



wwPDB EM Validation Summary Report ⓘ

Jun 17, 2026 – 06:40 PM EDT

PDB ID : 9ZJT / pdb_00009zjt
EMDB ID : EMD-74341
Title : PSI-IsiA Complex from Anabaena 7120
Authors : Mazor, Y.M.; Maqdisi, R.M.; Gorski, C.G.; Pakrasi, H.P.; Biswas, S.B.;
Niedzwiedzki, D.N.
Deposited on : 2025-12-05
Resolution : 2.22 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

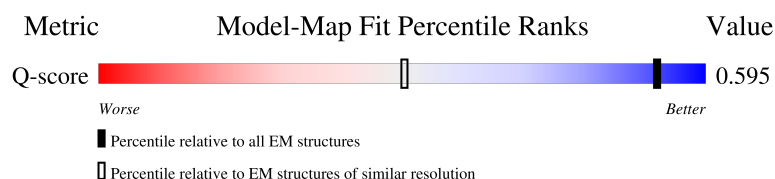
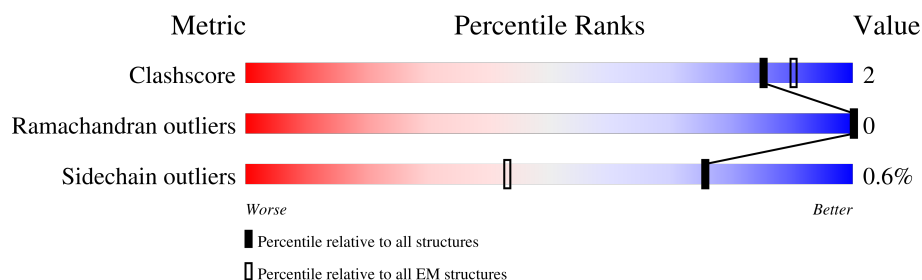
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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


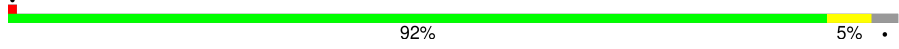
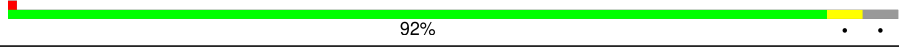
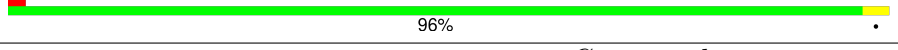
The reported resolution of this entry is 2.22 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3277 (1.73 - 2.72)

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

Mol	Chain	Length	Quality of chain
1	1	476	
2	2	342	
3	3	320	
4	4	342	

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Mol	Chain	Length	Quality of chain
4	5	342	
4	6	342	
4	7	342	
5	A	752	
6	B	740	
7	C	81	
8	D	139	
9	E	70	
10	F	164	
11	I	46	
12	J	49	
13	K	84	
14	M	32	
15	X	44	

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
17	LUT	1	518	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 49418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	465	Total	C	N	O	S	0	0
			3583	2375	577	623	8		

- Molecule 2 is a protein called Photosystem II CP43 protein PsbC homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	333	Total	C	N	O	S	0	0
			2607	1742	427	434	4		

- Molecule 3 is a protein called Photosystem II CP43 protein PsbC homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	306	Total	C	N	O	S	0	0
			2394	1595	396	399	4		

- Molecule 4 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	341	Total	C	N	O	S	0	0
			2660	1770	440	445	5		
4	5	332	Total	C	N	O	S	0	0
			2593	1728	429	431	5		
4	6	319	Total	C	N	O	S	0	0
			2469	1647	410	408	4		
4	7	314	Total	C	N	O	S	0	0
			2420	1615	401	400	4		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5824	3821	1003	979	21		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	135	Total	C	N	O	S	0	0
			1043	668	179	195	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	61	Total	C	N	O	0	0
			490	313	84	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	I	31	Total	C	N	O	0	0
			253	177	35	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	43	Total	C	N	O	0	0
			347	236	52	59		

- Molecule 13 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	72	Total	C	N	O	S	0	0
			524	352	82	89	1		

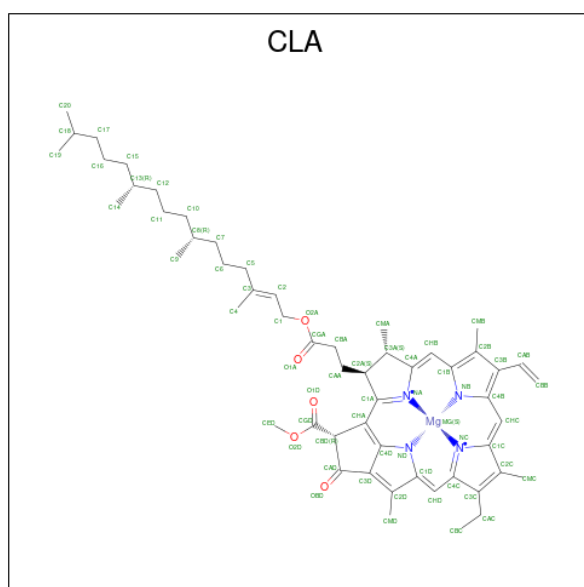
- Molecule 14 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	30	Total	C	N	O	0	0
			235	157	36	42		

- Molecule 15 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	29	Total	C	N	O	0	0
			243	170	37	36		

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			44	35	1	3	5	

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Mol	Chain	Residues	Atoms					AltConf
16	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	7	1	Total 63	C 53	Mg 1	N 4	O 5	0
16	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 59	C 49	Mg 1	N 4	O 5	0

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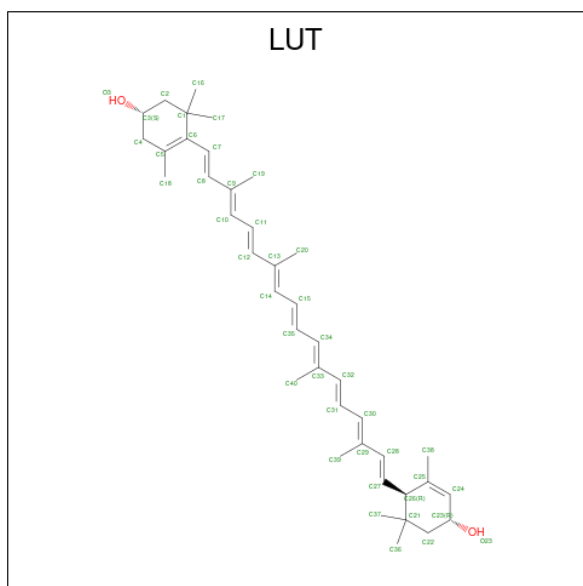
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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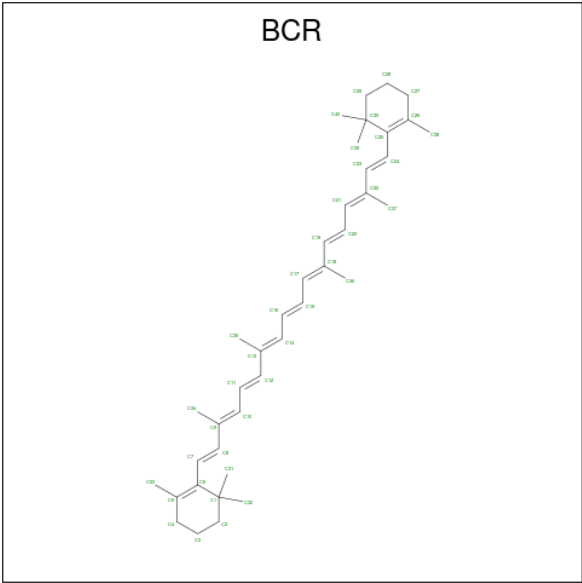
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 17 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
17	1	1	Total	C	O	0
			42	40	2	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	2	1	Total	C	0
			40	40	
18	2	1	Total	C	0
			40	40	
18	2	1	Total	C	0
			40	40	
18	3	1	Total	C	0
			40	40	
18	3	1	Total	C	0
			40	40	
18	3	1	Total	C	0
			40	40	

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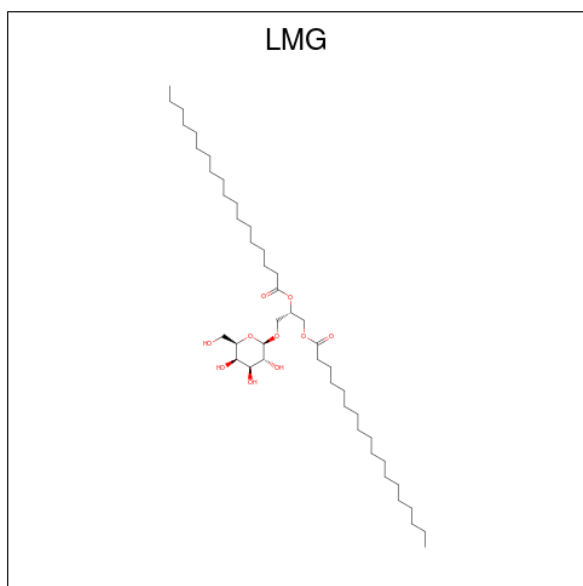
Mol	Chain	Residues	Atoms	AltConf
18	4	1	Total C 40 40	0
18	4	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	7	1	Total C 40 40	0
18	7	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0

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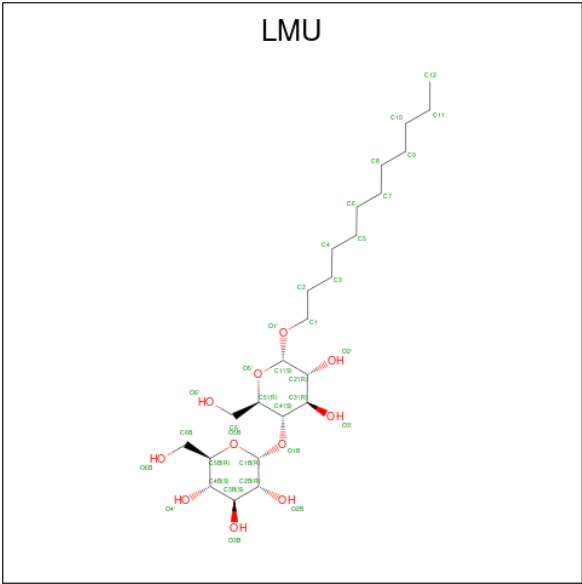
Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 40 40	0
18	M	1	Total C 40 40	0

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



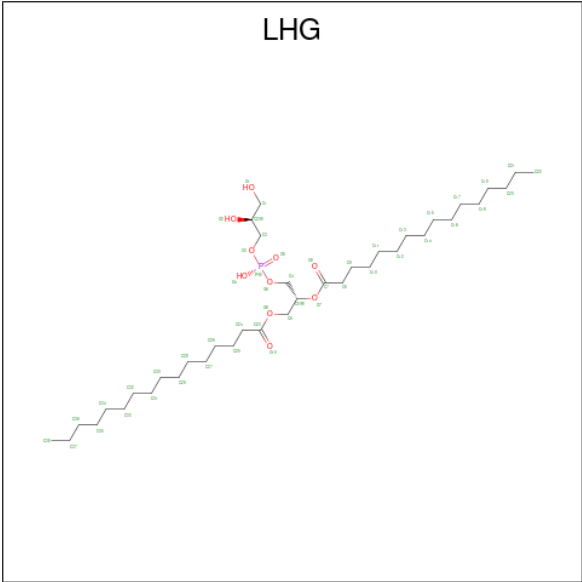
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			40	30	10	
19	5	1	Total	C	O	0
			43	33	10	
19	A	1	Total	C	O	0
			39	29	10	
19	B	1	Total	C	O	0
			54	44	10	

- Molecule 20 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



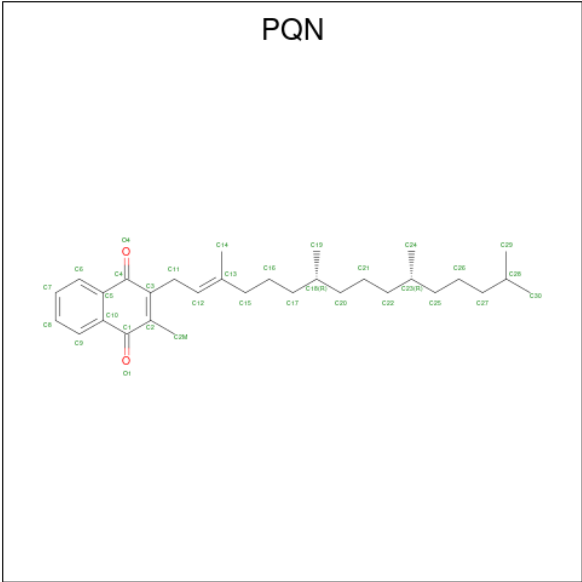
Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			35	24	11	
20	4	1	Total	C	O	0
			35	24	11	

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



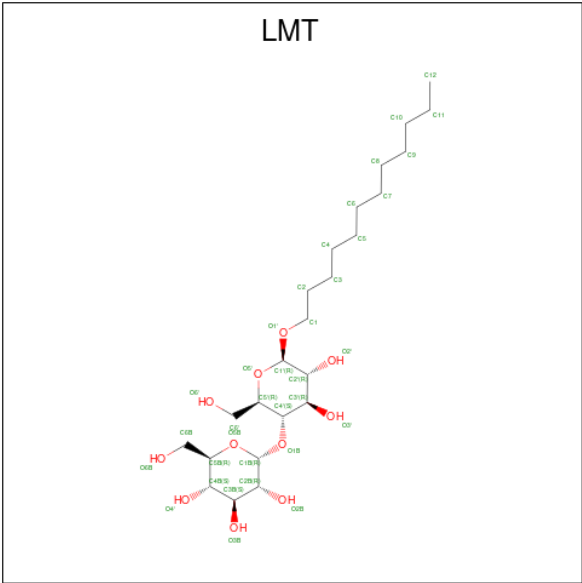
Mol	Chain	Residues	Atoms				AltConf
21	3	1	Total	C	O	P	0
			23	12	10	1	
21	4	1	Total	C	O	P	0
			23	12	10	1	
21	5	1	Total	C	O	P	0
			23	12	10	1	
21	5	1	Total	C	O	P	0
			23	12	10	1	
21	A	1	Total	C	O	P	0
			49	38	10	1	
21	A	1	Total	C	O	P	0
			27	16	10	1	
21	B	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Lig- and of Interest" by depositor).



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

- Molecule 23 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



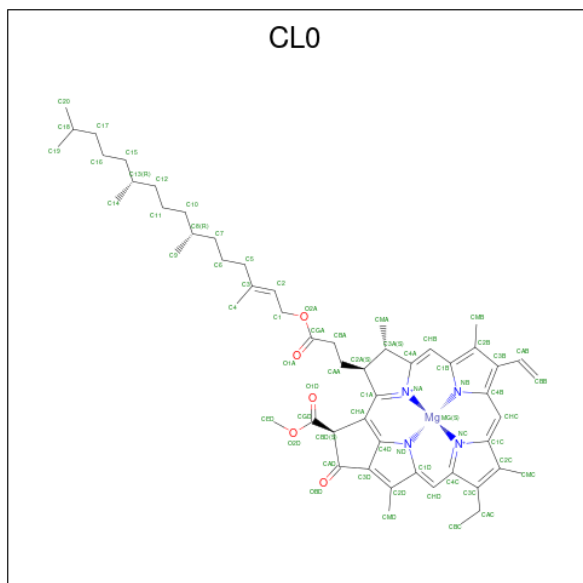
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			35	24	11	
23	B	1	Total	C	O	0
			35	24	11	

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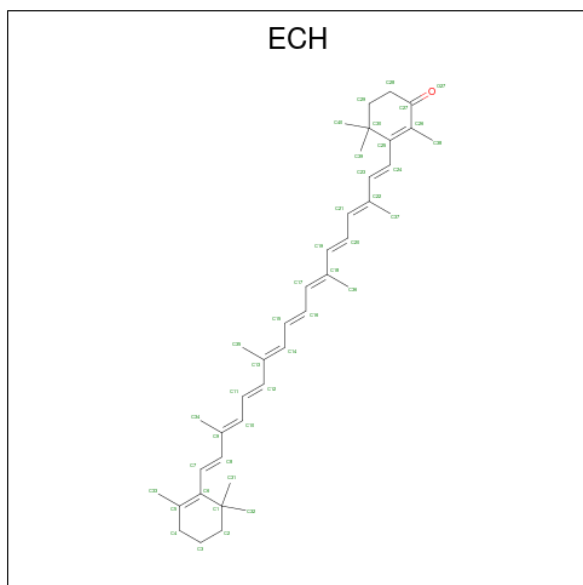
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			35	24	11	
23	I	1	Total	C	O	0
			35	24	11	

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



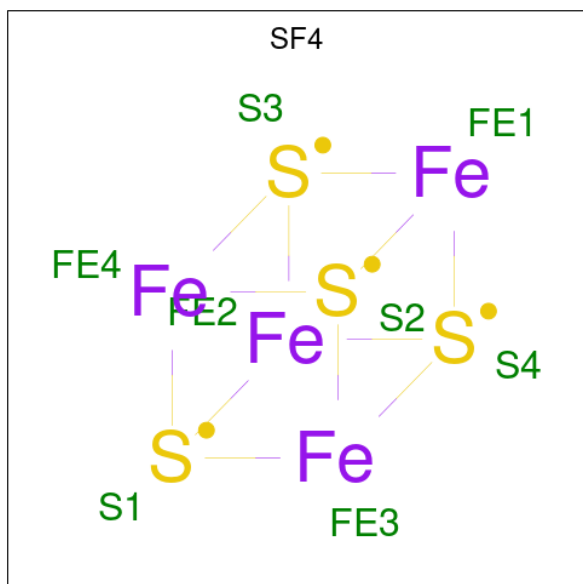
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			41	40	1	
25	A	1	Total	C	O	0
			41	40	1	
25	B	1	Total	C	O	0
			41	40	1	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

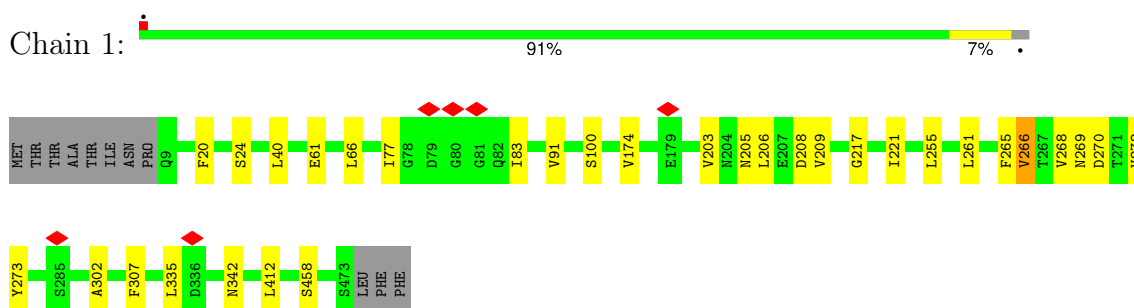


Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total 8	Fe 4	S 4	0
26	C	1	Total 8	Fe 4	S 4	0
26	C	1	Total 8	Fe 4	S 4	0

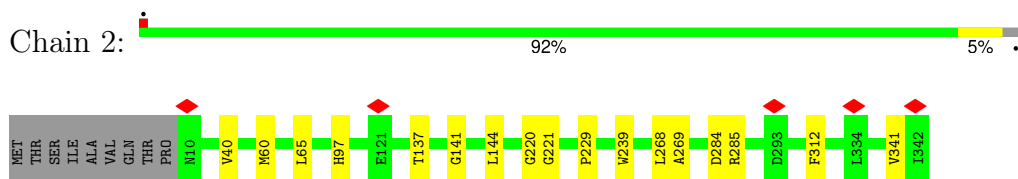
3 Residue-property plots

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

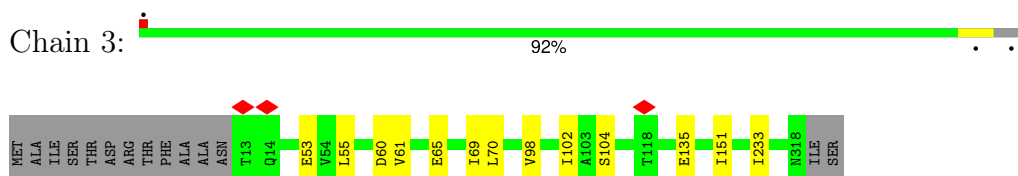
- Molecule 1: Photosystem I reaction center subunit XI



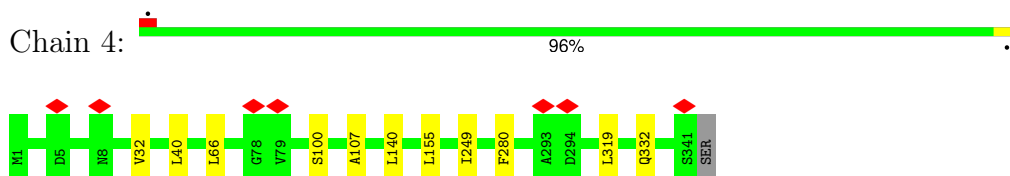
- Molecule 2: Photosystem II CP43 protein PsbC homolog



- Molecule 3: Photosystem II CP43 protein PsbC homolog



- Molecule 4: Iron stress-induced chlorophyll-binding protein



- Molecule 4: Iron stress-induced chlorophyll-binding protein





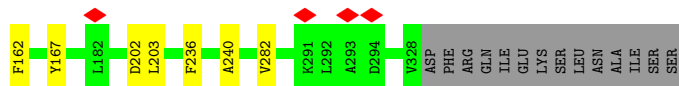
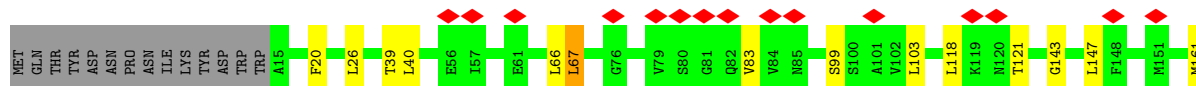
- Molecule 4: Iron stress-induced chlorophyll-binding protein

Chain 6: 89% 7%



- Molecule 4: Iron stress-induced chlorophyll-binding protein

Chain 7: 6% 86% 6% 8%



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 96%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B: 95% 5%



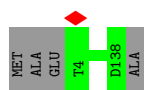
- Molecule 7: Photosystem I iron-sulfur center

Chain C: 99%



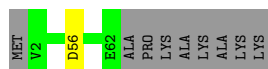
- Molecule 8: Photosystem I reaction center subunit II

Chain D: 97%



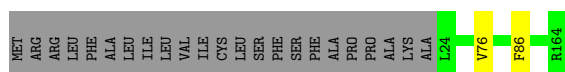
- Molecule 9: Photosystem I reaction center subunit IV

Chain E: 86% 13%



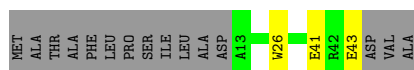
- Molecule 10: Photosystem I reaction center subunit III

Chain F: 85% 14%



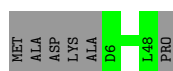
- Molecule 11: Photosystem I reaction center subunit VIII

Chain I: 61% 7% 33%



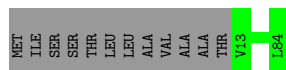
- Molecule 12: Photosystem I reaction center subunit IX

Chain J: 88% 12%



- Molecule 13: Photosystem I reaction center subunit PsaK

Chain K: 86% 14%



- Molecule 14: Photosystem I reaction center subunit XII

Chain M: 94% 6%



- Molecule 15: Photosystem I 4.8 kDa protein

Chain X: 61% 5% 34%

MET	ALA	LYS	ALA	LYS	ILE	SER	PRO	VAL	ALA	ASN	THR	GLY	ALA	LYS	P16	L34	I43	Q44
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	34.681	Depositor
Minimum map value	-14.026	Depositor
Average map value	0.021	Depositor
Map value standard deviation	1.154	Depositor
Recommended contour level	4.34	Depositor
Map size (\AA)	321.536, 321.536, 321.536	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.628, 0.628, 0.628	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1	0.10	0/3694	0.22	0/5048
2	2	0.09	0/2697	0.21	0/3680
3	3	0.11	0/2471	0.22	0/3379
4	4	0.11	0/2748	0.22	0/3747
4	5	0.12	0/2681	0.25	0/3657
4	6	0.11	0/2550	0.25	0/3476
4	7	0.09	0/2499	0.23	0/3407
5	A	0.12	0/6023	0.23	0/8216
6	B	0.11	0/6143	0.24	0/8398
7	C	0.10	0/609	0.24	0/826
8	D	0.09	0/1067	0.22	0/1441
9	E	0.09	0/499	0.21	0/677
10	F	0.10	0/1104	0.24	0/1500
11	I	0.13	0/262	0.29	0/358
12	J	0.10	0/358	0.20	0/490
13	K	0.10	0/539	0.23	0/739
14	M	0.09	0/239	0.18	0/326
15	X	0.09	0/253	0.22	0/347
All	All	0.11	0/36436	0.23	0/49712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3583	0	3560	23	0
2	2	2607	0	2581	10	0
3	3	2394	0	2396	8	0
4	4	2660	0	2643	9	0
4	5	2593	0	2570	8	0
4	6	2469	0	2465	8	0
4	7	2420	0	2414	16	0
5	A	5824	0	5703	17	0
6	B	5919	0	5679	22	0
7	C	599	0	585	0	0
8	D	1043	0	1049	0	0
9	E	490	0	484	1	0
10	F	1080	0	1076	1	0
11	I	253	0	255	4	0
12	J	347	0	352	0	0
13	K	524	0	558	0	0
14	M	235	0	251	0	0
15	X	243	0	244	1	0
16	1	1031	0	941	16	0
16	2	830	0	777	10	0
16	3	730	0	698	5	0
16	4	965	0	930	9	0
16	5	925	0	856	5	0
16	6	915	0	836	3	0
16	7	817	0	649	5	0
16	A	2379	0	2397	22	0
16	B	2493	0	2588	20	0
16	F	96	0	74	0	0
16	J	155	0	138	0	0
16	K	115	0	111	0	0
16	X	45	0	33	0	0
17	1	42	0	55	6	0
18	1	200	0	280	7	0
18	2	120	0	168	1	0
18	3	120	0	168	4	0
18	4	80	0	112	3	0
18	5	240	0	336	1	0
18	6	160	0	224	3	0
18	7	80	0	112	1	0
18	A	200	0	280	3	0
18	B	240	0	336	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	F	80	0	112	1	0
18	I	80	0	112	2	0
18	J	40	0	56	0	0
18	K	40	0	56	2	0
18	M	40	0	56	2	0
19	1	40	0	50	0	0
19	5	43	0	56	0	0
19	A	39	0	48	0	0
19	B	54	0	81	0	0
20	1	35	0	46	1	0
20	4	35	0	46	0	0
21	3	23	0	16	0	0
21	4	23	0	16	0	0
21	5	46	0	32	0	0
21	A	76	0	98	1	0
21	B	45	0	63	1	0
22	A	33	0	46	1	0
22	B	33	0	46	1	0
23	A	35	0	46	0	0
23	B	70	0	92	0	0
23	I	35	0	46	0	0
24	A	65	0	72	6	0
25	A	82	0	108	2	0
25	B	41	0	54	0	0
26	B	8	0	0	0	0
26	C	16	0	0	0	0
All	All	49418	0	49418	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 218 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)
17:1:518:LUT:H371	17:1:518:LUT:H28	1.66	0.75
4:5:291:LYS:HA	4:5:291:LYS:HE2	1.72	0.71
16:A:835:CLA:H143	22:B:803:PQN:H191	1.74	0.69
1:1:272:VAL:HG21	16:1:504:CLA:HMA2	1.76	0.65
4:6:258:TYR:O	4:6:262:VAL:HG22	1.97	0.65

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	463/476 (97%)	458 (99%)	5 (1%)	0	100	100
2	2	331/342 (97%)	321 (97%)	10 (3%)	0	100	100
3	3	304/320 (95%)	297 (98%)	7 (2%)	0	100	100
4	4	339/342 (99%)	330 (97%)	9 (3%)	0	100	100
4	5	330/342 (96%)	324 (98%)	6 (2%)	0	100	100
4	6	317/342 (93%)	312 (98%)	5 (2%)	0	100	100
4	7	312/342 (91%)	305 (98%)	7 (2%)	0	100	100
5	A	740/752 (98%)	726 (98%)	14 (2%)	0	100	100
6	B	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
9	E	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
10	F	139/164 (85%)	136 (98%)	3 (2%)	0	100	100
11	I	29/46 (63%)	29 (100%)	0	0	100	100
12	J	41/49 (84%)	41 (100%)	0	0	100	100
13	K	70/84 (83%)	68 (97%)	2 (3%)	0	100	100
14	M	28/32 (88%)	28 (100%)	0	0	100	100
15	X	27/44 (61%)	27 (100%)	0	0	100	100
All	All	4477/4707 (95%)	4389 (98%)	88 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	363/373 (97%)	356 (98%)	7 (2%)	50	64
2	2	263/271 (97%)	263 (100%)	0	100	100
3	3	243/254 (96%)	241 (99%)	2 (1%)	73	84
4	4	264/265 (100%)	262 (99%)	2 (1%)	73	84
4	5	256/265 (97%)	255 (100%)	1 (0%)	84	91
4	6	243/265 (92%)	242 (100%)	1 (0%)	84	91
4	7	237/265 (89%)	234 (99%)	3 (1%)	61	75
5	A	595/605 (98%)	595 (100%)	0	100	100
6	B	601/602 (100%)	598 (100%)	3 (0%)	81	89
7	C	68/69 (99%)	68 (100%)	0	100	100
8	D	108/110 (98%)	108 (100%)	0	100	100
9	E	54/60 (90%)	54 (100%)	0	100	100
10	F	110/129 (85%)	110 (100%)	0	100	100
11	I	28/39 (72%)	28 (100%)	0	100	100
12	J	38/42 (90%)	38 (100%)	0	100	100
13	K	57/66 (86%)	57 (100%)	0	100	100
14	M	25/27 (93%)	25 (100%)	0	100	100
15	X	24/34 (71%)	23 (96%)	1 (4%)	26	34
All	All	3577/3741 (96%)	3557 (99%)	20 (1%)	76	88

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	7	66	LEU
6	B	319	PHE
15	X	43	ILE
6	B	583	PHE
1	1	266	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
4	4	193	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	F	38	GLN
4	6	144	HIS
15	X	41	HIS
7	C	16	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

274 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	4	404	4	49,53,73	1.17	4 (8%)	58,89,113	0.98	2 (3%)
16	CLA	7	515	4	64,70,73	0.94	4 (6%)	74,108,113	0.95	4 (5%)
16	CLA	B	809	6	69,73,73	1.00	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	7	508	-	54,58,73	1.14	4 (7%)	64,95,113	1.08	5 (7%)
16	CLA	6	510	-	69,73,73	0.99	4 (5%)	82,113,113	0.86	1 (1%)
16	CLA	7	517	-	49,53,73	1.19	4 (8%)	58,89,113	1.06	4 (6%)
16	CLA	A	825	-	61,65,73	1.07	4 (6%)	72,103,113	1.00	3 (4%)
18	BCR	3	515	-	41,41,41	0.29	0	56,56,56	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LHG	5	425	16	22,22,48	0.70	0	25,28,54	0.63	0
16	CLA	6	515	4	69,73,73	1.00	4 (5%)	82,113,113	0.90	3 (3%)
16	CLA	7	502	-	49,53,73	1.21	5 (10%)	58,89,113	1.00	4 (6%)
16	CLA	5	403	4	49,53,73	1.19	4 (8%)	58,89,113	0.98	2 (3%)
16	CLA	7	507	-	49,53,73	1.19	4 (8%)	58,89,113	1.06	4 (6%)
21	LHG	A	803	16	26,26,48	0.67	0	29,32,54	0.61	0
16	CLA	B	838	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	5 (6%)
16	CLA	3	502	3	59,63,73	1.08	5 (8%)	70,101,113	0.90	2 (2%)
16	CLA	7	503	-	49,53,73	1.19	4 (8%)	58,89,113	1.15	5 (8%)
16	CLA	3	503	3	49,53,73	1.18	4 (8%)	58,89,113	0.92	1 (1%)
16	CLA	6	507	4	69,73,73	0.99	5 (7%)	82,113,113	0.93	4 (4%)
16	CLA	B	834	6	69,73,73	1.00	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	2	407	2	59,63,73	1.07	5 (8%)	70,101,113	1.08	6 (8%)
16	CLA	4	414	-	49,53,73	1.18	4 (8%)	58,89,113	1.13	3 (5%)
18	BCR	6	521	-	41,41,41	0.30	0	56,56,56	0.45	0
16	CLA	B	819	6	49,53,73	1.18	4 (8%)	58,89,113	0.95	1 (1%)
16	CLA	B	847	-	69,73,73	1.00	4 (5%)	82,113,113	0.96	6 (7%)
16	CLA	B	843	-	49,53,73	1.17	4 (8%)	58,89,113	0.98	1 (1%)
18	BCR	A	847	-	41,41,41	0.29	0	56,56,56	0.44	0
16	CLA	4	408	4	69,73,73	0.99	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	3	511	3	49,53,73	1.18	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	5	412	-	69,73,73	1.01	5 (7%)	82,113,113	0.89	3 (3%)
16	CLA	A	819	-	49,53,73	1.19	4 (8%)	58,89,113	0.97	0
16	CLA	6	512	-	49,53,73	1.20	4 (8%)	58,89,113	1.01	3 (5%)
16	CLA	4	416	4	69,73,73	1.00	4 (5%)	82,113,113	0.99	6 (7%)
16	CLA	6	505	4	69,73,73	1.00	5 (7%)	82,113,113	0.98	6 (7%)
16	CLA	A	822	5	69,73,73	0.97	4 (5%)	82,113,113	0.92	2 (2%)
16	CLA	A	826	5	55,59,73	1.11	4 (7%)	64,96,113	0.99	4 (6%)
16	CLA	1	526	21	49,53,73	1.18	4 (8%)	58,89,113	0.99	2 (3%)
16	CLA	4	410	4	64,68,73	1.04	4 (6%)	76,107,113	0.90	4 (5%)
16	CLA	A	837	5	55,59,73	1.10	4 (7%)	64,96,113	0.97	3 (4%)
18	BCR	1	519	-	41,41,41	0.27	0	56,56,56	0.61	0
18	BCR	3	516	-	41,41,41	0.29	0	56,56,56	0.52	0
16	CLA	A	810	5	54,58,73	1.11	4 (7%)	64,95,113	0.99	4 (6%)
18	BCR	6	520	-	41,41,41	0.29	0	56,56,56	0.60	0
18	BCR	M	101	-	41,41,41	0.30	0	56,56,56	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	4	413	4	49,53,73	1.18	4 (8%)	58,89,113	1.05	2 (3%)
16	CLA	7	509	4	64,68,73	1.04	4 (6%)	76,107,113	0.91	3 (3%)
16	CLA	1	511	1	49,53,73	1.20	4 (8%)	58,89,113	1.10	5 (8%)
16	CLA	A	833	5	69,73,73	0.98	5 (7%)	82,113,113	0.89	2 (2%)
16	CLA	B	813	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	1	515	1	50,54,73	1.16	4 (8%)	59,90,113	0.97	2 (3%)
16	CLA	4	403	4	59,63,73	1.08	4 (6%)	70,101,113	0.93	2 (2%)
16	CLA	B	824	6	63,67,73	1.03	4 (6%)	74,105,113	0.99	5 (6%)
16	CLA	B	829	-	59,63,73	1.08	4 (6%)	70,101,113	0.95	5 (7%)
16	CLA	1	517	-	59,63,73	1.08	4 (6%)	70,101,113	0.96	4 (5%)
16	CLA	B	841	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	3 (3%)
16	CLA	J	1102	12	49,53,73	1.18	4 (8%)	58,89,113	1.00	4 (6%)
16	CLA	3	504	3	69,73,73	1.01	5 (7%)	82,113,113	1.00	6 (7%)
16	CLA	A	827	5	51,55,73	1.15	4 (7%)	60,91,113	0.97	3 (5%)
16	CLA	B	839	6	69,73,73	0.99	4 (5%)	82,113,113	0.92	4 (4%)
16	CLA	2	406	-	69,73,73	1.00	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	3	512	3	49,53,73	1.20	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	1	503	-	69,73,73	1.00	4 (5%)	82,113,113	0.86	1 (1%)
16	CLA	B	820	6	69,73,73	0.99	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	B	826	-	69,73,73	1.00	5 (7%)	82,113,113	0.91	4 (4%)
16	CLA	B	828	6	49,53,73	1.21	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	A	842	5	69,73,73	0.98	3 (4%)	82,113,113	0.98	4 (4%)
18	BCR	4	419	-	41,41,41	0.31	0	56,56,56	0.56	0
21	LHG	4	421	-	22,22,48	0.69	0	25,28,54	0.66	0
26	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	A	828	-	69,73,73	1.00	3 (4%)	82,113,113	1.03	6 (7%)
16	CLA	A	840	5	69,73,73	1.00	5 (7%)	82,113,113	0.95	4 (4%)
16	CLA	B	812	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	4	411	-	69,73,73	1.00	4 (5%)	82,113,113	0.86	2 (2%)
16	CLA	6	508	4	59,63,73	1.08	4 (6%)	70,101,113	0.98	4 (5%)
16	CLA	6	514	-	49,53,73	1.19	4 (8%)	58,89,113	1.00	1 (1%)
16	CLA	A	841	5	69,73,73	0.98	3 (4%)	82,113,113	0.94	3 (3%)
18	BCR	F	203	-	41,41,41	0.30	0	56,56,56	0.82	1 (1%)
16	CLA	4	409	4	59,63,73	1.08	5 (8%)	70,101,113	1.01	4 (5%)
18	BCR	2	416	-	41,41,41	0.31	0	56,56,56	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	4	402	4	54,58,73	1.11	4 (7%)	64,95,113	1.01	3 (4%)
16	CLA	A	811	5	69,73,73	0.99	4 (5%)	82,113,113	1.04	5 (6%)
23	LMT	I	103	-	36,36,36	0.52	0	47,47,47	0.70	0
16	CLA	1	525	5	59,63,73	1.07	5 (8%)	70,101,113	0.98	3 (4%)
16	CLA	5	410	21,4	59,63,73	1.07	4 (6%)	70,101,113	1.03	5 (7%)
26	SF4	B	802	-	0,12,12	-	-	-	-	-
16	CLA	2	404	2	69,73,73	0.99	4 (5%)	82,113,113	0.91	2 (2%)
16	CLA	4	406	4	69,73,73	0.99	4 (5%)	82,113,113	1.00	4 (4%)
16	CLA	B	844	6	64,68,73	1.03	3 (4%)	76,107,113	0.99	6 (7%)
16	CLA	A	809	5	69,73,73	1.00	4 (5%)	82,113,113	0.95	3 (3%)
18	BCR	B	854	-	41,41,41	0.30	0	56,56,56	0.68	0
16	CLA	1	516	1	64,68,73	1.02	4 (6%)	76,107,113	0.94	1 (1%)
16	CLA	2	412	-	49,53,73	1.18	4 (8%)	58,89,113	1.00	2 (3%)
16	CLA	1	505	-	64,68,73	1.04	5 (7%)	76,107,113	1.03	6 (7%)
18	BCR	2	418	-	41,41,41	0.28	0	56,56,56	0.52	0
21	LHG	5	424	-	22,22,48	0.71	0	25,28,54	0.63	0
16	CLA	4	417	-	64,68,73	1.04	4 (6%)	76,107,113	0.95	5 (6%)
16	CLA	A	823	5	54,58,73	1.13	5 (9%)	64,95,113	1.06	6 (9%)
16	CLA	B	816	6	69,73,73	0.99	4 (5%)	82,113,113	0.88	1 (1%)
16	CLA	B	835	6	69,73,73	0.99	4 (5%)	82,113,113	0.94	6 (7%)
16	CLA	2	405	2	69,73,73	0.99	4 (5%)	82,113,113	0.98	4 (4%)
16	CLA	3	507	-	59,63,73	1.08	4 (6%)	70,101,113	0.92	3 (4%)
16	CLA	7	505	4	49,53,73	1.19	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	7	510	-	49,53,73	1.19	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	5	418	4	49,53,73	1.18	4 (8%)	58,89,113	1.06	5 (8%)
16	CLA	B	814	6	69,73,73	1.01	6 (8%)	82,113,113	0.94	4 (4%)
16	CLA	6	504	4	69,73,73	1.00	5 (7%)	82,113,113	0.98	5 (6%)
18	BCR	5	421	-	41,41,41	0.28	0	56,56,56	0.71	0
18	BCR	5	422	-	41,41,41	0.28	0	56,56,56	0.68	2 (3%)
16	CLA	A	852	-	69,73,73	1.00	4 (5%)	82,113,113	0.94	4 (4%)
18	BCR	5	402	-	41,41,41	0.29	0	56,56,56	0.46	0
19	LMG	A	851	-	39,39,55	0.55	0	47,47,63	0.62	0
16	CLA	B	833	6	69,73,73	1.00	4 (5%)	82,113,113	0.90	4 (4%)
16	CLA	A	818	5	49,53,73	1.18	4 (8%)	58,89,113	0.97	3 (5%)
16	CLA	2	414	2	49,53,73	1.18	5 (10%)	58,89,113	1.04	1 (1%)
16	CLA	1	510	1	64,68,73	1.04	4 (6%)	76,107,113	0.98	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	4	401	-	36,36,36	0.45	0	47,47,47	0.81	1 (2%)
16	CLA	B	825	6	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
16	CLA	4	415	-	69,73,73	1.01	4 (5%)	82,113,113	0.92	4 (4%)
16	CLA	A	843	5	69,73,73	0.99	4 (5%)	82,113,113	0.91	5 (6%)
16	CLA	A	806	-	69,73,73	1.01	4 (5%)	82,113,113	0.93	5 (6%)
16	CLA	2	408	2	64,68,73	1.05	4 (6%)	76,107,113	0.89	3 (3%)
16	CLA	1	506	1	69,73,73	0.99	4 (5%)	82,113,113	0.89	4 (4%)
16	CLA	5	417	4	69,73,73	1.00	5 (7%)	82,113,113	0.94	4 (4%)
16	CLA	6	509	4	64,68,73	1.05	5 (7%)	76,107,113	0.95	2 (2%)
16	CLA	2	410	2	64,68,73	1.04	5 (7%)	76,107,113	1.09	5 (6%)
16	CLA	7	512	4	49,53,73	1.18	4 (8%)	58,89,113	1.05	1 (1%)
25	ECH	A	853	-	42,42,42	0.35	0	55,58,58	0.69	0
16	CLA	B	815	6	69,73,73	0.99	4 (5%)	82,113,113	1.00	4 (4%)
18	BCR	B	853	-	41,41,41	0.29	0	56,56,56	0.44	0
18	BCR	B	850	-	41,41,41	0.29	0	56,56,56	0.54	0
21	LHG	B	806	-	44,44,48	0.53	0	47,50,54	0.51	0
16	CLA	B	846	6	69,73,73	0.99	4 (5%)	82,113,113	0.92	4 (4%)
16	CLA	2	403	-	69,73,73	1.01	4 (5%)	82,113,113	0.93	3 (3%)
18	BCR	A	845	-	41,41,41	0.32	0	56,56,56	0.71	1 (1%)
16	CLA	1	512	-	49,53,73	1.19	4 (8%)	58,89,113	1.01	3 (5%)
18	BCR	K	101	-	41,41,41	0.30	0	56,56,56	0.44	0
16	CLA	F	201	-	55,59,73	1.10	4 (7%)	64,96,113	1.02	5 (7%)
25	ECH	A	848	-	42,42,42	0.35	0	55,58,58	0.71	0
16	CLA	A	832	5	69,73,73	0.99	5 (7%)	82,113,113	0.94	5 (6%)
25	ECH	B	851	-	42,42,42	0.36	0	55,58,58	0.92	2 (3%)
16	CLA	3	508	3	64,68,73	1.04	4 (6%)	76,107,113	0.91	2 (2%)
16	CLA	B	830	6	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	A	808	5	69,73,73	0.99	4 (5%)	82,113,113	0.96	4 (4%)
16	CLA	5	408	4	64,68,73	1.03	5 (7%)	76,107,113	0.94	1 (1%)
16	CLA	B	801	-	69,73,73	0.99	4 (5%)	82,113,113	0.90	2 (2%)
16	CLA	5	407	4	69,73,73	0.99	4 (5%)	82,113,113	0.90	3 (3%)
16	CLA	6	513	-	49,53,73	1.18	5 (10%)	58,89,113	1.06	4 (6%)
16	CLA	A	812	5	69,73,73	0.98	4 (5%)	82,113,113	0.92	2 (2%)
16	CLA	2	411	2	49,53,73	1.17	4 (8%)	58,89,113	1.02	3 (5%)
16	CLA	6	501	4	54,58,73	1.12	4 (7%)	64,95,113	1.06	5 (7%)
18	BCR	4	420	-	41,41,41	0.29	0	56,56,56	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LMG	B	805	-	54,54,55	0.50	0	62,62,63	0.57	0
24	CL0	A	805	5	58,73,73	1.87	6 (10%)	60,113,113	1.48	9 (15%)
16	CLA	1	504	1	69,73,73	1.00	4 (5%)	82,113,113	1.00	2 (2%)
16	CLA	2	402	2	49,53,73	1.20	5 (10%)	58,89,113	1.07	3 (5%)
16	CLA	6	506	4	64,68,73	1.02	4 (6%)	76,107,113	0.95	4 (5%)
18	BCR	1	523	-	41,41,41	0.31	0	56,56,56	0.50	0
18	BCR	5	423	-	41,41,41	0.29	0	56,56,56	0.46	0
16	CLA	B	842	-	49,53,73	1.18	4 (8%)	58,89,113	0.97	3 (5%)
20	LMU	1	527	-	36,36,36	0.46	0	47,47,47	0.62	0
16	CLA	5	405	4	49,53,73	1.19	4 (8%)	58,89,113	0.95	0
16	CLA	5	414	4	49,53,73	1.19	4 (8%)	58,89,113	1.07	2 (3%)
16	CLA	B	837	6	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
16	CLA	A	814	5,16	69,73,73	0.99	4 (5%)	82,113,113	0.97	4 (4%)
21	LHG	A	802	-	48,48,48	0.51	0	51,54,54	0.49	0
16	CLA	5	419	4	49,53,73	1.18	4 (8%)	58,89,113	1.00	2 (3%)
16	CLA	B	836	6	69,73,73	0.98	4 (5%)	82,113,113	0.98	5 (6%)
18	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.49	0
23	LMT	B	807	-	36,36,36	0.52	0	47,47,47	0.71	0
22	PQN	A	801	-	34,34,34	0.36	0	43,45,45	0.66	1 (2%)
18	BCR	6	518	-	41,41,41	0.32	0	56,56,56	0.51	0
18	BCR	A	850	-	41,41,41	0.28	0	56,56,56	0.48	0
16	CLA	A	829	-	59,63,73	1.06	4 (6%)	70,101,113	0.95	5 (7%)
16	CLA	A	836	5	69,73,73	0.99	4 (5%)	82,113,113	0.95	5 (6%)
18	BCR	5	420	-	41,41,41	0.32	0	56,56,56	0.68	1 (1%)
16	CLA	5	406	4	69,73,73	1.00	4 (5%)	82,113,113	0.95	5 (6%)
16	CLA	J	1103	12	49,53,73	1.19	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	K	103	13	69,73,73	1.00	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	A	807	5,16	58,62,73	1.08	4 (6%)	68,99,113	0.99	3 (4%)
16	CLA	4	405	4	69,73,73	0.99	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	7	516	4	49,53,73	1.20	5 (10%)	58,89,113	1.04	3 (5%)
16	CLA	A	839	5	55,59,73	1.11	4 (7%)	64,96,113	1.00	3 (4%)
18	BCR	3	514	-	41,41,41	0.28	0	56,56,56	0.56	0
17	LUT	1	518	-	42,43,43	0.81	0	51,60,60	1.61	9 (17%)
16	CLA	3	509	-	69,73,73	1.00	5 (7%)	82,113,113	1.02	7 (8%)
16	CLA	5	411	4	64,68,73	1.04	5 (7%)	76,107,113	0.96	5 (6%)
16	CLA	K	102	-	54,58,73	1.12	4 (7%)	64,95,113	1.01	4 (6%)
16	CLA	4	412	4	54,58,73	1.13	4 (7%)	64,95,113	1.01	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMT	B	808	-	36,36,36	0.53	0	47,47,47	0.78	1 (2%)
16	CLA	B	832	-	69,73,73	0.98	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	5	409	4	69,73,73	1.00	4 (5%)	82,113,113	0.93	5 (6%)
23	LMT	A	804	-	36,36,36	0.53	0	47,47,47	0.74	0
16	CLA	A	821	5	58,62,73	1.07	5 (8%)	68,99,113	0.97	3 (4%)
16	CLA	7	504	4	49,53,73	1.19	4 (8%)	58,89,113	0.99	2 (3%)
16	CLA	2	413	2	64,68,73	1.04	4 (6%)	76,107,113	0.98	4 (5%)
19	LMG	5	426	-	43,43,55	0.54	0	51,51,63	0.64	0
21	LHG	3	517	-	22,22,48	0.70	0	25,28,54	0.64	0
16	CLA	3	505	3	69,73,73	0.99	5 (7%)	82,113,113	1.00	3 (3%)
16	CLA	A	816	5	69,73,73	0.99	5 (7%)	82,113,113	0.97	4 (4%)
16	CLA	A	838	5	59,63,73	1.08	4 (6%)	70,101,113	0.96	4 (5%)
16	CLA	1	502	1	59,63,73	1.09	4 (6%)	70,101,113	0.89	3 (4%)
16	CLA	A	835	5	69,73,73	1.00	5 (7%)	82,113,113	0.97	4 (4%)
16	CLA	B	818	6	69,73,73	1.01	4 (5%)	82,113,113	0.91	1 (1%)
16	CLA	1	509	1	64,68,73	1.03	4 (6%)	76,107,113	0.94	3 (3%)
16	CLA	2	415	2	49,53,73	1.17	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	B	845	-	69,73,73	0.98	4 (5%)	82,113,113	0.91	4 (4%)
19	LMG	1	524	-	40,40,55	0.56	0	48,48,63	0.62	0
18	BCR	1	520	-	41,41,41	0.28	0	56,56,56	0.68	1 (1%)
16	CLA	6	502	4	54,58,73	1.11	4 (7%)	64,95,113	1.02	5 (7%)
16	CLA	1	514	1	54,58,73	1.14	4 (7%)	64,95,113	0.94	5 (7%)
16	CLA	5	404	4	54,58,73	1.12	4 (7%)	64,95,113	0.99	4 (6%)
18	BCR	6	519	-	41,41,41	0.31	0	56,56,56	0.43	0
16	CLA	A	831	5	69,73,73	1.00	5 (7%)	82,113,113	0.93	5 (6%)
18	BCR	A	849	-	41,41,41	0.29	0	56,56,56	0.61	0
18	BCR	A	846	-	41,41,41	0.28	0	56,56,56	0.45	0
18	BCR	B	804	-	41,41,41	0.29	0	56,56,56	0.53	0
18	BCR	1	521	-	41,41,41	0.30	0	56,56,56	0.58	1 (1%)
16	CLA	4	418	4	49,53,73	1.19	5 (10%)	58,89,113	1.06	5 (8%)
18	BCR	2	417	-	41,41,41	0.28	0	56,56,56	0.54	0
16	CLA	B	810	-	69,73,73	1.00	5 (7%)	82,113,113	0.97	4 (4%)
16	CLA	3	506	-	69,73,73	1.00	3 (4%)	82,113,113	0.87	4 (4%)
16	CLA	1	508	-	69,73,73	1.01	4 (5%)	82,113,113	1.03	6 (7%)
16	CLA	6	511	4	49,53,73	1.18	5 (10%)	58,89,113	0.96	2 (3%)
16	CLA	4	407	4	69,73,73	0.99	5 (7%)	82,113,113	1.03	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	6	517	4	49,53,73	1.18	4 (8%)	58,89,113	1.06	3 (5%)
18	BCR	F	204	-	41,41,41	0.29	0	56,56,56	0.49	0
16	CLA	5	413	4	64,68,73	1.05	5 (7%)	76,107,113	0.99	5 (6%)
16	CLA	3	513	3	49,53,73	1.18	4 (8%)	58,89,113	0.96	1 (1%)
16	CLA	A	830	5	69,73,73	1.01	4 (5%)	82,113,113	0.92	5 (6%)
16	CLA	J	1101	5	69,73,73	1.00	4 (5%)	82,113,113	0.84	3 (3%)
16	CLA	A	813	5	59,63,73	1.06	4 (6%)	70,101,113	1.04	4 (5%)
16	CLA	6	503	4	49,53,73	1.18	4 (8%)	58,89,113	0.98	0
16	CLA	1	501	1	49,53,73	1.18	4 (8%)	58,89,113	0.96	2 (3%)
18	BCR	5	401	-	41,41,41	0.29	0	56,56,56	0.70	0
16	CLA	7	514	-	49,53,73	1.19	4 (8%)	58,89,113	1.04	2 (3%)
16	CLA	A	834	5	64,68,73	1.03	4 (6%)	76,107,113	0.88	2 (2%)
18	BCR	1	522	-	41,41,41	0.30	0	56,56,56	0.74	0
16	CLA	A	844	-	69,73,73	0.98	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	B	822	6	49,53,73	1.18	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	A	815	5	64,68,73	1.03	5 (7%)	76,107,113	1.08	7 (9%)
16	CLA	B	821	6	60,64,73	1.06	4 (6%)	71,102,113	0.98	5 (7%)
18	BCR	I	101	-	41,41,41	0.30	0	56,56,56	0.66	0
16	CLA	B	840	6	62,66,73	1.04	4 (6%)	73,104,113	0.92	1 (1%)
26	SF4	C	101	-	0,12,12	-	-	-	-	-
16	CLA	7	501	-	49,53,73	1.22	5 (10%)	58,89,113	0.99	2 (3%)
16	CLA	3	510	3	59,63,73	1.09	4 (6%)	70,101,113	1.06	5 (7%)
16	CLA	7	506	4	64,68,73	1.06	5 (7%)	76,107,113	0.94	4 (5%)
16	CLA	3	501	3	69,73,73	1.00	4 (5%)	82,113,113	0.98	3 (3%)
16	CLA	7	511	4	41,50,73	1.40	3 (7%)	49,79,113	1.22	2 (4%)
16	CLA	2	401	2	59,63,73	1.08	5 (8%)	70,101,113	0.92	3 (4%)
16	CLA	5	415	-	49,53,73	1.19	4 (8%)	58,89,113	1.00	2 (3%)
16	CLA	7	513	-	49,53,73	1.19	5 (10%)	58,89,113	1.10	4 (6%)
16	CLA	B	817	6	64,68,73	1.04	4 (6%)	76,107,113	0.90	2 (2%)
18	BCR	B	849	-	41,41,41	0.32	0	56,56,56	0.85	3 (5%)
16	CLA	B	848	6	69,73,73	0.98	3 (4%)	82,113,113	1.07	6 (7%)
16	CLA	B	823	6	59,63,73	1.06	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	1	507	1	49,53,73	1.17	5 (10%)	58,89,113	0.98	3 (5%)
16	CLA	6	516	4	49,53,73	1.16	4 (8%)	58,89,113	0.99	1 (1%)
16	CLA	1	513	1	49,53,73	1.19	4 (8%)	58,89,113	0.99	1 (1%)
16	CLA	B	827	6	60,64,73	1.07	4 (6%)	71,102,113	0.92	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	811	6	58,62,73	1.07	4 (6%)	68,99,113	0.94	2 (2%)
16	CLA	A	817	5	59,63,73	1.07	5 (8%)	70,101,113	0.96	3 (4%)
16	CLA	2	409	-	59,63,73	1.08	4 (6%)	70,101,113	1.01	3 (4%)
16	CLA	A	820	5	58,62,73	1.08	4 (6%)	68,99,113	0.97	4 (5%)
16	CLA	X	101	15	49,53,73	1.19	4 (8%)	58,89,113	0.99	2 (3%)
18	BCR	B	852	-	41,41,41	0.28	0	56,56,56	0.68	0
18	BCR	J	1104	-	41,41,41	0.29	0	56,56,56	0.64	0
18	BCR	7	519	-	41,41,41	0.29	0	56,56,56	0.51	0
18	BCR	7	518	-	41,41,41	0.30	0	56,56,56	0.44	0
22	PQN	B	803	-	34,34,34	0.37	0	43,45,45	0.69	1 (2%)
16	CLA	F	202	-	49,53,73	1.18	4 (8%)	58,89,113	0.94	2 (3%)
16	CLA	B	831	6	69,73,73	1.00	5 (7%)	82,113,113	0.95	3 (3%)
16	CLA	5	416	-	49,53,73	1.18	4 (8%)	58,89,113	1.04	2 (3%)
16	CLA	A	824	-	69,73,73	0.97	4 (5%)	82,113,113	0.95	4 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	4	404	4	-	2/15/91/115	-
16	CLA	7	515	4	-	12/33/109/115	-
16	CLA	B	809	6	-	7/39/115/115	-
16	CLA	7	508	-	-	10/21/97/115	-
16	CLA	6	510	-	-	9/39/115/115	-
16	CLA	7	517	-	-	4/15/91/115	-
16	CLA	A	825	-	-	2/30/106/115	-
18	BCR	3	515	-	-	10/29/63/63	0/2/2/2
21	LHG	5	425	16	-	2/27/27/53	-
16	CLA	6	515	4	-	11/39/115/115	-
16	CLA	7	502	-	-	5/15/91/115	-
16	CLA	5	403	4	-	4/15/91/115	-
16	CLA	7	507	-	-	6/15/91/115	-
21	LHG	A	803	16	-	5/31/31/53	-
16	CLA	B	838	6	-	9/39/115/115	-
16	CLA	3	502	3	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	7	503	-	-	5/15/91/115	-
16	CLA	3	503	3	-	4/15/91/115	-
16	CLA	6	507	4	-	12/39/115/115	-
16	CLA	B	834	6	-	9/39/115/115	-
16	CLA	2	407	2	-	11/27/103/115	-
16	CLA	4	414	-	-	7/15/91/115	-
18	BCR	6	521	-	-	8/29/63/63	0/2/2/2
16	CLA	B	819	6	-	5/15/91/115	-
16	CLA	B	847	-	-	8/39/115/115	-
16	CLA	B	843	-	-	5/15/91/115	-
18	BCR	A	847	-	-	3/29/63/63	0/2/2/2
16	CLA	4	408	4	-	9/39/115/115	-
16	CLA	3	511	3	-	7/15/91/115	-
16	CLA	5	412	-	-	14/39/115/115	-
16	CLA	A	819	-	-	3/15/91/115	-
16	CLA	6	512	-	-	7/15/91/115	-
16	CLA	4	416	4	-	9/39/115/115	-
16	CLA	6	505	4	-	11/39/115/115	-
16	CLA	A	822	5	-	5/39/115/115	-
16	CLA	A	826	5	-	2/23/99/115	-
16	CLA	1	526	21	-	4/15/91/115	-
16	CLA	4	410	4	-	9/33/109/115	-
16	CLA	A	837	5	-	7/23/99/115	-
18	BCR	1	519	-	-	3/29/63/63	0/2/2/2
18	BCR	3	516	-	-	2/29/63/63	0/2/2/2
16	CLA	A	810	5	-	6/21/97/115	-
18	BCR	6	520	-	-	3/29/63/63	0/2/2/2
18	BCR	M	101	-	-	5/29/63/63	0/2/2/2
16	CLA	4	413	4	-	2/15/91/115	-
16	CLA	7	509	4	-	12/33/109/115	-
16	CLA	1	511	1	-	5/15/91/115	-
16	CLA	A	833	5	-	10/39/115/115	-
16	CLA	B	813	6	-	11/39/115/115	-
16	CLA	1	515	1	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	4	403	4	-	5/27/103/115	-
16	CLA	B	824	6	-	5/32/108/115	-
16	CLA	B	829	-	-	4/27/103/115	-
16	CLA	1	517	-	-	10/27/103/115	-
16	CLA	B	841	6	-	11/39/115/115	-
16	CLA	J	1102	12	-	3/15/91/115	-
16	CLA	3	504	3	-	10/39/115/115	-
16	CLA	A	827	5	-	8/18/94/115	-
16	CLA	B	839	6	-	12/39/115/115	-
16	CLA	2	406	-	-	15/39/115/115	-
16	CLA	3	512	3	-	10/15/91/115	-
16	CLA	1	503	-	-	10/39/115/115	-
16	CLA	B	820	6	-	6/39/115/115	-
16	CLA	B	826	-	-	6/39/115/115	-
16	CLA	B	828	6	-	6/15/91/115	-
16	CLA	A	842	5	-	16/39/115/115	-
18	BCR	4	419	-	-	11/29/63/63	0/2/2/2
21	LHG	4	421	-	-	5/27/27/53	-
26	SF4	C	102	-	-	-	0/6/5/5
16	CLA	A	828	-	-	14/39/115/115	-
16	CLA	A	840	5	-	15/39/115/115	-
16	CLA	B	812	6	-	8/39/115/115	-
16	CLA	4	411	-	-	16/39/115/115	-
16	CLA	6	508	4	-	15/27/103/115	-
16	CLA	6	514	-	-	5/15/91/115	-
16	CLA	A	841	5	-	15/39/115/115	-
18	BCR	F	203	-	-	6/29/63/63	0/2/2/2
16	CLA	4	409	4	-	9/27/103/115	-
18	BCR	2	416	-	-	7/29/63/63	0/2/2/2
16	CLA	4	402	4	-	6/21/97/115	-
16	CLA	A	811	5	-	11/39/115/115	-
23	LMT	I	103	-	-	10/21/61/61	0/2/2/2
16	CLA	1	525	5	-	4/27/103/115	-
16	CLA	5	410	21,4	-	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SF4	B	802	-	-	-	0/6/5/5
16	CLA	2	404	2	-	14/39/115/115	-
16	CLA	4	406	4	-	15/39/115/115	-
16	CLA	B	844	6	-	5/33/109/115	-
16	CLA	A	809	5	-	12/39/115/115	-
18	BCR	B	854	-	-	0/29/63/63	0/2/2/2
16	CLA	1	516	1	-	9/33/109/115	-
16	CLA	2	412	-	-	7/15/91/115	-
16	CLA	1	505	-	-	13/33/109/115	-
18	BCR	2	418	-	-	7/29/63/63	0/2/2/2
21	LHG	5	424	-	-	8/27/27/53	-
16	CLA	4	417	-	-	10/33/109/115	-
16	CLA	A	823	5	-	4/21/97/115	-
16	CLA	B	816	6	-	16/39/115/115	-
16	CLA	B	835	6	-	11/39/115/115	-
16	CLA	2	405	2	-	5/39/115/115	-
16	CLA	3	507	-	-	6/27/103/115	-
16	CLA	7	505	4	-	8/15/91/115	-
16	CLA	7	510	-	-	8/15/91/115	-
16	CLA	5	418	4	-	7/15/91/115	-
16	CLA	B	814	6	-	9/39/115/115	-
16	CLA	6	504	4	-	12/39/115/115	-
18	BCR	5	421	-	-	4/29/63/63	0/2/2/2
18	BCR	5	422	-	-	2/29/63/63	0/2/2/2
16	CLA	A	852	-	-	7/39/115/115	-
18	BCR	5	402	-	-	2/29/63/63	0/2/2/2
19	LMG	A	851	-	-	9/34/54/70	0/1/1/1
16	CLA	B	833	6	-	3/39/115/115	-
16	CLA	A	818	5	-	4/15/91/115	-
16	CLA	2	414	2	-	8/15/91/115	-
16	CLA	1	510	1	-	8/33/109/115	-
20	LMU	4	401	-	-	5/21/61/61	0/2/2/2
16	CLA	B	825	6	-	14/39/115/115	-
16	CLA	4	415	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	843	5	-	6/39/115/115	-
16	CLA	A	806	-	-	5/39/115/115	-
16	CLA	2	408	2	-	13/33/109/115	-
16	CLA	1	506	1	-	6/39/115/115	-
16	CLA	5	417	4	-	14/39/115/115	-
16	CLA	6	509	4	-	9/33/109/115	-
16	CLA	2	410	2	-	11/33/109/115	-
16	CLA	7	512	4	-	4/15/91/115	-
25	ECH	A	853	-	-	8/29/66/66	0/2/2/2
16	CLA	B	815	6	-	11/39/115/115	-
18	BCR	B	853	-	-	6/29/63/63	0/2/2/2
18	BCR	B	850	-	-	9/29/63/63	0/2/2/2
21	LHG	B	806	-	-	7/49/49/53	-
16	CLA	B	846	6	-	11/39/115/115	-
16	CLA	2	403	-	-	10/39/115/115	-
18	BCR	A	845	-	-	5/29/63/63	0/2/2/2
16	CLA	1	512	-	-	4/15/91/115	-
18	BCR	K	101	-	-	4/29/63/63	0/2/2/2
16	CLA	F	201	-	-	5/23/99/115	-
25	ECH	A	848	-	-	3/29/66/66	0/2/2/2
16	CLA	A	832	5	-	3/39/115/115	-
25	ECH	B	851	-	-	11/29/66/66	0/2/2/2
16	CLA	3	508	3	-	7/33/109/115	-
16	CLA	B	830	6	-	9/39/115/115	-
16	CLA	A	808	5	-	10/39/115/115	-
16	CLA	5	408	4	-	11/33/109/115	-
16	CLA	B	801	-	-	2/39/115/115	-
16	CLA	5	407	4	-	15/39/115/115	-
16	CLA	6	513	-	-	6/15/91/115	-
16	CLA	A	812	5	-	14/39/115/115	-
16	CLA	2	411	2	-	5/15/91/115	-
16	CLA	6	501	4	-	5/21/97/115	-
18	BCR	4	420	-	-	2/29/63/63	0/2/2/2
19	LMG	B	805	-	-	11/49/69/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CL0	A	805	5	-	9/37/135/135	-
16	CLA	1	504	1	-	7/39/115/115	-
16	CLA	2	402	2	-	4/15/91/115	-
16	CLA	6	506	4	-	6/33/109/115	-
18	BCR	1	523	-	-	5/29/63/63	0/2/2/2
18	BCR	5	423	-	-	3/29/63/63	0/2/2/2
16	CLA	B	842	-	-	1/15/91/115	-
20	LMU	1	527	-	-	9/21/61/61	0/2/2/2
16	CLA	5	405	4	-	3/15/91/115	-
16	CLA	5	414	4	-	6/15/91/115	-
16	CLA	B	837	6	-	17/39/115/115	-
16	CLA	A	814	5,16	-	12/39/115/115	-
21	LHG	A	802	-	-	15/53/53/53	-
16	CLA	5	419	4	-	2/15/91/115	-
16	CLA	B	836	6	-	10/39/115/115	-
18	BCR	I	102	-	-	9/29/63/63	0/2/2/2
23	LMT	B	807	-	-	6/21/61/61	0/2/2/2
22	PQN	A	801	-	-	3/23/43/43	0/2/2/2
18	BCR	6	518	-	-	9/29/63/63	0/2/2/2
18	BCR	A	850	-	-	10/29/63/63	0/2/2/2
16	CLA	A	829	-	-	6/27/103/115	-
16	CLA	A	836	5	-	7/39/115/115	-
18	BCR	5	420	-	-	9/29/63/63	0/2/2/2
16	CLA	5	406	4	-	9/39/115/115	-
16	CLA	J	1103	12	-	3/15/91/115	-
16	CLA	K	103	13	-	6/39/115/115	-
16	CLA	A	807	5,16	-	6/26/102/115	-
16	CLA	4	405	4	-	9/39/115/115	-
16	CLA	7	516	4	-	6/15/91/115	-
16	CLA	A	839	5	-	5/23/99/115	-
18	BCR	3	514	-	-	6/29/63/63	0/2/2/2
17	LUT	1	518	-	1/1/12/27	9/29/67/67	0/2/2/2
16	CLA	3	509	-	-	19/39/115/115	-
16	CLA	5	411	4	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	K	102	-	-	5/21/97/115	-
16	CLA	4	412	4	-	8/21/97/115	-
23	LMT	B	808	-	-	5/21/61/61	0/2/2/2
16	CLA	B	832	-	-	10/39/115/115	-
16	CLA	5	409	4	-	9/39/115/115	-
23	LMT	A	804	-	-	5/21/61/61	0/2/2/2
16	CLA	A	821	5	-	5/26/102/115	-
16	CLA	7	504	4	-	6/15/91/115	-
16	CLA	2	413	2	-	16/33/109/115	-
19	LMG	5	426	-	-	6/38/58/70	0/1/1/1
21	LHG	3	517	-	-	7/27/27/53	-
16	CLA	3	505	3	-	14/39/115/115	-
16	CLA	A	816	5	-	11/39/115/115	-
16	CLA	A	838	5	-	5/27/103/115	-
16	CLA	1	502	1	-	7/27/103/115	-
16	CLA	A	835	5	-	8/39/115/115	-
16	CLA	B	818	6	-	9/39/115/115	-
16	CLA	1	509	1	-	10/33/109/115	-
16	CLA	2	415	2	-	4/15/91/115	-
16	CLA	B	845	-	-	8/39/115/115	-
19	LMG	1	524	-	-	5/35/55/70	0/1/1/1
18	BCR	1	520	-	-	2/29/63/63	0/2/2/2
16	CLA	6	502	4	-	5/21/97/115	-
16	CLA	1	514	1	-	5/21/97/115	-
16	CLA	5	404	4	-	6/21/97/115	-
18	BCR	6	519	-	-	8/29/63/63	0/2/2/2
16	CLA	A	831	5	-	8/39/115/115	-
18	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	BCR	A	846	-	-	3/29/63/63	0/2/2/2
18	BCR	B	804	-	-	10/29/63/63	0/2/2/2
18	BCR	1	521	-	-	4/29/63/63	0/2/2/2
16	CLA	4	418	4	-	4/15/91/115	-
18	BCR	2	417	-	-	5/29/63/63	0/2/2/2
16	CLA	B	810	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	3	506	-	-	15/39/115/115	-
16	CLA	1	508	-	-	12/39/115/115	-
16	CLA	6	511	4	-	6/15/91/115	-
16	CLA	4	407	4	-	10/39/115/115	-
16	CLA	6	517	4	-	4/15/91/115	-
18	BCR	F	204	-	-	6/29/63/63	0/2/2/2
16	CLA	5	413	4	-	14/33/109/115	-
16	CLA	3	513	3	-	4/15/91/115	-
16	CLA	A	830	5	-	10/39/115/115	-
16	CLA	J	1101	5	-	15/39/115/115	-
16	CLA	A	813	5	-	9/27/103/115	-
16	CLA	6	503	4	-	4/15/91/115	-
16	CLA	1	501	1	-	5/15/91/115	-
18	BCR	5	401	-	-	1/29/63/63	0/2/2/2
16	CLA	7	514	-	-	7/15/91/115	-
16	CLA	A	834	5	-	2/33/109/115	-
18	BCR	1	522	-	-	9/29/63/63	0/2/2/2
16	CLA	A	844	-	-	10/39/115/115	-
16	CLA	B	822	6	-	7/15/91/115	-
16	CLA	A	815	5	-	5/33/109/115	-
16	CLA	B	821	6	-	9/29/105/115	-
18	BCR	I	101	-	-	8/29/63/63	0/2/2/2
16	CLA	B	840	6	-	9/31/107/115	-
26	SF4	C	101	-	-	-	0/6/5/5
16	CLA	7	501	-	-	5/15/91/115	-
16	CLA	3	510	3	-	10/27/103/115	-
16	CLA	7	506	4	-	7/33/109/115	-
16	CLA	3	501	3	-	9/39/115/115	-
16	CLA	7	511	4	-	10/27/77/115	-
16	CLA	2	401	2	-	7/27/103/115	-
16	CLA	5	415	-	-	1/15/91/115	-
16	CLA	7	513	-	-	6/15/91/115	-
16	CLA	B	817	6	-	4/33/109/115	-
18	BCR	B	849	-	-	6/29/63/63	0/2/2/2
16	CLA	B	848	6	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	823	6	-	4/27/103/115	-
16	CLA	1	507	1	-	4/15/91/115	-
16	CLA	6	516	4	-	4/15/91/115	-
16	CLA	1	513	1	-	8/15/91/115	-
16	CLA	B	827	6	-	10/29/105/115	-
16	CLA	B	811	6	-	3/26/102/115	-
16	CLA	A	817	5	-	6/27/103/115	-
16	CLA	2	409	-	-	10/27/103/115	-
16	CLA	A	820	5	-	7/26/102/115	-
16	CLA	X	101	15	-	8/15/91/115	-
18	BCR	B	852	-	-	6/29/63/63	0/2/2/2
18	BCR	J	1104	-	-	4/29/63/63	0/2/2/2
18	BCR	7	519	-	-	2/29/63/63	0/2/2/2
18	BCR	7	518	-	-	5/29/63/63	0/2/2/2
22	PQN	B	803	-	-	3/23/43/43	0/2/2/2
16	CLA	F	202	-	-	1/15/91/115	-
16	CLA	B	831	6	-	14/39/115/115	-
16	CLA	5	416	-	-	6/15/91/115	-
16	CLA	A	824	-	-	12/39/115/115	-

The worst 5 of 861 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	805	CL0	C1B-C2B	8.60	1.49	1.39
24	A	805	CL0	C3B-C4B	8.12	1.49	1.41
16	7	511	CLA	C1B-C2B	5.54	1.49	1.34
24	A	805	CL0	C3D-C4D	3.90	1.47	1.41
16	J	1101	CLA	C1D-ND	3.64	1.42	1.37

The worst 5 of 733 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	805	CL0	C1B-CHB-C4A	6.30	125.38	121.32
17	1	518	LUT	C7-C8-C9	-5.72	117.77	126.23
16	7	511	CLA	CMB-C2B-C3B	4.62	123.98	116.53
16	2	410	CLA	C4A-NA-C1A	4.39	108.68	106.68
17	1	518	LUT	C21-C26-C27	4.37	117.85	112.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	518	LUT	C26

5 of 2026 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	501	CLA	C4B-C3B-CAB-CBB
16	1	502	CLA	C2B-C3B-CAB-CBB
16	1	502	CLA	C4B-C3B-CAB-CBB
16	1	505	CLA	C1A-C2A-CAA-CBA
16	1	505	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

104 monomers are involved in 140 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	515	BCR	1	0
21	A	803	LHG	1	0
16	2	407	CLA	1	0
18	6	521	BCR	1	0
16	B	847	CLA	1	0
16	5	412	CLA	2	0
16	4	416	CLA	1	0
16	4	410	CLA	5	0
16	A	837	CLA	2	0
18	1	519	BCR	1	0
18	3	516	BCR	2	0
18	M	101	BCR	2	0
16	4	403	CLA	1	0
16	B	829	CLA	1	0
16	1	517	CLA	1	0
16	B	841	CLA	1	0
16	3	504	CLA	2	0
16	A	827	CLA	1	0
16	2	406	CLA	3	0
16	1	503	CLA	1	0
16	B	820	CLA	1	0
18	4	419	BCR	3	0
16	A	828	CLA	3	0
16	B	812	CLA	1	0
16	4	411	CLA	2	0
16	A	841	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	F	203	BCR	1	0
16	4	402	CLA	1	0
16	A	811	CLA	1	0
16	1	525	CLA	1	0
16	5	410	CLA	1	0
16	B	844	CLA	1	0
16	A	809	CLA	1	0
16	1	505	CLA	1	0
18	2	418	BCR	1	0
16	B	835	CLA	2	0
16	2	405	CLA	1	0
16	3	507	CLA	1	0
16	7	510	CLA	1	0
16	B	814	CLA	2	0
16	A	852	CLA	2	0
16	A	818	CLA	1	0
16	2	414	CLA	3	0
16	1	510	CLA	1	0
16	A	806	CLA	2	0
16	2	408	CLA	1	0
16	1	506	CLA	4	0
16	6	509	CLA	1	0
16	7	512	CLA	2	0
25	A	853	ECH	1	0
16	B	815	CLA	1	0
18	B	853	BCR	2	0
18	B	850	BCR	1	0
21	B	806	LHG	1	0
16	B	846	CLA	1	0
18	A	845	BCR	2	0
18	K	101	BCR	2	0
25	A	848	ECH	1	0
16	3	508	CLA	1	0
16	A	808	CLA	1	0
16	B	801	CLA	2	0
16	6	501	CLA	1	0
24	A	805	CL0	6	0
16	1	504	CLA	3	0
16	6	506	CLA	1	0
18	1	523	BCR	1	0
20	1	527	LMU	1	0
16	B	837	CLA	1	0

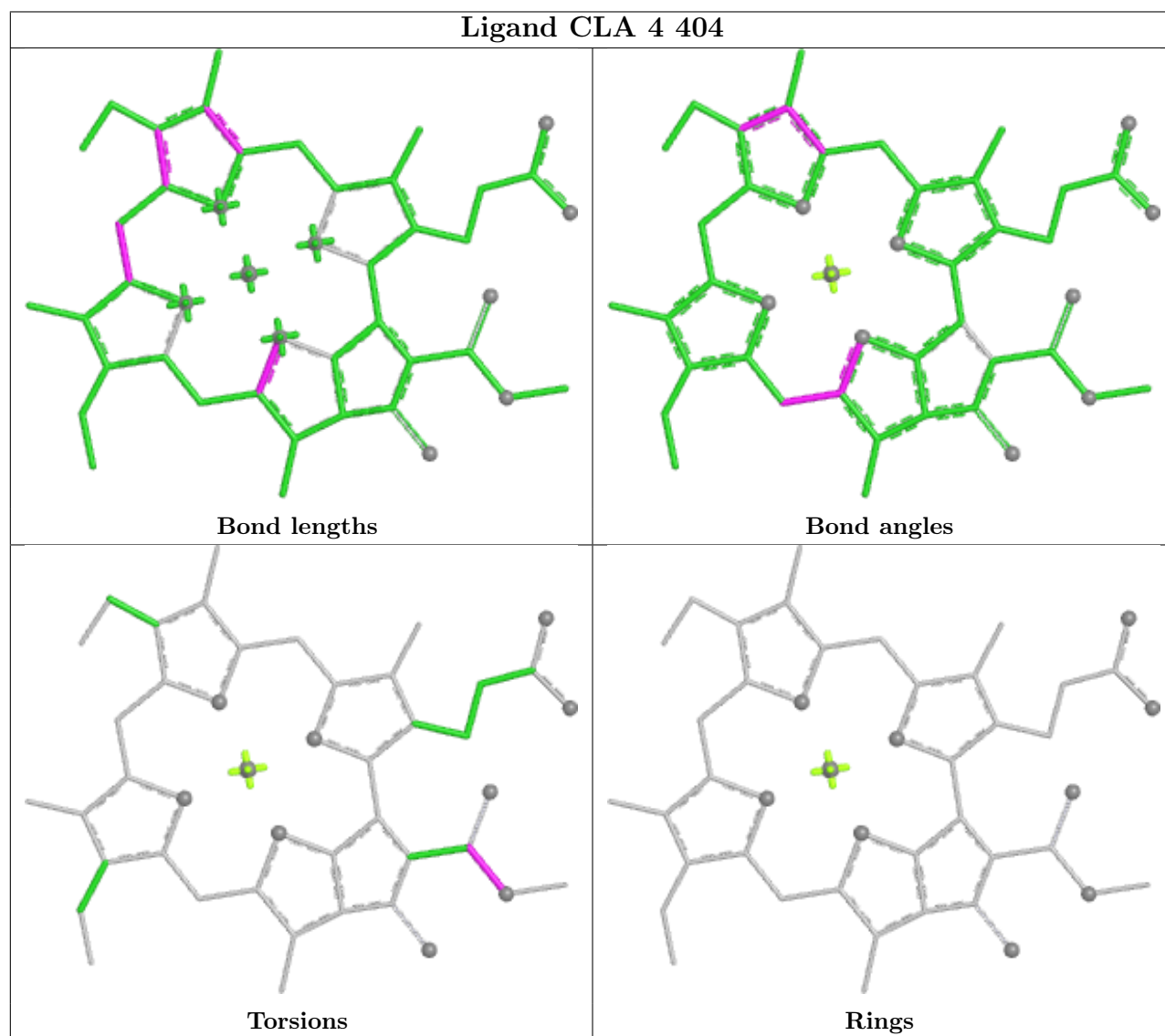
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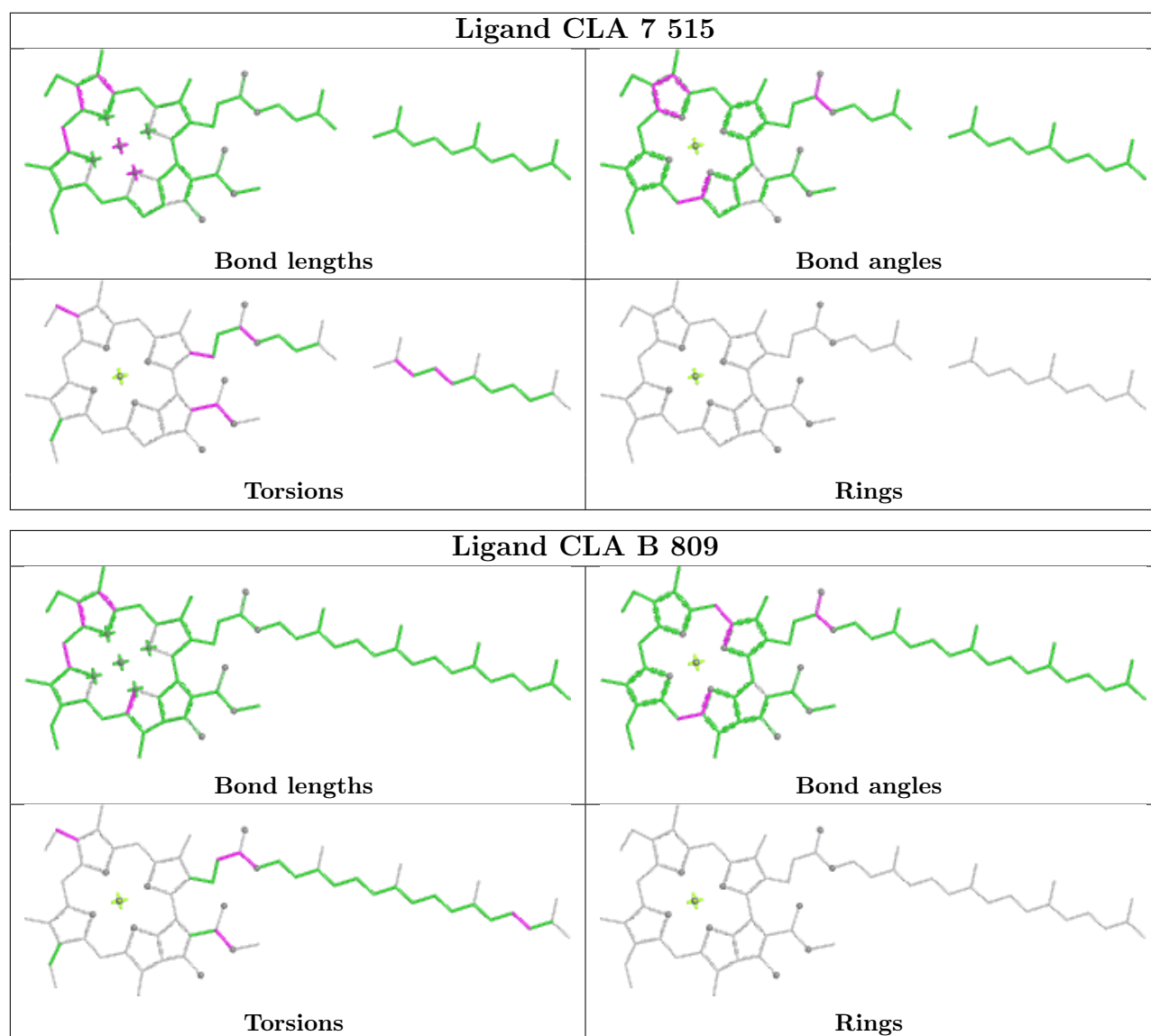
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	814	CLA	1	0
18	I	102	BCR	2	0
22	A	801	PQN	1	0
18	6	518	BCR	2	0
18	A	850	BCR	1	0
18	5	420	BCR	1	0
16	A	807	CLA	1	0
16	4	405	CLA	1	0
16	A	839	CLA	1	0
18	3	514	BCR	1	0
17	1	518	LUT	6	0
16	5	411	CLA	3	0
16	B	832	CLA	4	0
16	A	816	CLA	1	0
16	A	835	CLA	1	0
16	1	509	CLA	2	0
16	B	845	CLA	1	0
18	1	520	BCR	2	0
16	5	404	CLA	1	0
16	A	831	CLA	1	0
18	B	804	BCR	1	0
18	1	521	BCR	2	0
16	B	810	CLA	1	0
16	3	506	CLA	2	0
16	A	830	CLA	1	0
18	1	522	BCR	1	0
16	A	844	CLA	1	0
16	B	822	CLA	1	0
16	7	511	CLA	2	0
16	B	817	CLA	1	0
18	B	849	BCR	1	0
16	1	507	CLA	3	0
16	2	409	CLA	1	0
18	B	852	BCR	2	0
18	7	518	BCR	1	0
22	B	803	PQN	1	0

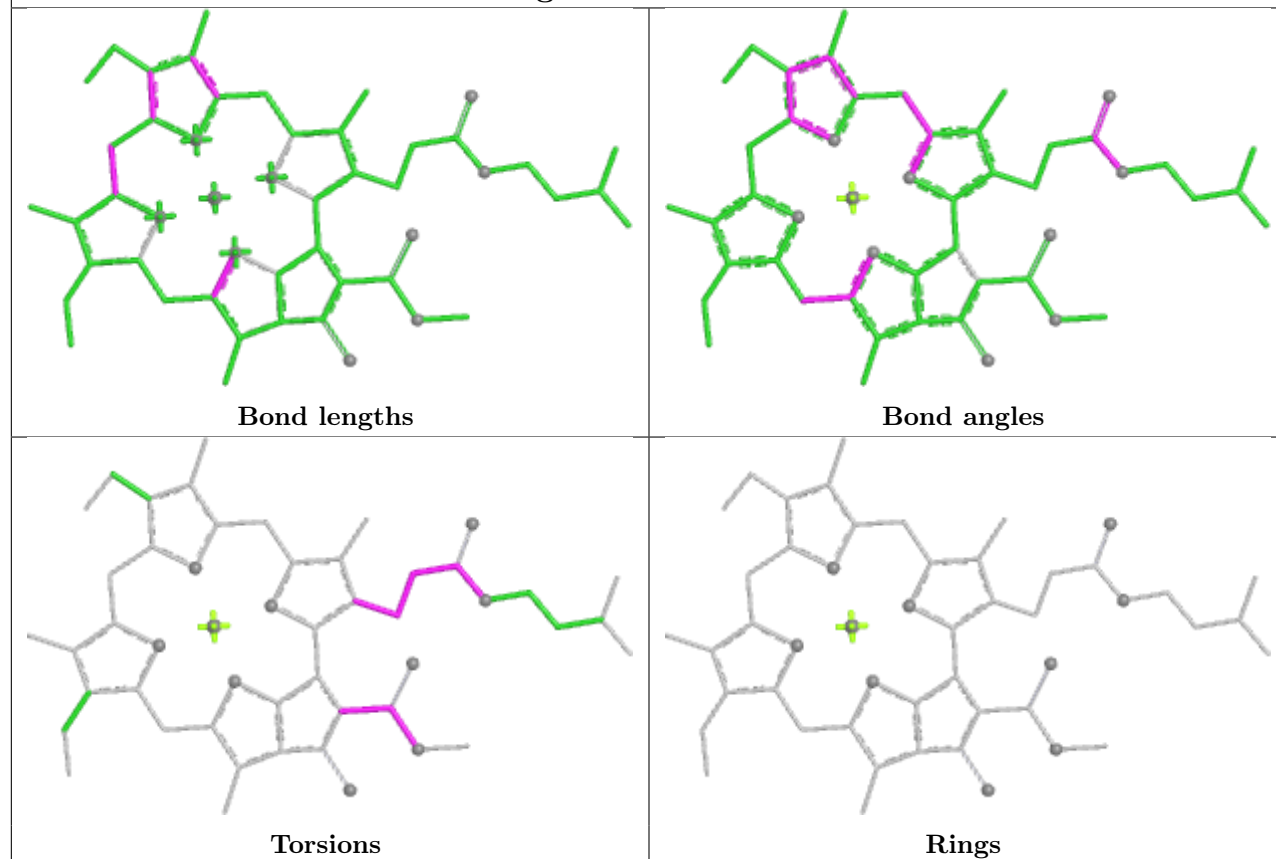
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

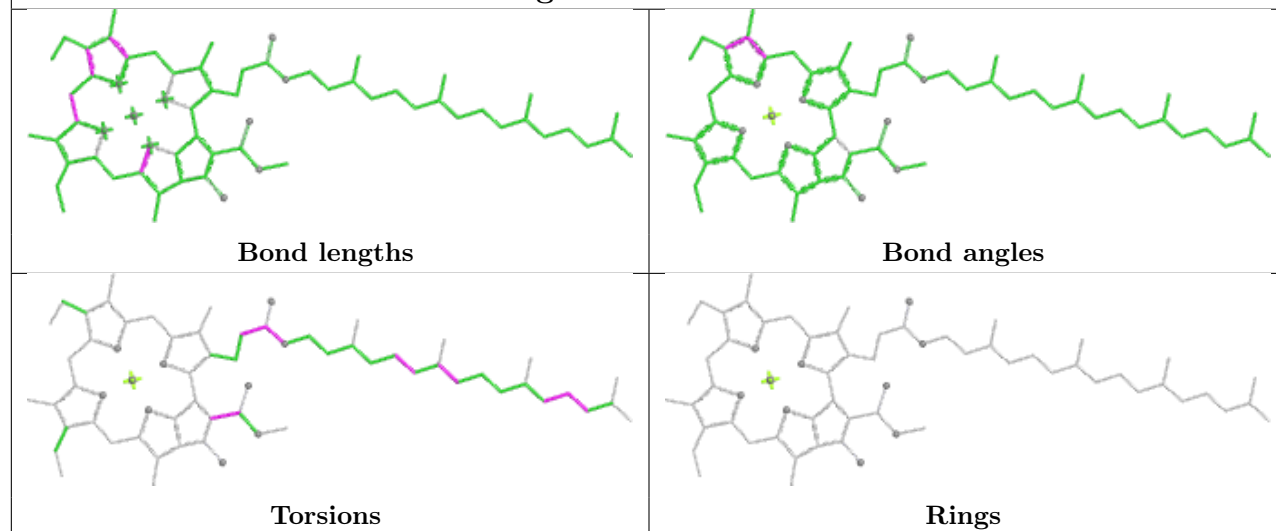




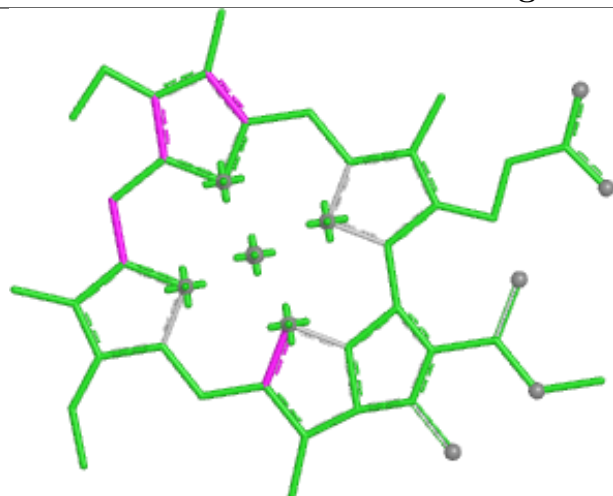
Ligand CLA 7 508



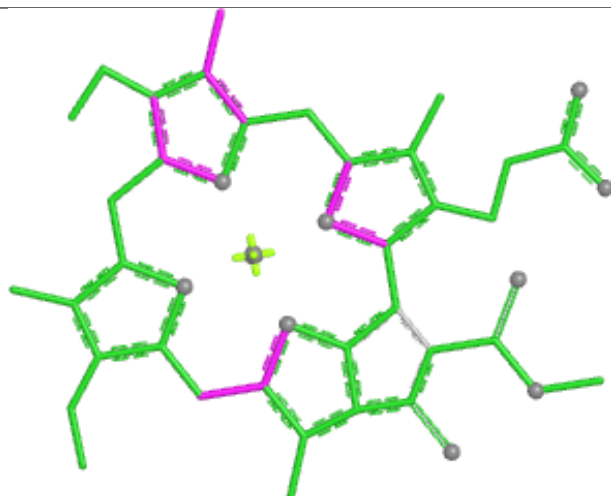
Ligand CLA 6 510



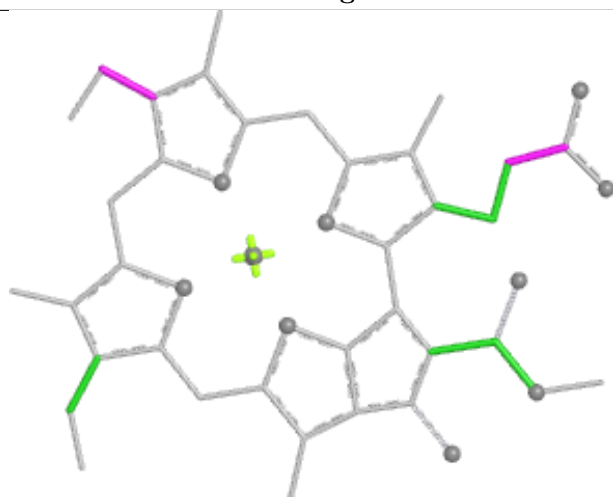
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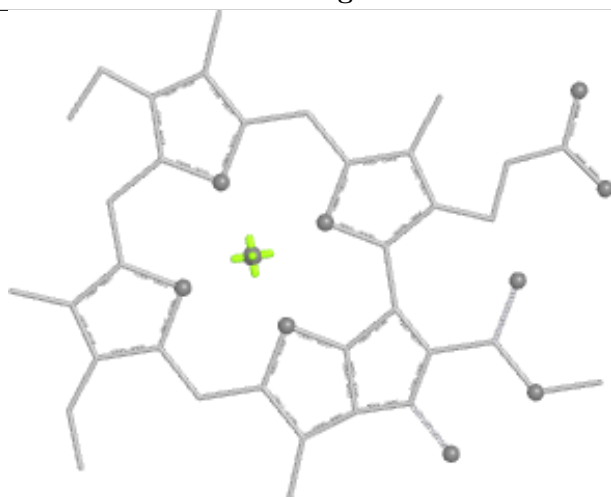
Bond lengths



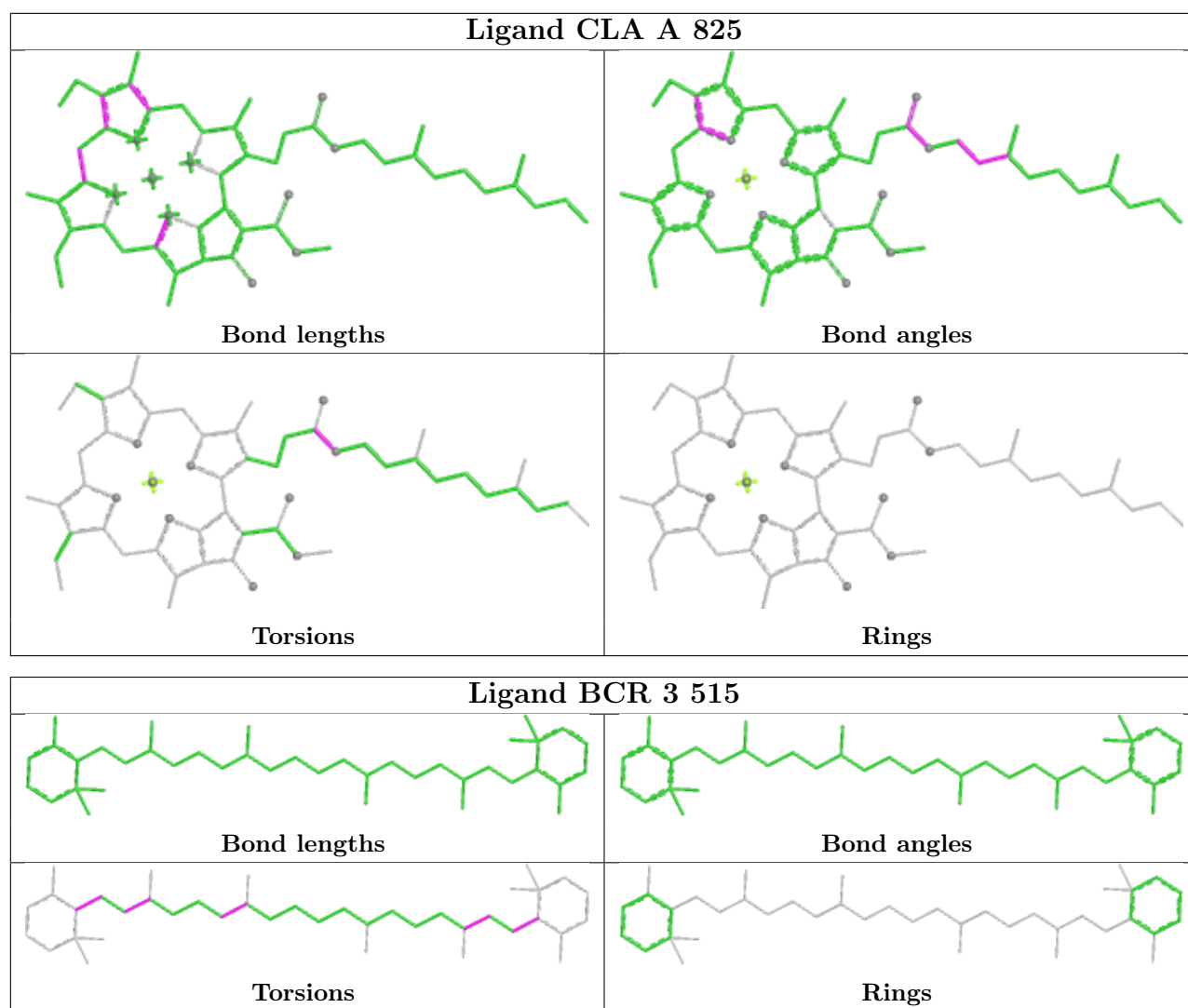
Bond angles

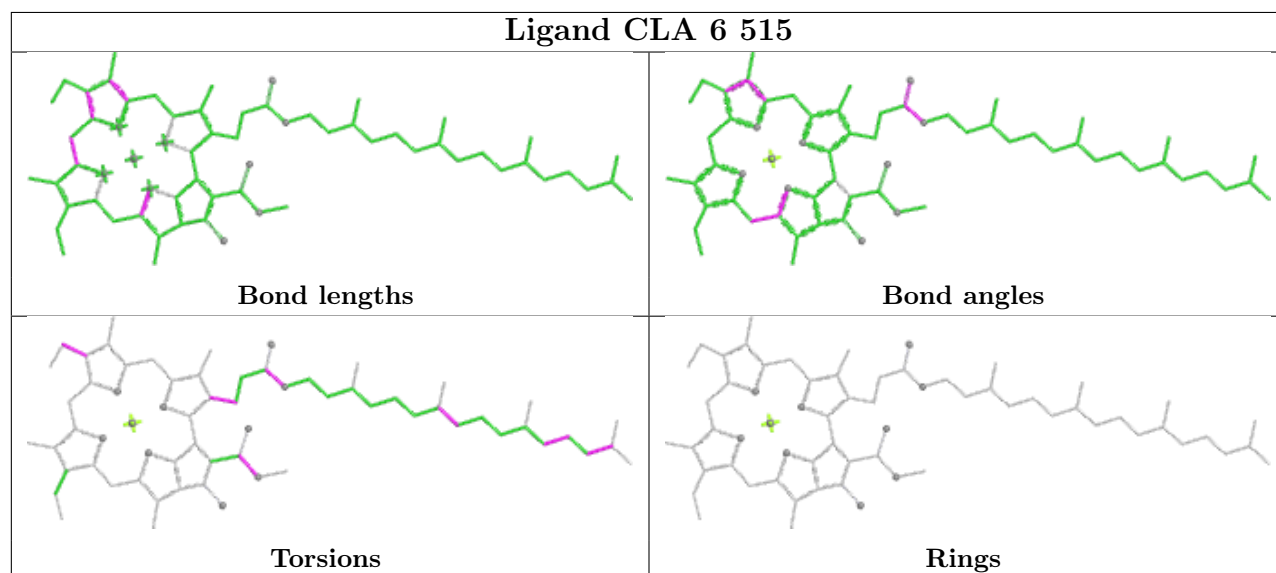
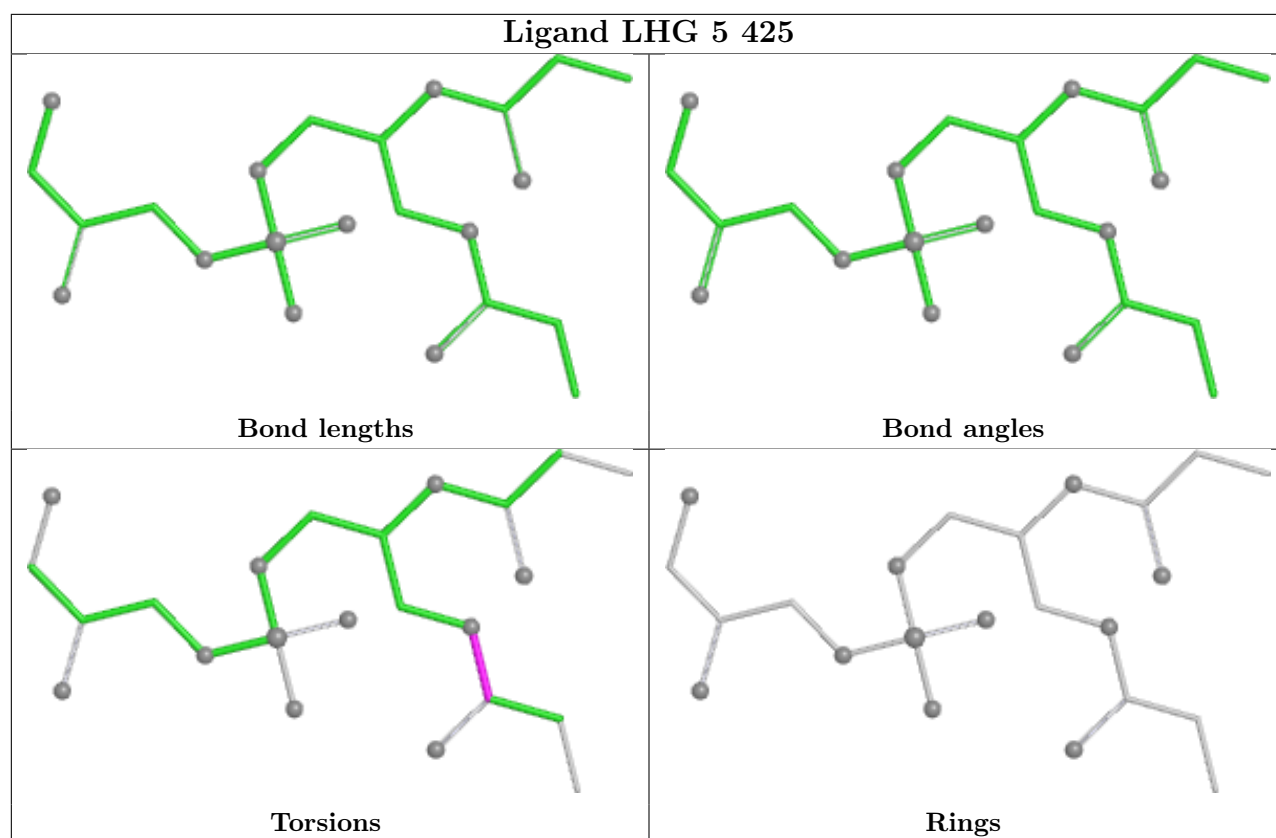


Torsions

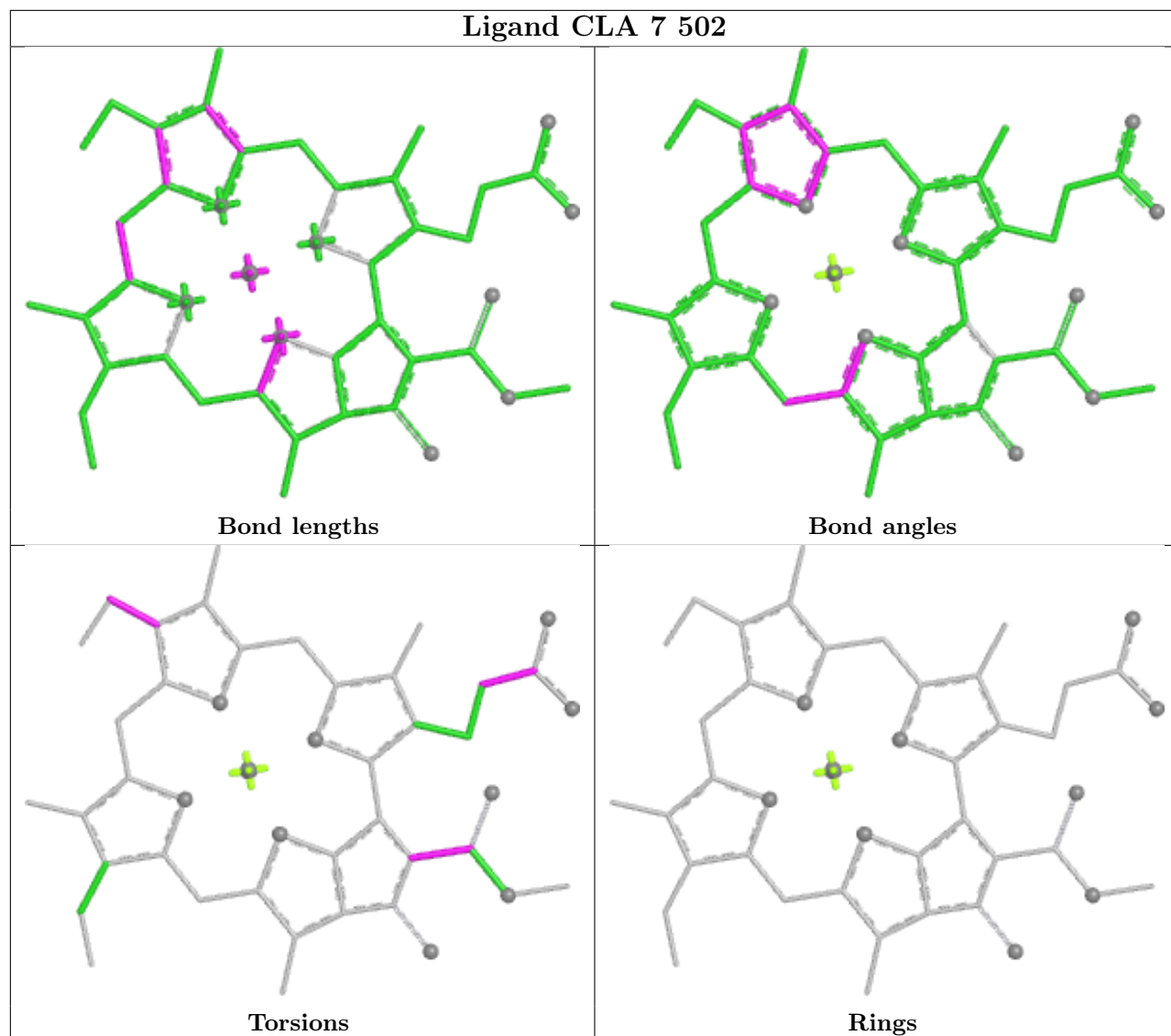


Rings

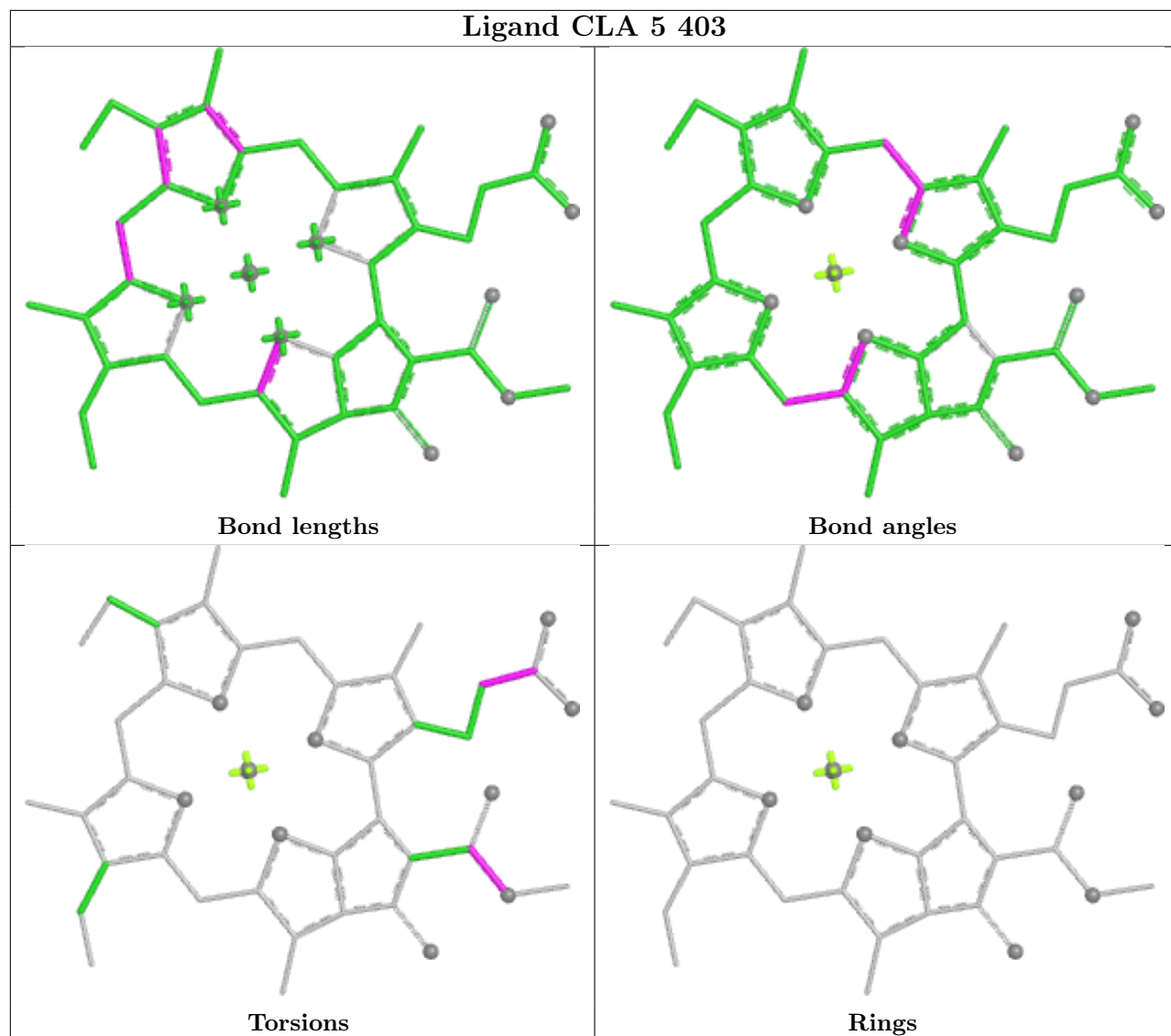




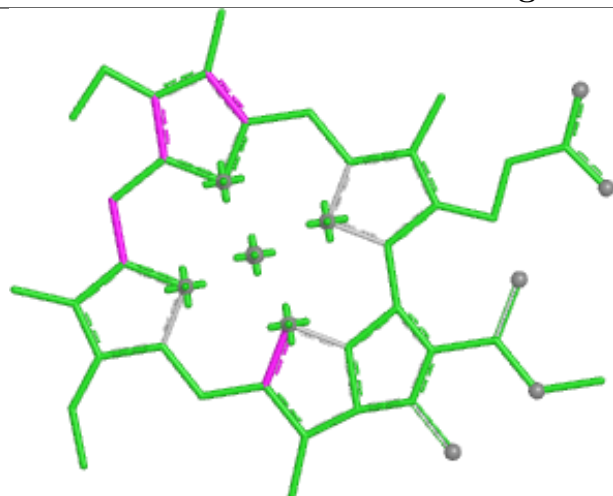
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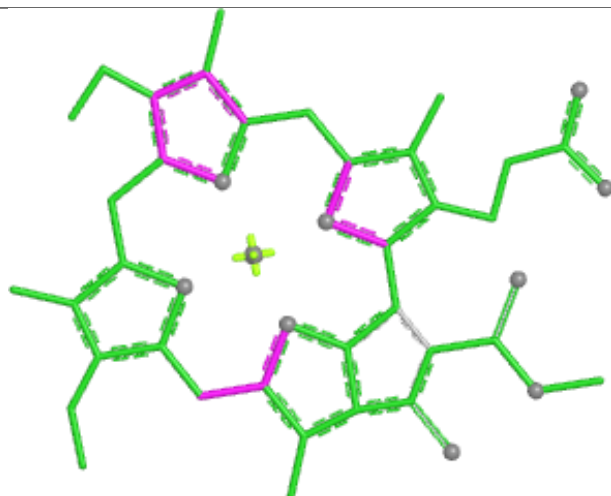
Ligand CLA 5 403



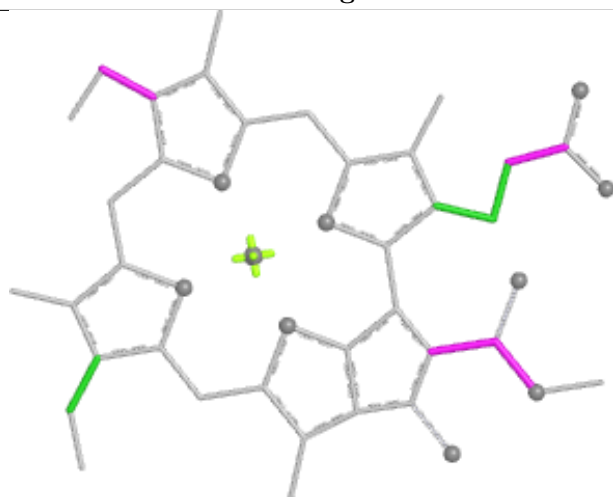
Ligand CLA 7 507



Bond lengths



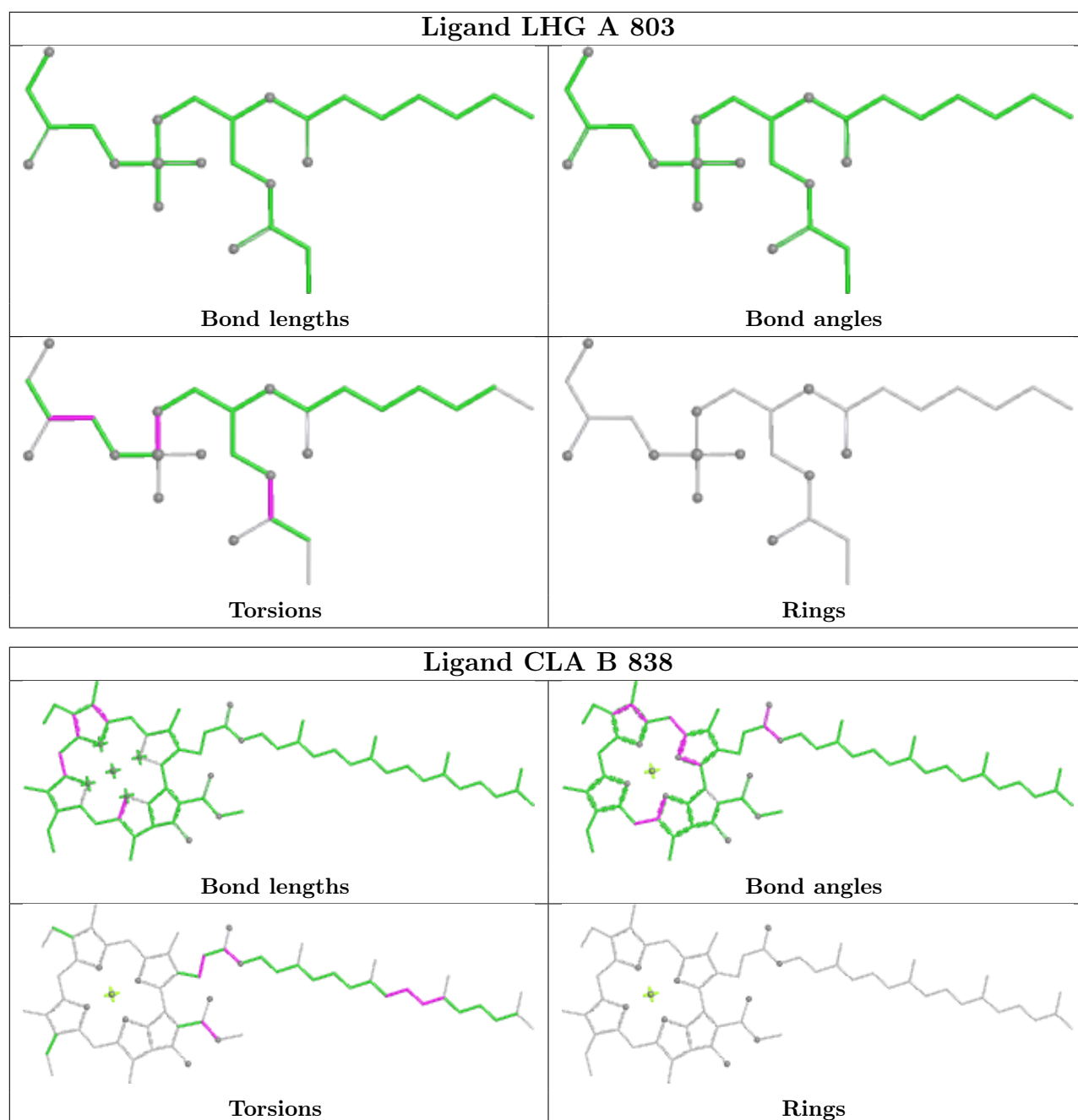
Bond angles

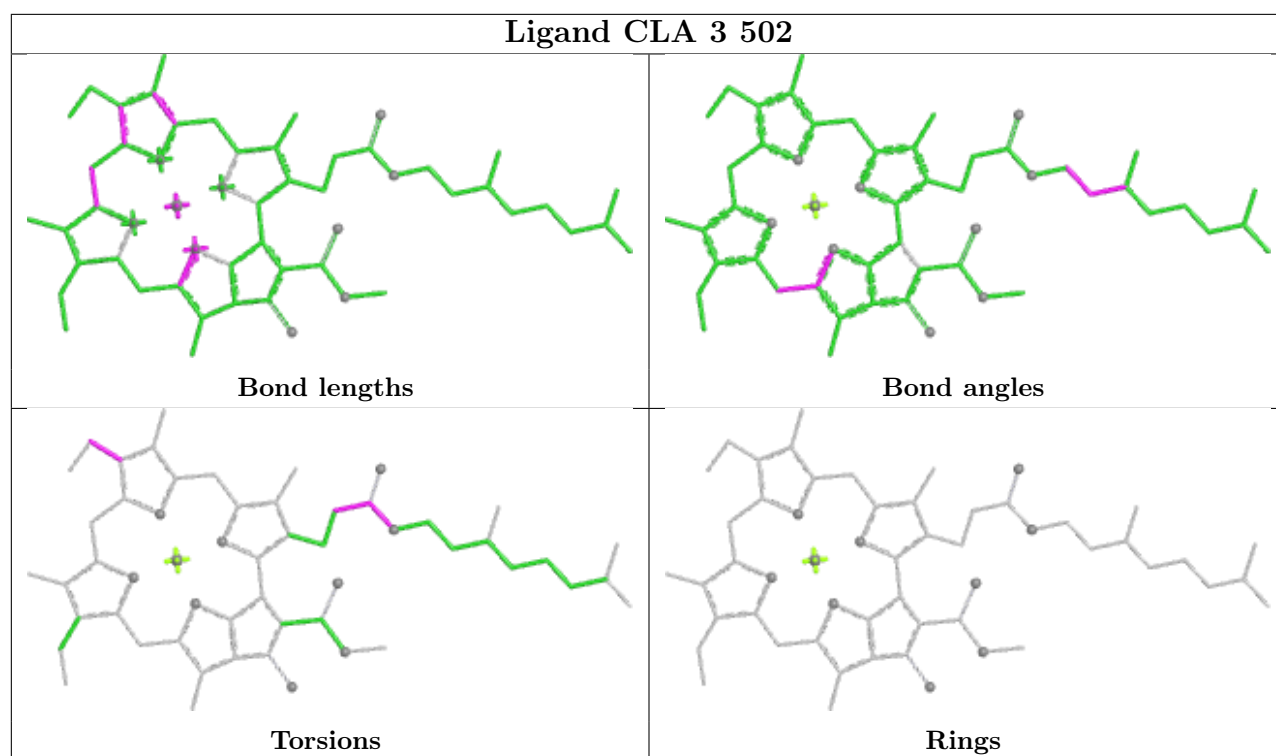


Torsions

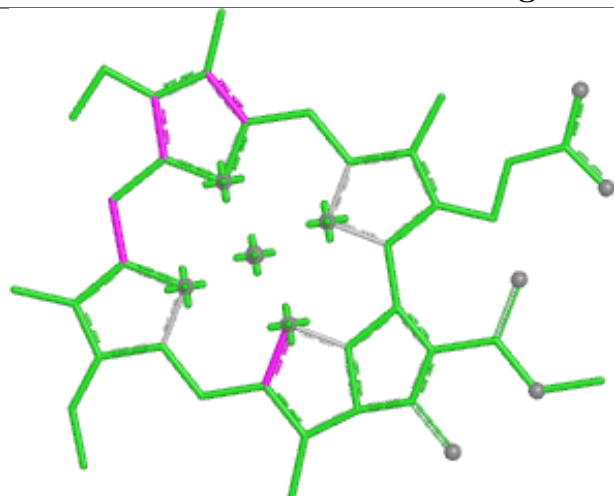


Rings

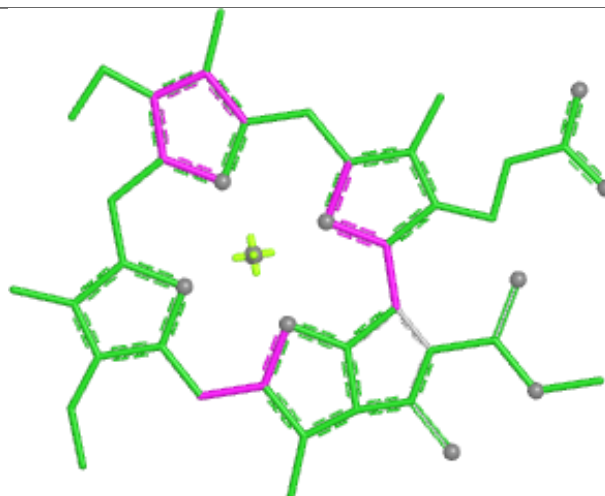




Ligand CLA 7 503



Bond lengths



Bond angles

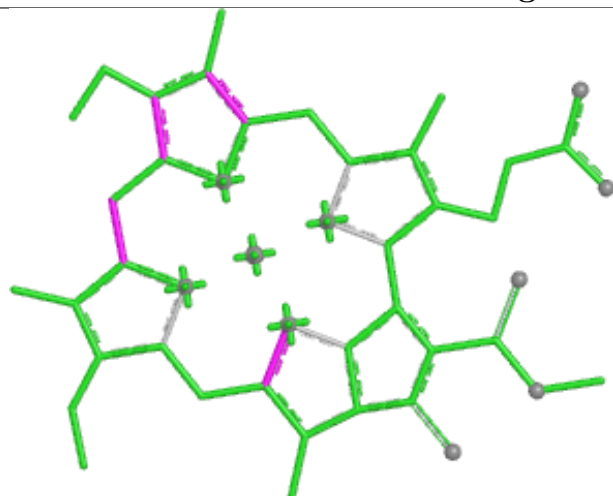


Torsions

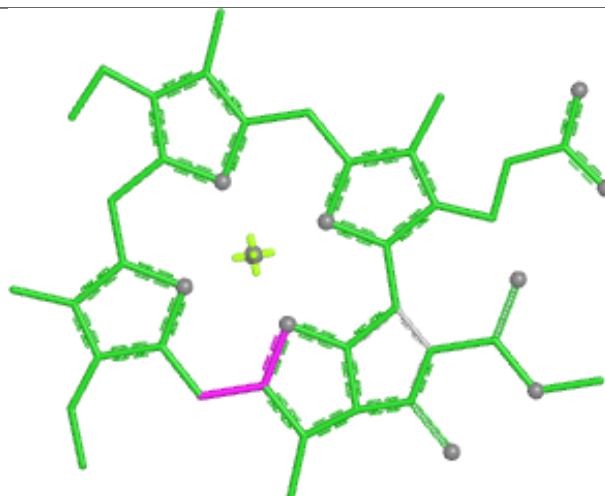


Rings

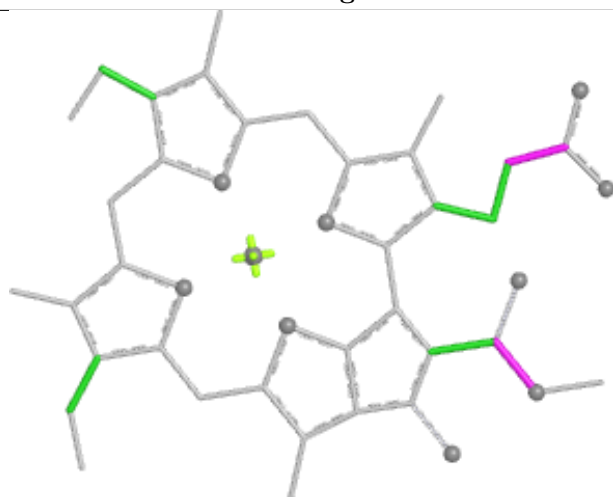
Ligand CLA 3 503



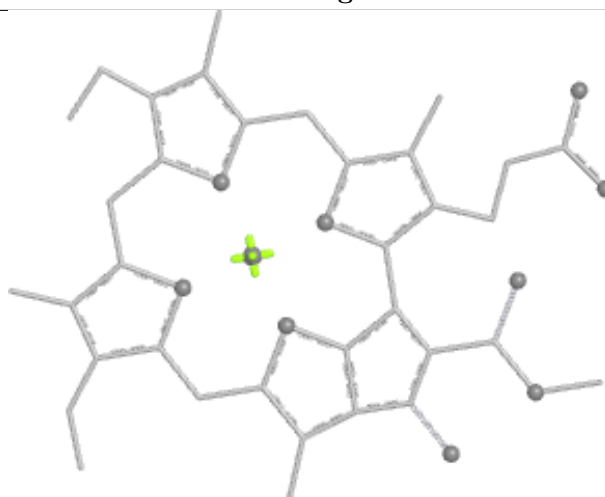
Bond lengths



Bond angles

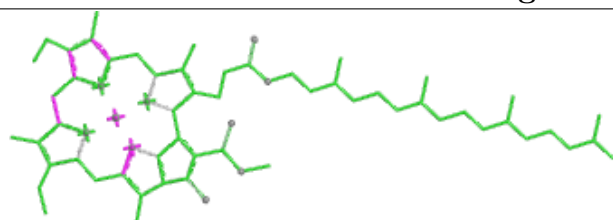


Torsions

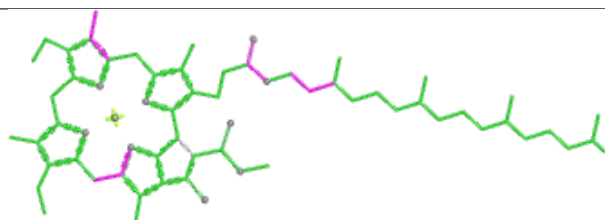


Rings

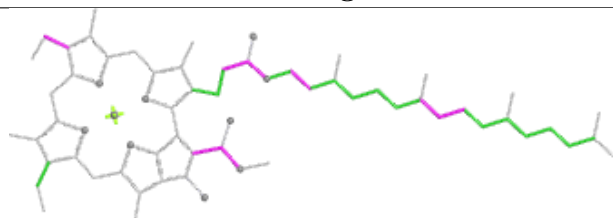
Ligand CLA 6 507



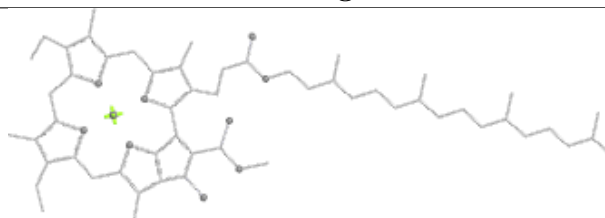
Bond lengths



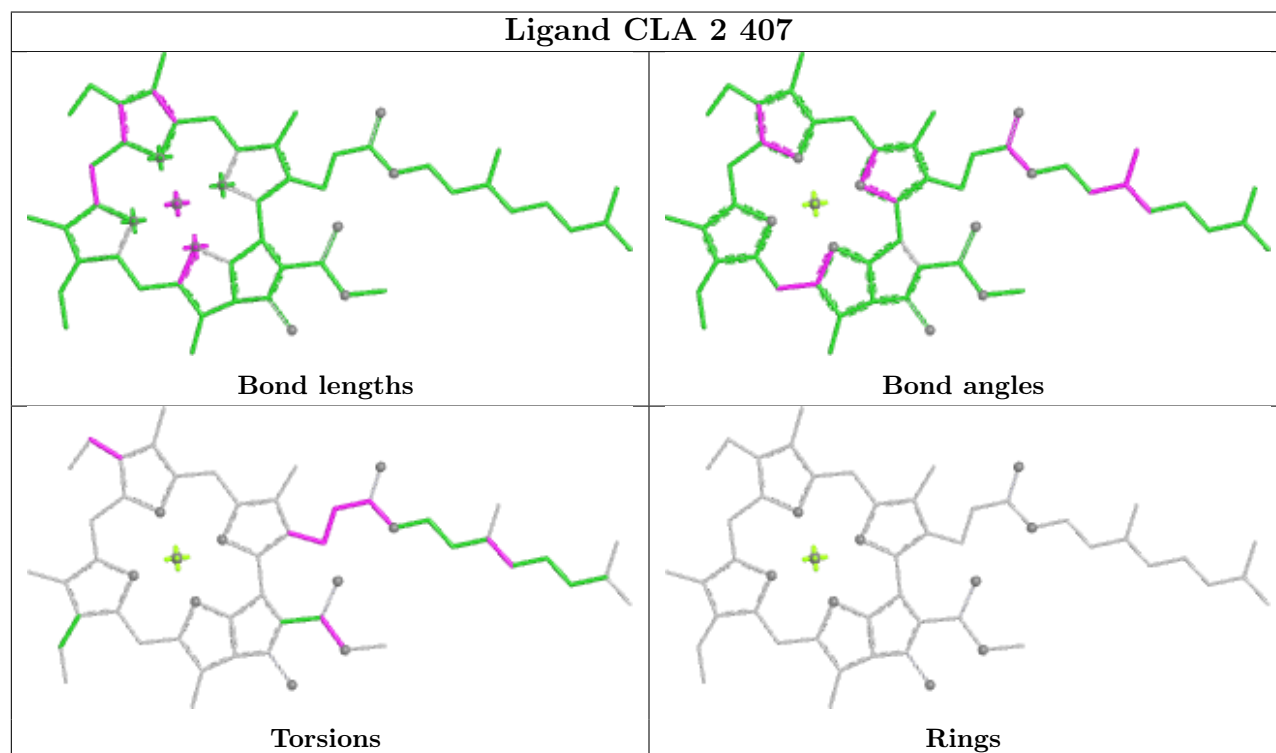
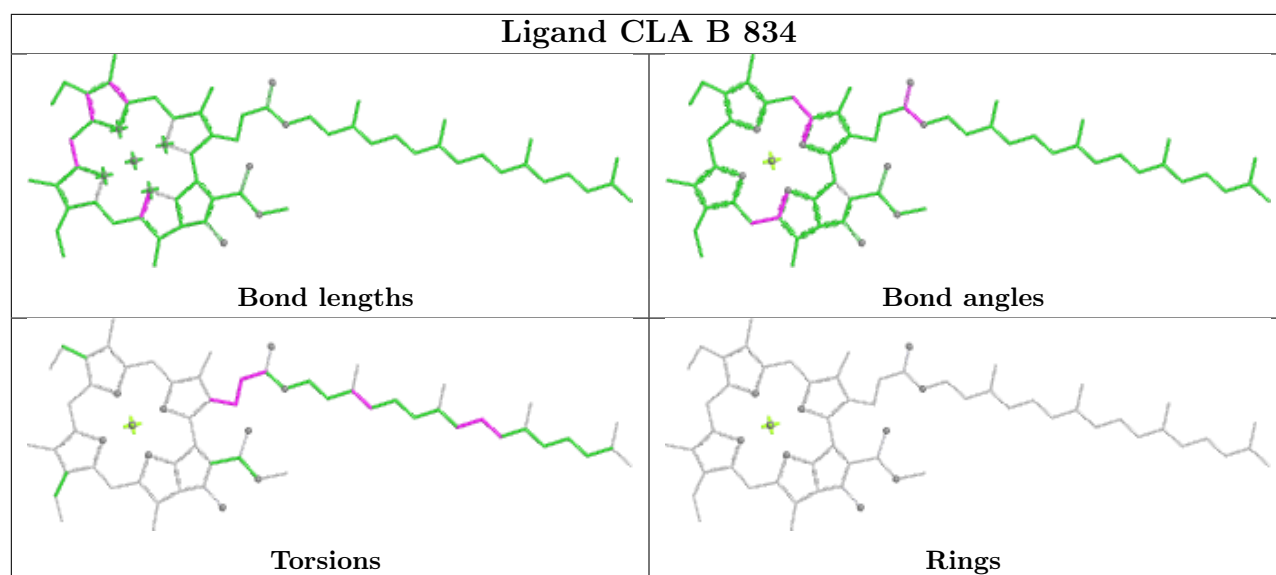
Bond angles

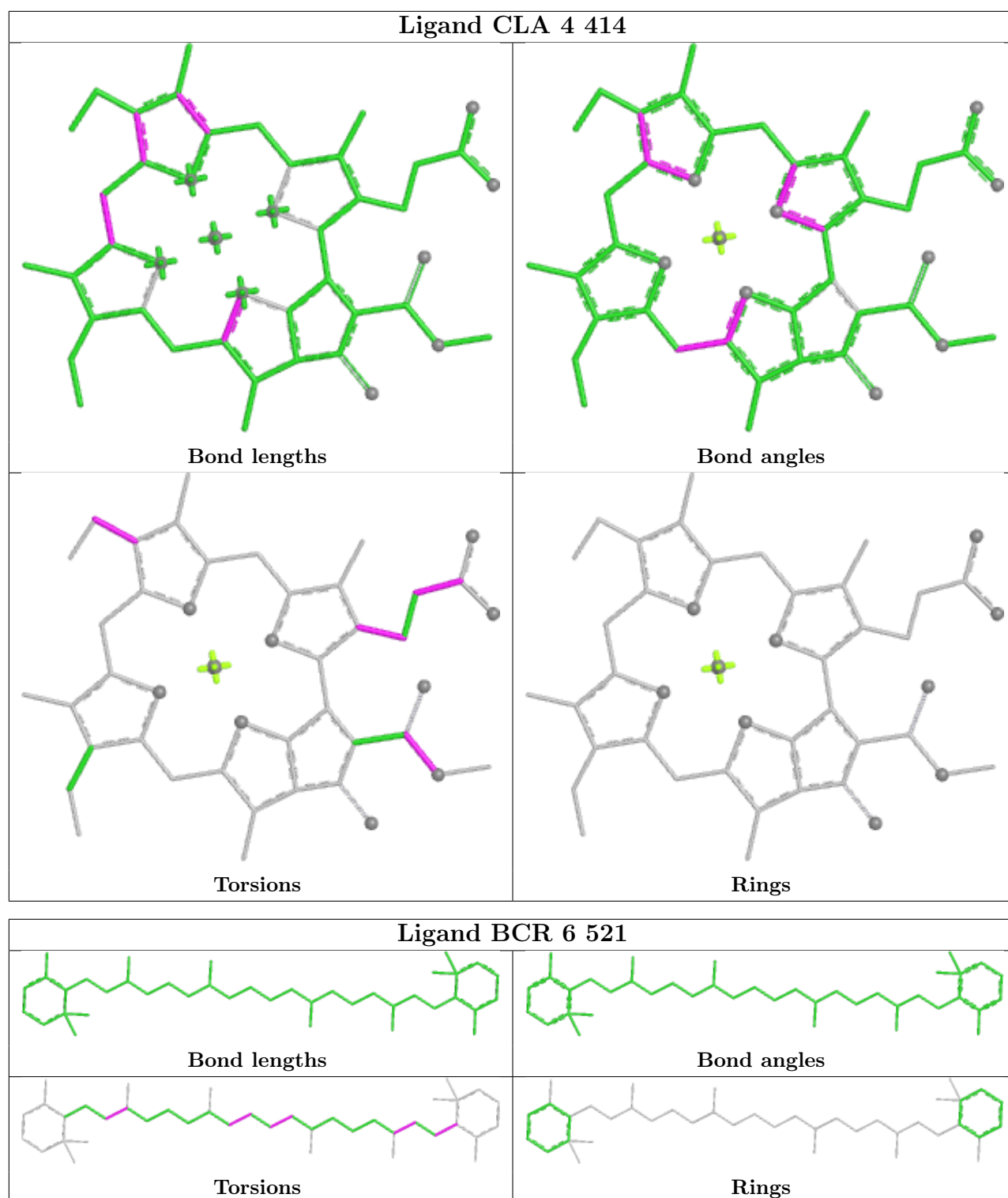


Torsions

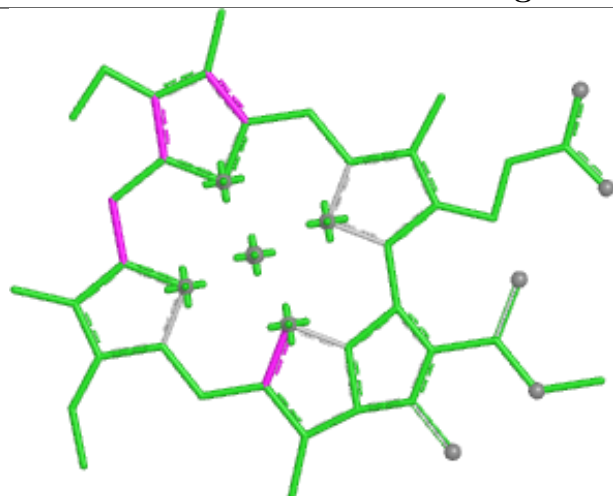


Rings

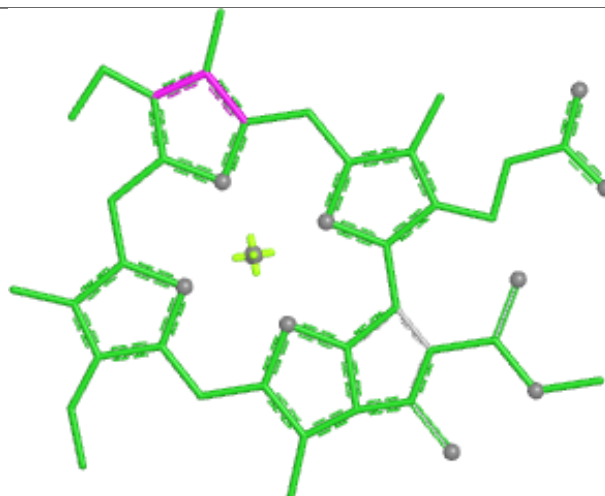




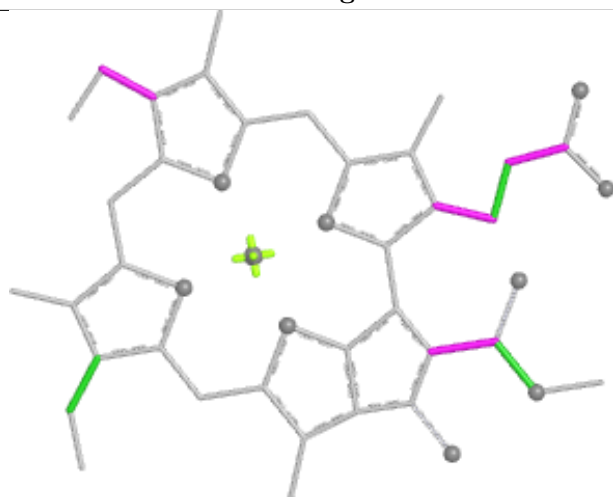
Ligand CLA B 819



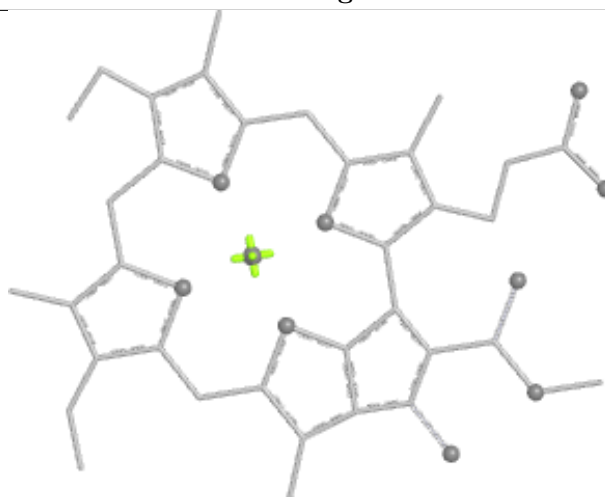
Bond lengths



Bond angles

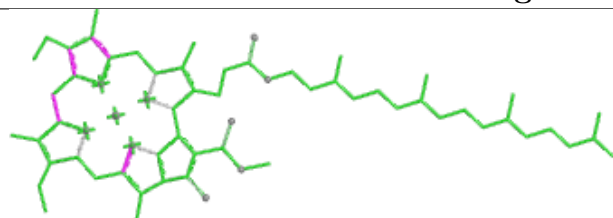


Torsions

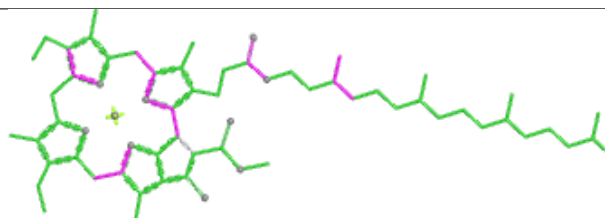


Rings

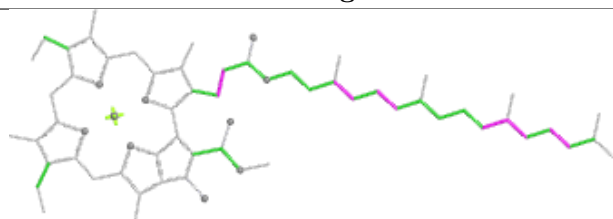
Ligand CLA B 847



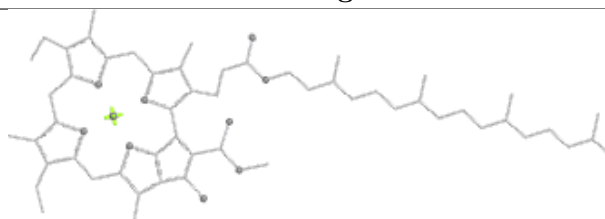
Bond lengths



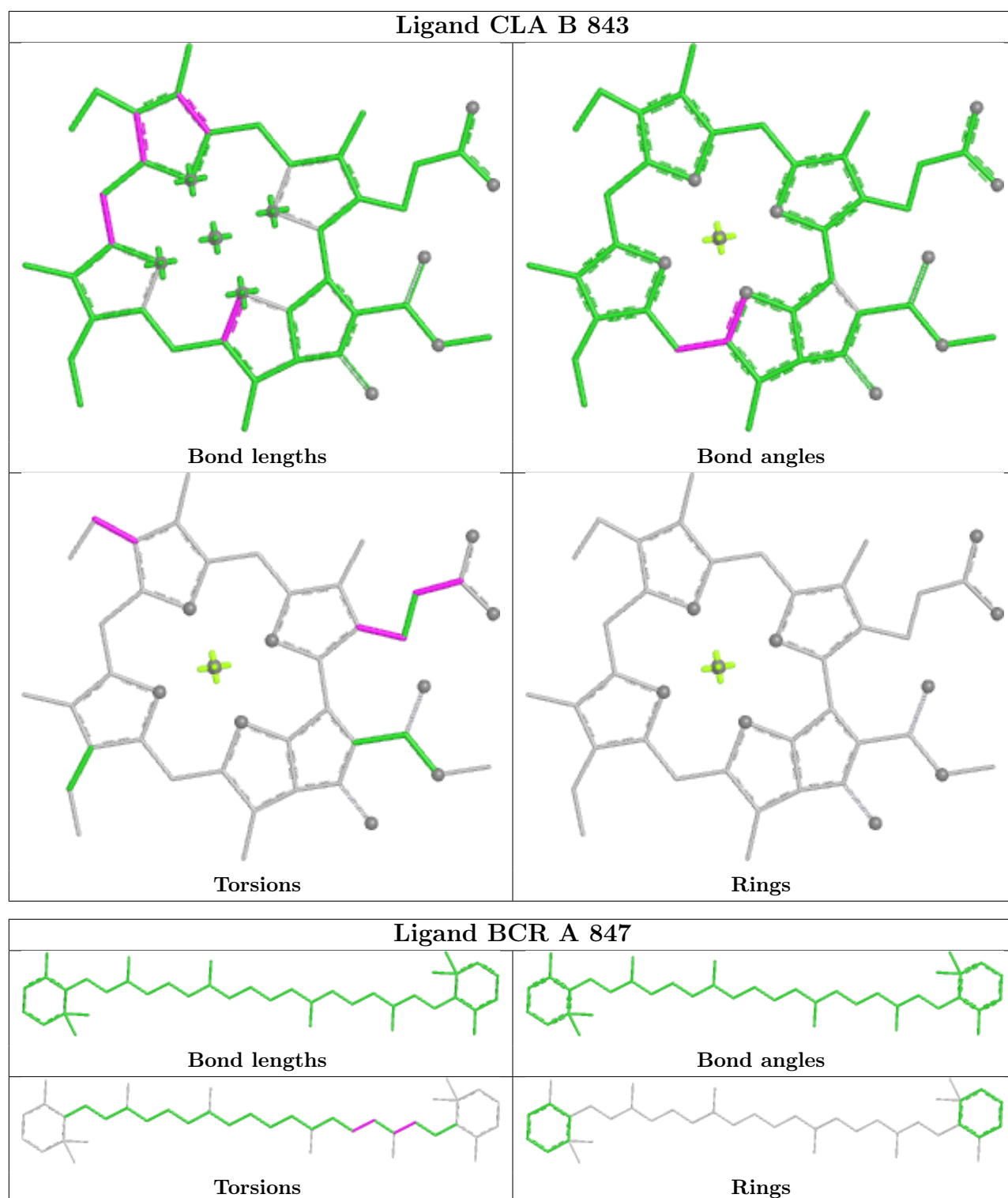
Bond angles



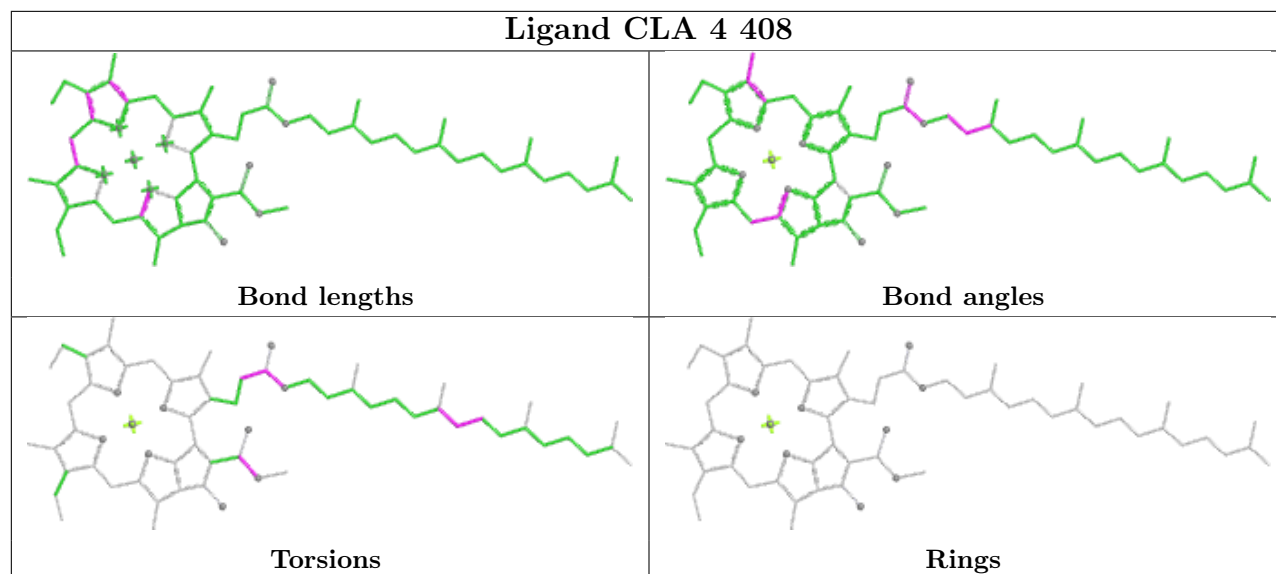
Torsions



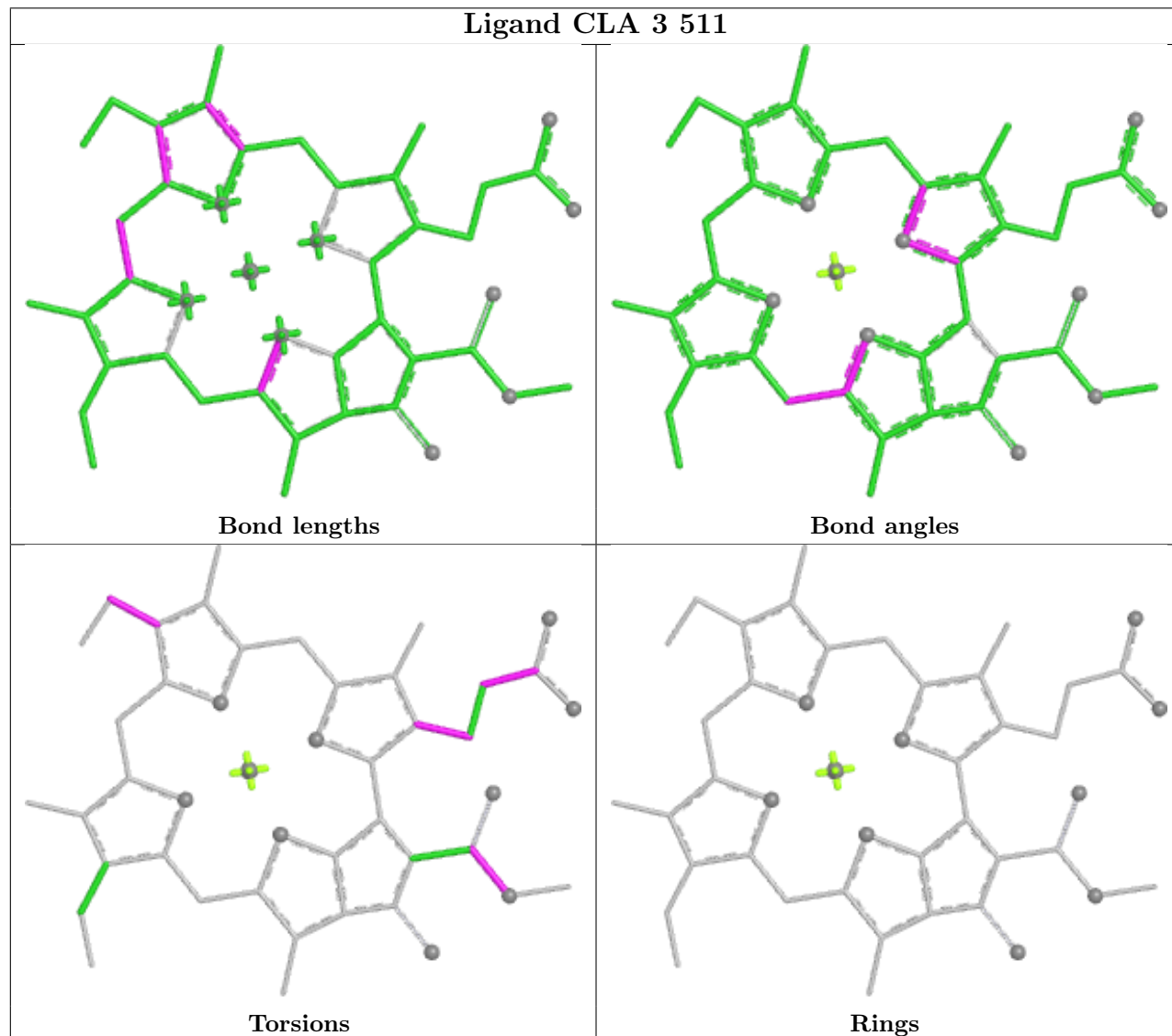
Rings



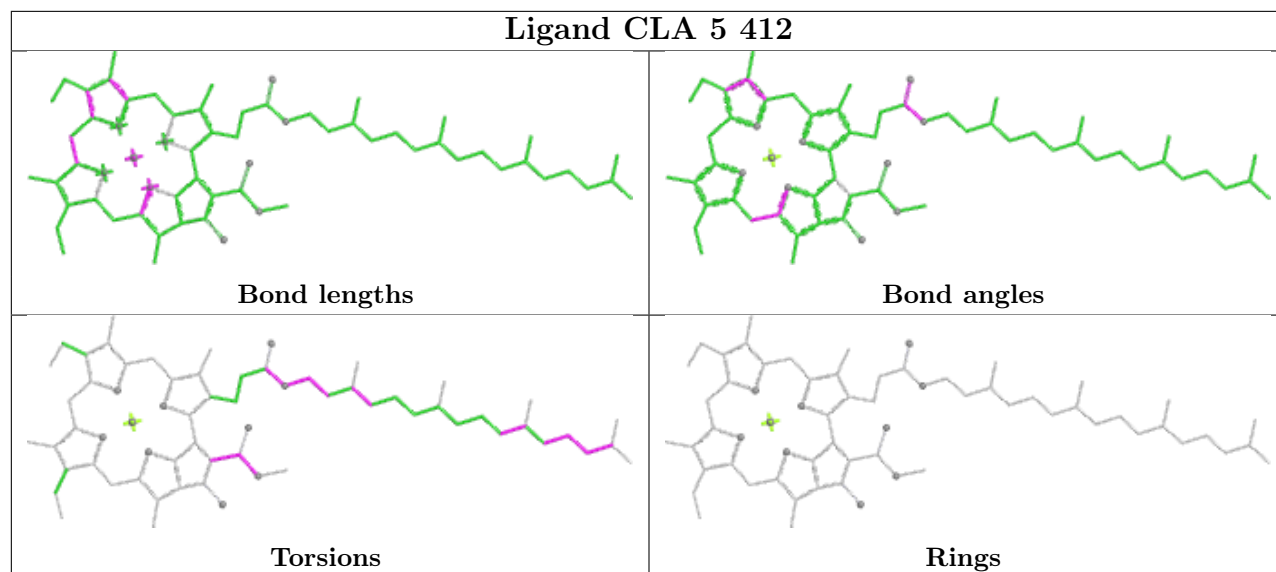
Ligand CLA 4 408



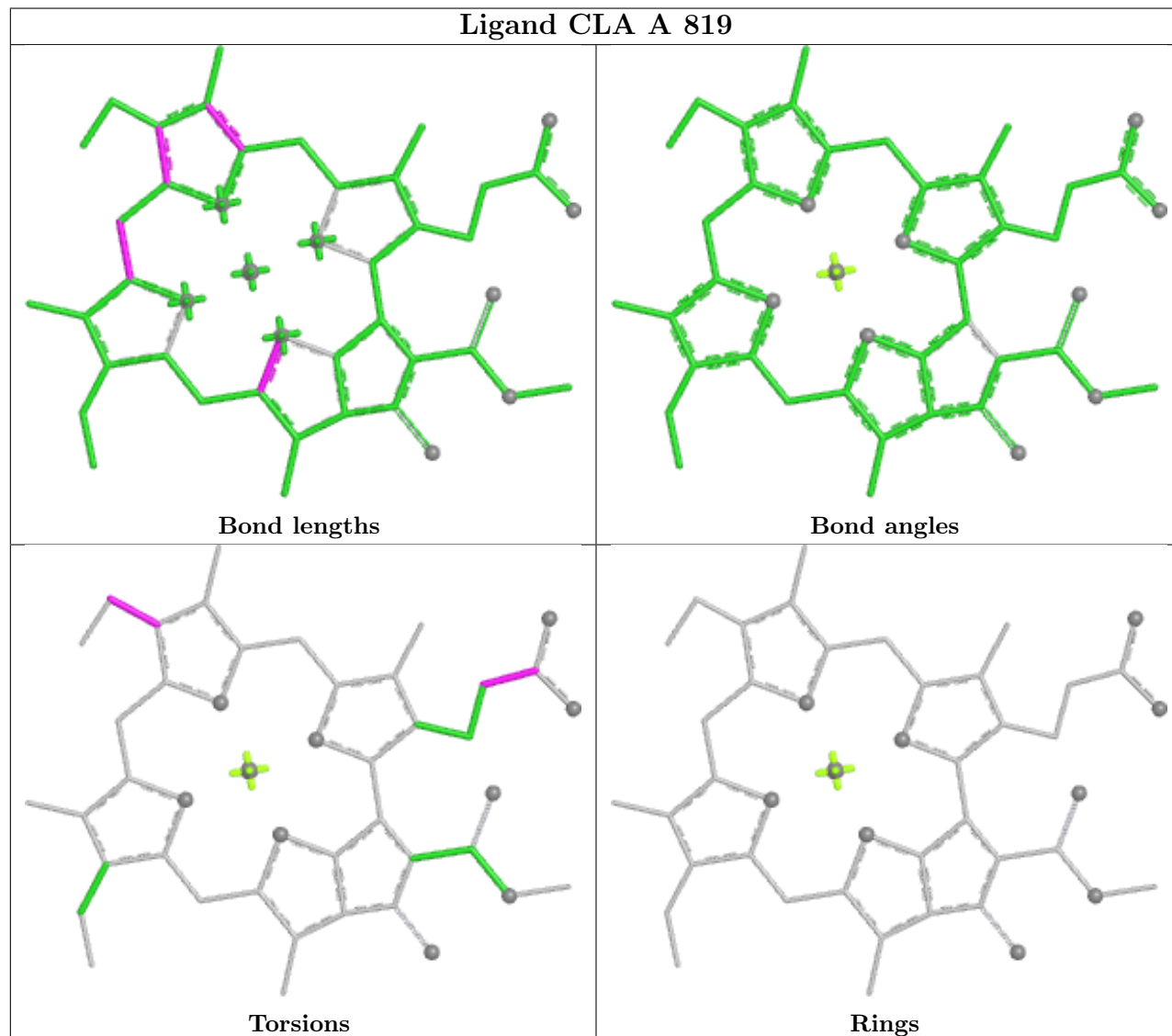
Ligand CLA 3 511



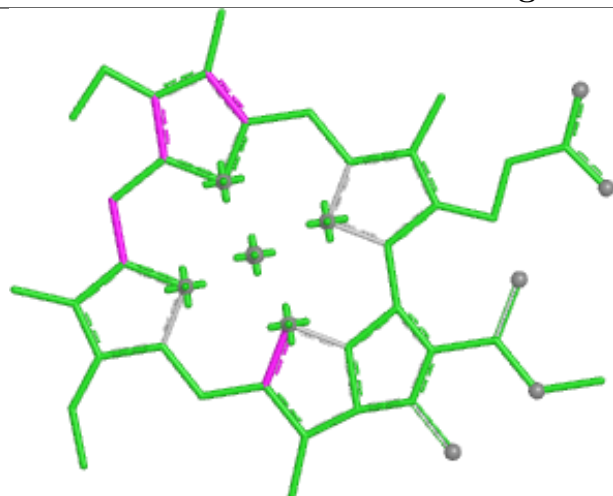
Ligand CLA 5 412



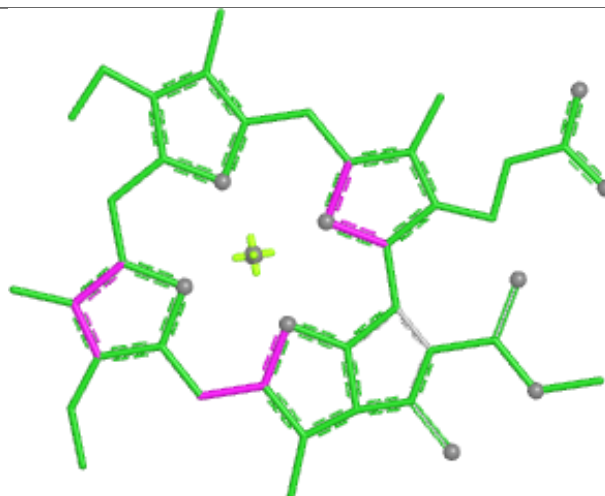
Ligand CLA A 819



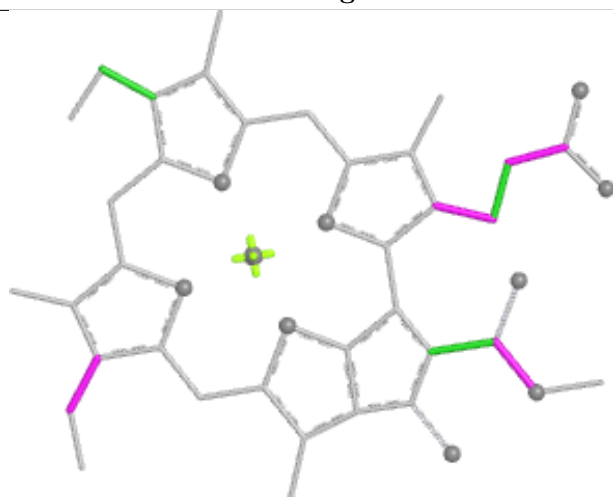
Ligand CLA 6 512



Bond lengths



Bond angles

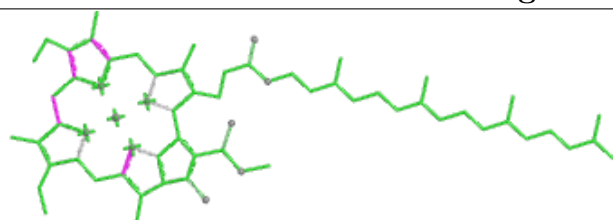


Torsions

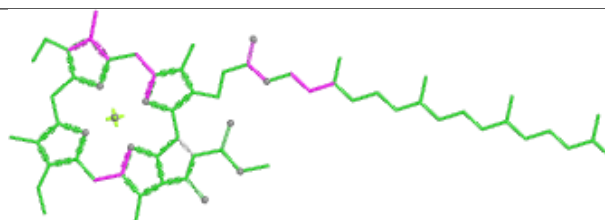


Rings

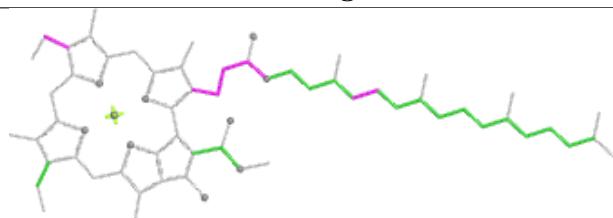
Ligand CLA 4 416



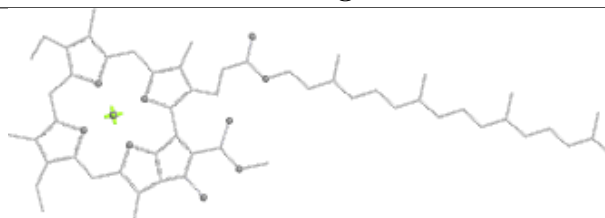
Bond lengths



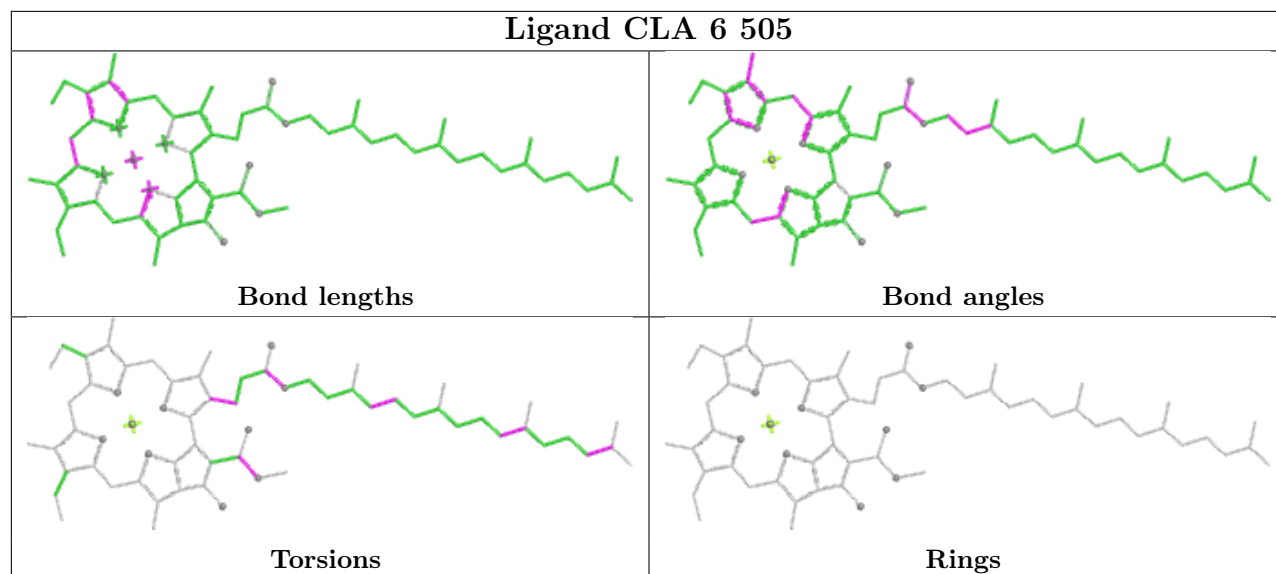
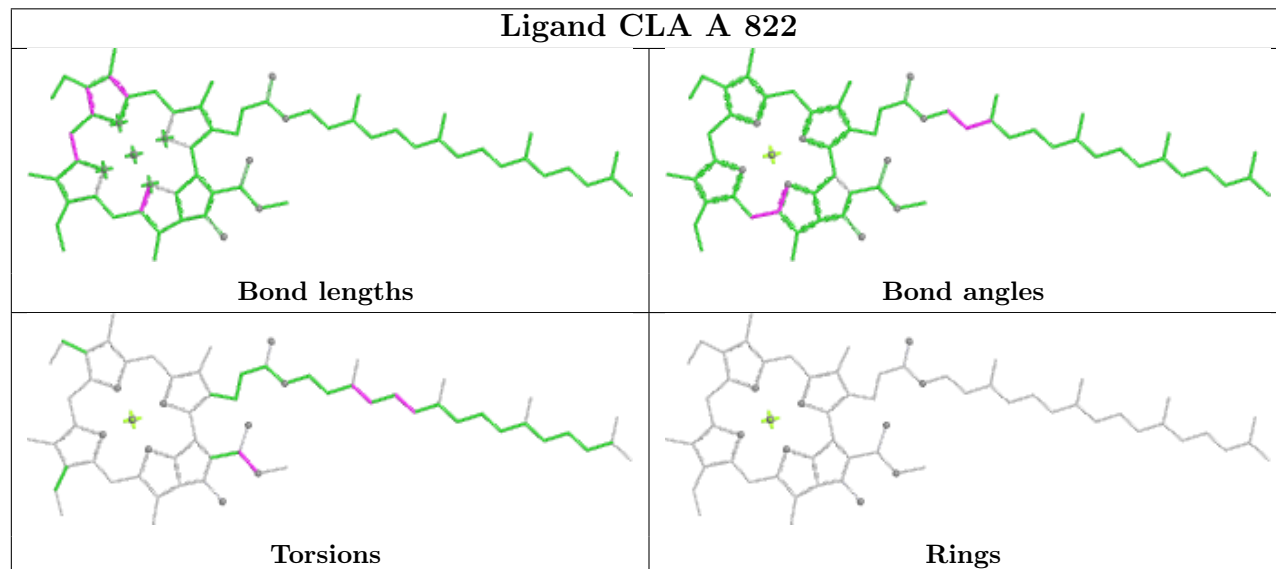
Bond angles

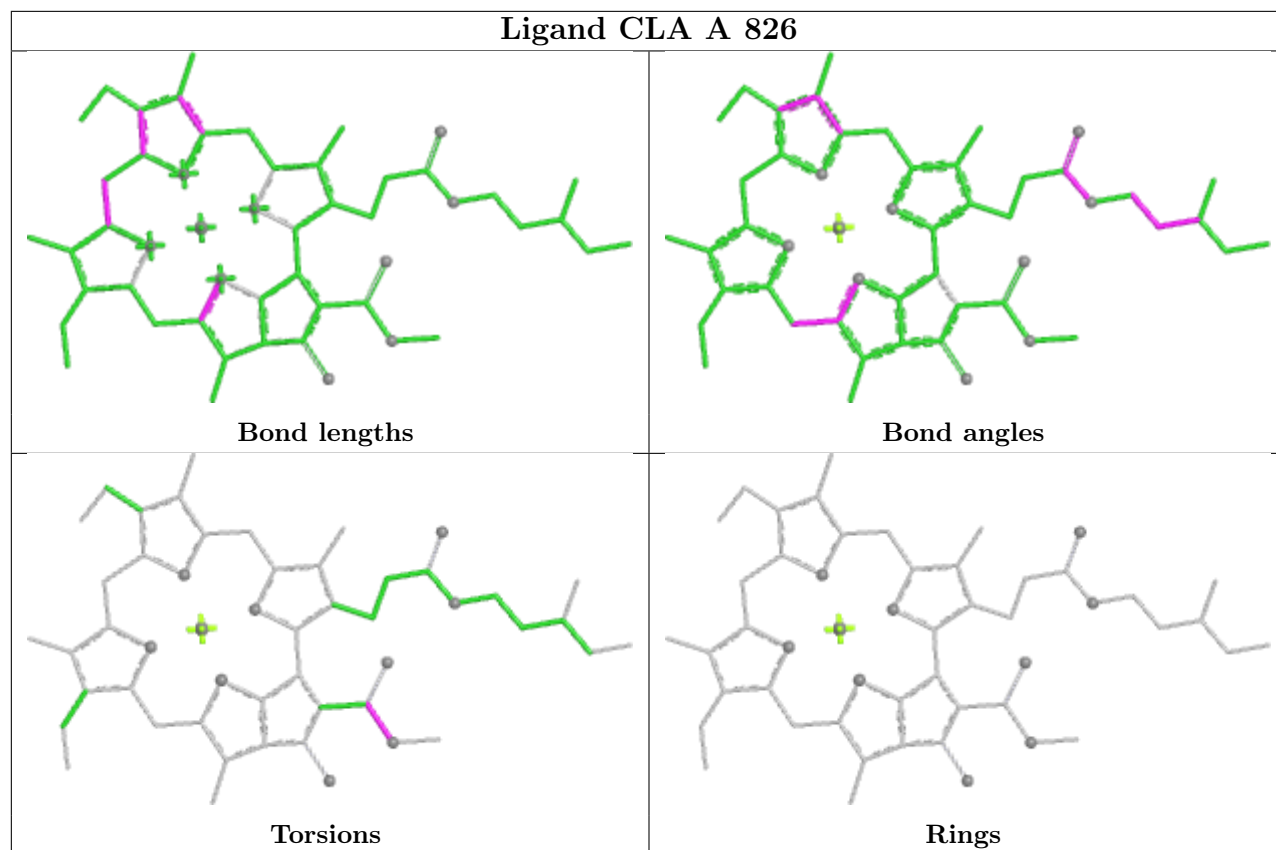


Torsions

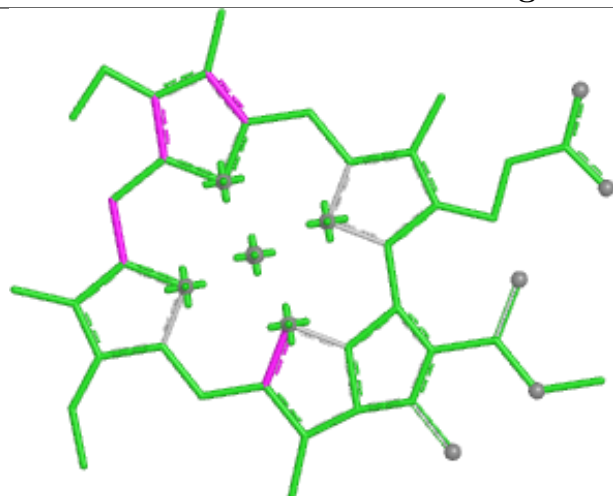


Rings

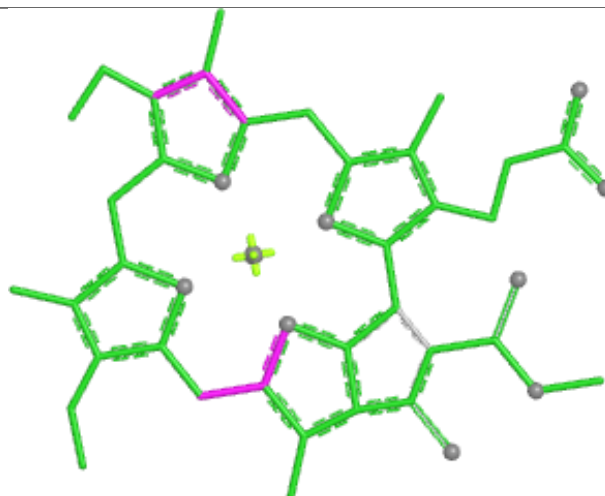
Ligand CLA 6 505**Ligand CLA A 822**



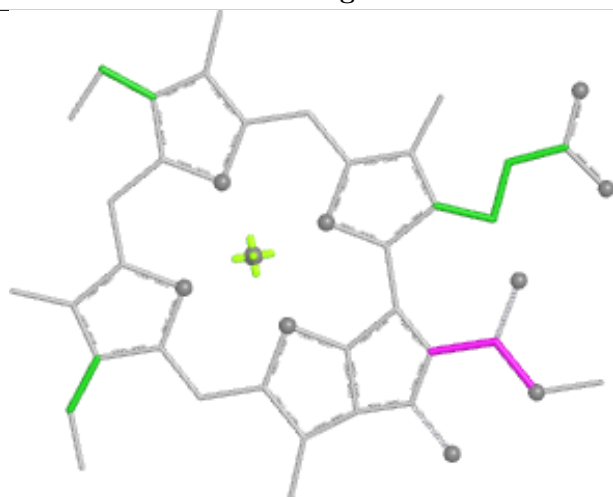
Ligand CLA 1 526



Bond lengths



Bond angles

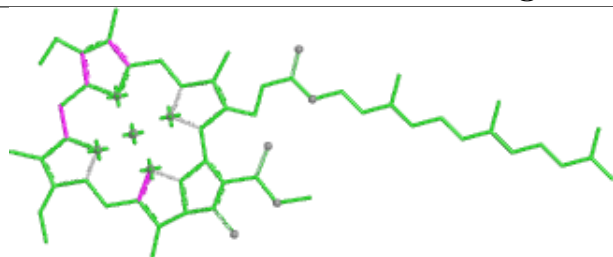


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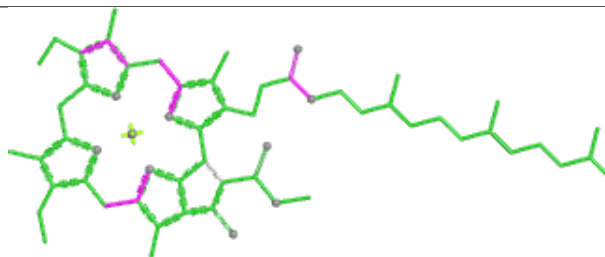


Rings

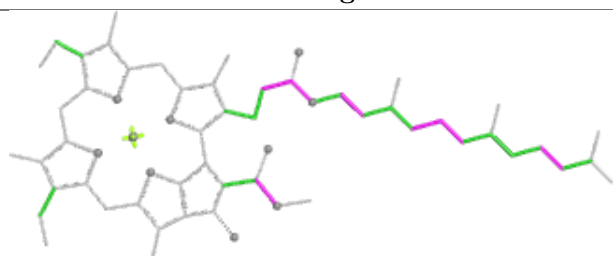
Ligand CLA 4 410



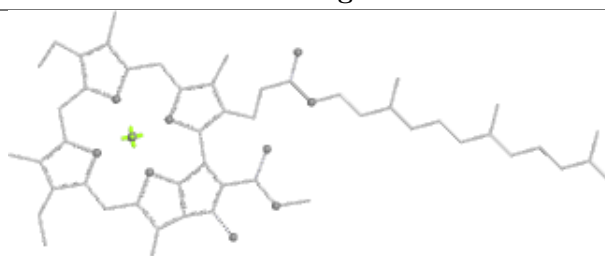
Bond lengths



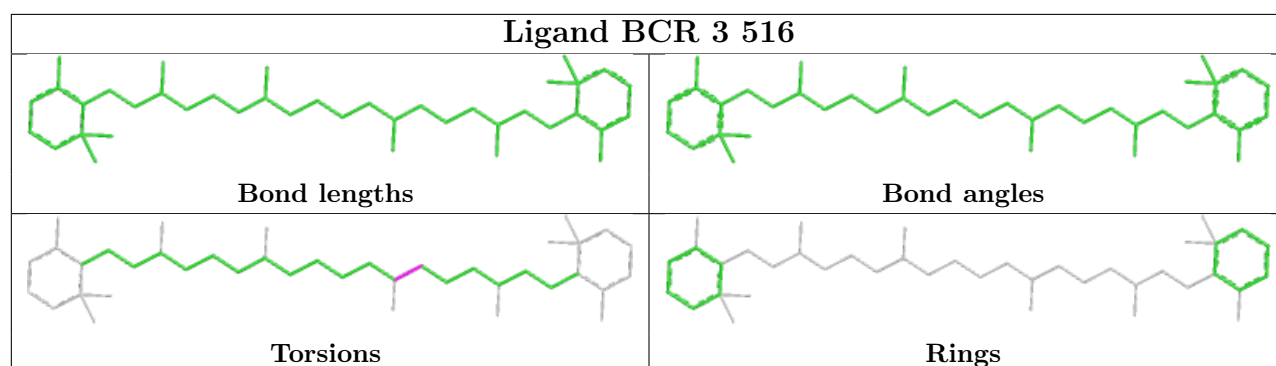
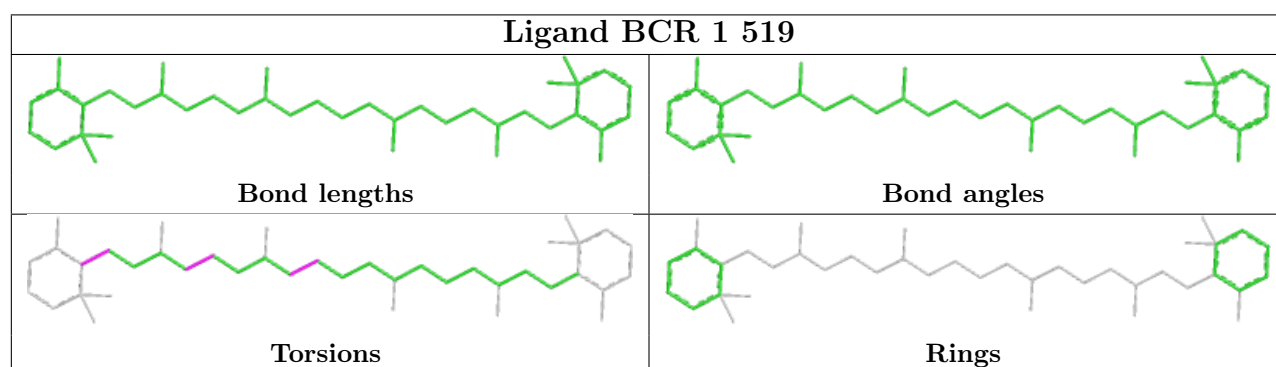
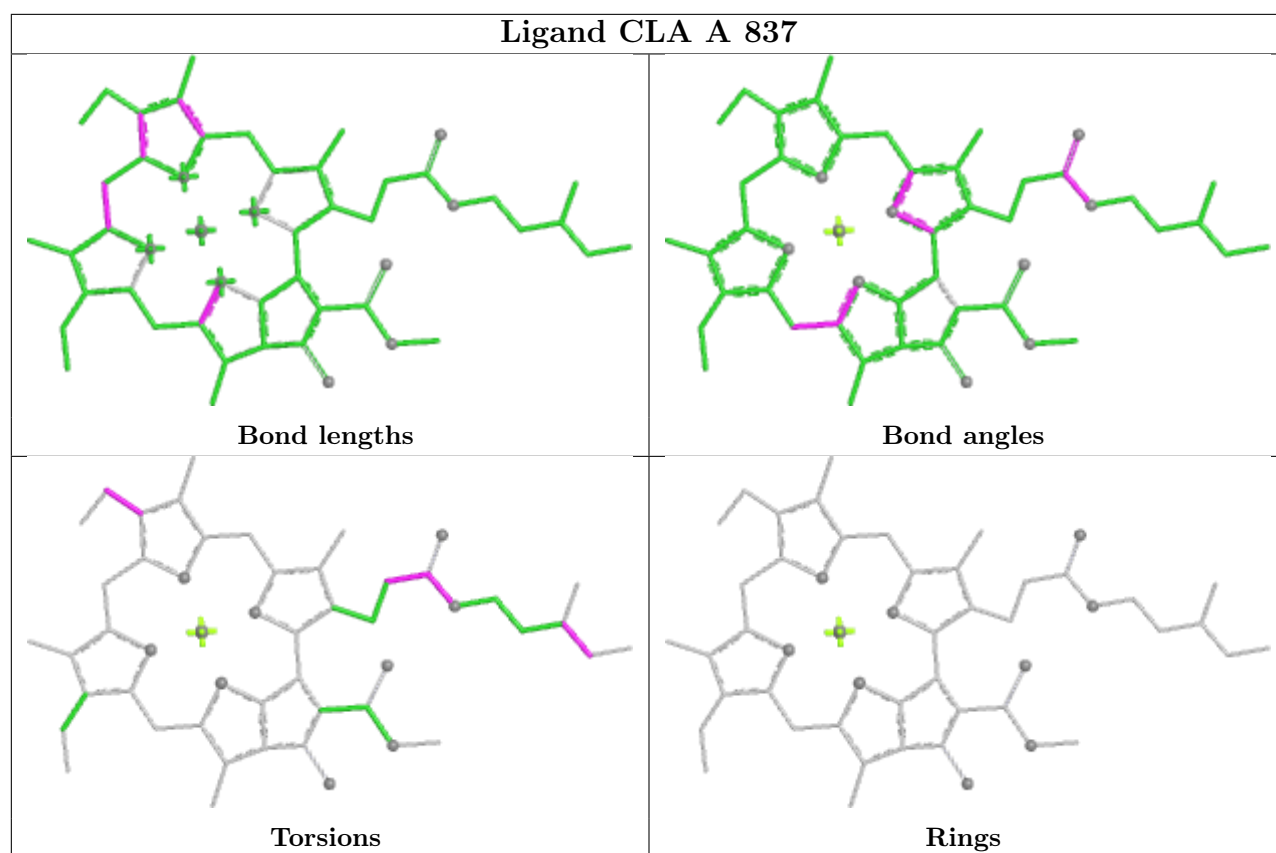
Bond angles

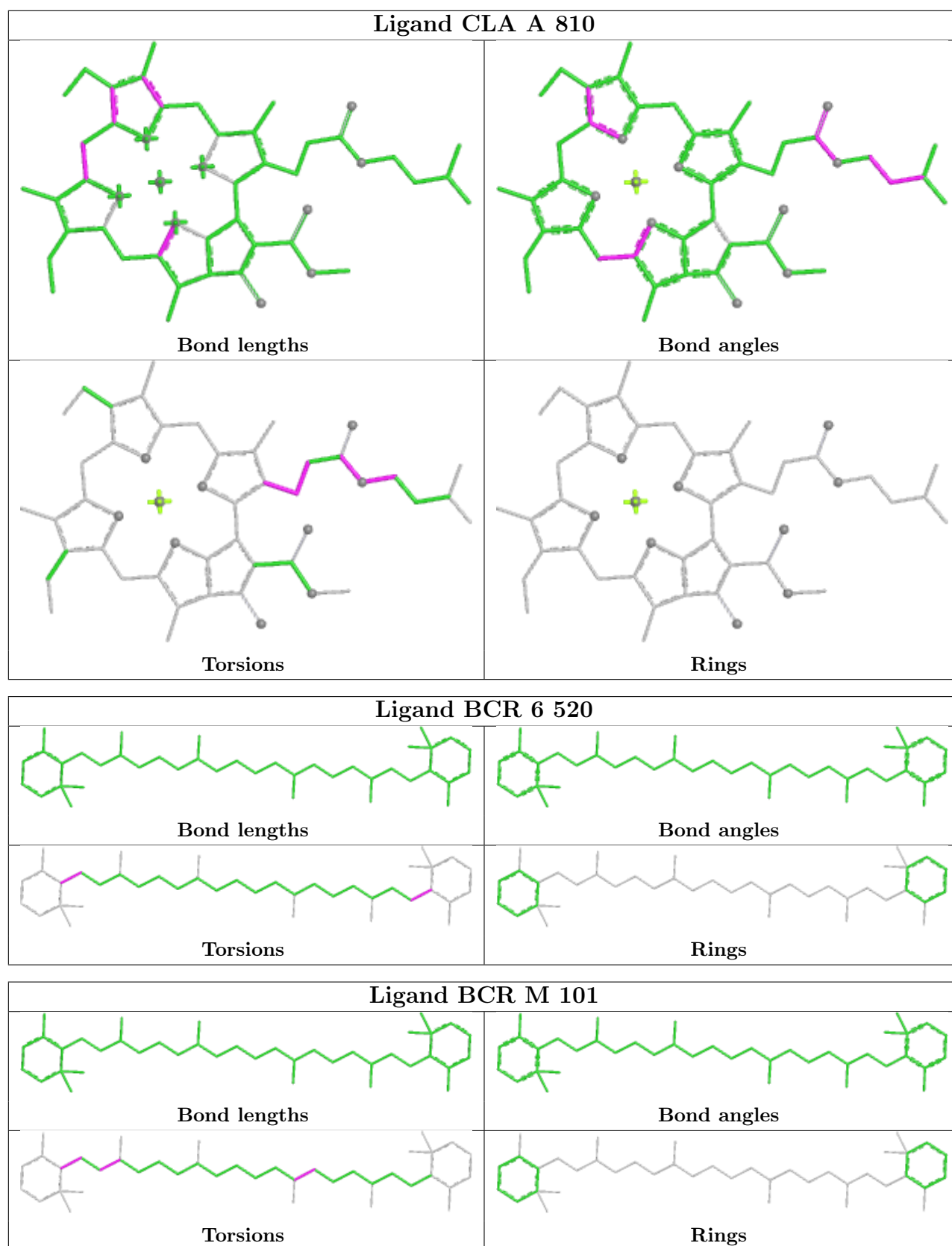


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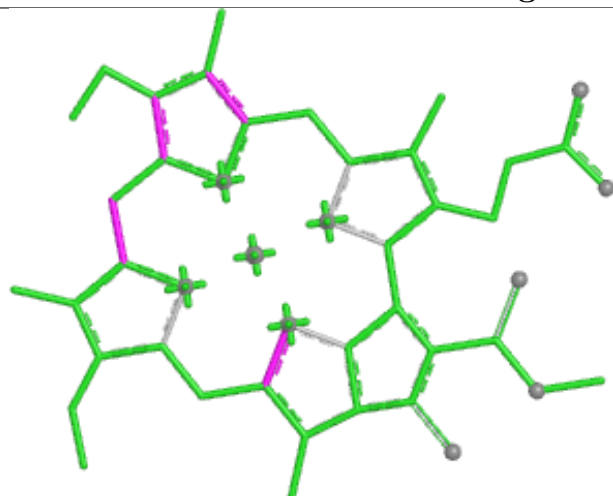


Rings

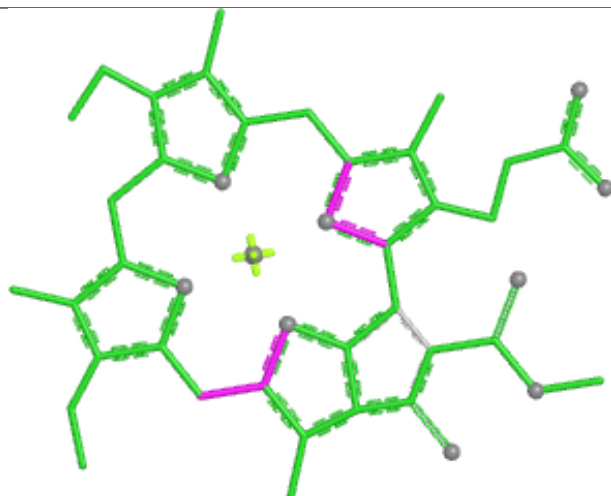




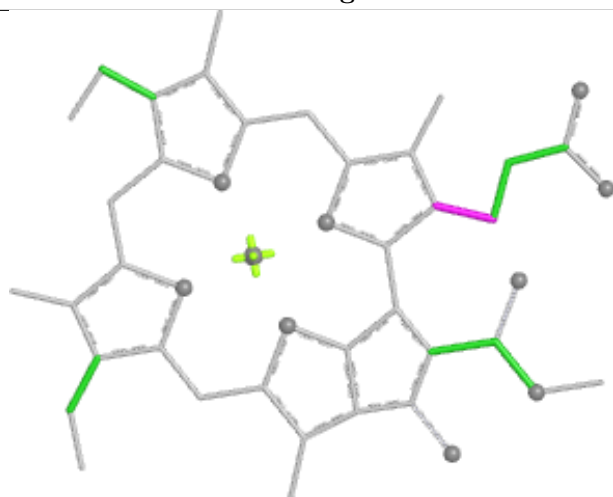
Ligand CLA 4 413



Bond lengths



Bond angles

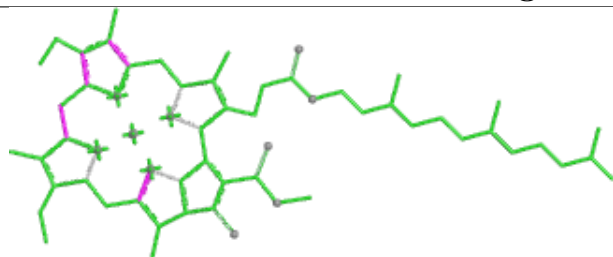


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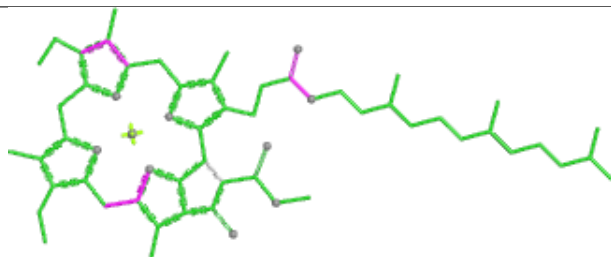


Rings

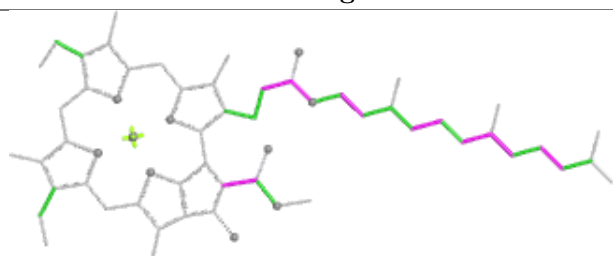
Ligand CLA 7 509



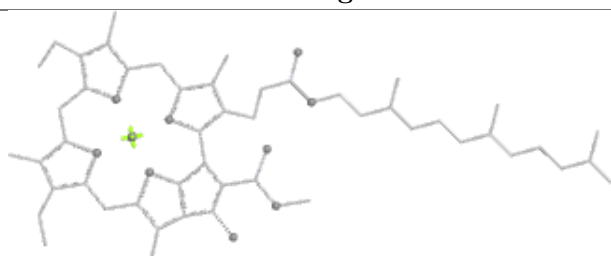
Bond lengths



Bond angles

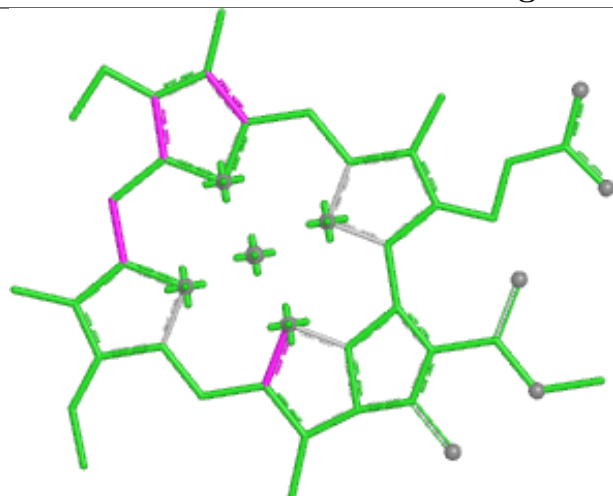


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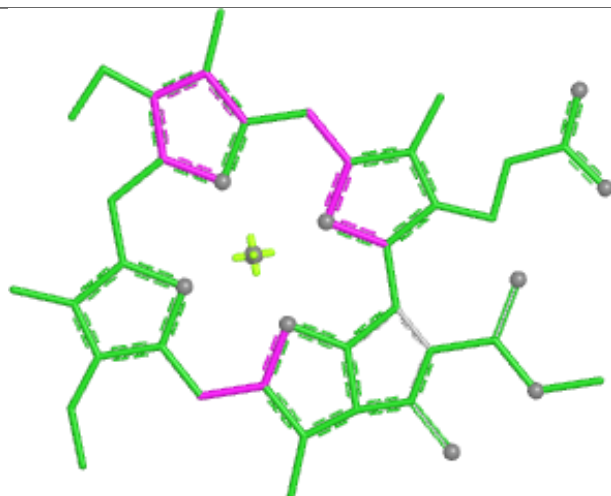


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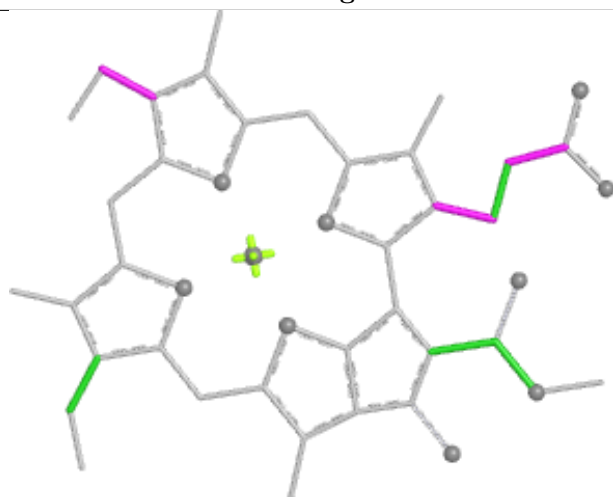
Ligand CLA 1 511



Bond lengths



Bond angles

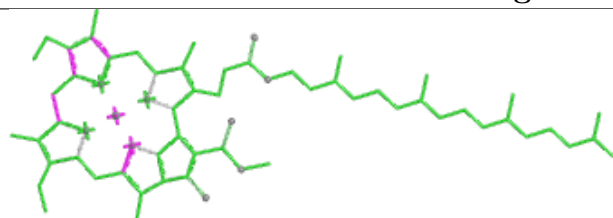


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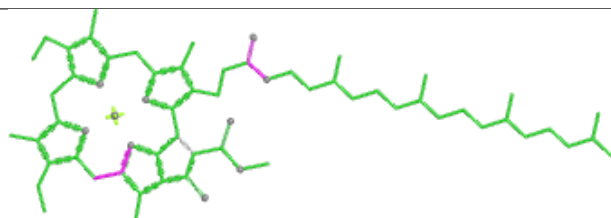


Rings

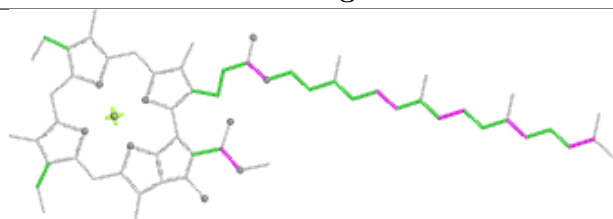
Ligand CLA A 833



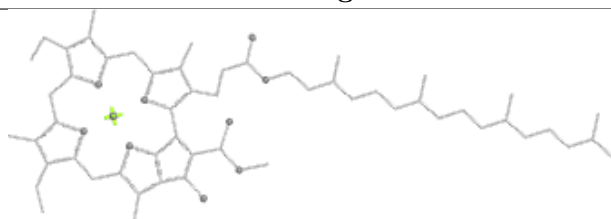
Bond lengths



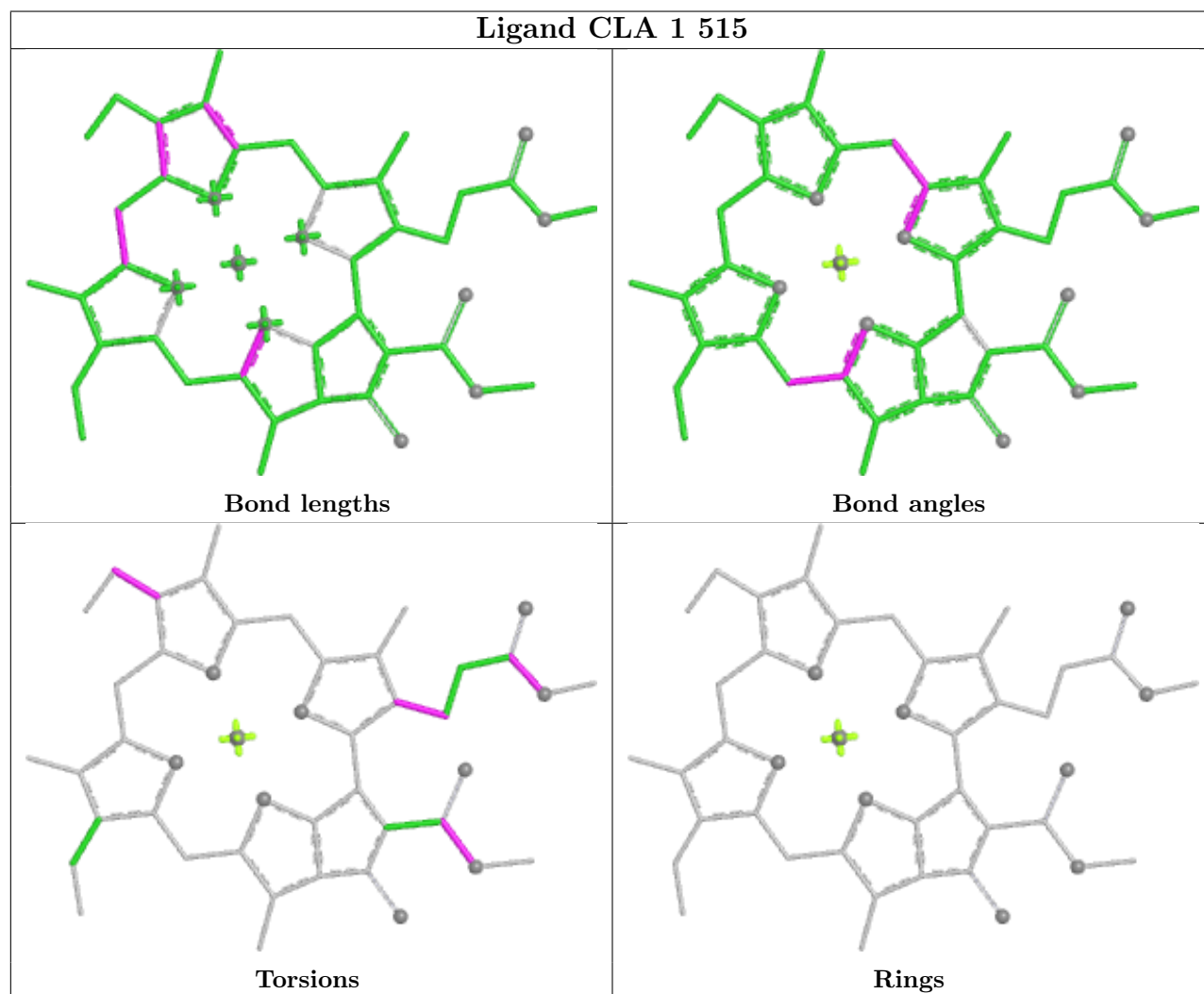
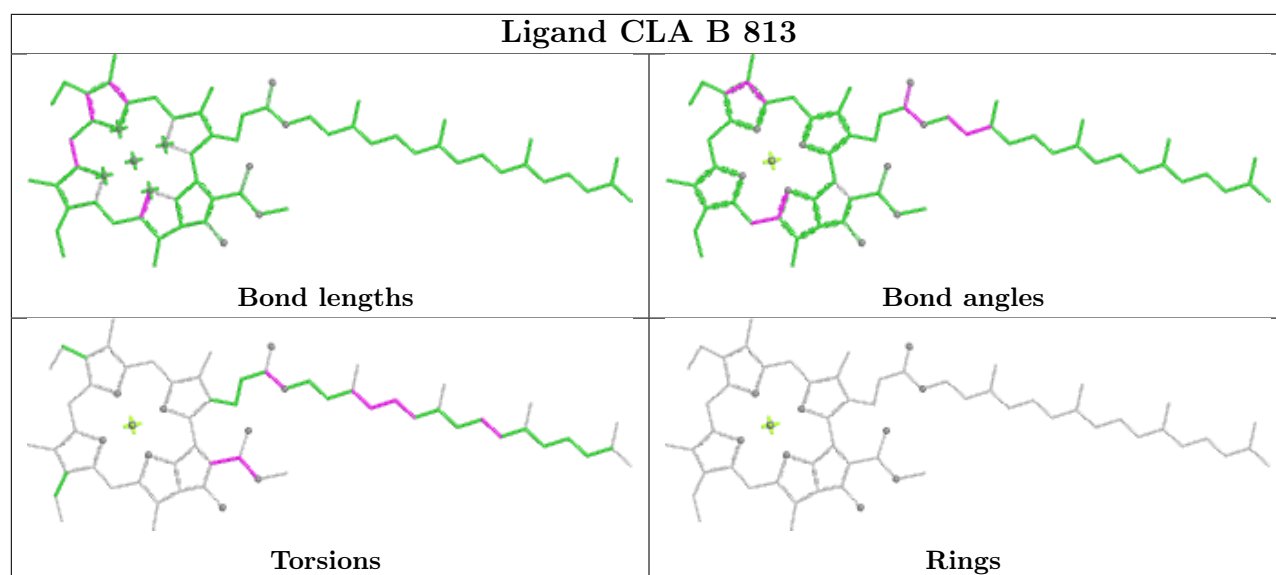
Bond angles

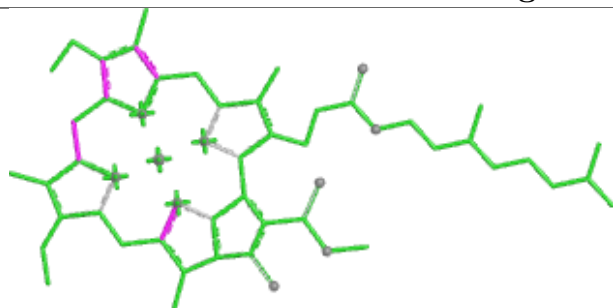


Torsions

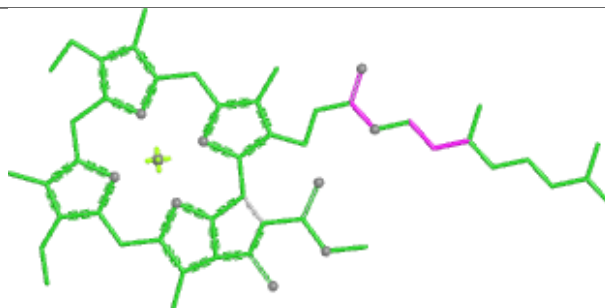


Rings

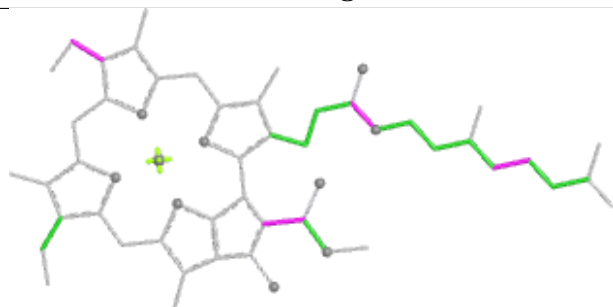


Ligand CLA 4 403

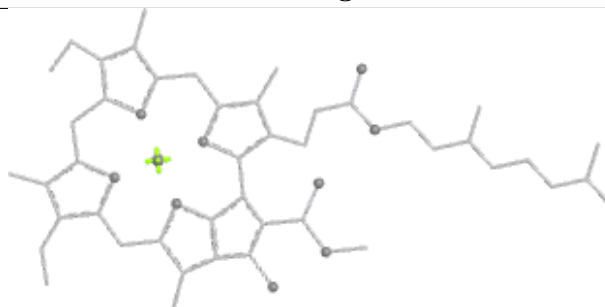
Bond lengths



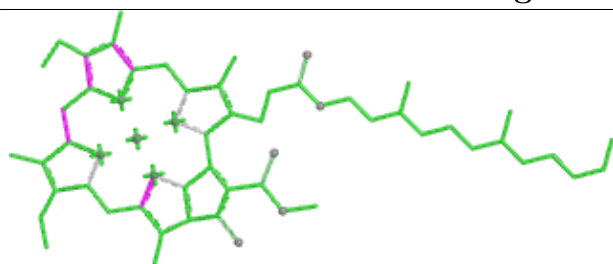
Bond angles



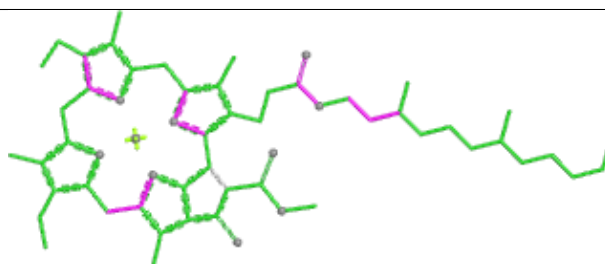
Torsions



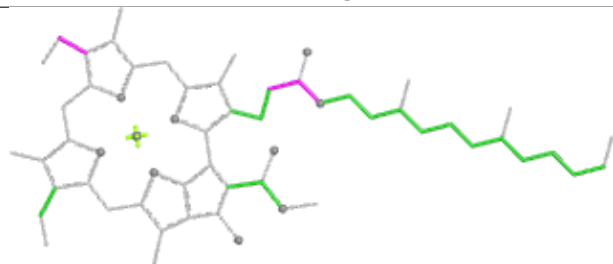
Rings

Ligand CLA B 824

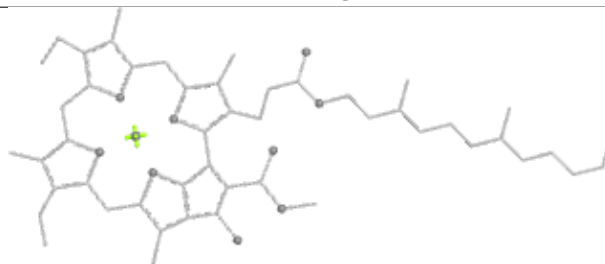
Bond lengths



Bond angles

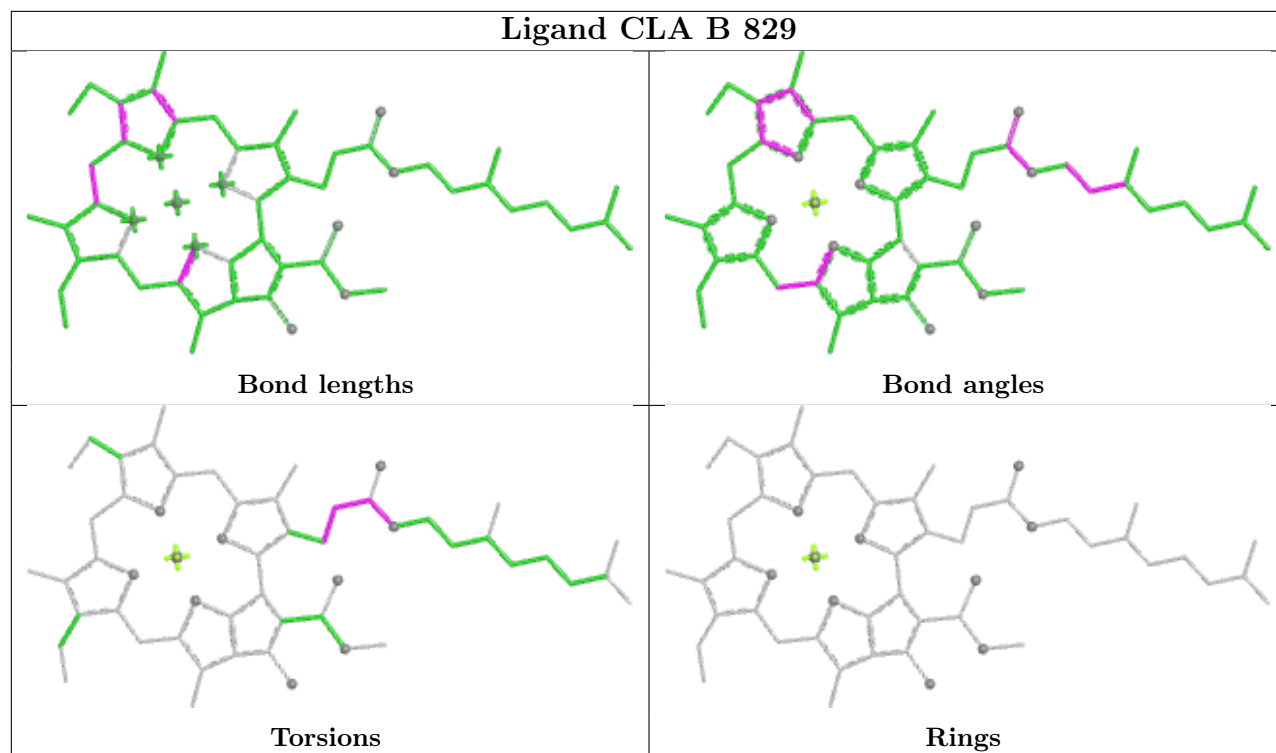


Torsions

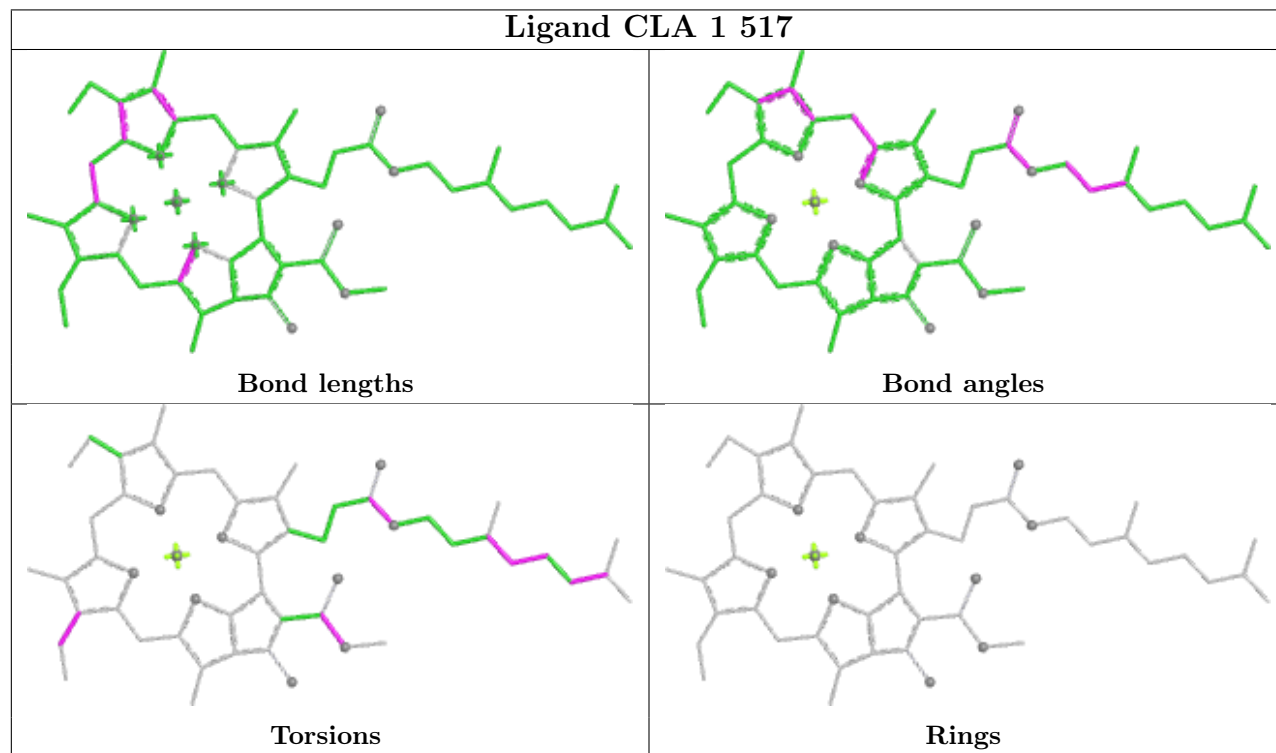


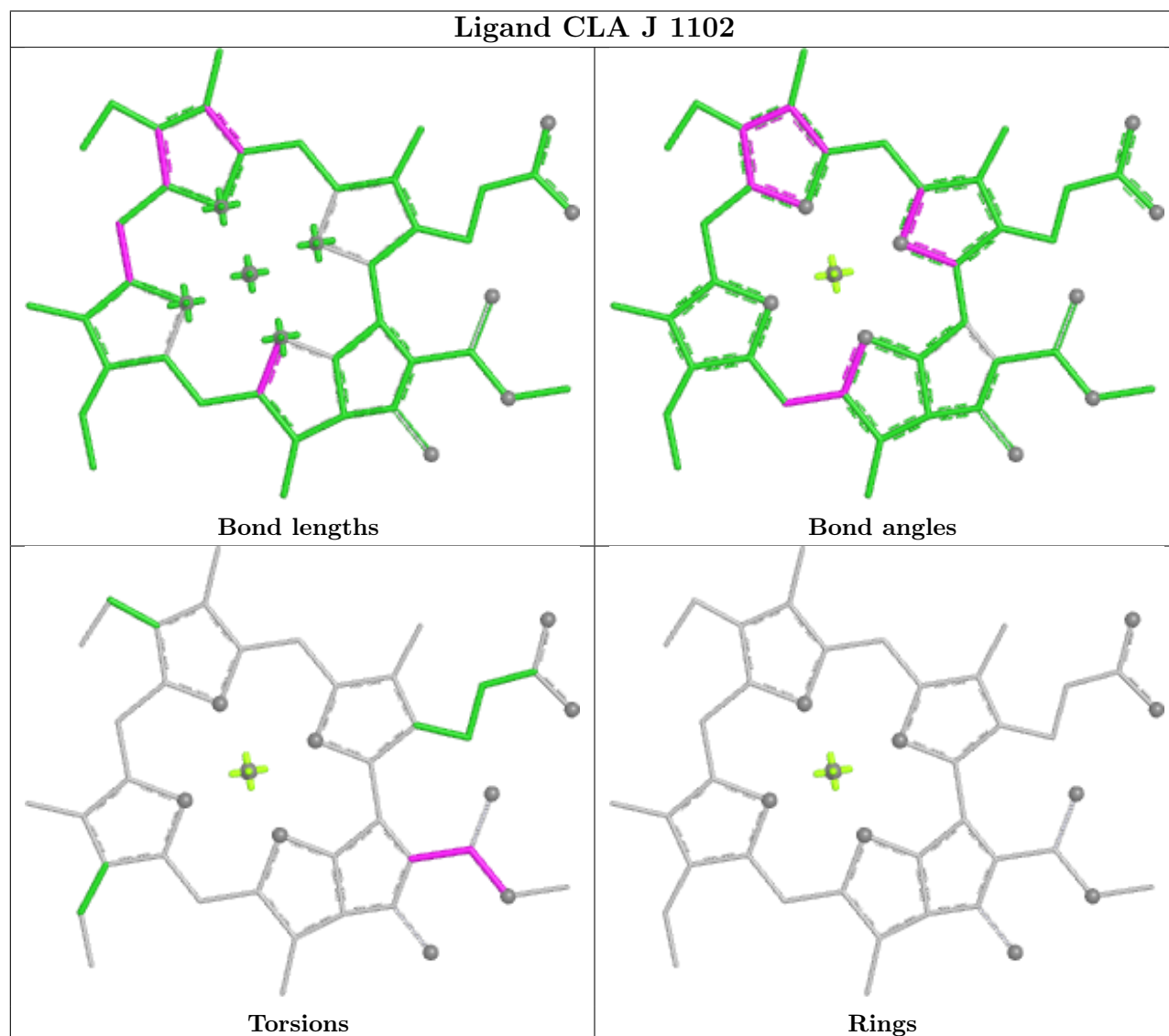
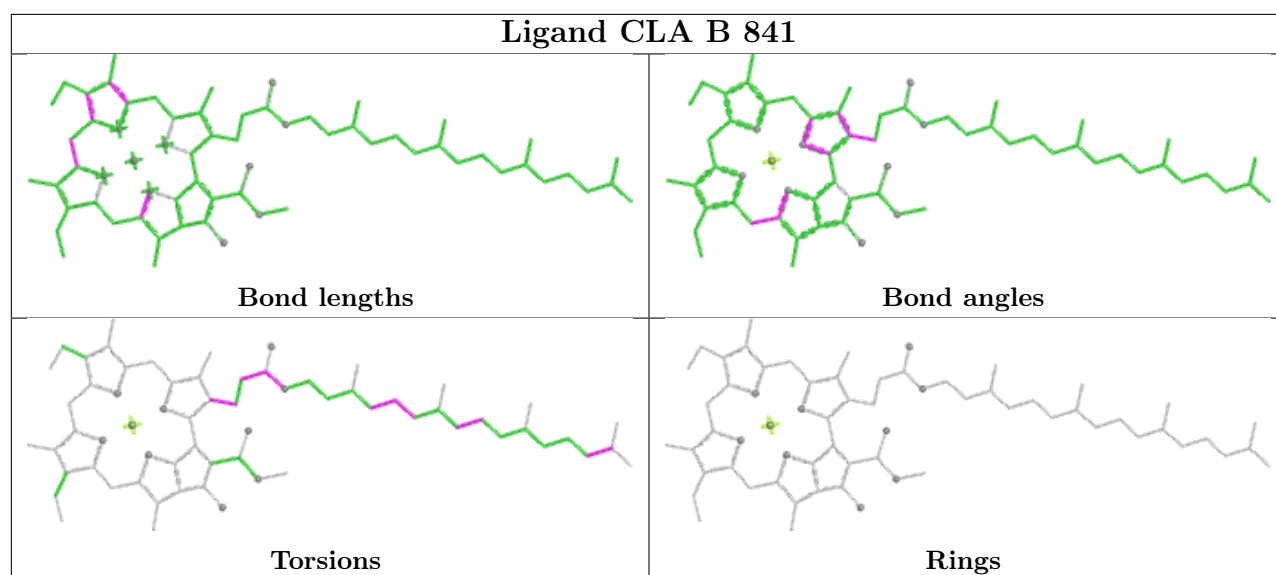
Rings

Ligand CLA B 829

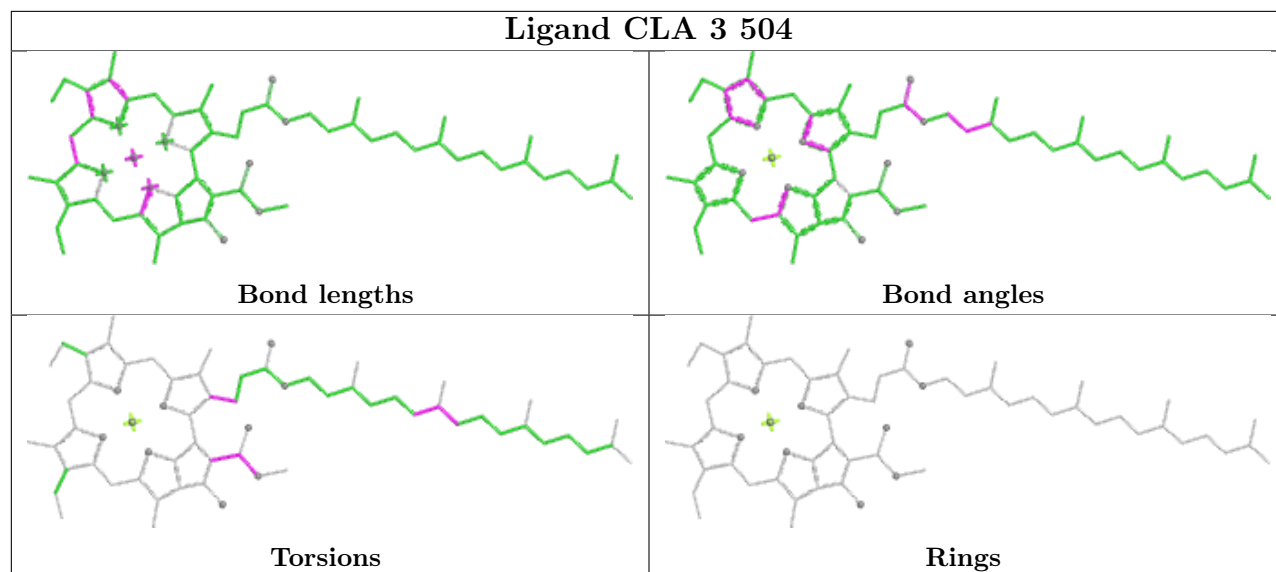


Ligand CLA 1 517

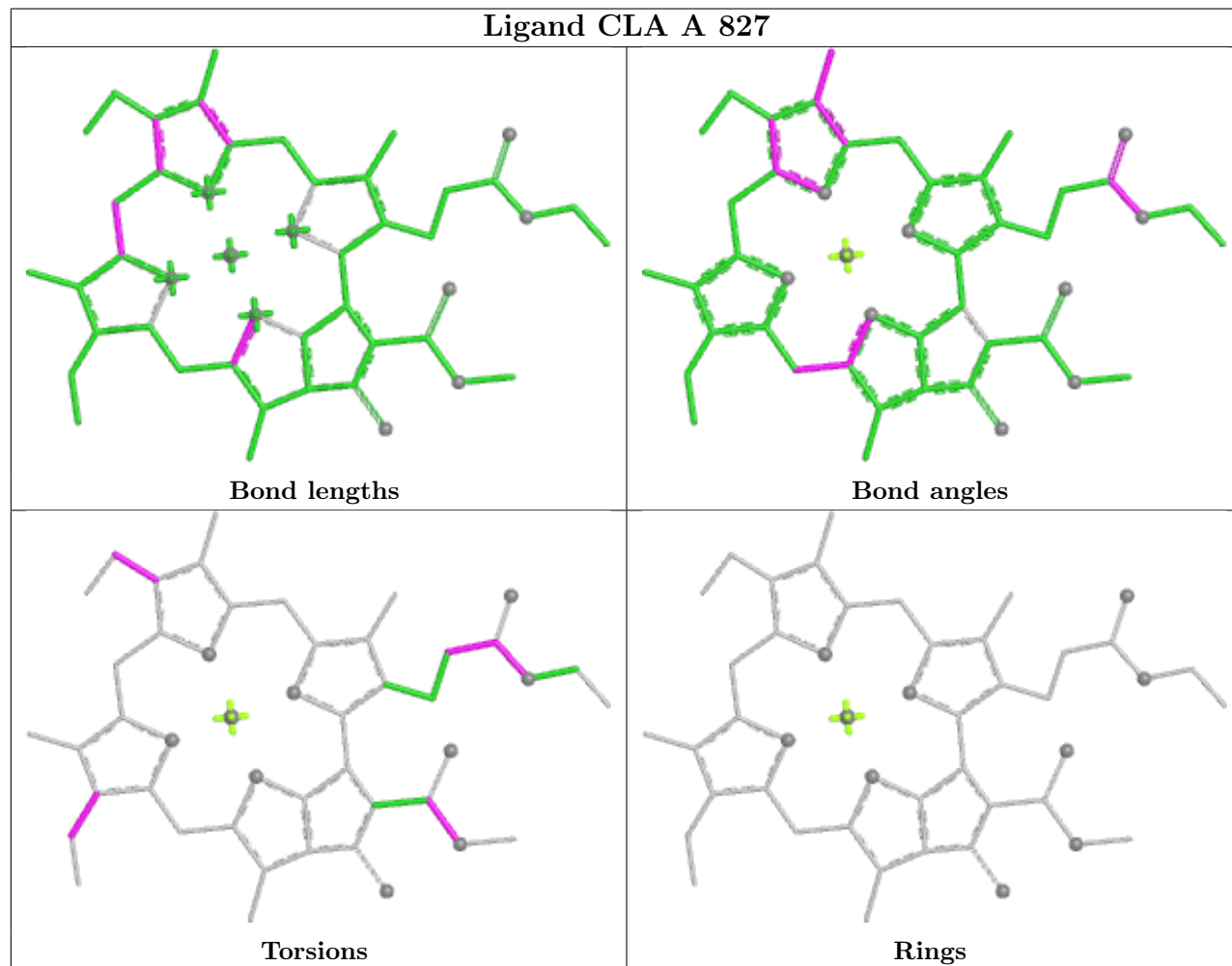


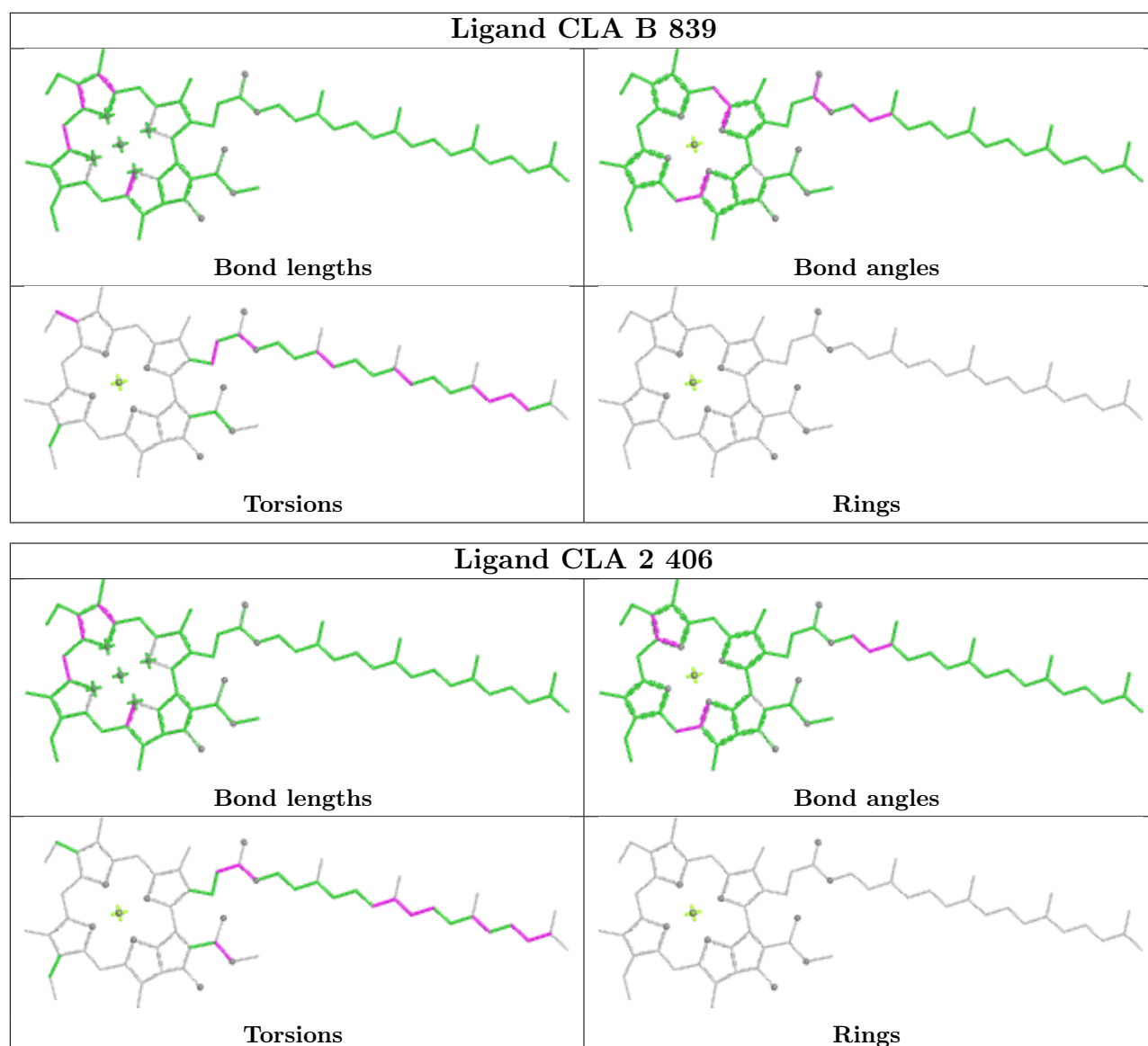


Ligand CLA 3 504

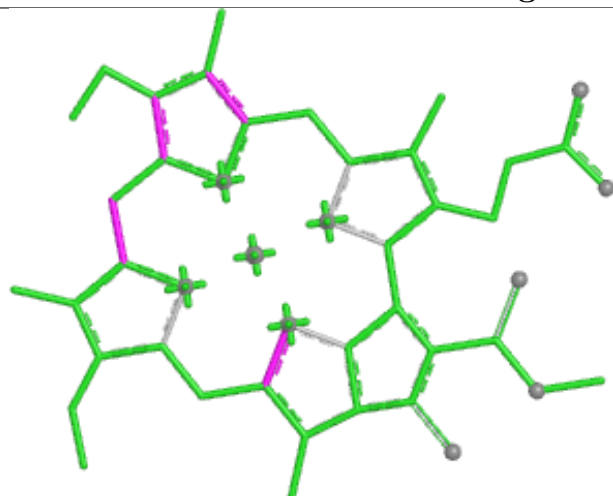


Ligand CLA A 827

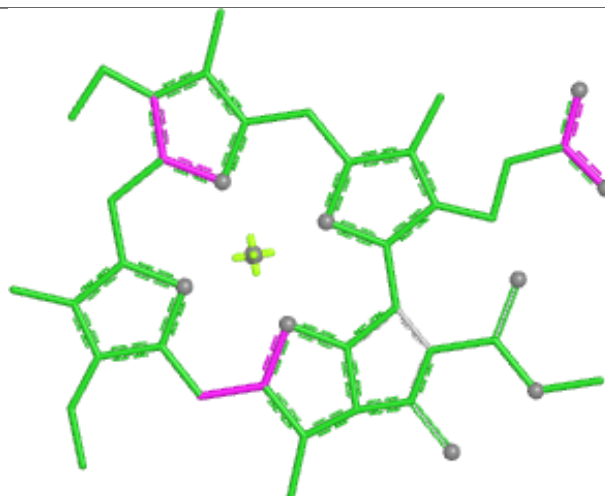




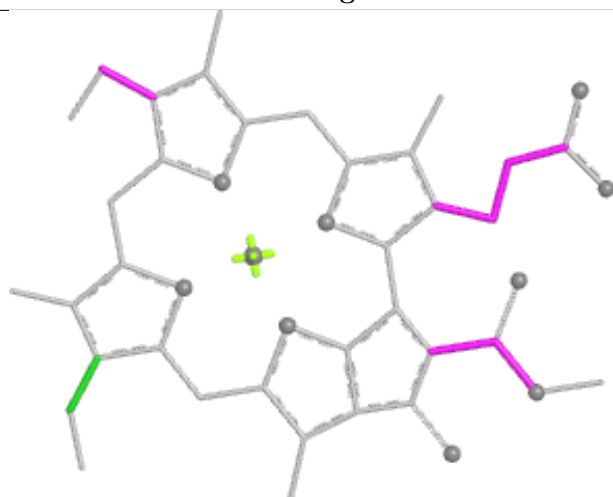
Ligand CLA 3 512



Bond lengths



Bond angles

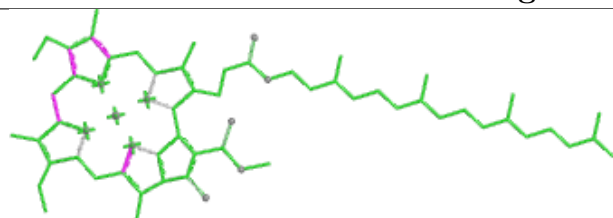


Torsions

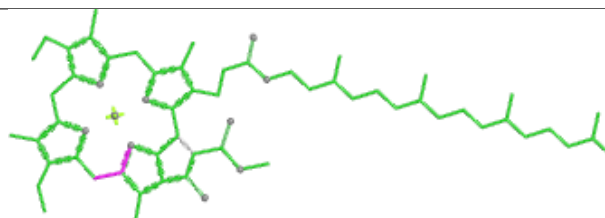


Rings

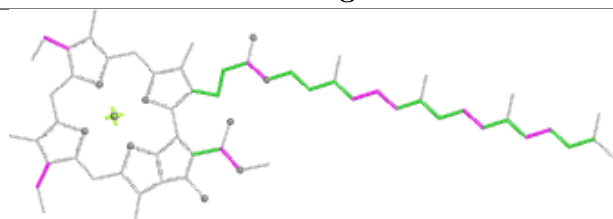
Ligand CLA 1 503



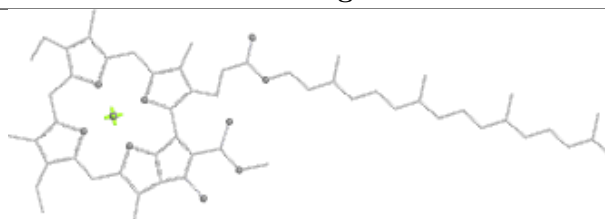
Bond lengths



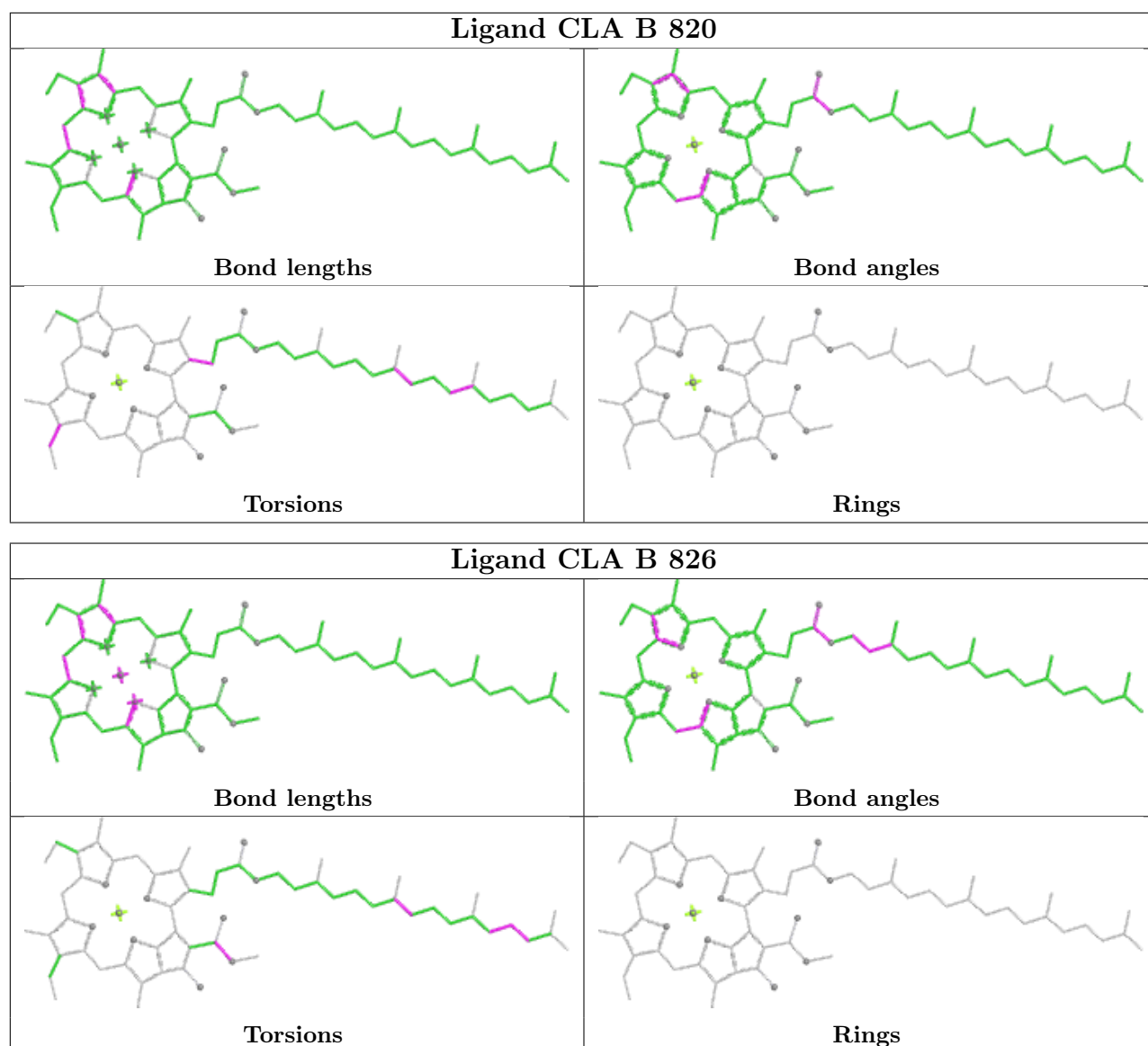
Bond angles



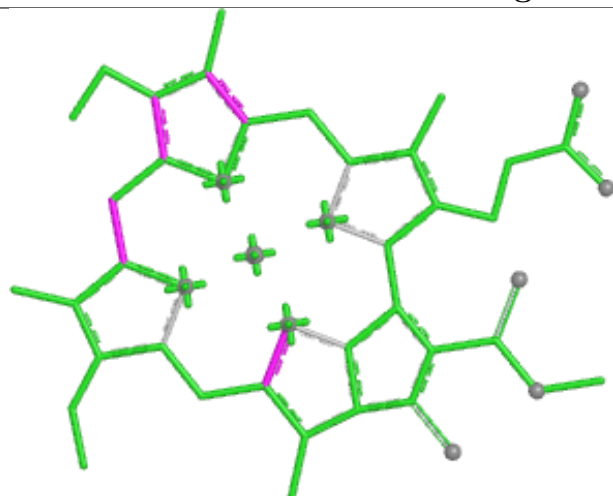
Torsions



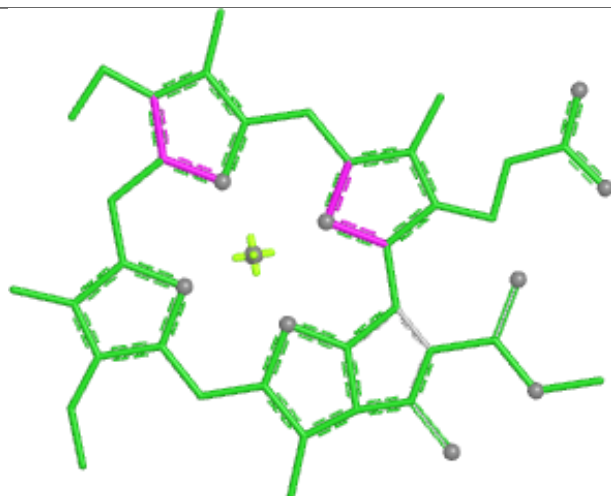
Rings



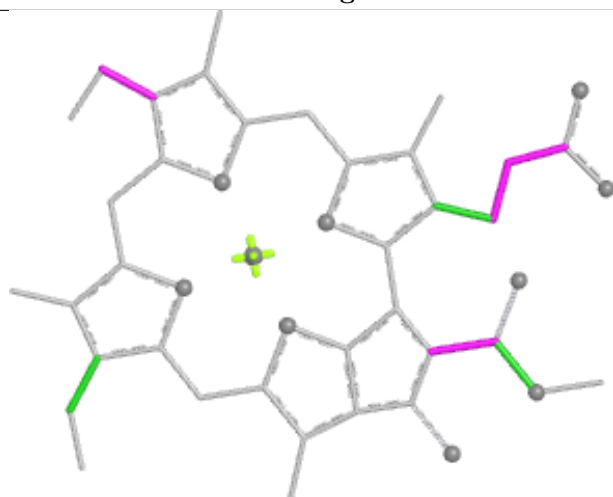
Ligand CLA B 828



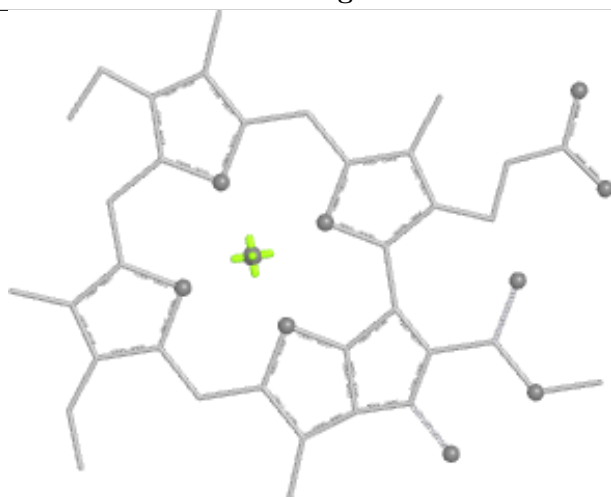
Bond lengths



Bond angles

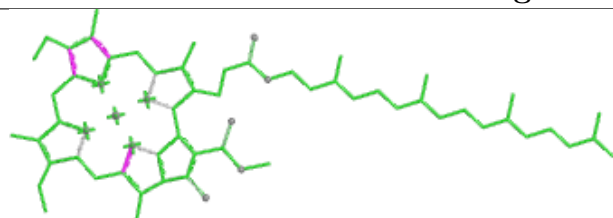


Torsions

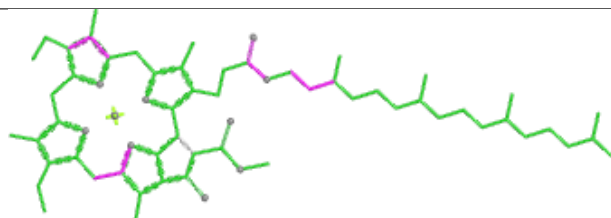


Rings

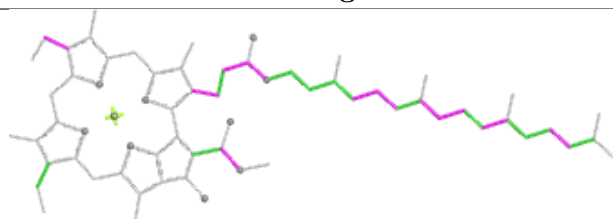
Ligand CLA A 842



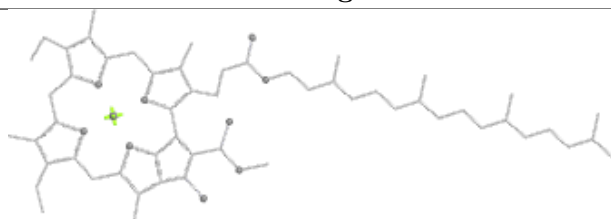
Bond lengths



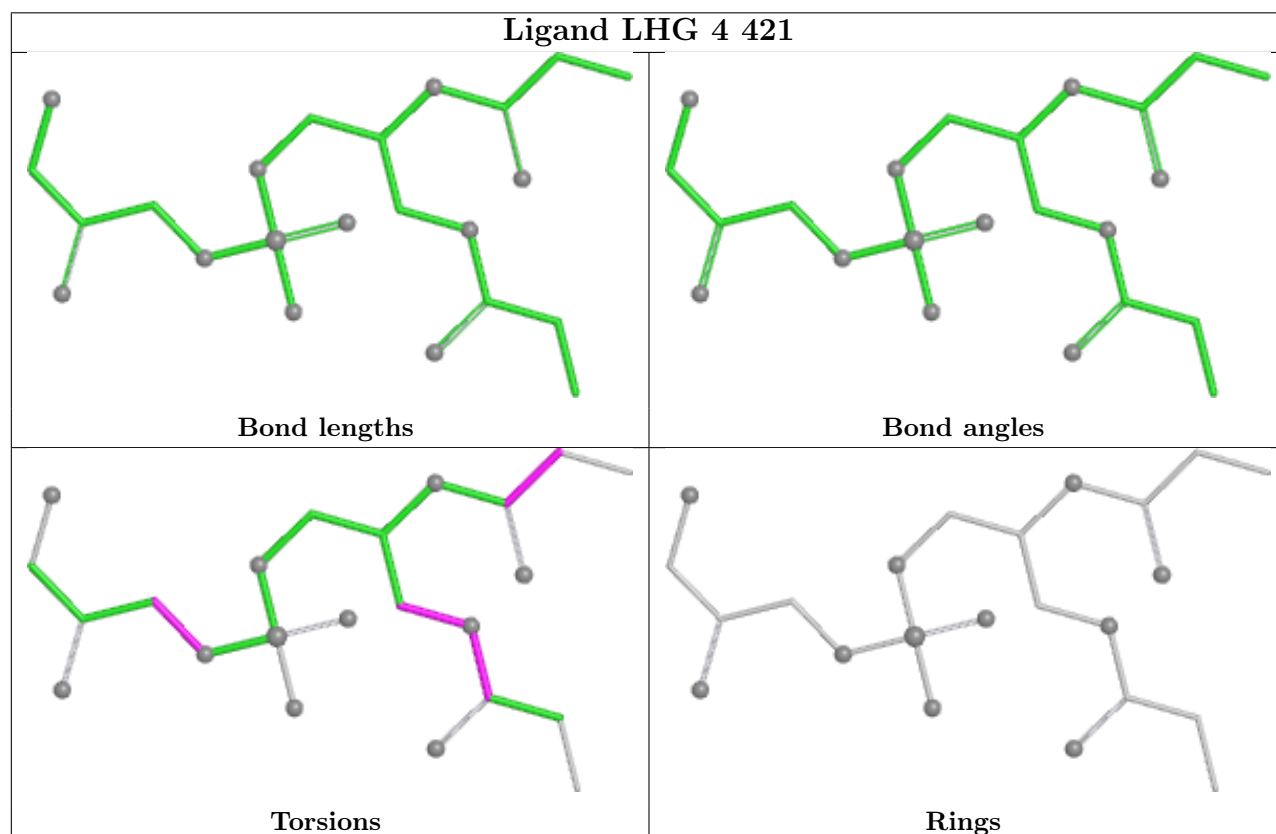
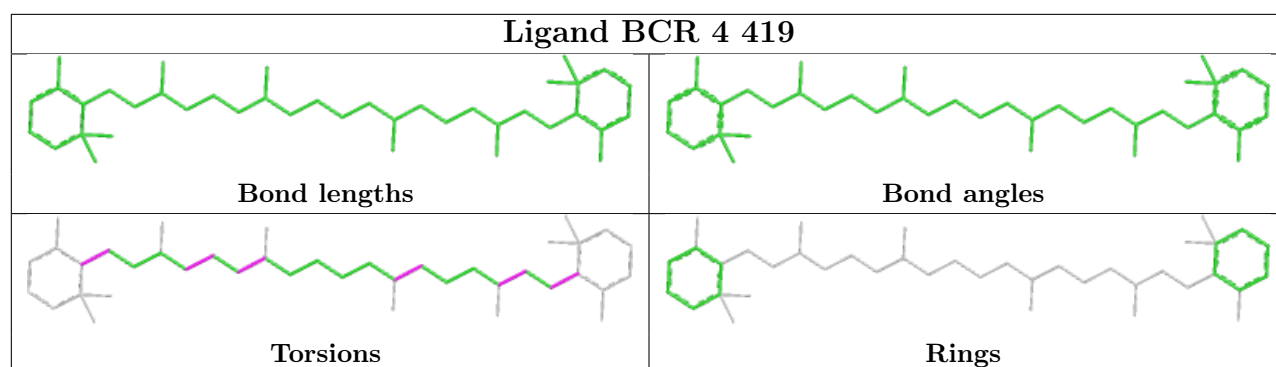
Bond angles

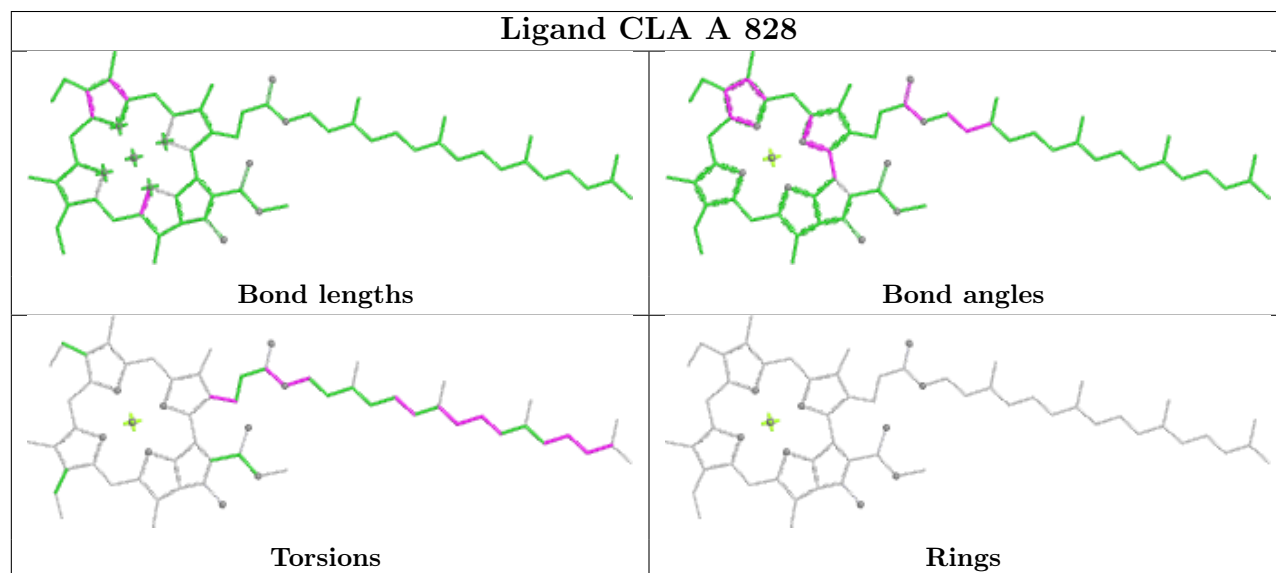
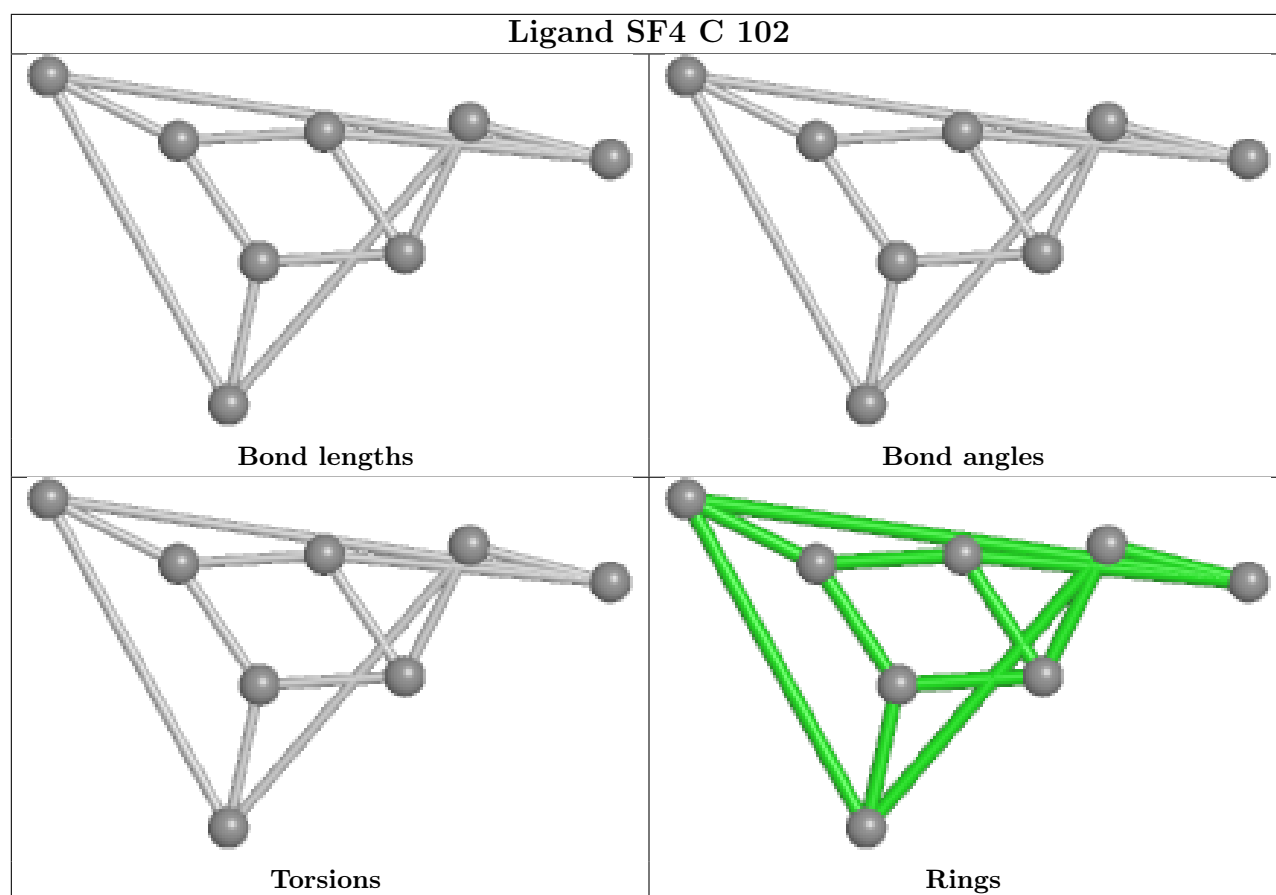


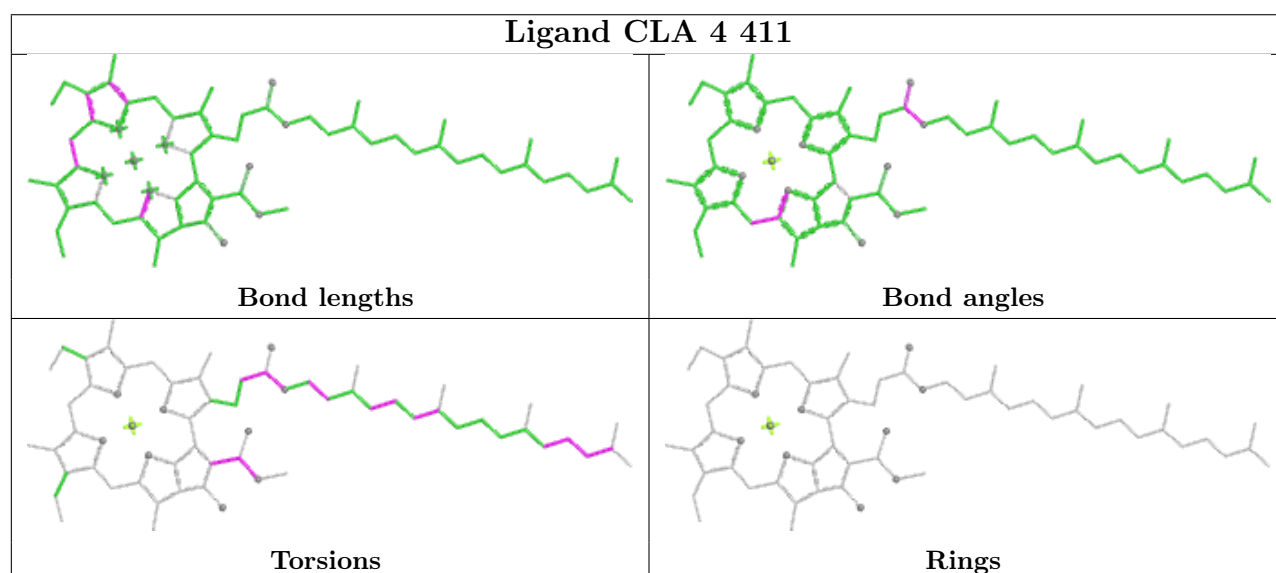
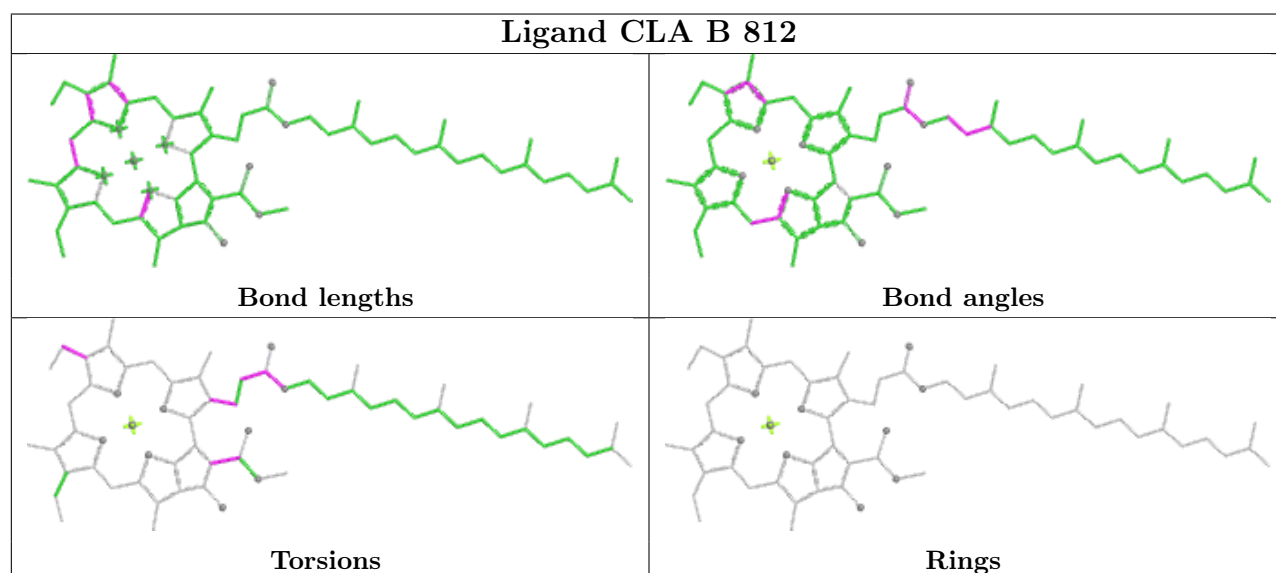
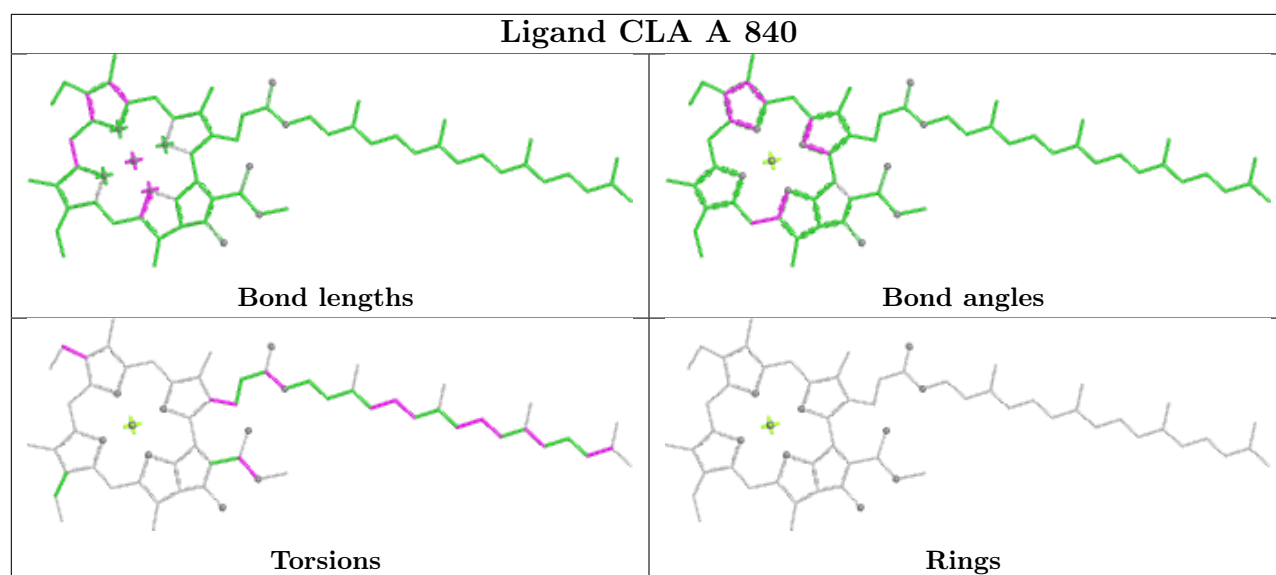
Torsions

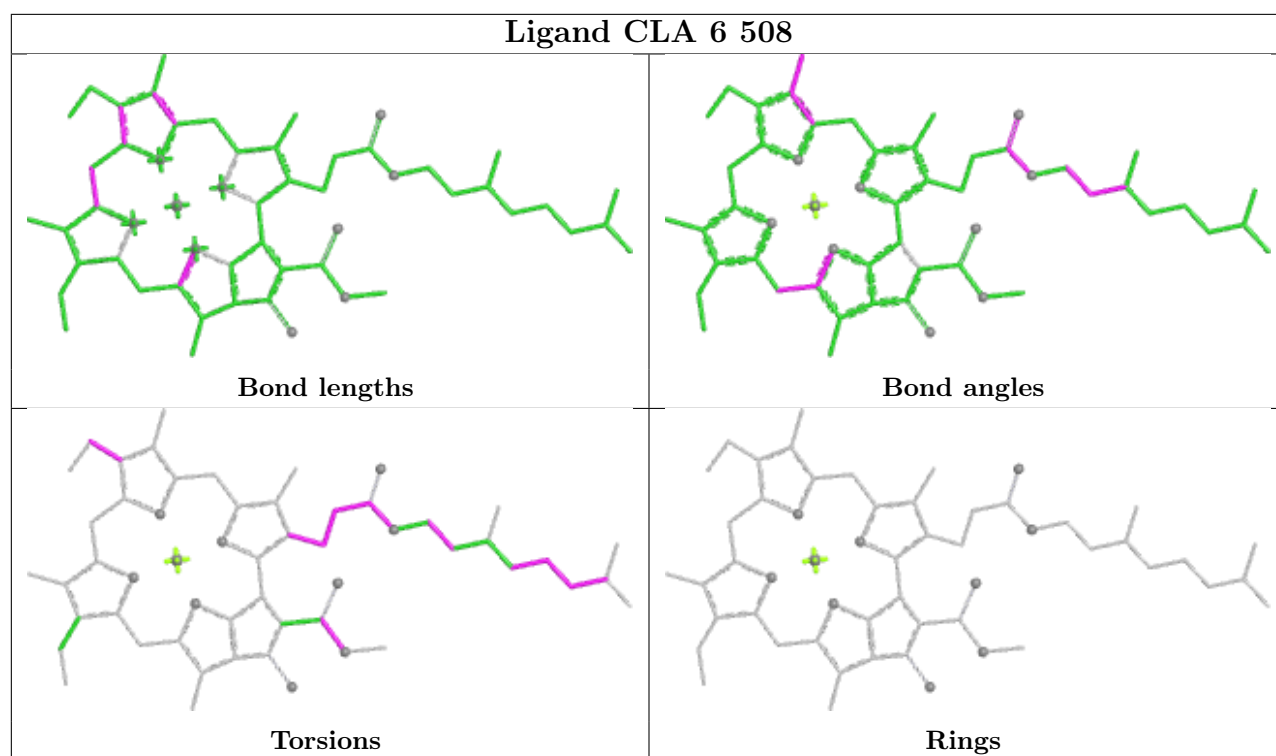


Rings

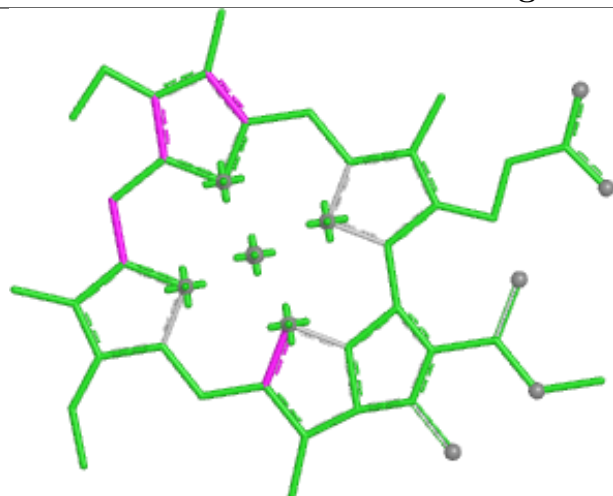




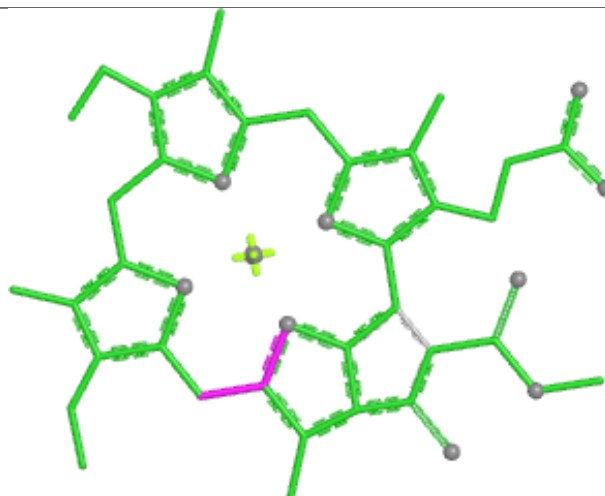




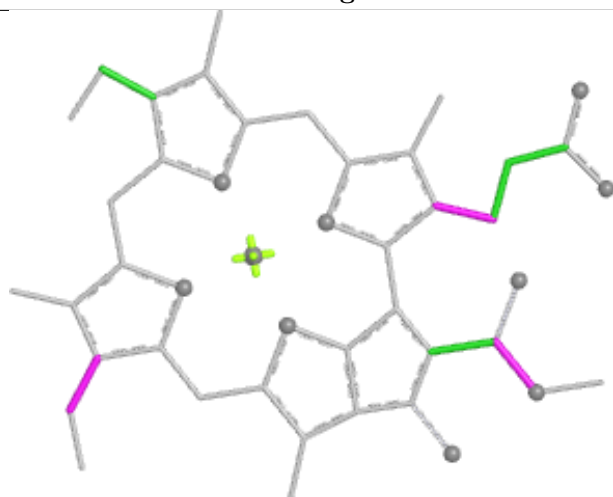
Ligand CLA 6 514



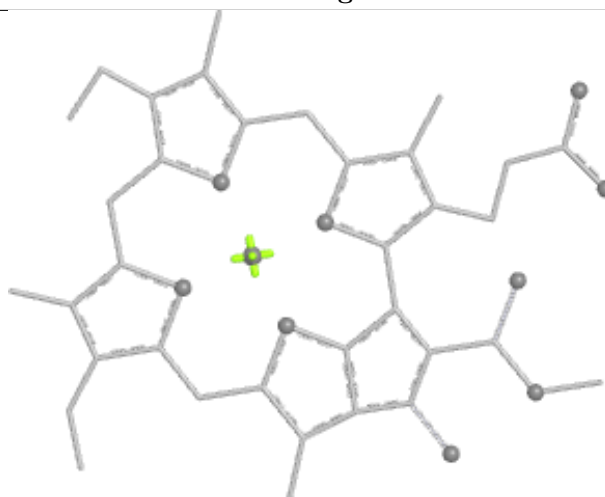
Bond lengths



Bond angles

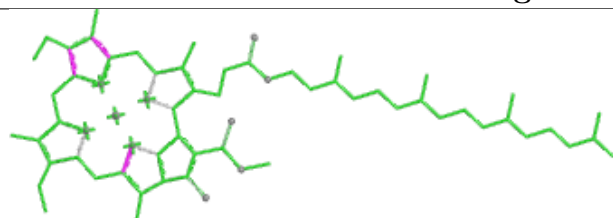


Torsions

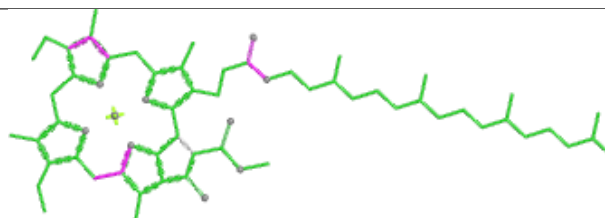


Rings

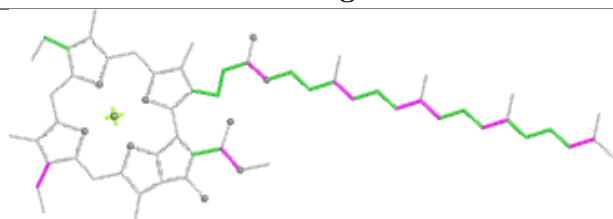
Ligand CLA A 841



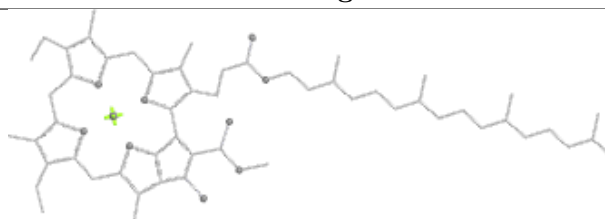
Bond lengths



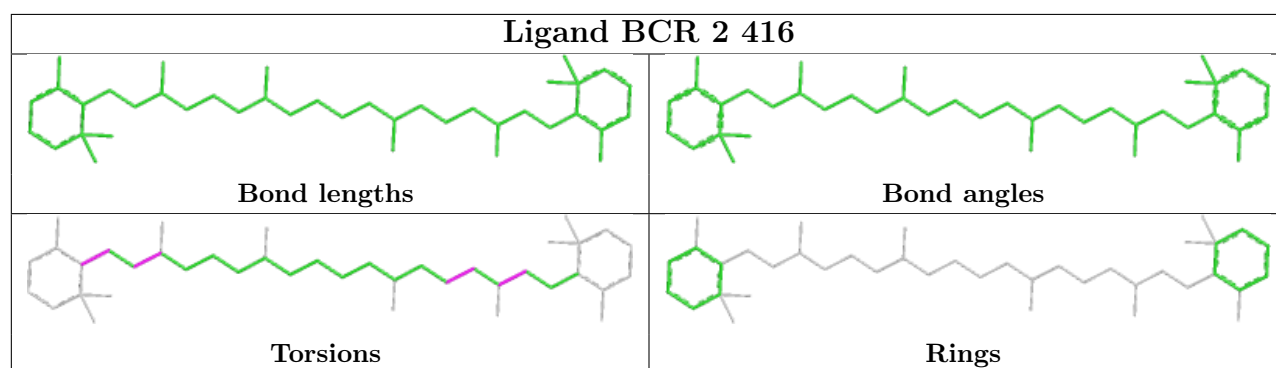
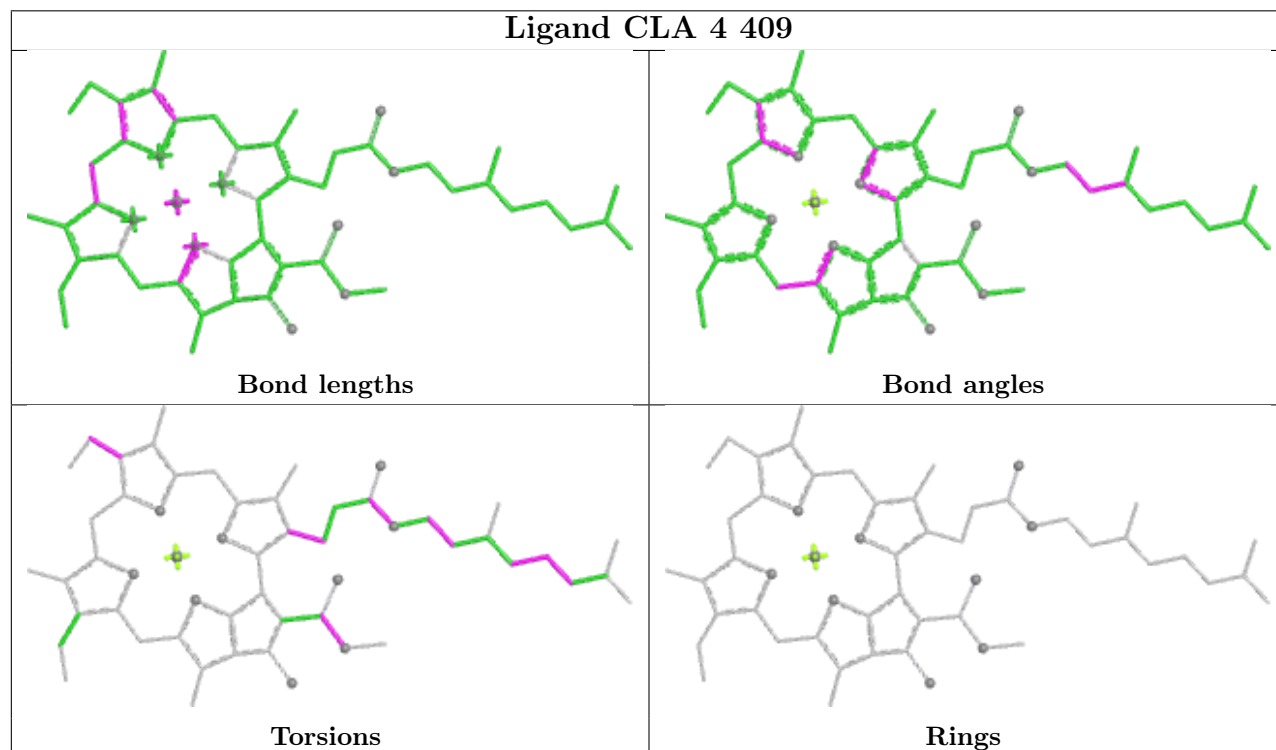
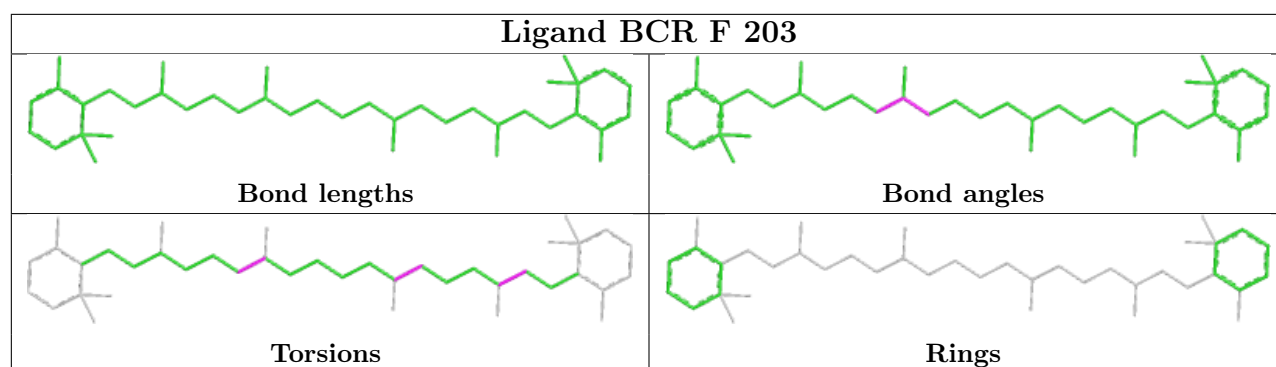
Bond angles



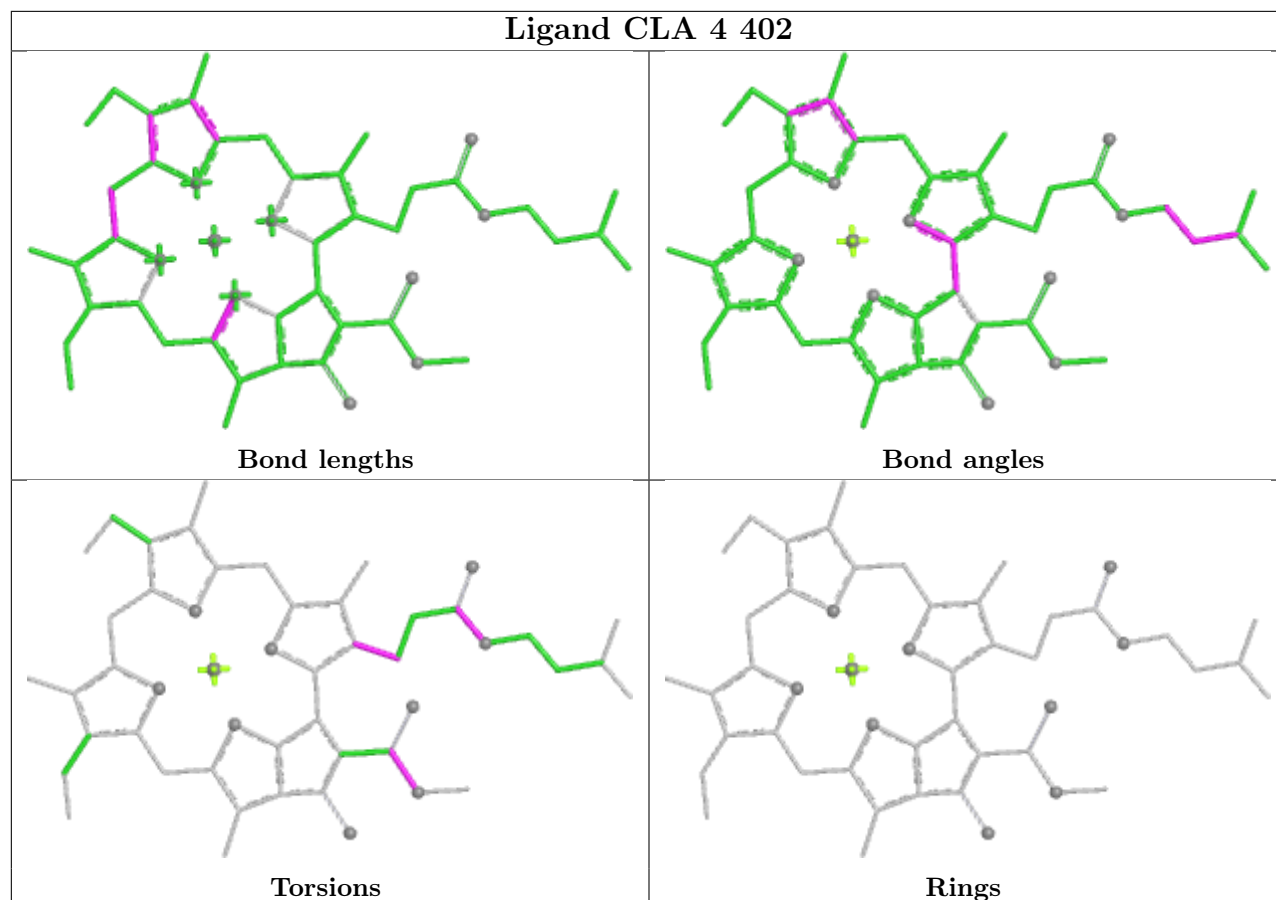
Torsions



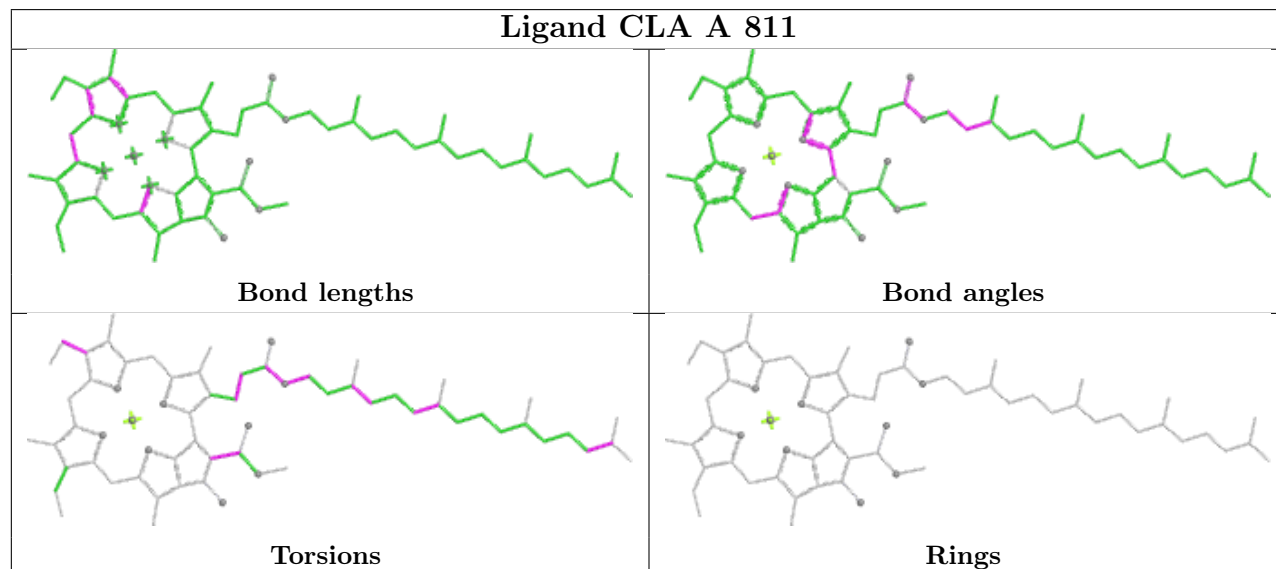
Rings

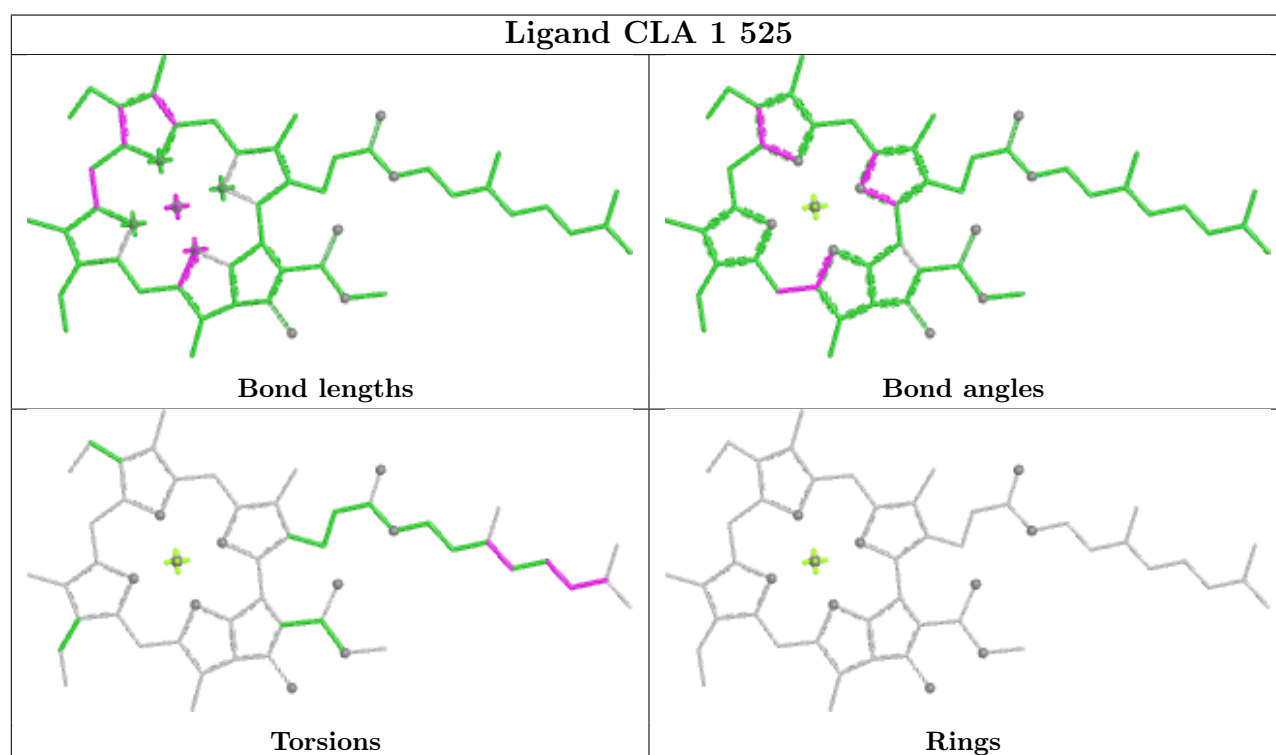
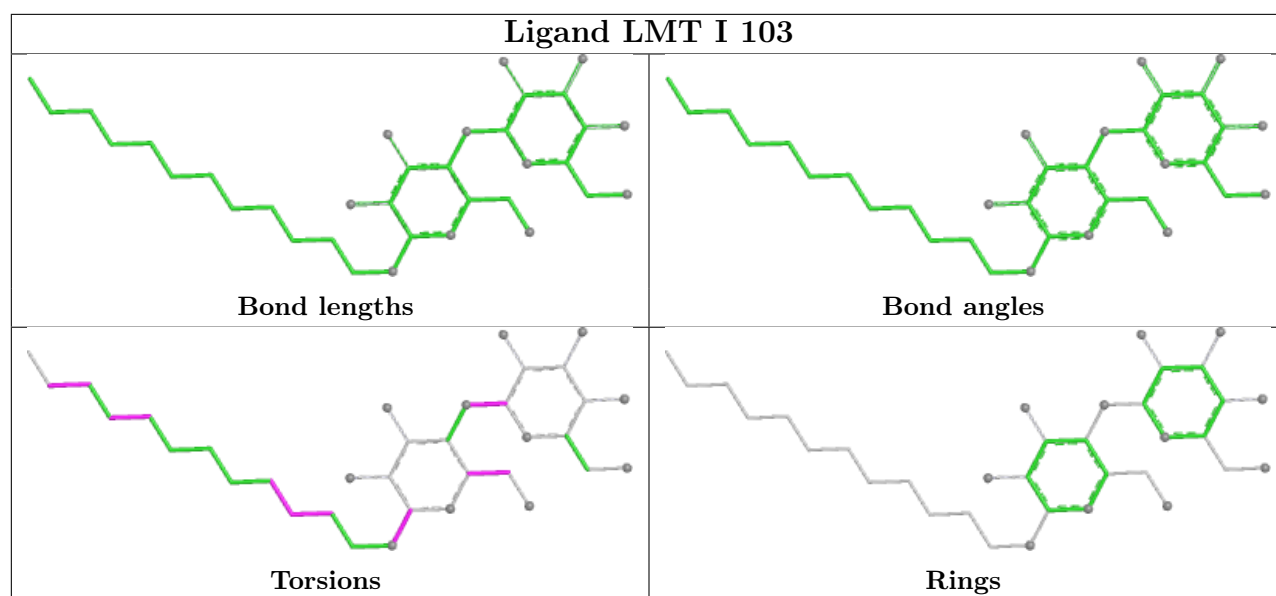


Ligand CLA 4 402

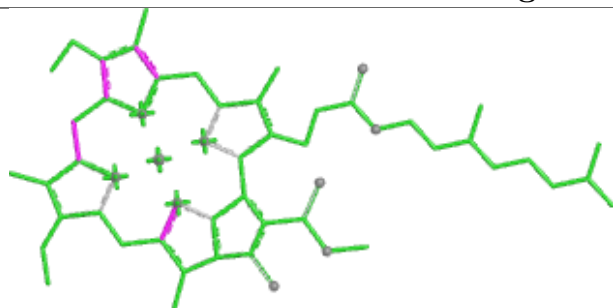


Ligand CLA A 811

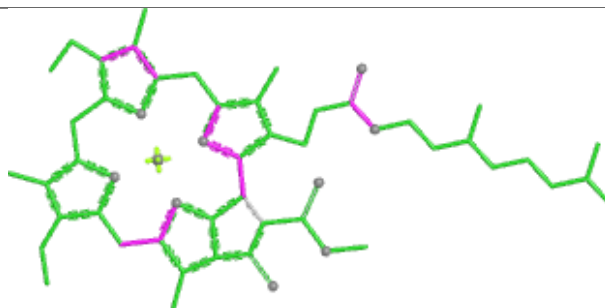




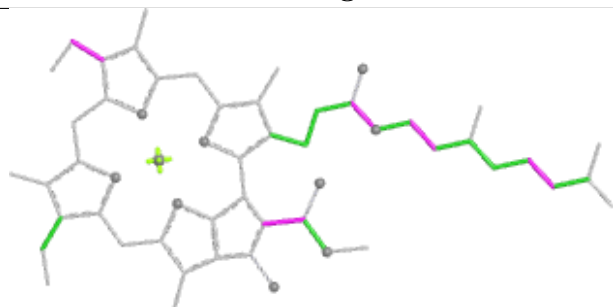
Ligand CLA 5 410



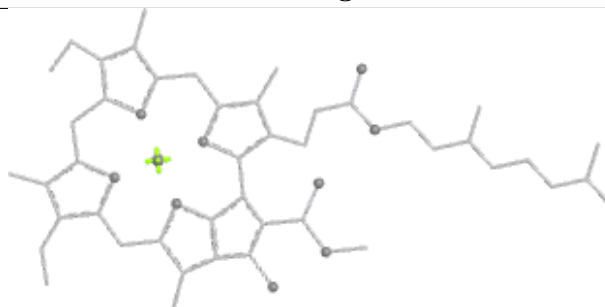
Bond lengths



Bond angles

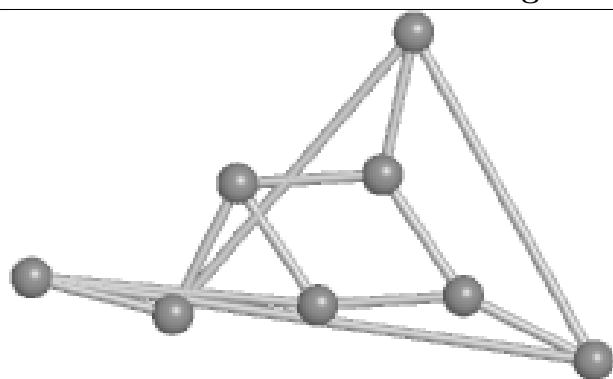


Torsions

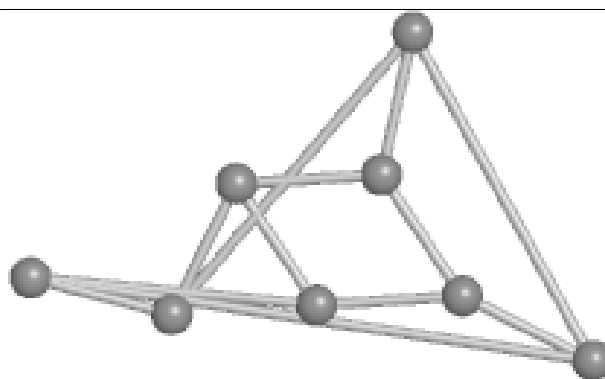


Rings

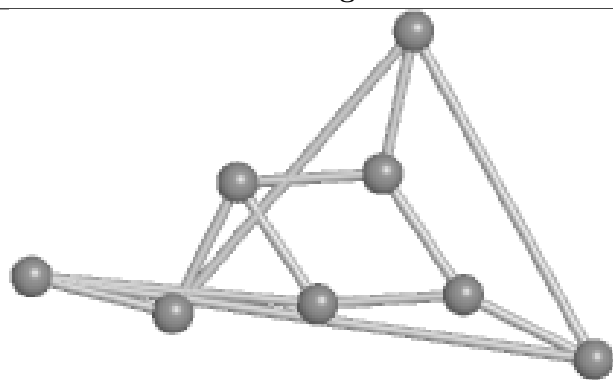
Ligand SF4 B 802



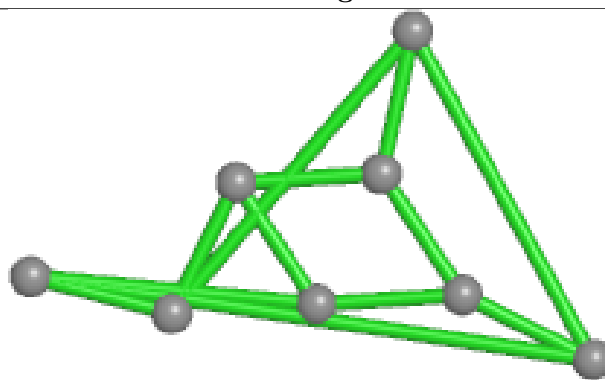
Bond lengths



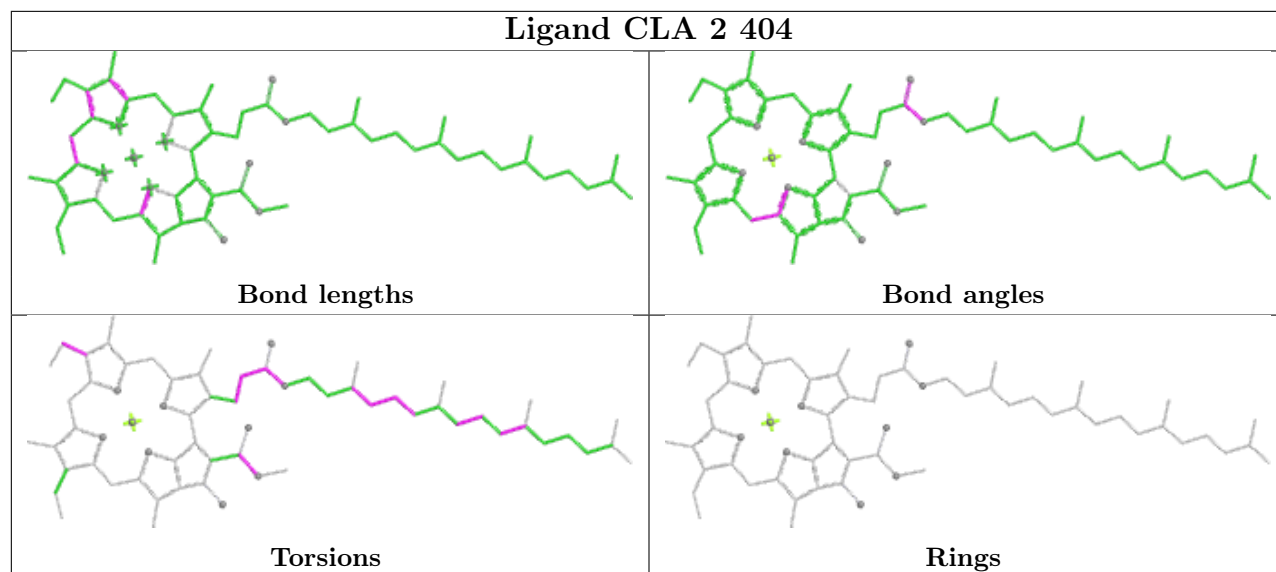
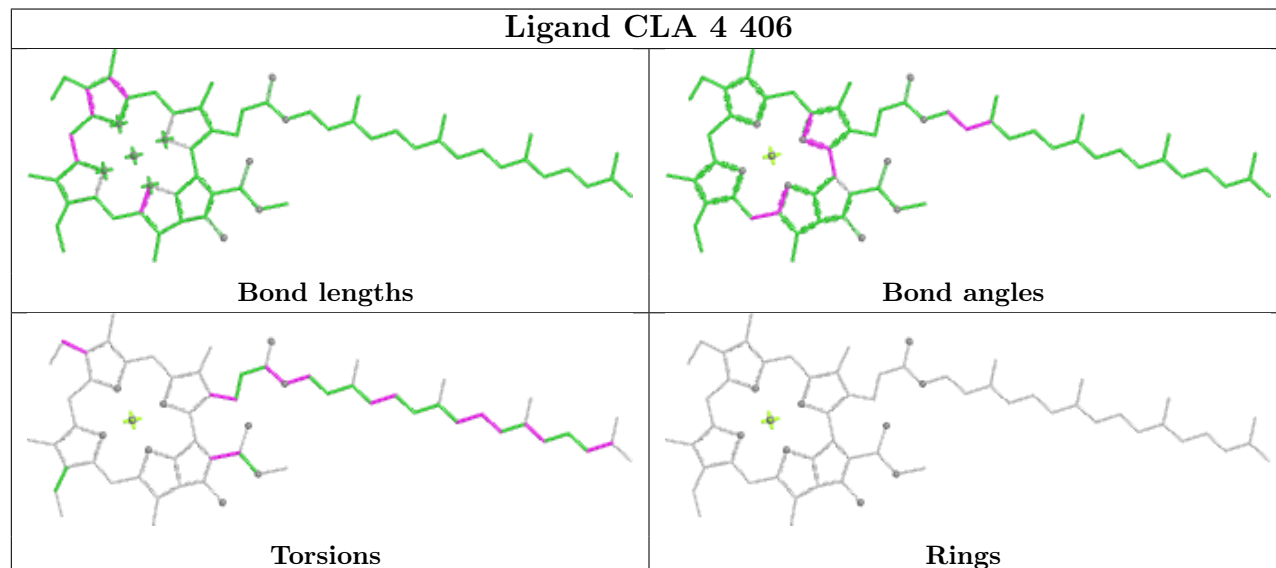
Bond angles

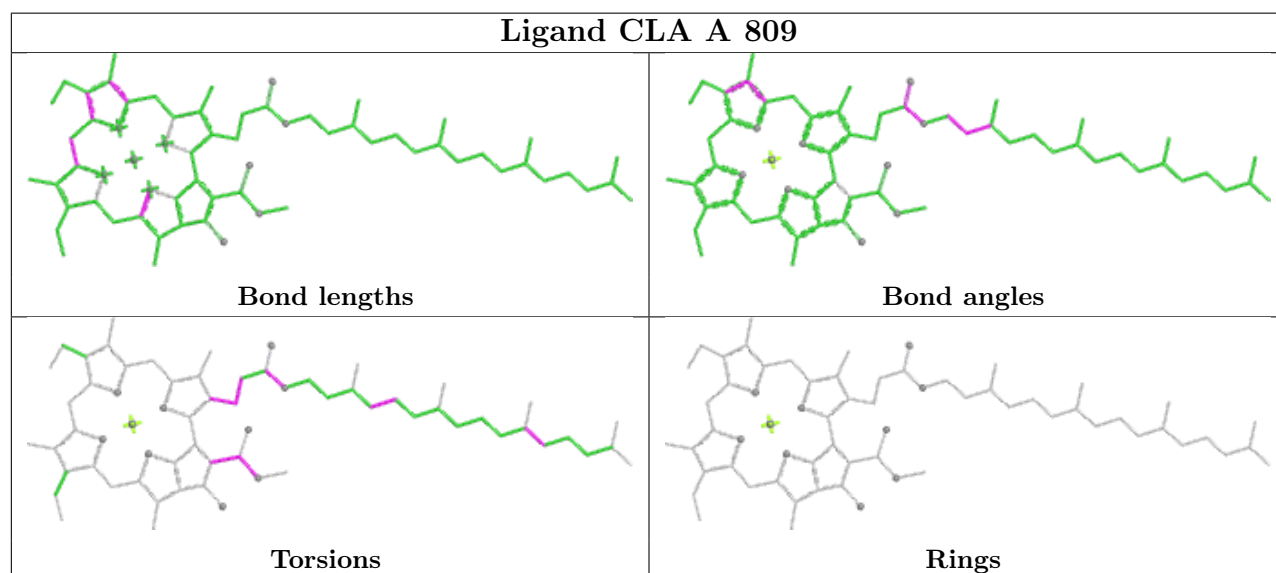
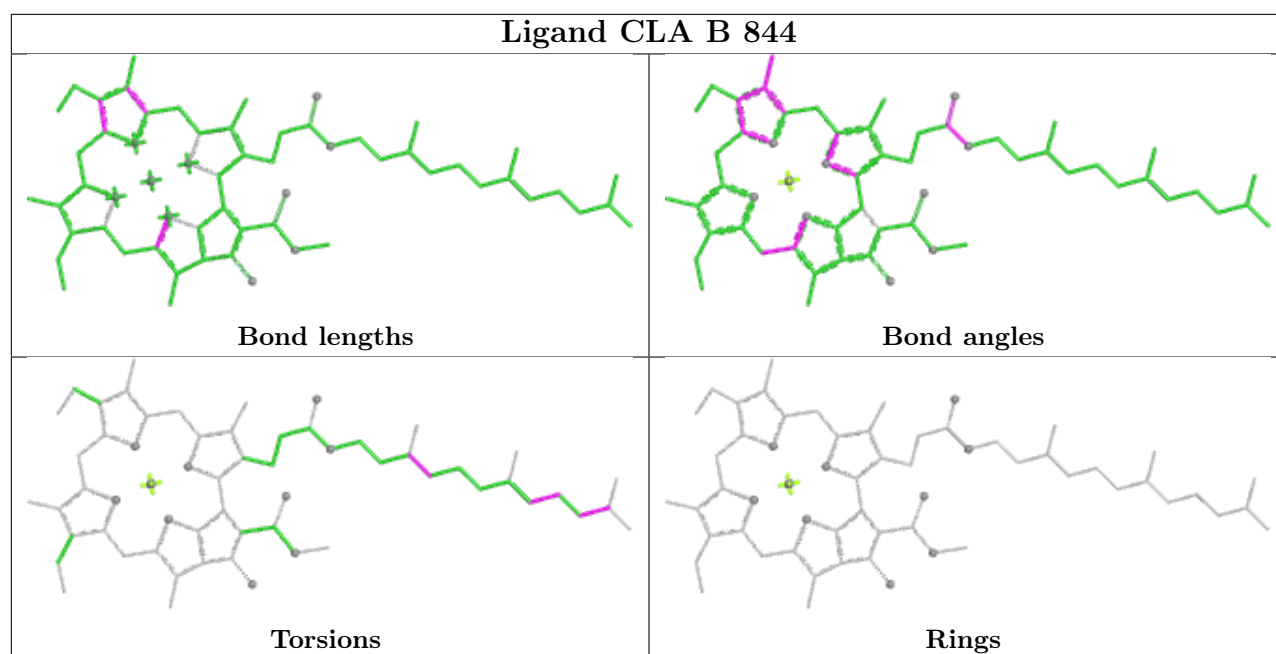


Torsions

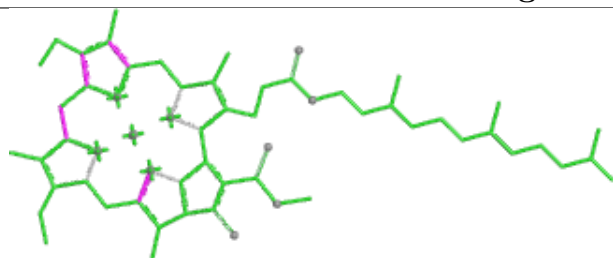


Rings

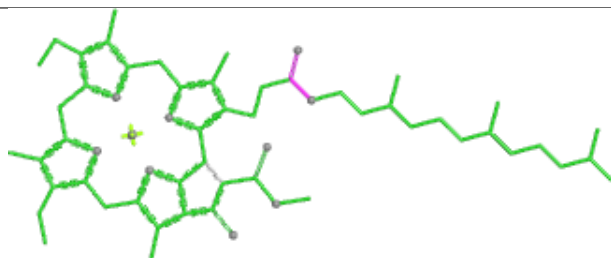
Ligand CLA 2 404**Ligand CLA 4 406**



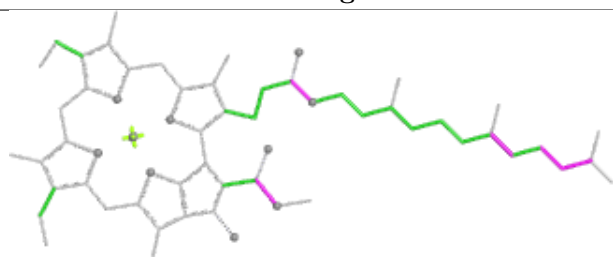
Ligand CLA 1 516



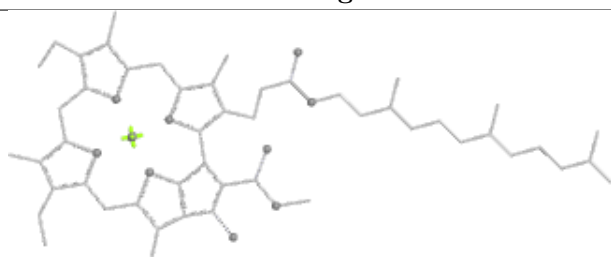
Bond lengths



Bond angles

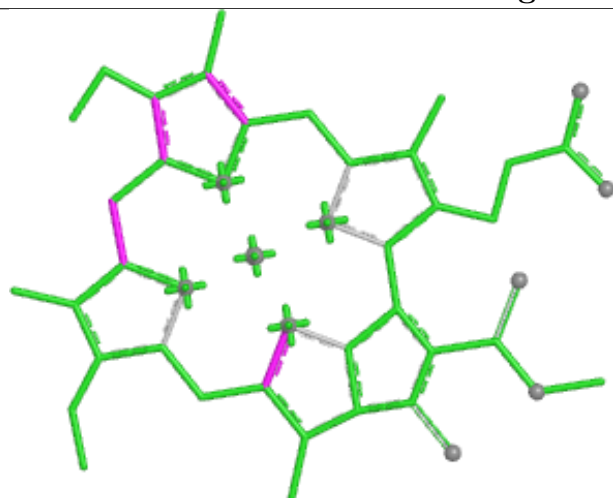


Torsions

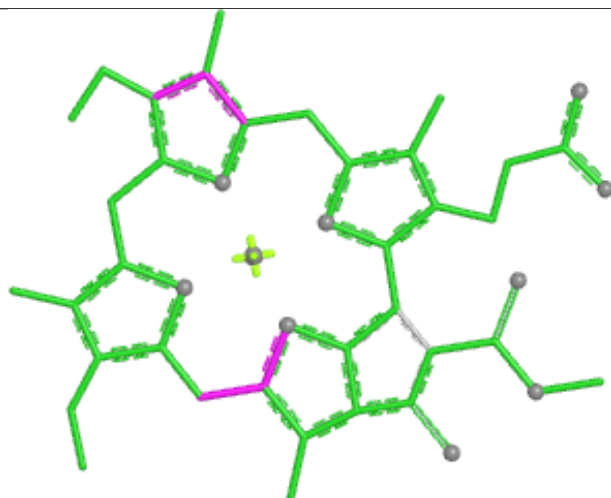


Rings

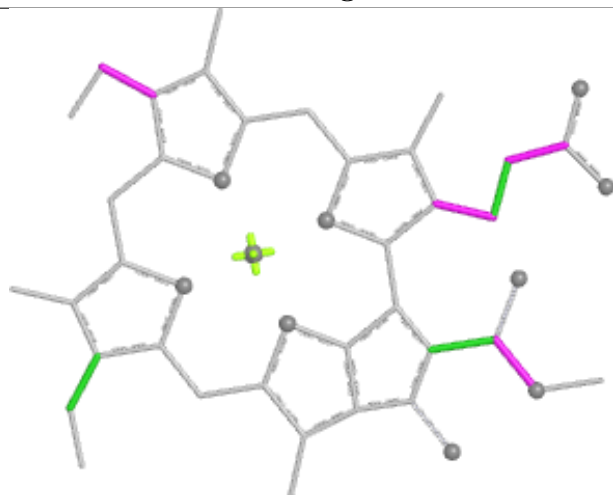
Ligand CLA 2 412



Bond lengths



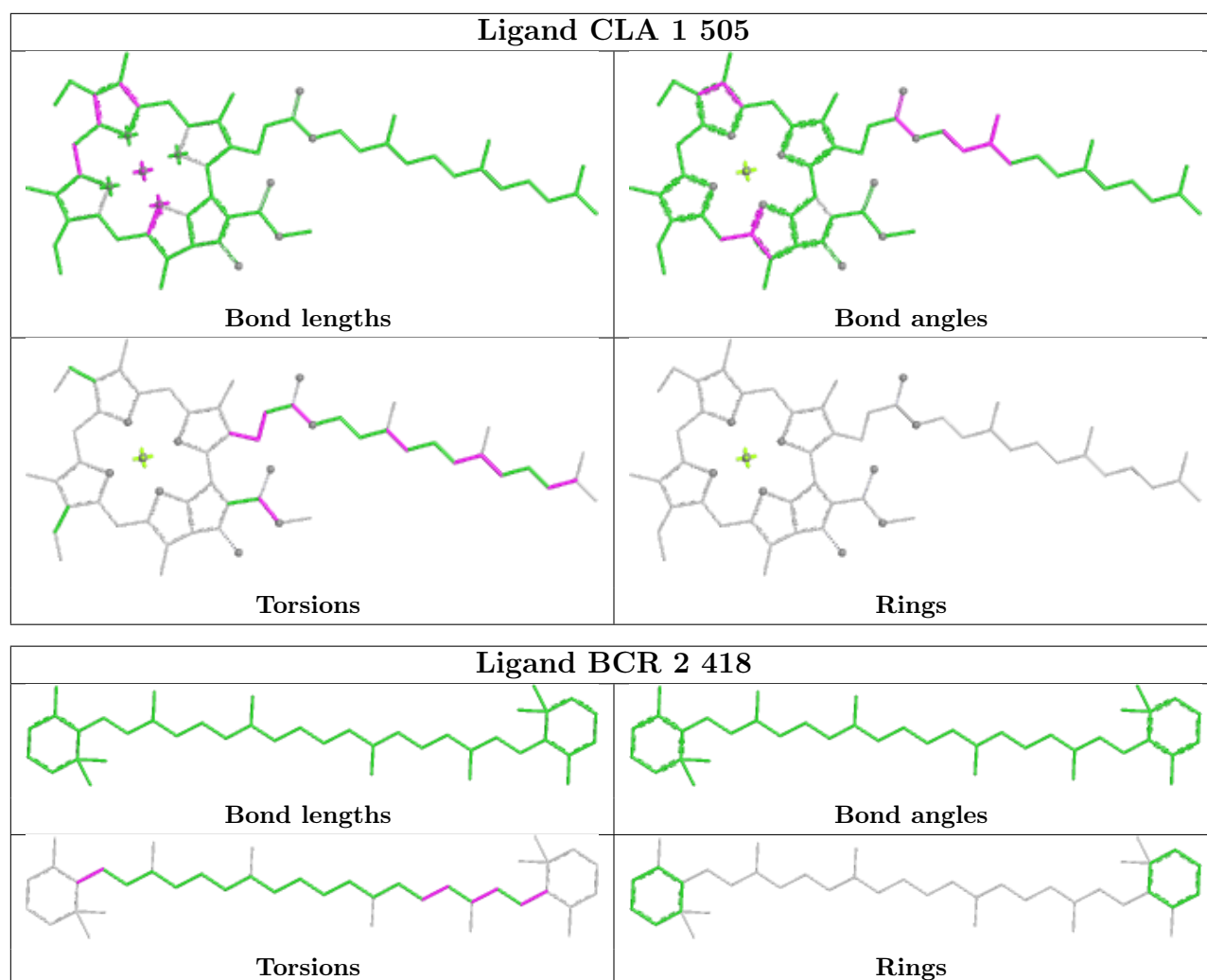
Bond angles

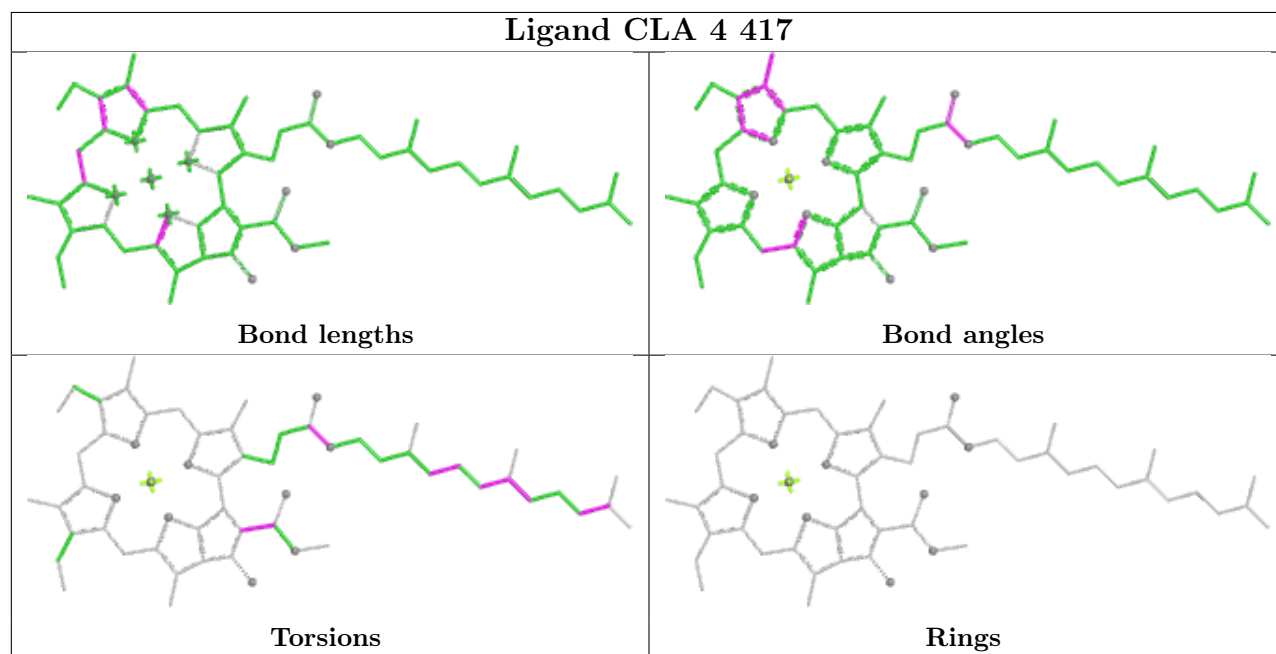
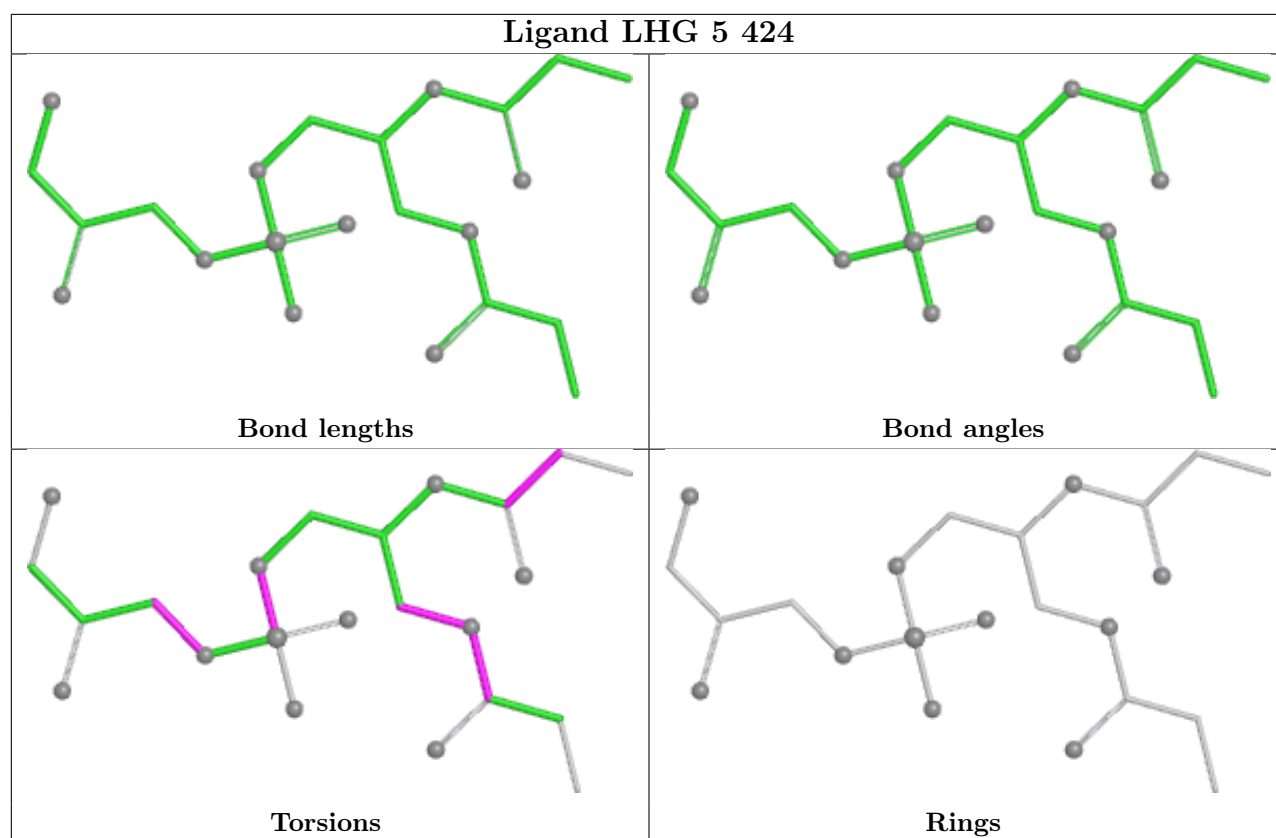


Torsions

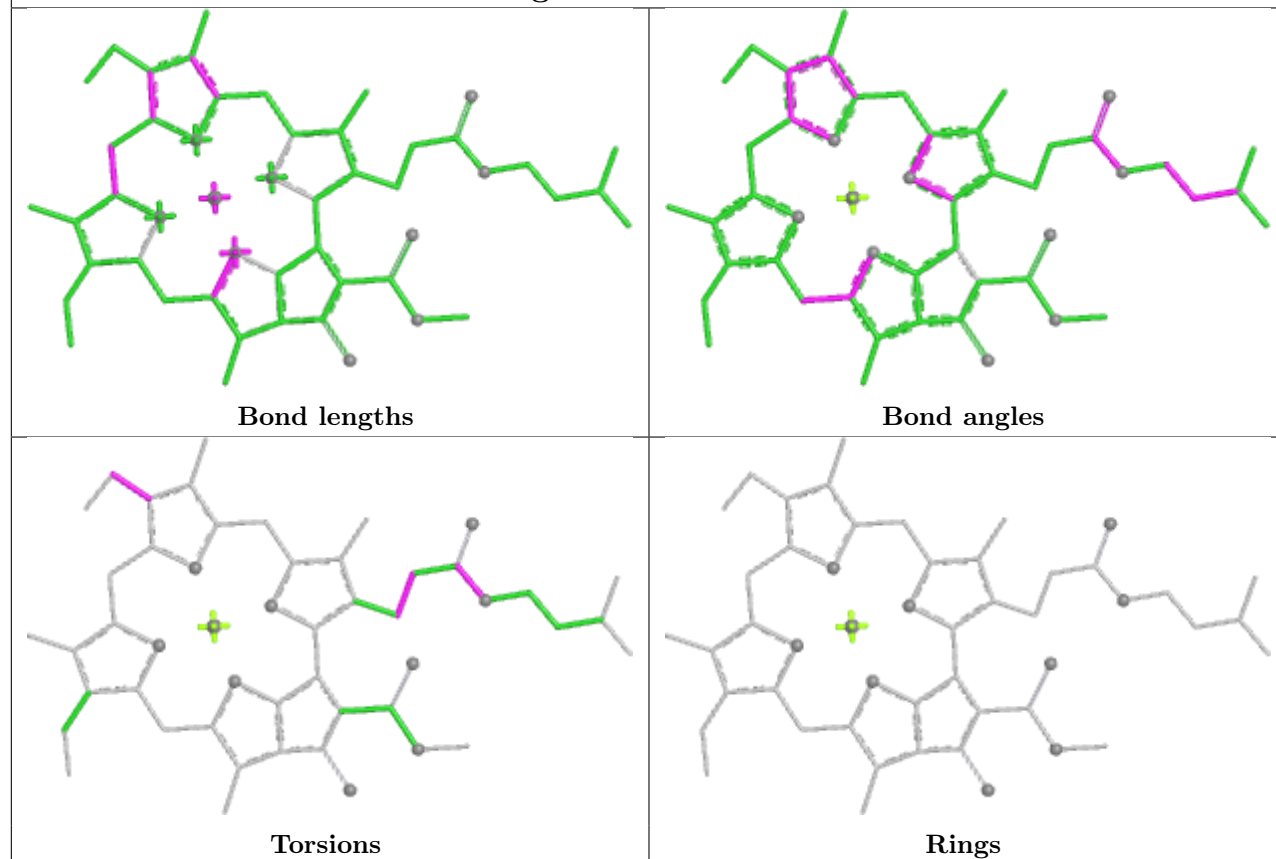


Rings

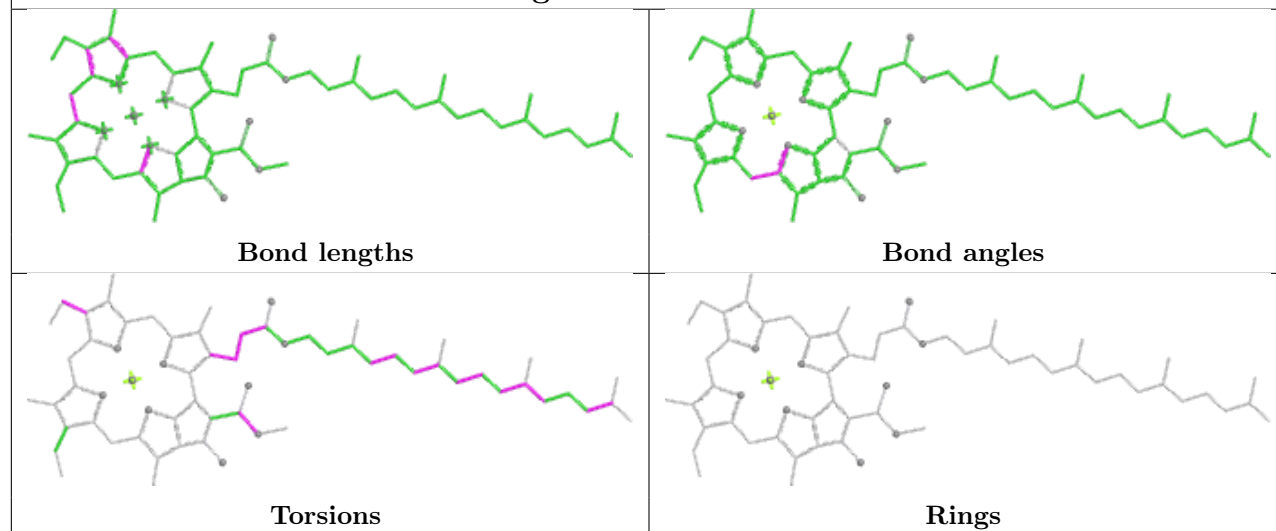


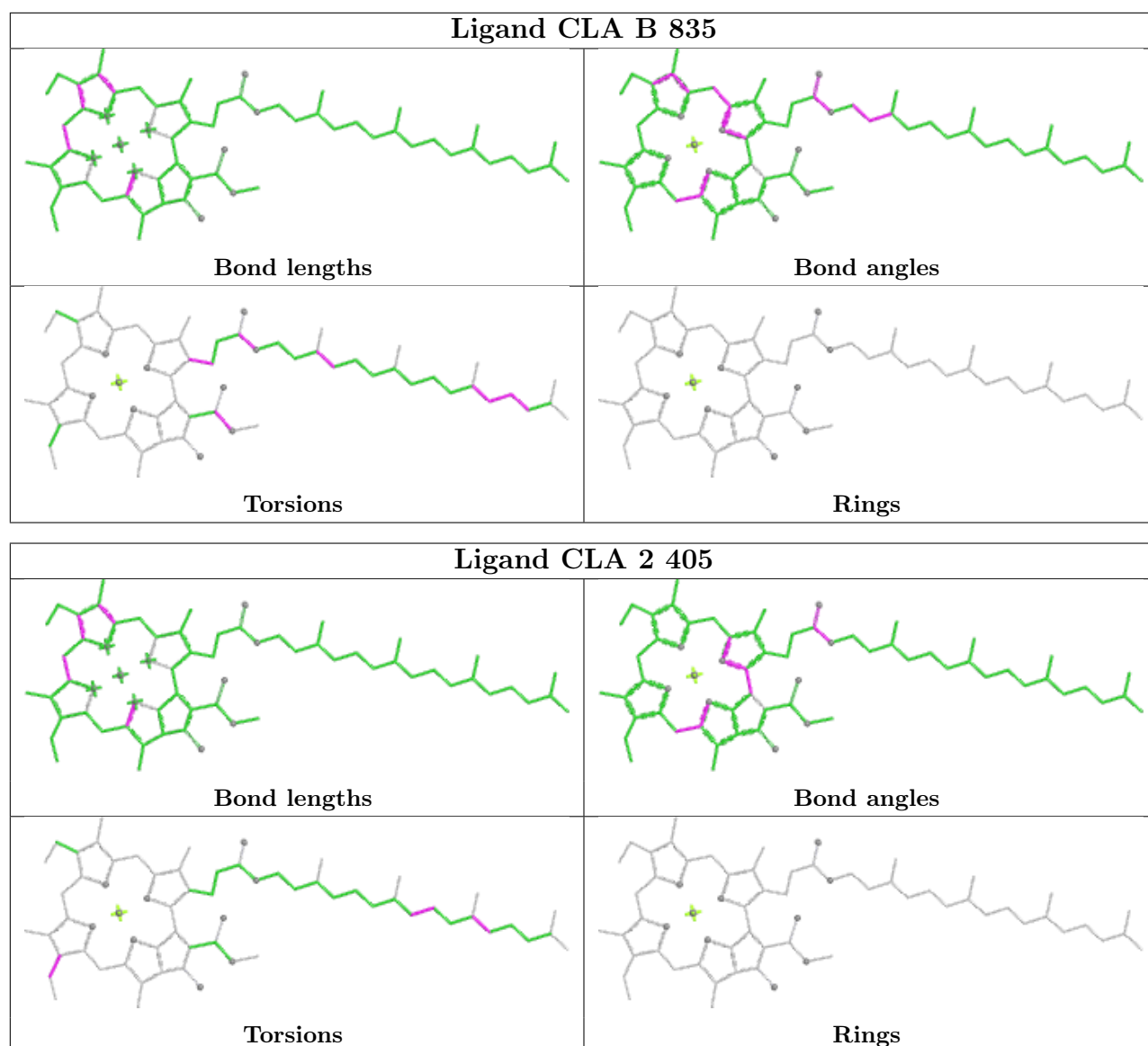


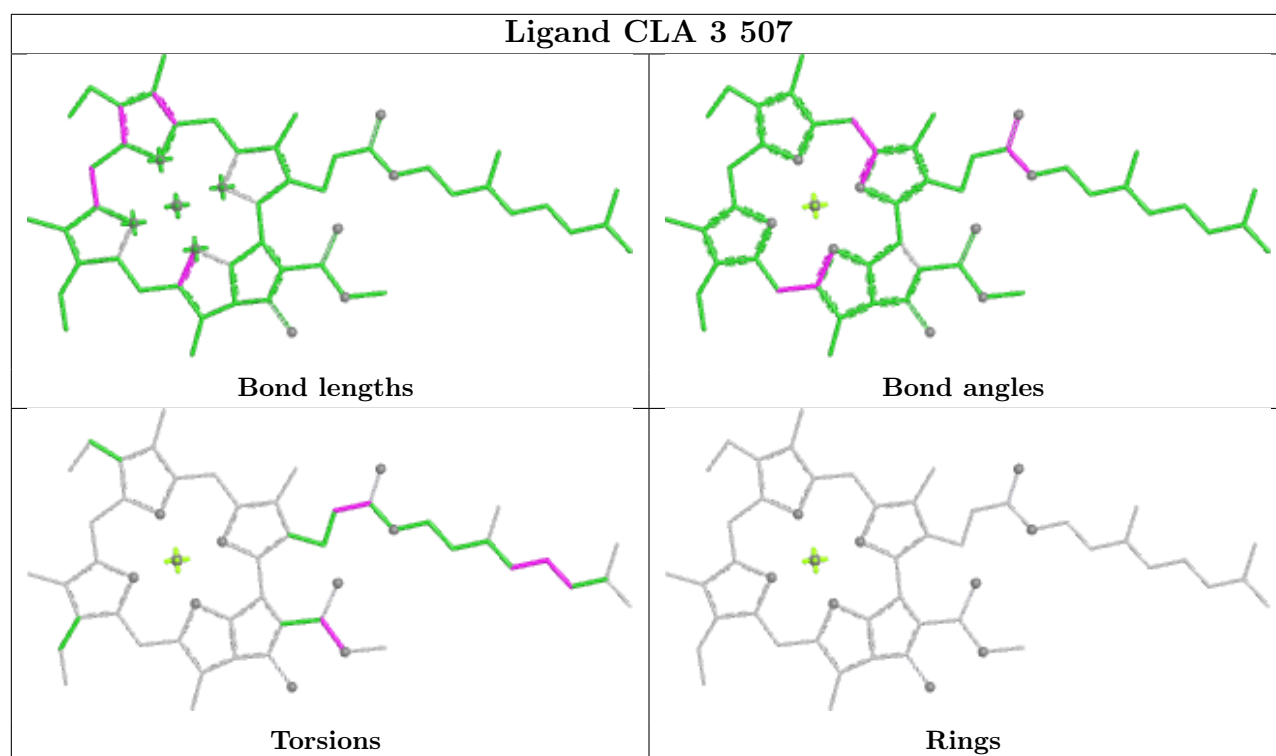
Ligand CLA A 823



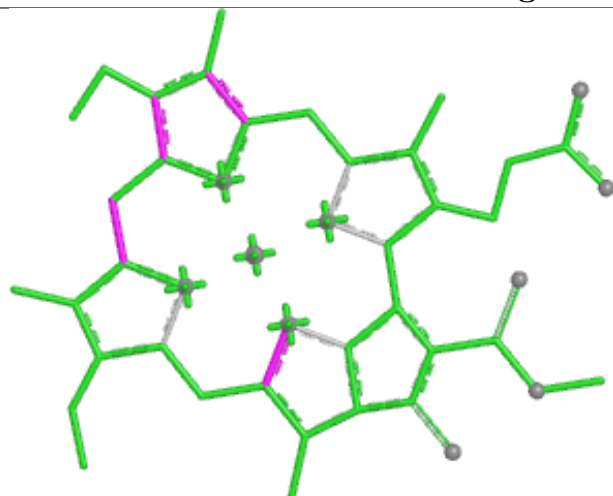
Ligand CLA B 816



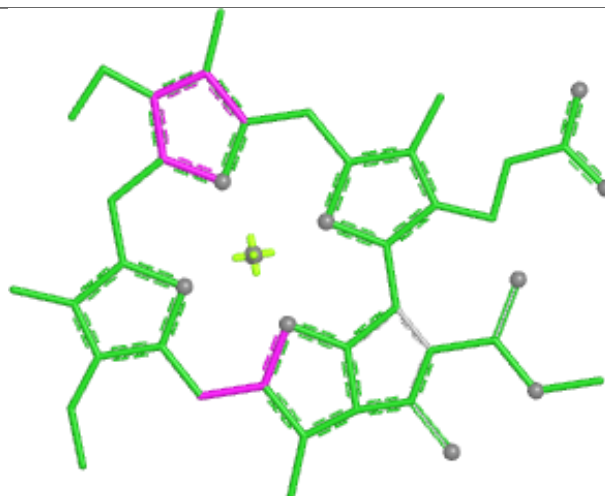




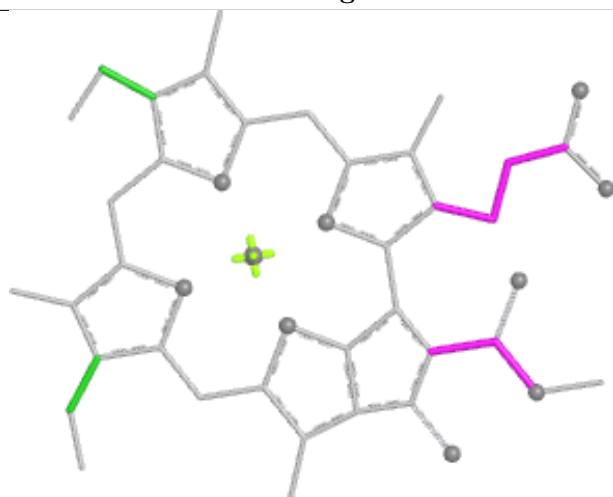
Ligand CLA 7 505



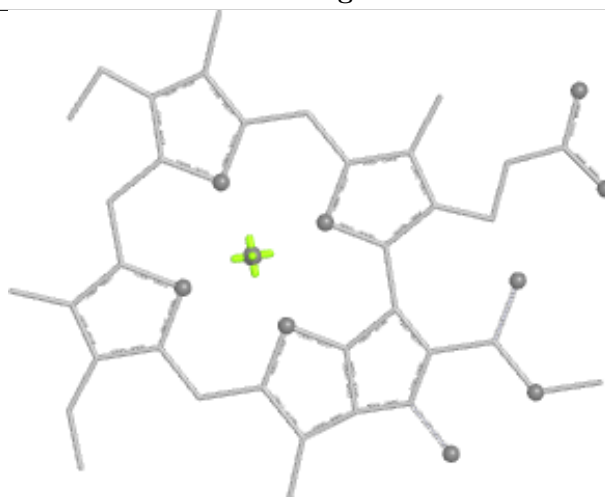
Bond lengths



Bond angles

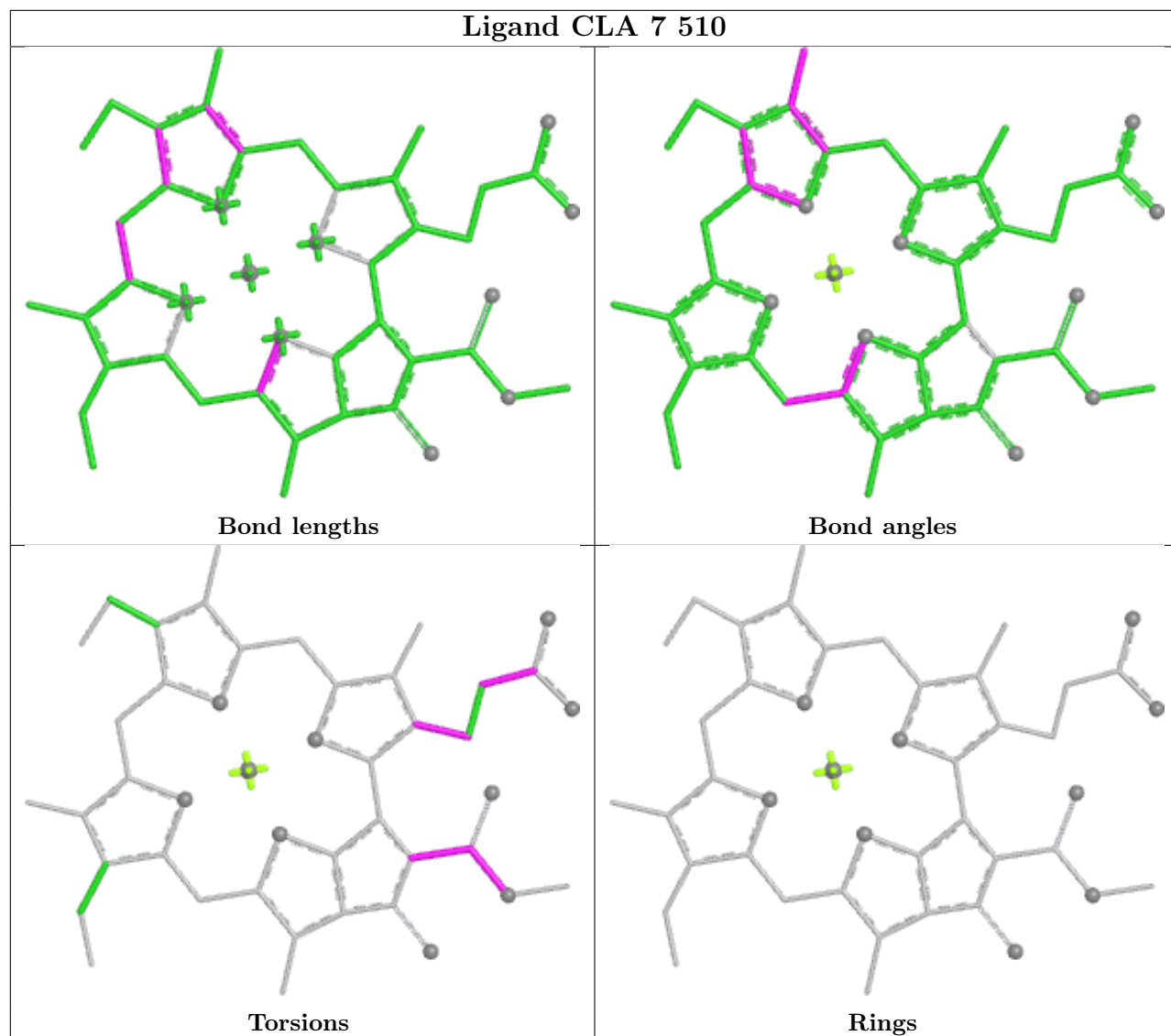


Torsions

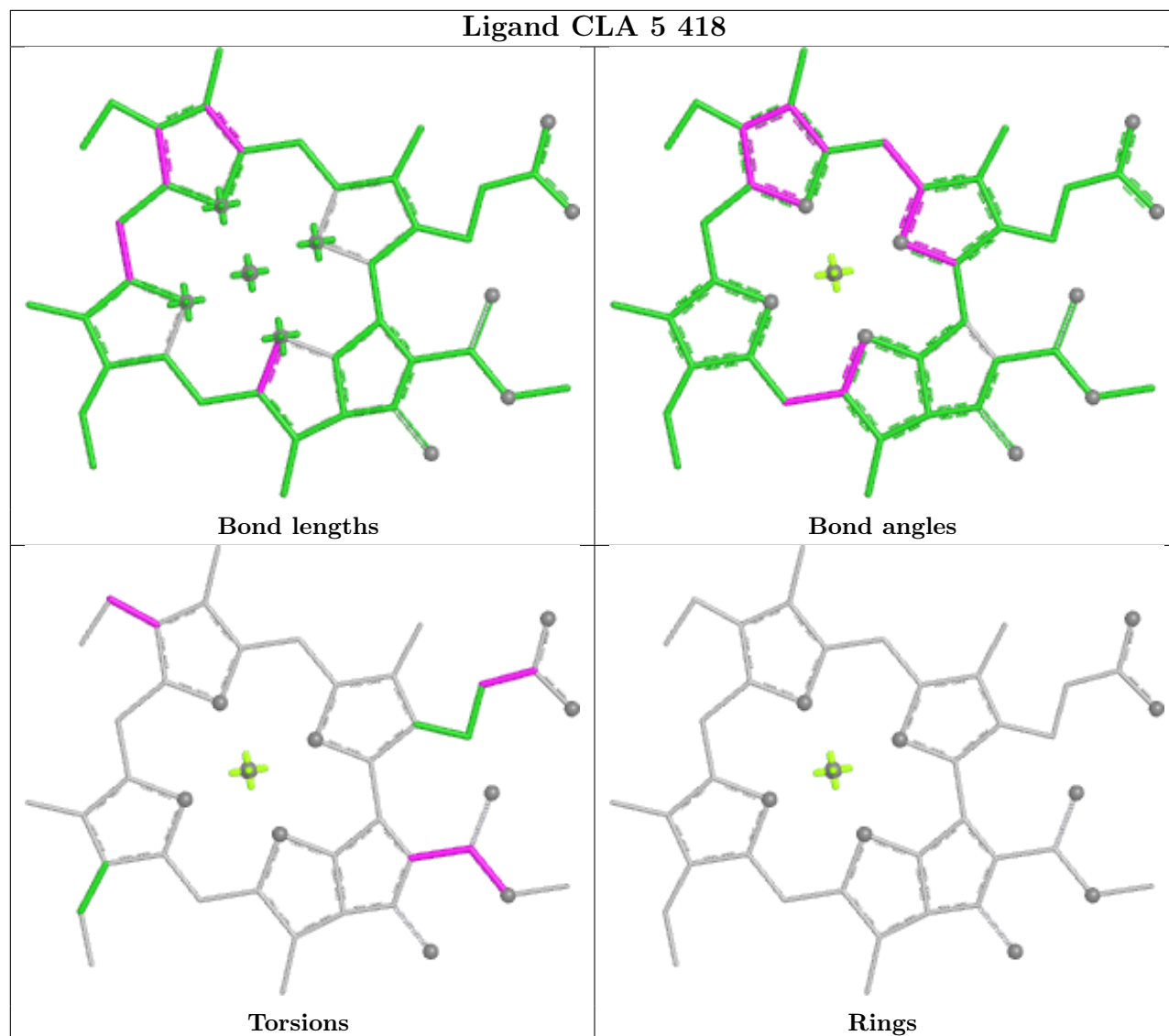


Rings

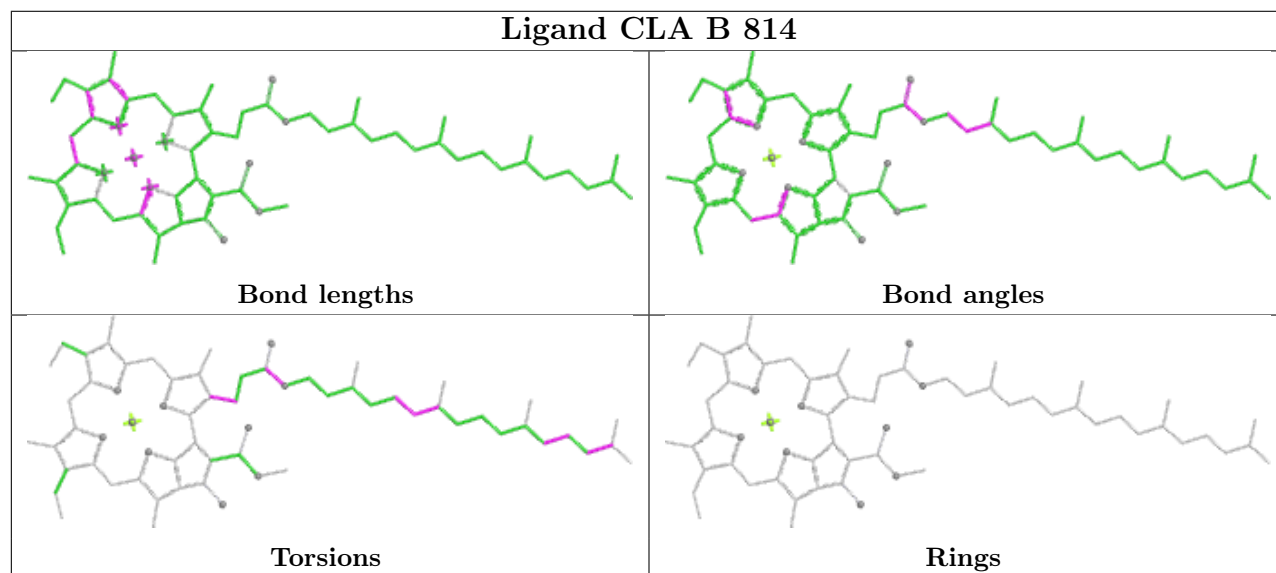
Ligand CLA 7 510

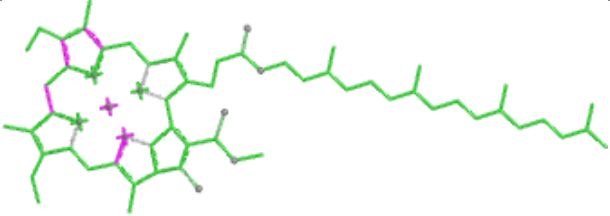
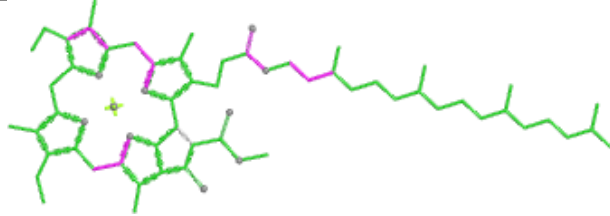
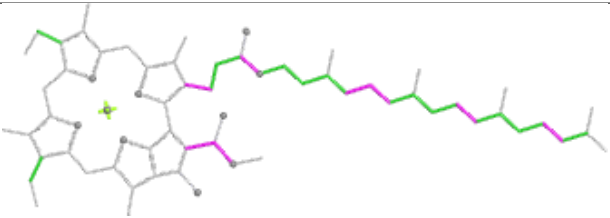
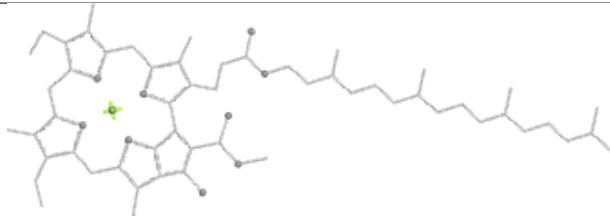
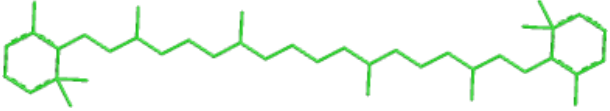
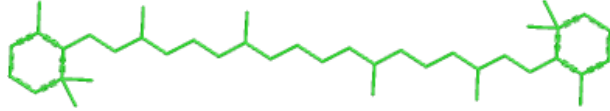

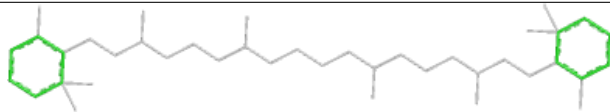
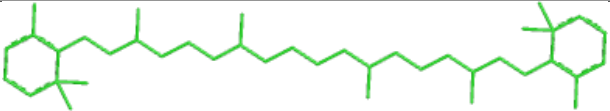
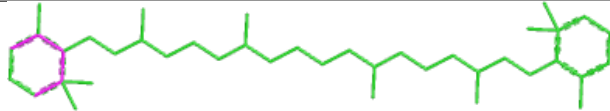
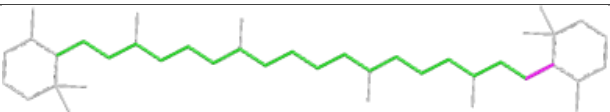
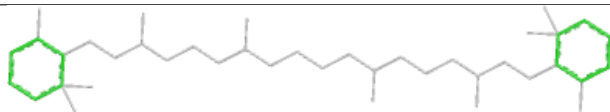


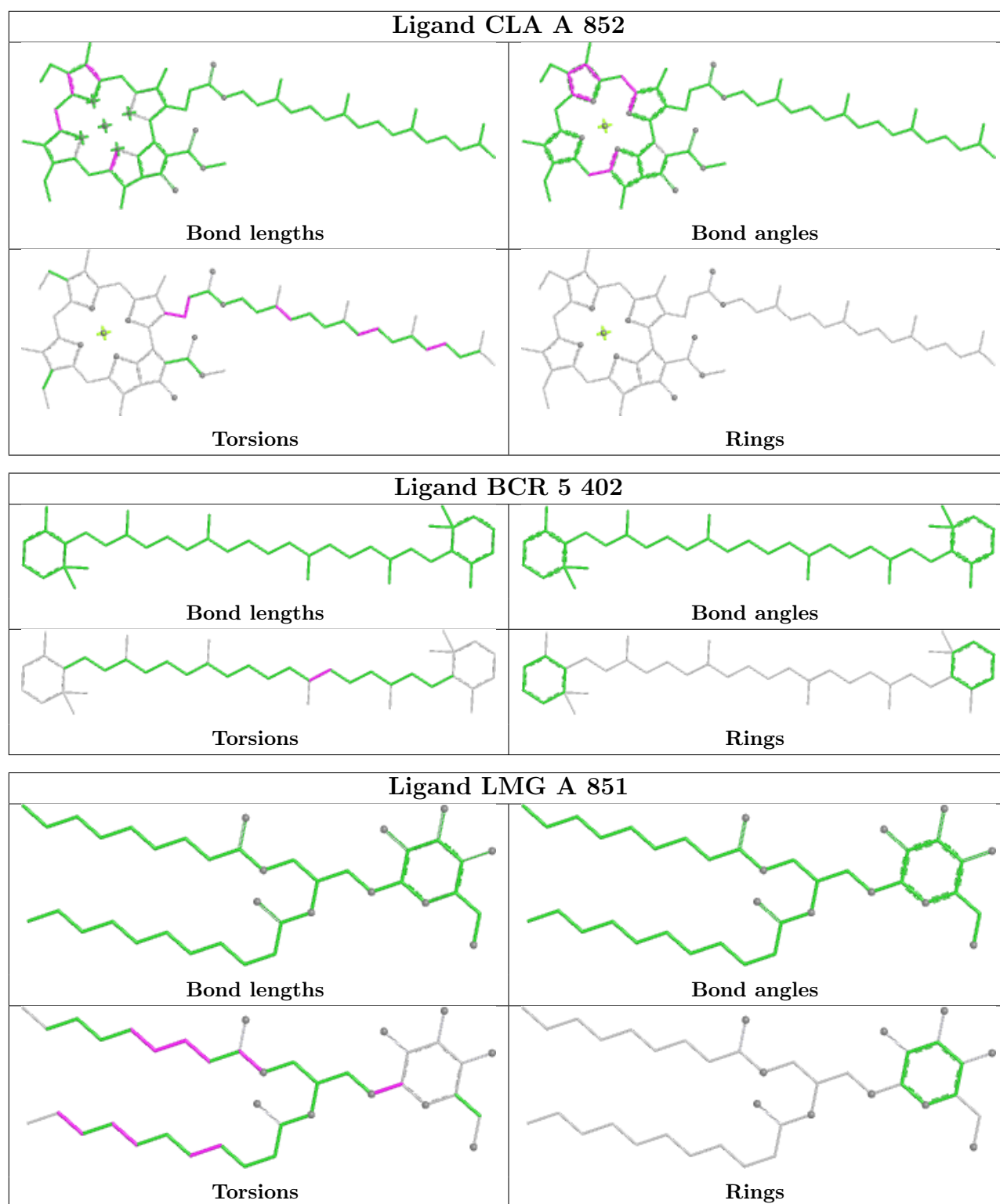
Ligand CLA 5 418



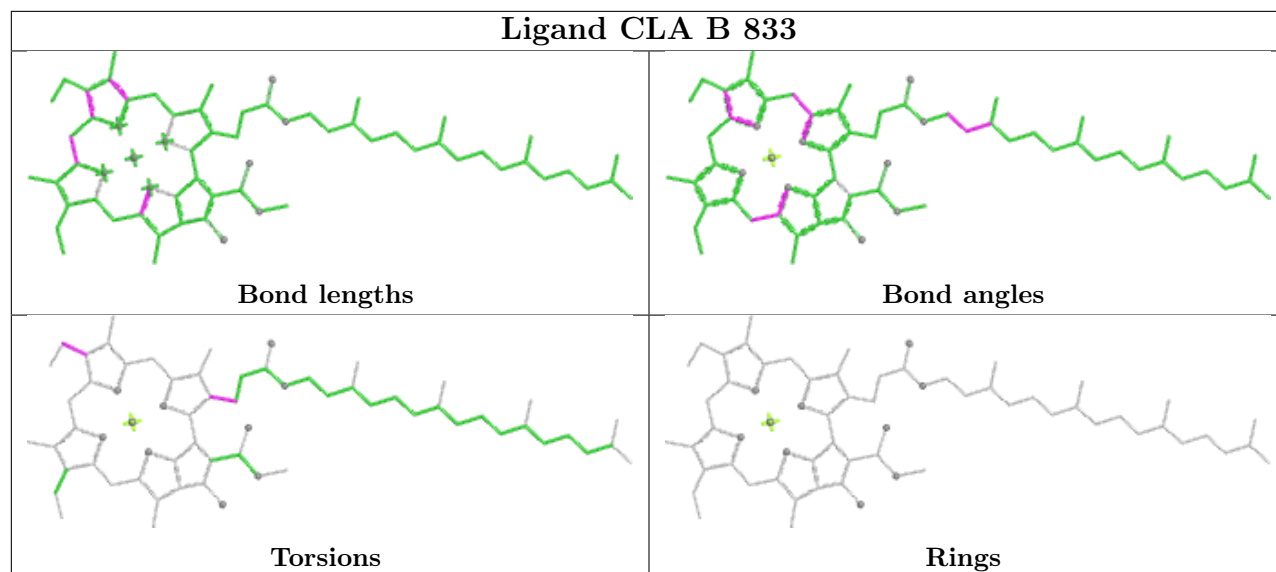
Ligand CLA B 814



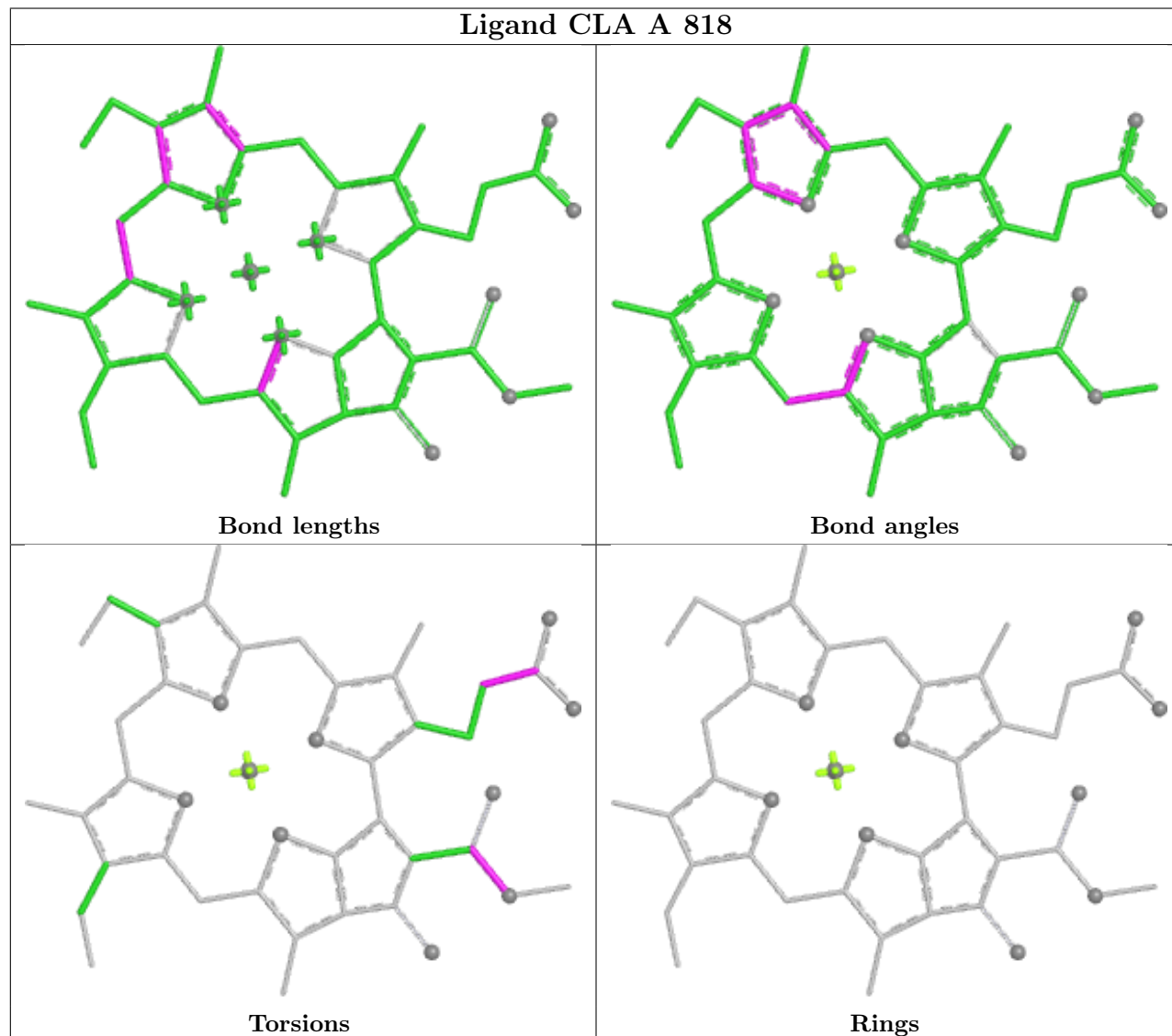
Ligand CLA 6 504	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR 5 421	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR 5 422	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



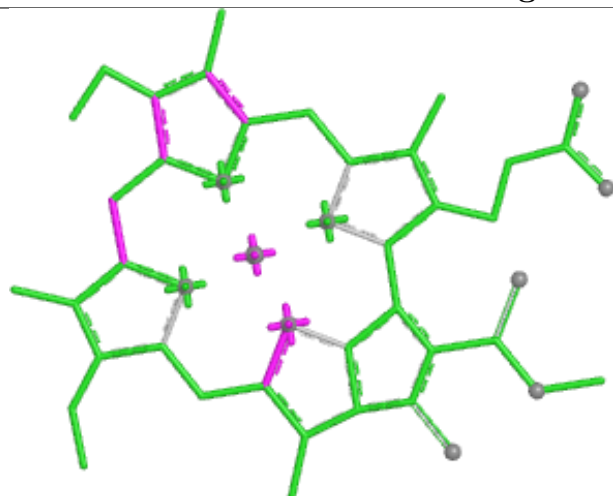
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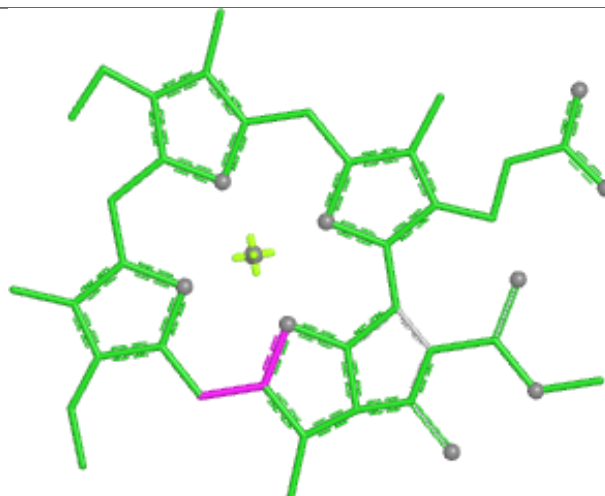
Ligand CLA A 818



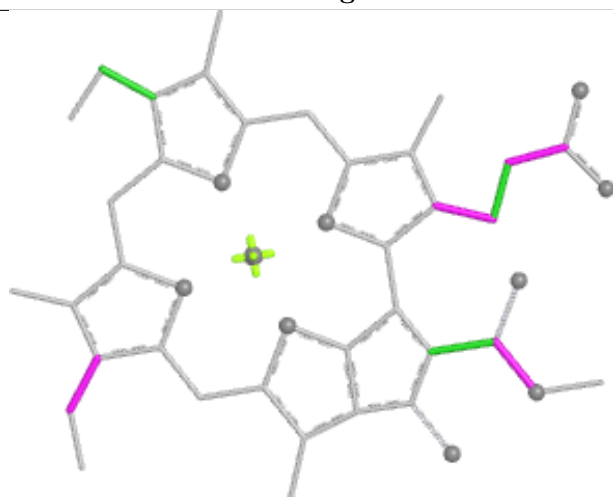
Ligand CLA 2 414



Bond lengths



Bond angles

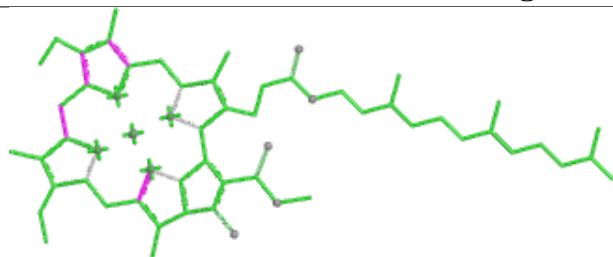


Torsions

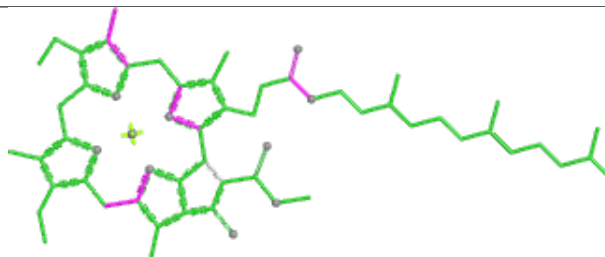


Rings

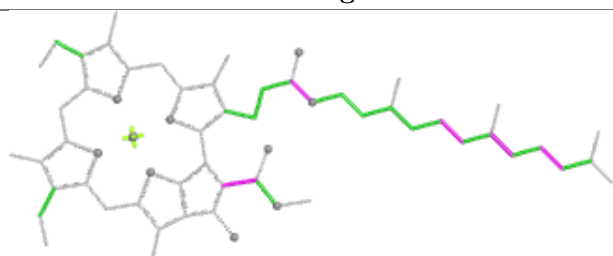
Ligand CLA 1 510



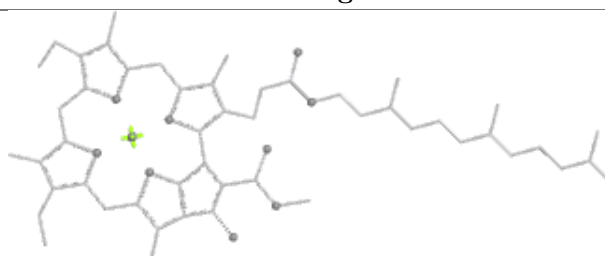
Bond lengths



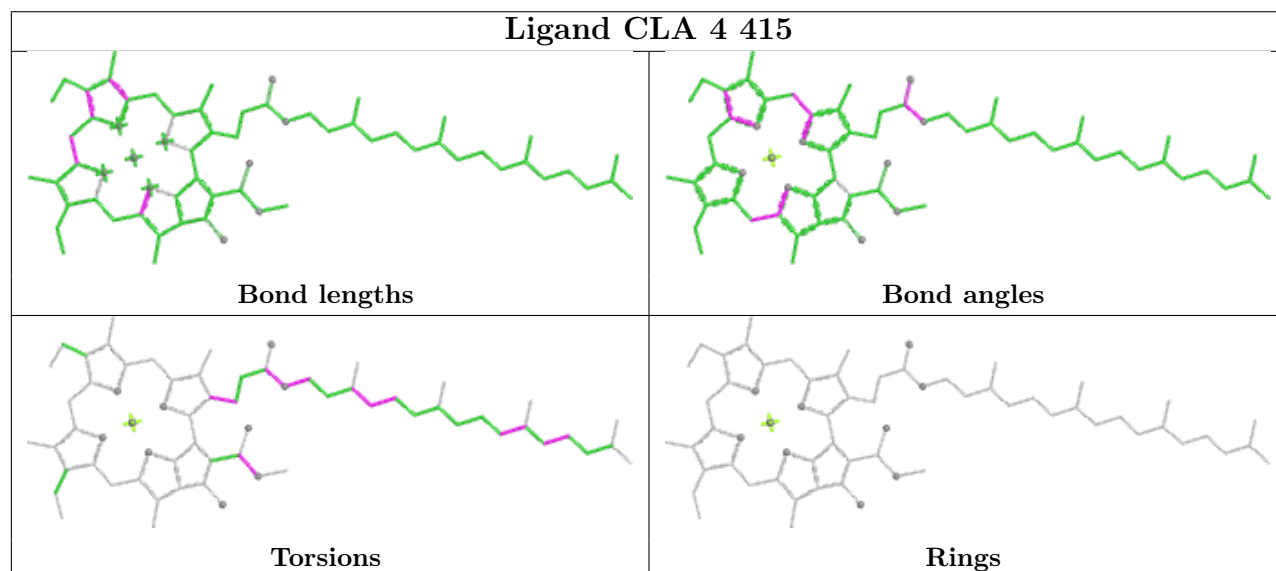
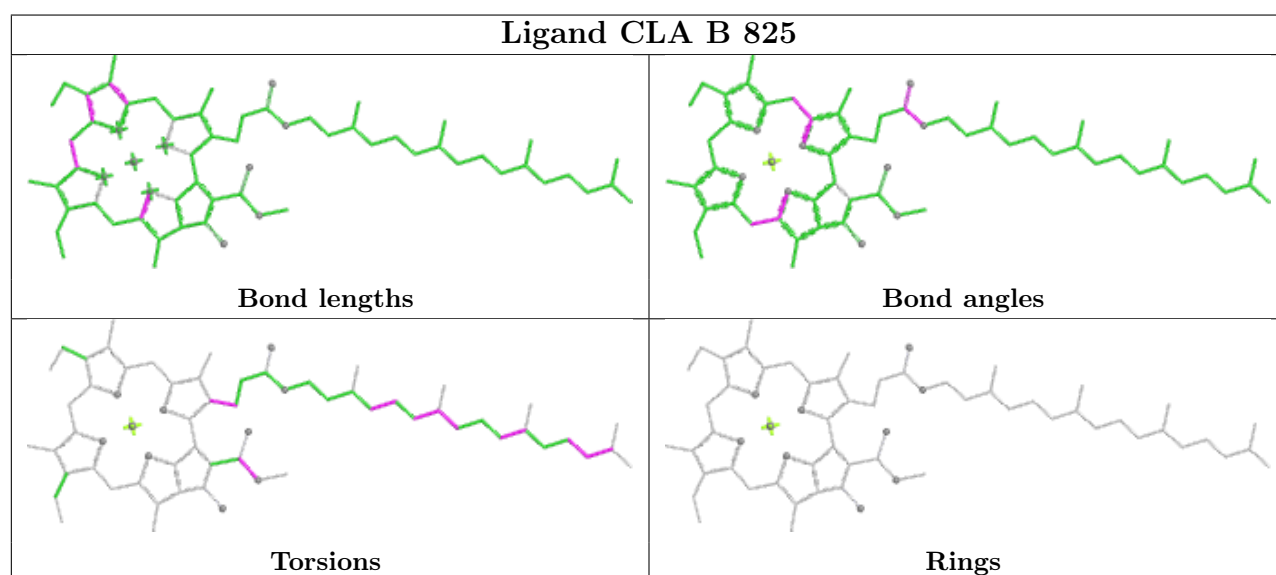
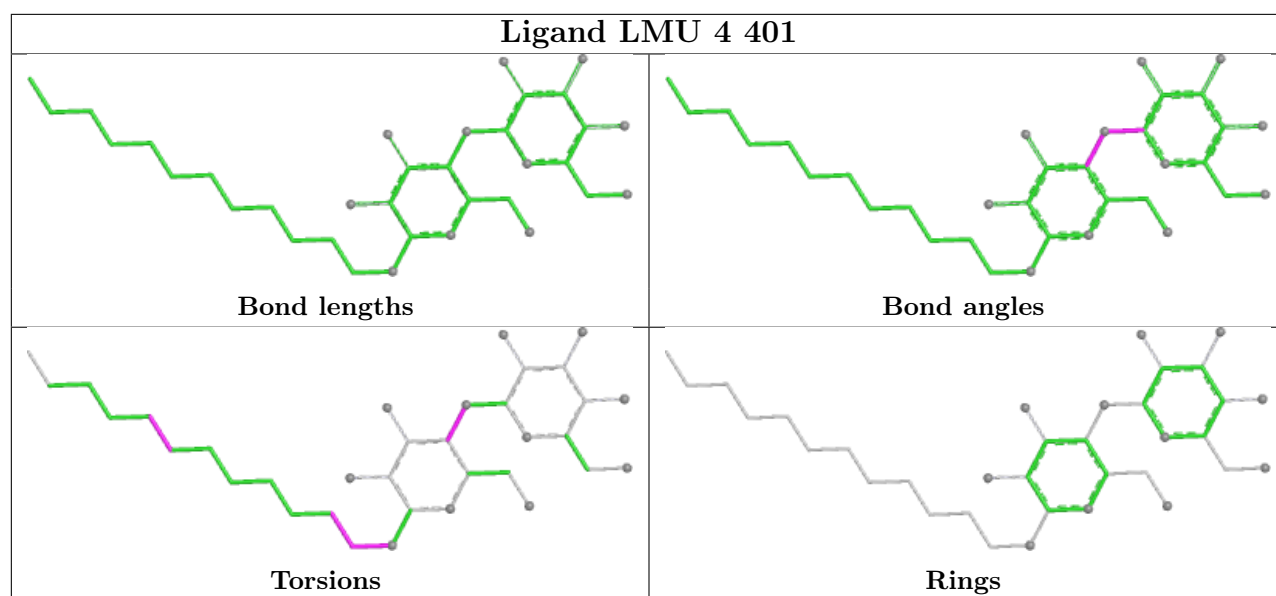
Bond angles

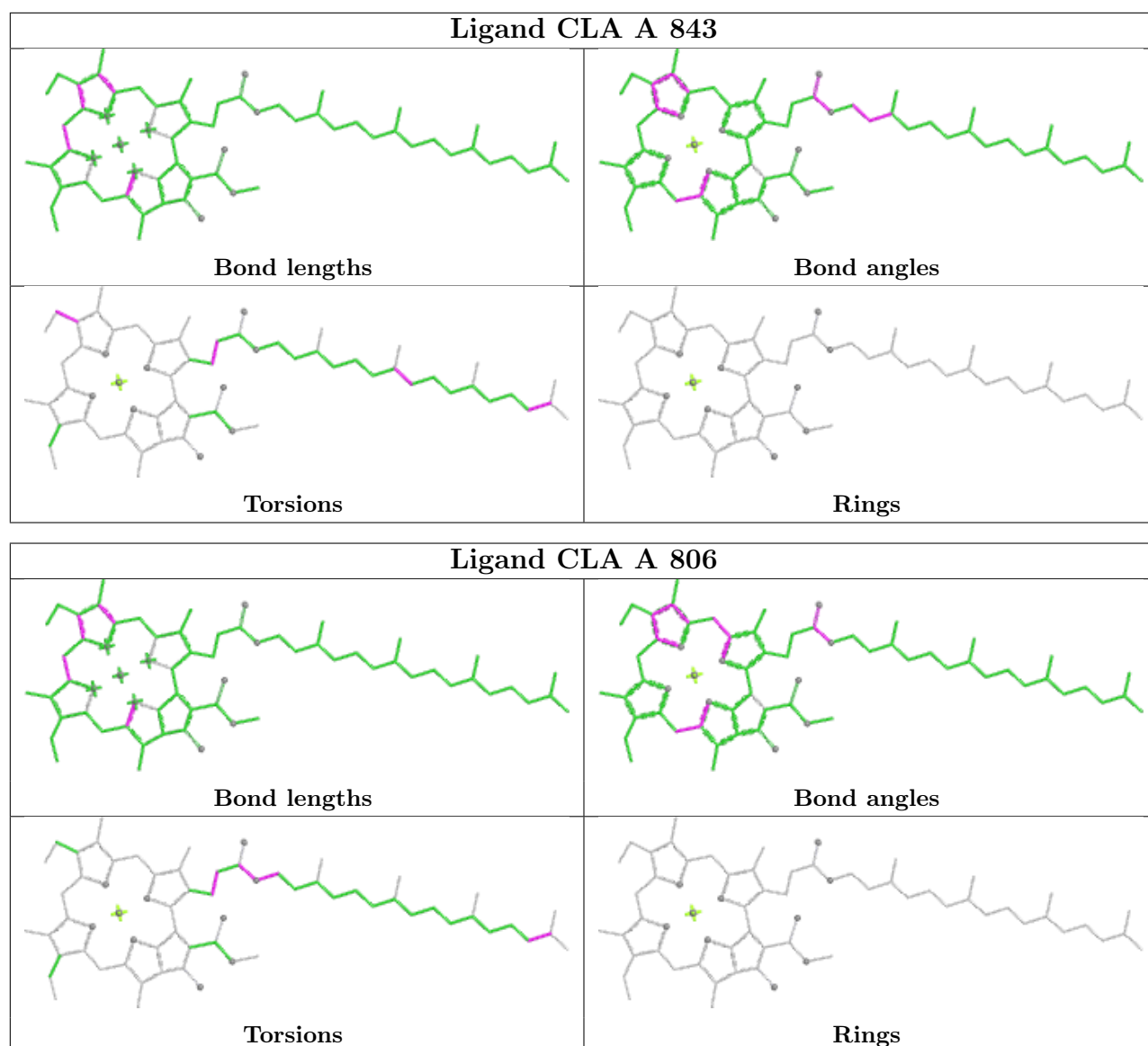


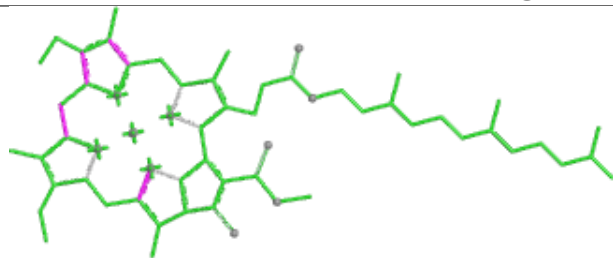
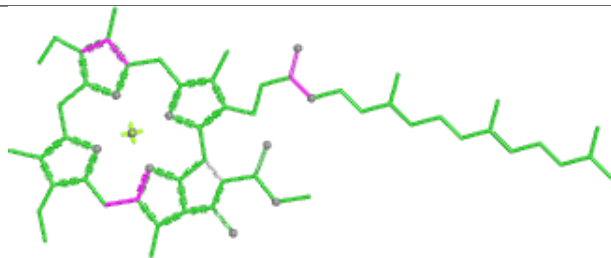
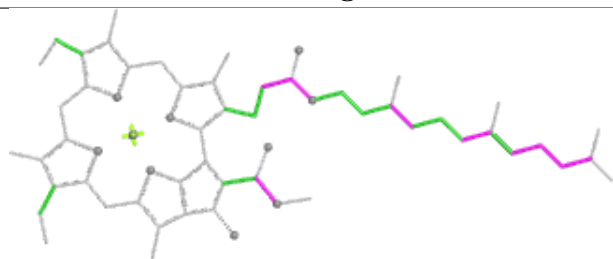
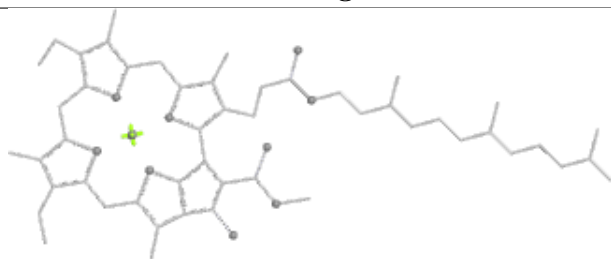
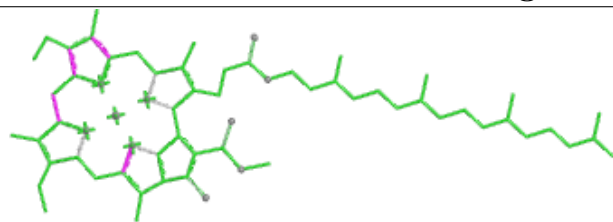
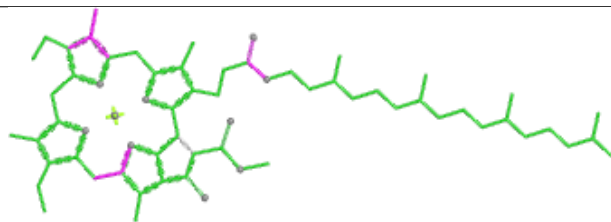
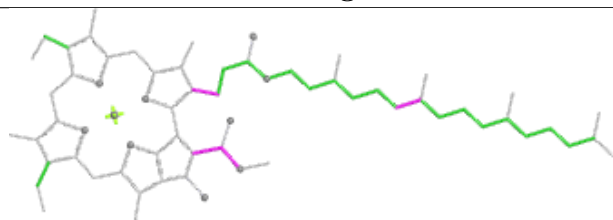
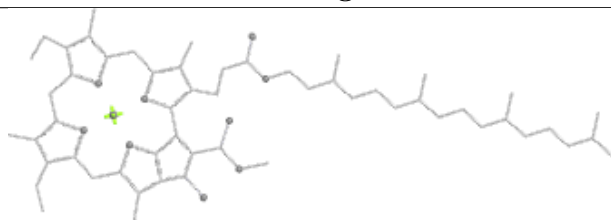
Torsions

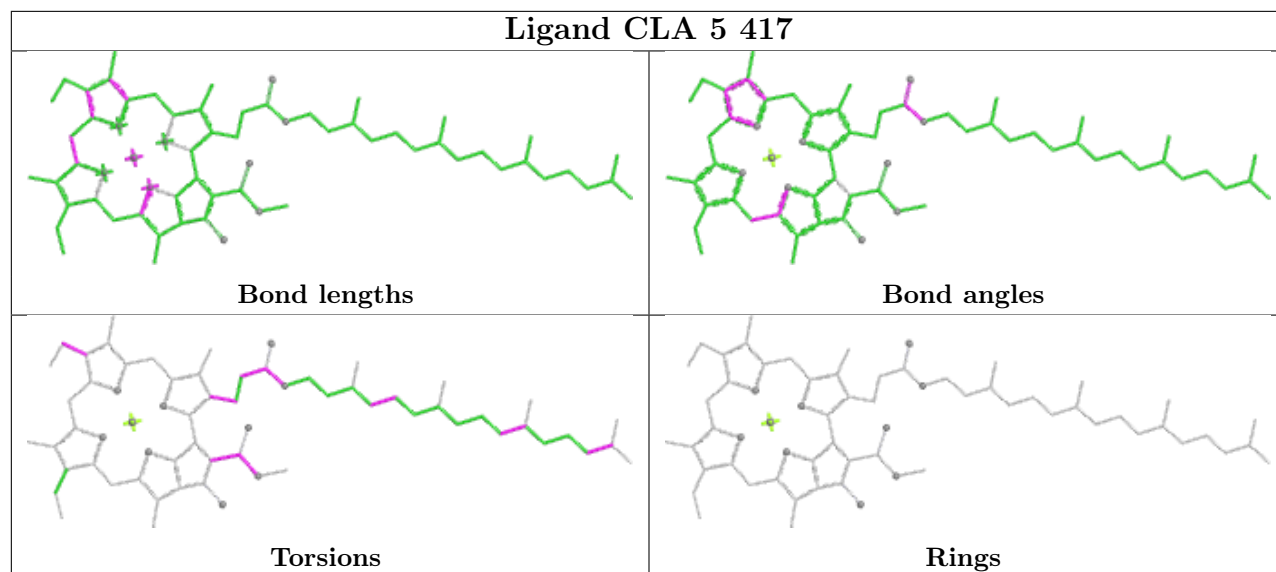
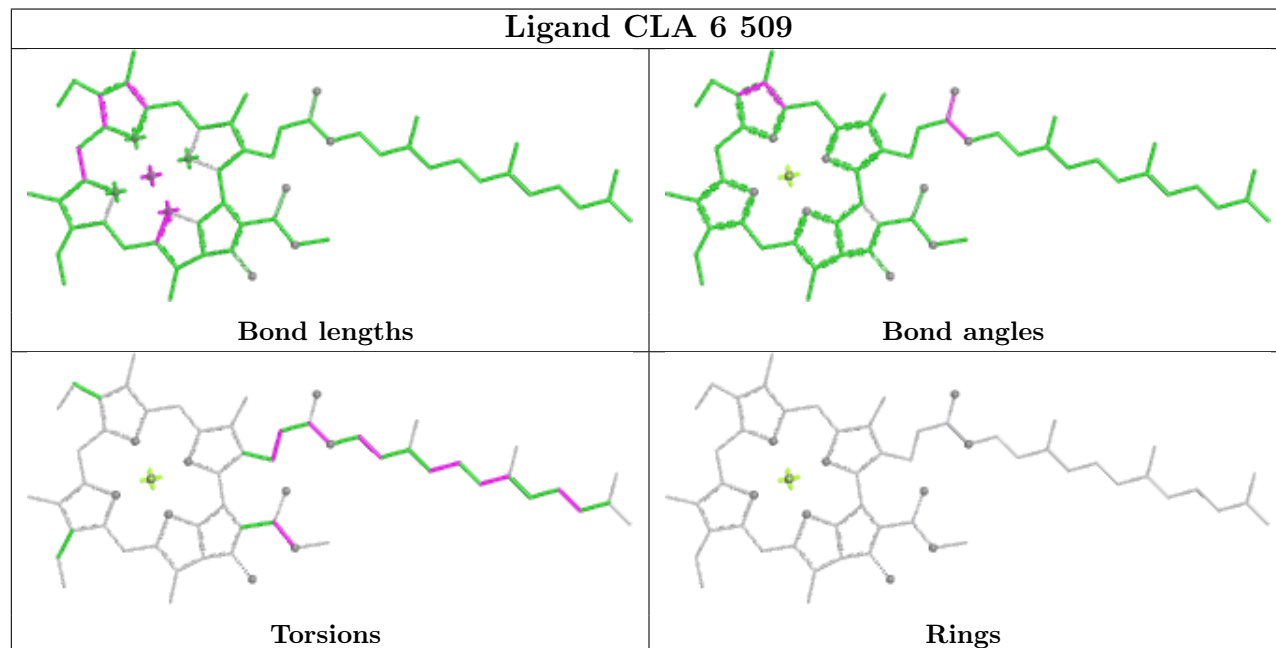


Rings

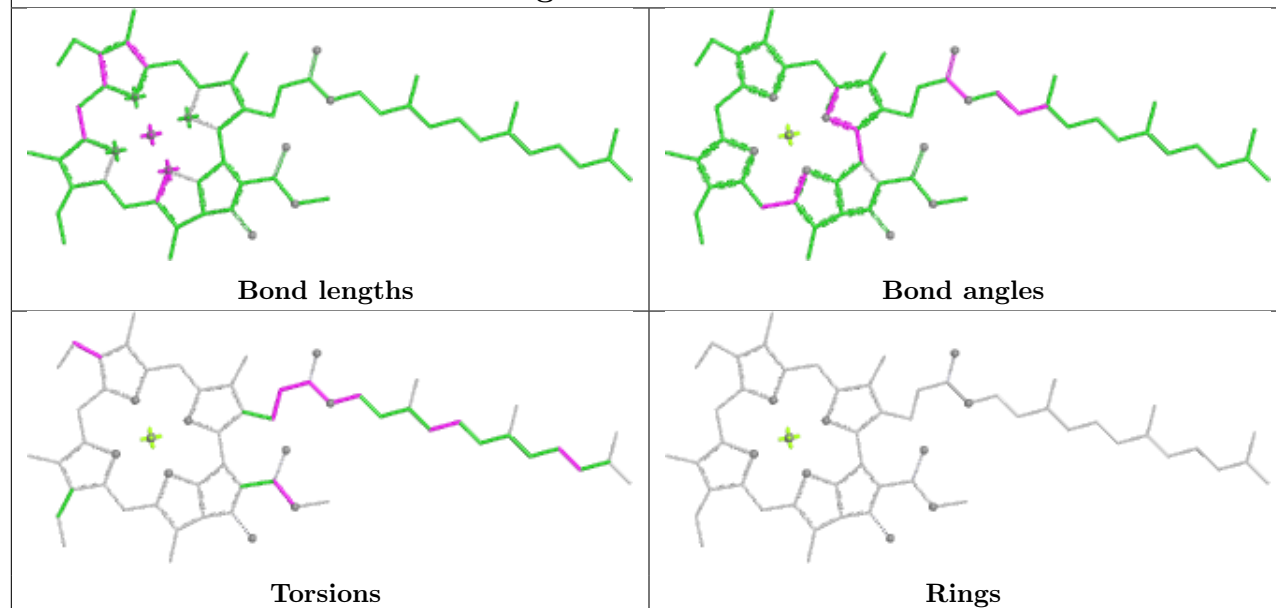




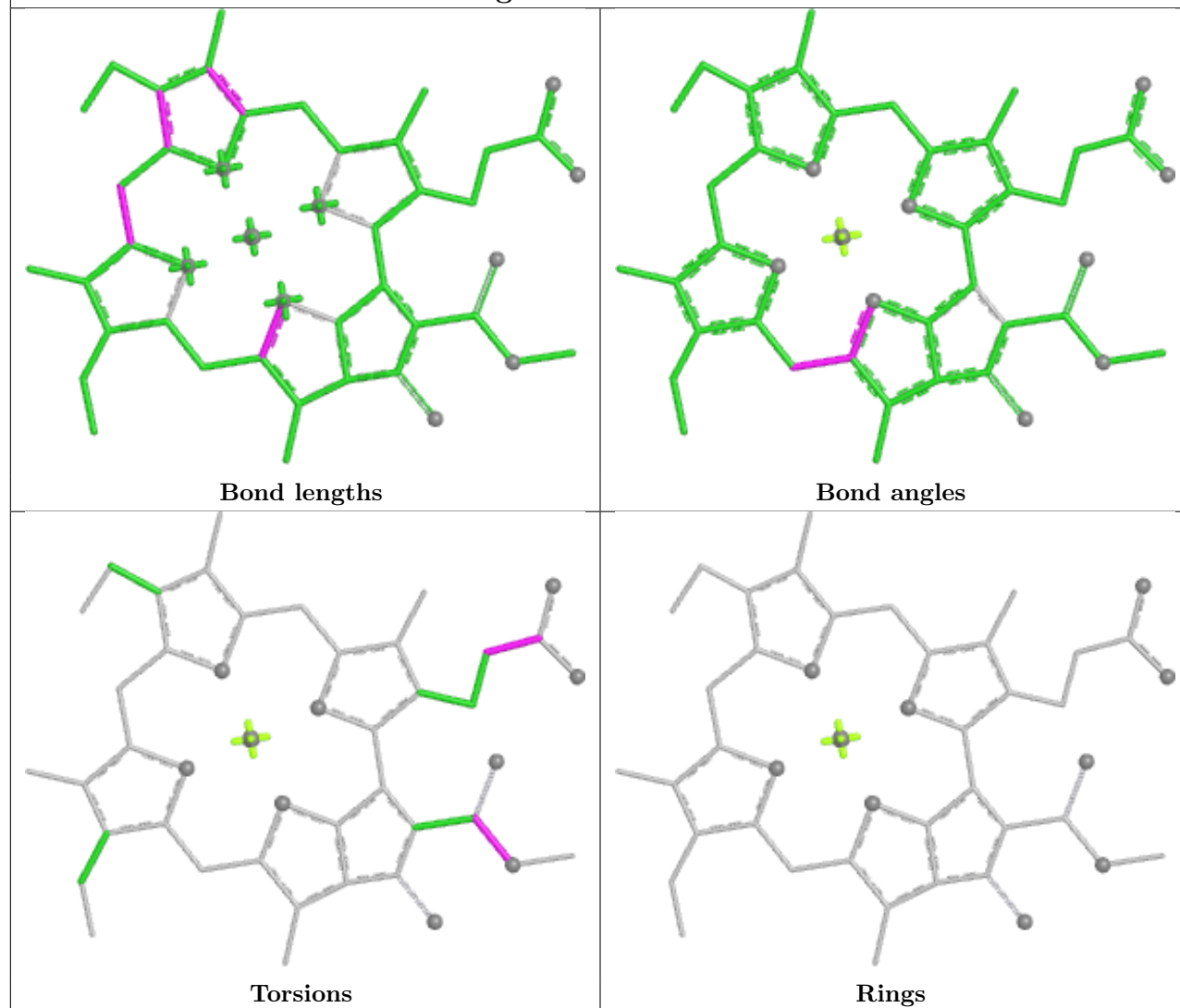
Ligand CLA 2 408**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 1 506****Bond lengths****Bond angles****Torsions****Rings**

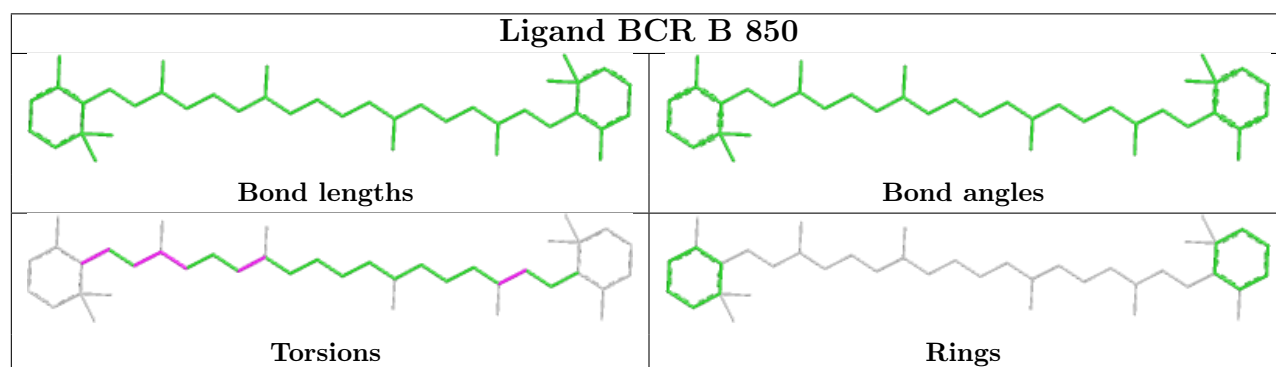
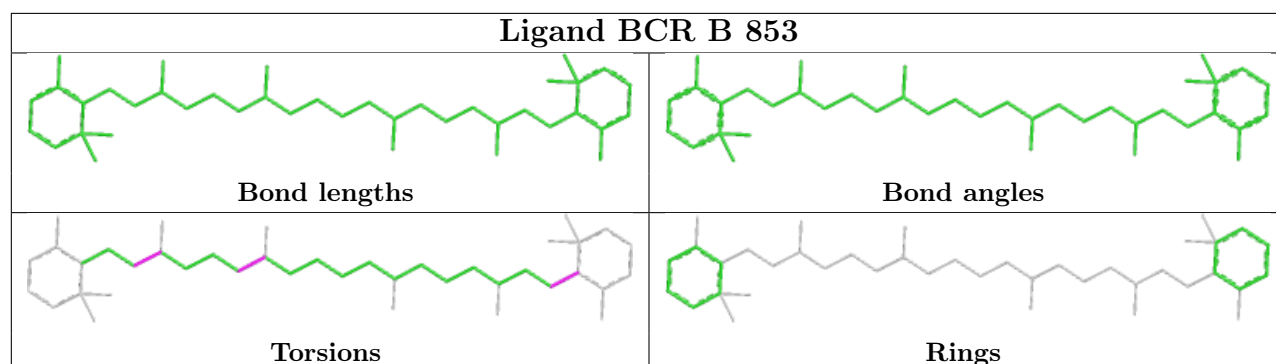
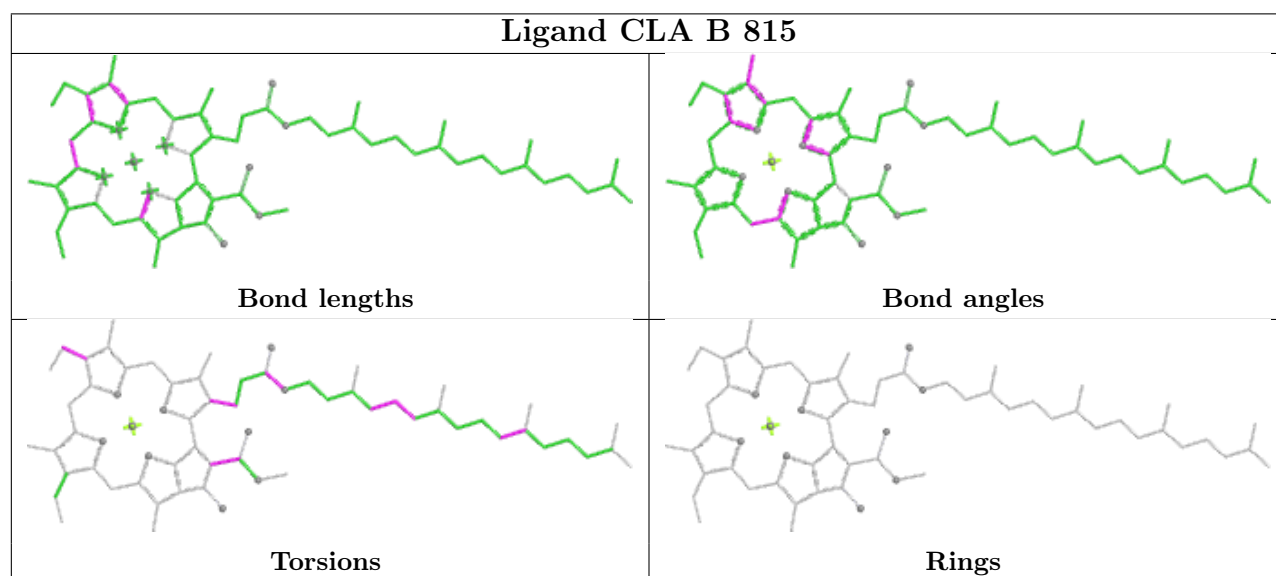
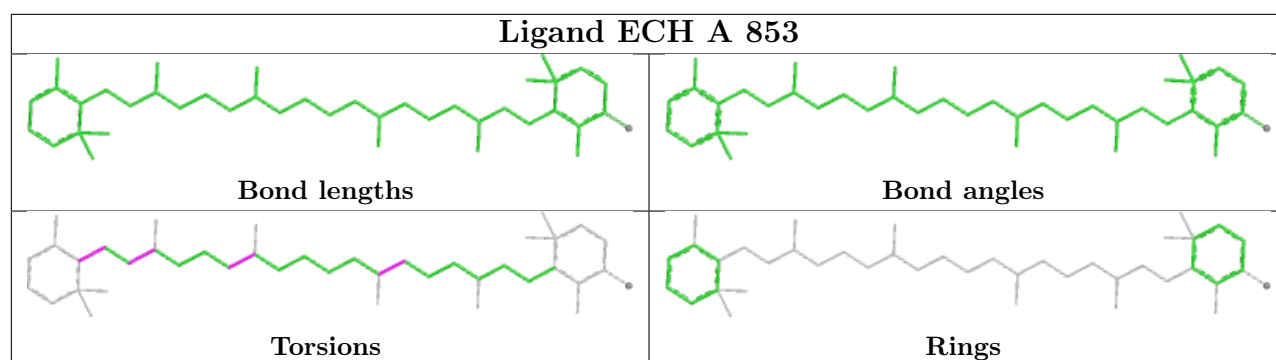
Ligand CLA 5 417**Ligand CLA 6 509**

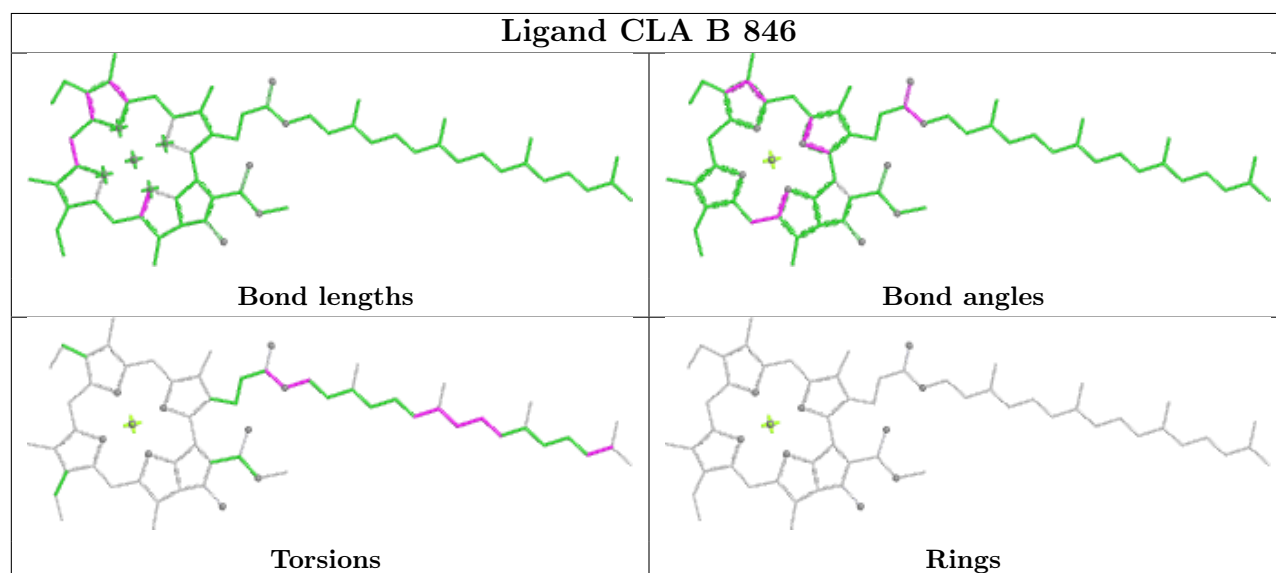
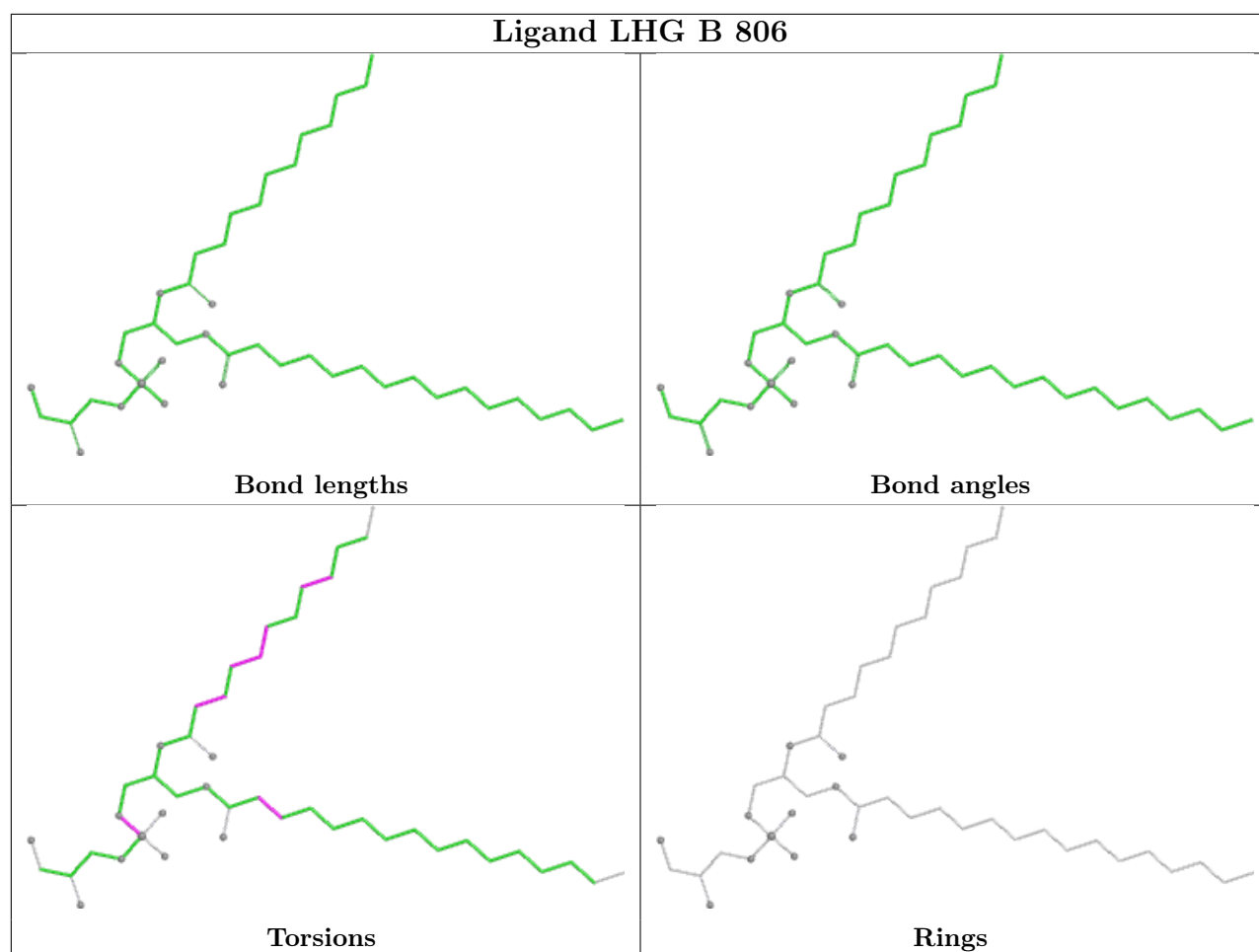
Ligand CLA 2 410

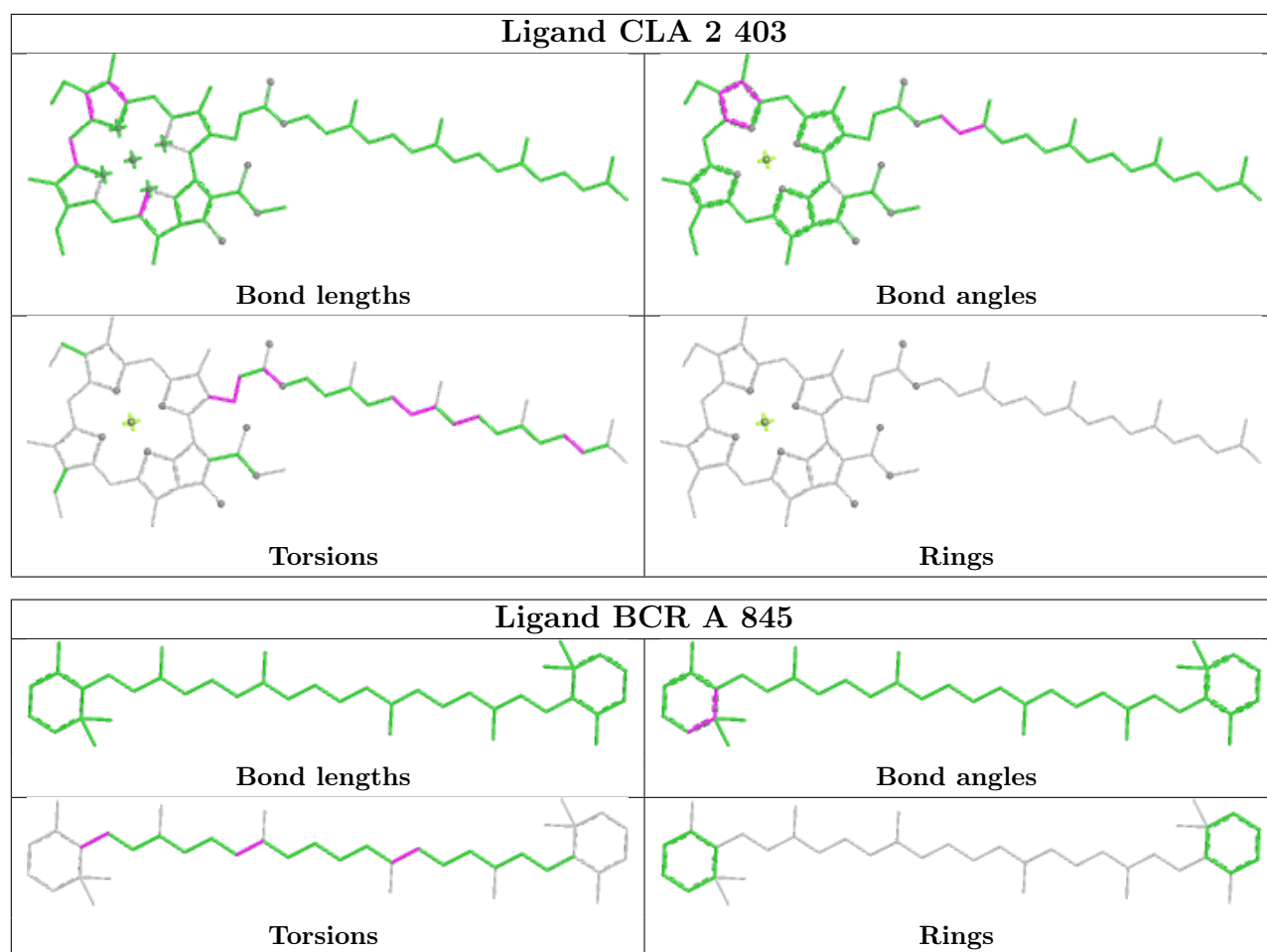


Ligand CLA 7 512

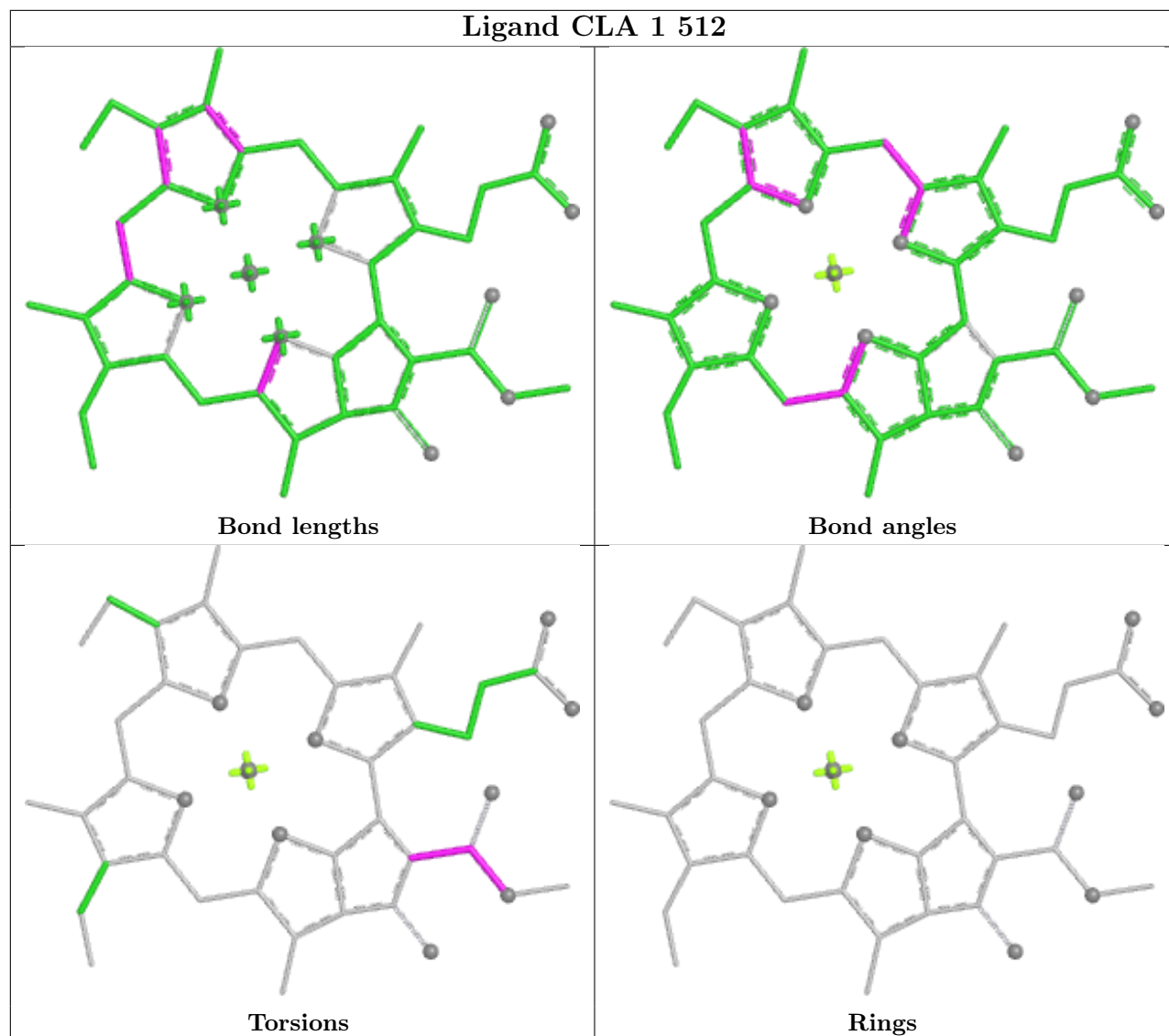




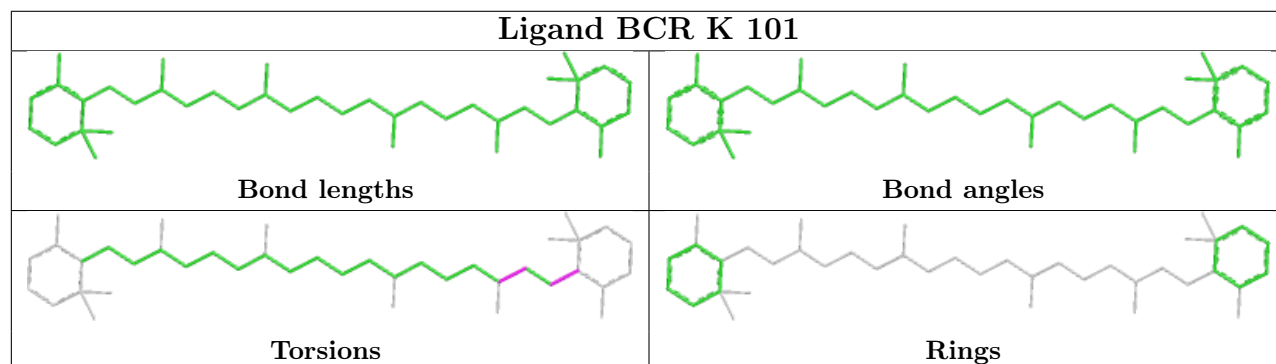


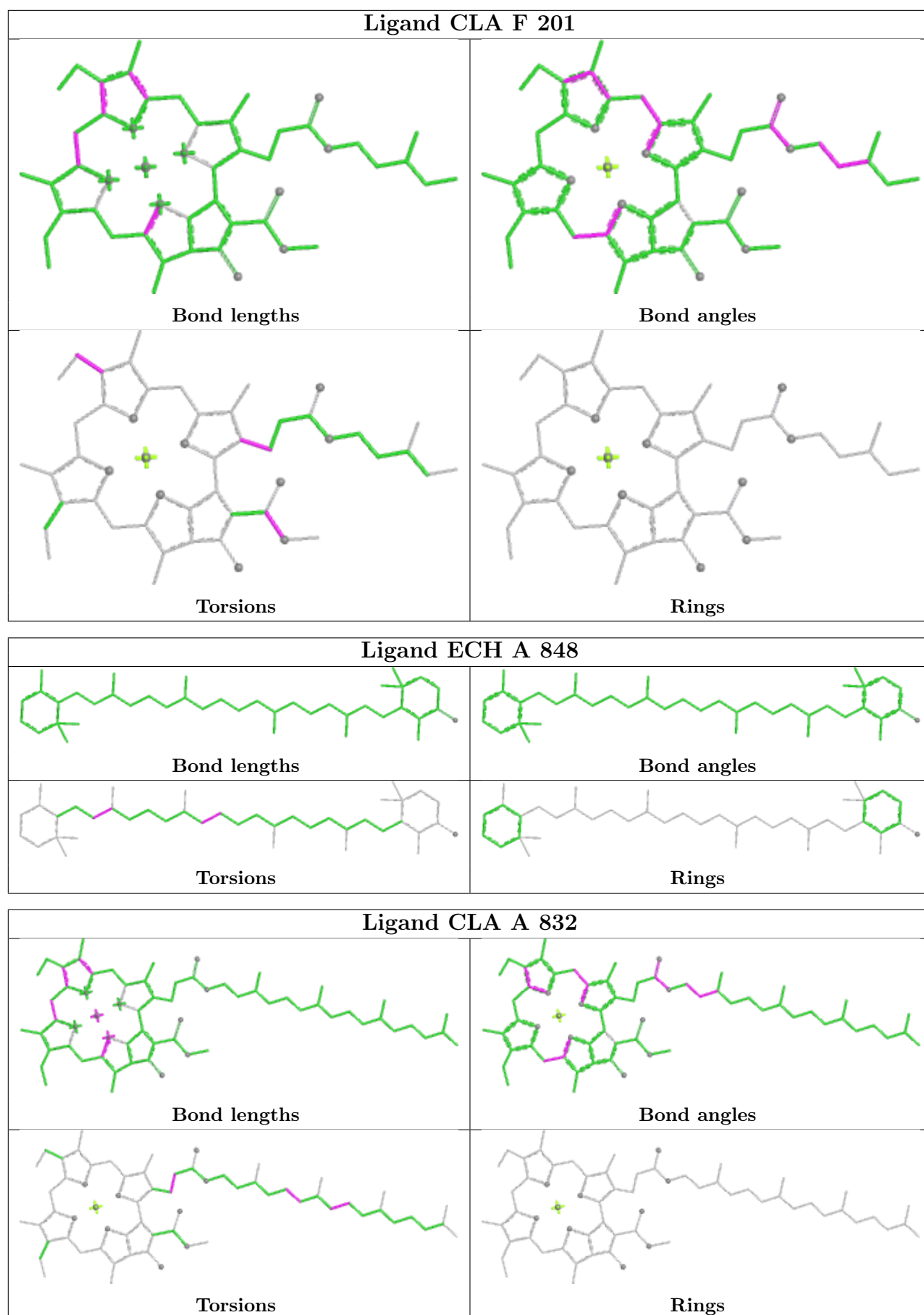


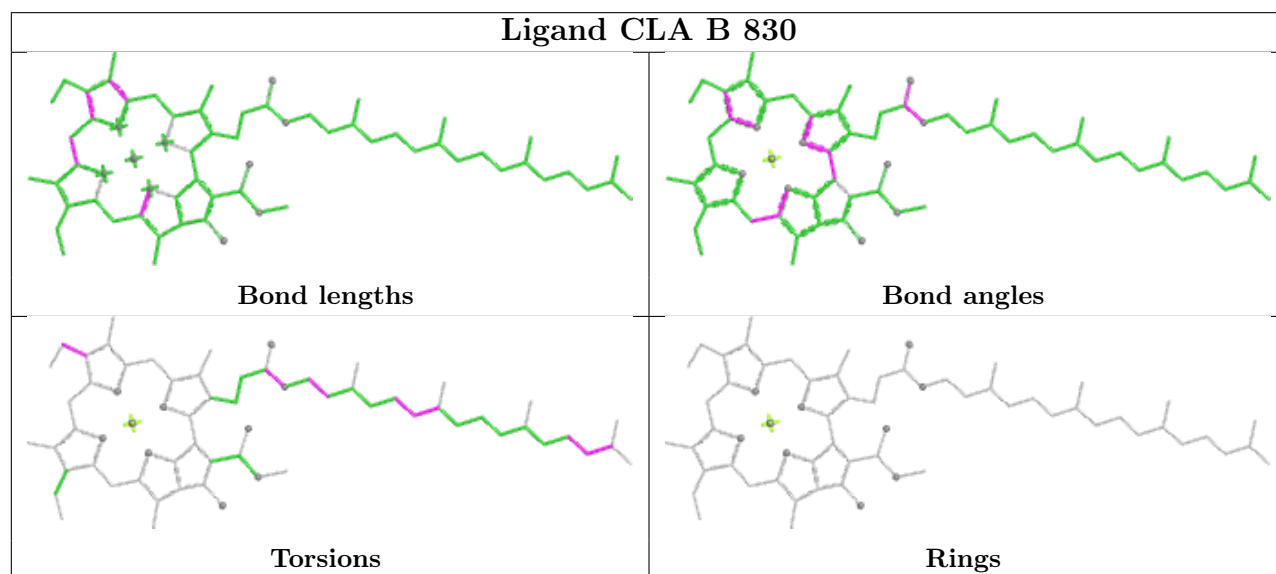
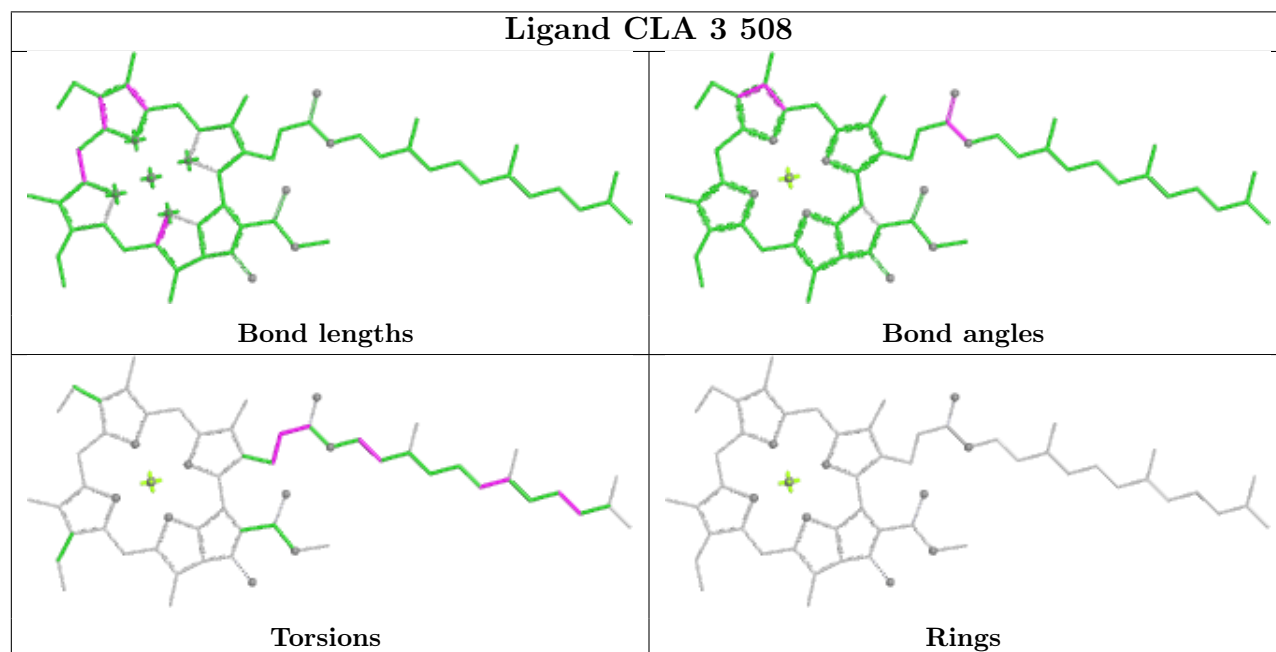
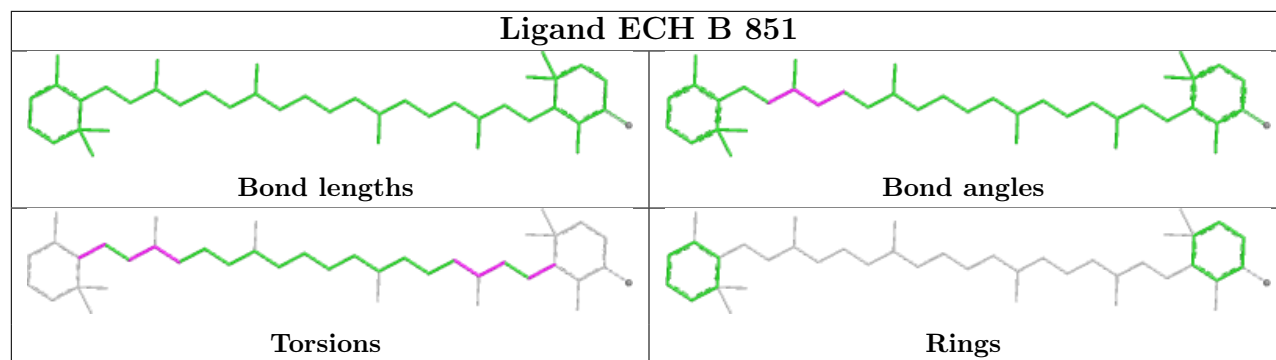
Ligand CLA 1 512

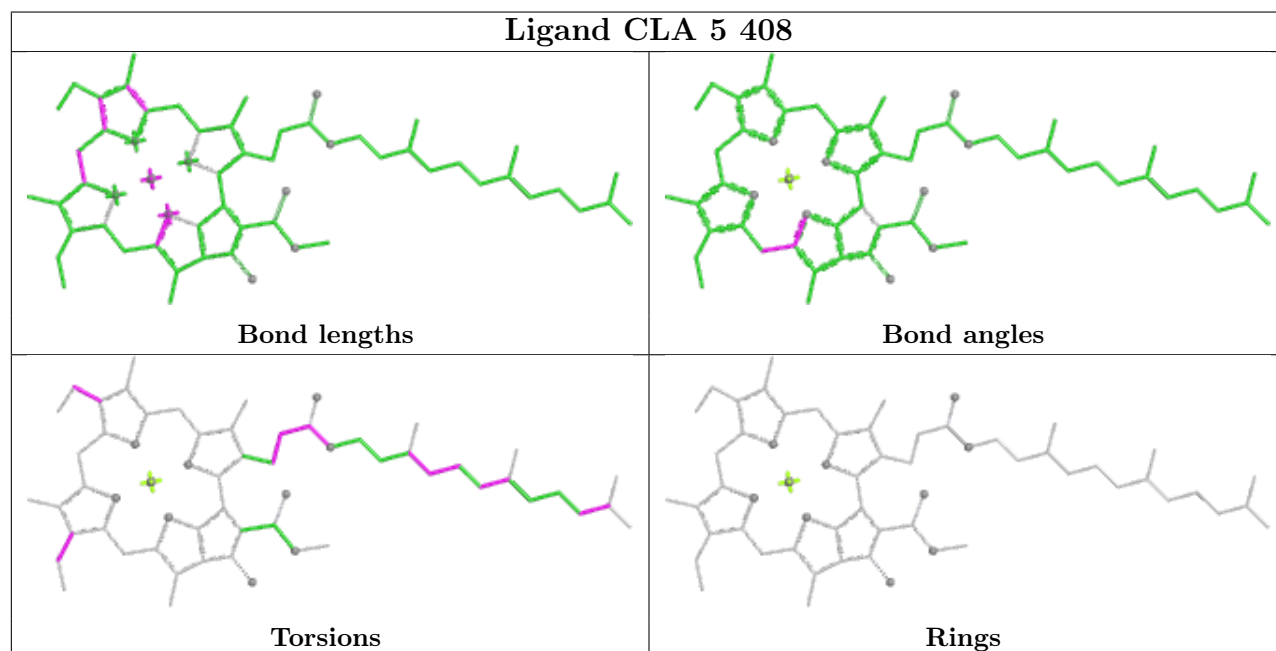
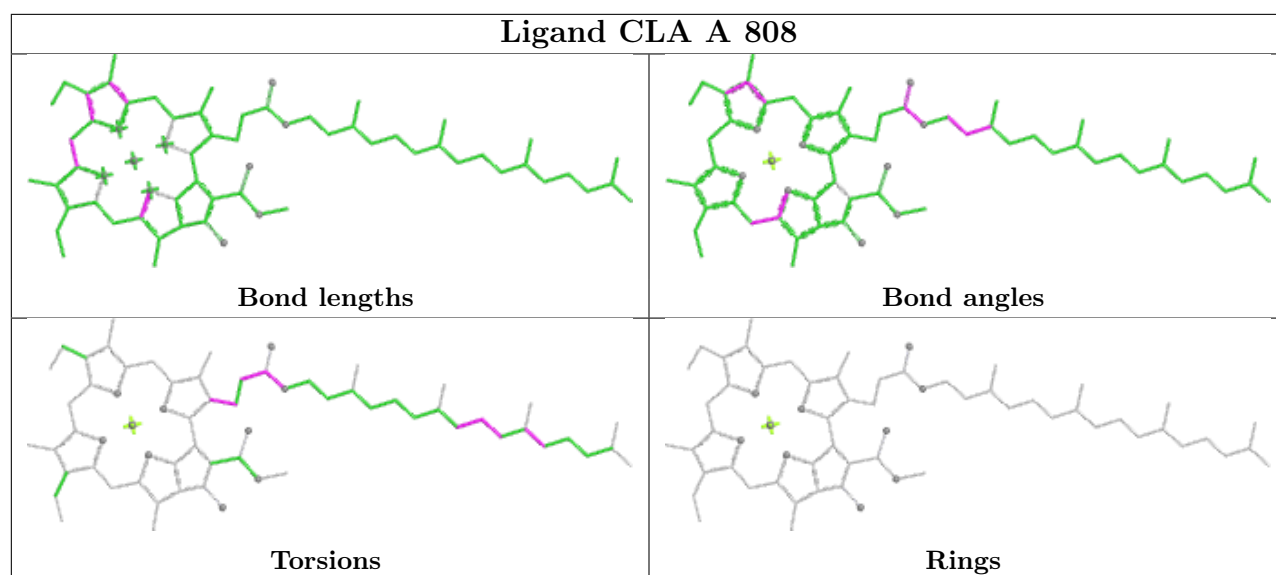


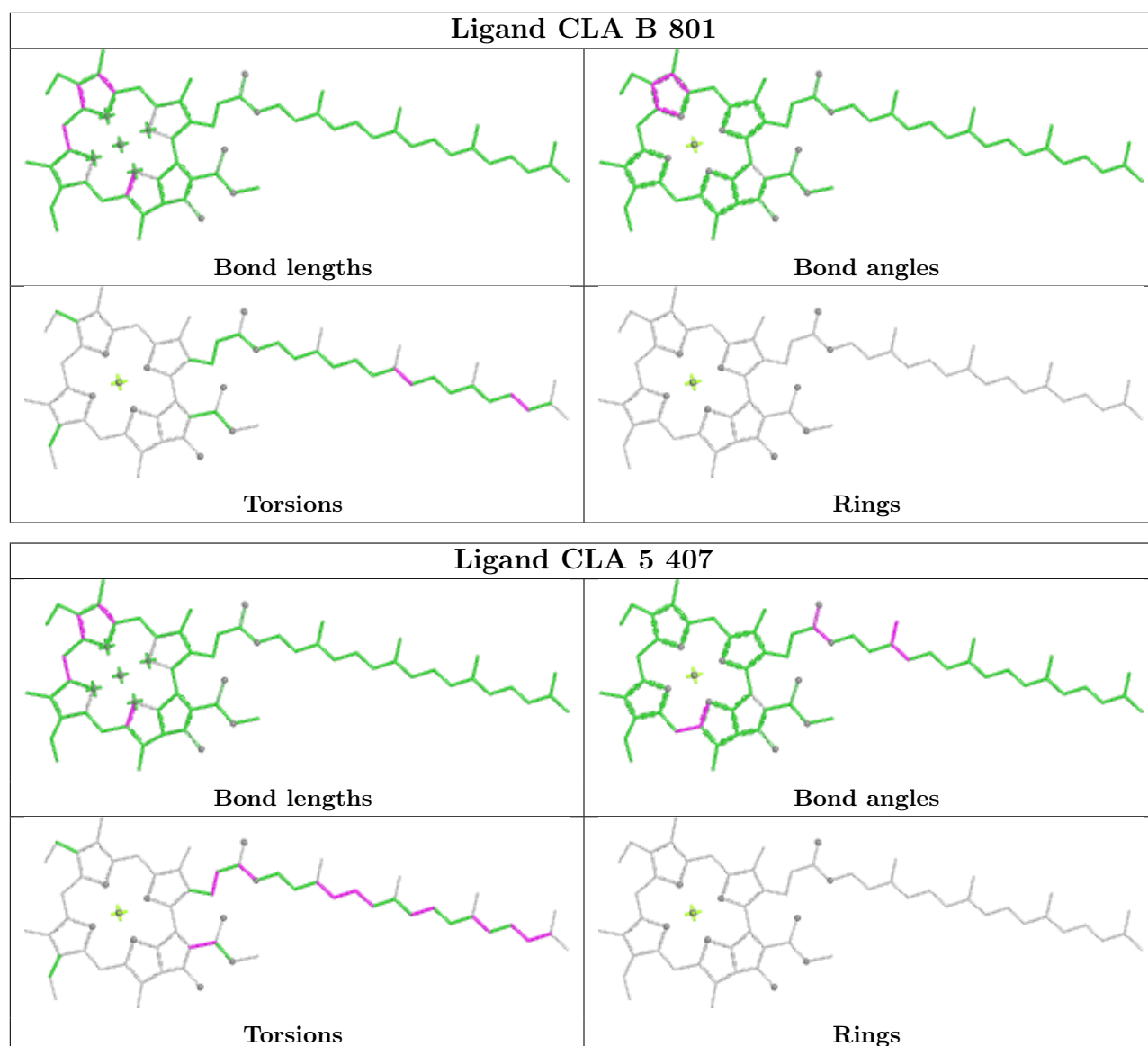
Ligand BCR K 101



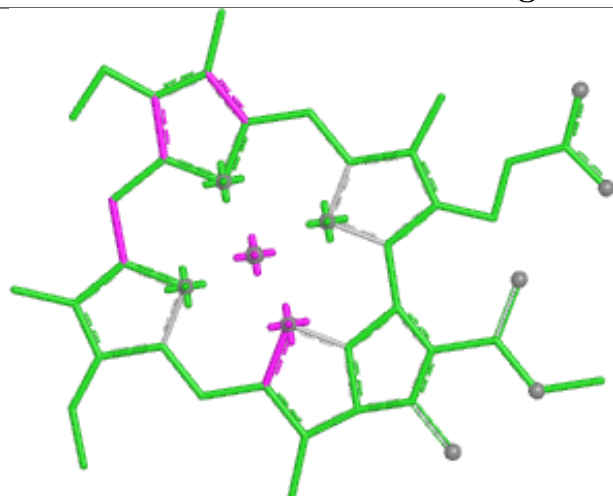




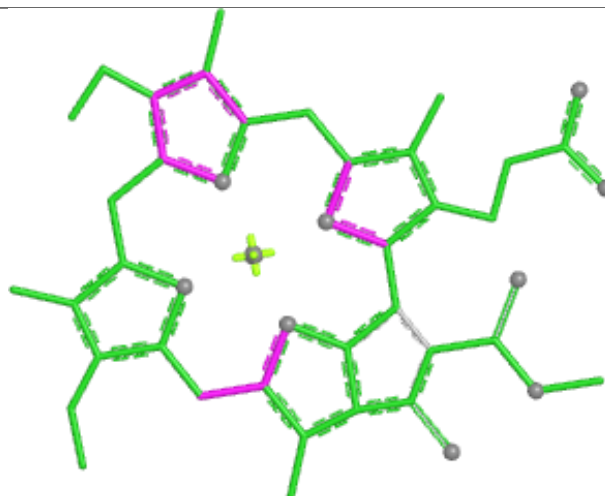




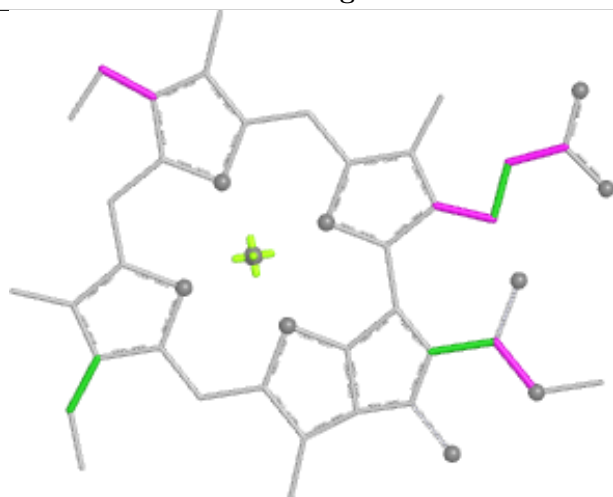
Ligand CLA 6 513



Bond lengths



Bond angles

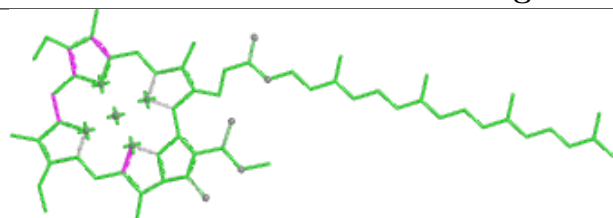


Torsions

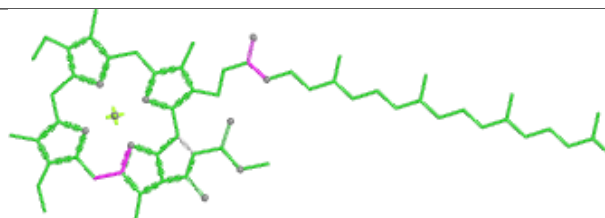


Rings

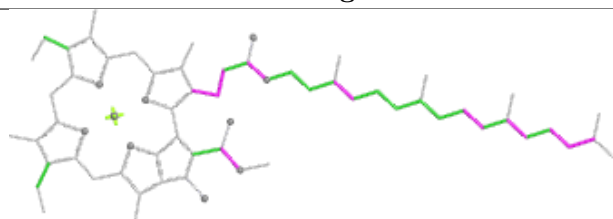
Ligand CLA A 812



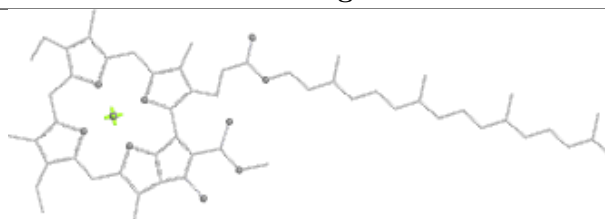
Bond lengths



Bond angles

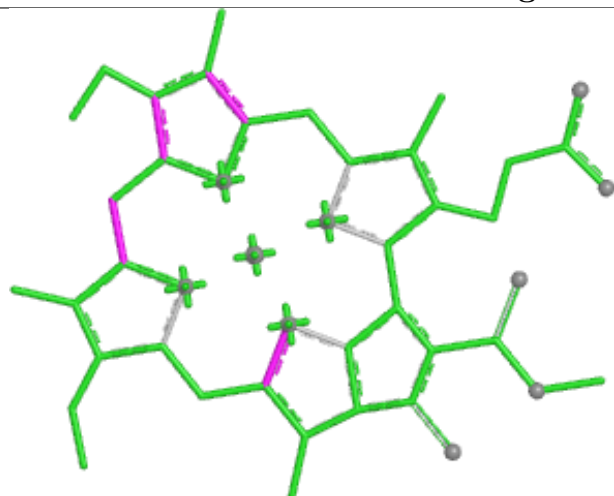


Torsions

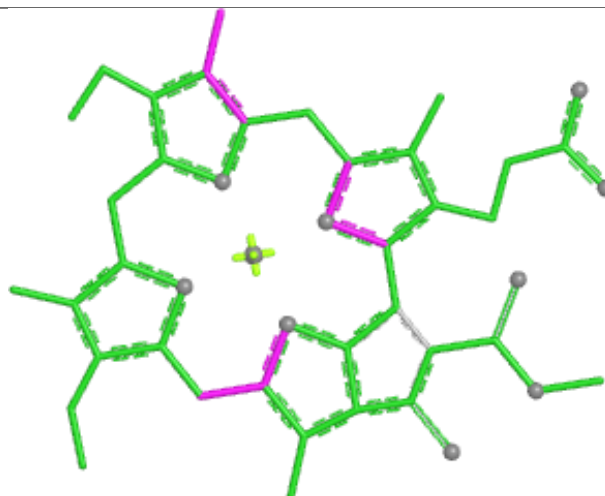


Rings

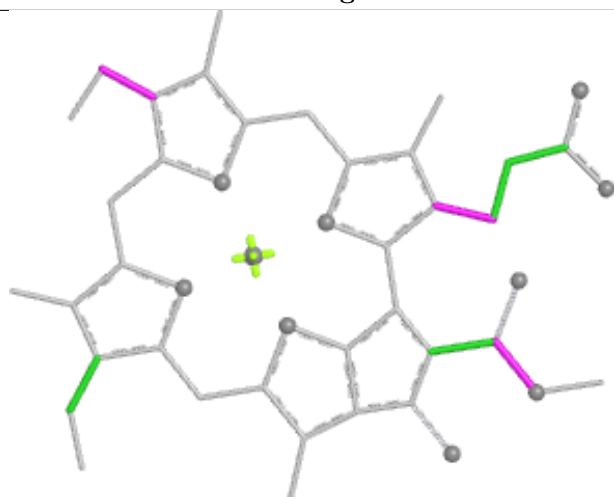
Ligand CLA 2 411



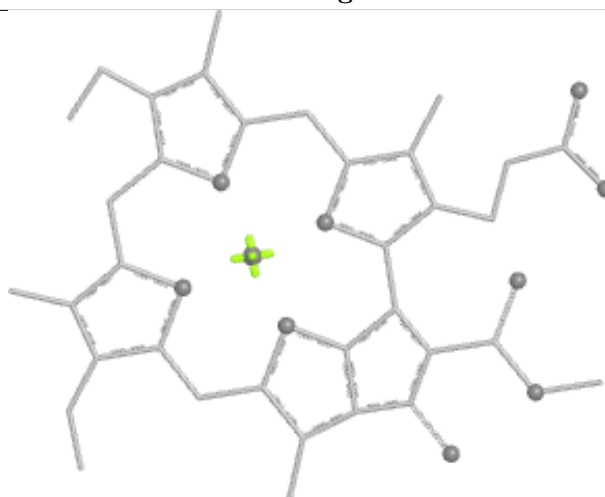
Bond lengths



Bond angles

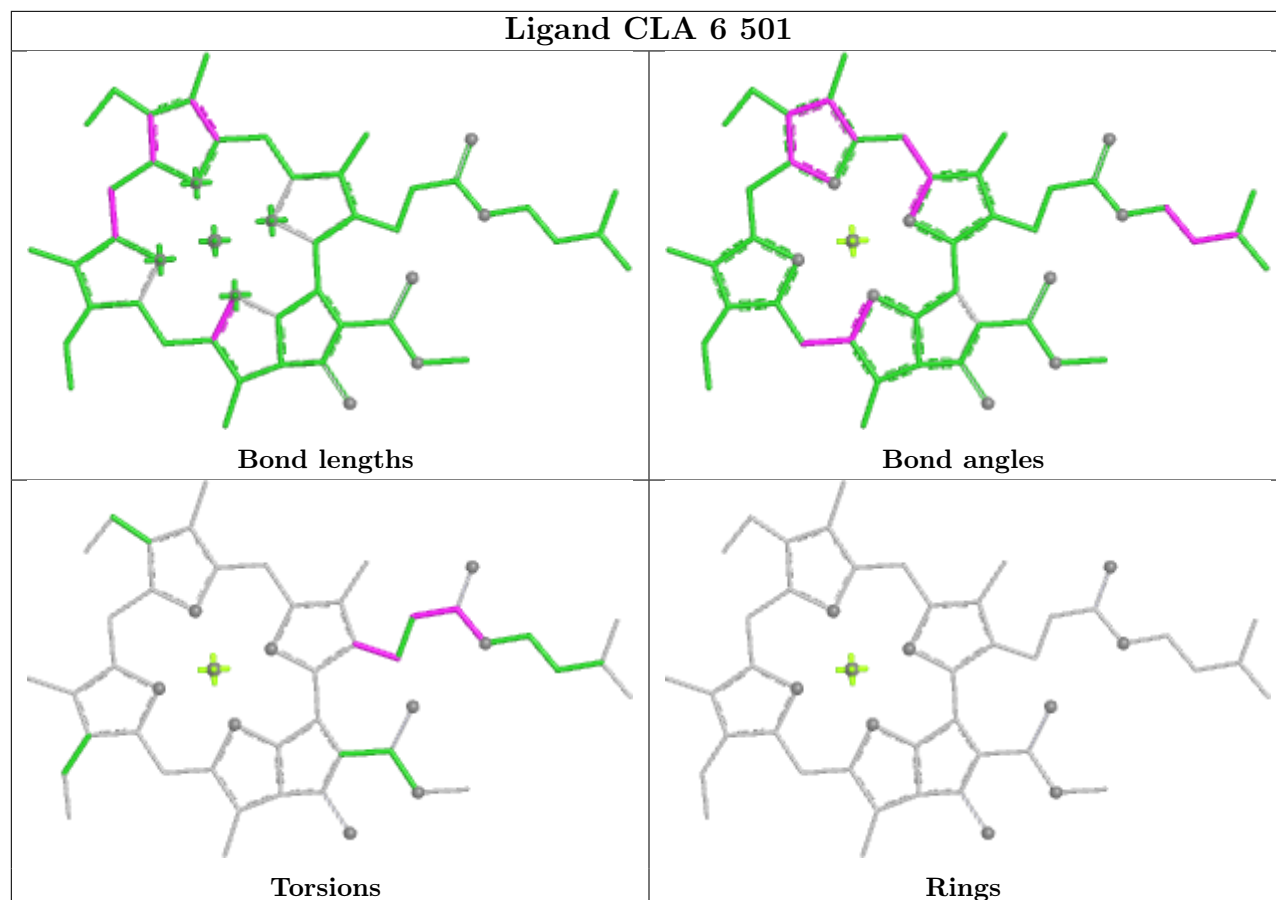


Torsions

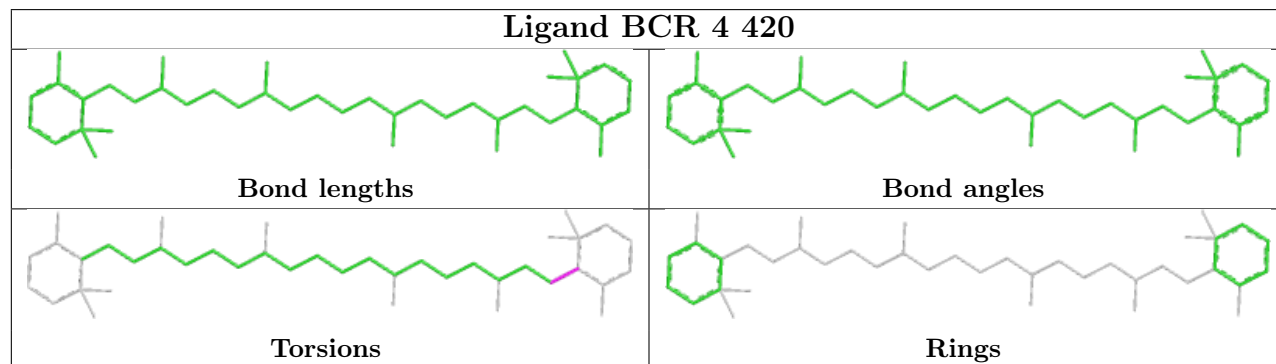


Rings

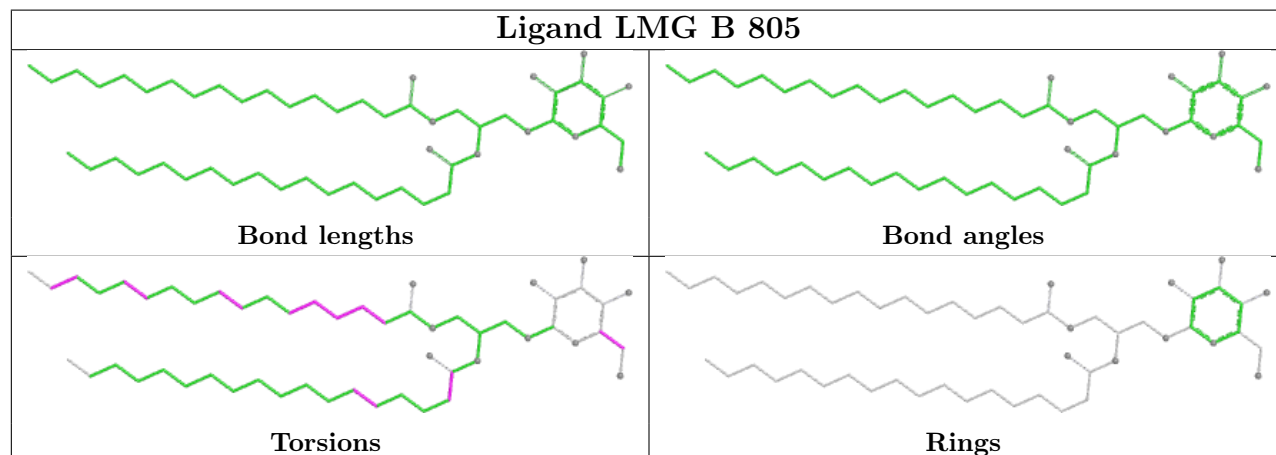
Ligand CLA 6 501

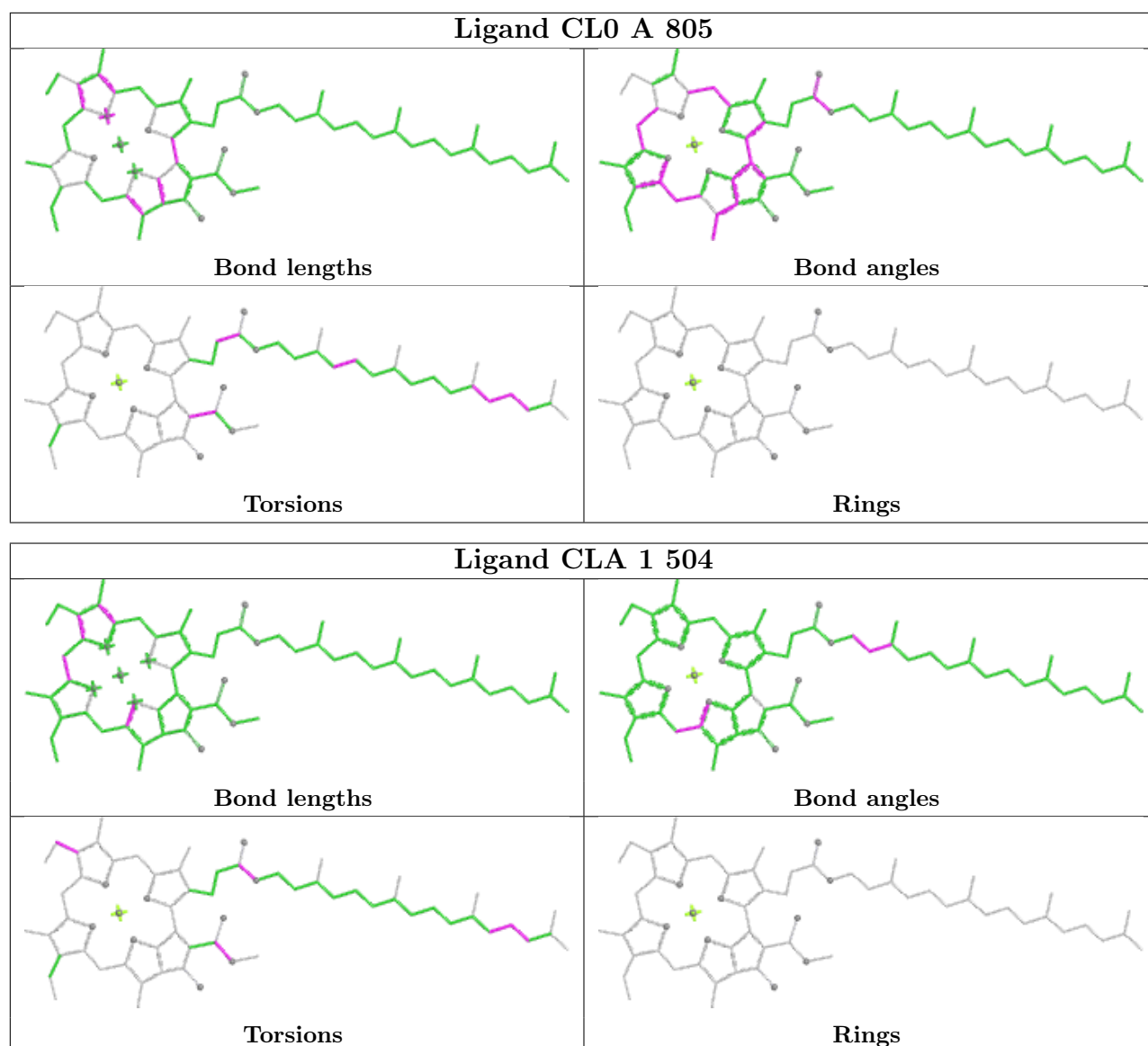


Ligand BCR 4 420

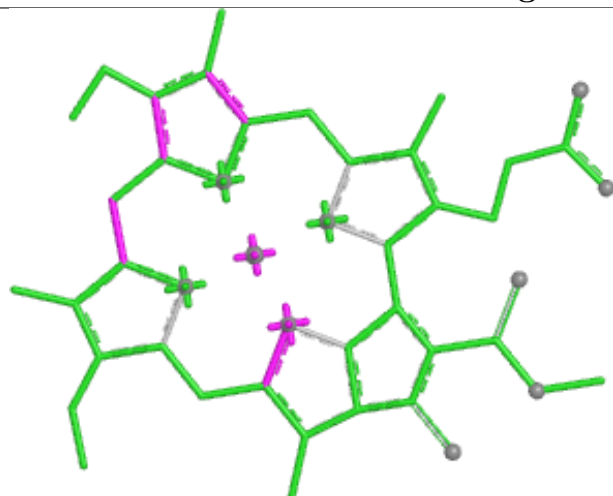


Ligand LMG B 805

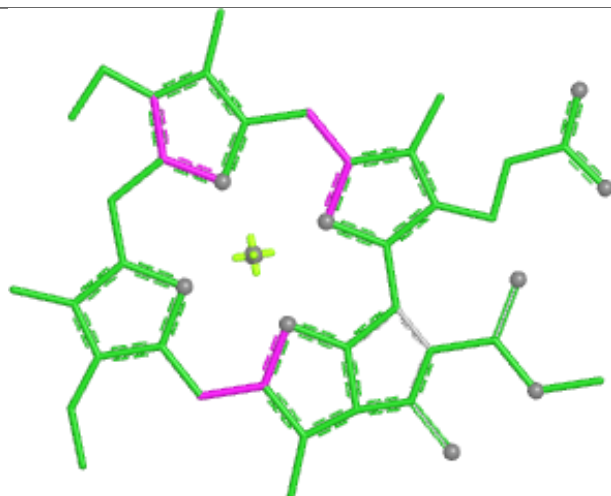




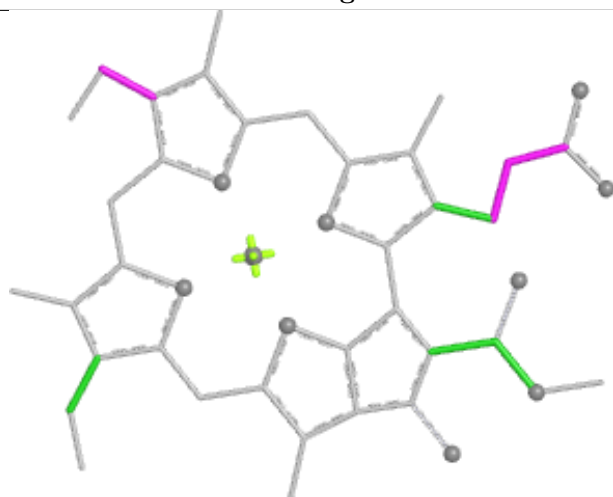
Ligand CLA 2 402



Bond lengths



Bond angles

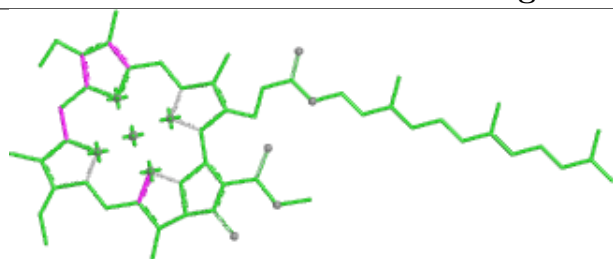


Torsions

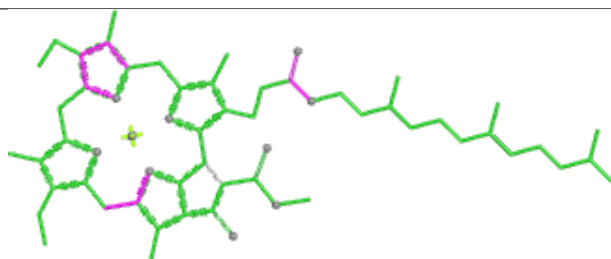


Rings

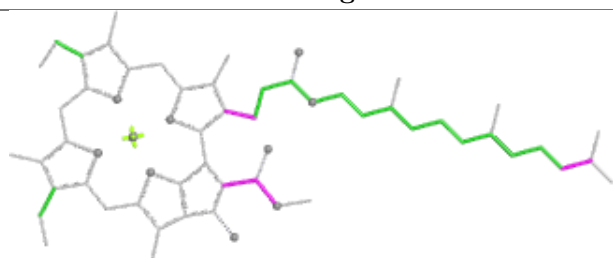
Ligand CLA 6 506



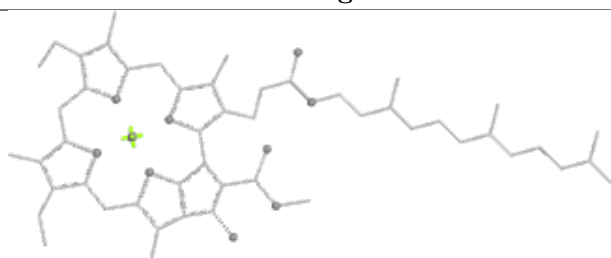
Bond lengths



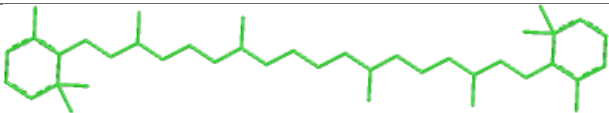
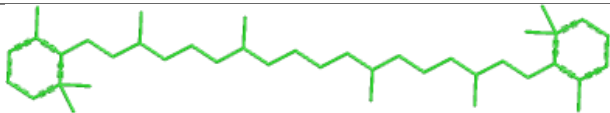
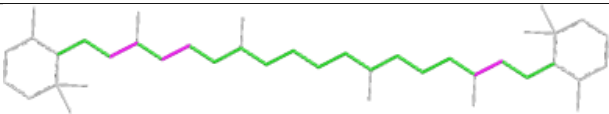
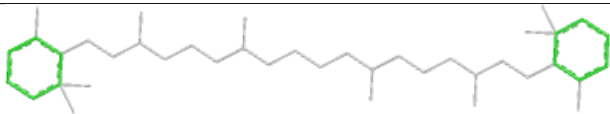
Bond angles



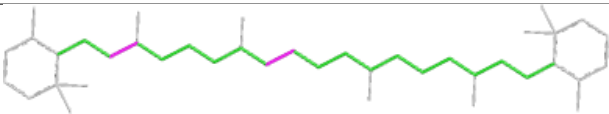
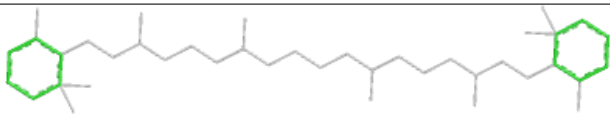


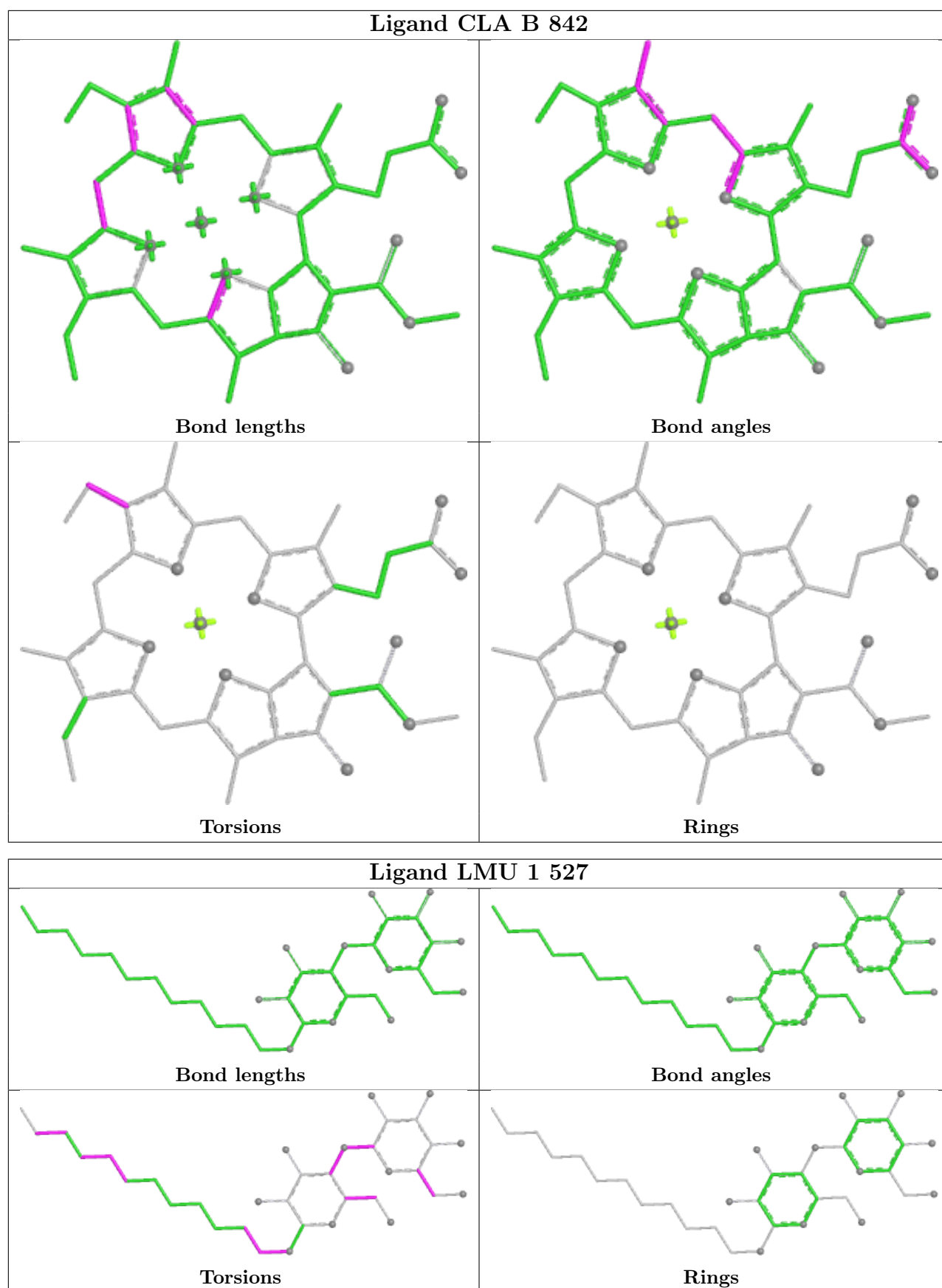
Torsions



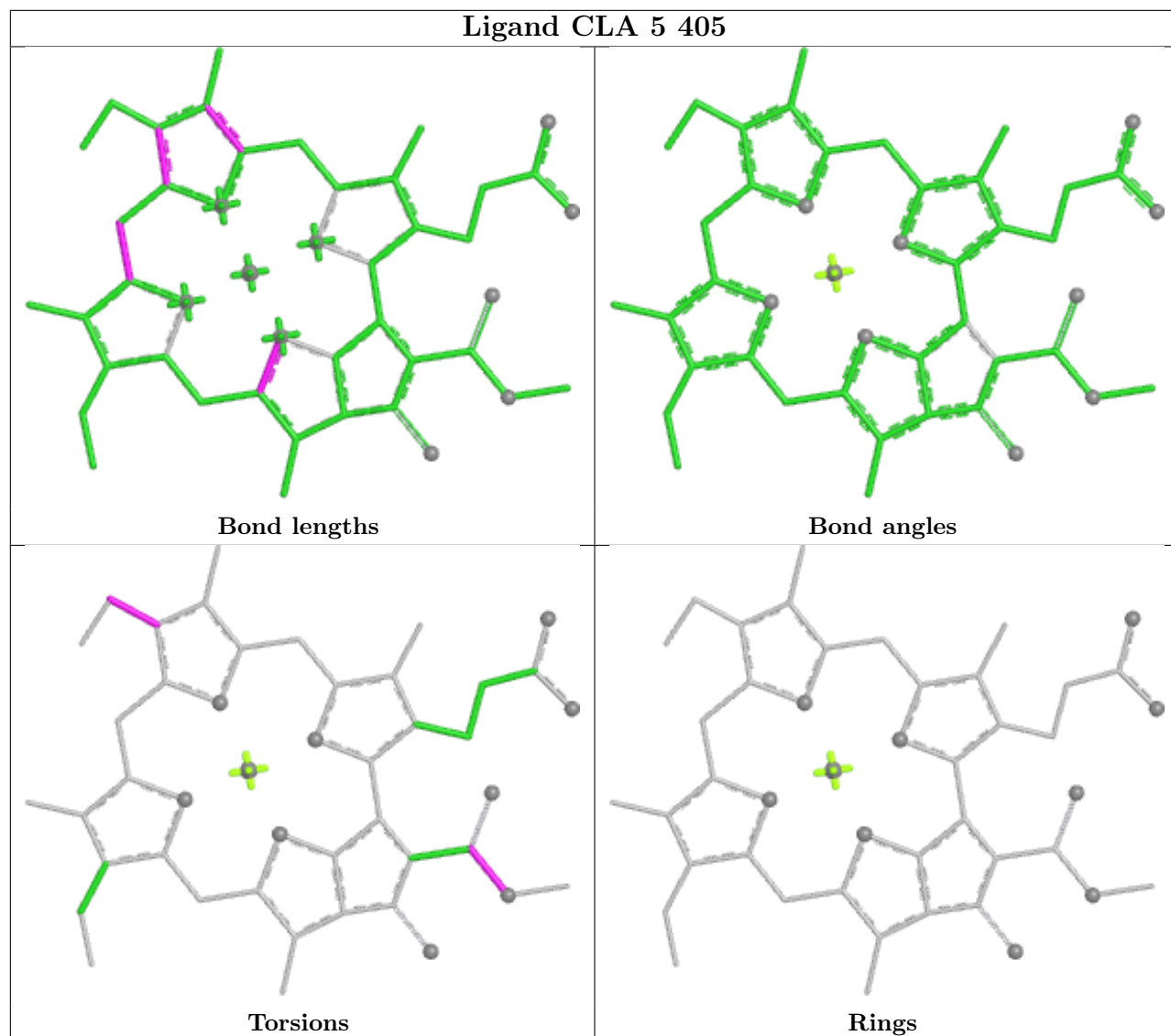
Rings

Ligand BCR 1 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

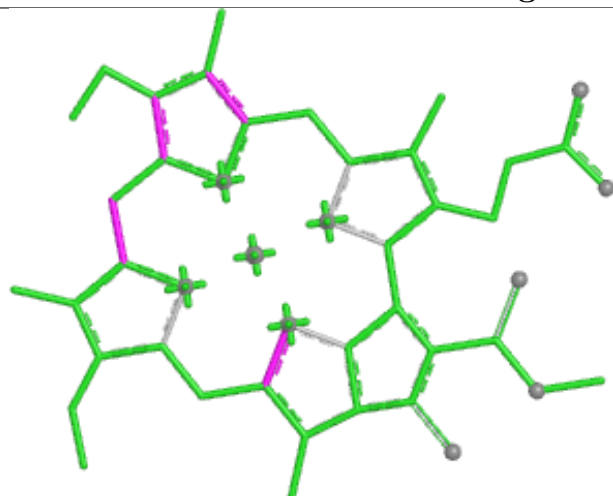
Ligand BCR 5 423	
	
Bond lengths	Bond angles
	
Torsions	Rings



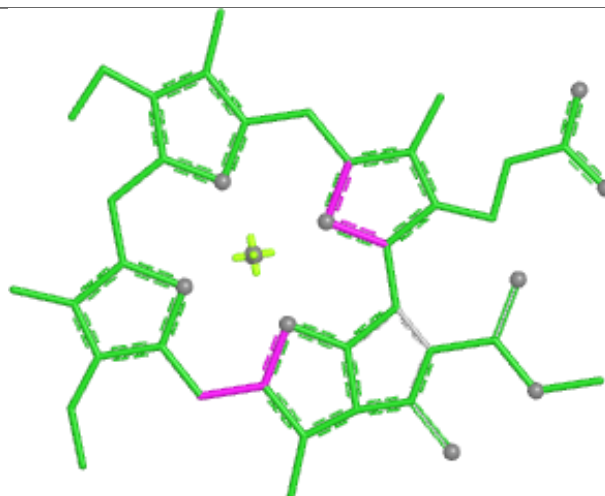
Ligand CLA 5 405



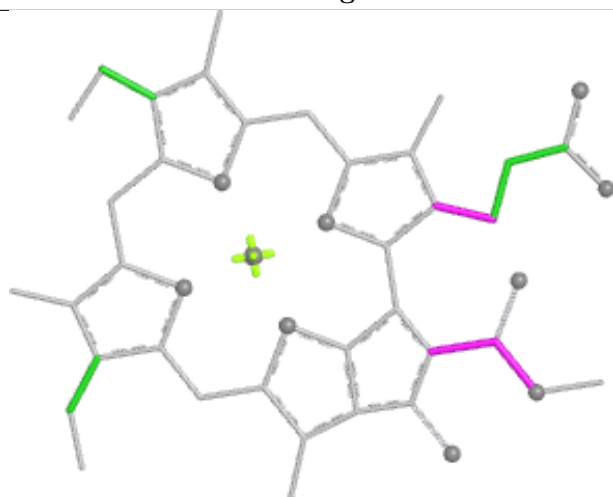
Ligand CLA 5 414



Bond lengths



Bond angles

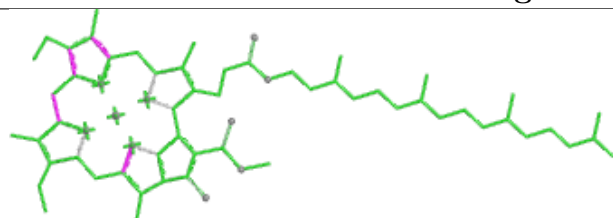


Torsions

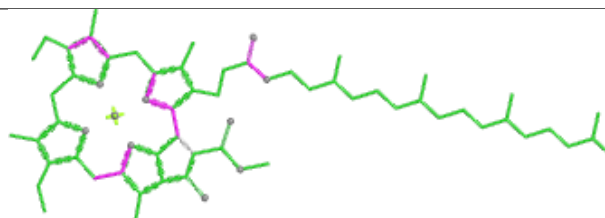


Rings

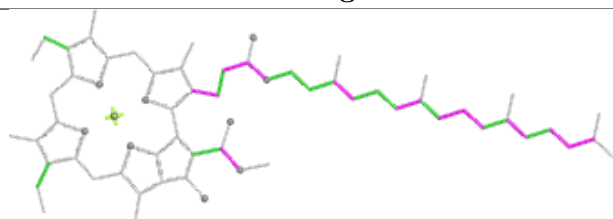
Ligand CLA B 837



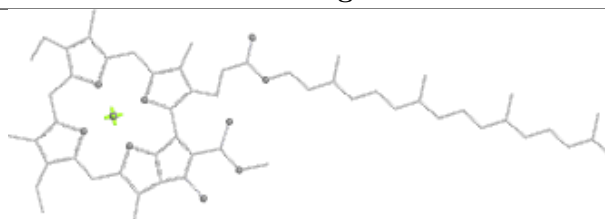
Bond lengths



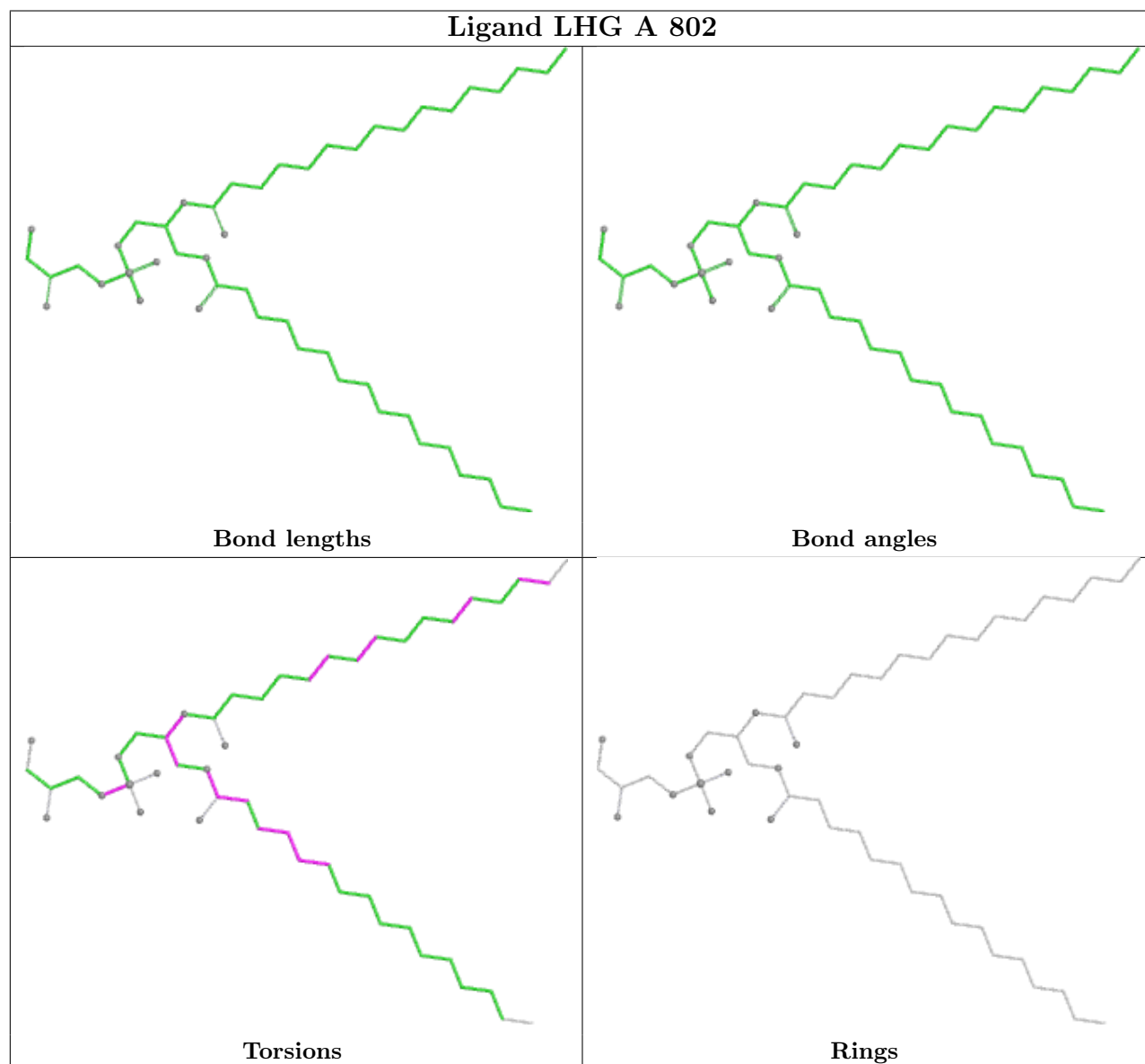
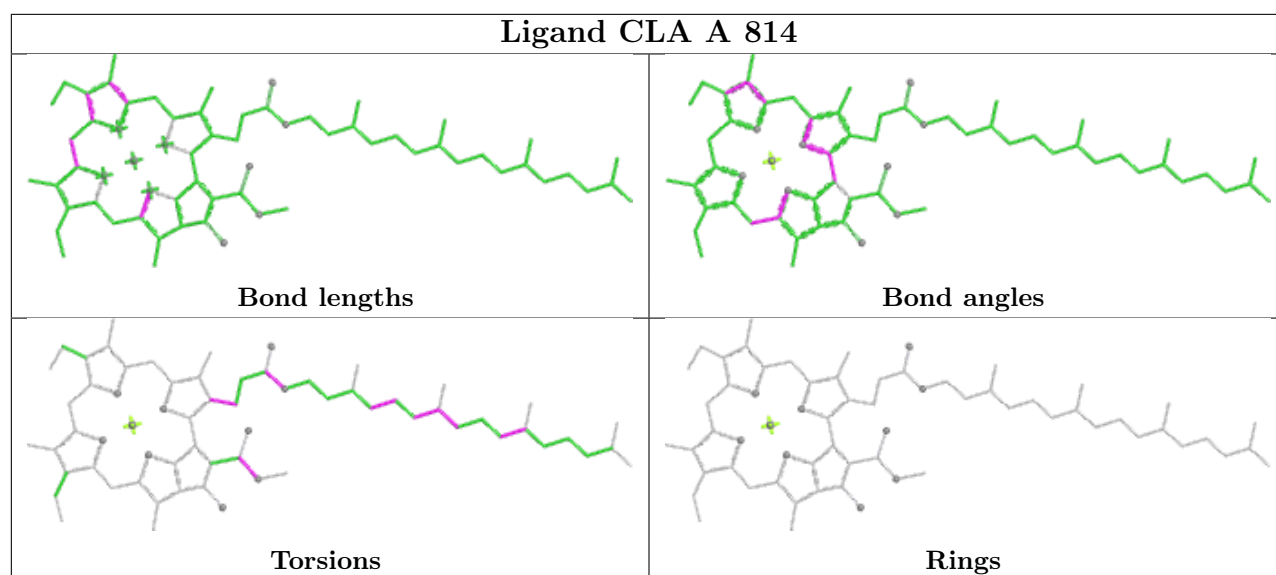
Bond angles



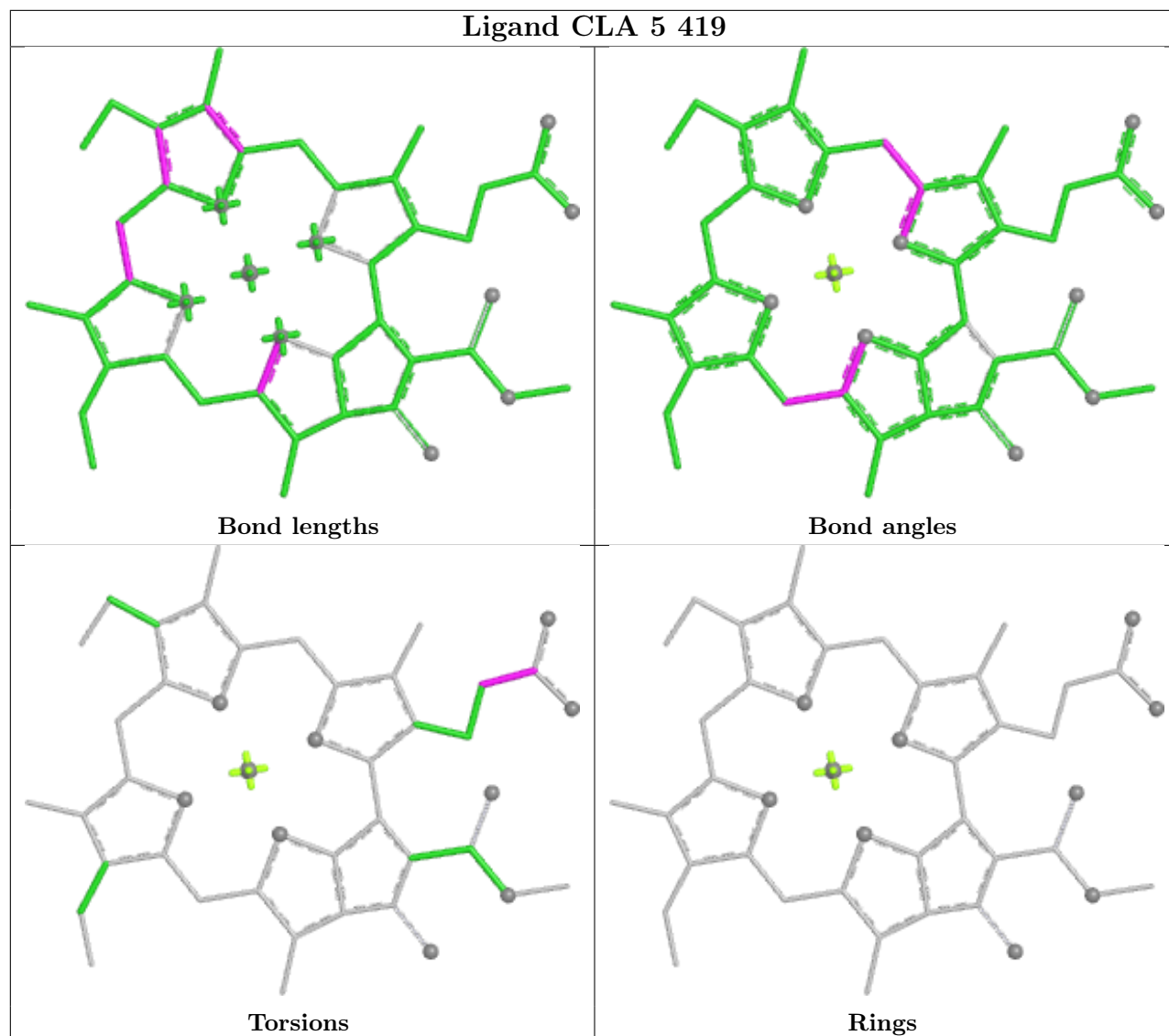
Torsions



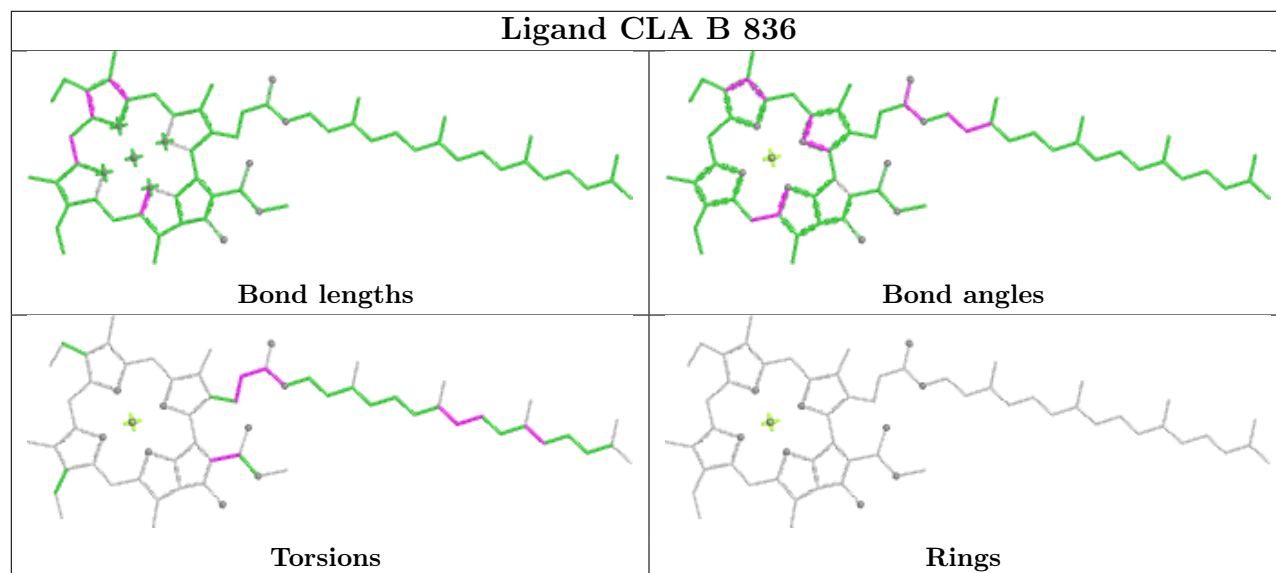
Rings

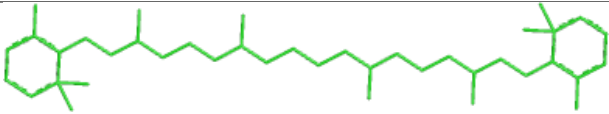
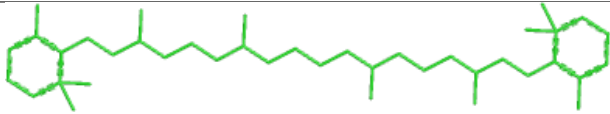
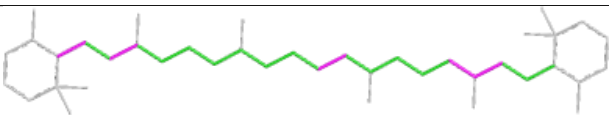
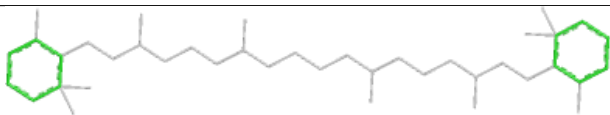


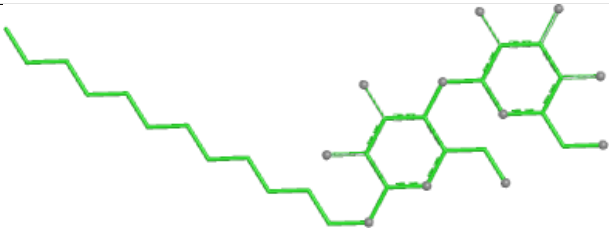
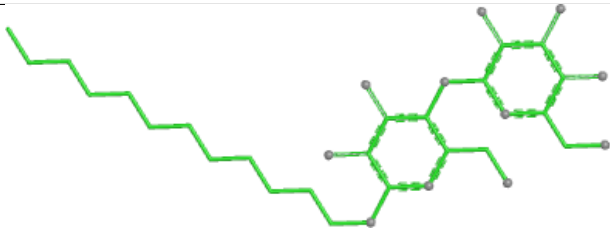
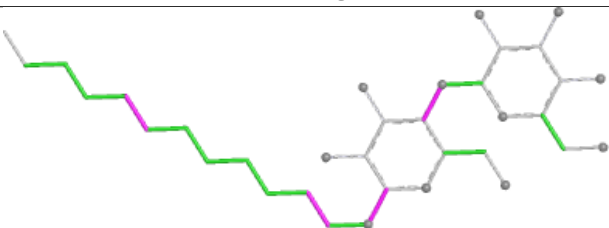
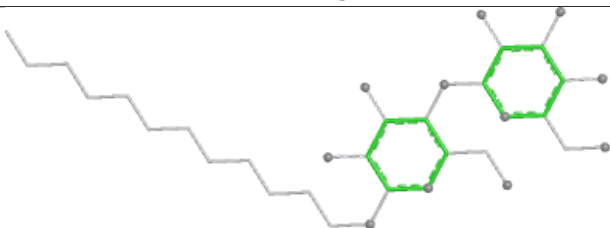
Ligand CLA 5 419

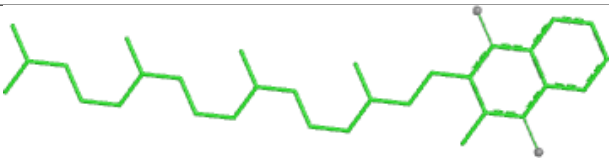
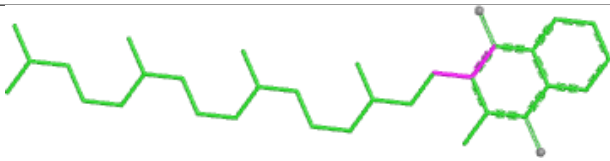
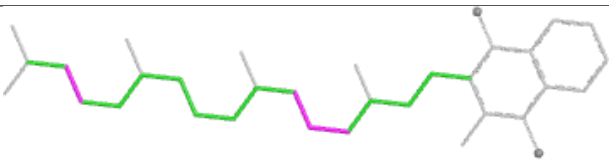
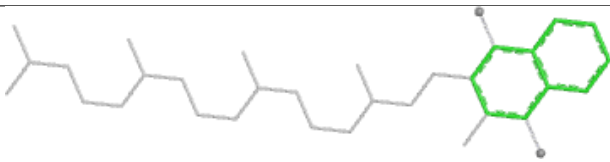


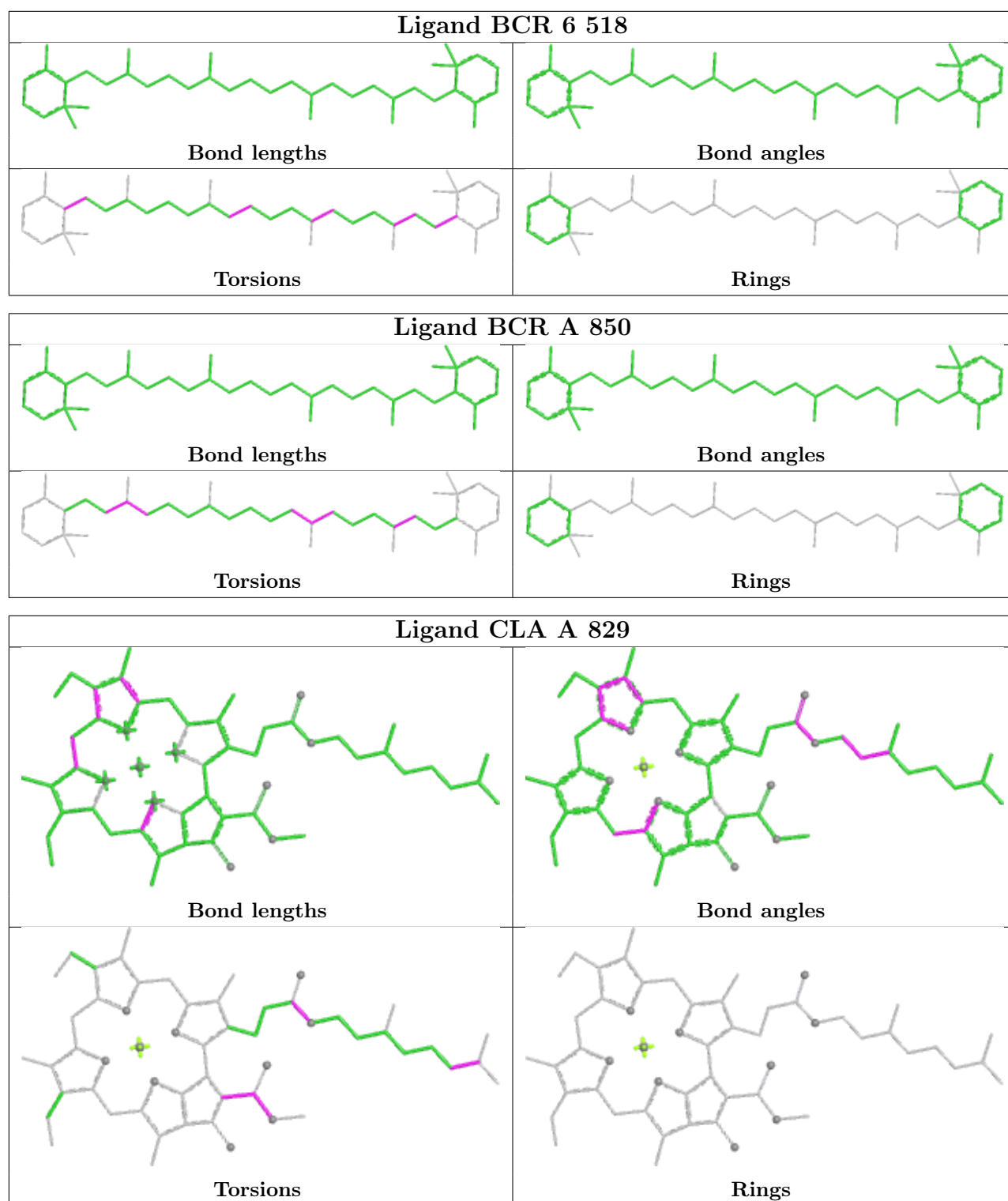
Ligand CLA B 836

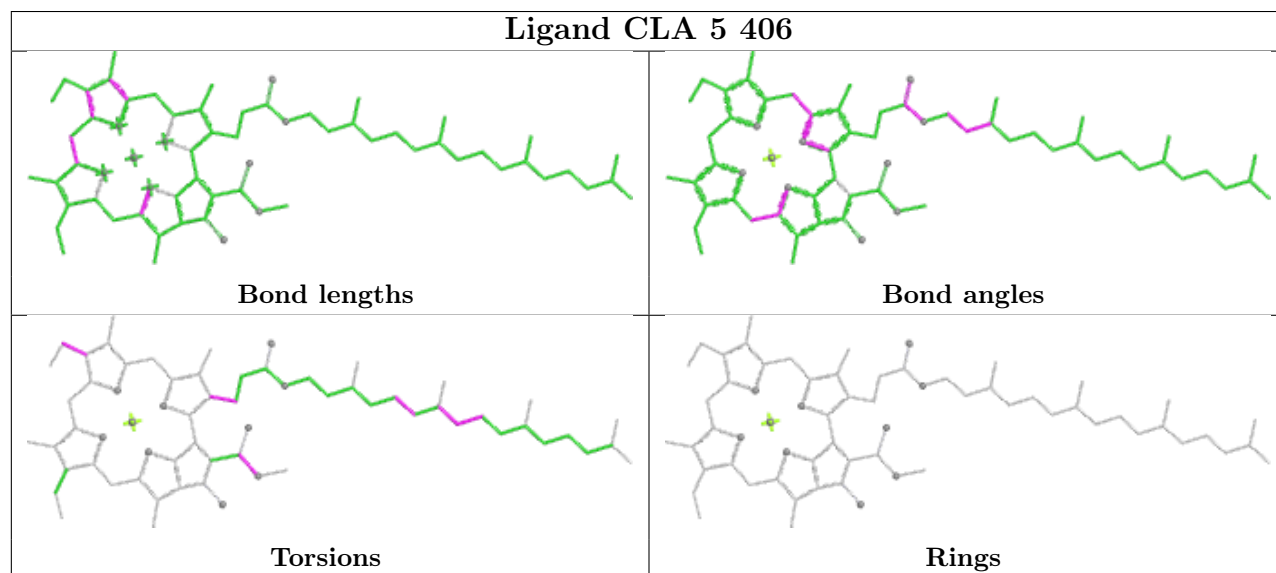
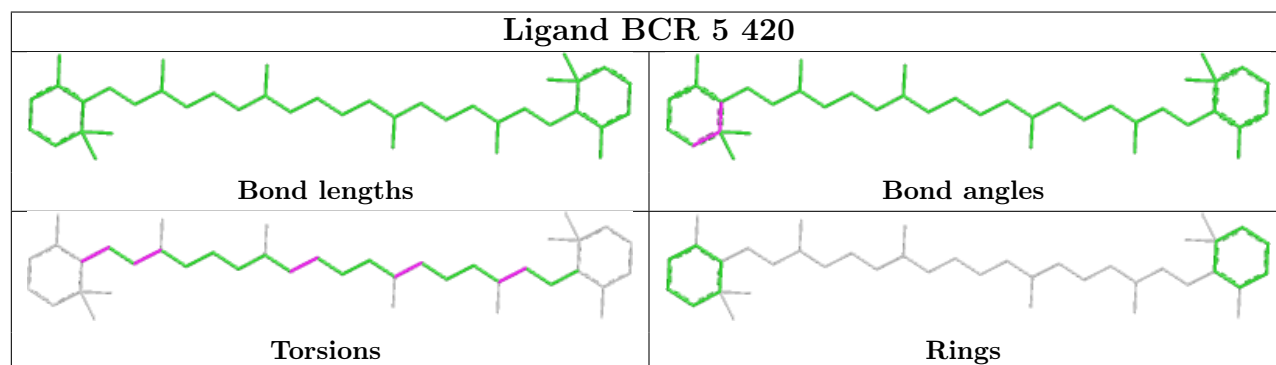
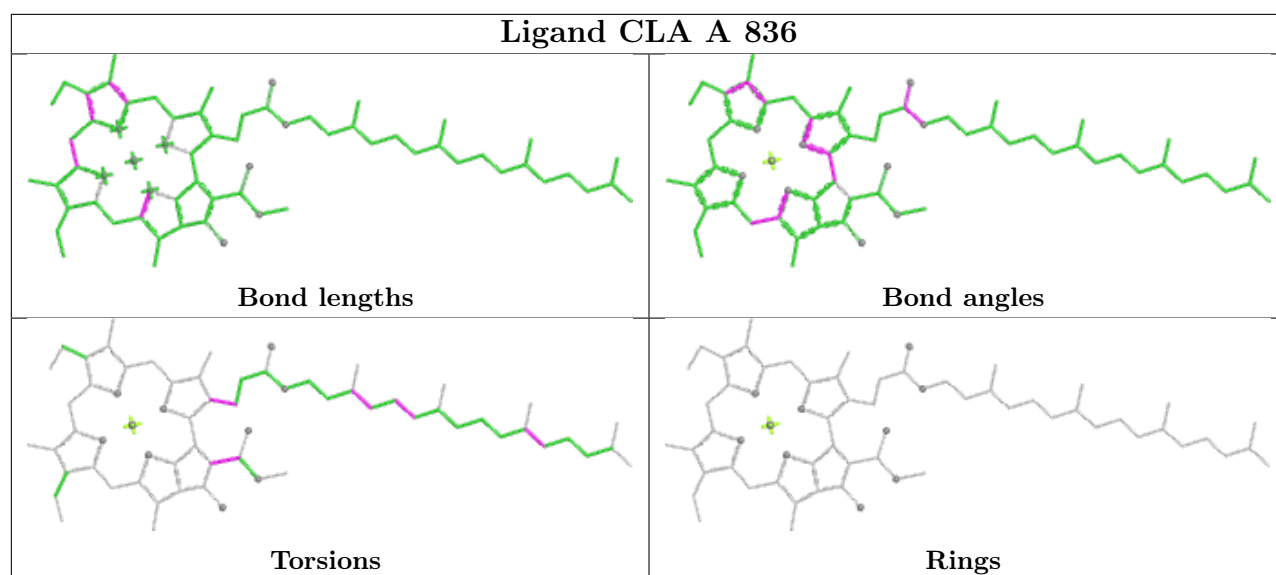


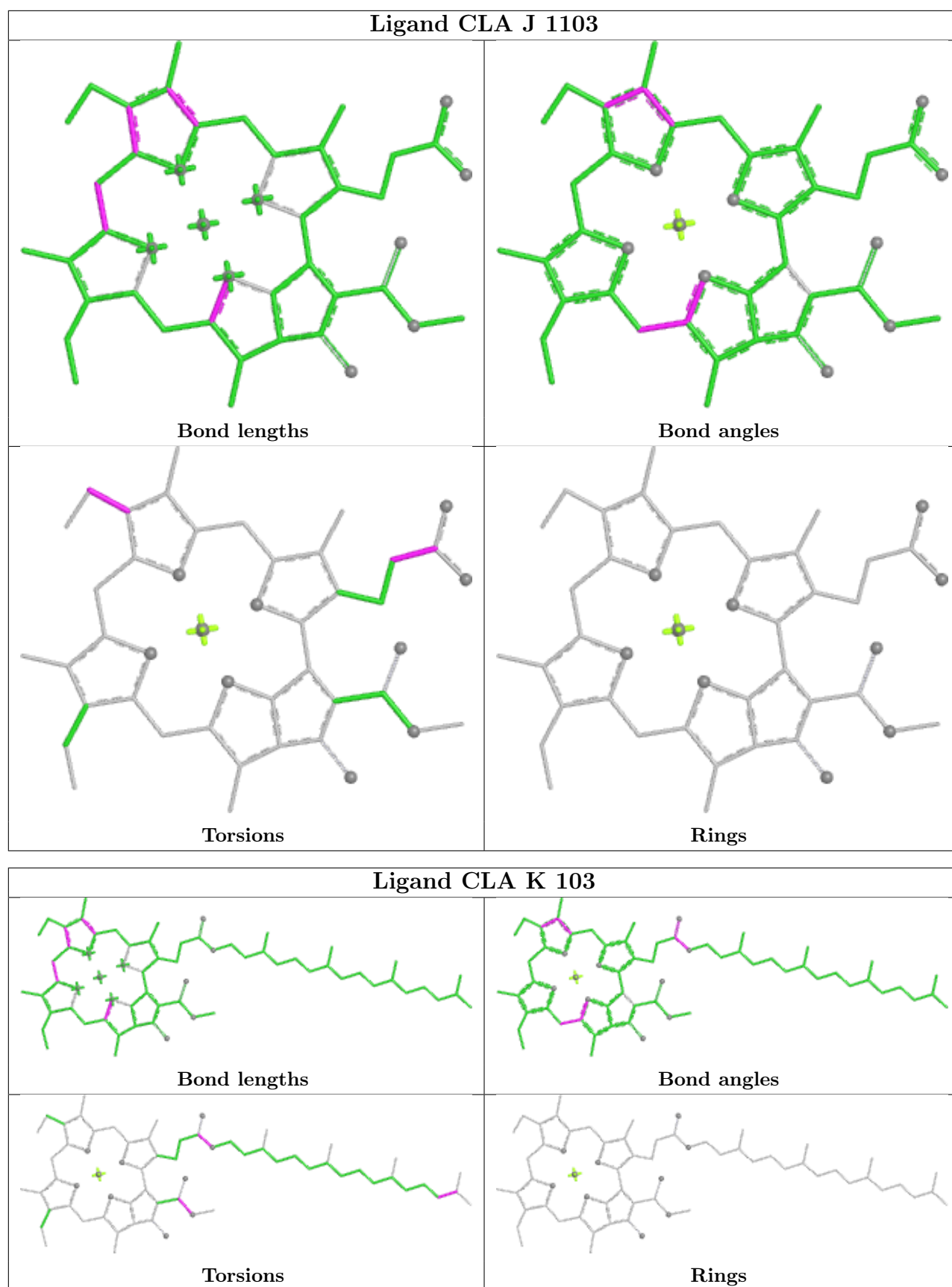
Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

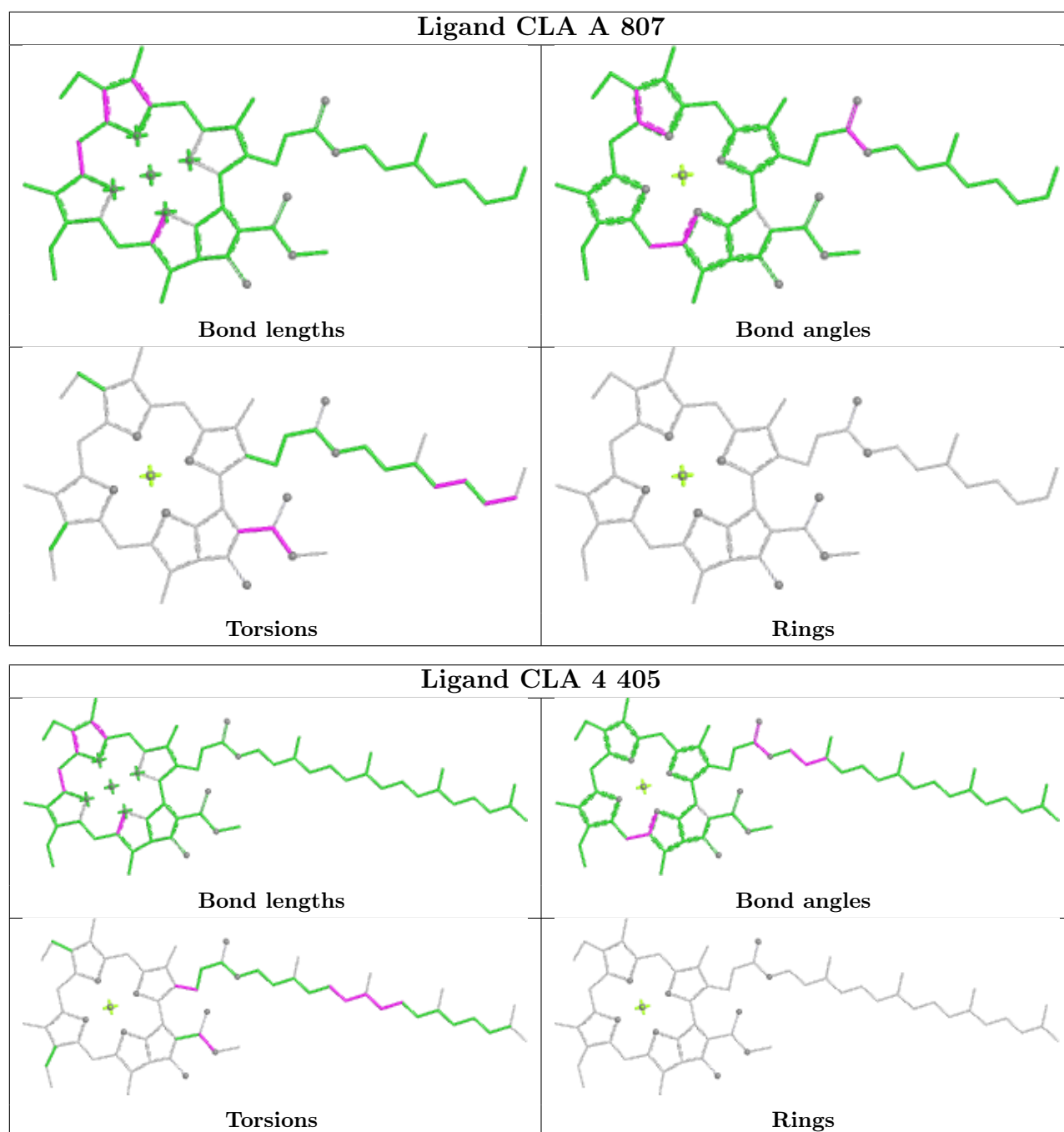
Ligand LMT B 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

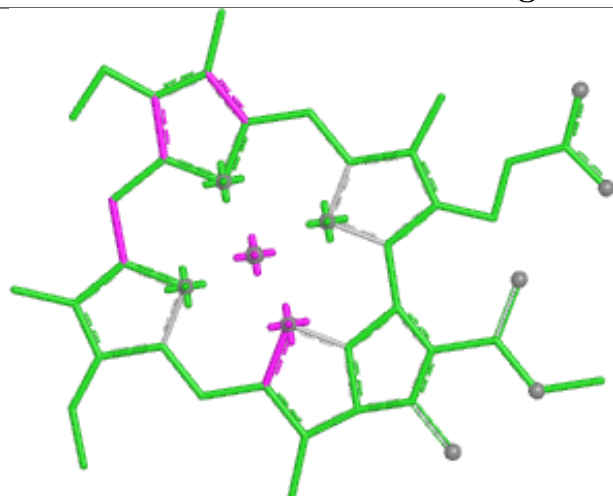




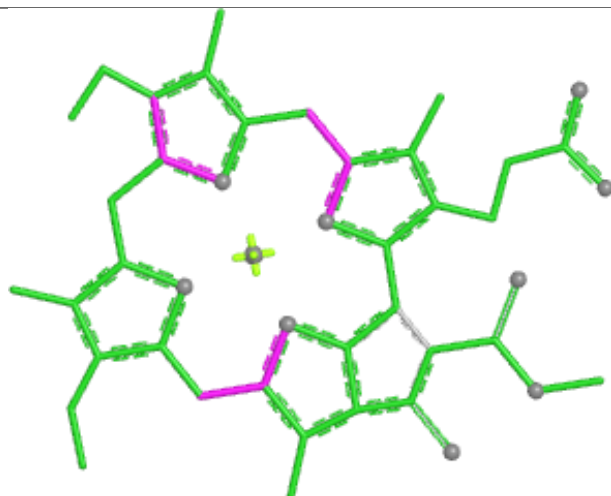




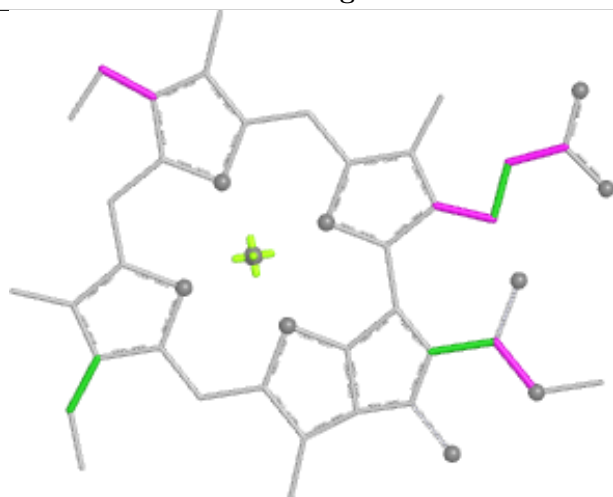
Ligand CLA 7 516



Bond lengths



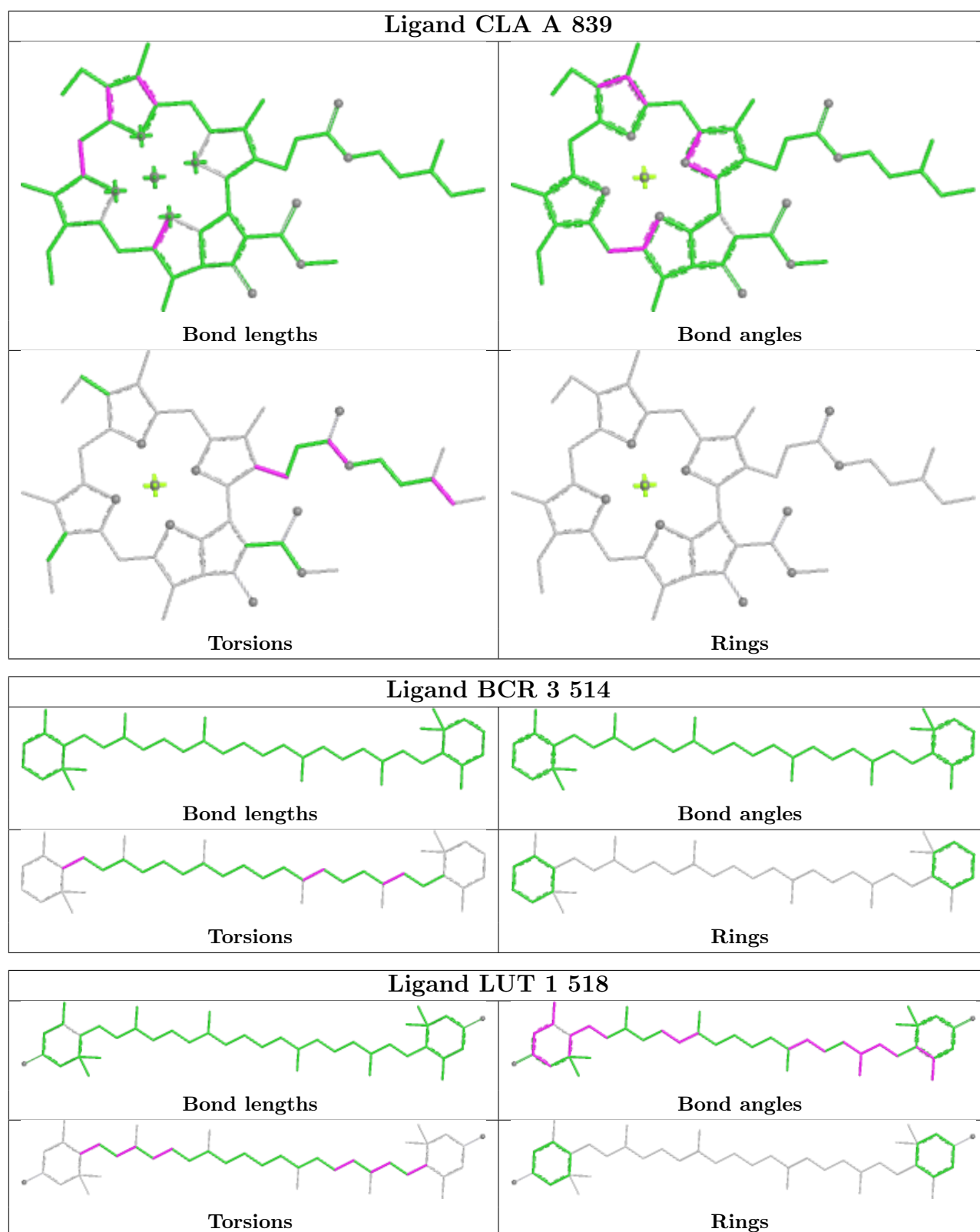
Bond angles

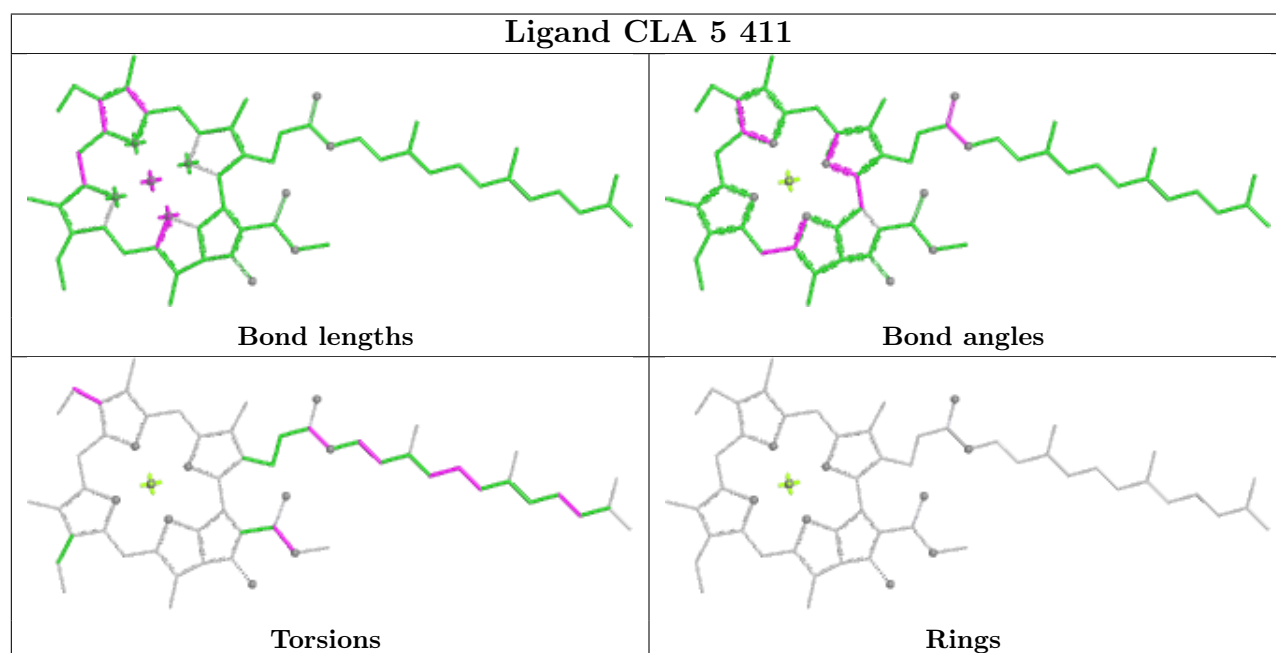
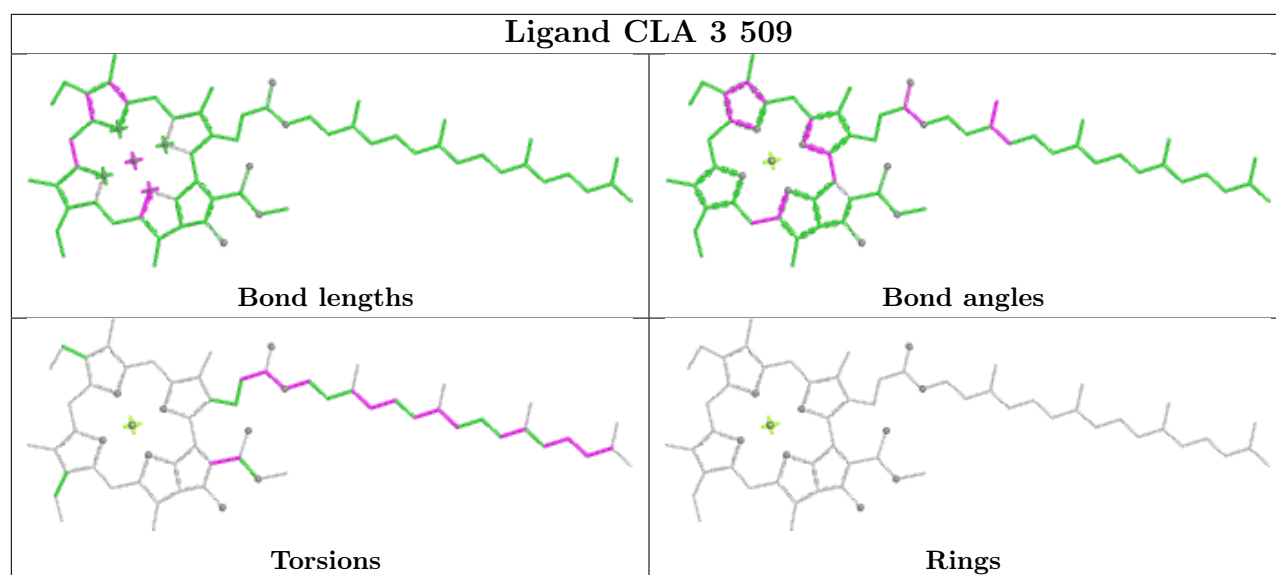


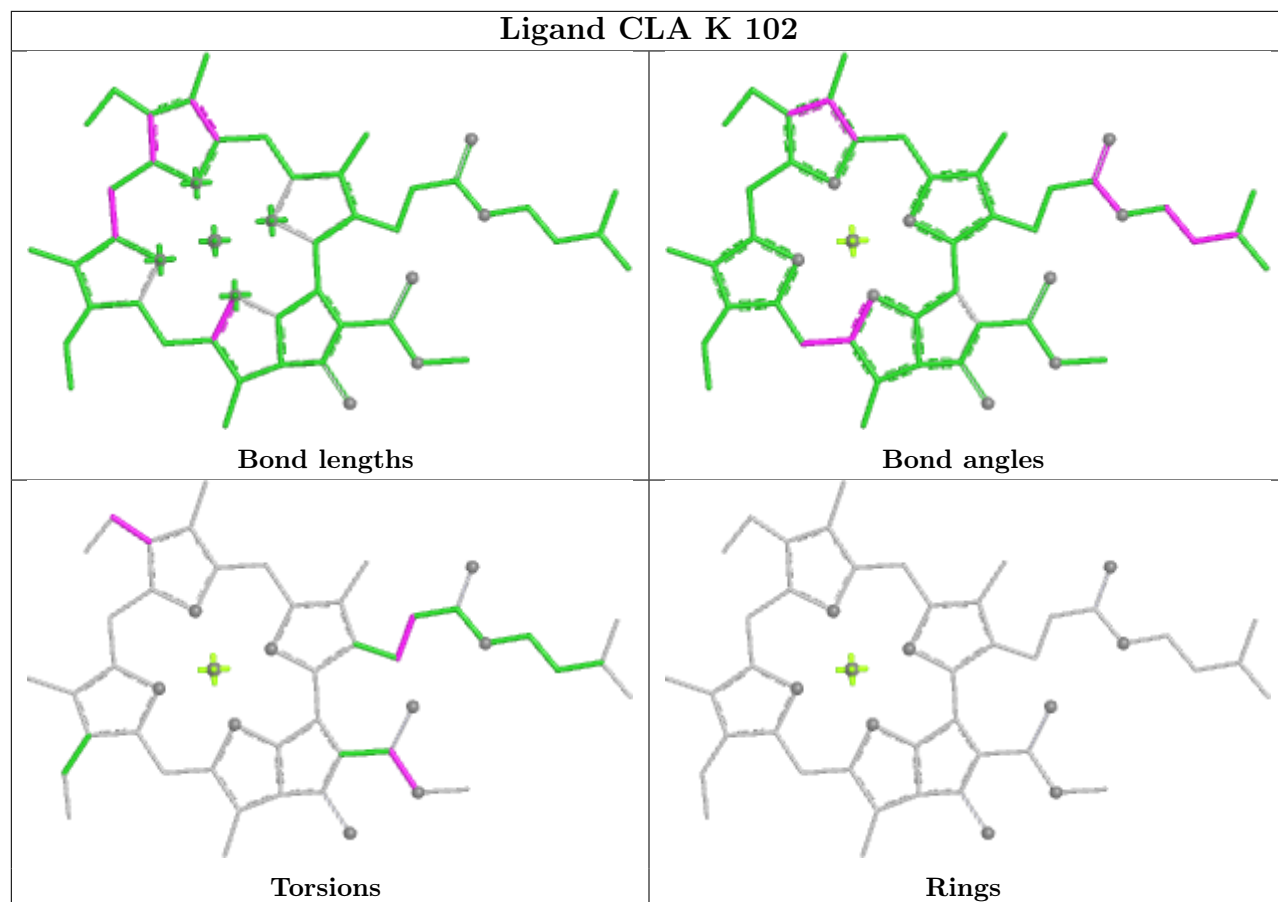
Torsions



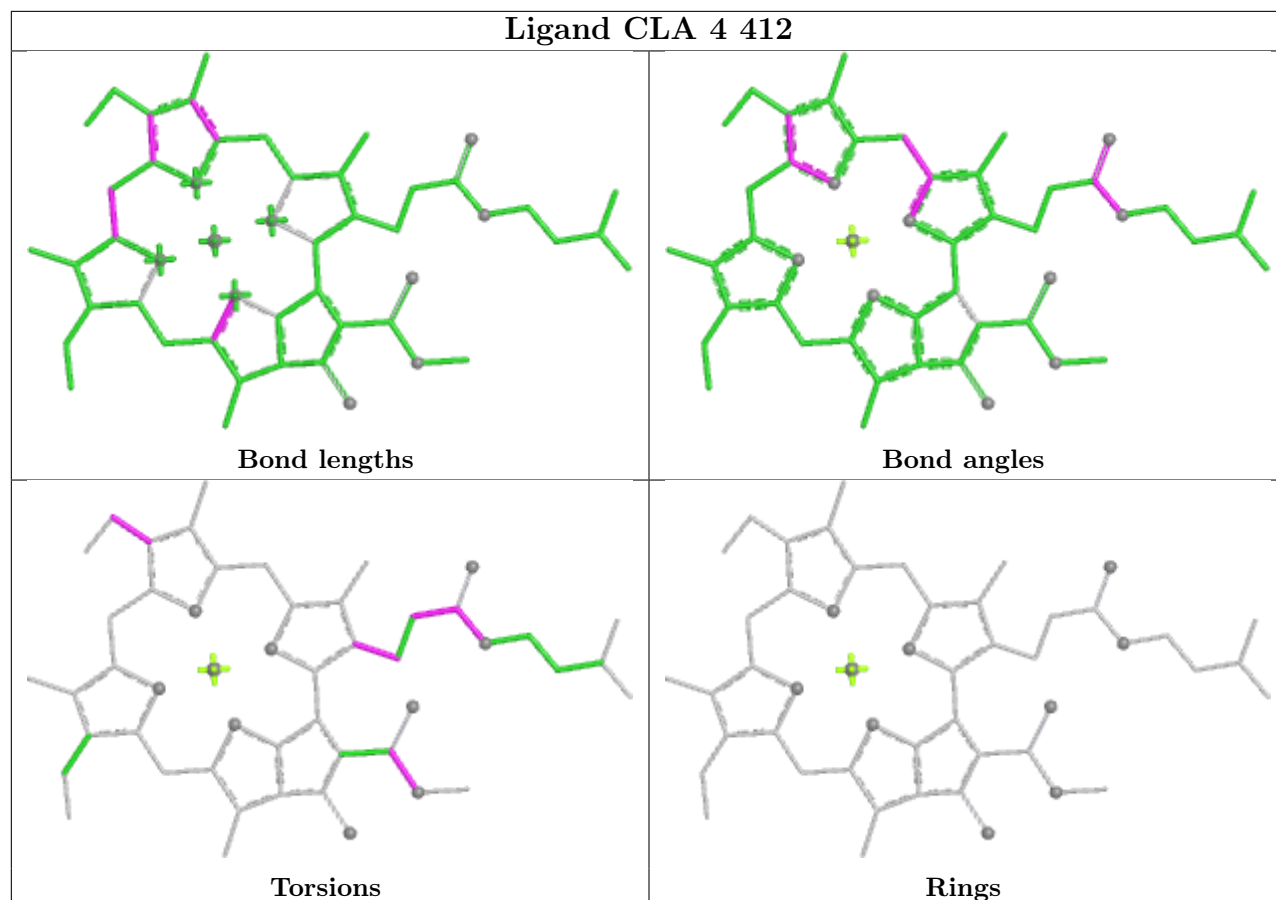
Rings



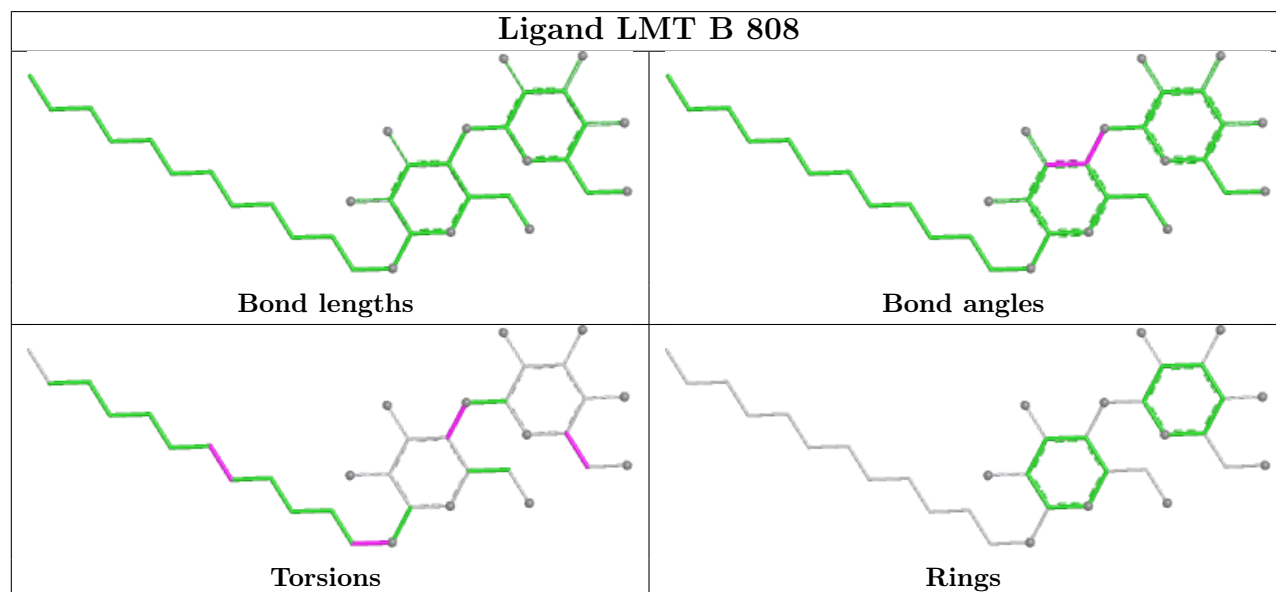


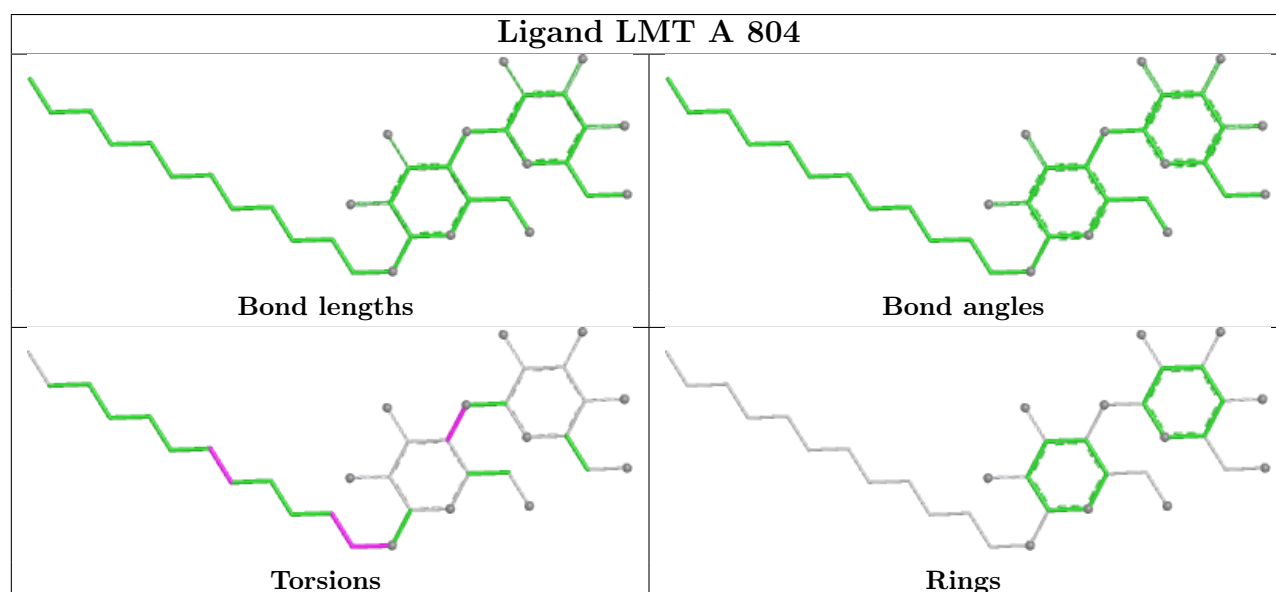
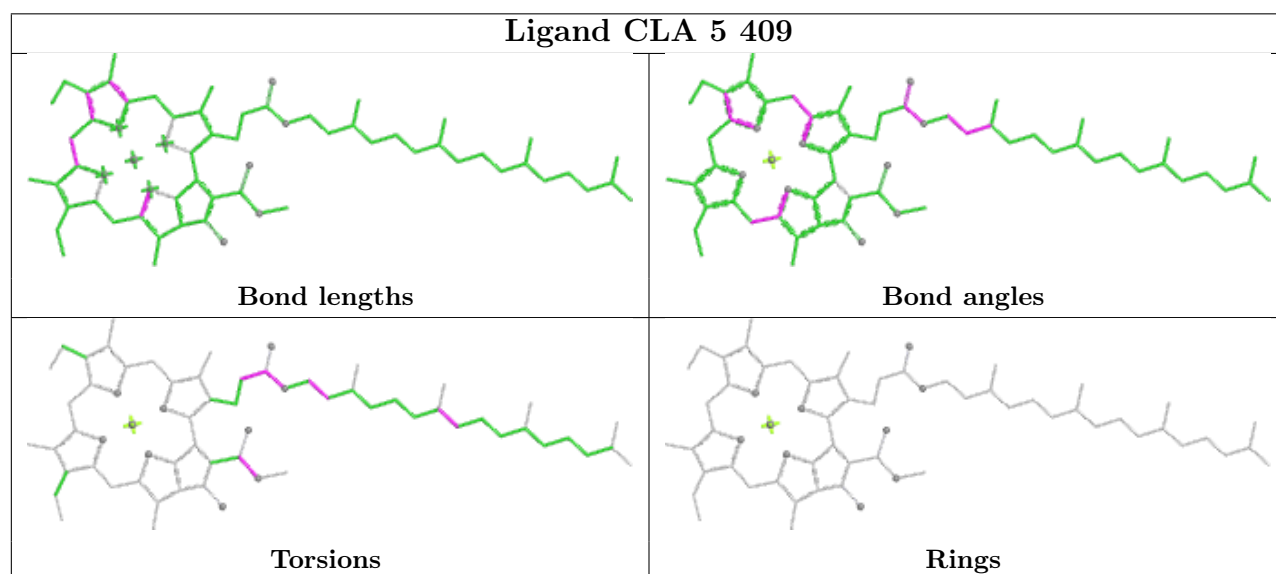
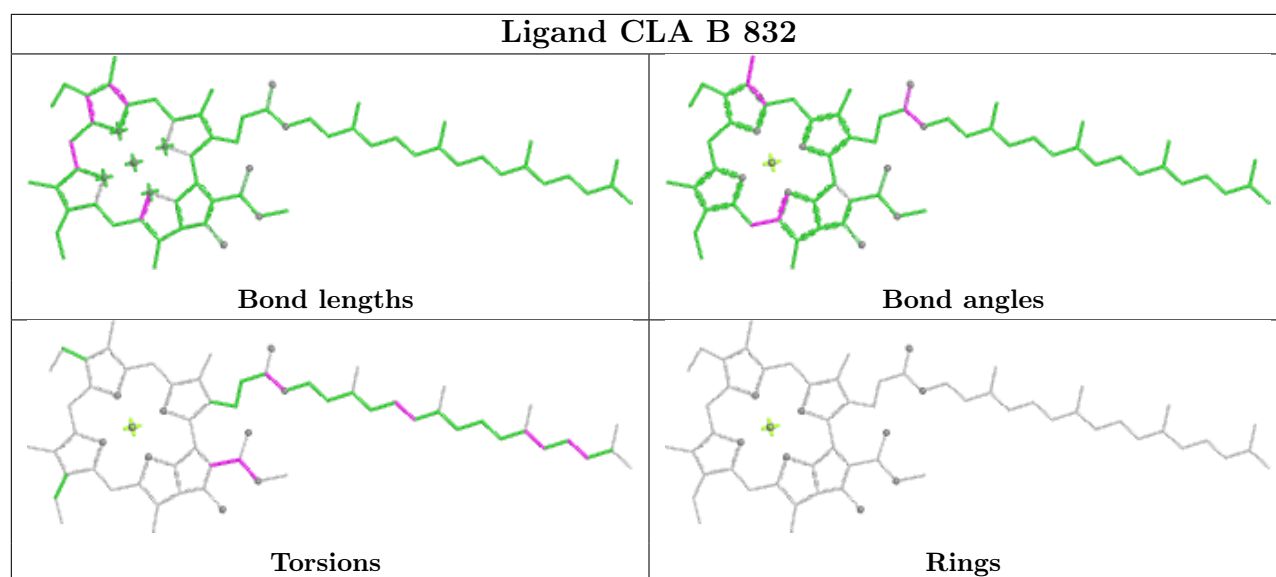


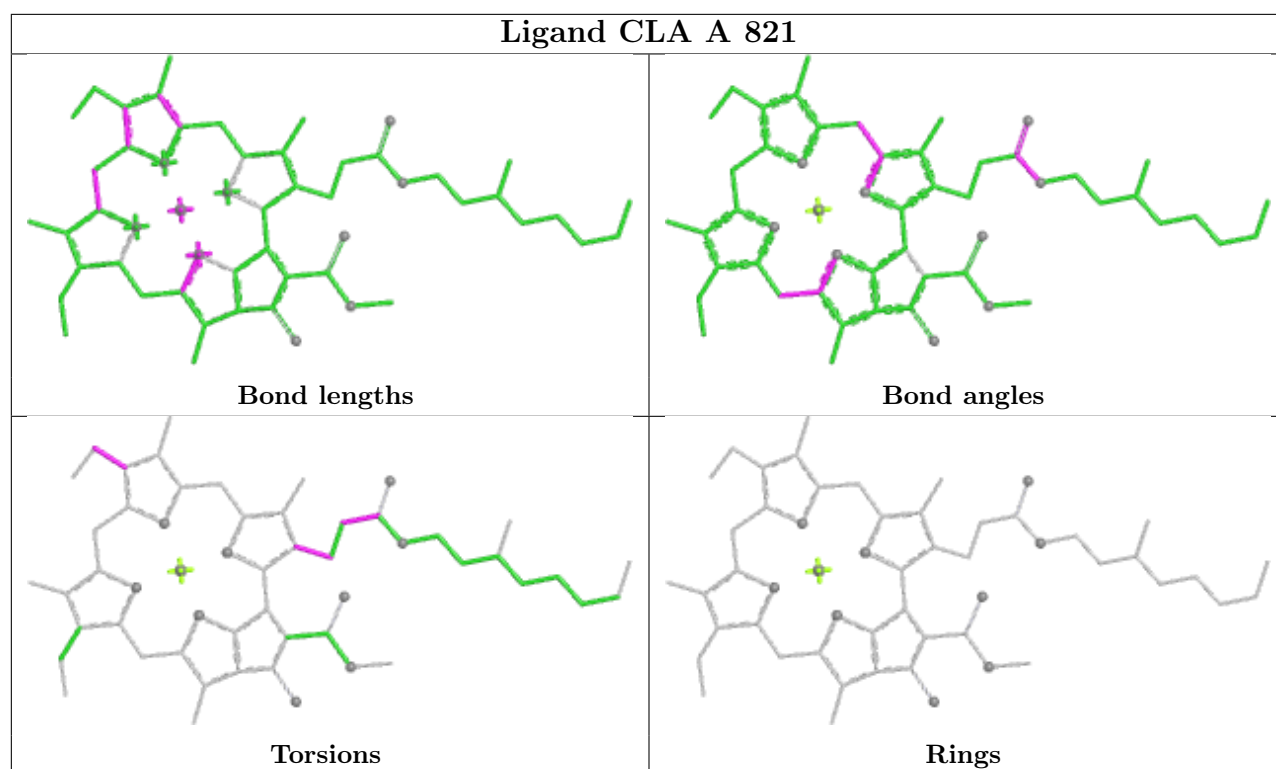
Ligand CLA 4 412



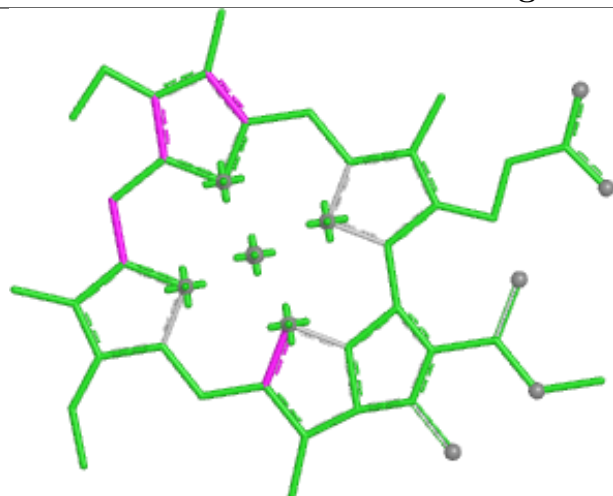
Ligand LMT B 808



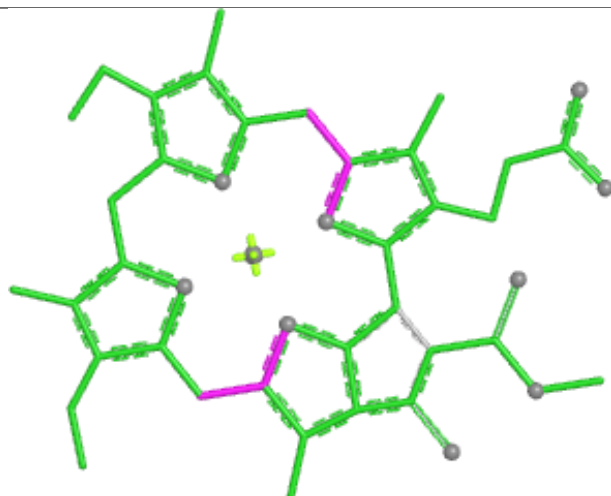




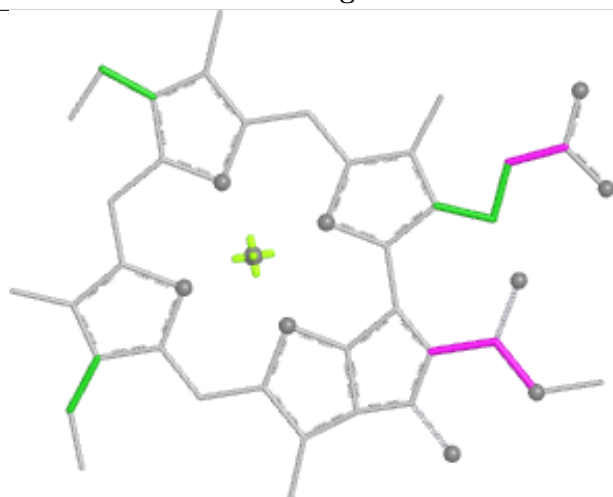
Ligand CLA 7 504



Bond lengths



Bond angles

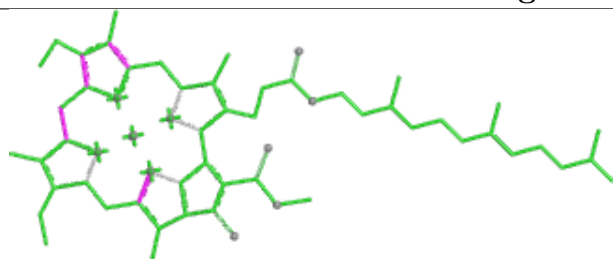


Torsions

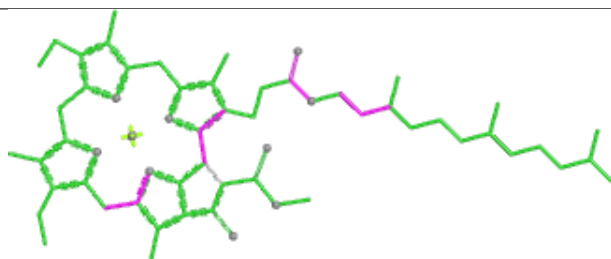


Rings

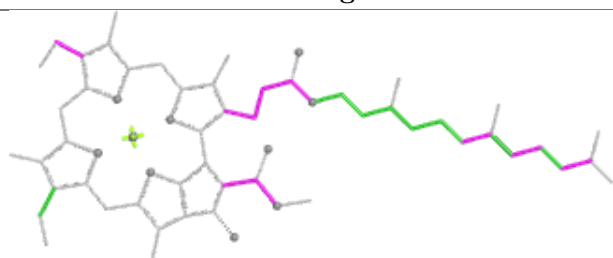
Ligand CLA 2 413



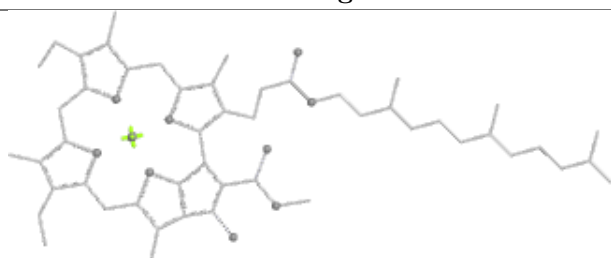
Bond lengths



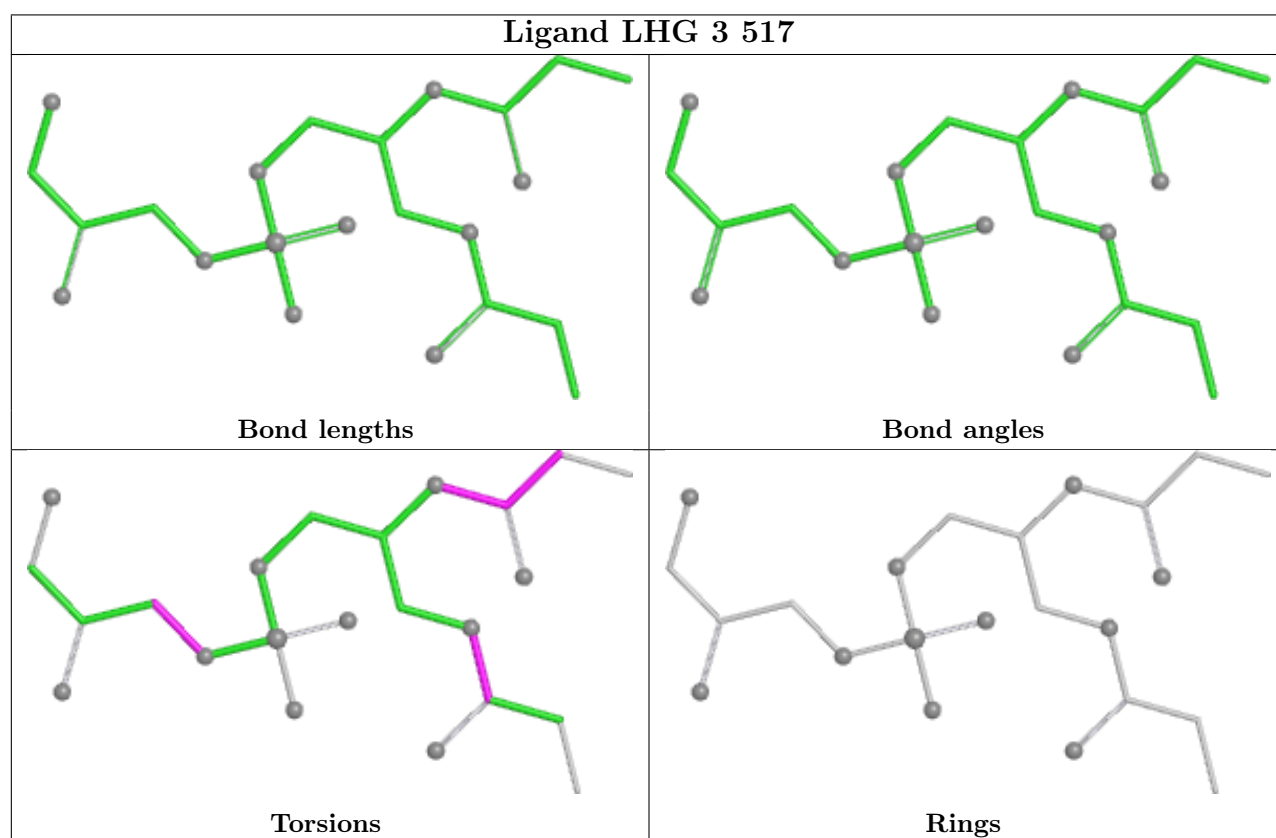
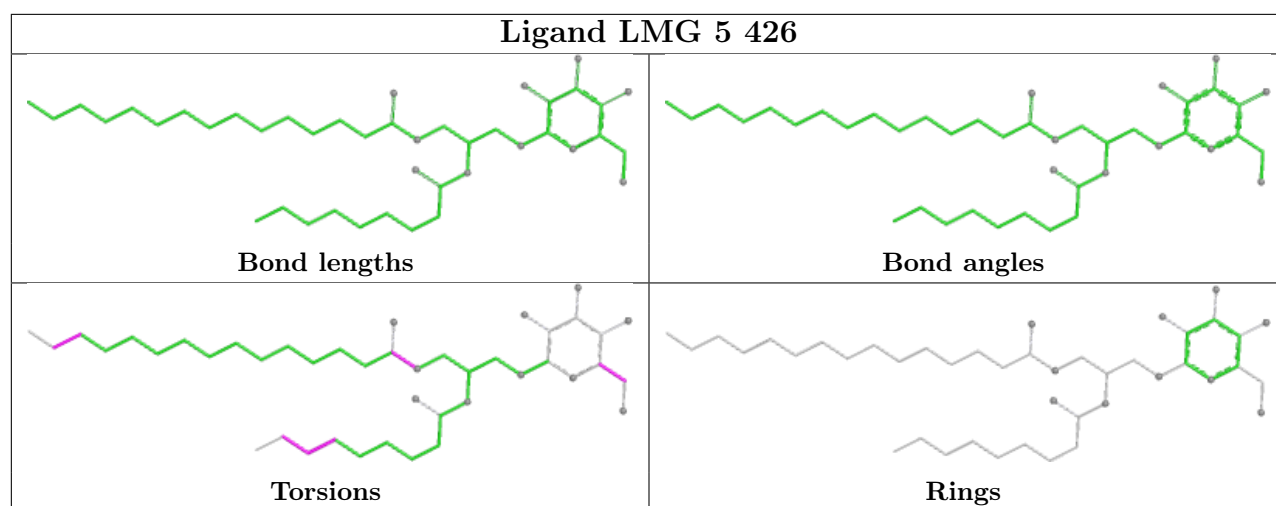
Bond angles

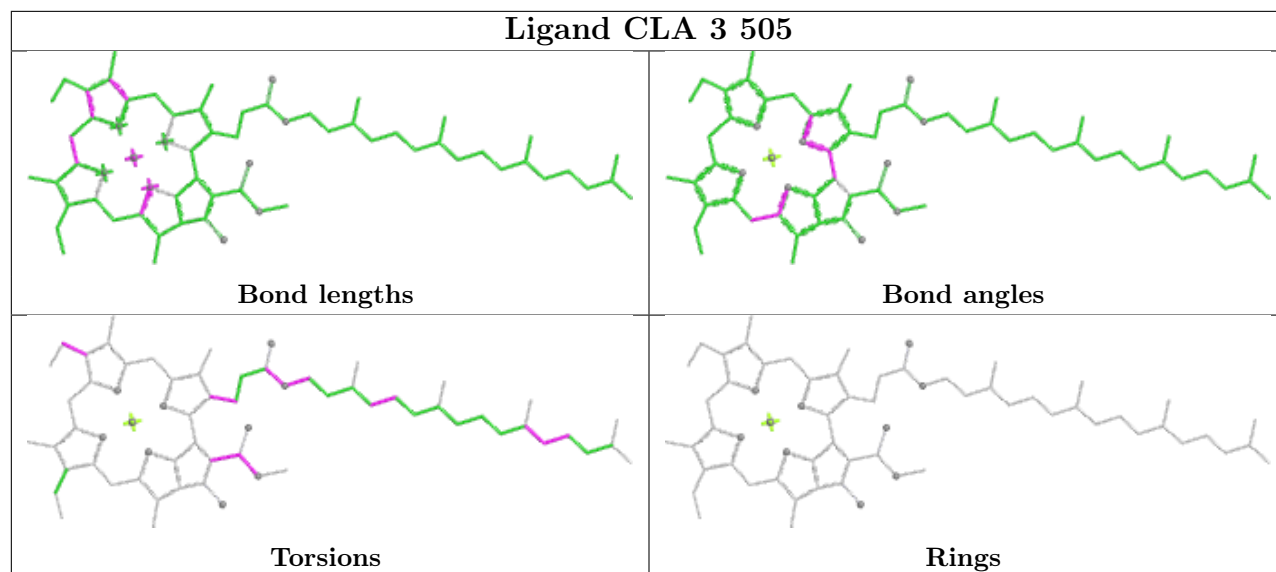
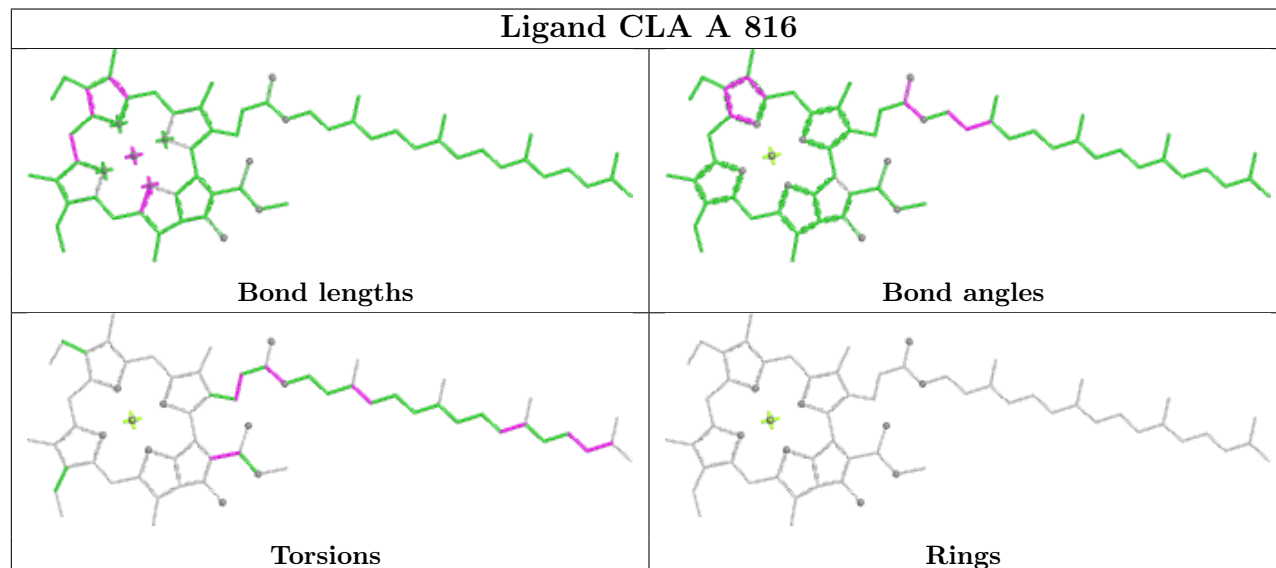


Torsions

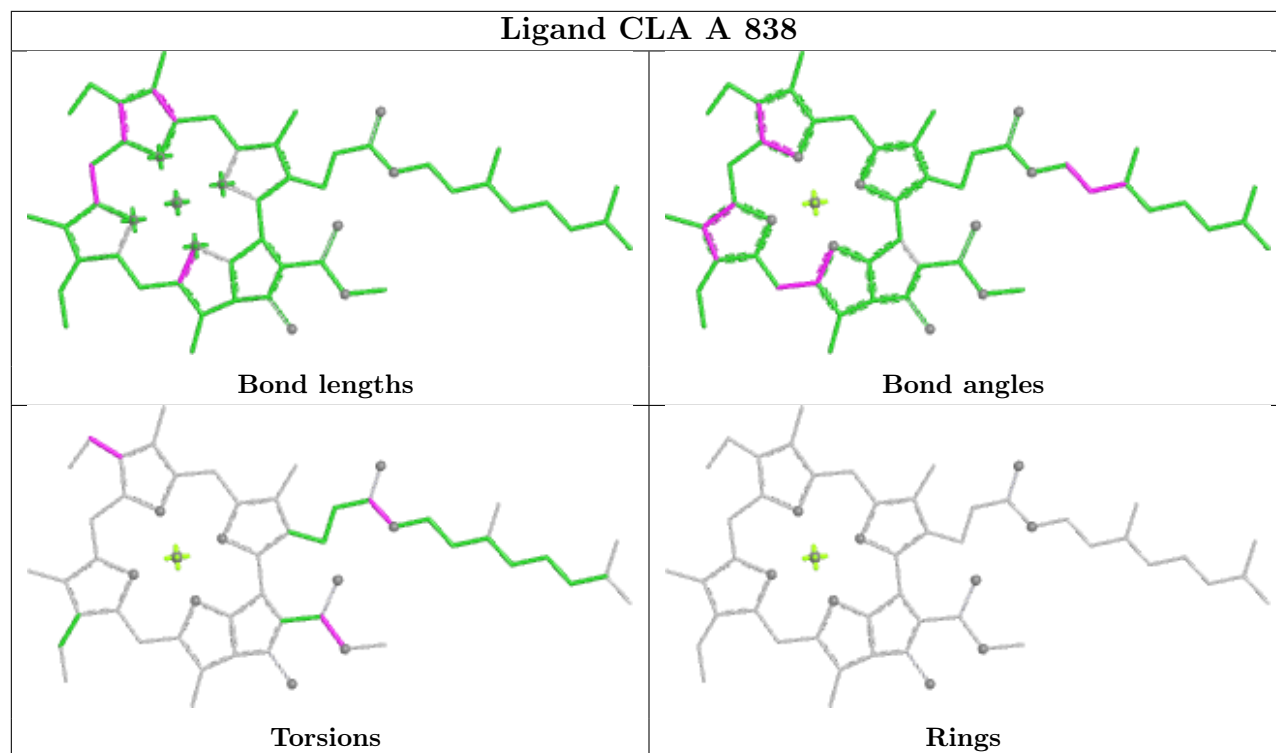


Rings

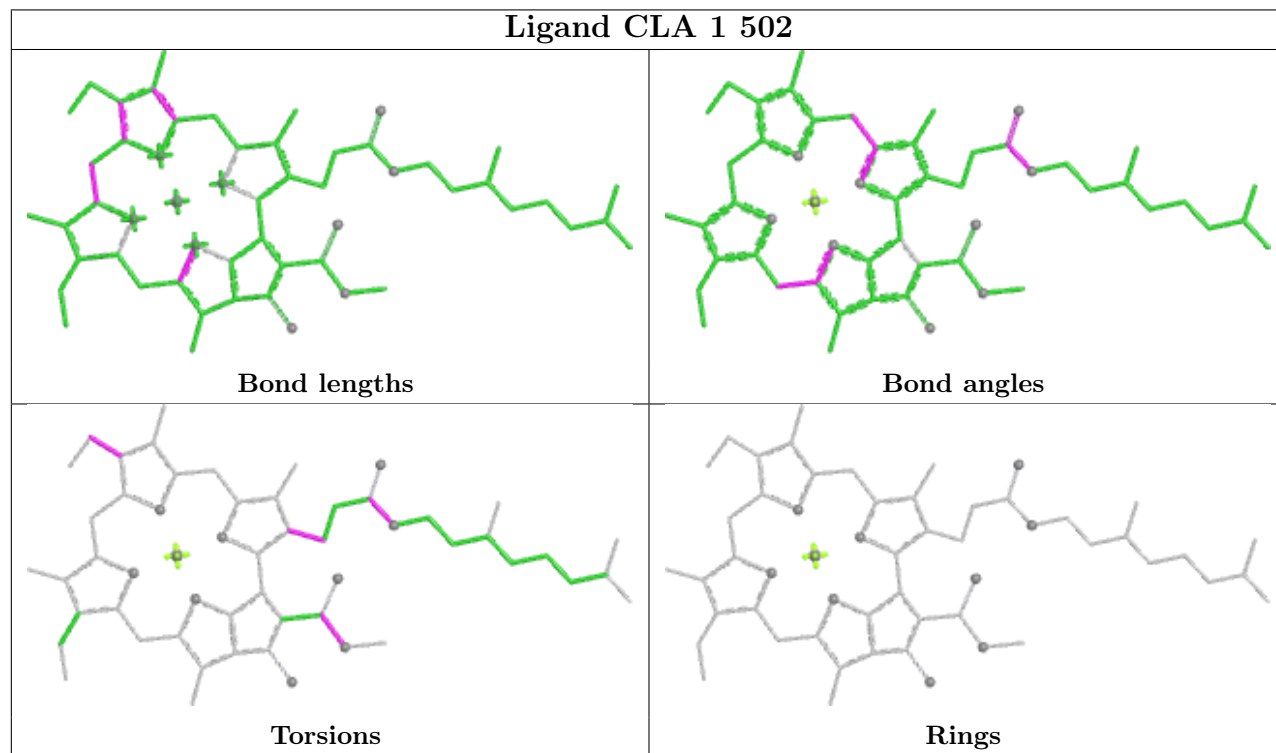


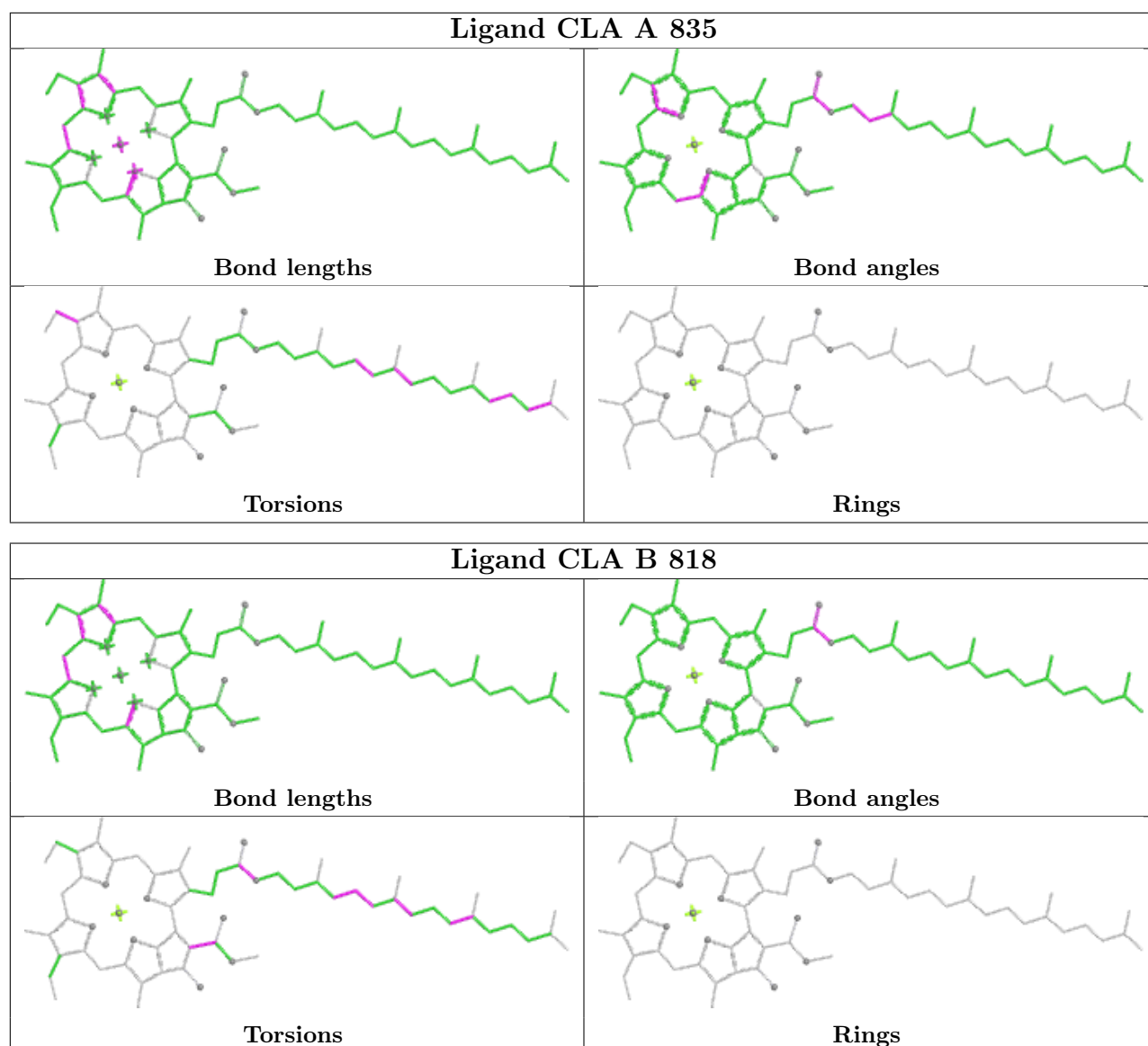
Ligand CLA 3 505**Ligand CLA A 816**

Ligand CLA A 838

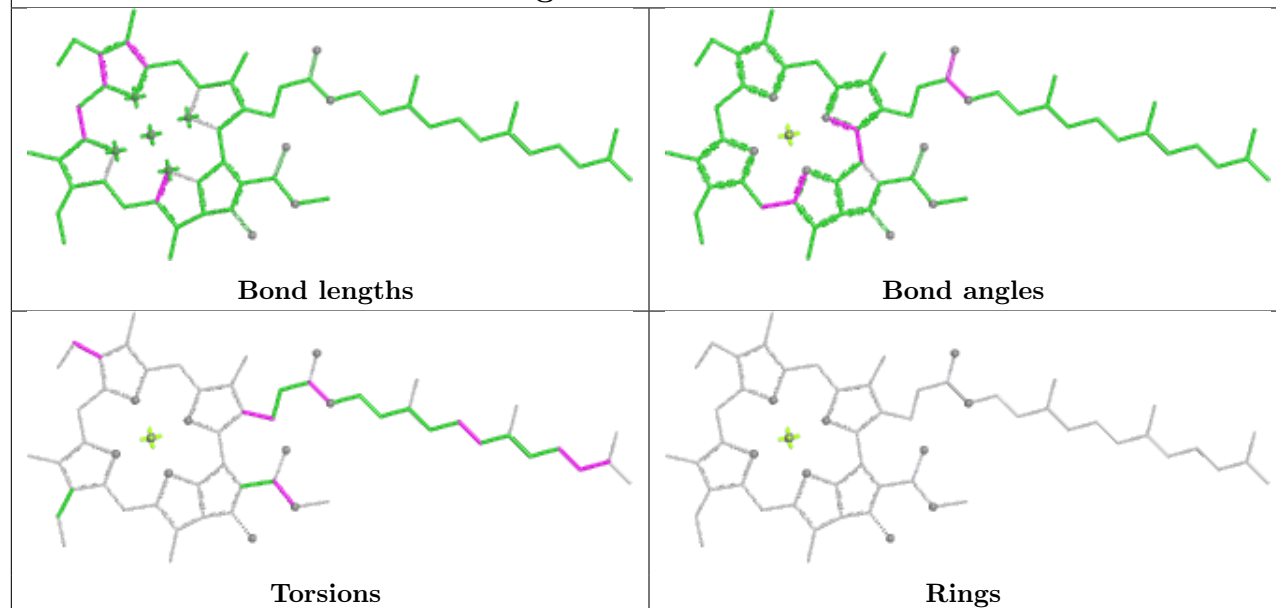


Ligand CLA 1 502

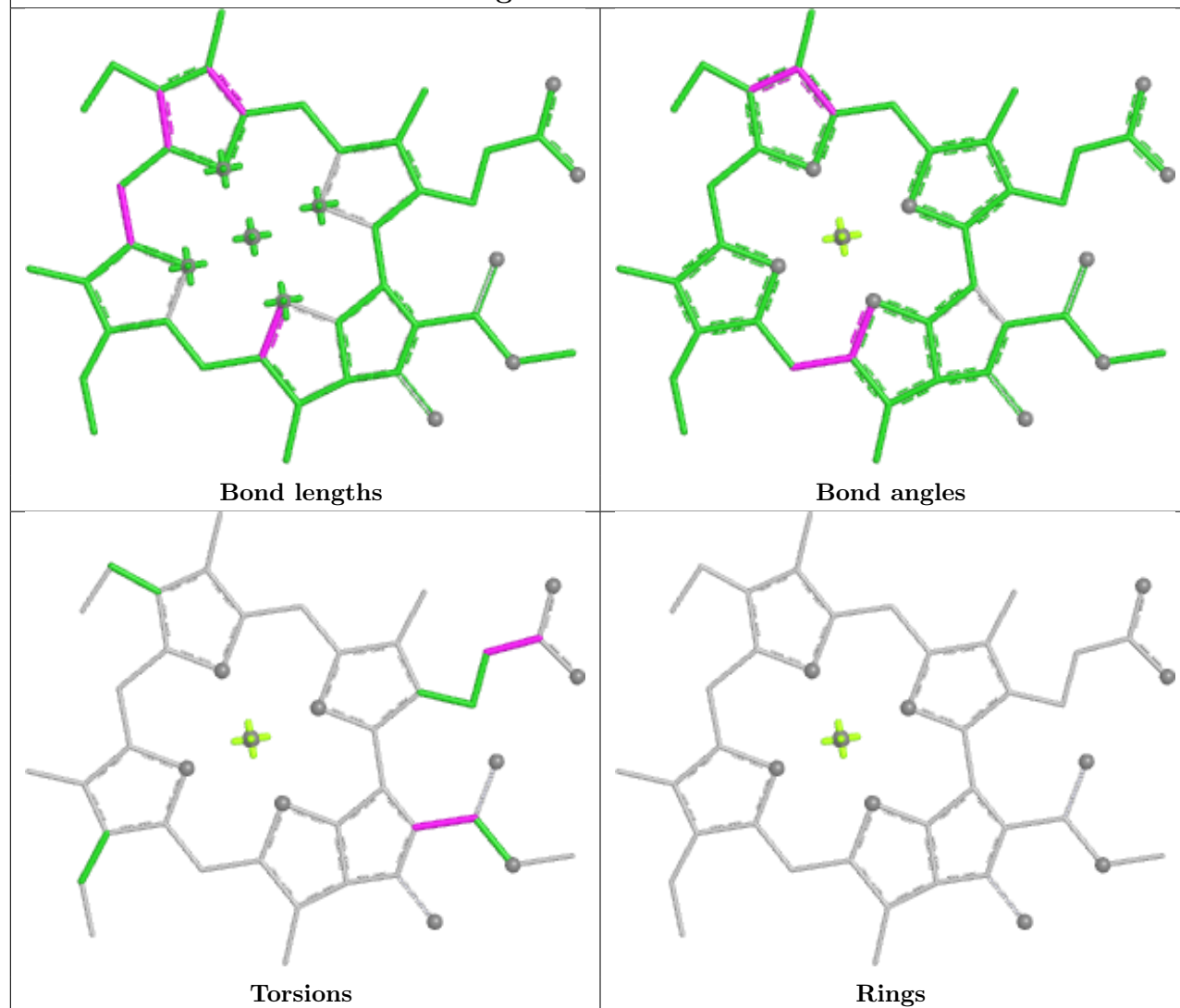


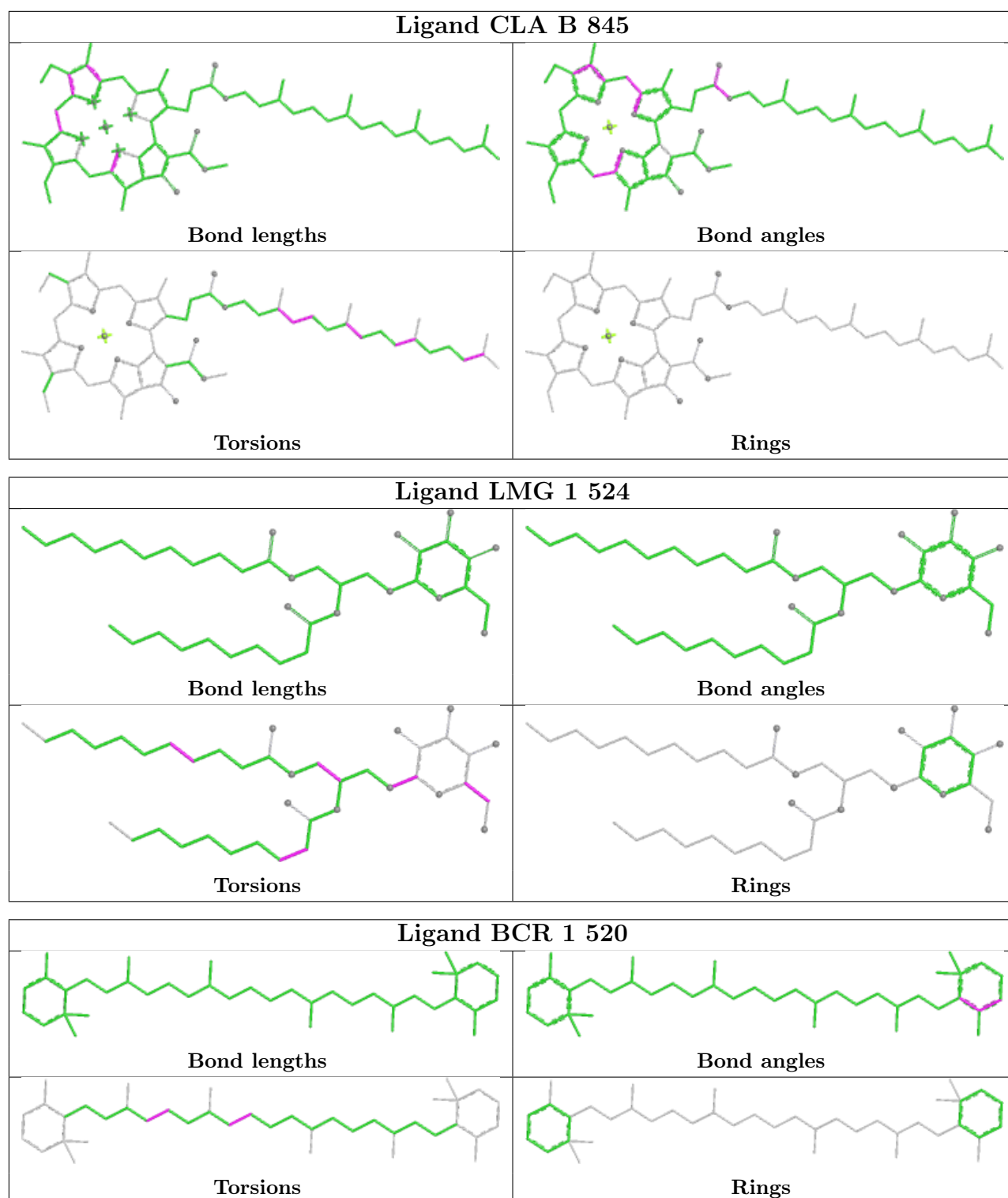


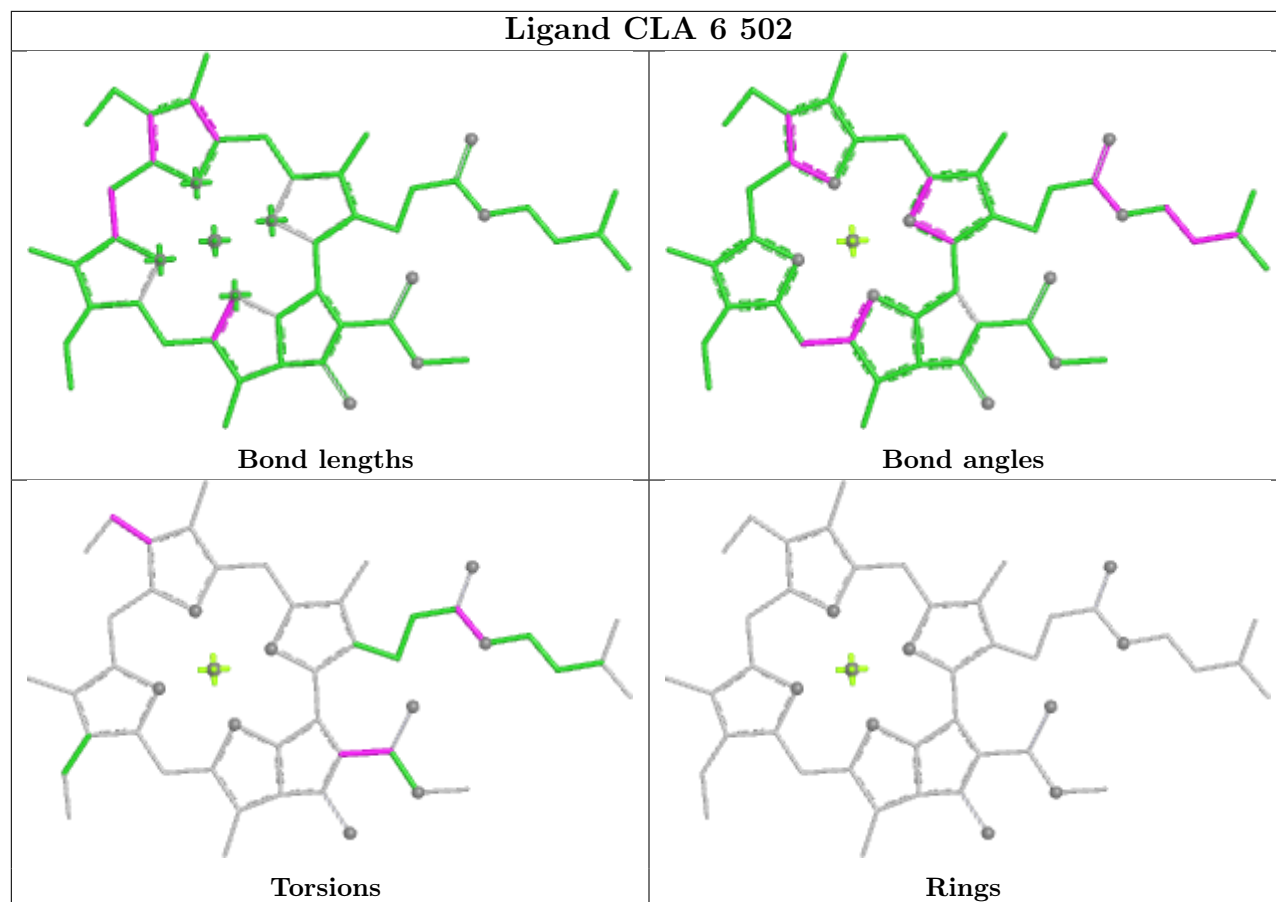
Ligand CLA 1 509



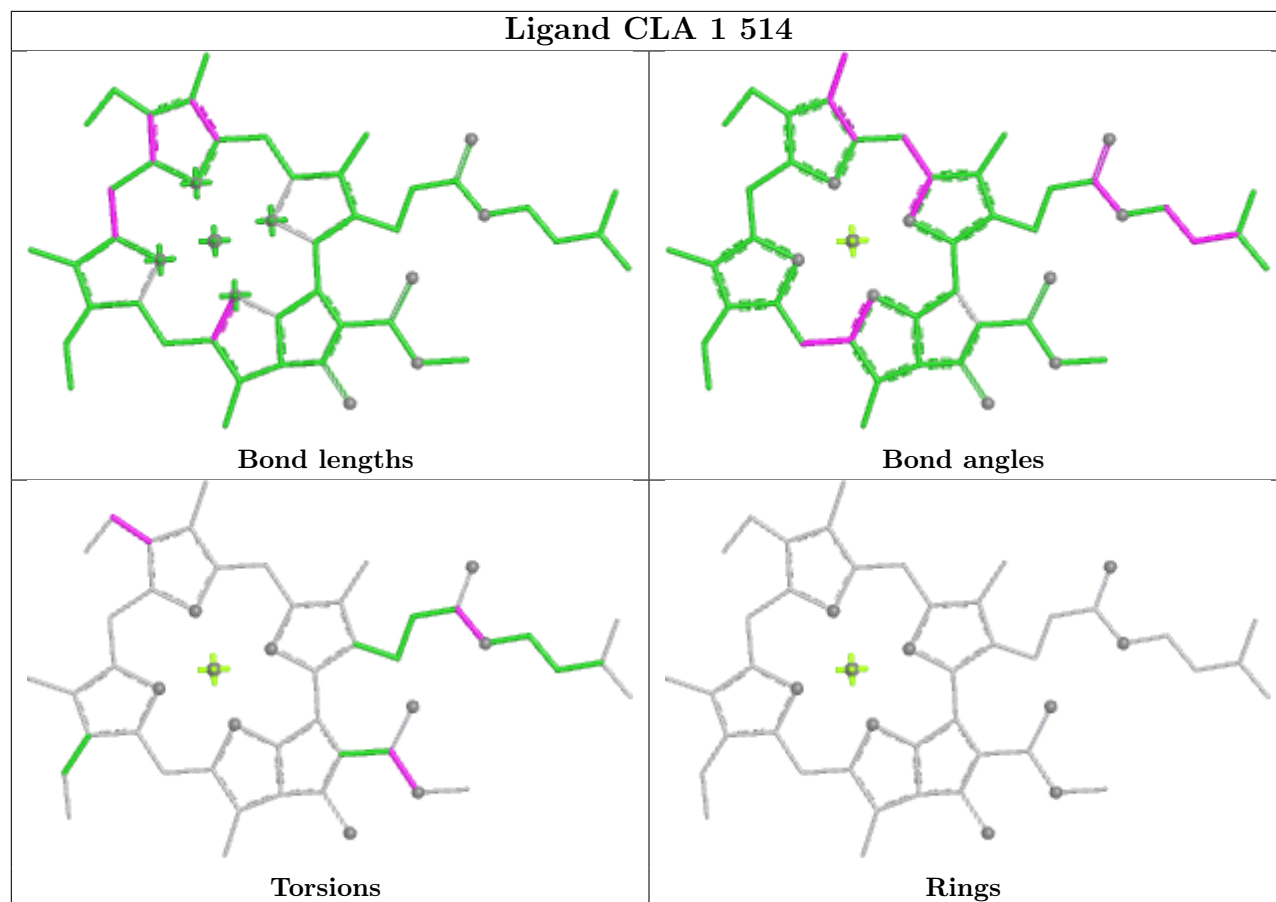
Ligand CLA 2 415



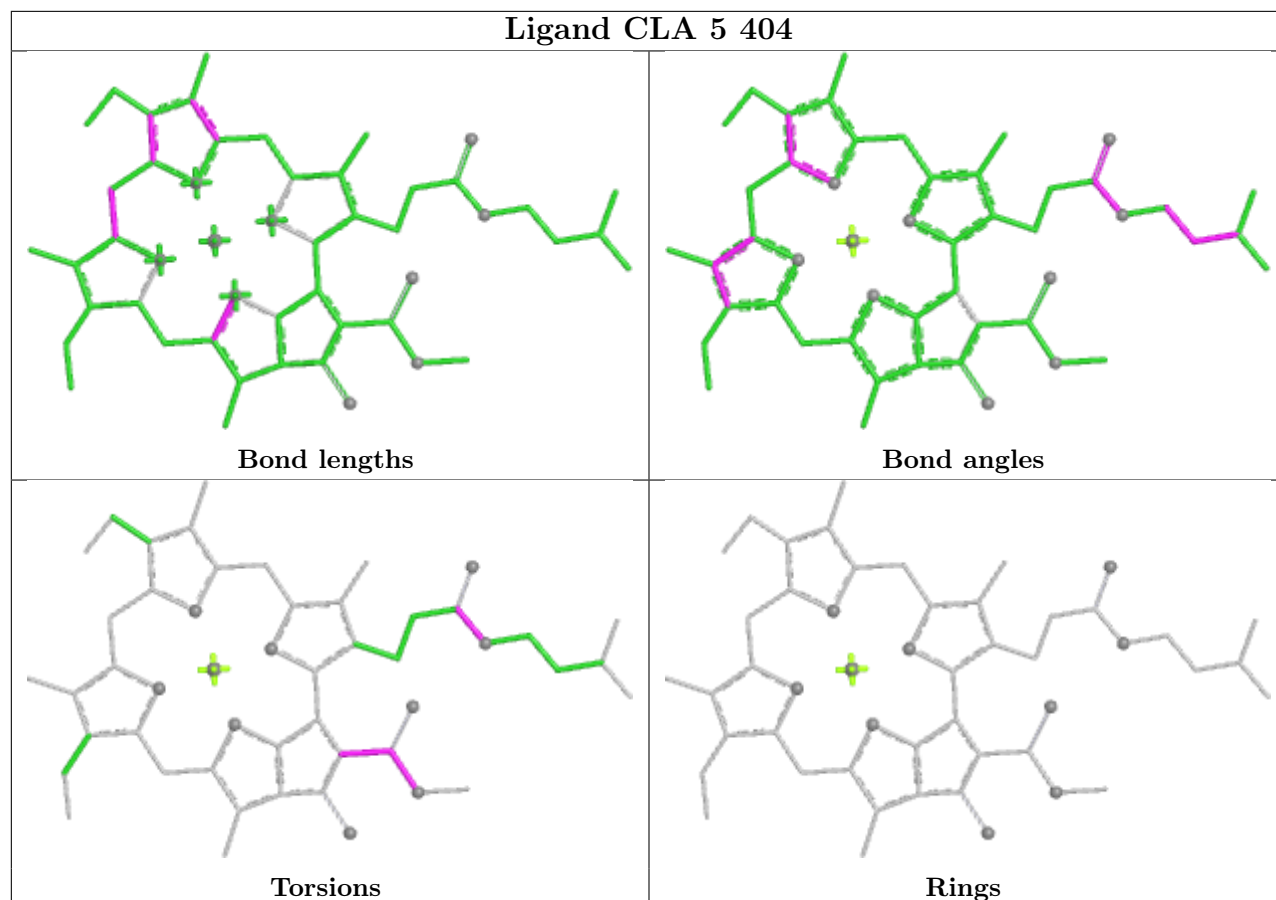




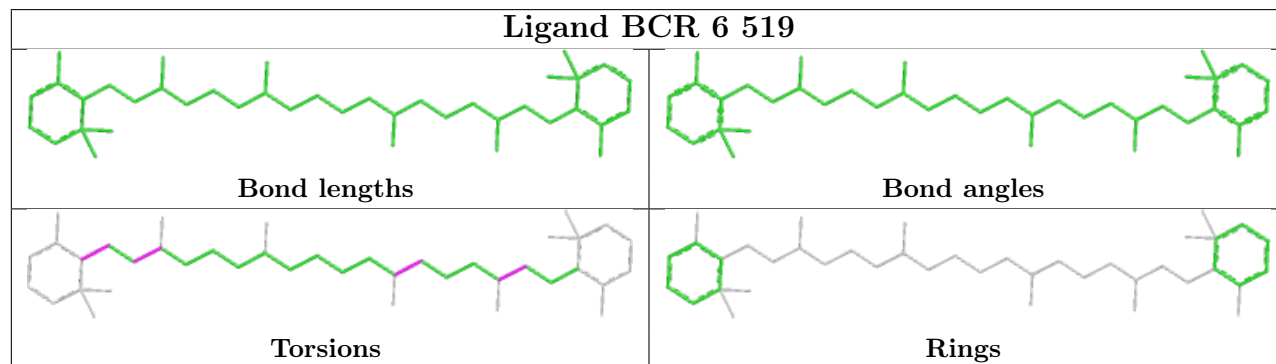
Ligand CLA 1 514

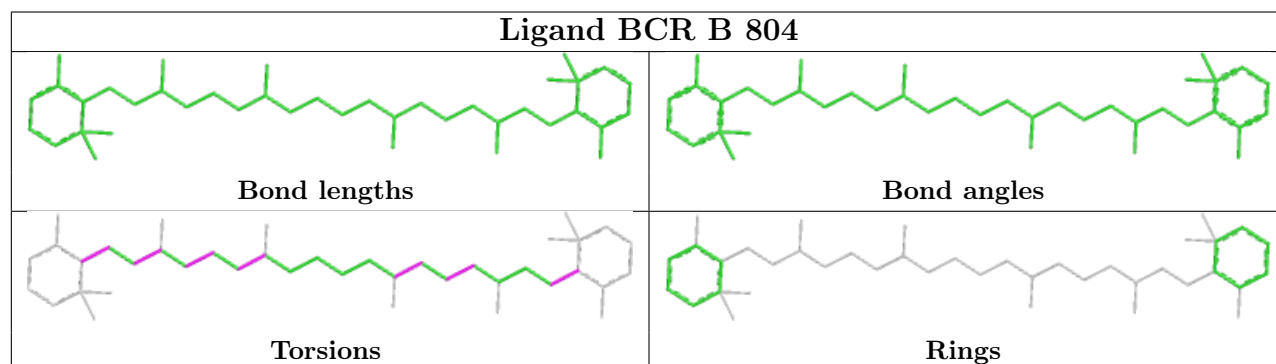
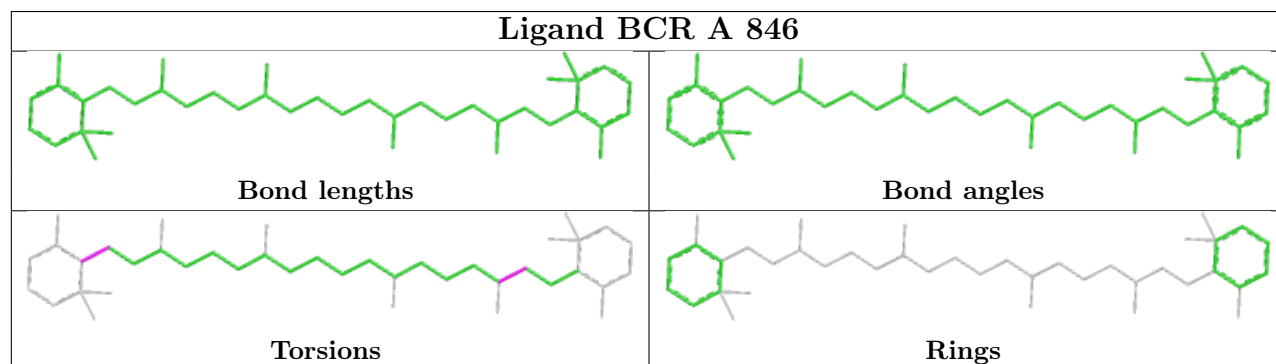
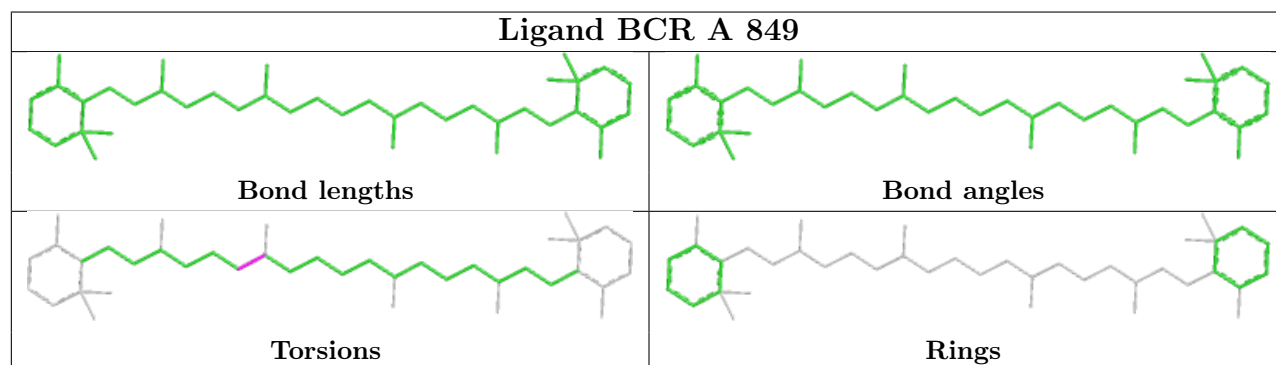
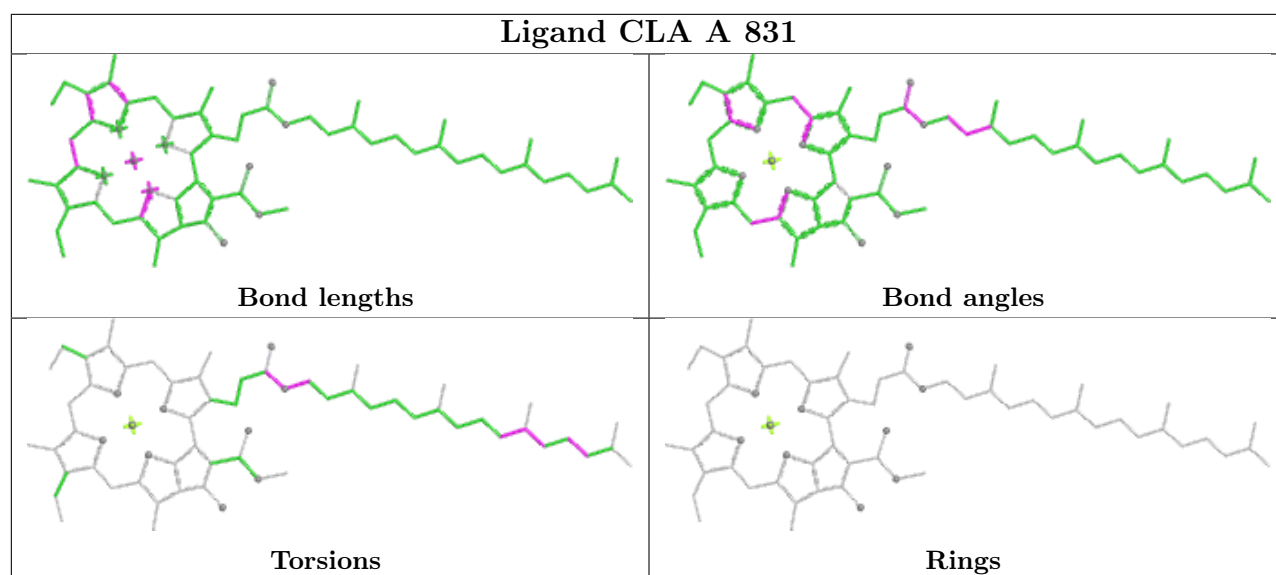


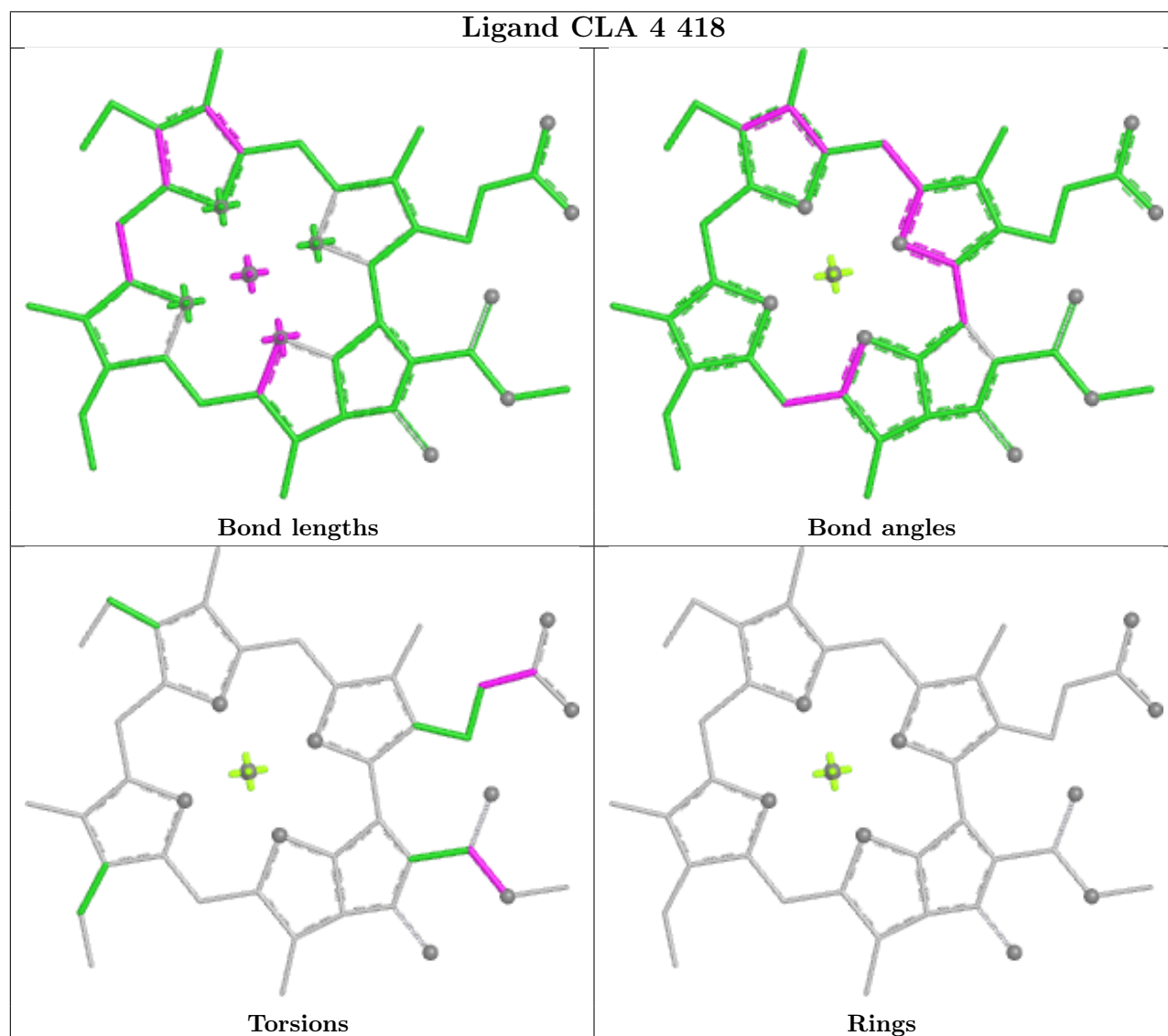
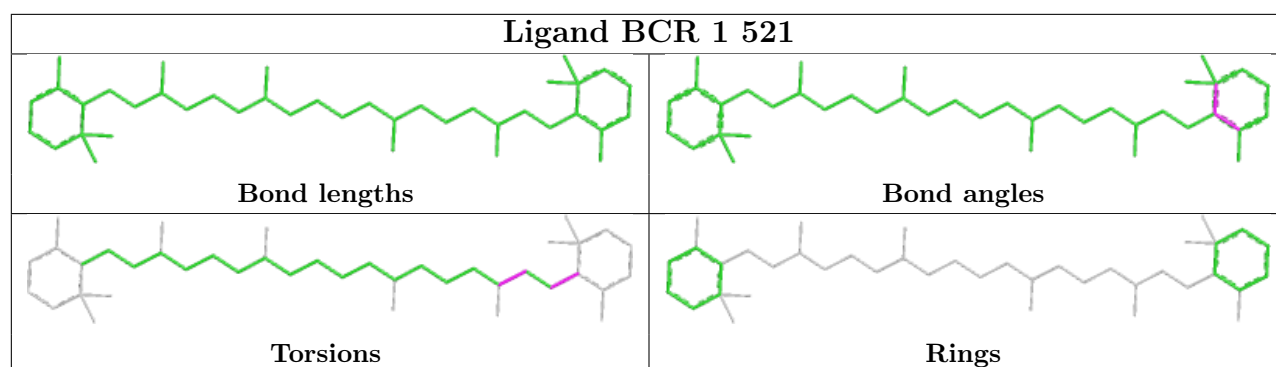
Ligand CLA 5 404

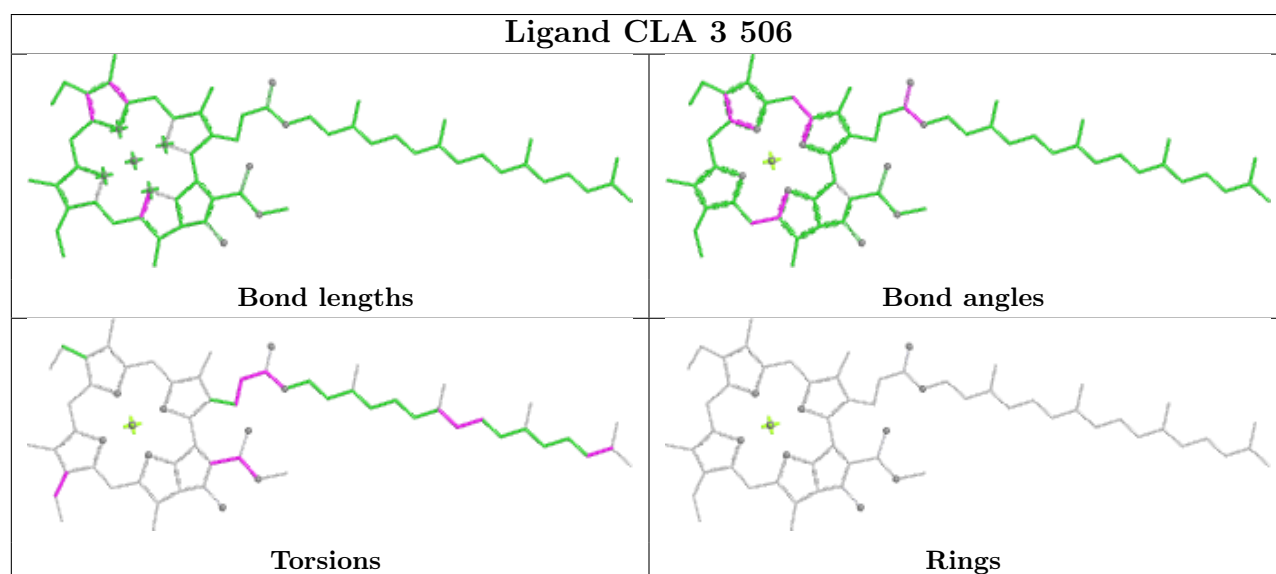
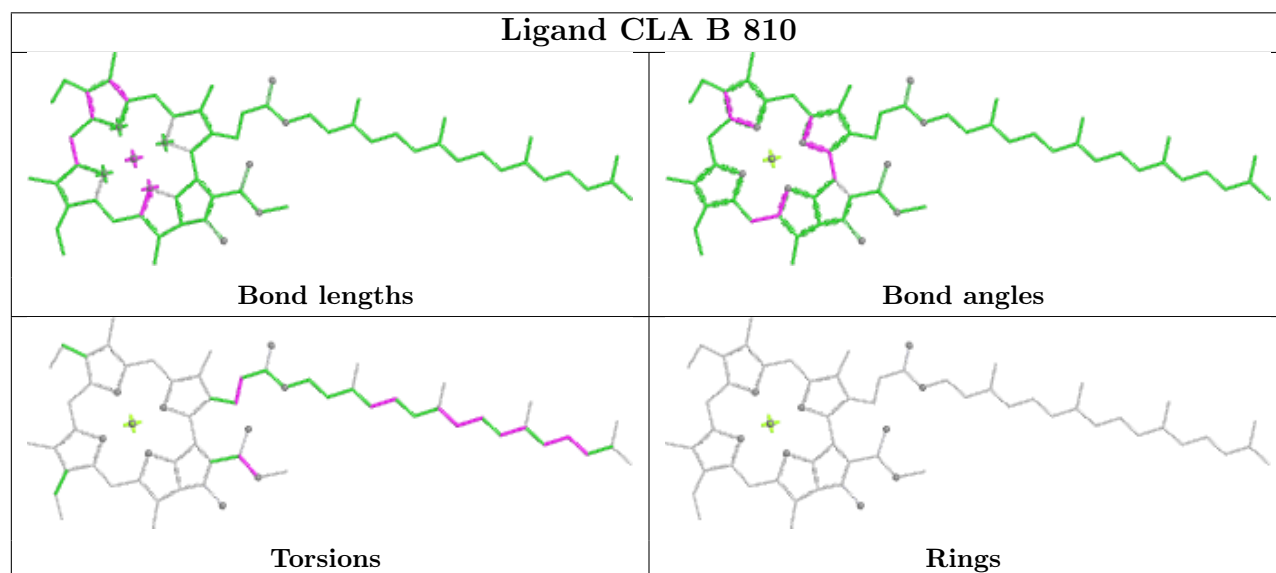
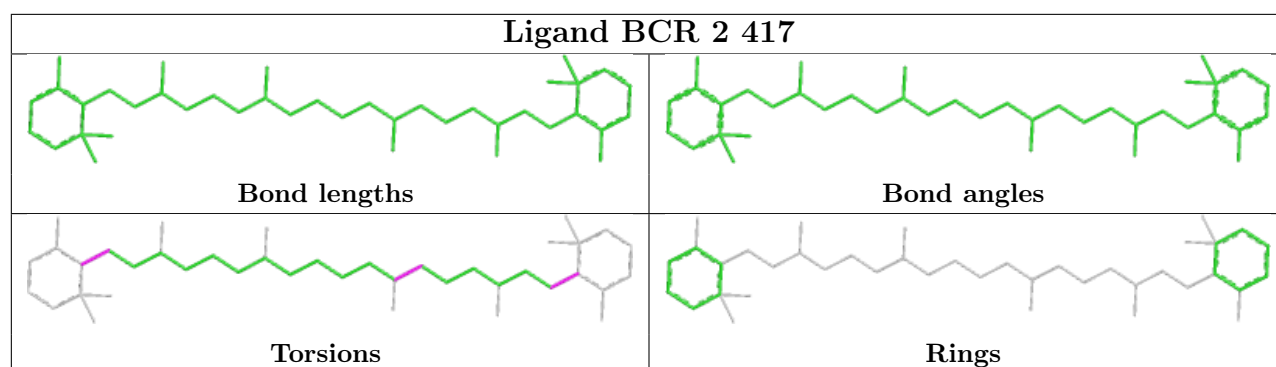


Ligand BCR 6 519

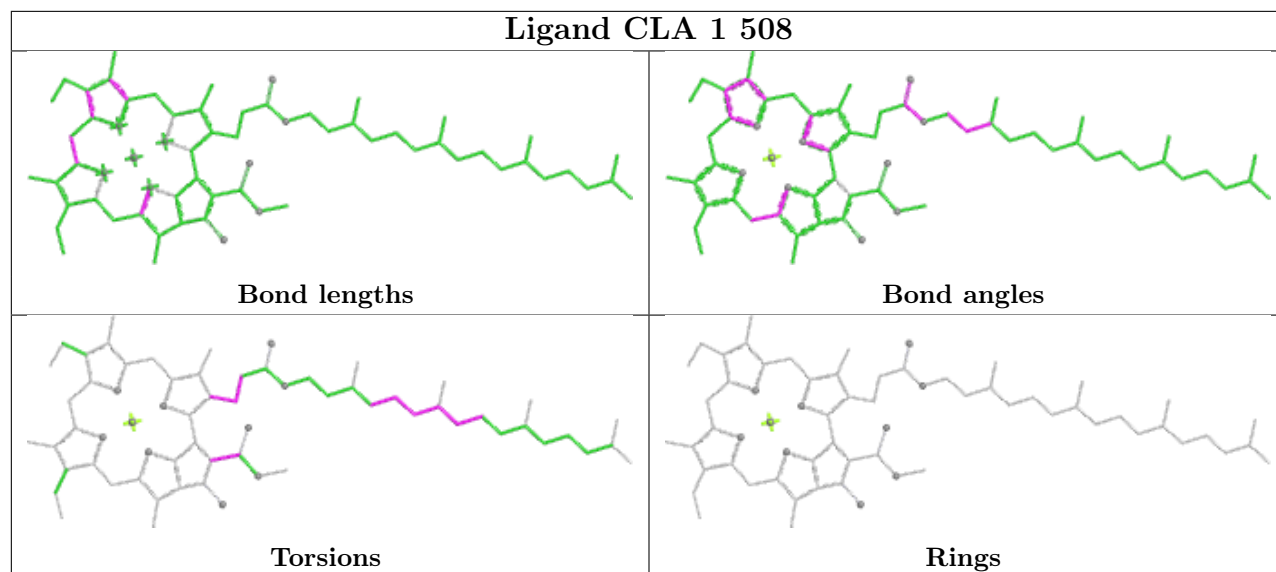




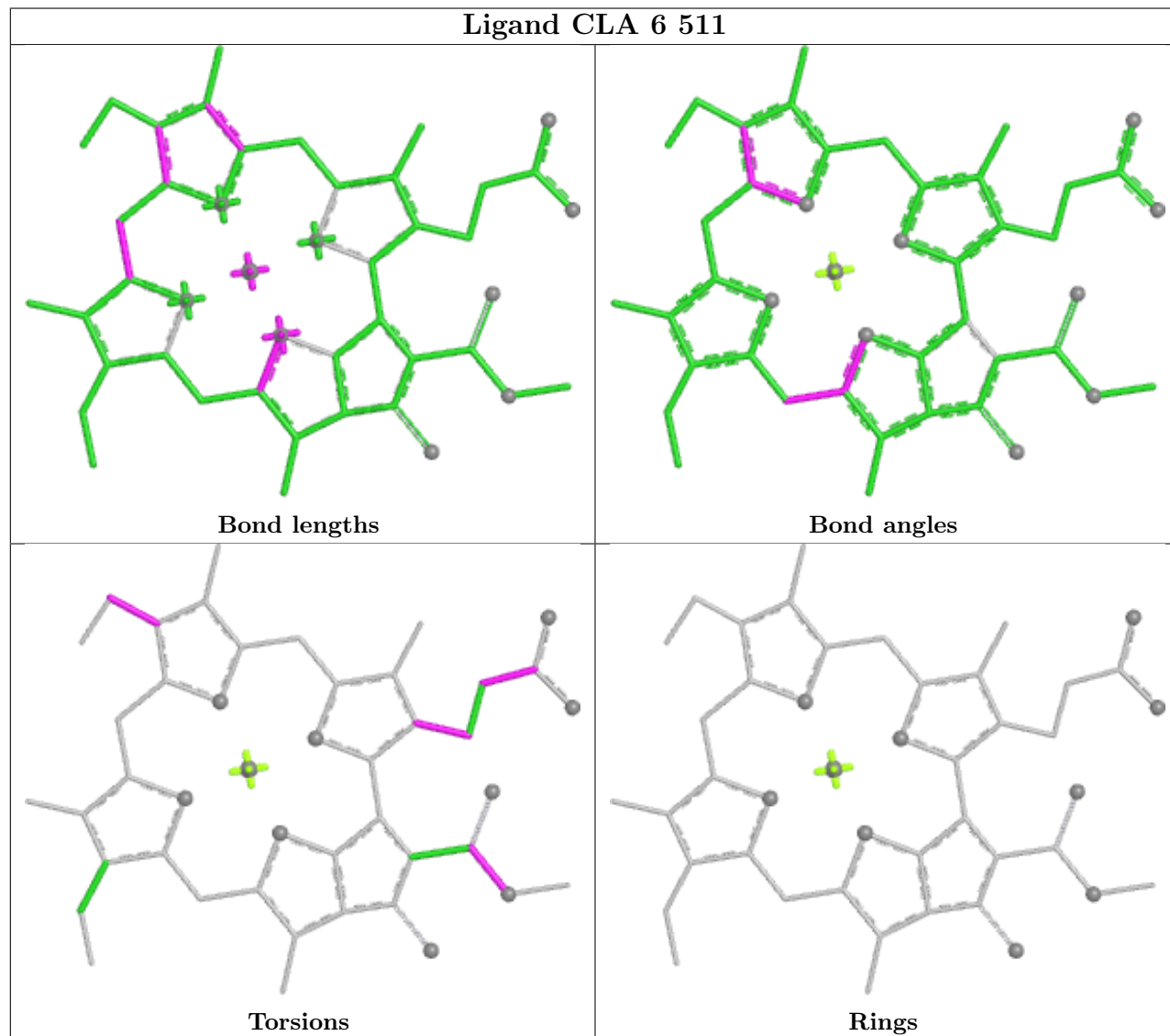




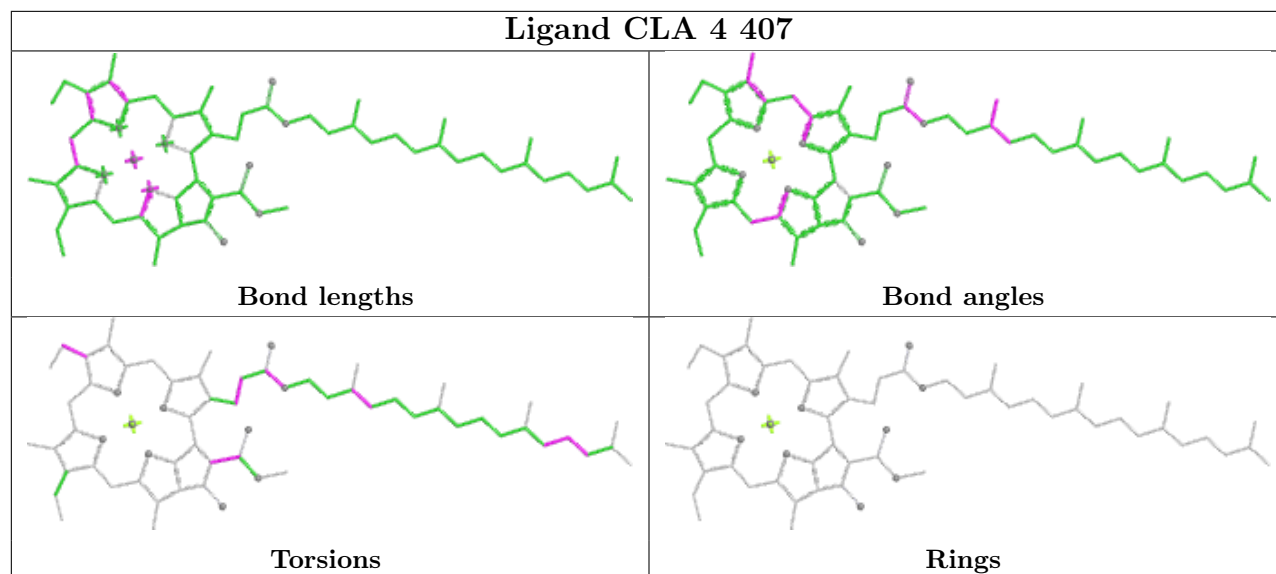
Ligand CLA 1 508



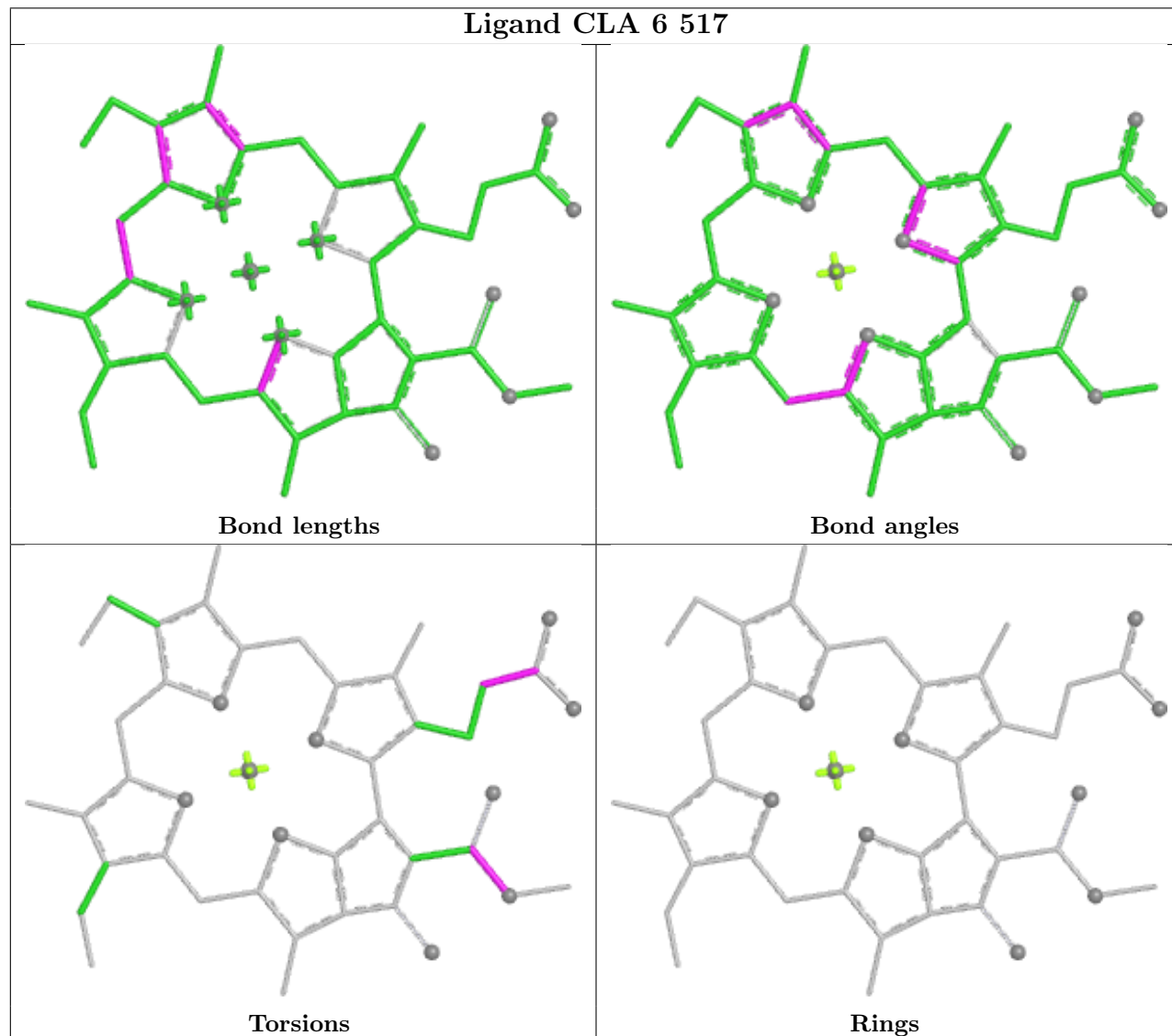
Ligand CLA 6 511

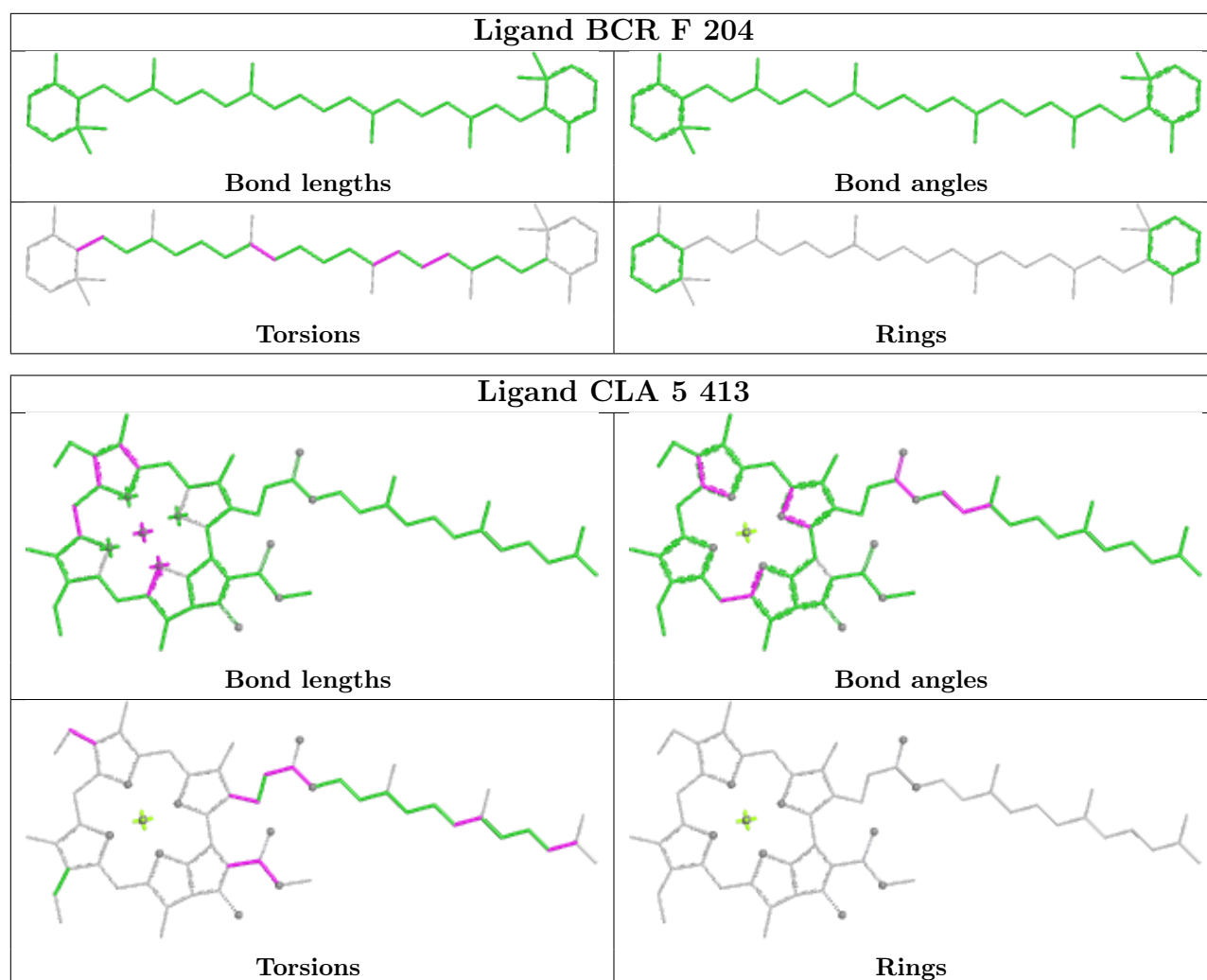


Ligand CLA 4 407

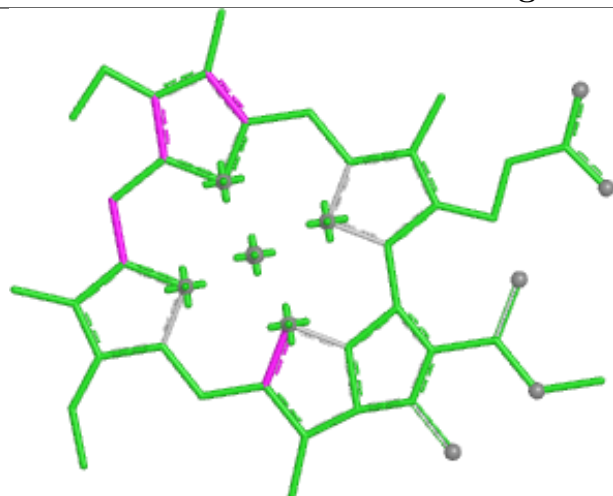


Ligand CLA 6 517

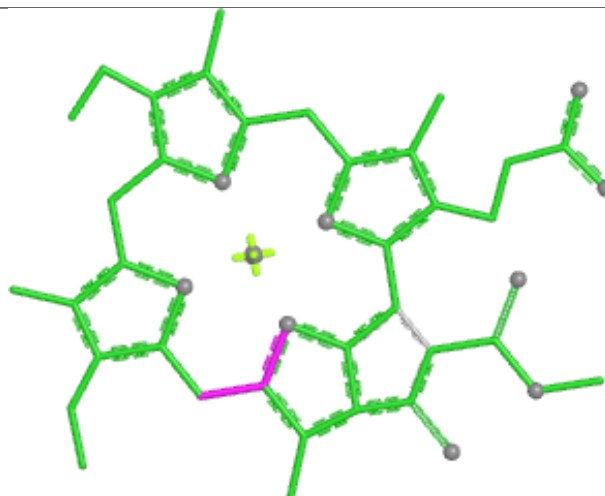




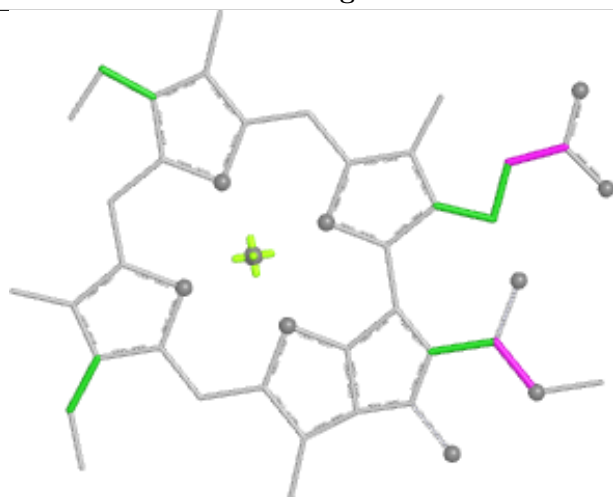
Ligand CLA 3 513



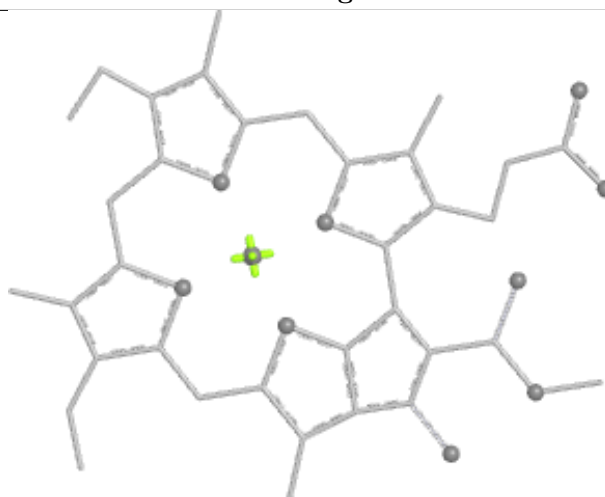
Bond lengths



Bond angles

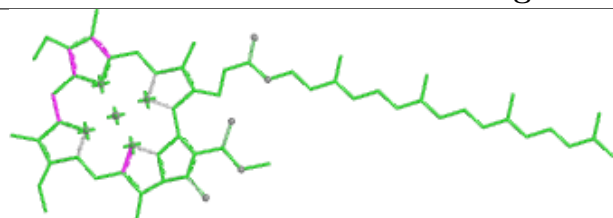


Torsions

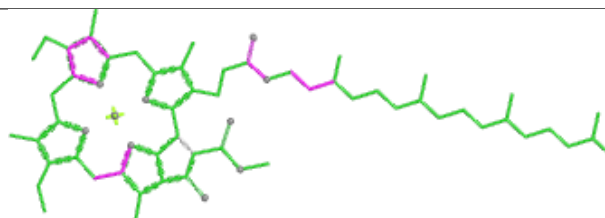


Rings

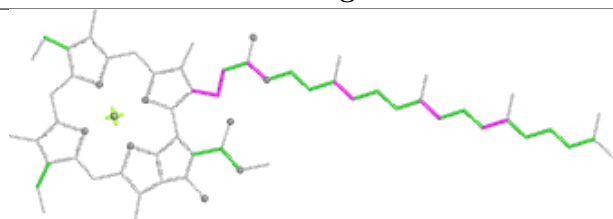
Ligand CLA A 830



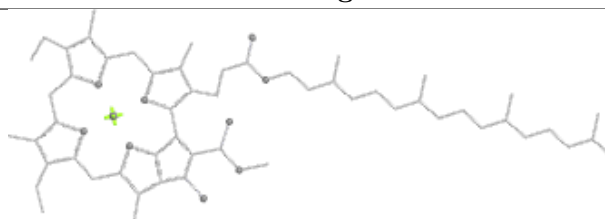
Bond lengths



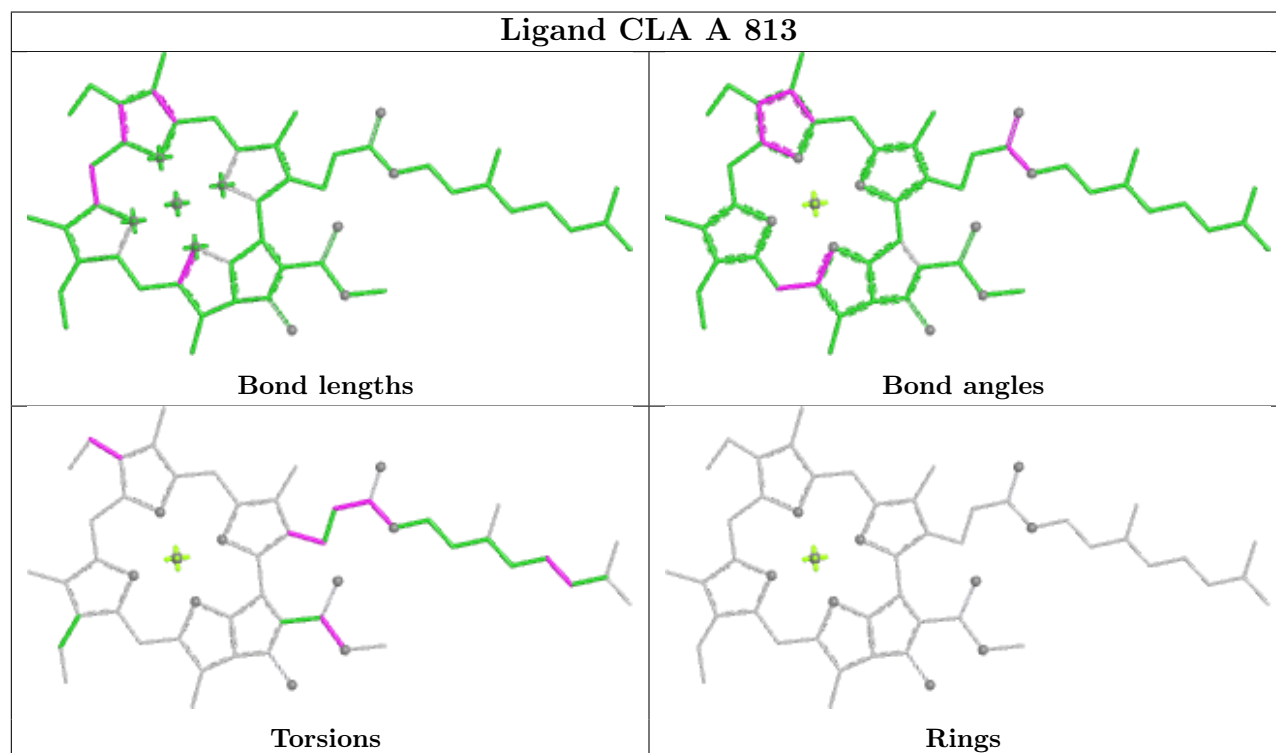
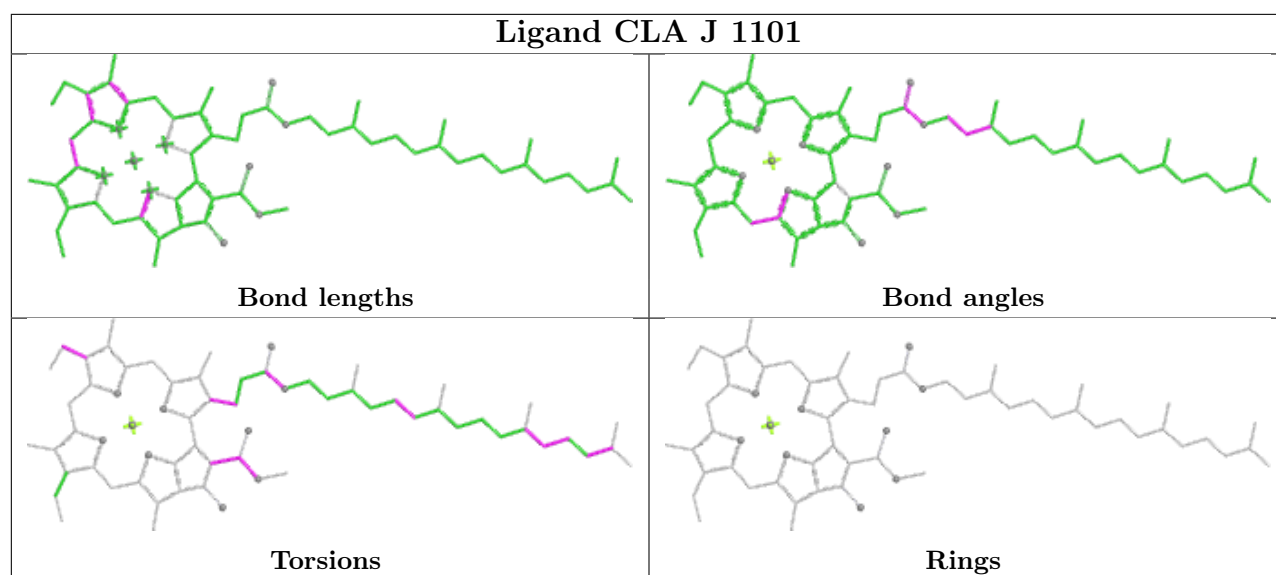
Bond angles



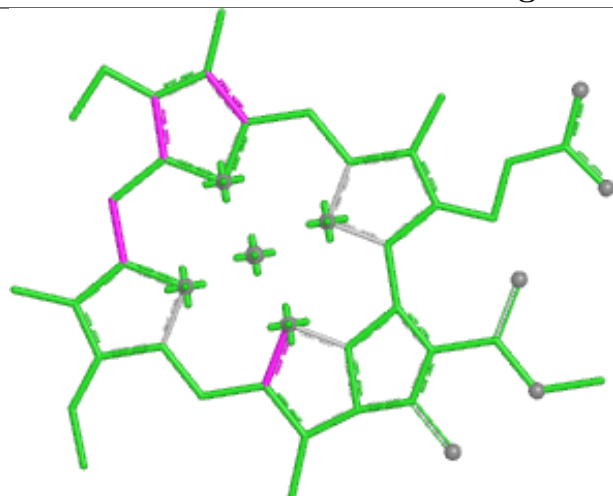
Torsions



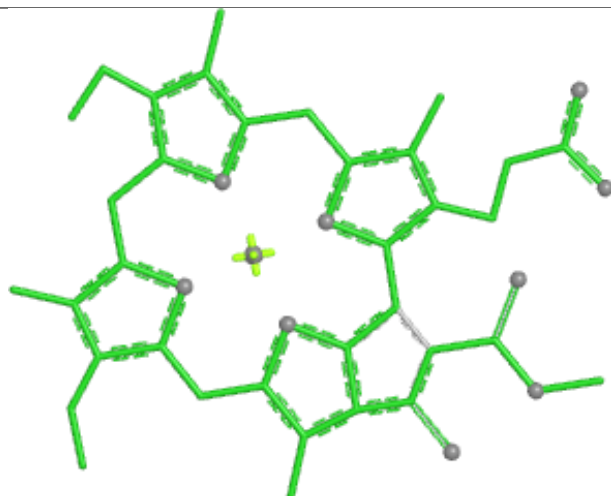
Rings



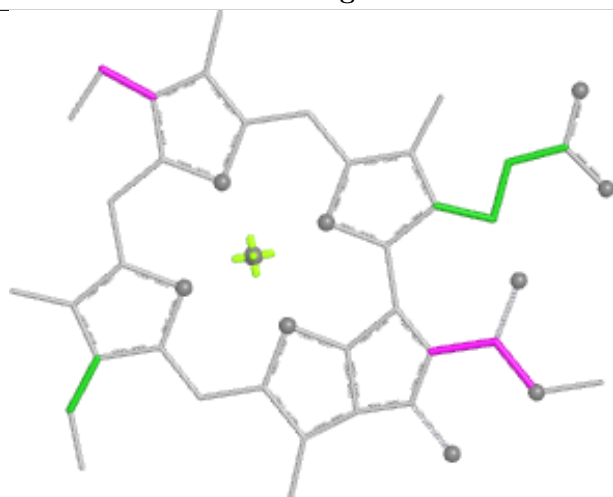
Ligand CLA 6 503



Bond lengths



Bond angles

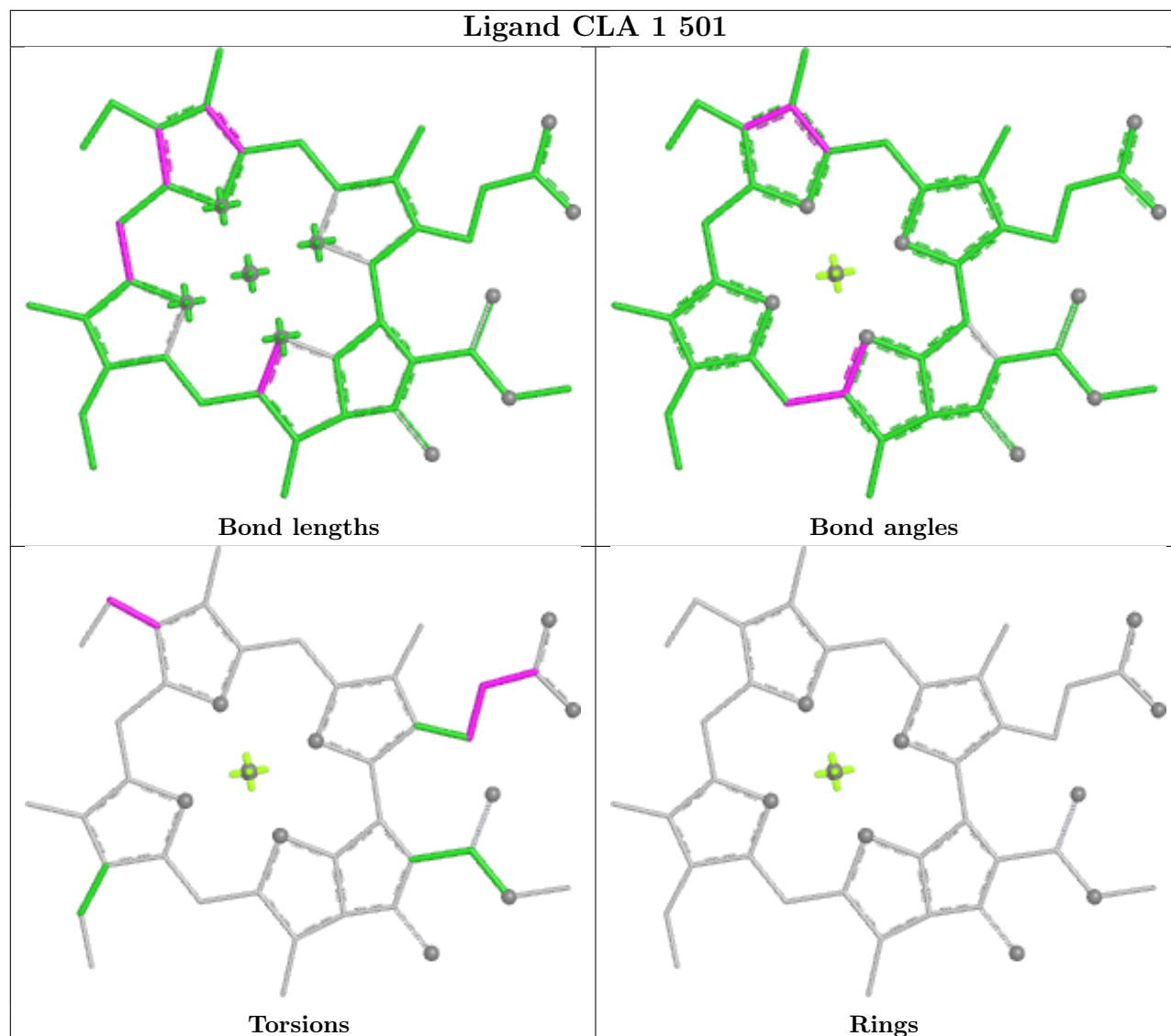


Torsions

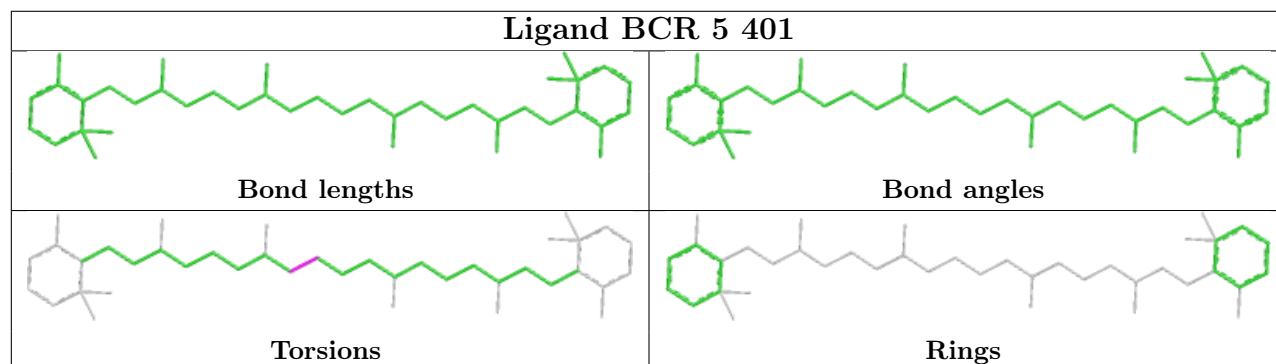


Rings

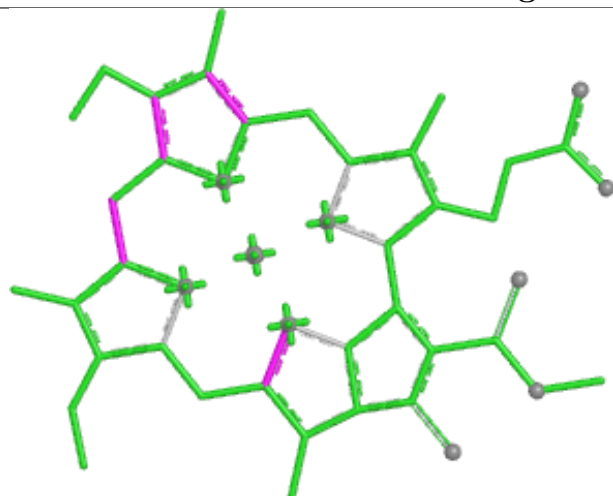
Ligand CLA 1 501



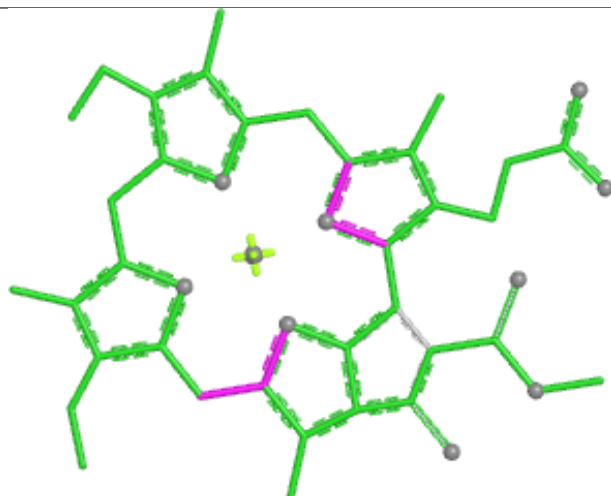
Ligand BCR 5 401



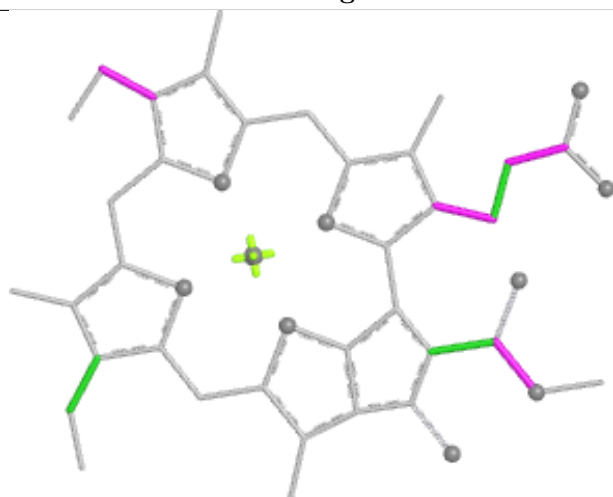
Ligand CLA 7 514



Bond lengths



Bond angles

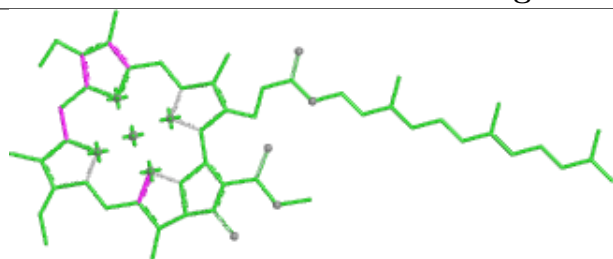


Torsions

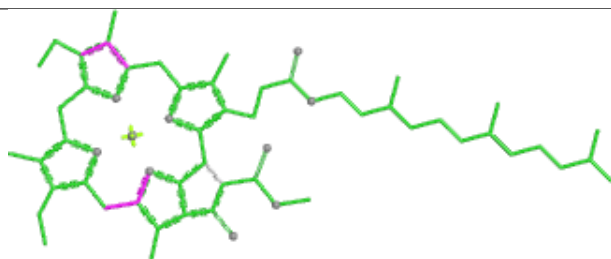


Rings

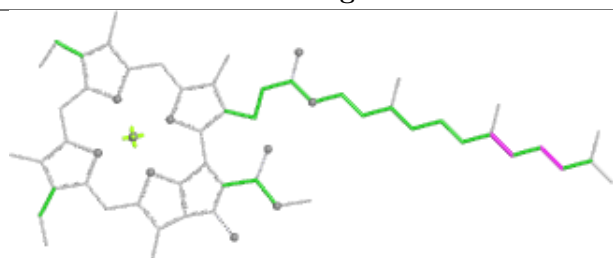
Ligand CLA A 834



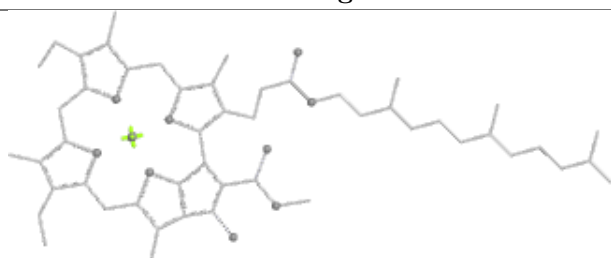
Bond lengths



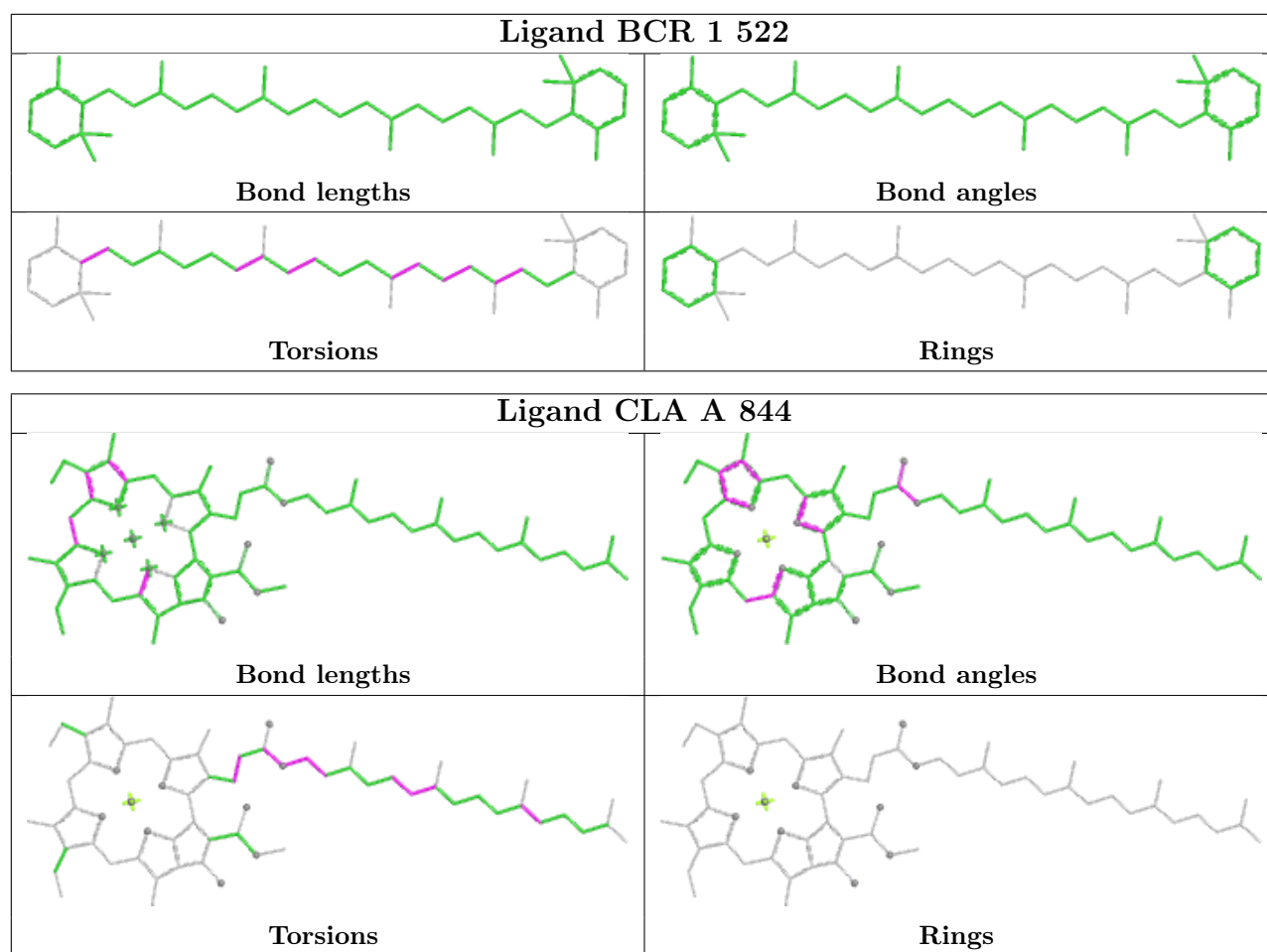
Bond angles



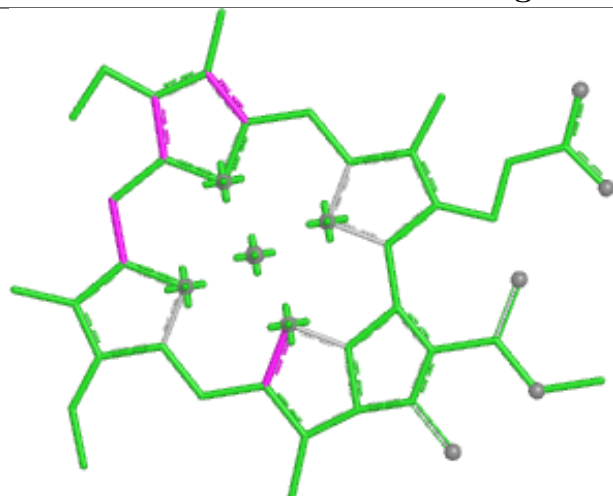
Torsions



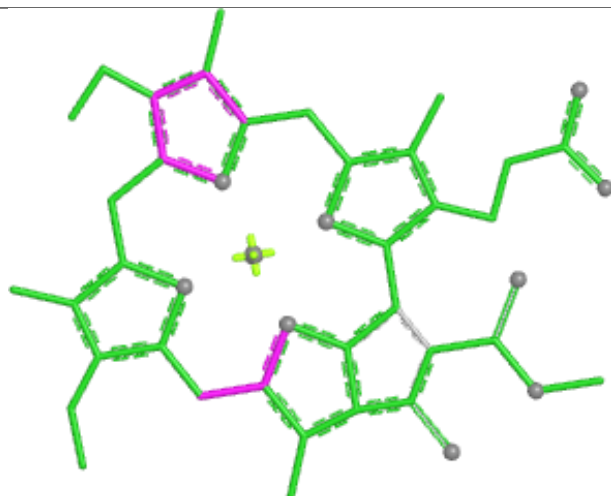
Rings



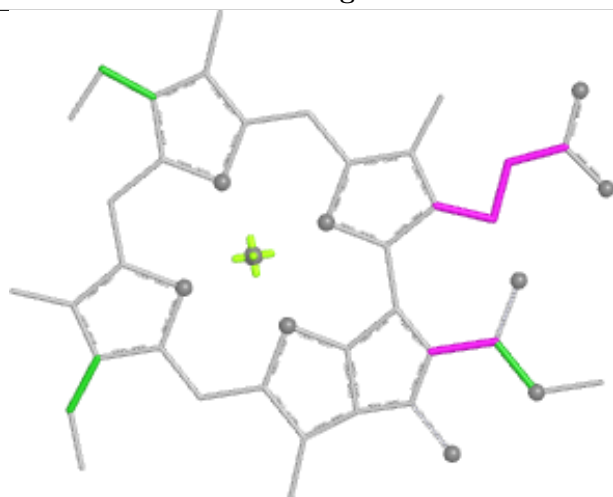
Ligand CLA B 822



Bond lengths



Bond angles

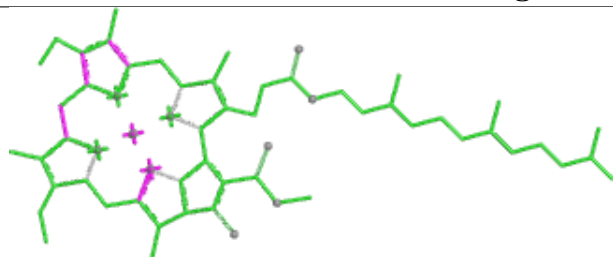


Torsions

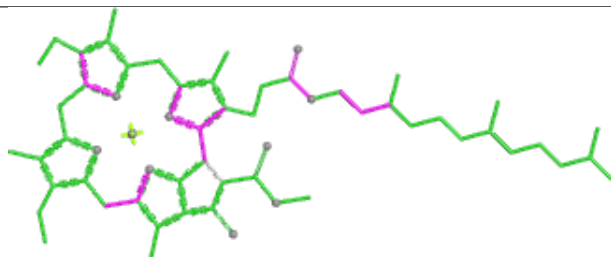


Rings

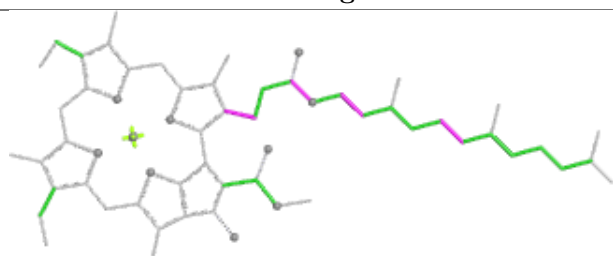
Ligand CLA A 815



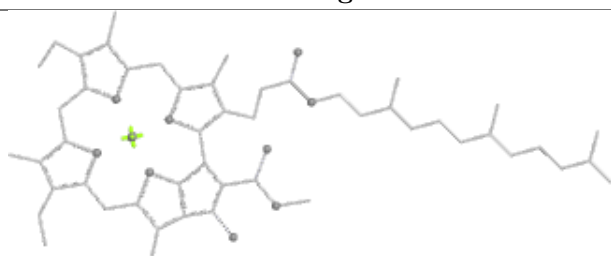
Bond lengths



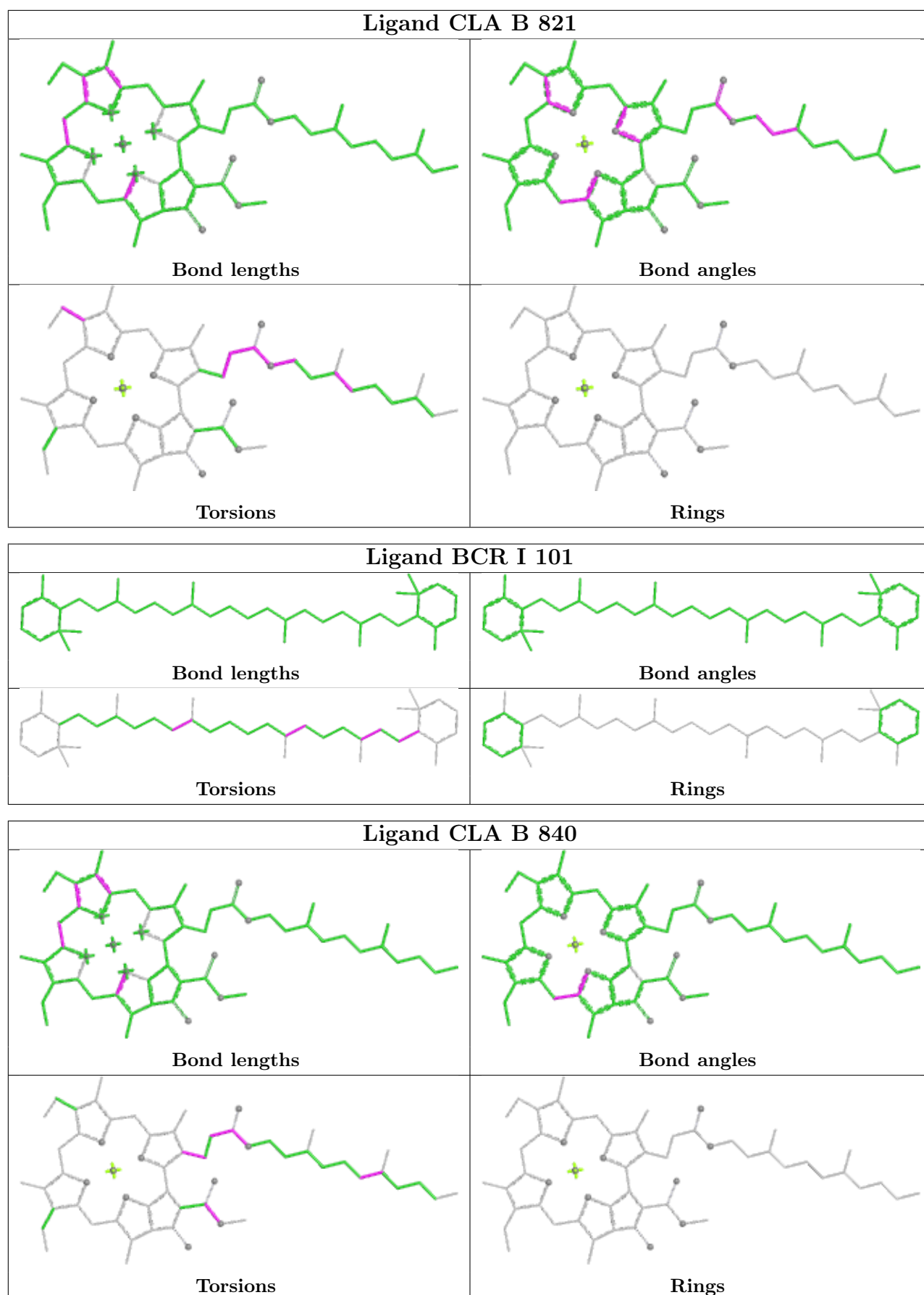
Bond angles

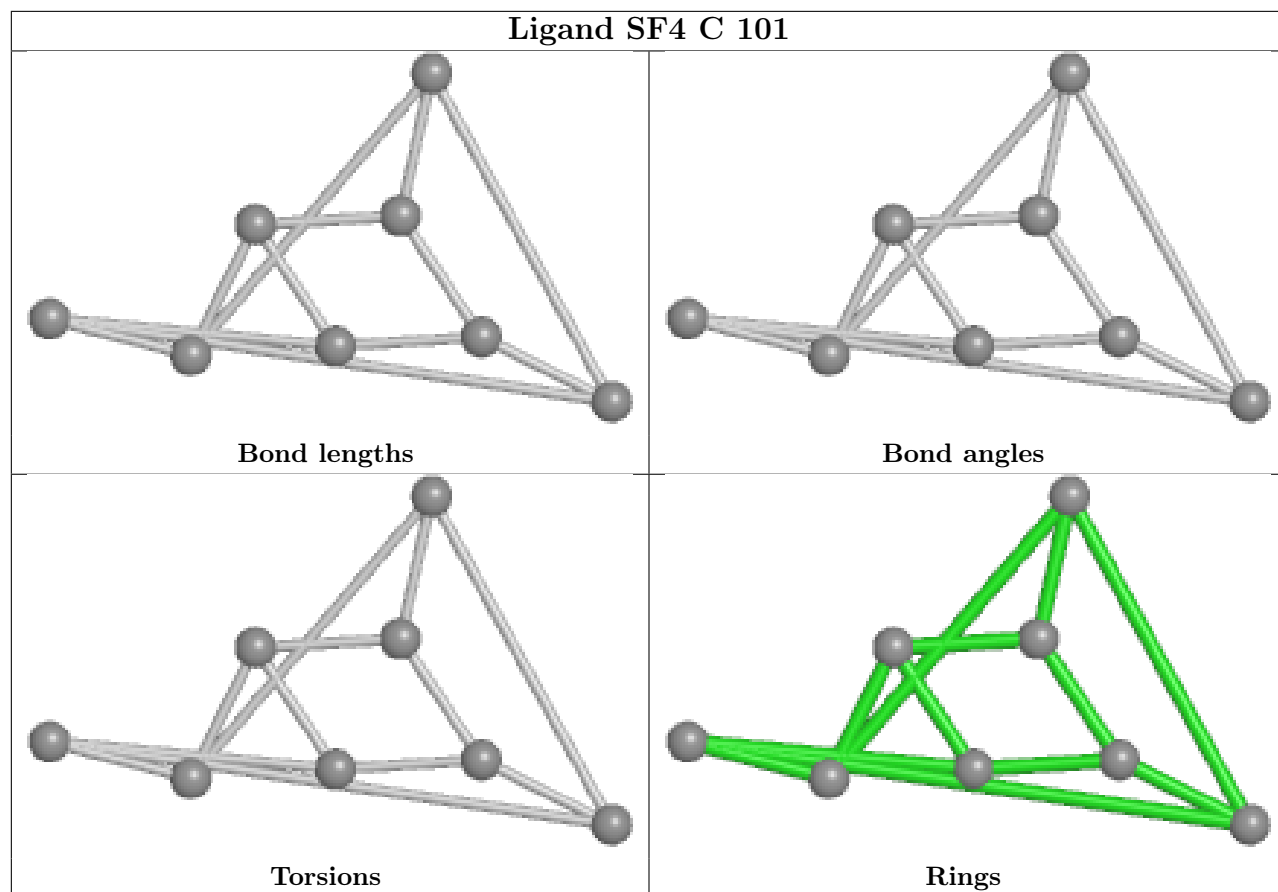


Torsions

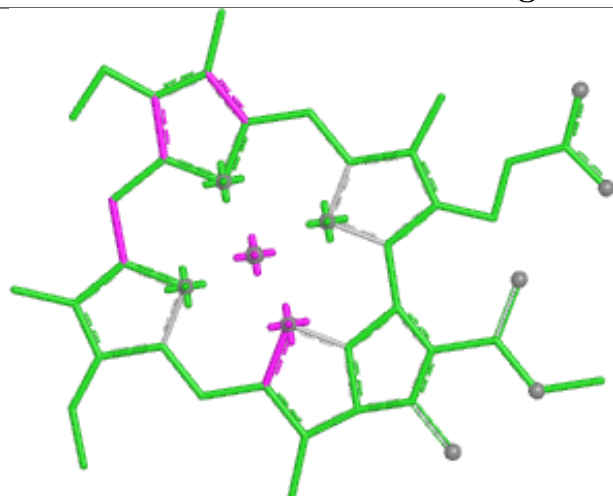


Rings

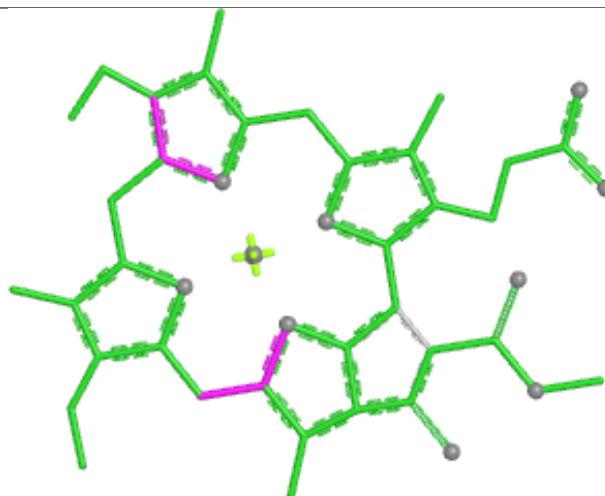




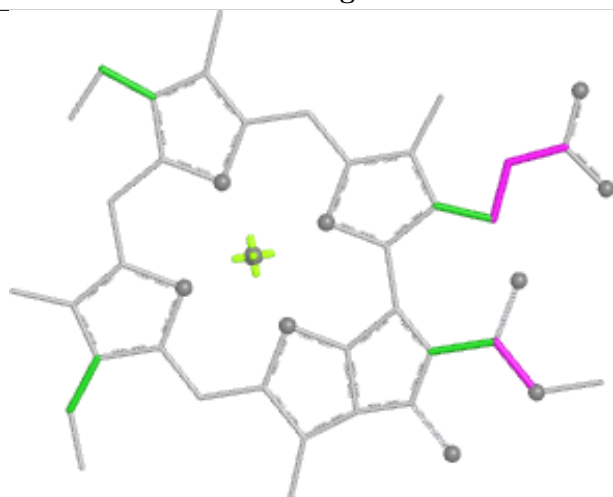
Ligand CLA 7 501



Bond lengths



Bond angles

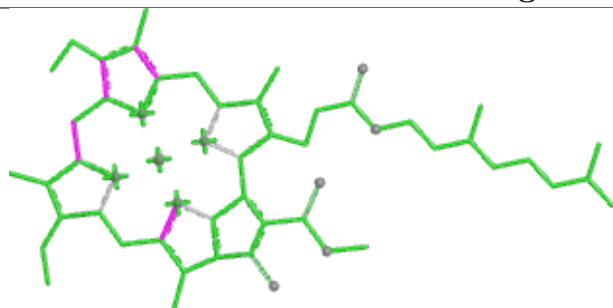


Torsions

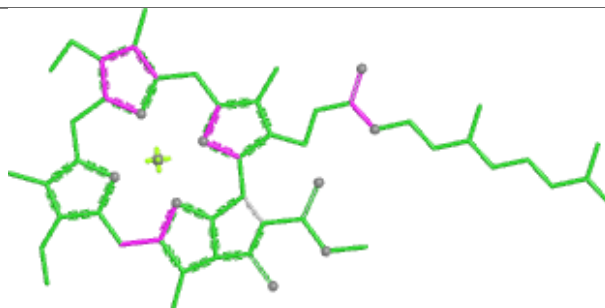


Rings

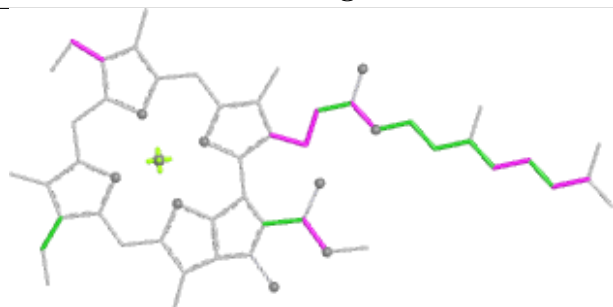
Ligand CLA 3 510



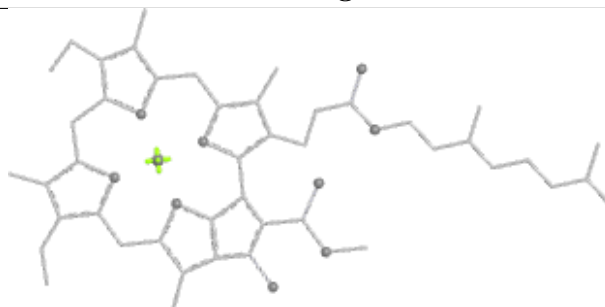
Bond lengths



Bond angles

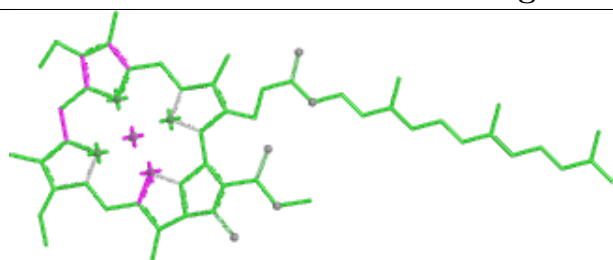


Torsions

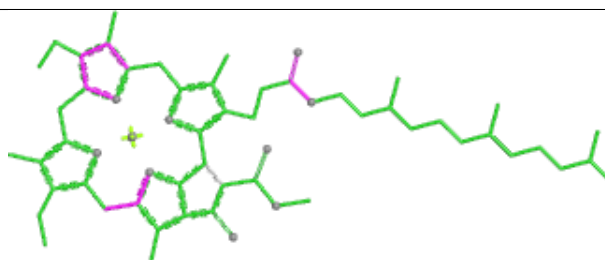


Rings

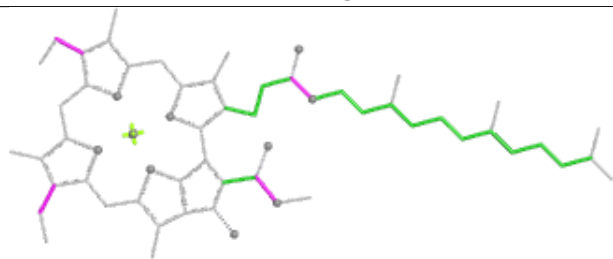
Ligand CLA 7 506



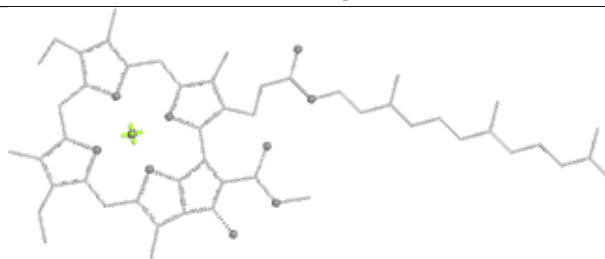
Bond lengths



Bond angles

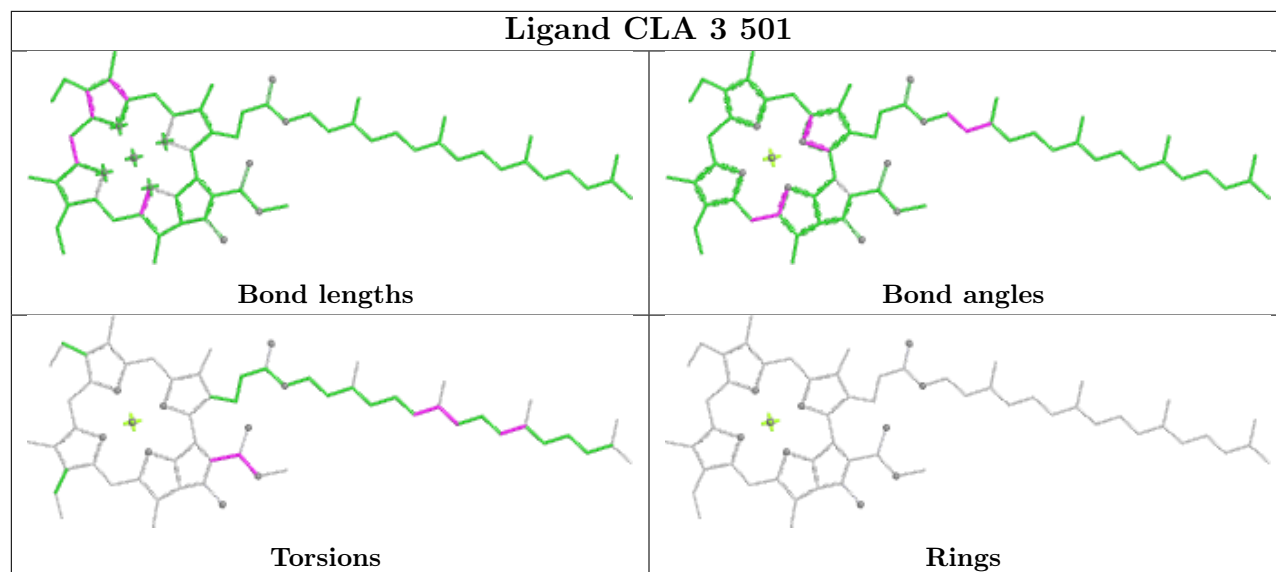


Torsions

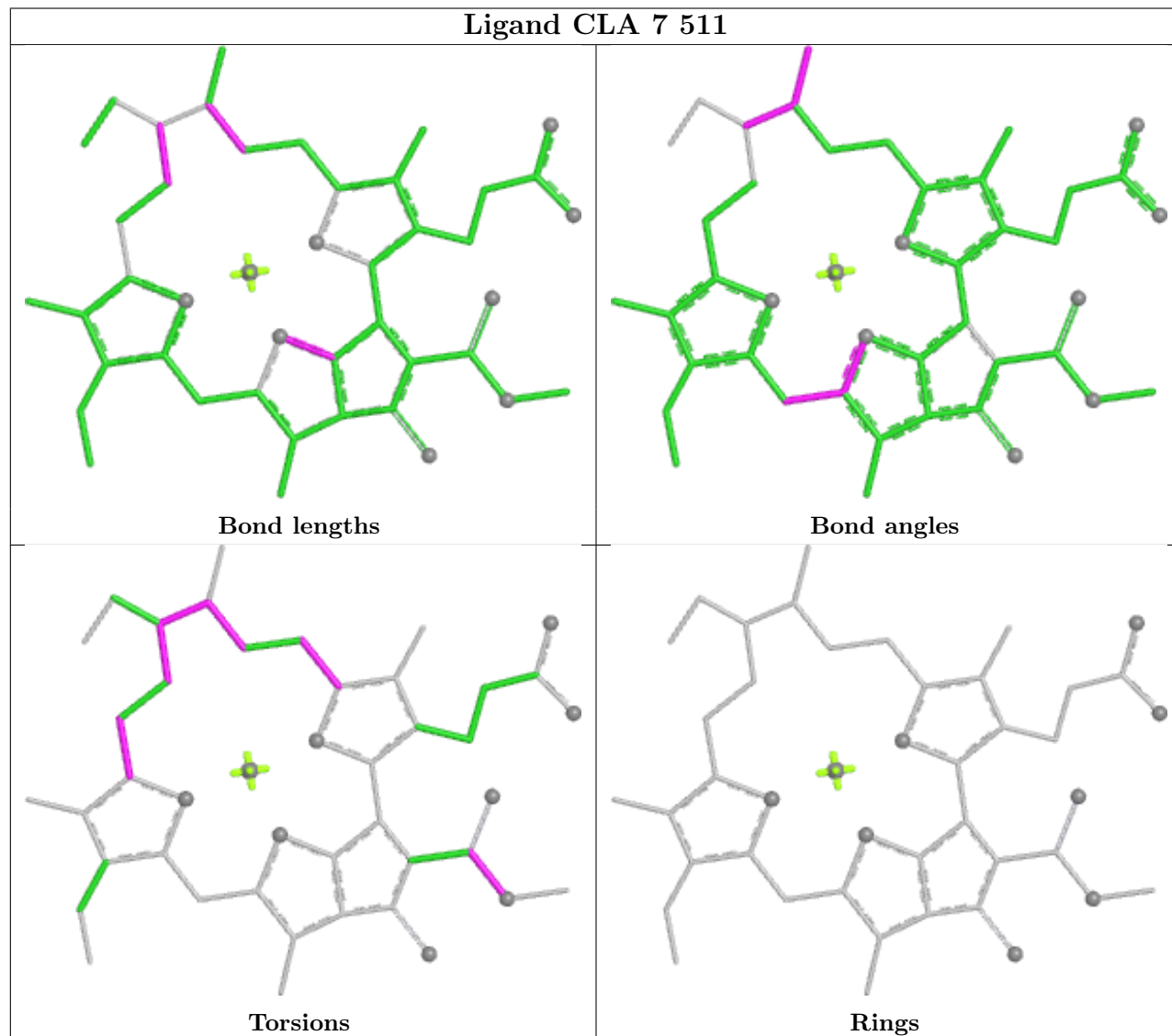


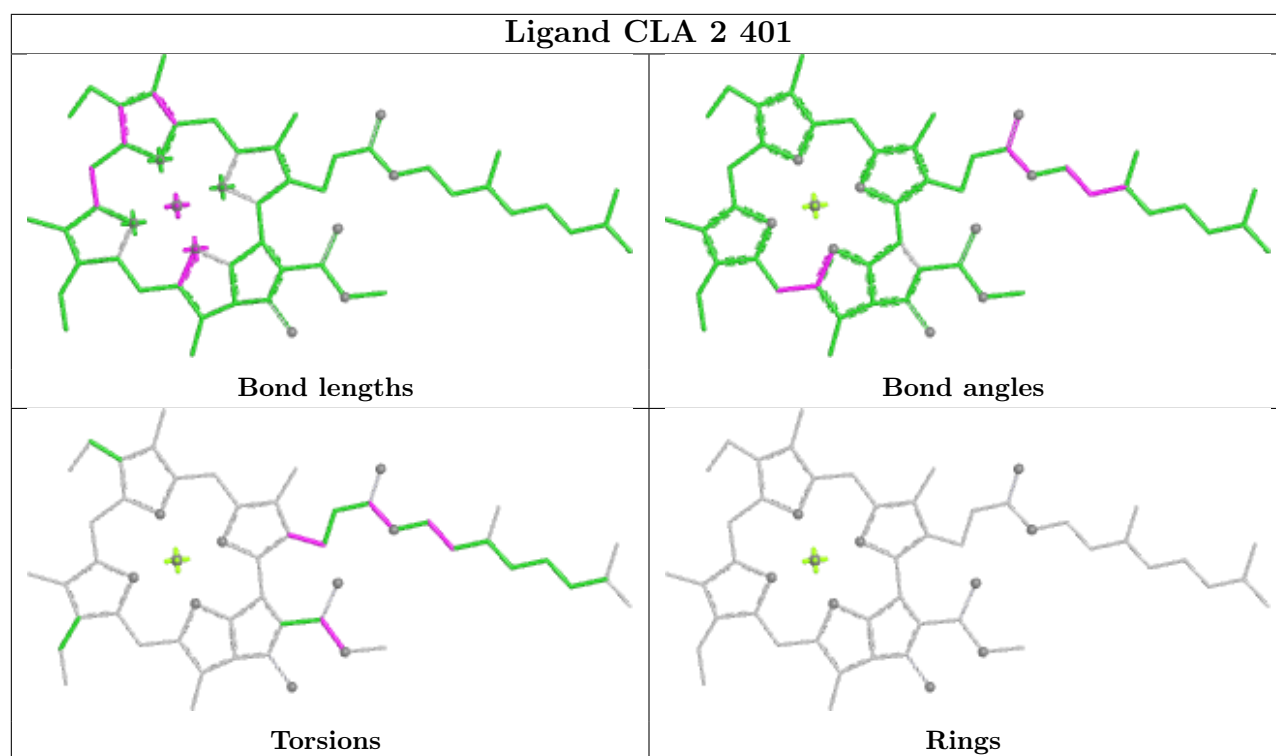
Rings

Ligand CLA 3 501

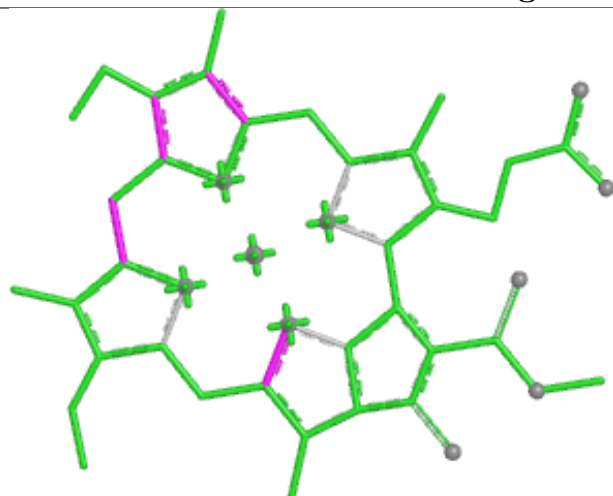


Ligand CLA 7 511

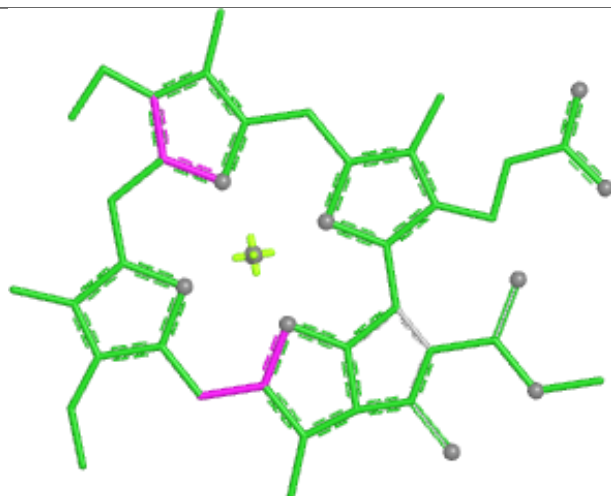




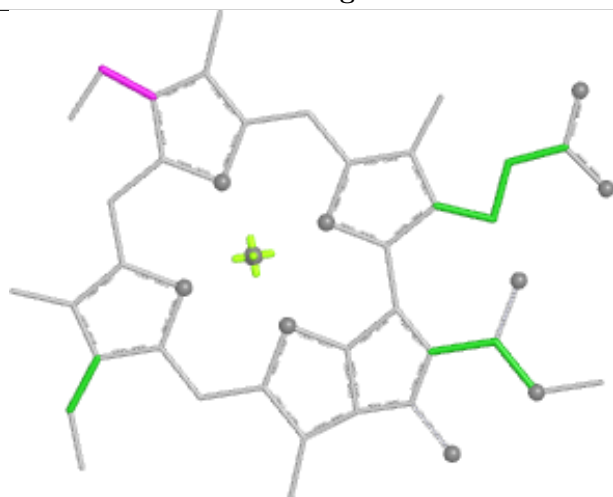
Ligand CLA 5 415



Bond lengths



Bond angles

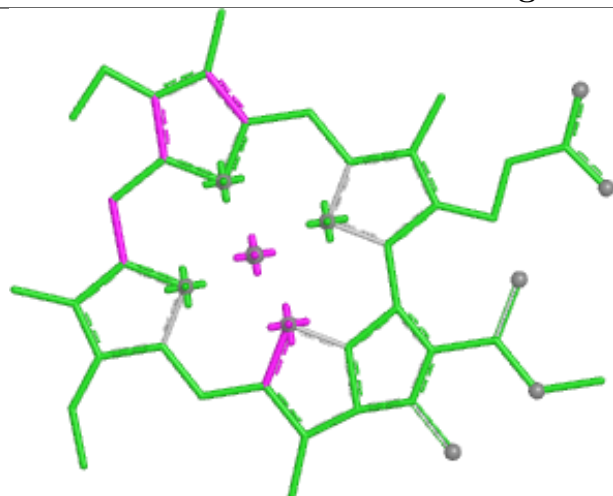


Torsions

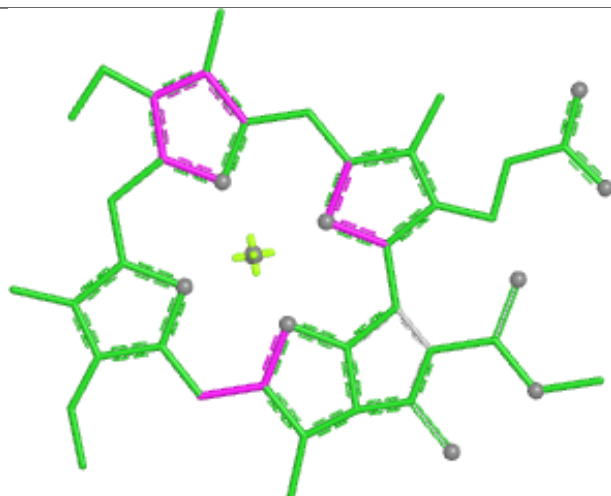


Rings

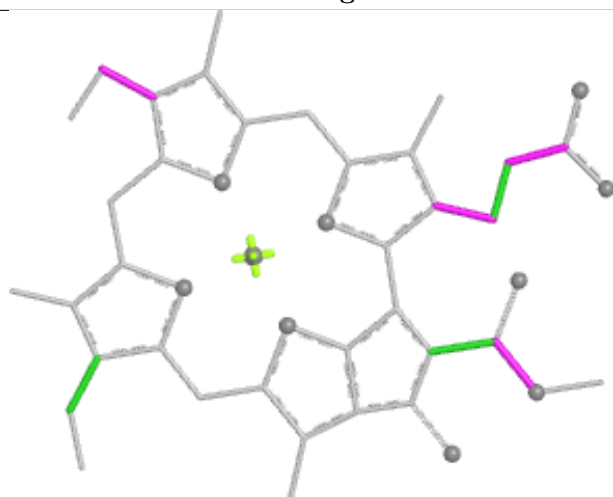
Ligand CLA 7 513



Bond lengths



Bond angles

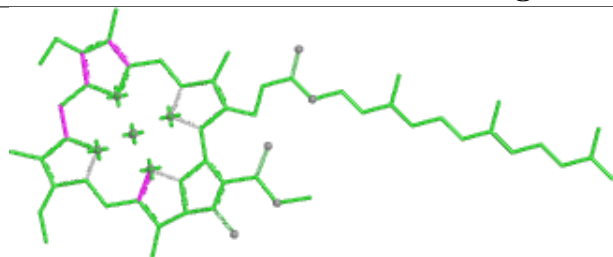


Torsions

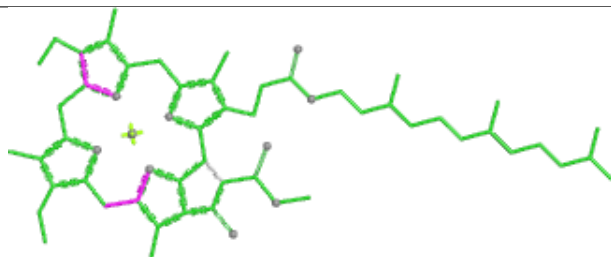


Rings

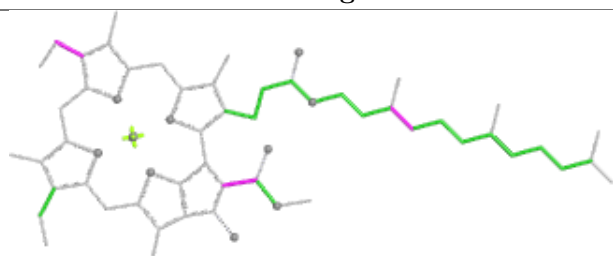
Ligand CLA B 817



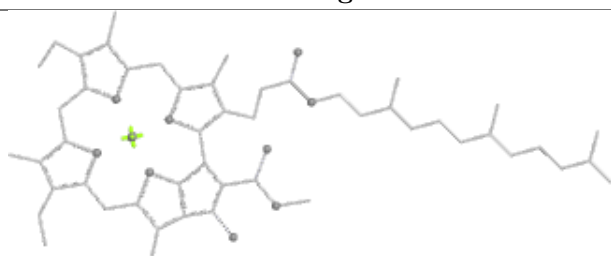
Bond lengths



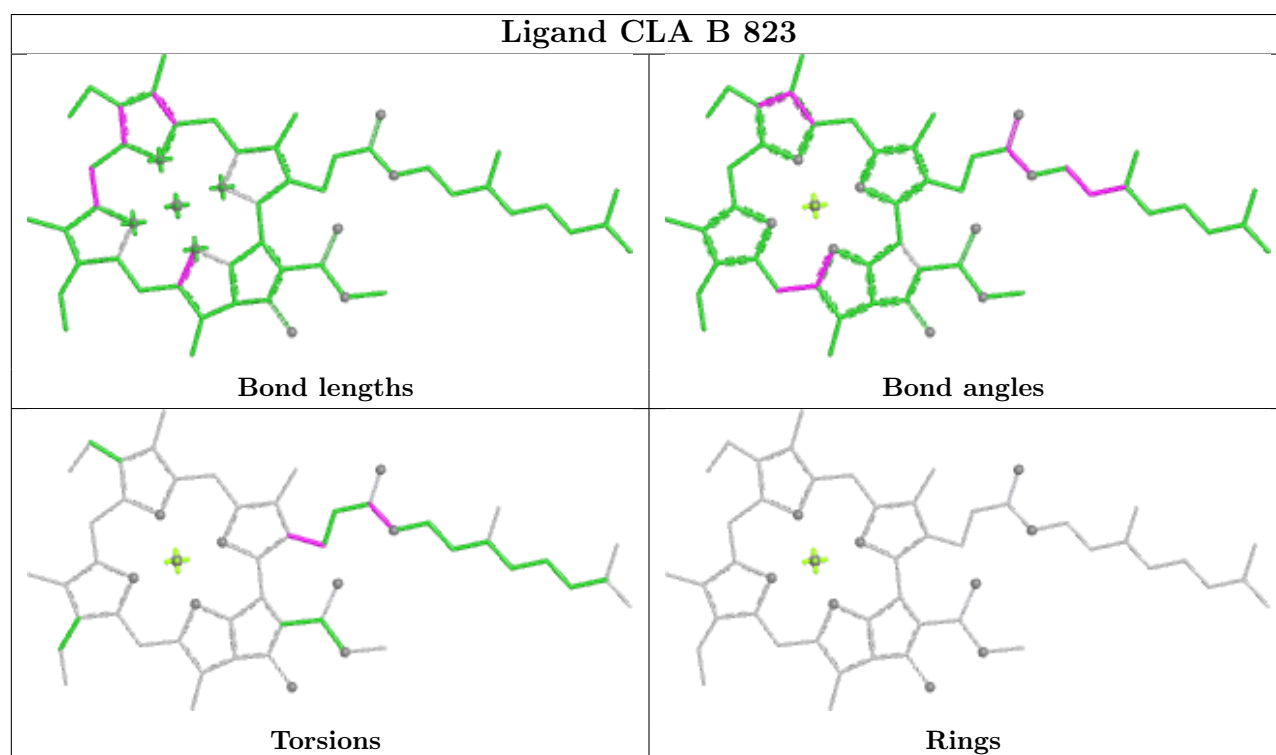
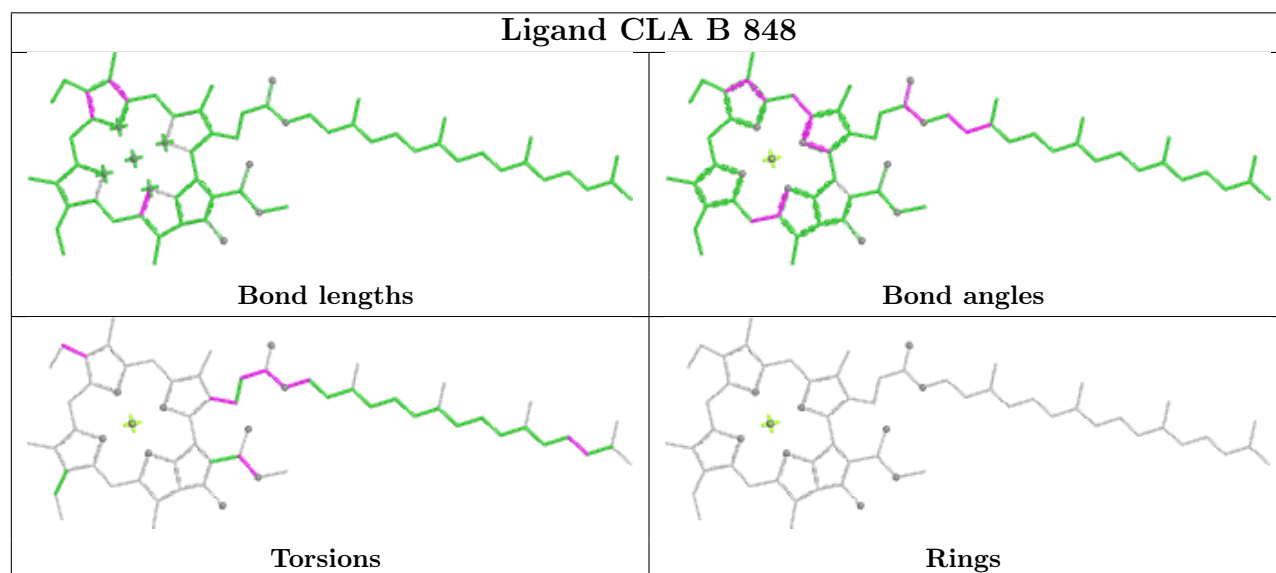
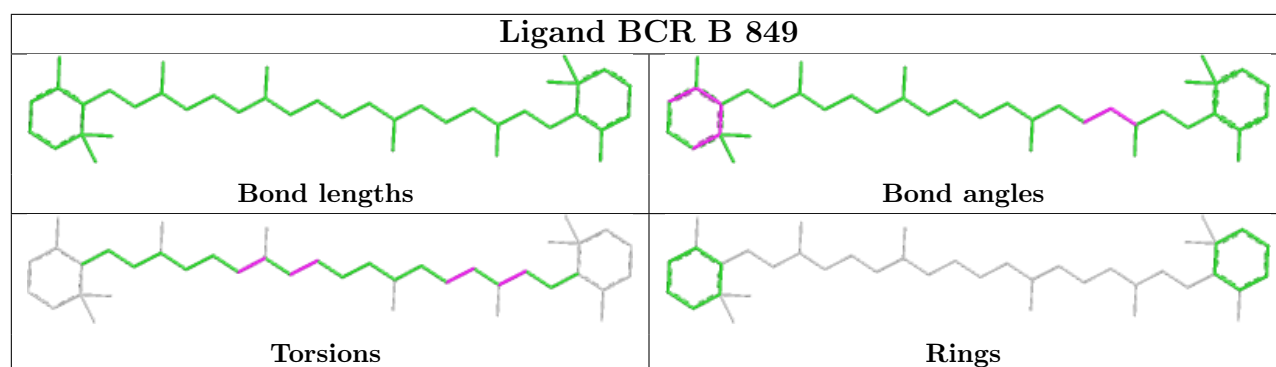
Bond angles



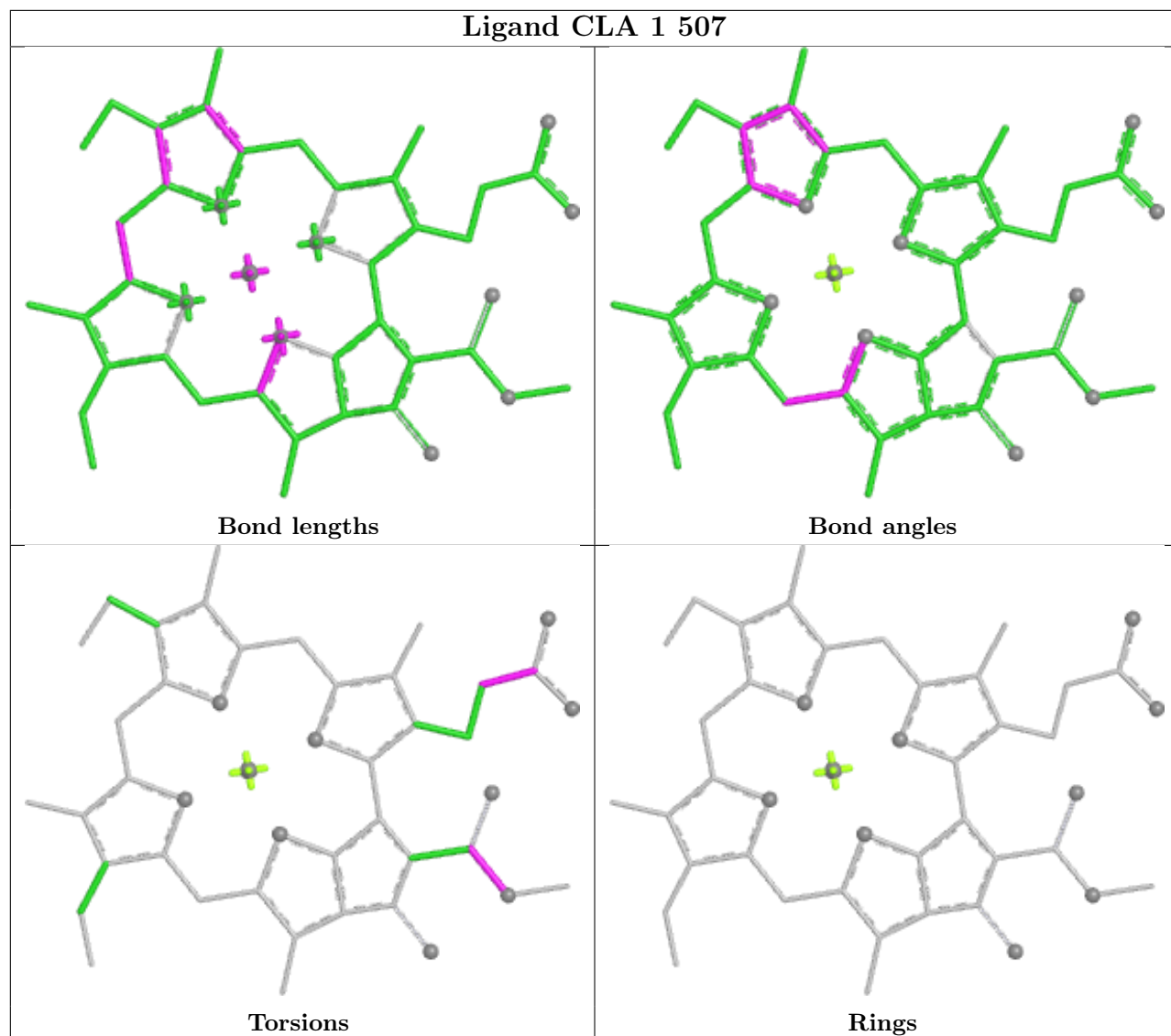
Torsions



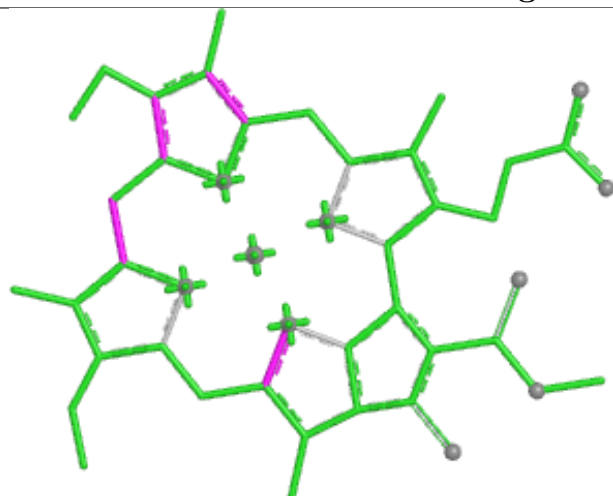
Rings



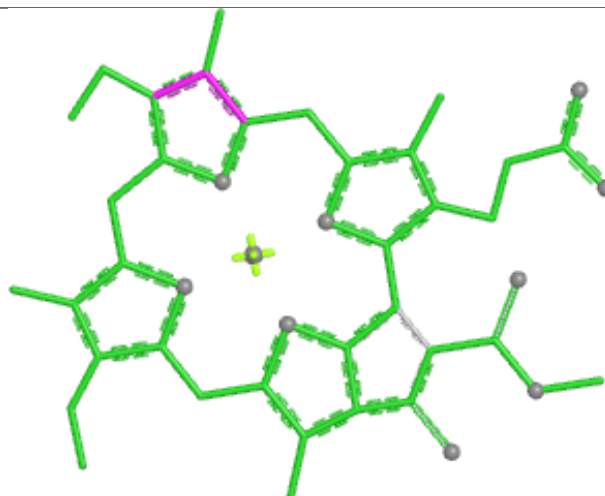
Ligand CLA 1 507



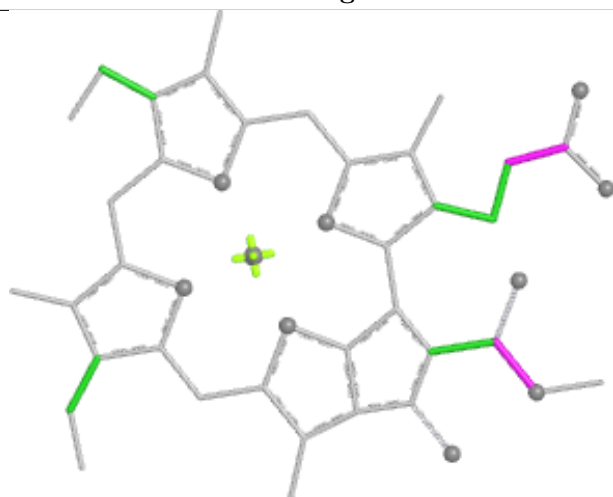
Ligand CLA 6 516



Bond lengths



Bond angles

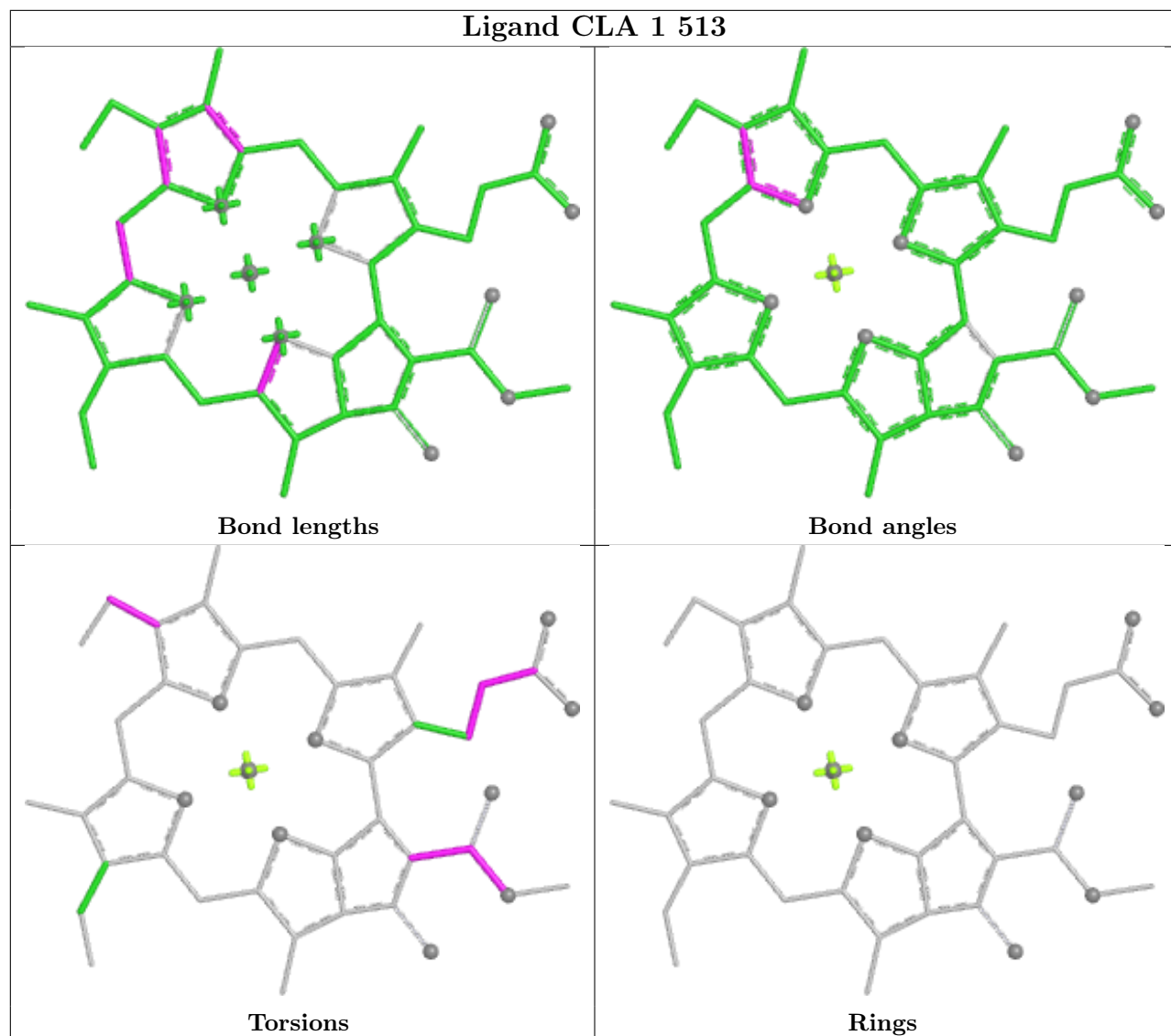


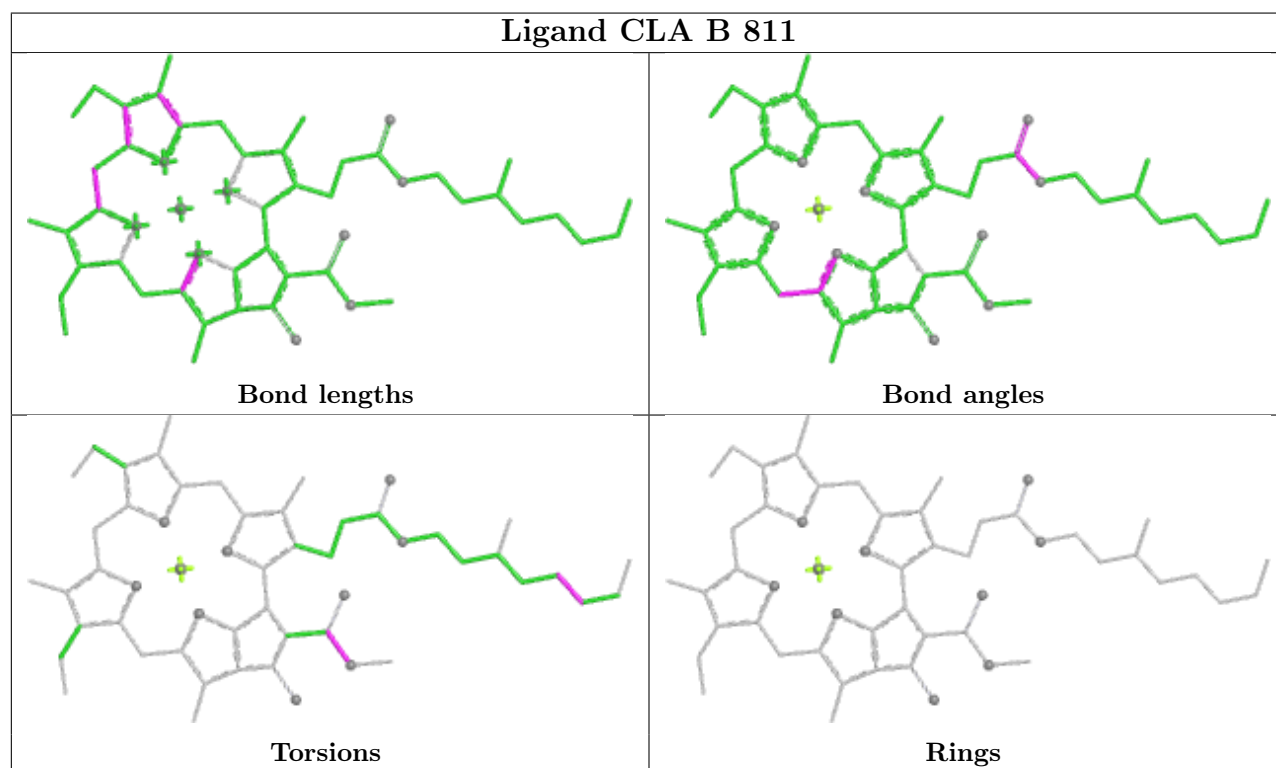
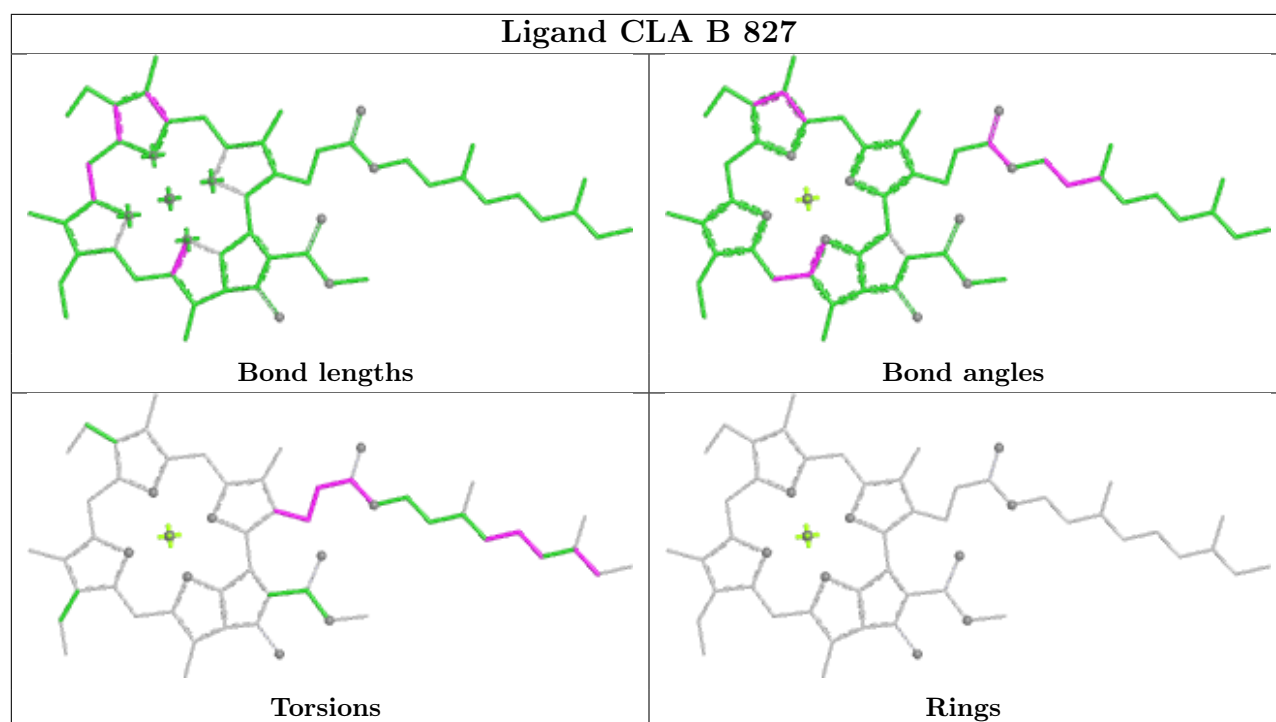
Torsions



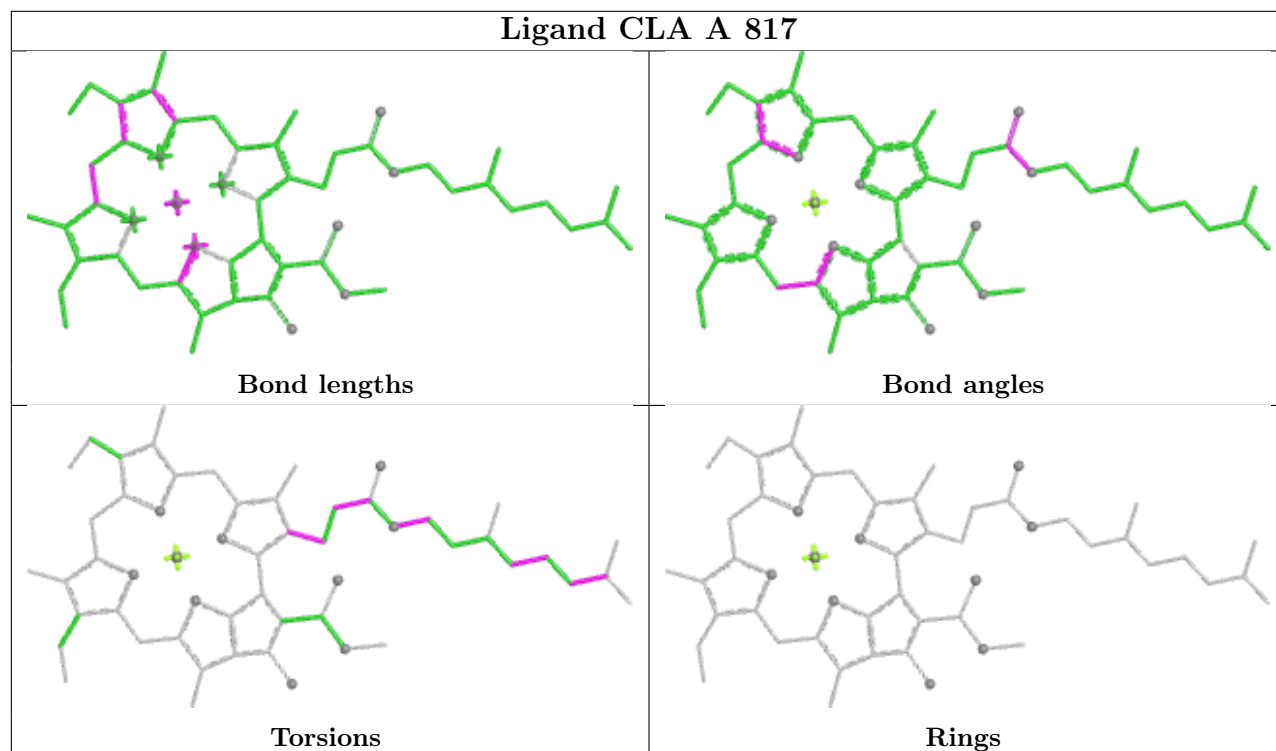
Rings

Ligand CLA 1 513

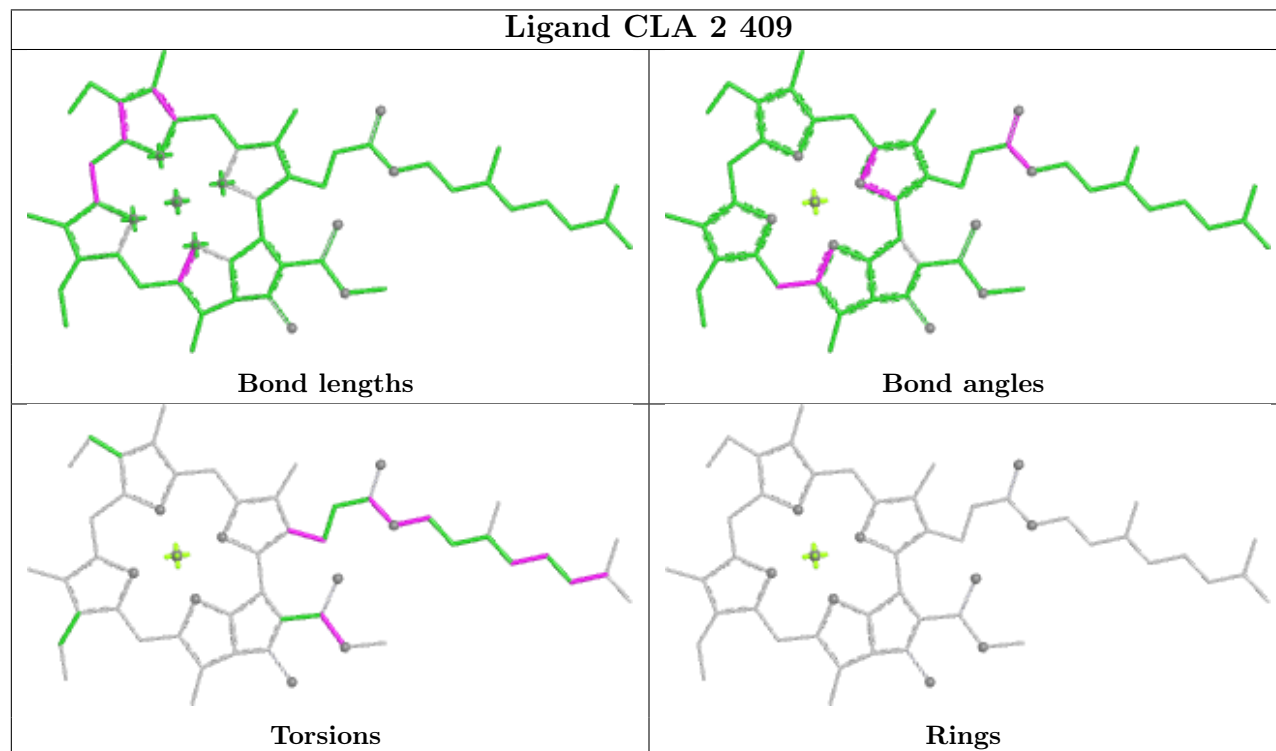


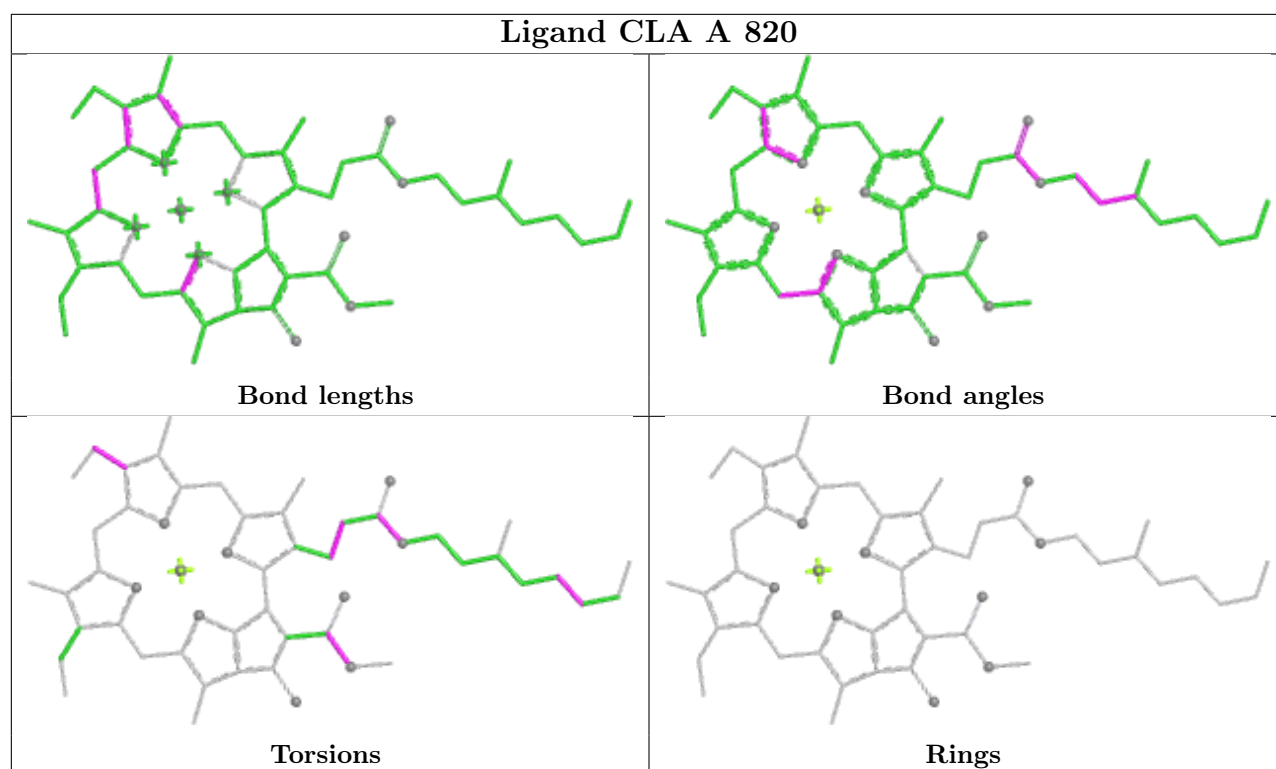


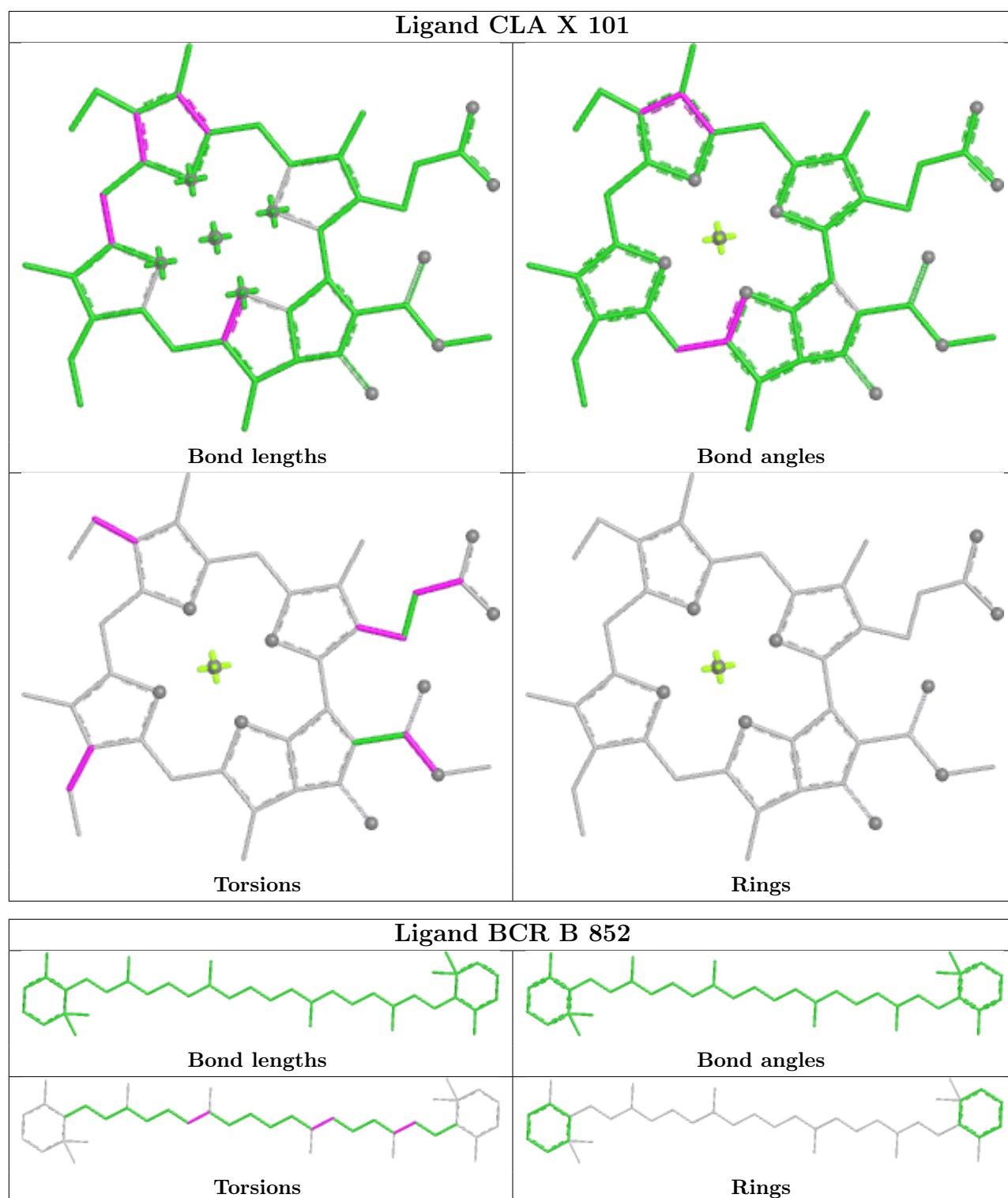
Ligand CLA A 817

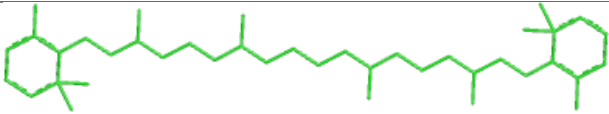
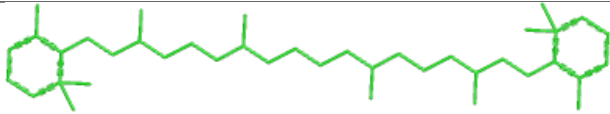
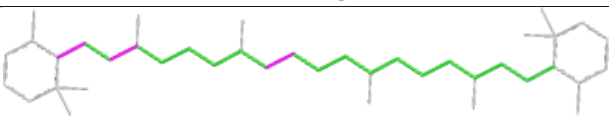
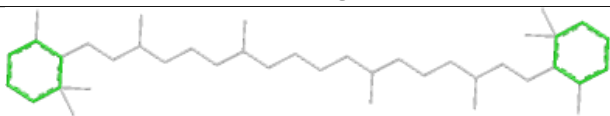





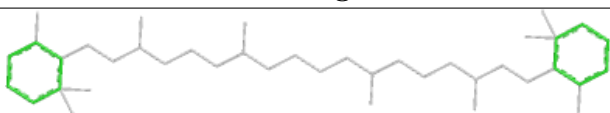
Ligand CLA 2 409

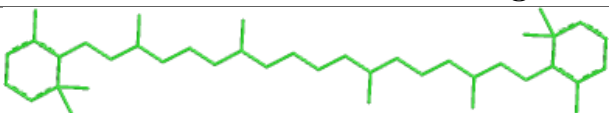
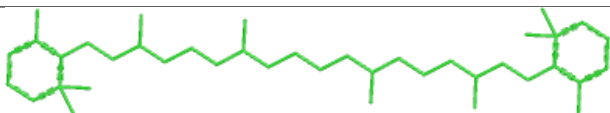
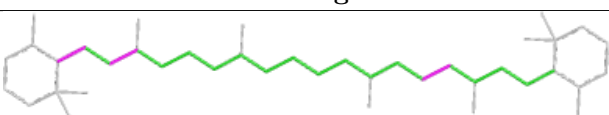
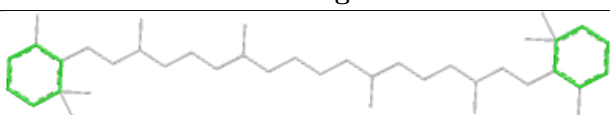


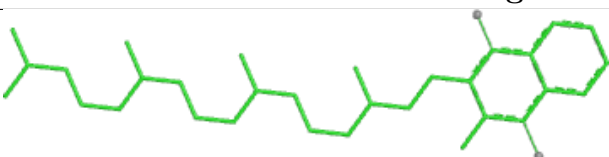
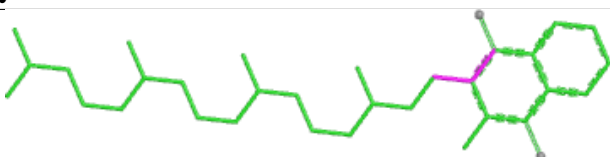
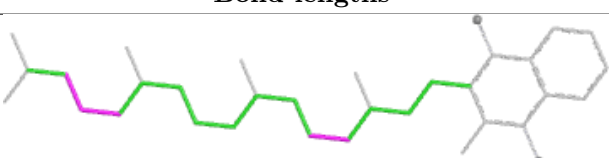
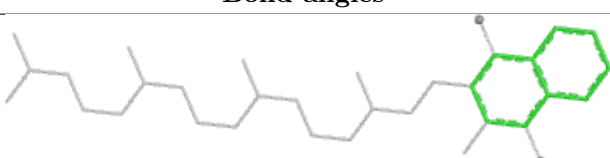




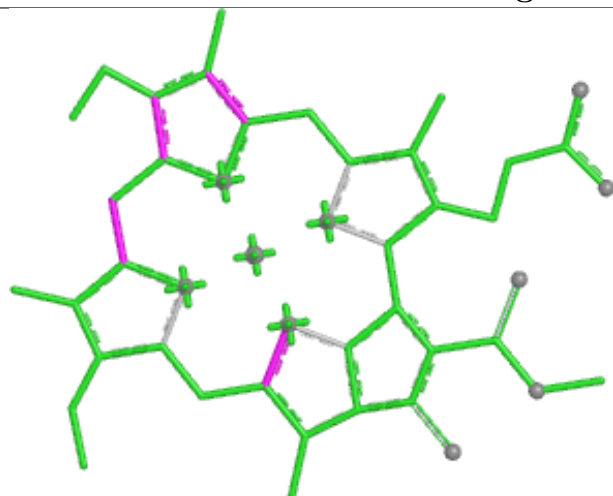
Ligand BCR J 1104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 7 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

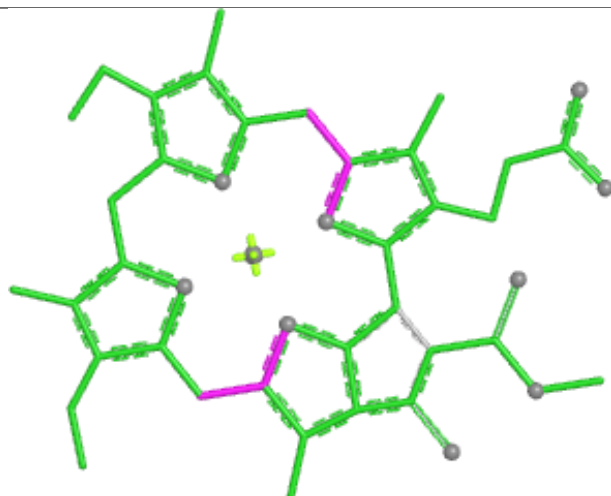
Ligand BCR 7 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PQN B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

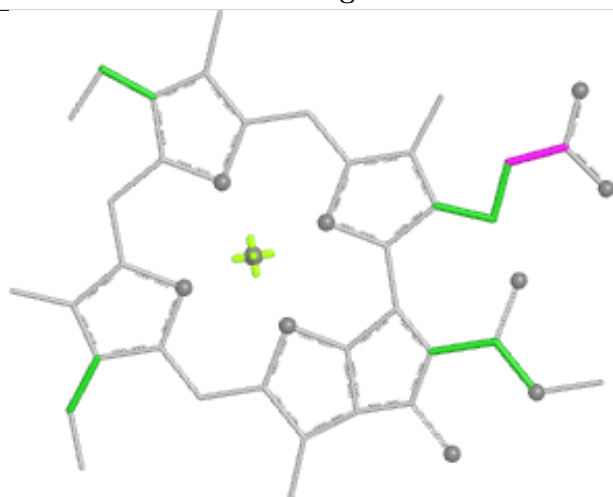
Ligand CLA F 202



Bond lengths



Bond angles

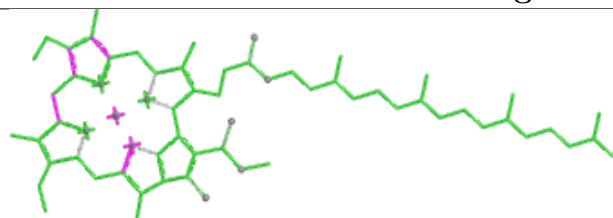


Torsions

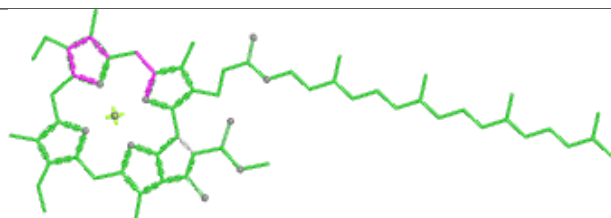


Rings

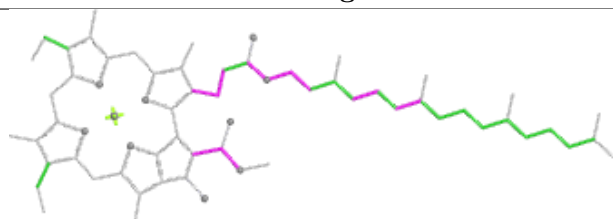
Ligand CLA B 831



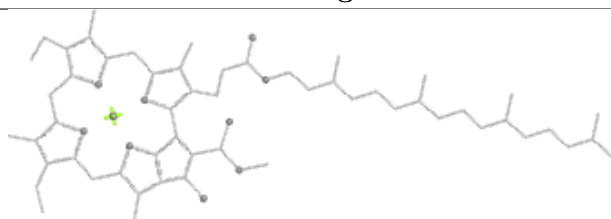
Bond lengths



Bond angles

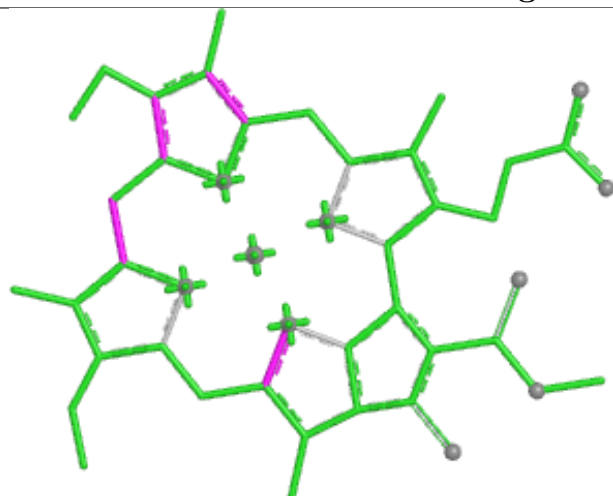


Torsions

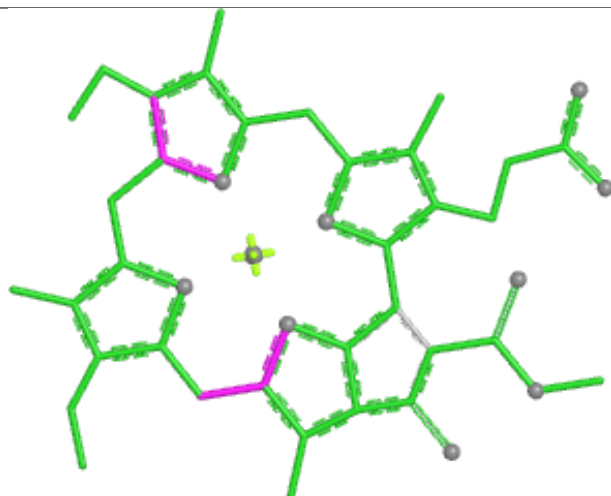


Rings

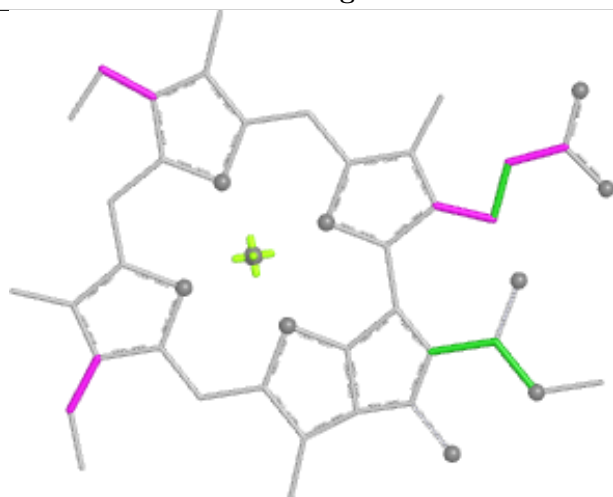
Ligand CLA 5 416



Bond lengths



Bond angles

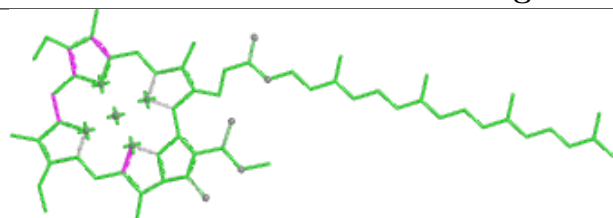


Torsions

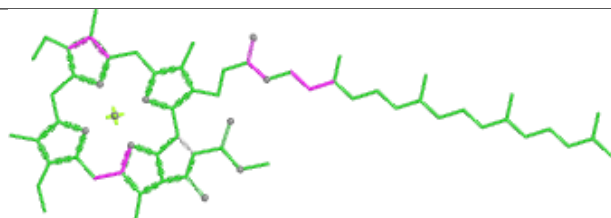


Rings

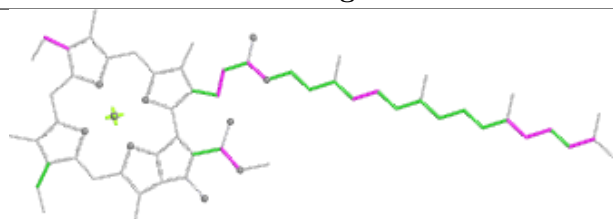
Ligand CLA A 824



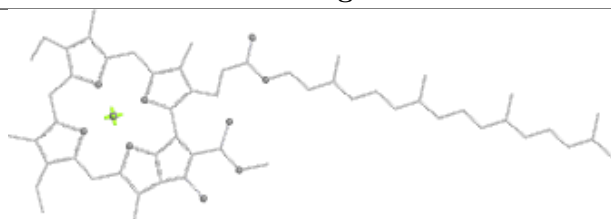
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

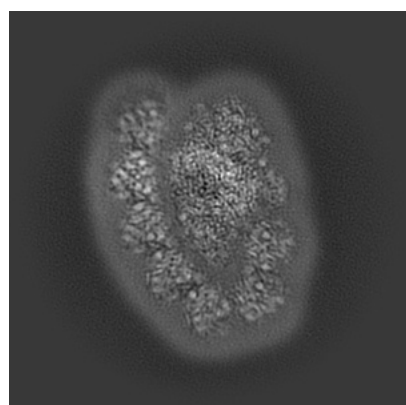
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74341. These allow visual inspection of the internal detail of the map and identification of artifacts.

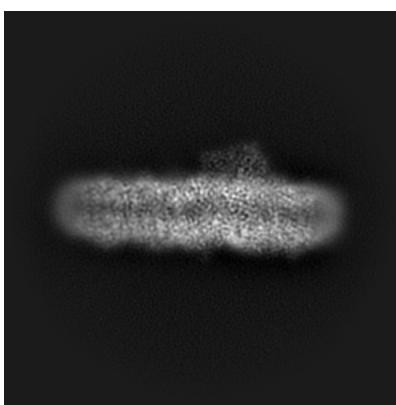
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

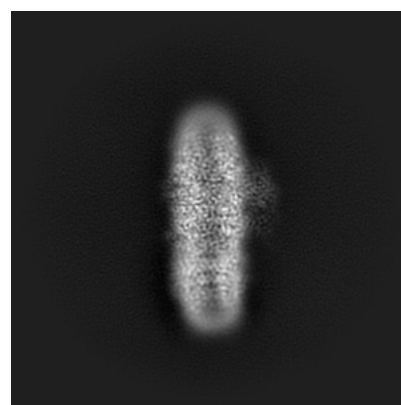
6.1.1 Primary map



X



Y

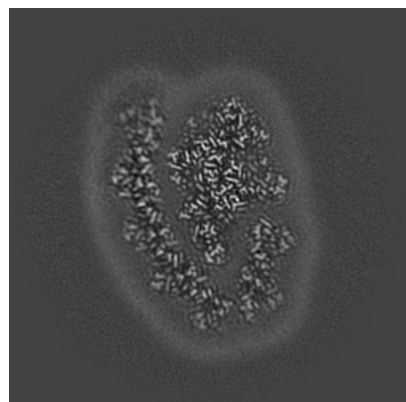


Z

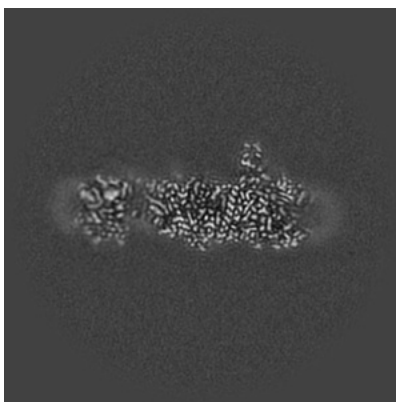
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

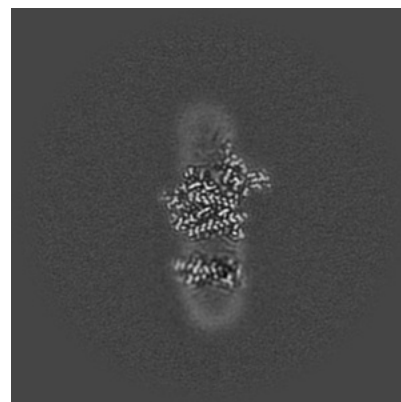
6.2.1 Primary map



X Index: 256



Y Index: 256

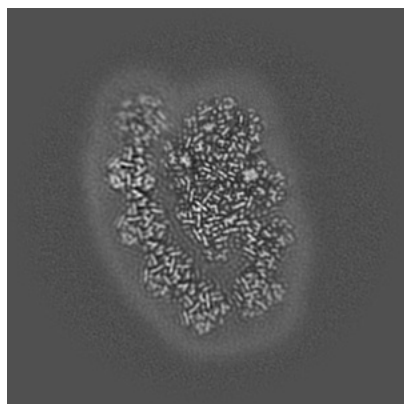


Z Index: 256

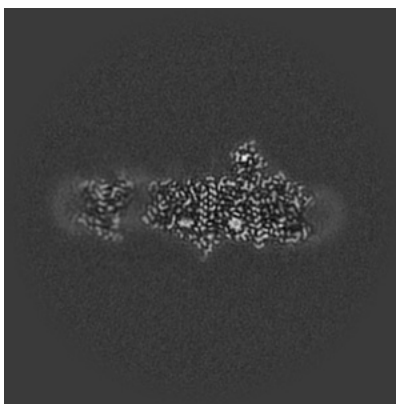
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

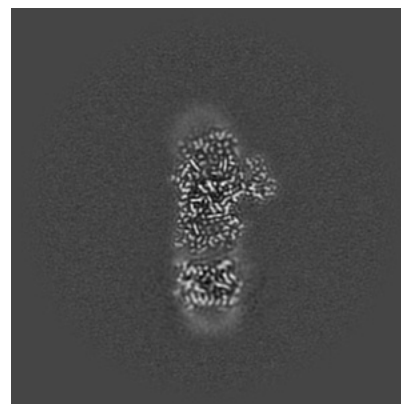
6.3.1 Primary map



X Index: 273



Y Index: 266

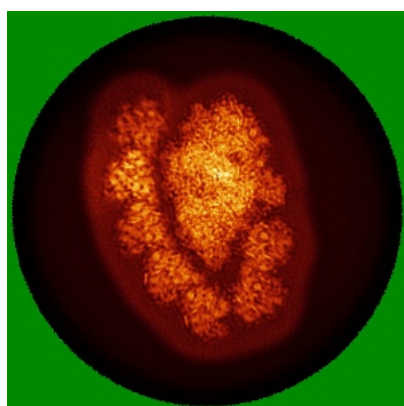


Z Index: 293

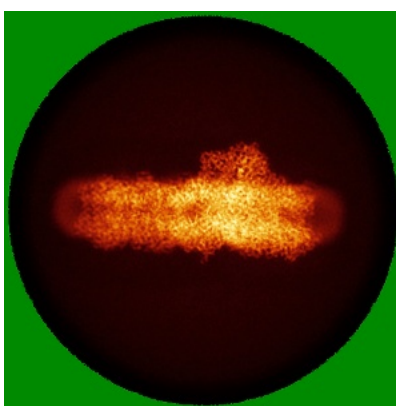
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

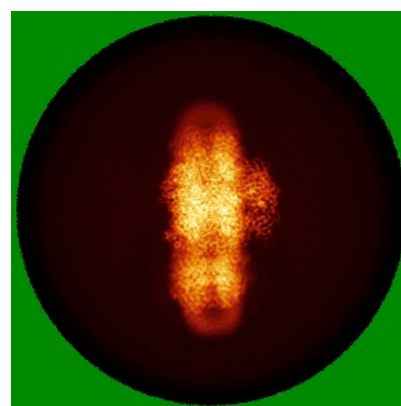
6.4.1 Primary map



X



Y

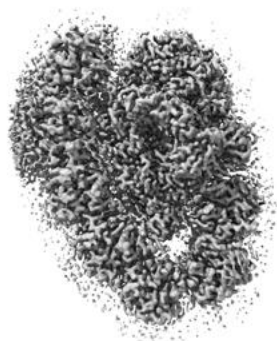


Z

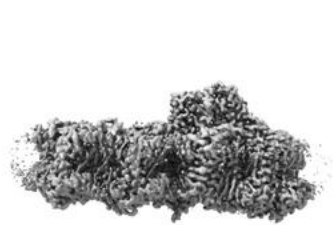
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

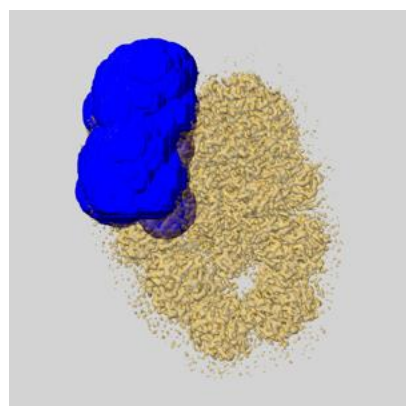
6.6 Mask visualisation [i](#)

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

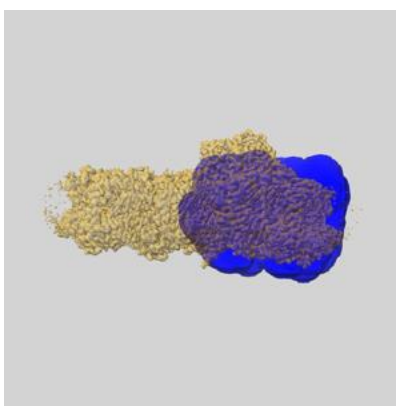
A mask typically either:

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

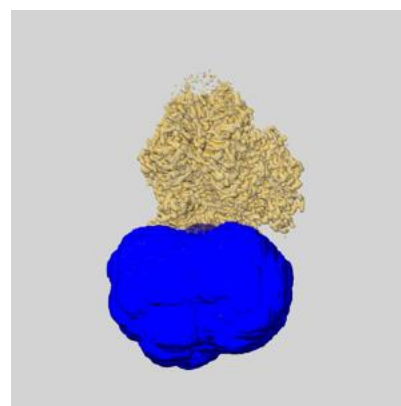
6.6.1 emd_74341_msk_1.map [i](#)



X

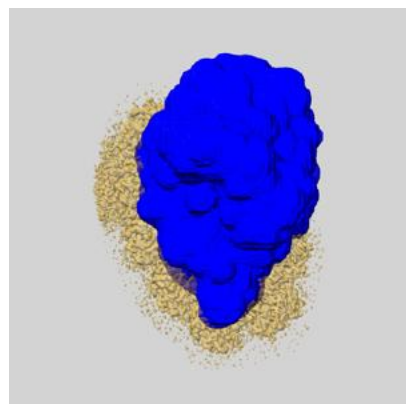


Y

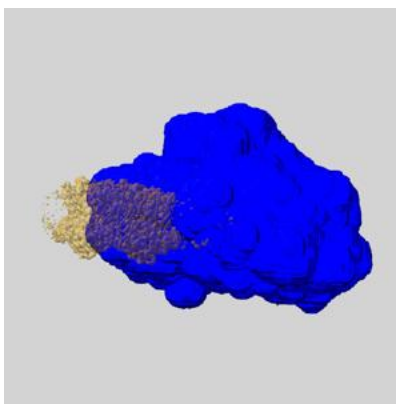


Z

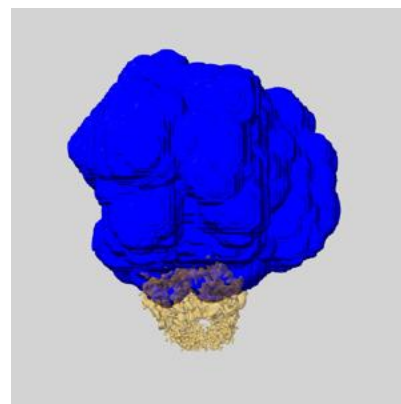
6.6.2 emd_74341_msk_2.map [i](#)



X

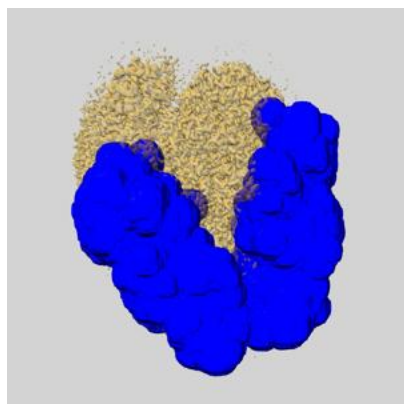


Y

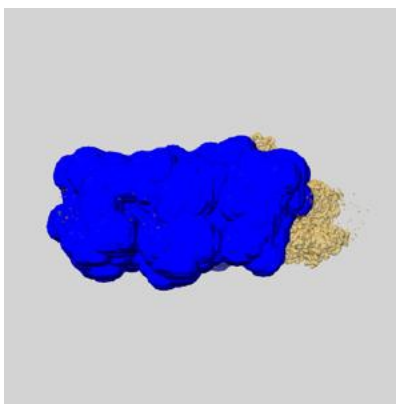


Z

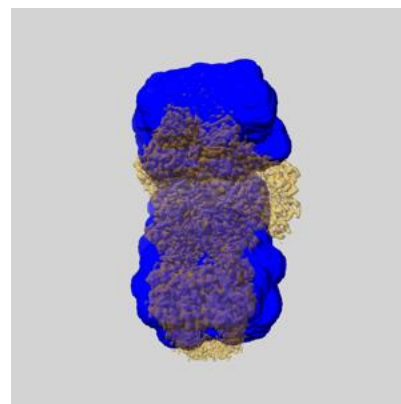
6.6.3 emd_74341_msk_3.map [i](#)



X



Y

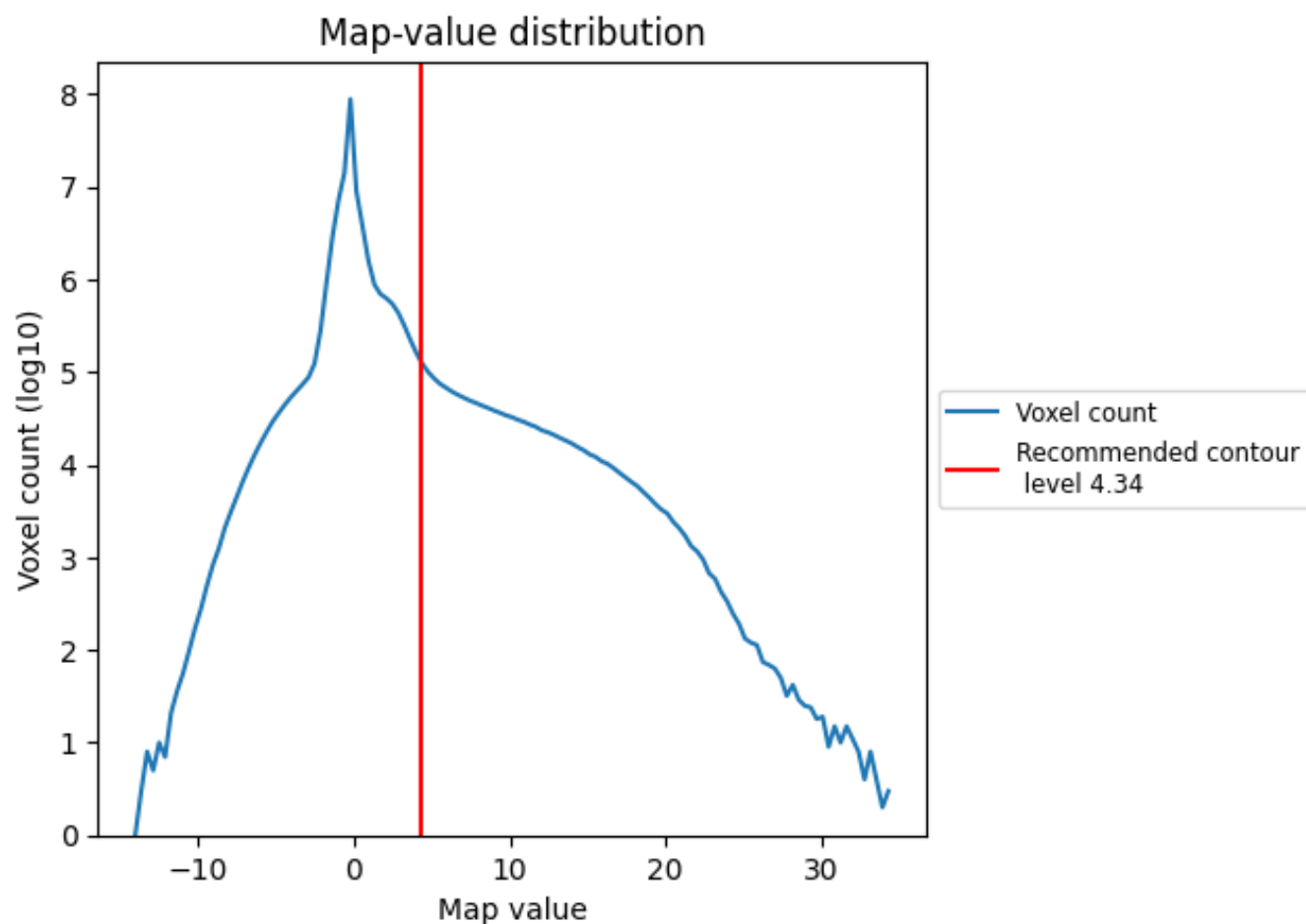


Z

7 Map analysis [i](#)

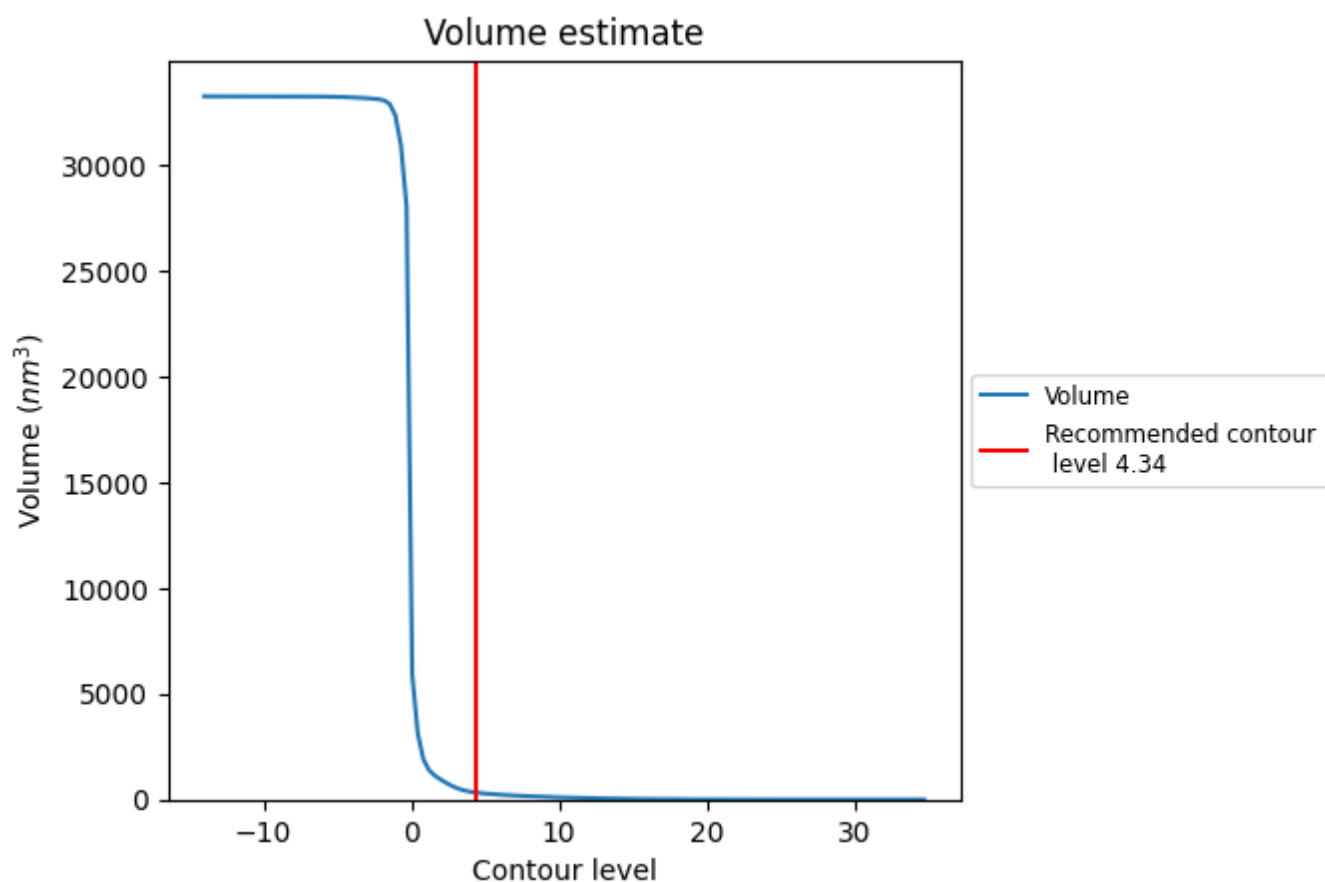
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

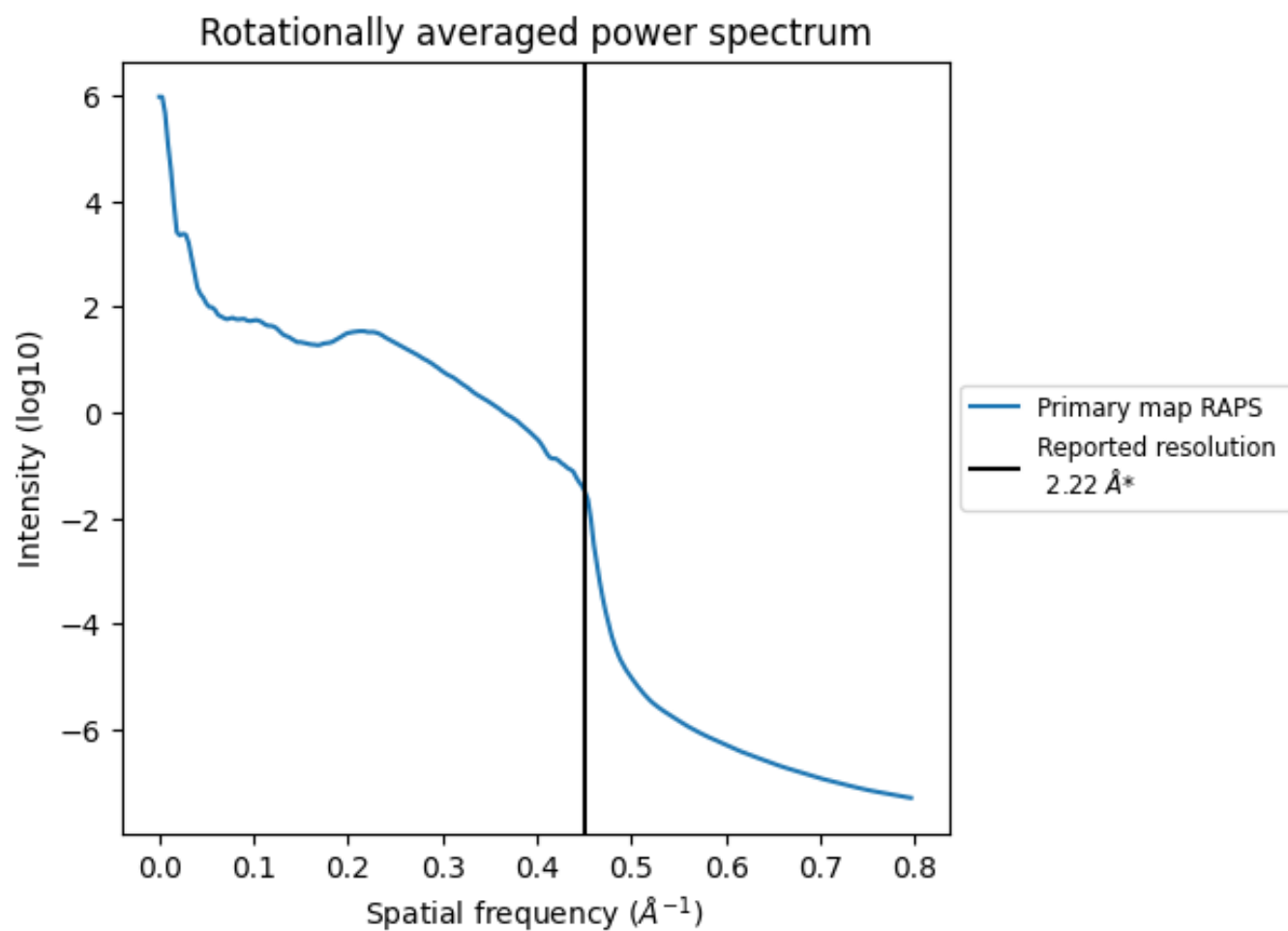
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm^3 ; this corresponds to an approximate mass of 301 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.450 Å⁻¹

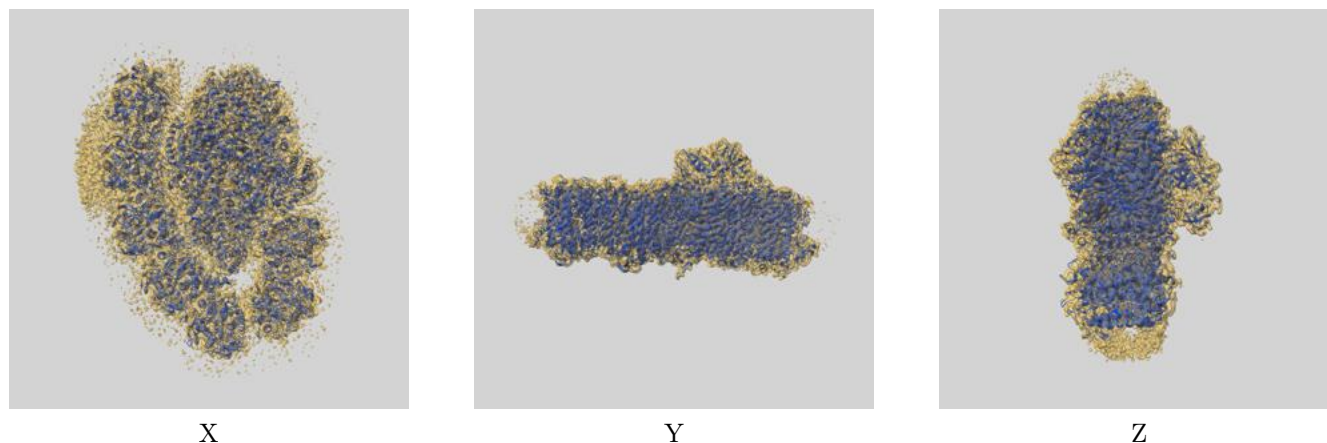
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

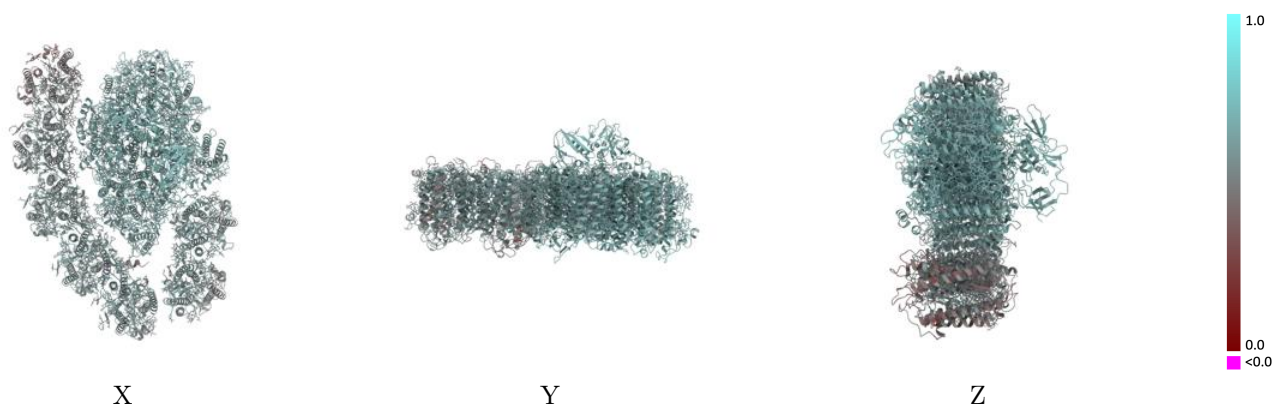
This section contains information regarding the fit between EMDB map EMD-74341 and PDB model 9ZJT. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



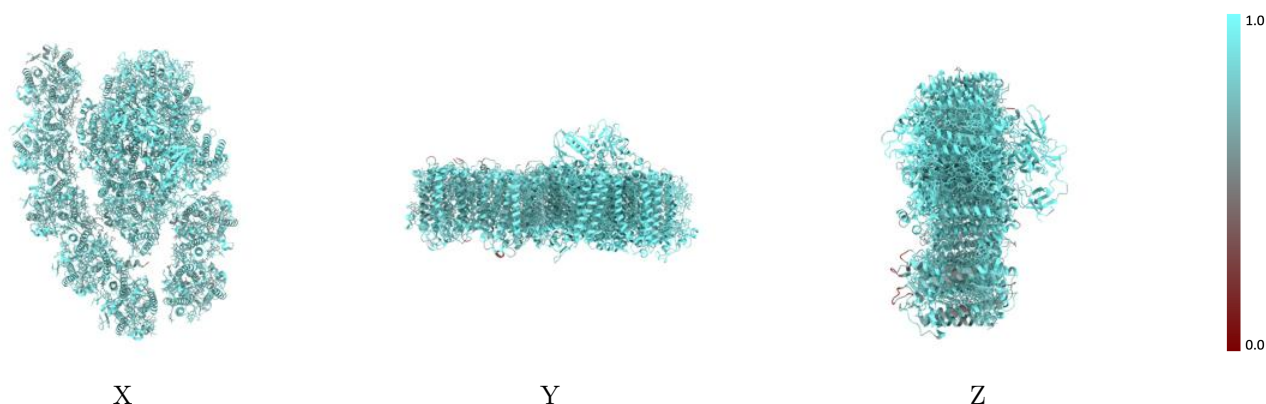
The images above show the 3D surface view of the map at the recommended contour level 4.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



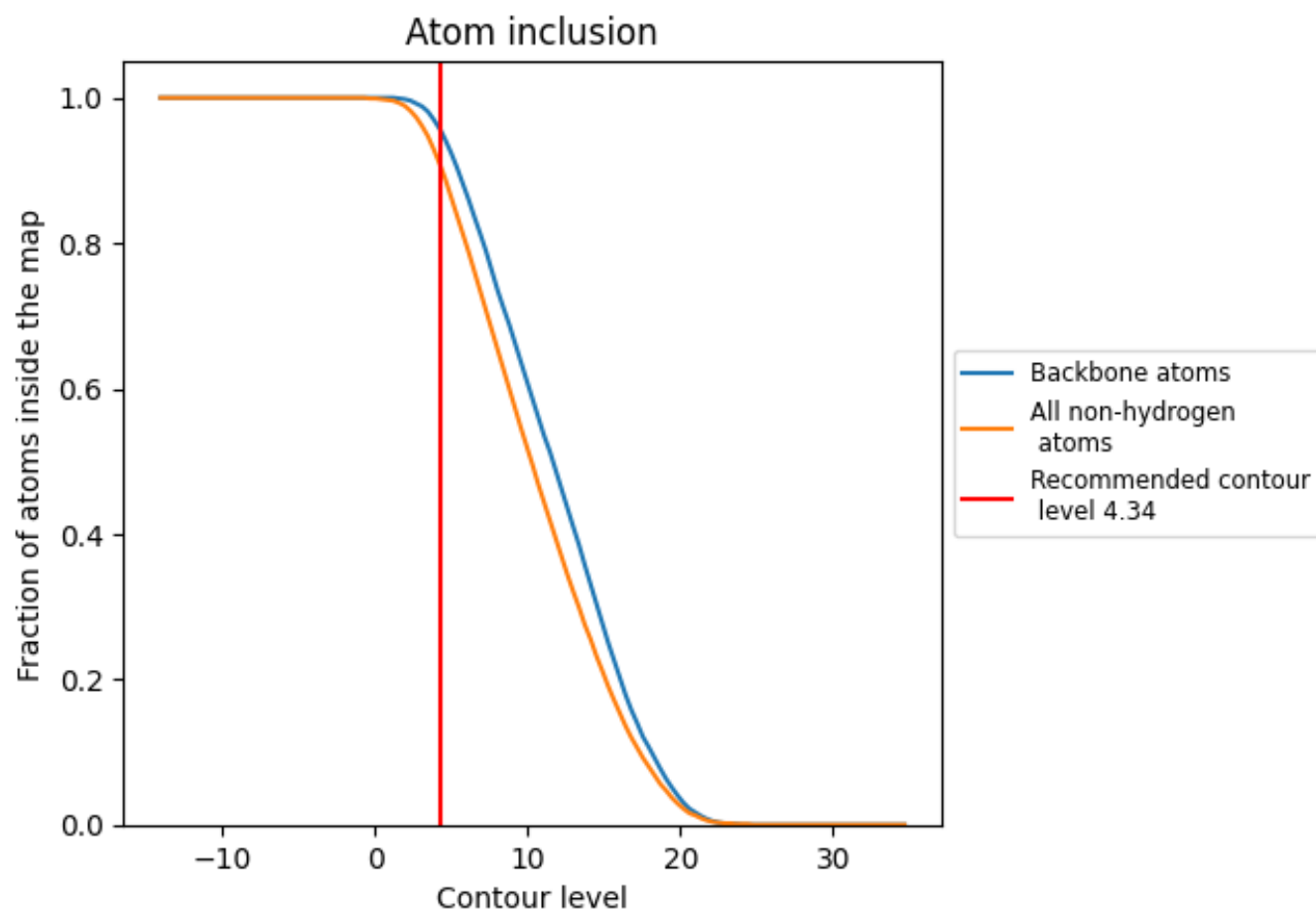
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.34).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.5950
1	 0.8670	 0.5670
2	 0.8270	 0.5480
3	 0.8560	 0.5600
4	 0.8830	 0.5690
5	 0.8750	 0.5580
6	 0.9130	 0.5280
7	 0.7690	 0.4610
A	 0.9670	 0.6610
B	 0.9560	 0.6520
C	 0.9850	 0.6620
D	 0.9530	 0.6440
E	 0.9350	 0.6350
F	 0.9390	 0.6410
I	 0.9370	 0.6230
J	 0.9600	 0.6390
K	 0.9110	 0.6230
M	 0.9520	 0.6390
X	 0.9280	 0.6300

