wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 05:25 PM EDT

PDB ID	:	1JB0
Title	:	Crystal Structure of Photosystem I: a Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria
Authors	:	Jordan, P.; Fromme, P.; Witt, H.T.; Klukas, O.; Saenger, W.; Krauss, N.
Deposited on	:	2001-06-01
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

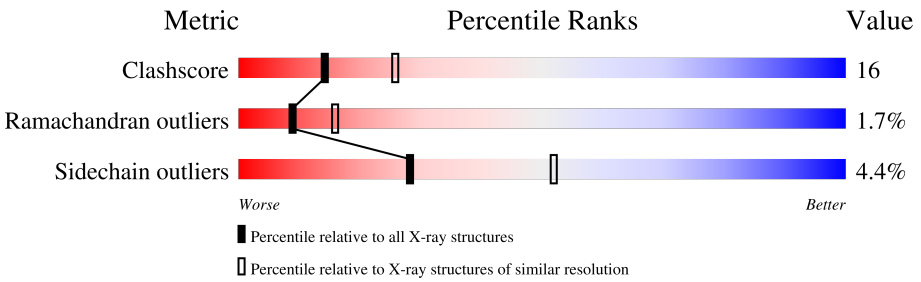
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	755	71% 24% • •
2	B	740	71% 26% •
3	C	80	74% 25% •
4	D	138	67% 28% •
5	E	75	72% 16% • 8%
6	F	164	57% 28% • 14%
7	I	38	74% 21% 5%
8	J	41	54% 41% 5%

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Mol	Chain	Length	Quality of chain
9	K	83	42% 12% • 45%
10	L	154	79% 16% • •
11	M	31	74% 19% • •
12	X	35	54% 26% • 17%

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
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
13	CLA	A	1111	X	-	-	-
13	CLA	A	1112	X	-	-	-
13	CLA	A	1113	X	-	-	-
13	CLA	A	1114	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
13	CLA	A	1118	X	-	-	-
13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-
13	CLA	A	1123	X	-	-	-
13	CLA	A	1124	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-
13	CLA	A	1127	X	-	-	-
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1130	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1402	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1207	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-
13	CLA	B	1224	X	-	-	-
13	CLA	B	1226	X	-	-	-
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1233	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1235	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	J	1303	X	-	-	-
13	CLA	L	1501	X	-	-	-
13	CLA	L	1503	X	-	-	-
13	CLA	M	1601	X	-	-	-
13	CLA	X	1701	X	-	-	-
17	LHG	A	5003	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 24198 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	740	5784	3794	988	976	26	0	0	0

- Molecule 2 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	739	5879	3867	986	1005	21	0	0	0

- Molecule 3 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

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

- Molecule 4 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II.

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

- Molecule 5 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV.

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

- Molecule 6 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III.

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

- Molecule 7 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII.

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

- Molecule 8 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX.

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

- Molecule 9 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X.

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

- Molecule 10 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ARG	PRO	conflict	UNP P25902
L	144	VAL	-	SEE REMARK 999	UNP P25902
L	145	VAL	-	SEE REMARK 999	UNP P25902
L	146	ASP	-	SEE REMARK 999	UNP P25902
L	147	GLY	-	SEE REMARK 999	UNP P25902
L	148	ILE	-	SEE REMARK 999	UNP P25902
L	149	MET	-	SEE REMARK 999	UNP P25902
L	150	THR	-	SEE REMARK 999	UNP P25902
L	151	GLY	-	SEE REMARK 999	UNP P25902
L	152	LEU	-	SEE REMARK 999	UNP P25902
L	153	PHE	-	SEE REMARK 999	UNP P25902
L	154	ASN	-	SEE REMARK 999	UNP P25902

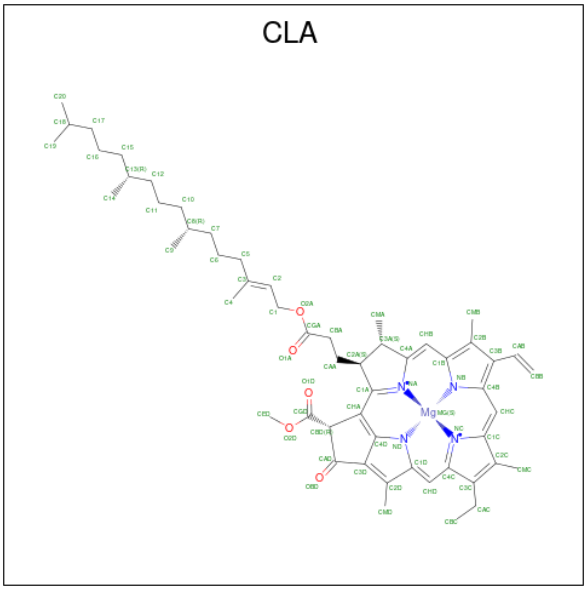
- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	M	31	241	161	36	43	1	0	0	0

- Molecule 12 is a protein called PHOTOSYSTEM I SUBUNIT PSAX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	X	29	233	164	34	35	0	0	0

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	59	49	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	B	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	59	49	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	47	37	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	54	44	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	B	1	46	36	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	49	39	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	58	48	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	47	37	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	F	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	J	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	J	1	37	31	1	4	1	0	0
			Total	C	Mg	N	O		
13	K	1	45	35	1	4	5	0	0

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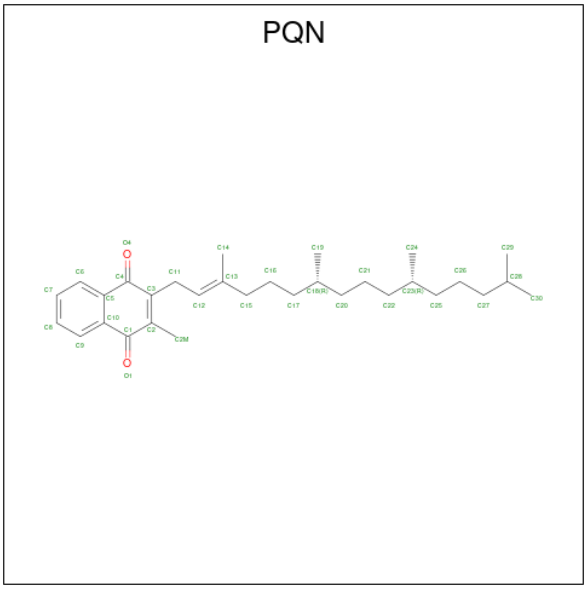
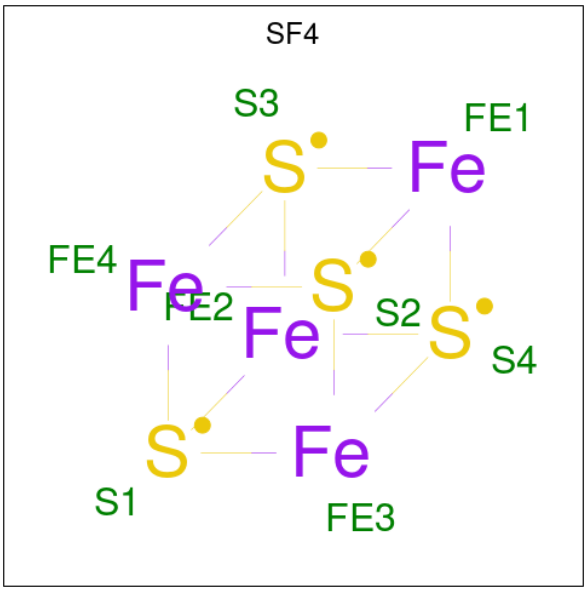
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	M	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	X	1	45	35	1	4	5	0	0

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



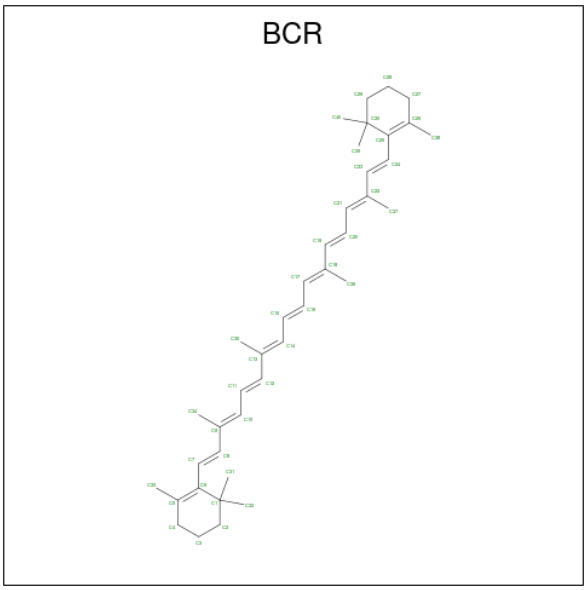
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	A	1	33	31	2	0	0
			Total	C	O		
14	B	1	33	31	2	0	0

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
15	A	1	8	4	4	0	0
			Total	Fe	S		
15	C	1	8	4	4	0	0
			Total	Fe	S		
15	C	1	8	4	4	0	0

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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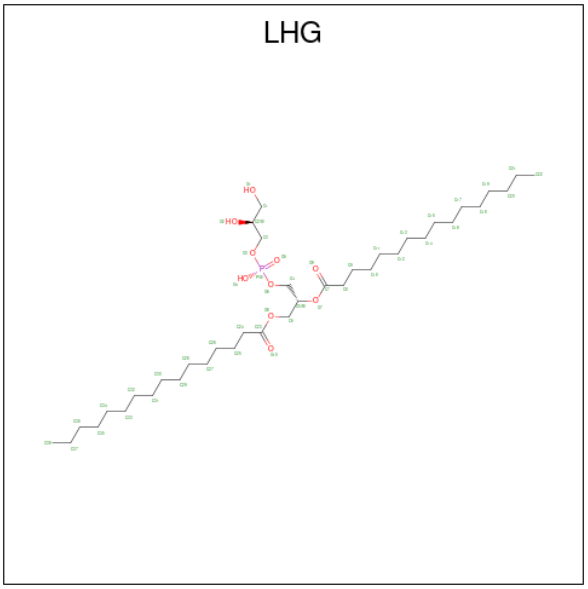
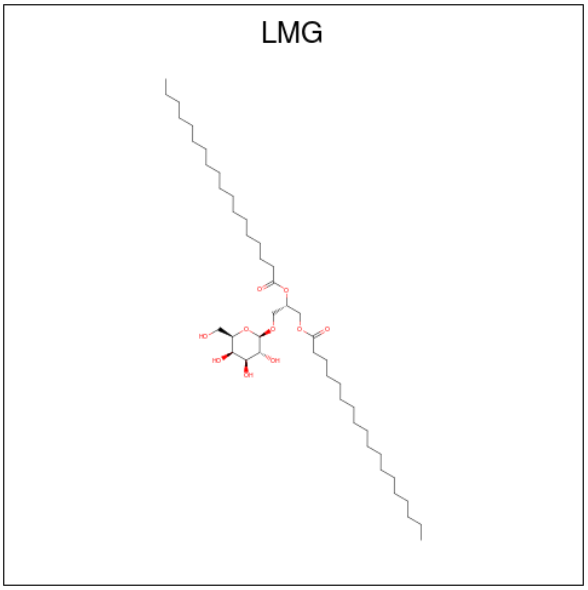
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1	25	25	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	F	1	40	40	0	0
			Total	C		
16	I	1	40	40	0	0
			Total	C		
16	I	1	40	40	0	0
			Total	C		
16	J	1	40	40	0	0
			Total	C		
16	J	1	40	40	0	0
			Total	C		
16	J	1	40	40	0	0
			Total	C		
16	L	1	40	40	0	0
			Total	C		
16	L	1	40	40	0	0
			Total	C		
16	M	1	40	40	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
17	A	1	49	38	10	1	0	0
			Total	C	O	P		
17	A	1	27	16	10	1	0	0
			Total	C	O	P		
17	B	1	23	12	10	1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	B	1	55	45	10	0	0

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
19	L	1	1	1	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	A	53	53	53	0	0
20	B	65	65	65	0	0
20	C	21	21	21	0	0
20	D	17	17	17	0	0
20	E	5	5	5	0	0
20	F	6	6	6	0	0
20	I	3	3	3	0	0
20	J	1	1	1	0	0
20	L	27	27	27	0	0
20	M	3	3	3	0	0

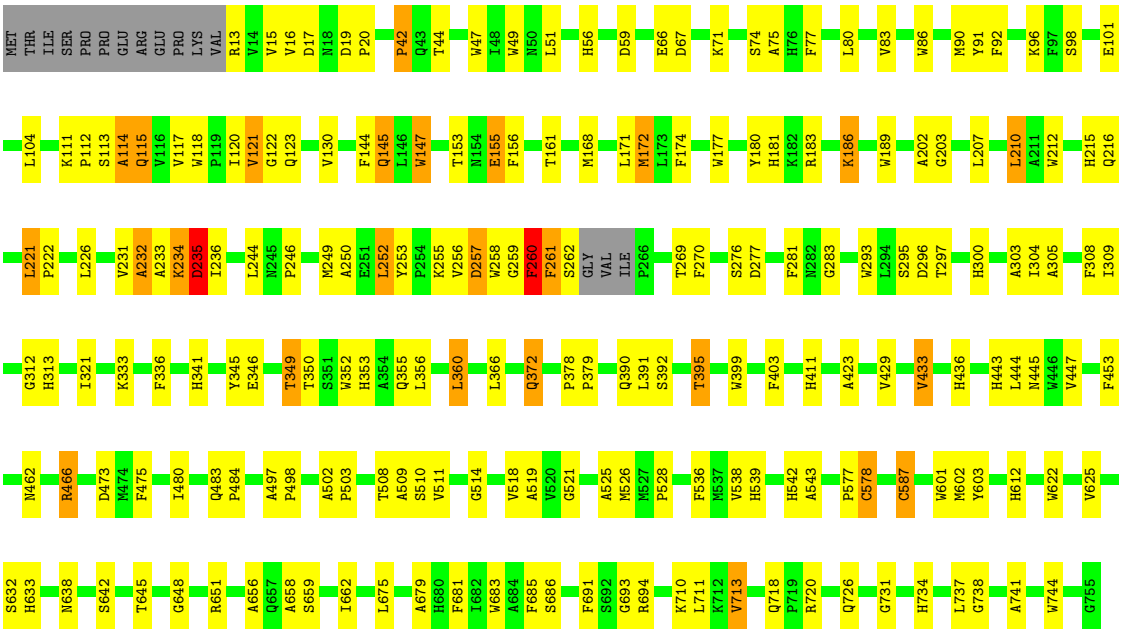
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

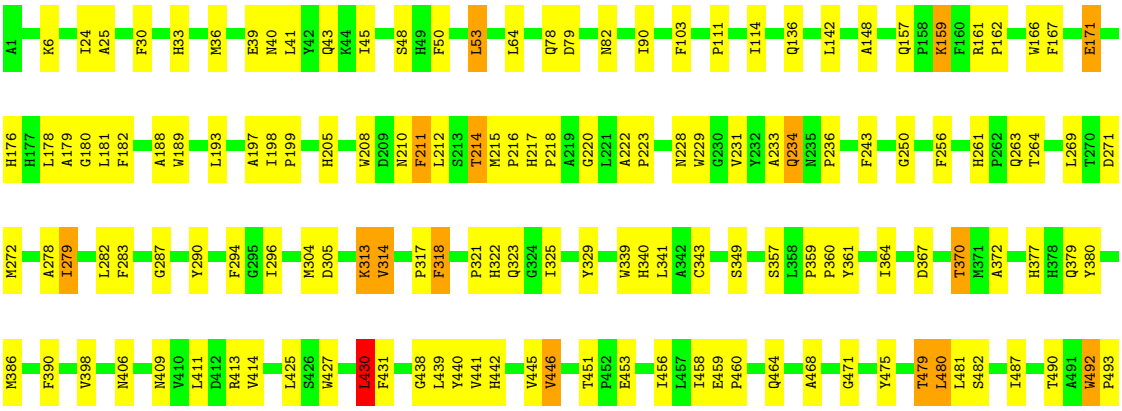
• Molecule 1: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

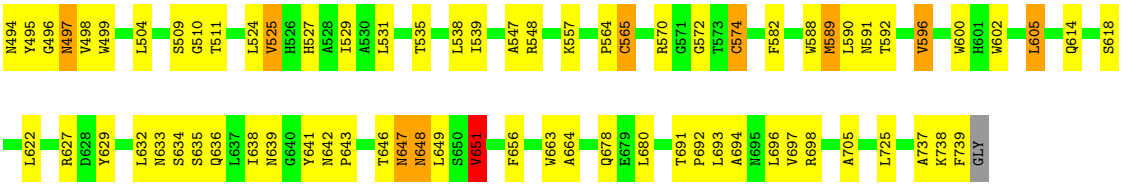
Chain A: 71% 24%



• Molecule 2: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

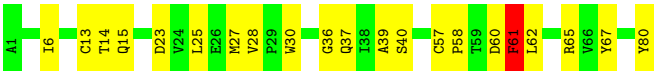
Chain B: 71% 26%





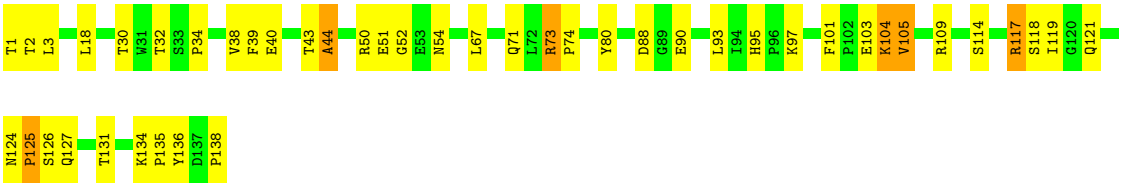
- Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C:



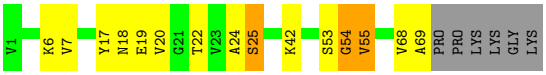
- Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D:



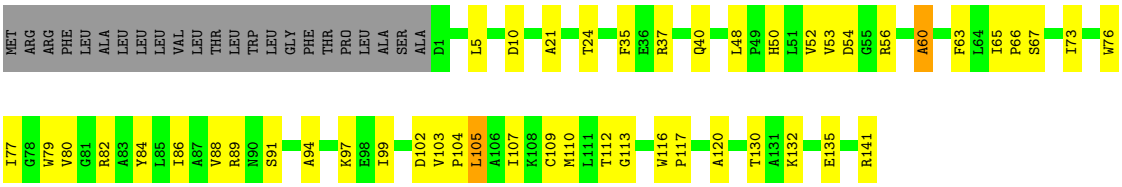
- Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E:



- Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F:



- Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

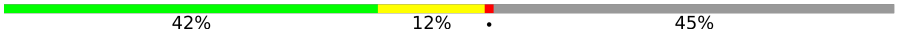
Chain I:

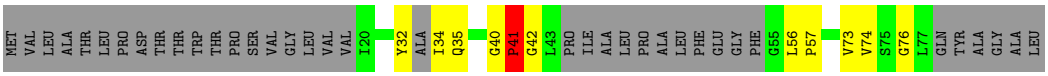
- Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX

Chain J:

• Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X

Chain K:



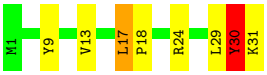


• Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI

Chain L:

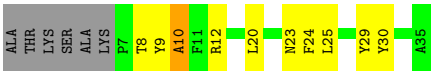
• Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII

Chain M:



• Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX

Chain X:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (30.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.199 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24198	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

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: PQN, SF4, CA, BCR, CLA, LHG, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.66	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.55	0/242	0.67	0/332
All	All	0.55	0/17941	0.70	15/24453 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	80	TYR	CA-C-O	9.95	140.99	120.10
11	M	30	TYR	N-CA-C	7.84	132.18	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.52	131.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	GLY	N-CA-C	-6.39	97.13	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	215	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	40	0
5	E	539	0	528	10	0
6	F	1065	0	1079	42	0
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	0
10	L	1119	0	1125	22	0
11	M	241	0	264	13	0
12	X	233	0	231	6	0
13	A	2687	0	2675	143	0
13	B	2349	0	2304	152	0
13	F	45	0	33	1	0
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	11	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	265	0	369	17	0
16	F	40	0	56	2	0
16	I	80	0	112	3	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	0
20	A	53	0	0	5	0
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	1
20	M	3	0	0	1	0
All	All	24198	0	23804	743	1

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 16.

The worst 5 of 743 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)
8:J:31:ARG:HD3	16:J:4013:BCR:H312	1.25	1.17
2:B:622:LEU:HD12	13:B:1012:CLA:H11	1.29	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.05
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:4048:HOH:O	20:L:4048:HOH:O[2_655]	1.94	0.26

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	695 (94%)	31 (4%)	10 (1%)	11	20
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	13	24
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	12	21
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	6	10
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	1	1
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	6	10
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	1
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	12	21
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	5
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	3	4
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	9	16

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
1	A	261	PHE
2	B	234	GLN

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	565 (96%)	24 (4%)	30	55
2	B	595/597 (100%)	567 (95%)	28 (5%)	26	49
3	C	67/67 (100%)	66 (98%)	1 (2%)	65	85
4	D	115/115 (100%)	107 (93%)	8 (7%)	15	29
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	107 (98%)	2 (2%)	59	81
7	I	32/32 (100%)	30 (94%)	2 (6%)	18	34
8	J	36/36 (100%)	34 (94%)	2 (6%)	21	40
10	L	117/119 (98%)	109 (93%)	8 (7%)	16	30
11	M	26/26 (100%)	25 (96%)	1 (4%)	33	58
12	X	20/24 (83%)	18 (90%)	2 (10%)	7	15
All	All	1765/1811 (98%)	1687 (96%)	78 (4%)	28	52

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	105	VAL
10	L	48	LEU
4	D	125	PRO
8	J	1	MET
11	M	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	678	GLN
6	F	40	GLN
2	B	688	HIS
4	D	71	GLN
10	L	16	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 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	$\#\|Z\| > 2$
13	CLA	M	1601	20	45,53,73	1.59	7 (15%)	52,89,113	2.21	8 (15%)
13	CLA	A	1114	20	49,57,73	1.48	7 (14%)	55,93,113	2.06	10 (18%)
16	BCR	A	4001	-	41,41,41	1.37	5 (12%)	56,56,56	1.88	16 (28%)
16	BCR	J	4013	-	41,41,41	1.28	4 (9%)	56,56,56	1.83	19 (33%)
13	CLA	B	1238	20	65,73,73	1.31	8 (12%)	76,113,113	1.65	12 (15%)
13	CLA	B	1210	-	65,73,73	1.43	7 (10%)	76,113,113	1.70	11 (14%)
13	CLA	A	1117	-	65,73,73	1.40	12 (18%)	76,113,113	1.89	14 (18%)
13	CLA	B	1216	20	65,73,73	1.36	7 (10%)	76,113,113	1.73	11 (14%)
13	CLA	A	1128	-	65,73,73	1.57	11 (16%)	76,113,113	1.69	9 (11%)
16	BCR	B	4009	-	25,25,41	1.36	4 (16%)	33,33,56	1.86	11 (33%)
13	CLA	J	1302	8	45,53,73	1.64	7 (15%)	52,89,113	2.15	10 (19%)
13	CLA	A	1022	20	65,73,73	1.41	11 (16%)	76,113,113	1.62	8 (10%)
13	CLA	B	1226	-	65,73,73	1.41	10 (15%)	76,113,113	1.79	12 (15%)
13	CLA	B	1211	-	65,73,73	1.34	8 (12%)	76,113,113	1.80	10 (13%)
13	CLA	B	1225	-	65,73,73	1.55	13 (20%)	76,113,113	1.70	13 (17%)
13	CLA	A	1131	-	65,73,73	1.20	5 (7%)	76,113,113	1.70	14 (18%)
13	CLA	A	1138	-	65,73,73	1.35	7 (10%)	76,113,113	1.74	10 (13%)
13	CLA	A	1108	-	45,53,73	1.59	7 (15%)	52,89,113	1.97	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	BCR	B	4017	-	41,41,41	1.28	4 (9%)	56,56,56	1.74	17 (30%)
13	CLA	X	1701	12	45,53,73	1.60	5 (11%)	52,89,113	2.12	11 (21%)
13	CLA	A	1121	-	51,59,73	1.57	10 (19%)	59,96,113	1.94	11 (18%)
13	CLA	B	1239	-	65,73,73	1.17	9 (13%)	76,113,113	1.73	10 (13%)
13	CLA	B	1214	-	59,67,73	1.45	8 (13%)	68,105,113	1.84	13 (19%)
15	SF4	C	3003	3	0,12,12	-	-	-		
13	CLA	B	1203	-	65,73,73	1.29	6 (9%)	76,113,113	1.64	10 (13%)
13	CLA	A	1103	-	65,73,73	1.20	4 (6%)	76,113,113	1.81	15 (19%)
13	CLA	B	1208	-	45,53,73	1.54	8 (17%)	52,89,113	2.00	10 (19%)
13	CLA	A	1136	-	65,73,73	1.36	8 (12%)	76,113,113	1.66	8 (10%)
13	CLA	A	1119	20	65,73,73	1.33	8 (12%)	76,113,113	1.82	12 (15%)
16	BCR	J	4012	-	41,41,41	1.29	5 (12%)	56,56,56	1.91	16 (28%)
13	CLA	B	1230	-	58,66,73	1.45	11 (18%)	67,104,113	1.98	12 (17%)
13	CLA	A	1104	-	65,73,73	1.39	8 (12%)	76,113,113	1.90	14 (18%)
13	CLA	B	1217	-	47,55,73	1.53	8 (17%)	54,91,113	2.22	11 (20%)
13	CLA	A	1120	-	49,57,73	1.47	6 (12%)	55,93,113	2.12	12 (21%)
13	CLA	A	1237	20	65,73,73	1.34	10 (15%)	76,113,113	1.67	10 (13%)
13	CLA	B	1232	20	45,53,73	1.70	8 (17%)	52,89,113	1.99	12 (23%)
13	CLA	A	1115	-	54,62,73	1.57	10 (18%)	62,99,113	1.81	9 (14%)
13	CLA	B	1228	-	49,57,73	1.53	7 (14%)	55,93,113	1.99	7 (12%)
16	BCR	B	4010	-	41,41,41	1.25	5 (12%)	56,56,56	1.88	18 (32%)
13	CLA	A	1105	-	51,59,73	1.62	10 (19%)	59,96,113	1.97	10 (16%)
16	BCR	B	4014	-	41,41,41	1.23	5 (12%)	56,56,56	1.99	20 (35%)
16	BCR	J	4015	-	41,41,41	1.40	5 (12%)	56,56,56	1.88	14 (25%)
13	CLA	J	1303	-	38,45,73	1.79	7 (18%)	43,78,113	2.16	8 (18%)
13	CLA	A	1402	-	42,49,73	1.67	9 (21%)	48,83,113	1.99	7 (14%)
18	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.30	3 (4%)
16	BCR	F	4016	-	41,41,41	1.27	4 (9%)	56,56,56	1.81	17 (30%)
13	CLA	A	1110	-	54,62,73	1.48	9 (16%)	62,99,113	2.02	11 (17%)
13	CLA	B	1023	-	65,73,73	1.50	9 (13%)	76,113,113	1.65	7 (9%)
13	CLA	B	1234	-	60,68,73	1.48	8 (13%)	70,107,113	1.76	11 (15%)
13	CLA	A	1132	-	65,73,73	1.37	9 (13%)	76,113,113	1.71	11 (14%)
13	CLA	A	1111	-	60,68,73	1.32	7 (11%)	70,107,113	1.88	14 (20%)
13	CLA	A	1101	-	65,73,73	1.32	6 (9%)	76,113,113	1.75	9 (11%)
13	CLA	A	1126	-	65,73,73	1.28	7 (10%)	76,113,113	1.65	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	PQN	B	2002	-	34,34,34	3.46	16 (47%)	42,45,45	2.10	4 (9%)
16	BCR	A	4008	-	41,41,41	1.26	8 (19%)	56,56,56	1.90	18 (32%)
13	CLA	A	1139	20	51,59,73	1.47	7 (13%)	59,96,113	1.91	10 (16%)
13	CLA	B	1235	-	65,73,73	1.31	8 (12%)	76,113,113	1.81	13 (17%)
15	SF4	A	3001	2,1	0,12,12	-	-	-		
13	CLA	B	1236	-	47,55,73	1.55	8 (17%)	54,91,113	1.86	10 (18%)
13	CLA	A	1113	-	45,53,73	1.50	6 (13%)	52,89,113	2.24	14 (26%)
13	CLA	B	1222	20	46,54,73	1.43	8 (17%)	53,90,113	2.13	12 (22%)
16	BCR	L	4019	-	41,41,41	1.43	8 (19%)	56,56,56	1.81	15 (26%)
16	BCR	L	4022	-	41,41,41	1.60	7 (17%)	56,56,56	1.72	12 (21%)
13	CLA	A	1106	1	65,73,73	1.35	7 (10%)	76,113,113	1.80	9 (11%)
13	CLA	K	1401	-	45,53,73	1.62	8 (17%)	52,89,113	1.95	7 (13%)
13	CLA	A	1118	-	61,69,73	1.46	9 (14%)	71,108,113	1.95	11 (15%)
13	CLA	B	1219	20	55,63,73	1.47	7 (12%)	64,101,113	1.95	9 (14%)
13	CLA	B	1218	-	45,53,73	1.61	8 (17%)	52,89,113	2.19	12 (23%)
13	CLA	B	1209	-	45,53,73	1.55	6 (13%)	52,89,113	2.16	10 (19%)
13	CLA	A	1122	-	59,67,73	1.36	7 (11%)	68,105,113	1.79	13 (19%)
13	CLA	B	1224	-	65,73,73	1.54	9 (13%)	76,113,113	1.81	13 (17%)
13	CLA	A	1013	-	65,73,73	1.36	9 (13%)	76,113,113	1.80	14 (18%)
16	BCR	A	4007	-	41,41,41	1.37	6 (14%)	56,56,56	1.78	14 (25%)
16	BCR	B	4005	-	41,41,41	1.57	7 (17%)	56,56,56	2.09	19 (33%)
17	LHG	B	5004	-	22,22,48	2.80	5 (22%)	25,28,54	1.13	1 (4%)
13	CLA	B	1227	-	45,53,73	1.55	8 (17%)	52,89,113	2.16	11 (21%)
13	CLA	L	1501	10	65,73,73	1.51	9 (13%)	76,113,113	1.74	10 (13%)
13	CLA	A	1107	1	65,73,73	1.38	8 (12%)	76,113,113	1.84	14 (18%)
14	PQN	A	2001	-	34,34,34	3.54	17 (50%)	42,45,45	2.21	3 (7%)
13	CLA	A	1134	1	45,53,73	1.50	8 (17%)	52,89,113	2.15	10 (19%)
13	CLA	B	1229	-	65,73,73	1.36	7 (10%)	76,113,113	1.75	8 (10%)
16	BCR	B	4006	-	41,41,41	1.26	5 (12%)	56,56,56	2.01	20 (35%)
13	CLA	A	1123	20	65,73,73	1.42	7 (10%)	76,113,113	1.70	12 (15%)
13	CLA	A	1137	-	47,55,73	1.64	6 (12%)	54,91,113	1.94	10 (18%)
13	CLA	B	1220	-	45,53,73	1.58	5 (11%)	52,89,113	1.97	9 (17%)
13	CLA	B	1021	-	65,73,73	1.40	6 (9%)	76,113,113	1.71	9 (11%)
13	CLA	B	1012	20	65,73,73	1.46	6 (9%)	76,113,113	1.71	11 (14%)
13	CLA	A	1112	-	45,53,73	1.65	9 (20%)	52,89,113	2.02	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CLA	B	1213	-	55,63,73	1.58	11 (20%)	64,101,113	1.84	9 (14%)
13	CLA	B	1204	-	65,73,73	1.25	8 (12%)	76,113,113	1.78	9 (11%)
13	CLA	L	1502	-	65,73,73	1.43	8 (12%)	76,113,113	1.76	10 (13%)
13	CLA	B	1215	-	60,68,73	1.44	9 (15%)	70,107,113	1.96	11 (15%)
16	BCR	A	4011	-	41,41,41	1.39	6 (14%)	56,56,56	2.03	19 (33%)
13	CLA	A	1102	13	59,67,73	1.41	7 (11%)	68,105,113	1.89	12 (17%)
13	CLA	A	1109	13	65,73,73	1.30	8 (12%)	76,113,113	1.78	10 (13%)
13	CLA	A	1133	-	54,62,73	1.40	10 (18%)	62,99,113	2.00	11 (17%)
13	CLA	A	1129	-	50,58,73	1.53	7 (14%)	58,95,113	2.08	14 (24%)
13	CLA	B	1207	2	65,73,73	1.43	9 (13%)	76,113,113	1.79	14 (18%)
13	CLA	A	1135	-	51,59,73	1.34	4 (7%)	59,96,113	2.08	13 (22%)
16	BCR	I	4020	-	41,41,41	1.28	7 (17%)	56,56,56	1.82	17 (30%)
13	CLA	L	1503	20	65,73,73	1.44	8 (12%)	76,113,113	1.68	9 (11%)
13	CLA	A	1125	-	65,73,73	1.39	6 (9%)	76,113,113	1.77	11 (14%)
16	BCR	I	4018	-	41,41,41	1.30	7 (17%)	56,56,56	1.79	15 (26%)
13	CLA	B	1202	-	65,73,73	1.33	7 (10%)	76,113,113	1.68	10 (13%)
16	BCR	M	4021	-	41,41,41	1.34	6 (14%)	56,56,56	1.79	15 (26%)
13	CLA	B	1231	-	45,53,73	1.56	9 (20%)	52,89,113	2.07	12 (23%)
13	CLA	A	1140	-	65,73,73	1.38	8 (12%)	76,113,113	1.81	14 (18%)
13	CLA	A	1130	-	65,73,73	1.23	7 (10%)	76,113,113	1.90	10 (13%)
13	CLA	A	1801	17	52,60,73	1.61	11 (21%)	60,97,113	2.15	13 (21%)
13	CLA	B	1223	-	65,73,73	1.44	7 (10%)	76,113,113	1.80	11 (14%)
13	CLA	B	1205	-	65,73,73	1.33	7 (10%)	76,113,113	1.71	11 (14%)
13	CLA	B	1206	2	65,73,73	1.36	5 (7%)	76,113,113	1.71	10 (13%)
13	CLA	B	1212	-	45,53,73	1.57	10 (22%)	52,89,113	2.06	9 (17%)
13	CLA	B	1221	2	54,62,73	1.74	12 (22%)	62,99,113	1.91	10 (16%)
13	CLA	A	1124	20	65,73,73	1.25	7 (10%)	76,113,113	1.76	10 (13%)
16	BCR	A	4002	-	41,41,41	1.27	4 (9%)	56,56,56	1.77	17 (30%)
16	BCR	A	4003	-	41,41,41	1.41	6 (14%)	56,56,56	1.93	17 (30%)
13	CLA	A	1116	-	54,62,73	1.57	10 (18%)	62,99,113	1.90	11 (17%)
13	CLA	B	1233	20	45,53,73	1.52	6 (13%)	52,89,113	2.09	10 (19%)
13	CLA	A	1127	-	65,73,73	1.43	7 (10%)	76,113,113	1.73	7 (9%)
13	CLA	F	1301	20	45,53,73	1.64	7 (15%)	52,89,113	2.06	7 (13%)
17	LHG	A	5003	13	26,26,48	2.32	5 (19%)	29,32,54	1.59	5 (17%)
15	SF4	C	3002	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	BCR	B	4004	-	41,41,41	1.52	5 (12%)	56,56,56	2.02	16 (28%)
17	LHG	A	5001	-	48,48,48	1.76	6 (12%)	51,54,54	1.30	3 (5%)
13	CLA	B	1201	-	54,62,73	1.47	8 (14%)	62,99,113	2.02	12 (19%)
13	CLA	A	1011	-	65,73,73	1.42	7 (10%)	76,113,113	2.04	17 (22%)

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
13	CLA	M	1601	20	1/1/11/20	9/13/91/115	-
13	CLA	A	1114	20	1/1/11/20	9/18/96/115	-
16	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1238	20	1/1/15/20	2/37/115/115	-
13	CLA	B	1210	-	1/1/15/20	13/37/115/115	-
13	CLA	A	1117	-	1/1/15/20	14/37/115/115	-
13	CLA	B	1216	20	1/1/15/20	4/37/115/115	-
13	CLA	A	1128	-	1/1/15/20	6/37/115/115	-
16	BCR	B	4009	-	-	6/18/35/63	0/1/1/2
13	CLA	J	1302	8	1/1/11/20	11/13/91/115	-
13	CLA	A	1022	20	1/1/15/20	4/37/115/115	-
13	CLA	B	1226	-	1/1/15/20	9/37/115/115	-
13	CLA	B	1211	-	1/1/15/20	11/37/115/115	-
13	CLA	B	1225	-	-	10/37/115/115	-
13	CLA	A	1131	-	-	5/37/115/115	-
13	CLA	A	1138	-	1/1/15/20	7/37/115/115	-
13	CLA	A	1108	-	-	9/13/91/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	X	1701	12	1/1/11/20	5/13/91/115	-
13	CLA	A	1121	-	1/1/12/20	10/21/99/115	-
13	CLA	B	1239	-	-	8/37/115/115	-
13	CLA	B	1214	-	1/1/13/20	7/30/108/115	-
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	B	1203	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1103	-	1/1/15/20	16/37/115/115	-
13	CLA	B	1208	-	1/1/11/20	3/13/91/115	-
13	CLA	A	1136	-	1/1/15/20	8/37/115/115	-
13	CLA	A	1119	20	1/1/15/20	6/37/115/115	-
16	BCR	J	4012	-	-	3/29/63/63	0/2/2/2
13	CLA	B	1230	-	1/1/13/20	6/29/107/115	-
13	CLA	A	1104	-	1/1/15/20	14/37/115/115	-
13	CLA	B	1217	-	1/1/11/20	6/16/94/115	-
13	CLA	A	1120	-	1/1/11/20	10/18/96/115	-
13	CLA	A	1237	20	1/1/15/20	10/37/115/115	-
13	CLA	B	1232	20	1/1/11/20	0/13/91/115	-
13	CLA	A	1115	-	-	1/24/102/115	-
13	CLA	B	1228	-	1/1/11/20	9/18/96/115	-
16	BCR	B	4010	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1105	-	1/1/12/20	6/21/99/115	-
16	BCR	B	4014	-	-	1/29/63/63	0/2/2/2
16	BCR	J	4015	-	-	2/29/63/63	0/2/2/2
13	CLA	J	1303	-	1/1/8/20	0/2/76/115	-
13	CLA	A	1402	-	1/1/9/20	3/7/81/115	-
18	LMG	B	5002	-	-	8/50/70/70	0/1/1/1
16	BCR	F	4016	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1110	-	1/1/12/20	8/24/102/115	-
13	CLA	B	1023	-	-	2/37/115/115	-
13	CLA	B	1234	-	1/1/14/20	9/31/109/115	-
13	CLA	A	1132	-	1/1/15/20	8/37/115/115	-
13	CLA	A	1111	-	1/1/14/20	11/31/109/115	-
13	CLA	A	1101	-	1/1/15/20	6/37/115/115	-
13	CLA	A	1126	-	1/1/15/20	8/37/115/115	-
14	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
16	BCR	A	4008	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1139	20	1/1/12/20	8/21/99/115	-
13	CLA	B	1235	-	1/1/15/20	0/37/115/115	-
15	SF4	A	3001	2,1	-	-	0/6/5/5
13	CLA	B	1236	-	-	4/16/94/115	-
13	CLA	A	1113	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1222	20	1/1/11/20	6/15/93/115	-
16	BCR	L	4019	-	-	1/29/63/63	0/2/2/2
16	BCR	L	4022	-	-	1/29/63/63	0/2/2/2
13	CLA	A	1106	1	1/1/15/20	16/37/115/115	-
13	CLA	K	1401	-	-	6/13/91/115	-
13	CLA	A	1118	-	1/1/14/20	14/33/111/115	-
13	CLA	B	1219	20	1/1/13/20	8/25/103/115	-
13	CLA	B	1218	-	1/1/11/20	5/13/91/115	-
13	CLA	B	1209	-	1/1/11/20	3/13/91/115	-
13	CLA	A	1122	-	1/1/13/20	12/30/108/115	-
13	CLA	B	1224	-	1/1/15/20	14/37/115/115	-
13	CLA	A	1013	-	1/1/15/20	10/37/115/115	-
16	BCR	A	4007	-	-	2/29/63/63	0/2/2/2
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
17	LHG	B	5004	-	-	7/26/26/53	-
13	CLA	B	1227	-	1/1/11/20	8/13/91/115	-
13	CLA	L	1501	10	1/1/15/20	11/37/115/115	-
13	CLA	A	1107	1	1/1/15/20	13/37/115/115	-
14	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
13	CLA	A	1134	1	1/1/11/20	5/13/91/115	-
13	CLA	B	1229	-	1/1/15/20	16/37/115/115	-
16	BCR	B	4006	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1123	20	1/1/15/20	11/37/115/115	-
13	CLA	A	1137	-	1/1/11/20	5/16/94/115	-
13	CLA	B	1220	-	1/1/11/20	3/13/91/115	-
13	CLA	B	1021	-	1/1/15/20	10/37/115/115	-
13	CLA	B	1012	20	1/1/15/20	7/37/115/115	-
13	CLA	A	1112	-	1/1/11/20	1/13/91/115	-
13	CLA	B	1213	-	1/1/13/20	8/25/103/115	-
13	CLA	B	1204	-	1/1/15/20	2/37/115/115	-
13	CLA	L	1502	-	-	7/37/115/115	-
13	CLA	B	1215	-	1/1/14/20	10/31/109/115	-
16	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
13	CLA	A	1102	13	1/1/13/20	12/30/108/115	-
13	CLA	A	1109	13	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1133	-	1/1/12/20	6/24/102/115	-
13	CLA	A	1129	-	1/1/12/20	4/19/97/115	-
13	CLA	B	1207	2	1/1/15/20	7/37/115/115	-
13	CLA	A	1135	-	1/1/12/20	6/21/99/115	-
16	BCR	I	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	L	1503	20	1/1/15/20	8/37/115/115	-
13	CLA	A	1125	-	1/1/15/20	7/37/115/115	-
16	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
13	CLA	B	1202	-	1/1/15/20	13/37/115/115	-
16	BCR	M	4021	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1231	-	1/1/11/20	4/13/91/115	-
13	CLA	A	1140	-	1/1/15/20	8/37/115/115	-
13	CLA	A	1130	-	1/1/15/20	7/37/115/115	-
13	CLA	A	1801	17	1/1/12/20	15/22/100/115	-
13	CLA	B	1223	-	1/1/15/20	12/37/115/115	-
13	CLA	B	1205	-	1/1/15/20	9/37/115/115	-
13	CLA	B	1206	2	1/1/15/20	14/37/115/115	-
13	CLA	B	1212	-	-	8/13/91/115	-
13	CLA	B	1221	2	1/1/12/20	7/24/102/115	-
13	CLA	A	1124	20	1/1/15/20	12/37/115/115	-
16	BCR	A	4002	-	-	4/29/63/63	0/2/2/2
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1116	-	1/1/12/20	9/24/102/115	-
13	CLA	B	1233	20	1/1/11/20	4/13/91/115	-
13	CLA	A	1127	-	1/1/15/20	9/37/115/115	-
13	CLA	F	1301	20	1/1/11/20	4/13/91/115	-
17	LHG	A	5003	13	1/1/5/5	10/31/31/53	-
15	SF4	C	3002	3	-	-	0/6/5/5
16	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
17	LHG	A	5001	-	-	19/53/53/53	-
13	CLA	B	1201	-	1/1/12/20	4/24/102/115	-
13	CLA	A	1011	-	1/1/15/20	1/37/115/115	-

The worst 5 of 932 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	2001	PQN	O4-C4	9.27	1.42	1.23
14	B	2002	PQN	O4-C4	8.95	1.42	1.23
14	A	2001	PQN	O1-C1	8.92	1.42	1.23
17	B	5004	LHG	P-O5	8.61	1.81	1.50
14	B	2002	PQN	O1-C1	8.42	1.41	1.23

The worst 5 of 1417 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1217	CLA	C4A-NA-C1A	12.31	112.24	106.71
13	A	1130	CLA	C4A-NA-C1A	12.24	112.21	106.71
13	M	1601	CLA	C4A-NA-C1A	12.18	112.18	106.71
13	A	1113	CLA	C4A-NA-C1A	12.01	112.10	106.71
13	A	1118	CLA	C4A-NA-C1A	11.91	112.06	106.71

5 of 87 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1011	CLA	ND
13	A	1022	CLA	ND
13	A	1013	CLA	ND
13	A	1101	CLA	ND
13	A	1102	CLA	ND

5 of 864 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1013	CLA	O2A-C1-C2-C3
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	C1A-C2A-CAA-CBA
13	A	1103	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	CBA-CGA-O2A-C1

There are no ring outliers.

114 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1601	CLA	1	0
13	A	1114	CLA	2	0
16	A	4001	BCR	2	0
16	J	4013	BCR	7	0
13	B	1238	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1210	CLA	6	0
13	A	1117	CLA	6	0
13	B	1216	CLA	5	0
13	A	1128	CLA	7	0
16	B	4009	BCR	5	0
13	J	1302	CLA	1	0
13	A	1022	CLA	3	0
13	B	1226	CLA	7	0
13	B	1211	CLA	6	0
13	B	1225	CLA	8	0
13	A	1138	CLA	2	0
13	A	1108	CLA	4	0
16	B	4017	BCR	1	0
13	X	1701	CLA	1	0
13	A	1121	CLA	1	0
13	B	1214	CLA	8	0
13	B	1203	CLA	6	0
13	A	1103	CLA	6	0
13	B	1208	CLA	1	0
13	A	1136	CLA	7	0
13	A	1119	CLA	4	0
16	J	4012	BCR	4	0
13	B	1230	CLA	7	0
13	A	1104	CLA	4	0
13	B	1217	CLA	2	0
13	A	1120	CLA	2	0
13	A	1237	CLA	5	0
13	B	1232	CLA	3	0
13	B	1228	CLA	2	0
16	B	4010	BCR	3	0
13	A	1105	CLA	2	0
16	B	4014	BCR	1	0
16	J	4015	BCR	5	0
13	A	1402	CLA	1	0
18	B	5002	LMG	5	0
16	F	4016	BCR	2	0
13	B	1023	CLA	4	0
13	B	1234	CLA	3	0
13	A	1132	CLA	4	0
13	A	1111	CLA	1	0
13	A	1101	CLA	2	0
13	A	1126	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	2002	PQN	1	0
16	A	4008	BCR	1	0
13	B	1235	CLA	2	0
13	B	1236	CLA	4	0
13	B	1222	CLA	2	0
16	L	4022	BCR	1	0
13	A	1106	CLA	6	0
13	K	1401	CLA	1	0
13	A	1118	CLA	5	0
13	B	1219	CLA	4	0
13	B	1218	CLA	1	0
13	B	1209	CLA	1	0
13	A	1122	CLA	2	0
13	B	1224	CLA	5	0
13	A	1013	CLA	10	0
16	A	4007	BCR	4	0
16	B	4005	BCR	1	0
17	B	5004	LHG	1	0
13	B	1227	CLA	5	0
13	L	1501	CLA	2	0
13	A	1107	CLA	4	0
14	A	2001	PQN	1	0
13	A	1134	CLA	2	0
13	B	1229	CLA	6	0
16	B	4006	BCR	5	0
13	A	1123	CLA	4	0
13	A	1137	CLA	3	0
13	B	1220	CLA	3	0
13	B	1021	CLA	8	0
13	B	1012	CLA	17	0
13	A	1112	CLA	5	0
13	B	1213	CLA	3	0
13	B	1204	CLA	1	0
13	L	1502	CLA	8	0
13	B	1215	CLA	6	0
16	A	4011	BCR	13	0
13	A	1102	CLA	1	0
13	A	1109	CLA	1	0
13	A	1133	CLA	4	0
13	A	1129	CLA	1	0
13	B	1207	CLA	5	0
13	A	1135	CLA	2	0

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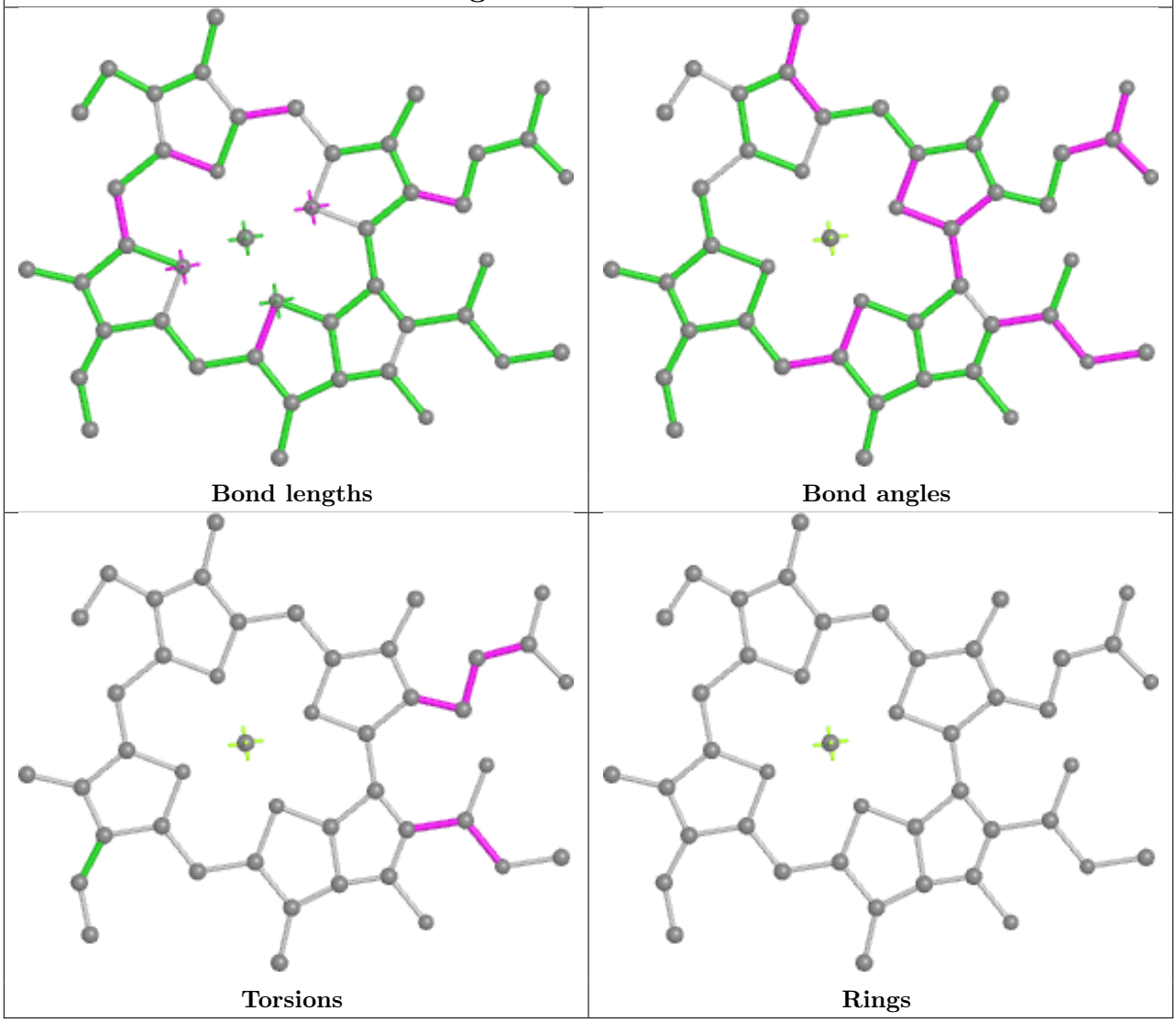
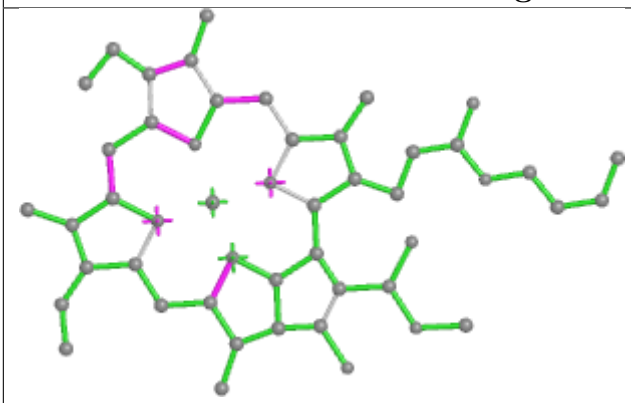
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	1503	CLA	2	0
13	A	1125	CLA	3	0
16	I	4018	BCR	3	0
13	B	1202	CLA	3	0
16	M	4021	BCR	2	0
13	A	1140	CLA	8	0
13	A	1130	CLA	2	0
13	A	1801	CLA	5	0
13	B	1223	CLA	3	0
13	B	1205	CLA	3	0
13	B	1206	CLA	2	0
13	B	1212	CLA	2	0
13	B	1221	CLA	10	0
13	A	1124	CLA	5	0
16	A	4002	BCR	2	0
16	A	4003	BCR	1	0
13	A	1116	CLA	5	0
13	B	1233	CLA	2	0
13	A	1127	CLA	1	0
13	F	1301	CLA	1	0
17	A	5003	LHG	2	0
16	B	4004	BCR	1	0
17	A	5001	LHG	4	0
13	B	1201	CLA	2	0
13	A	1011	CLA	9	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.

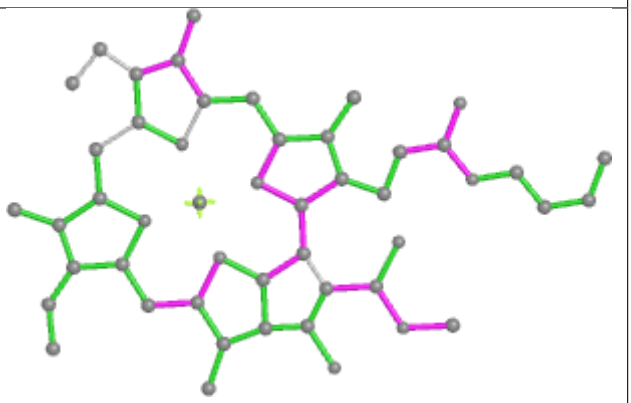
Ligand CLA M 1601



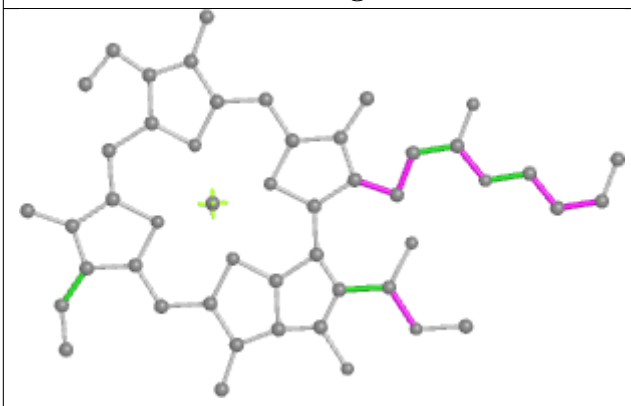
Ligand CLA A 1114



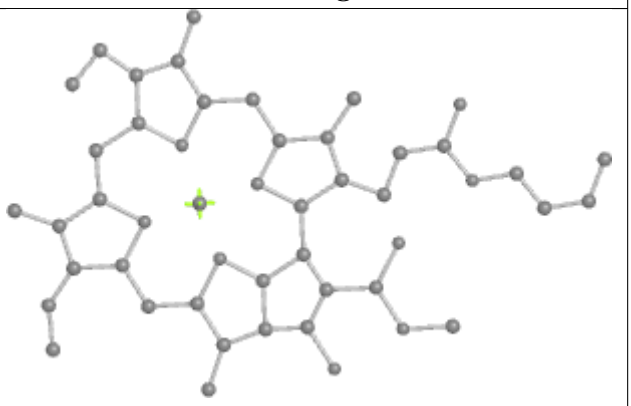
Bond lengths



Bond angles

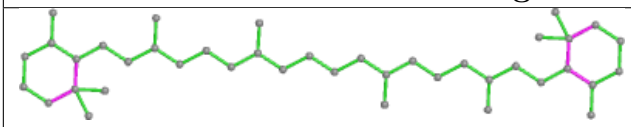


Torsions

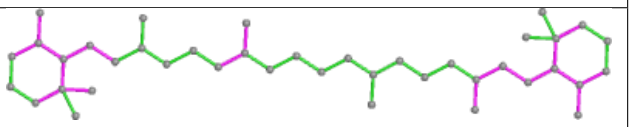


Rings

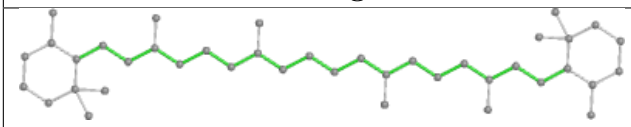
Ligand BCR A 4001



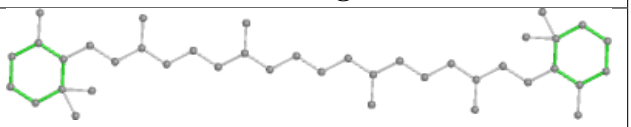
Bond lengths



Bond angles

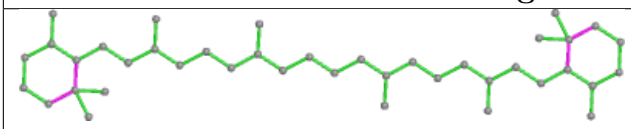


Torsions

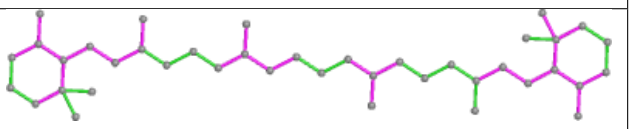


Rings

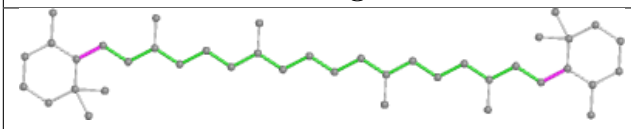
Ligand BCR J 4013



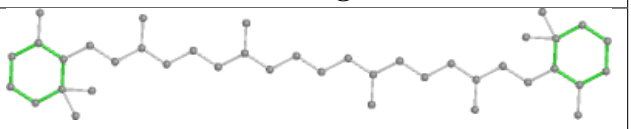
Bond lengths



Bond angles

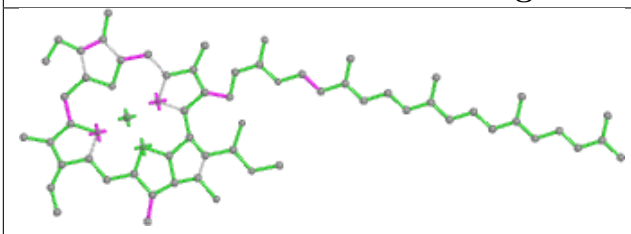


Torsions

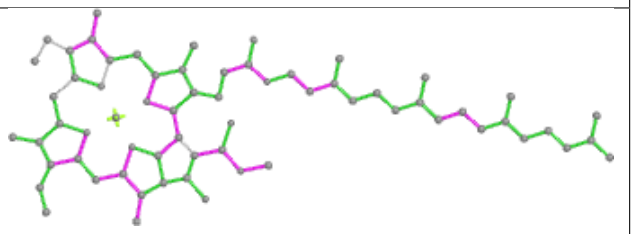


Rings

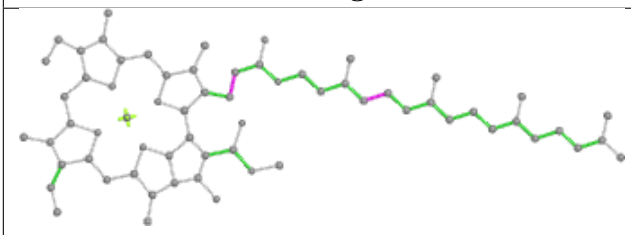
Ligand CLA B 1238



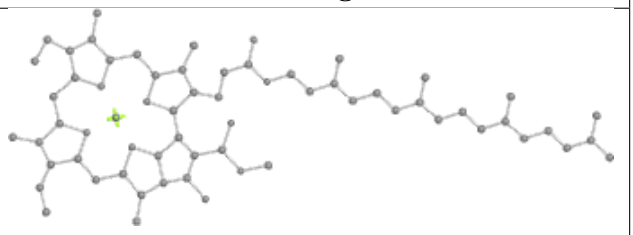
Bond lengths



Bond angles

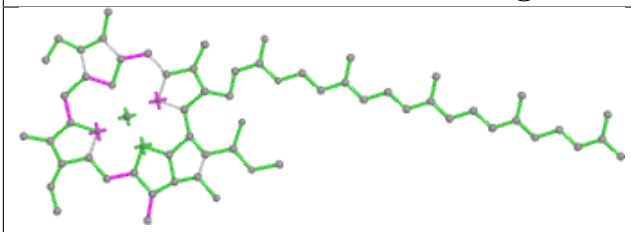


Torsions

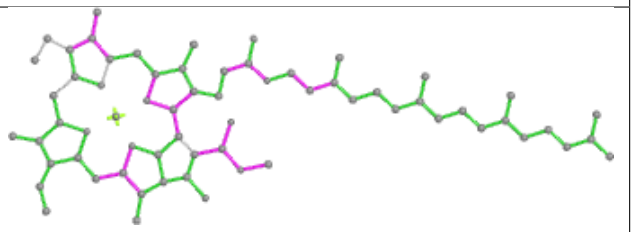


Rings

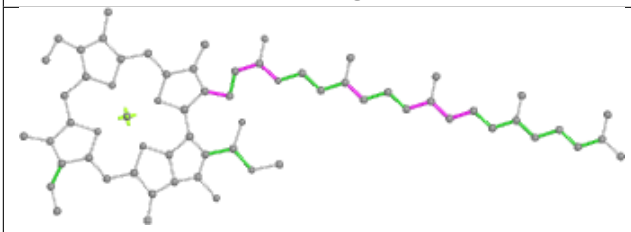
Ligand CLA B 1210



Bond lengths



Bond angles



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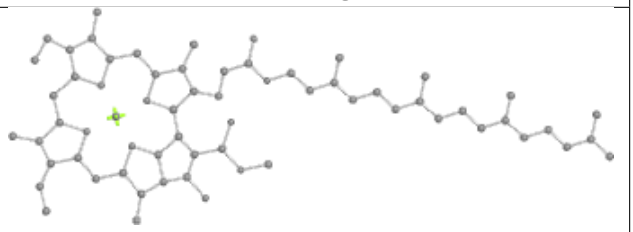
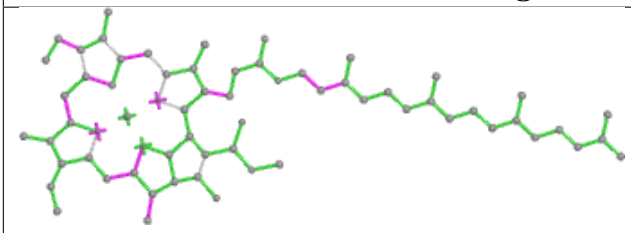


Rings

Ligand CLA A 1117



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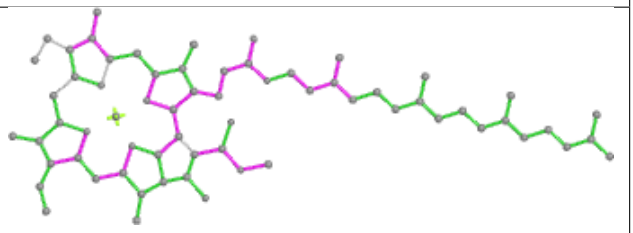
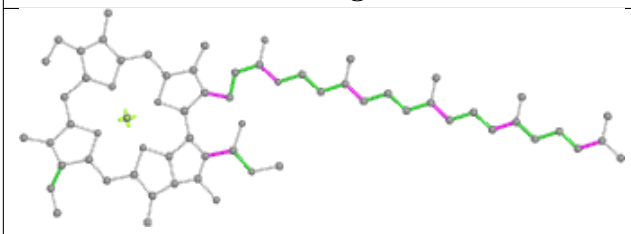


Bond angles



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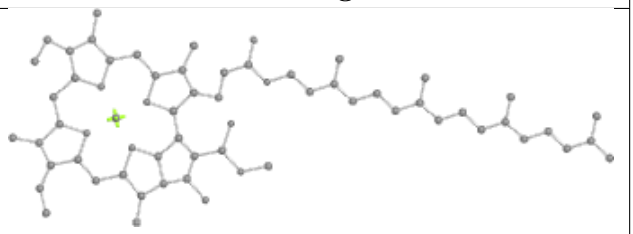
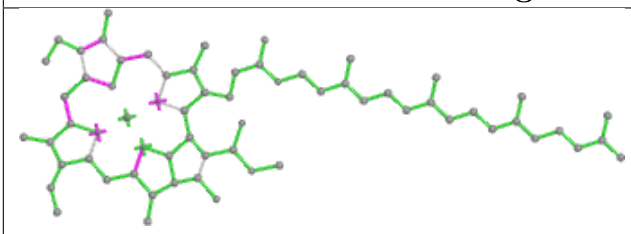
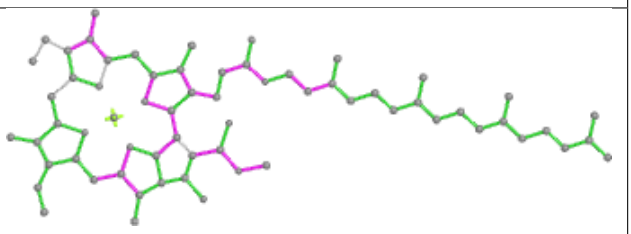


Rings

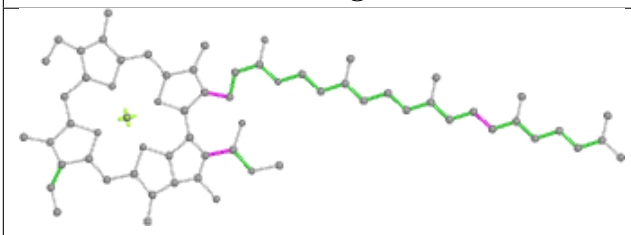
Ligand CLA B 1216



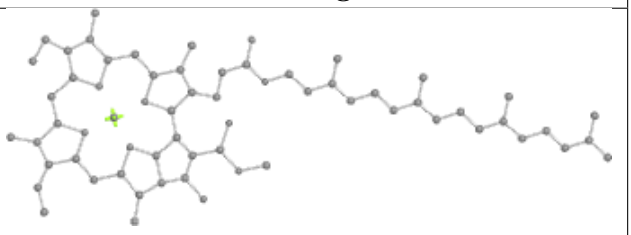
Bond lengths



Bond angles

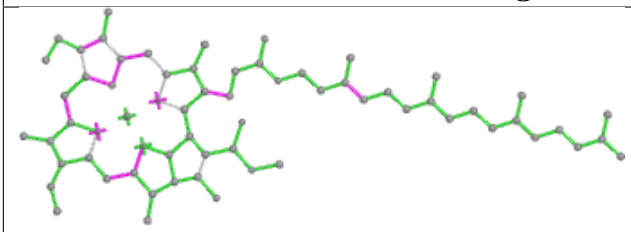


Torsions

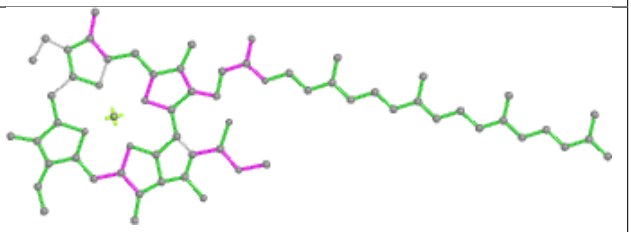


Rings

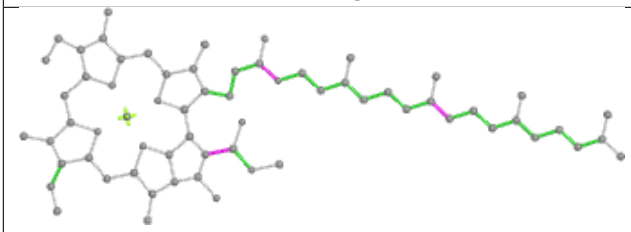
Ligand CLA A 1128



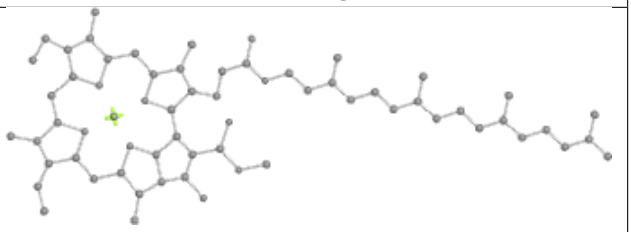
Bond lengths



Bond angles

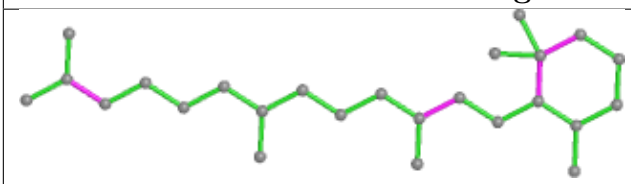


Torsions



Rings

Ligand BCR B 4009



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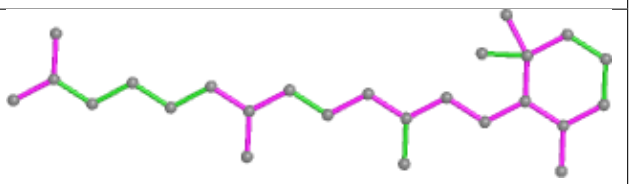
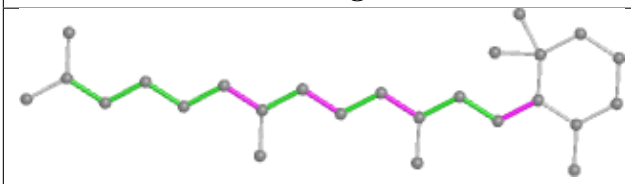


Bond angles



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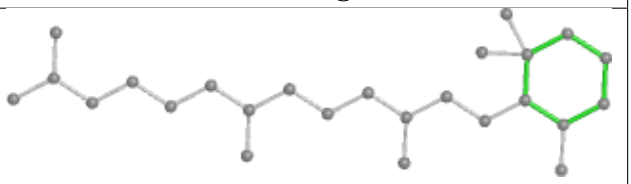
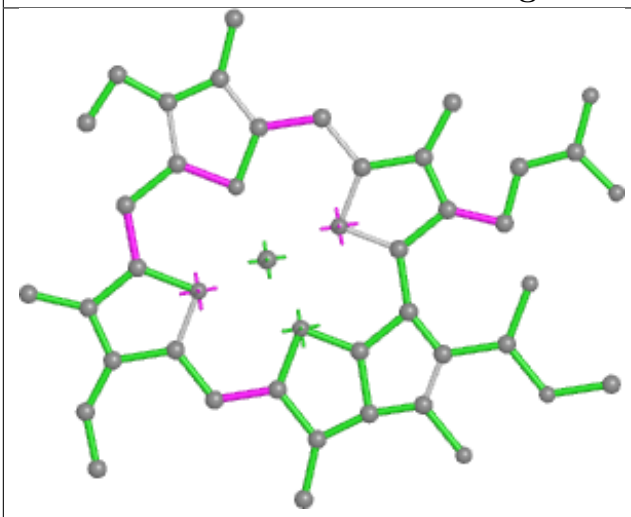


Rings

Ligand CLA J 1302



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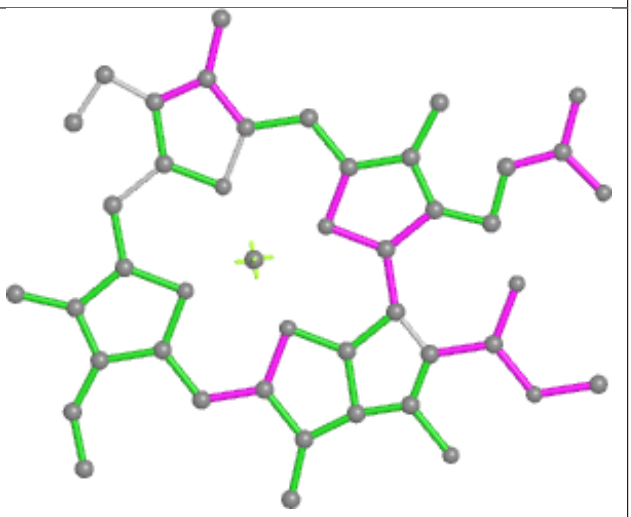
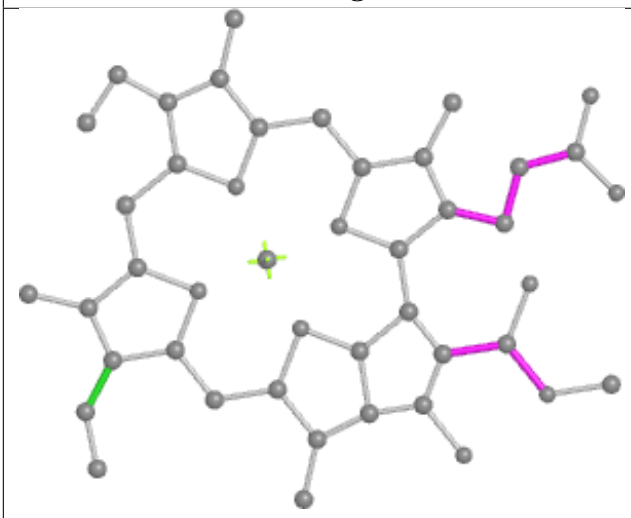
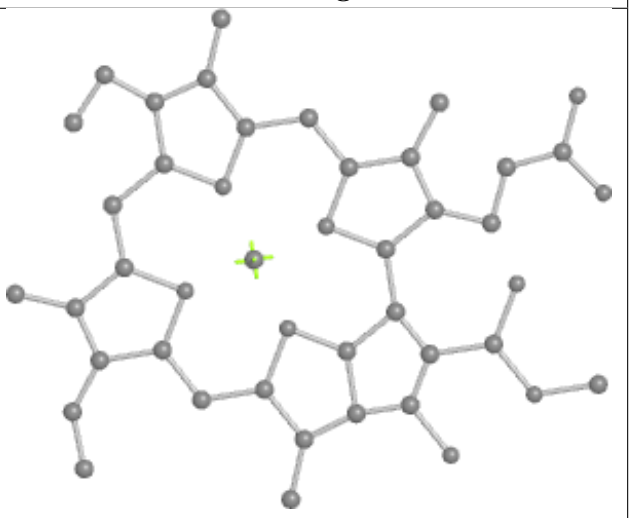


Bond angles

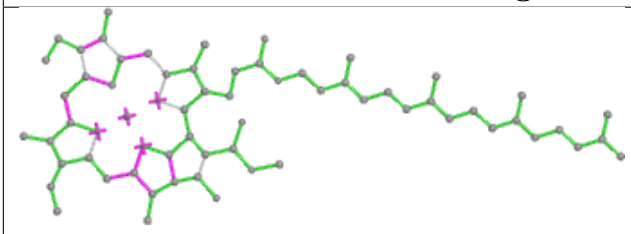


Torsions



Rings

Ligand CLA A 1022



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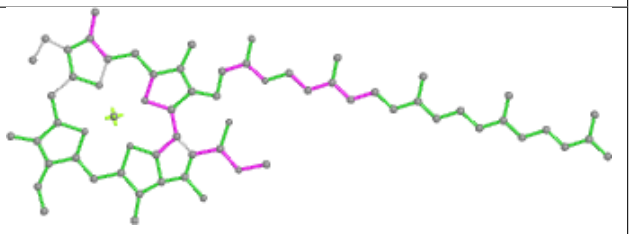
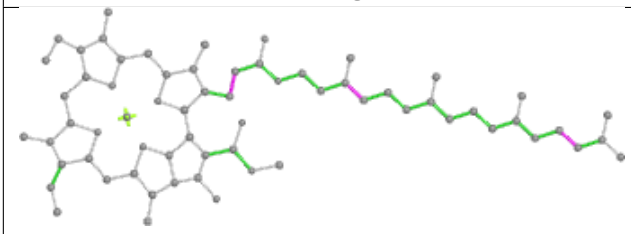


Bond angles



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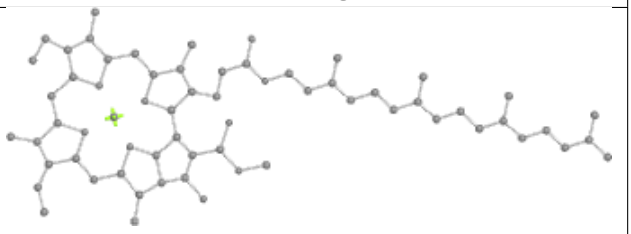
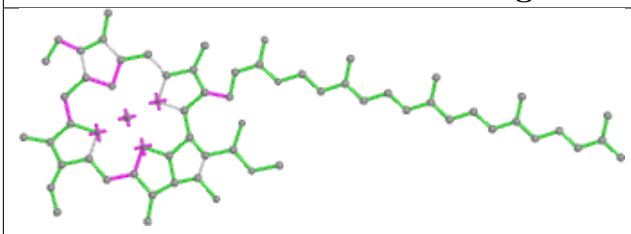


Rings

Ligand CLA B 1226



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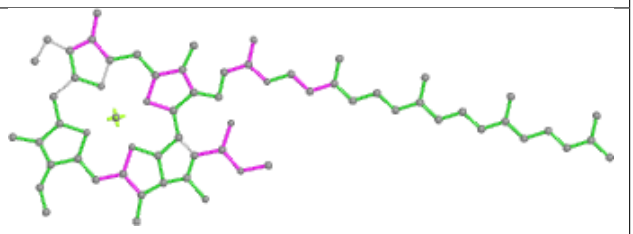
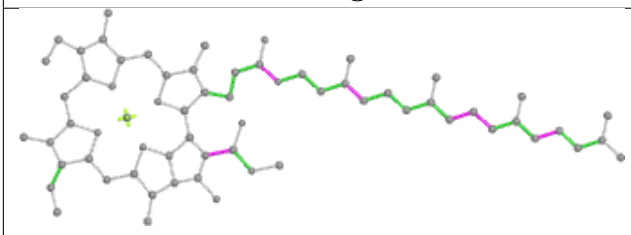


Bond angles



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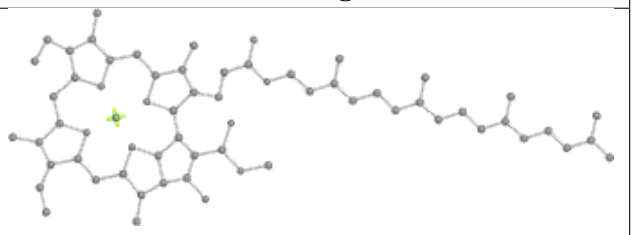
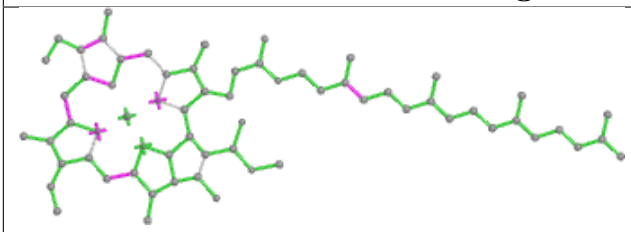


Rings

Ligand CLA B 1211



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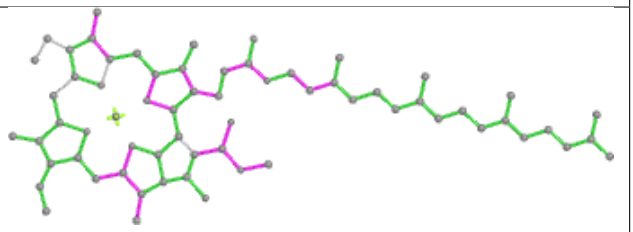
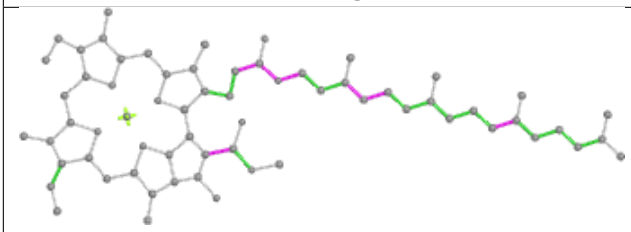


Bond angles



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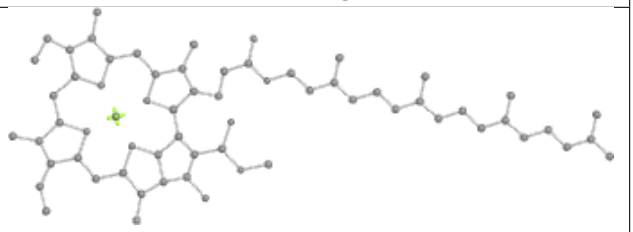
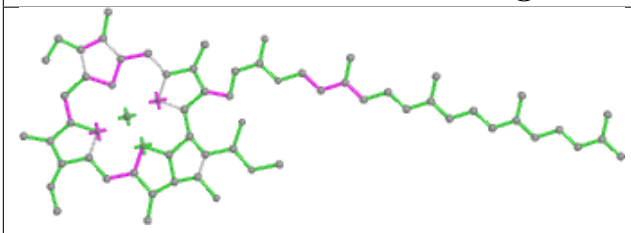


Rings

Ligand CLA B 1225



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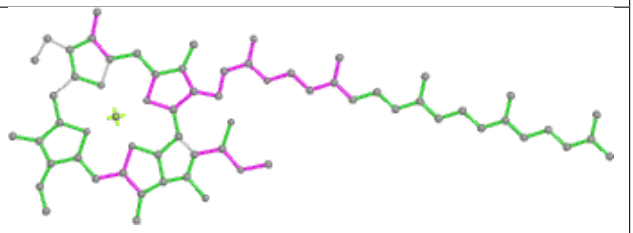
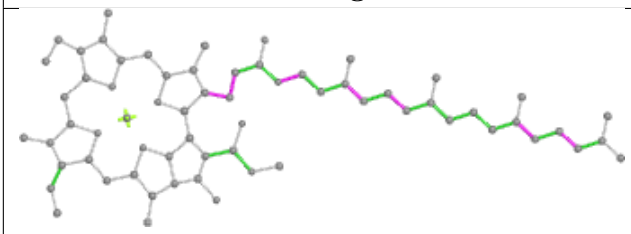


Bond angles



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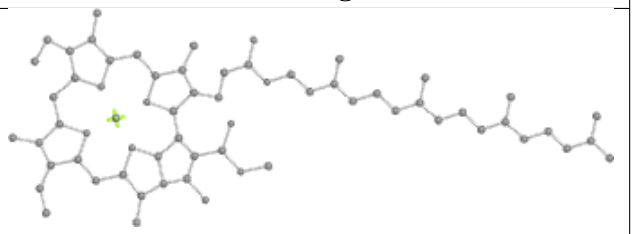
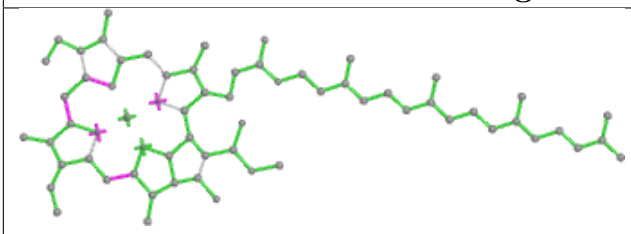
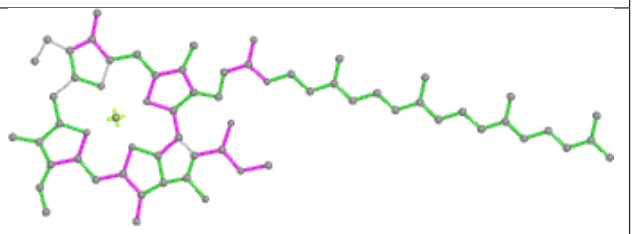
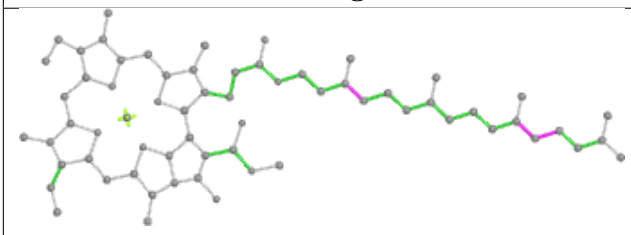
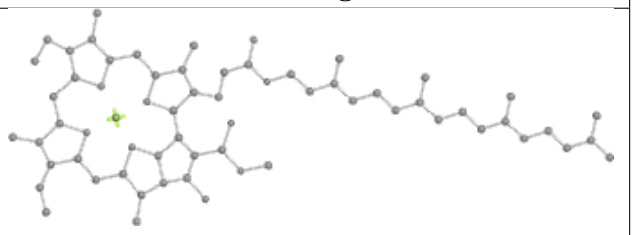
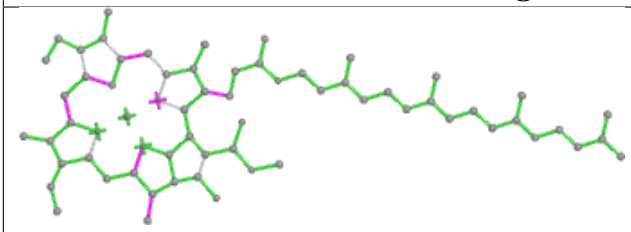
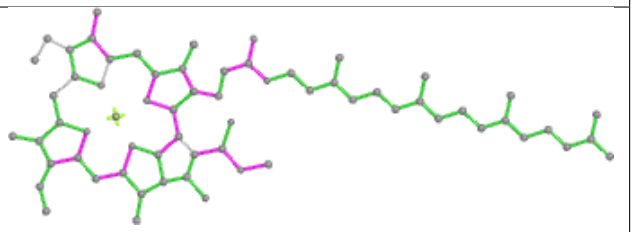
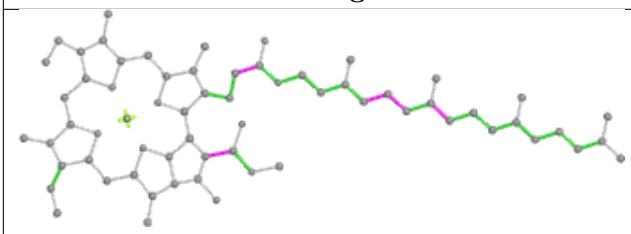
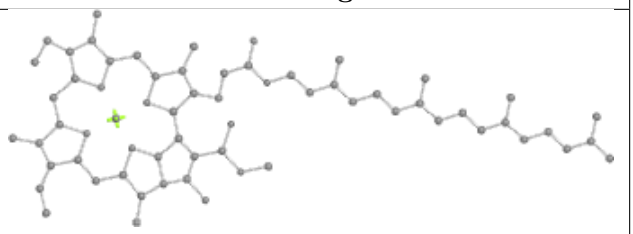
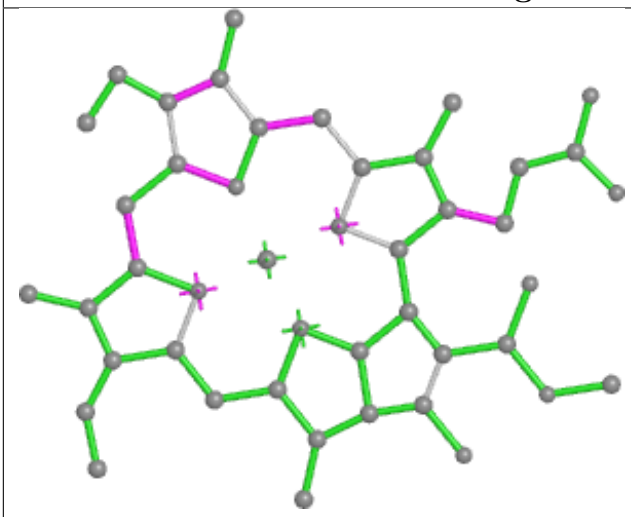


Rings

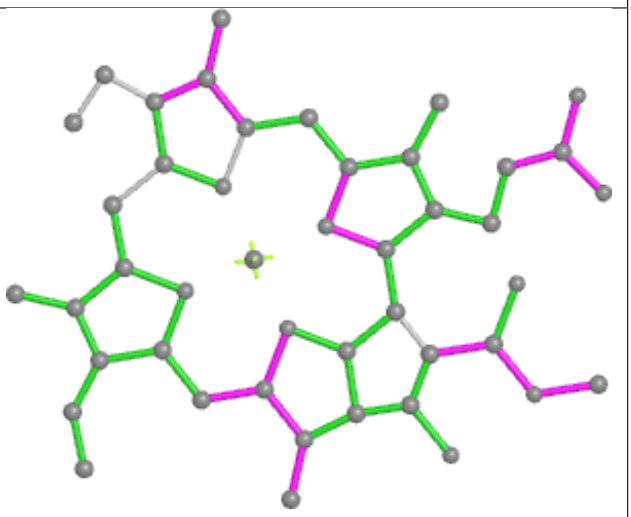
Ligand CLA A 1131	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1138	
 Bond lengths	 Bond angles
 Torsions	 Rings

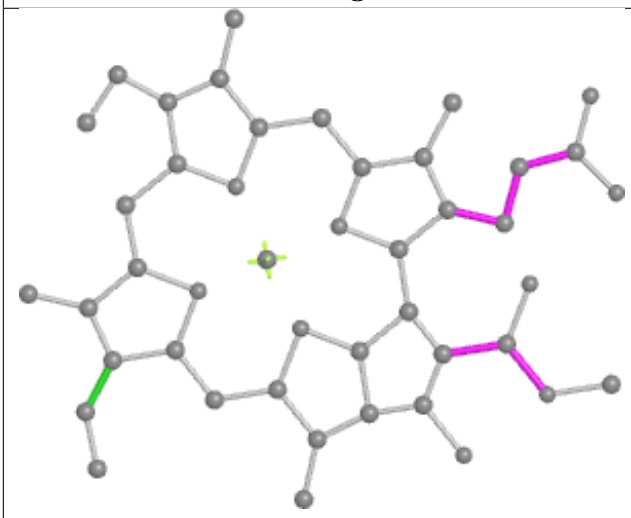
Ligand CLA A 1108



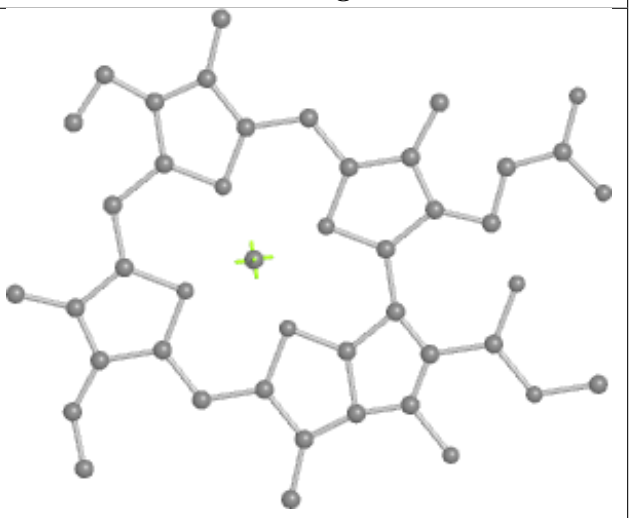
Bond lengths



Bond angles

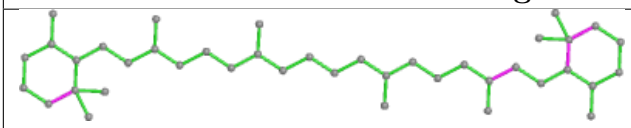


Torsions



Rings

Ligand BCR B 4017



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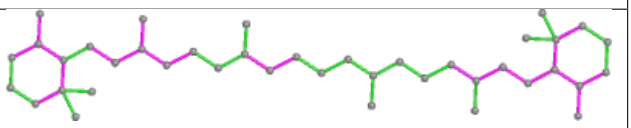
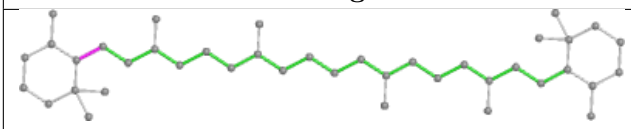


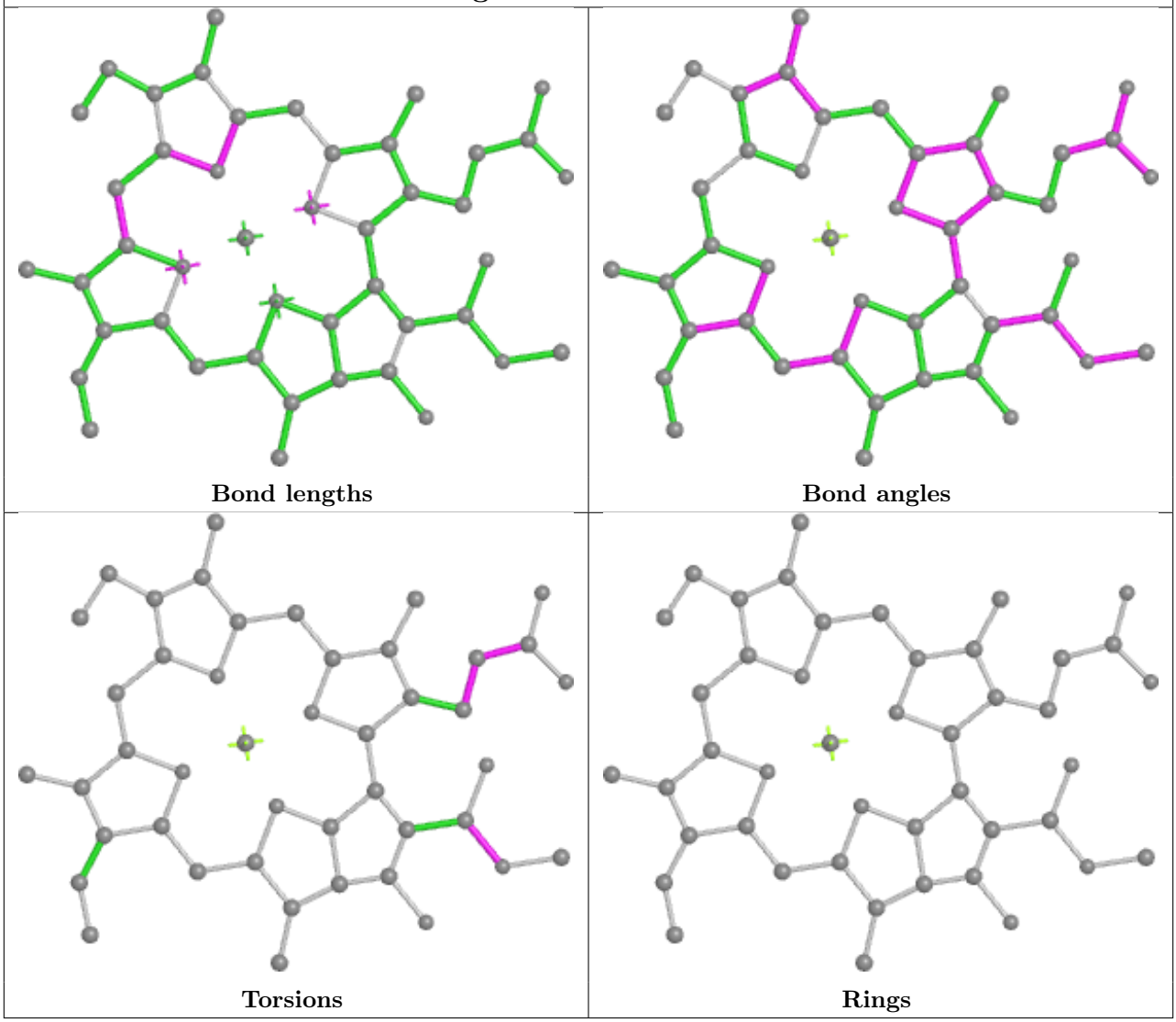
Bond angles



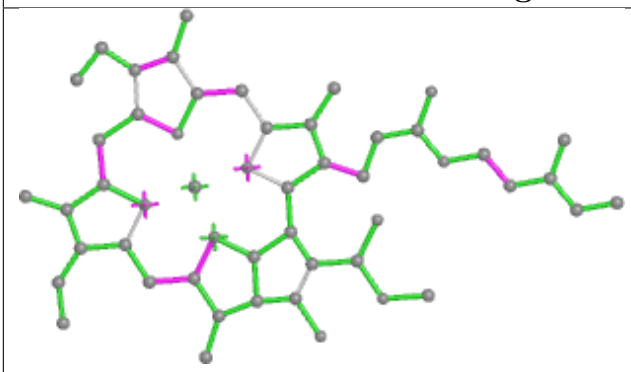
Torsions

Rings

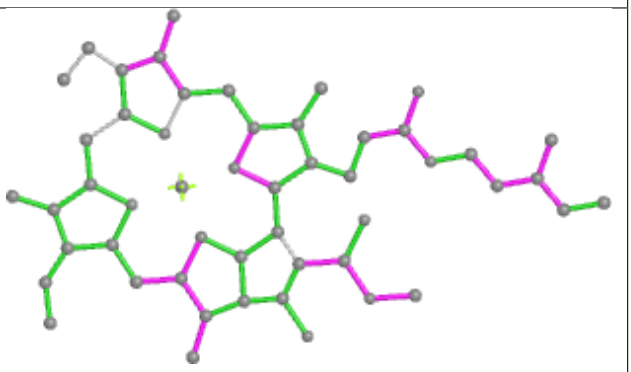
Ligand CLA X 1701



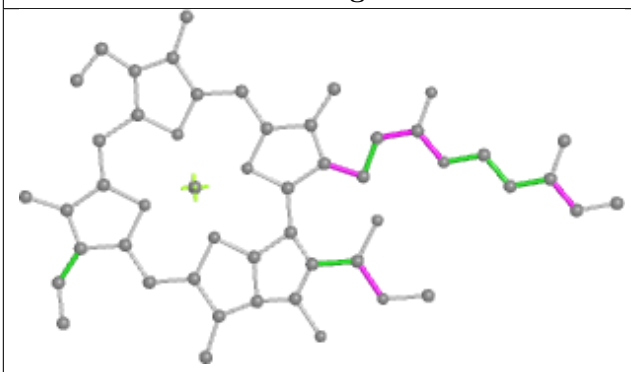
Ligand CLA A 1121



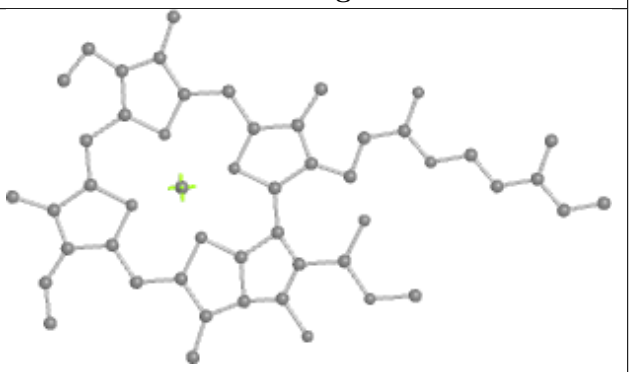
Bond lengths



Bond angles

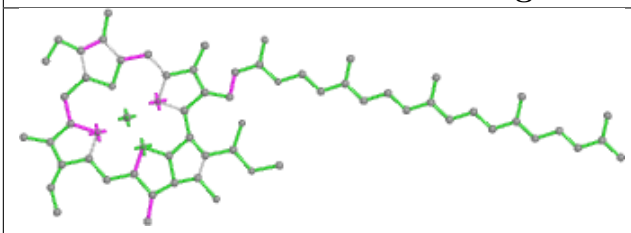


Torsions

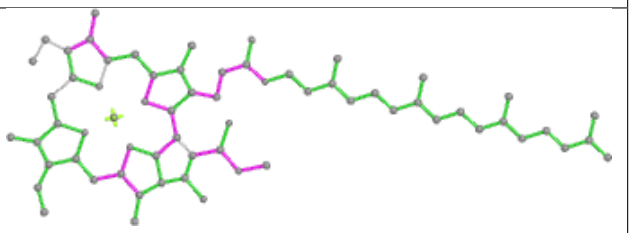


Rings

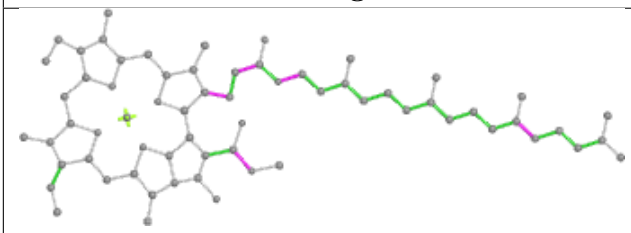
Ligand CLA B 1239



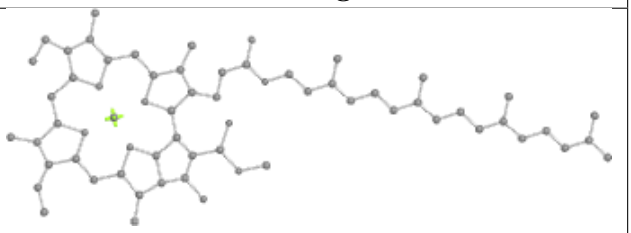
Bond lengths



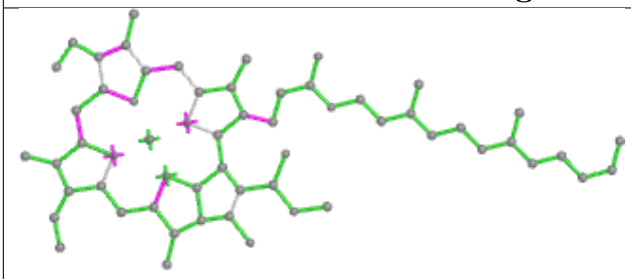
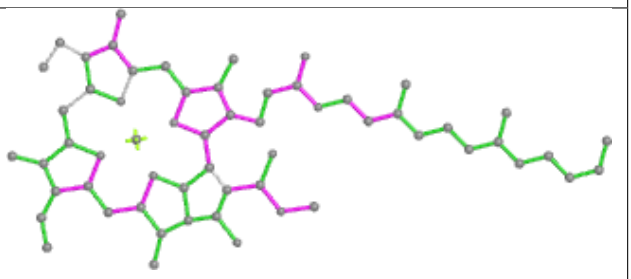
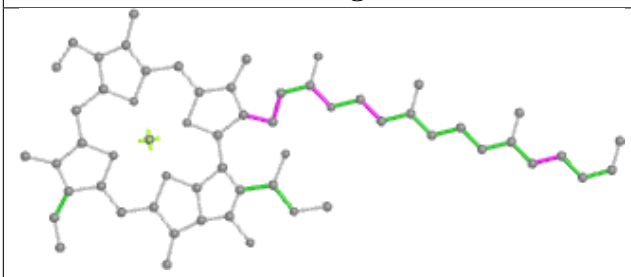
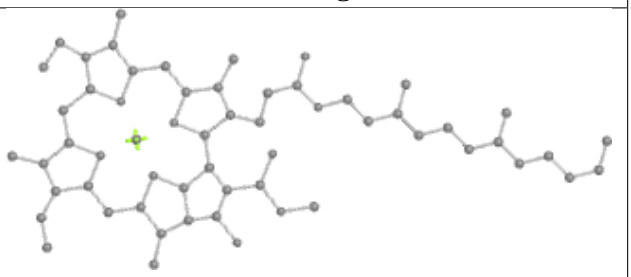
Bond angles

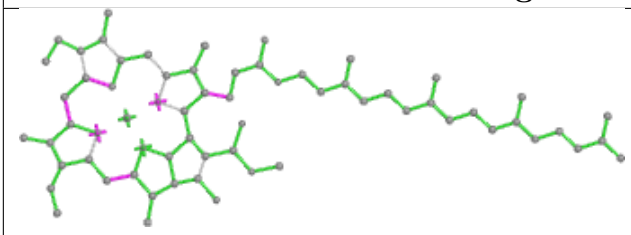
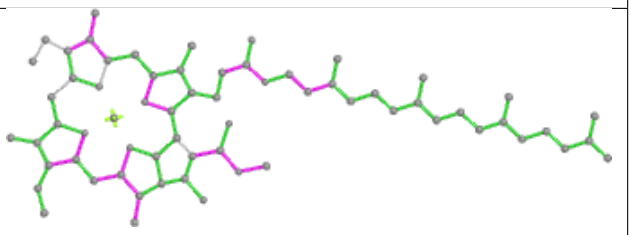
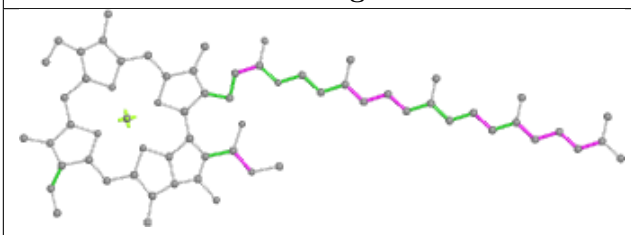
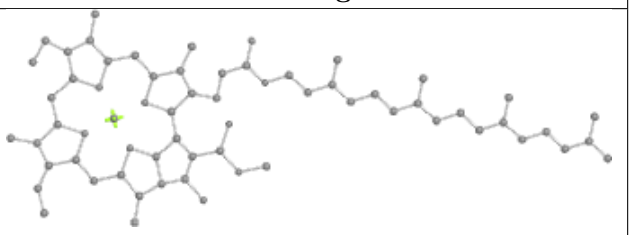


Torsions

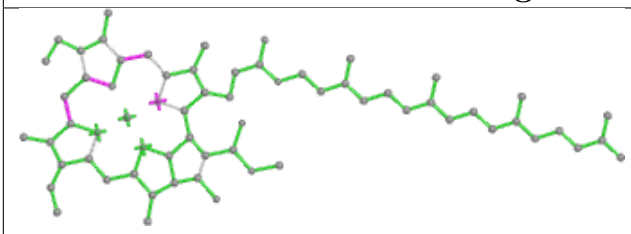


Rings

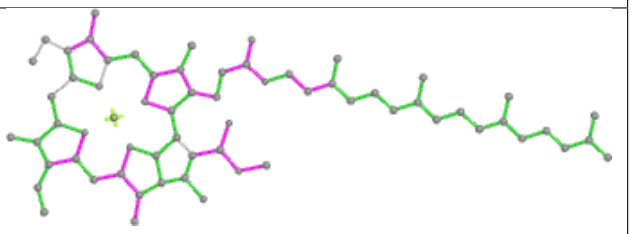
Ligand CLA B 1214	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

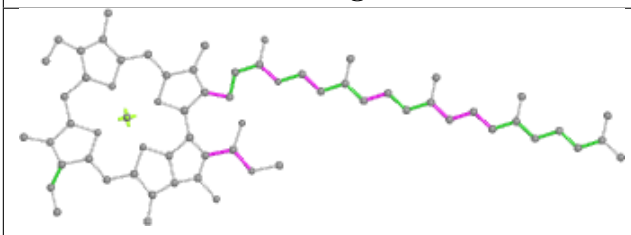
Ligand CLA A 1103



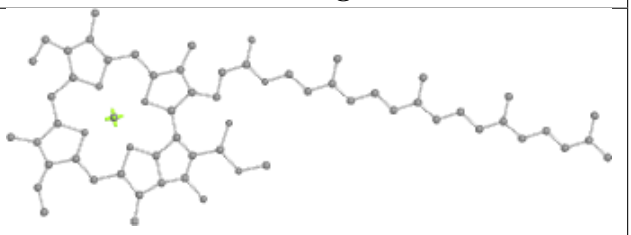
Bond lengths



Bond angles

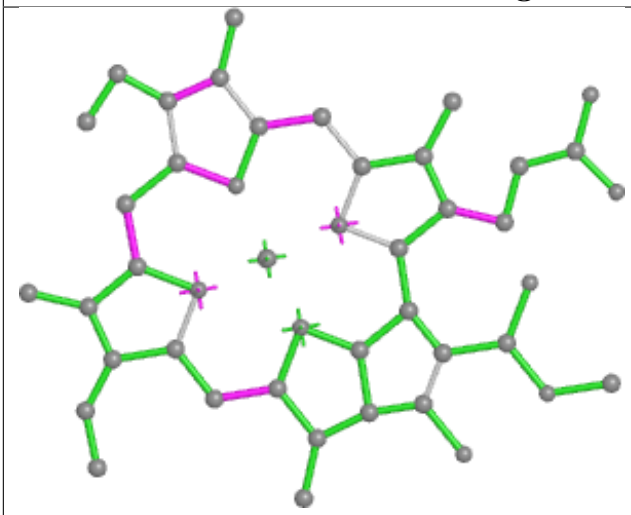


Torsions



Rings

Ligand CLA B 1208



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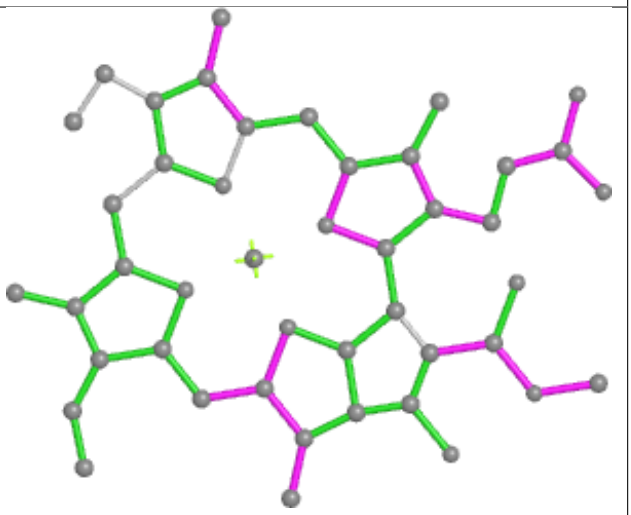
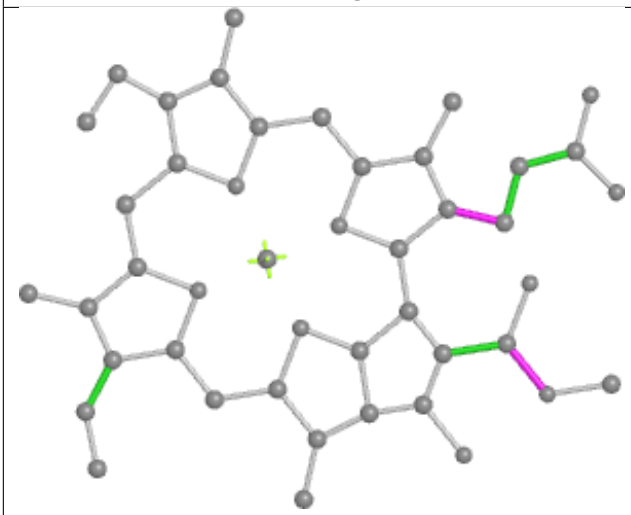


Bond angles



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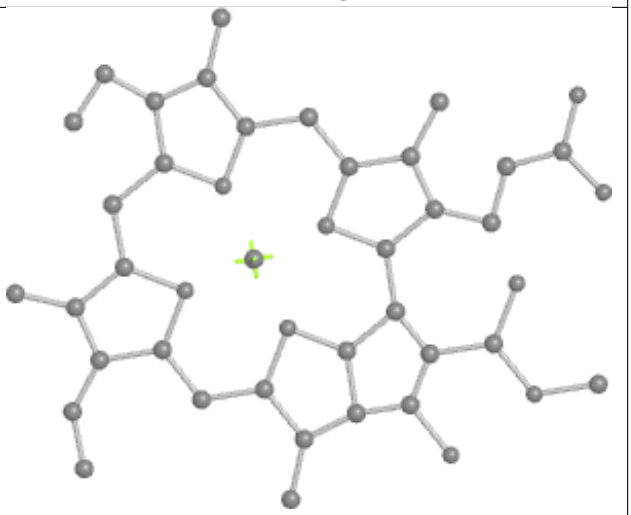
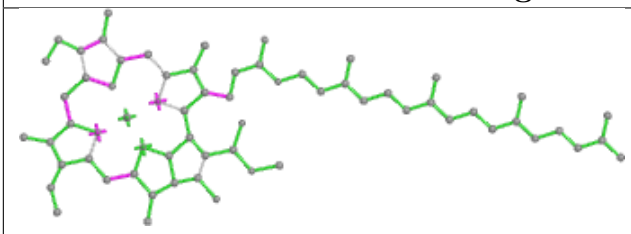


Rings

Ligand CLA A 1136



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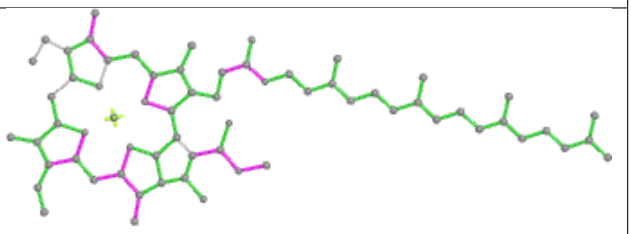
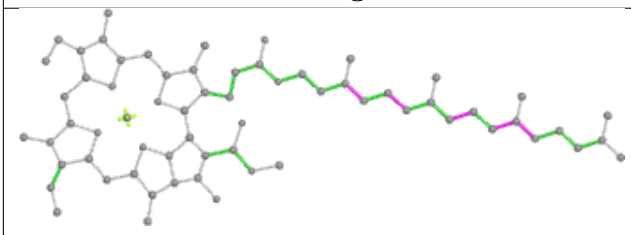


Bond angles



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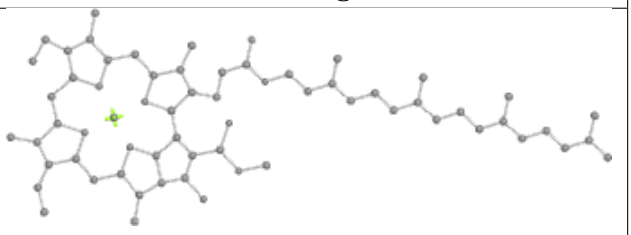
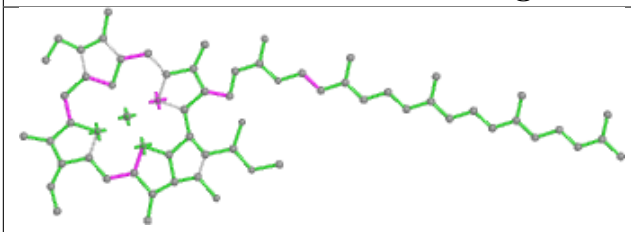


Rings

Ligand CLA A 1119



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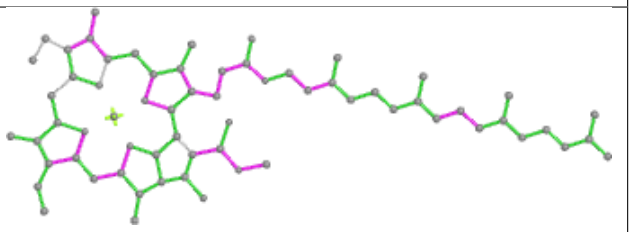
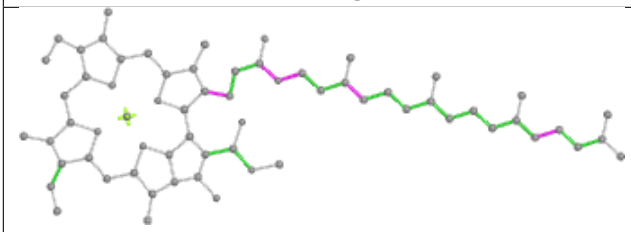


Bond angles



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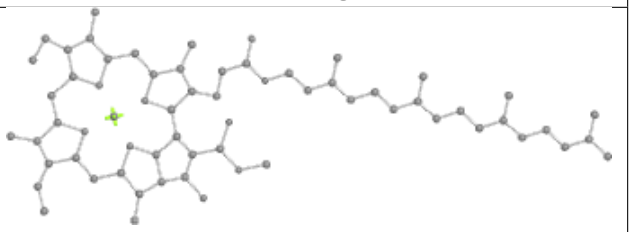
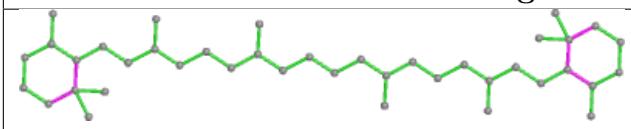
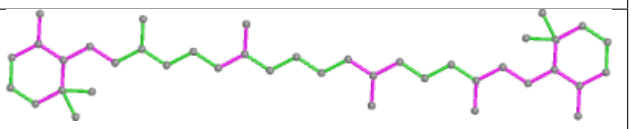


Rings

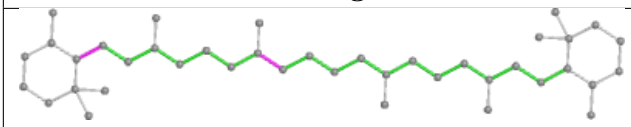
Ligand BCR J 4012



Bond lengths

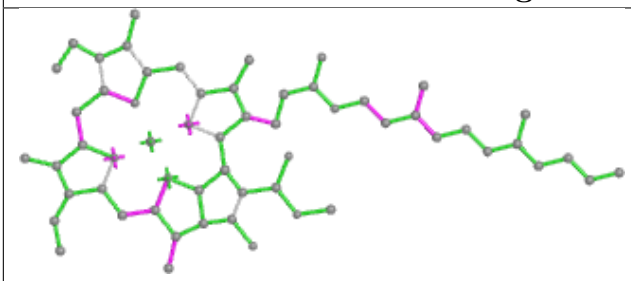
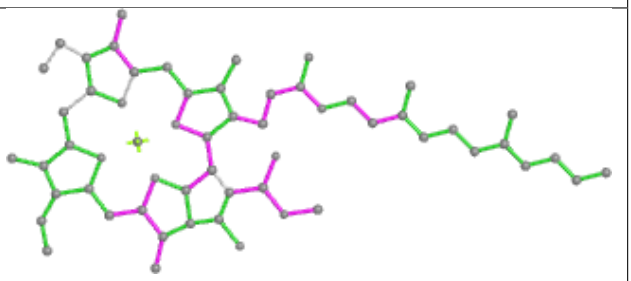
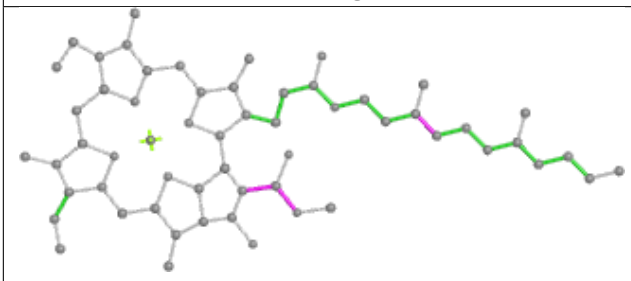
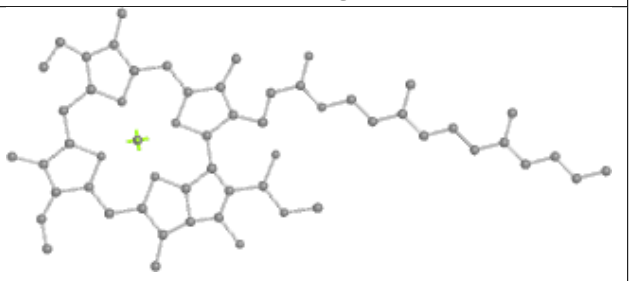


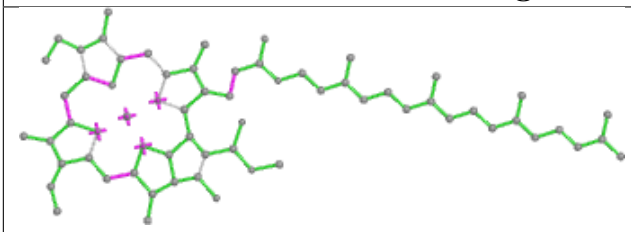
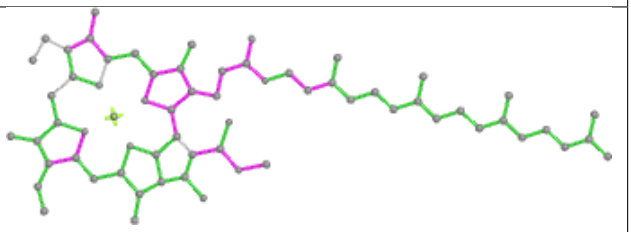
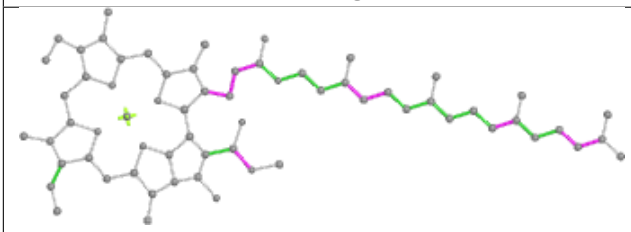
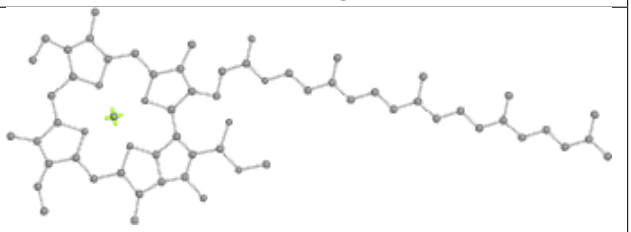
Bond angles



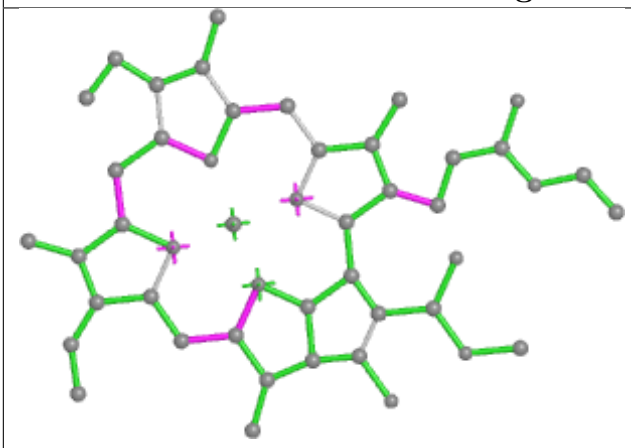
Torsions

Rings

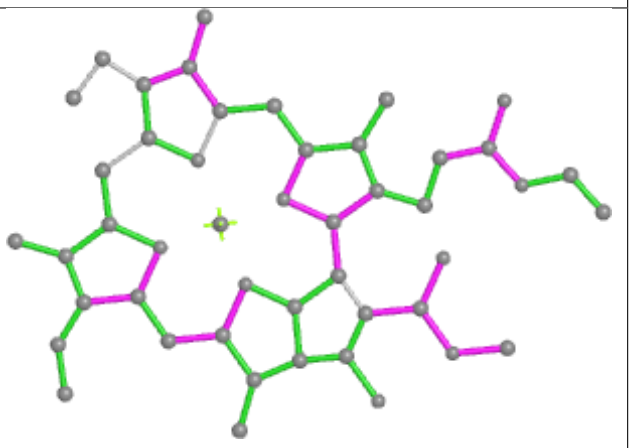
Ligand CLA B 1230	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1104	
 Bond lengths	 Bond angles
 Torsions	 Rings

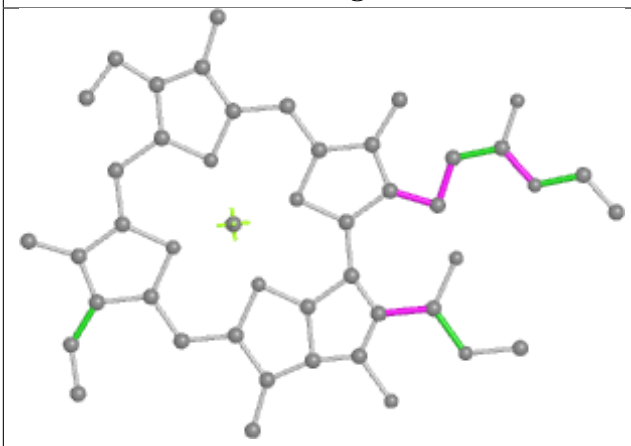
Ligand CLA B 1217



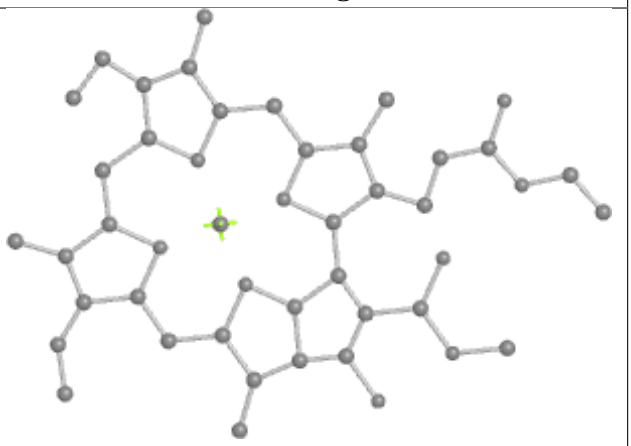
Bond lengths



Bond angles

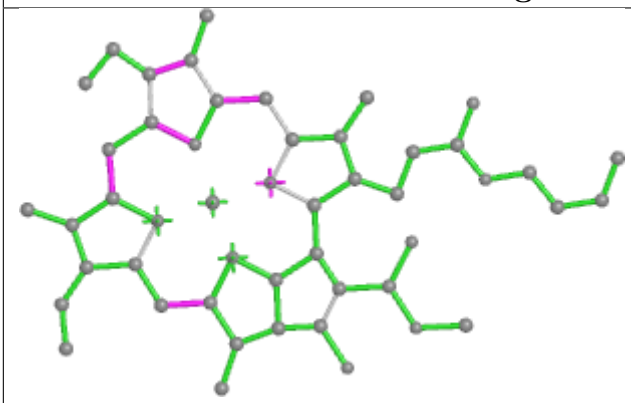


Torsions



Rings

Ligand CLA A 1120



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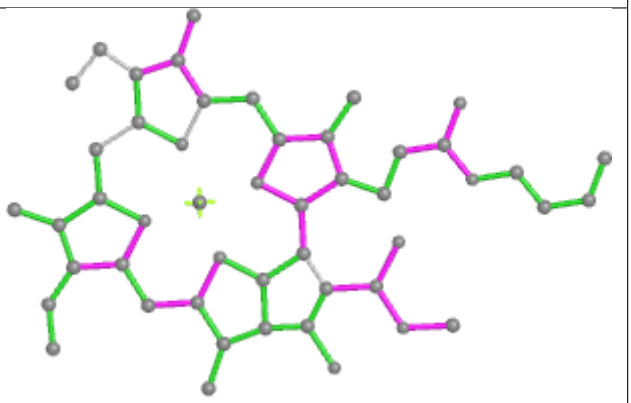
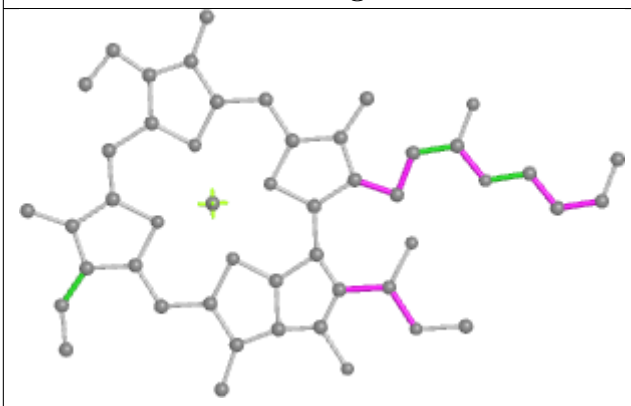


Bond angles



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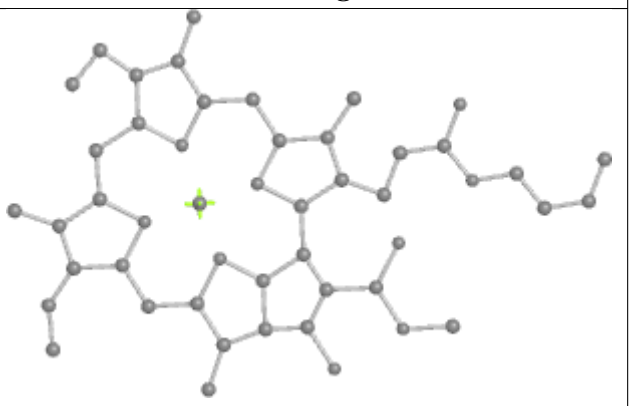
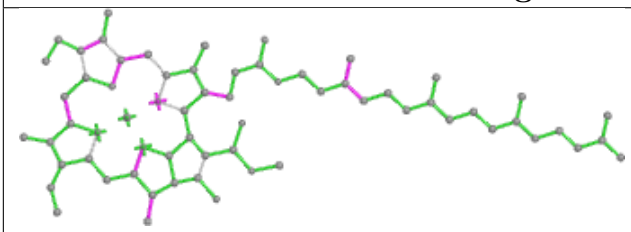


Rings

Ligand CLA A 1237



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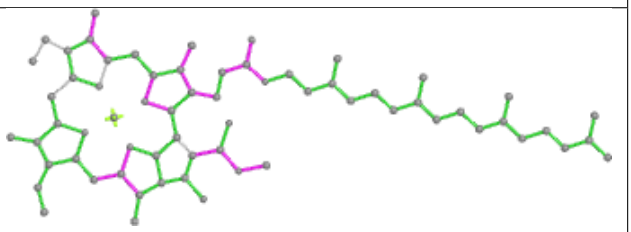
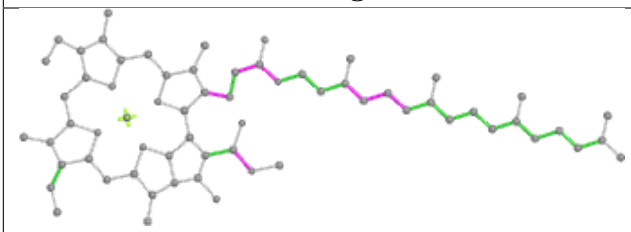
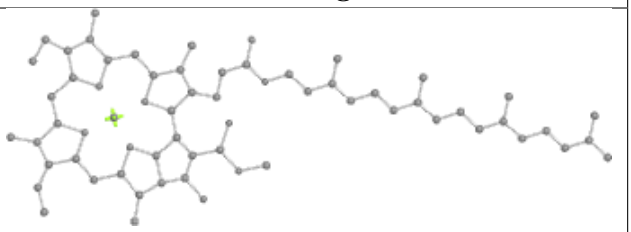


Bond angles

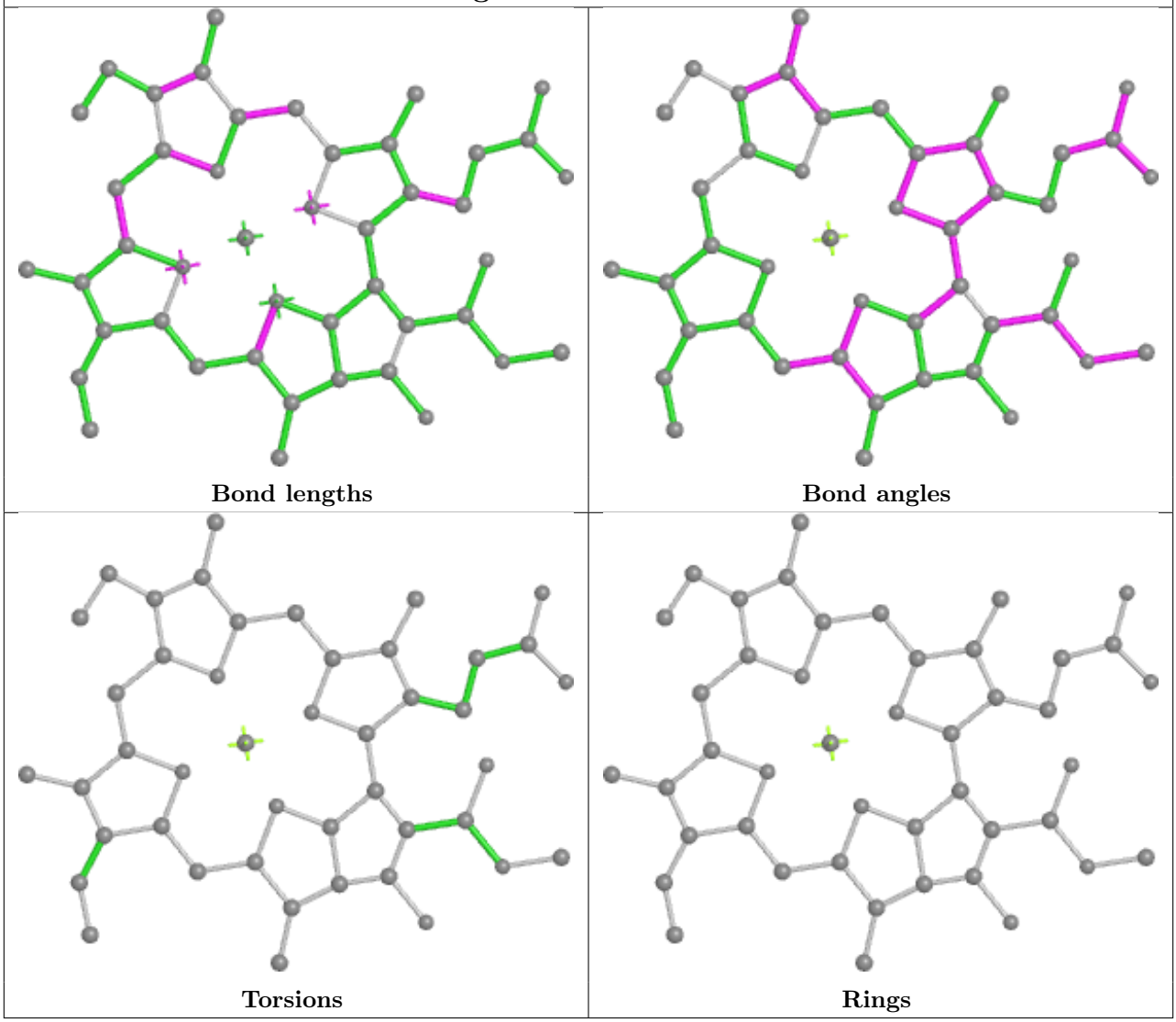


Torsions

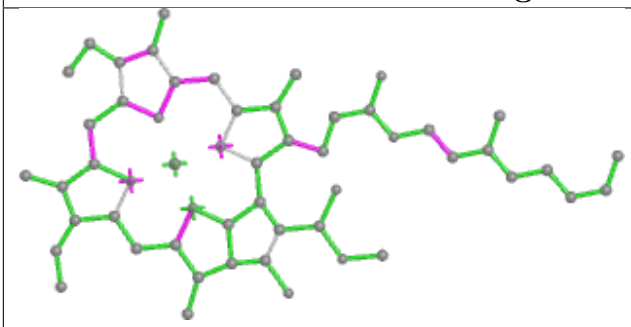


Rings

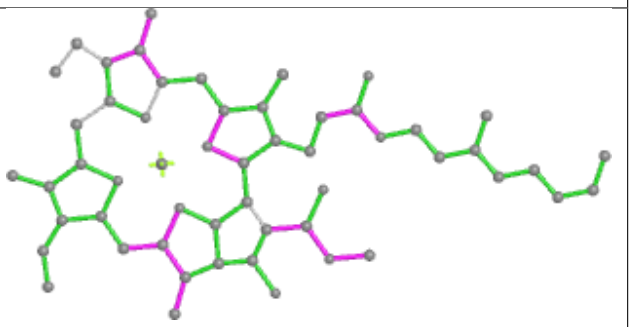
Ligand CLA B 1232



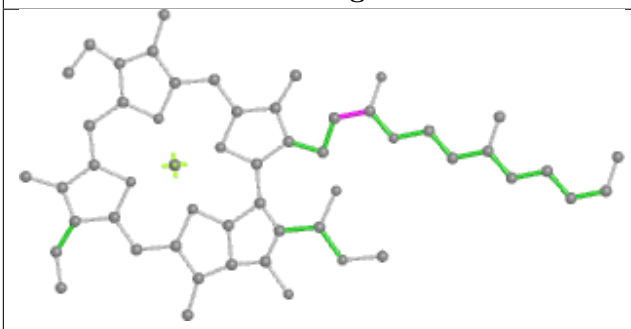
Ligand CLA A 1115



Bond lengths



Bond angles



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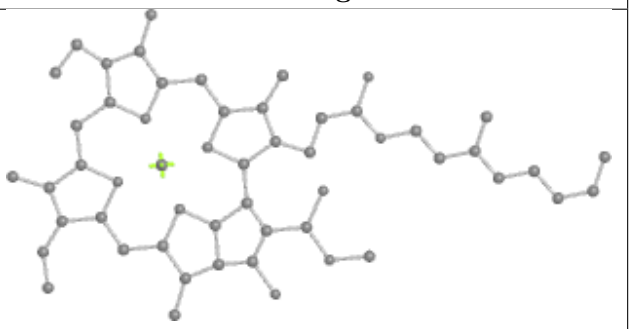
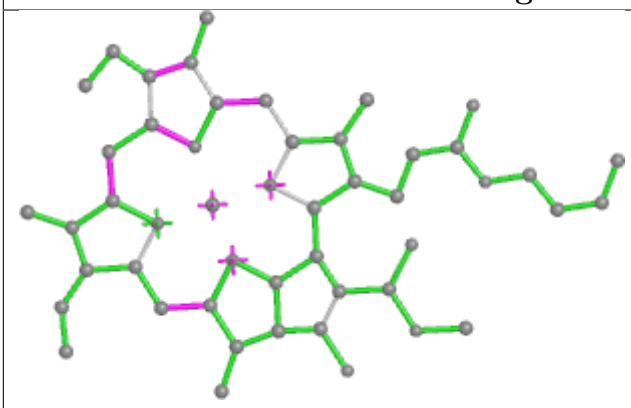
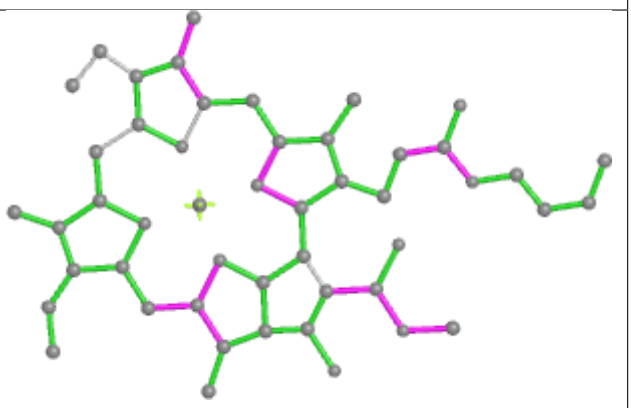


Rings

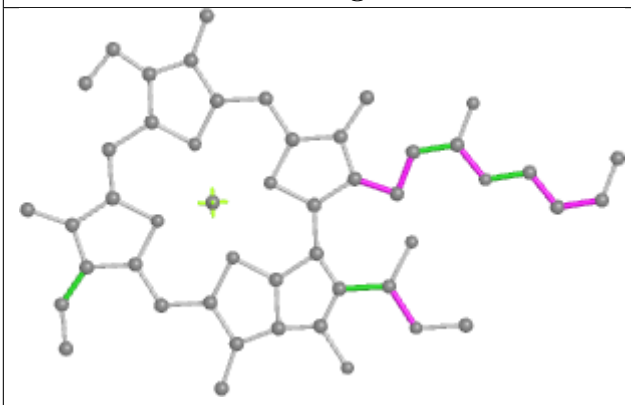
Ligand CLA B 1228



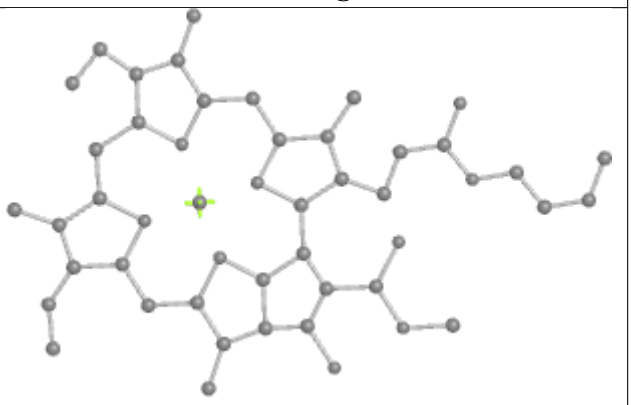
Bond lengths



Bond angles

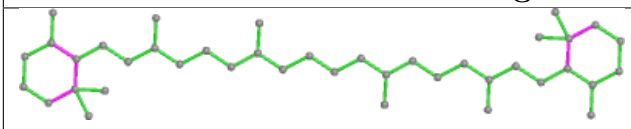


Torsions

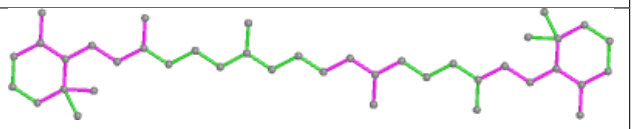


Rings

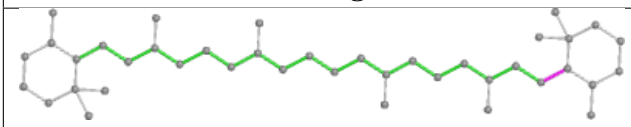
Ligand BCR B 4010



Bond lengths



Bond angles



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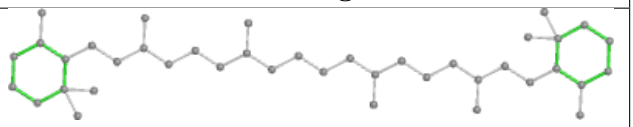
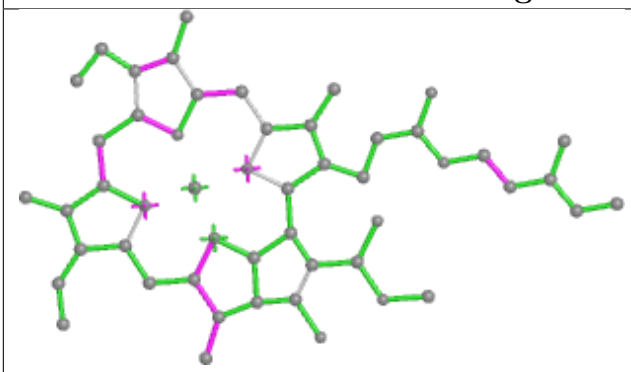


Rings

Ligand CLA A 1105



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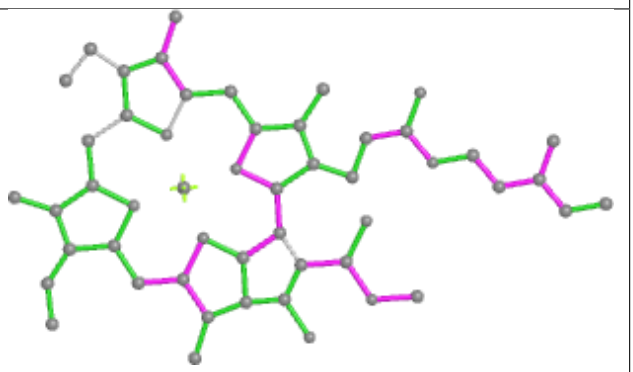
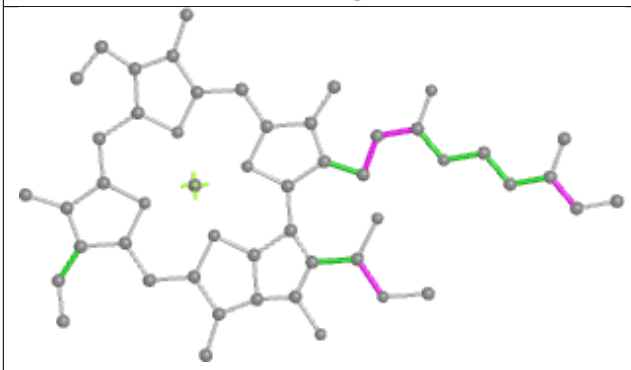
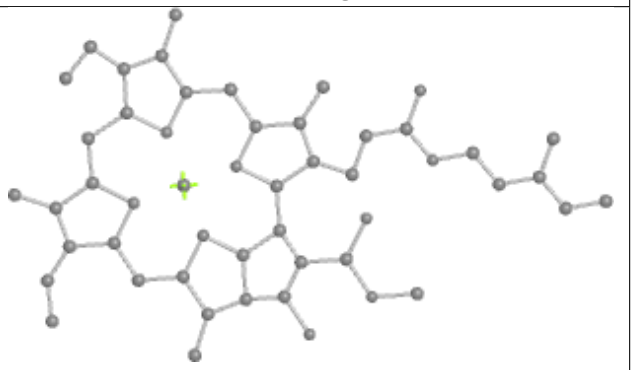


Bond angles

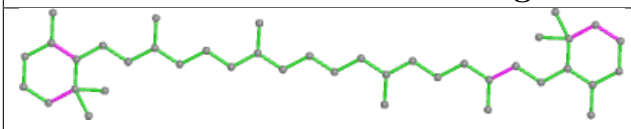


Torsions



Rings

Ligand BCR B 4014



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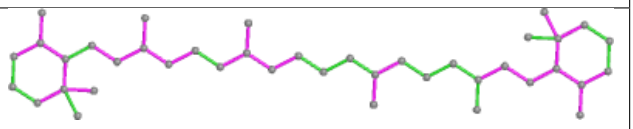
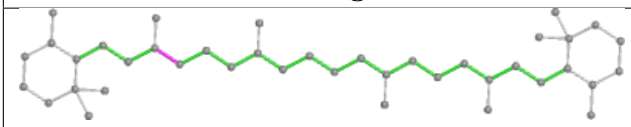


Bond angles



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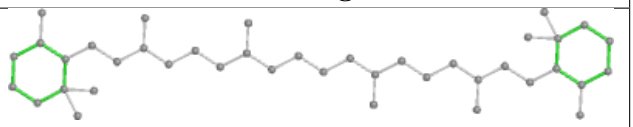
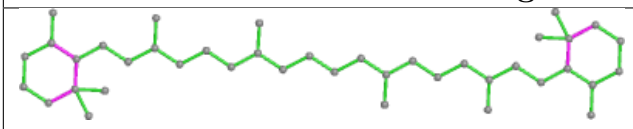


Rings

Ligand BCR J 4015



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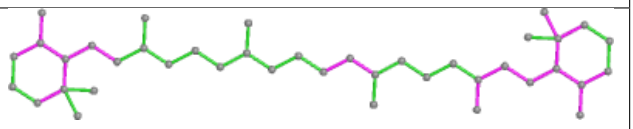
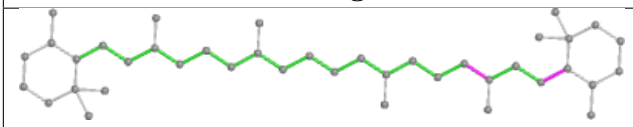


Bond angles



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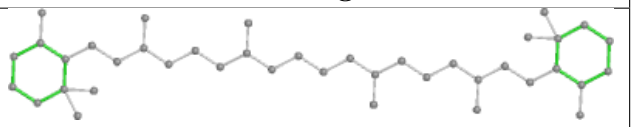
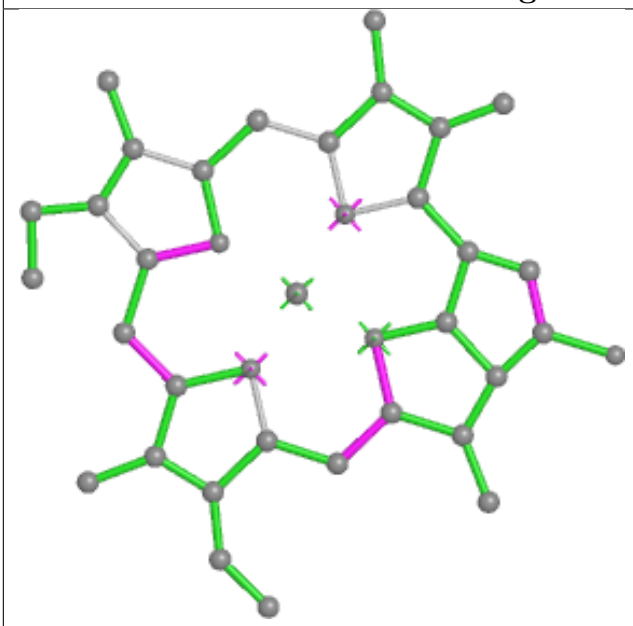


Rings

Ligand CLA J 1303



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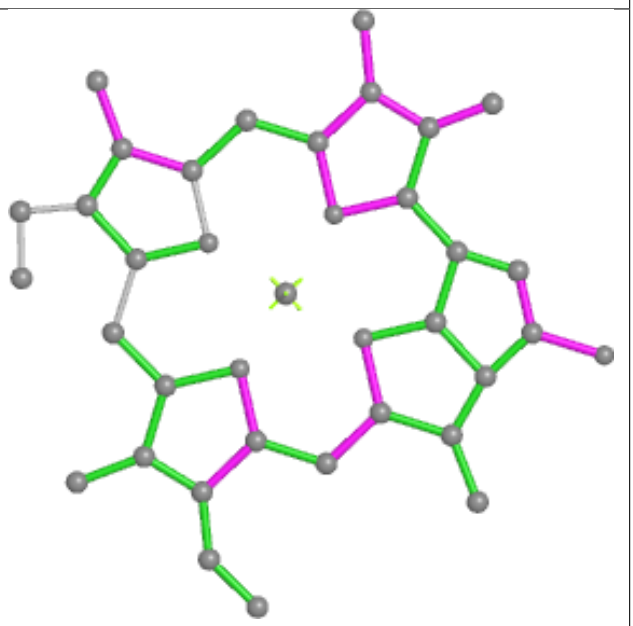
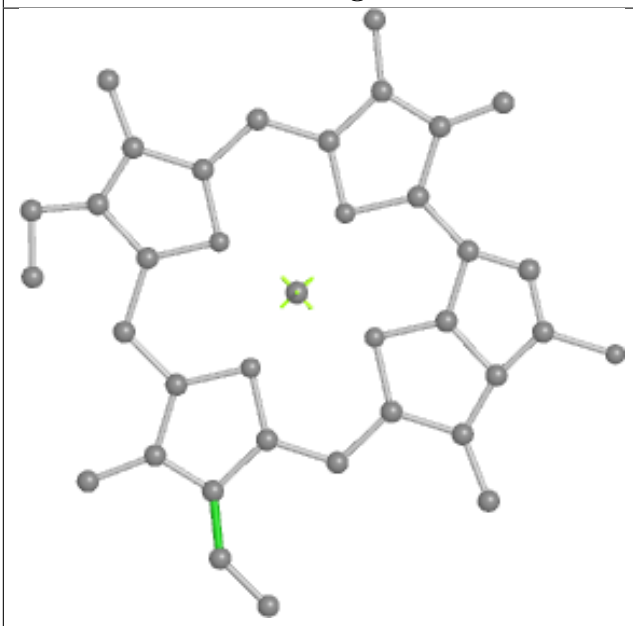


Bond angles



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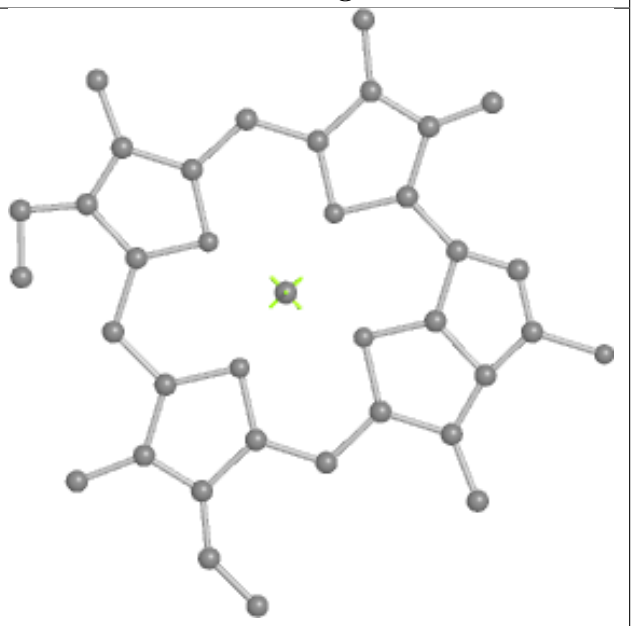
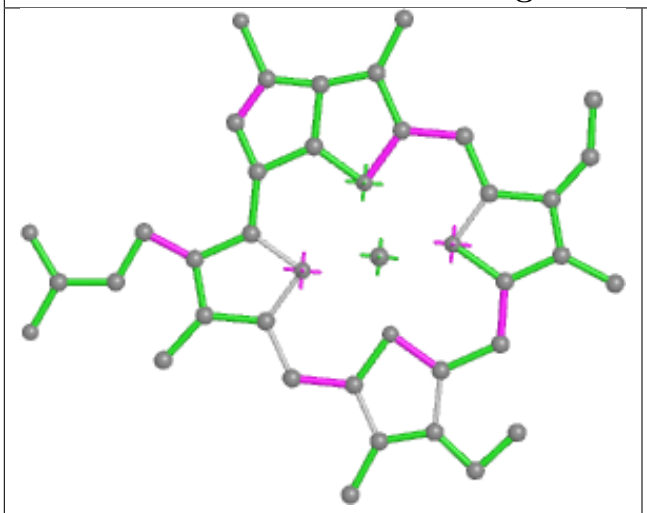


Rings

Ligand CLA A 1402



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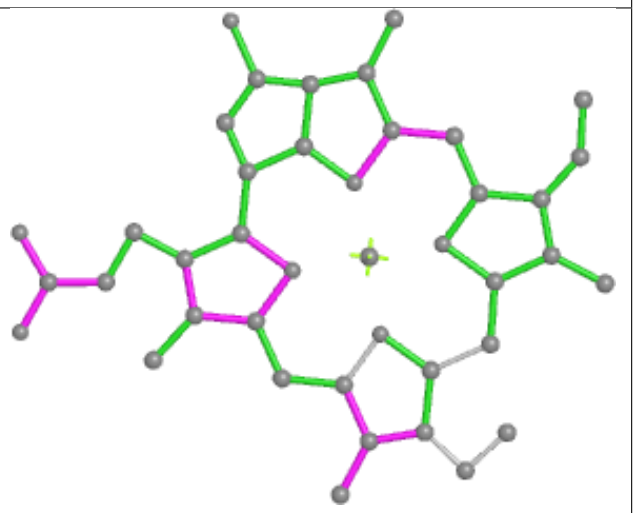

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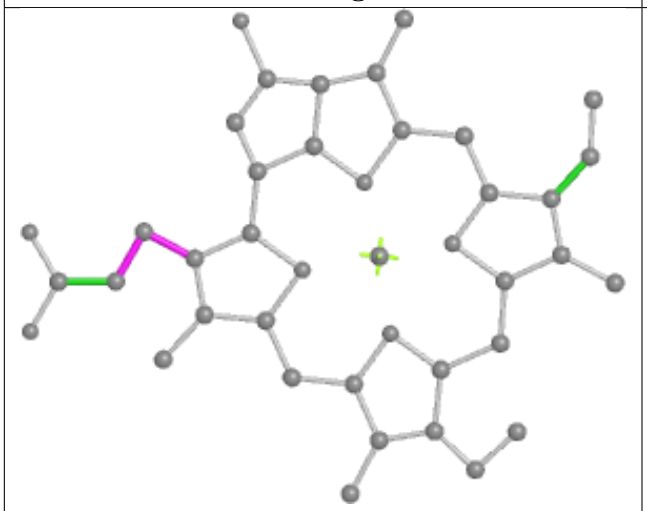

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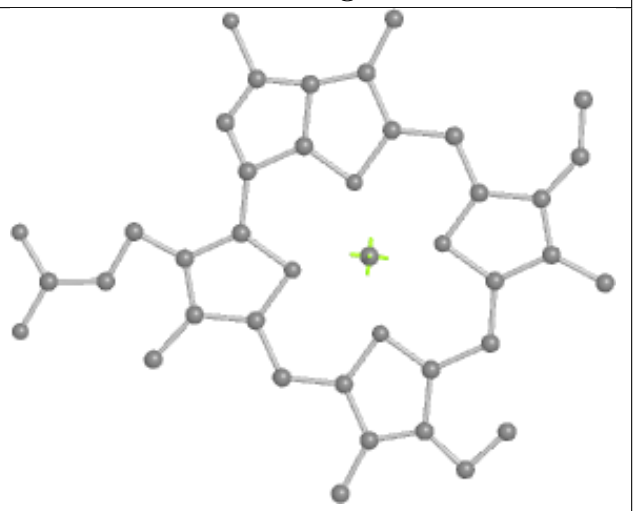
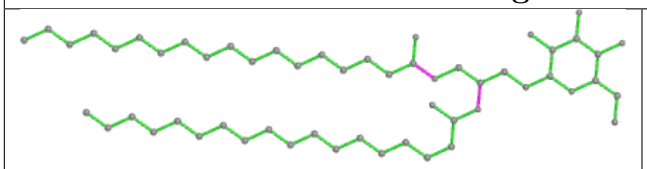


Rings

Ligand LMG B 5002



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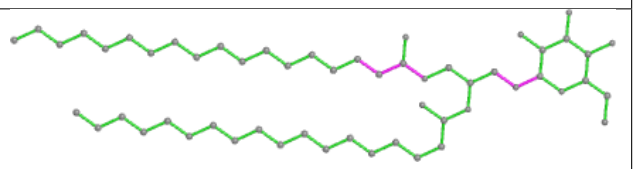
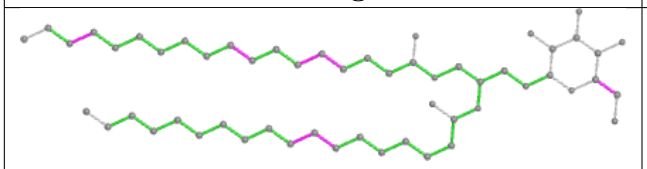


Bond angles



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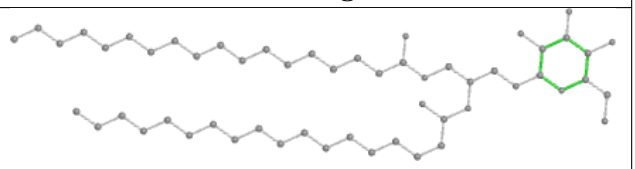
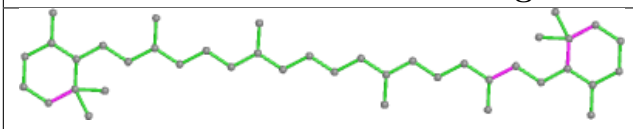


Rings

Ligand BCR F 4016



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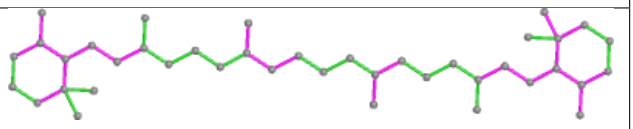
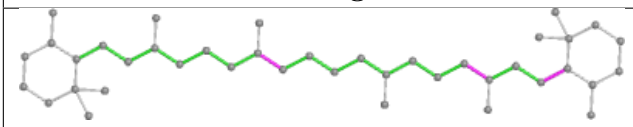
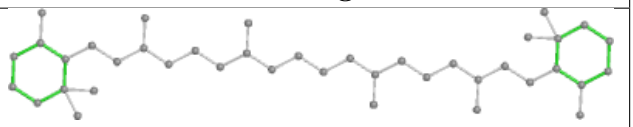


Bond angles

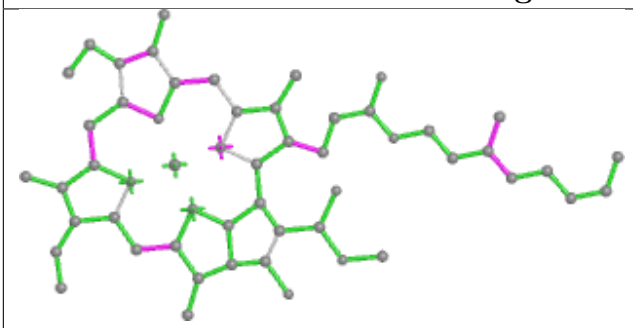


Torsions



Rings

Ligand CLA A 1110



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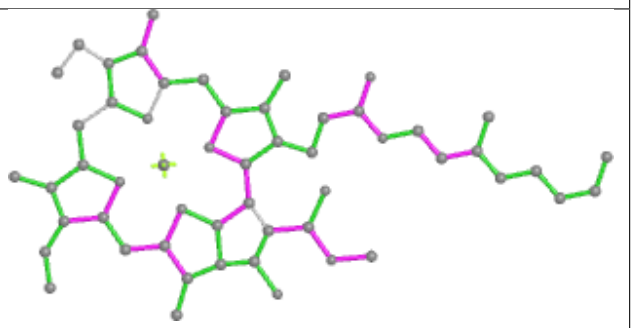
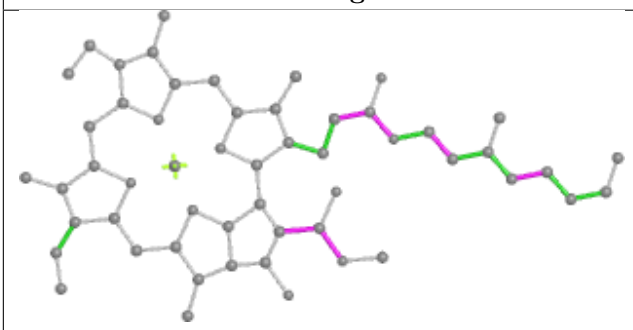


Bond angles



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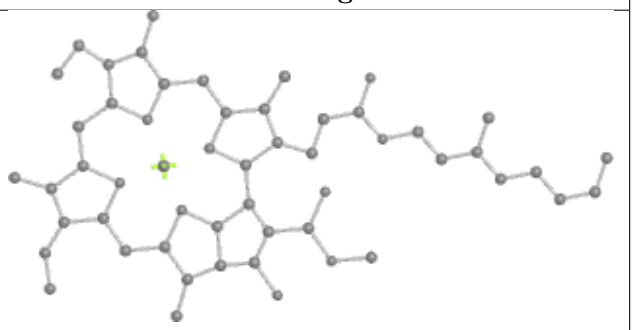
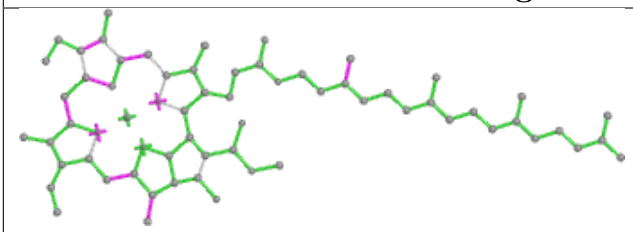


Rings

Ligand CLA B 1023



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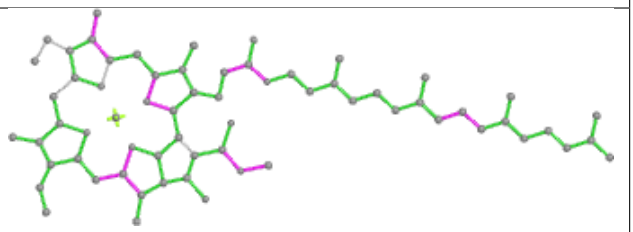
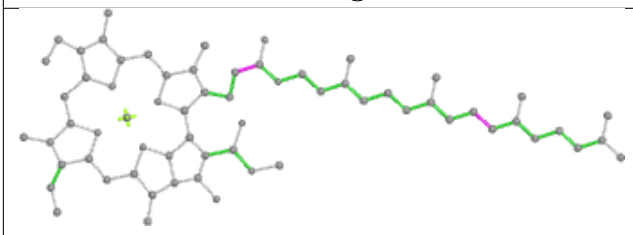


Bond angles



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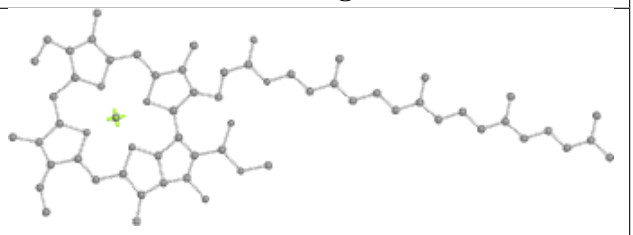
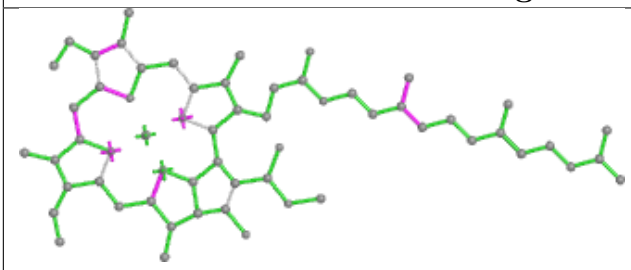


Rings

Ligand CLA B 1234



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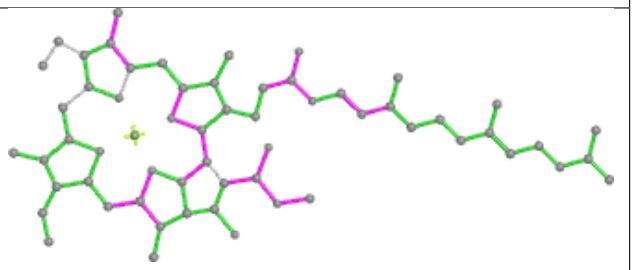
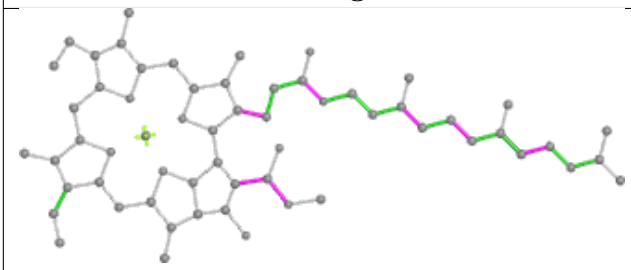


Bond angles



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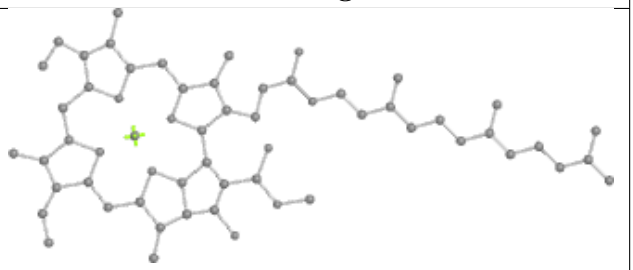
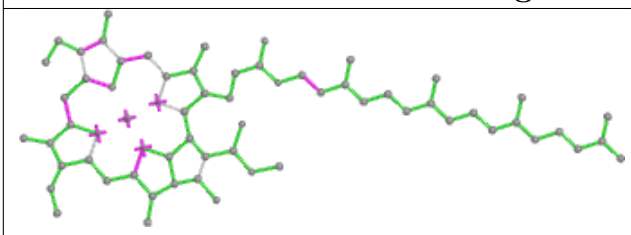
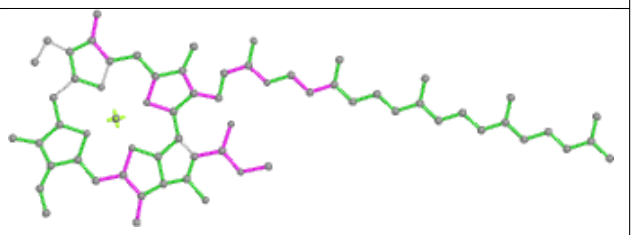


Rings

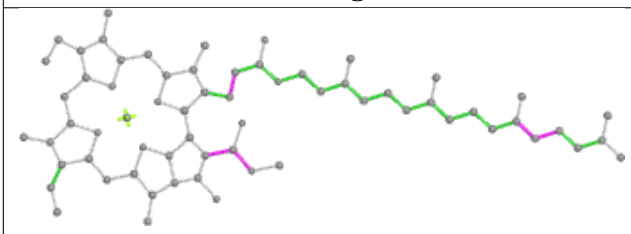
Ligand CLA A 1132



Bond lengths



Bond angles



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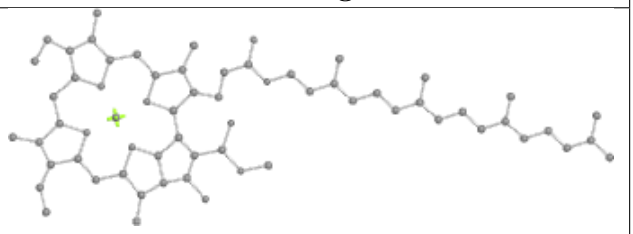
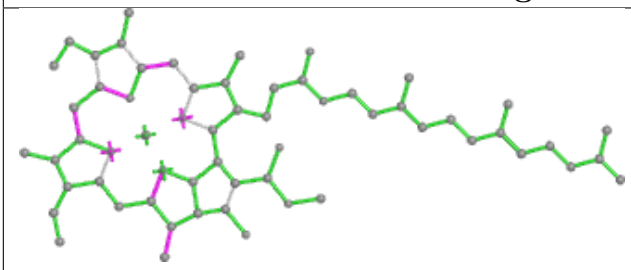
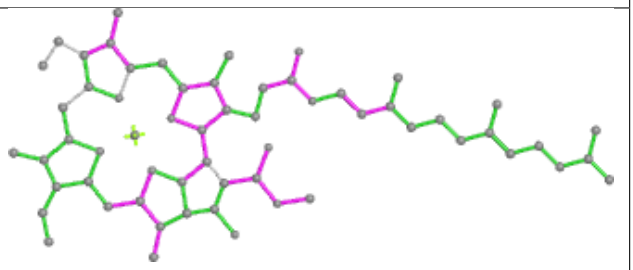
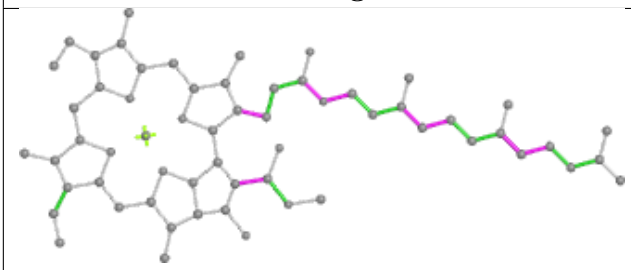
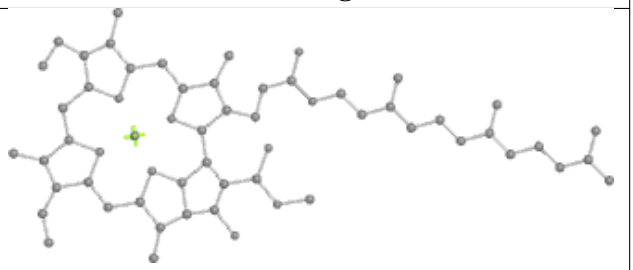


Rings

Ligand CLA A 1111	
 Bond lengths	 Bond angles
 Torsions	 Rings

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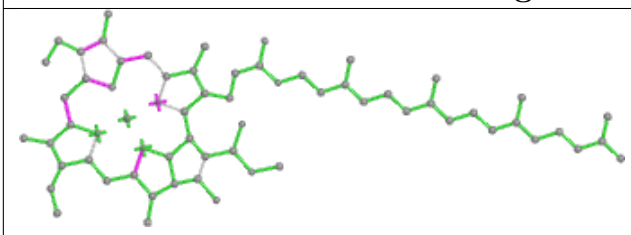
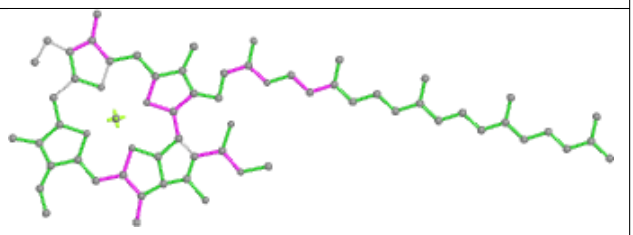
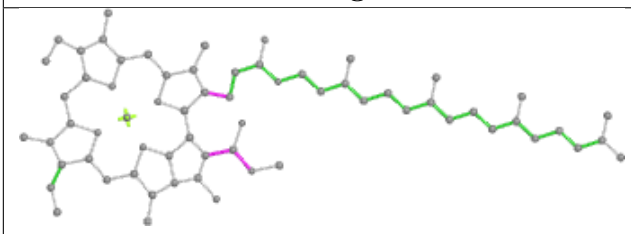
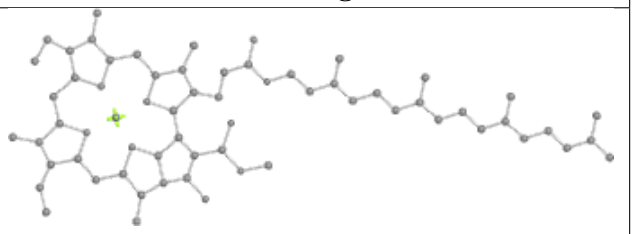
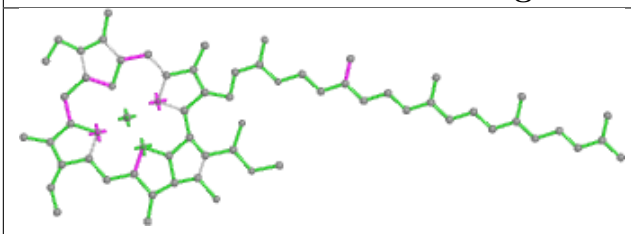
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1126



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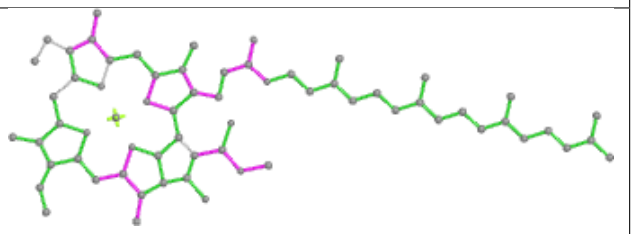

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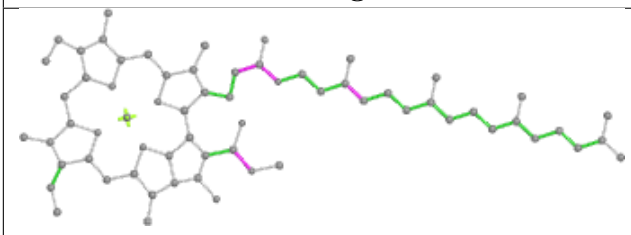
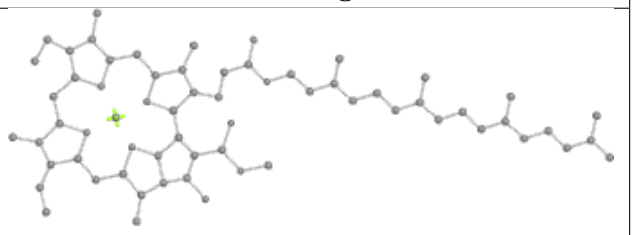
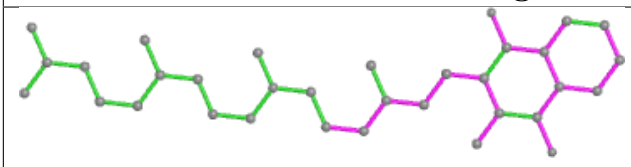


Torsions



Rings

Ligand PQN B 2002



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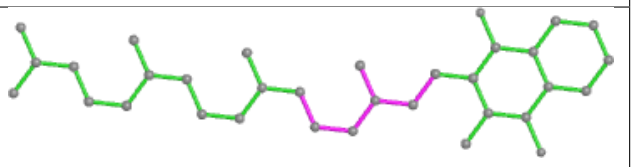

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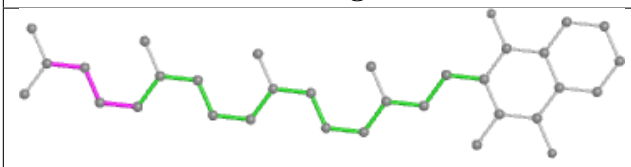

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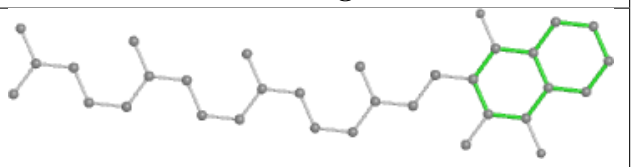
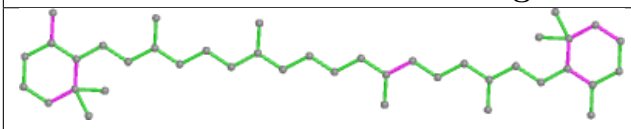


Rings

Ligand BCR A 4008



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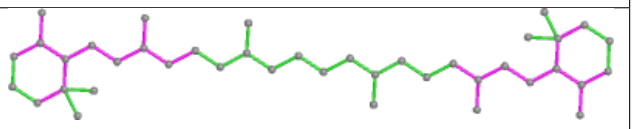

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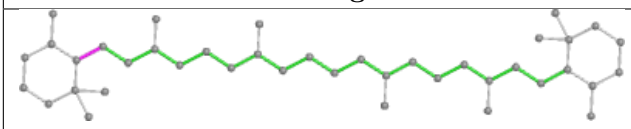

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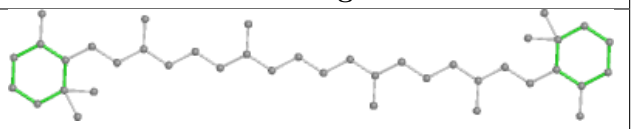
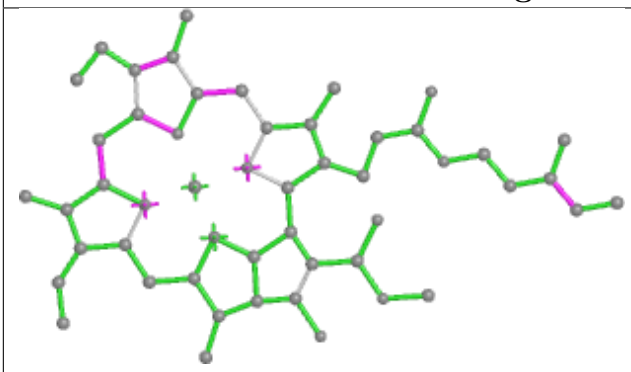


Rings

Ligand CLA A 1139



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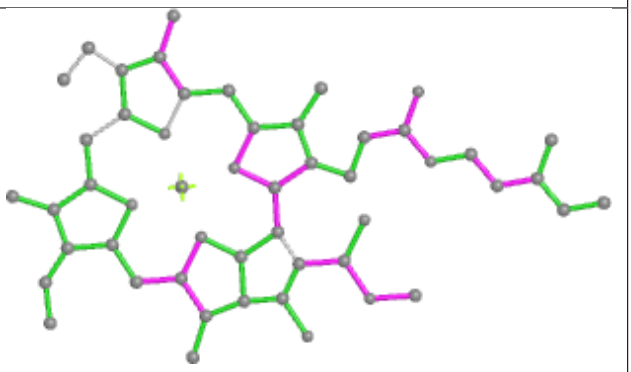

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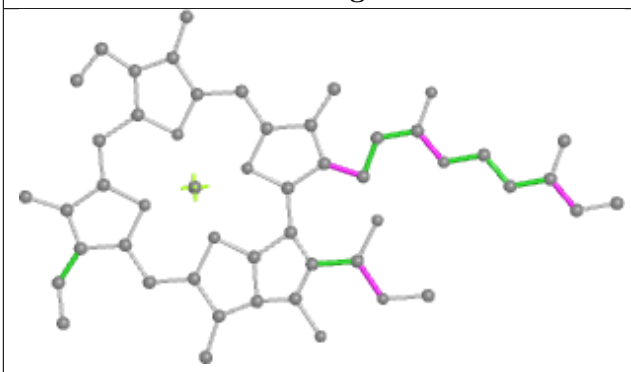

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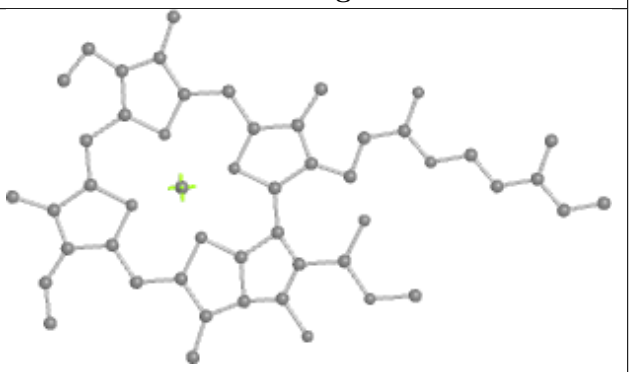
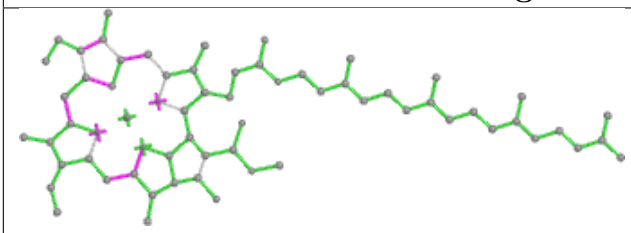


Rings

Ligand CLA B 1235



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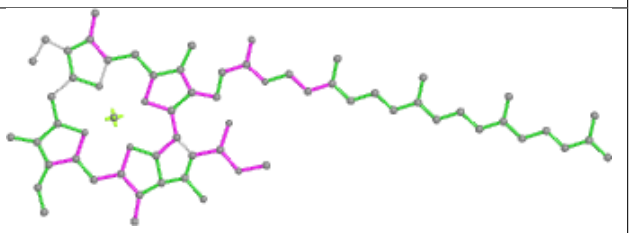

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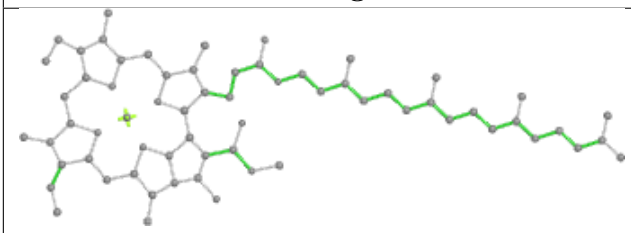

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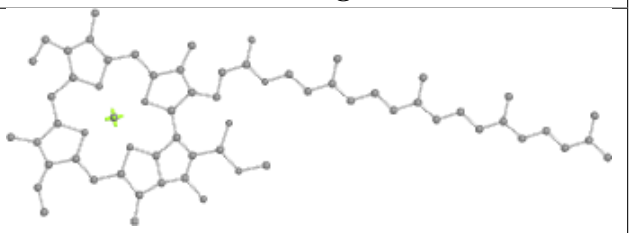
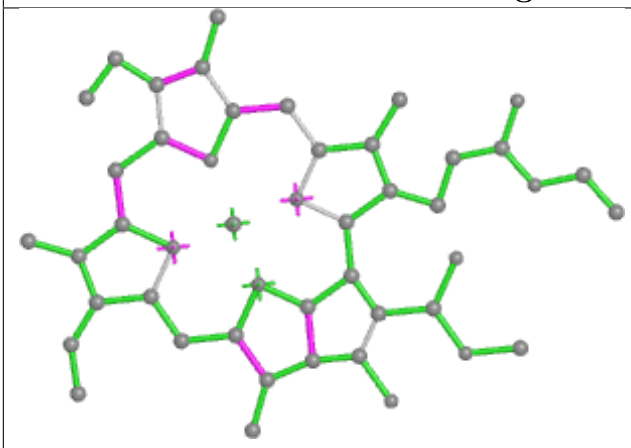


Rings

Ligand CLA B 1236



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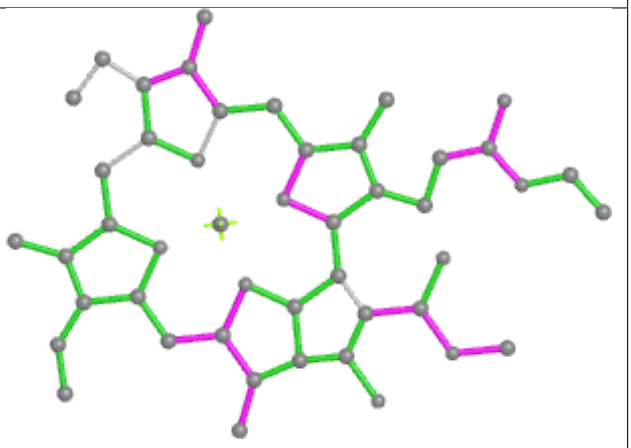

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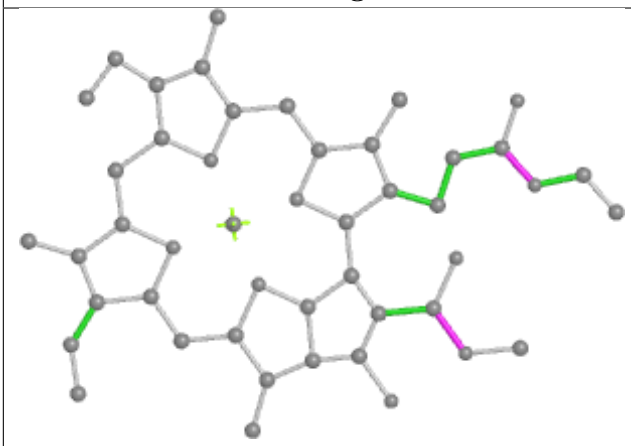

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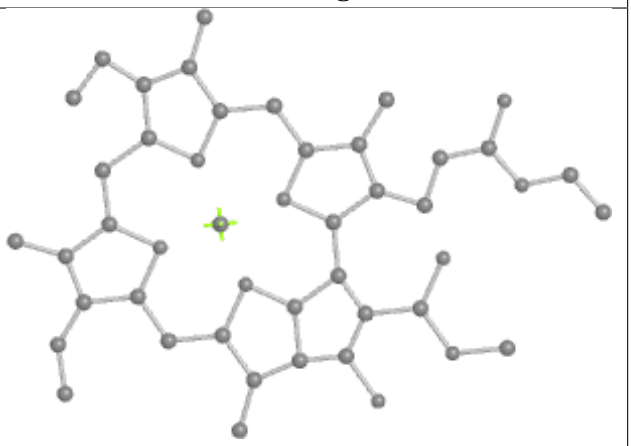
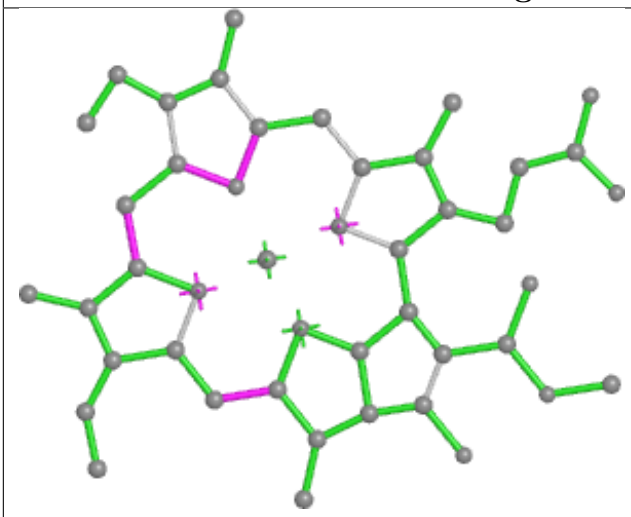


Rings

Ligand CLA A 1113



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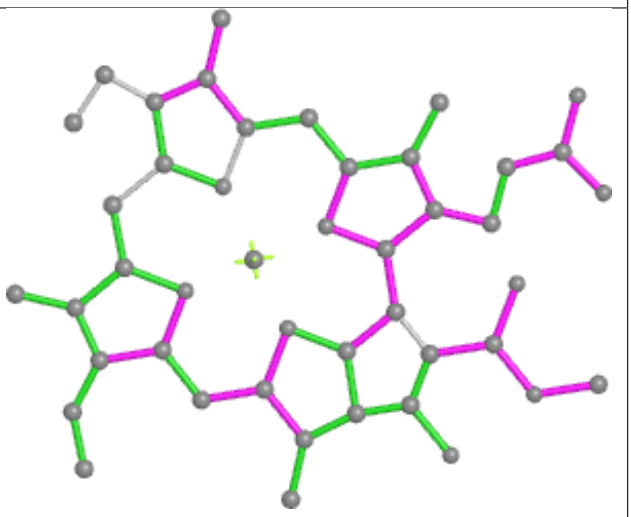

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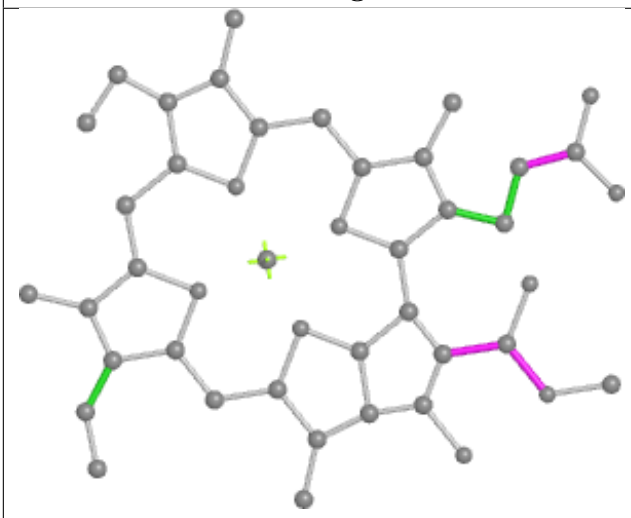

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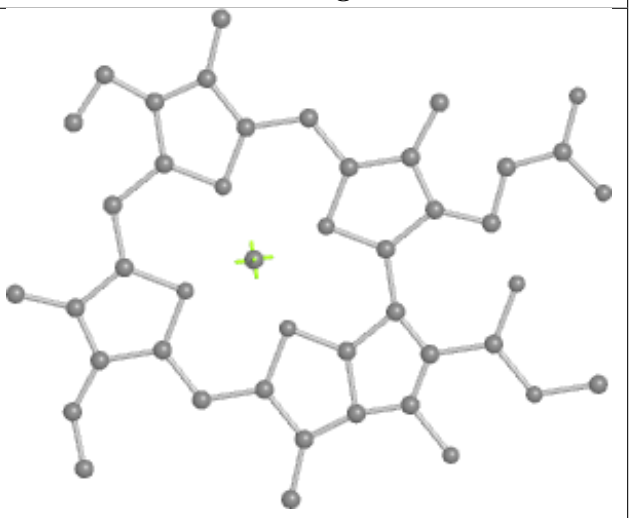
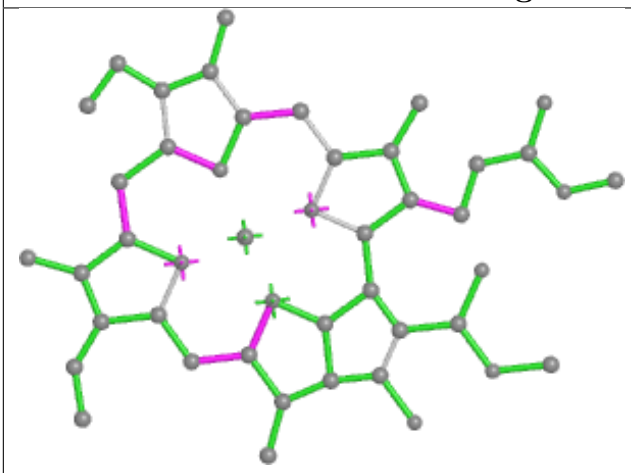


Rings

Ligand CLA B 1222



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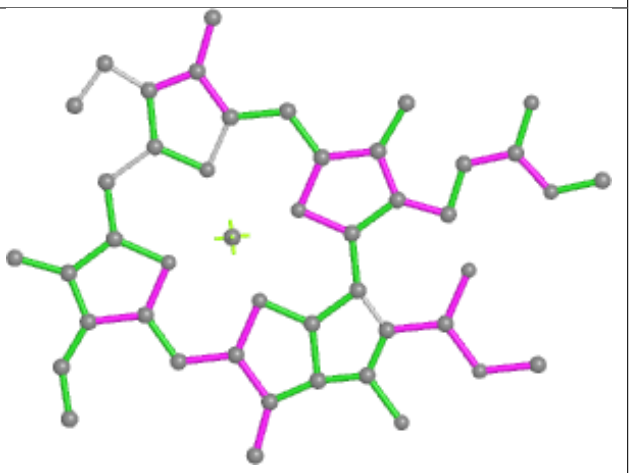

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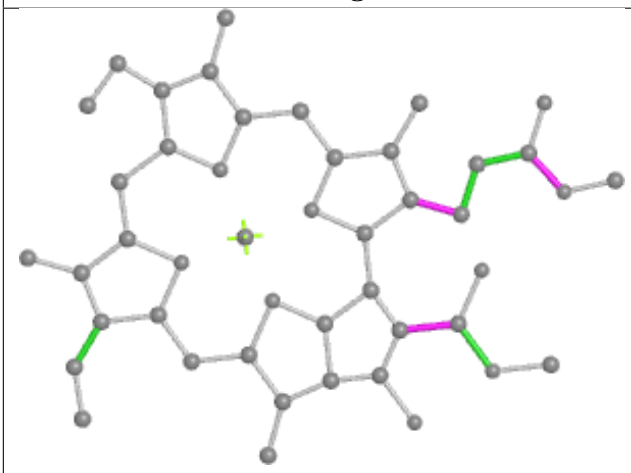

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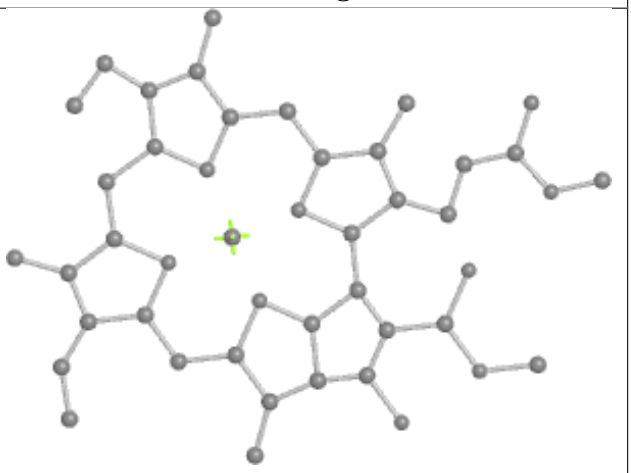
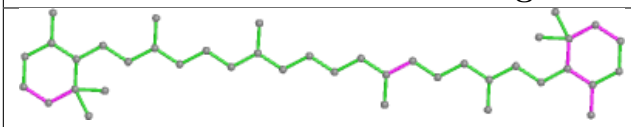


Rings

Ligand BCR L 4019



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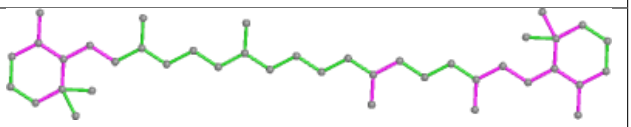
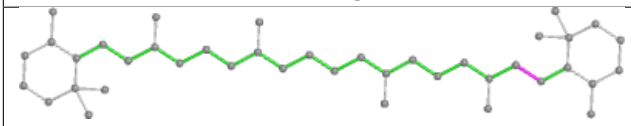


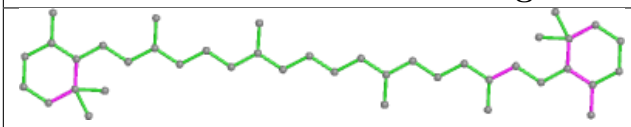
Bond angles



Torsions

Rings

Ligand BCR L 4022



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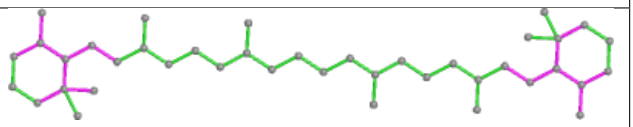
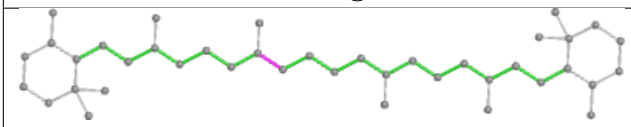
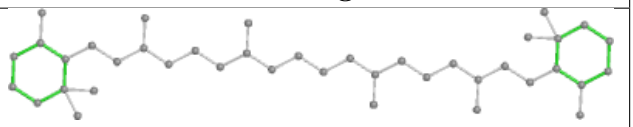


Bond angles

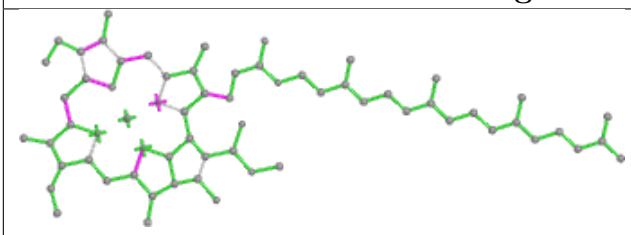


Torsions



Rings

Ligand CLA A 1106



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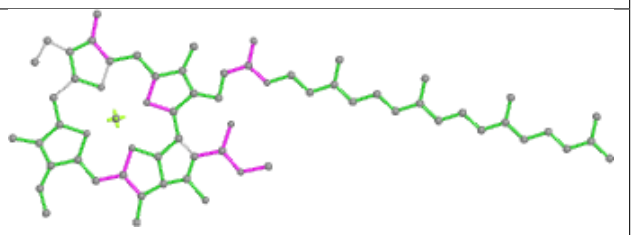
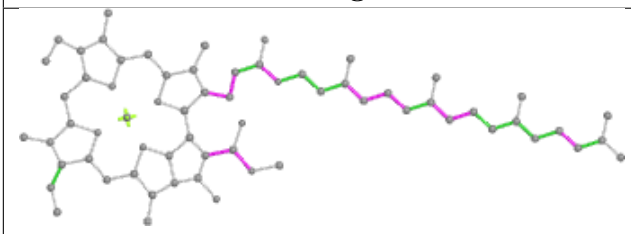


Bond angles



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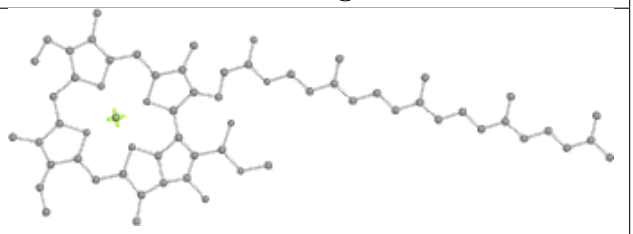
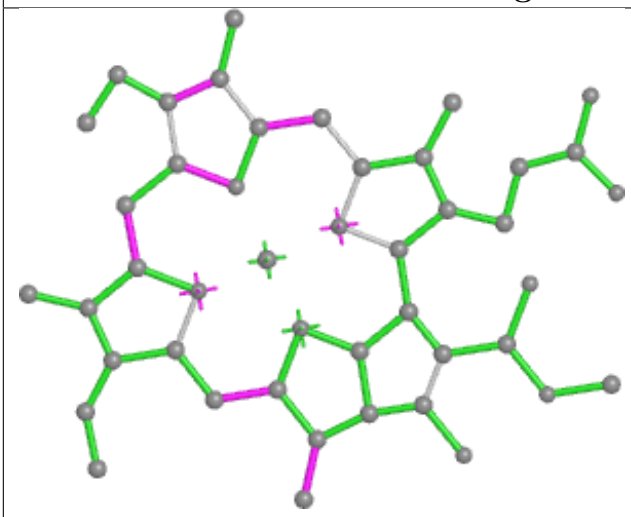


Rings

Ligand CLA K 1401



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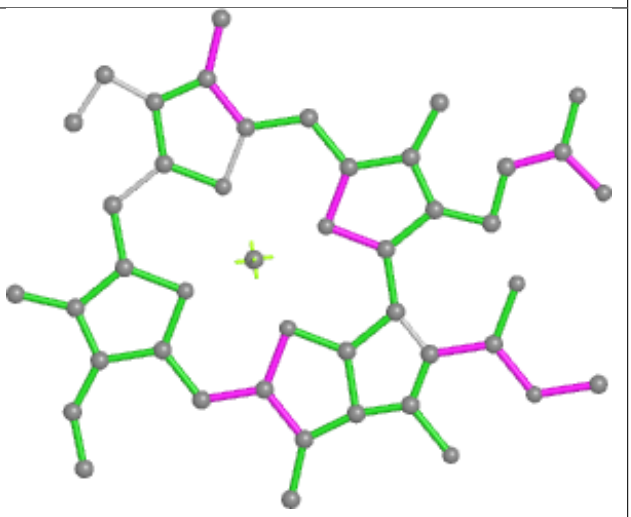
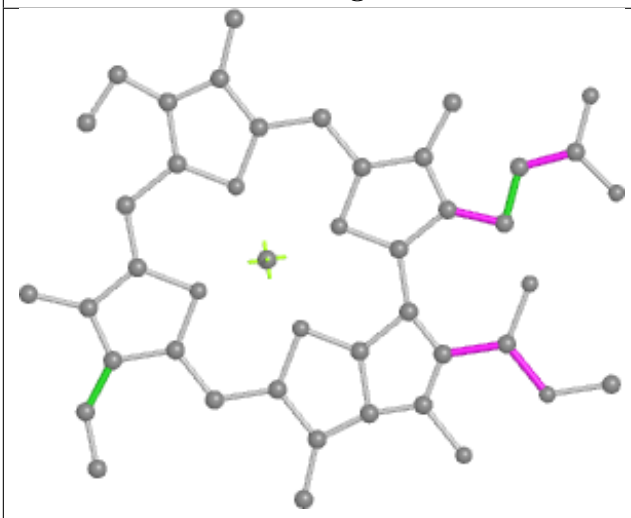
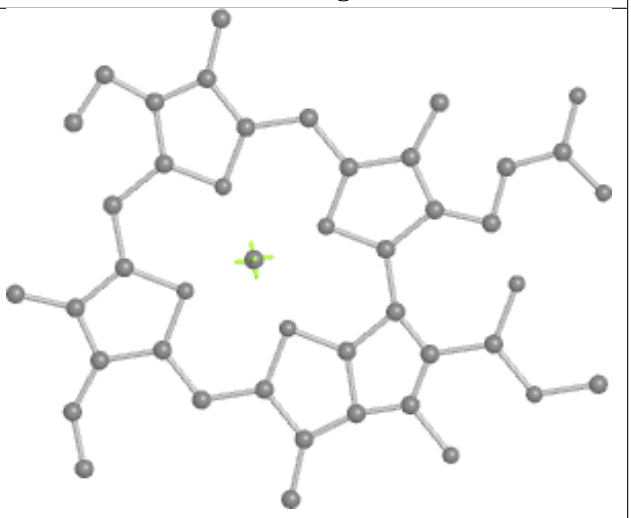


Bond angles

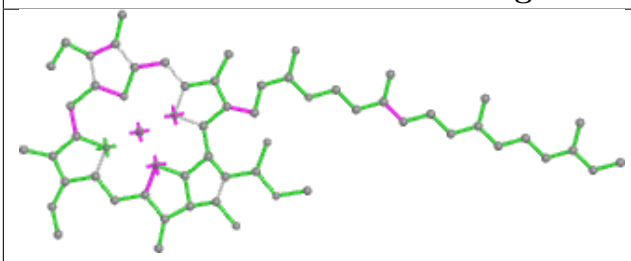


Torsions

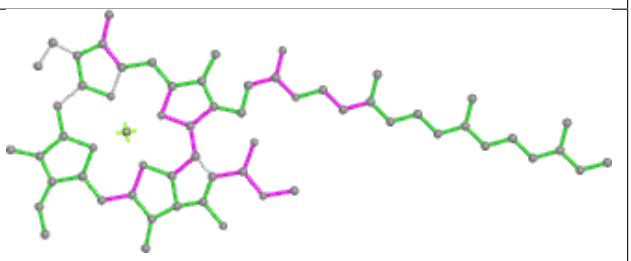


Rings

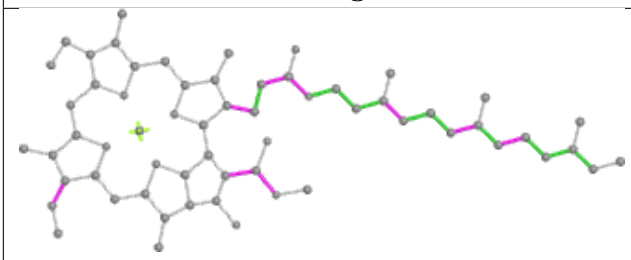
Ligand CLA A 1118



Bond lengths



Bond angles



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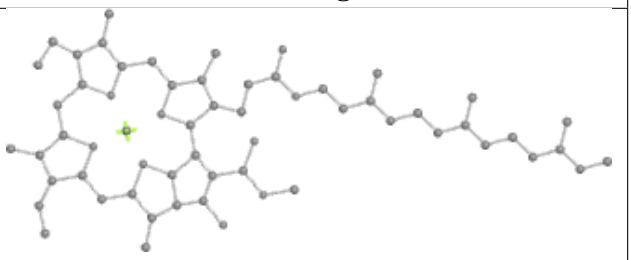
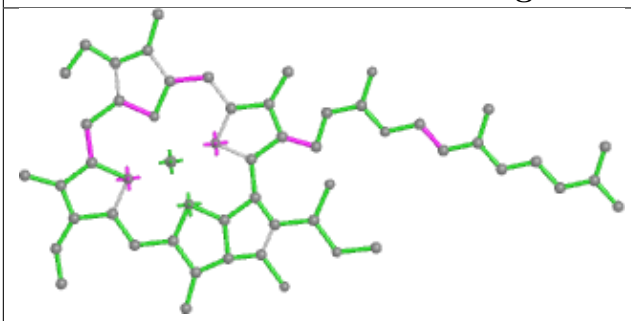
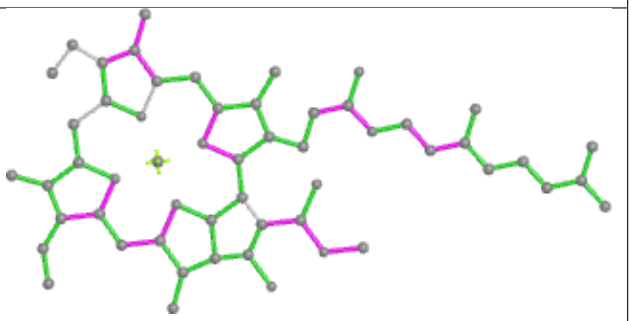


Rings

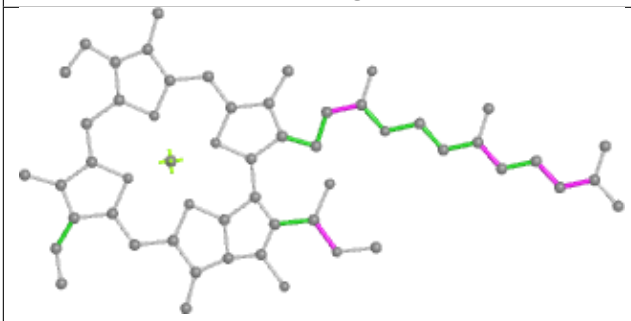
Ligand CLA B 1219



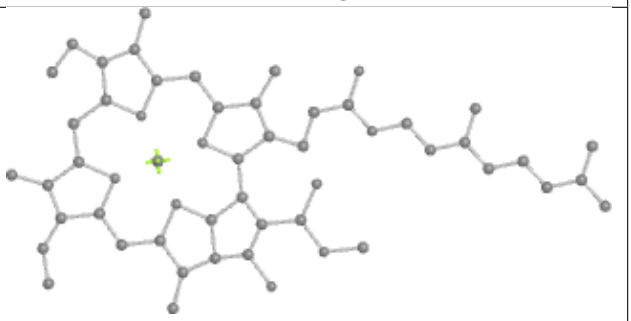
Bond lengths



Bond angles

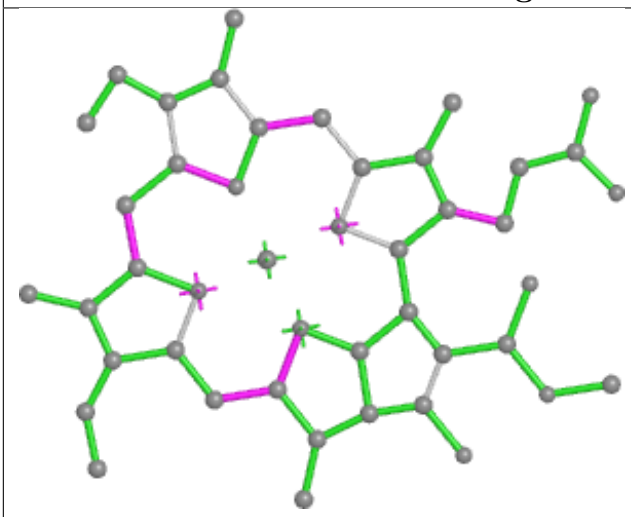


Torsions

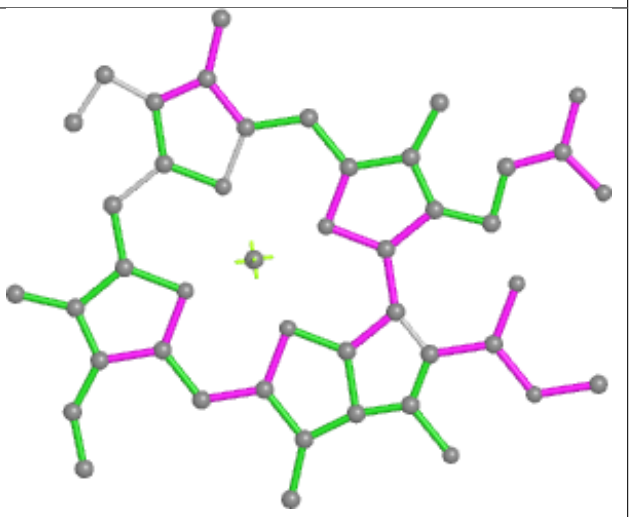


Rings

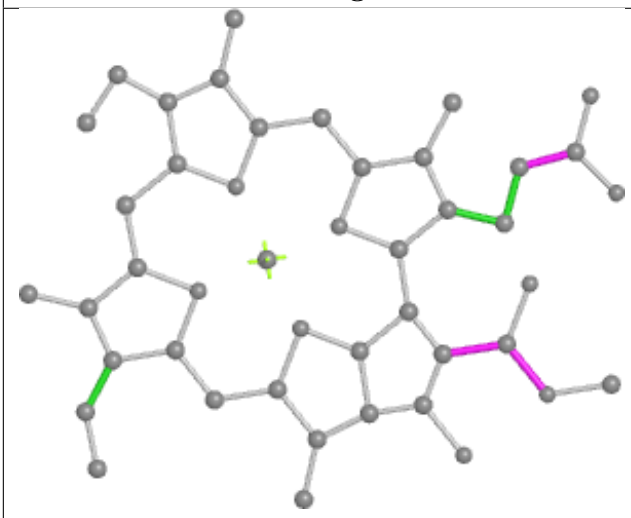
Ligand CLA B 1218



Bond lengths



Bond angles



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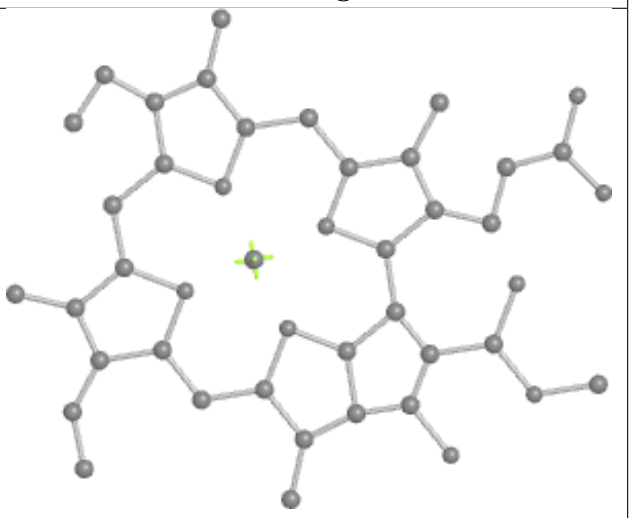
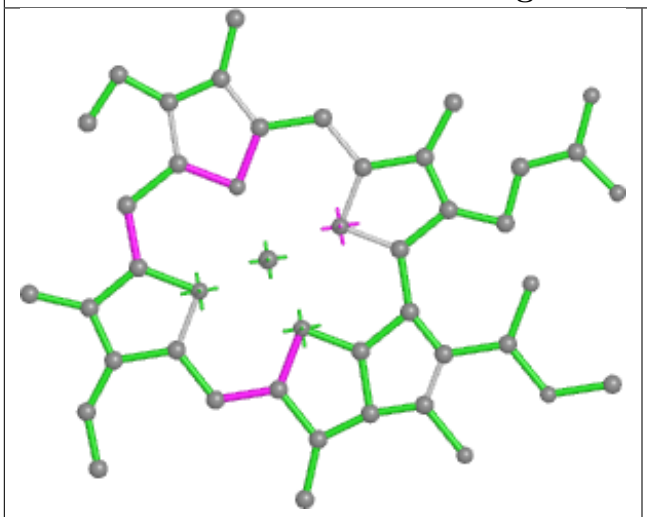


Rings

Ligand CLA B 1209



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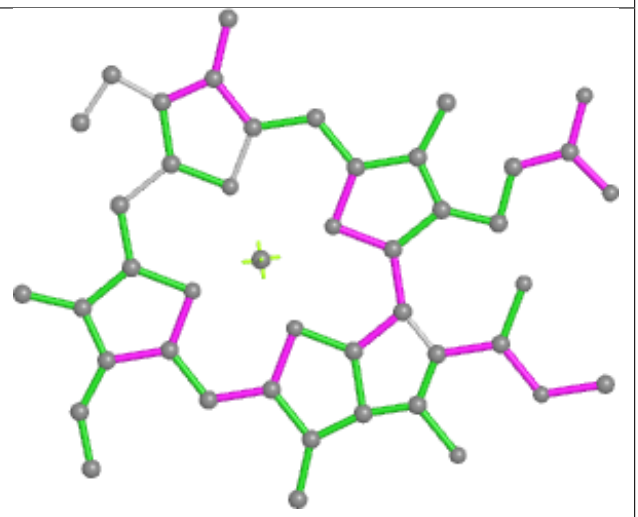
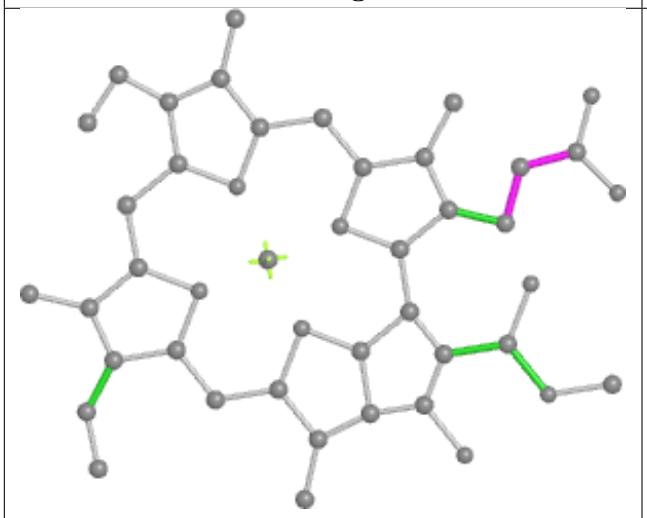
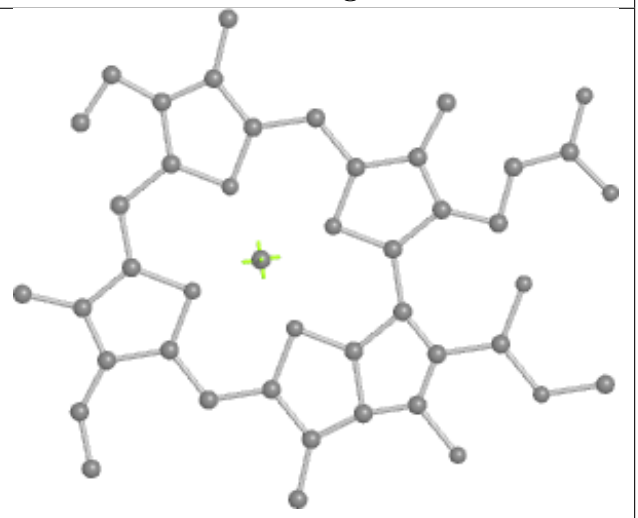


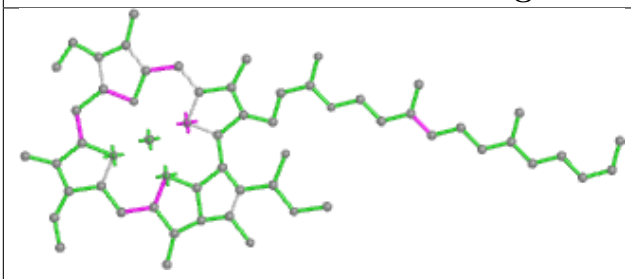
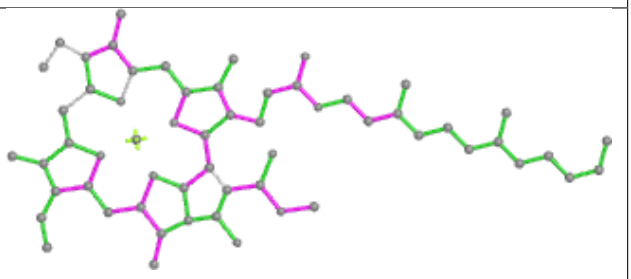
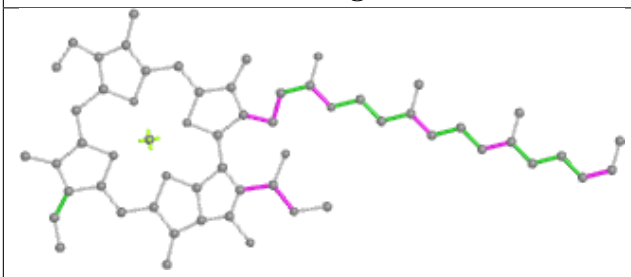
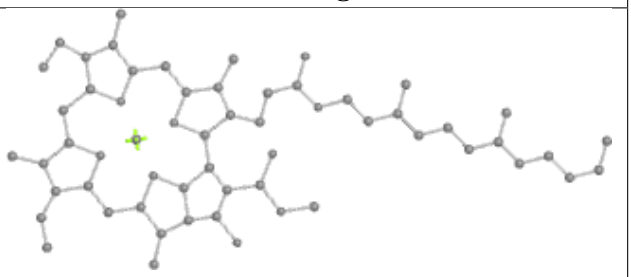
Bond angles



Torsions



Rings

Ligand CLA A 1122	
 Bond lengths	 Bond angles
 Torsions	 Rings

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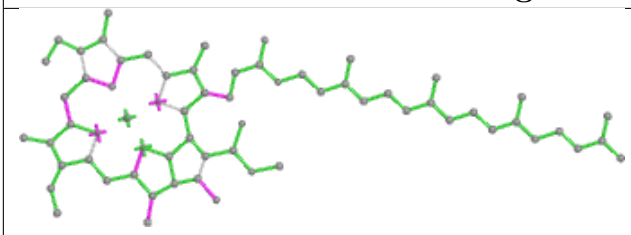
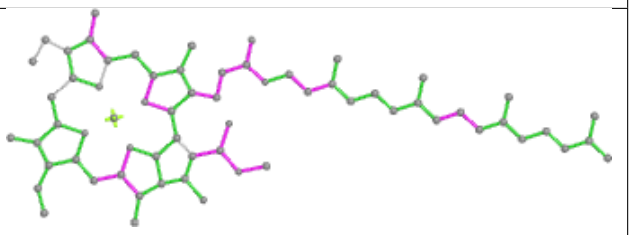
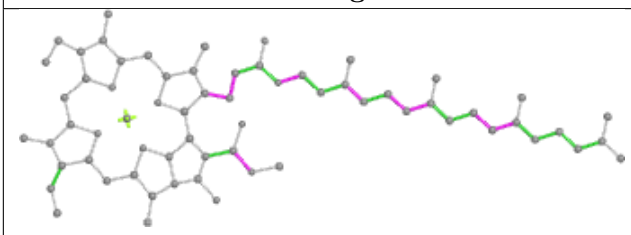
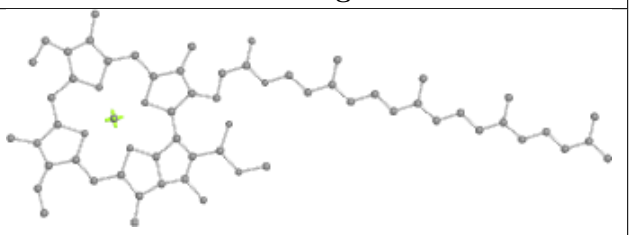
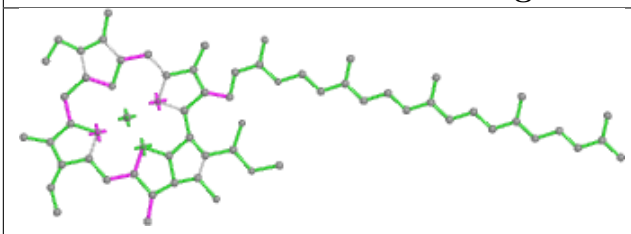
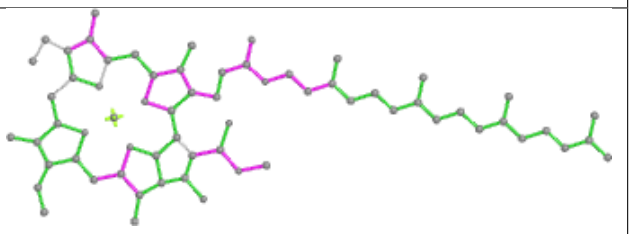
 Bond lengths	 Bond angles
 Torsions	 Rings

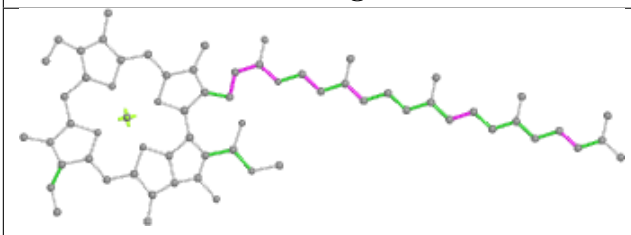
Ligand CLA A 1013



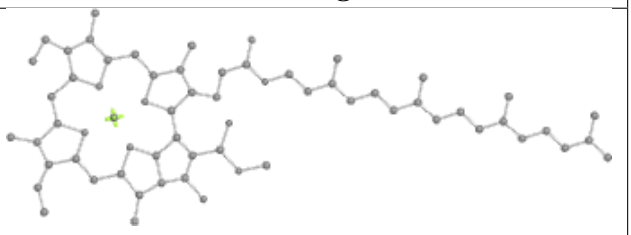
Bond lengths



Bond angles

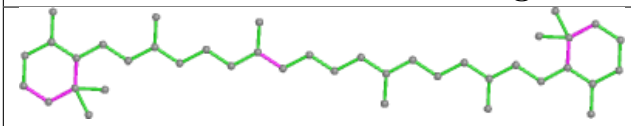


Torsions



Rings

Ligand BCR A 4007



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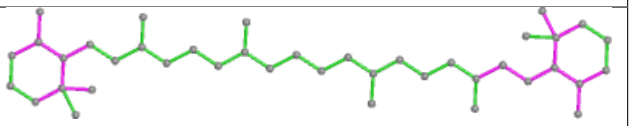
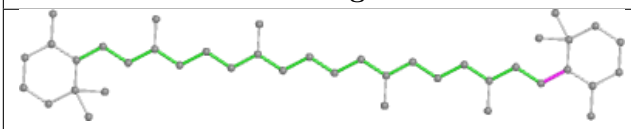


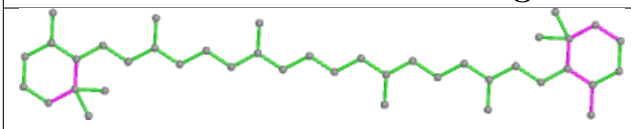
Bond angles



Torsions

Rings

Ligand BCR B 4005



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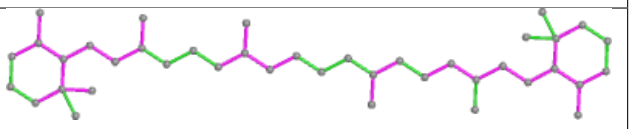
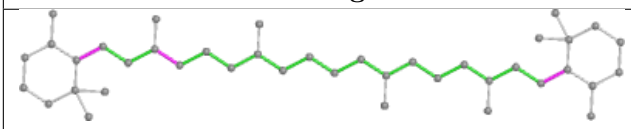


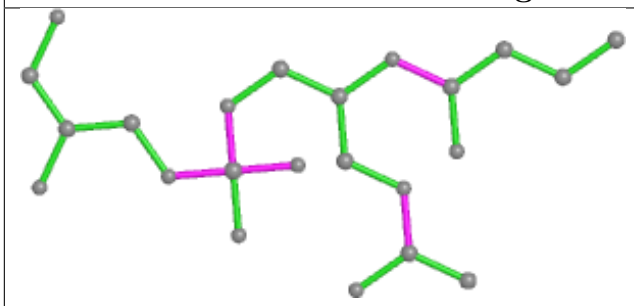
Bond angles



Torsions

Rings

Ligand LHG B 5004



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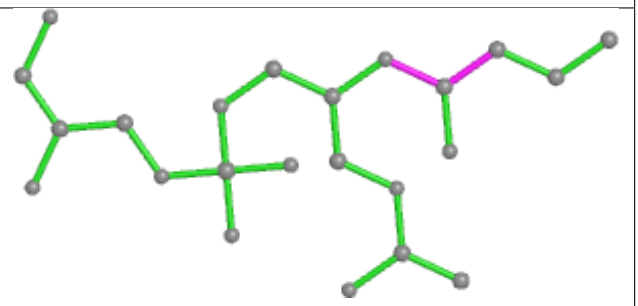
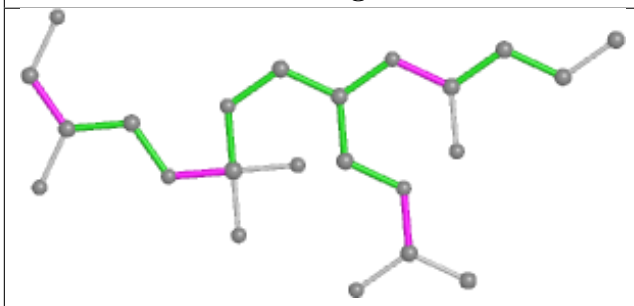
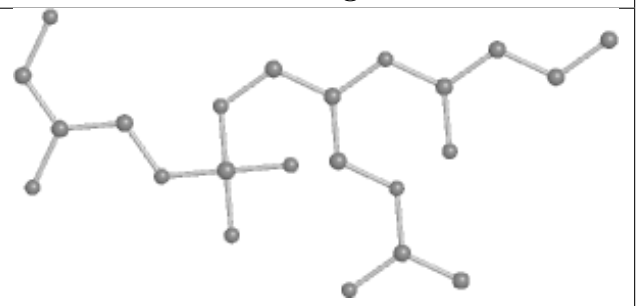


Bond angles

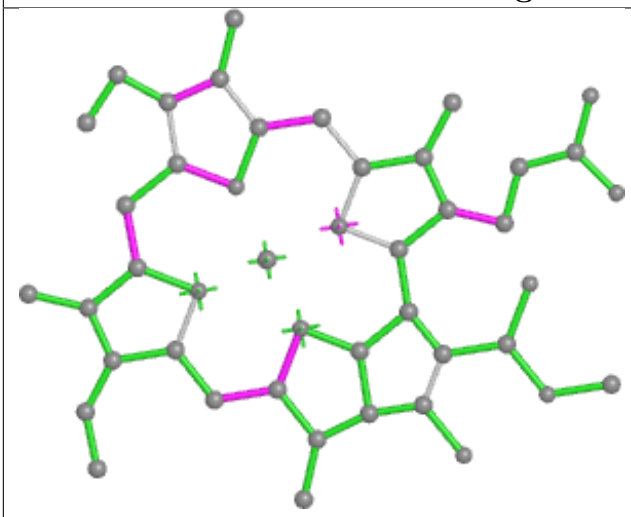


Torsions



Rings

Ligand CLA B 1227



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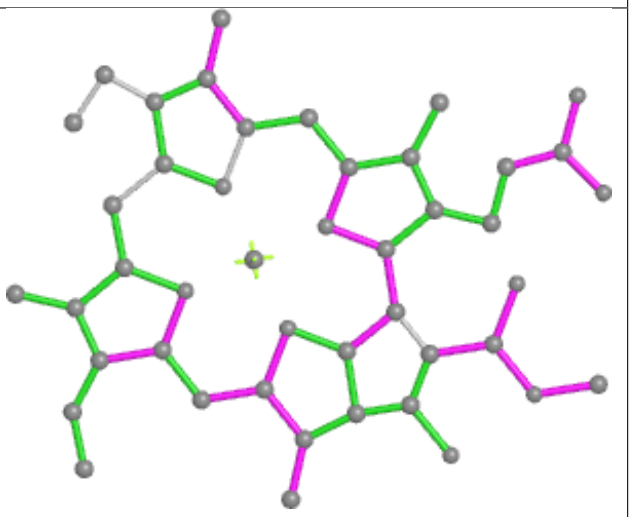
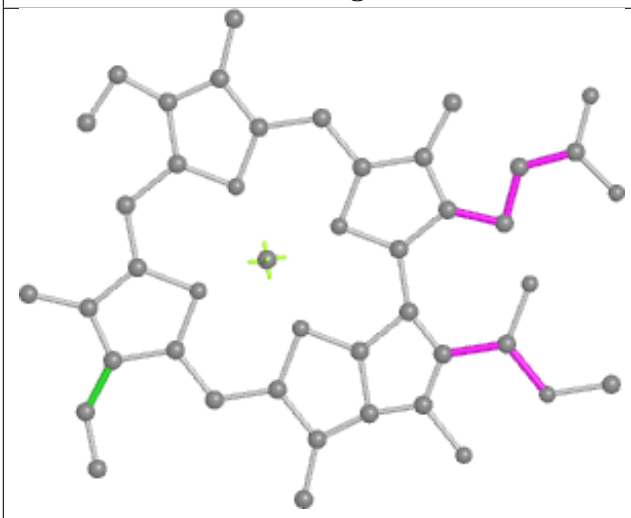
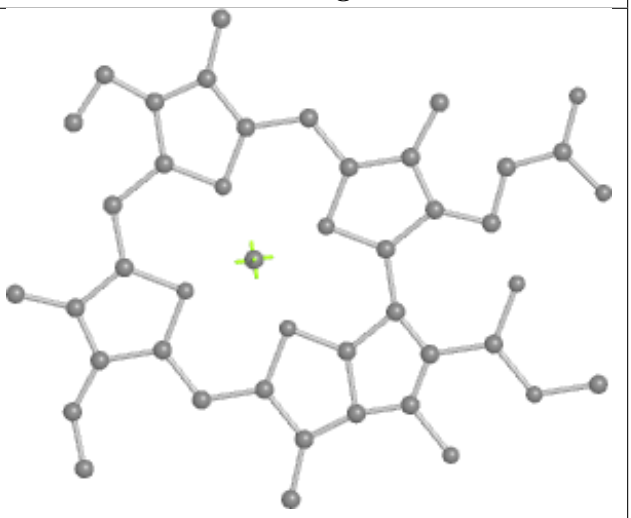


Bond angles

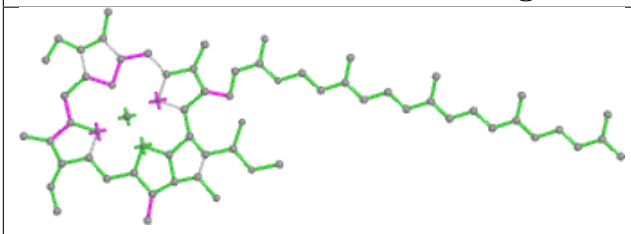


Torsions



Rings

Ligand CLA L 1501



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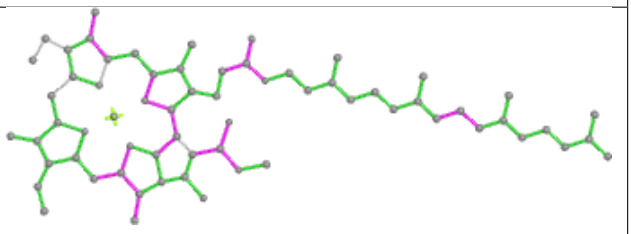
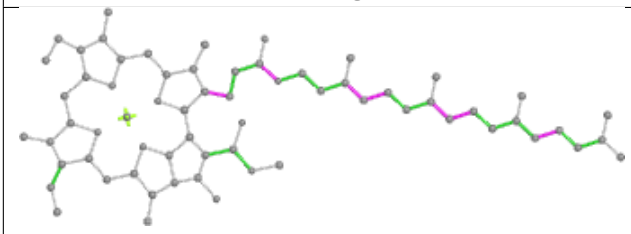
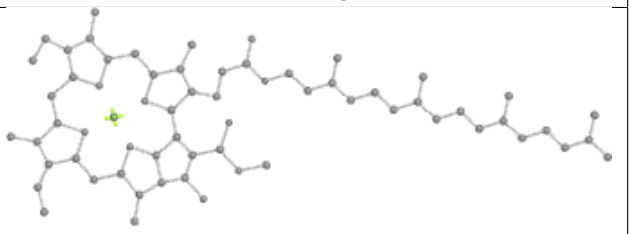


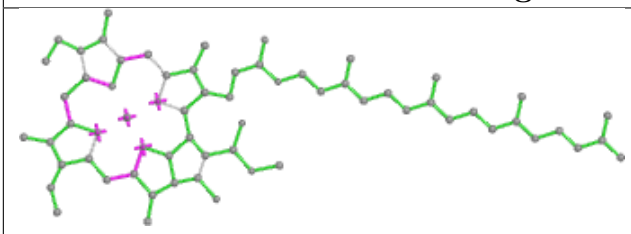
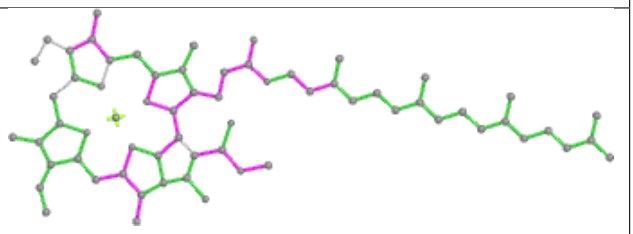
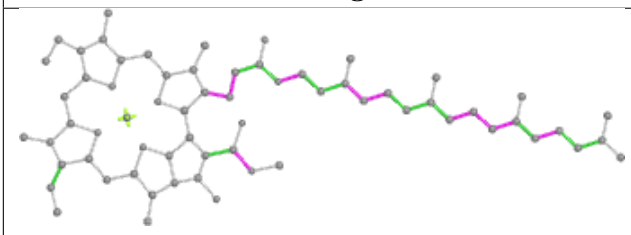
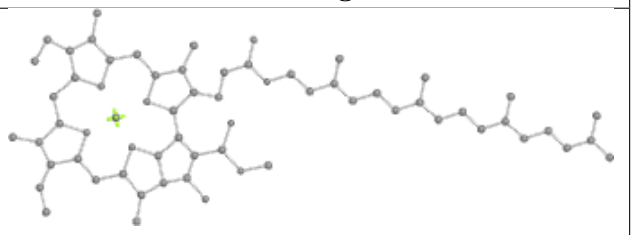
Bond angles



Torsions



Rings

Ligand CLA A 1107	
 Bond lengths	 Bond angles
 Torsions	 Rings

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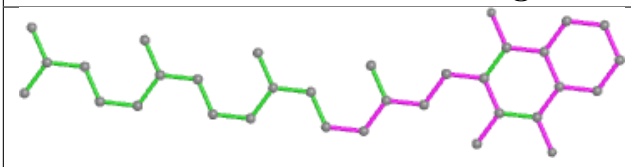
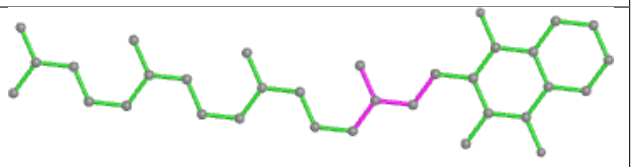
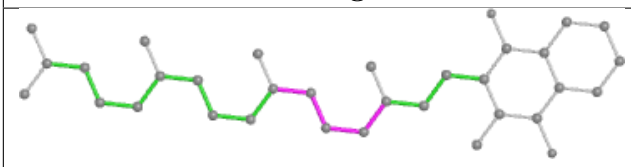
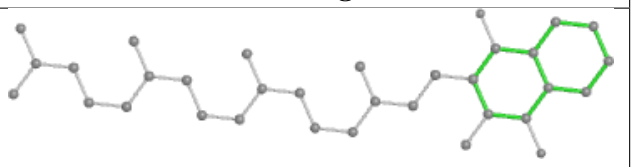
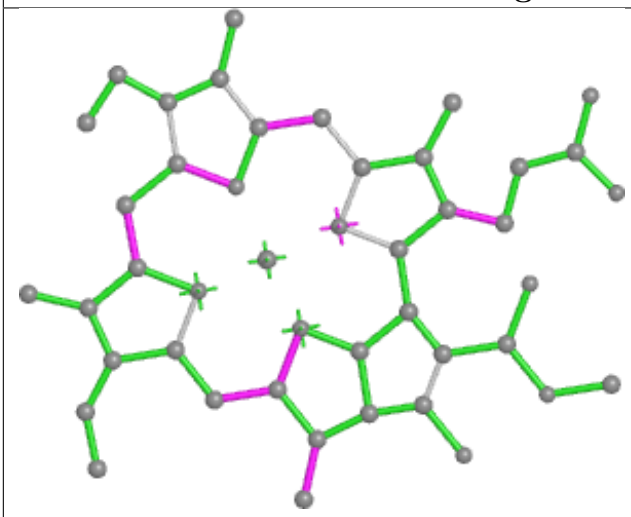
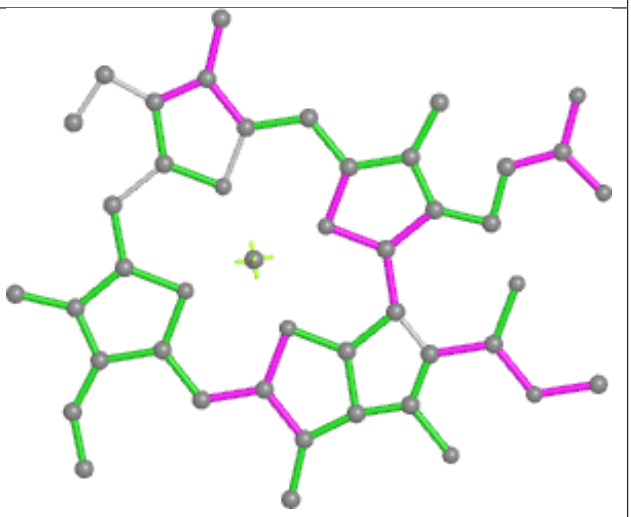
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1134



Bond lengths



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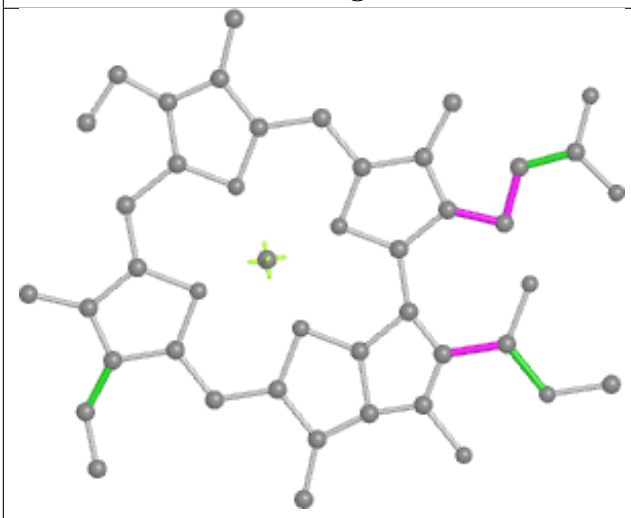
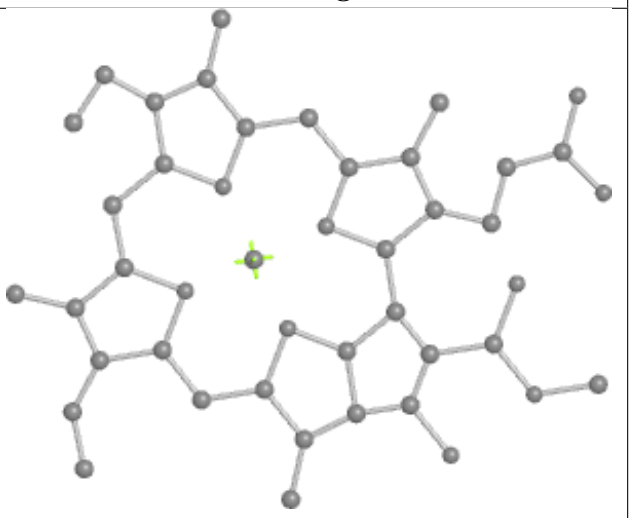
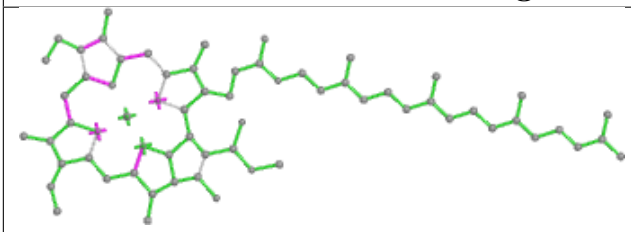


Torsions



Rings

Ligand CLA B 1229



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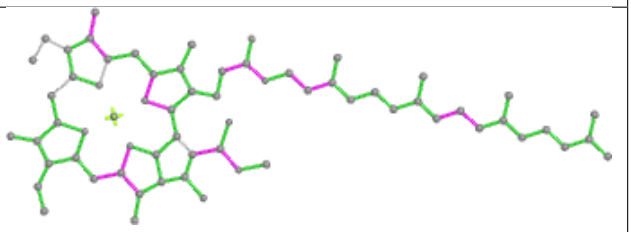

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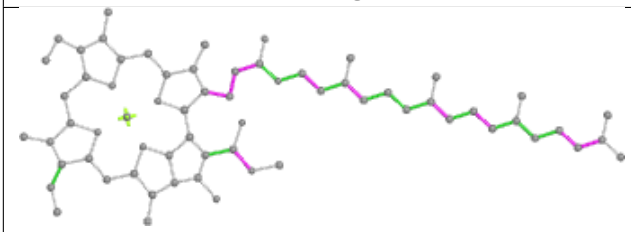
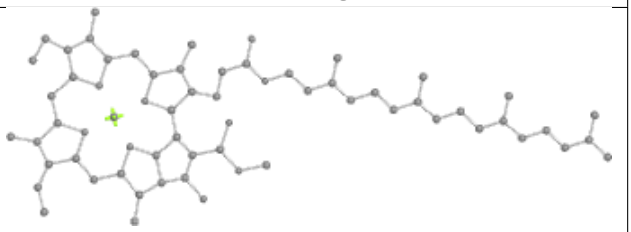
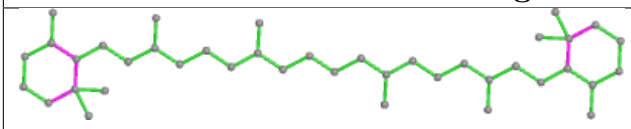
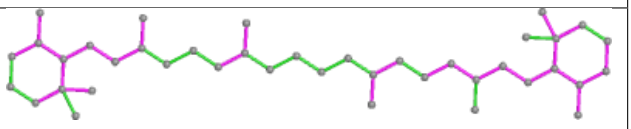
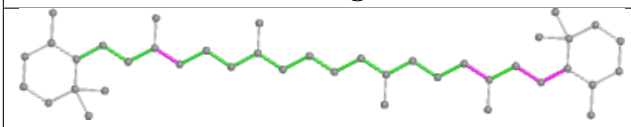
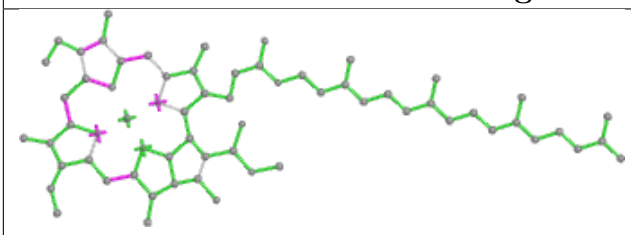
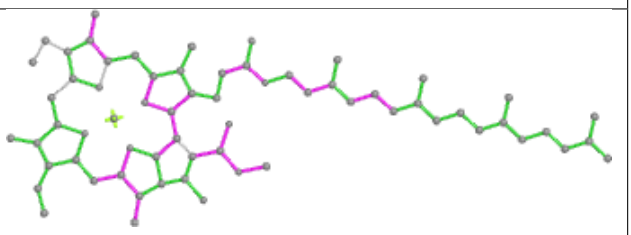
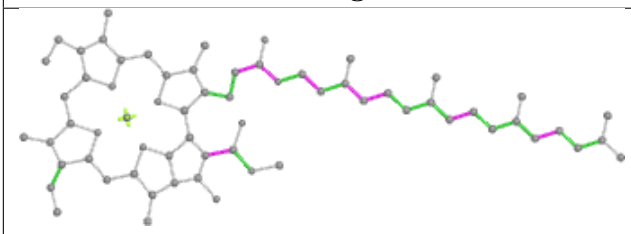
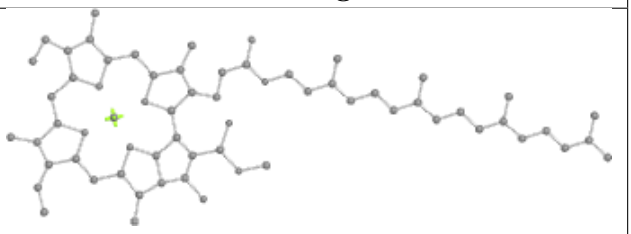


Torsions

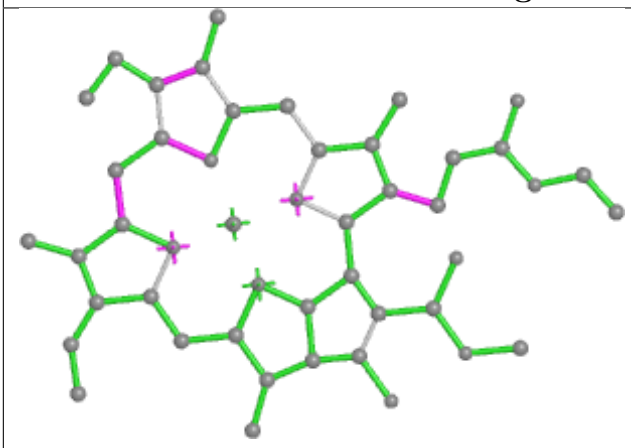


Rings

Ligand BCR B 4006	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA A 1123	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1137



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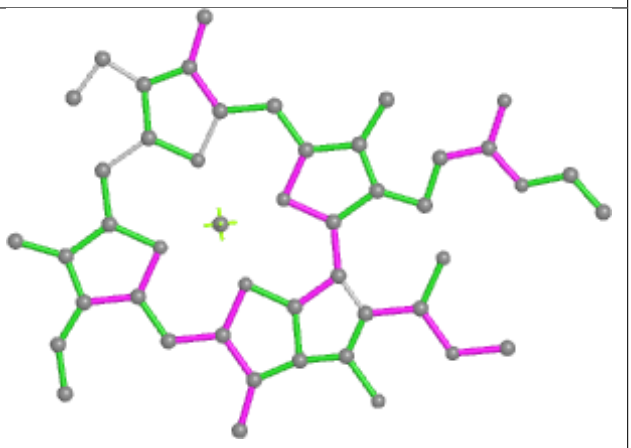
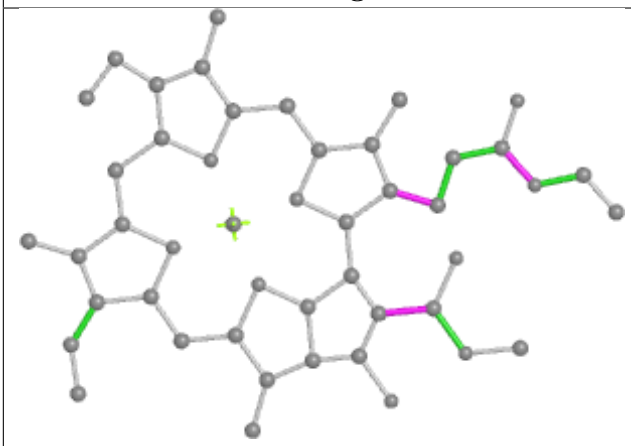


Bond angles



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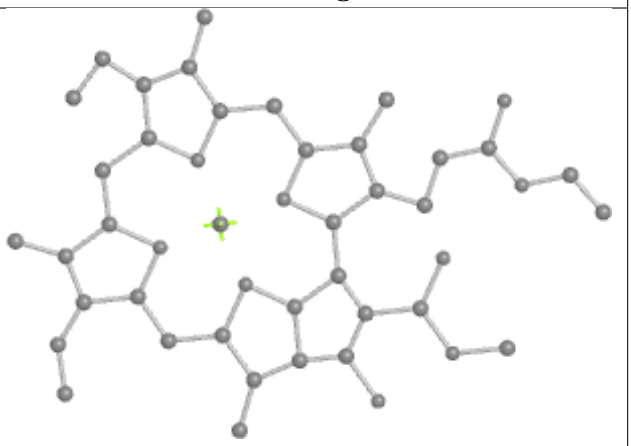
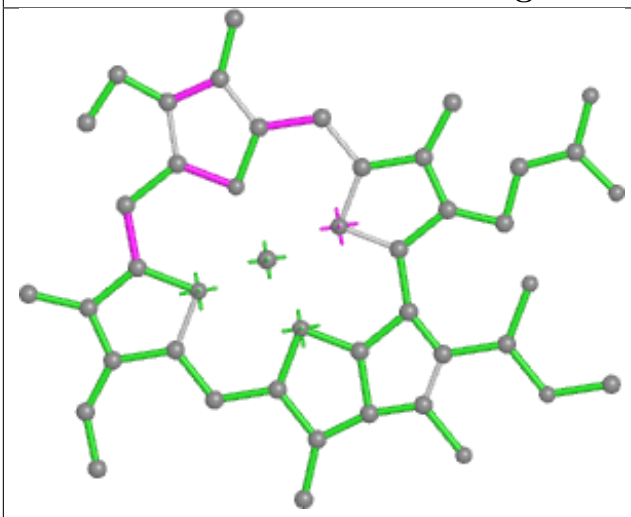


Rings

Ligand CLA B 1220



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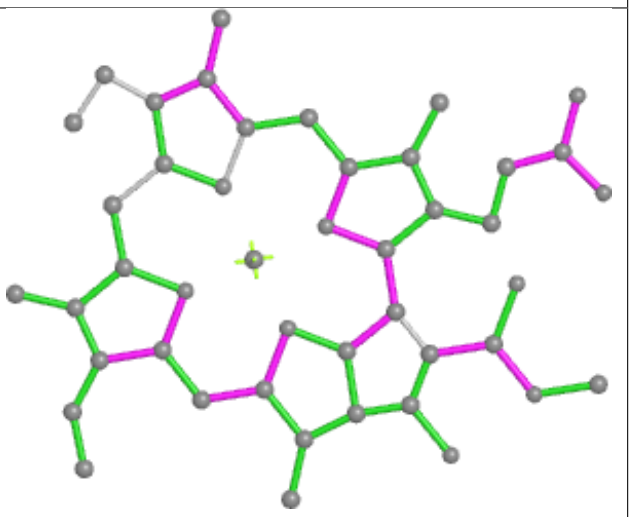

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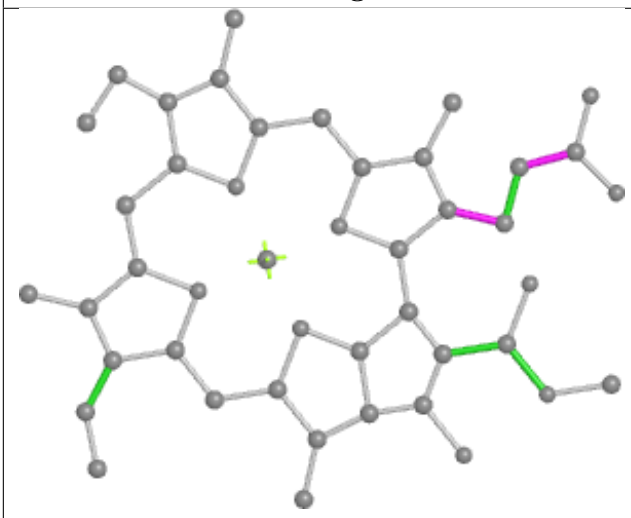

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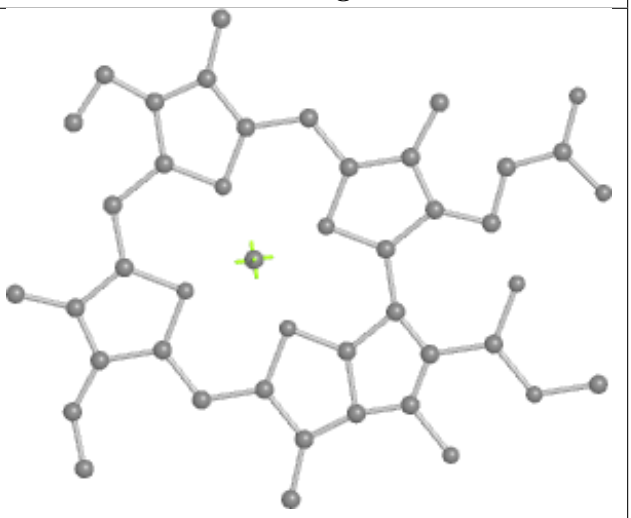
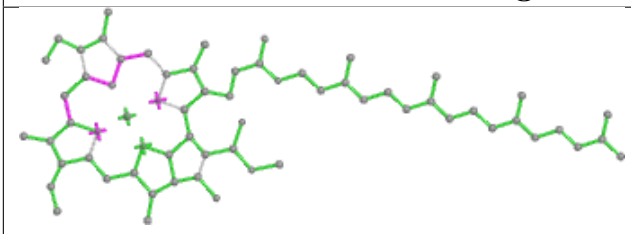


Rings

Ligand CLA B 1021



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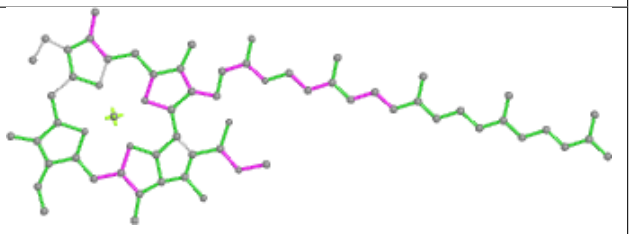

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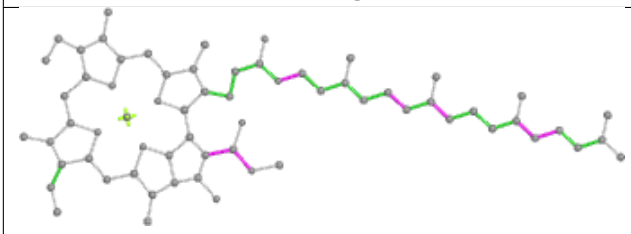

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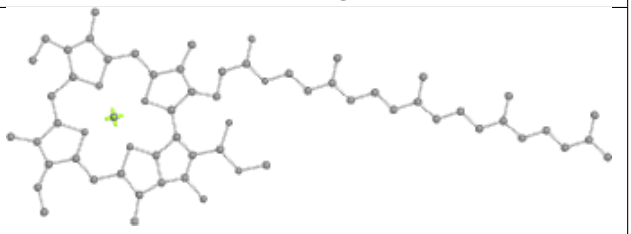

Rings

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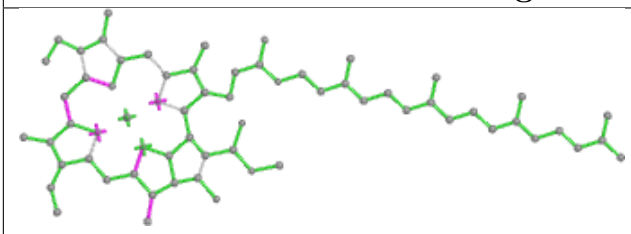

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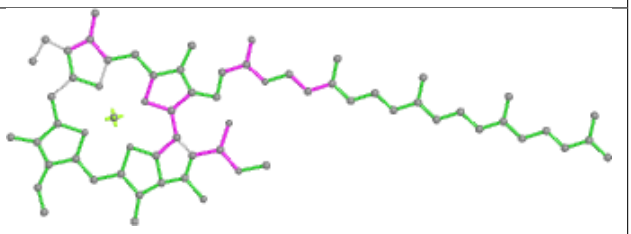

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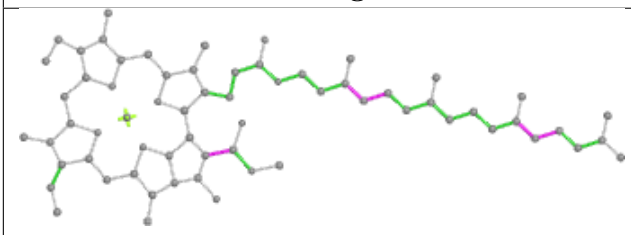

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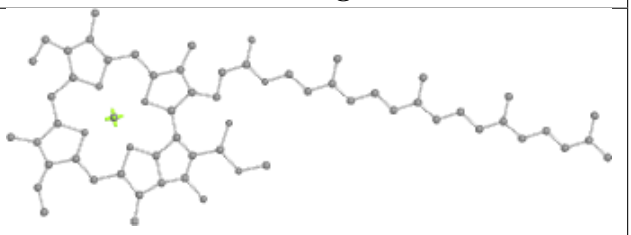
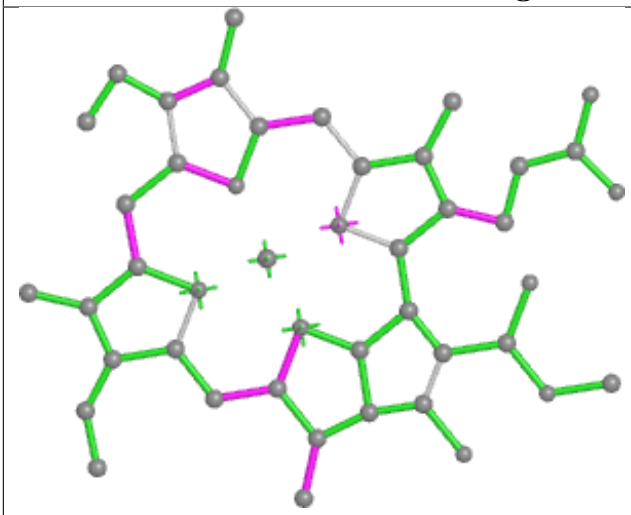


Rings

Ligand CLA A 1112



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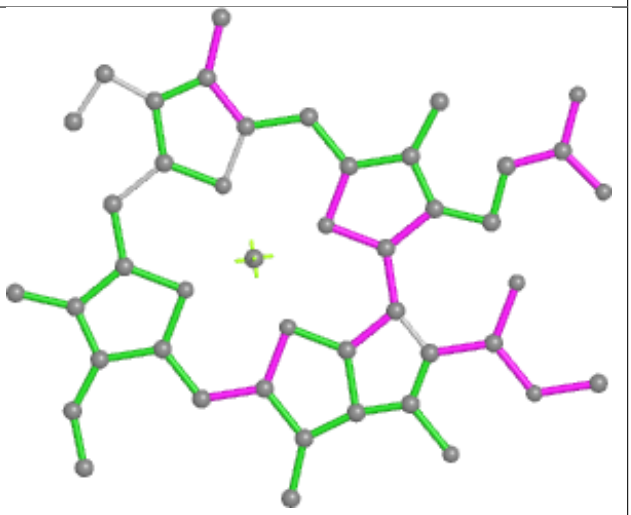
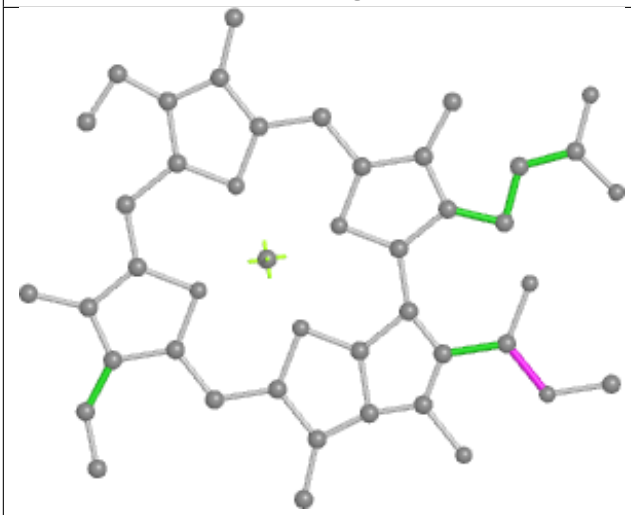


Bond angles



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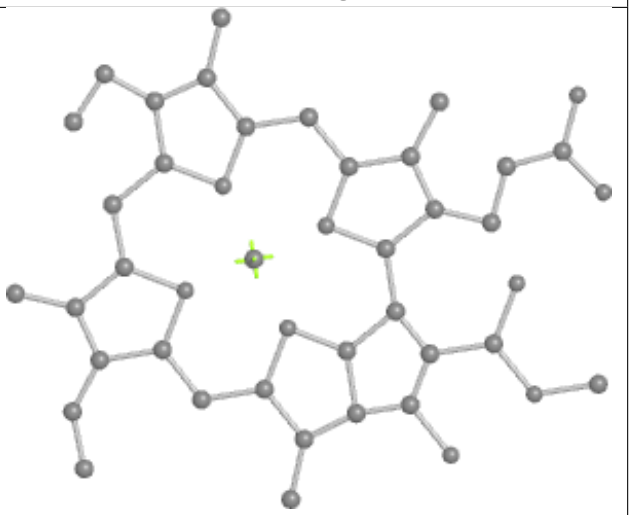
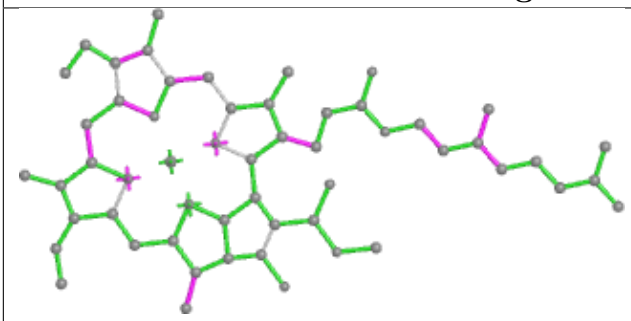


Rings

Ligand CLA B 1213



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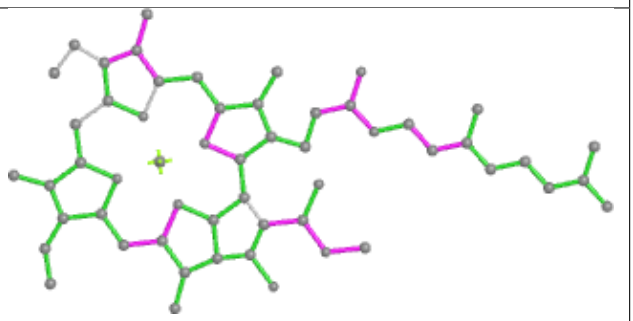
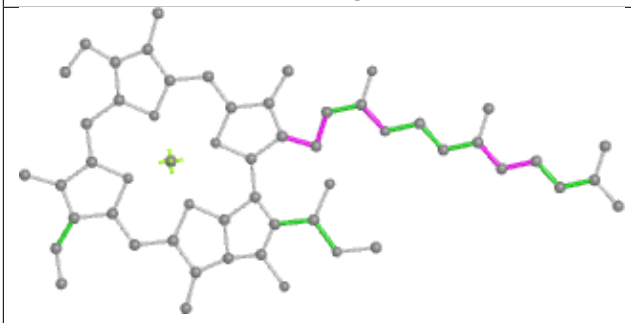


Bond angles



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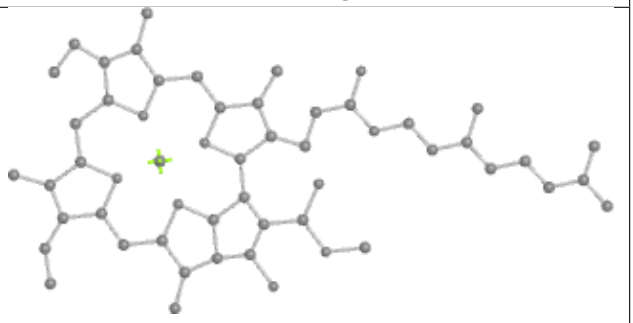

Rings

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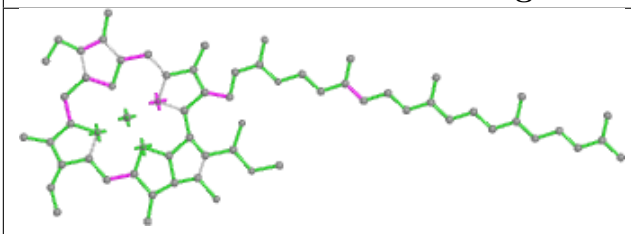

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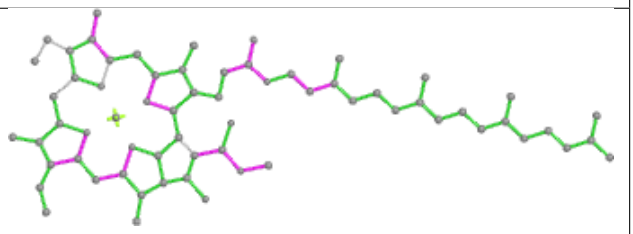
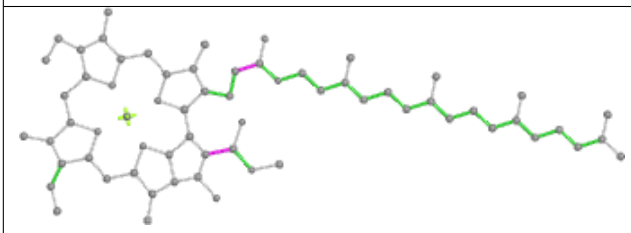


Bond angles



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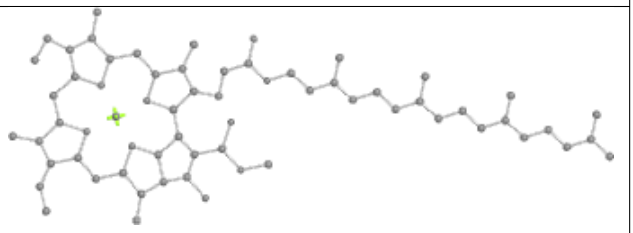
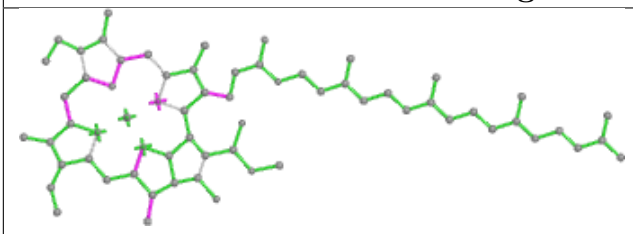


Rings

Ligand CLA L 1502



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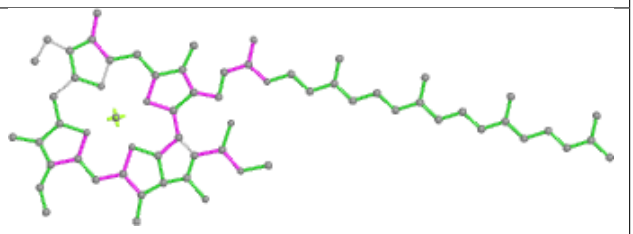
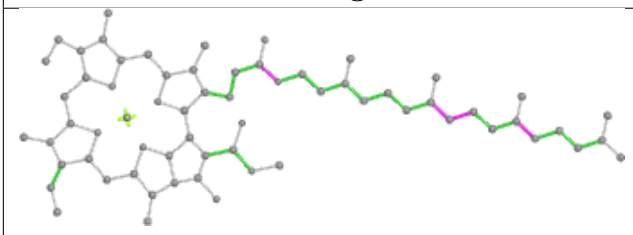


Bond angles



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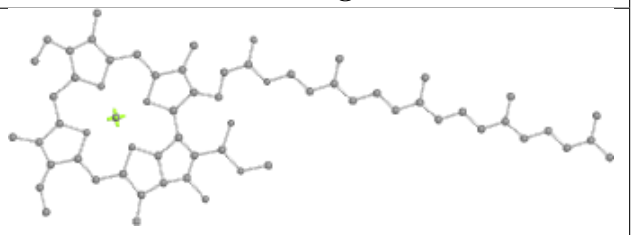
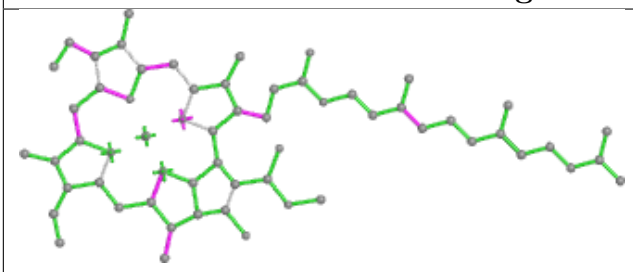


Rings

Ligand CLA B 1215



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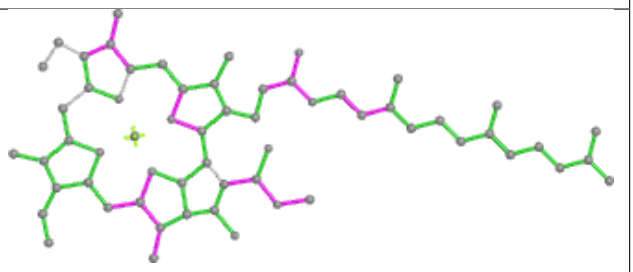
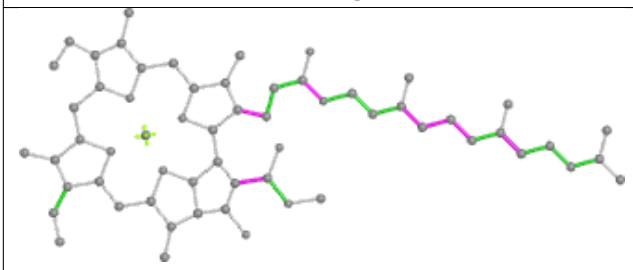
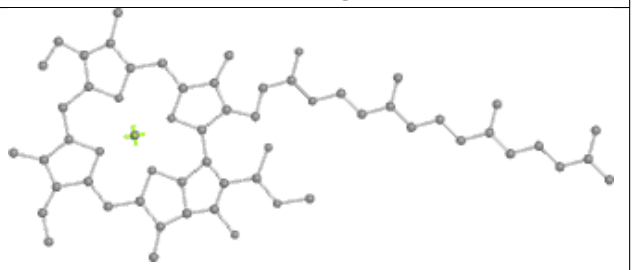


Bond angles

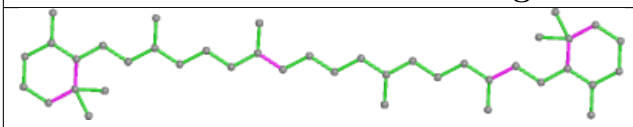


Torsions

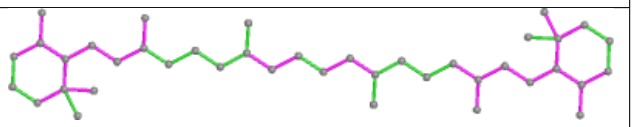


Rings

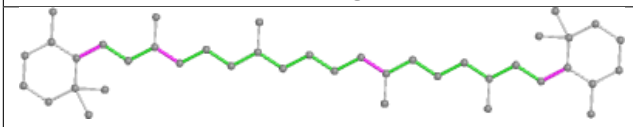
Ligand BCR A 4011



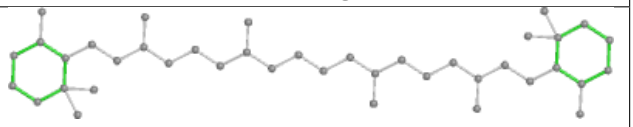
Bond lengths



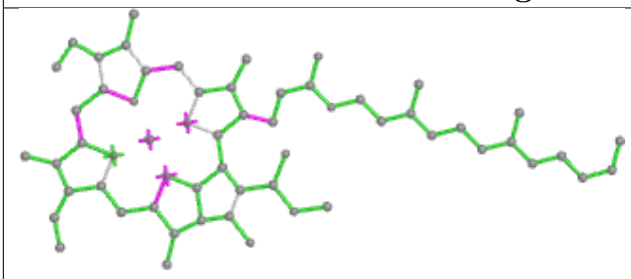
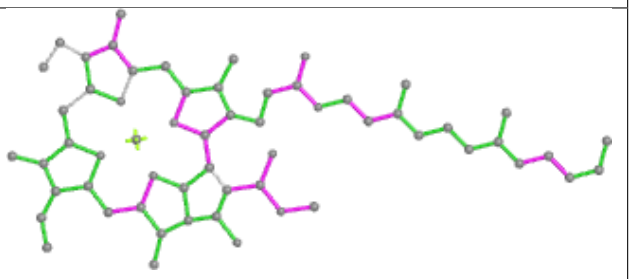
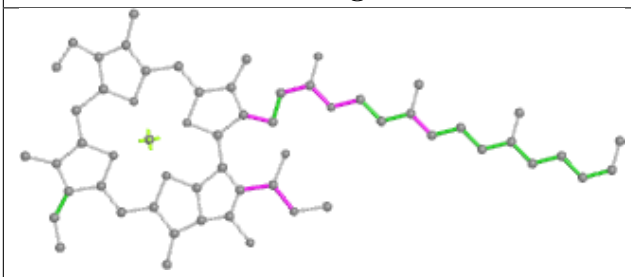
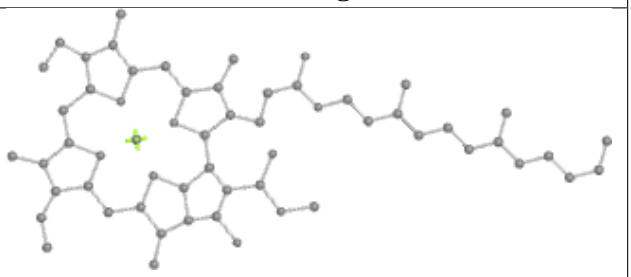
Bond angles

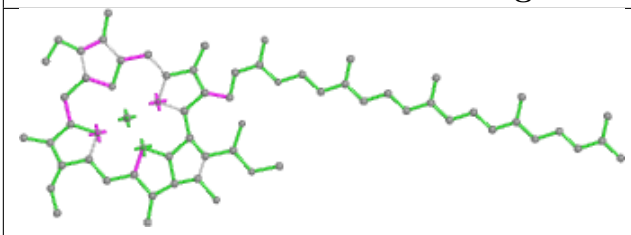
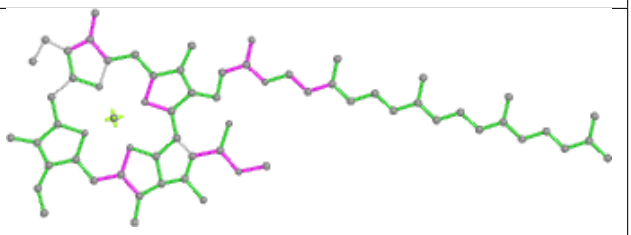
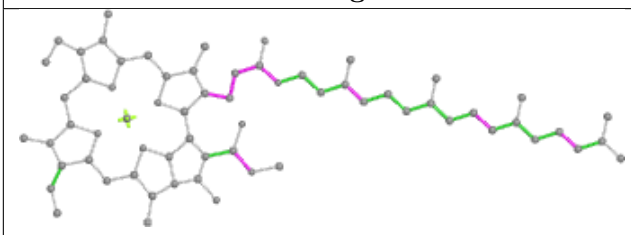
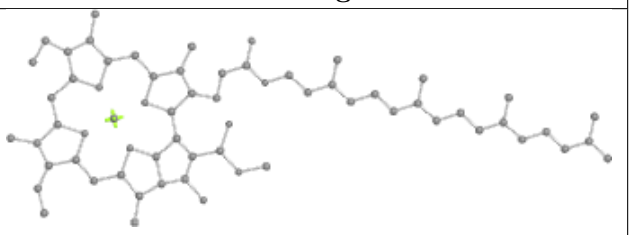


Torsions

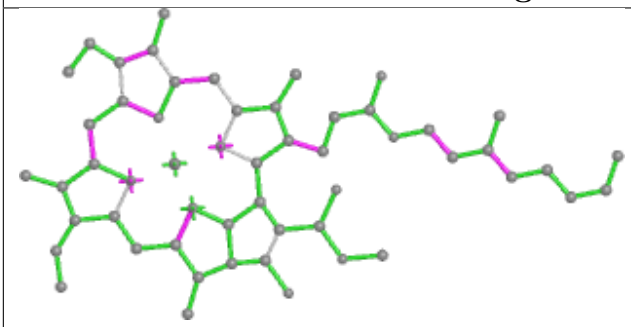


Rings

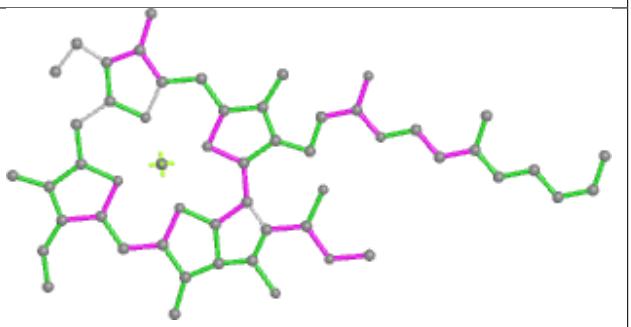
Ligand CLA A 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1109	
 Bond lengths	 Bond angles
 Torsions	 Rings

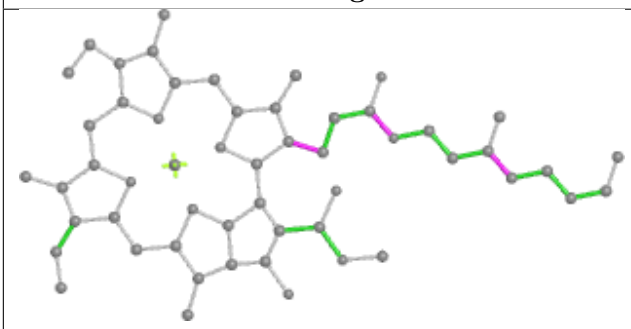
Ligand CLA A 1133



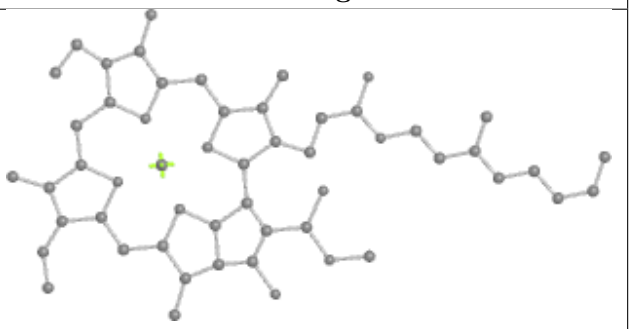
Bond lengths



Bond angles

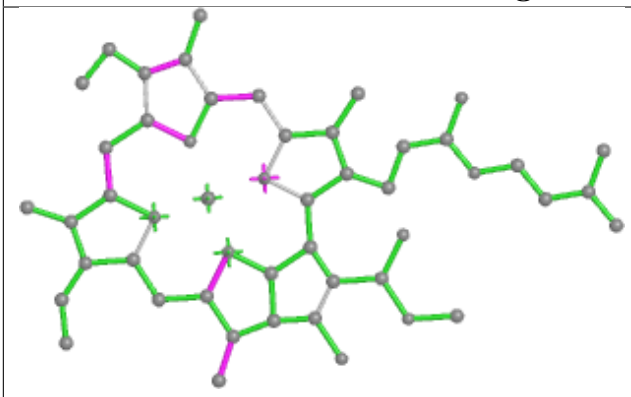


Torsions

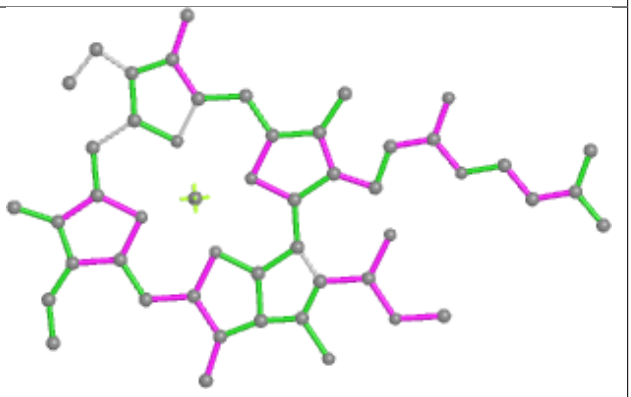


Rings

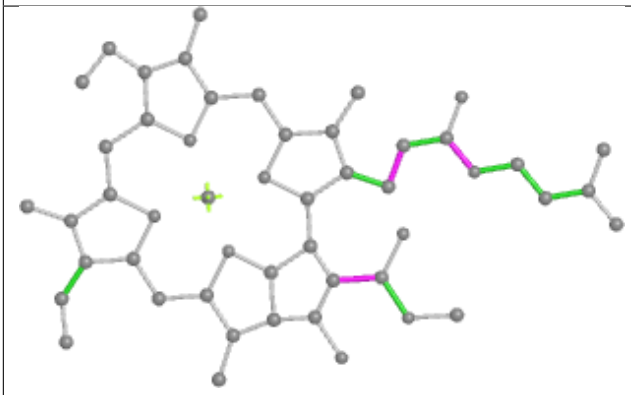
Ligand CLA A 1129



Bond lengths



Bond angles



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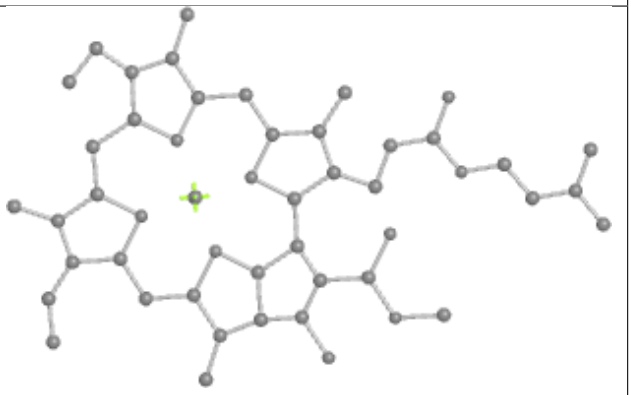
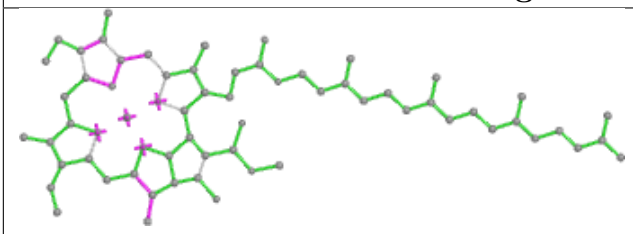
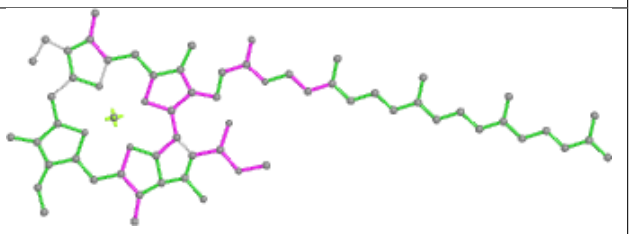


Rings

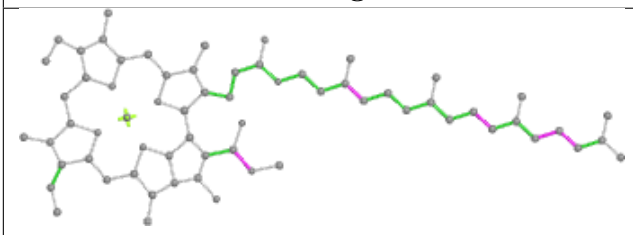
Ligand CLA B 1207



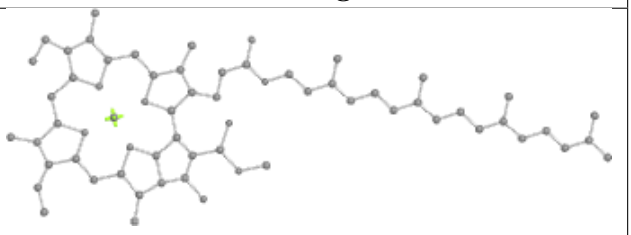
Bond lengths



Bond angles

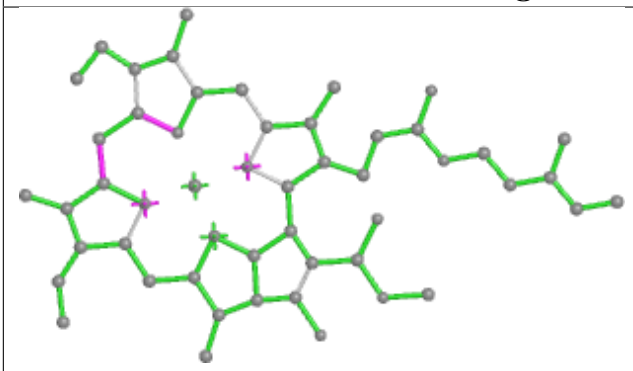


Torsions

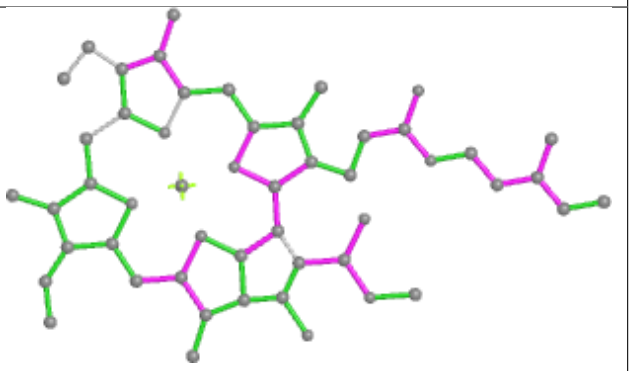


Rings

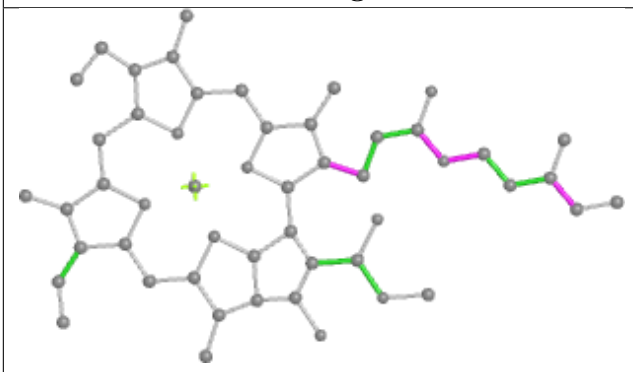
Ligand CLA A 1135



Bond lengths



Bond angles



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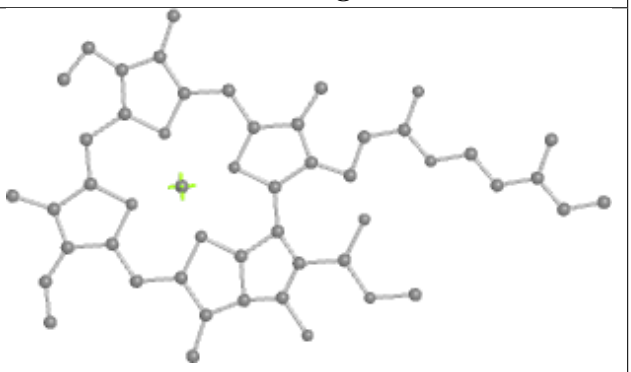
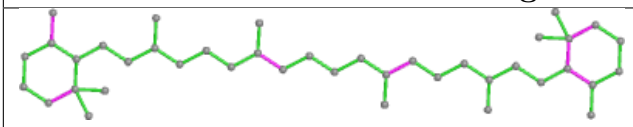


Rings

Ligand BCR I 4020



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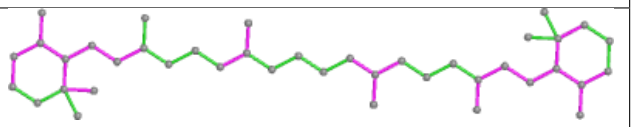
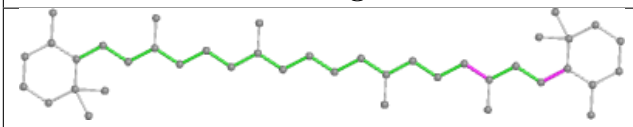


Bond angles



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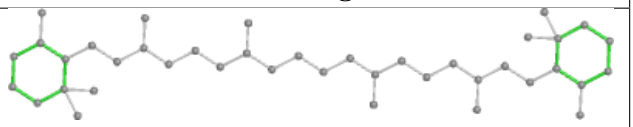
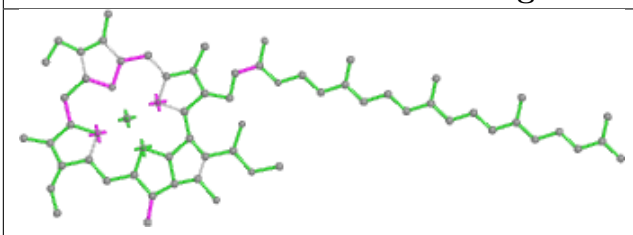


Rings

Ligand CLA L 1503



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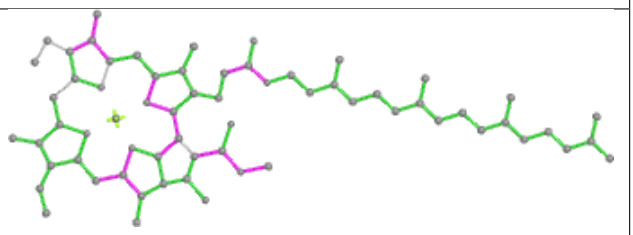
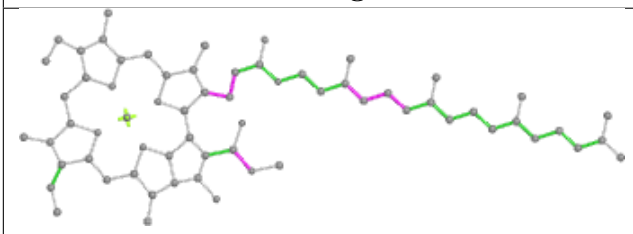


Bond angles



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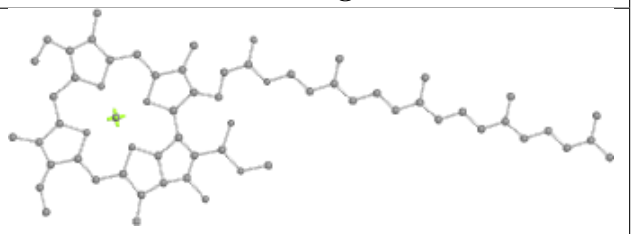
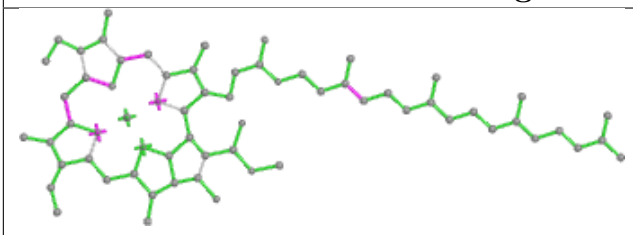


Rings

Ligand CLA A 1125



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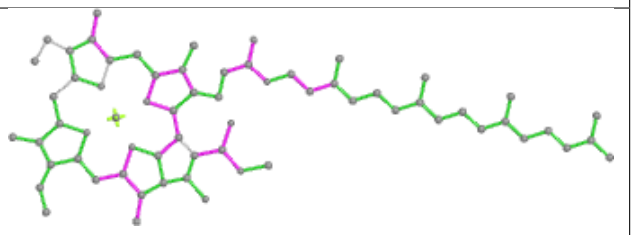
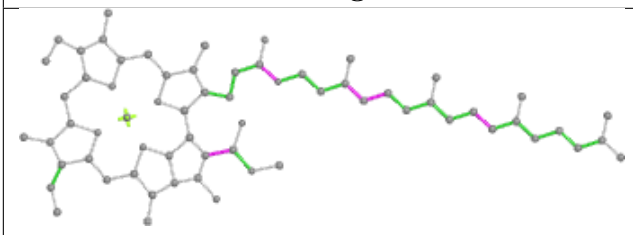


Bond angles



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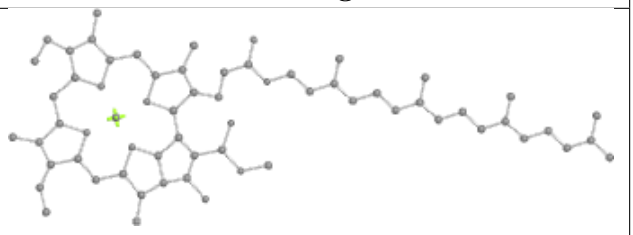
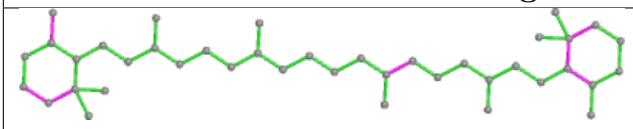


Rings

Ligand BCR I 4018



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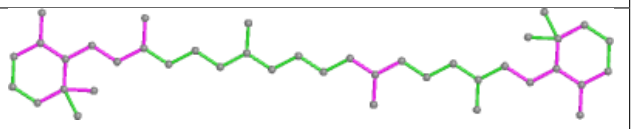
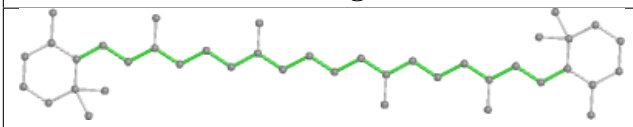


Bond angles



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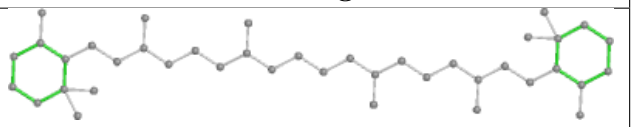
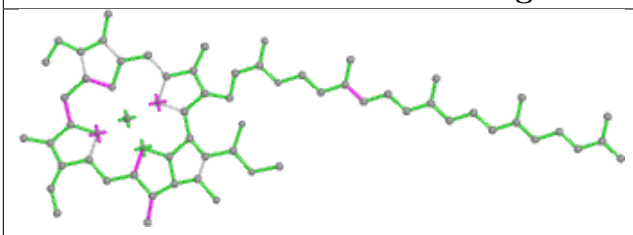
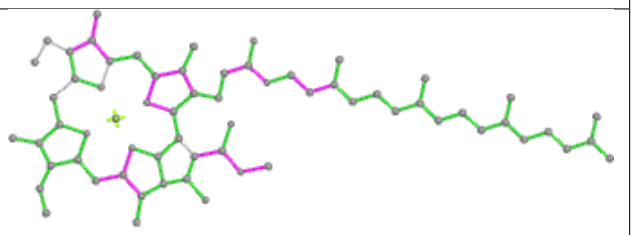


Rings

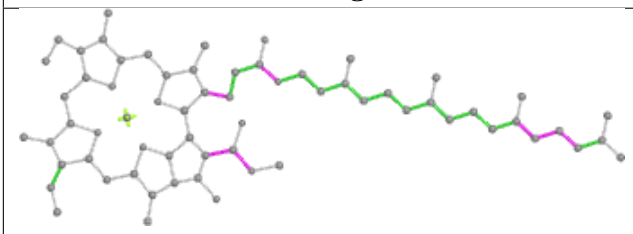
Ligand CLA B 1202



Bond lengths



Bond angles



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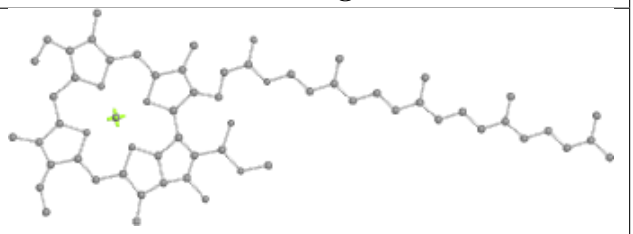
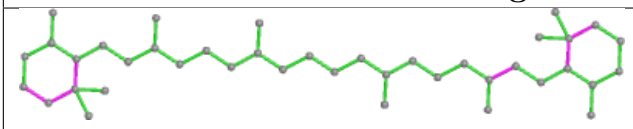
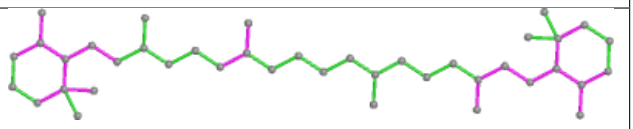


Rings

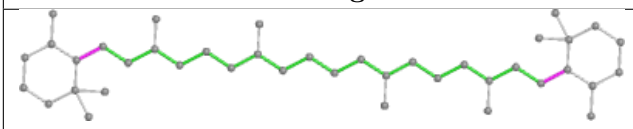
Ligand BCR M 4021



Bond lengths



Bond angles



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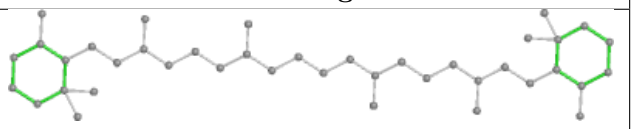
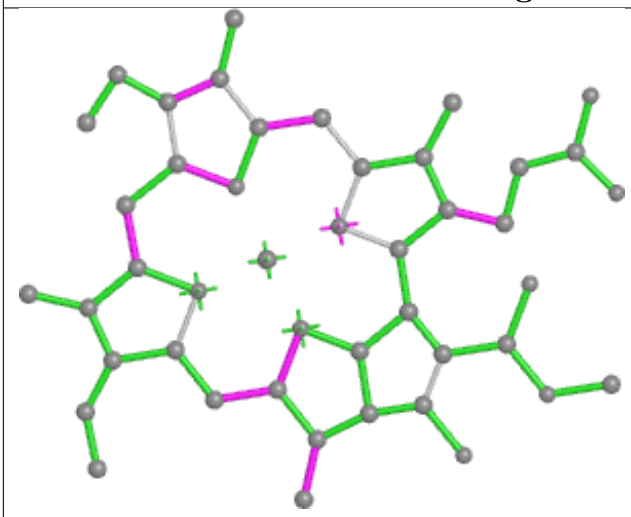
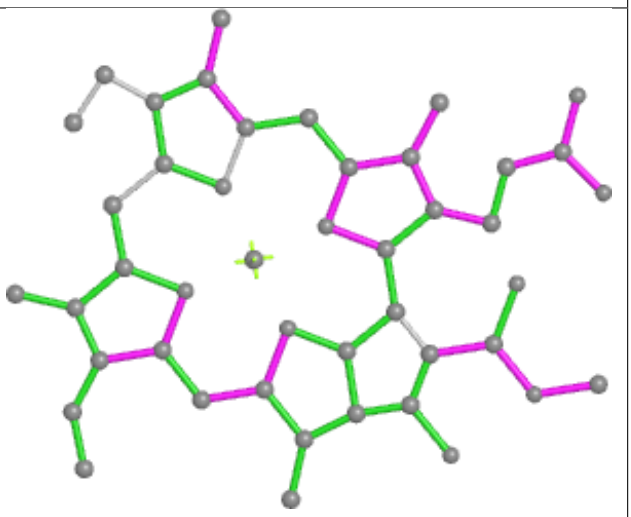


Rings

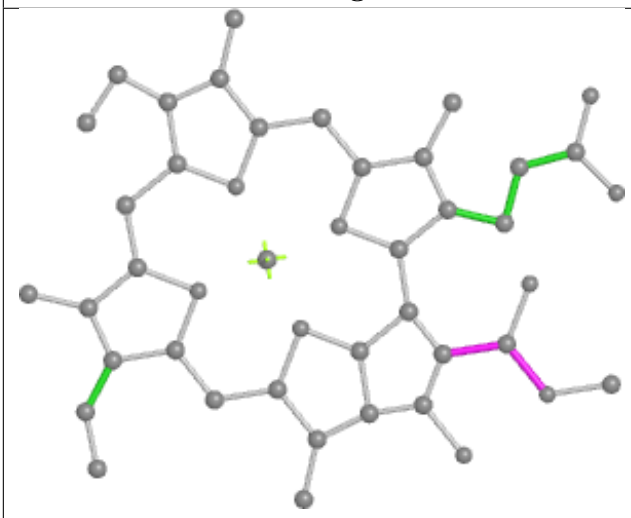
Ligand CLA B 1231



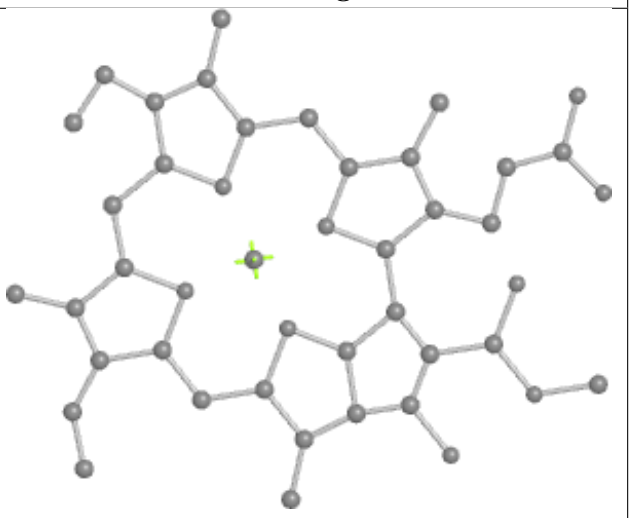
Bond lengths



Bond angles

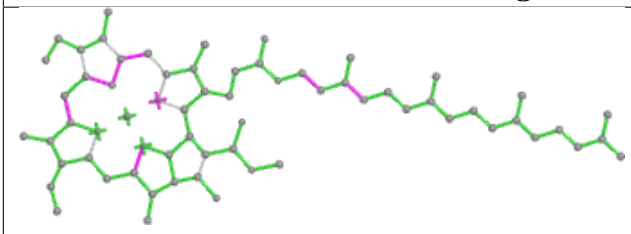


Torsions

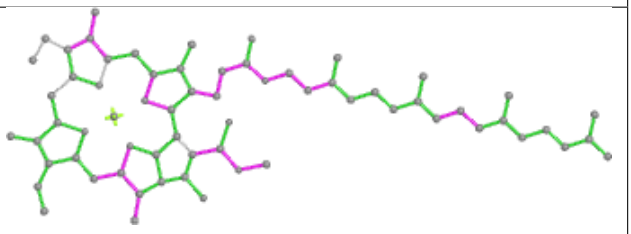


Rings

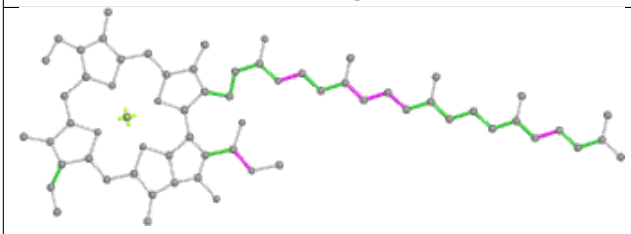
Ligand CLA A 1140



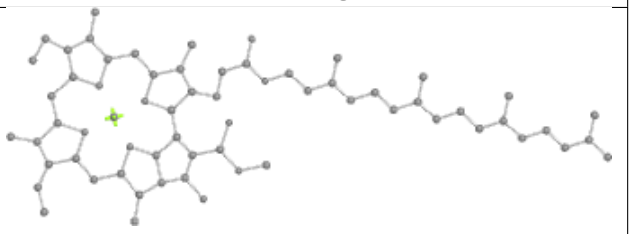
Bond lengths



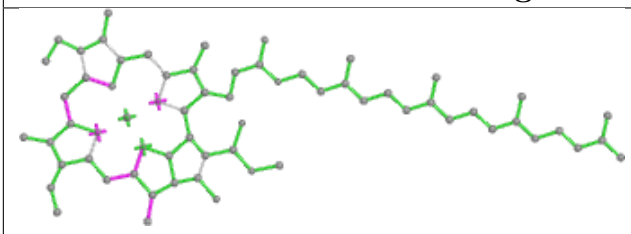
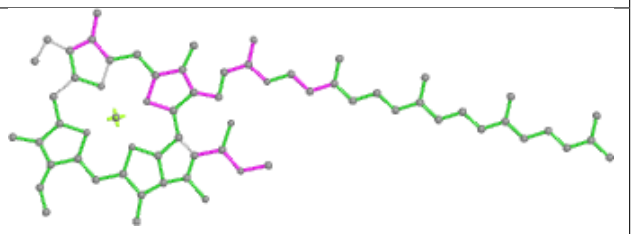
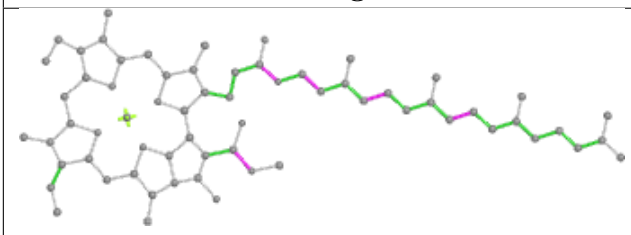
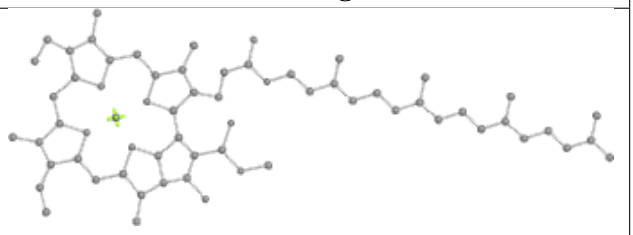
Bond angles

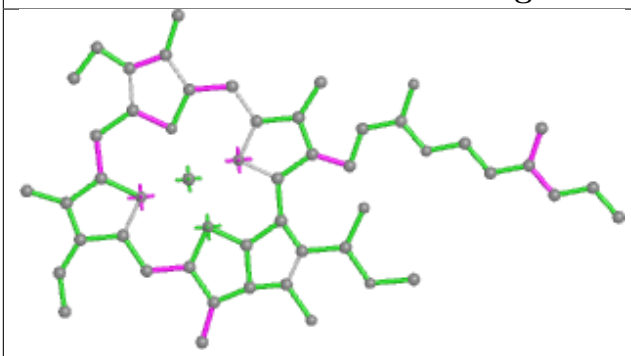
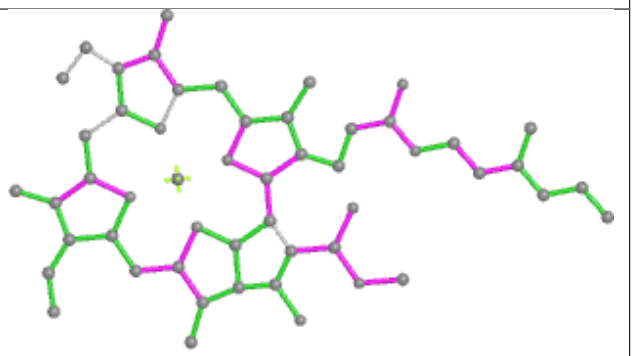
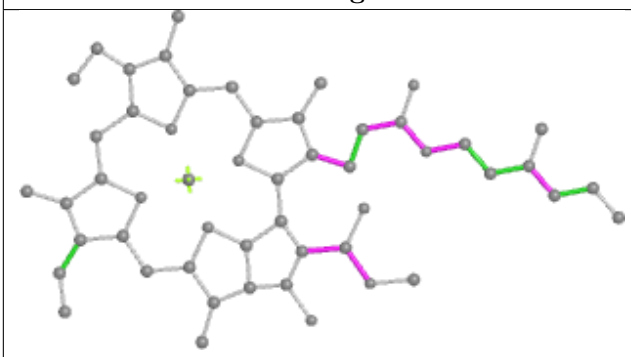
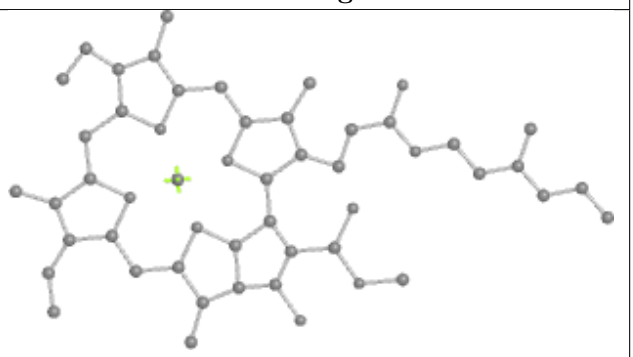


Torsions

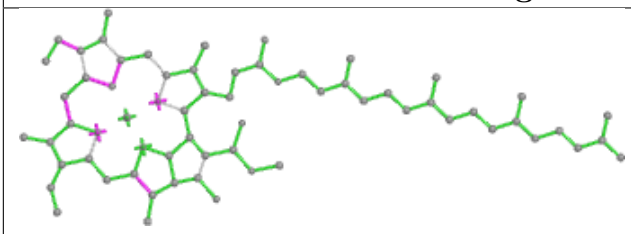


Rings

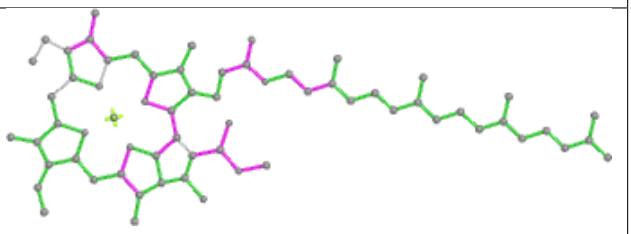
Ligand CLA A 1130	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1801	
 Bond lengths	 Bond angles
 Torsions	 Rings

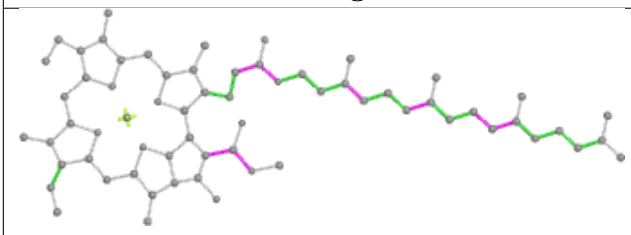
Ligand CLA B 1223



Bond lengths



Bond angles



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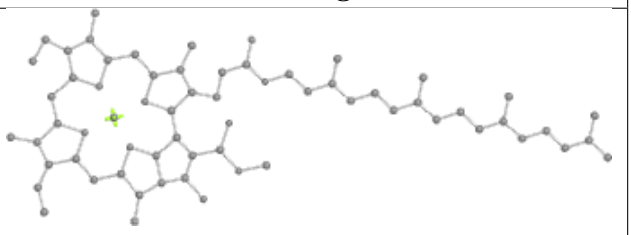
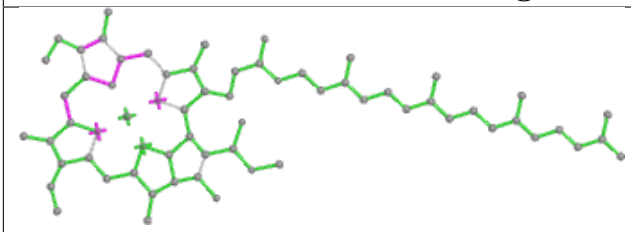
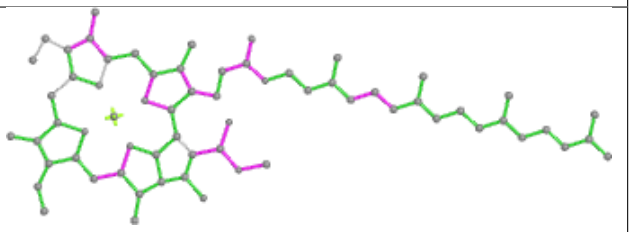


Rings

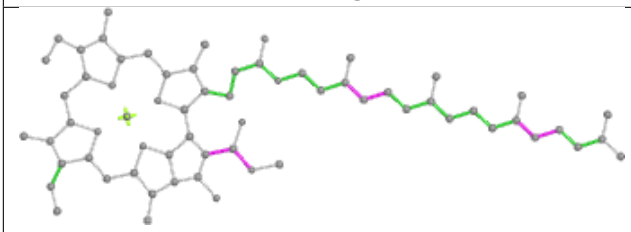
Ligand CLA B 1205



Bond lengths



Bond angles



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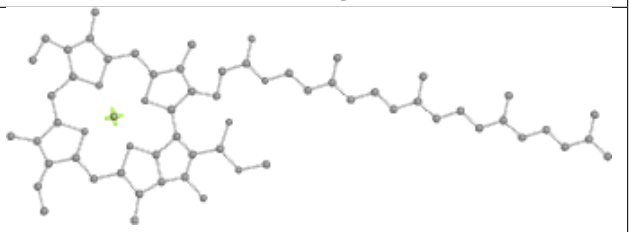
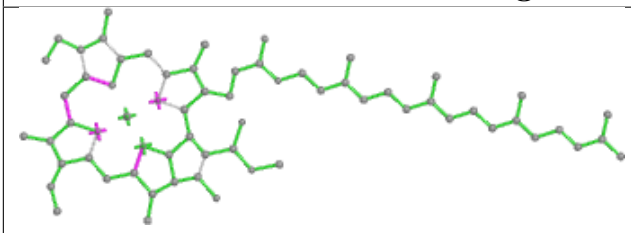


Rings

Ligand CLA B 1206



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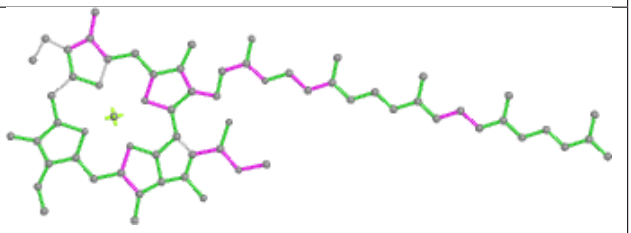
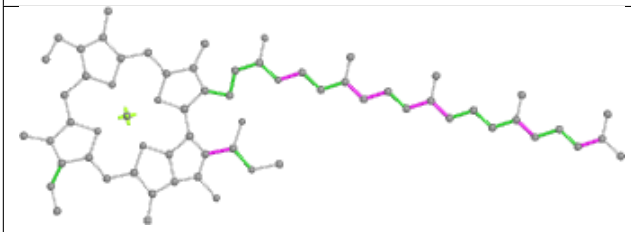


Bond angles



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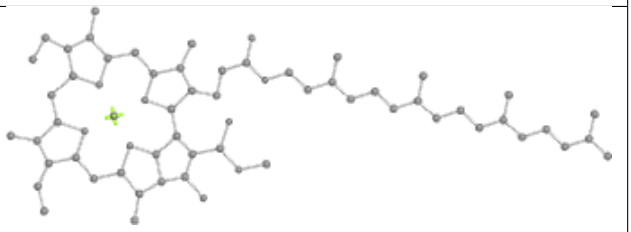
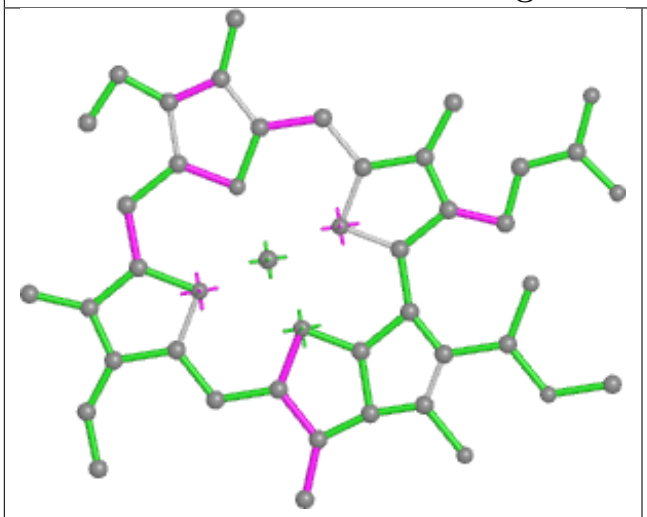
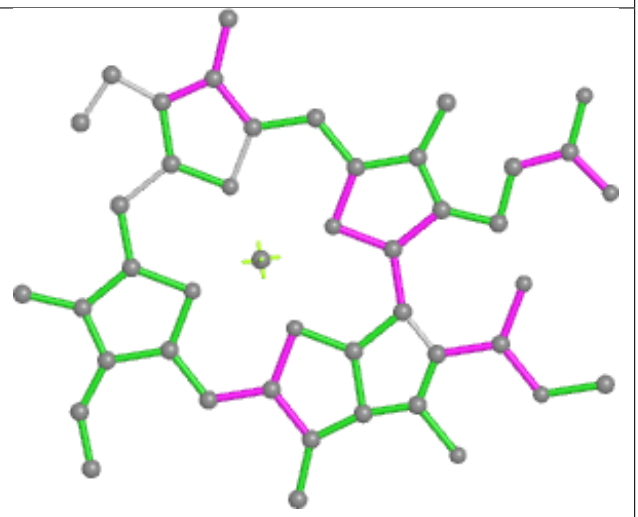


Rings

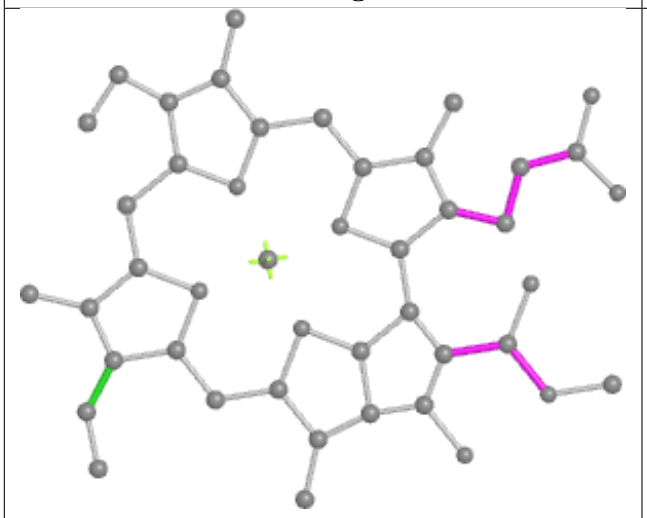
Ligand CLA B 1212



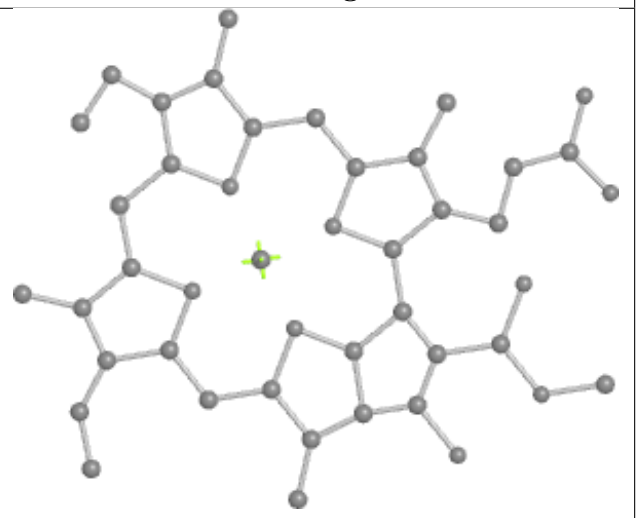
Bond lengths



Bond angles

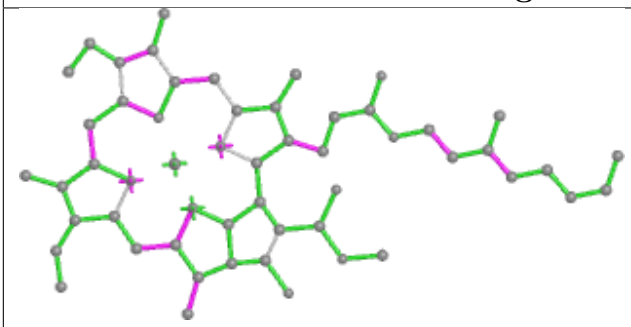


Torsions

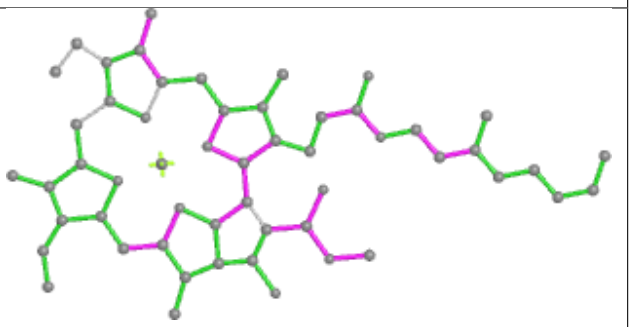


Rings

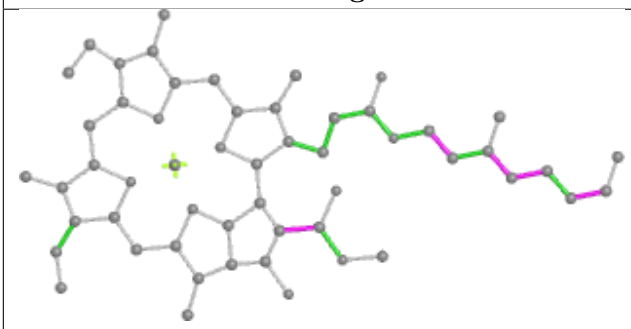
Ligand CLA B 1221



Bond lengths



Bond angles



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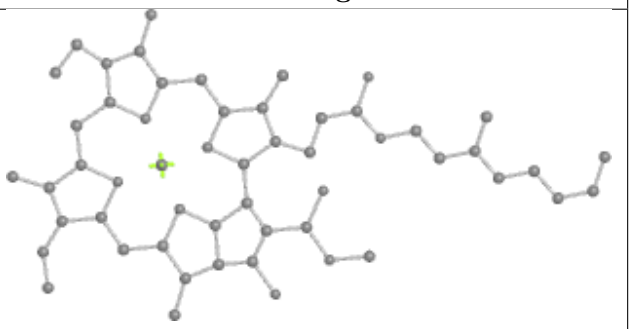
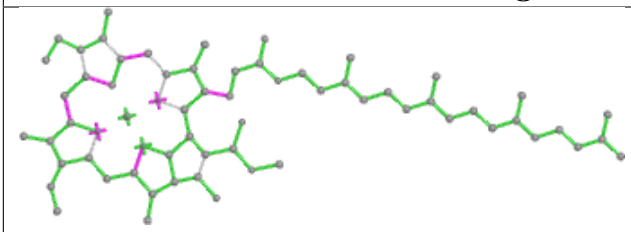


Rings

Ligand CLA A 1124



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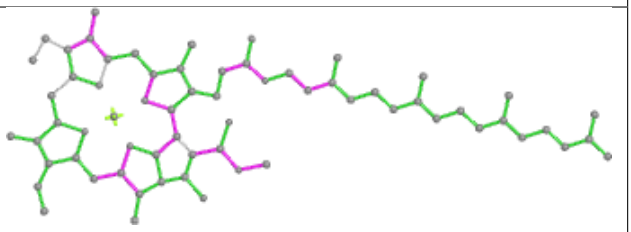
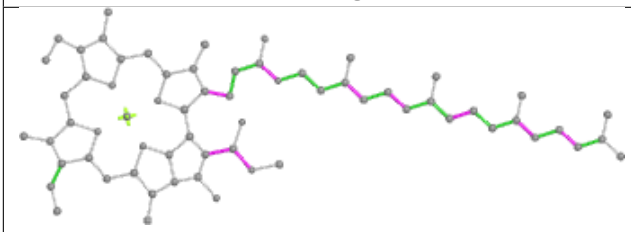


Bond angles



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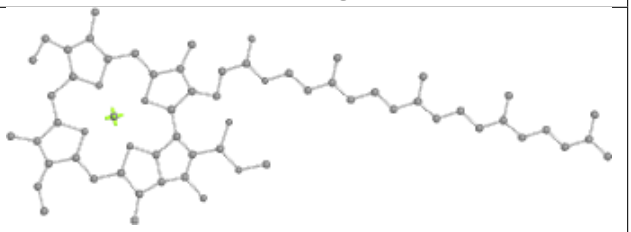
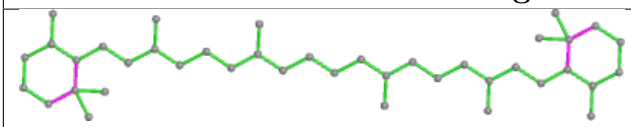


Rings

Ligand BCR A 4002



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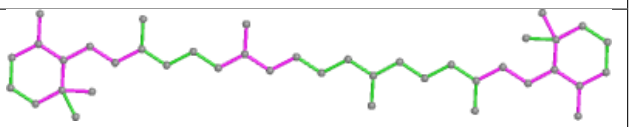
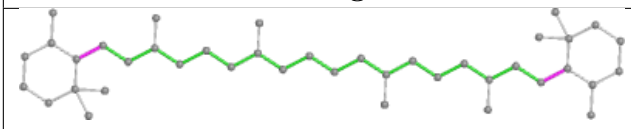


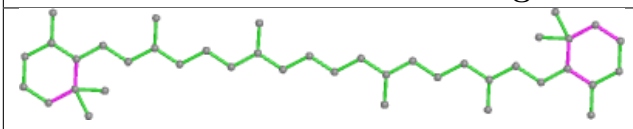
Bond angles



Torsions

Rings

Ligand BCR A 4003



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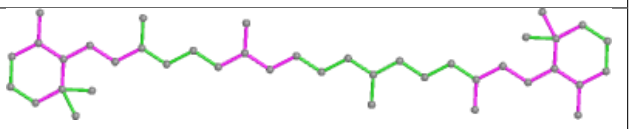
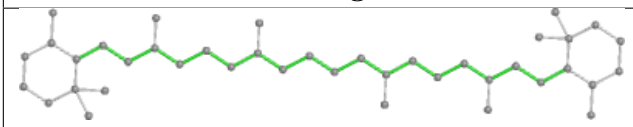


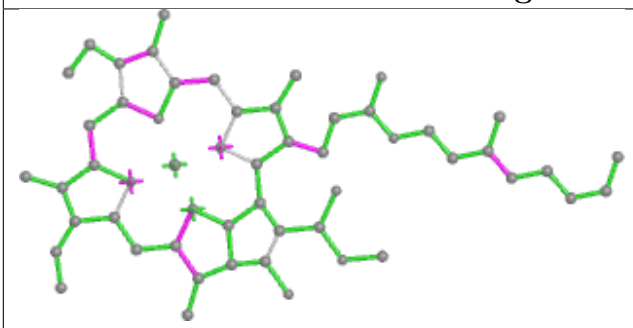
Bond angles



Torsions

Rings

Ligand CLA A 1116



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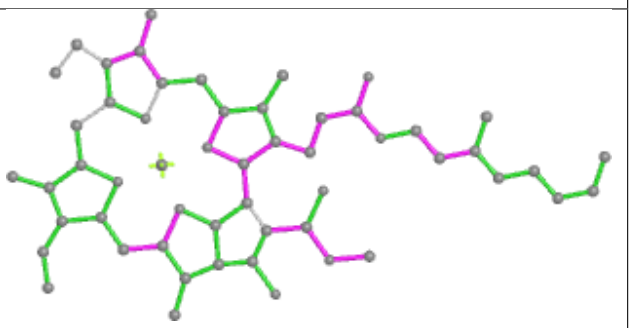
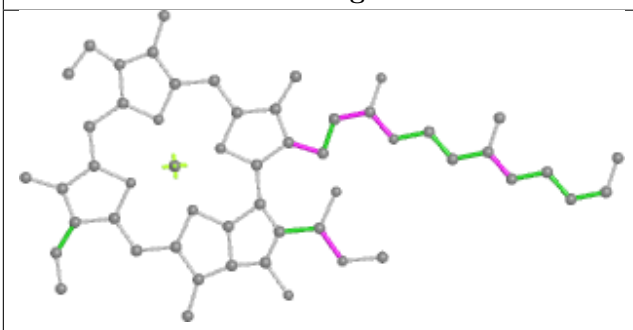
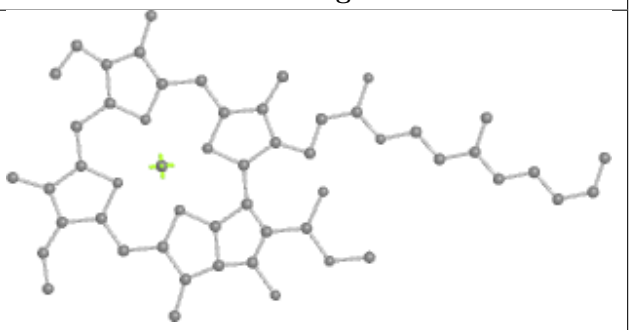


Bond angles

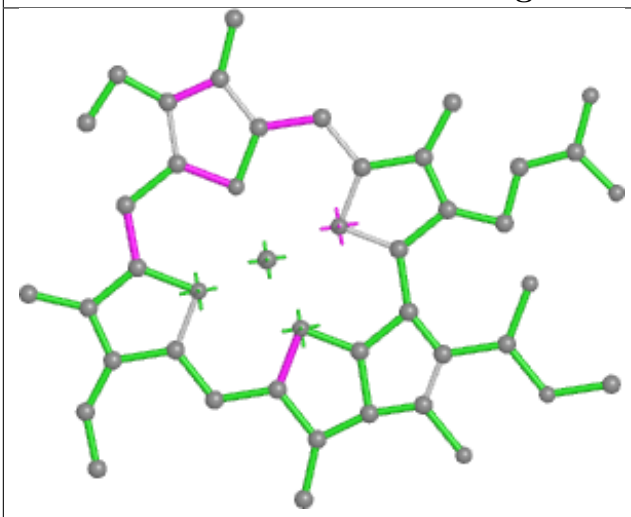


Torsions



Rings

Ligand CLA B 1233



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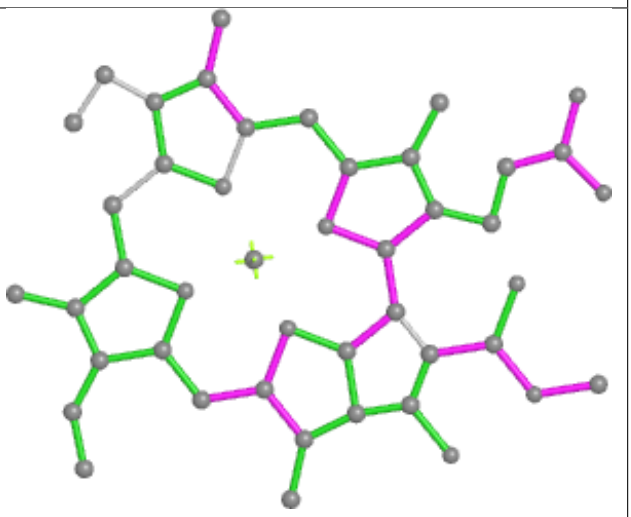
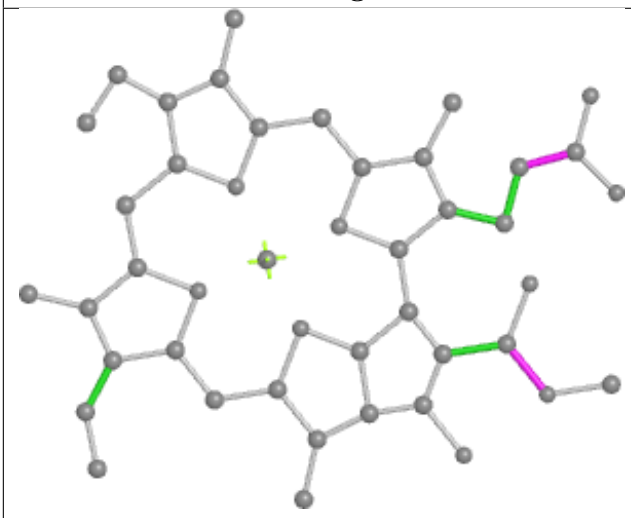
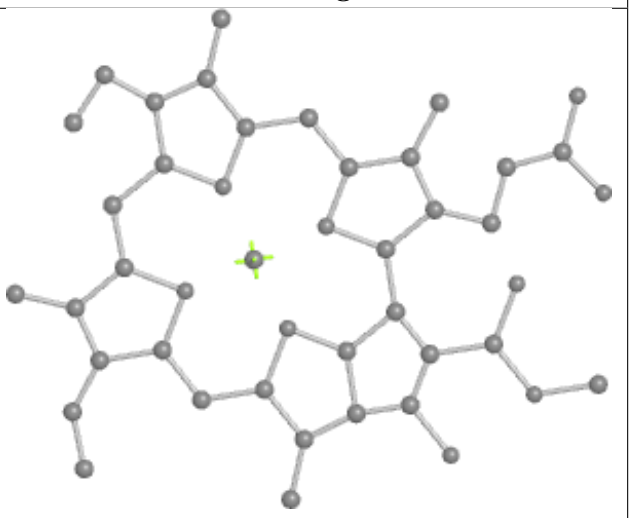


Bond angles

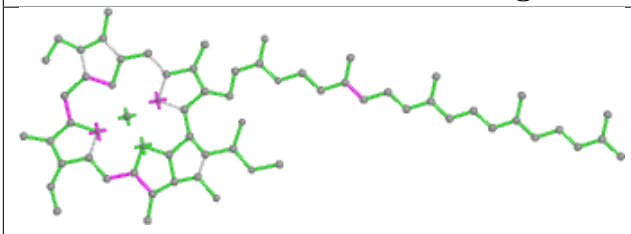


Torsions

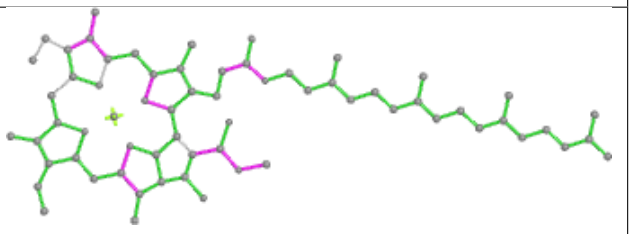


Rings

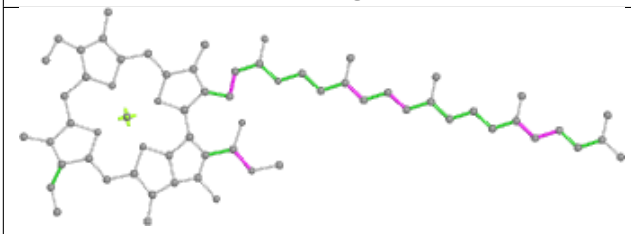
Ligand CLA A 1127



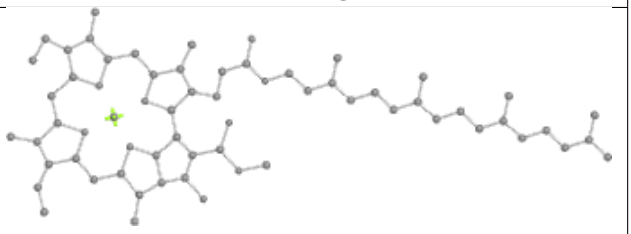
Bond lengths



Bond angles

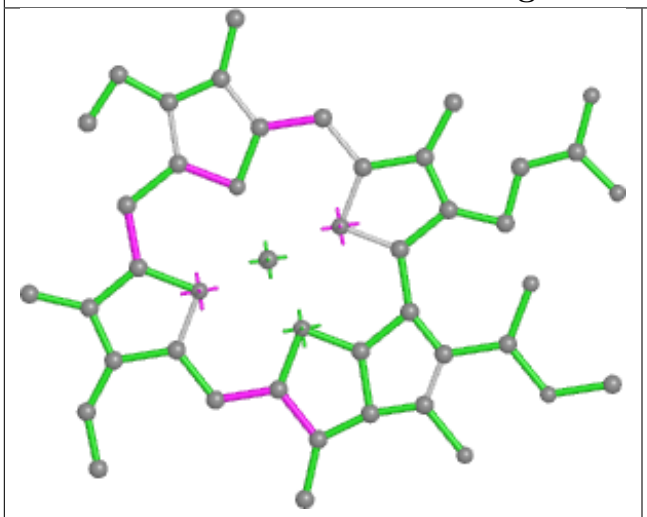


Torsions

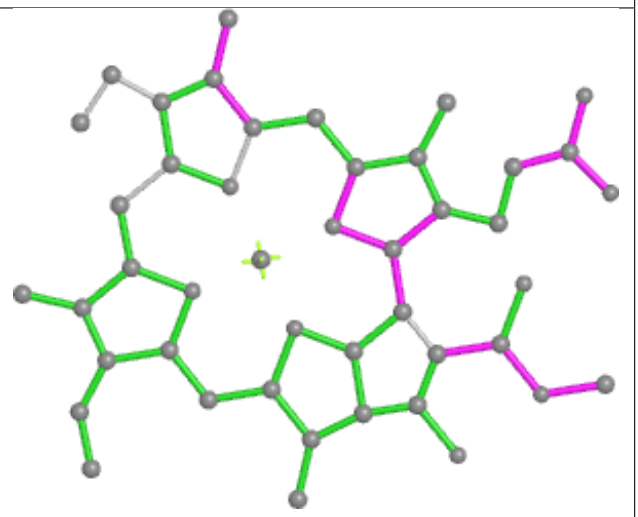


Rings

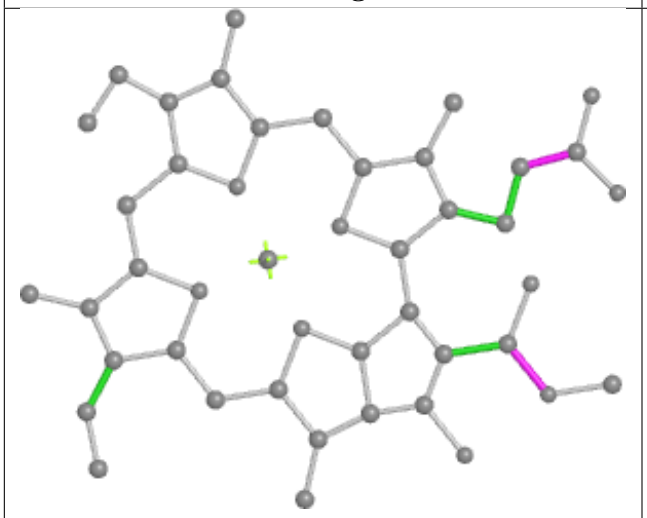
Ligand CLA F 1301



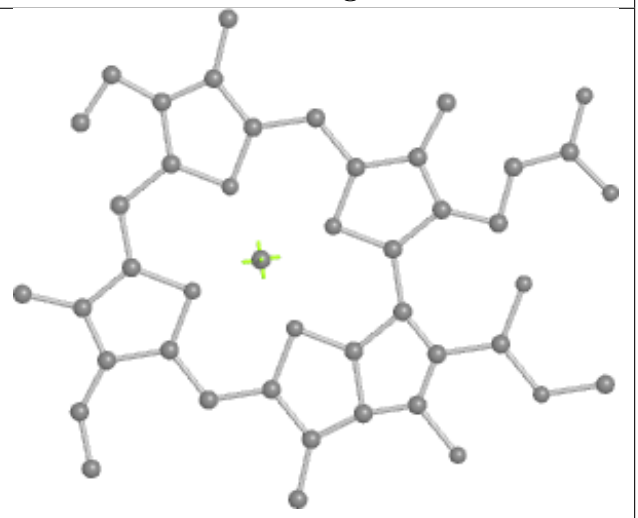
Bond lengths



Bond angles

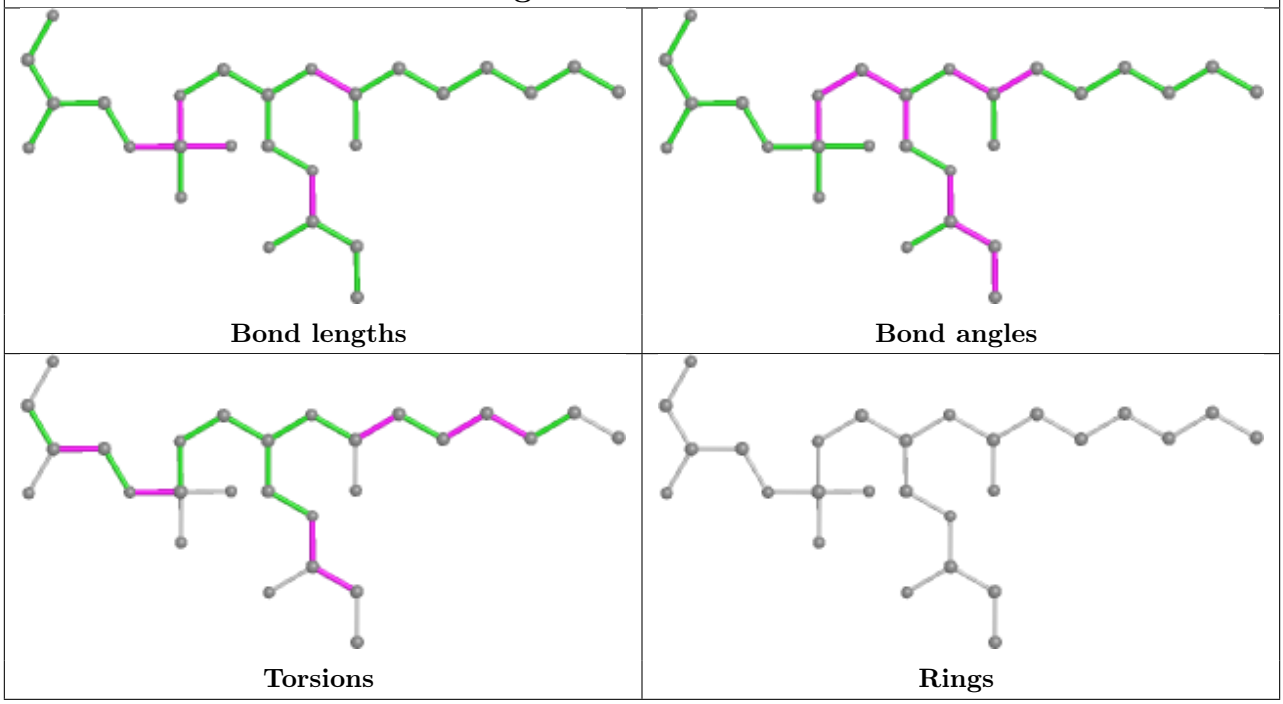


Torsions

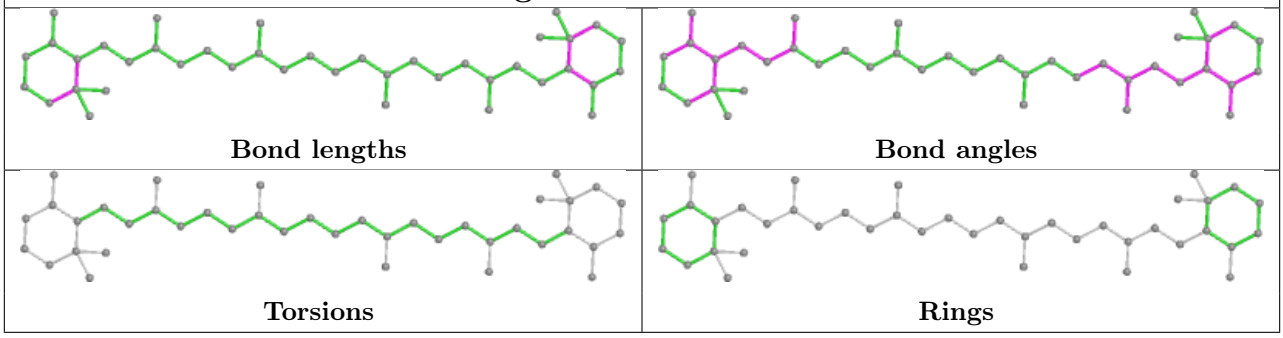


Rings

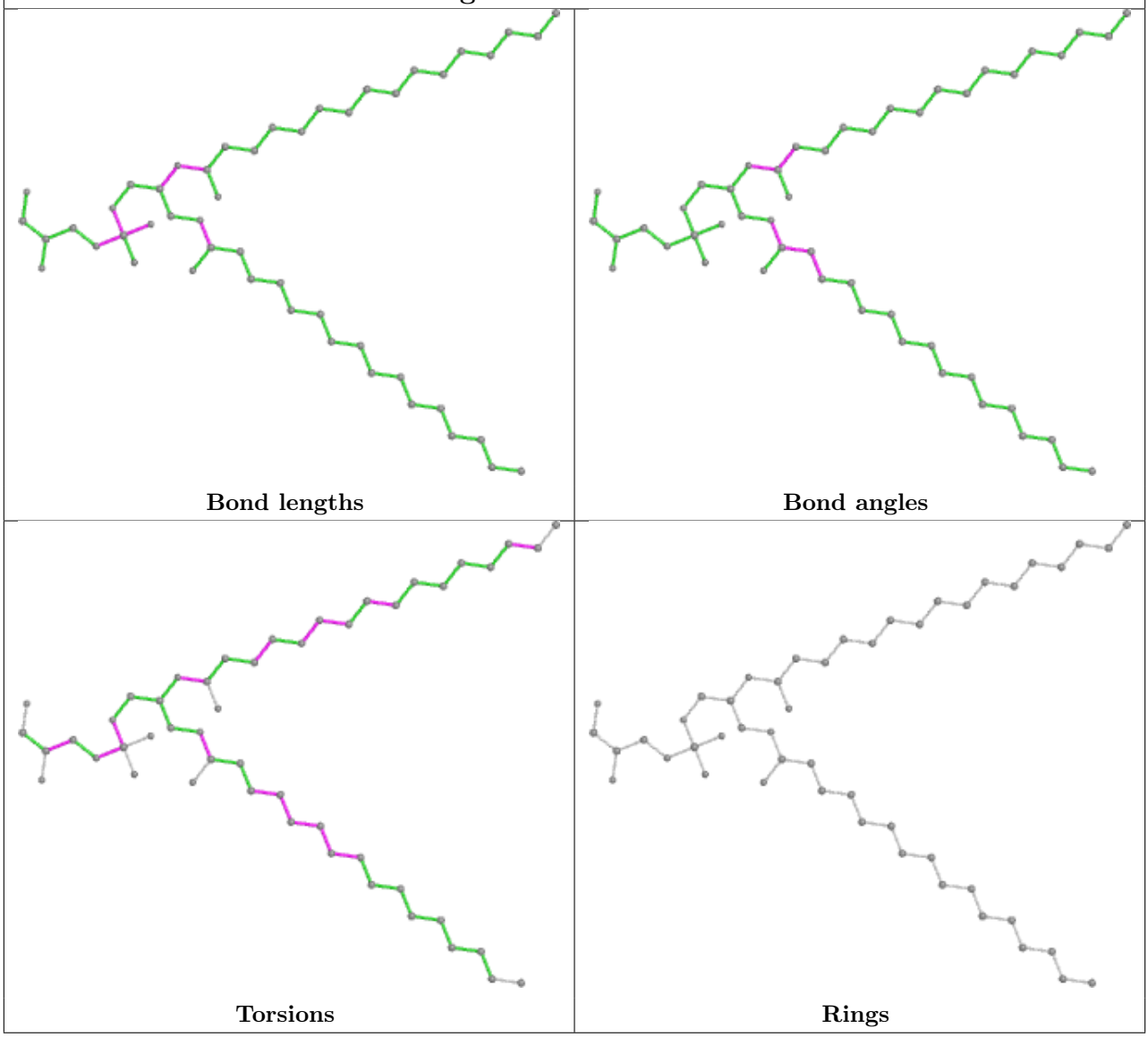
Ligand LHG A 5003



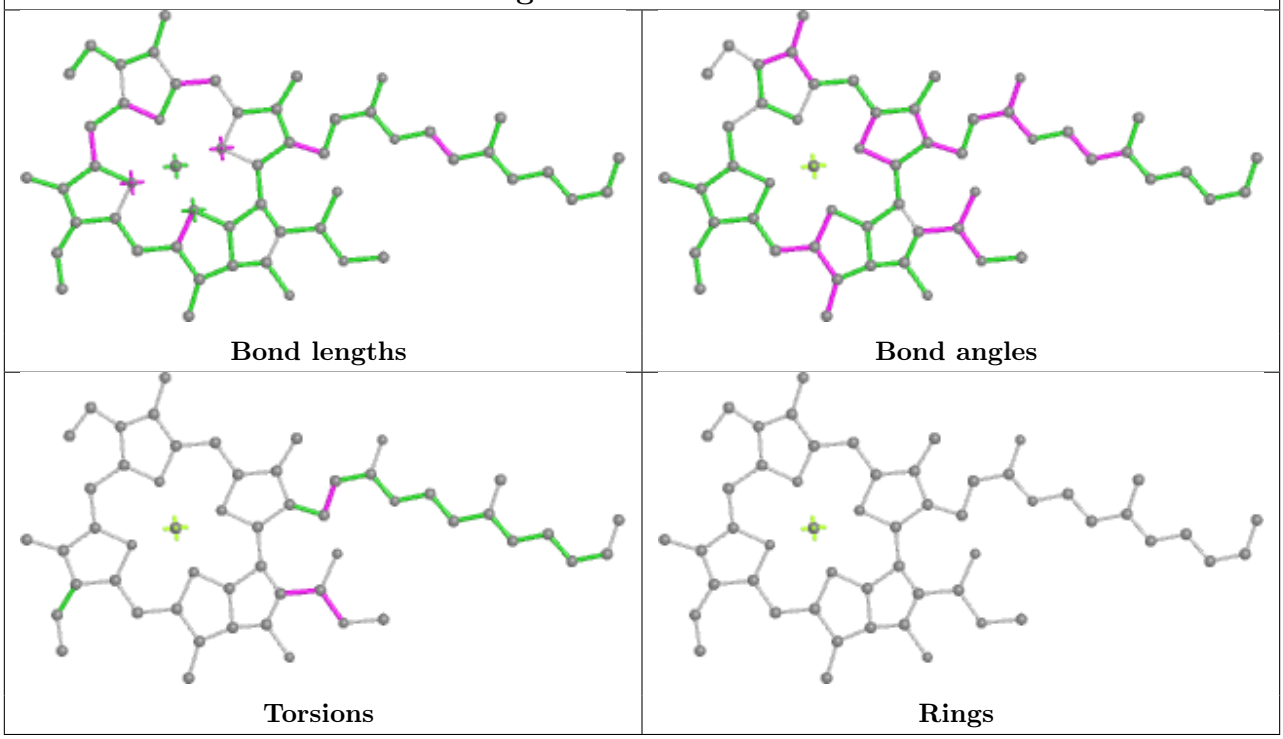
Ligand BCR B 4004



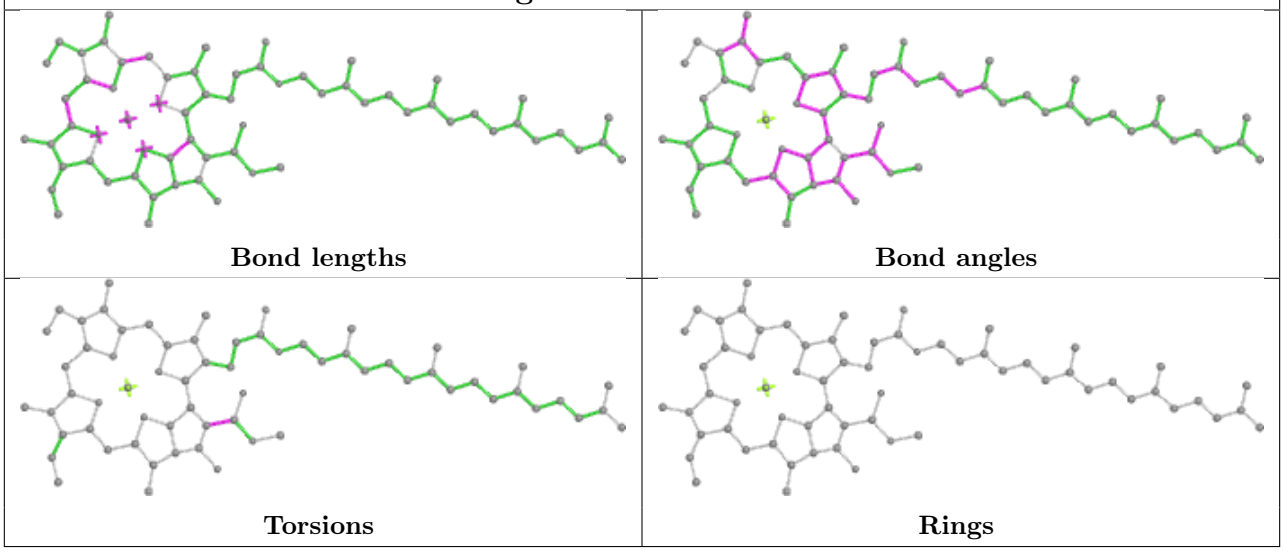
Ligand LHG A 5001



Ligand CLA B 1201



Ligand CLA A 1011



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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.