



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:19 PM UTC

PDB ID : 8ZOA / pdb_00008zoa
EMDB ID : EMD-60286
Title : Structure of the wild-type PSI-8VCPI supercomplex in *Nannochloropsis oceanica*
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 2.95 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

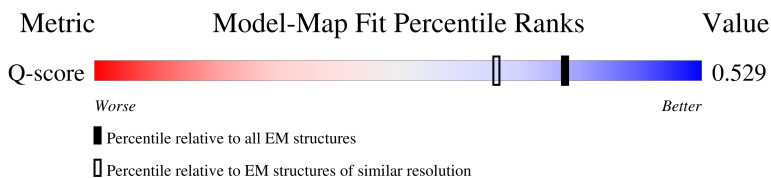
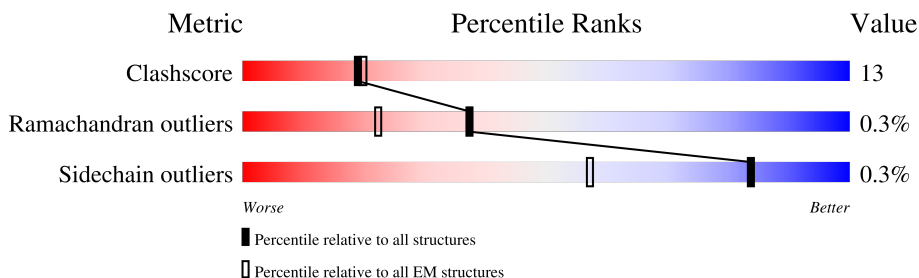
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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	13114 (2.45 - 3.45)

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	5	244	
2	9	232	
3	8	200	
4	4	202	

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Mol	Chain	Length	Quality of chain
4	7	202	
5	3	220	
6	2	223	
7	1	208	
8	a	745	
9	b	737	
10	d	136	
11	e	67	
12	f	185	
13	h	128	
14	i	45	
15	j	41	
16	l	172	
17	m	30	
18	g	55	
19	c	81	

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
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	312	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	1	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	306	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	2	309	X	-	-	-
22	CLA	2	310	X	-	-	-
22	CLA	2	311	X	-	-	-
22	CLA	2	312	X	-	-	-
22	CLA	2	313	X	-	-	-
22	CLA	2	314	X	-	-	-
22	CLA	2	315	X	-	-	-
22	CLA	2	316	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	314	X	-	-	-
22	CLA	3	315	X	-	-	-
22	CLA	4	306	X	-	-	-
22	CLA	4	307	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	4	311	X	-	-	-
22	CLA	4	312	X	-	-	-
22	CLA	4	313	X	-	-	-
22	CLA	4	314	X	-	-	-
22	CLA	4	315	X	-	-	-
22	CLA	4	316	X	-	-	-
22	CLA	4	317	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	306	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	315	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	308	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-
22	CLA	8	305	X	-	-	-
22	CLA	8	306	X	-	-	-
22	CLA	8	307	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	311	X	-	-	-
22	CLA	8	312	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	314	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	312	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	9	314	X	-	-	-
22	CLA	9	315	X	-	-	-
22	CLA	9	316	X	-	-	-
22	CLA	9	318	X	-	-	-
22	CLA	a	801	X	-	-	-
22	CLA	a	802	X	-	-	-
22	CLA	a	803	X	-	-	-
22	CLA	a	804	X	-	-	-
22	CLA	a	805	X	-	-	-
22	CLA	a	806	X	-	-	-
22	CLA	a	807	X	-	-	-
22	CLA	a	808	X	-	-	-
22	CLA	a	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	810	X	-	-	-
22	CLA	a	811	X	-	-	-
22	CLA	a	812	X	-	-	-
22	CLA	a	813	X	-	-	-
22	CLA	a	814	X	-	-	-
22	CLA	a	815	X	-	-	-
22	CLA	a	816	X	-	-	-
22	CLA	a	817	X	-	-	-
22	CLA	a	818	X	-	-	-
22	CLA	a	819	X	-	-	-
22	CLA	a	820	X	-	-	-
22	CLA	a	821	X	-	-	-
22	CLA	a	822	X	-	-	-
22	CLA	a	823	X	-	-	-
22	CLA	a	824	X	-	-	-
22	CLA	a	825	X	-	-	-
22	CLA	a	826	X	-	-	-
22	CLA	a	827	X	-	-	-
22	CLA	a	828	X	-	-	-
22	CLA	a	829	X	-	-	-
22	CLA	a	830	X	-	-	-
22	CLA	a	831	X	-	-	-
22	CLA	a	832	X	-	-	-
22	CLA	a	833	X	-	-	-
22	CLA	a	834	X	-	-	-
22	CLA	a	835	X	-	-	-
22	CLA	a	836	X	-	-	-
22	CLA	a	837	X	-	-	-
22	CLA	a	838	X	-	-	-
22	CLA	a	839	X	-	-	-
22	CLA	a	840	X	-	-	-
22	CLA	a	841	X	-	-	-
22	CLA	a	842	X	-	-	-
22	CLA	a	844	X	-	-	-
22	CLA	a	854	X	-	-	-
22	CLA	b	801	X	-	-	-
22	CLA	b	802	X	-	-	-
22	CLA	b	803	X	-	-	-
22	CLA	b	804	X	-	-	-
22	CLA	b	805	X	-	-	-
22	CLA	b	806	X	-	-	-
22	CLA	b	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	b	808	X	-	-	-
22	CLA	b	809	X	-	-	-
22	CLA	b	810	X	-	-	-
22	CLA	b	811	X	-	-	-
22	CLA	b	812	X	-	-	-
22	CLA	b	813	X	-	-	-
22	CLA	b	814	X	-	-	-
22	CLA	b	815	X	-	-	-
22	CLA	b	816	X	-	-	-
22	CLA	b	817	X	-	-	-
22	CLA	b	818	X	-	-	-
22	CLA	b	819	X	-	-	-
22	CLA	b	820	X	-	-	-
22	CLA	b	821	X	-	-	-
22	CLA	b	822	X	-	-	-
22	CLA	b	823	X	-	-	-
22	CLA	b	824	X	-	-	-
22	CLA	b	825	X	-	-	-
22	CLA	b	826	X	-	-	-
22	CLA	b	827	X	-	-	-
22	CLA	b	828	X	-	-	-
22	CLA	b	829	X	-	-	-
22	CLA	b	830	X	-	-	-
22	CLA	b	831	X	-	-	-
22	CLA	b	832	X	-	-	-
22	CLA	b	833	X	-	-	-
22	CLA	b	834	X	-	-	-
22	CLA	b	835	X	-	-	-
22	CLA	b	836	X	-	-	-
22	CLA	b	837	X	-	-	-
22	CLA	b	838	X	-	-	-
22	CLA	b	839	X	-	-	-
22	CLA	b	840	X	-	-	-
22	CLA	f	802	X	-	-	-
22	CLA	f	803	X	-	-	-
22	CLA	h	203	X	-	-	-
22	CLA	h	205	X	-	-	-
22	CLA	j	102	X	-	-	-
22	CLA	j	103	X	-	-	-
22	CLA	l	202	X	-	-	-
22	CLA	l	203	X	-	-	-
22	CLA	l	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SF4	c	102	-	-	X	-

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 41637 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 VCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	169	Total	C	N	O	S	0	0
			1317	867	222	222	6		

- Molecule 2 is a protein called VCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	201	Total	C	N	O	S	0	0
			1466	936	256	269	5		

- Molecule 3 is a protein called VCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	164	Total	C	N	O	S	0	0
			1258	822	203	227	6		

- Molecule 4 is a protein called VCPI-4/7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		
4	7	166	Total	C	N	O	S	0	0
			1220	791	202	222	5		

- Molecule 5 is a protein called VCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	177	Total	C	N	O	S	0	0
			1324	846	225	245	8		

- Molecule 6 is a protein called VCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 7 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	739	Total	C	N	O	S	0	0
			5827	3828	982	1000	17		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	735	Total	C	N	O	S	0	0
			5865	3874	985	989	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	130	Total	C	N	O	S	0	0
			1014	652	175	184	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	61	Total	C	N	O	0	0
			494	314	86	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	160	Total	C	N	O	S	0	0
			1266	815	213	235	3		

- Molecule 13 is a protein called Psar.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	h	85	Total	C	N	O	S	0	0
			646	427	100	117	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	i	34	Total	C	N	O	S	0	0
			271	189	36	45	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	j	41	Total	C	N	O	S	0	0
			339	233	48	57	1		

- Molecule 16 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	171	Total	C	N	O		0	0
			1283	848	203	232			

- Molecule 17 is a protein called PsaM.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	m	30	Total	C	N	O	0	0
			210	137	35	38		

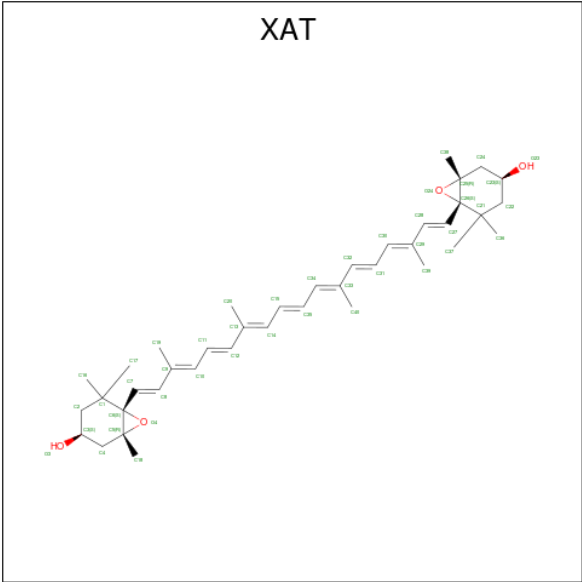
- Molecule 18 is a protein called PsaS.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	g	55	Total	C	N	O	0	0
			275	165	55	55		

- Molecule 19 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	80	Total	C	N	O	S	0	0
			596	366	103	117	10		

- Molecule 20 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



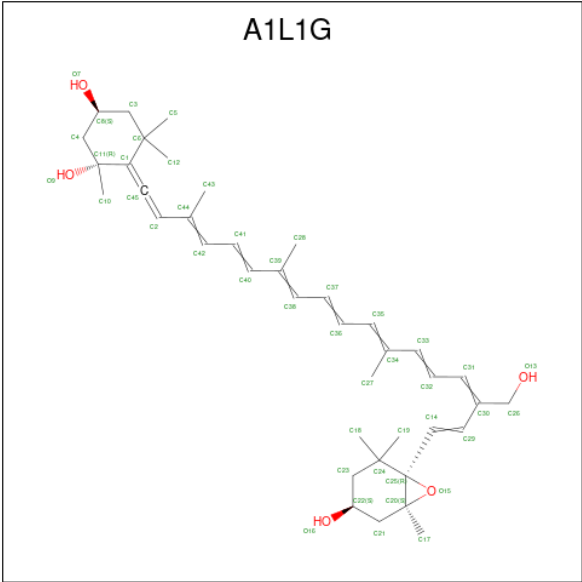
Mol	Chain	Residues	Atoms			AltConf
20	5	1	Total	C	O	0
			44	40	4	
20	5	1	Total	C	O	0
			44	40	4	
20	5	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	

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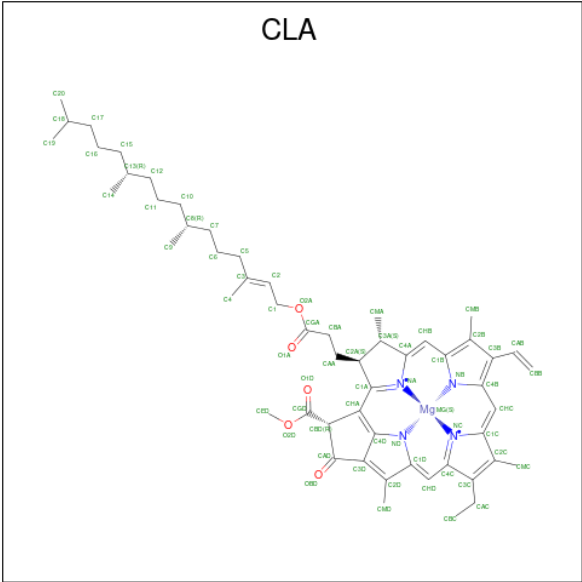
Mol	Chain	Residues	Atoms			AltConf
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	1	1	Total	C	O	0
			44	40	4	
20	1	1	Total	C	O	0
			44	40	4	
20	a	1	Total	C	O	0
			44	40	4	
20	j	1	Total	C	O	0
			44	40	4	

- Molecule 21 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxa bicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	5	1	Total	C	O	0
			45	40	5	
21	9	1	Total	C	O	0
			45	40	5	
21	9	1	Total	C	O	0
			45	40	5	
21	3	1	Total	C	O	0
			45	40	5	
21	3	1	Total	C	O	0
			45	40	5	
21	7	1	Total	C	O	0
			45	40	5	
21	1	1	Total	C	O	0
			45	40	5	

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	9	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	2	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	2	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 54	C 44	Mg 1	N 4	O 5	0

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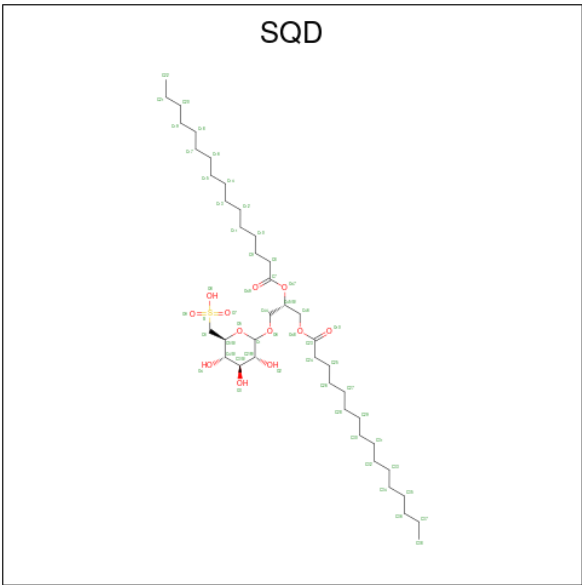
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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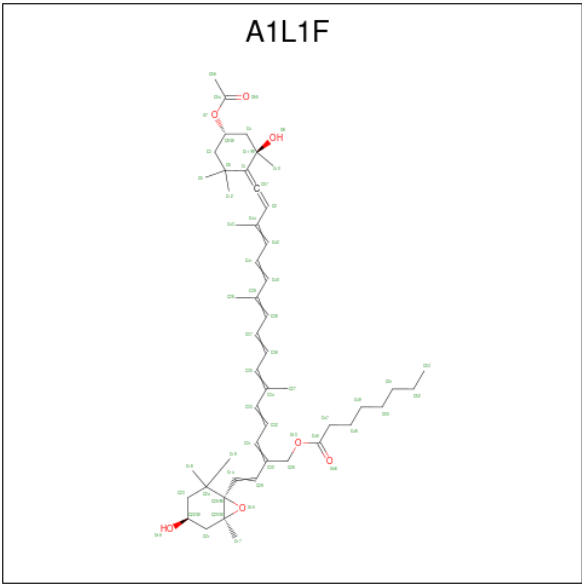
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



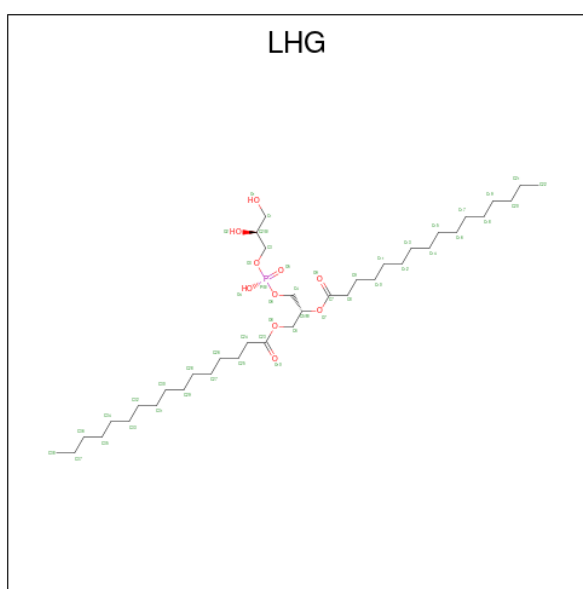
Mol	Chain	Residues	Atoms				AltConf
23	5	1	Total	C	O	S	0
			35	22	12	1	
23	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 24 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyl oxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S}, 6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,1 0,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C₅₀H₇₂O₇) (labeled as "Ligand of Interest" by depositor).



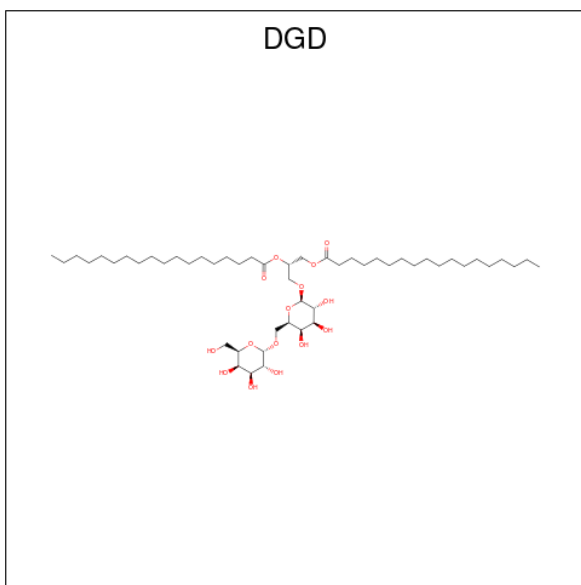
Mol	Chain	Residues	Atoms			AltConf
24	9	1	Total	C	O	0
			57	50	7	
24	8	1	Total	C	O	0
			57	50	7	
24	1	1	Total	C	O	0
			57	50	7	
24	h	1	Total	C	O	0
			57	50	7	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



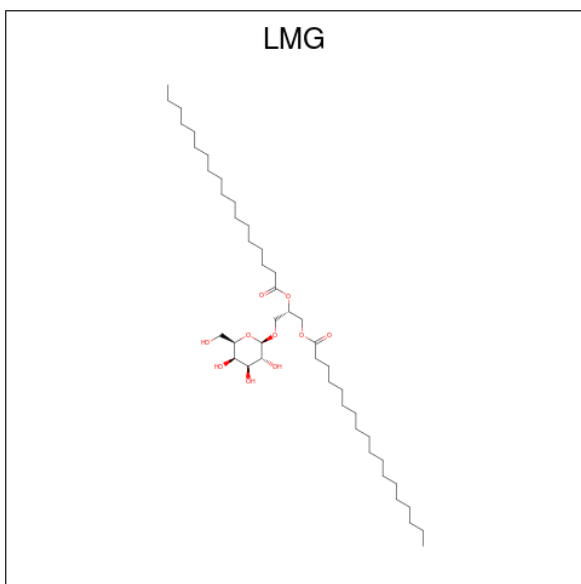
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O	P	0
			36	25	10	1	
25	9	1	Total	C	O	P	0
			46	35	10	1	
25	a	1	Total	C	O	P	0
			48	37	10	1	
25	a	1	Total	C	O	P	0
			27	16	10	1	
25	b	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



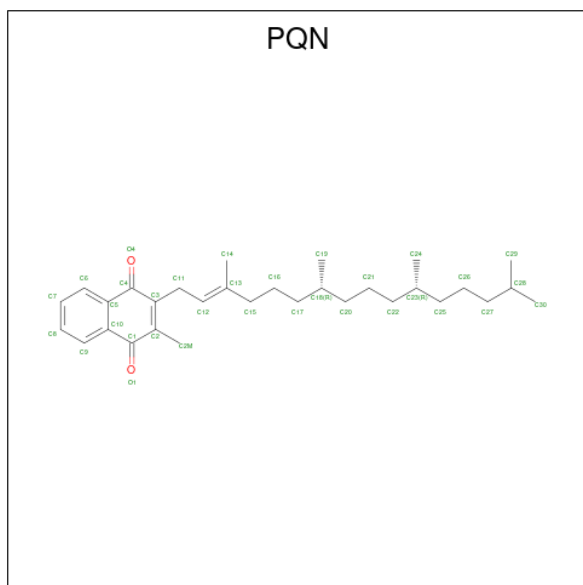
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	8	1	40	25	15	0
26	4	1	40	25	15	0
26	b	1	57	42	15	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



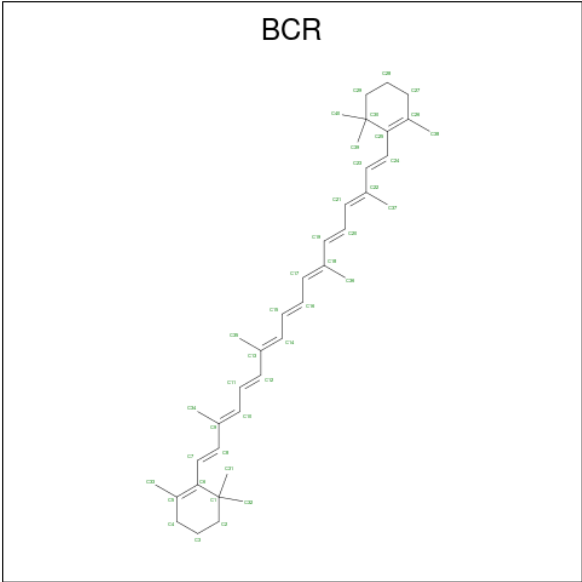
Mol	Chain	Residues	Atoms			AltConf
27	2	1	Total	C	O	0
			35	25	10	
27	a	1	Total	C	O	0
			34	24	10	
27	j	1	Total	C	O	0
			32	22	10	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	a	1	Total	C	O	0
			33	31	2	
28	b	1	Total	C	O	0
			33	31	2	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



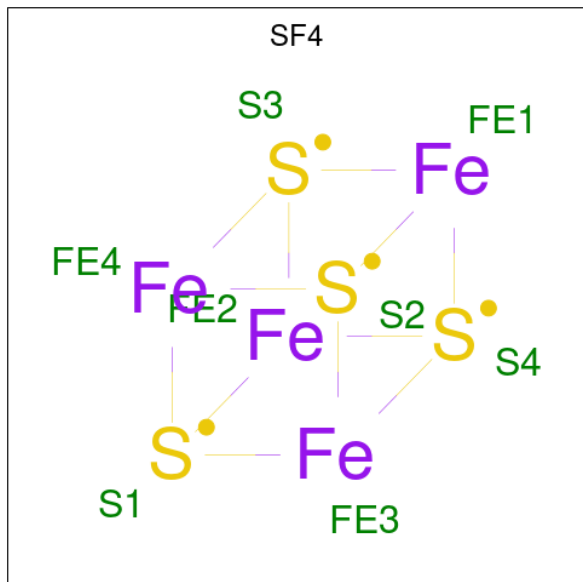
Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	C	0
			40	40	
29	a	1	Total	C	0
			40	40	
29	a	1	Total	C	0
			40	40	
29	a	1	Total	C	0
			40	40	
29	b	1	Total	C	0
			40	40	
29	b	1	Total	C	0
			40	40	
29	b	1	Total	C	0
			40	40	
29	b	1	Total	C	0
			40	40	
29	b	1	Total	C	0
			40	40	
29	f	1	Total	C	0
			40	40	
29	f	1	Total	C	0
			40	40	
29	h	1	Total	C	0
			40	40	
29	h	1	Total	C	0
			40	40	

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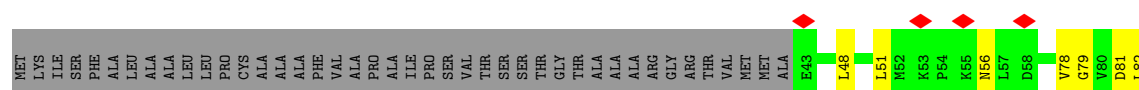
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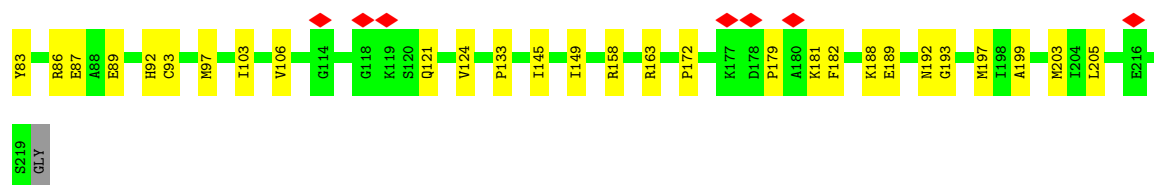
Mol	Chain	Residues	Atoms	AltConf
29	i	1	Total C 40 40	0
29	j	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	m	1	Total C 40 40	0

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

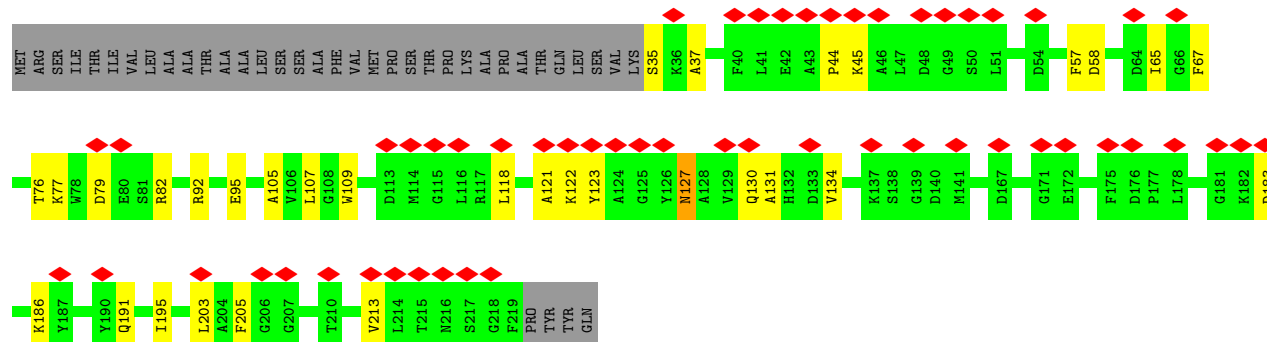


Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total Fe S 8 4 4	0
30	c	1	Total Fe S 8 4 4	0
30	c	1	Total Fe S 8 4 4	0

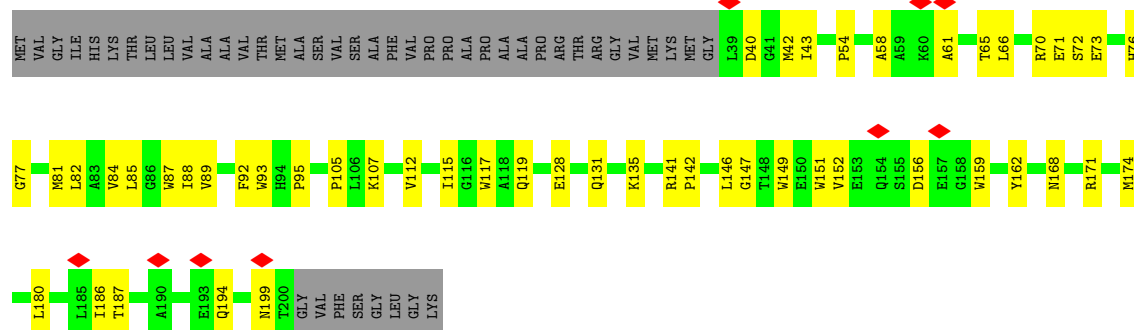




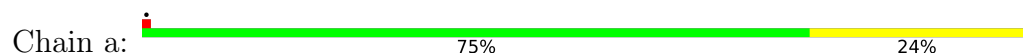
• Molecule 6: VCPI-2

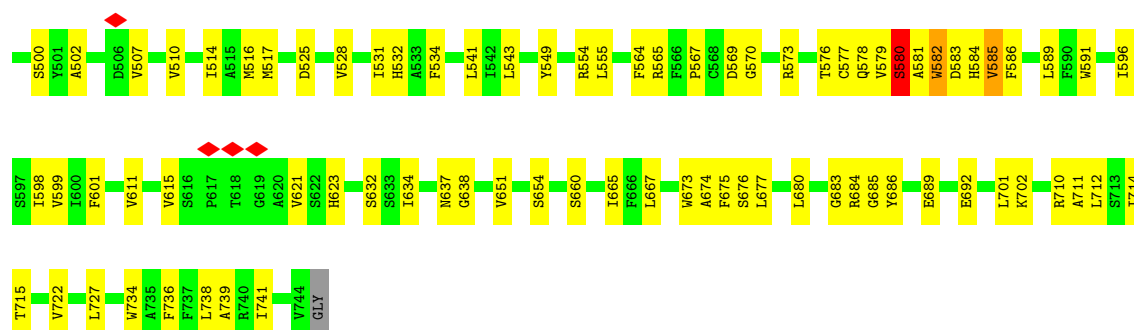


• Molecule 7: VCPI-1

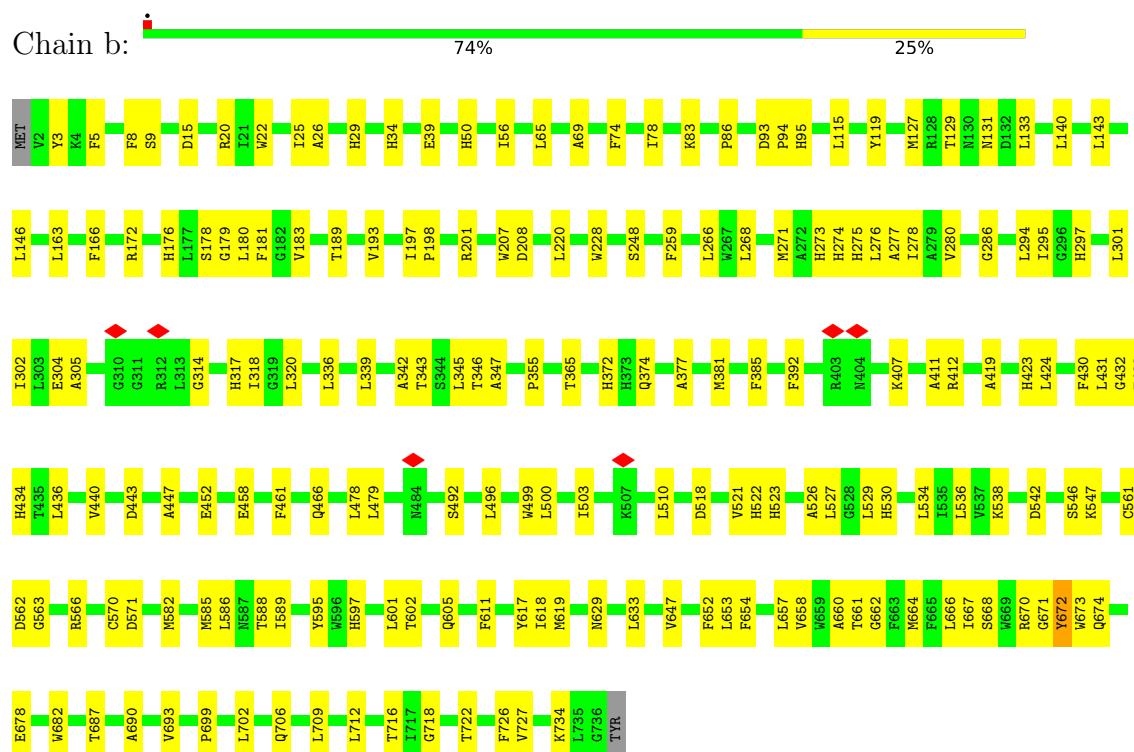


• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A1

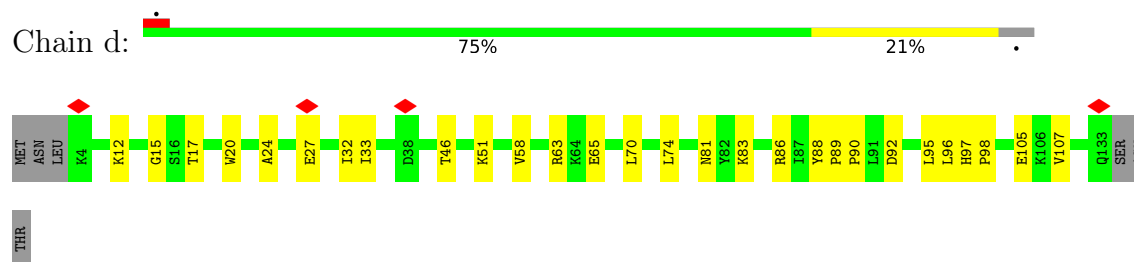




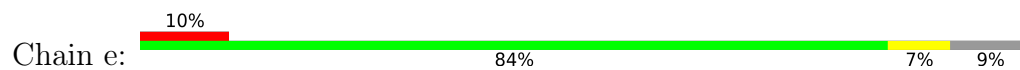
• Molecule 9: Photosystem I P700 chlorophyll a apoprotein A2

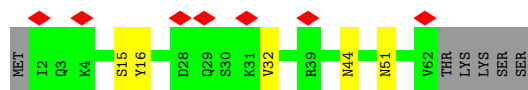


• Molecule 10: Photosystem I reaction center subunit II



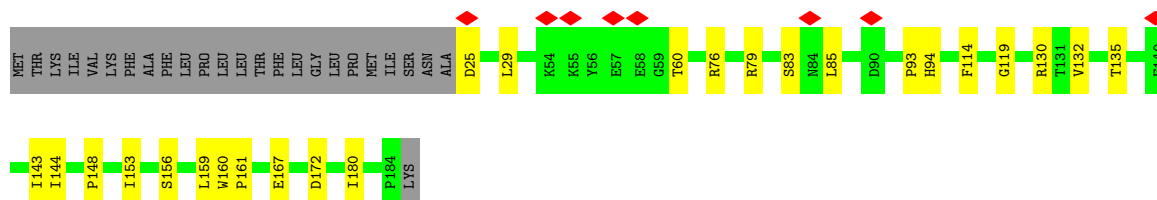
• Molecule 11: Photosystem I reaction center subunit IV





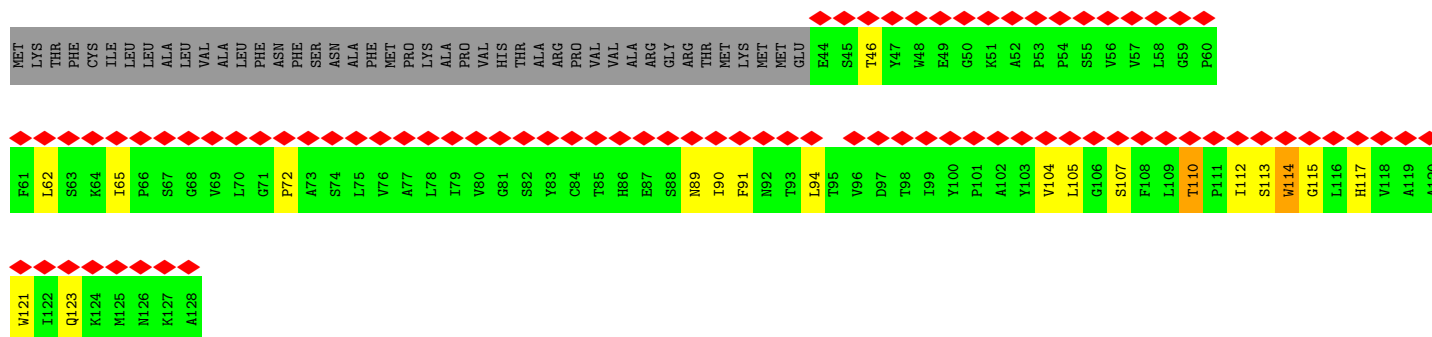
- Molecule 12: Photosystem I reaction center subunit III

Chain f: 73% 14% 14%



- Molecule 13: PsaR

Chain h: 52% 13% 34%



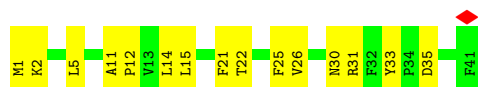
- Molecule 14: Photosystem I reaction center subunit VIII

Chain i: 7% 53% 22% 24%



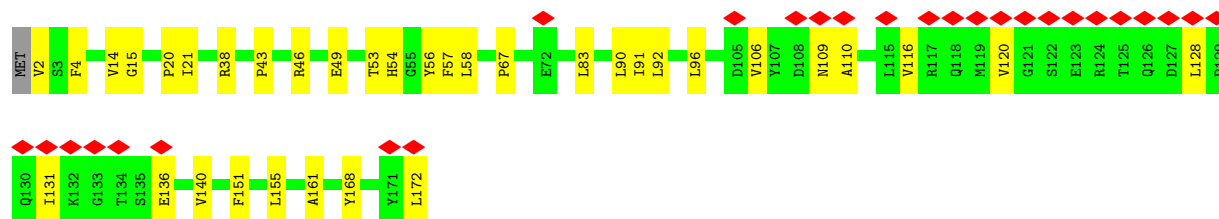
- Molecule 15: Photosystem I reaction center subunit IX

Chain j: 63% 37%



- Molecule 16: PSI subunit V

Chain l: 16% 79% 20%



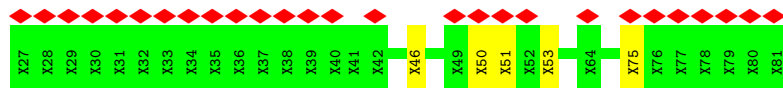
- Molecule 17: PsaM

Chain m: 90% 10%



- Molecule 18: PsaS

Chain g: 49% 91% 9%



- Molecule 19: Photosystem I iron-sulfur center

Chain c: 70% 28%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60260	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.545	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.295	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: BCR, PQN, A1L1F, SF4, DGD, LMG, XAT, SQD, LHG, A1L1G, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	5	0.14	0/1353	0.29	0/1823
2	9	0.34	0/1496	0.34	0/2032
3	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
4	4	0.17	0/1298	0.31	0/1761
4	7	0.19	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.27	0/1821
6	2	0.14	0/1405	0.36	0/1904
7	1	0.13	0/1293	0.33	0/1759
8	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
9	b	0.20	0/6080	0.32	1/8302 (0.0%)
10	d	0.12	0/1040	0.32	0/1402
11	e	0.09	0/502	0.20	0/681
12	f	0.14	0/1297	0.30	0/1762
13	h	0.52	1/667 (0.1%)	0.52	0/915
14	i	0.15	0/278	0.33	0/378
15	j	0.15	0/351	0.36	0/478
16	l	0.14	0/1315	0.31	0/1796
17	m	0.09	0/210	0.28	0/288
19	c	0.13	0/606	0.34	0/822
All	All	0.24	5/29099 (0.0%)	0.33	8/39586 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	580	SER	CA-C	-7.02	1.43	1.52
3	8	44	LEU	C-O	-6.16	1.15	1.23
8	a	581	ALA	CA-C	-5.42	1.45	1.52
13	h	114	TRP	C-O	-5.28	1.18	1.24
8	a	582	TRP	CA-C	-5.08	1.45	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	581	ALA	N-CA-C	-8.63	102.50	113.72
8	a	448	LEU	N-CA-C	-6.11	104.18	111.69
3	8	39	LYS	N-CA-C	-6.10	105.66	113.23
8	a	584	HIS	N-CA-C	-5.81	106.53	113.97
9	b	672	TYR	N-CA-C	-5.59	106.30	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5	1317	0	1318	37	0
2	9	1466	0	1470	46	0
3	8	1258	0	1280	33	0
4	4	1268	0	1288	22	0
4	7	1220	0	1209	41	0
5	3	1324	0	1340	25	0
6	2	1372	0	1347	21	0
7	1	1262	0	1237	37	0
8	a	5827	0	5697	140	0
9	b	5865	0	5710	157	0
10	d	1014	0	1015	22	0
11	e	494	0	495	5	0
12	f	1266	0	1262	21	0
13	h	646	0	649	18	0
14	i	271	0	292	12	0
15	j	339	0	342	20	0
16	l	1283	0	1278	28	0
17	m	210	0	226	3	0
18	g	275	0	62	3	0
19	c	596	0	583	20	0
20	1	88	0	112	7	0
20	2	220	0	280	20	0
20	3	176	0	224	19	0
20	4	220	0	280	31	0
20	5	132	0	168	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	7	176	0	224	25	0
20	8	132	0	168	12	0
20	9	132	0	168	17	0
20	a	44	0	56	6	0
20	j	44	0	56	7	0
21	1	45	0	0	1	0
21	3	90	0	0	0	0
21	5	45	0	0	1	0
21	7	45	0	0	2	0
21	9	90	0	0	3	0
22	1	547	0	508	15	0
22	2	544	0	452	13	0
22	3	458	0	378	9	0
22	4	613	0	522	32	0
22	5	563	0	472	22	0
22	7	576	0	444	23	0
22	8	507	0	429	20	0
22	9	519	0	452	34	0
22	a	2579	0	2562	138	0
22	b	2410	0	2464	133	0
22	f	117	0	115	2	0
22	h	120	0	121	6	0
22	j	100	0	86	9	0
22	l	148	0	123	3	0
23	1	45	0	54	2	0
23	5	35	0	34	1	0
24	1	57	0	0	2	0
24	8	57	0	0	2	0
24	9	57	0	0	2	0
24	h	57	0	0	4	0
25	9	82	0	110	5	0
25	a	75	0	93	6	0
25	b	31	0	32	0	0
26	4	40	0	38	11	0
26	8	40	0	38	2	0
26	b	57	0	72	6	0
27	2	35	0	40	3	0
27	a	34	0	38	10	0
27	j	32	0	34	7	0
28	a	33	0	46	4	0
28	b	33	0	46	3	0
29	a	160	0	224	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	b	240	0	336	24	0
29	f	80	0	112	14	0
29	h	80	0	112	6	0
29	i	40	0	56	3	0
29	j	40	0	56	9	0
29	l	80	0	112	14	0
29	m	40	0	56	2	0
30	a	8	0	0	0	0
30	c	16	0	0	3	0
All	All	41637	0	40703	1052	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 13.

The worst 5 of 1052 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:193:ALA:HB1	26:4:318:DGD:HE62	1.13	1.13
4:4:193:ALA:HB1	26:4:318:DGD:C6E	1.84	1.07
26:4:318:DGD:O4E	26:4:318:DGD:O5E	1.61	0.91
20:2:303:XAT:H32	22:2:308:CLA:HAB	1.52	0.90
20:5:302:XAT:H12	22:5:307:CLA:HAB	1.53	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	24	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	21	45
4	7	164/202 (81%)	144 (88%)	20 (12%)	0	100	100
5	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
6	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	7	21
7	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
8	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	72
9	b	633/737 (86%)	606 (96%)	27 (4%)	0	100	100
10	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
11	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
12	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
13	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	10	28
14	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
15	j	39/41 (95%)	39 (100%)	0	0	100	100
16	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	10	28
17	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
19	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3520/4098 (86%)	3297 (94%)	214 (6%)	9 (0%)	37	59

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR
6	2	45	LYS
16	1	120	VAL
6	2	127	ASN
6	2	213	VAL

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	5	133/182 (73%)	133 (100%)	0	100	100
2	9	91/167 (54%)	91 (100%)	0	100	100
3	8	84/160 (52%)	83 (99%)	1 (1%)	63	79
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	121/159 (76%)	120 (99%)	1 (1%)	73	85
5	3	17/164 (10%)	17 (100%)	0	100	100
6	2	36/172 (21%)	36 (100%)	0	100	100
7	1	128/165 (78%)	128 (100%)	0	100	100
8	a	607/613 (99%)	603 (99%)	4 (1%)	76	87
9	b	599/602 (100%)	599 (100%)	0	100	100
10	d	107/113 (95%)	107 (100%)	0	100	100
11	e	56/62 (90%)	56 (100%)	0	100	100
12	f	138/162 (85%)	138 (100%)	0	100	100
13	h	71/107 (66%)	70 (99%)	1 (1%)	59	77
14	i	32/43 (74%)	32 (100%)	0	100	100
15	j	36/36 (100%)	36 (100%)	0	100	100
16	l	130/141 (92%)	130 (100%)	0	100	100
17	m	21/24 (88%)	21 (100%)	0	100	100
19	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2607/3299 (79%)	2600 (100%)	7 (0%)	84	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	a	448	LEU
8	a	579	VAL
13	h	110	THR
8	a	580	SER
8	a	428	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
9	b	605	GLN
12	f	166	GLN

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Mol	Chain	Res	Type
10	d	7	GLN
8	a	435	ASN
9	b	373	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

257 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	$\# Z > 2$
20	XAT	3	303	-	41,47,47	0.89	2 (4%)	54,74,74	2.60	20 (37%)
20	XAT	a	852	-	41,47,47	0.92	2 (4%)	54,74,74	2.71	18 (33%)
22	CLA	7	310	-	50,54,73	1.37	7 (14%)	59,90,113	1.40	4 (6%)
22	CLA	b	806	-	69,73,73	1.16	6 (8%)	82,113,113	1.30	6 (7%)
22	CLA	l	202	-	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)
29	BCR	b	842	-	41,41,41	0.64	0	56,56,56	2.31	21 (37%)
20	XAT	9	303	-	41,47,47	0.95	2 (4%)	54,74,74	2.62	20 (37%)
20	XAT	2	301	-	41,47,47	0.92	2 (4%)	54,74,74	2.72	18 (33%)
22	CLA	7	313	-	58,62,73	1.29	7 (12%)	68,99,113	1.35	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	838	-	55,59,73	1.31	8 (14%)	64,96,113	1.40	6 (9%)
22	CLA	b	817	-	63,67,73	1.23	8 (12%)	74,105,113	1.36	9 (12%)
22	CLA	b	838	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	f	802	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	a	816	-	54,58,73	1.32	8 (14%)	64,95,113	1.41	7 (10%)
22	CLA	a	827	-	69,73,73	1.16	7 (10%)	82,113,113	1.31	7 (8%)
20	XAT	8	301	-	41,47,47	0.92	2 (4%)	54,74,74	2.55	18 (33%)
22	CLA	9	309	2	50,54,73	1.36	8 (16%)	59,90,113	1.36	5 (8%)
22	CLA	1	310	7	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
22	CLA	a	840	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
29	BCR	a	849	-	41,41,41	0.67	0	56,56,56	2.19	22 (39%)
21	A1L1G	1	301	-	40,47,47	1.14	5 (12%)	49,71,71	1.46	10 (20%)
26	DGD	b	848	-	58,58,67	1.13	4 (6%)	72,72,81	1.50	10 (13%)
22	CLA	4	312	-	50,54,73	1.37	8 (16%)	59,90,113	1.37	4 (6%)
29	BCR	l	201	-	41,41,41	0.68	0	56,56,56	1.98	17 (30%)
22	CLA	a	842	-	69,73,73	1.19	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	3	312	5	63,67,73	1.23	8 (12%)	74,105,113	1.29	4 (5%)
22	CLA	a	804	-	59,63,73	1.27	7 (11%)	70,101,113	1.40	8 (11%)
22	CLA	2	316	6	50,54,73	1.37	8 (16%)	59,90,113	1.40	4 (6%)
22	CLA	a	810	8	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
29	BCR	m	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	6 (10%)
22	CLA	b	822	-	64,68,73	1.21	7 (10%)	76,107,113	1.26	5 (6%)
20	XAT	5	302	-	41,47,47	0.95	2 (4%)	54,74,74	2.59	19 (35%)
22	CLA	a	813	-	58,62,73	1.28	8 (13%)	68,99,113	1.31	5 (7%)
22	CLA	a	854	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
29	BCR	l	205	-	41,41,41	0.66	0	56,56,56	2.04	15 (26%)
22	CLA	2	312	-	51,55,73	1.36	8 (15%)	60,91,113	1.41	5 (8%)
20	XAT	5	304	-	41,47,47	0.86	2 (4%)	54,74,74	2.85	20 (37%)
22	CLA	7	307	-	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
22	CLA	7	306	4	52,56,73	1.36	7 (13%)	61,92,113	1.36	5 (8%)
22	CLA	a	830	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
20	XAT	4	301	-	41,47,47	0.97	2 (4%)	54,74,74	2.63	19 (35%)
20	XAT	7	305	-	41,47,47	0.87	2 (4%)	54,74,74	2.66	19 (35%)
29	BCR	j	104	-	41,41,41	0.68	0	56,56,56	2.09	17 (30%)
22	CLA	5	314	-	56,60,73	1.30	6 (10%)	65,97,113	1.40	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	f	804	-	41,41,41	0.69	0	56,56,56	2.05	14 (25%)
22	CLA	b	809	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
22	CLA	5	307	1	64,68,73	1.20	6 (9%)	76,107,113	1.28	6 (7%)
20	XAT	3	305	-	41,47,47	0.89	2 (4%)	54,74,74	2.58	18 (33%)
20	XAT	7	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.64	19 (35%)
22	CLA	a	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
22	CLA	b	810	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
22	CLA	1	312	7	56,60,73	1.32	7 (12%)	65,97,113	1.36	5 (7%)
20	XAT	4	303	-	41,47,47	0.92	2 (4%)	54,74,74	2.58	17 (31%)
20	XAT	8	302	-	41,47,47	0.94	2 (4%)	54,74,74	2.66	18 (33%)
22	CLA	b	820	-	54,58,73	1.32	7 (12%)	64,95,113	1.44	7 (10%)
22	CLA	b	837	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	6 (7%)
22	CLA	l	203	-	64,68,73	1.21	9 (14%)	76,107,113	1.35	5 (6%)
22	CLA	4	311	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	5 (8%)
22	CLA	b	832	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	b	839	-	69,73,73	1.18	6 (8%)	82,113,113	1.31	6 (7%)
29	BCR	b	845	-	41,41,41	0.65	0	56,56,56	2.22	22 (39%)
20	XAT	8	303	-	41,47,47	0.87	2 (4%)	54,74,74	2.66	18 (33%)
22	CLA	a	802	-	62,66,73	1.22	8 (12%)	73,104,113	1.35	7 (9%)
22	CLA	j	102	-	62,66,73	1.24	6 (9%)	73,104,113	1.30	5 (6%)
22	CLA	4	313	-	57,61,73	1.29	7 (12%)	67,98,113	1.31	7 (10%)
21	A1L1G	9	306	-	40,47,47	1.14	4 (10%)	49,71,71	1.44	7 (14%)
22	CLA	8	310	-	50,54,73	1.38	8 (16%)	59,90,113	1.38	5 (8%)
22	CLA	a	819	-	58,62,73	1.28	8 (13%)	68,99,113	1.33	5 (7%)
22	CLA	3	314	5	51,55,73	1.36	7 (13%)	60,91,113	1.40	4 (6%)
22	CLA	b	801	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	b	831	-	53,57,73	1.32	6 (11%)	61,93,113	1.39	5 (8%)
22	CLA	8	314	-	45,49,73	1.43	7 (15%)	54,84,113	1.47	5 (9%)
22	CLA	a	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	9	310	-	50,54,73	1.37	7 (14%)	59,90,113	1.48	4 (6%)
22	CLA	4	307	-	60,64,73	1.27	6 (10%)	71,102,113	1.32	6 (8%)
22	CLA	b	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
22	CLA	8	307	3	69,73,73	1.17	6 (8%)	82,113,113	1.25	5 (6%)
22	CLA	8	309	-	61,65,73	1.25	7 (11%)	72,103,113	1.33	6 (8%)
25	LHG	a	846	22	26,26,48	1.30	5 (19%)	29,32,54	1.18	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	305	1	50,54,73	1.37	7 (14%)	59,90,113	1.39	4 (6%)
22	CLA	a	805	22	59,63,73	1.26	7 (11%)	70,101,113	1.35	6 (8%)
22	CLA	3	315	5	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)
20	XAT	2	303	-	41,47,47	1.01	2 (4%)	54,74,74	2.63	17 (31%)
22	CLA	b	802	-	69,73,73	1.17	7 (10%)	82,113,113	1.18	5 (6%)
24	A1L1F	1	304	-	52,59,59	1.41	6 (11%)	63,85,85	2.26	18 (28%)
22	CLA	j	103	15	46,50,73	1.40	7 (15%)	53,85,113	1.48	4 (7%)
24	A1L1F	h	204	-	52,59,59	1.47	6 (11%)	63,85,85	2.59	22 (34%)
20	XAT	j	101	-	41,47,47	0.87	2 (4%)	54,74,74	2.73	18 (33%)
20	XAT	7	303	-	41,47,47	1.00	2 (4%)	54,74,74	2.60	18 (33%)
22	CLA	4	306	4	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
24	A1L1F	9	302	-	52,59,59	1.48	6 (11%)	63,85,85	2.55	20 (31%)
22	CLA	b	823	-	57,61,73	1.29	7 (12%)	67,98,113	1.35	6 (8%)
22	CLA	7	311	-	50,54,73	1.38	8 (16%)	59,90,113	1.40	5 (8%)
29	BCR	b	846	-	41,41,41	0.69	0	56,56,56	1.81	14 (25%)
21	A1L1G	5	303	-	40,47,47	1.15	3 (7%)	49,71,71	1.38	7 (14%)
22	CLA	1	204	-	50,54,73	1.37	9 (18%)	59,90,113	1.40	4 (6%)
22	CLA	5	308	-	59,63,73	1.28	7 (11%)	70,101,113	1.35	6 (8%)
27	LMG	j	105	-	32,32,55	1.13	2 (6%)	40,40,63	1.15	4 (10%)
22	CLA	9	311	-	50,54,73	1.36	7 (14%)	59,90,113	1.45	5 (8%)
22	CLA	1	307	-	58,62,73	1.28	8 (13%)	68,99,113	1.35	6 (8%)
22	CLA	a	835	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
22	CLA	a	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
21	A1L1G	3	306	-	40,47,47	1.18	4 (10%)	49,71,71	1.41	8 (16%)
22	CLA	4	317	-	59,63,73	1.28	8 (13%)	70,101,113	1.35	5 (7%)
22	CLA	1	305	-	65,69,73	1.21	6 (9%)	77,108,113	1.29	5 (6%)
22	CLA	2	306	-	45,50,73	1.42	6 (13%)	52,85,113	1.40	4 (7%)
22	CLA	5	309	1	69,73,73	1.17	7 (10%)	82,113,113	1.25	4 (4%)
24	A1L1F	8	304	-	52,59,59	1.41	5 (9%)	63,85,85	2.75	22 (34%)
22	CLA	2	314	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	4 (5%)
22	CLA	a	831	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	8 (9%)
22	CLA	7	312	-	52,56,73	1.35	7 (13%)	61,92,113	1.39	5 (8%)
23	SQD	1	315	-	43,45,54	1.22	3 (6%)	53,56,65	1.12	2 (3%)
22	CLA	b	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
22	CLA	4	309	-	54,58,73	1.31	6 (11%)	64,95,113	1.40	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	306	23	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
22	CLA	a	808	-	55,59,73	1.32	8 (14%)	64,96,113	1.37	5 (7%)
22	CLA	8	308	-	59,63,73	1.28	8 (13%)	70,101,113	1.36	8 (11%)
22	CLA	b	808	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
22	CLA	b	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.25	7 (8%)
22	CLA	a	825	-	59,63,73	1.26	6 (10%)	70,101,113	1.32	5 (7%)
22	CLA	b	816	-	59,63,73	1.26	6 (10%)	70,101,113	1.33	6 (8%)
22	CLA	b	833	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
26	DGD	8	315	22	41,41,67	1.06	2 (4%)	55,55,81	1.12	5 (9%)
22	CLA	8	312	3	56,60,73	1.29	8 (14%)	65,97,113	1.38	5 (7%)
23	SQD	5	316	22	33,35,54	1.39	3 (9%)	43,46,65	1.30	5 (11%)
22	CLA	5	312	-	56,60,73	1.30	8 (14%)	65,97,113	1.39	6 (9%)
25	LHG	a	845	-	47,47,48	1.15	6 (12%)	50,53,54	0.98	2 (4%)
20	XAT	3	304	-	41,47,47	0.93	2 (4%)	54,74,74	2.63	17 (31%)
22	CLA	b	813	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
27	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.17	3 (7%)
27	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.31	4 (9%)
22	CLA	a	820	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
22	CLA	2	311	-	62,66,73	1.25	9 (14%)	73,104,113	1.27	5 (6%)
22	CLA	f	803	12	56,60,73	1.30	8 (14%)	65,97,113	1.38	5 (7%)
22	CLA	b	814	-	59,63,73	1.27	6 (10%)	70,101,113	1.40	8 (11%)
22	CLA	b	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
30	SF4	a	851	-	0,12,12	-	-	-		
22	CLA	2	309	-	50,54,73	1.37	7 (14%)	59,90,113	1.39	4 (6%)
22	CLA	9	313	2	50,54,73	1.36	6 (12%)	59,90,113	1.47	4 (6%)
22	CLA	2	313	6	45,49,73	1.43	7 (15%)	54,84,113	1.51	5 (9%)
29	BCR	f	801	-	41,41,41	0.66	0	56,56,56	2.16	16 (28%)
28	PQN	a	843	-	34,34,34	1.62	2 (5%)	43,45,45	1.16	4 (9%)
22	CLA	b	805	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	5	310	-	50,54,73	1.36	7 (14%)	59,90,113	1.41	4 (6%)
22	CLA	3	309	5	60,64,73	1.25	7 (11%)	71,102,113	1.30	5 (7%)
22	CLA	9	308	2	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
29	BCR	h	201	-	41,41,41	0.66	0	56,56,56	1.99	21 (37%)
22	CLA	5	313	1	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	b	811	-	58,62,73	1.35	9 (15%)	71,100,113	1.34	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	a	850	-	41,41,41	0.70	0	56,56,56	2.17	14 (25%)
21	A1L1G	7	302	-	40,47,47	1.14	3 (7%)	49,71,71	1.41	8 (16%)
21	A1L1G	9	301	-	40,47,47	1.16	5 (12%)	49,71,71	1.48	9 (18%)
25	LHG	9	307	-	35,35,48	1.27	6 (17%)	38,41,54	0.92	2 (5%)
22	CLA	1	306	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
22	CLA	4	314	4	49,53,73	1.40	9 (18%)	58,89,113	1.42	4 (6%)
22	CLA	b	815	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	a	829	-	66,70,73	1.20	6 (9%)	78,109,113	1.24	7 (8%)
29	BCR	a	848	-	41,41,41	0.68	0	56,56,56	1.95	18 (32%)
22	CLA	a	812	22	66,70,73	1.19	7 (10%)	78,109,113	1.30	5 (6%)
22	CLA	b	812	-	57,61,73	1.29	8 (14%)	67,98,113	1.35	5 (7%)
20	XAT	1	302	-	41,47,47	0.90	2 (4%)	54,74,74	2.61	18 (33%)
22	CLA	a	815	-	49,53,73	1.39	6 (12%)	58,89,113	1.42	4 (6%)
22	CLA	7	314	-	49,53,73	1.40	8 (16%)	58,89,113	1.50	5 (8%)
29	BCR	i	101	-	41,41,41	0.72	0	56,56,56	2.15	13 (23%)
22	CLA	a	803	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	6 (7%)
20	XAT	1	303	-	41,47,47	0.90	2 (4%)	54,74,74	2.53	19 (35%)
22	CLA	9	314	-	59,63,73	1.26	6 (10%)	70,101,113	1.34	6 (8%)
22	CLA	b	824	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
22	CLA	7	309	-	50,55,73	1.36	7 (14%)	58,91,113	1.35	5 (8%)
29	BCR	h	202	-	41,41,41	0.67	0	56,56,56	1.90	17 (30%)
22	CLA	9	312	-	50,54,73	1.36	7 (14%)	59,90,113	1.49	6 (10%)
22	CLA	1	311	-	57,61,73	1.28	8 (14%)	67,98,113	1.36	7 (10%)
22	CLA	b	819	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
28	PQN	b	841	-	34,34,34	1.58	2 (5%)	43,45,45	1.24	5 (11%)
22	CLA	8	305	3	47,51,73	1.40	7 (14%)	55,86,113	1.45	6 (10%)
22	CLA	9	315	2	46,50,73	1.41	6 (13%)	53,85,113	1.42	4 (7%)
22	CLA	b	830	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
29	BCR	b	844	-	41,41,41	0.66	0	56,56,56	2.09	16 (28%)
22	CLA	4	315	4	45,49,73	1.43	7 (15%)	54,84,113	1.49	5 (9%)
29	BCR	b	843	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
20	XAT	9	305	-	41,47,47	1.03	3 (7%)	54,74,74	2.33	17 (31%)
22	CLA	a	826	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
22	CLA	1	313	-	45,49,73	1.41	7 (15%)	54,84,113	1.47	5 (9%)
25	LHG	9	317	-	45,45,48	1.19	6 (13%)	48,51,54	0.96	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	a	847	-	41,41,41	0.68	0	56,56,56	1.95	17 (30%)
22	CLA	7	315	4	45,49,73	1.43	8 (17%)	54,84,113	1.49	5 (9%)
29	BCR	b	849	-	41,41,41	0.70	0	56,56,56	2.06	13 (23%)
20	XAT	2	304	-	41,47,47	0.89	2 (4%)	54,74,74	2.55	20 (37%)
22	CLA	4	308	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	7 (8%)
22	CLA	2	310	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
22	CLA	a	818	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	7 (9%)
22	CLA	3	308	-	51,55,73	1.36	8 (15%)	60,91,113	1.43	6 (10%)
20	XAT	5	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.59	19 (35%)
22	CLA	a	841	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	6 (7%)
22	CLA	1	308	7	69,73,73	1.16	6 (8%)	82,113,113	1.29	6 (7%)
22	CLA	a	814	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	a	839	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
22	CLA	7	317	-	49,53,73	1.40	7 (14%)	58,89,113	1.45	4 (6%)
22	CLA	b	827	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
20	XAT	4	302	-	41,47,47	0.89	2 (4%)	54,74,74	2.59	19 (35%)
25	LHG	b	847	22	30,30,48	1.38	6 (20%)	33,36,54	1.17	2 (6%)
22	CLA	a	834	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	3	307	5	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
22	CLA	b	826	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	5 (6%)
26	DGD	4	318	-	41,41,67	1.07	2 (4%)	55,55,81	1.79	6 (10%)
22	CLA	a	809	8	69,73,73	1.16	7 (10%)	82,113,113	1.29	8 (9%)
30	SF4	c	101	-	0,12,12	-	-	-		
22	CLA	8	306	26	50,54,73	1.36	8 (16%)	59,90,113	1.40	4 (6%)
22	CLA	b	835	-	62,66,73	1.24	7 (11%)	73,104,113	1.37	8 (10%)
20	XAT	2	302	-	41,47,47	0.93	2 (4%)	54,74,74	2.52	18 (33%)
22	CLA	5	311	-	55,59,73	1.30	8 (14%)	64,96,113	1.36	7 (10%)
20	XAT	4	304	-	41,47,47	0.91	2 (4%)	54,74,74	2.57	18 (33%)
22	CLA	4	316	-	50,54,73	1.36	6 (12%)	59,90,113	1.43	4 (6%)
22	CLA	7	308	-	64,68,73	1.22	6 (9%)	76,107,113	1.27	6 (7%)
22	CLA	a	806	-	69,73,73	1.21	10 (14%)	82,113,113	1.55	12 (14%)
20	XAT	3	301	-	41,47,47	0.91	2 (4%)	54,74,74	2.56	19 (35%)
22	CLA	b	836	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
20	XAT	4	305	-	41,47,47	0.91	2 (4%)	54,74,74	2.76	18 (33%)
22	CLA	4	310	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	9	318	-	66,70,73	1.21	8 (12%)	78,109,113	1.27	6 (7%)
22	CLA	8	313	-	50,54,73	1.38	9 (18%)	59,90,113	1.40	4 (6%)
22	CLA	a	837	8	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	7	316	-	55,59,73	1.31	7 (12%)	64,96,113	1.45	7 (10%)
22	CLA	a	832	-	54,58,73	1.32	8 (14%)	64,95,113	1.39	6 (9%)
20	XAT	9	304	-	41,47,47	0.96	2 (4%)	54,74,74	2.43	18 (33%)
22	CLA	b	825	-	68,72,73	1.17	8 (11%)	80,111,113	1.30	8 (10%)
22	CLA	2	307	-	51,55,73	1.36	8 (15%)	60,91,113	1.45	8 (13%)
20	XAT	7	304	-	41,47,47	0.94	2 (4%)	54,74,74	2.67	17 (31%)
22	CLA	h	205	-	59,63,73	1.27	8 (13%)	70,101,113	1.34	7 (10%)
22	CLA	a	823	-	53,57,73	1.32	7 (13%)	61,93,113	1.43	6 (9%)
22	CLA	b	818	-	64,68,73	1.22	7 (10%)	76,107,113	1.27	5 (6%)
22	CLA	b	840	25	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	a	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.28	5 (6%)
22	CLA	a	821	-	49,53,73	1.39	7 (14%)	58,89,113	1.46	4 (6%)
20	XAT	2	305	-	41,47,47	0.94	2 (4%)	54,74,74	2.43	18 (33%)
22	CLA	2	315	-	46,50,73	1.42	8 (17%)	53,85,113	1.38	4 (7%)
22	CLA	a	824	-	50,54,73	1.37	8 (16%)	59,90,113	1.35	4 (6%)
22	CLA	3	310	-	60,64,73	1.26	6 (10%)	71,102,113	1.30	5 (7%)
22	CLA	3	311	-	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
22	CLA	a	811	-	60,64,73	1.26	6 (10%)	71,102,113	1.34	6 (8%)
22	CLA	a	844	25	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
22	CLA	8	311	-	60,64,73	1.24	7 (11%)	71,102,113	1.33	8 (11%)
22	CLA	3	313	-	56,60,73	1.30	8 (14%)	65,97,113	1.38	6 (9%)
22	CLA	b	834	-	57,61,73	1.30	8 (14%)	67,98,113	1.36	5 (7%)
21	A1L1G	3	302	-	40,47,47	1.16	5 (12%)	49,71,71	1.33	7 (14%)
22	CLA	1	309	7	50,54,73	1.37	8 (16%)	59,90,113	1.35	4 (6%)
22	CLA	a	836	-	54,58,73	1.32	7 (12%)	64,95,113	1.38	6 (9%)
22	CLA	h	203	-	69,73,73	1.18	6 (8%)	82,113,113	1.33	6 (7%)
22	CLA	5	315	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
22	CLA	1	314	-	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
22	CLA	a	817	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
22	CLA	b	829	-	69,73,73	1.20	8 (11%)	82,113,113	1.31	9 (10%)
30	SF4	c	102	-	0,12,12	-	-	-	-	-
22	CLA	b	821	-	55,59,73	1.31	7 (12%)	64,96,113	1.41	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	833	-	59,63,73	1.25	7 (11%)	70,101,113	1.40	8 (11%)
22	CLA	2	308	6	58,62,73	1.28	7 (12%)	68,99,113	1.29	6 (8%)
22	CLA	9	316	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	8 (9%)

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
20	XAT	3	303	-	-	3/31/93/93	0/4/4/4
20	XAT	a	852	-	-	7/31/93/93	0/4/4/4
22	CLA	7	310	-	1/1/11/20	6/17/93/115	-
22	CLA	b	806	-	1/1/15/20	13/39/115/115	-
22	CLA	l	202	-	1/1/10/20	0/12/88/115	-
29	BCR	b	842	-	-	2/29/63/63	0/2/2/2
20	XAT	9	303	-	-	4/31/93/93	0/4/4/4
20	XAT	2	301	-	-	3/31/93/93	0/4/4/4
22	CLA	7	313	-	1/1/12/20	5/26/102/115	-
22	CLA	a	838	-	1/1/12/20	6/23/99/115	-
22	CLA	b	817	-	1/1/13/20	11/32/108/115	-
22	CLA	b	838	-	1/1/15/20	15/39/115/115	-
22	CLA	f	802	-	1/1/15/20	13/39/115/115	-
22	CLA	a	816	-	1/1/12/20	4/21/97/115	-
22	CLA	a	827	-	1/1/15/20	6/39/115/115	-
20	XAT	8	301	-	-	3/31/93/93	0/4/4/4
22	CLA	9	309	2	1/1/11/20	5/17/93/115	-
22	CLA	1	310	7	1/1/15/20	17/39/115/115	-
22	CLA	a	840	-	1/1/15/20	8/39/115/115	-
29	BCR	a	849	-	-	0/29/63/63	0/2/2/2
21	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
26	DGD	b	848	-	-	20/46/86/95	0/2/2/2
22	CLA	4	312	-	1/1/11/20	6/17/93/115	-
29	BCR	l	201	-	-	4/29/63/63	0/2/2/2
22	CLA	a	842	-	1/1/15/20	8/39/115/115	-
22	CLA	3	312	5	1/1/13/20	10/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	804	-	1/1/13/20	9/27/103/115	-
22	CLA	2	316	6	1/1/11/20	6/17/93/115	-
22	CLA	a	810	8	1/1/15/20	15/39/115/115	-
29	BCR	m	101	-	-	8/29/63/63	0/2/2/2
22	CLA	b	822	-	1/1/14/20	7/33/109/115	-
22	CLA	a	854	-	1/1/15/20	14/39/115/115	-
22	CLA	a	813	-	1/1/12/20	9/26/102/115	-
20	XAT	5	302	-	-	3/31/93/93	0/4/4/4
29	BCR	l	205	-	-	8/29/63/63	0/2/2/2
22	CLA	2	312	-	1/1/11/20	4/18/94/115	-
22	CLA	7	307	-	1/1/11/20	6/15/91/115	-
20	XAT	5	304	-	-	1/31/93/93	0/4/4/4
22	CLA	7	306	4	1/1/11/20	10/19/95/115	-
22	CLA	a	830	-	1/1/15/20	13/39/115/115	-
20	XAT	4	301	-	-	4/31/93/93	0/4/4/4
20	XAT	7	305	-	-	2/31/93/93	0/4/4/4
29	BCR	j	104	-	-	2/29/63/63	0/2/2/2
22	CLA	5	314	-	1/1/12/20	4/24/100/115	-
29	BCR	f	804	-	-	4/29/63/63	0/2/2/2
22	CLA	b	809	-	1/1/15/20	13/39/115/115	-
22	CLA	5	307	1	1/1/14/20	5/33/109/115	-
20	XAT	3	305	-	-	0/31/93/93	0/4/4/4
22	CLA	a	807	-	1/1/15/20	18/39/115/115	-
20	XAT	7	301	-	-	6/31/93/93	0/4/4/4
22	CLA	b	810	-	1/1/15/20	14/39/115/115	-
22	CLA	1	312	7	1/1/12/20	3/24/100/115	-
20	XAT	4	303	-	-	3/31/93/93	0/4/4/4
22	CLA	b	837	-	1/1/15/20	9/39/115/115	-
22	CLA	b	820	-	1/1/12/20	5/21/97/115	-
20	XAT	8	302	-	-	4/31/93/93	0/4/4/4
22	CLA	l	203	-	1/1/14/20	4/33/109/115	-
22	CLA	4	311	-	1/1/11/20	9/17/93/115	-
22	CLA	b	832	-	1/1/15/20	13/39/115/115	-
22	CLA	b	839	-	1/1/15/20	15/39/115/115	-
29	BCR	b	845	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	XAT	8	303	-	-	0/31/93/93	0/4/4/4
22	CLA	a	802	-	1/1/13/20	5/31/107/115	-
22	CLA	j	102	-	1/1/13/20	18/31/107/115	-
22	CLA	4	313	-	1/1/12/20	4/25/101/115	-
22	CLA	a	819	-	1/1/12/20	6/26/102/115	-
22	CLA	8	310	-	1/1/11/20	6/17/93/115	-
21	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
22	CLA	3	314	5	1/1/11/20	8/18/94/115	-
22	CLA	b	801	-	1/1/15/20	20/39/115/115	-
22	CLA	b	831	-	1/1/11/20	5/20/96/115	-
22	CLA	8	314	-	1/1/10/20	6/10/86/115	-
22	CLA	a	822	-	1/1/15/20	5/39/115/115	-
22	CLA	9	310	-	1/1/11/20	6/17/93/115	-
22	CLA	4	307	-	1/1/13/20	9/29/105/115	-
22	CLA	b	807	-	1/1/15/20	18/39/115/115	-
22	CLA	8	307	3	1/1/15/20	11/39/115/115	-
22	CLA	8	309	-	1/1/13/20	7/30/106/115	-
25	LHG	a	846	22	-	15/31/31/53	-
22	CLA	5	305	1	1/1/11/20	6/17/93/115	-
22	CLA	a	805	22	1/1/13/20	6/27/103/115	-
22	CLA	3	315	5	1/1/11/20	9/17/93/115	-
20	XAT	2	303	-	-	6/31/93/93	0/4/4/4
22	CLA	b	802	-	1/1/15/20	15/39/115/115	-
24	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
22	CLA	j	103	15	1/1/10/20	7/12/88/115	-
24	A1L1F	h	204	-	-	11/43/99/99	1/3/3/3
20	XAT	j	101	-	-	5/31/93/93	0/4/4/4
20	XAT	7	303	-	-	7/31/93/93	0/4/4/4
22	CLA	4	306	4	1/1/11/20	9/15/91/115	-
24	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
22	CLA	b	823	-	1/1/12/20	6/25/101/115	-
22	CLA	7	311	-	1/1/11/20	4/17/93/115	-
29	BCR	b	846	-	-	2/29/63/63	0/2/2/2
22	CLA	l	204	-	1/1/11/20	3/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
22	CLA	5	308	-	1/1/13/20	6/27/103/115	-
27	LMG	j	105	-	-	11/27/47/70	0/1/1/1
22	CLA	9	311	-	1/1/11/20	6/17/93/115	-
22	CLA	1	307	-	1/1/12/20	5/26/102/115	-
22	CLA	a	835	-	1/1/15/20	11/39/115/115	-
22	CLA	a	828	-	1/1/15/20	8/39/115/115	-
21	A1L1G	3	306	-	-	19/29/85/85	0/3/3/3
22	CLA	4	317	-	1/1/13/20	9/27/103/115	-
22	CLA	1	305	-	1/1/14/20	9/35/111/115	-
22	CLA	2	306	-	1/1/10/20	4/11/87/115	-
22	CLA	5	309	1	1/1/15/20	10/39/115/115	-
24	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
22	CLA	2	314	-	1/1/13/20	14/29/105/115	-
22	CLA	a	831	-	1/1/15/20	11/39/115/115	-
22	CLA	7	312	-	1/1/11/20	3/19/95/115	-
23	SQD	1	315	-	-	19/40/60/69	0/1/1/1
22	CLA	b	804	-	1/1/15/20	7/39/115/115	-
22	CLA	4	309	-	1/1/12/20	4/21/97/115	-
22	CLA	5	306	23	1/1/11/20	8/15/91/115	-
22	CLA	a	808	-	1/1/12/20	4/23/99/115	-
22	CLA	8	308	-	1/1/13/20	7/27/103/115	-
22	CLA	b	808	-	1/1/15/20	11/39/115/115	-
22	CLA	b	803	-	1/1/15/20	17/39/115/115	-
22	CLA	a	825	-	1/1/13/20	8/27/103/115	-
22	CLA	b	816	-	1/1/13/20	3/27/103/115	-
22	CLA	b	833	-	1/1/15/20	13/39/115/115	-
26	DGD	8	315	22	-	10/29/69/95	0/2/2/2
22	CLA	8	312	3	1/1/12/20	2/24/100/115	-
23	SQD	5	316	22	-	11/30/50/69	0/1/1/1
22	CLA	5	312	-	1/1/12/20	0/24/100/115	-
25	LHG	a	845	-	-	26/52/52/53	-
22	CLA	b	813	-	1/1/15/20	13/39/115/115	-
20	XAT	3	304	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	a	853	-	-	13/29/49/70	0/1/1/1
27	LMG	2	317	-	-	11/30/50/70	0/1/1/1
22	CLA	a	820	-	1/1/15/20	13/39/115/115	-
22	CLA	2	311	-	1/1/13/20	5/31/107/115	-
22	CLA	f	803	12	1/1/12/20	5/24/100/115	-
22	CLA	b	814	-	1/1/13/20	10/27/103/115	-
22	CLA	b	828	-	1/1/15/20	13/39/115/115	-
30	SF4	a	851	-	-	-	0/6/5/5
22	CLA	2	309	-	1/1/11/20	3/17/93/115	-
22	CLA	9	313	2	1/1/11/20	12/17/93/115	-
22	CLA	2	313	6	1/1/10/20	2/10/86/115	-
29	BCR	f	801	-	-	3/29/63/63	0/2/2/2
28	PQN	a	843	-	-	5/23/43/43	0/2/2/2
22	CLA	b	805	-	1/1/15/20	11/39/115/115	-
22	CLA	5	310	-	1/1/11/20	8/17/93/115	-
22	CLA	3	309	5	1/1/13/20	3/29/105/115	-
22	CLA	9	308	2	1/1/15/20	14/39/115/115	-
29	BCR	h	201	-	-	0/29/63/63	0/2/2/2
22	CLA	5	313	1	1/1/11/20	6/15/91/115	-
22	CLA	b	811	-	1/1/13/20	4/25/101/115	-
29	BCR	a	850	-	-	4/29/63/63	0/2/2/2
21	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
21	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
25	LHG	9	307	-	-	20/40/40/53	-
22	CLA	1	306	-	1/1/15/20	15/39/115/115	-
22	CLA	4	314	4	1/1/11/20	6/15/91/115	-
22	CLA	b	815	-	1/1/11/20	3/15/91/115	-
22	CLA	a	829	-	1/1/14/20	13/36/112/115	-
29	BCR	a	848	-	-	0/29/63/63	0/2/2/2
22	CLA	a	812	22	1/1/14/20	9/36/112/115	-
22	CLA	b	812	-	1/1/12/20	5/25/101/115	-
20	XAT	1	302	-	-	0/31/93/93	0/4/4/4
22	CLA	a	815	-	1/1/11/20	0/15/91/115	-
22	CLA	7	314	-	1/1/11/20	5/15/91/115	-
29	BCR	i	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	803	-	1/1/15/20	3/39/115/115	-
20	XAT	1	303	-	-	0/31/93/93	0/4/4/4
22	CLA	9	314	-	1/1/13/20	10/27/103/115	-
22	CLA	b	824	-	1/1/15/20	15/39/115/115	-
22	CLA	7	309	-	1/1/11/20	5/17/93/115	-
29	BCR	h	202	-	-	0/29/63/63	0/2/2/2
22	CLA	9	312	-	1/1/11/20	7/17/93/115	-
22	CLA	1	311	-	1/1/12/20	4/25/101/115	-
22	CLA	b	819	-	1/1/13/20	5/27/103/115	-
28	PQN	b	841	-	-	1/23/43/43	0/2/2/2
22	CLA	8	305	3	1/1/10/20	2/13/89/115	-
22	CLA	9	315	2	1/1/10/20	5/12/88/115	-
22	CLA	b	830	-	1/1/10/20	2/10/86/115	-
29	BCR	b	844	-	-	6/29/63/63	0/2/2/2
22	CLA	4	315	4	1/1/10/20	6/10/86/115	-
29	BCR	b	843	-	-	2/29/63/63	0/2/2/2
20	XAT	9	305	-	-	3/31/93/93	0/4/4/4
22	CLA	a	826	-	1/1/15/20	8/39/115/115	-
22	CLA	1	313	-	1/1/10/20	6/10/86/115	-
25	LHG	9	317	-	-	28/50/50/53	-
29	BCR	a	847	-	-	0/29/63/63	0/2/2/2
22	CLA	7	315	4	1/1/10/20	4/10/86/115	-
29	BCR	b	849	-	-	4/29/63/63	0/2/2/2
20	XAT	2	304	-	-	3/31/93/93	0/4/4/4
22	CLA	4	308	-	1/1/15/20	13/39/115/115	-
22	CLA	2	310	-	1/1/15/20	14/39/115/115	-
22	CLA	a	818	-	1/1/13/20	11/29/105/115	-
22	CLA	3	308	-	1/1/11/20	7/18/94/115	-
22	CLA	a	841	-	1/1/15/20	15/39/115/115	-
20	XAT	5	301	-	-	3/31/93/93	0/4/4/4
22	CLA	1	308	7	1/1/15/20	13/39/115/115	-
22	CLA	a	814	-	1/1/15/20	19/39/115/115	-
22	CLA	a	839	-	1/1/15/20	14/39/115/115	-
22	CLA	7	317	-	1/1/11/20	7/15/91/115	-
22	CLA	b	827	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	XAT	4	302	-	-	0/31/93/93	0/4/4/4
25	LHG	b	847	22	-	20/35/35/53	-
22	CLA	a	834	-	1/1/15/20	9/39/115/115	-
22	CLA	3	307	5	1/1/11/20	2/15/91/115	-
22	CLA	b	826	-	1/1/15/20	3/39/115/115	-
26	DGD	4	318	-	-	10/29/69/95	0/2/2/2
22	CLA	a	809	8	1/1/15/20	15/39/115/115	-
30	SF4	c	101	-	-	-	0/6/5/5
22	CLA	8	306	26	1/1/11/20	4/17/93/115	-
22	CLA	b	835	-	1/1/13/20	10/31/107/115	-
22	CLA	5	311	-	1/1/12/20	7/23/99/115	-
22	CLA	4	316	-	1/1/11/20	7/17/93/115	-
22	CLA	7	308	-	1/1/14/20	12/33/109/115	-
22	CLA	a	806	-	1/1/15/20	11/39/115/115	-
20	XAT	4	304	-	-	0/31/93/93	0/4/4/4
20	XAT	2	302	-	-	0/31/93/93	0/4/4/4
20	XAT	3	301	-	-	3/31/93/93	0/4/4/4
22	CLA	b	836	-	1/1/15/20	7/39/115/115	-
20	XAT	4	305	-	-	4/31/93/93	0/4/4/4
22	CLA	4	310	-	1/1/15/20	15/39/115/115	-
22	CLA	9	318	-	1/1/14/20	11/36/112/115	-
22	CLA	8	313	-	1/1/11/20	5/17/93/115	-
22	CLA	a	837	8	1/1/11/20	4/15/91/115	-
22	CLA	7	316	-	1/1/12/20	10/23/99/115	-
22	CLA	a	832	-	1/1/12/20	7/21/97/115	-
20	XAT	9	304	-	-	1/31/93/93	0/4/4/4
22	CLA	b	825	-	1/1/14/20	4/38/114/115	-
22	CLA	2	307	-	1/1/11/20	7/18/94/115	-
22	CLA	h	205	-	1/1/13/20	9/27/103/115	-
20	XAT	7	304	-	-	6/31/93/93	0/4/4/4
22	CLA	a	823	-	1/1/11/20	7/20/96/115	-
22	CLA	b	818	-	1/1/14/20	15/33/109/115	-
22	CLA	b	840	25	1/1/15/20	11/39/115/115	-
22	CLA	a	801	-	1/1/15/20	22/39/115/115	-
22	CLA	a	821	-	1/1/11/20	1/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	XAT	2	305	-	-	2/31/93/93	0/4/4/4
22	CLA	2	315	-	1/1/10/20	3/12/88/115	-
22	CLA	a	824	-	1/1/11/20	5/17/93/115	-
22	CLA	3	310	-	1/1/13/20	3/29/105/115	-
22	CLA	3	311	-	1/1/12/20	4/21/97/115	-
22	CLA	a	811	-	1/1/13/20	6/29/105/115	-
22	CLA	a	844	25	1/1/15/20	15/39/115/115	-
22	CLA	8	311	-	1/1/13/20	7/29/105/115	-
22	CLA	3	313	-	1/1/12/20	1/24/100/115	-
22	CLA	b	834	-	1/1/12/20	9/25/101/115	-
21	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
22	CLA	1	309	7	1/1/11/20	7/17/93/115	-
22	CLA	a	836	-	1/1/12/20	8/21/97/115	-
22	CLA	h	203	-	1/1/15/20	9/39/115/115	-
22	CLA	5	315	-	1/1/11/20	5/17/93/115	-
22	CLA	1	314	-	1/1/11/20	7/15/91/115	-
22	CLA	a	817	-	1/1/11/20	8/15/91/115	-
22	CLA	b	829	-	1/1/15/20	11/39/115/115	-
30	SF4	c	102	-	-	-	0/6/5/5
22	CLA	b	821	-	1/1/12/20	4/23/99/115	-
22	CLA	a	833	-	1/1/13/20	2/27/103/115	-
22	CLA	2	308	6	1/1/12/20	3/26/102/115	-
22	CLA	9	316	-	1/1/15/20	16/39/115/115	-

The worst 5 of 1485 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	843	PQN	C3-C2	7.72	1.49	1.35
28	b	841	PQN	C3-C2	7.50	1.48	1.35
28	a	843	PQN	C10-C5	4.93	1.48	1.40
28	b	841	PQN	C10-C5	4.92	1.48	1.40
24	h	204	A1L1F	O7-C54	4.68	1.45	1.35

The worst 5 of 2072 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	302	A1L1F	O15-C20-C21	10.50	123.33	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	318	DGD	C6E-C5E-C4E	-8.98	90.97	113.02
24	9	302	A1L1F	C17-C20-C25	-8.66	108.05	122.30
24	h	204	A1L1F	C17-C20-C25	-8.53	108.27	122.30
24	8	304	A1L1F	C17-C20-C25	-8.39	108.49	122.30

5 of 178 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	5	305	CLA	ND
22	5	306	CLA	ND
22	5	307	CLA	ND
22	5	308	CLA	ND
22	5	309	CLA	ND

5 of 1966 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	5	302	XAT	O4-C6-C7-C8
20	5	302	XAT	C7-C8-C9-C10
20	5	302	XAT	C7-C8-C9-C19
20	9	303	XAT	O4-C6-C7-C8
20	9	304	XAT	O24-C26-C27-C28

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	h	204	A1L1F	C1-C11-C3-C4-C6-C8

217 monomers are involved in 660 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	303	XAT	3	0
20	a	852	XAT	6	0
22	b	806	CLA	3	0
22	l	202	CLA	1	0
29	b	842	BCR	4	0
20	9	303	XAT	7	0
20	2	301	XAT	3	0
22	7	313	CLA	4	0
22	a	838	CLA	1	0
22	b	817	CLA	8	0
22	b	838	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	f	802	CLA	2	0
22	a	816	CLA	2	0
22	a	827	CLA	3	0
20	8	301	XAT	2	0
22	9	309	CLA	1	0
22	1	310	CLA	1	0
22	a	840	CLA	6	0
29	a	849	BCR	3	0
21	1	301	A1L1G	1	0
26	b	848	DGD	6	0
22	4	312	CLA	1	0
29	l	201	BCR	3	0
22	a	842	CLA	4	0
22	3	312	CLA	2	0
22	a	804	CLA	4	0
22	2	316	CLA	2	0
22	a	810	CLA	4	0
29	m	101	BCR	2	0
22	b	822	CLA	7	0
20	5	302	XAT	6	0
22	a	854	CLA	3	0
29	l	205	BCR	11	0
20	5	304	XAT	3	0
22	7	307	CLA	2	0
22	7	306	CLA	3	0
22	a	830	CLA	5	0
20	4	301	XAT	6	0
20	7	305	XAT	2	0
29	j	104	BCR	9	0
22	5	314	CLA	1	0
29	f	804	BCR	5	0
22	b	809	CLA	4	0
22	5	307	CLA	7	0
20	3	305	XAT	6	0
20	7	301	XAT	3	0
22	a	807	CLA	4	0
22	1	312	CLA	2	0
20	4	303	XAT	11	0
20	8	302	XAT	6	0
22	b	820	CLA	3	0
22	b	837	CLA	5	0
22	l	203	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	311	CLA	1	0
22	b	832	CLA	3	0
22	b	839	CLA	4	0
29	b	845	BCR	7	0
20	8	303	XAT	4	0
22	a	802	CLA	5	0
22	j	102	CLA	7	0
22	4	313	CLA	4	0
21	9	306	A1L1G	1	0
22	a	819	CLA	5	0
22	b	801	CLA	3	0
22	b	831	CLA	2	0
22	a	822	CLA	5	0
22	9	310	CLA	2	0
22	4	307	CLA	1	0
22	b	807	CLA	7	0
22	8	307	CLA	4	0
25	a	846	LHG	3	0
22	5	305	CLA	3	0
20	2	303	XAT	12	0
22	b	802	CLA	3	0
24	1	304	A1L1F	2	0
22	j	103	CLA	2	0
24	h	204	A1L1F	4	0
20	j	101	XAT	7	0
20	7	303	XAT	12	0
22	4	306	CLA	2	0
24	9	302	A1L1F	2	0
22	b	823	CLA	6	0
22	7	311	CLA	3	0
29	b	846	BCR	3	0
21	5	303	A1L1G	1	0
22	5	308	CLA	1	0
27	j	105	LMG	7	0
22	9	311	CLA	2	0
22	a	835	CLA	5	0
22	a	828	CLA	5	0
22	4	317	CLA	6	0
22	5	309	CLA	4	0
24	8	304	A1L1F	2	0
22	2	314	CLA	2	0
22	a	831	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	312	CLA	1	0
23	1	315	SQD	2	0
22	b	804	CLA	5	0
22	4	309	CLA	3	0
22	a	808	CLA	1	0
22	8	308	CLA	2	0
22	b	808	CLA	1	0
22	b	803	CLA	2	0
22	a	825	CLA	4	0
22	b	816	CLA	6	0
22	b	833	CLA	4	0
26	8	315	DGD	2	0
22	8	312	CLA	2	0
23	5	316	SQD	1	0
22	5	312	CLA	3	0
25	a	845	LHG	3	0
20	3	304	XAT	6	0
22	b	813	CLA	7	0
27	a	853	LMG	10	0
27	2	317	LMG	3	0
22	a	820	CLA	6	0
22	b	814	CLA	2	0
22	b	828	CLA	4	0
22	2	309	CLA	2	0
22	9	313	CLA	2	0
29	f	801	BCR	9	0
28	a	843	PQN	4	0
22	b	805	CLA	3	0
22	5	310	CLA	1	0
22	3	309	CLA	1	0
22	9	308	CLA	5	0
29	h	201	BCR	2	0
22	b	811	CLA	3	0
29	a	850	BCR	2	0
21	7	302	A1L1G	2	0
21	9	301	A1L1G	2	0
25	9	307	LHG	2	0
22	1	306	CLA	6	0
22	4	314	CLA	1	0
22	a	829	CLA	6	0
29	a	848	BCR	7	0
22	b	812	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	302	XAT	3	0
22	a	815	CLA	1	0
22	7	314	CLA	3	0
29	i	101	BCR	3	0
22	a	803	CLA	5	0
20	1	303	XAT	4	0
22	9	314	CLA	7	0
22	b	824	CLA	6	0
29	h	202	BCR	4	0
22	9	312	CLA	4	0
22	1	311	CLA	2	0
22	b	819	CLA	2	0
28	b	841	PQN	3	0
22	8	305	CLA	5	0
22	9	315	CLA	1	0
22	b	830	CLA	6	0
29	b	844	BCR	5	0
22	4	315	CLA	1	0
20	9	305	XAT	3	0
22	a	826	CLA	7	0
25	9	317	LHG	3	0
29	a	847	BCR	1	0
22	7	315	CLA	2	0
29	b	849	BCR	5	0
22	4	308	CLA	6	0
22	2	310	CLA	3	0
22	a	818	CLA	10	0
22	3	308	CLA	2	0
20	5	301	XAT	4	0
22	a	841	CLA	7	0
22	1	308	CLA	4	0
22	a	814	CLA	3	0
22	a	839	CLA	4	0
22	b	827	CLA	5	0
20	4	302	XAT	6	0
22	a	834	CLA	6	0
22	b	826	CLA	3	0
26	4	318	DGD	11	0
22	a	809	CLA	3	0
22	8	306	CLA	1	0
22	b	835	CLA	4	0
20	2	302	XAT	3	0

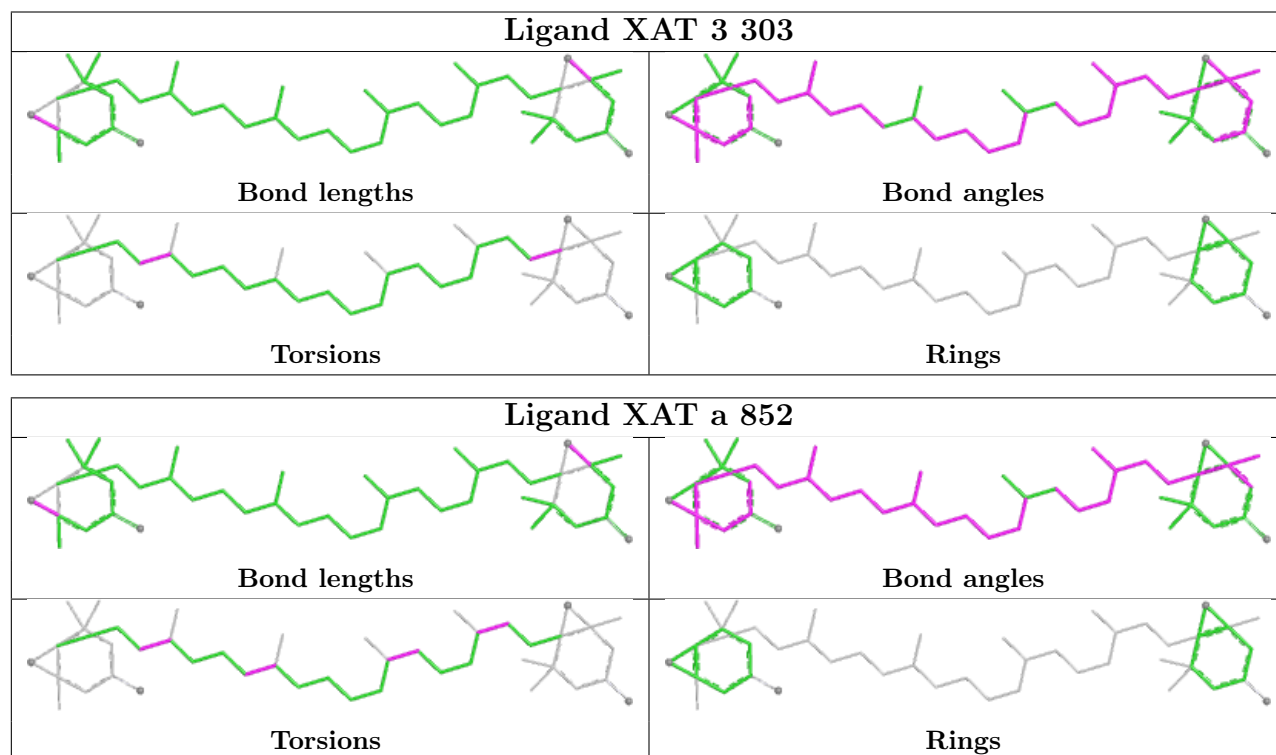
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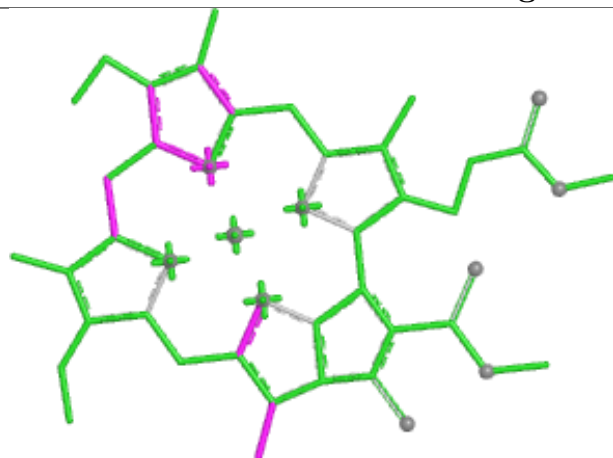
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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20	4	304	XAT	5	0
22	4	316	CLA	1	0
22	7	308	CLA	6	0
22	a	806	CLA	10	0
20	3	301	XAT	4	0
22	b	836	CLA	7	0
20	4	305	XAT	3	0
22	4	310	CLA	7	0
22	9	318	CLA	6	0
22	8	313	CLA	3	0
22	a	837	CLA	1	0
22	7	316	CLA	1	0
22	a	832	CLA	2	0
20	9	304	XAT	7	0
22	b	825	CLA	3	0
22	2	307	CLA	1	0
20	7	304	XAT	8	0
22	h	205	CLA	2	0
22	a	823	CLA	3	0
22	b	818	CLA	4	0
22	b	840	CLA	5	0
22	a	801	CLA	5	0
20	2	305	XAT	2	0
22	a	824	CLA	1	0
22	3	311	CLA	1	0
22	a	844	CLA	5	0
22	8	311	CLA	3	0
22	3	313	CLA	3	0
22	b	834	CLA	1	0
22	h	203	CLA	4	0
22	5	315	CLA	1	0
22	b	829	CLA	4	0
30	c	102	SF4	3	0
22	b	821	CLA	3	0
22	a	833	CLA	2	0
22	2	308	CLA	5	0
22	9	316	CLA	5	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

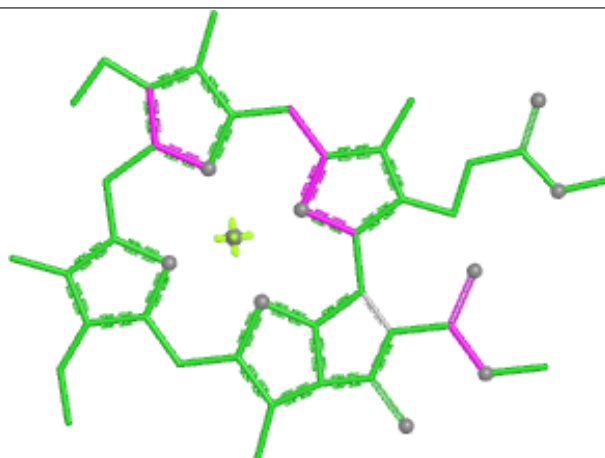
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



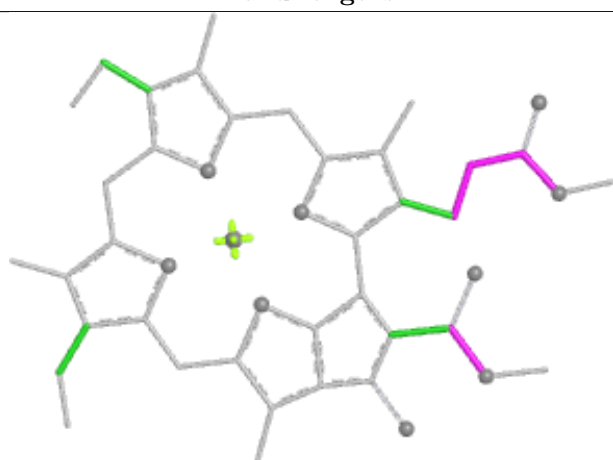
Ligand CLA 7 310



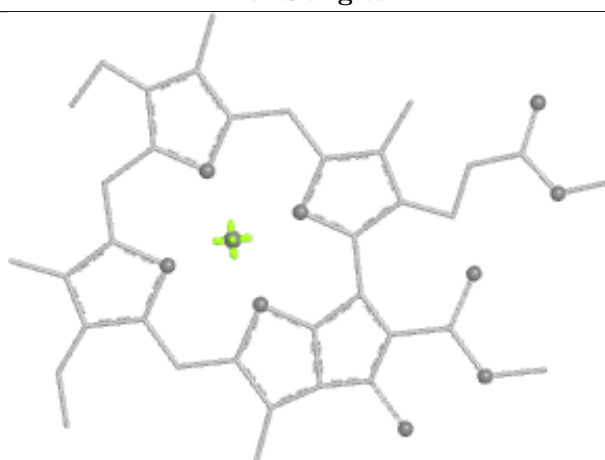
Bond lengths



Bond angles

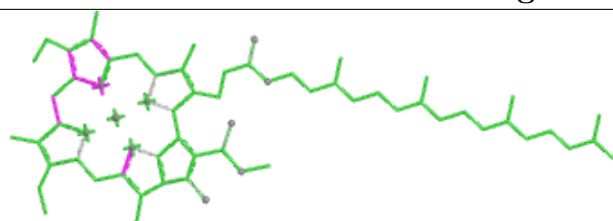


Torsions

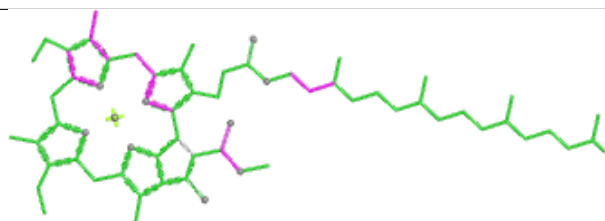


Rings

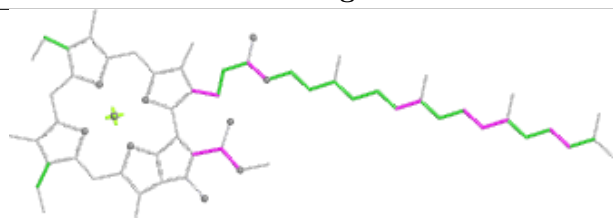
Ligand CLA b 806



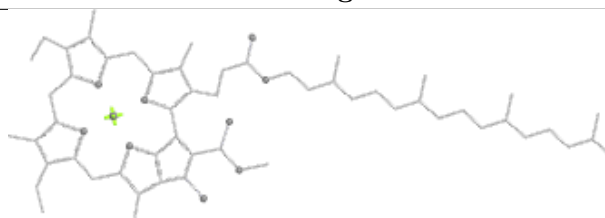
Bond lengths



Bond angles

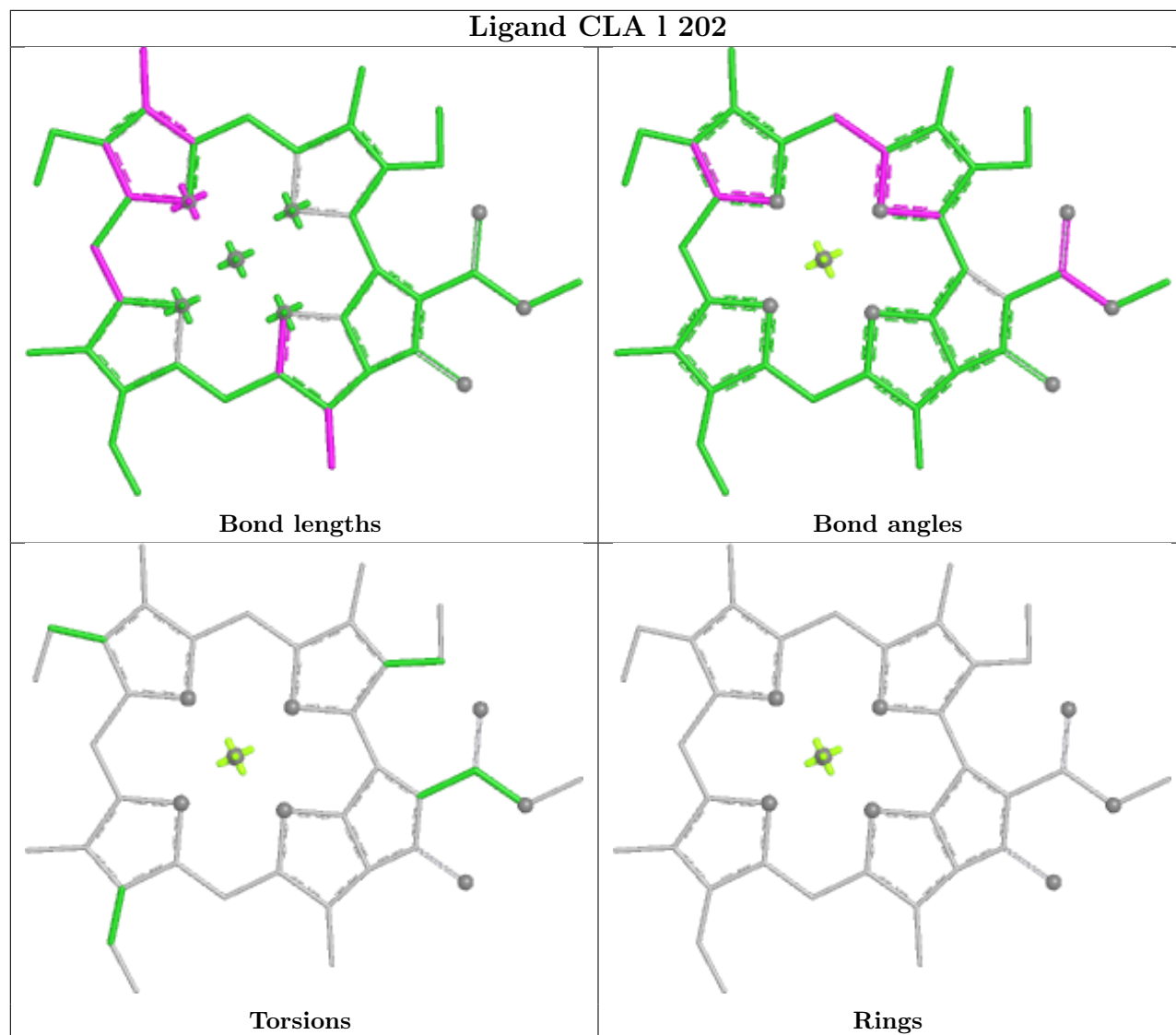


Torsions

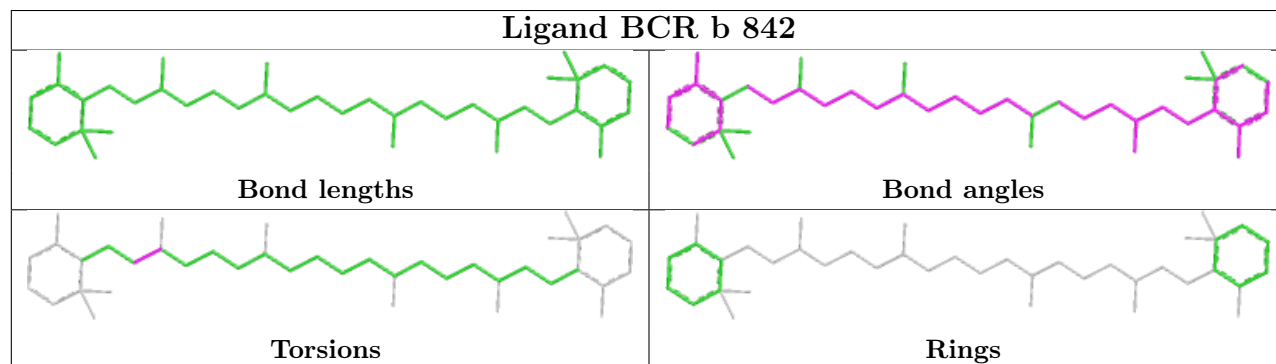


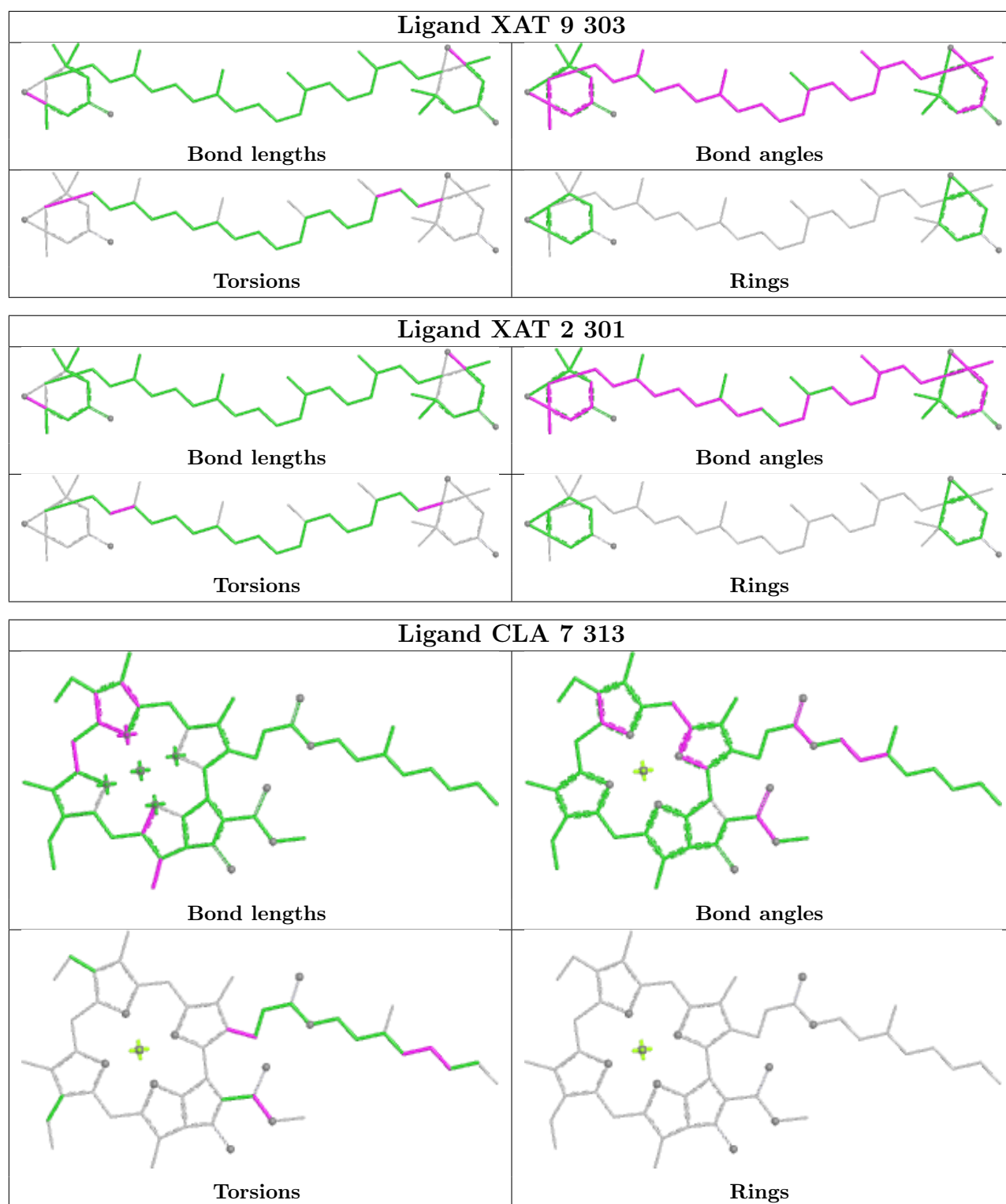
Rings

Ligand CLA 1 202

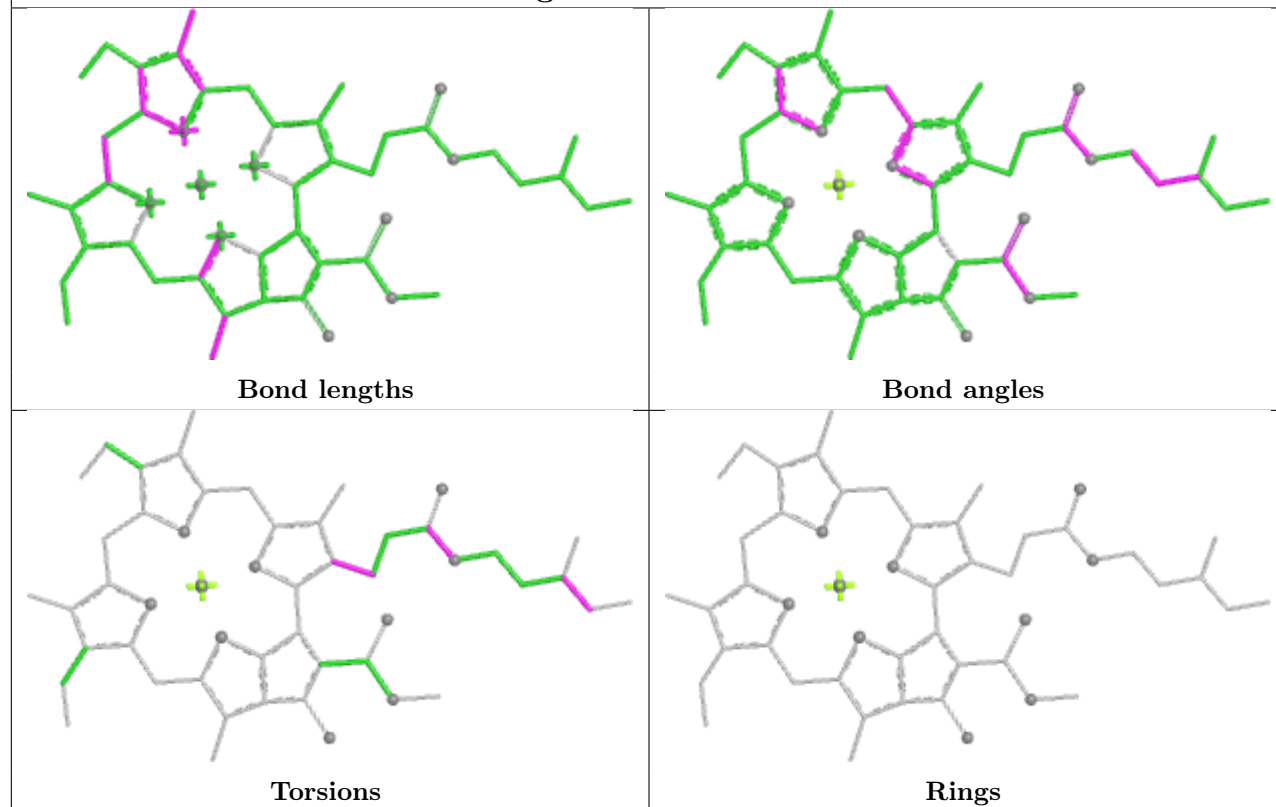


Ligand BCR b 842

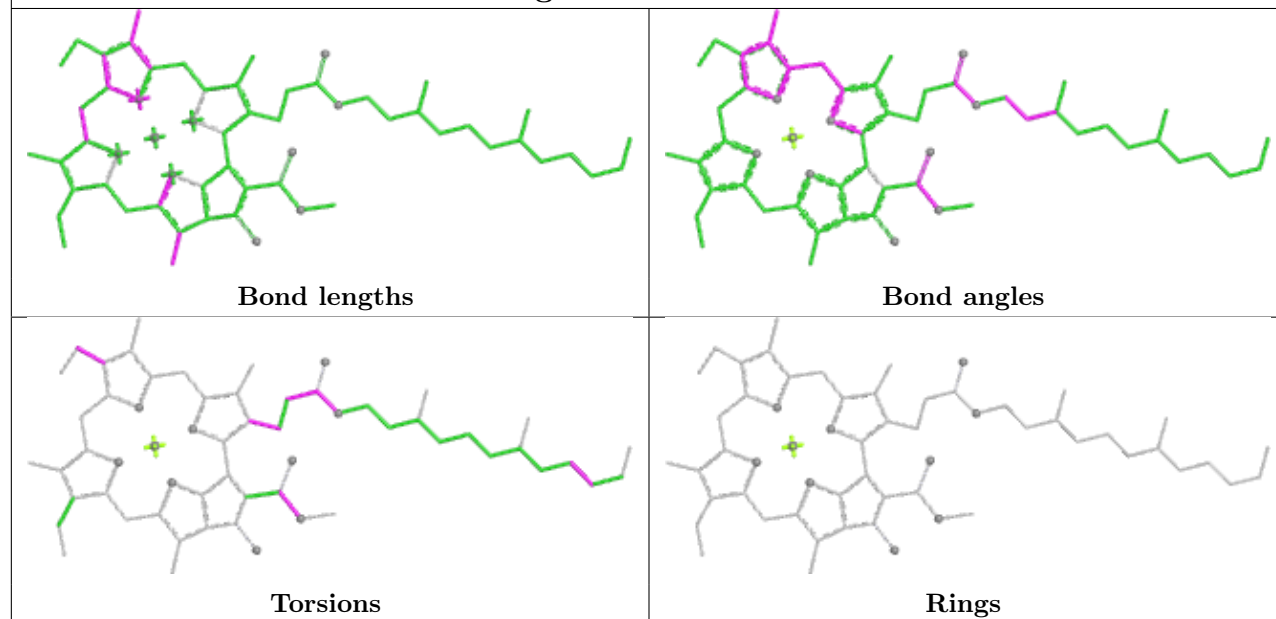


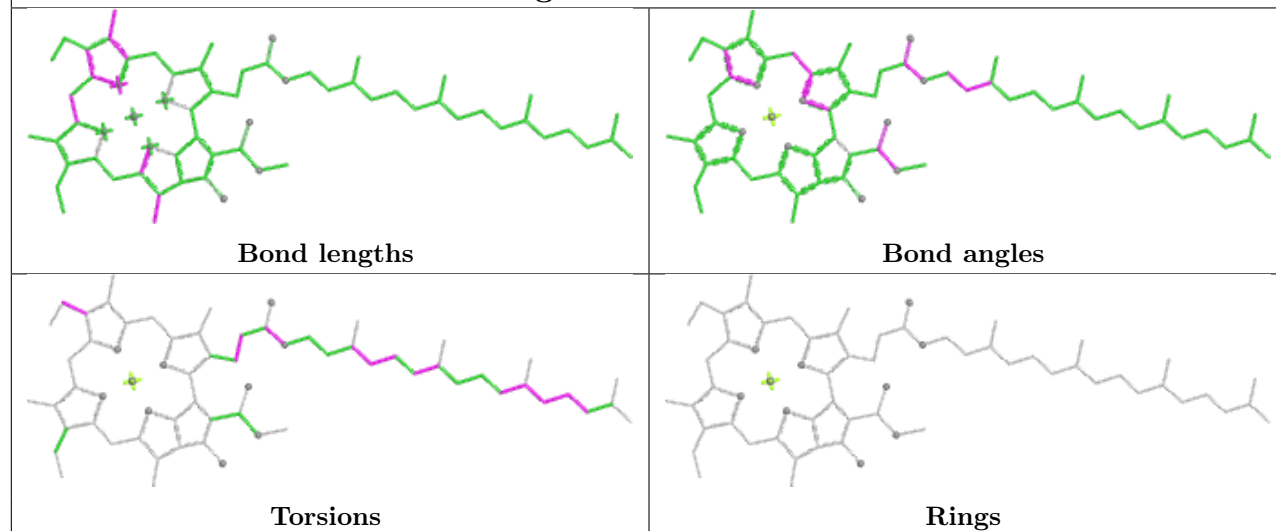
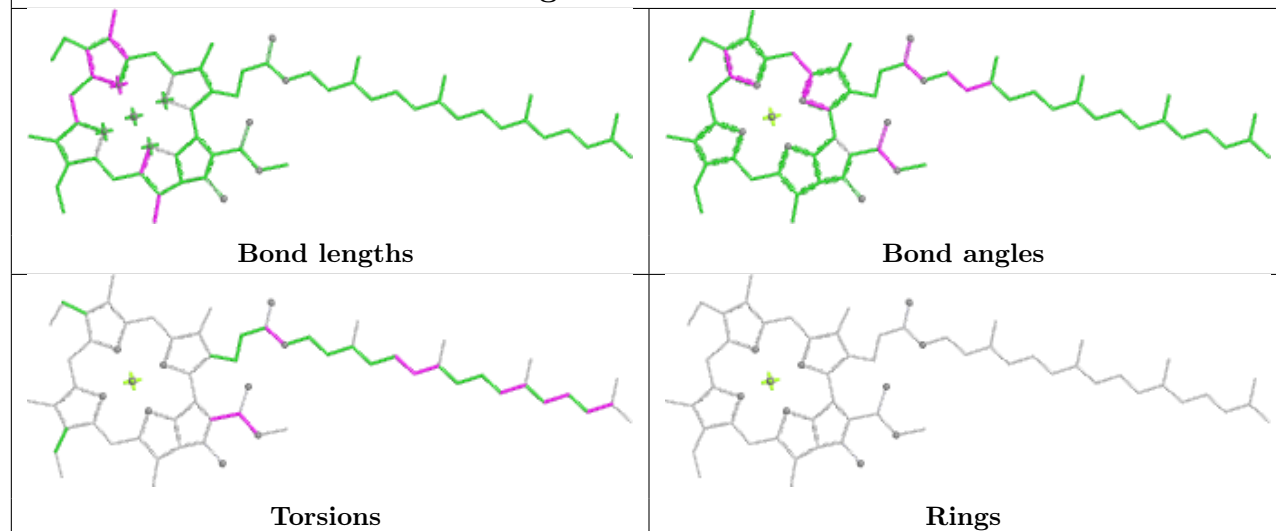


Ligand CLA a 838

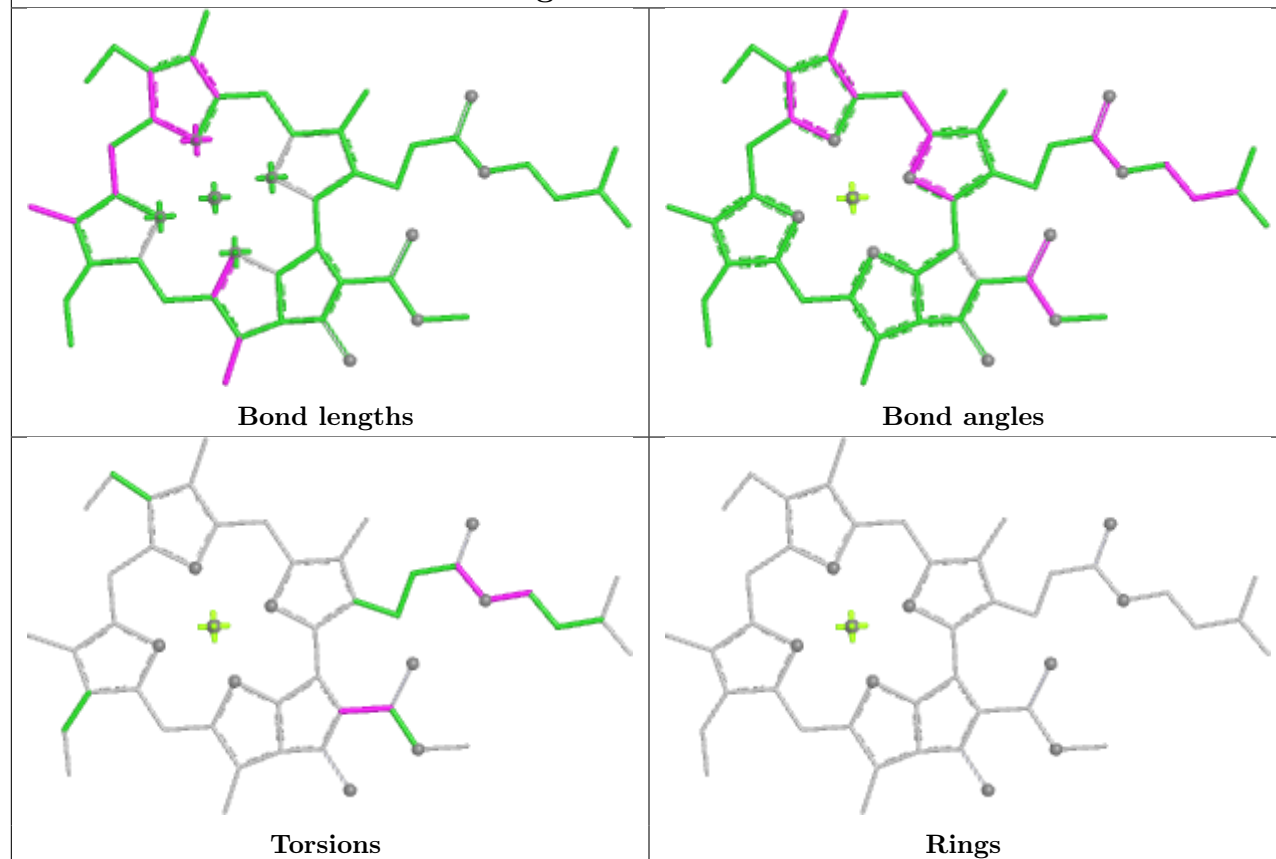


Ligand CLA b 817

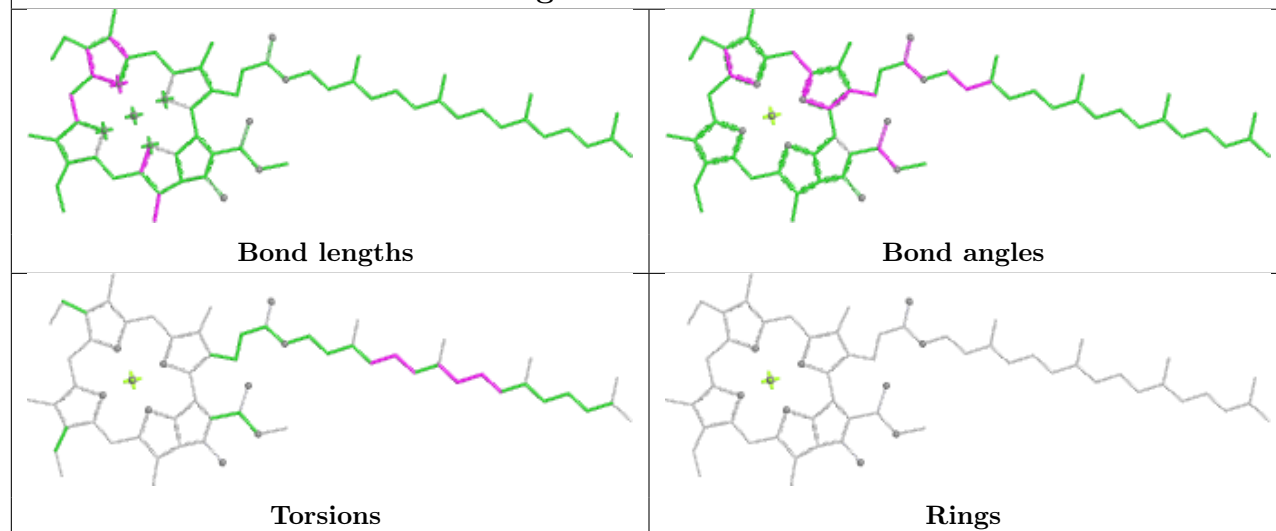


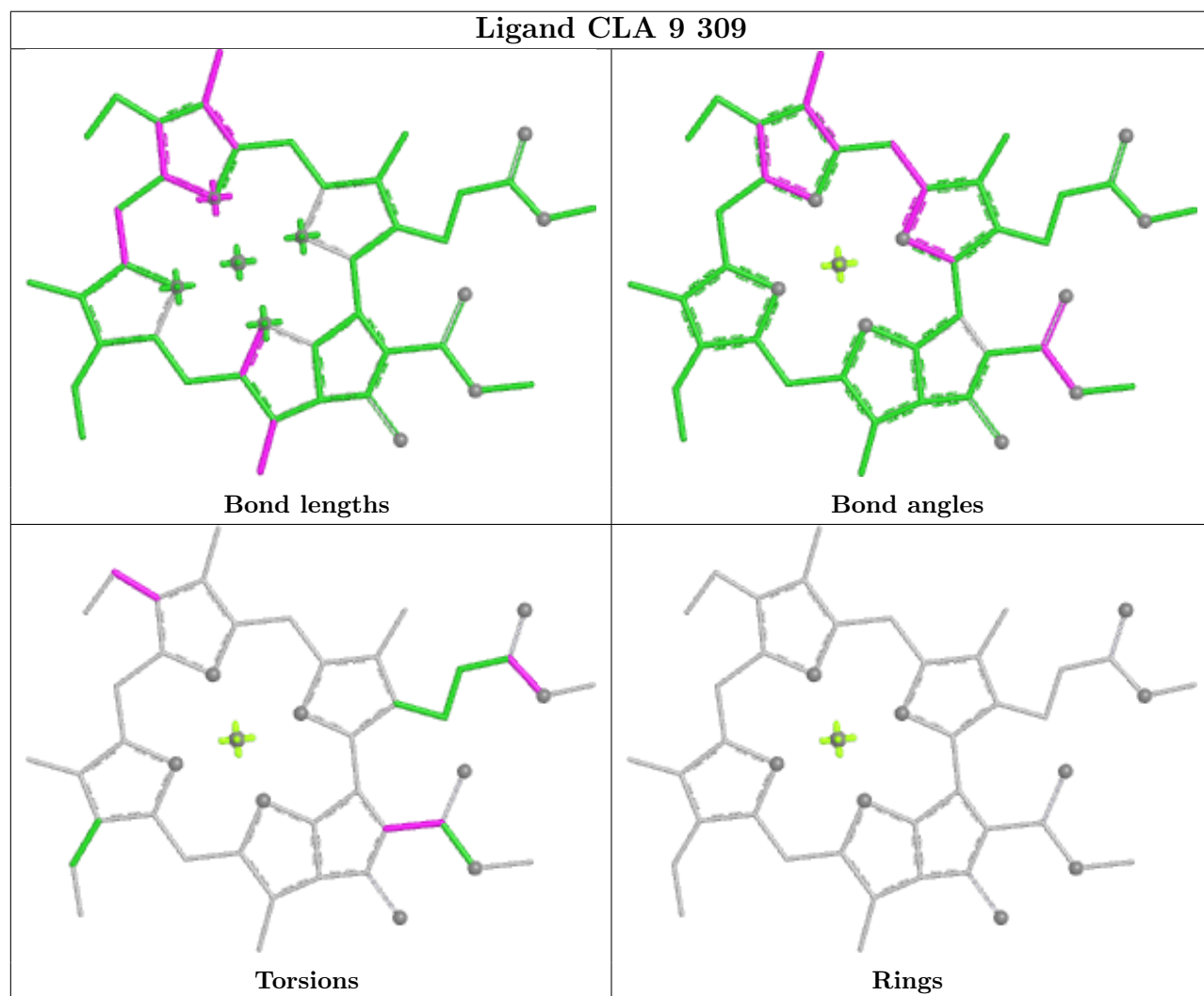
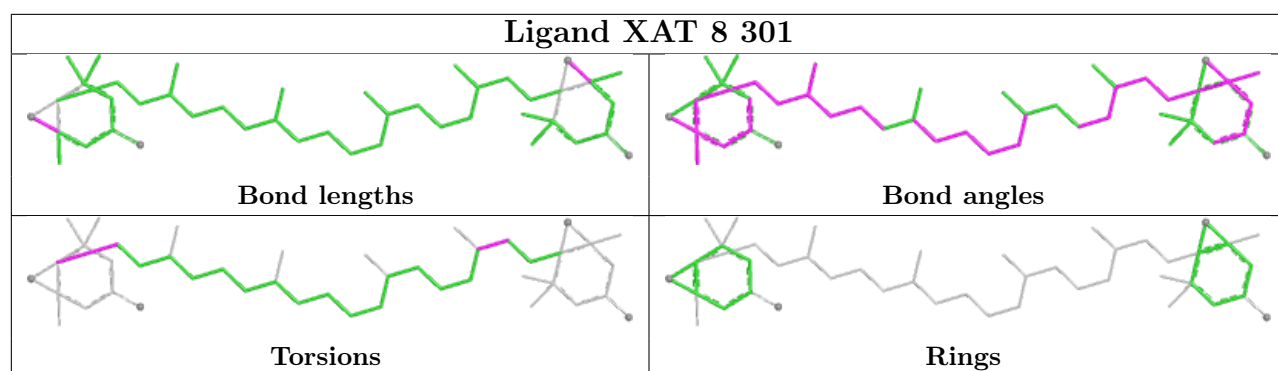
Ligand CLA b 838**Ligand CLA f 802**

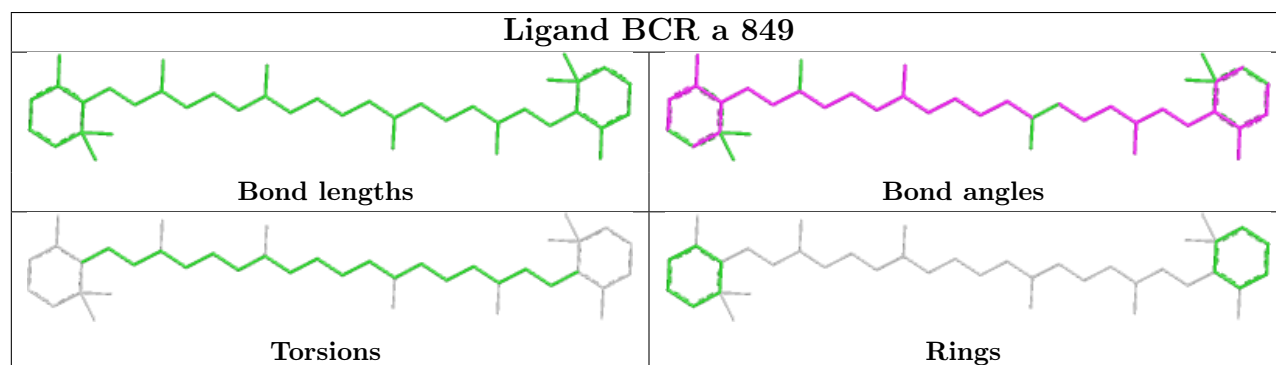
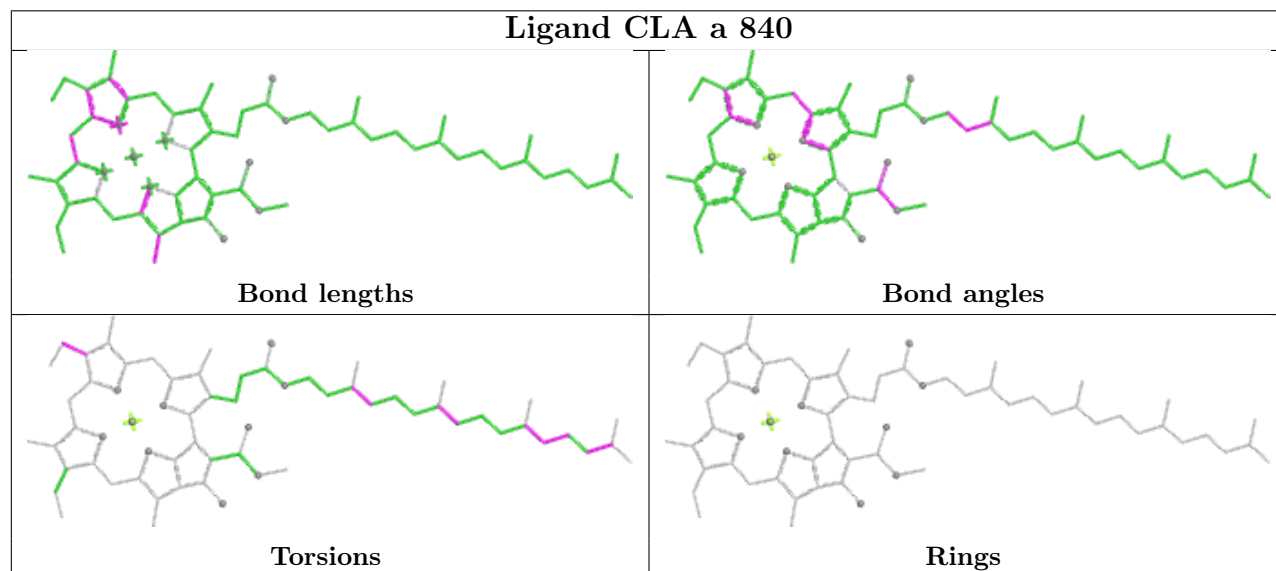
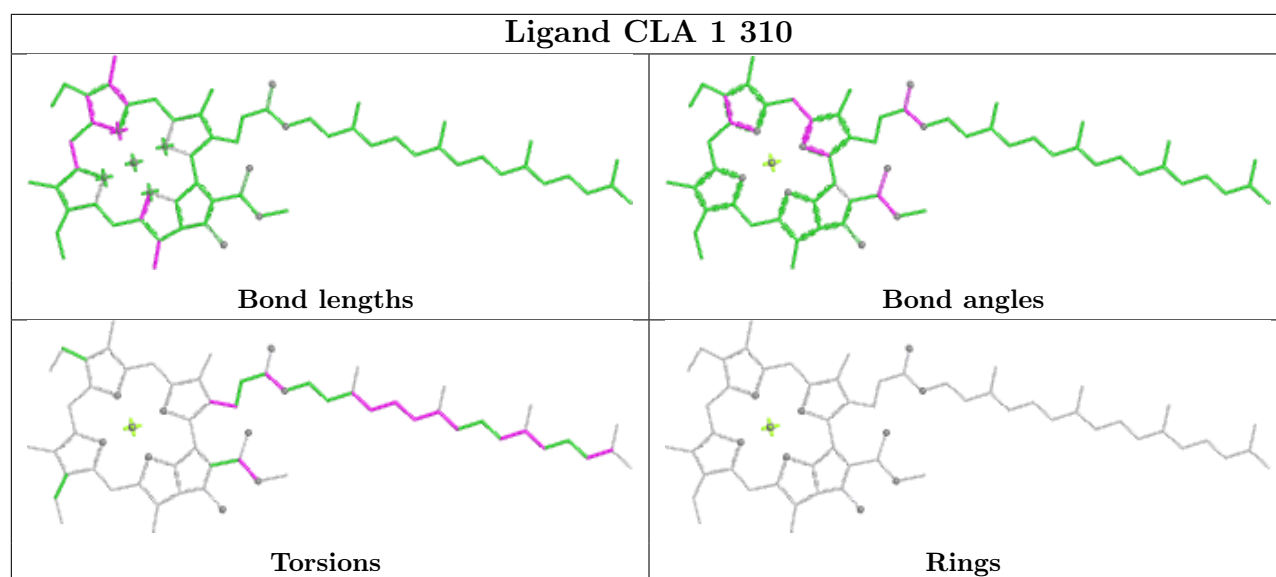
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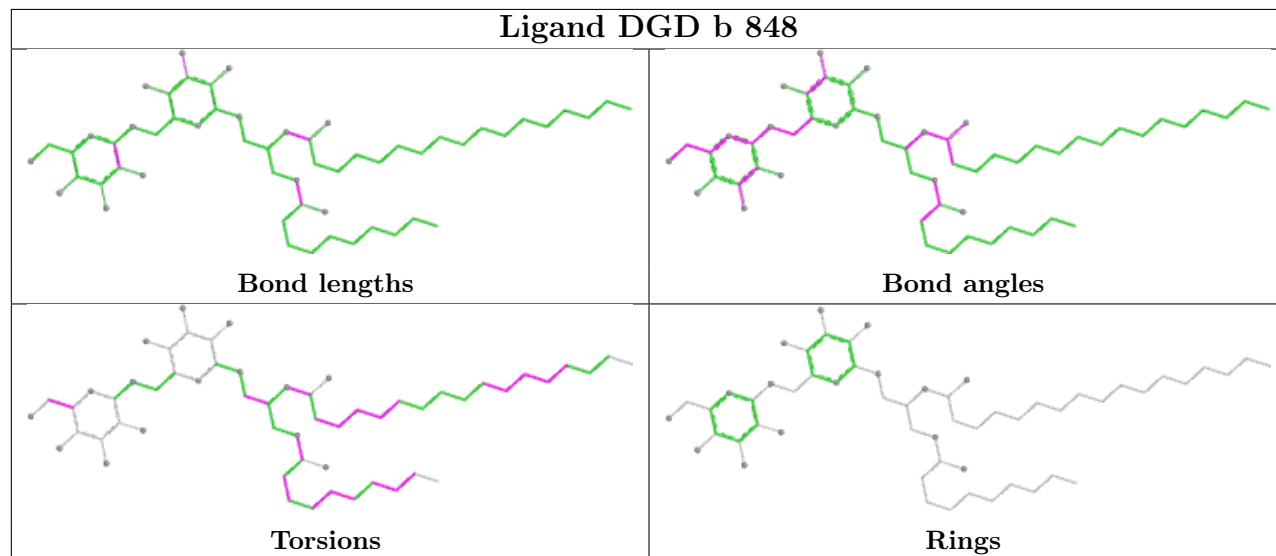
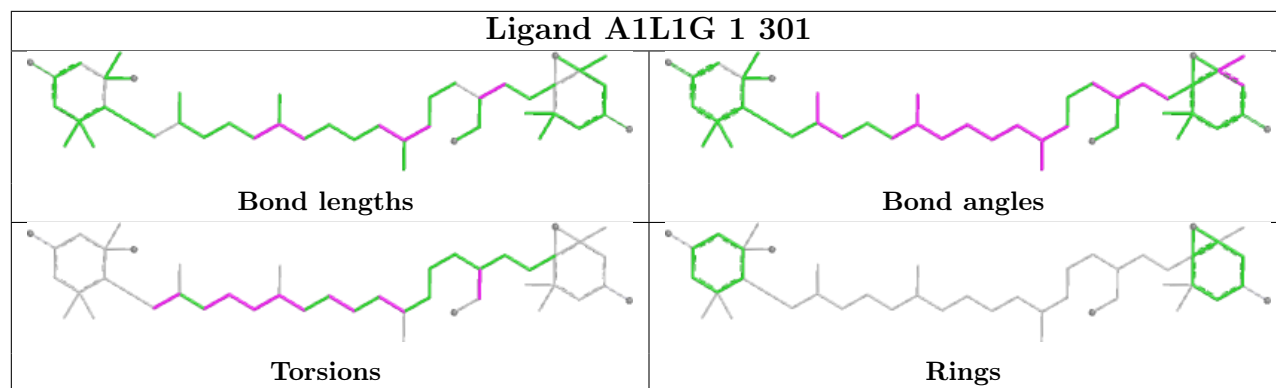


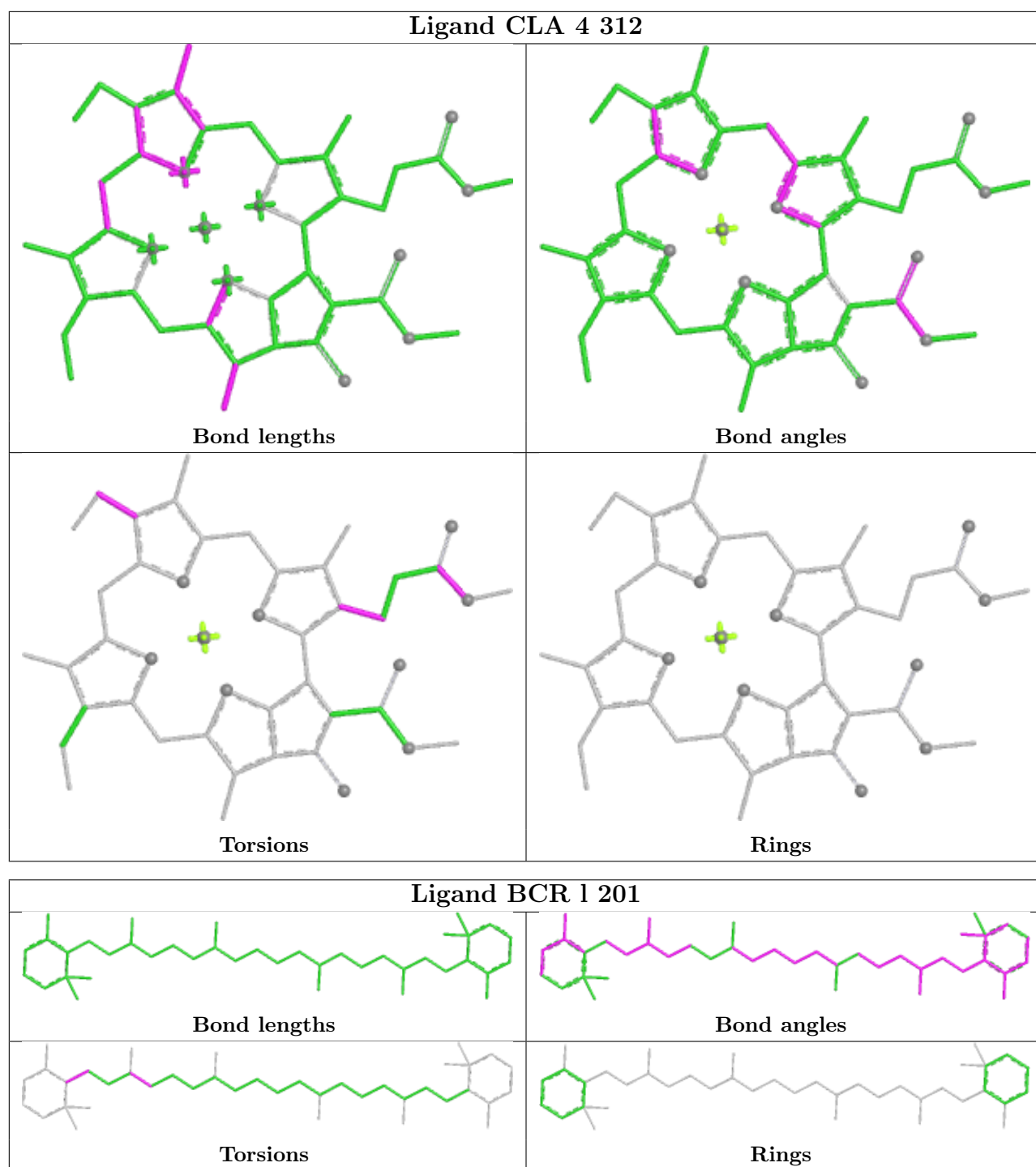
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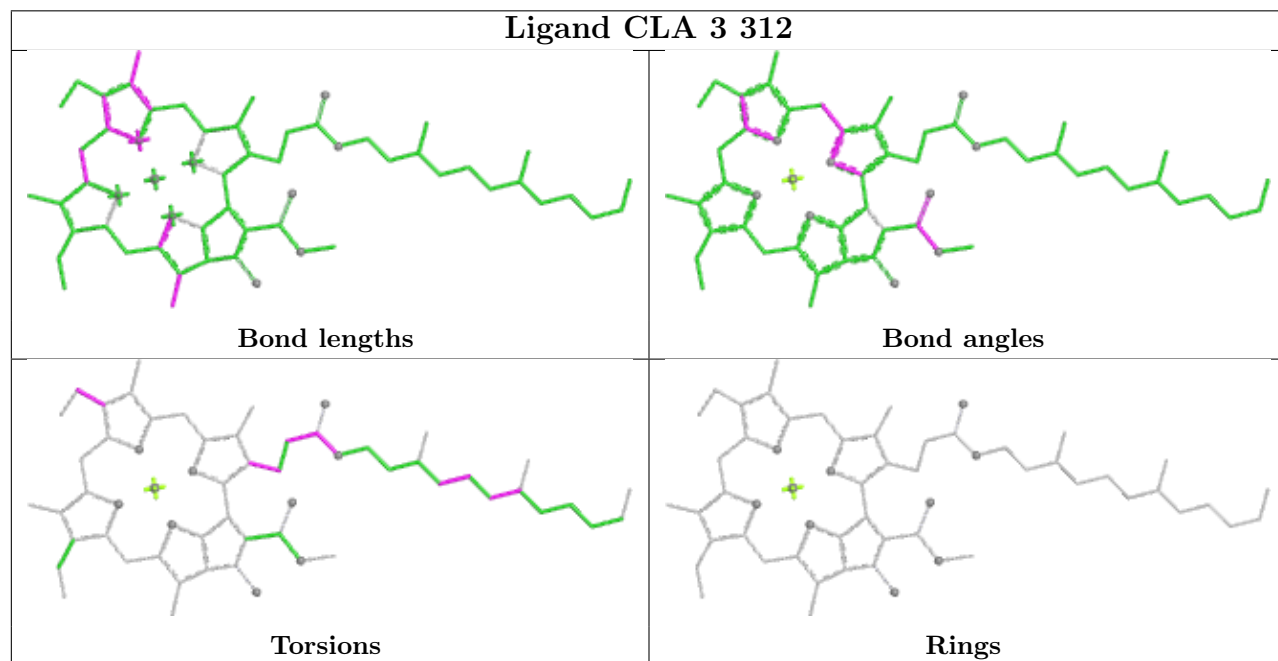
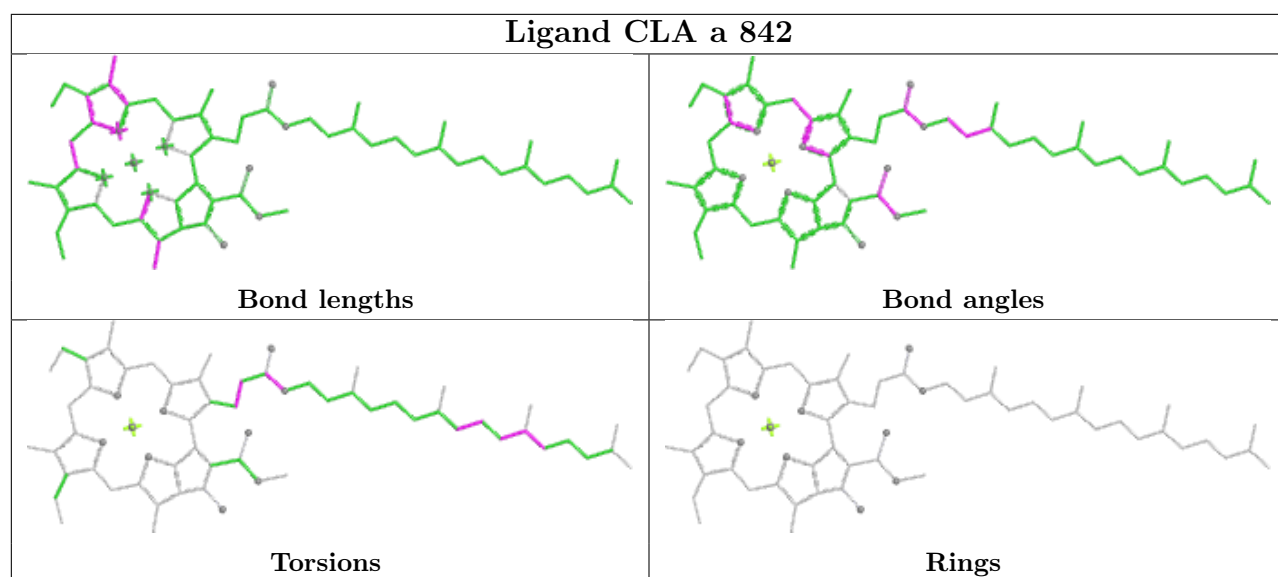


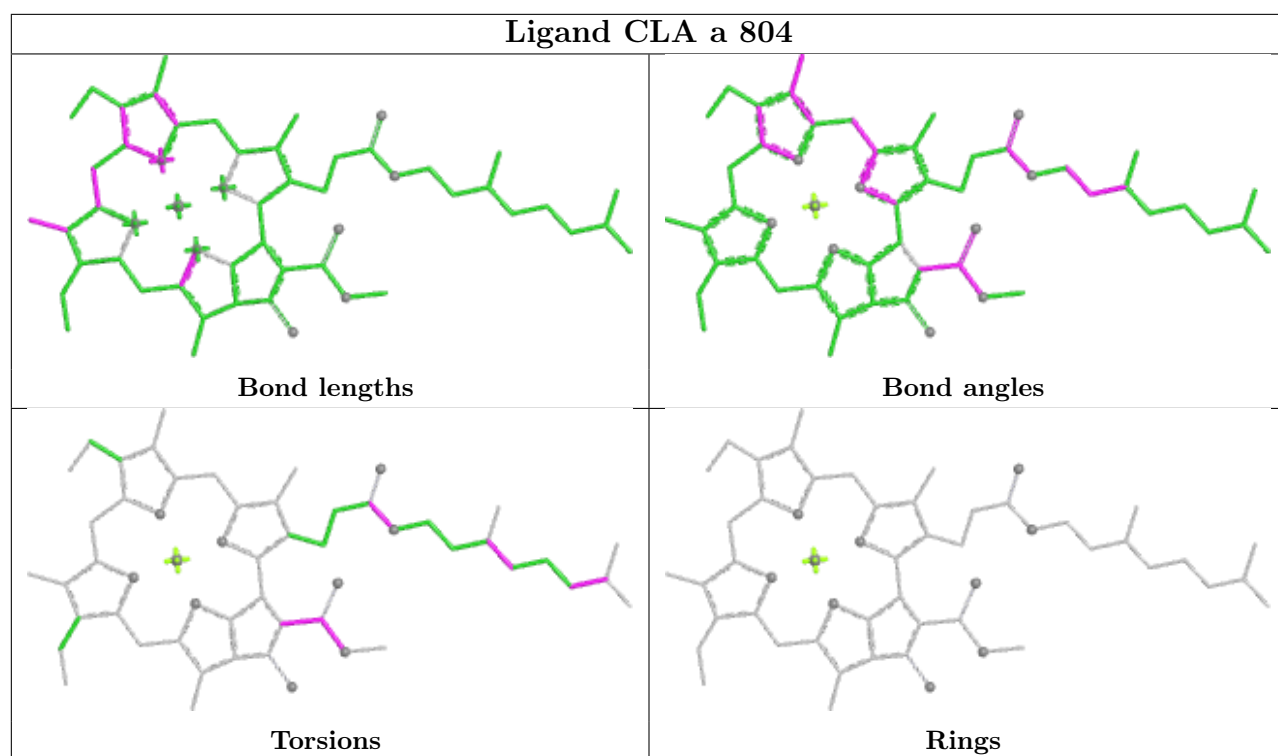




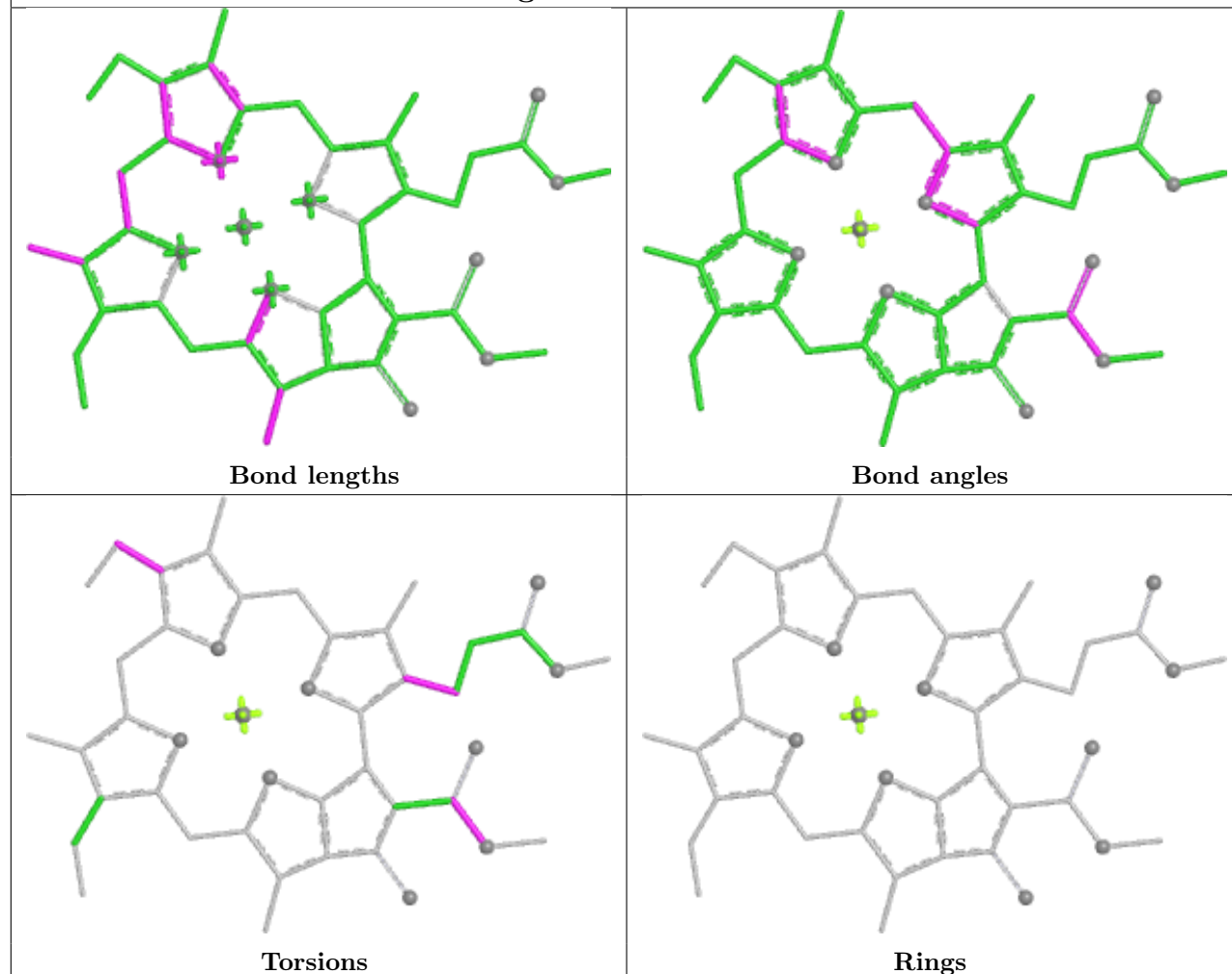




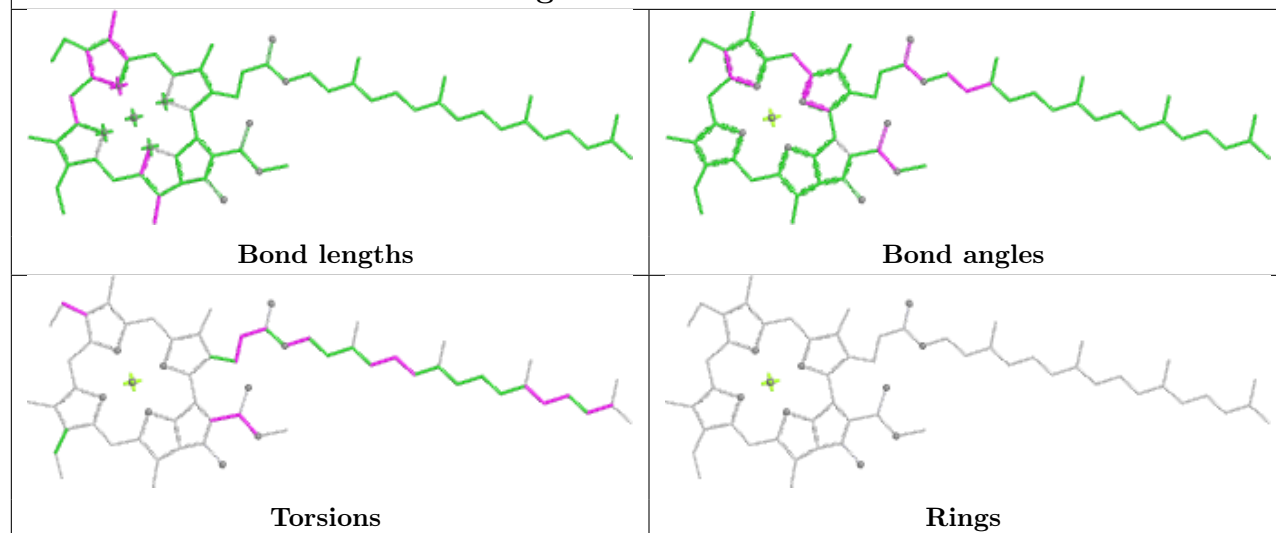


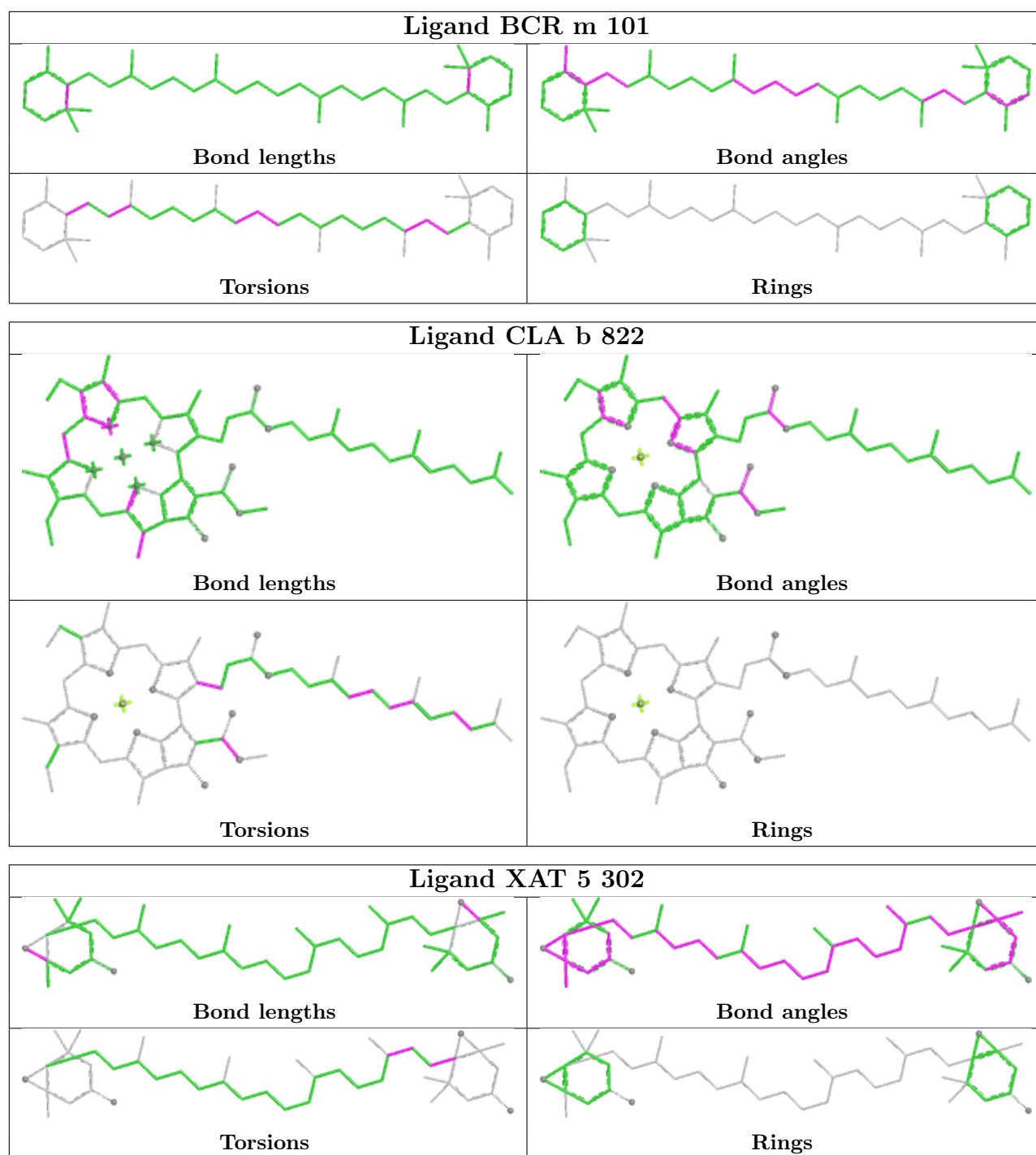


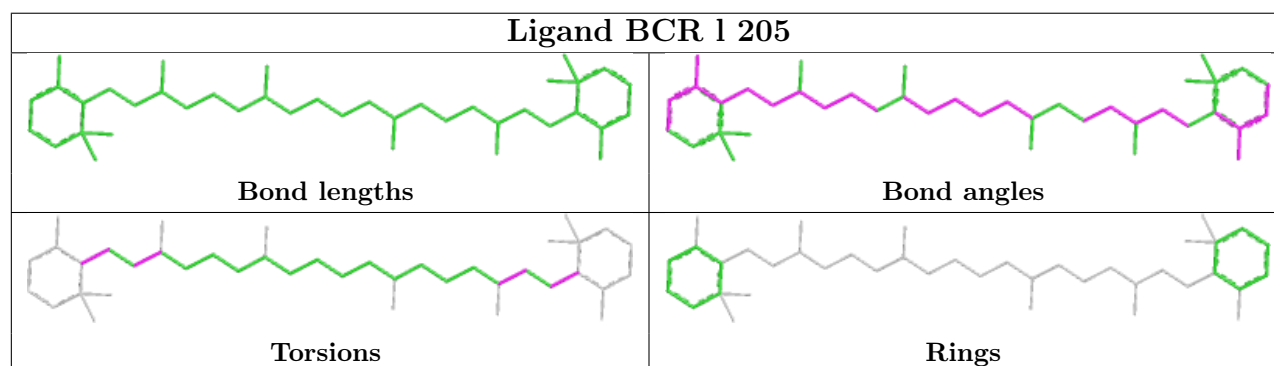
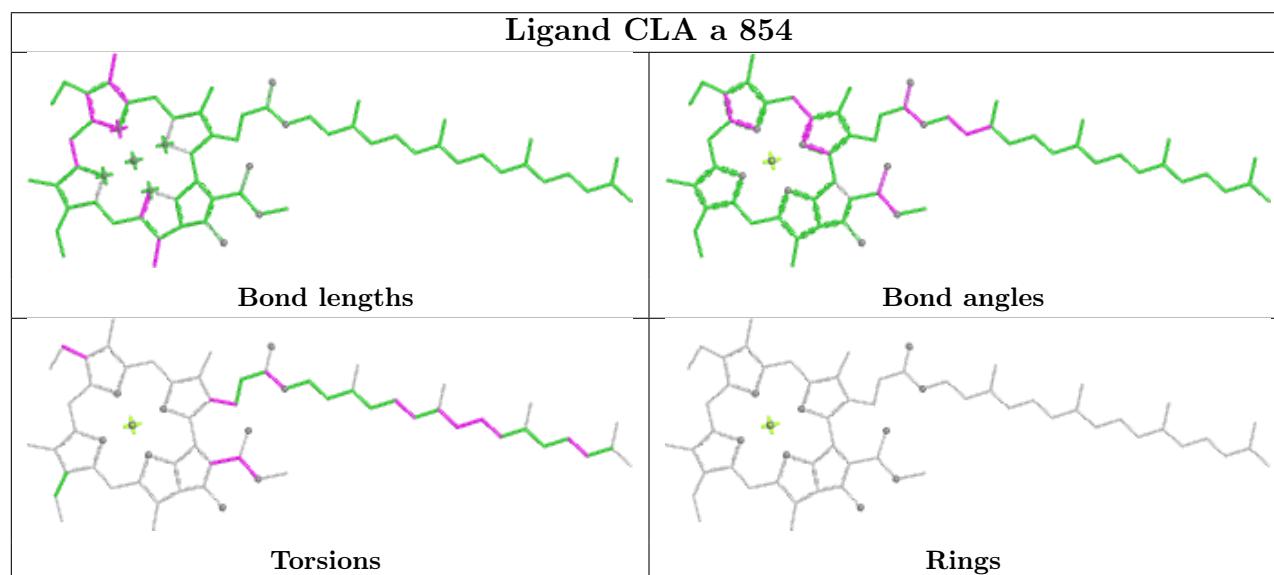
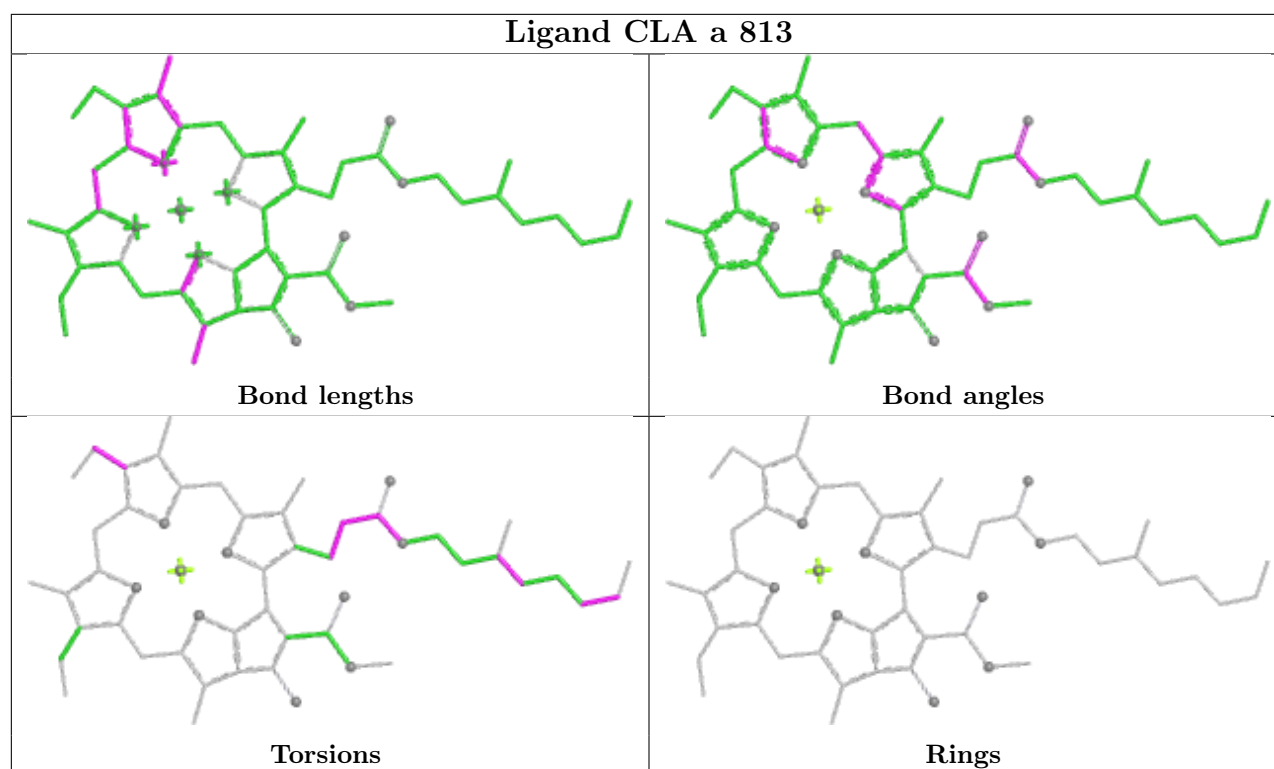
Ligand CLA 2 316



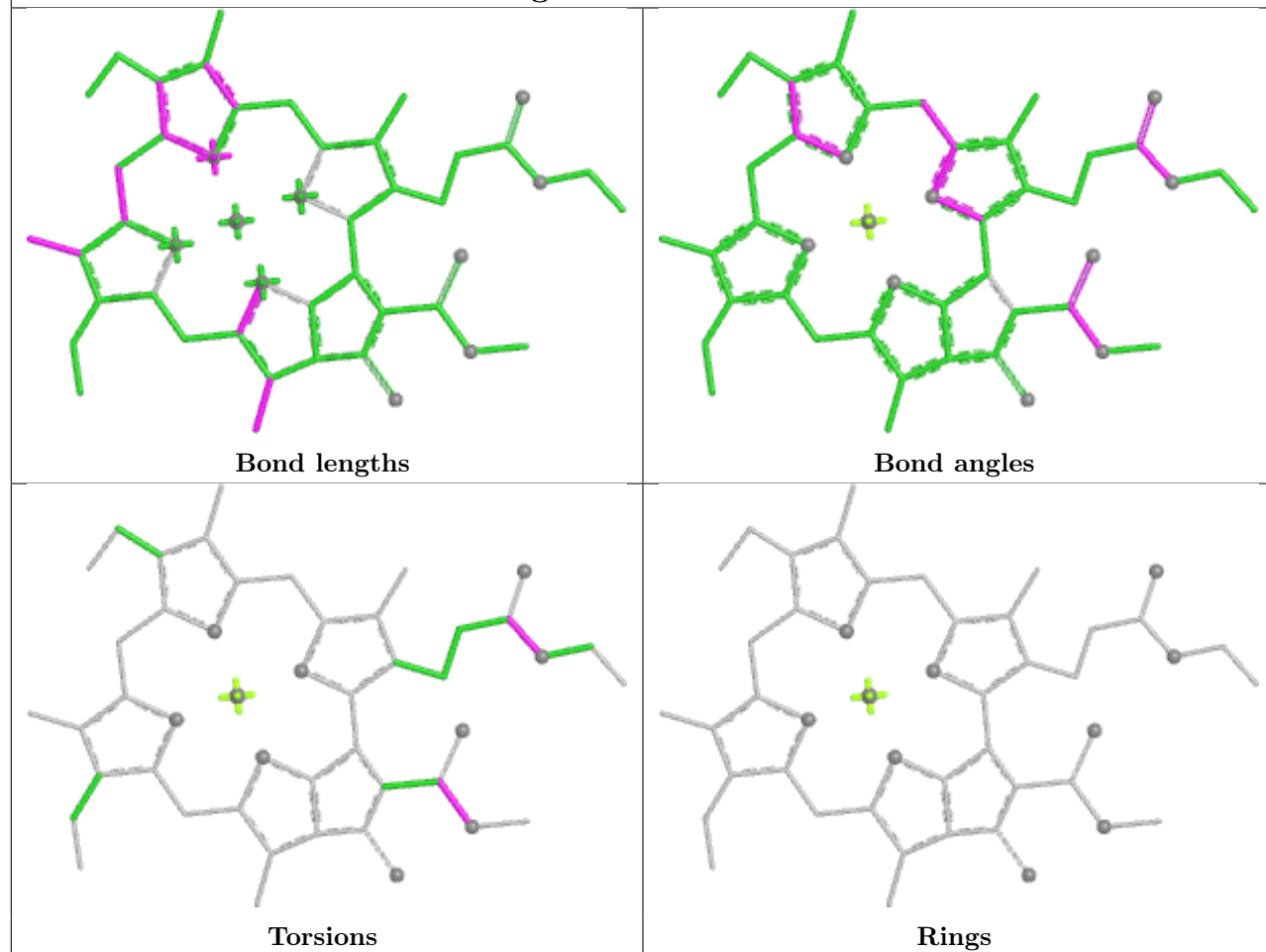
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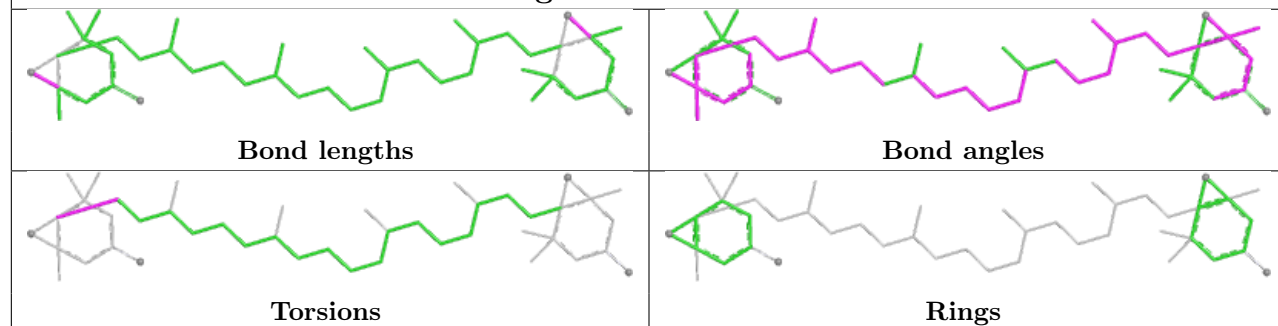




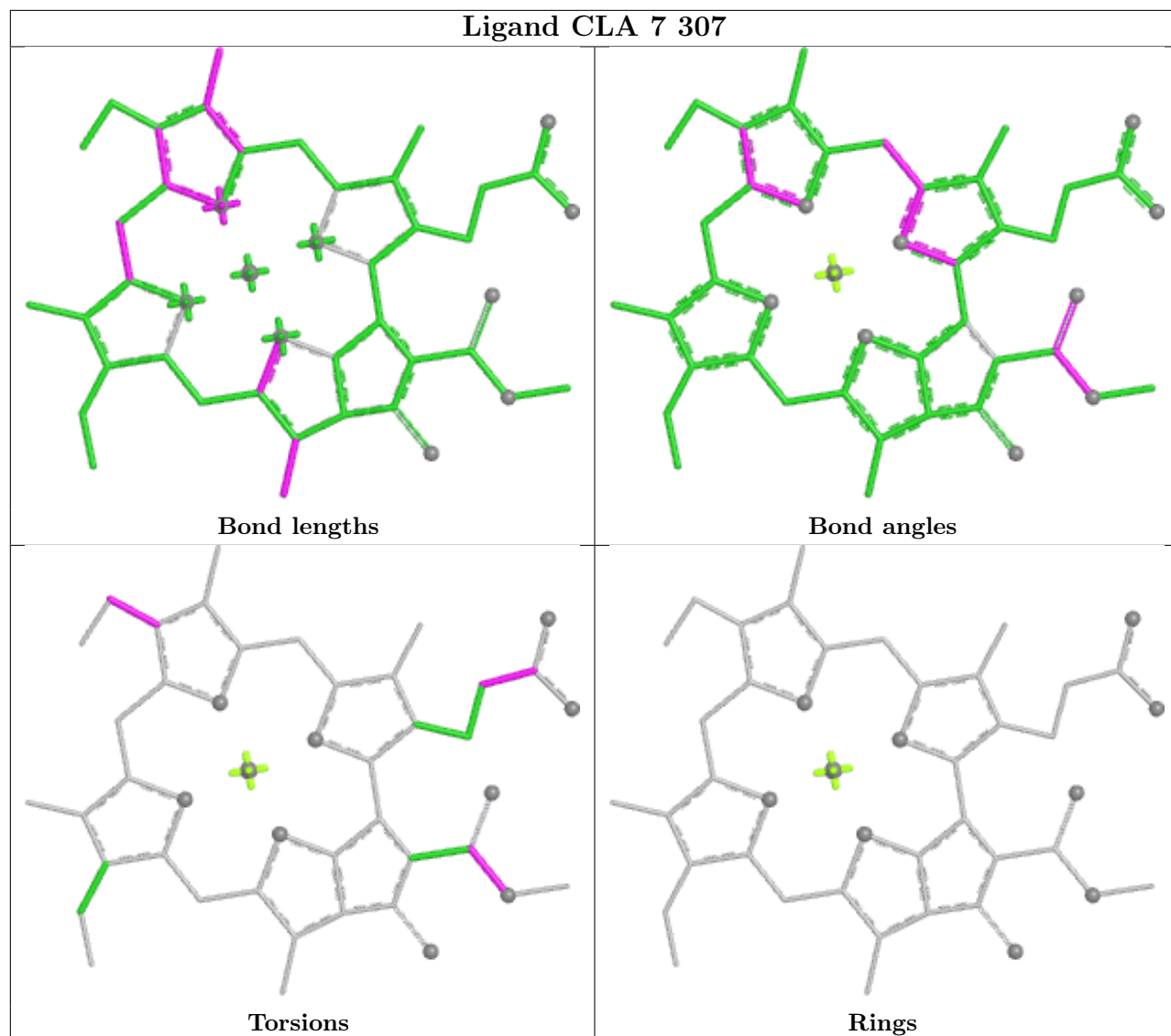
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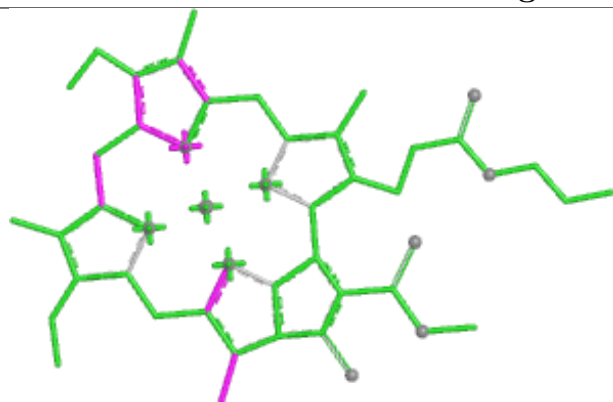
Ligand XAT 5 304



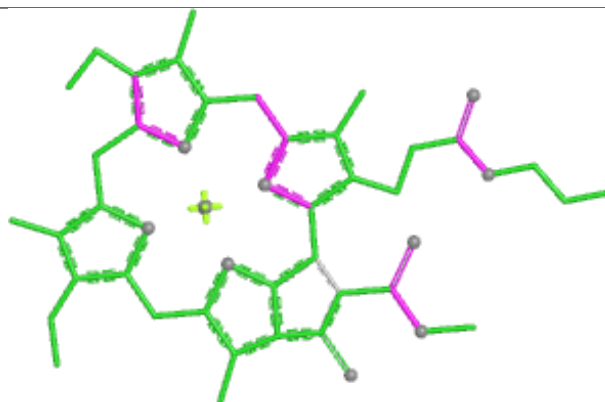
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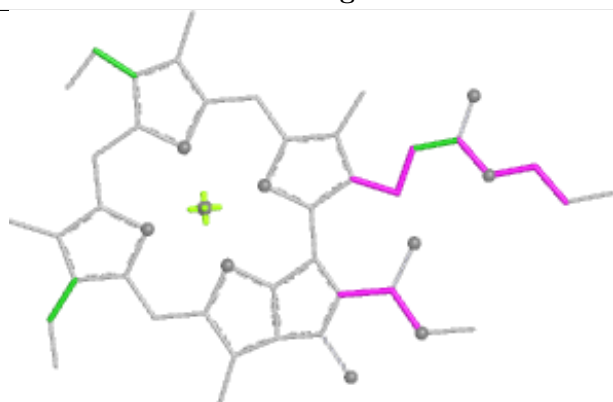
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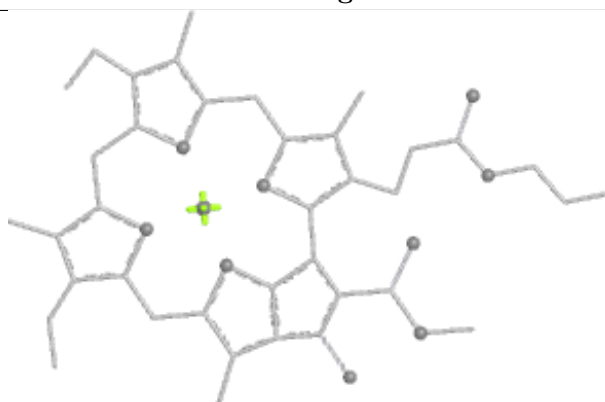
Bond lengths



Bond angles

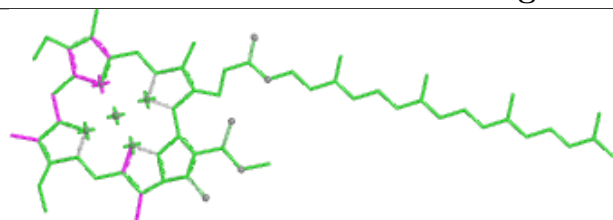


Torsions

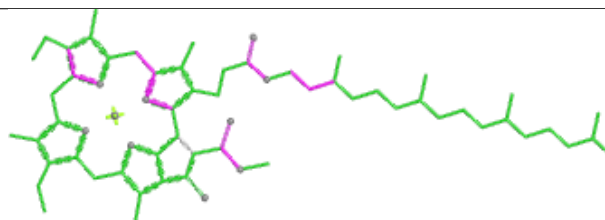


Rings

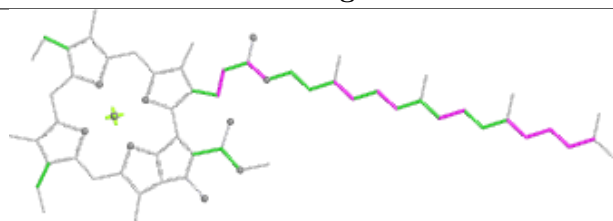
Ligand CLA a 830



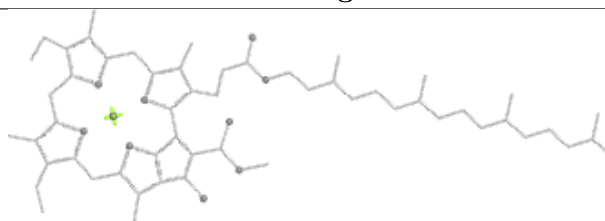
Bond lengths



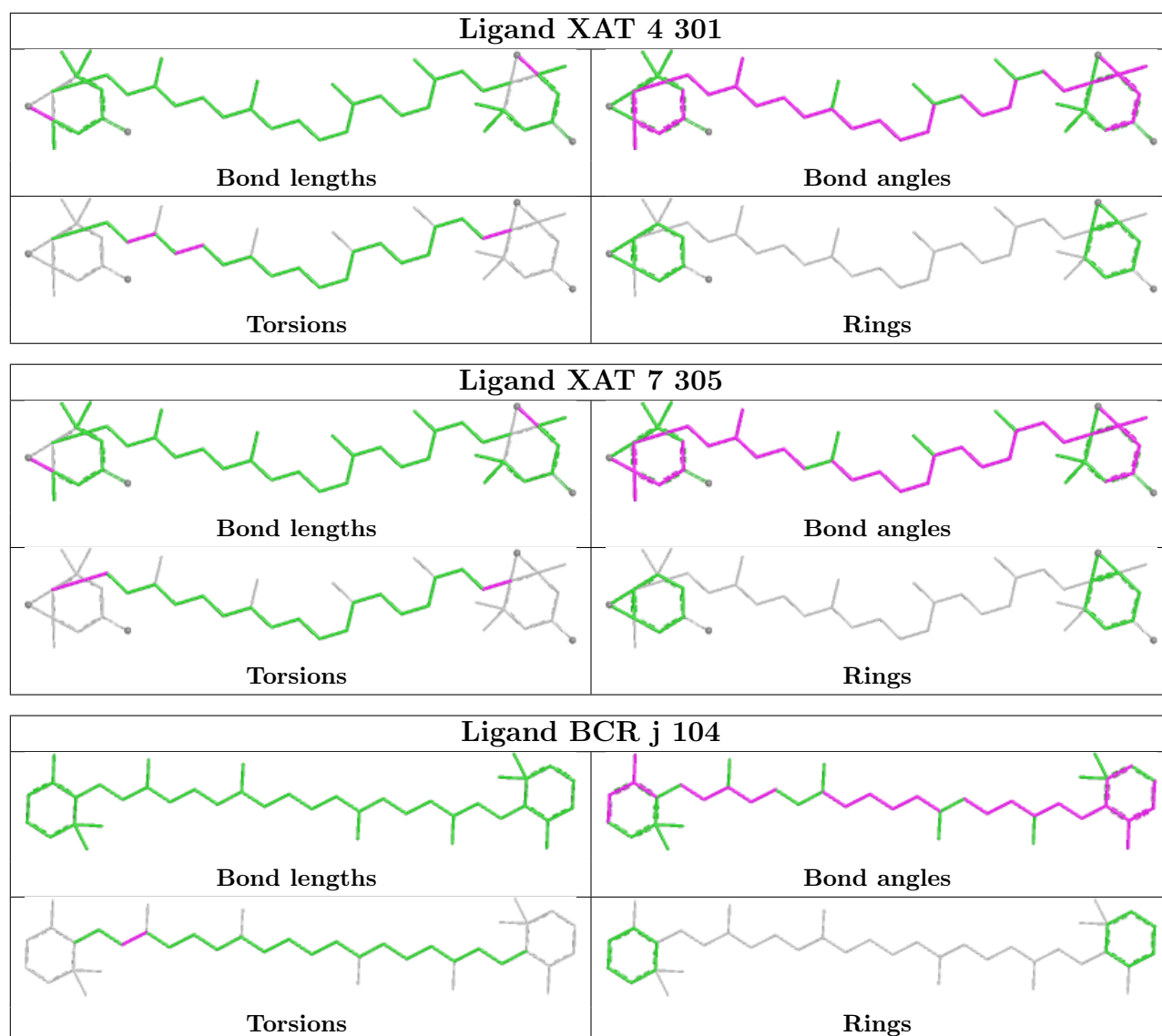
Bond angles

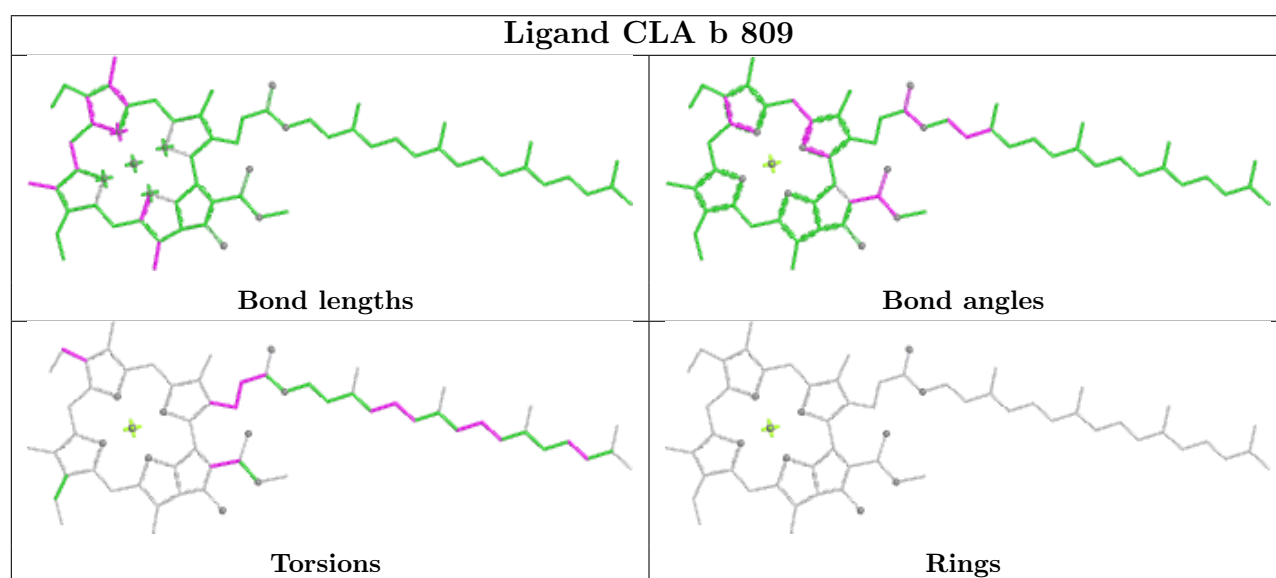
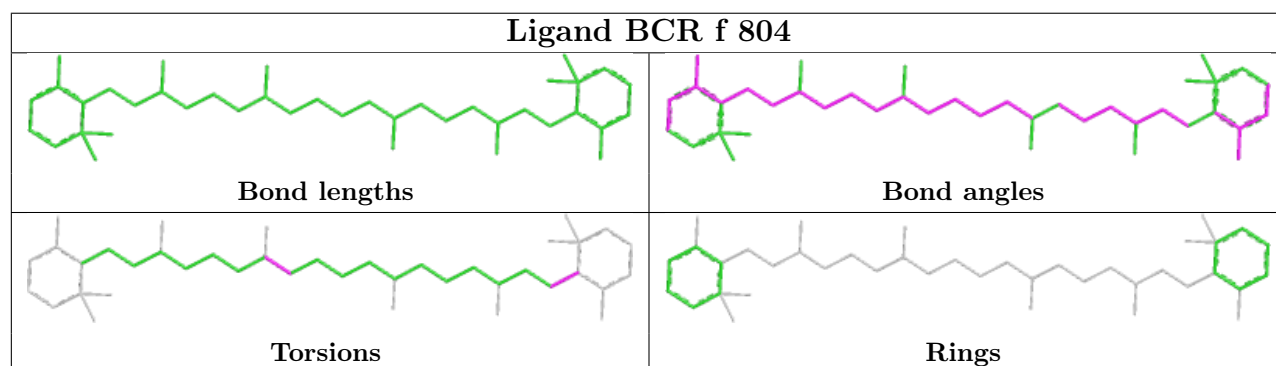
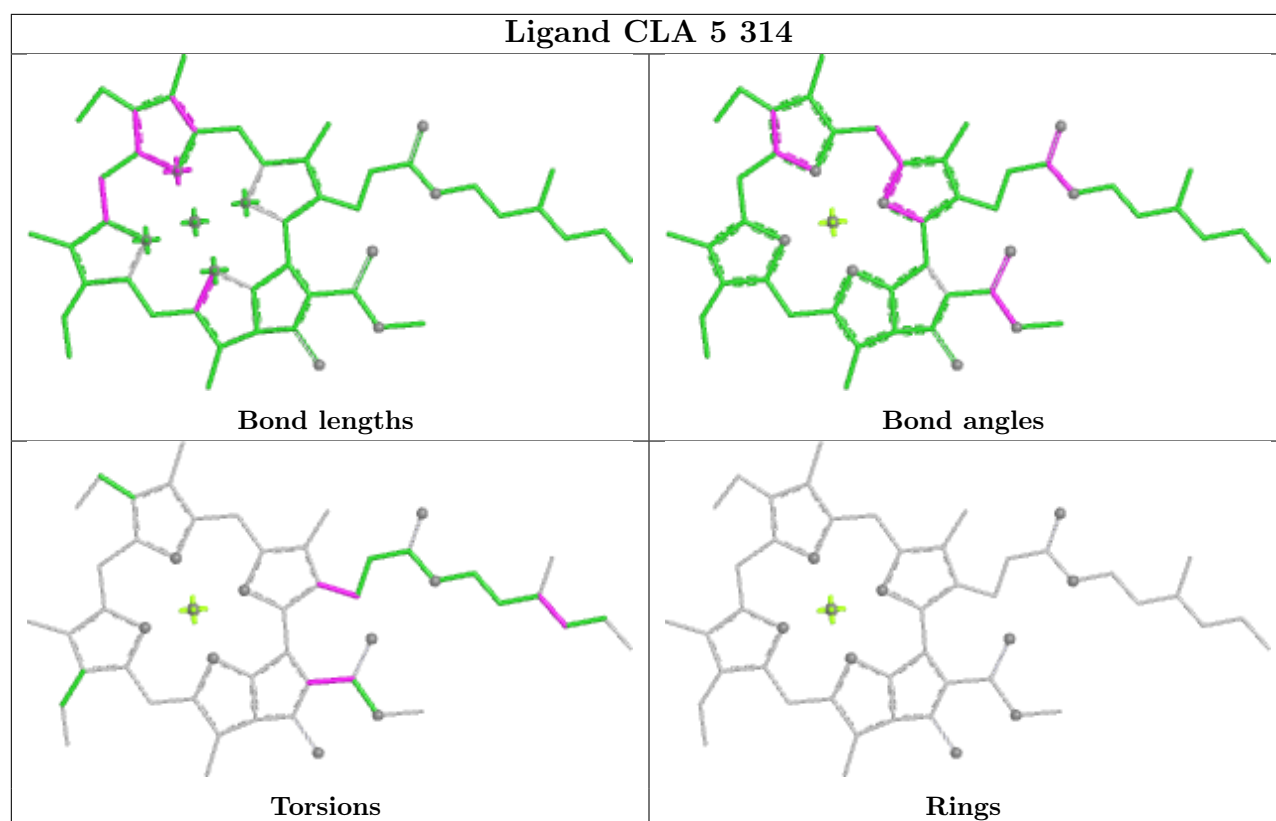


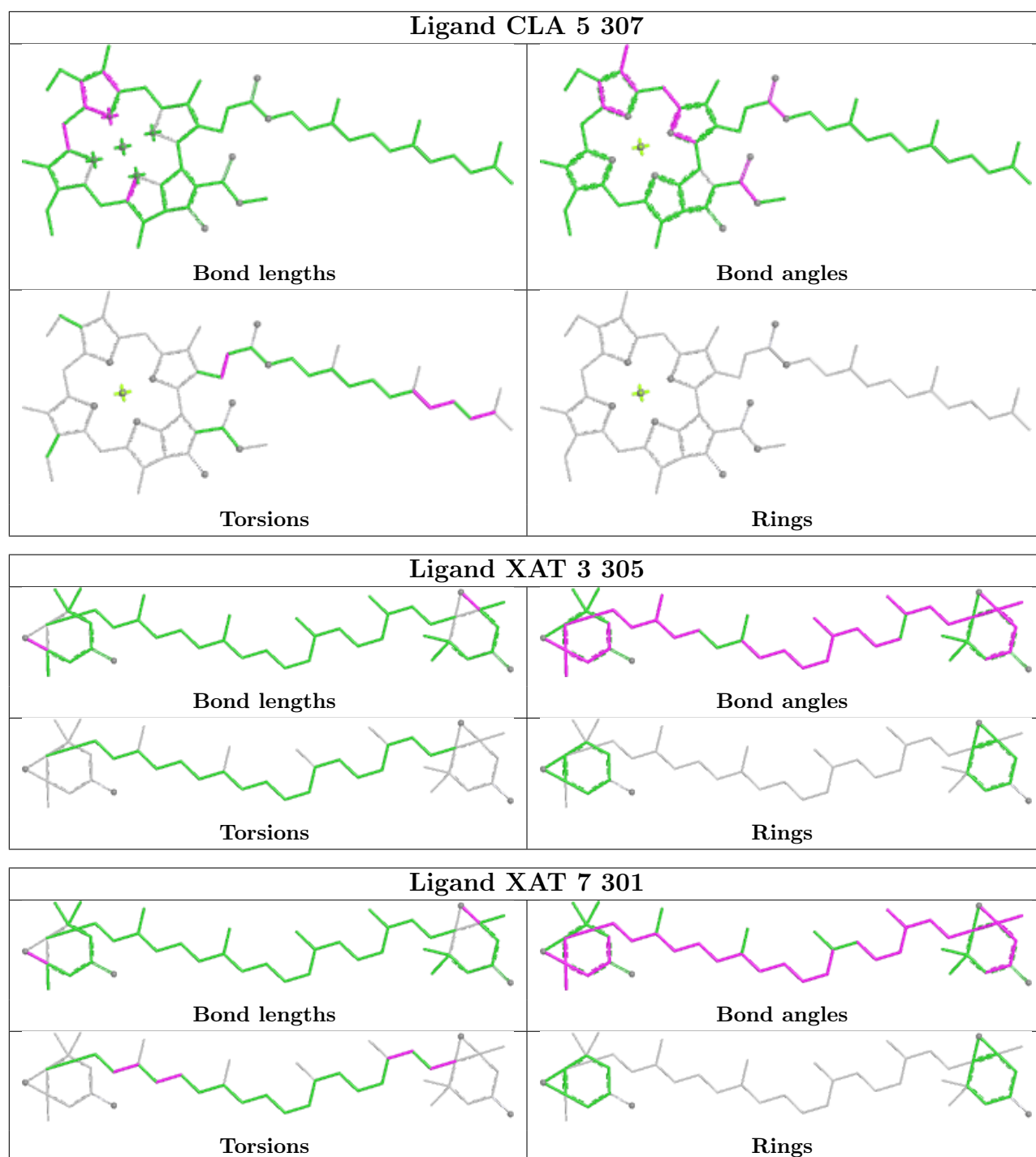
Torsions

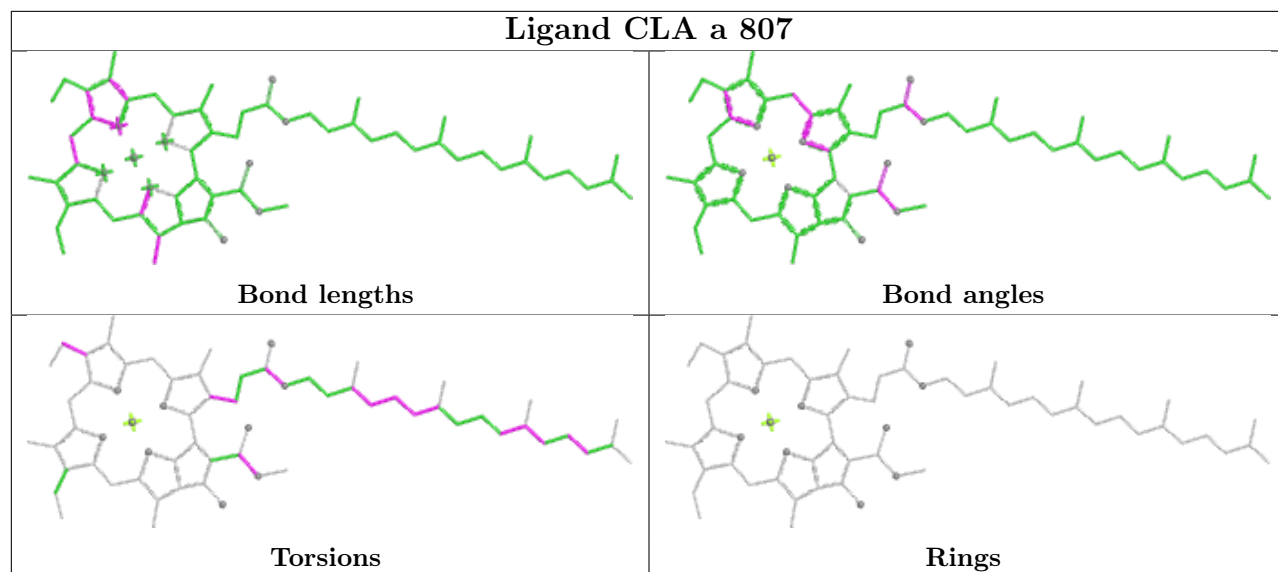
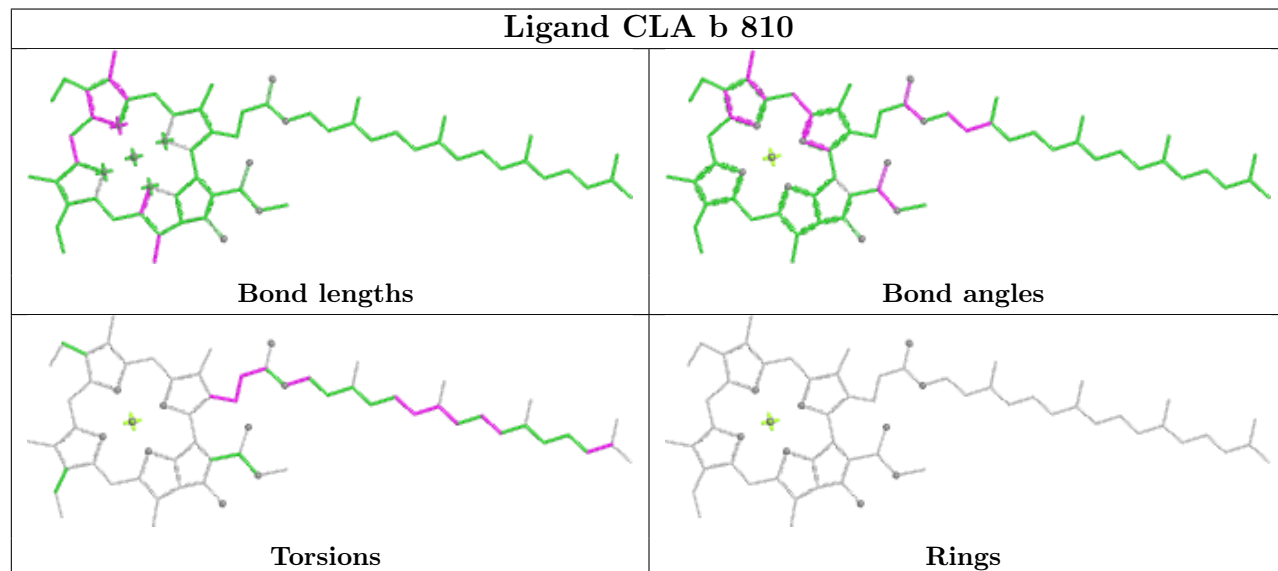


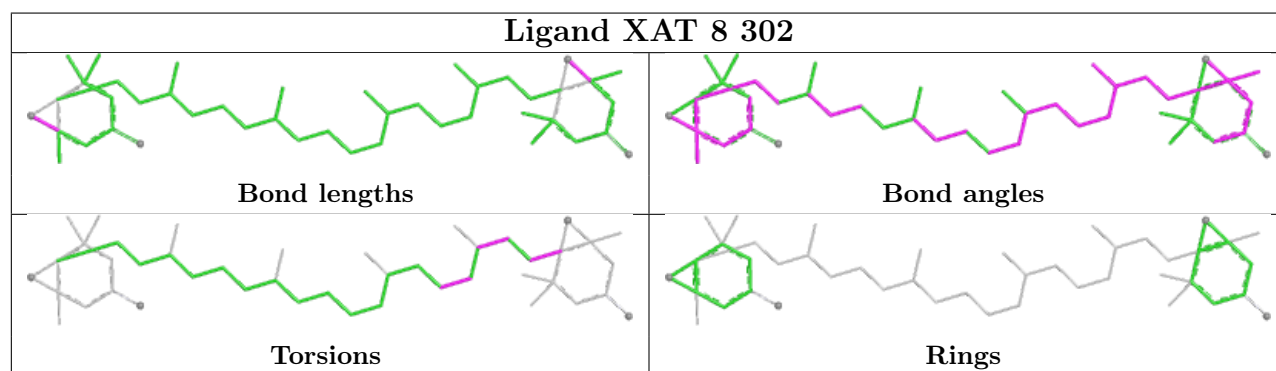
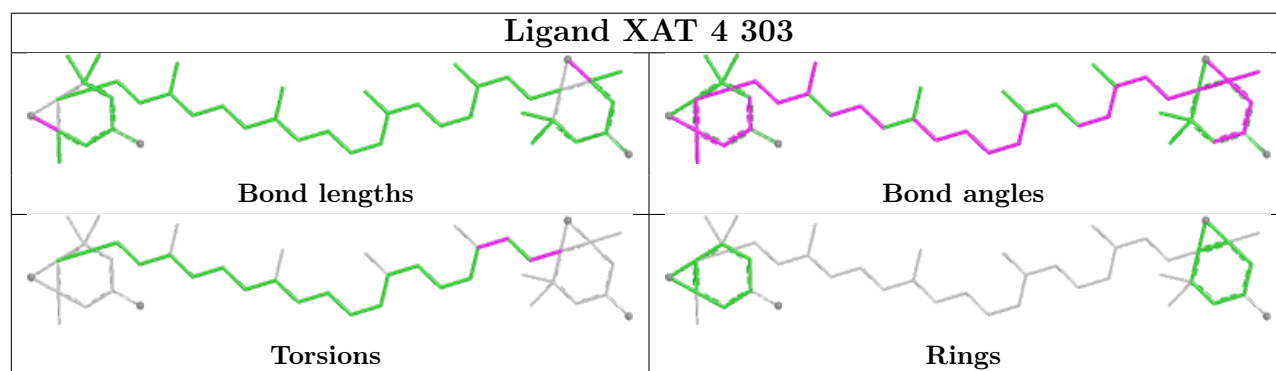
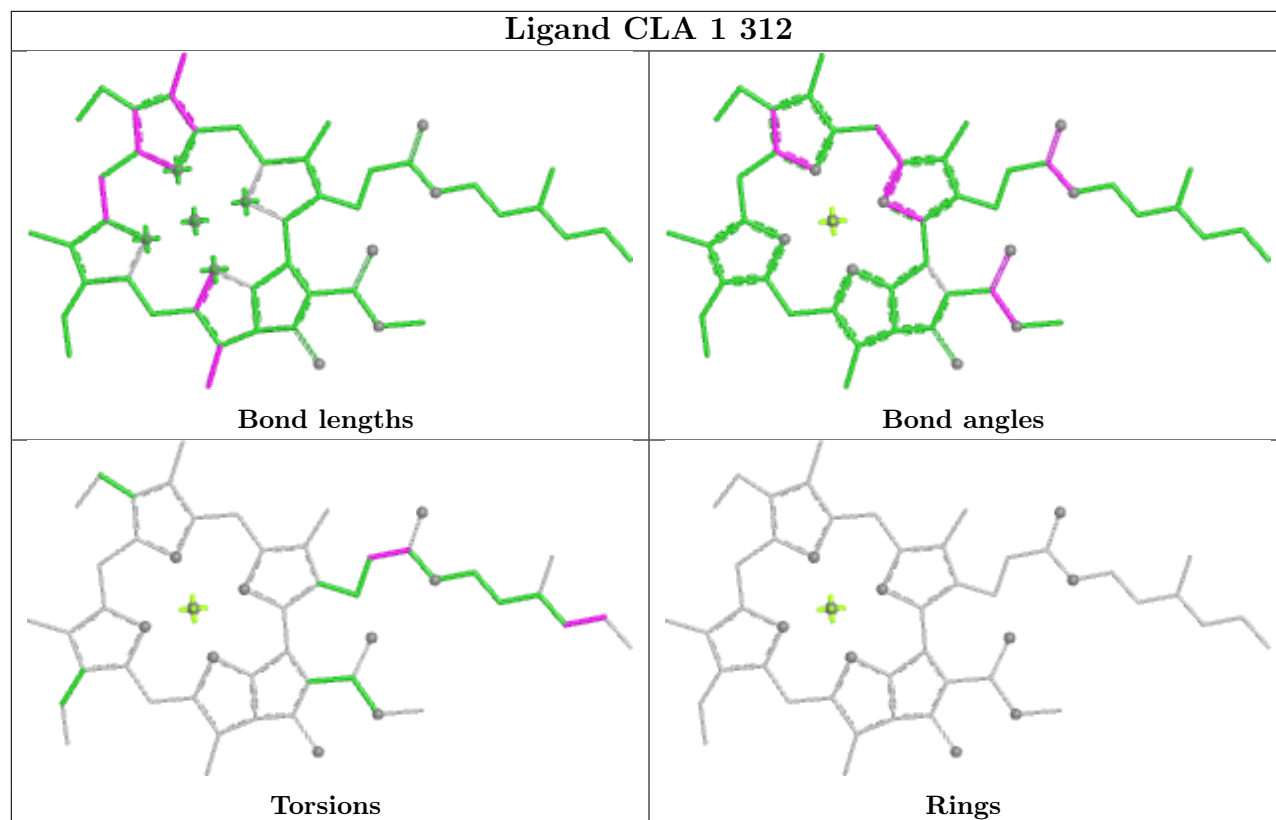
Rings



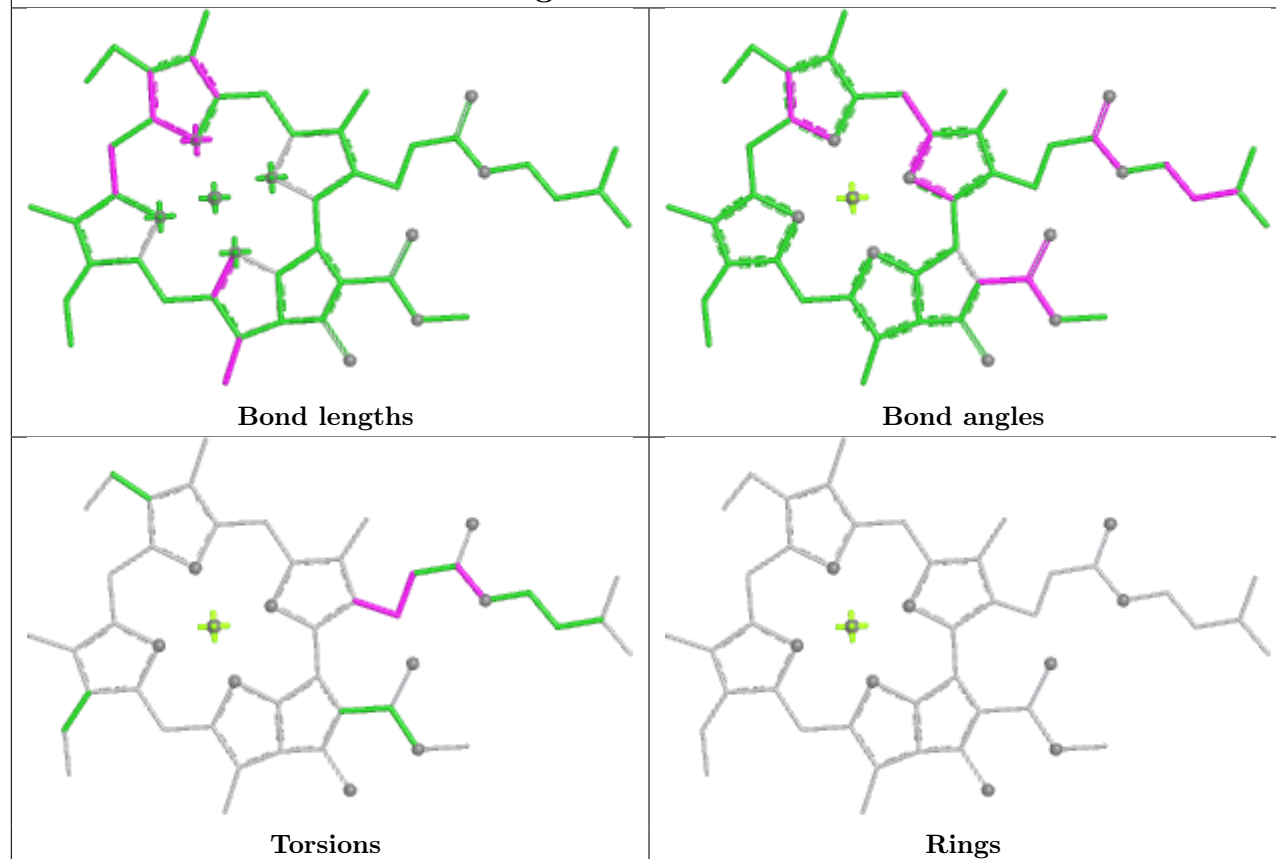




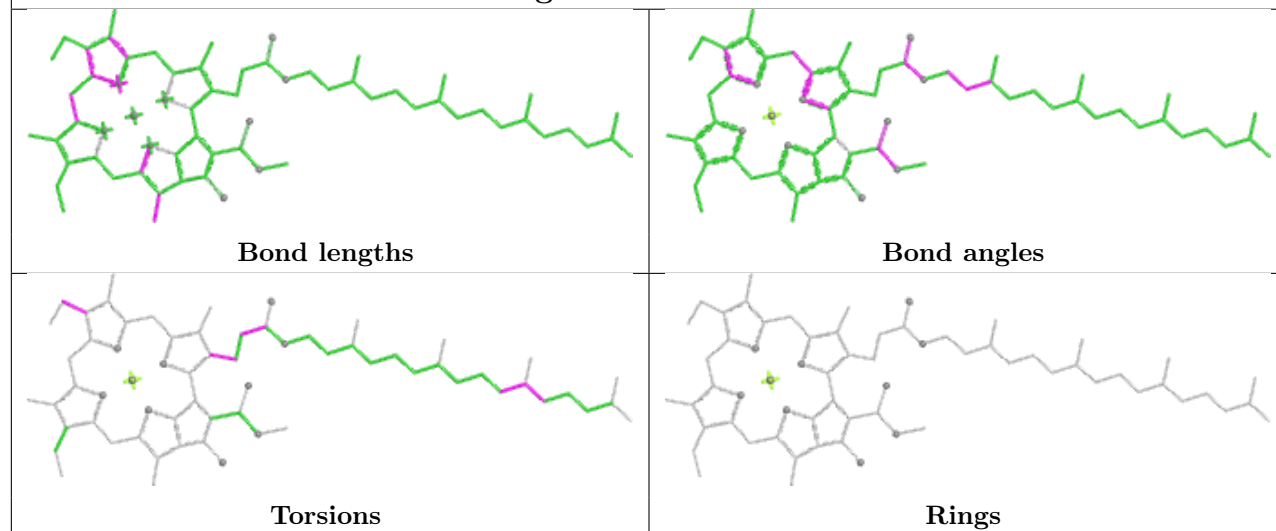
Ligand CLA a 807**Ligand CLA b 810**



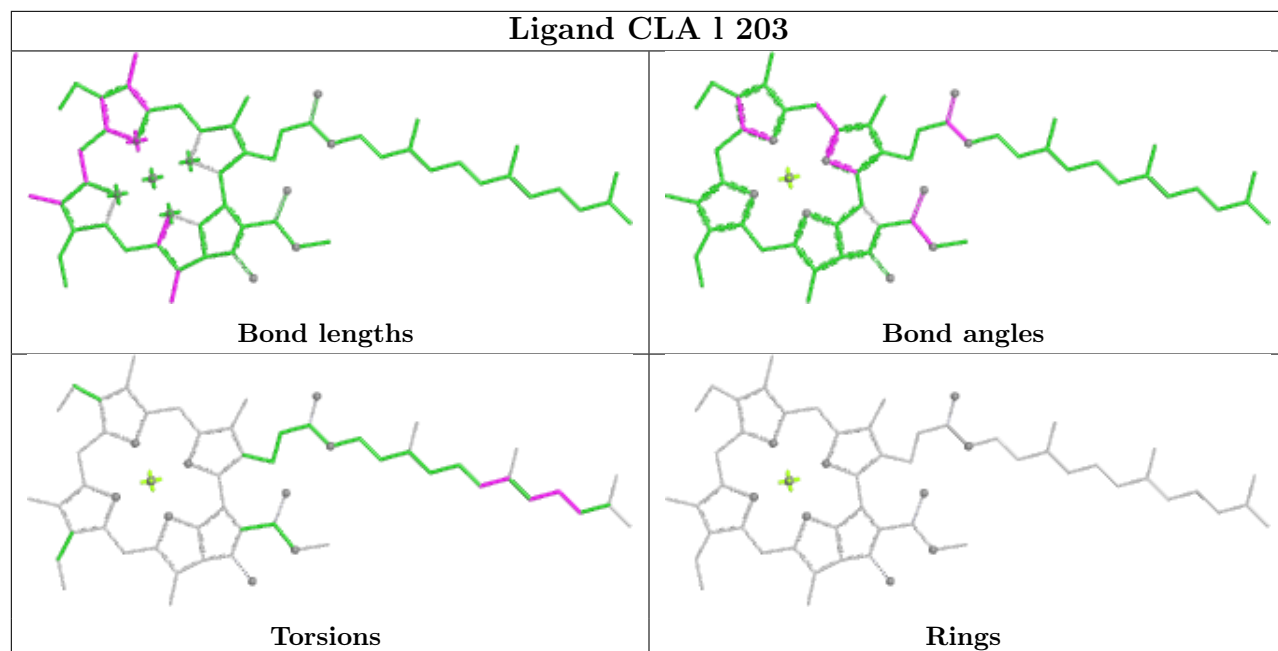
Ligand CLA b 820



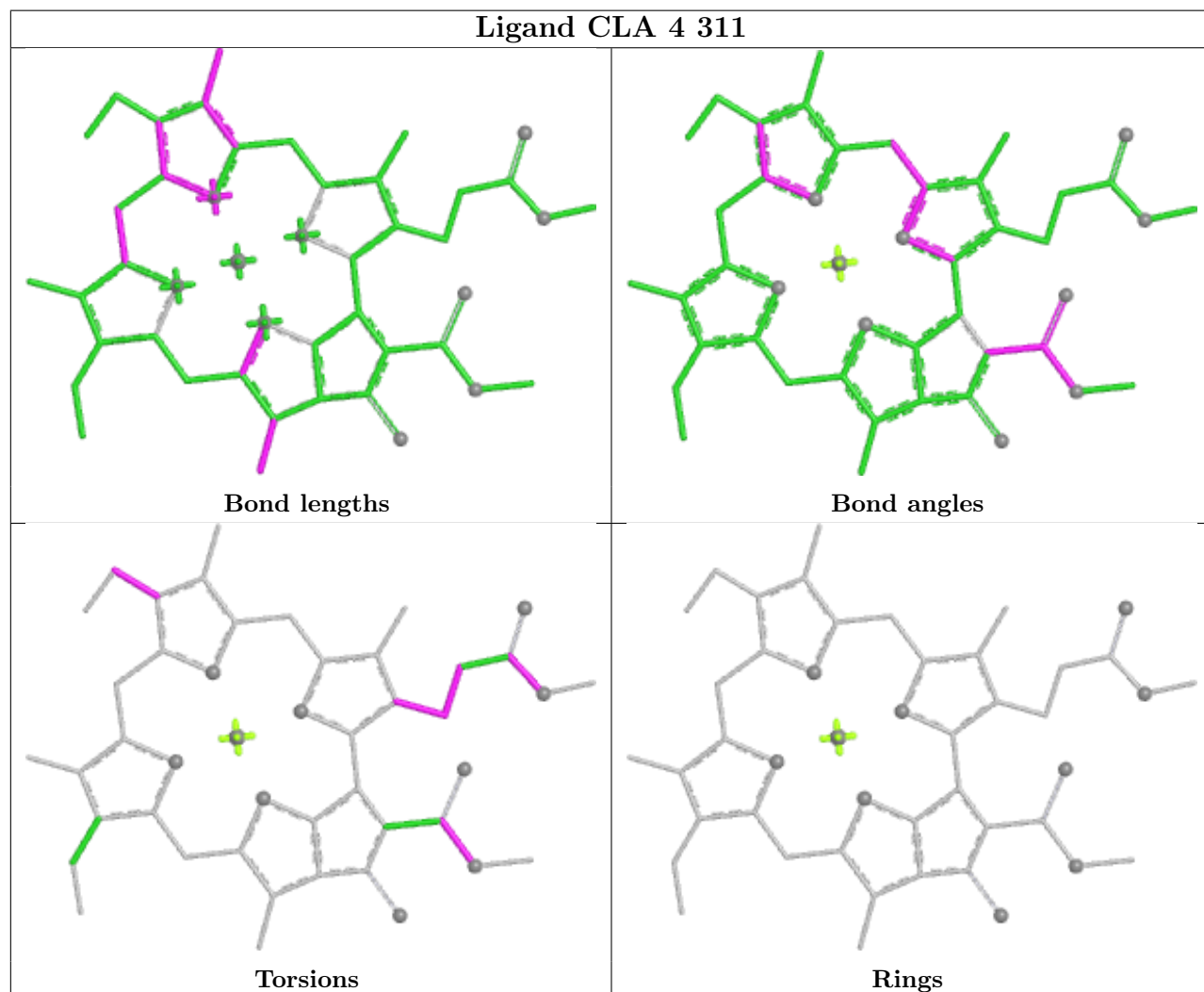
Ligand CLA b 837

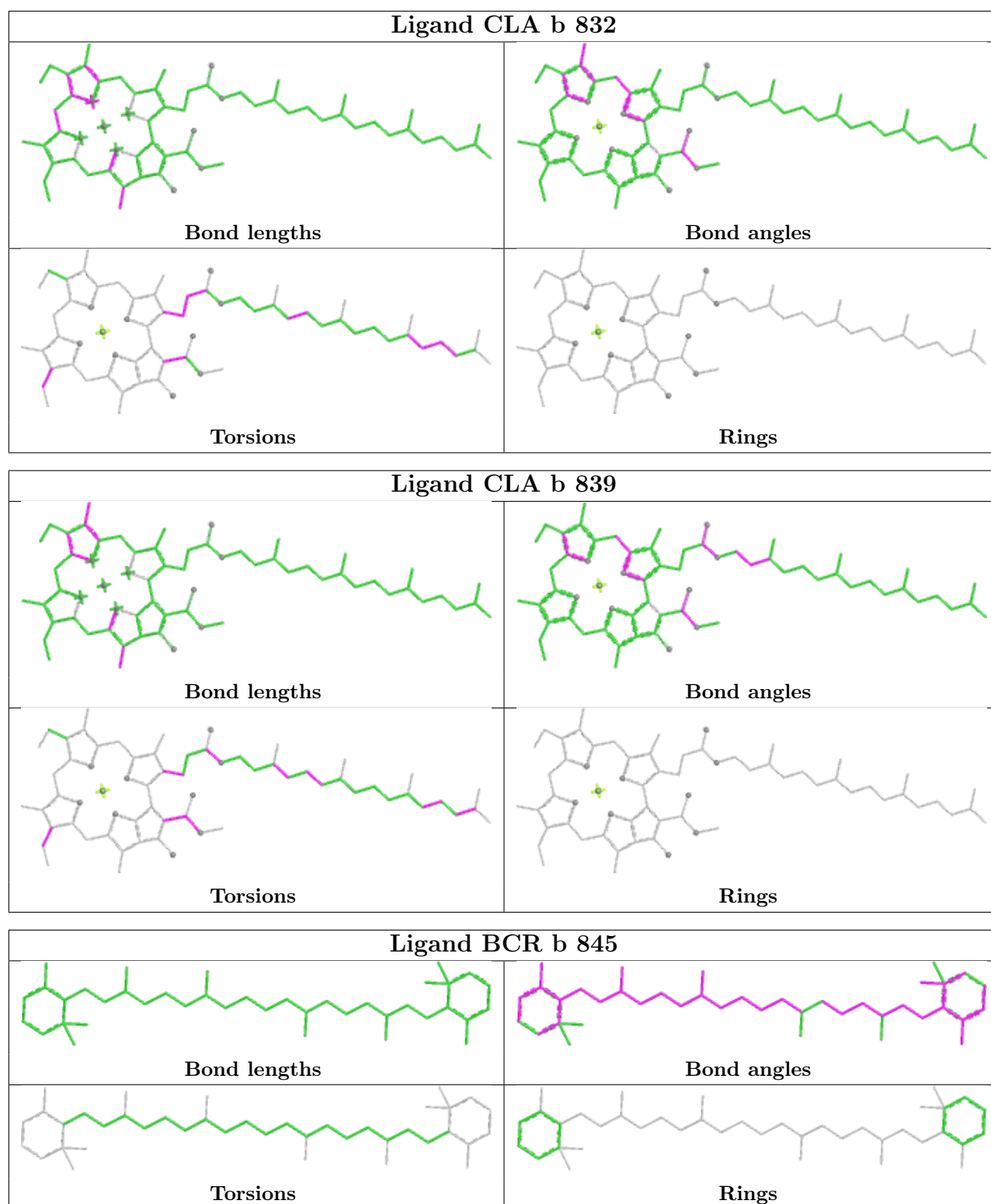


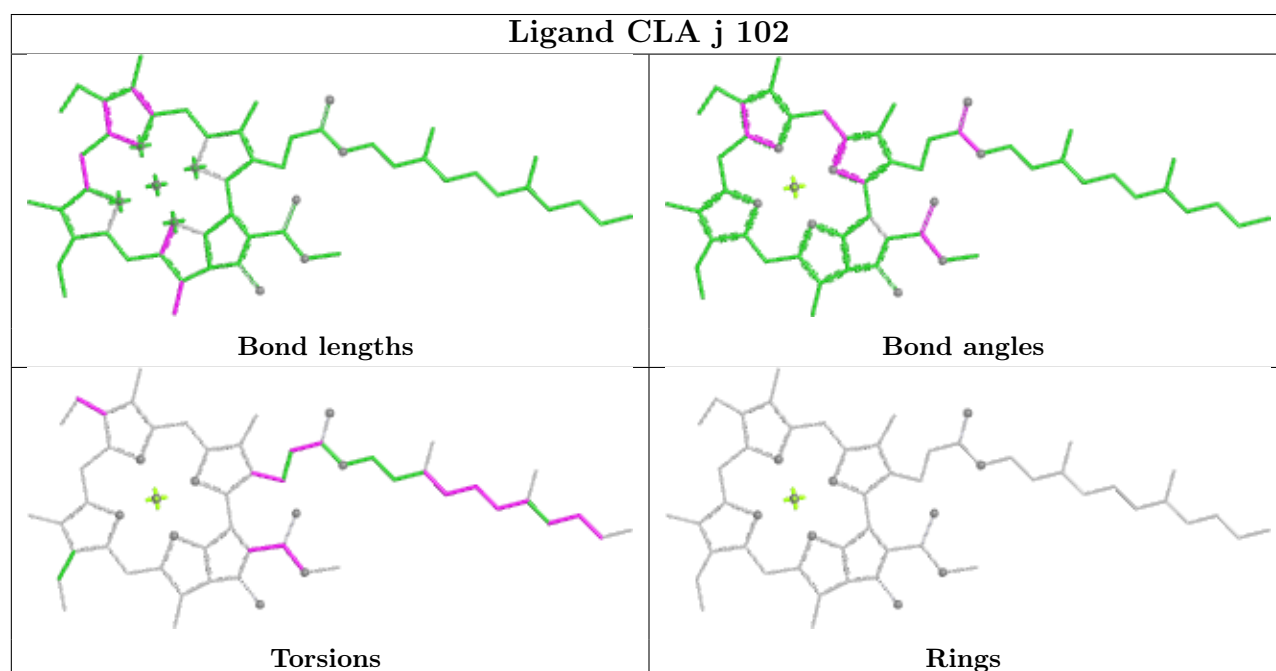
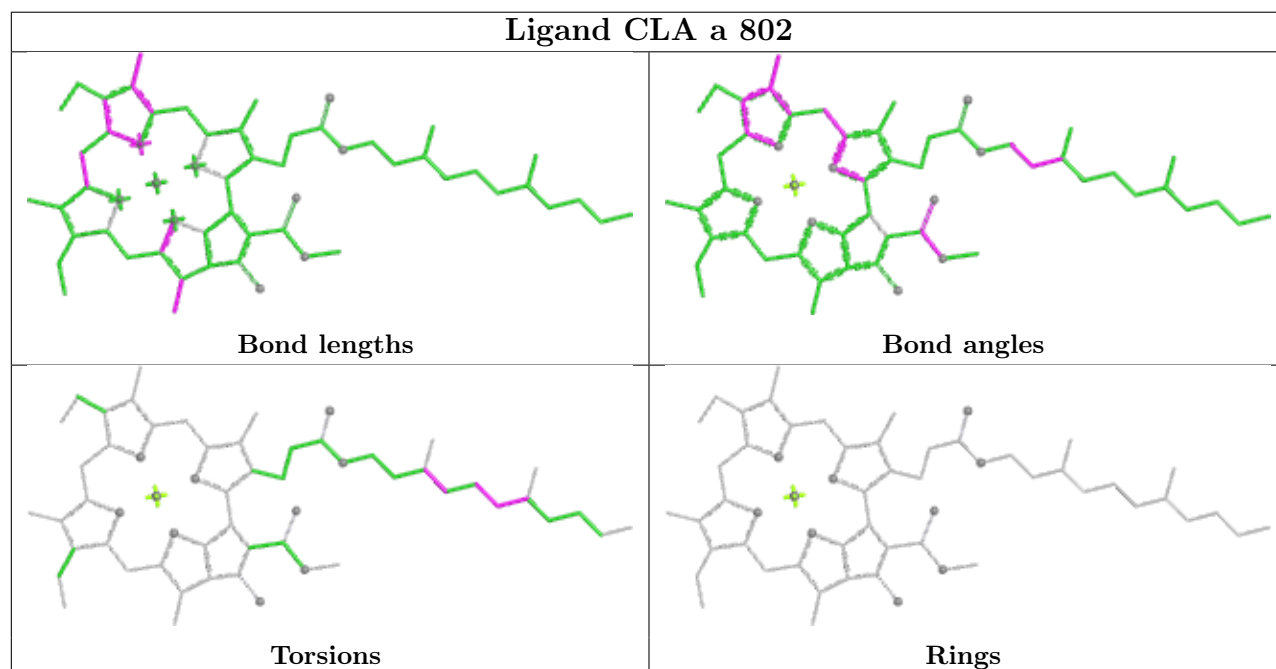
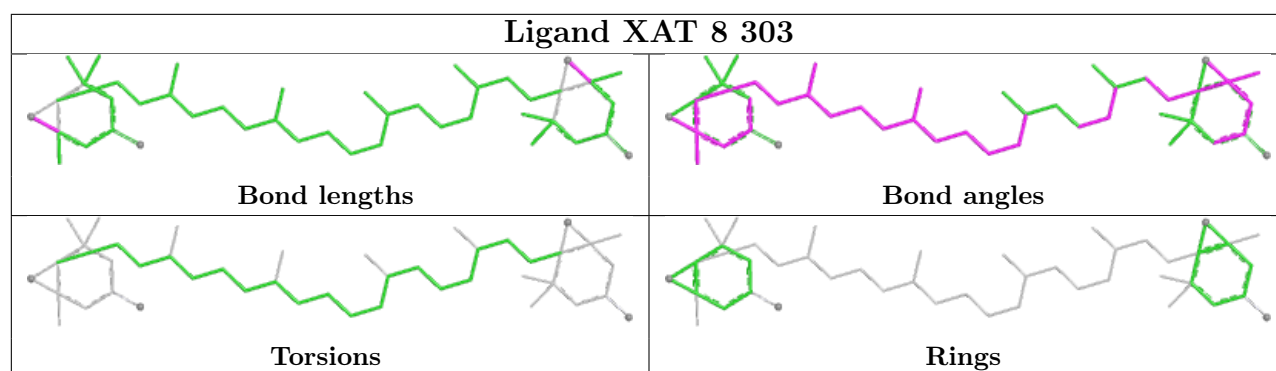
Ligand CLA 1 203

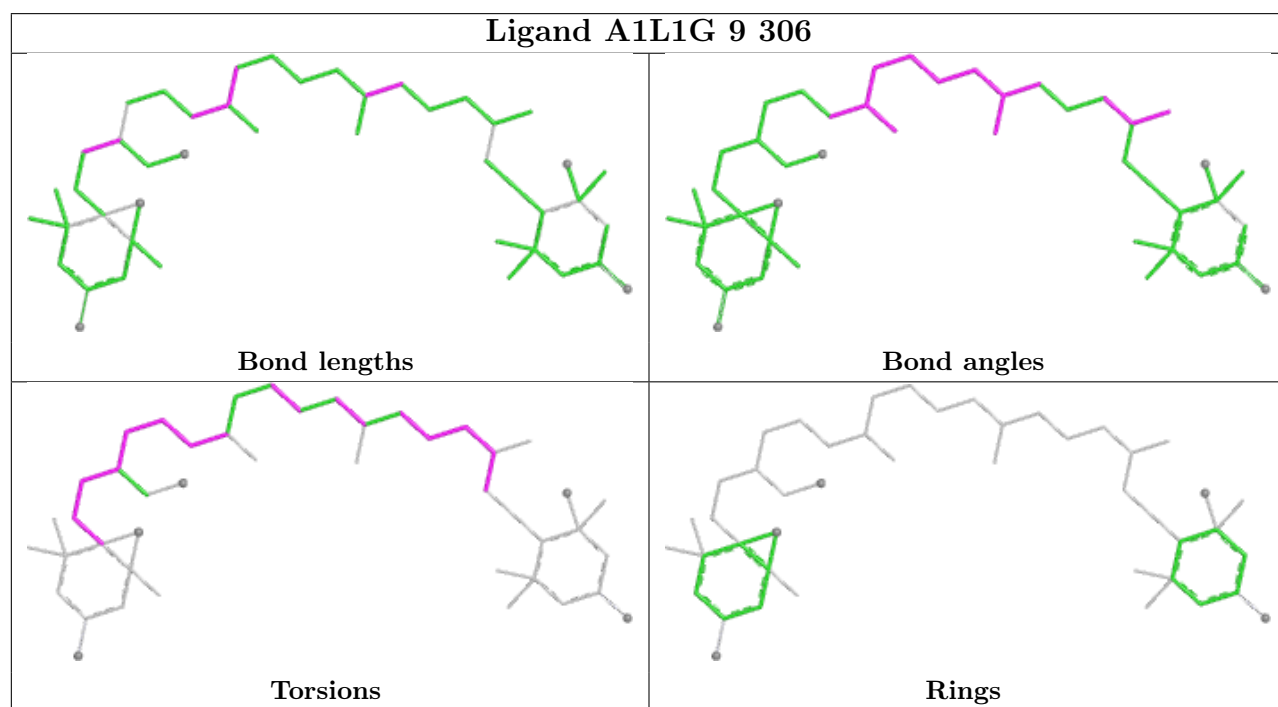
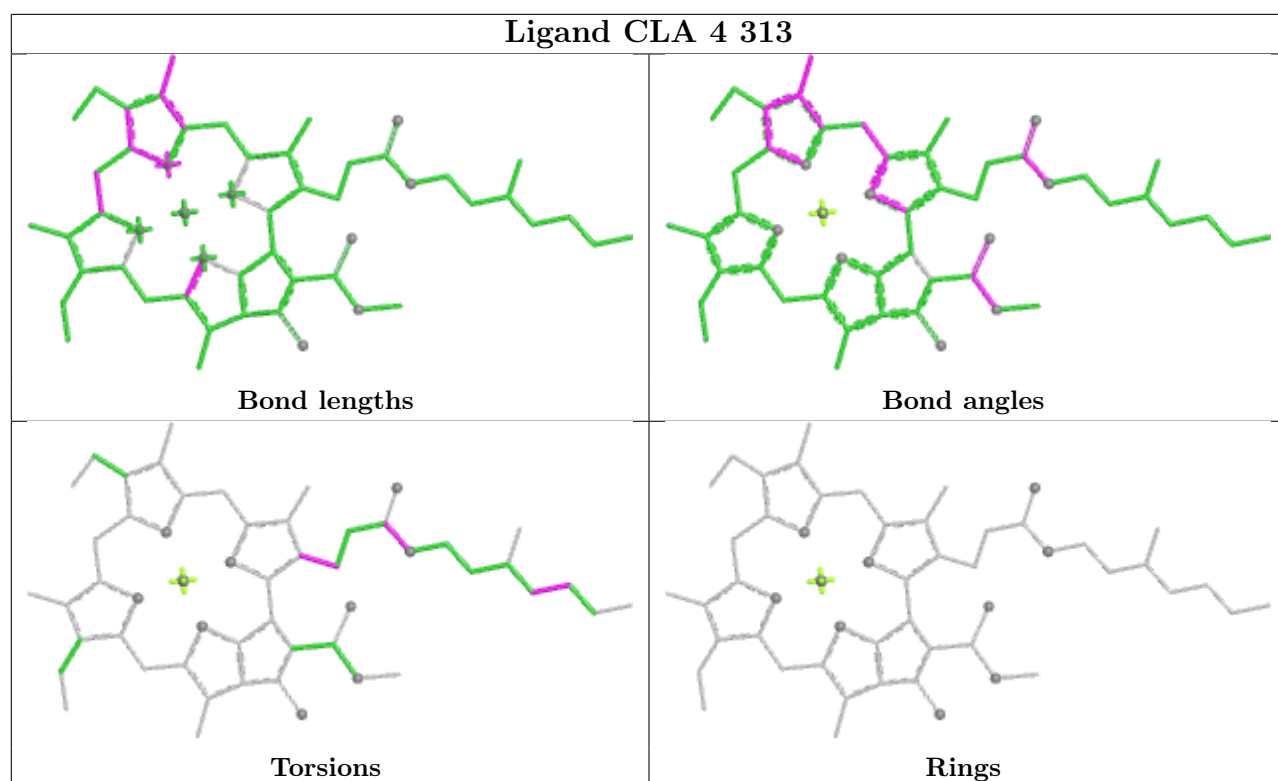


Ligand CLA 4 311

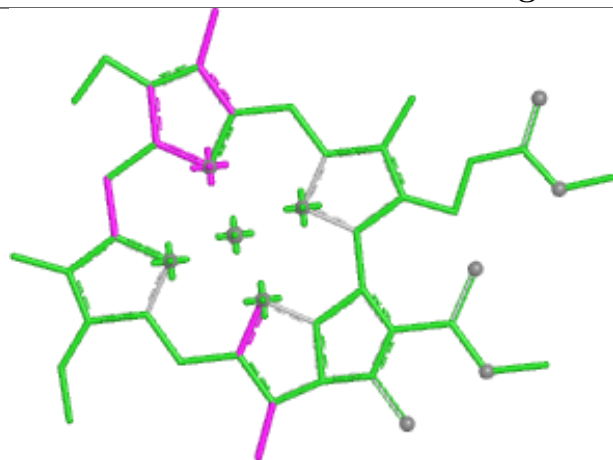




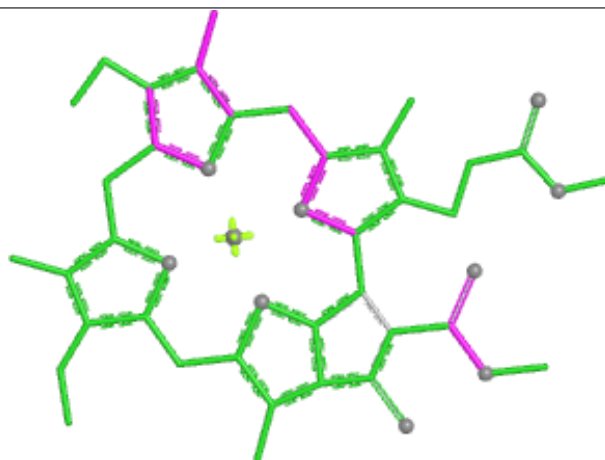




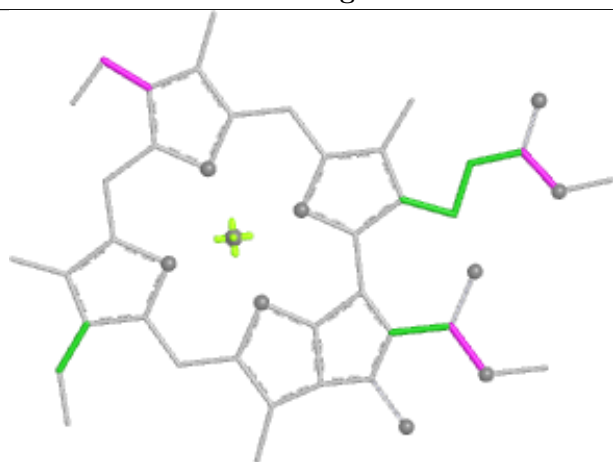
Ligand CLA 8 310



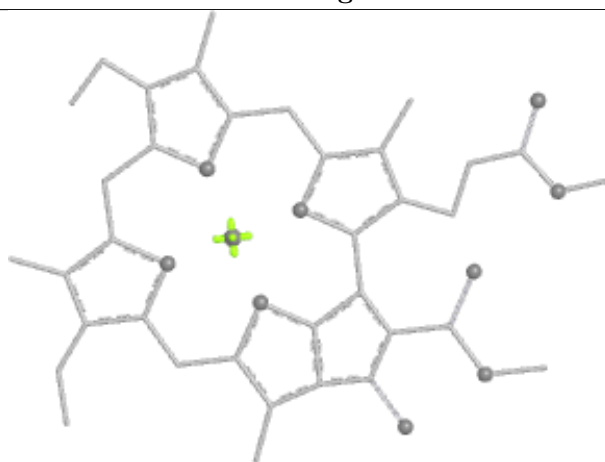
Bond lengths



Bond angles

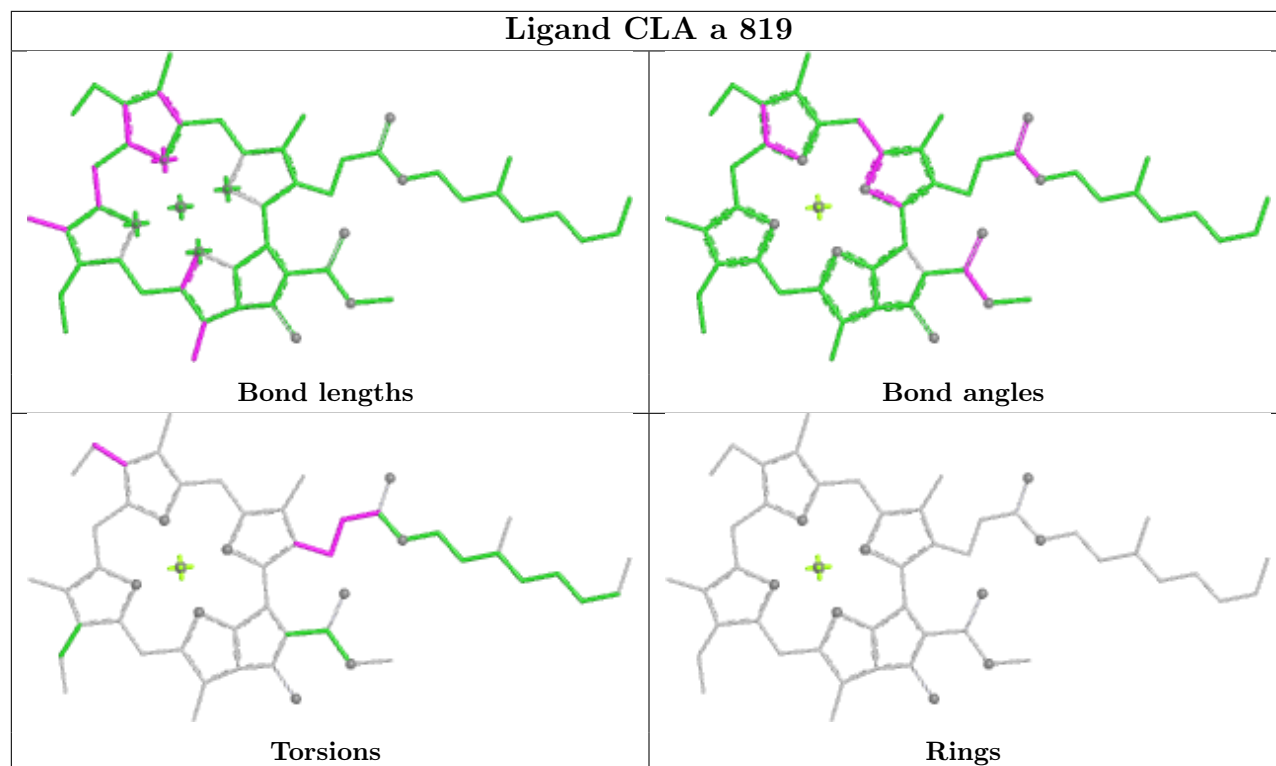


Torsions

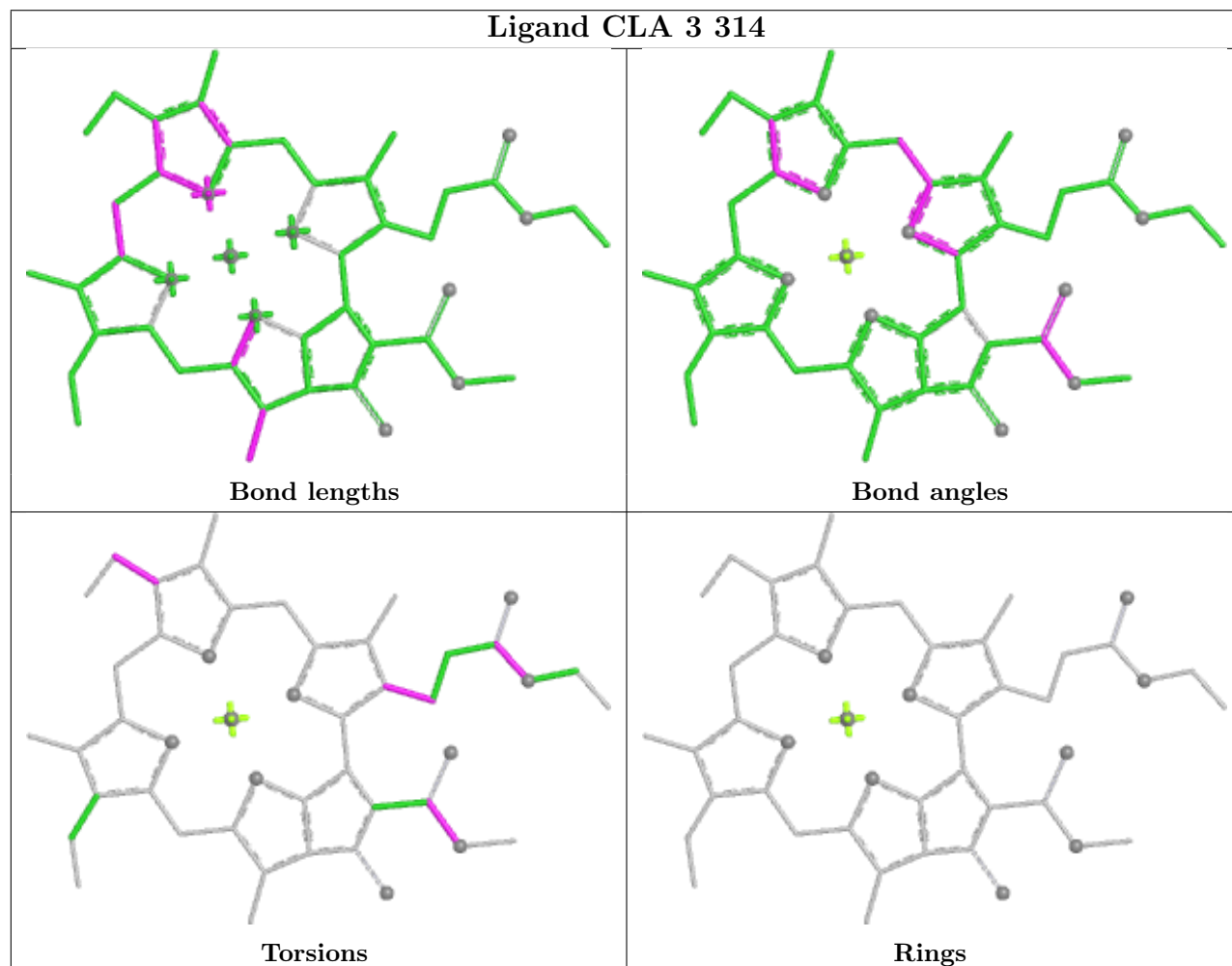


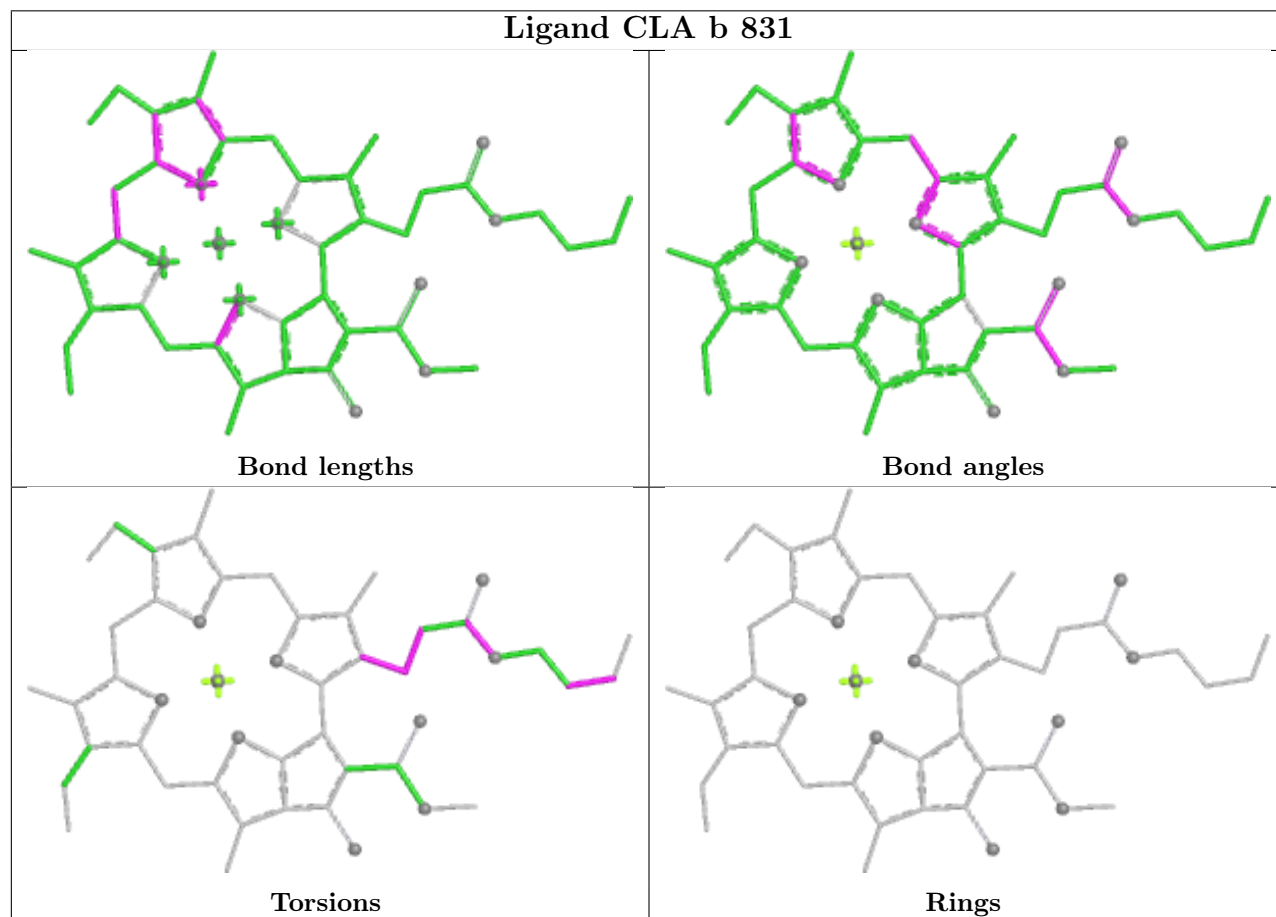
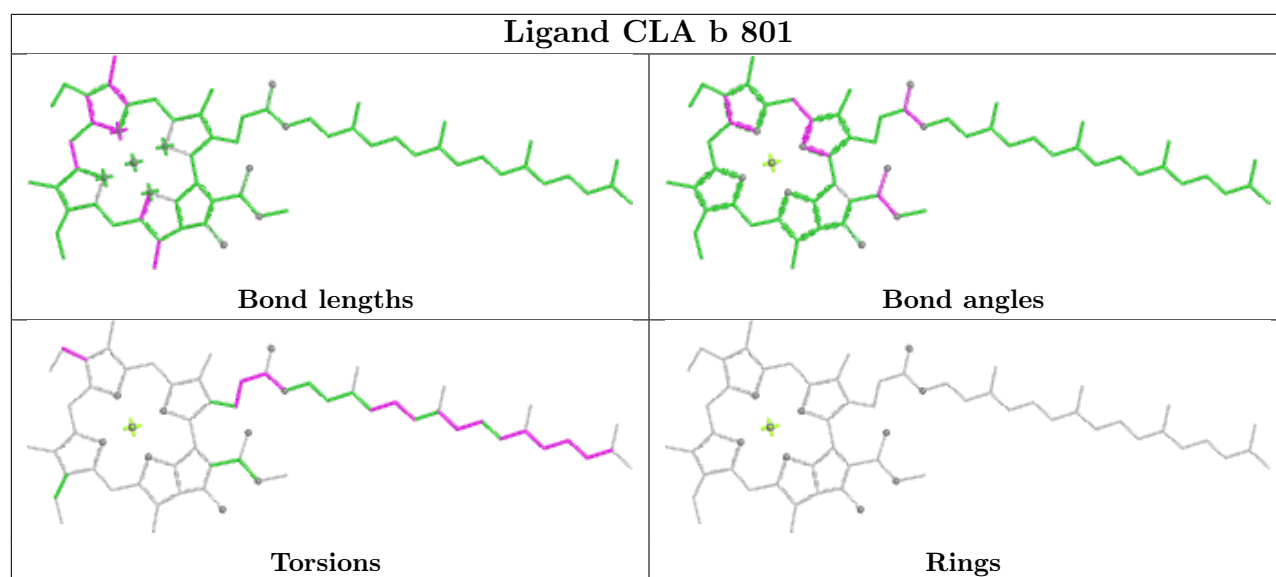
Rings

Ligand CLA a 819

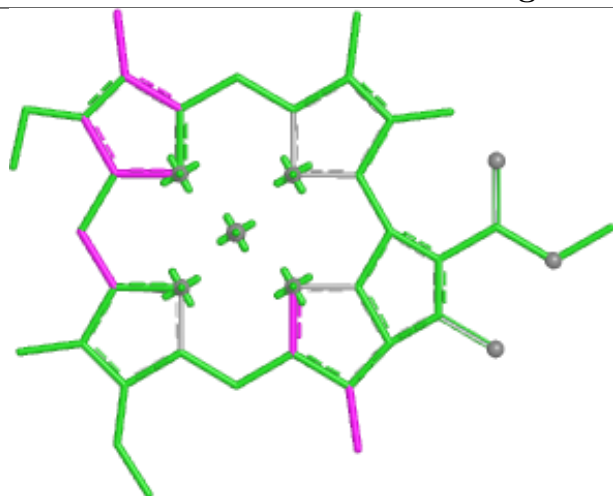


Ligand CLA 3 314

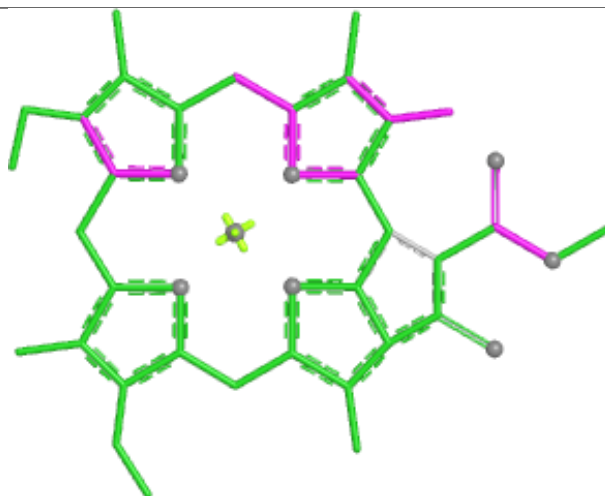




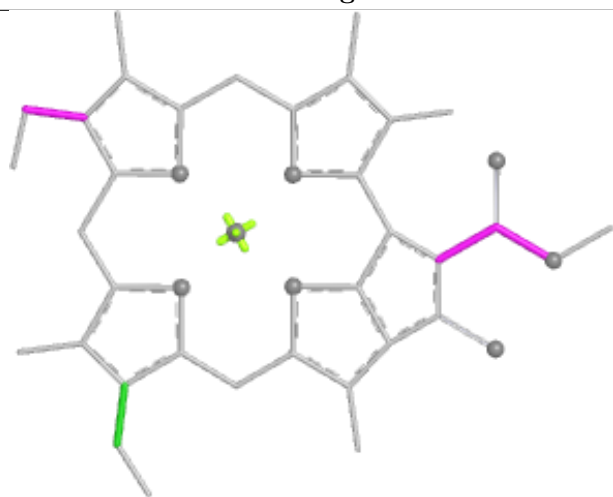
Ligand CLA 8 314



Bond lengths



Bond angles

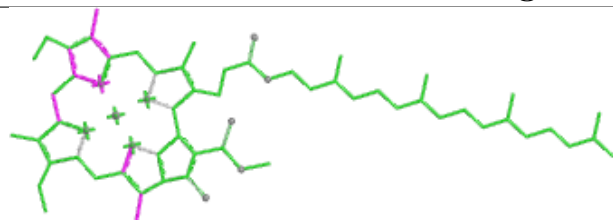


Torsions

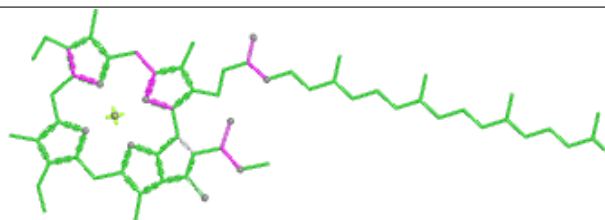


Rings

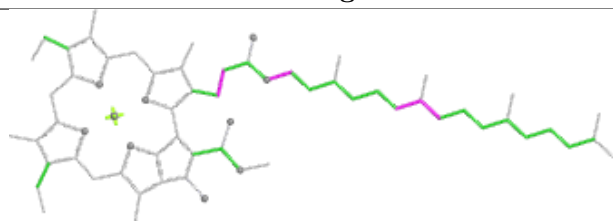
Ligand CLA a 822



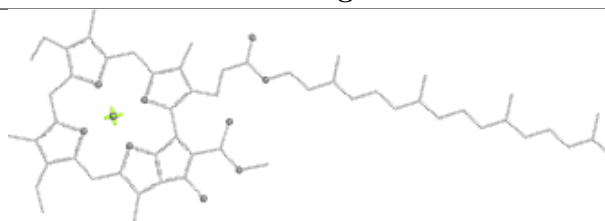
Bond lengths



Bond angles

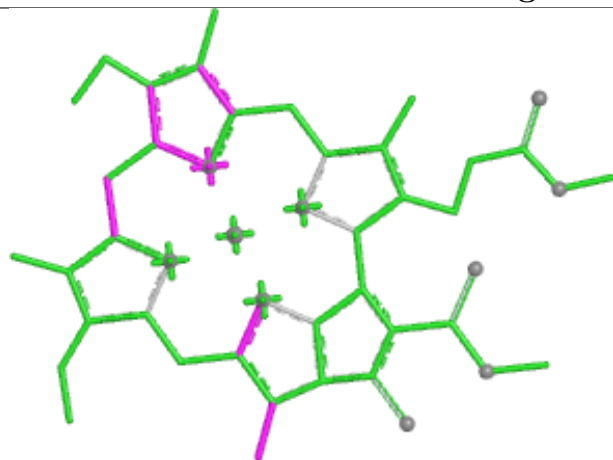


Torsions

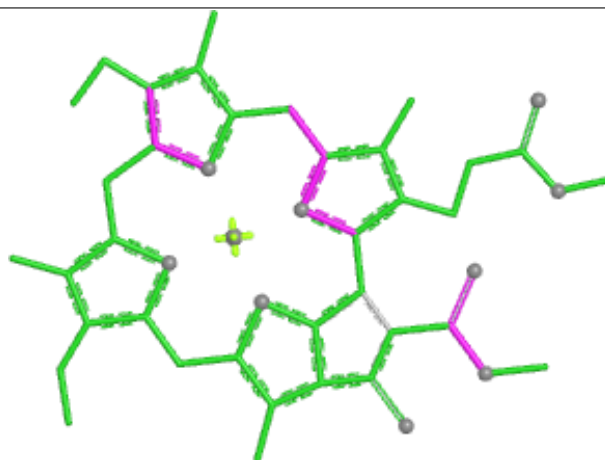


Rings

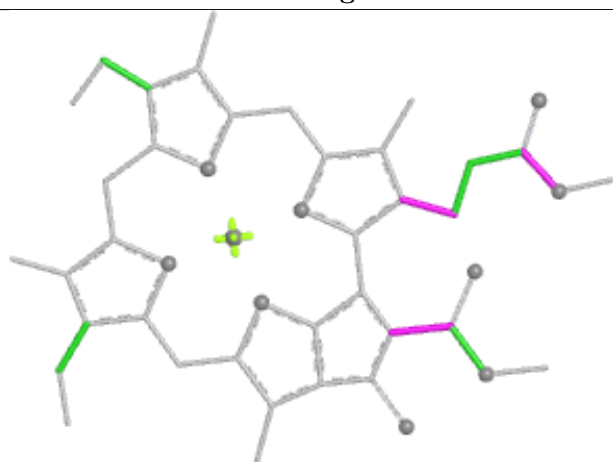
Ligand CLA 9 310



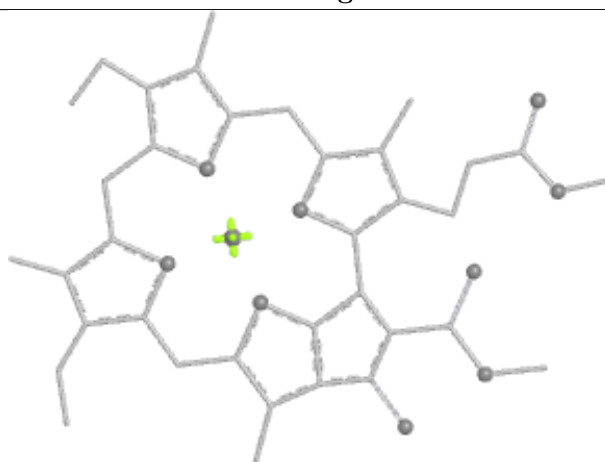
Bond lengths



Bond angles

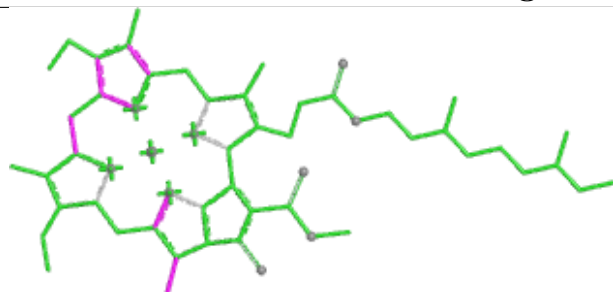


Torsions

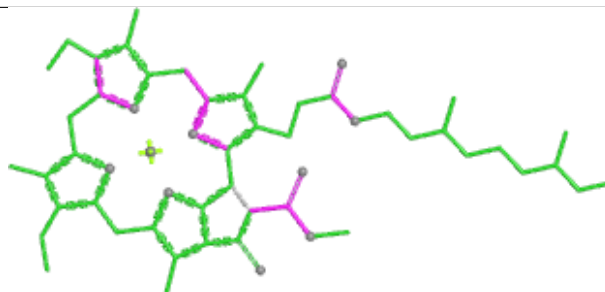


Rings

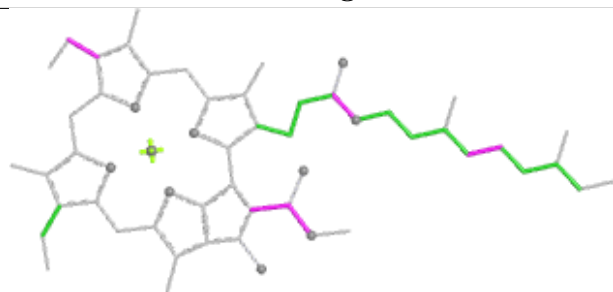
Ligand CLA 4 307



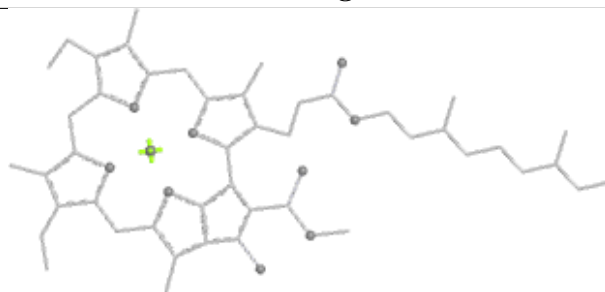
Bond lengths



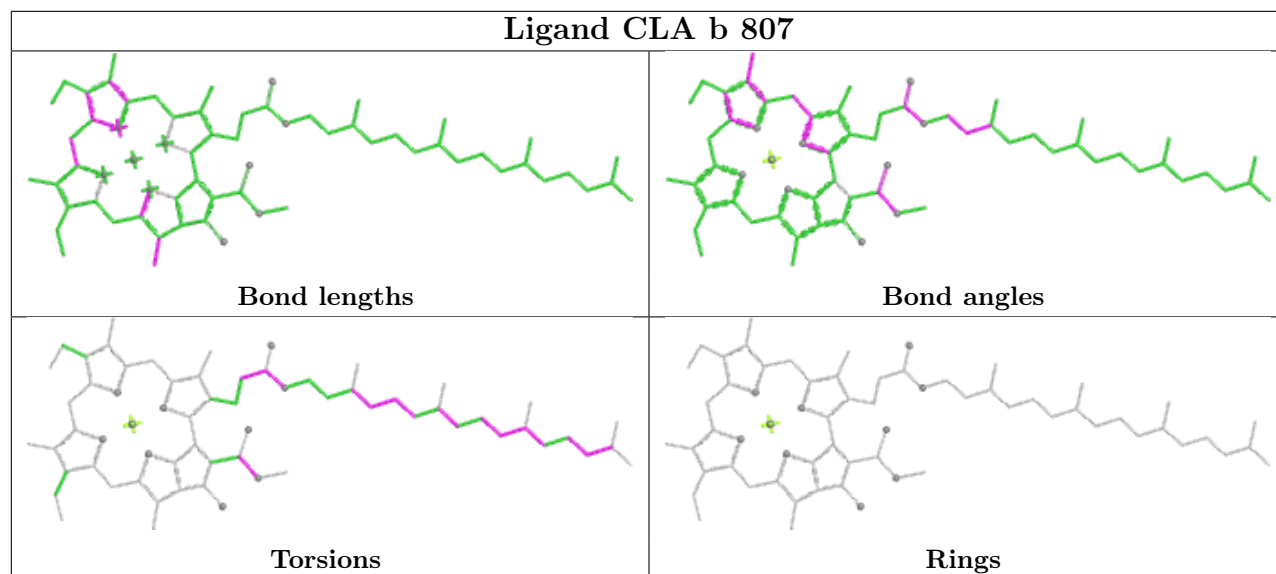
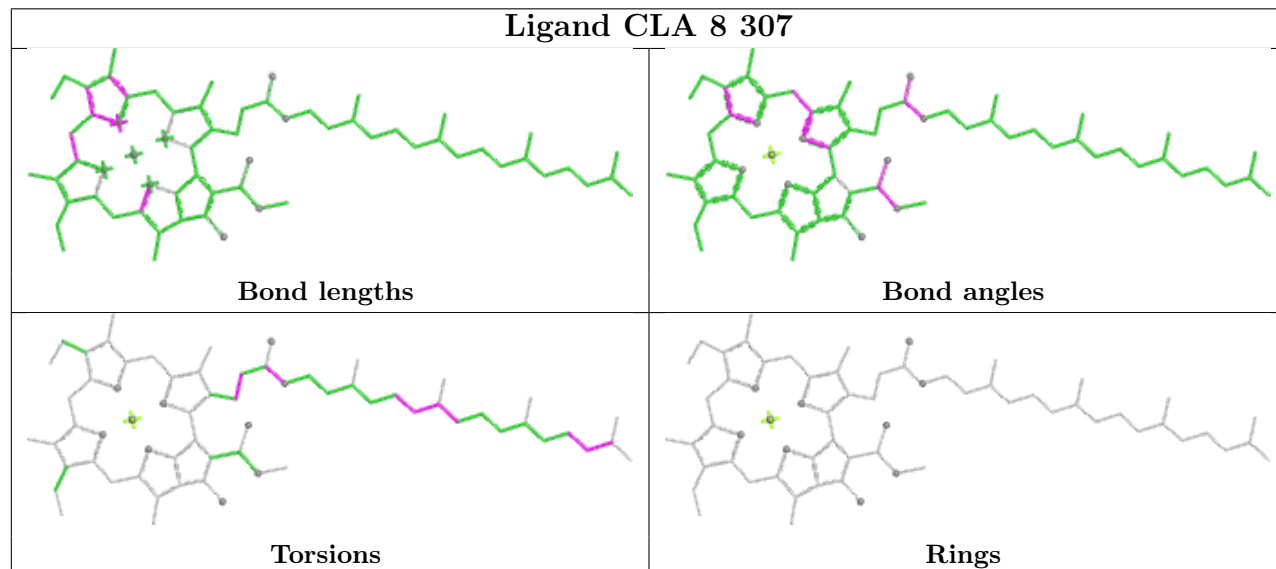
Bond angles



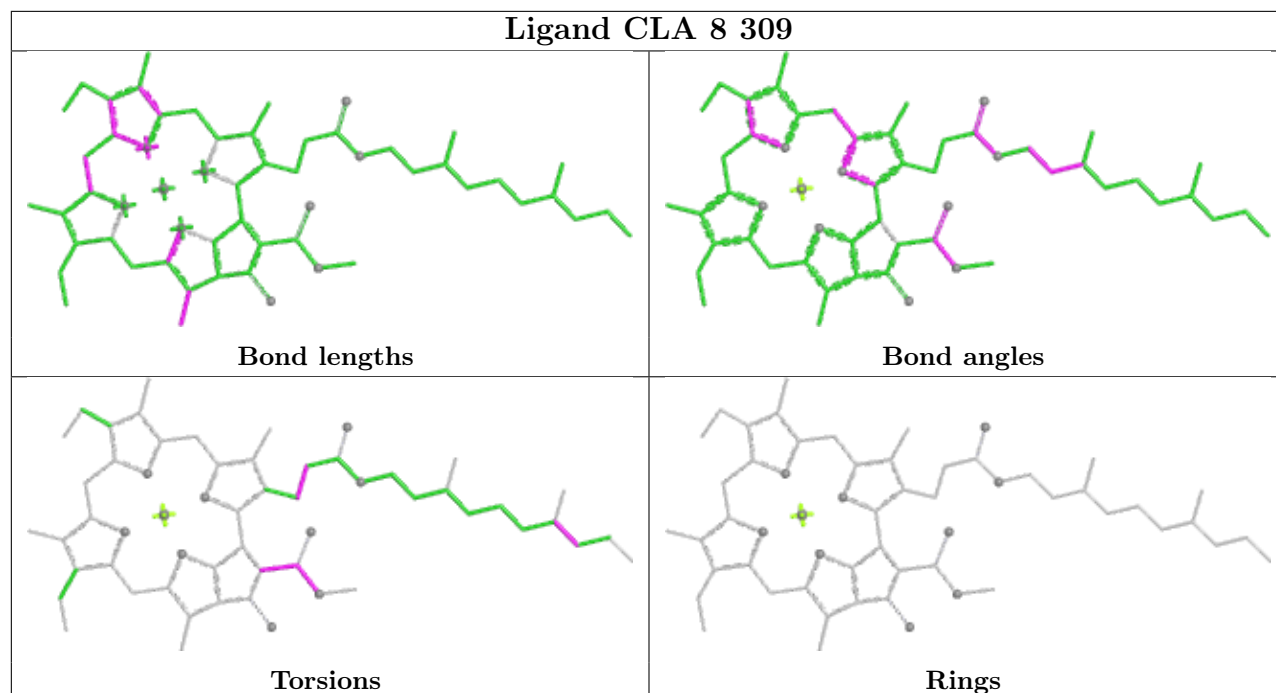
Torsions



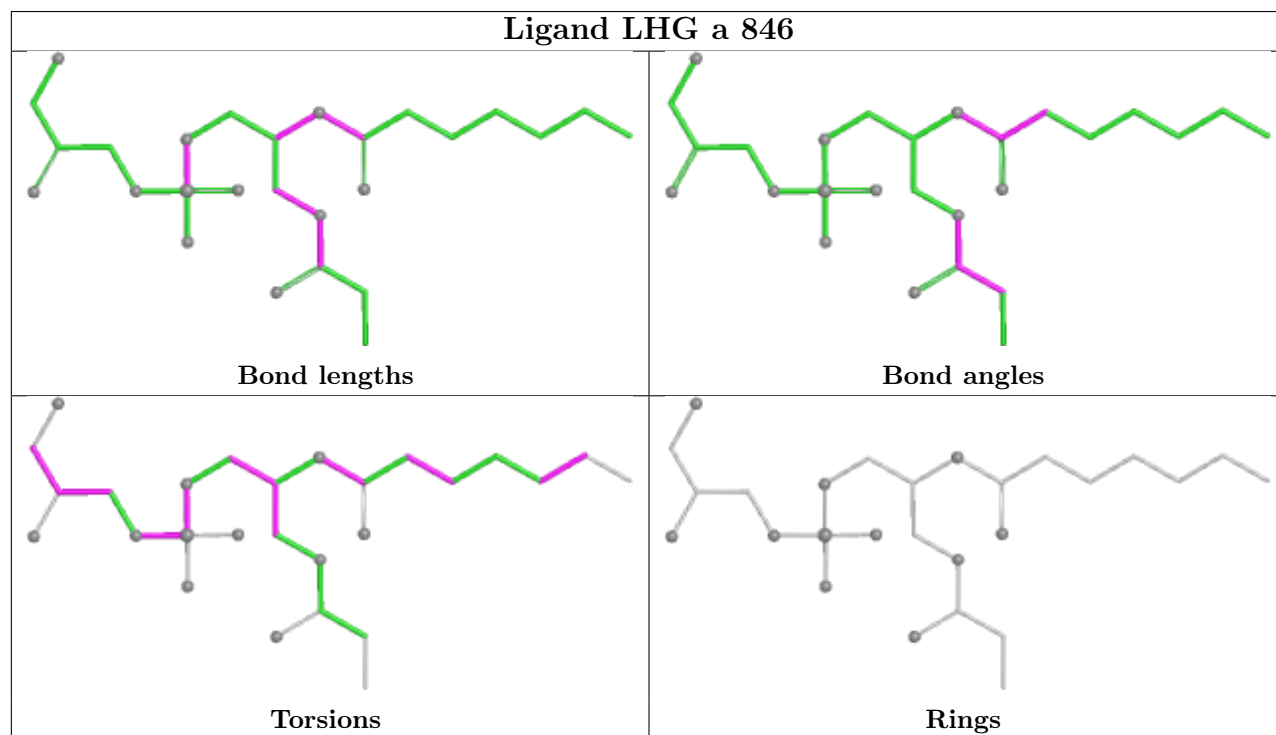
Rings

Ligand CLA b 807**Ligand CLA 8 307**

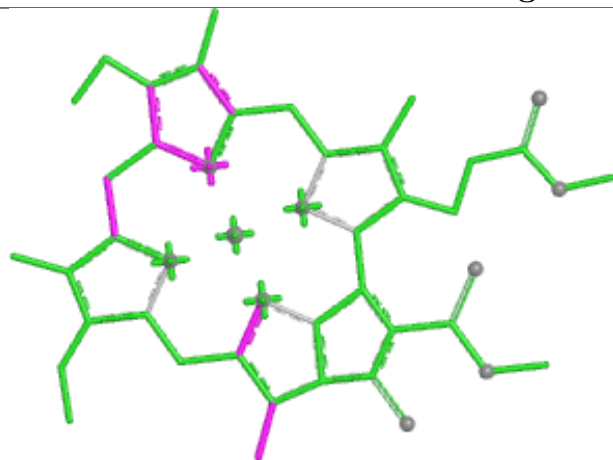
Ligand CLA 8 309



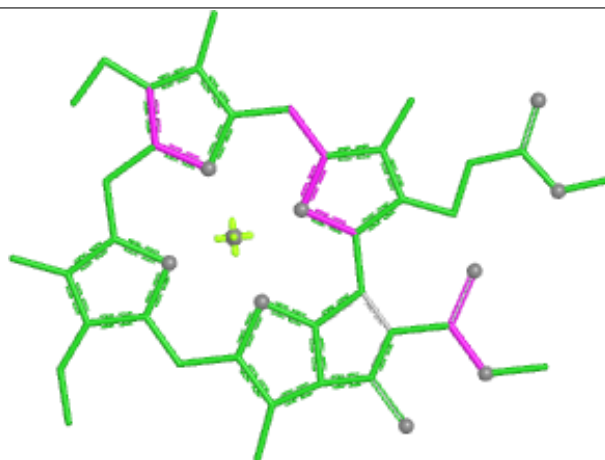
Ligand LHG a 846



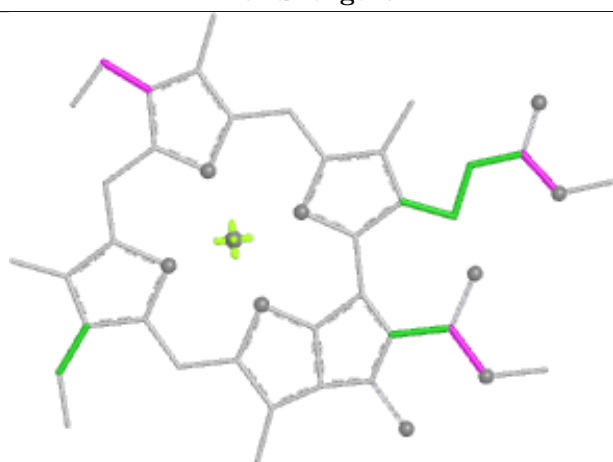
Ligand CLA 5 305



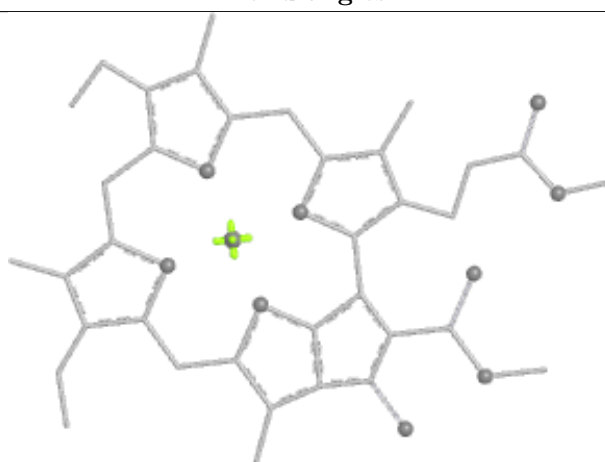
Bond lengths



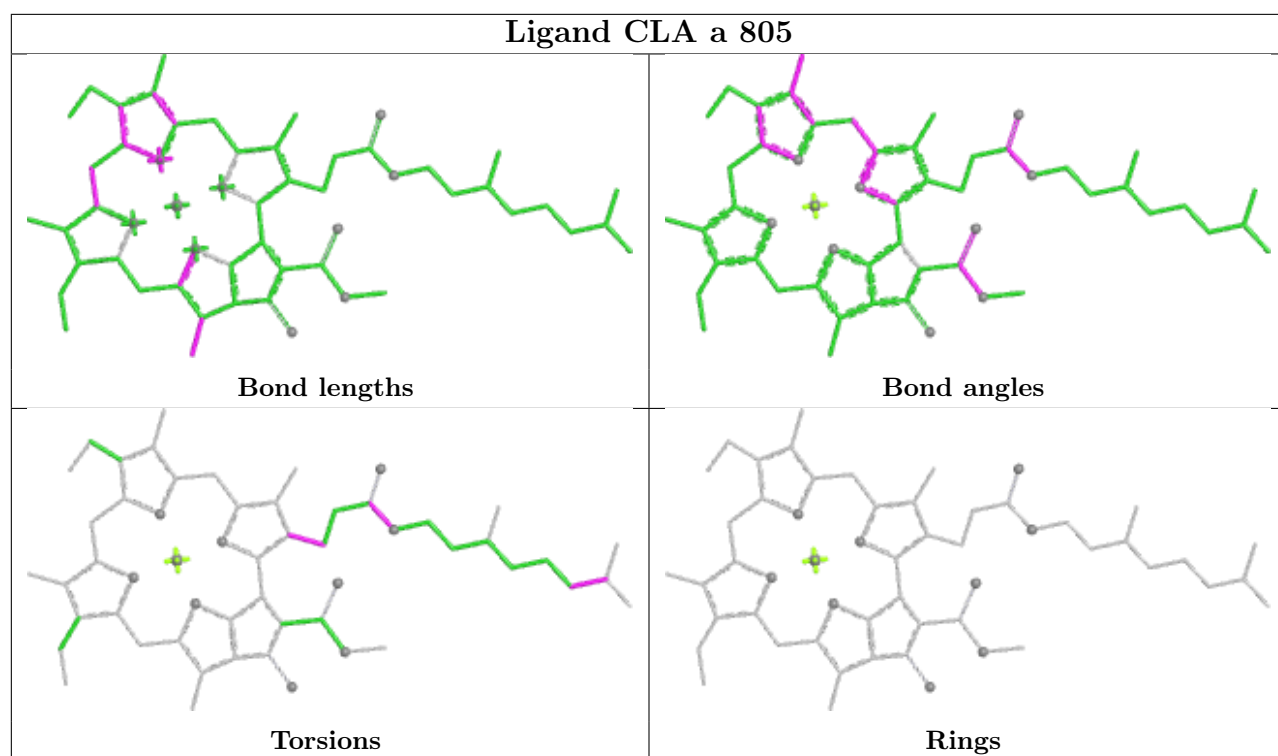
Bond angles



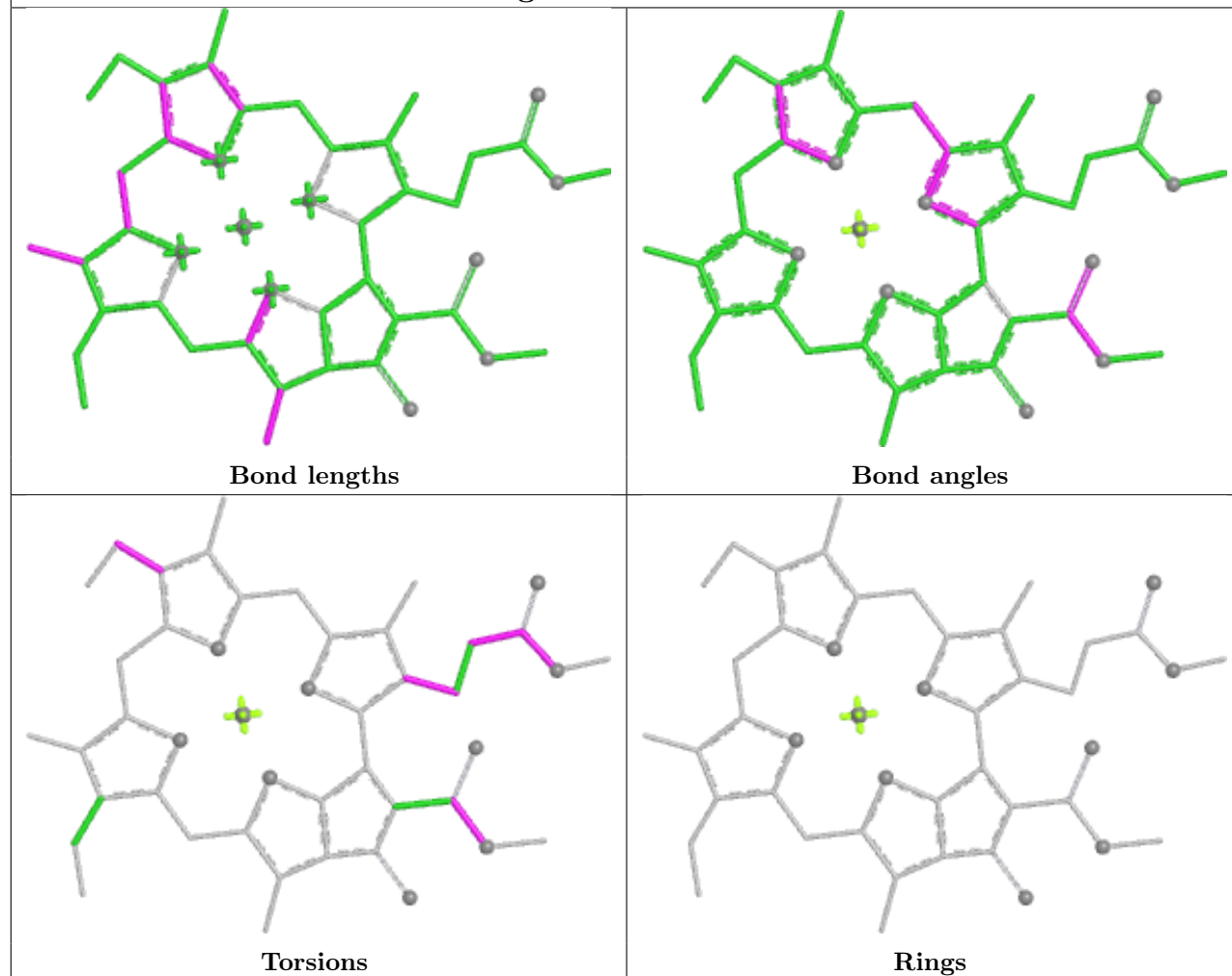
Torsions



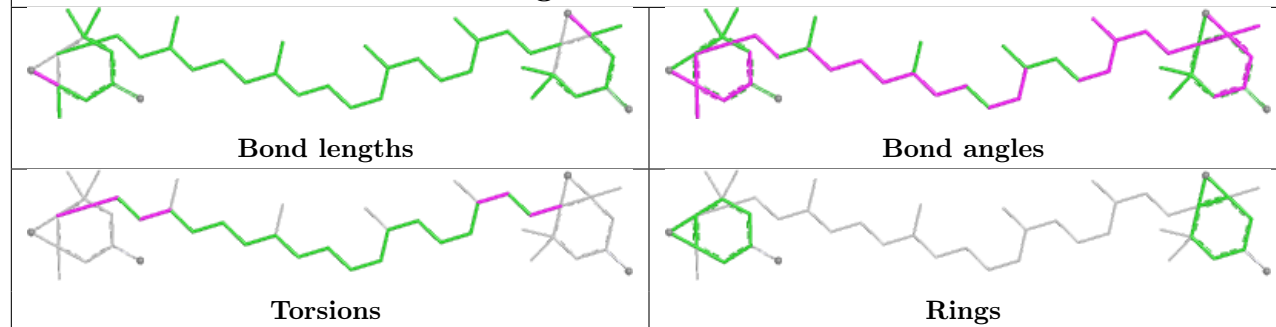
Rings

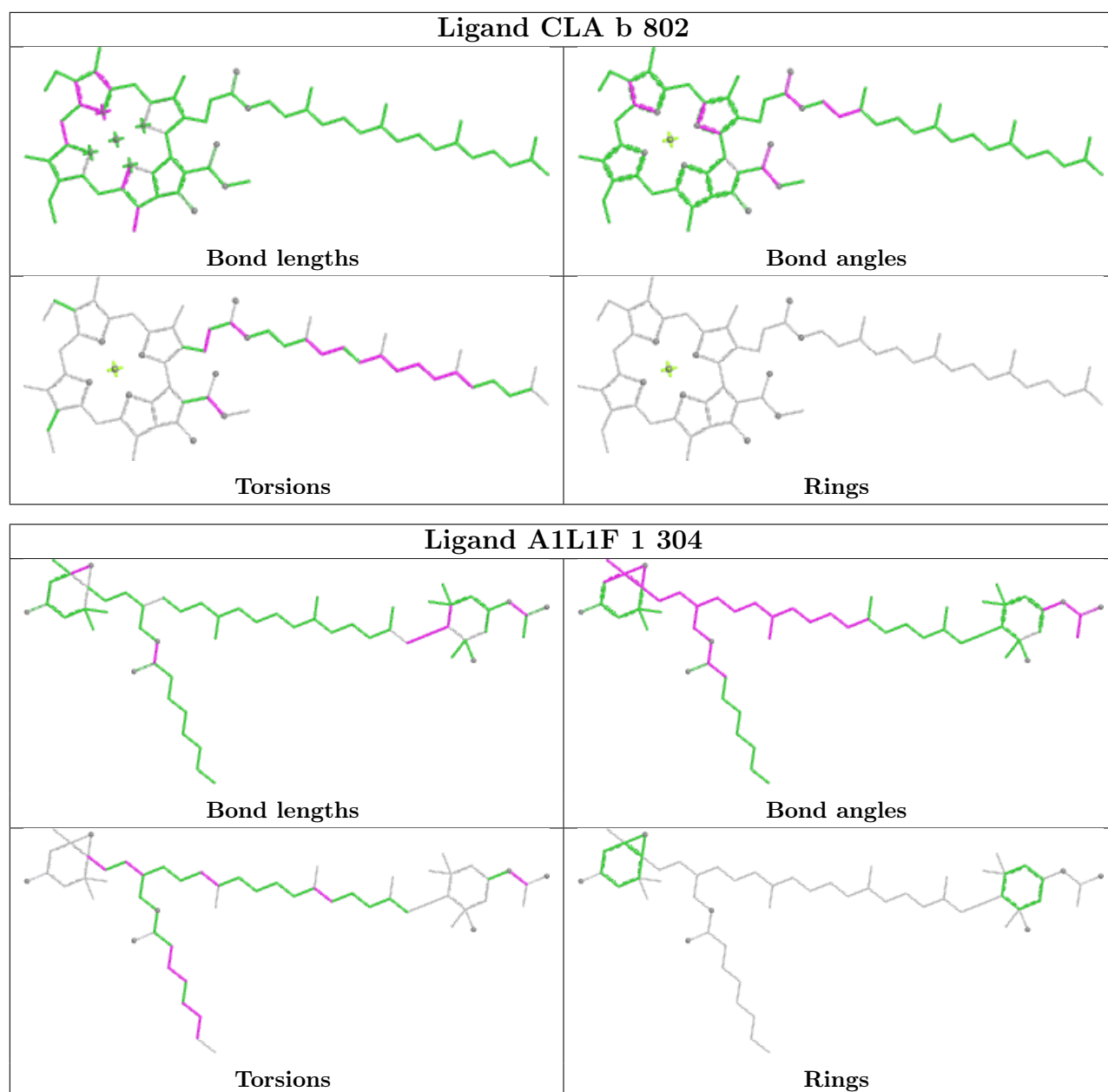


Ligand CLA 3 315

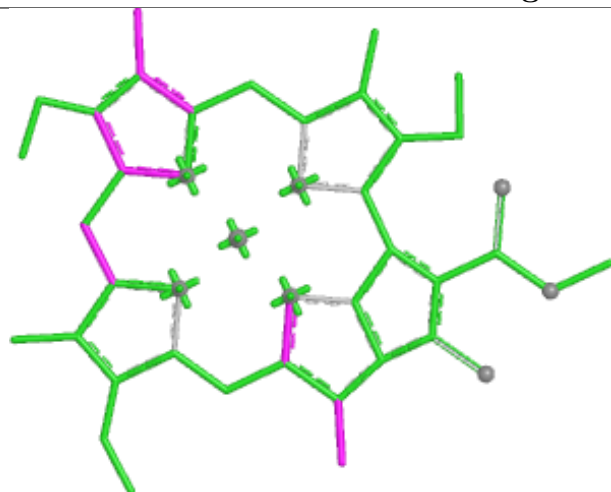


Ligand XAT 2 303

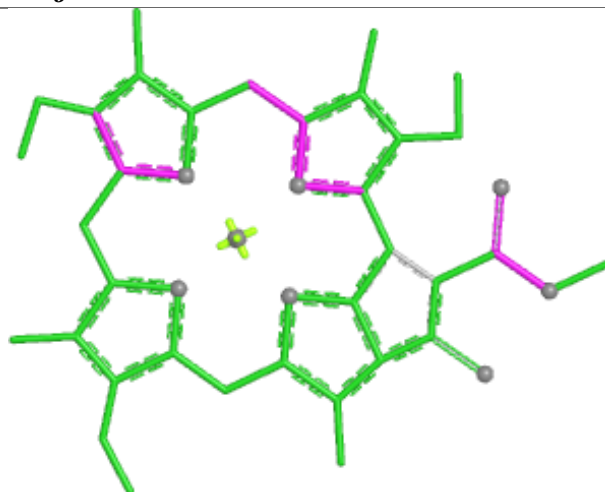




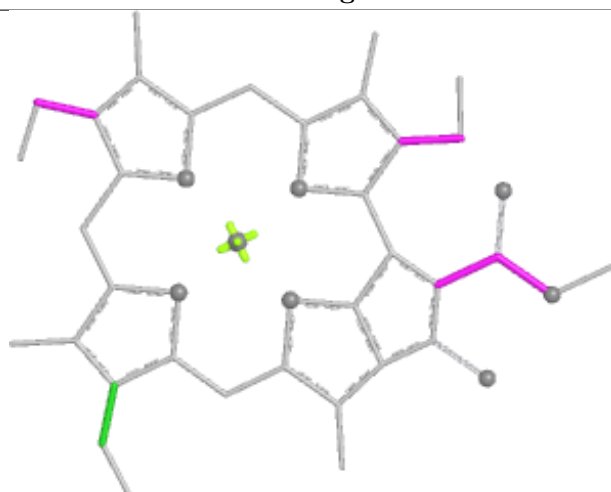
Ligand CLA j 103



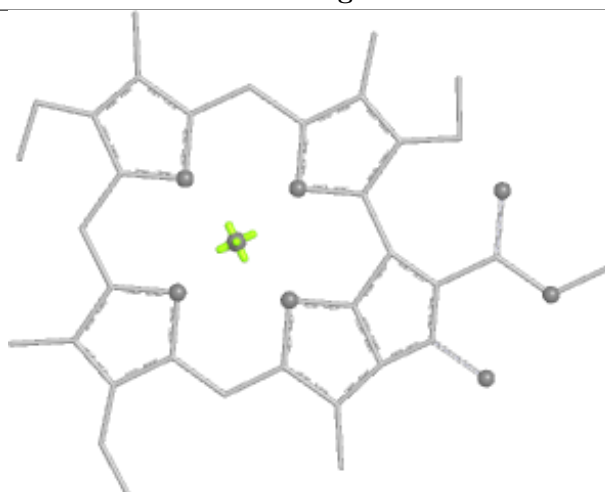
Bond lengths



Bond angles

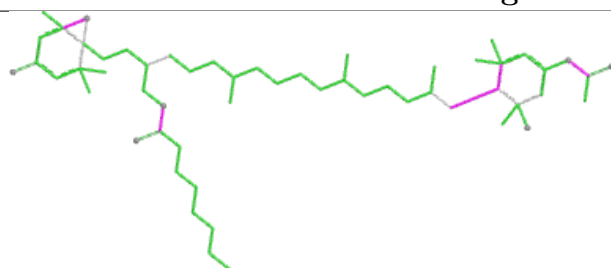


Torsions

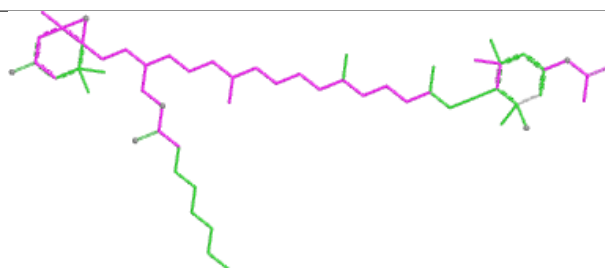


Rings

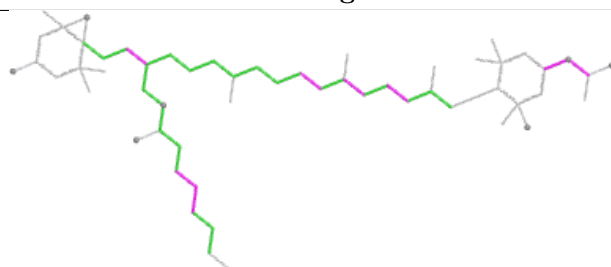
Ligand A1L1F h 204



Bond lengths



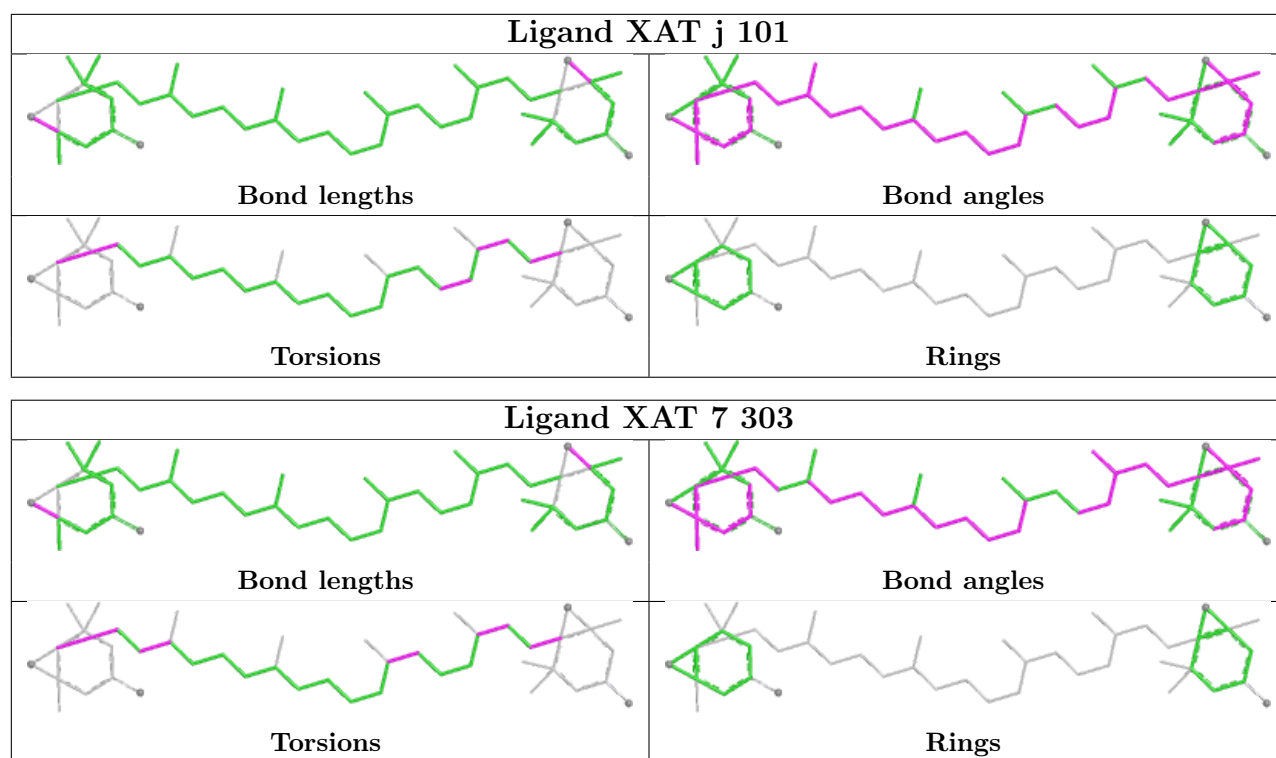
Bond angles



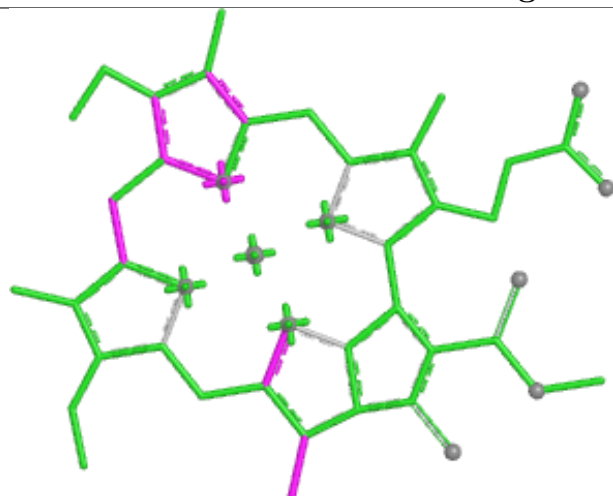
Torsions



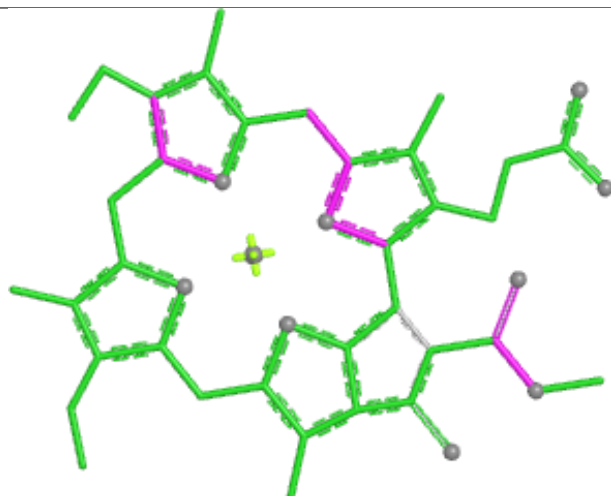
Rings



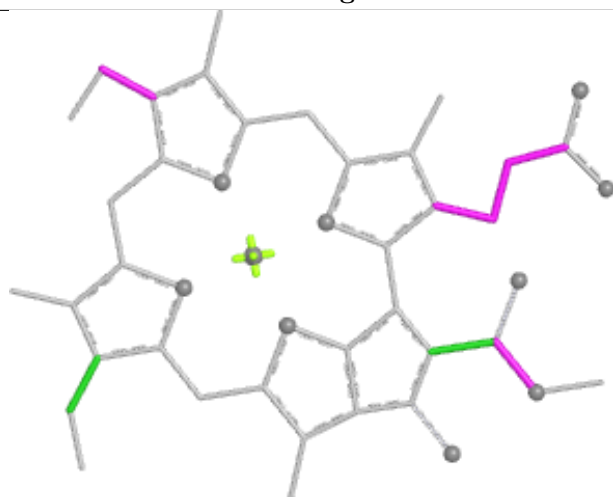
Ligand CLA 4 306



Bond lengths



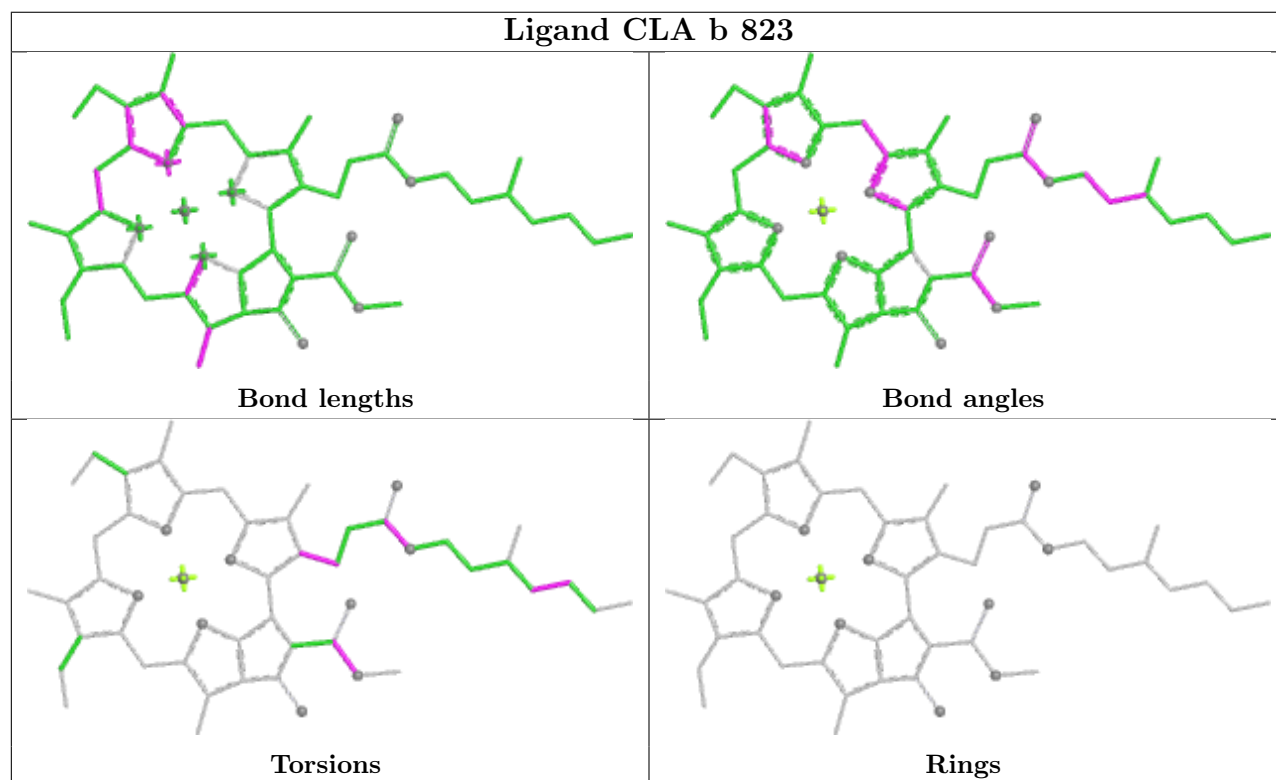
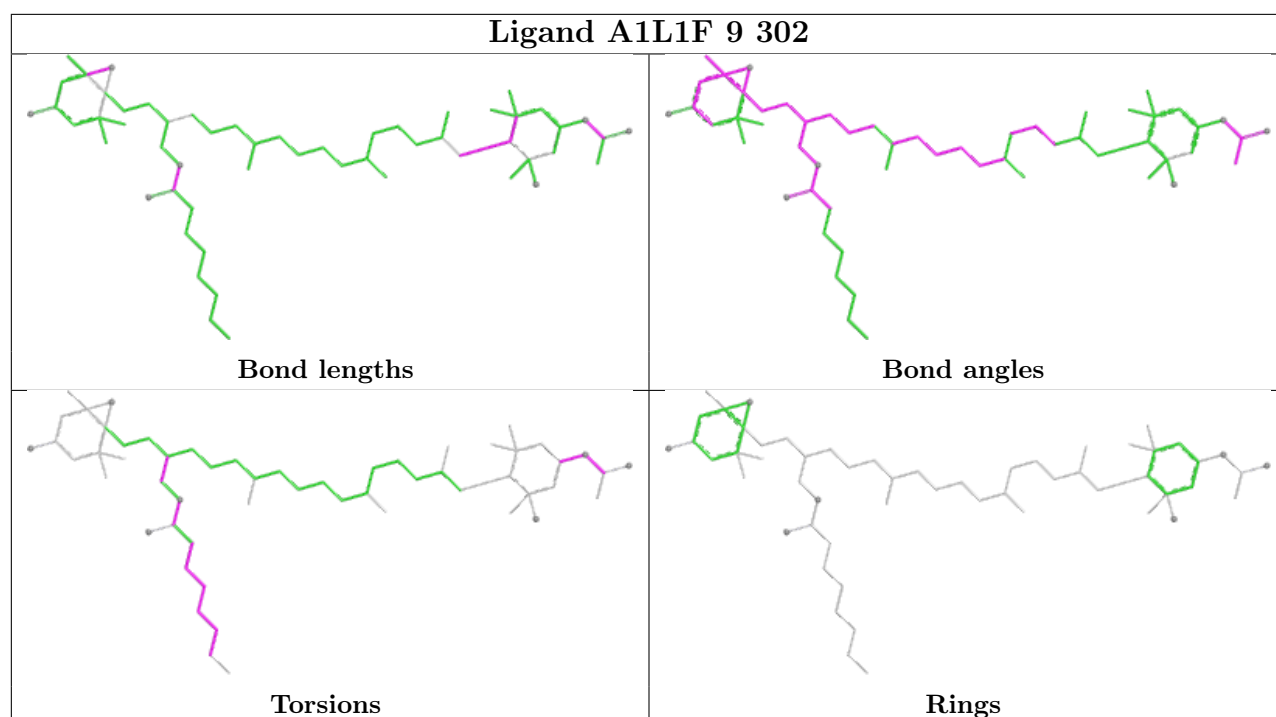
Bond angles



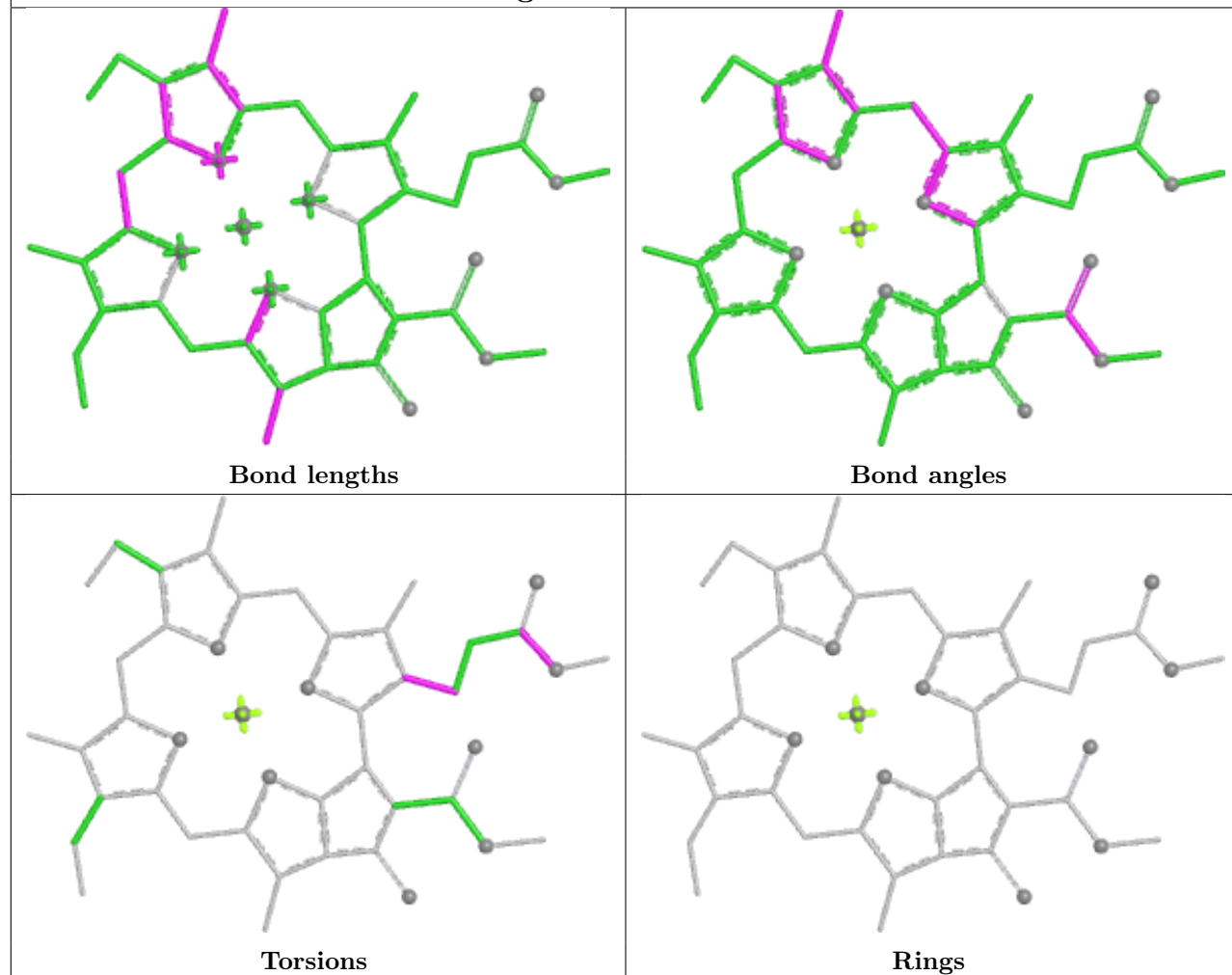
Torsions



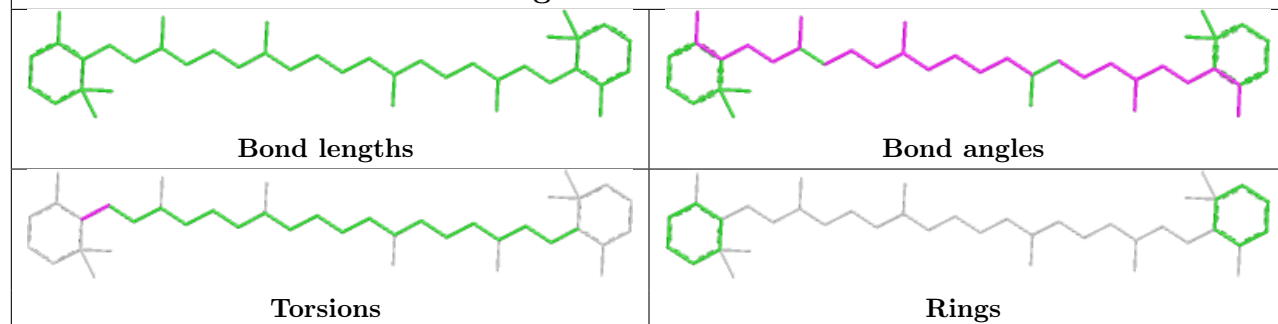
Rings

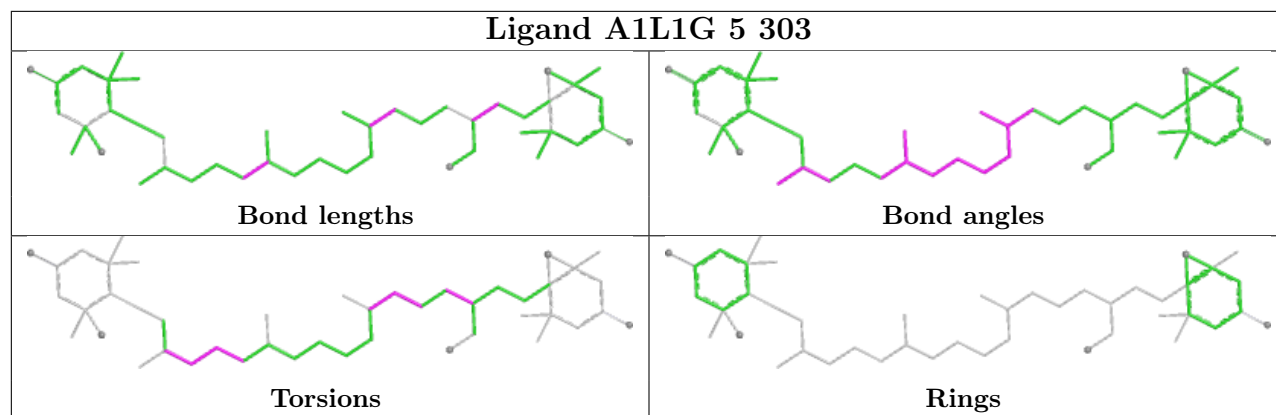
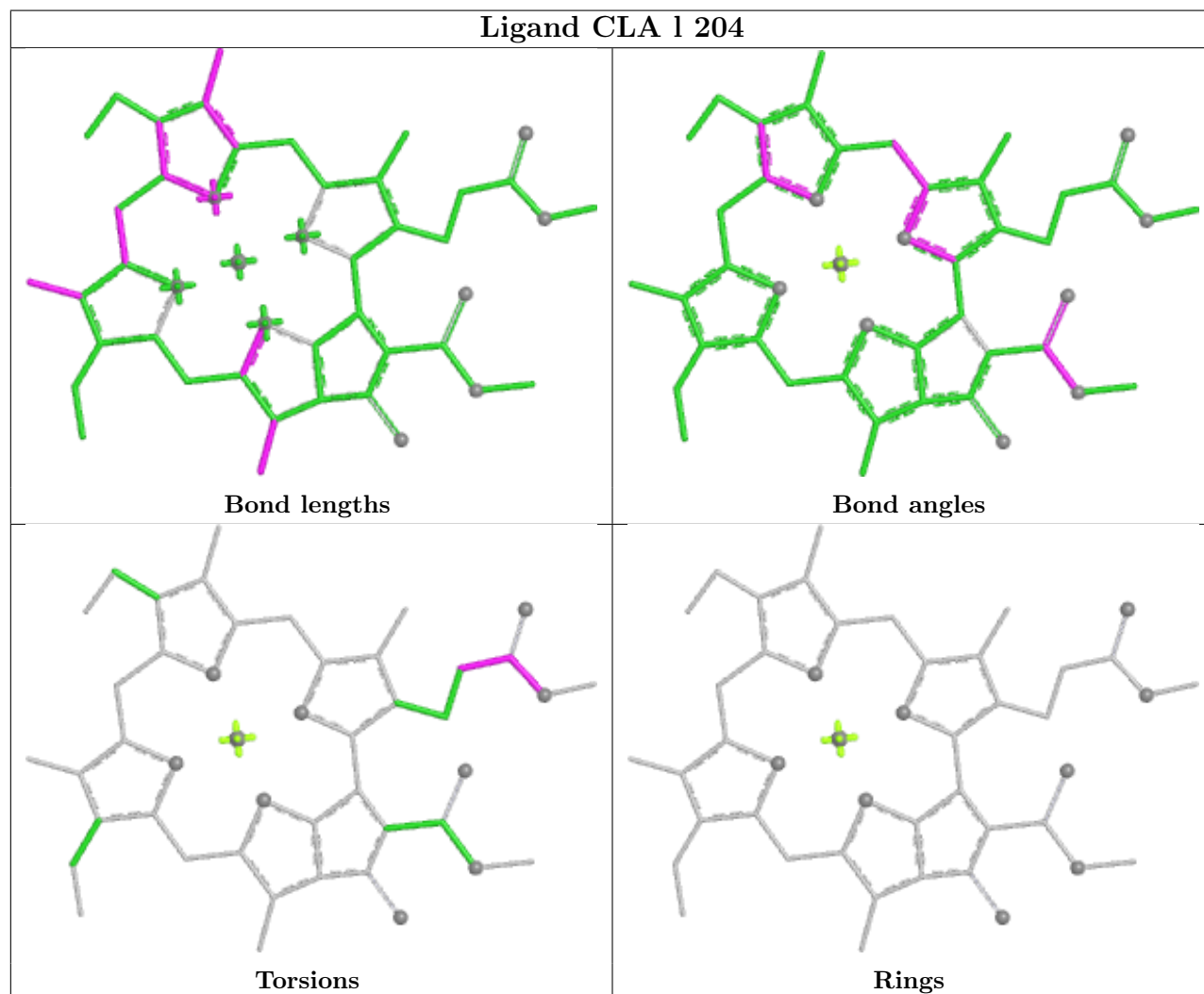


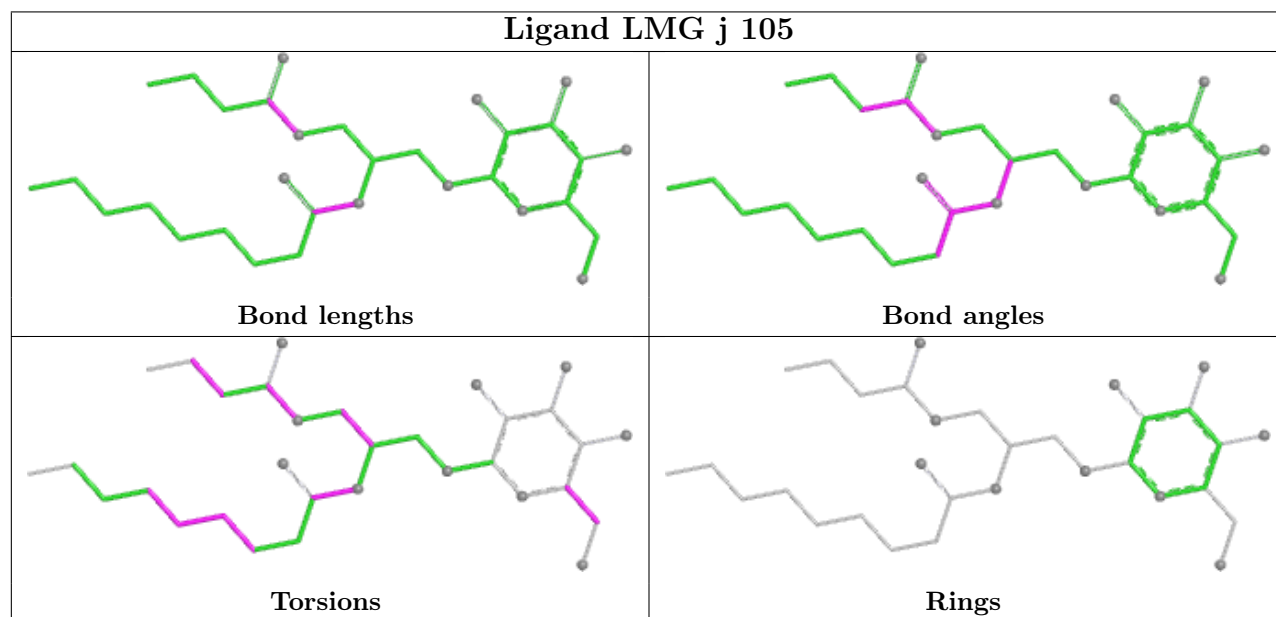
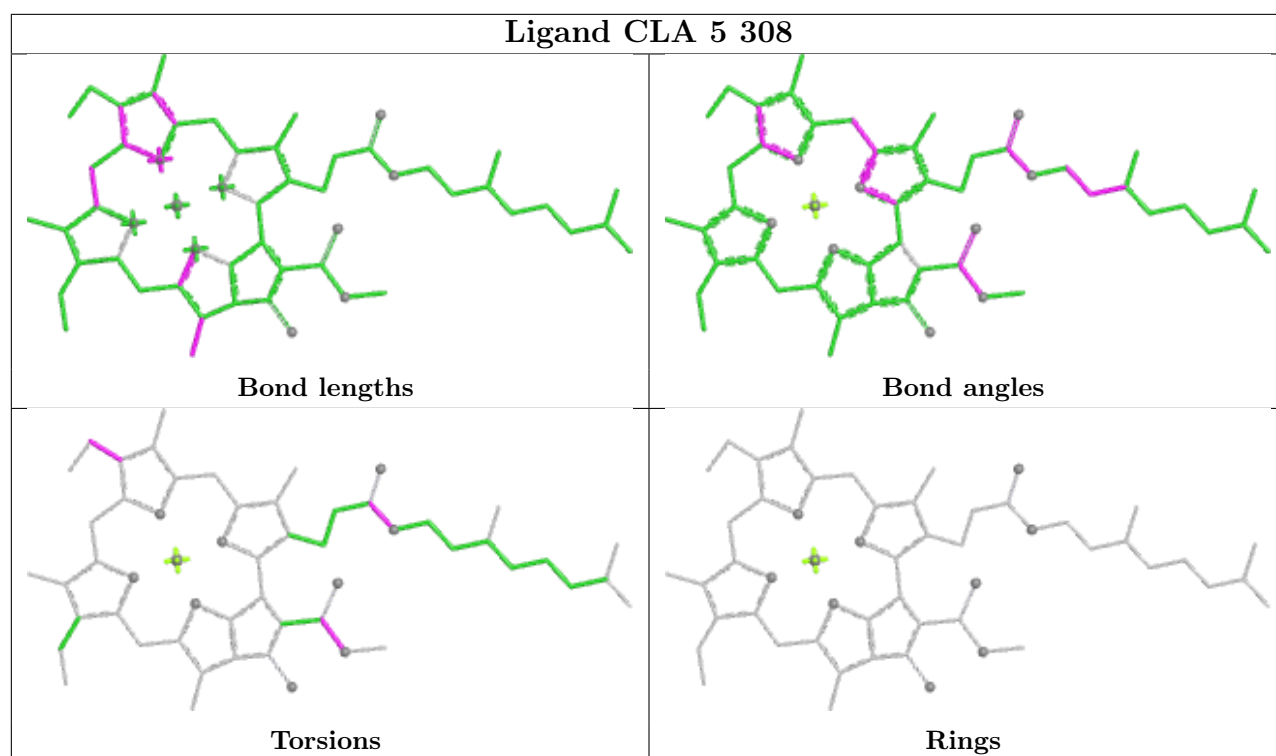
Ligand CLA 7 311



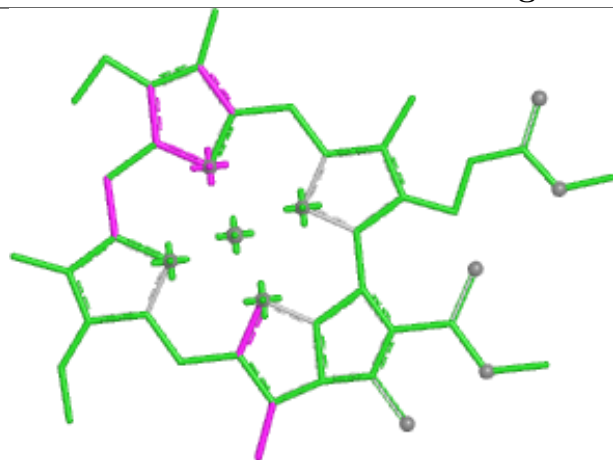
Ligand BCR b 846



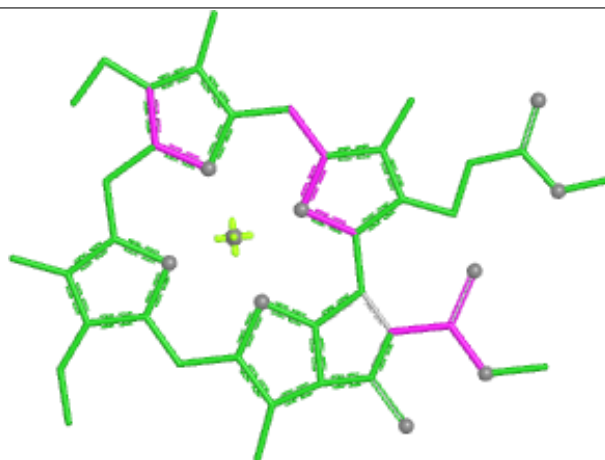
Ligand A1L1G 5 303**Ligand CLA 1 204**



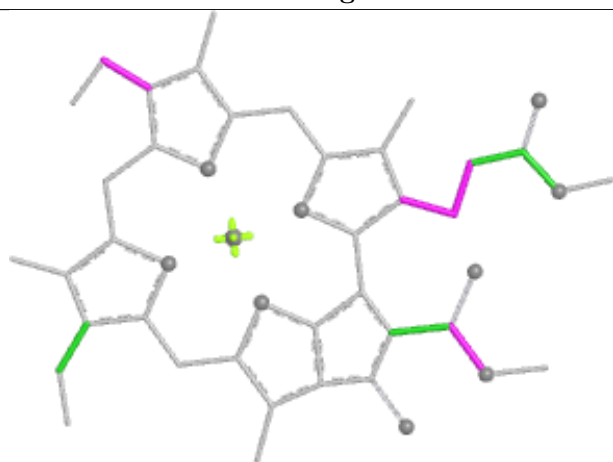
Ligand CLA 9 311



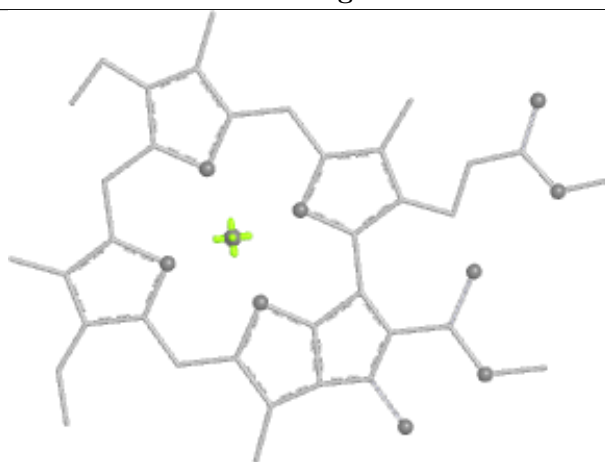
Bond lengths



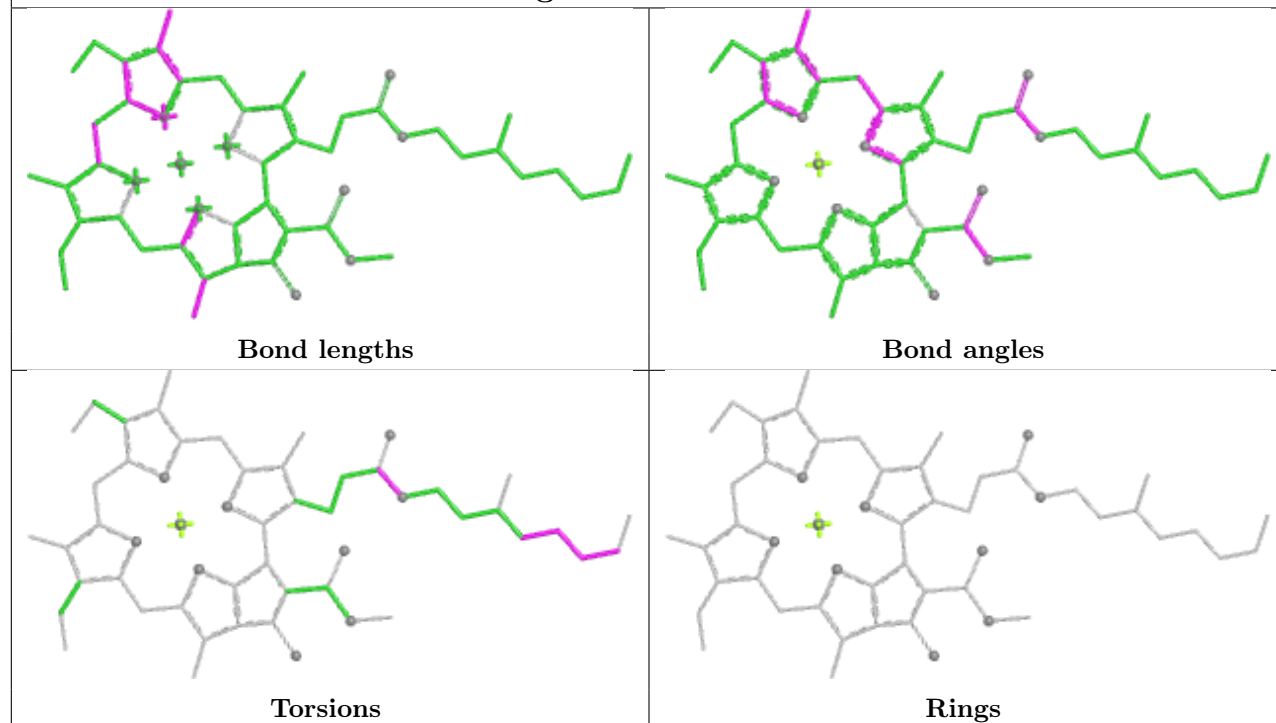
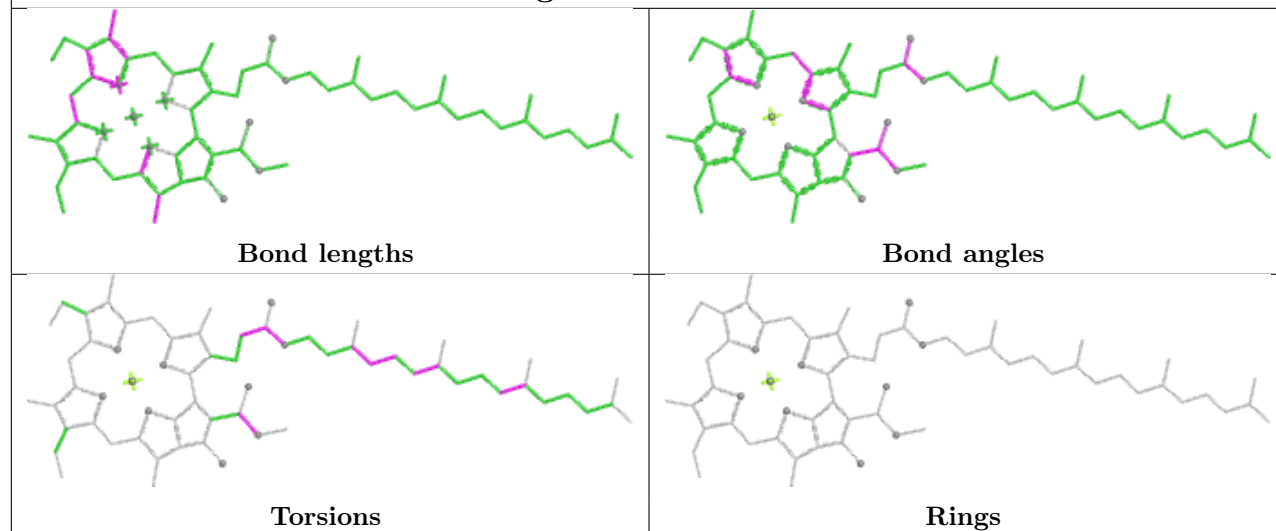
Bond angles

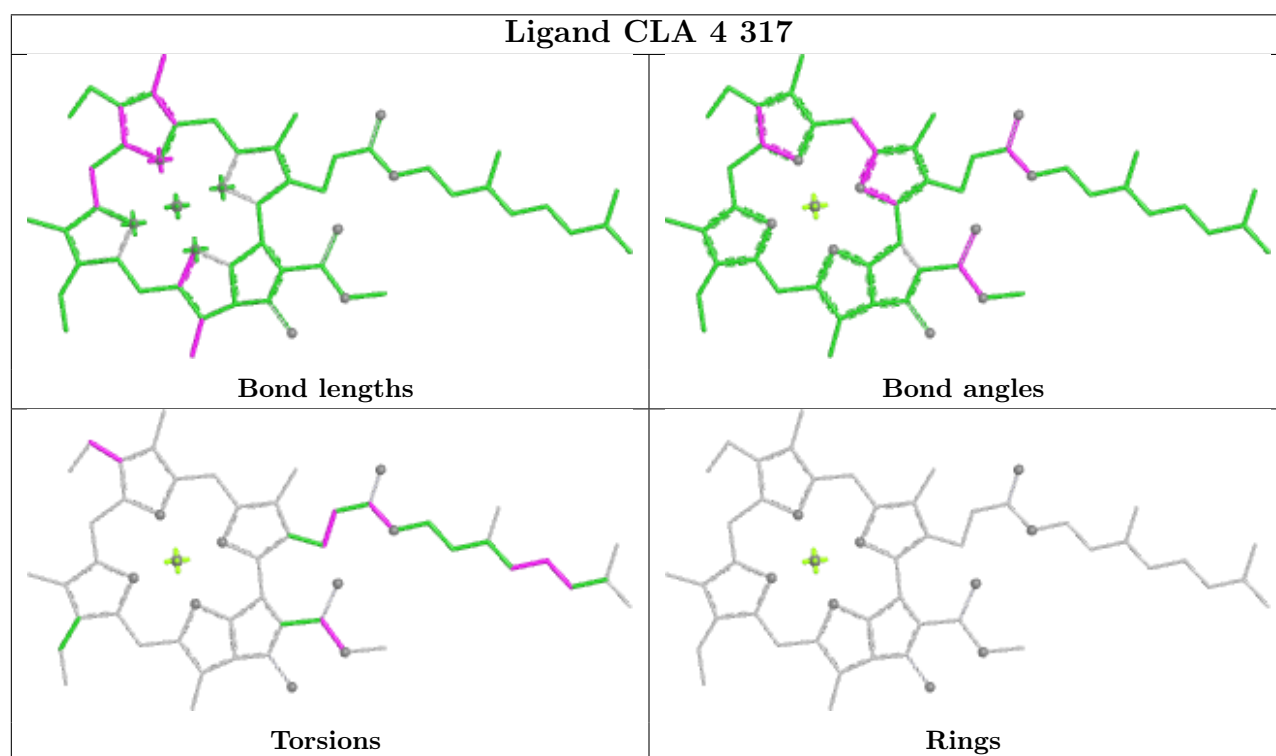
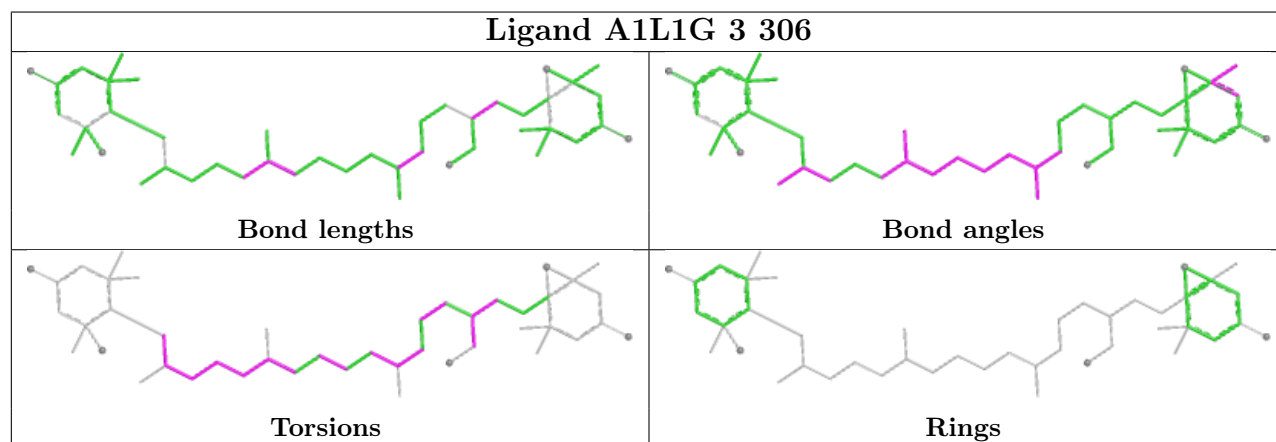
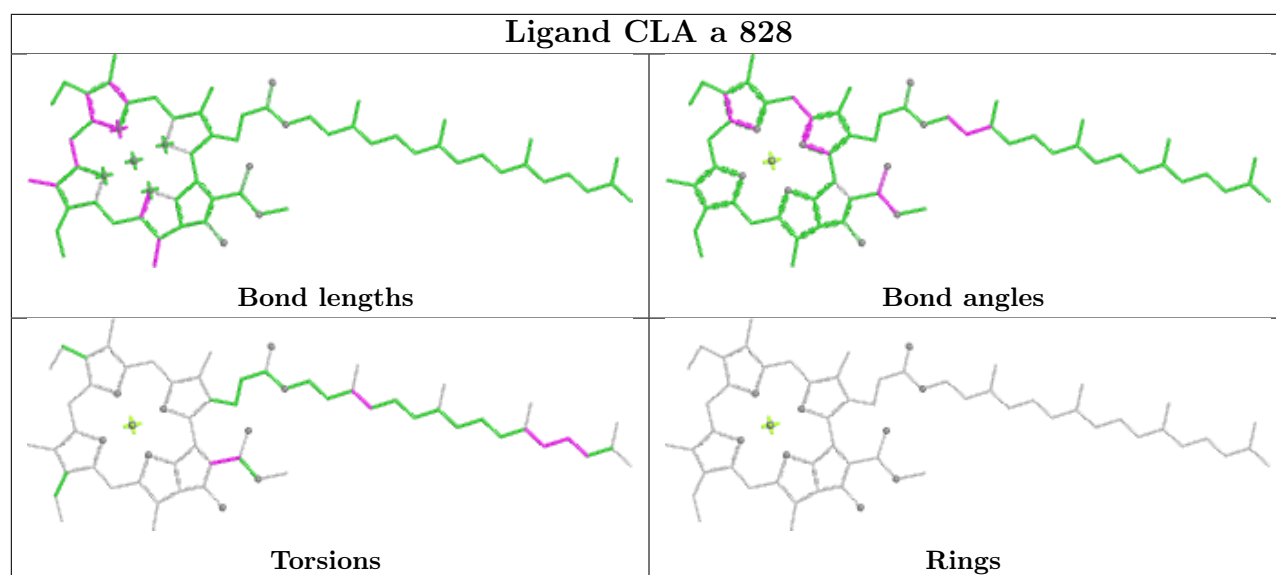


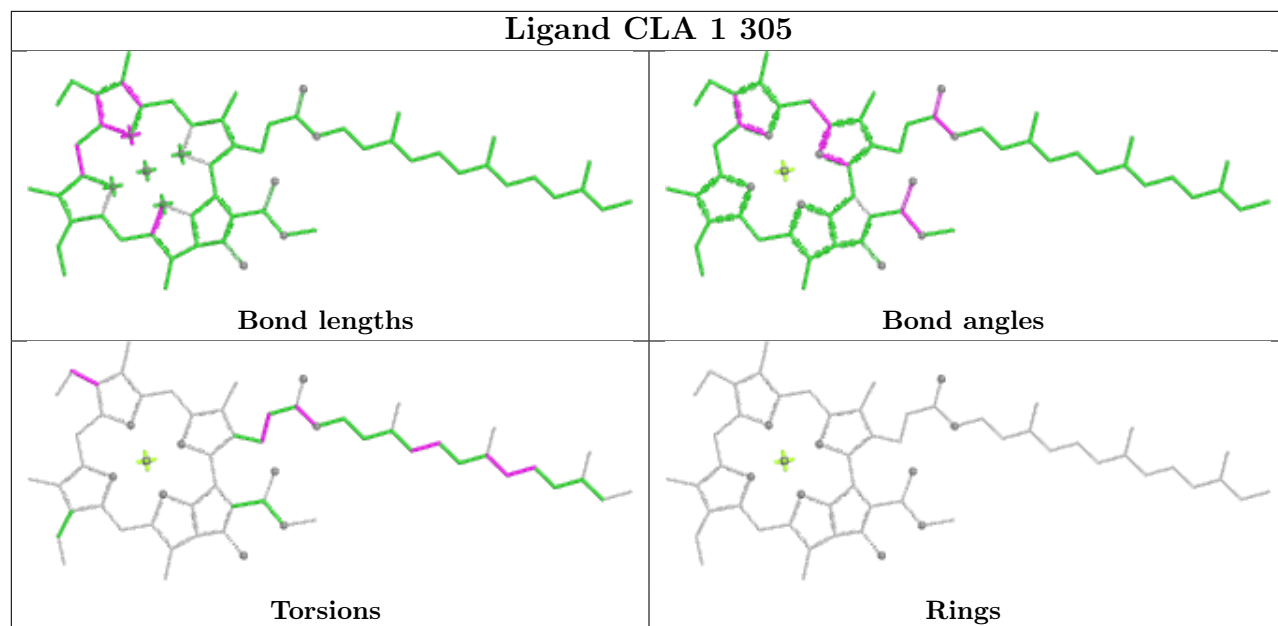
Torsions



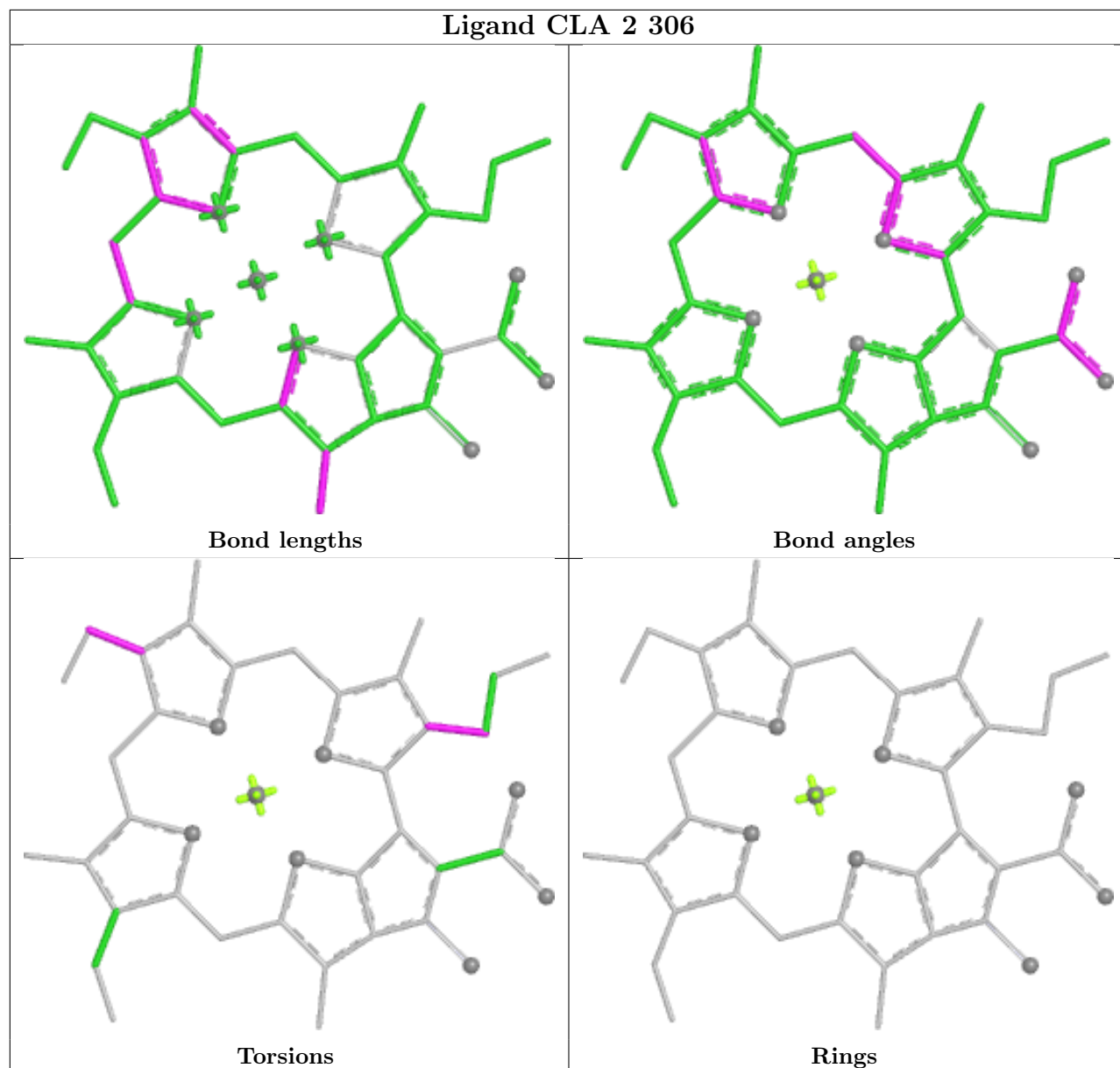
Rings

Ligand CLA 1 307**Ligand CLA a 835**

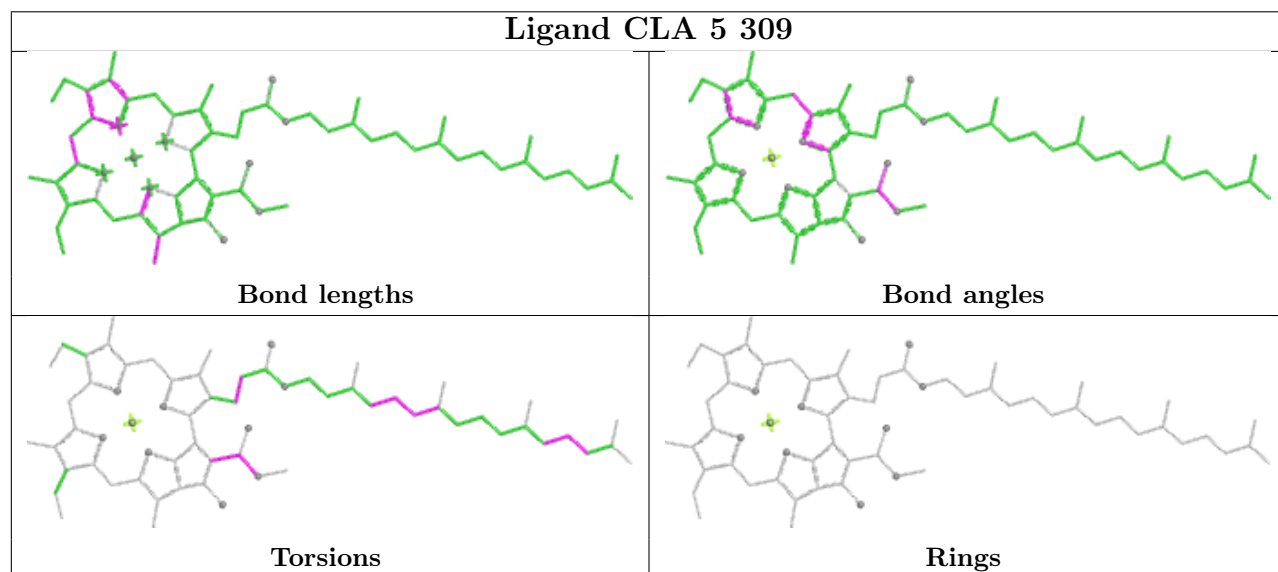


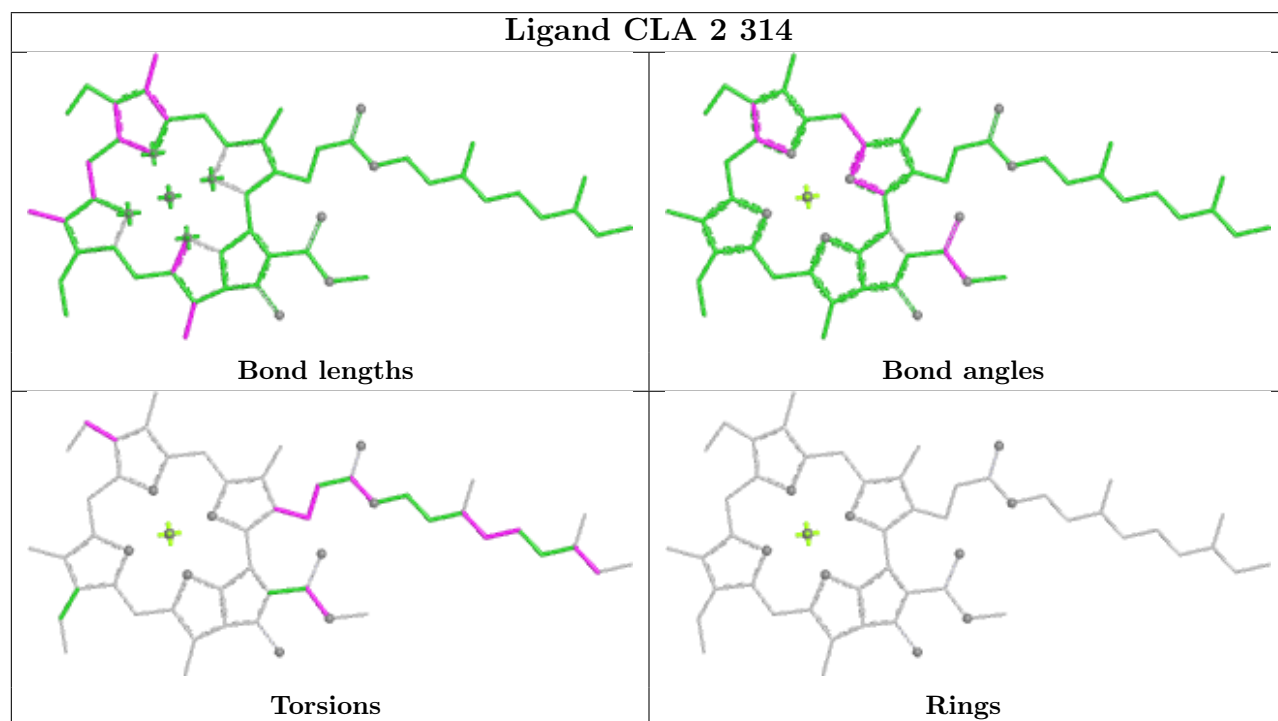
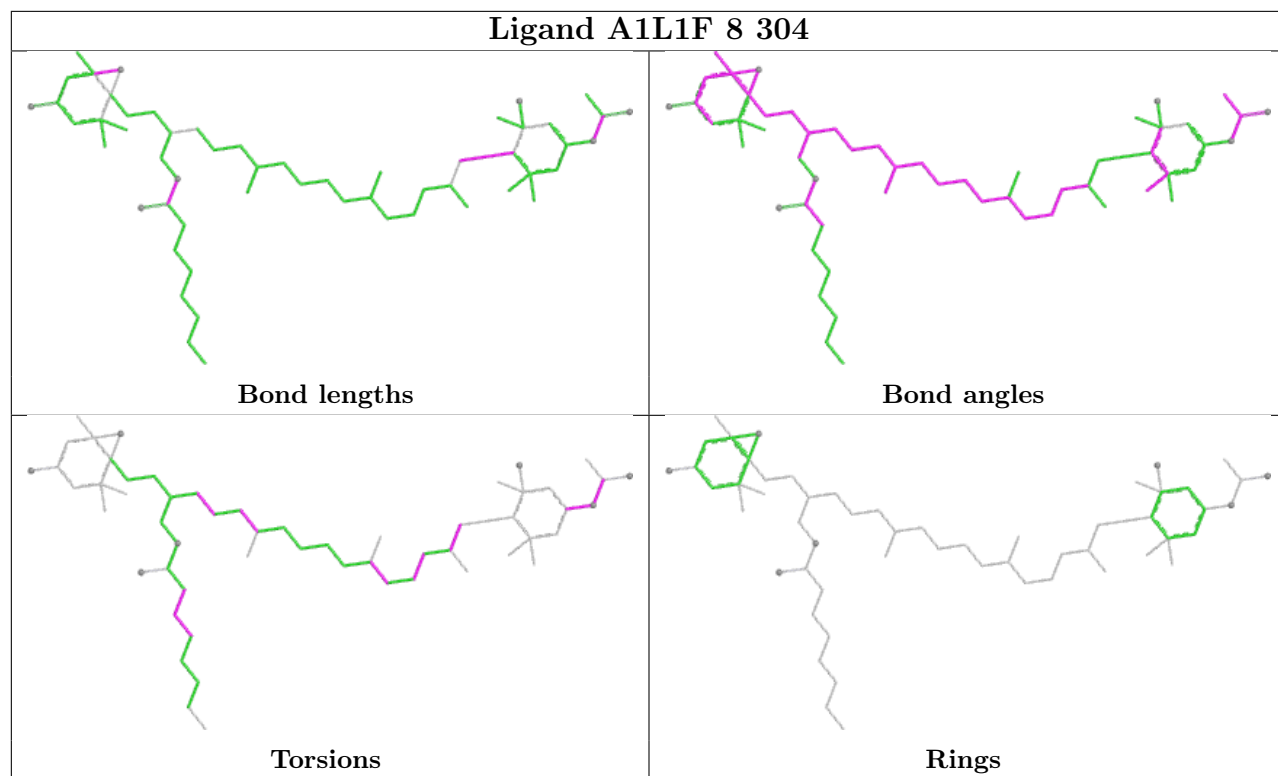


Ligand CLA 2 306

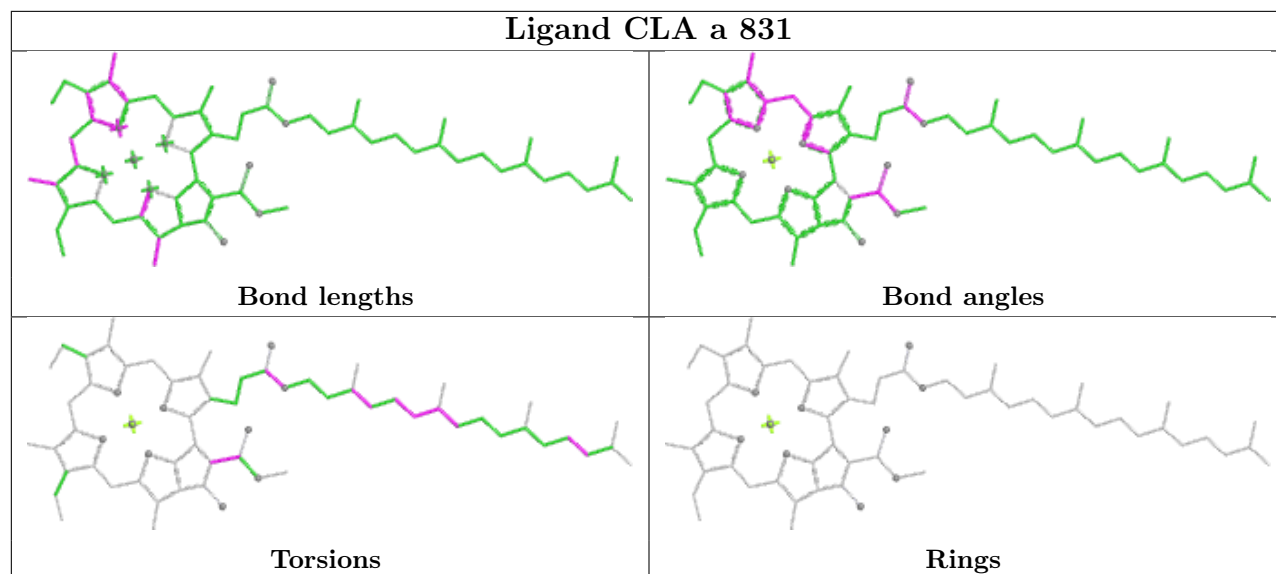


Ligand CLA 5 309

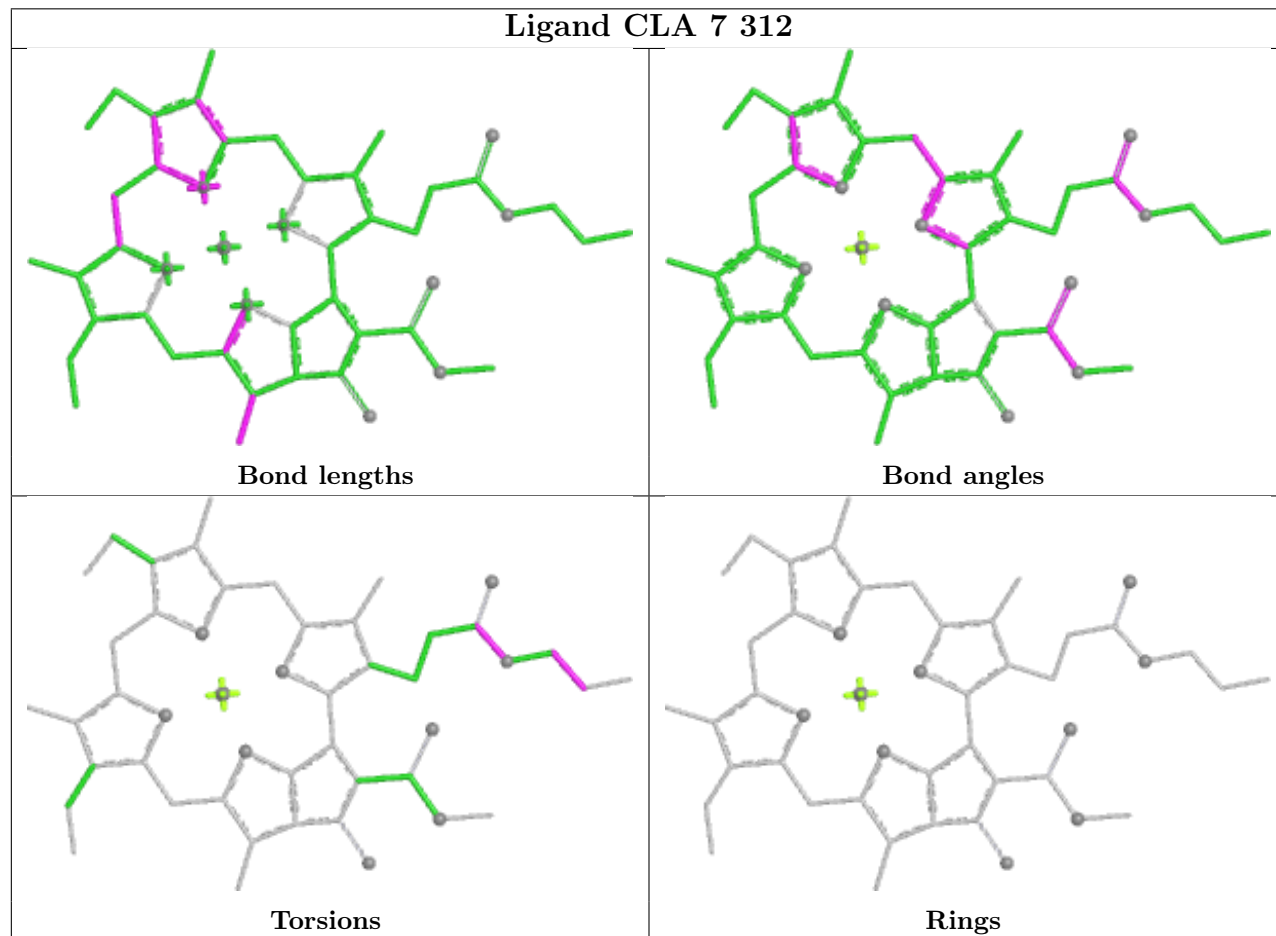


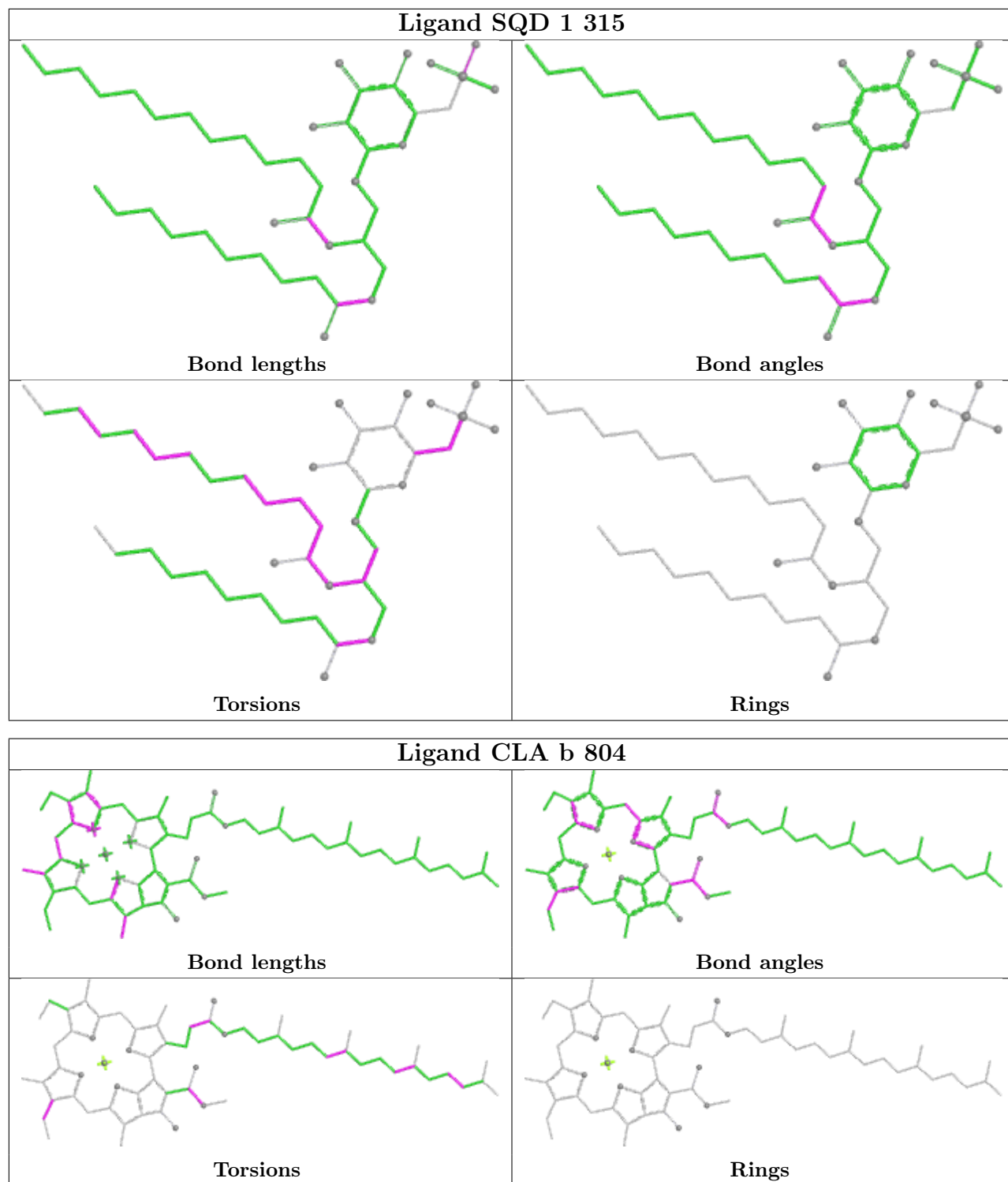


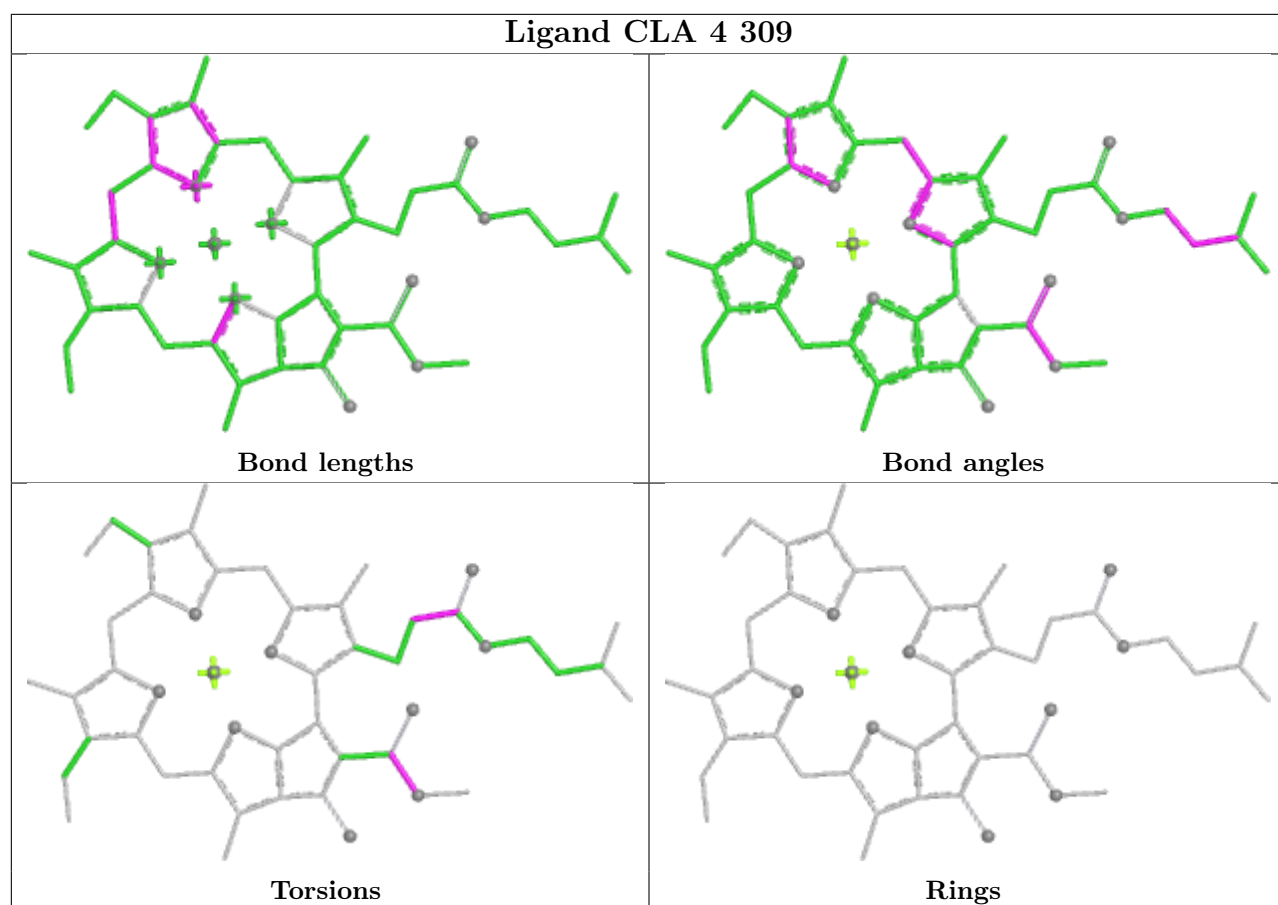
Ligand CLA a 831



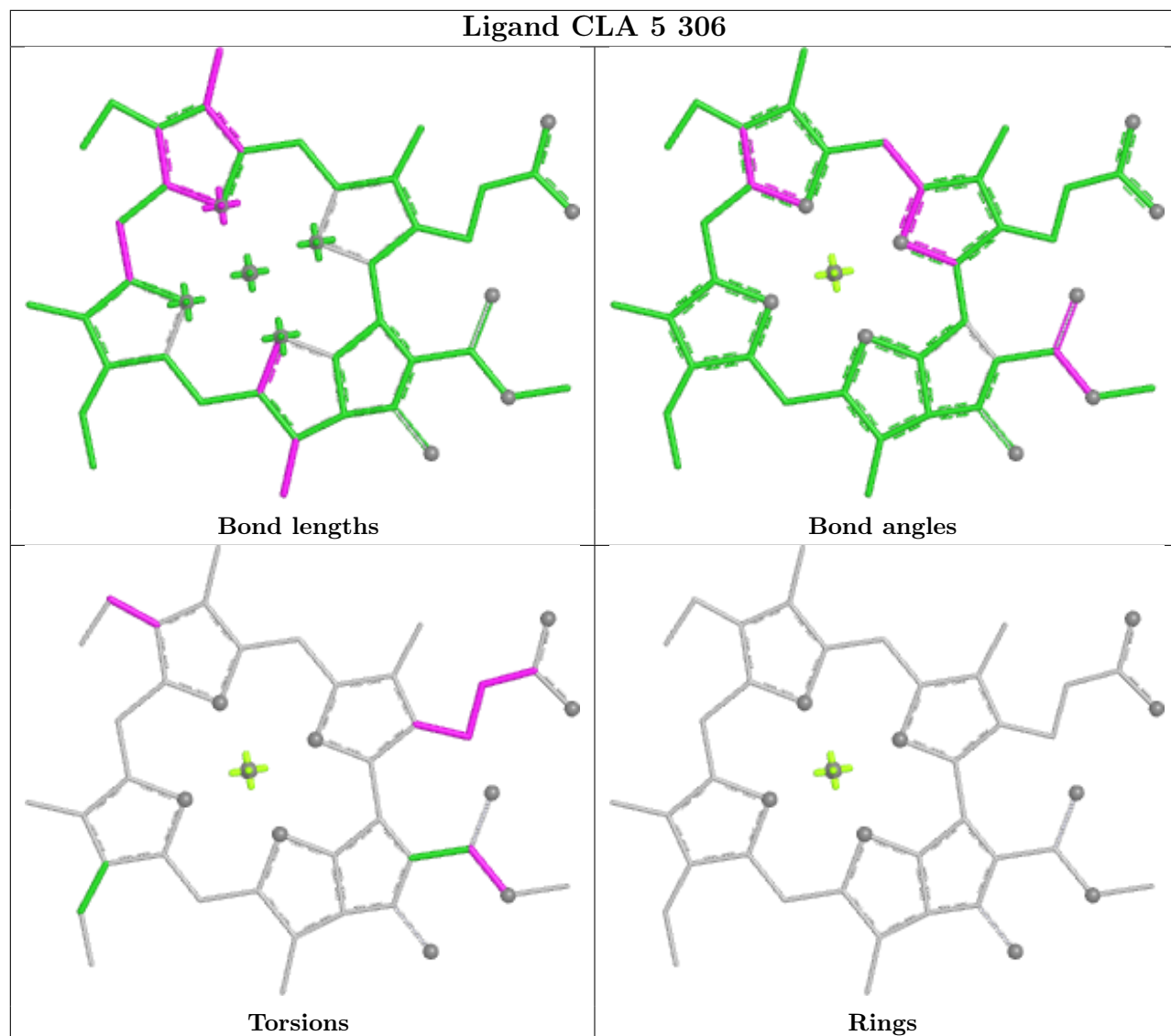
Ligand CLA 7 312



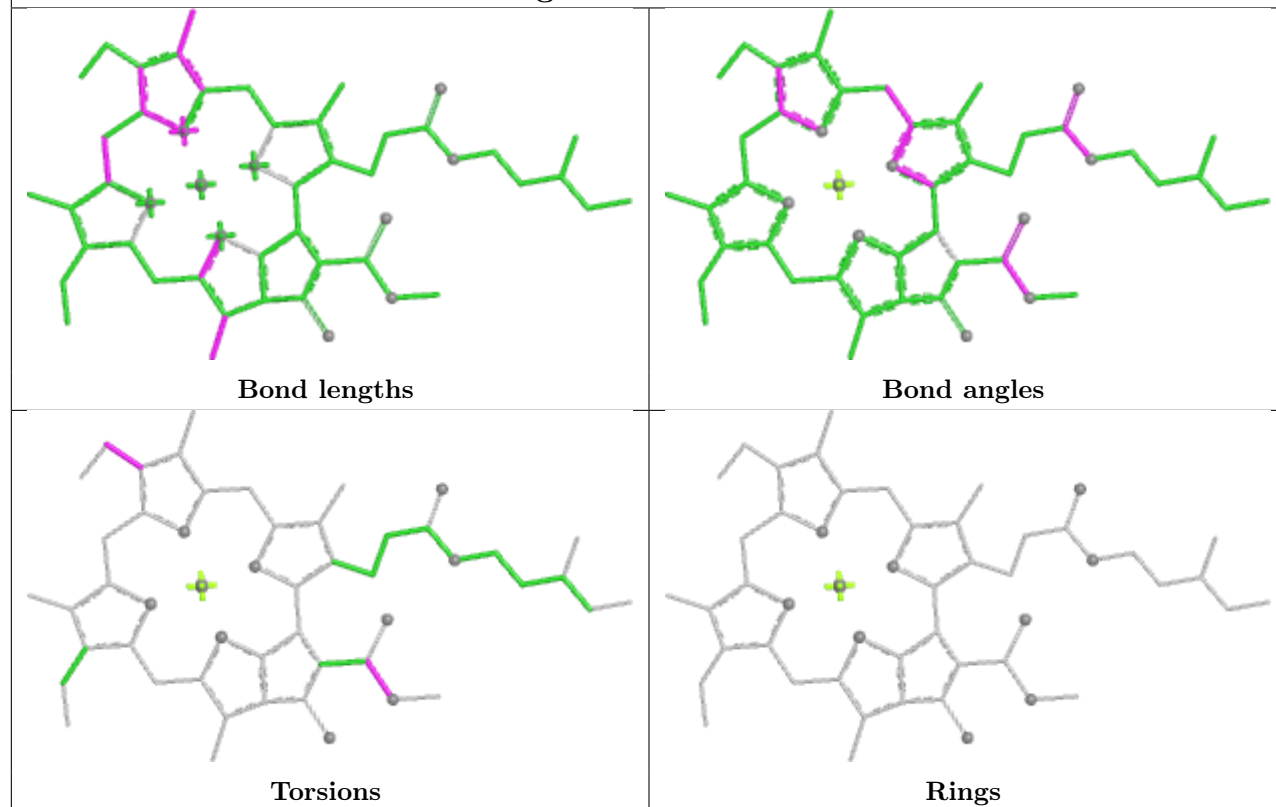




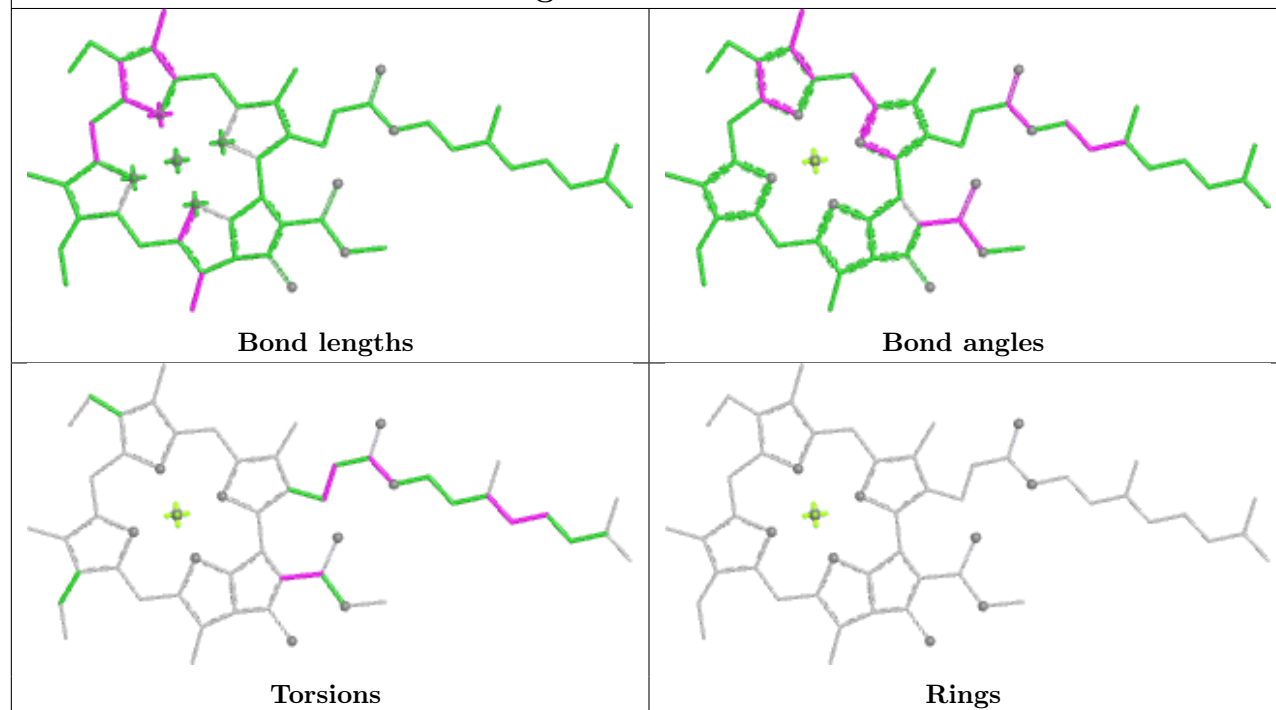
Ligand CLA 5 306

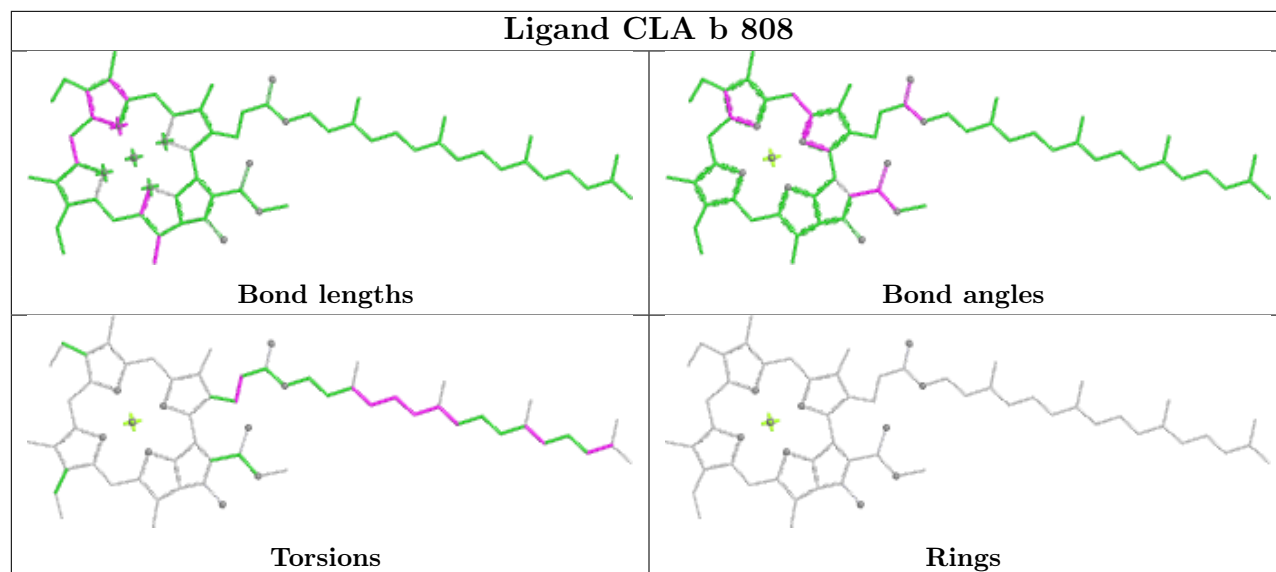
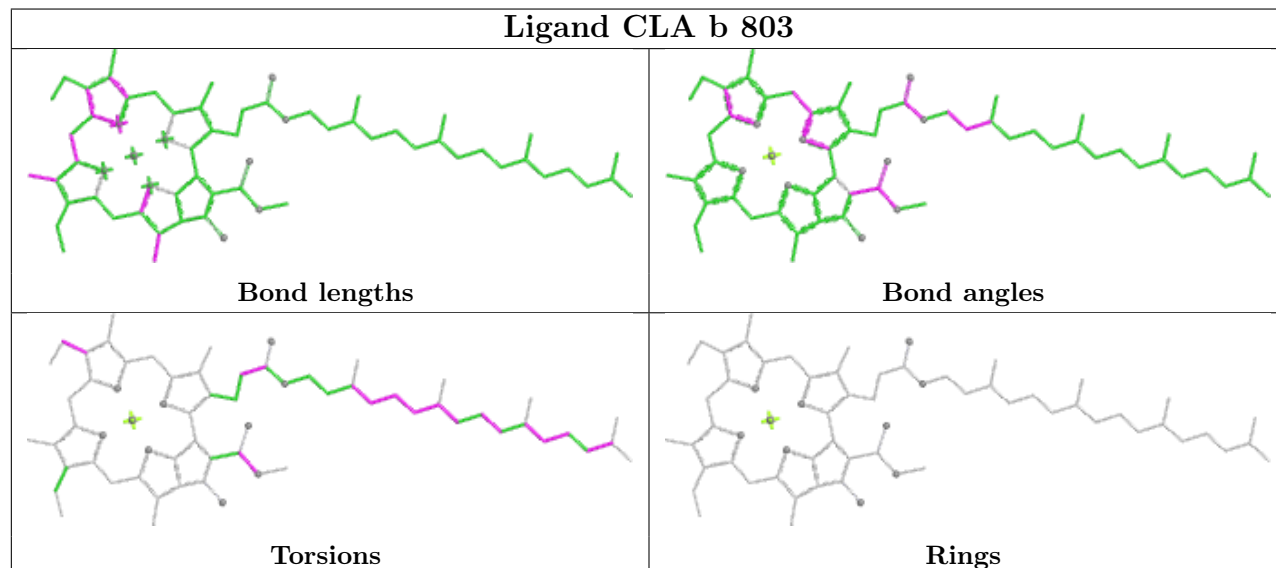


Ligand CLA a 808

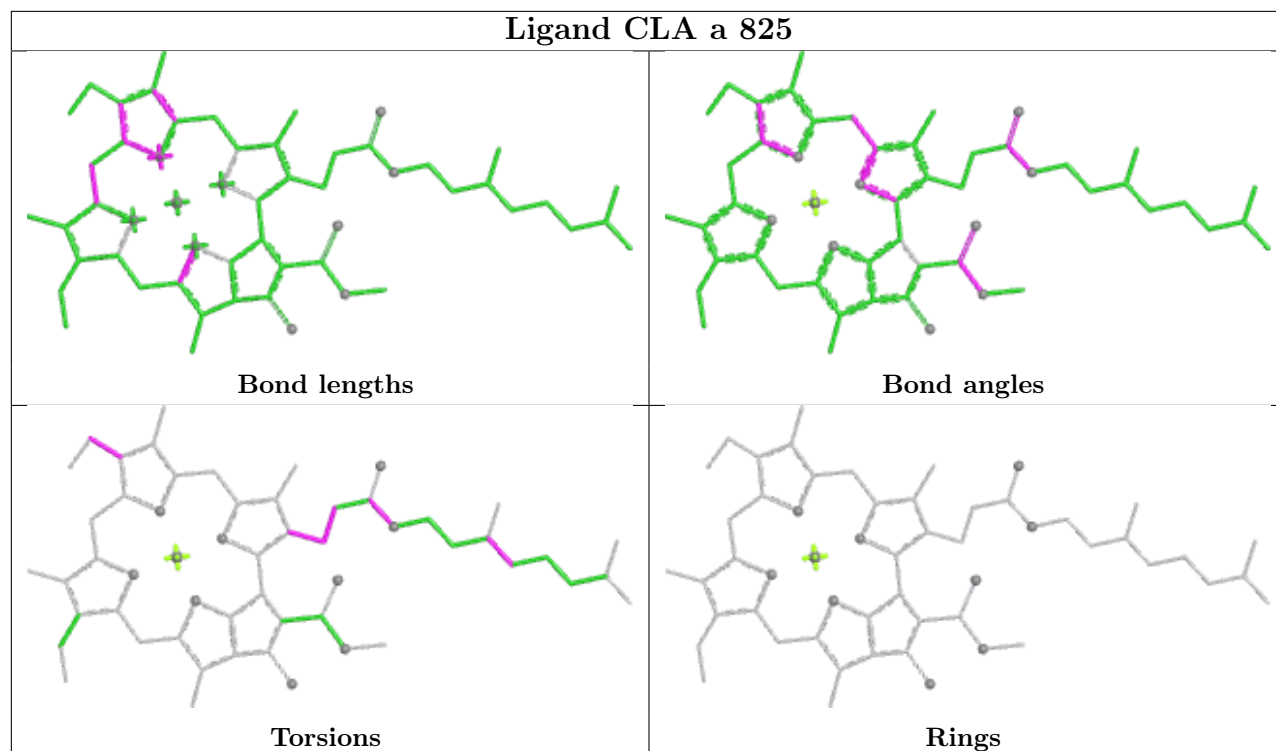


Ligand CLA 8 308

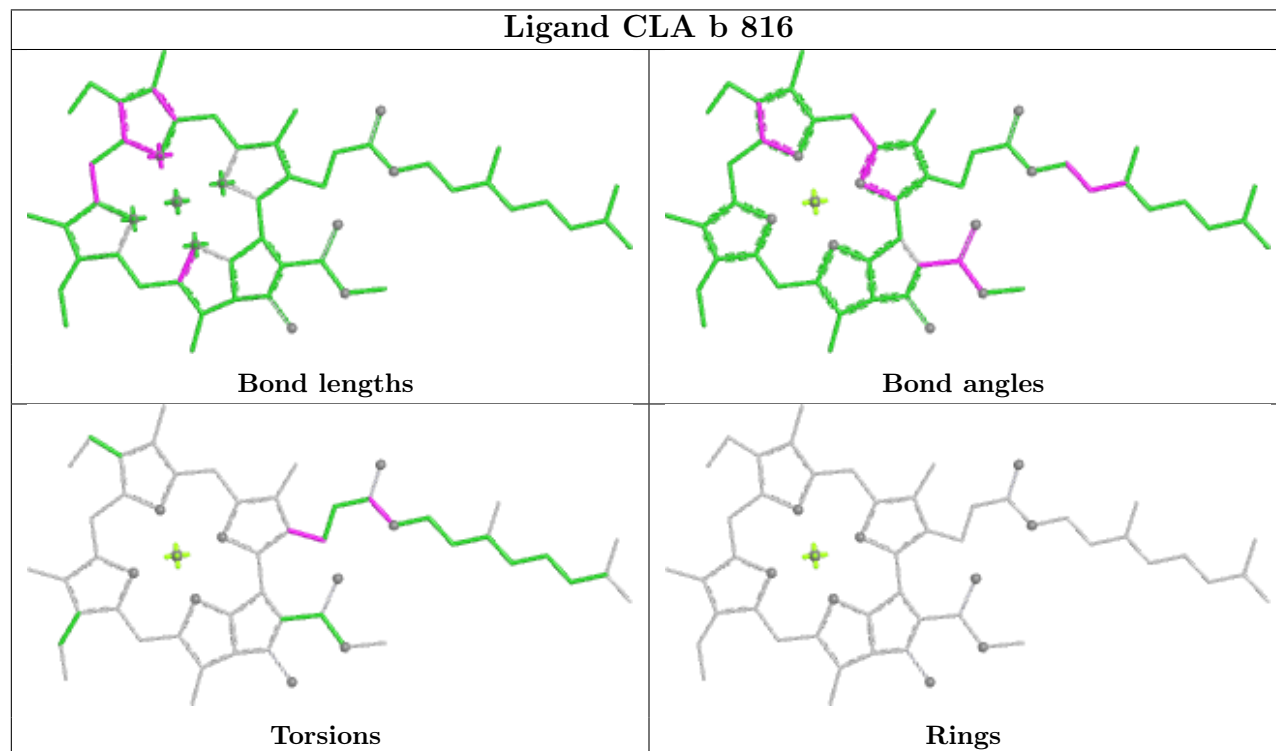


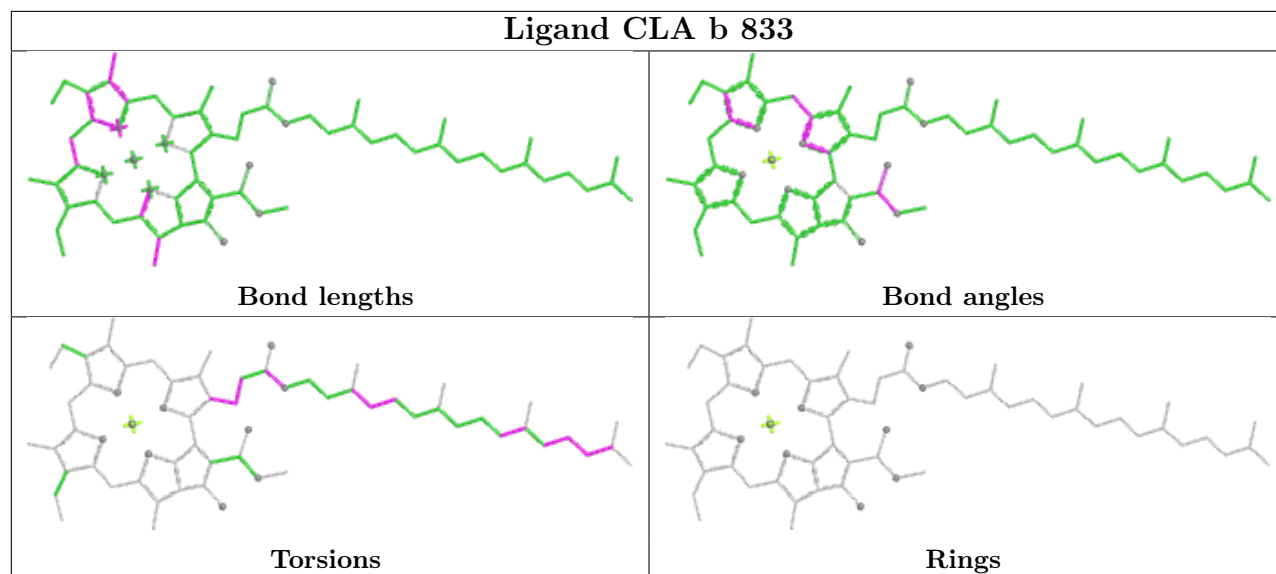
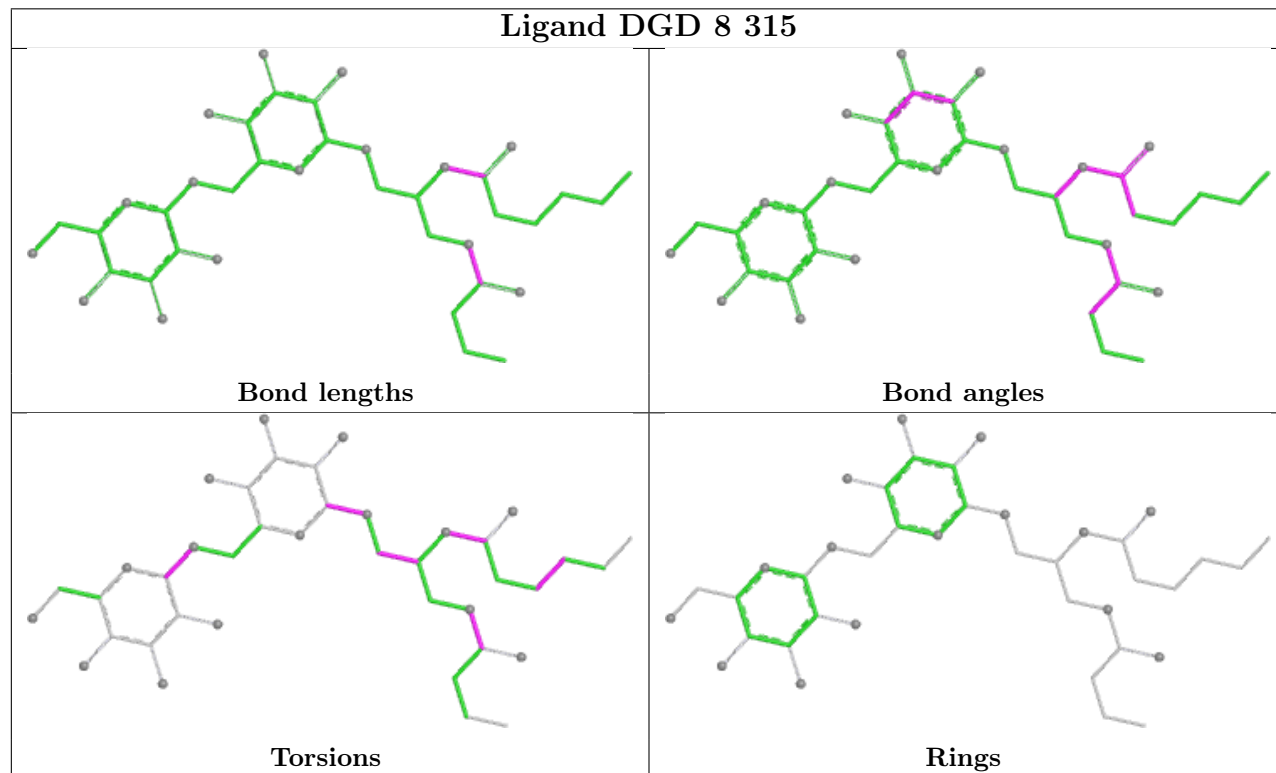
Ligand CLA b 808**Ligand CLA b 803**

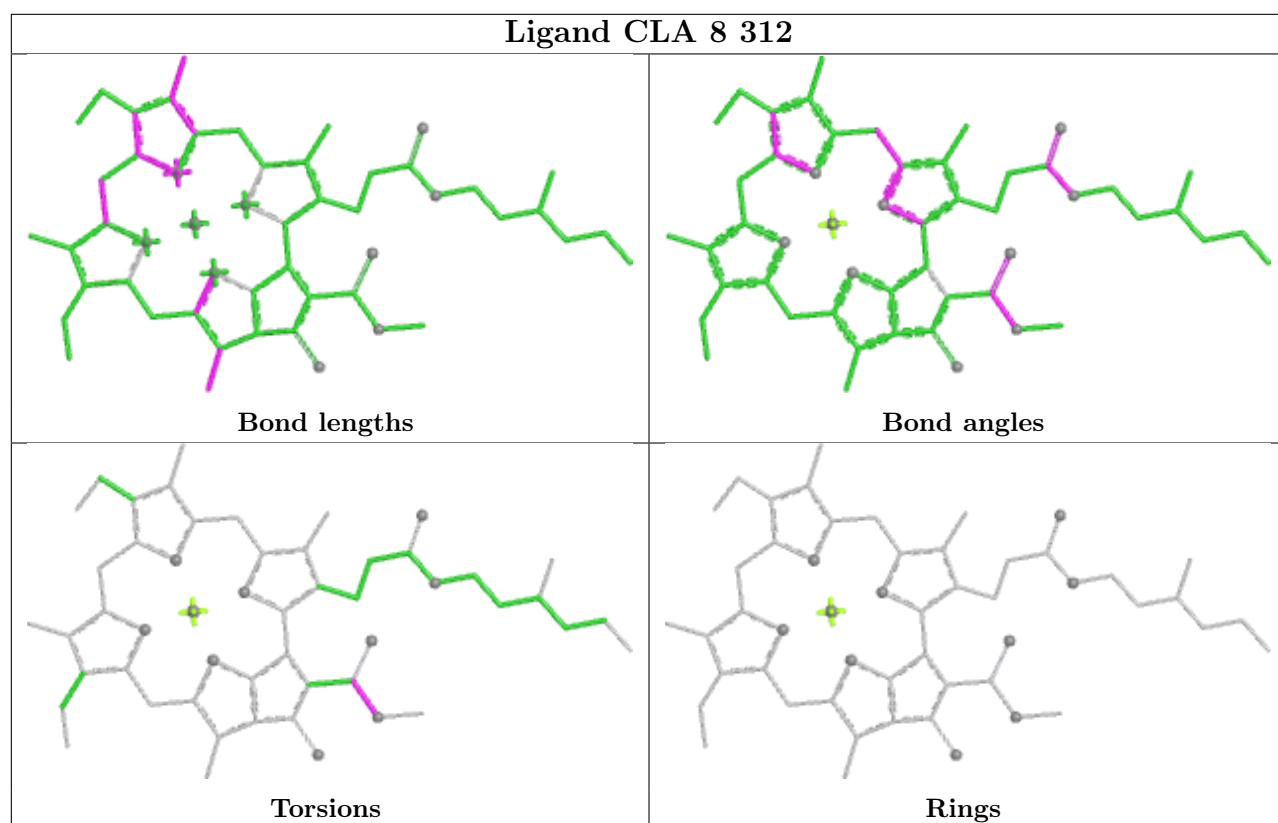
Ligand CLA a 825



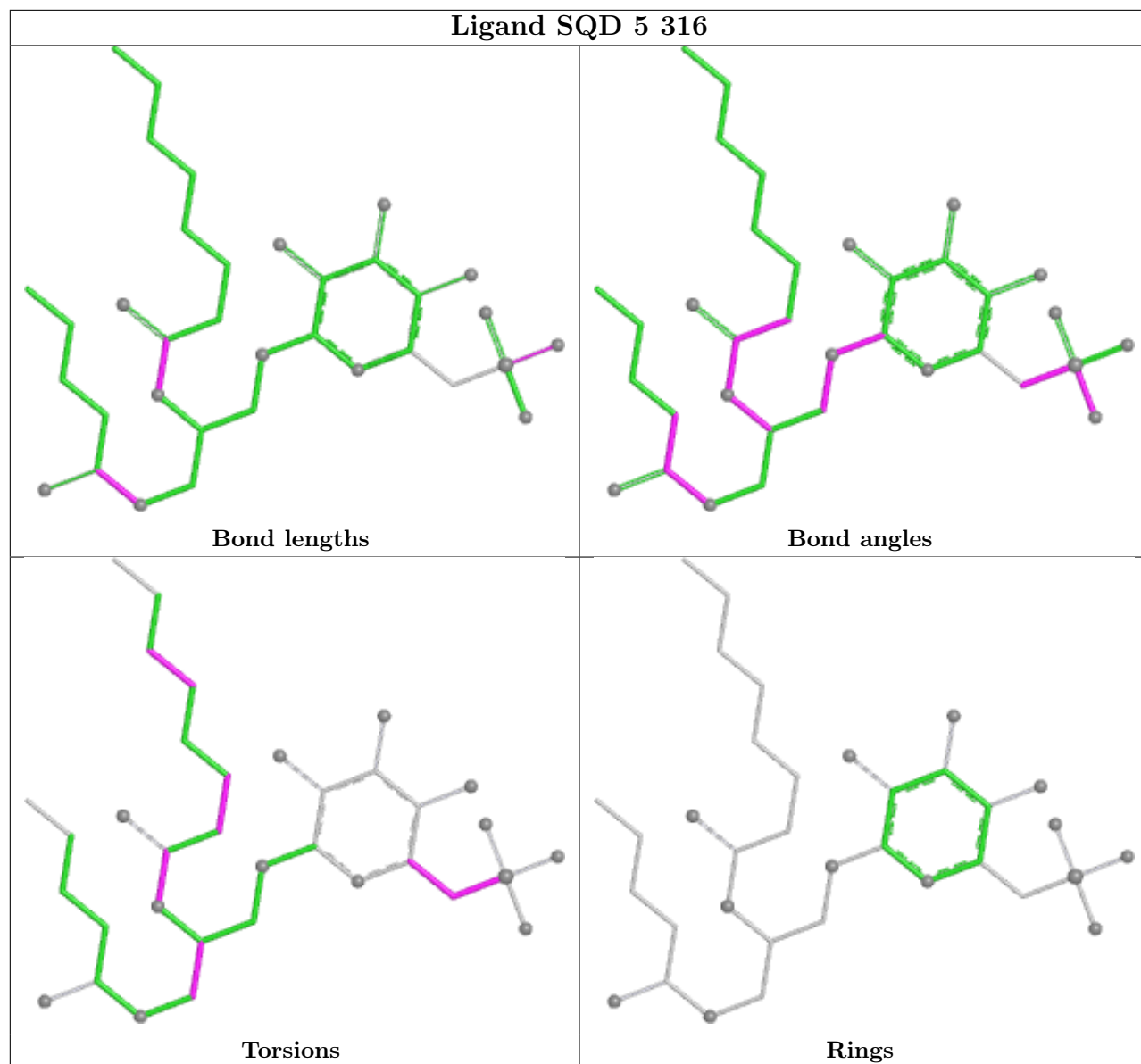
Ligand CLA b 816



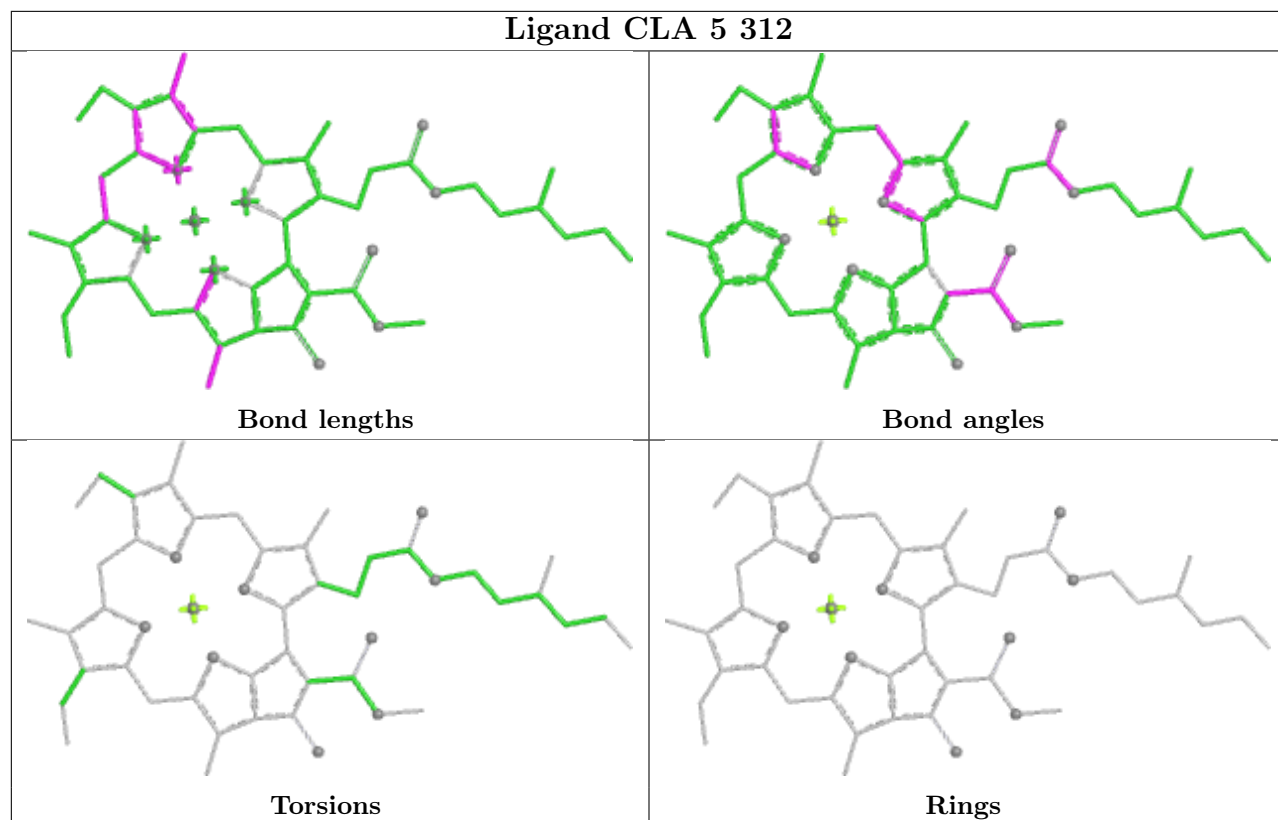
Ligand CLA b 833**Ligand DGD 8 315**

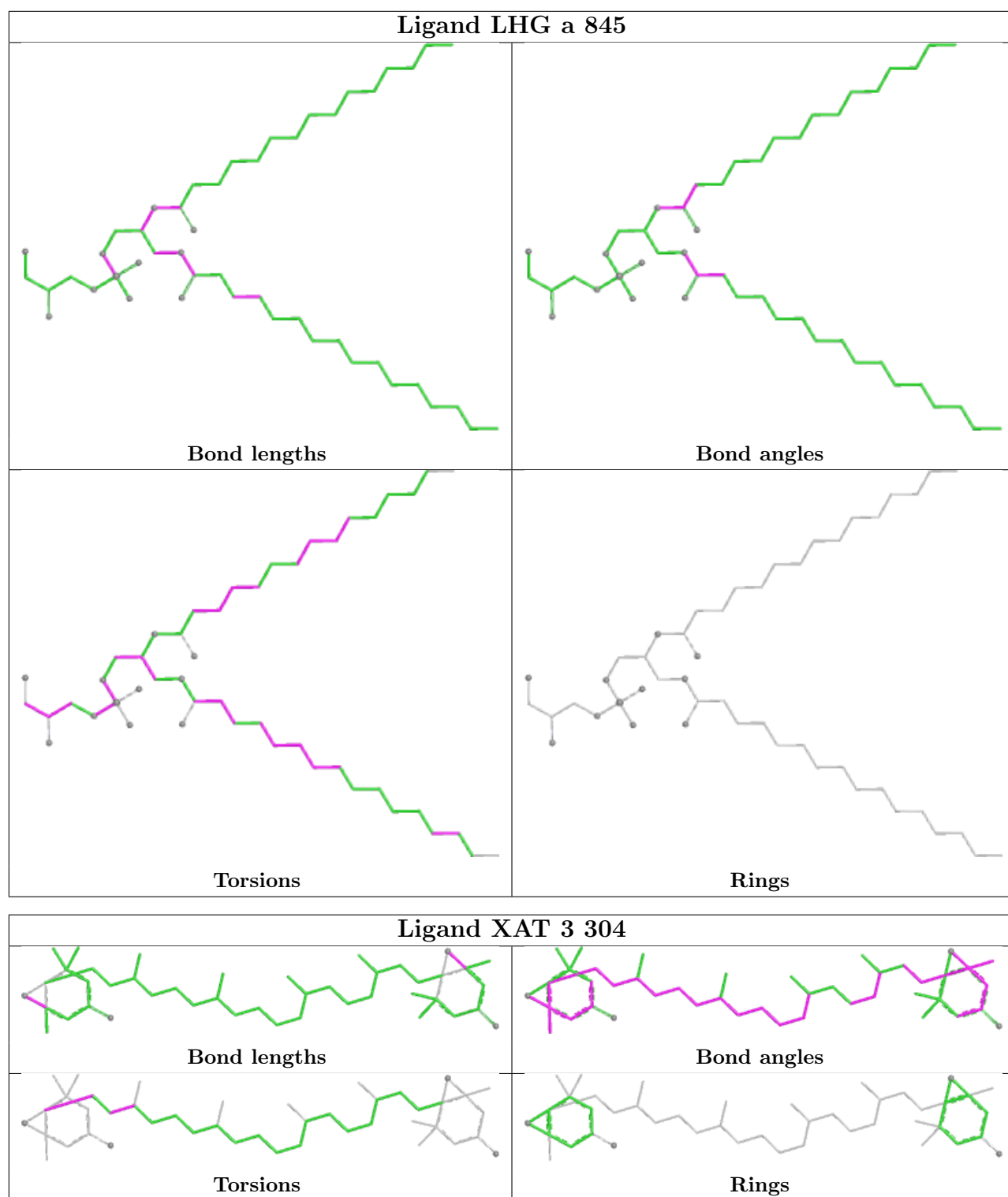


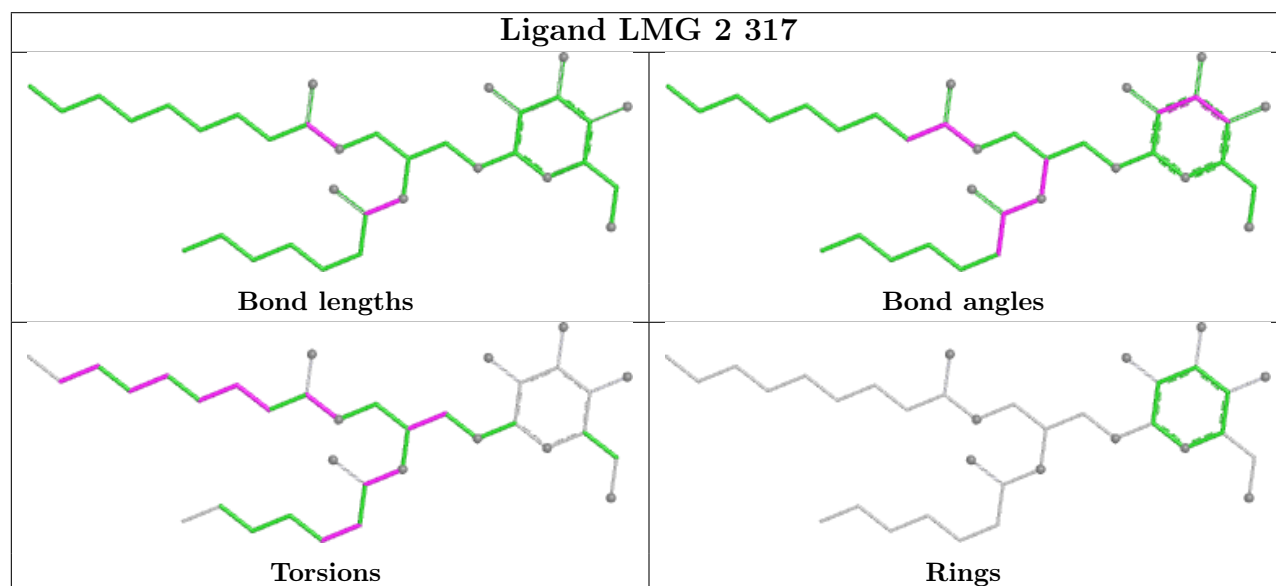
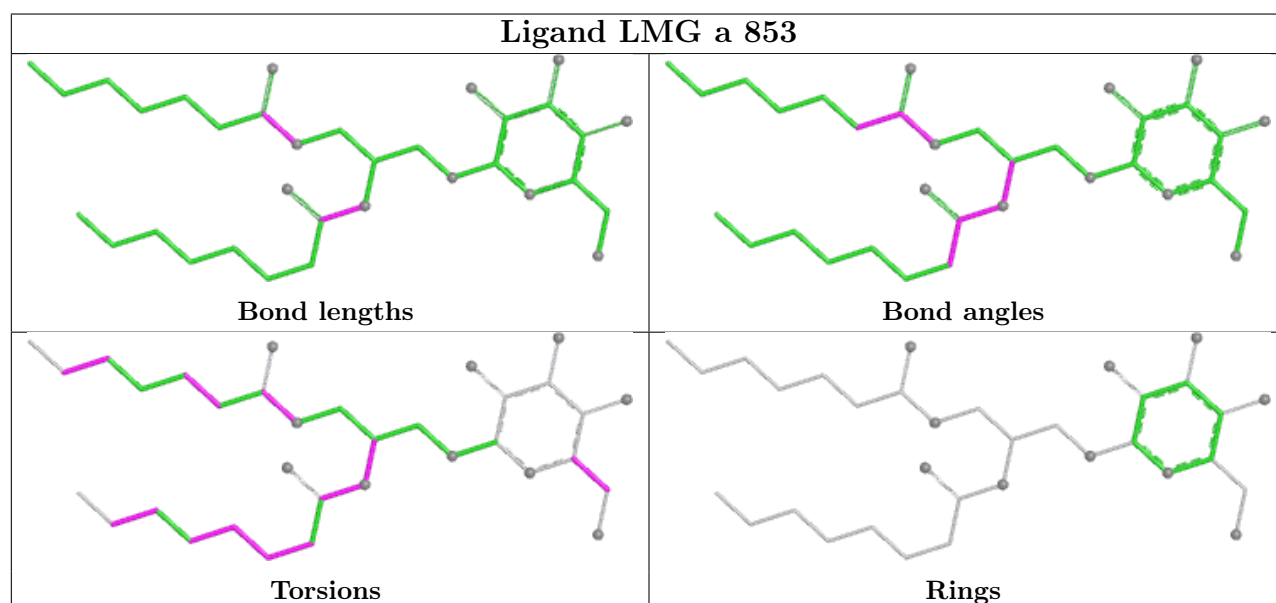
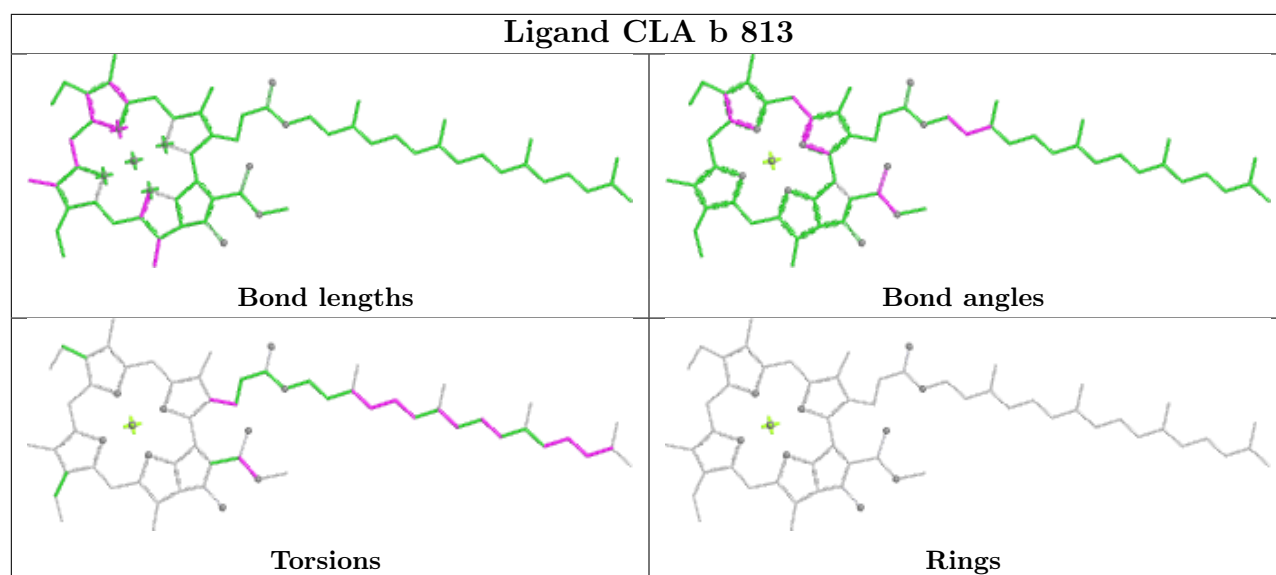
Ligand SQD 5 316

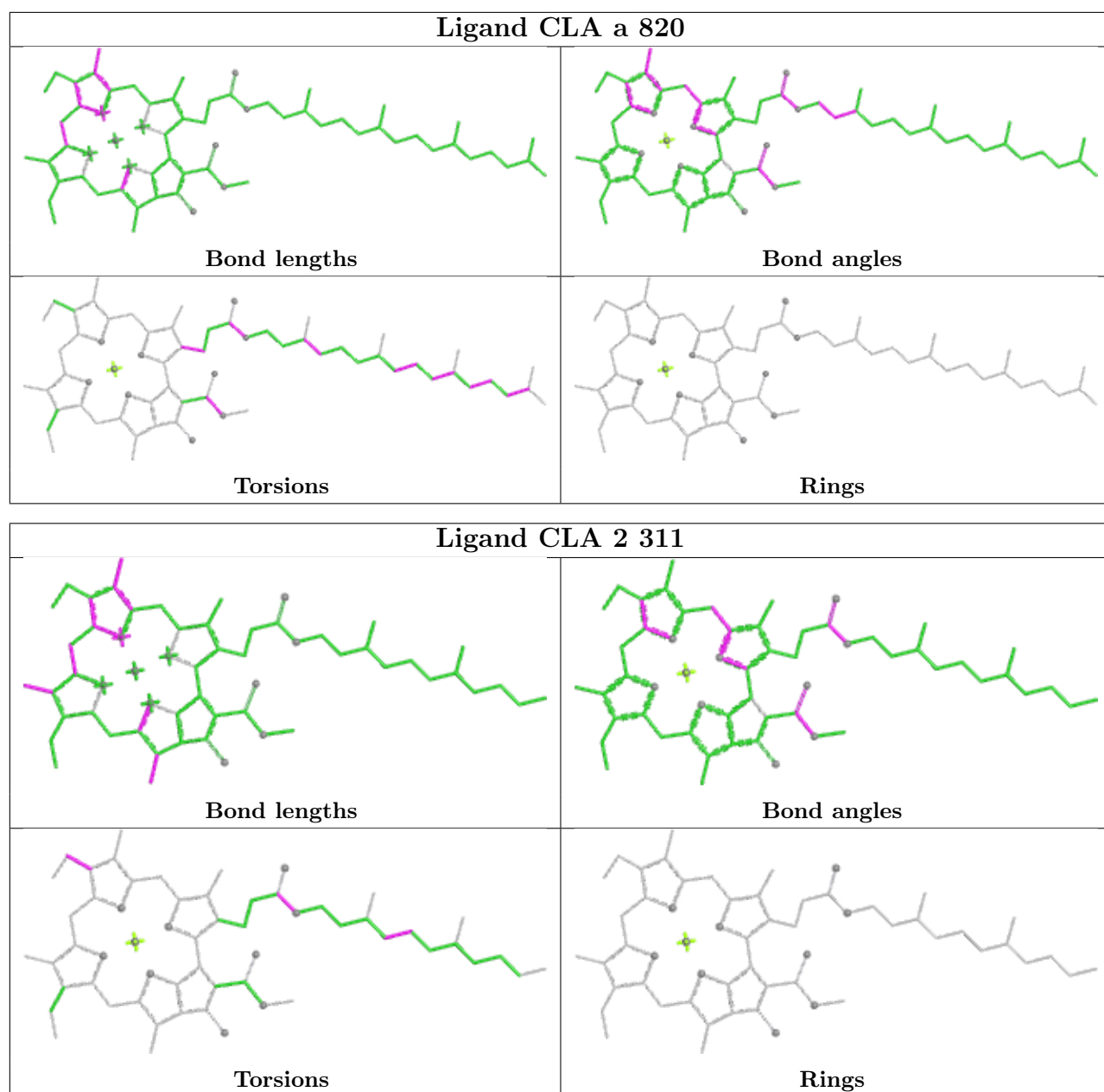


Ligand CLA 5 312

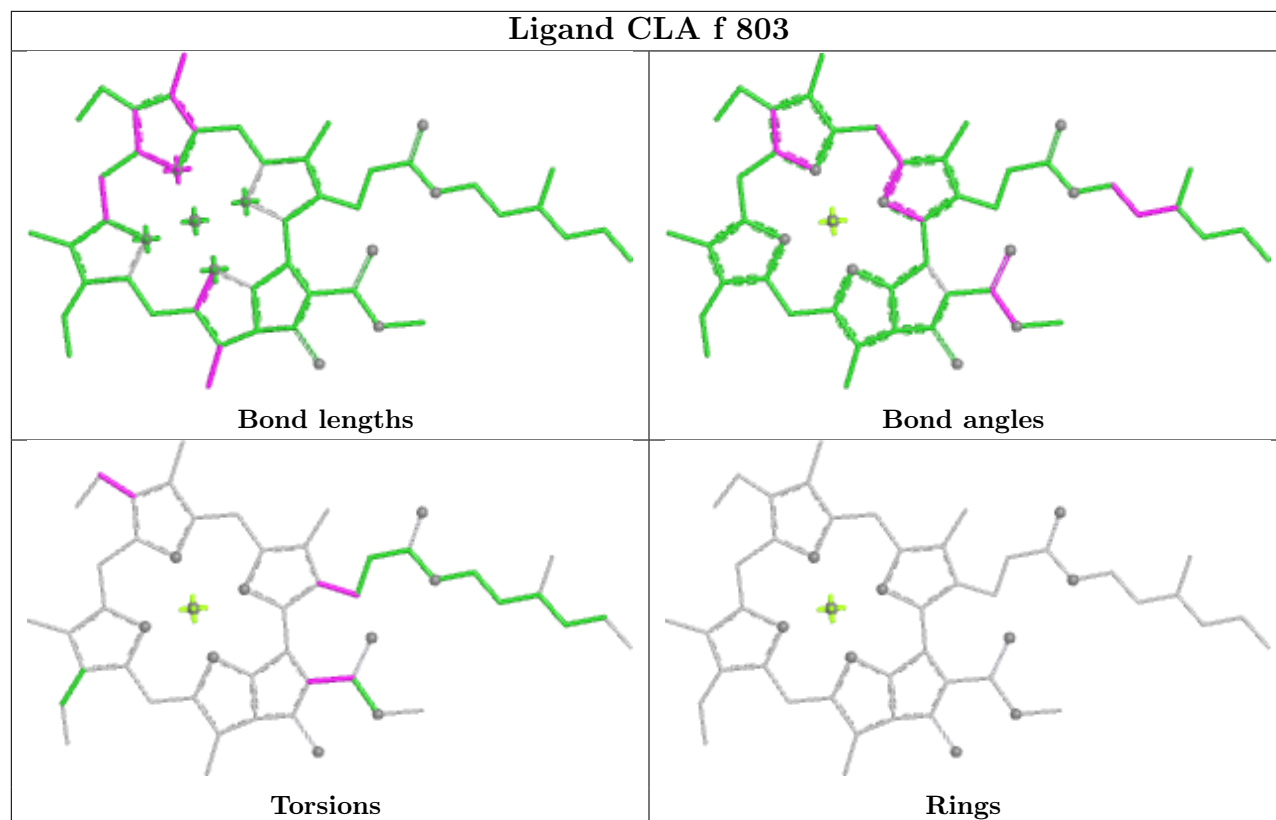




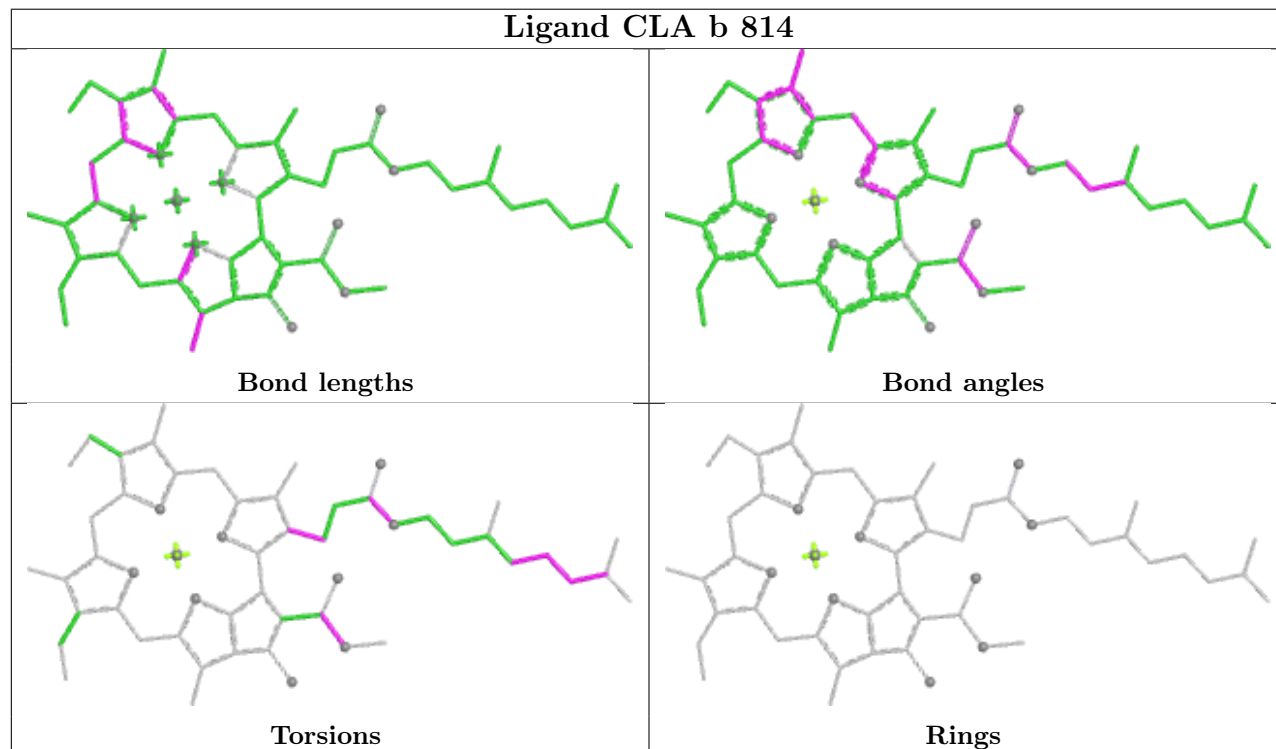




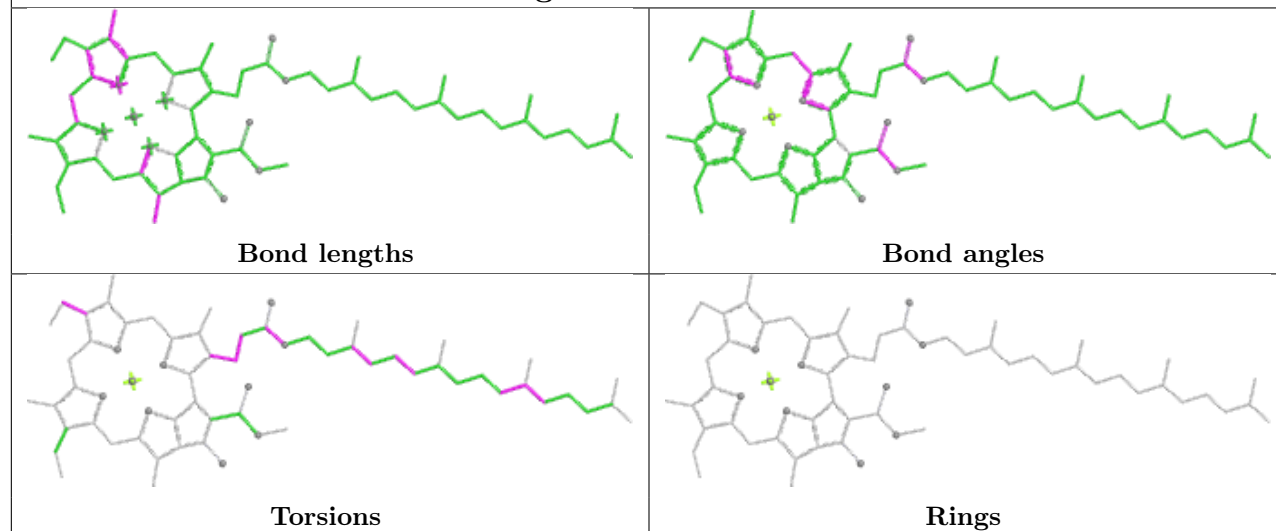
Ligand CLA f 803



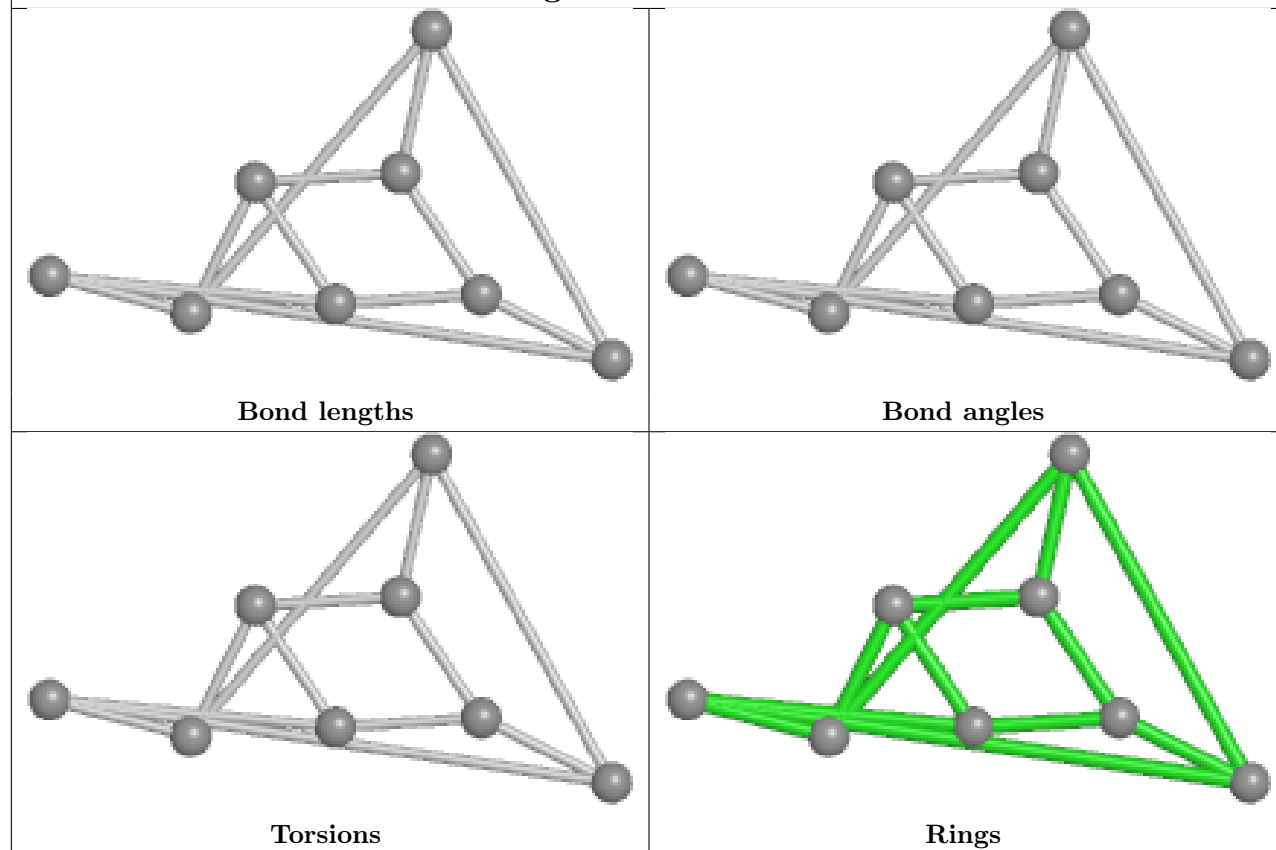
Ligand CLA b 814



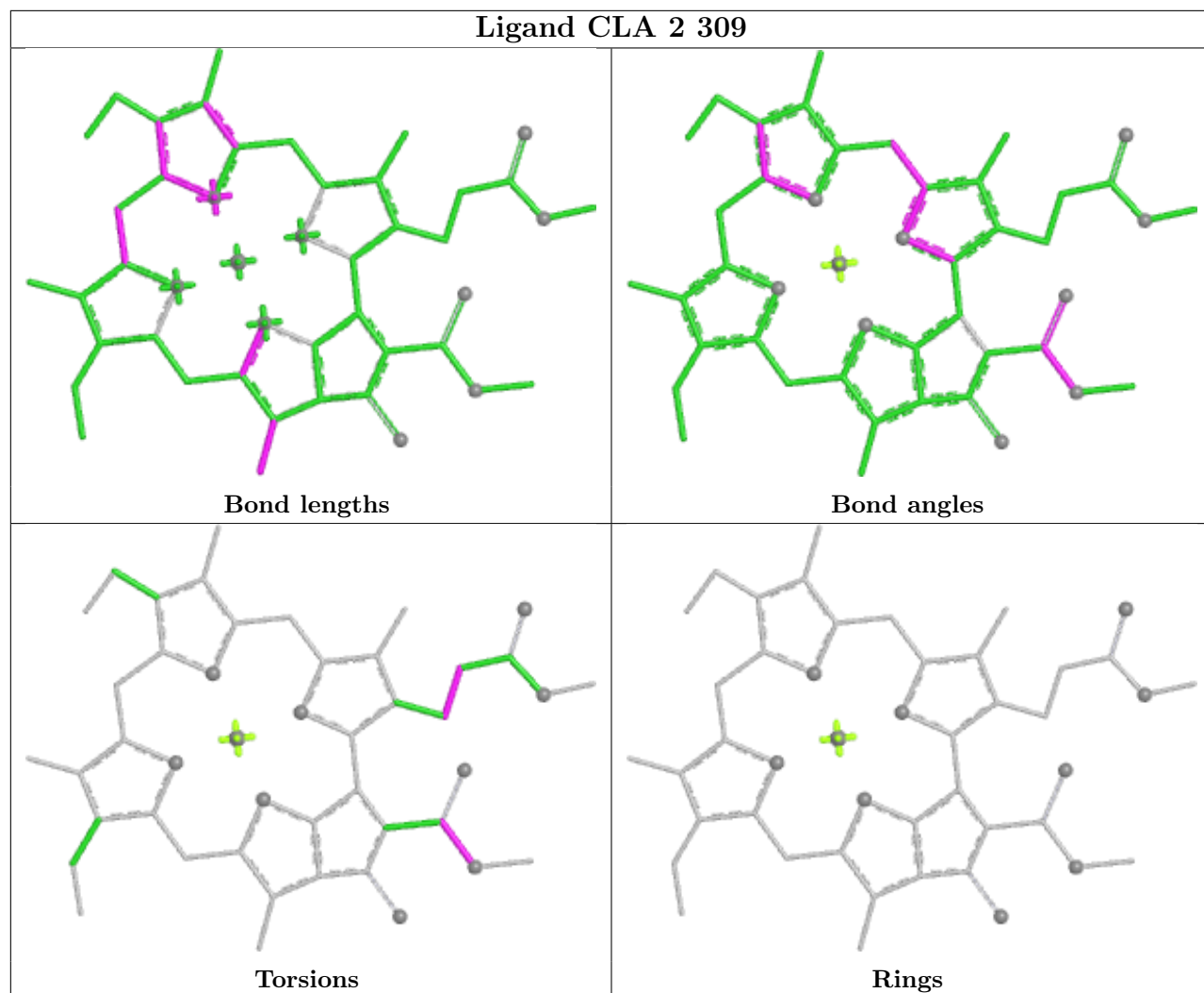
Ligand CLA b 828



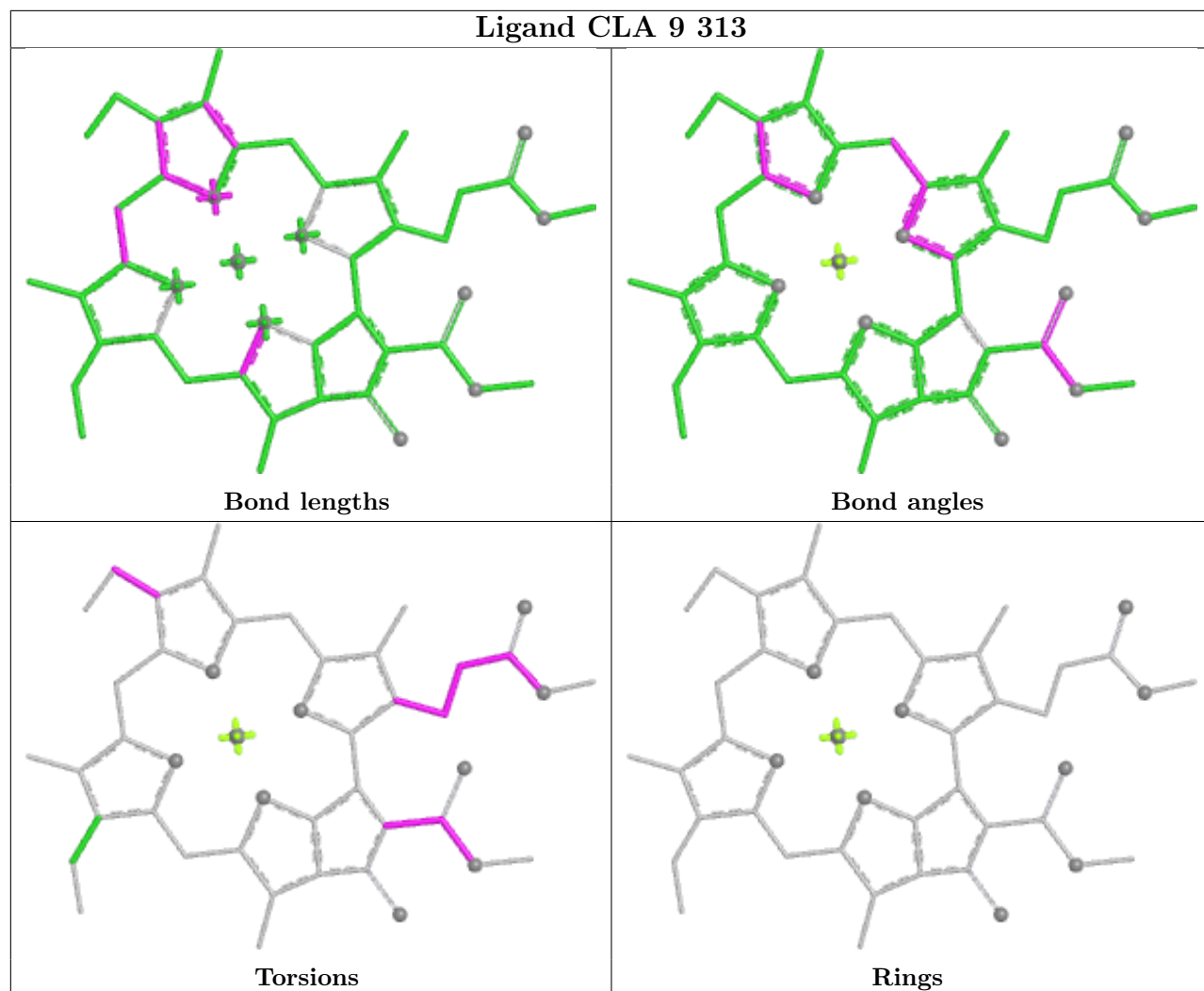
Ligand SF4 a 851



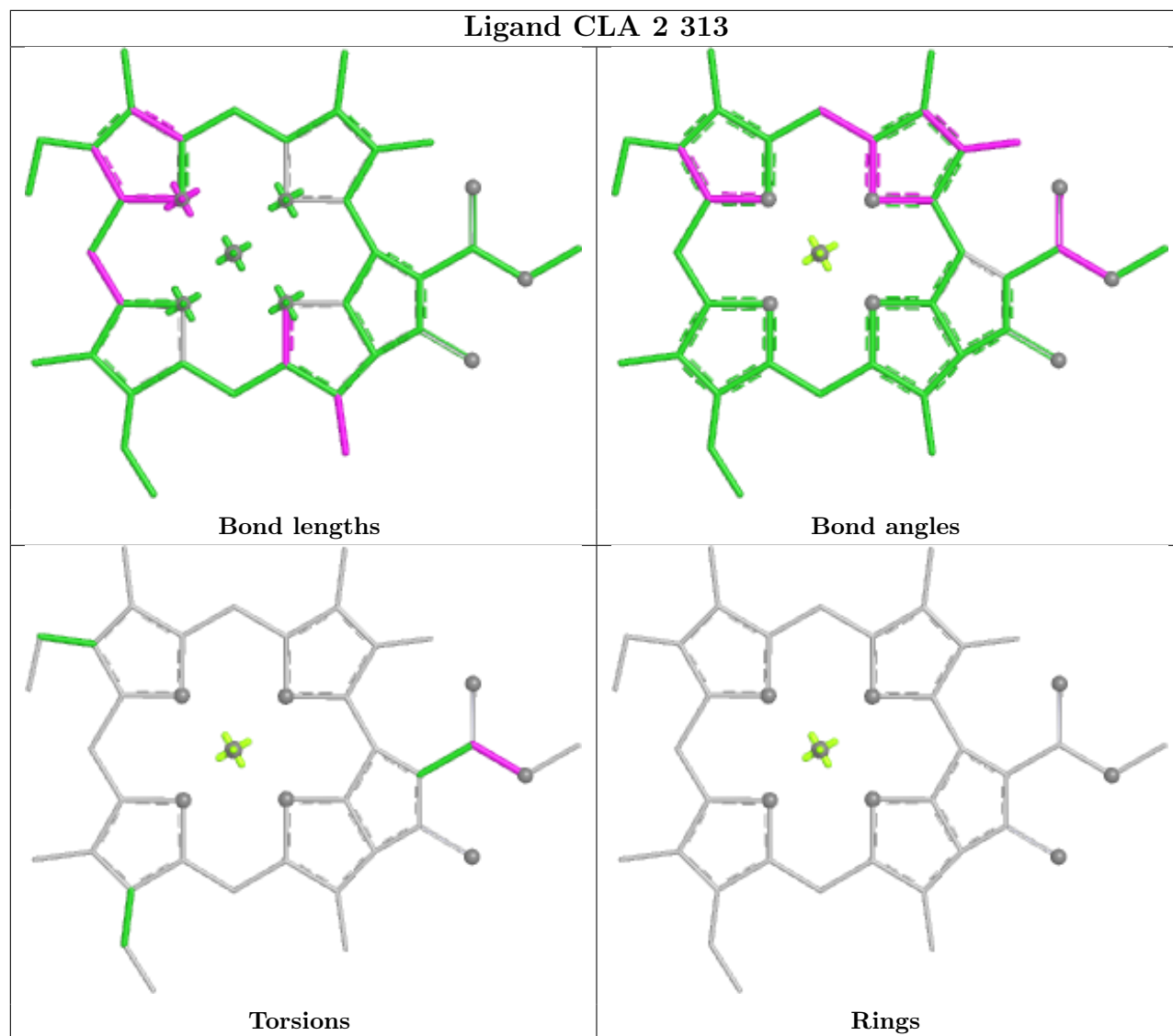
Ligand CLA 2 309



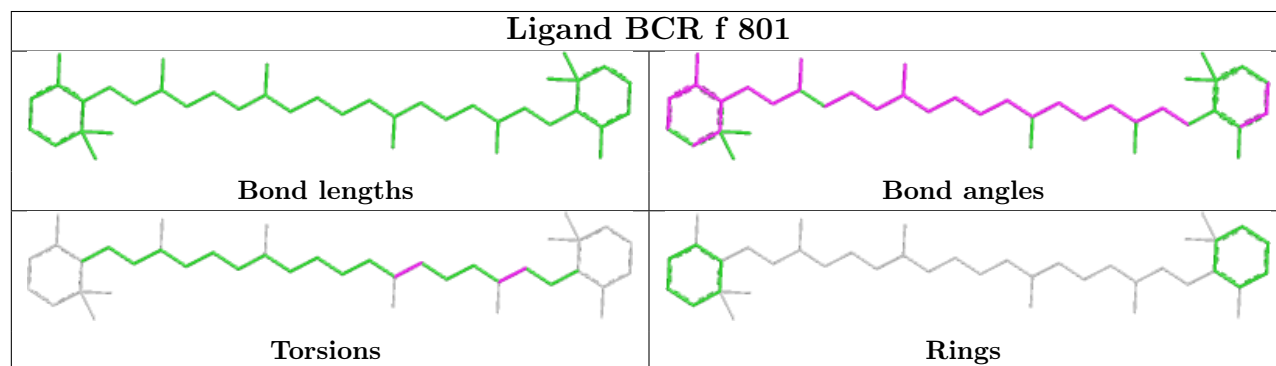
Ligand CLA 9 313

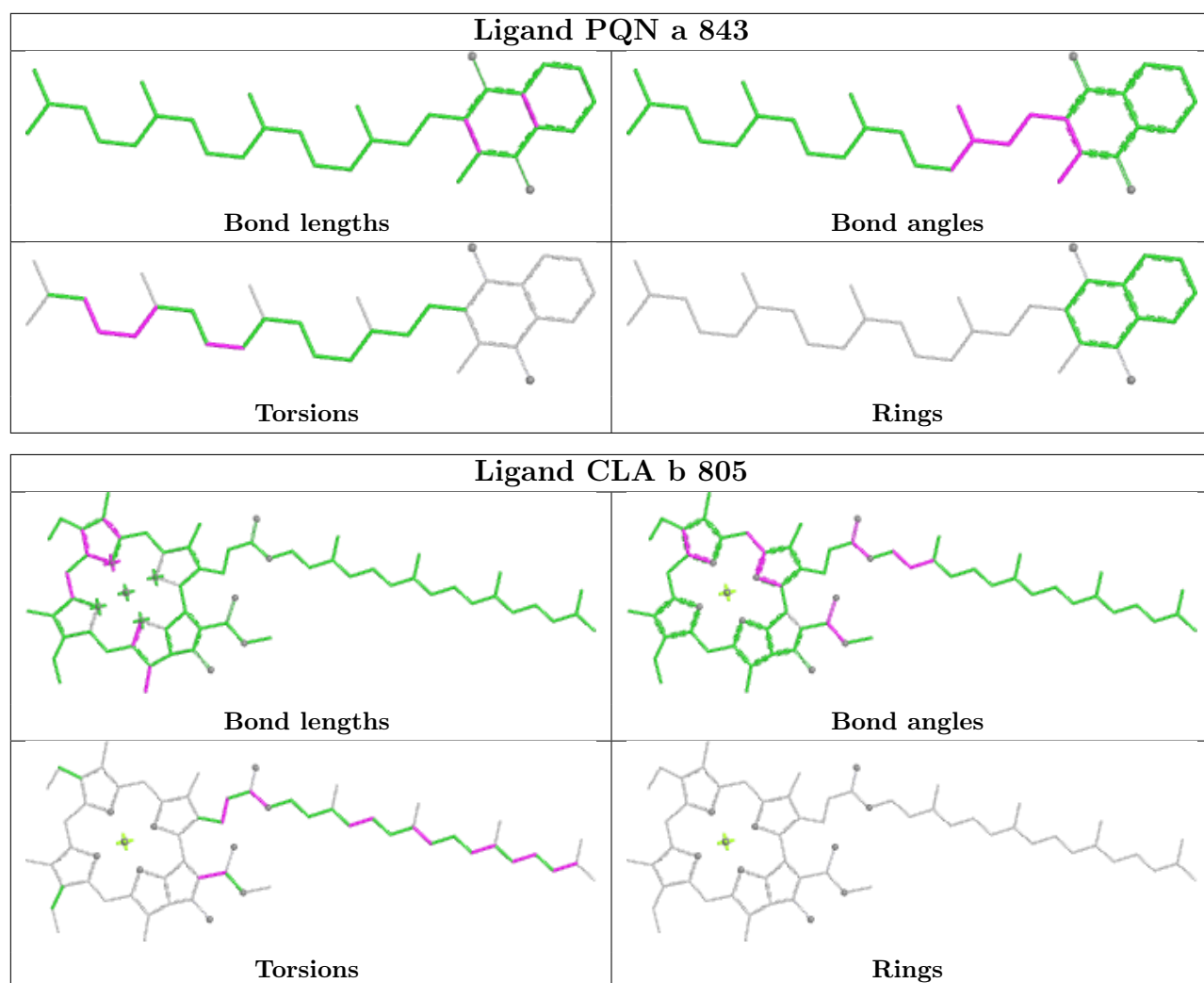


Ligand CLA 2 313

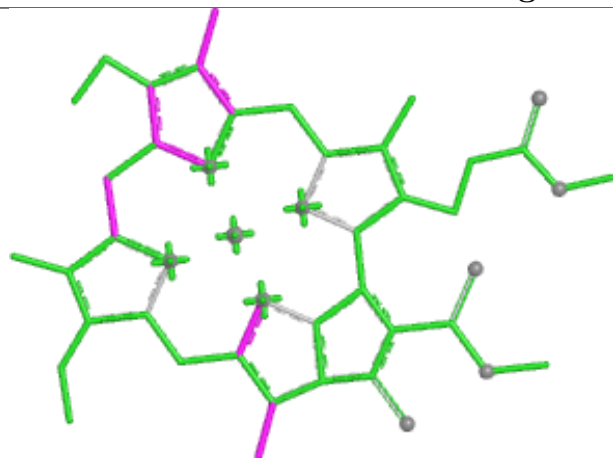


Ligand BCR f 801

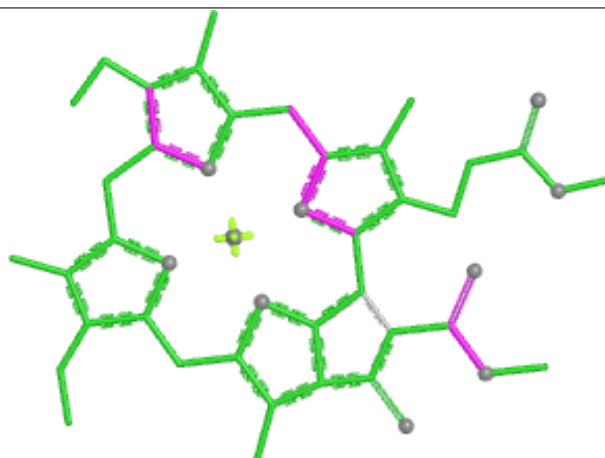




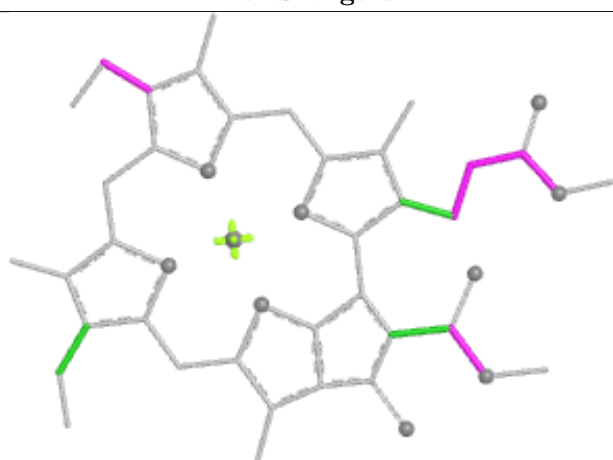
Ligand CLA 5 310



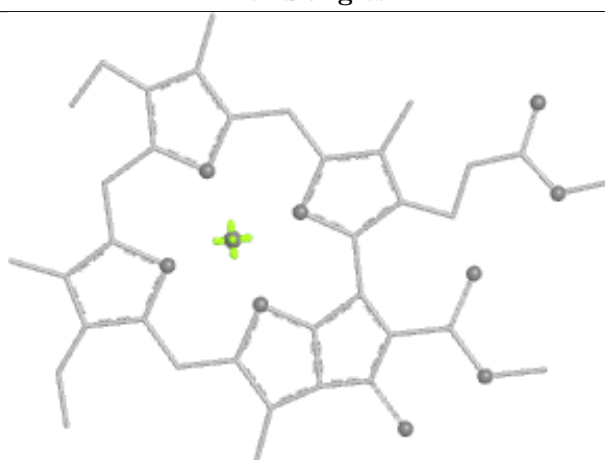
Bond lengths



Bond angles

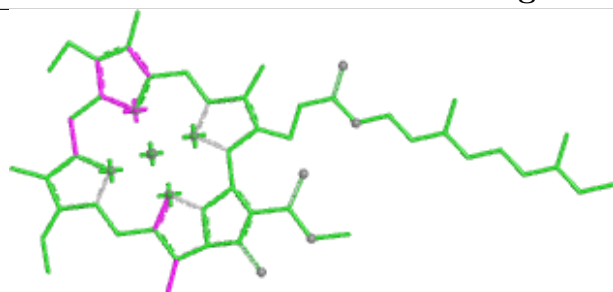


Torsions

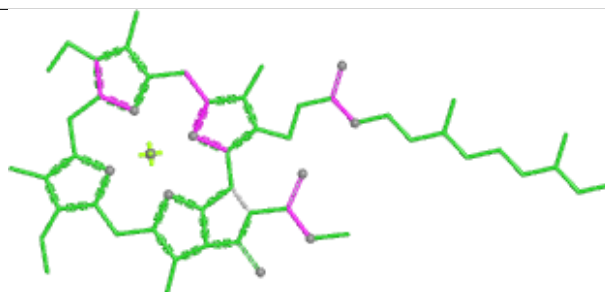


Rings

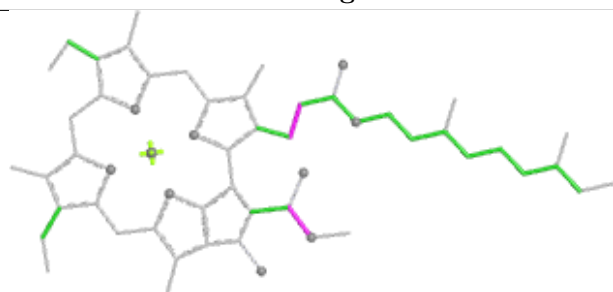
Ligand CLA 3 309



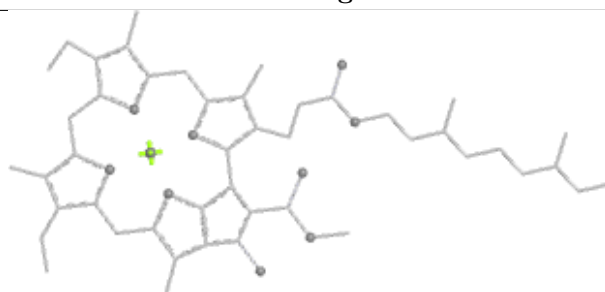
Bond lengths



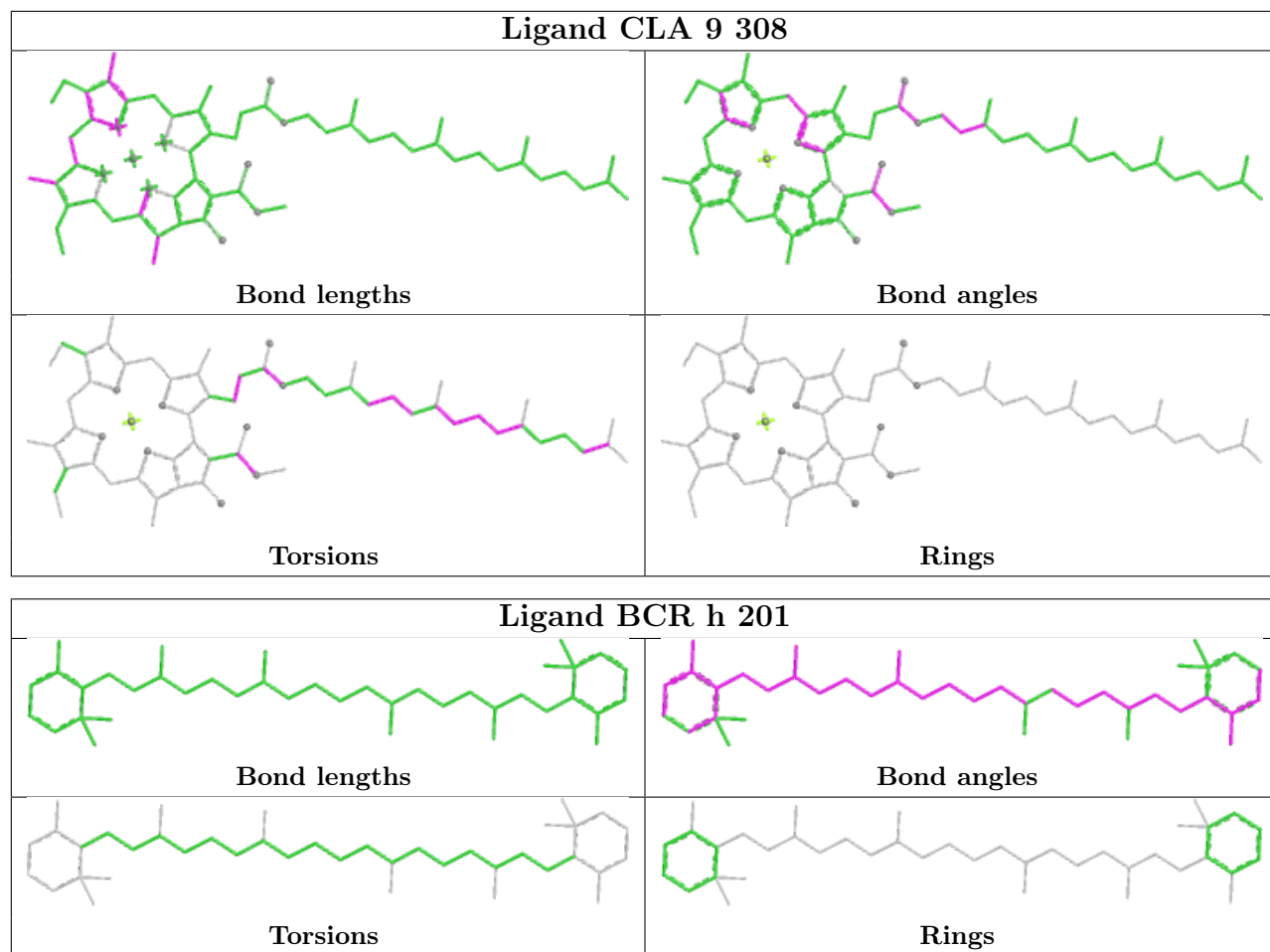
Bond angles



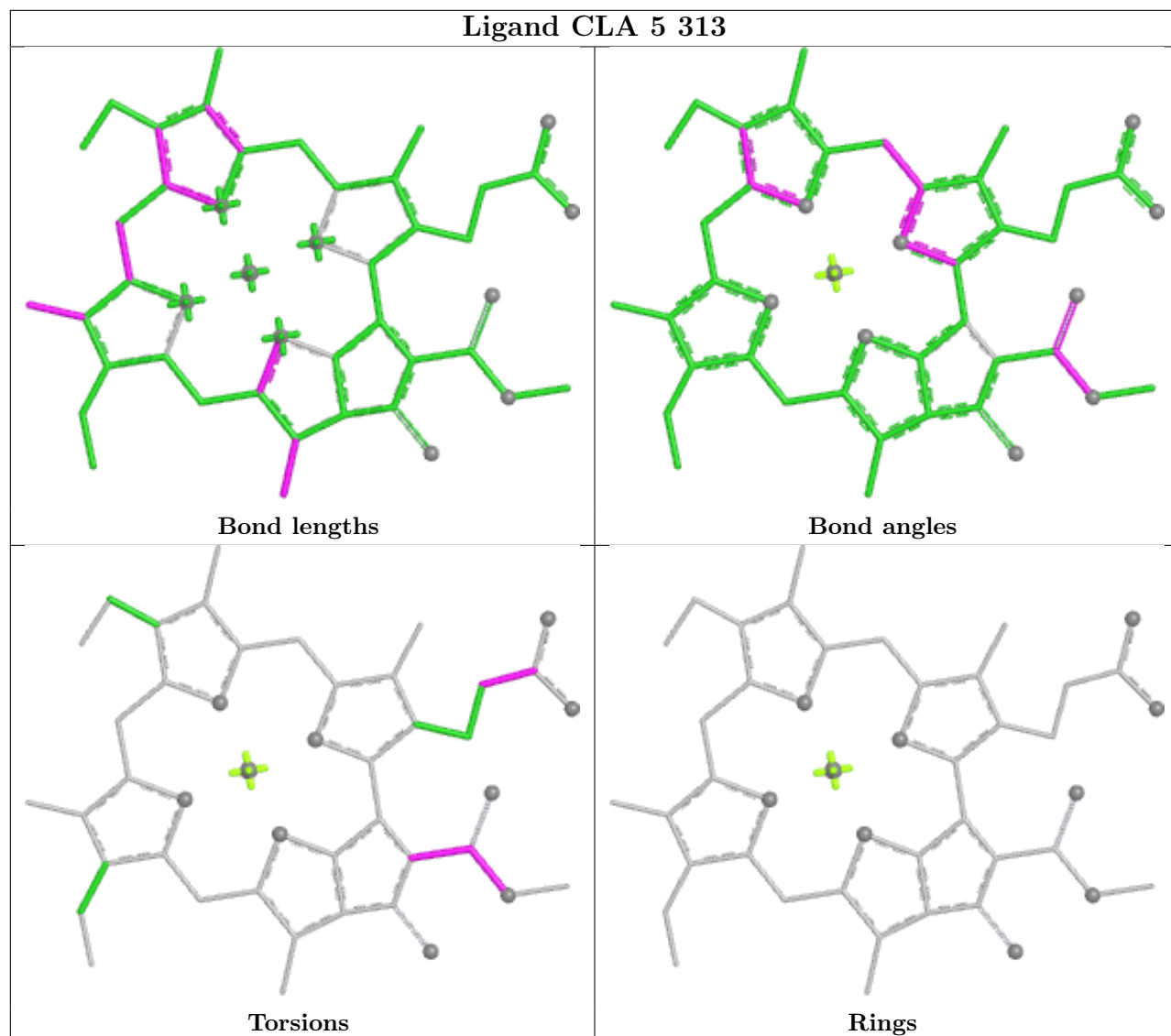
Torsions

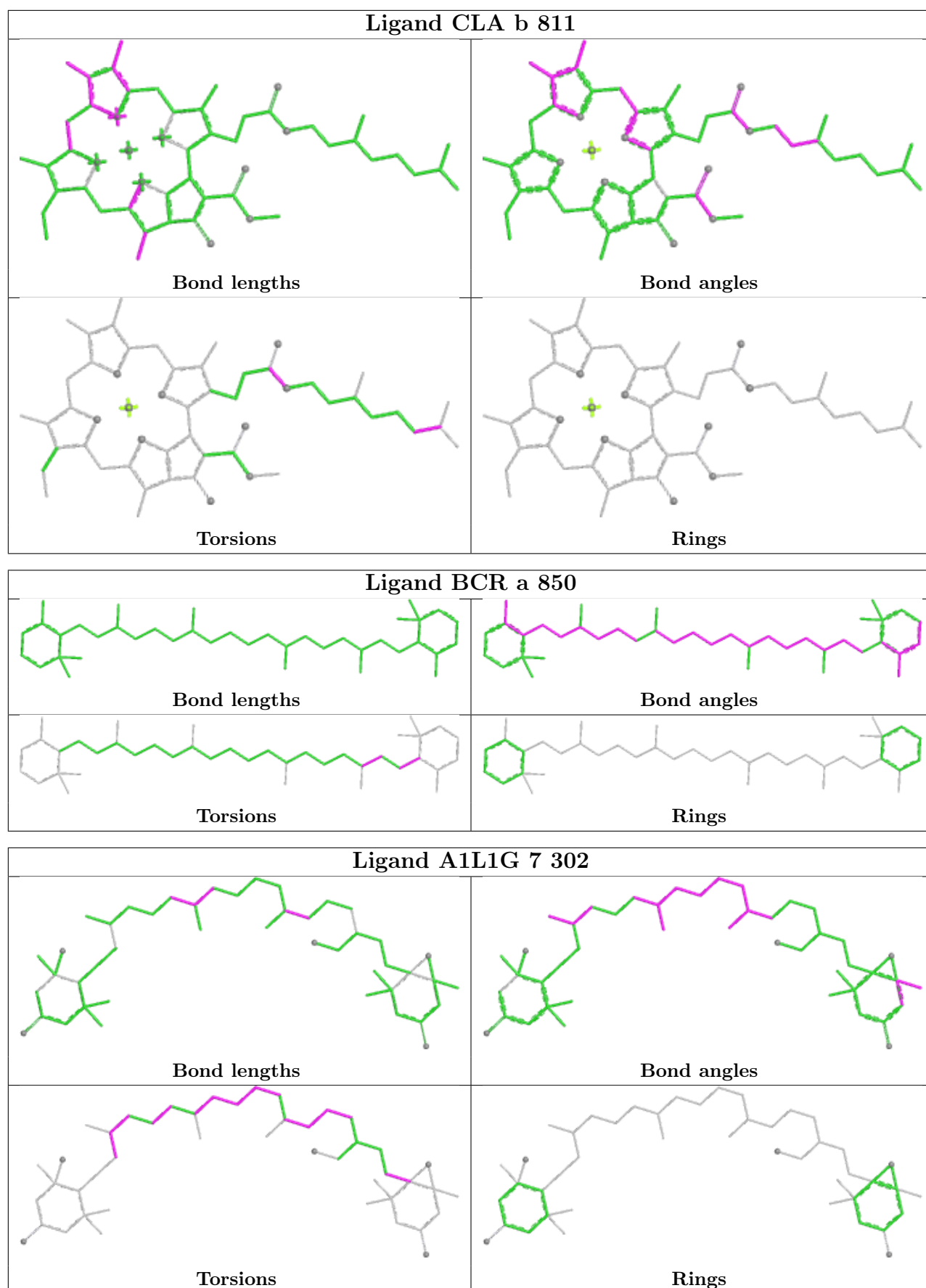


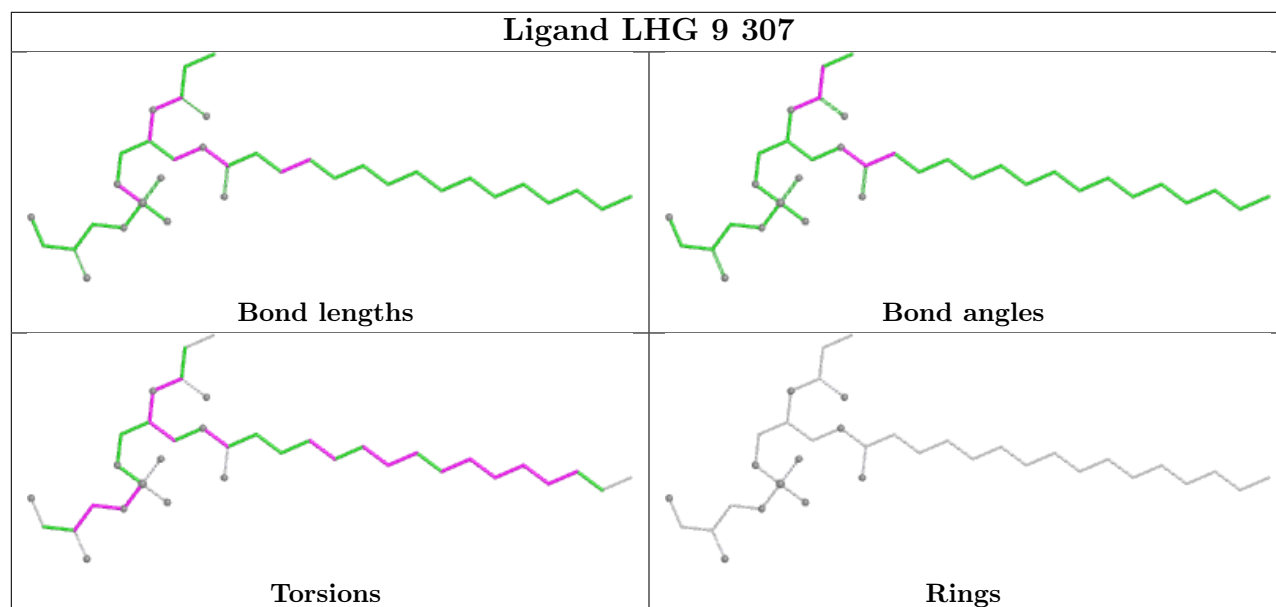
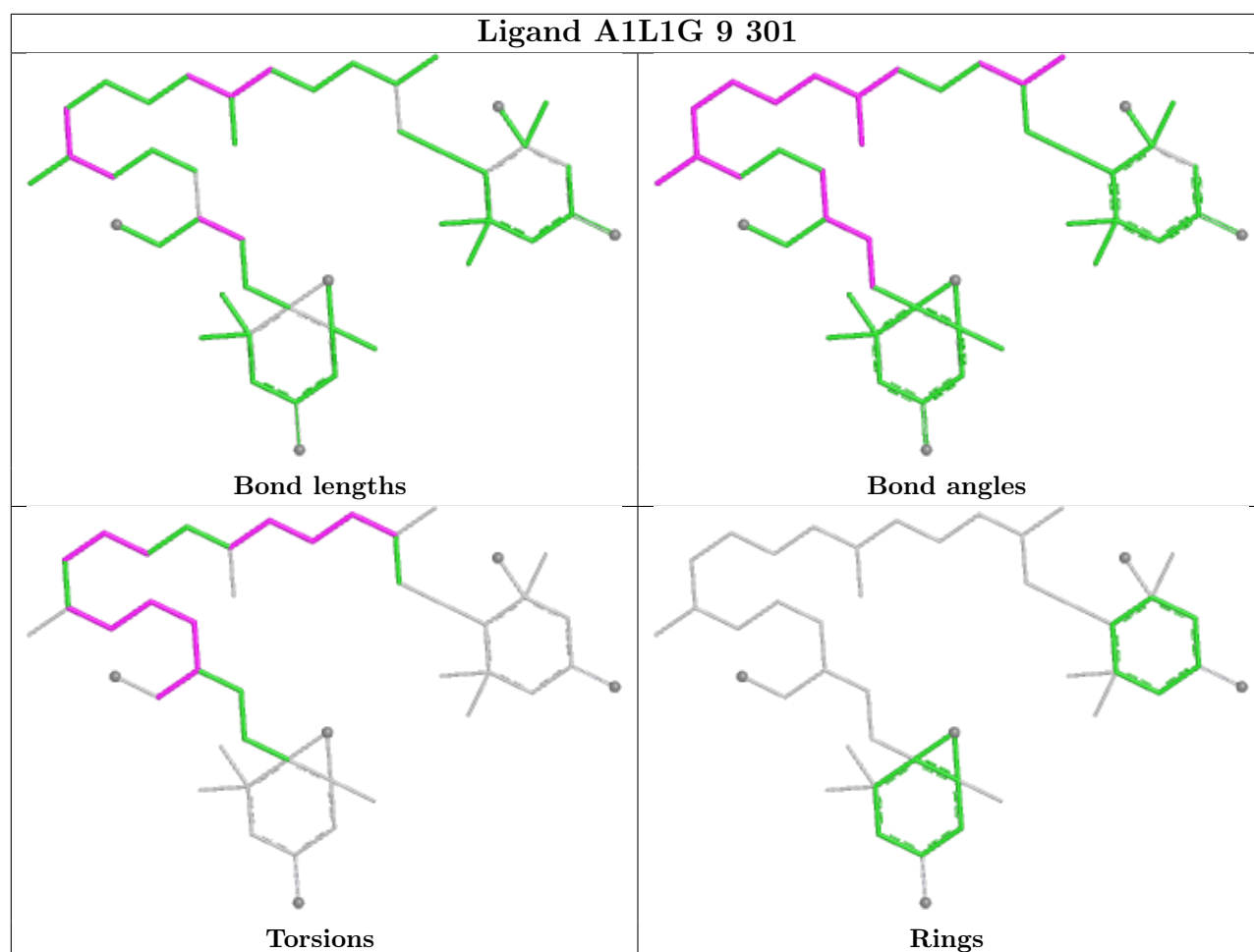
Rings



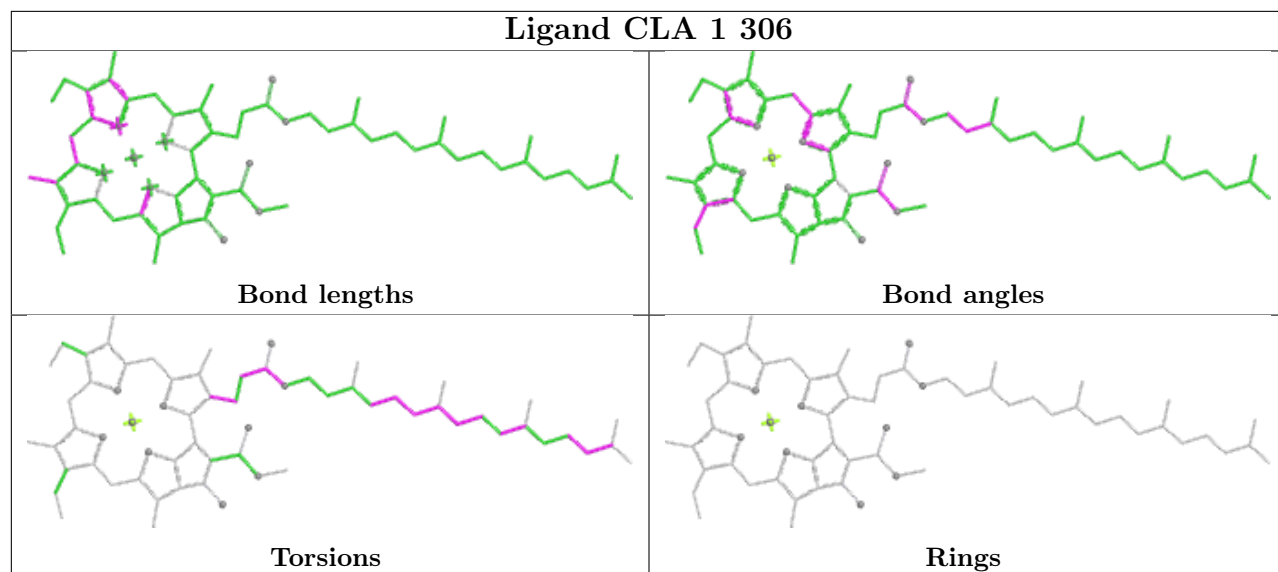
Ligand CLA 5 313



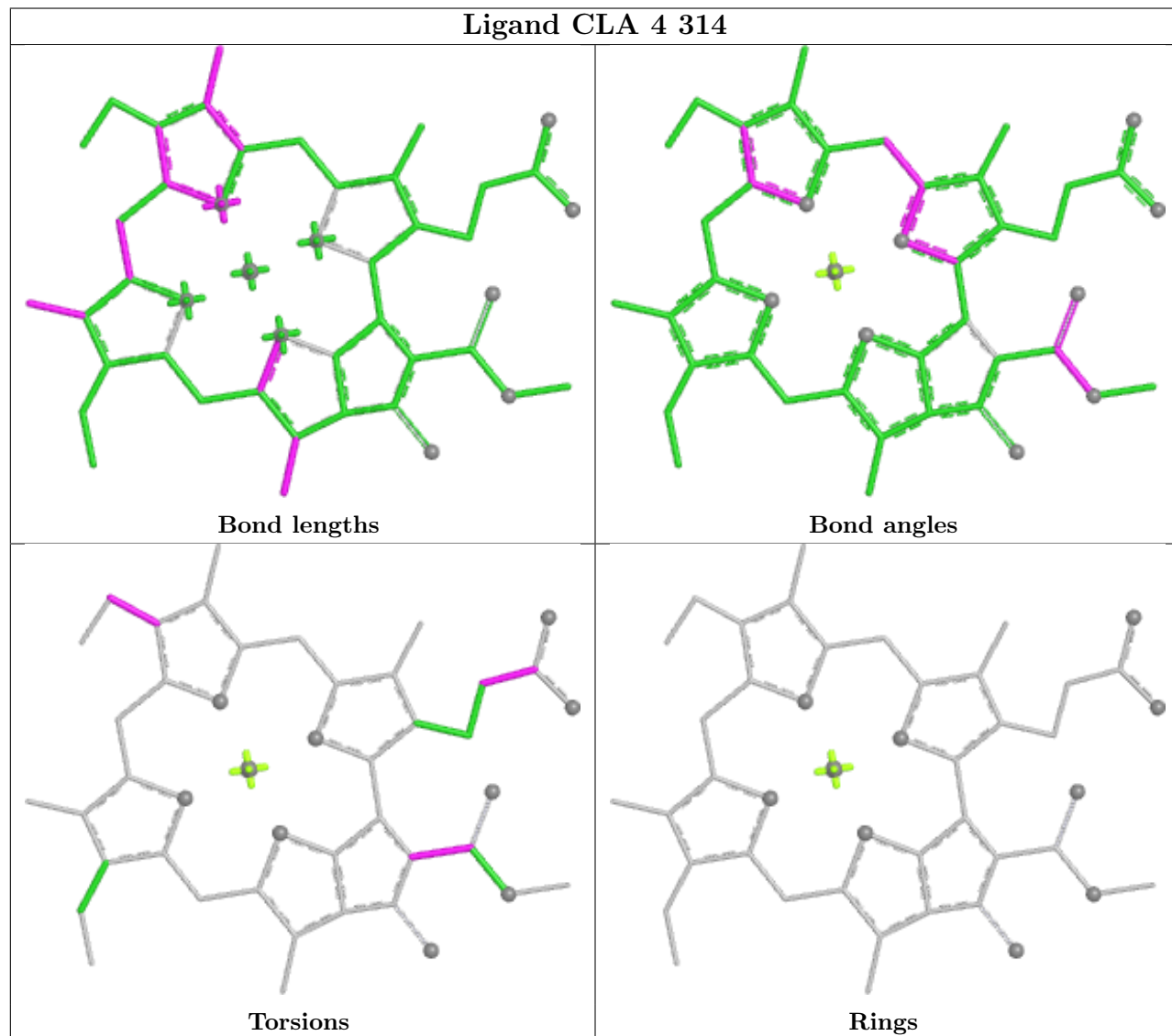




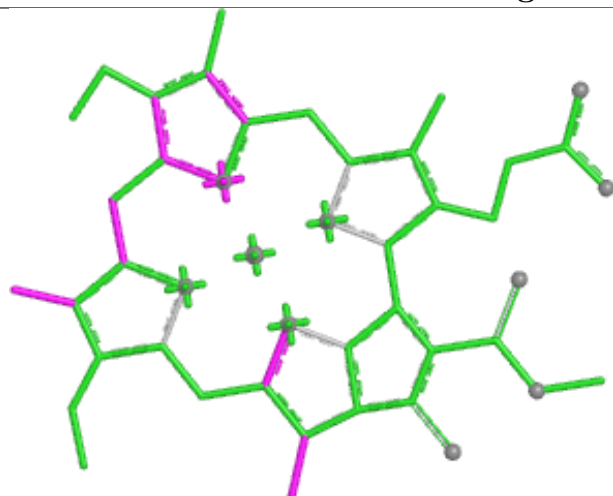
Ligand CLA 1 306



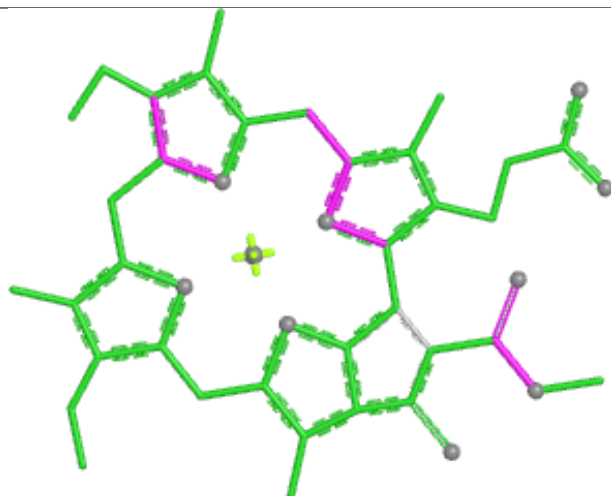
Ligand CLA 4 314



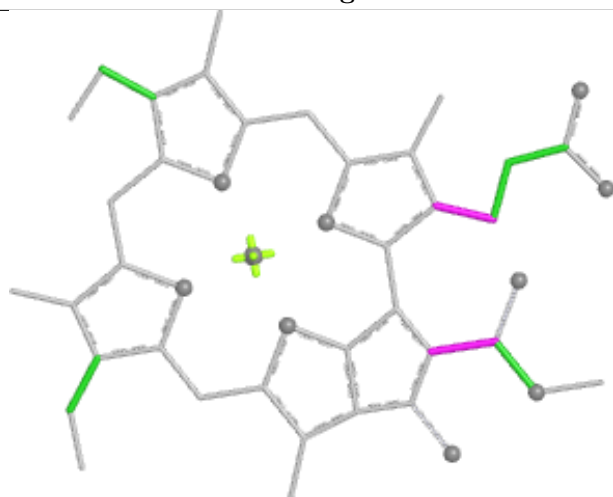
Ligand CLA b 815



Bond lengths



Bond angles

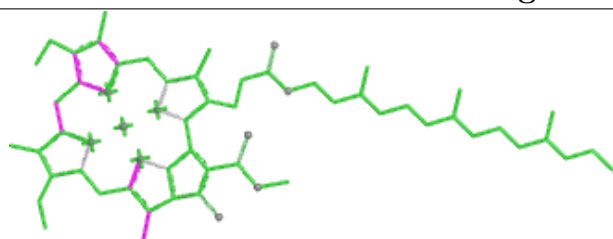


Torsions

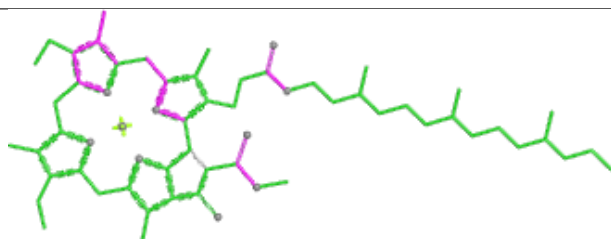


Rings

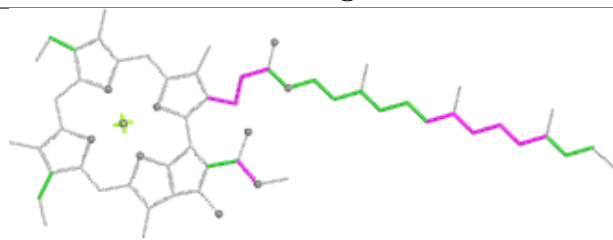
Ligand CLA a 829



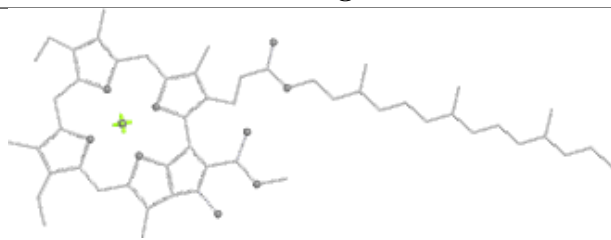
Bond lengths



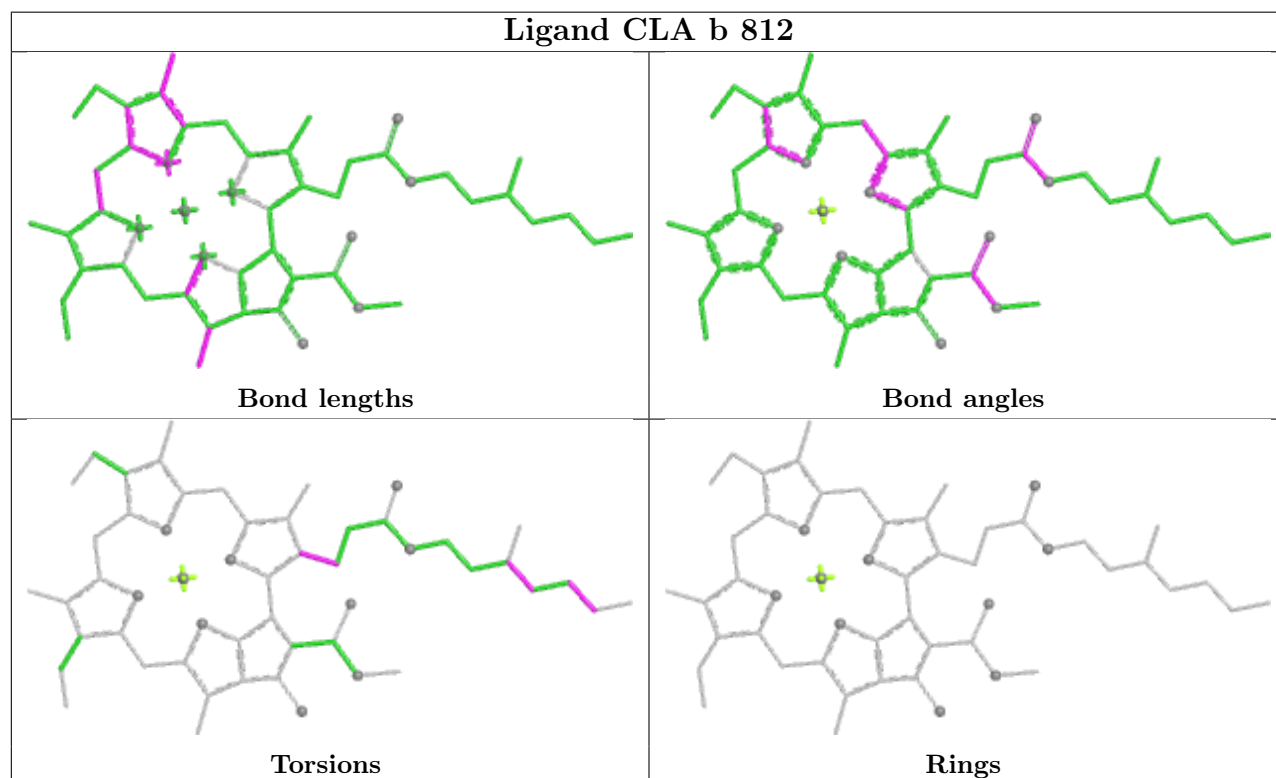
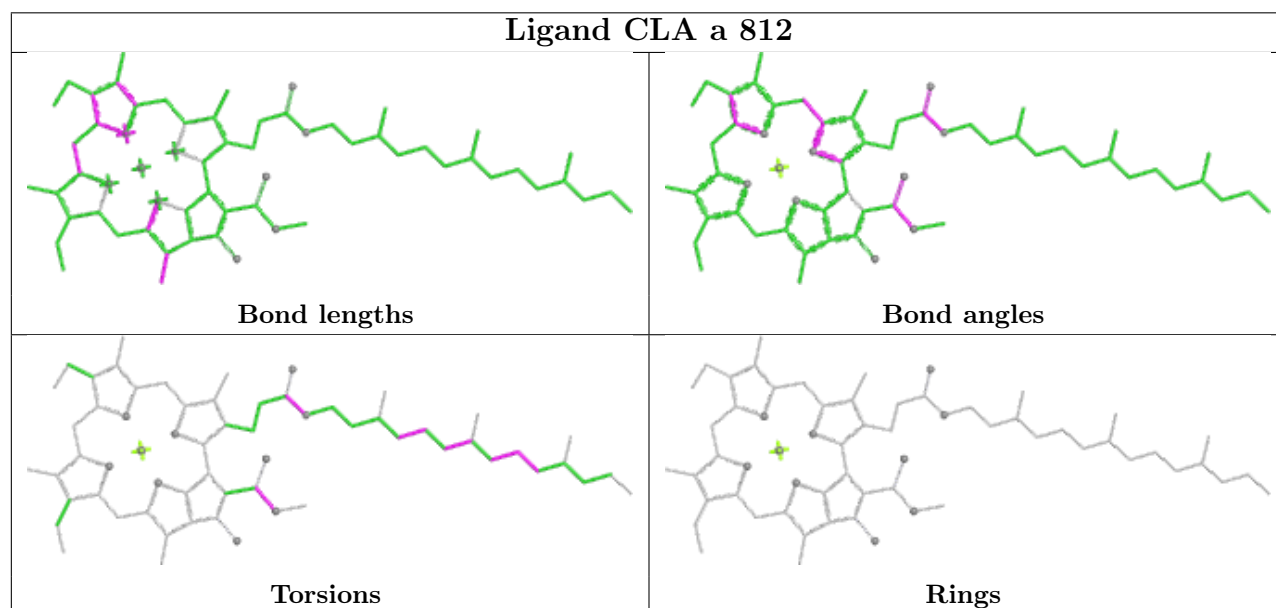
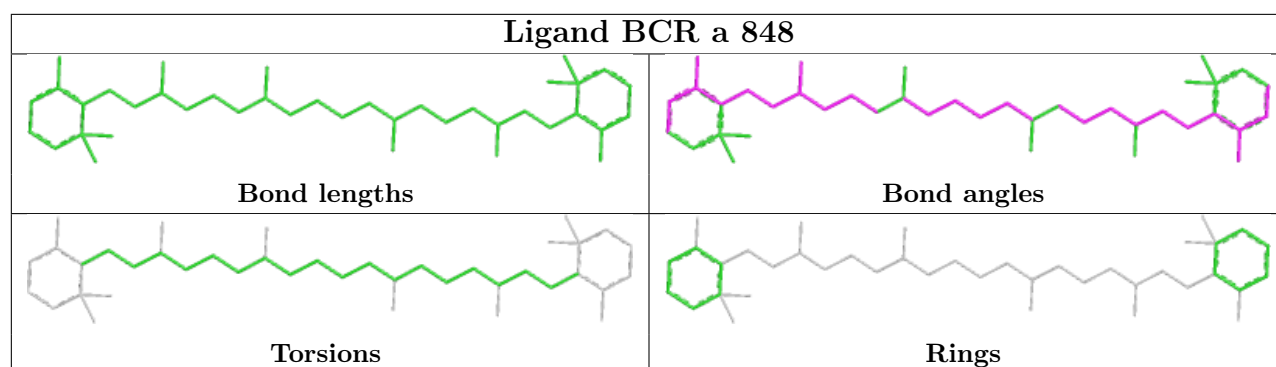
Bond angles

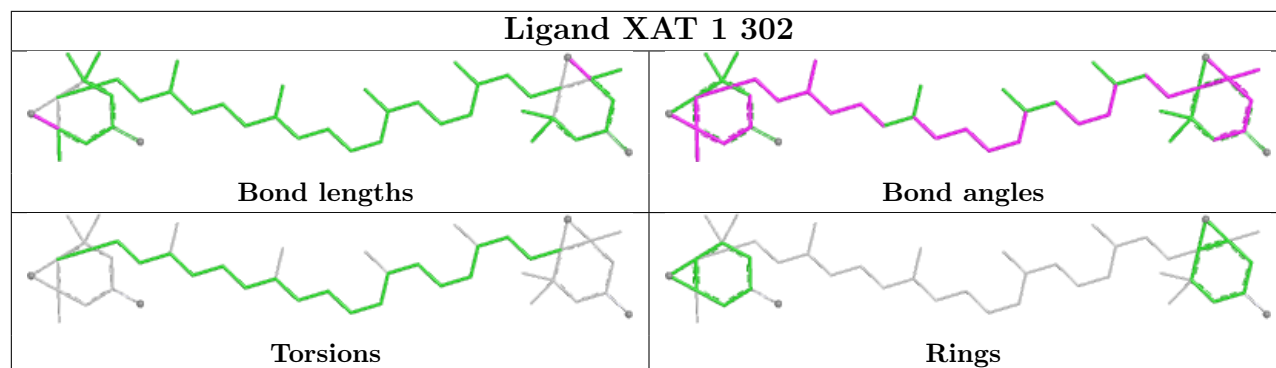
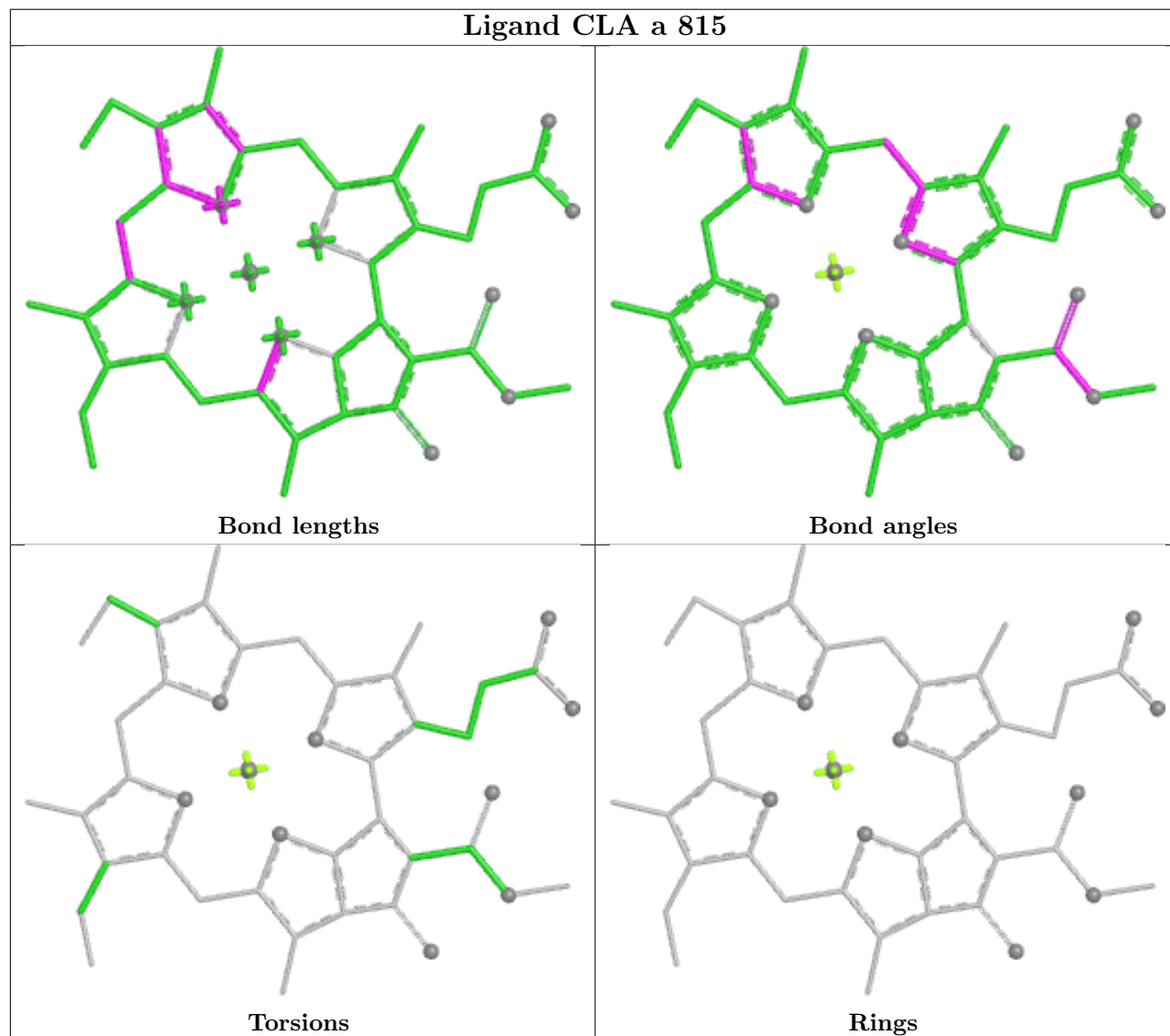


Torsions

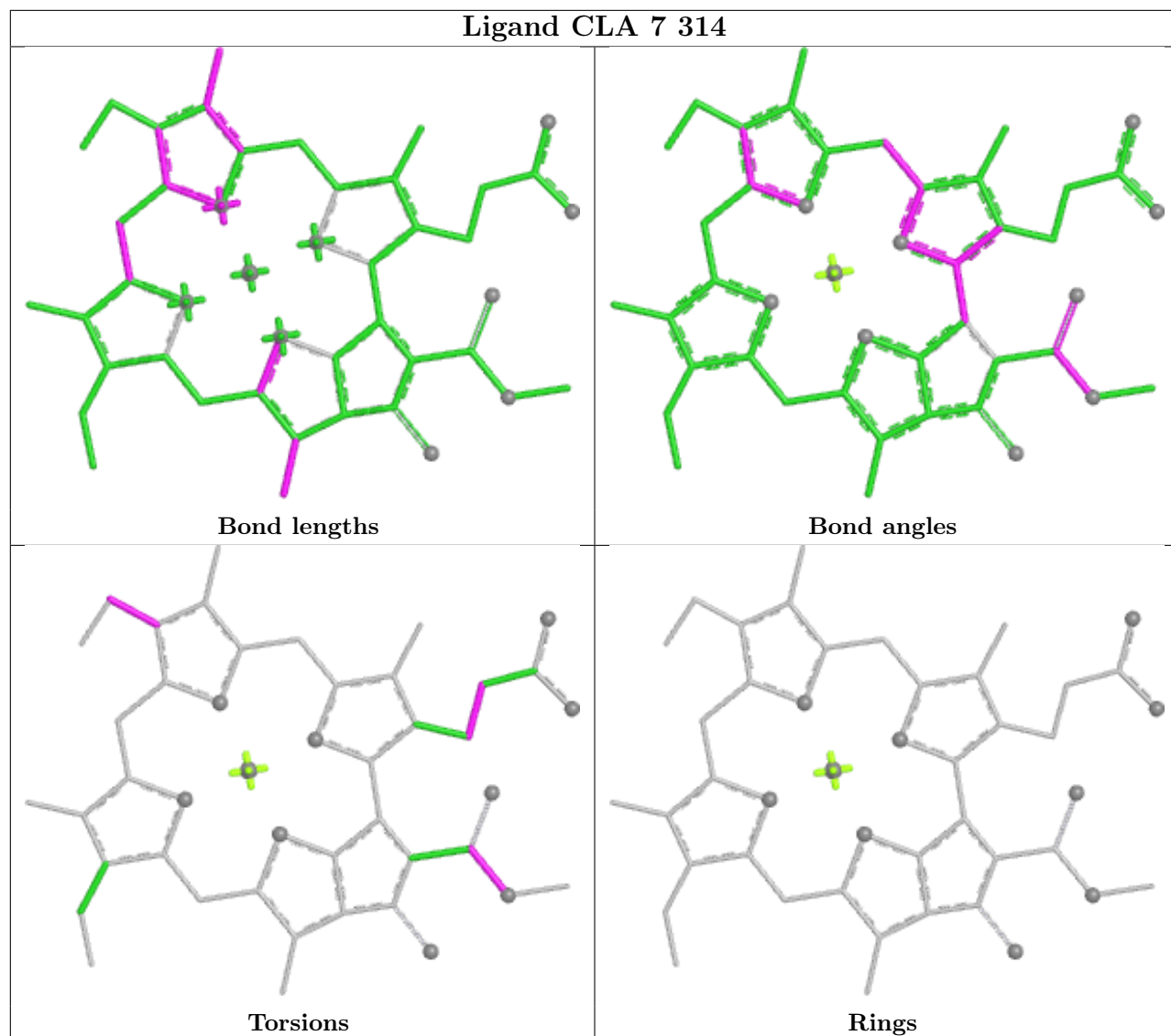


Rings

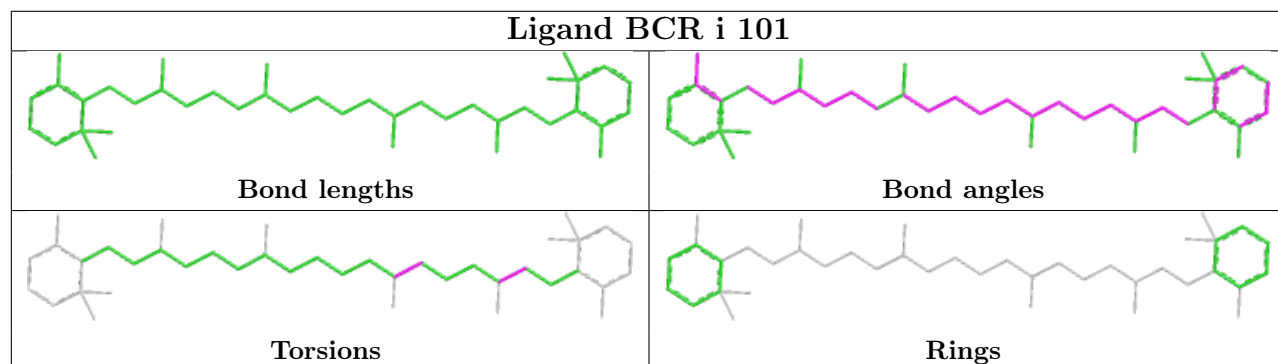


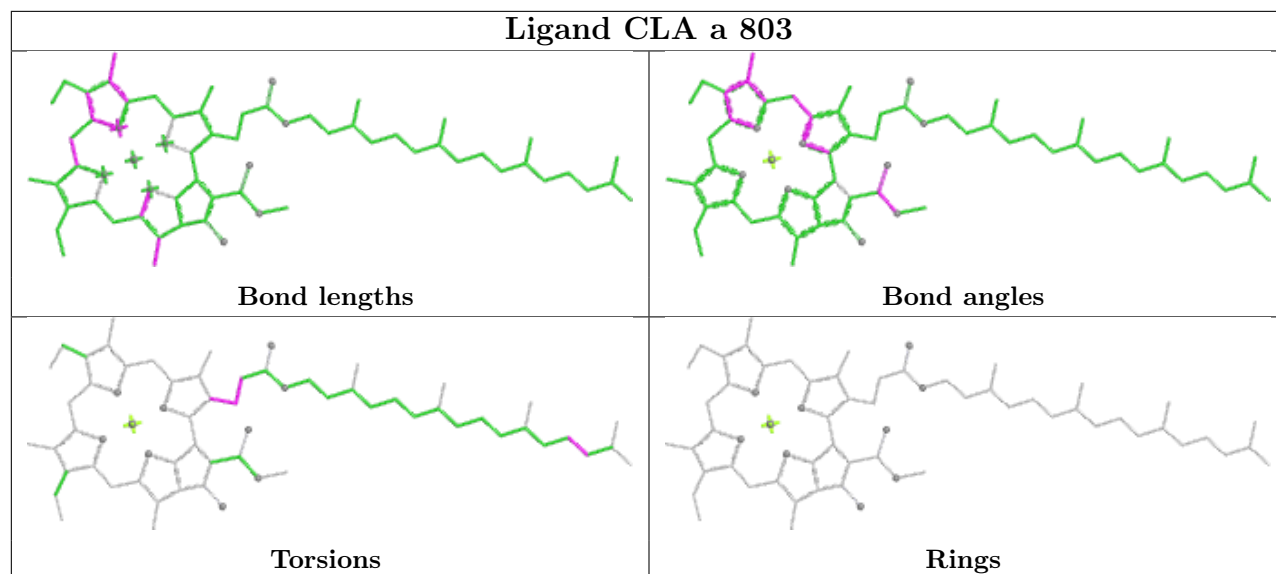
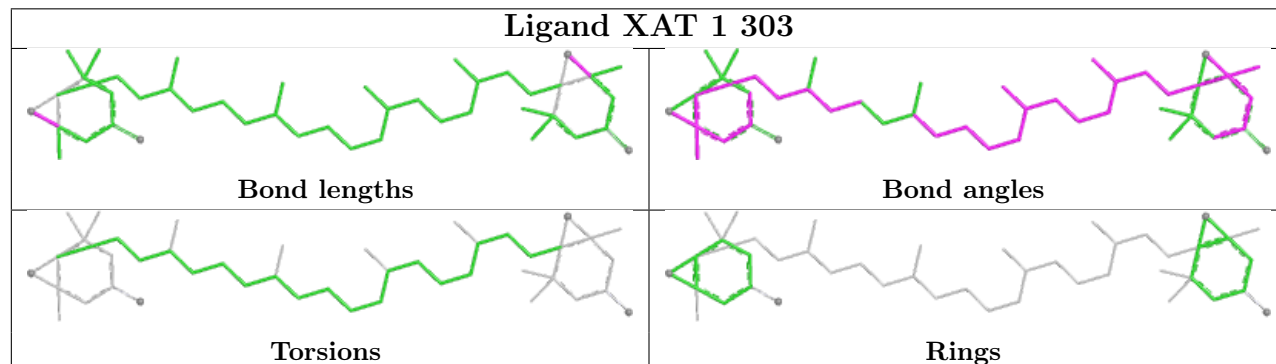
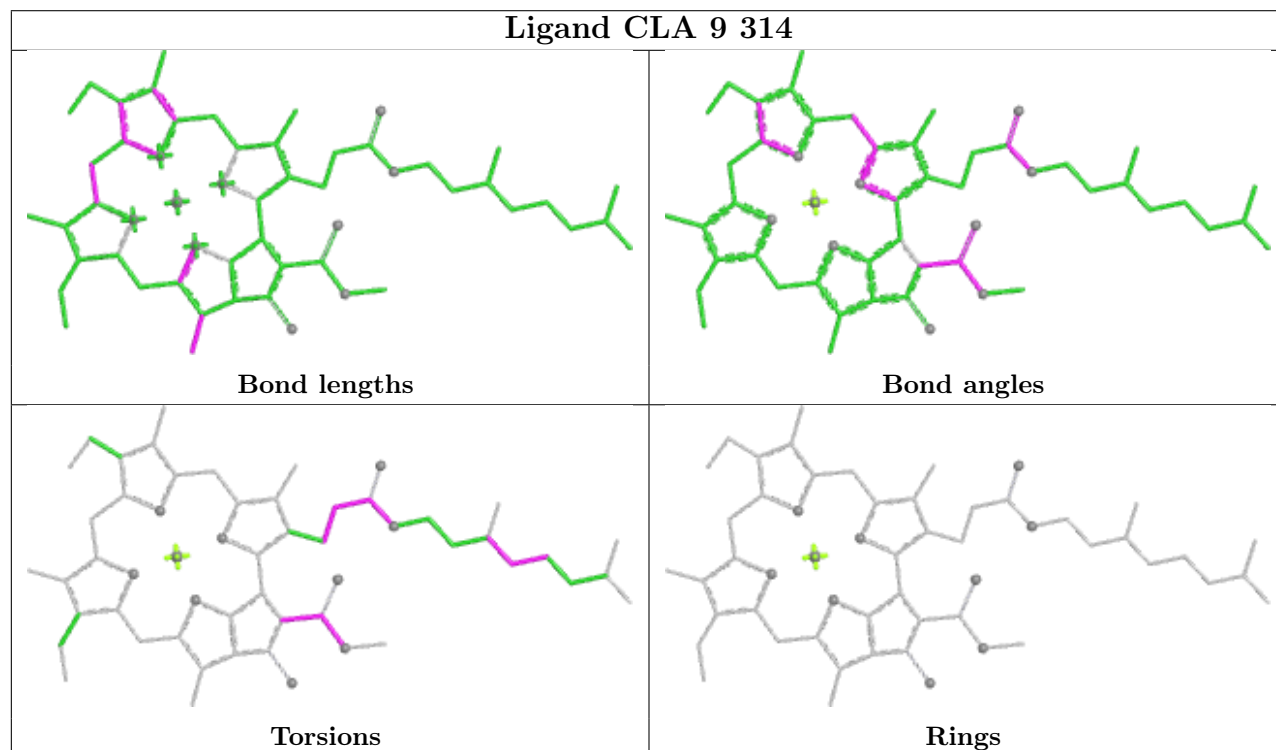
Ligand XAT 1 302**Ligand CLA a 815**

Ligand CLA 7 314

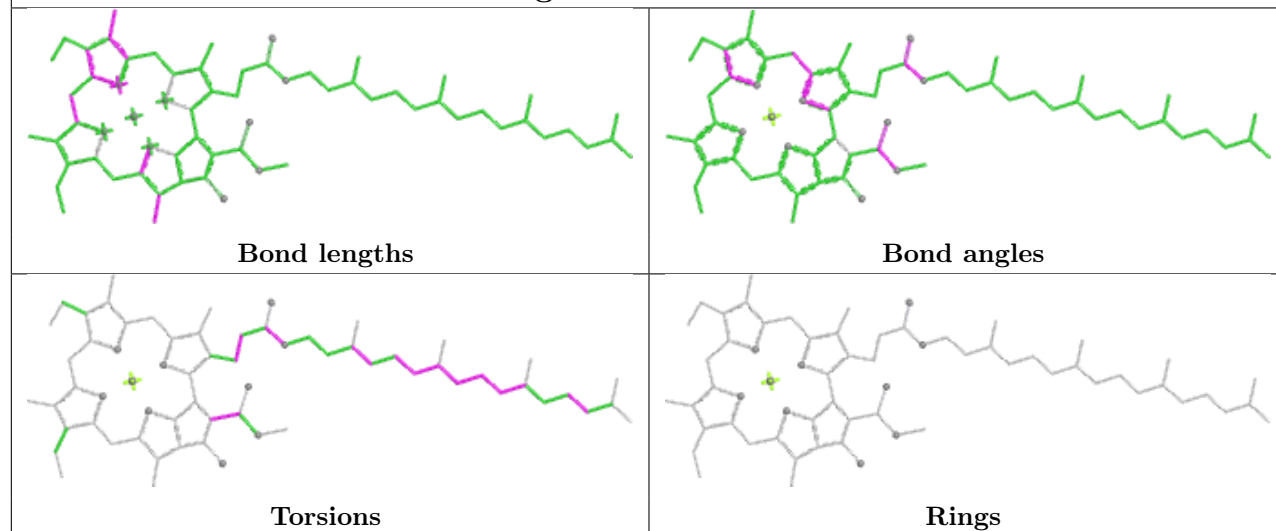


Ligand BCR i 101

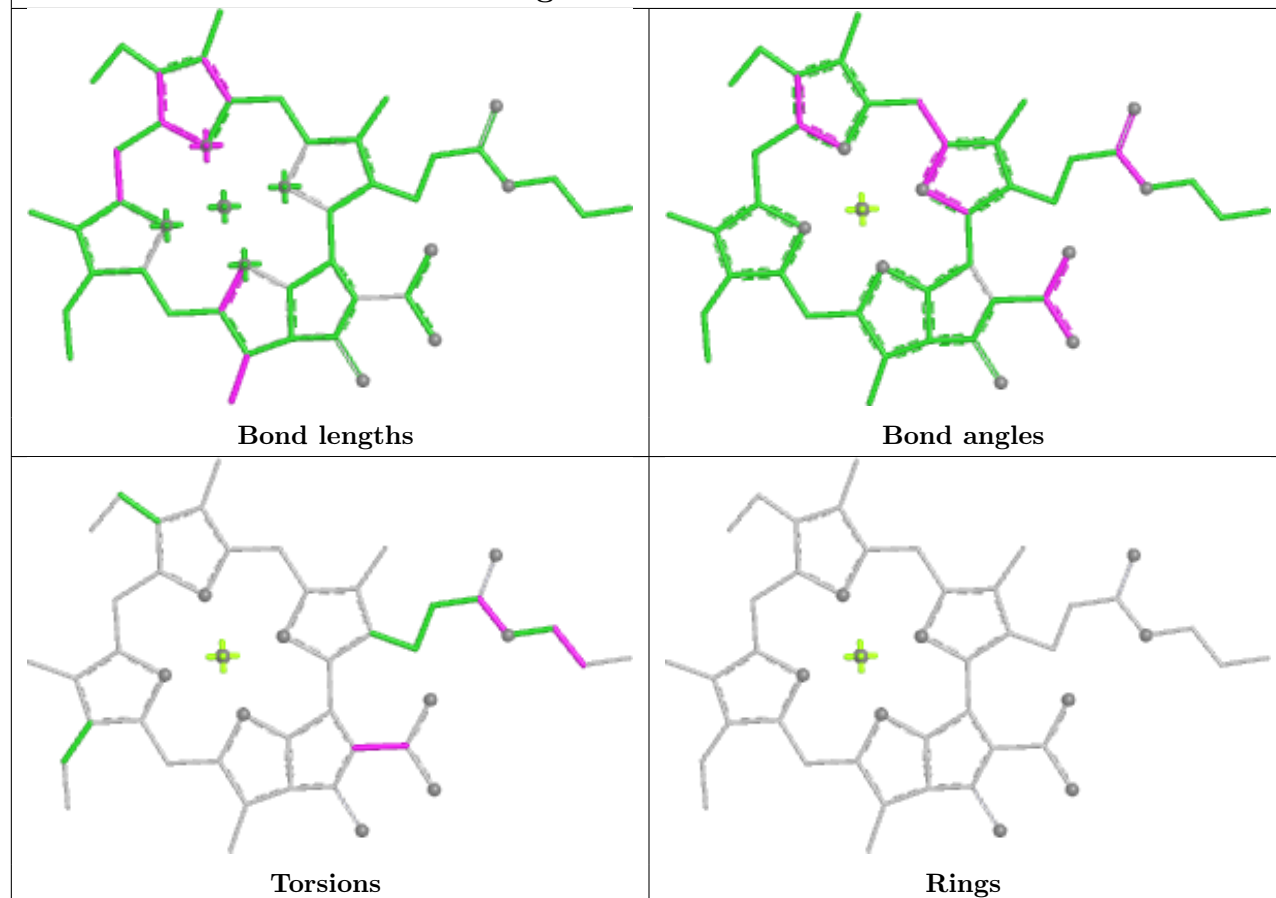


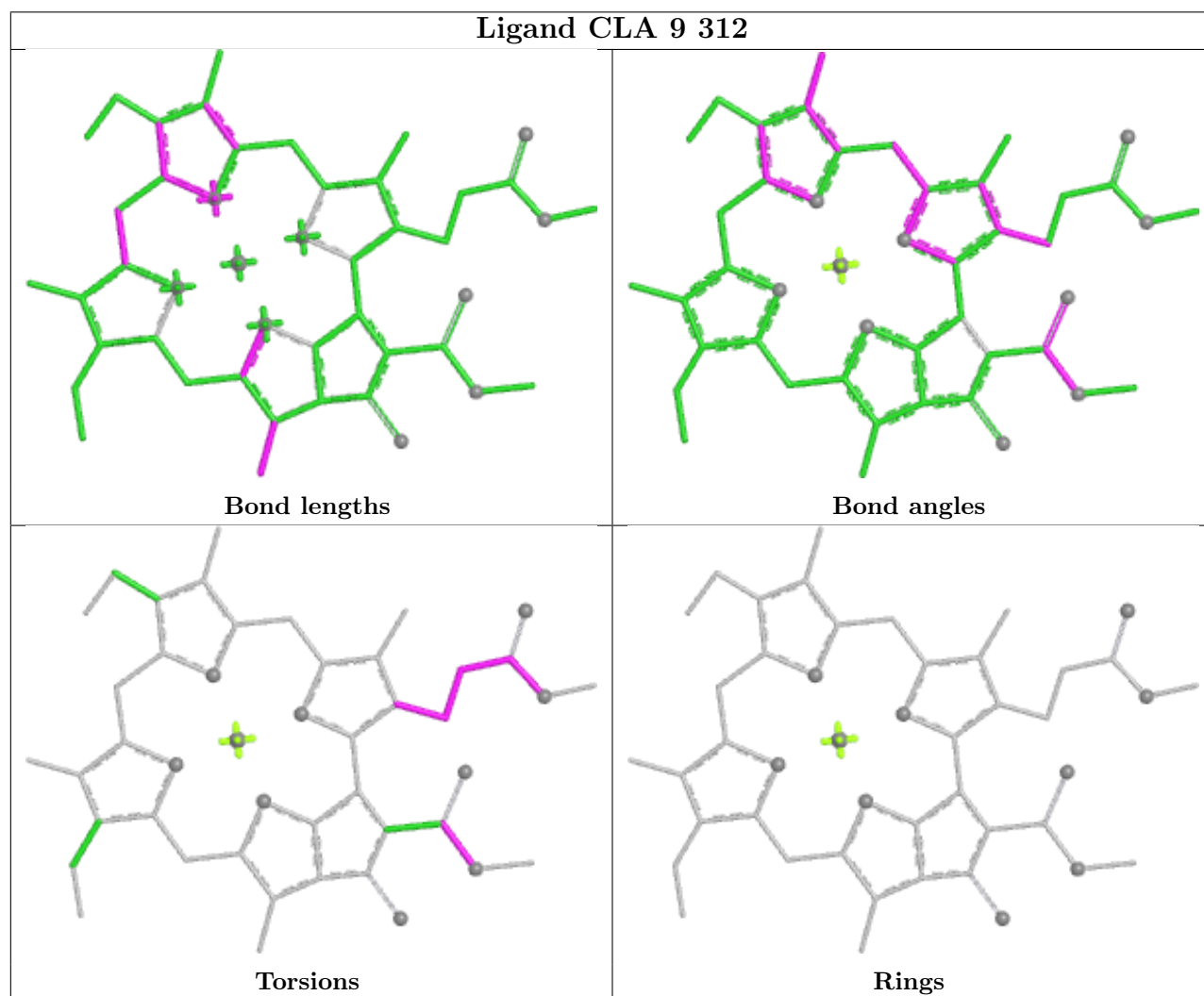
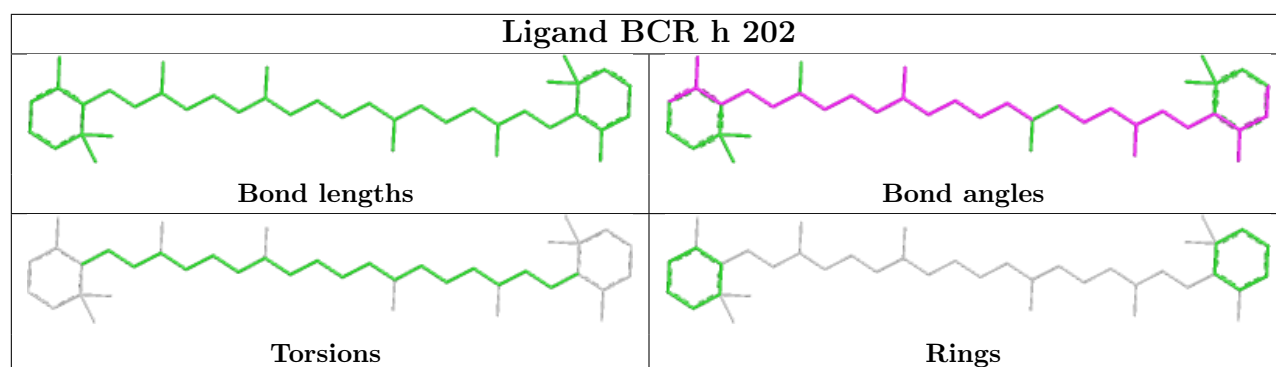
Ligand CLA a 803**Ligand XAT 1 303****Ligand CLA 9 314**

Ligand CLA b 824

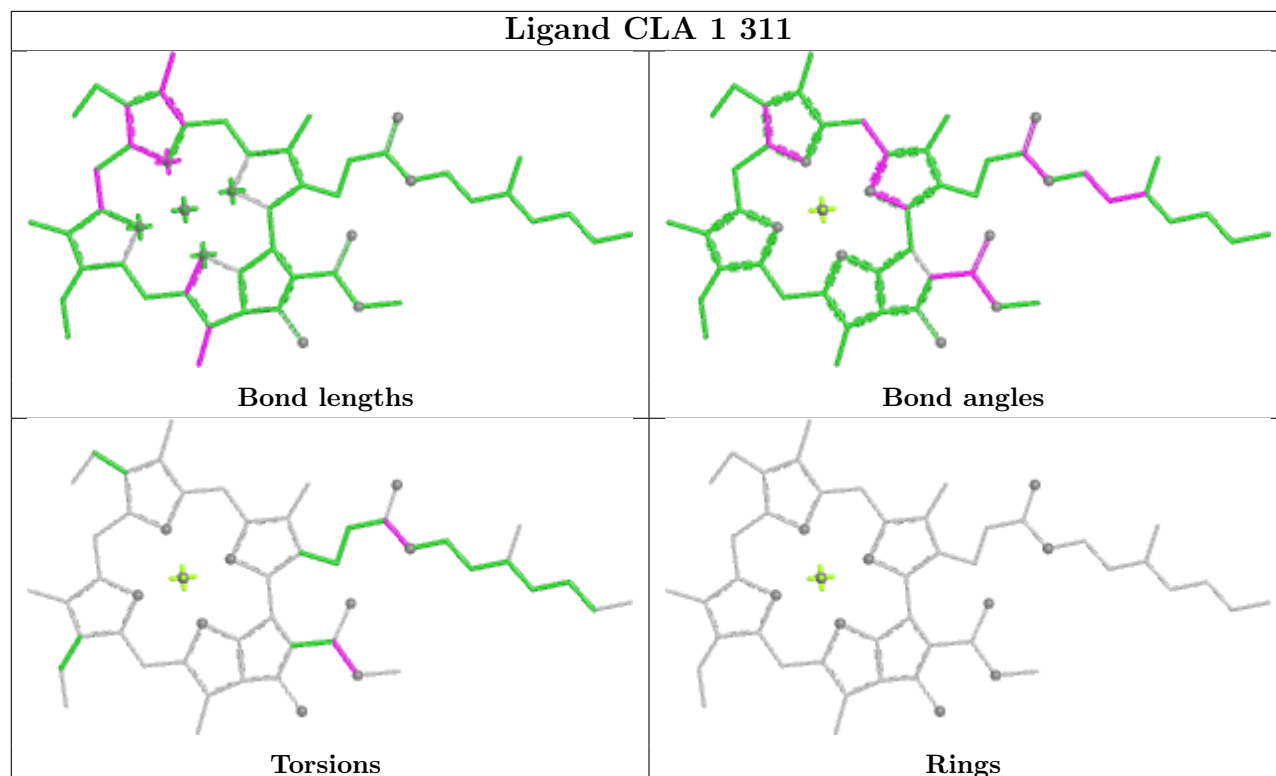


Ligand CLA 7 309

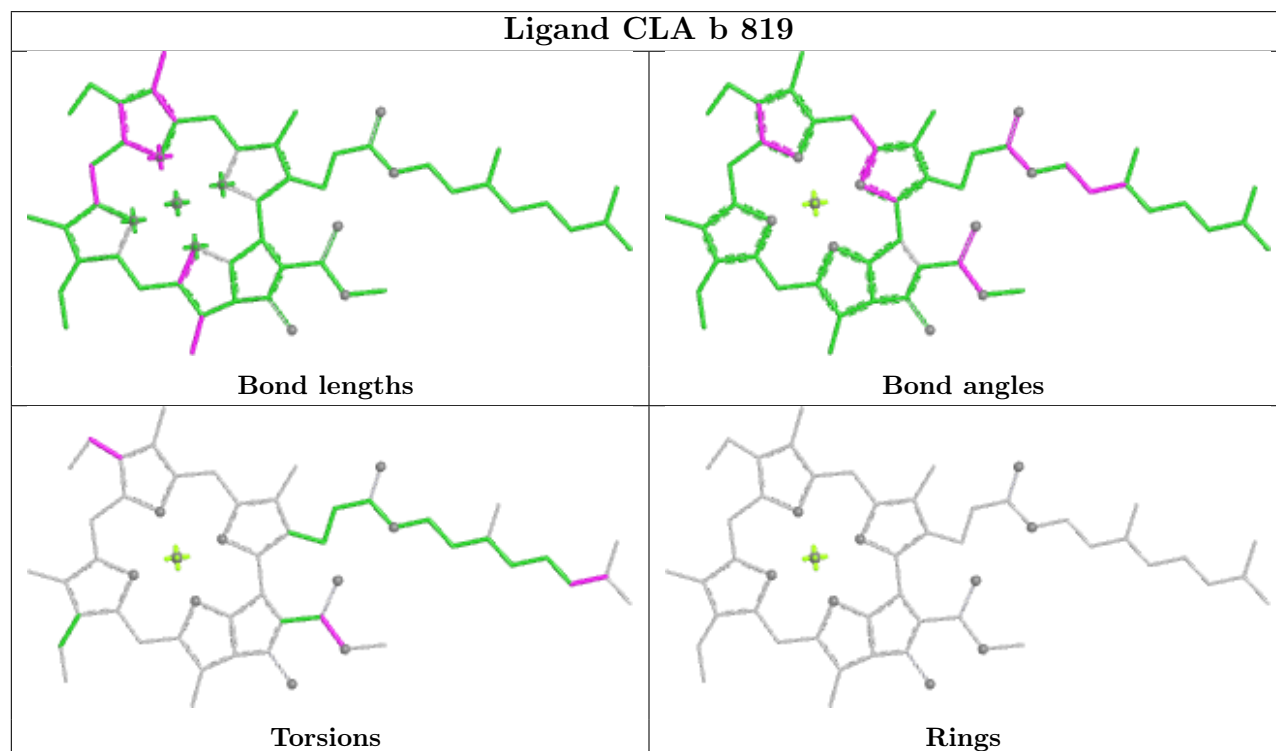


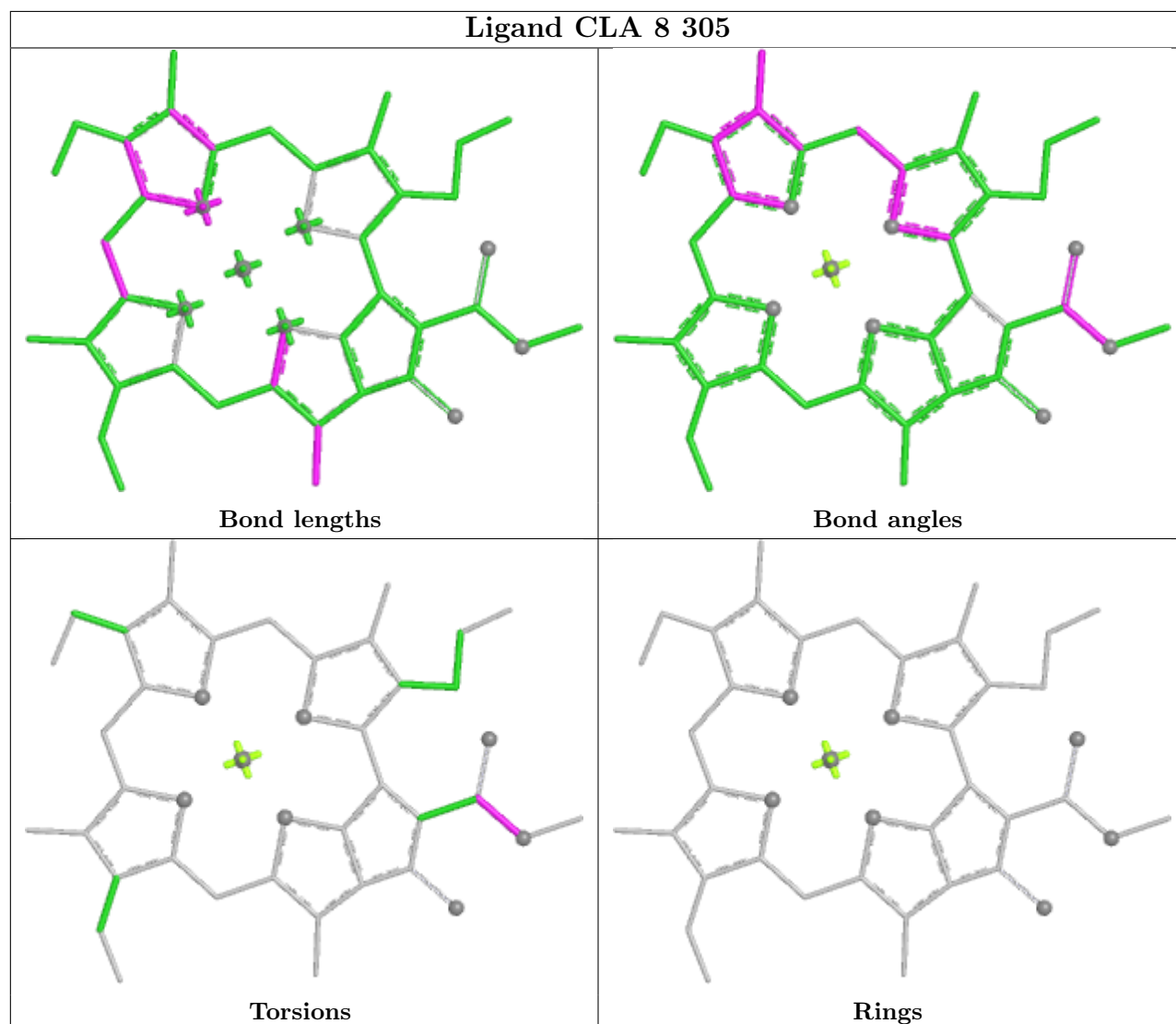
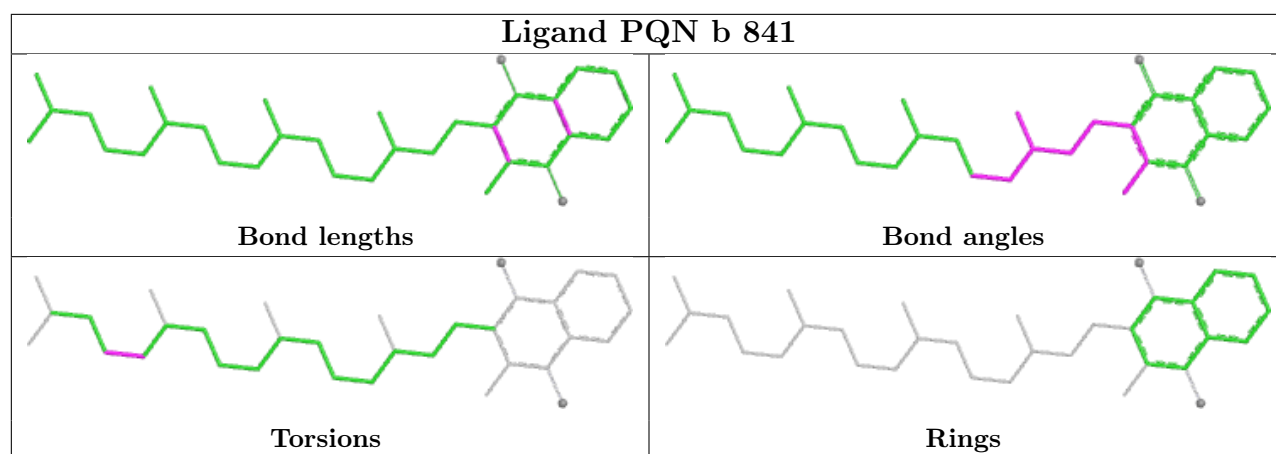


Ligand CLA 1 311

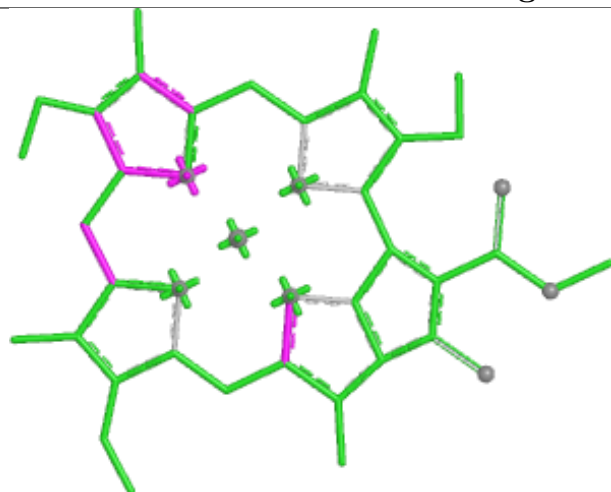


Ligand CLA b 819

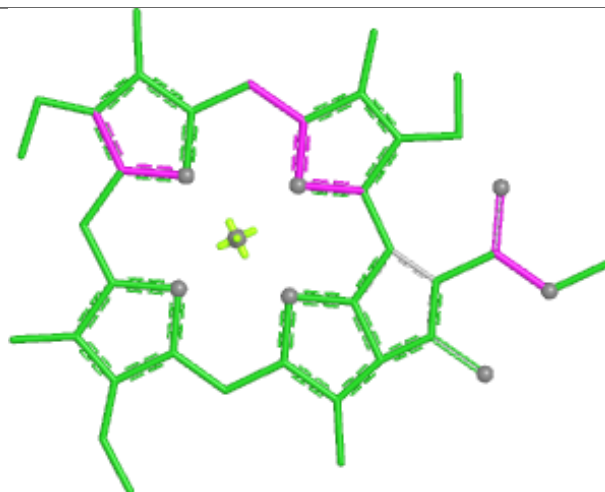




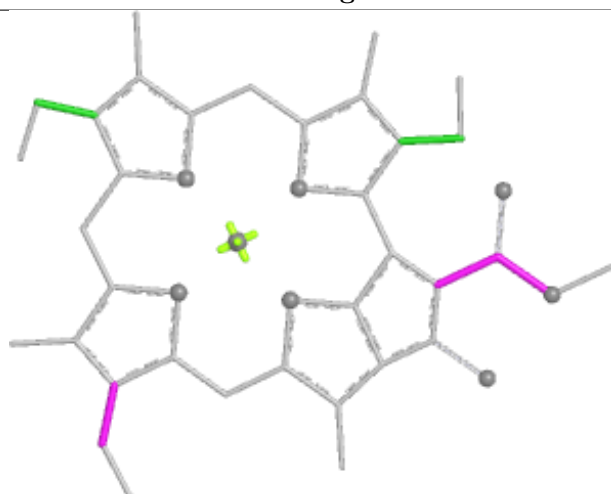
Ligand CLA 9 315



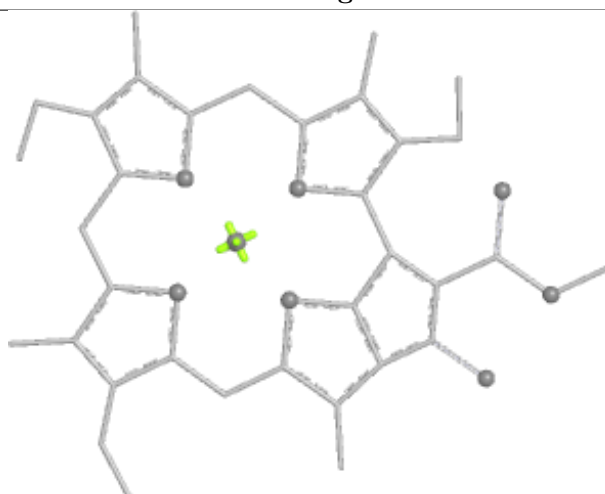
Bond lengths



Bond angles

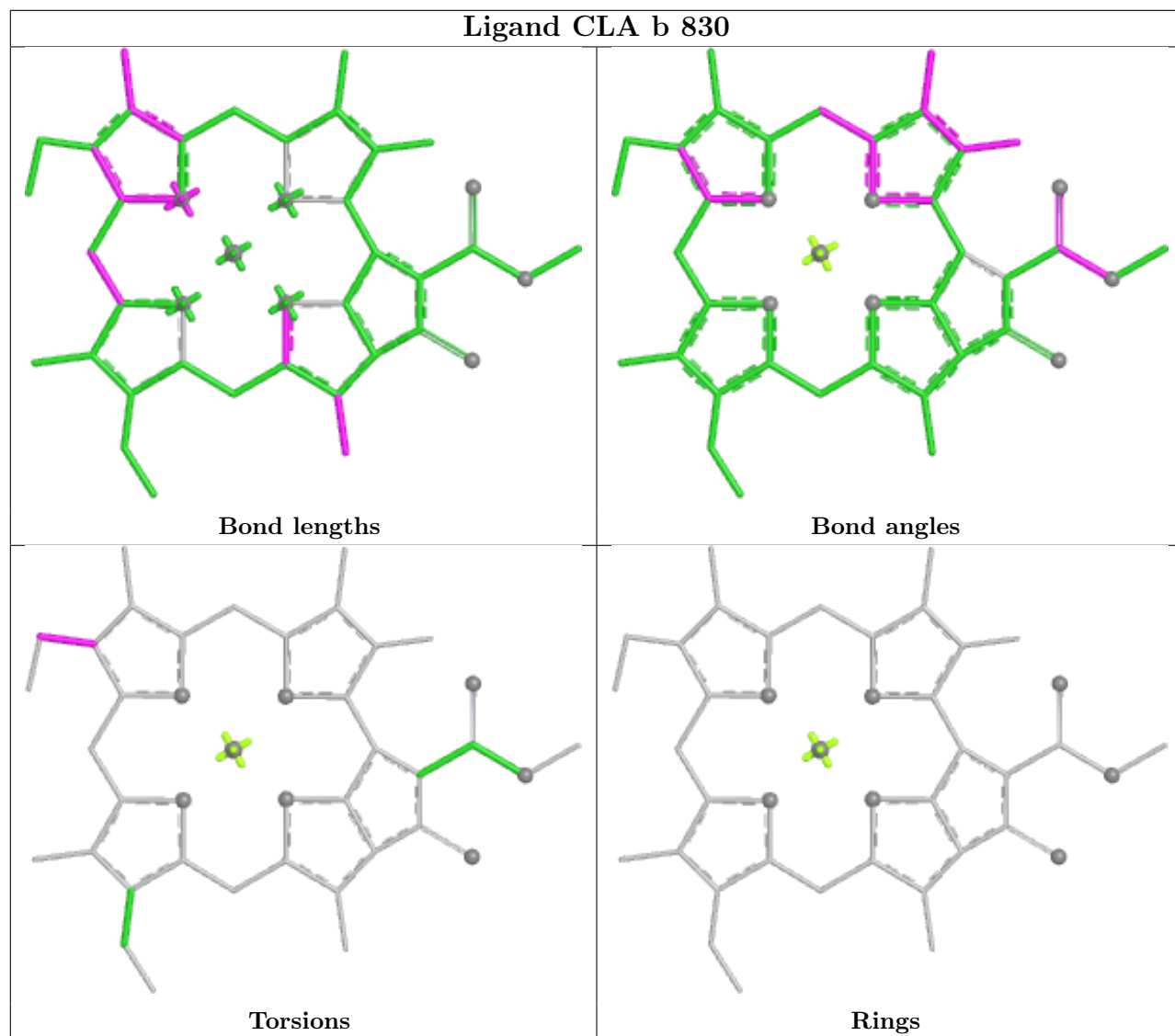


Torsions

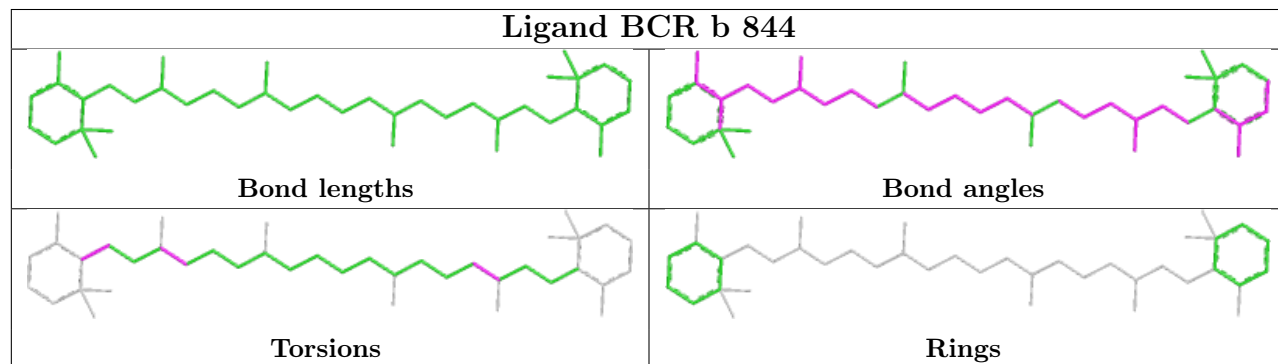


Rings

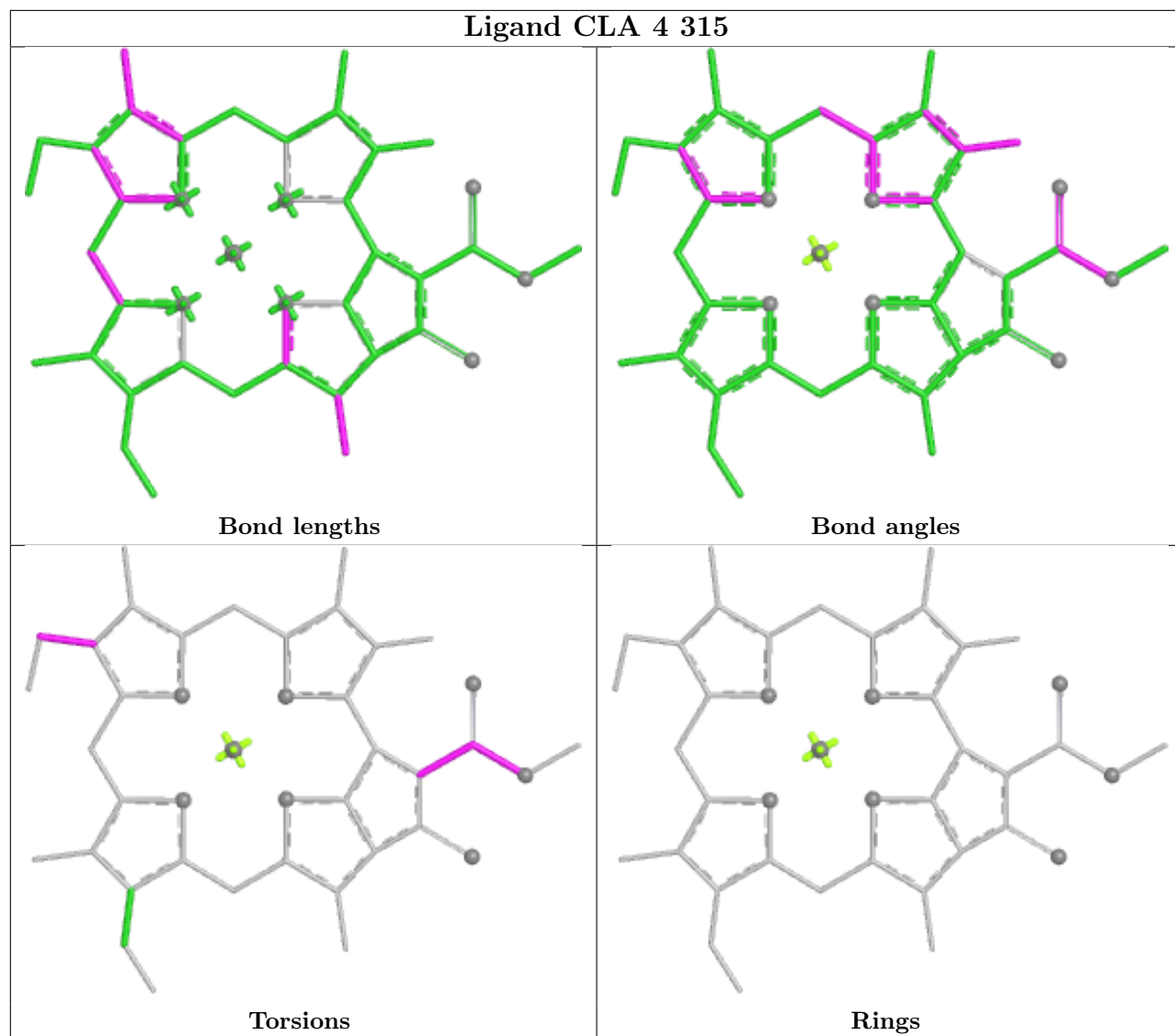
Ligand CLA b 830



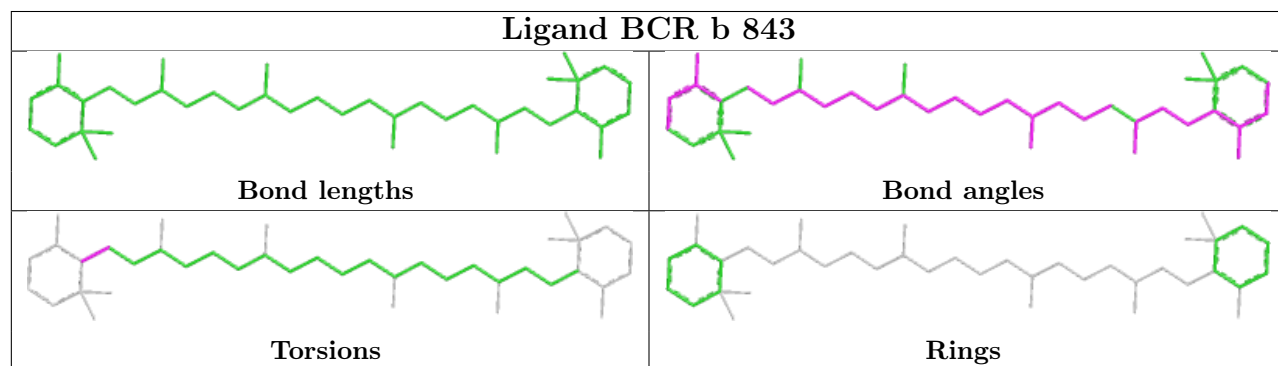
Ligand BCR b 844

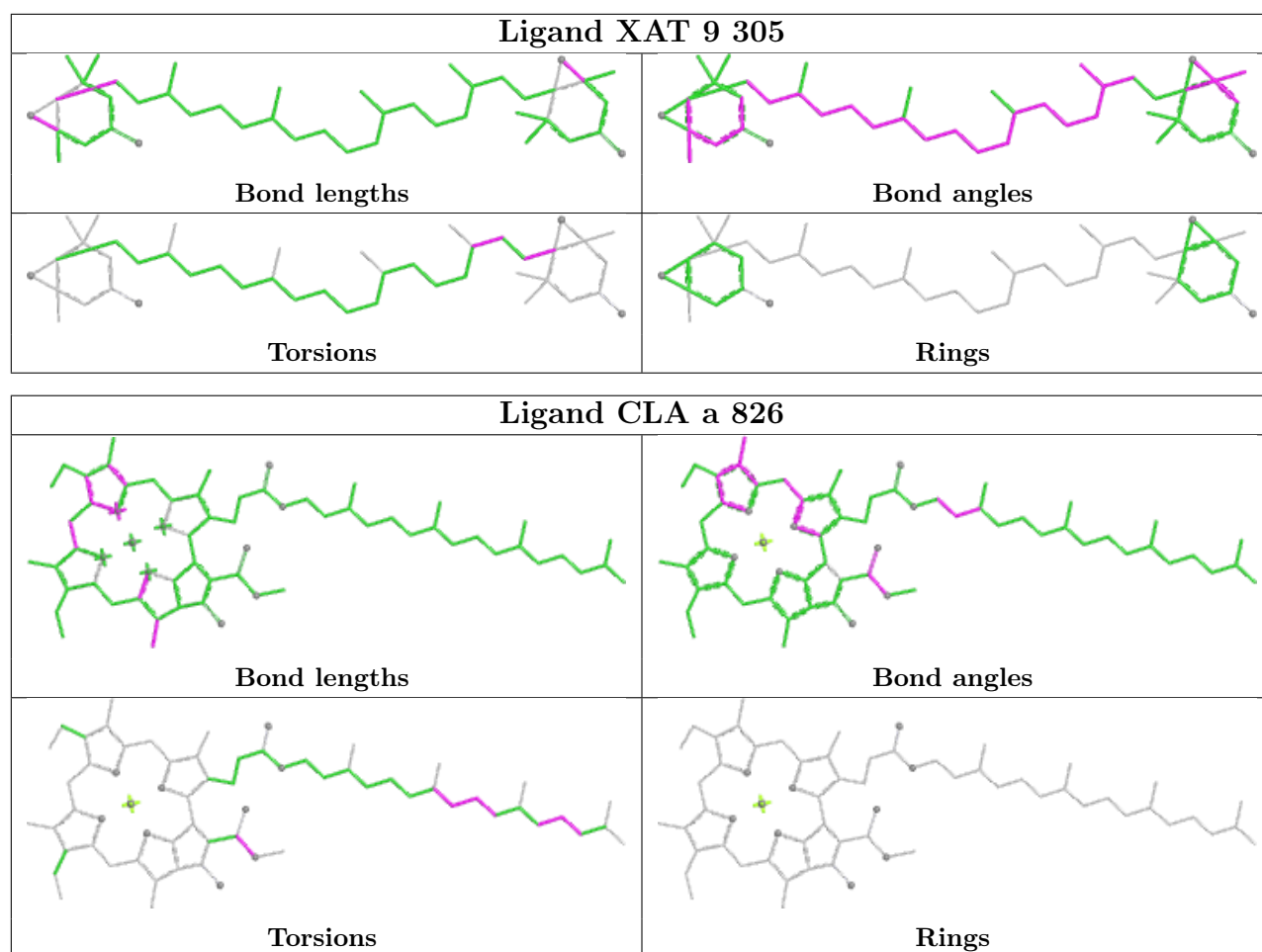


Ligand CLA 4 315

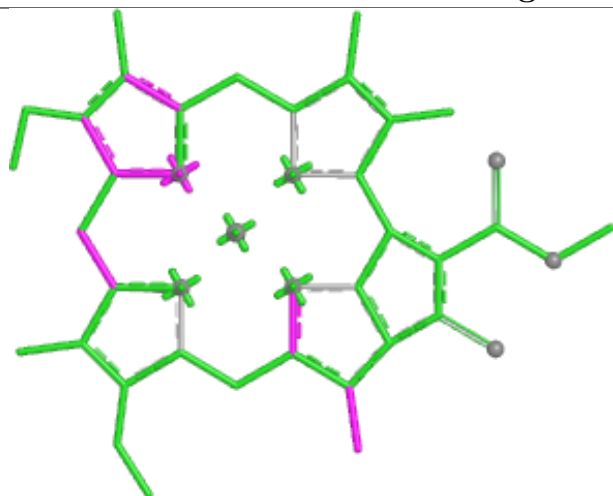


Ligand BCR b 843

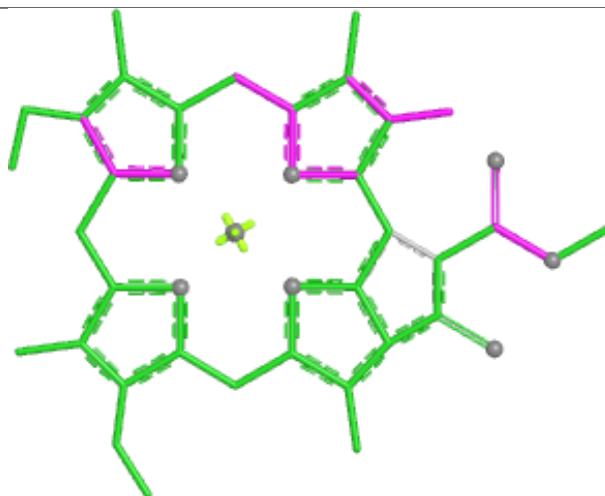




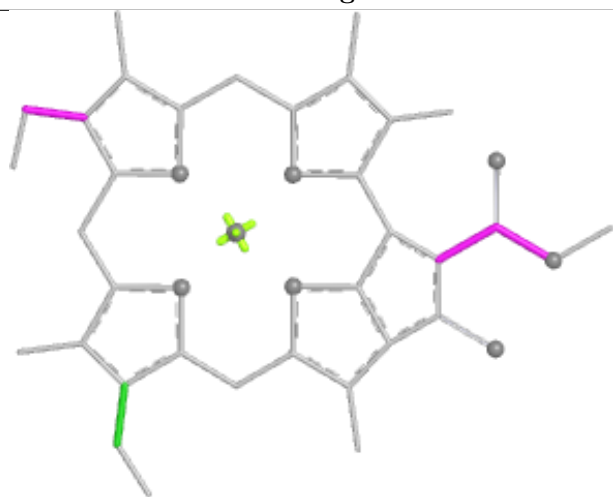
Ligand CLA 1 313



Bond lengths



Bond angles

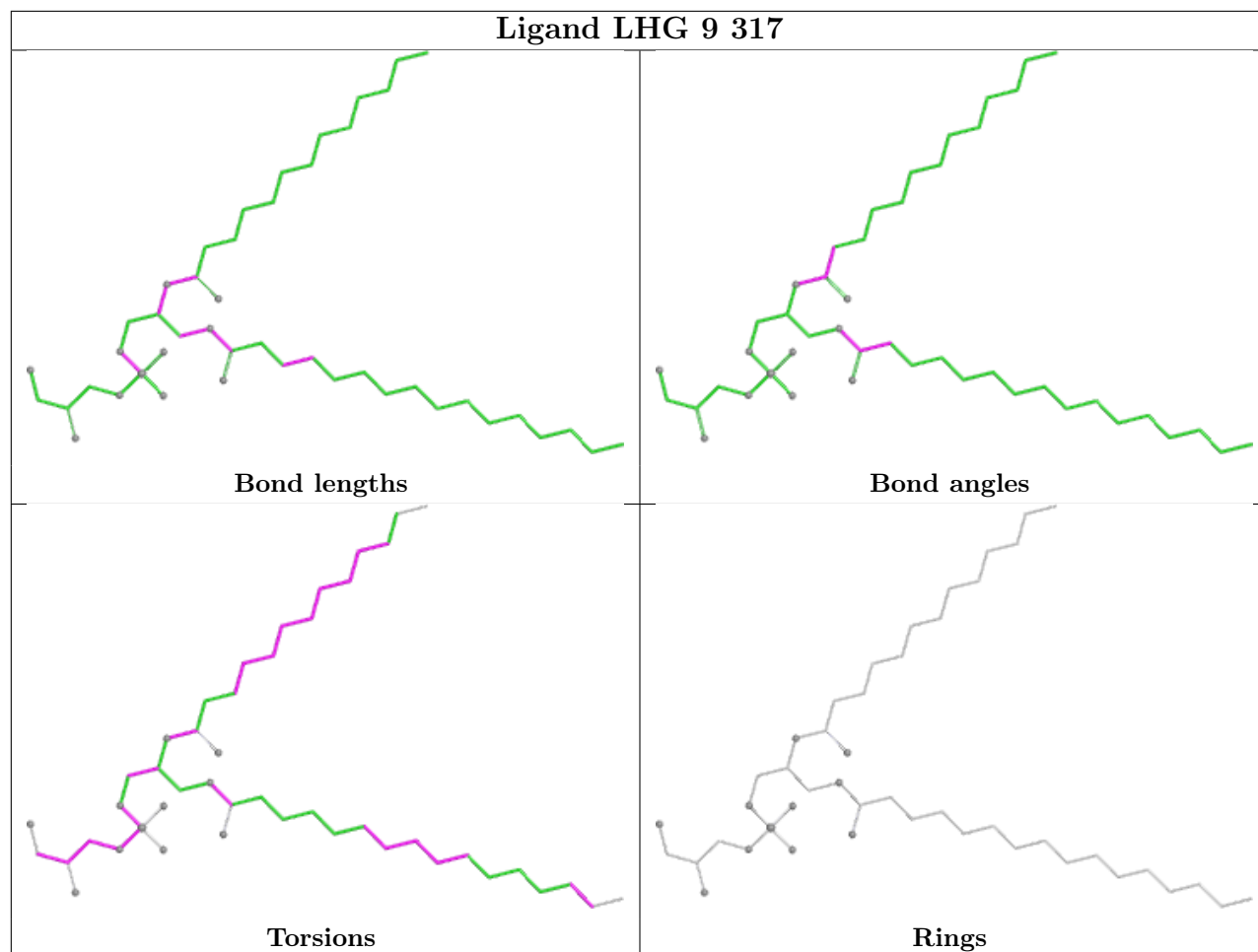


Torsions

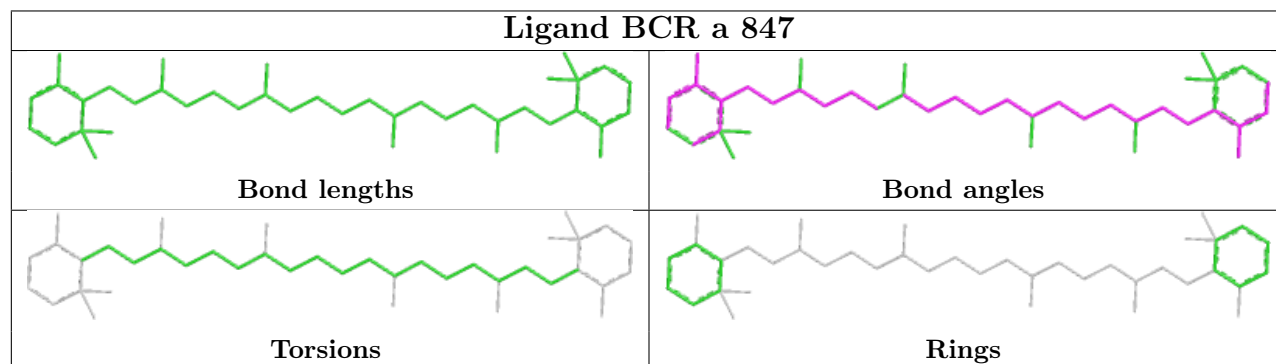


Rings

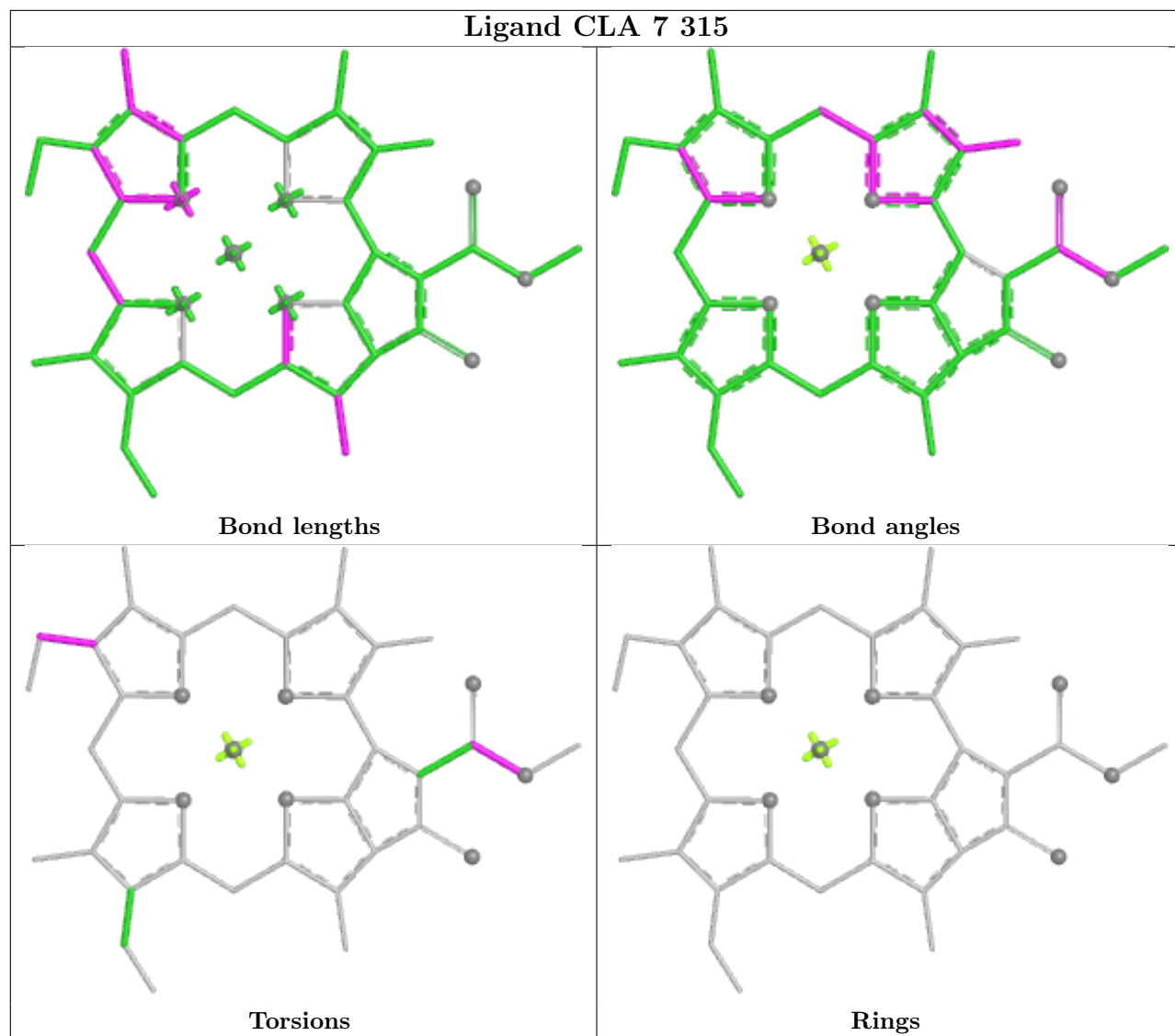
Ligand LHG 9 317



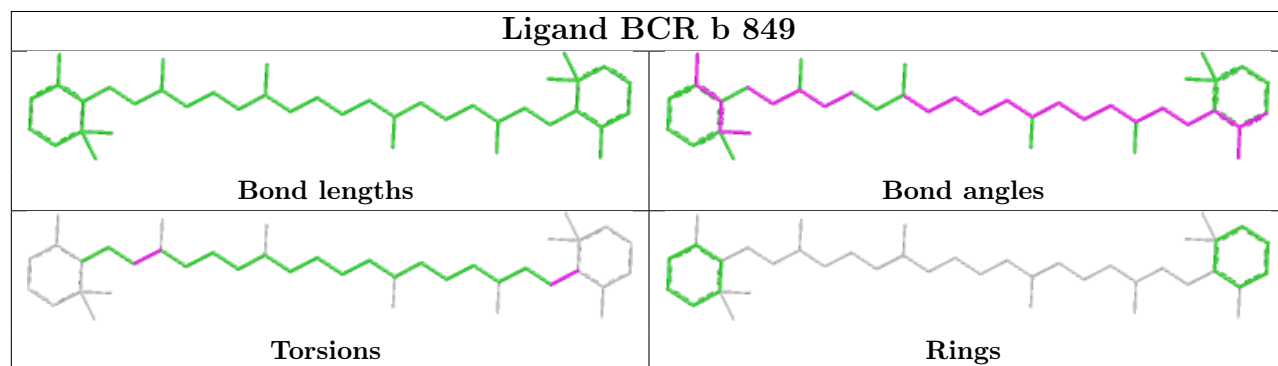
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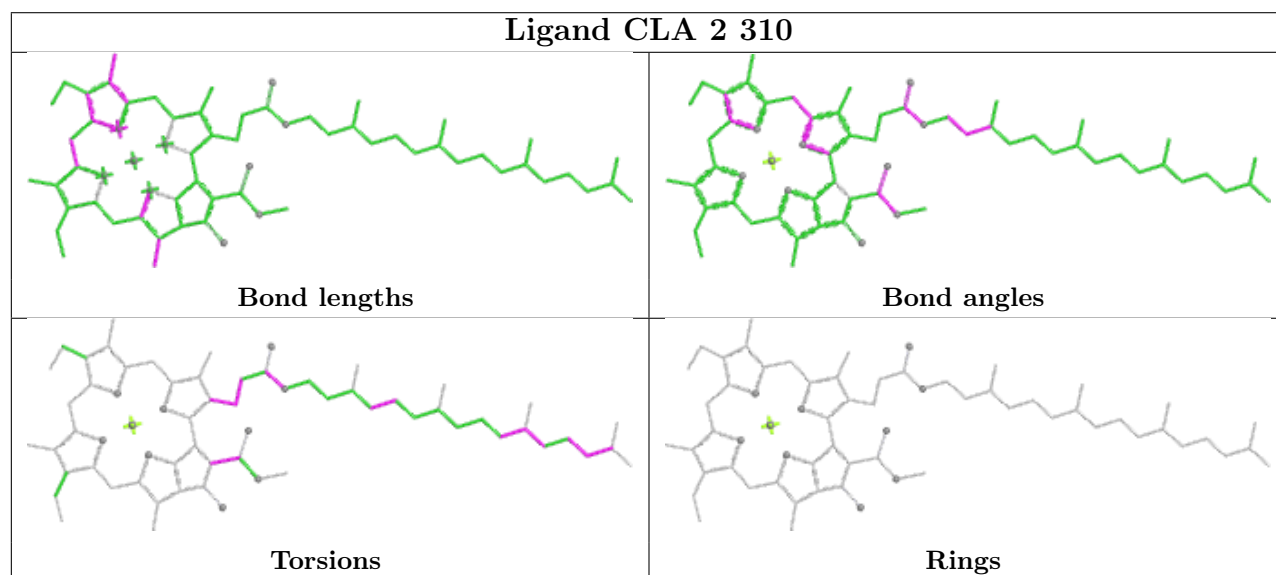
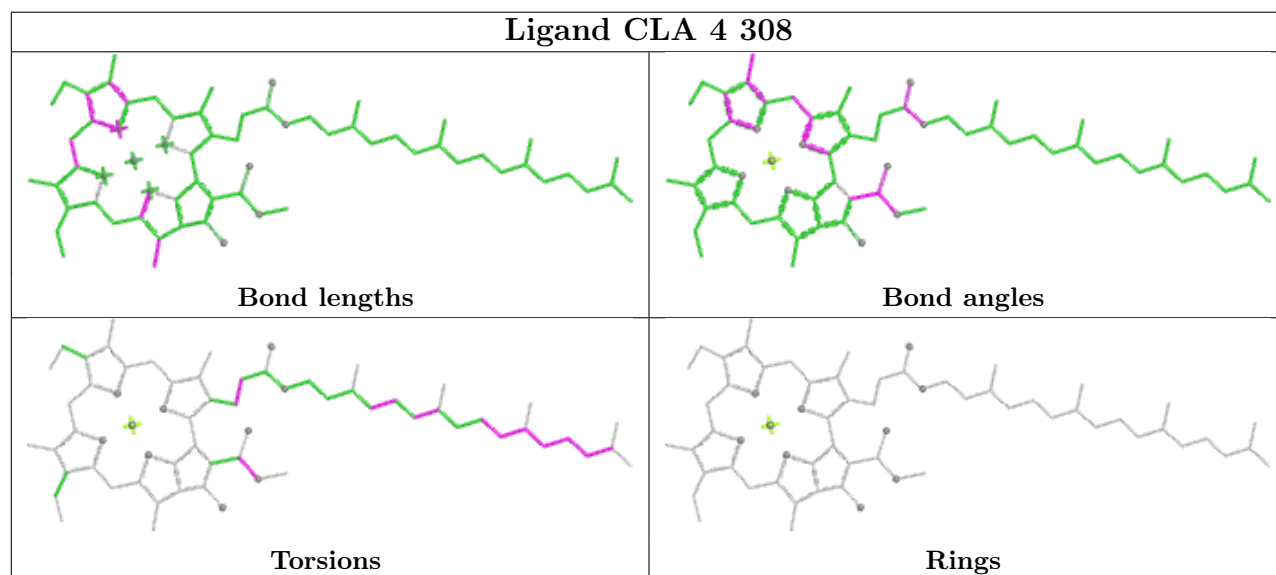
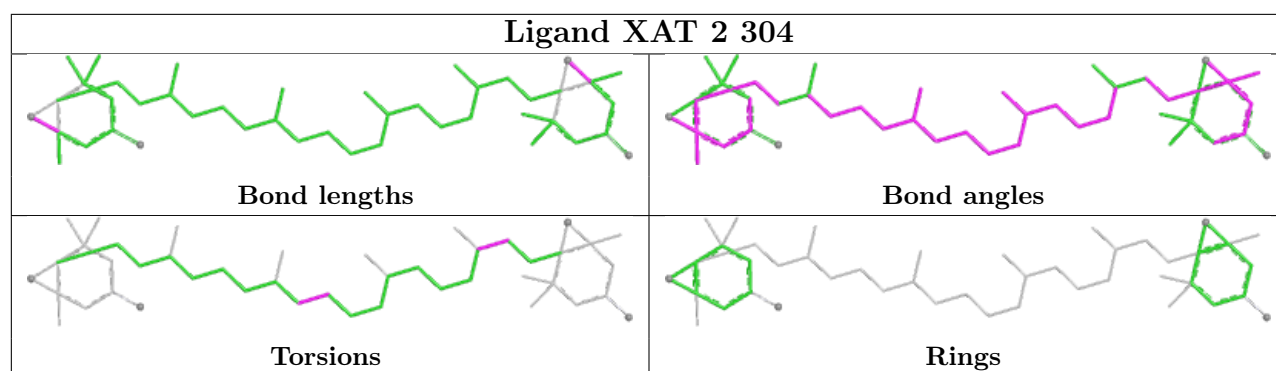


Ligand CLA 7 315

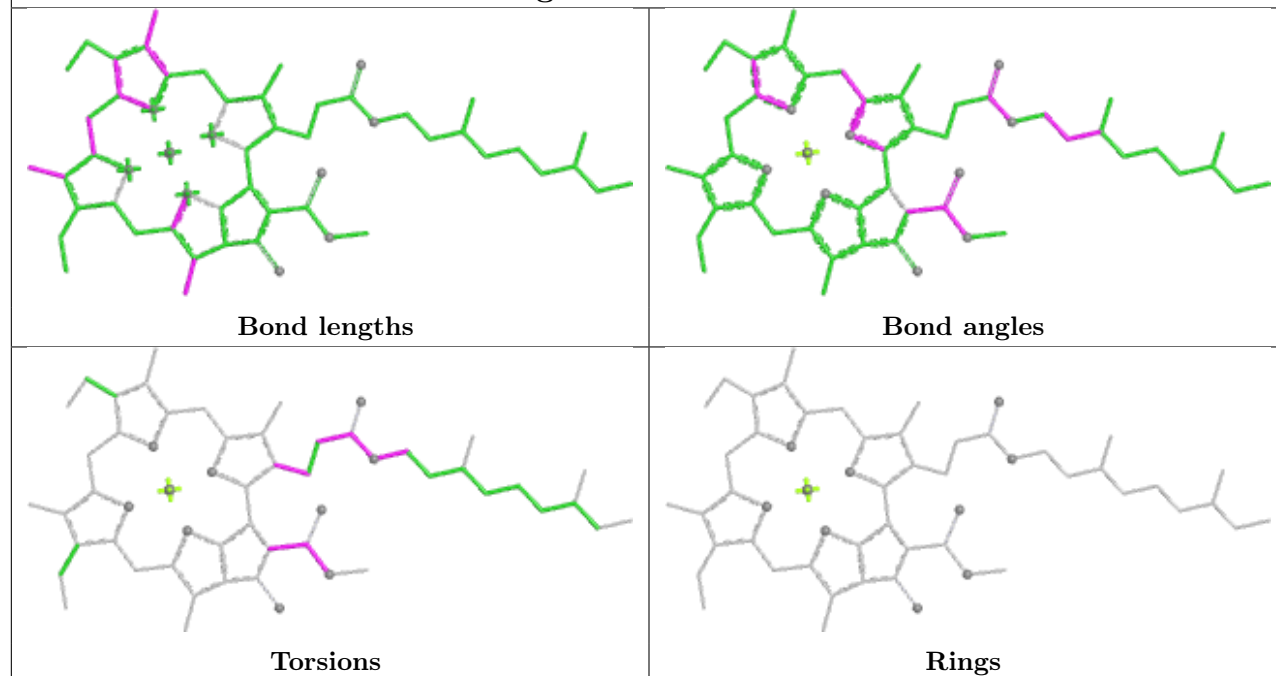


Ligand BCR b 849

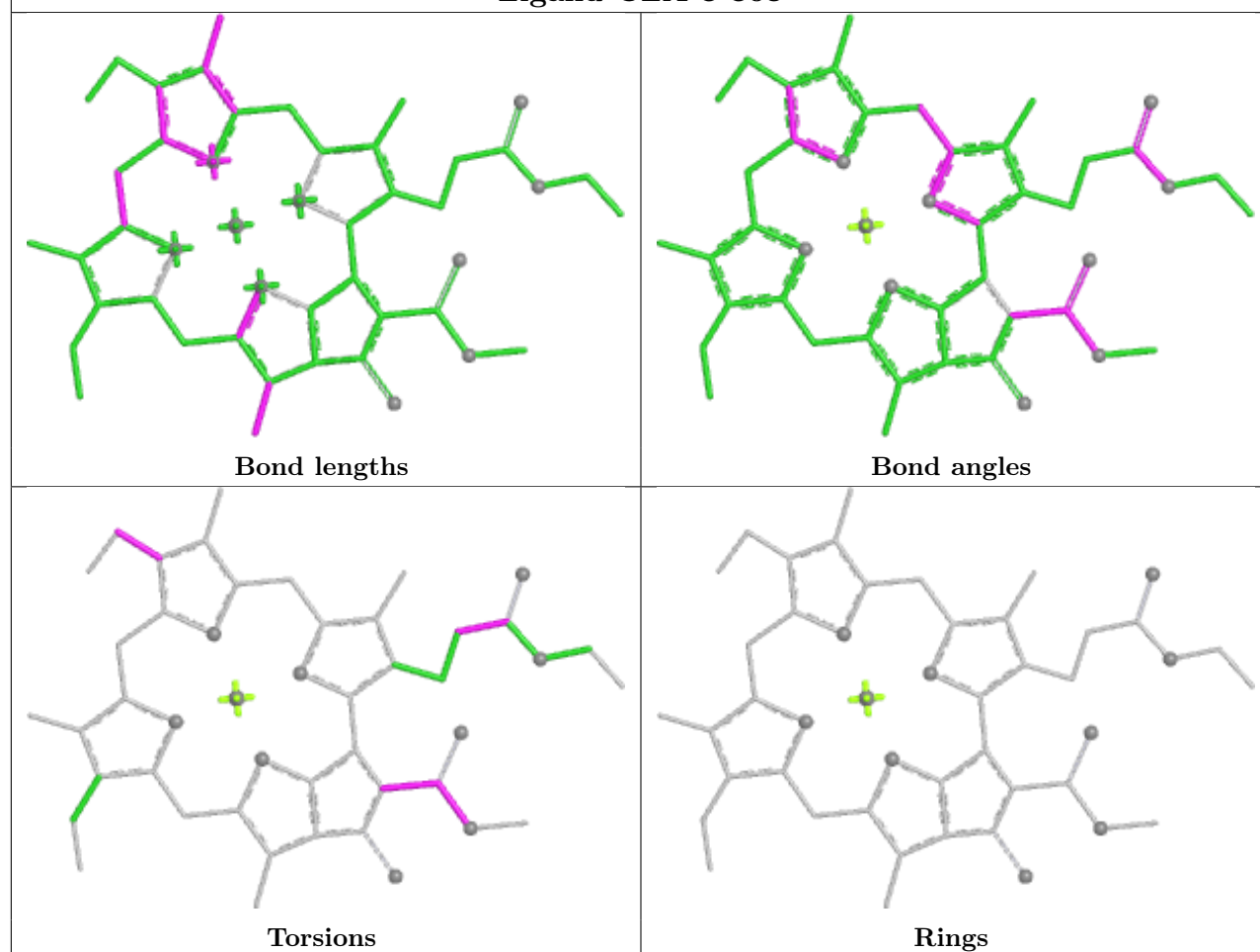


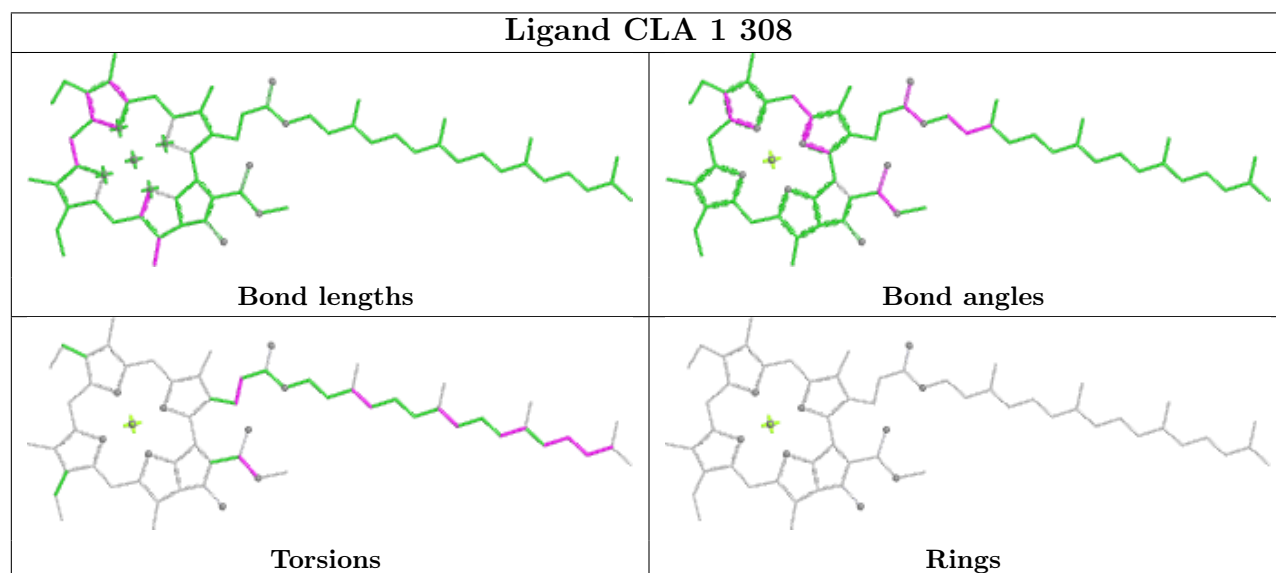
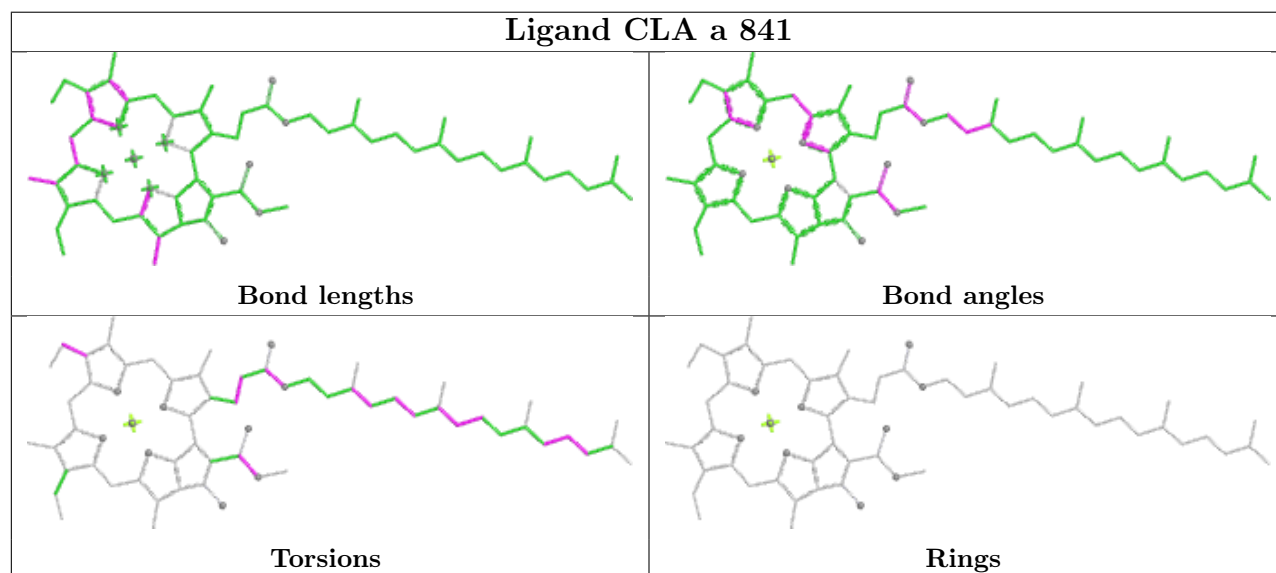
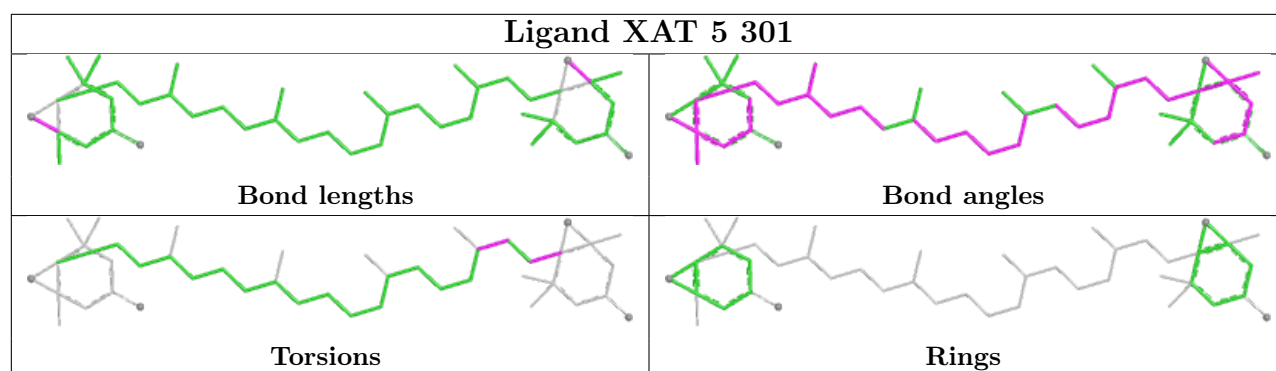


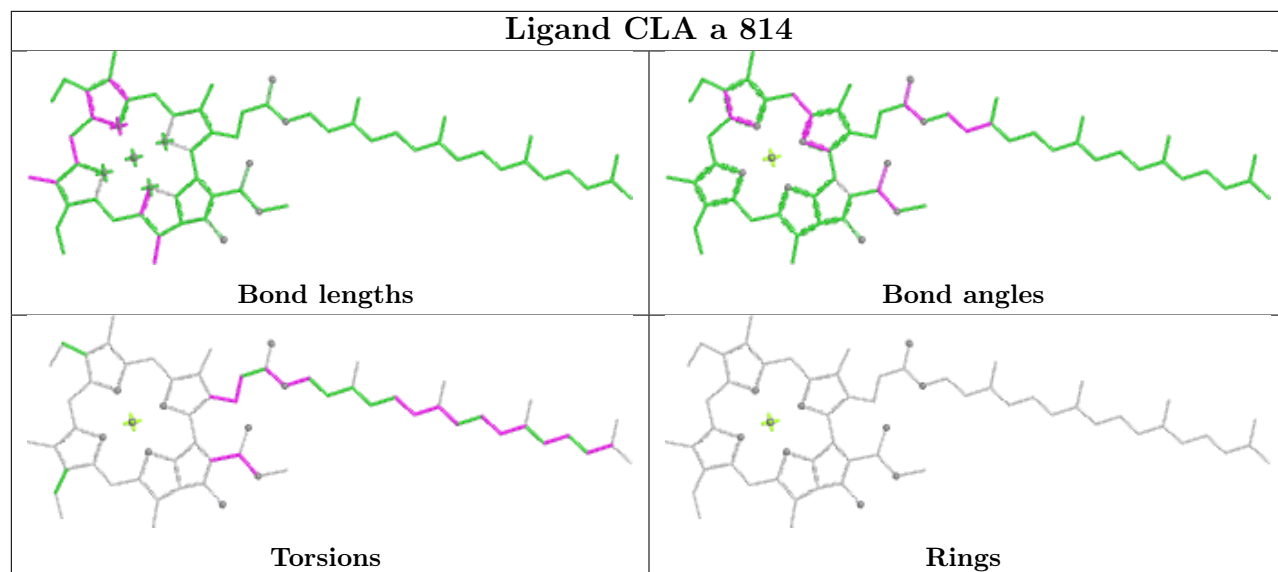
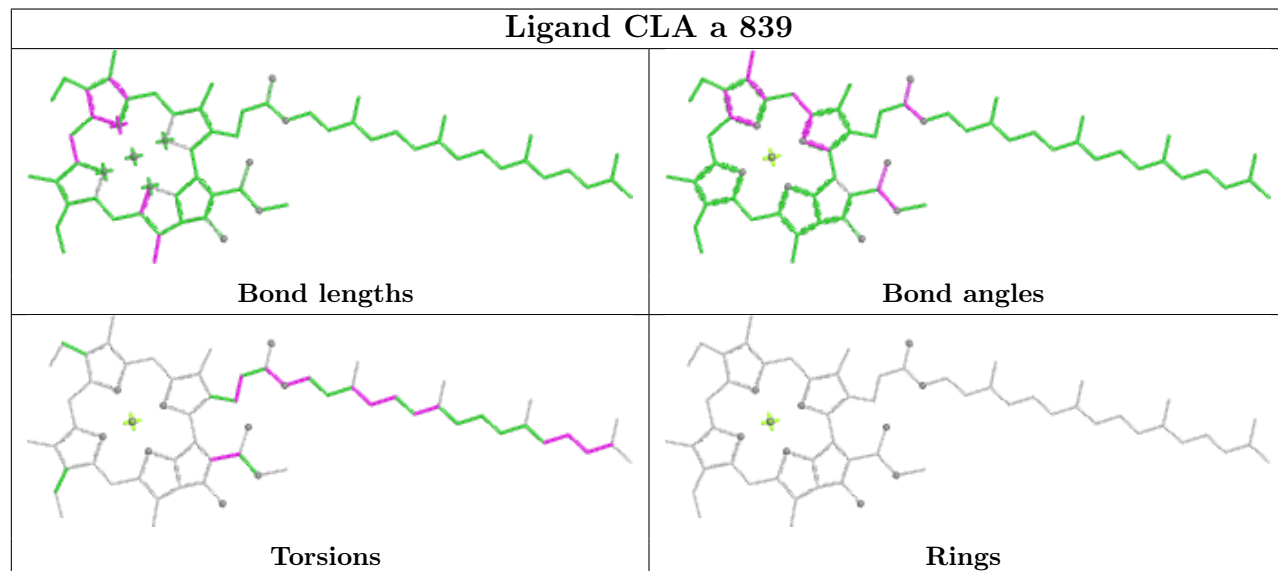
Ligand CLA a 818



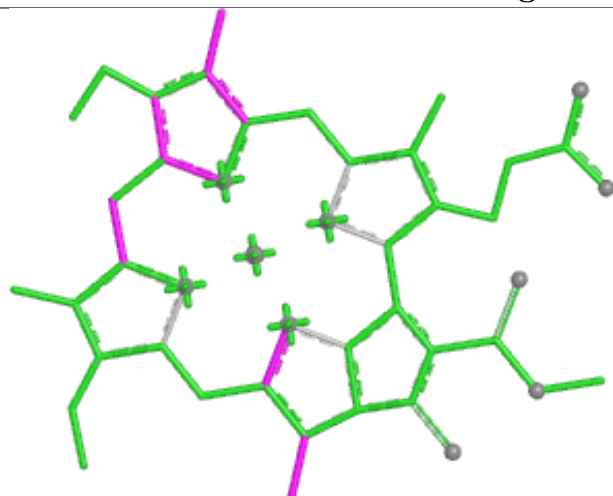
Ligand CLA 3 308



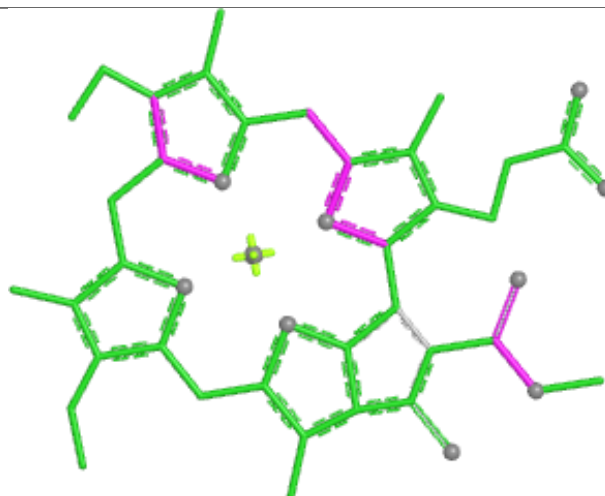


Ligand CLA a 814**Ligand CLA a 839**

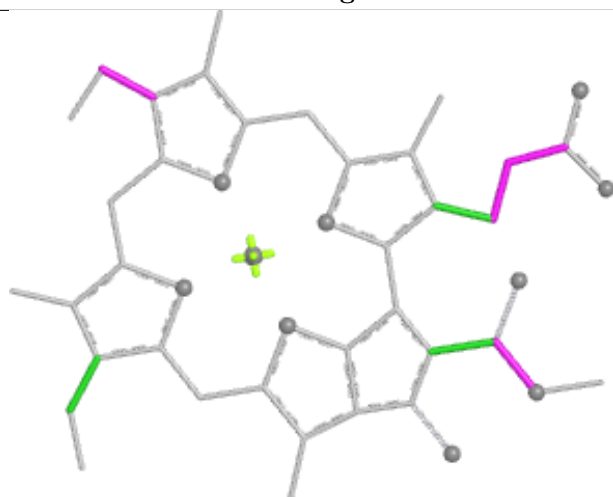
Ligand CLA 7 317



Bond lengths



Bond angles

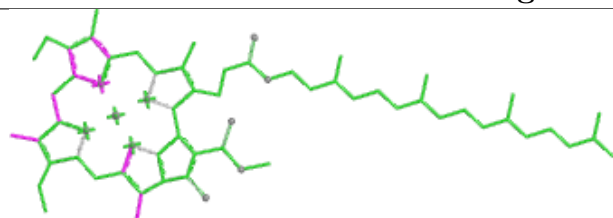


Torsions

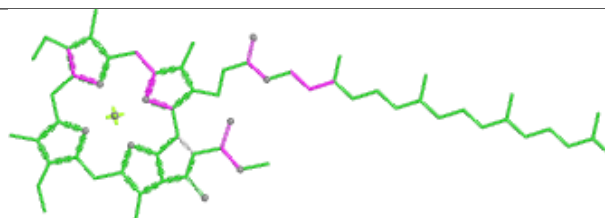


Rings

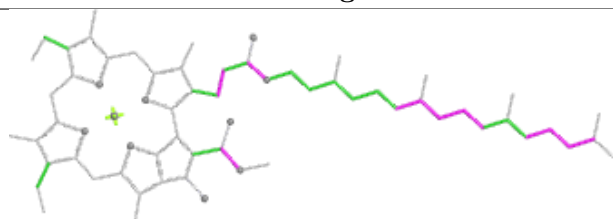
Ligand CLA b 827



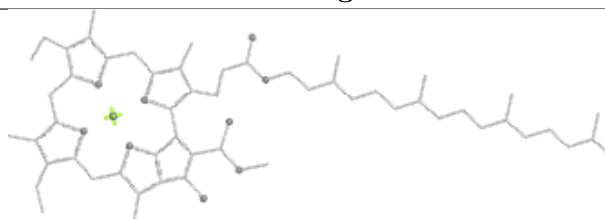
Bond lengths



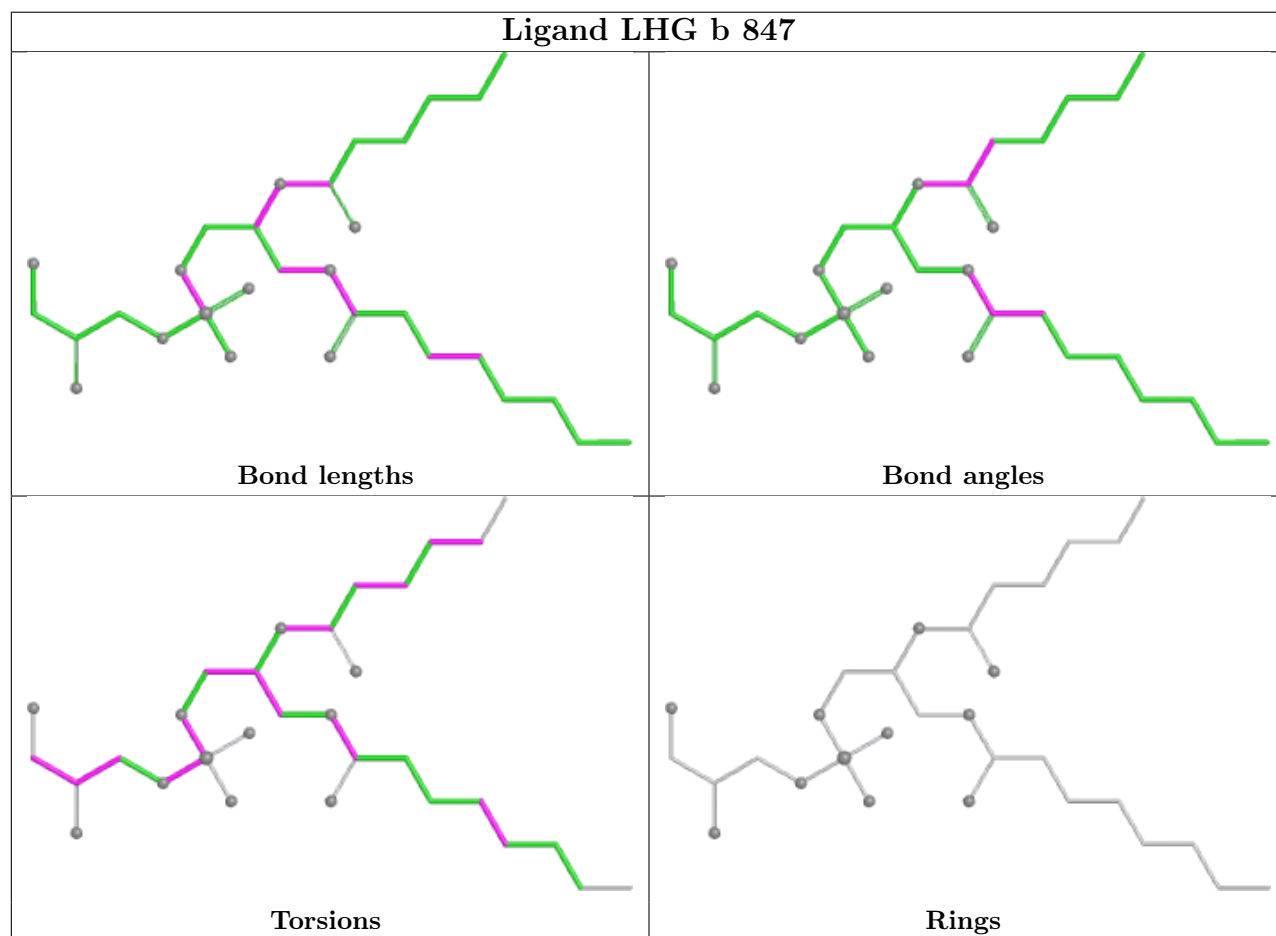
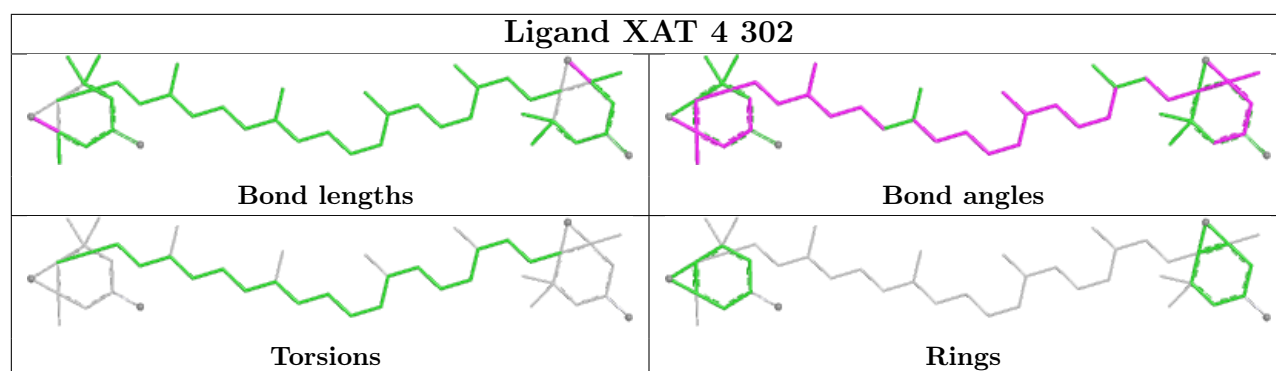
Bond angles



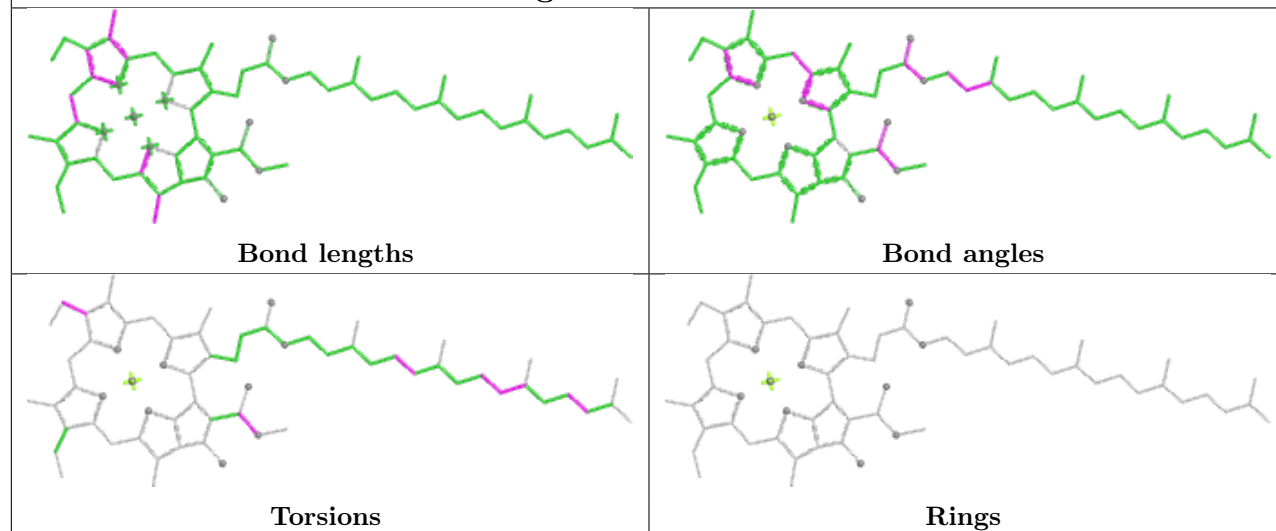
Torsions



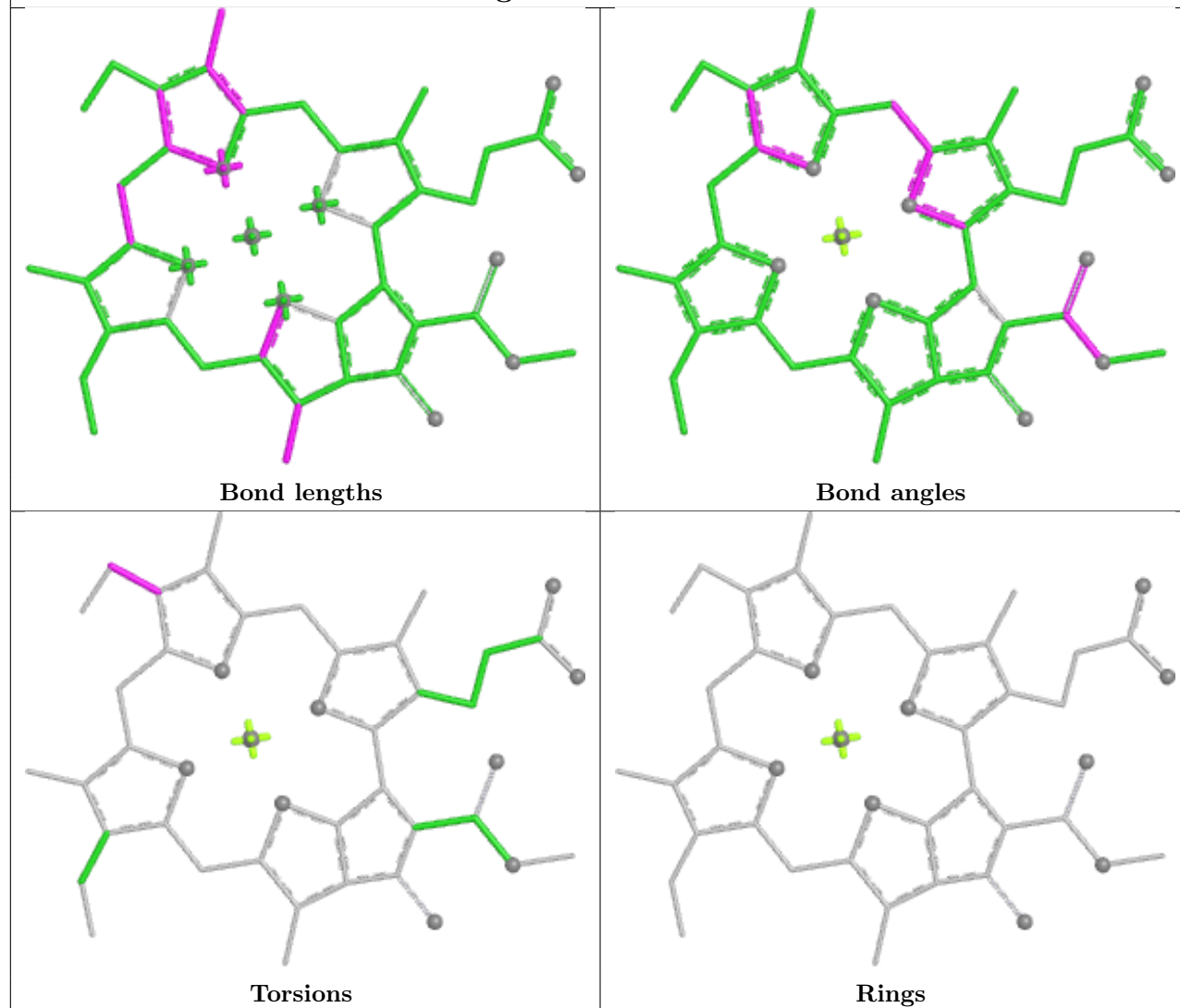
Rings



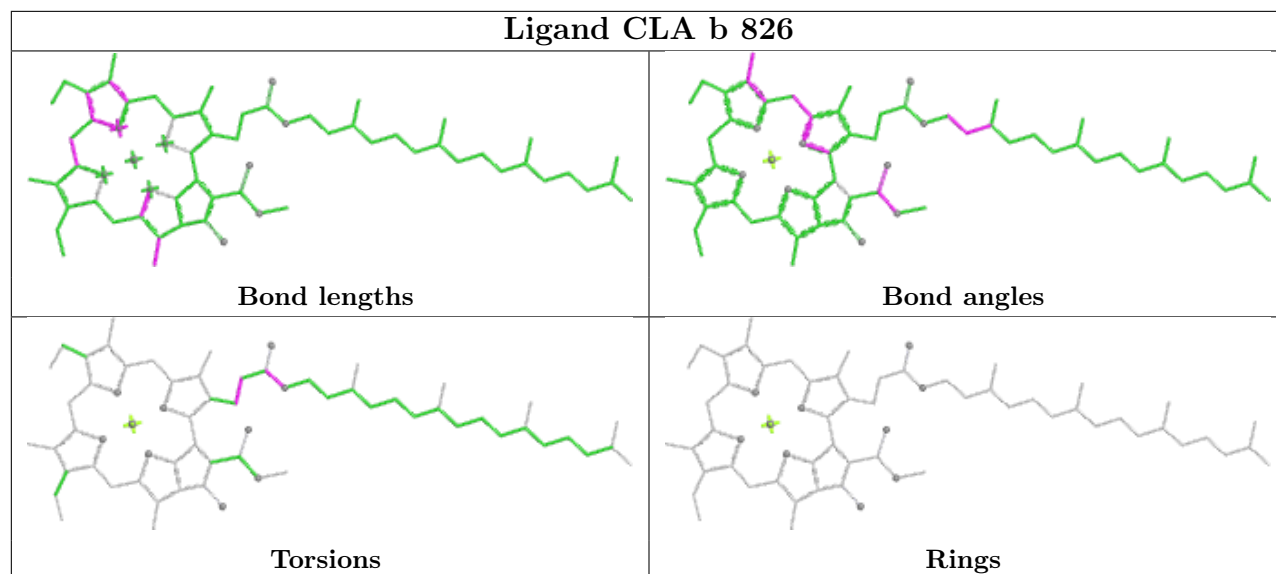
Ligand CLA a 834



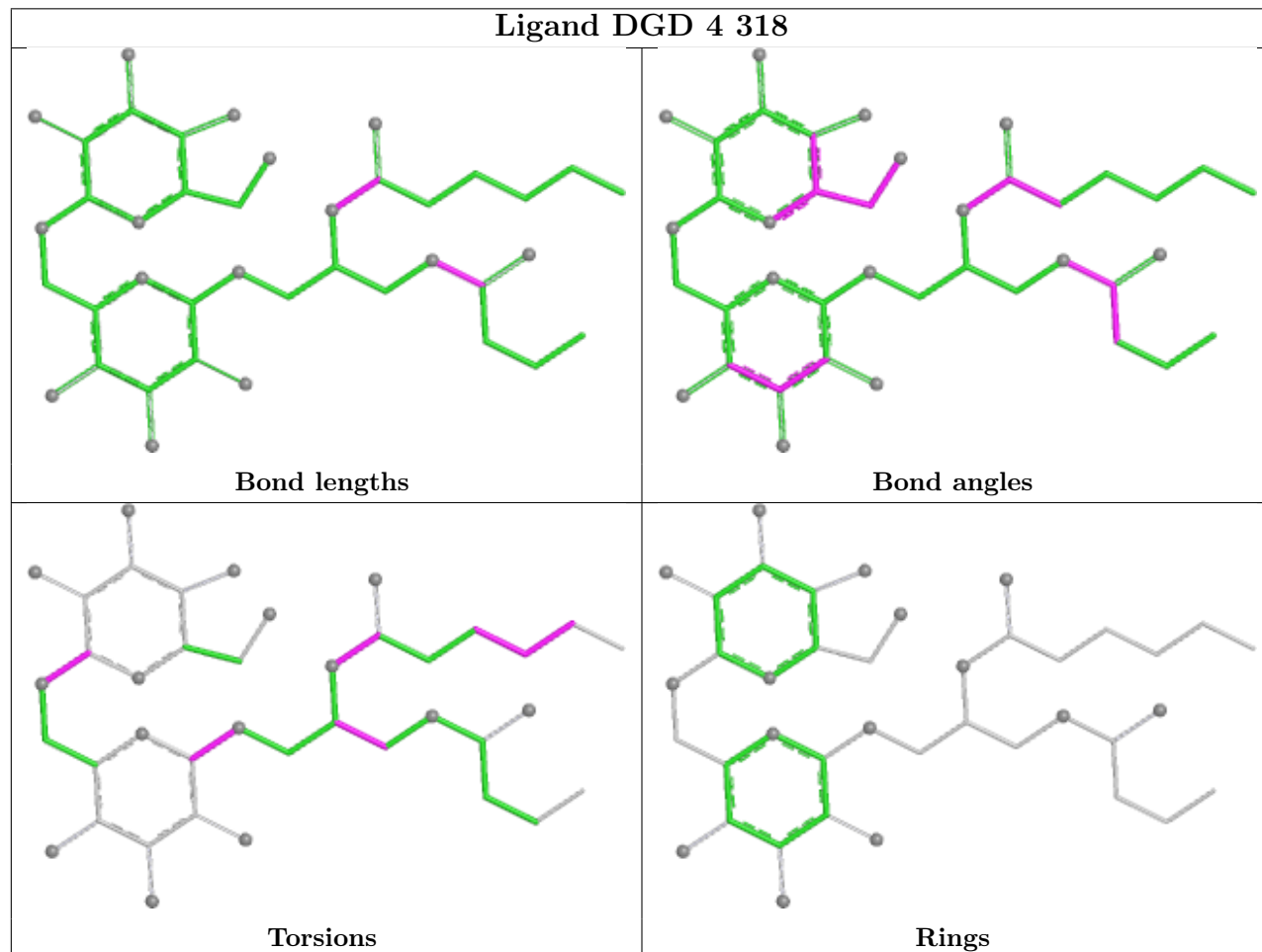
Ligand CLA 3 307



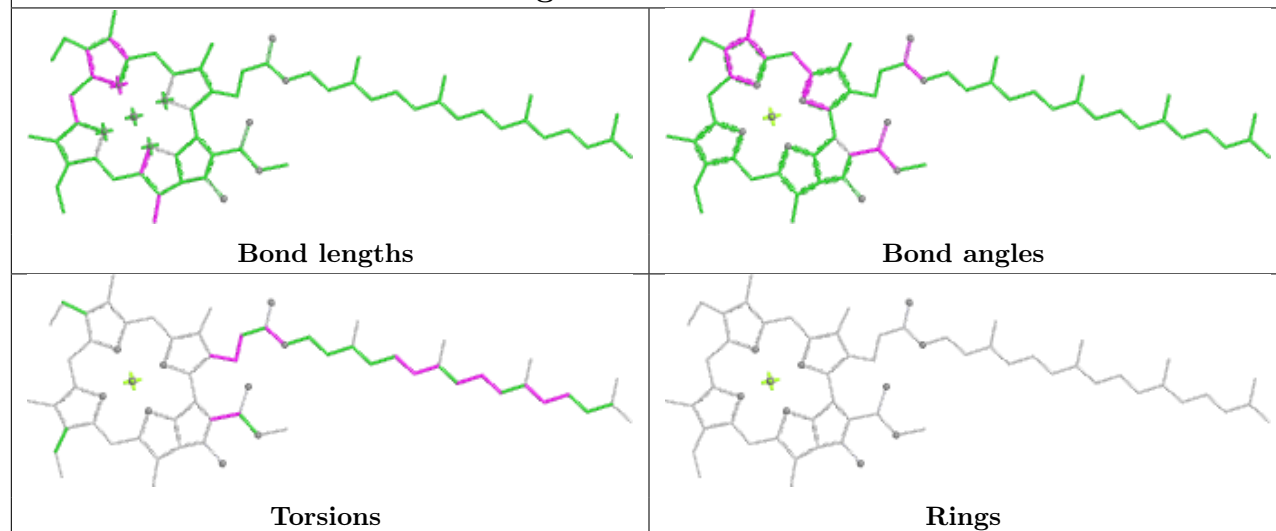
Ligand CLA b 826



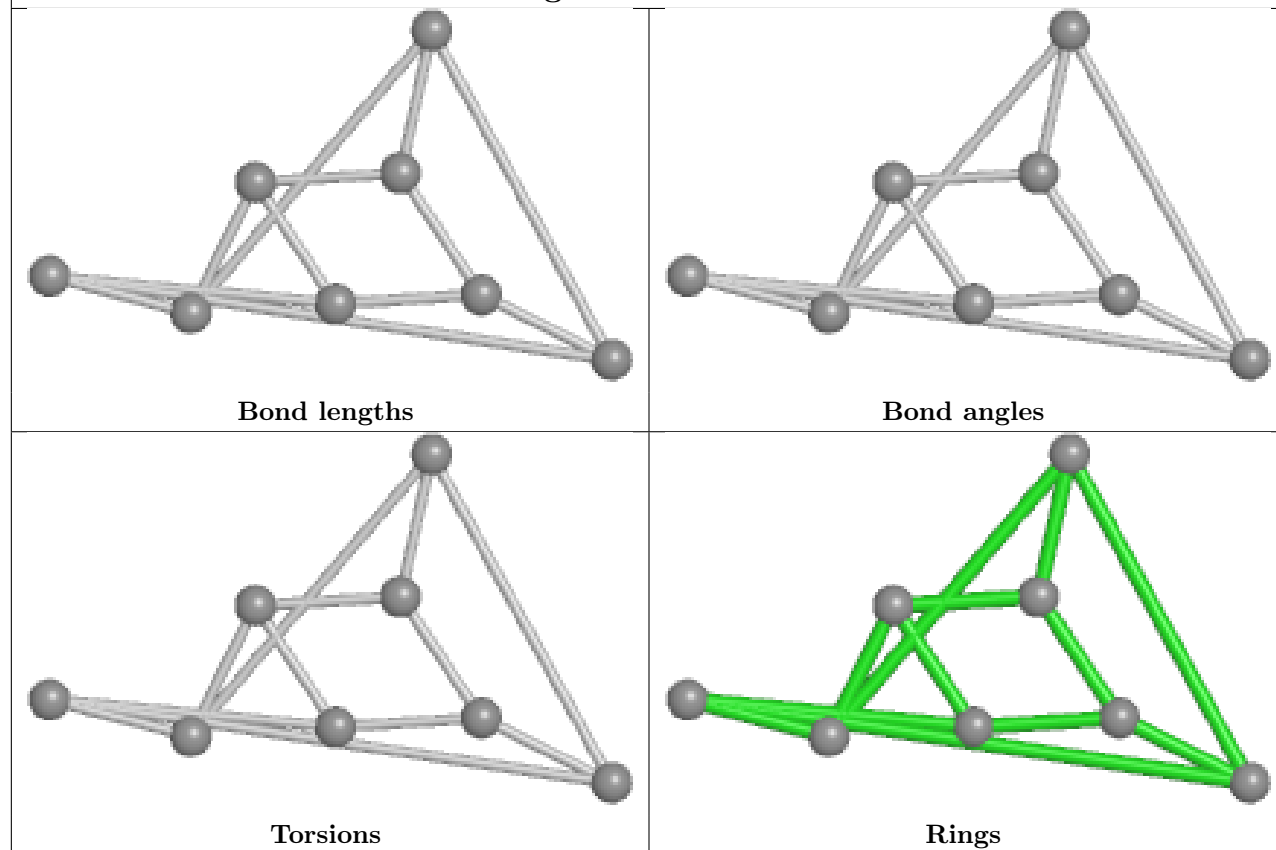
Ligand DGD 4 318



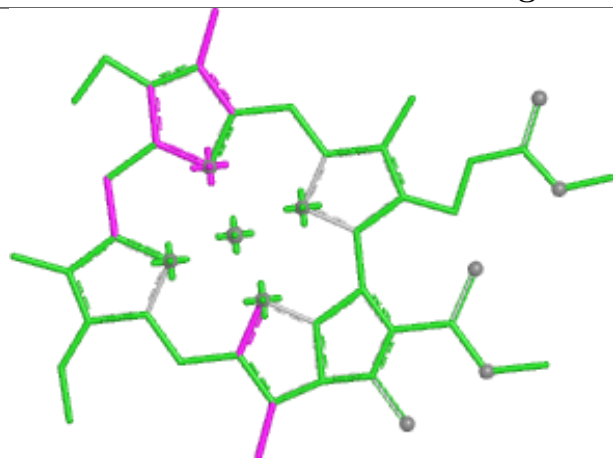
Ligand CLA a 809



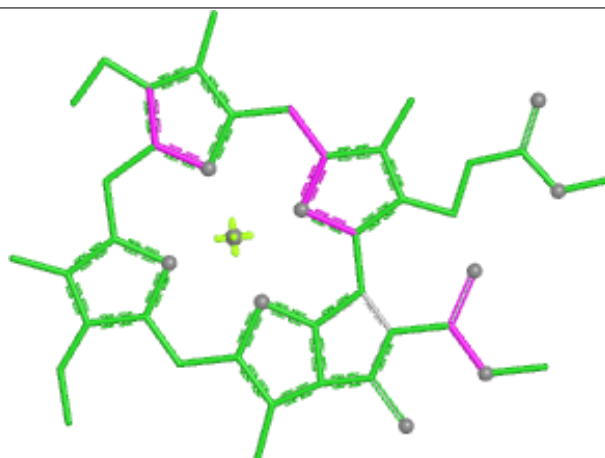
Ligand SF4 c 101



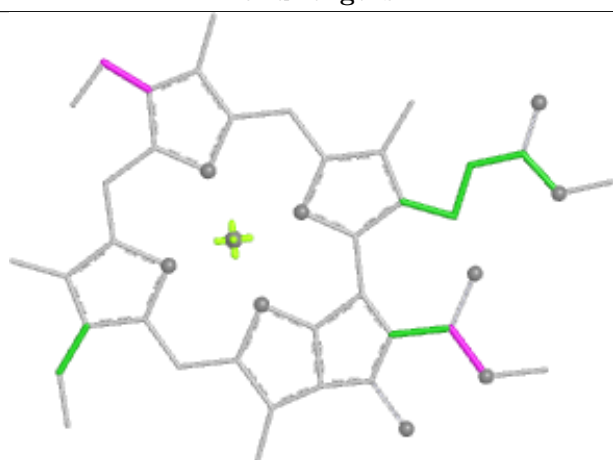
Ligand CLA 8 306



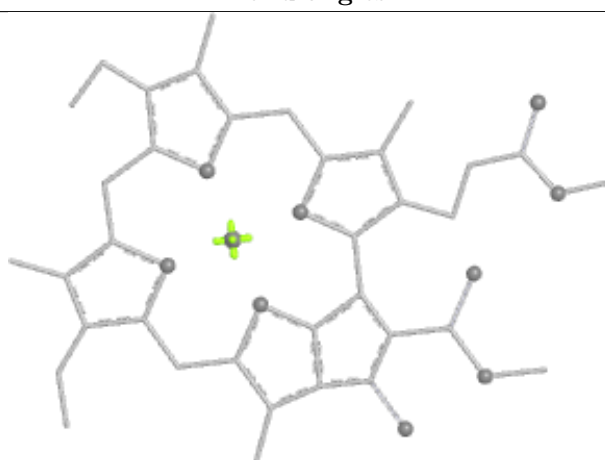
Bond lengths



Bond angles

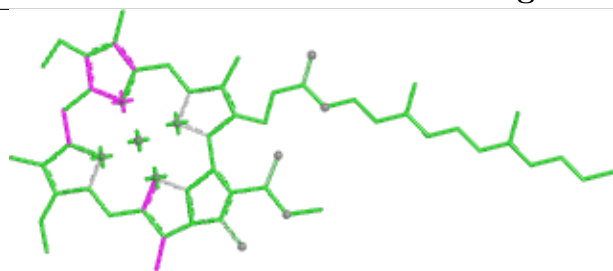


Torsions

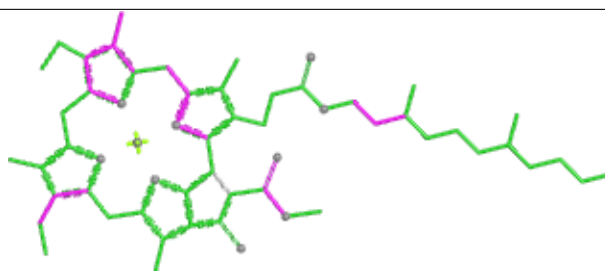


Rings

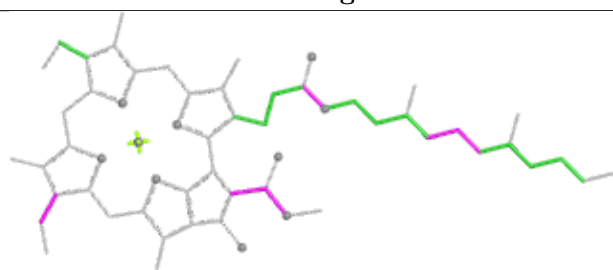
Ligand CLA b 835



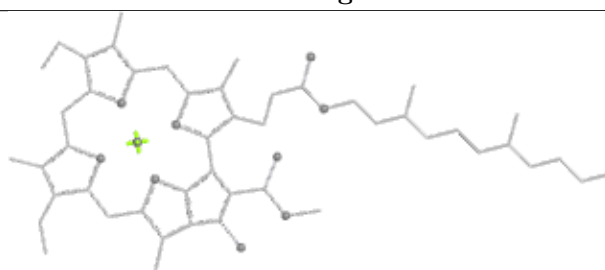
Bond lengths



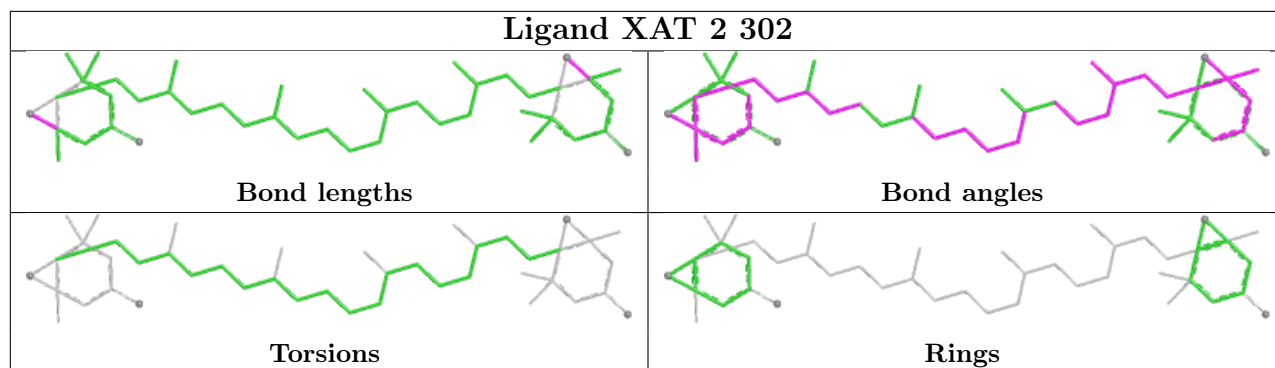
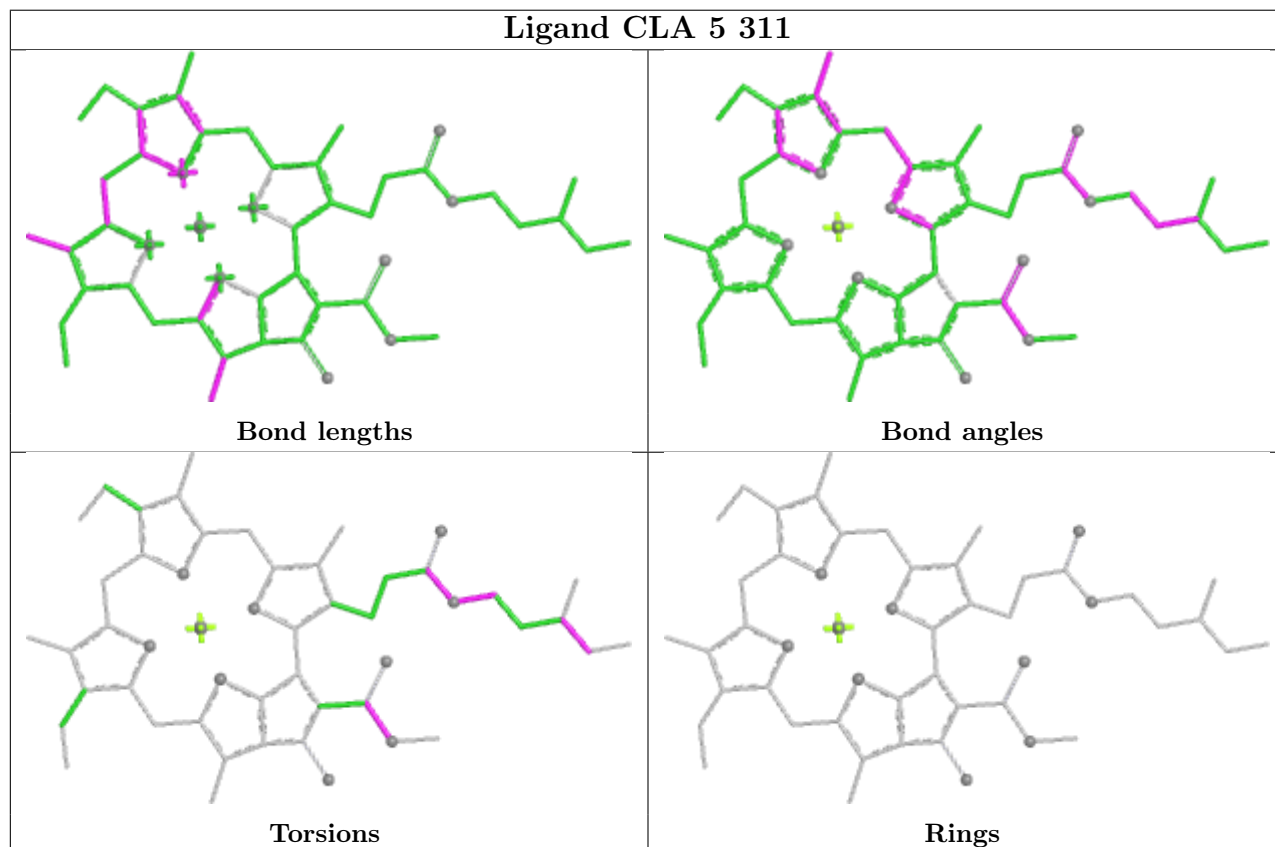
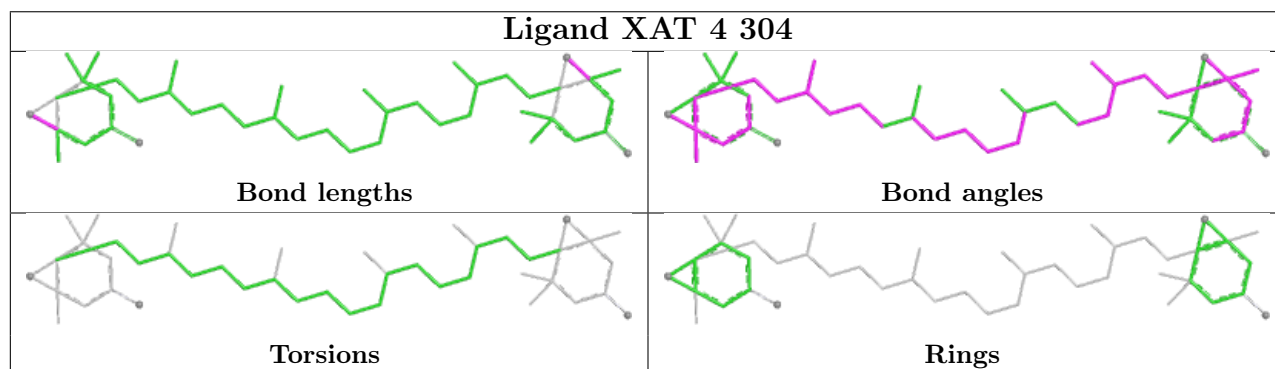
Bond angles



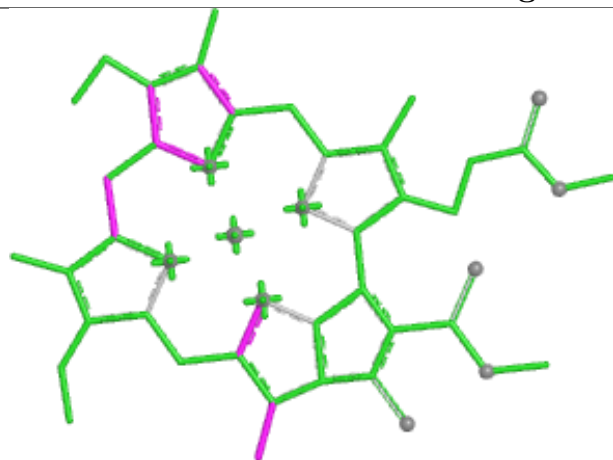
Torsions



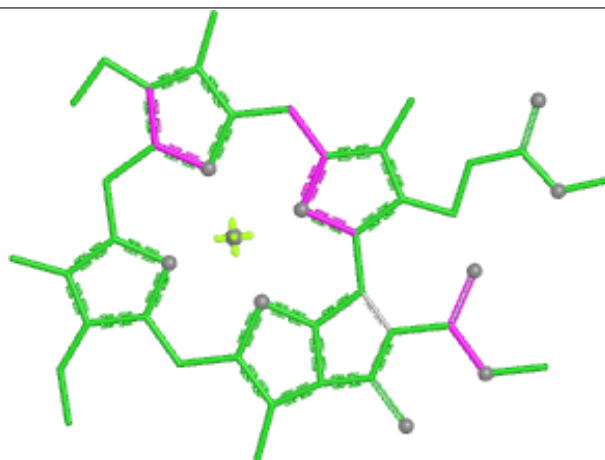
Rings

Ligand XAT 2 302**Ligand CLA 5 311****Ligand XAT 4 304**

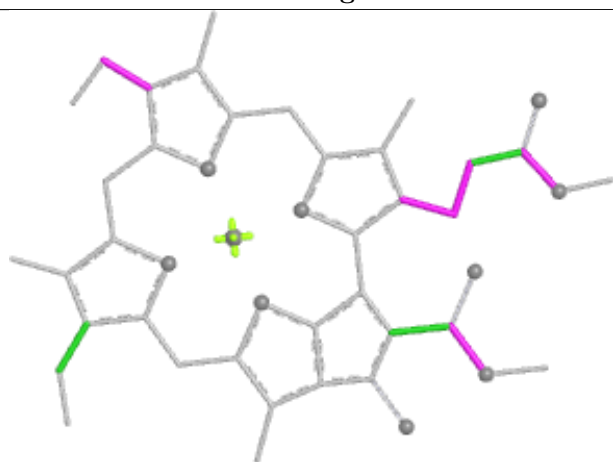
Ligand CLA 4 316



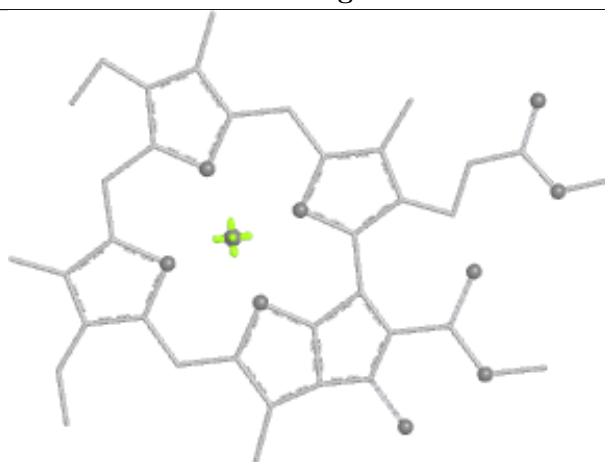
Bond lengths



Bond angles

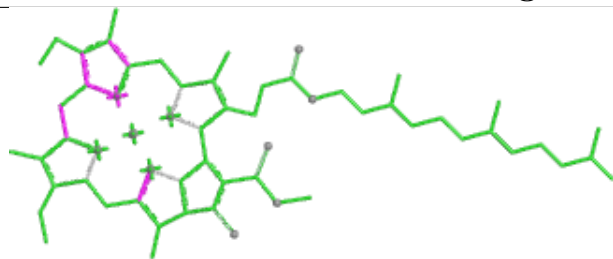


Torsions

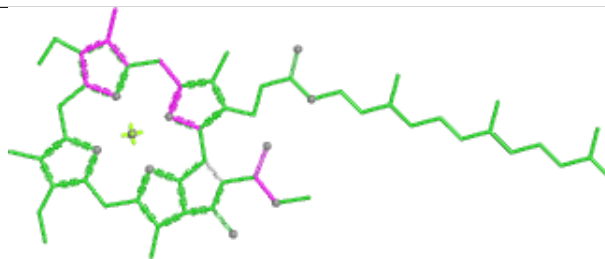


Rings

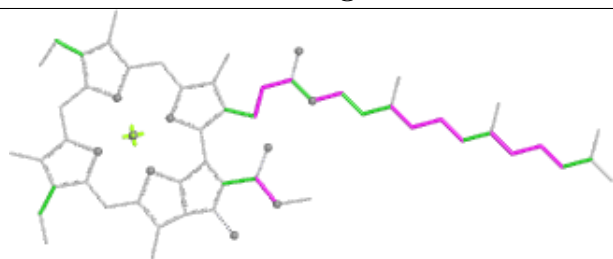
Ligand CLA 7 308



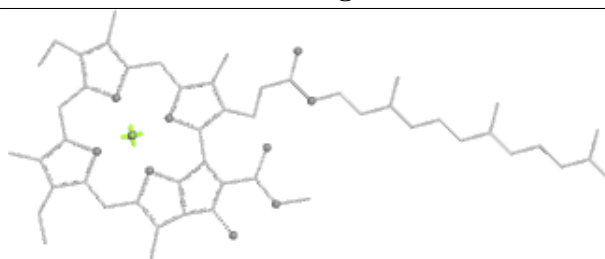
Bond lengths



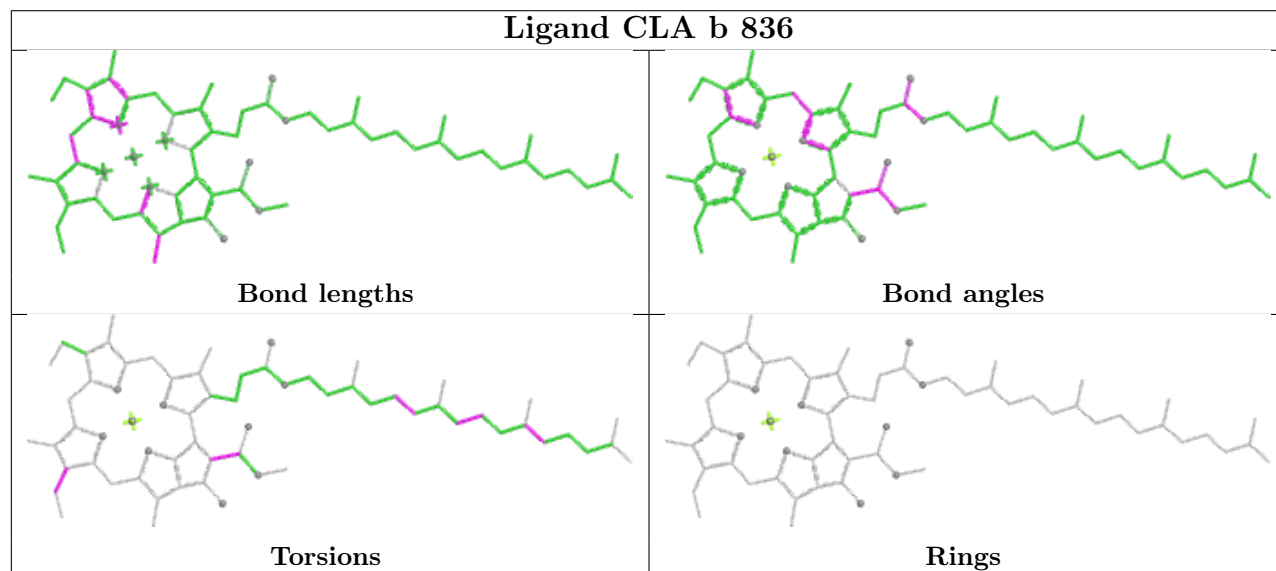
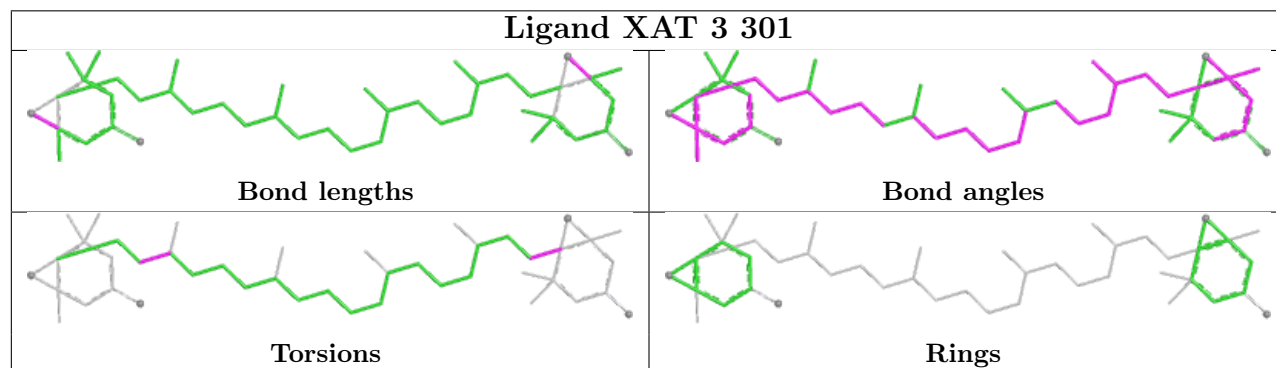
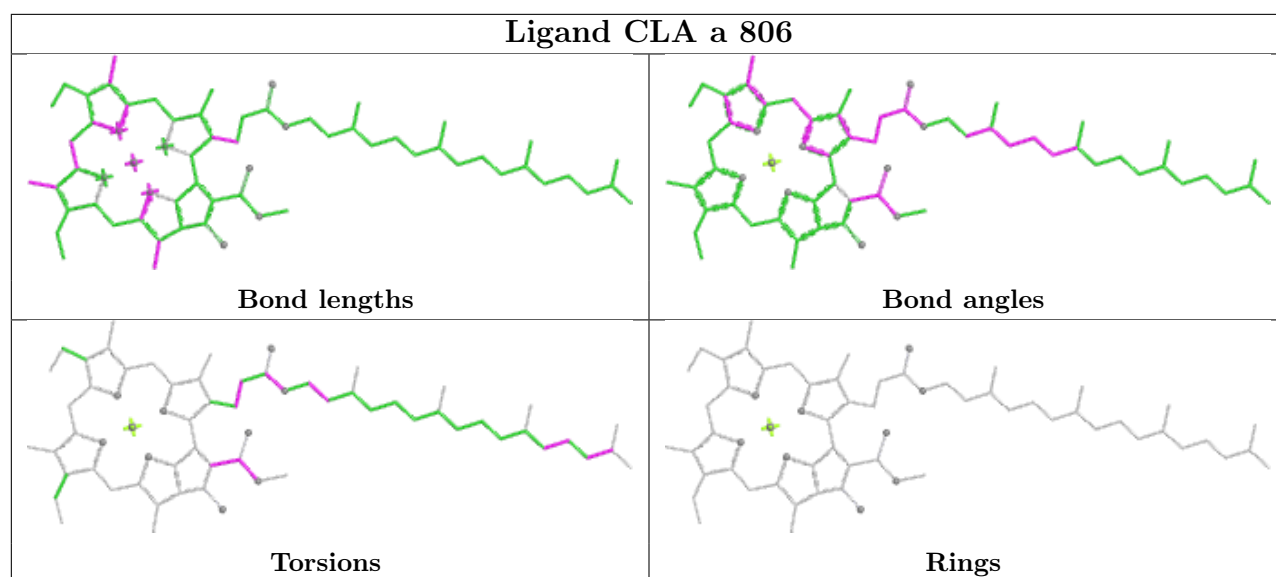
Bond angles

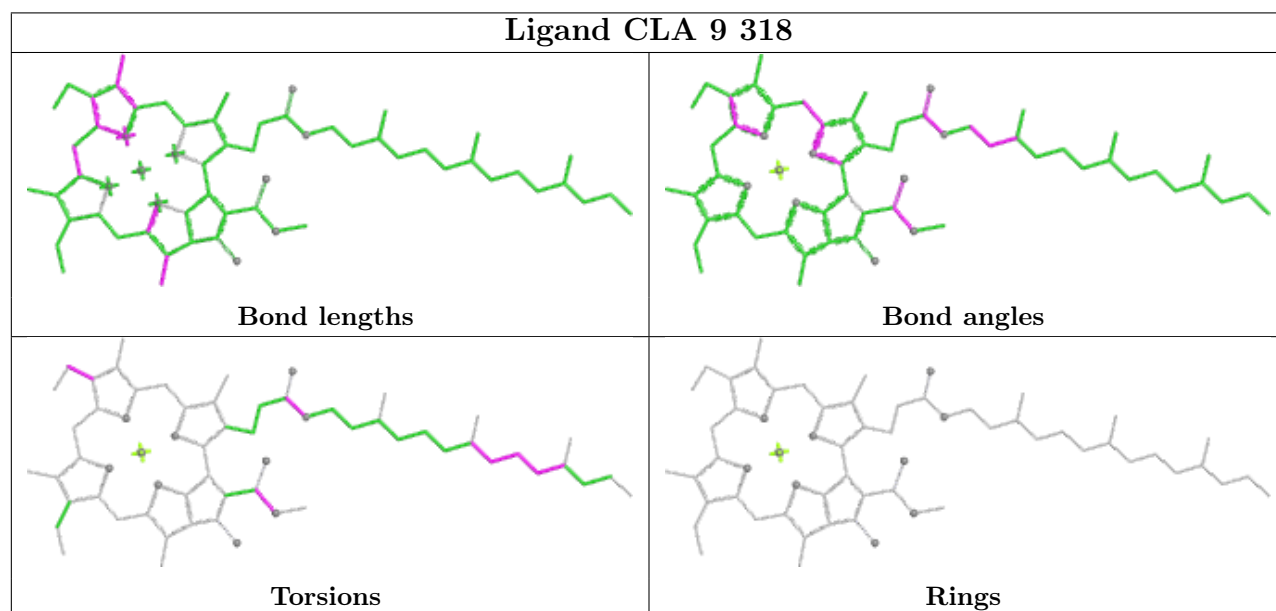
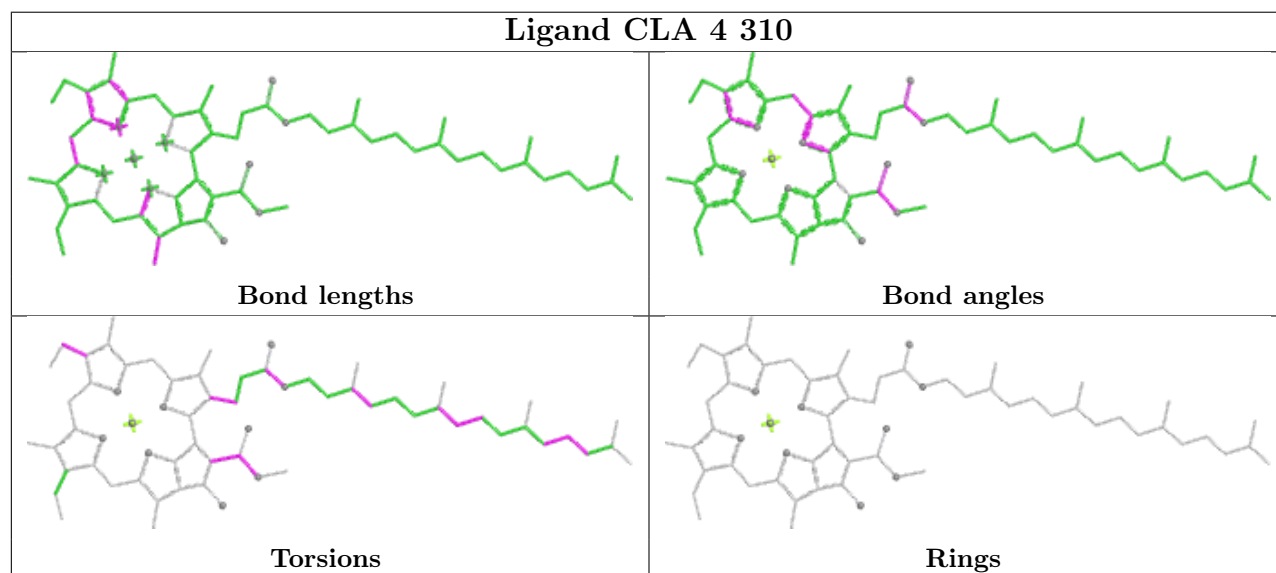
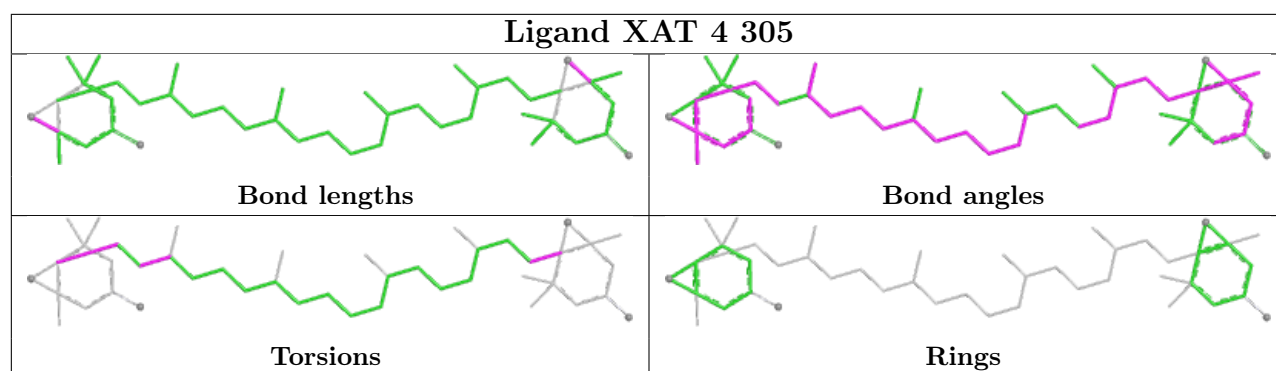


Torsions

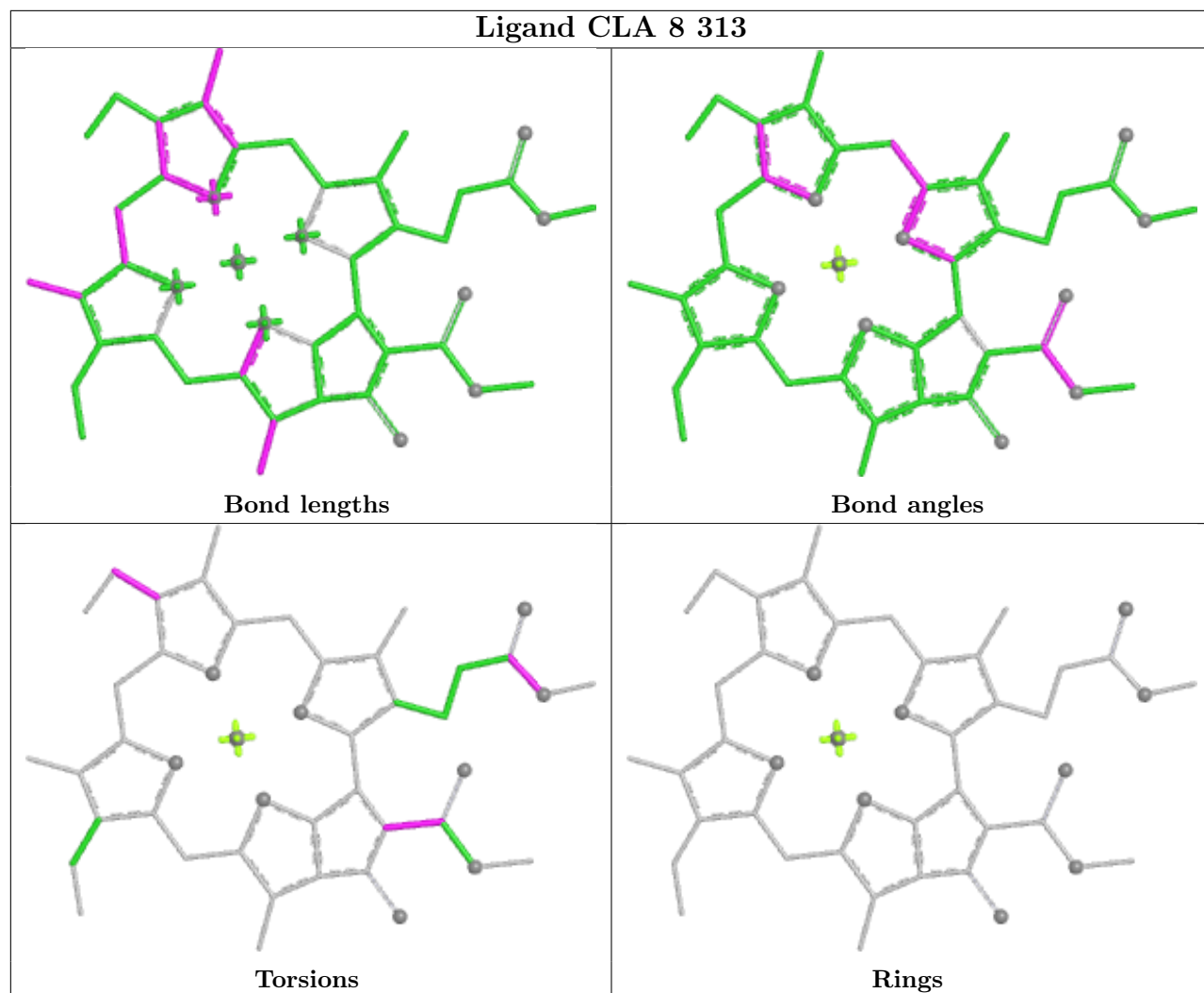


Rings

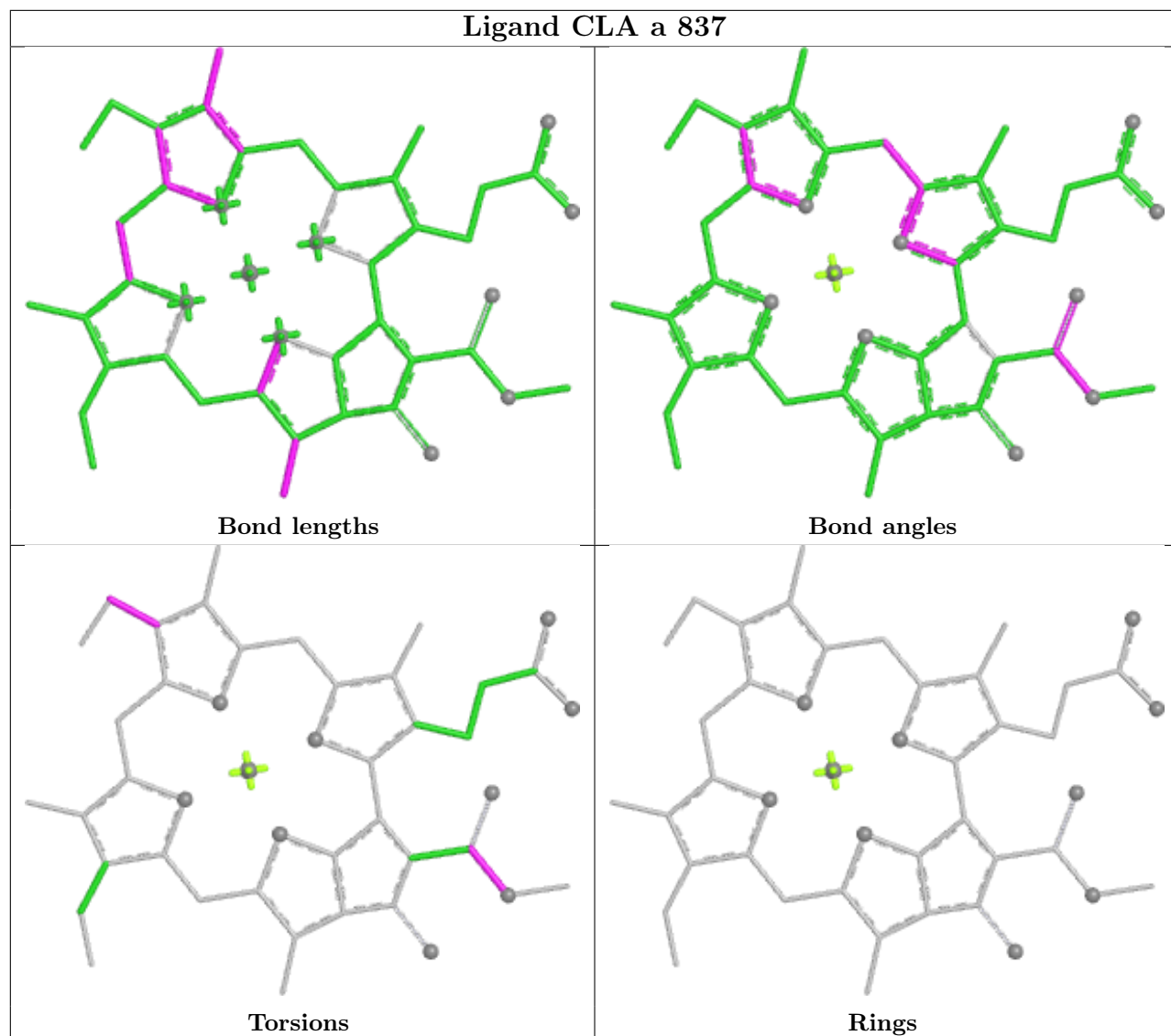




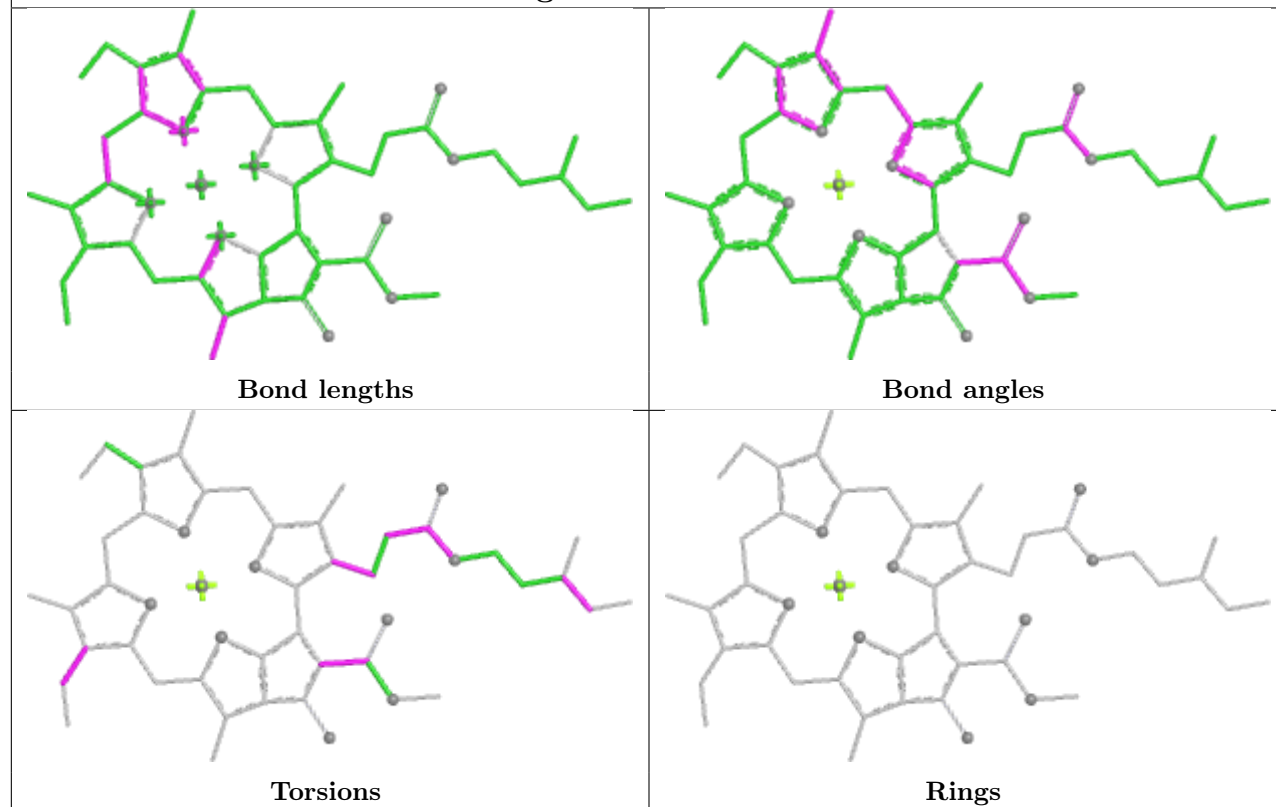
Ligand CLA 8 313



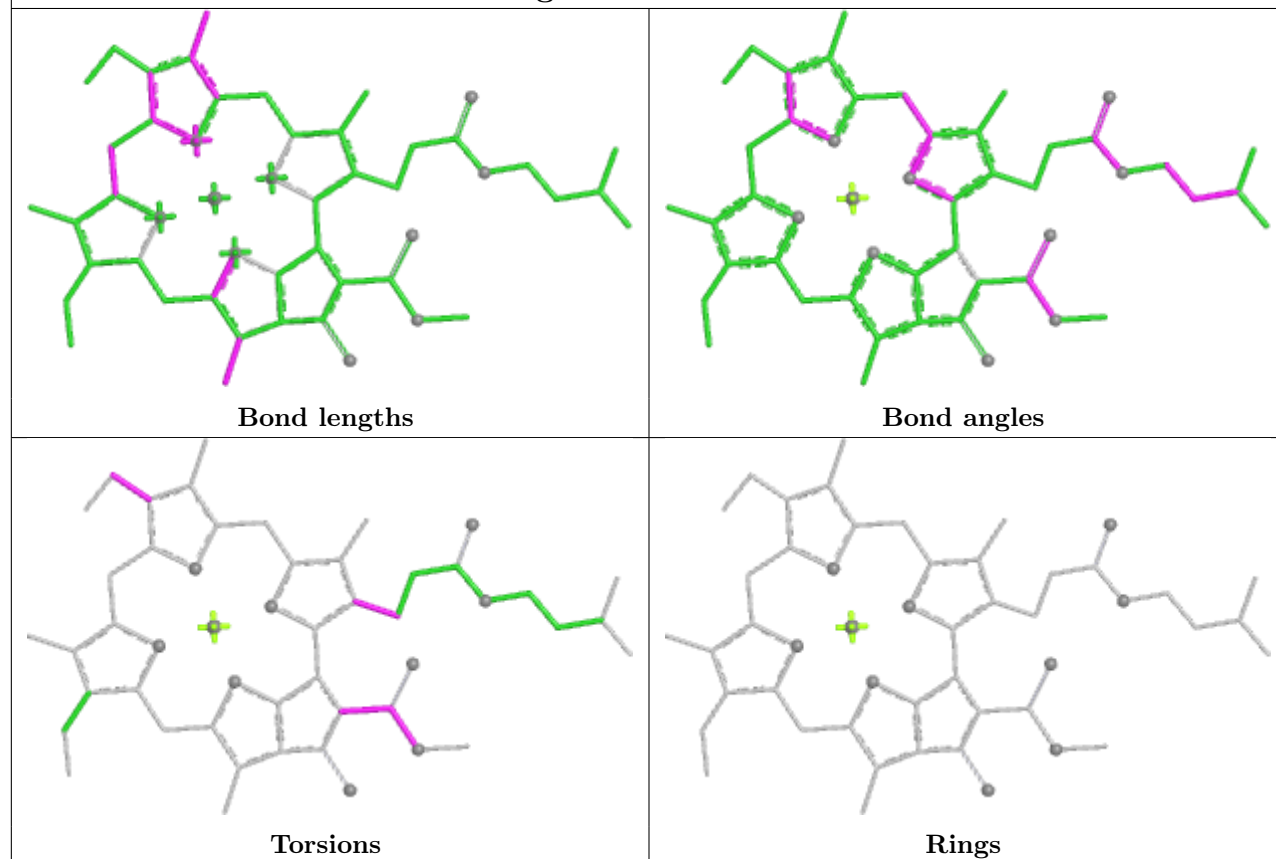
Ligand CLA a 837

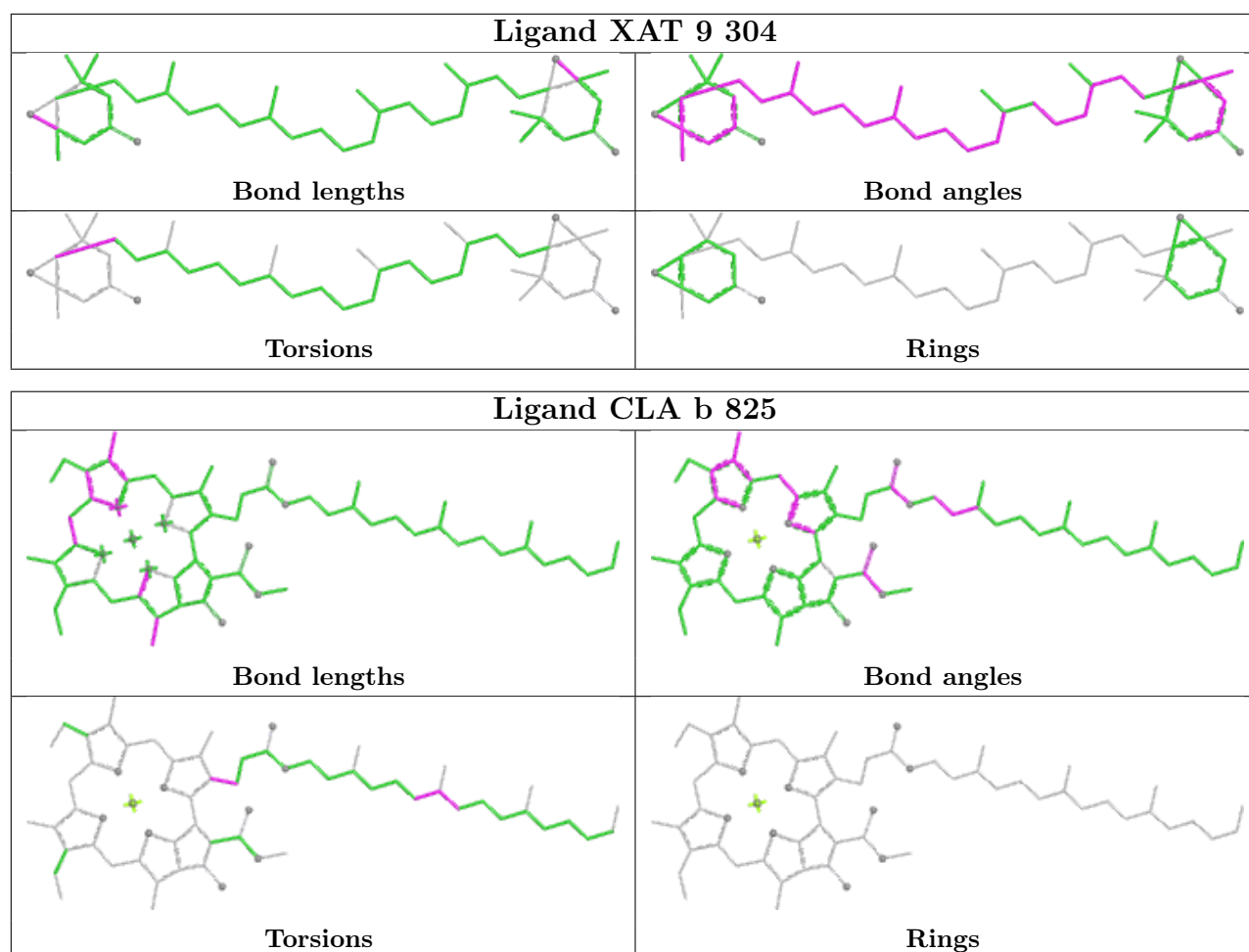


Ligand CLA 7 316

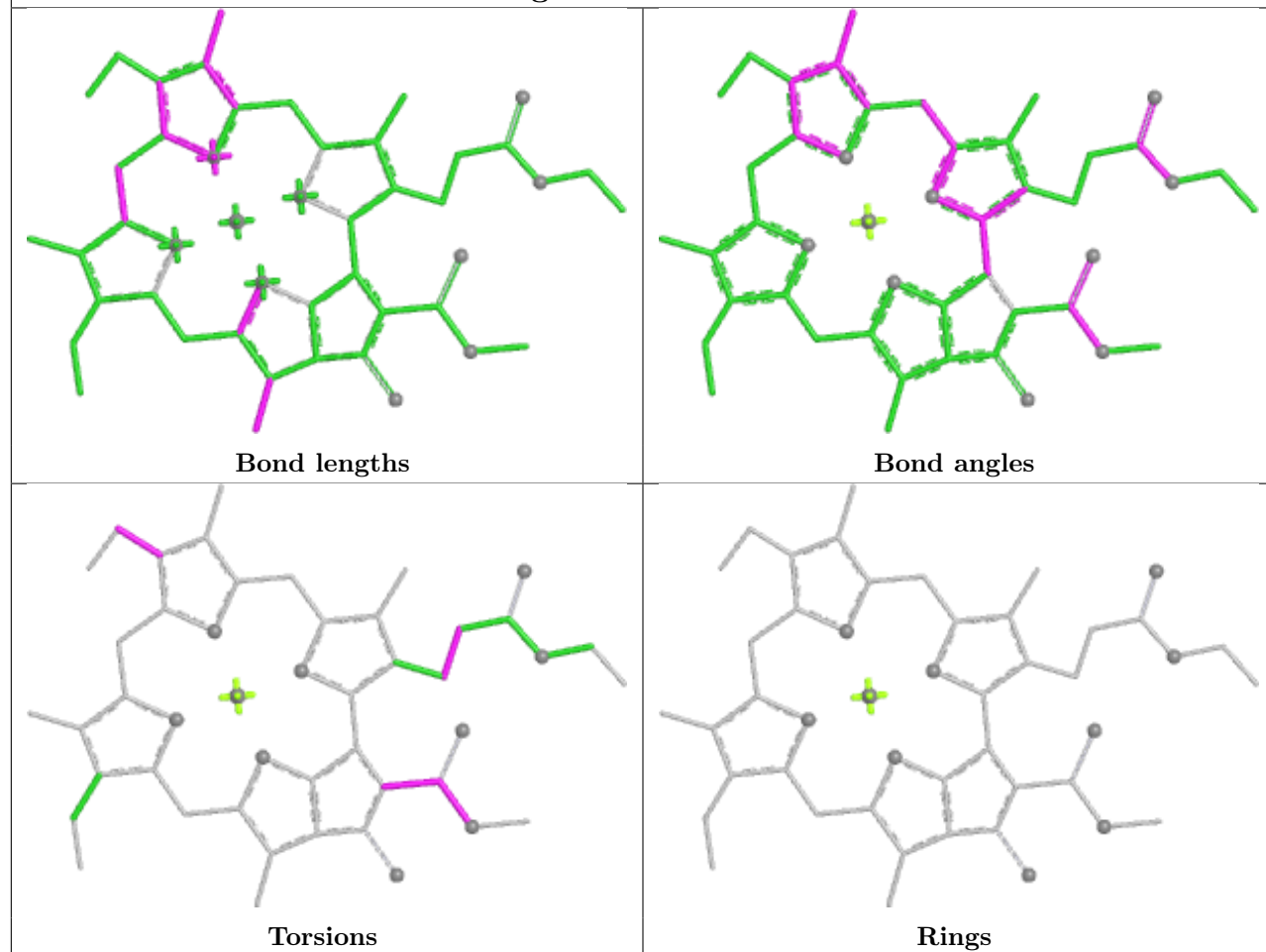


Ligand CLA a 832

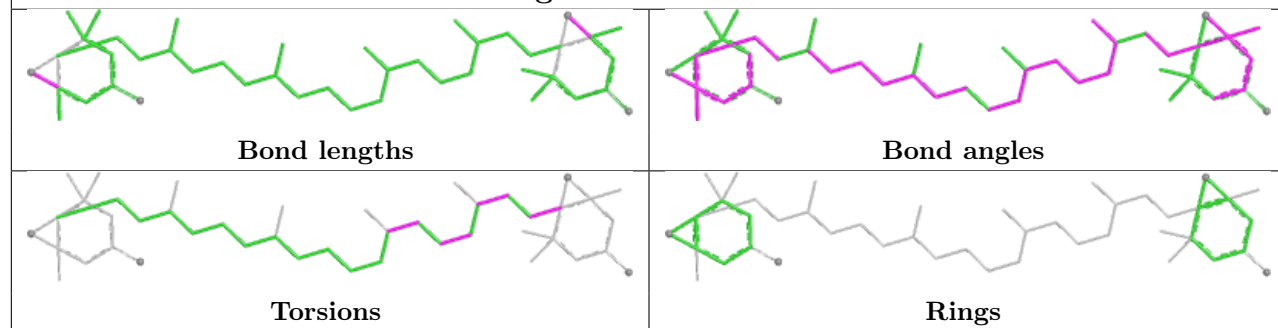




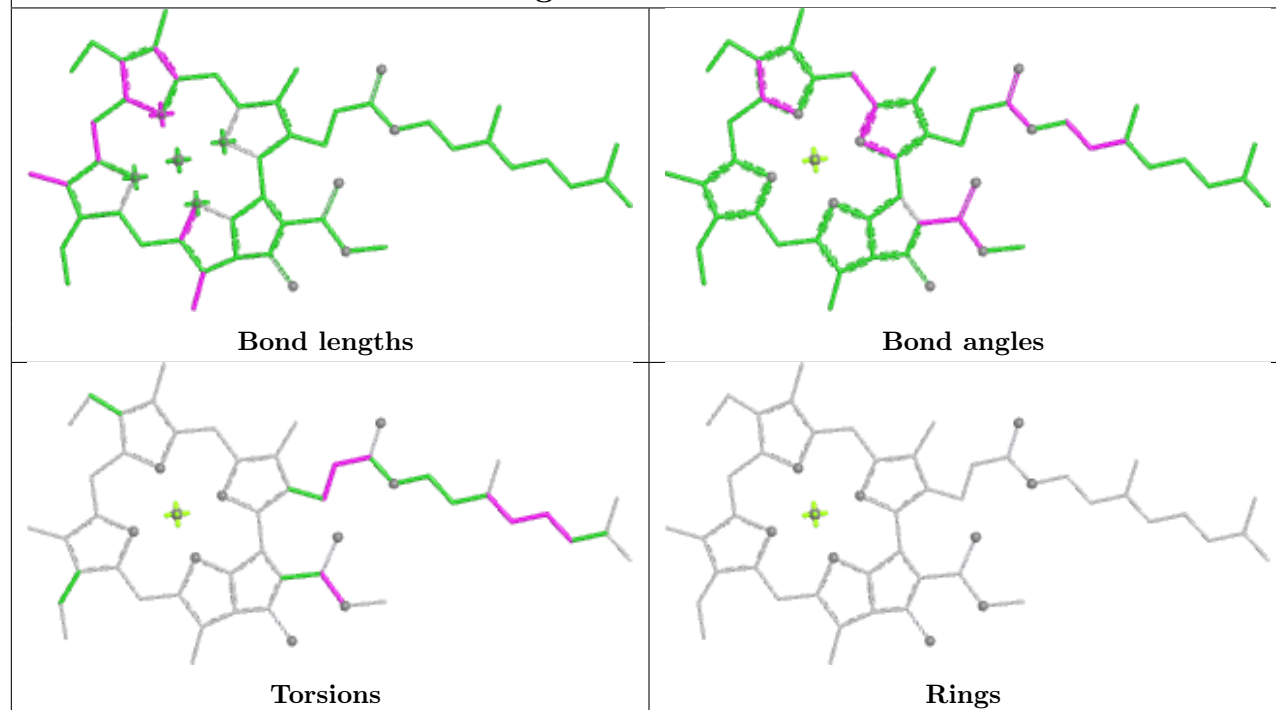
Ligand CLA 2 307



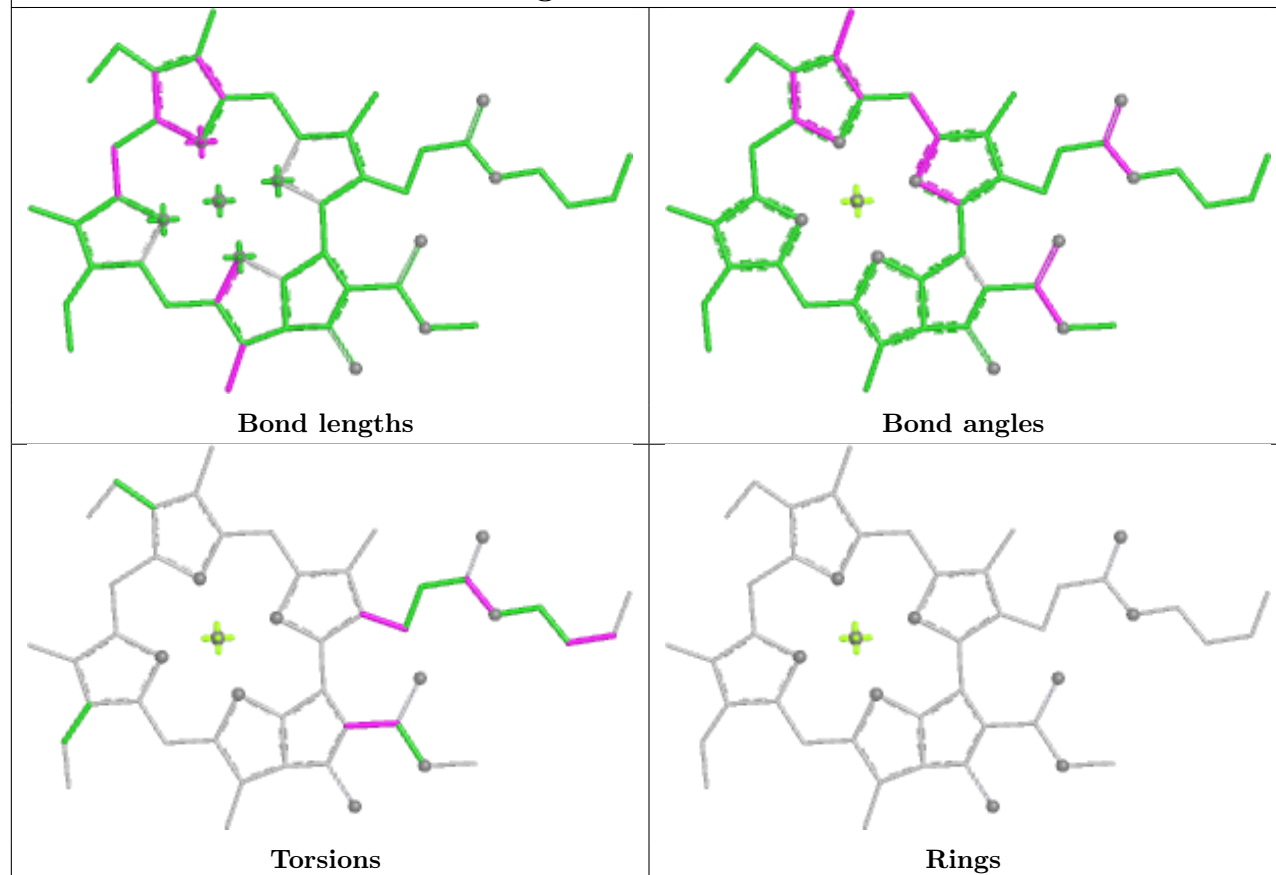
Ligand XAT 7 304

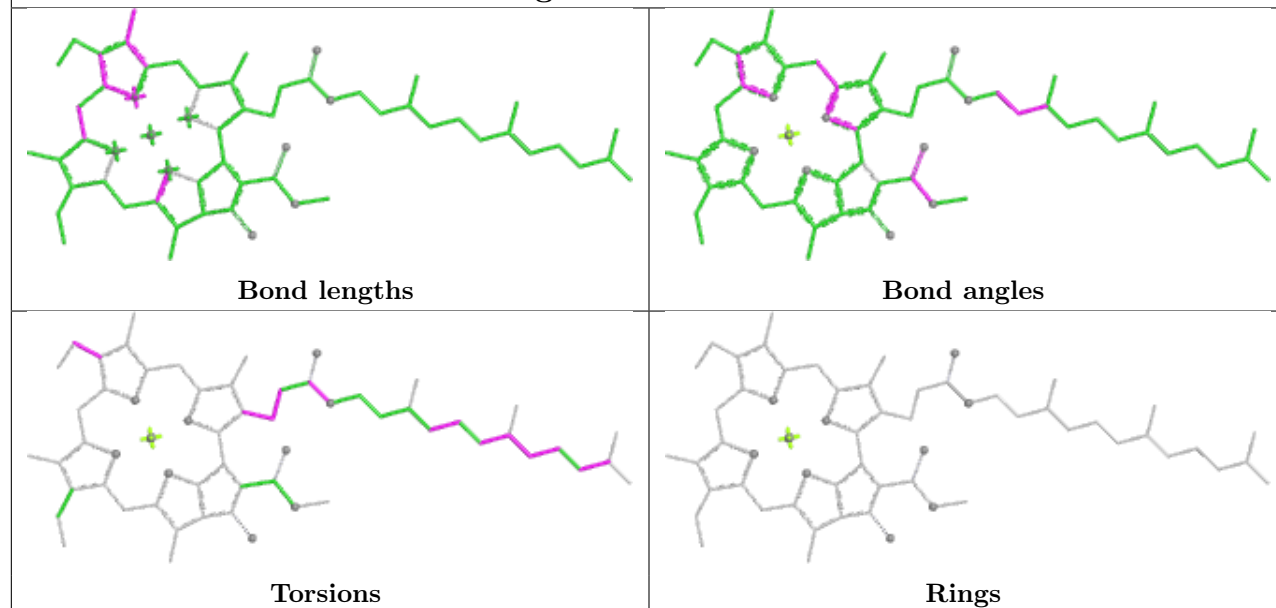
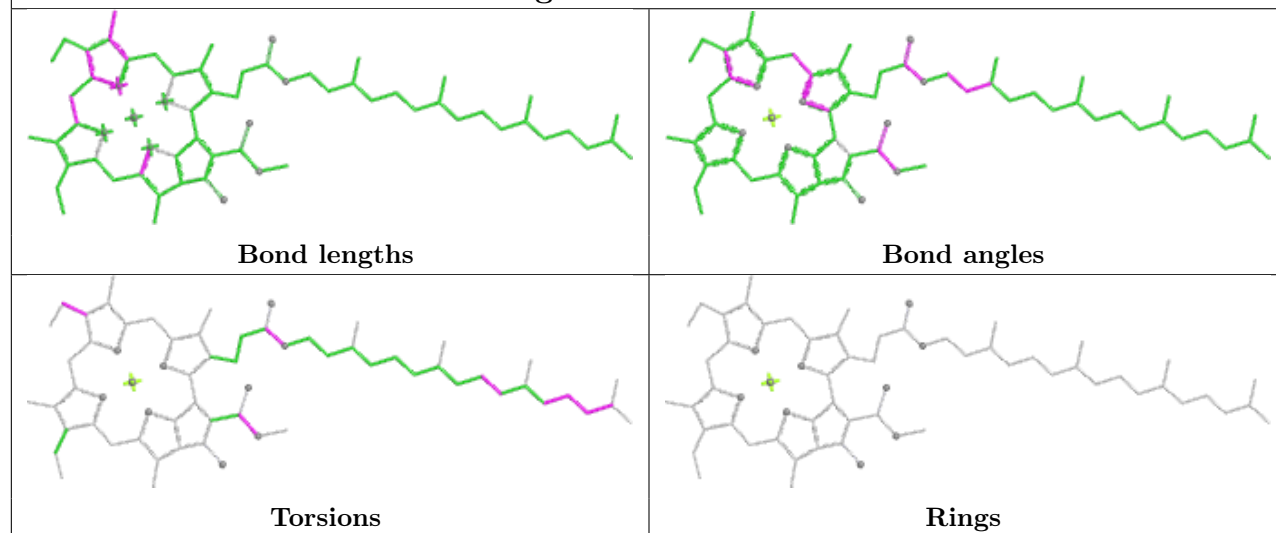


Ligand CLA h 205

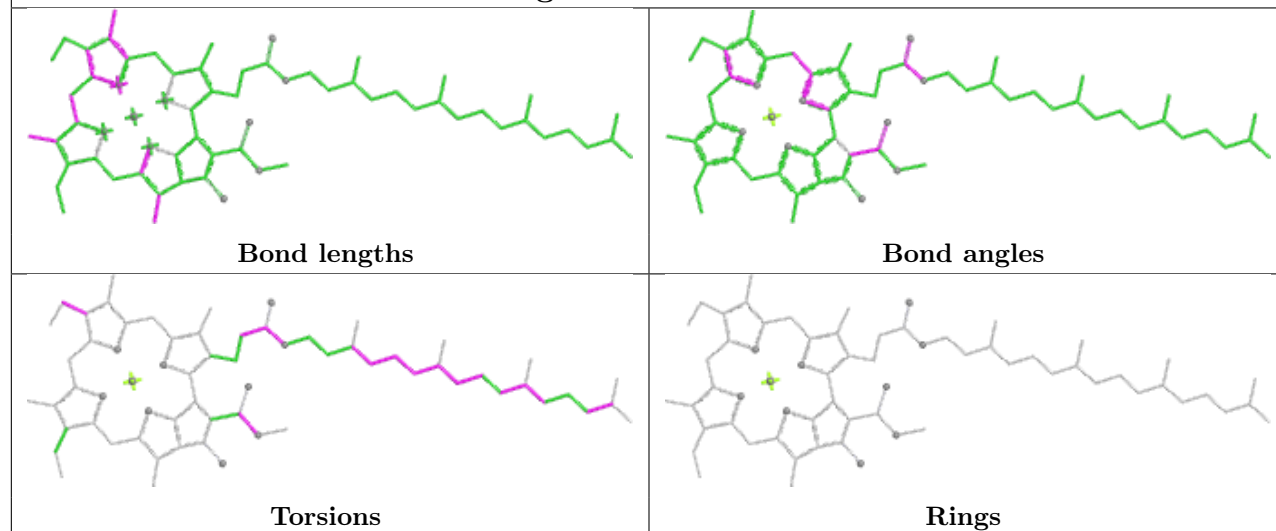


Ligand CLA a 823

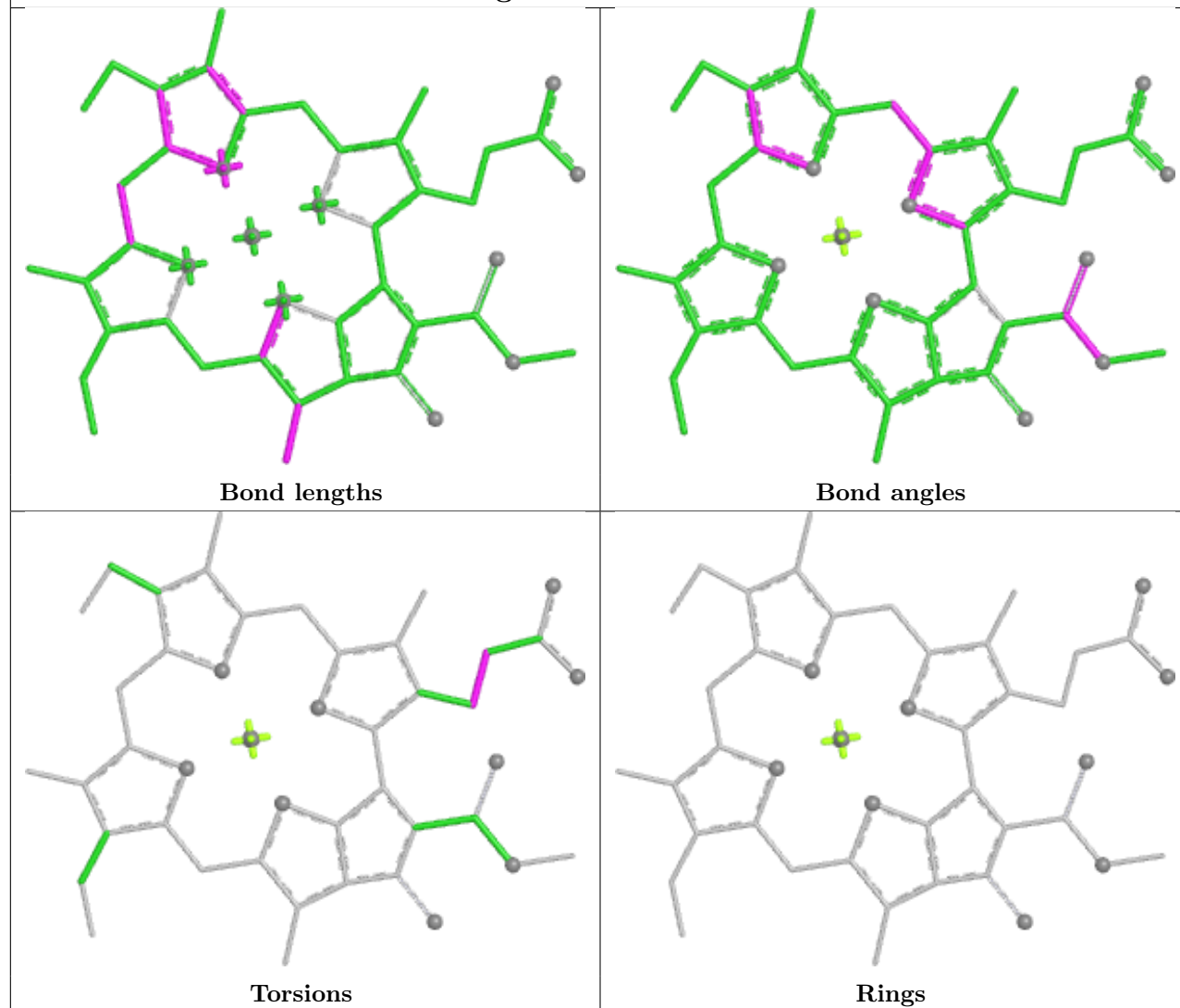


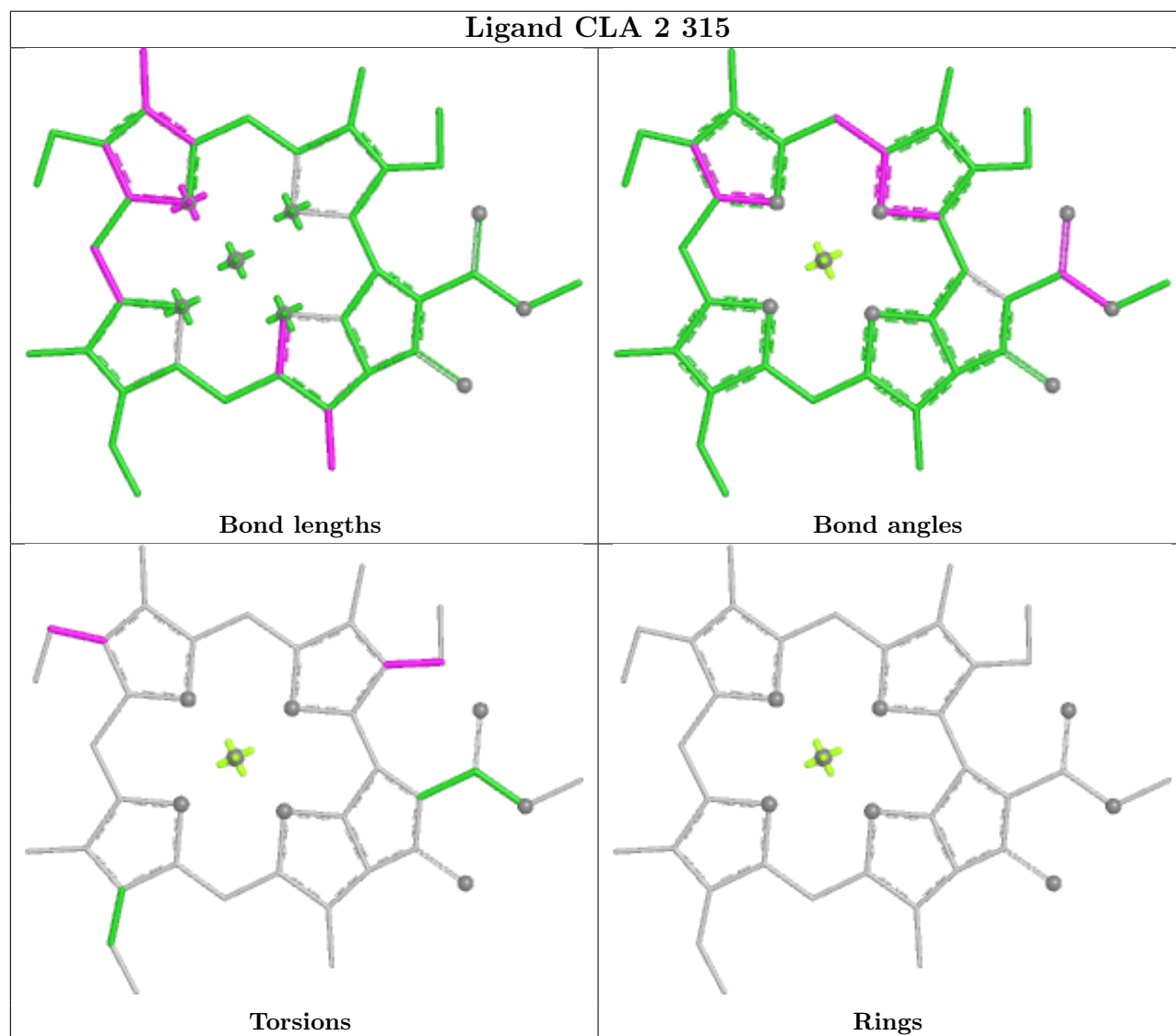
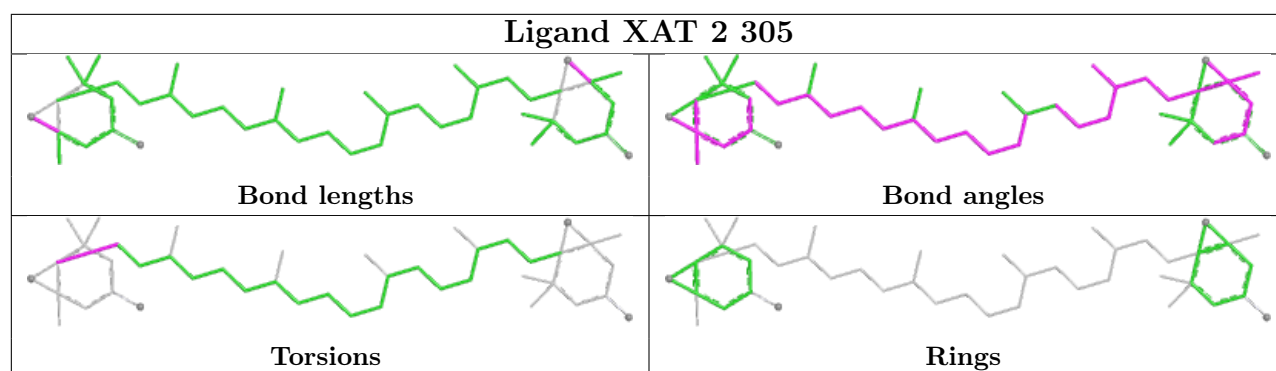
Ligand CLA b 818**Ligand CLA b 840**

Ligand CLA a 801

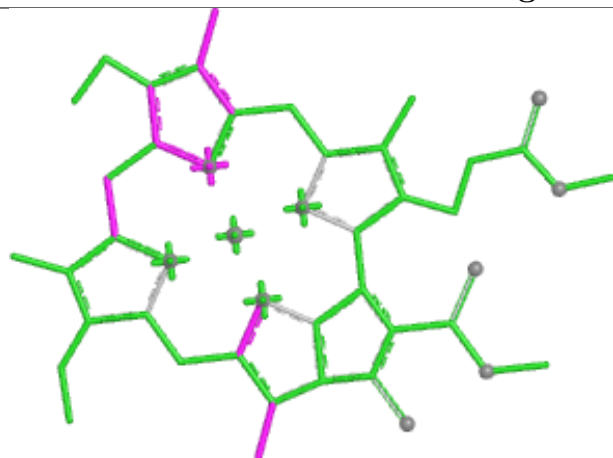


Ligand CLA a 821

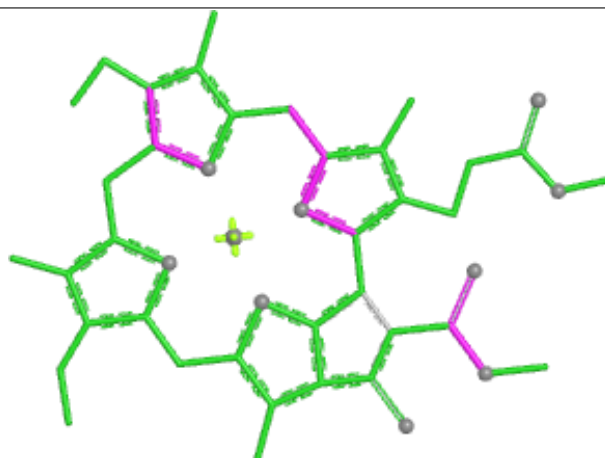




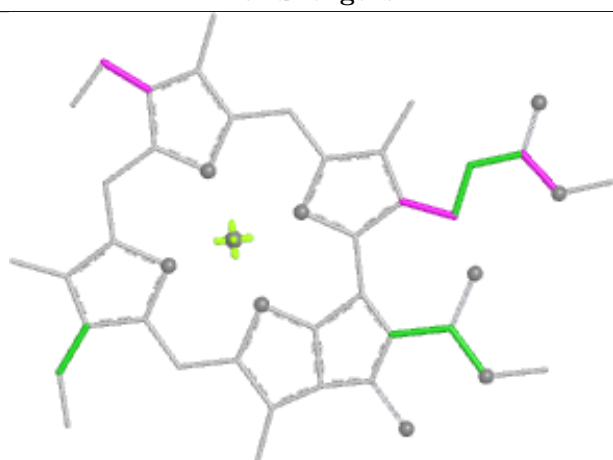
Ligand CLA a 824



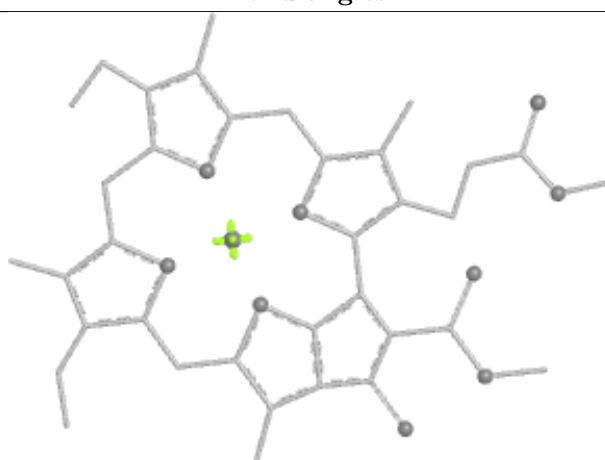
Bond lengths



Bond angles

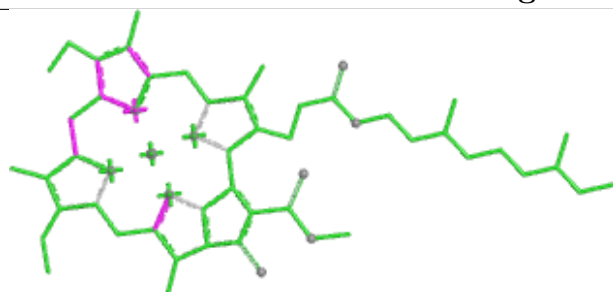


Torsions

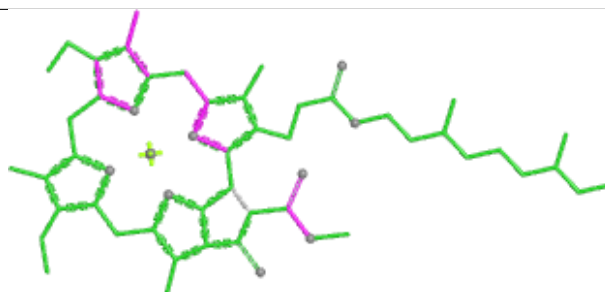


Rings

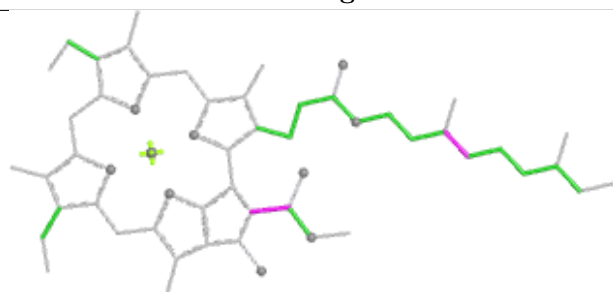
Ligand CLA 3 310



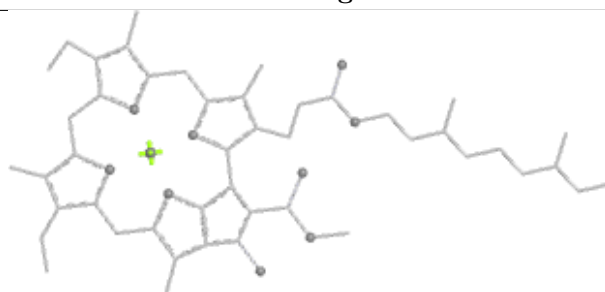
Bond lengths



Bond angles

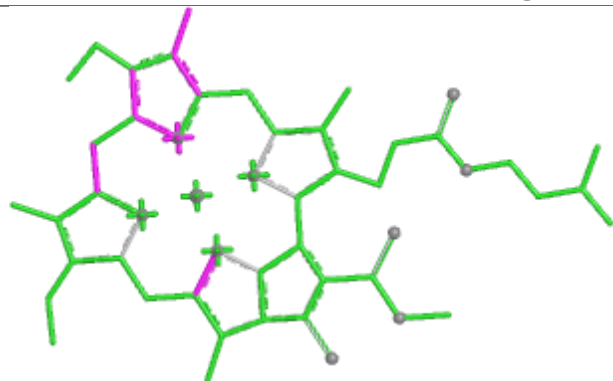


Torsions

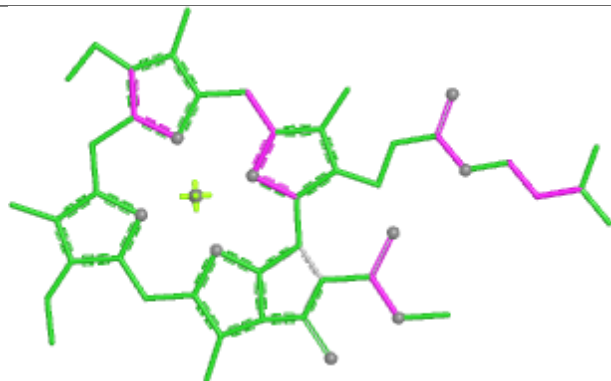


Rings

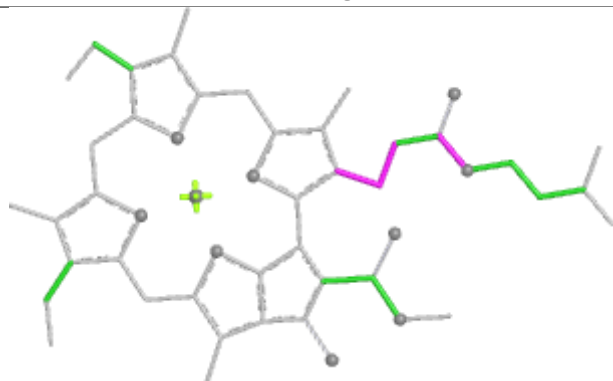
Ligand CLA 3 311



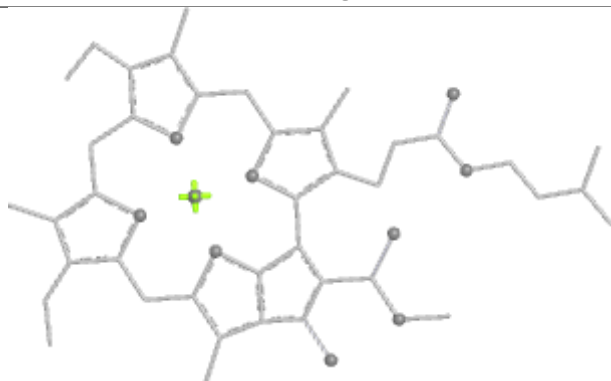
Bond lengths



Bond angles

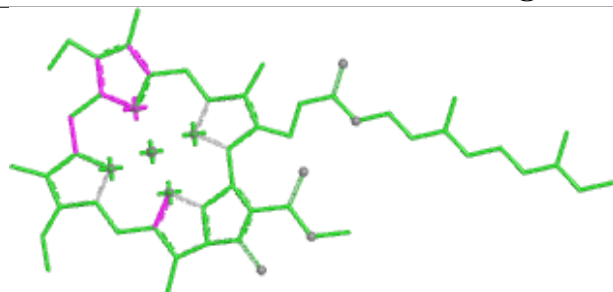


Torsions

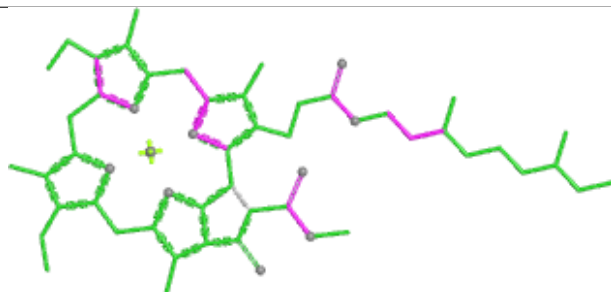


Rings

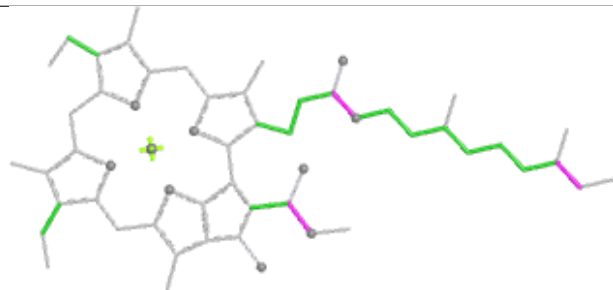
Ligand CLA a 811



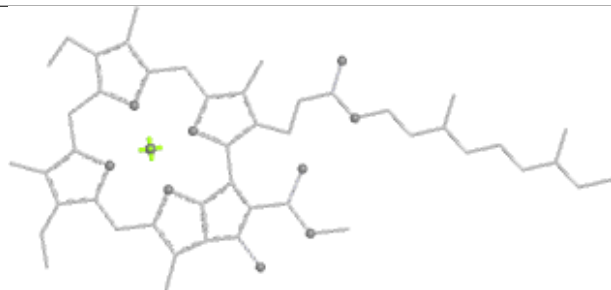
Bond lengths



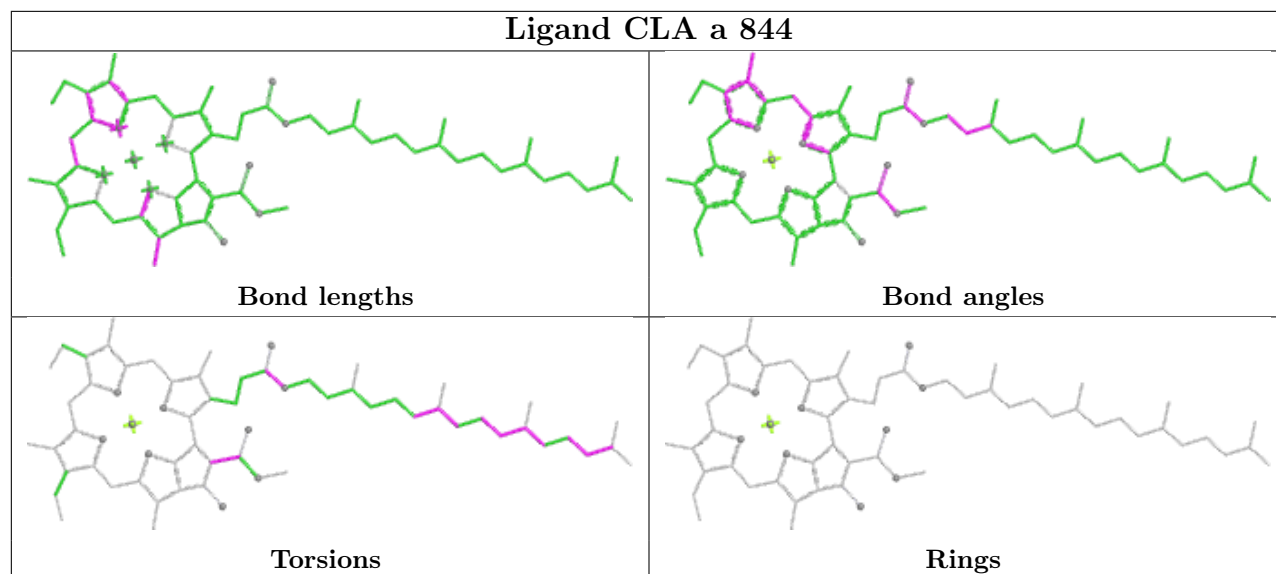
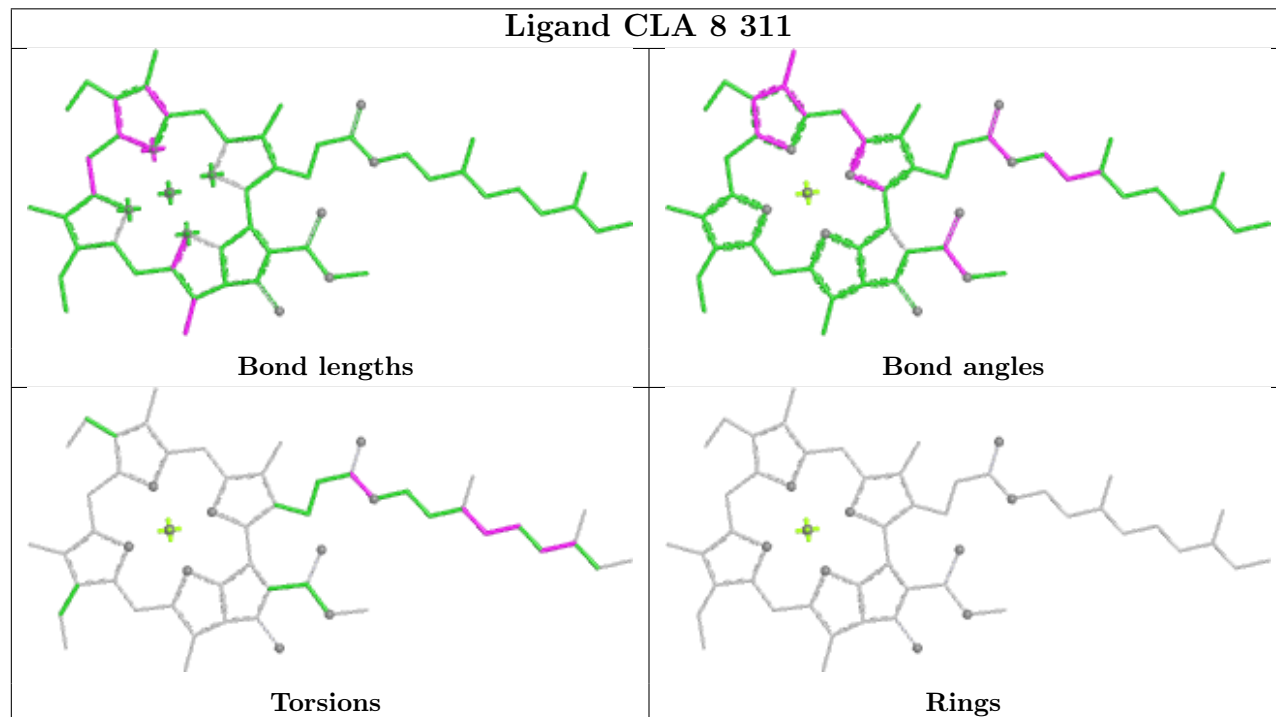
Bond angles



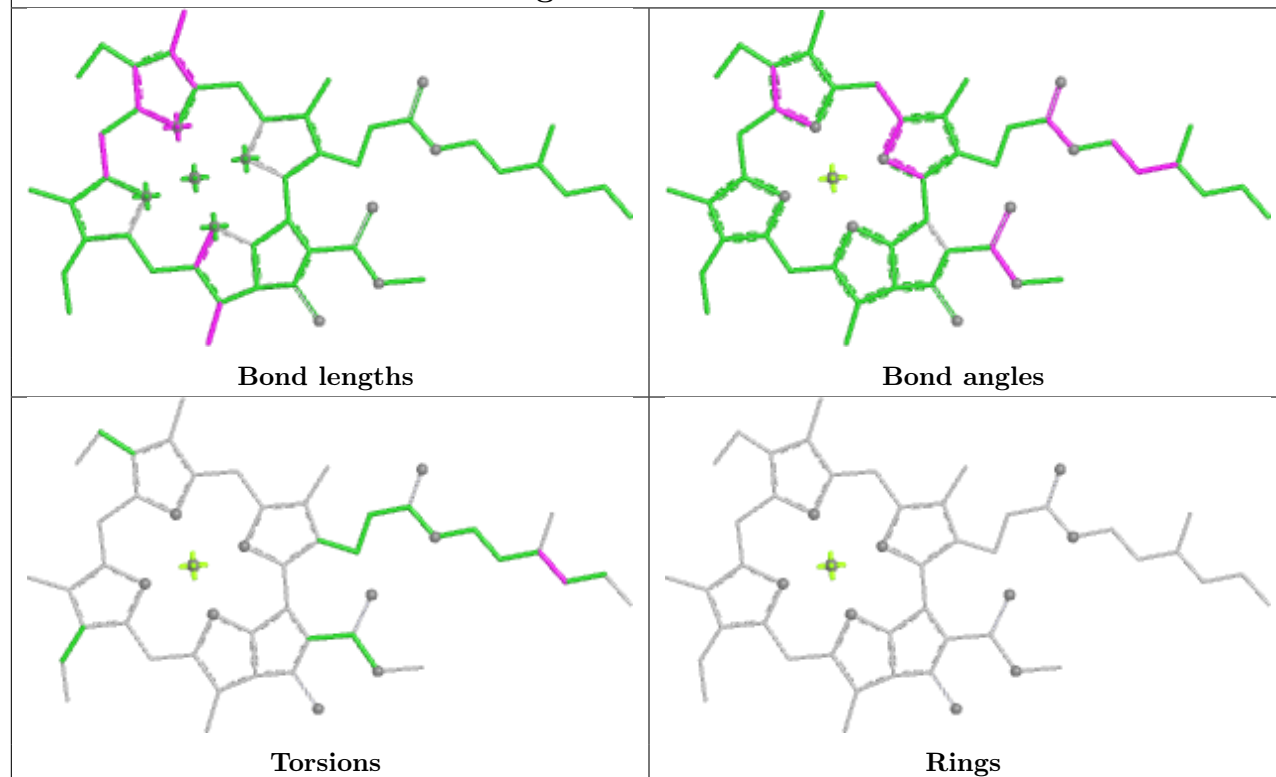
Torsions



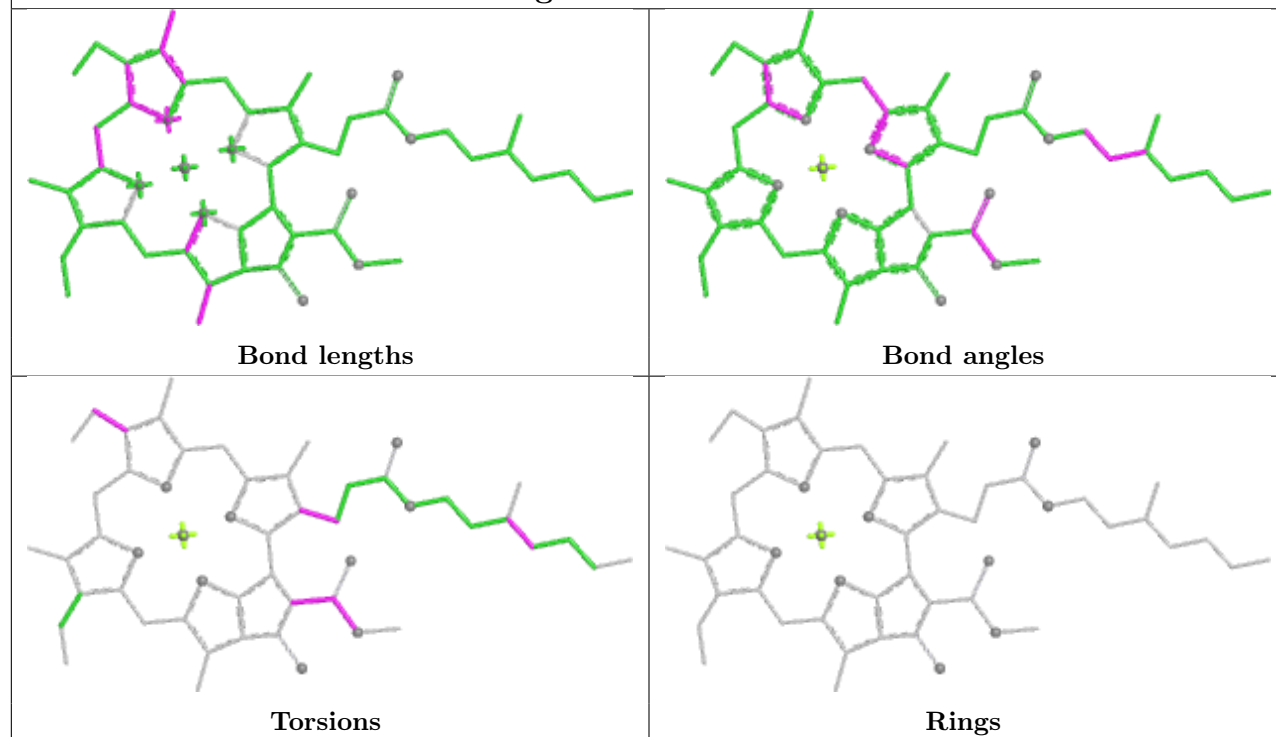
Rings

Ligand CLA a 844**Ligand CLA 8 311**

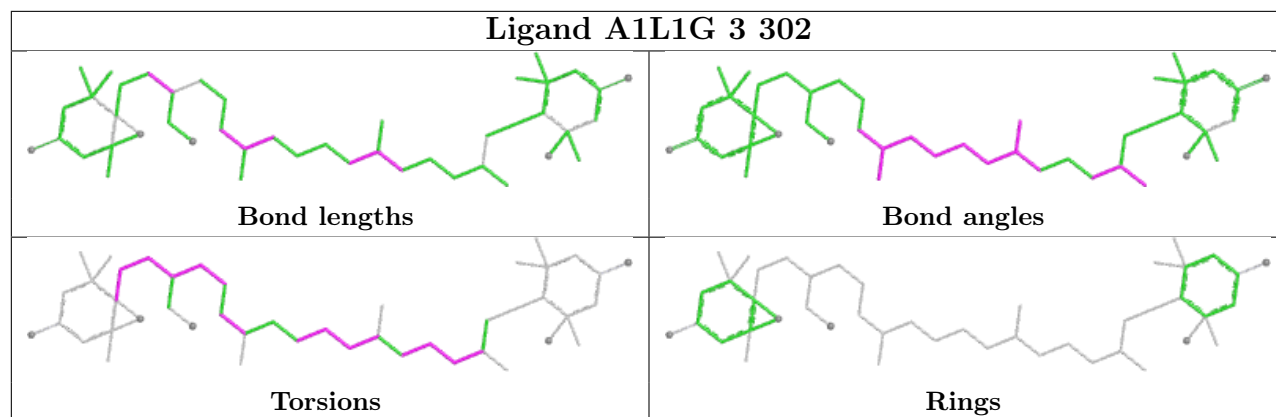
Ligand CLA 3 313



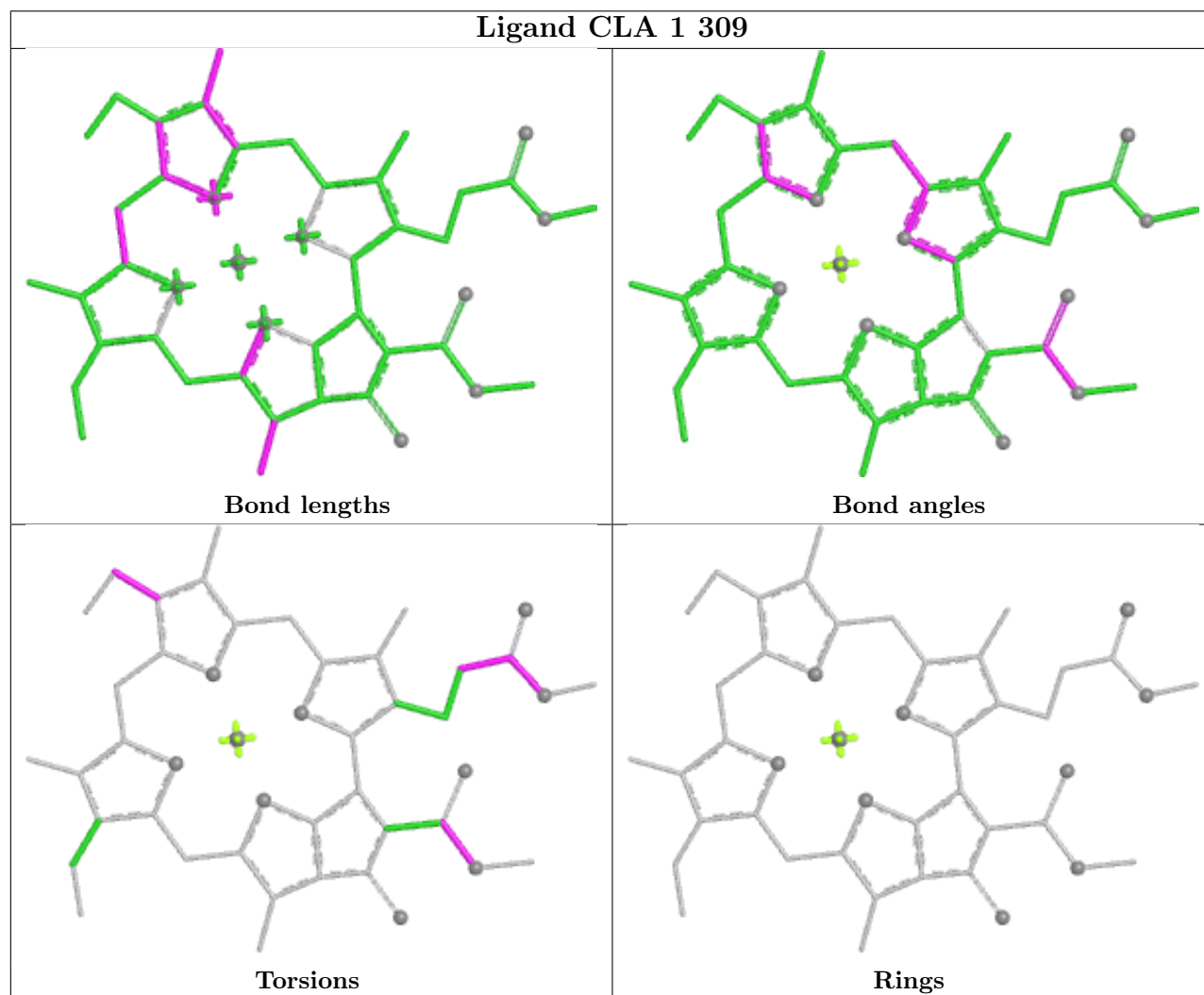
Ligand CLA b 834



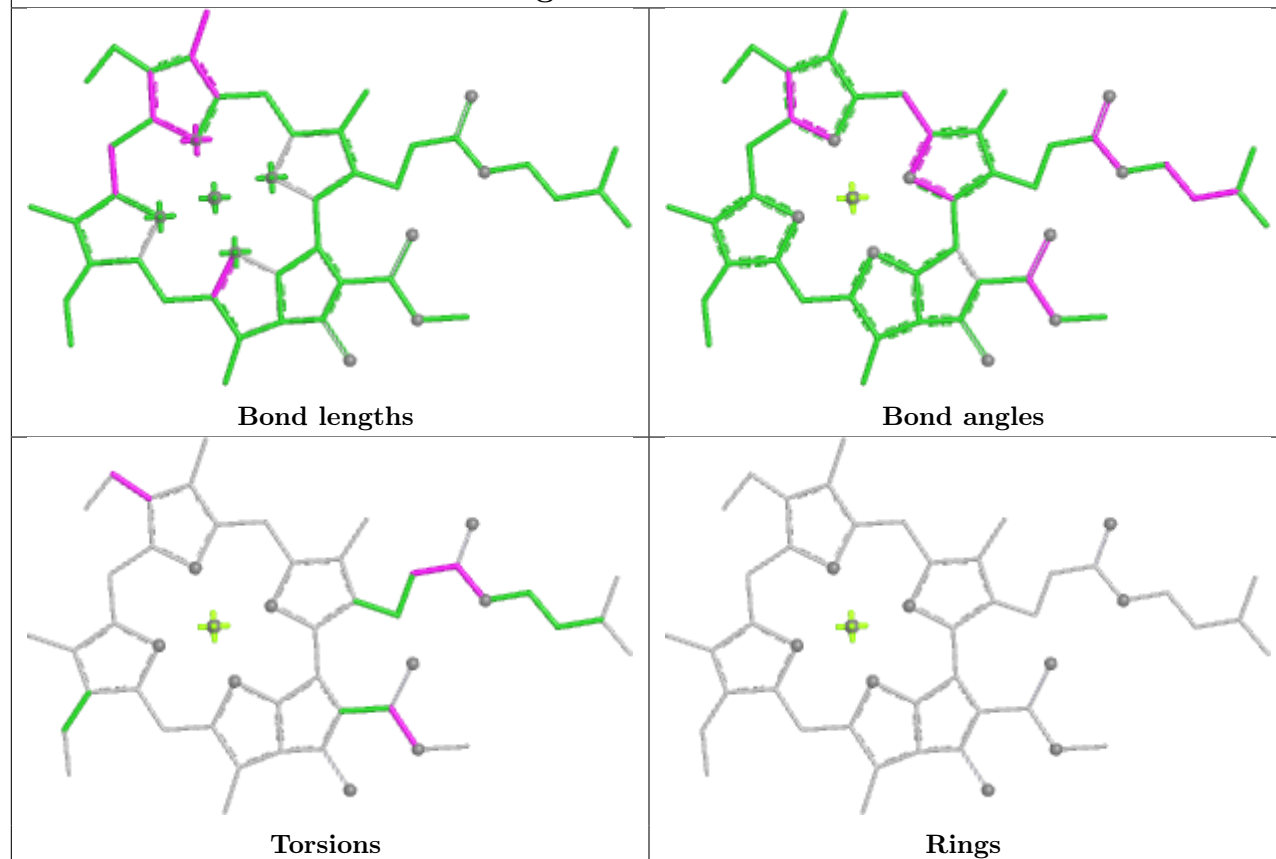
Ligand A1L1G 3 302



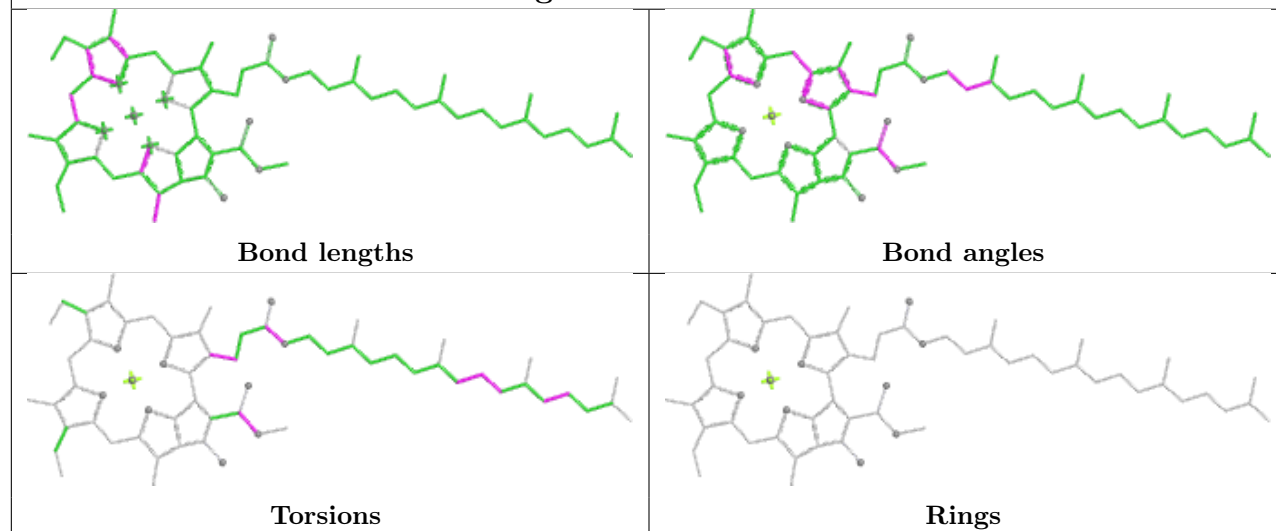
Ligand CLA 1 309



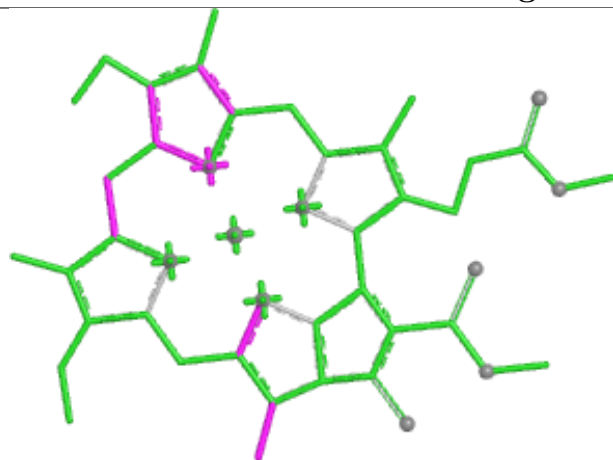
Ligand CLA a 836



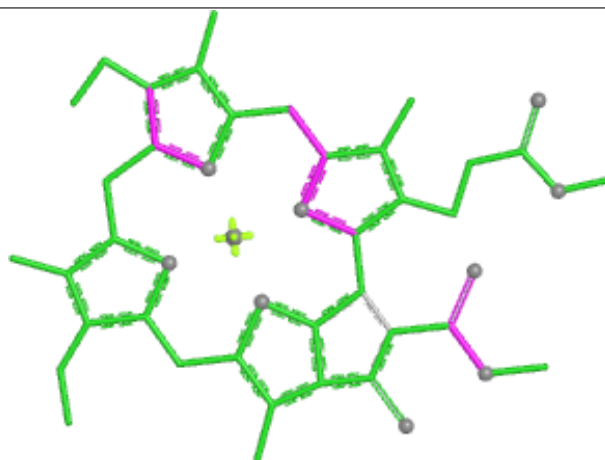
Ligand CLA h 203



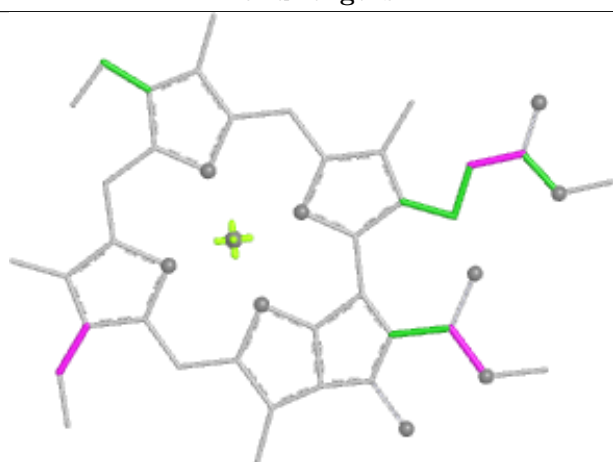
Ligand CLA 5 315



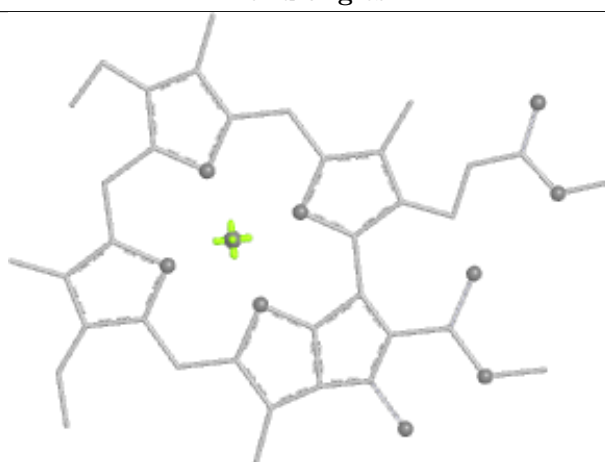
Bond lengths



Bond angles

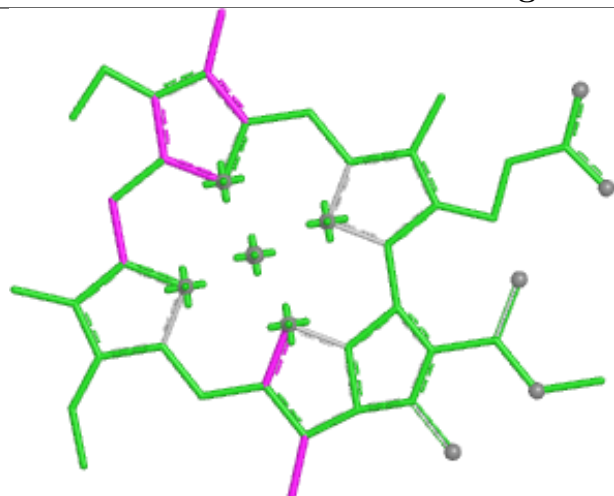


Torsions

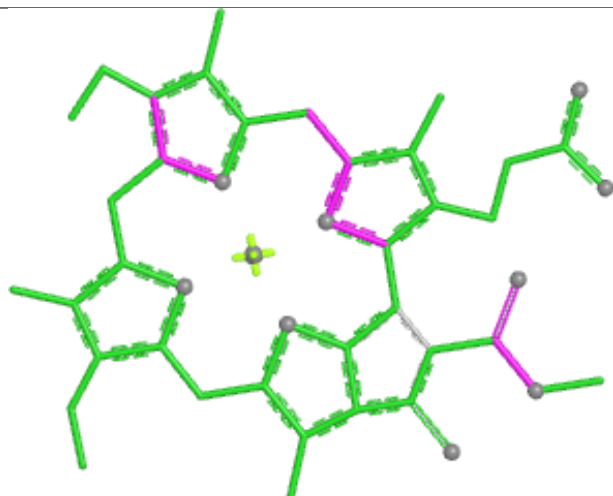


Rings

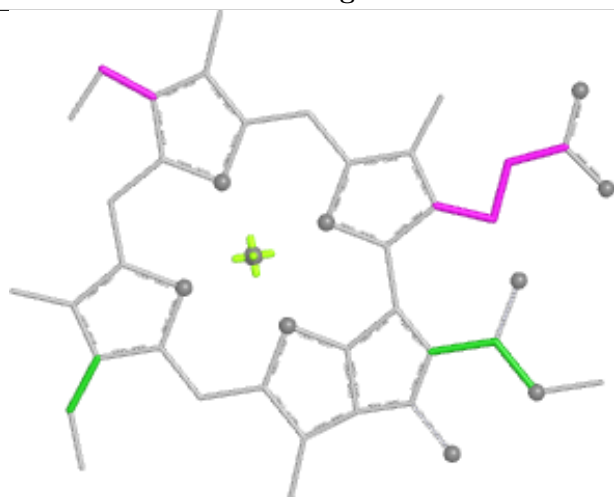
Ligand CLA 1 314



Bond lengths



Bond angles

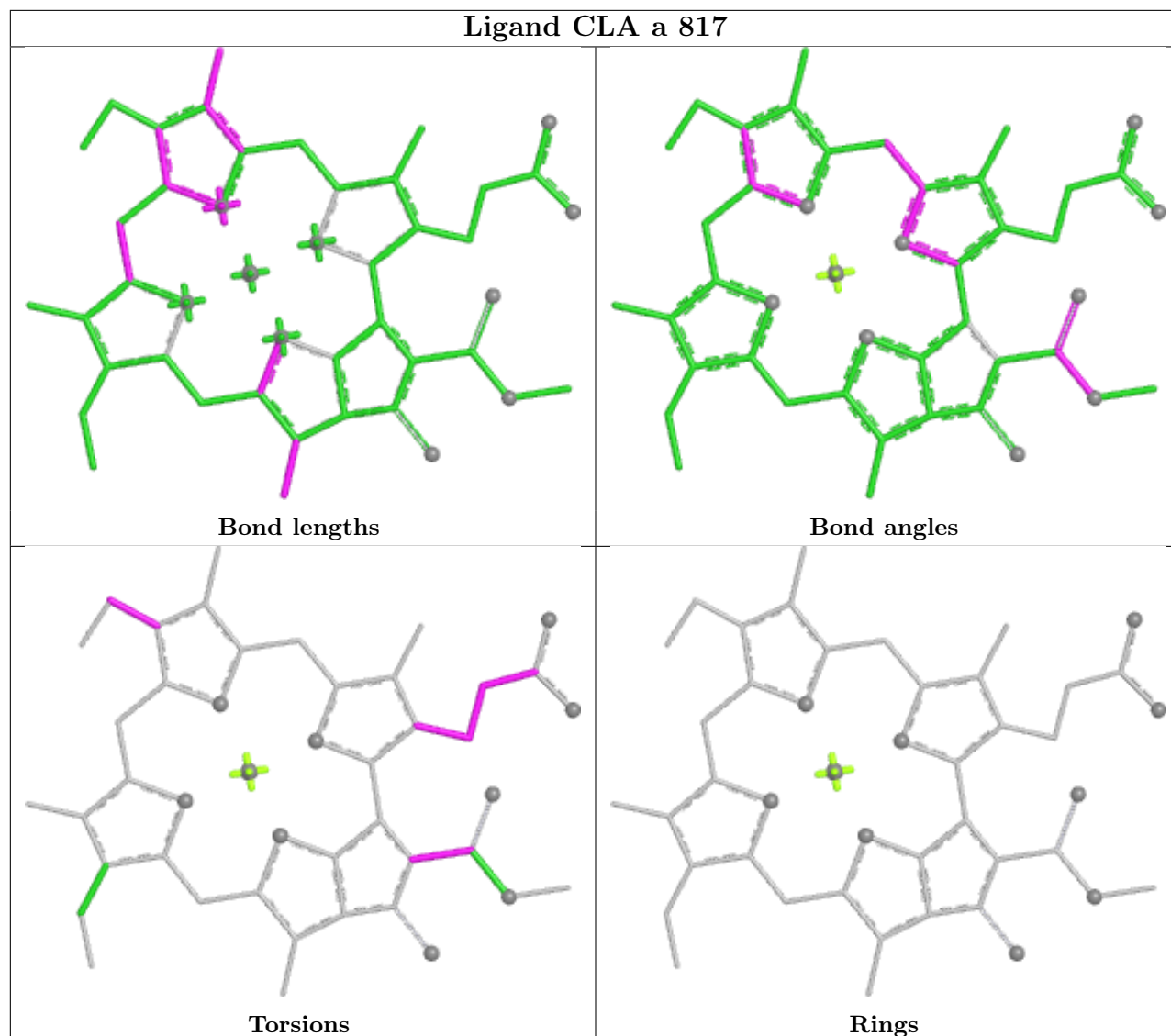


Torsions

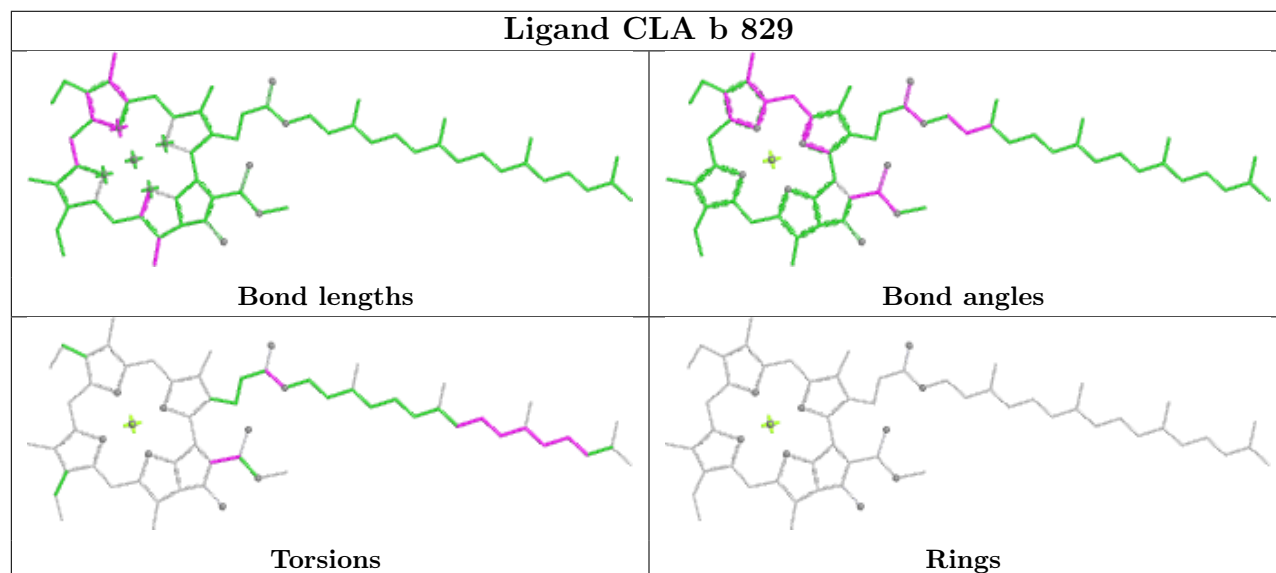


Rings

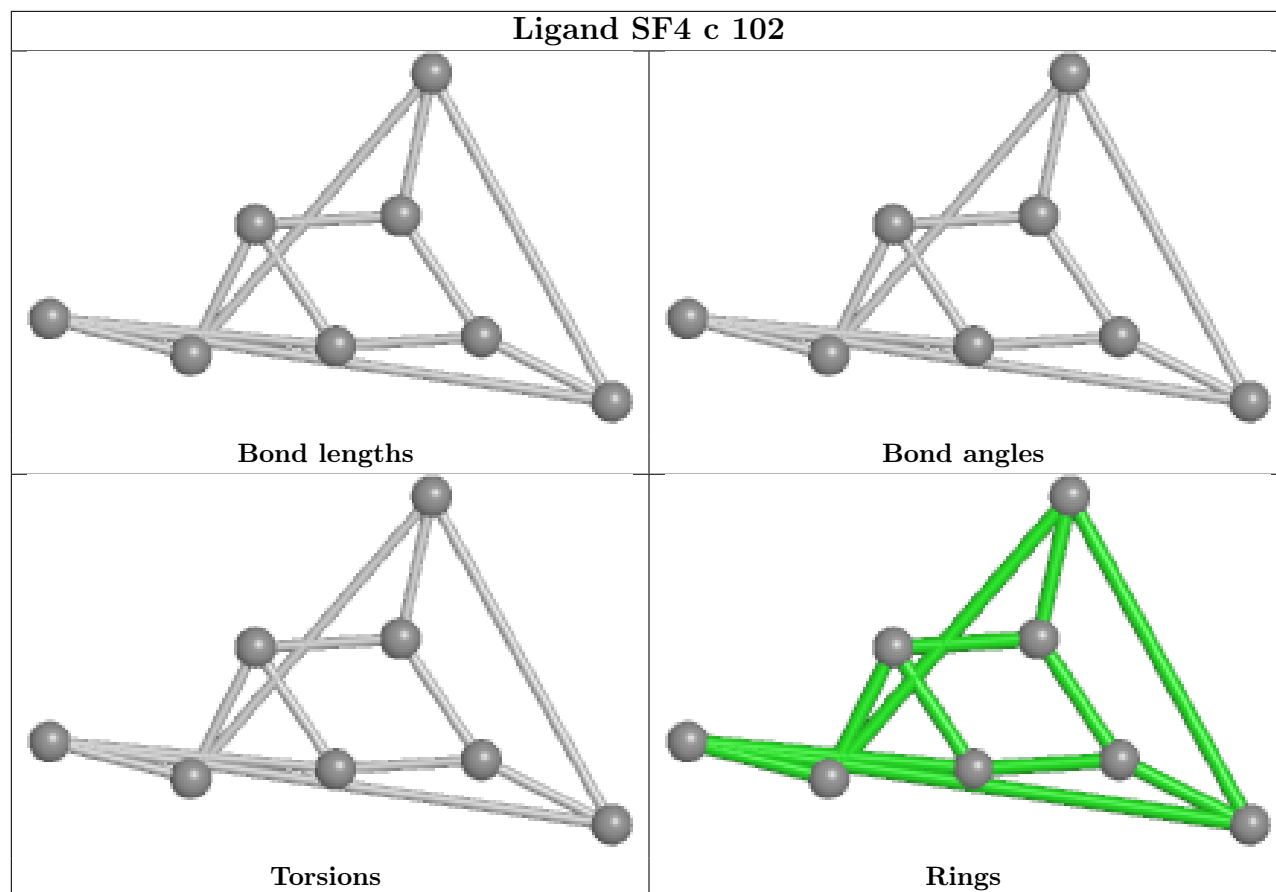
Ligand CLA a 817



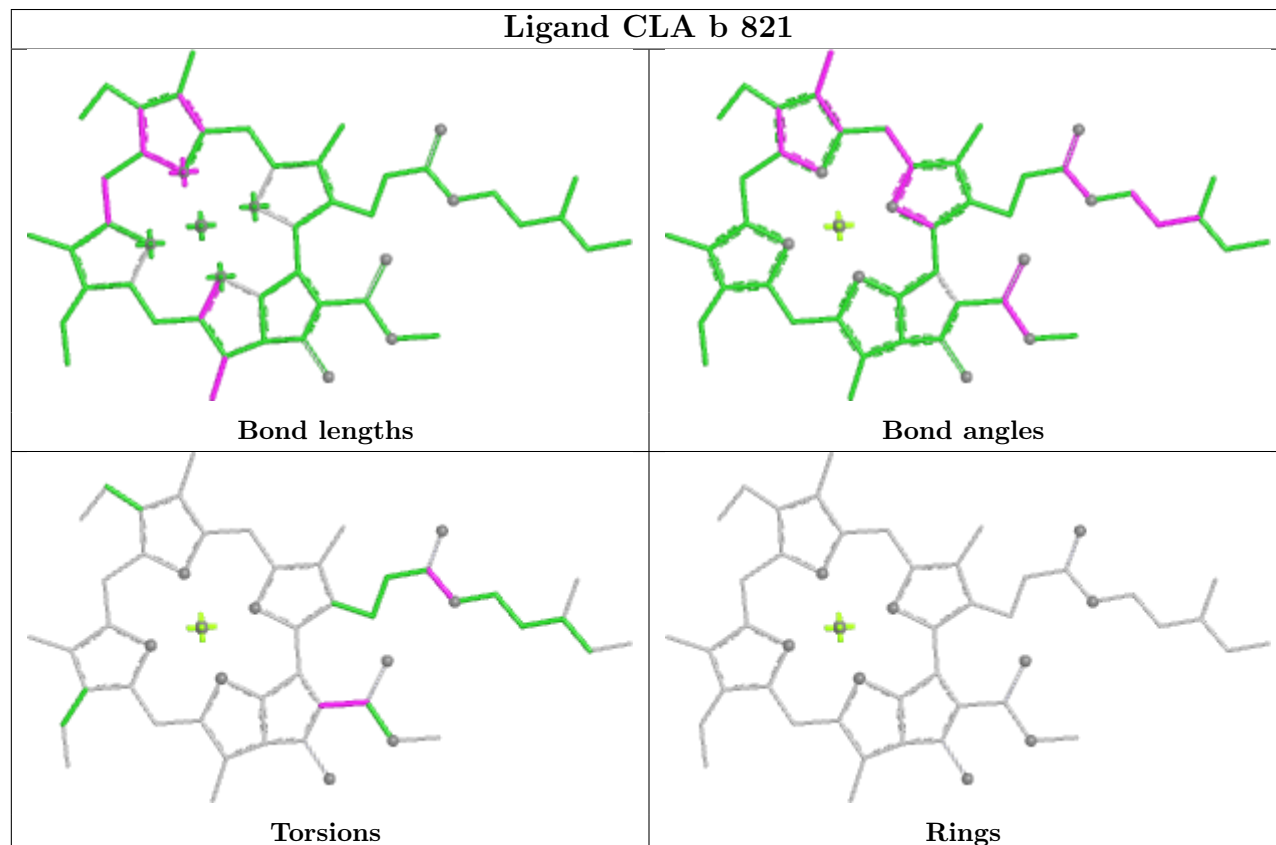
Ligand CLA b 829

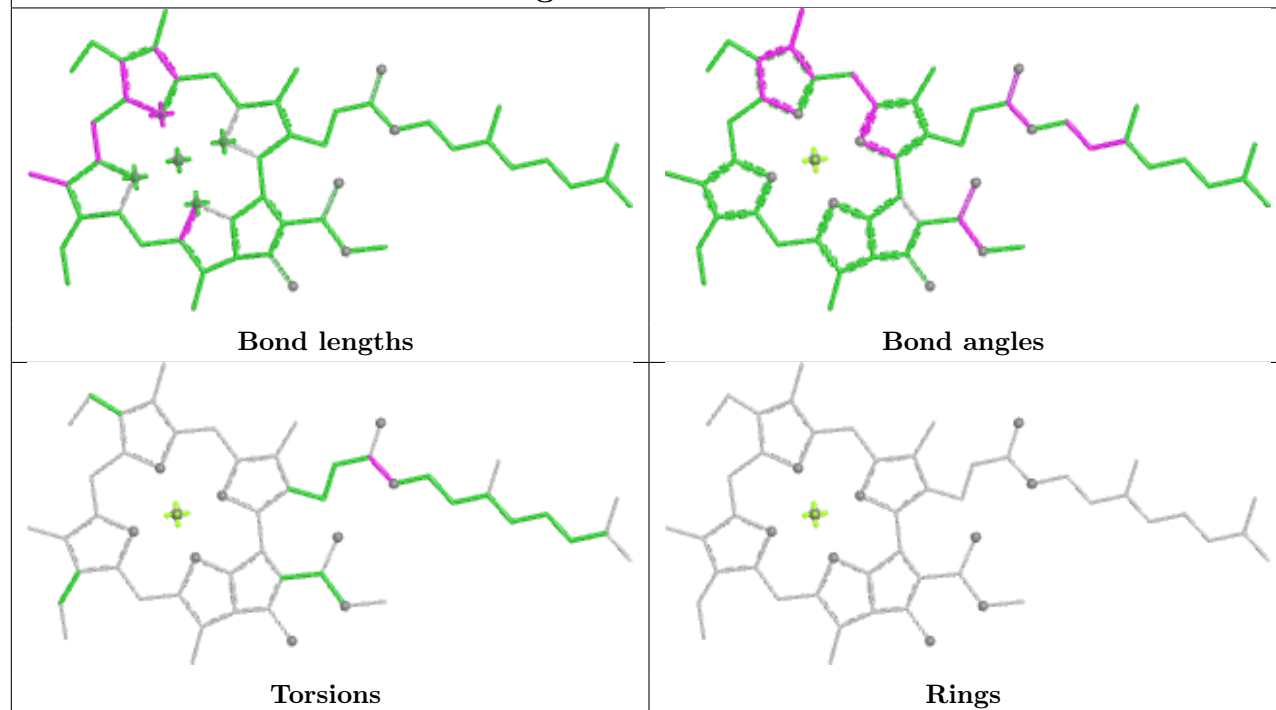
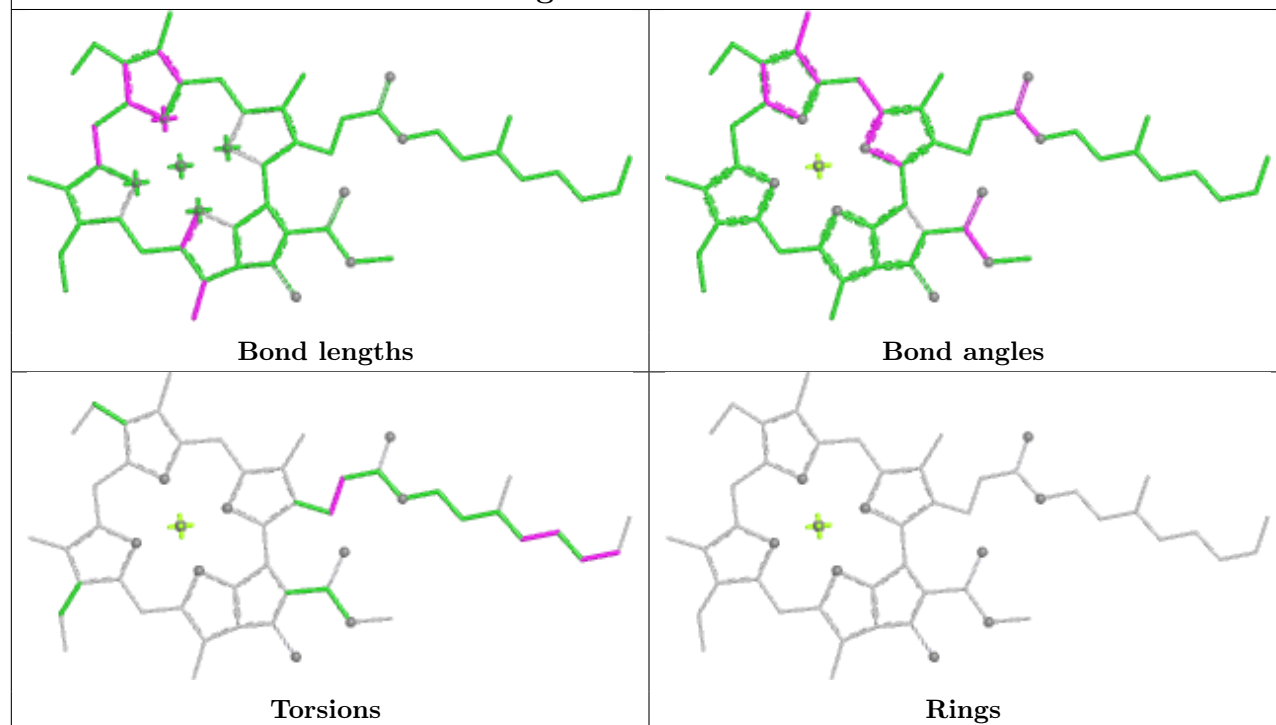


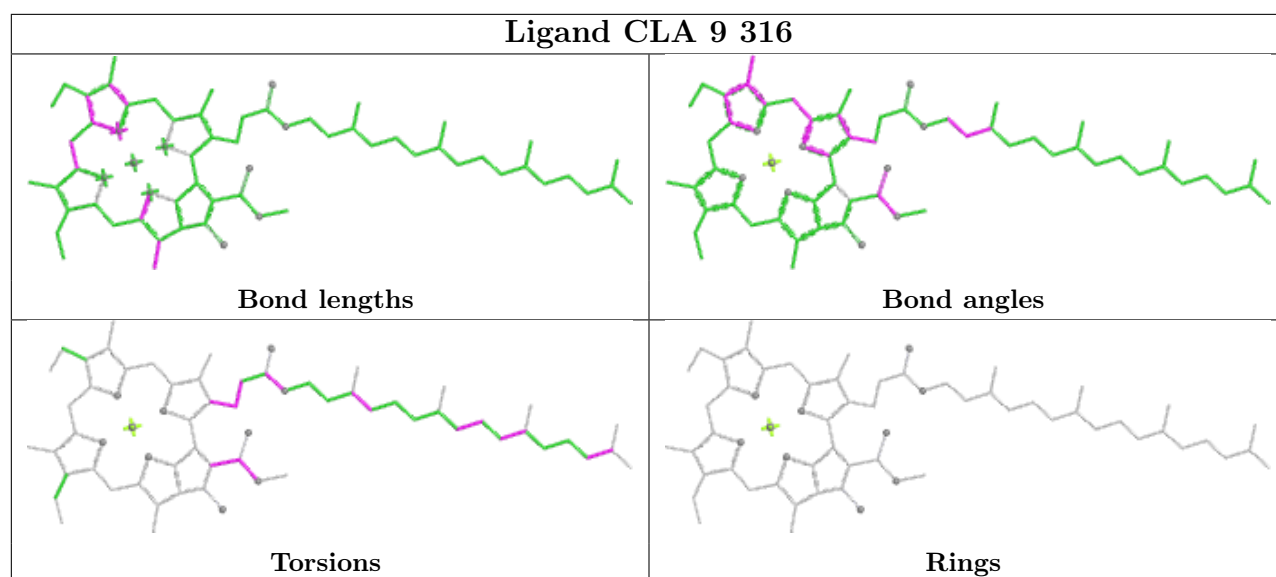
Ligand SF4 c 102



Ligand CLA b 821



Ligand CLA a 833**Ligand CLA 2 308**



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.

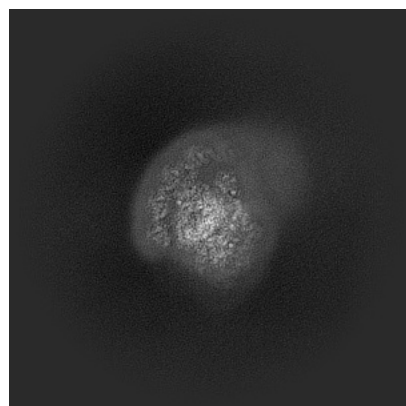
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60286. These allow visual inspection of the internal detail of the map and identification of artifacts.

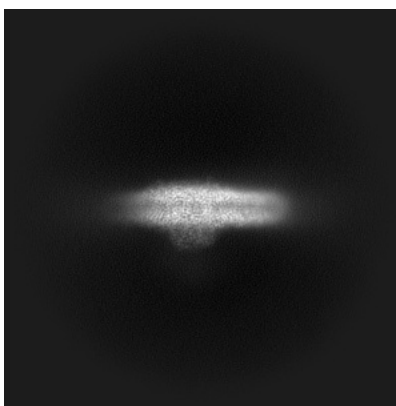
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

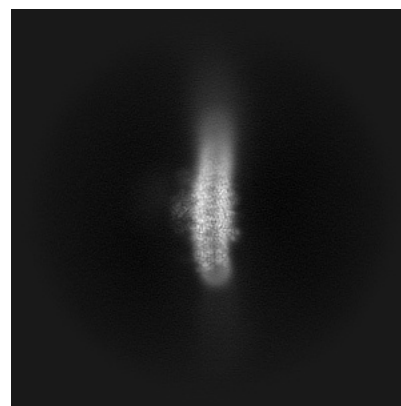
6.1.1 Primary map



X

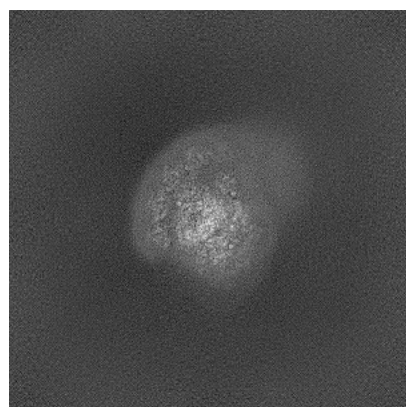


Y

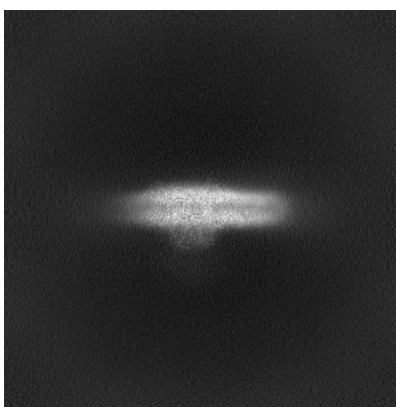


Z

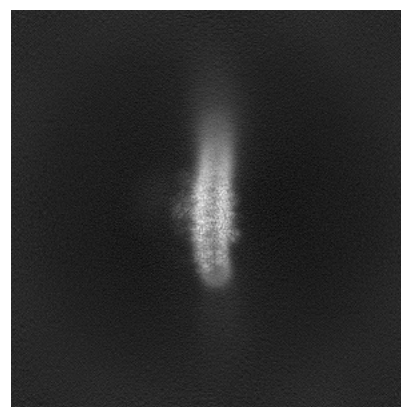
6.1.2 Raw map



X



Y

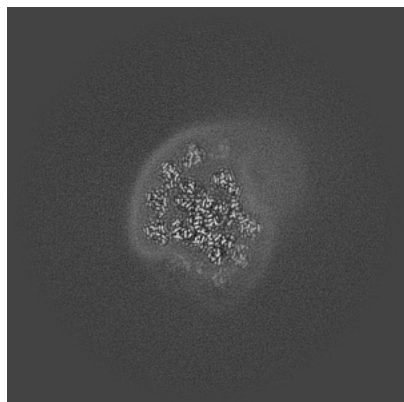


Z

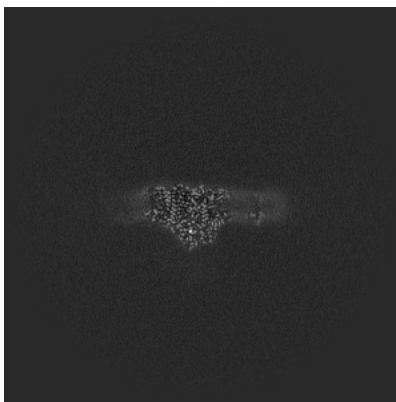
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

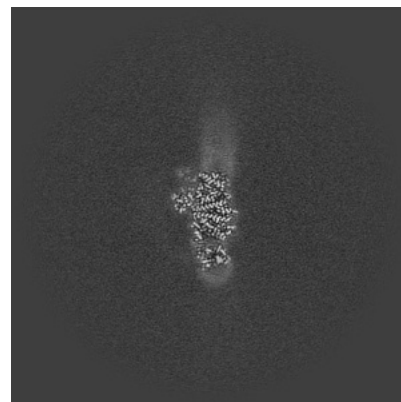
6.2.1 Primary map



X Index: 256

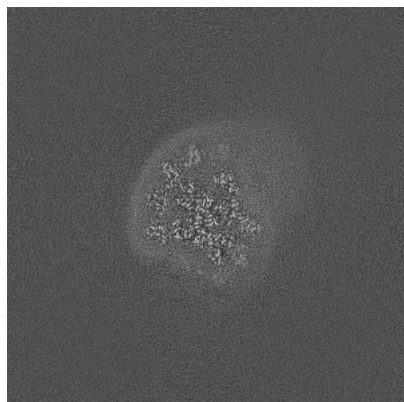


Y Index: 256

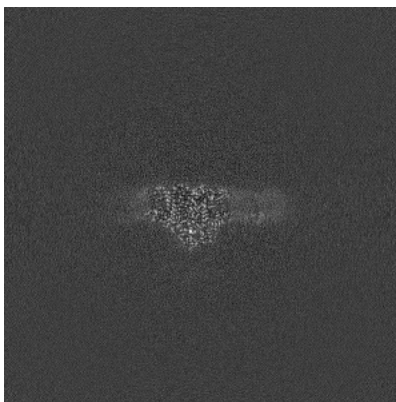


Z Index: 256

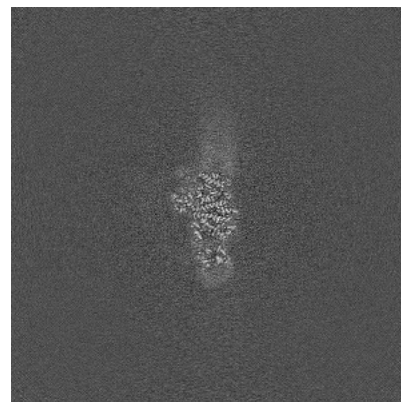
6.2.2 Raw map



X Index: 256



Y Index: 256

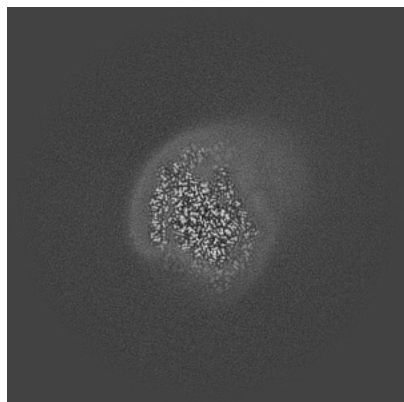


Z Index: 256

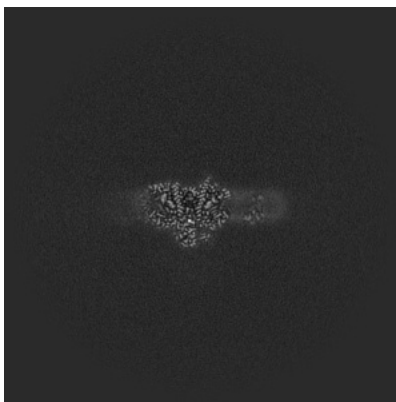
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

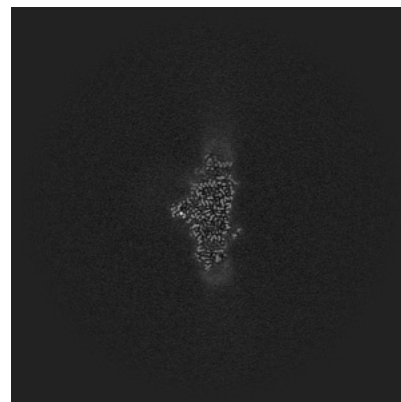
6.3.1 Primary map



X Index: 268

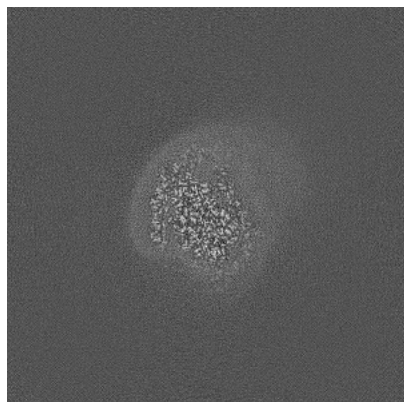


Y Index: 251

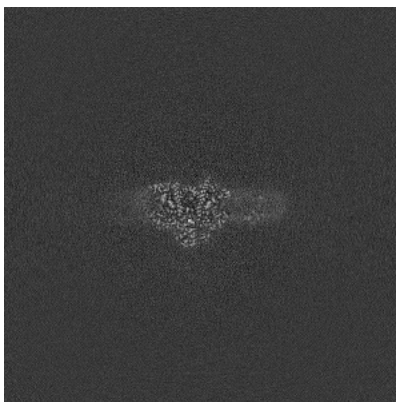


Z Index: 234

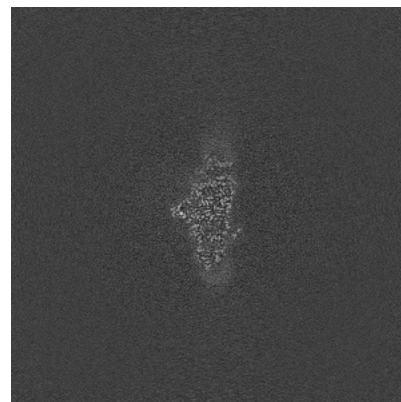
6.3.2 Raw map



X Index: 268



Y Index: 251

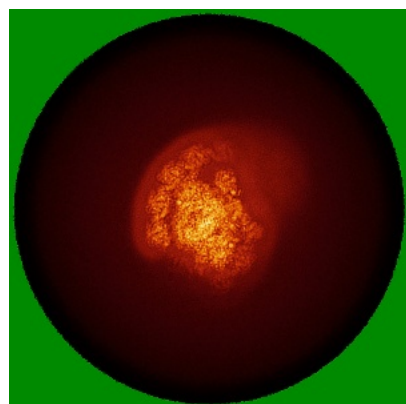


Z Index: 234

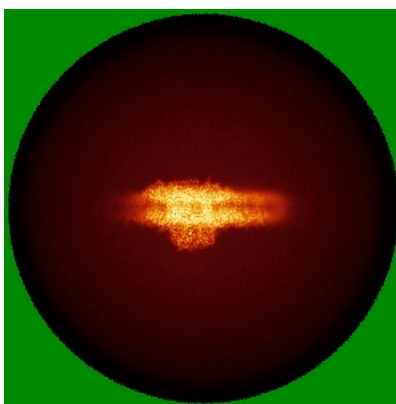
The images above show the largest variance slices of the map in three orthogonal directions.

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

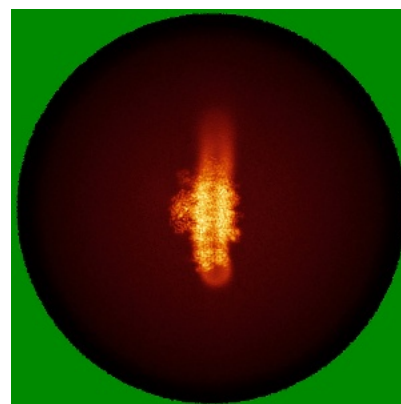
6.4.1 Primary map



X

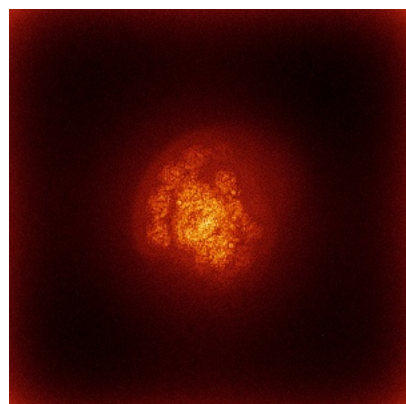


Y

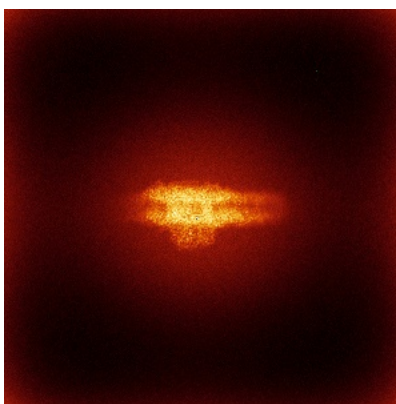


Z

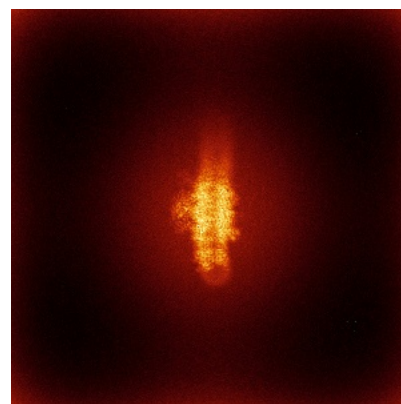
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.295. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

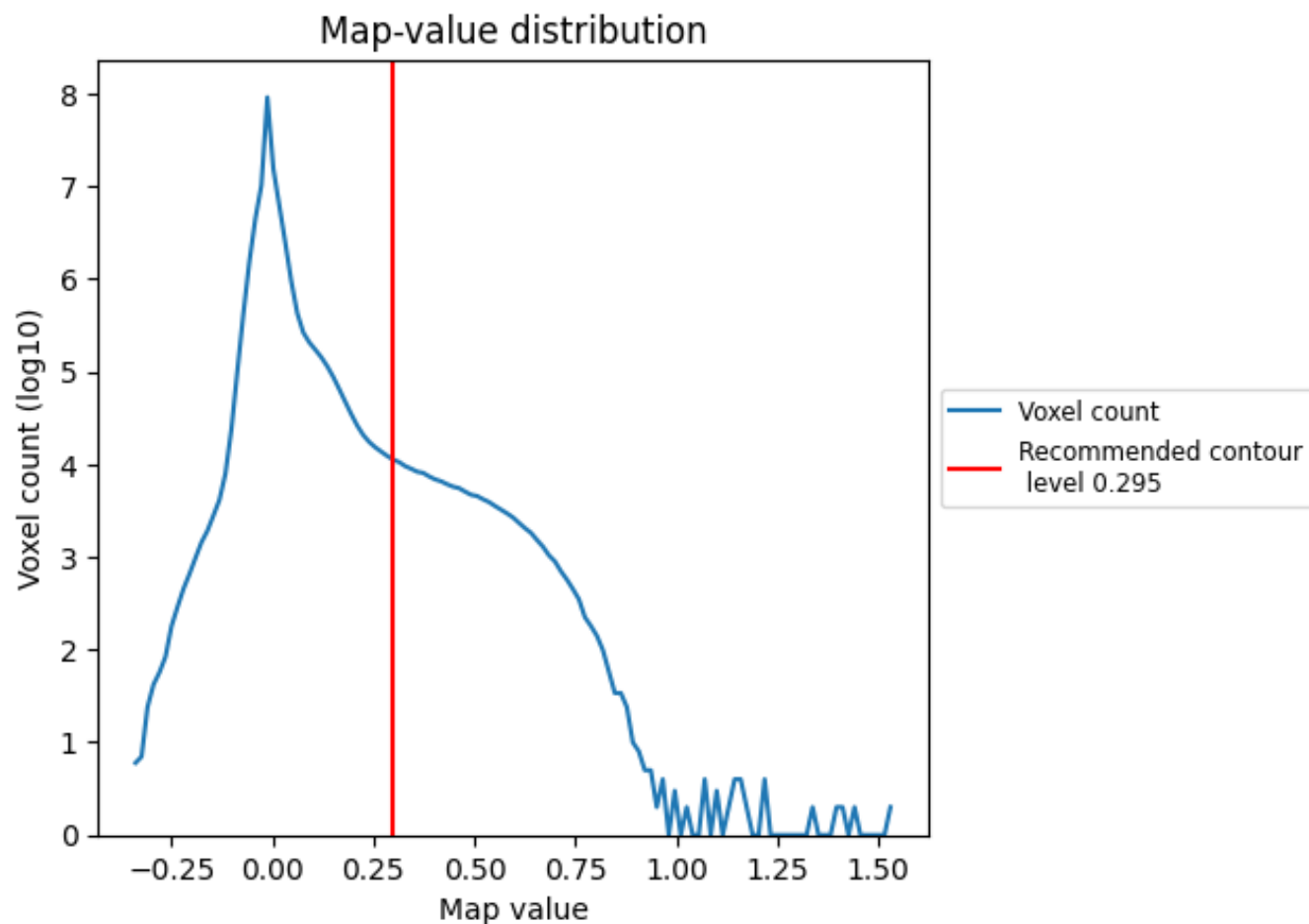
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

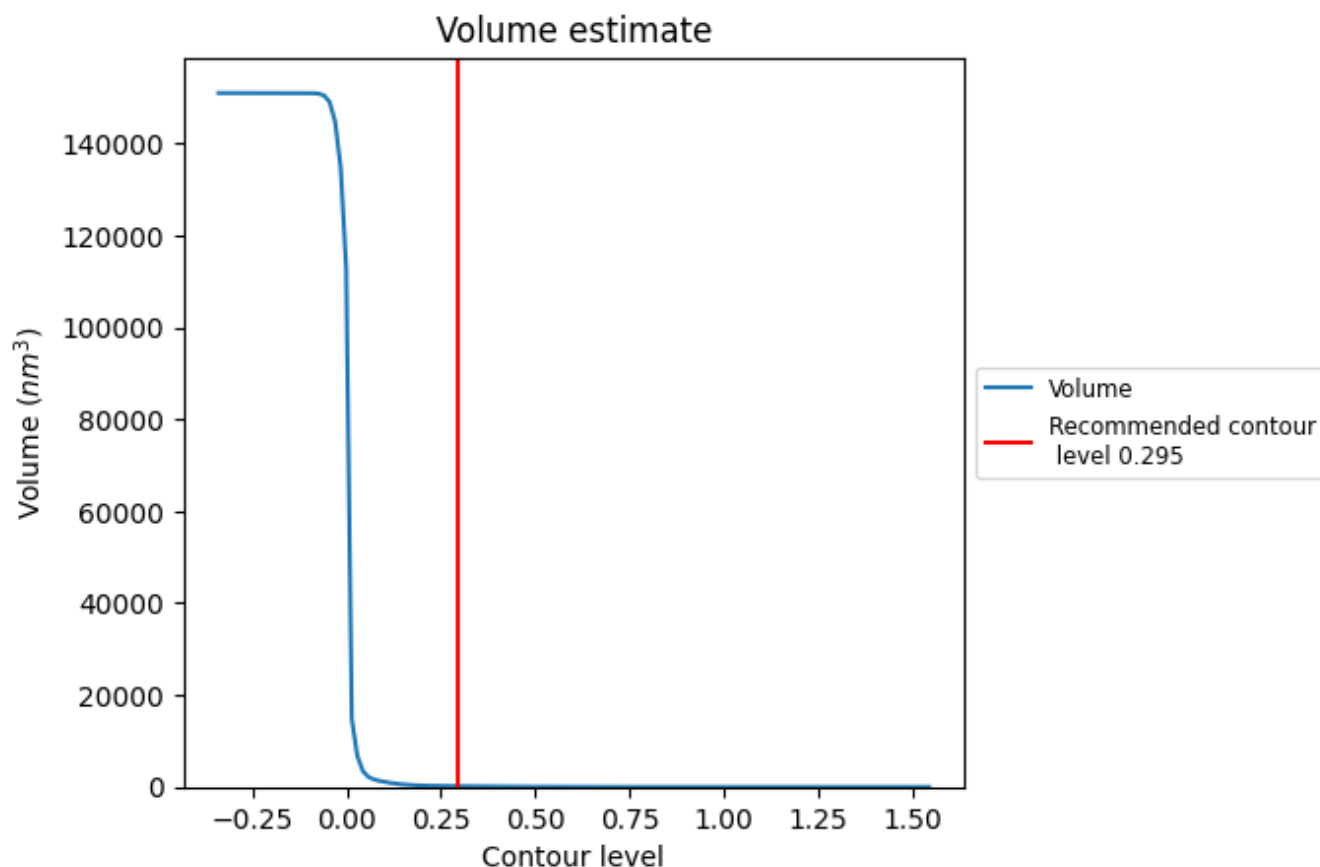
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

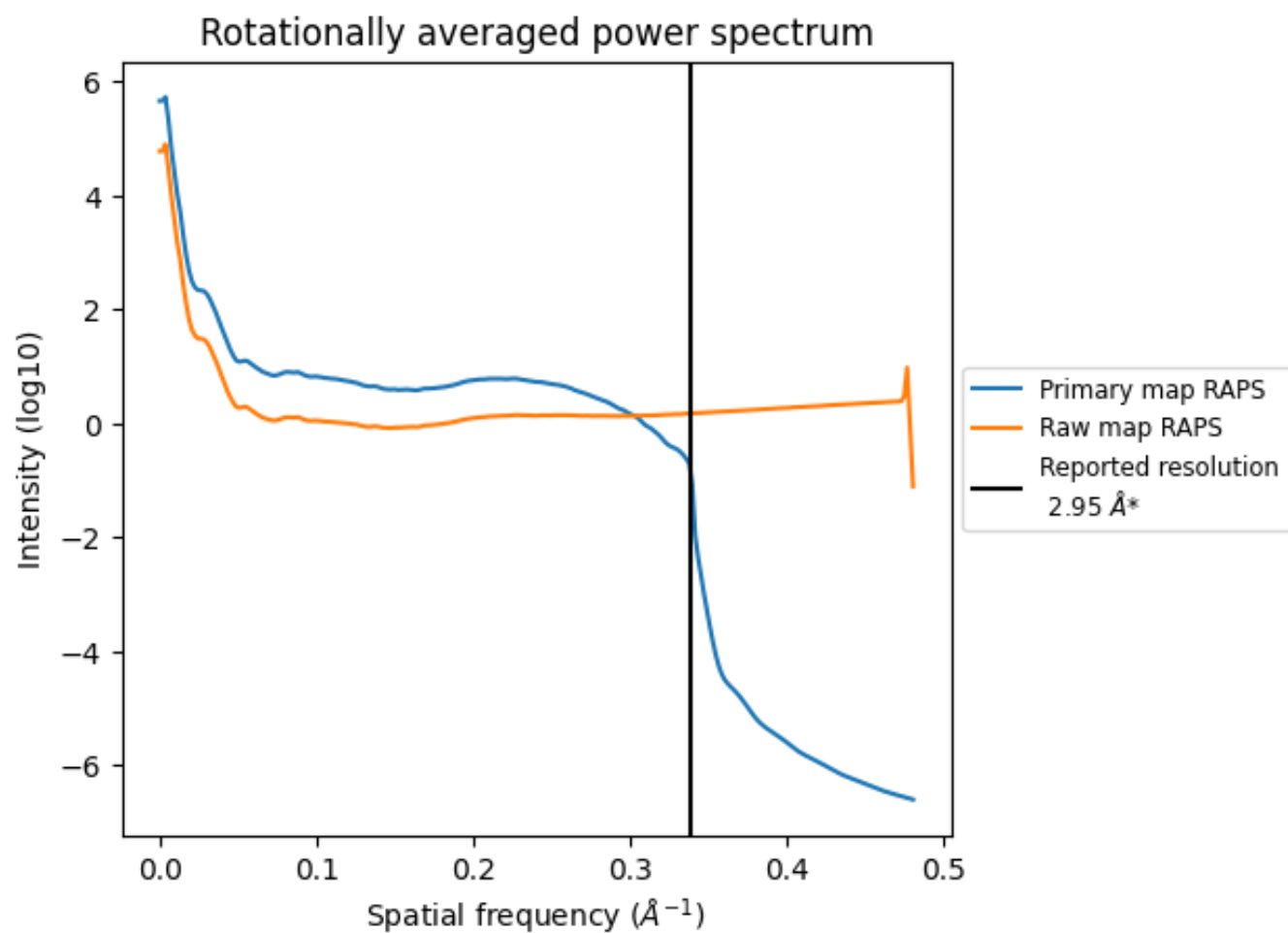
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm^3 ; this corresponds to an approximate mass of 149 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 ⓘ

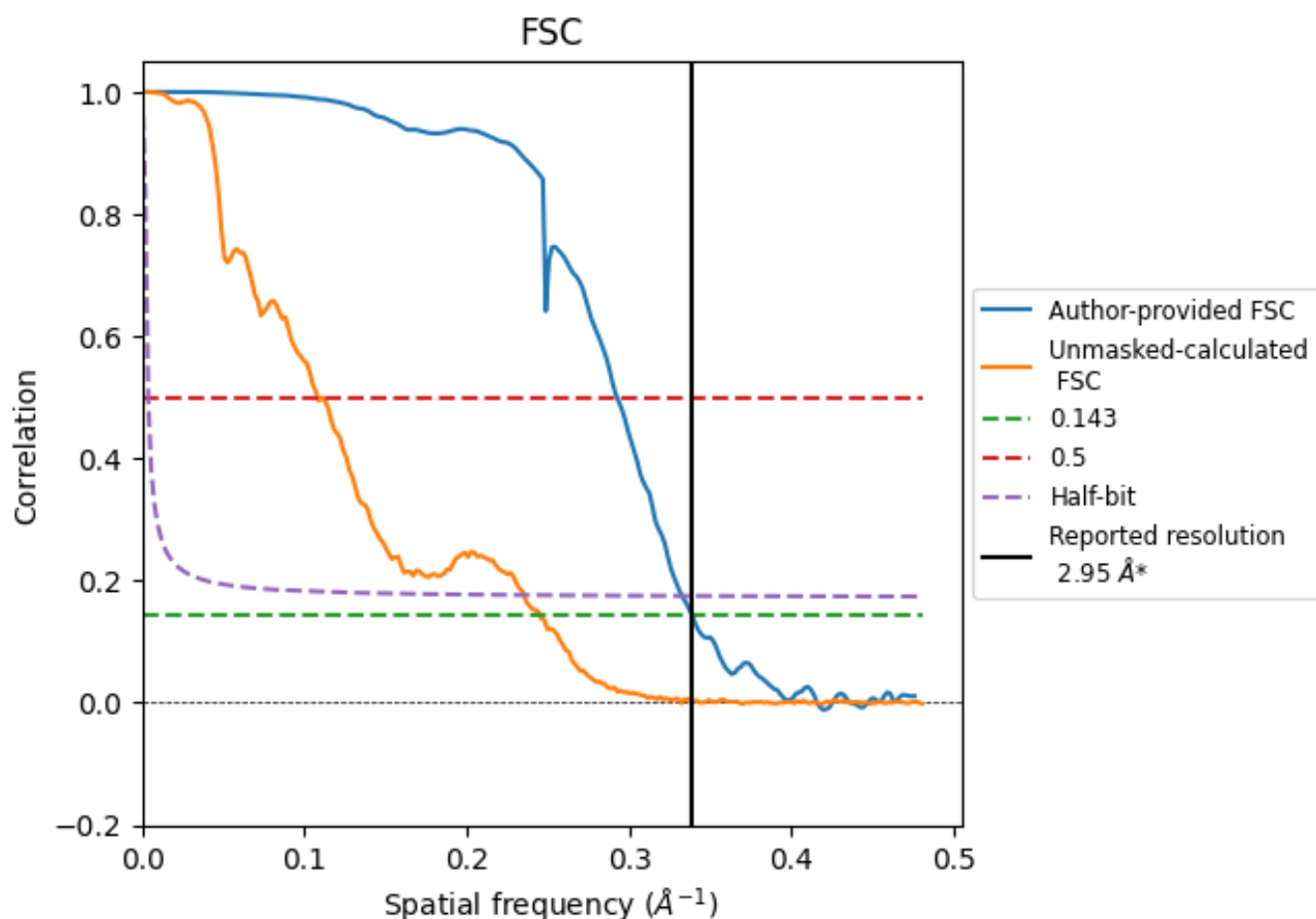


*Reported resolution corresponds to spatial frequency of 0.339 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.339 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

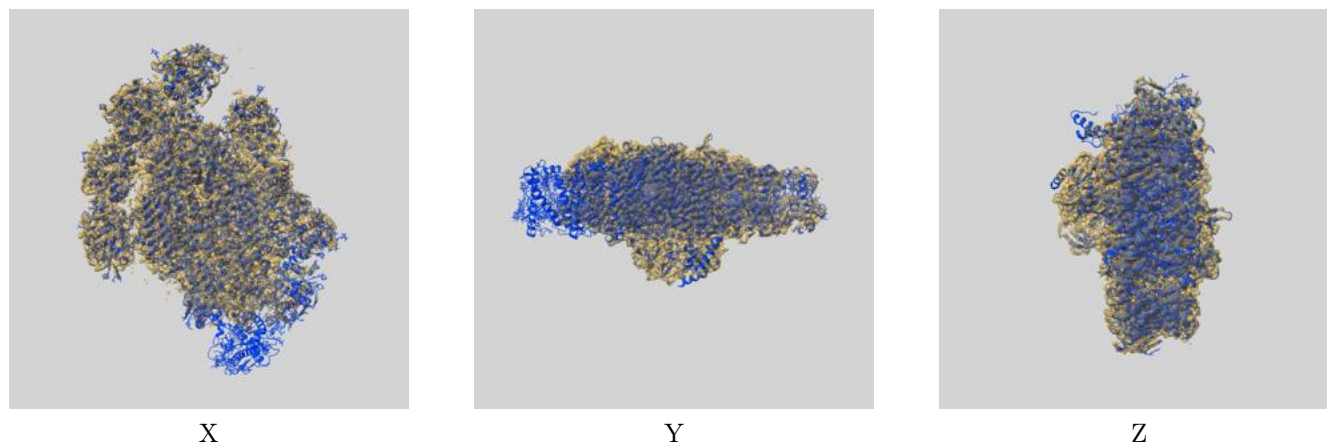
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.42	3.00
Unmasked-calculated*	4.08	9.24	4.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

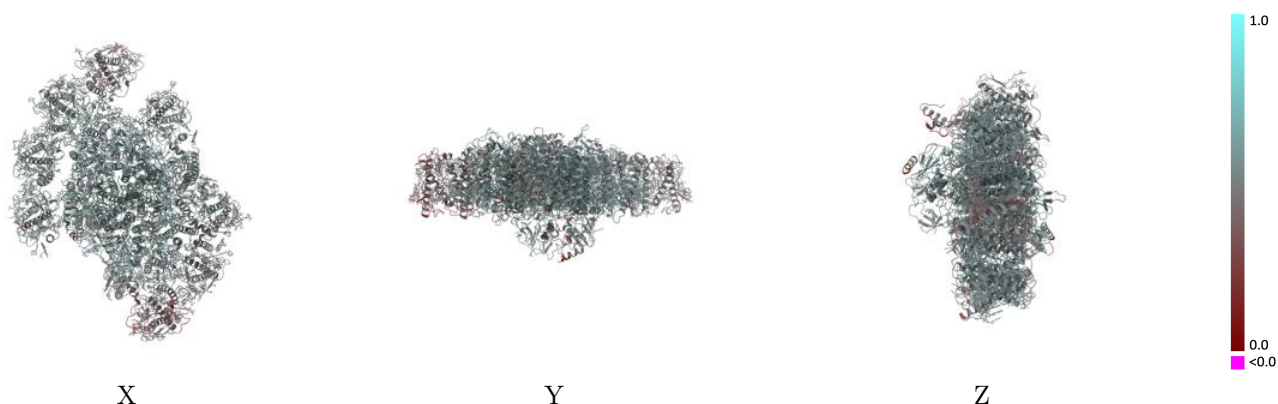
This section contains information regarding the fit between EMDB map EMD-60286 and PDB model 8ZOA. Per-residue inclusion information can be found in section 3 on page 30.

9.1 Map-model overlay [i](#)



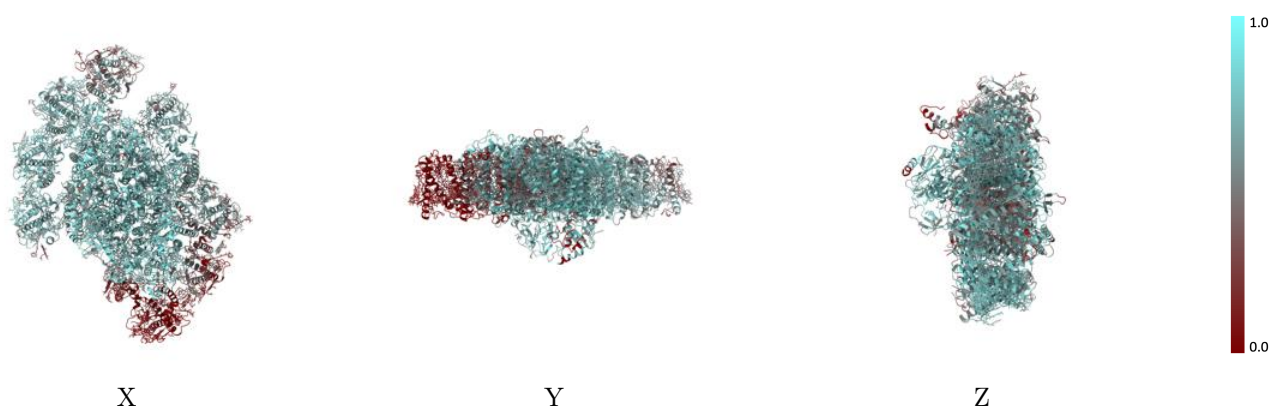
The images above show the 3D surface view of the map at the recommended contour level 0.295 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



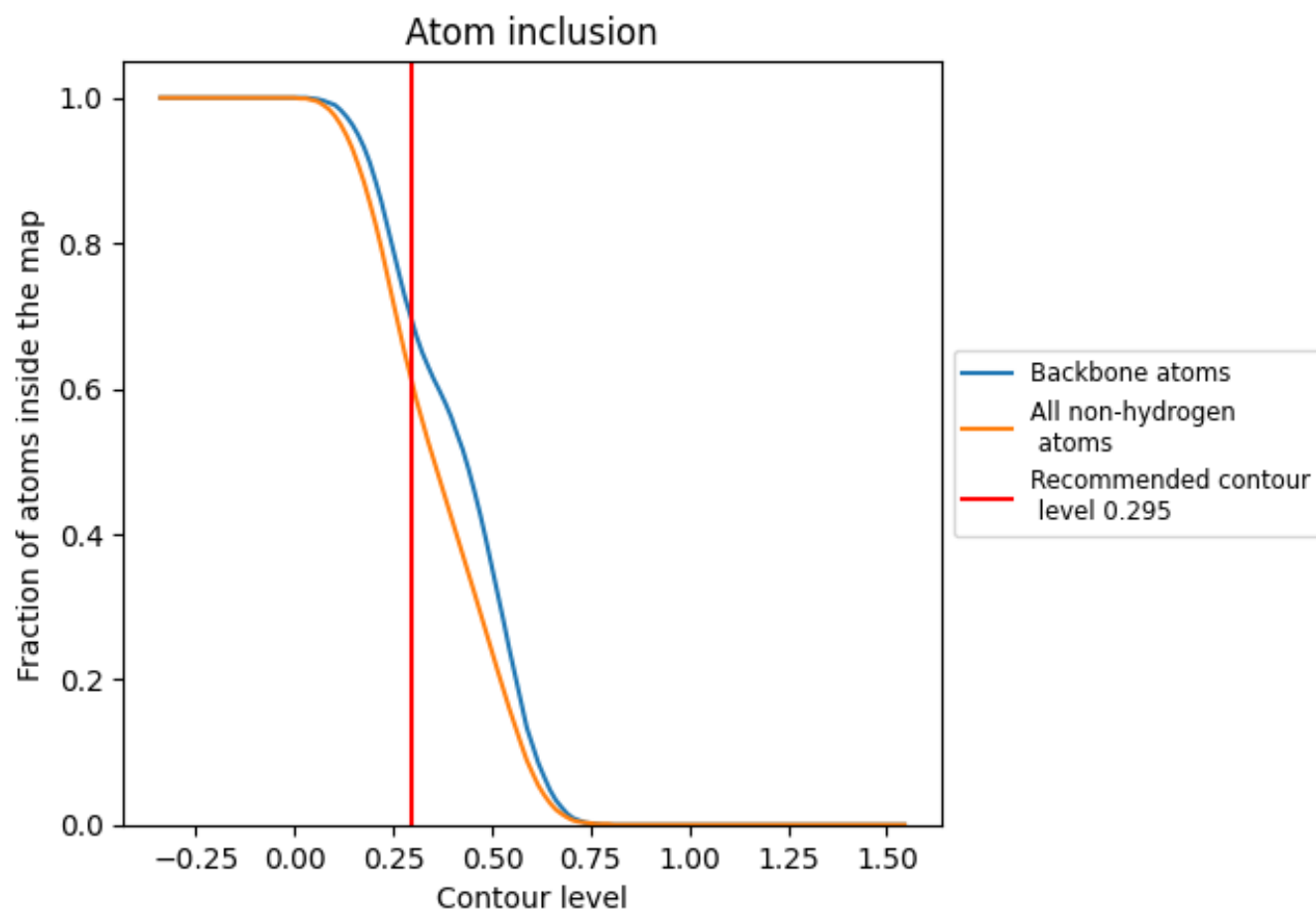
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.295).

9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.295) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.5290
1	0.6330	0.5250
2	0.4790	0.4640
3	0.6590	0.5320
4	0.6850	0.5340
5	0.6530	0.5180
7	0.0110	0.3890
8	0.2650	0.4850
9	0.4640	0.4980
a	0.7450	0.5690
b	0.7440	0.5620
c	0.7780	0.5450
d	0.6890	0.5510
e	0.6530	0.5370
f	0.6770	0.5320
g	0.4180	0.4380
h	0.0880	0.4680
i	0.6840	0.5390
j	0.7160	0.5590
l	0.6510	0.5180
m	0.6600	0.5110

1.0

0.0

<0.0