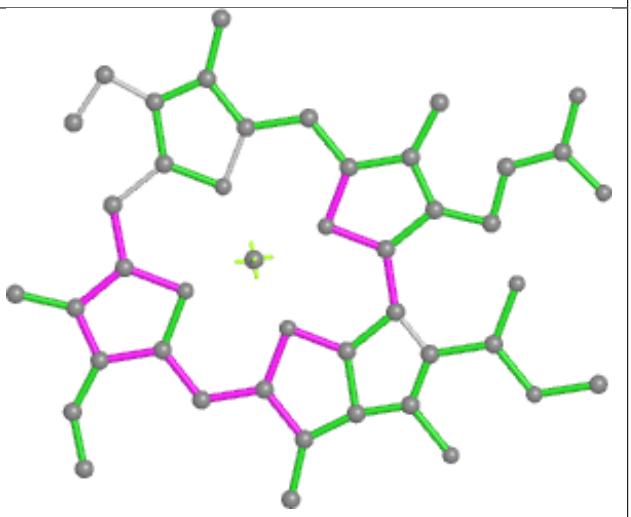


Rings

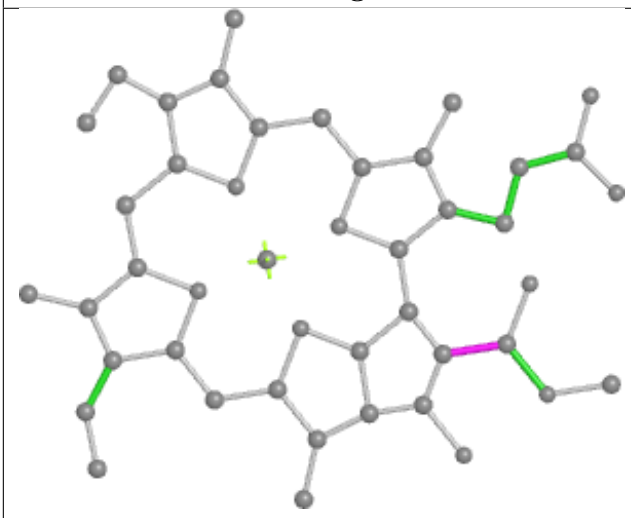
Ligand CLA B3 836



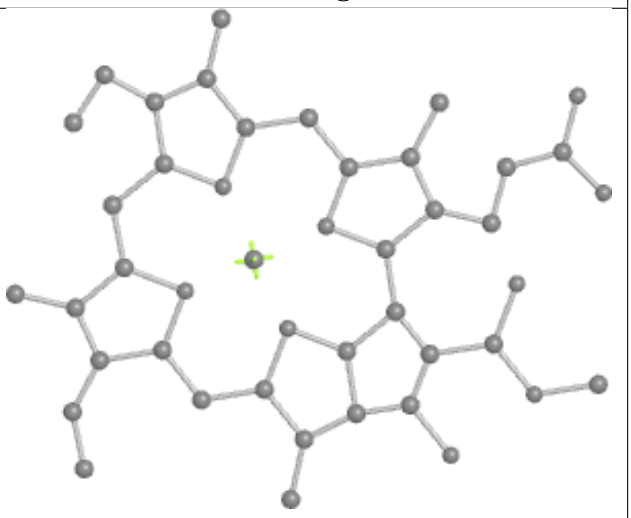
Bond lengths



Bond angles

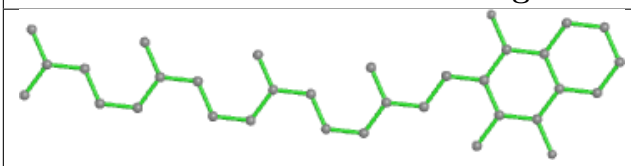


Torsions

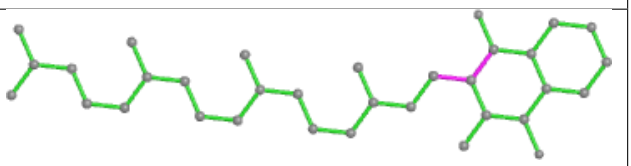


Rings

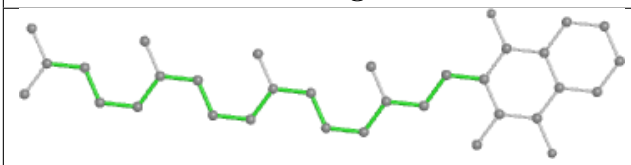
Ligand PQN A3 845



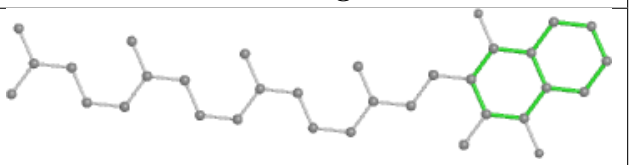
Bond lengths



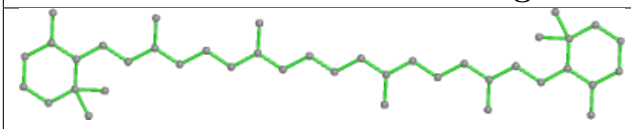
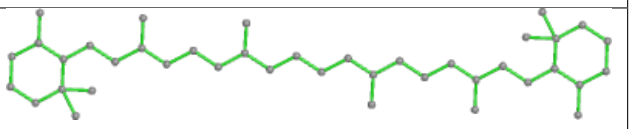
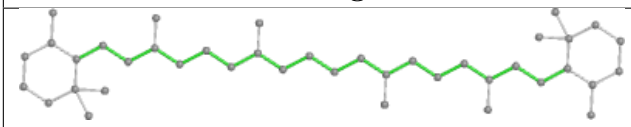
Bond angles

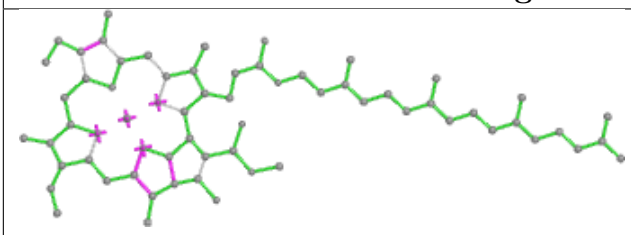
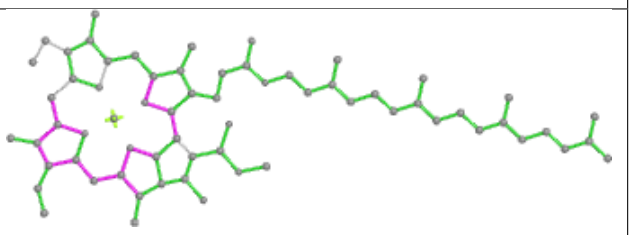
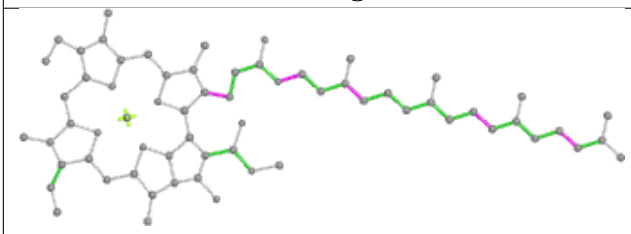
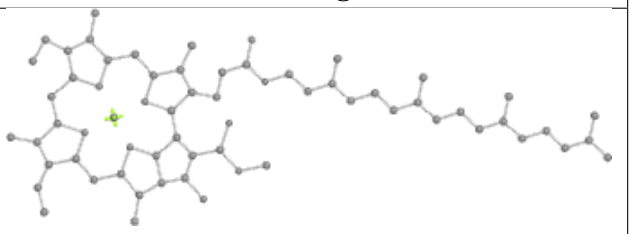


Torsions

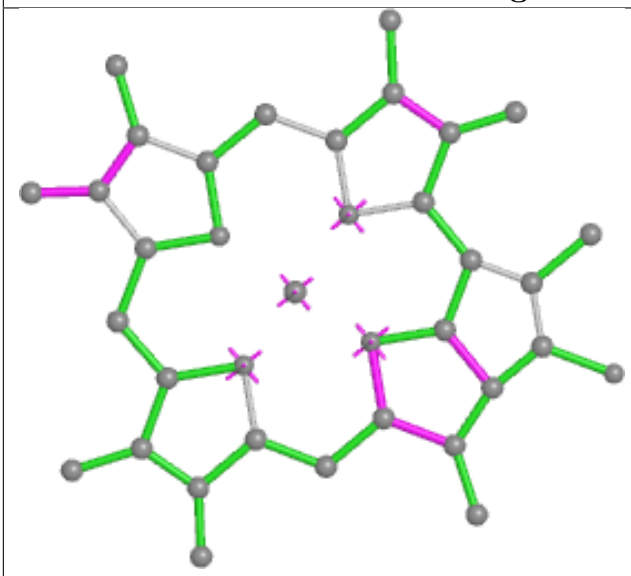


Rings

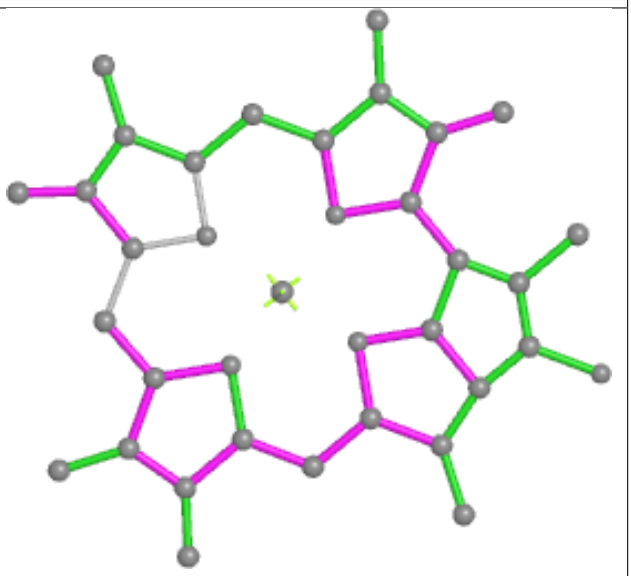
Ligand BCR B3 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

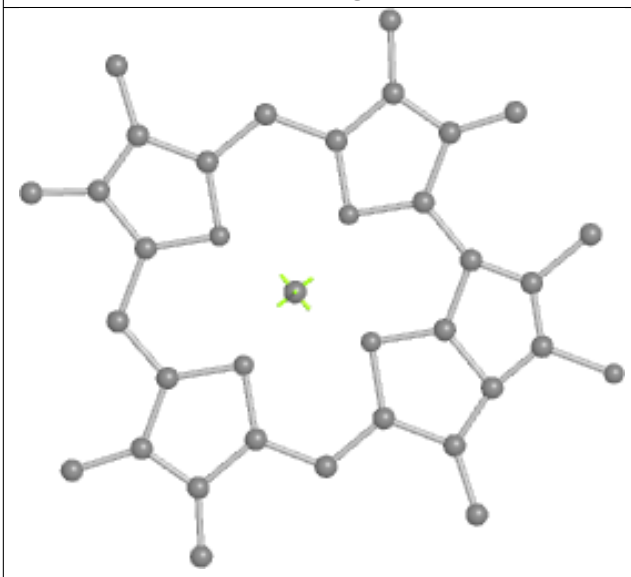
Ligand CLA J1 1303



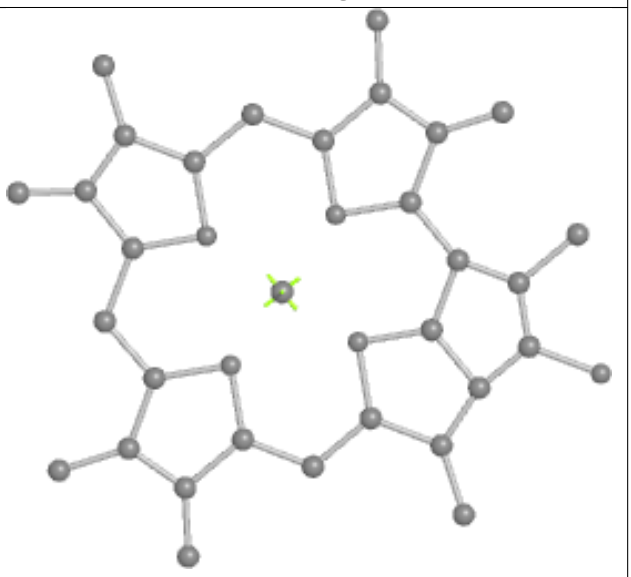
Bond lengths



Bond angles

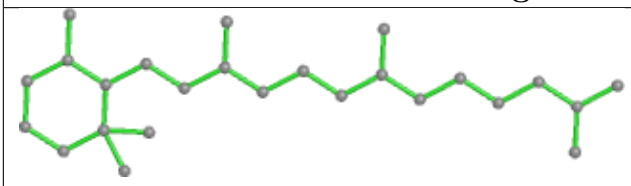


Torsions

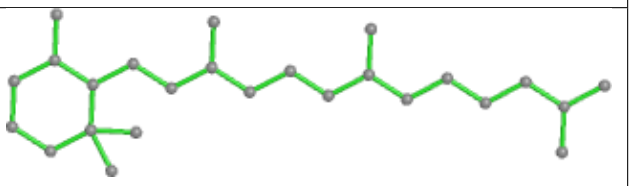


Rings

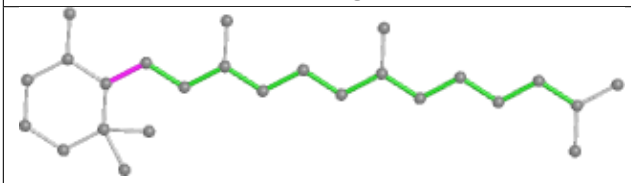
Ligand BCR K1 102



Bond lengths



Bond angles



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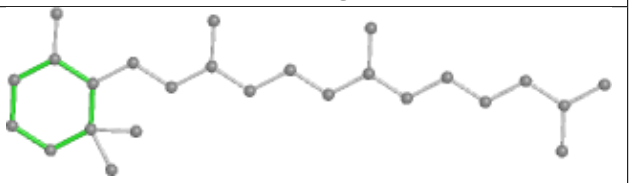
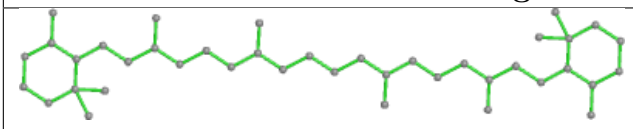
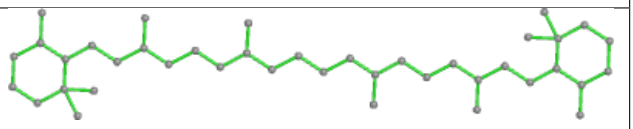


Rings

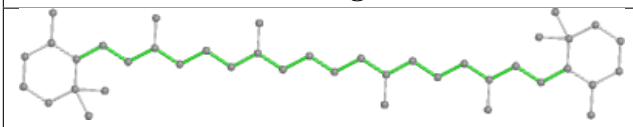
Ligand BCR A2 849



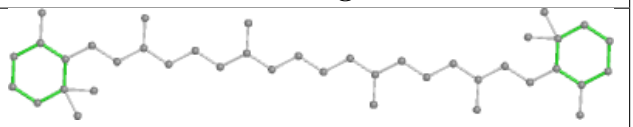
Bond lengths



Bond angles

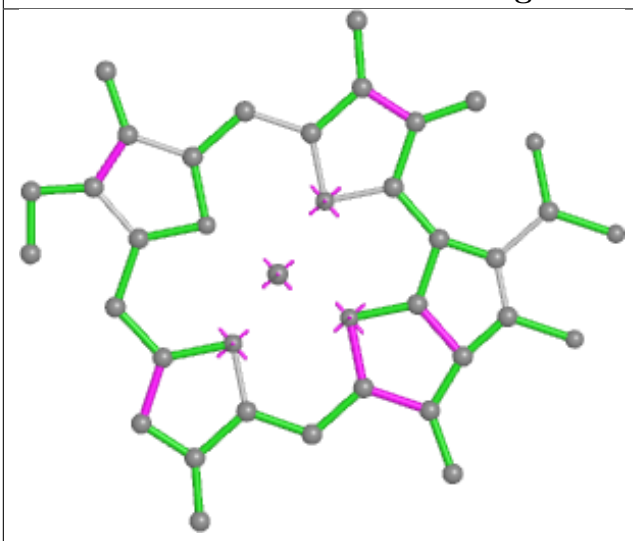


Torsions

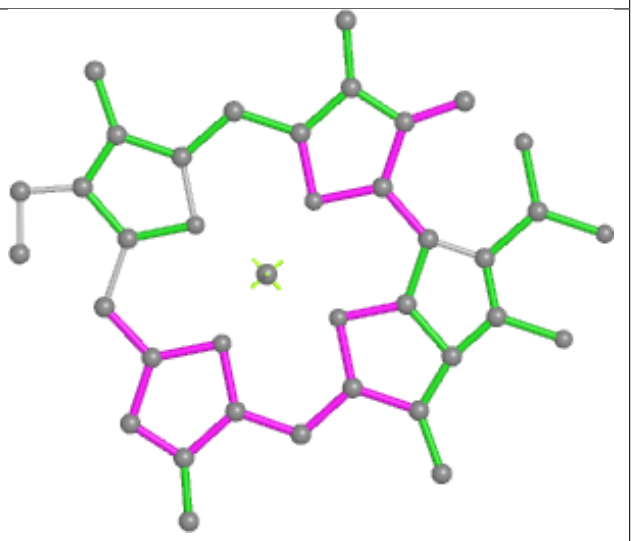


Rings

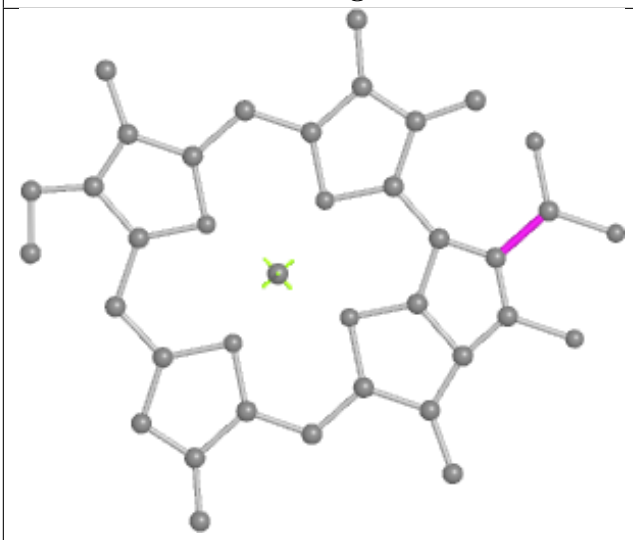
Ligand CLA A3 810



Bond lengths



Bond angles



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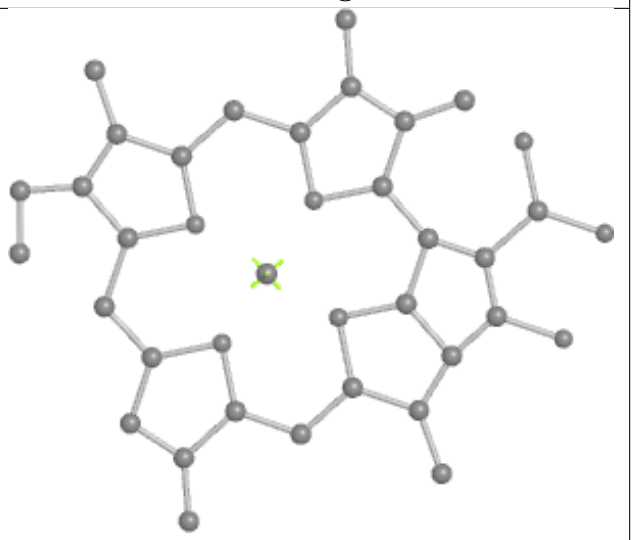
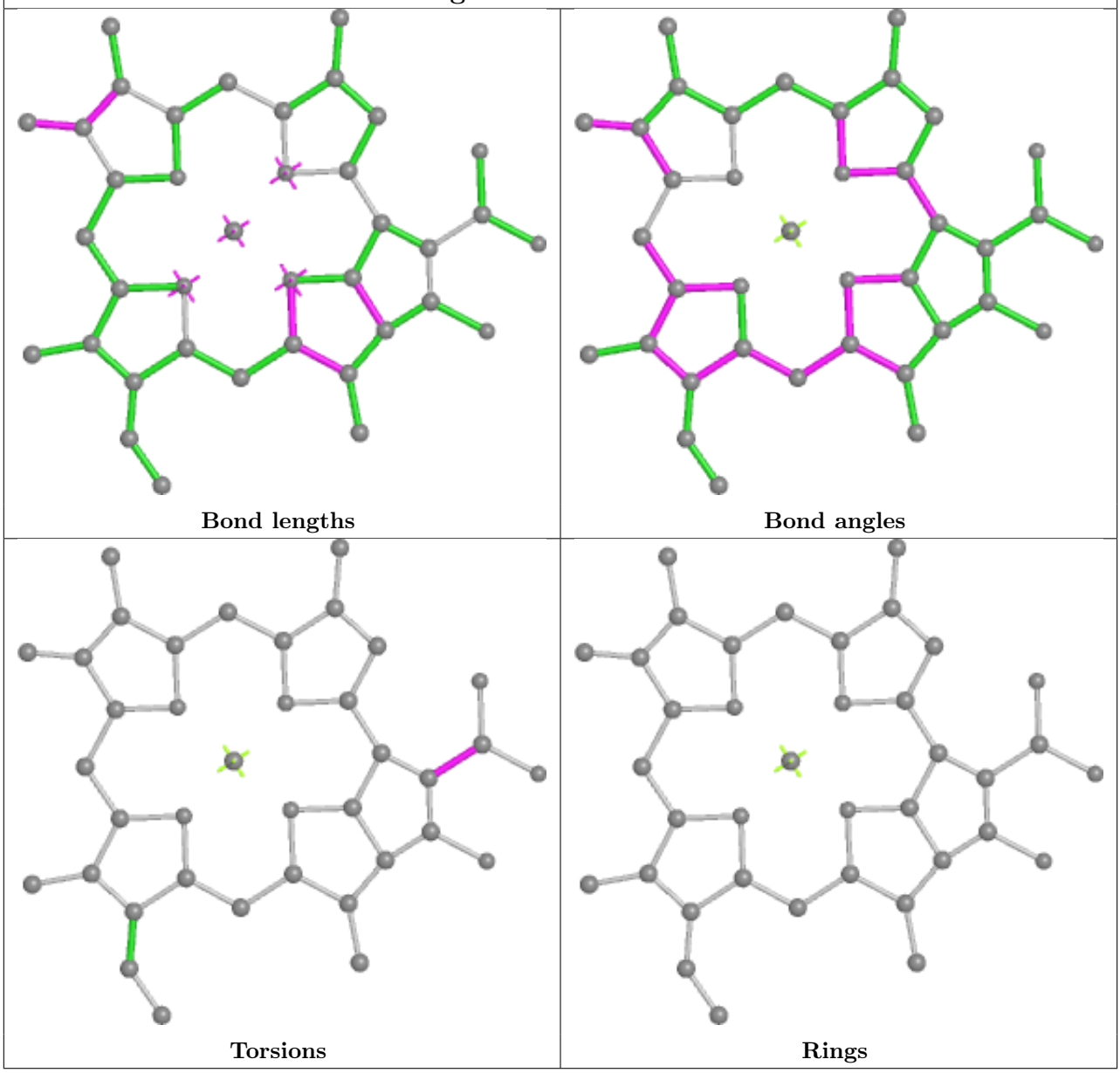
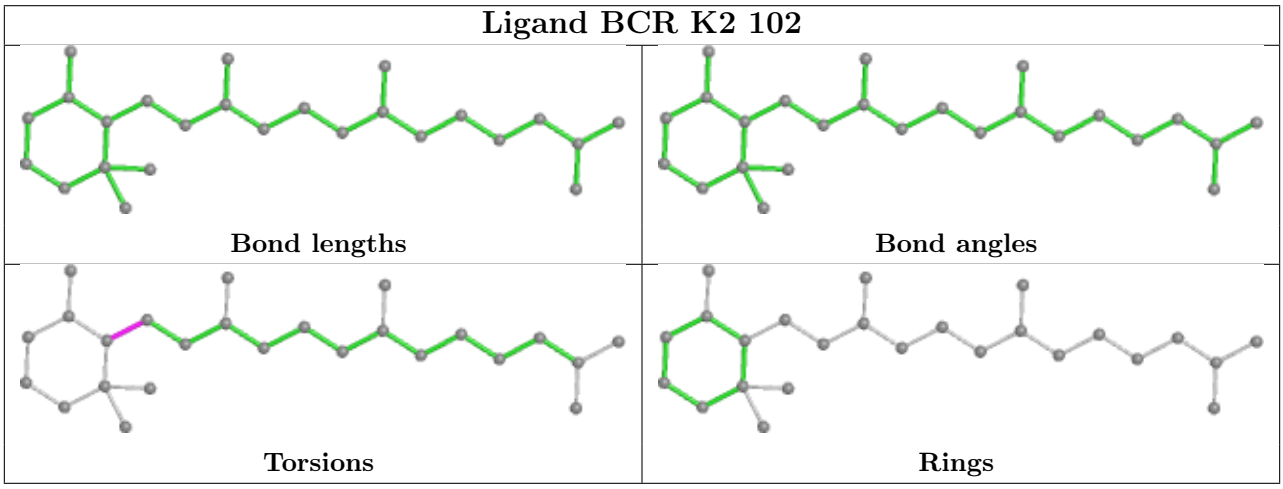


Rings

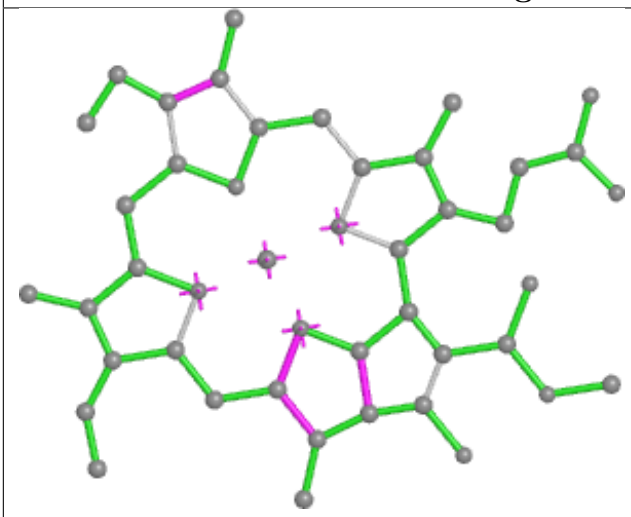
Ligand CLA A1 820



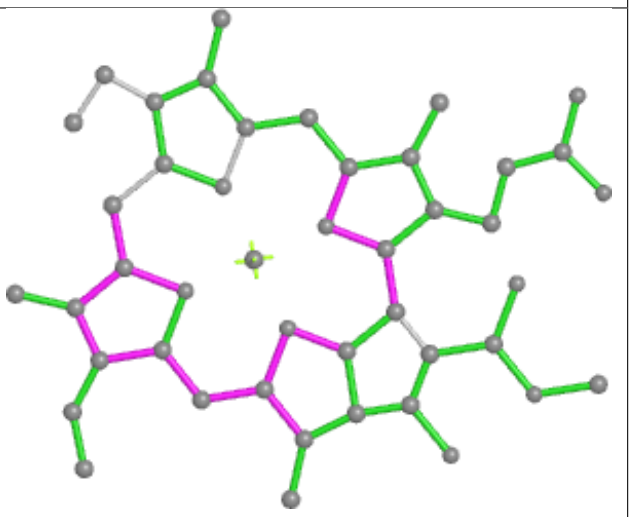
Ligand BCR K2 102



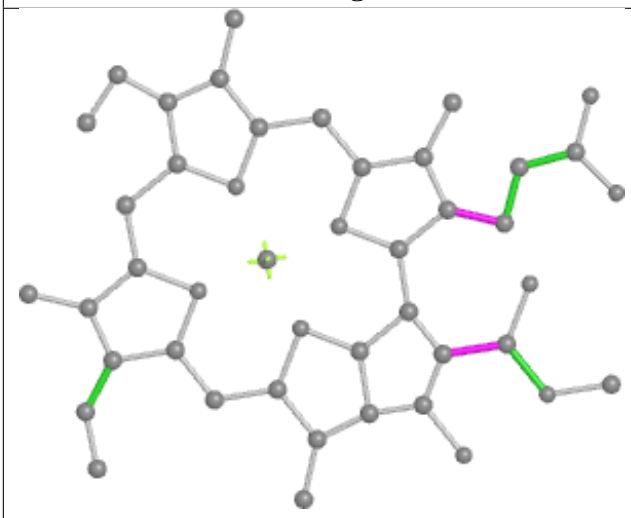
Ligand CLA A1 844



Bond lengths



Bond angles



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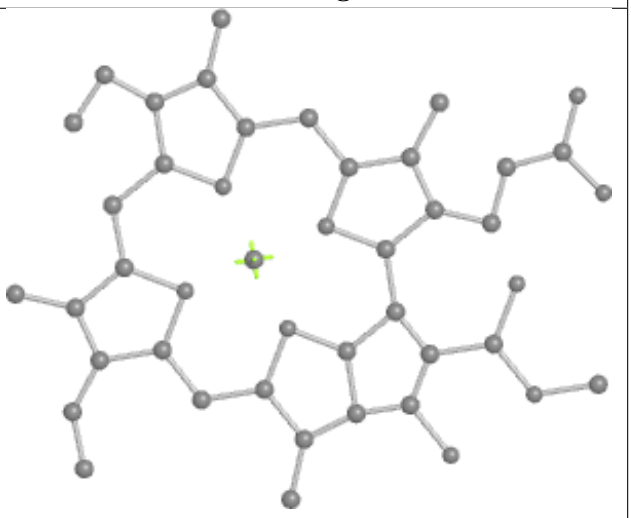
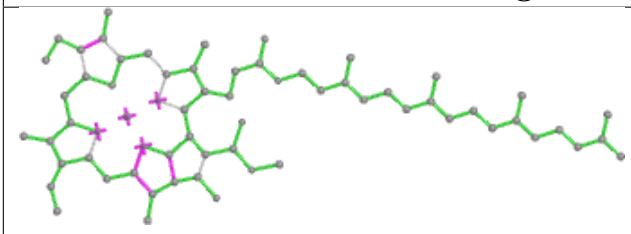


Rings

Ligand CLA B2 827



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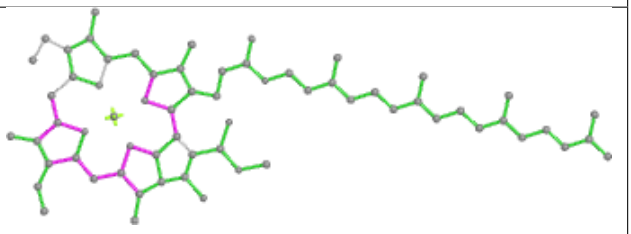
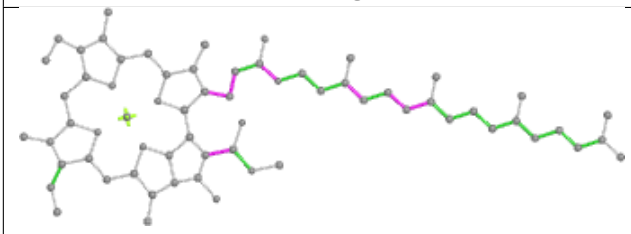


Bond angles



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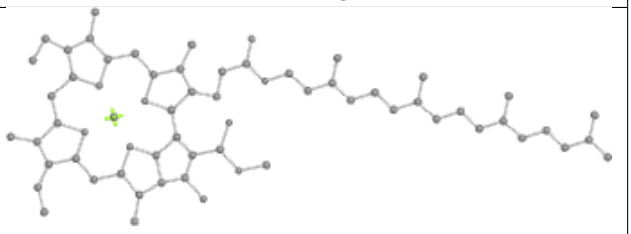
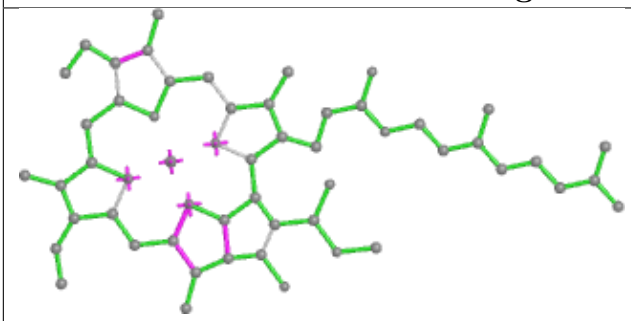


Rings

Ligand CLA B2 804



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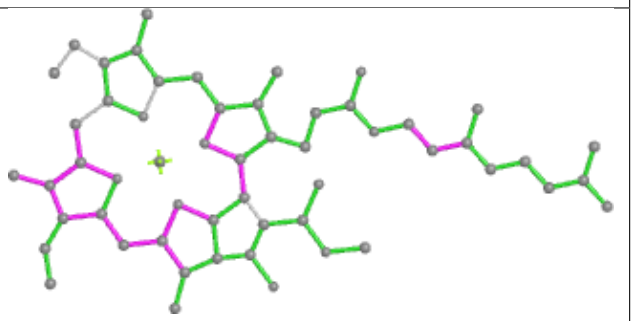
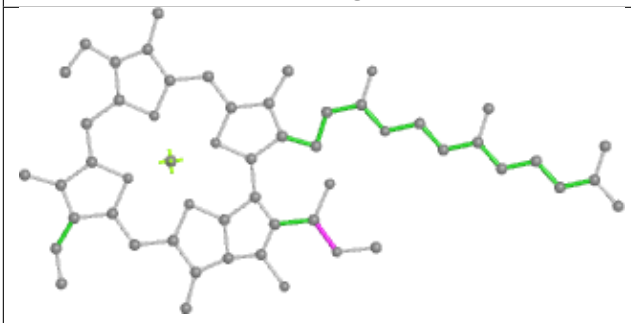


Bond angles



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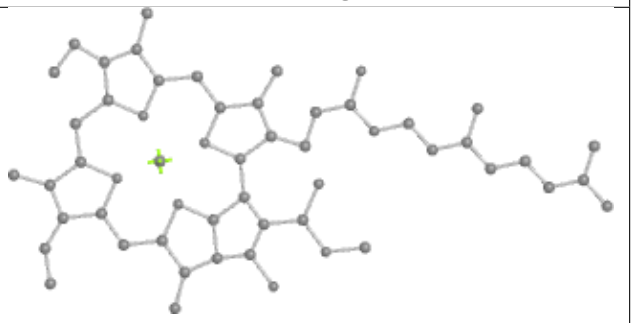
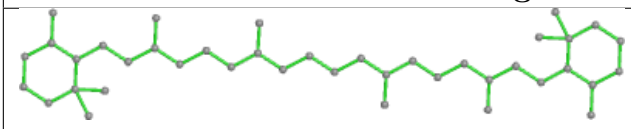


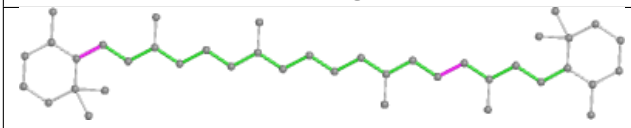
Rings

Ligand BCR B2 841



Bond lengths

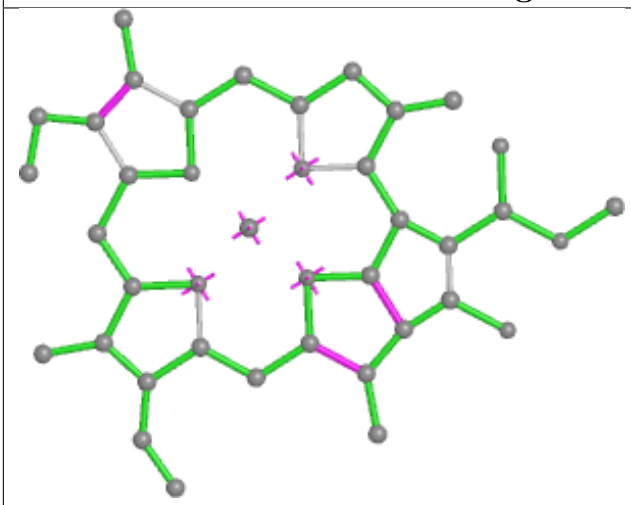
Bond angles



Torsions

Rings

Ligand CLA B1 832



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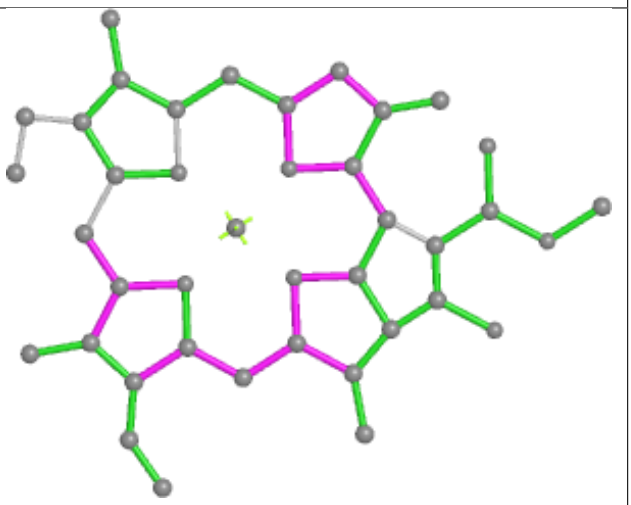
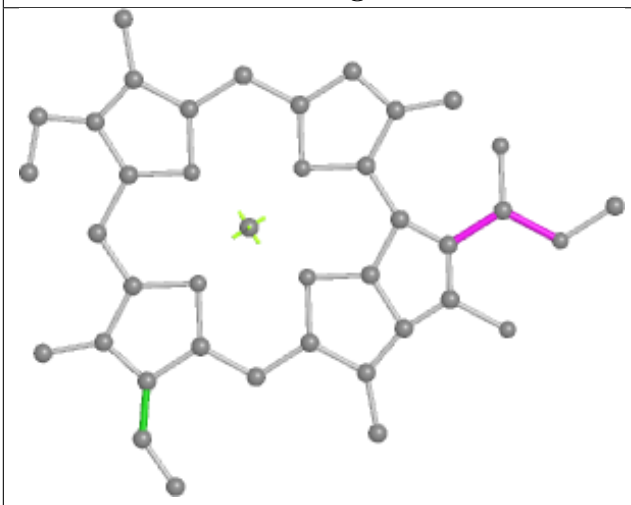


Bond angles



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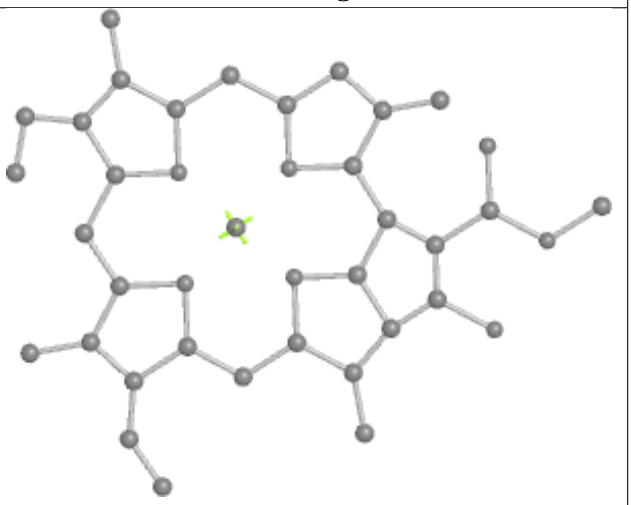
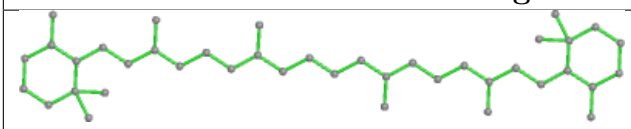


Rings

Ligand BCR A3 852



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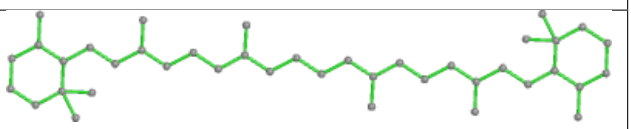

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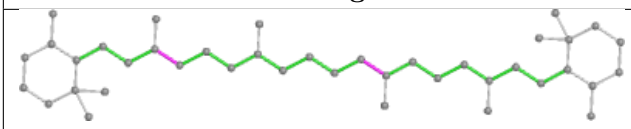
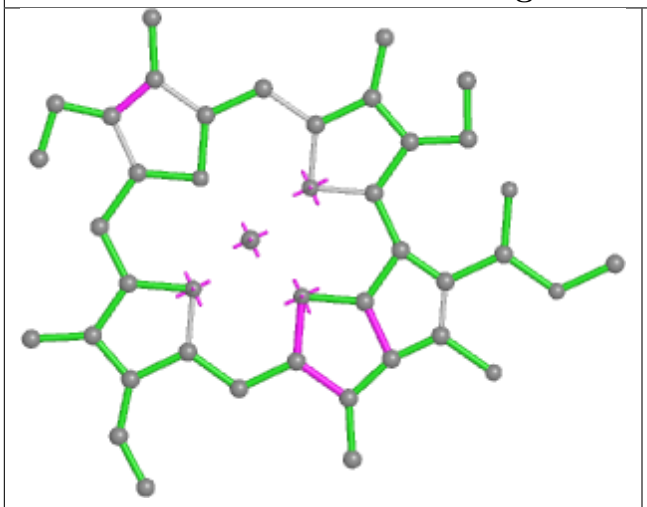


Torsions

Rings

Ligand CLA A2 828



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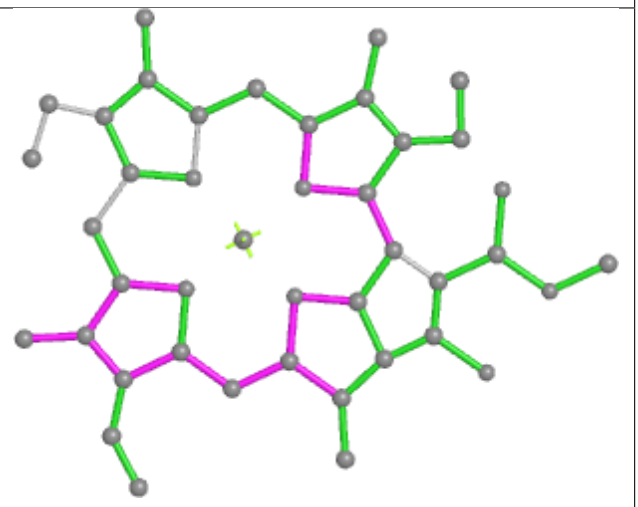
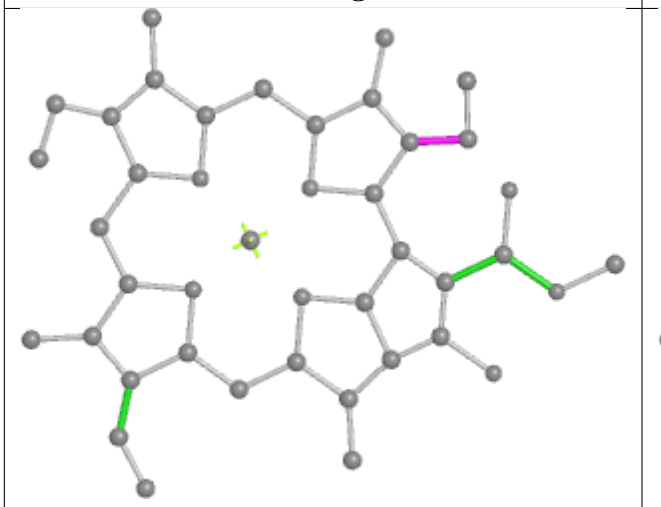


Bond angles



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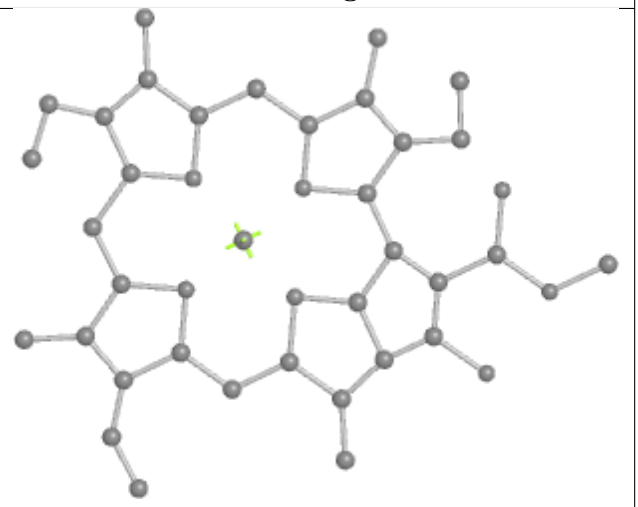
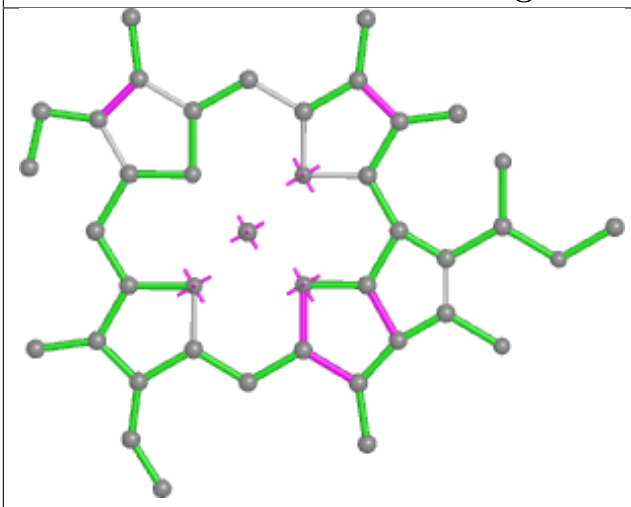


Rings

Ligand CLA B1 823



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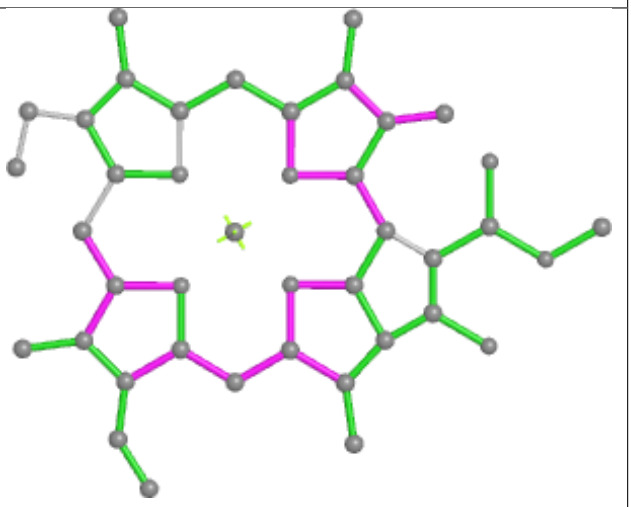
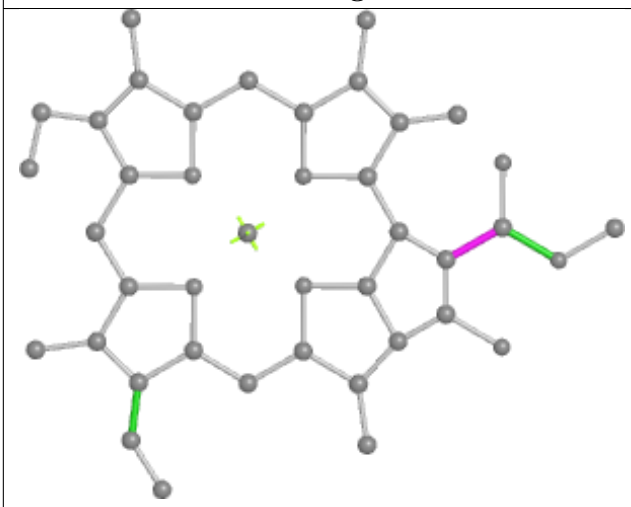


Bond angles



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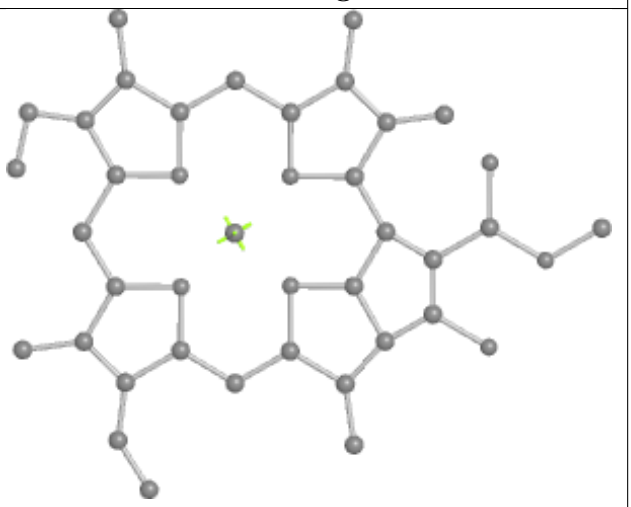
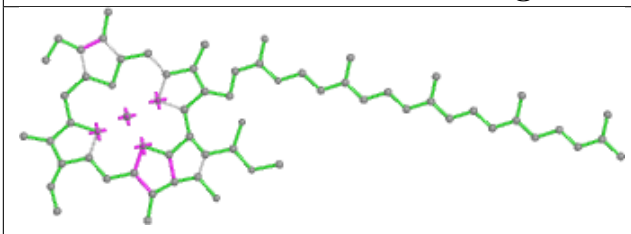
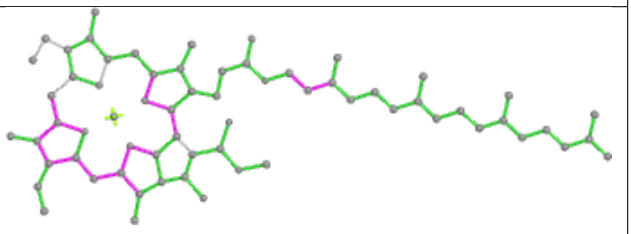


Rings

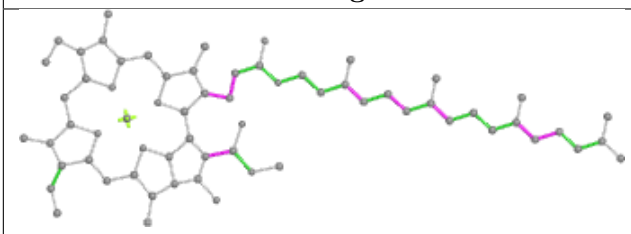
Ligand CLA A3 809



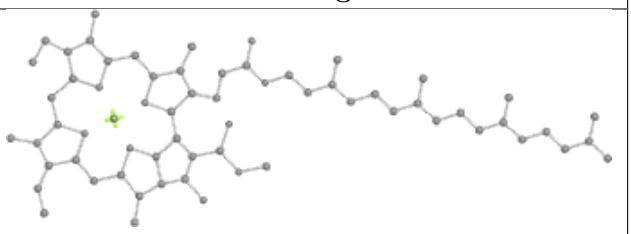
Bond lengths



Bond angles

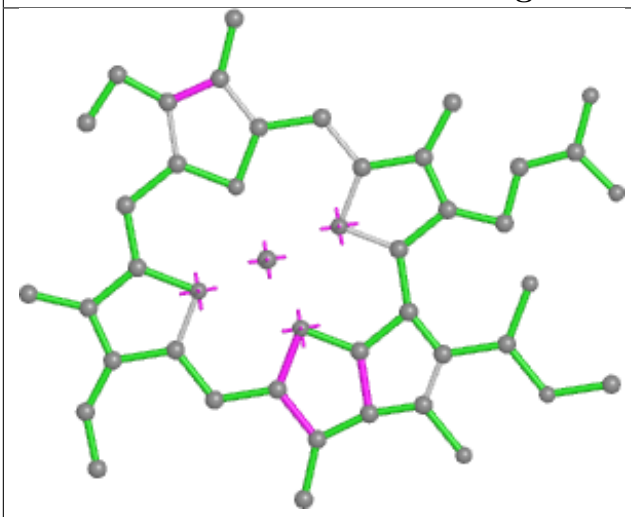


Torsions



Rings

Ligand CLA B2 836



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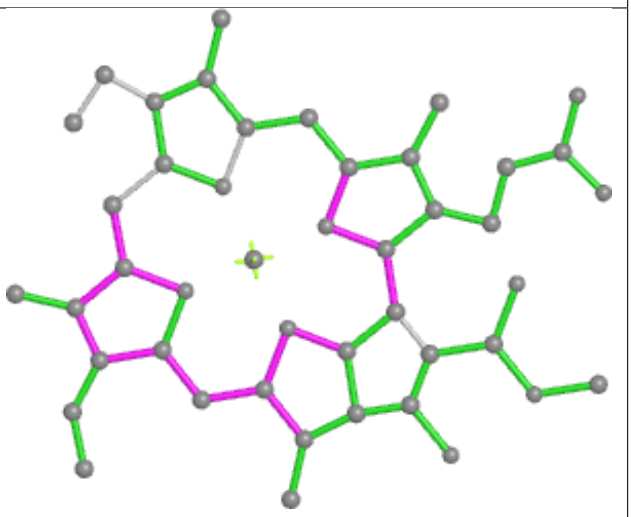
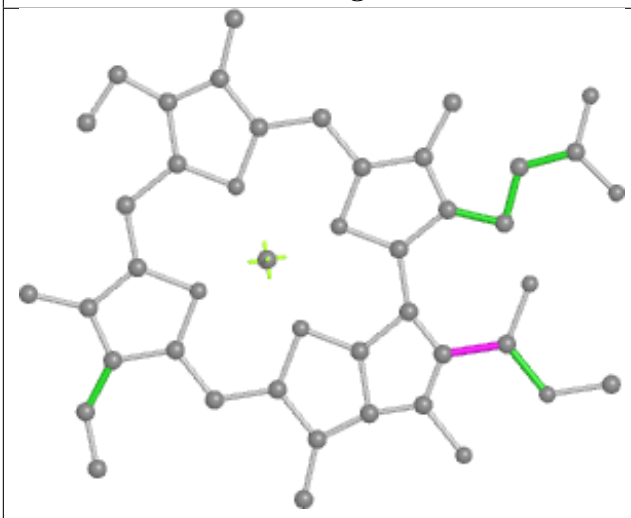


Bond angles



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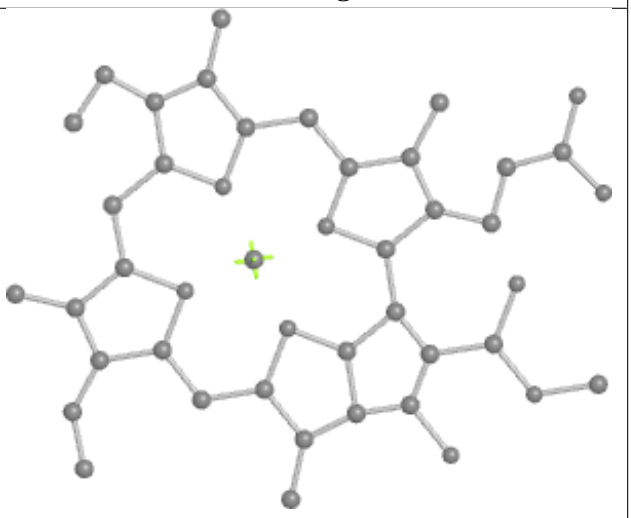
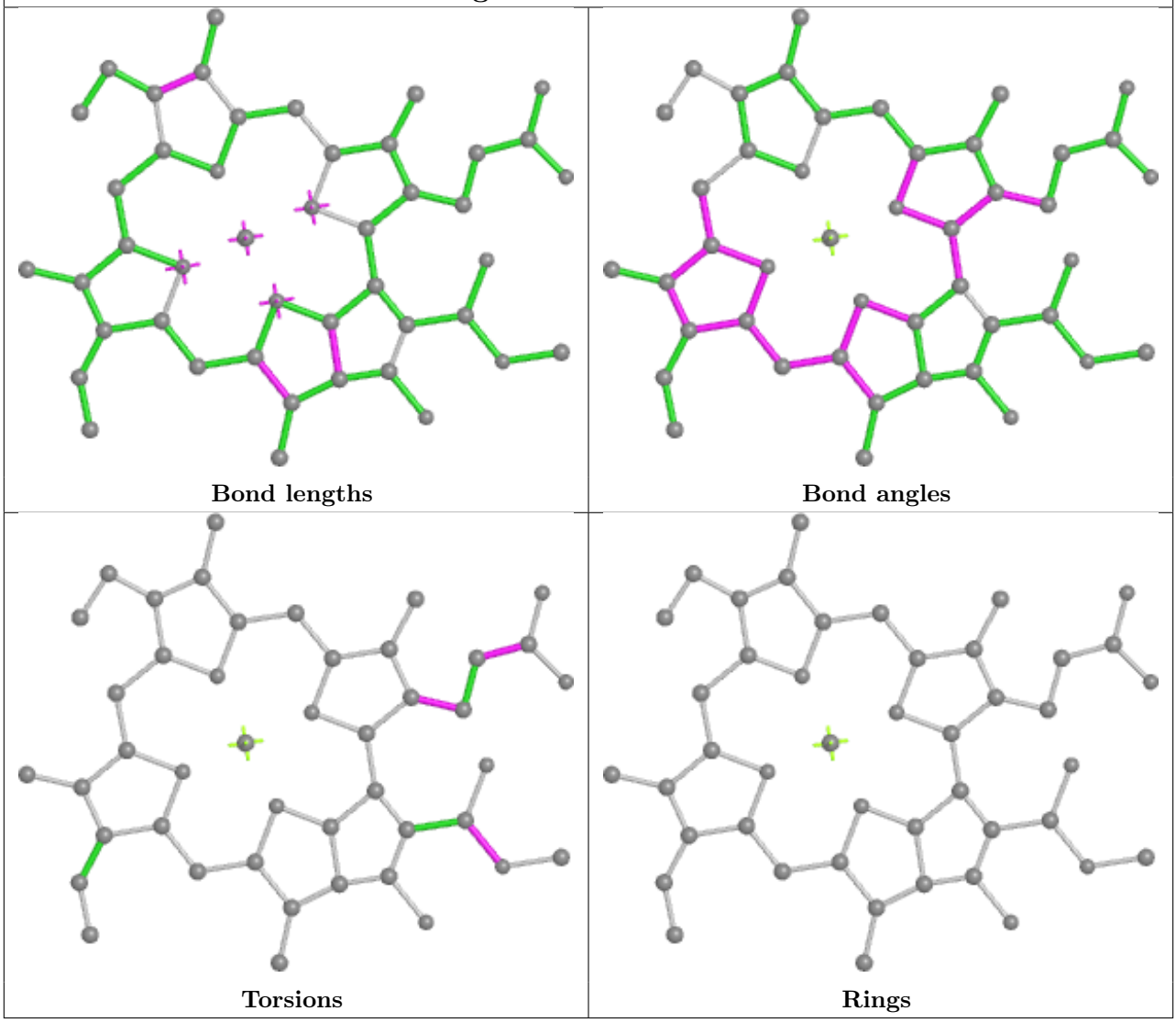
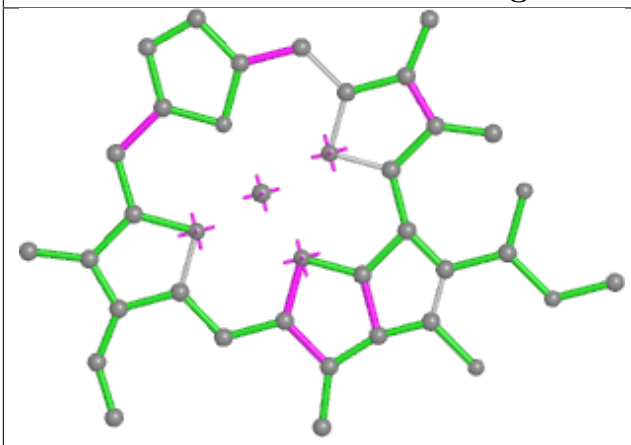
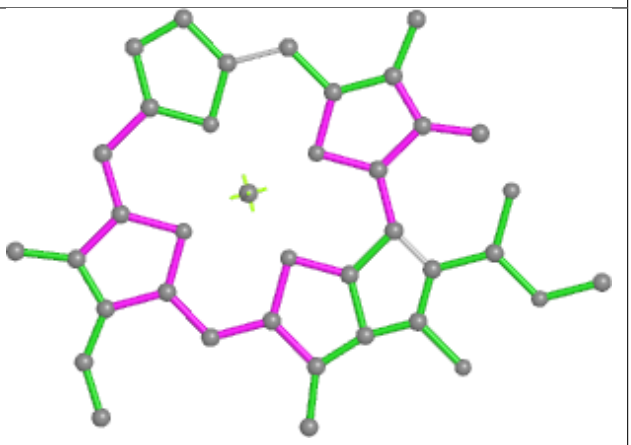
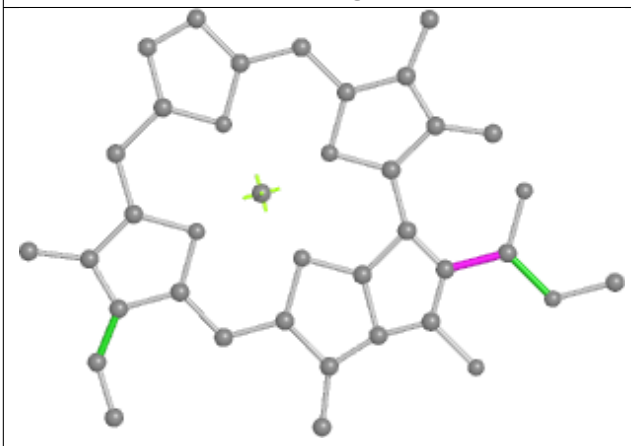
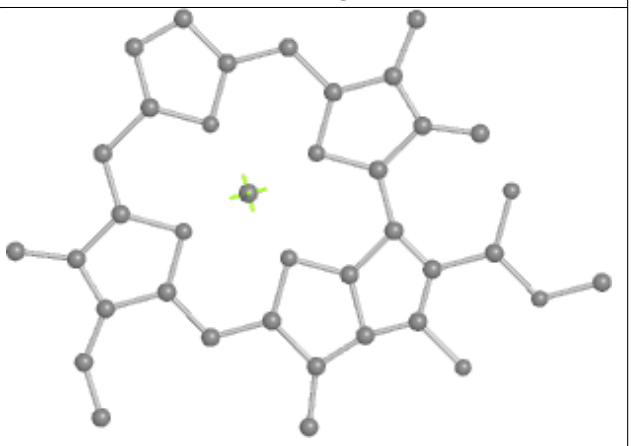


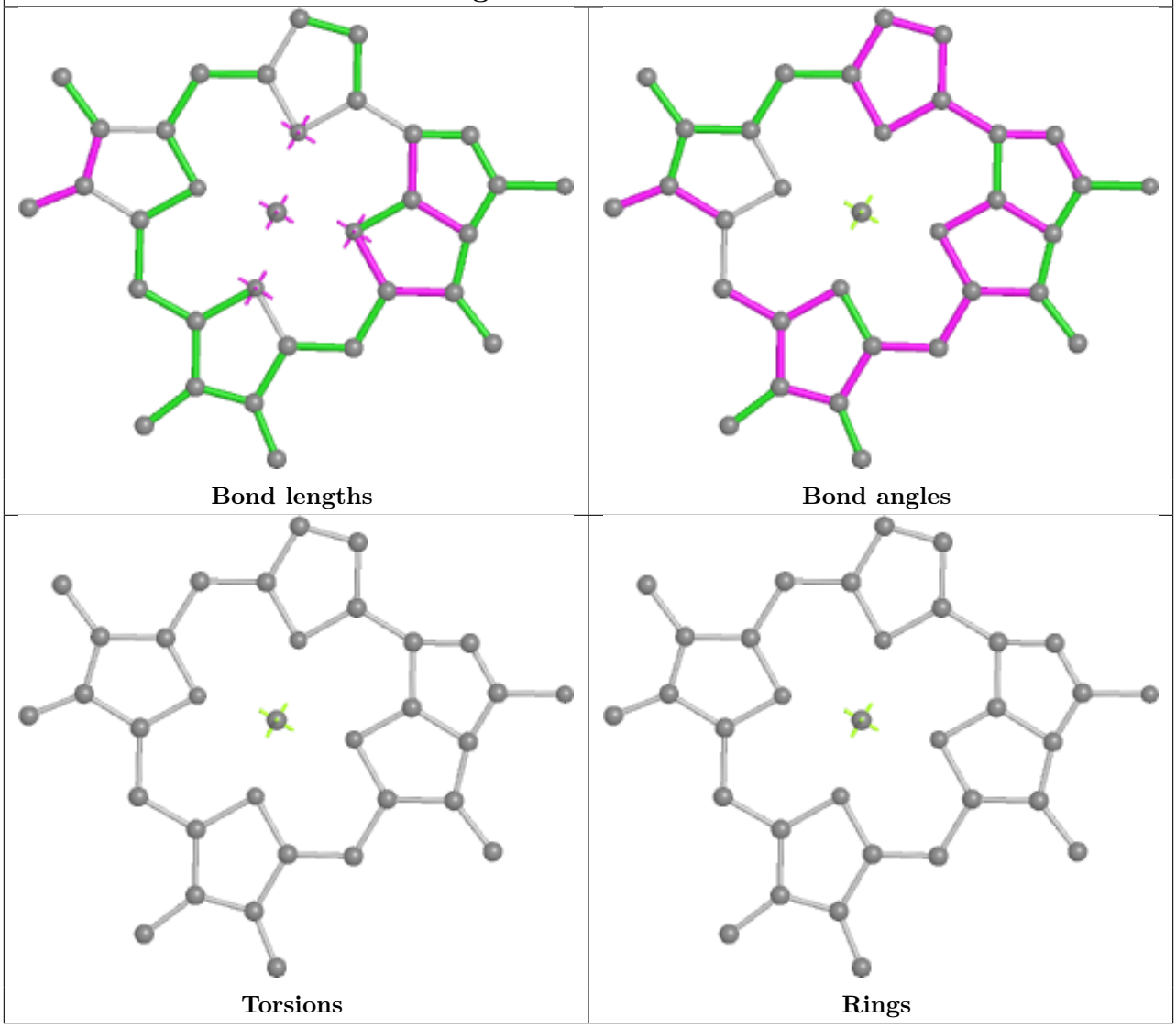
Rings

Ligand CLA A3 832

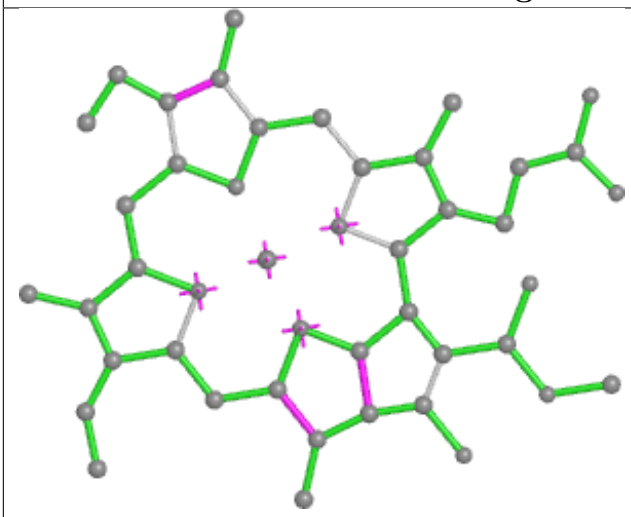


Ligand CLA J2 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

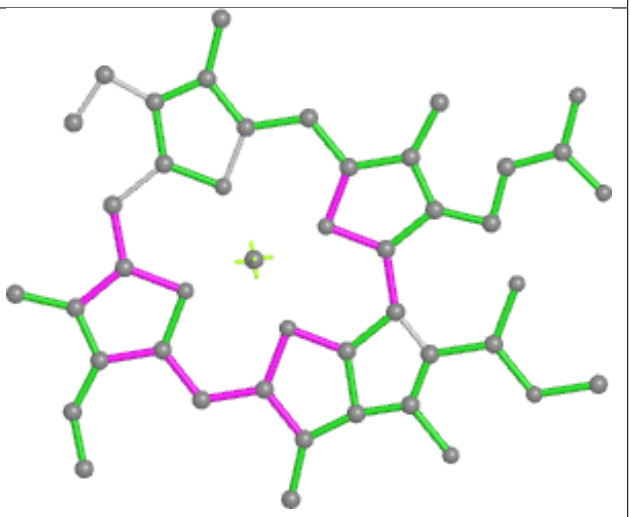
Ligand CLA A3 814



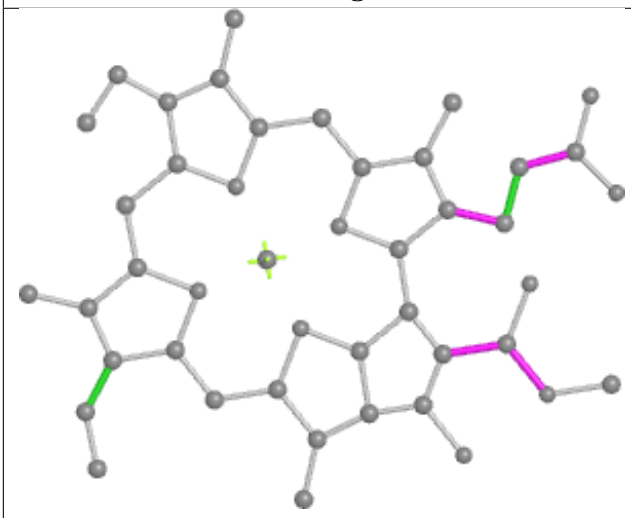
Ligand CLA B2 849



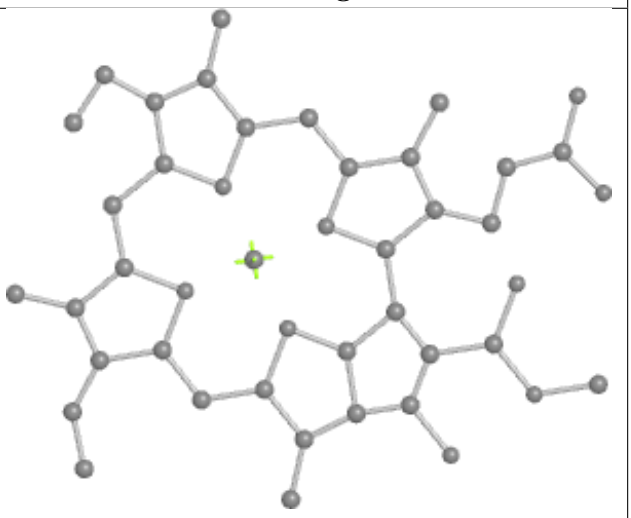
Bond lengths



Bond angles

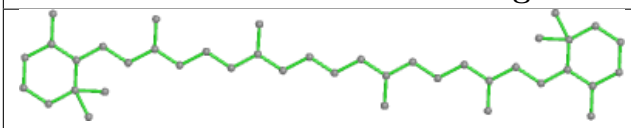


Torsions

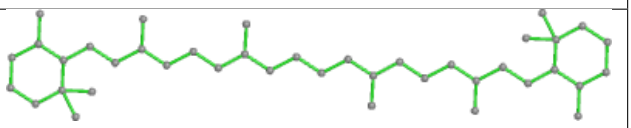


Rings

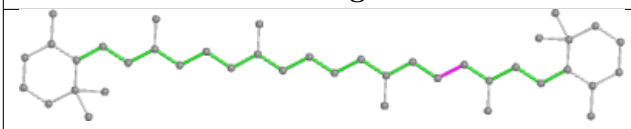
Ligand BCR A1 847



Bond lengths



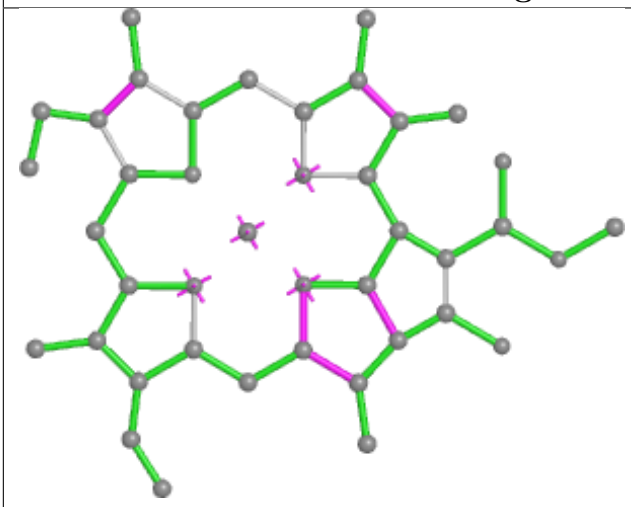
Bond angles



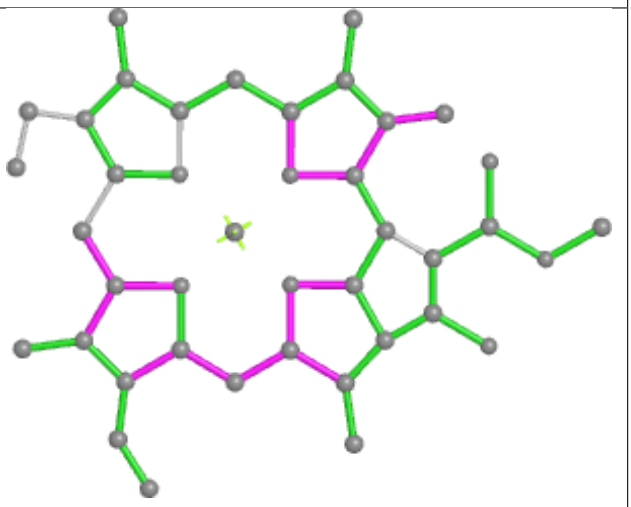
Torsions

Rings

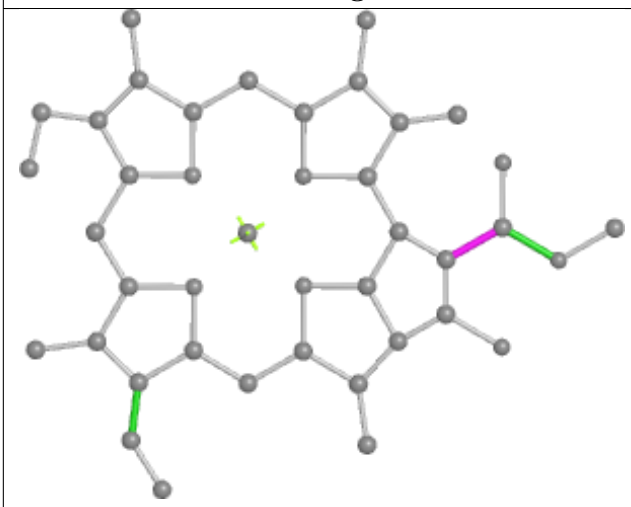
Ligand CLA A3 823



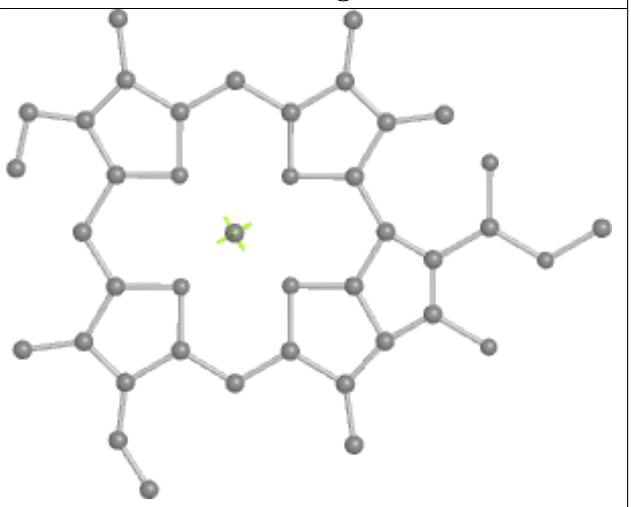
Bond lengths



Bond angles

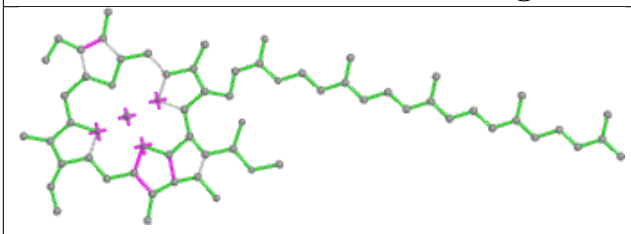


Torsions

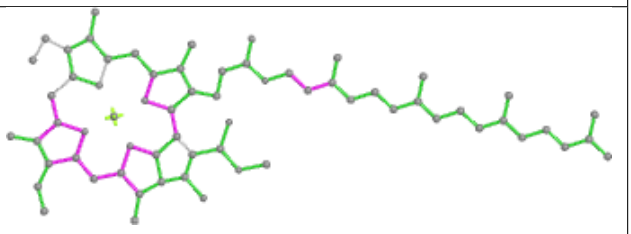


Rings

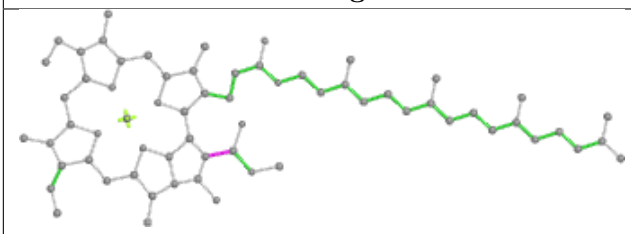
Ligand CLA B2 825



Bond lengths



Bond angles



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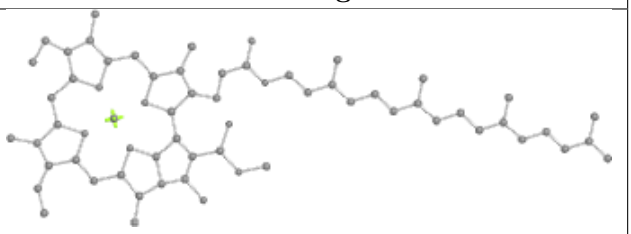
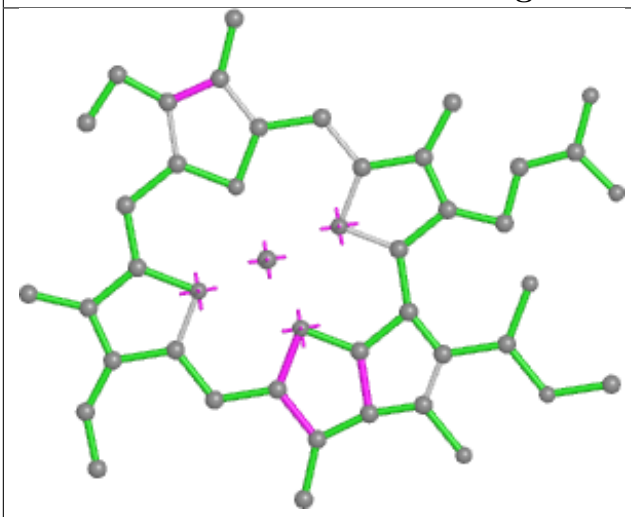


Rings

Ligand CLA B2 813



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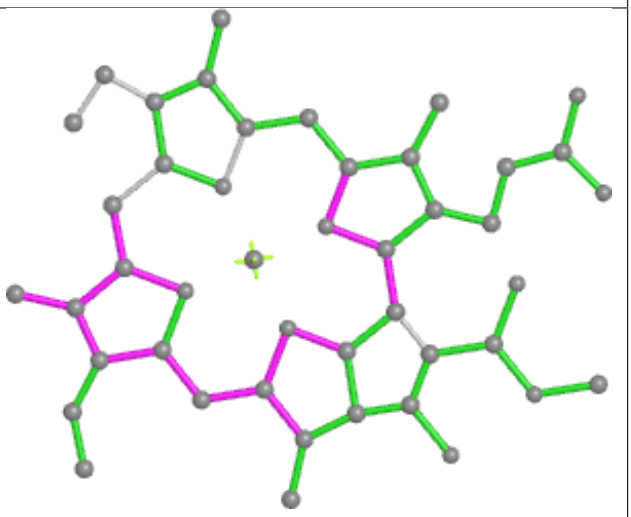
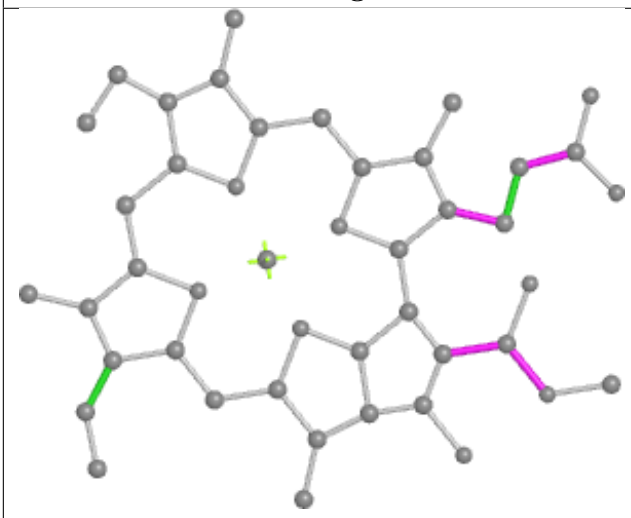
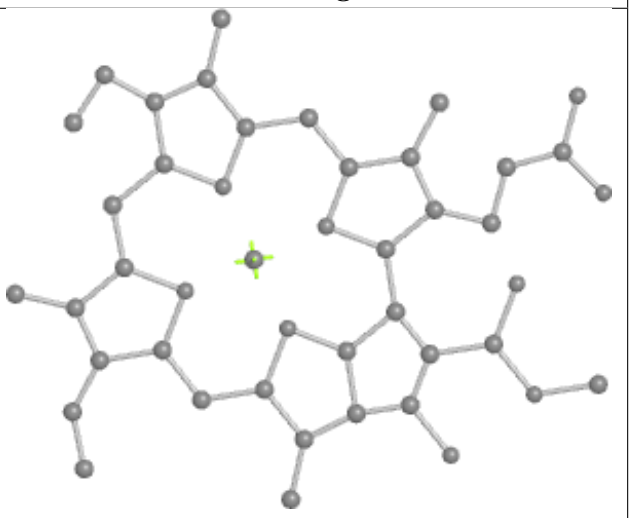


Bond angles

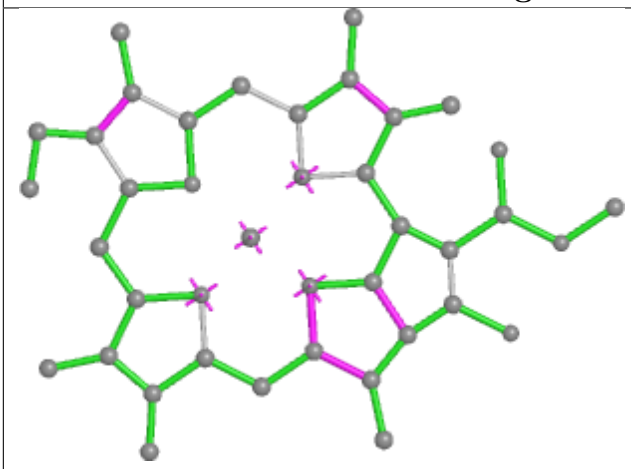


Torsions



Rings

Ligand CLA X1 102



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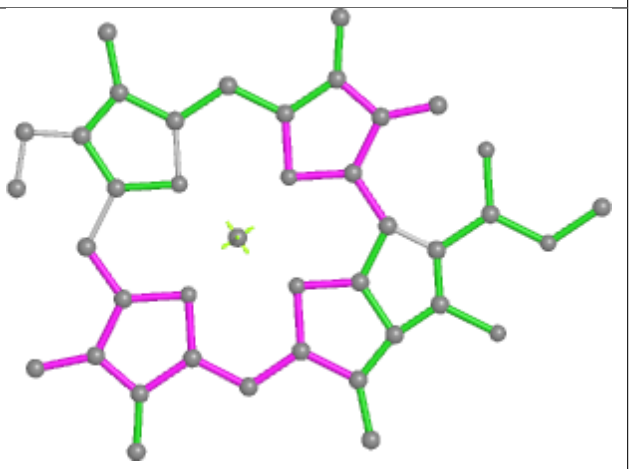
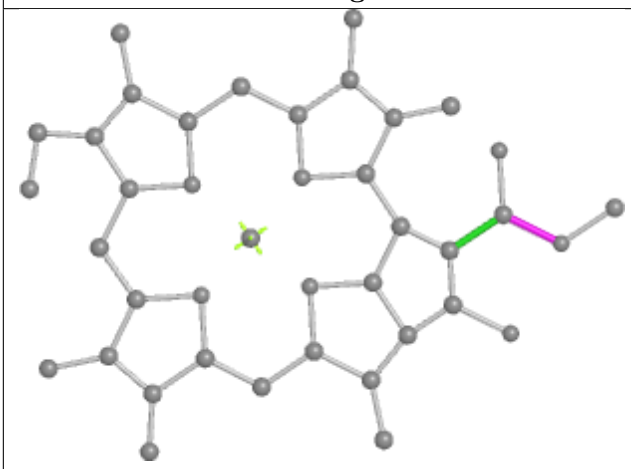


Bond angles



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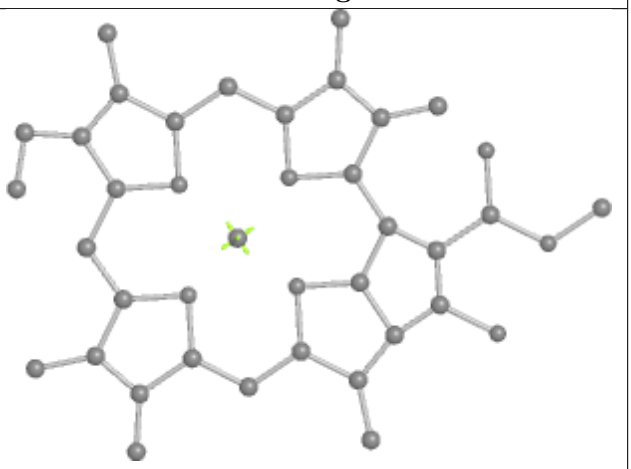
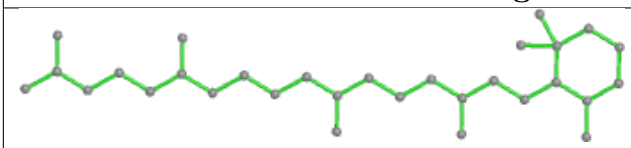


Rings

Ligand BCR A3 855



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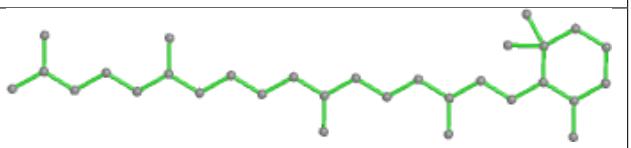
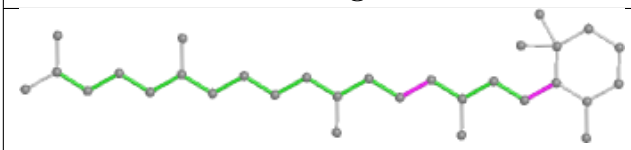


Bond angles



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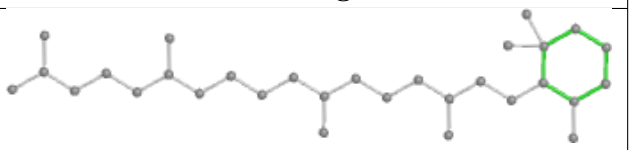
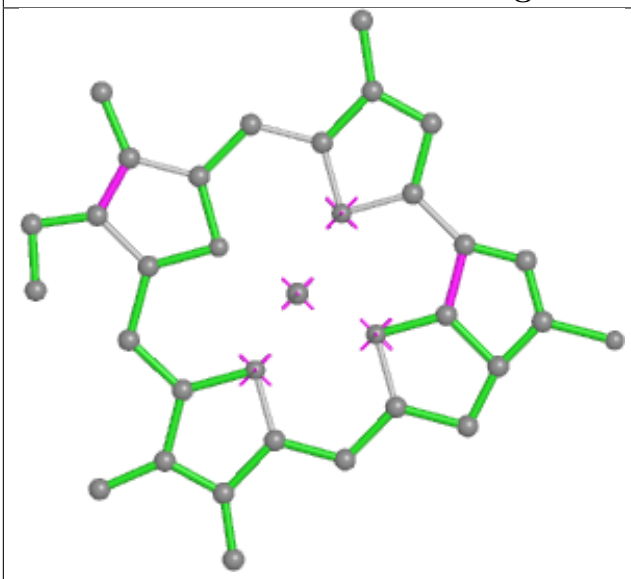


Rings

Ligand CLA K2 101



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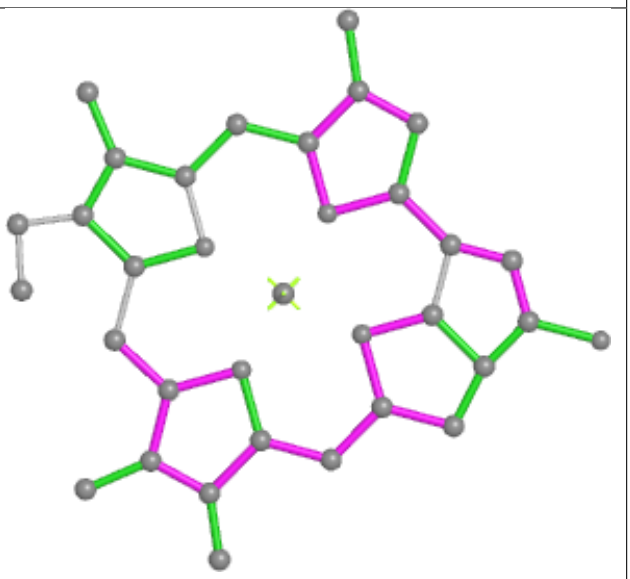
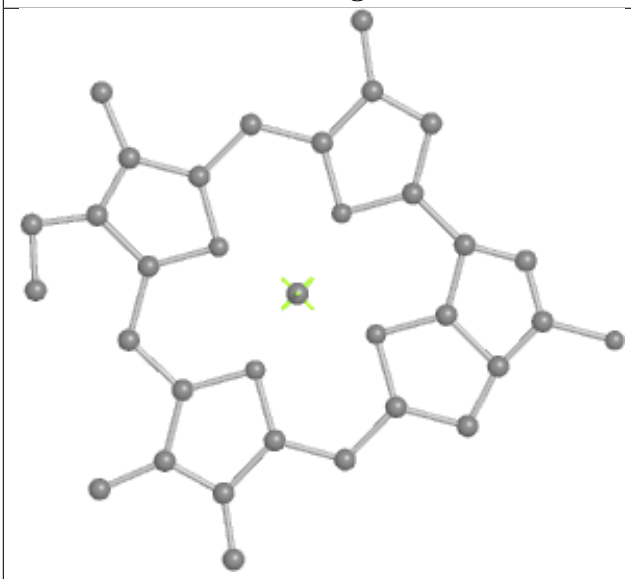


Bond angles



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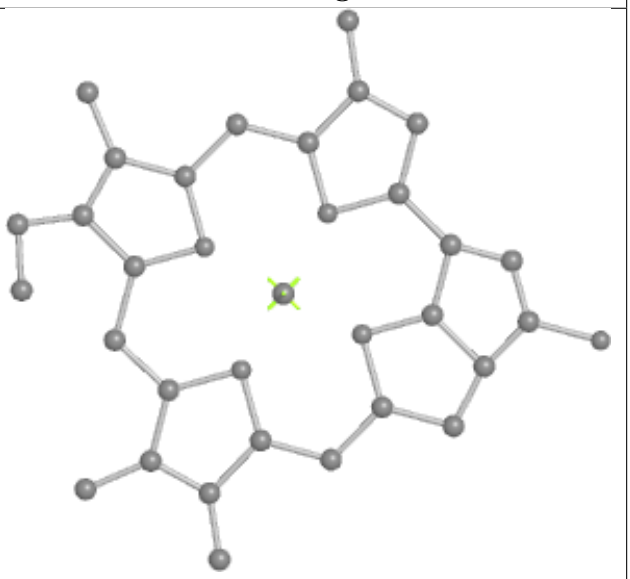
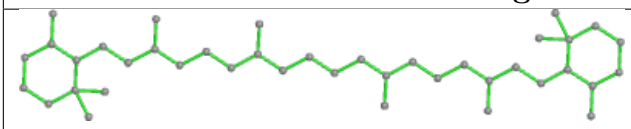


Rings

Ligand BCR A1 851



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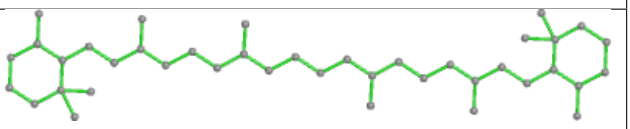
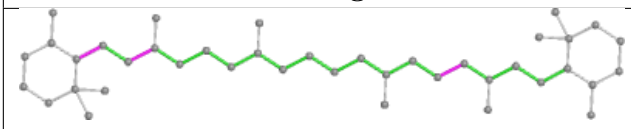
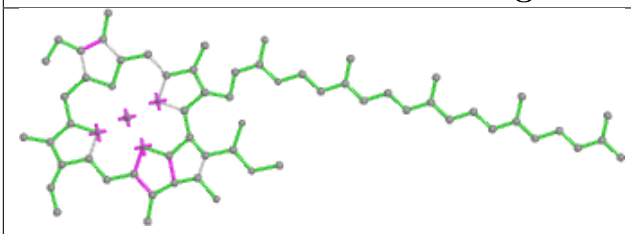
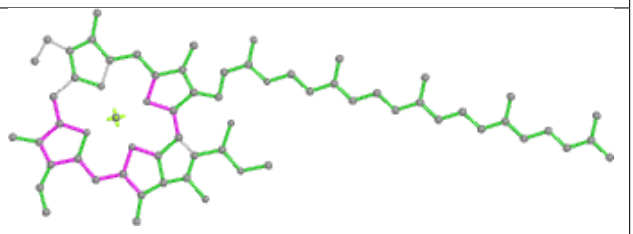
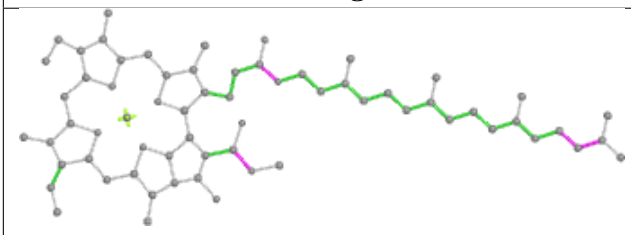
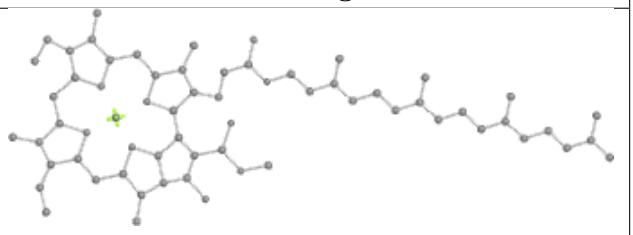


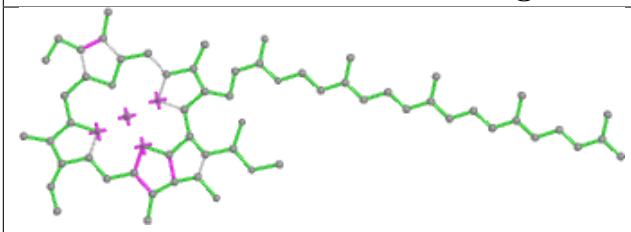
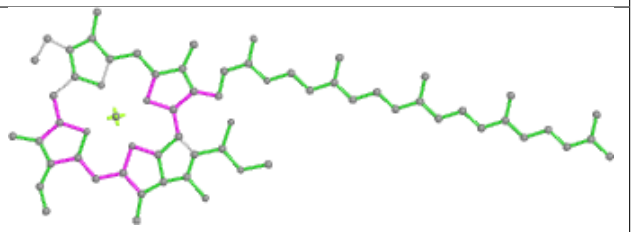
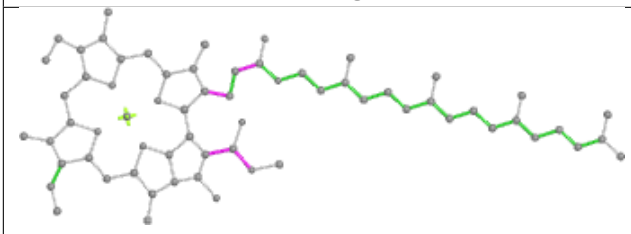
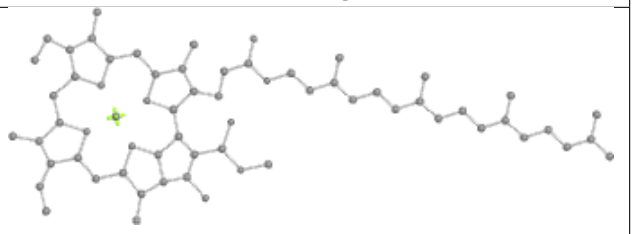
Bond angles



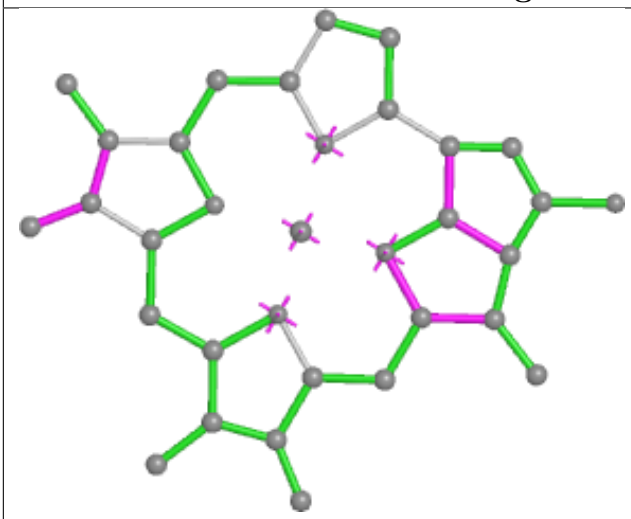
Torsions

Rings

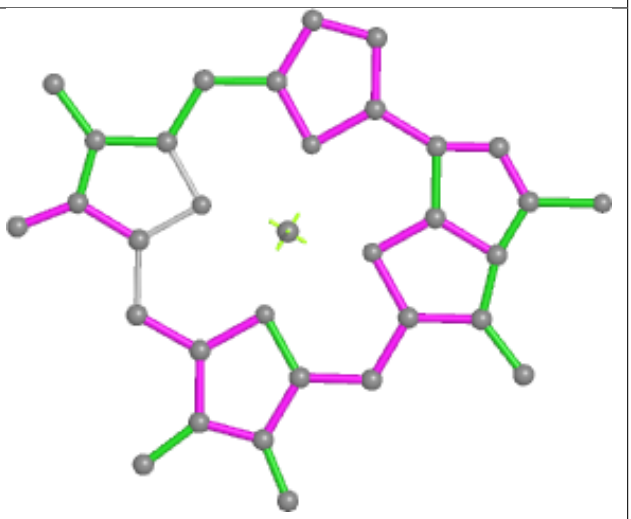
Ligand CLA B2 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

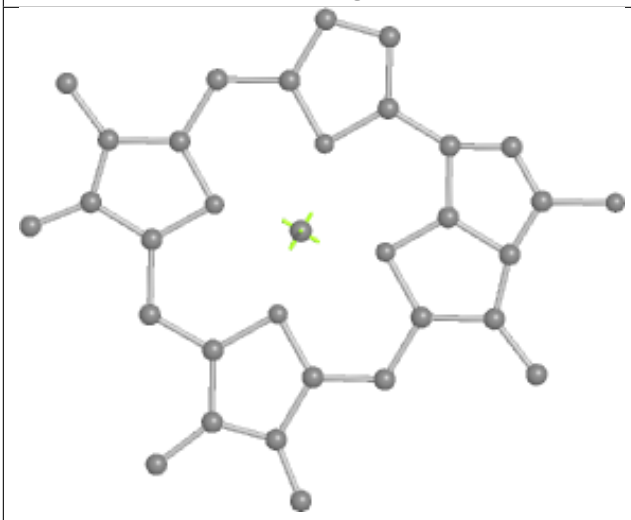
Ligand CLA A1 814



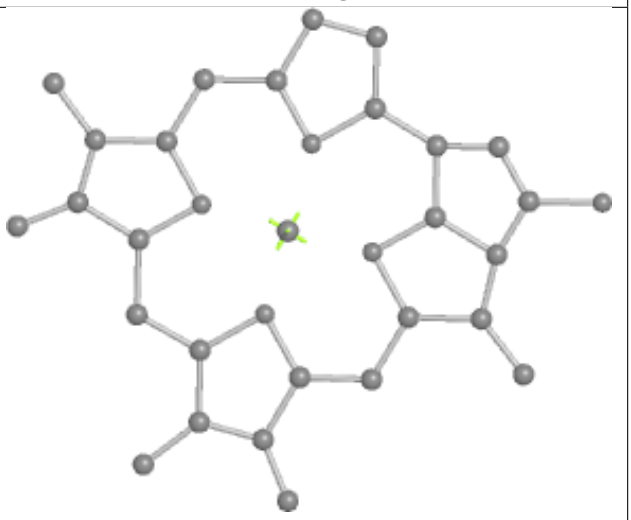
Bond lengths



Bond angles

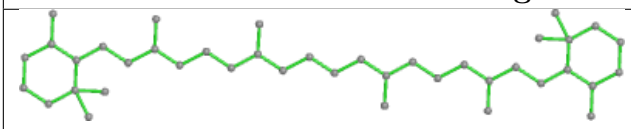


Torsions

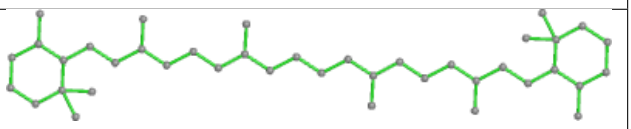


Rings

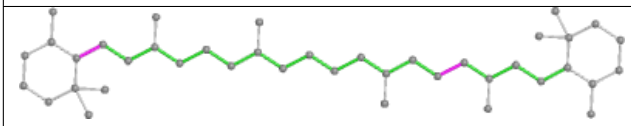
Ligand BCR B2 844



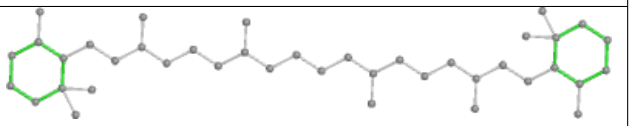
Bond lengths



Bond angles

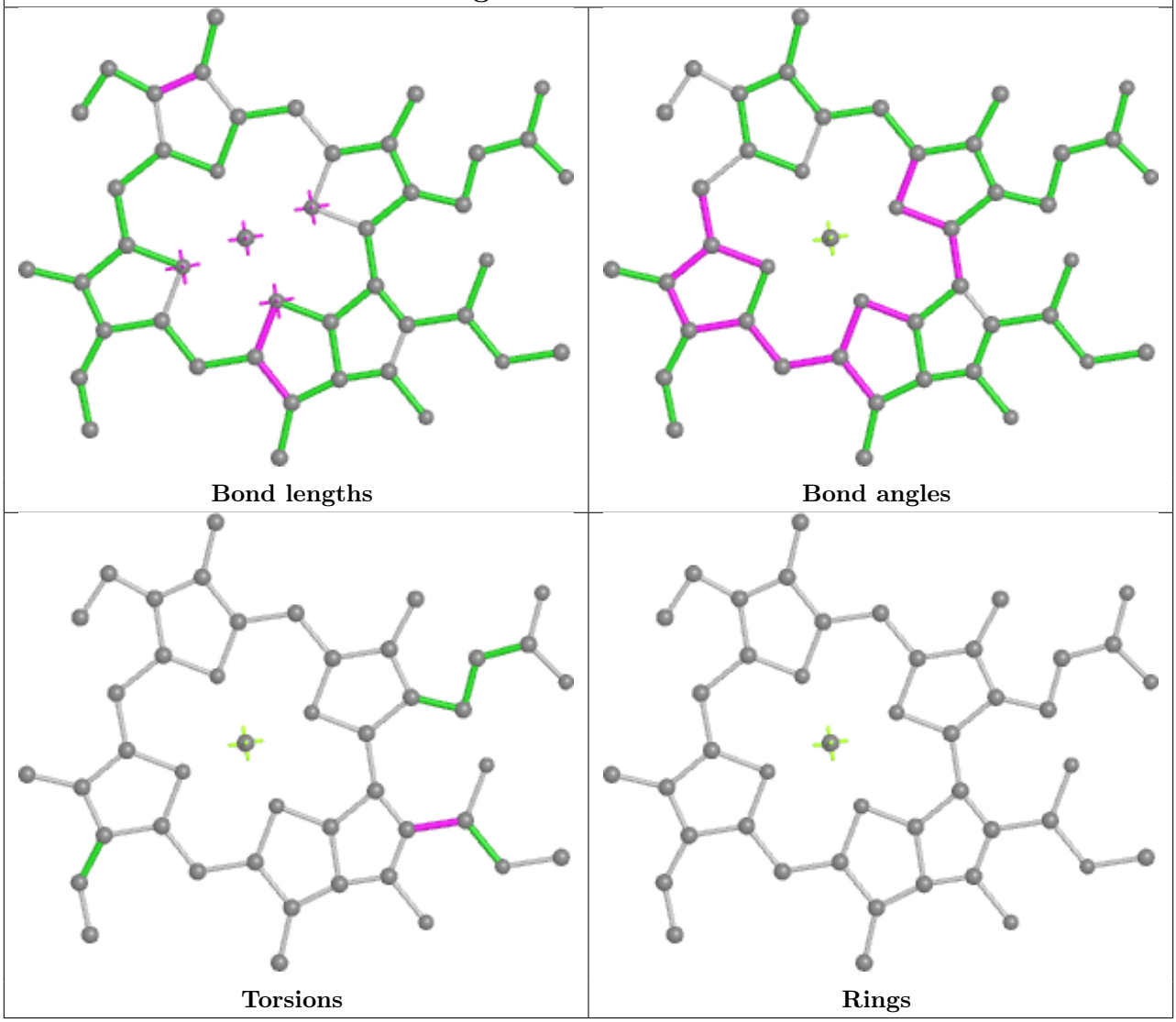


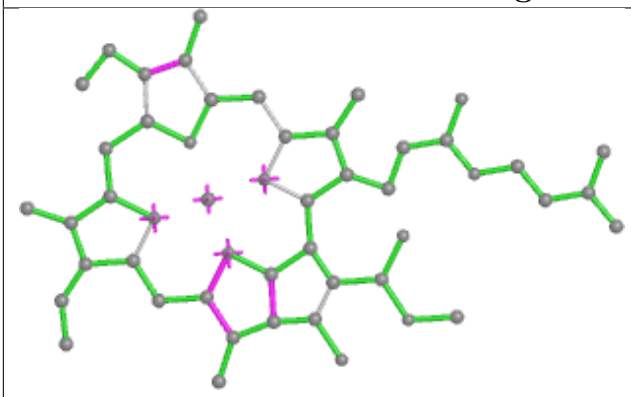
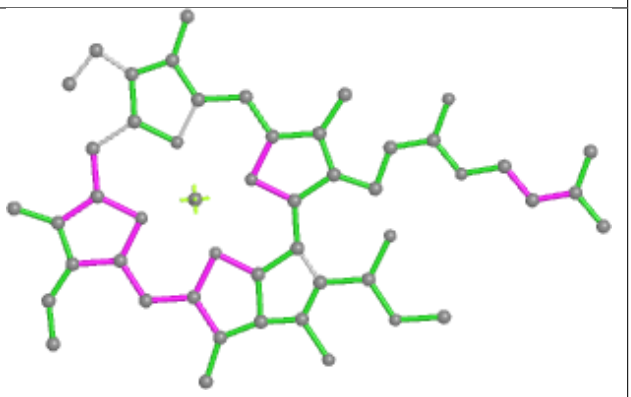
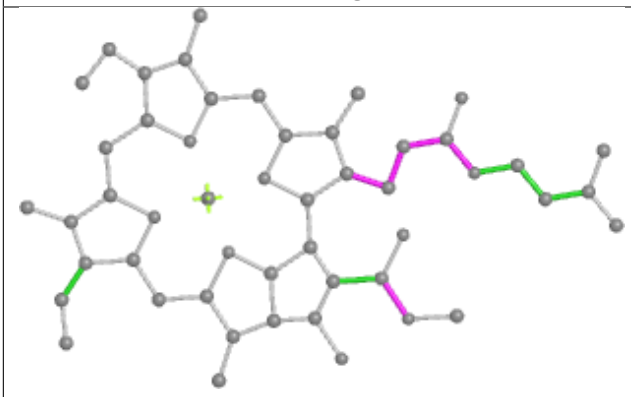
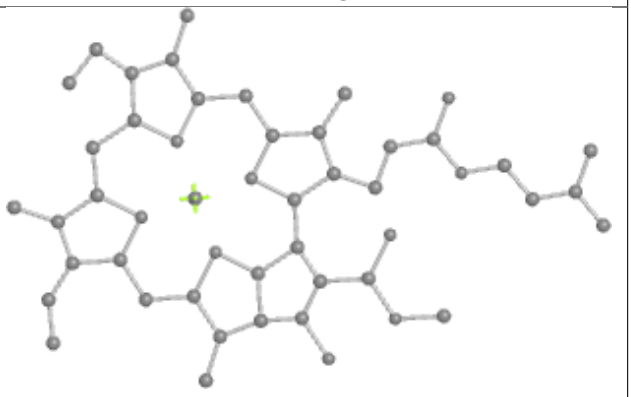
Torsions



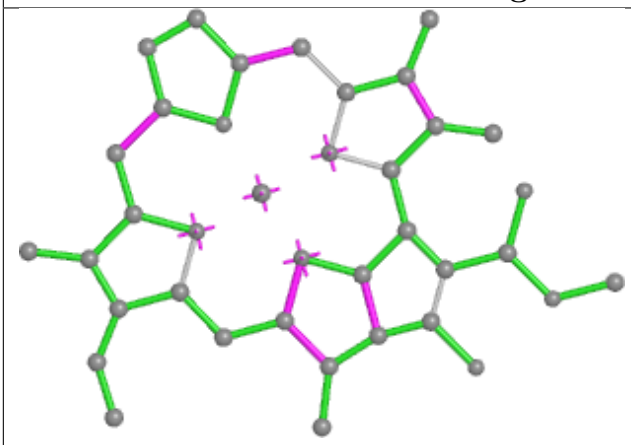
Rings

Ligand CLA B1 811

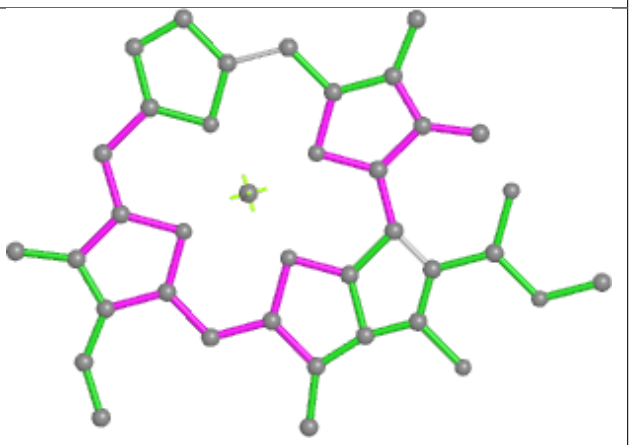


Ligand CLA A3 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

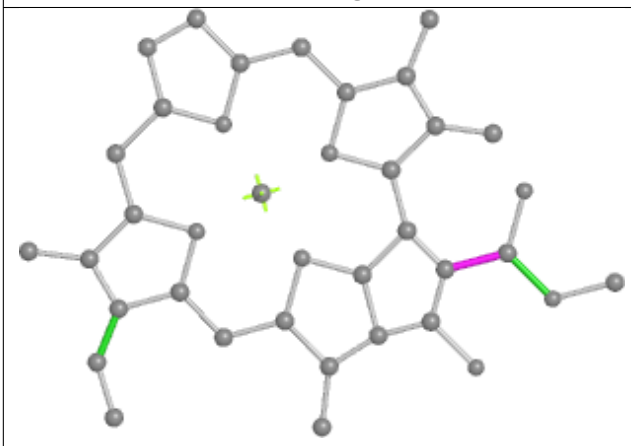
Ligand CLA J1 1301



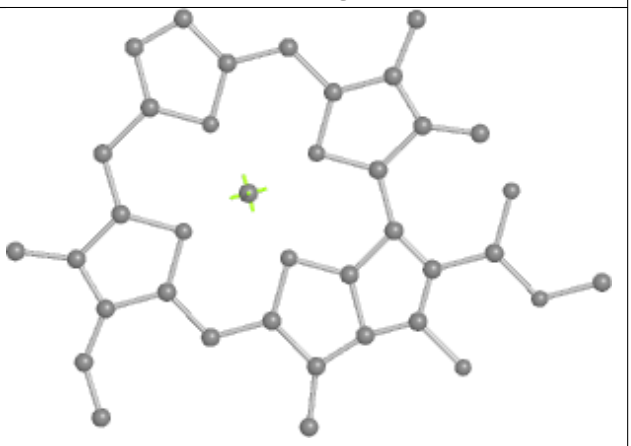
Bond lengths



Bond angles

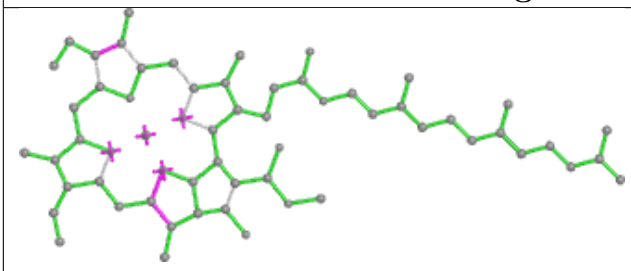


Torsions

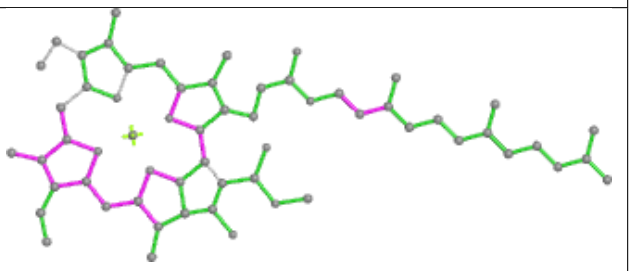


Rings

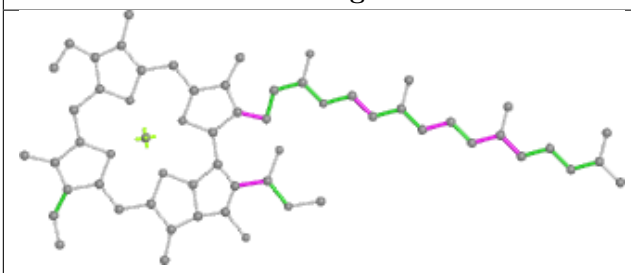
Ligand CLA A1 825



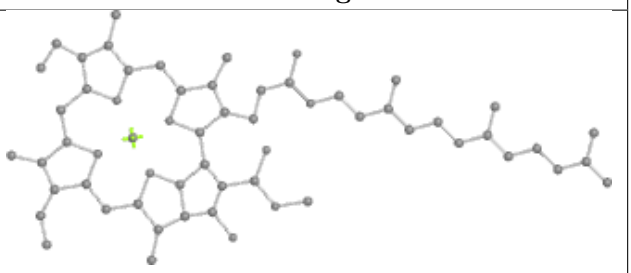
Bond lengths



Bond angles

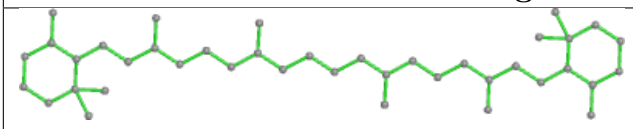


Torsions

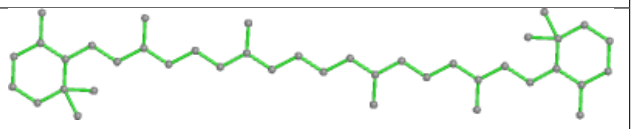


Rings

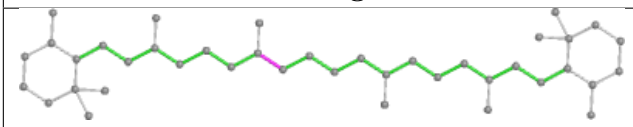
Ligand BCR F1 201



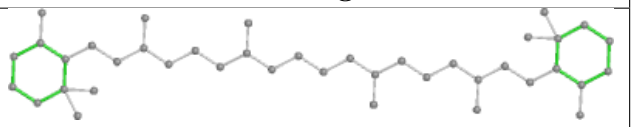
Bond lengths



Bond angles

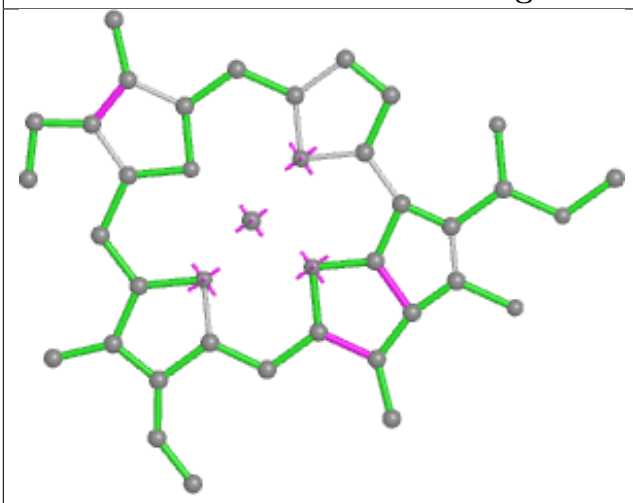


Torsions

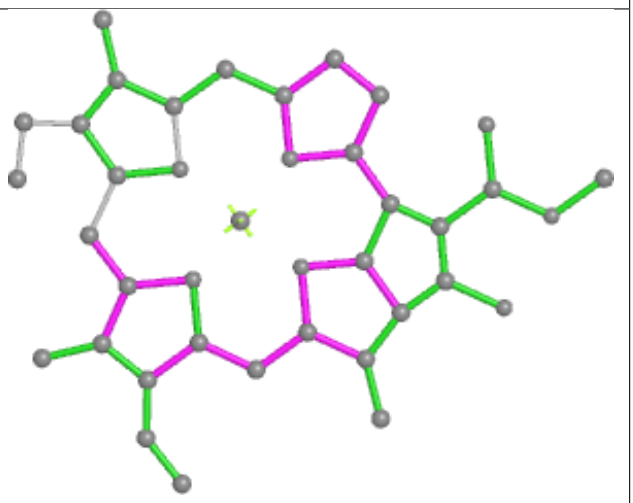


Rings

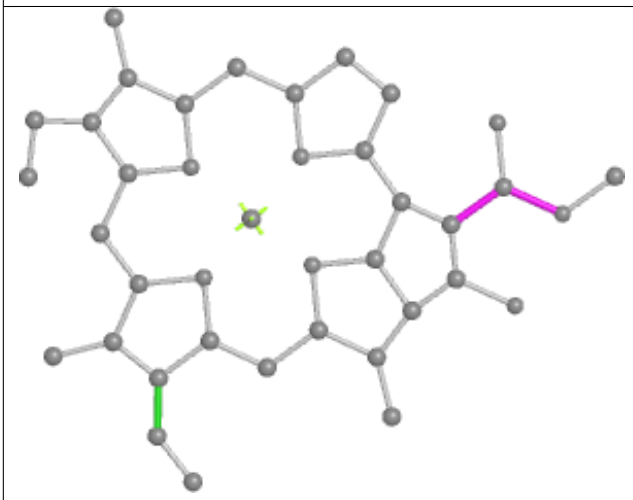
Ligand CLA B2 821



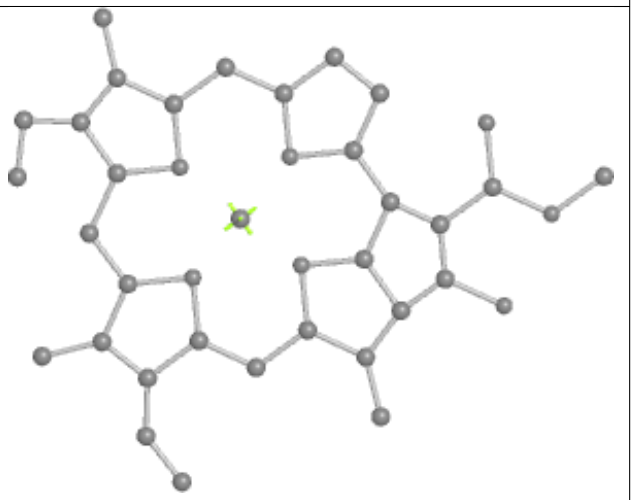
Bond lengths



Bond angles

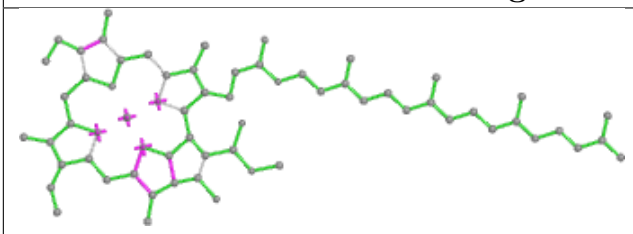


Torsions

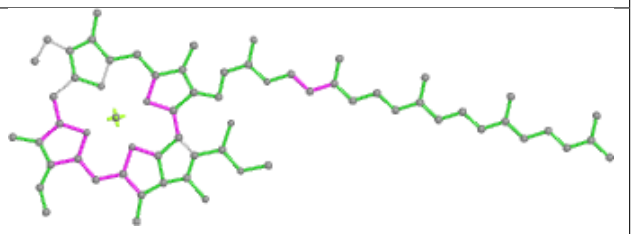


Rings

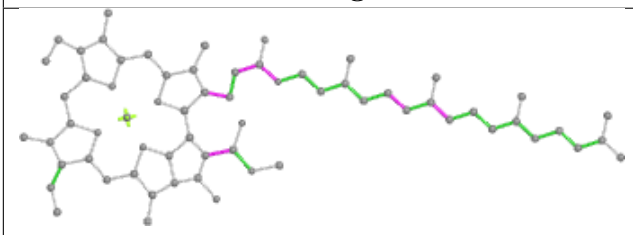
Ligand CLA L1 1002



Bond lengths



Bond angles



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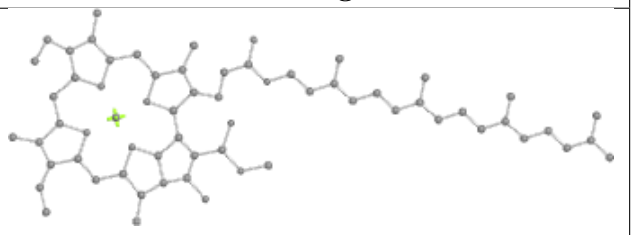
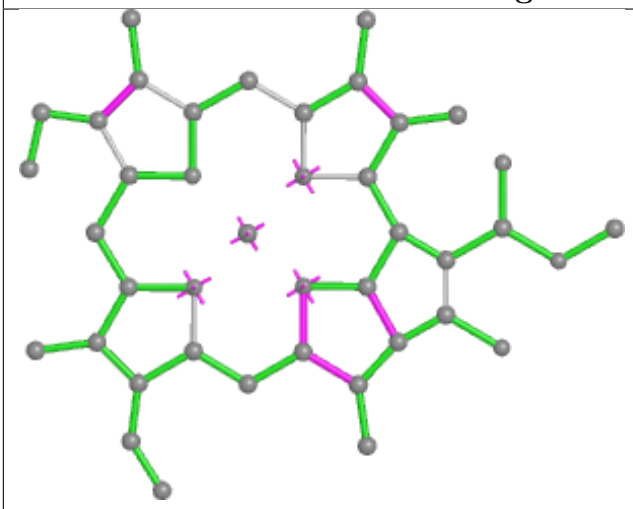


Rings

Ligand CLA B3 837



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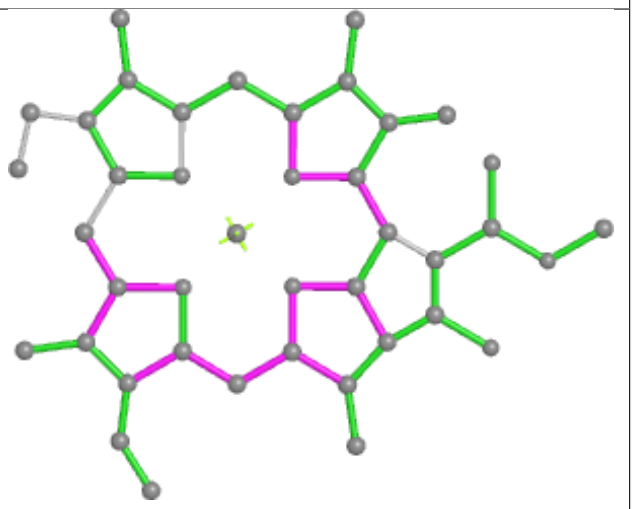

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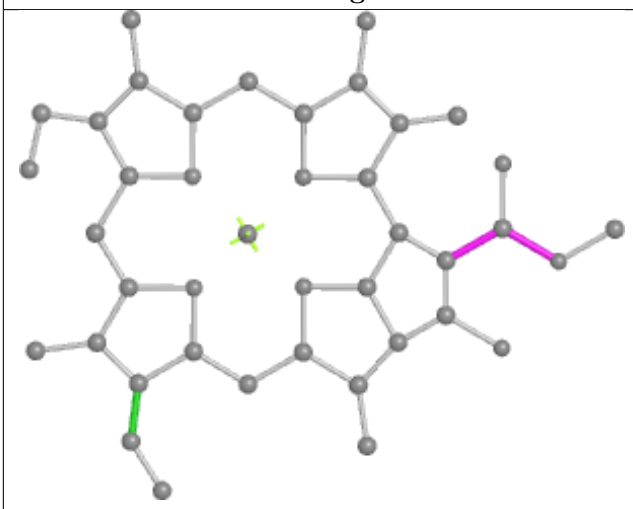

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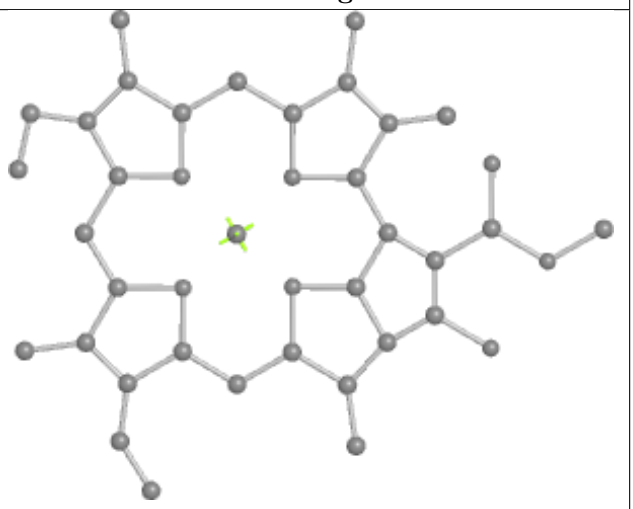
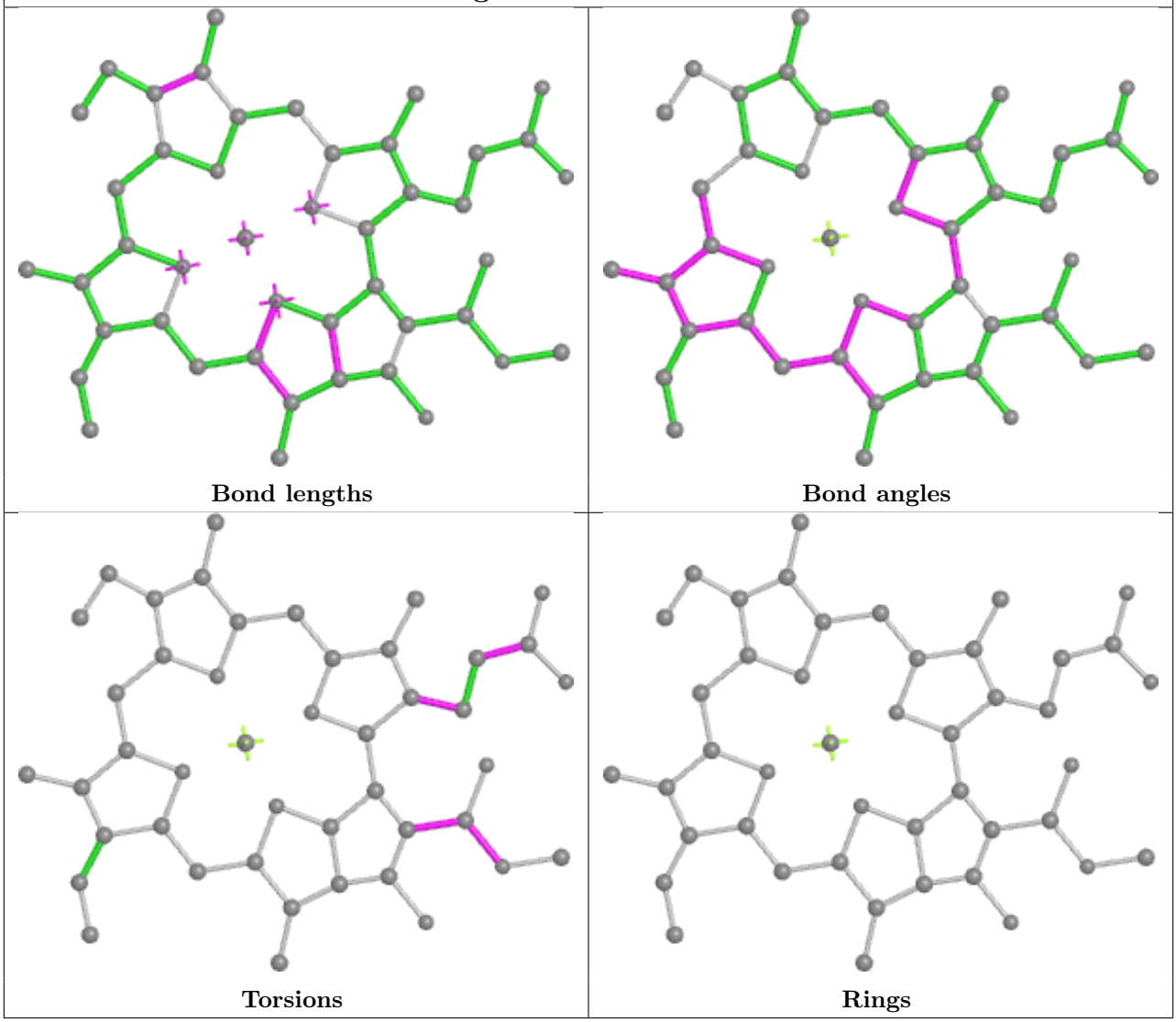
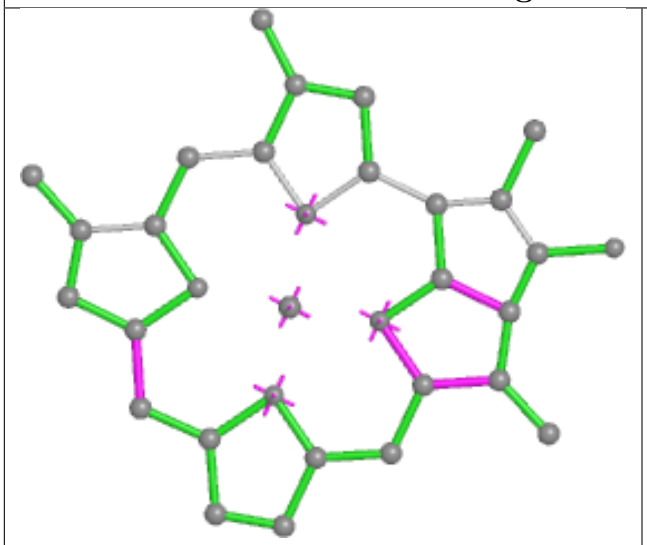


Rings

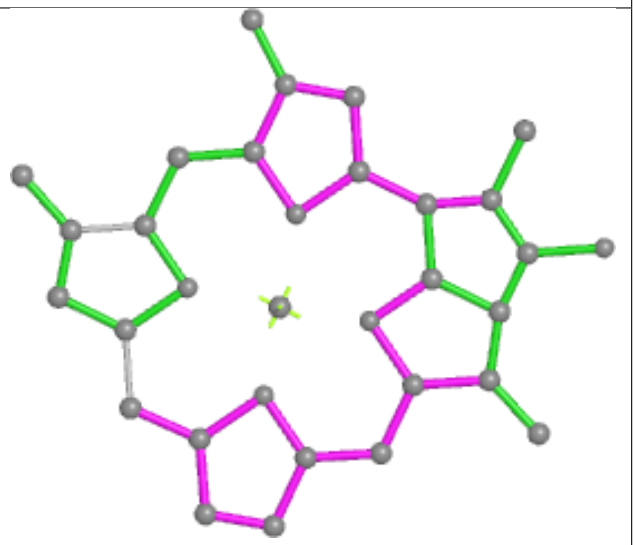
Ligand CLA B1 813



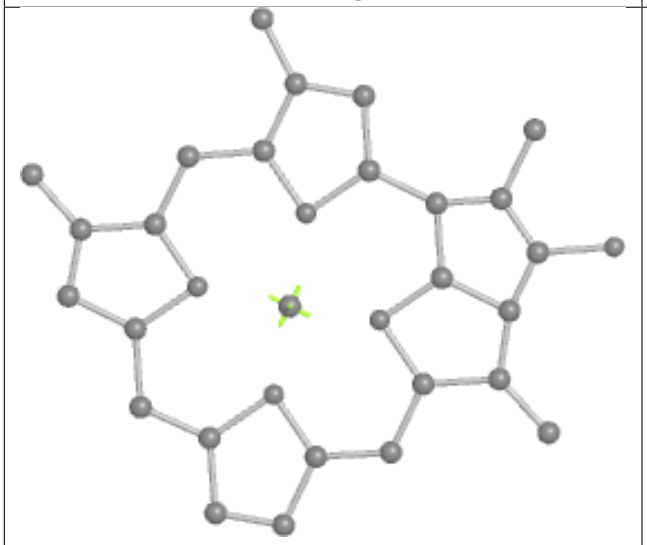
Ligand CLA K2 103



Bond lengths



Bond angles



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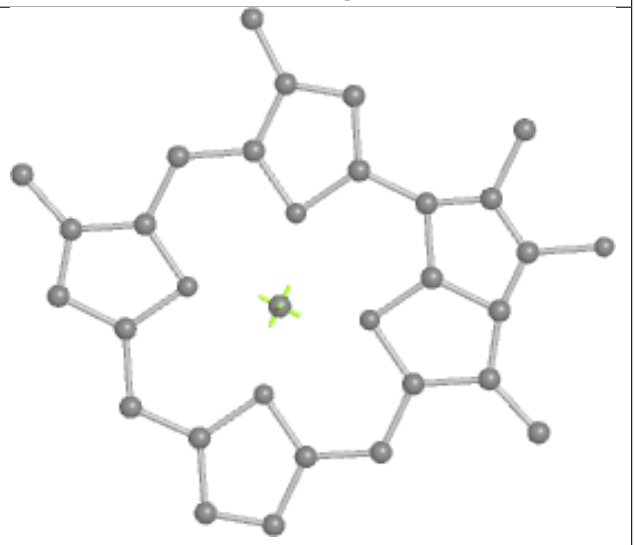
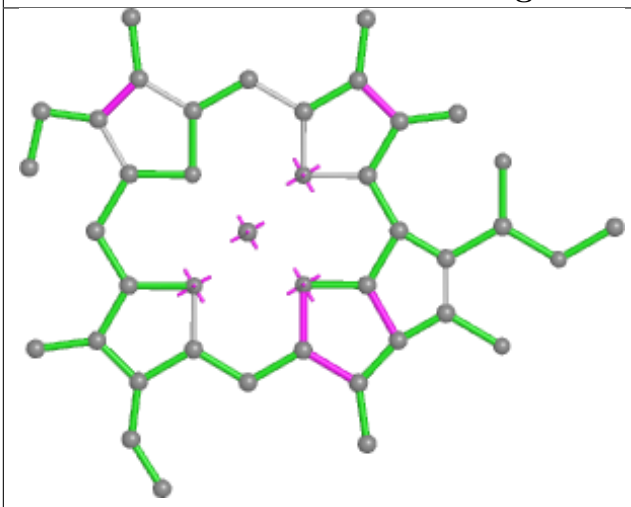
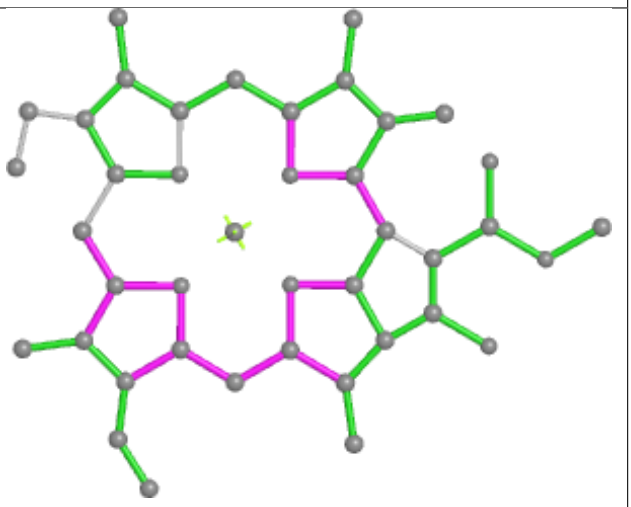


Rings

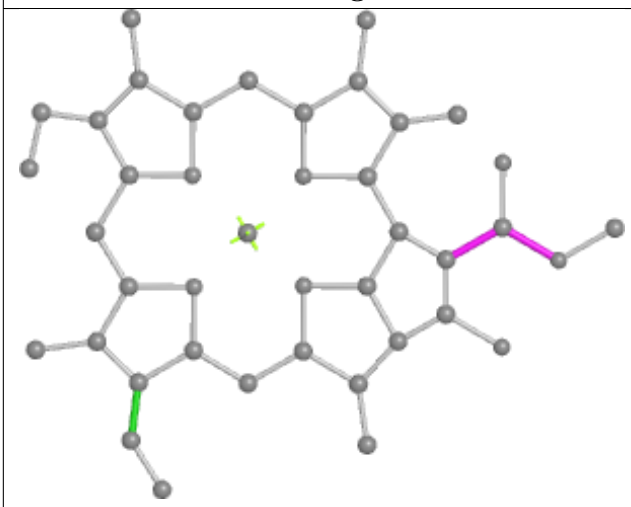
Ligand CLA B3 814



Bond lengths



Bond angles



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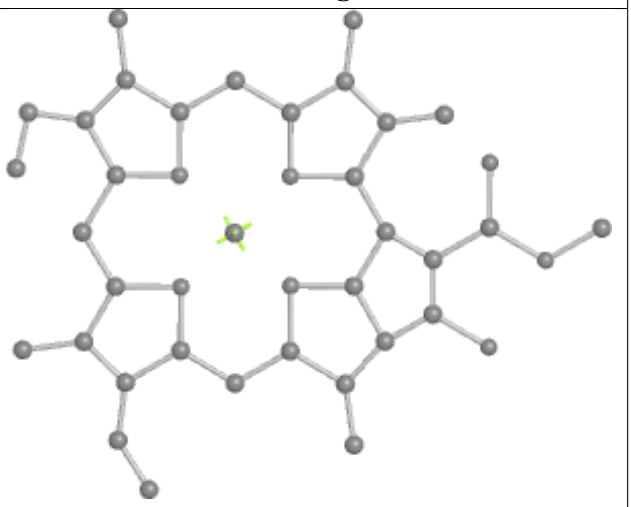
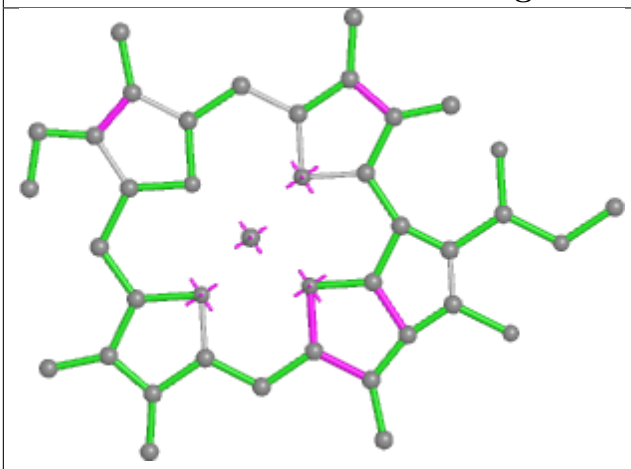


Rings

Ligand CLA X3 102



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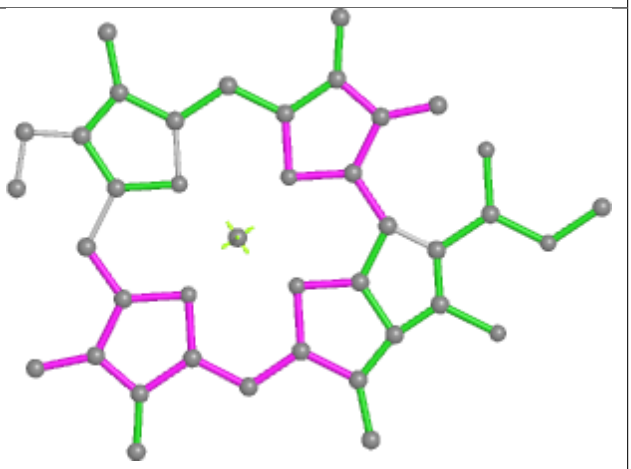
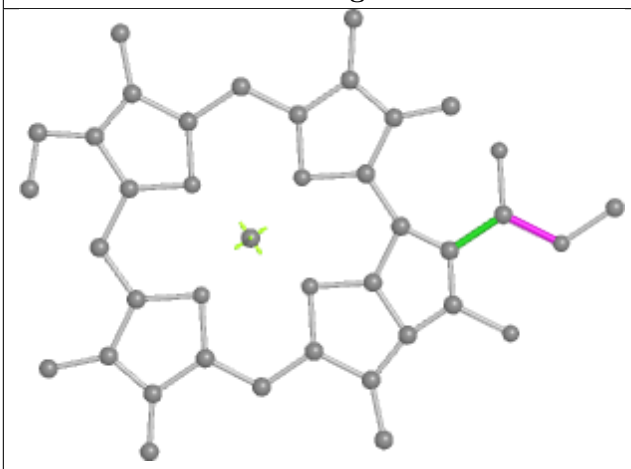


Bond angles



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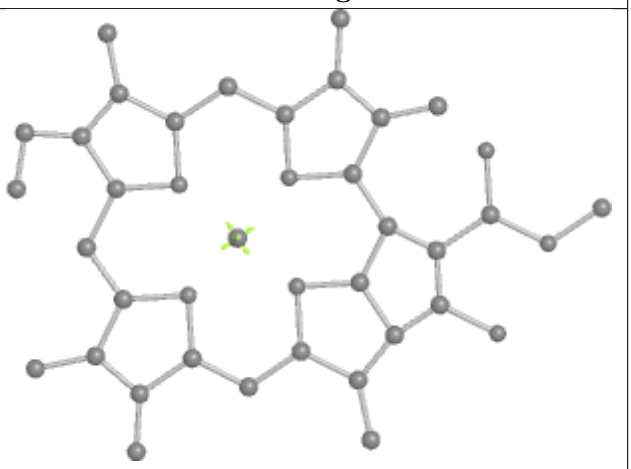
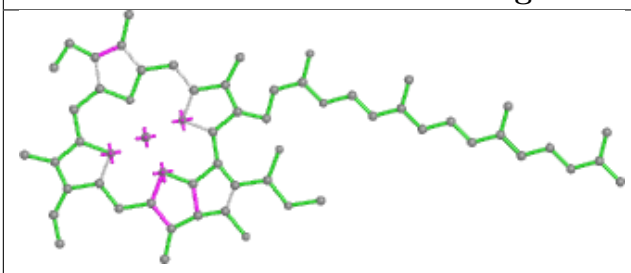
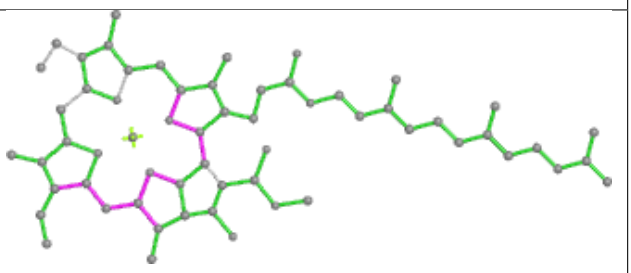


Rings

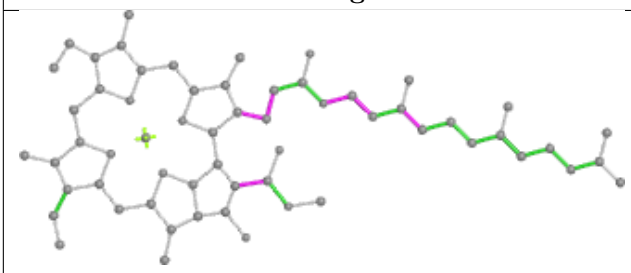
Ligand CLA A3 827



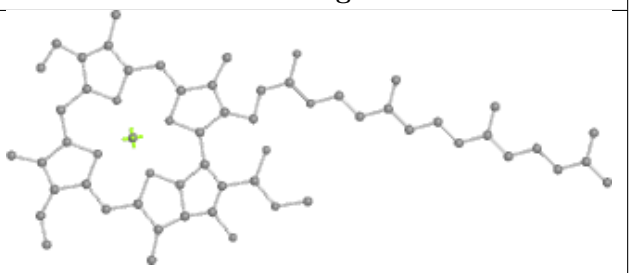
Bond lengths



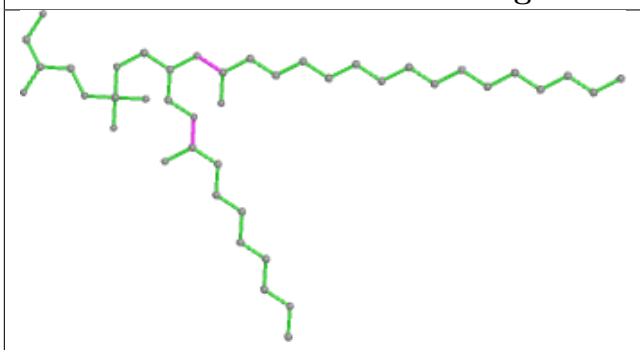
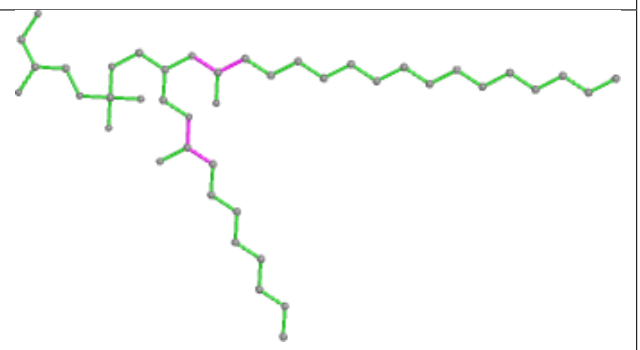
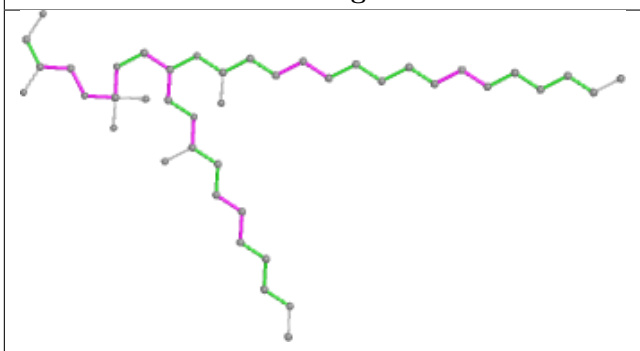
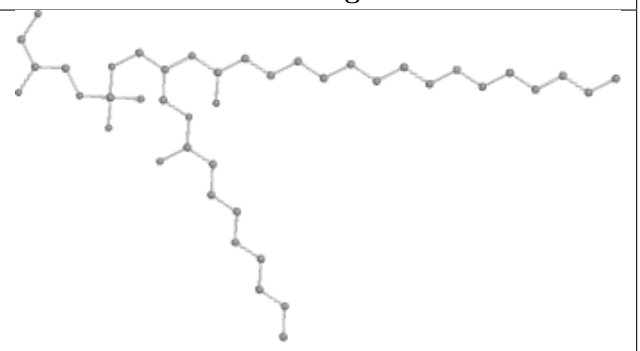
Bond angles

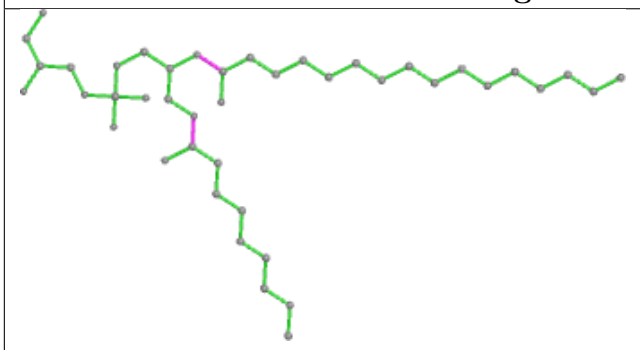
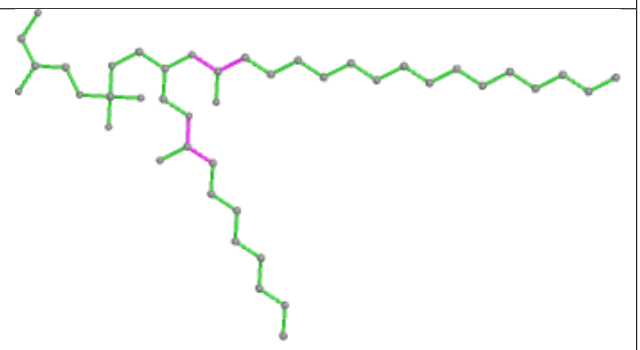
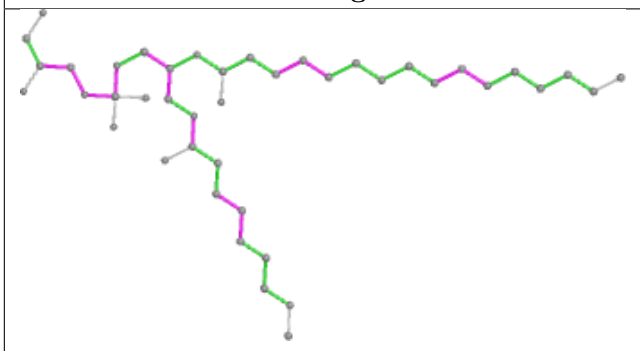
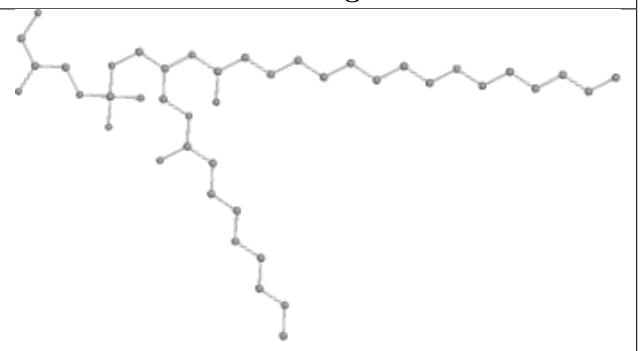


Torsions

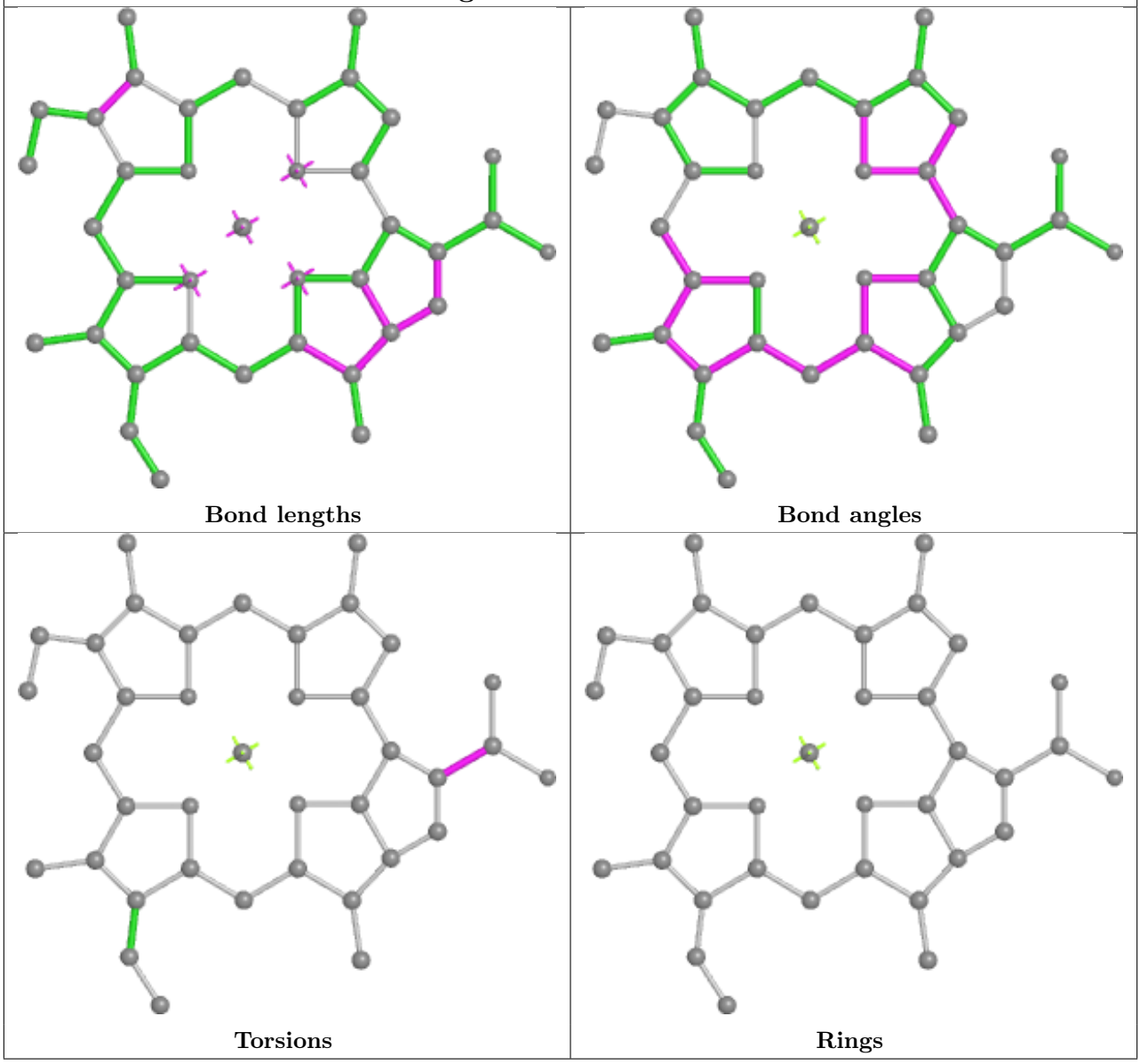


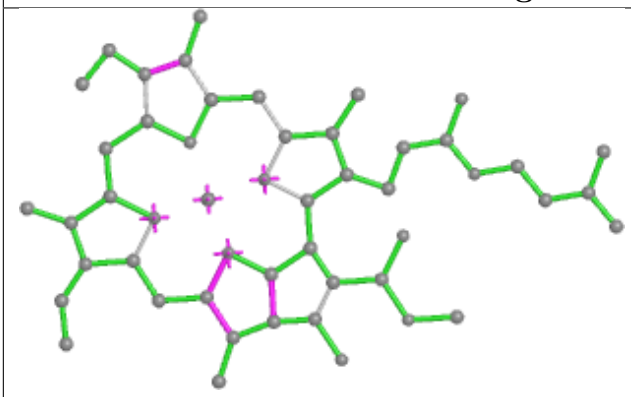
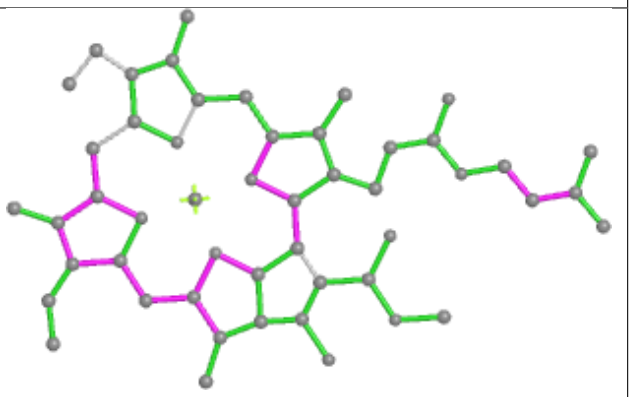
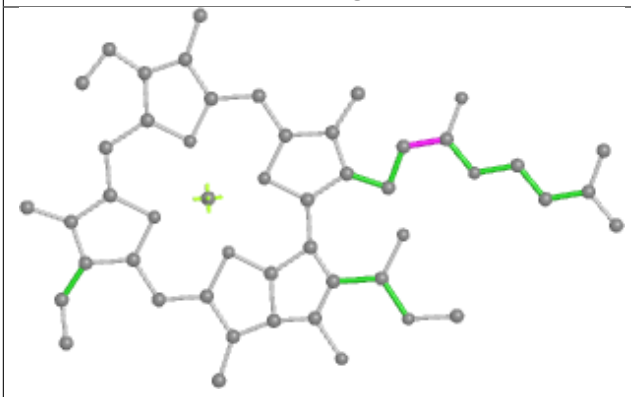
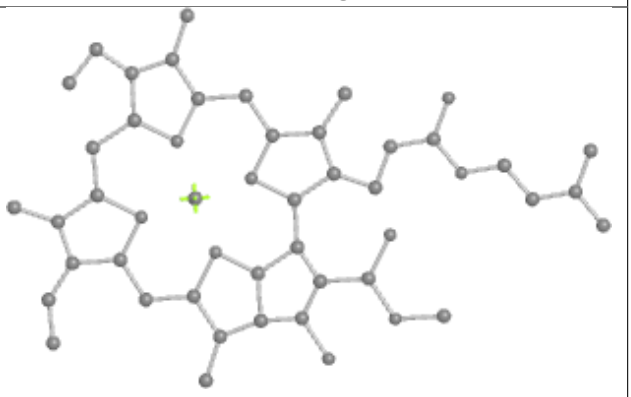
Rings

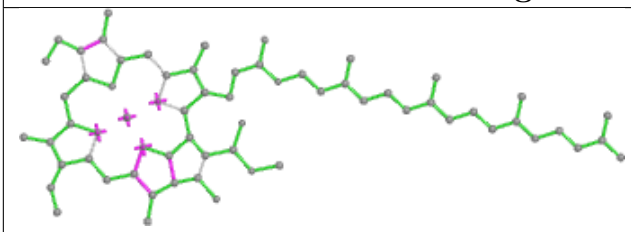
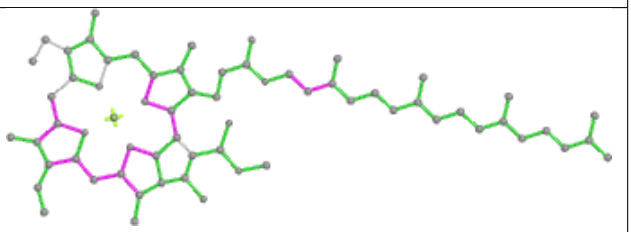
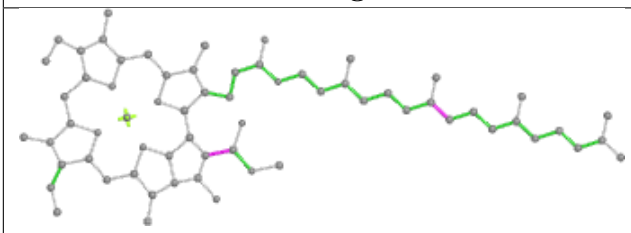
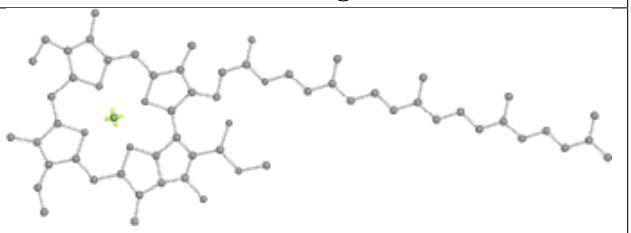
Ligand LHG X3 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG X2 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

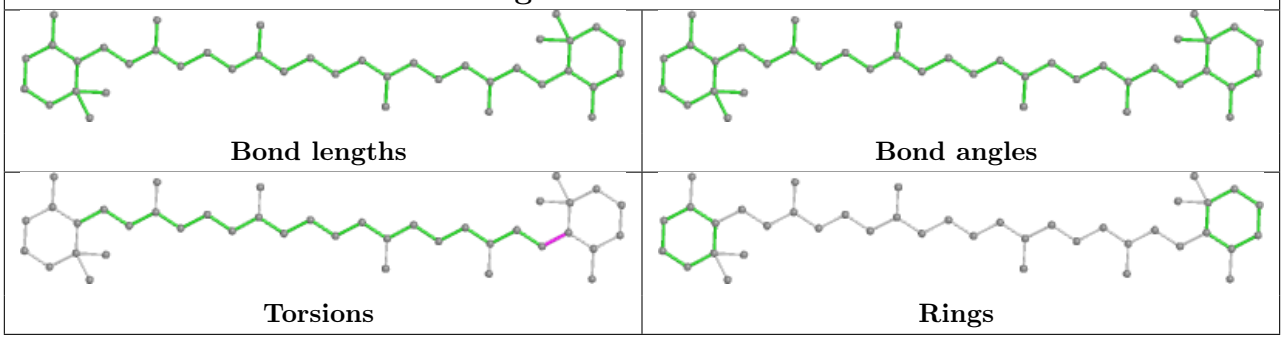
Ligand CLA B3 816



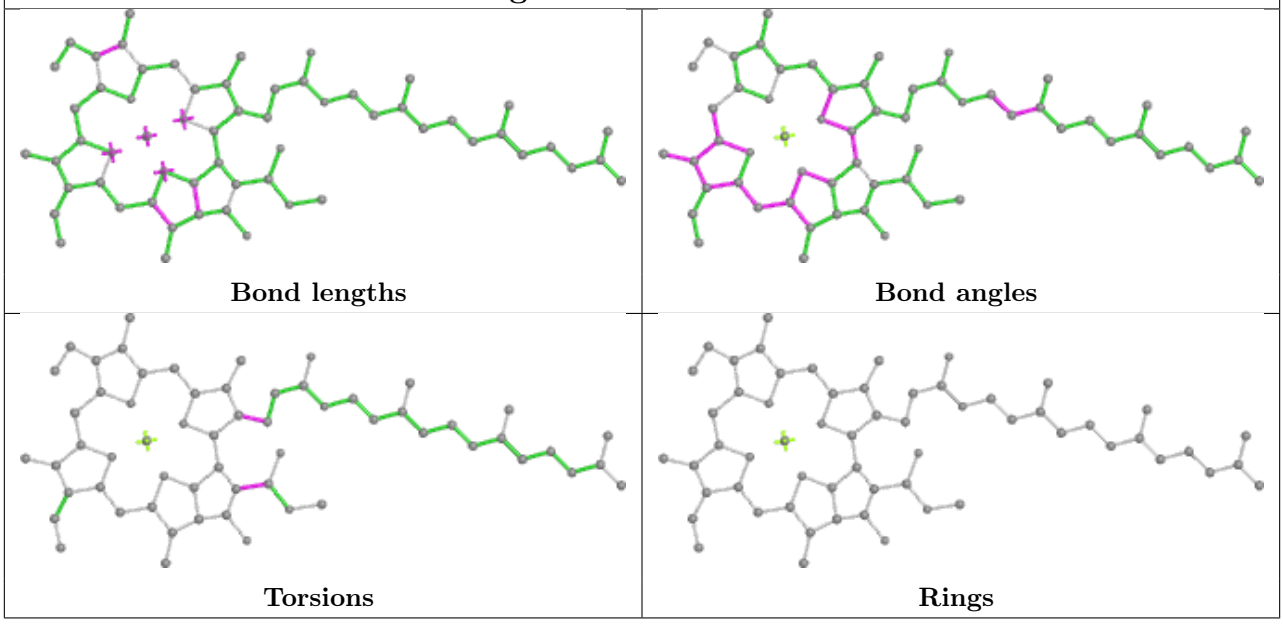
Ligand CLA B2 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A3 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

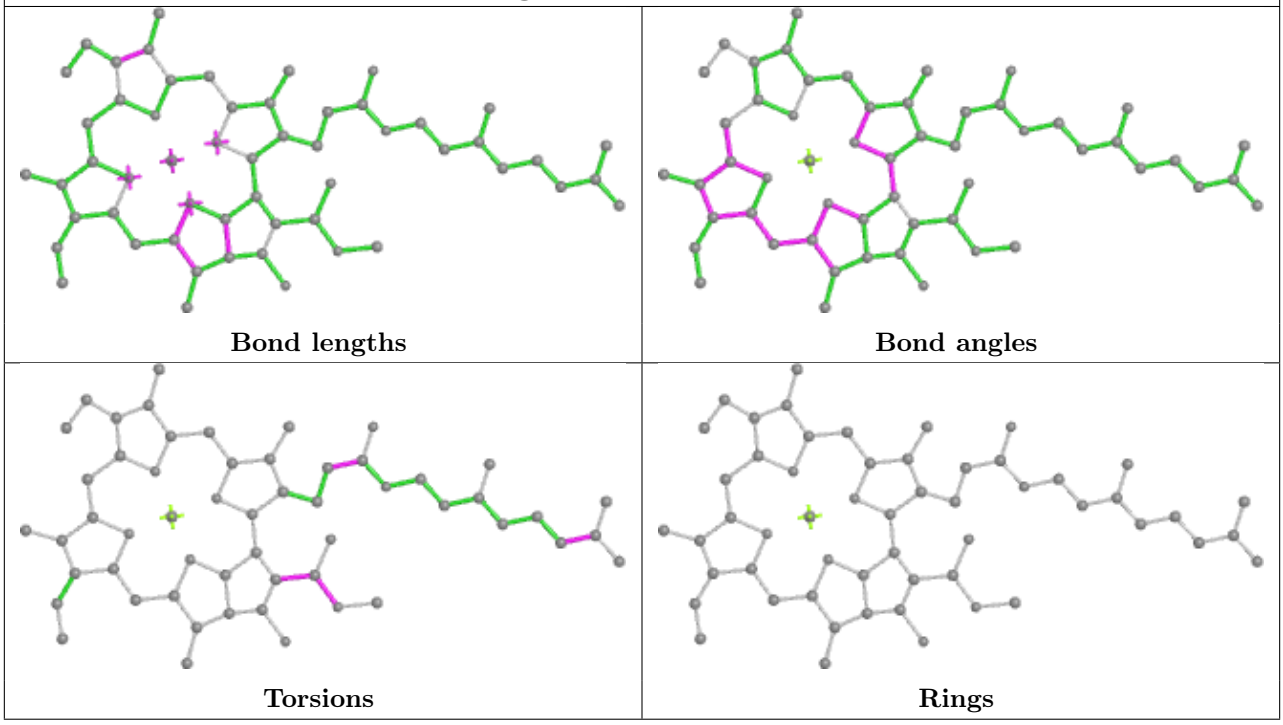
Ligand BCR B2 845

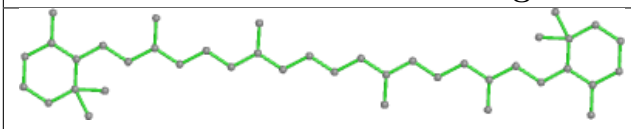
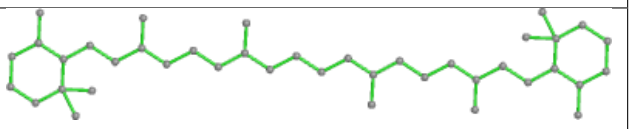
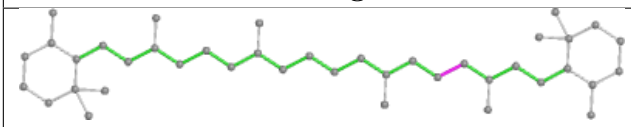


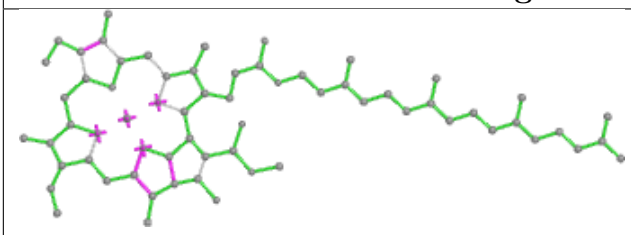
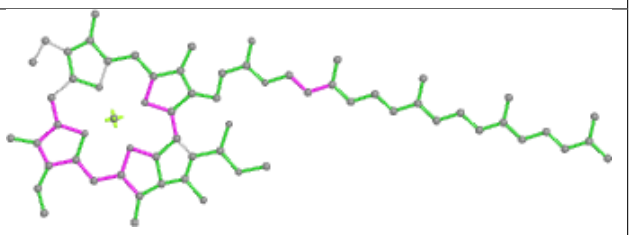
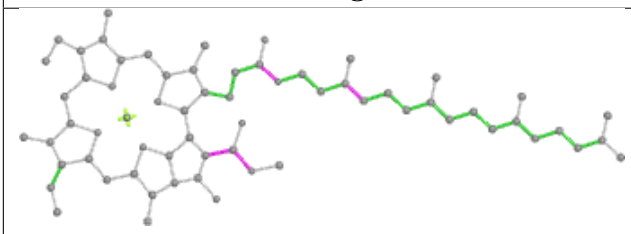
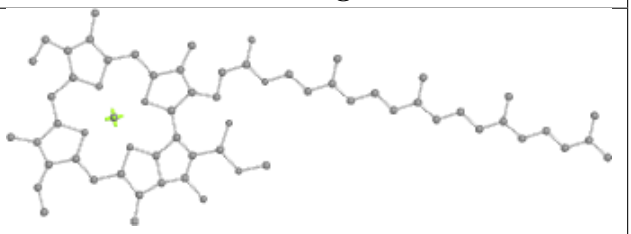
Ligand CLA L1 1003



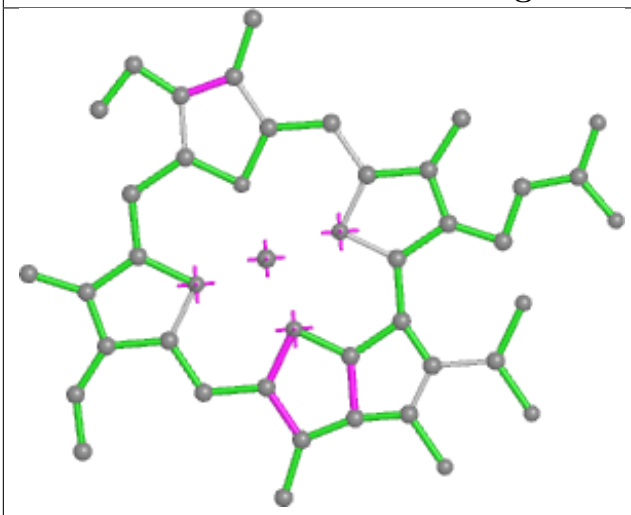
Ligand CLA A3 839



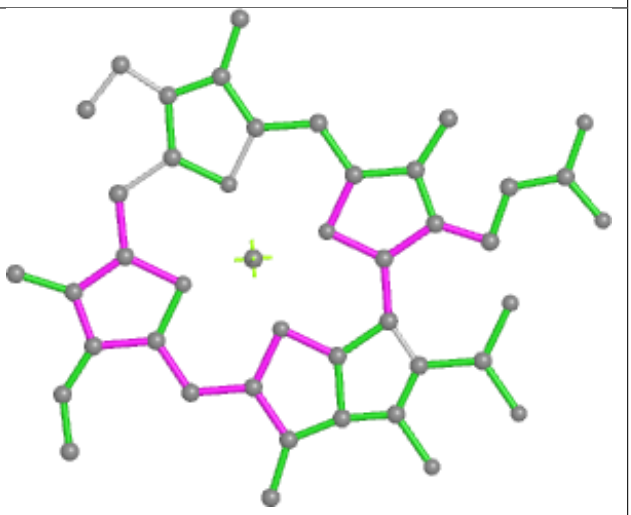
Ligand BCR A3 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

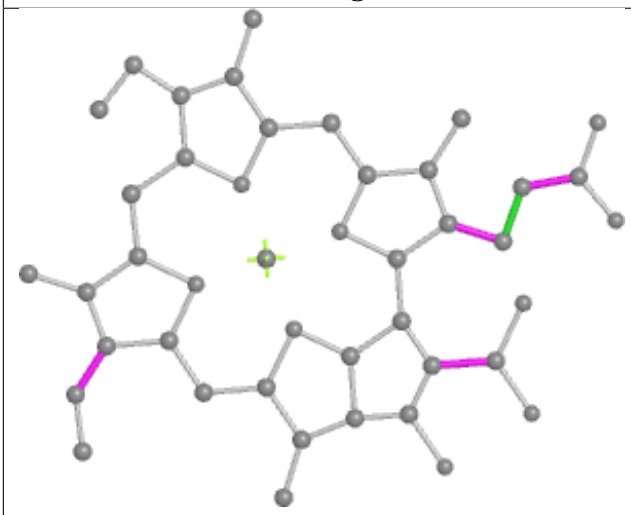
Ligand CLA A1 807



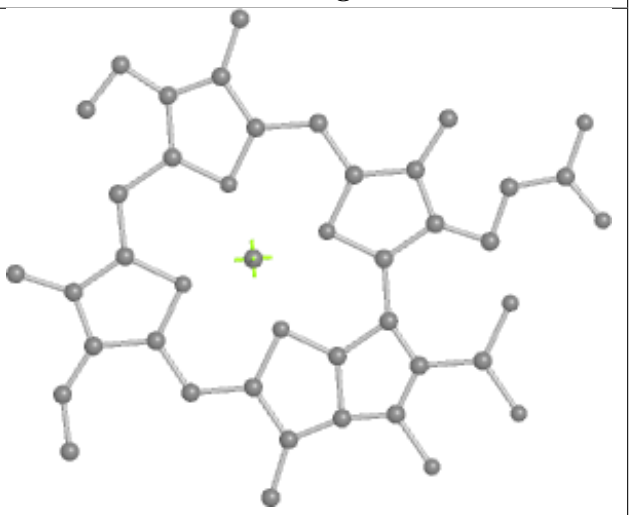
Bond lengths



Bond angles

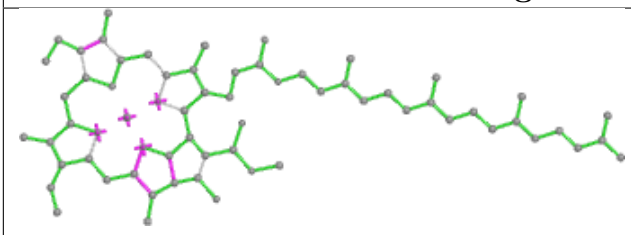


Torsions

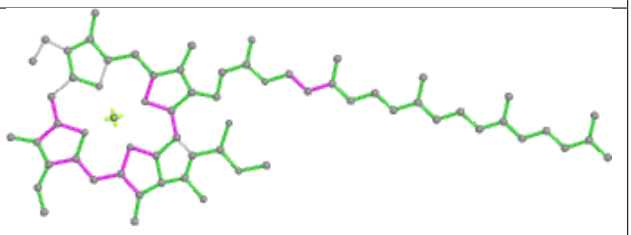


Rings

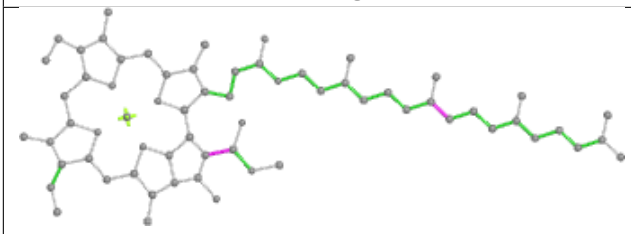
Ligand CLA A1 808



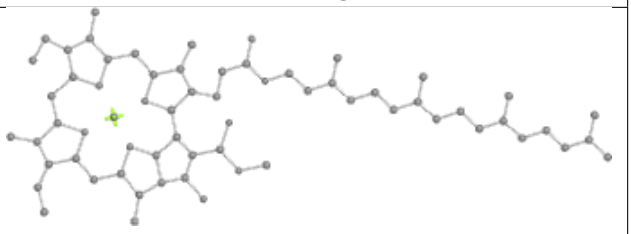
Bond lengths



Bond angles

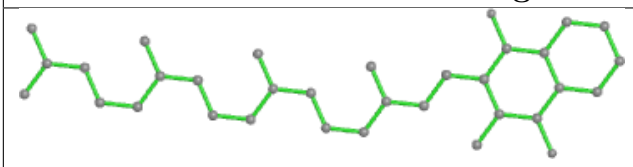


Torsions

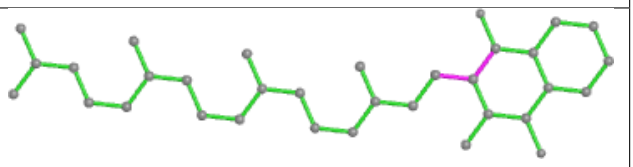


Rings

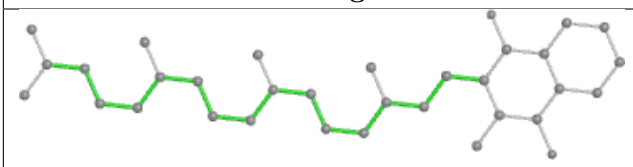
Ligand PQN B3 840



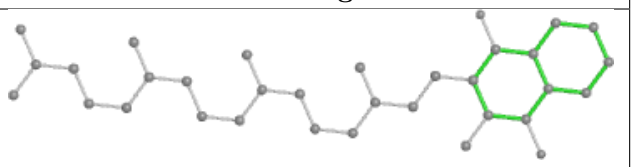
Bond lengths



Bond angles

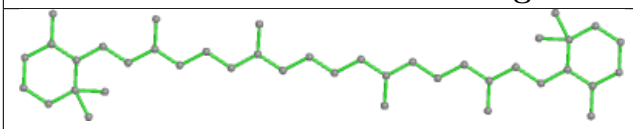


Torsions



Rings

Ligand BCR B3 841



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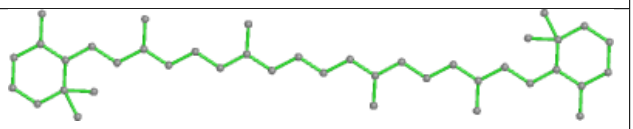
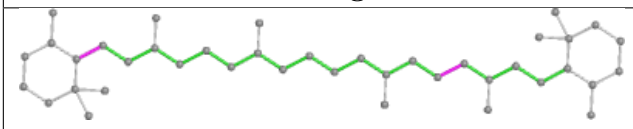
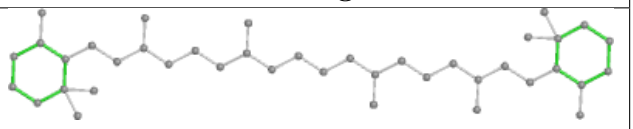


Bond angles

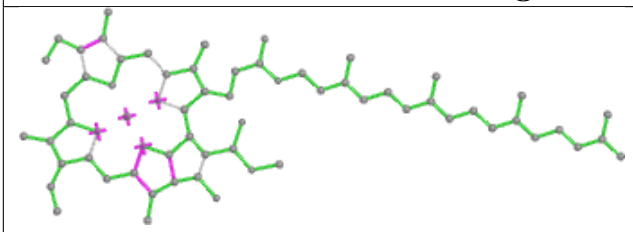


Torsions



Rings

Ligand CLA A1 802



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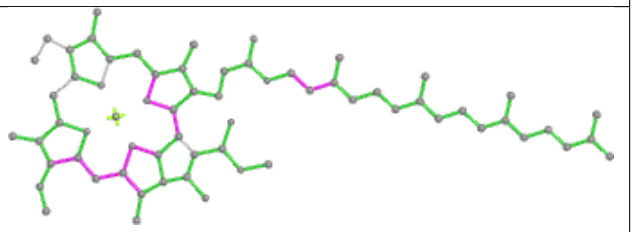
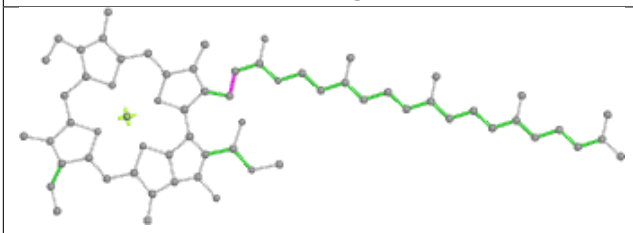


Bond angles



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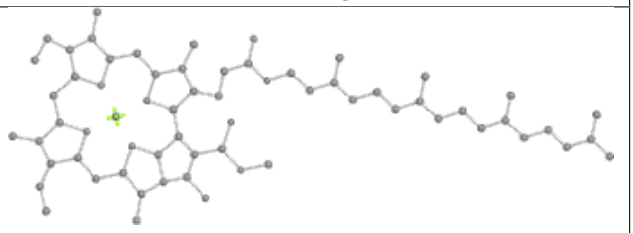
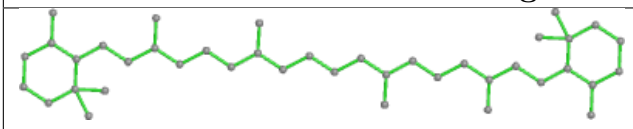


Rings

Ligand BCR I1 102



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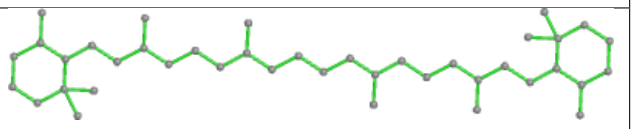
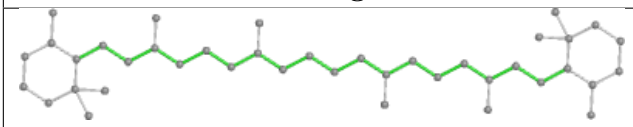


Bond angles



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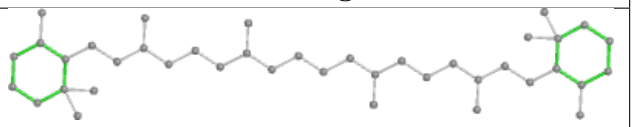
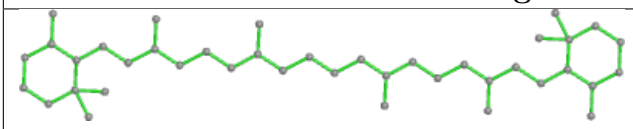


Rings

Ligand BCR B2 846



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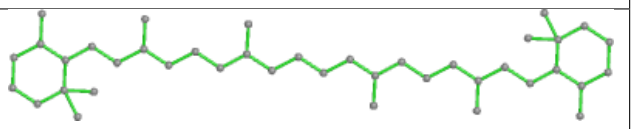
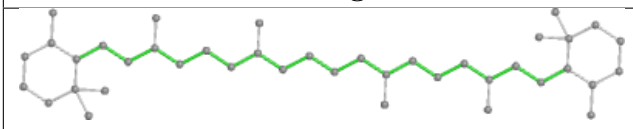


Bond angles



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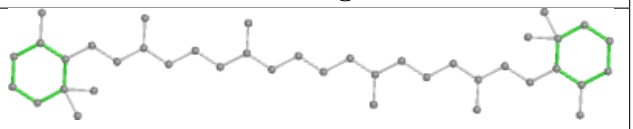
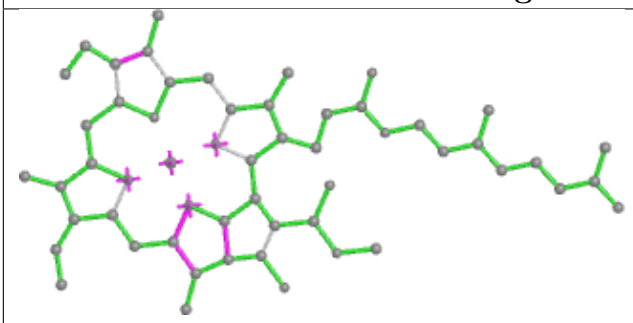


Rings

Ligand CLA A1 826



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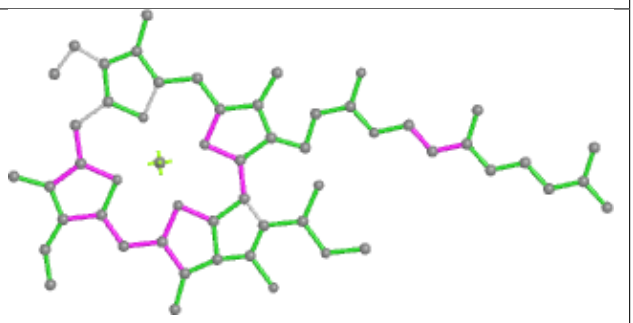
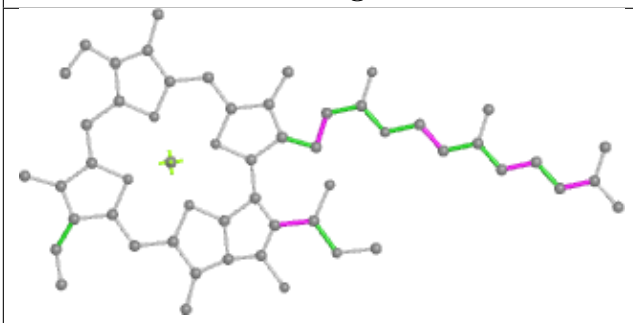


Bond angles



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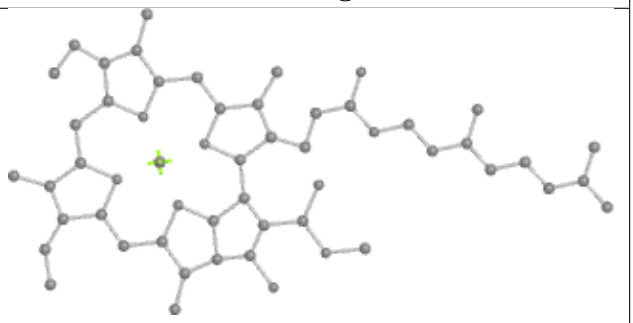
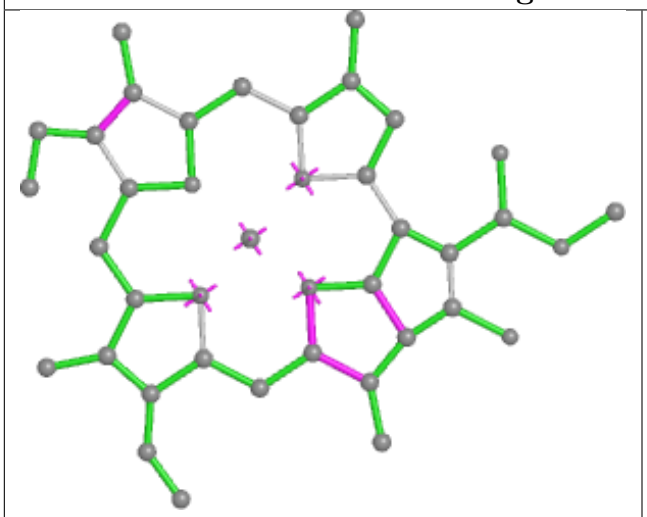


Rings

Ligand CLA B1 822



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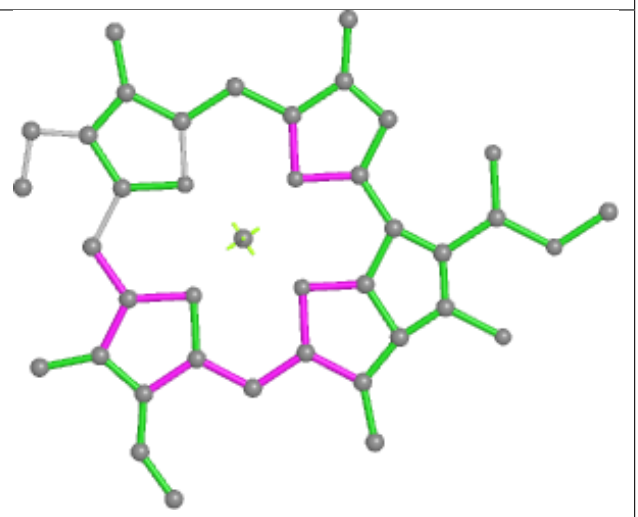
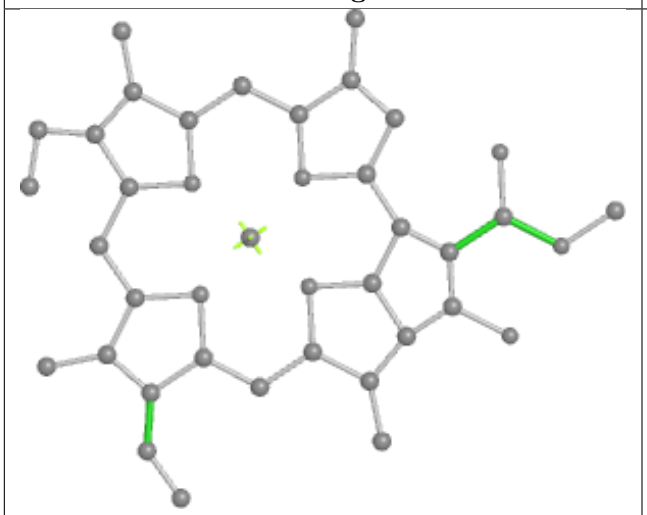


Bond angles



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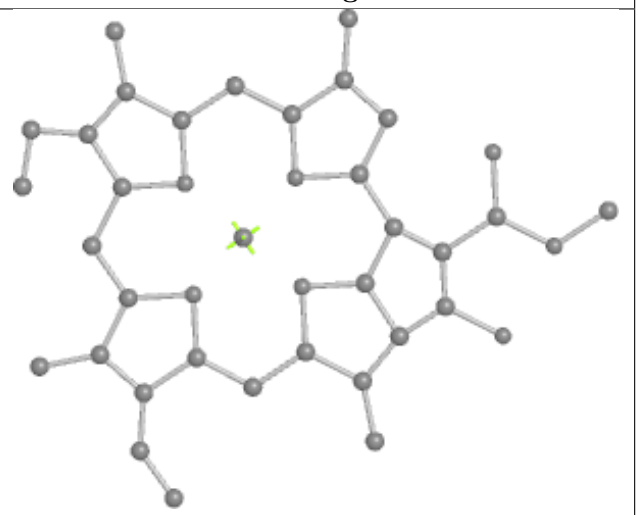
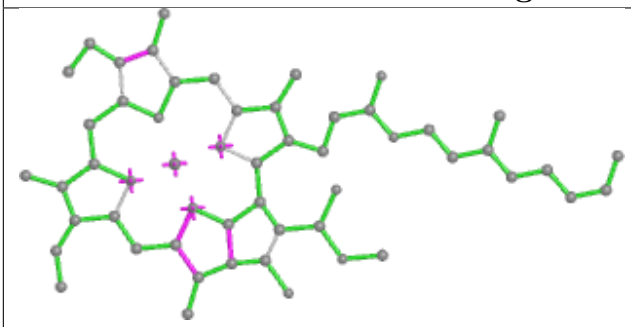
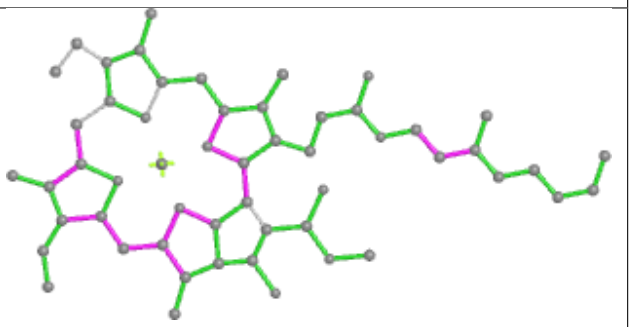


Rings

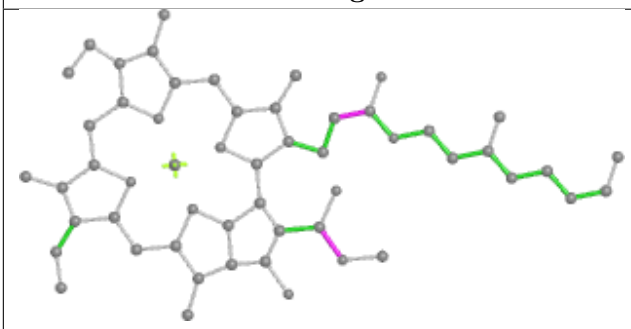
Ligand CLA B1 803



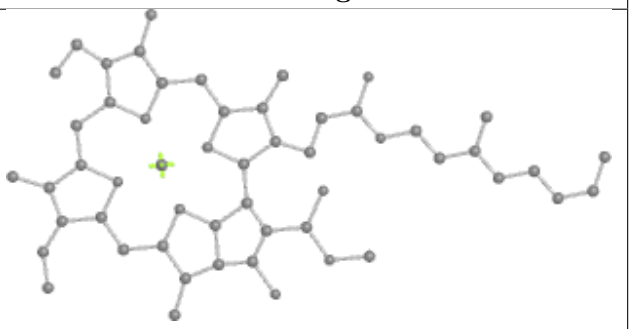
Bond lengths



Bond angles

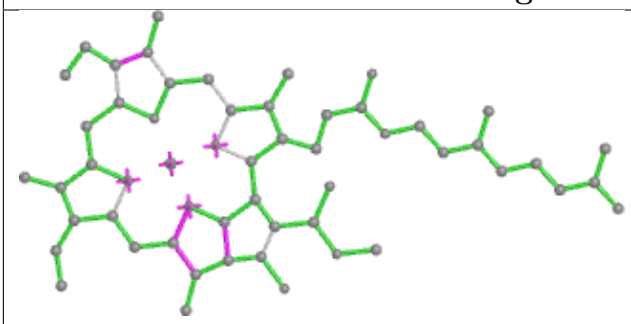


Torsions

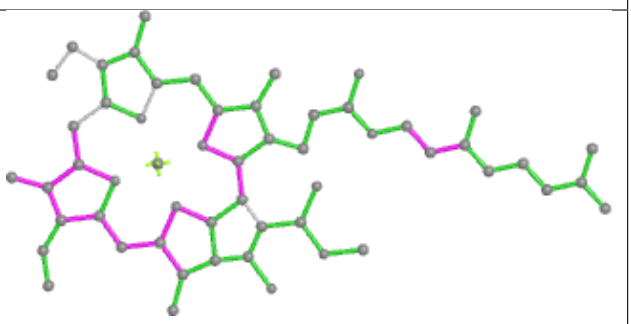


Rings

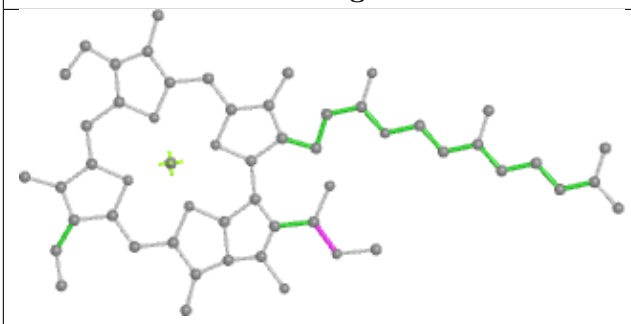
Ligand CLA B1 804



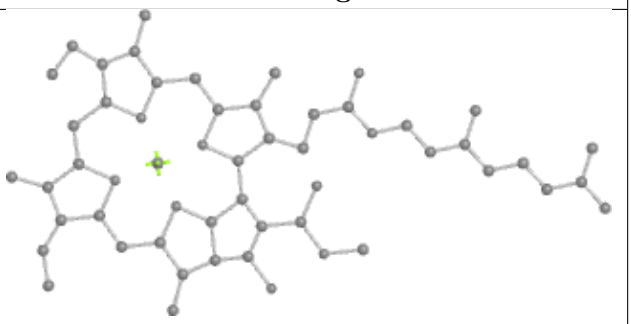
Bond lengths



Bond angles

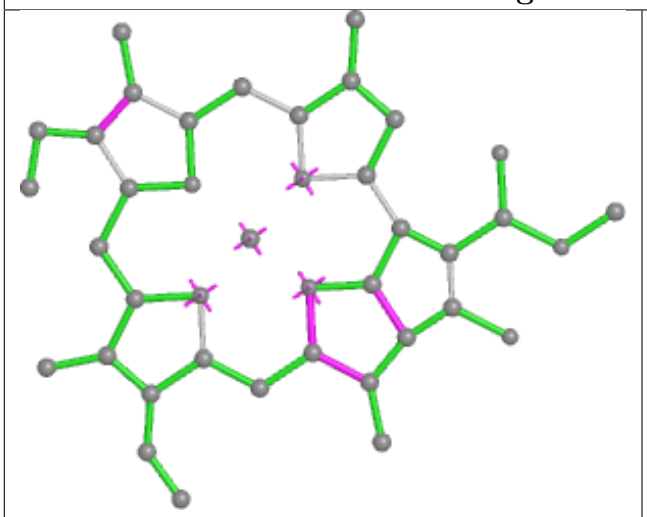


Torsions

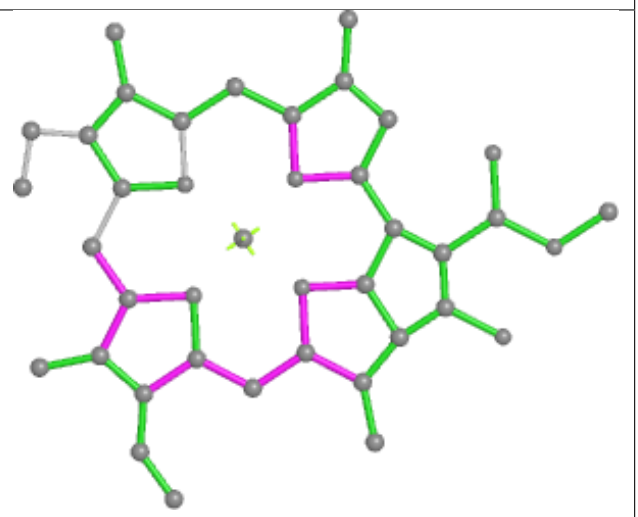


Rings

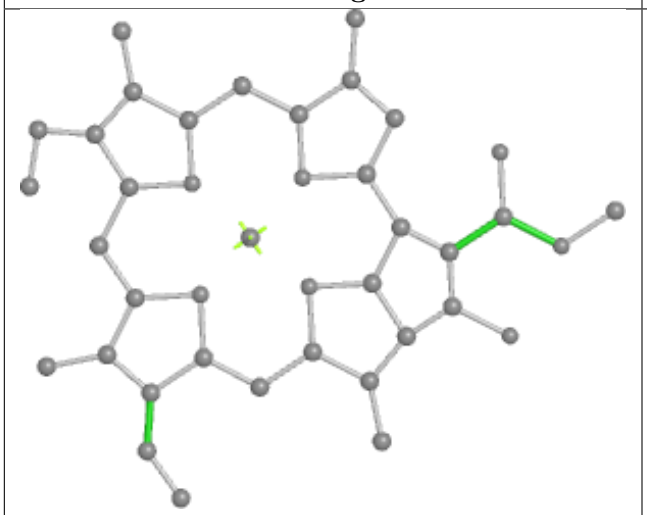
Ligand CLA B2 822



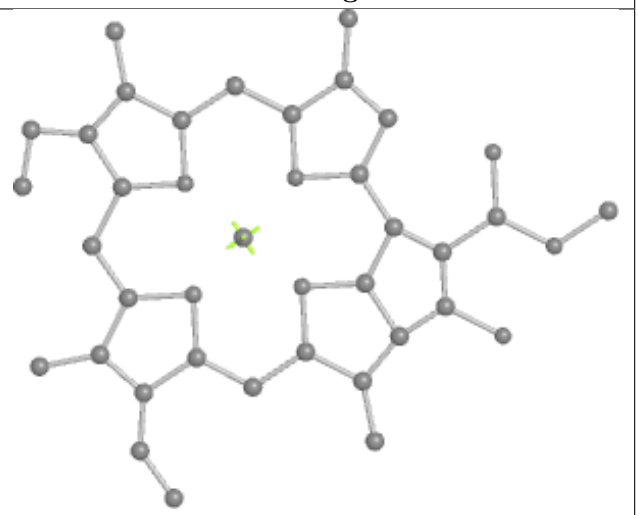
Bond lengths



Bond angles

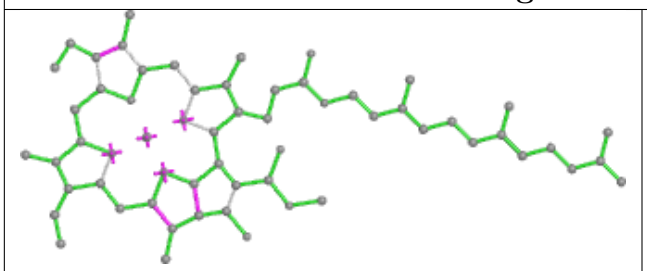


Torsions

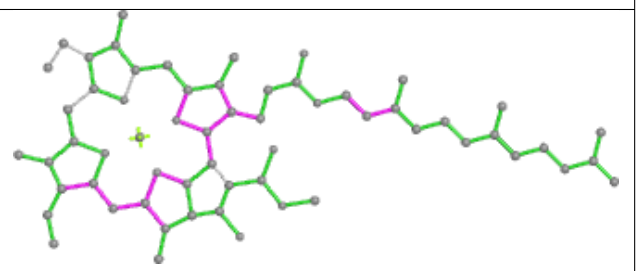


Rings

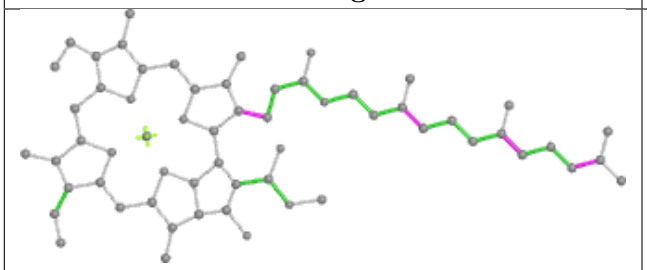
Ligand CLA B2 807



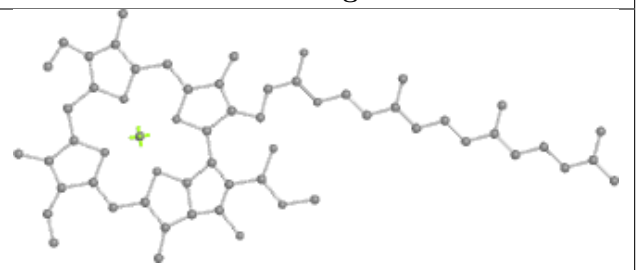
Bond lengths



Bond angles

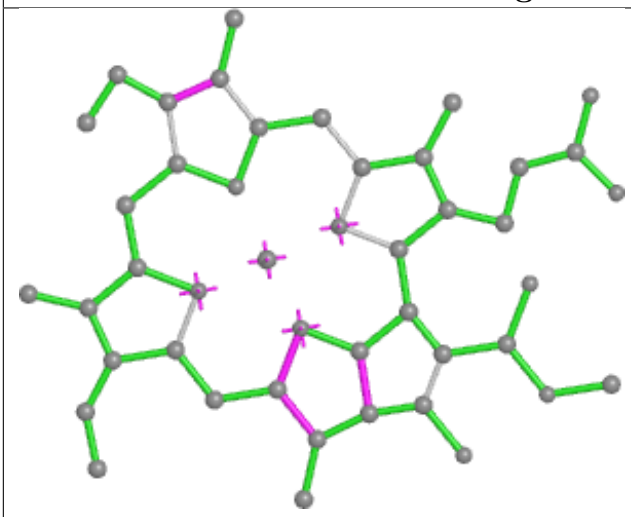


Torsions

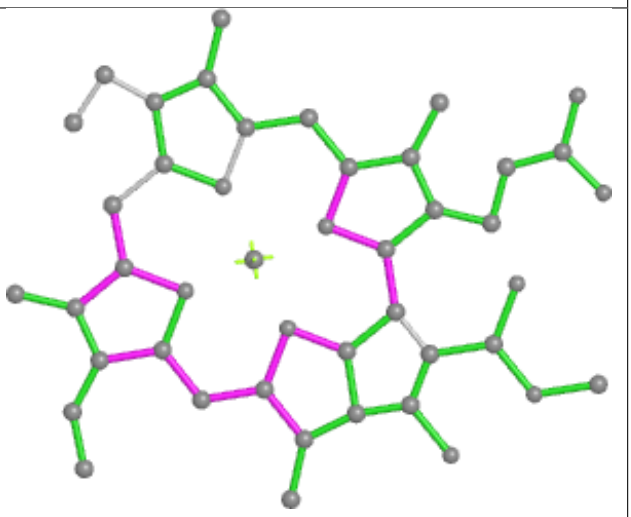


Rings

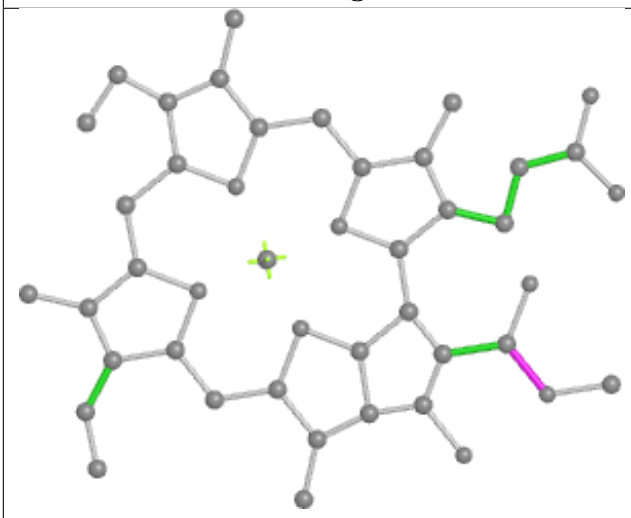
Ligand CLA B2 824



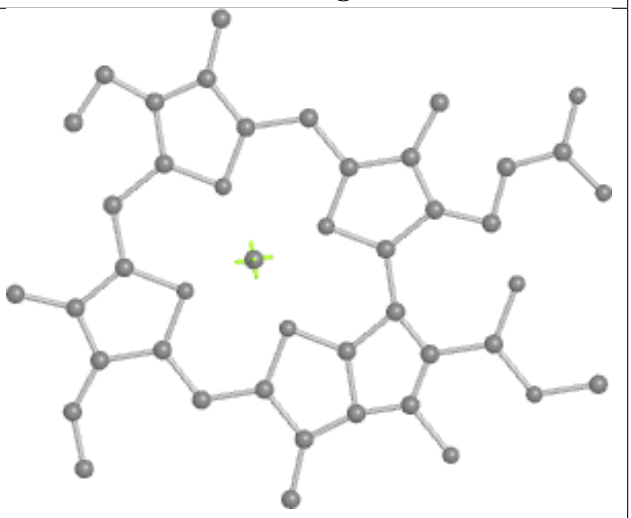
Bond lengths



Bond angles

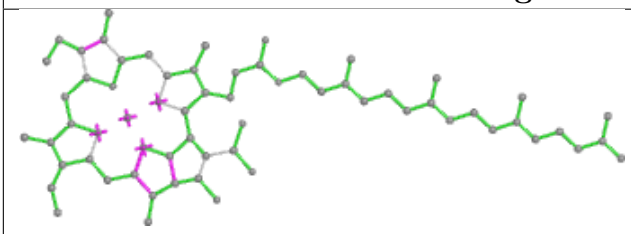


Torsions

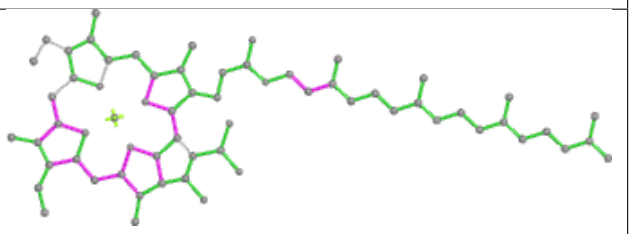


Rings

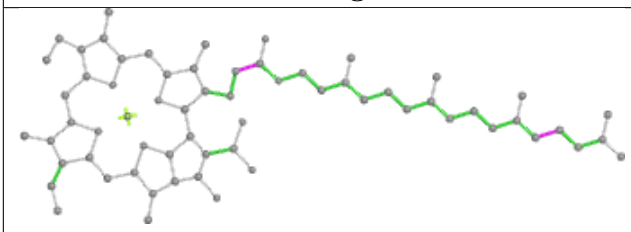
Ligand CLA A3 803



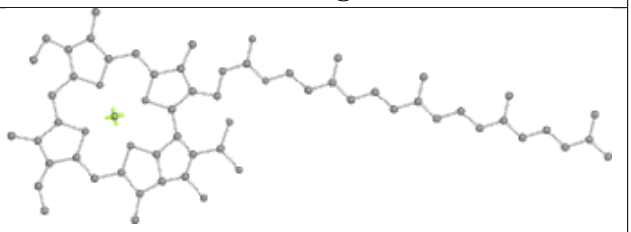
Bond lengths



Bond angles

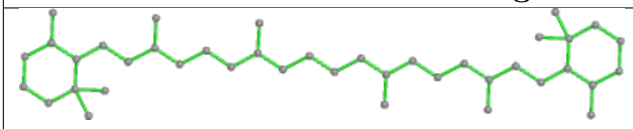


Torsions

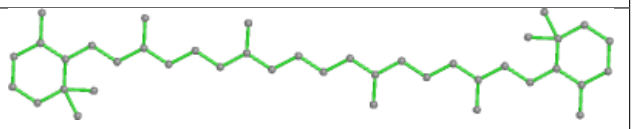


Rings

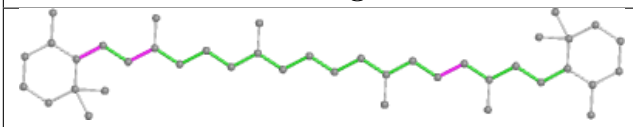
Ligand BCR A3 851



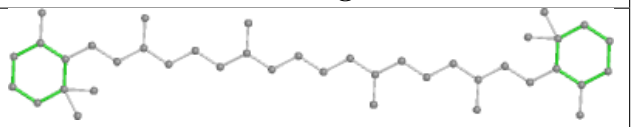
Bond lengths



Bond angles

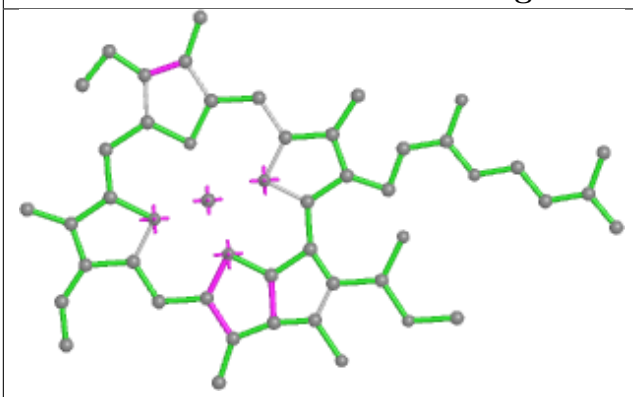


Torsions

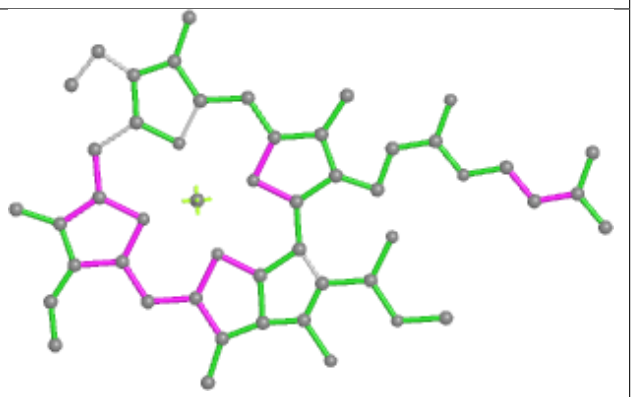


Rings

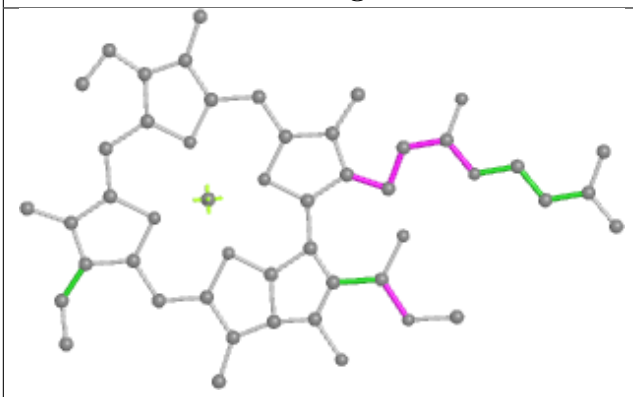
Ligand CLA A1 818



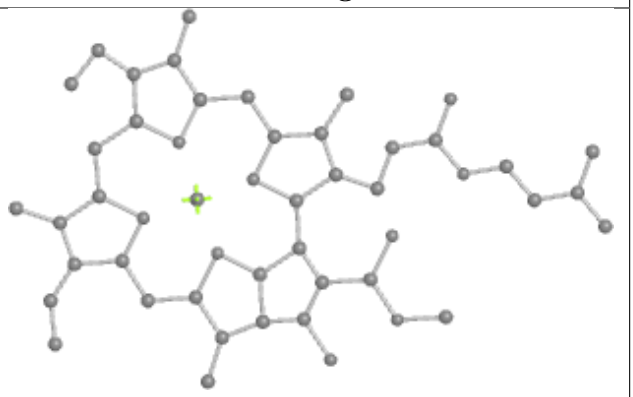
Bond lengths



Bond angles

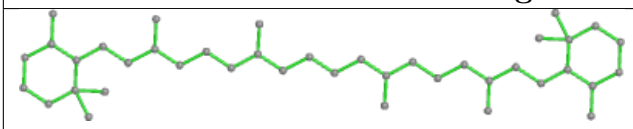


Torsions

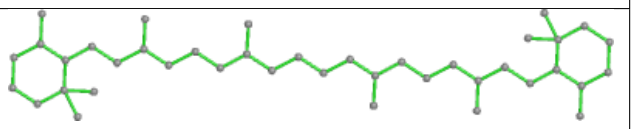


Rings

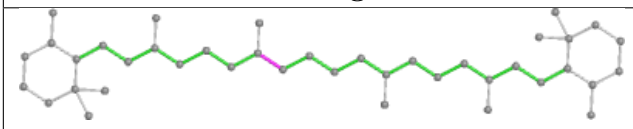
Ligand BCR F2 201



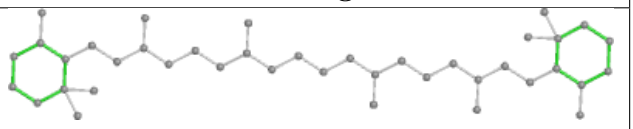
Bond lengths



Bond angles

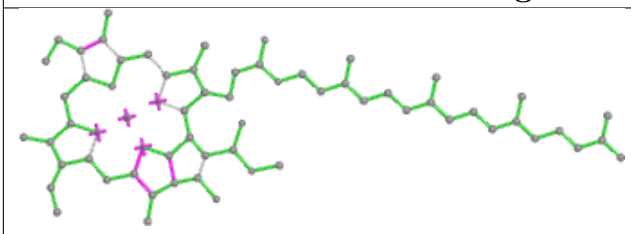


Torsions



Rings

Ligand CLA A3 804



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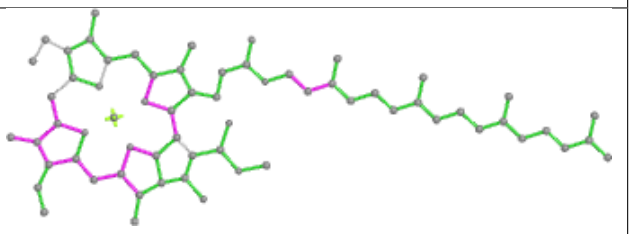
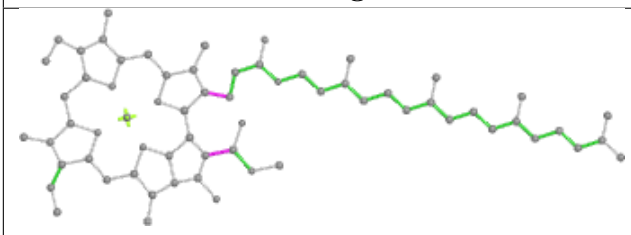


Bond angles



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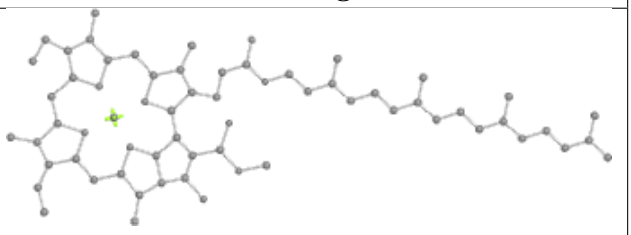
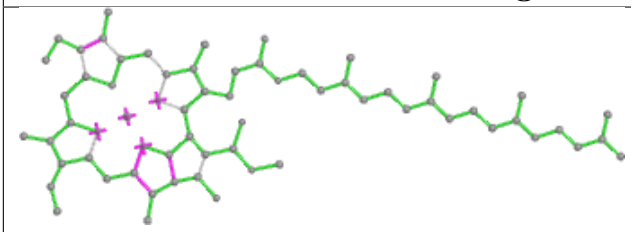
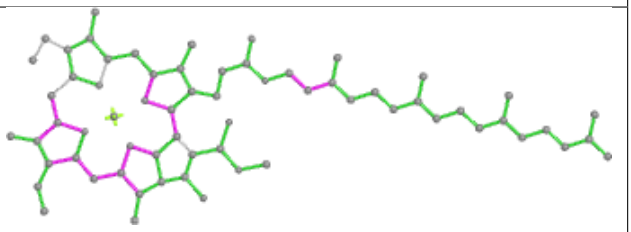


Rings

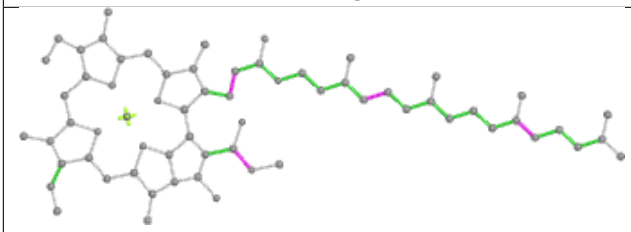
Ligand CLA B1 838



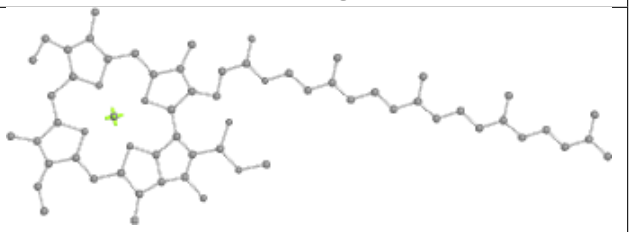
Bond lengths



Bond angles

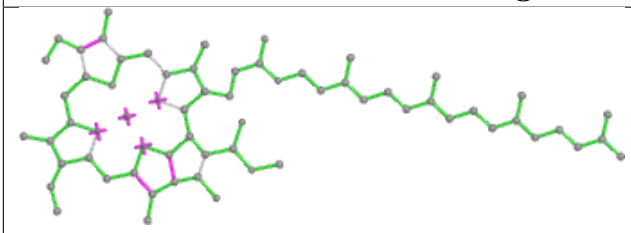


Torsions

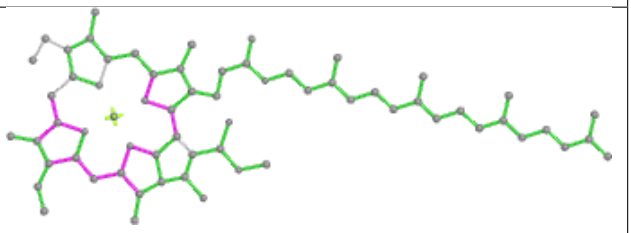


Rings

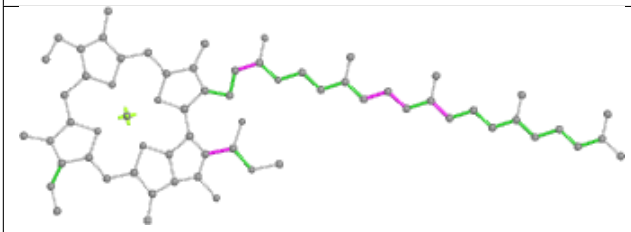
Ligand CLA A3 856



Bond lengths



Bond angles



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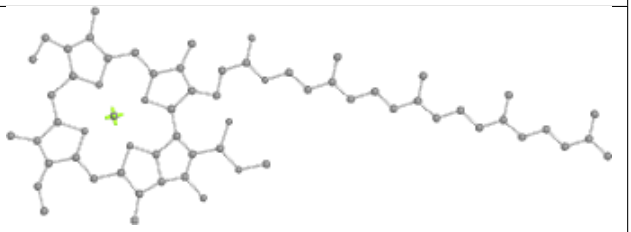
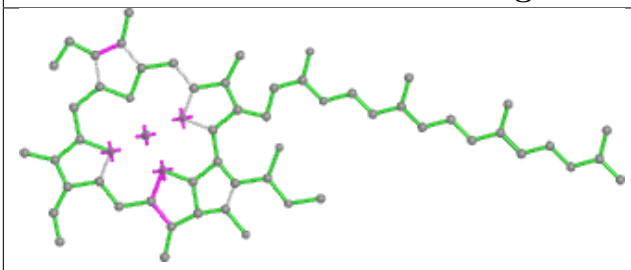
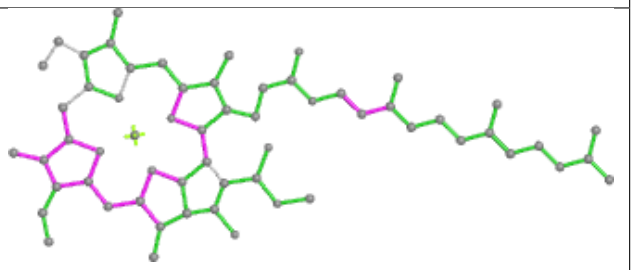
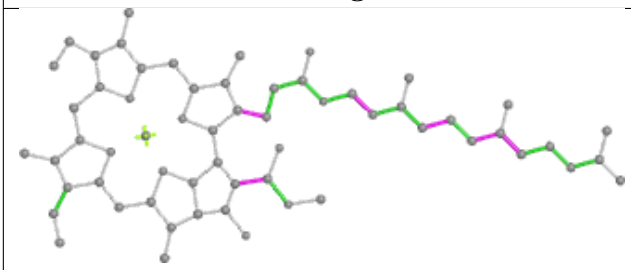
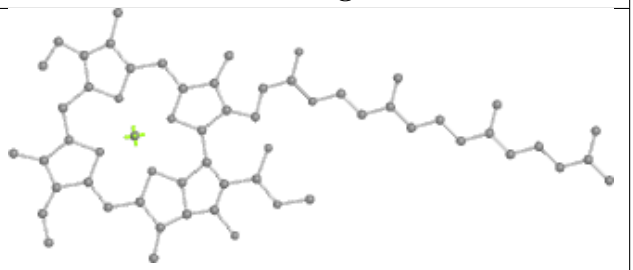
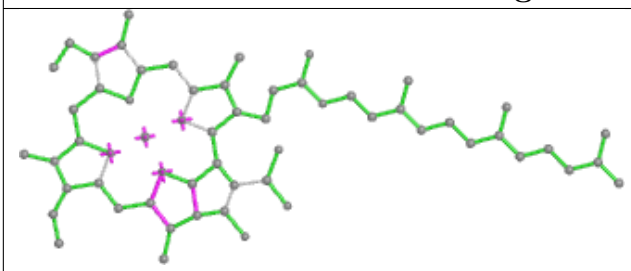
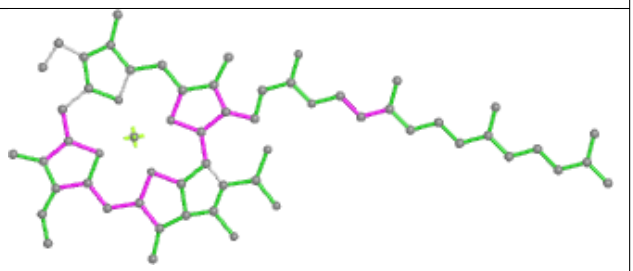
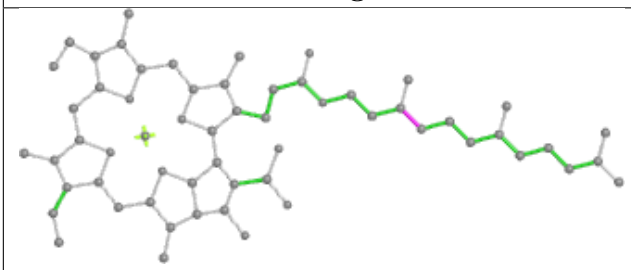
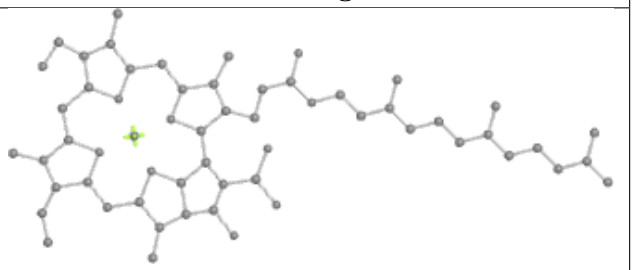
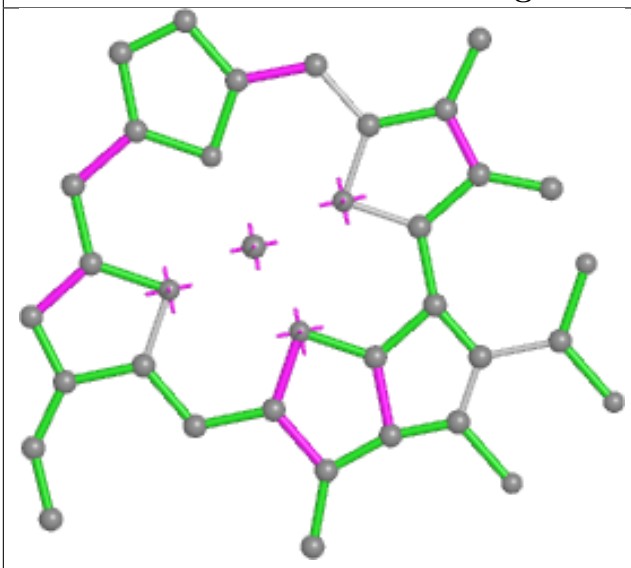


Rings

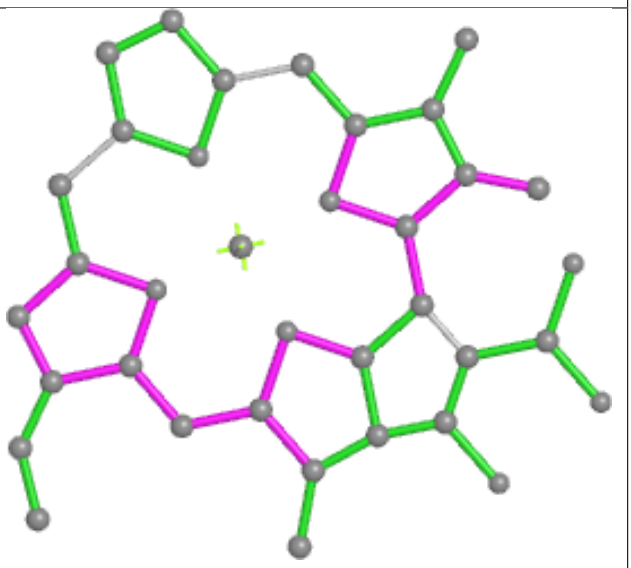
Ligand CLA A2 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

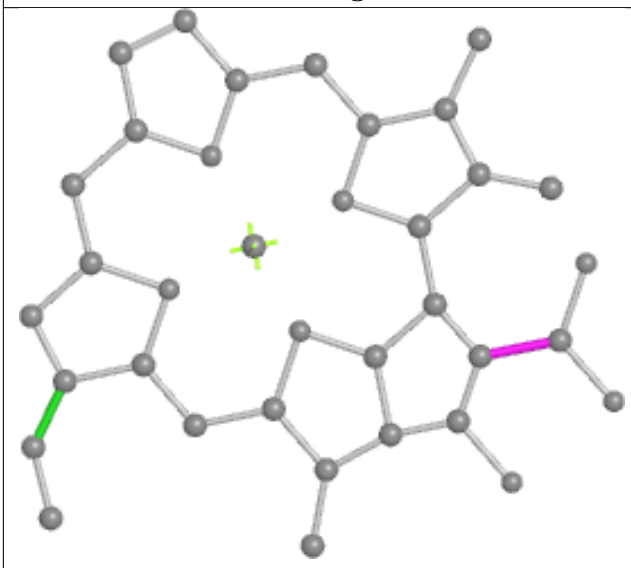
Ligand CLA A2 815



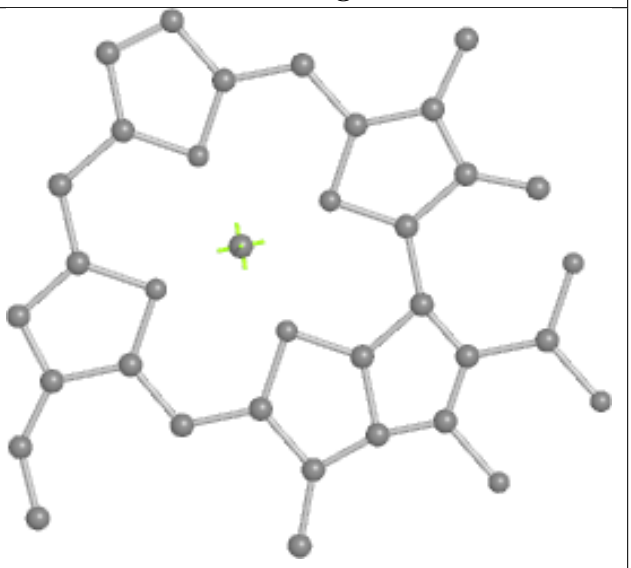
Bond lengths



Bond angles

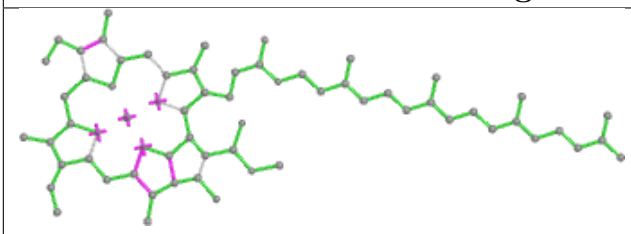


Torsions

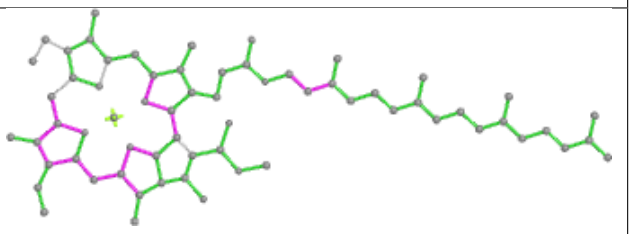


Rings

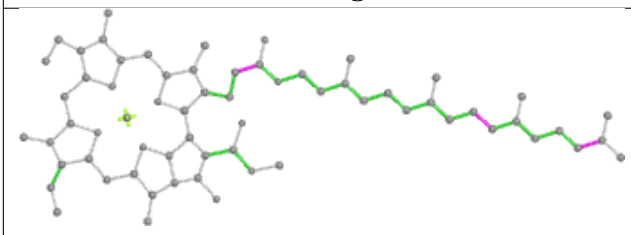
Ligand CLA A1 806



Bond lengths



Bond angles



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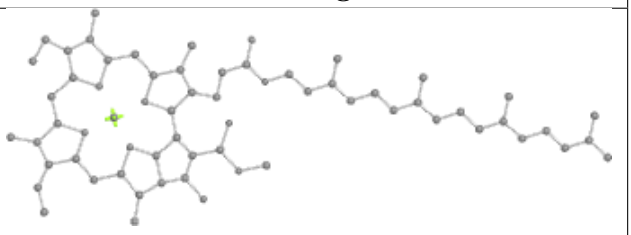
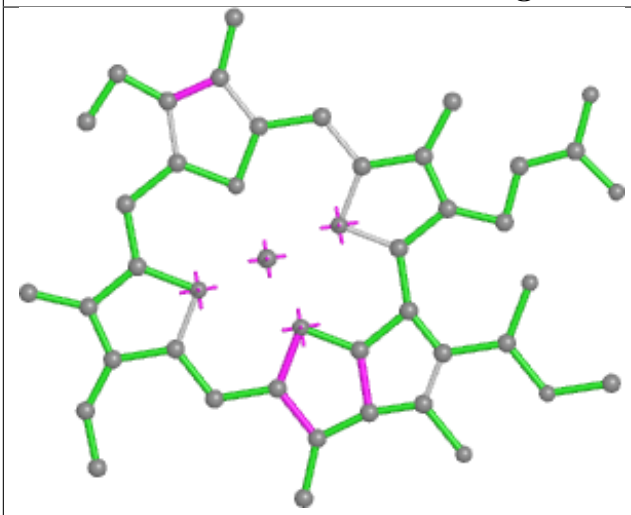
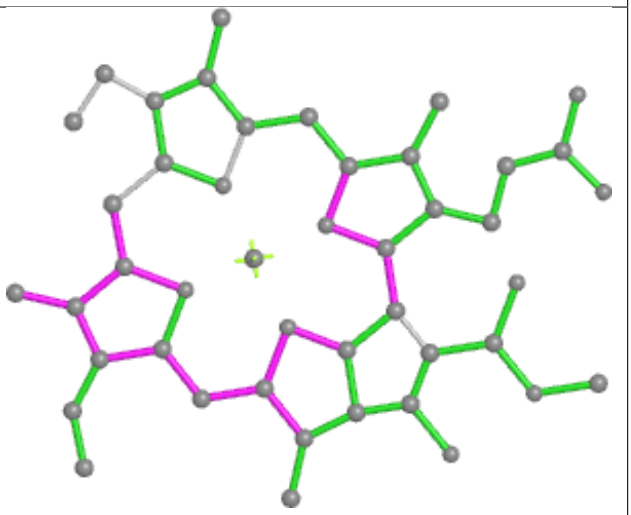


Rings

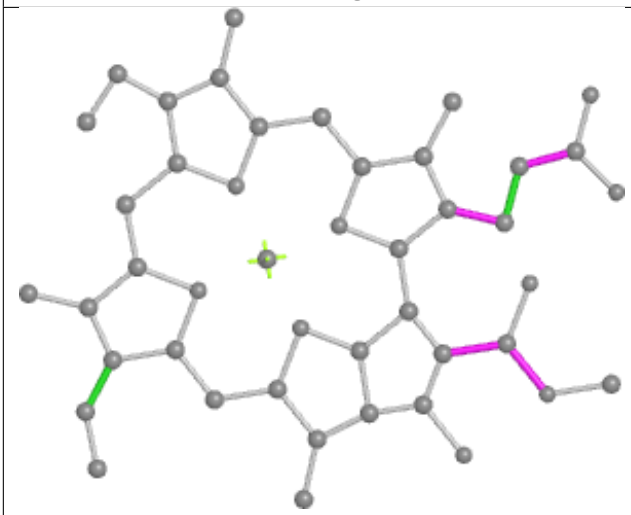
Ligand CLA B3 813



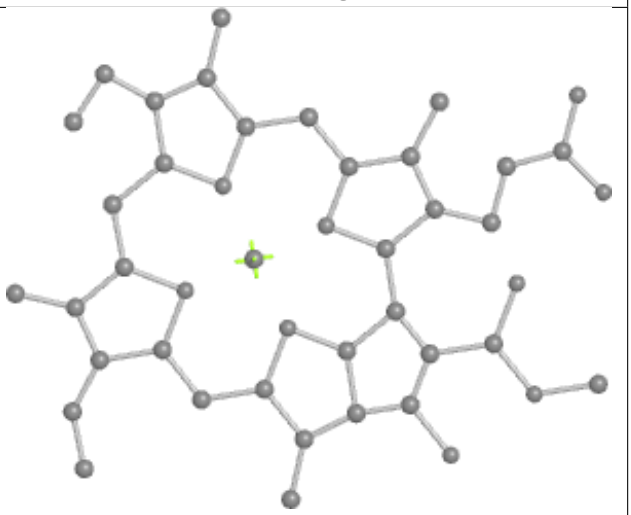
Bond lengths



Bond angles

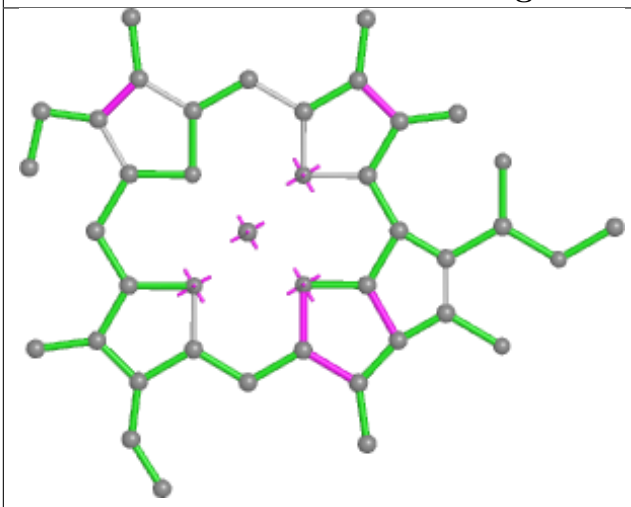


Torsions

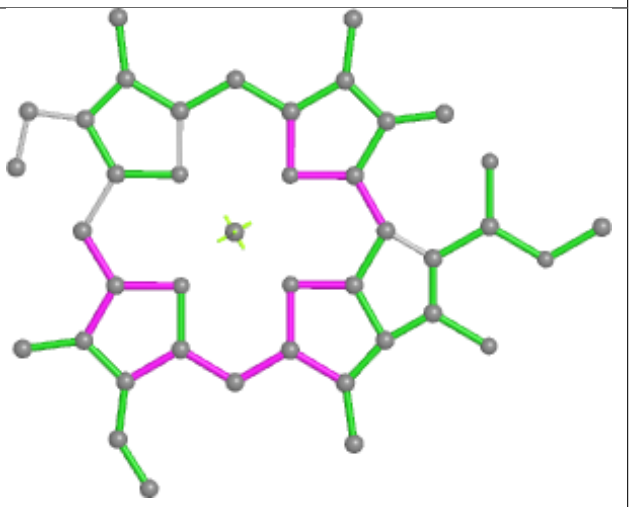


Rings

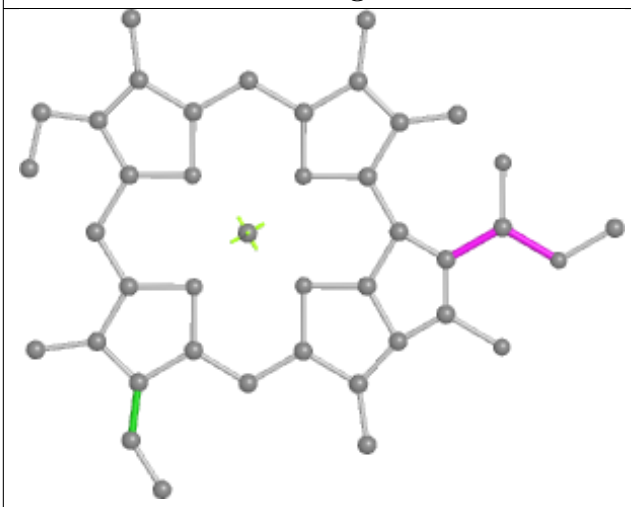
Ligand CLA B3 830



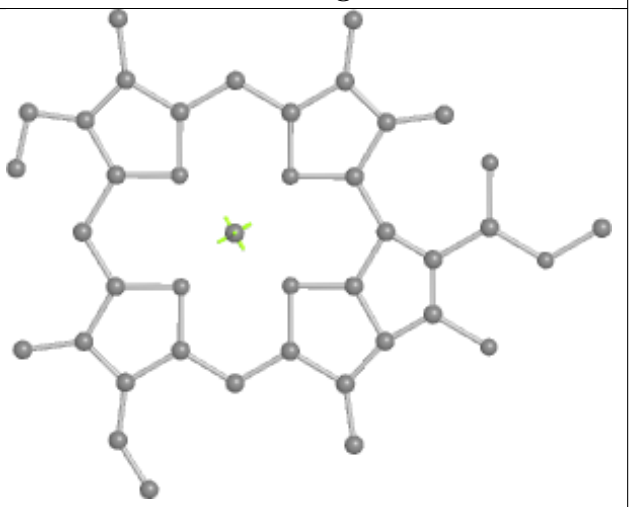
Bond lengths



Bond angles

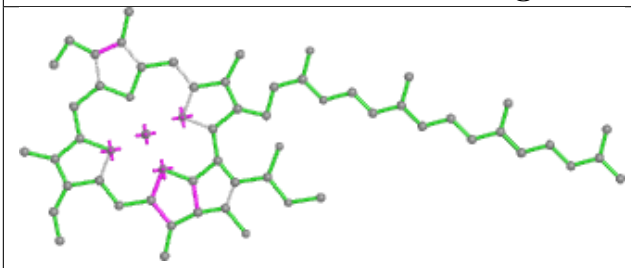


Torsions

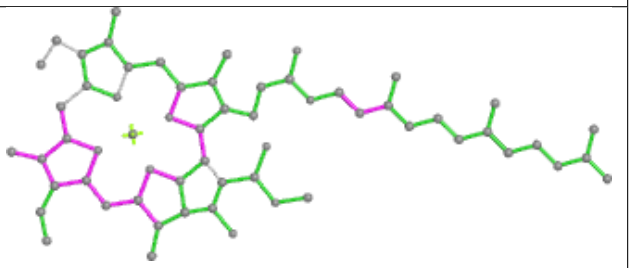


Rings

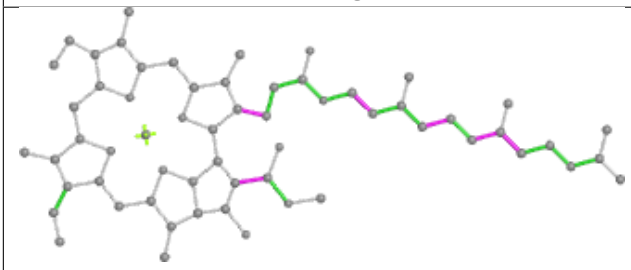
Ligand CLA A3 825



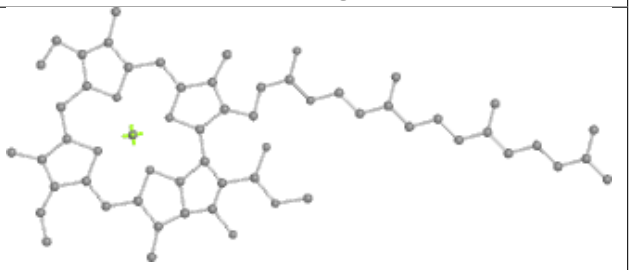
Bond lengths



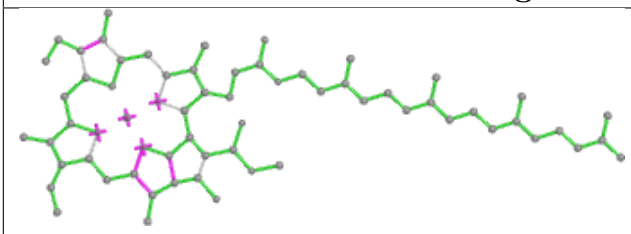
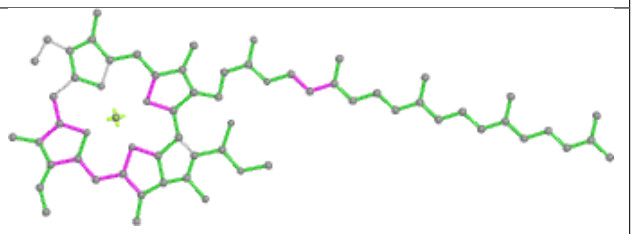
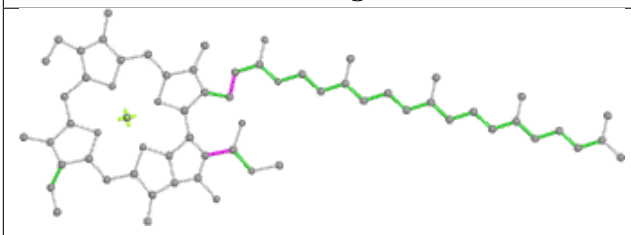
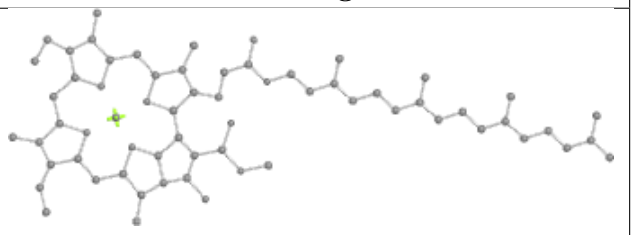
Bond angles

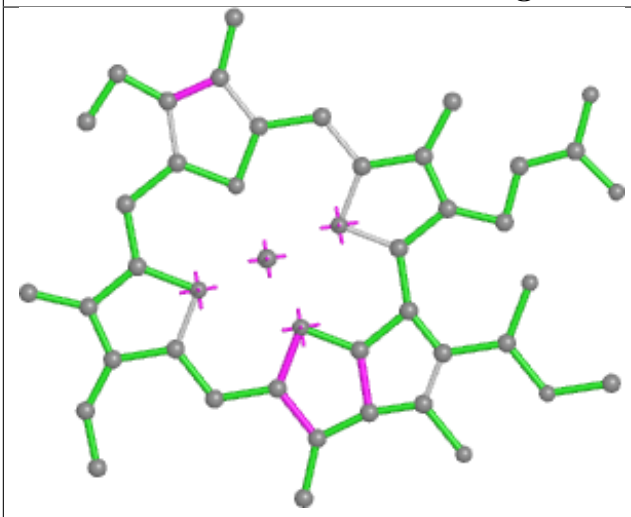
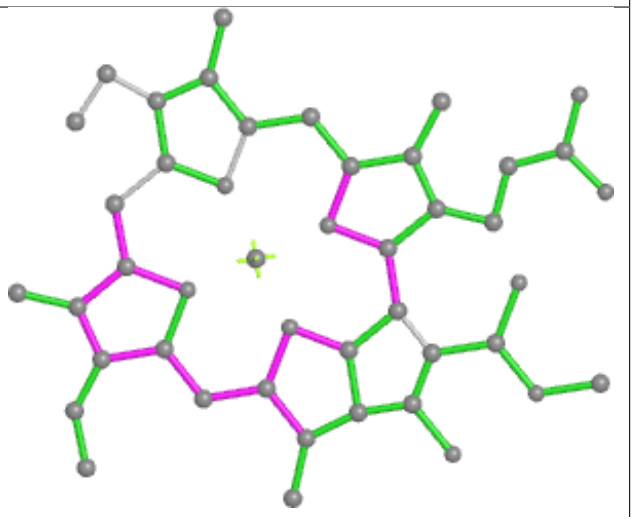
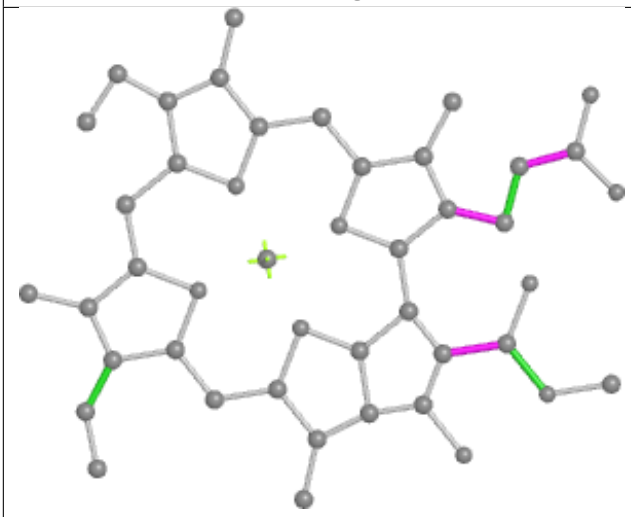
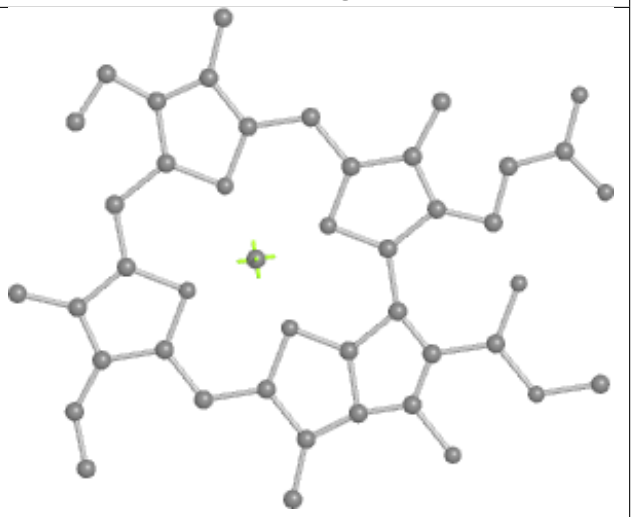


Torsions

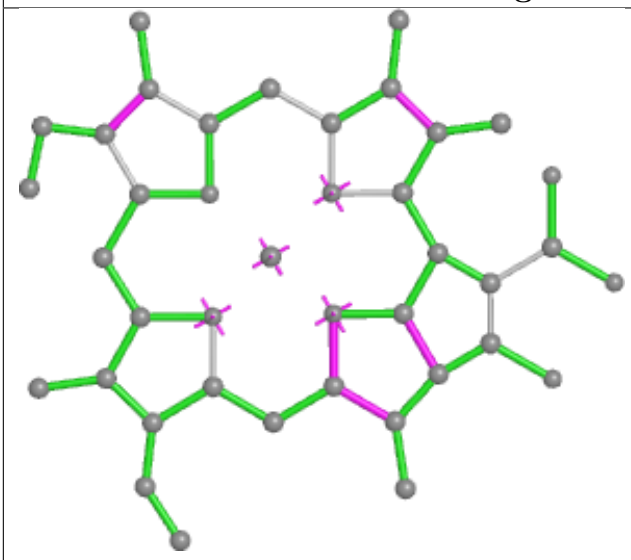


Rings

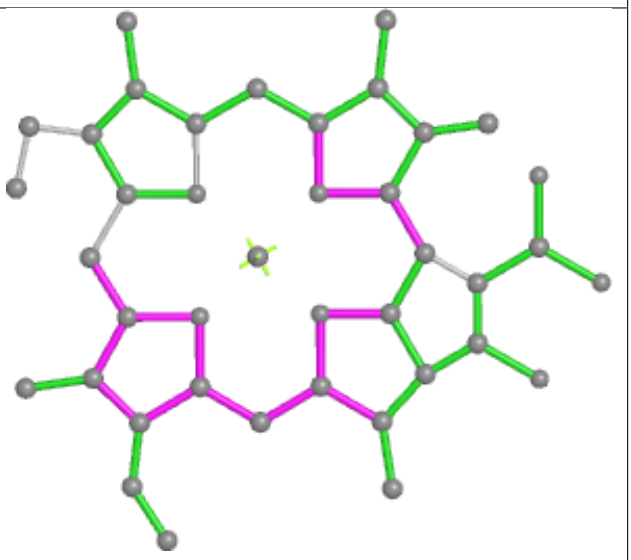
Ligand CLA A2 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

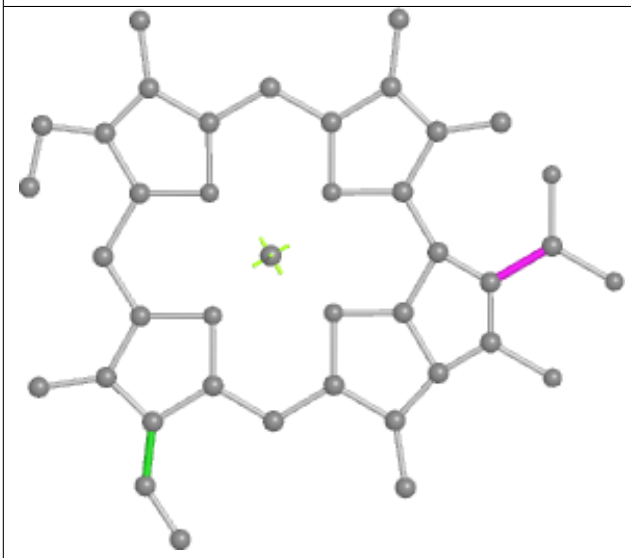
Ligand CLA A1 841



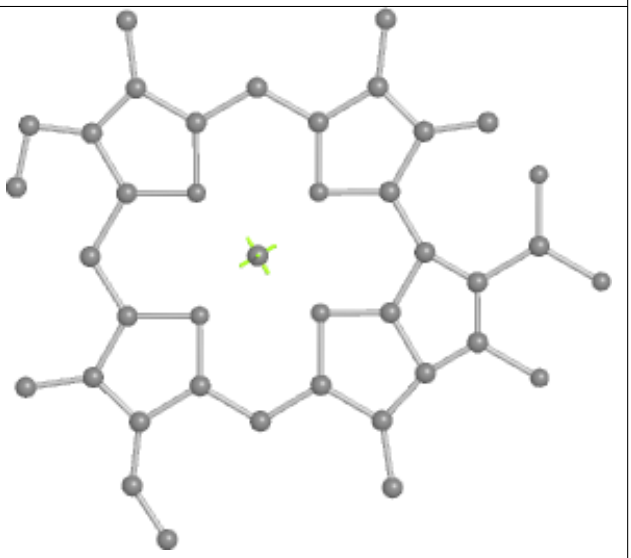
Bond lengths



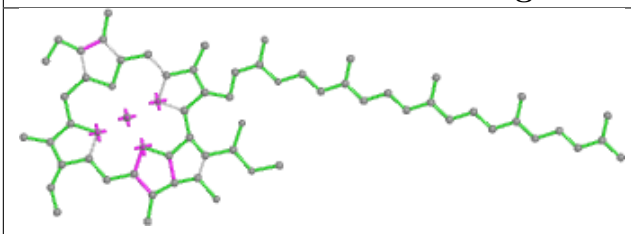
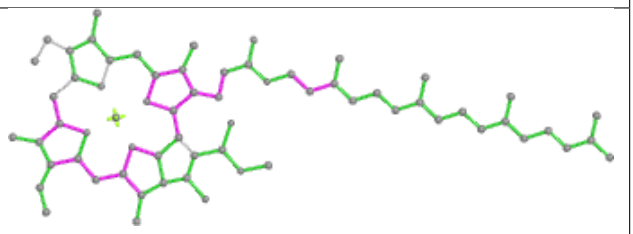
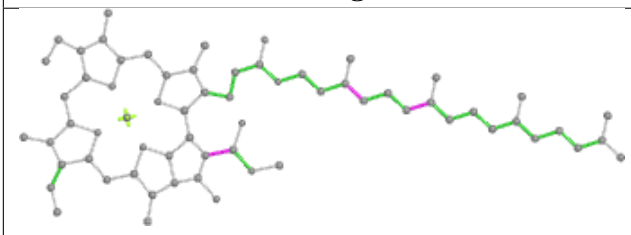
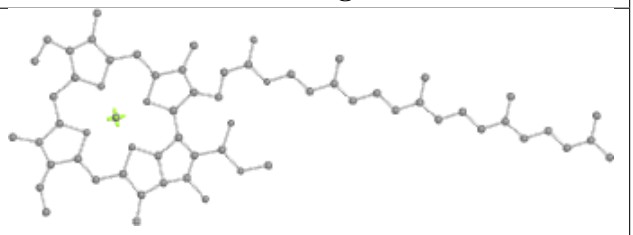
Bond angles

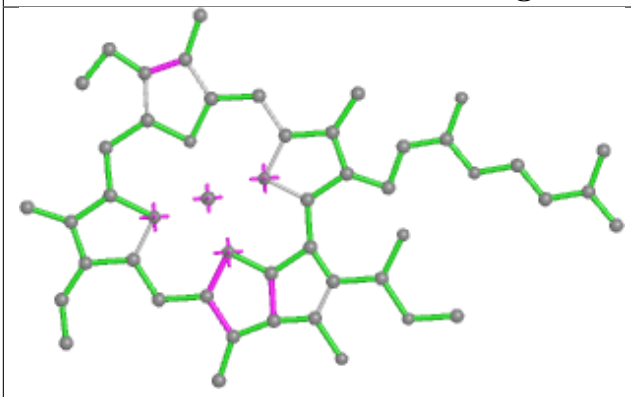
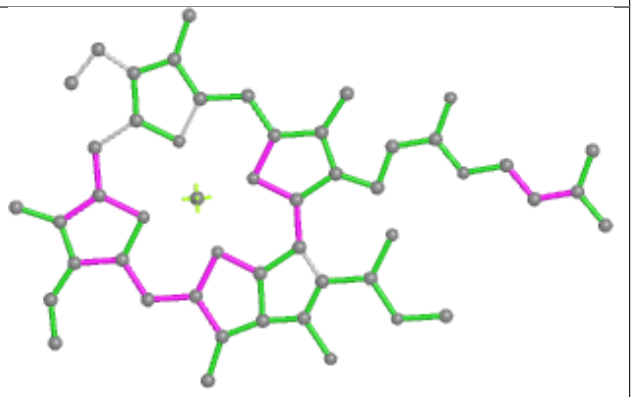
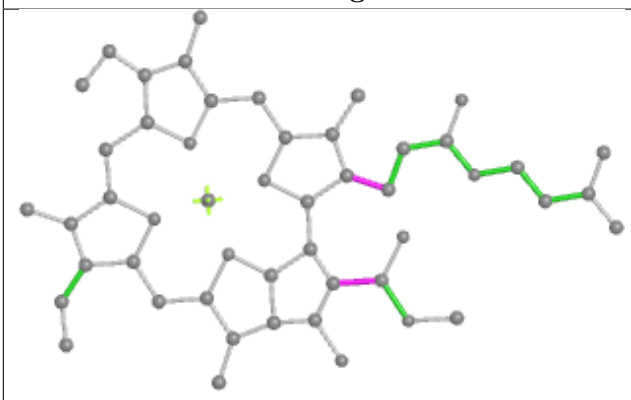
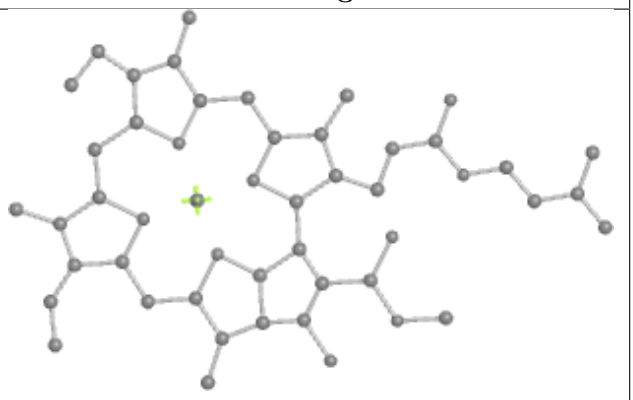


Torsions

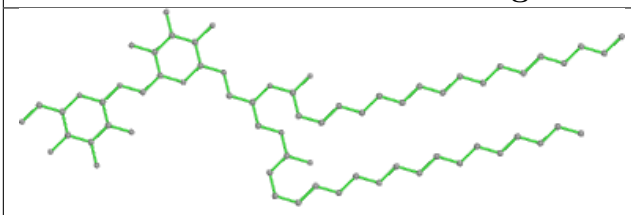


Rings

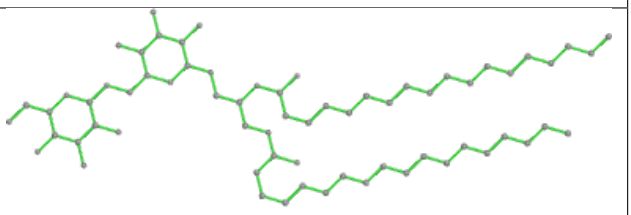
Ligand CLA B3 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B3 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

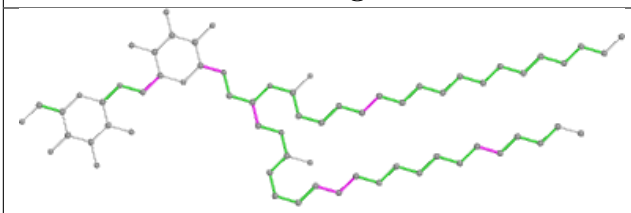
Ligand DGD B1 848



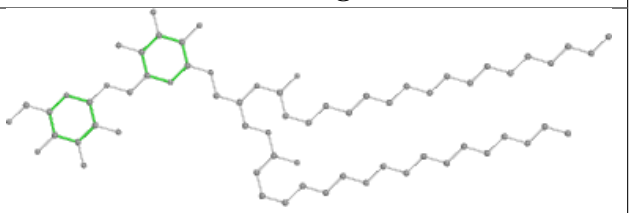
Bond lengths



Bond angles

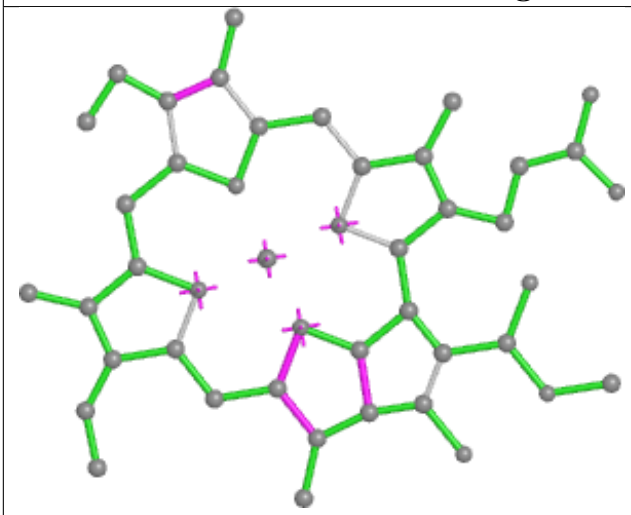


Torsions

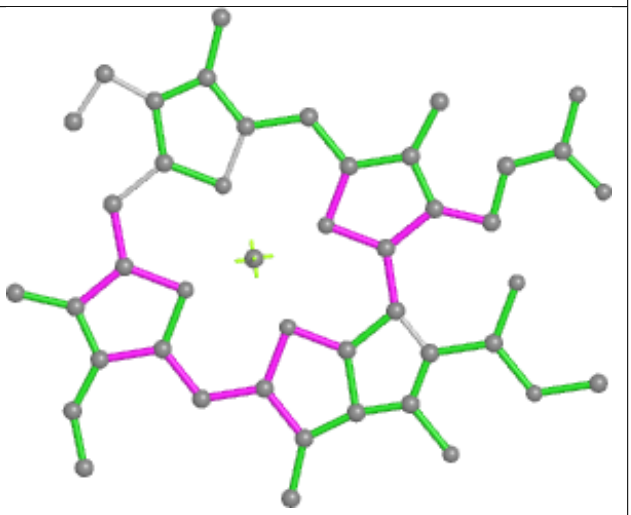


Rings

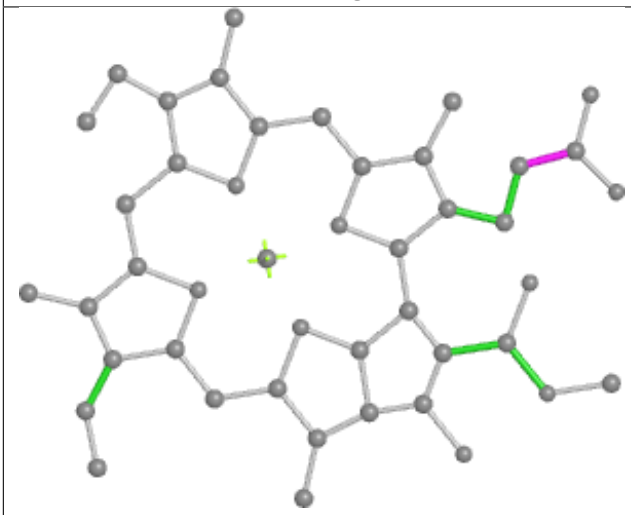
Ligand CLA A1 822



Bond lengths



Bond angles



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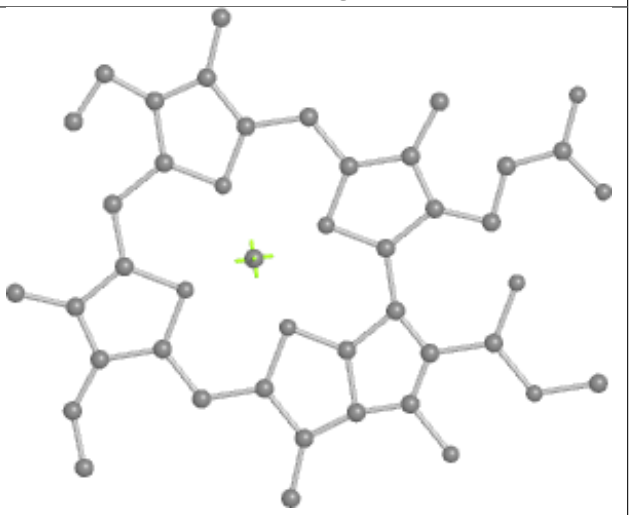
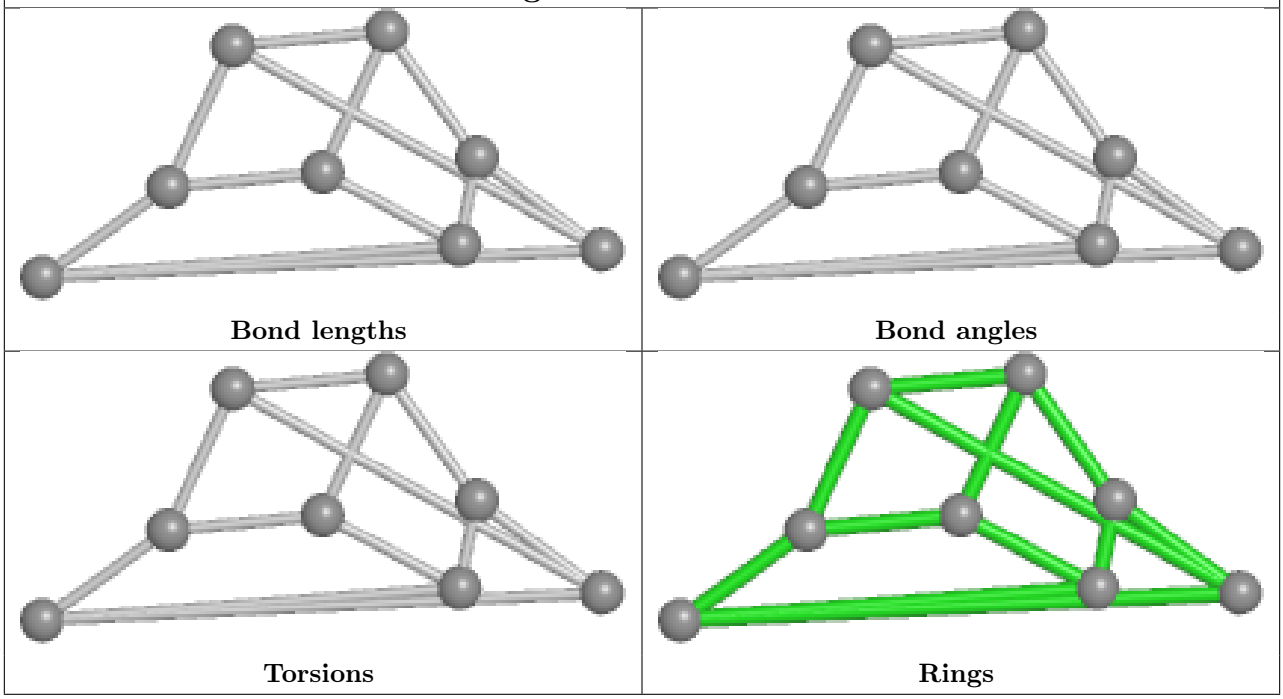
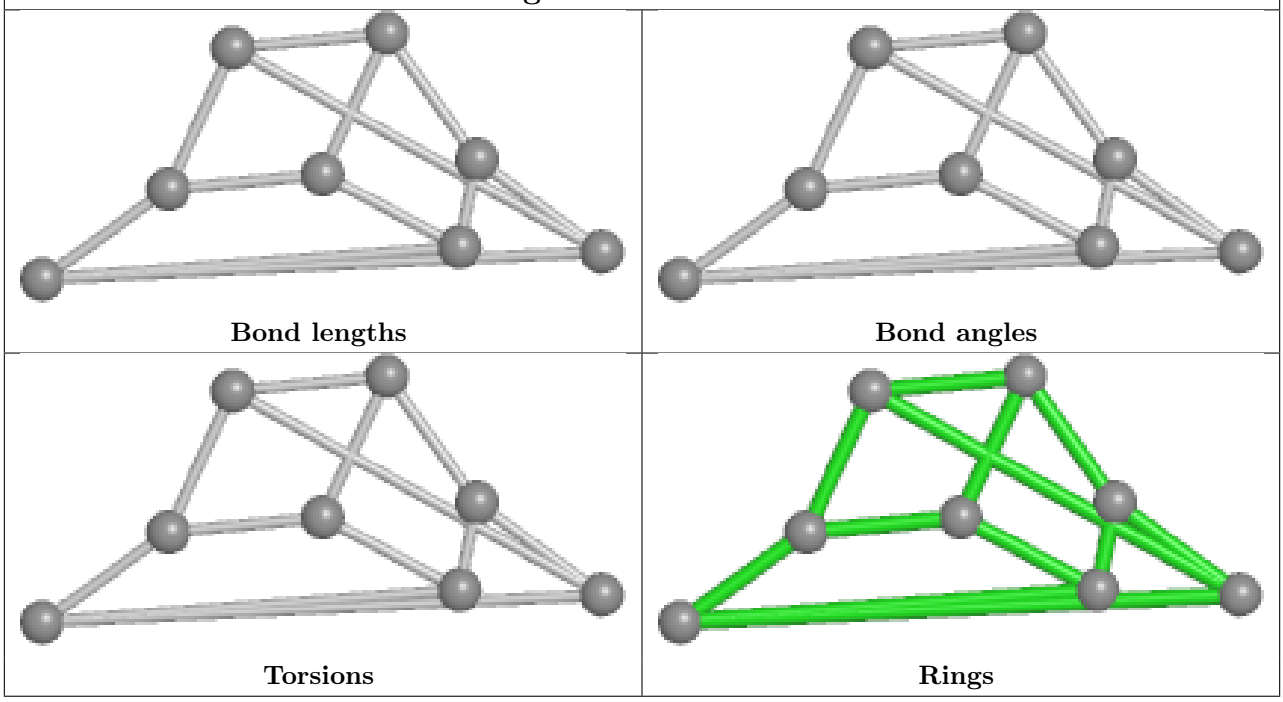


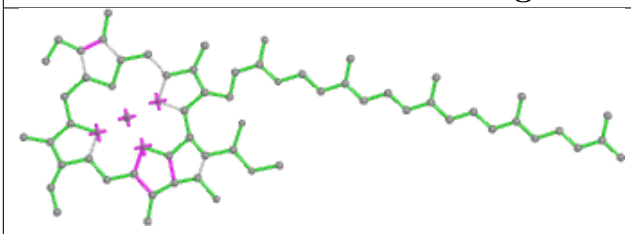
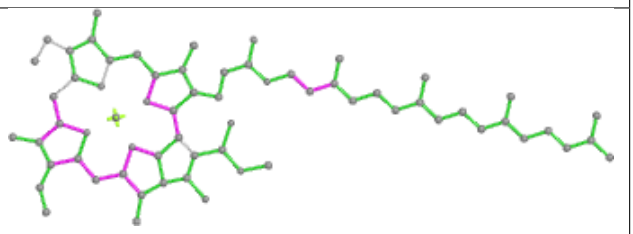
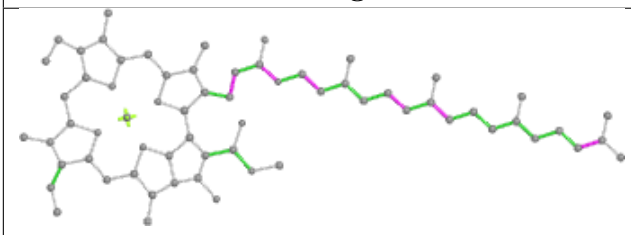
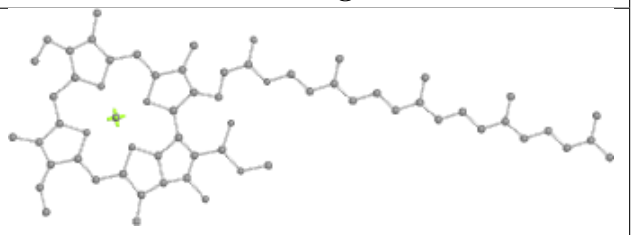
Rings

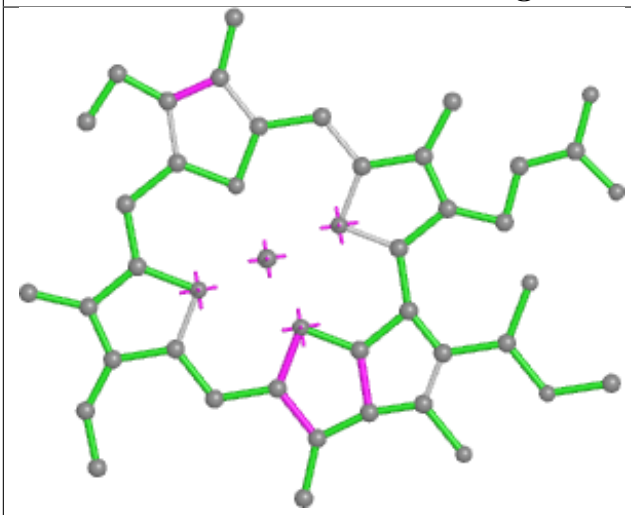
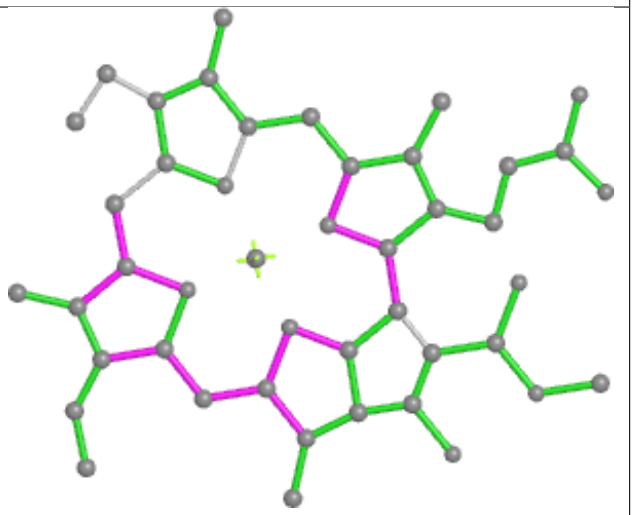
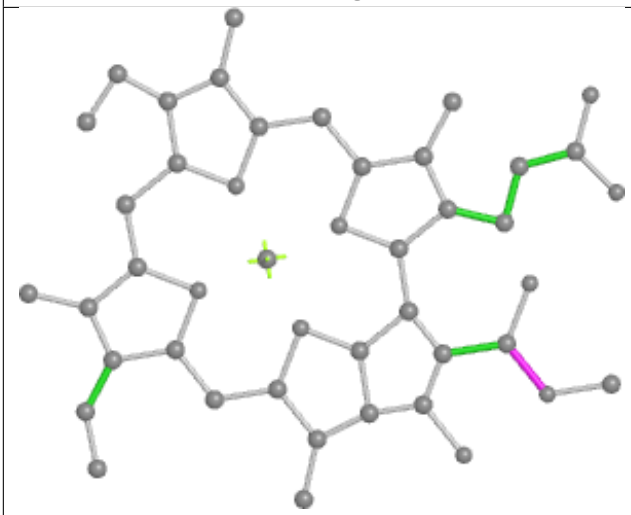
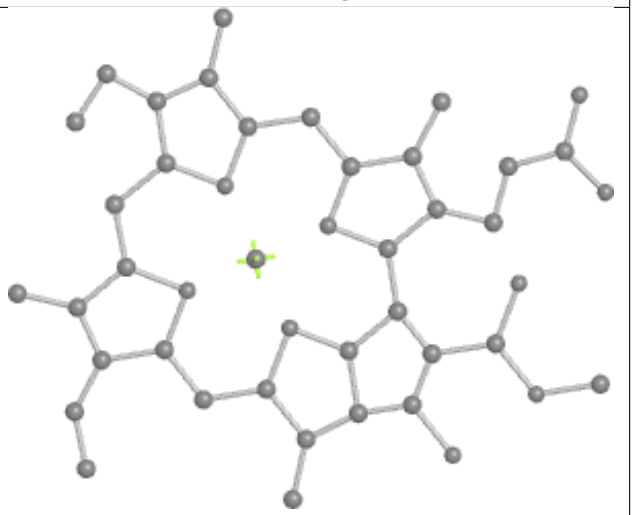
Ligand SF4 C1 101



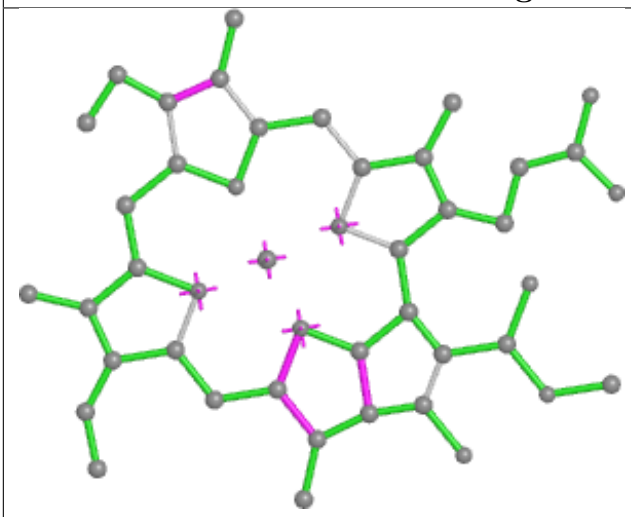
Ligand SF4 C3 101



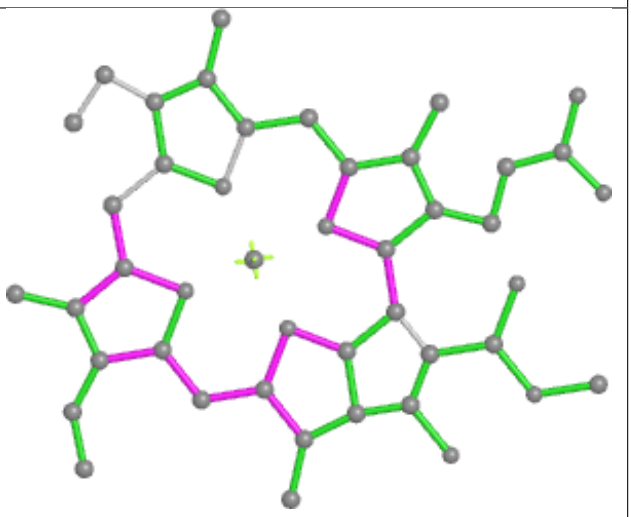
Ligand CLA A1 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

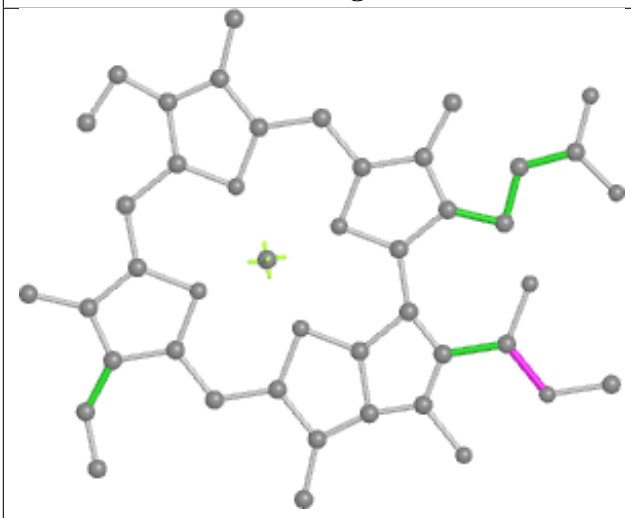
Ligand CLA B3 826



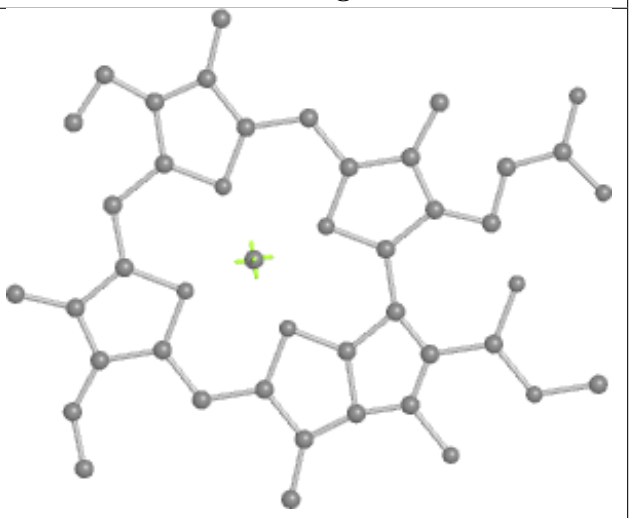
Bond lengths



Bond angles

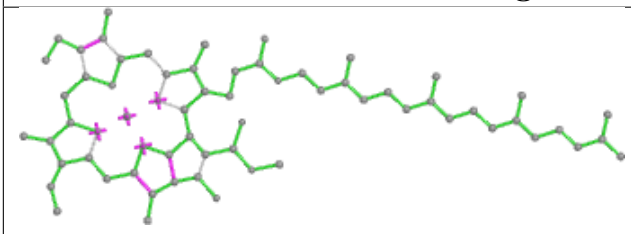


Torsions

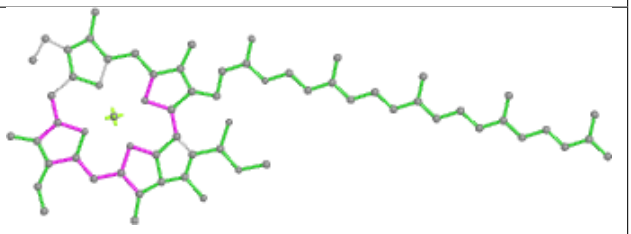


Rings

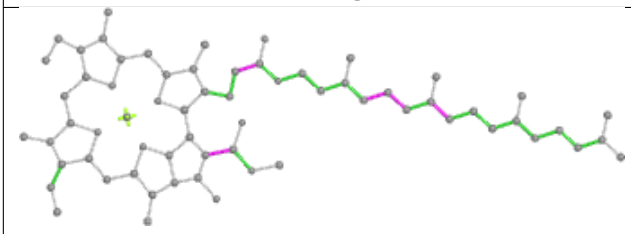
Ligand CLA A2 856



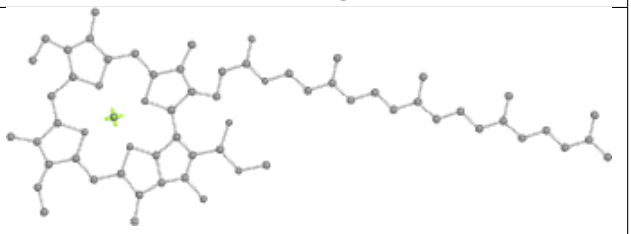
Bond lengths



Bond angles

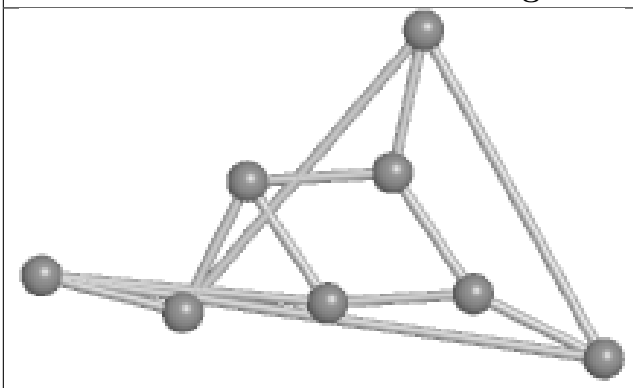


Torsions

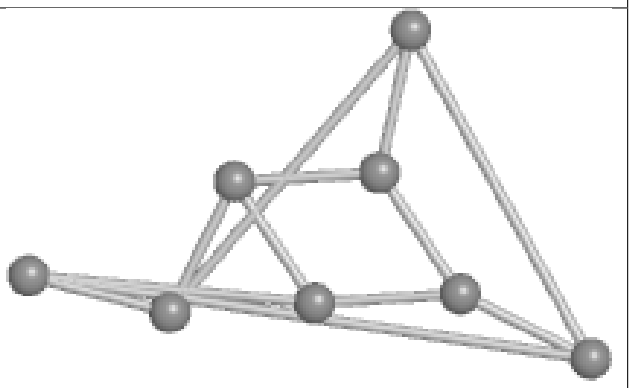


Rings

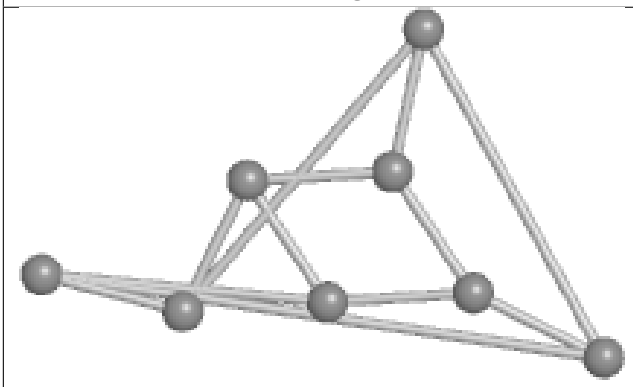
Ligand SF4 C2 102



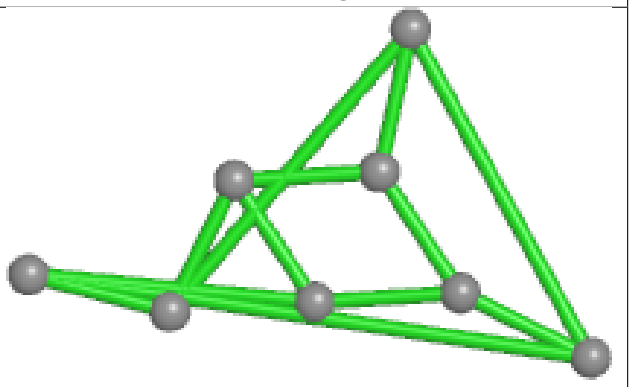
Bond lengths



Bond angles

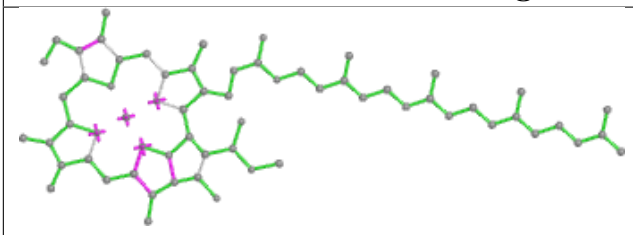


Torsions

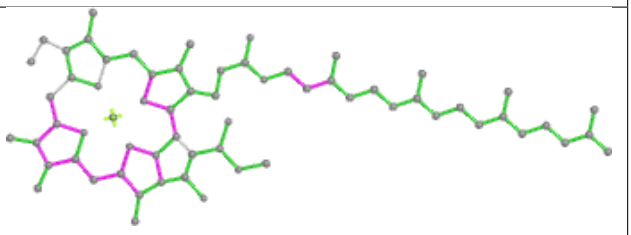


Rings

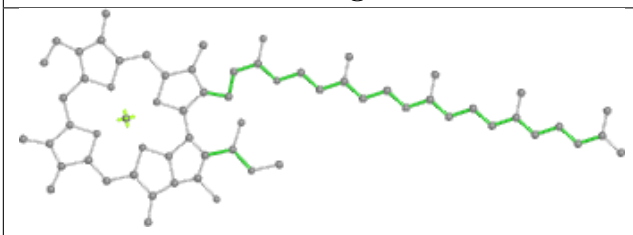
Ligand CLA A2 821



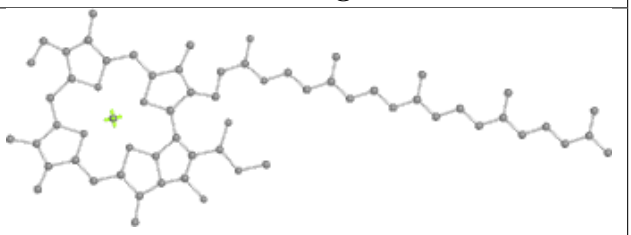
Bond lengths



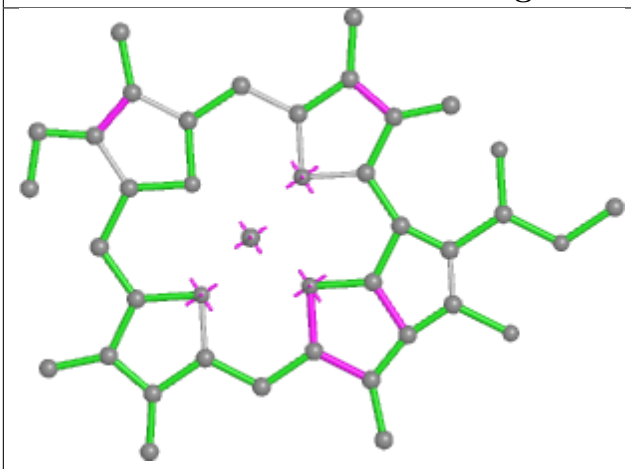
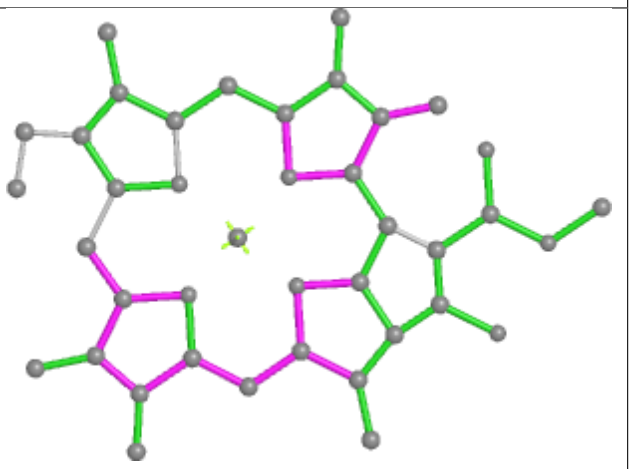
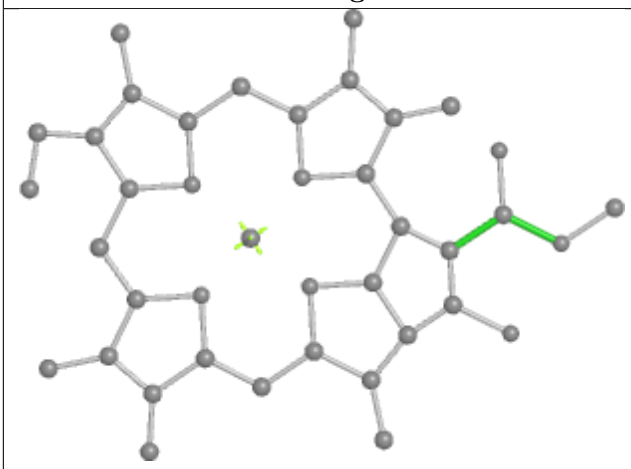
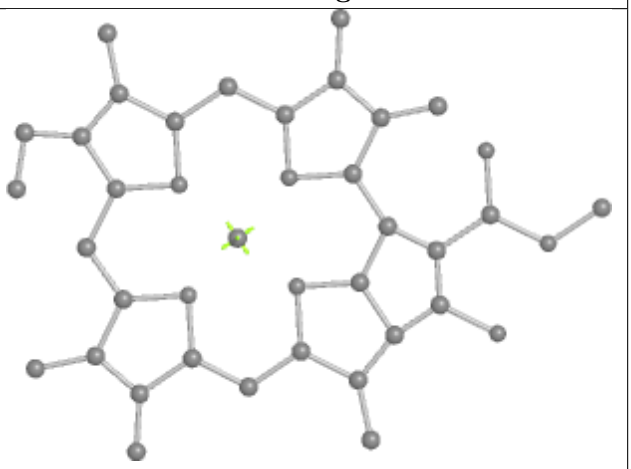
Bond angles



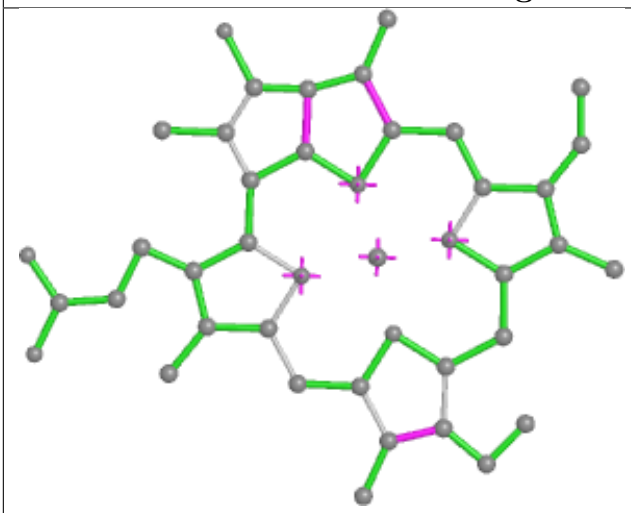
Torsions



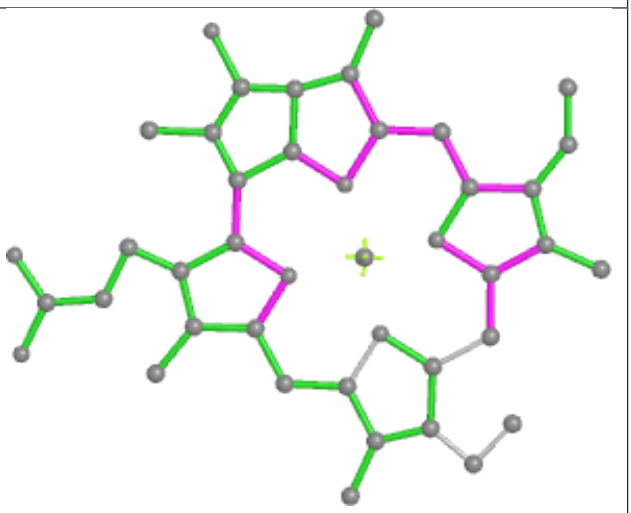
Rings

Ligand CLA A1 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

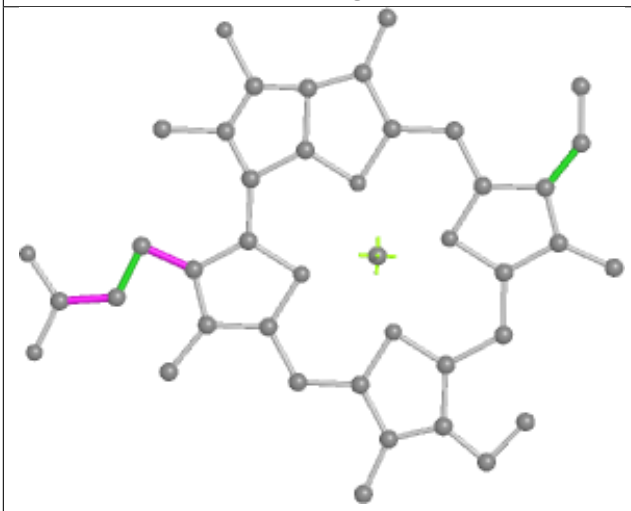
Ligand CLA B1 828



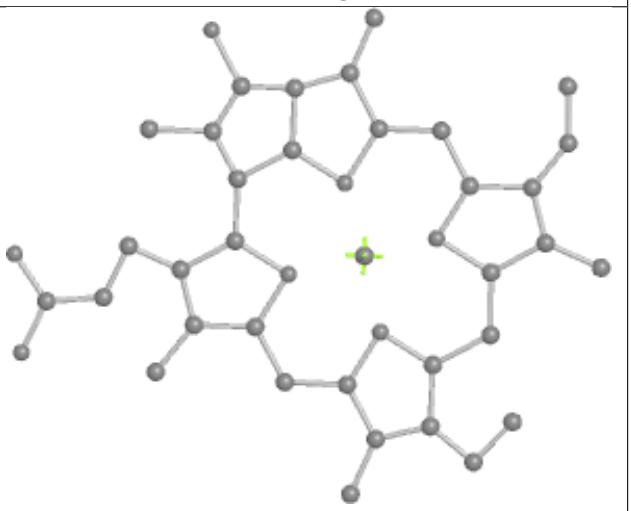
Bond lengths



Bond angles

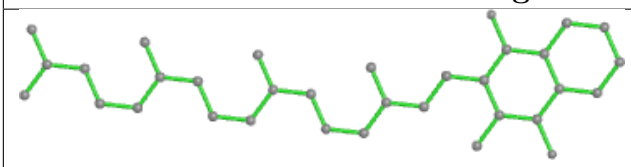


Torsions

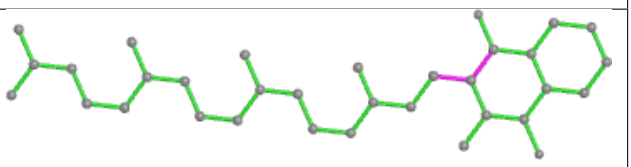


Rings

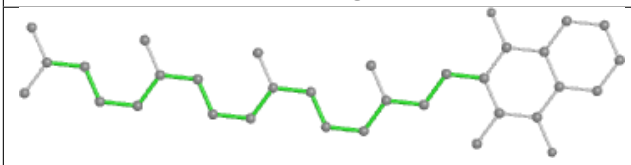
Ligand PQN A1 845



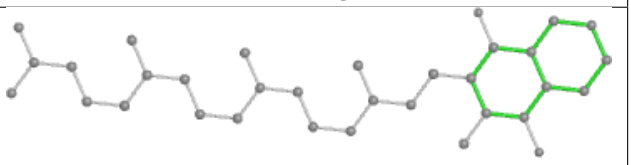
Bond lengths



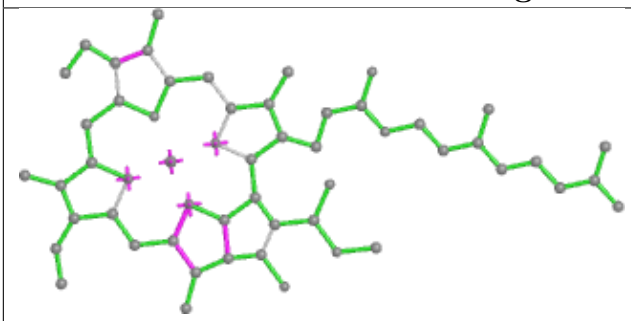
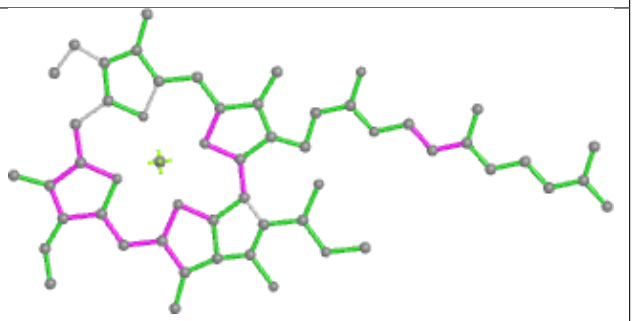
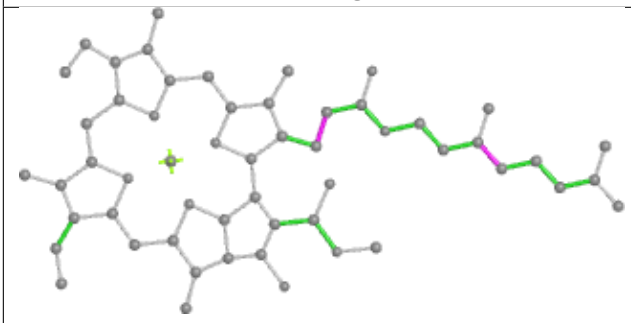
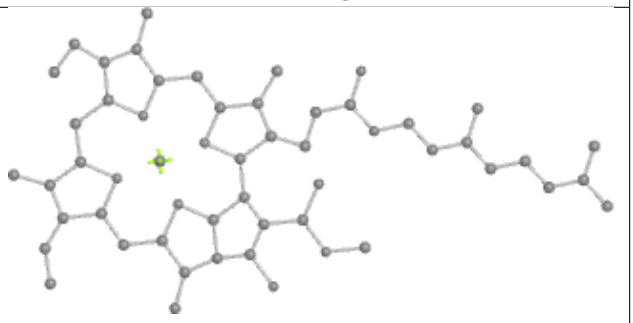
Bond angles



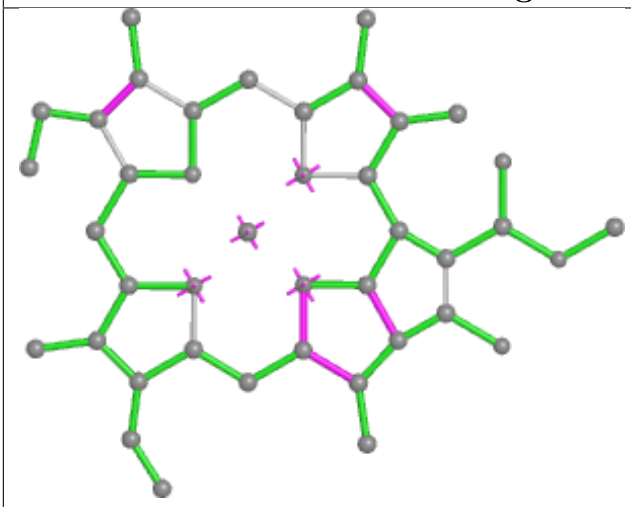
Torsions



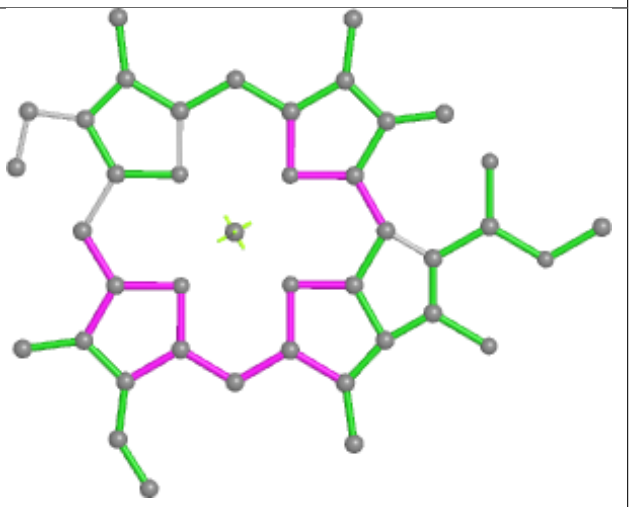
Rings

Ligand CLA A2 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

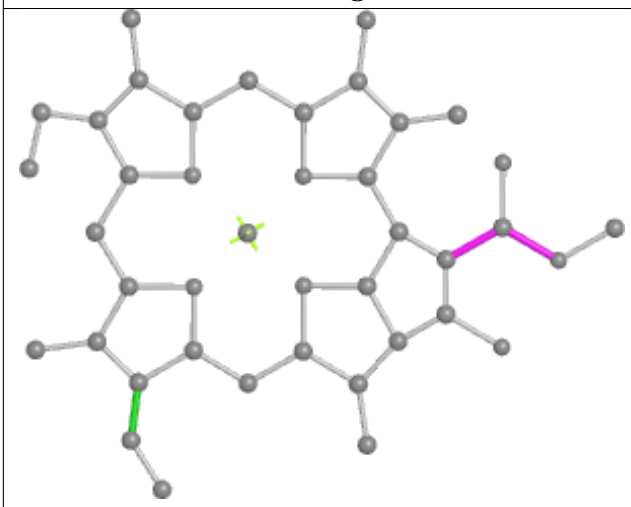
Ligand CLA B1 814



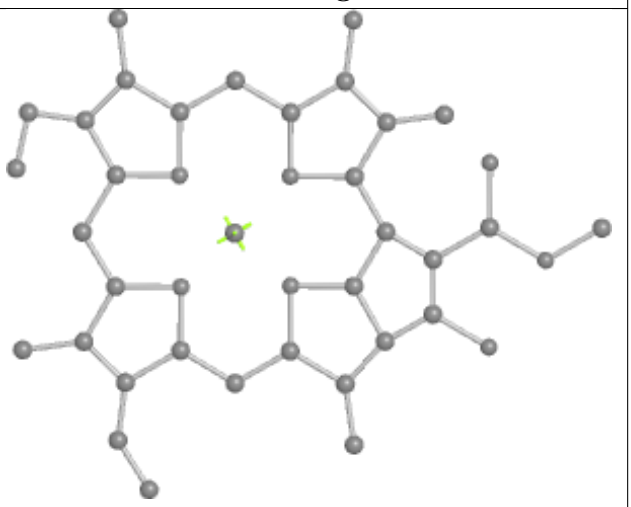
Bond lengths



Bond angles

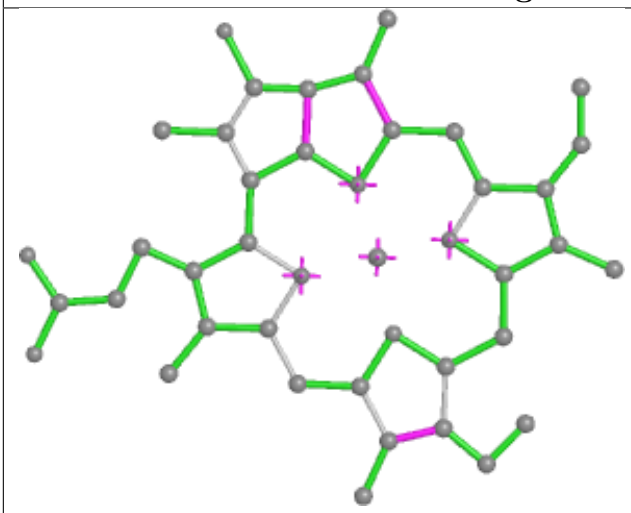


Torsions

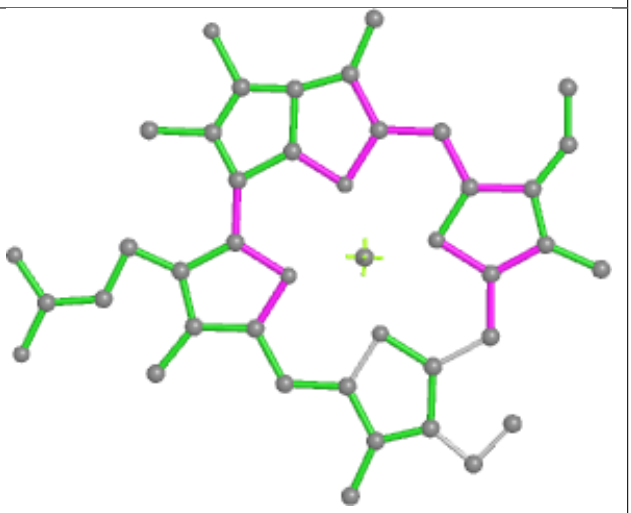


Rings

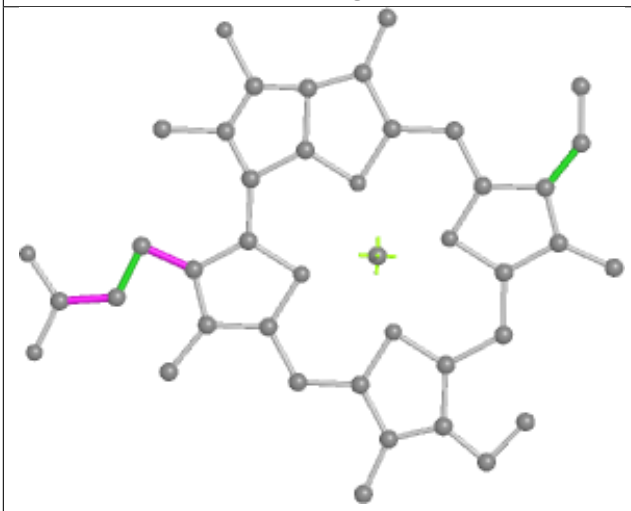
Ligand CLA B2 828



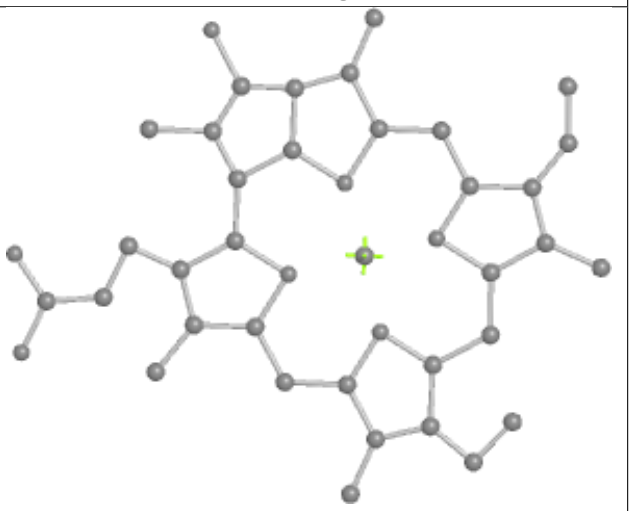
Bond lengths



Bond angles

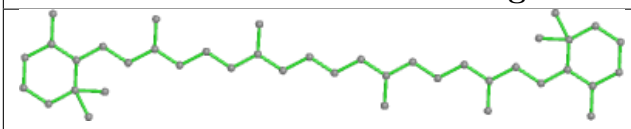


Torsions

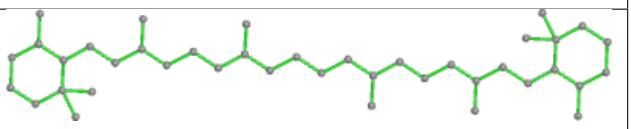


Rings

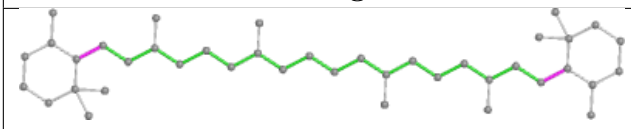
Ligand BCR J2 1305



Bond lengths

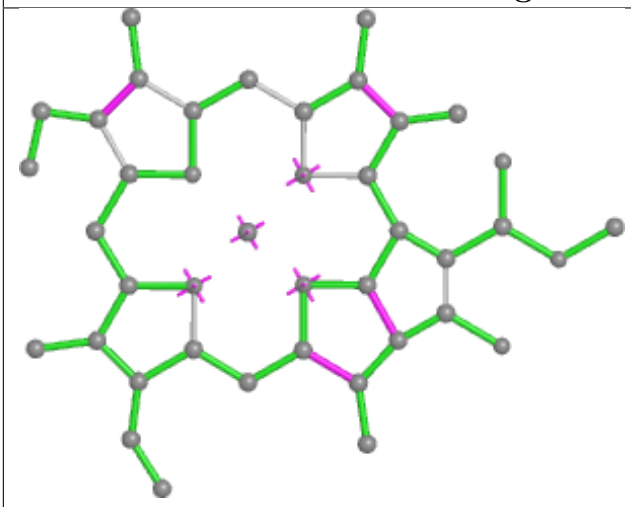
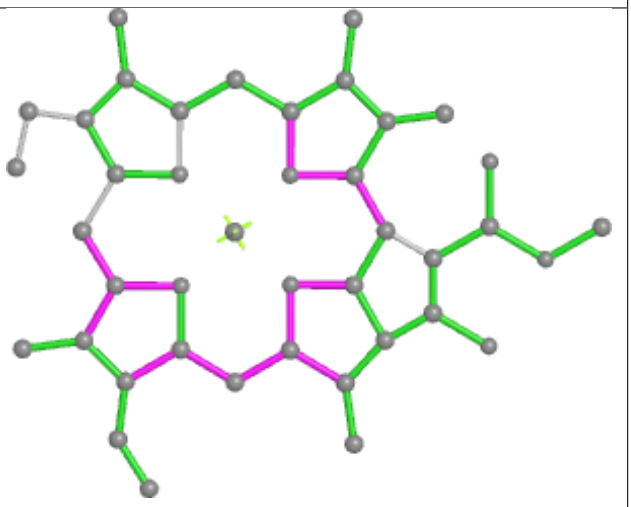
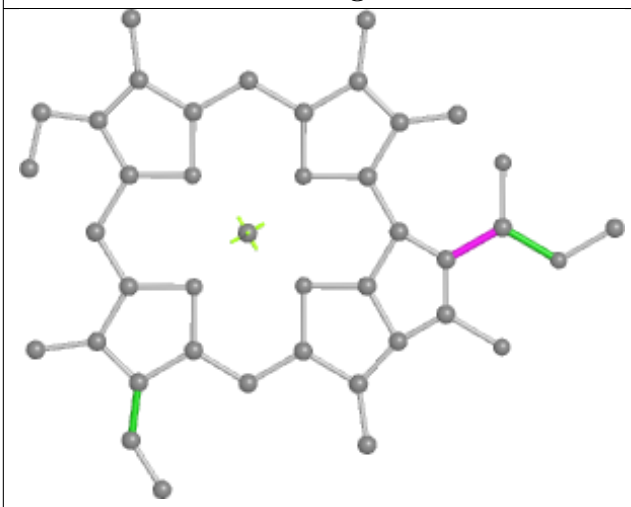
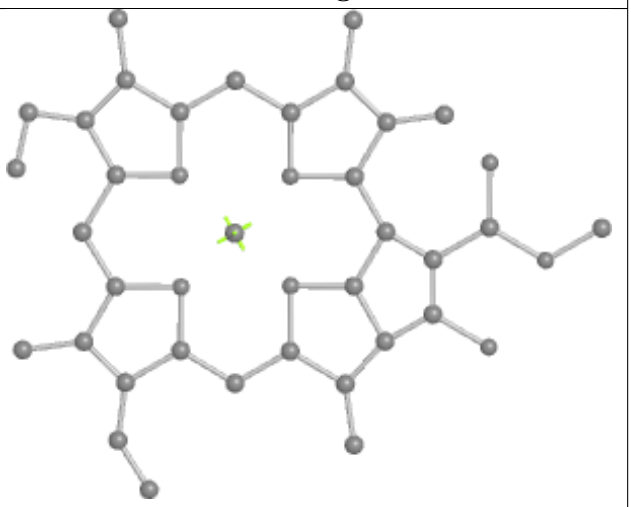


Bond angles

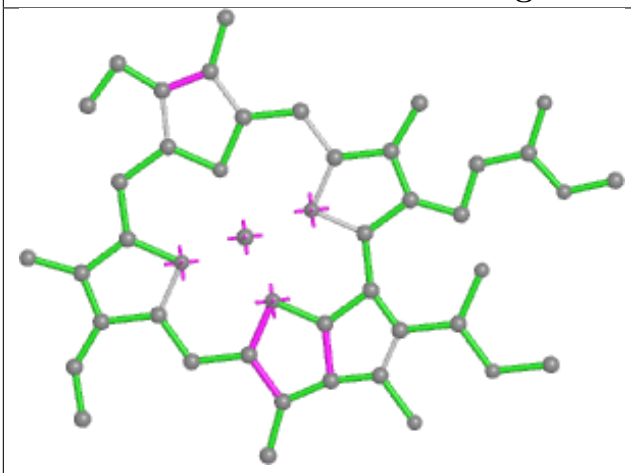


Torsions

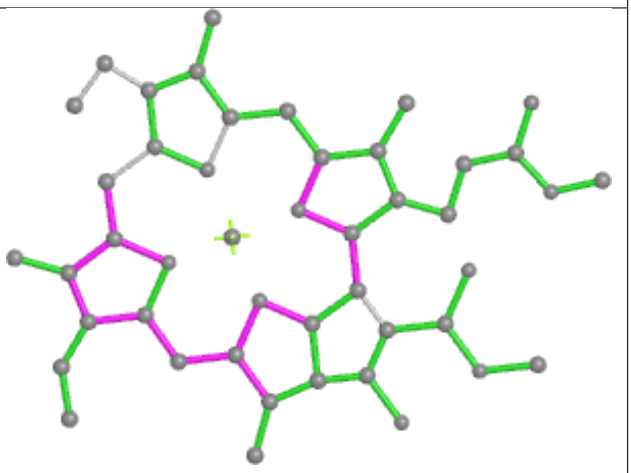
Rings

Ligand CLA A2 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

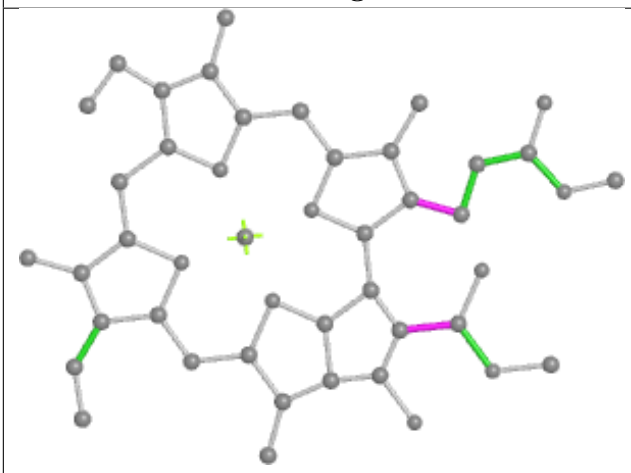
Ligand CLA B3 835



Bond lengths



Bond angles



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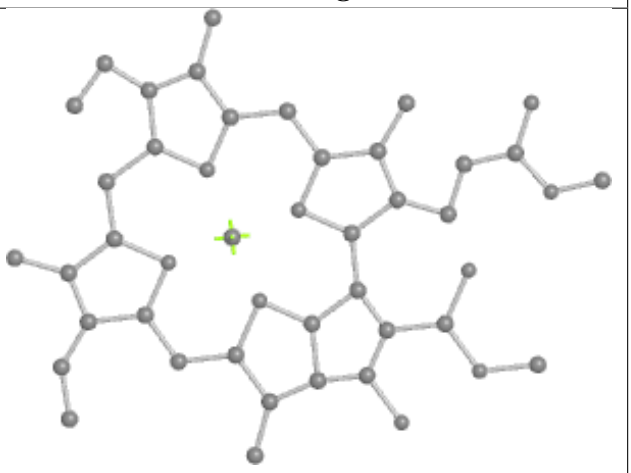
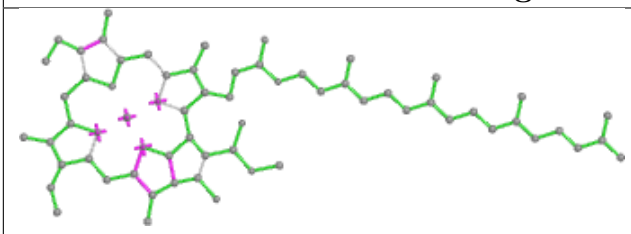
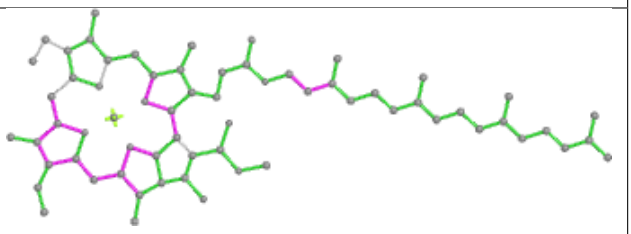


Rings

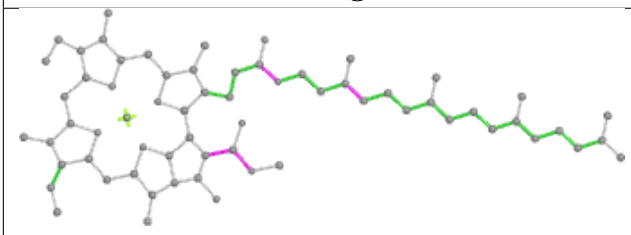
Ligand CLA A3 833



Bond lengths



Bond angles



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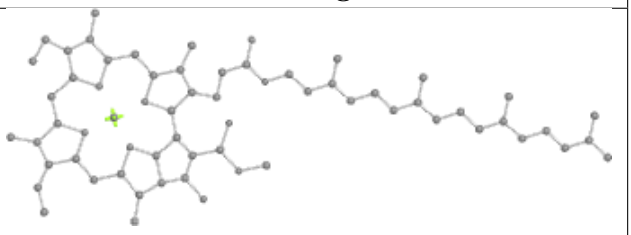
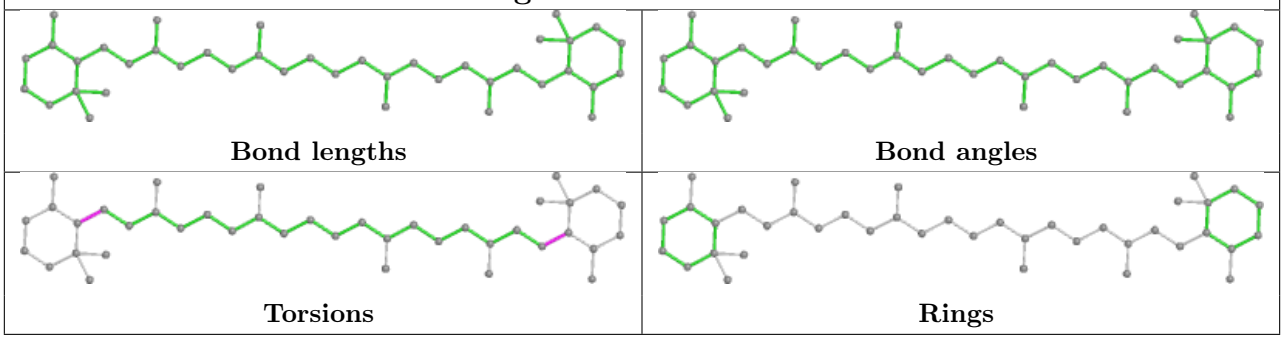
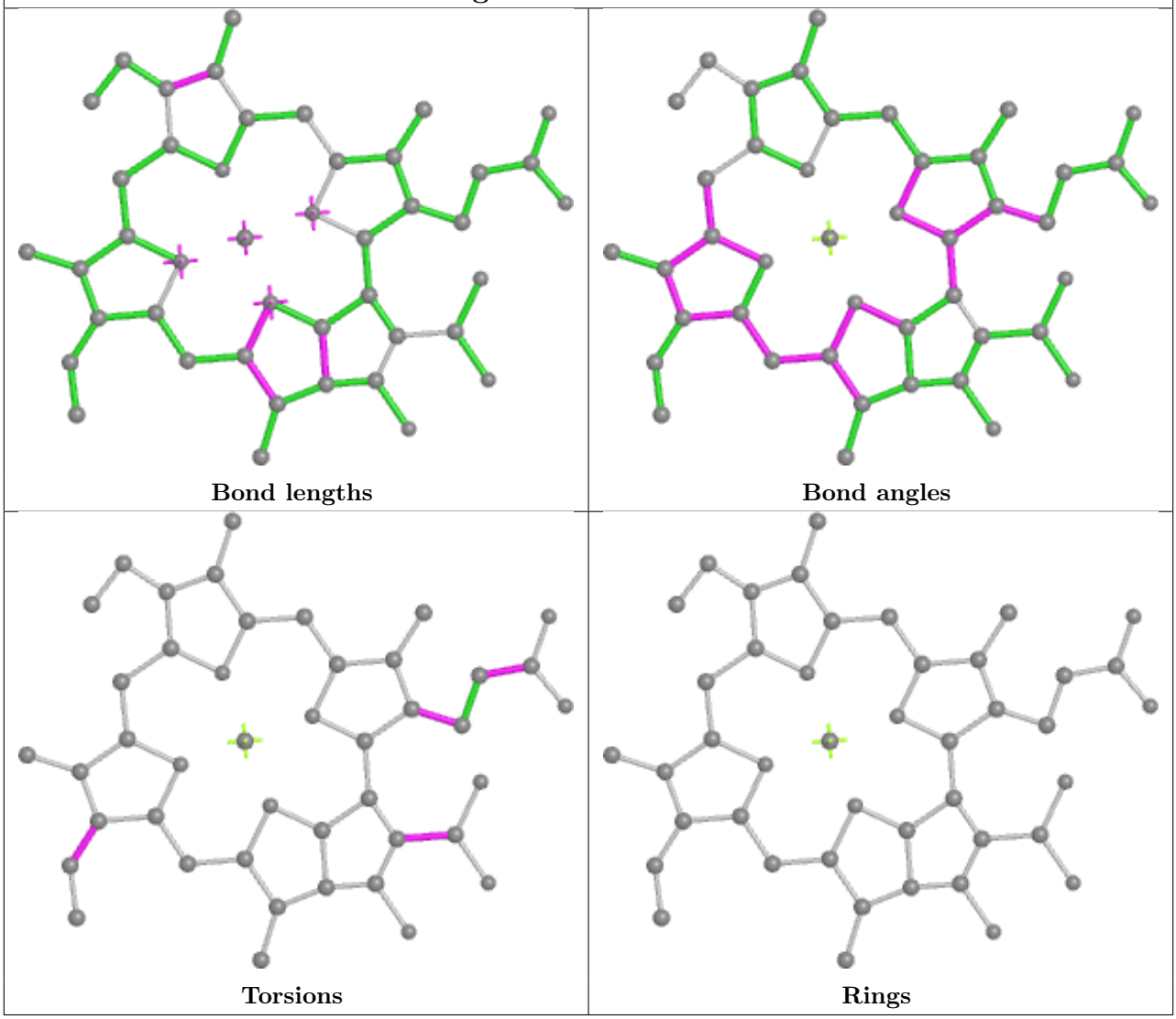


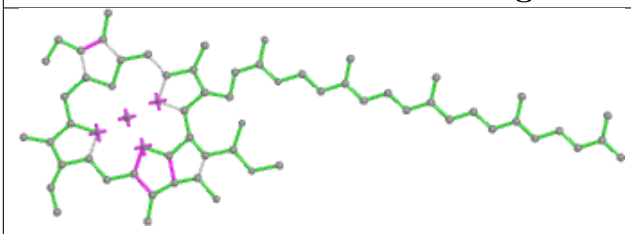
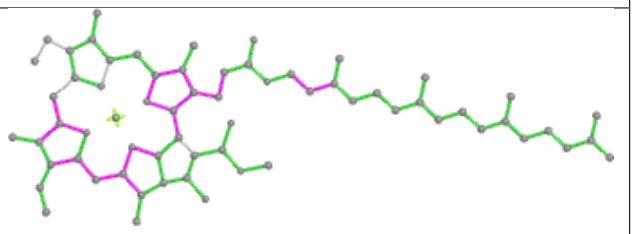
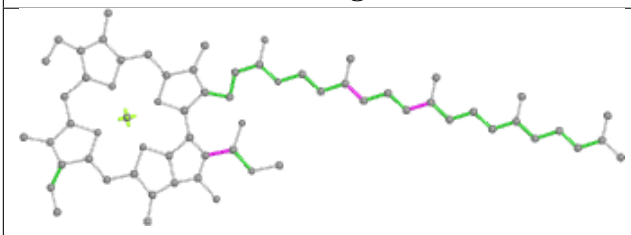
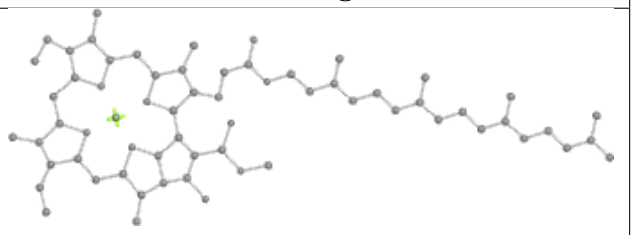
Rings

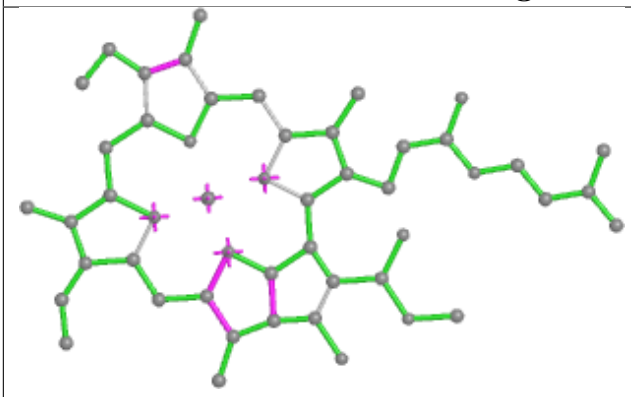
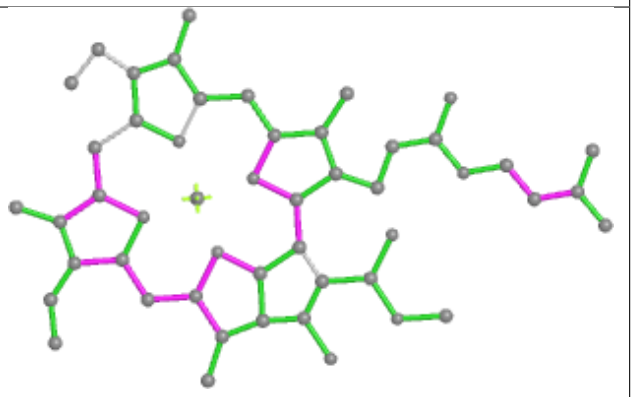
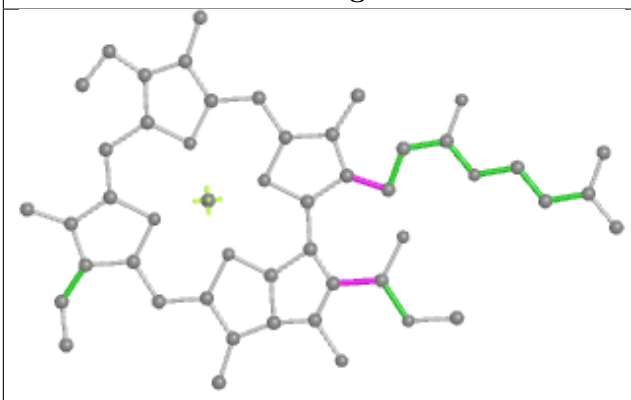
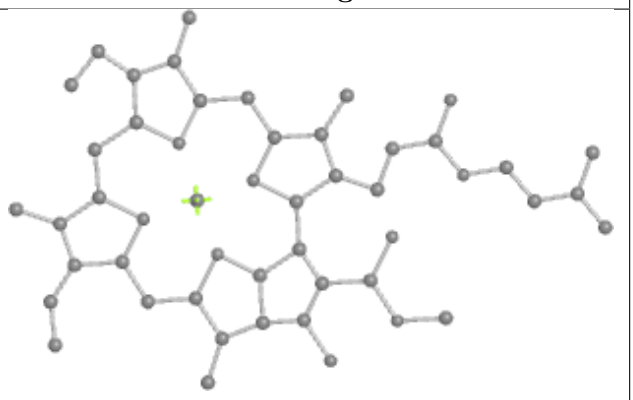
Ligand BCR A2 848



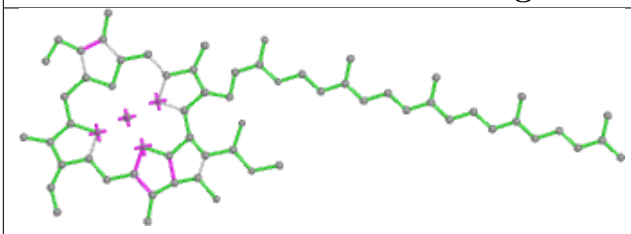
Ligand CLA A3 807



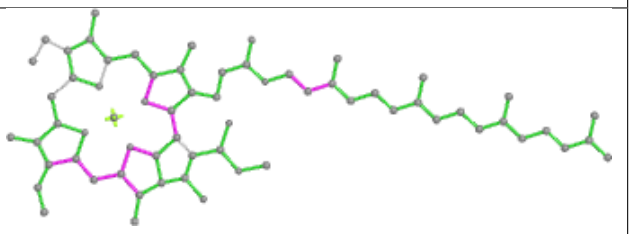
Ligand CLA B1 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

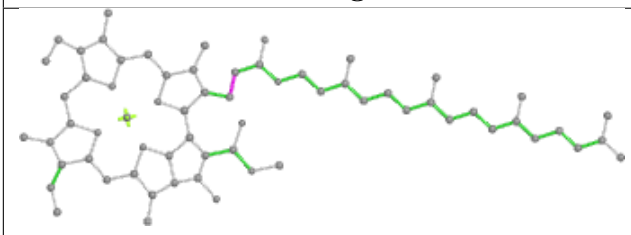
Ligand CLA A3 802



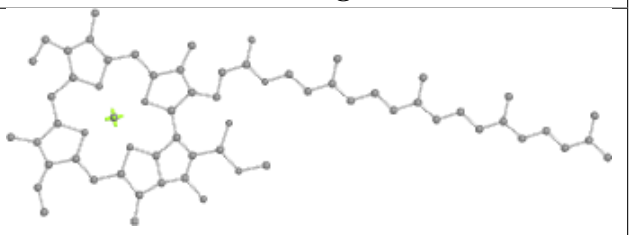
Bond lengths



Bond angles

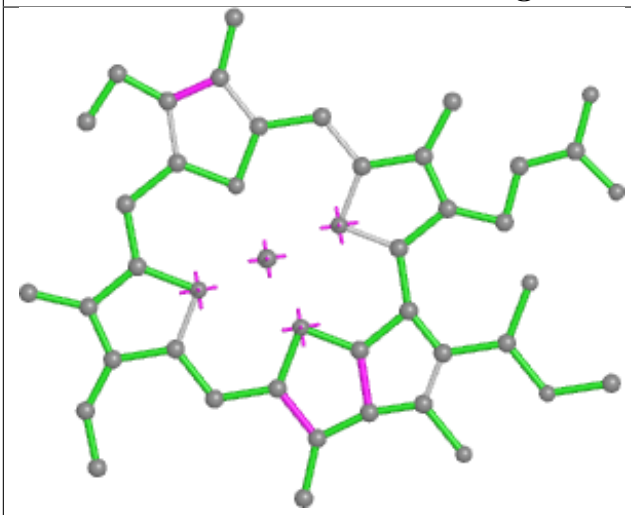


Torsions

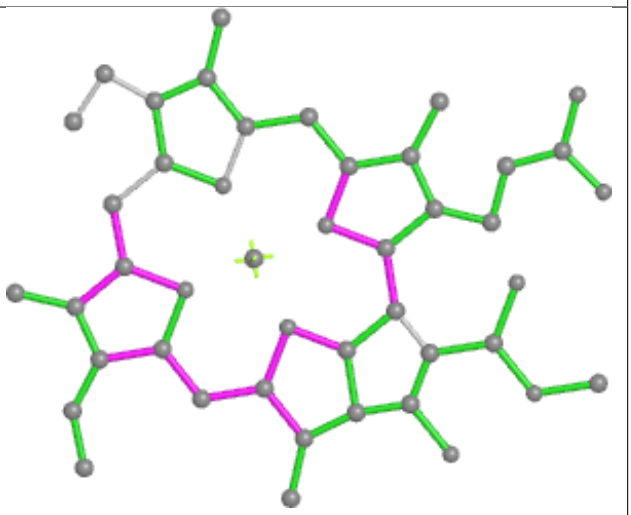


Rings

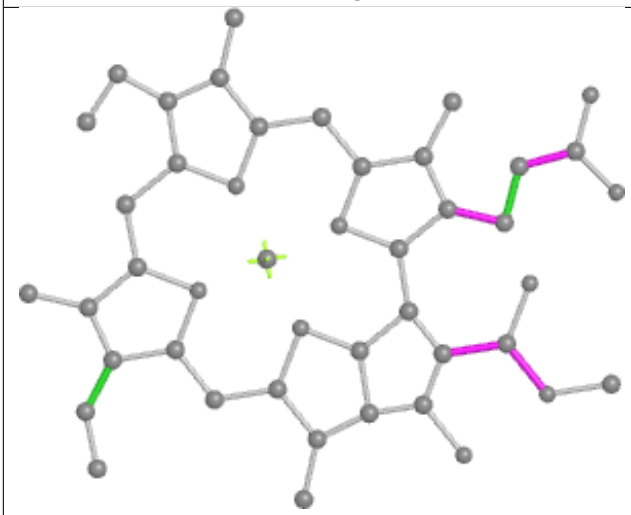
Ligand CLA B1 849



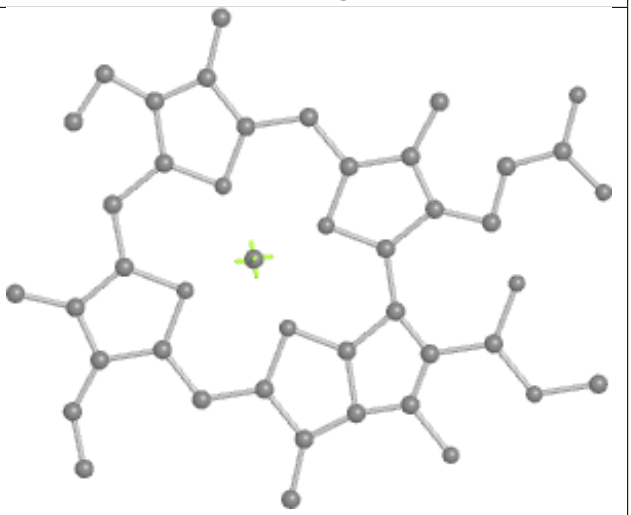
Bond lengths



Bond angles

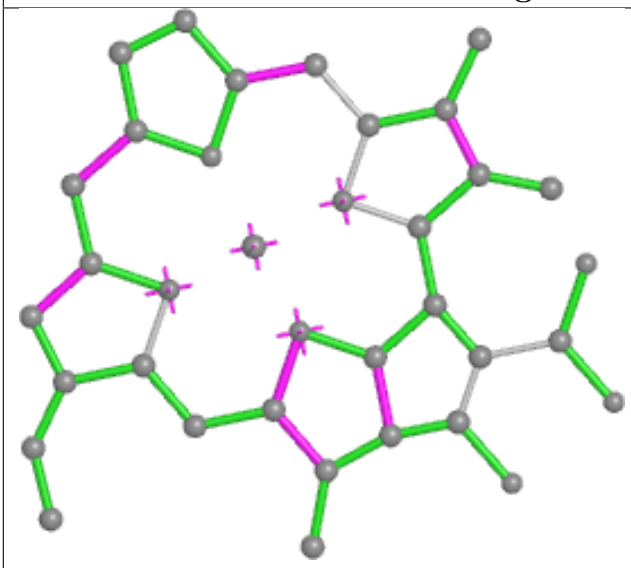


Torsions

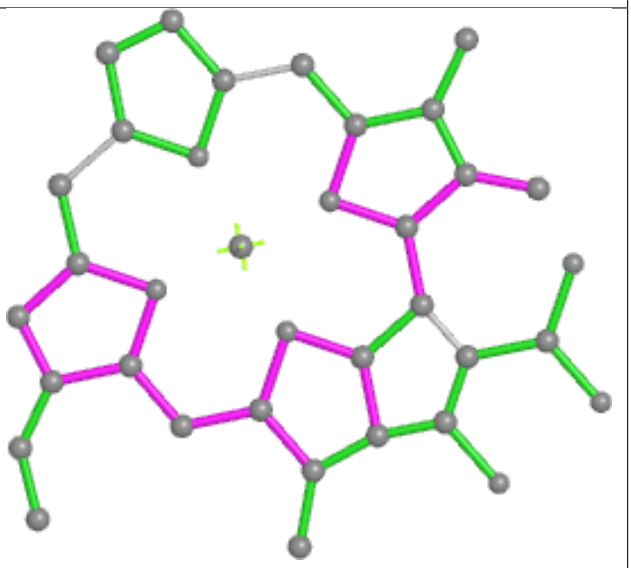


Rings

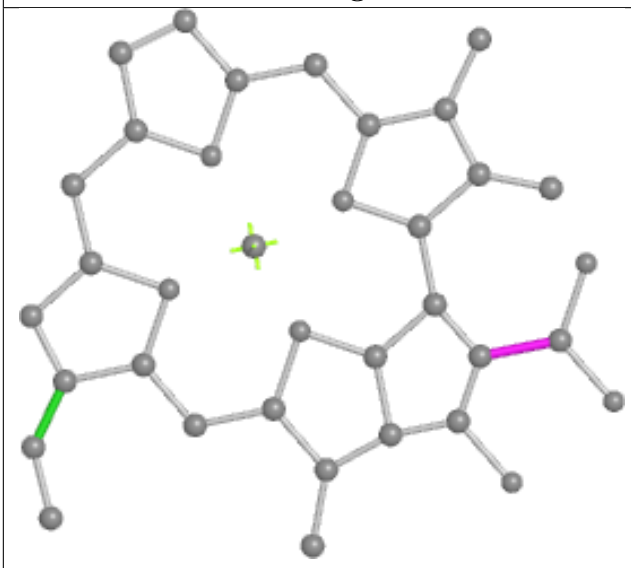
Ligand CLA A3 815



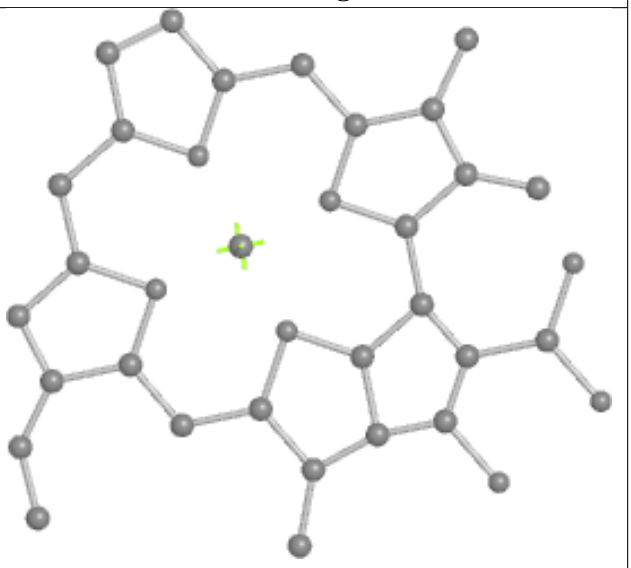
Bond lengths



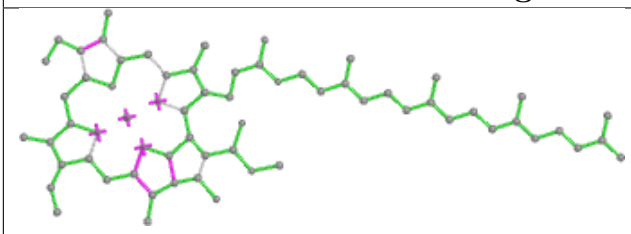
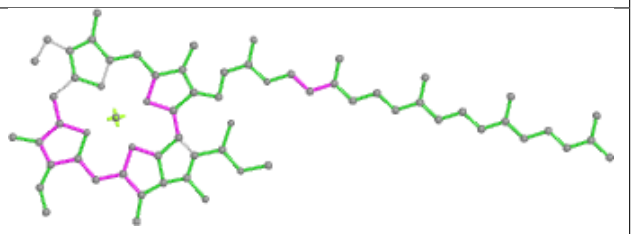
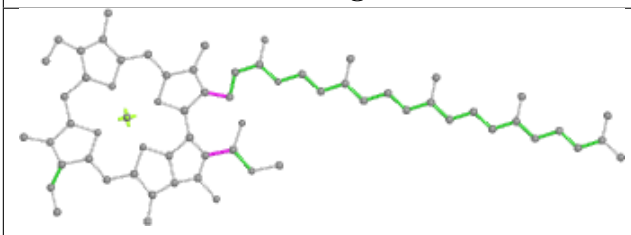
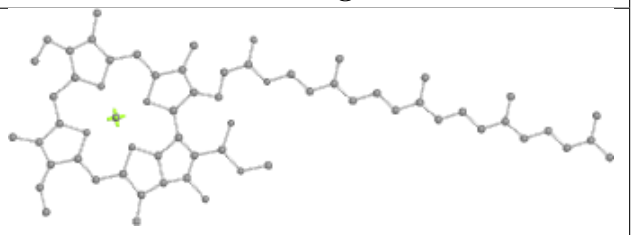
Bond angles

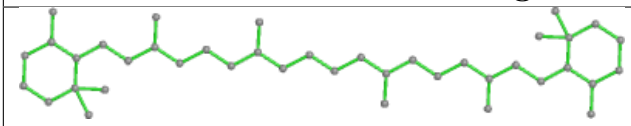
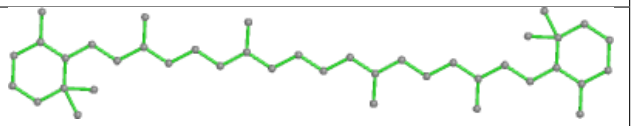
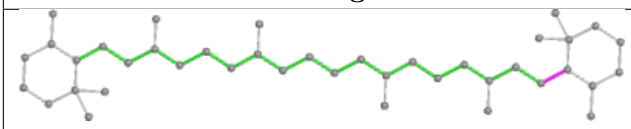
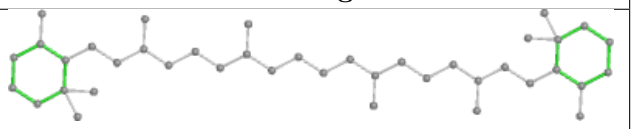


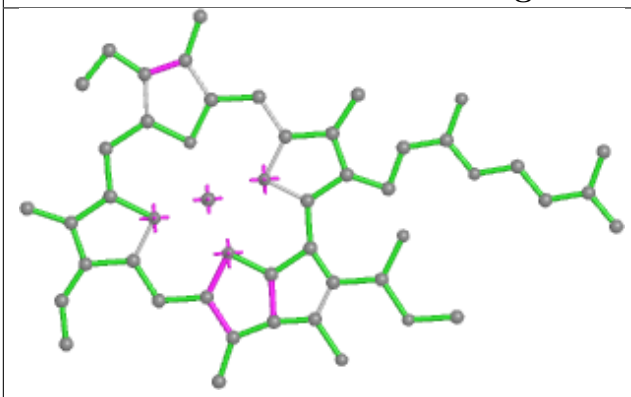
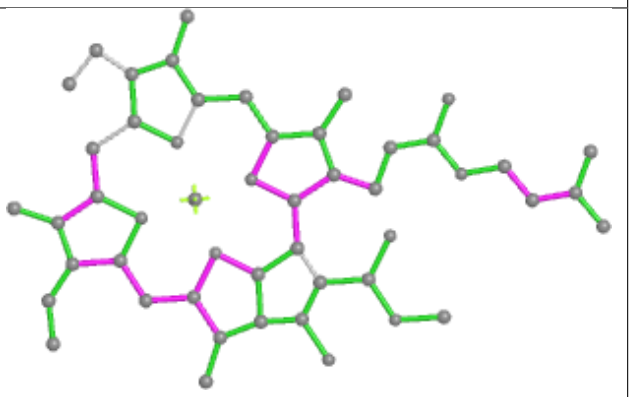
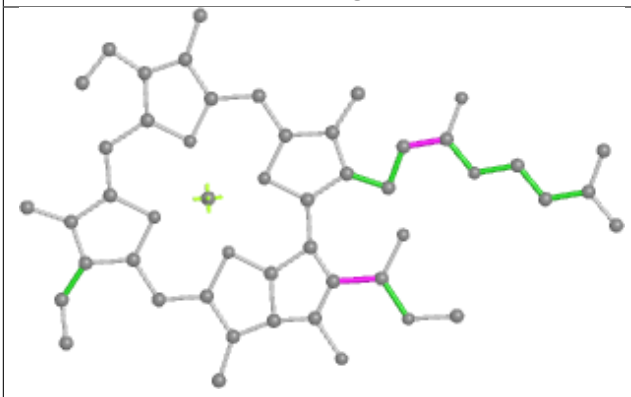
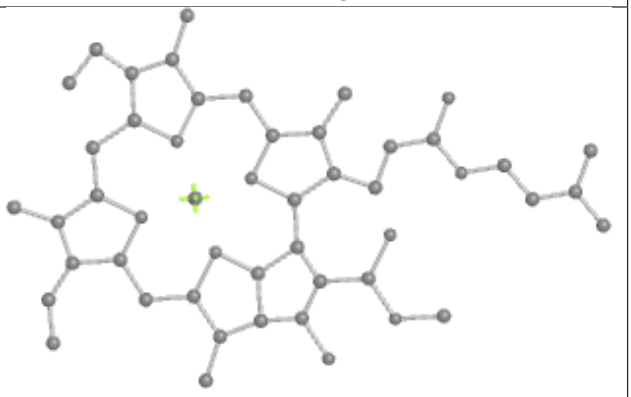
Torsions

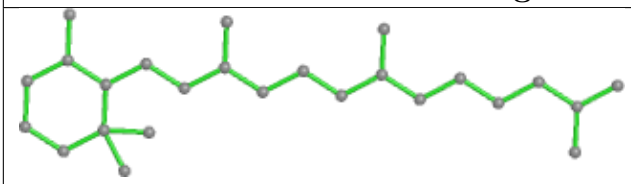
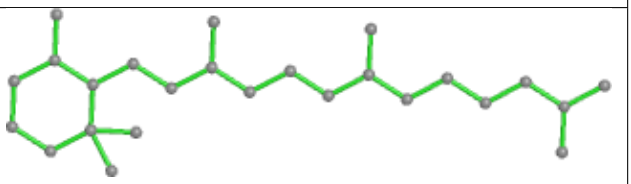
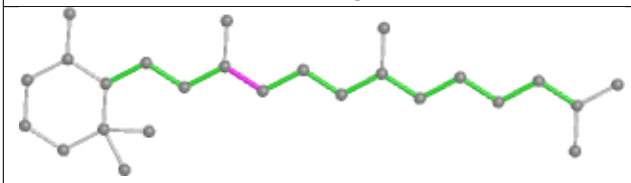
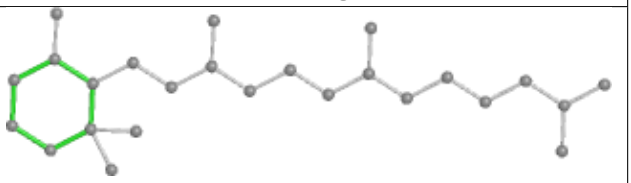


Rings

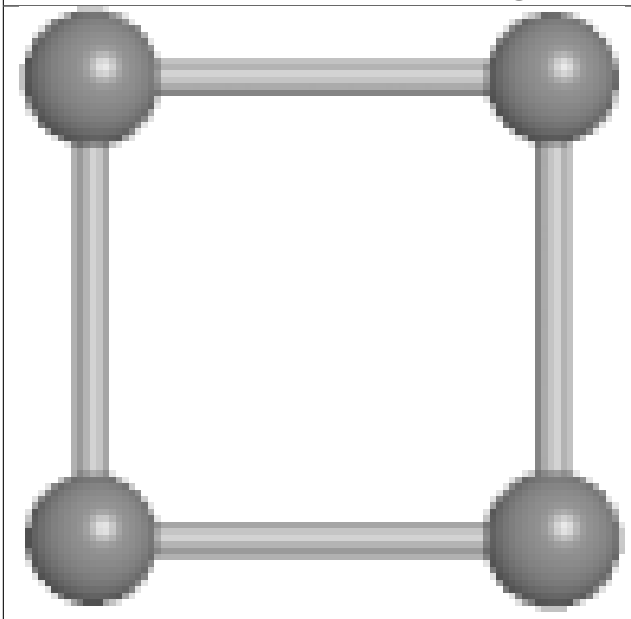
Ligand CLA A2 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B3 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

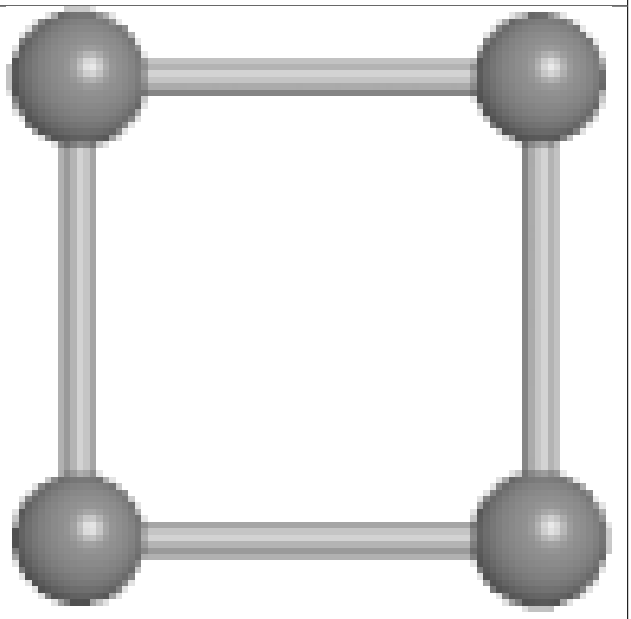
Ligand CLA A2 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B1 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

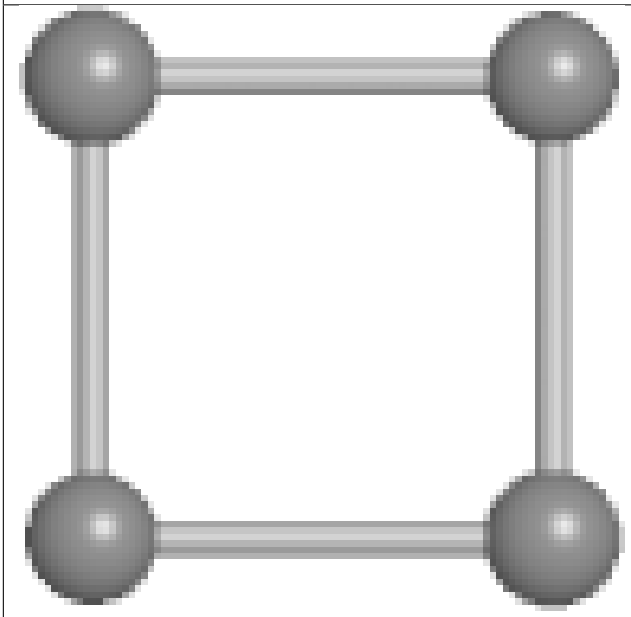
Ligand GAK R3 101



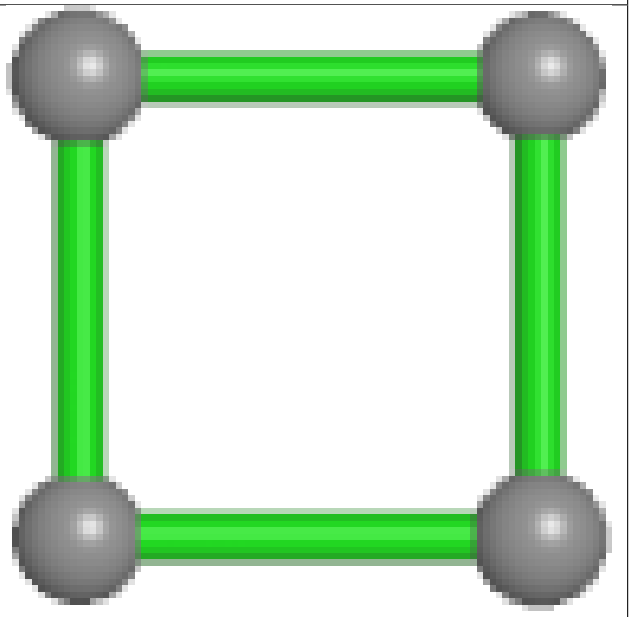
Bond lengths



Bond angles

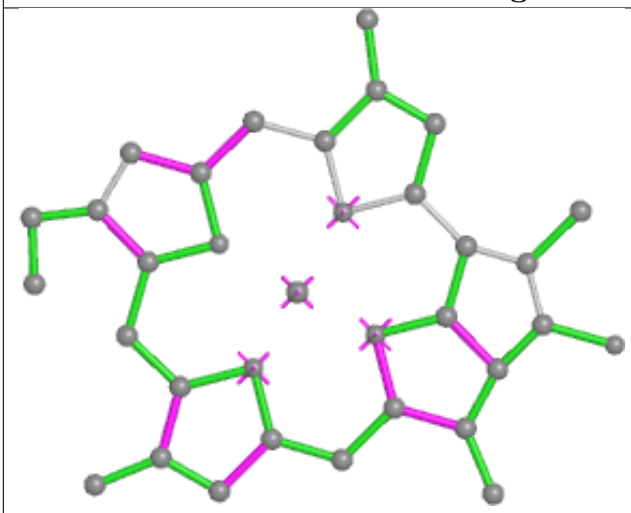


Torsions



Rings

Ligand CLA J2 1307



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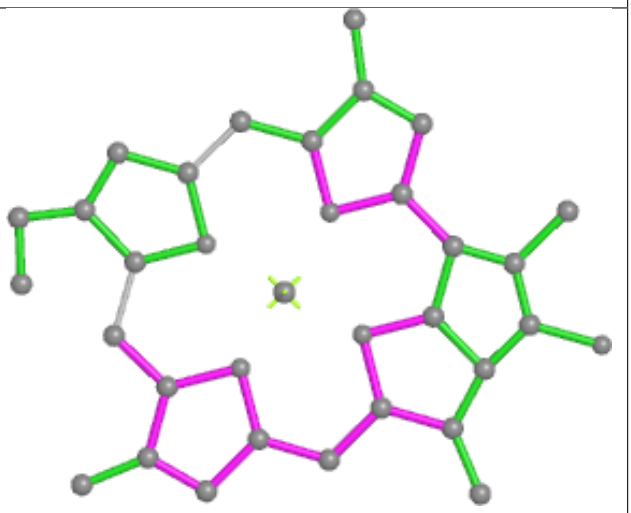
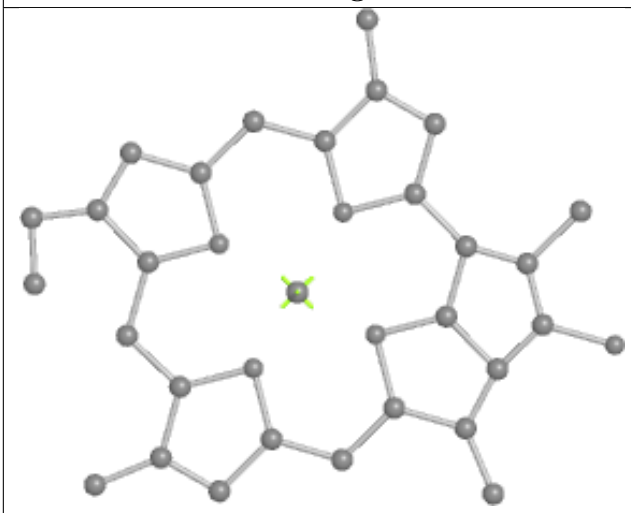


Bond angles



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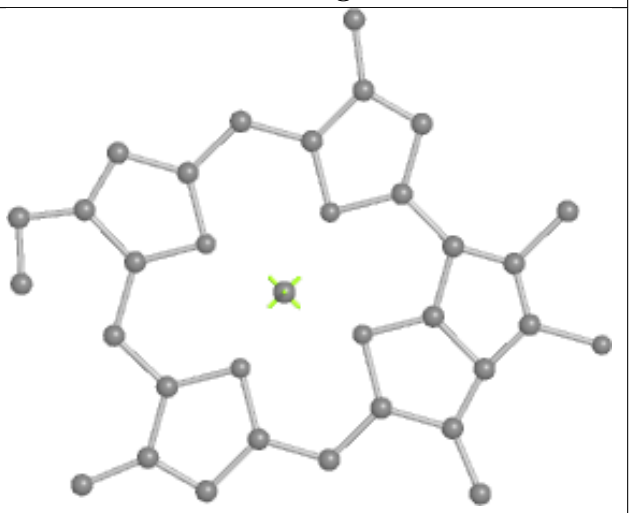
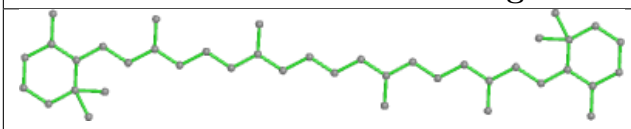


Rings

Ligand BCR L3 1005



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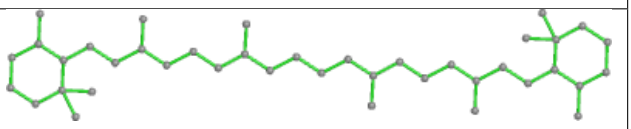
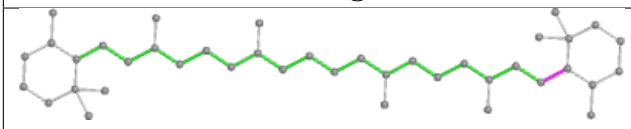


Bond angles



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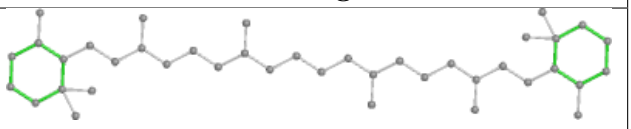
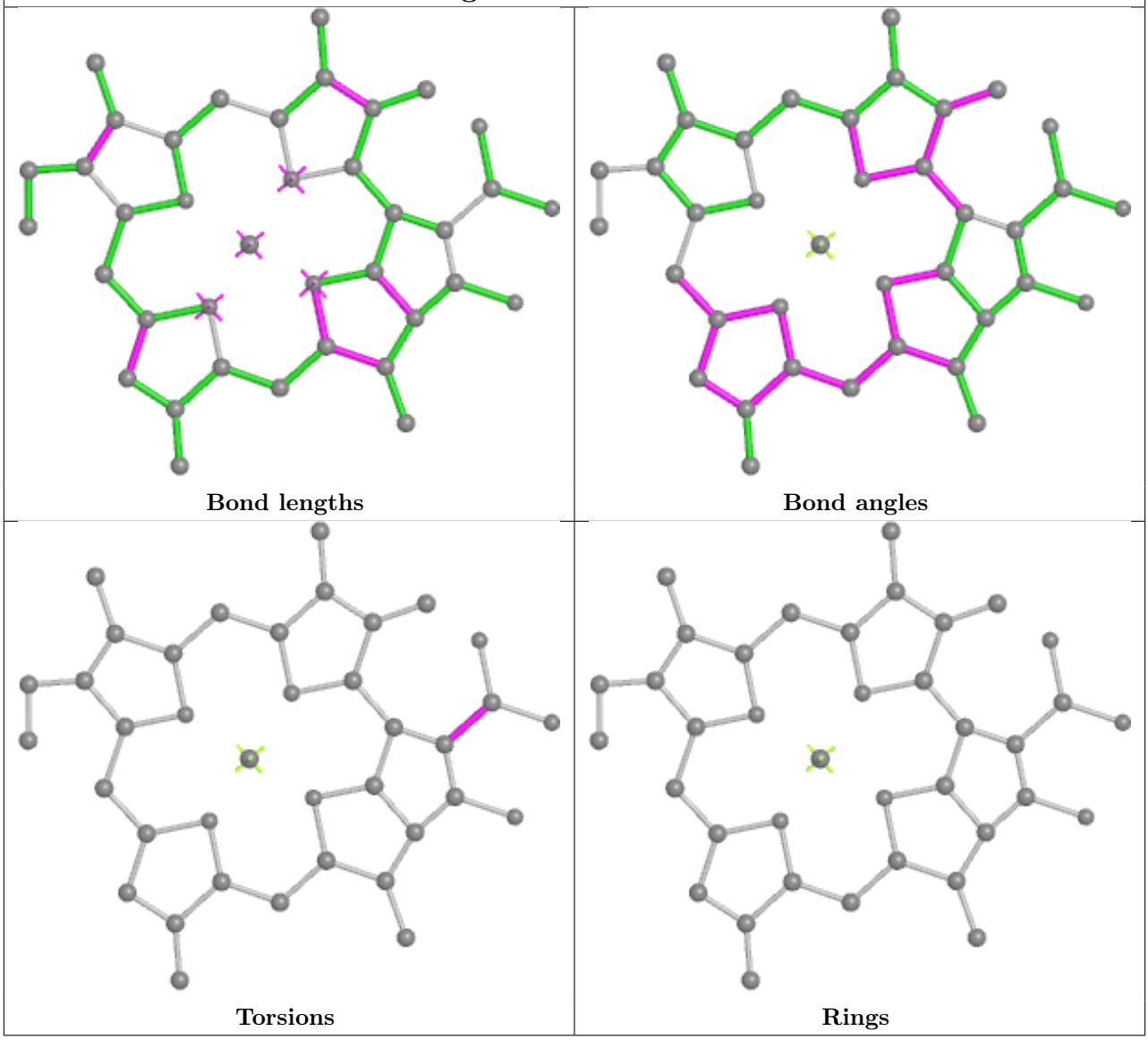
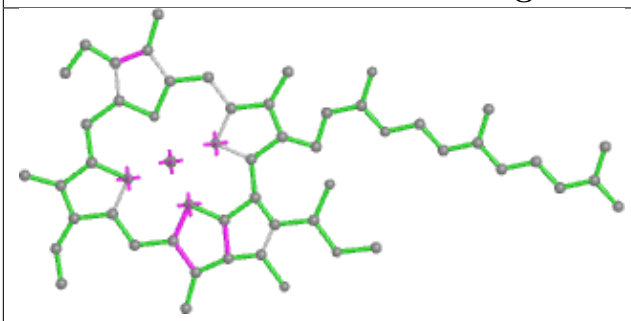
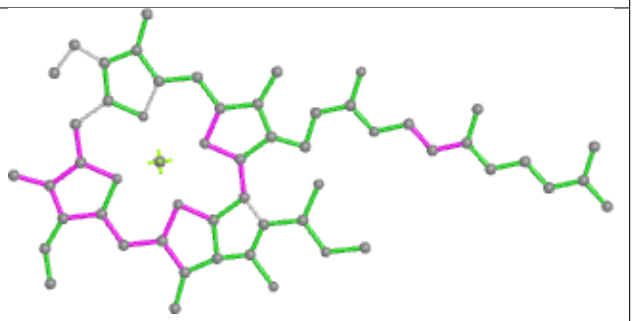
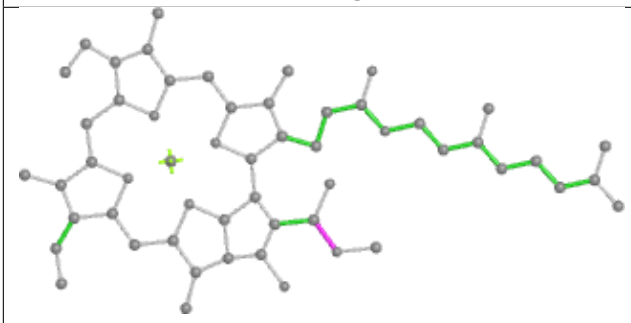
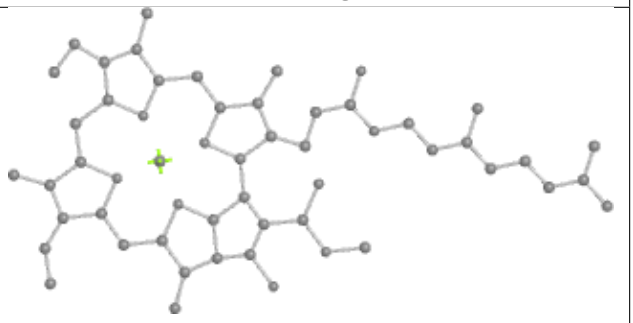


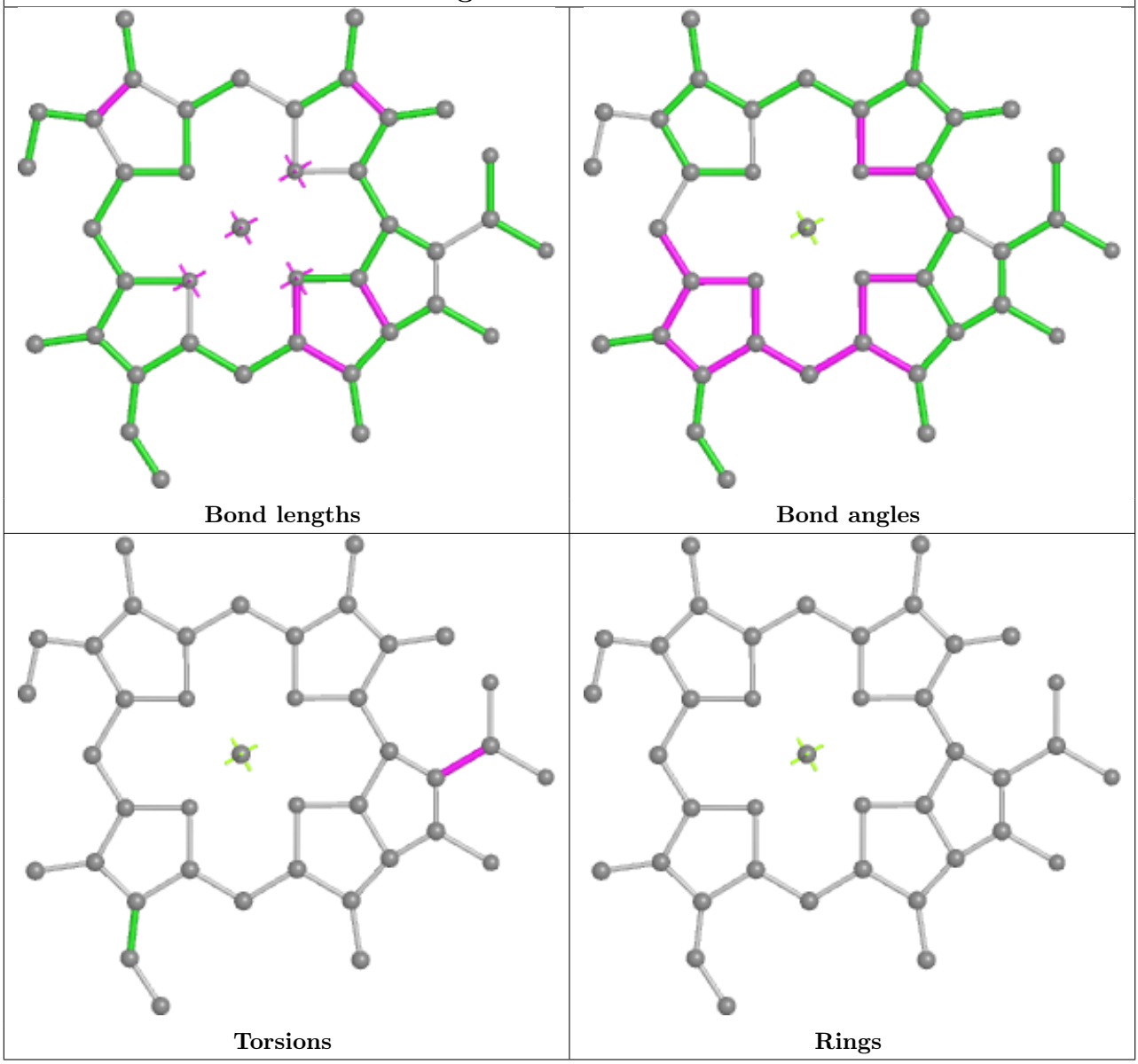
Rings

Ligand CLA A2 810

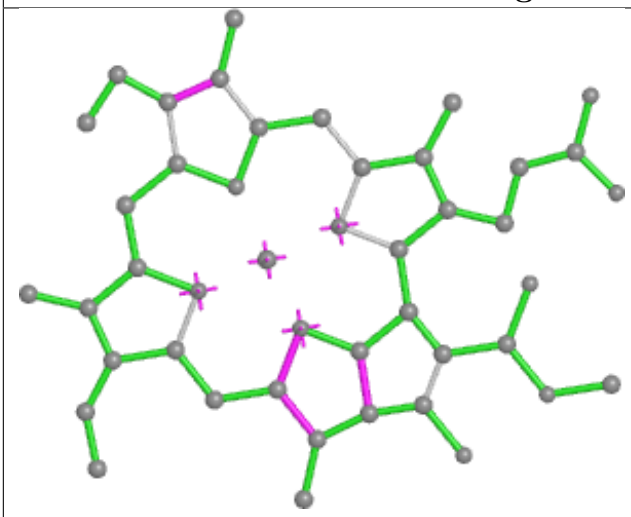


Ligand CLA B3 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

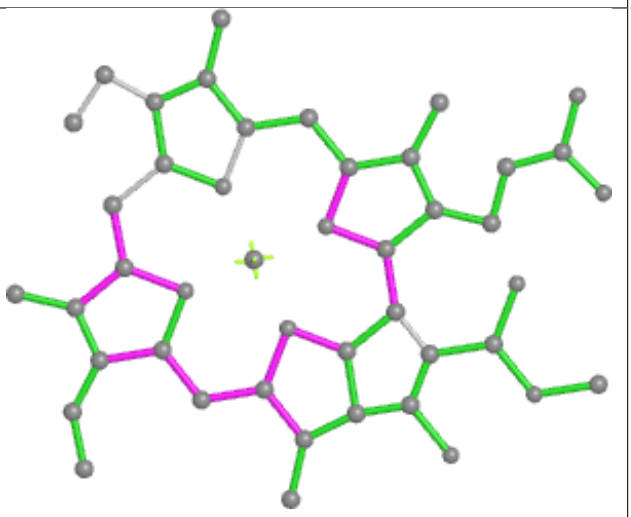
Ligand CLA A3 841



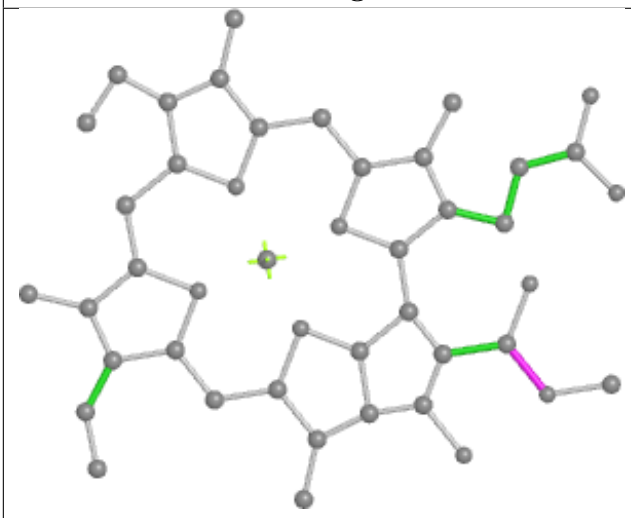
Ligand CLA B3 824



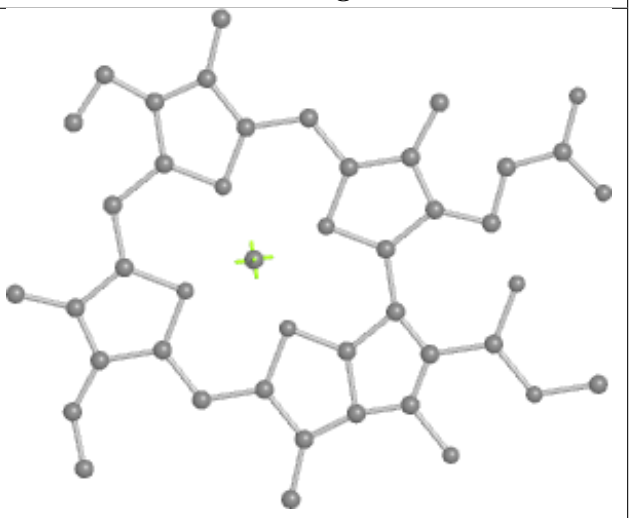
Bond lengths



Bond angles

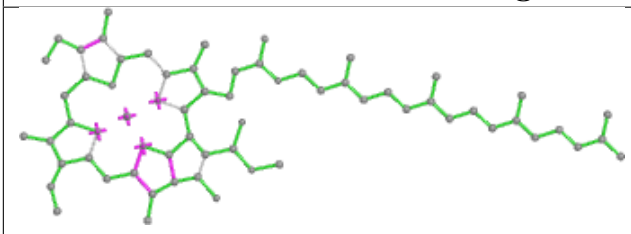


Torsions



Rings

Ligand CLA A1 805



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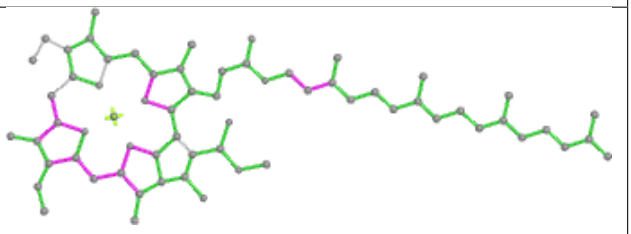
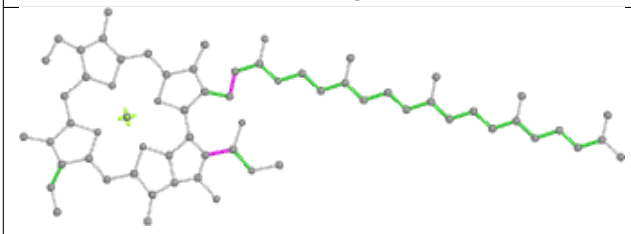
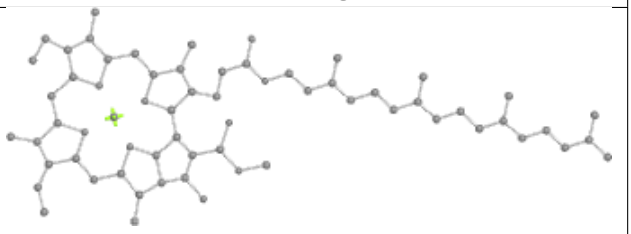


Bond angles

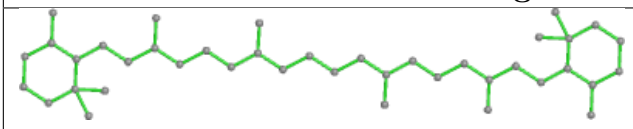


Torsions

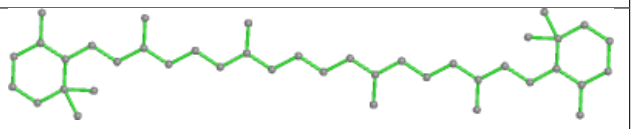


Rings

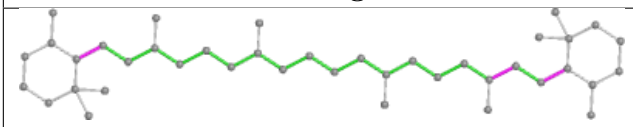
Ligand BCR B2 847



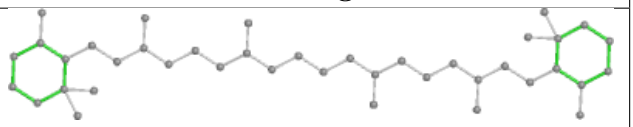
Bond lengths



Bond angles

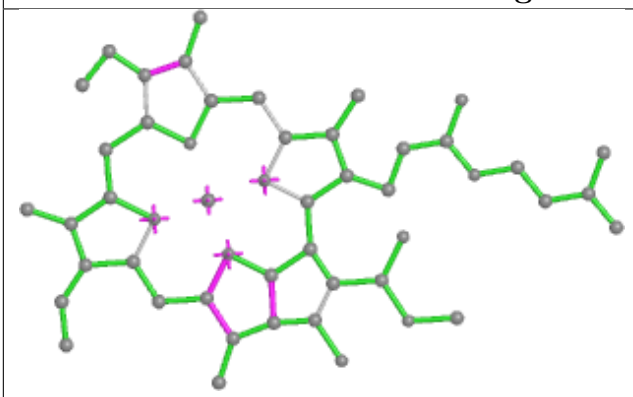


Torsions

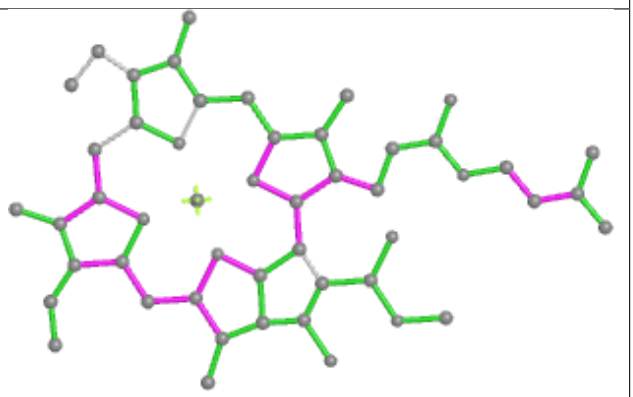


Rings

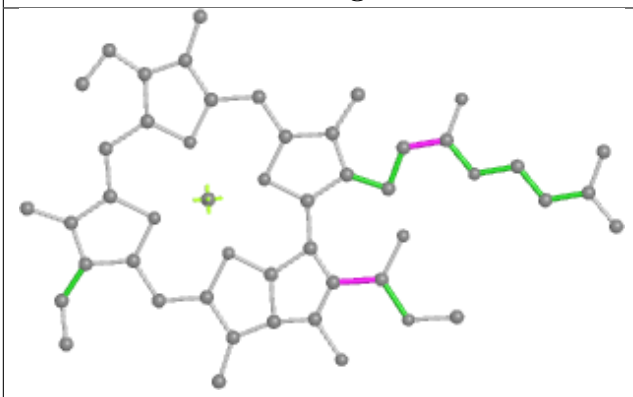
Ligand CLA A3 831



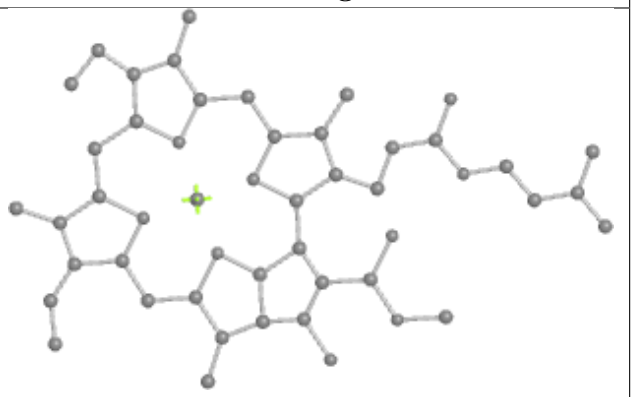
Bond lengths



Bond angles

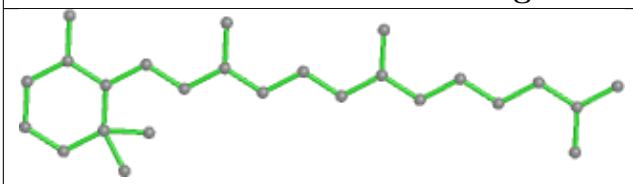


Torsions

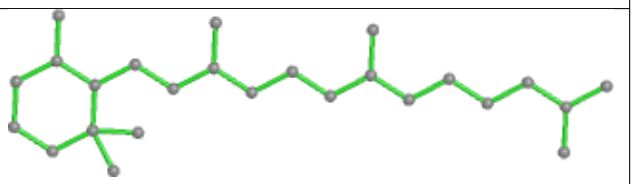


Rings

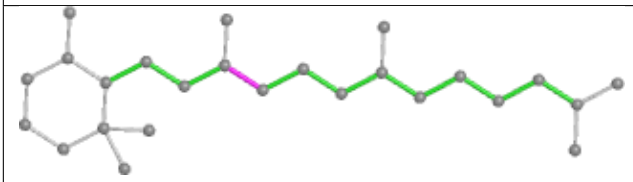
Ligand BCR B3 843



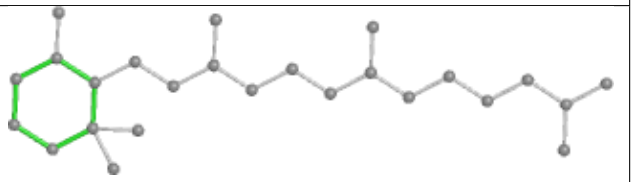
Bond lengths



Bond angles

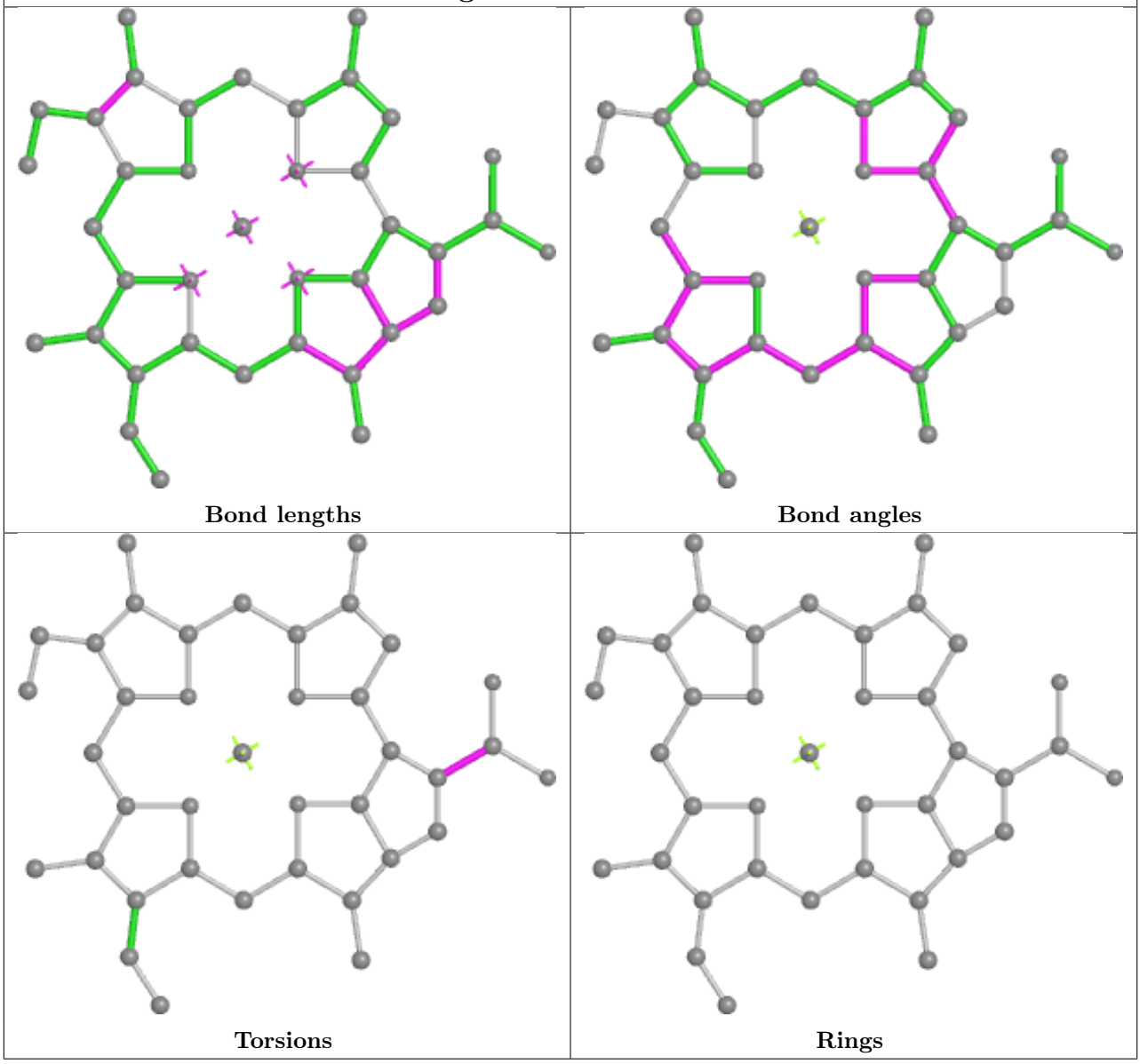


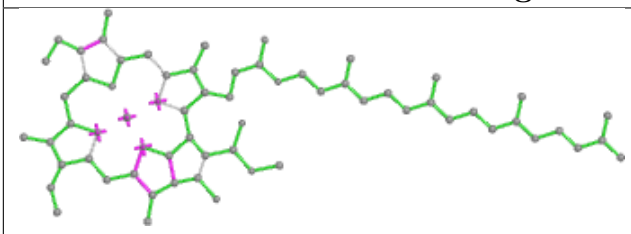
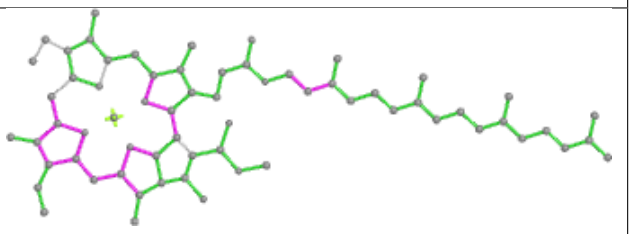
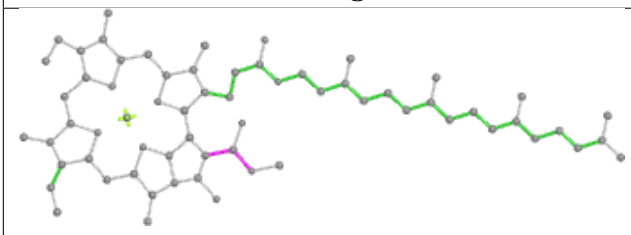
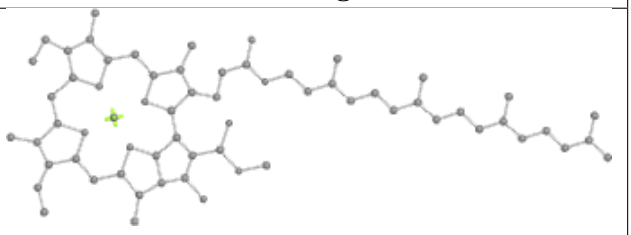
Torsions

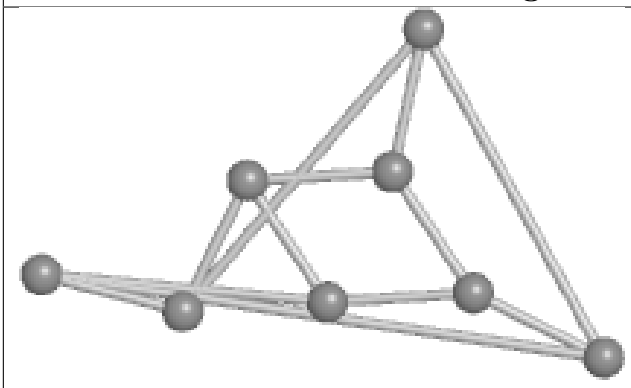
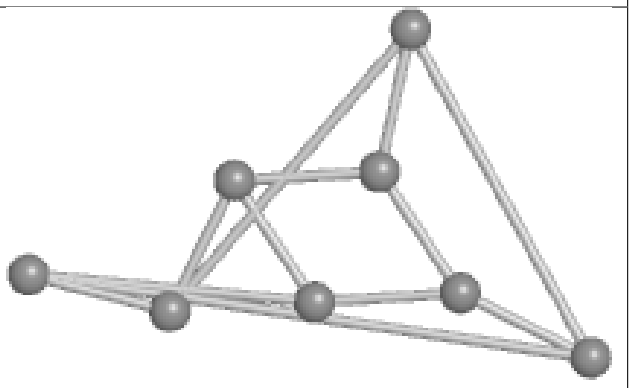
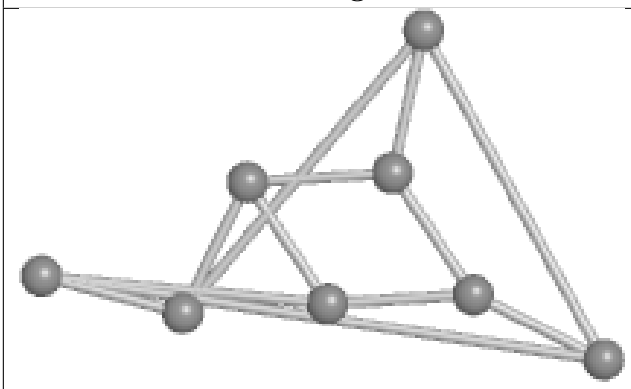
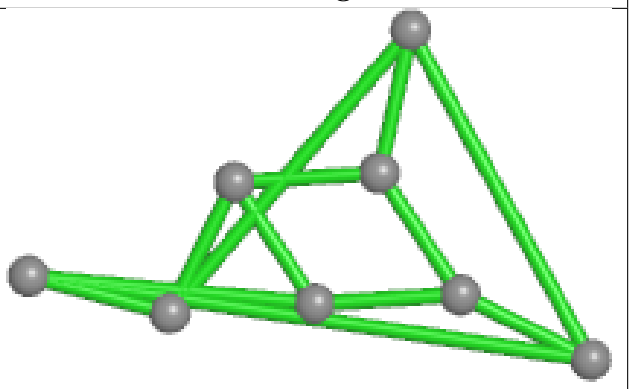


Rings

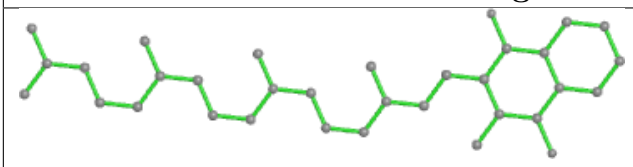
Ligand CLA B2 816



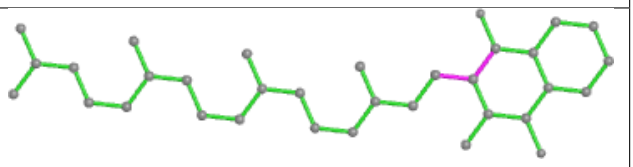
Ligand CLA A2 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 C1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

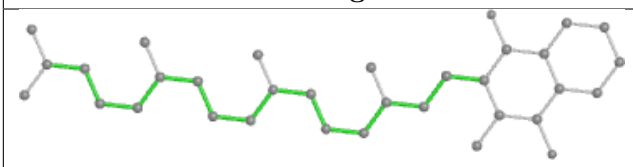
Ligand PQN A2 845



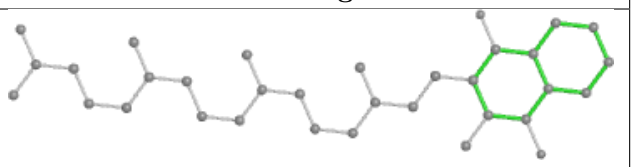
Bond lengths



Bond angles

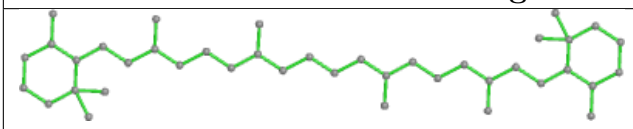


Torsions

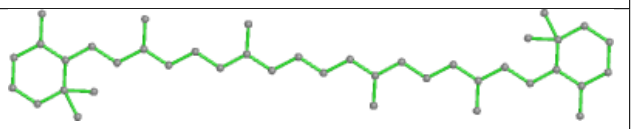


Rings

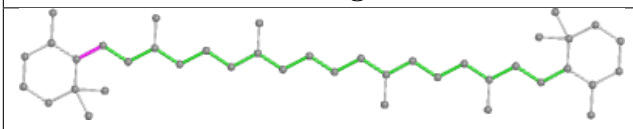
Ligand BCR M1 101



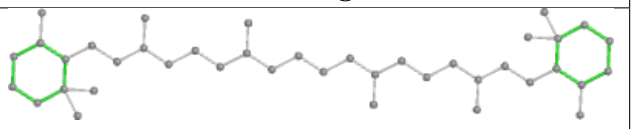
Bond lengths



Bond angles

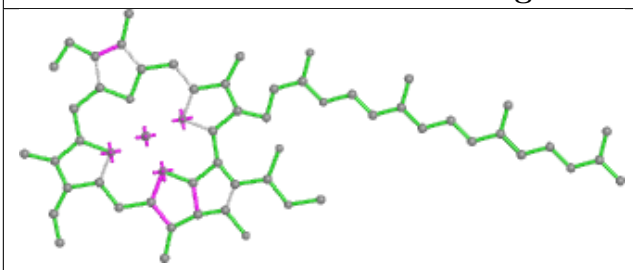


Torsions

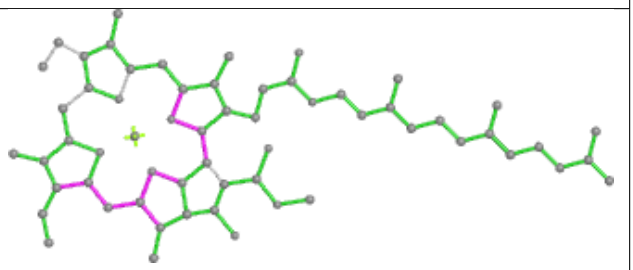


Rings

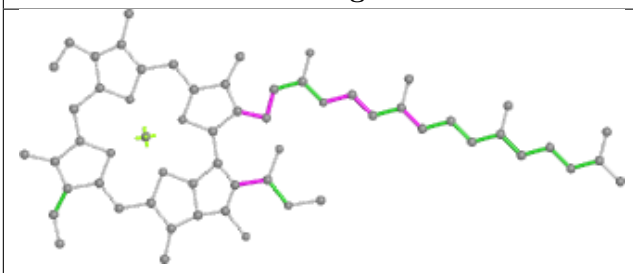
Ligand CLA A1 827



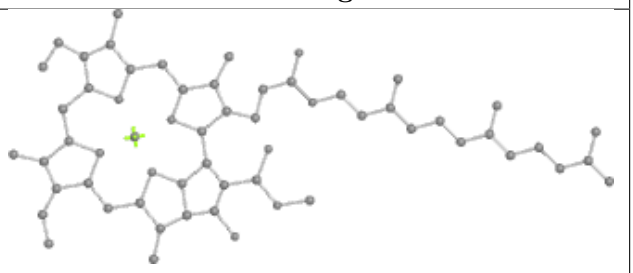
Bond lengths



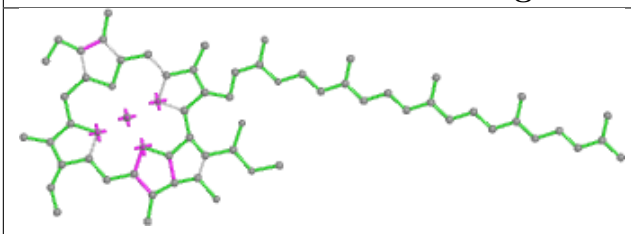
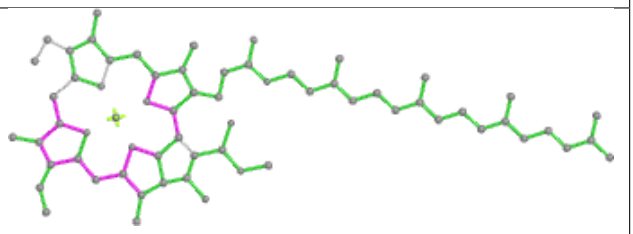
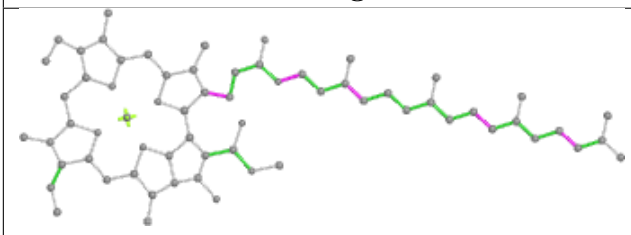
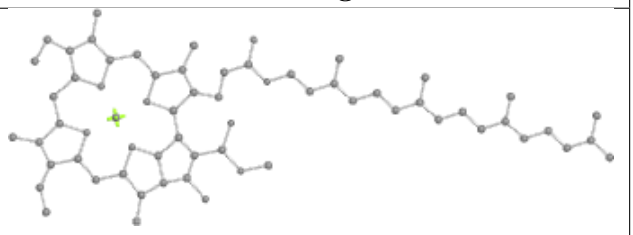
Bond angles

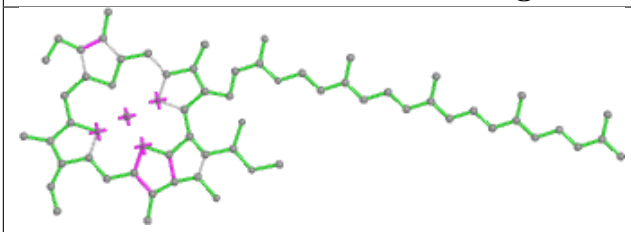
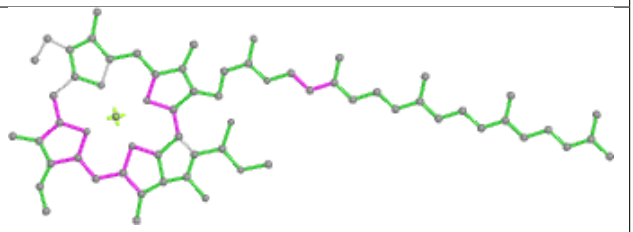
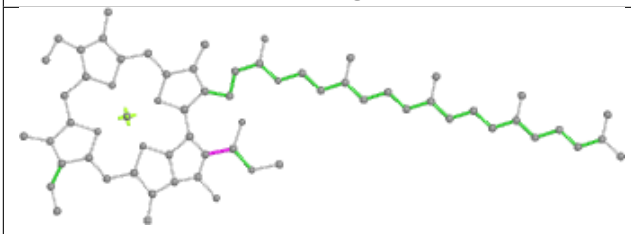
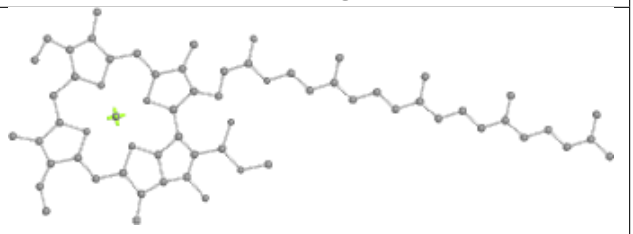


Torsions

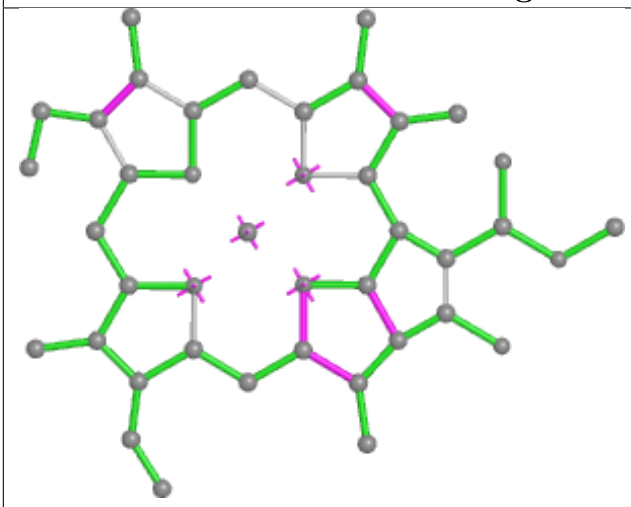


Rings

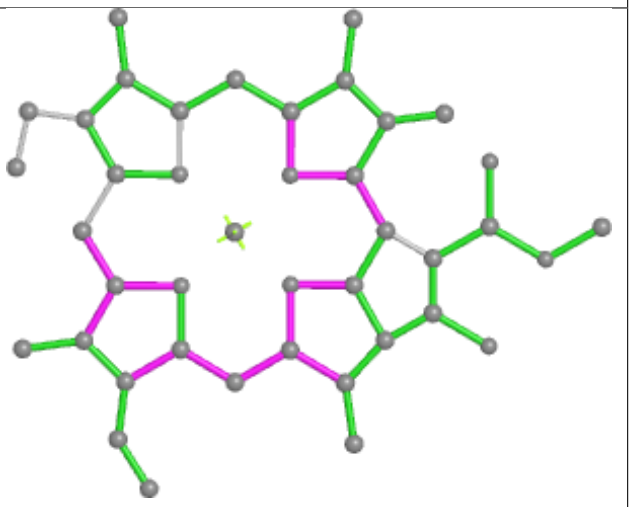
Ligand CLA A2 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B3 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

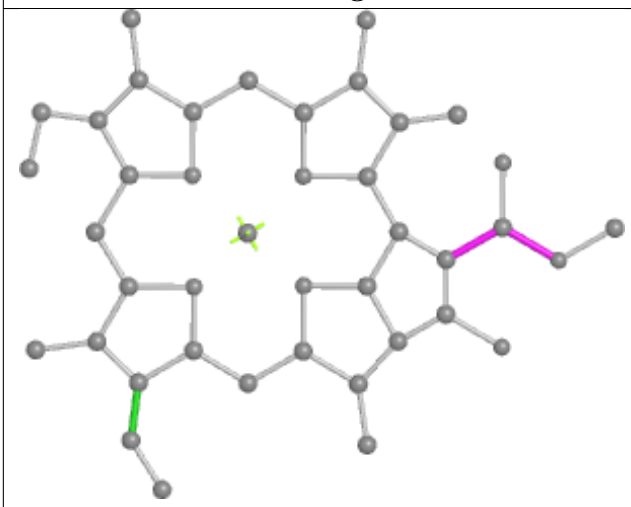
Ligand CLA B2 814



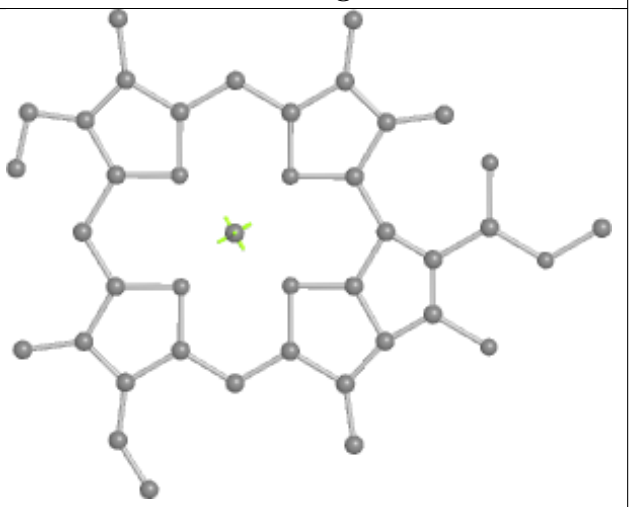
Bond lengths



Bond angles

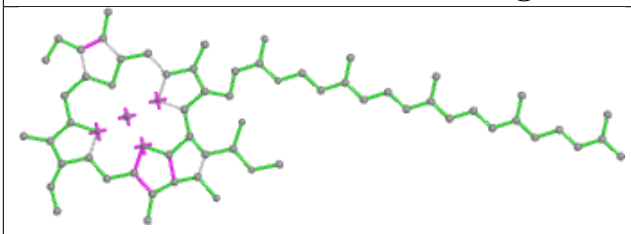


Torsions

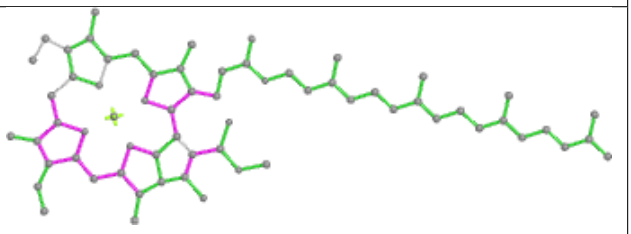


Rings

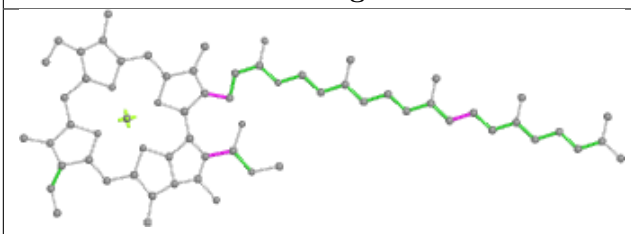
Ligand CLA B2 812



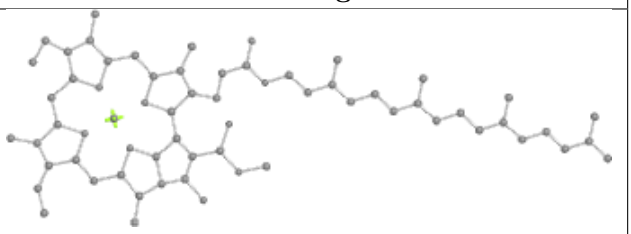
Bond lengths



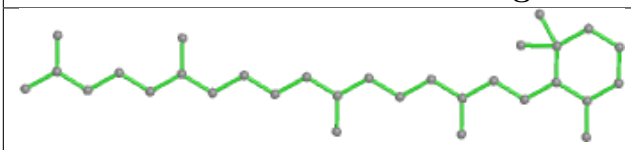
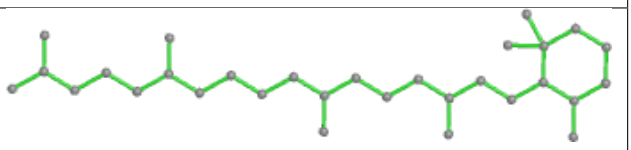
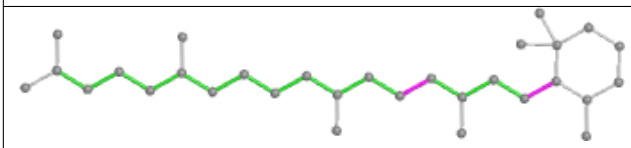
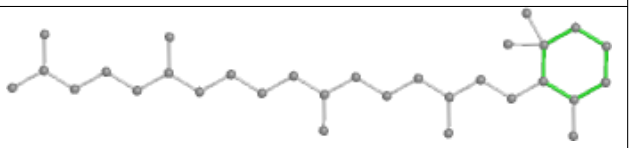
Bond angles

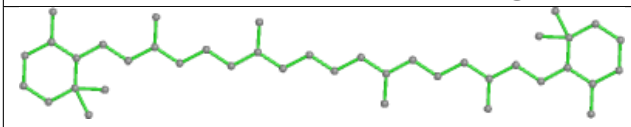
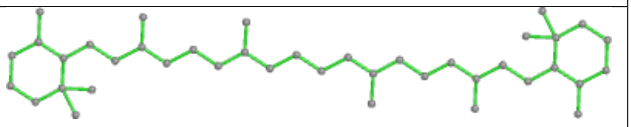
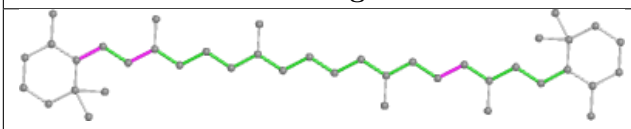
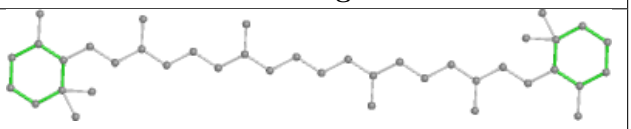


Torsions

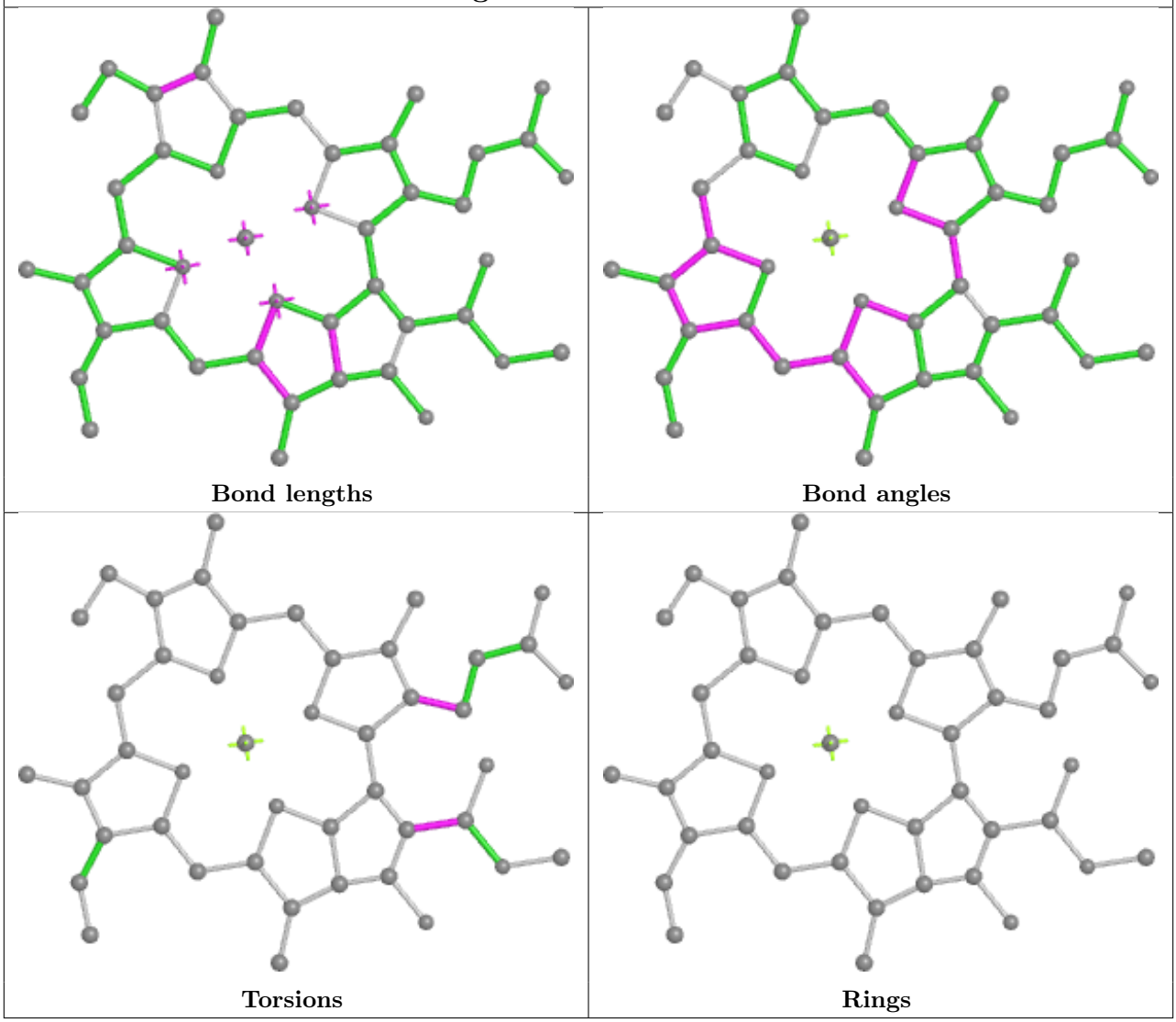


Rings

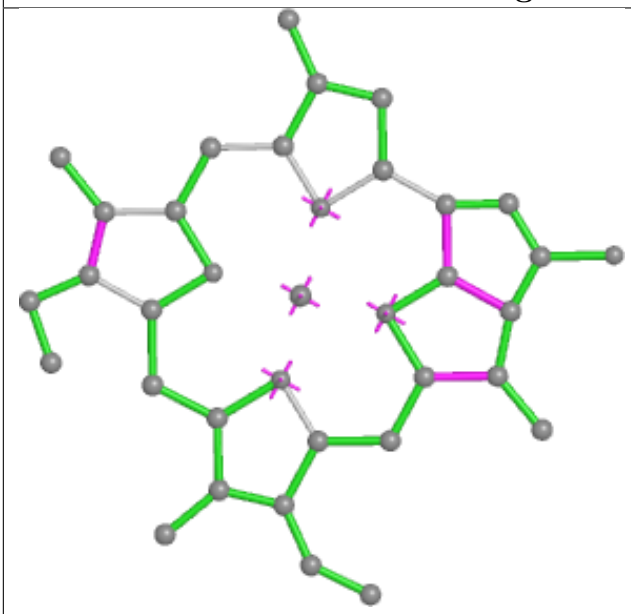
Ligand BCR A2 855	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J1 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

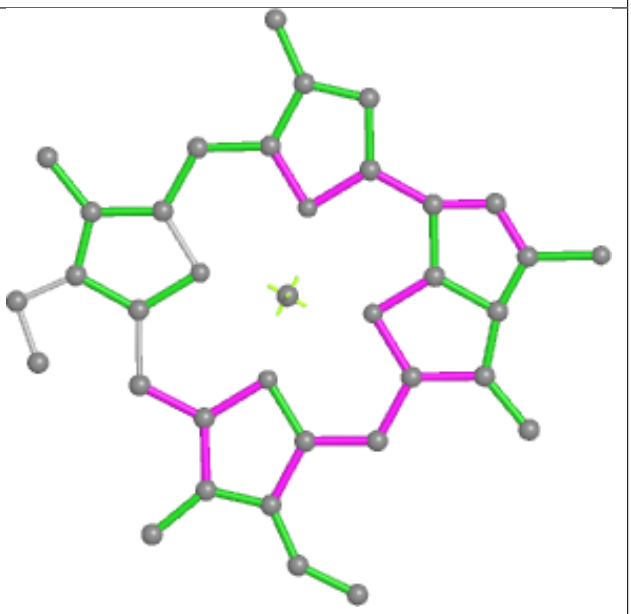
Ligand CLA A2 844



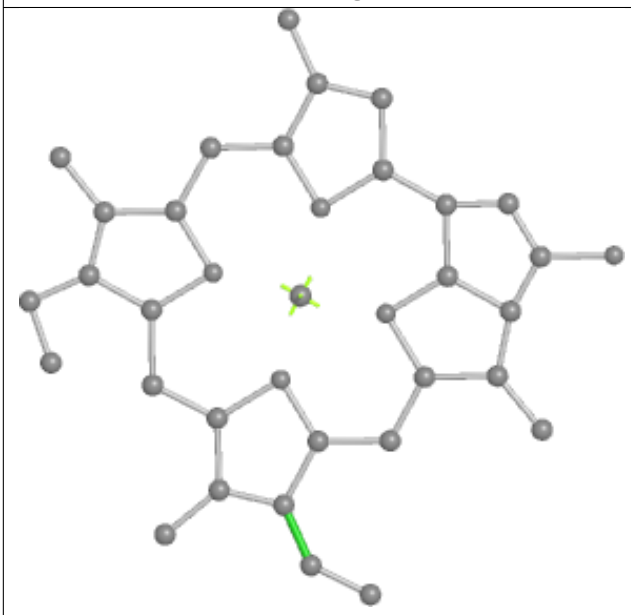
Ligand CLA B3 815



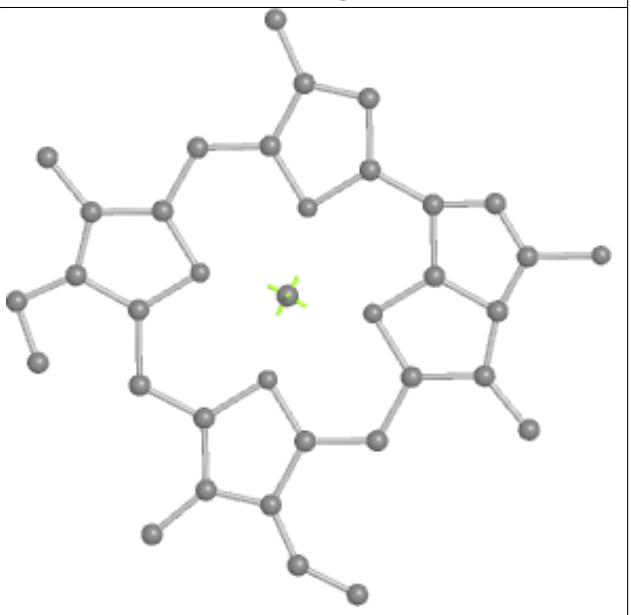
Bond lengths



Bond angles

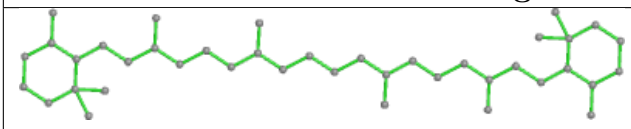


Torsions

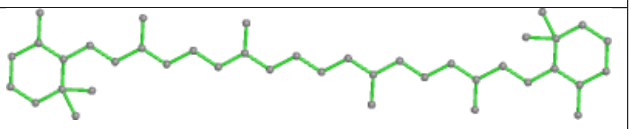


Rings

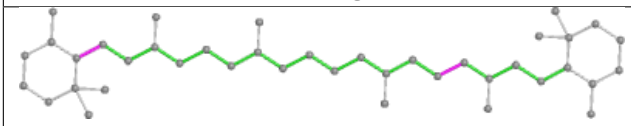
Ligand BCR B3 844



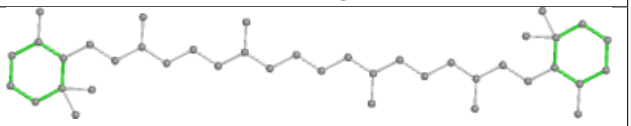
Bond lengths



Bond angles

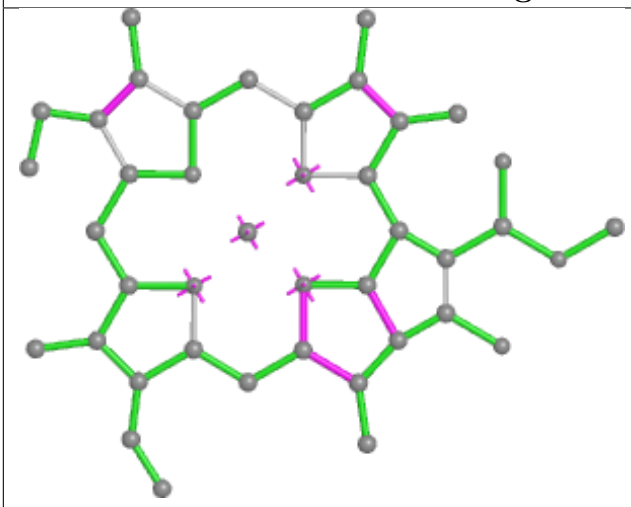


Torsions

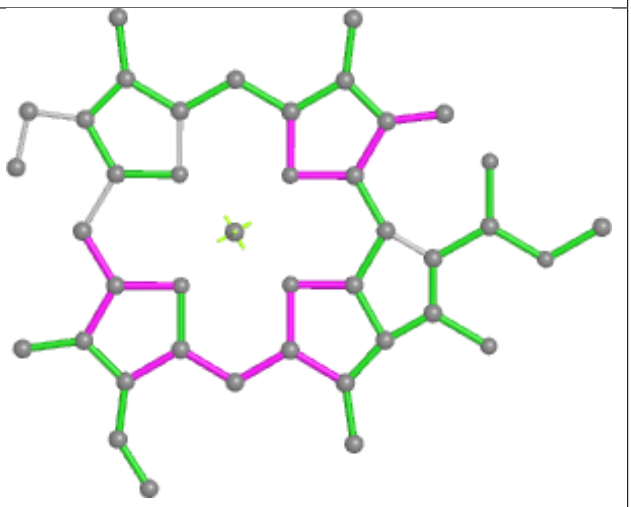


Rings

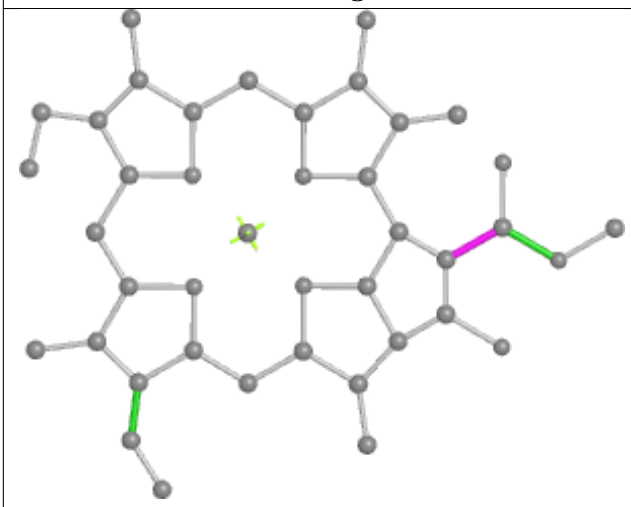
Ligand CLA A2 823



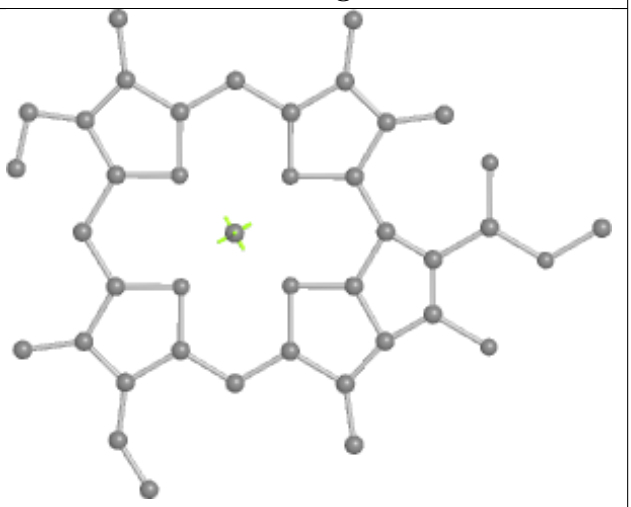
Bond lengths



Bond angles

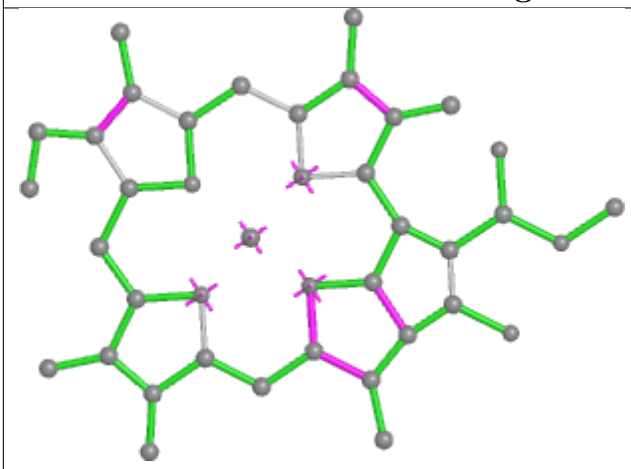


Torsions

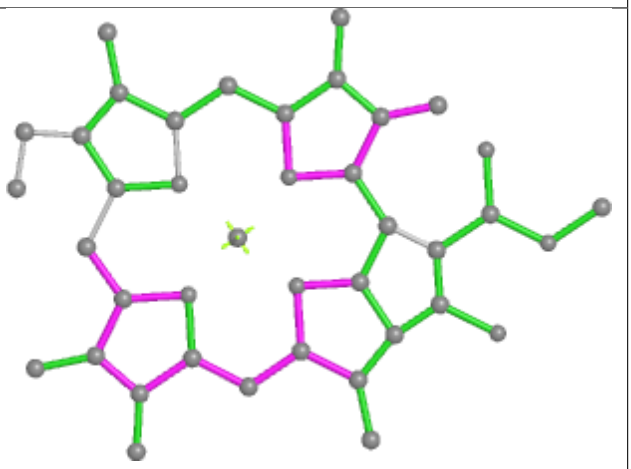


Rings

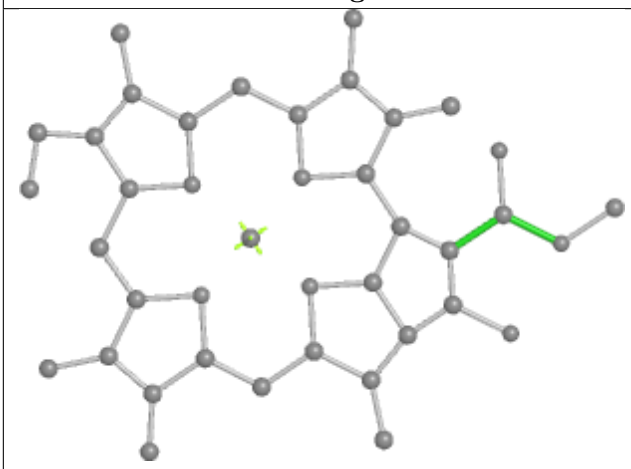
Ligand CLA A3 812



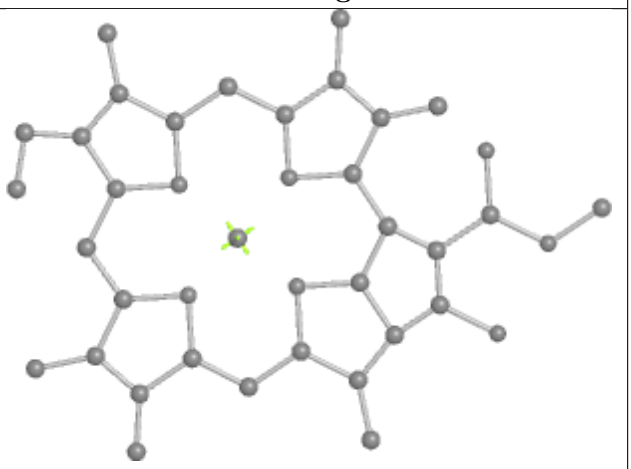
Bond lengths



Bond angles

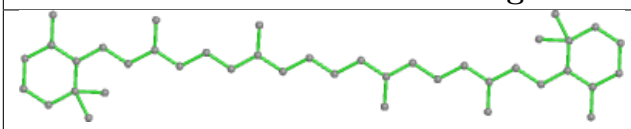


Torsions



Rings

Ligand BCR L1 1005



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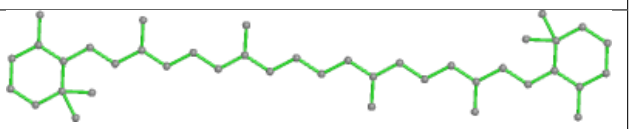
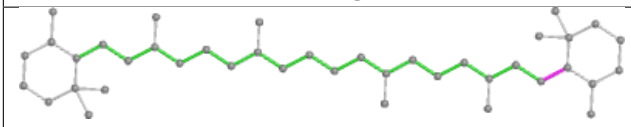


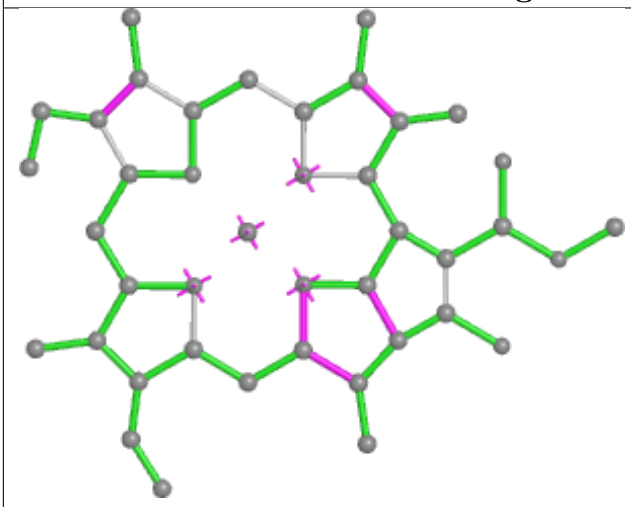
Bond angles



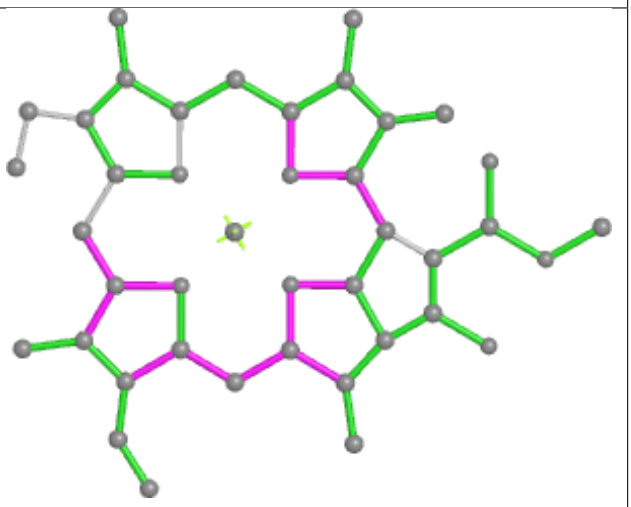
Torsions

Rings

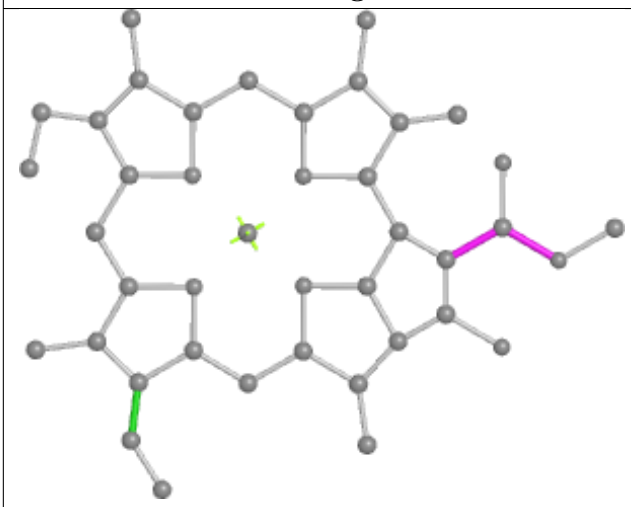
Ligand CLA B2 830



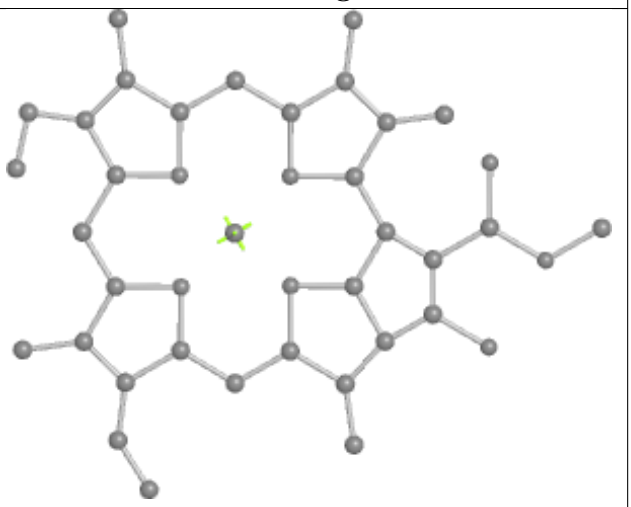
Bond lengths



Bond angles

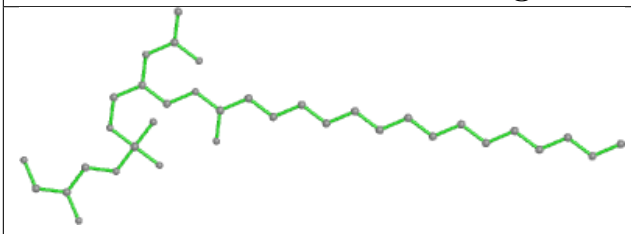


Torsions

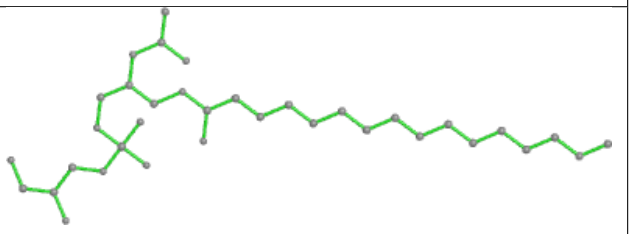


Rings

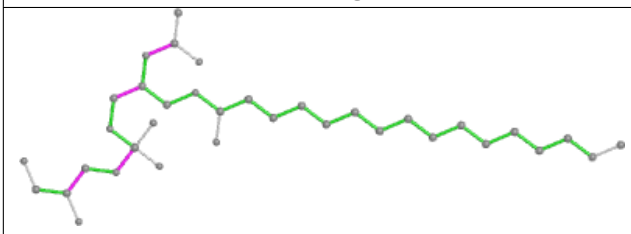
Ligand LHG A1 854



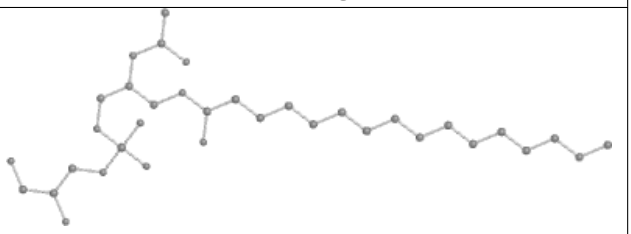
Bond lengths



Bond angles

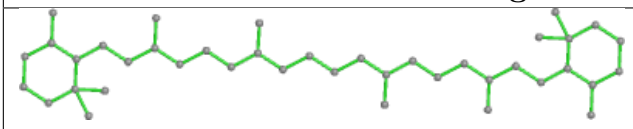


Torsions

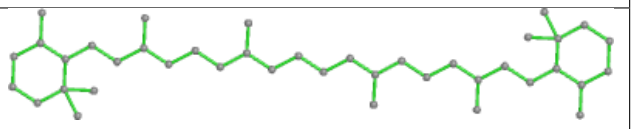


Rings

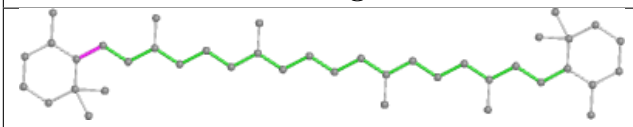
Ligand BCR M3 101



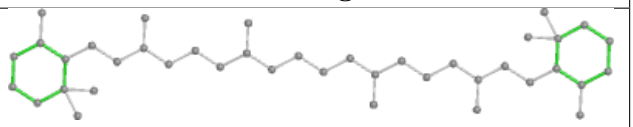
Bond lengths



Bond angles

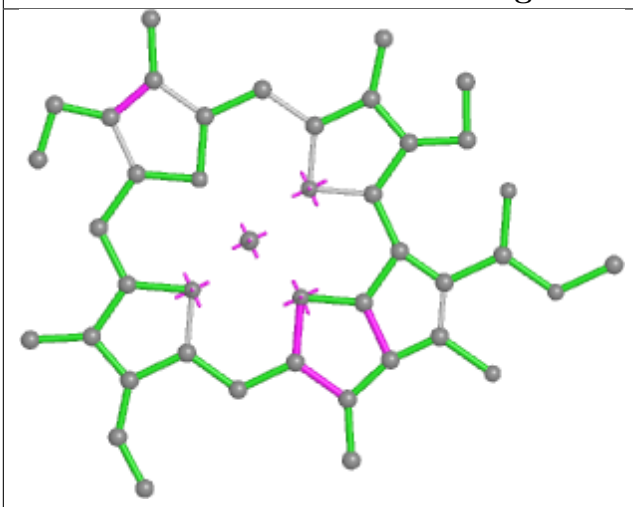


Torsions

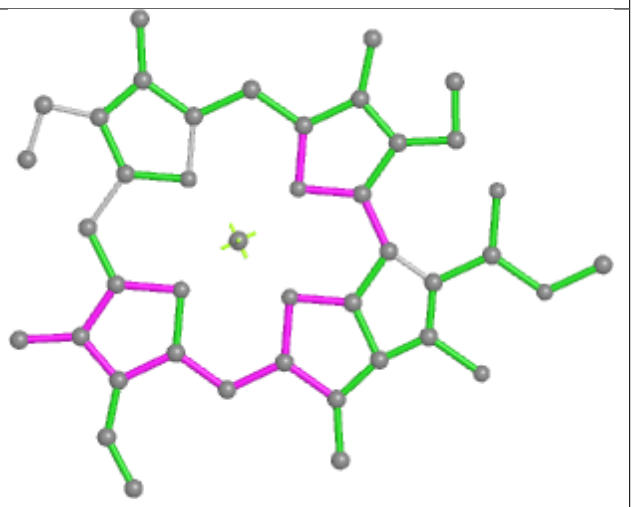


Rings

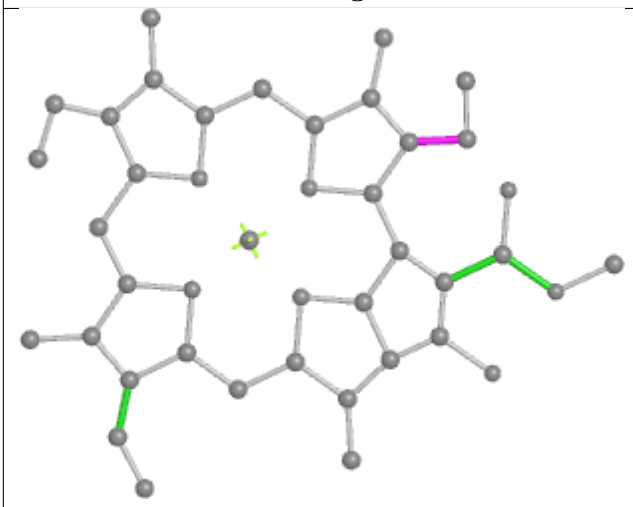
Ligand CLA A3 828



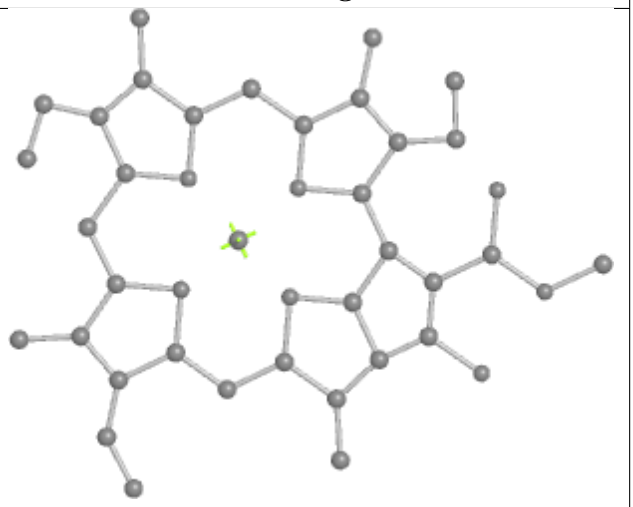
Bond lengths



Bond angles

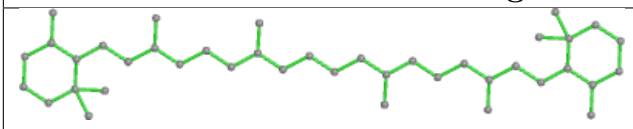


Torsions

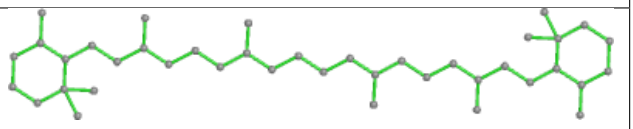


Rings

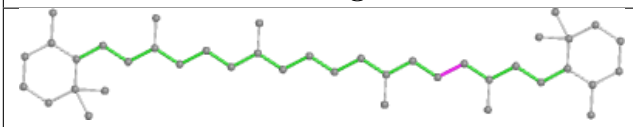
Ligand BCR L1 1006



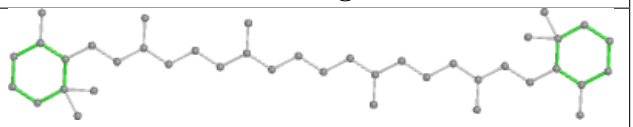
Bond lengths



Bond angles

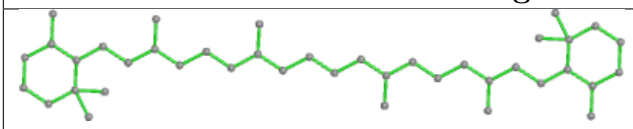


Torsions



Rings

Ligand BCR A2 847



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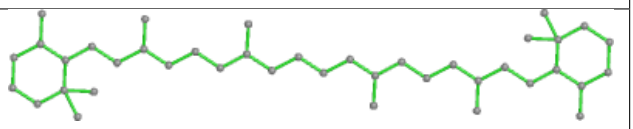

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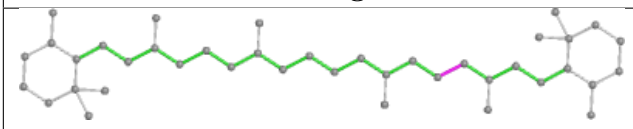

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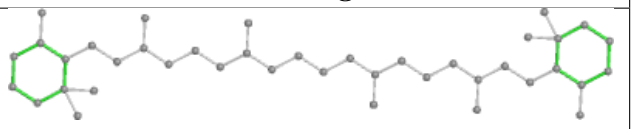
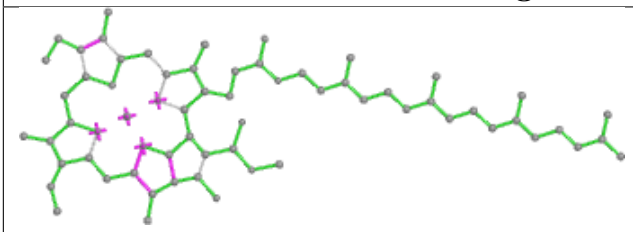


Rings

Ligand CLA B1 825



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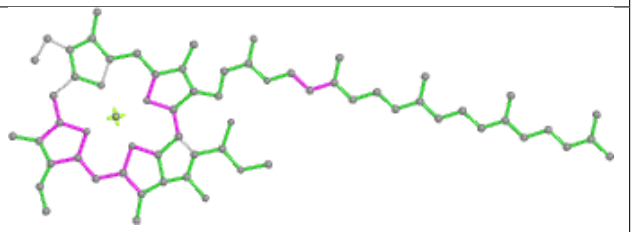
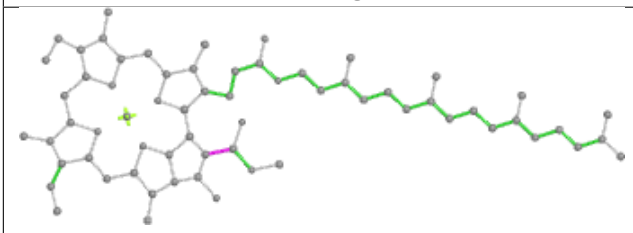
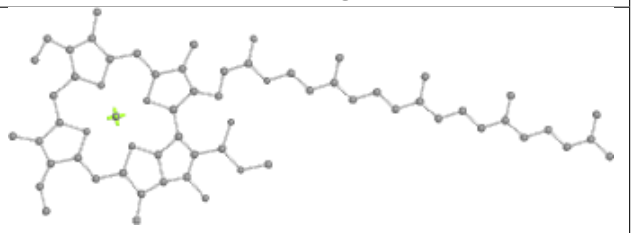


Bond angles

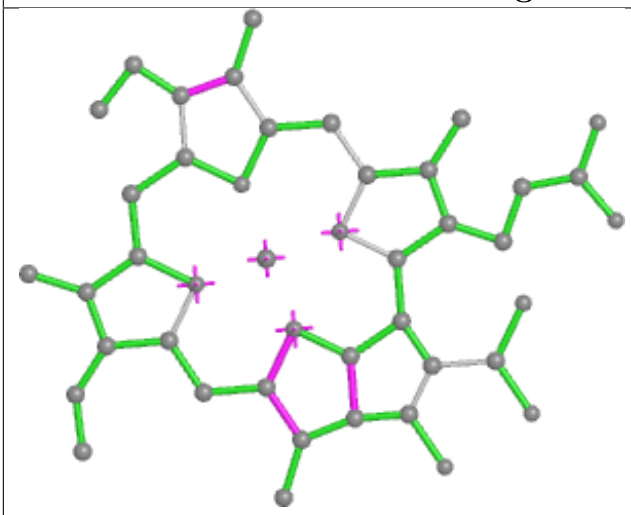


Torsions

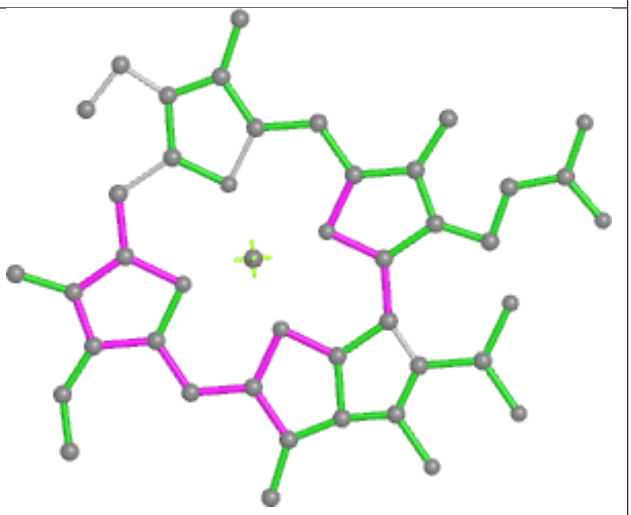


Rings

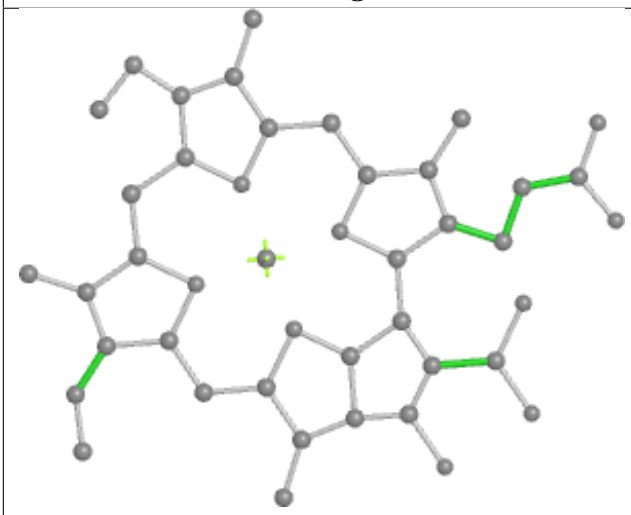
Ligand CLA B2 810



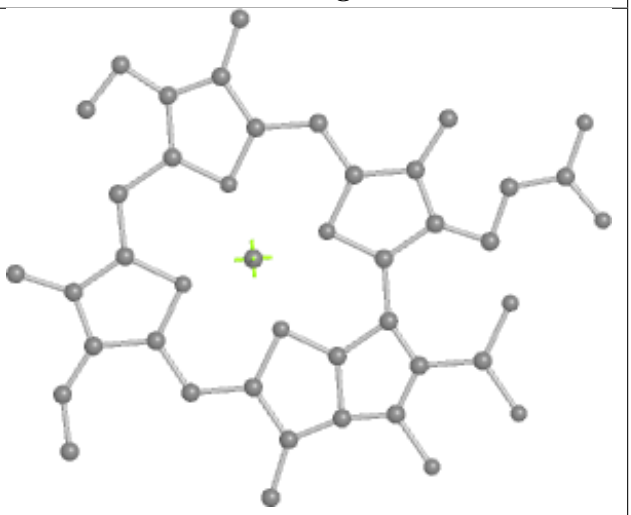
Bond lengths



Bond angles

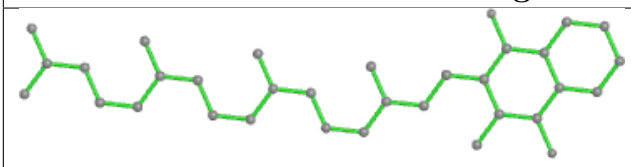


Torsions



Rings

Ligand PQN B2 840



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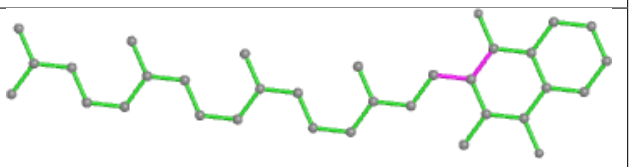

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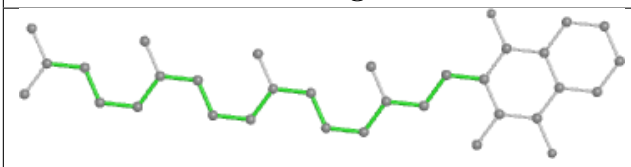

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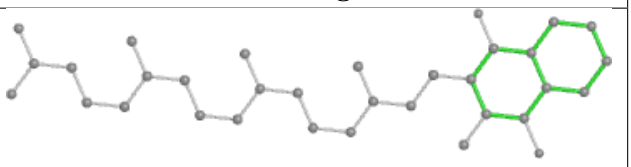
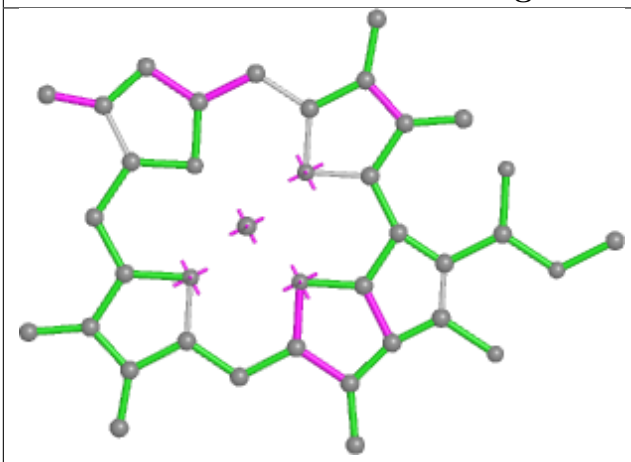


Rings

Ligand CLA A2 817



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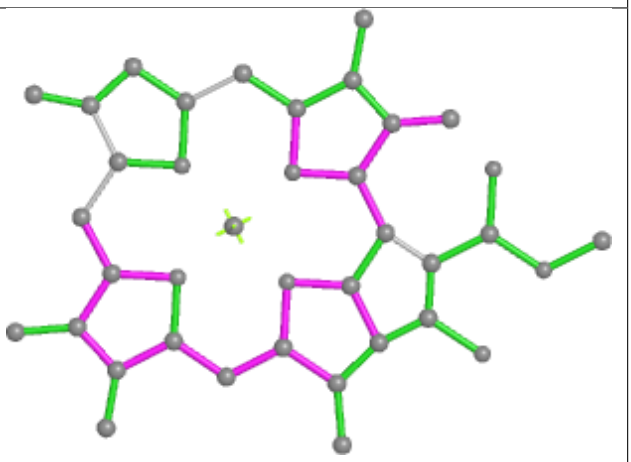
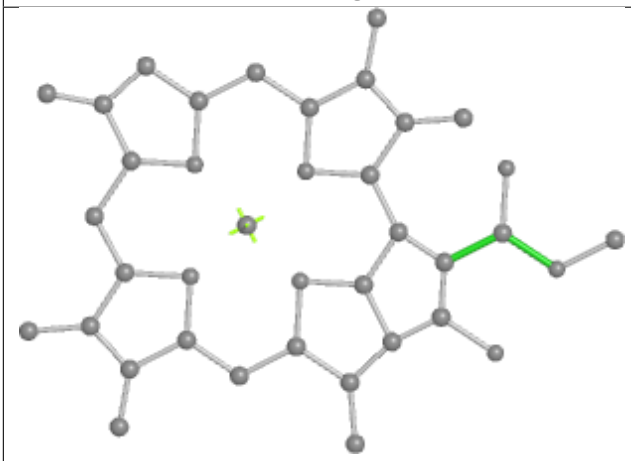


Bond angles



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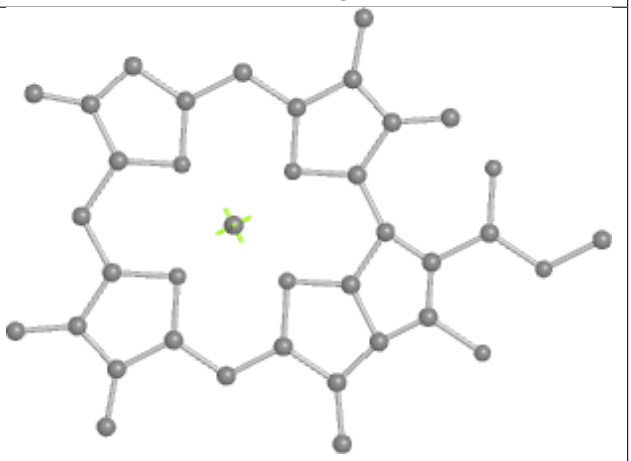
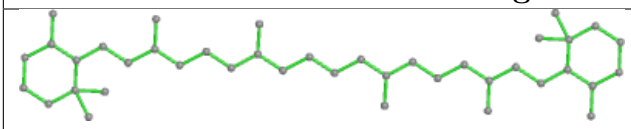


Rings

Ligand BCR A1 848



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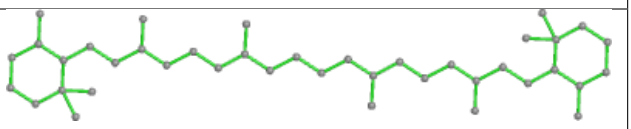
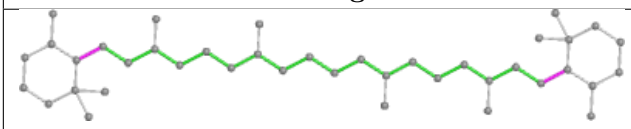


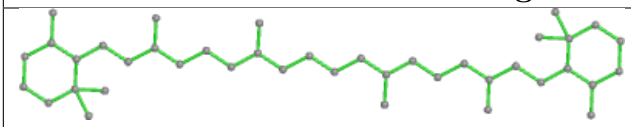
Bond angles



Torsions

Rings

Ligand BCR F3 201



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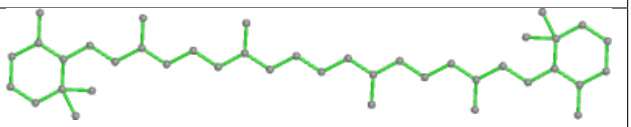
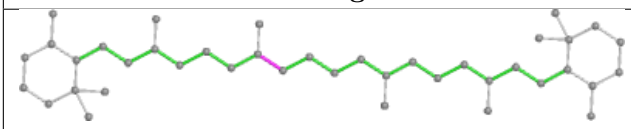


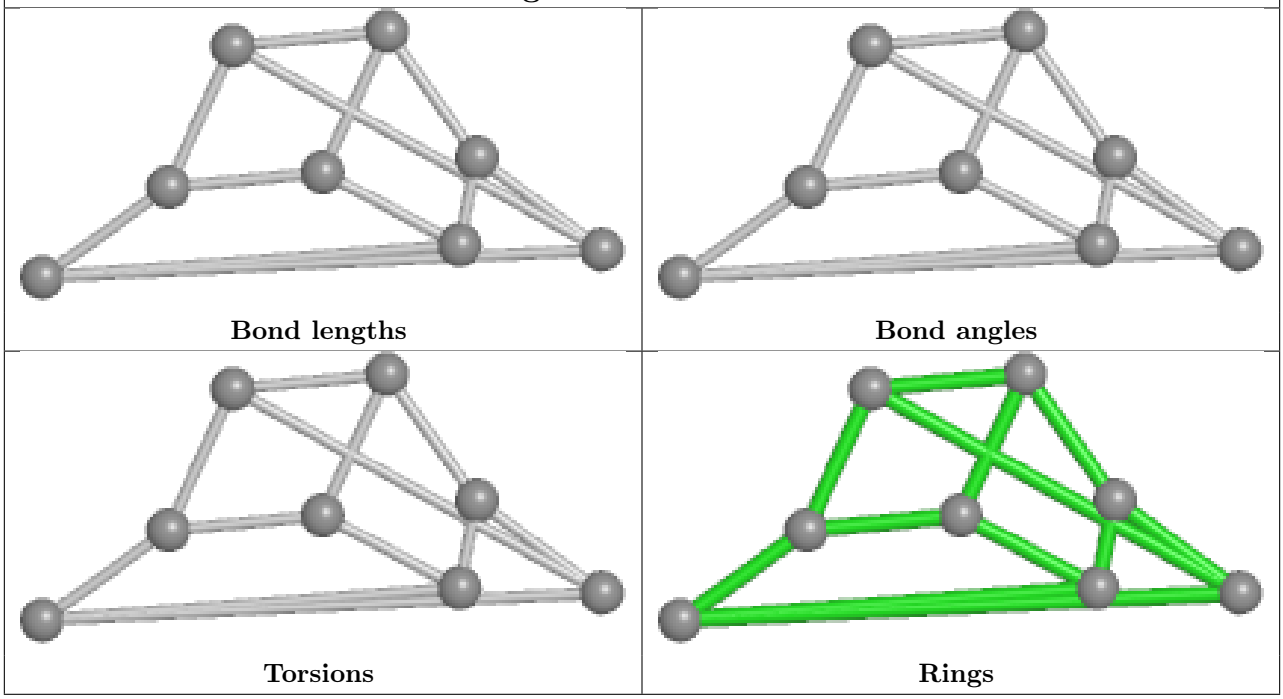
Bond angles



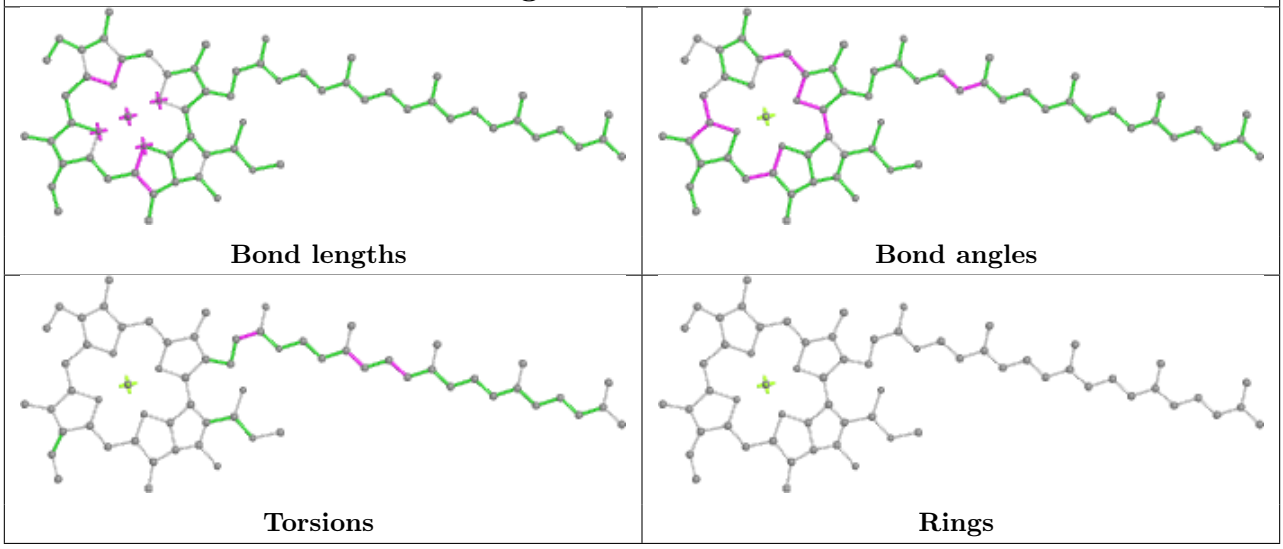
Torsions

Rings

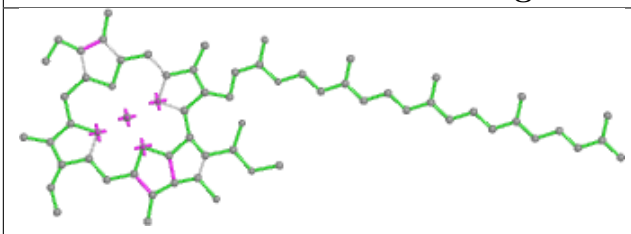
Ligand SF4 A2 846



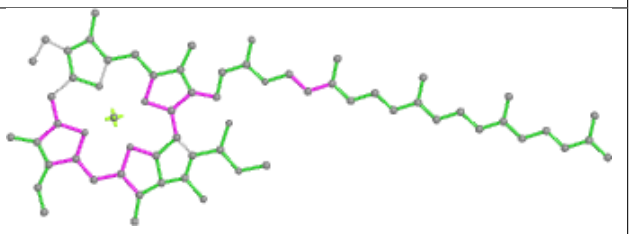
Ligand CL0 A1 801



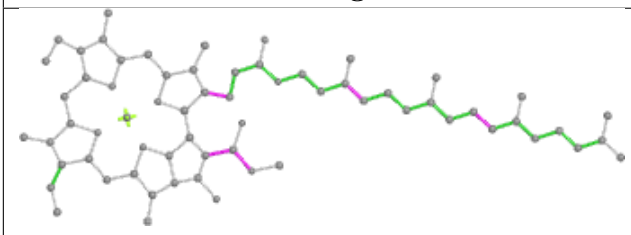
Ligand CLA A1 830



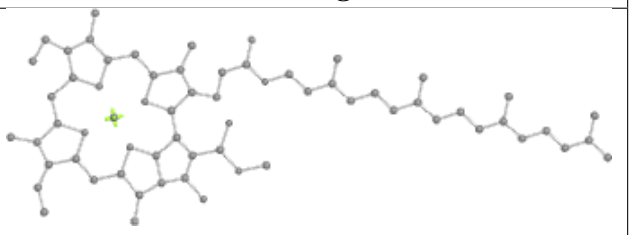
Bond lengths



Bond angles

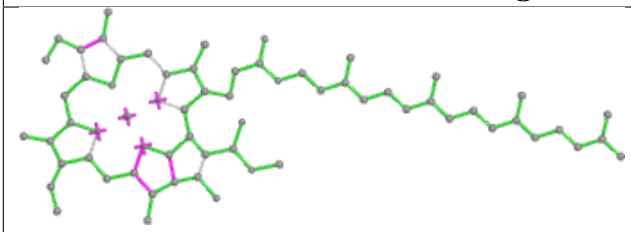


Torsions

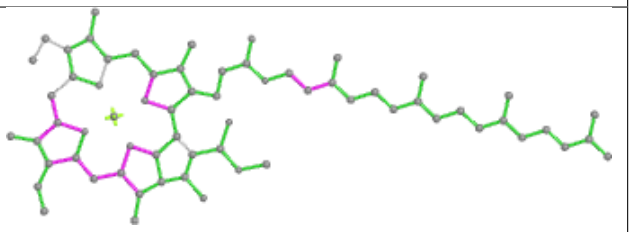


Rings

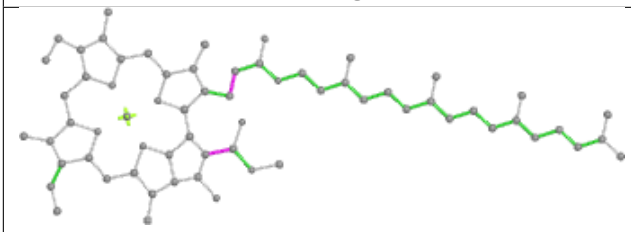
Ligand CLA A3 805



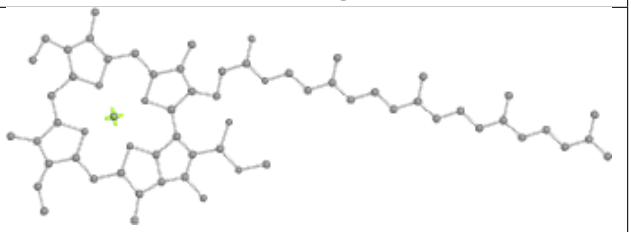
Bond lengths



Bond angles

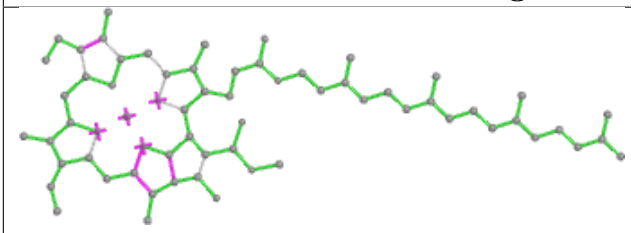


Torsions



Rings

Ligand CLA L3 1002



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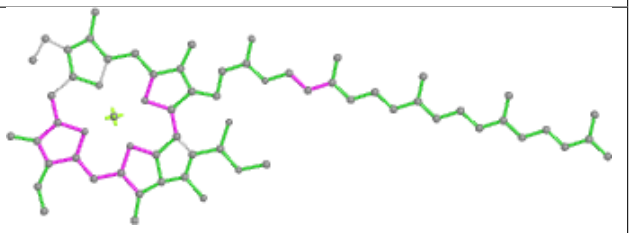
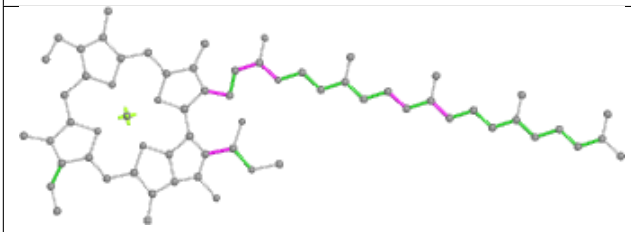


Bond angles



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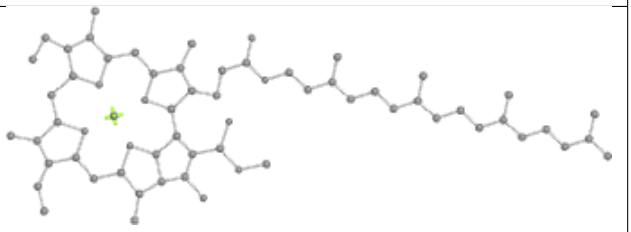
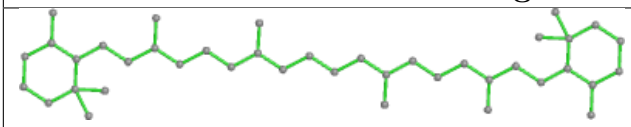
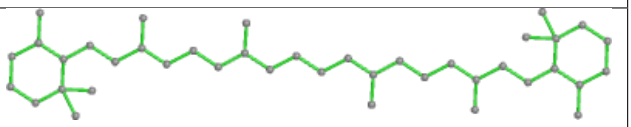
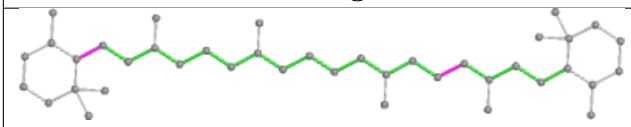
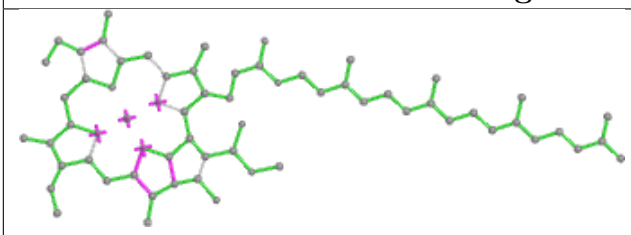
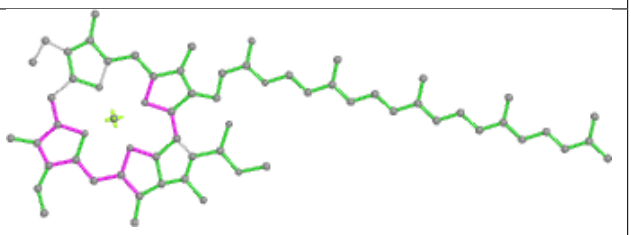
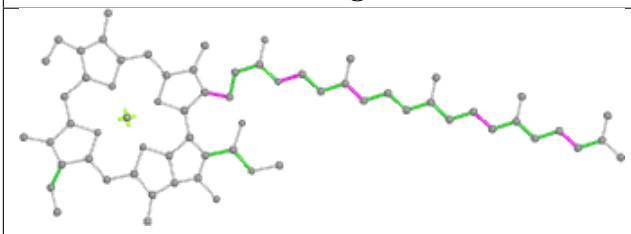
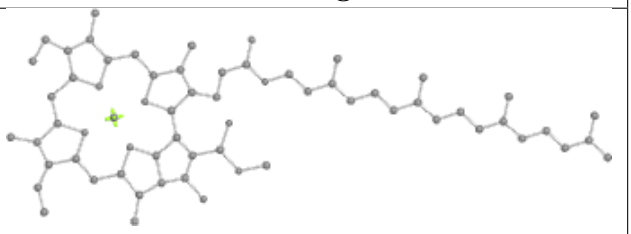
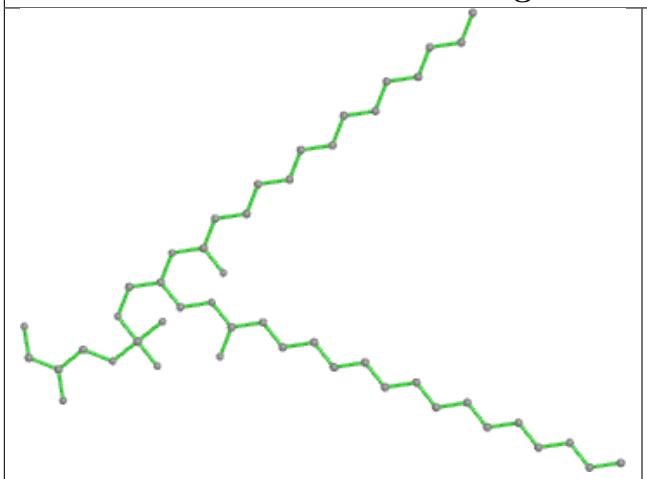


Rings

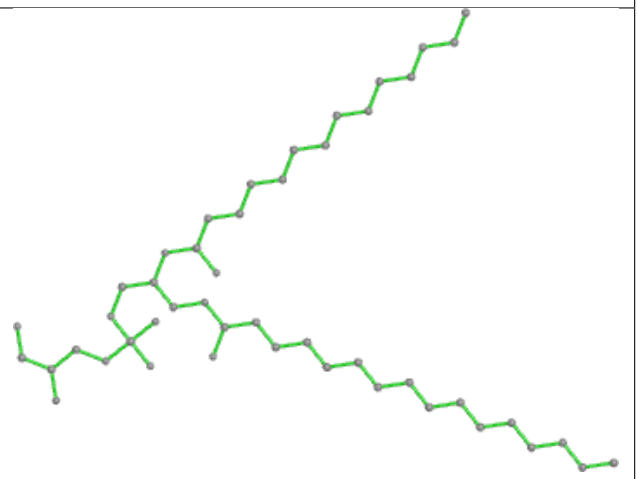
Ligand BCR B1 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A3 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

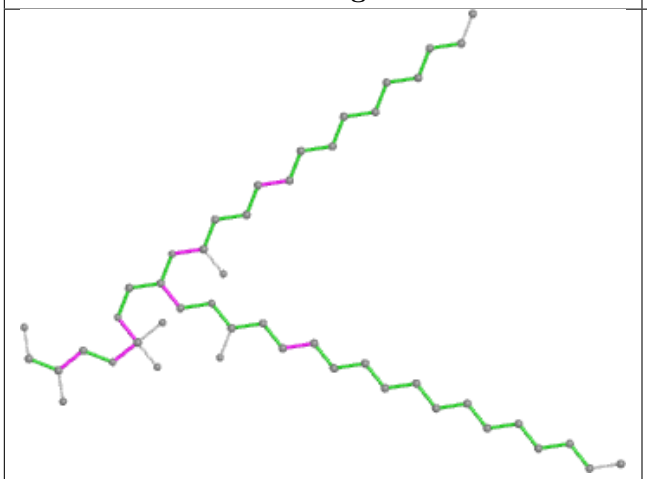
Ligand LHG A3 853



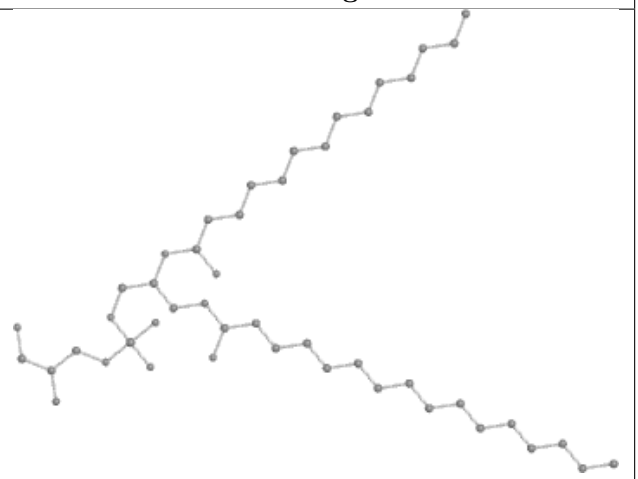
Bond lengths



Bond angles

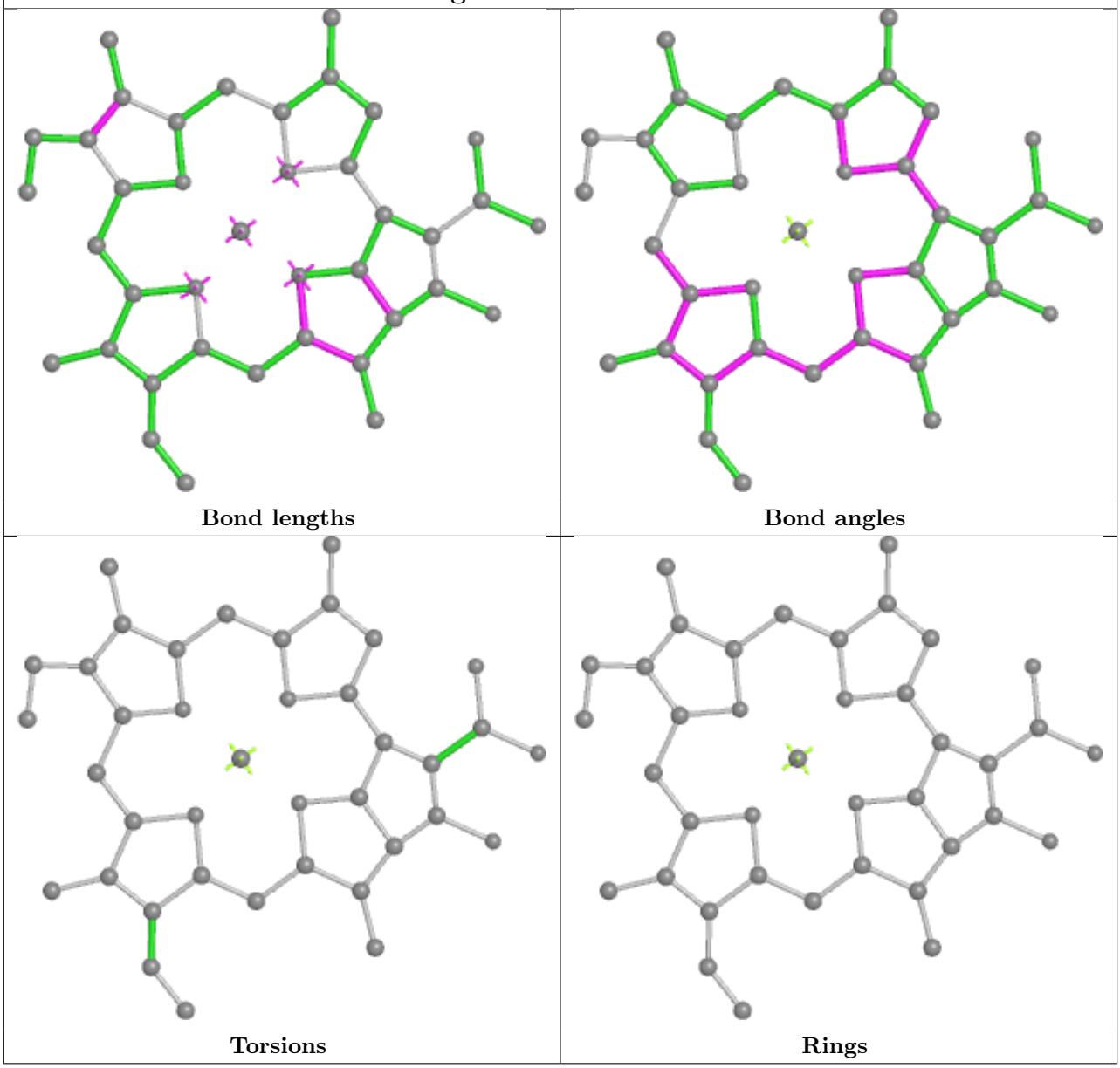


Torsions

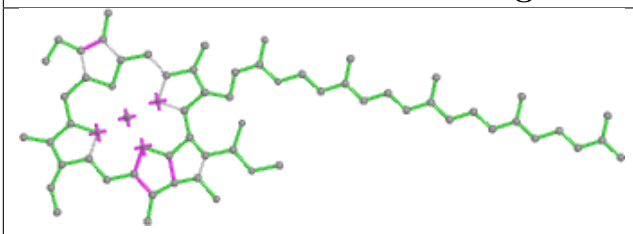


Rings

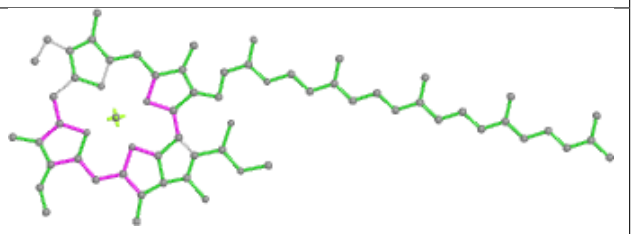
Ligand CLA B2 834



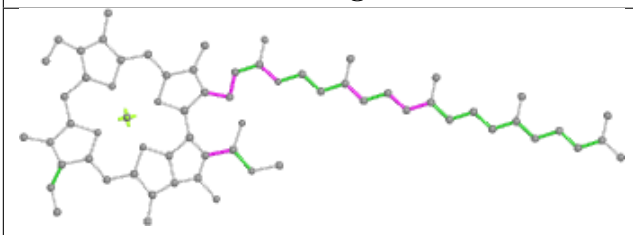
Ligand CLA B1 827



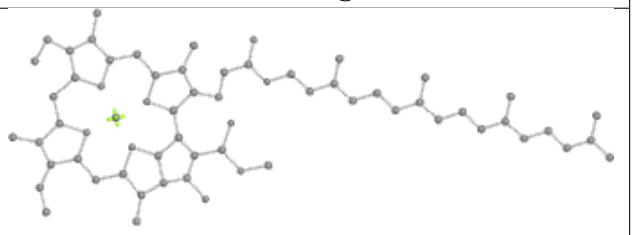
Bond lengths



Bond angles

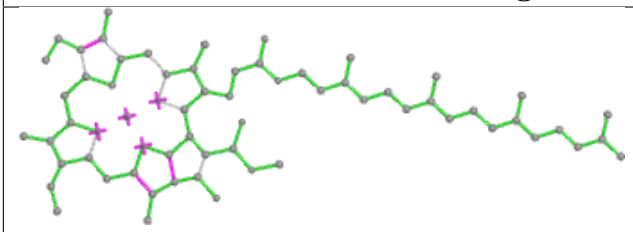


Torsions

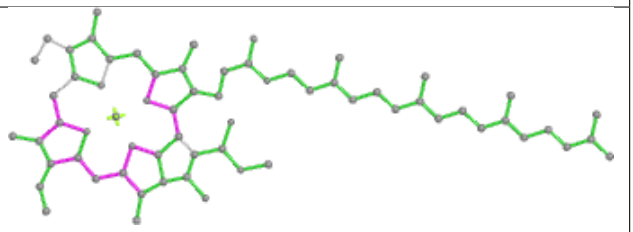


Rings

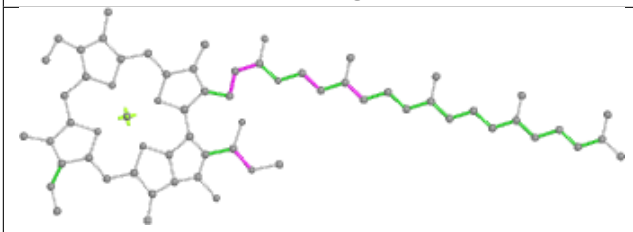
Ligand CLA B3 801



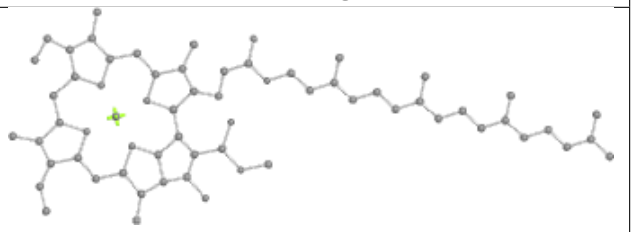
Bond lengths



Bond angles

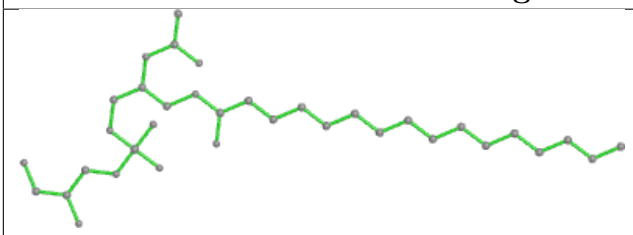


Torsions

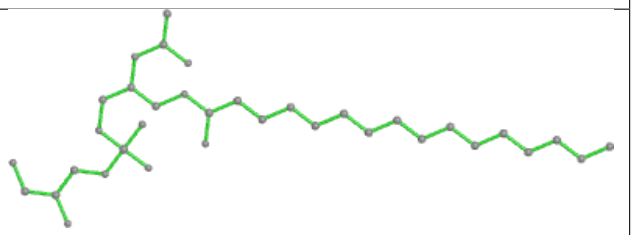


Rings

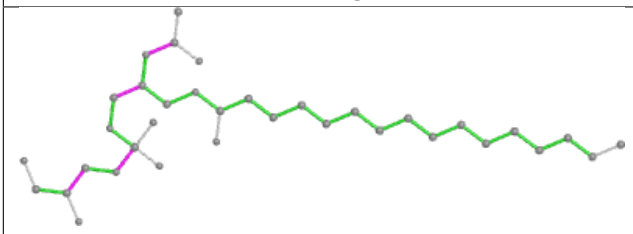
Ligand LHG A2 854



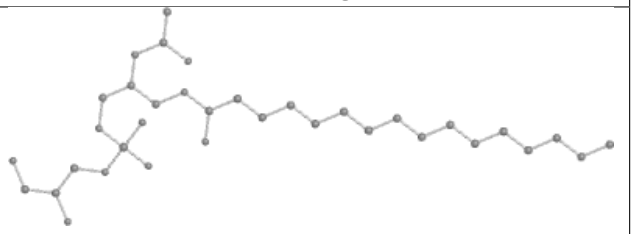
Bond lengths



Bond angles

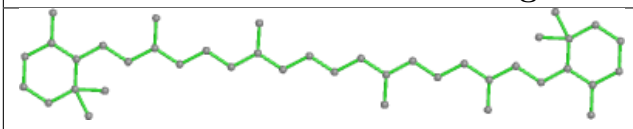


Torsions

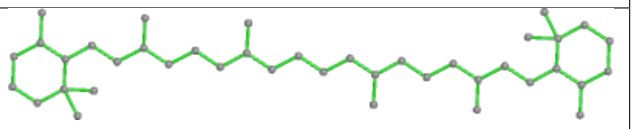


Rings

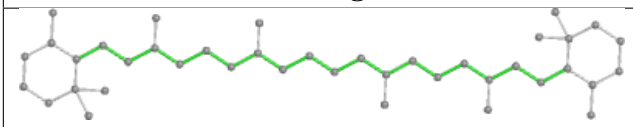
Ligand BCR I3 102



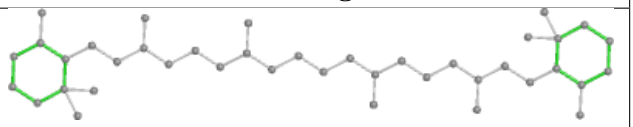
Bond lengths



Bond angles

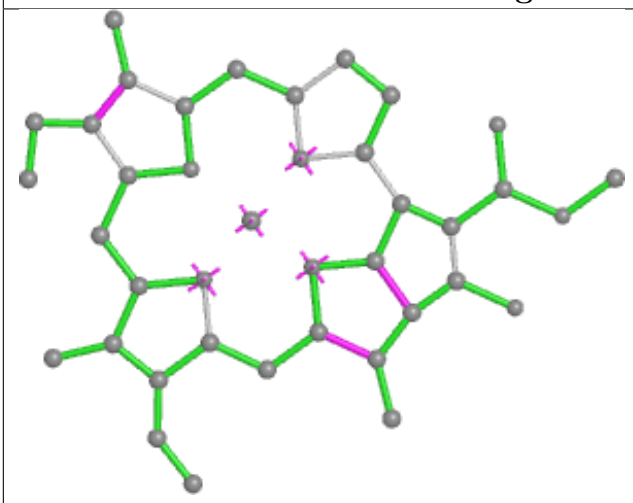


Torsions

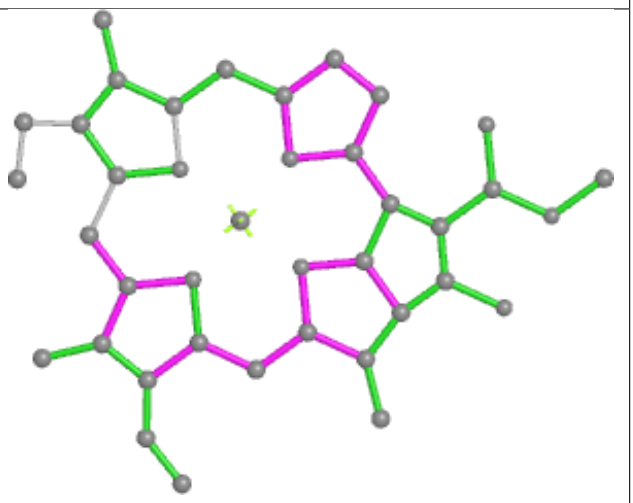


Rings

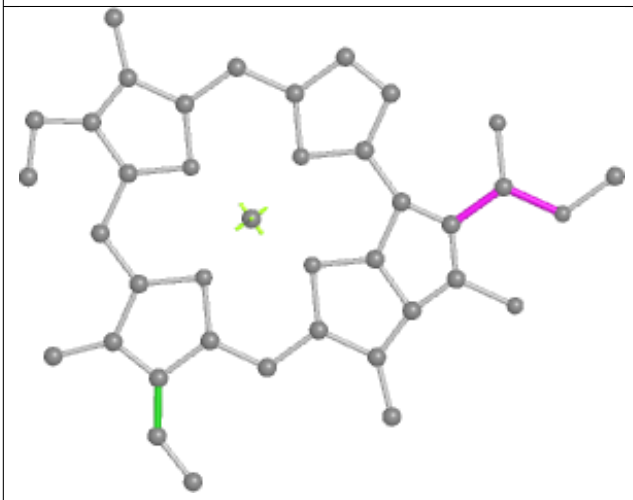
Ligand CLA B1 821



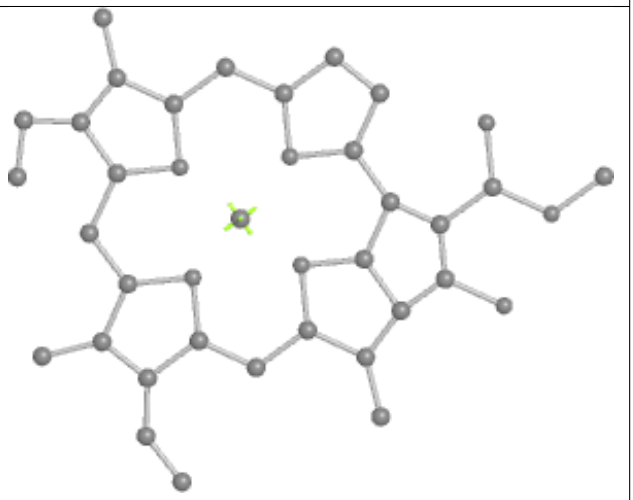
Bond lengths



Bond angles

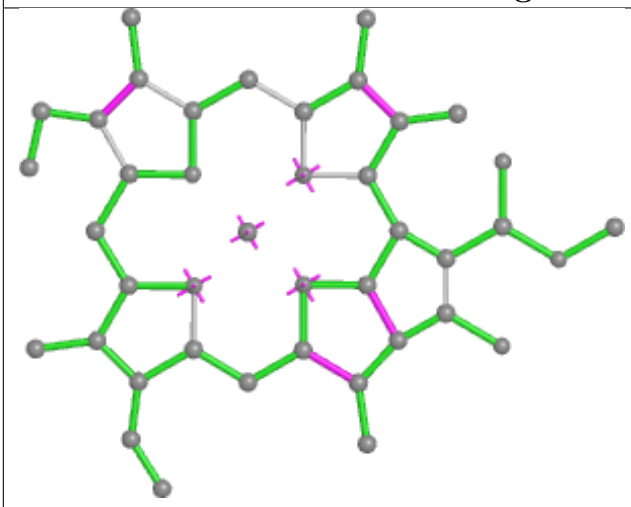


Torsions

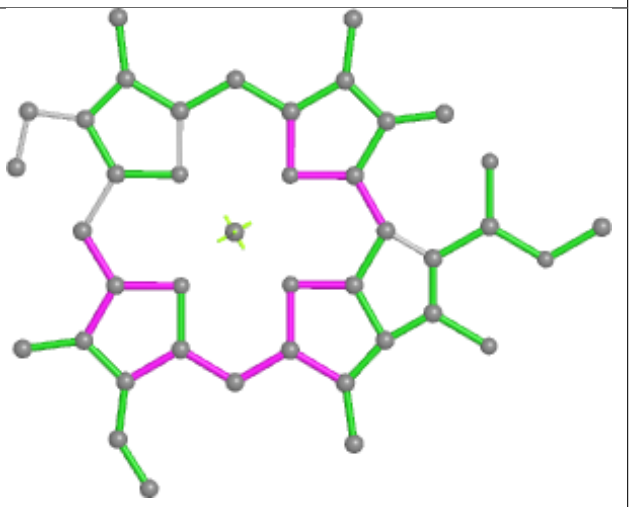


Rings

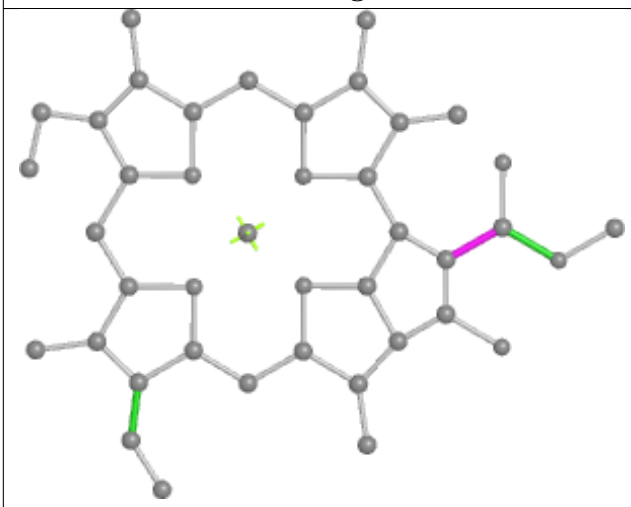
Ligand CLA A1 836



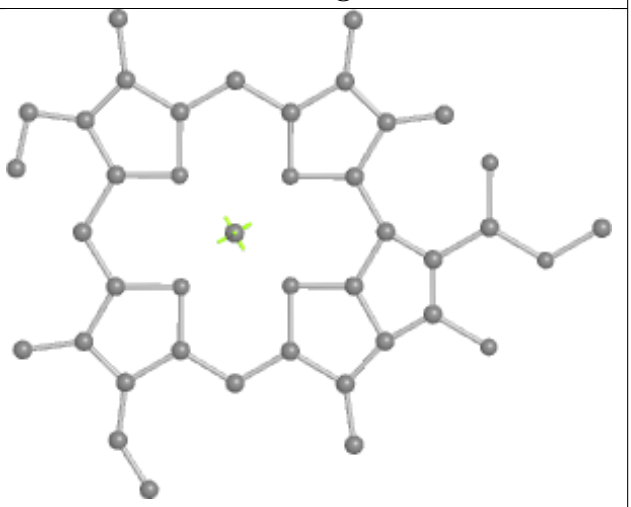
Bond lengths



Bond angles

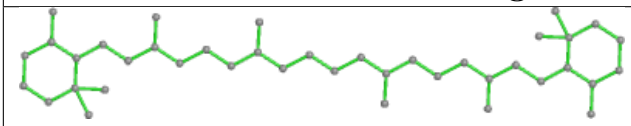


Torsions

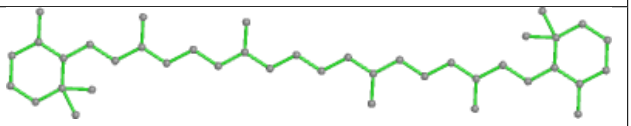


Rings

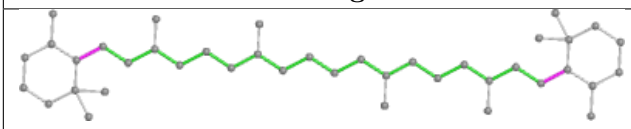
Ligand BCR J1 1305



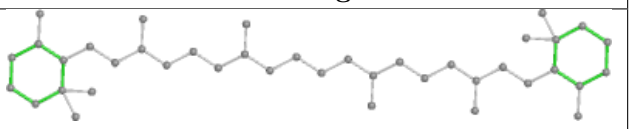
Bond lengths



Bond angles

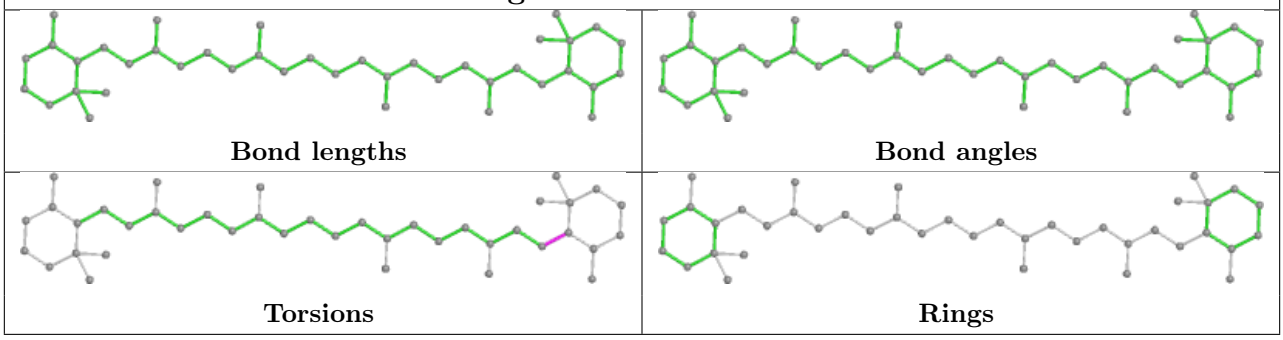


Torsions

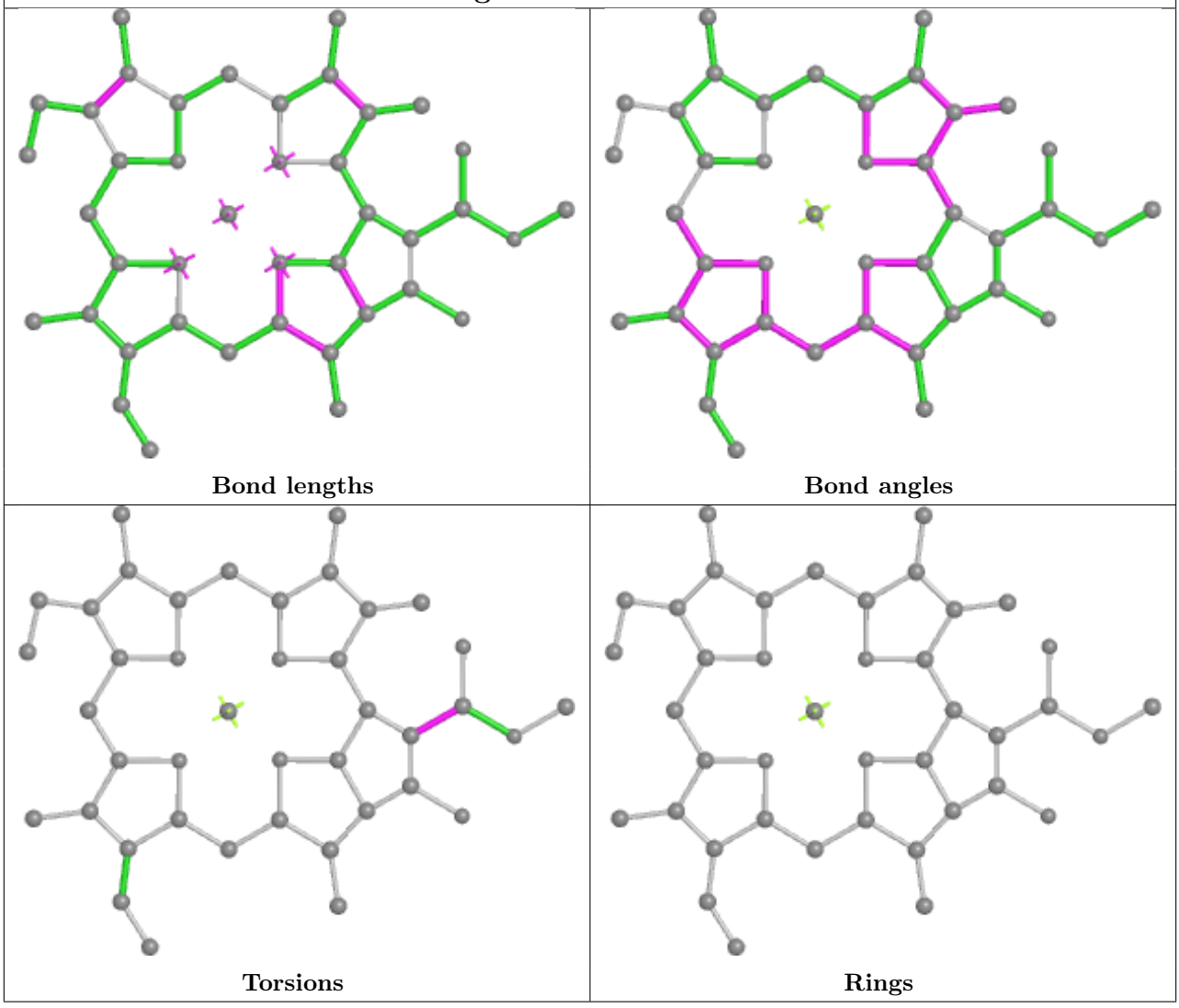


Rings

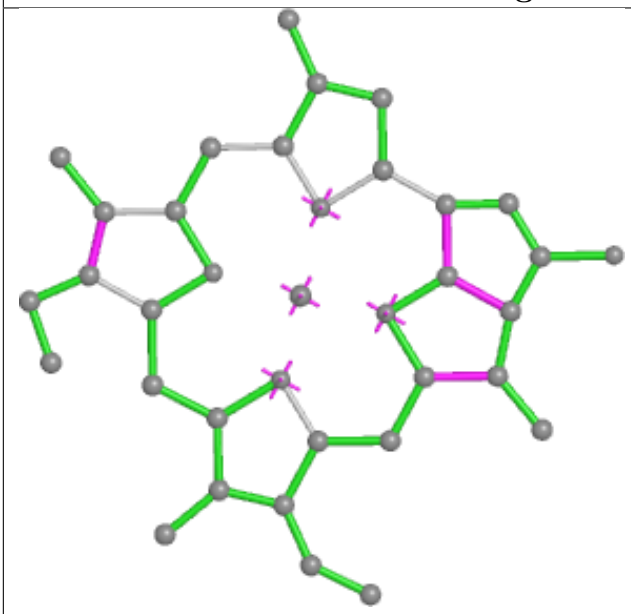
Ligand BCR L2 1005



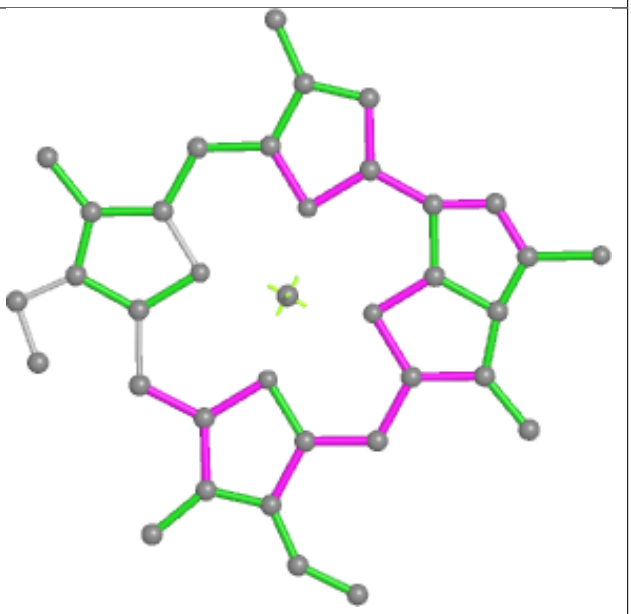
Ligand CLA B1 831



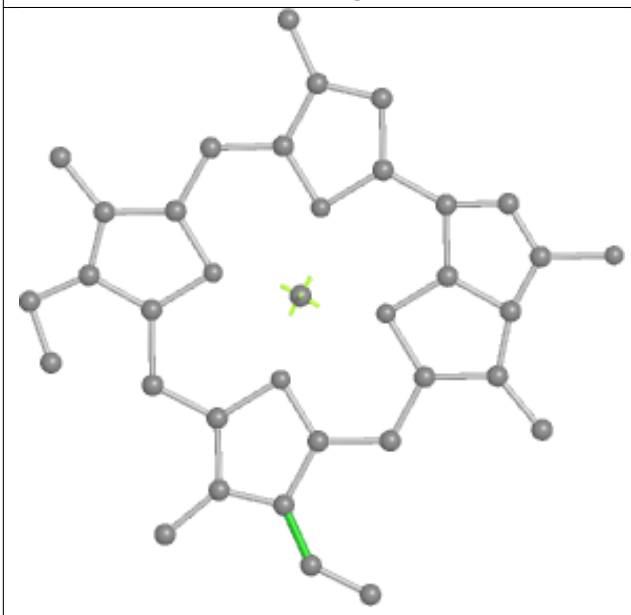
Ligand CLA B2 820



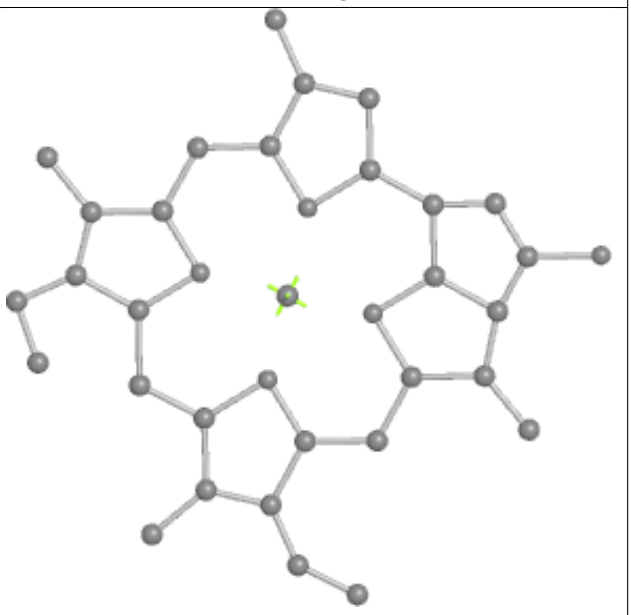
Bond lengths



Bond angles

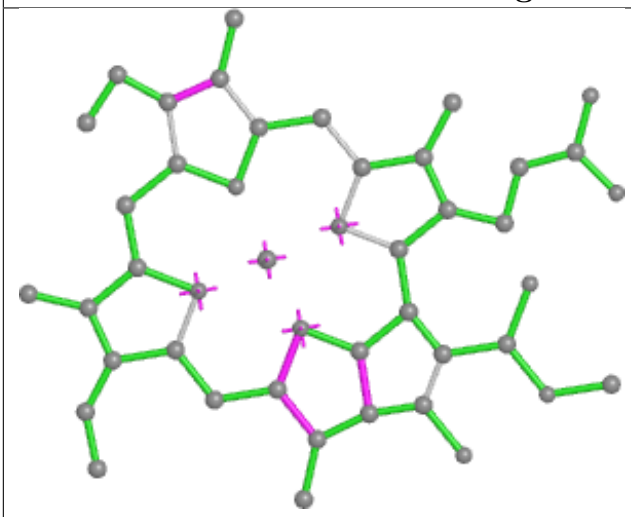


Torsions

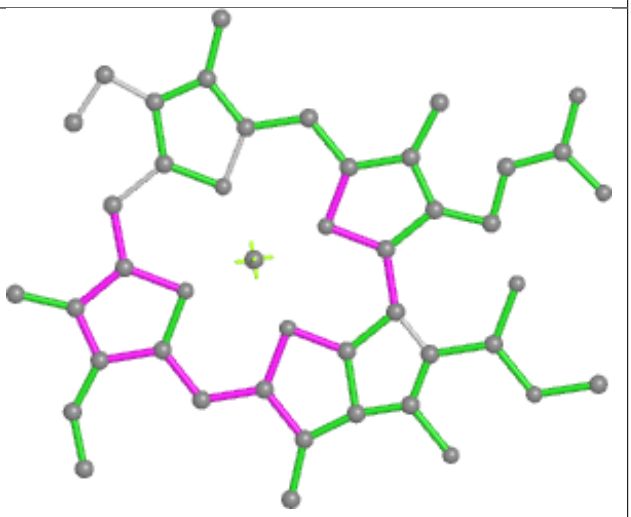


Rings

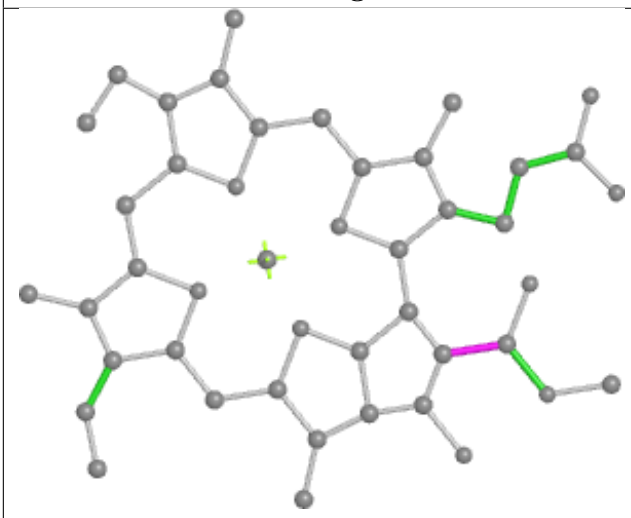
Ligand CLA B1 836



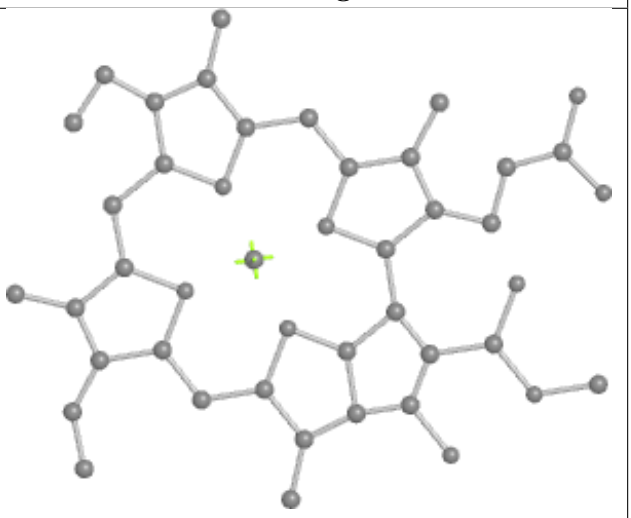
Bond lengths



Bond angles

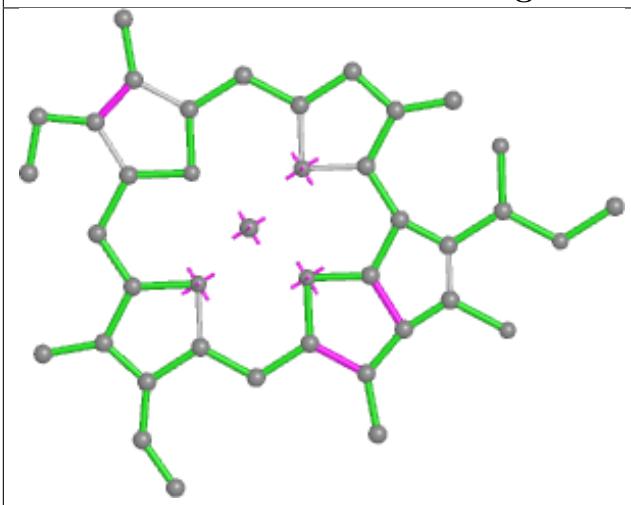


Torsions

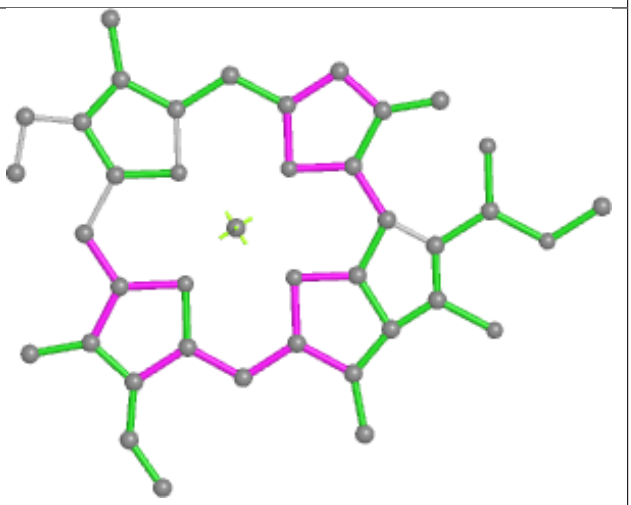


Rings

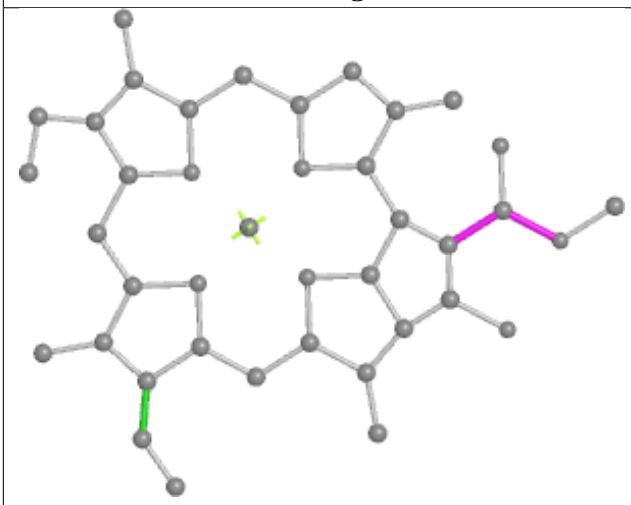
Ligand CLA B2 832



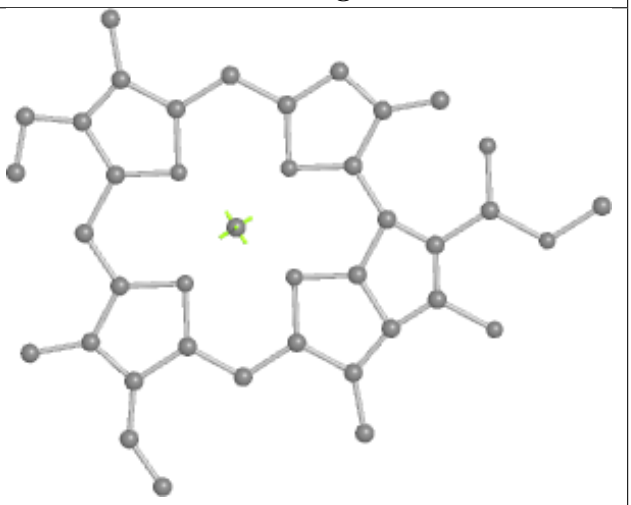
Bond lengths



Bond angles

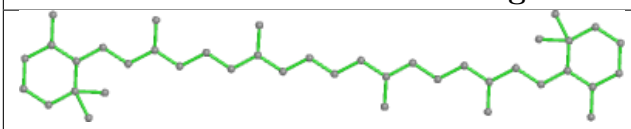


Torsions

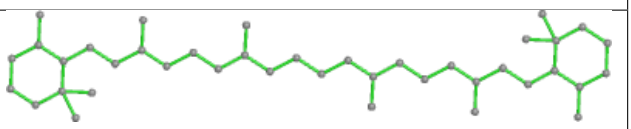


Rings

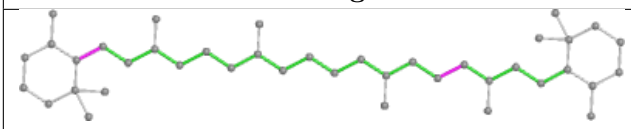
Ligand BCR J3 1304



Bond lengths



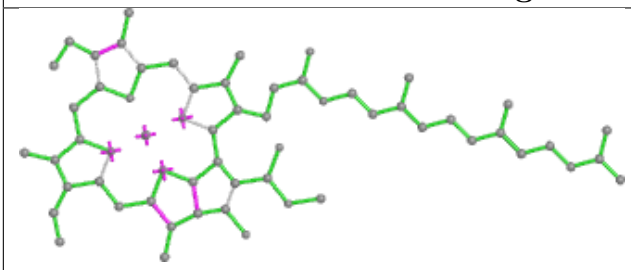
Bond angles



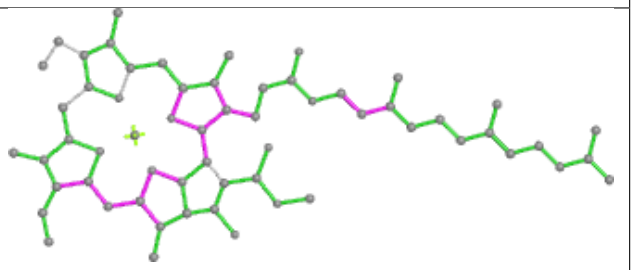
Torsions

Rings

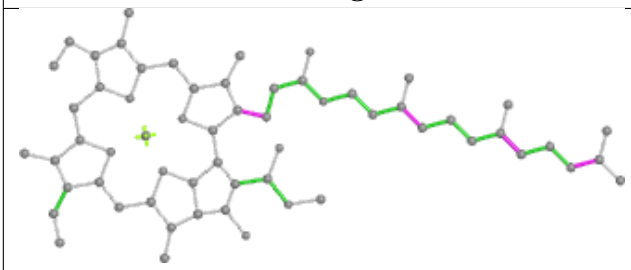
Ligand CLA B1 807



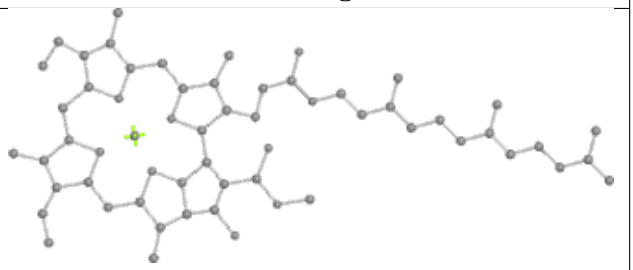
Bond lengths



Bond angles

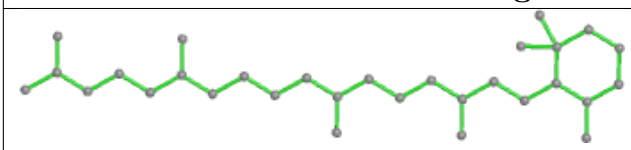


Torsions

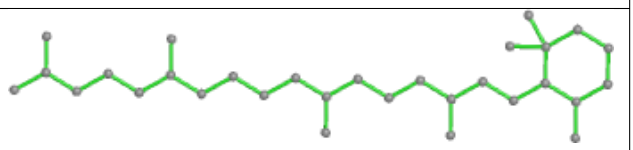


Rings

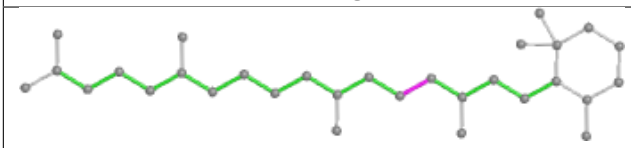
Ligand BCR B1 842



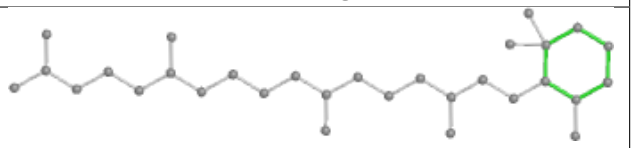
Bond lengths



Bond angles

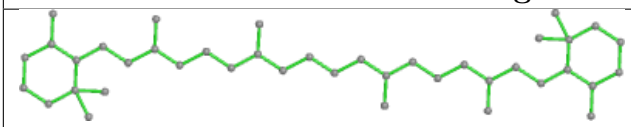


Torsions

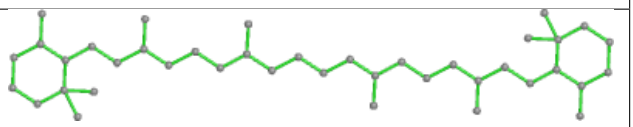


Rings

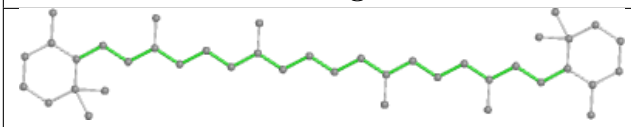
Ligand BCR B1 846



Bond lengths

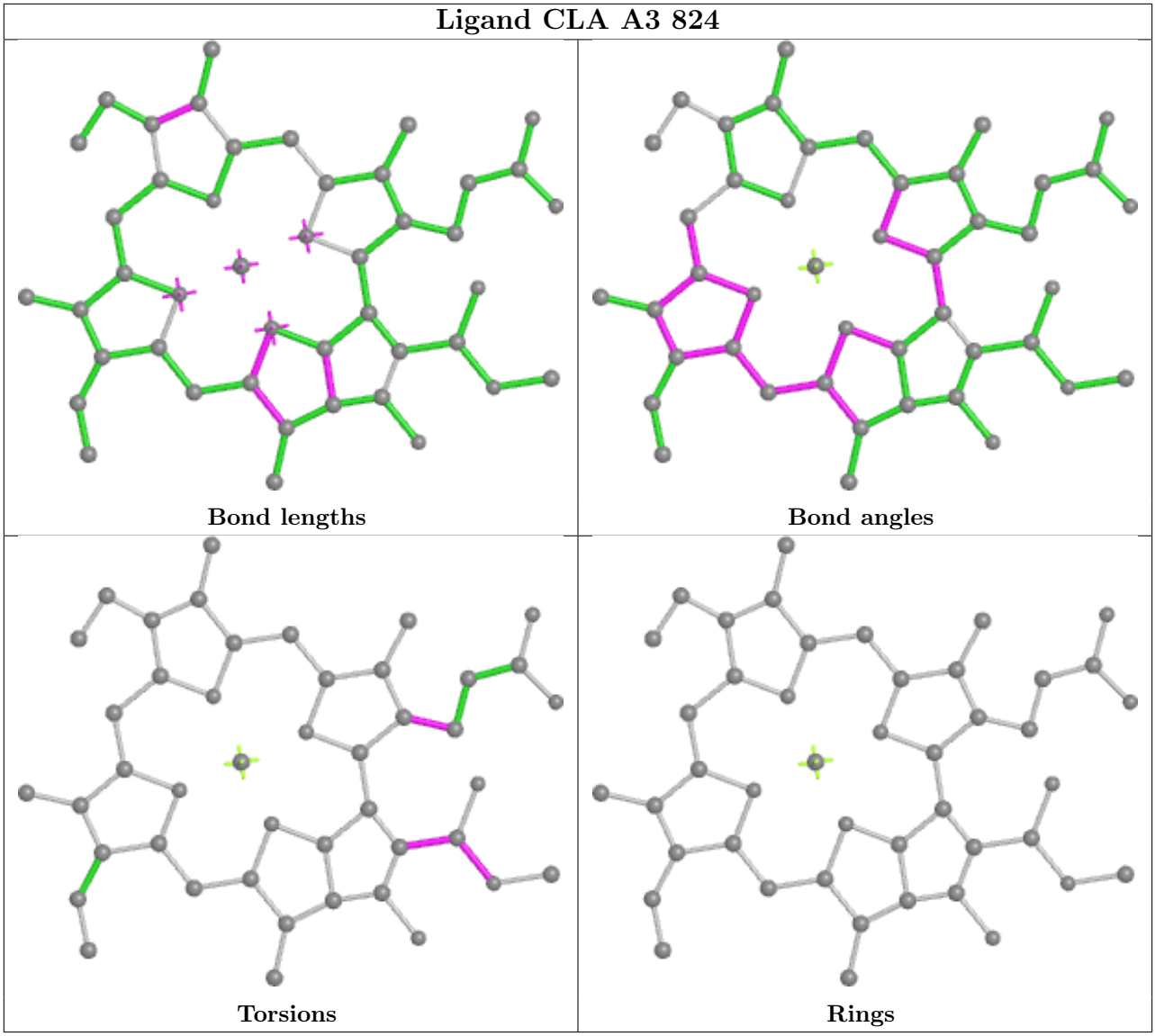


Bond angles



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.

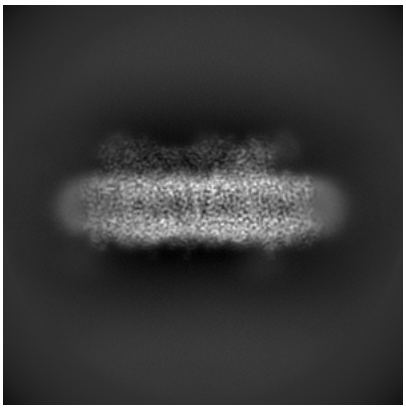
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31605. These allow visual inspection of the internal detail of the map and identification of artifacts.

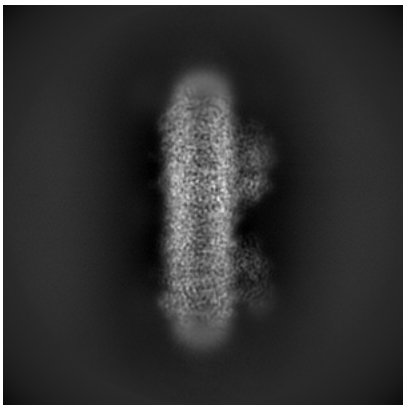
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

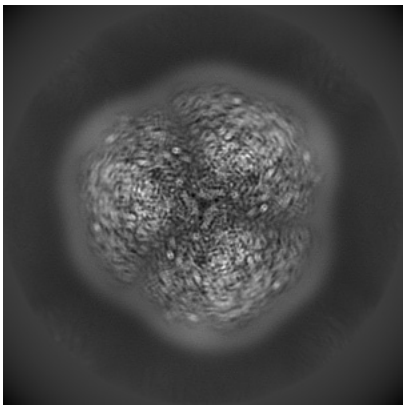
6.1.1 Primary map



X

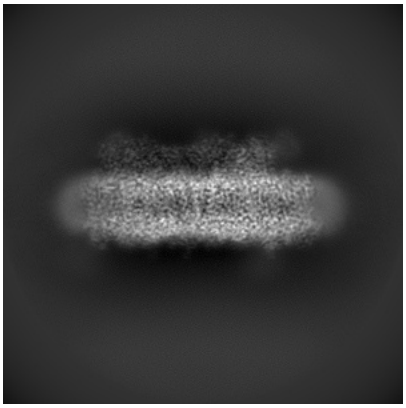


Y

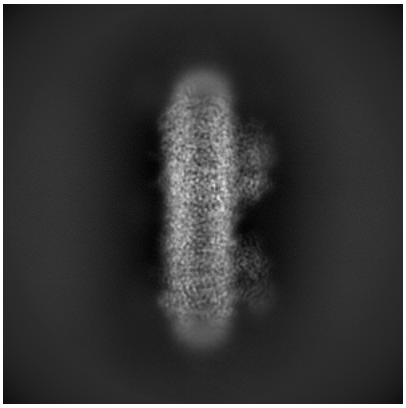


Z

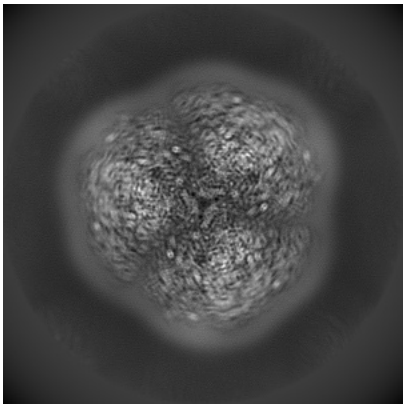
6.1.2 Raw map



X



Y

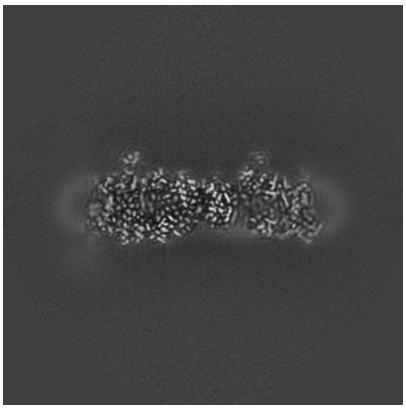


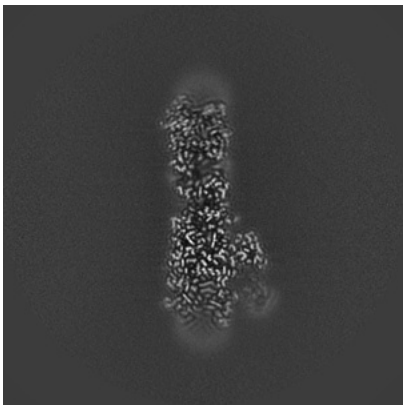
Z

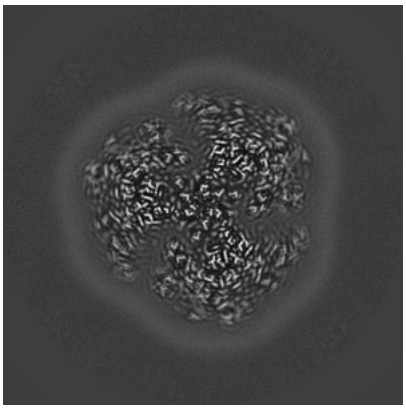
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

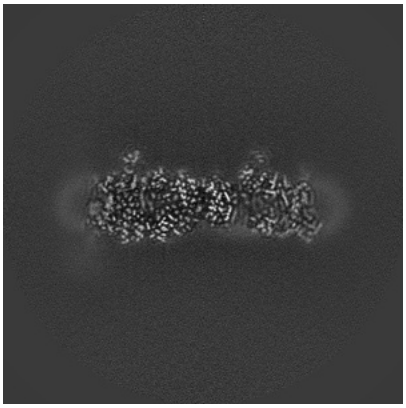
6.2.1 Primary map

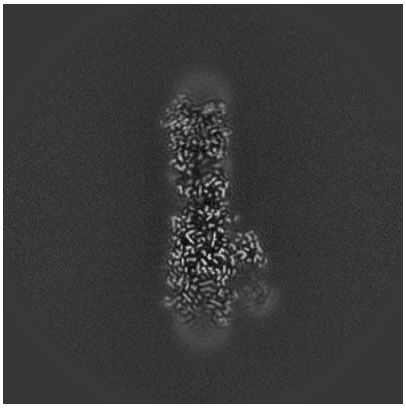

X Index: 200

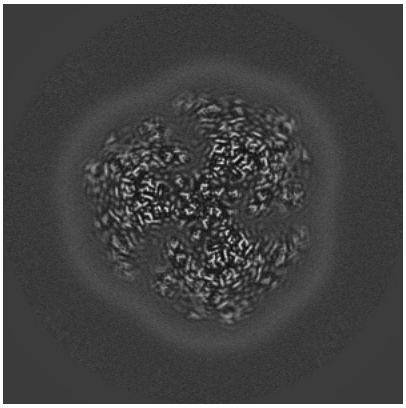

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

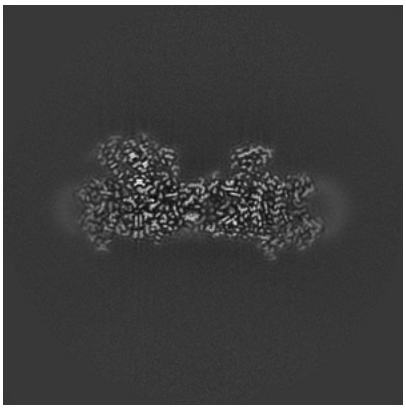

Y Index: 200

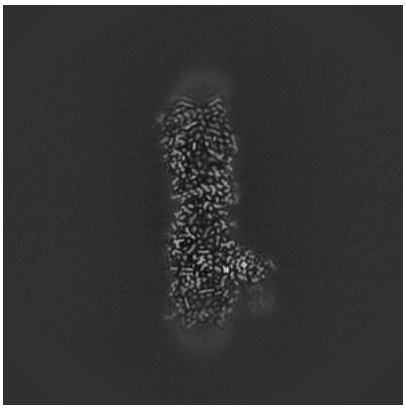

Z Index: 200

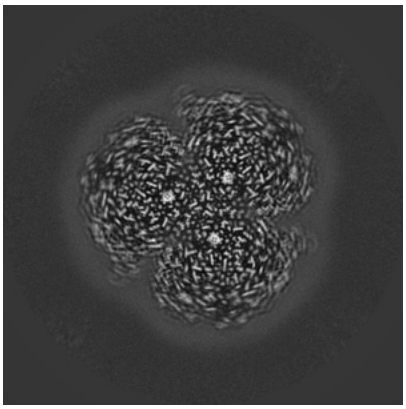
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

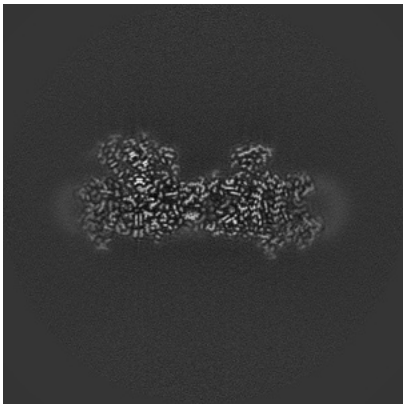
6.3.1 Primary map

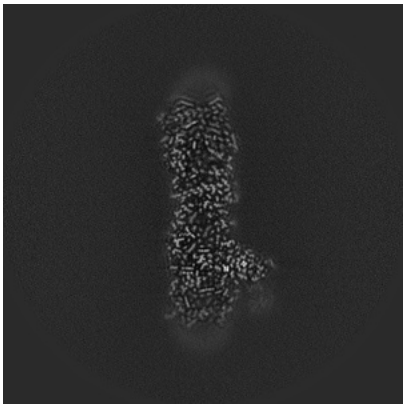

X Index: 221

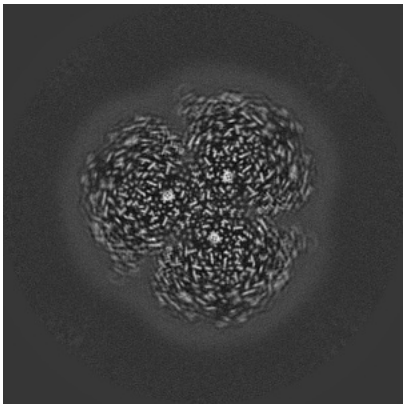

Y Index: 213


Z Index: 215

6.3.2 Raw map


X Index: 221

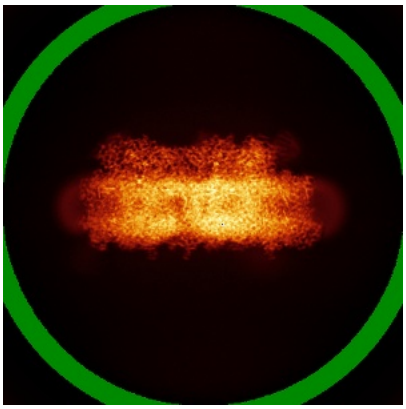

Y Index: 213

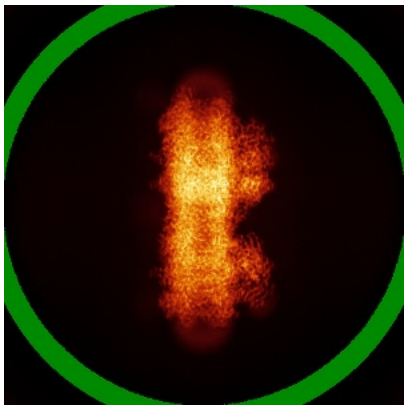

Z Index: 215

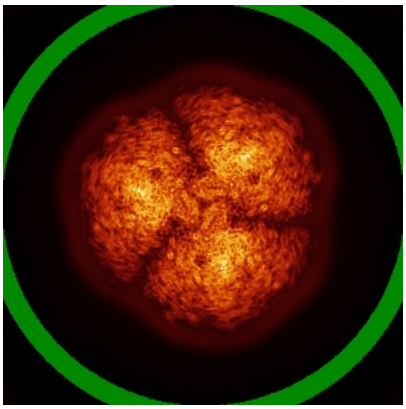
The images above show the largest variance slices of the map in three orthogonal directions.

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

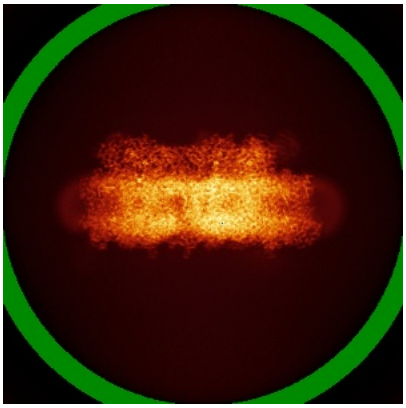
6.4.1 Primary map

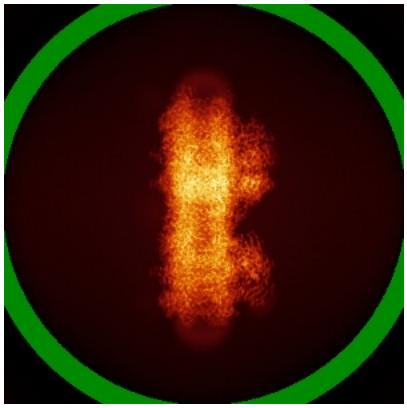

X

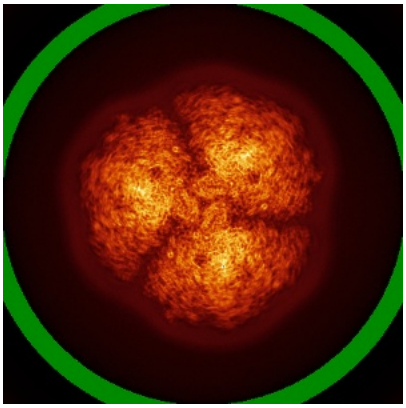

Y


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.

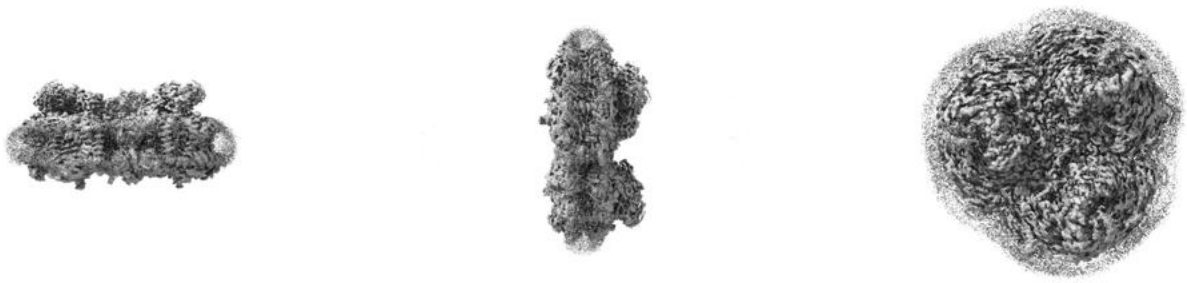
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

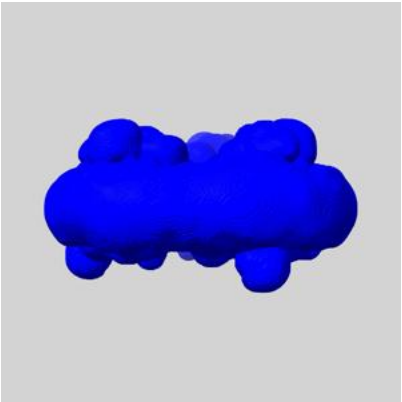
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

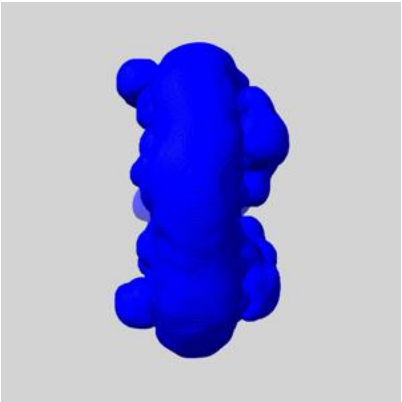
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

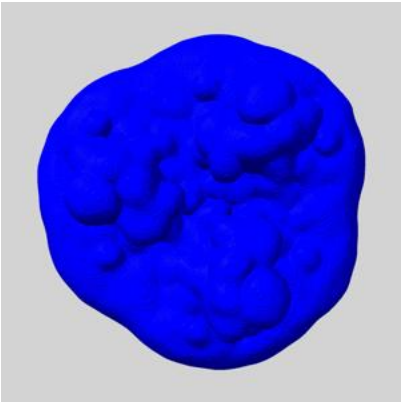
6.6.1 emd_31605_msk_1.map (i)



X



Y

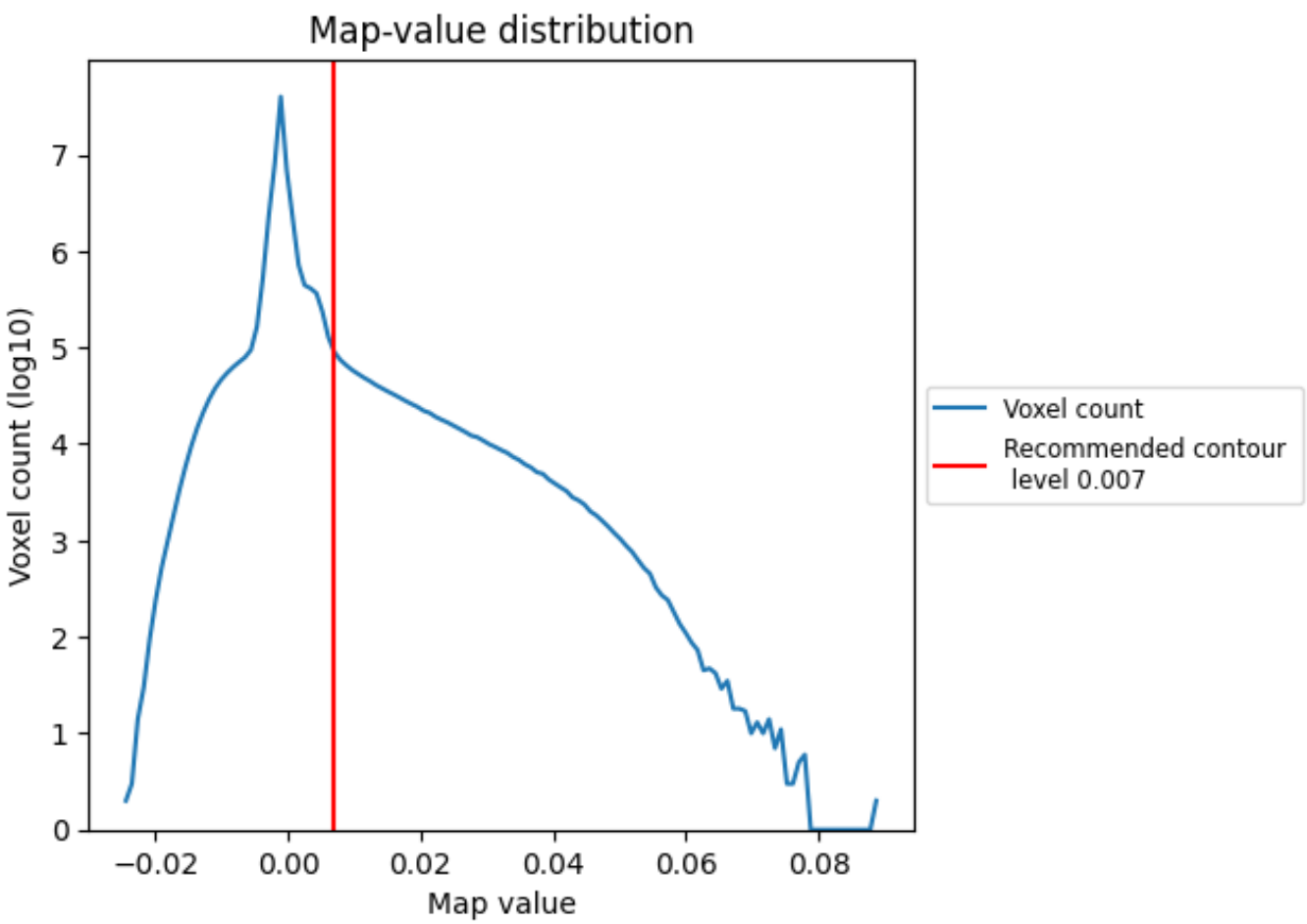


Z

7 Map analysis (i)

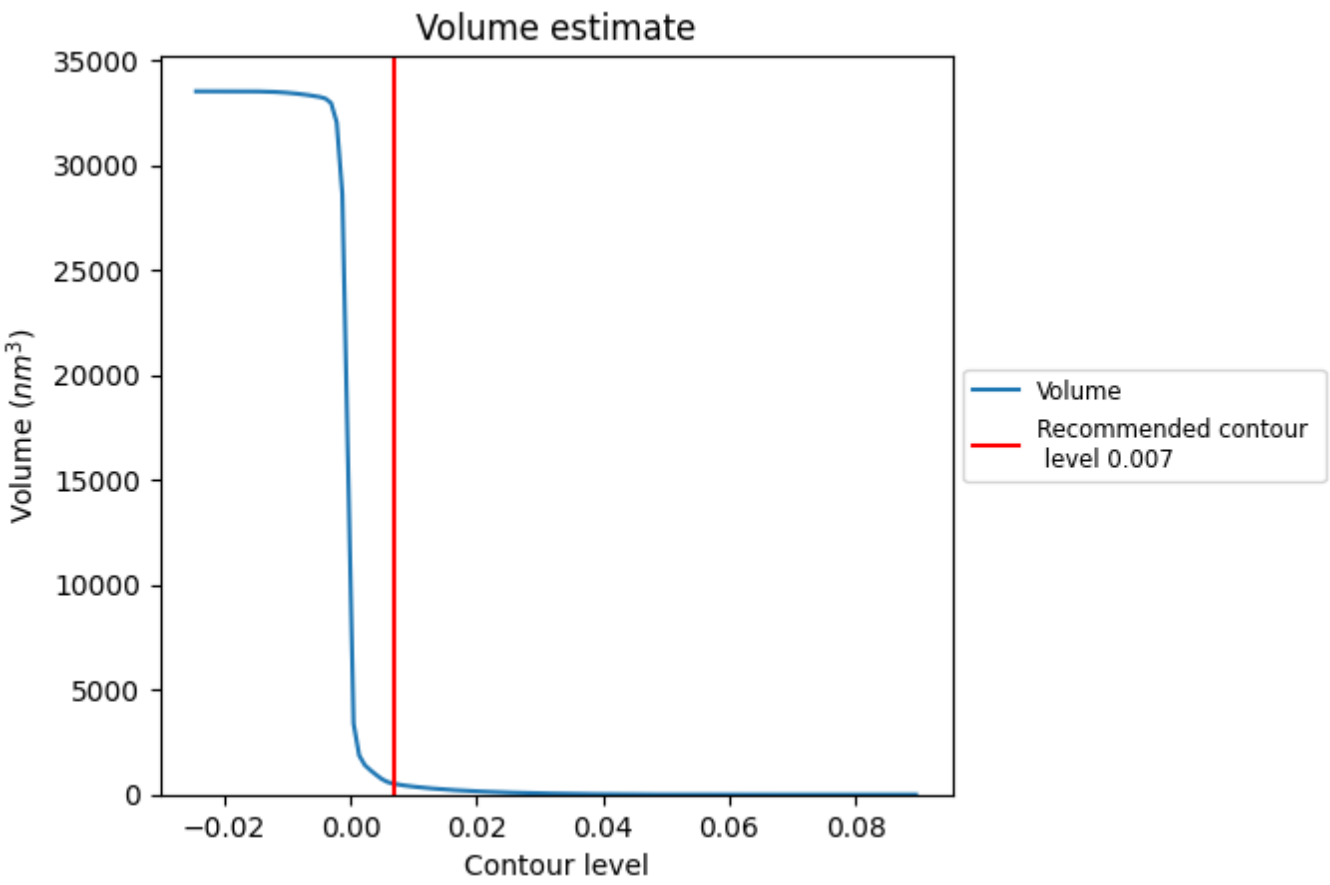
This section contains the results of statistical analysis of the map.

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.

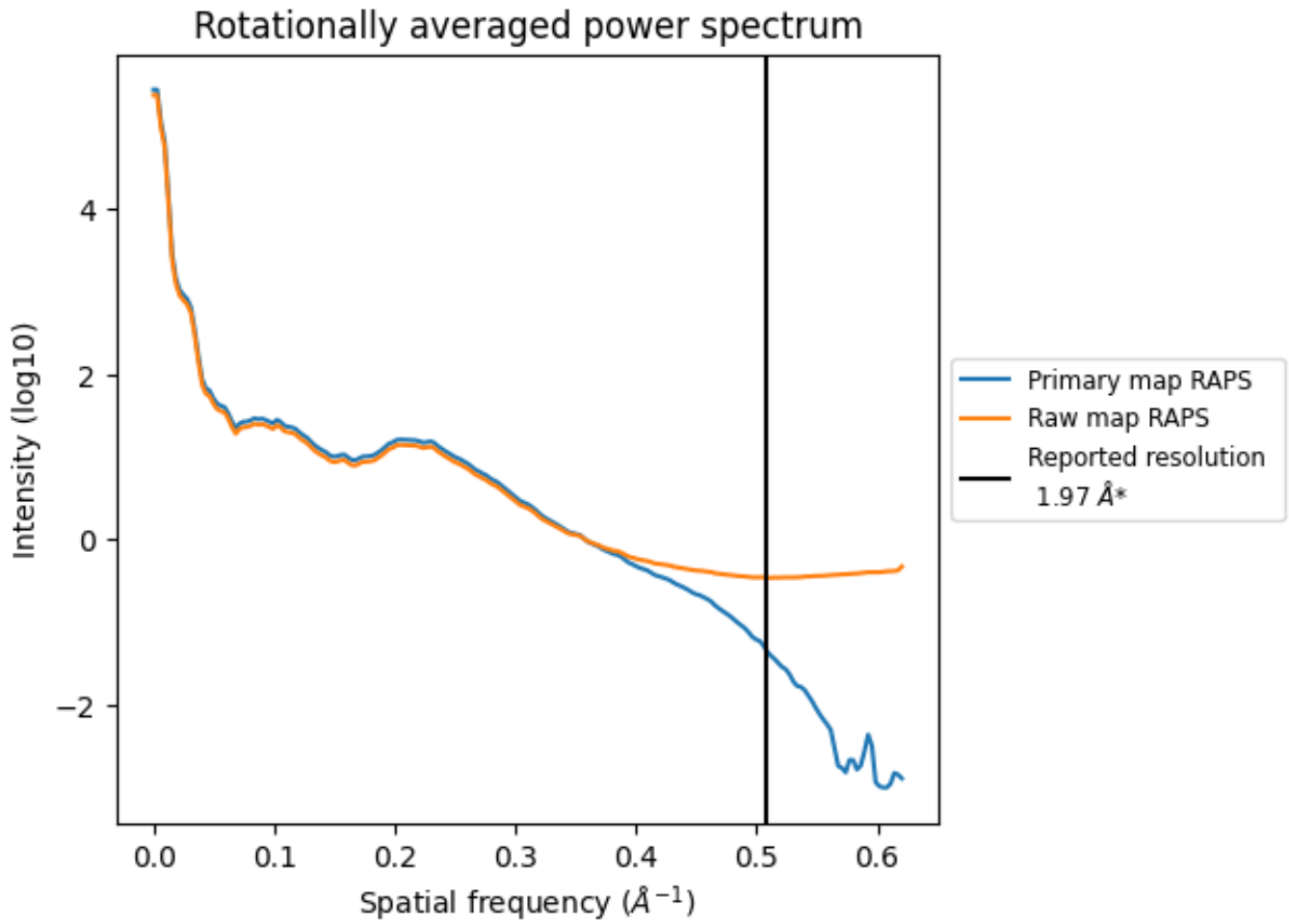
7.2 Volume estimate (i)



The volume at the recommended contour level is 511 nm^3; this corresponds to an approximate mass of 461 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)

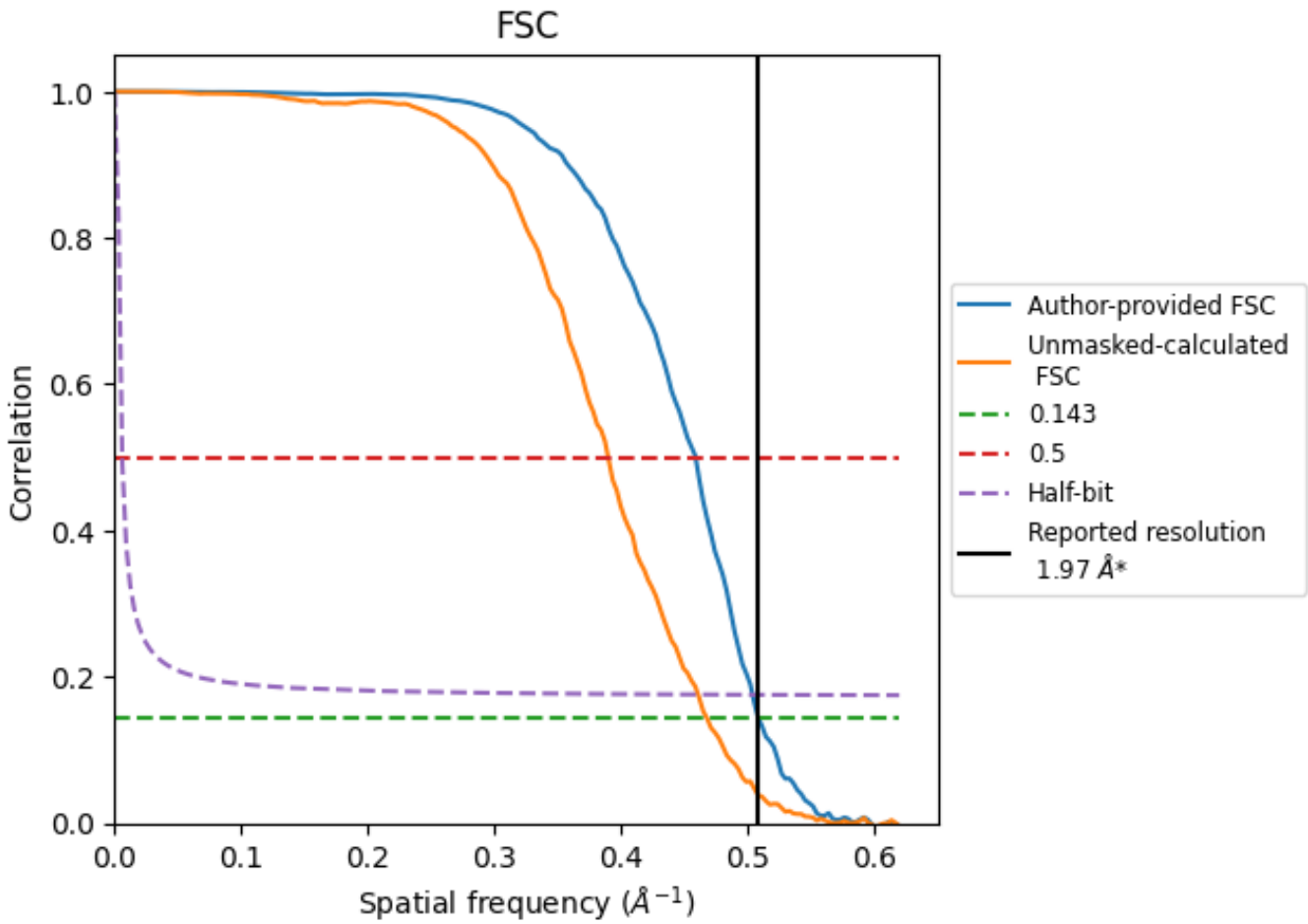


*Reported resolution corresponds to spatial frequency of 0.508 Å^{-1}

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 0.508 Å^{-1}

8.2 Resolution estimates (i)

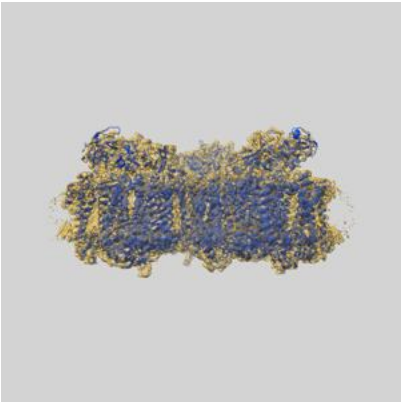
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.97	-	-
Author-provided FSC curve	1.96	2.18	1.98
Unmasked-calculated*	2.14	2.56	2.17

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

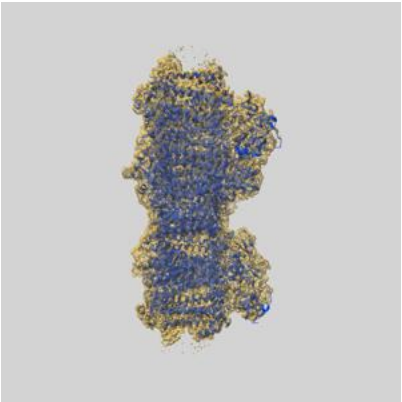
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31605 and PDB model 7FIX. Per-residue inclusion information can be found in section 3 on page 42.

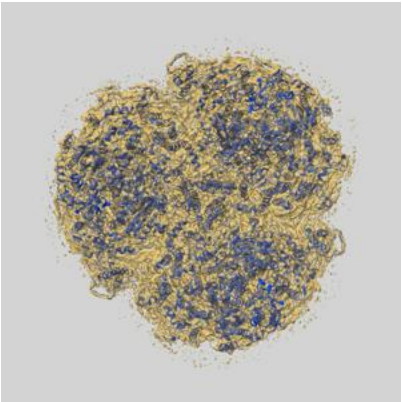
9.1 Map-model overlay (i)



X



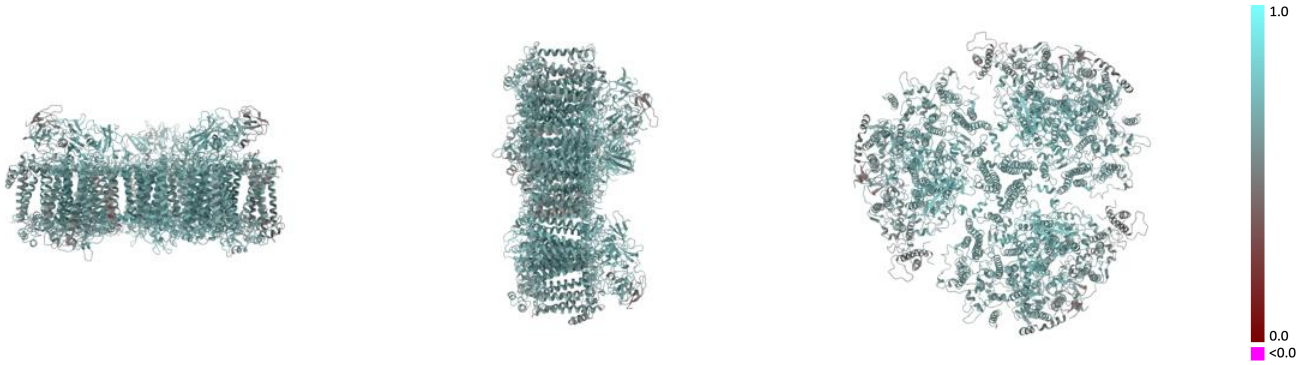
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

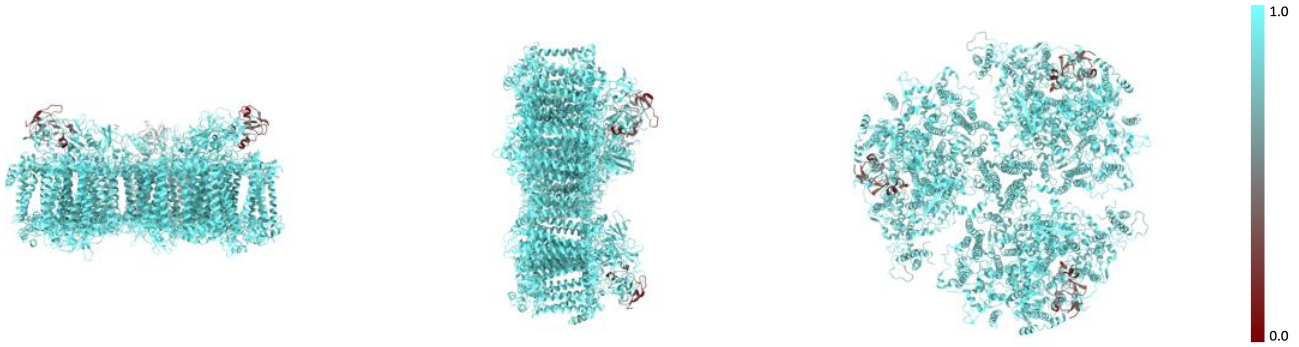
9.2 Q-score mapped to coordinate model (i)



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.

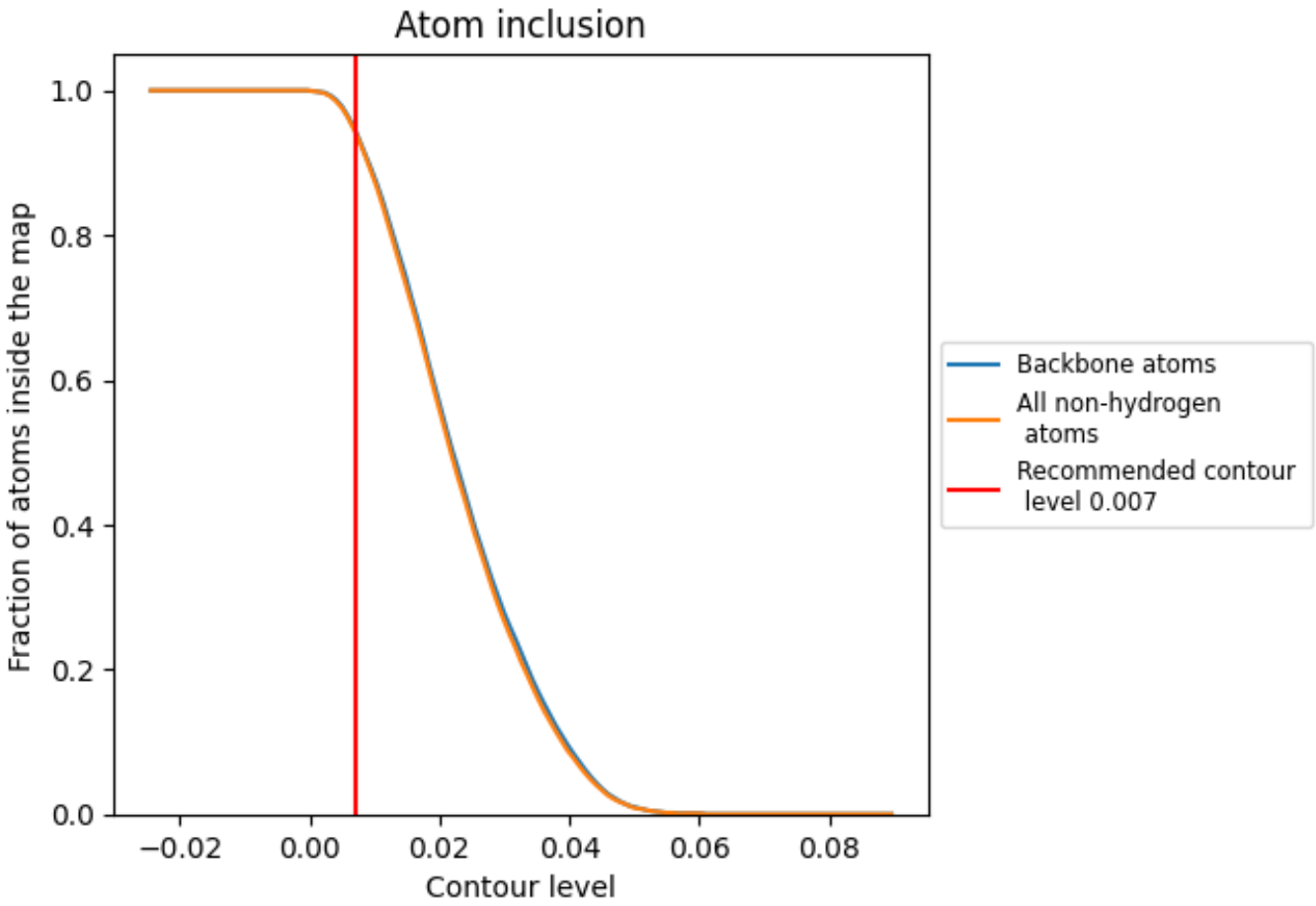
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9430	0.6510
A1	0.9630	0.6500
A2	0.9630	0.6500
A3	0.9630	0.6480
B1	0.9770	0.6710
B2	0.9770	0.6700
B3	0.9760	0.6690
C1	0.9880	0.7040
C2	0.9870	0.7030
C3	0.9870	0.7030
D1	0.9550	0.6810
D2	0.9530	0.6810
D3	0.9530	0.6800
E1	0.9520	0.6450
E2	0.9560	0.6500
E3	0.9600	0.6450
F1	0.9010	0.5810
F2	0.8930	0.5760
F3	0.9010	0.5770
I1	0.9820	0.7090
I2	0.9880	0.7080
I3	0.9880	0.7050
J1	0.9120	0.5770
J2	0.9190	0.5750
J3	0.9100	0.5750
K1	0.8390	0.4810
K2	0.8400	0.4870
K3	0.8320	0.4860
L1	0.9770	0.7110
L2	0.9780	0.7100
L3	0.9800	0.7100
M1	0.9680	0.6650
M2	0.9680	0.6660
M3	0.9680	0.6620
R1	0.3870	0.5300

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Continued from previous page...

Chain	Atom inclusion	Q-score
R2	0.4020	0.5250
R3	0.4020	0.5250
X1	0.9260	0.5940
X2	0.9120	0.5900
X3	0.9290	0.5910