



# wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 06:11 AM UTC

PDB ID : 9LUU / pdb\_00009luu  
EMDB ID : EMD-63405  
Title : PSI-4 LHCI dimer supercomplex from M. polymorpha  
Authors : Tsai, P.-C.; La Rocca, R.; Shen, J.-R.; Akita, F.  
Deposited on : 2025-02-10  
Resolution : 2.52 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](mailto: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>.

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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

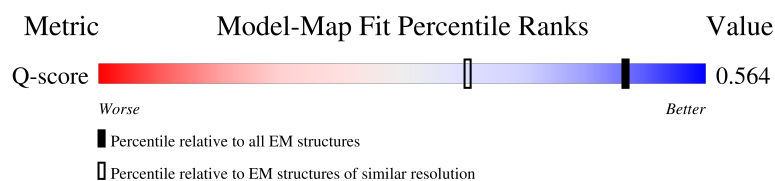
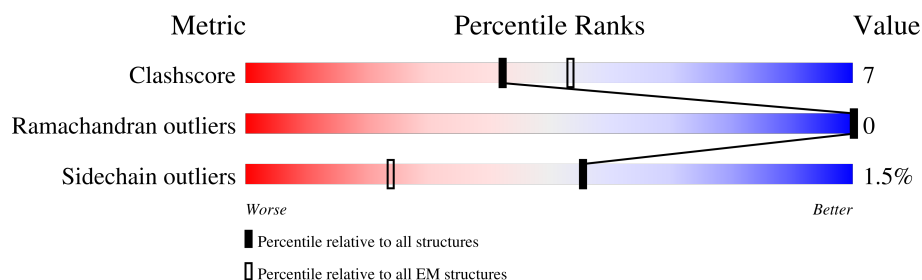
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.52 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.






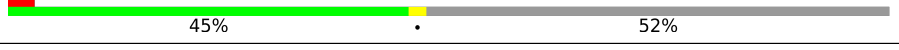


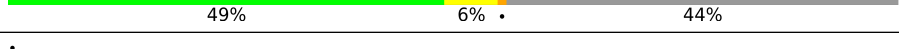
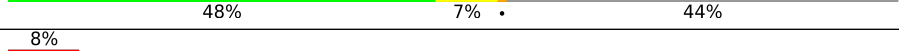
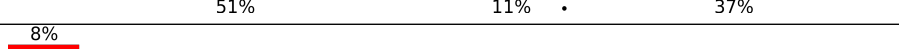
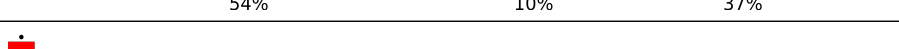
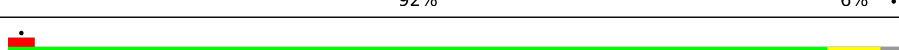
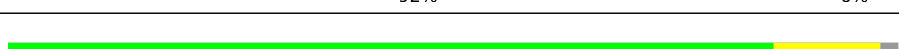
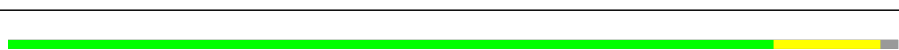

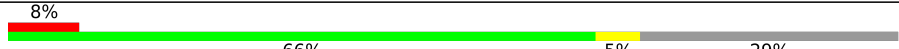





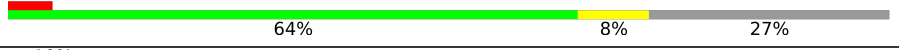
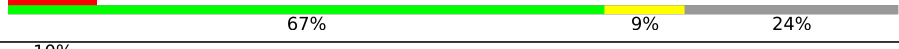



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7226 ( 2.02 - 3.02 )

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  $\geq 3$ , 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	B	734	
1	b	734	
2	C	81	
2	c	81	





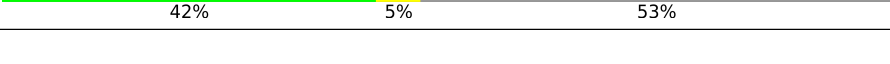
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Mol	Chain	Length	Quality of chain
3	D	215	
3	d	215	
4	E	132	
4	e	132	
5	F	246	
5	f	246	
6	G	161	
6	g	161	
7	H	142	
7	h	142	
8	I	36	
8	i	36	
9	J	42	
9	j	42	
10	L	221	
10	l	221	
11	M	32	
11	m	32	
12	A	750	
12	a	750	
13	2a	267	
13	2b	267	
14	3a	279	
14	3b	279	
15	5a	249	

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Mol	Chain	Length	Quality of chain
15	5b	249	
16	6a	243	
16	6b	243	
17	K	135	
17	k	135	

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
18	CLA	2a	301	X	-	-	-
18	CLA	2a	302	X	-	-	-
18	CLA	2a	303	X	-	-	-
18	CLA	2a	307	X	-	-	-
18	CLA	2a	308	X	-	-	-
18	CLA	2a	309	X	-	-	-
18	CLA	2a	310	X	-	-	-
18	CLA	2a	312	X	-	-	-
18	CLA	2b	301	X	-	-	-
18	CLA	2b	302	X	-	-	-
18	CLA	2b	303	X	-	-	-
18	CLA	2b	307	X	-	-	-
18	CLA	2b	308	X	-	-	-
18	CLA	2b	309	X	-	-	-
18	CLA	2b	310	X	-	-	-
18	CLA	2b	312	X	-	-	-
18	CLA	3a	303	X	-	-	-
18	CLA	3a	304	X	-	-	-
18	CLA	3a	306	X	-	-	-
18	CLA	3a	308	X	-	-	-
18	CLA	3a	310	X	-	-	-
18	CLA	3a	311	X	-	-	-
18	CLA	3a	313	X	-	-	-
18	CLA	3a	314	X	-	-	-
18	CLA	3b	303	X	-	-	-
18	CLA	3b	304	X	-	-	-
18	CLA	3b	306	X	-	-	-
18	CLA	3b	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3b	310	X	-	-	-
18	CLA	3b	311	X	-	-	-
18	CLA	3b	313	X	-	-	-
18	CLA	3b	314	X	-	-	-
18	CLA	5a	303	X	-	-	-
18	CLA	5a	308	X	-	-	-
18	CLA	5a	310	X	-	-	-
18	CLA	5a	311	X	-	-	-
18	CLA	5a	313	X	-	-	-
18	CLA	5b	303	X	-	-	-
18	CLA	5b	308	X	-	-	-
18	CLA	5b	310	X	-	-	-
18	CLA	5b	311	X	-	-	-
18	CLA	5b	313	X	-	-	-
18	CLA	6a	306	X	-	-	-
18	CLA	6a	308	X	-	-	-
18	CLA	6a	310	X	-	-	-
18	CLA	6a	311	X	-	-	-
18	CLA	6a	313	X	-	-	-
18	CLA	6a	314	X	-	-	-
18	CLA	6a	315	X	-	-	-
18	CLA	6a	317	X	-	-	-
18	CLA	6b	306	X	-	-	-
18	CLA	6b	308	X	-	-	-
18	CLA	6b	310	X	-	-	-
18	CLA	6b	311	X	-	-	-
18	CLA	6b	313	X	-	-	-
18	CLA	6b	314	X	-	-	-
18	CLA	6b	315	X	-	-	-
18	CLA	6b	317	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	818	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	853	X	-	-	-
18	CLA	B	854	X	-	-	-
18	CLA	F	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	F	303	X	-	-	-
18	CLA	F	305	X	-	-	-
18	CLA	G	202	X	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	L	301	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	a	803	X	-	-	-
18	CLA	a	804	X	-	-	-
18	CLA	a	805	X	-	-	-
18	CLA	a	806	X	-	-	-
18	CLA	a	807	X	-	-	-
18	CLA	a	808	X	-	-	-
18	CLA	a	809	X	-	-	-
18	CLA	a	811	X	-	-	-
18	CLA	a	812	X	-	-	-
18	CLA	a	813	X	-	-	-
18	CLA	a	814	X	-	-	-
18	CLA	a	817	X	-	-	-
18	CLA	a	818	X	-	-	-
18	CLA	a	822	X	-	-	-
18	CLA	a	824	X	-	-	-
18	CLA	a	825	X	-	-	-
18	CLA	a	826	X	-	-	-
18	CLA	a	827	X	-	-	-
18	CLA	a	831	X	-	-	-
18	CLA	a	832	X	-	-	-
18	CLA	a	835	X	-	-	-
18	CLA	a	836	X	-	-	-
18	CLA	a	837	X	-	-	-
18	CLA	a	838	X	-	-	-
18	CLA	a	840	X	-	-	-
18	CLA	a	841	X	-	-	-
18	CLA	b	801	X	-	-	-
18	CLA	b	802	X	-	-	-
18	CLA	b	803	X	-	-	-
18	CLA	b	804	X	-	-	-
18	CLA	b	805	X	-	-	-
18	CLA	b	807	X	-	-	-
18	CLA	b	808	X	-	-	-
18	CLA	b	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	b	812	X	-	-	-
18	CLA	b	816	X	-	-	-
18	CLA	b	817	X	-	-	-
18	CLA	b	819	X	-	-	-
18	CLA	b	821	X	-	-	-
18	CLA	b	823	X	-	-	-
18	CLA	b	824	X	-	-	-
18	CLA	b	825	X	-	-	-
18	CLA	b	826	X	-	-	-
18	CLA	b	830	X	-	-	-
18	CLA	b	831	X	-	-	-
18	CLA	b	833	X	-	-	-
18	CLA	b	834	X	-	-	-
18	CLA	b	835	X	-	-	-
18	CLA	b	836	X	-	-	-
18	CLA	b	837	X	-	-	-
18	CLA	b	840	X	-	-	-
18	CLA	b	853	X	-	-	-
18	CLA	b	854	X	-	-	-
18	CLA	f	302	X	-	-	-
18	CLA	f	303	X	-	-	-
18	CLA	f	305	X	-	-	-
18	CLA	g	202	X	-	-	-
18	CLA	g	203	X	-	-	-
18	CLA	j	101	X	-	-	-
18	CLA	k	201	X	-	-	-
18	CLA	l	301	X	-	-	-
18	CLA	l	303	X	-	-	-
29	CHL	2a	304	X	-	-	-
29	CHL	2a	305	X	-	-	-
29	CHL	2a	306	X	-	-	-
29	CHL	2a	313	X	-	-	-
29	CHL	2b	304	X	-	-	-
29	CHL	2b	305	X	-	-	-
29	CHL	2b	306	X	-	-	-
29	CHL	2b	313	X	-	-	-
29	CHL	3a	301	X	-	-	-
29	CHL	3a	307	X	-	-	-
29	CHL	3a	315	X	-	-	-
29	CHL	3b	301	X	-	-	-
29	CHL	3b	307	X	-	-	-
29	CHL	3b	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	5a	301	X	-	-	-
29	CHL	5a	305	X	-	-	-
29	CHL	5a	306	X	-	-	-
29	CHL	5a	307	X	-	-	-
29	CHL	5a	314	X	-	-	-
29	CHL	5b	301	X	-	-	-
29	CHL	5b	305	X	-	-	-
29	CHL	5b	306	X	-	-	-
29	CHL	5b	307	X	-	-	-
29	CHL	5b	314	X	-	-	-
29	CHL	6a	304	X	-	-	-
29	CHL	6a	309	X	-	-	-
29	CHL	6b	304	X	-	-	-
29	CHL	6b	309	X	-	-	-

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 70242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	733	Total	C	N	O	S	0	0
			5854	3839	998	1003	14		
1	b	733	Total	C	N	O	S	0	0
			5854	3839	998	1003	14		

- Molecule 2 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	80	Total	C	N	O	S	0	0
			602	368	104	119	11		
2	c	80	Total	C	N	O	S	0	0
			602	368	104	119	11		

- Molecule 3 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	140	Total	C	N	O	S	0	0
			1094	706	189	196	3		
3	d	140	Total	C	N	O	S	0	0
			1094	706	189	196	3		

- Molecule 4 is a protein called Photosystem I reaction centre subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	63	Total	C	N	O	S	0	0
			495	314	85	94	2		
4	e	63	Total	C	N	O	S	0	0
			495	314	85	94	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	161	Total	C	N	O	S	0	0
			1248	809	212	225	2		
5	f	161	Total	C	N	O	S	0	0
			1248	809	212	225	2		

- Molecule 6 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	90	Total	C	N	O	S	0	0
			673	432	117	123	1		
6	g	90	Total	C	N	O	S	0	0
			673	432	117	123	1		

- Molecule 7 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	90	Total	C	N	O	S	0	0
			680	438	113	127	2		
7	h	90	Total	C	N	O	S	0	0
			680	438	113	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			274	187	36	49	2		
8	i	35	Total	C	N	O	S	0	0
			274	187	36	49	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			328	225	48	54	1		
9	j	41	Total	C	N	O	S	0	0
			328	225	48	54	1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	158	Total	C	N	O	S	0	0
			1180	781	188	209	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	158	Total	C	N	O	S	0	0
			1180	781	188	209	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O		0	0
			242	159	37	46			
11	m	31	Total	C	N	O		0	0
			242	159	37	46			

- Molecule 12 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	737	Total	C	N	O	S	0	0
			5810	3818	983	992	17		
12	a	737	Total	C	N	O	S	0	0
			5810	3818	983	992	17		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2a	194	Total	C	N	O	S	0	0
			1520	1003	245	267	5		
13	2b	194	Total	C	N	O	S	0	0
			1520	1003	245	267	5		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3a	212	Total	C	N	O	S	0	0
			1633	1072	261	294	6		
14	3b	212	Total	C	N	O	S	0	0
			1633	1072	261	294	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5a	193	Total	C	N	O	S	0	0
			1516	1001	242	269	4		
15	5b	193	Total	C	N	O	S	0	0
			1516	1001	242	269	4		



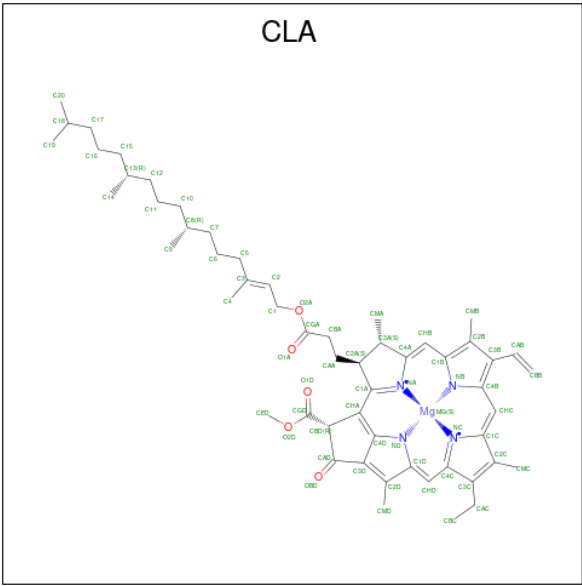
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6a	193	Total	C	N	O	S	0	0
			1491	973	249	266	3		
16	6b	193	Total	C	N	O	S	0	0
			1491	973	249	266	3		

- Molecule 17 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	64	Total	C	N	O	S	0	0
			441	280	73	84	4		
17	k	64	Total	C	N	O	S	0	0
			441	280	73	84	4		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
18	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
18	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	f	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	l	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	2a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2a	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	2a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3a	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	3a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3a	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	3a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3a	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	3a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3a	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	3a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3a	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5a	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	5a	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	5a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5a	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	5a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5a	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	5a	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	5a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5a	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	6a	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	6a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6a	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	a	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	a	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	2b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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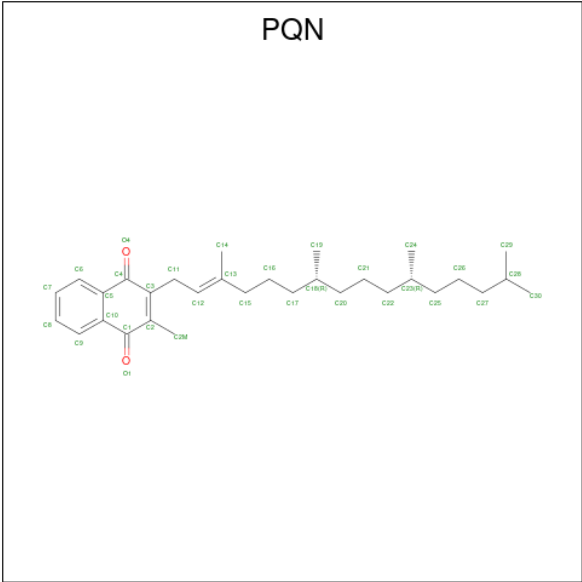
Mol	Chain	Residues	Atoms					AltConf
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	3b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3b	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5b	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	5b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	5b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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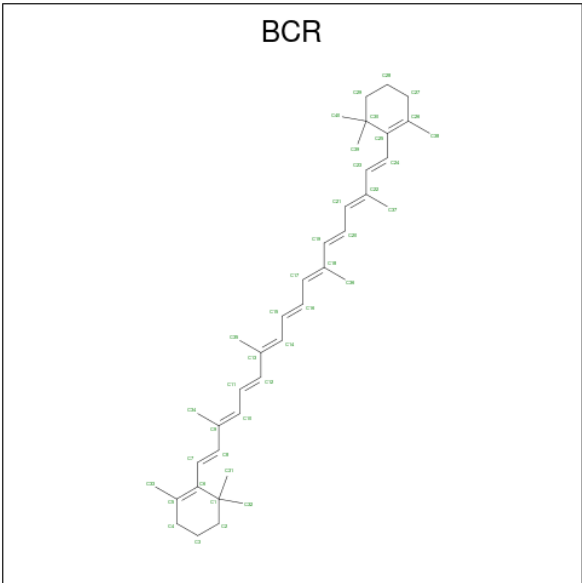
Mol	Chain	Residues	Atoms					AltConf
18	5b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	k	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	G	1	Total C 40 40	0
20	G	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	M	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0

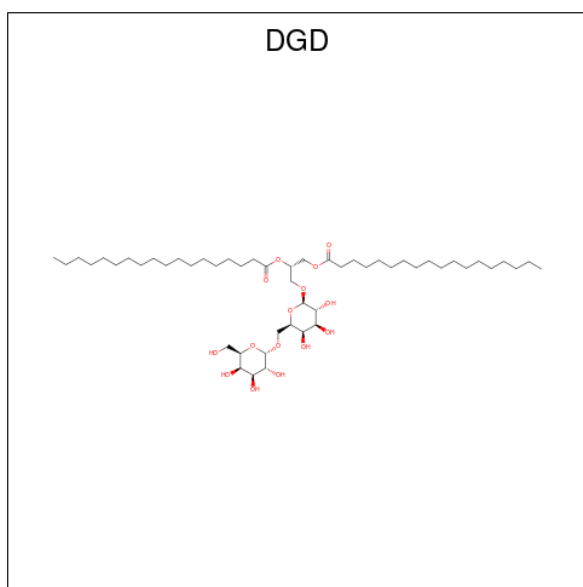
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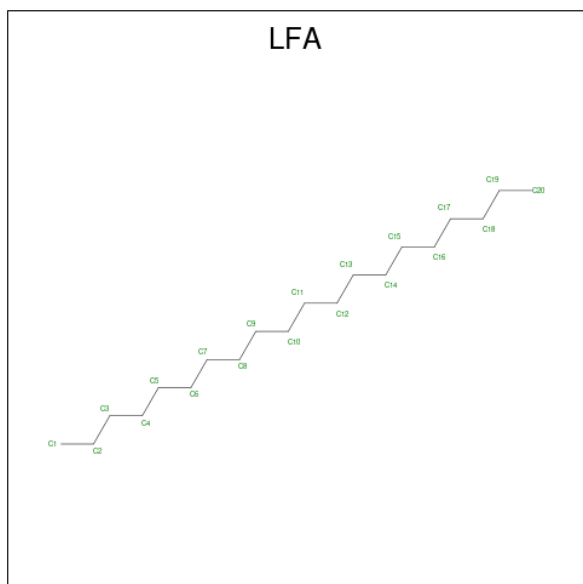
Mol	Chain	Residues	Atoms	AltConf
20	f	1	Total C 40 40	0
20	f	1	Total C 40 40	0
20	g	1	Total C 40 40	0
20	g	1	Total C 40 40	0
20	i	1	Total C 40 40	0
20	j	1	Total C 40 40	0
20	l	1	Total C 40 40	0
20	m	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	k	1	Total C 40 40	0

- Molecule 21 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
21	B	1	Total	C	O	0
			59	44	15	
21	b	1	Total	C	O	0
			59	44	15	

- Molecule 22 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ) (labeled as "Ligand of Interest" by depositor).



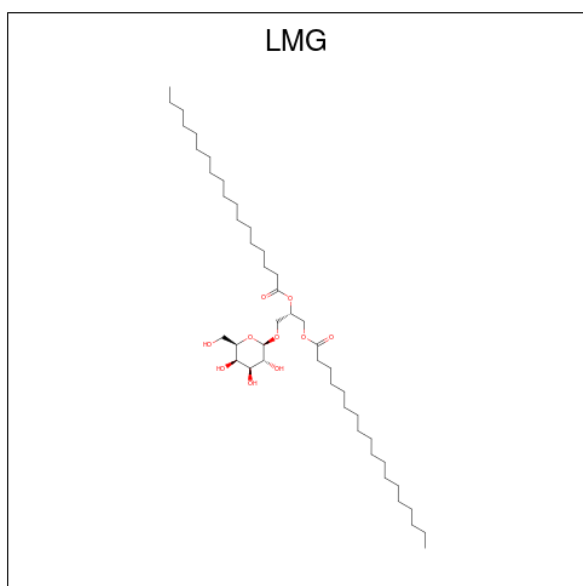
Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	C	0
			12	12	

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Mol	Chain	Residues	Atoms		AltConf
22	M	1	Total	C	0
			12	12	
22	b	1	Total	C	0
			12	12	
22	m	1	Total	C	0
			12	12	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



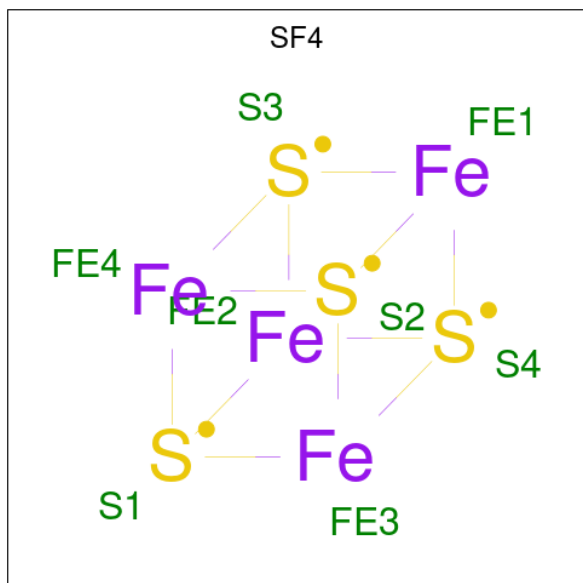
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			42	32	10	
23	I	1	Total	C	O	0
			31	21	10	
23	J	1	Total	C	O	0
			30	20	10	
23	J	1	Total	C	O	0
			41	31	10	
23	b	1	Total	C	O	0
			42	32	10	
23	i	1	Total	C	O	0
			31	21	10	
23	j	1	Total	C	O	0
			30	20	10	
23	j	1	Total	C	O	0
			41	31	10	

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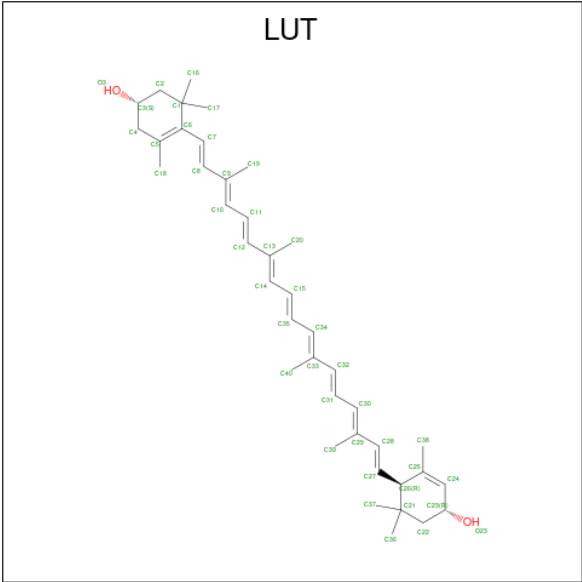
Mol	Chain	Residues	Atoms			AltConf
23	5a	1	Total	C	O	0
			35	25	10	
23	5b	1	Total	C	O	0
			35	25	10	

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	Fe	S	0
			8	4	4	
24	C	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	A	1	Total	Fe	S	0
			8	4	4	
24	a	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $\text{C}_{40}\text{H}_{56}\text{O}_2$ ) (labeled as "Ligand of Interest" by depositor).



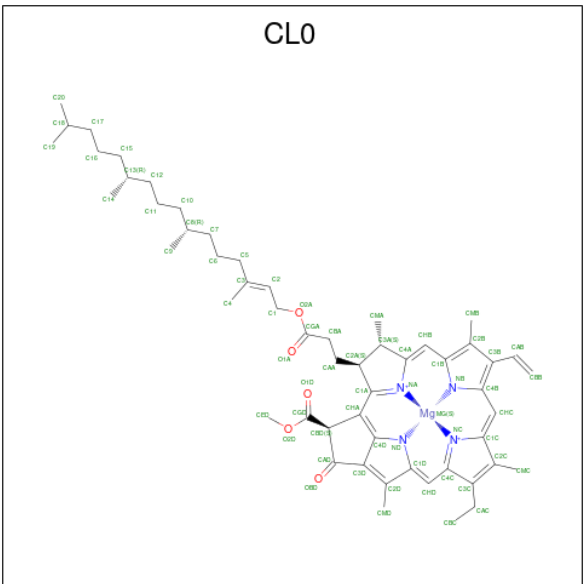
Mol	Chain	Residues	Atoms			AltConf
25	J	1	Total	C	O	0
			42	40	2	
25	j	1	Total	C	O	0
			42	40	2	
25	2a	1	Total	C	O	0
			42	40	2	
25	2a	1	Total	C	O	0
			42	40	2	
25	3a	1	Total	C	O	0
			42	40	2	
25	3a	1	Total	C	O	0
			42	40	2	
25	5a	1	Total	C	O	0
			42	40	2	
25	5a	1	Total	C	O	0
			42	40	2	
25	6a	1	Total	C	O	0
			42	40	2	
25	6a	1	Total	C	O	0
			42	40	2	
25	6a	1	Total	C	O	0
			42	40	2	
25	2b	1	Total	C	O	0
			42	40	2	
25	2b	1	Total	C	O	0
			42	40	2	
25	3b	1	Total	C	O	0
			42	40	2	

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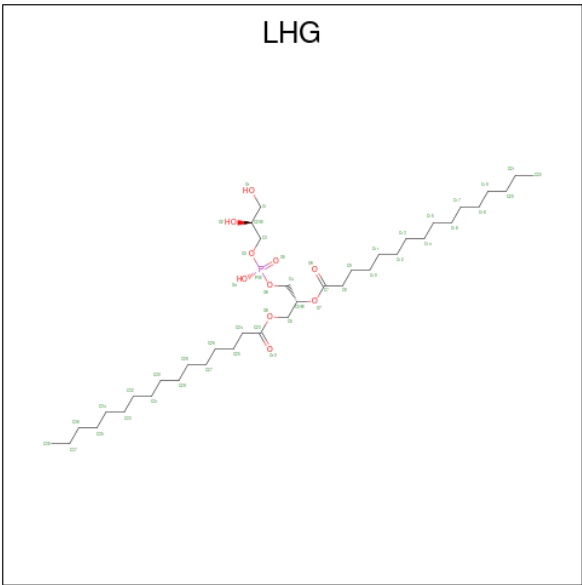
Mol	Chain	Residues	Atoms			AltConf
25	3b	1	Total	C	O	0
			42	40	2	
25	5b	1	Total	C	O	0
			42	40	2	
25	5b	1	Total	C	O	0
			42	40	2	
25	6b	1	Total	C	O	0
			42	40	2	
25	6b	1	Total	C	O	0
			42	40	2	
25	6b	1	Total	C	O	0
			42	40	2	

- Molecule 26 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



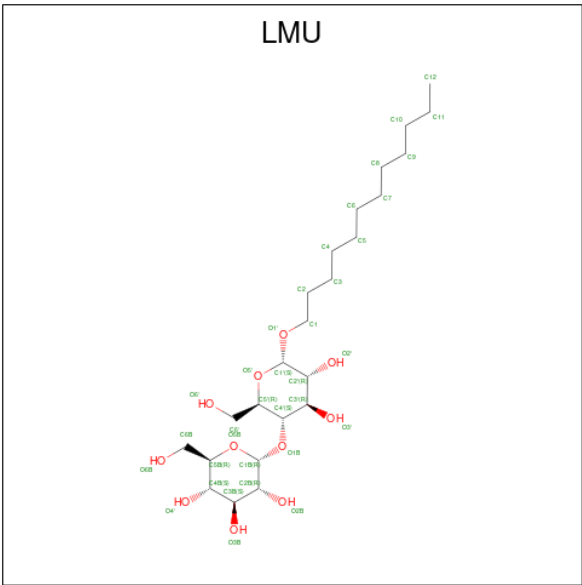
Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			34	23	10	1	
27	2a	1	Total	C	O	P	0
			32	21	10	1	
27	5a	1	Total	C	O	P	0
			32	21	10	1	
27	5a	1	Total	C	O	P	0
			37	26	10	1	
27	6a	1	Total	C	O	P	0
			39	28	10	1	
27	a	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			34	23	10	1	
27	2b	1	Total	C	O	P	0
			32	21	10	1	
27	5b	1	Total	C	O	P	0
			32	21	10	1	
27	5b	1	Total	C	O	P	0
			37	26	10	1	
27	6b	1	Total	C	O	P	0
			39	28	10	1	

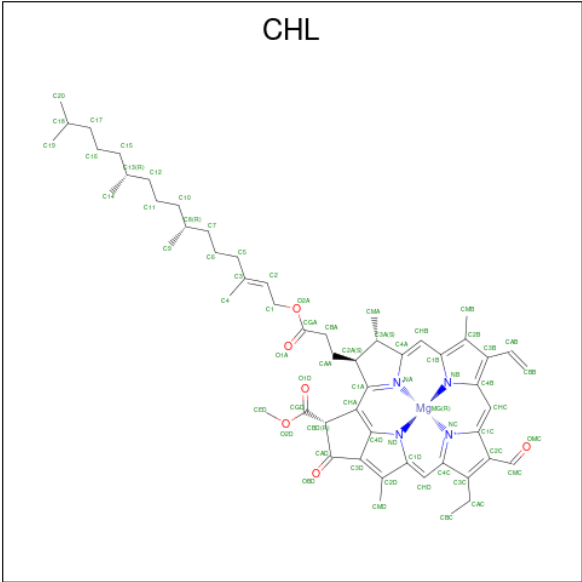
- Molecule 28 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	6a	1	Total	C	O	0
			35	24	11	
28	6a	1	Total	C	O	0
			33	22	11	
28	a	1	Total	C	O	0
			35	24	11	
28	6b	1	Total	C	O	0
			35	24	11	
28	6b	1	Total	C	O	0
			33	22	11	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms						AltConf
29	2a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	2a	1	Total	C	Mg	N	O		0
			43	34	1	4	4		
29	2a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	2a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	3a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	3a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	3a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	5a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	5a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	5a	1	Total	C	Mg	N	O		0
			43	34	1	4	4		
29	5a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	5a	1	Total	C	Mg	N	O		0
			43	34	1	4	4		
29	6a	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
29	6a	1	Total	C	Mg	N	O		0
			41	32	1	4	4		

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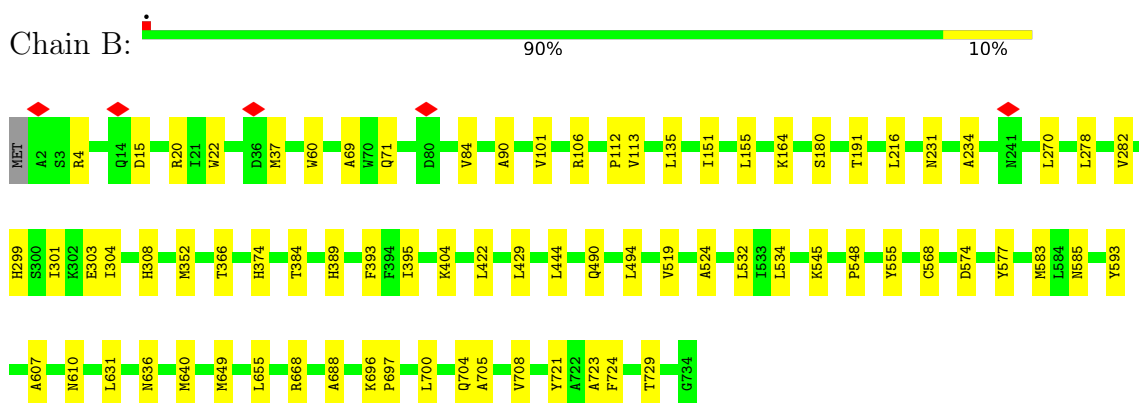
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Mol	Chain	Residues	Atoms					AltConf
29	2b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	2b	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	2b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	2b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	3b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	3b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	3b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5b	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	5b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5b	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	6b	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6b	1	Total 41	C 32	Mg 1	N 4	O 4	0

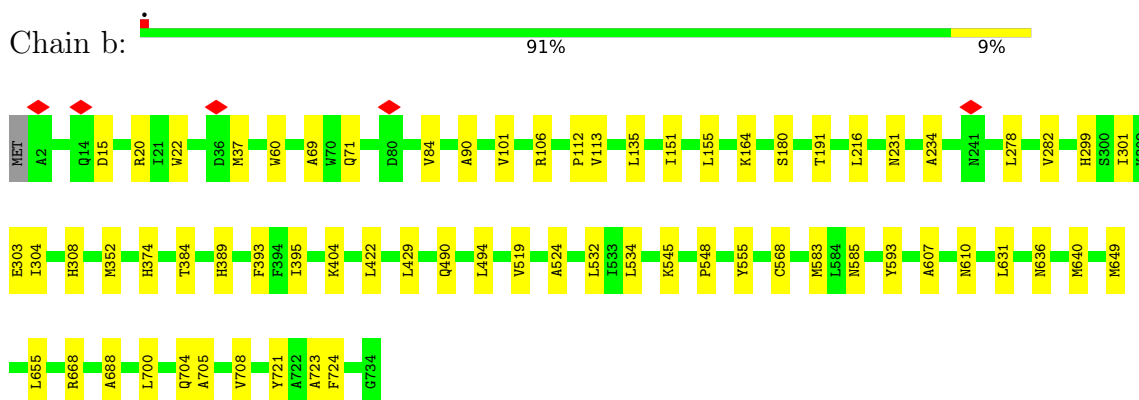
### 3 Residue-property plots [i](#)

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

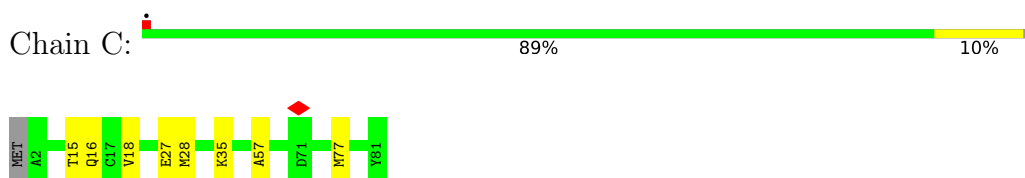
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I iron-sulfur center



- Molecule 2: Photosystem I iron-sulfur center



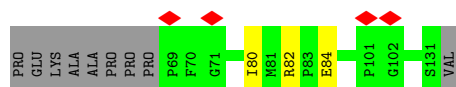
- Molecule 3: Photosystem I reaction center subunit II, chloroplastic



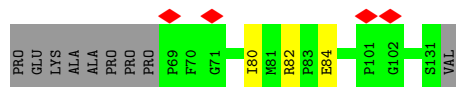
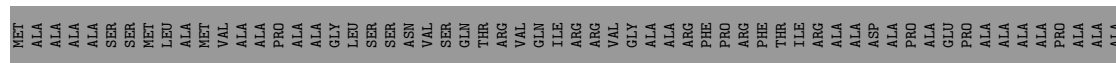
- Molecule 3: Photosystem I reaction center subunit II, chloroplastic



- Molecule 4: Photosystem I reaction centre subunit IV

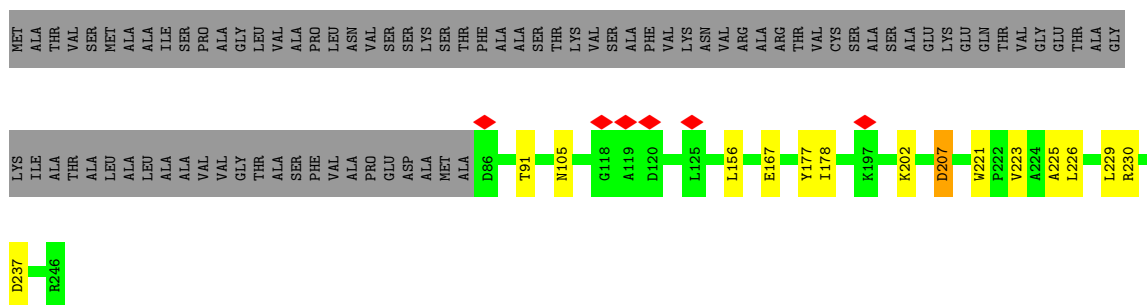


- Molecule 4: Photosystem I reaction centre subunit IV



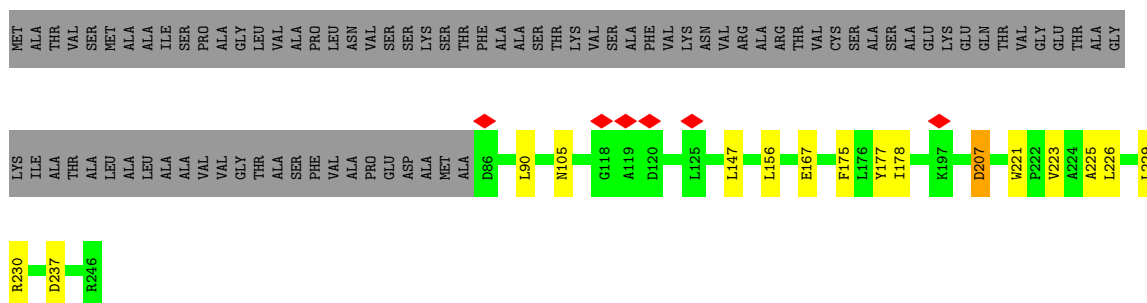
- Molecule 5: Photosystem I reaction center subunit III





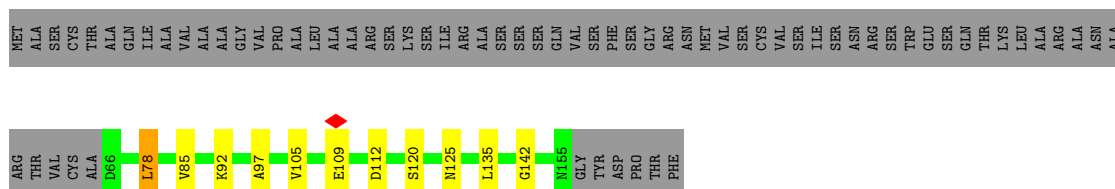
• Molecule 5: Photosystem I reaction center subunit III

Chain f: 59% 6% 35%



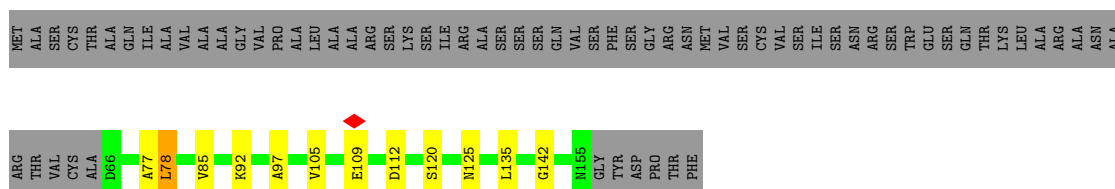
• Molecule 6: Photosystem I reaction center subunit V, chloroplastic

Chain G: 49% 6% 44%



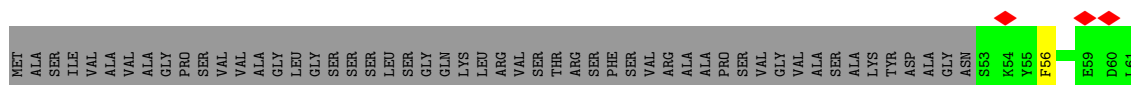
• Molecule 6: Photosystem I reaction center subunit V, chloroplastic

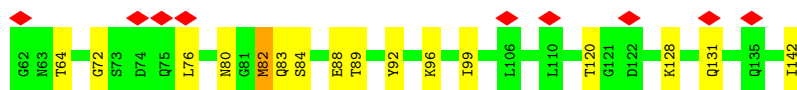
Chain g: 48% 7% 44%



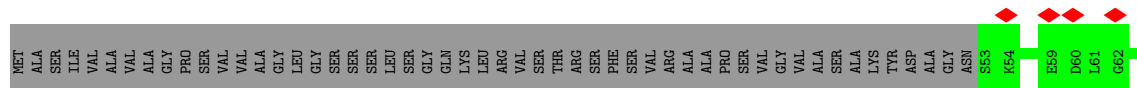
• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic

Chain H: 8% 51% 11% 37%

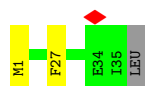




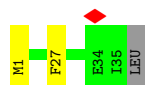
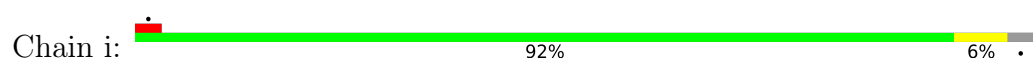
- Molecule 7: Photosystem I reaction center subunit VI, chloroplastic



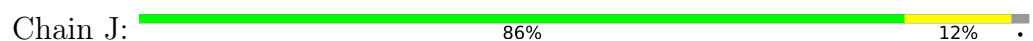
- Molecule 8: Photosystem I reaction center subunit VIII



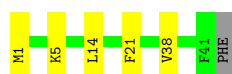
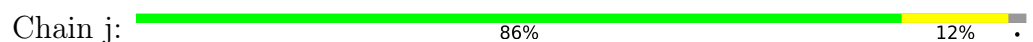
- Molecule 8: Photosystem I reaction center subunit VIII



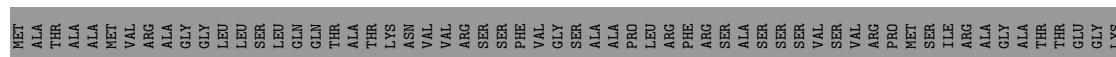
- Molecule 9: Photosystem I reaction center subunit IX

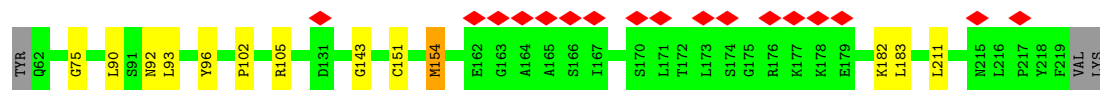


- Molecule 9: Photosystem I reaction center subunit IX

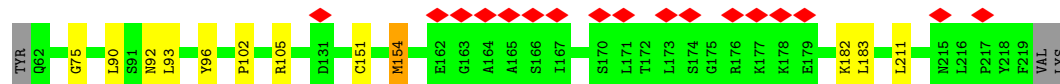
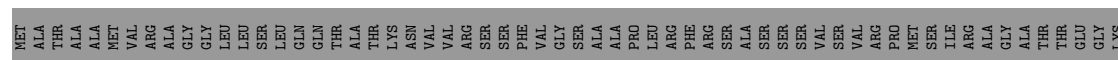


- Molecule 10: PSI subunit V

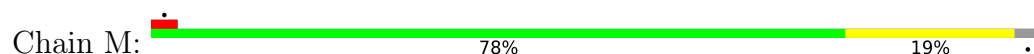




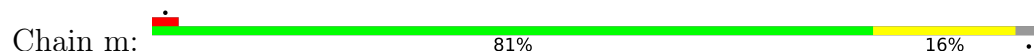
• Molecule 10: PSI subunit V



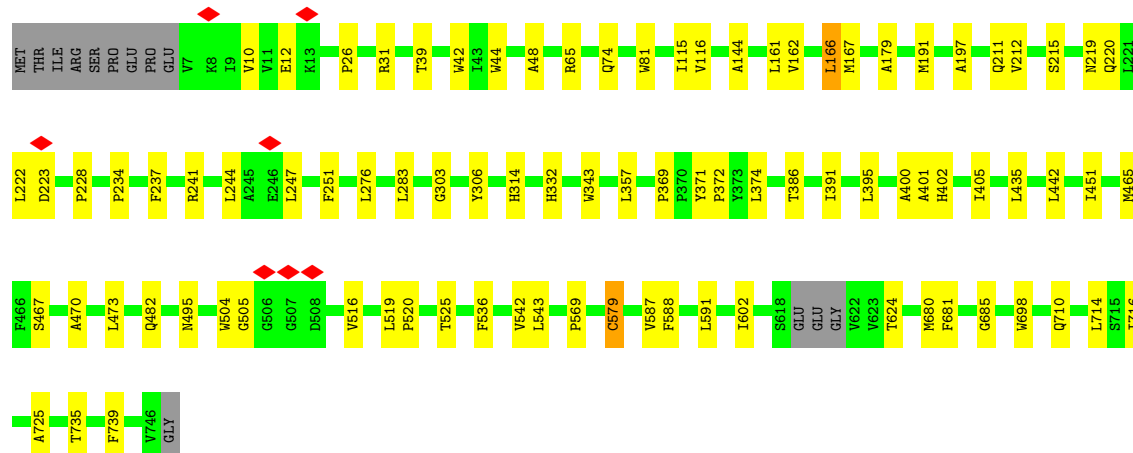
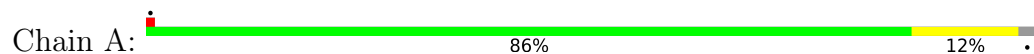
• Molecule 11: Photosystem I reaction center subunit XII



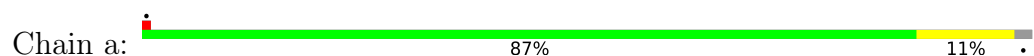
• Molecule 11: Photosystem I reaction center subunit XII

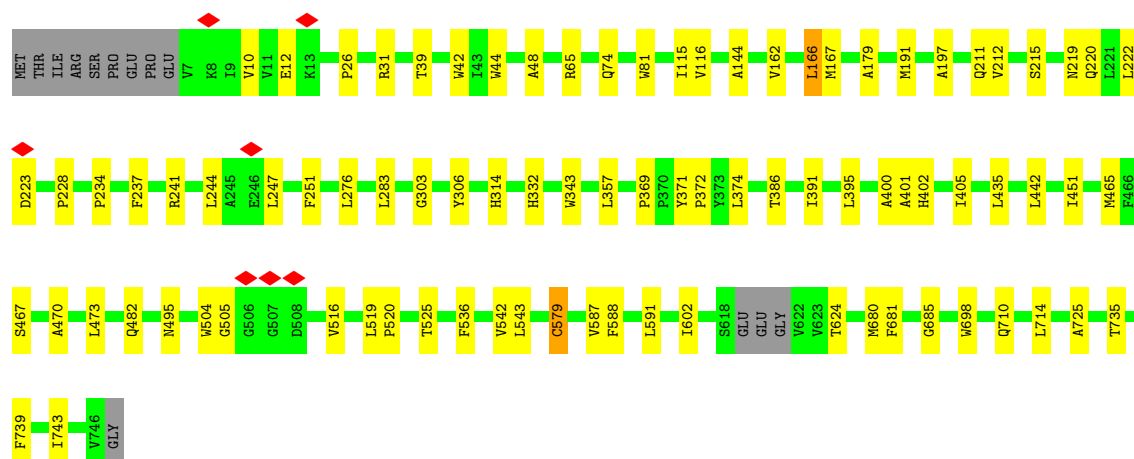


• Molecule 12: Photosystem I P700 chlorophyll a apoprotein A1

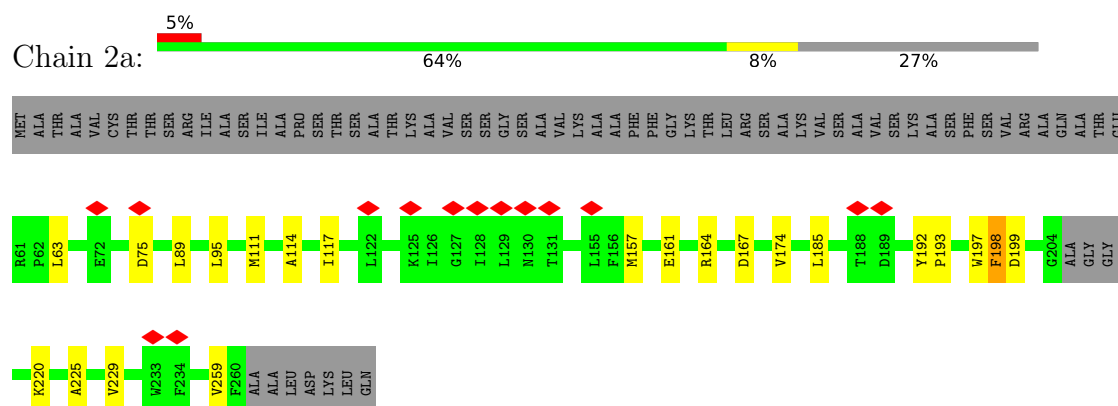


• Molecule 12: Photosystem I P700 chlorophyll a apoprotein A1

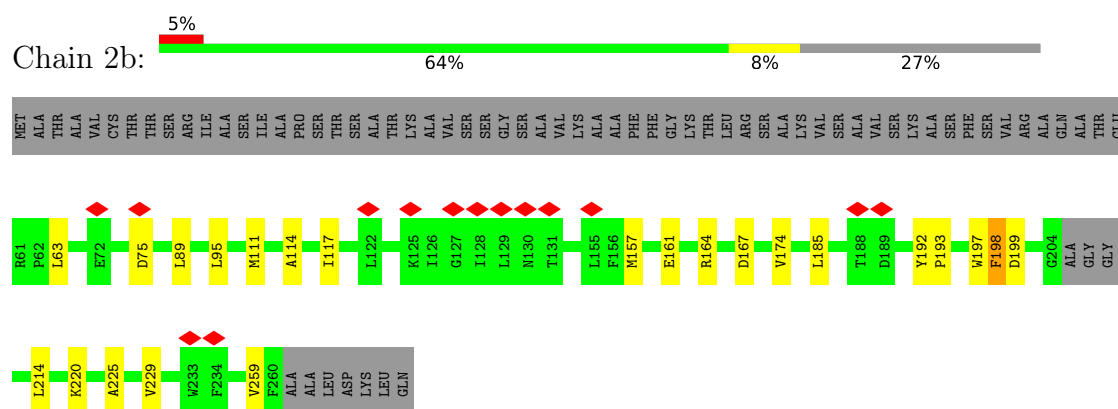




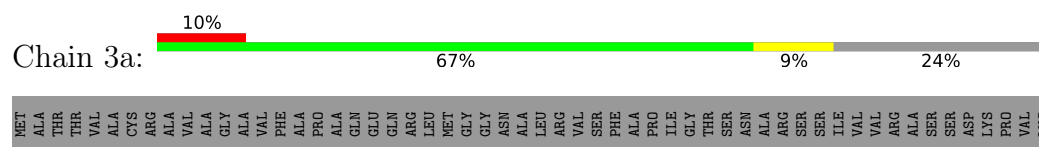
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



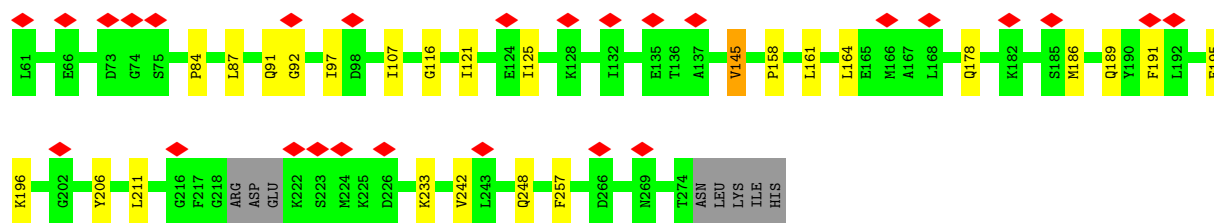
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



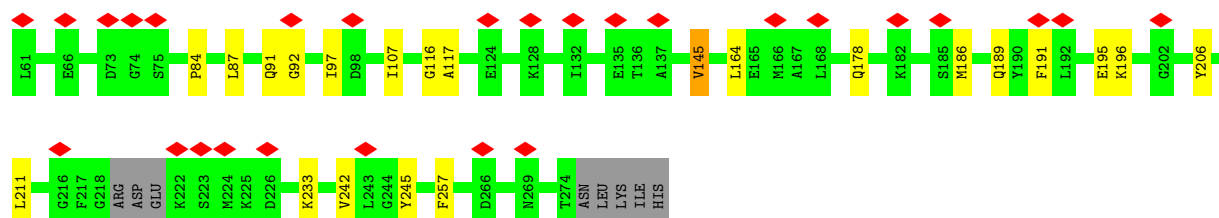
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



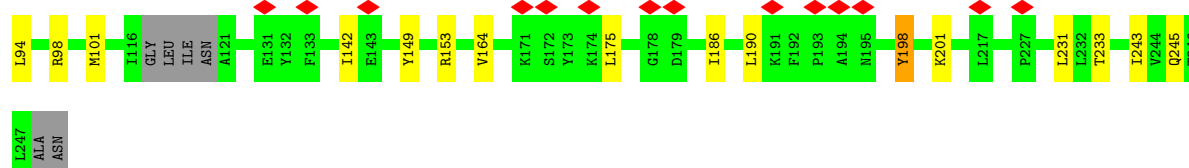
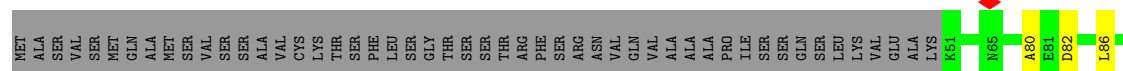
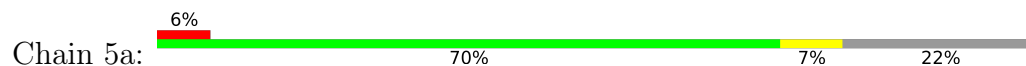




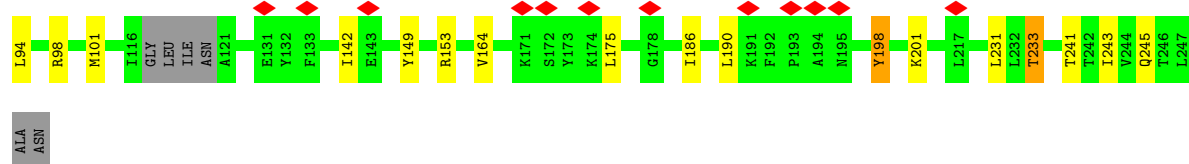
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



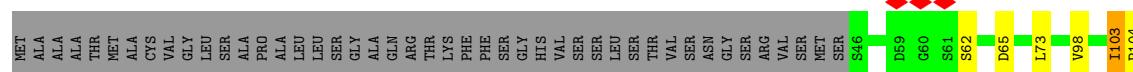
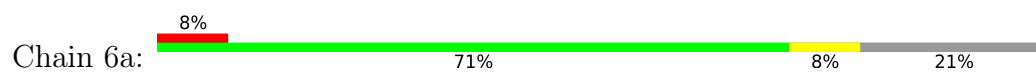
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



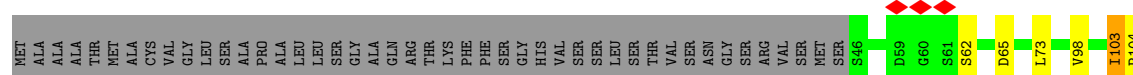
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



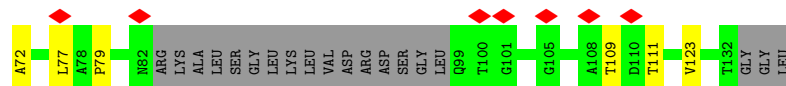
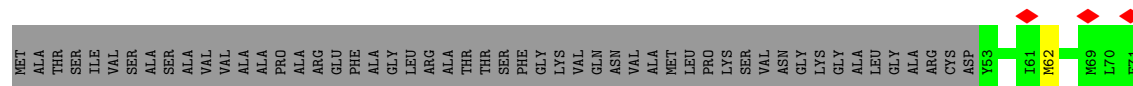
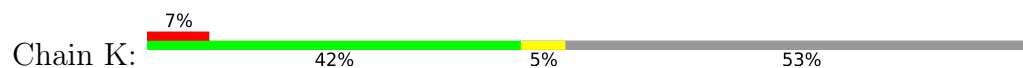
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



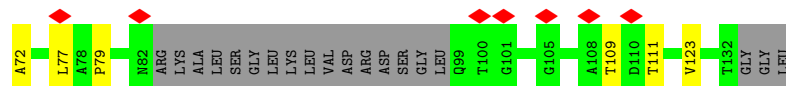
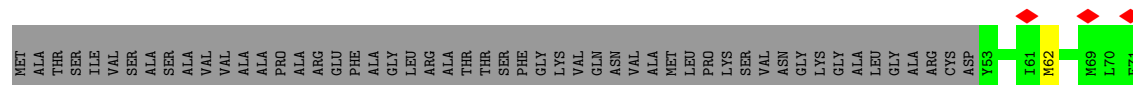
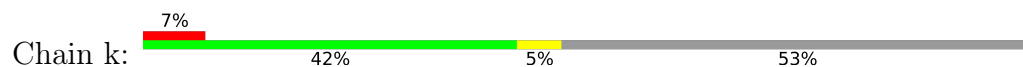
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: PSI-K



- Molecule 17: PSI-K



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	465.28, 465.28, 465.28	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, DGD, CHL, SF4, LMU, LMG, LUT, CLA, LFA, BCR, LHG, CLO

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	B	0.21	0/6066	0.44	0/8277
1	b	0.21	0/6066	0.44	0/8277
2	C	0.23	0/612	0.56	0/829
2	c	0.23	0/612	0.56	0/829
3	D	0.21	0/1122	0.56	0/1511
3	d	0.21	0/1122	0.56	0/1511
4	E	0.21	0/508	0.49	0/691
4	e	0.22	0/508	0.49	0/691
5	F	0.21	0/1275	0.47	2/1725 (0.1%)
5	f	0.21	0/1275	0.47	2/1725 (0.1%)
6	G	0.25	0/686	0.51	0/931
6	g	0.26	0/686	0.51	0/931
7	H	0.22	0/696	0.55	0/939
7	h	0.22	0/696	0.55	0/939
8	I	0.31	0/281	0.70	0/384
8	i	0.31	0/281	0.70	0/384
9	J	0.24	0/338	0.57	0/462
9	j	0.24	0/338	0.57	0/462
10	L	0.23	0/1215	0.58	0/1660
10	l	0.23	0/1215	0.58	0/1660
11	M	0.30	0/243	0.56	0/327
11	m	0.30	0/243	0.56	0/327
12	A	0.21	0/6007	0.46	2/8198 (0.0%)
12	a	0.21	0/6007	0.46	2/8198 (0.0%)
13	2a	0.21	0/1574	0.56	2/2151 (0.1%)
13	2b	0.21	0/1574	0.56	2/2151 (0.1%)
14	3a	0.24	0/1682	0.59	0/2281
14	3b	0.24	0/1682	0.59	0/2281
15	5a	0.19	0/1566	0.49	1/2137 (0.0%)
15	5b	0.19	0/1566	0.49	1/2137 (0.0%)
16	6a	0.22	0/1539	0.56	2/2100 (0.1%)
16	6b	0.23	0/1539	0.56	2/2100 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	K	0.26	0/446	0.58	0/604
17	k	0.26	0/446	0.58	0/604
All	All	0.22	0/51712	0.51	18/70414 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2a	198	PHE	CA-CB-CG	-6.88	106.92	113.80
13	2b	198	PHE	CA-CB-CG	-6.88	106.92	113.80
5	F	207	ASP	CA-C-N	6.41	124.28	120.24
5	F	207	ASP	C-N-CA	6.41	124.28	120.24
5	f	207	ASP	CA-C-N	6.41	124.28	120.24

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5854	0	5632	55	0
1	b	5854	0	5632	50	0
2	C	602	0	575	6	0
2	c	602	0	575	6	0
3	D	1094	0	1113	6	0
3	d	1094	0	1113	7	0
4	E	495	0	481	2	0
4	e	495	0	481	2	0
5	F	1248	0	1291	10	0
5	f	1248	0	1291	11	0
6	G	673	0	678	17	0
6	g	673	0	678	18	0
7	H	680	0	680	20	0
7	h	680	0	680	18	0
8	I	274	0	285	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	i	274	0	285	2	0
9	J	328	0	339	3	0
9	j	328	0	339	3	0
10	L	1180	0	1186	12	0
10	l	1180	0	1186	12	0
11	M	242	0	266	6	0
11	m	242	0	266	5	0
12	A	5810	0	5687	61	0
12	a	5810	0	5687	59	0
13	2a	1520	0	1470	18	0
13	2b	1520	0	1470	18	0
14	3a	1633	0	1594	17	0
14	3b	1633	0	1594	14	0
15	5a	1516	0	1491	12	0
15	5b	1516	0	1491	13	0
16	6a	1491	0	1471	13	0
16	6b	1491	0	1471	16	0
17	K	441	0	446	4	0
17	k	441	0	446	4	0
18	2a	425	0	329	14	0
18	2b	425	0	329	14	0
18	3a	566	0	438	13	0
18	3b	566	0	438	11	0
18	5a	479	0	367	14	0
18	5b	479	0	367	14	0
18	6a	590	0	478	21	0
18	6b	590	0	478	22	0
18	A	2387	0	2303	72	0
18	B	2483	0	2431	80	0
18	F	146	0	121	6	0
18	G	95	0	72	4	0
18	J	45	0	33	2	0
18	K	44	0	30	0	0
18	L	147	0	123	5	0
18	a	2387	0	2303	72	0
18	b	2483	0	2431	84	0
18	f	146	0	121	6	0
18	g	95	0	72	4	0
18	j	45	0	33	2	0
18	k	44	0	30	0	0
18	l	147	0	123	5	0
19	A	33	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	33	0	46	3	0
19	a	33	0	46	1	0
19	b	33	0	46	3	0
20	A	200	0	280	15	0
20	B	280	0	392	19	0
20	F	80	0	112	3	0
20	G	80	0	112	5	0
20	I	40	0	56	3	0
20	J	40	0	56	4	0
20	K	40	0	56	3	0
20	L	40	0	56	2	0
20	M	40	0	56	4	0
20	a	200	0	280	16	0
20	b	280	0	392	18	0
20	f	80	0	112	5	0
20	g	80	0	112	6	0
20	i	40	0	56	3	0
20	j	40	0	56	5	0
20	k	40	0	56	2	0
20	l	40	0	56	2	0
20	m	40	0	56	3	0
21	B	59	0	79	3	0
21	b	59	0	79	3	0
22	B	12	0	23	0	0
22	M	12	0	23	0	0
22	b	12	0	23	0	0
22	m	12	0	23	0	0
23	5a	35	0	40	1	0
23	5b	35	0	40	1	0
23	B	42	0	54	1	0
23	I	31	0	32	1	0
23	J	71	0	85	2	0
23	b	42	0	54	1	0
23	i	31	0	32	1	0
23	j	71	0	85	2	0
24	A	8	0	0	1	0
24	C	16	0	0	0	0
24	a	8	0	0	1	0
24	c	16	0	0	0	0
25	2a	84	0	112	11	0
25	2b	84	0	112	11	0
25	3a	84	0	112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3b	84	0	112	8	0
25	5a	84	0	112	8	0
25	5b	84	0	112	5	0
25	6a	126	0	168	14	0
25	6b	126	0	168	12	0
25	J	42	0	56	4	0
25	j	42	0	56	3	0
26	A	65	0	72	3	0
26	a	65	0	72	3	0
27	2a	32	0	34	0	0
27	2b	32	0	34	0	0
27	5a	69	0	78	3	0
27	5b	69	0	78	3	0
27	6a	39	0	51	1	0
27	6b	39	0	51	1	0
27	A	83	0	112	7	0
27	a	83	0	112	7	0
28	6a	68	0	85	0	0
28	6b	68	0	85	0	0
28	A	35	0	46	0	0
28	a	35	0	46	0	0
29	2a	181	0	122	9	0
29	2b	181	0	122	8	0
29	3a	138	0	93	4	0
29	3b	138	0	93	4	0
29	5a	224	0	151	6	0
29	5b	224	0	151	6	0
29	6a	87	0	55	3	0
29	6b	87	0	55	3	0
All	All	70242	0	68946	937	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 7.

The worst 5 of 937 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)
7:H:92:TYR:CD1	6:g:125:ASN:ND2	1.83	1.41
6:G:125:ASN:ND2	7:h:92:TYR:CD1	1.81	1.40
7:H:92:TYR:CE1	6:g:125:ASN:ND2	1.83	1.39
6:G:125:ASN:ND2	7:h:92:TYR:CE1	1.83	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:120:SER:HB2	7:h:96:LYS:HE2	1.41	1.00

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	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
1	b	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
2	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
2	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	D	138/215 (64%)	132 (96%)	6 (4%)	0	100	100
3	d	138/215 (64%)	132 (96%)	6 (4%)	0	100	100
4	E	61/132 (46%)	57 (93%)	4 (7%)	0	100	100
4	e	61/132 (46%)	57 (93%)	4 (7%)	0	100	100
5	F	159/246 (65%)	157 (99%)	2 (1%)	0	100	100
5	f	159/246 (65%)	157 (99%)	2 (1%)	0	100	100
6	G	88/161 (55%)	86 (98%)	2 (2%)	0	100	100
6	g	88/161 (55%)	86 (98%)	2 (2%)	0	100	100
7	H	88/142 (62%)	84 (96%)	4 (4%)	0	100	100
7	h	88/142 (62%)	84 (96%)	4 (4%)	0	100	100
8	I	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
8	i	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
9	J	39/42 (93%)	37 (95%)	2 (5%)	0	100	100
9	j	39/42 (93%)	37 (95%)	2 (5%)	0	100	100
10	L	156/221 (71%)	147 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	l	156/221 (71%)	147 (94%)	9 (6%)	0	100	100
11	M	29/32 (91%)	29 (100%)	0	0	100	100
11	m	29/32 (91%)	29 (100%)	0	0	100	100
12	A	733/750 (98%)	716 (98%)	17 (2%)	0	100	100
12	a	733/750 (98%)	716 (98%)	17 (2%)	0	100	100
13	2a	190/267 (71%)	182 (96%)	8 (4%)	0	100	100
13	2b	190/267 (71%)	182 (96%)	8 (4%)	0	100	100
14	3a	208/279 (75%)	200 (96%)	8 (4%)	0	100	100
14	3b	208/279 (75%)	200 (96%)	8 (4%)	0	100	100
15	5a	189/249 (76%)	184 (97%)	5 (3%)	0	100	100
15	5b	189/249 (76%)	184 (97%)	5 (3%)	0	100	100
16	6a	189/243 (78%)	180 (95%)	9 (5%)	0	100	100
16	6b	189/243 (78%)	180 (95%)	9 (5%)	0	100	100
17	K	60/135 (44%)	58 (97%)	2 (3%)	0	100	100
17	k	60/135 (44%)	58 (97%)	2 (3%)	0	100	100
All	All	6338/7930 (80%)	6126 (97%)	212 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	597/598 (100%)	593 (99%)	4 (1%)	76	89
1	b	597/598 (100%)	593 (99%)	4 (1%)	76	89
2	C	68/69 (99%)	67 (98%)	1 (2%)	57	79
2	c	68/69 (99%)	67 (98%)	1 (2%)	57	79
3	D	114/161 (71%)	113 (99%)	1 (1%)	70	86
3	d	114/161 (71%)	113 (99%)	1 (1%)	70	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	56/99 (57%)	56 (100%)	0	100	100
4	e	56/99 (57%)	56 (100%)	0	100	100
5	F	129/189 (68%)	126 (98%)	3 (2%)	44	70
5	f	129/189 (68%)	127 (98%)	2 (2%)	55	78
6	G	70/125 (56%)	69 (99%)	1 (1%)	59	80
6	g	70/125 (56%)	69 (99%)	1 (1%)	59	80
7	H	70/107 (65%)	67 (96%)	3 (4%)	26	49
7	h	70/107 (65%)	68 (97%)	2 (3%)	37	63
8	I	31/32 (97%)	31 (100%)	0	100	100
8	i	31/32 (97%)	31 (100%)	0	100	100
9	J	35/36 (97%)	33 (94%)	2 (6%)	18	36
9	j	35/36 (97%)	33 (94%)	2 (6%)	18	36
10	L	121/169 (72%)	120 (99%)	1 (1%)	73	88
10	l	121/169 (72%)	120 (99%)	1 (1%)	73	88
11	M	29/30 (97%)	29 (100%)	0	100	100
11	m	29/30 (97%)	29 (100%)	0	100	100
12	A	600/611 (98%)	595 (99%)	5 (1%)	73	88
12	a	600/611 (98%)	595 (99%)	5 (1%)	73	88
13	2a	154/204 (76%)	152 (99%)	2 (1%)	61	81
13	2b	154/204 (76%)	152 (99%)	2 (1%)	61	81
14	3a	165/216 (76%)	158 (96%)	7 (4%)	26	49
14	3b	165/216 (76%)	158 (96%)	7 (4%)	26	49
15	5a	156/202 (77%)	151 (97%)	5 (3%)	34	60
15	5b	156/202 (77%)	151 (97%)	5 (3%)	34	60
16	6a	152/190 (80%)	149 (98%)	3 (2%)	48	73
16	6b	152/190 (80%)	149 (98%)	3 (2%)	48	73
17	K	45/96 (47%)	44 (98%)	1 (2%)	45	71
17	k	45/96 (47%)	44 (98%)	1 (2%)	45	71
All	All	5184/6268 (83%)	5108 (98%)	76 (2%)	55	79

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	a	624	THR
15	5b	233	THR
13	2b	259	VAL
14	3b	233	LYS
17	k	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
5	f	164	HIS
13	2b	221	ASN
10	l	129	ASN
13	2b	183	ASN
15	5b	240	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

412 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
18	CLA	B	822	1	49,53,73	1.35	6 (12%)	58,89,113	1.10	5 (8%)
20	BCR	k	202	-	41,41,41	1.45	7 (17%)	56,56,56	1.78	16 (28%)
20	BCR	f	304	-	41,41,41	1.44	8 (19%)	56,56,56	1.76	15 (26%)
18	CLA	b	808	1	51,55,73	1.38	8 (15%)	60,91,113	1.12	4 (6%)
18	CLA	b	813	1	59,63,73	1.26	6 (10%)	70,101,113	0.93	3 (4%)
18	CLA	3b	312	14	59,63,73	1.25	7 (11%)	70,101,113	1.11	5 (7%)
29	CHL	5a	305	-	40,54,74	1.15	3 (7%)	34,90,114	2.77	10 (29%)
18	CLA	a	840	12	69,73,73	1.19	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	B	823	-	69,73,73	1.17	6 (8%)	82,113,113	1.05	6 (7%)
18	CLA	a	823	12	69,73,73	1.20	8 (11%)	82,113,113	1.01	5 (6%)
18	CLA	3b	306	14	49,53,73	1.38	7 (14%)	58,89,113	1.15	4 (6%)
20	BCR	A	847	-	41,41,41	1.45	9 (21%)	56,56,56	1.86	17 (30%)
20	BCR	i	202	-	41,41,41	1.45	4 (9%)	56,56,56	1.62	13 (23%)
18	CLA	5a	311	15	48,52,73	1.38	7 (14%)	57,88,113	1.13	4 (7%)
29	CHL	2a	305	-	37,51,74	1.16	3 (8%)	30,86,114	2.93	10 (33%)
18	CLA	b	812	1	69,73,73	1.17	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	a	806	12	69,73,73	1.19	8 (11%)	82,113,113	0.88	3 (3%)
18	CLA	5a	310	-	49,53,73	1.39	7 (14%)	58,89,113	1.09	3 (5%)
18	CLA	5a	312	15	56,60,73	1.27	6 (10%)	65,97,113	1.15	6 (9%)
23	LMG	b	850	-	42,42,55	0.54	0	50,50,63	0.67	0
25	LUT	3a	317	-	42,43,43	1.36	8 (19%)	51,60,60	2.02	11 (21%)
18	CLA	2b	310	-	49,53,73	1.38	7 (14%)	58,89,113	1.20	4 (6%)
18	CLA	5b	302	15	60,64,73	1.22	6 (10%)	71,102,113	1.01	4 (5%)
18	CLA	6b	315	16	59,63,73	1.28	7 (11%)	70,101,113	1.04	4 (5%)
18	CLA	B	803	1	49,53,73	1.40	7 (14%)	58,89,113	1.04	4 (6%)
18	CLA	a	803	12	65,69,73	1.19	6 (9%)	77,108,113	1.00	4 (5%)
18	CLA	a	839	12	69,73,73	1.19	7 (10%)	82,113,113	0.87	3 (3%)
18	CLA	b	825	1	69,73,73	1.23	7 (10%)	82,113,113	0.94	3 (3%)
18	CLA	B	854	-	69,73,73	1.20	7 (10%)	82,113,113	1.00	6 (7%)
25	LUT	3b	316	-	42,43,43	1.31	6 (14%)	51,60,60	1.81	15 (29%)
18	CLA	A	840	12	69,73,73	1.19	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	5b	312	15	56,60,73	1.27	6 (10%)	65,97,113	1.16	6 (9%)
18	CLA	6b	308	16	49,53,73	1.47	7 (14%)	58,89,113	1.05	4 (6%)
20	BCR	A	849	-	41,41,41	1.45	8 (19%)	56,56,56	1.71	17 (30%)
18	CLA	5a	315	15	50,54,73	1.39	7 (14%)	59,90,113	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	BCR	g	201	-	41,41,41	1.48	4 (9%)	56,56,56	1.74	17 (30%)
18	CLA	B	831	1	69,73,73	1.18	7 (10%)	82,113,113	1.01	4 (4%)
18	CLA	b	822	1	49,53,73	1.35	6 (12%)	58,89,113	1.10	5 (8%)
18	CLA	b	802	-	69,73,73	1.13	6 (8%)	82,113,113	0.98	6 (7%)
20	BCR	G	204	-	41,41,41	1.46	7 (17%)	56,56,56	1.68	15 (26%)
20	BCR	B	848	-	41,41,41	1.40	10 (24%)	56,56,56	2.23	22 (39%)
20	BCR	a	848	-	41,41,41	1.46	7 (17%)	56,56,56	1.72	16 (28%)
18	CLA	B	807	1	65,69,73	1.19	7 (10%)	77,108,113	0.92	3 (3%)
18	CLA	A	804	12	59,63,73	1.25	6 (10%)	70,101,113	1.05	5 (7%)
18	CLA	B	828	1	59,63,73	1.27	7 (11%)	70,101,113	1.05	4 (5%)
18	CLA	B	829	1	49,53,73	1.37	6 (12%)	58,89,113	1.12	5 (8%)
18	CLA	5a	302	15	60,64,73	1.22	6 (10%)	71,102,113	1.01	4 (5%)
18	CLA	a	828	12	69,73,73	1.31	8 (11%)	82,113,113	0.92	3 (3%)
18	CLA	B	809	1	69,73,73	1.17	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	a	820	-	69,73,73	1.19	6 (8%)	82,113,113	0.97	4 (4%)
18	CLA	b	816	1	66,70,73	1.25	7 (10%)	78,109,113	1.06	5 (6%)
20	BCR	B	846	-	41,41,41	1.46	7 (17%)	56,56,56	1.67	13 (23%)
20	BCR	B	843	-	41,41,41	1.46	8 (19%)	56,56,56	2.16	13 (23%)
27	LHG	5b	318	-	31,31,48	0.32	0	34,37,54	0.42	0
25	LUT	6b	318	-	42,43,43	1.29	8 (19%)	51,60,60	1.76	12 (23%)
18	CLA	A	813	12	54,58,73	1.27	5 (9%)	64,95,113	1.10	5 (7%)
18	CLA	b	801	1	69,73,73	1.20	8 (11%)	82,113,113	0.88	3 (3%)
18	CLA	6a	305	16	65,69,73	1.17	6 (9%)	77,108,113	0.98	4 (5%)
18	CLA	A	825	-	59,63,73	1.25	7 (11%)	70,101,113	0.97	4 (5%)
28	LMU	6a	302	-	36,36,36	0.26	0	47,47,47	0.67	0
18	CLA	A	822	12	49,53,73	1.41	7 (14%)	58,89,113	1.14	6 (10%)
22	LFA	M	102	-	11,11,19	0.11	0	10,10,18	0.13	0
18	CLA	k	201	17	48,52,73	1.44	8 (16%)	59,88,113	1.06	4 (6%)
18	CLA	b	817	1	69,73,73	1.15	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	3a	305	14	50,54,73	1.36	6 (12%)	59,90,113	1.09	5 (8%)
25	LUT	2a	314	-	42,43,43	1.30	7 (16%)	51,60,60	2.29	15 (29%)
18	CLA	5b	310	-	49,53,73	1.39	7 (14%)	58,89,113	1.09	3 (5%)
18	CLA	6b	317	16	49,53,73	1.39	7 (14%)	58,89,113	1.08	3 (5%)
25	LUT	j	105	-	42,43,43	1.29	7 (16%)	51,60,60	3.07	21 (41%)
18	CLA	B	835	1	54,58,73	1.42	7 (12%)	64,95,113	1.10	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	b	807	1	65,69,73	1.20	7 (10%)	77,108,113	0.92	3 (3%)
18	CLA	6a	310	-	49,53,73	1.40	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	A	811	12	49,53,73	1.36	5 (10%)	58,89,113	1.03	4 (6%)
18	CLA	b	814	1	54,58,73	1.33	6 (11%)	64,95,113	1.04	4 (6%)
18	CLA	2b	309	27	49,53,73	1.39	7 (14%)	58,89,113	1.03	3 (5%)
20	BCR	b	848	-	41,41,41	1.40	10 (24%)	56,56,56	2.23	22 (39%)
20	BCR	a	847	-	41,41,41	1.45	9 (21%)	56,56,56	1.86	17 (30%)
28	LMU	6a	303	-	34,34,36	0.29	0	45,45,47	0.51	0
29	CHL	5b	306	-	37,51,74	1.19	3 (8%)	30,86,114	3.07	12 (40%)
18	CLA	5b	315	15	50,54,73	1.39	7 (14%)	59,90,113	1.03	3 (5%)
20	BCR	B	844	-	41,41,41	1.44	8 (19%)	56,56,56	1.81	17 (30%)
18	CLA	b	824	-	54,58,73	1.28	6 (11%)	64,95,113	1.07	5 (7%)
18	CLA	6a	315	16	59,63,73	1.28	7 (11%)	70,101,113	1.04	4 (5%)
27	LHG	A	846	-	33,33,48	0.34	0	36,39,54	0.47	0
18	CLA	3b	309	14	54,58,73	1.26	6 (11%)	64,95,113	1.07	4 (6%)
18	CLA	2b	308	13	59,63,73	1.22	6 (10%)	70,101,113	1.02	4 (5%)
18	CLA	a	810	12	69,73,73	1.19	6 (8%)	82,113,113	0.89	3 (3%)
20	BCR	A	850	-	41,41,41	1.47	5 (12%)	56,56,56	1.67	15 (26%)
18	CLA	5a	313	15	49,53,73	1.39	7 (14%)	58,89,113	1.04	3 (5%)
18	CLA	a	842	-	49,53,73	1.38	7 (14%)	58,89,113	1.10	5 (8%)
18	CLA	b	837	1	51,55,73	1.35	7 (13%)	60,91,113	1.02	4 (6%)
18	CLA	B	840	27	69,73,73	1.14	6 (8%)	82,113,113	1.03	6 (7%)
20	BCR	j	102	-	41,41,41	1.45	10 (24%)	56,56,56	2.15	21 (37%)
20	BCR	F	304	-	41,41,41	1.44	8 (19%)	56,56,56	1.76	14 (25%)
20	BCR	J	102	-	41,41,41	1.45	10 (24%)	56,56,56	2.15	21 (37%)
27	LHG	5b	320	-	36,36,48	0.31	0	39,42,54	0.47	0
18	CLA	A	853	-	55,59,73	1.29	6 (10%)	64,96,113	1.06	5 (7%)
18	CLA	6a	311	16	49,53,73	1.36	6 (12%)	58,89,113	1.11	3 (5%)
18	CLA	A	831	12	54,58,73	1.33	6 (11%)	64,95,113	0.96	4 (6%)
18	CLA	B	808	1	51,55,73	1.38	8 (15%)	60,91,113	1.11	4 (6%)
18	CLA	a	808	12	69,73,73	1.11	7 (10%)	82,113,113	0.90	4 (4%)
28	LMU	6b	303	-	34,34,36	0.29	0	45,45,47	0.51	0
18	CLA	b	835	1	54,58,73	1.42	7 (12%)	64,95,113	1.10	4 (6%)
25	LUT	6a	320	-	42,43,43	1.31	8 (19%)	51,60,60	1.69	14 (27%)
18	CLA	a	801	12	56,60,73	1.28	6 (10%)	65,97,113	1.05	5 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	6b	305	16	65,69,73	1.17	6 (9%)	77,108,113	0.98	4 (5%)
29	CHL	3b	301	13	40,54,74	1.11	2 (5%)	34,90,114	2.98	10 (29%)
18	CLA	A	821	12	49,53,73	1.39	7 (14%)	58,89,113	1.09	5 (8%)
25	LUT	2b	315	-	42,43,43	1.36	8 (19%)	51,60,60	2.44	14 (27%)
18	CLA	f	305	-	64,68,73	1.22	7 (10%)	76,107,113	1.02	7 (9%)
18	CLA	3a	312	14	59,63,73	1.25	7 (11%)	70,101,113	1.10	5 (7%)
18	CLA	B	830	1	64,68,73	1.22	7 (10%)	76,107,113	1.07	5 (6%)
18	CLA	b	832	1	64,68,73	1.22	7 (10%)	76,107,113	1.05	5 (6%)
18	CLA	A	824	-	69,73,73	1.24	8 (11%)	82,113,113	0.94	5 (6%)
18	CLA	A	830	12	54,58,73	1.33	7 (12%)	64,95,113	1.17	5 (7%)
18	CLA	g	203	6	49,53,73	1.38	7 (14%)	58,89,113	1.06	4 (6%)
18	CLA	b	818	-	57,61,73	1.30	6 (10%)	67,98,113	1.05	4 (5%)
18	CLA	2a	303	-	49,53,73	1.38	8 (16%)	58,89,113	1.14	5 (8%)
18	CLA	a	813	12	54,58,73	1.27	5 (9%)	64,95,113	1.11	5 (7%)
20	BCR	B	842	-	41,41,41	1.45	8 (19%)	56,56,56	1.83	18 (32%)
18	CLA	3b	311	14	47,51,73	1.44	7 (14%)	55,86,113	1.14	4 (7%)
18	CLA	A	829	12	69,73,73	1.20	7 (10%)	82,113,113	0.96	3 (3%)
25	LUT	2a	315	-	42,43,43	1.36	8 (19%)	51,60,60	2.44	14 (27%)
18	CLA	2a	310	-	49,53,73	1.38	7 (14%)	58,89,113	1.20	4 (6%)
18	CLA	3a	302	14	59,63,73	1.23	7 (11%)	70,101,113	0.96	3 (4%)
29	CHL	2b	305	-	37,51,74	1.16	3 (8%)	30,86,114	2.93	10 (33%)
18	CLA	A	837	12	59,63,73	1.26	7 (11%)	70,101,113	1.04	5 (7%)
18	CLA	a	825	-	59,63,73	1.24	7 (11%)	70,101,113	0.97	4 (5%)
29	CHL	2a	313	13	40,54,74	1.16	2 (5%)	34,90,114	2.91	11 (32%)
18	CLA	3a	314	-	49,53,73	1.36	7 (14%)	58,89,113	1.08	4 (6%)
18	CLA	b	827	1	64,68,73	1.24	7 (10%)	75,106,113	0.90	4 (5%)
24	SF4	c	101	2	0,12,12	-	-	-	-	-
18	CLA	6a	307	-	53,57,73	1.33	7 (13%)	61,93,113	1.07	5 (8%)
18	CLA	B	806	1	64,68,73	1.22	7 (10%)	76,107,113	1.03	4 (5%)
20	BCR	M	101	-	41,41,41	1.45	8 (19%)	56,56,56	1.69	14 (25%)
23	LMG	B	850	-	42,42,55	0.54	0	50,50,63	0.67	0
18	CLA	3b	308	14	49,53,73	1.38	7 (14%)	58,89,113	1.01	3 (5%)
18	CLA	B	816	1	66,70,73	1.25	7 (10%)	78,109,113	1.06	5 (6%)
18	CLA	b	830	1	64,68,73	1.22	6 (9%)	76,107,113	1.07	5 (6%)
18	CLA	f	302	-	49,53,73	1.39	6 (12%)	58,89,113	1.09	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	b	838	-	69,73,73	1.14	6 (8%)	82,113,113	1.01	7 (8%)
18	CLA	2b	302	13	49,53,73	1.42	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	5a	304	-	49,53,73	1.43	7 (14%)	58,89,113	1.11	5 (8%)
20	BCR	F	301	-	41,41,41	1.45	5 (12%)	56,56,56	1.79	16 (28%)
27	LHG	a	846	-	33,33,48	0.34	0	36,39,54	0.46	0
29	CHL	5a	301	15	40,54,74	1.13	2 (5%)	34,90,114	2.82	10 (29%)
18	CLA	b	805	1	69,73,73	1.20	7 (10%)	82,113,113	0.95	4 (4%)
27	LHG	2b	316	18	31,31,48	0.33	0	34,37,54	0.46	0
25	LUT	6b	319	-	42,43,43	1.34	8 (19%)	51,60,60	2.66	20 (39%)
20	BCR	a	849	-	41,41,41	1.45	7 (17%)	56,56,56	1.71	17 (30%)
18	CLA	2b	312	13	49,53,73	1.40	7 (14%)	58,89,113	1.12	5 (8%)
18	CLA	B	821	1	59,63,73	1.25	7 (11%)	70,101,113	0.93	5 (7%)
25	LUT	6a	319	-	42,43,43	1.34	8 (19%)	51,60,60	2.66	20 (39%)
18	CLA	A	835	12	49,53,73	1.35	6 (12%)	58,89,113	1.13	4 (6%)
18	CLA	3b	302	14	59,63,73	1.23	7 (11%)	70,101,113	0.96	3 (4%)
18	CLA	b	804	1	69,73,73	1.17	6 (8%)	82,113,113	0.96	4 (4%)
18	CLA	B	833	1	69,73,73	1.13	6 (8%)	82,113,113	0.95	4 (4%)
18	CLA	3a	303	14	54,58,73	1.40	7 (12%)	64,95,113	1.10	5 (7%)
18	CLA	a	811	12	49,53,73	1.36	5 (10%)	58,89,113	1.03	4 (6%)
18	CLA	g	202	6	54,58,73	1.34	8 (14%)	64,95,113	1.04	3 (4%)
18	CLA	5b	308	15	49,53,73	1.34	6 (12%)	58,89,113	1.14	4 (6%)
18	CLA	a	814	12	46,50,73	1.40	7 (15%)	53,85,113	1.08	4 (7%)
18	CLA	6a	308	16	49,53,73	1.47	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	B	853	-	69,73,73	1.17	7 (10%)	82,113,113	0.93	4 (4%)
18	CLA	a	809	12	59,63,73	1.29	6 (10%)	70,101,113	1.09	5 (7%)
18	CLA	a	853	-	55,59,73	1.29	6 (10%)	64,96,113	1.06	5 (7%)
29	CHL	2a	306	-	40,54,74	1.13	4 (10%)	34,90,114	2.40	8 (23%)
18	CLA	a	831	12	54,58,73	1.33	6 (11%)	64,95,113	0.96	4 (6%)
18	CLA	b	811	1	49,53,73	1.39	6 (12%)	58,89,113	1.10	4 (6%)
18	CLA	5a	308	15	49,53,73	1.34	6 (12%)	58,89,113	1.14	4 (6%)
18	CLA	B	811	1	49,53,73	1.39	6 (12%)	58,89,113	1.10	4 (6%)
20	BCR	A	851	-	41,41,41	1.49	7 (17%)	56,56,56	1.78	13 (23%)
18	CLA	L	302	10	64,68,73	1.22	7 (10%)	76,107,113	0.86	3 (3%)
29	CHL	5a	307	-	40,54,74	1.16	3 (7%)	34,90,114	1.99	9 (26%)
18	CLA	j	101	-	49,53,73	1.39	7 (14%)	58,89,113	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	A	827	12	69,73,73	1.21	7 (10%)	82,113,113	0.94	4 (4%)
18	CLA	J	101	-	49,53,73	1.39	7 (14%)	58,89,113	1.11	4 (6%)
18	CLA	B	839	1	69,73,73	1.24	8 (11%)	82,113,113	0.97	5 (6%)
27	LHG	2a	316	18	31,31,48	0.33	0	34,37,54	0.46	0
27	LHG	5a	320	-	36,36,48	0.31	0	39,42,54	0.47	0
18	CLA	a	821	12	49,53,73	1.39	7 (14%)	58,89,113	1.08	5 (8%)
18	CLA	A	838	12	54,58,73	1.37	7 (12%)	64,95,113	1.03	4 (6%)
20	BCR	a	850	-	41,41,41	1.47	5 (12%)	56,56,56	1.67	15 (26%)
18	CLA	B	820	1	49,53,73	1.41	7 (14%)	58,89,113	1.09	4 (6%)
20	BCR	l	304	-	41,41,41	1.48	9 (21%)	56,56,56	1.93	16 (28%)
18	CLA	6a	314	16	49,53,73	1.42	7 (14%)	58,89,113	1.10	3 (5%)
18	CLA	b	803	1	49,53,73	1.41	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	3a	313	14	46,50,73	1.45	7 (15%)	53,85,113	1.14	4 (7%)
18	CLA	b	834	-	49,53,73	1.41	8 (16%)	58,89,113	1.09	5 (8%)
18	CLA	l	301	10	49,53,73	1.40	7 (14%)	58,89,113	1.18	5 (8%)
18	CLA	a	804	12	59,63,73	1.25	6 (10%)	70,101,113	1.05	5 (7%)
18	CLA	5a	309	15	55,59,73	1.28	6 (10%)	64,96,113	1.11	3 (4%)
18	CLA	G	203	6	49,53,73	1.38	7 (14%)	58,89,113	1.06	4 (6%)
18	CLA	5b	304	-	49,53,73	1.43	7 (14%)	58,89,113	1.12	5 (8%)
20	BCR	b	846	-	41,41,41	1.45	7 (17%)	56,56,56	1.66	13 (23%)
18	CLA	A	814	12	46,50,73	1.40	7 (15%)	53,85,113	1.08	4 (7%)
28	LMU	6b	302	-	36,36,36	0.26	0	47,47,47	0.67	0
29	CHL	3a	307	-	40,54,74	1.13	3 (7%)	34,90,114	3.08	12 (35%)
18	CLA	5a	303	15	54,58,73	1.39	7 (12%)	64,95,113	1.03	4 (6%)
18	CLA	2b	303	-	49,53,73	1.38	8 (16%)	58,89,113	1.14	5 (8%)
18	CLA	3a	309	14	54,58,73	1.26	6 (11%)	64,95,113	1.07	4 (6%)
18	CLA	a	818	12	69,73,73	1.17	5 (7%)	82,113,113	1.00	4 (4%)
18	CLA	b	823	-	69,73,73	1.17	6 (8%)	82,113,113	1.05	6 (7%)
22	LFA	m	102	-	11,11,19	0.11	0	10,10,18	0.13	0
19	PQN	B	841	-	34,34,34	0.45	0	43,45,45	0.73	0
18	CLA	2a	312	13	49,53,73	1.40	7 (14%)	58,89,113	1.12	5 (8%)
18	CLA	b	828	1	59,63,73	1.27	7 (11%)	70,101,113	1.05	4 (5%)
23	LMG	5b	319	-	35,35,55	0.58	0	43,43,63	0.72	0
29	CHL	2b	313	13	40,54,74	1.16	2 (5%)	34,90,114	2.91	11 (32%)
18	CLA	L	303	-	46,50,73	1.42	7 (15%)	53,85,113	1.12	4 (7%)
18	CLA	2a	308	13	59,63,73	1.22	6 (10%)	70,101,113	1.02	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	PQN	A	843	-	34,34,34	0.37	0	43,45,45	0.64	1 (2%)
18	CLA	b	809	1	69,73,73	1.17	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	b	806	1	64,68,73	1.22	7 (10%)	76,107,113	1.03	4 (5%)
24	SF4	A	844	12,1	0,12,12	-	-	-		
18	CLA	F	303	5	45,49,73	1.47	7 (15%)	54,84,113	1.19	5 (9%)
18	CLA	A	805	12	69,73,73	1.14	7 (10%)	82,113,113	0.92	4 (4%)
18	CLA	3b	313	14	46,50,73	1.46	7 (15%)	53,85,113	1.14	4 (7%)
18	CLA	B	810	1	64,68,73	1.25	7 (10%)	76,107,113	0.89	3 (3%)
18	CLA	a	841	-	69,73,73	1.18	7 (10%)	82,113,113	0.90	2 (2%)
22	LFA	b	849	-	11,11,19	0.10	0	10,10,18	0.08	0
27	LHG	5a	318	-	31,31,48	0.32	0	34,37,54	0.42	0
25	LUT	2b	314	-	42,43,43	1.30	7 (16%)	51,60,60	2.30	15 (29%)
18	CLA	A	816	12	64,68,73	1.26	8 (12%)	76,107,113	1.07	6 (7%)
18	CLA	a	805	12	69,73,73	1.14	7 (10%)	82,113,113	0.92	4 (4%)
18	CLA	B	832	1	64,68,73	1.22	7 (10%)	76,107,113	1.05	5 (6%)
20	BCR	G	201	-	41,41,41	1.48	4 (9%)	56,56,56	1.74	17 (30%)
18	CLA	A	841	-	69,73,73	1.18	7 (10%)	82,113,113	0.90	2 (2%)
18	CLA	A	803	12	65,69,73	1.19	6 (9%)	77,108,113	1.00	4 (5%)
20	BCR	B	845	-	41,41,41	1.49	7 (17%)	56,56,56	1.79	18 (32%)
18	CLA	K	201	17	48,52,73	1.44	8 (16%)	59,88,113	1.05	4 (6%)
18	CLA	b	819	1	47,51,73	1.39	6 (12%)	55,86,113	1.12	4 (7%)
18	CLA	A	832	12	69,73,73	1.22	6 (8%)	82,113,113	0.87	2 (2%)
18	CLA	3b	305	14	50,54,73	1.36	6 (12%)	59,90,113	1.09	5 (8%)
20	BCR	I	202	-	41,41,41	1.45	4 (9%)	56,56,56	1.62	13 (23%)
18	CLA	6b	306	16	59,63,73	1.28	7 (11%)	70,101,113	0.98	4 (5%)
28	LMU	A	852	-	36,36,36	0.29	0	47,47,47	0.72	1 (2%)
18	CLA	b	815	1	61,65,73	1.30	7 (11%)	72,103,113	0.99	5 (6%)
25	LUT	5a	316	-	42,43,43	1.32	8 (19%)	51,60,60	1.57	12 (23%)
29	CHL	5b	314	15	37,51,74	1.16	2 (5%)	30,86,114	3.17	11 (36%)
18	CLA	A	815	-	49,53,73	1.37	5 (10%)	58,89,113	1.20	5 (8%)
18	CLA	a	835	12	49,53,73	1.35	6 (12%)	58,89,113	1.13	4 (6%)
18	CLA	5b	313	15	49,53,73	1.39	7 (14%)	58,89,113	1.04	3 (5%)
18	CLA	6a	306	16	59,63,73	1.28	7 (11%)	70,101,113	0.98	4 (5%)
18	CLA	6b	312	16	59,63,73	1.25	6 (10%)	70,101,113	1.12	7 (10%)
26	CL0	a	802	12	58,73,73	0.85	4 (6%)	60,113,113	1.69	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LHG	6b	301	18	38,38,48	0.29	0	41,44,54	0.38	0
18	CLA	A	817	12	61,65,73	1.26	7 (11%)	72,103,113	0.98	4 (5%)
18	CLA	2b	307	13	49,53,73	1.37	6 (12%)	58,89,113	1.09	3 (5%)
22	LFA	B	849	-	11,11,19	0.10	0	10,10,18	0.08	0
29	CHL	3a	315	14	40,54,74	1.12	2 (5%)	34,90,114	2.63	9 (26%)
18	CLA	6a	312	16	59,63,73	1.24	6 (10%)	70,101,113	1.12	8 (11%)
18	CLA	3a	304	-	49,53,73	1.36	7 (14%)	58,89,113	1.07	5 (8%)
20	BCR	m	101	-	41,41,41	1.45	8 (19%)	56,56,56	1.69	14 (25%)
18	CLA	b	836	1	69,73,73	1.14	6 (8%)	82,113,113	0.95	5 (6%)
18	CLA	a	832	12	69,73,73	1.22	6 (8%)	82,113,113	0.87	2 (2%)
18	CLA	a	807	12	52,56,73	1.37	7 (13%)	61,92,113	1.05	3 (4%)
21	DGD	b	847	-	60,60,67	0.56	0	74,74,81	0.74	1 (1%)
18	CLA	B	826	1	62,66,73	1.24	7 (11%)	73,104,113	0.93	3 (4%)
18	CLA	B	824	-	54,58,73	1.28	6 (11%)	64,95,113	1.07	5 (7%)
18	CLA	B	827	1	64,68,73	1.24	7 (10%)	75,106,113	0.90	4 (5%)
18	CLA	a	827	12	69,73,73	1.21	7 (10%)	82,113,113	0.94	4 (4%)
23	LMG	I	201	-	31,31,55	0.59	0	39,39,63	0.82	1 (2%)
18	CLA	A	834	12	64,68,73	1.20	6 (9%)	76,107,113	0.95	3 (3%)
18	CLA	a	830	12	54,58,73	1.33	7 (12%)	64,95,113	1.17	6 (9%)
18	CLA	b	810	1	64,68,73	1.25	7 (10%)	76,107,113	0.89	3 (3%)
25	LUT	6b	320	-	42,43,43	1.31	8 (19%)	51,60,60	1.69	14 (27%)
18	CLA	b	852	-	69,73,73	1.18	8 (11%)	82,113,113	0.85	4 (4%)
18	CLA	a	815	-	49,53,73	1.37	5 (10%)	58,89,113	1.20	5 (8%)
23	LMG	j	103	-	30,30,55	0.64	0	38,38,63	0.74	0
18	CLA	A	801	12	56,60,73	1.28	6 (10%)	65,97,113	1.05	5 (7%)
18	CLA	A	819	12	49,53,73	1.39	7 (14%)	58,89,113	1.06	4 (6%)
29	CHL	2b	304	-	40,54,74	1.13	2 (5%)	34,90,114	2.88	11 (32%)
20	BCR	b	845	-	41,41,41	1.49	7 (17%)	56,56,56	1.79	18 (32%)
29	CHL	5a	306	-	37,51,74	1.19	3 (8%)	30,86,114	3.07	12 (40%)
19	PQN	b	841	-	34,34,34	0.45	0	43,45,45	0.73	0
18	CLA	l	303	-	46,50,73	1.42	7 (15%)	53,85,113	1.12	4 (7%)
18	CLA	B	804	1	69,73,73	1.17	6 (8%)	82,113,113	0.96	4 (4%)
25	LUT	3a	316	-	42,43,43	1.31	6 (14%)	51,60,60	1.81	15 (29%)
29	CHL	3b	315	14	40,54,74	1.12	2 (5%)	34,90,114	2.63	9 (26%)
18	CLA	A	836	12	55,59,73	1.41	7 (12%)	64,96,113	1.12	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	LUT	6a	318	-	42,43,43	1.29	8 (19%)	51,60,60	1.76	12 (23%)
18	CLA	5b	303	15	54,58,73	1.39	7 (12%)	64,95,113	1.04	4 (6%)
18	CLA	6b	311	16	49,53,73	1.36	6 (12%)	58,89,113	1.11	3 (5%)
18	CLA	3b	303	14	54,58,73	1.40	7 (12%)	64,95,113	1.10	5 (7%)
18	CLA	6b	313	-	49,53,73	1.36	6 (12%)	58,89,113	1.11	4 (6%)
18	CLA	b	826	1	62,66,73	1.24	7 (11%)	73,104,113	0.93	3 (4%)
29	CHL	2a	304	-	40,54,74	1.14	2 (5%)	34,90,114	2.88	11 (32%)
24	SF4	C	102	2	0,12,12	-	-	-	-	-
18	CLA	B	805	1	69,73,73	1.20	7 (10%)	82,113,113	0.95	4 (4%)
18	CLA	3a	311	14	47,51,73	1.44	7 (14%)	55,86,113	1.14	4 (7%)
26	CL0	A	802	12	58,73,73	0.85	4 (6%)	60,113,113	1.69	8 (13%)
18	CLA	5b	311	15	48,52,73	1.39	7 (14%)	57,88,113	1.13	4 (7%)
18	CLA	A	809	12	59,63,73	1.30	6 (10%)	70,101,113	1.09	5 (7%)
18	CLA	a	816	12	64,68,73	1.26	8 (12%)	76,107,113	1.07	6 (7%)
20	BCR	b	842	-	41,41,41	1.45	8 (19%)	56,56,56	1.83	18 (32%)
18	CLA	3b	314	-	49,53,73	1.36	7 (14%)	58,89,113	1.08	4 (6%)
18	CLA	B	834	-	49,53,73	1.41	8 (16%)	58,89,113	1.09	5 (8%)
29	CHL	5b	307	-	40,54,74	1.16	3 (7%)	34,90,114	2.00	9 (26%)
19	PQN	a	843	-	34,34,34	0.37	0	43,45,45	0.63	1 (2%)
29	CHL	5b	301	15	40,54,74	1.13	2 (5%)	34,90,114	2.82	10 (29%)
18	CLA	l	302	10	64,68,73	1.22	7 (10%)	76,107,113	0.86	3 (3%)
20	BCR	a	851	-	41,41,41	1.49	7 (17%)	56,56,56	1.78	13 (23%)
29	CHL	5b	305	-	40,54,74	1.15	3 (7%)	34,90,114	2.77	10 (29%)
18	CLA	B	802	-	69,73,73	1.13	6 (8%)	82,113,113	0.98	6 (7%)
25	LUT	5b	317	-	42,43,43	1.31	8 (19%)	51,60,60	1.78	14 (27%)
18	CLA	A	808	12	69,73,73	1.11	7 (10%)	82,113,113	0.90	4 (4%)
20	BCR	b	851	-	41,41,41	1.43	8 (19%)	56,56,56	1.78	16 (28%)
18	CLA	a	817	12	61,65,73	1.26	7 (11%)	72,103,113	0.98	4 (5%)
29	CHL	6b	309	16	35,49,74	1.41	2 (5%)	28,84,114	3.04	10 (35%)
18	CLA	A	826	12	69,73,73	1.21	7 (10%)	82,113,113	0.87	3 (3%)
18	CLA	5b	309	15	55,59,73	1.28	6 (10%)	64,96,113	1.11	3 (4%)
18	CLA	a	838	12	54,58,73	1.36	7 (12%)	64,95,113	1.03	3 (4%)
18	CLA	B	815	1	61,65,73	1.30	7 (11%)	72,103,113	0.99	5 (6%)
18	CLA	6a	313	-	49,53,73	1.36	6 (12%)	58,89,113	1.11	4 (6%)
18	CLA	b	839	1	69,73,73	1.25	8 (11%)	82,113,113	0.97	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	A	812	12	69,73,73	1.18	7 (10%)	82,113,113	0.91	3 (3%)
29	CHL	5a	314	15	37,51,74	1.16	2 (5%)	30,86,114	3.17	11 (36%)
29	CHL	6a	309	16	35,49,74	1.40	2 (5%)	28,84,114	3.05	10 (35%)
18	CLA	A	818	12	69,73,73	1.17	5 (7%)	82,113,113	1.00	4 (4%)
29	CHL	2b	306	-	40,54,74	1.13	4 (10%)	34,90,114	2.40	8 (23%)
24	SF4	c	102	2	0,12,12	-	-	-		
18	CLA	6b	307	-	53,57,73	1.33	7 (13%)	61,93,113	1.07	5 (8%)
18	CLA	F	302	-	49,53,73	1.39	6 (12%)	58,89,113	1.09	3 (5%)
18	CLA	a	834	12	64,68,73	1.20	6 (9%)	76,107,113	0.95	3 (3%)
23	LMG	J	103	-	30,30,55	0.64	0	38,38,63	0.74	0
18	CLA	2a	302	13	49,53,73	1.43	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	b	821	1	59,63,73	1.25	7 (11%)	70,101,113	0.93	5 (7%)
27	LHG	6a	301	18	38,38,48	0.29	0	41,44,54	0.38	0
18	CLA	6b	316	16	49,53,73	1.37	6 (12%)	58,89,113	1.09	4 (6%)
28	LMU	a	852	-	36,36,36	0.29	0	47,47,47	0.72	1 (2%)
18	CLA	b	854	-	69,73,73	1.20	7 (10%)	82,113,113	1.00	6 (7%)
18	CLA	a	819	12	49,53,73	1.40	7 (14%)	58,89,113	1.06	4 (6%)
18	CLA	b	833	1	69,73,73	1.13	6 (8%)	82,113,113	0.95	4 (4%)
18	CLA	a	826	12	69,73,73	1.21	7 (10%)	82,113,113	0.87	3 (3%)
20	BCR	B	851	-	41,41,41	1.43	8 (19%)	56,56,56	1.78	16 (28%)
18	CLA	a	837	12	59,63,73	1.26	7 (11%)	70,101,113	1.04	5 (7%)
18	CLA	2b	311	13	49,53,73	1.39	8 (16%)	58,89,113	1.12	5 (8%)
18	CLA	b	853	-	69,73,73	1.18	7 (10%)	82,113,113	0.94	4 (4%)
29	CHL	3a	301	13	40,54,74	1.11	2 (5%)	34,90,114	2.98	10 (29%)
24	SF4	C	101	2	0,12,12	-	-	-		
18	CLA	b	831	1	69,73,73	1.18	7 (10%)	82,113,113	1.01	4 (4%)
18	CLA	B	817	1	69,73,73	1.15	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	A	810	12	69,73,73	1.19	6 (8%)	82,113,113	0.89	3 (3%)
18	CLA	B	838	-	69,73,73	1.14	6 (8%)	82,113,113	1.02	7 (8%)
18	CLA	A	823	12	69,73,73	1.20	8 (11%)	82,113,113	1.00	5 (6%)
18	CLA	A	807	12	52,56,73	1.37	7 (13%)	61,92,113	1.05	3 (4%)
29	CHL	6a	304	16	40,54,74	1.19	2 (5%)	34,90,114	2.66	10 (29%)
18	CLA	b	829	1	49,53,73	1.37	6 (12%)	58,89,113	1.12	5 (8%)
18	CLA	B	836	1	69,73,73	1.14	6 (8%)	82,113,113	0.95	5 (6%)
18	CLA	a	836	12	55,59,73	1.41	7 (12%)	64,96,113	1.12	5 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	a	822	12	49,53,73	1.41	7 (14%)	58,89,113	1.14	6 (10%)
18	CLA	B	814	1	54,58,73	1.33	6 (11%)	64,95,113	1.04	3 (4%)
18	CLA	2b	301	13	59,63,73	1.24	7 (11%)	70,101,113	0.97	4 (5%)
21	DGD	B	847	-	60,60,67	0.56	0	74,74,81	0.74	1 (1%)
25	LUT	J	105	-	42,43,43	1.30	7 (16%)	51,60,60	3.07	21 (41%)
18	CLA	a	833	12	69,73,73	1.20	7 (10%)	82,113,113	0.90	3 (3%)
23	LMG	i	201	-	31,31,55	0.59	0	39,39,63	0.82	1 (2%)
18	CLA	b	820	1	49,53,73	1.41	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	2a	311	13	49,53,73	1.39	8 (16%)	58,89,113	1.12	5 (8%)
18	CLA	A	839	12	69,73,73	1.19	7 (10%)	82,113,113	0.87	3 (3%)
18	CLA	f	303	5	45,49,73	1.47	7 (15%)	54,84,113	1.19	5 (9%)
20	BCR	b	843	-	41,41,41	1.46	8 (19%)	56,56,56	2.16	13 (23%)
23	LMG	5a	319	-	35,35,55	0.58	0	43,43,63	0.72	0
18	CLA	a	812	12	69,73,73	1.18	7 (10%)	82,113,113	0.91	3 (3%)
18	CLA	B	819	1	47,51,73	1.39	6 (12%)	55,86,113	1.12	4 (7%)
18	CLA	A	820	-	69,73,73	1.18	6 (8%)	82,113,113	0.97	4 (4%)
18	CLA	6b	314	16	49,53,73	1.43	7 (14%)	58,89,113	1.10	3 (5%)
20	BCR	b	844	-	41,41,41	1.44	8 (19%)	56,56,56	1.81	17 (30%)
18	CLA	3a	306	14	49,53,73	1.38	7 (14%)	58,89,113	1.15	4 (6%)
18	CLA	2a	307	13	49,53,73	1.37	6 (12%)	58,89,113	1.09	3 (5%)
18	CLA	B	852	-	69,73,73	1.18	8 (11%)	82,113,113	0.86	4 (4%)
18	CLA	B	837	1	51,55,73	1.35	7 (13%)	60,91,113	1.02	4 (6%)
20	BCR	f	301	-	41,41,41	1.45	5 (12%)	56,56,56	1.79	16 (28%)
18	CLA	2a	301	13	59,63,73	1.24	7 (11%)	70,101,113	0.97	4 (5%)
29	CHL	6b	304	16	40,54,74	1.19	2 (5%)	34,90,114	2.66	10 (29%)
20	BCR	L	304	-	41,41,41	1.48	9 (21%)	56,56,56	1.93	16 (28%)
18	CLA	3a	310	-	49,53,73	1.36	6 (12%)	58,89,113	1.09	4 (6%)
24	SF4	a	844	12,1	0,12,12	-	-	-	-	-
18	CLA	2a	309	27	49,53,73	1.39	7 (14%)	58,89,113	1.03	3 (5%)
18	CLA	B	813	1	59,63,73	1.26	6 (10%)	70,101,113	0.93	3 (4%)
29	CHL	3b	307	-	40,54,74	1.14	3 (7%)	34,90,114	3.07	12 (35%)
18	CLA	L	301	10	49,53,73	1.40	7 (14%)	58,89,113	1.18	5 (8%)
20	BCR	A	848	-	41,41,41	1.46	7 (17%)	56,56,56	1.72	16 (28%)
25	LUT	5b	316	-	42,43,43	1.32	8 (19%)	51,60,60	1.57	12 (23%)
23	LMG	j	104	-	41,41,55	0.54	0	49,49,63	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	A	833	12	69,73,73	1.20	7 (10%)	82,113,113	0.90	3 (3%)
18	CLA	A	828	12	69,73,73	1.31	8 (11%)	82,113,113	0.92	3 (3%)
23	LMG	J	104	-	41,41,55	0.54	0	49,49,63	0.63	0
18	CLA	F	305	-	64,68,73	1.22	7 (10%)	76,107,113	1.02	7 (9%)
18	CLA	G	202	6	54,58,73	1.34	8 (14%)	64,95,113	1.03	3 (4%)
18	CLA	A	842	-	49,53,73	1.38	7 (14%)	58,89,113	1.10	5 (8%)
27	LHG	a	845	-	48,48,48	0.28	0	51,54,54	0.35	0
18	CLA	A	806	12	69,73,73	1.19	8 (11%)	82,113,113	0.87	3 (3%)
20	BCR	K	202	-	41,41,41	1.46	7 (17%)	56,56,56	1.78	16 (28%)
18	CLA	6a	317	16	49,53,73	1.39	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	B	812	1	69,73,73	1.18	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	a	829	12	69,73,73	1.20	7 (10%)	82,113,113	0.96	3 (3%)
25	LUT	5a	317	-	42,43,43	1.31	8 (19%)	51,60,60	1.78	14 (27%)
18	CLA	B	801	1	69,73,73	1.20	8 (11%)	82,113,113	0.88	3 (3%)
18	CLA	6b	310	-	49,53,73	1.40	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	6a	316	16	49,53,73	1.37	6 (12%)	58,89,113	1.08	4 (6%)
25	LUT	3b	317	-	42,43,43	1.36	8 (19%)	51,60,60	2.02	11 (21%)
18	CLA	B	818	-	57,61,73	1.30	6 (10%)	67,98,113	1.05	4 (5%)
18	CLA	3a	308	14	49,53,73	1.37	7 (14%)	58,89,113	1.01	3 (5%)
18	CLA	b	840	27	69,73,73	1.14	6 (8%)	82,113,113	1.03	6 (7%)
18	CLA	a	824	-	69,73,73	1.24	8 (11%)	82,113,113	0.94	5 (6%)
20	BCR	g	204	-	41,41,41	1.45	7 (17%)	56,56,56	1.68	15 (26%)
18	CLA	3b	310	-	49,53,73	1.36	6 (12%)	58,89,113	1.09	4 (6%)
27	LHG	A	845	-	48,48,48	0.28	0	51,54,54	0.35	0
18	CLA	B	825	1	69,73,73	1.23	7 (10%)	82,113,113	0.94	3 (3%)
18	CLA	3b	304	-	49,53,73	1.36	7 (14%)	58,89,113	1.07	5 (8%)

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
18	CLA	B	822	1	-	2/15/91/115	-
20	BCR	k	202	-	-	3/29/63/63	0/2/2/2
20	BCR	f	304	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	808	1	1/1/11/20	2/18/94/115	-
18	CLA	b	813	1	-	2/27/103/115	-
18	CLA	3b	312	14	-	5/27/103/115	-
29	CHL	5a	305	-	3/3/16/26	2/15/113/137	-
18	CLA	a	840	12	1/1/15/20	0/39/115/115	-
18	CLA	B	823	-	1/1/15/20	8/39/115/115	-
18	CLA	a	823	12	-	1/39/115/115	-
18	CLA	3b	306	14	1/1/11/20	0/15/91/115	-
20	BCR	A	847	-	-	3/29/63/63	0/2/2/2
20	BCR	i	202	-	-	2/29/63/63	0/2/2/2
18	CLA	5a	311	15	1/1/11/20	3/13/89/115	-
29	CHL	2a	305	-	3/3/15/26	2/12/110/137	-
18	CLA	b	812	1	1/1/15/20	5/39/115/115	-
18	CLA	a	806	12	1/1/15/20	8/39/115/115	-
18	CLA	5a	310	-	1/1/11/20	2/15/91/115	-
18	CLA	5a	312	15	-	5/24/100/115	-
23	LMG	b	850	-	-	18/37/57/70	0/1/1/1
25	LUT	3a	317	-	-	4/29/67/67	0/2/2/2
18	CLA	2b	310	-	1/1/11/20	2/15/91/115	-
18	CLA	5b	302	15	-	8/29/105/115	-
18	CLA	6b	315	16	1/1/13/20	2/27/103/115	-
18	CLA	B	803	1	1/1/11/20	2/15/91/115	-
18	CLA	a	803	12	1/1/14/20	3/35/111/115	-
18	CLA	a	839	12	-	3/39/115/115	-
18	CLA	b	825	1	1/1/15/20	0/39/115/115	-
18	CLA	B	854	-	1/1/15/20	6/39/115/115	-
25	LUT	3b	316	-	-	0/29/67/67	0/2/2/2
18	CLA	A	840	12	1/1/15/20	0/39/115/115	-
18	CLA	5b	312	15	-	5/24/100/115	-
18	CLA	6b	308	16	1/1/11/20	2/15/91/115	-
20	BCR	A	849	-	-	3/29/63/63	0/2/2/2
18	CLA	5a	315	15	-	2/17/93/115	-
20	BCR	g	201	-	-	4/29/63/63	0/2/2/2
18	CLA	B	831	1	1/1/15/20	2/39/115/115	-
18	CLA	b	822	1	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	802	-	1/1/15/20	1/39/115/115	-
20	BCR	G	204	-	-	2/29/63/63	0/2/2/2
20	BCR	B	848	-	-	6/29/63/63	0/2/2/2
20	BCR	a	848	-	-	3/29/63/63	0/2/2/2
18	CLA	B	807	1	1/1/14/20	0/35/111/115	-
18	CLA	A	804	12	1/1/13/20	3/27/103/115	-
18	CLA	a	828	12	-	3/39/115/115	-
18	CLA	B	828	1	-	5/27/103/115	-
18	CLA	B	829	1	-	2/15/91/115	-
18	CLA	5a	302	15	-	8/29/105/115	-
18	CLA	B	809	1	1/1/15/20	8/39/115/115	-
18	CLA	a	820	-	-	3/39/115/115	-
18	CLA	b	816	1	1/1/14/20	6/36/112/115	-
20	BCR	B	846	-	-	1/29/63/63	0/2/2/2
20	BCR	B	843	-	-	11/29/63/63	0/2/2/2
27	LHG	5b	318	-	-	6/36/36/53	-
25	LUT	6b	318	-	-	3/29/67/67	0/2/2/2
18	CLA	A	813	12	1/1/12/20	1/21/97/115	-
18	CLA	b	801	1	1/1/15/20	7/39/115/115	-
18	CLA	6a	305	16	-	4/35/111/115	-
18	CLA	A	825	-	1/1/13/20	0/27/103/115	-
28	LMU	6a	302	-	-	8/21/61/61	0/2/2/2
18	CLA	A	822	12	1/1/11/20	2/15/91/115	-
22	LFA	M	102	-	-	0/9/9/17	-
18	CLA	k	201	17	1/1/11/20	2/13/89/115	-
18	CLA	b	817	1	1/1/15/20	5/39/115/115	-
18	CLA	3a	305	14	-	3/17/93/115	-
25	LUT	2a	314	-	-	8/29/67/67	0/2/2/2
18	CLA	5b	310	-	1/1/11/20	2/15/91/115	-
18	CLA	6b	317	16	1/1/11/20	3/15/91/115	-
25	LUT	j	105	-	-	10/29/67/67	0/2/2/2
18	CLA	B	835	1	1/1/12/20	0/21/97/115	-
18	CLA	b	807	1	1/1/14/20	0/35/111/115	-
18	CLA	6a	310	-	1/1/11/20	2/15/91/115	-
18	CLA	A	811	12	1/1/11/20	4/15/91/115	-
18	CLA	b	814	1	-	1/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2b	309	27	1/1/11/20	2/15/91/115	-
20	BCR	b	848	-	-	6/29/63/63	0/2/2/2
20	BCR	a	847	-	-	3/29/63/63	0/2/2/2
28	LMU	6a	303	-	-	4/19/59/61	0/2/2/2
29	CHL	5b	306	-	3/3/15/26	4/12/110/137	-
18	CLA	5b	315	15	-	2/17/93/115	-
20	BCR	B	844	-	-	3/29/63/63	0/2/2/2
18	CLA	b	824	-	1/1/12/20	2/21/97/115	-
18	CLA	6a	315	16	1/1/13/20	2/27/103/115	-
27	LHG	A	846	-	-	13/38/38/53	-
18	CLA	3b	309	14	-	1/21/97/115	-
18	CLA	2b	308	13	1/1/13/20	6/27/103/115	-
18	CLA	a	810	12	-	4/39/115/115	-
20	BCR	A	850	-	-	0/29/63/63	0/2/2/2
18	CLA	5a	313	15	1/1/11/20	1/15/91/115	-
18	CLA	a	842	-	-	3/15/91/115	-
18	CLA	b	837	1	1/1/11/20	0/18/94/115	-
18	CLA	B	840	27	1/1/15/20	10/39/115/115	-
20	BCR	j	102	-	-	6/29/63/63	0/2/2/2
20	BCR	F	304	-	-	5/29/63/63	0/2/2/2
20	BCR	J	102	-	-	6/29/63/63	0/2/2/2
27	LHG	5b	320	-	-	5/41/41/53	-
18	CLA	A	853	-	-	1/23/99/115	-
18	CLA	6a	311	16	1/1/11/20	0/15/91/115	-
18	CLA	A	831	12	1/1/12/20	0/21/97/115	-
18	CLA	B	808	1	1/1/11/20	2/18/94/115	-
18	CLA	a	808	12	1/1/15/20	3/39/115/115	-
28	LMU	6b	303	-	-	4/19/59/61	0/2/2/2
18	CLA	b	835	1	1/1/12/20	0/21/97/115	-
25	LUT	6a	320	-	-	3/29/67/67	0/2/2/2
18	CLA	a	801	12	-	2/24/100/115	-
18	CLA	6b	305	16	-	4/35/111/115	-
29	CHL	3b	301	13	3/3/16/26	0/15/113/137	-
18	CLA	A	821	12	-	2/15/91/115	-
25	LUT	2b	315	-	-	4/29/67/67	0/2/2/2
18	CLA	f	305	-	1/1/14/20	3/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3a	312	14	-	5/27/103/115	-
18	CLA	B	830	1	1/1/14/20	11/33/109/115	-
18	CLA	A	824	-	1/1/15/20	2/39/115/115	-
18	CLA	b	832	1	-	7/33/109/115	-
18	CLA	A	830	12	-	5/21/97/115	-
18	CLA	g	203	6	1/1/11/20	4/15/91/115	-
18	CLA	b	818	-	-	0/25/101/115	-
18	CLA	2a	303	-	1/1/11/20	2/15/91/115	-
18	CLA	a	813	12	1/1/12/20	1/21/97/115	-
20	BCR	B	842	-	-	2/29/63/63	0/2/2/2
18	CLA	3b	311	14	1/1/10/20	0/13/89/115	-
18	CLA	A	829	12	-	6/39/115/115	-
25	LUT	2a	315	-	-	4/29/67/67	0/2/2/2
18	CLA	2a	310	-	1/1/11/20	2/15/91/115	-
29	CHL	2b	305	-	3/3/15/26	2/12/110/137	-
18	CLA	3a	302	14	-	4/27/103/115	-
18	CLA	A	837	12	1/1/13/20	3/27/103/115	-
18	CLA	a	825	-	1/1/13/20	0/27/103/115	-
29	CHL	2a	313	13	3/3/16/26	6/15/113/137	-
18	CLA	3a	314	-	1/1/11/20	2/15/91/115	-
18	CLA	b	827	1	-	1/33/109/115	-
24	SF4	c	101	2	-	-	0/6/5/5
18	CLA	6a	307	-	-	2/20/96/115	-
18	CLA	B	806	1	-	2/33/109/115	-
20	BCR	M	101	-	-	4/29/63/63	0/2/2/2
23	LMG	B	850	-	-	18/37/57/70	0/1/1/1
18	CLA	3b	308	14	1/1/11/20	0/15/91/115	-
18	CLA	B	816	1	1/1/14/20	6/36/112/115	-
18	CLA	b	830	1	1/1/14/20	11/33/109/115	-
18	CLA	f	302	-	1/1/11/20	2/15/91/115	-
18	CLA	b	838	-	-	6/39/115/115	-
18	CLA	2b	302	13	1/1/11/20	2/15/91/115	-
29	CHL	5a	301	15	3/3/16/26	2/15/113/137	-
18	CLA	5a	304	-	-	2/15/91/115	-
20	BCR	F	301	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	a	846	-	-	13/38/38/53	-
18	CLA	b	805	1	1/1/15/20	10/39/115/115	-
27	LHG	2b	316	18	-	5/36/36/53	-
25	LUT	6b	319	-	-	16/29/67/67	0/2/2/2
20	BCR	a	849	-	-	3/29/63/63	0/2/2/2
18	CLA	2b	312	13	1/1/11/20	2/15/91/115	-
18	CLA	B	821	1	1/1/13/20	4/27/103/115	-
25	LUT	6a	319	-	-	16/29/67/67	0/2/2/2
18	CLA	A	835	12	1/1/11/20	3/15/91/115	-
18	CLA	3b	302	14	-	4/27/103/115	-
18	CLA	b	804	1	1/1/15/20	4/39/115/115	-
18	CLA	B	833	1	1/1/15/20	5/39/115/115	-
18	CLA	3a	303	14	1/1/12/20	4/21/97/115	-
18	CLA	a	811	12	1/1/11/20	4/15/91/115	-
18	CLA	g	202	6	1/1/12/20	1/21/97/115	-
18	CLA	5b	308	15	1/1/11/20	2/15/91/115	-
18	CLA	a	814	12	1/1/10/20	0/12/88/115	-
18	CLA	6a	308	16	1/1/11/20	2/15/91/115	-
18	CLA	a	853	-	-	1/23/99/115	-
18	CLA	B	853	-	1/1/15/20	3/39/115/115	-
18	CLA	a	809	12	1/1/13/20	3/27/103/115	-
29	CHL	2a	306	-	2/2/16/26	10/15/113/137	-
18	CLA	a	831	12	1/1/12/20	0/21/97/115	-
18	CLA	b	811	1	-	3/15/91/115	-
18	CLA	5a	308	15	1/1/11/20	2/15/91/115	-
18	CLA	B	811	1	-	3/15/91/115	-
20	BCR	A	851	-	-	8/29/63/63	0/2/2/2
18	CLA	L	302	10	-	0/33/109/115	-
29	CHL	5a	307	-	2/2/16/26	7/15/113/137	-
18	CLA	j	101	-	1/1/11/20	2/15/91/115	-
18	CLA	A	827	12	1/1/15/20	5/39/115/115	-
18	CLA	J	101	-	1/1/11/20	2/15/91/115	-
18	CLA	B	839	1	-	2/39/115/115	-
27	LHG	2a	316	18	-	5/36/36/53	-
27	LHG	5a	320	-	-	5/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	821	12	-	2/15/91/115	-
18	CLA	A	838	12	1/1/12/20	0/21/97/115	-
20	BCR	a	850	-	-	0/29/63/63	0/2/2/2
18	CLA	B	820	1	-	2/15/91/115	-
20	BCR	l	304	-	-	2/29/63/63	0/2/2/2
18	CLA	6a	314	16	1/1/11/20	2/15/91/115	-
18	CLA	b	803	1	1/1/11/20	2/15/91/115	-
18	CLA	3a	313	14	1/1/10/20	0/12/88/115	-
18	CLA	b	834	-	1/1/11/20	0/15/91/115	-
18	CLA	l	301	10	1/1/11/20	4/15/91/115	-
18	CLA	a	804	12	1/1/13/20	3/27/103/115	-
18	CLA	5a	309	15	-	2/23/99/115	-
18	CLA	G	203	6	1/1/11/20	4/15/91/115	-
18	CLA	5b	304	-	-	2/15/91/115	-
20	BCR	b	846	-	-	1/29/63/63	0/2/2/2
18	CLA	A	814	12	1/1/10/20	0/12/88/115	-
28	LMU	6b	302	-	-	8/21/61/61	0/2/2/2
29	CHL	3a	307	-	3/3/16/26	3/15/113/137	-
18	CLA	5a	303	15	1/1/12/20	6/21/97/115	-
18	CLA	2b	303	-	1/1/11/20	2/15/91/115	-
18	CLA	3a	309	14	-	1/21/97/115	-
18	CLA	a	818	12	1/1/15/20	4/39/115/115	-
18	CLA	b	823	-	1/1/15/20	8/39/115/115	-
22	LFA	m	102	-	-	0/9/9/17	-
19	PQN	B	841	-	-	0/23/43/43	0/2/2/2
18	CLA	2a	312	13	1/1/11/20	2/15/91/115	-
18	CLA	b	828	1	-	4/27/103/115	-
23	LMG	5b	319	-	-	5/30/50/70	0/1/1/1
29	CHL	2b	313	13	3/3/16/26	6/15/113/137	-
18	CLA	L	303	-	1/1/10/20	1/12/88/115	-
18	CLA	2a	308	13	1/1/13/20	6/27/103/115	-
19	PQN	A	843	-	-	4/23/43/43	0/2/2/2
18	CLA	b	809	1	1/1/15/20	8/39/115/115	-
18	CLA	b	806	1	-	2/33/109/115	-
24	SF4	A	844	12,1	-	-	0/6/5/5
18	CLA	F	303	5	1/1/10/20	0/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	805	12	1/1/15/20	5/39/115/115	-
18	CLA	3b	313	14	1/1/10/20	0/12/88/115	-
18	CLA	B	810	1	-	5/33/109/115	-
18	CLA	a	841	-	1/1/15/20	6/39/115/115	-
22	LFA	b	849	-	-	1/9/9/17	-
27	LHG	5a	318	-	-	6/36/36/53	-
25	LUT	2b	314	-	-	8/29/67/67	0/2/2/2
18	CLA	A	816	12	-	6/33/109/115	-
18	CLA	a	805	12	1/1/15/20	5/39/115/115	-
18	CLA	B	832	1	-	7/33/109/115	-
20	BCR	G	201	-	-	4/29/63/63	0/2/2/2
18	CLA	A	841	-	1/1/15/20	6/39/115/115	-
18	CLA	A	803	12	1/1/14/20	3/35/111/115	-
20	BCR	B	845	-	-	4/29/63/63	0/2/2/2
18	CLA	K	201	17	1/1/11/20	2/13/89/115	-
18	CLA	b	819	1	1/1/10/20	1/13/89/115	-
18	CLA	A	832	12	1/1/15/20	2/39/115/115	-
18	CLA	3b	305	14	-	3/17/93/115	-
20	BCR	I	202	-	-	2/29/63/63	0/2/2/2
18	CLA	6b	306	16	1/1/13/20	4/27/103/115	-
28	LMU	A	852	-	-	4/21/61/61	0/2/2/2
18	CLA	b	815	1	-	0/30/106/115	-
25	LUT	5a	316	-	-	0/29/67/67	0/2/2/2
29	CHL	5b	314	15	3/3/15/26	1/12/110/137	-
18	CLA	A	815	-	-	5/15/91/115	-
18	CLA	a	835	12	1/1/11/20	3/15/91/115	-
18	CLA	5b	313	15	1/1/11/20	1/15/91/115	-
18	CLA	6a	306	16	1/1/13/20	4/27/103/115	-
18	CLA	6b	312	16	-	3/27/103/115	-
26	CL0	a	802	12	-	7/37/135/135	-
27	LHG	6b	301	18	-	11/43/43/53	-
18	CLA	A	817	12	1/1/13/20	8/30/106/115	-
18	CLA	2b	307	13	1/1/11/20	0/15/91/115	-
29	CHL	3a	315	14	3/3/16/26	2/15/113/137	-
22	LFA	B	849	-	-	1/9/9/17	-
18	CLA	6a	312	16	-	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3a	304	-	1/1/11/20	1/15/91/115	-
20	BCR	m	101	-	-	4/29/63/63	0/2/2/2
18	CLA	b	836	1	1/1/15/20	5/39/115/115	-
18	CLA	a	832	12	1/1/15/20	2/39/115/115	-
18	CLA	a	807	12	1/1/11/20	0/19/95/115	-
21	DGD	b	847	-	-	19/48/88/95	0/2/2/2
18	CLA	B	826	1	1/1/13/20	1/31/107/115	-
18	CLA	B	824	-	1/1/12/20	2/21/97/115	-
18	CLA	a	827	12	1/1/15/20	5/39/115/115	-
18	CLA	B	827	1	-	1/33/109/115	-
23	LMG	I	201	-	-	16/26/46/70	0/1/1/1
18	CLA	A	834	12	-	4/33/109/115	-
18	CLA	a	830	12	-	5/21/97/115	-
18	CLA	b	810	1	-	5/33/109/115	-
25	LUT	6b	320	-	-	3/29/67/67	0/2/2/2
18	CLA	b	852	-	-	4/39/115/115	-
18	CLA	a	815	-	-	5/15/91/115	-
23	LMG	j	103	-	-	7/25/45/70	0/1/1/1
18	CLA	A	801	12	-	2/24/100/115	-
18	CLA	A	819	12	-	0/15/91/115	-
29	CHL	2b	304	-	3/3/16/26	4/15/113/137	-
20	BCR	b	845	-	-	4/29/63/63	0/2/2/2
29	CHL	5a	306	-	3/3/15/26	4/12/110/137	-
19	PQN	b	841	-	-	0/23/43/43	0/2/2/2
18	CLA	l	303	-	1/1/10/20	1/12/88/115	-
18	CLA	B	804	1	1/1/15/20	4/39/115/115	-
25	LUT	3a	316	-	-	0/29/67/67	0/2/2/2
29	CHL	3b	315	14	3/3/16/26	2/15/113/137	-
18	CLA	A	836	12	1/1/12/20	4/23/99/115	-
25	LUT	6a	318	-	-	3/29/67/67	0/2/2/2
18	CLA	5b	303	15	1/1/12/20	6/21/97/115	-
18	CLA	6b	311	16	1/1/11/20	0/15/91/115	-
18	CLA	3b	303	14	1/1/12/20	4/21/97/115	-
18	CLA	6b	313	-	1/1/11/20	4/15/91/115	-
18	CLA	b	826	1	1/1/13/20	1/31/107/115	-
29	CHL	2a	304	-	3/3/16/26	4/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	SF4	C	102	2	-	-	0/6/5/5
18	CLA	B	805	1	1/1/15/20	10/39/115/115	-
18	CLA	3a	311	14	1/1/10/20	0/13/89/115	-
26	CL0	A	802	12	-	7/37/135/135	-
18	CLA	5b	311	15	1/1/11/20	3/13/89/115	-
18	CLA	A	809	12	1/1/13/20	3/27/103/115	-
18	CLA	a	816	12	-	6/33/109/115	-
20	BCR	b	842	-	-	2/29/63/63	0/2/2/2
18	CLA	3b	314	-	1/1/11/20	2/15/91/115	-
18	CLA	B	834	-	1/1/11/20	0/15/91/115	-
29	CHL	5b	307	-	2/2/16/26	7/15/113/137	-
19	PQN	a	843	-	-	4/23/43/43	0/2/2/2
29	CHL	5b	301	15	3/3/16/26	2/15/113/137	-
18	CLA	l	302	10	-	0/33/109/115	-
20	BCR	a	851	-	-	8/29/63/63	0/2/2/2
29	CHL	5b	305	-	3/3/16/26	2/15/113/137	-
18	CLA	B	802	-	1/1/15/20	1/39/115/115	-
25	LUT	5b	317	-	-	2/29/67/67	0/2/2/2
18	CLA	A	808	12	1/1/15/20	3/39/115/115	-
20	BCR	b	851	-	-	8/29/63/63	0/2/2/2
18	CLA	a	817	12	1/1/13/20	8/30/106/115	-
29	CHL	6b	309	16	3/3/15/26	2/8/106/137	-
18	CLA	A	826	12	1/1/15/20	2/39/115/115	-
18	CLA	5b	309	15	-	2/23/99/115	-
18	CLA	a	838	12	1/1/12/20	0/21/97/115	-
18	CLA	B	815	1	-	0/30/106/115	-
18	CLA	6a	313	-	1/1/11/20	4/15/91/115	-
18	CLA	b	839	1	-	2/39/115/115	-
18	CLA	A	812	12	1/1/15/20	6/39/115/115	-
29	CHL	5a	314	15	3/3/15/26	1/12/110/137	-
29	CHL	6a	309	16	3/3/15/26	2/8/106/137	-
18	CLA	A	818	12	1/1/15/20	4/39/115/115	-
29	CHL	2b	306	-	2/2/16/26	10/15/113/137	-
24	SF4	c	102	2	-	-	0/6/5/5
18	CLA	6b	307	-	-	2/20/96/115	-
18	CLA	F	302	-	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	834	12	-	4/33/109/115	-
23	LMG	J	103	-	-	7/25/45/70	0/1/1/1
18	CLA	2a	302	13	1/1/11/20	2/15/91/115	-
18	CLA	b	821	1	1/1/13/20	4/27/103/115	-
27	LHG	6a	301	18	-	11/43/43/53	-
18	CLA	6b	316	16	-	2/15/91/115	-
28	LMU	a	852	-	-	4/21/61/61	0/2/2/2
18	CLA	b	854	-	1/1/15/20	6/39/115/115	-
18	CLA	a	819	12	-	0/15/91/115	-
18	CLA	b	833	1	1/1/15/20	5/39/115/115	-
18	CLA	a	826	12	1/1/15/20	2/39/115/115	-
20	BCR	B	851	-	-	8/29/63/63	0/2/2/2
18	CLA	a	837	12	1/1/13/20	3/27/103/115	-
18	CLA	2b	311	13	-	3/15/91/115	-
18	CLA	b	853	-	1/1/15/20	3/39/115/115	-
29	CHL	3a	301	13	3/3/16/26	0/15/113/137	-
24	SF4	C	101	2	-	-	0/6/5/5
18	CLA	b	831	1	1/1/15/20	2/39/115/115	-
18	CLA	B	817	1	1/1/15/20	5/39/115/115	-
18	CLA	A	810	12	-	4/39/115/115	-
18	CLA	B	838	-	-	6/39/115/115	-
18	CLA	A	823	12	-	1/39/115/115	-
18	CLA	A	807	12	1/1/11/20	0/19/95/115	-
29	CHL	6a	304	16	3/3/16/26	4/15/113/137	-
18	CLA	b	829	1	-	2/15/91/115	-
18	CLA	B	836	1	1/1/15/20	5/39/115/115	-
18	CLA	a	836	12	1/1/12/20	4/23/99/115	-
18	CLA	a	822	12	1/1/11/20	2/15/91/115	-
18	CLA	B	814	1	-	1/21/97/115	-
18	CLA	2b	301	13	1/1/13/20	6/27/103/115	-
21	DGD	B	847	-	-	19/48/88/95	0/2/2/2
25	LUT	J	105	-	-	10/29/67/67	0/2/2/2
18	CLA	a	833	12	-	6/39/115/115	-
23	LMG	i	201	-	-	16/26/46/70	0/1/1/1
18	CLA	b	820	1	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2a	311	13	-	3/15/91/115	-
18	CLA	A	839	12	-	3/39/115/115	-
18	CLA	f	303	5	1/1/10/20	0/10/86/115	-
20	BCR	b	843	-	-	11/29/63/63	0/2/2/2
23	LMG	5a	319	-	-	5/30/50/70	0/1/1/1
18	CLA	a	812	12	1/1/15/20	6/39/115/115	-
18	CLA	B	819	1	1/1/10/20	1/13/89/115	-
18	CLA	6b	314	16	1/1/11/20	2/15/91/115	-
18	CLA	A	820	-	-	3/39/115/115	-
20	BCR	b	844	-	-	3/29/63/63	0/2/2/2
18	CLA	3a	306	14	1/1/11/20	0/15/91/115	-
18	CLA	2a	307	13	1/1/11/20	0/15/91/115	-
18	CLA	B	852	-	-	4/39/115/115	-
18	CLA	B	837	1	1/1/11/20	0/18/94/115	-
20	BCR	f	301	-	-	3/29/63/63	0/2/2/2
18	CLA	2a	301	13	1/1/13/20	6/27/103/115	-
29	CHL	6b	304	16	3/3/16/26	4/15/113/137	-
20	BCR	L	304	-	-	2/29/63/63	0/2/2/2
18	CLA	3a	310	-	1/1/11/20	2/15/91/115	-
24	SF4	a	844	12,1	-	-	0/6/5/5
18	CLA	2a	309	27	1/1/11/20	2/15/91/115	-
29	CHL	3b	307	-	3/3/16/26	3/15/113/137	-
18	CLA	B	813	1	-	2/27/103/115	-
18	CLA	L	301	10	1/1/11/20	4/15/91/115	-
20	BCR	A	848	-	-	3/29/63/63	0/2/2/2
25	LUT	5b	316	-	-	0/29/67/67	0/2/2/2
23	LMG	j	104	-	-	7/36/56/70	0/1/1/1
18	CLA	A	833	12	-	6/39/115/115	-
18	CLA	A	828	12	-	3/39/115/115	-
23	LMG	J	104	-	-	7/36/56/70	0/1/1/1
18	CLA	F	305	-	1/1/14/20	3/33/109/115	-
18	CLA	G	202	6	1/1/12/20	1/21/97/115	-
18	CLA	A	842	-	-	3/15/91/115	-
27	LHG	a	845	-	-	4/53/53/53	-
18	CLA	A	806	12	1/1/15/20	8/39/115/115	-
20	BCR	K	202	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	6a	317	16	1/1/11/20	3/15/91/115	-
18	CLA	B	812	1	1/1/15/20	5/39/115/115	-
18	CLA	a	829	12	-	6/39/115/115	-
25	LUT	5a	317	-	-	2/29/67/67	0/2/2/2
18	CLA	B	801	1	1/1/15/20	7/39/115/115	-
18	CLA	6b	310	-	1/1/11/20	2/15/91/115	-
18	CLA	6a	316	16	-	2/15/91/115	-
25	LUT	3b	317	-	-	4/29/67/67	0/2/2/2
18	CLA	B	818	-	-	0/25/101/115	-
18	CLA	3a	308	14	1/1/11/20	0/15/91/115	-
18	CLA	b	840	27	1/1/15/20	10/39/115/115	-
18	CLA	a	824	-	1/1/15/20	2/39/115/115	-
20	BCR	g	204	-	-	2/29/63/63	0/2/2/2
18	CLA	3b	310	-	1/1/11/20	2/15/91/115	-
27	LHG	A	845	-	-	4/53/53/53	-
18	CLA	B	825	1	1/1/15/20	0/39/115/115	-
18	CLA	3b	304	-	1/1/11/20	1/15/91/115	-

The worst 5 of 2398 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6b	309	CHL	C2C-C3C	5.68	1.41	1.36
29	6a	309	CHL	C2C-C3C	5.65	1.41	1.36
18	A	828	CLA	MG-NA	5.28	2.18	2.06
18	a	828	CLA	MG-NA	5.28	2.18	2.06
18	B	835	CLA	MG-NA	5.26	2.18	2.06

The worst 5 of 2426 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3a	301	CHL	C1B-CHB-C4A	13.84	130.22	121.32
29	3b	301	CHL	C1B-CHB-C4A	13.84	130.22	121.32
29	5b	314	CHL	C1B-CHB-C4A	13.76	130.17	121.32
29	5a	314	CHL	C1B-CHB-C4A	13.75	130.17	121.32
29	2a	313	CHL	C1B-CHB-C4A	13.42	129.96	121.32

5 of 262 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	B	801	CLA	ND
18	B	802	CLA	ND
18	B	803	CLA	ND
18	B	804	CLA	ND
18	B	805	CLA	ND

5 of 1475 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	B	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D
18	B	808	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

360 monomers are involved in 665 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	822	CLA	1	0
20	k	202	BCR	2	0
20	f	304	BCR	1	0
18	b	808	CLA	2	0
18	b	813	CLA	1	0
18	3b	312	CLA	1	0
29	5a	305	CHL	1	0
18	a	840	CLA	2	0
18	B	823	CLA	3	0
18	a	823	CLA	5	0
18	3b	306	CLA	2	0
20	A	847	BCR	3	0
20	i	202	BCR	3	0
18	5a	311	CLA	1	0
18	b	812	CLA	2	0
18	a	806	CLA	4	0
18	5a	310	CLA	1	0
18	5a	312	CLA	2	0
23	b	850	LMG	1	0
25	3a	317	LUT	6	0
18	2b	310	CLA	2	0
18	5b	302	CLA	1	0
18	6b	315	CLA	2	0
18	B	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a	803	CLA	3	0
18	a	839	CLA	2	0
18	b	825	CLA	1	0
18	B	854	CLA	3	0
25	3b	316	LUT	3	0
18	A	840	CLA	2	0
18	5b	312	CLA	3	0
18	6b	308	CLA	3	0
20	A	849	BCR	3	0
18	5a	315	CLA	2	0
20	g	201	BCR	2	0
18	B	831	CLA	2	0
18	b	822	CLA	2	0
18	b	802	CLA	1	0
20	G	204	BCR	3	0
20	B	848	BCR	3	0
20	a	848	BCR	4	0
18	B	807	CLA	2	0
18	A	804	CLA	1	0
18	B	828	CLA	3	0
18	B	829	CLA	1	0
18	5a	302	CLA	1	0
18	a	828	CLA	1	0
18	B	809	CLA	3	0
18	a	820	CLA	3	0
18	b	816	CLA	1	0
20	B	846	BCR	1	0
20	B	843	BCR	1	0
25	6b	318	LUT	3	0
18	b	801	CLA	7	0
18	6a	305	CLA	3	0
18	A	822	CLA	1	0
18	b	817	CLA	2	0
25	2a	314	LUT	6	0
18	5b	310	CLA	1	0
18	6b	317	CLA	1	0
25	j	105	LUT	3	0
18	b	807	CLA	2	0
18	6a	310	CLA	2	0
18	A	811	CLA	1	0
18	b	814	CLA	2	0
18	2b	309	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	b	848	BCR	1	0
20	a	847	BCR	5	0
29	5b	306	CHL	1	0
18	5b	315	CLA	2	0
20	B	844	BCR	3	0
18	b	824	CLA	2	0
18	6a	315	CLA	2	0
27	A	846	LHG	4	0
18	3b	309	CLA	2	0
18	2b	308	CLA	4	0
18	a	810	CLA	3	0
20	A	850	BCR	3	0
18	5a	313	CLA	1	0
18	B	840	CLA	2	0
20	j	102	BCR	5	0
20	J	102	BCR	4	0
27	5b	320	LHG	3	0
18	A	853	CLA	1	0
18	6a	311	CLA	1	0
18	A	831	CLA	4	0
18	B	808	CLA	1	0
18	a	808	CLA	3	0
18	b	835	CLA	1	0
25	6a	320	LUT	5	0
18	a	801	CLA	2	0
18	6b	305	CLA	3	0
29	3b	301	CHL	1	0
18	A	821	CLA	2	0
25	2b	315	LUT	6	0
18	f	305	CLA	2	0
18	3a	312	CLA	2	0
18	B	830	CLA	3	0
18	b	832	CLA	4	0
18	A	824	CLA	2	0
18	g	203	CLA	3	0
18	b	818	CLA	1	0
18	2a	303	CLA	1	0
20	B	842	BCR	2	0
18	3b	311	CLA	1	0
18	A	829	CLA	2	0
25	2a	315	LUT	5	0
18	2a	310	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3a	302	CLA	1	0
18	A	837	CLA	1	0
29	2a	313	CHL	2	0
18	3a	314	CLA	1	0
18	b	827	CLA	2	0
18	6a	307	CLA	2	0
18	B	806	CLA	7	0
20	M	101	BCR	4	0
23	B	850	LMG	1	0
18	B	816	CLA	1	0
18	b	830	CLA	3	0
18	f	302	CLA	3	0
18	b	838	CLA	4	0
18	2b	302	CLA	1	0
20	F	301	BCR	3	0
27	a	846	LHG	4	0
29	5a	301	CHL	2	0
18	b	805	CLA	3	0
25	6b	319	LUT	6	0
20	a	849	BCR	1	0
18	2b	312	CLA	2	0
18	B	821	CLA	3	0
25	6a	319	LUT	5	0
18	A	835	CLA	4	0
18	3b	302	CLA	1	0
18	b	804	CLA	3	0
18	B	833	CLA	1	0
18	3a	303	CLA	2	0
18	g	202	CLA	1	0
18	5b	308	CLA	2	0
18	a	814	CLA	1	0
18	6a	308	CLA	3	0
18	B	853	CLA	1	0
18	a	809	CLA	1	0
18	a	853	CLA	1	0
29	2a	306	CHL	6	0
18	a	831	CLA	4	0
18	b	811	CLA	1	0
18	5a	308	CLA	2	0
18	B	811	CLA	2	0
20	A	851	BCR	5	0
18	L	302	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	5a	307	CHL	2	0
18	j	101	CLA	2	0
18	A	827	CLA	1	0
18	J	101	CLA	2	0
18	B	839	CLA	2	0
27	5a	320	LHG	3	0
18	a	821	CLA	2	0
18	A	838	CLA	1	0
20	a	850	BCR	3	0
18	B	820	CLA	1	0
20	l	304	BCR	2	0
18	6a	314	CLA	1	0
18	b	803	CLA	1	0
18	3a	313	CLA	2	0
18	l	301	CLA	2	0
18	a	804	CLA	1	0
18	5a	309	CLA	2	0
18	G	203	CLA	3	0
20	b	846	BCR	1	0
18	A	814	CLA	1	0
29	3a	307	CHL	2	0
18	5a	303	CLA	3	0
18	2b	303	CLA	1	0
18	3a	309	CLA	2	0
18	a	818	CLA	2	0
18	b	823	CLA	3	0
19	B	841	PQN	3	0
18	2a	312	CLA	2	0
18	b	828	CLA	4	0
23	5b	319	LMG	1	0
29	2b	313	CHL	2	0
18	L	303	CLA	1	0
18	2a	308	CLA	3	0
19	A	843	PQN	1	0
18	b	809	CLA	3	0
18	b	806	CLA	7	0
24	A	844	SF4	1	0
18	F	303	CLA	1	0
18	A	805	CLA	5	0
18	3b	313	CLA	1	0
18	B	810	CLA	2	0
18	a	841	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	2b	314	LUT	5	0
18	A	816	CLA	2	0
18	a	805	CLA	5	0
18	B	832	CLA	3	0
20	G	201	BCR	3	0
18	A	841	CLA	5	0
18	A	803	CLA	3	0
20	B	845	BCR	5	0
18	b	819	CLA	2	0
20	I	202	BCR	3	0
18	6b	306	CLA	1	0
18	b	815	CLA	3	0
25	5a	316	LUT	5	0
29	5b	314	CHL	1	0
18	A	815	CLA	2	0
18	a	835	CLA	4	0
18	5b	313	CLA	1	0
18	6a	306	CLA	1	0
26	a	802	CL0	3	0
27	6b	301	LHG	1	0
18	A	817	CLA	4	0
18	2b	307	CLA	1	0
29	3a	315	CHL	1	0
20	m	101	BCR	3	0
18	b	836	CLA	2	0
18	a	807	CLA	1	0
21	b	847	DGD	3	0
18	B	826	CLA	2	0
18	B	824	CLA	2	0
18	B	827	CLA	1	0
18	a	827	CLA	1	0
23	I	201	LMG	1	0
18	A	834	CLA	2	0
18	b	810	CLA	2	0
25	6b	320	LUT	3	0
18	b	852	CLA	1	0
18	a	815	CLA	2	0
23	j	103	LMG	1	0
18	A	801	CLA	2	0
18	A	819	CLA	2	0
29	2b	304	CHL	1	0
20	b	845	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	5a	306	CHL	1	0
19	b	841	PQN	3	0
18	l	303	CLA	1	0
18	B	804	CLA	4	0
25	3a	316	LUT	2	0
29	3b	315	CHL	1	0
18	A	836	CLA	1	0
25	6a	318	LUT	4	0
18	5b	303	CLA	3	0
18	6b	311	CLA	1	0
18	3b	303	CLA	1	0
18	6b	313	CLA	3	0
18	b	826	CLA	2	0
29	2a	304	CHL	1	0
18	B	805	CLA	2	0
18	3a	311	CLA	1	0
26	A	802	CL0	3	0
18	5b	311	CLA	1	0
18	A	809	CLA	1	0
18	a	816	CLA	3	0
20	b	842	BCR	3	0
18	3b	314	CLA	1	0
29	5b	307	CHL	2	0
19	a	843	PQN	1	0
29	5b	301	CHL	2	0
18	l	302	CLA	2	0
20	a	851	BCR	4	0
29	5b	305	CHL	1	0
18	B	802	CLA	2	0
25	5b	317	LUT	1	0
18	A	808	CLA	3	0
20	b	851	BCR	5	0
18	a	817	CLA	4	0
29	6b	309	CHL	1	0
18	5b	309	CLA	1	0
18	a	838	CLA	1	0
18	B	815	CLA	3	0
18	6a	313	CLA	3	0
18	b	839	CLA	2	0
18	A	812	CLA	4	0
29	5a	314	CHL	1	0
29	6a	309	CHL	1	0

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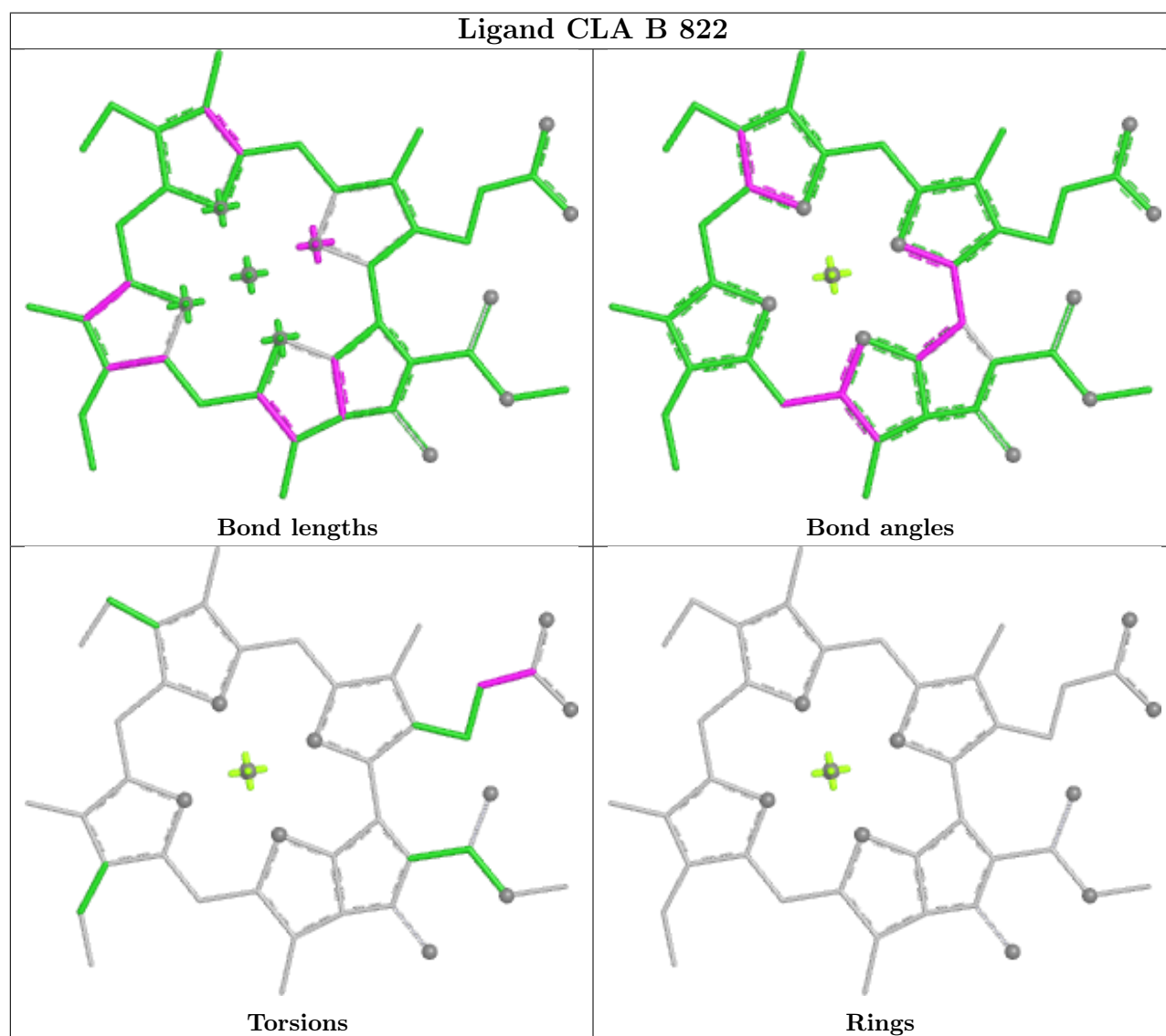
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	818	CLA	2	0
29	2b	306	CHL	5	0
18	6b	307	CLA	2	0
18	F	302	CLA	3	0
18	a	834	CLA	2	0
23	J	103	LMG	1	0
18	2a	302	CLA	1	0
18	b	821	CLA	2	0
27	6a	301	LHG	1	0
18	6b	316	CLA	2	0
18	b	854	CLA	4	0
18	a	819	CLA	2	0
18	b	833	CLA	1	0
20	B	851	BCR	5	0
18	a	837	CLA	1	0
18	2b	311	CLA	1	0
18	b	853	CLA	1	0
29	3a	301	CHL	1	0
18	b	831	CLA	3	0
18	B	817	CLA	2	0
18	A	810	CLA	3	0
18	B	838	CLA	4	0
18	A	823	CLA	5	0
18	A	807	CLA	1	0
29	6a	304	CHL	2	0
18	b	829	CLA	1	0
18	B	836	CLA	2	0
18	a	822	CLA	1	0
18	B	814	CLA	2	0
18	2b	301	CLA	1	0
21	B	847	DGD	3	0
25	J	105	LUT	4	0
18	a	833	CLA	2	0
23	i	201	LMG	1	0
18	b	820	CLA	1	0
18	2a	311	CLA	1	0
18	A	839	CLA	2	0
18	f	303	CLA	1	0
20	b	843	BCR	1	0
23	5a	319	LMG	1	0
18	a	812	CLA	3	0
18	B	819	CLA	2	0



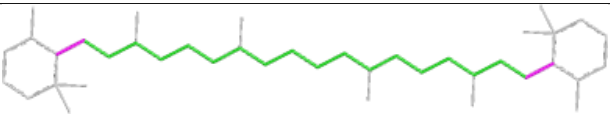
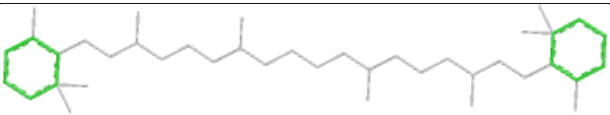
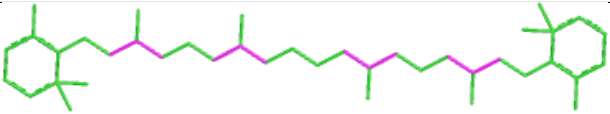
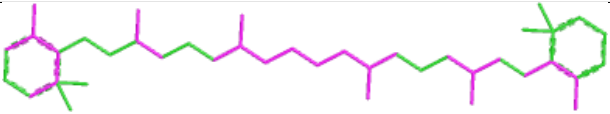
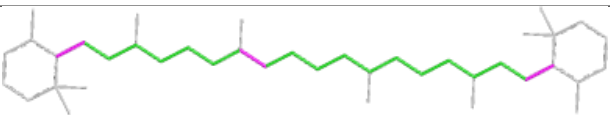
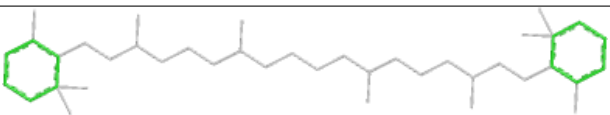
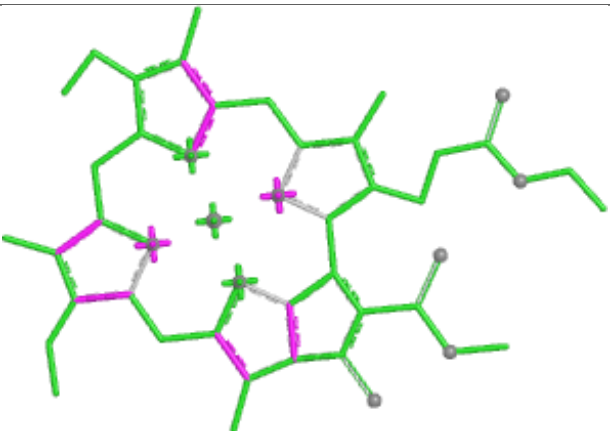
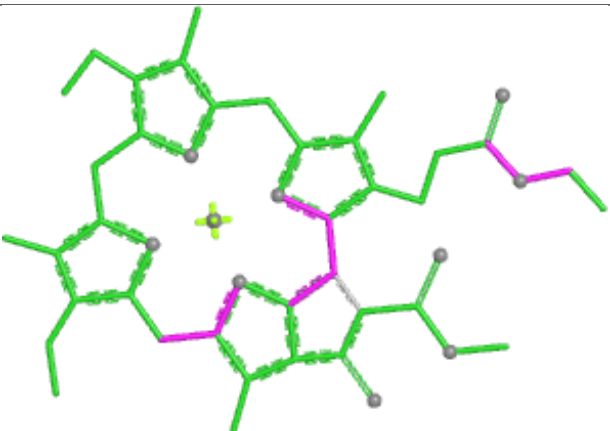
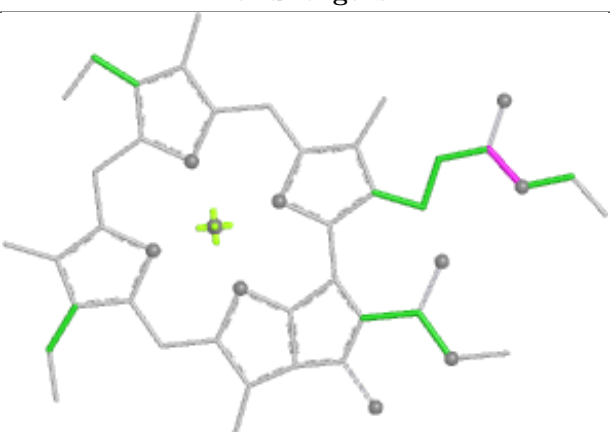
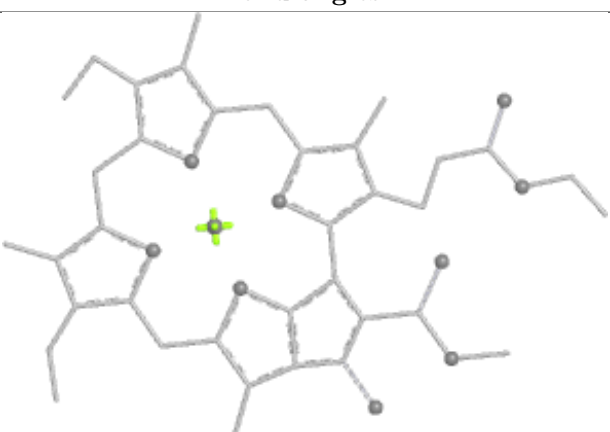
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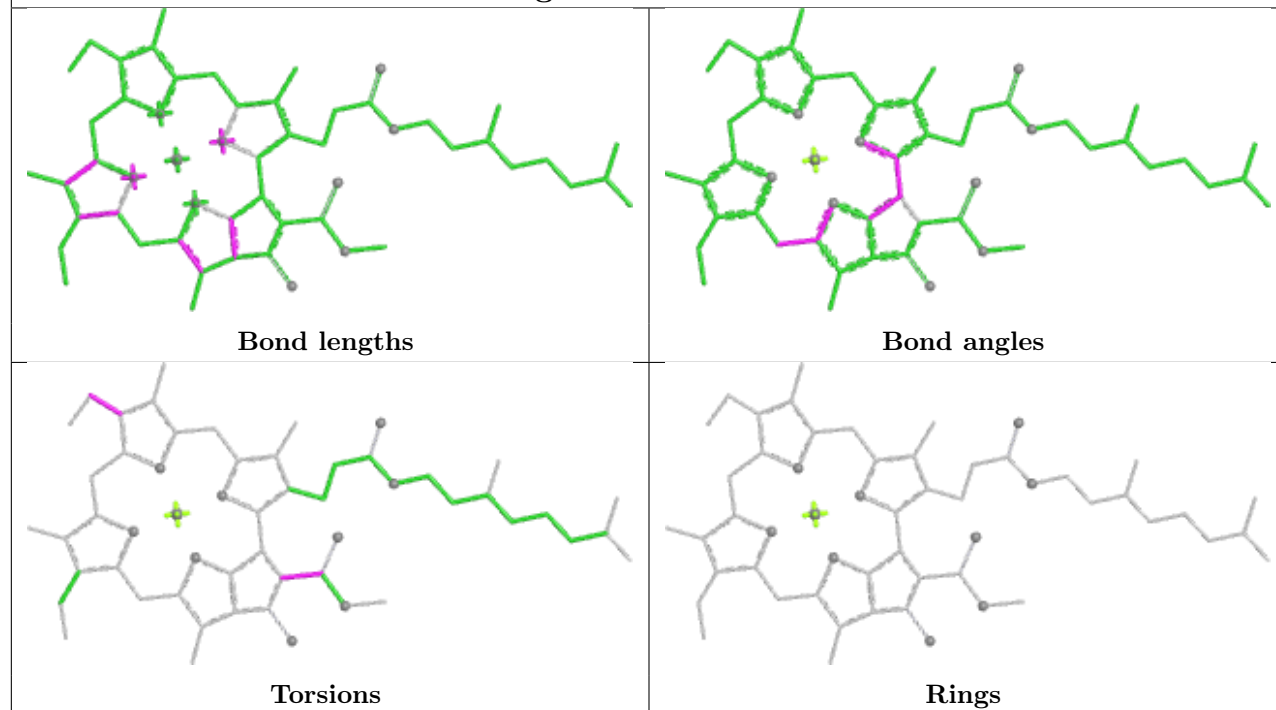
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	820	CLA	2	0
18	6b	314	CLA	1	0
20	b	844	BCR	3	0
18	3a	306	CLA	2	0
18	2a	307	CLA	1	0
18	B	852	CLA	1	0
20	f	301	BCR	4	0
18	2a	301	CLA	2	0
29	6b	304	CHL	2	0
20	L	304	BCR	2	0
18	3a	310	CLA	1	0
24	a	844	SF4	1	0
18	2a	309	CLA	1	0
18	B	813	CLA	1	0
29	3b	307	CHL	2	0
18	L	301	CLA	2	0
20	A	848	BCR	2	0
25	5b	316	LUT	4	0
23	j	104	LMG	1	0
18	A	833	CLA	2	0
18	A	828	CLA	1	0
23	J	104	LMG	1	0
18	F	305	CLA	2	0
18	G	202	CLA	1	0
27	a	845	LHG	3	0
18	A	806	CLA	4	0
20	K	202	BCR	3	0
18	6a	317	CLA	1	0
18	B	812	CLA	2	0
18	a	829	CLA	2	0
25	5a	317	LUT	3	0
18	B	801	CLA	8	0
18	6b	310	CLA	3	0
18	6a	316	CLA	2	0
25	3b	317	LUT	5	0
18	B	818	CLA	1	0
18	b	840	CLA	3	0
18	a	824	CLA	2	0
20	g	204	BCR	5	0
18	3b	310	CLA	1	0
27	A	845	LHG	3	0
18	B	825	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

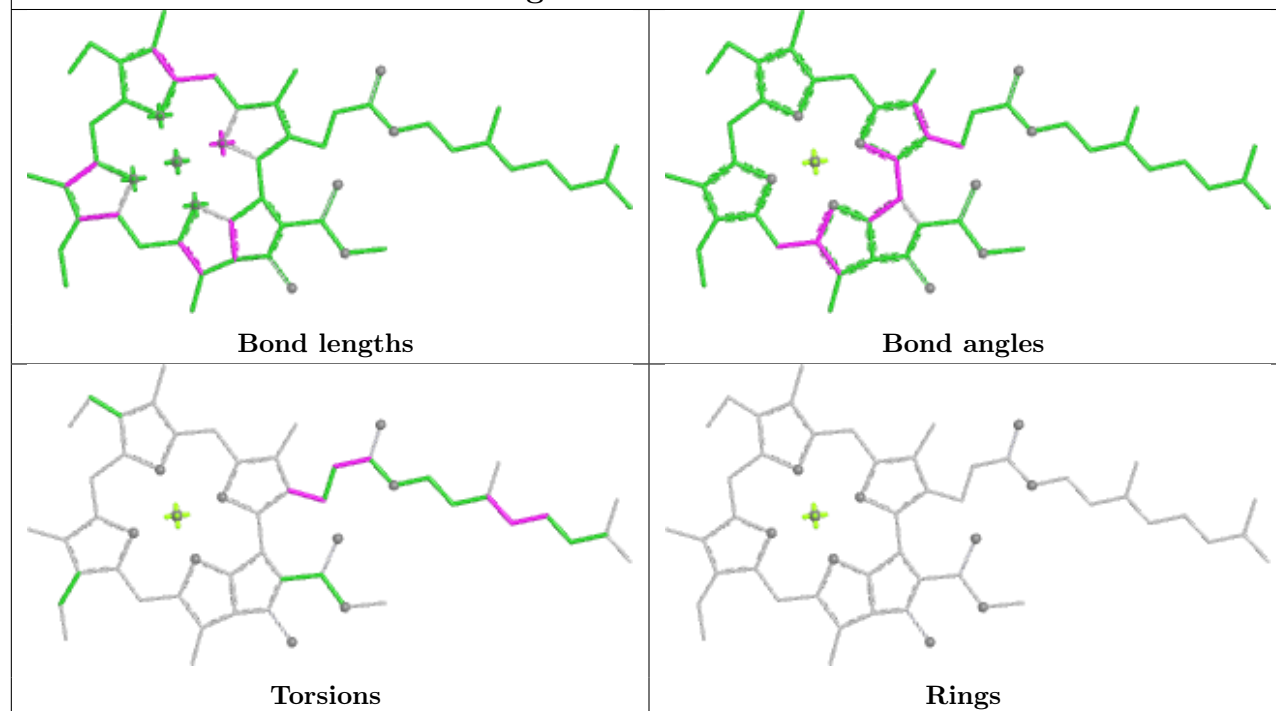


Ligand BCR k 202	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR f 304	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b 808	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

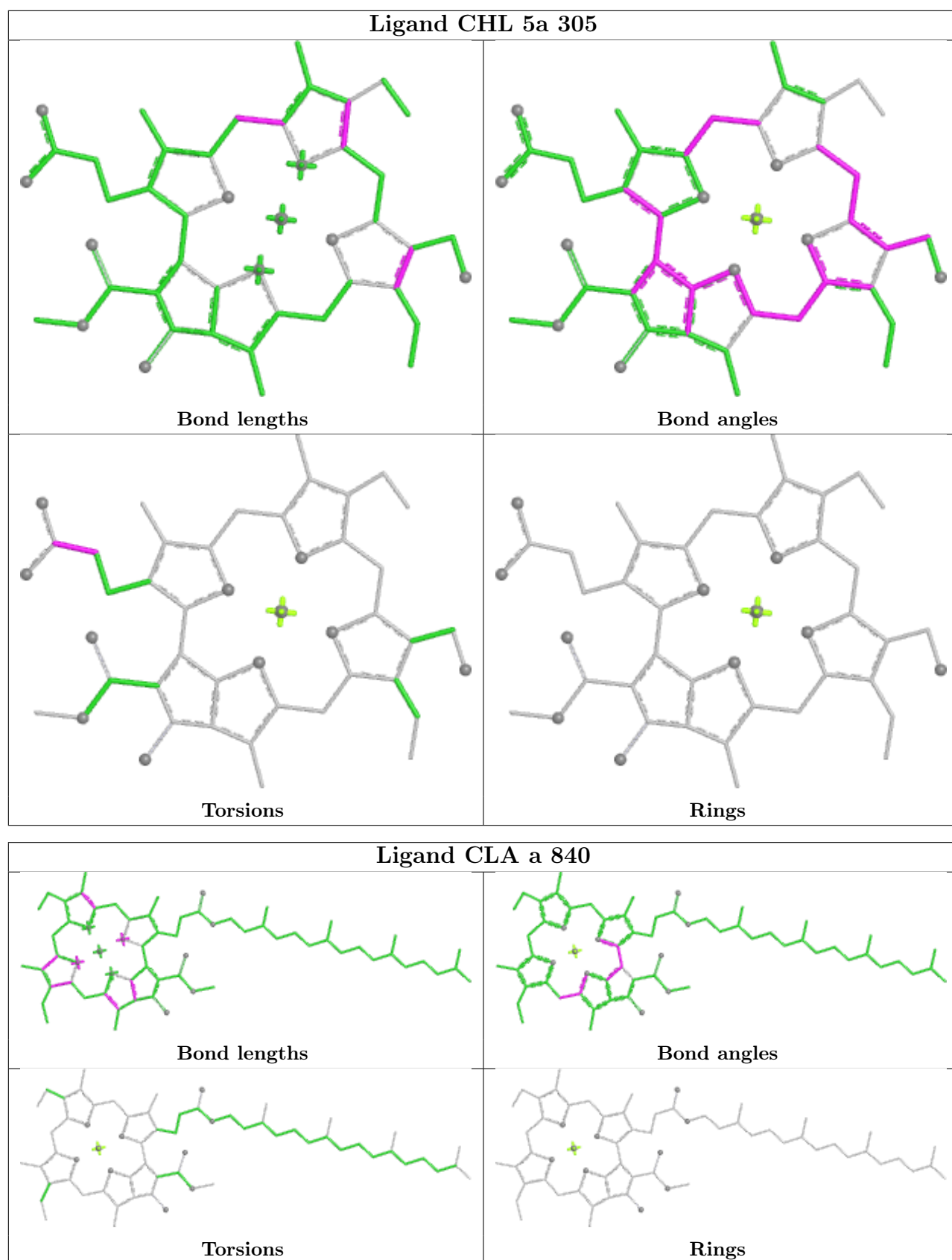
## Ligand CLA b 813

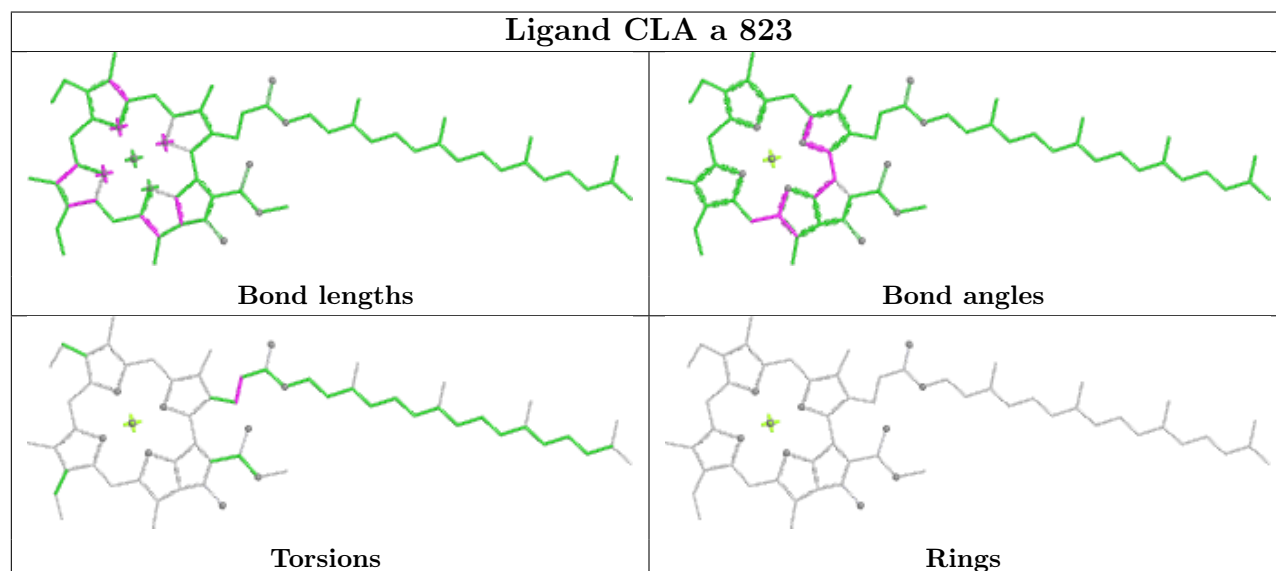
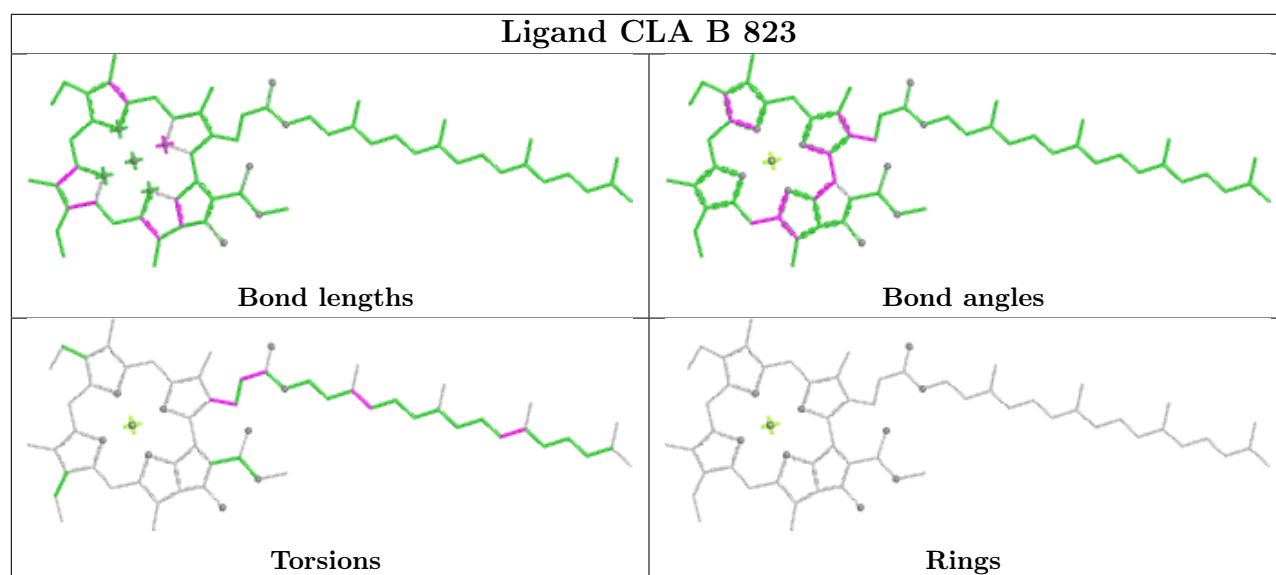


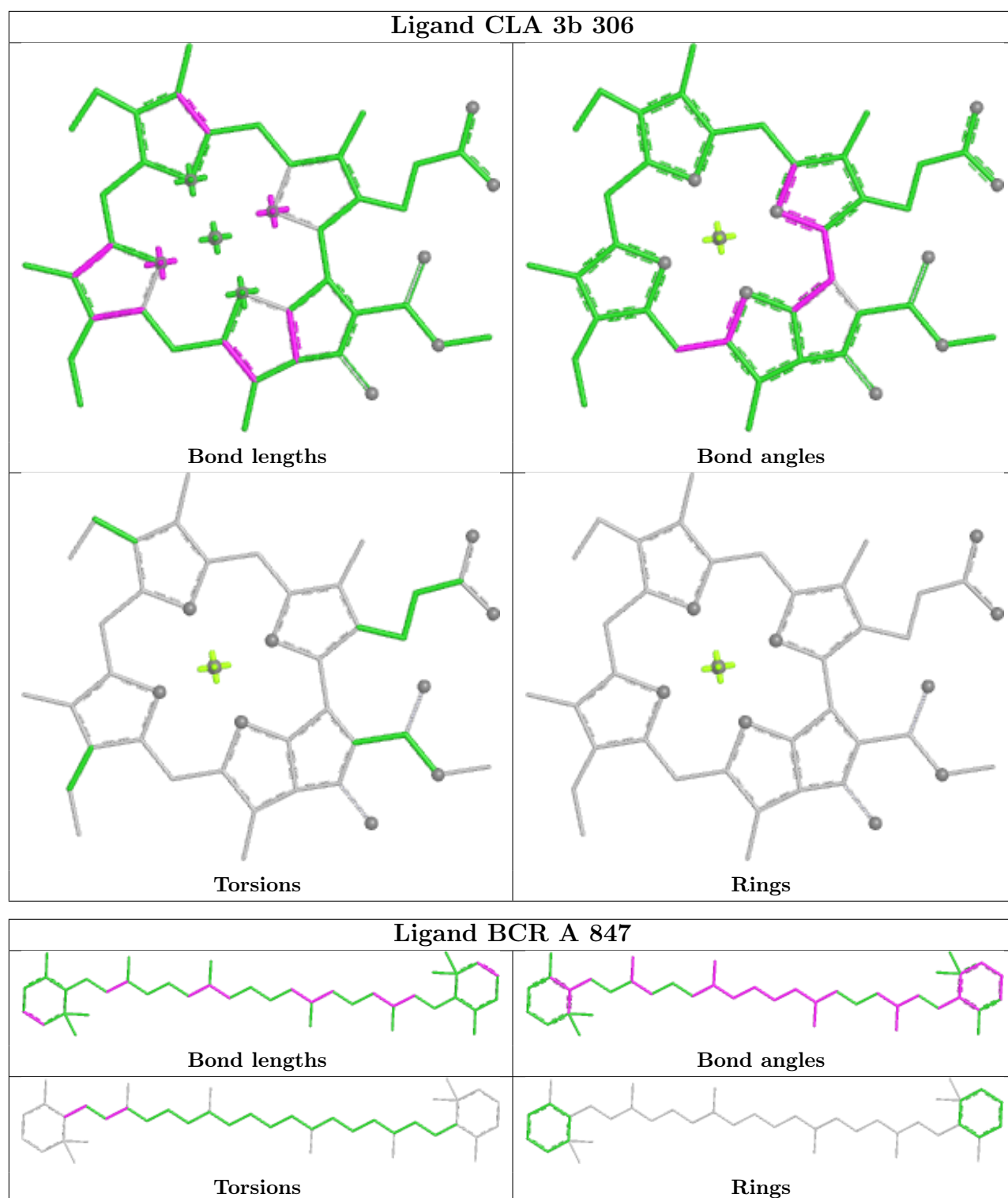
## Ligand CLA 3b 312

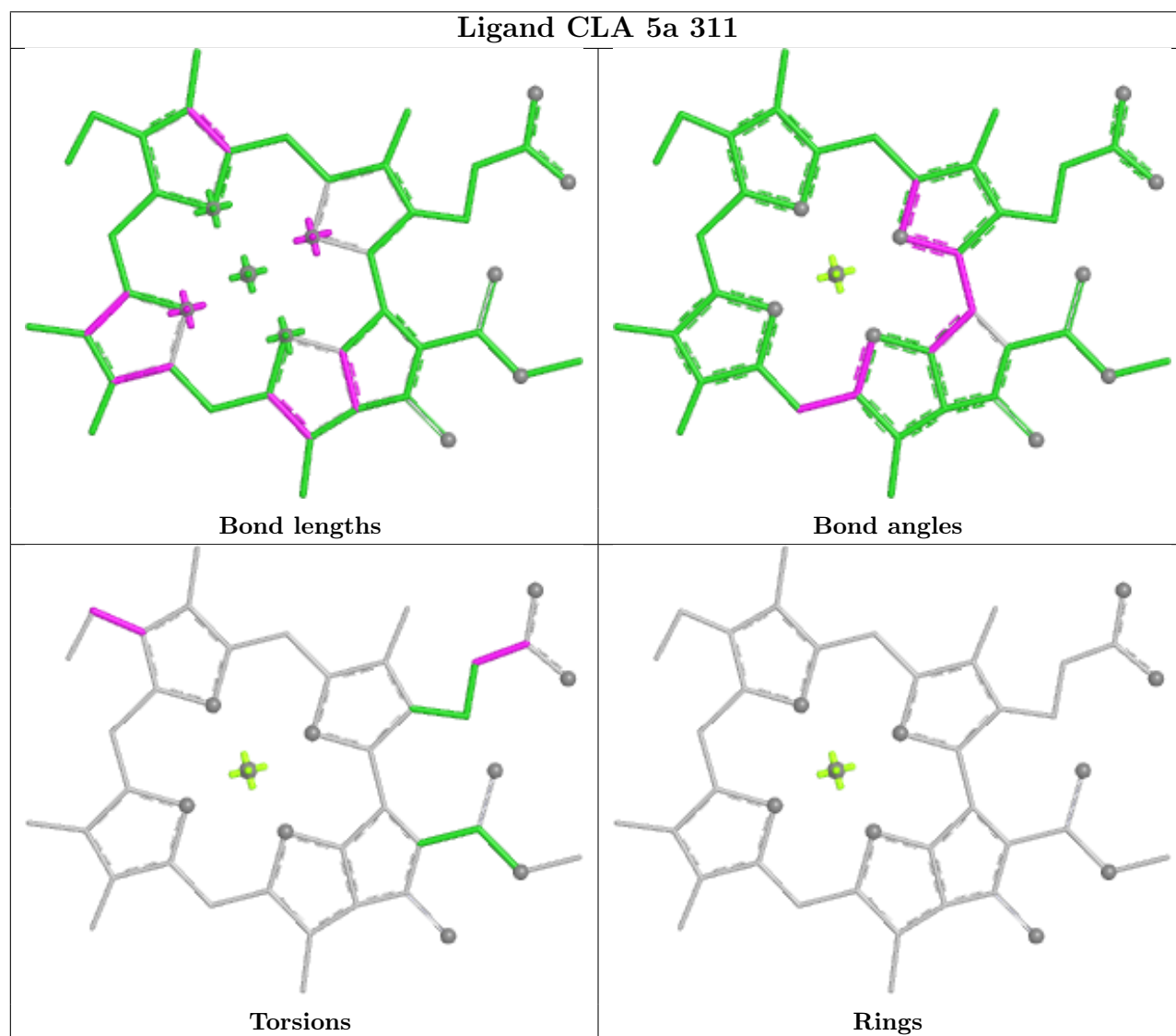
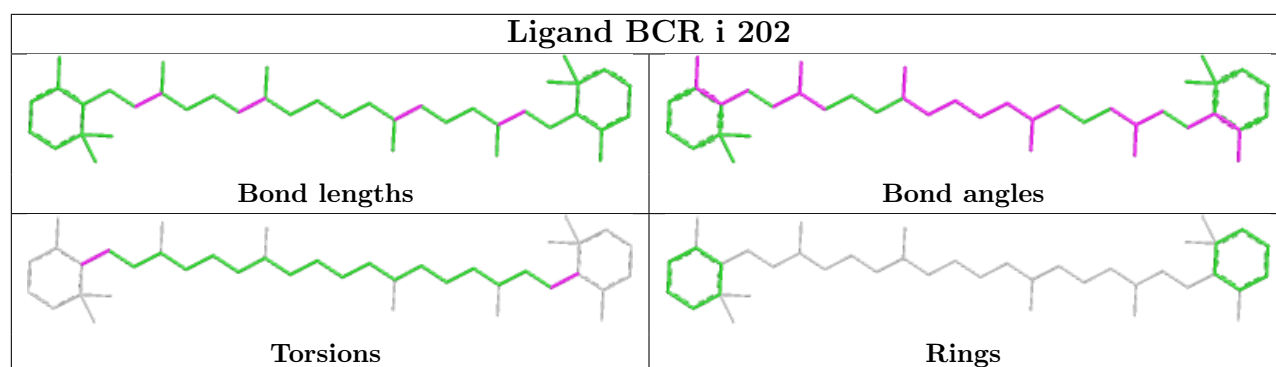


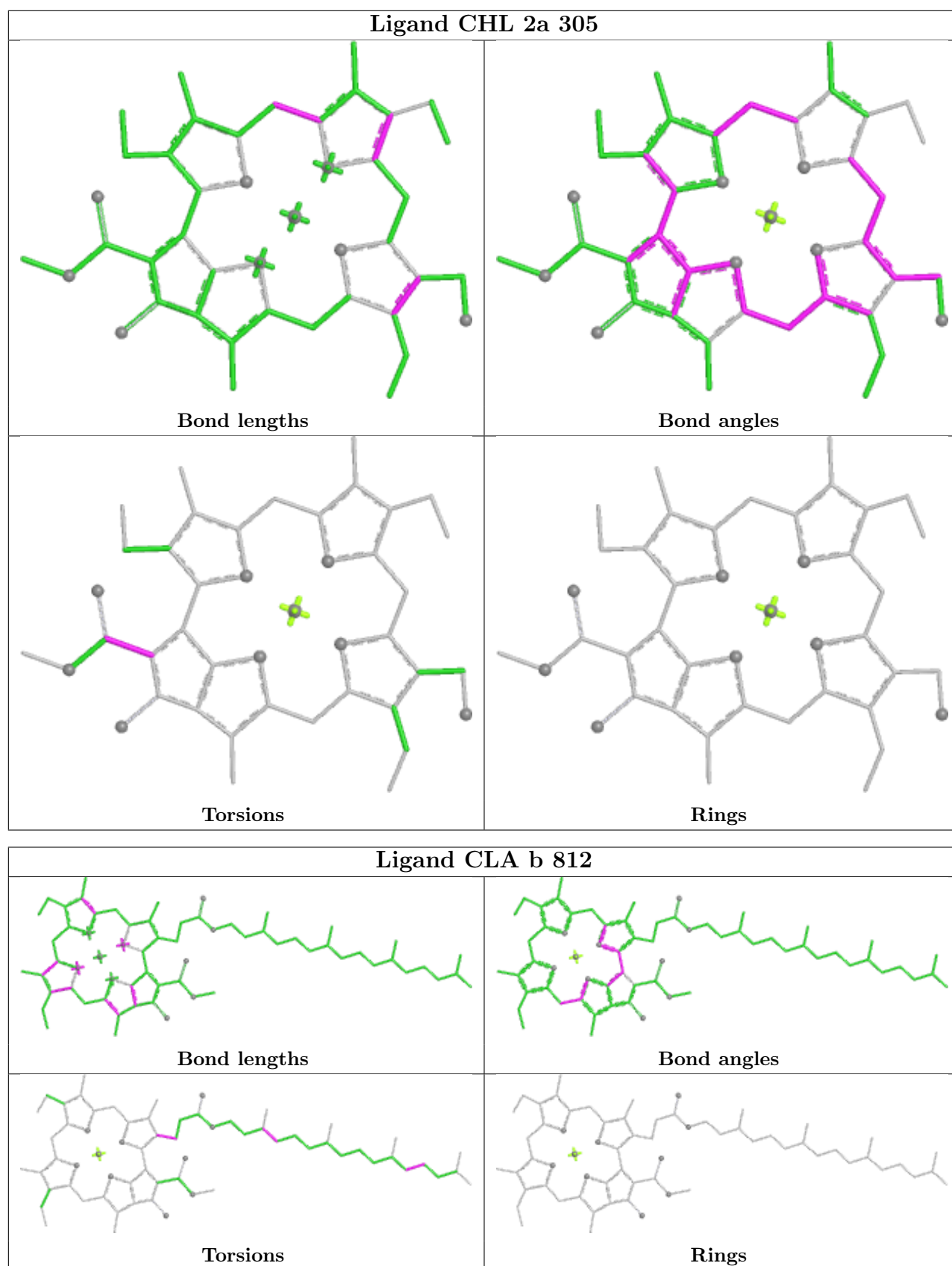


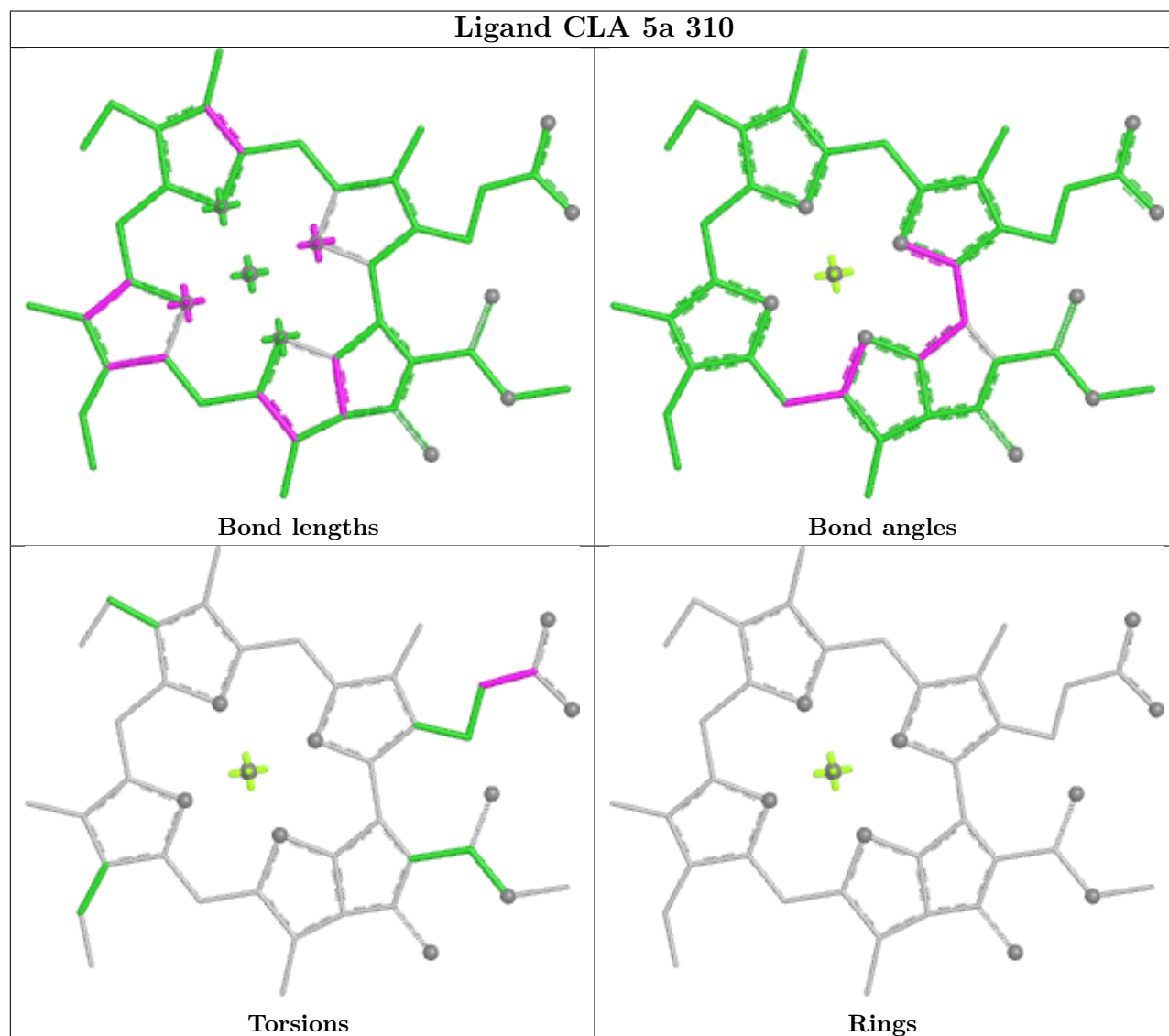
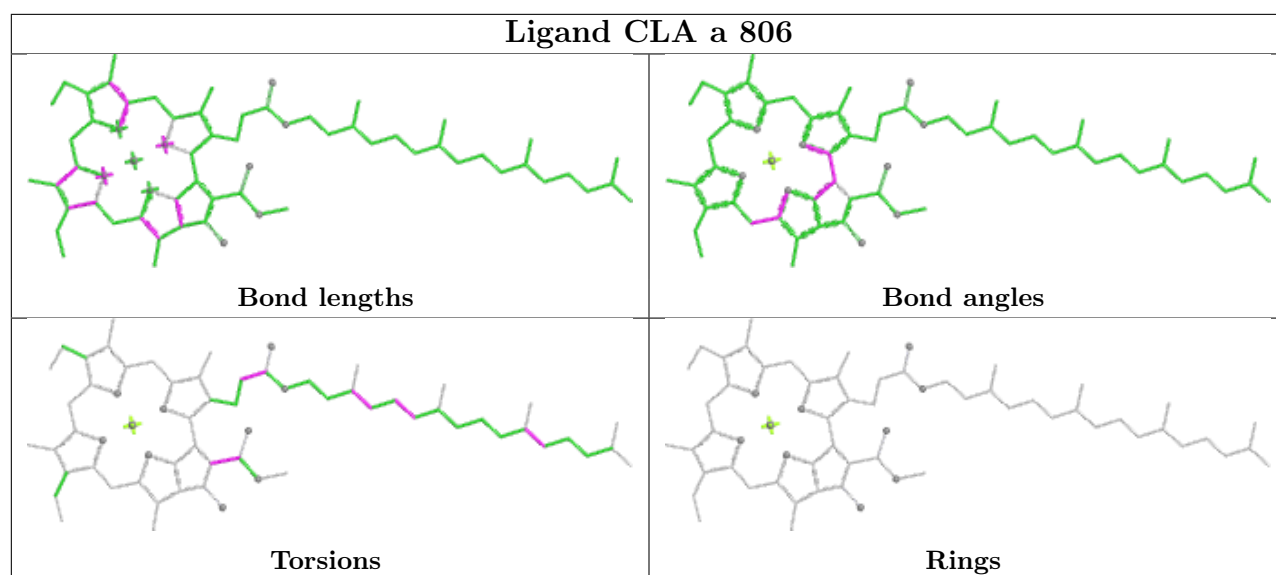


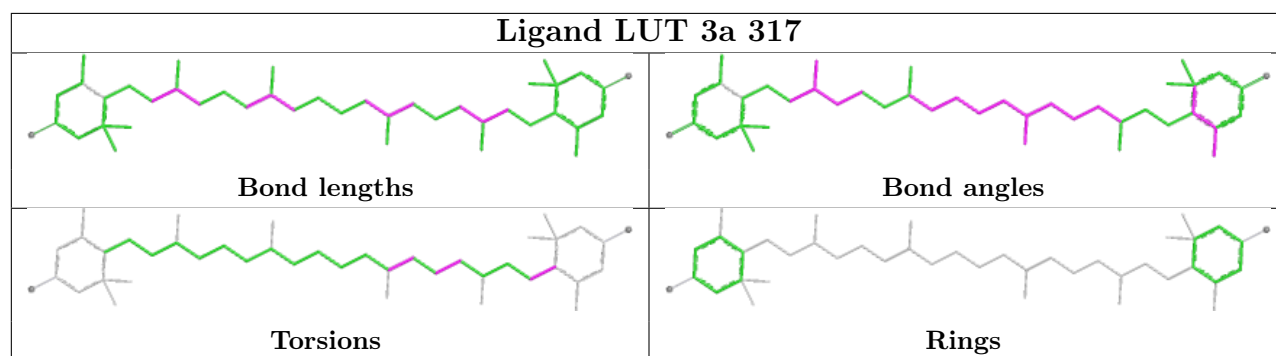
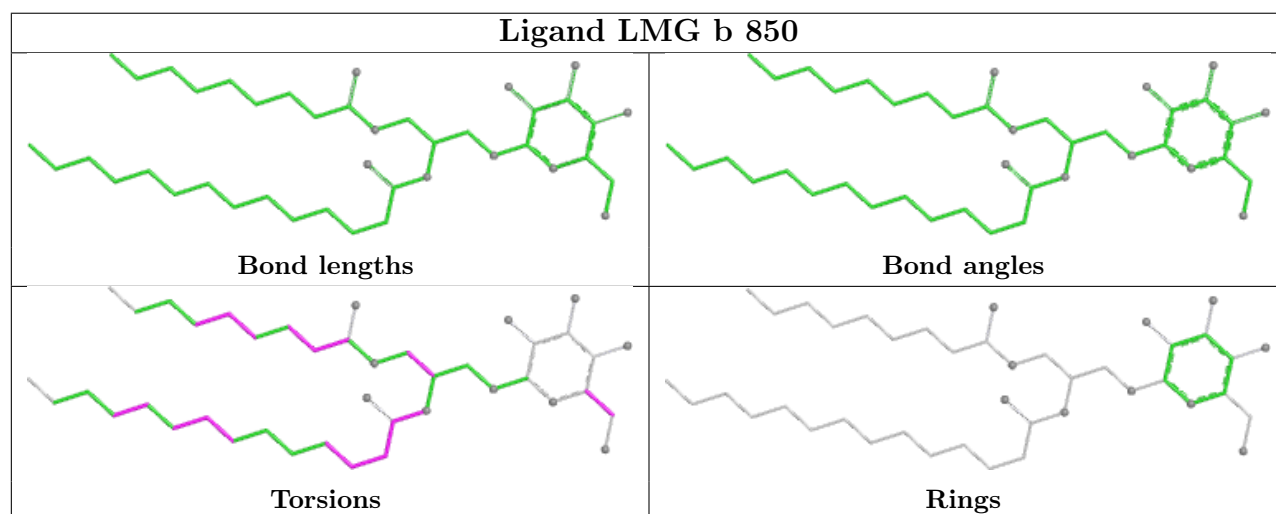
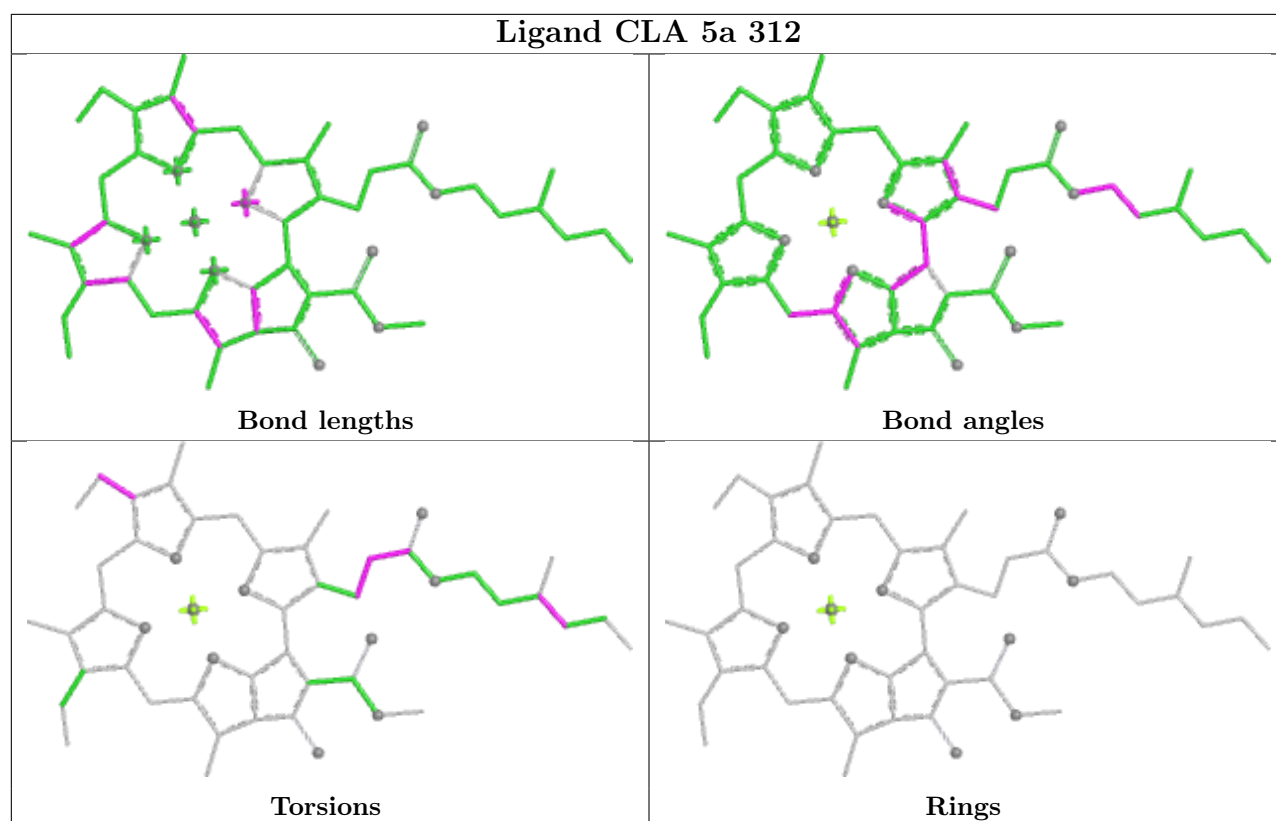


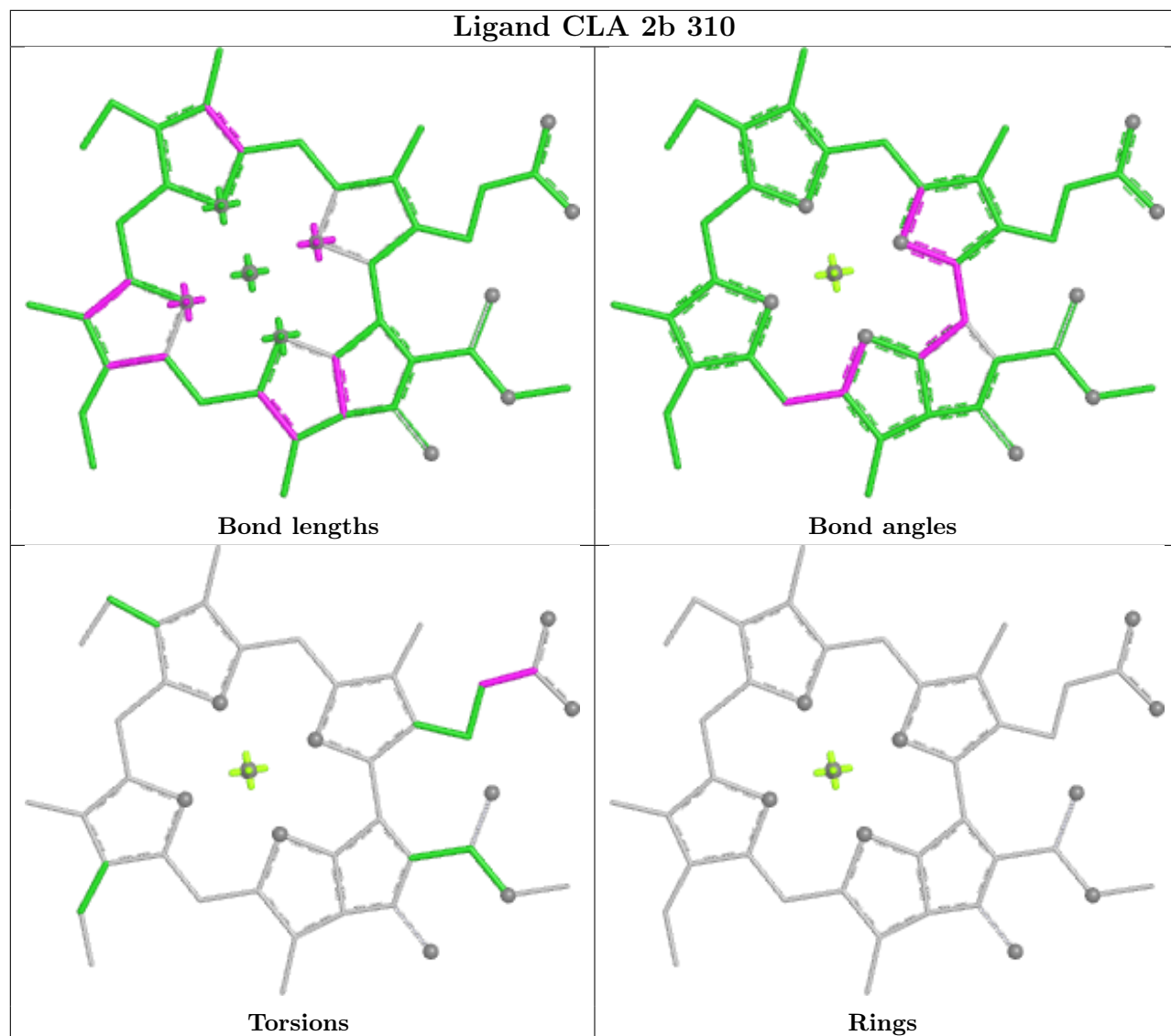




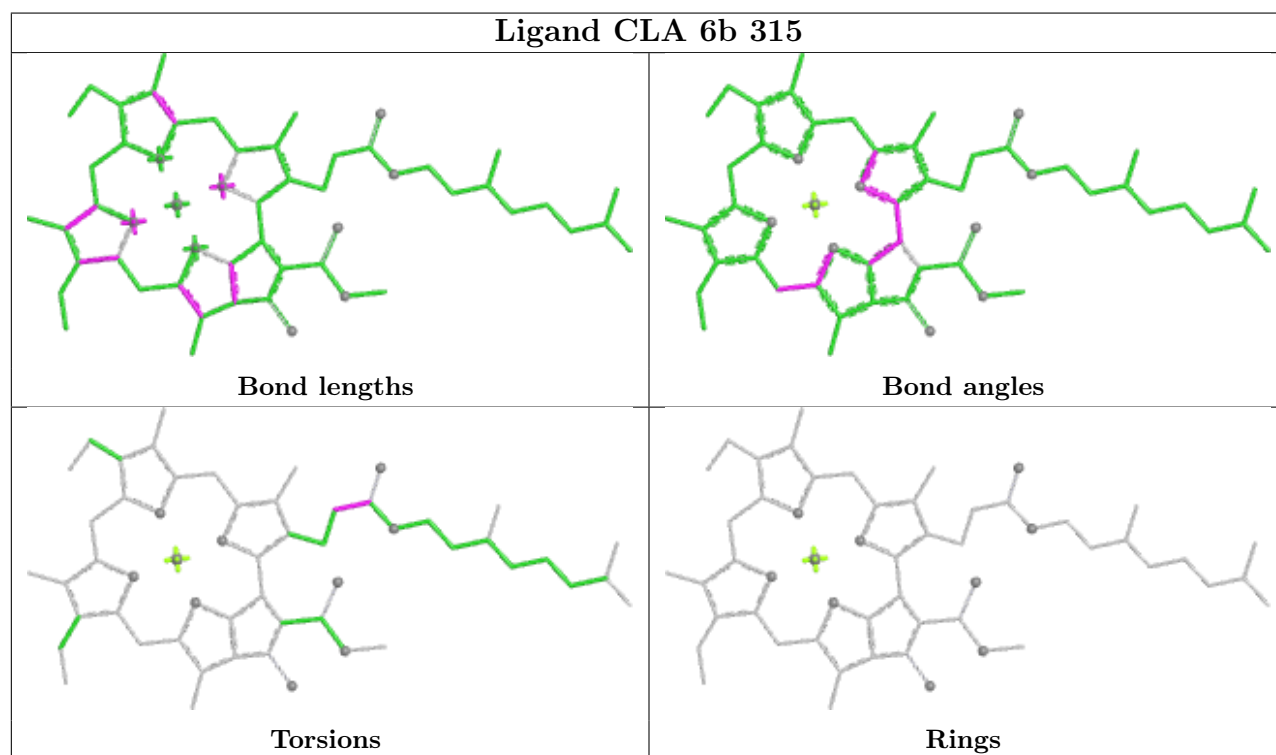
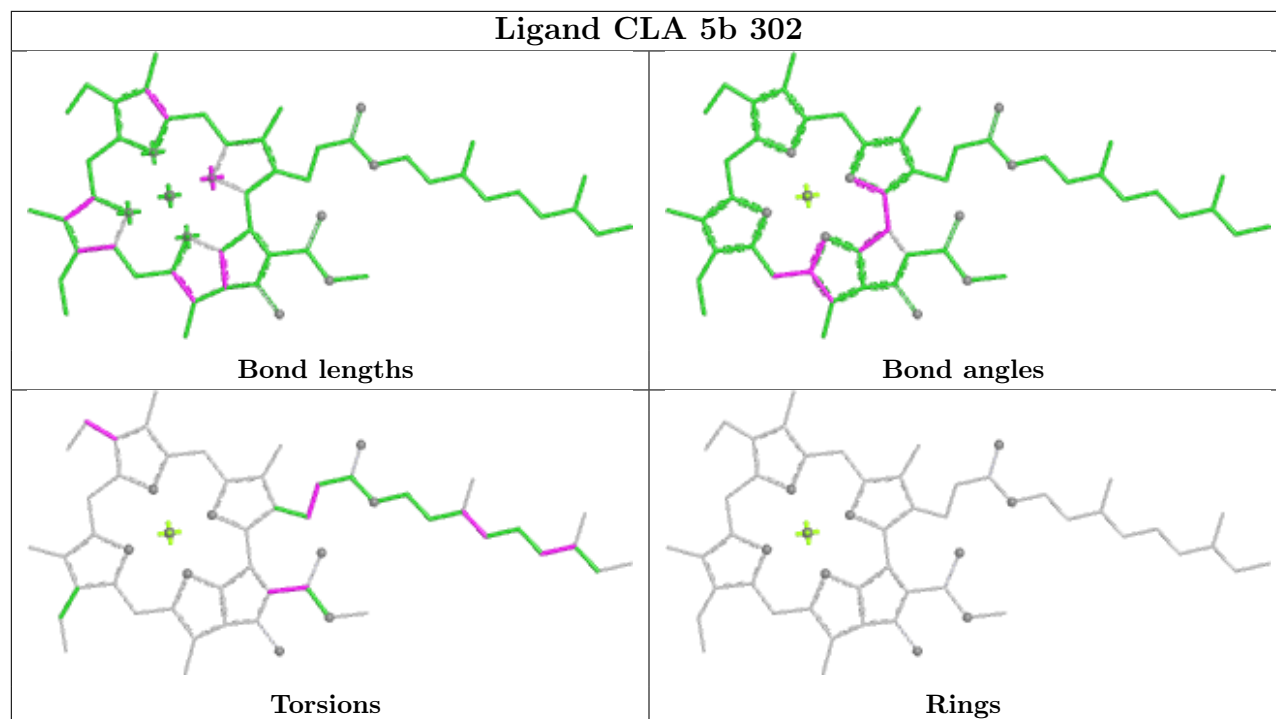




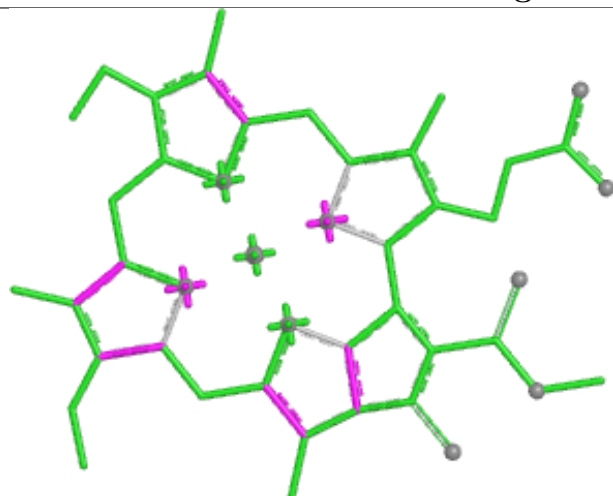




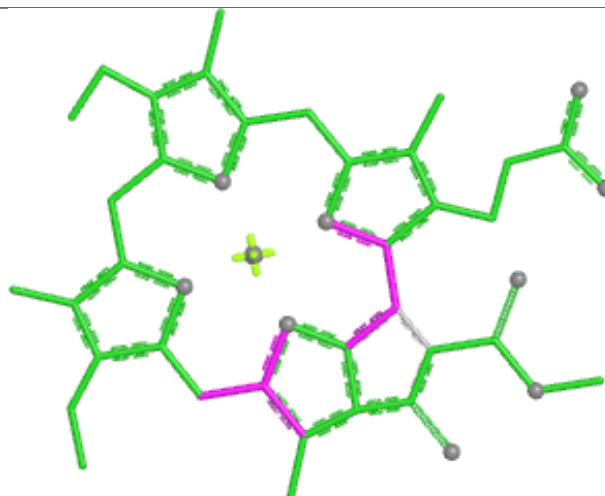




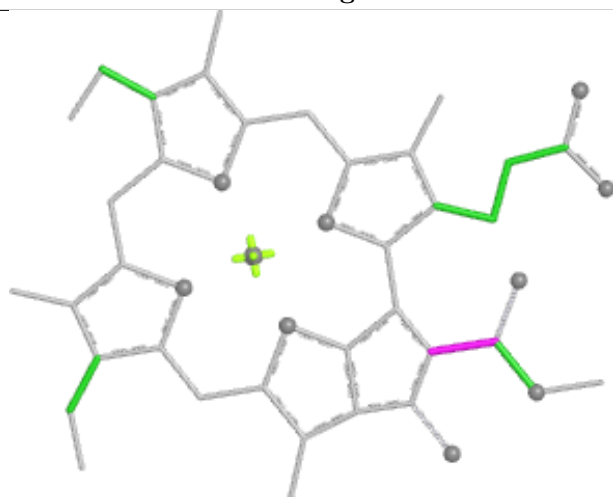
## Ligand CLA B 803



Bond lengths



Bond angles

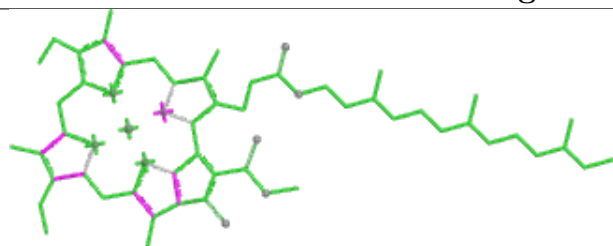


Torsions

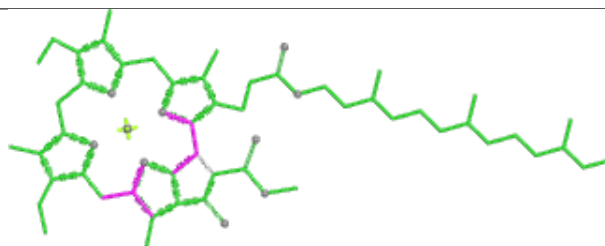


Rings

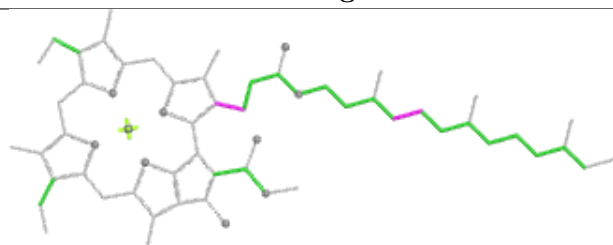
## Ligand CLA a 803



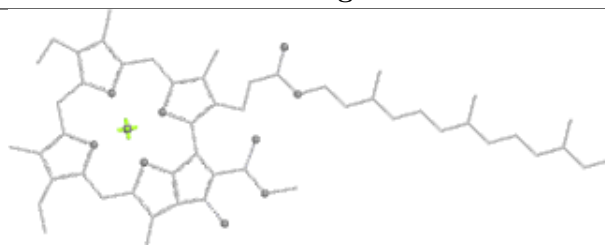
Bond lengths



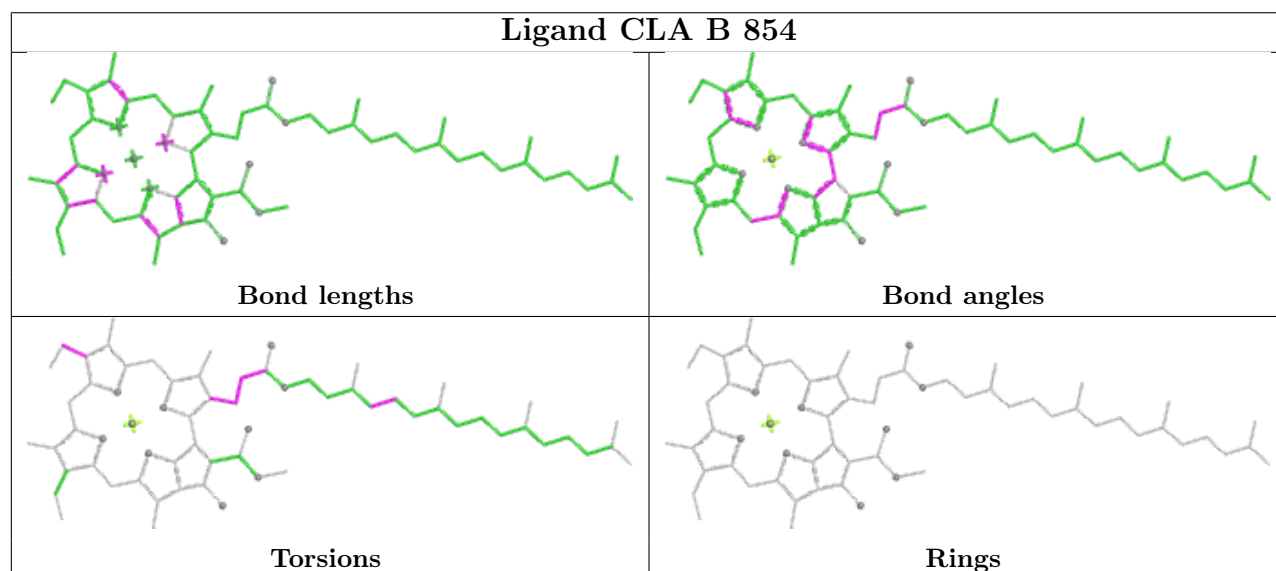
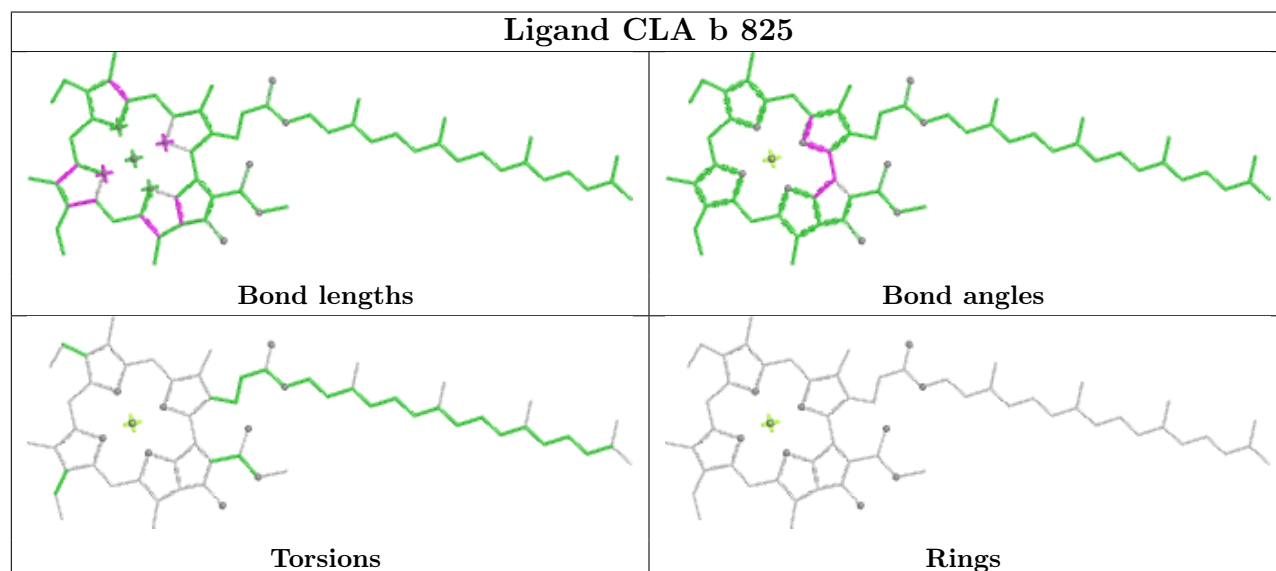
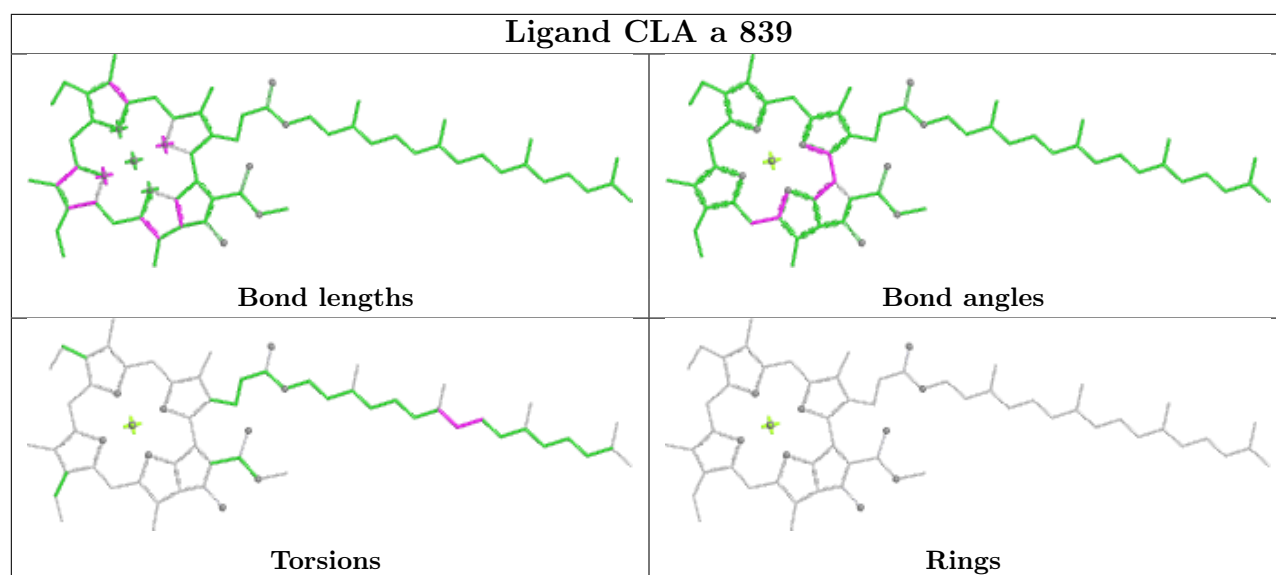
Bond angles

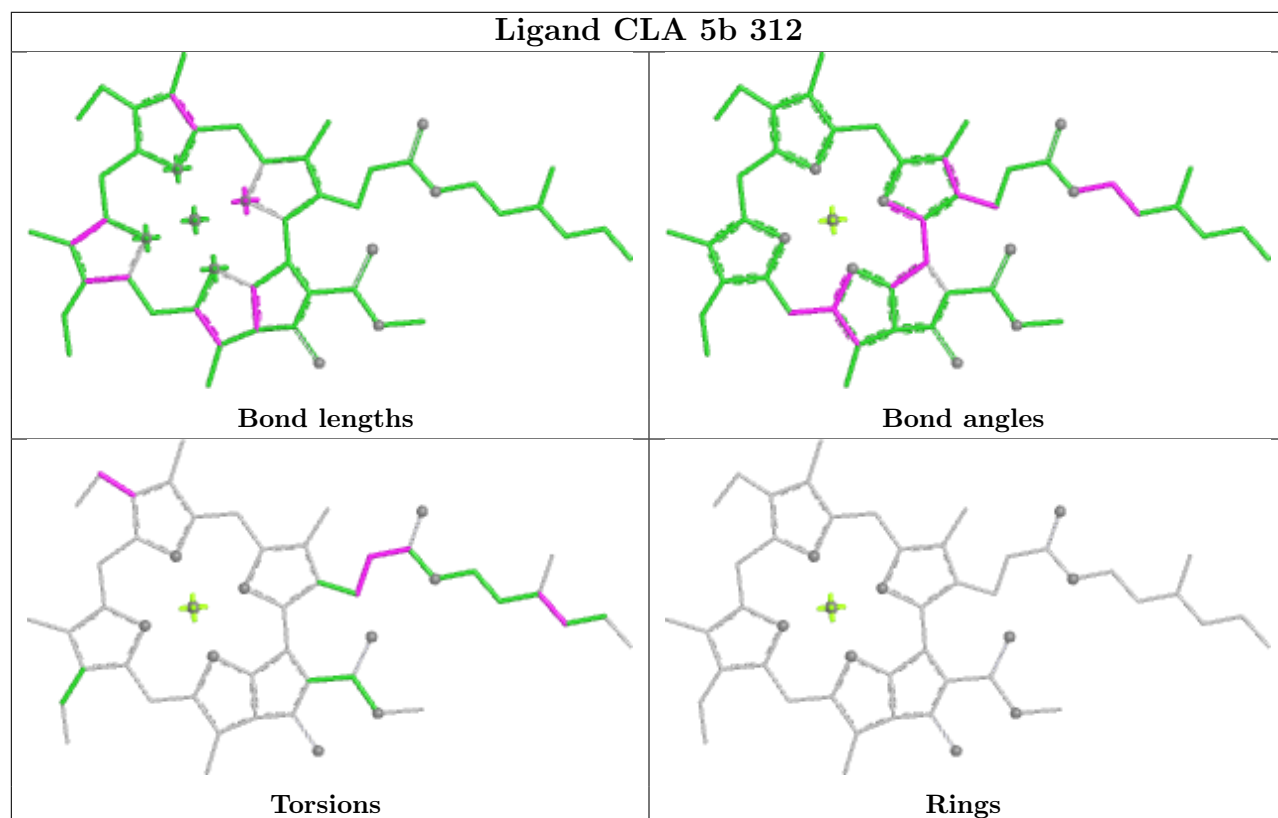
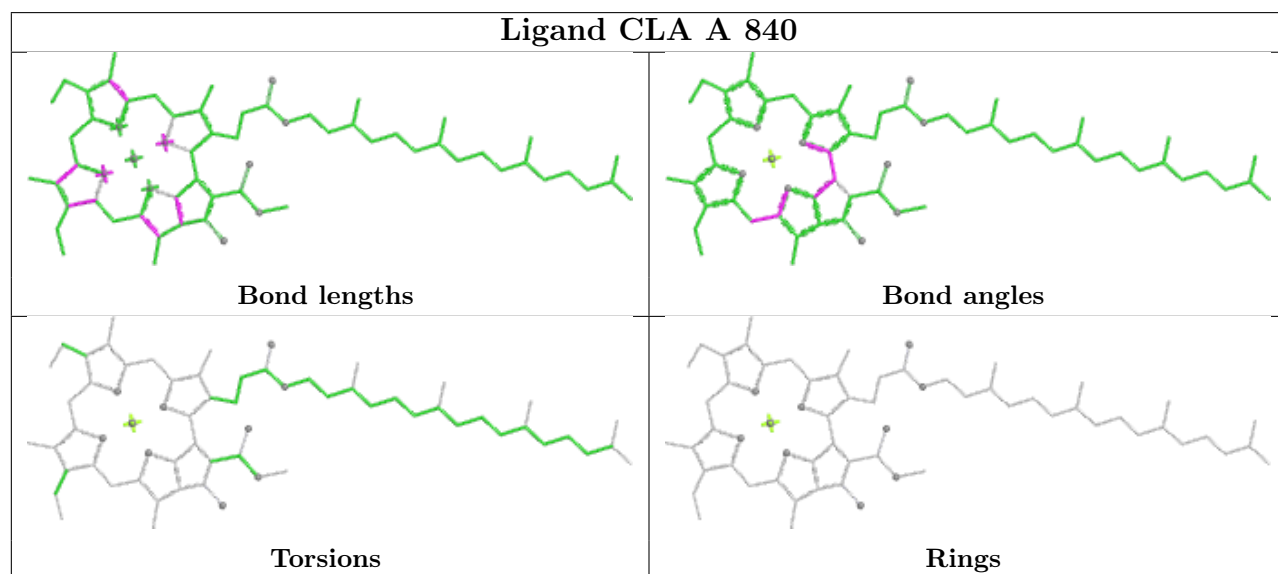
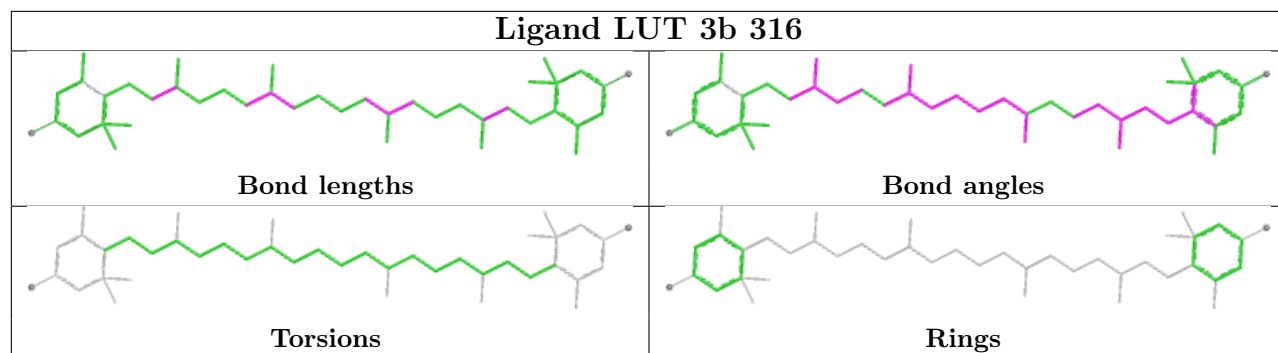


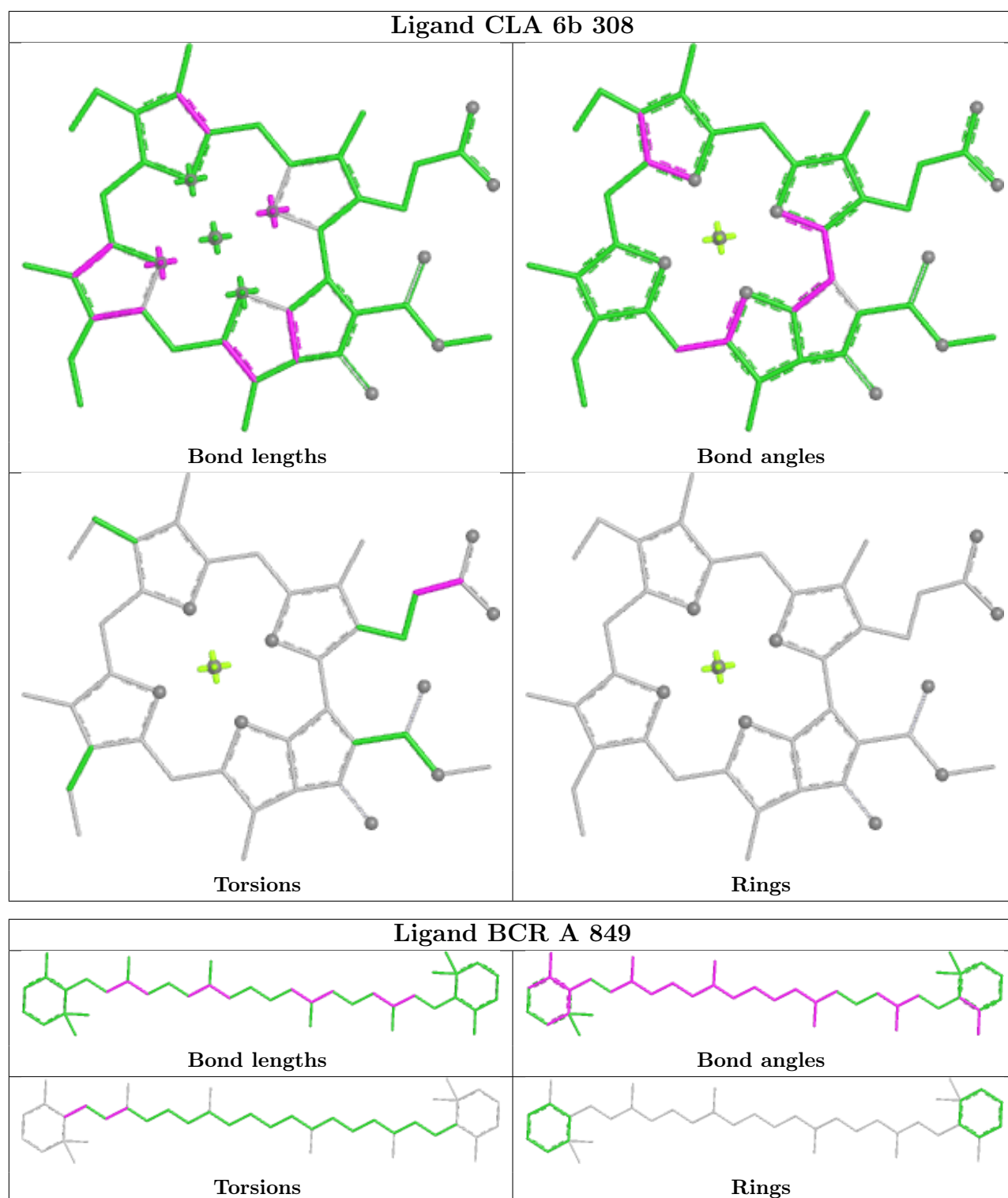
Torsions

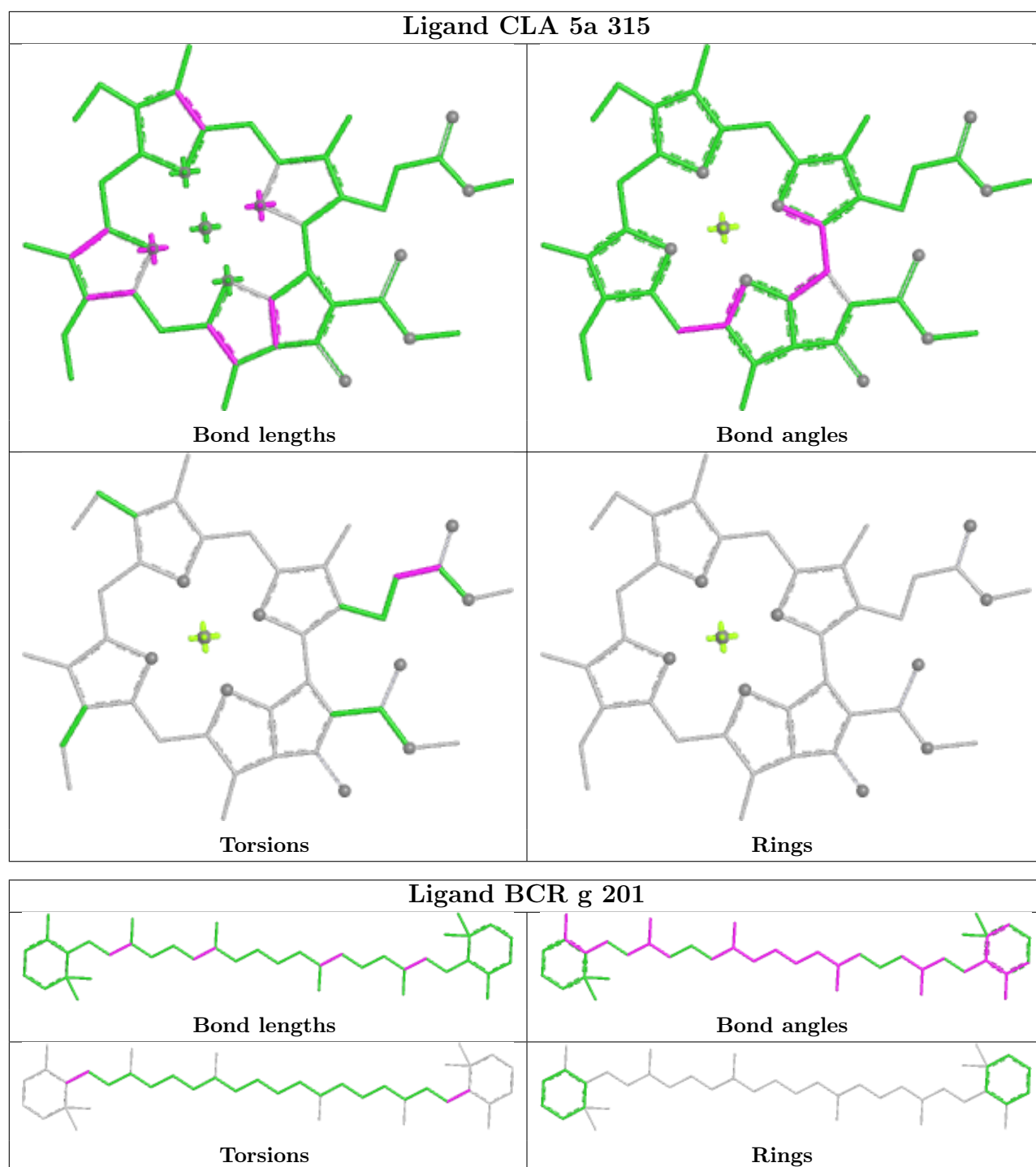


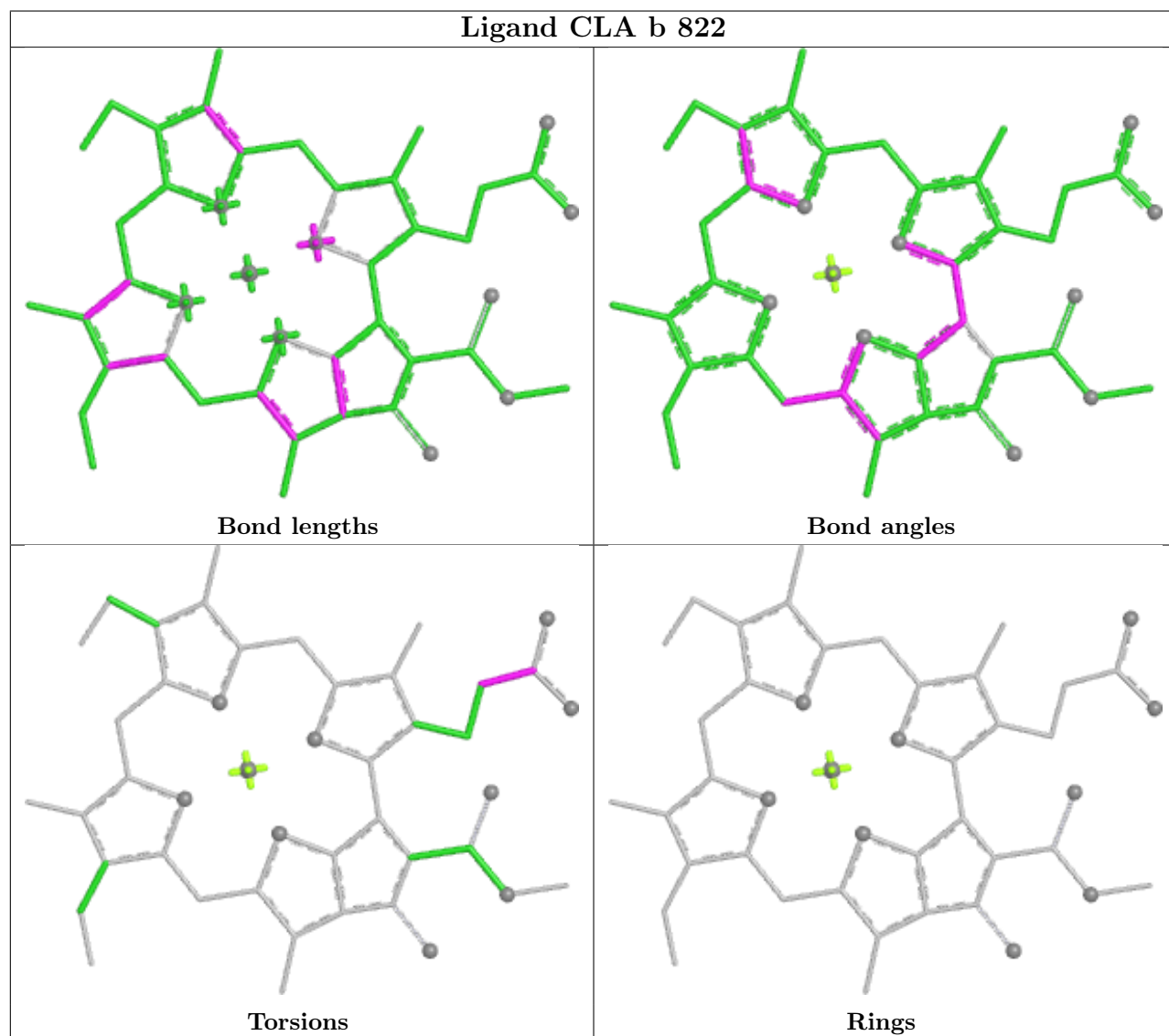
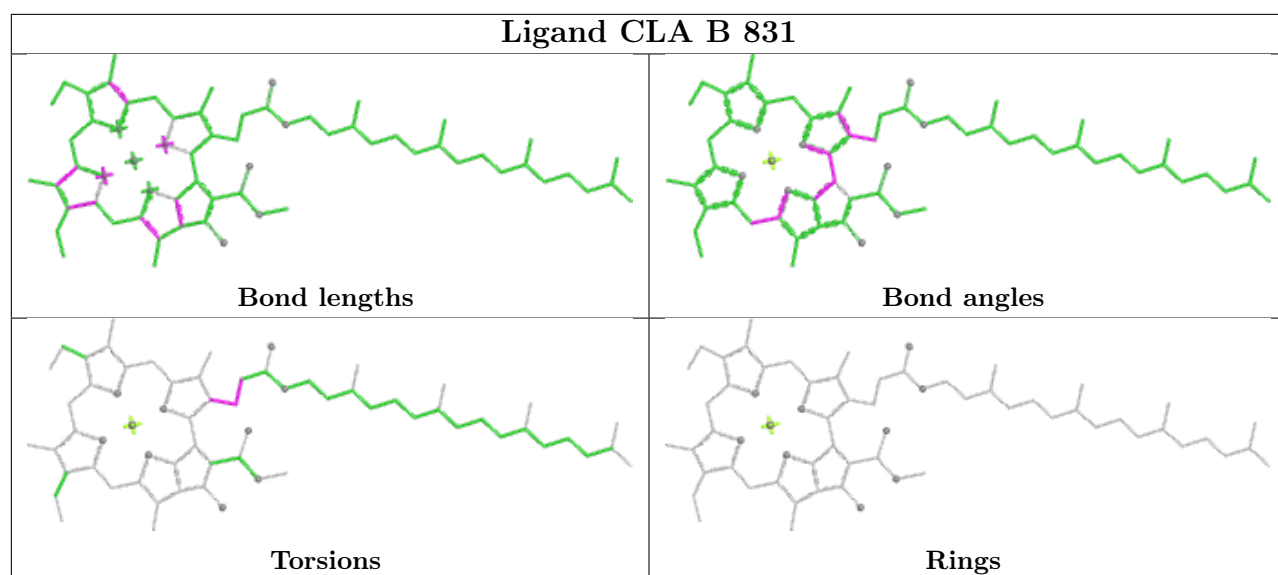
Rings

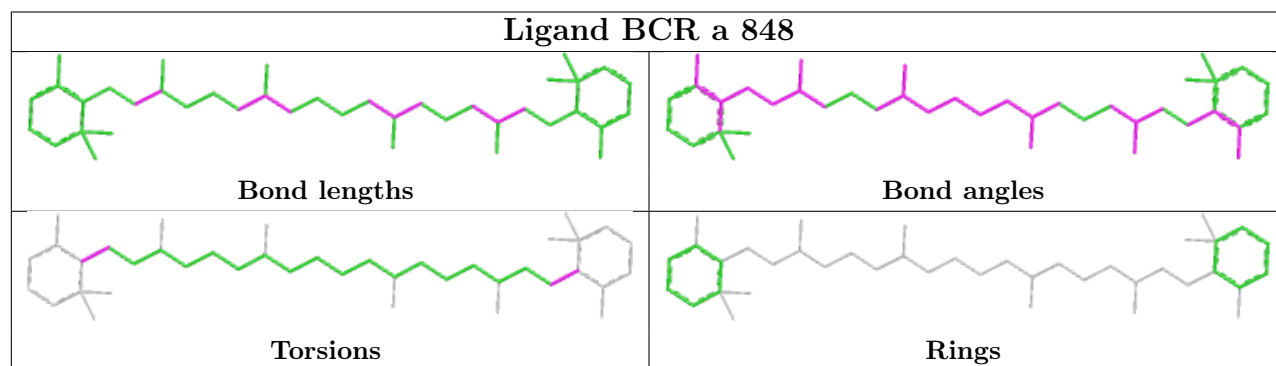
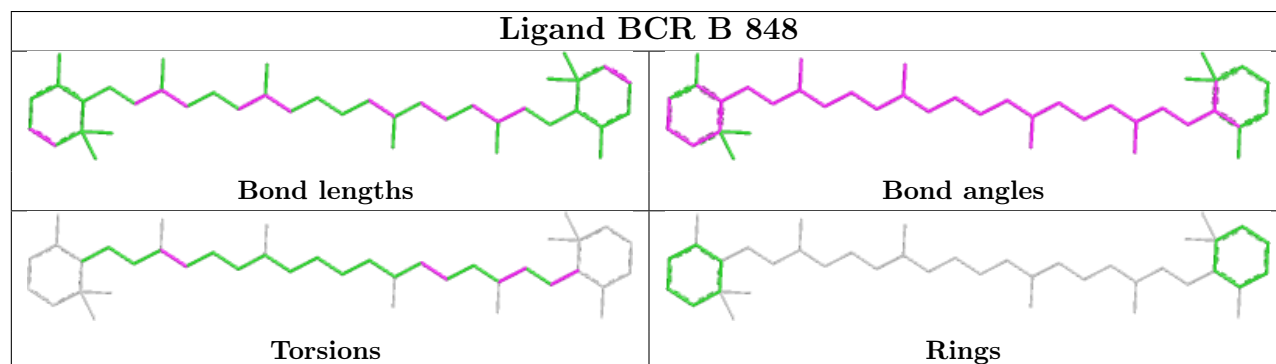
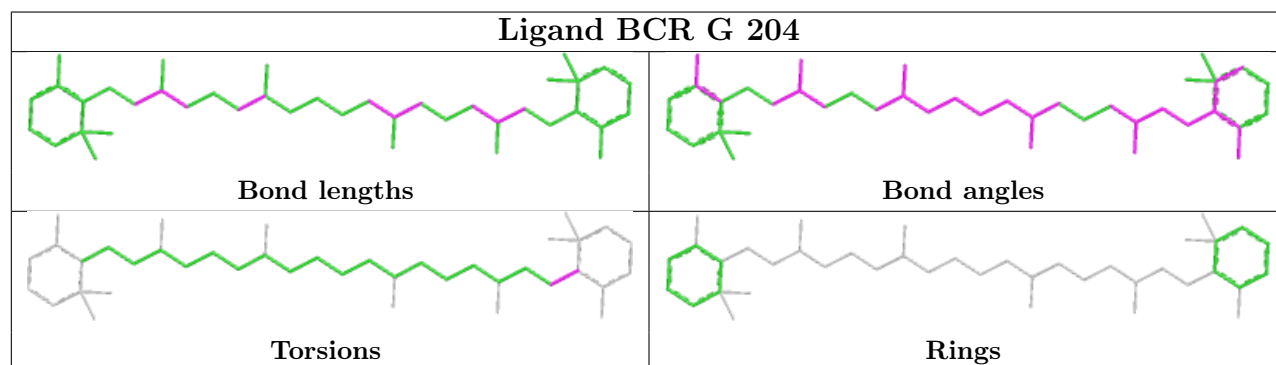
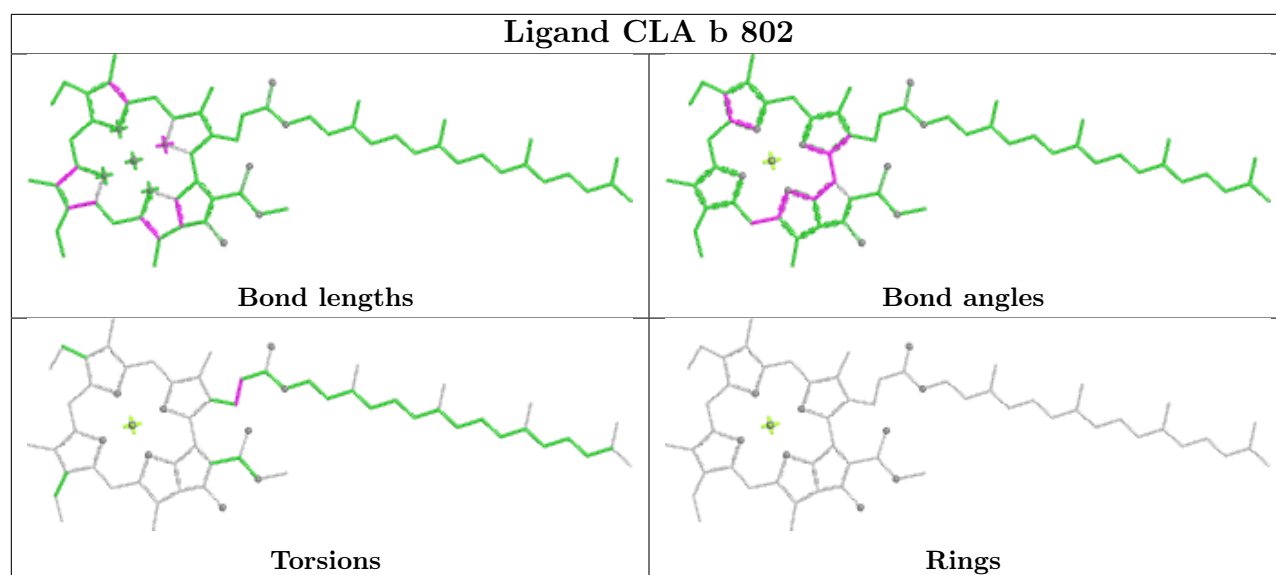




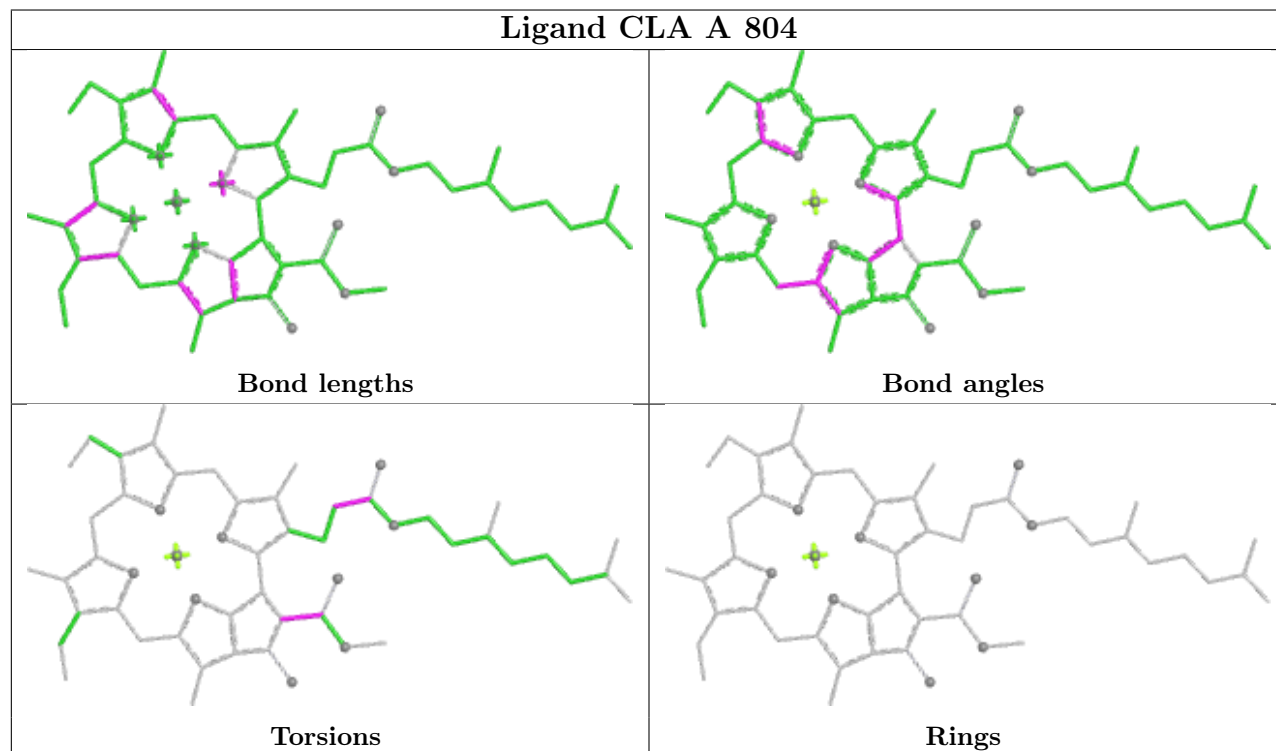
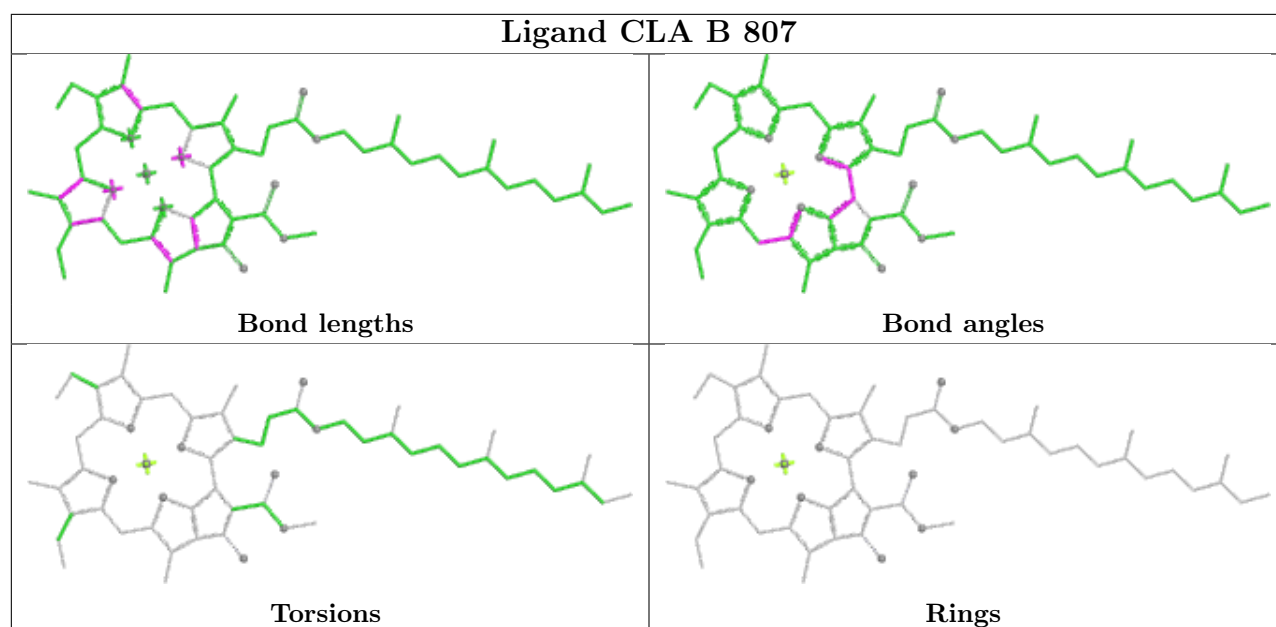


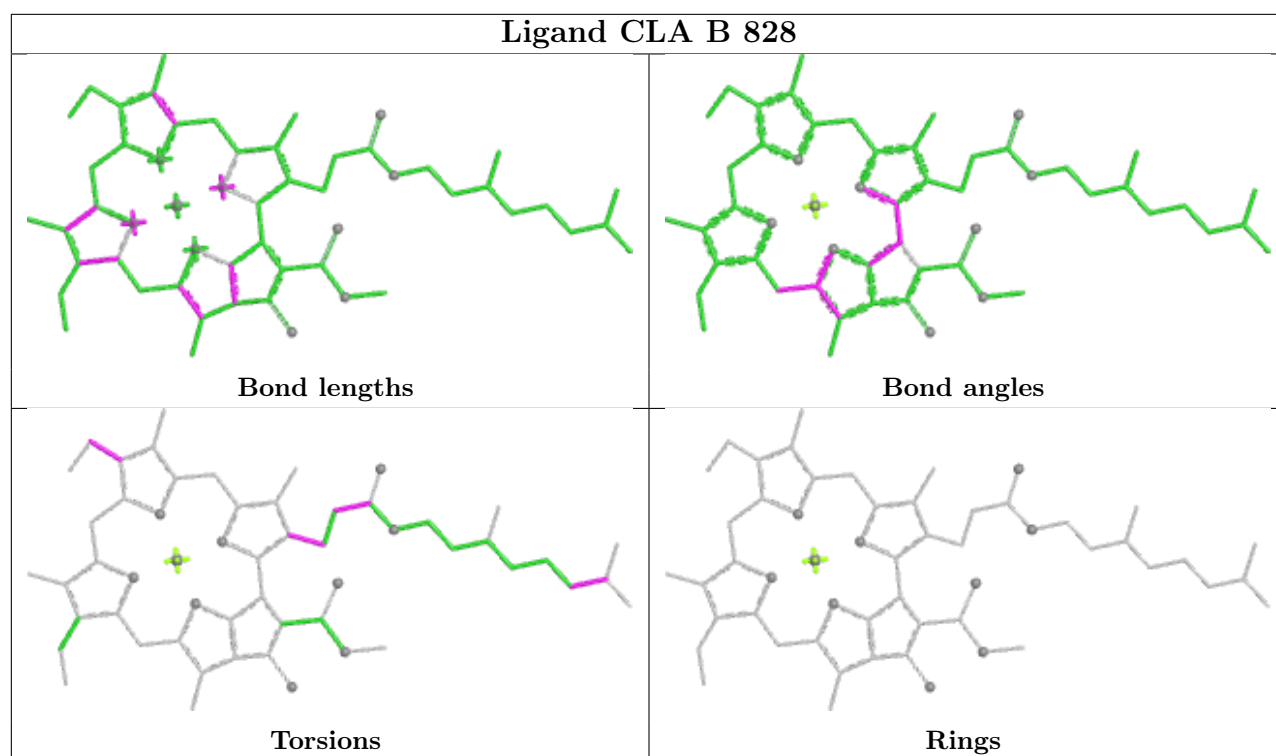




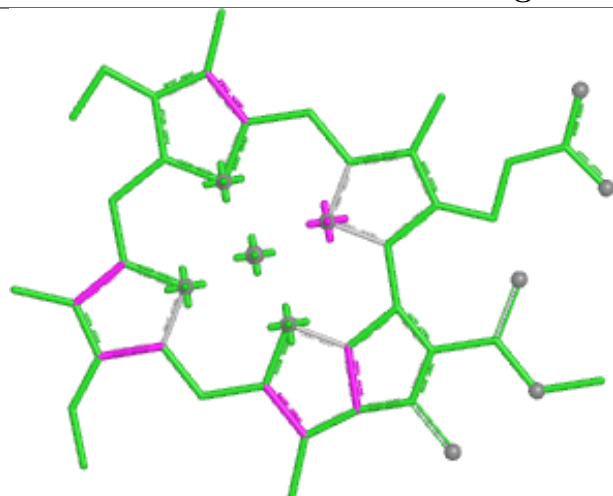




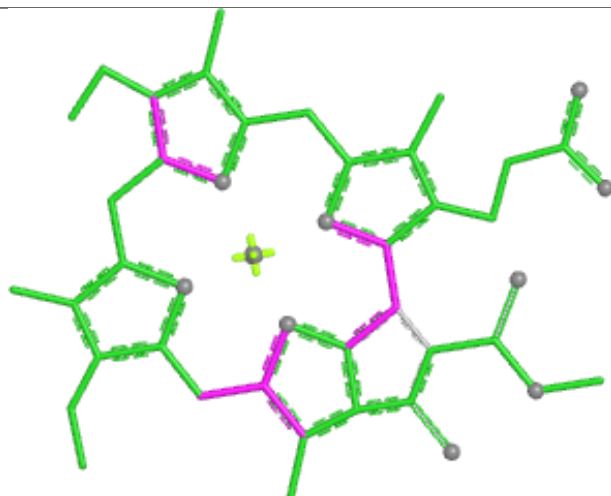




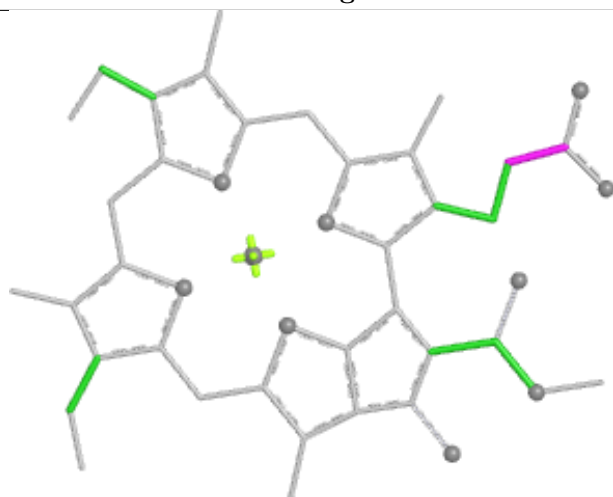
## Ligand CLA B 829



Bond lengths



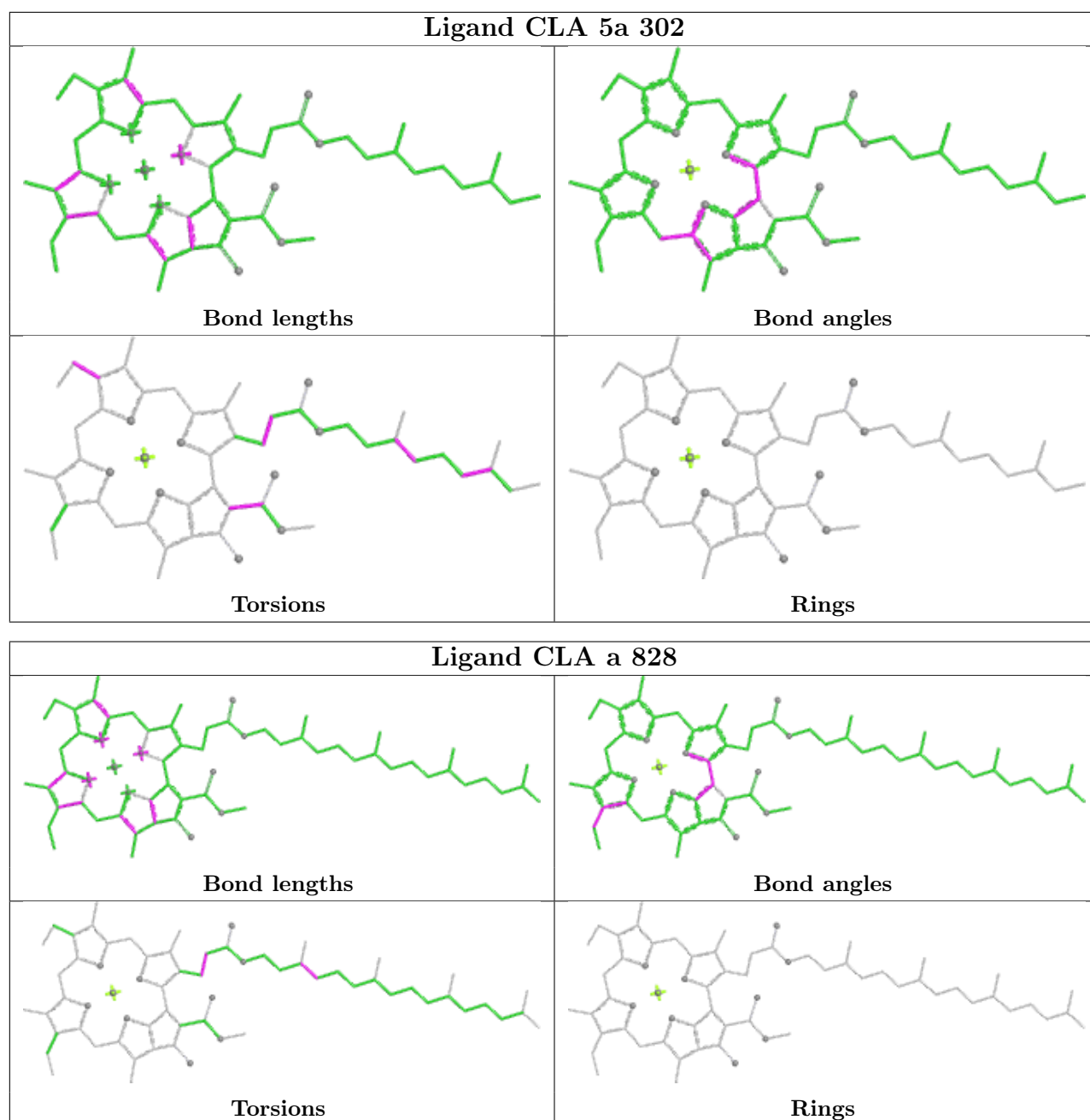
Bond angles

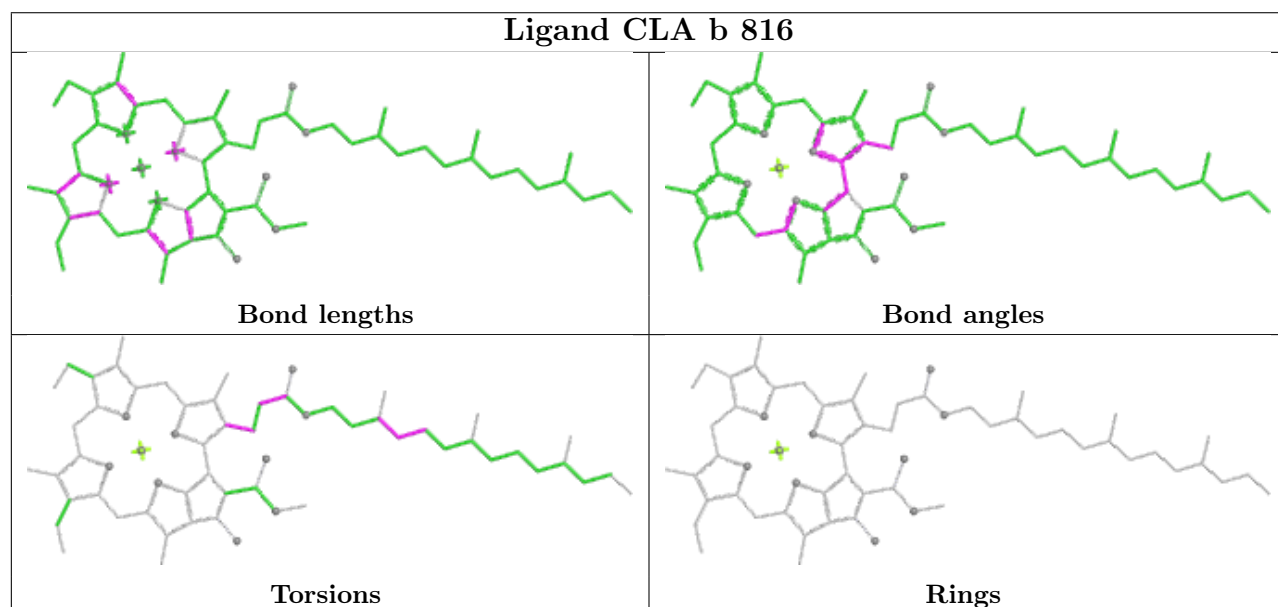
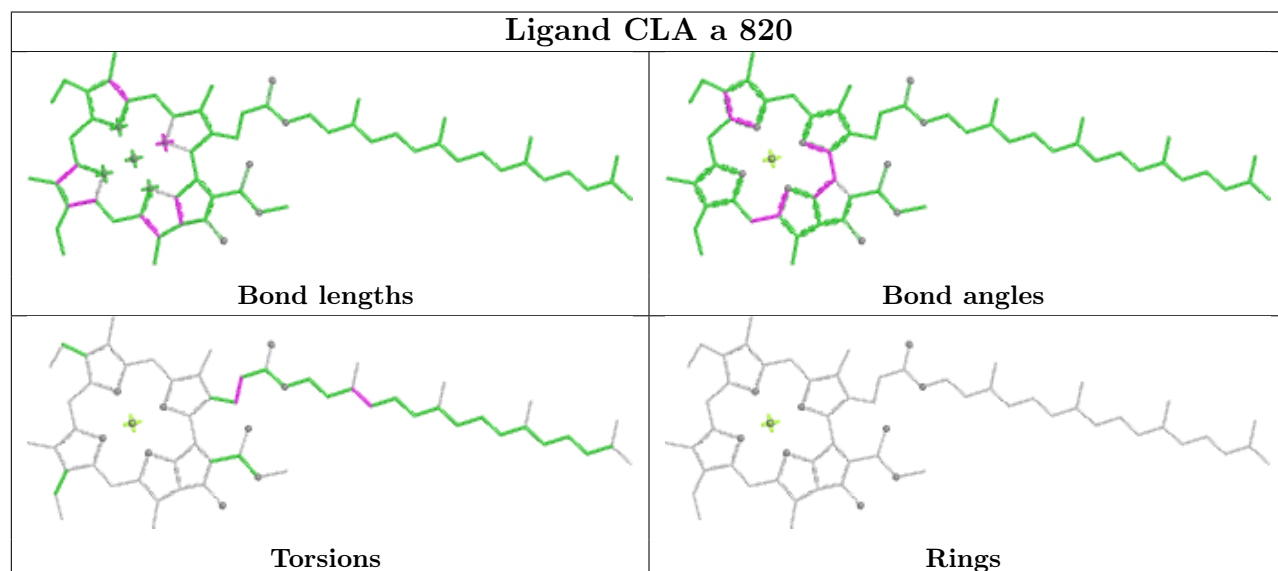
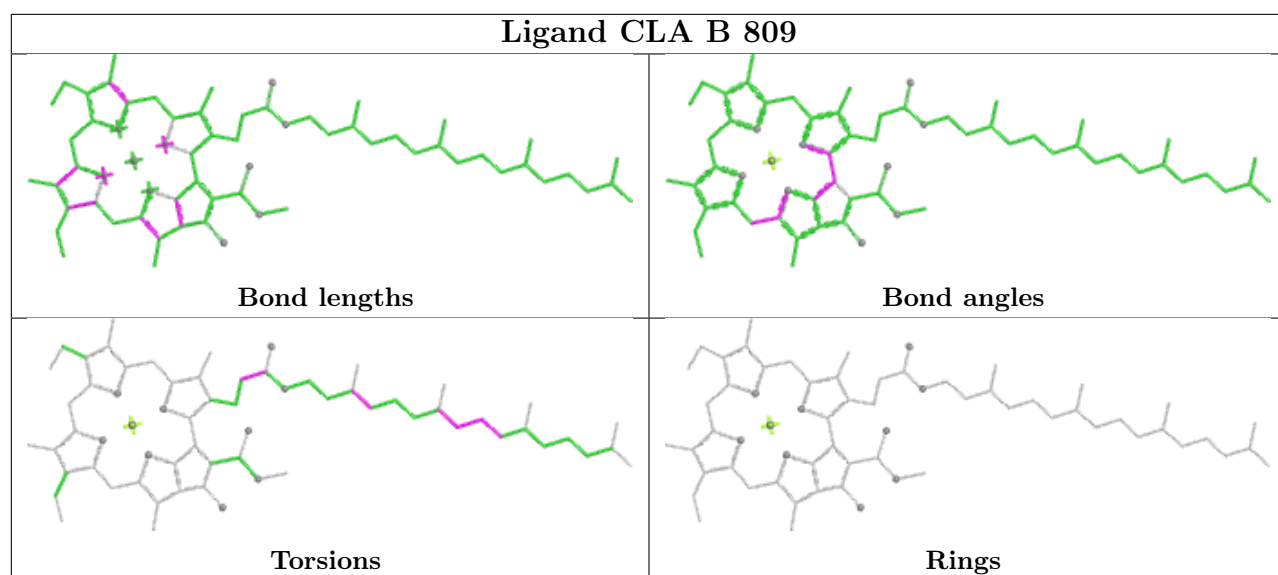


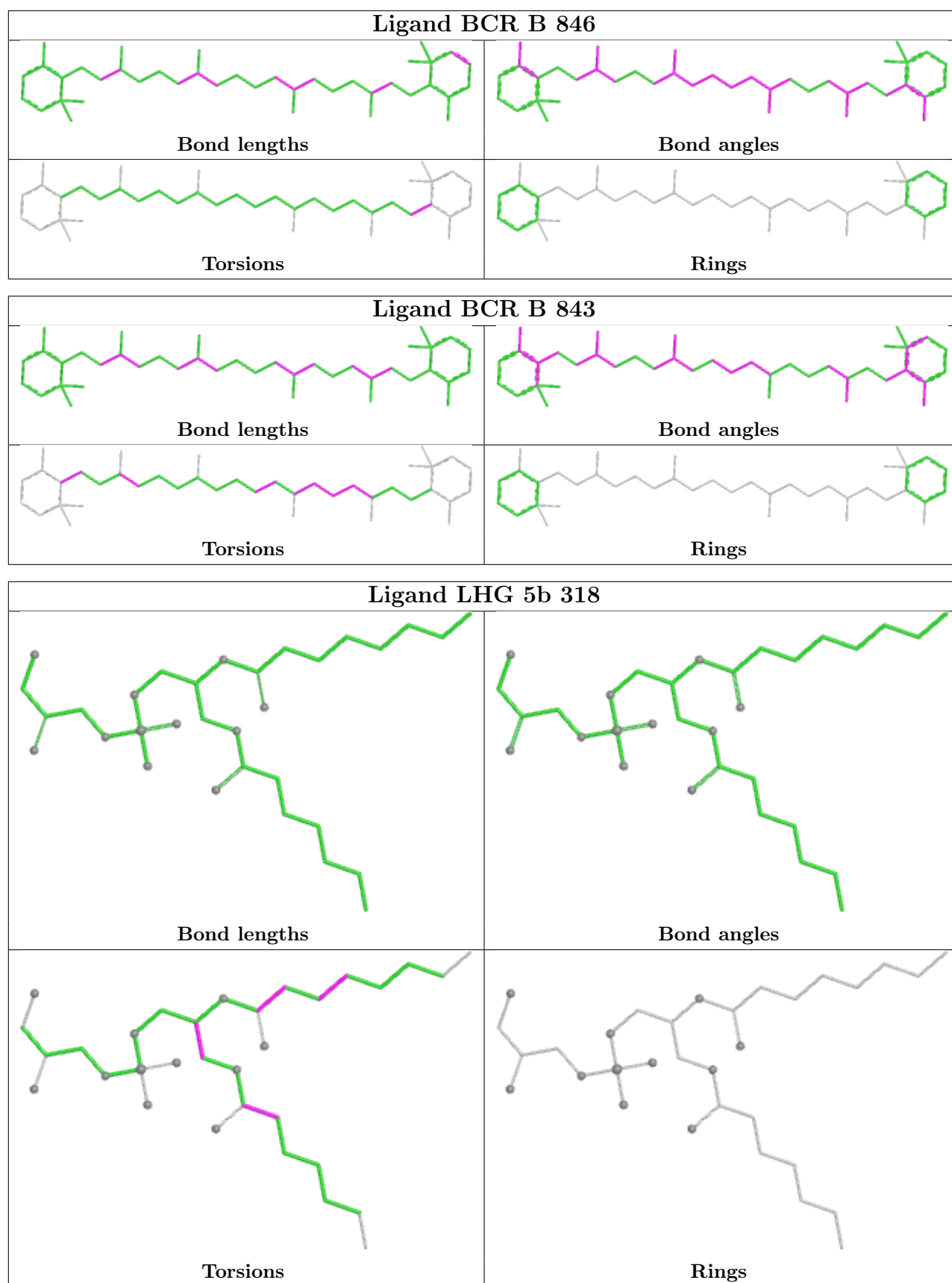
Torsions

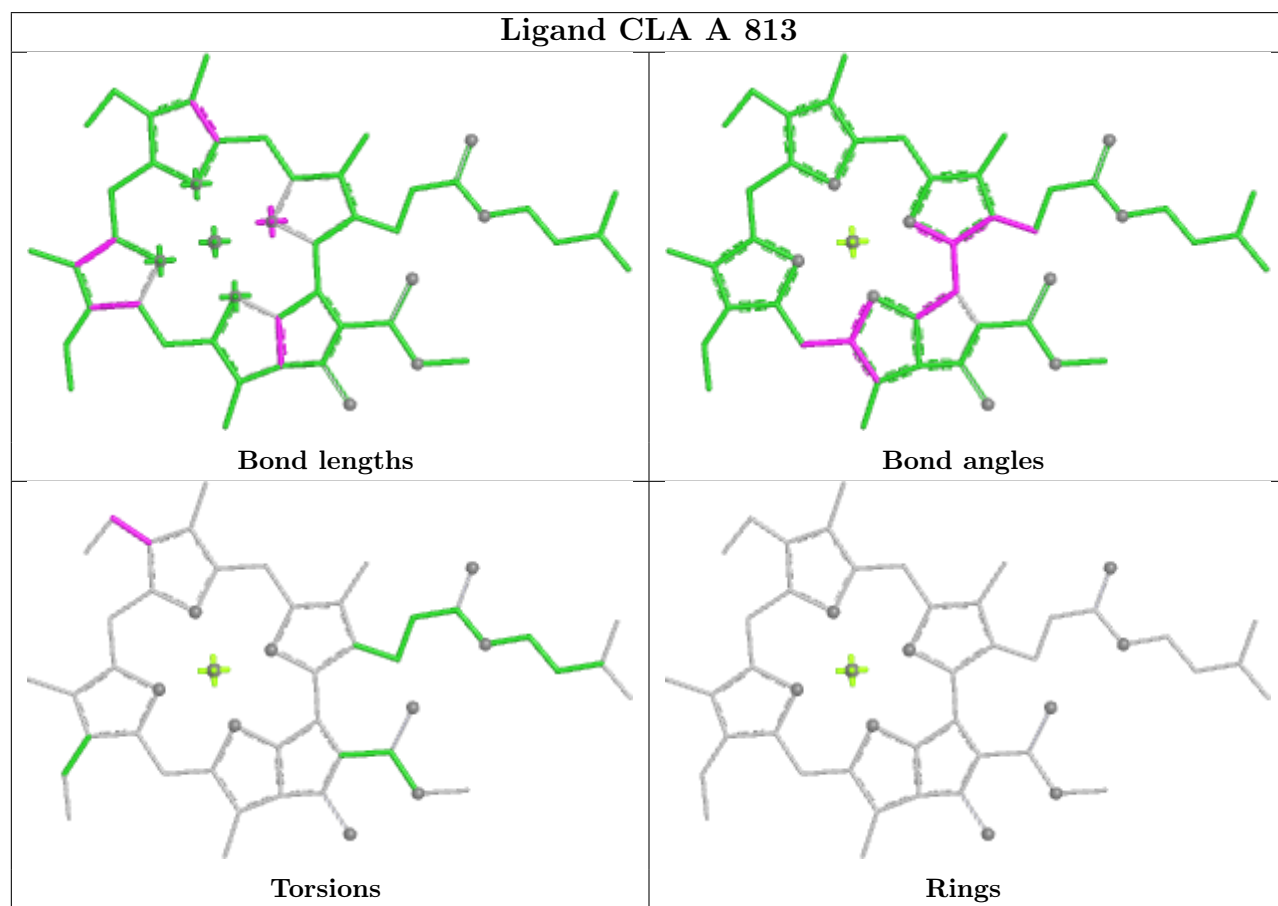
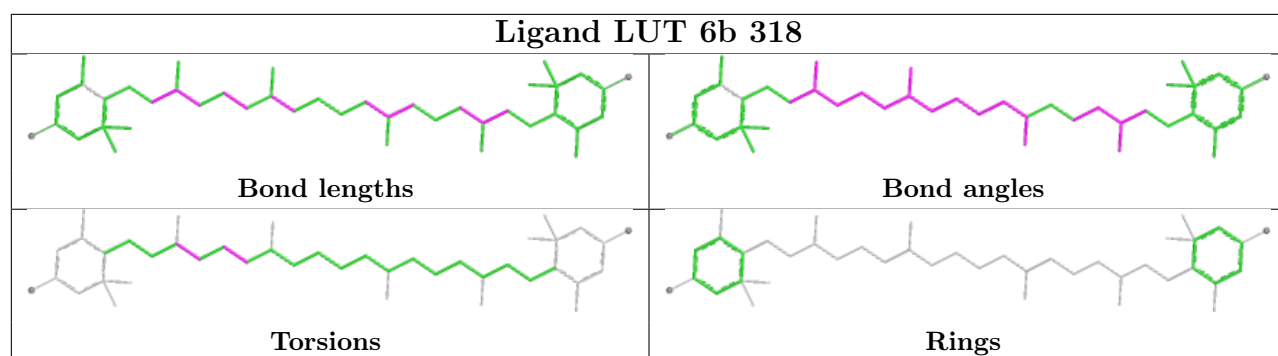


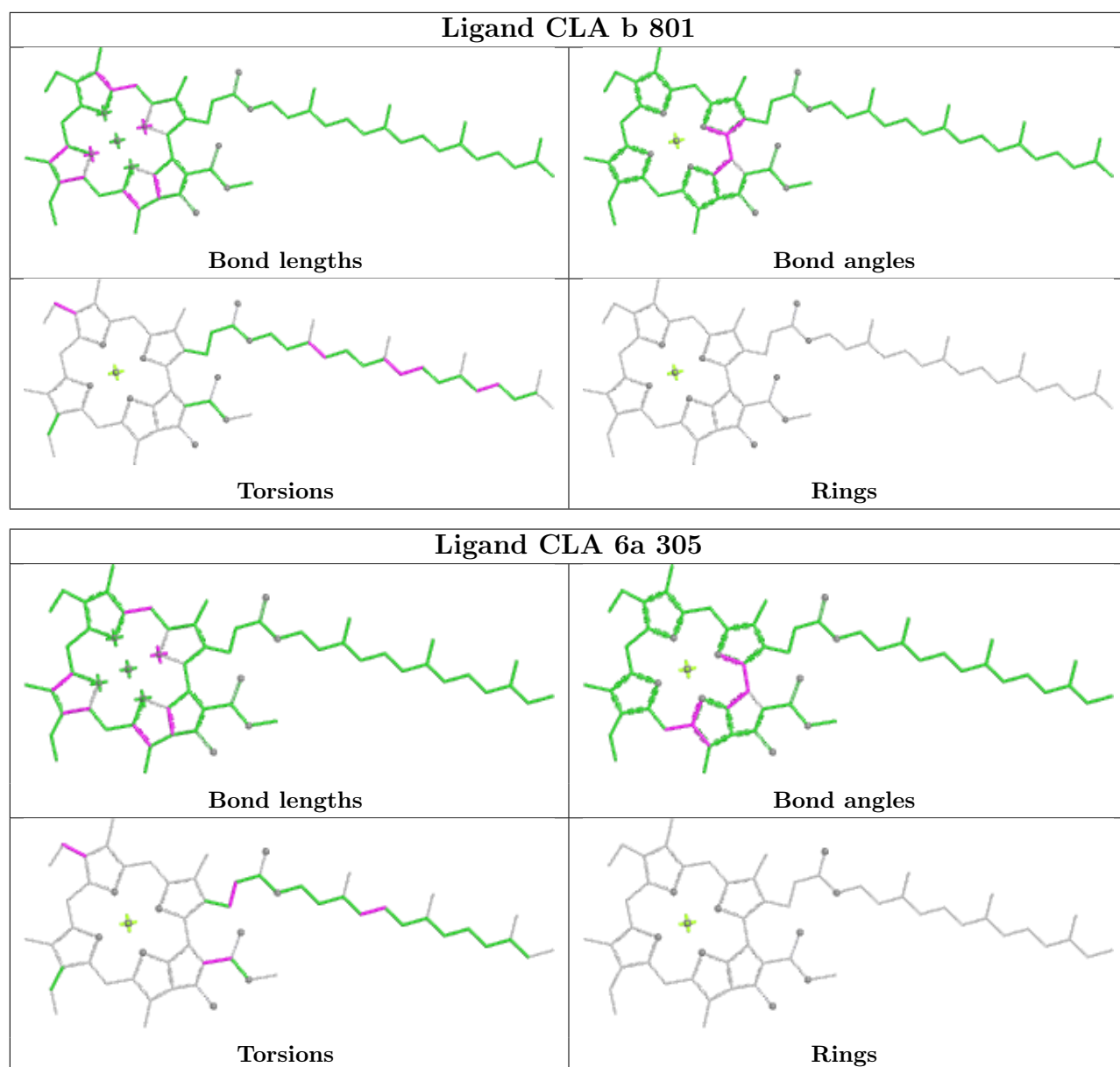
Rings



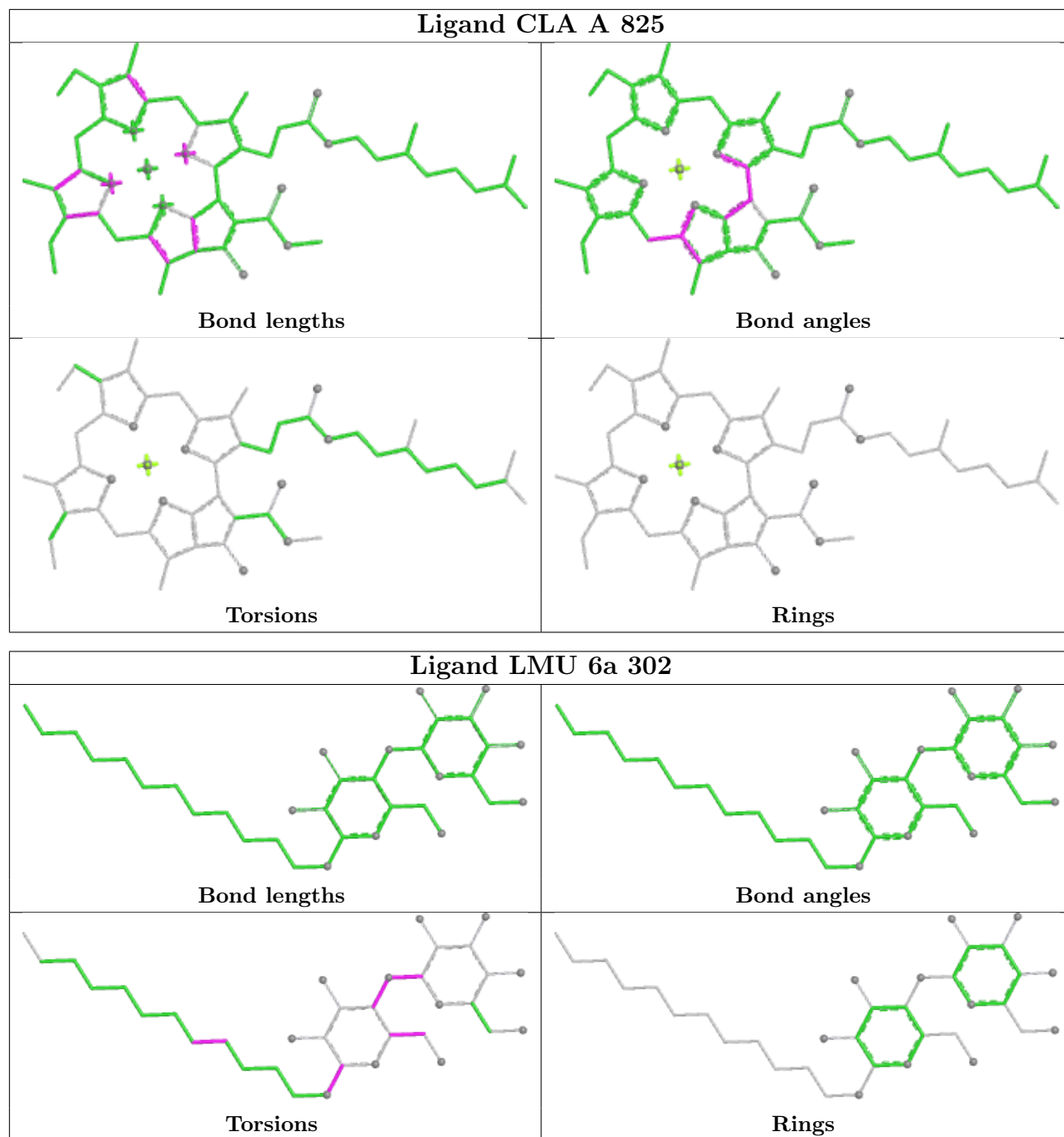


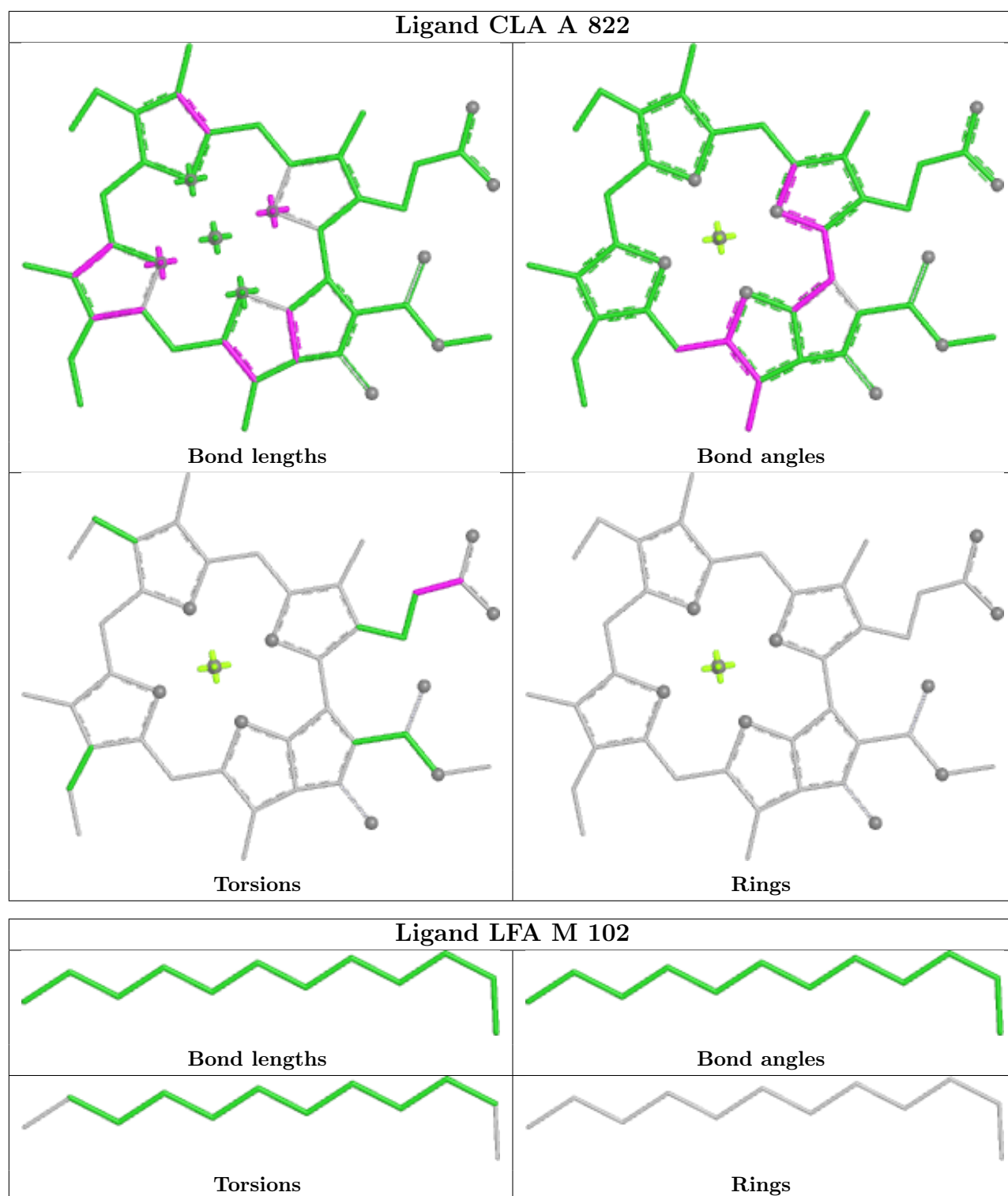




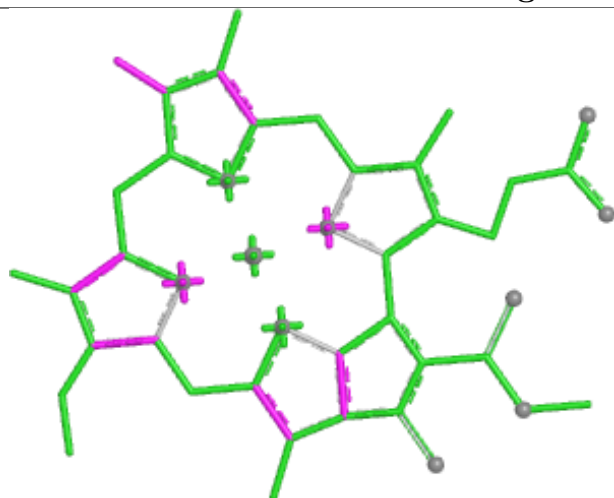




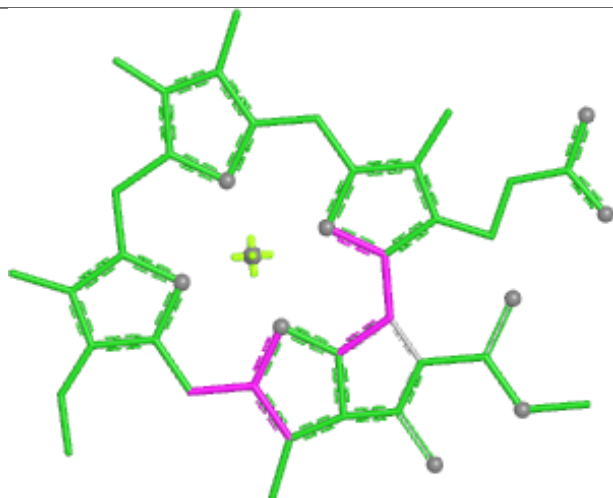




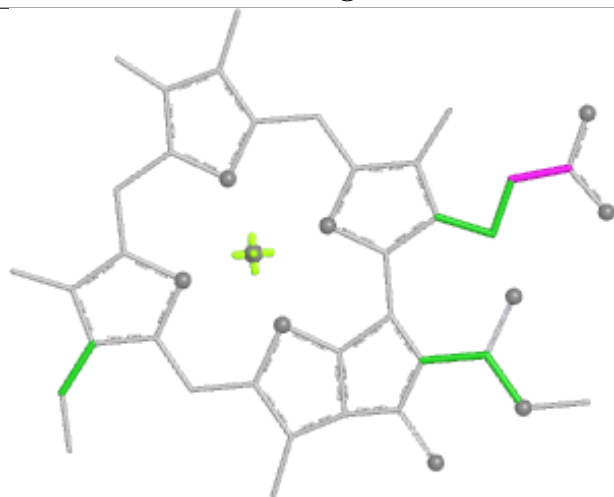
## Ligand CLA k 201



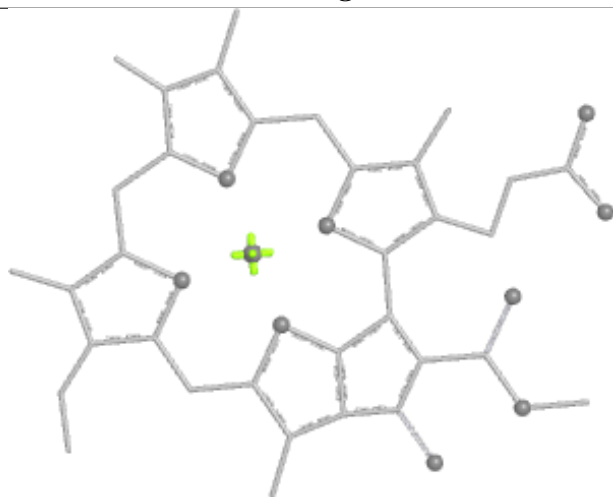
Bond lengths



Bond angles

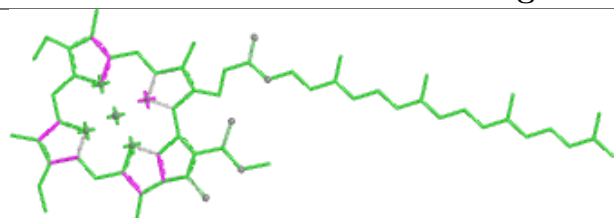


Torsions

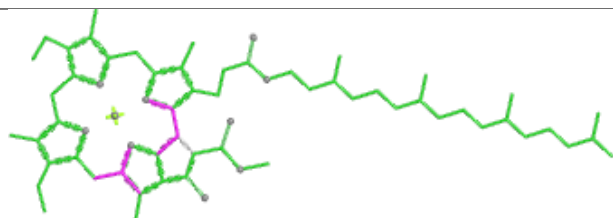


Rings

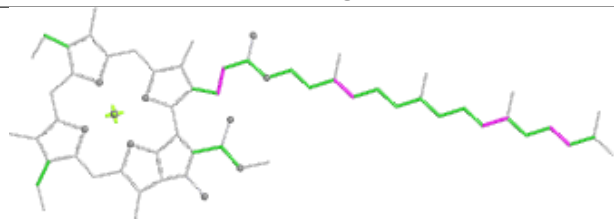
## Ligand CLA b 817



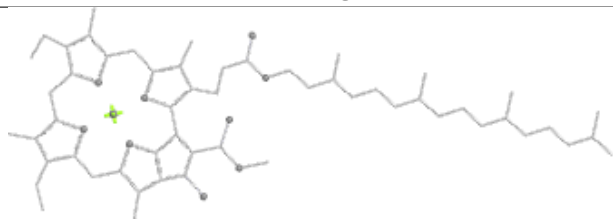
Bond lengths



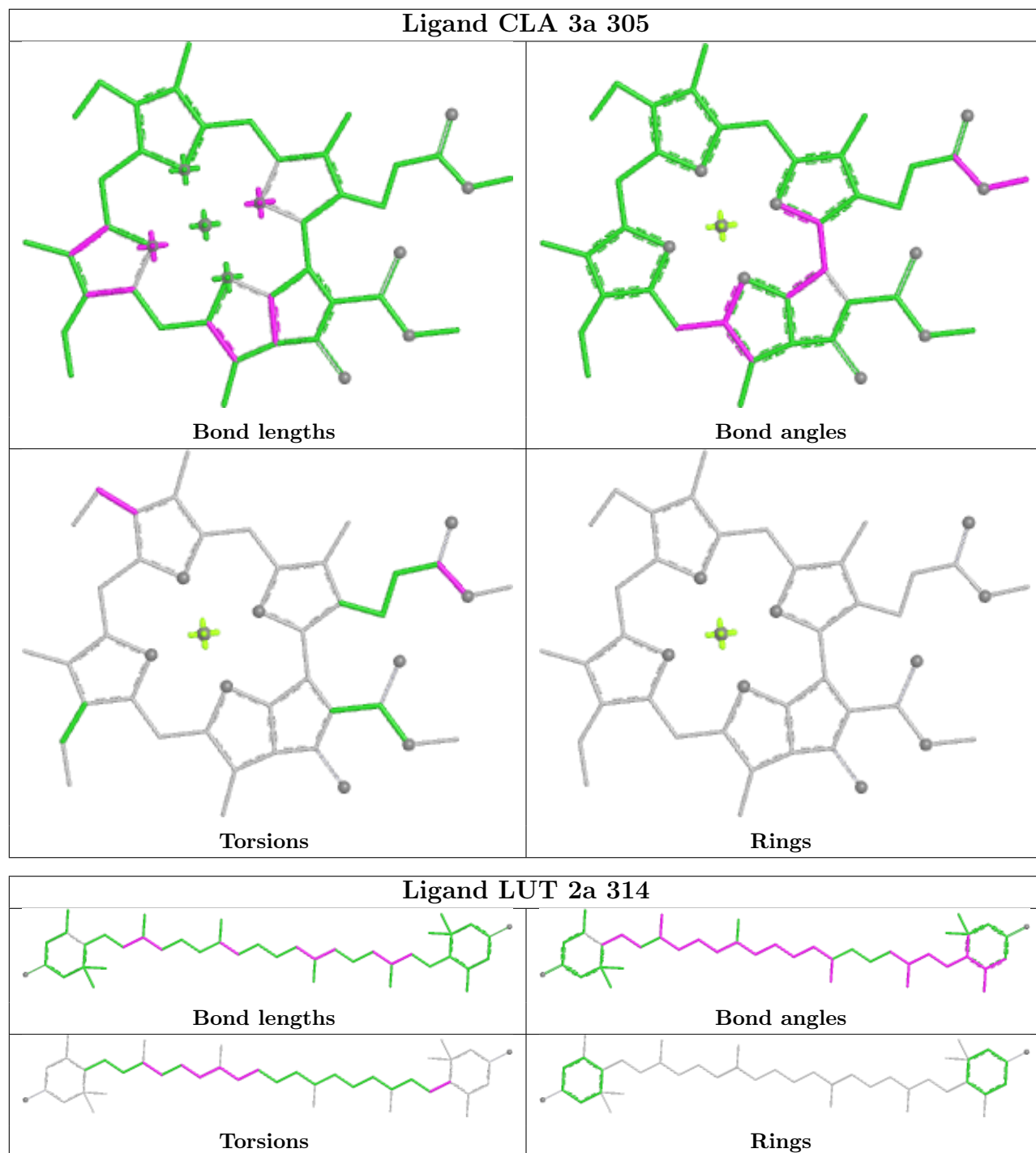
Bond angles

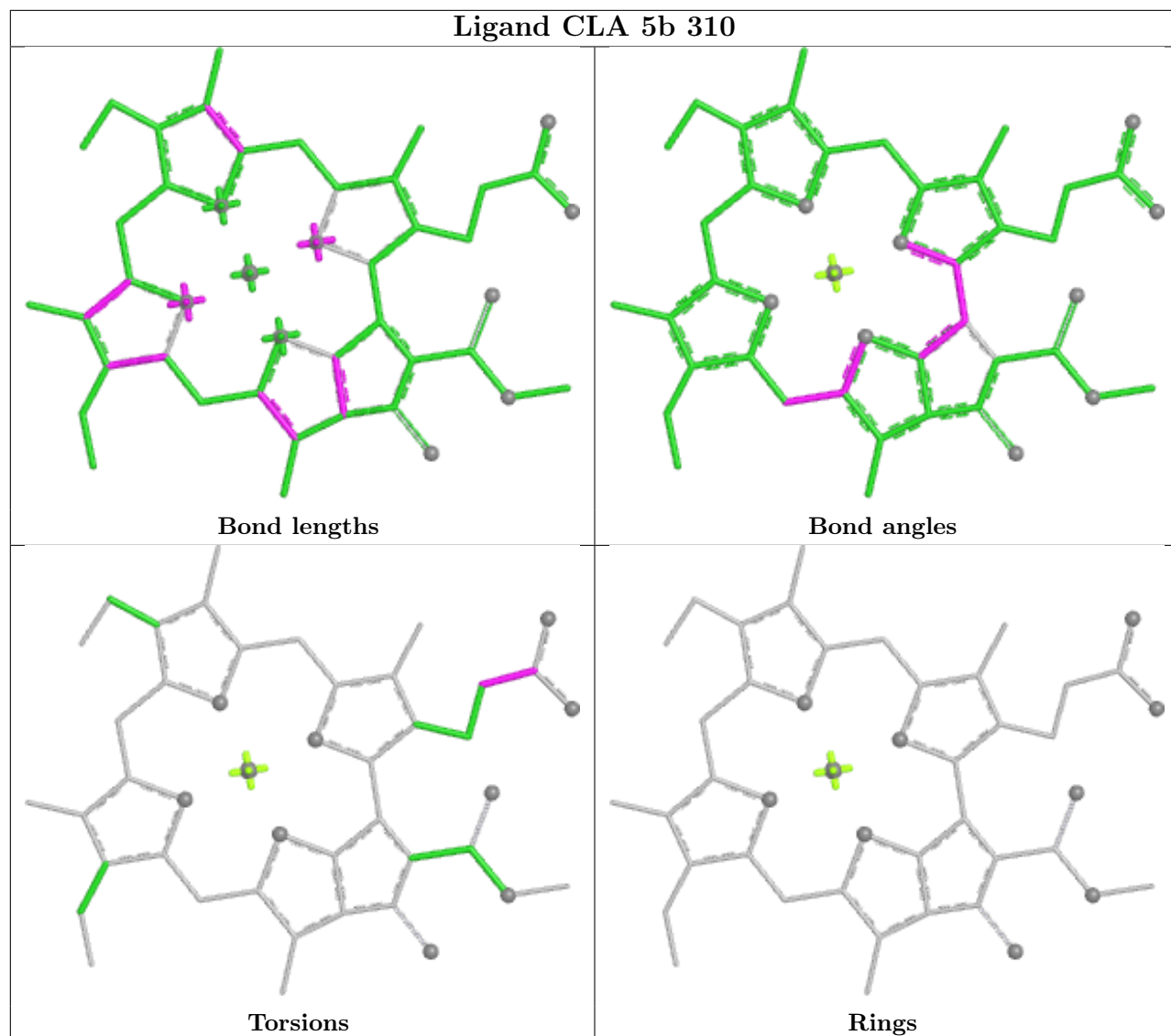


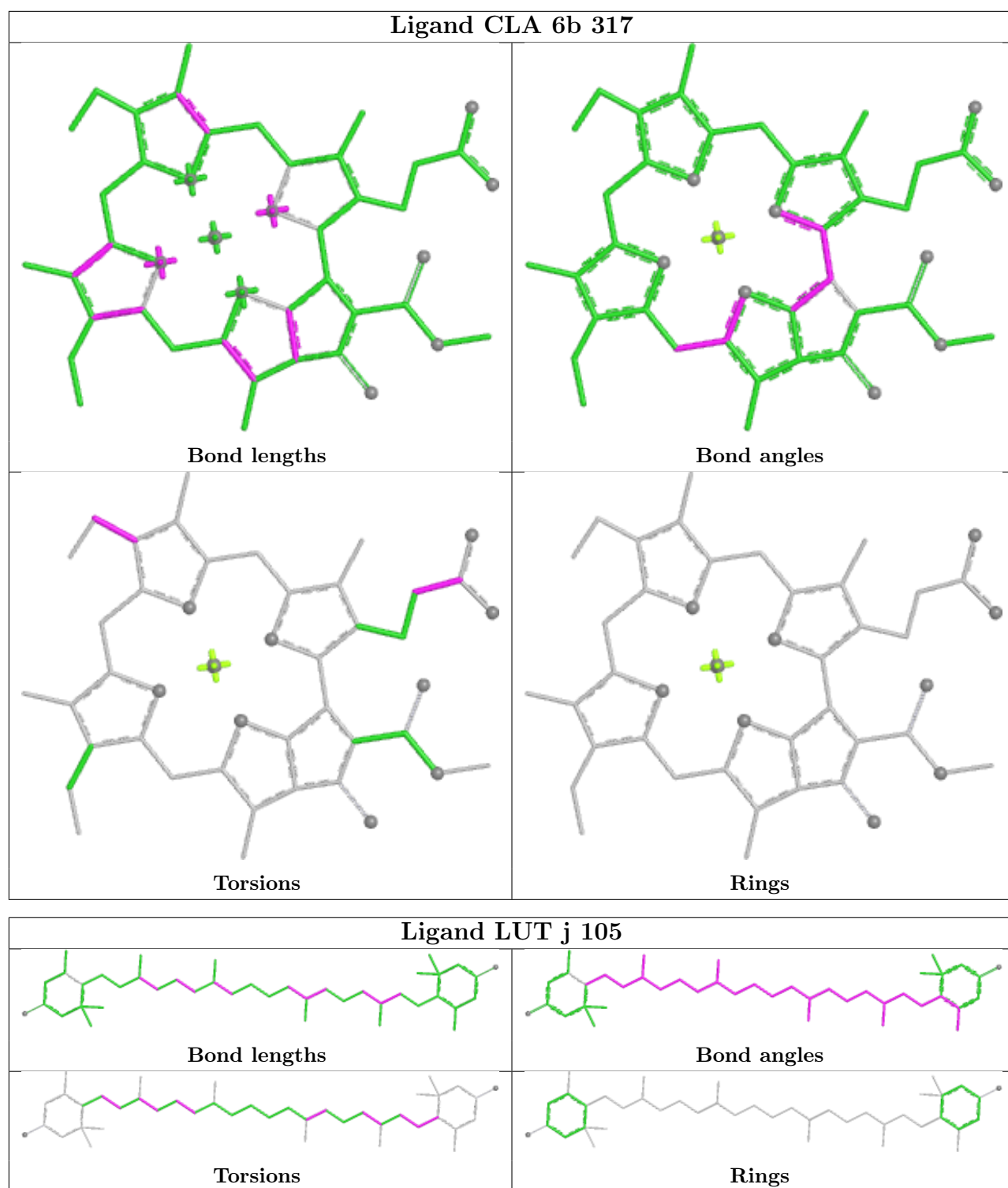
Torsions



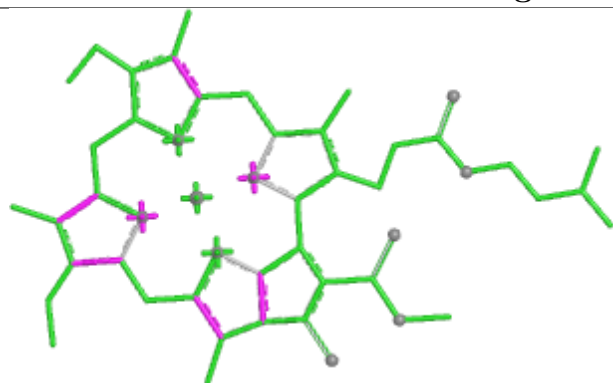
Rings



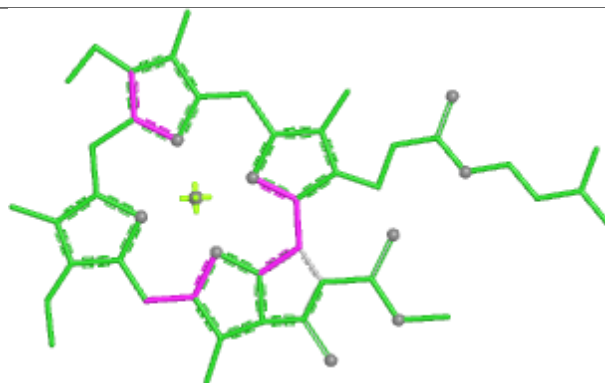




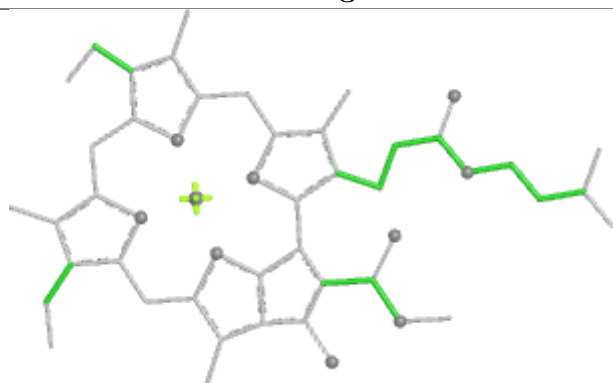
## Ligand CLA B 835



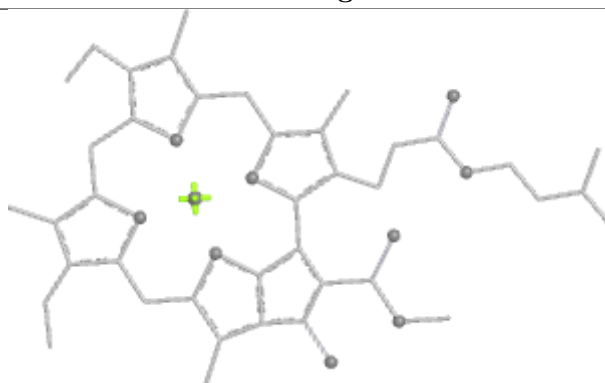
Bond lengths



Bond angles

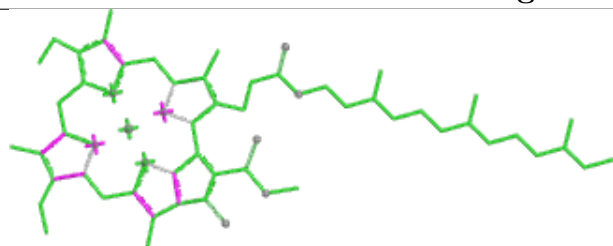


Torsions

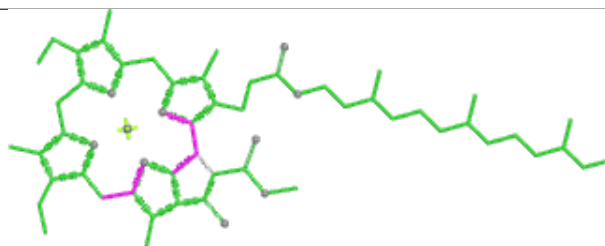


Rings

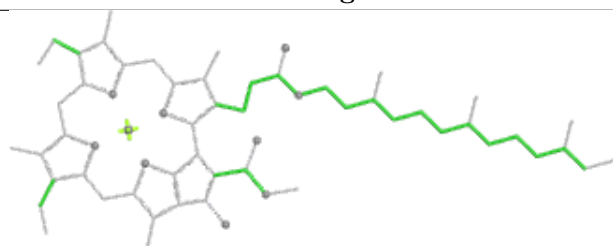
## Ligand CLA b 807



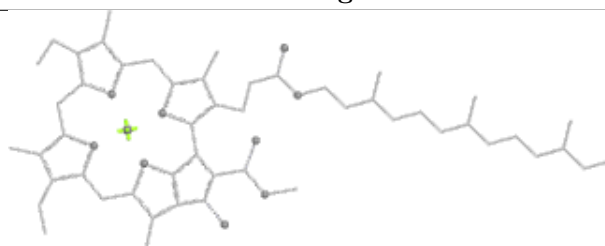
Bond lengths



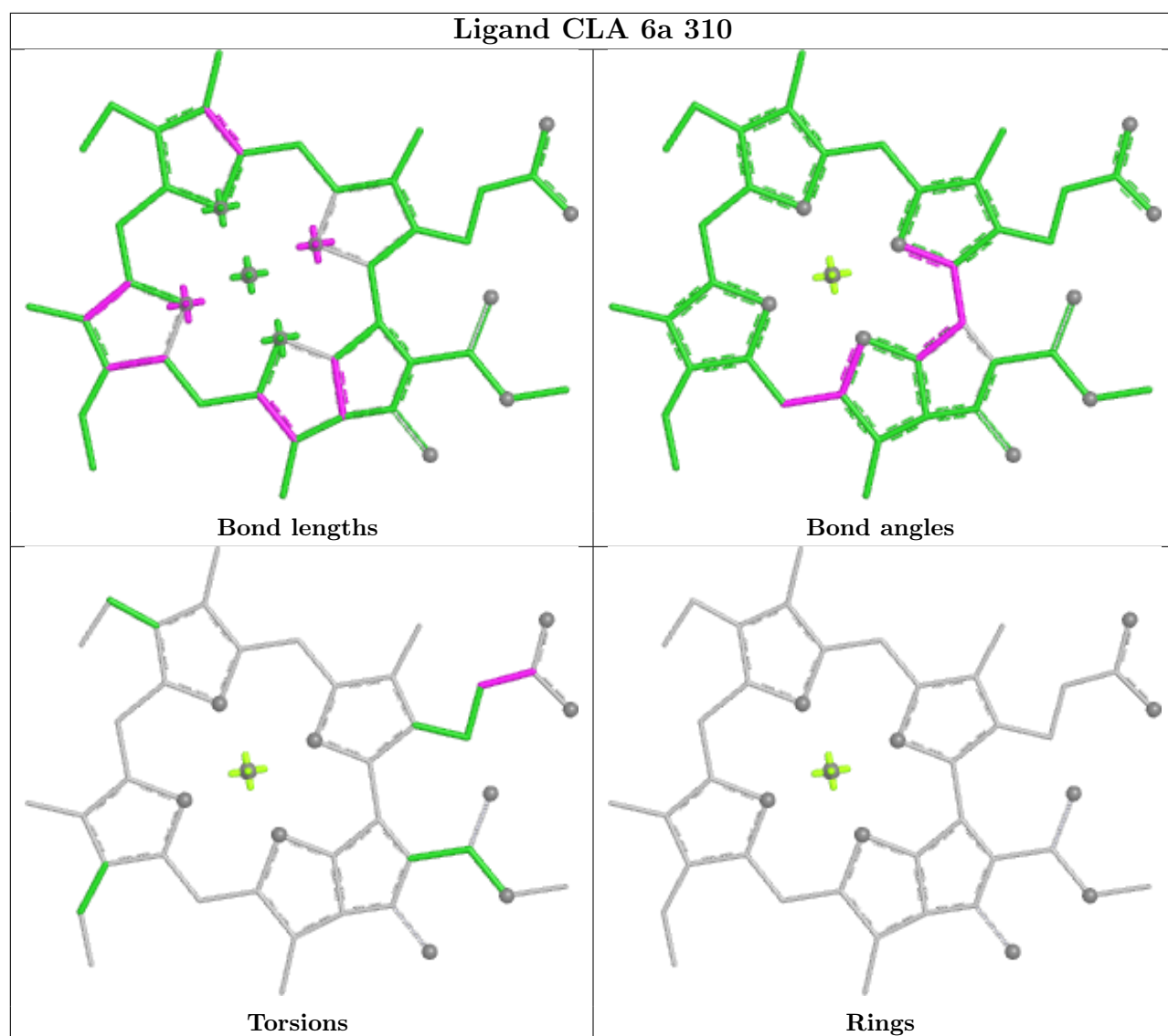
Bond angles



Torsions

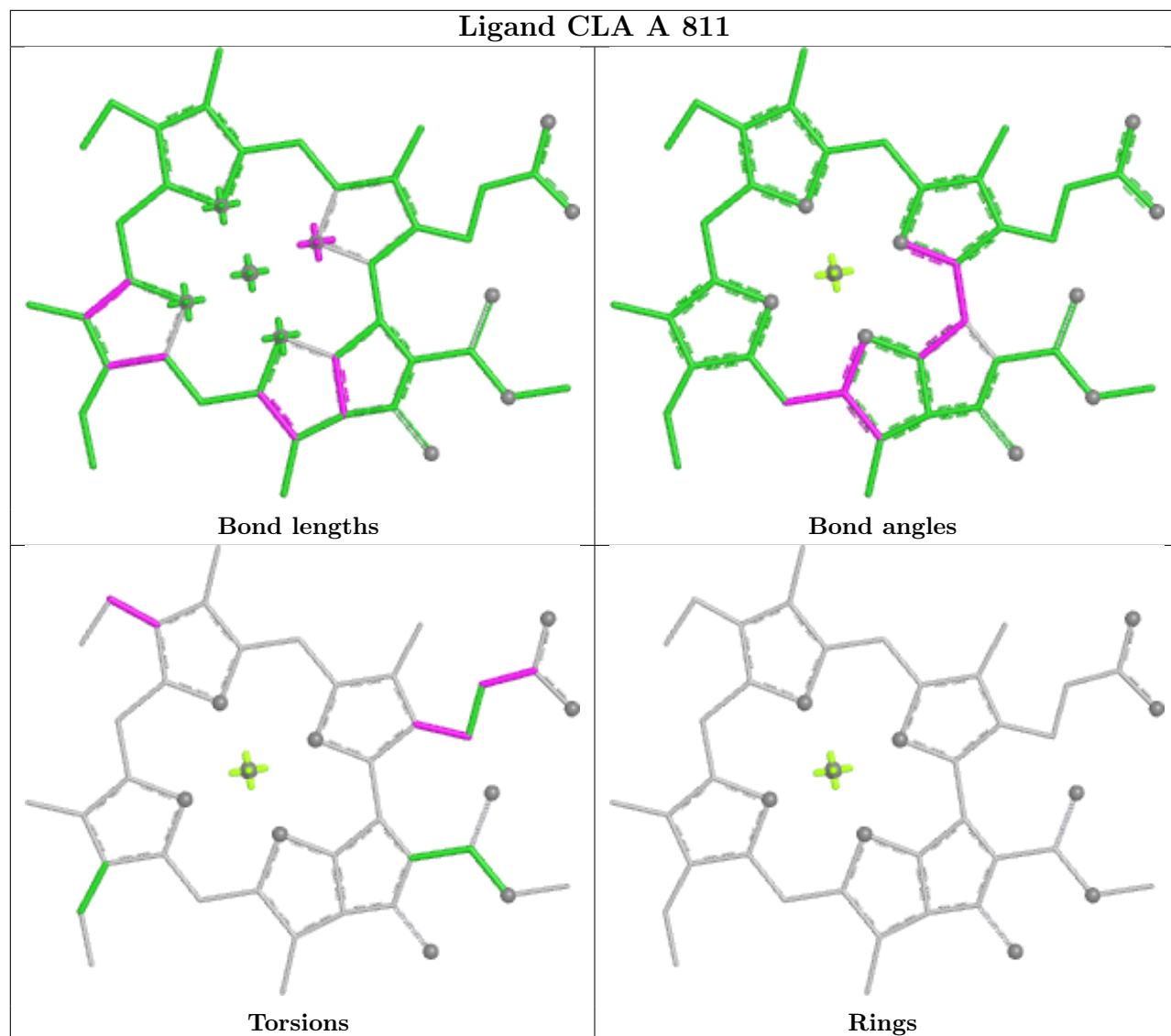


Rings

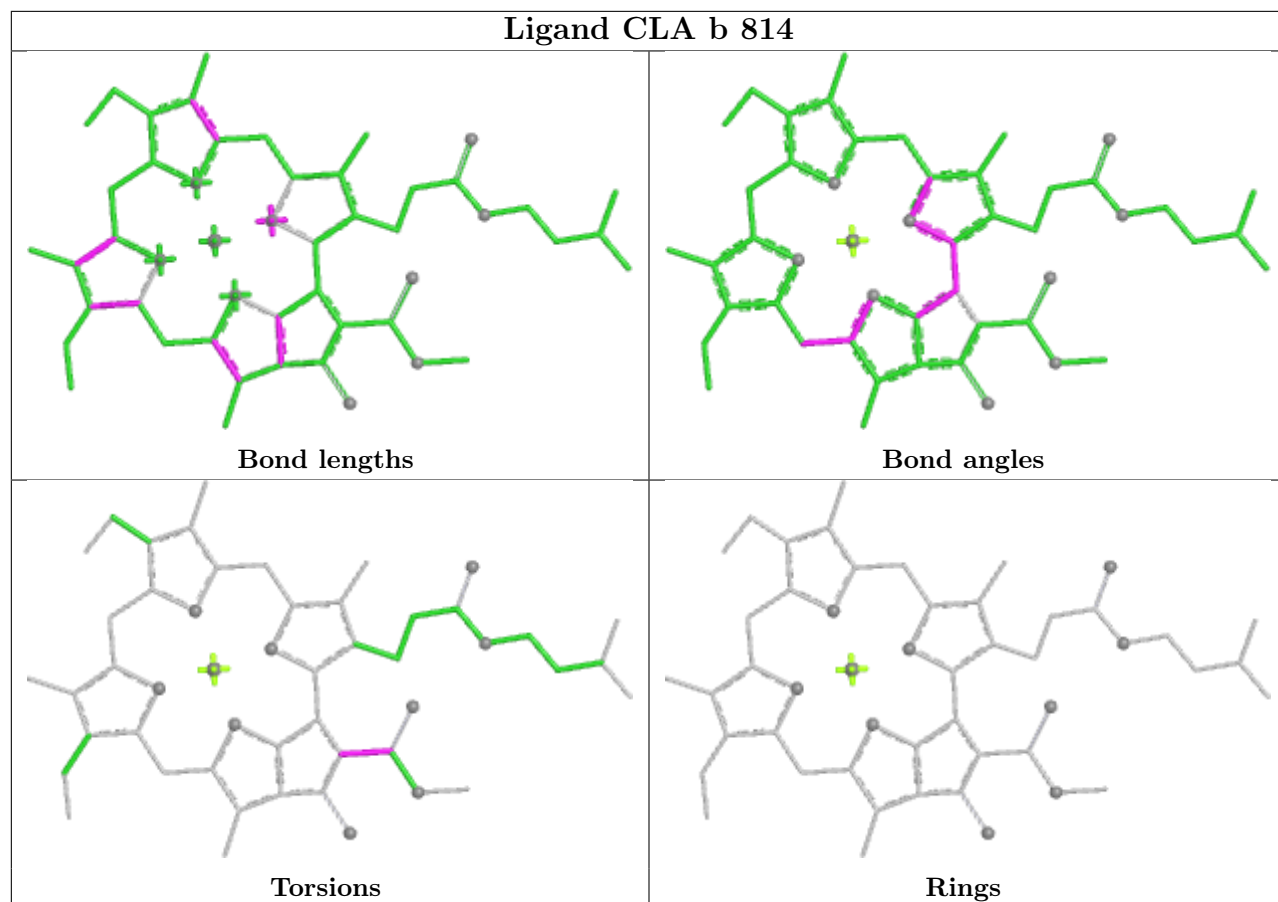


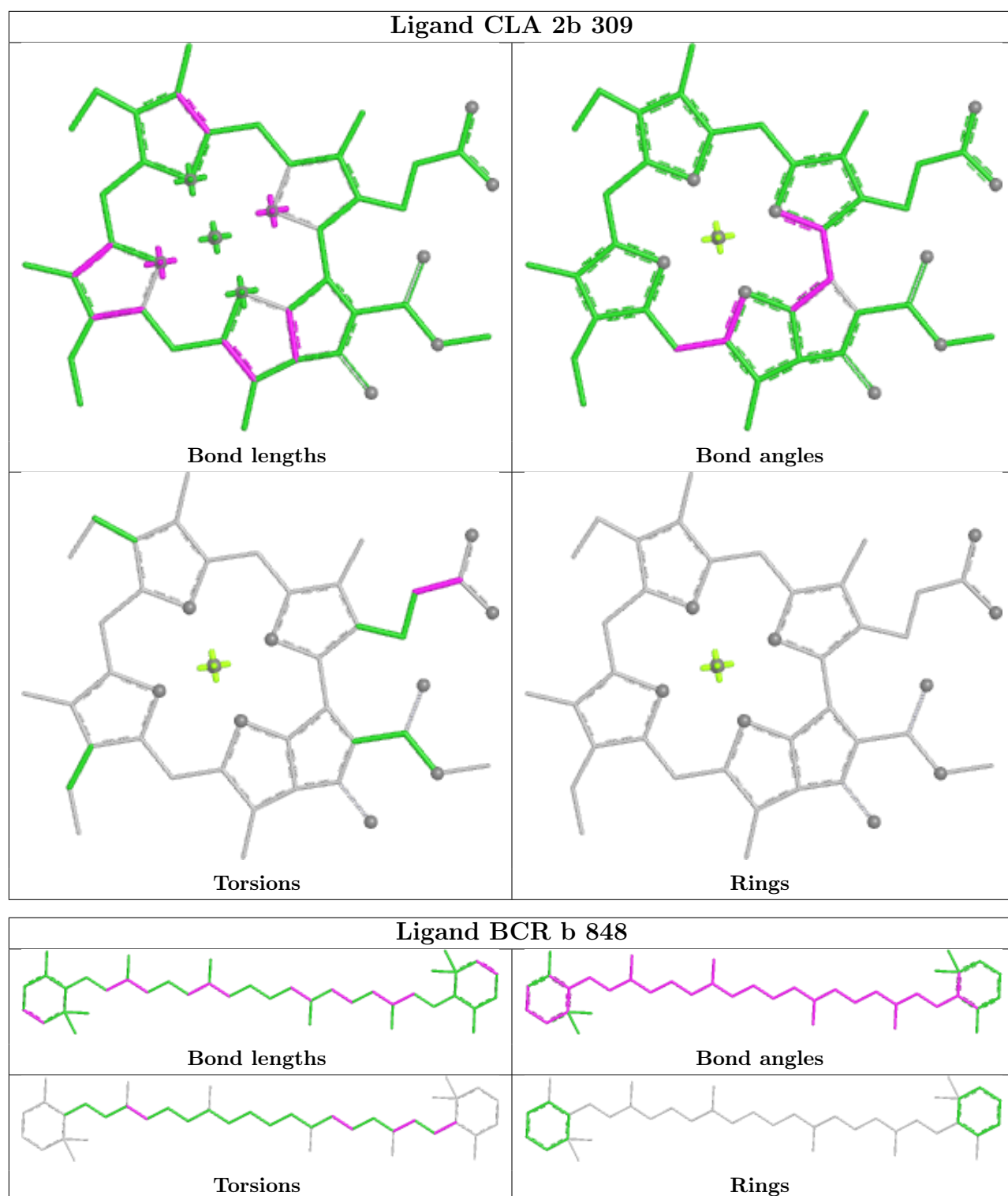


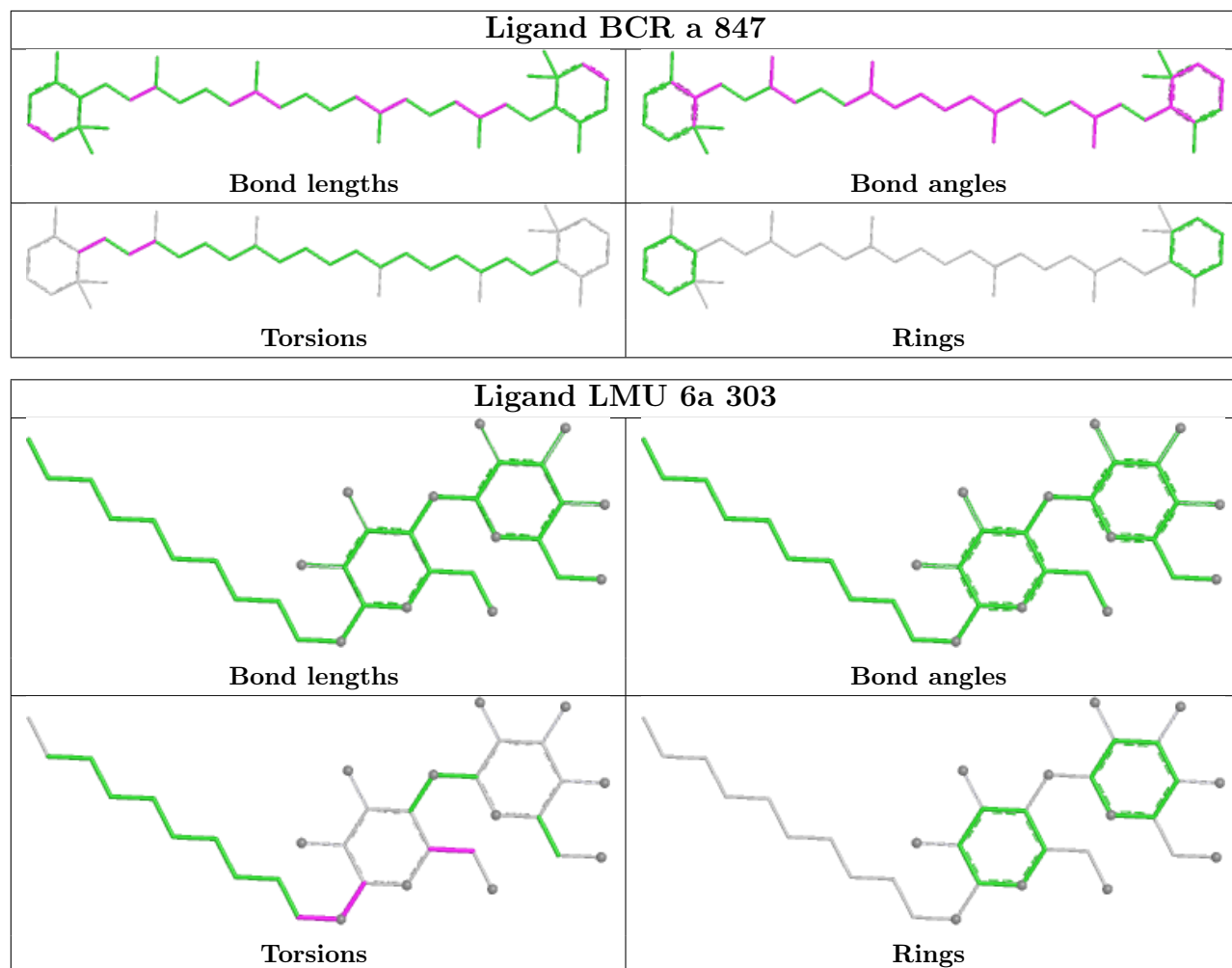
## Ligand CLA A 811

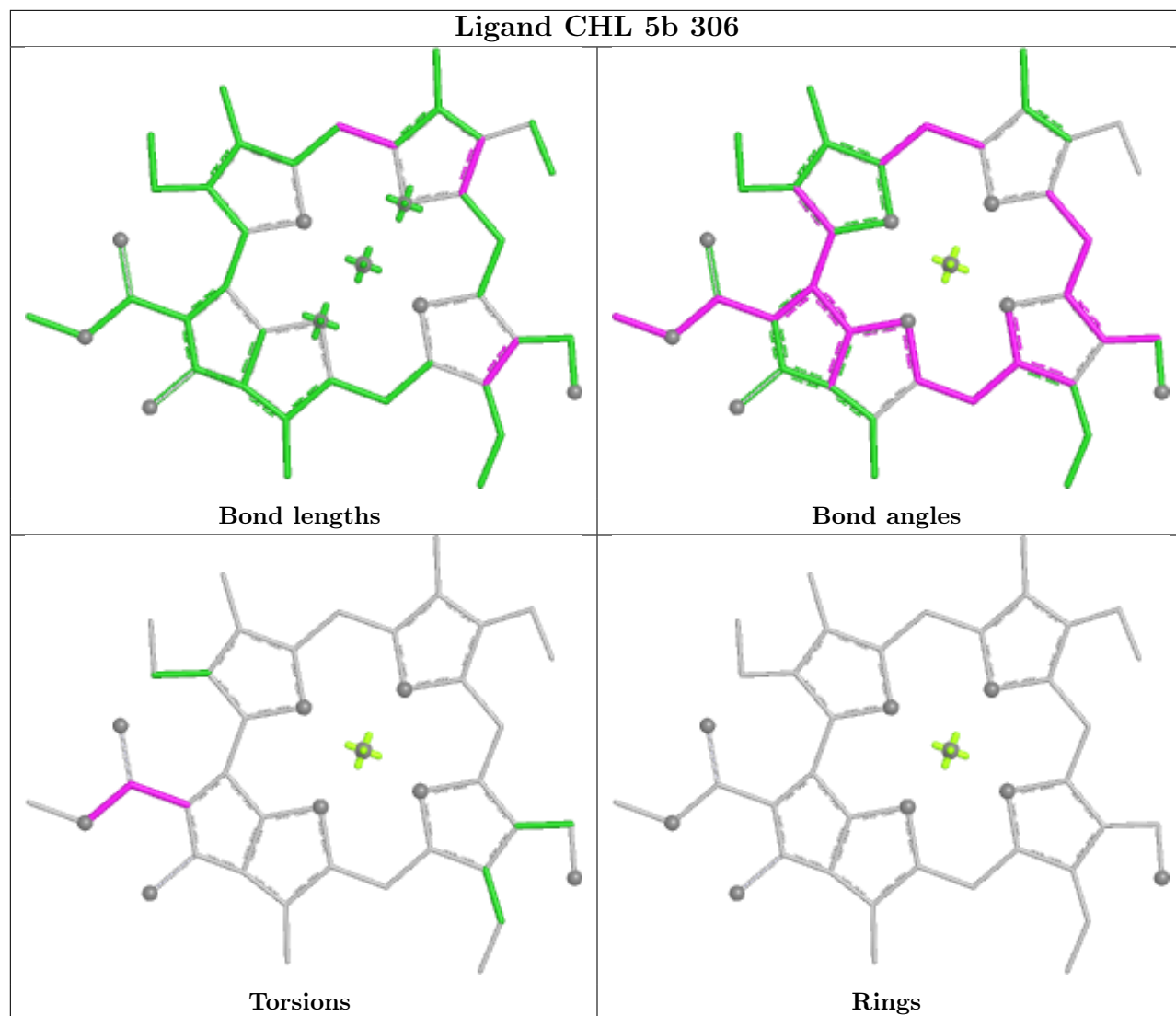


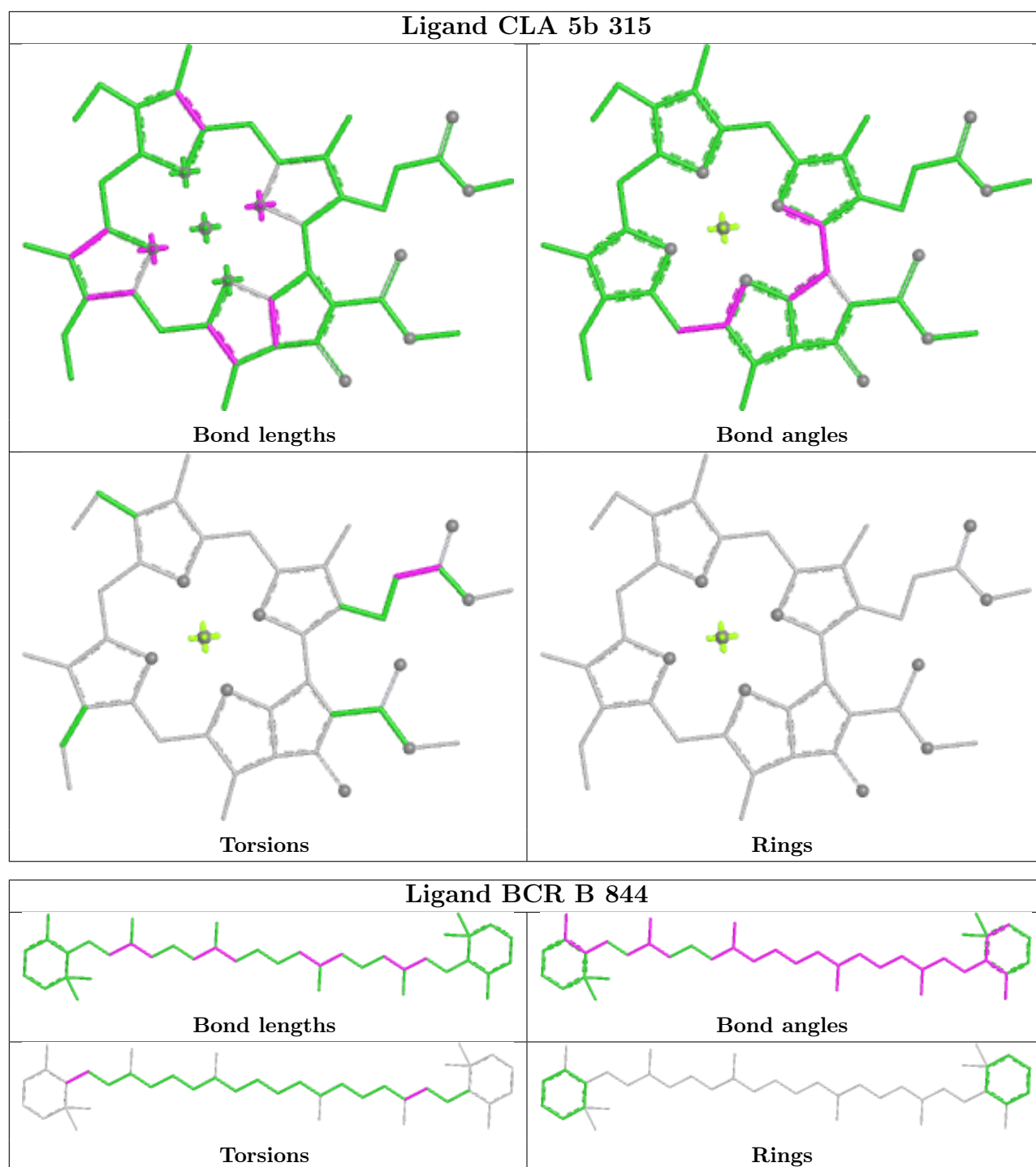
## Ligand CLA b 814



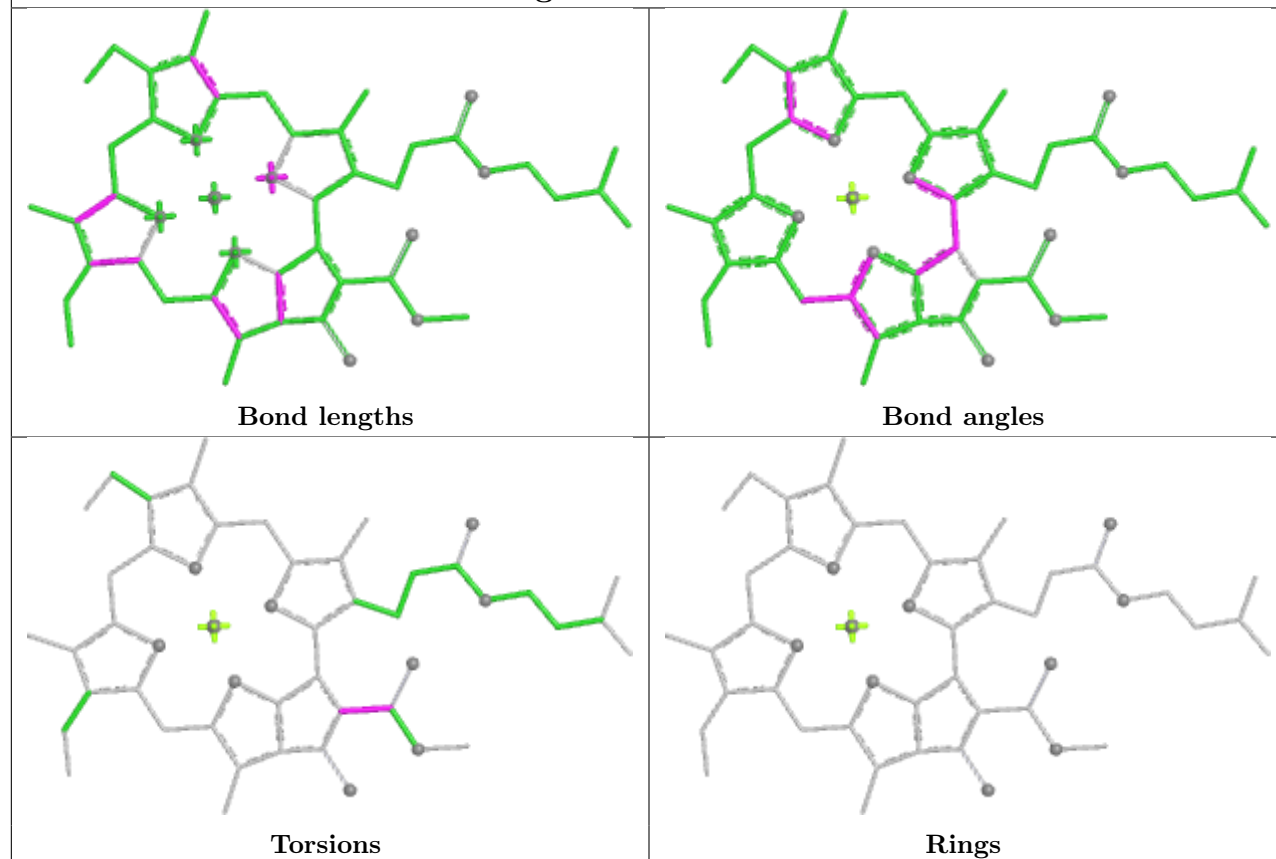




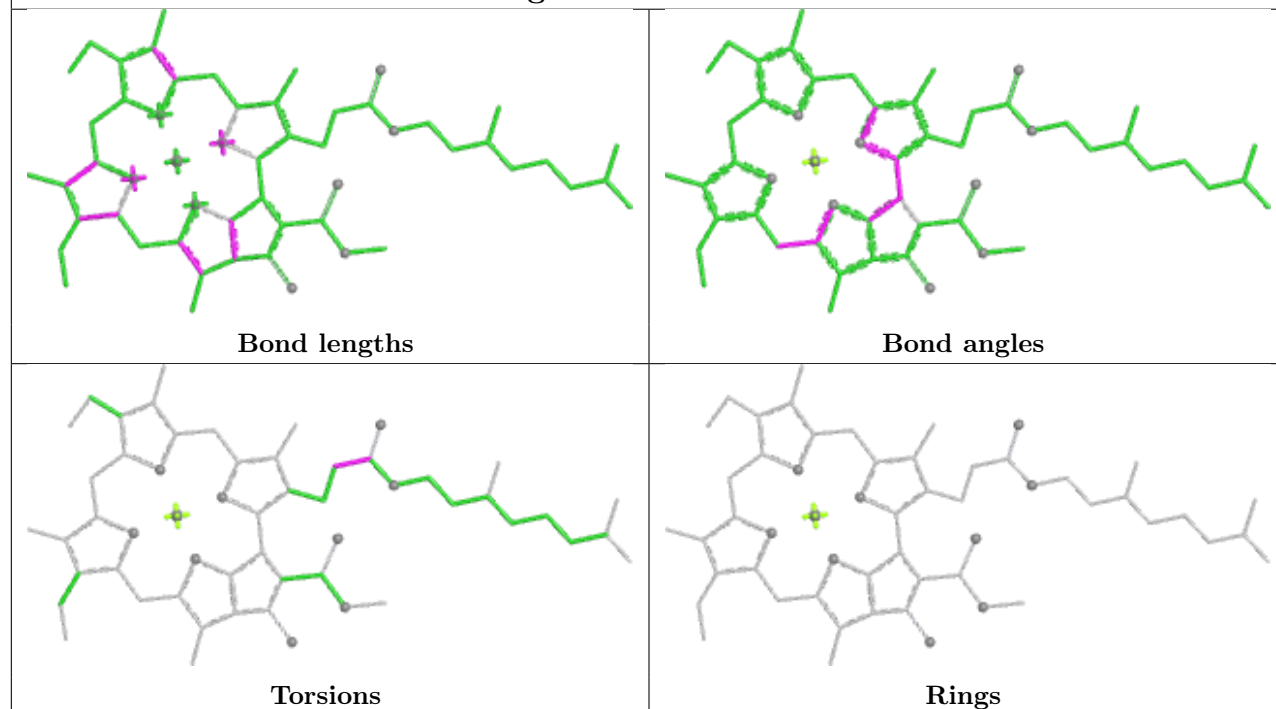


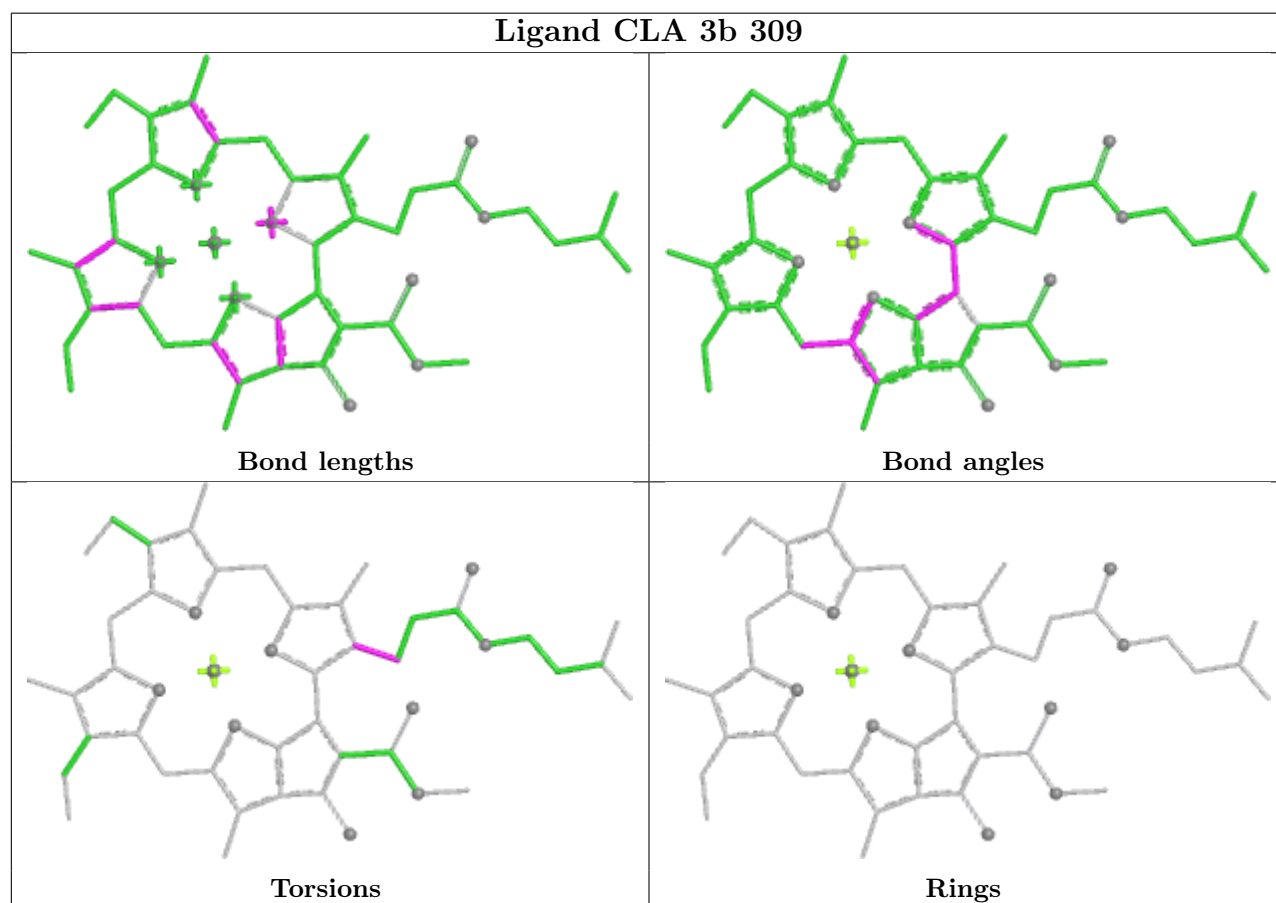
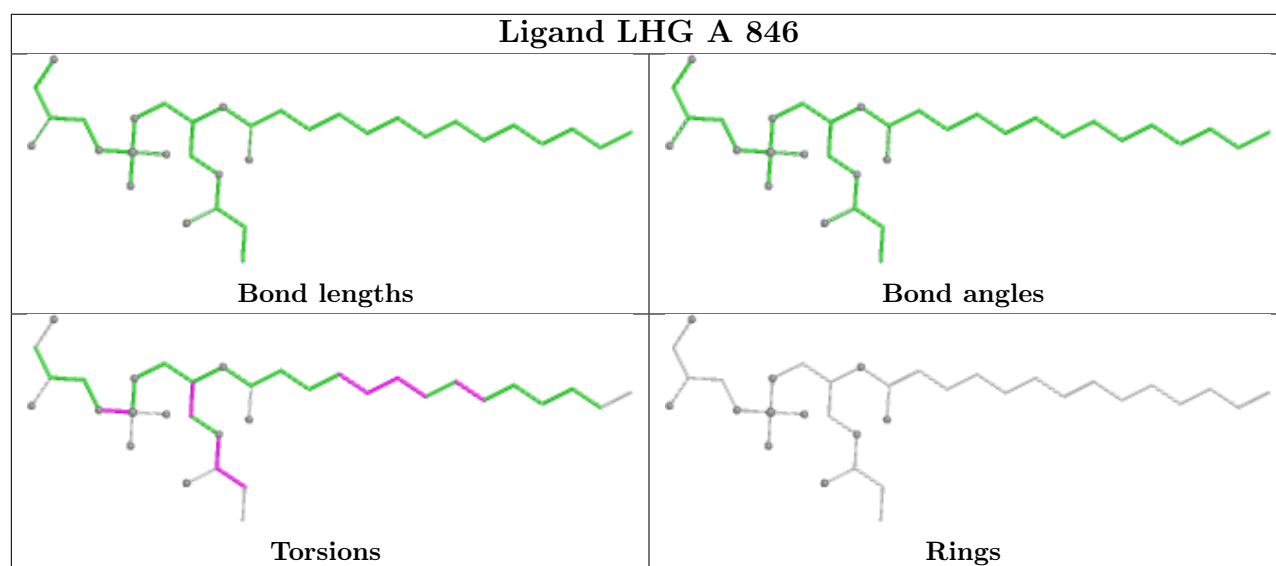


## Ligand CLA b 824

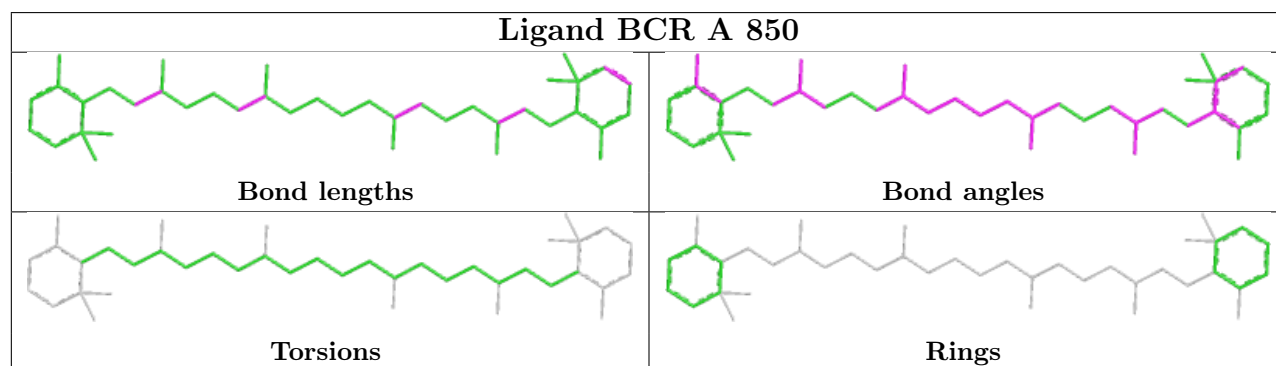
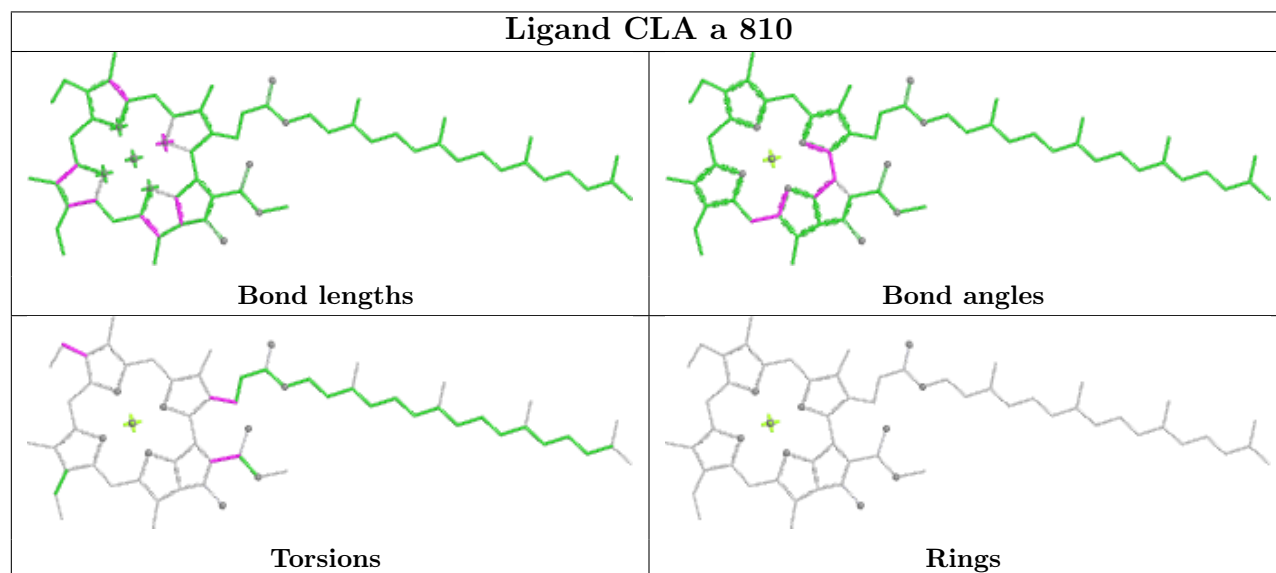
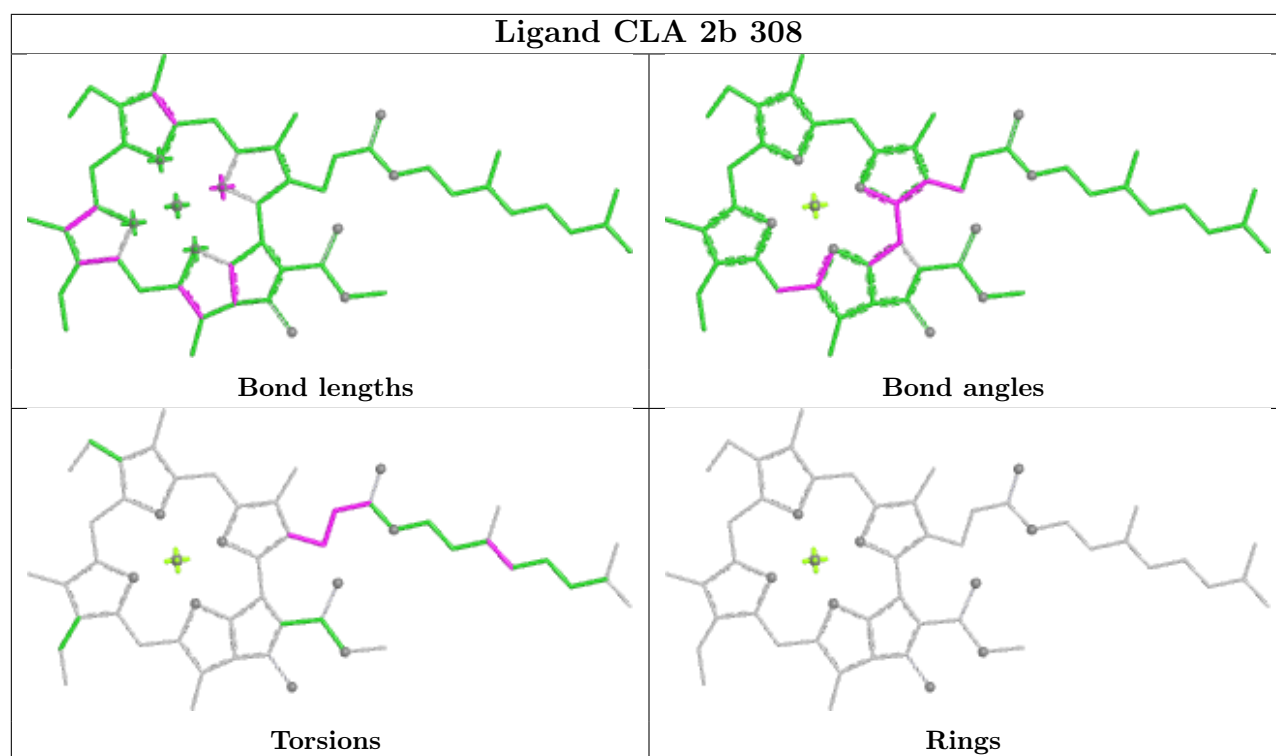


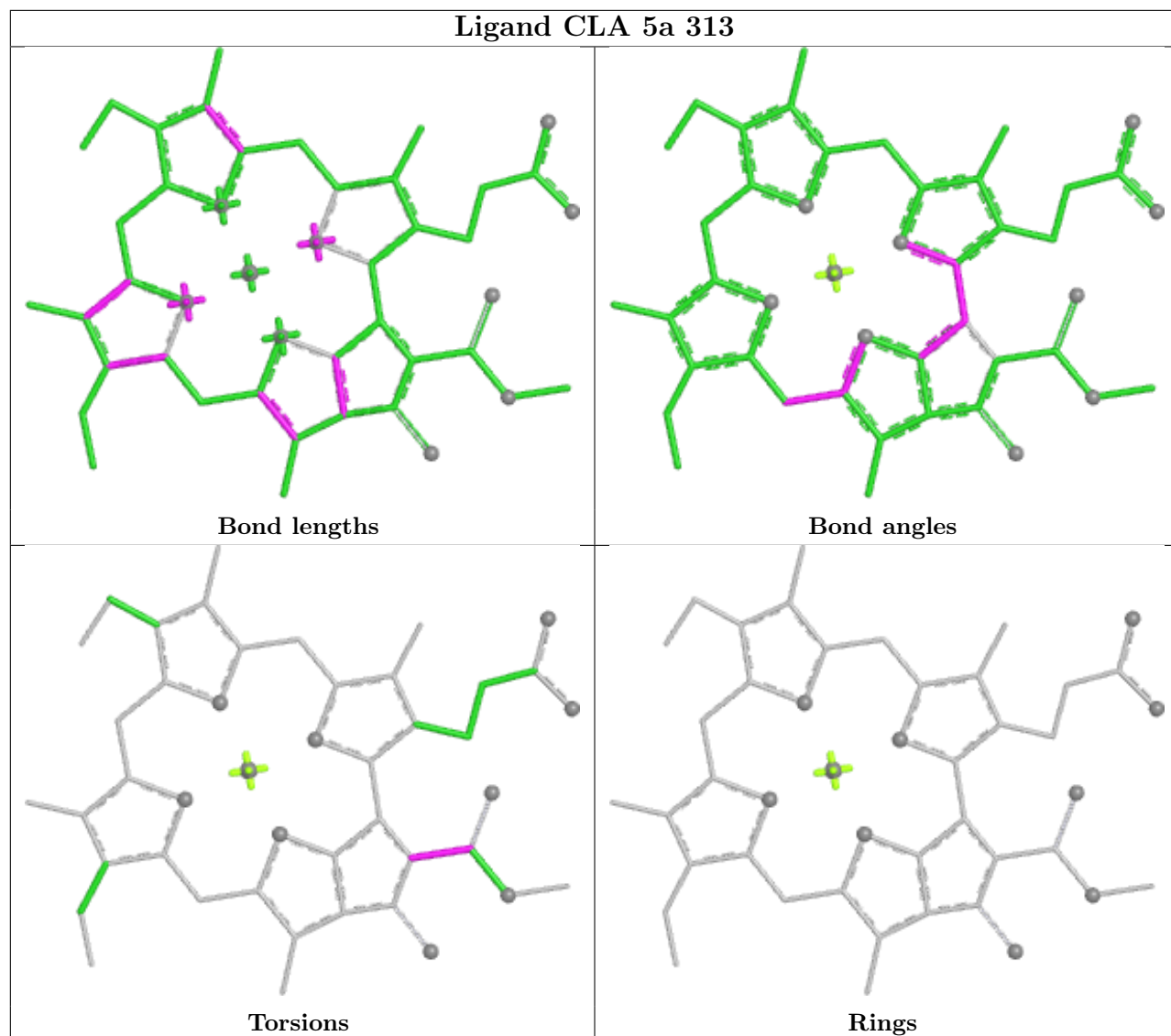
## Ligand CLA 6a 315



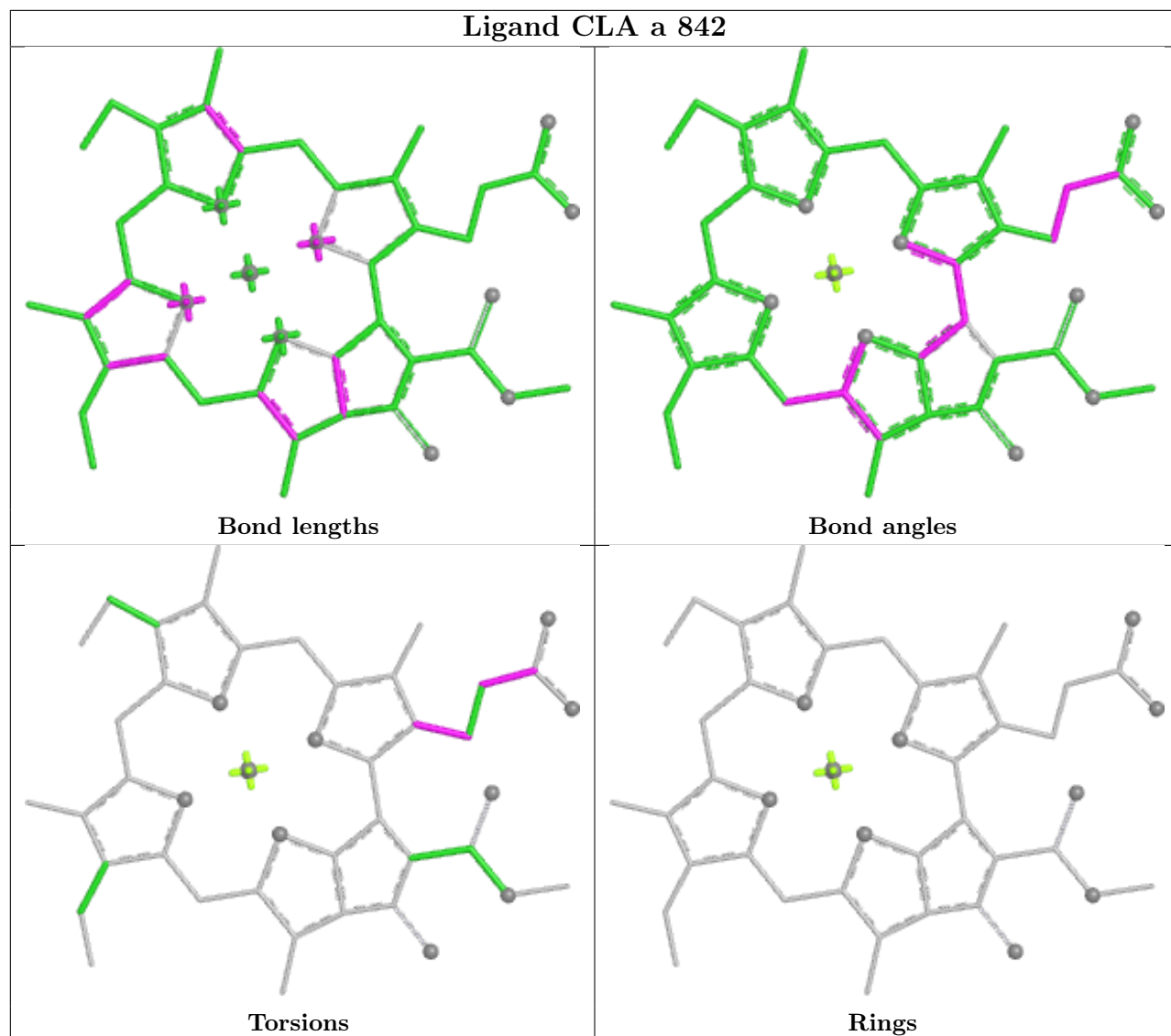




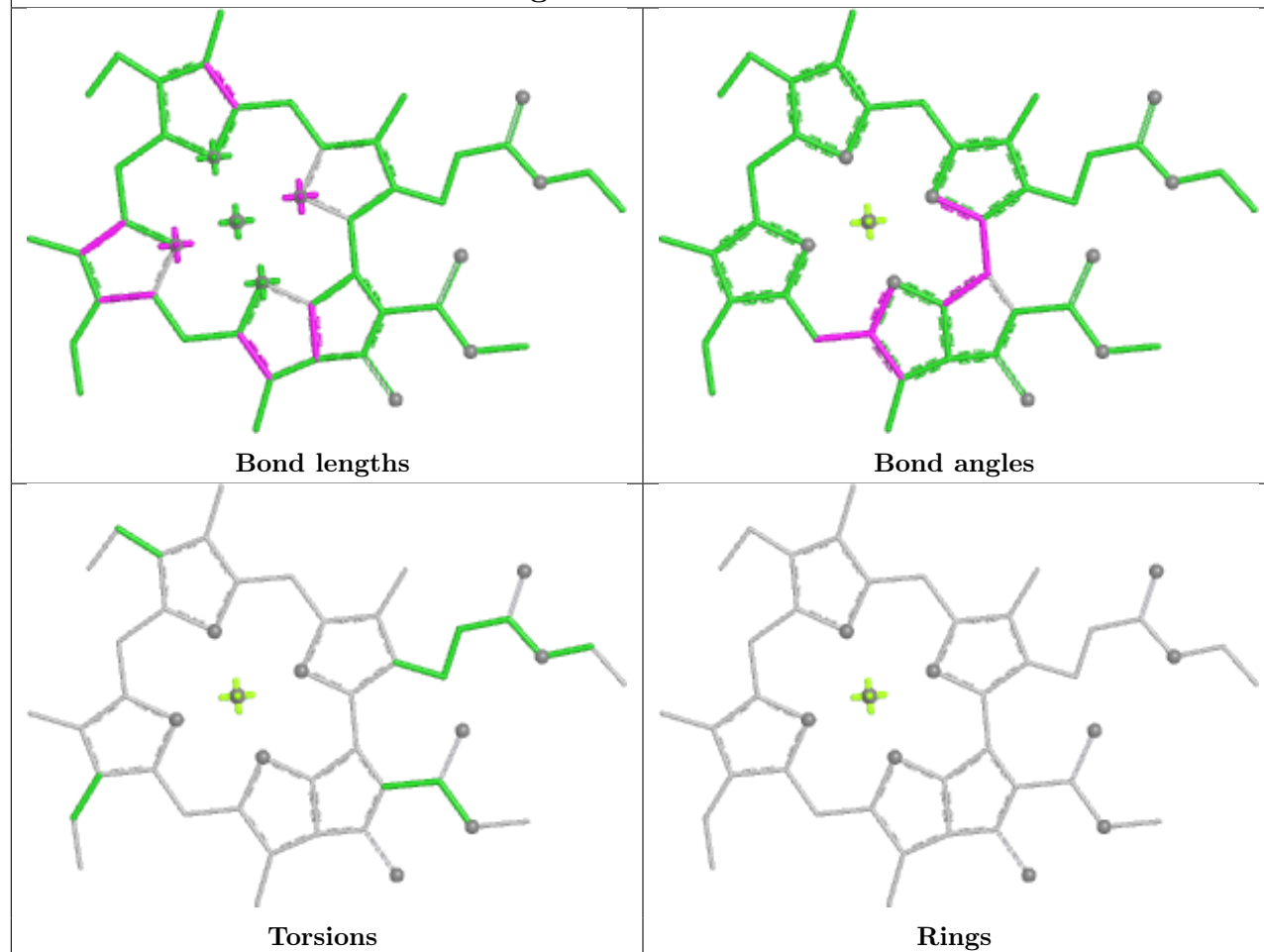




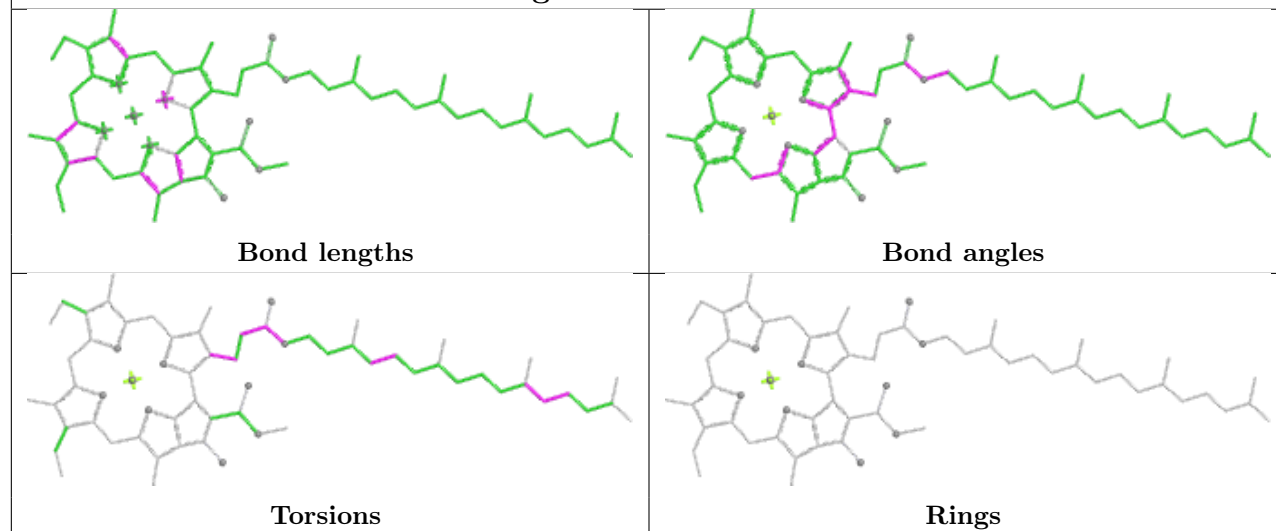
## Ligand CLA a 842

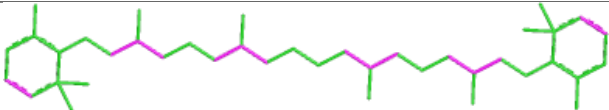
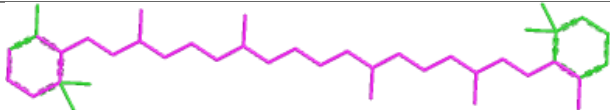
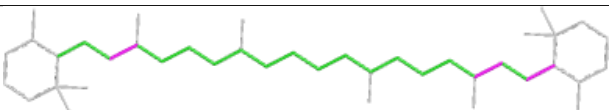
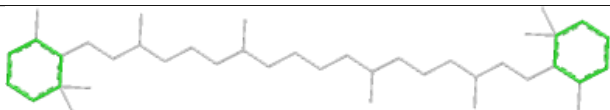



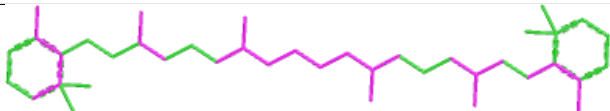
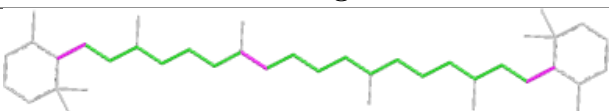
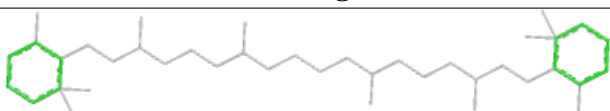
## Ligand CLA b 837

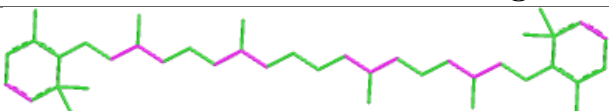
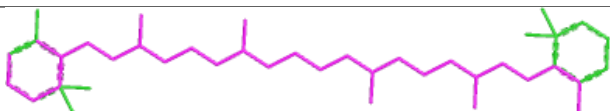
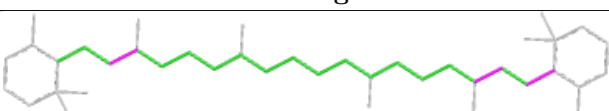
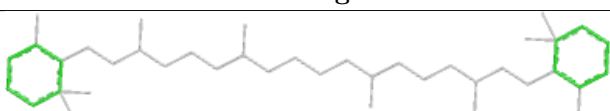


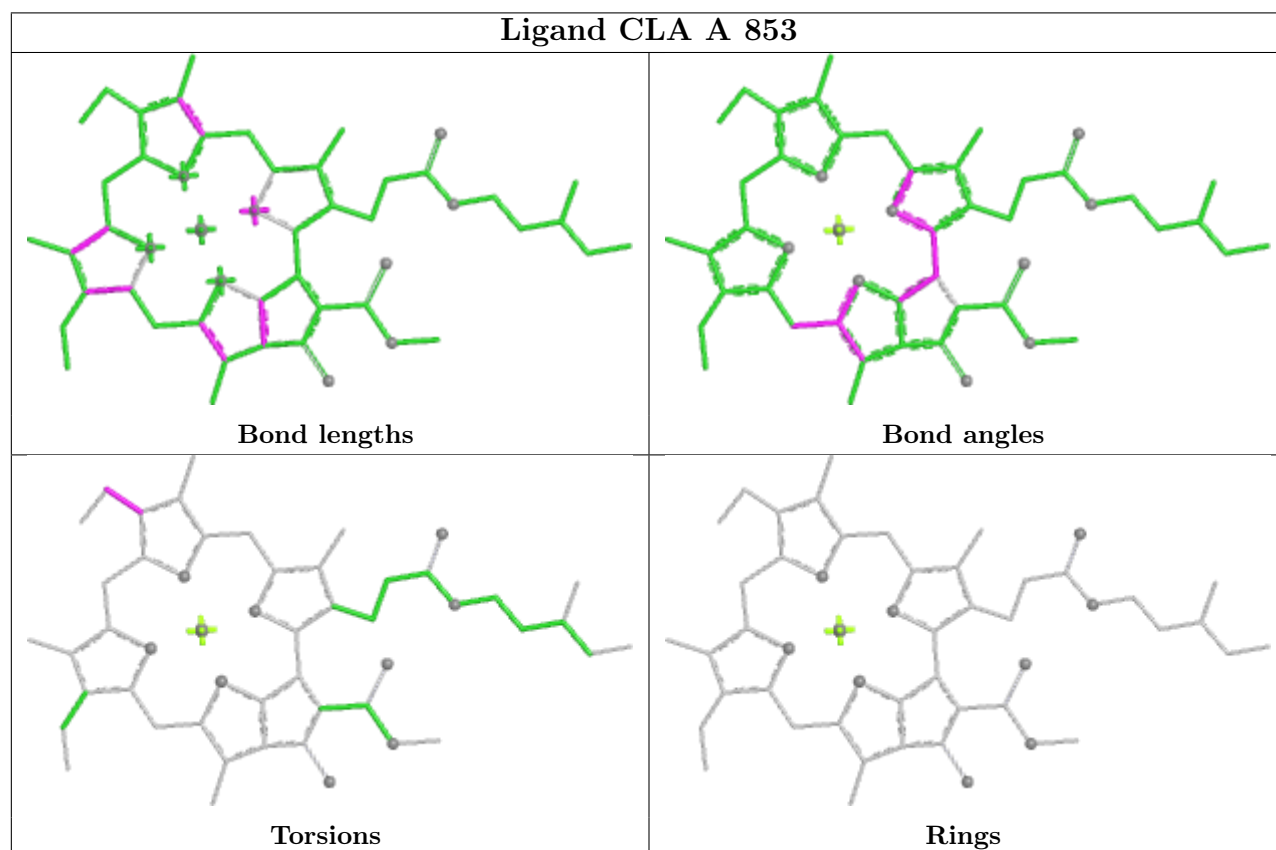
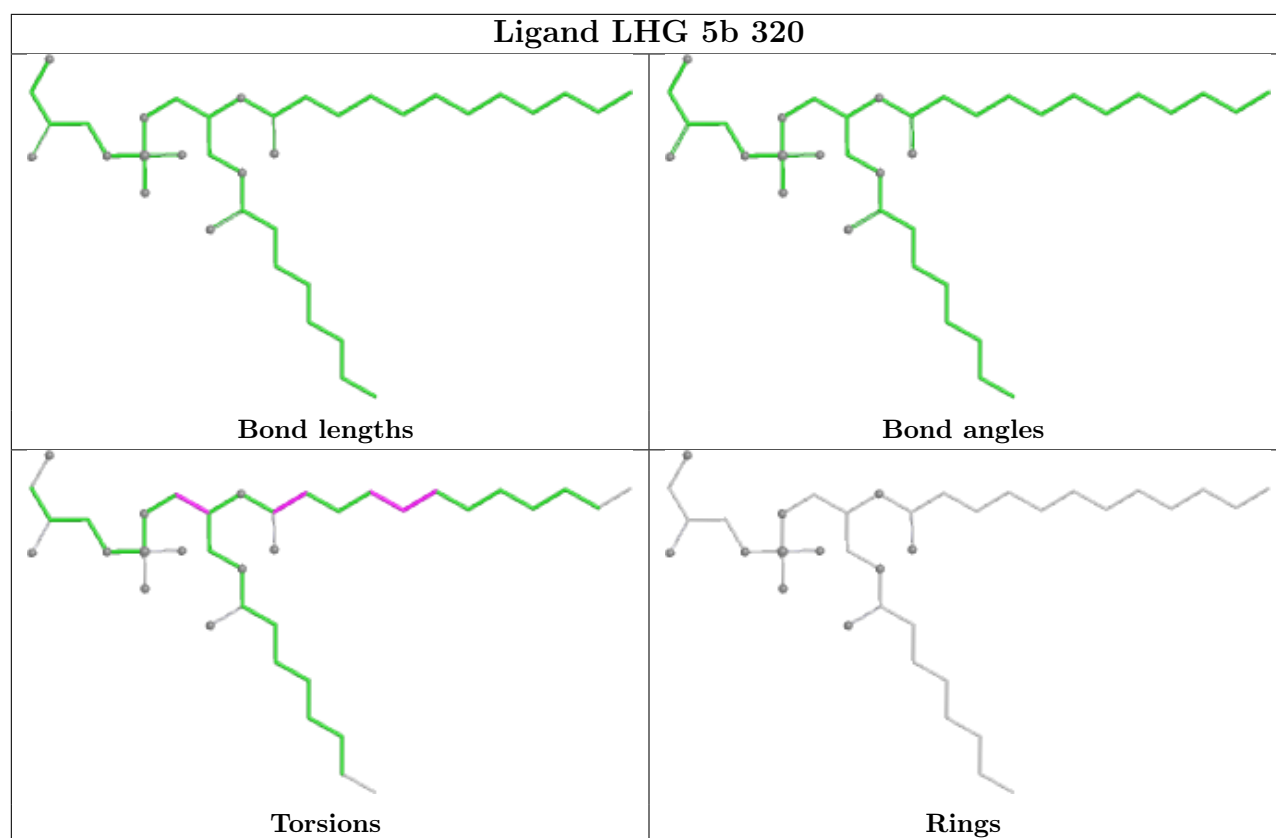
## Ligand CLA B 840

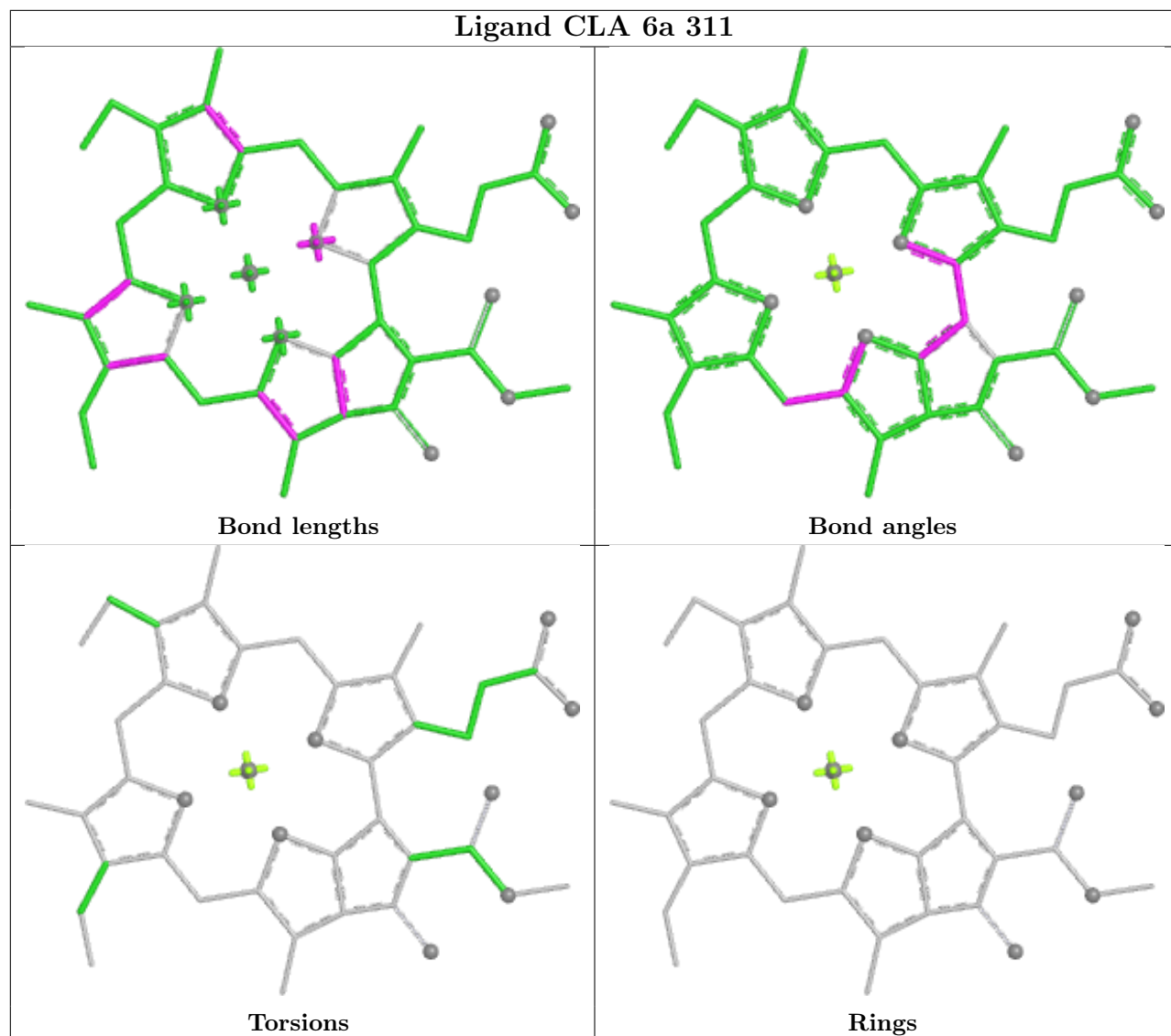


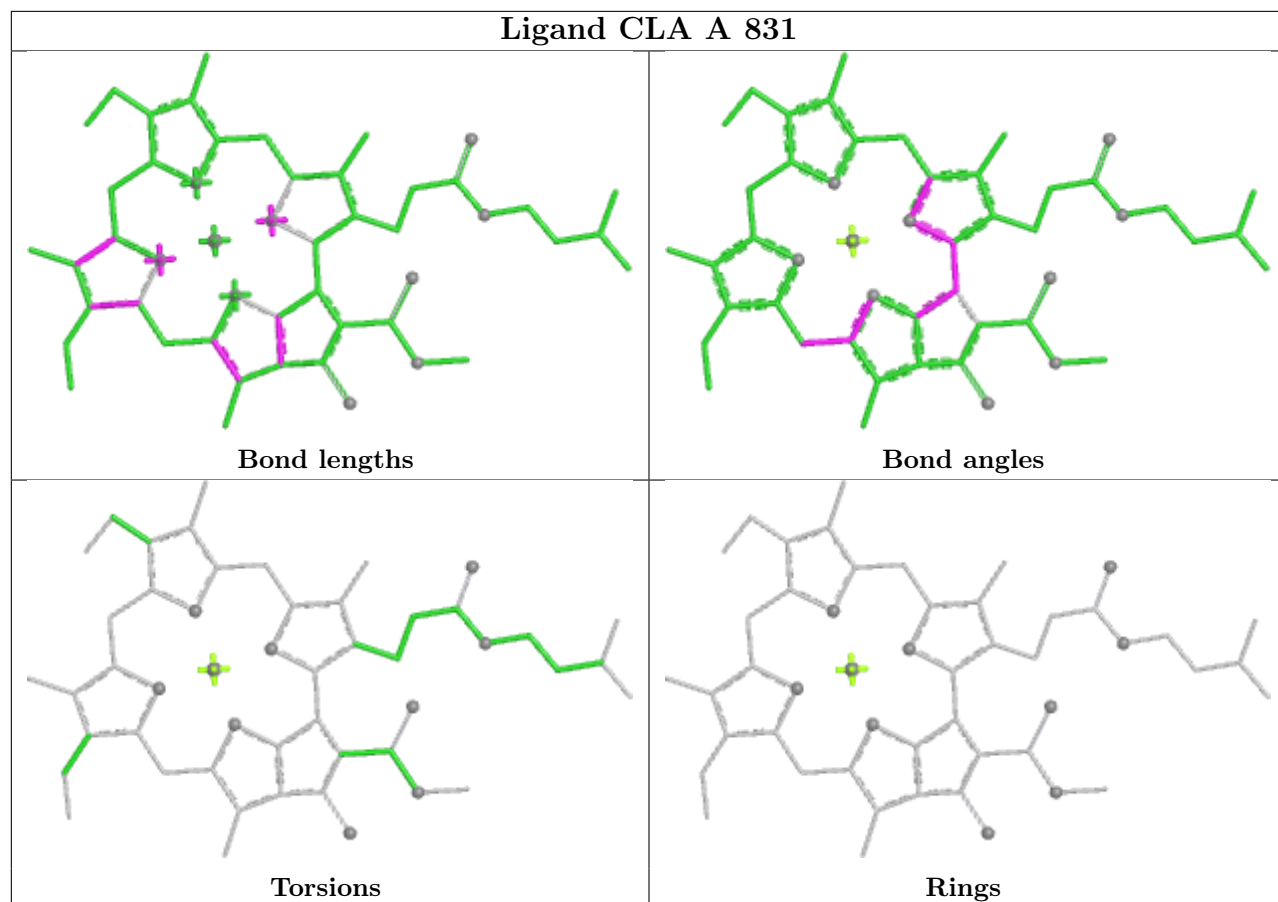
Ligand BCR j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

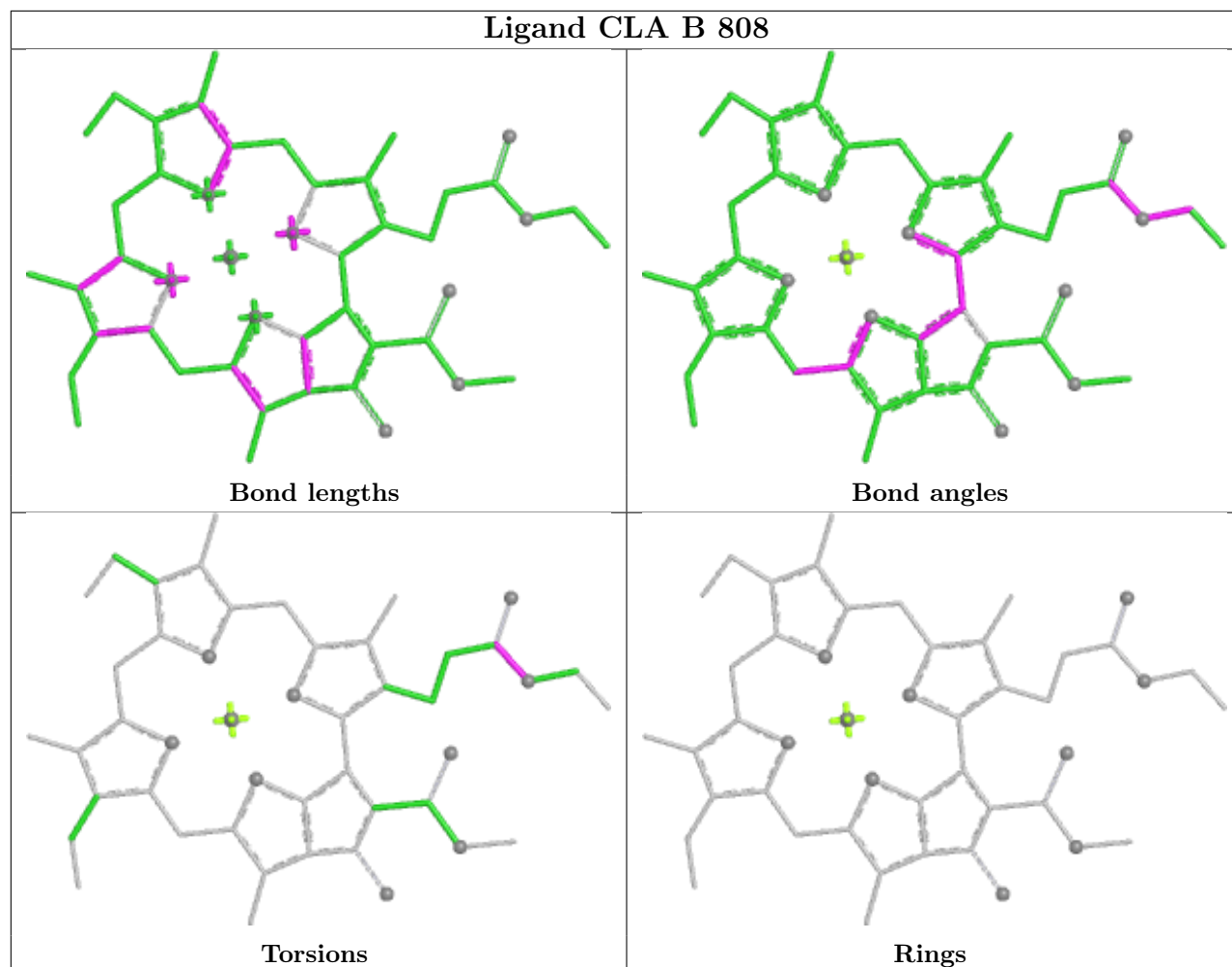




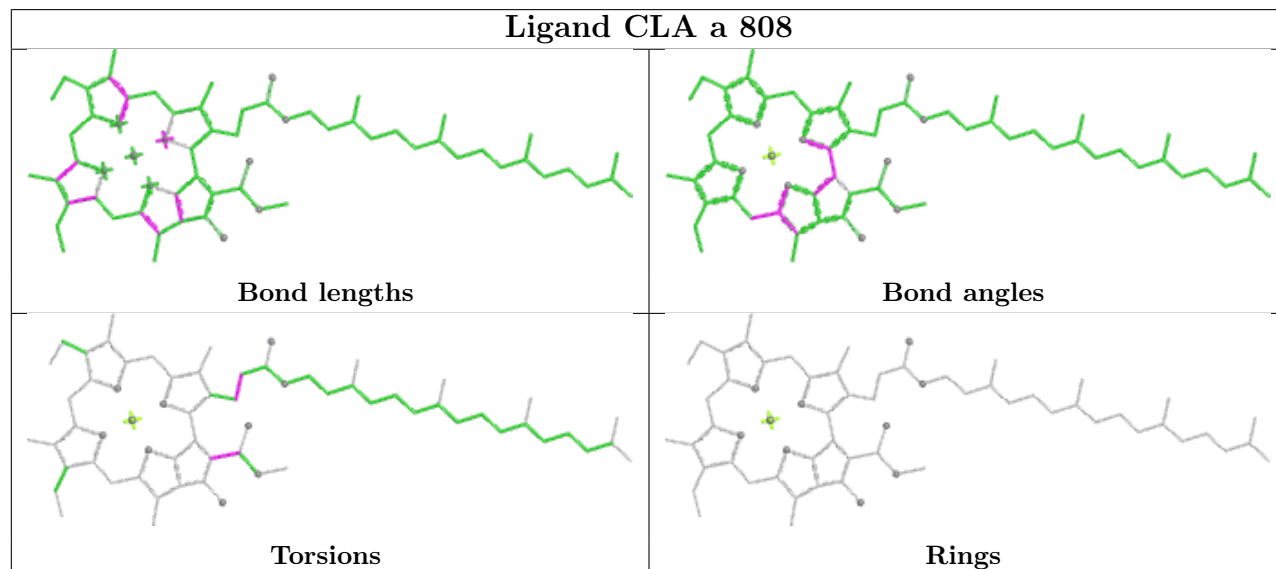


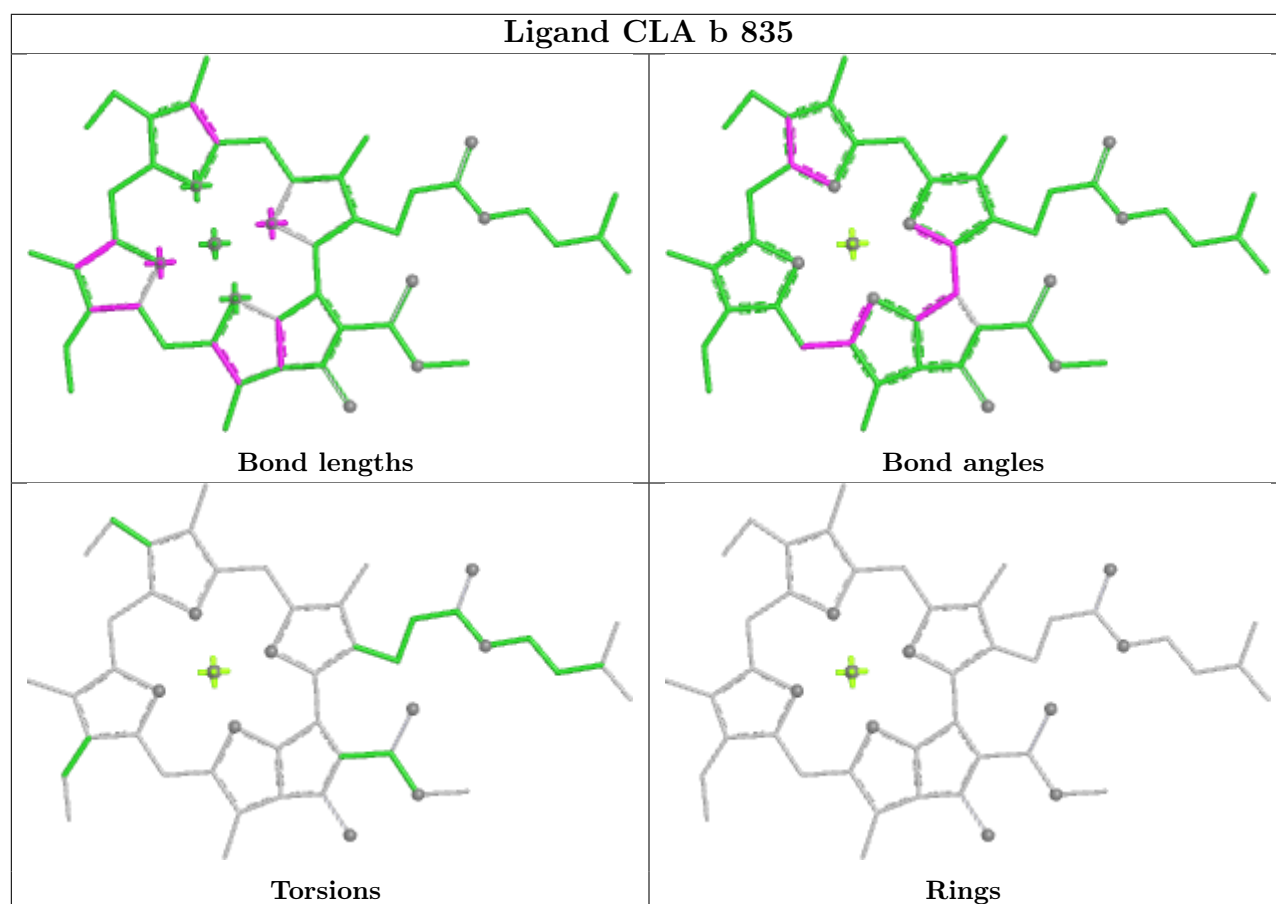
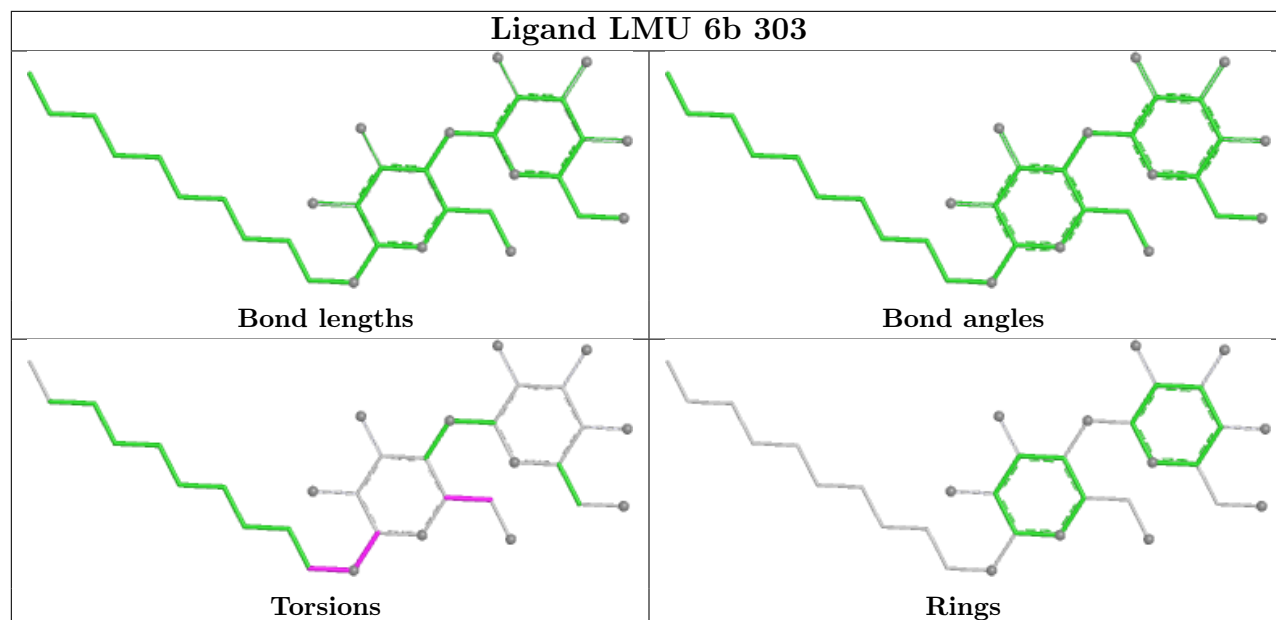


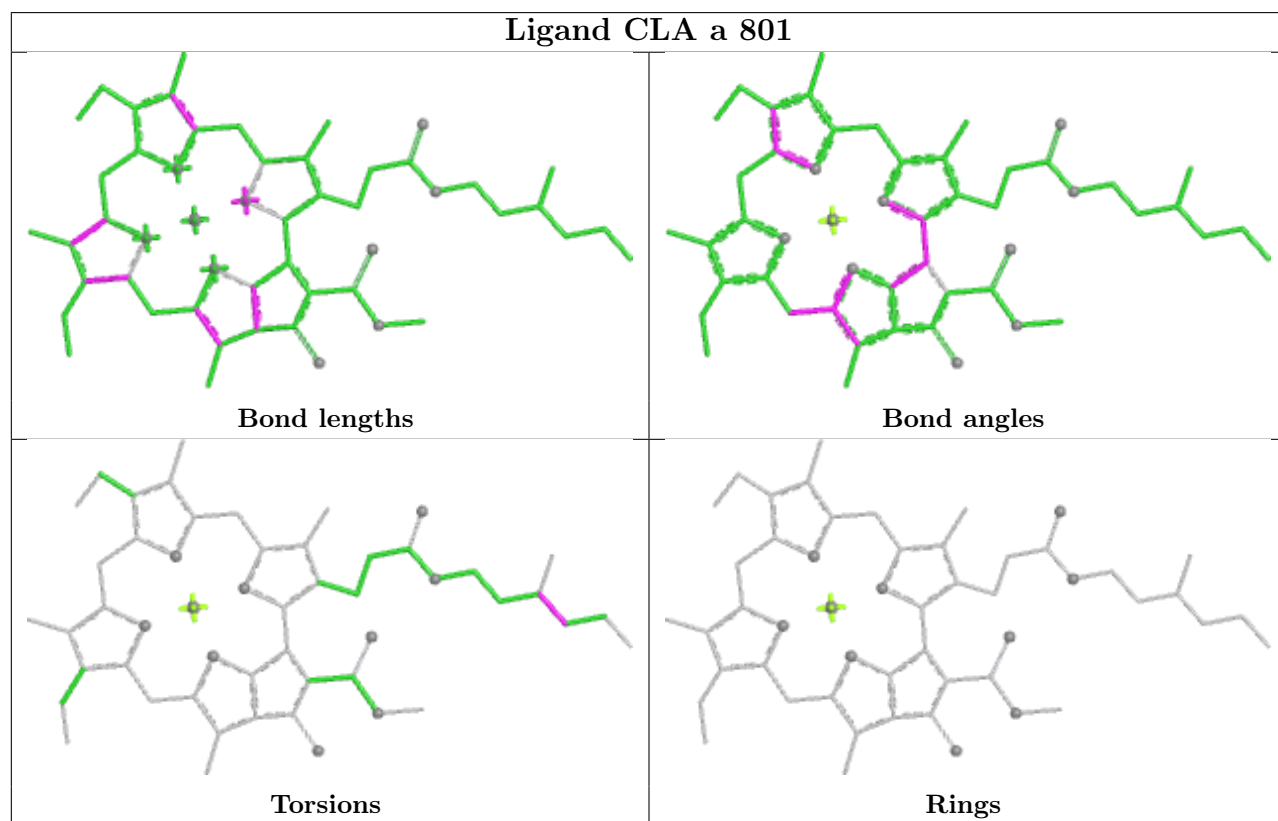
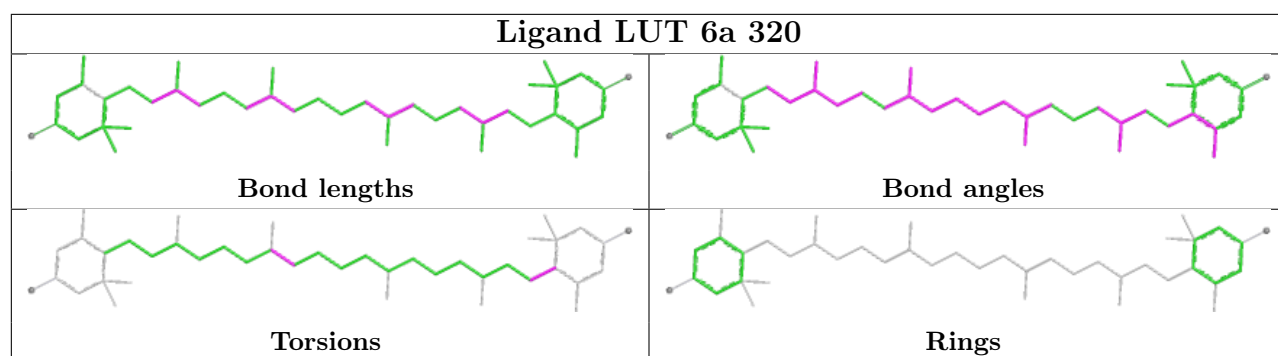
## Ligand CLA B 808

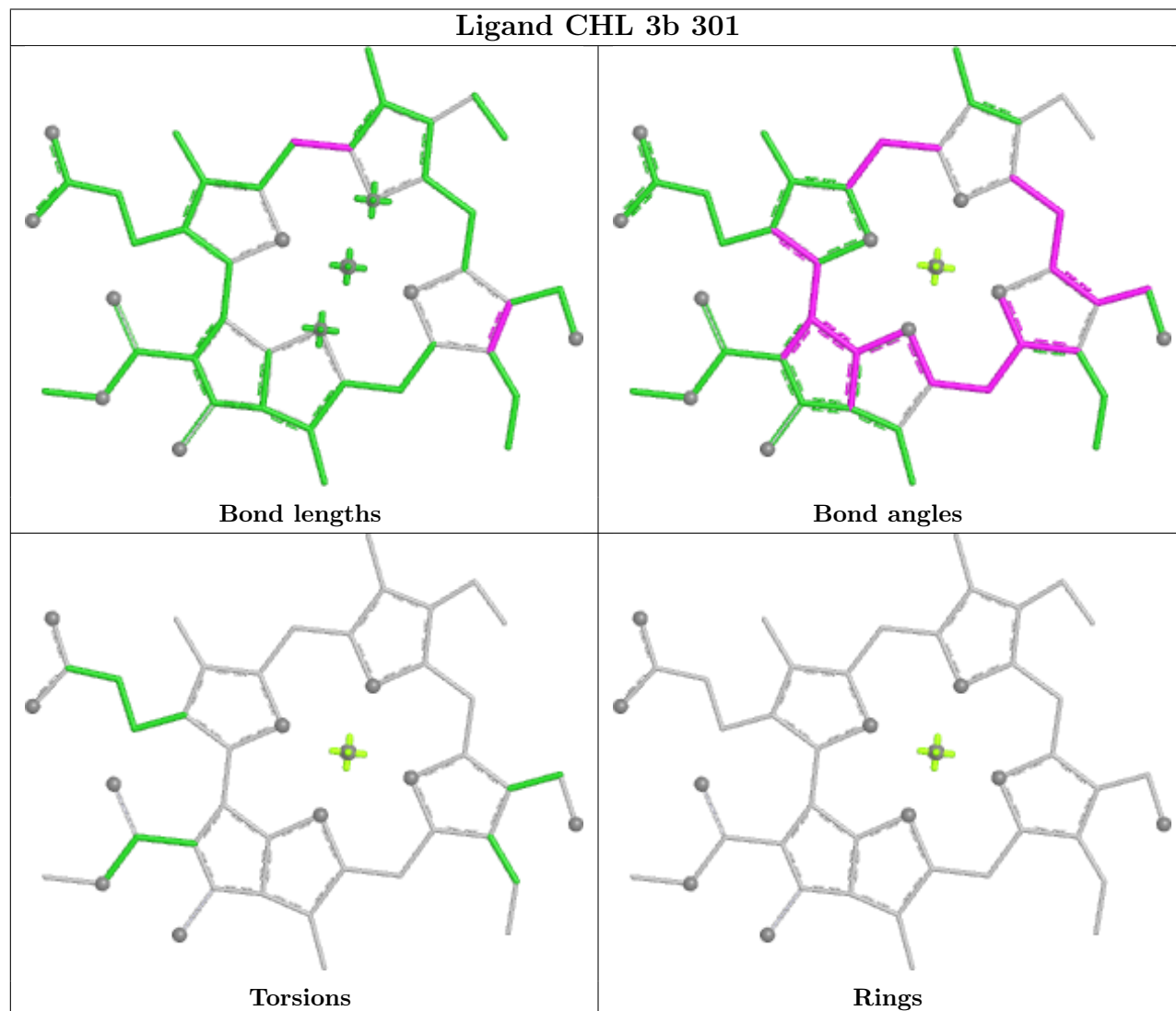
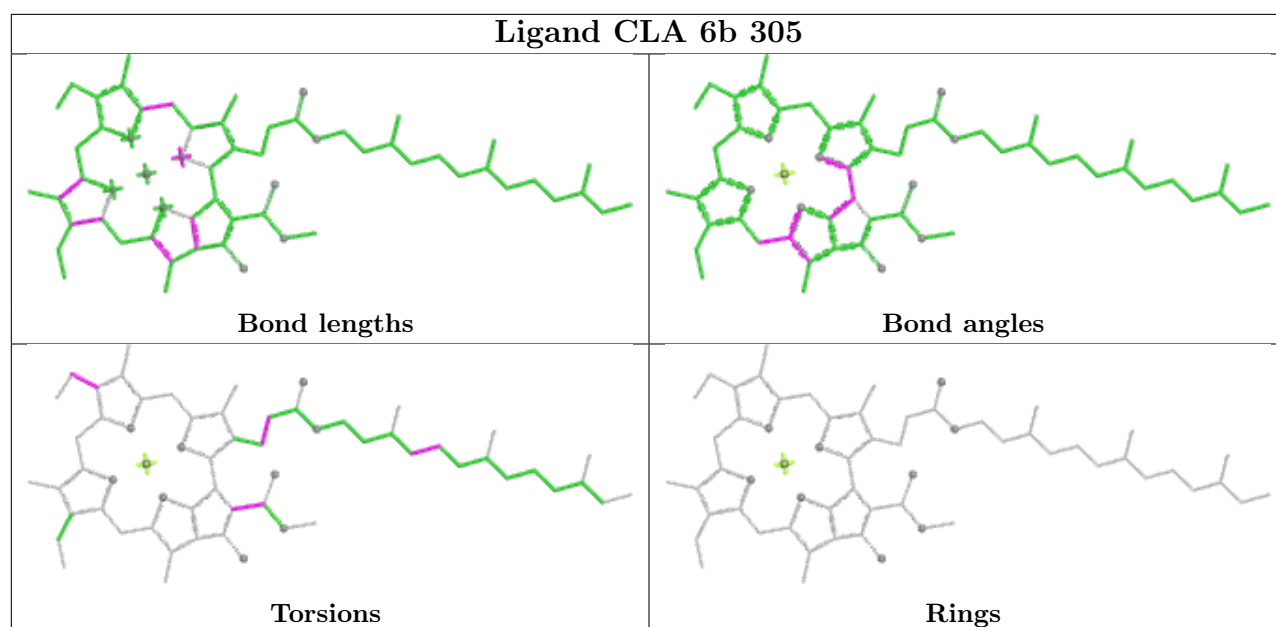


## Ligand CLA a 808

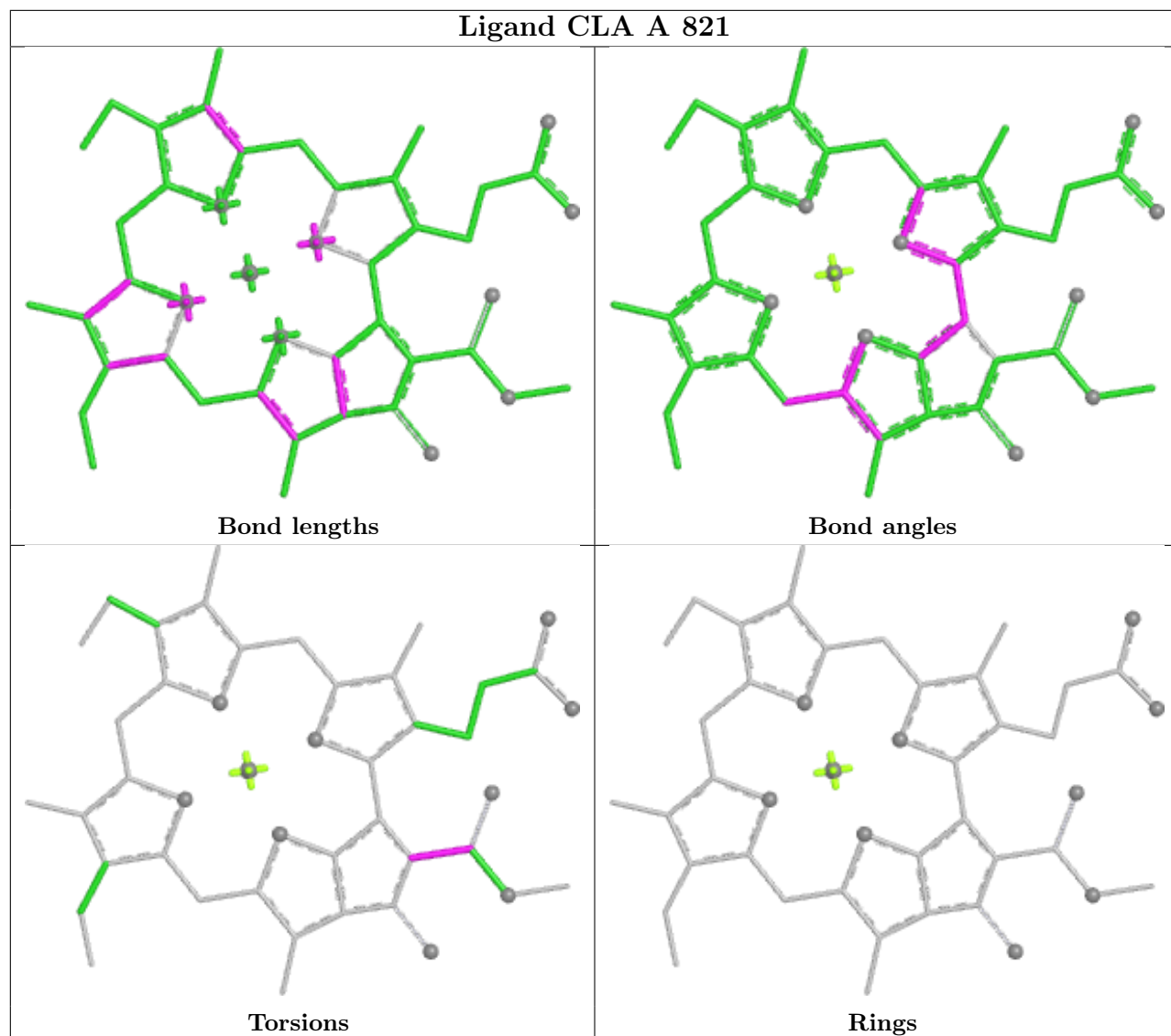




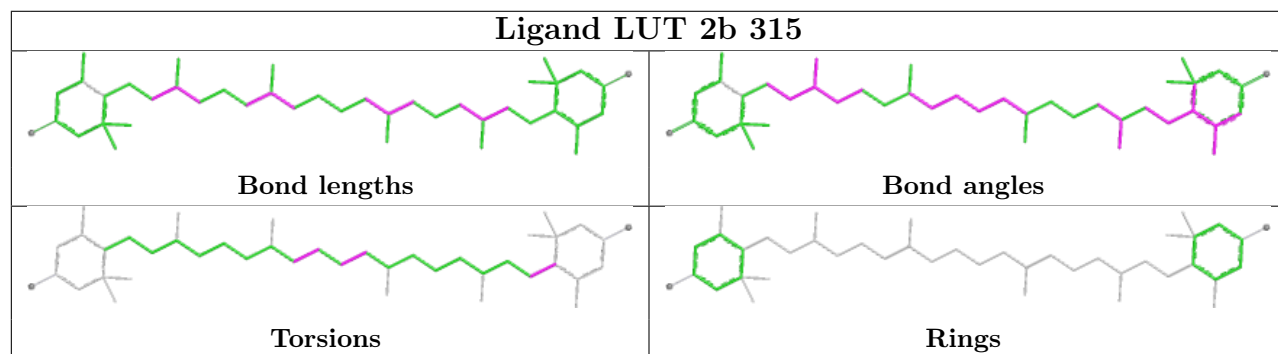




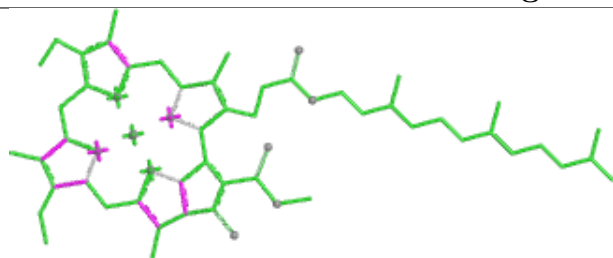
## Ligand CLA A 821



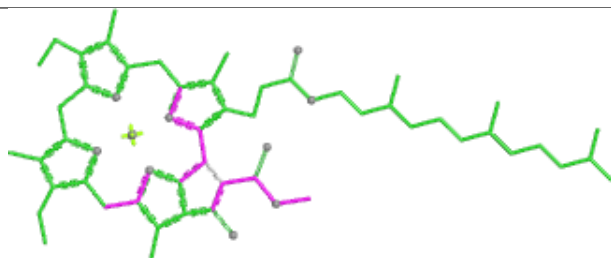
## Ligand LUT 2b 315



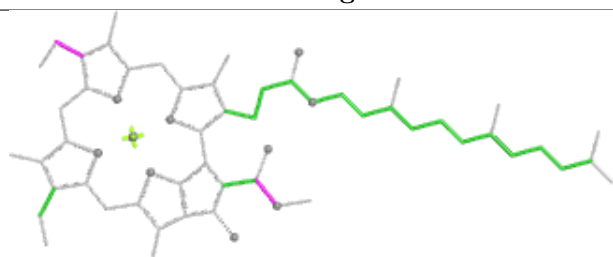
## Ligand CLA f 305



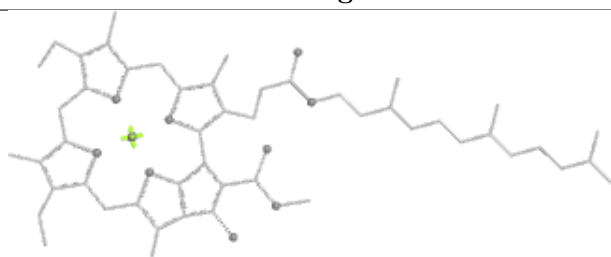
Bond lengths



Bond angles

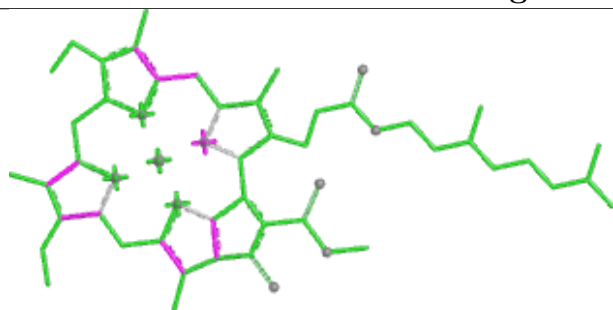


Torsions

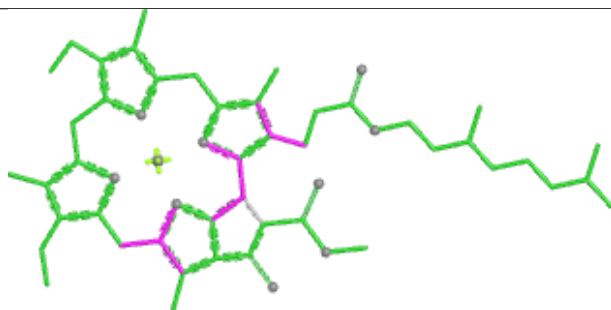


Rings

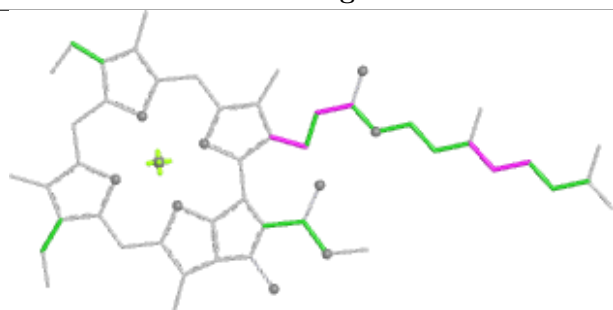
## Ligand CLA 3a 312



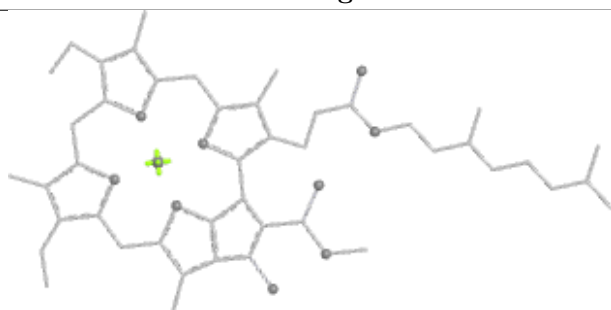
Bond lengths



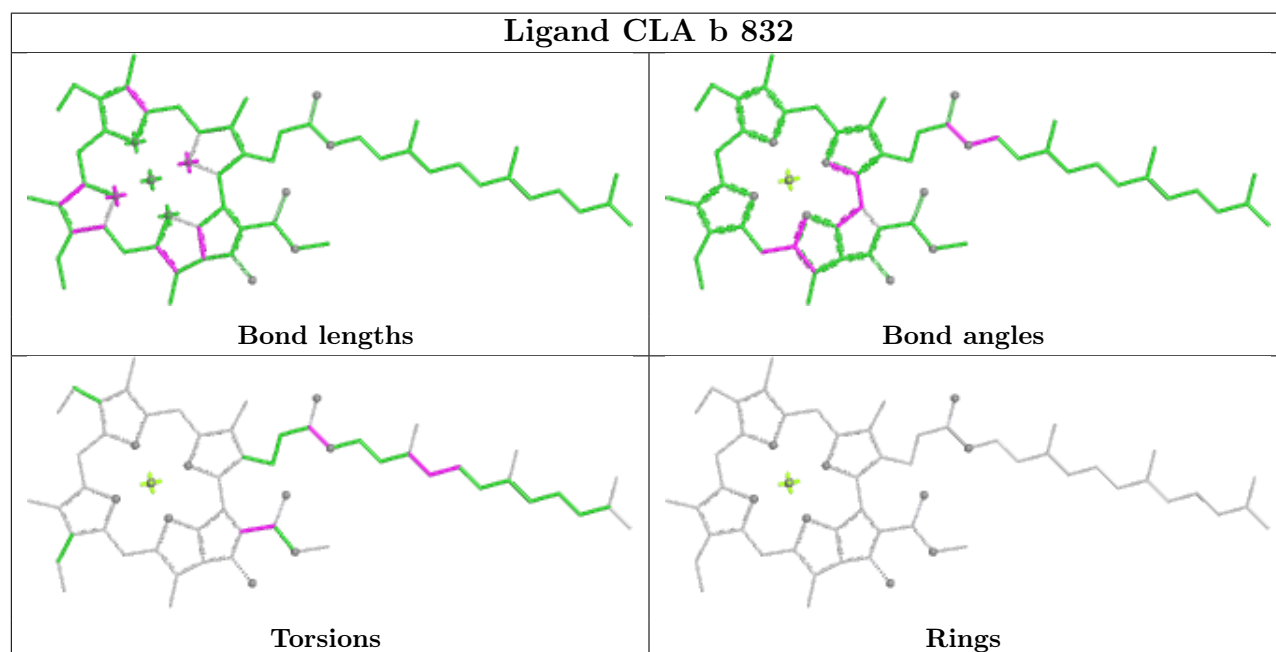
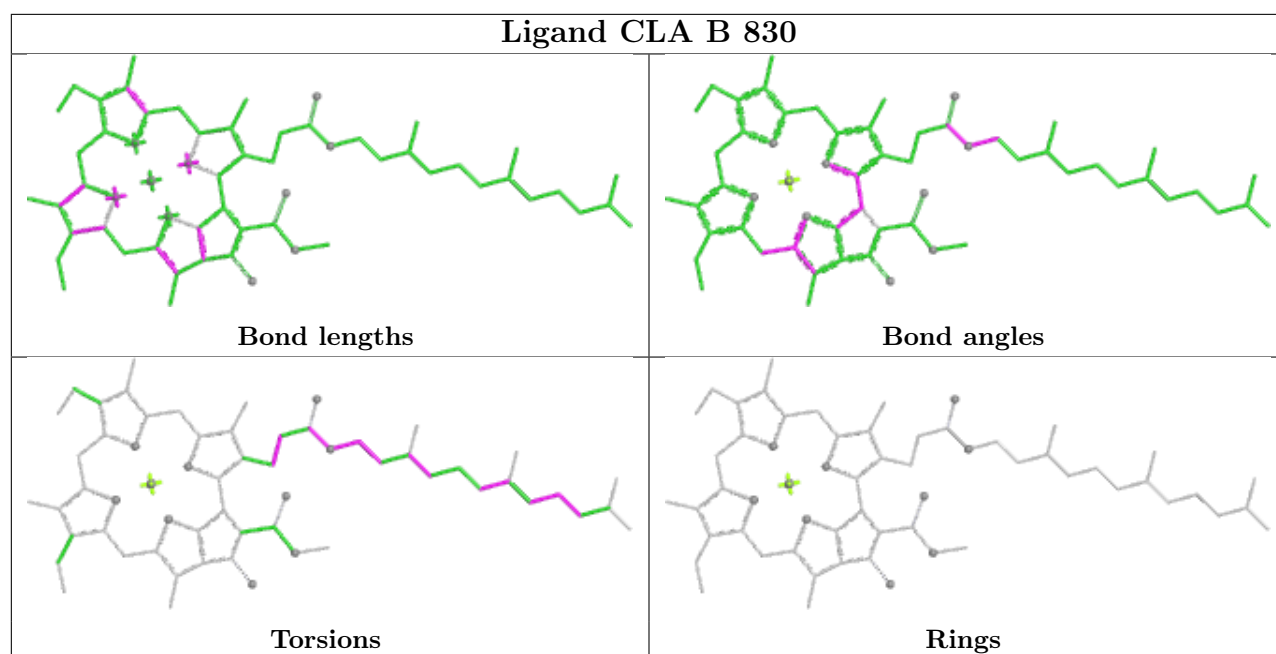
Bond angles

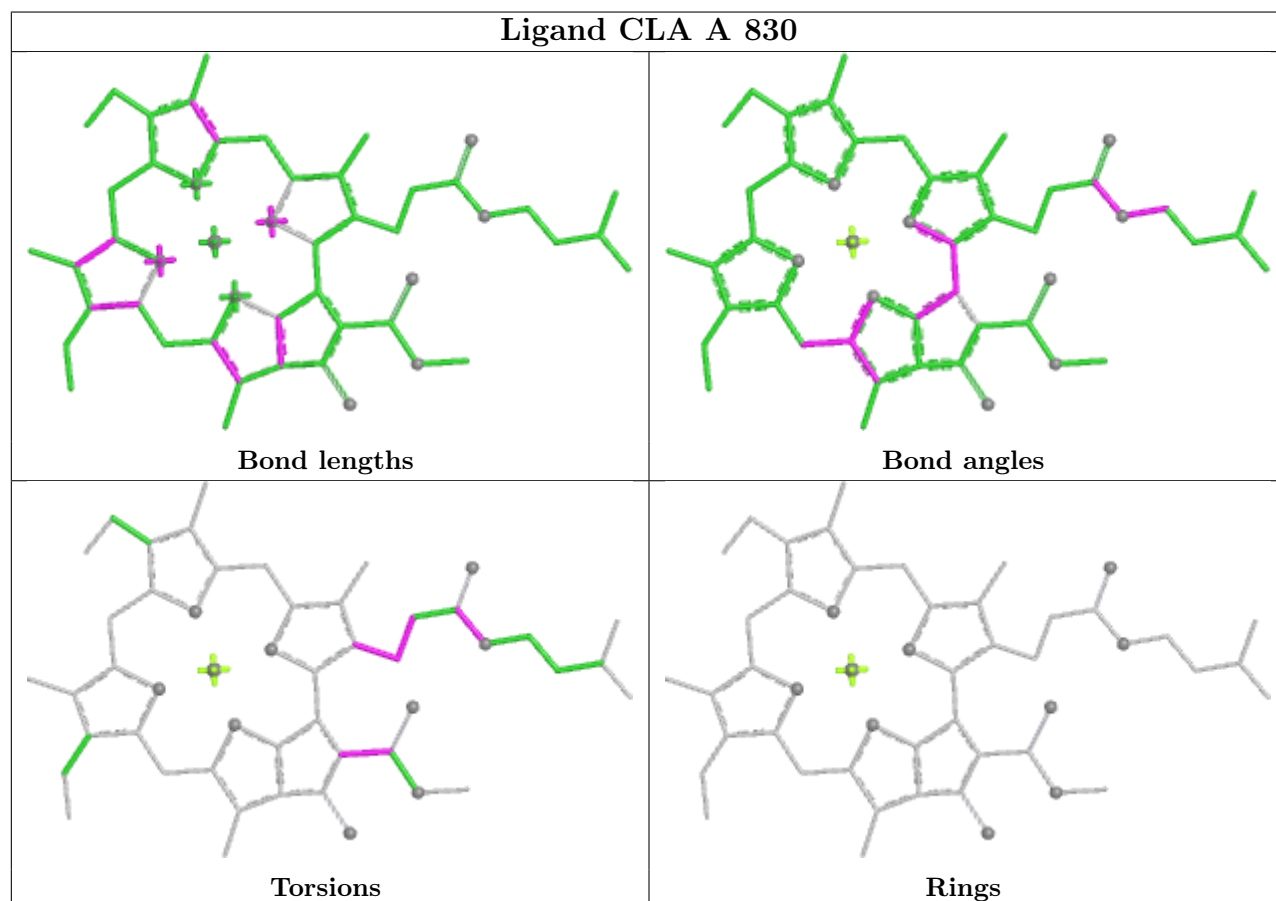
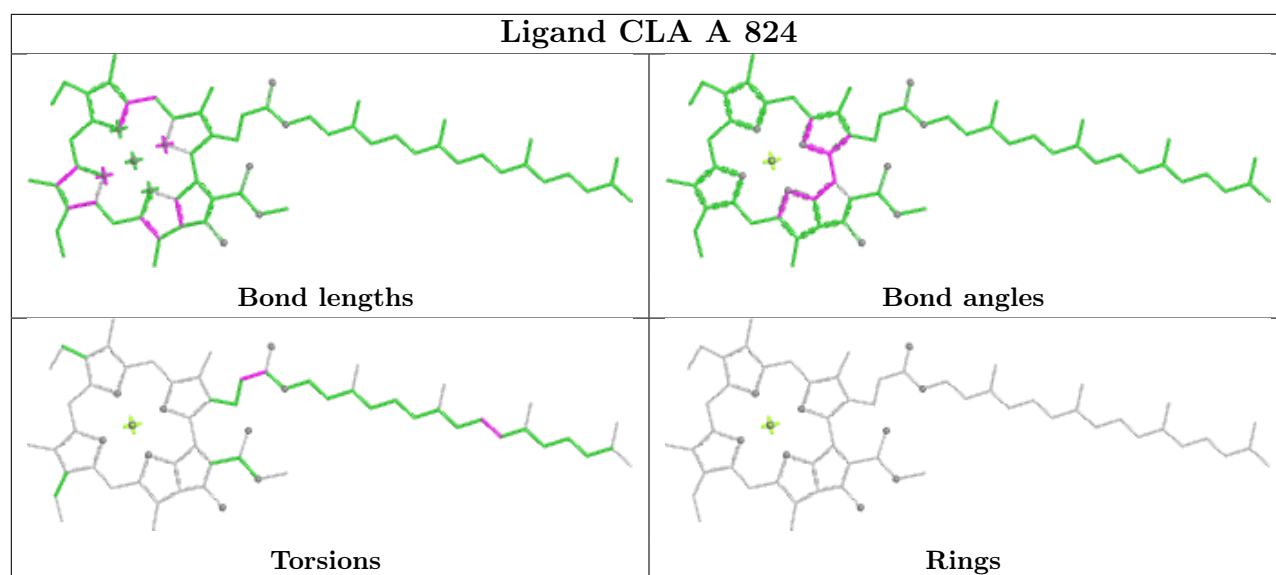


Torsions



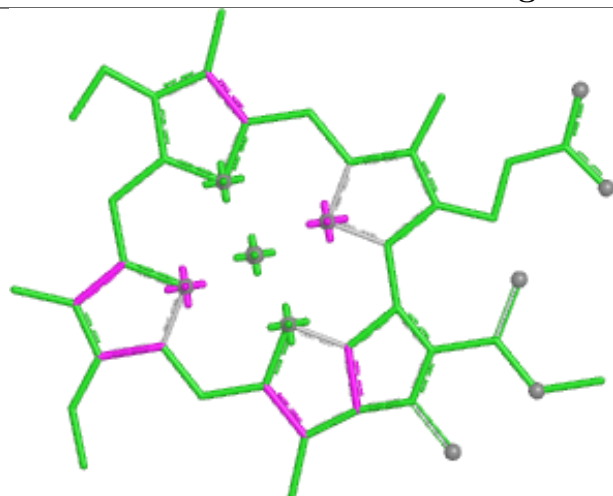
Rings



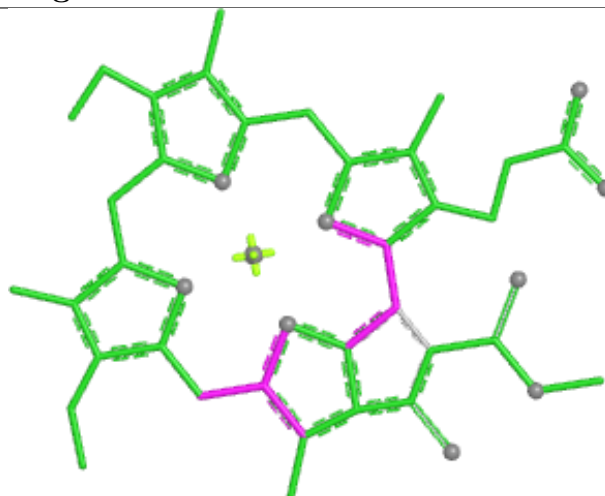




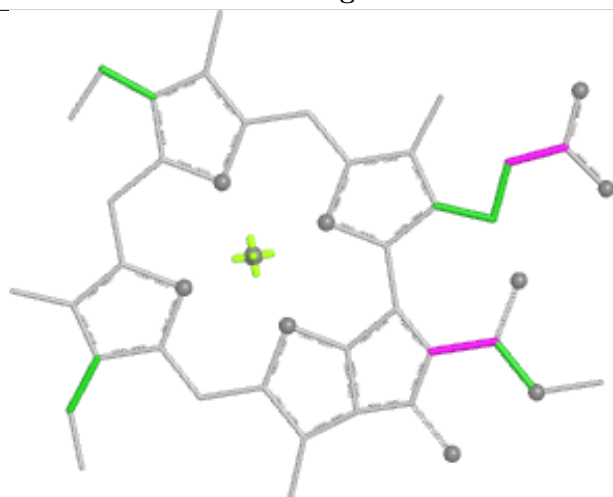
## Ligand CLA g 203



Bond lengths



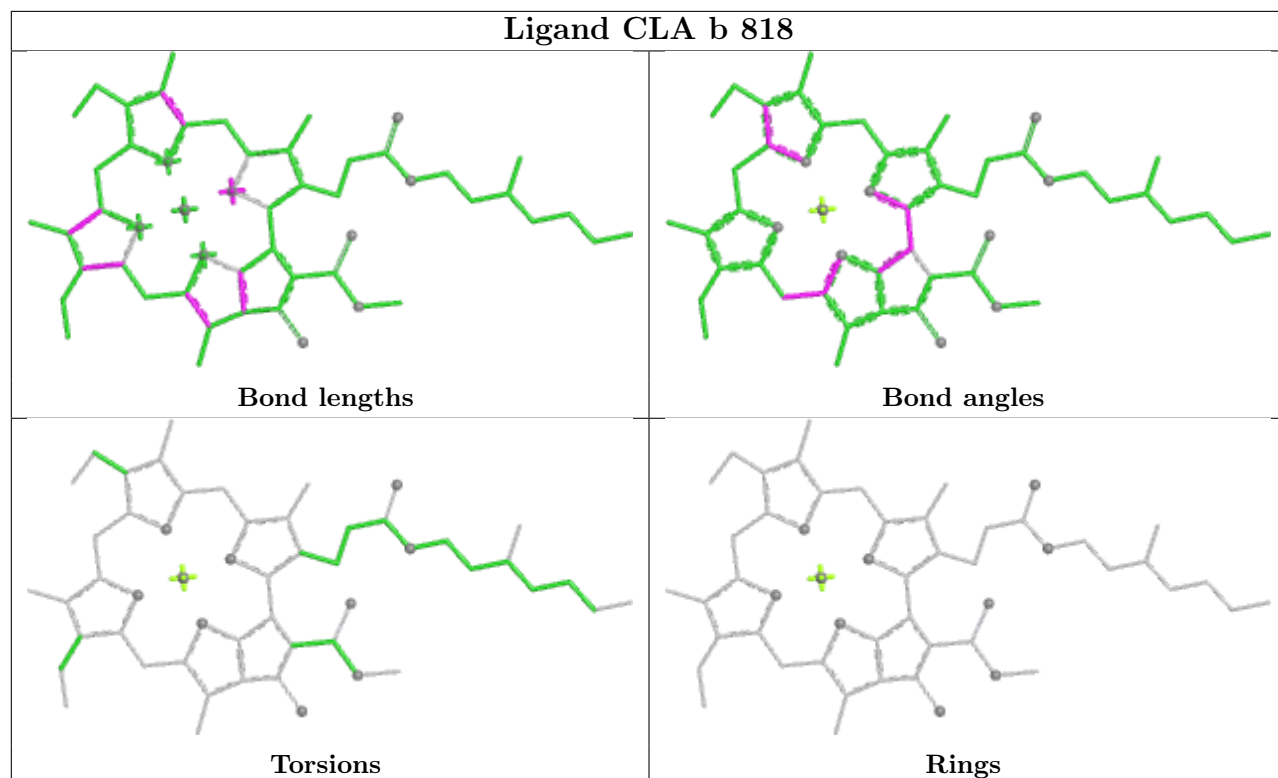
Bond angles

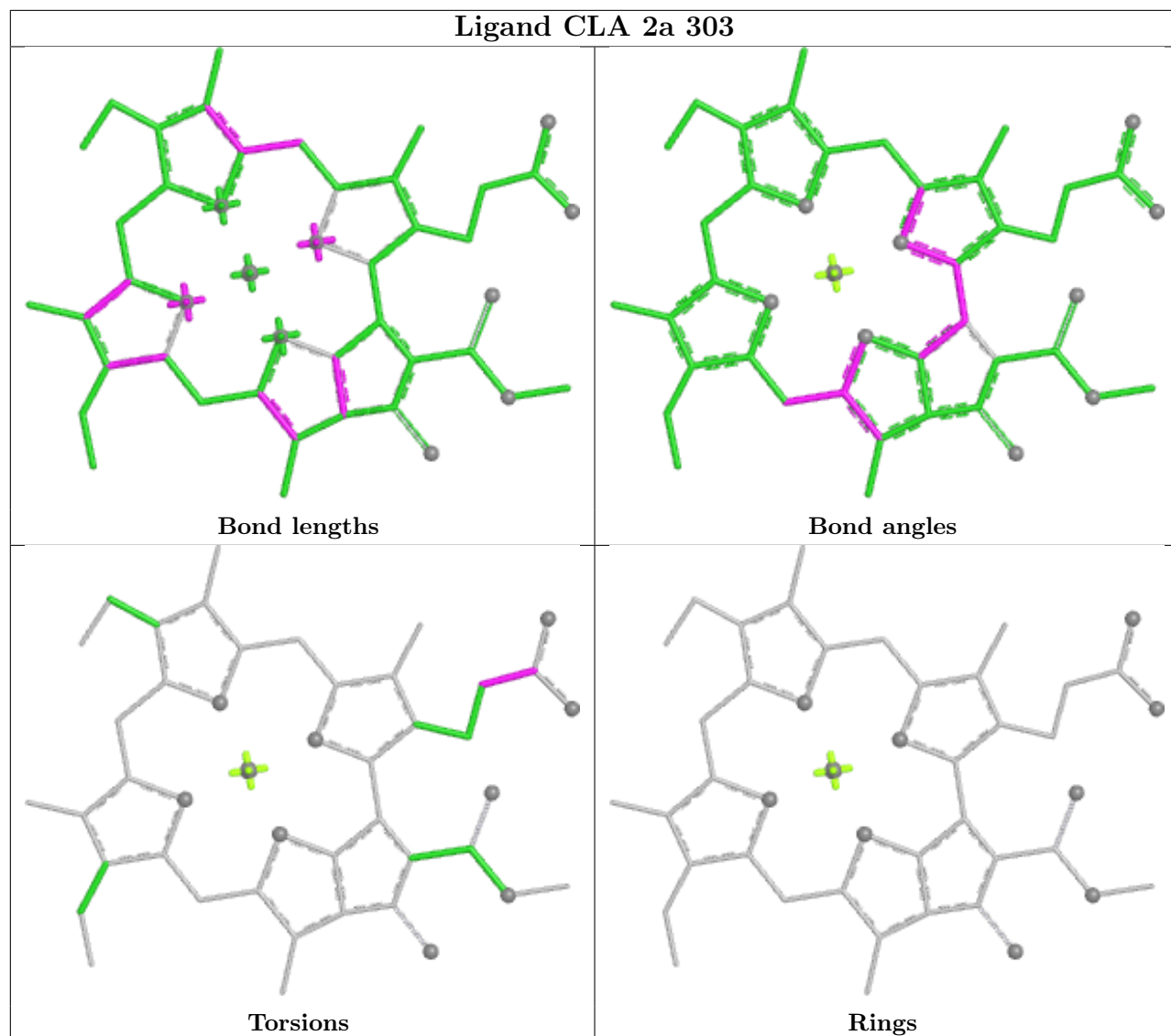


Torsions

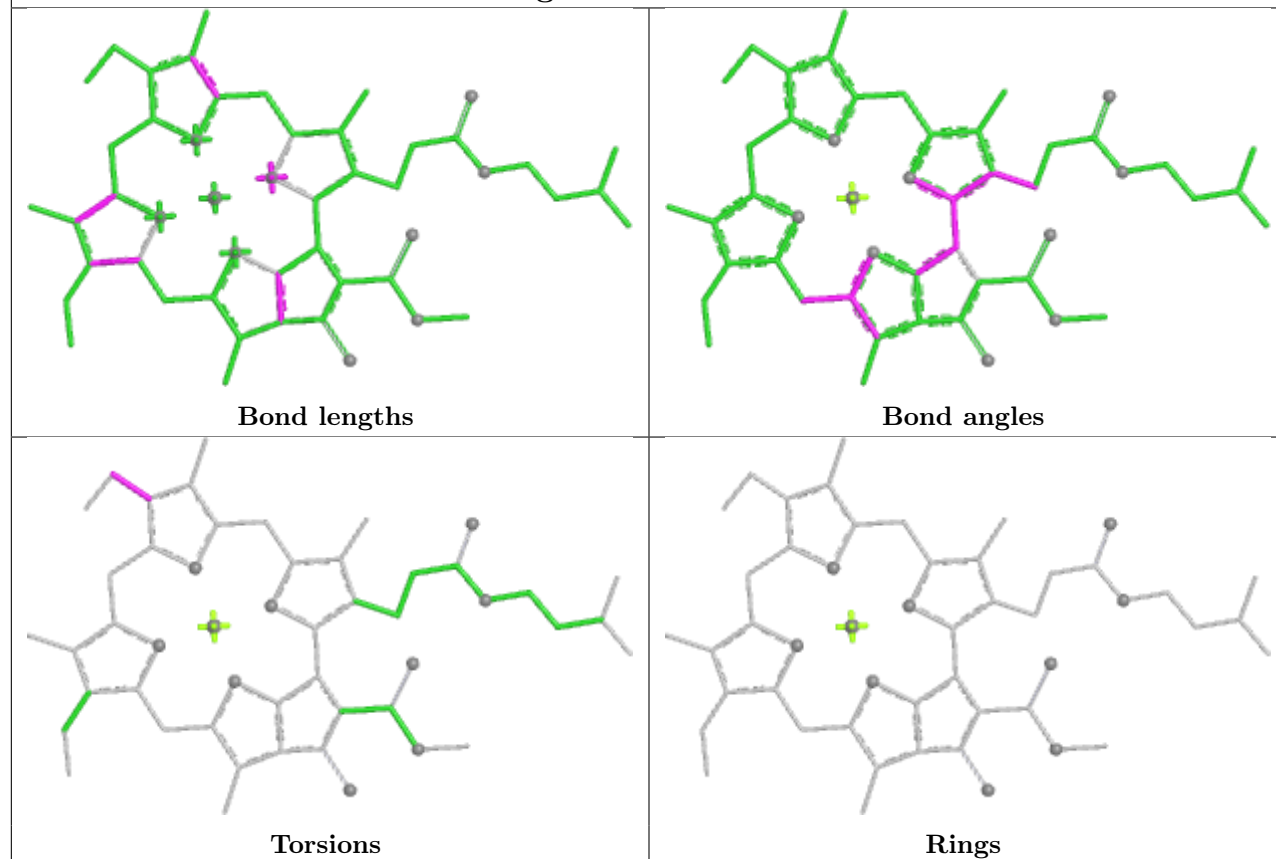


Rings

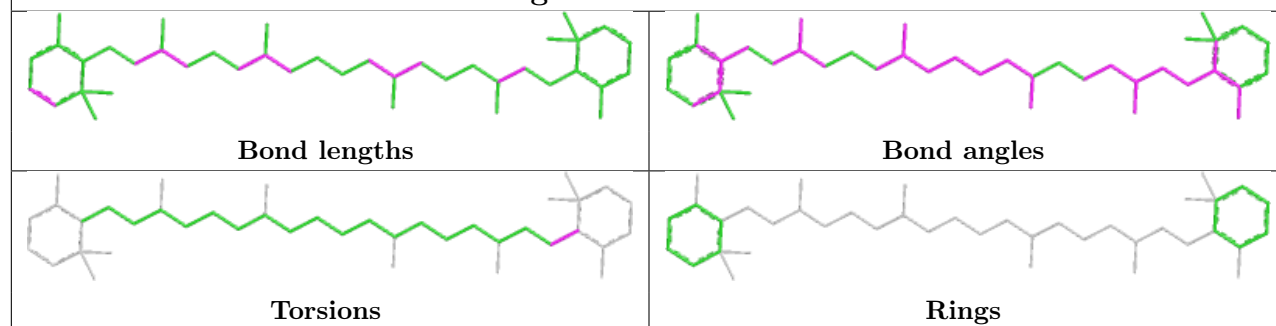


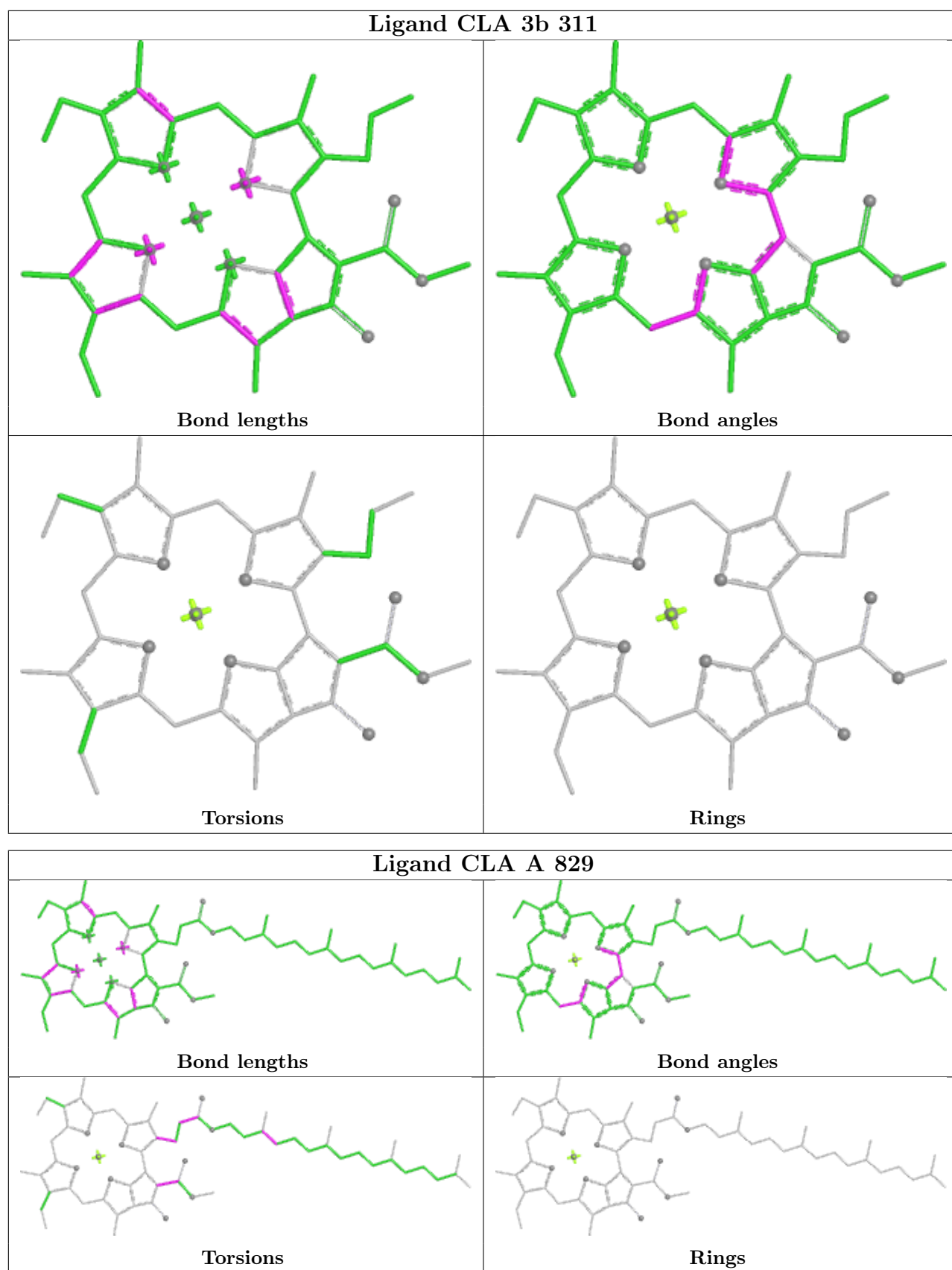


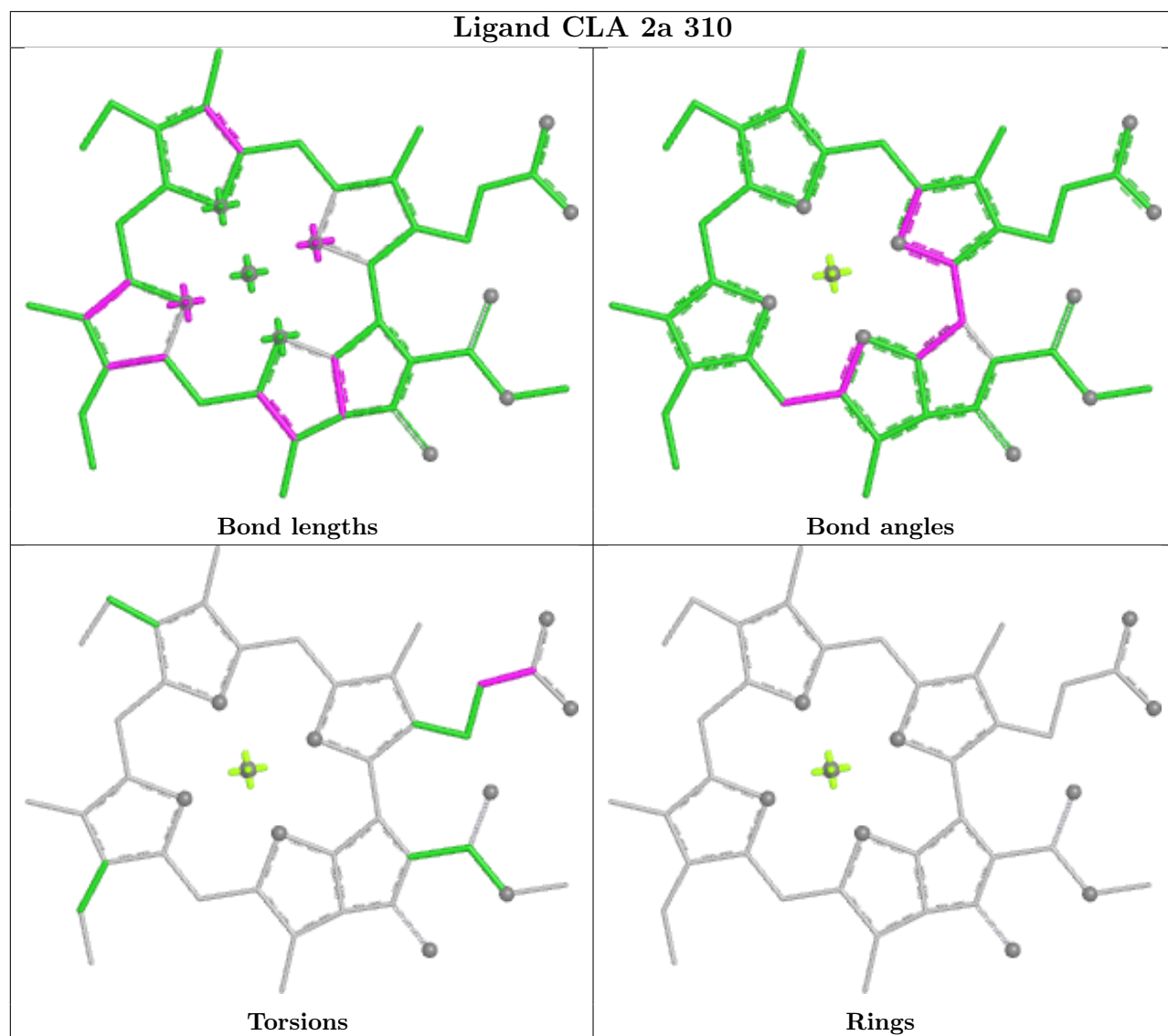
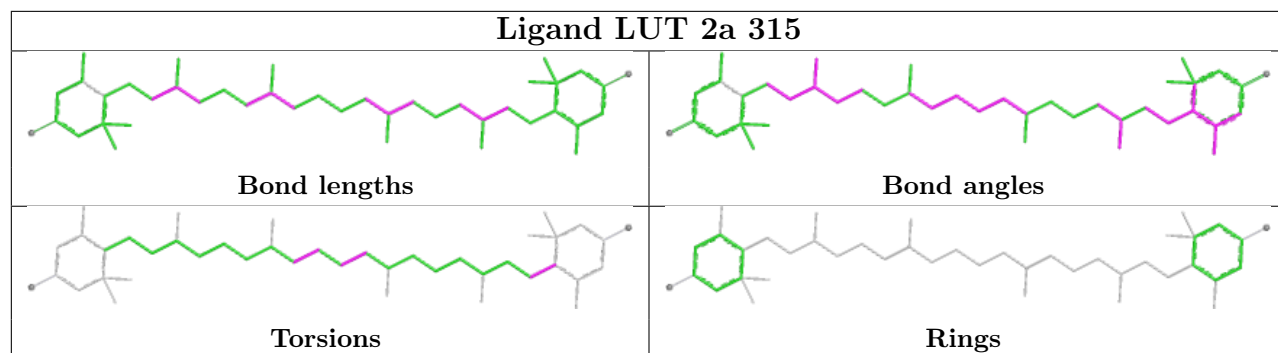
## Ligand CLA a 813

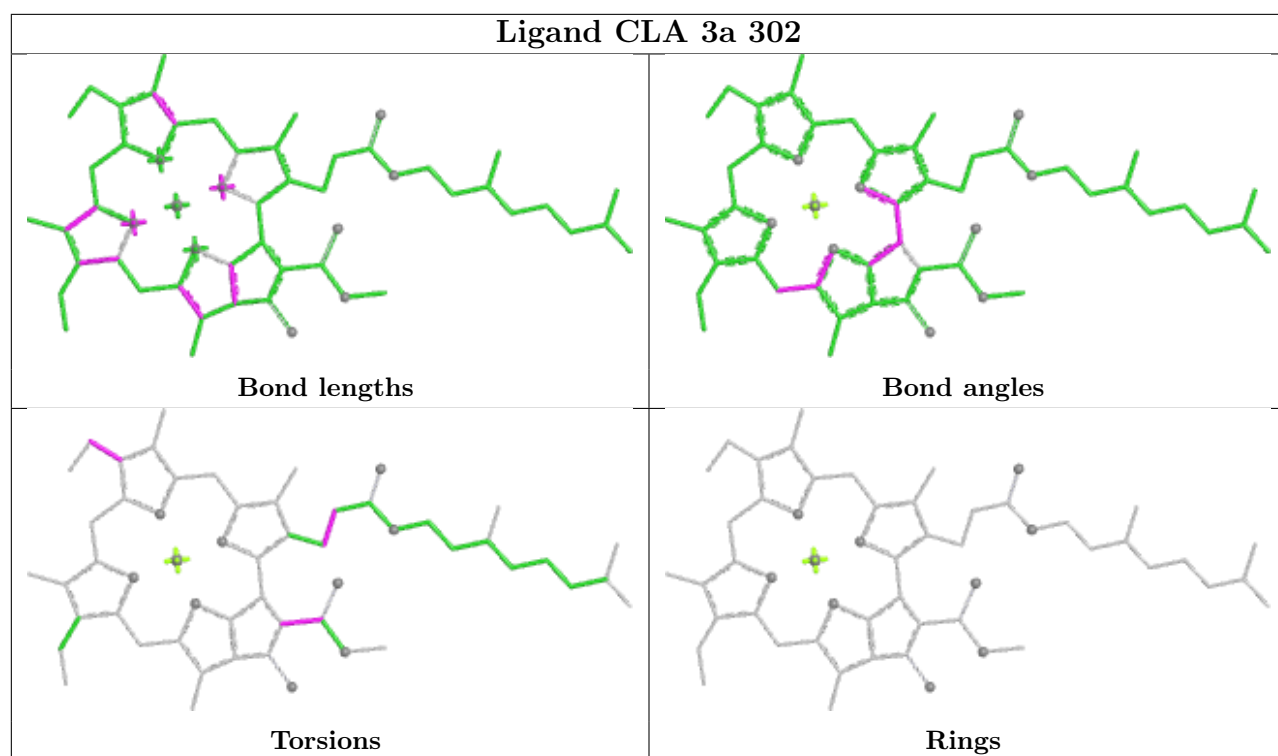


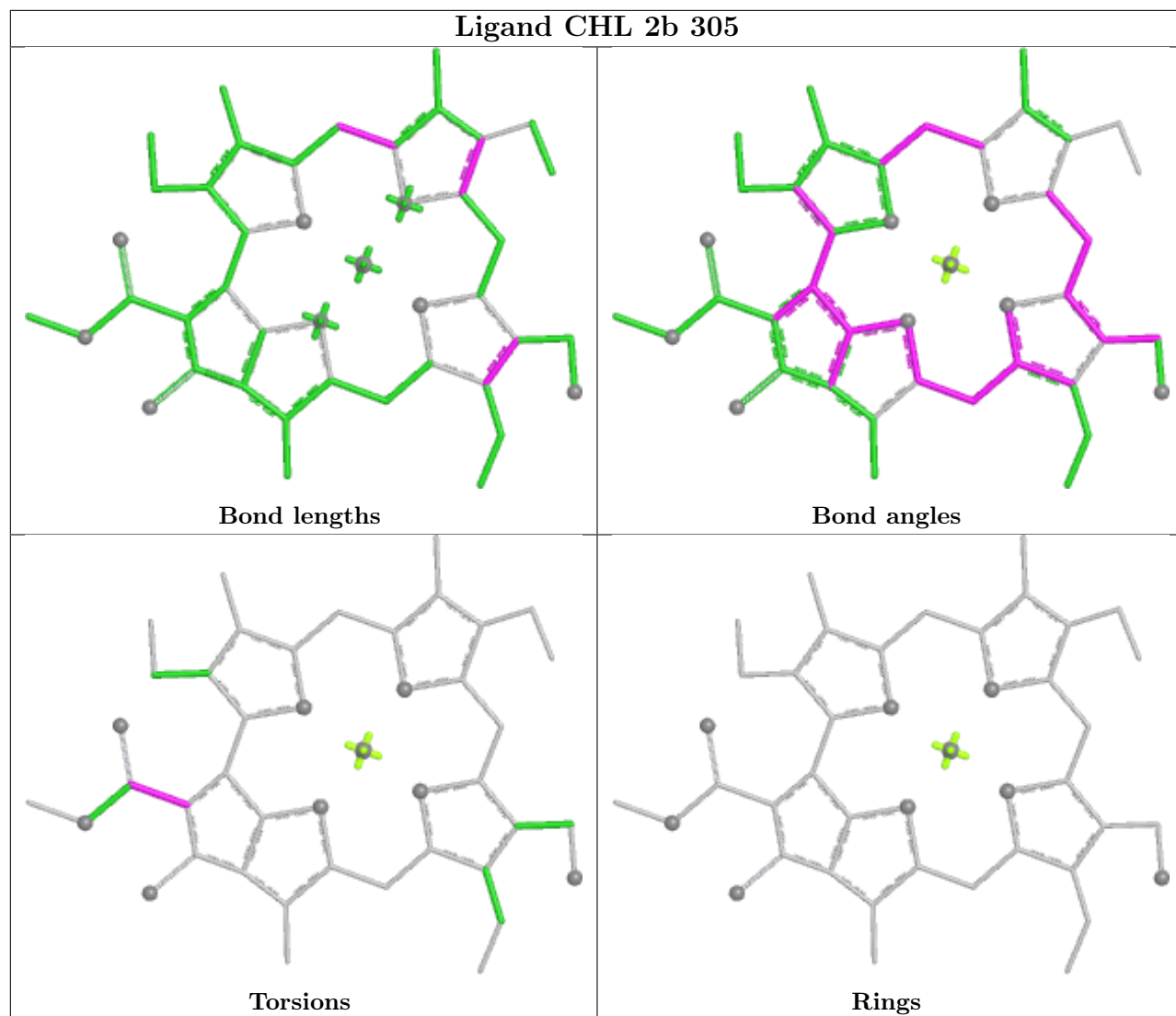
## Ligand BCR B 842





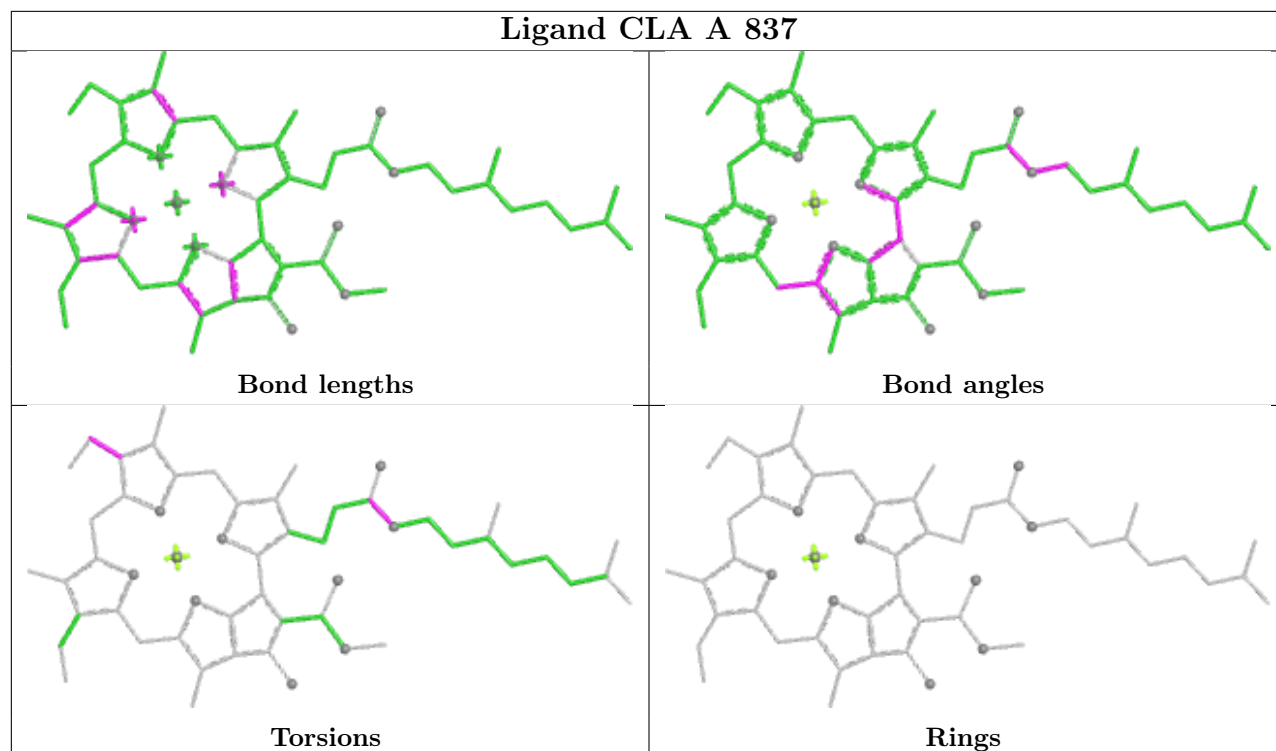




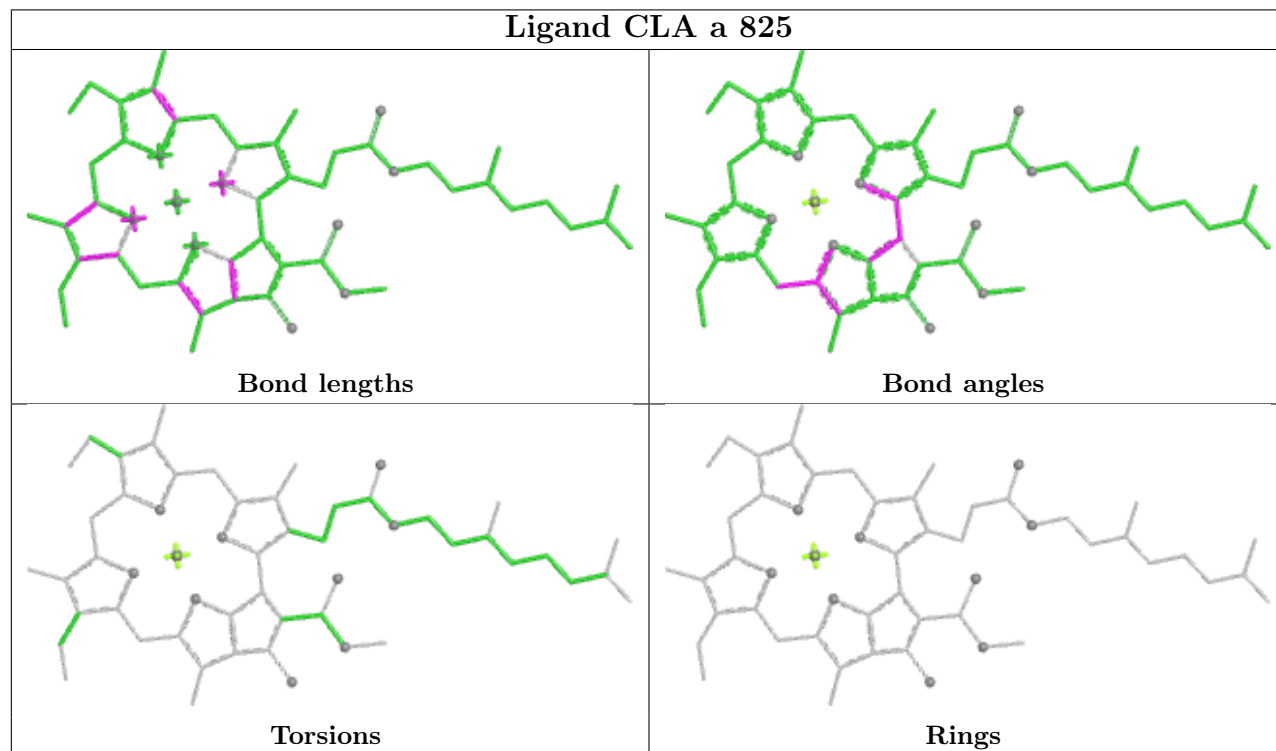


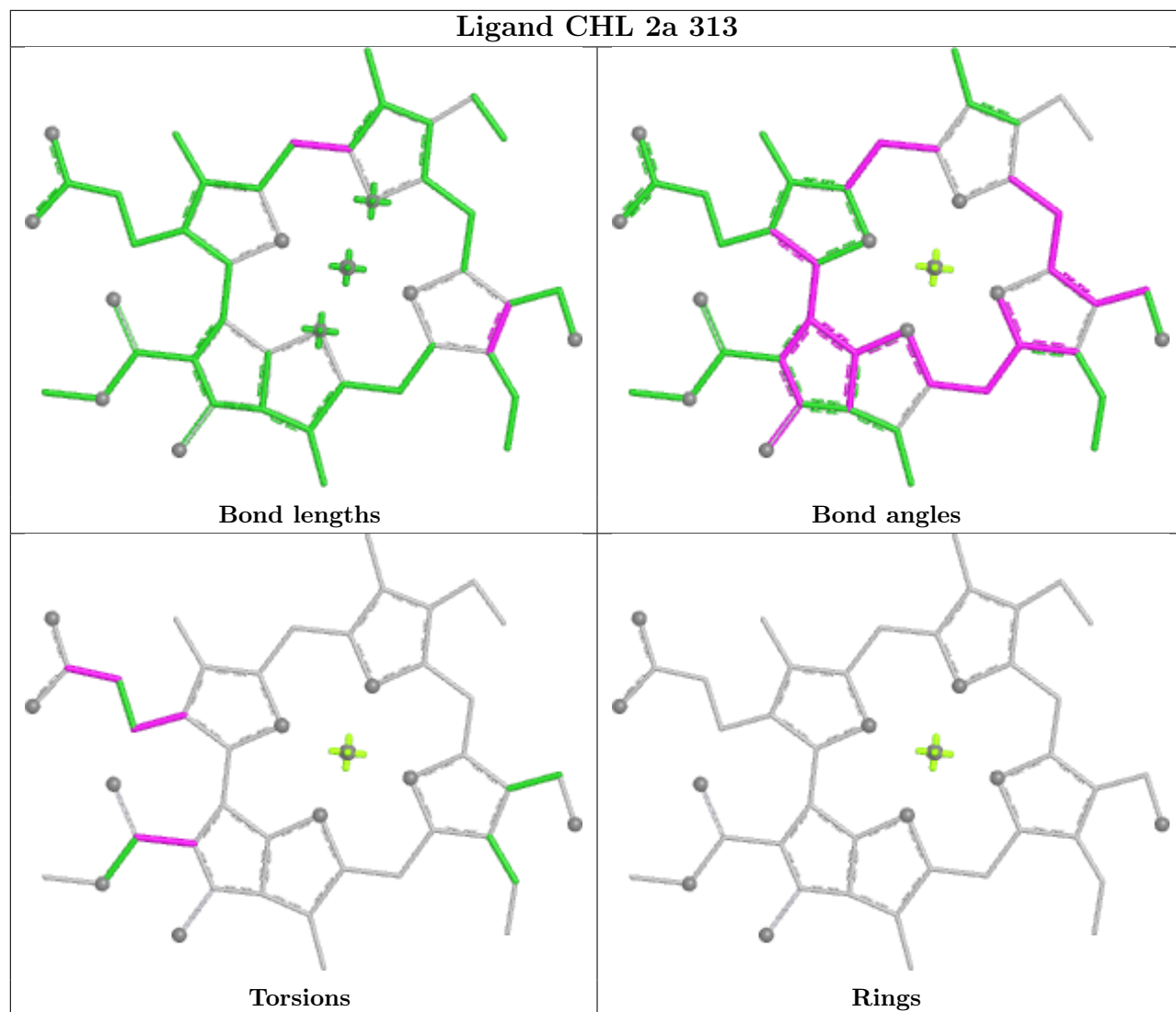


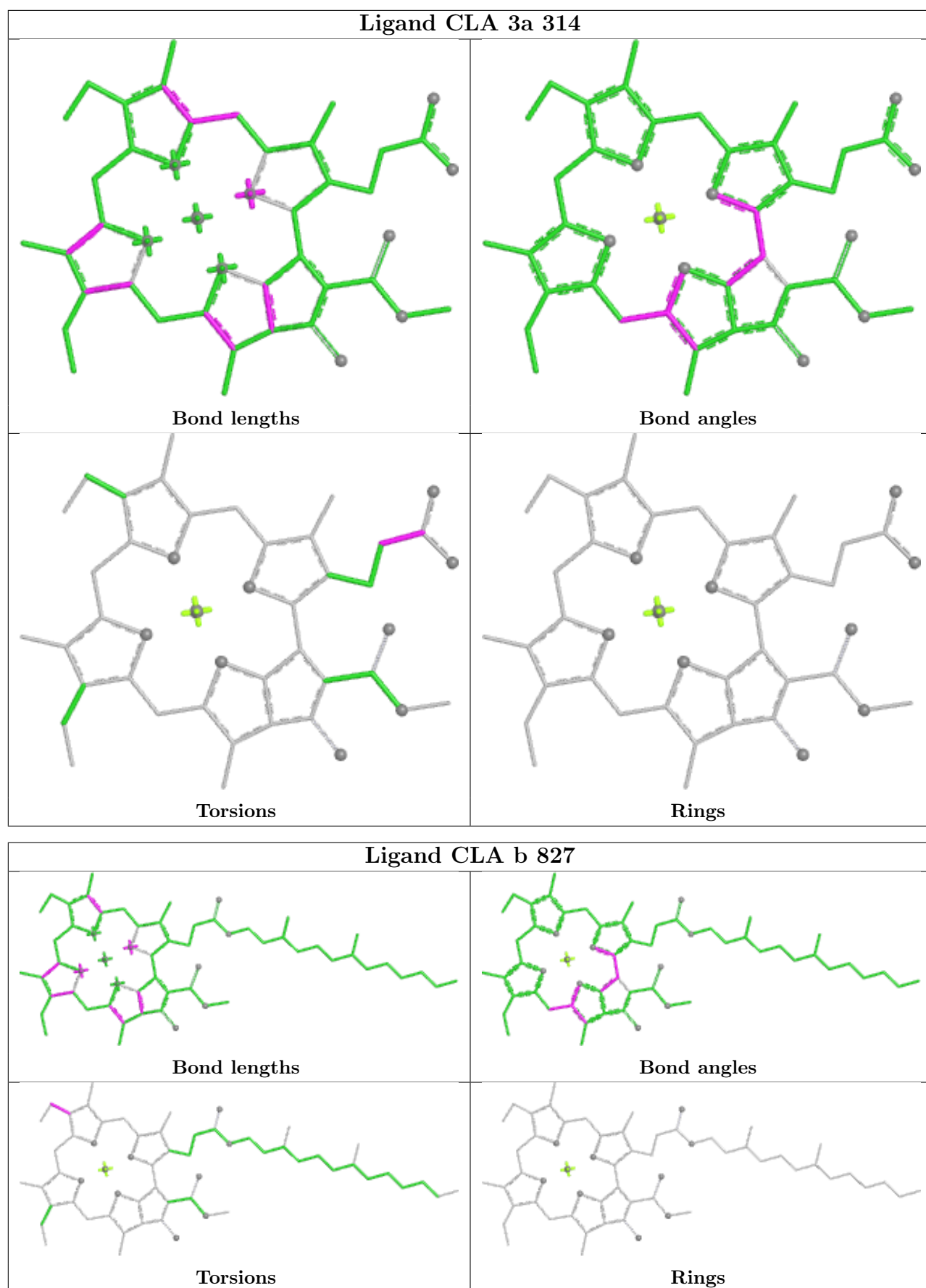
## Ligand CLA A 837

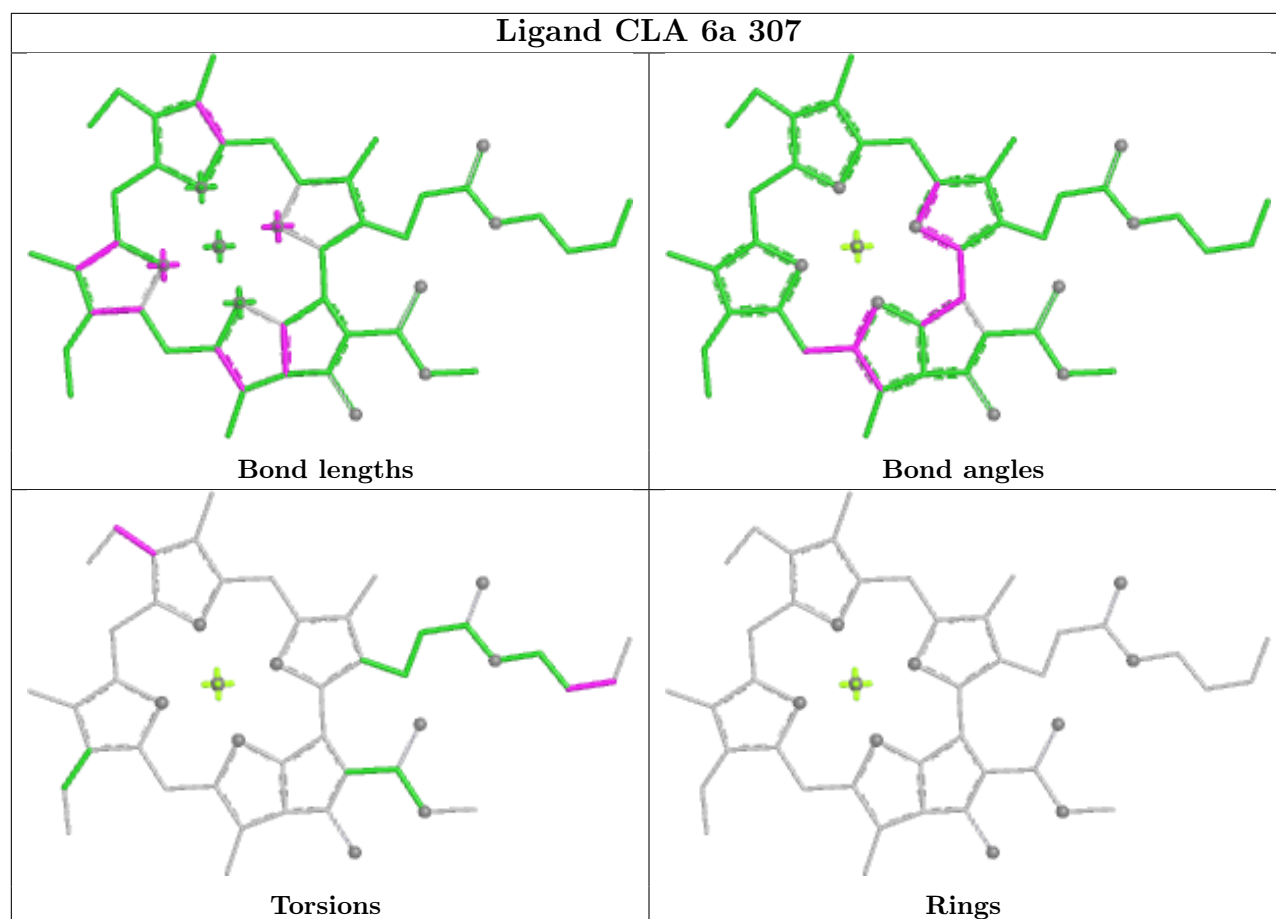
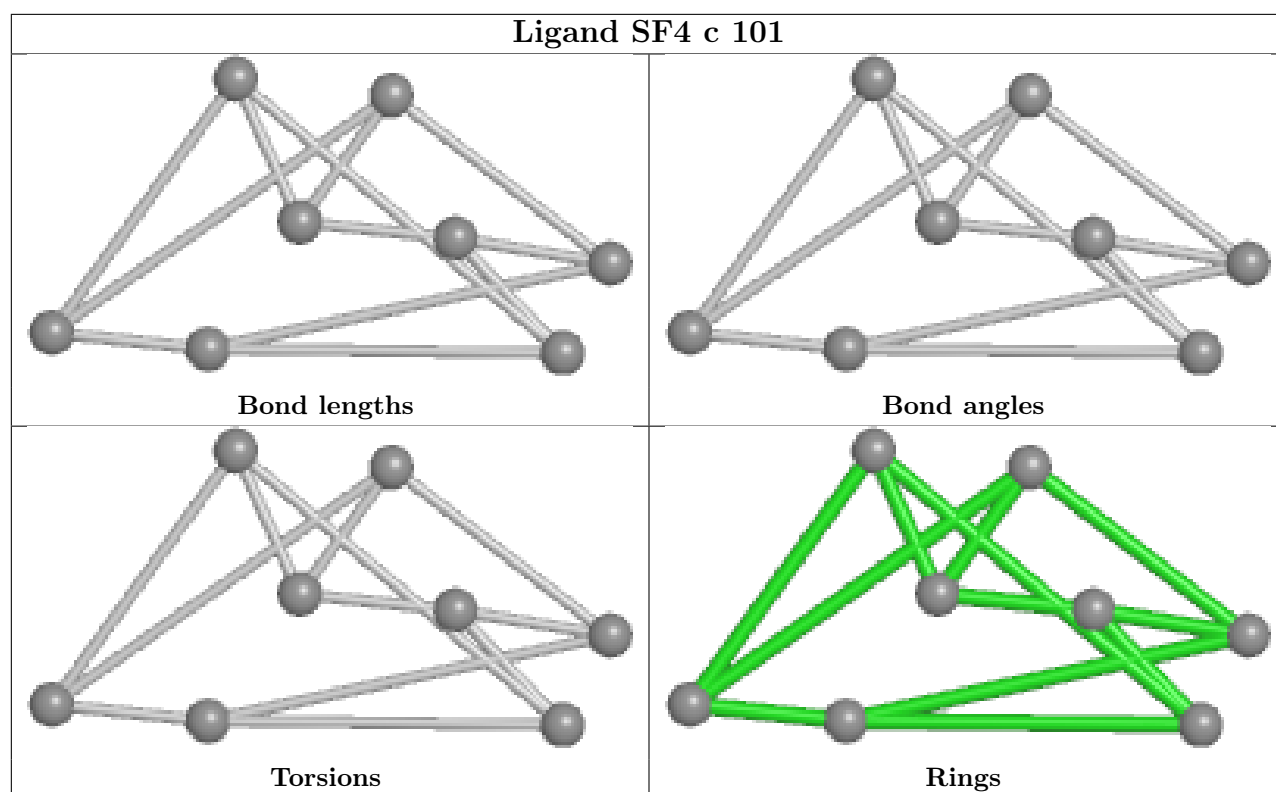


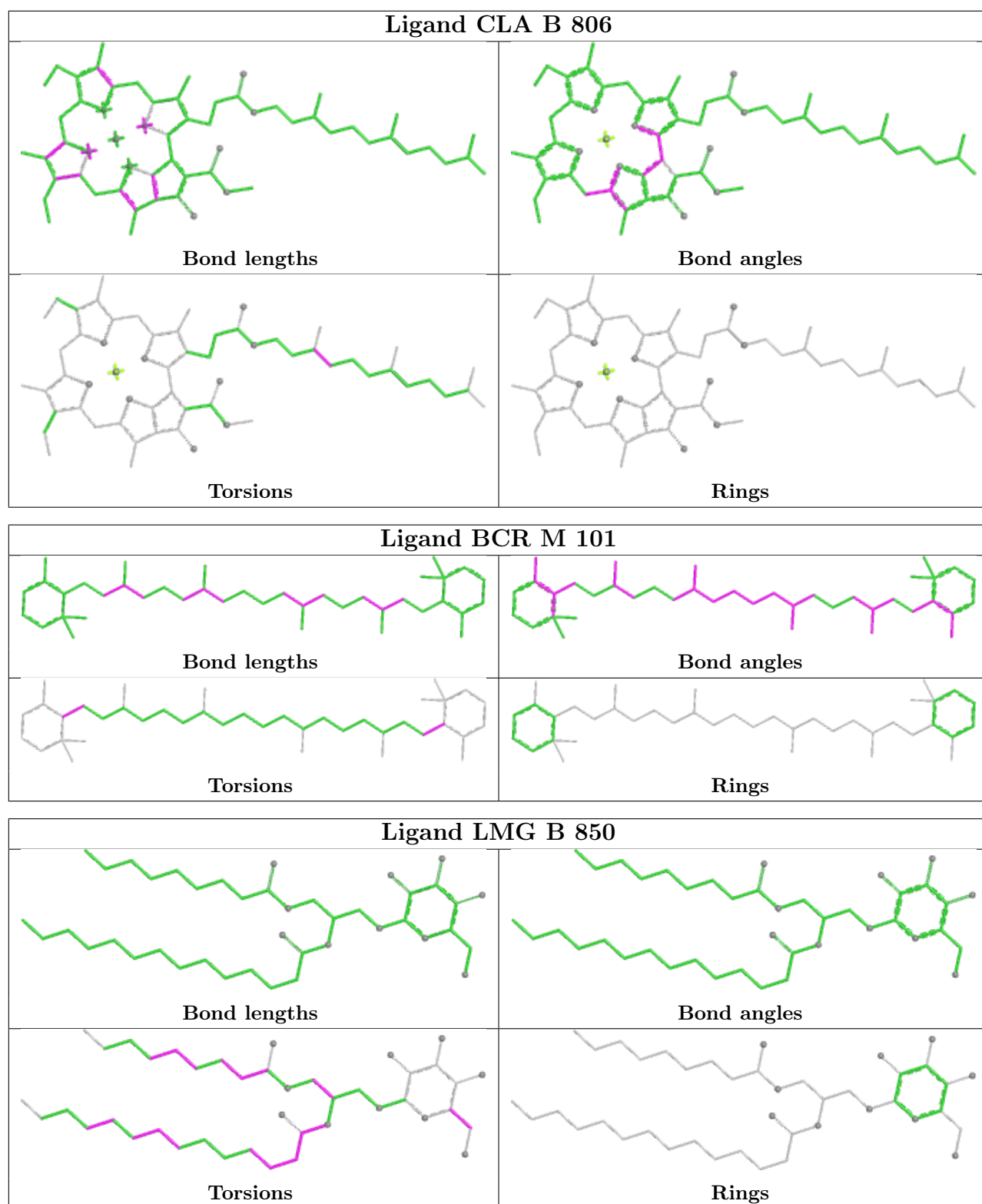
## Ligand CLA a 825



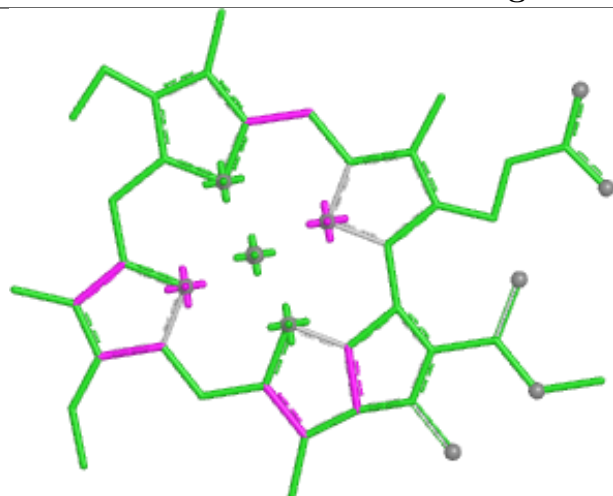




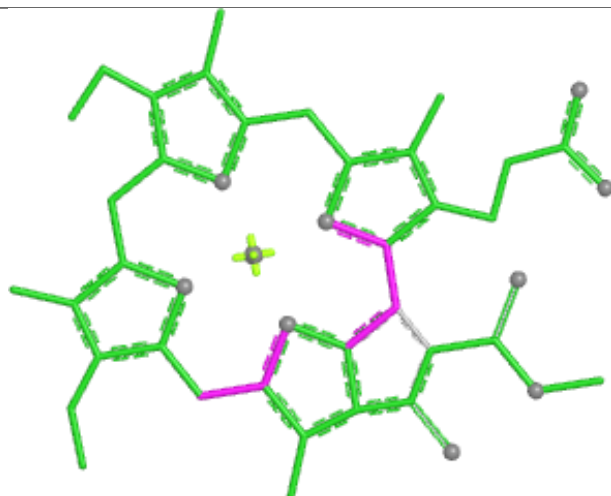




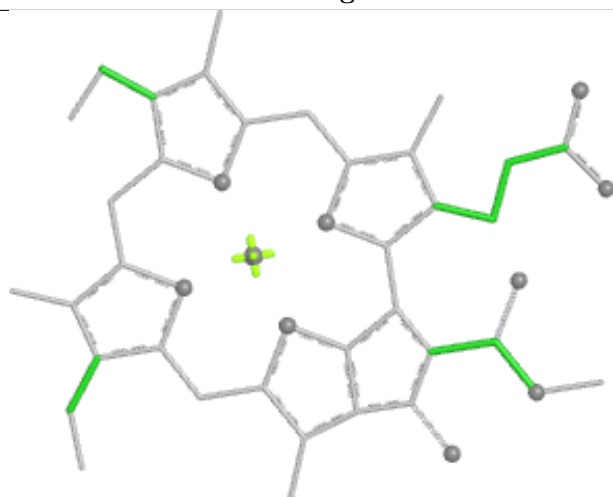
## Ligand CLA 3b 308



Bond lengths



Bond angles

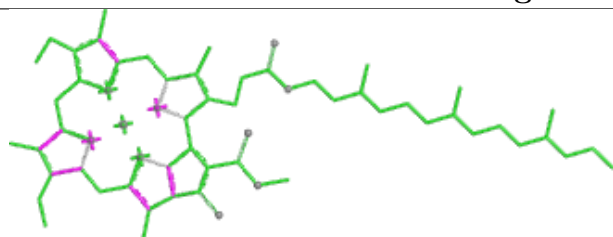


Torsions

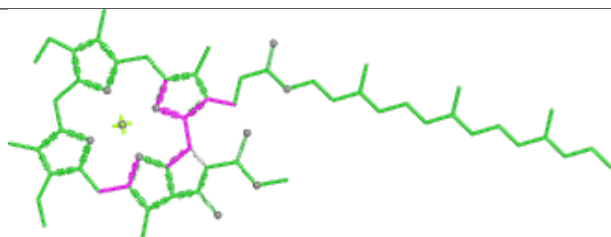


Rings

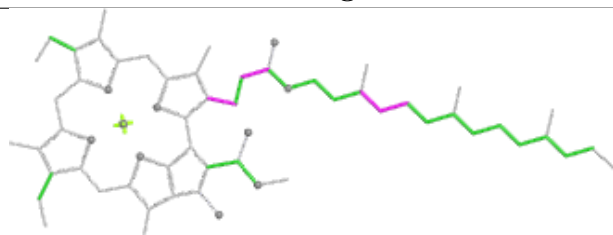
## Ligand CLA B 816



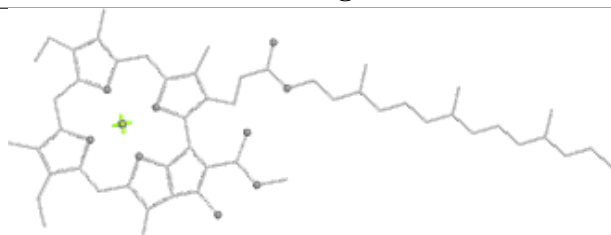
Bond lengths



Bond angles

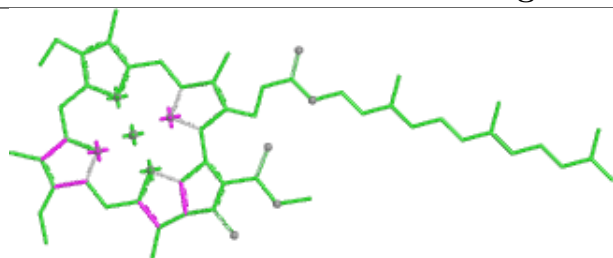


Torsions

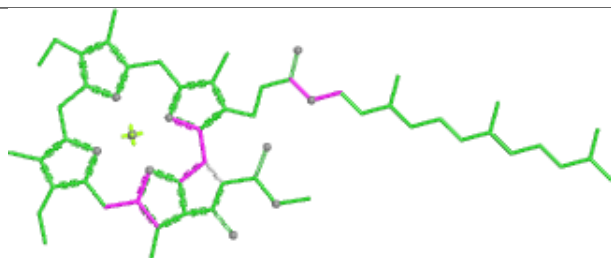


Rings

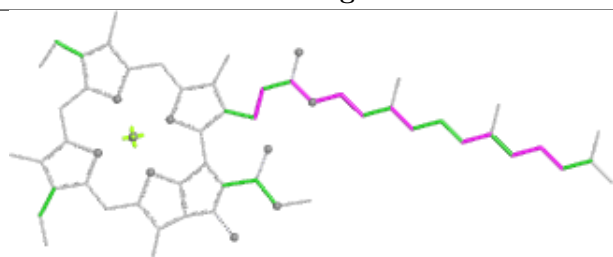
## Ligand CLA b 830



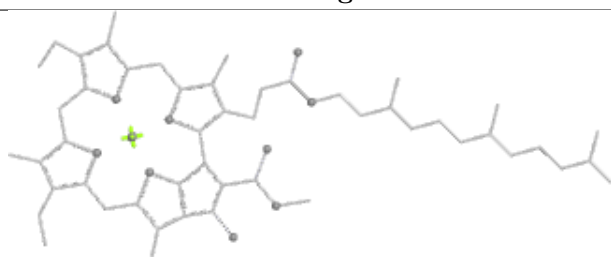
Bond lengths



Bond angles

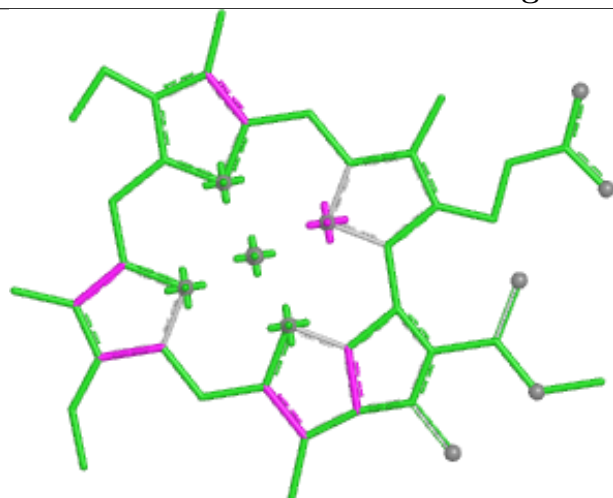


Torsions

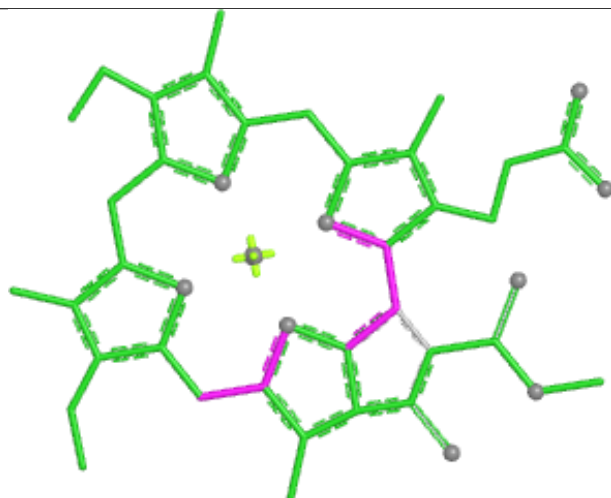


Rings

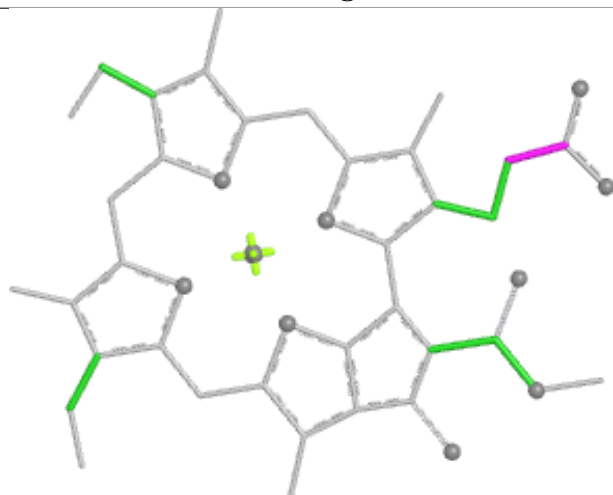
## Ligand CLA f 302



Bond lengths



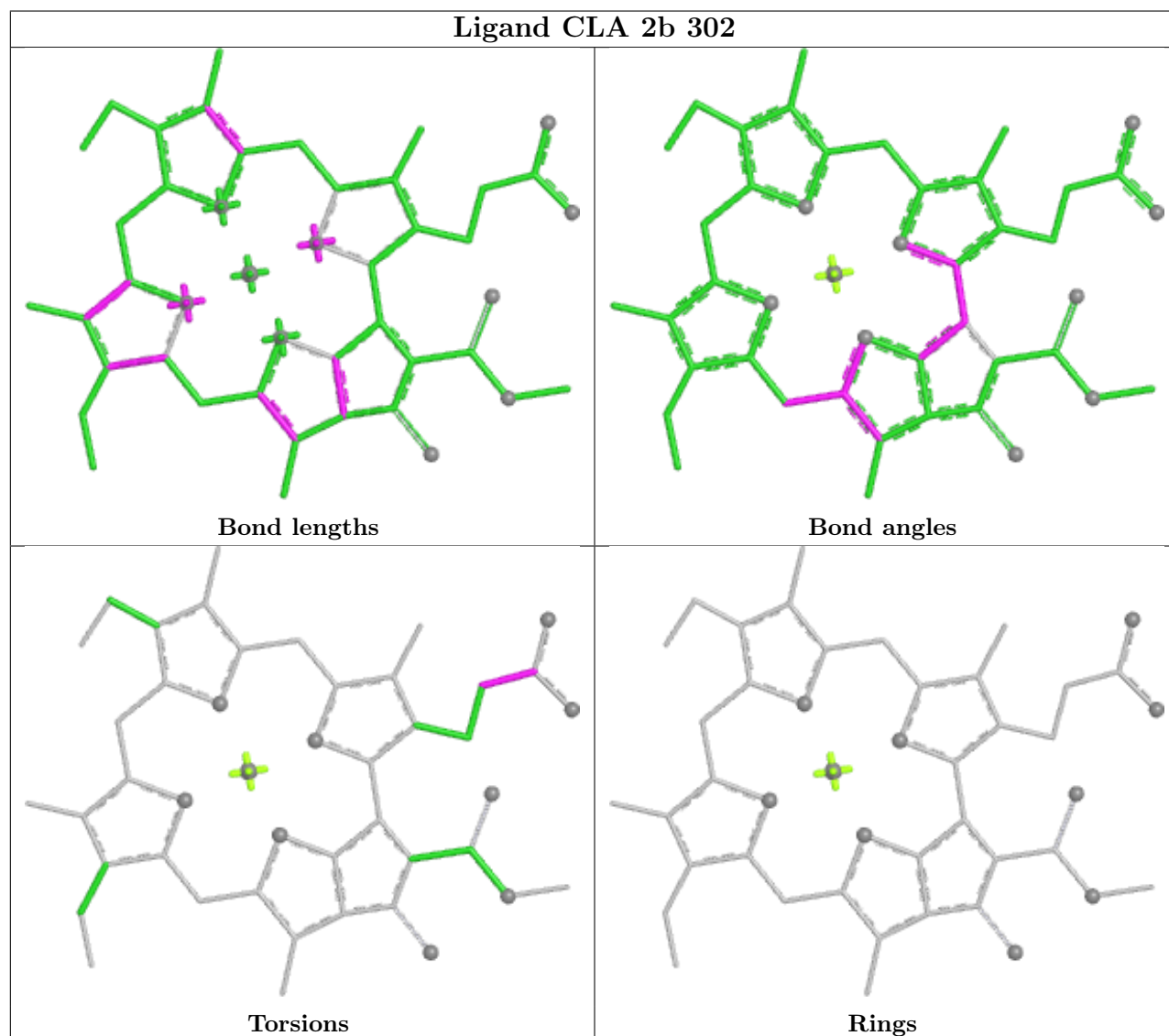
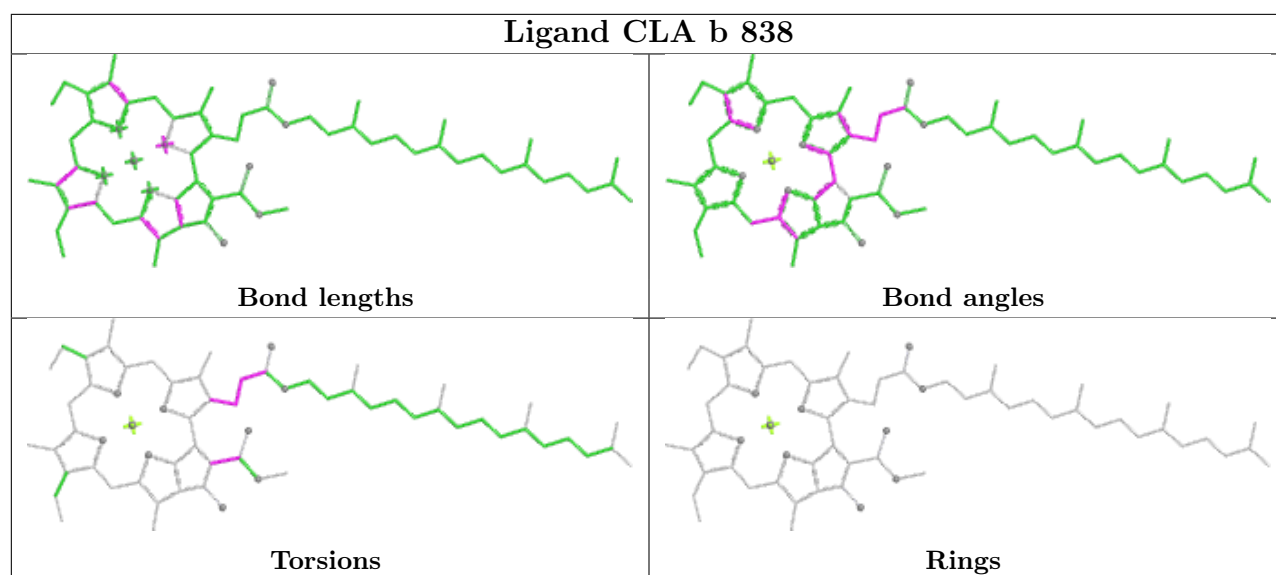
Bond angles



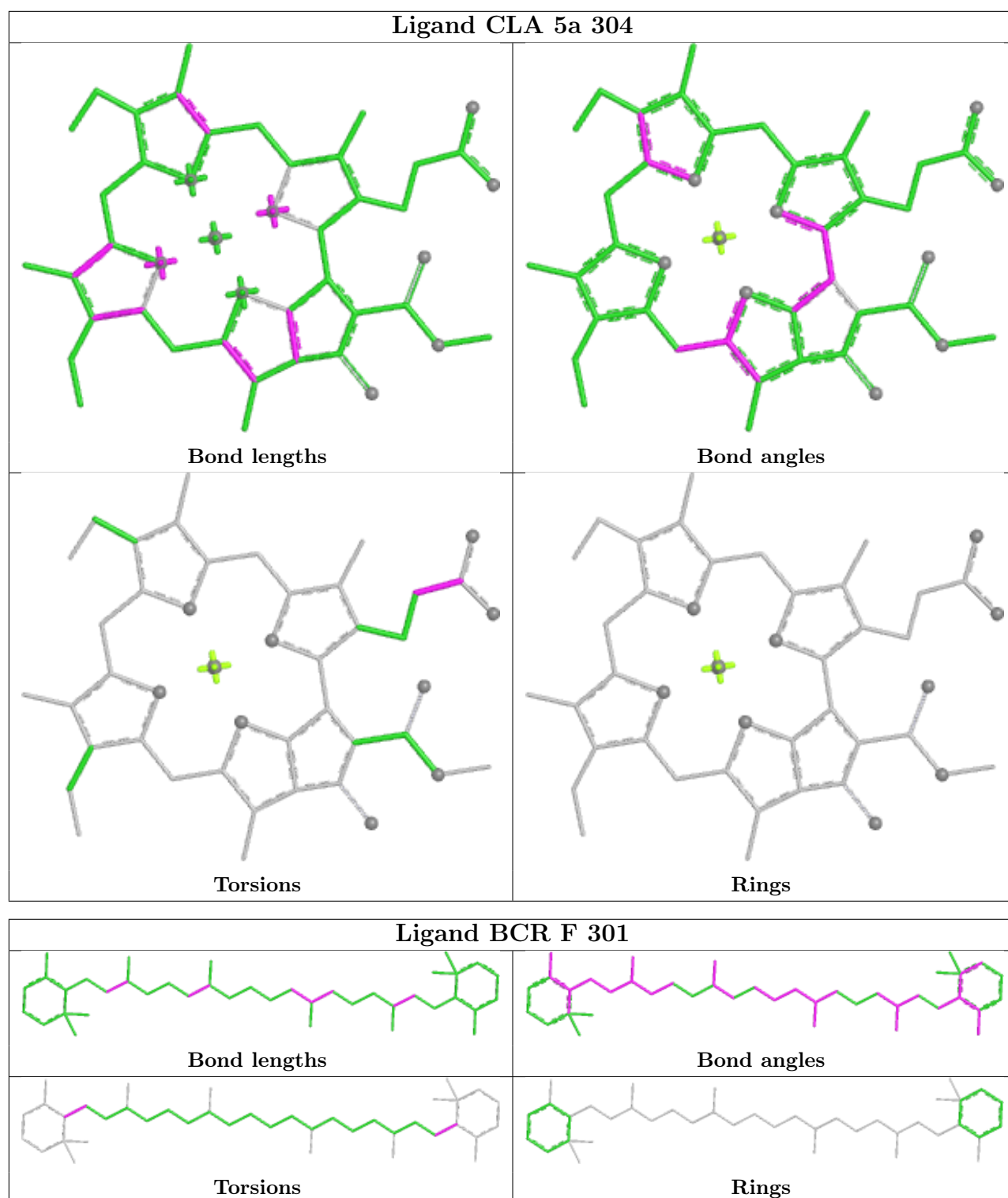
Torsions

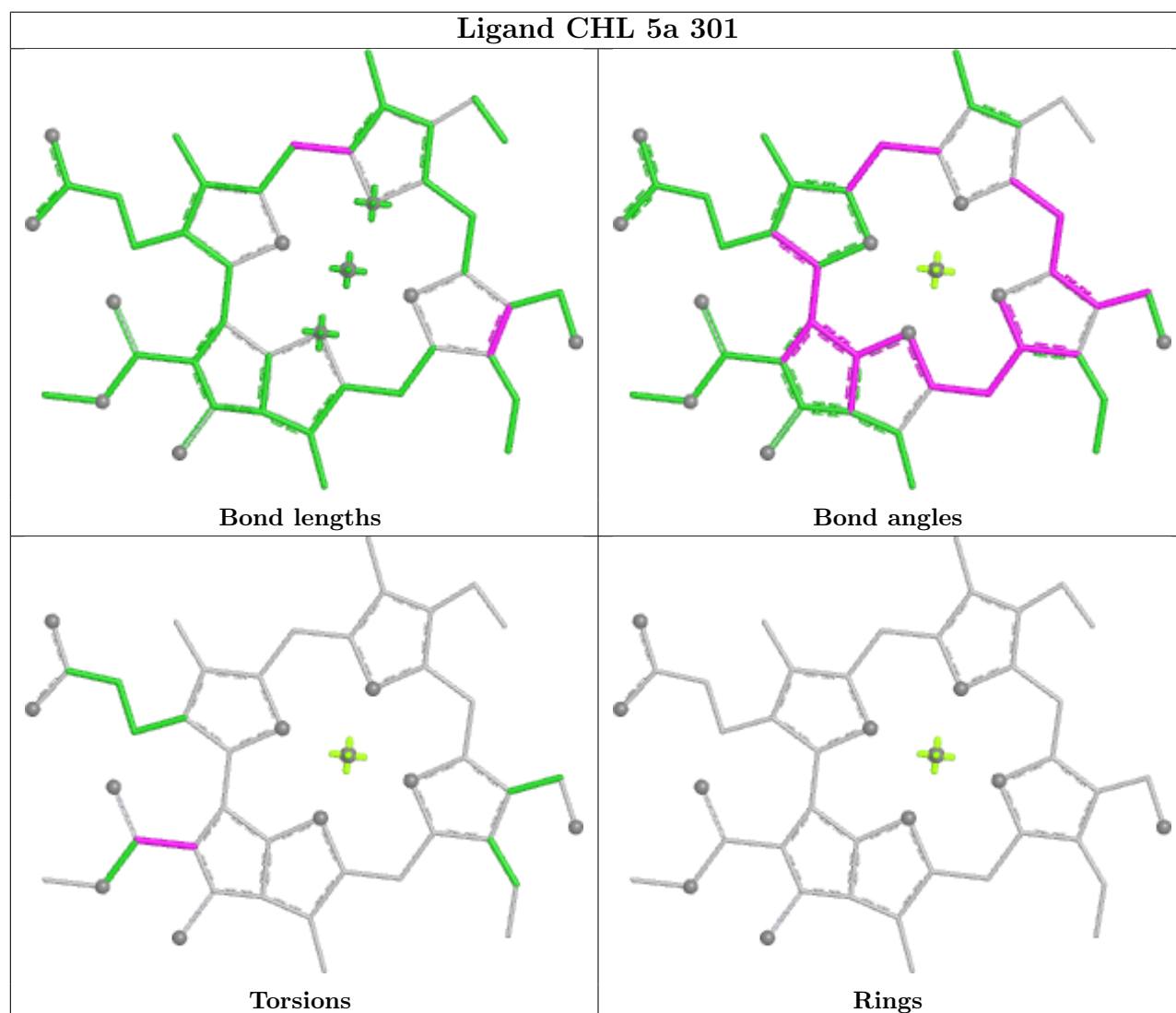
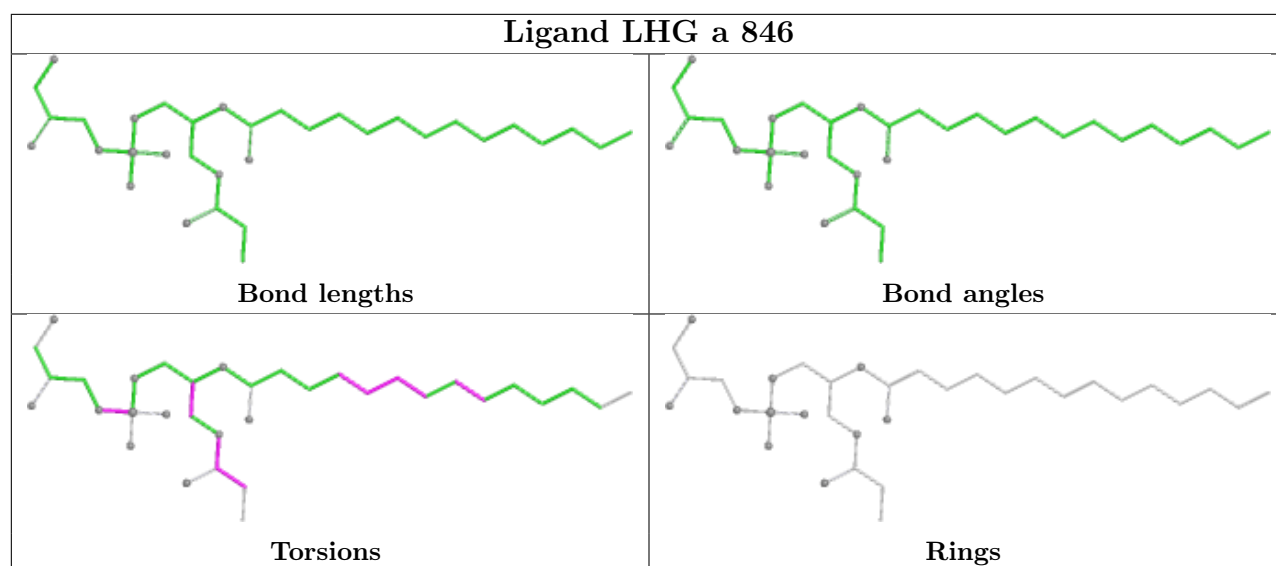


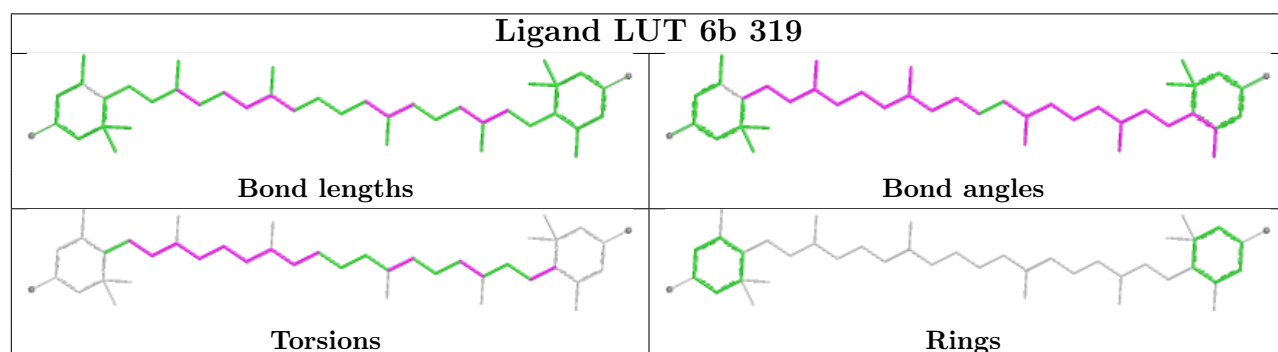
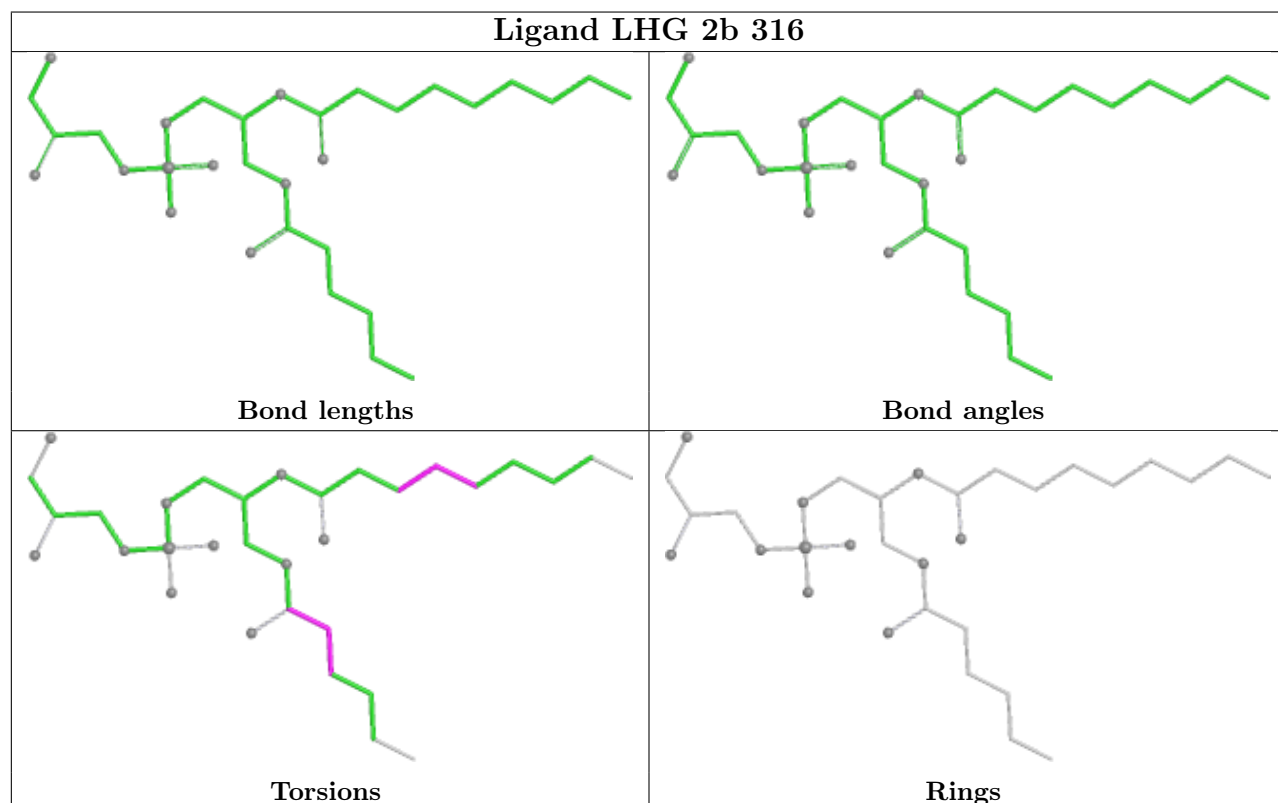
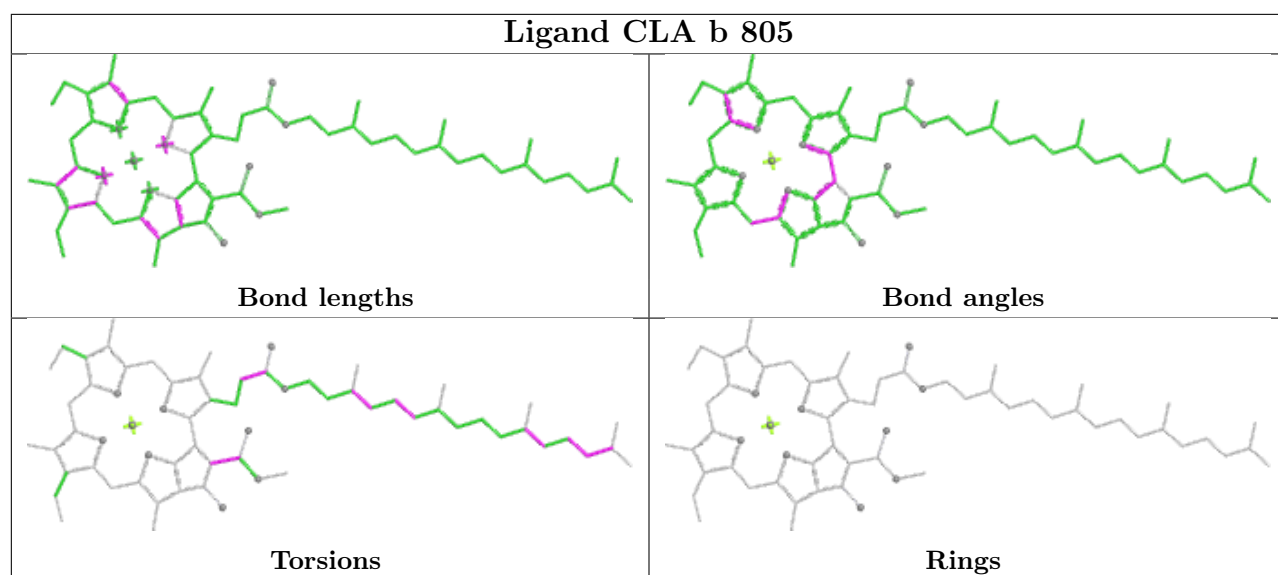
Rings

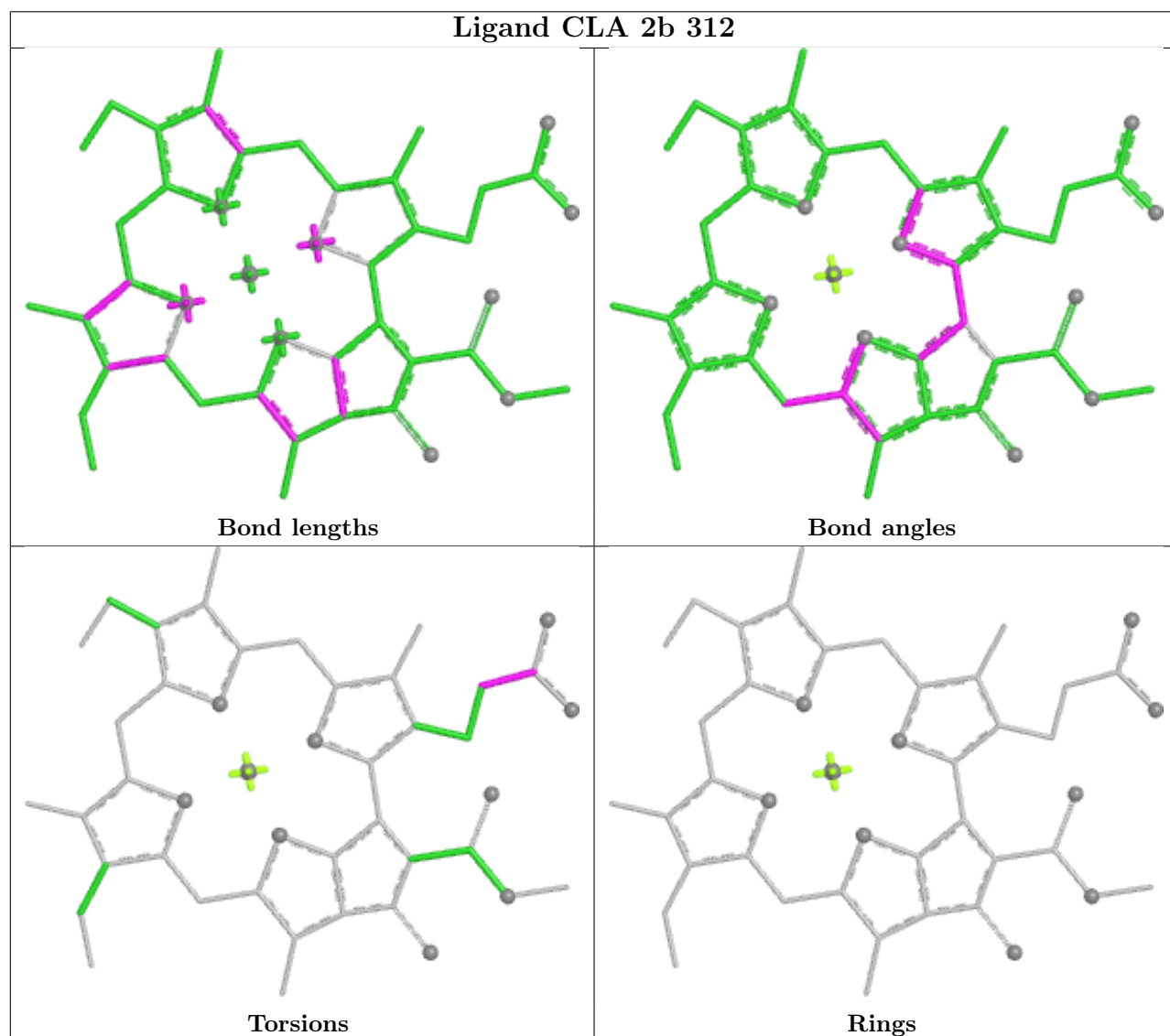
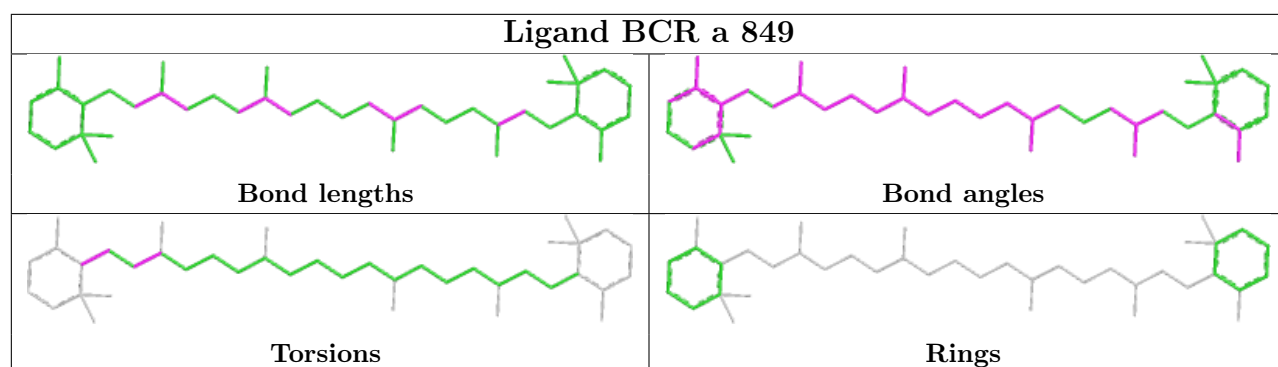


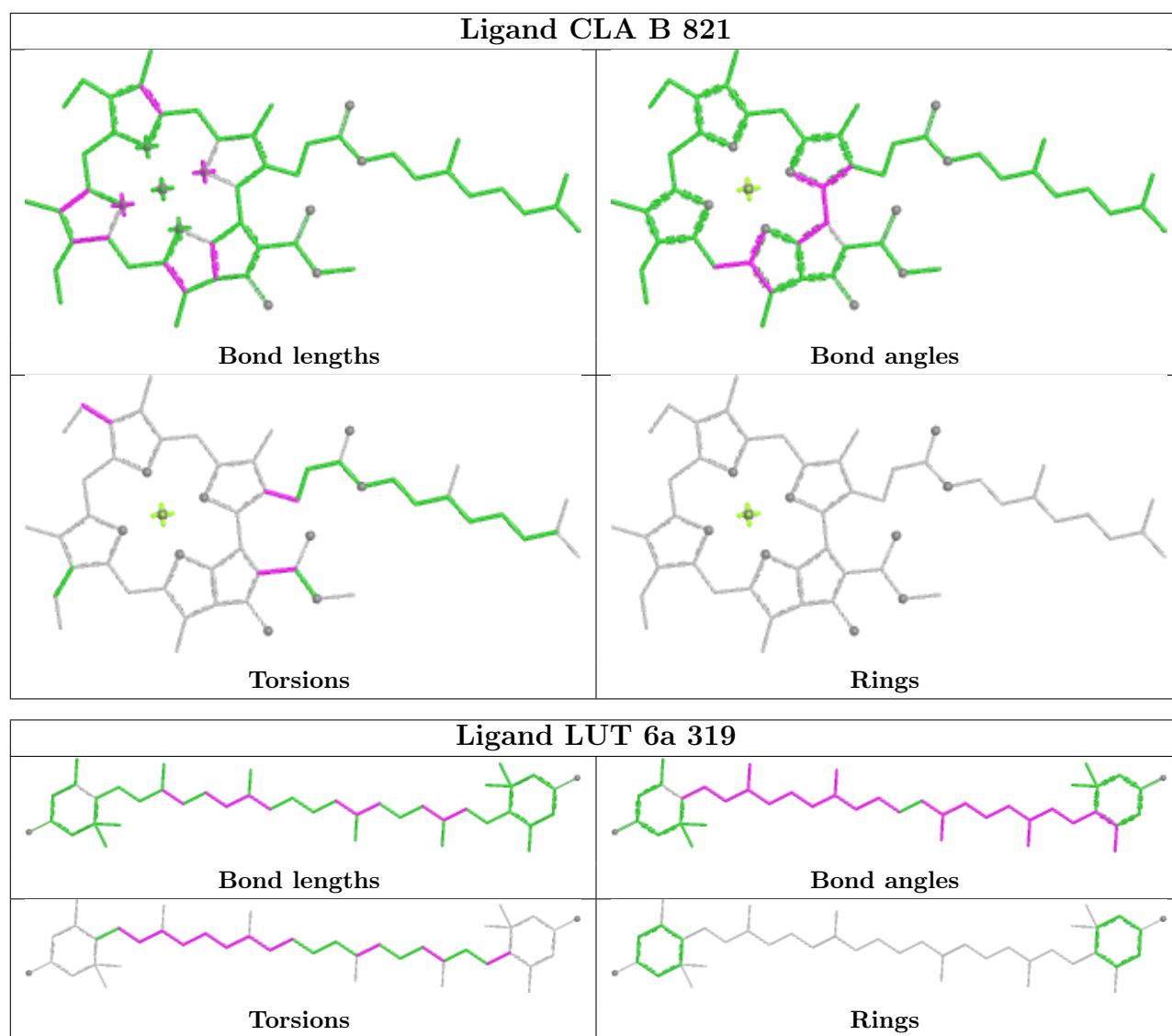




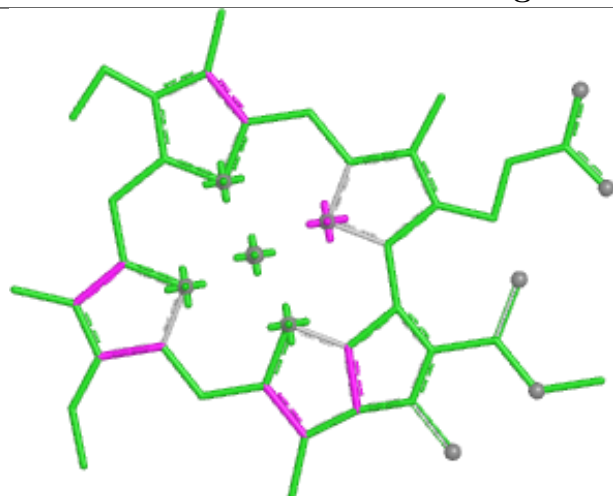




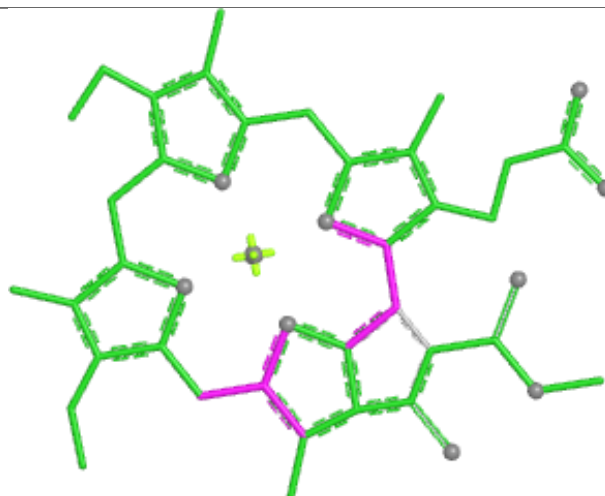




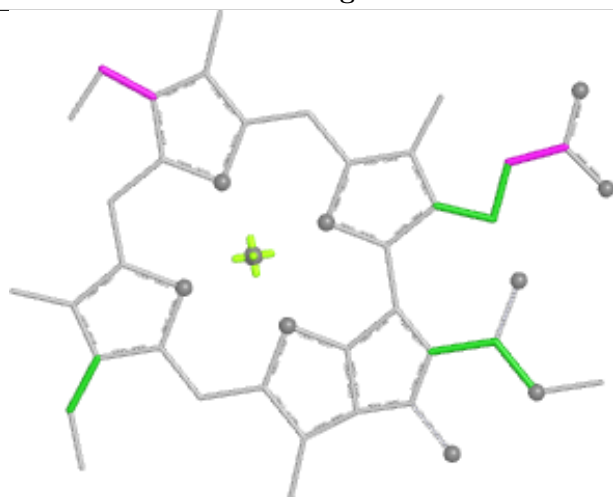
## Ligand CLA A 835



Bond lengths



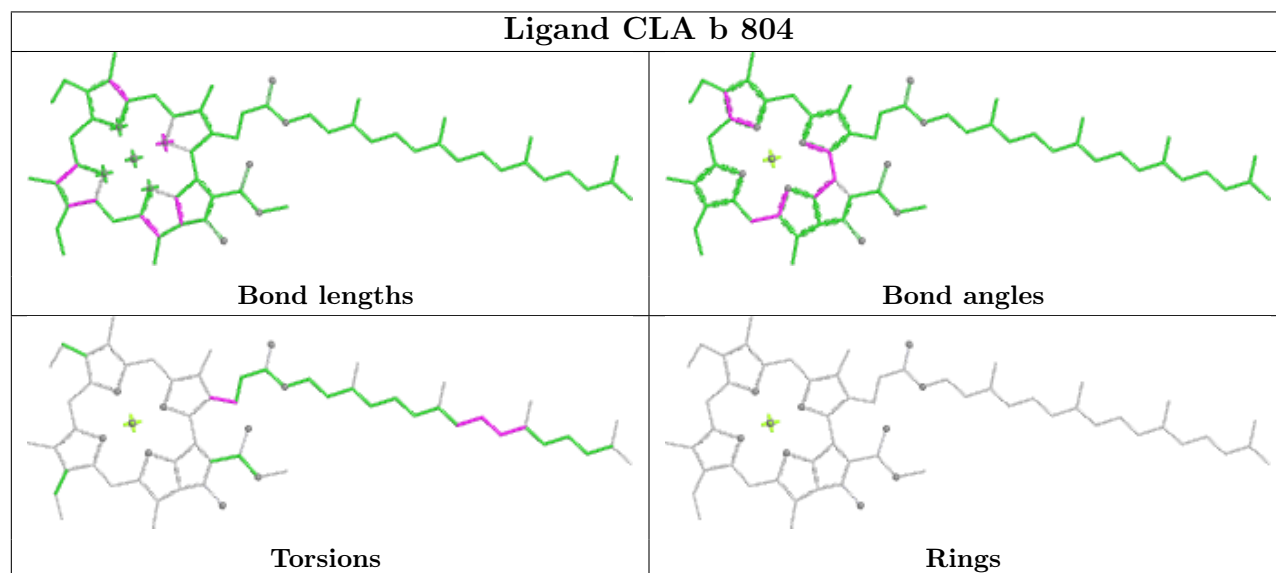
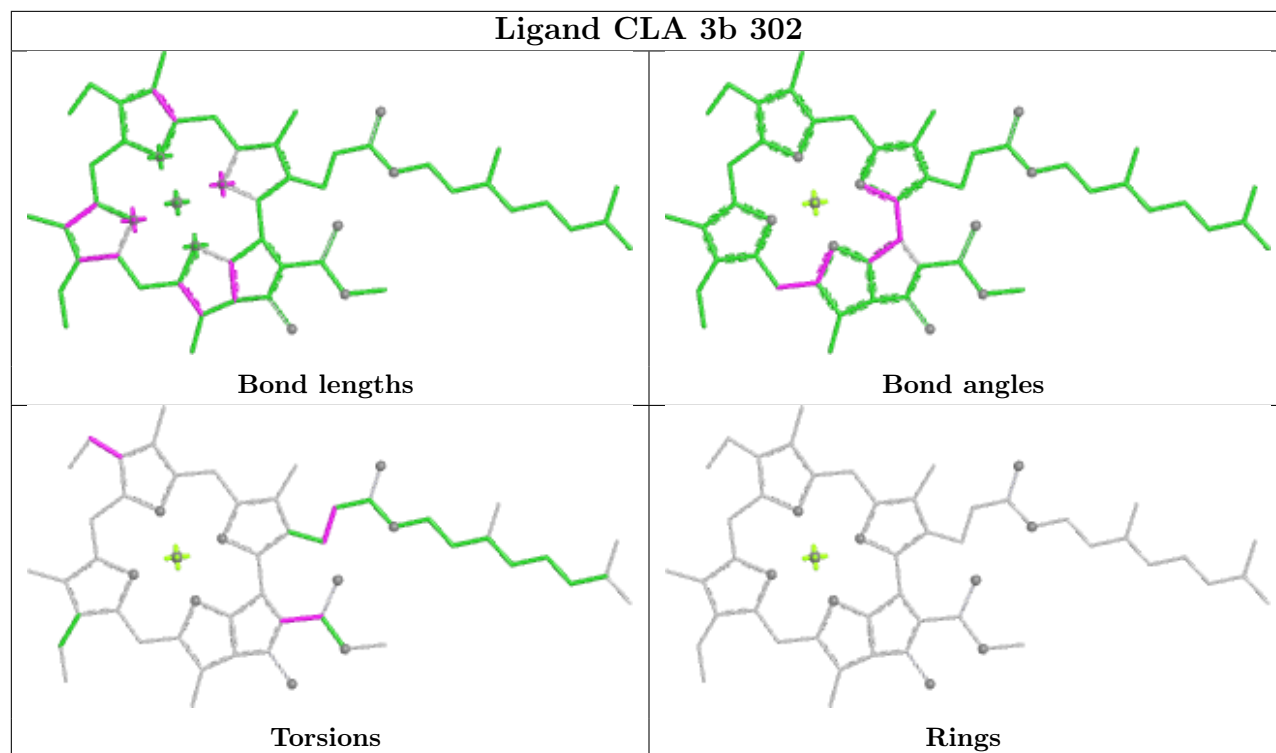
Bond angles

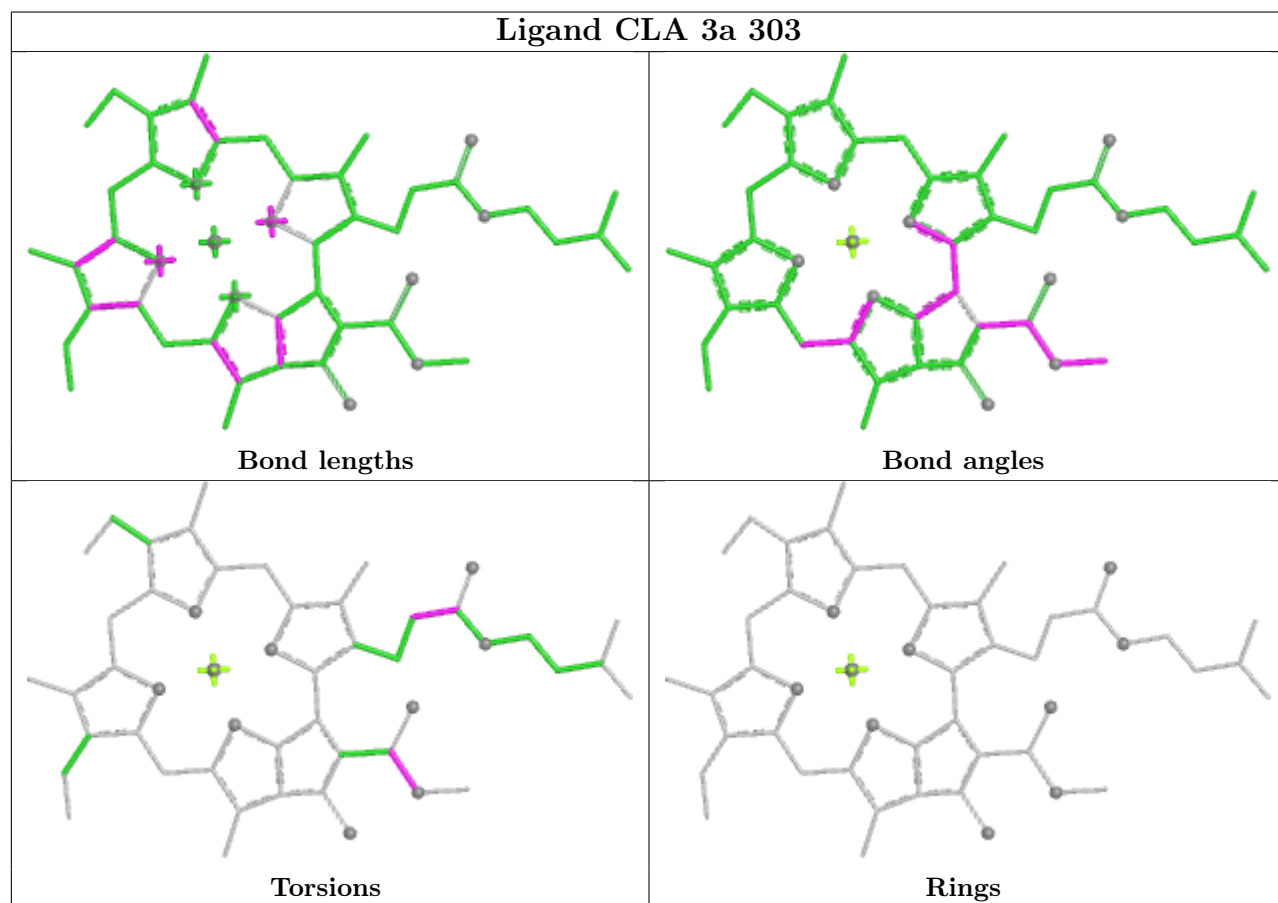
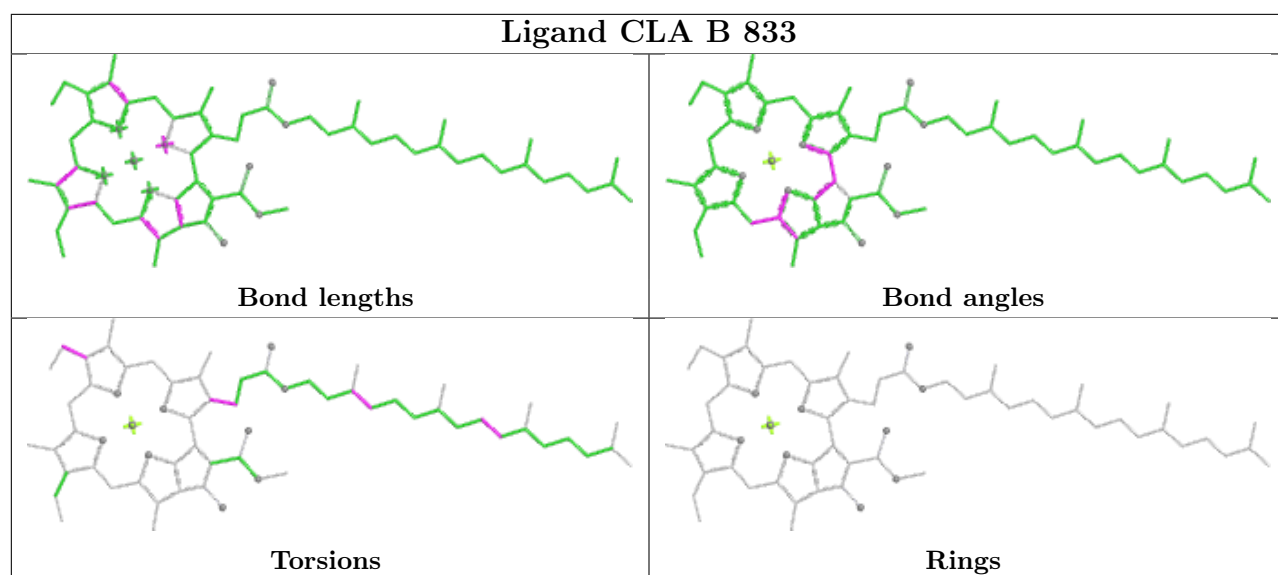


Torsions



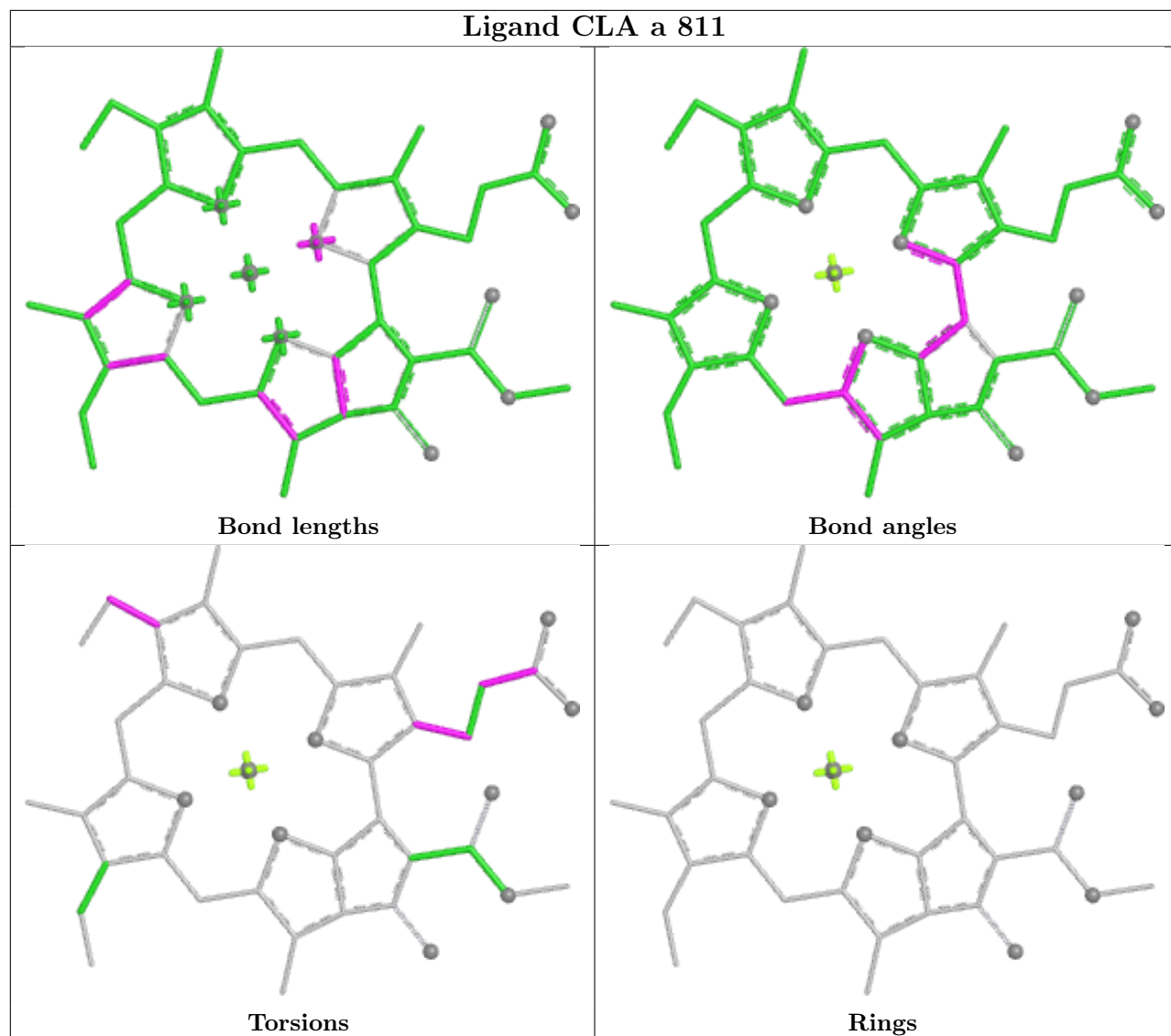
Rings



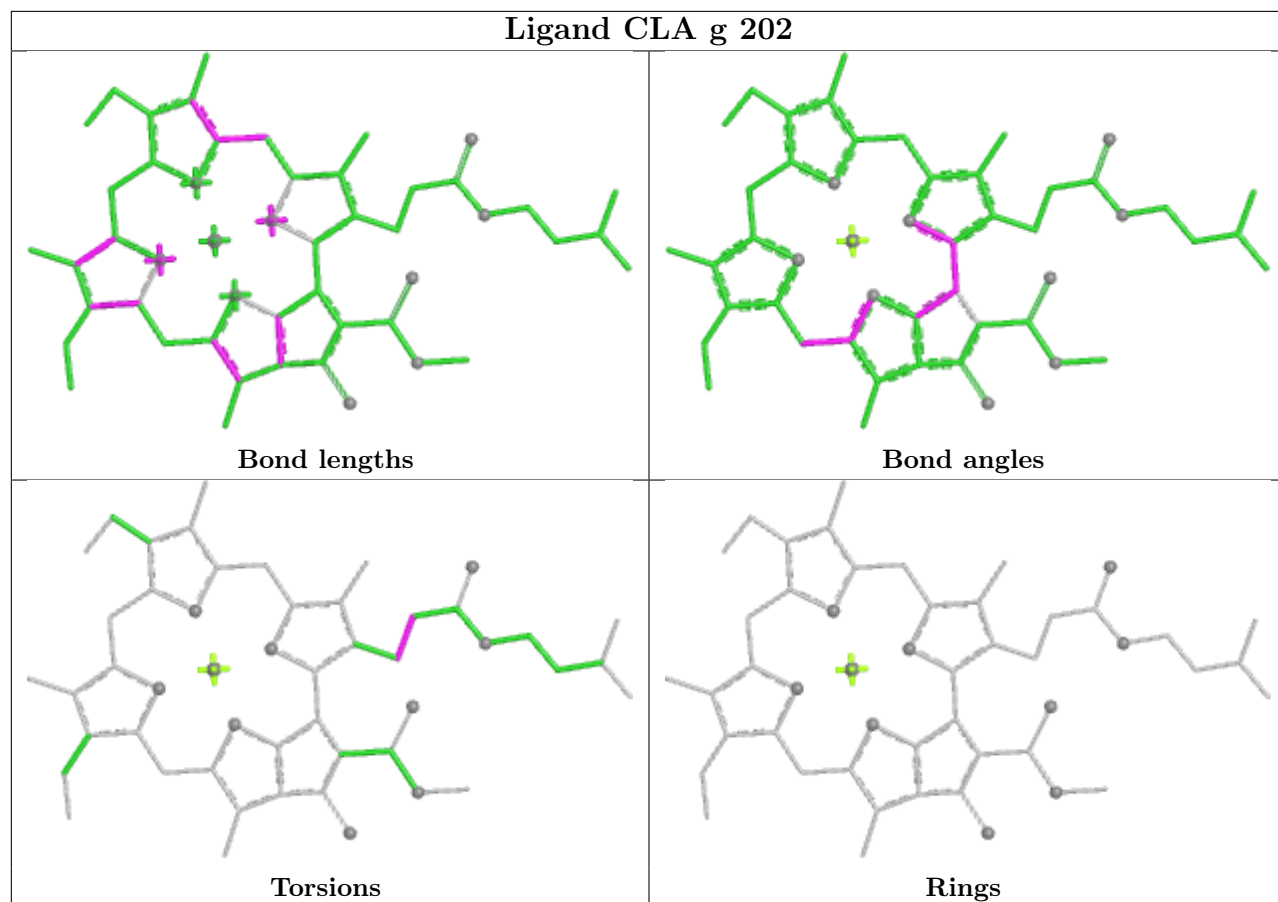


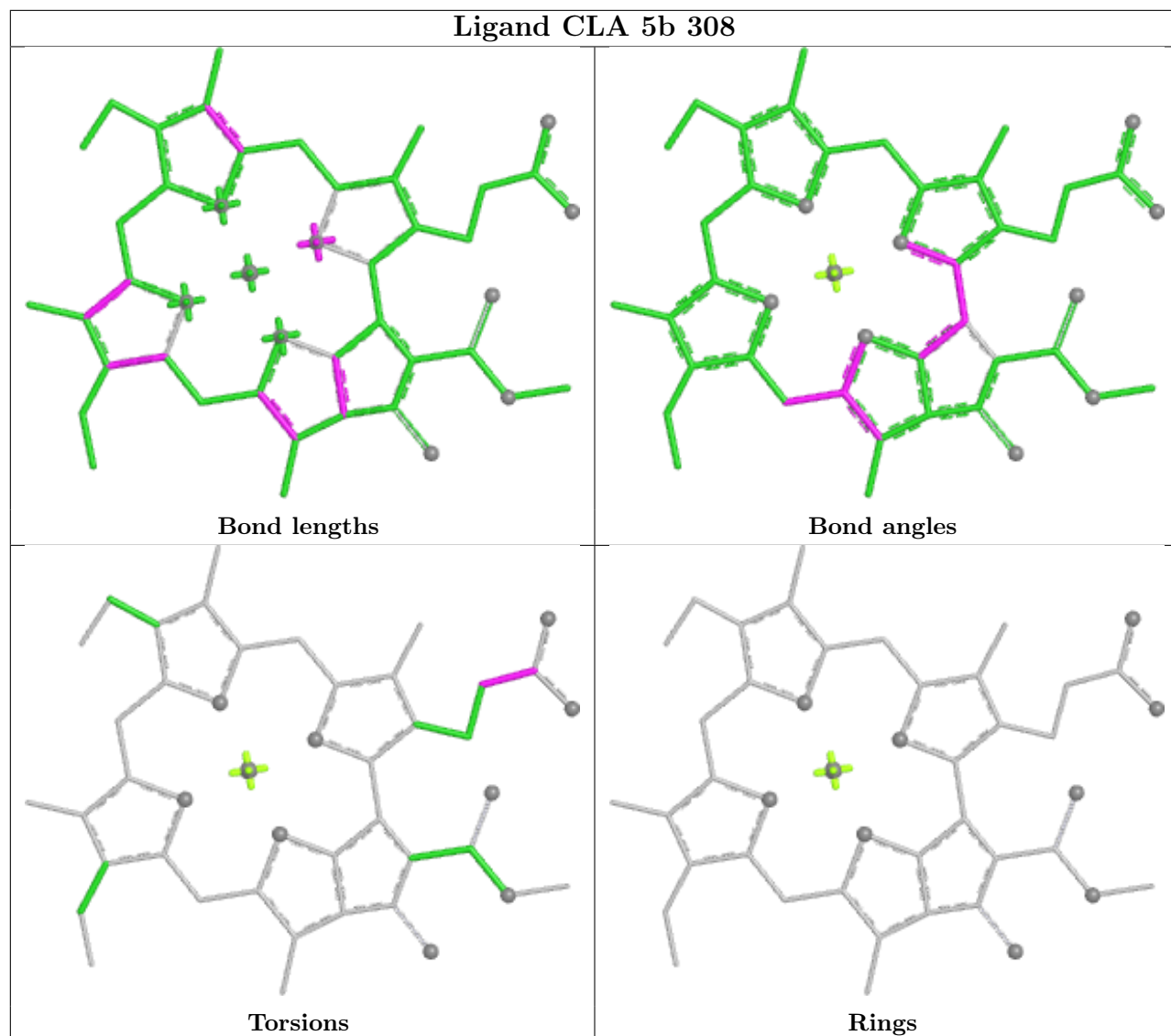


## Ligand CLA a 811

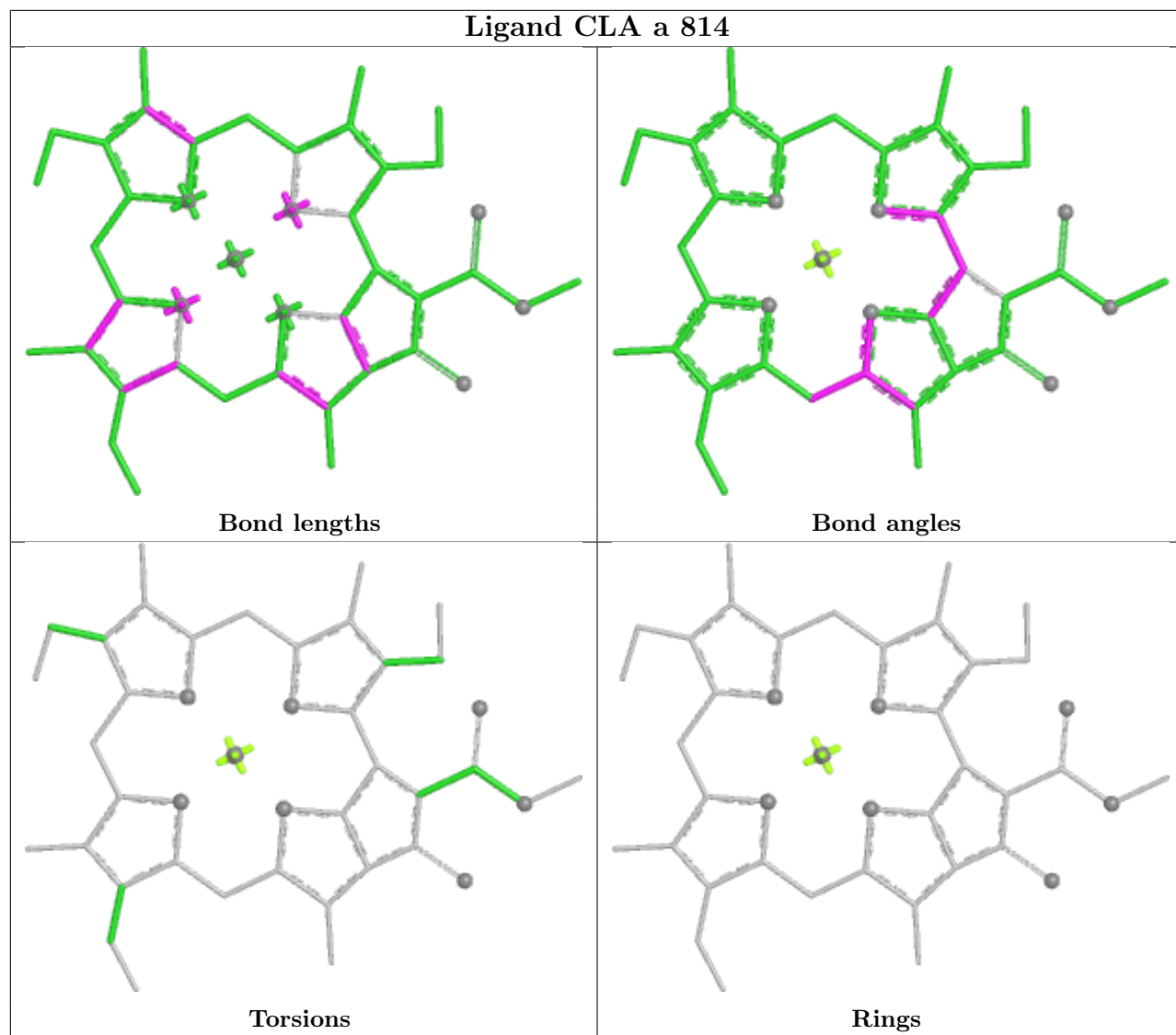


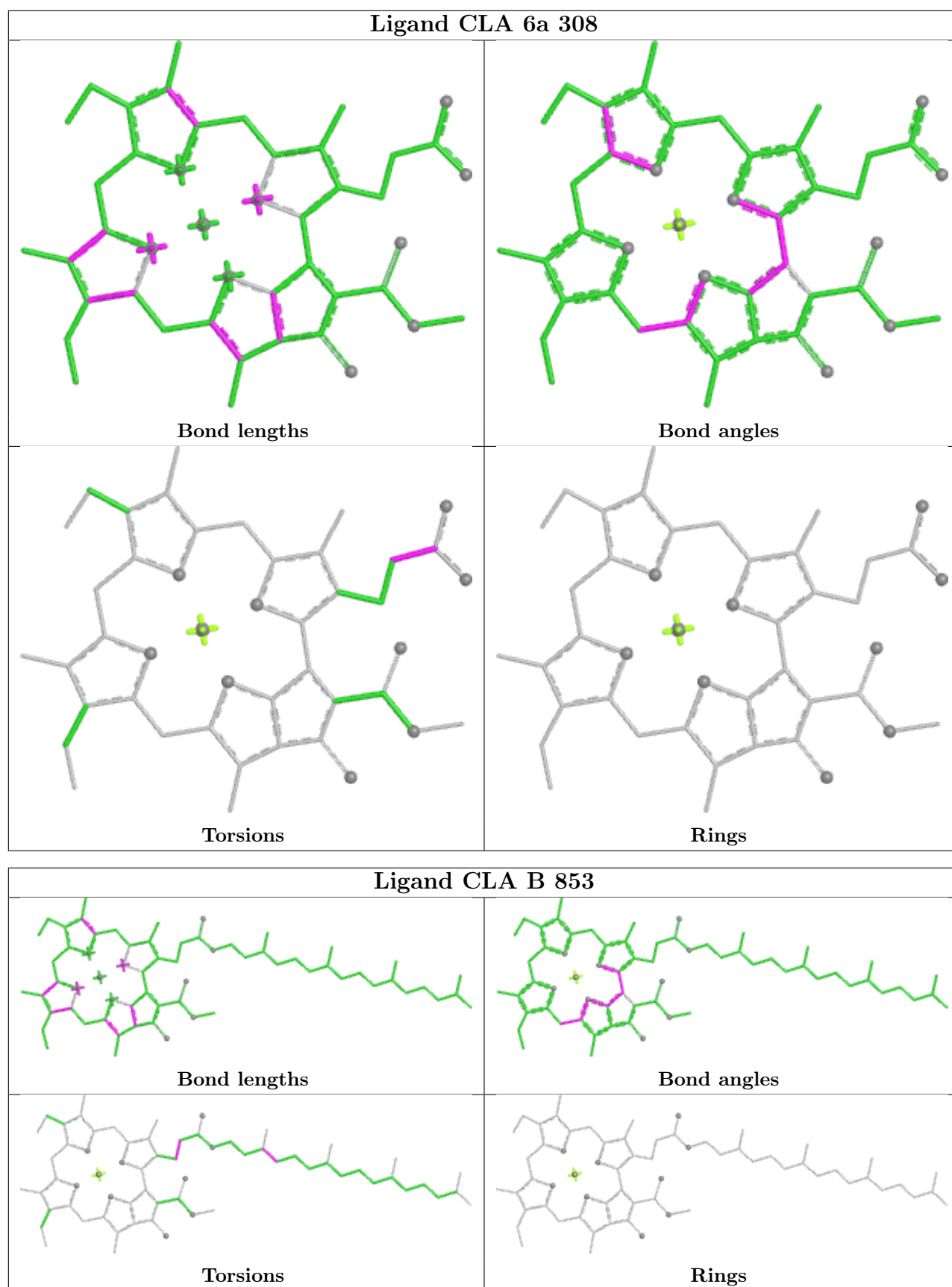
## Ligand CLA g 202



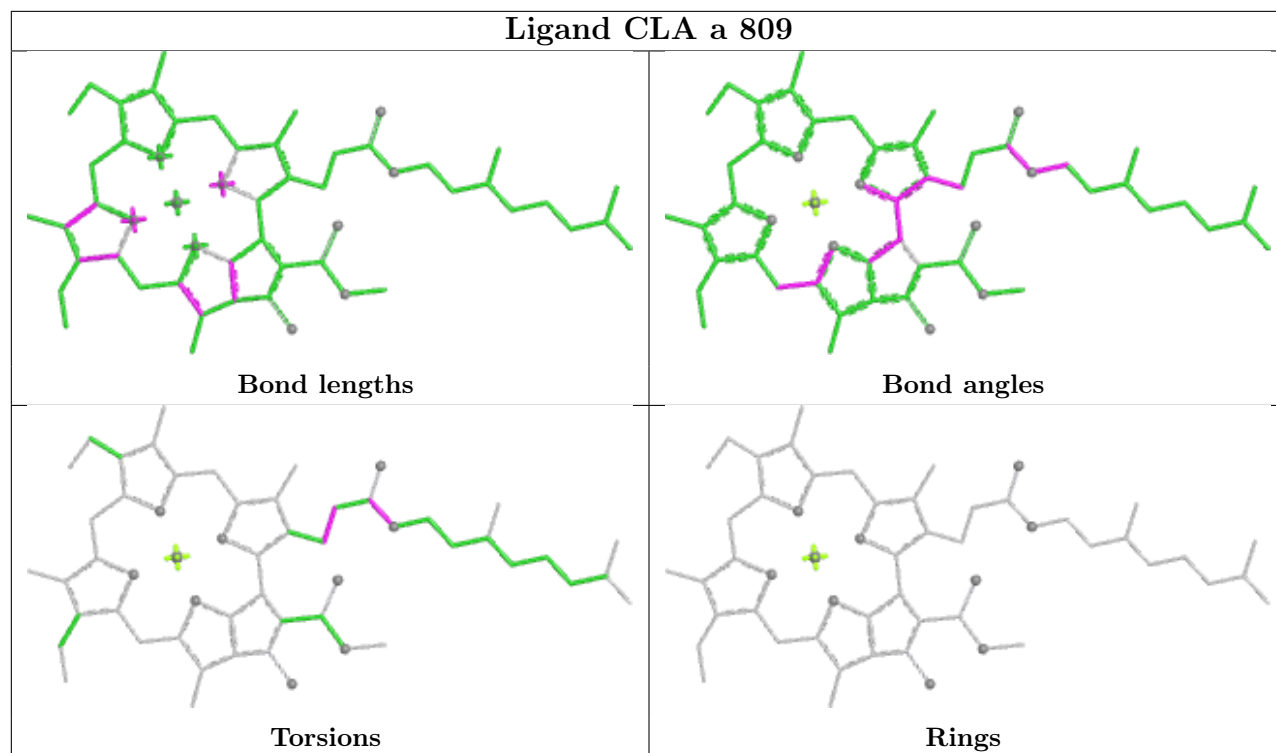


## Ligand CLA a 814

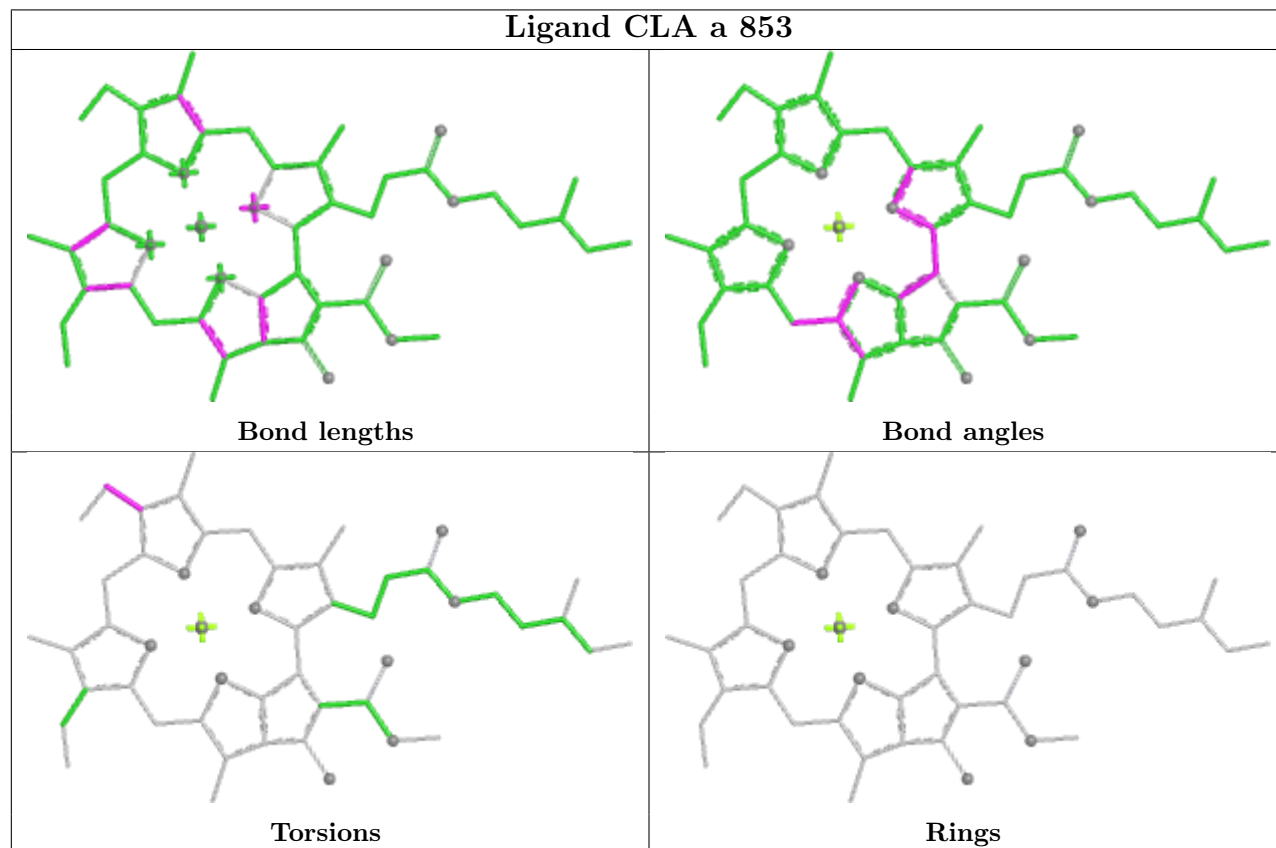


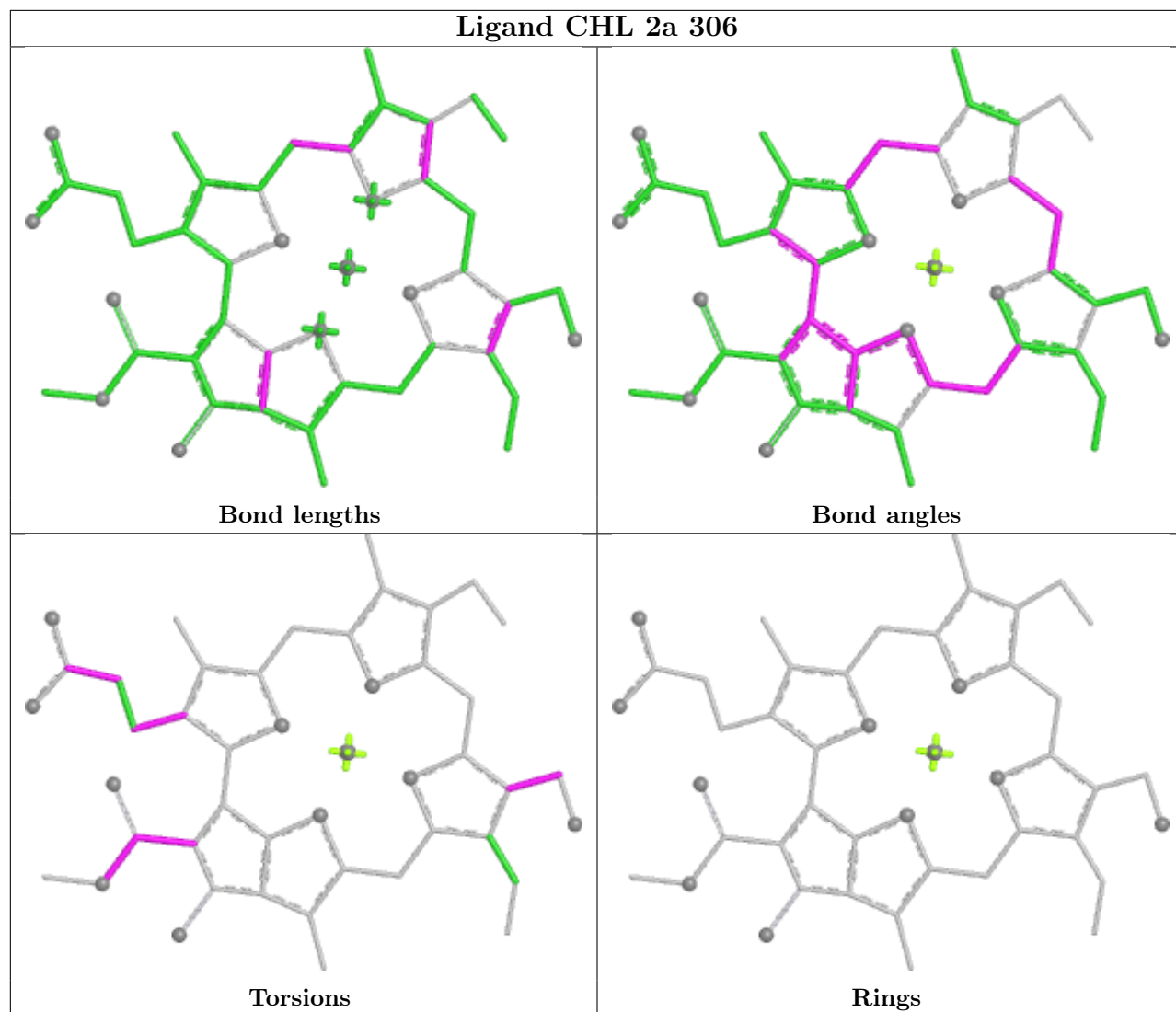


## Ligand CLA a 809

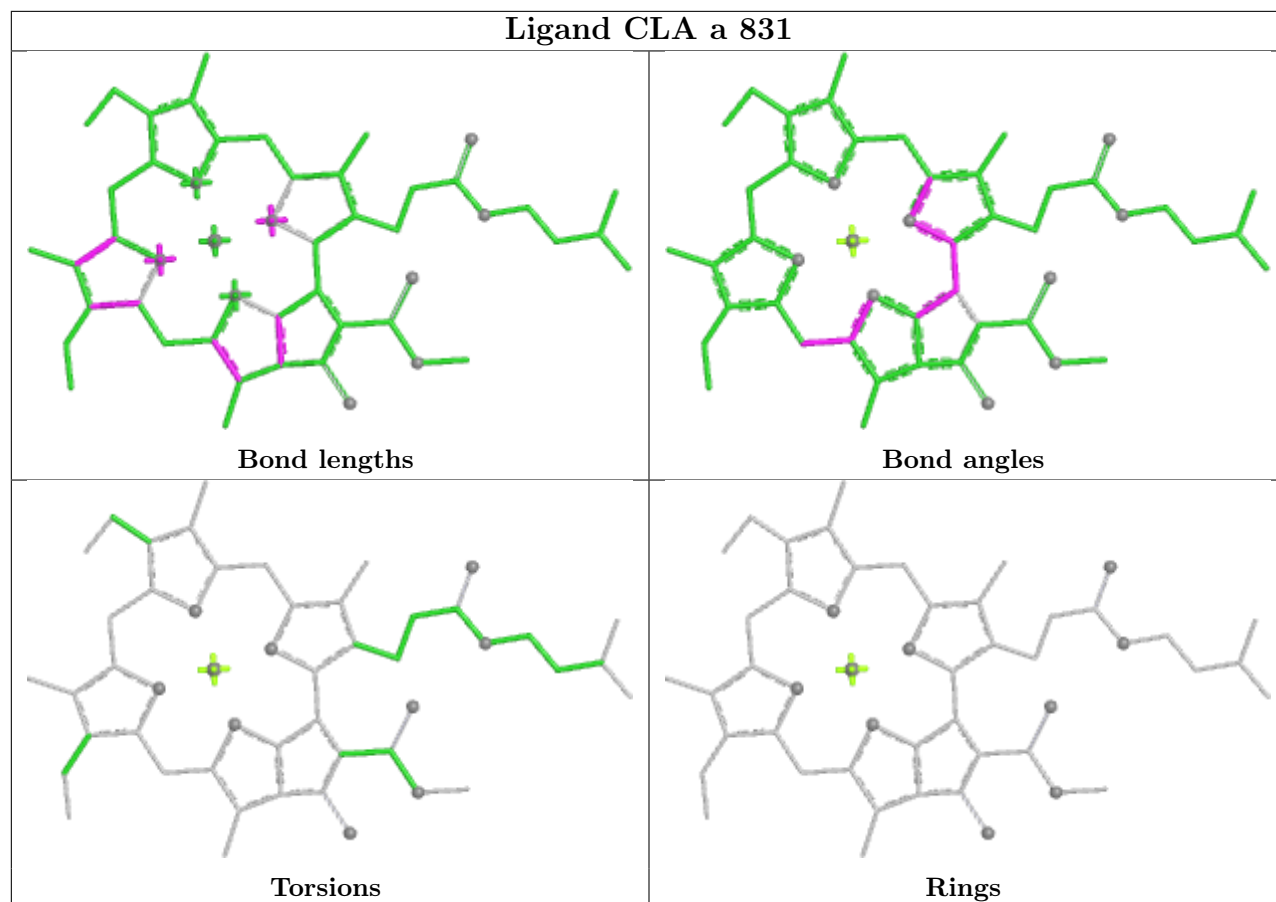


## Ligand CLA a 853



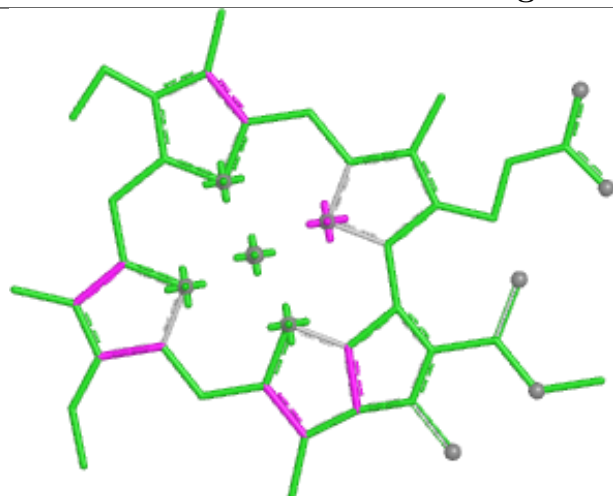


## Ligand CLA a 831

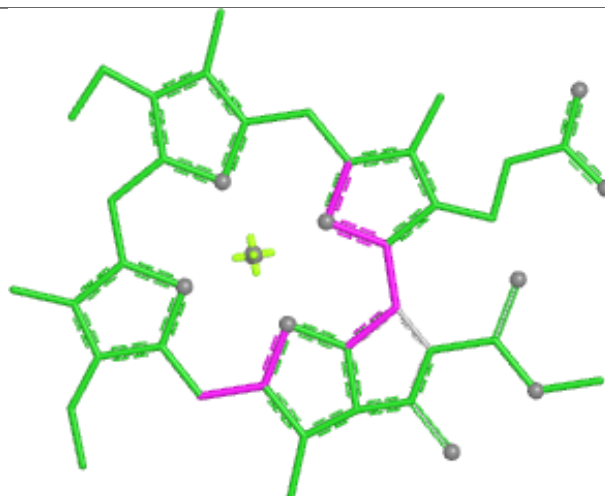




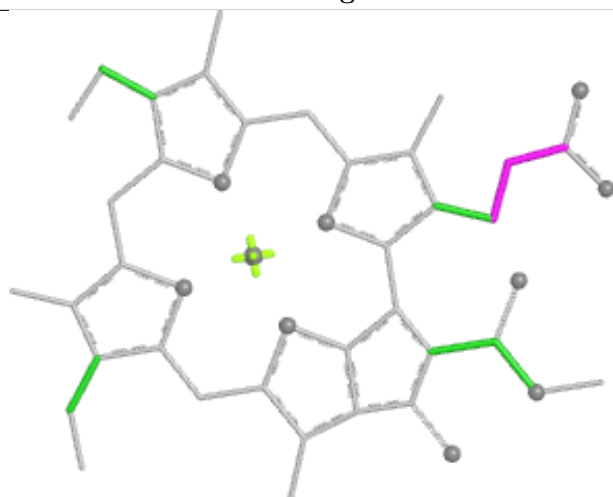
## Ligand CLA b 811



Bond lengths



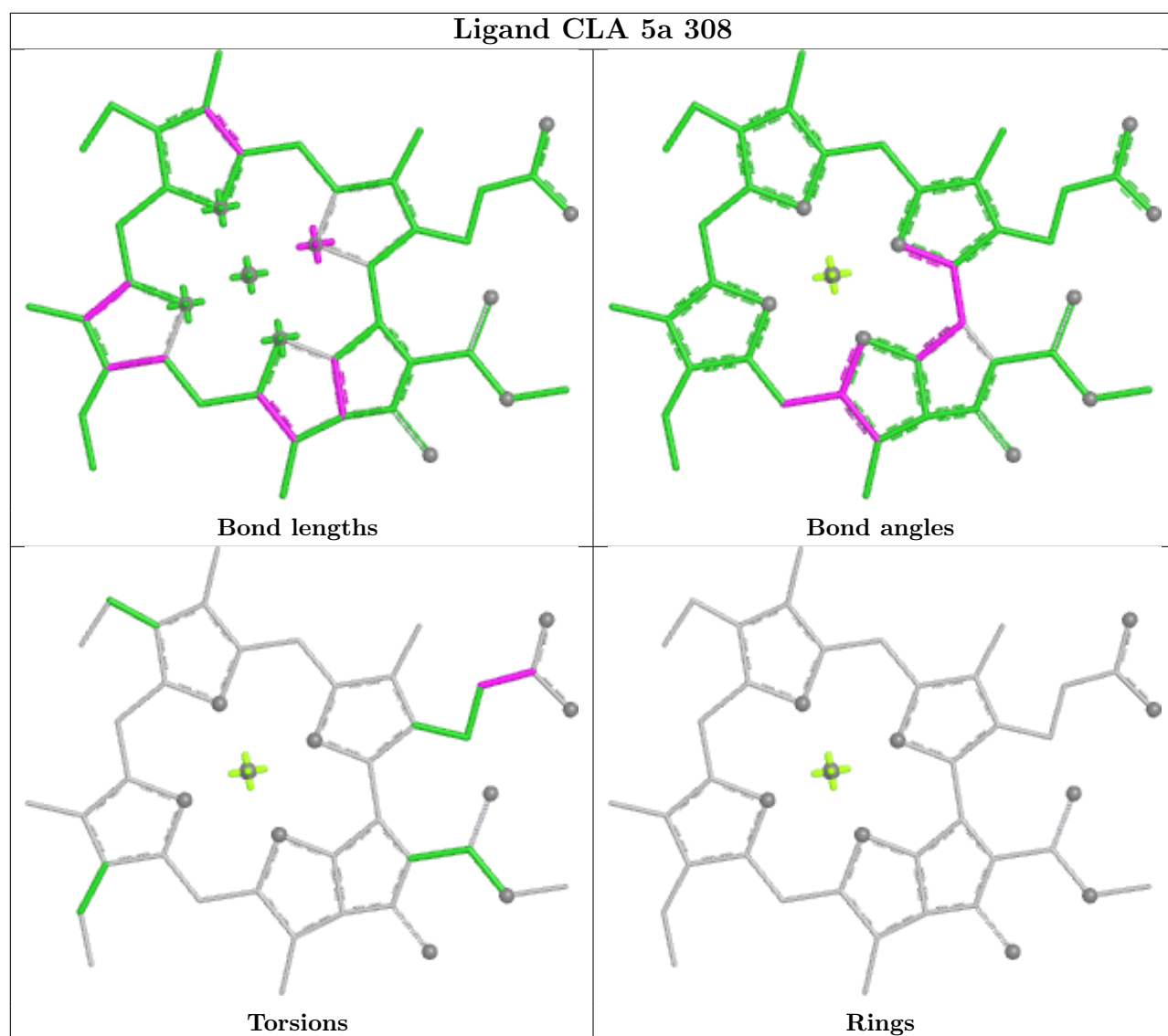
Bond angles



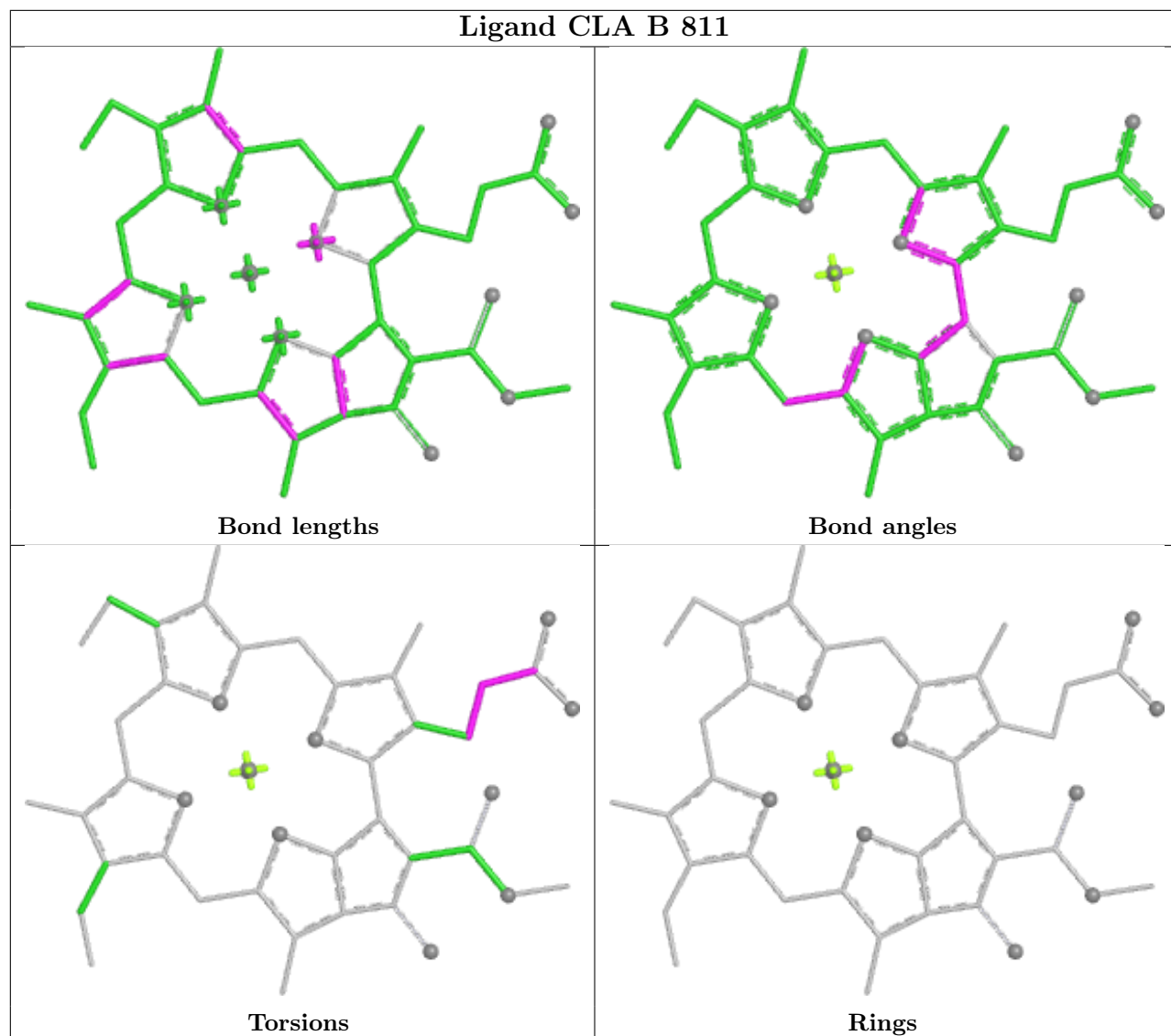
Torsions



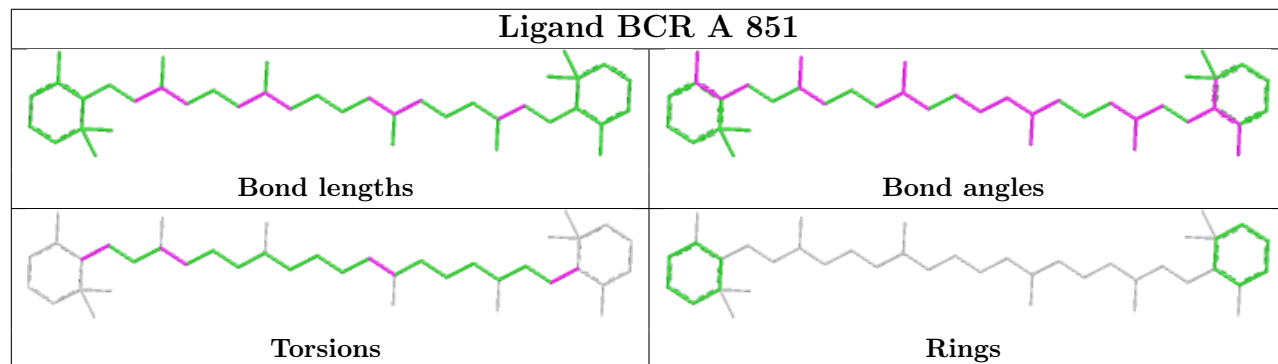
Rings



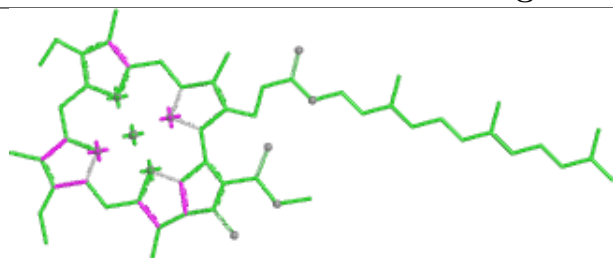
## Ligand CLA B 811



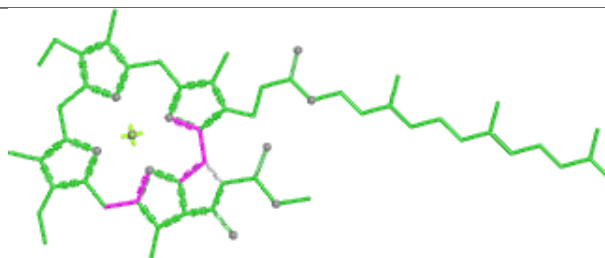
## Ligand BCR A 851



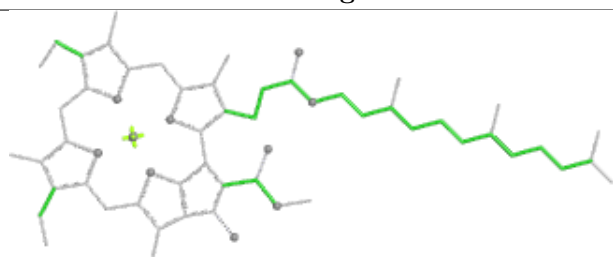
## Ligand CLA L 302



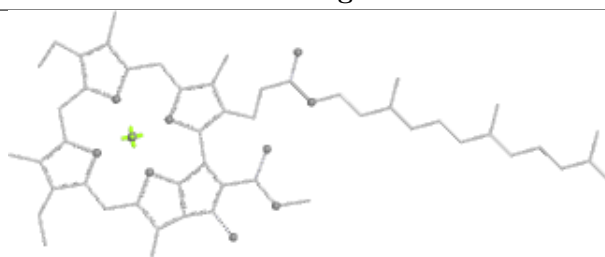
Bond lengths



Bond angles

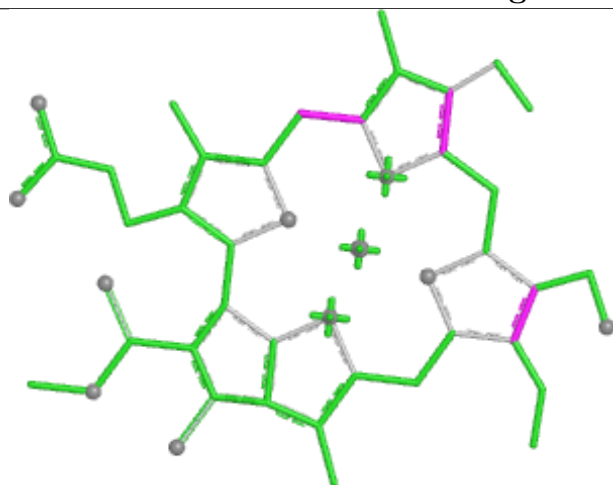


Torsions

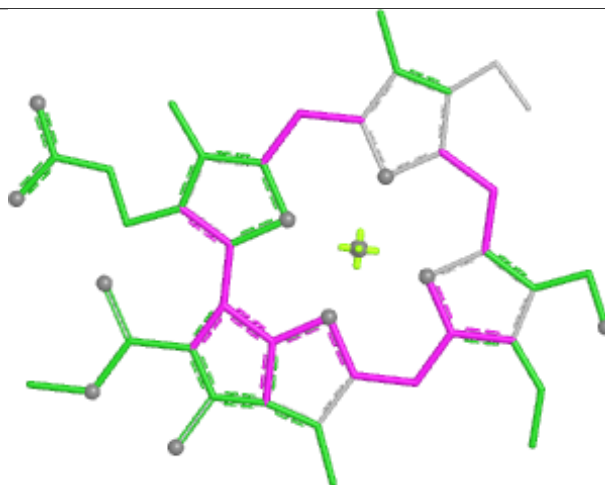


Rings

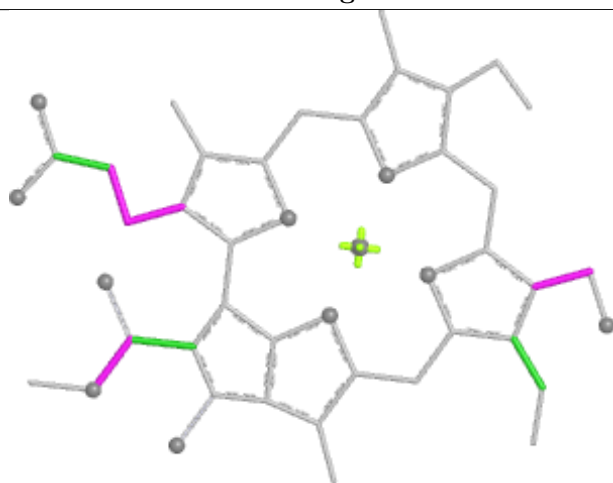
## Ligand CHL 5a 307



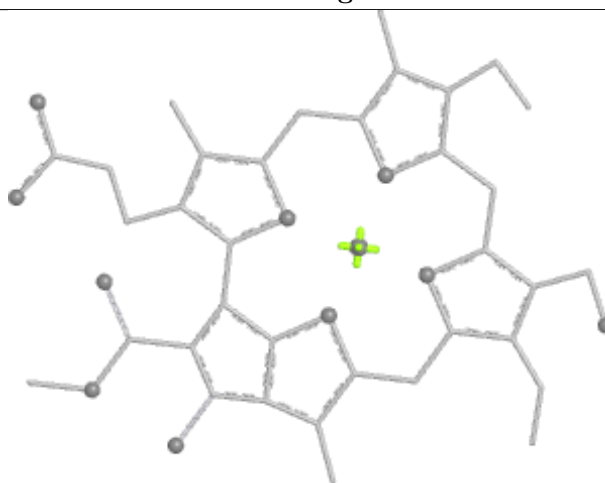
Bond lengths



Bond angles

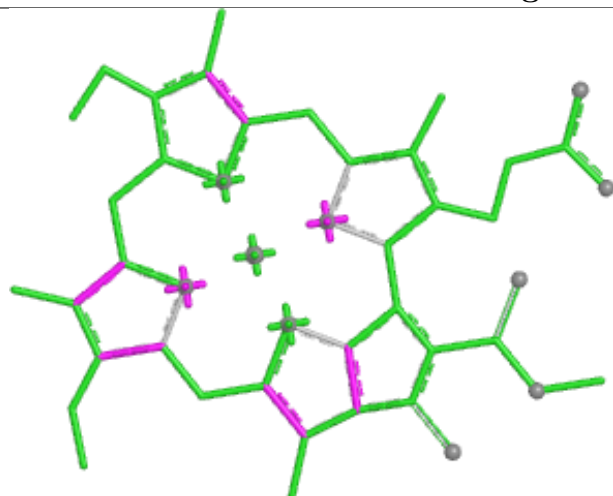


Torsions

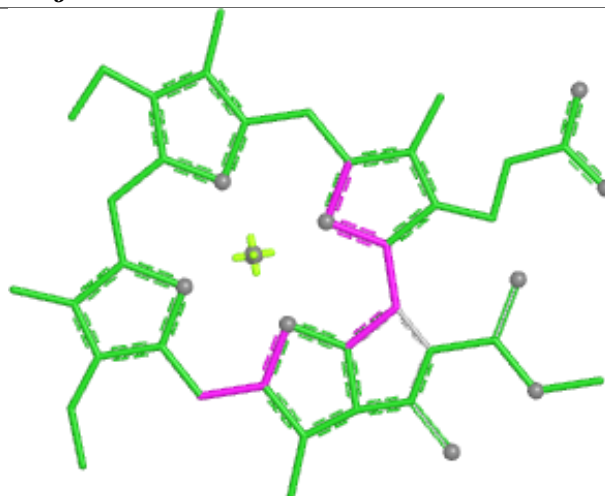


Rings

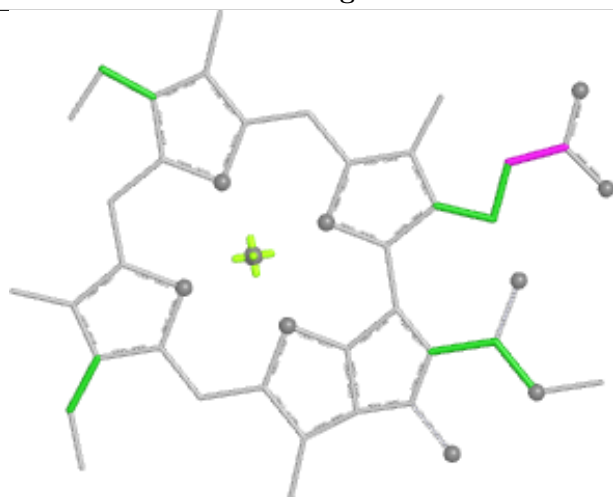
## Ligand CLA j 101



Bond lengths



Bond angles

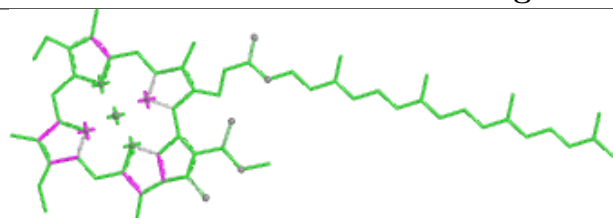


Torsions

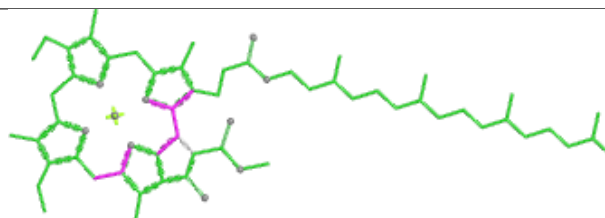


Rings

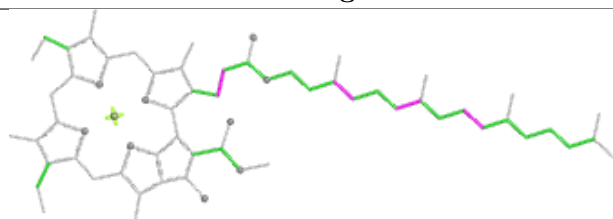
## Ligand CLA A 827



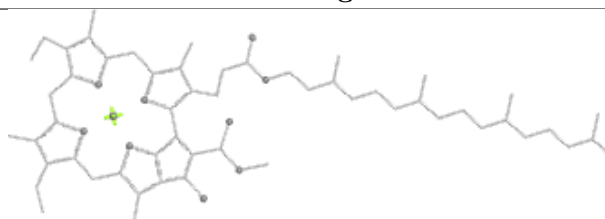
Bond lengths



Bond angles

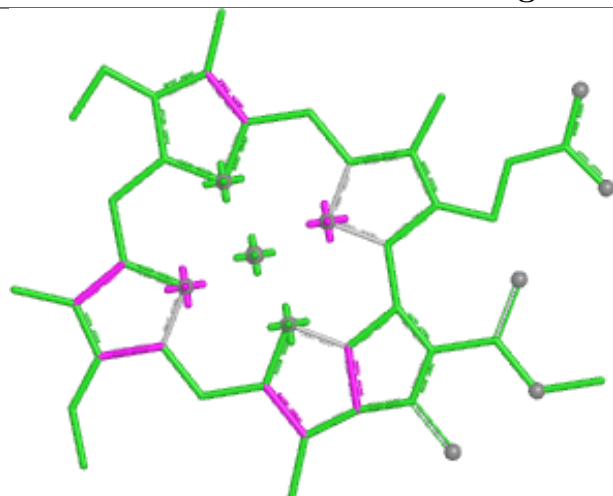


Torsions

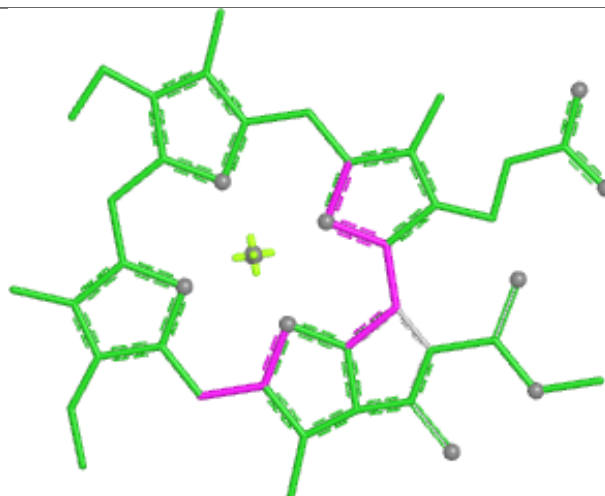


Rings

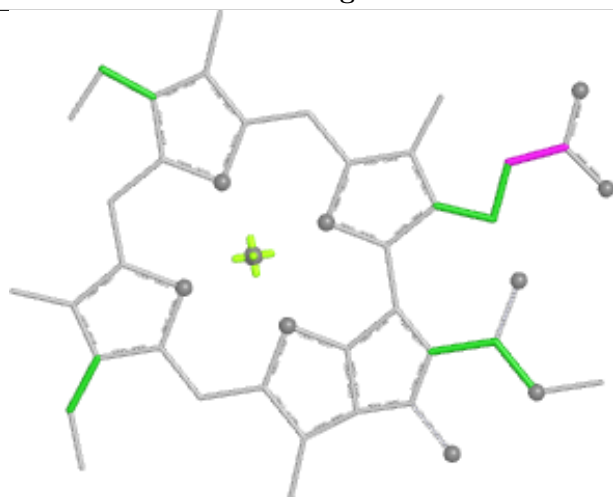
## Ligand CLA J 101



Bond lengths



Bond angles

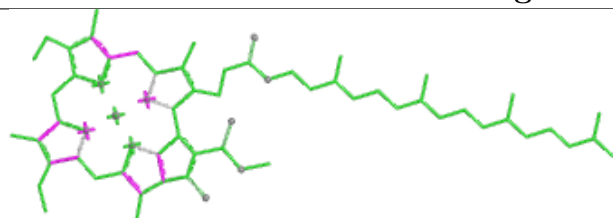


Torsions

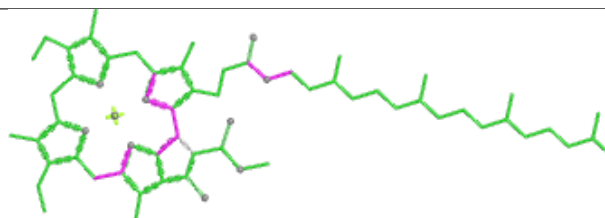


Rings

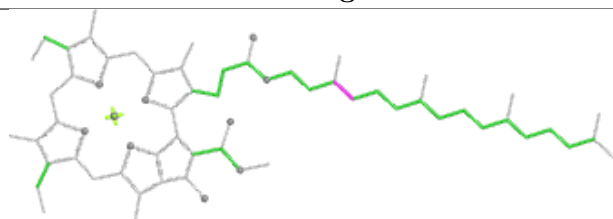
## Ligand CLA B 839



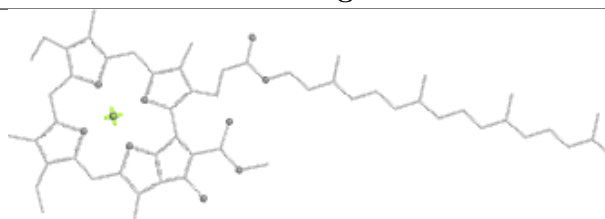
Bond lengths



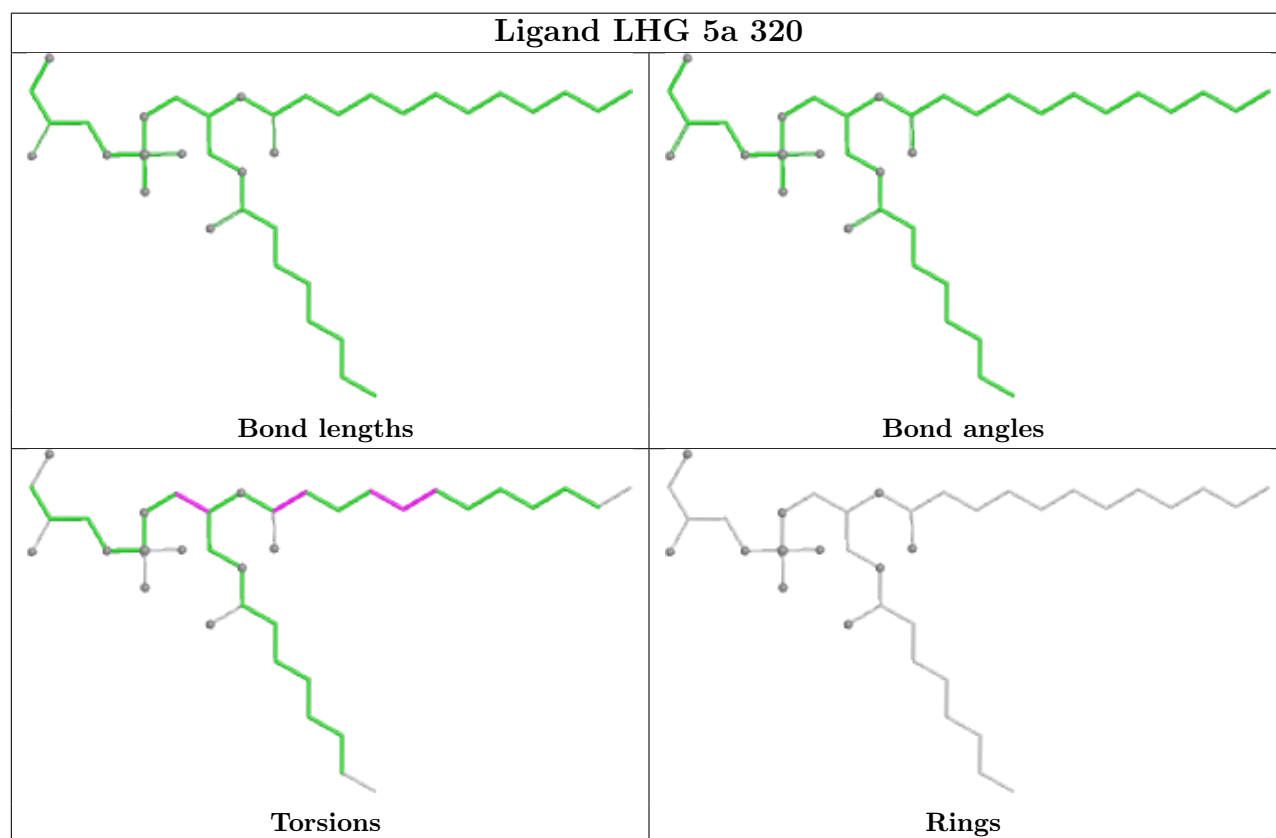
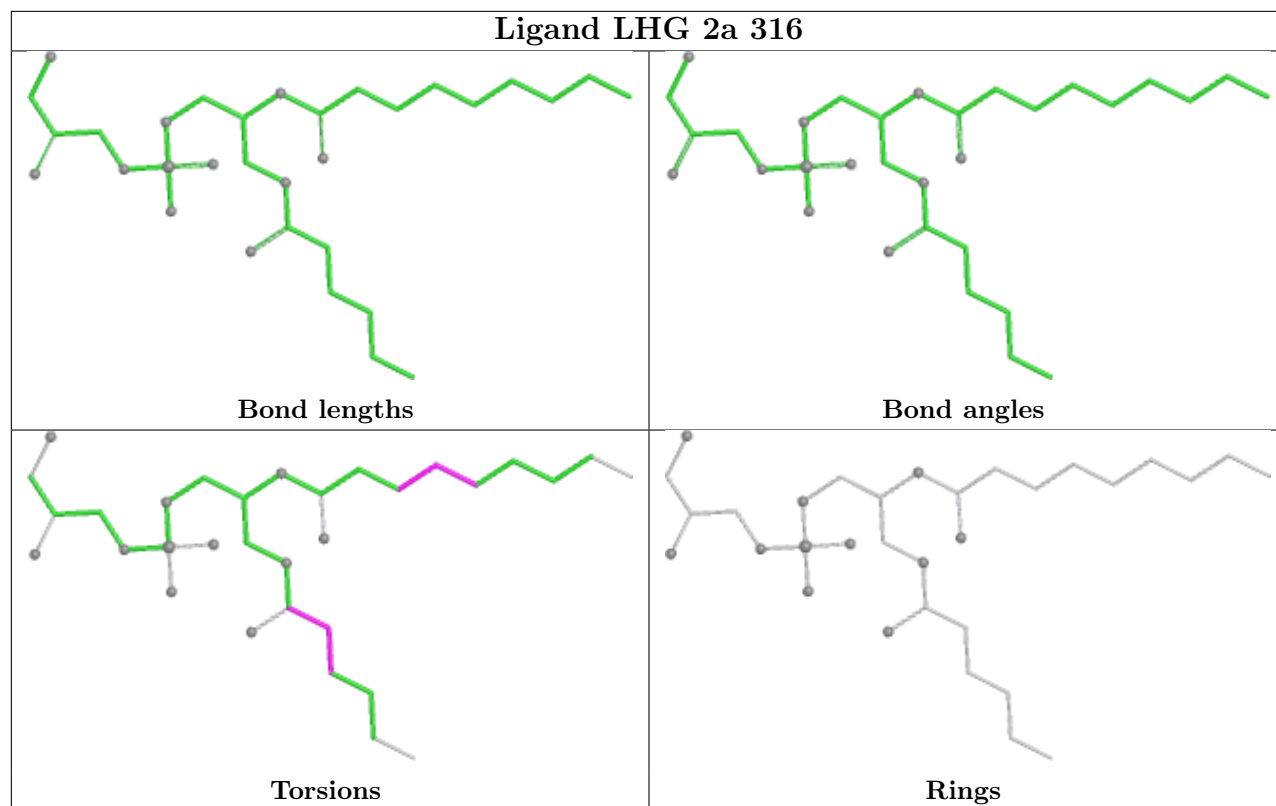
Bond angles



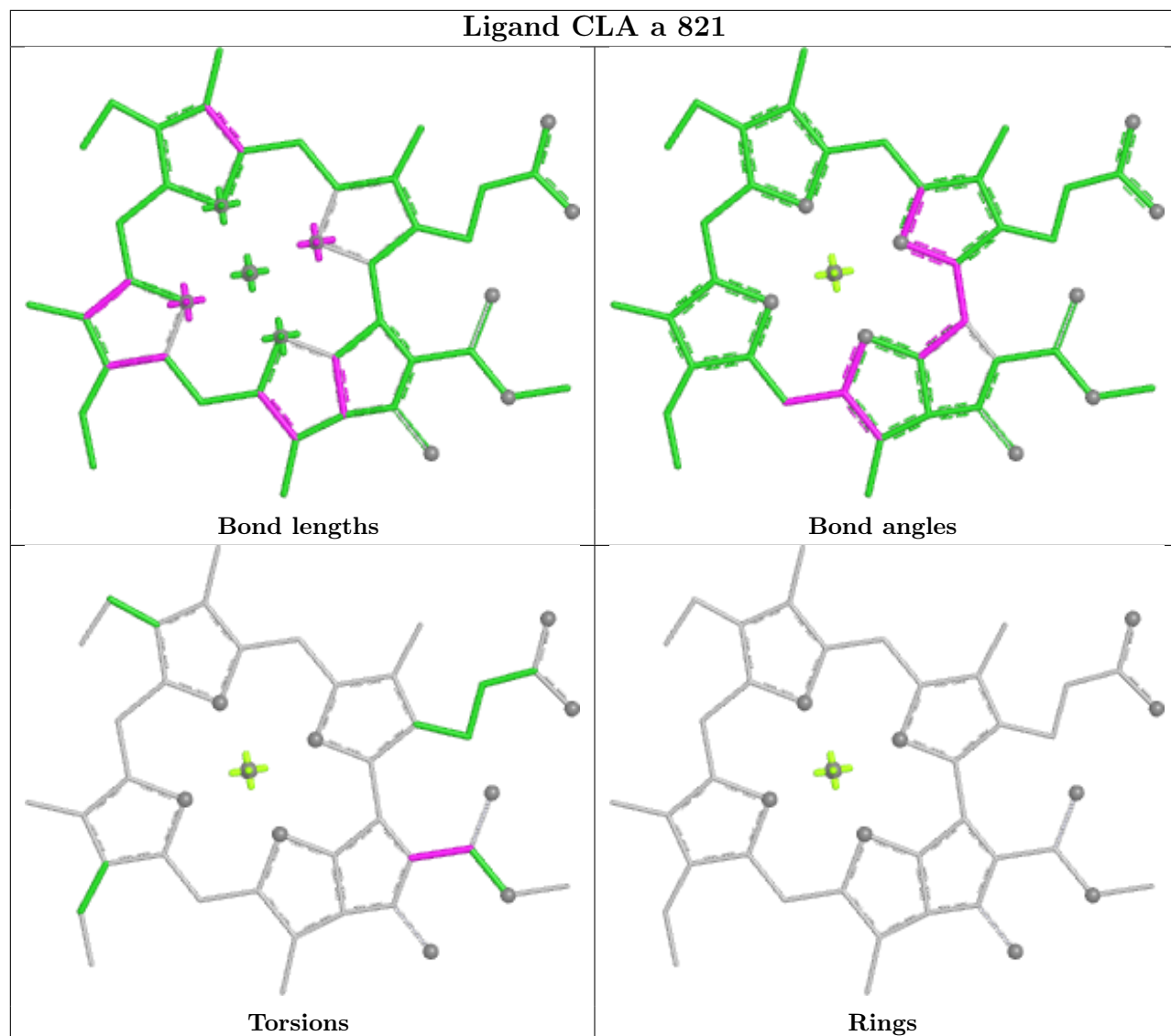
Torsions



Rings

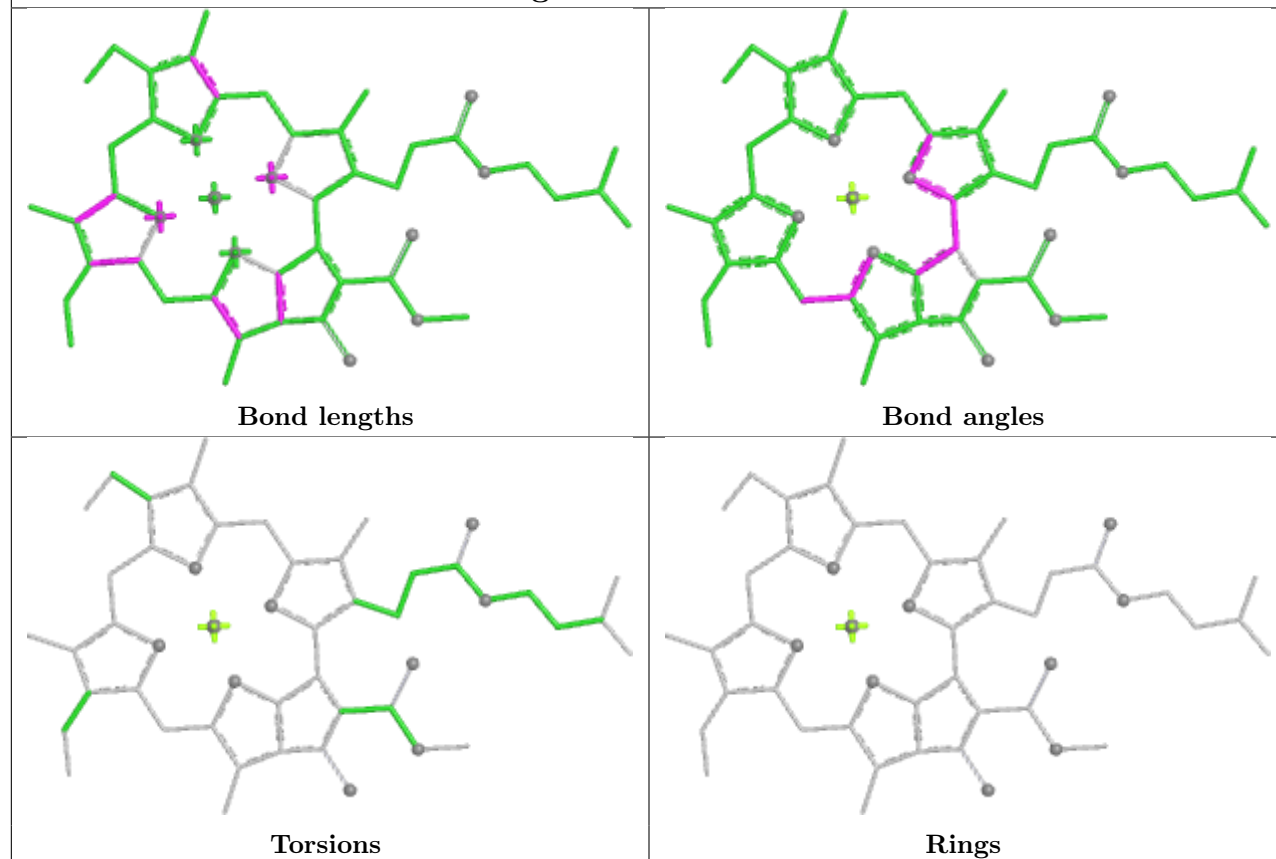


## Ligand CLA a 821

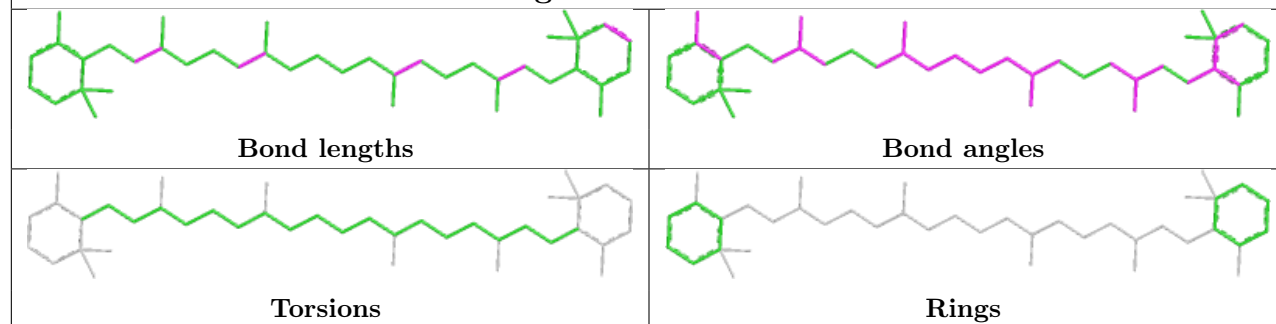




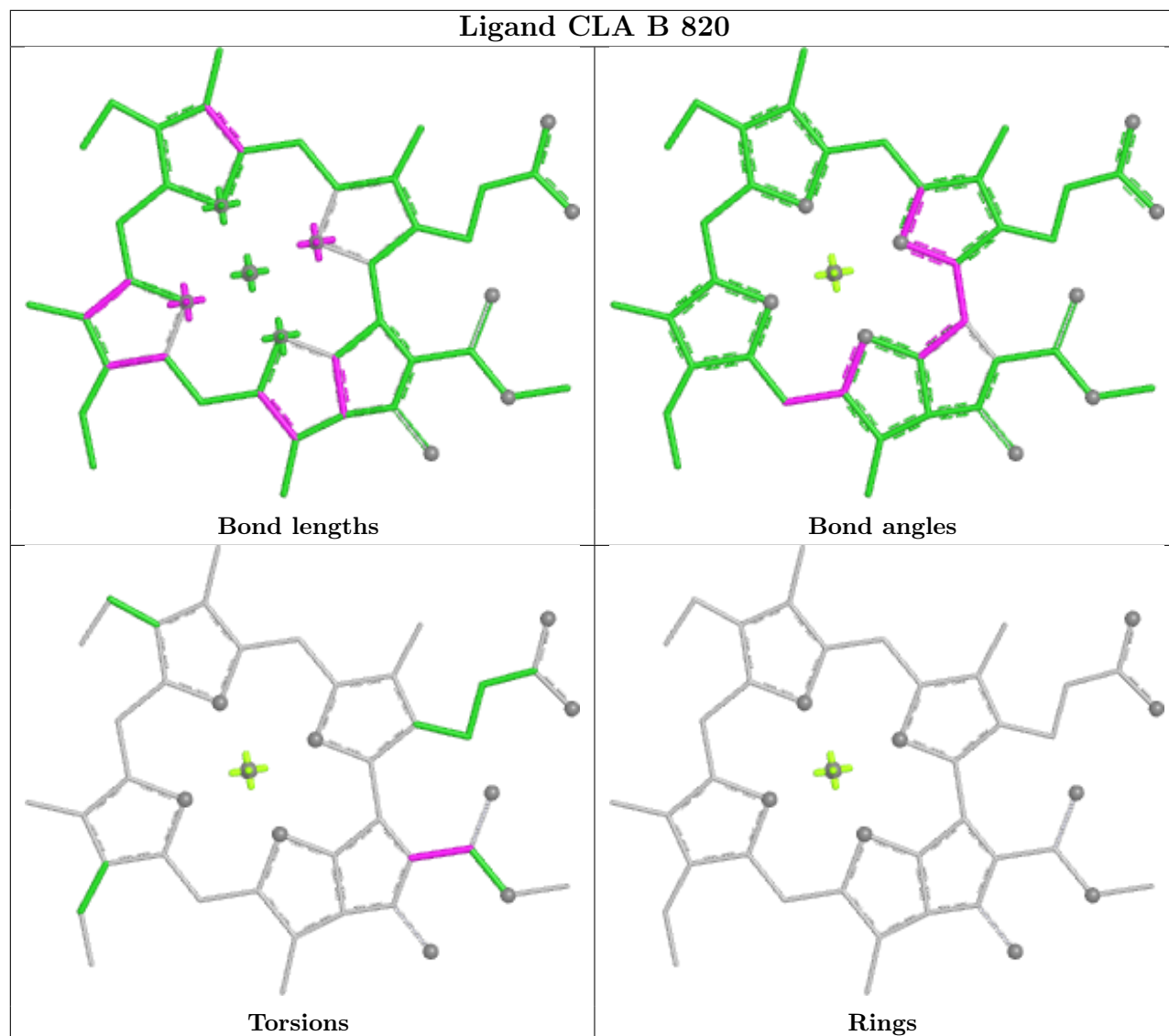
## Ligand CLA A 838



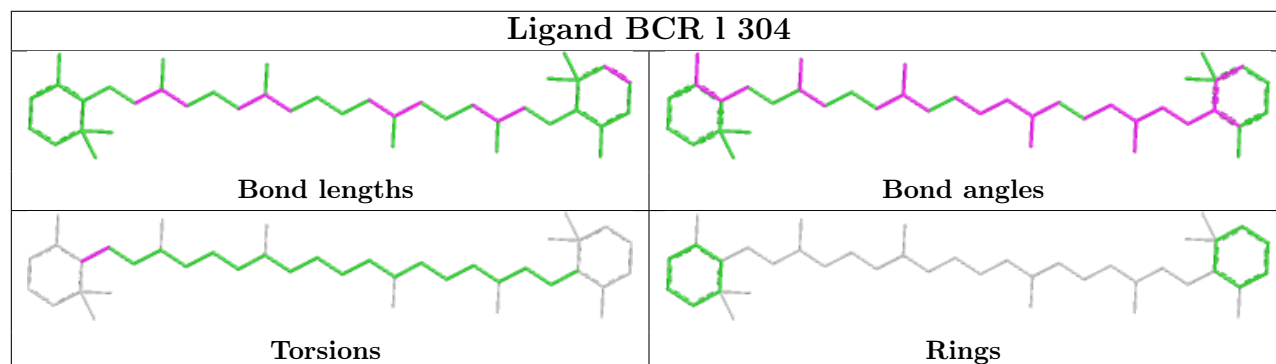
## Ligand BCR a 850

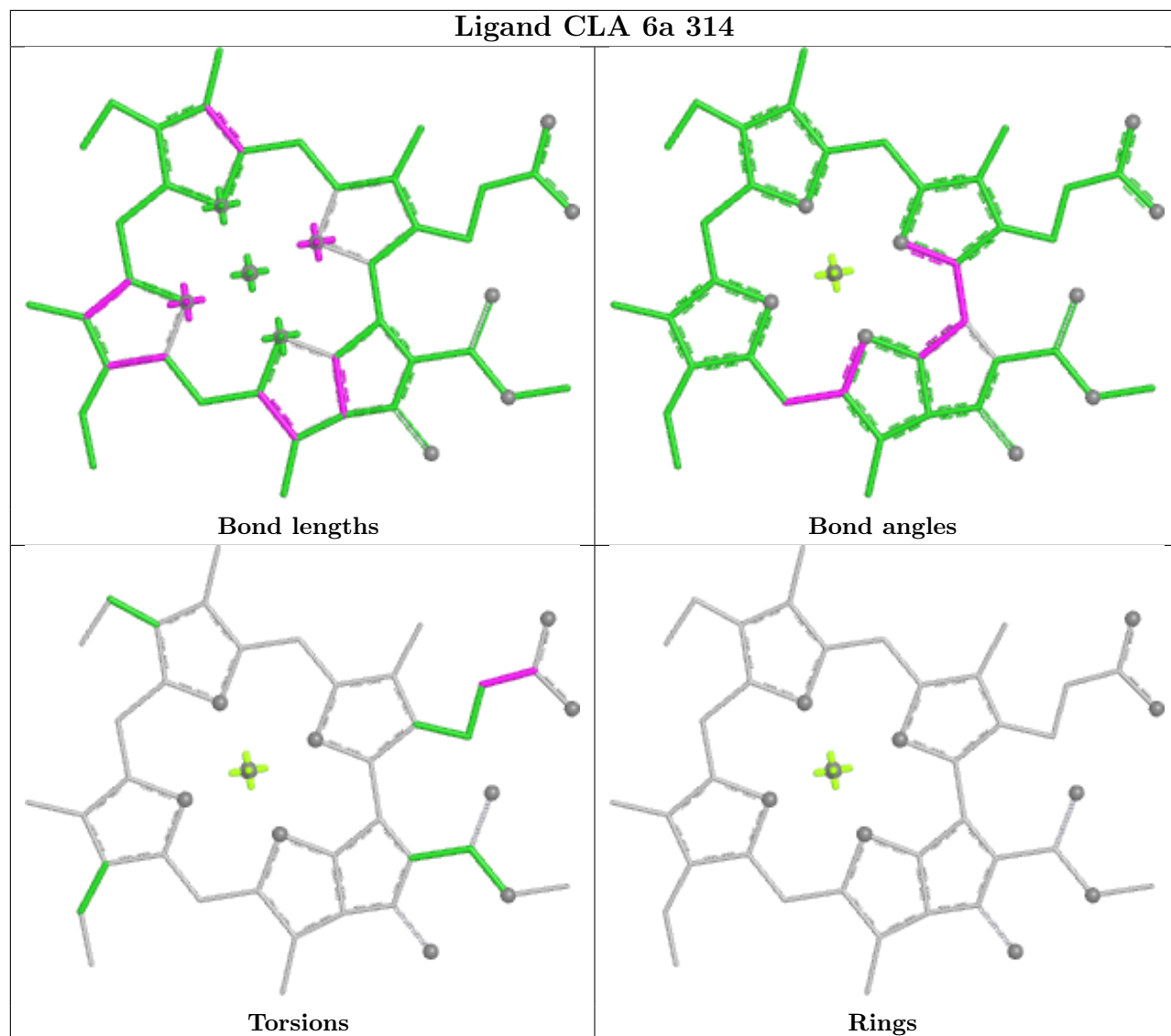


## Ligand CLA B 820

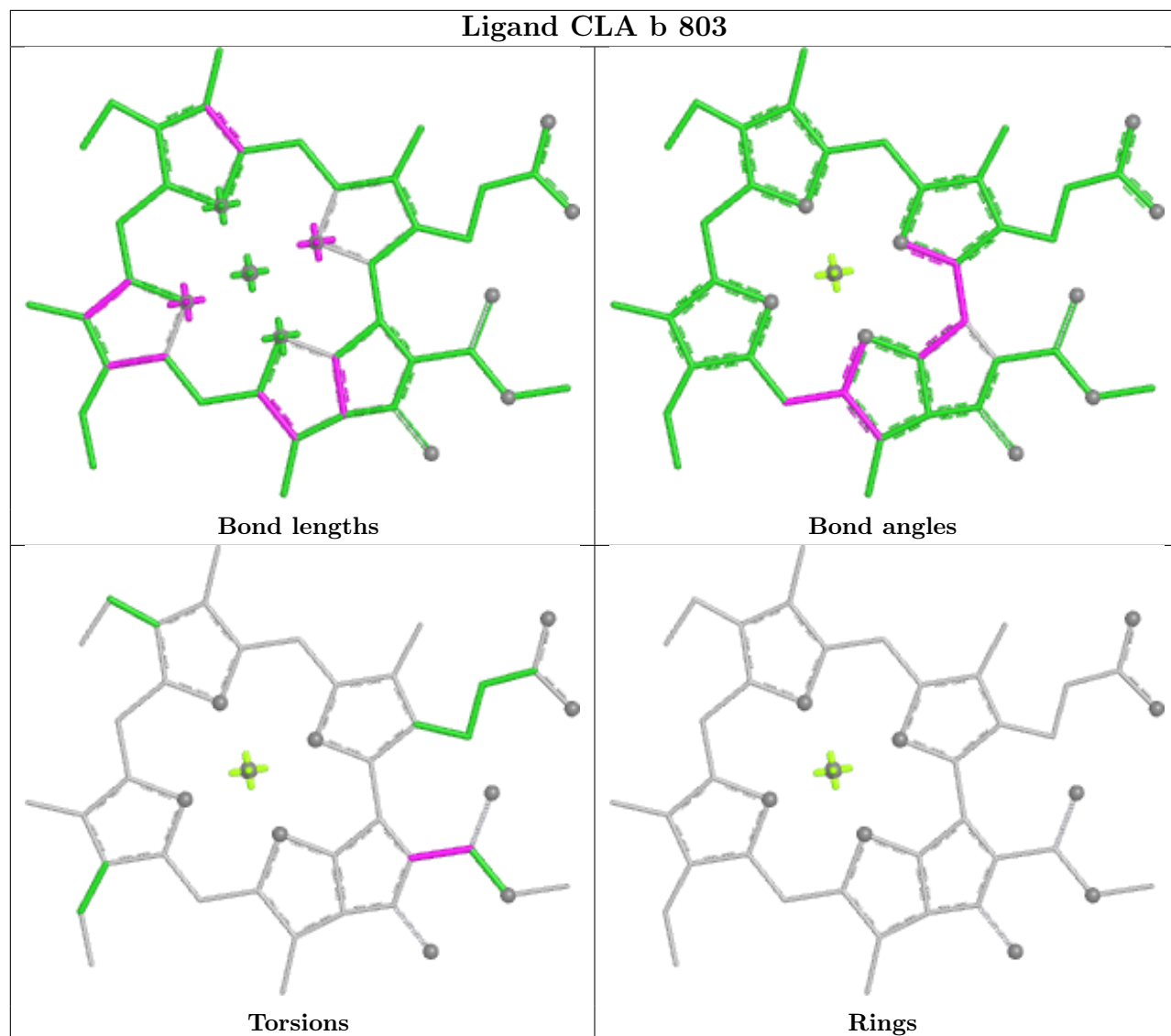


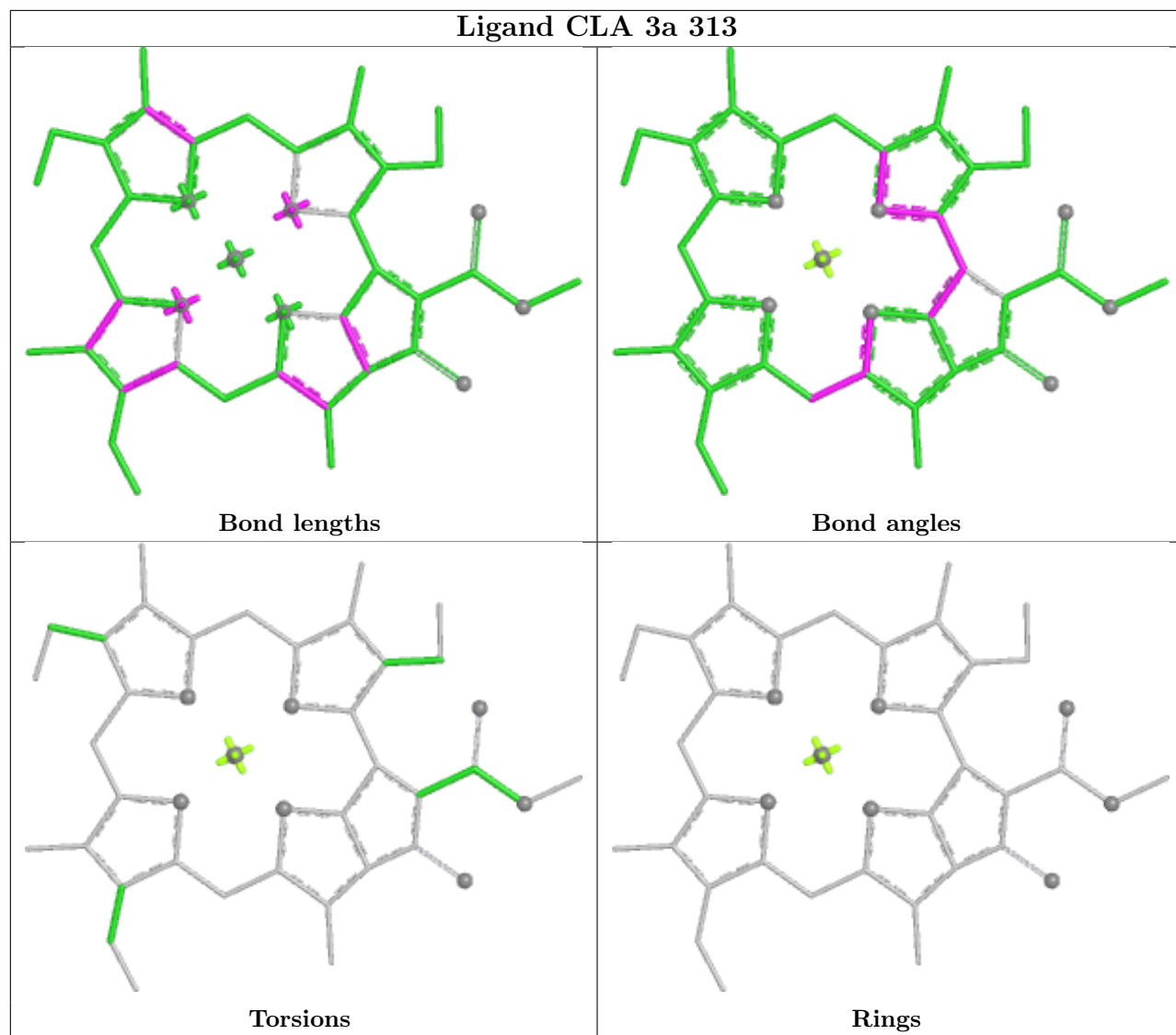
## Ligand BCR 1 304



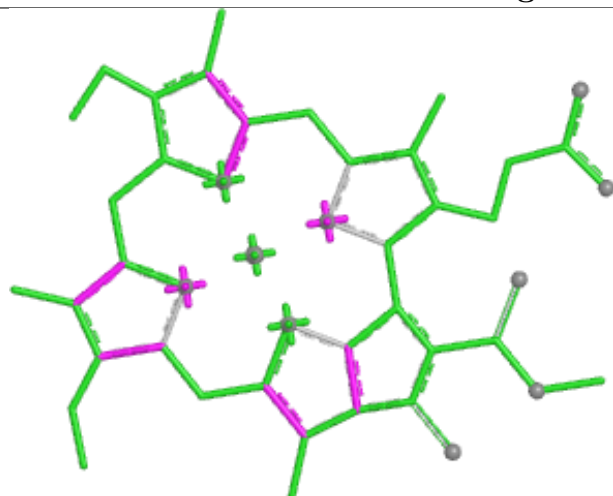


## Ligand CLA b 803

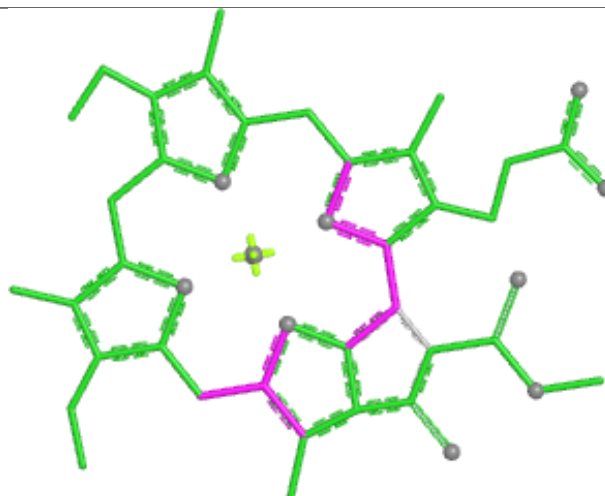




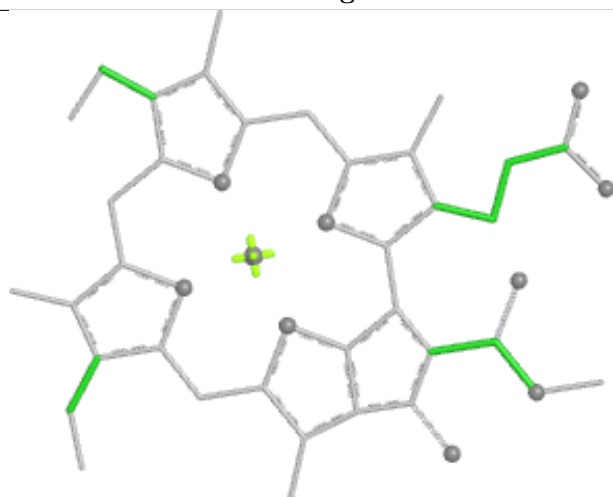
## Ligand CLA b 834



Bond lengths



Bond angles

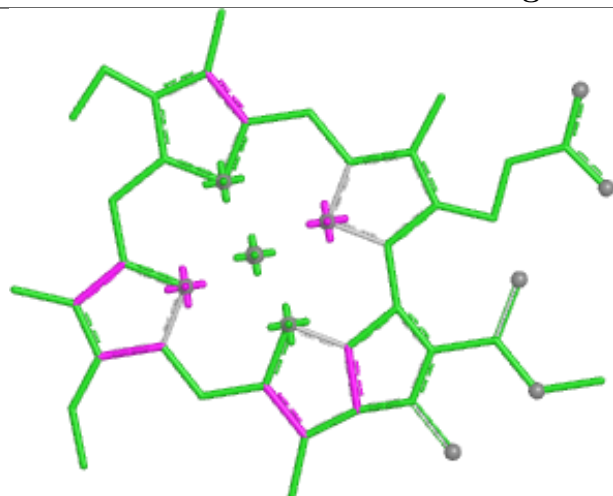


Torsions

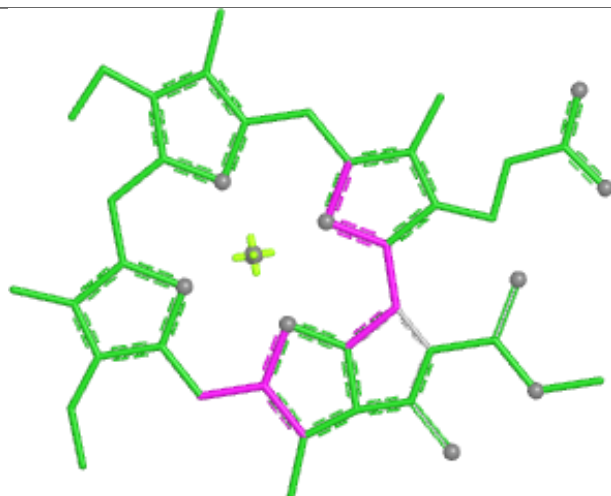


Rings

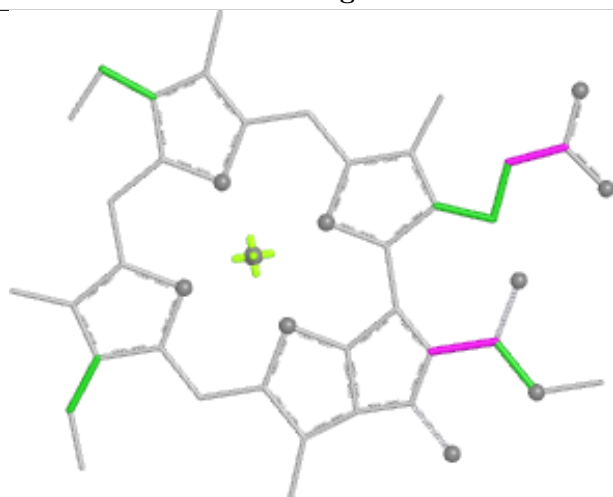
## Ligand CLA 1 301



Bond lengths



Bond angles

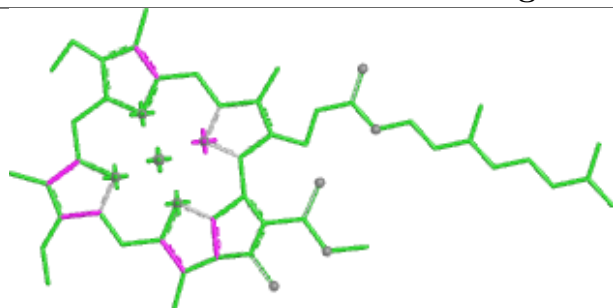


Torsions

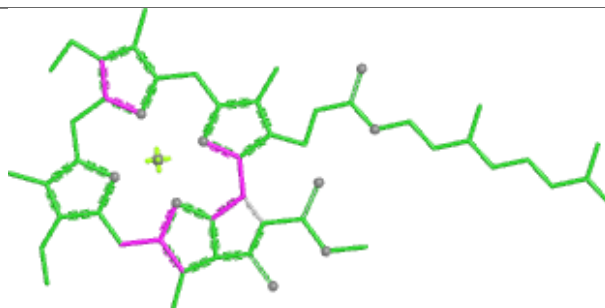


Rings

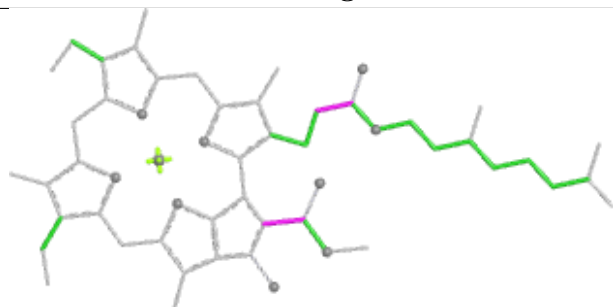
## Ligand CLA a 804



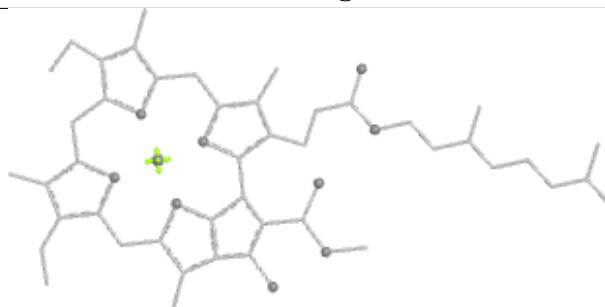
Bond lengths



Bond angles

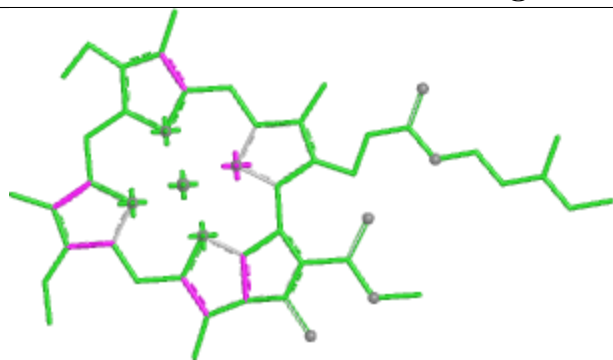


Torsions

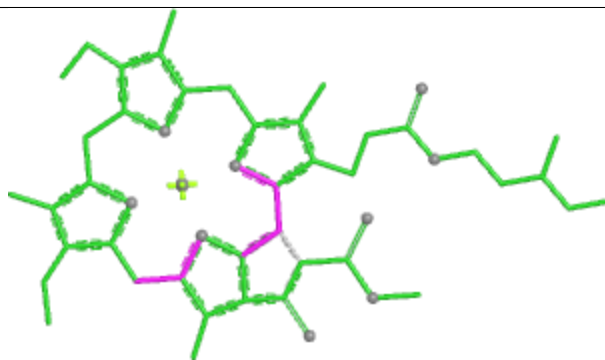


Rings

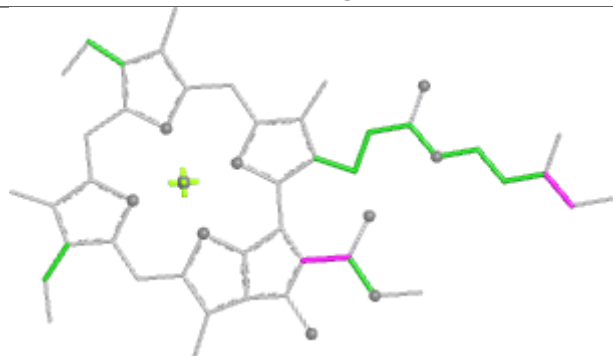
## Ligand CLA 5a 309



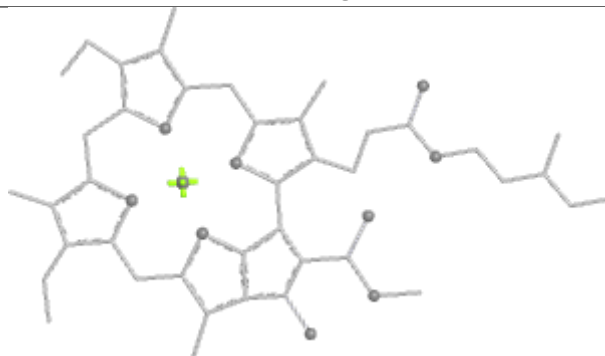
Bond lengths



Bond angles

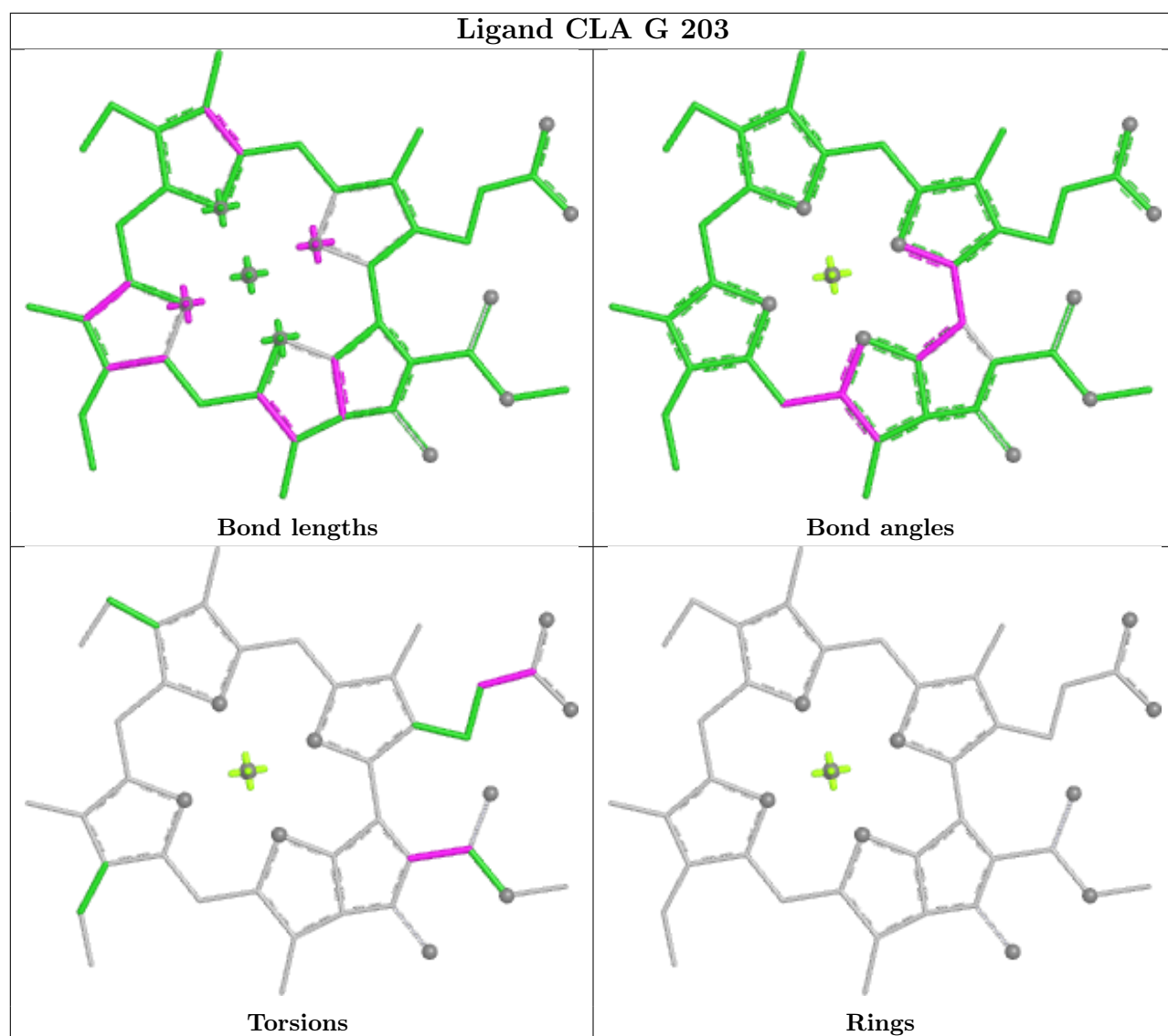


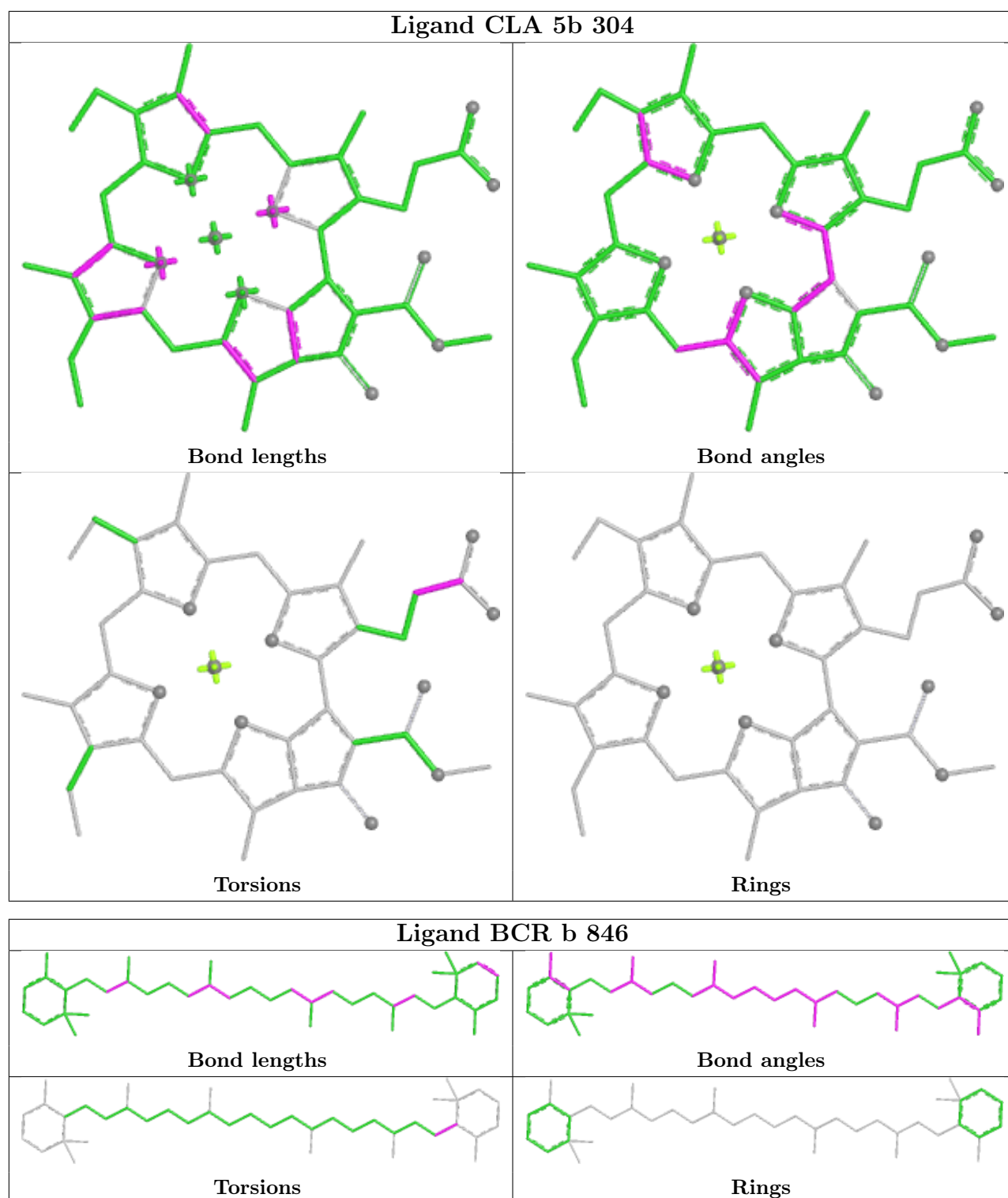
Torsions



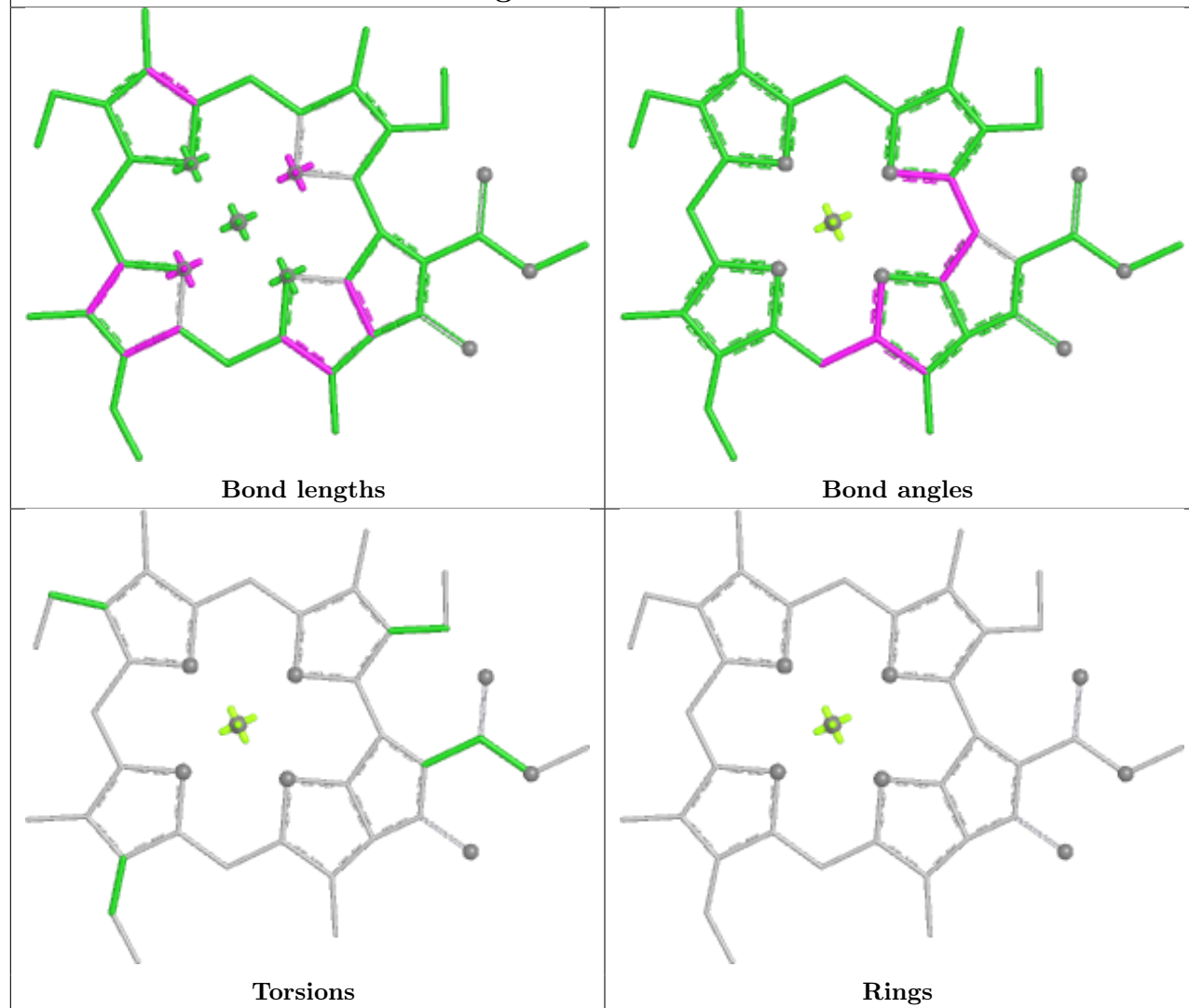
Rings



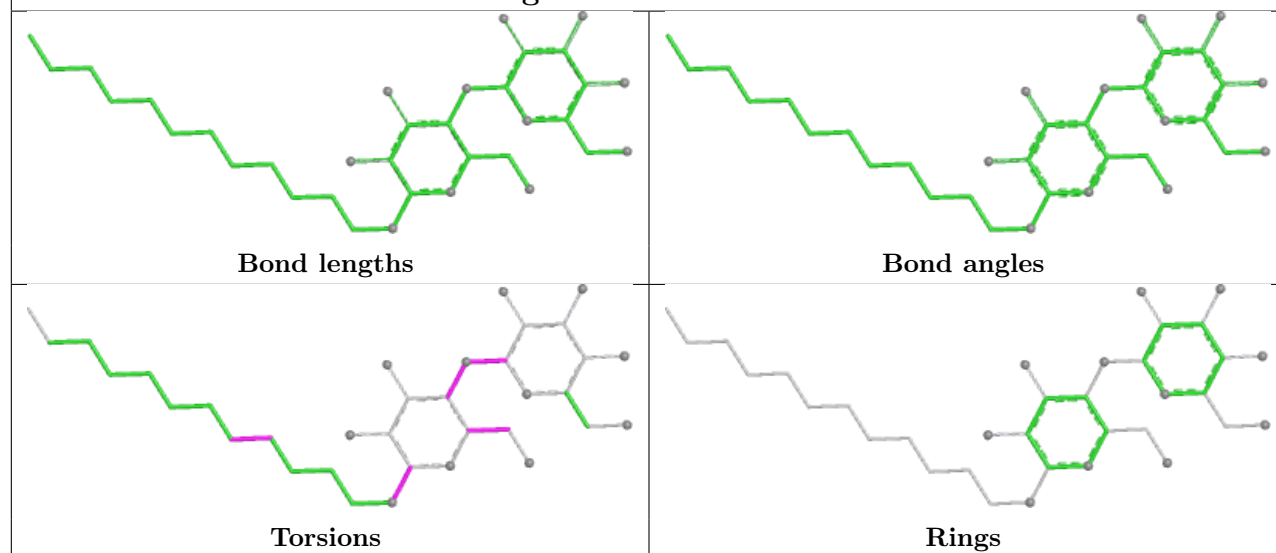


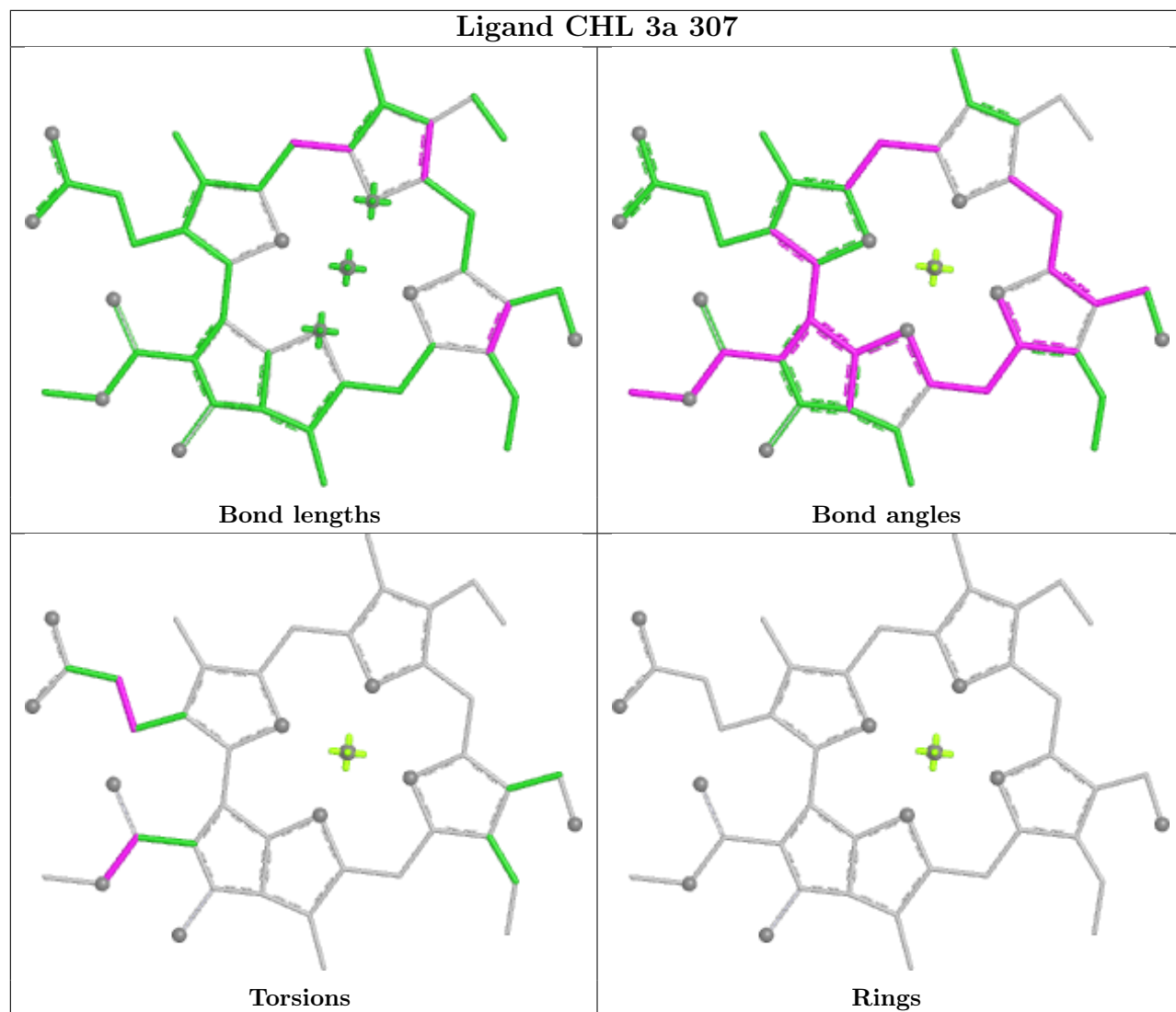


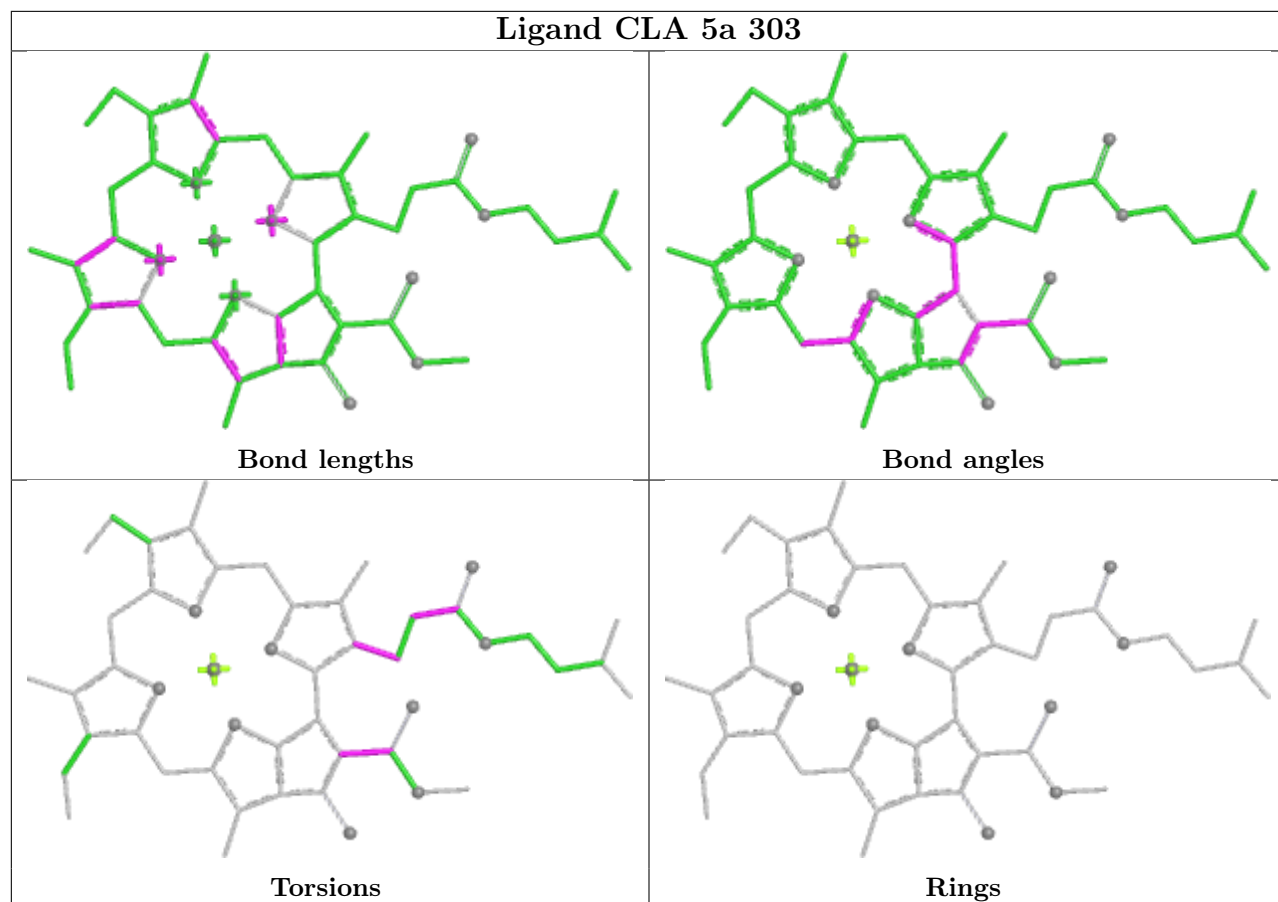
## Ligand CLA A 814

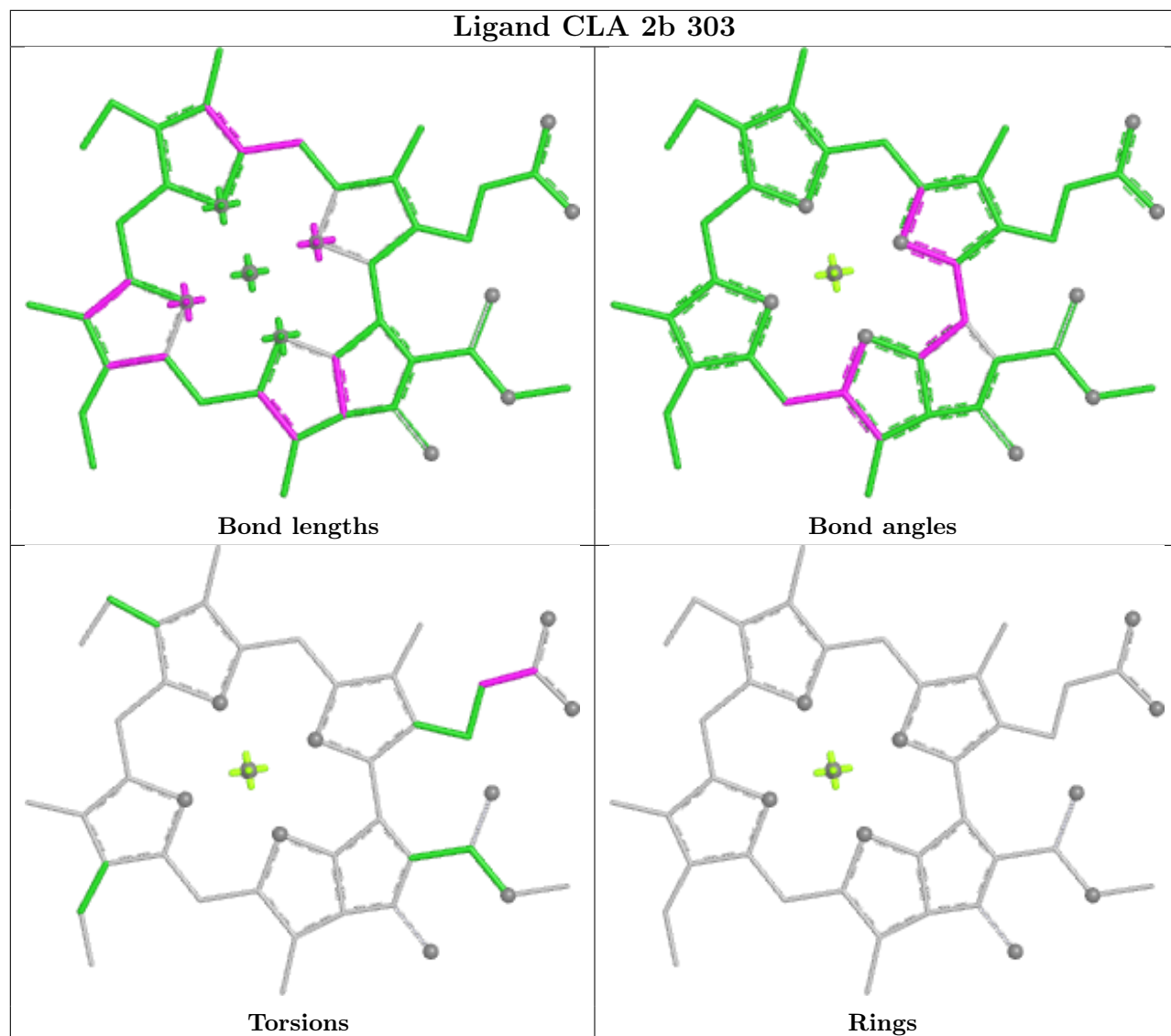


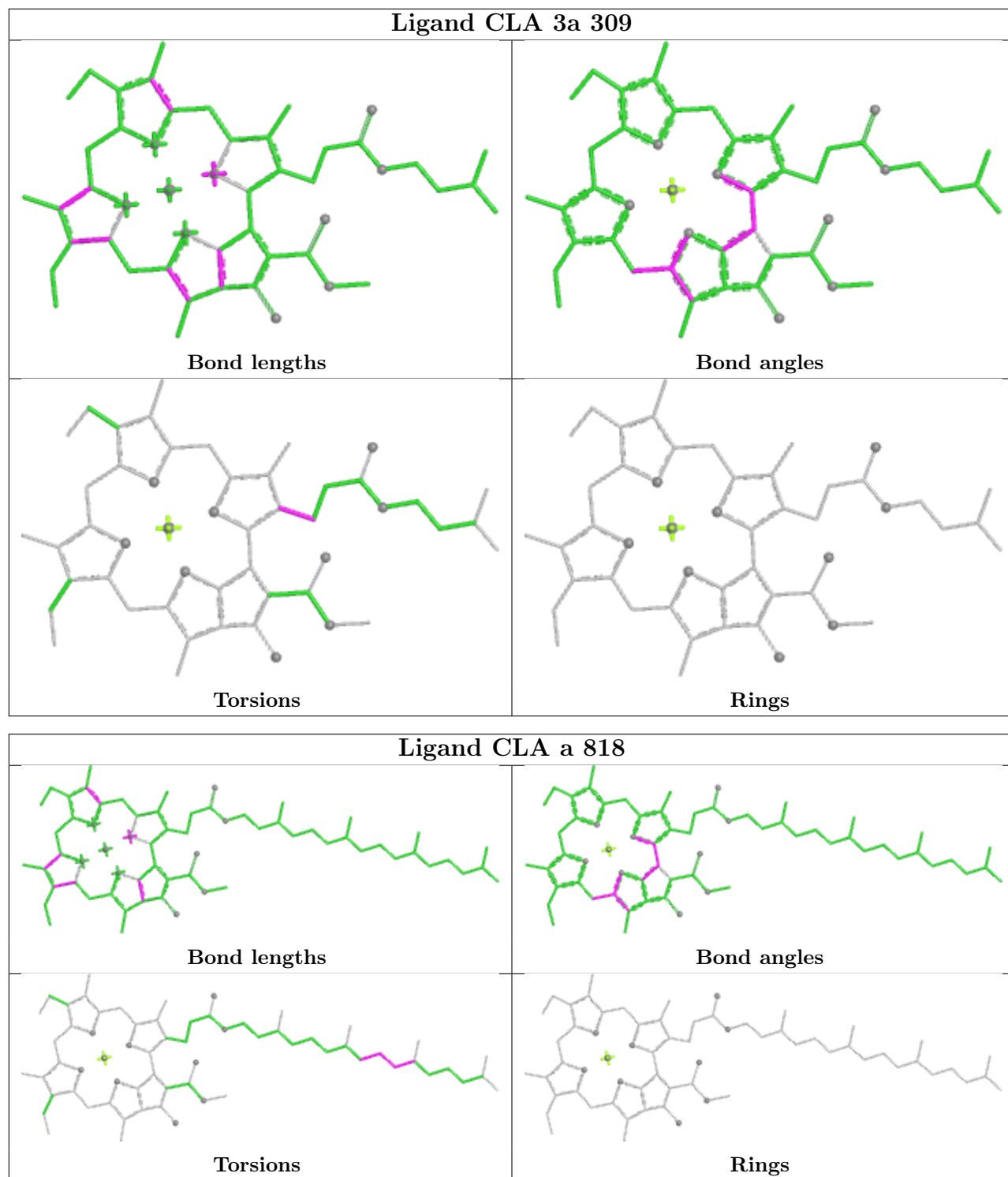
## Ligand LMU 6b 302

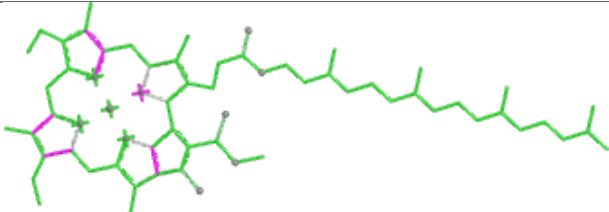
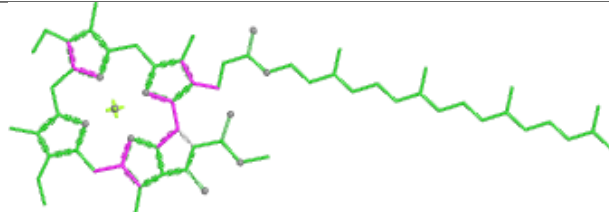
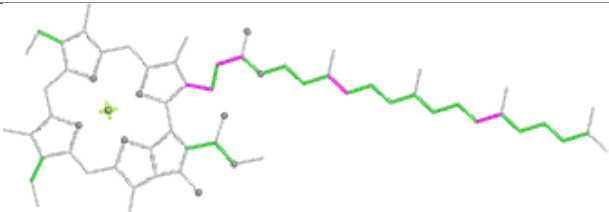
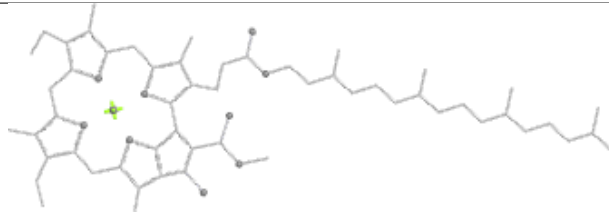


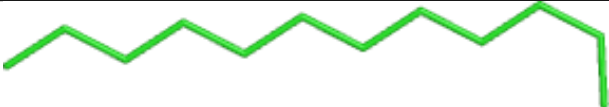
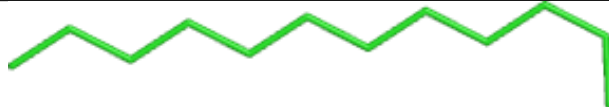
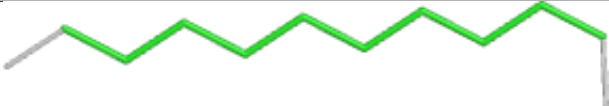
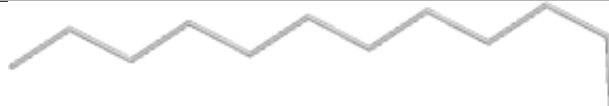


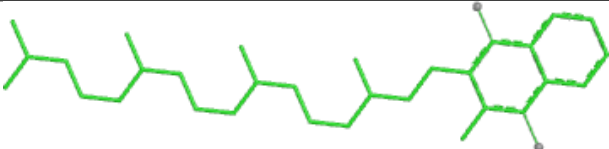
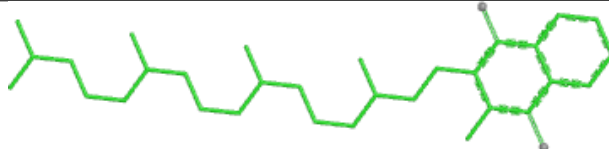
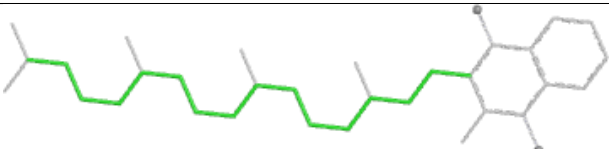
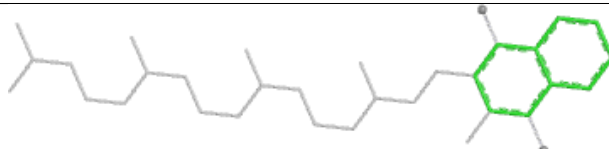




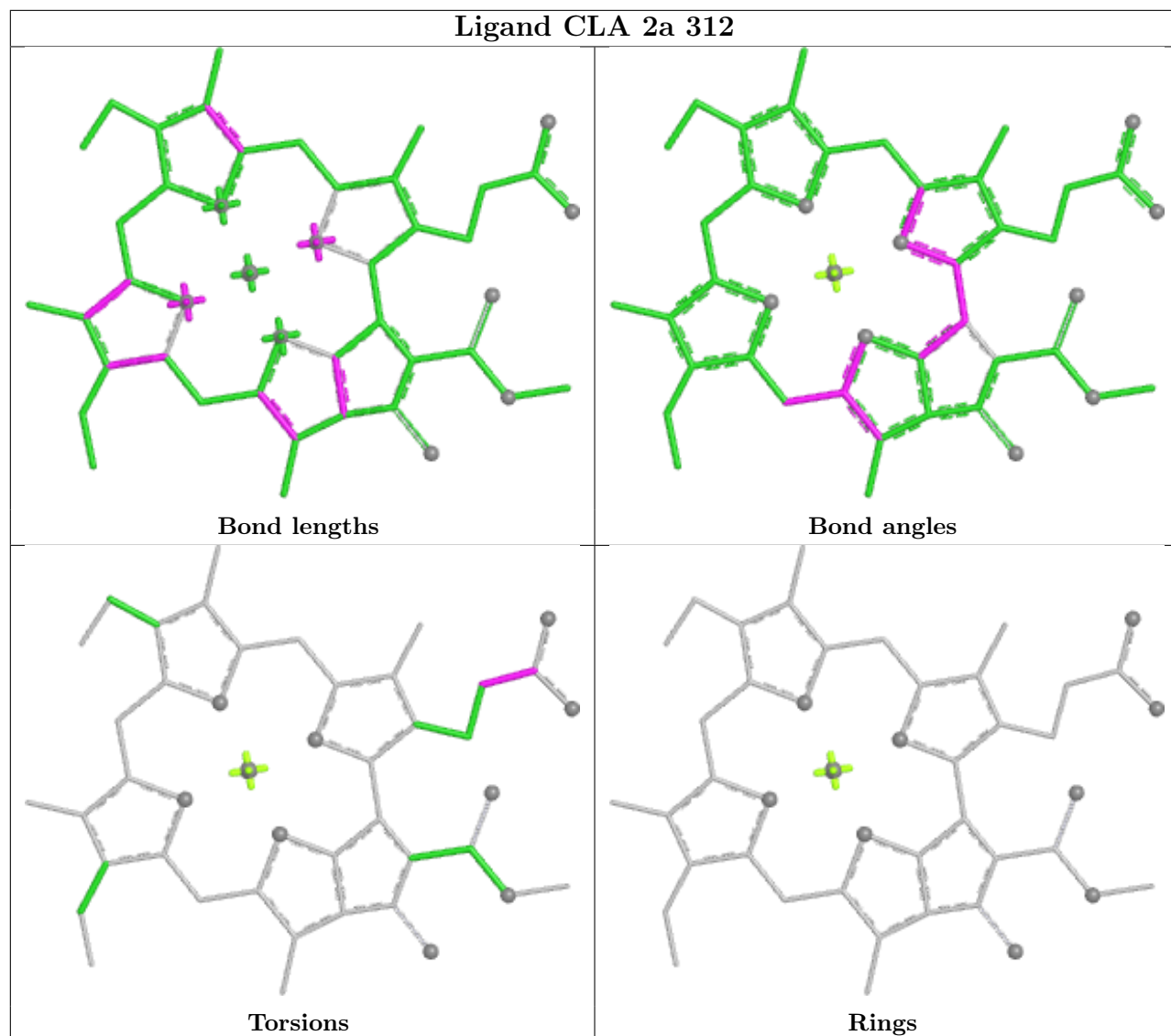


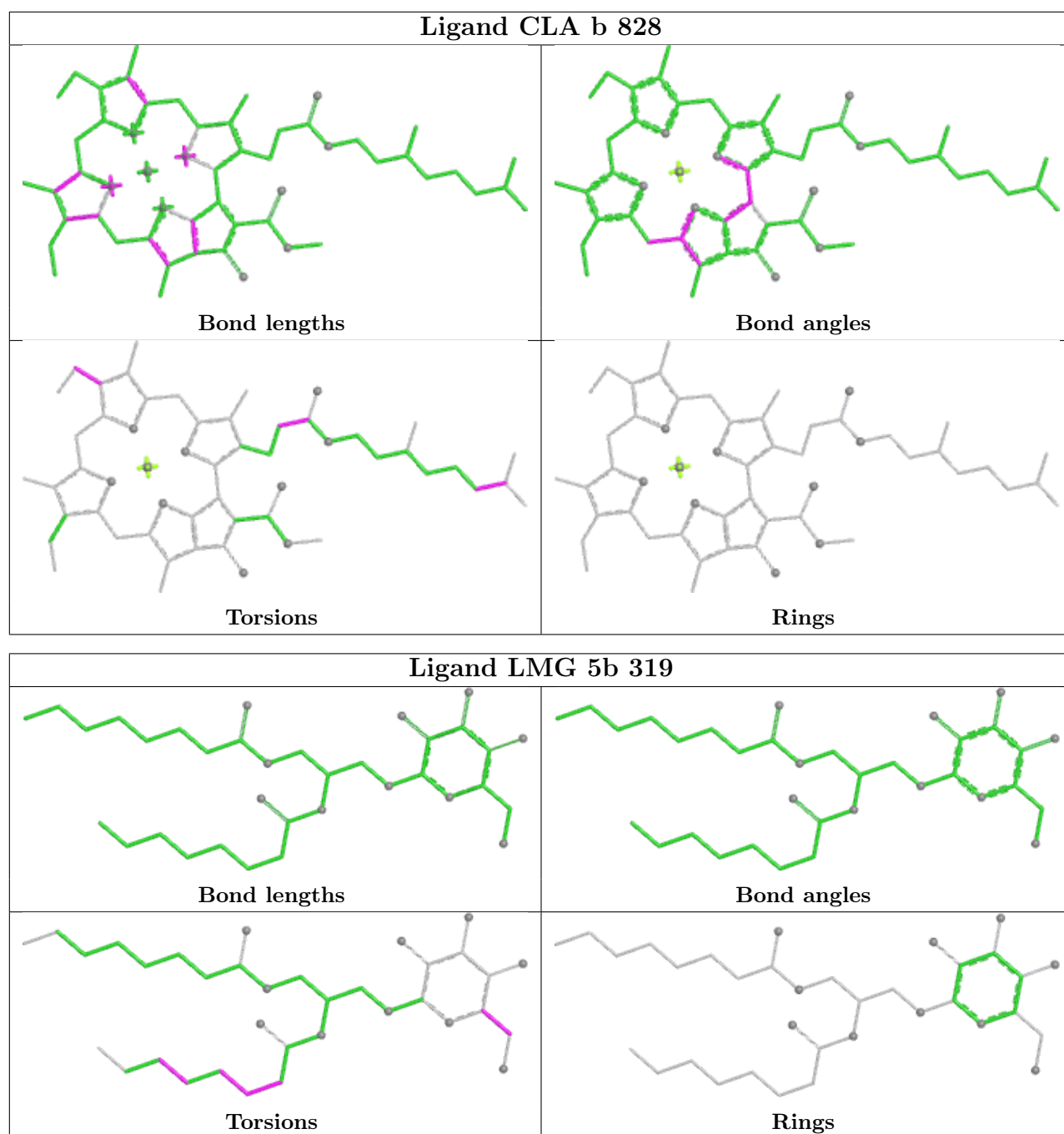
Ligand CLA b 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

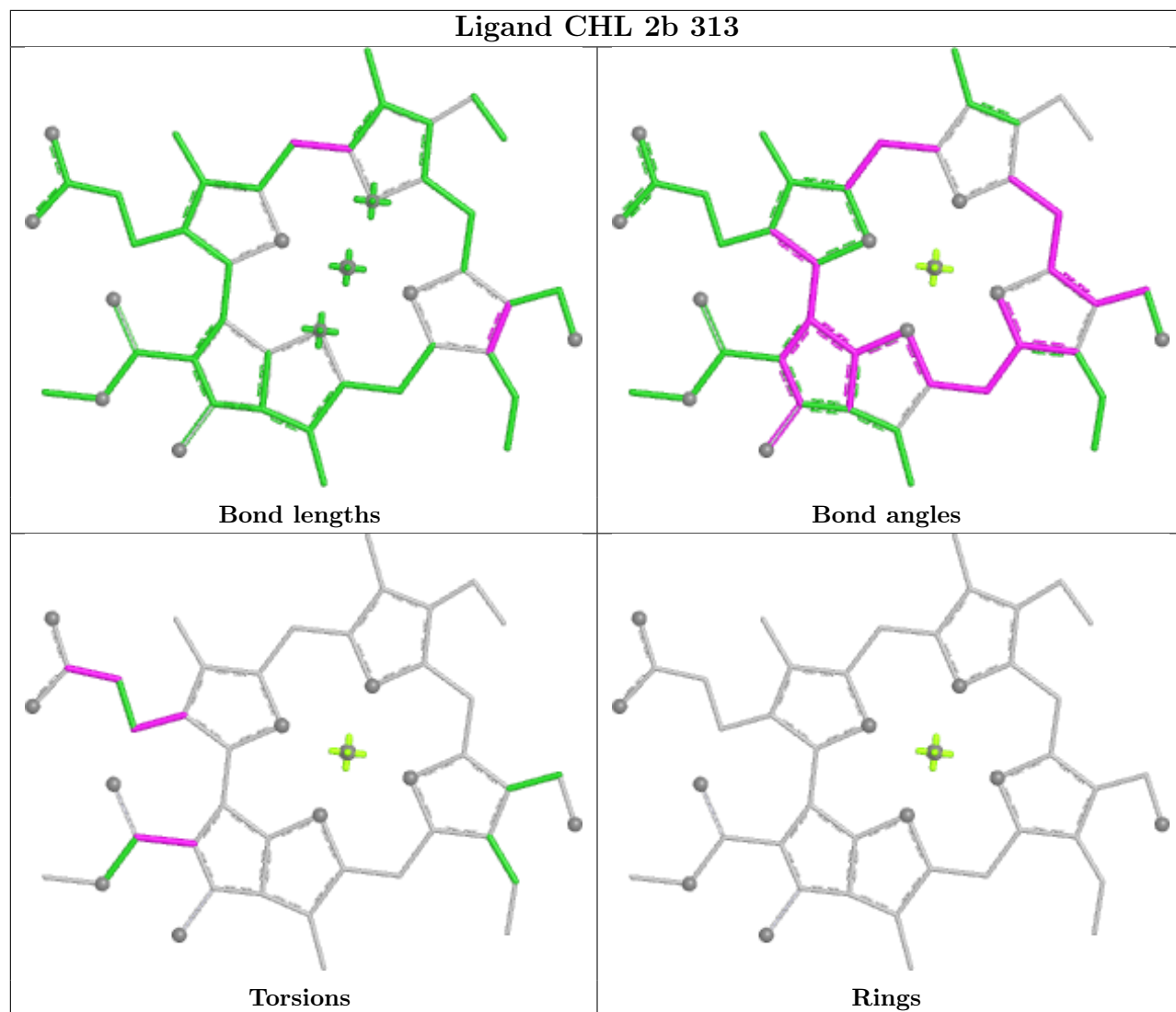
Ligand LFA m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN B 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

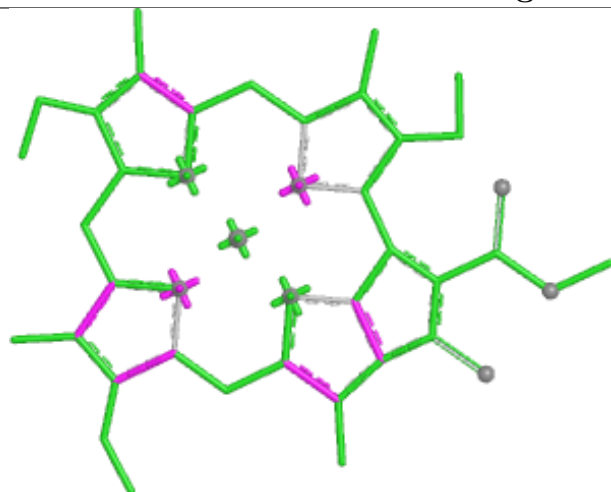




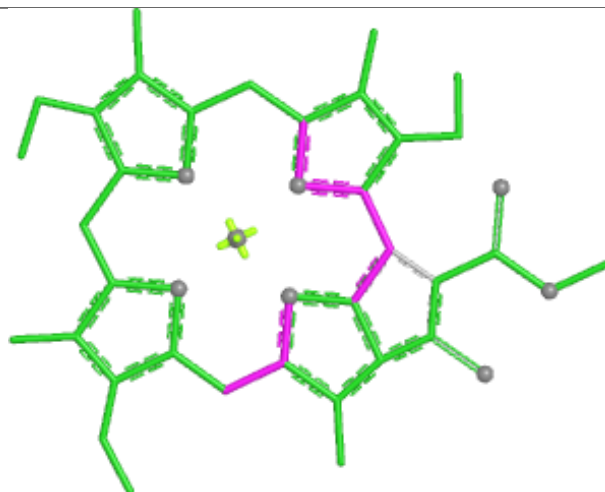




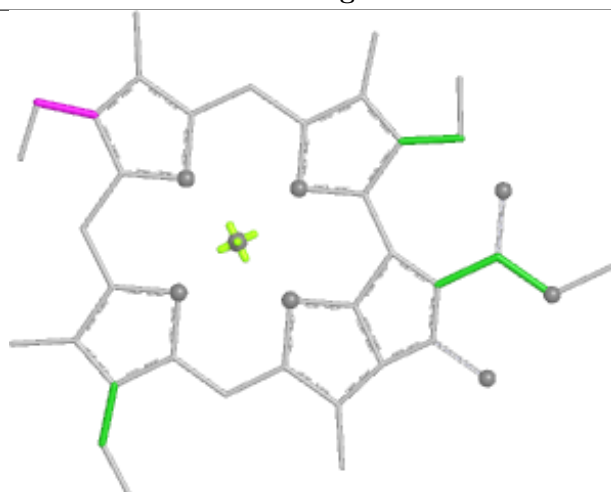
## Ligand CLA L 303



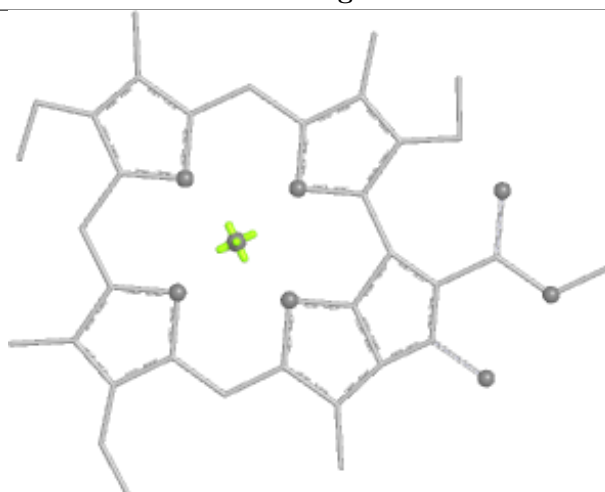
Bond lengths



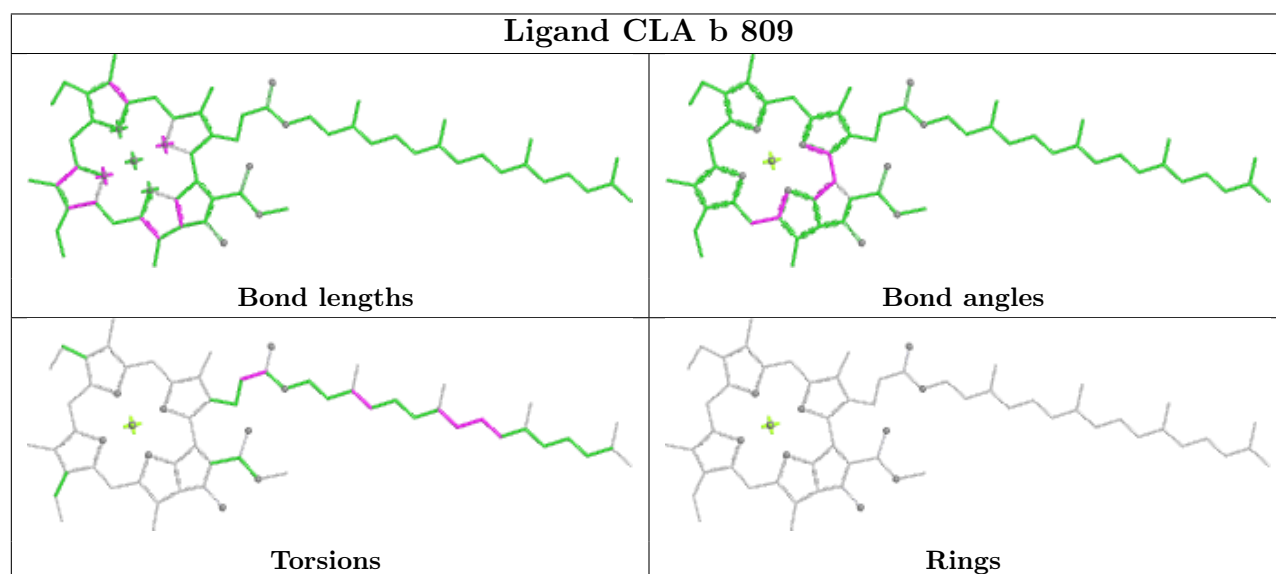
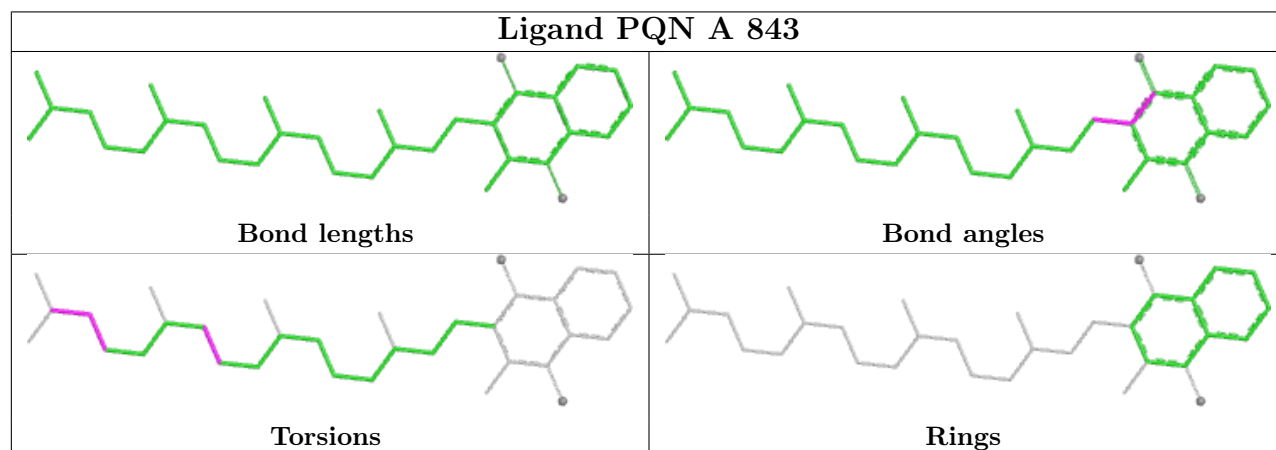
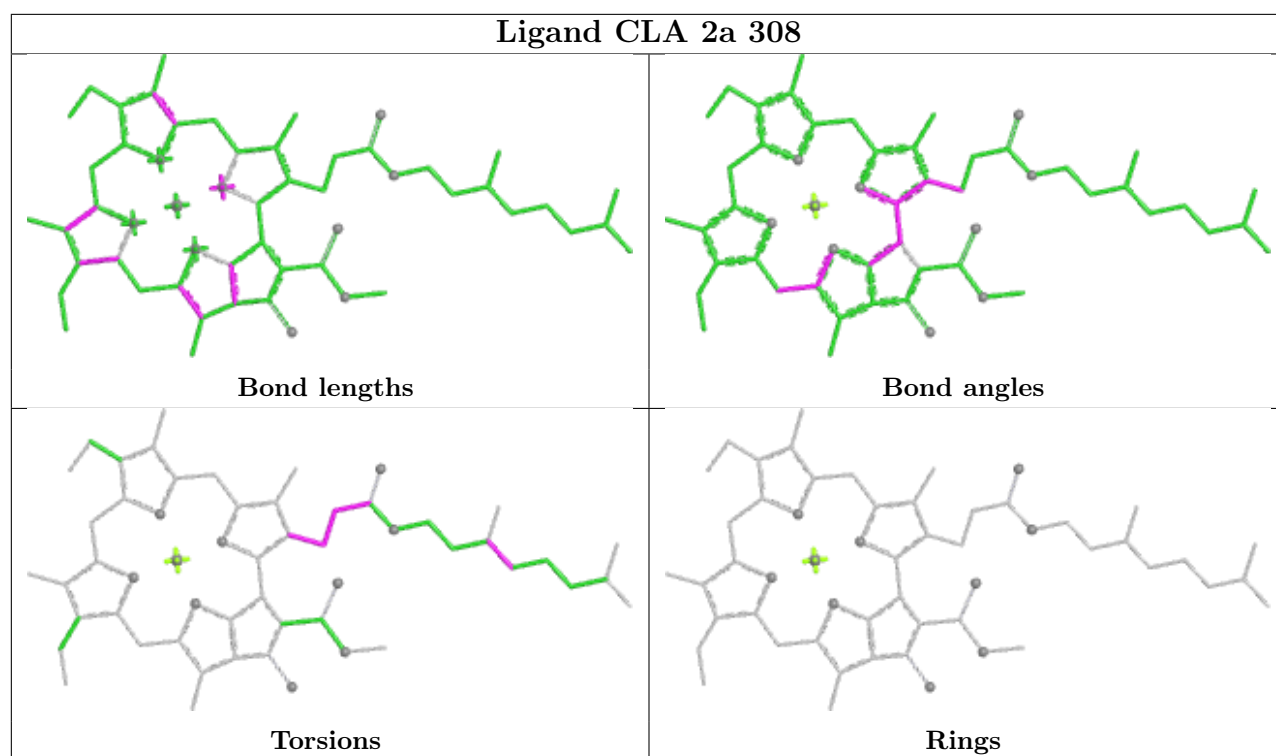
Bond angles

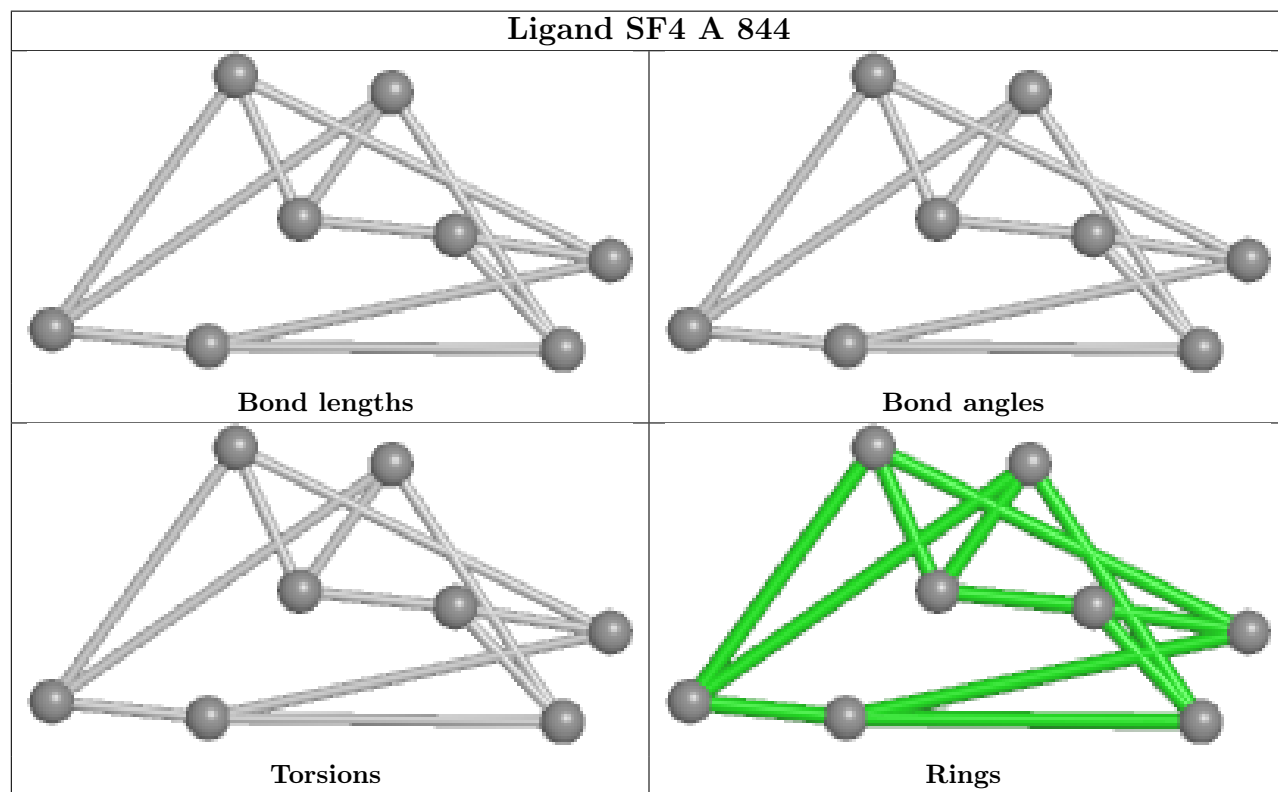
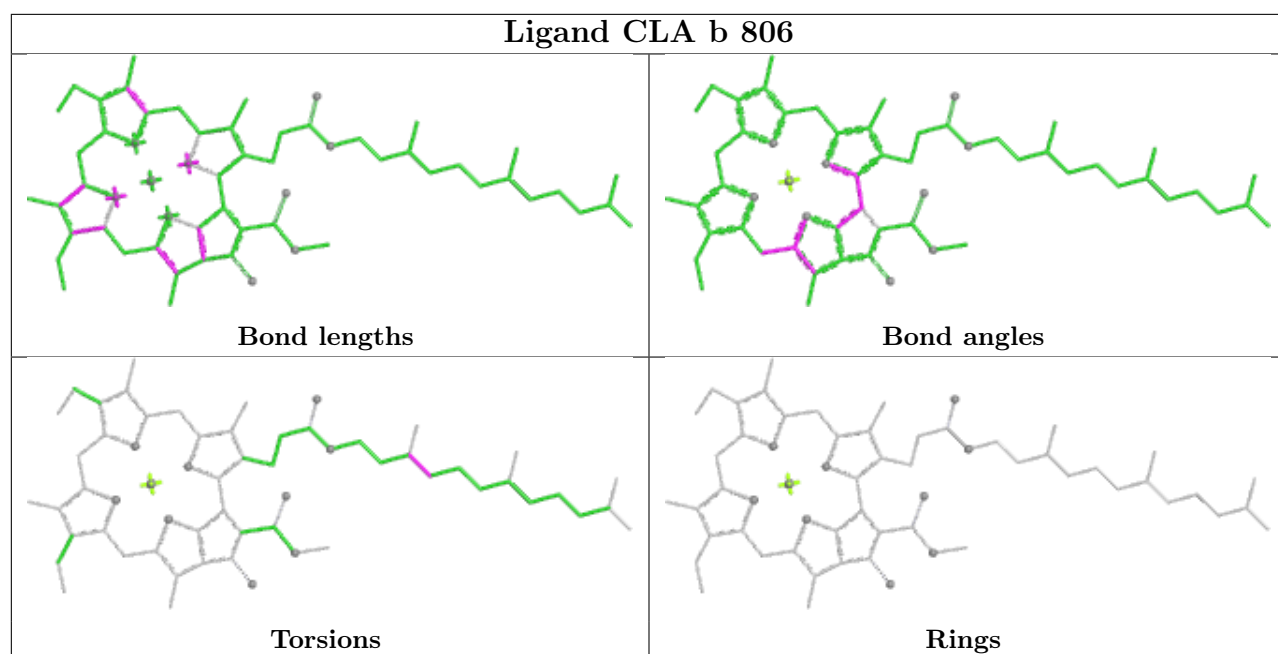


Torsions

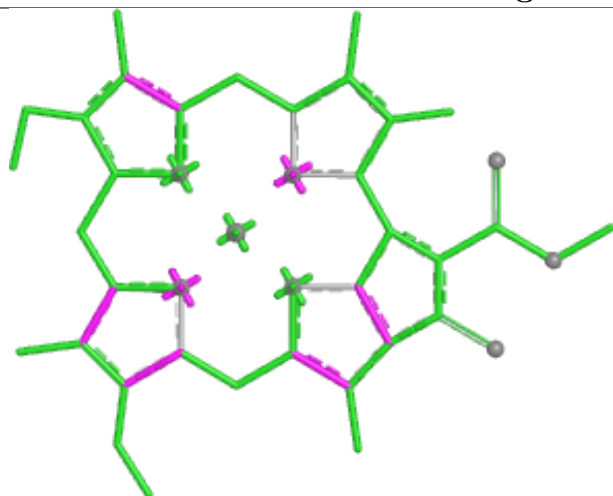


Rings

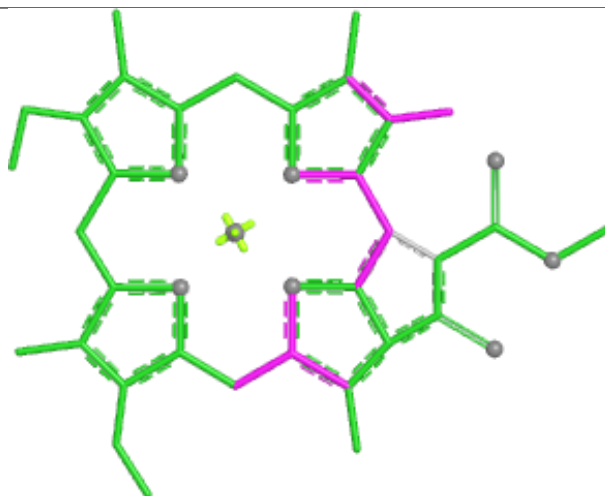




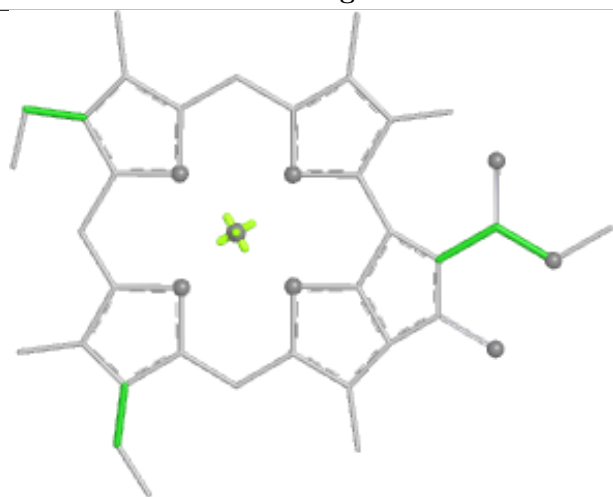
## Ligand CLA F 303



Bond lengths



Bond angles

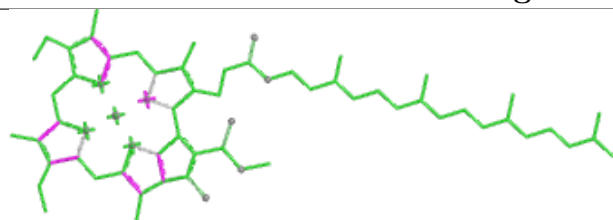


Torsions

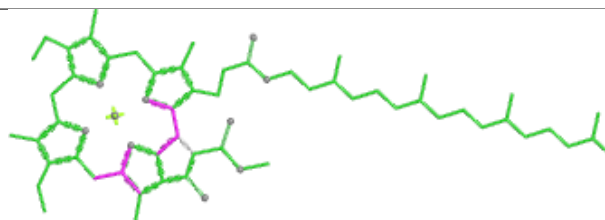


Rings

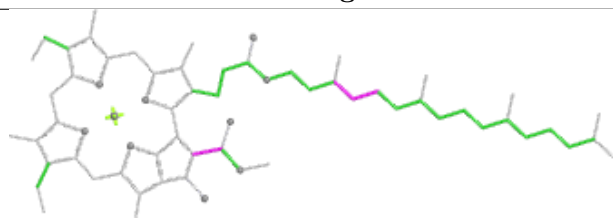
## Ligand CLA A 805



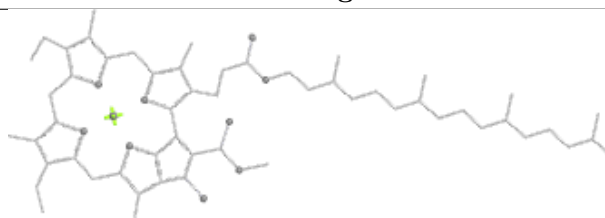
Bond lengths



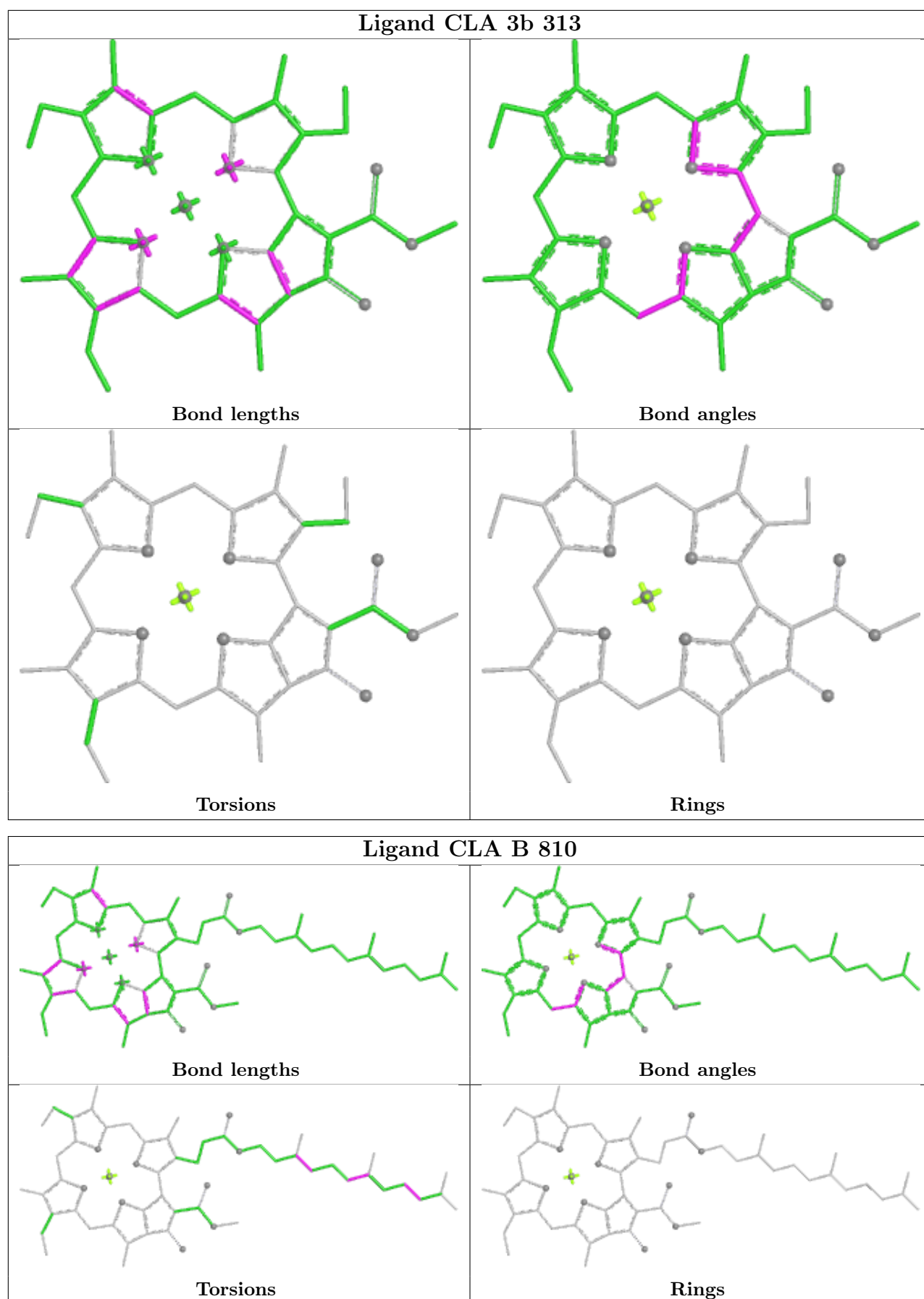
Bond angles



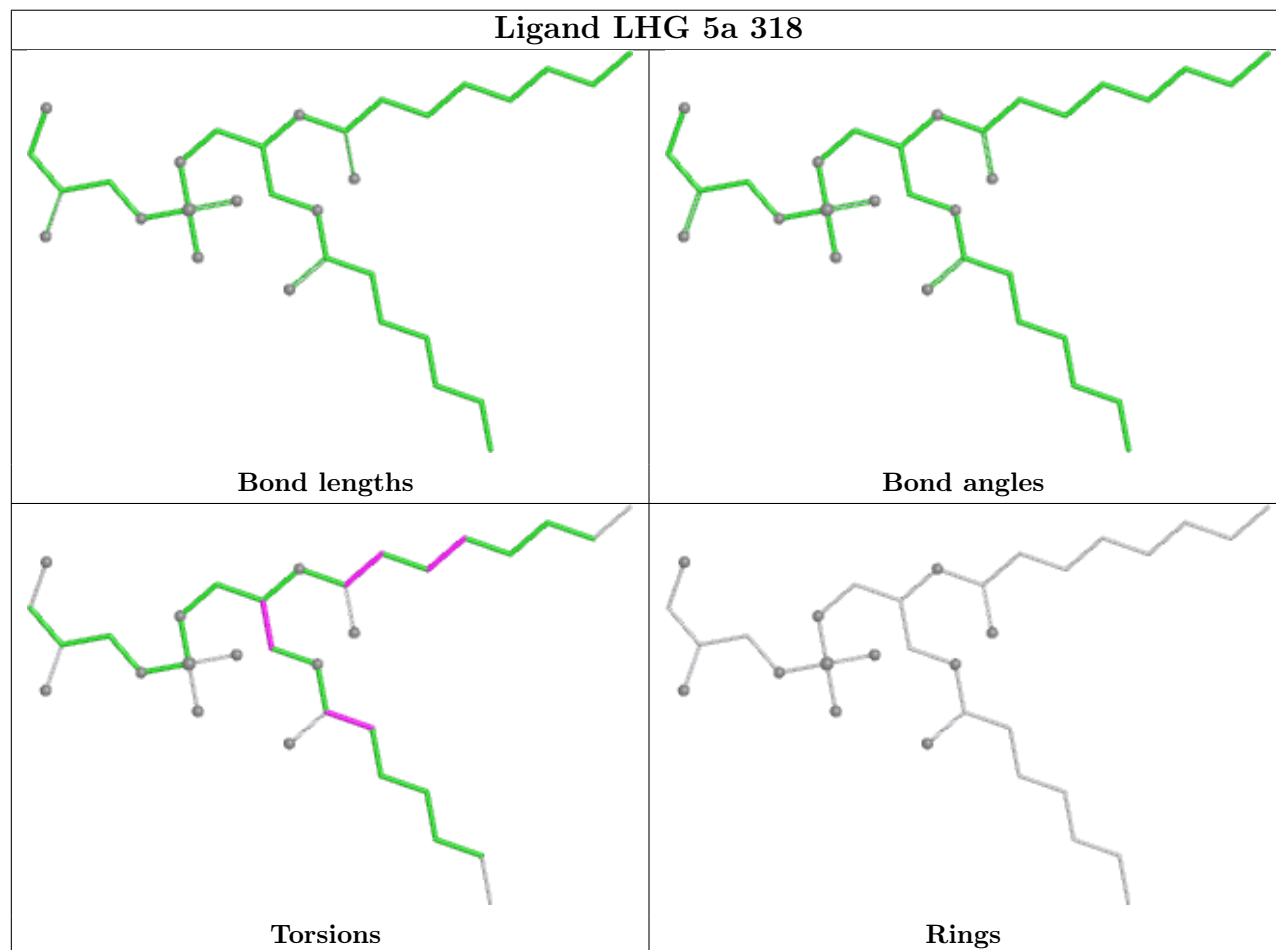
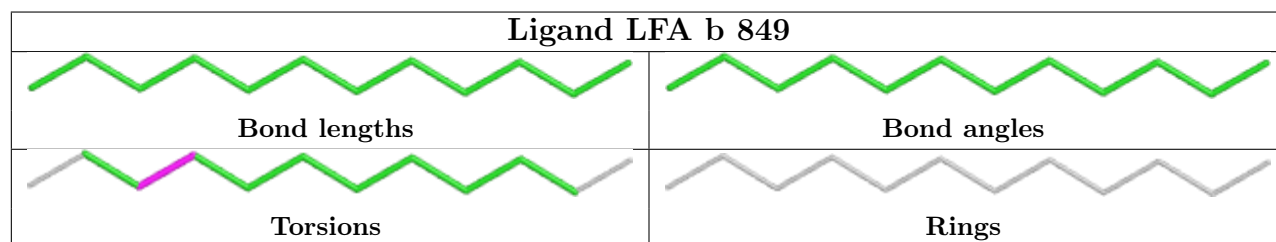
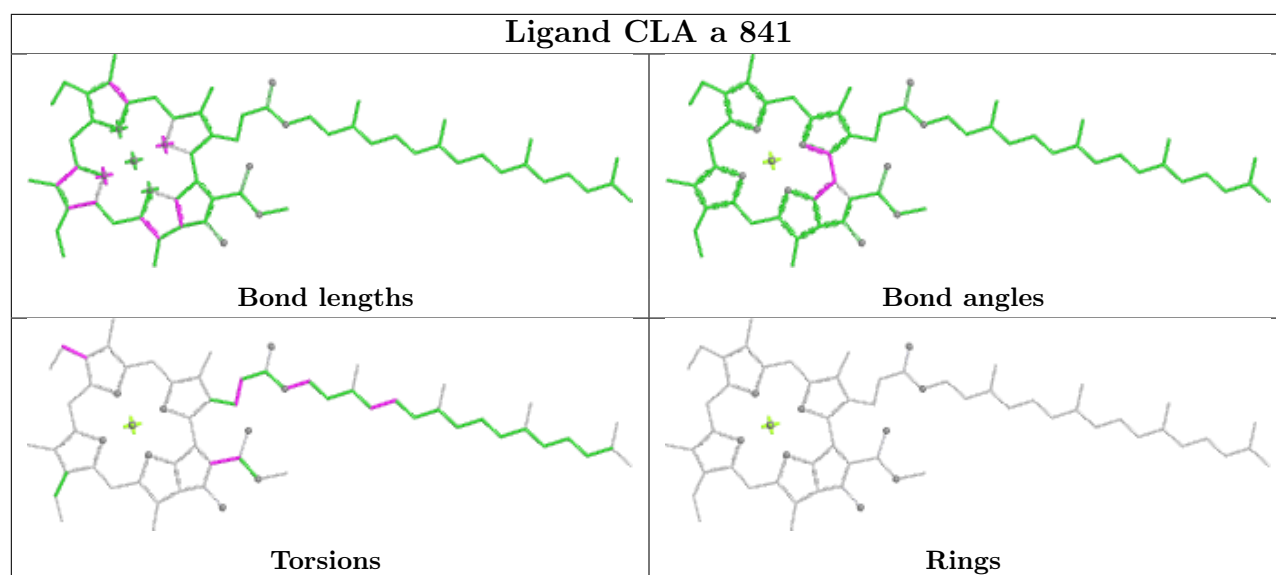
Torsions

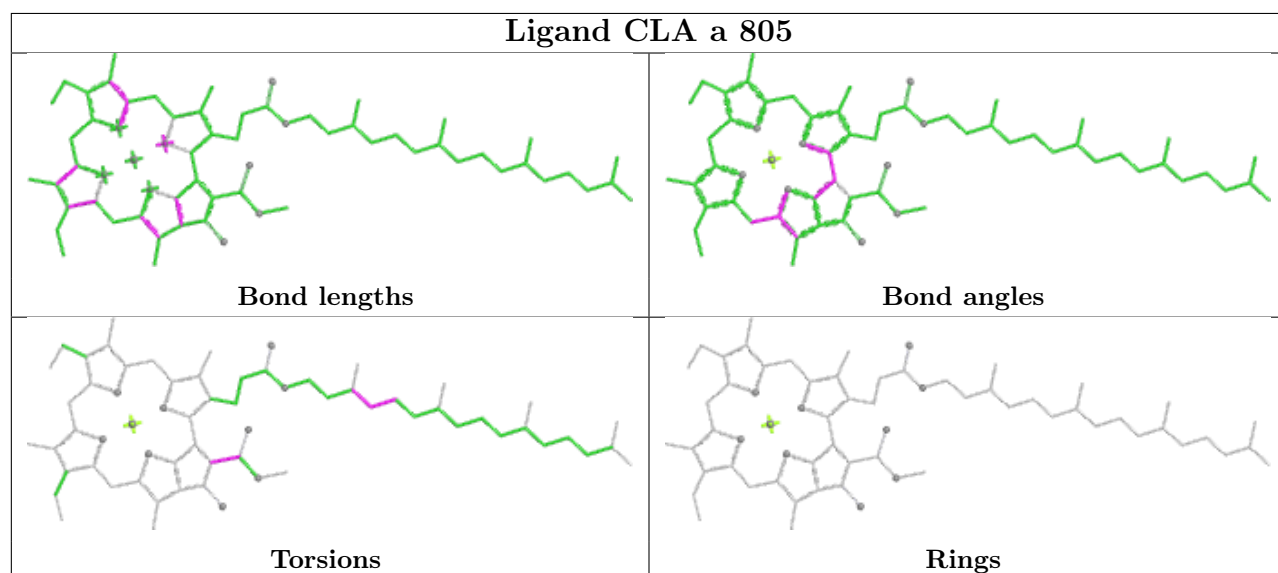
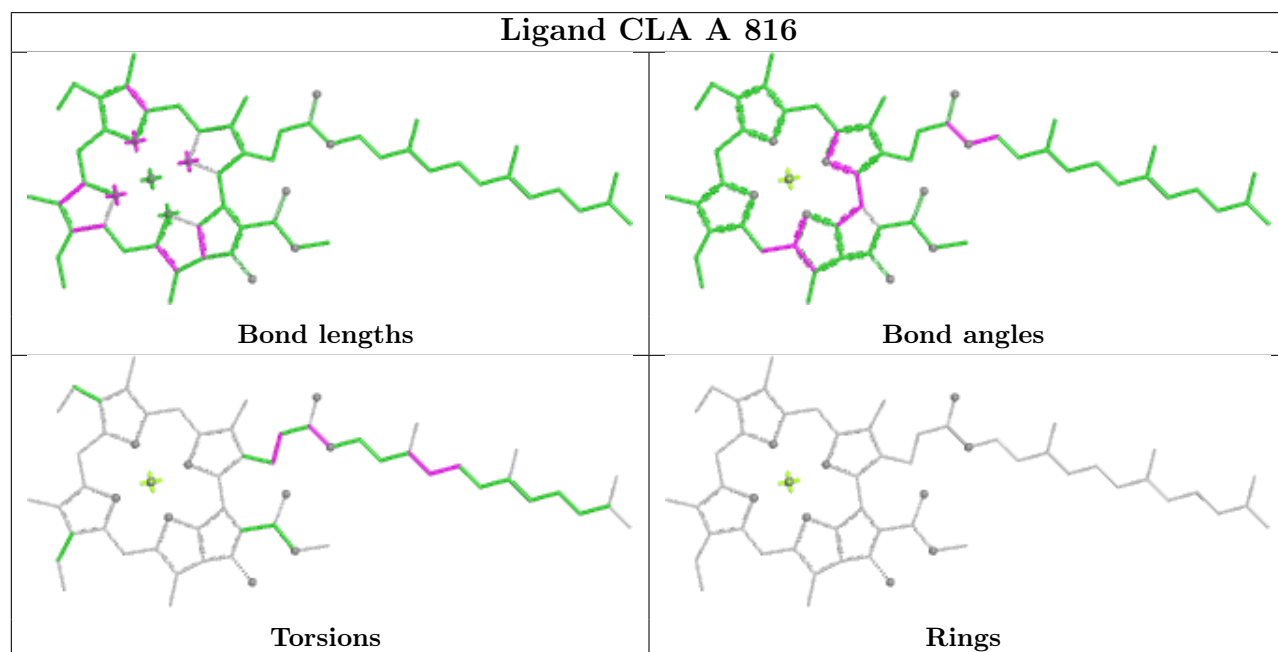
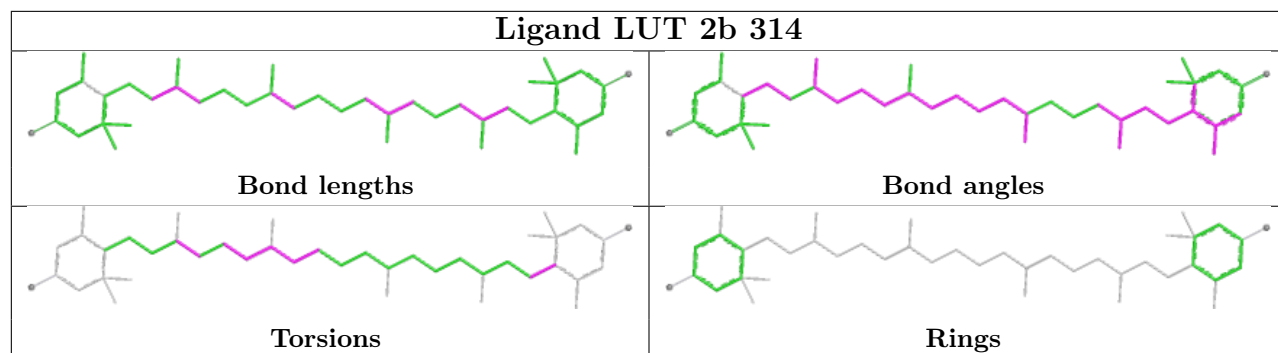


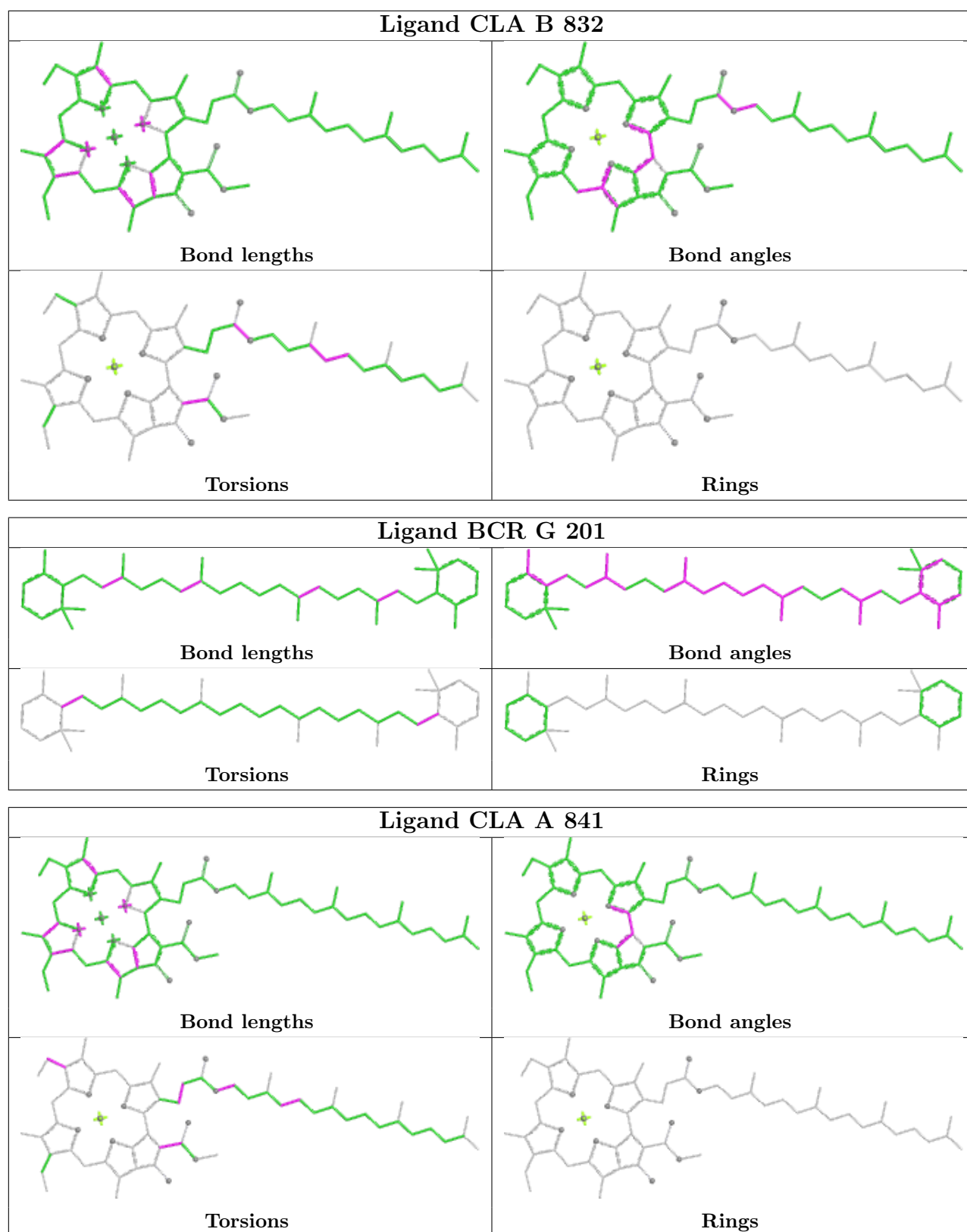
Rings

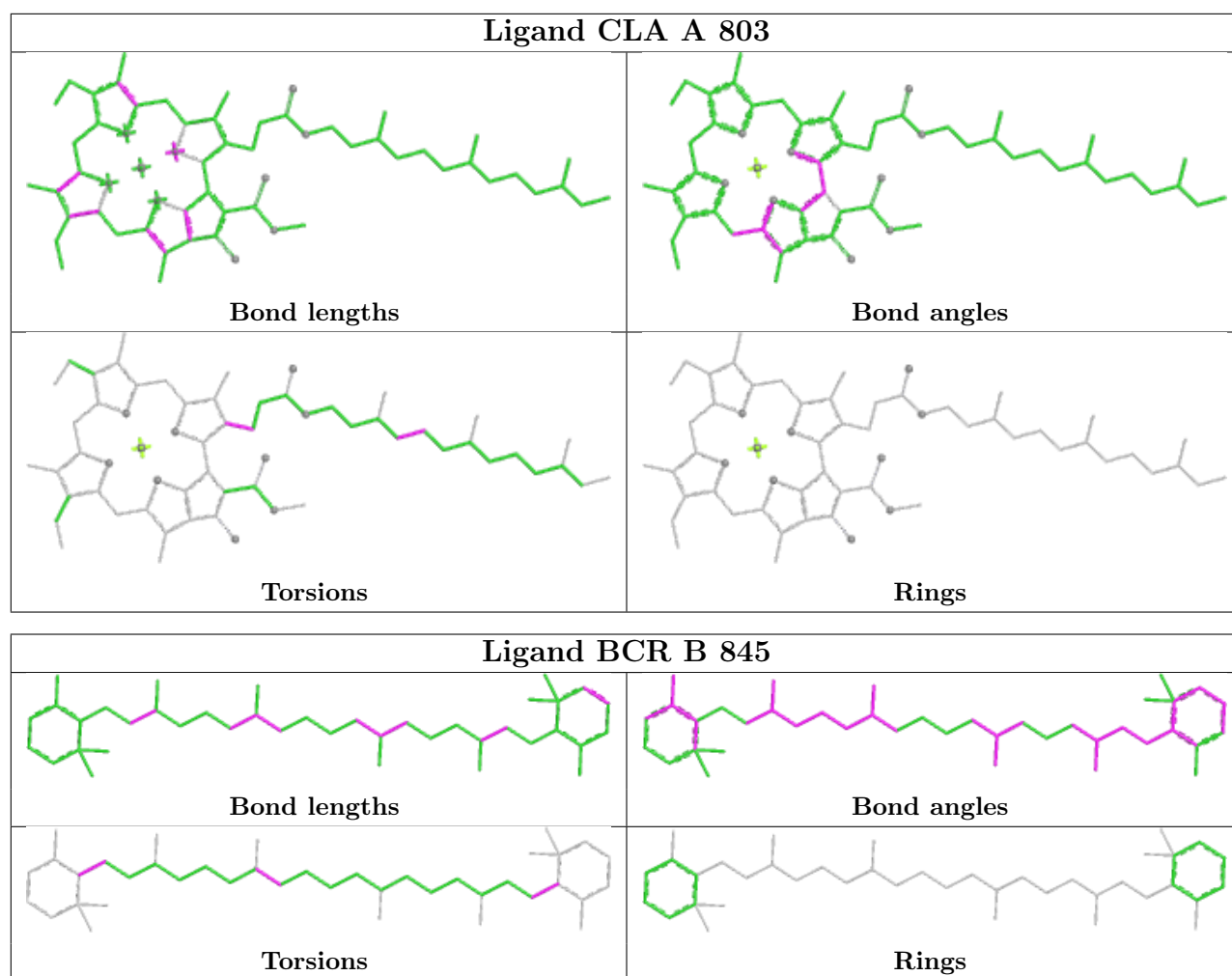




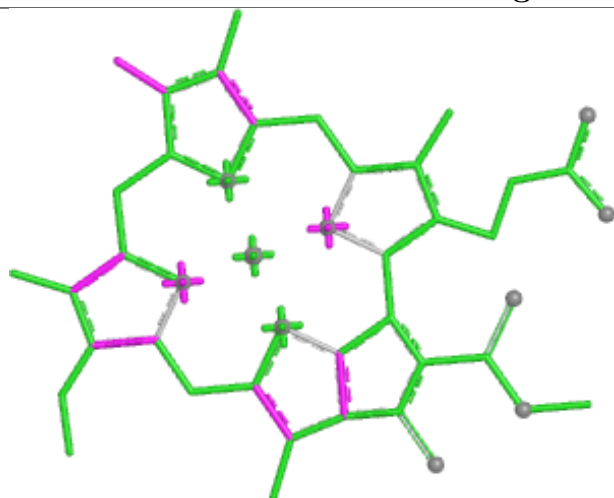




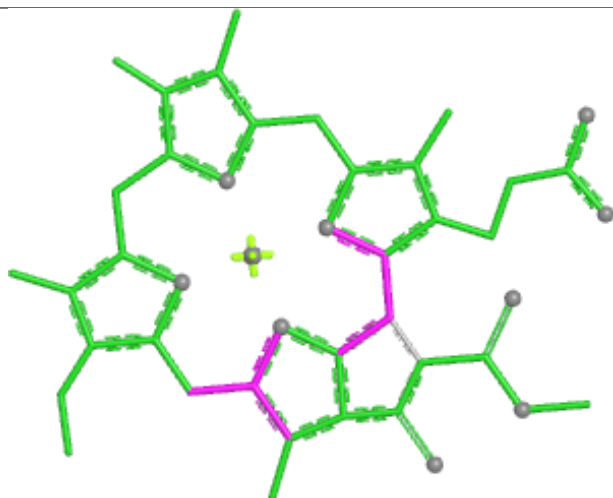




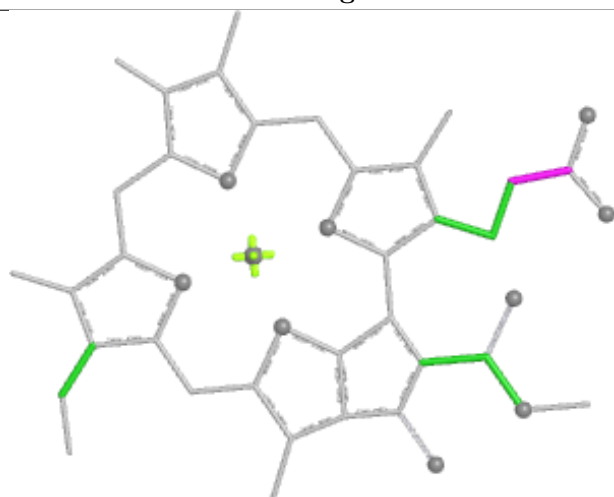
## Ligand CLA K 201



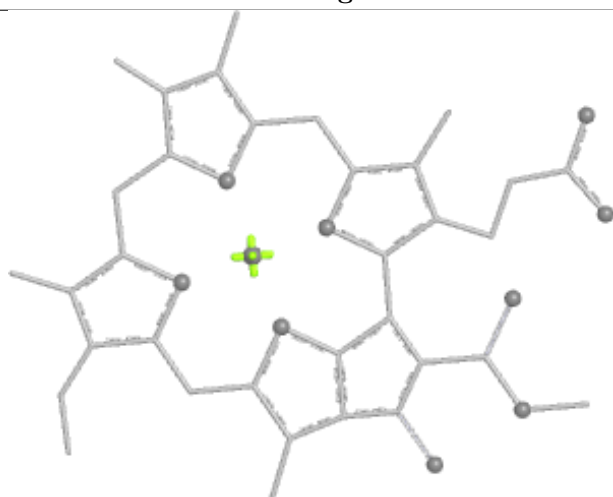
Bond lengths



Bond angles

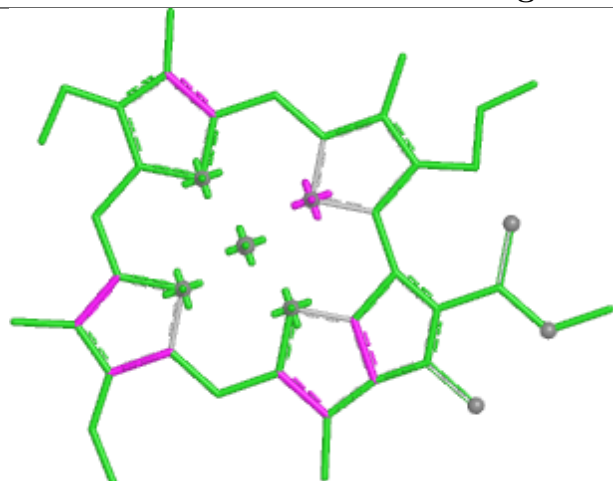


Torsions

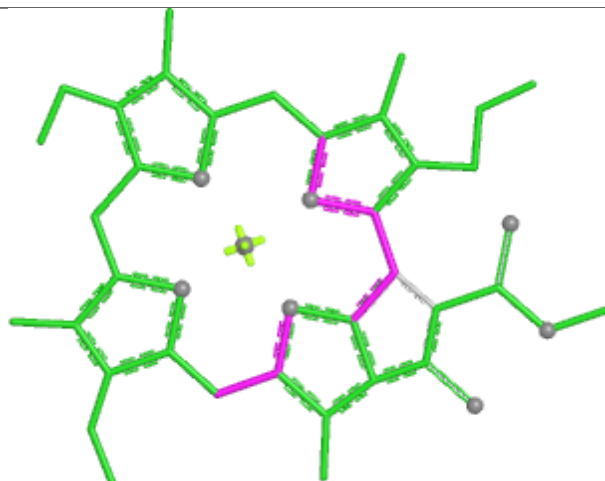


Rings

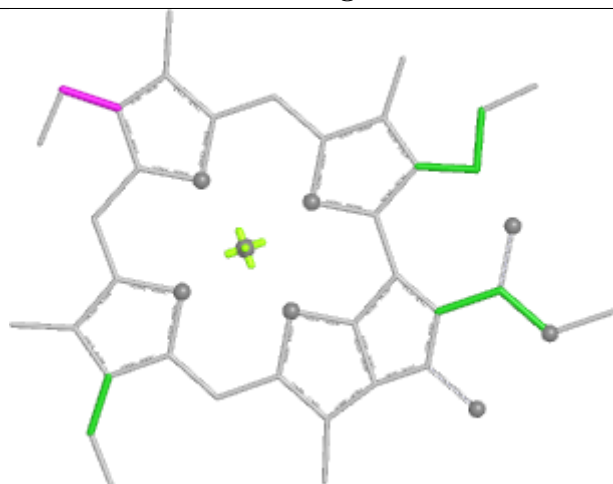
## Ligand CLA b 819



Bond lengths



Bond angles

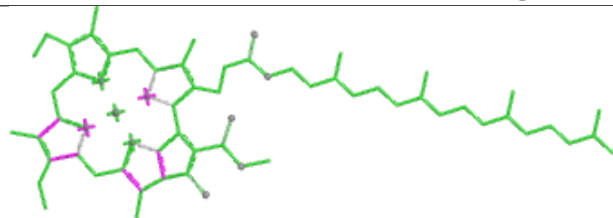


Torsions

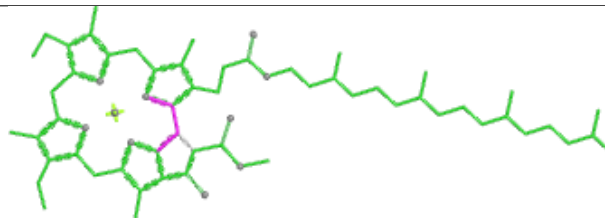


Rings

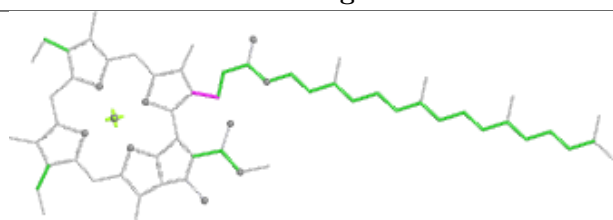
## Ligand CLA A 832



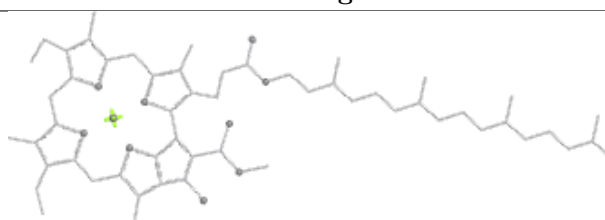
Bond lengths



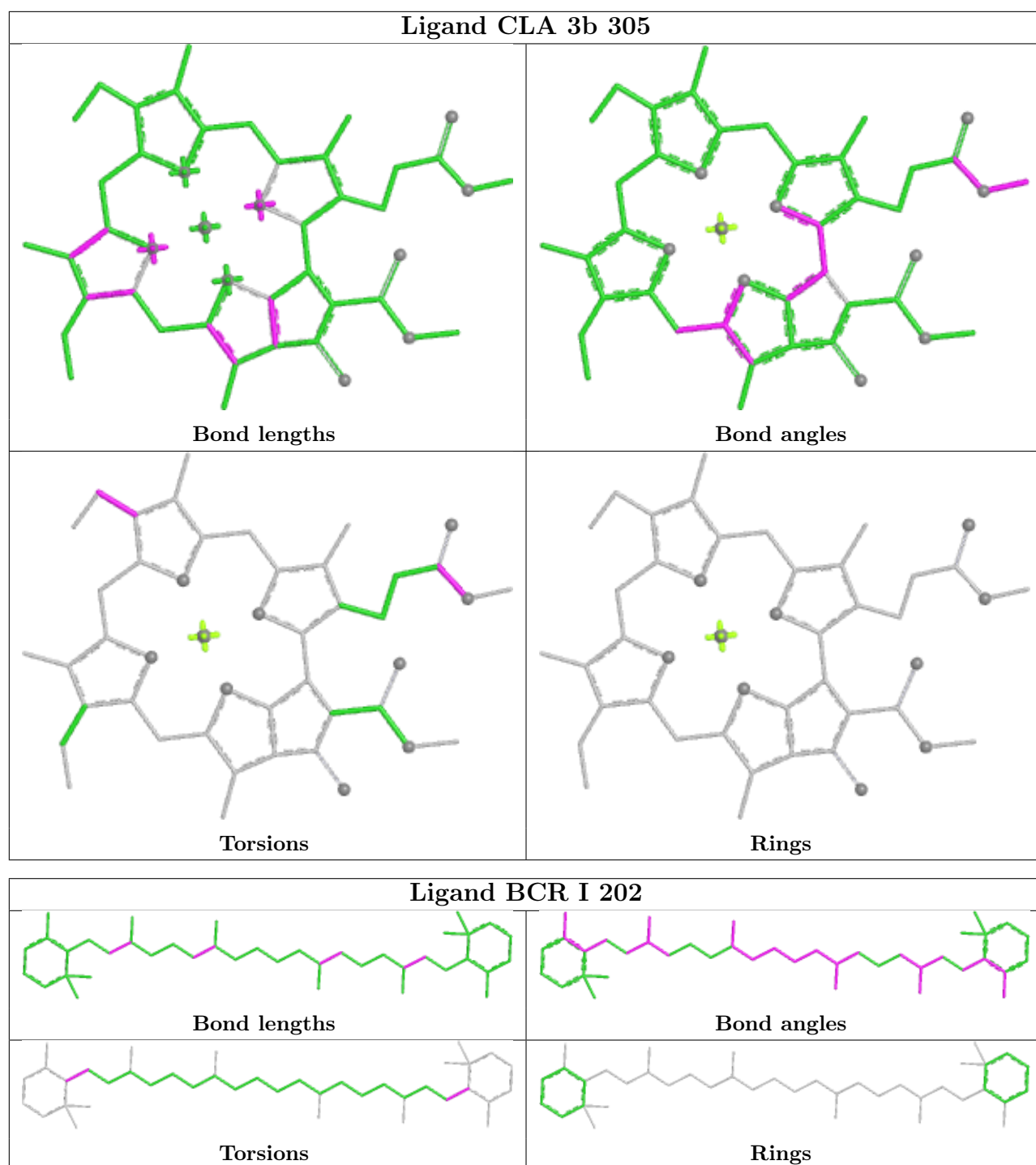
Bond angles

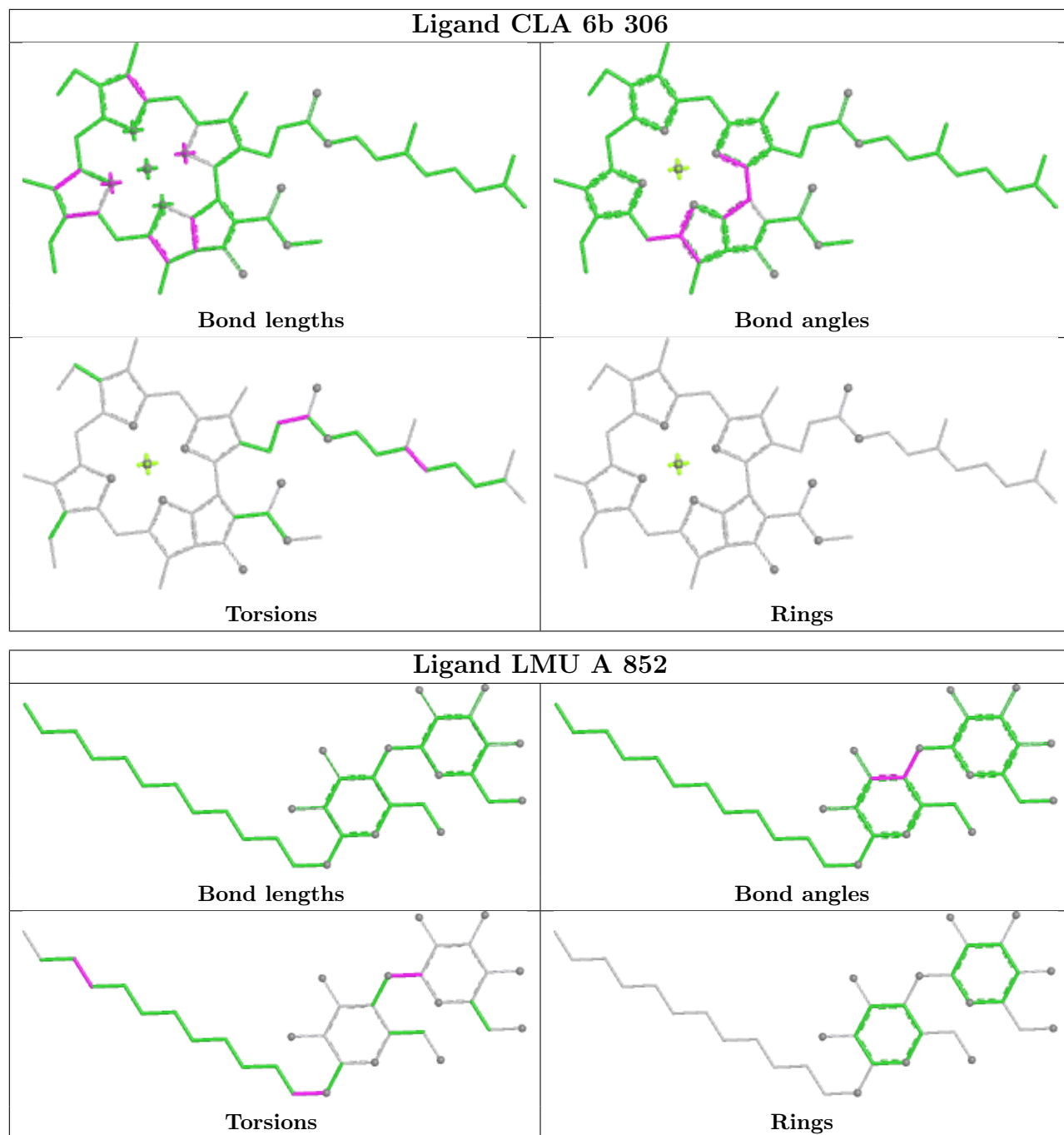


Torsions

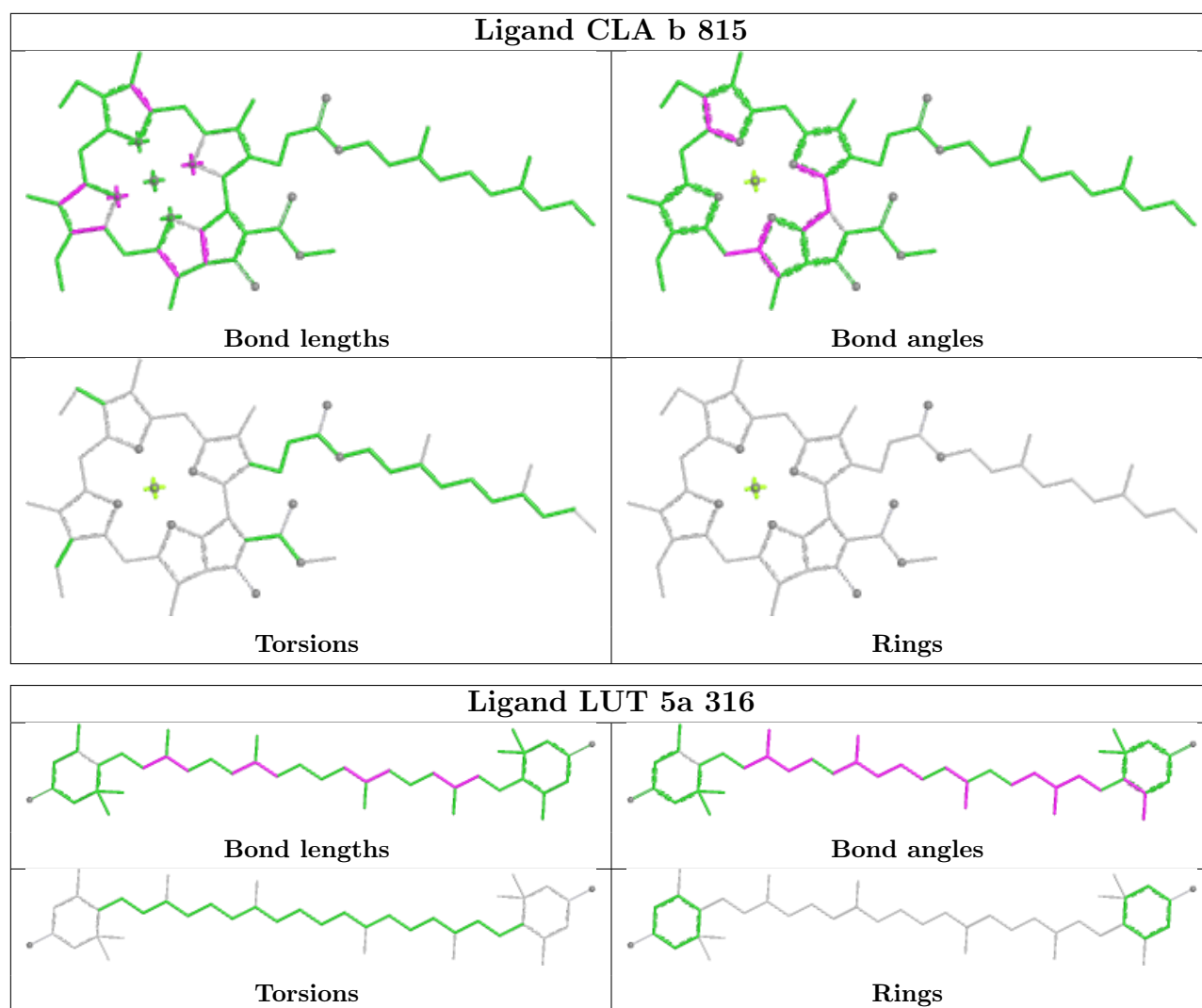


Rings

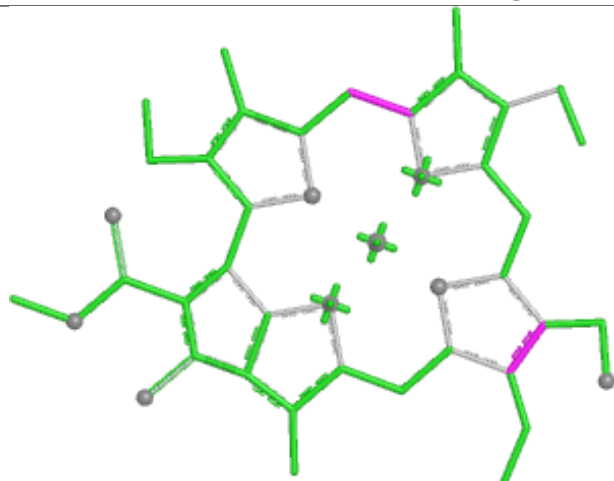




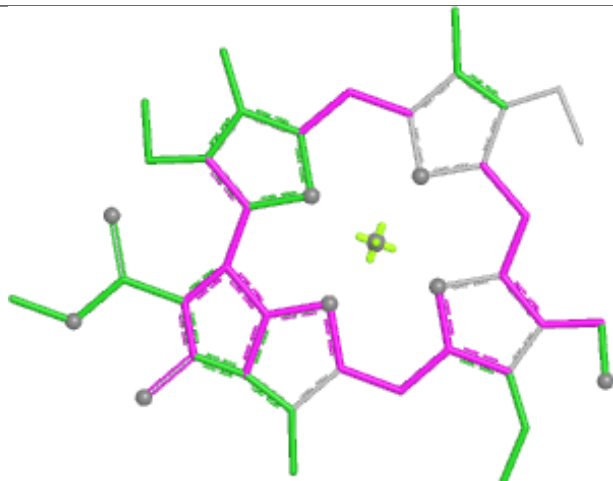




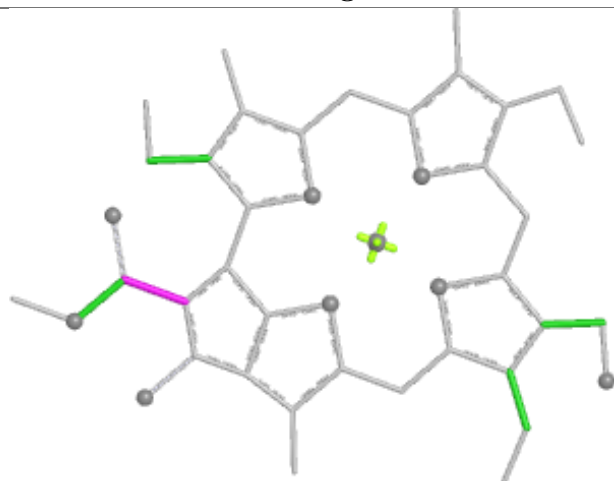
## Ligand CHL 5b 314



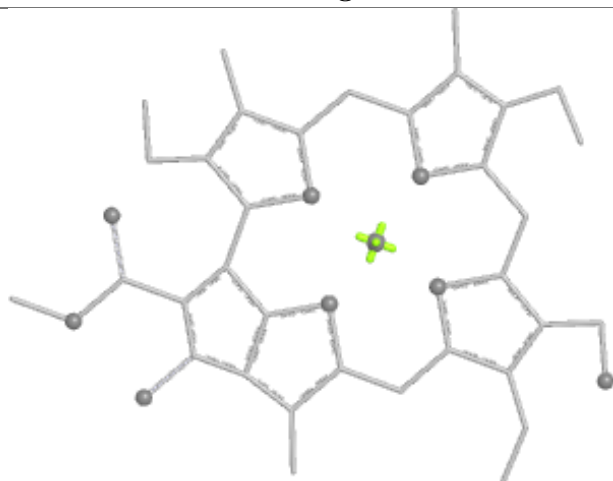
Bond lengths



Bond angles

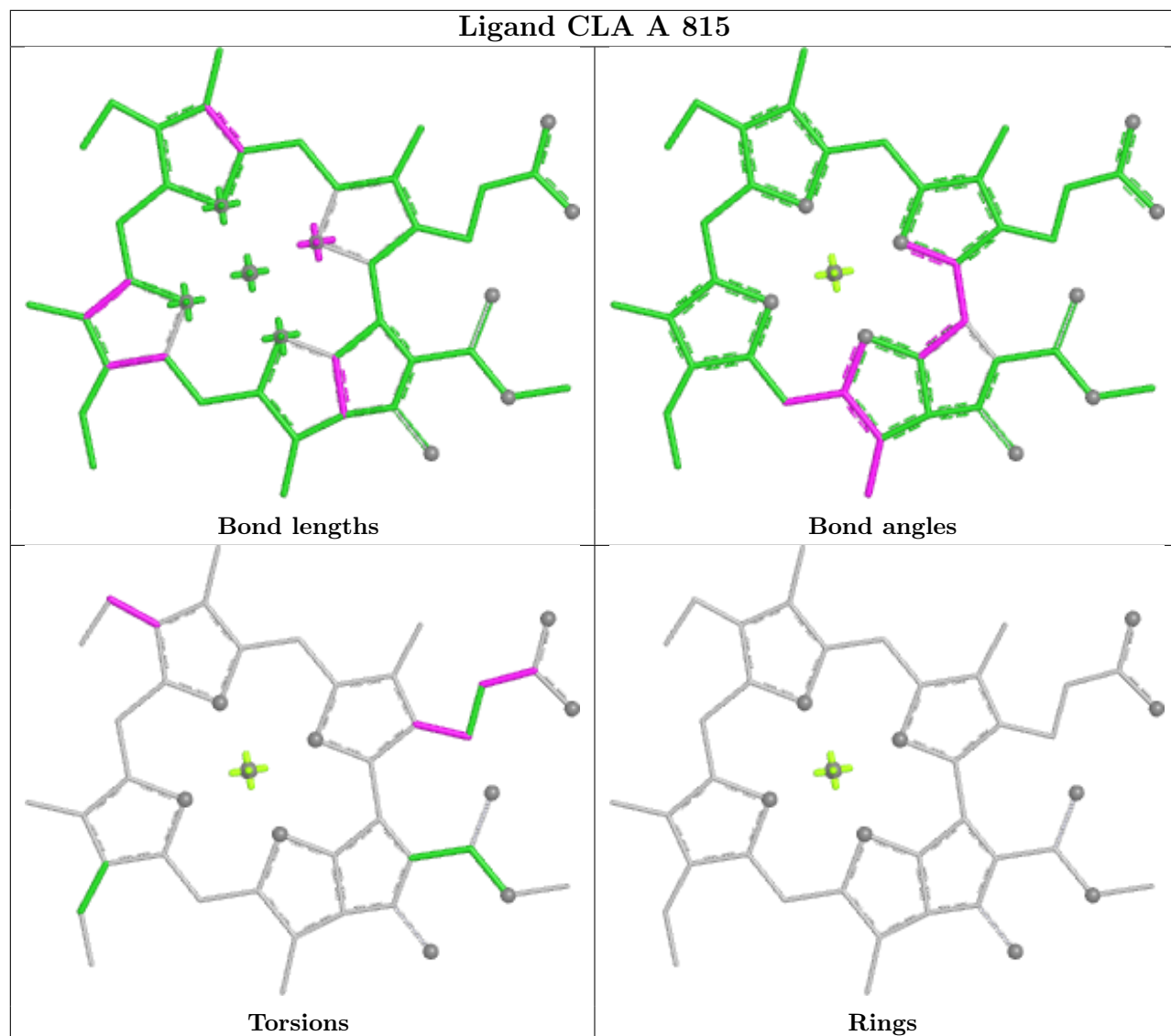


Torsions

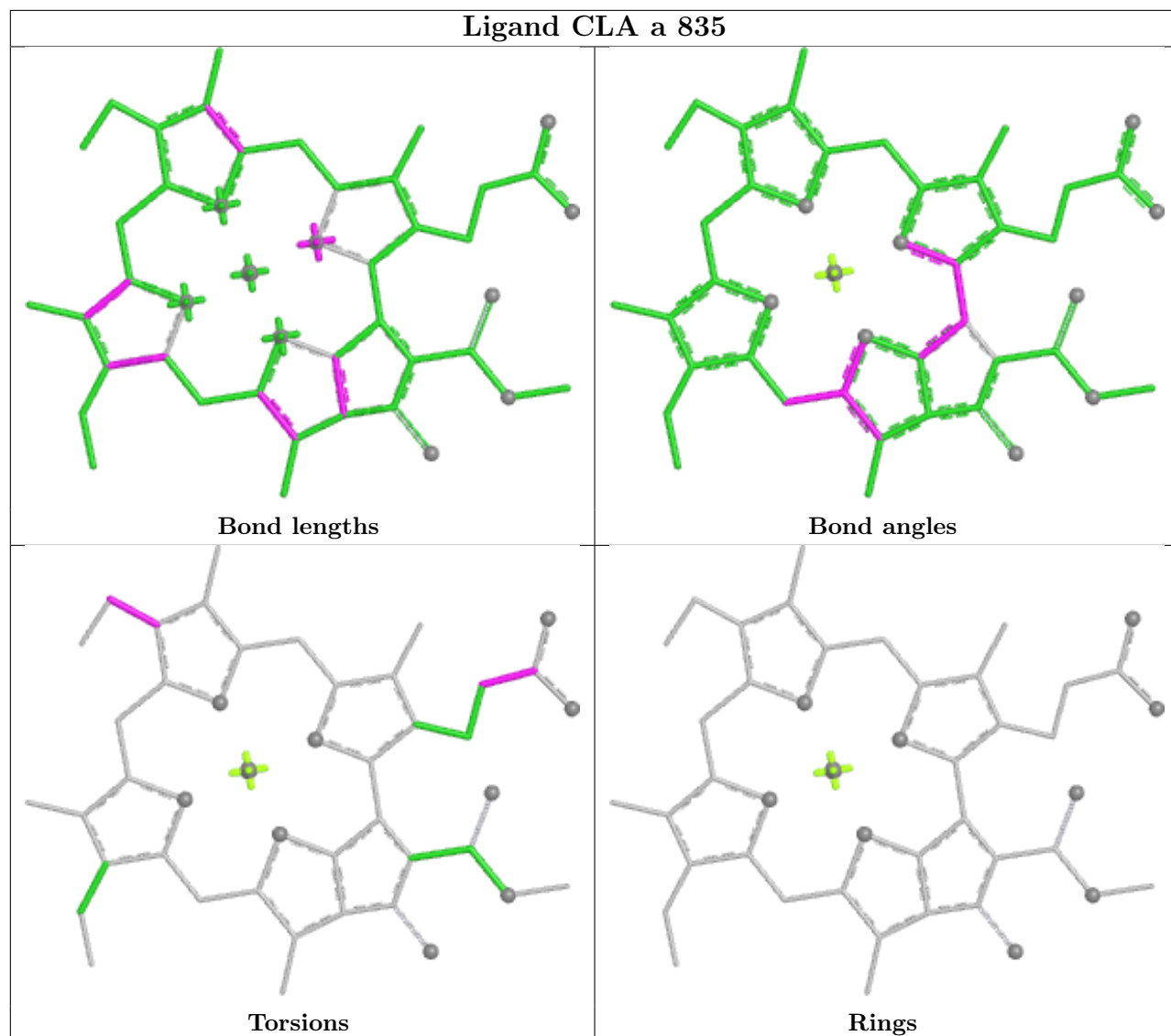


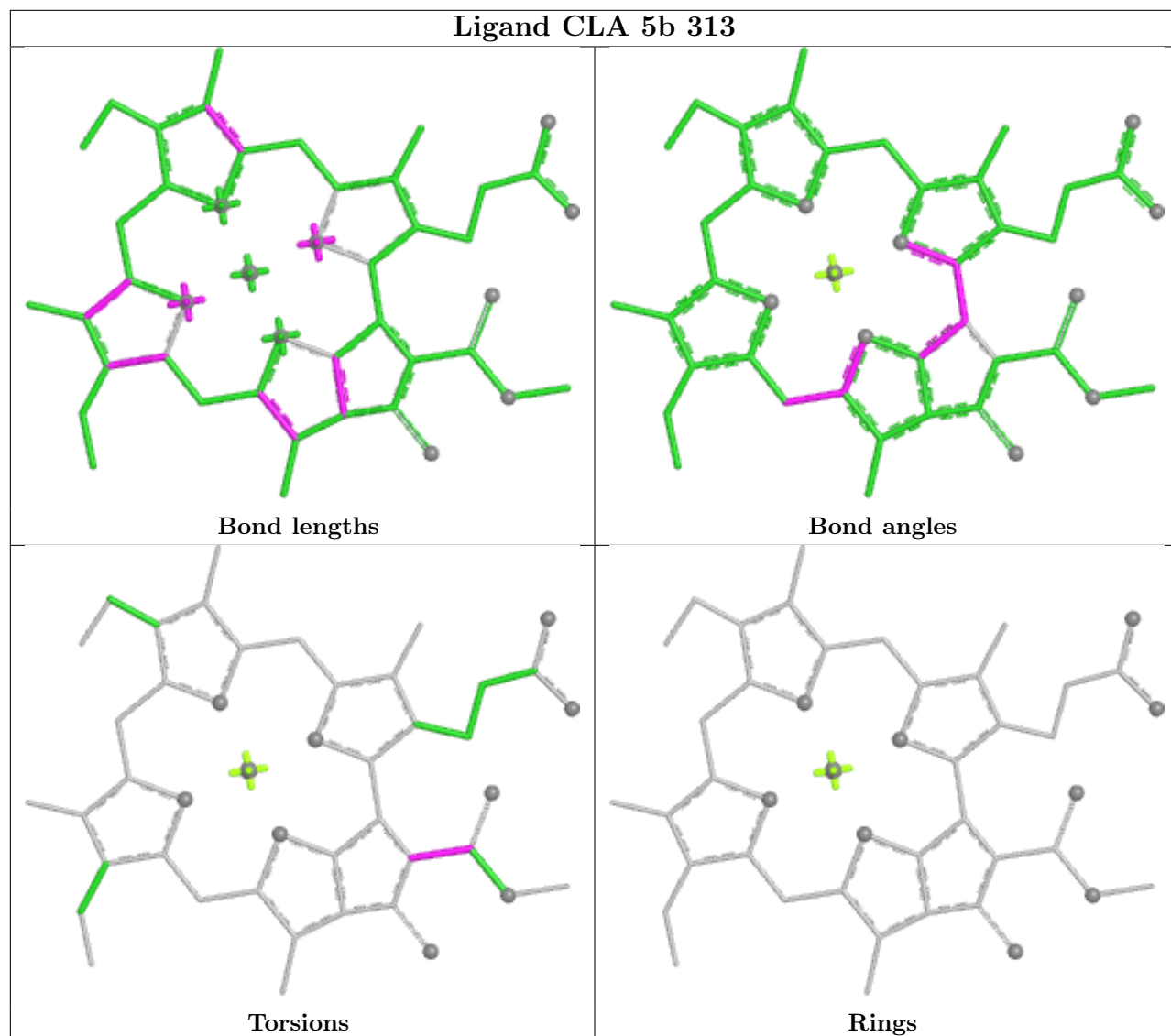
Rings

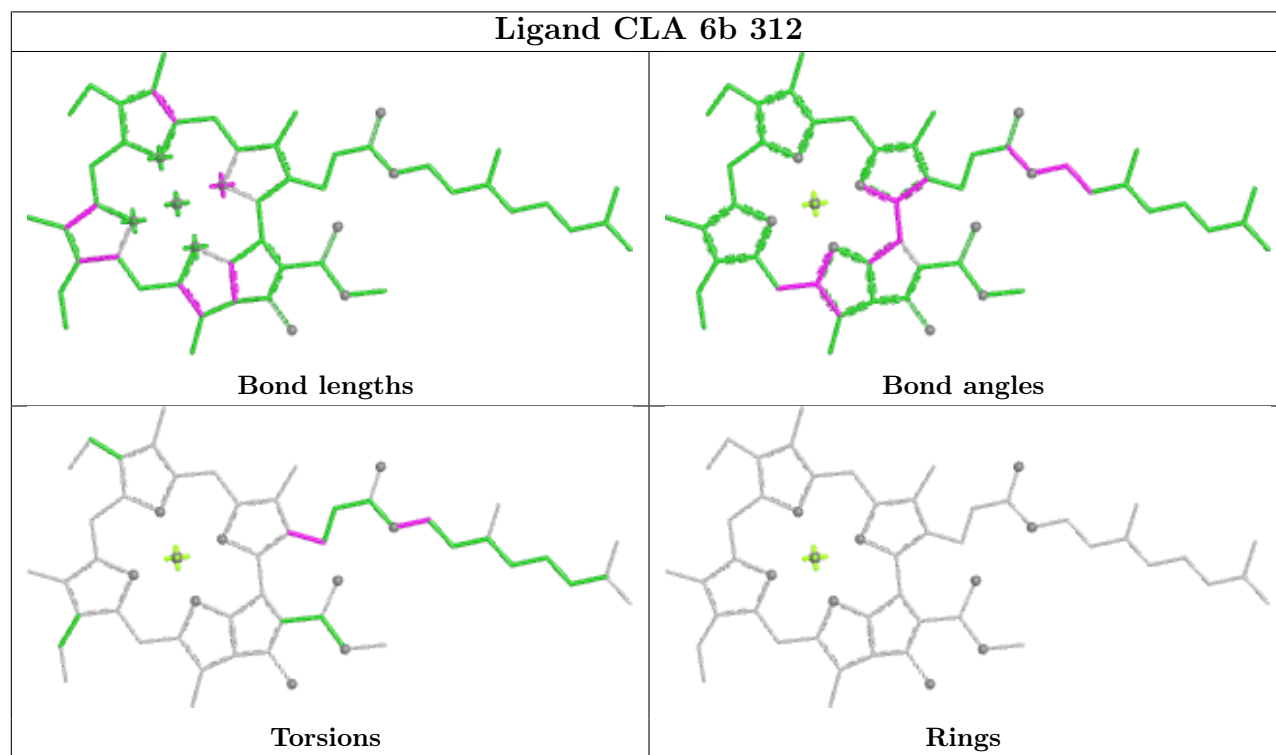
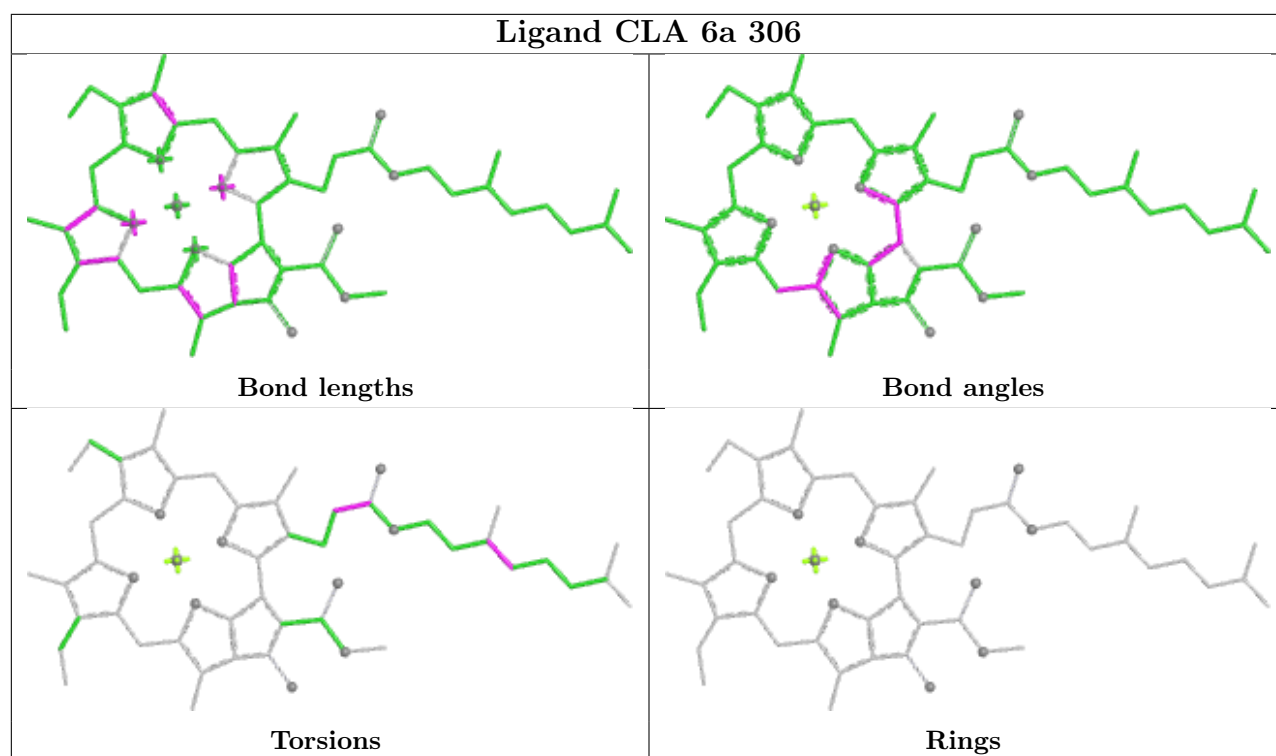
## Ligand CLA A 815

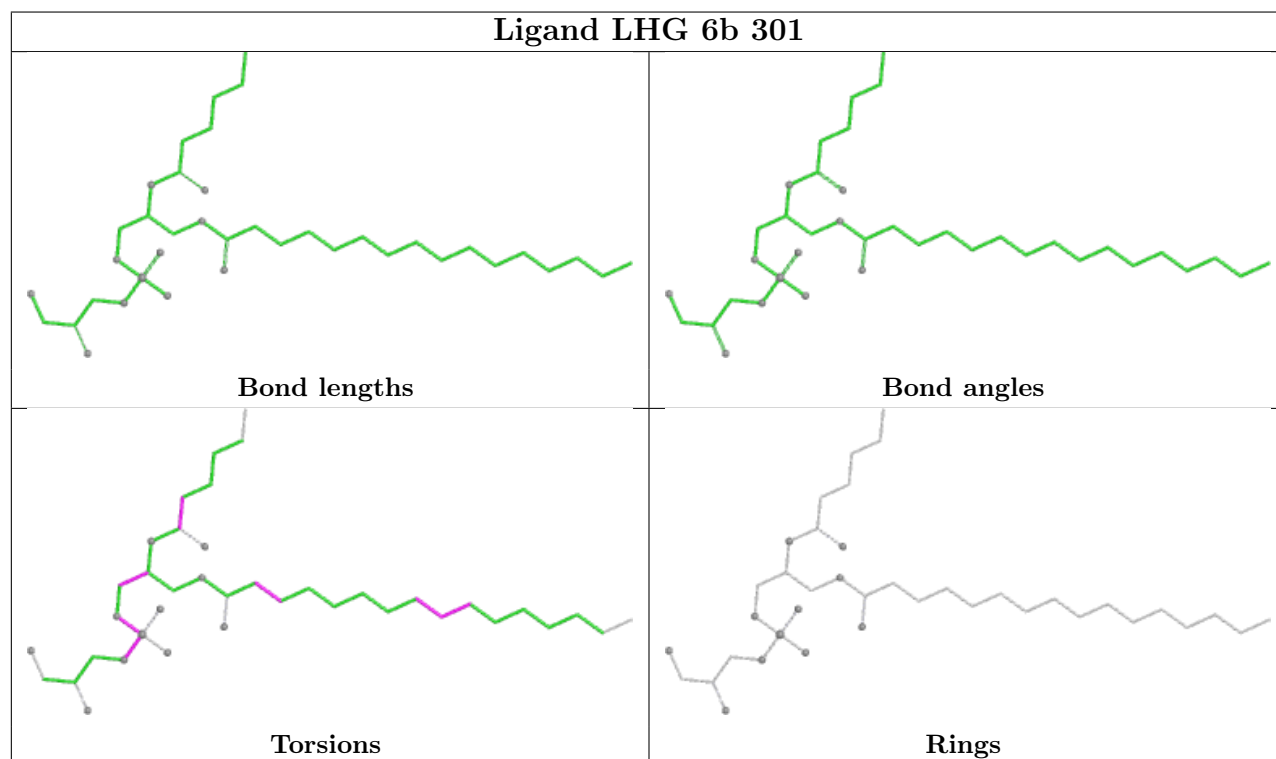
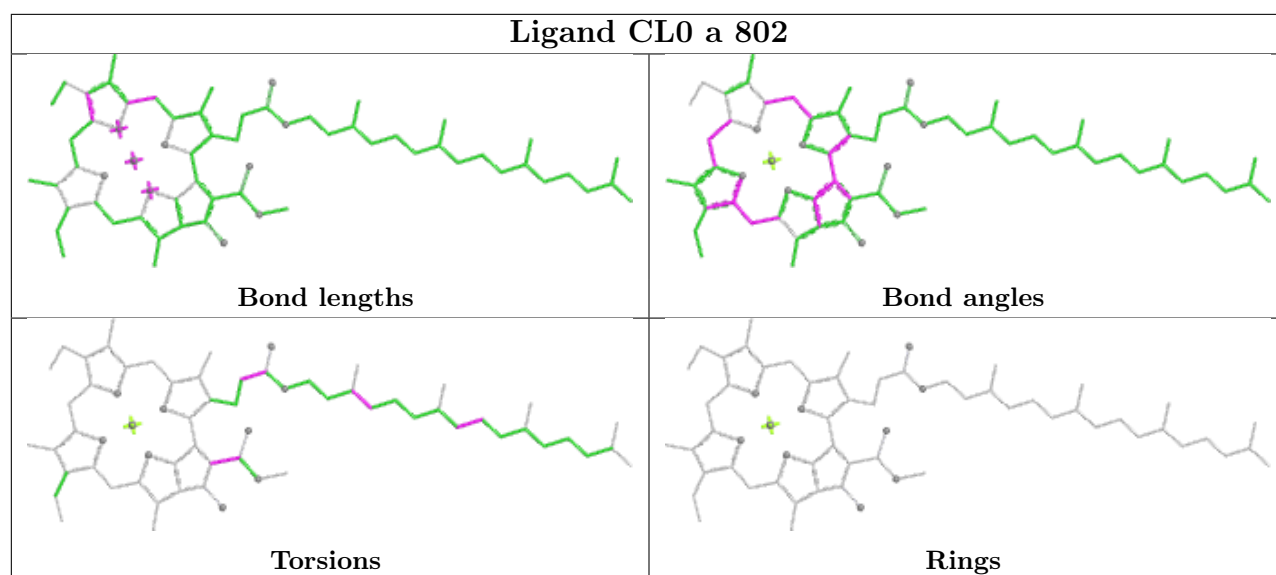


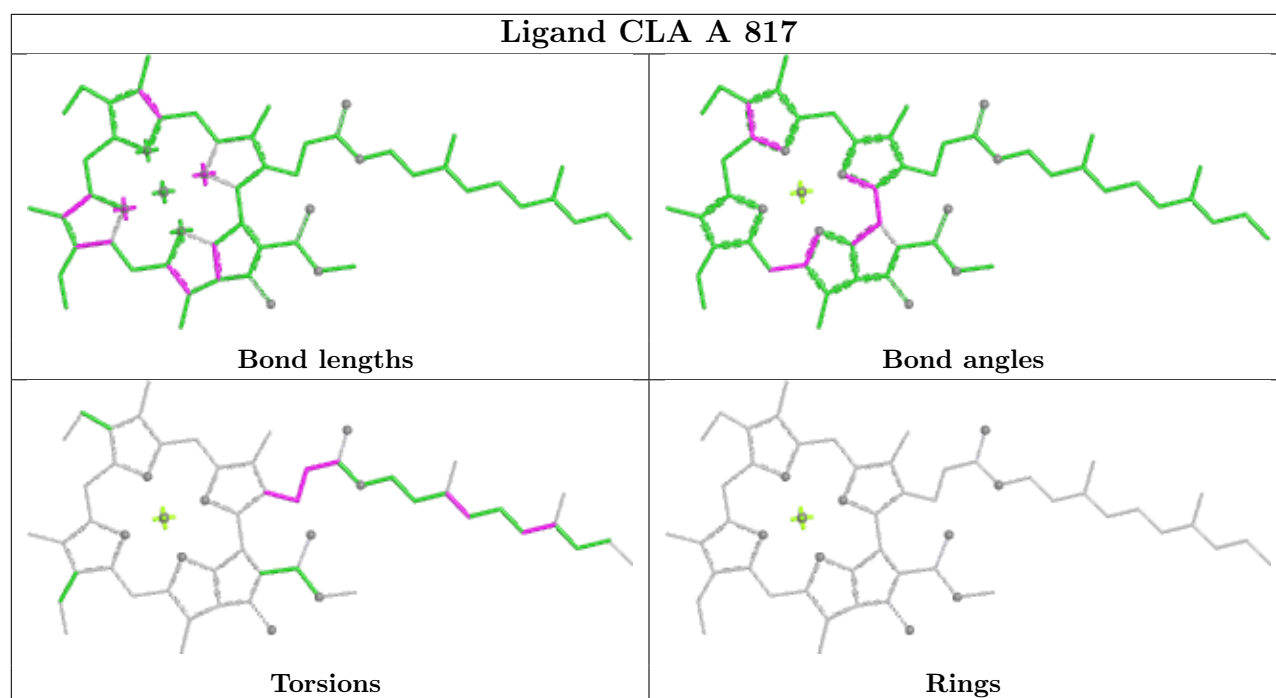
## Ligand CLA a 835



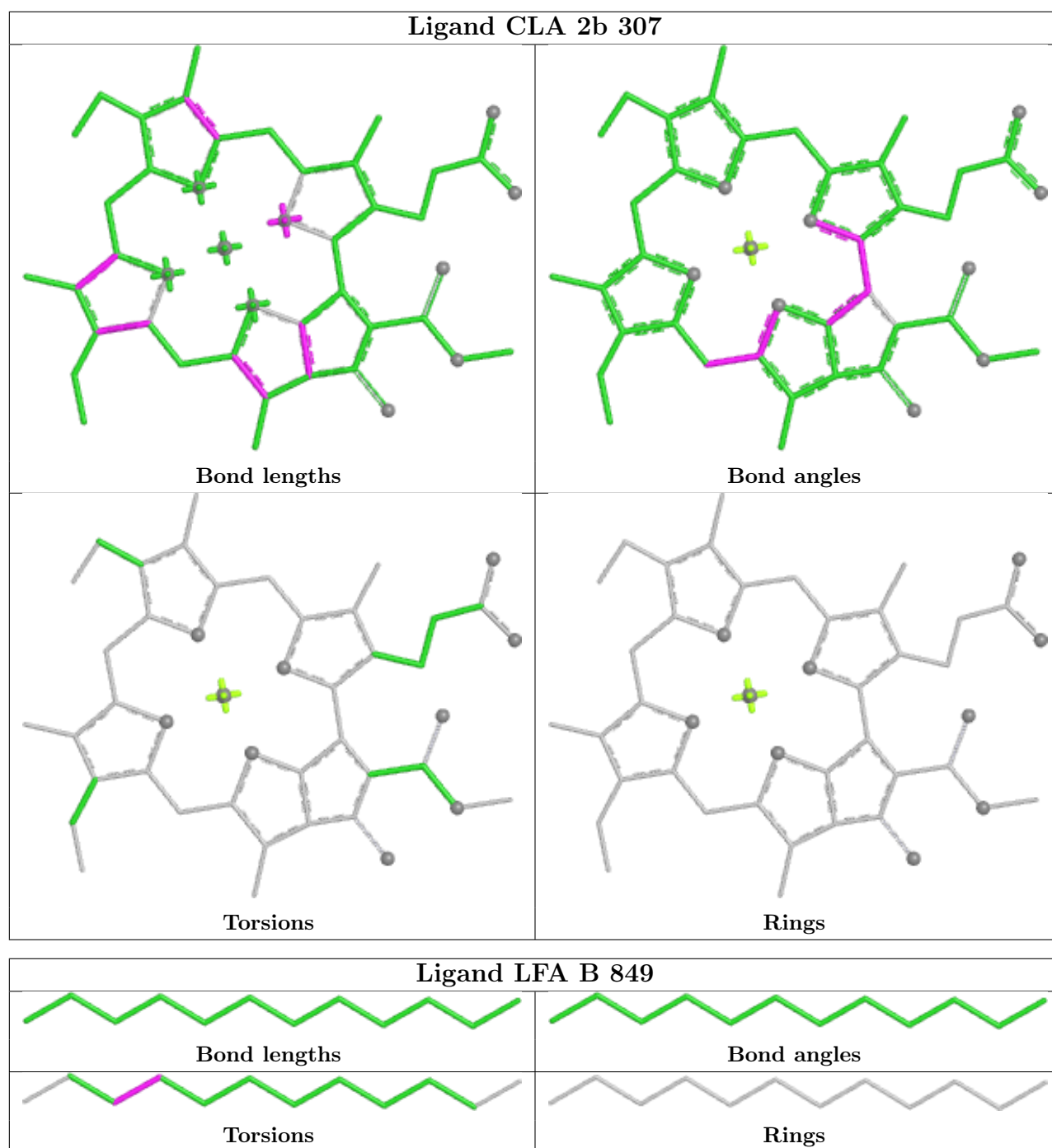


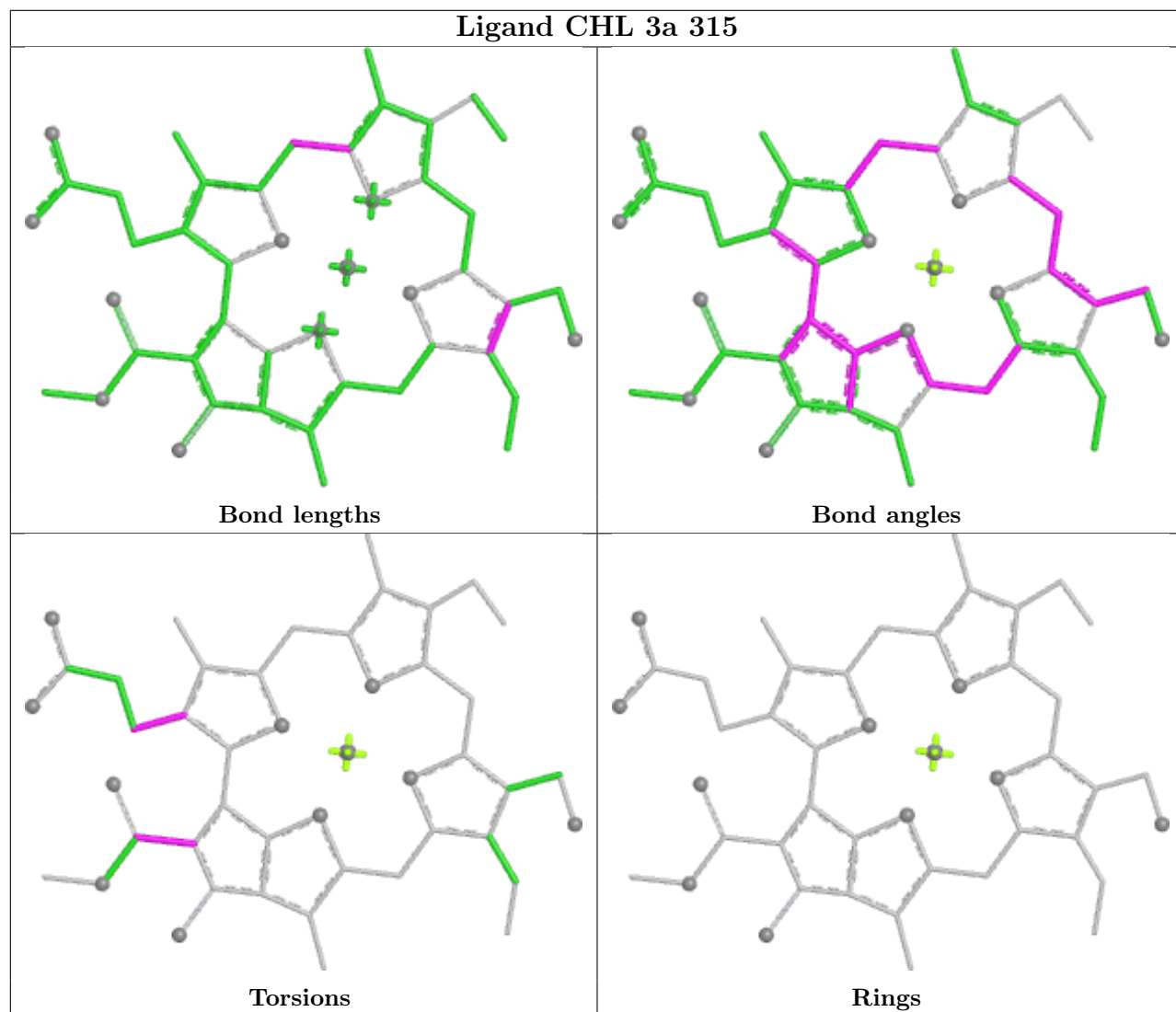


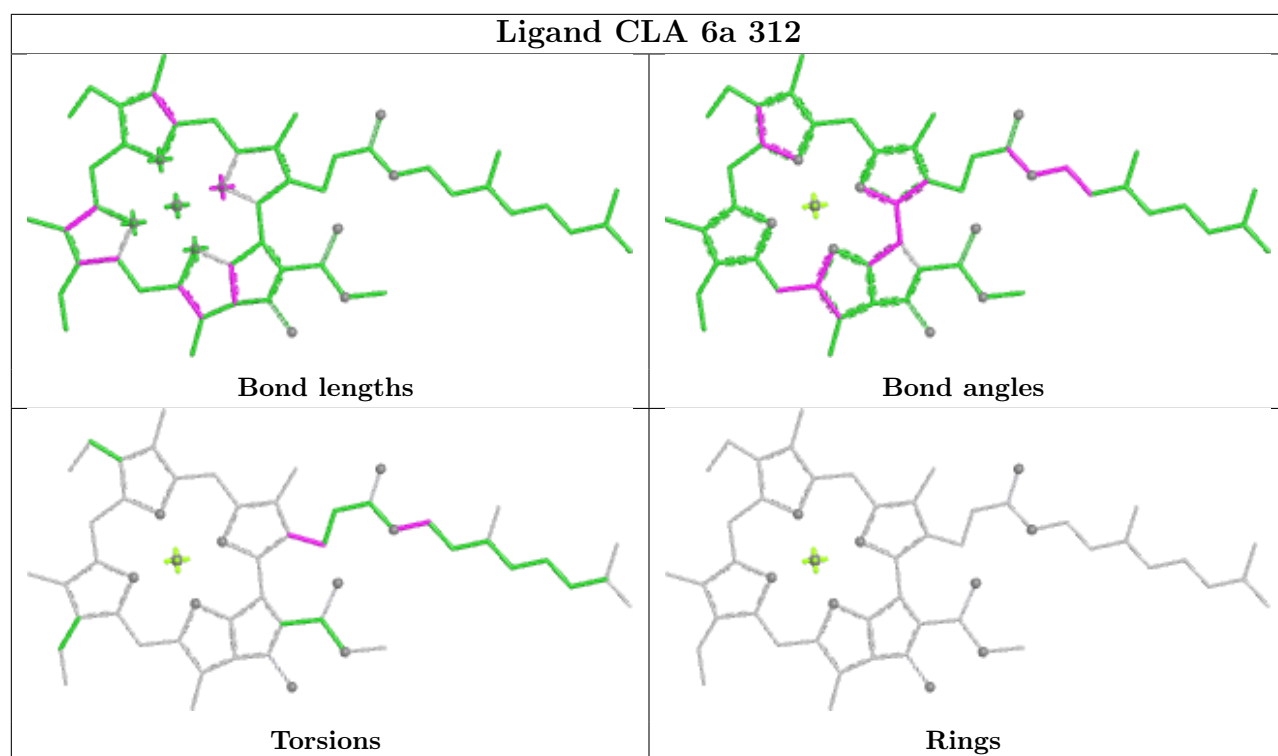


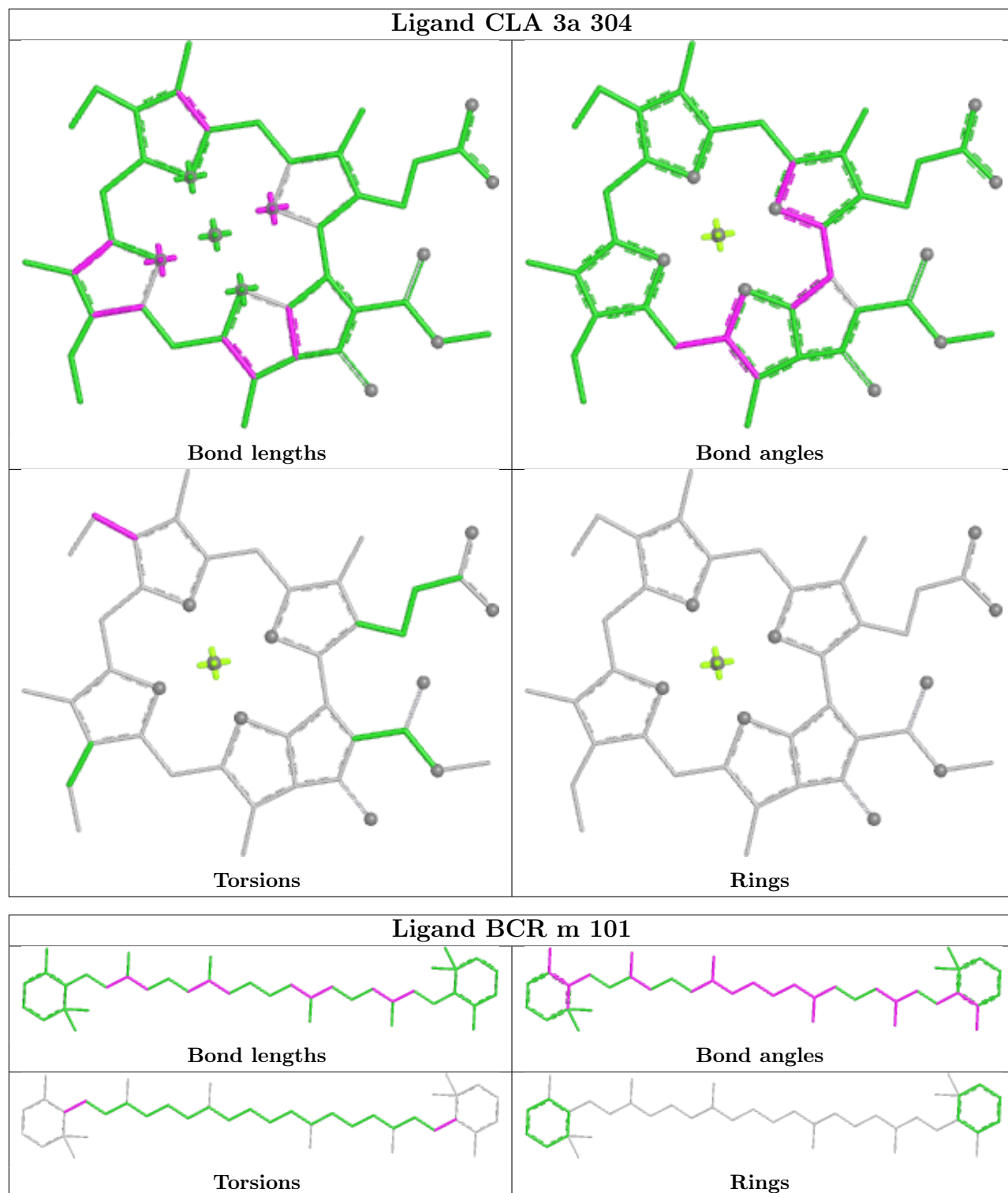


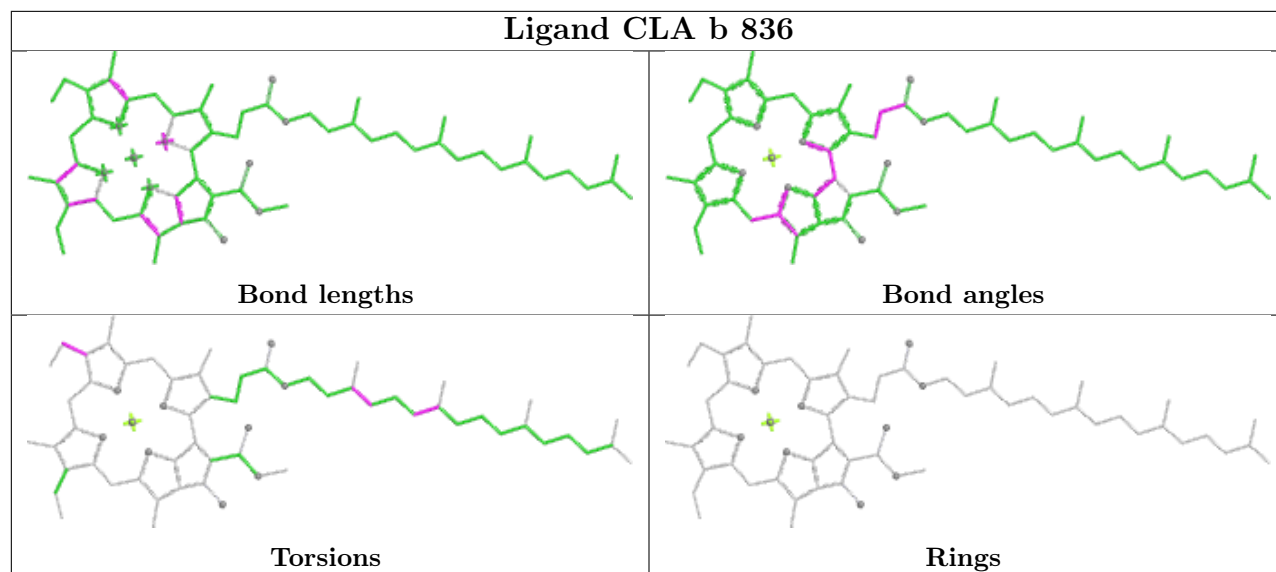
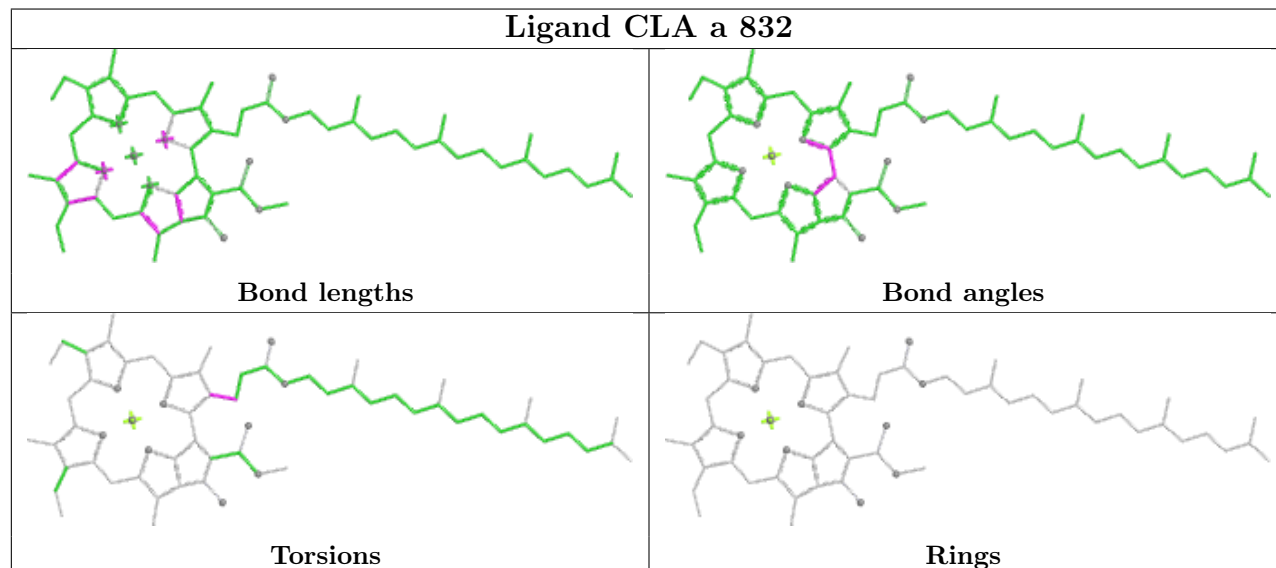


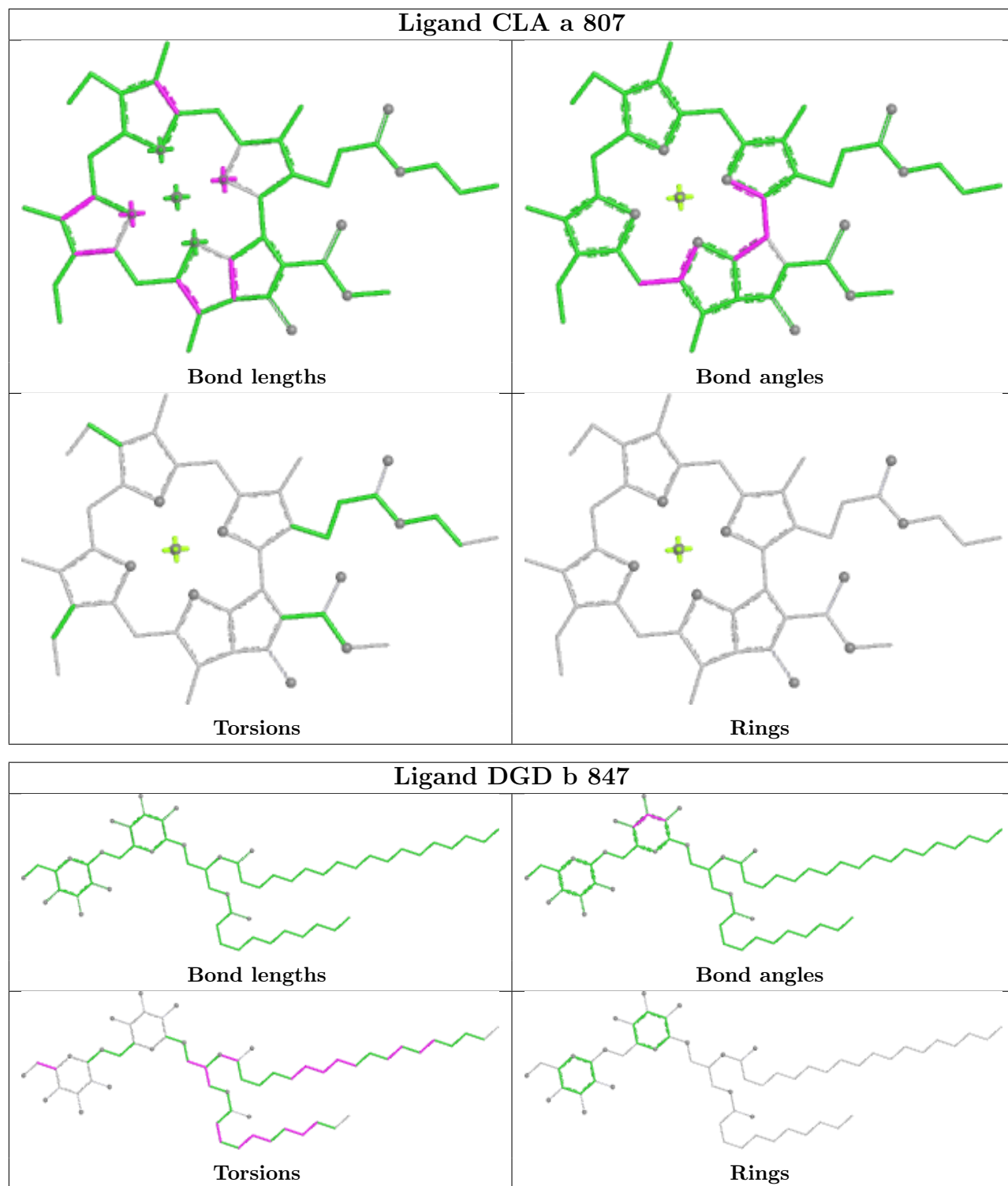




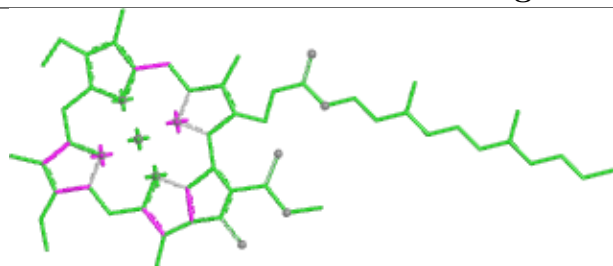




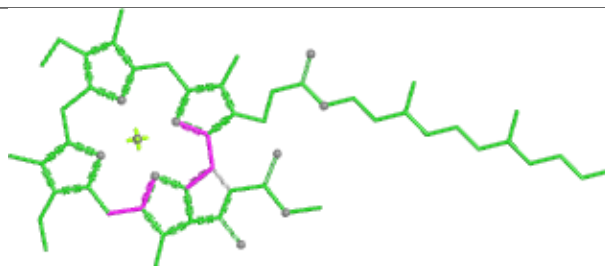
**Ligand CLA b 836****Ligand CLA a 832**



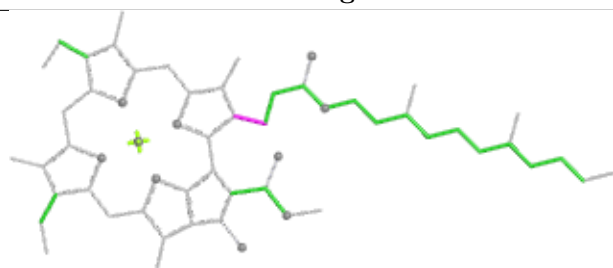
## Ligand CLA B 826



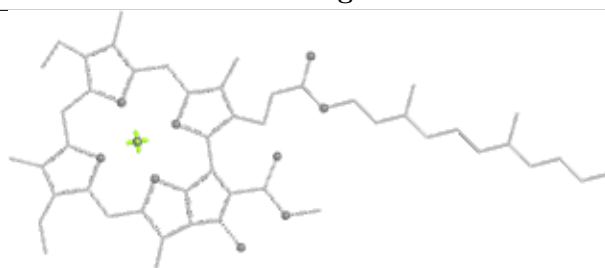
Bond lengths



Bond angles

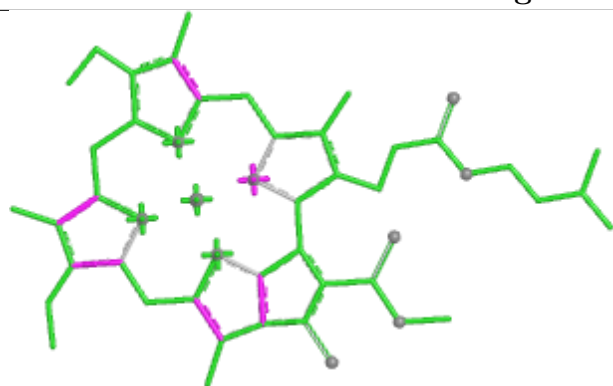


Torsions

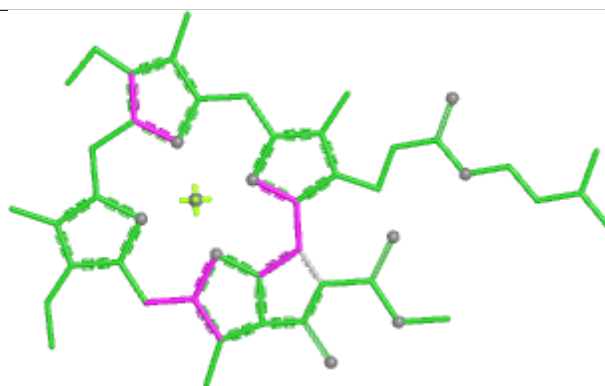


Rings

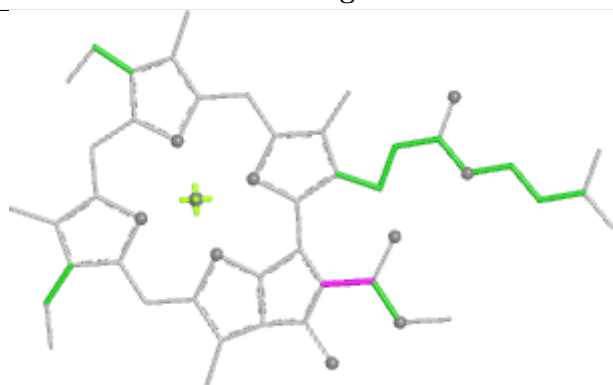
## Ligand CLA B 824



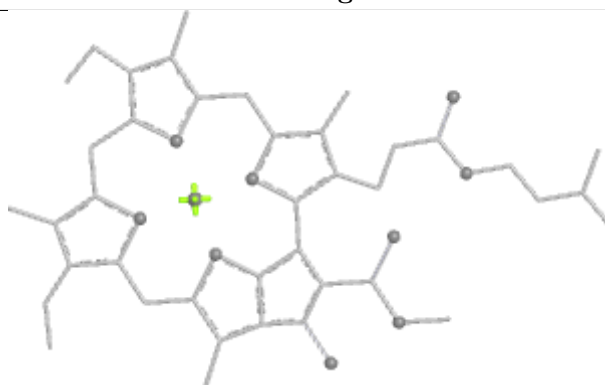
Bond lengths



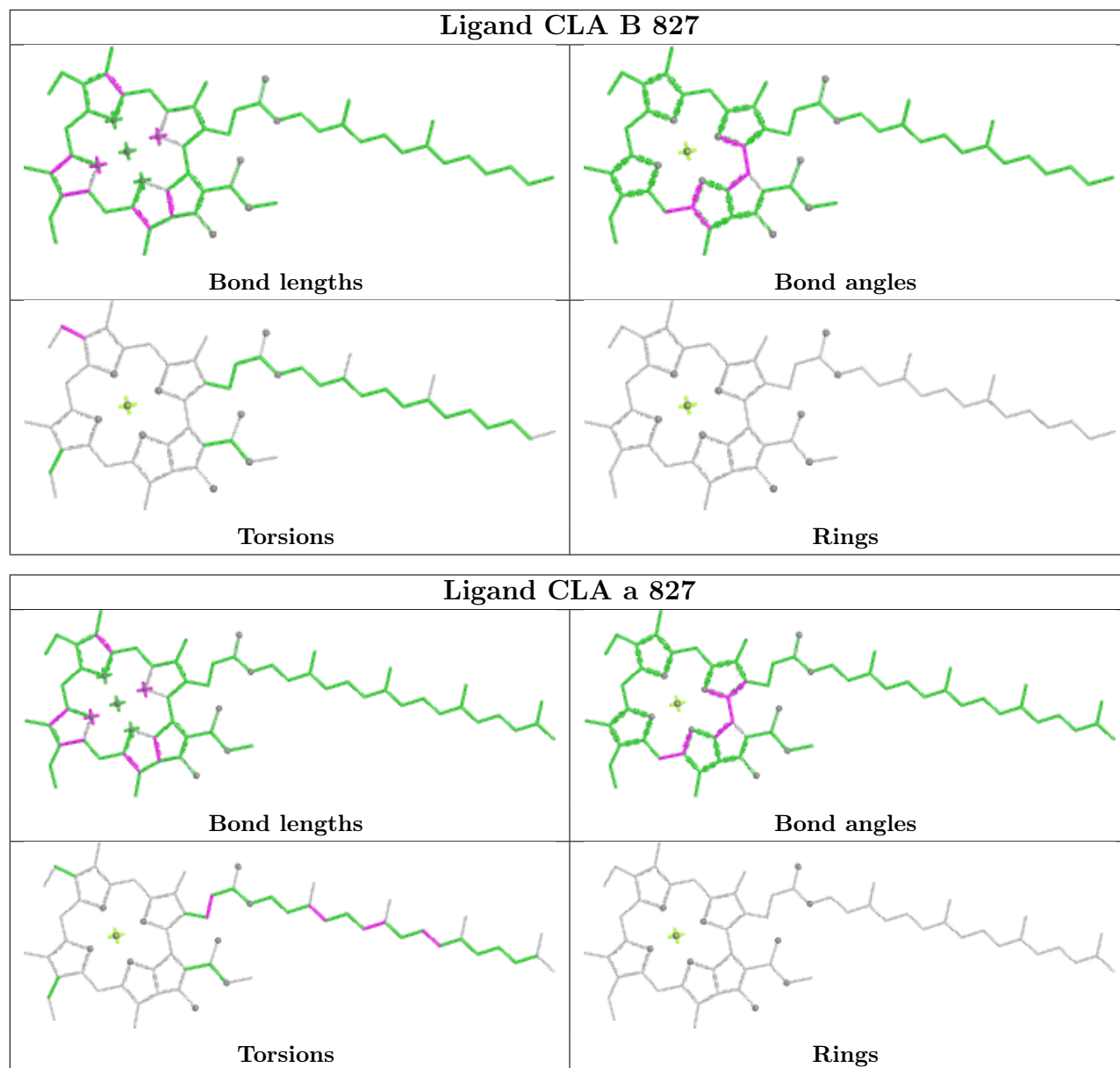
Bond angles



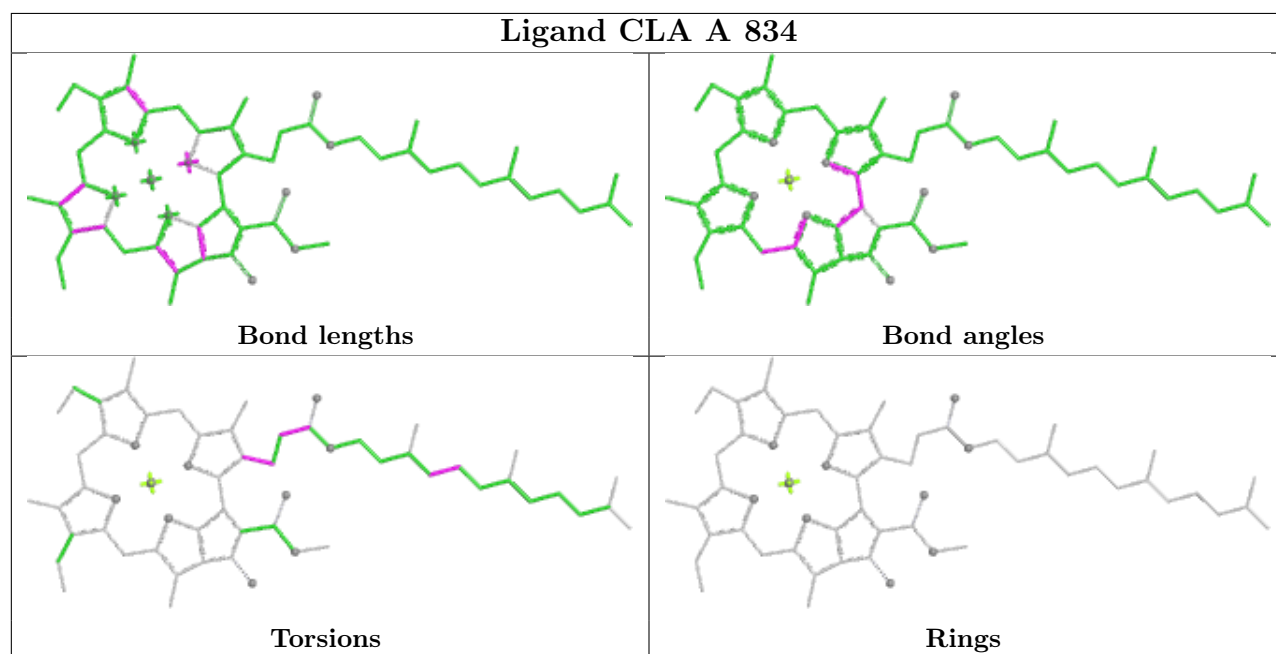
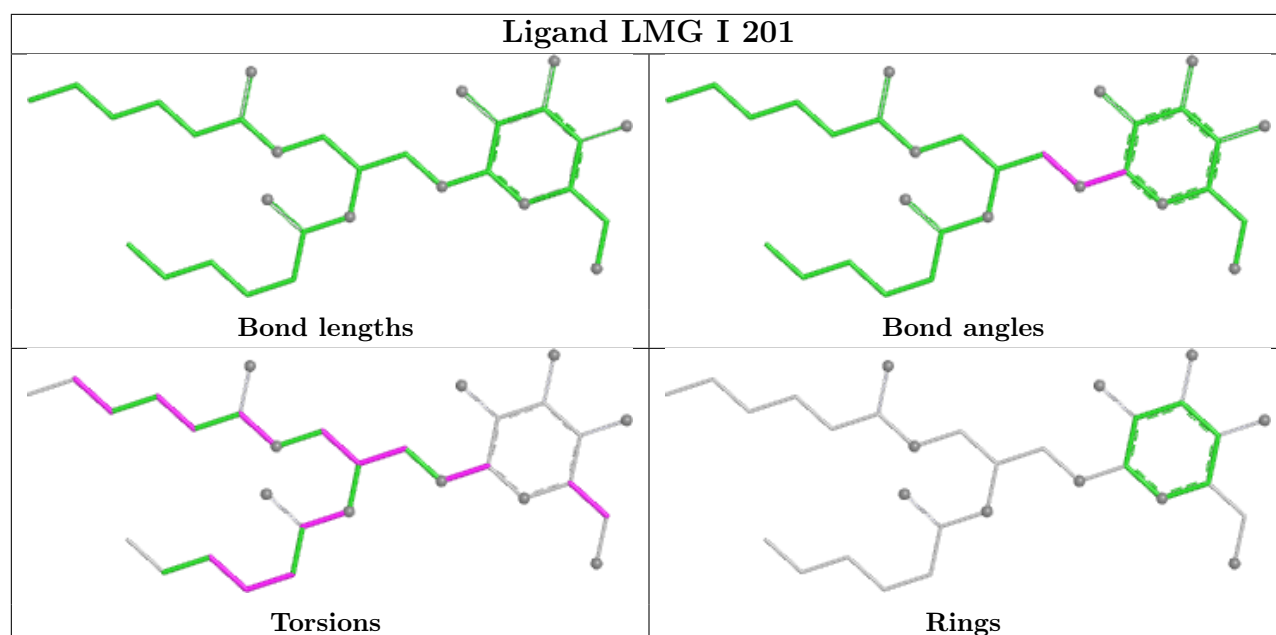
Torsions



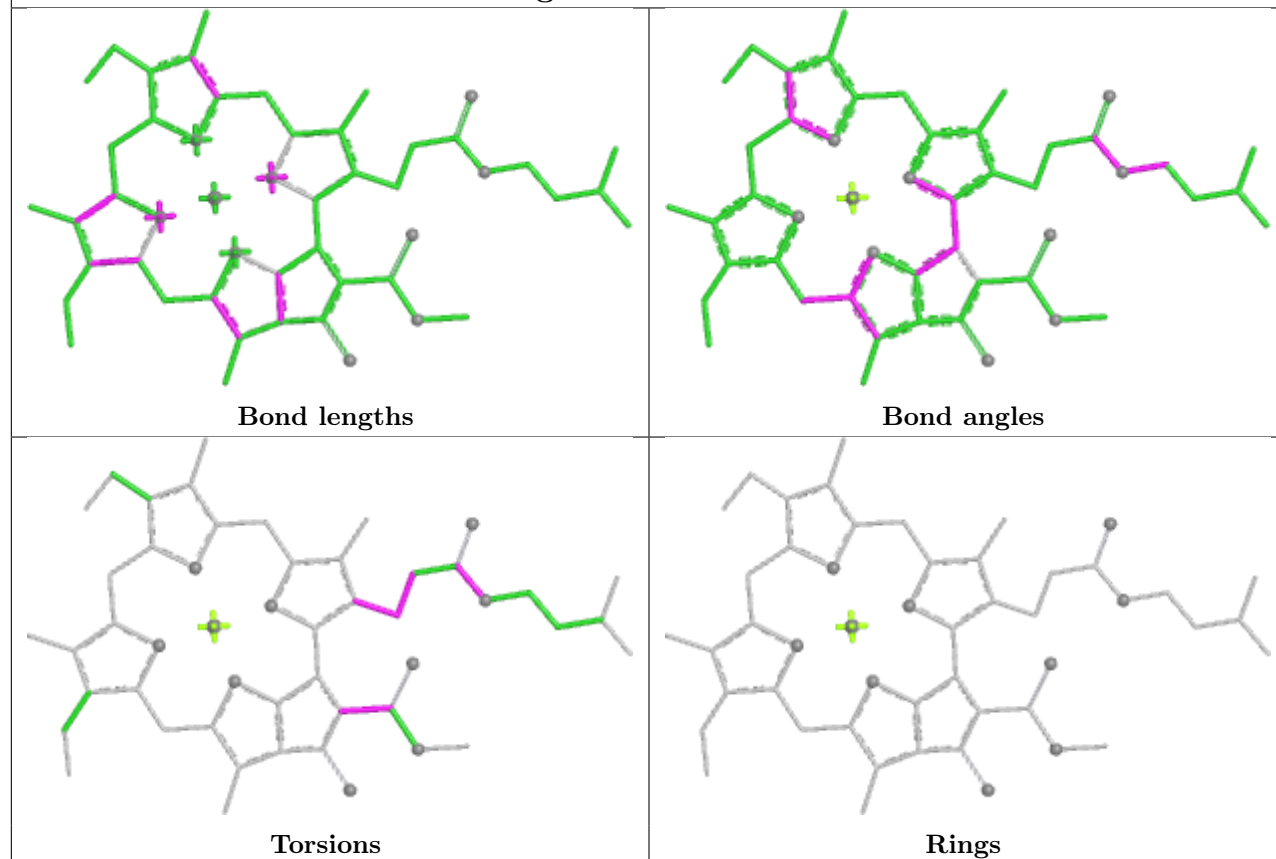
Rings



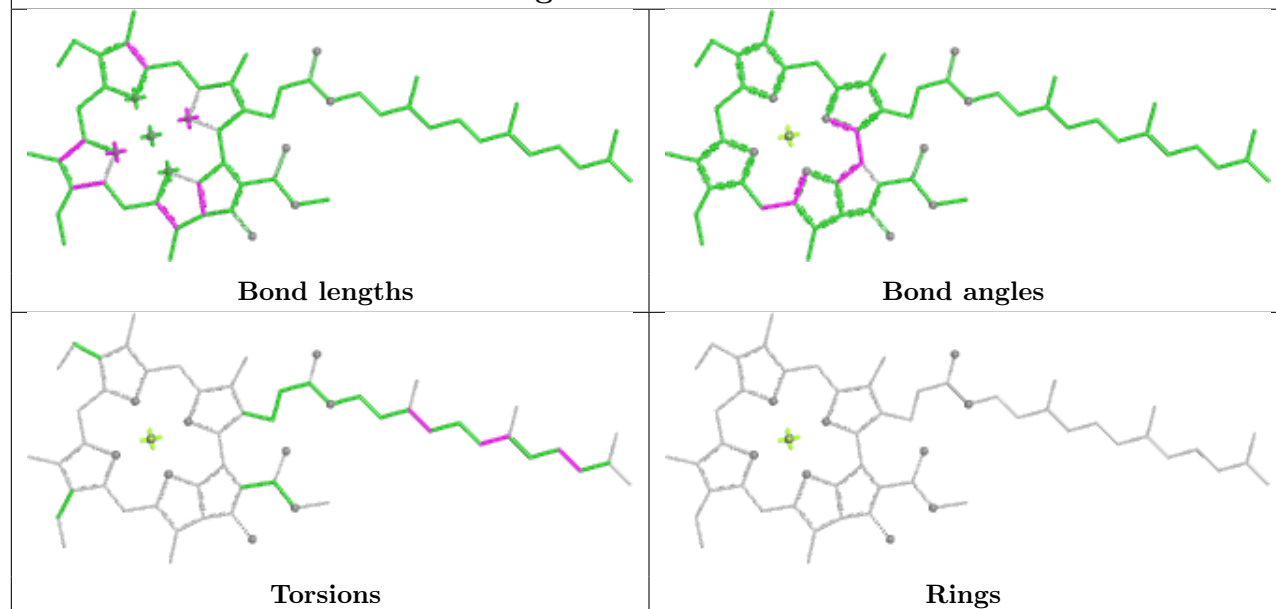


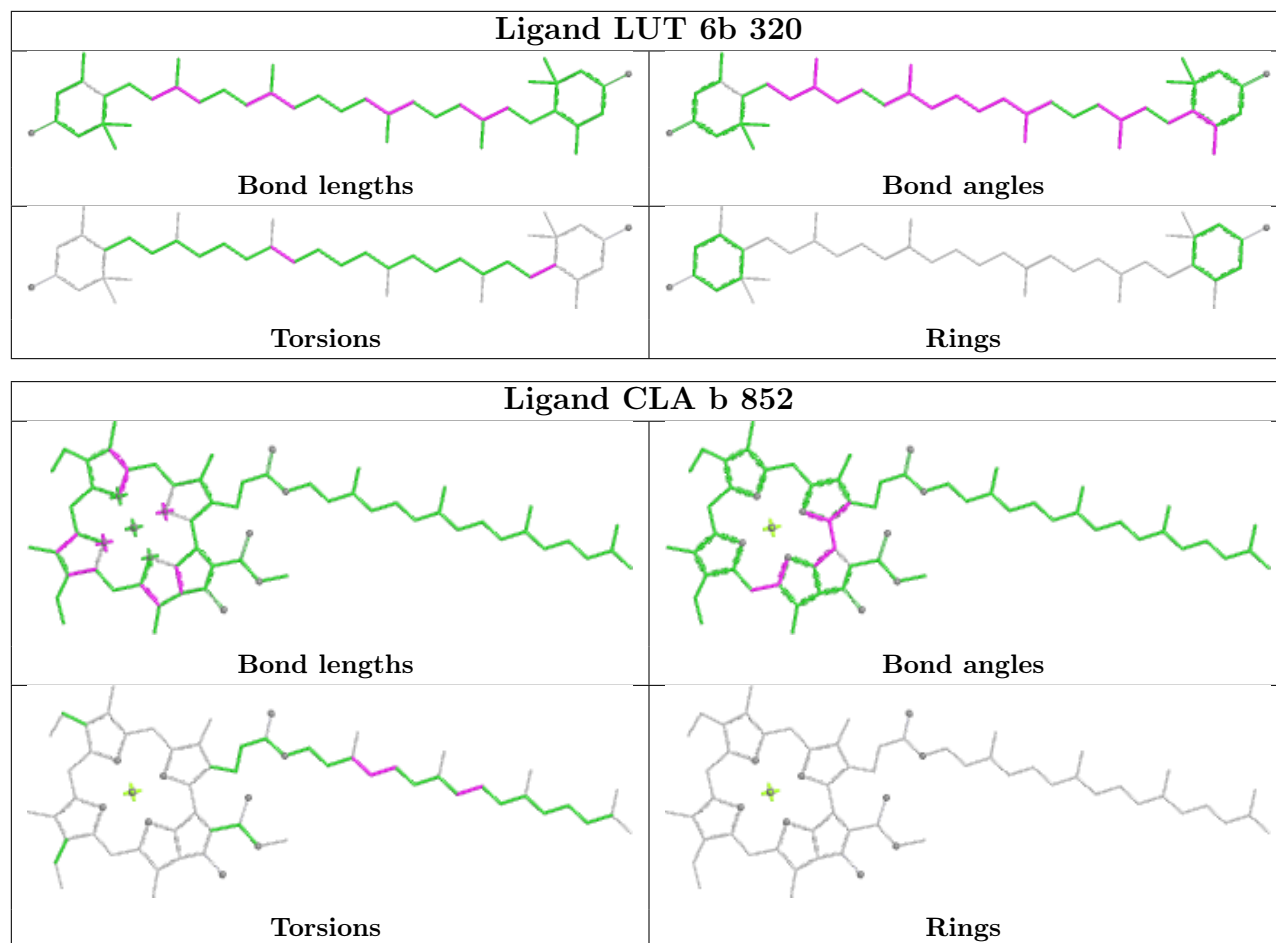


## Ligand CLA a 830

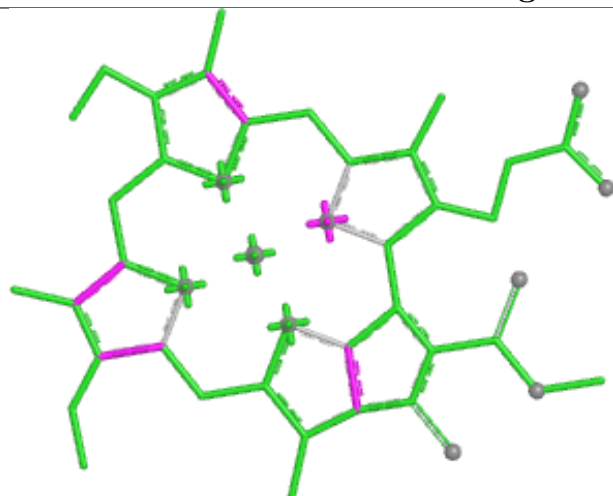


## Ligand CLA b 810

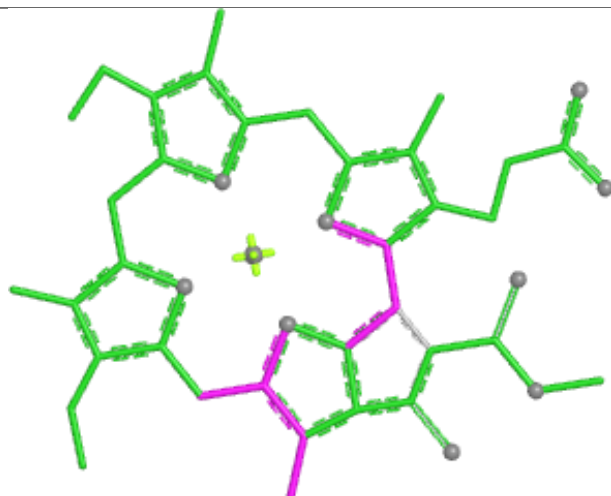




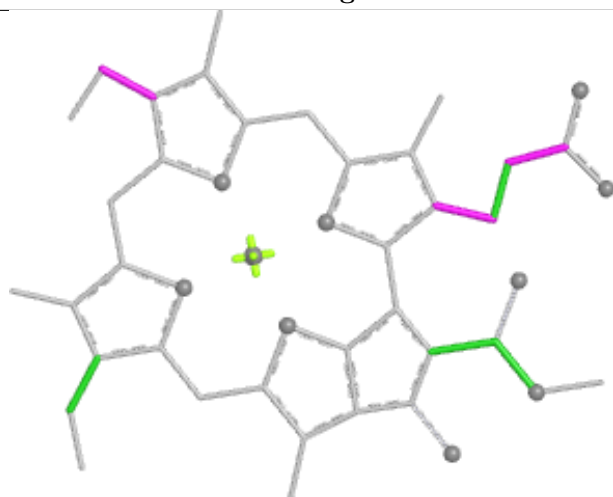
## Ligand CLA a 815



Bond lengths



Bond angles

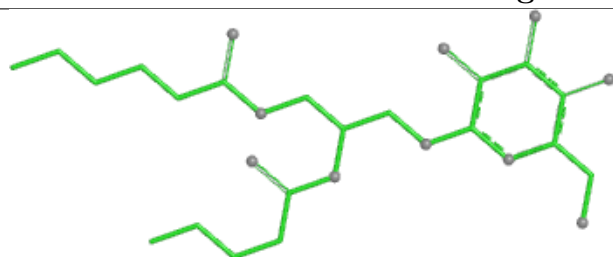


Torsions

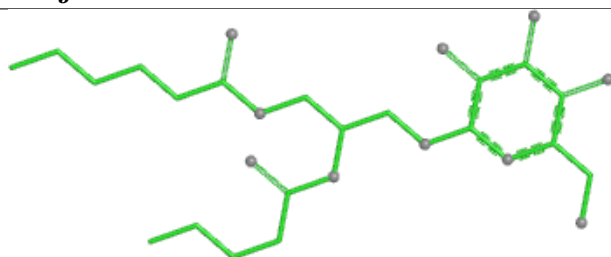


Rings

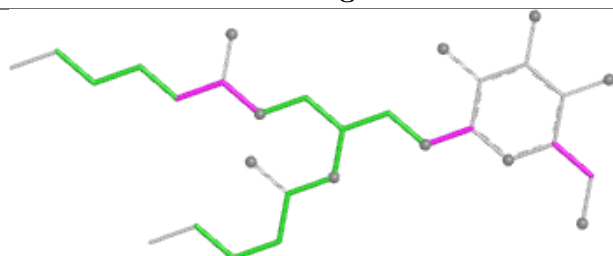
## Ligand LMG j 103



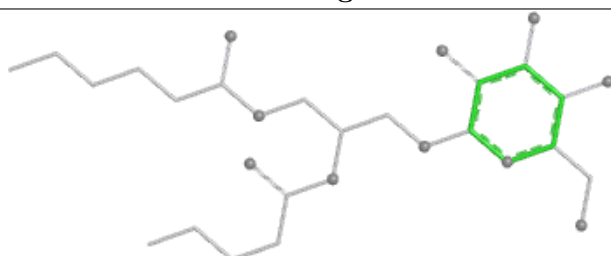
Bond lengths



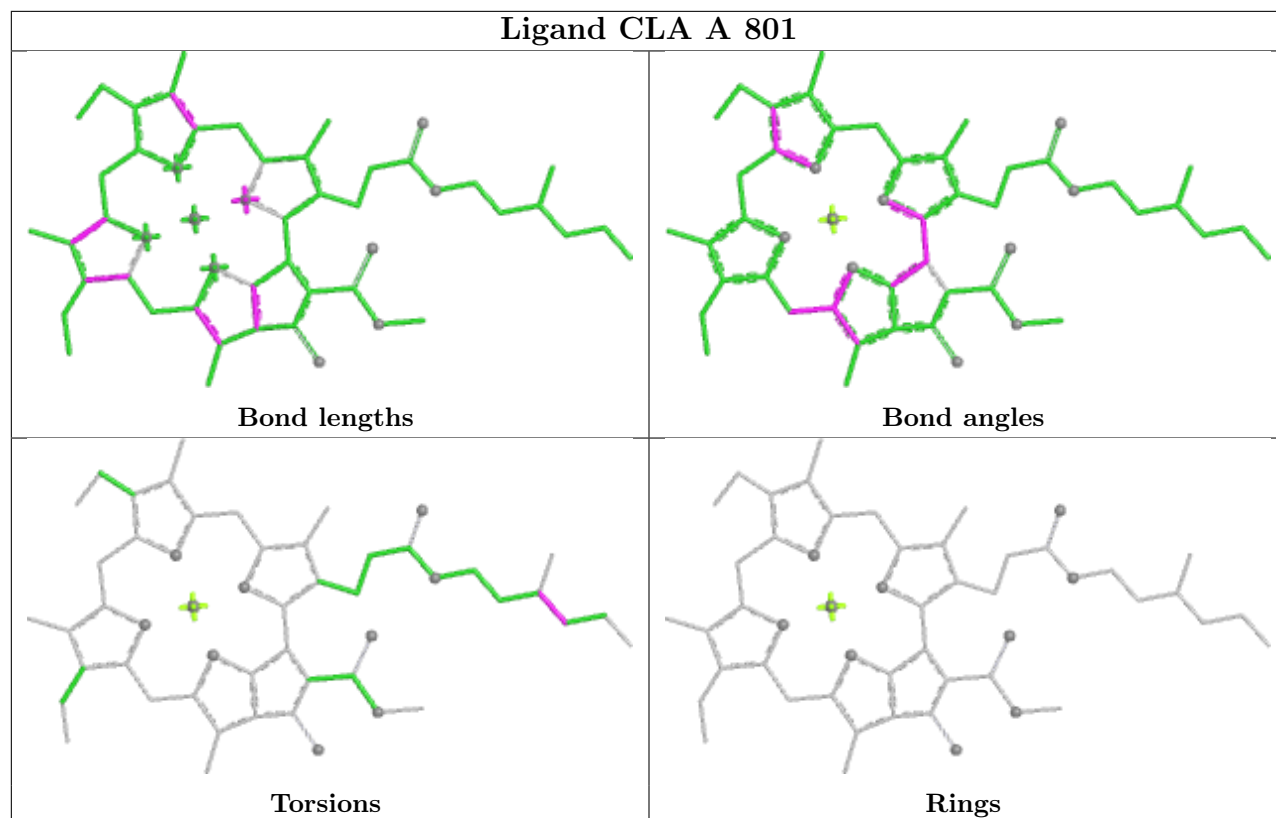
Bond angles



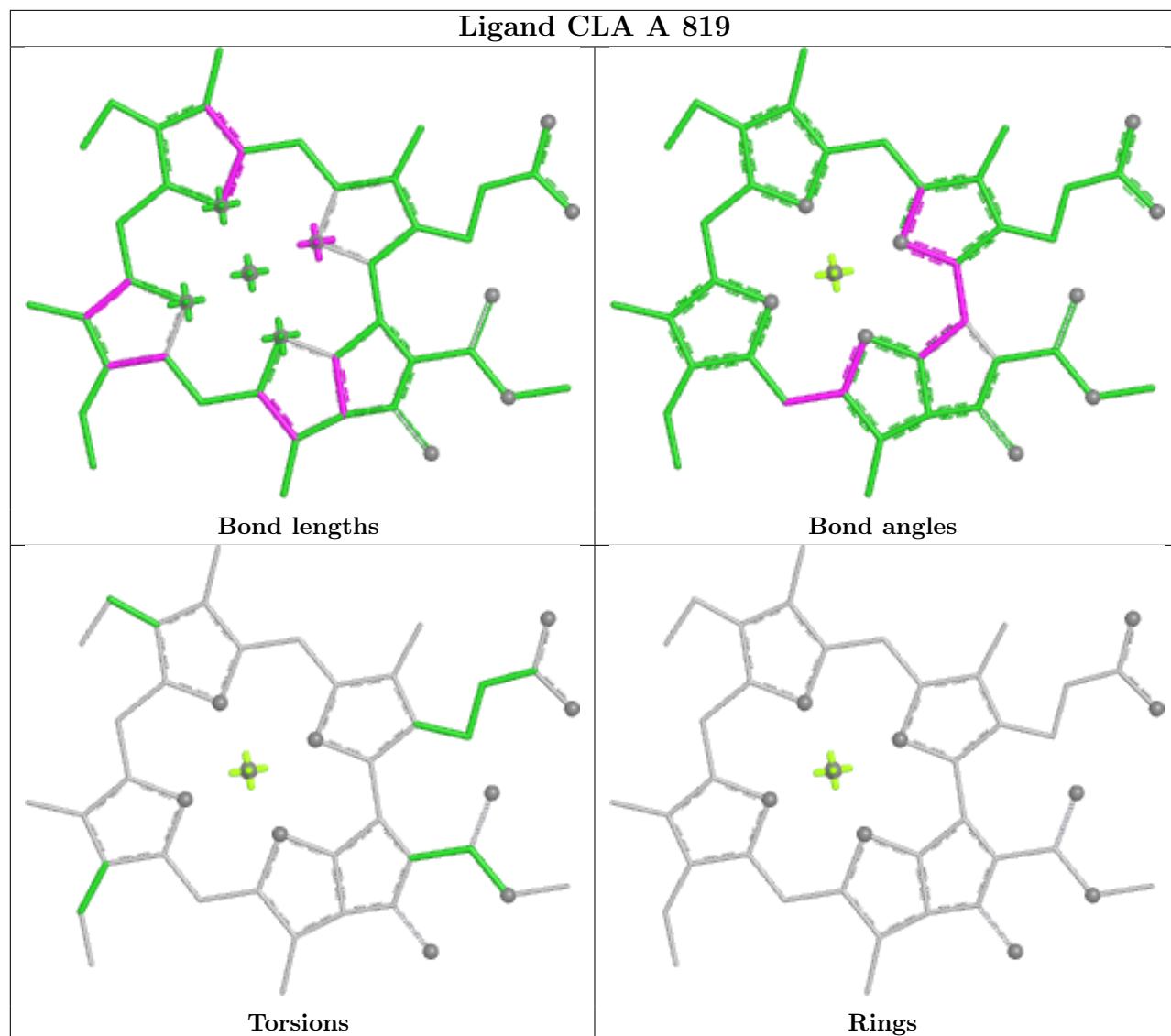
Torsions

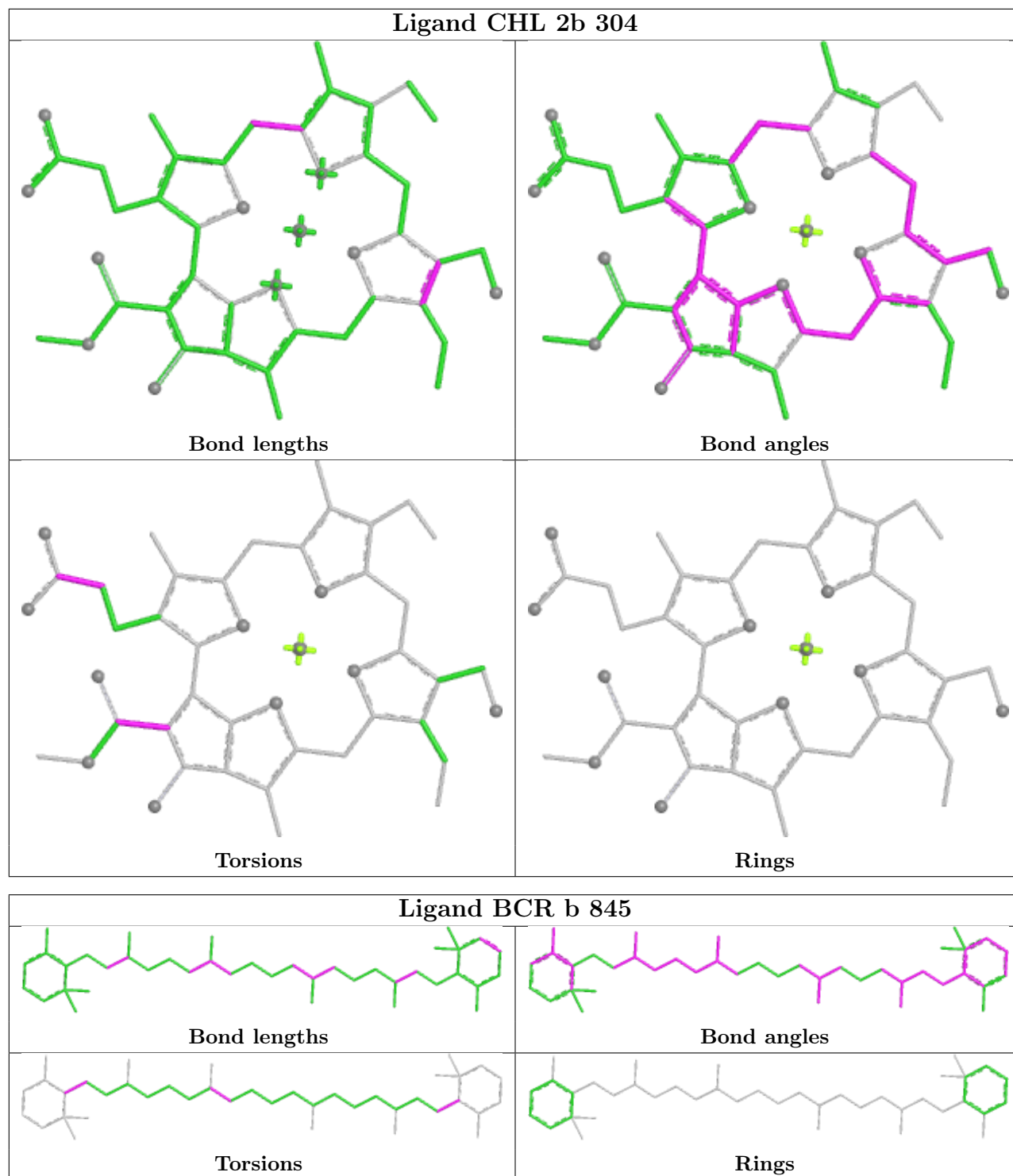


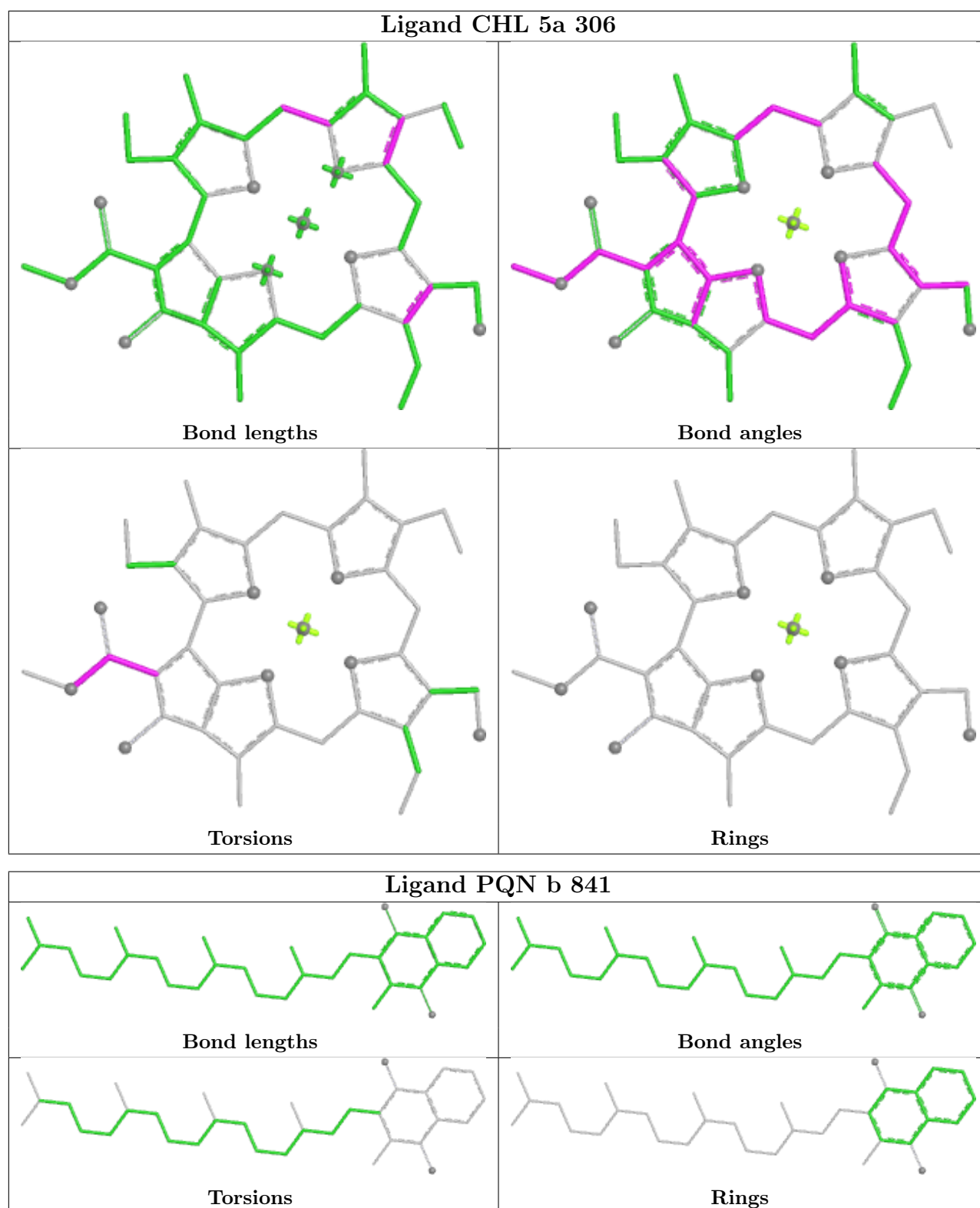
Rings



## Ligand CLA A 819

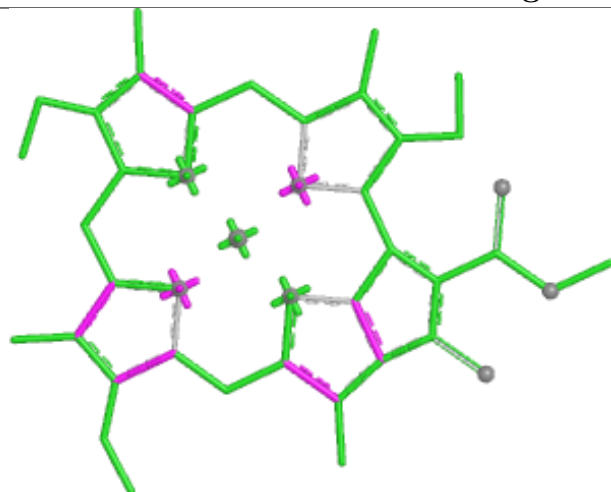




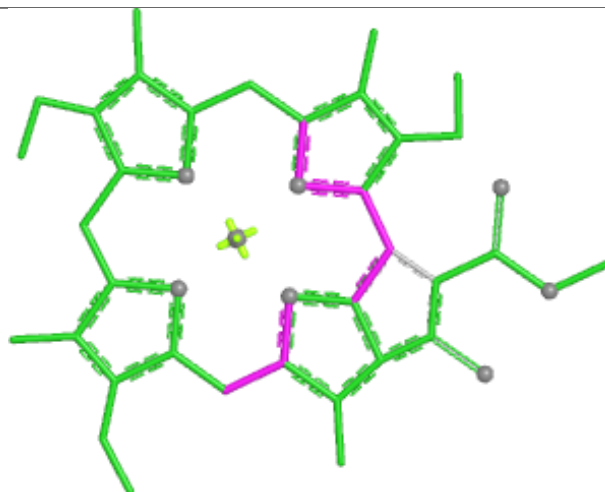




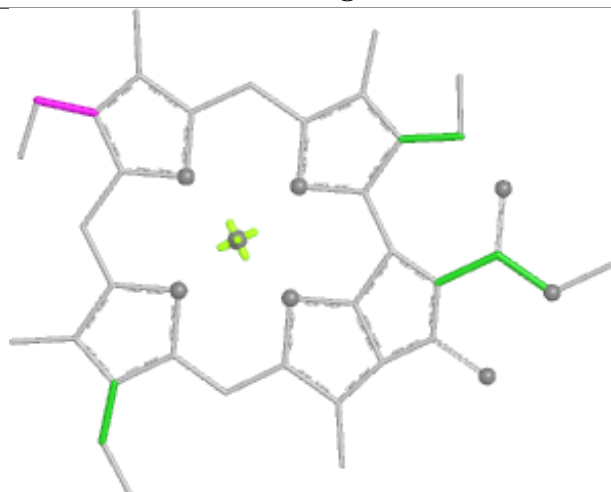
## Ligand CLA 1 303



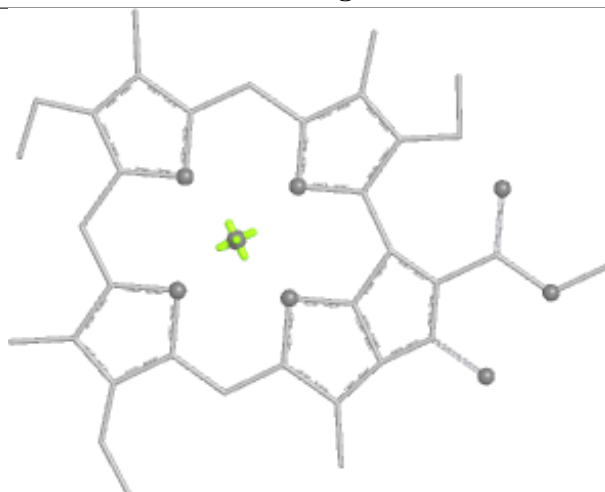
Bond lengths



Bond angles

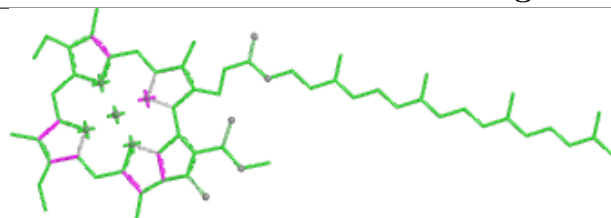


Torsions

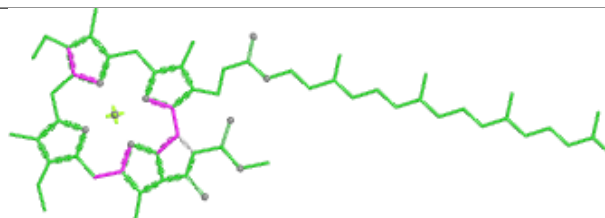


Rings

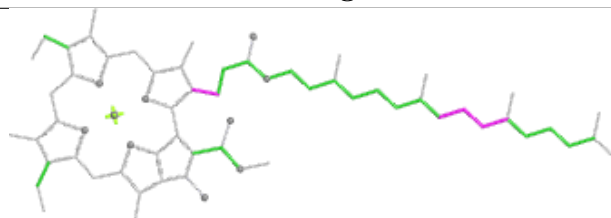
## Ligand CLA B 804



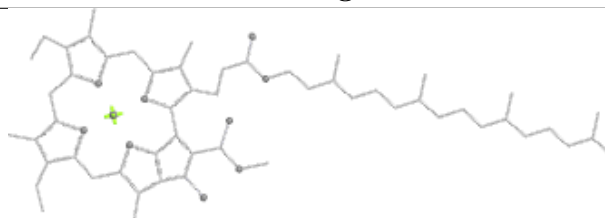
Bond lengths



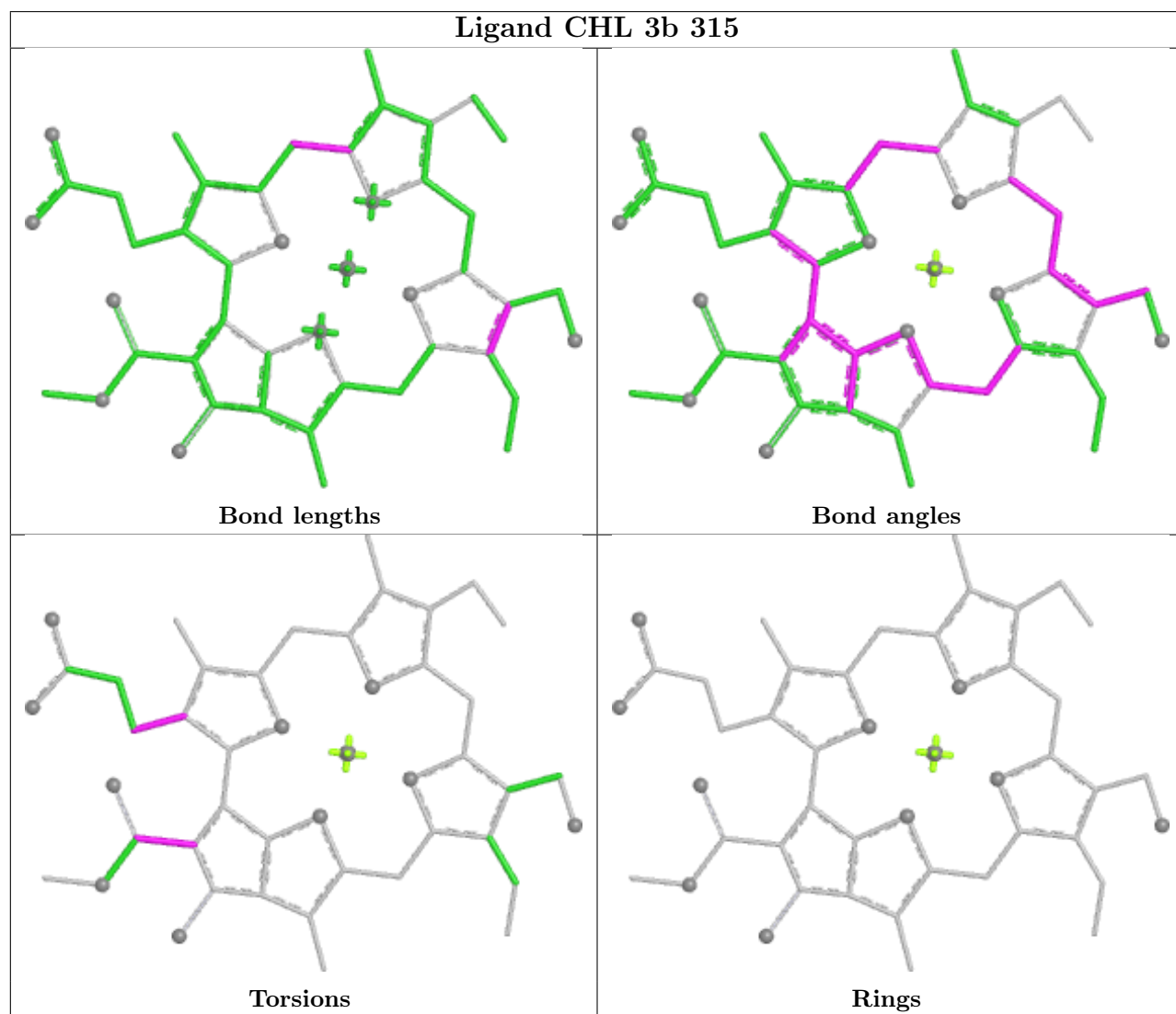
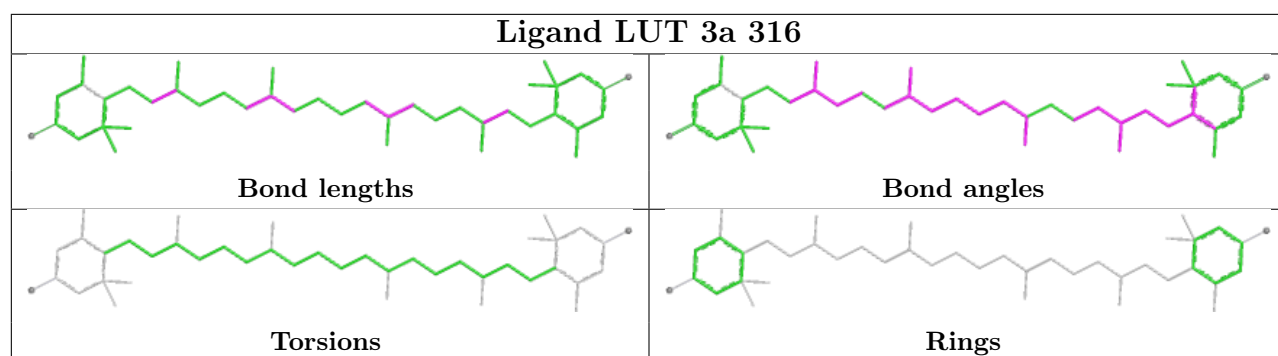
Bond angles



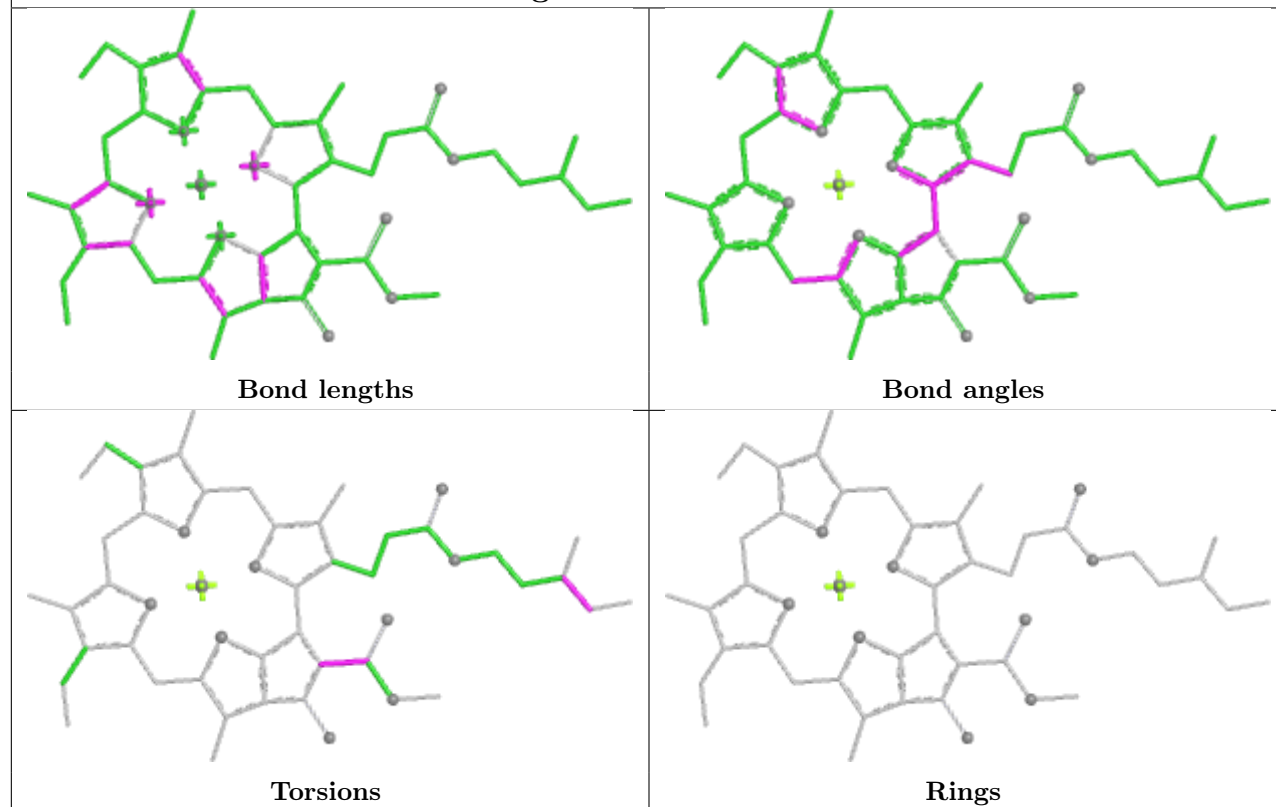
Torsions



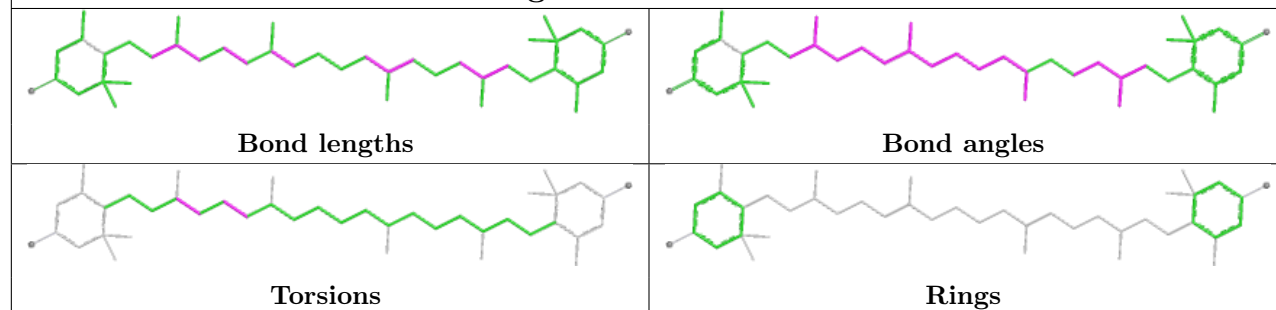
Rings

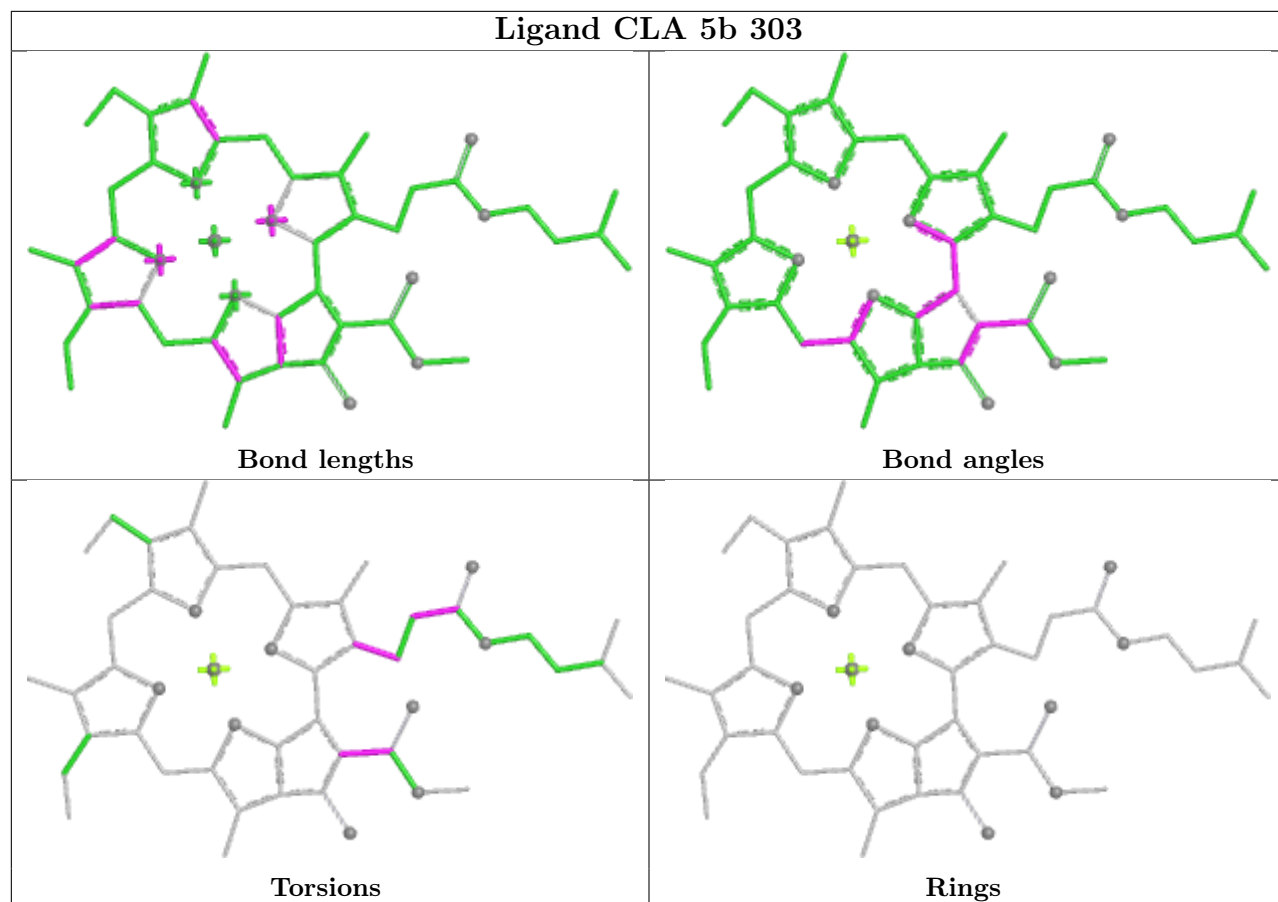


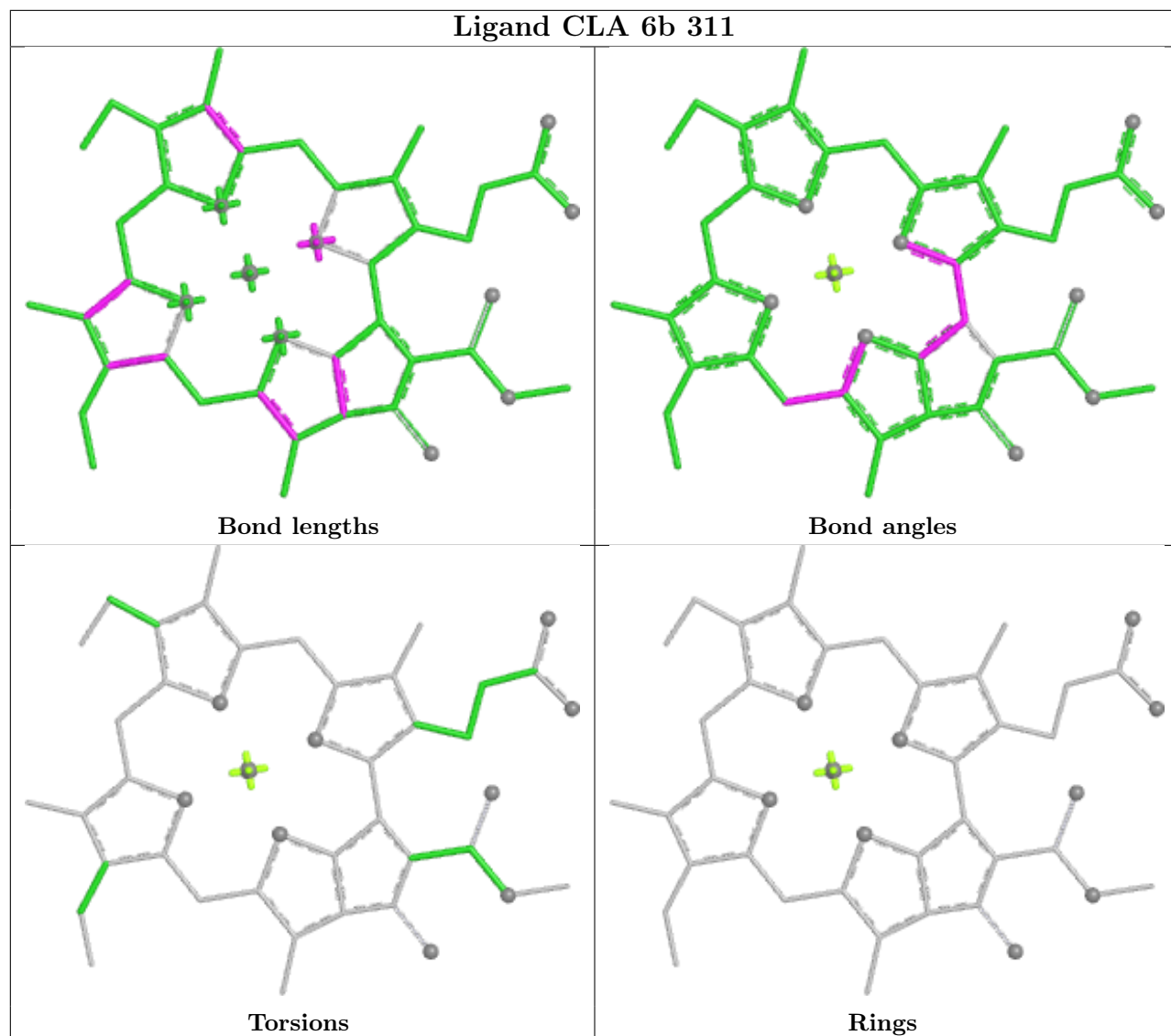
## Ligand CLA A 836

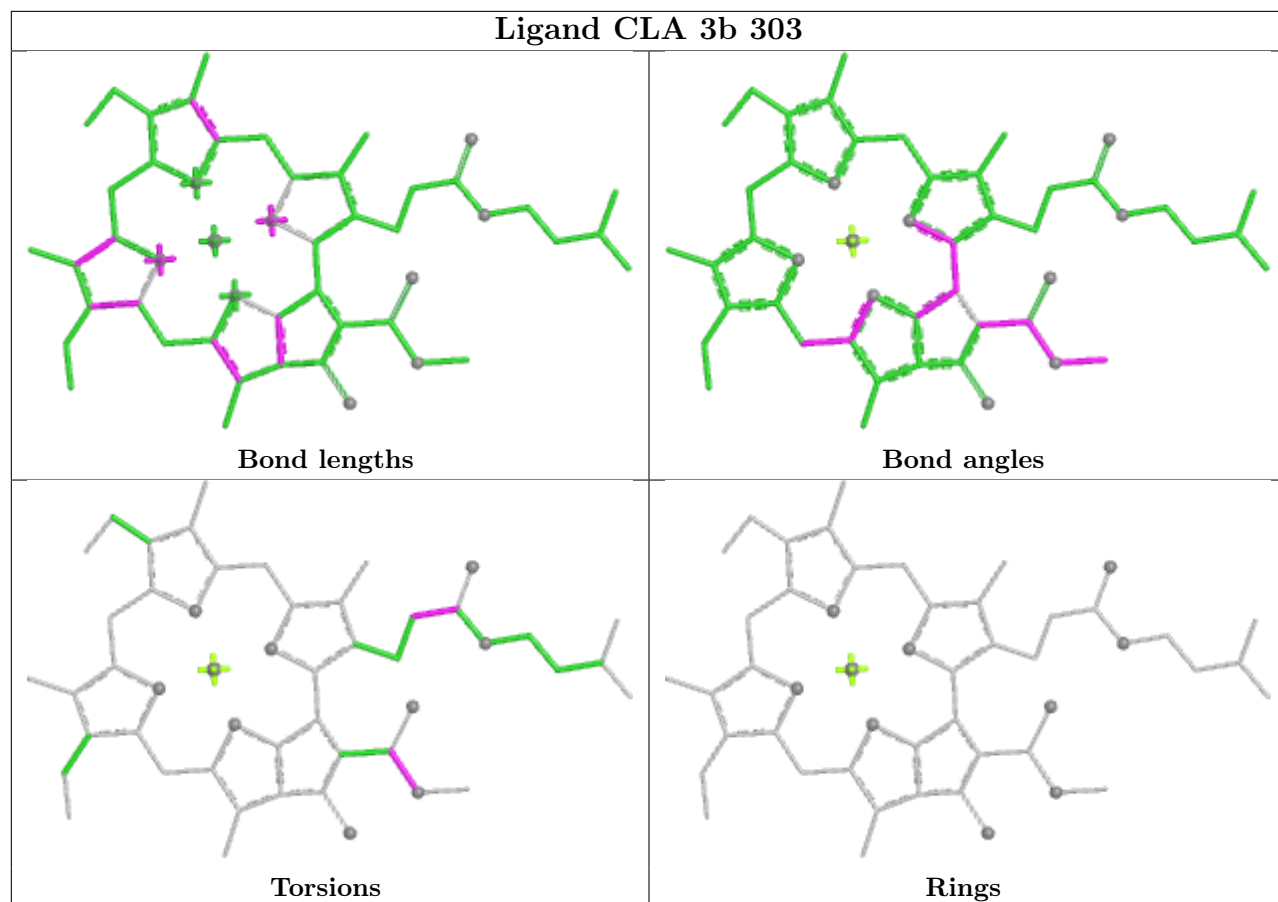


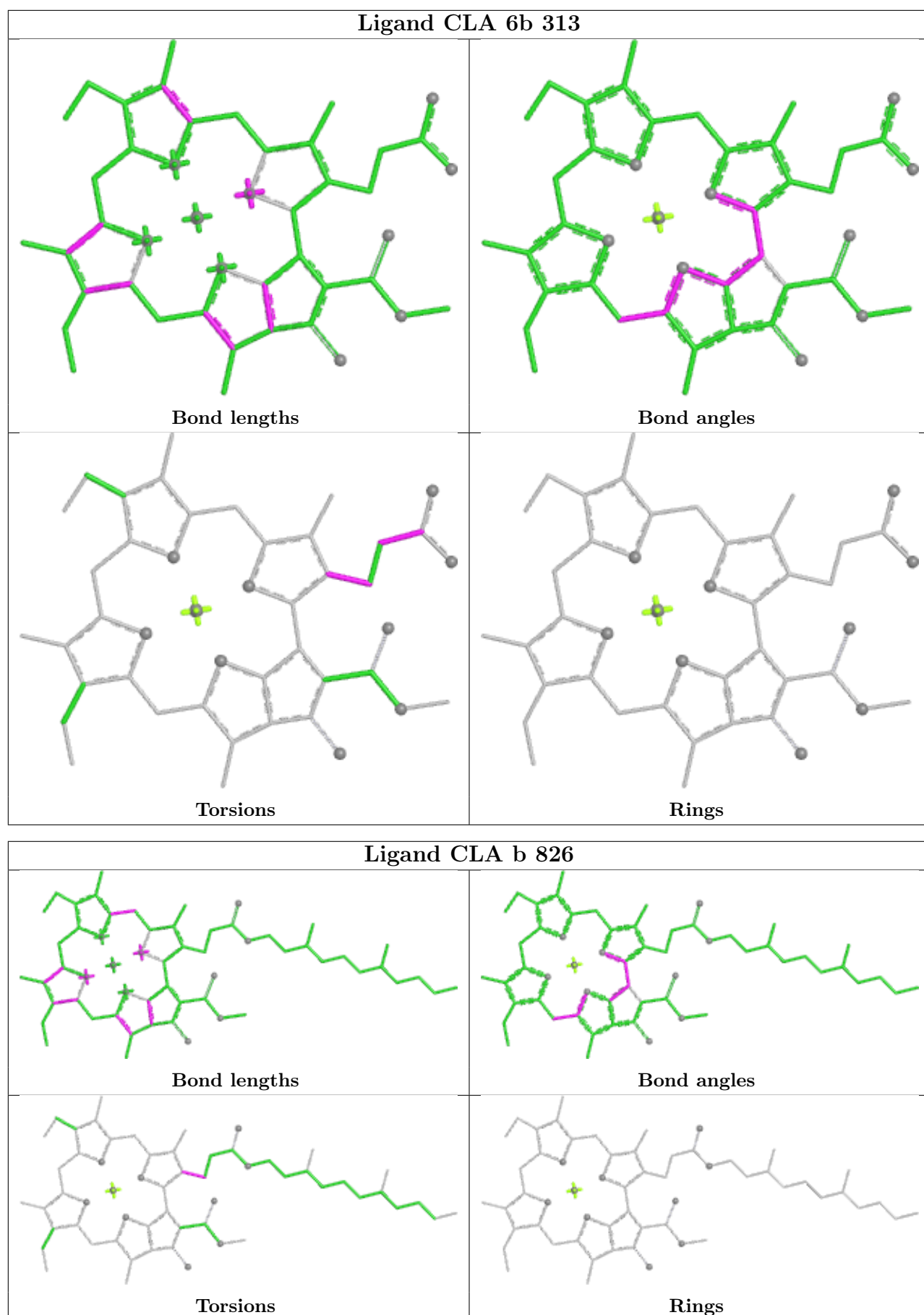
## Ligand LUT 6a 318

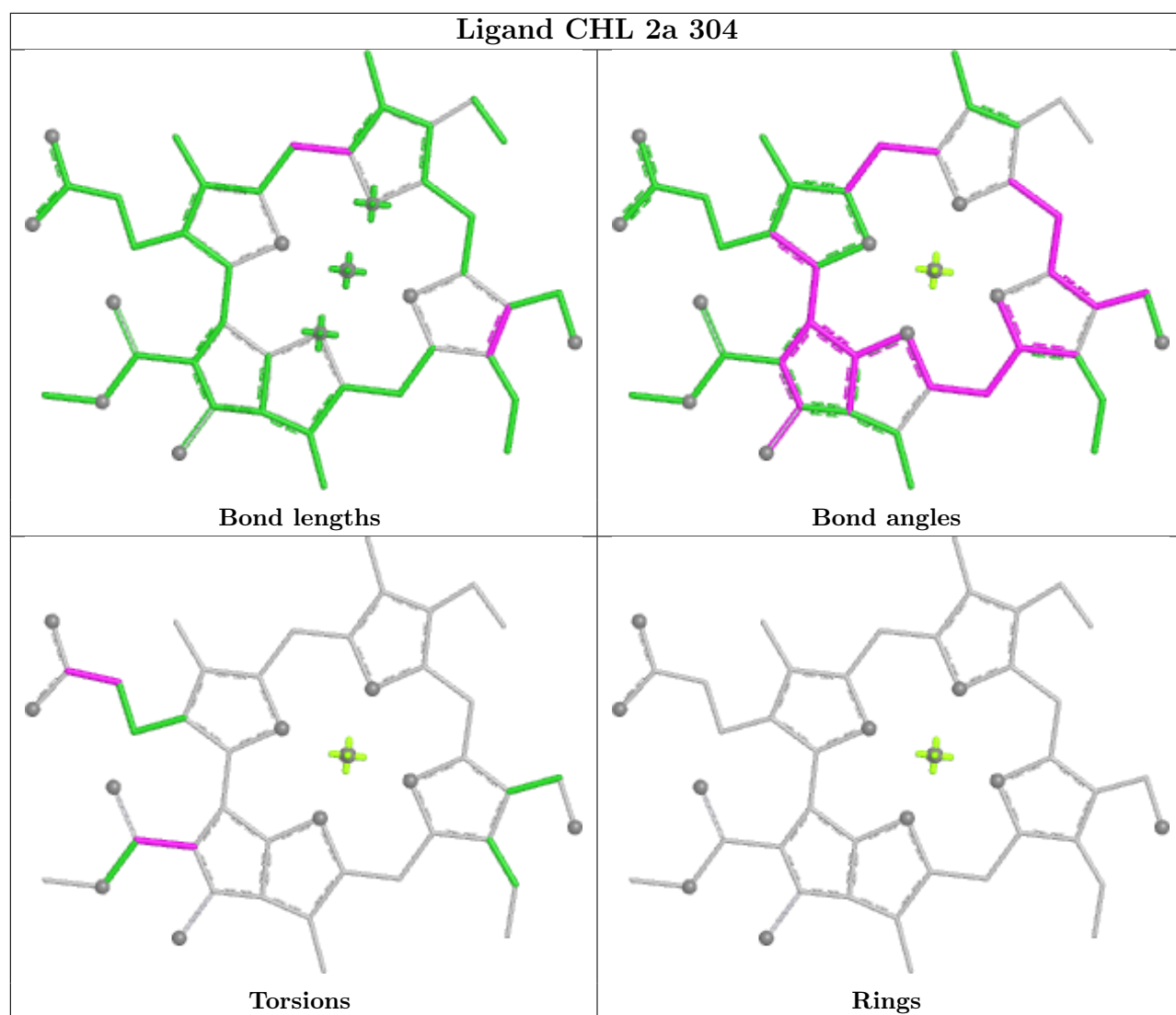






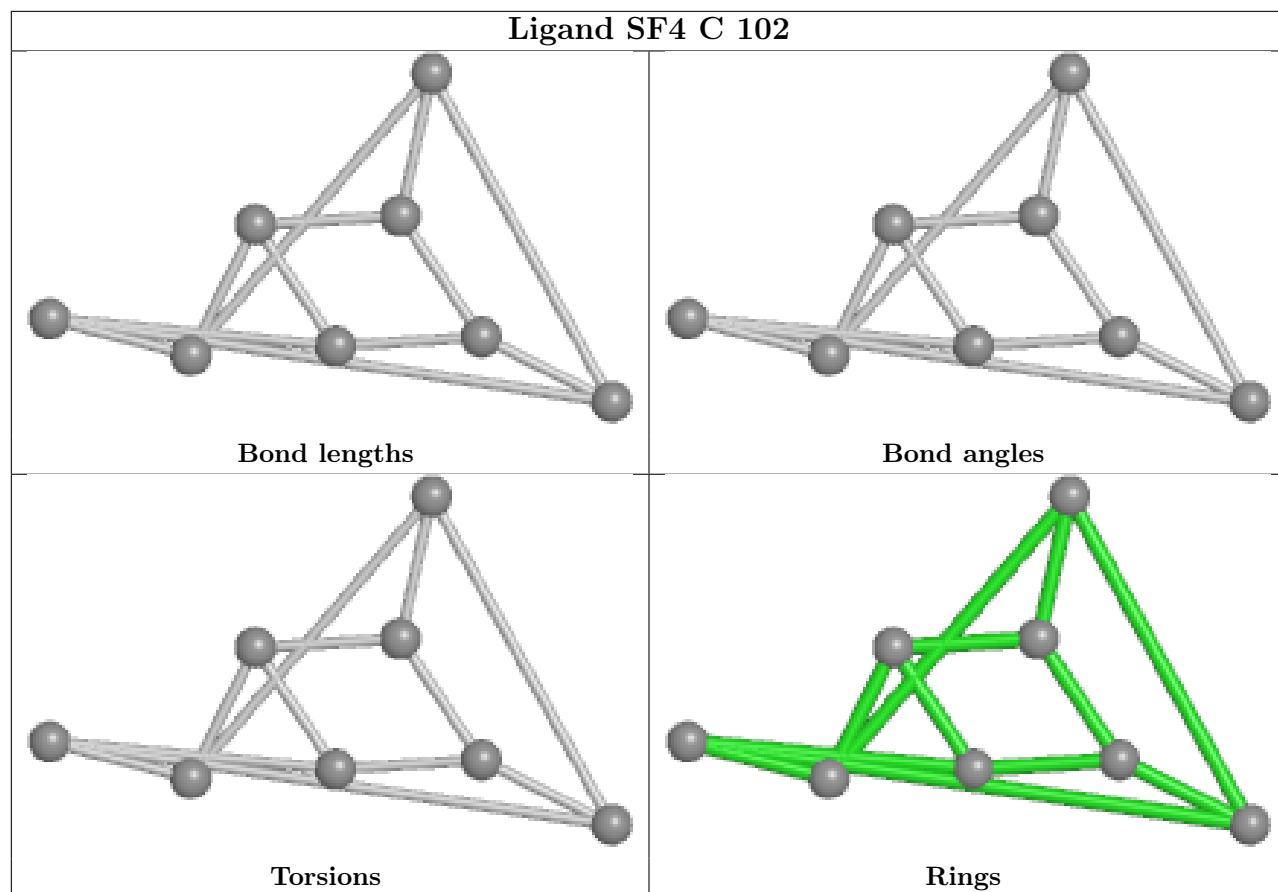




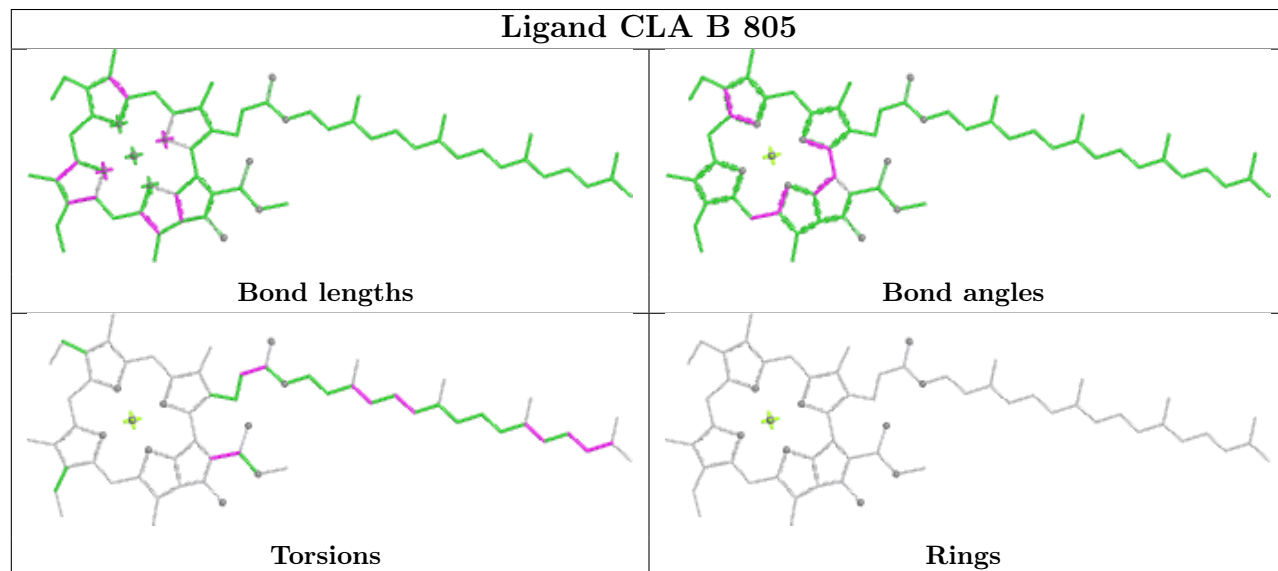


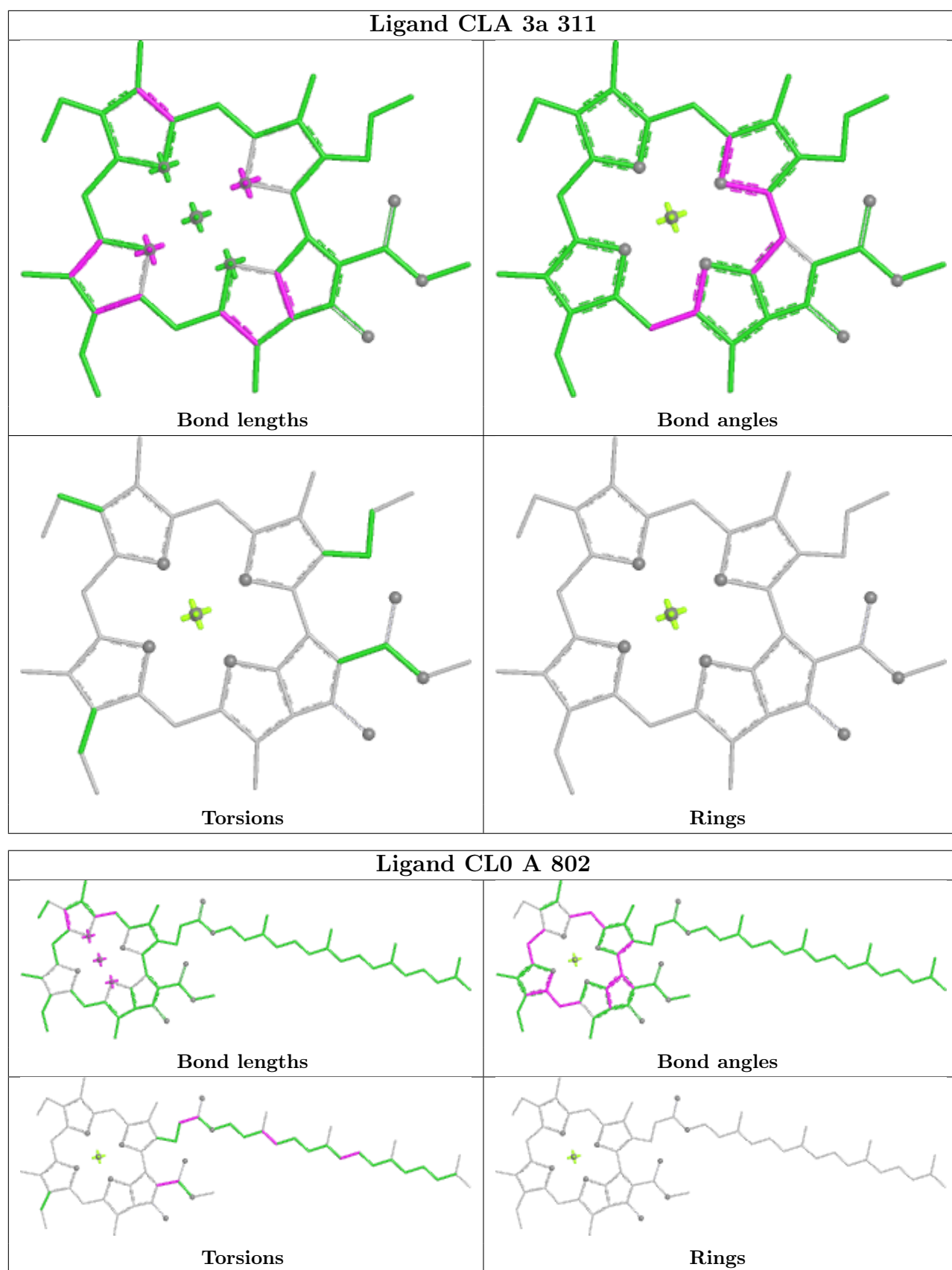


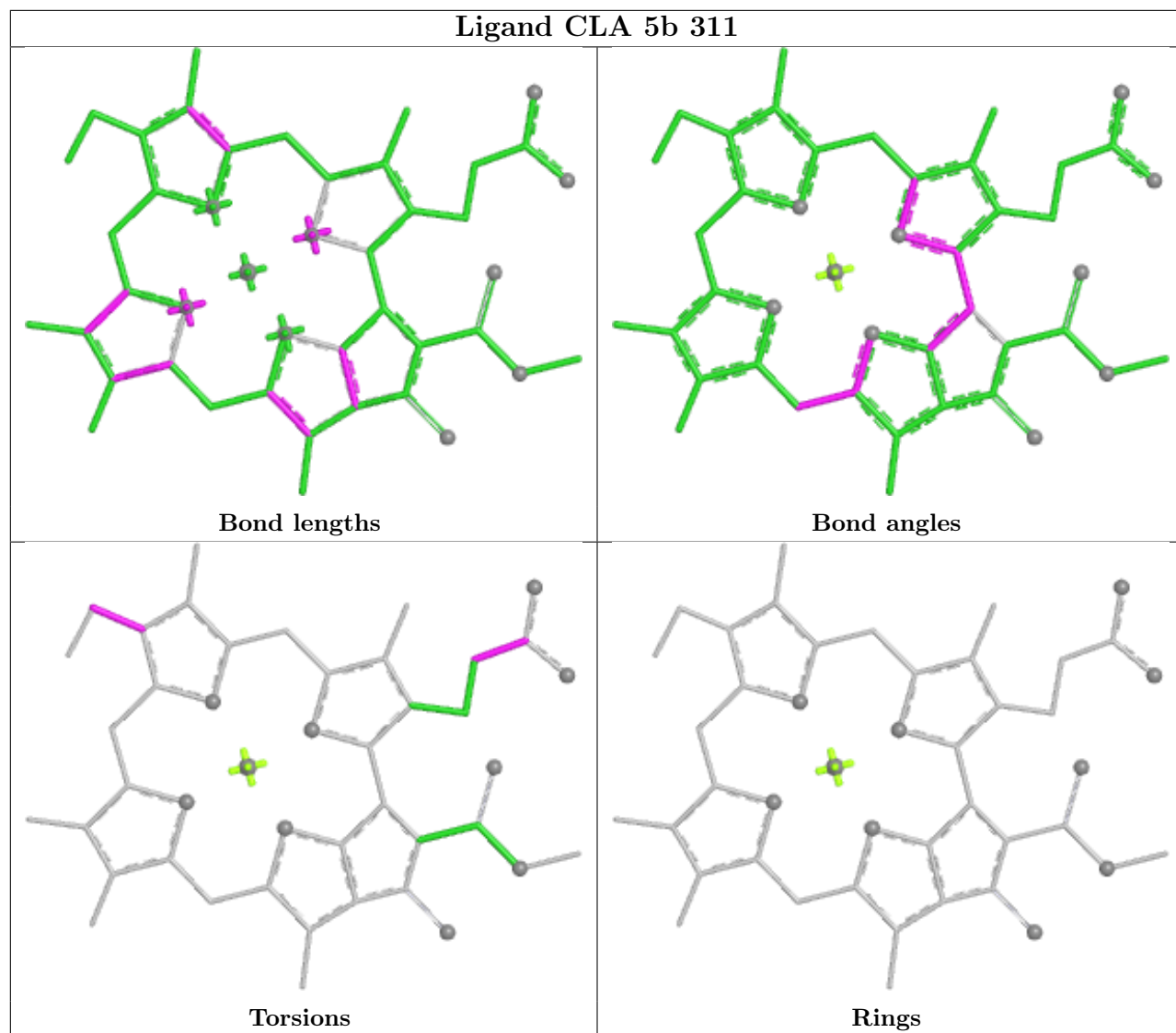
## Ligand SF4 C 102

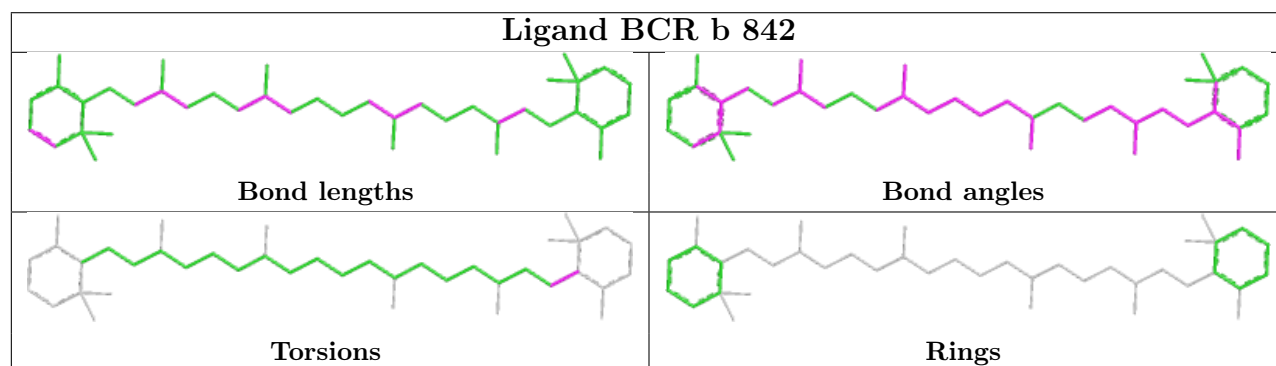
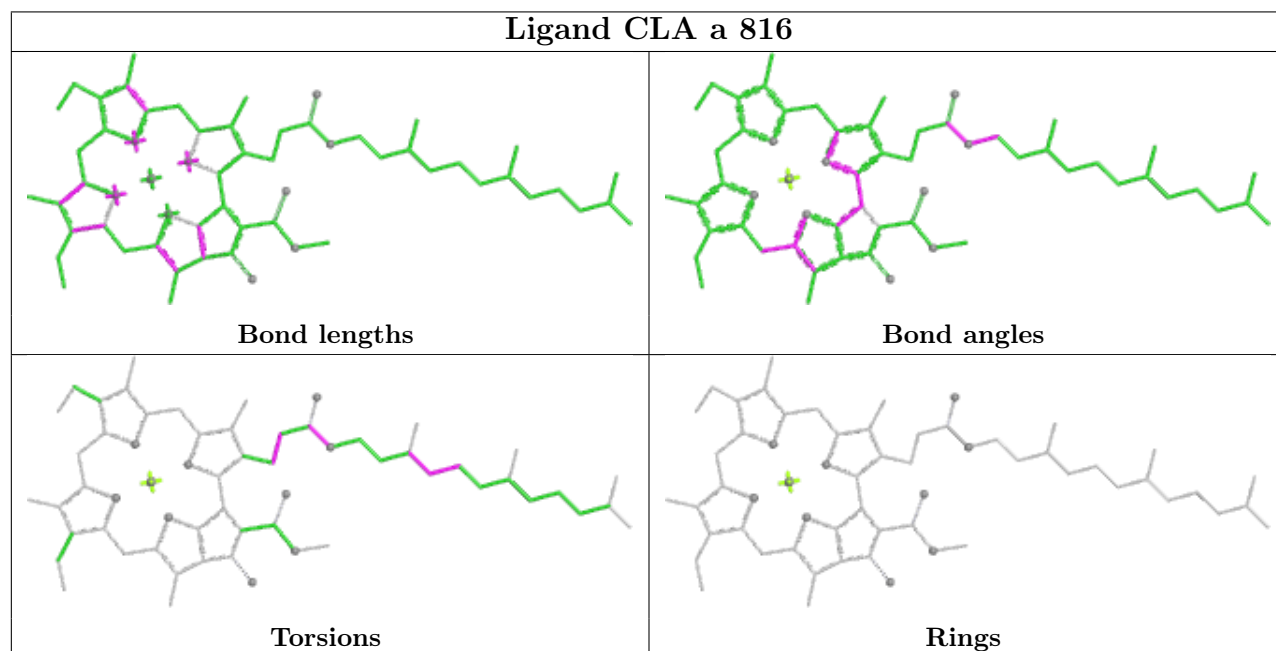
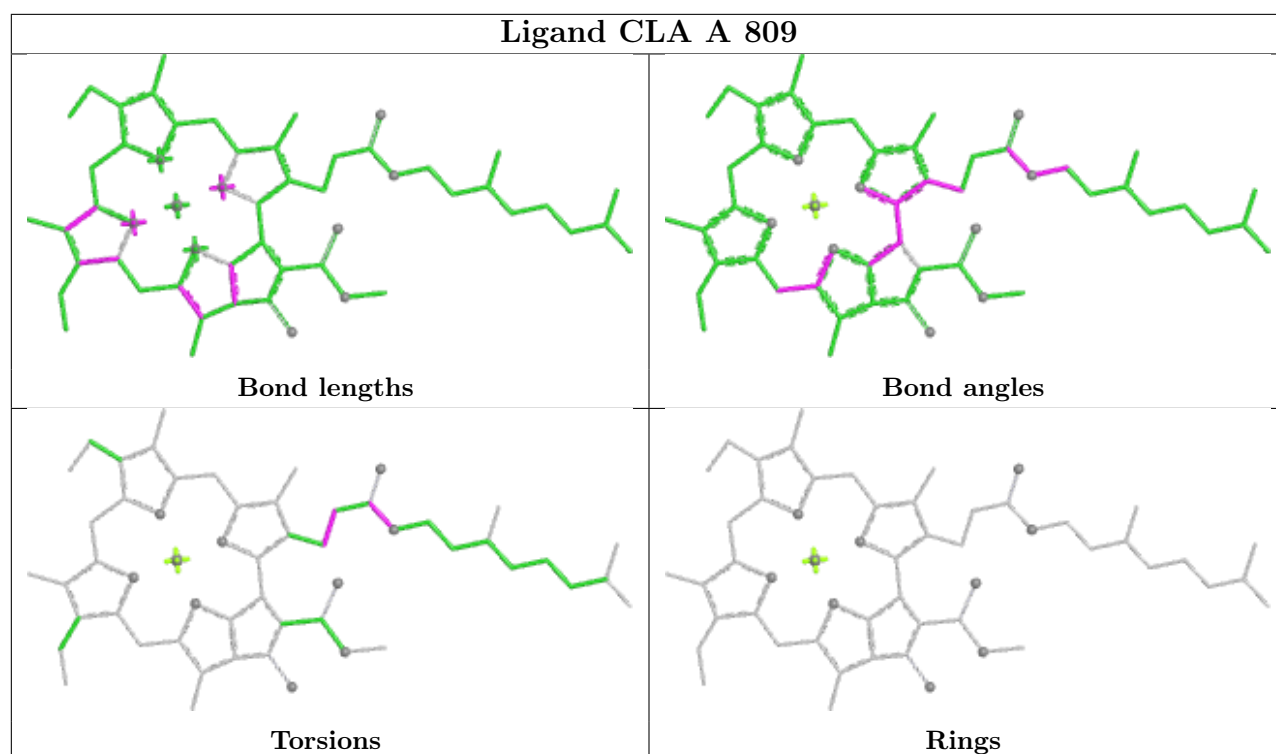


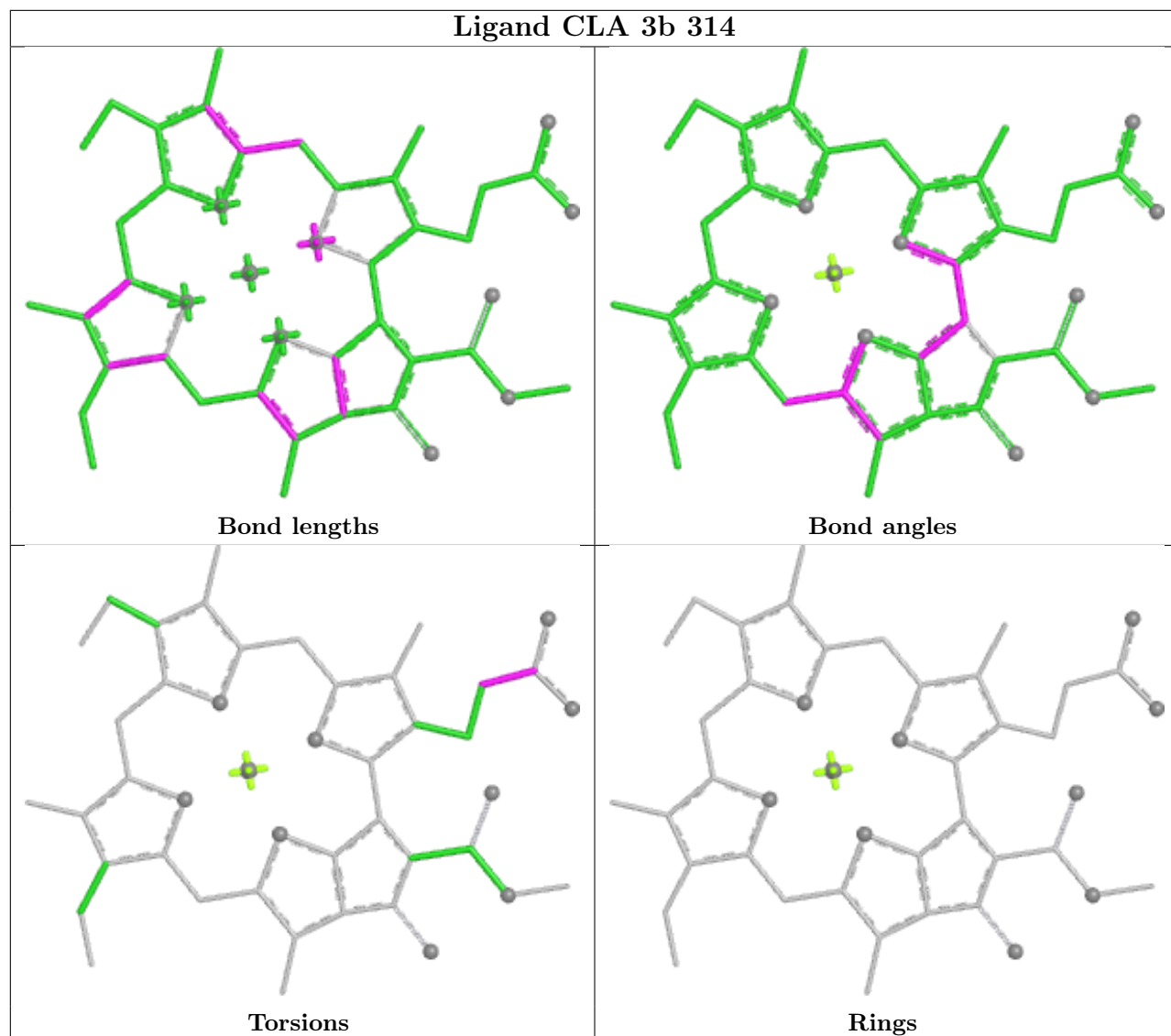
## Ligand CLA B 805



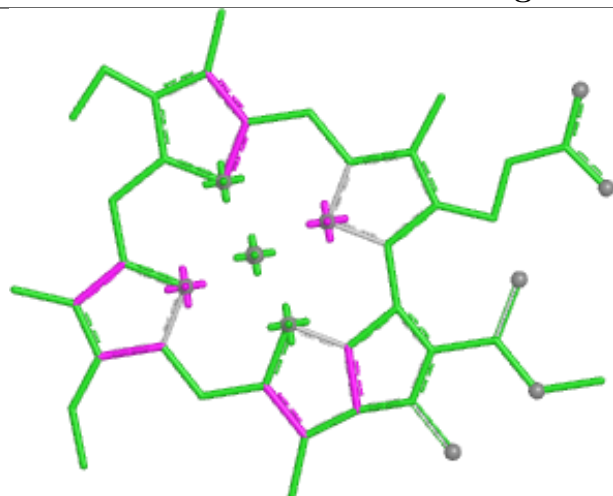




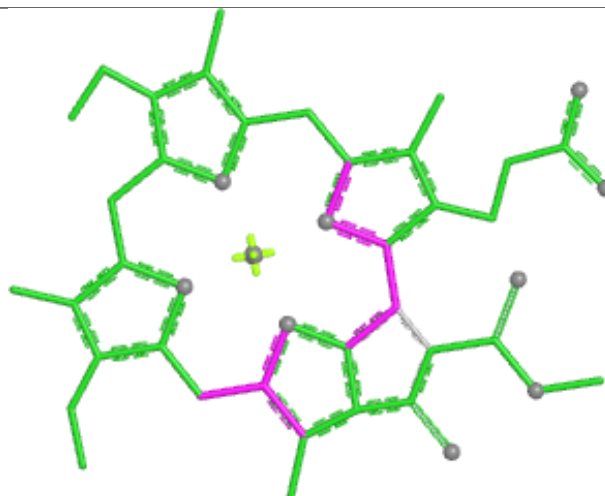




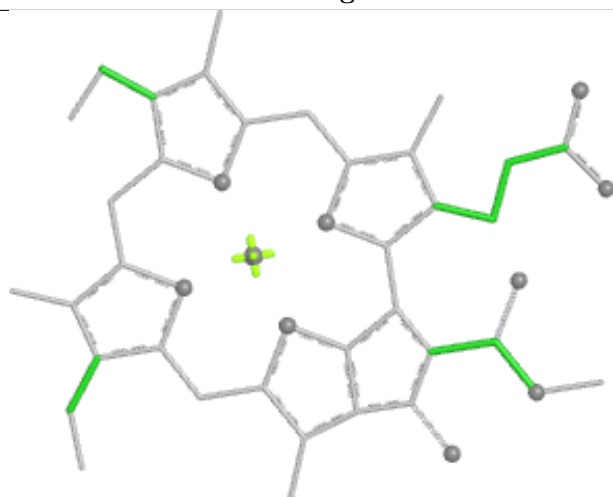
## Ligand CLA B 834



Bond lengths



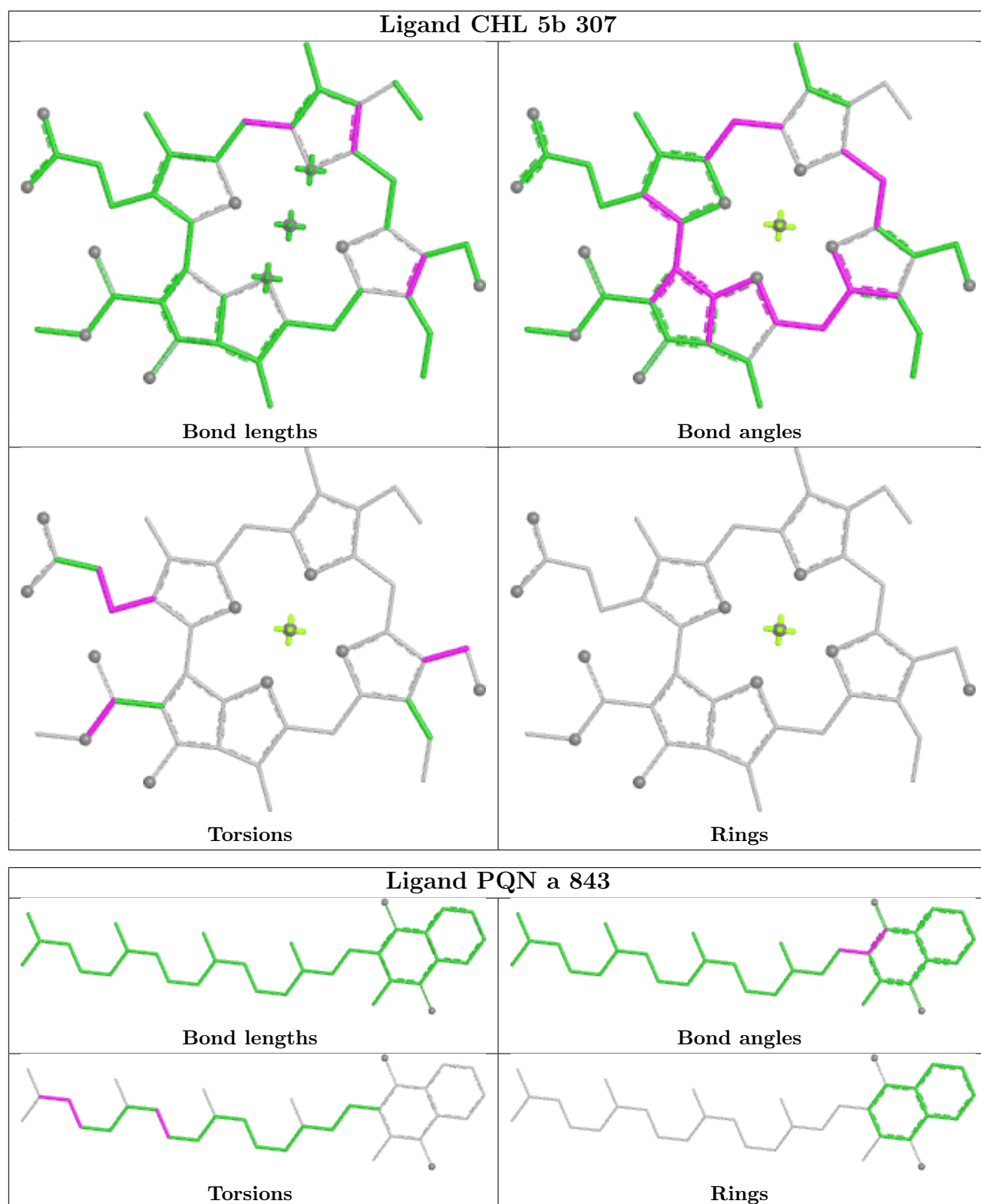
Bond angles

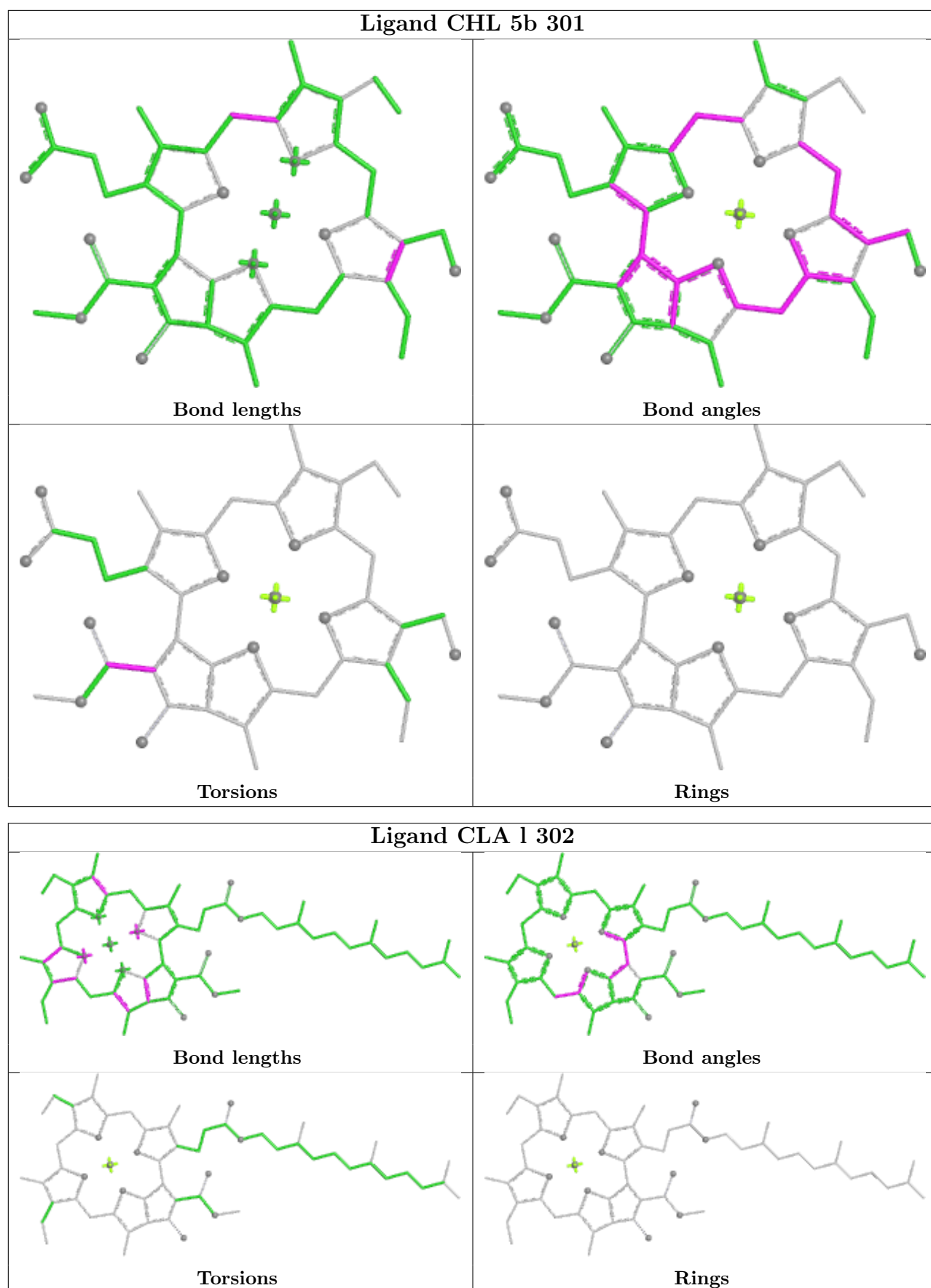


Torsions

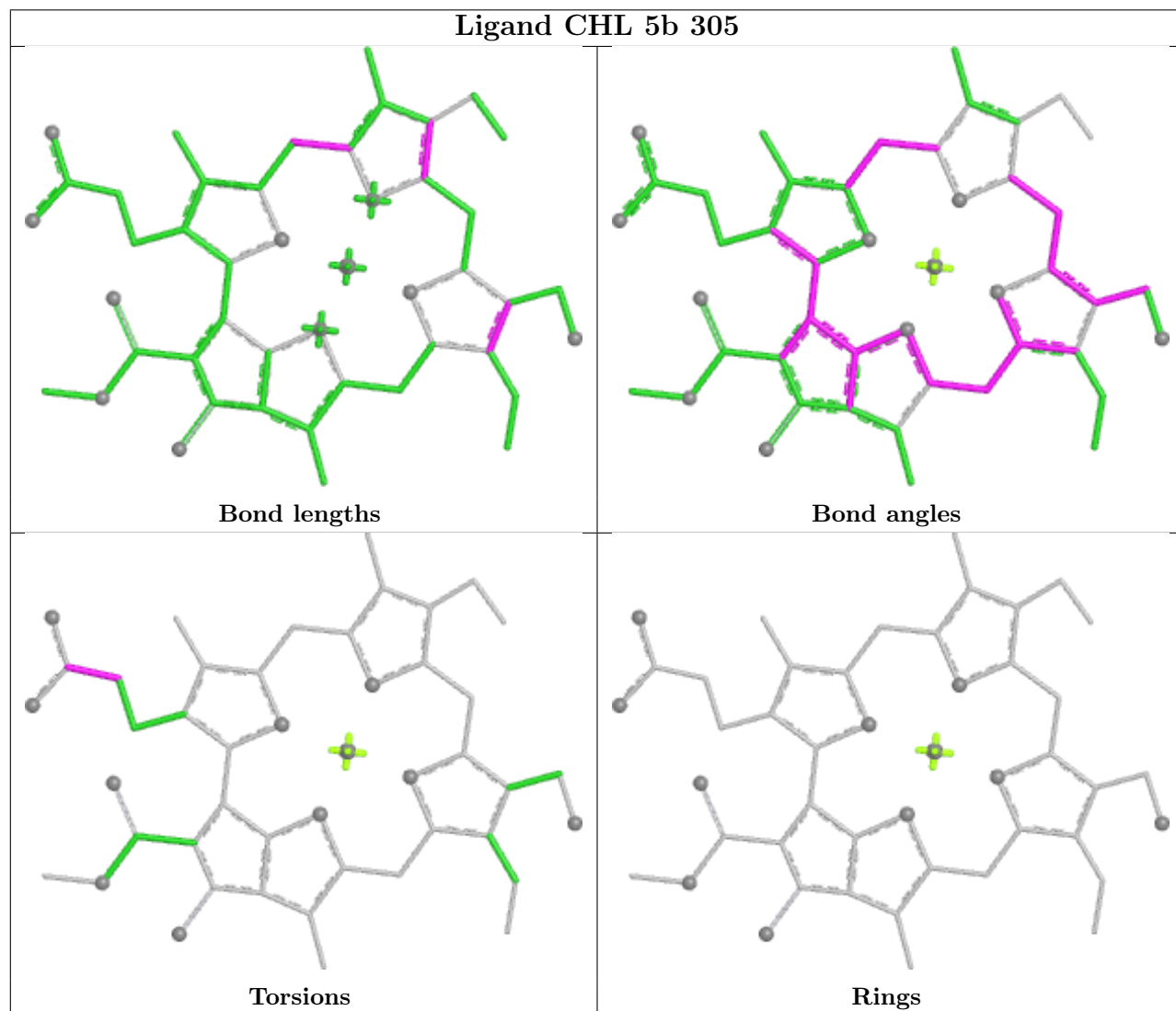
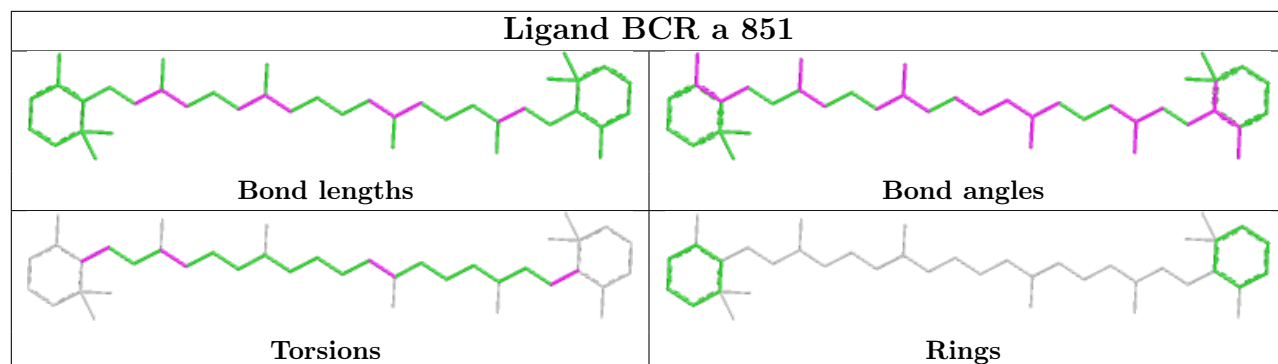


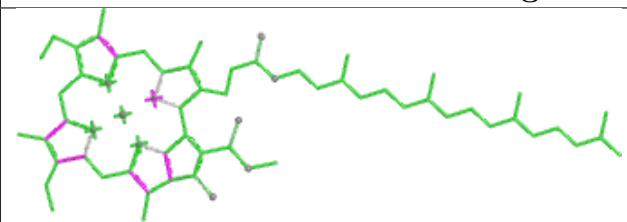
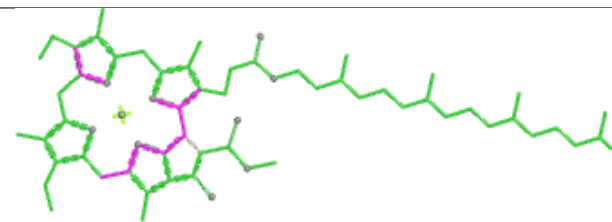
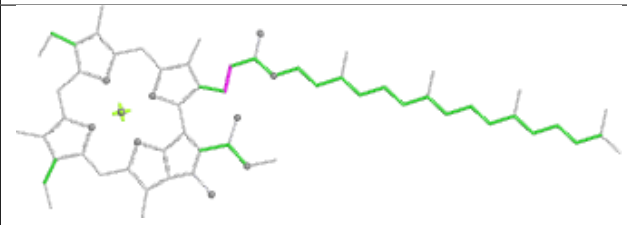
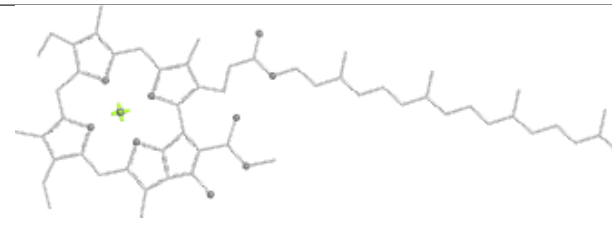
Rings

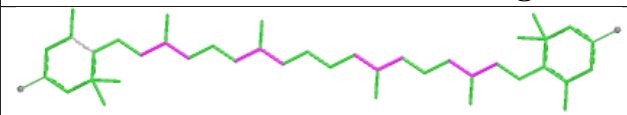
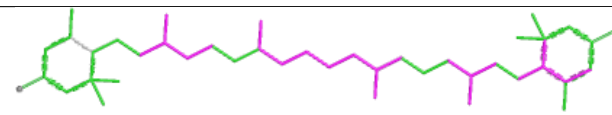
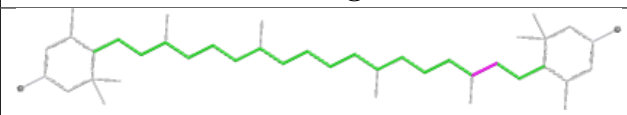
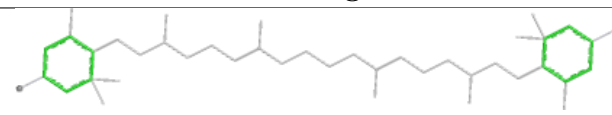


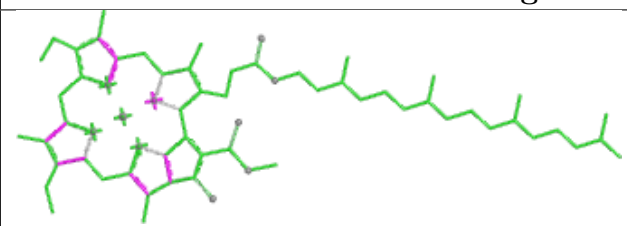
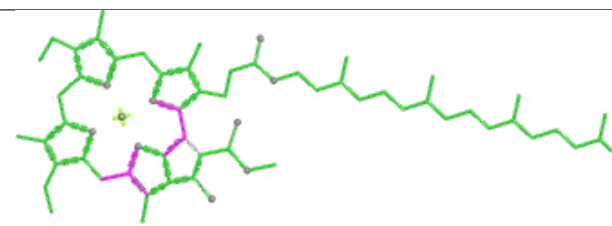
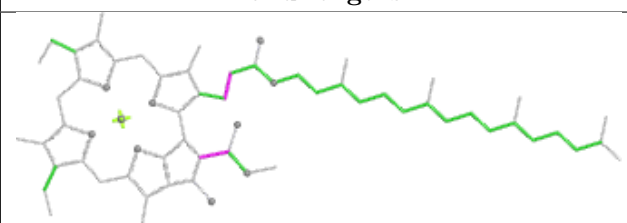
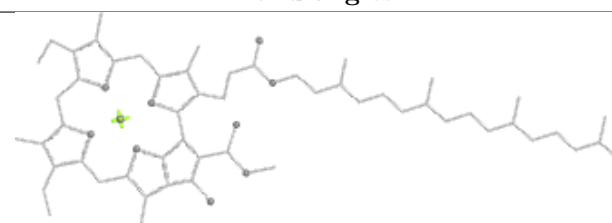


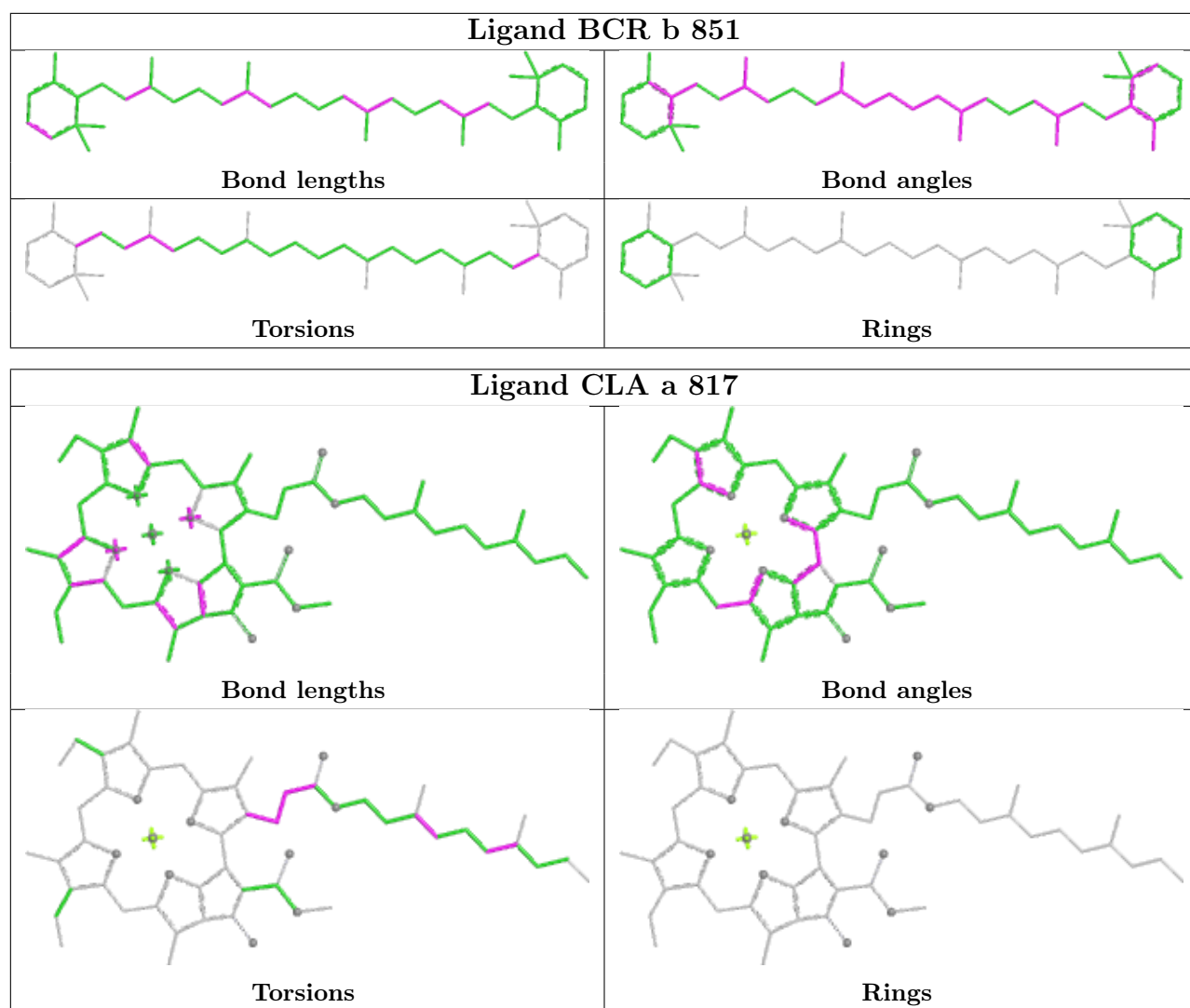


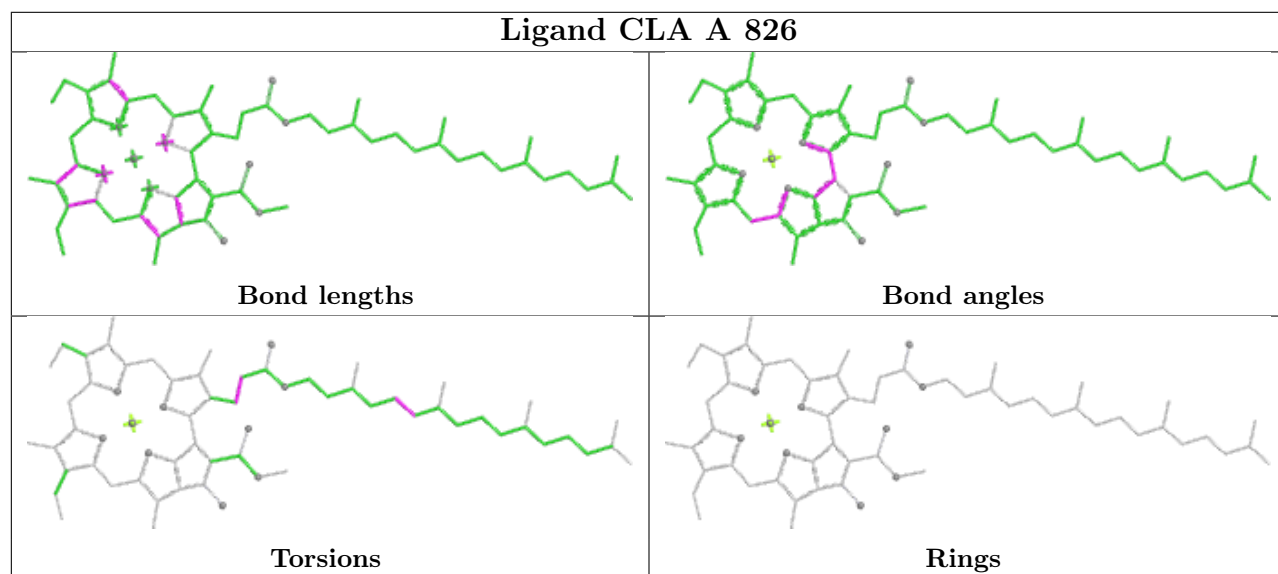
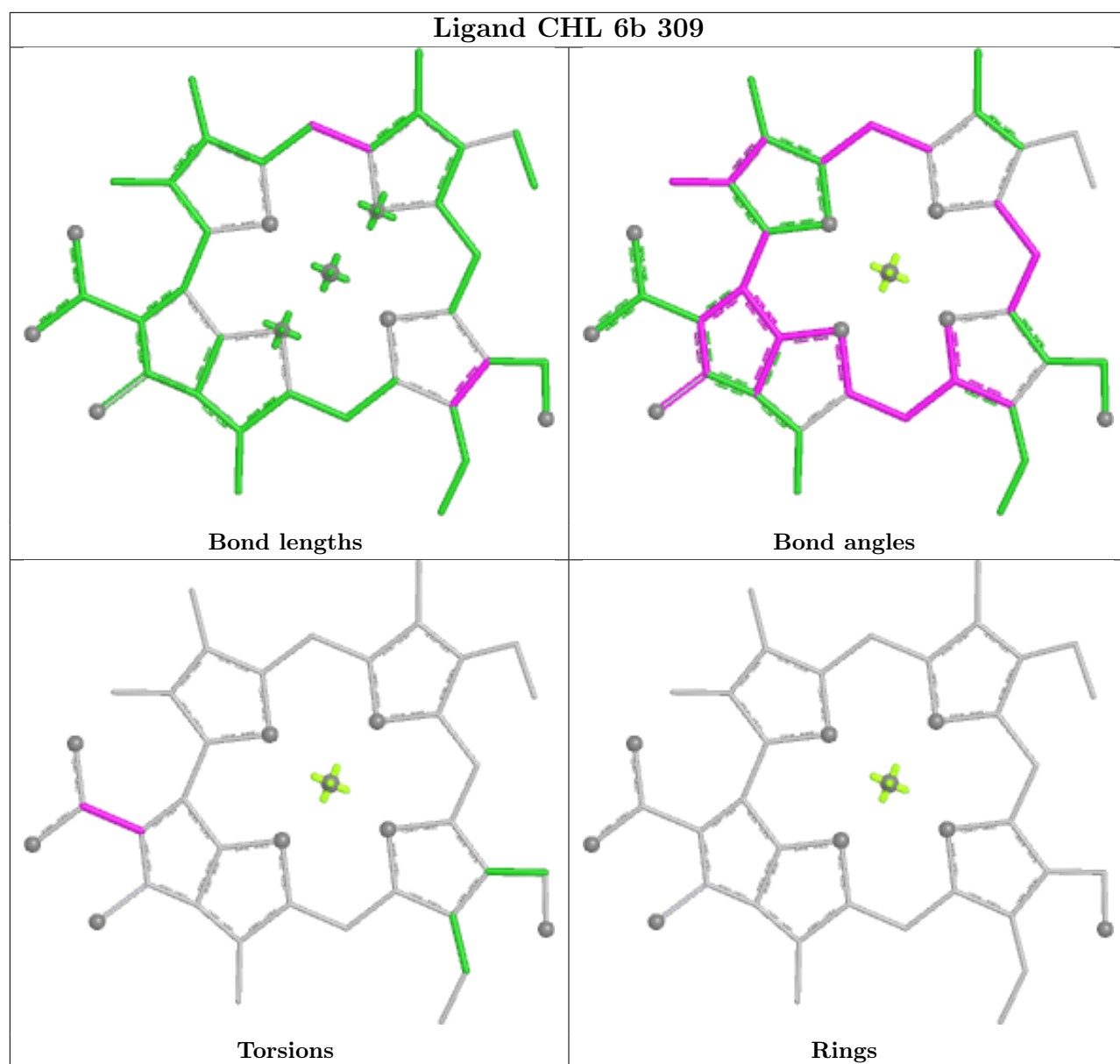


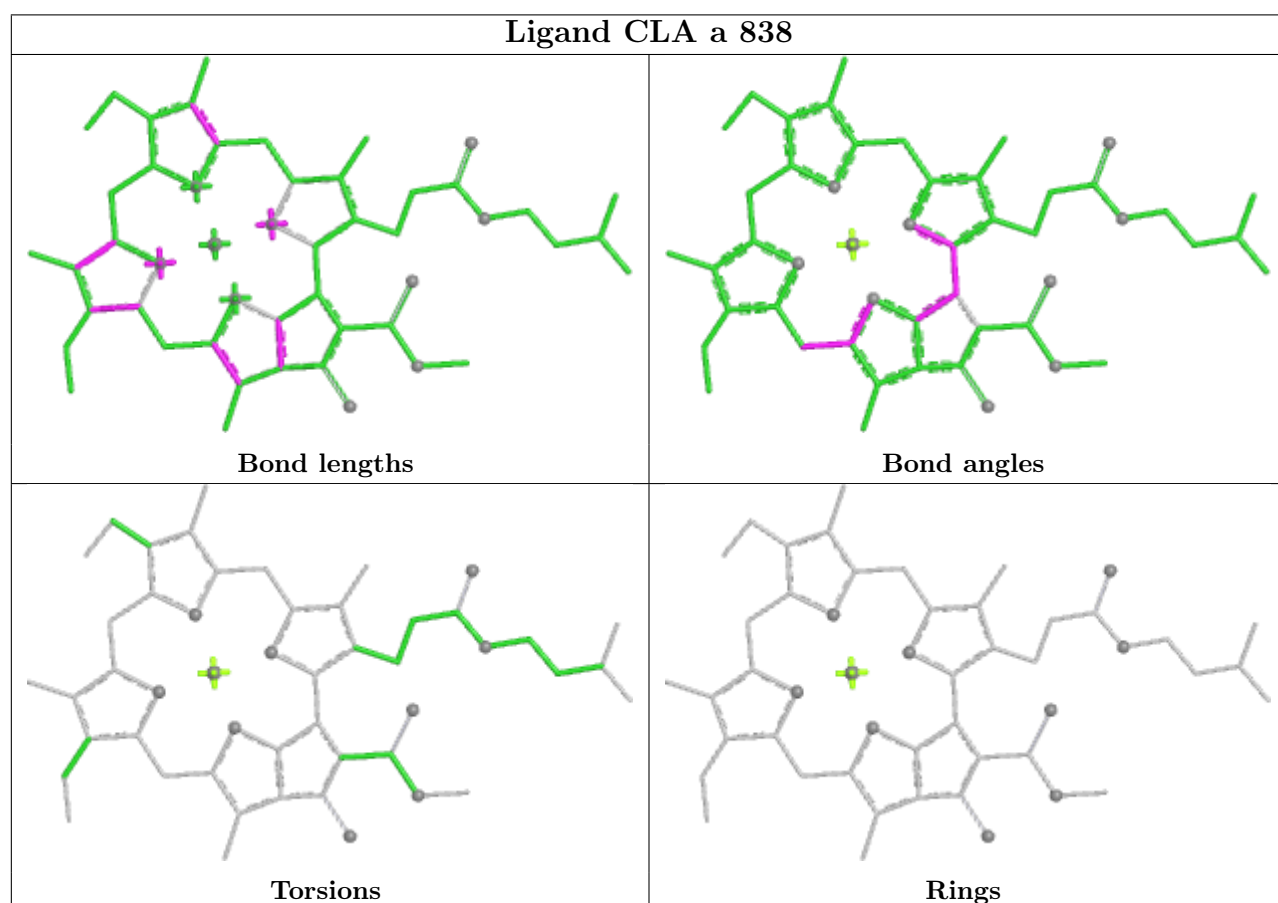
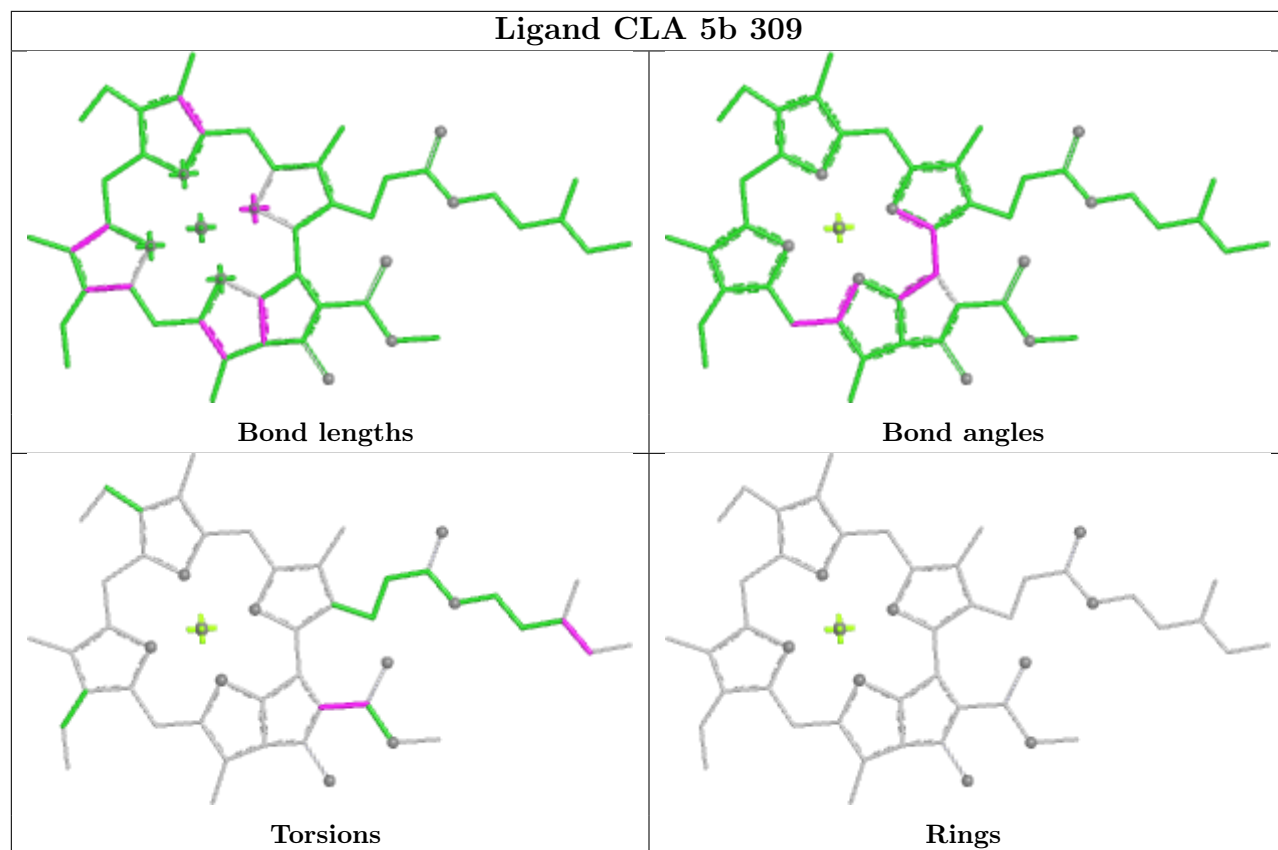
Ligand CLA B 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

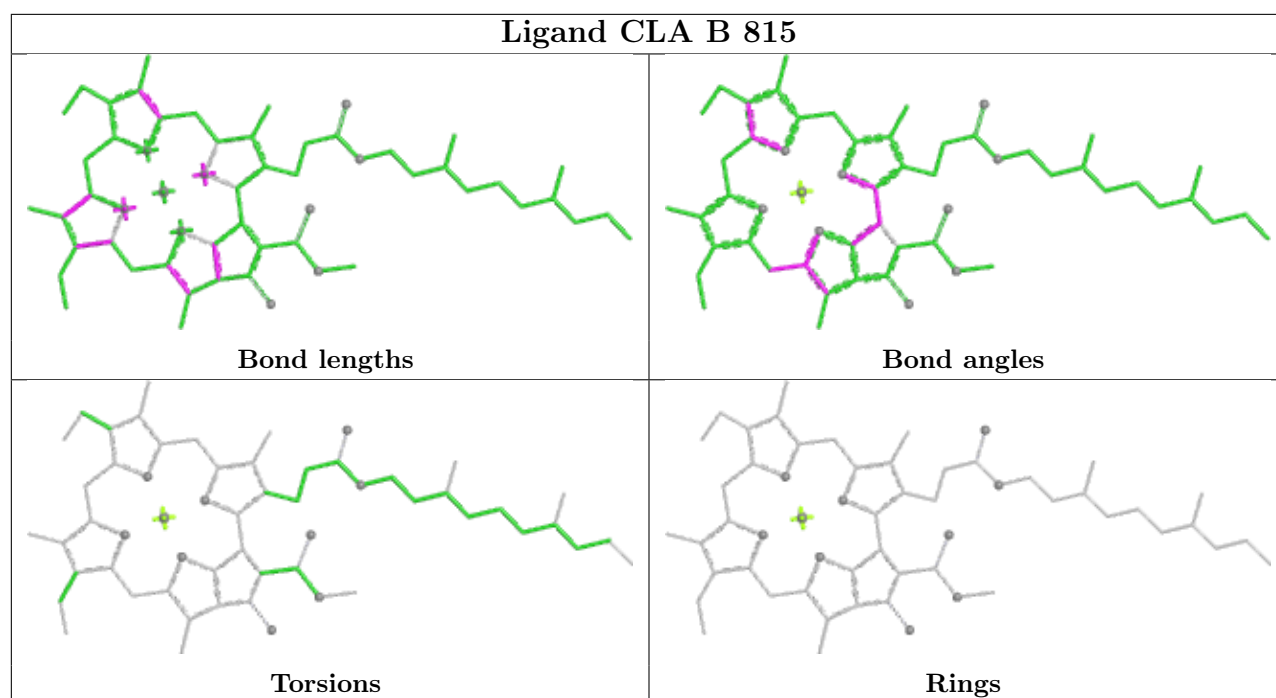
Ligand LUT 5b 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

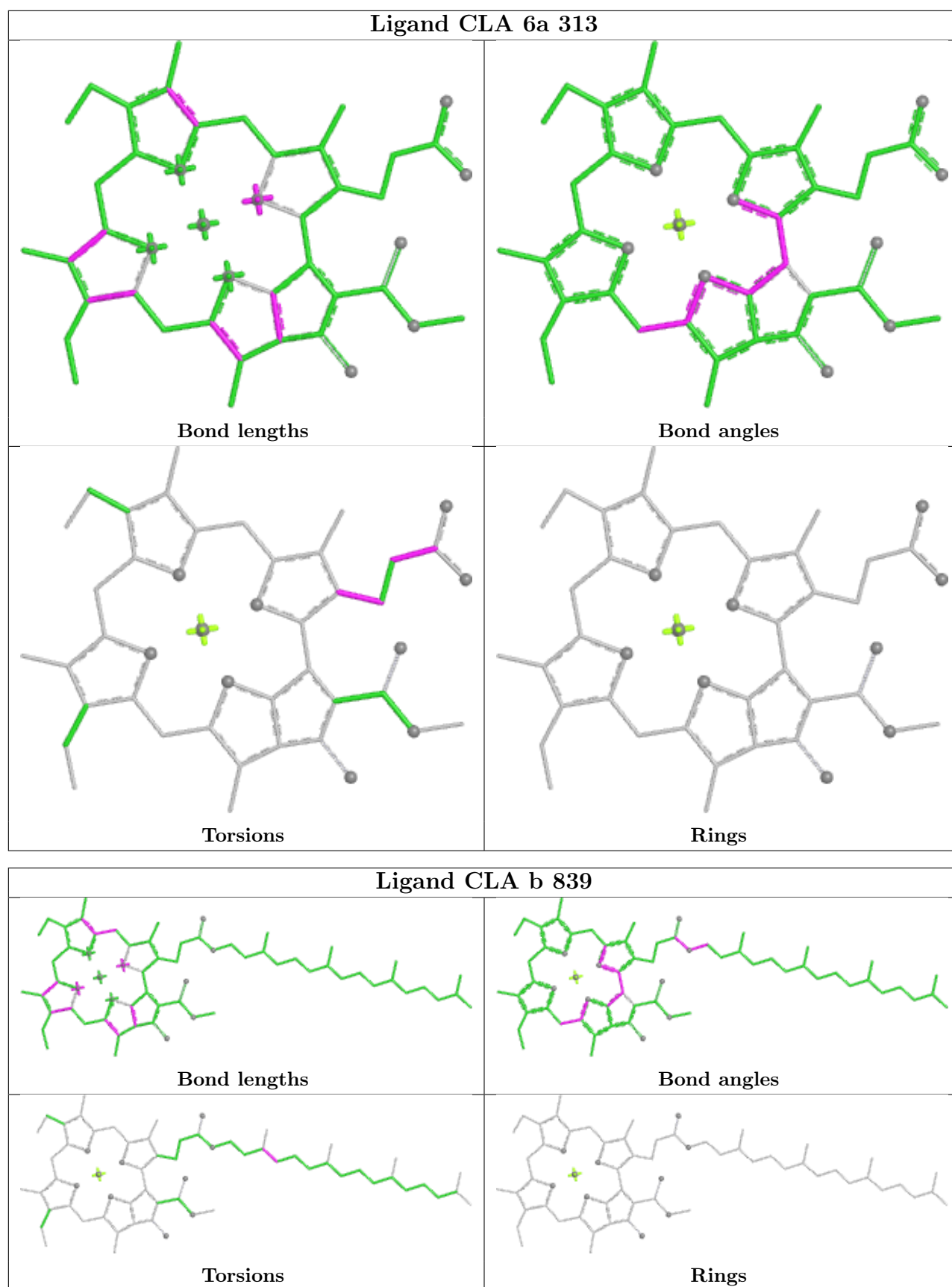
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

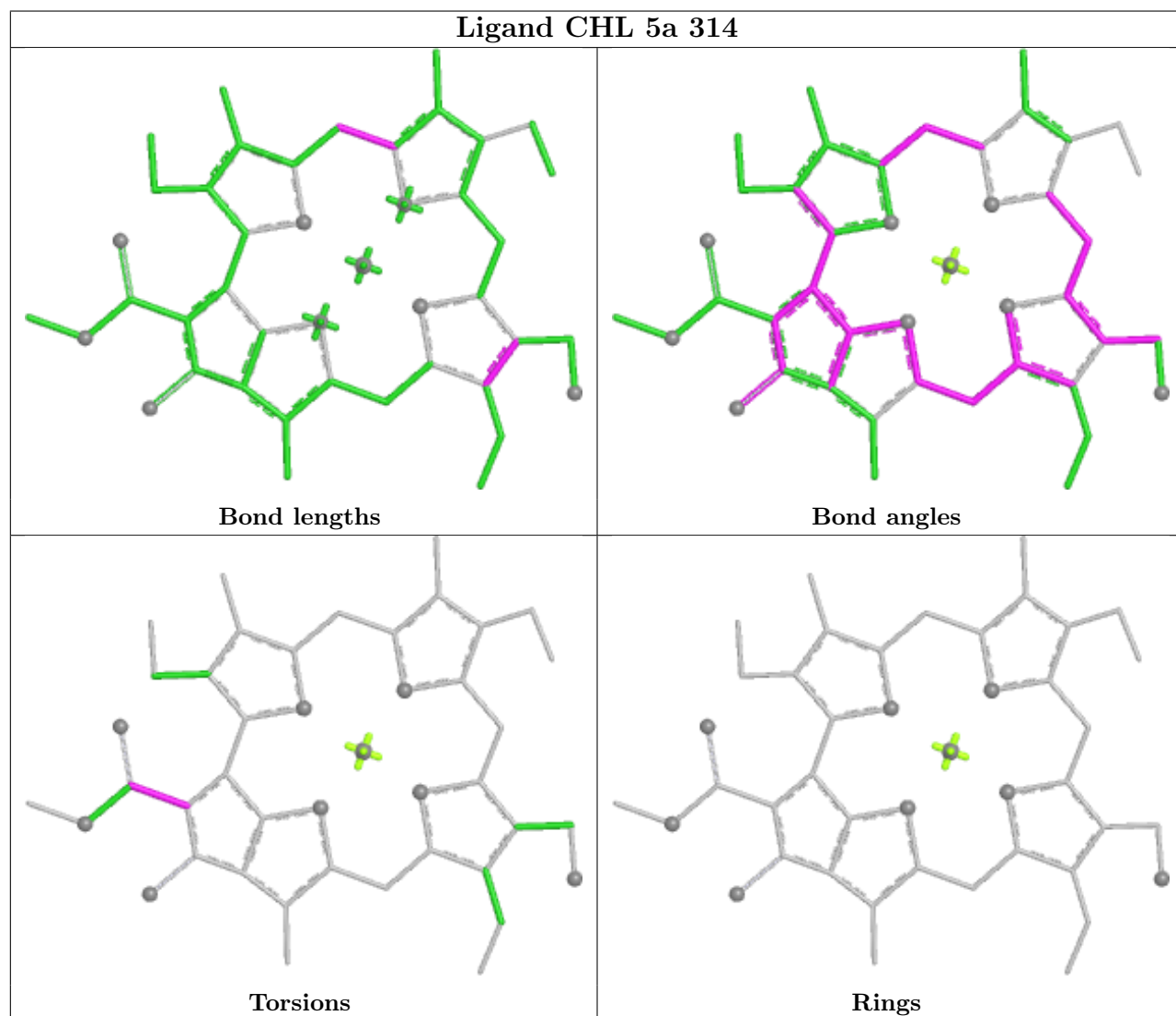
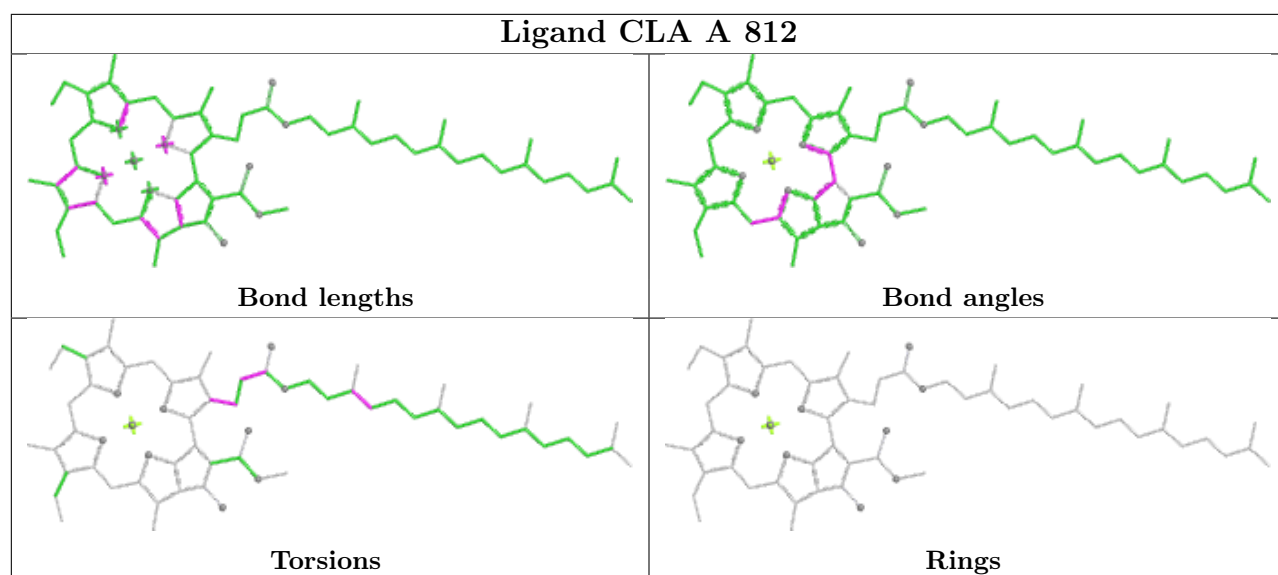




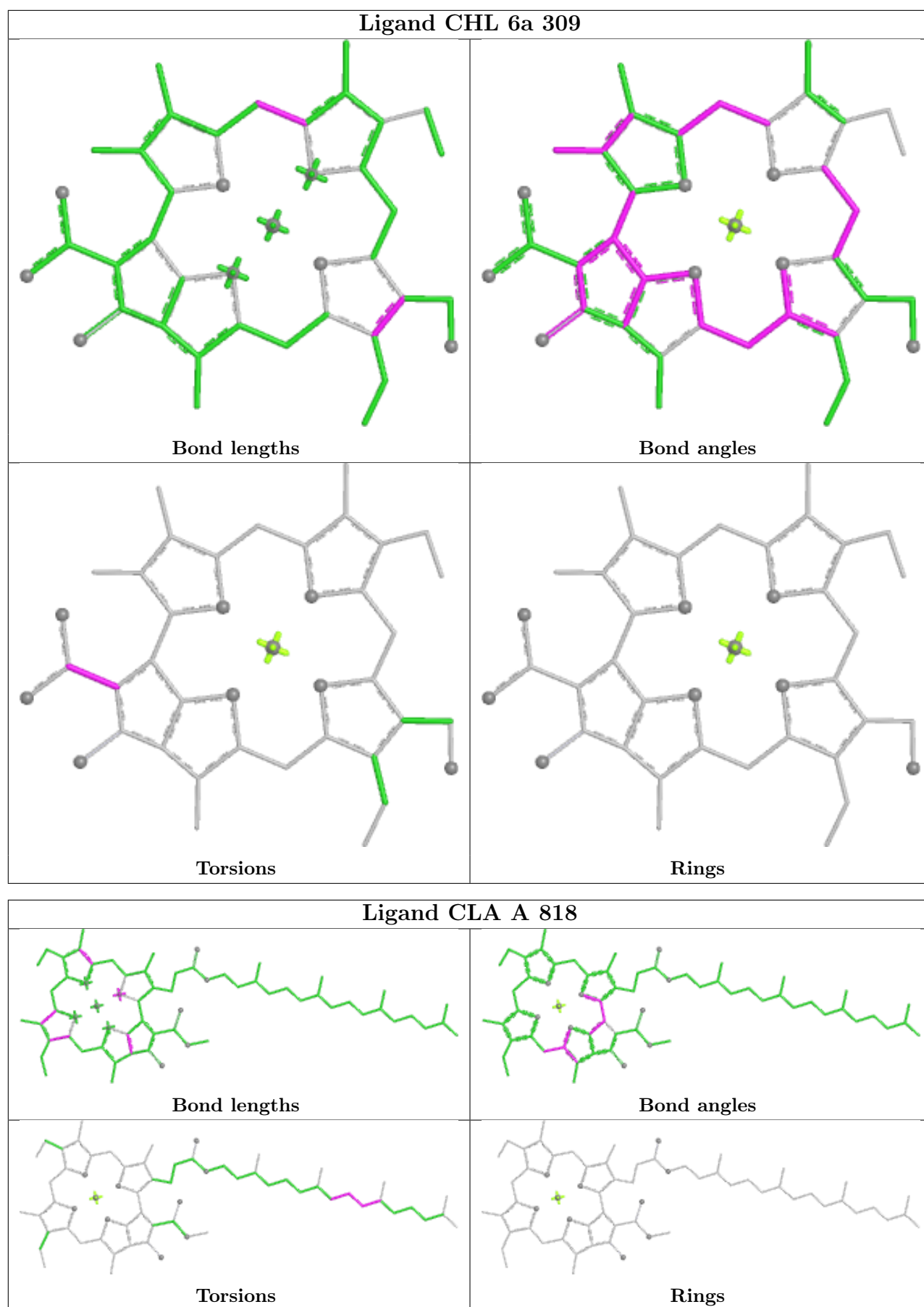


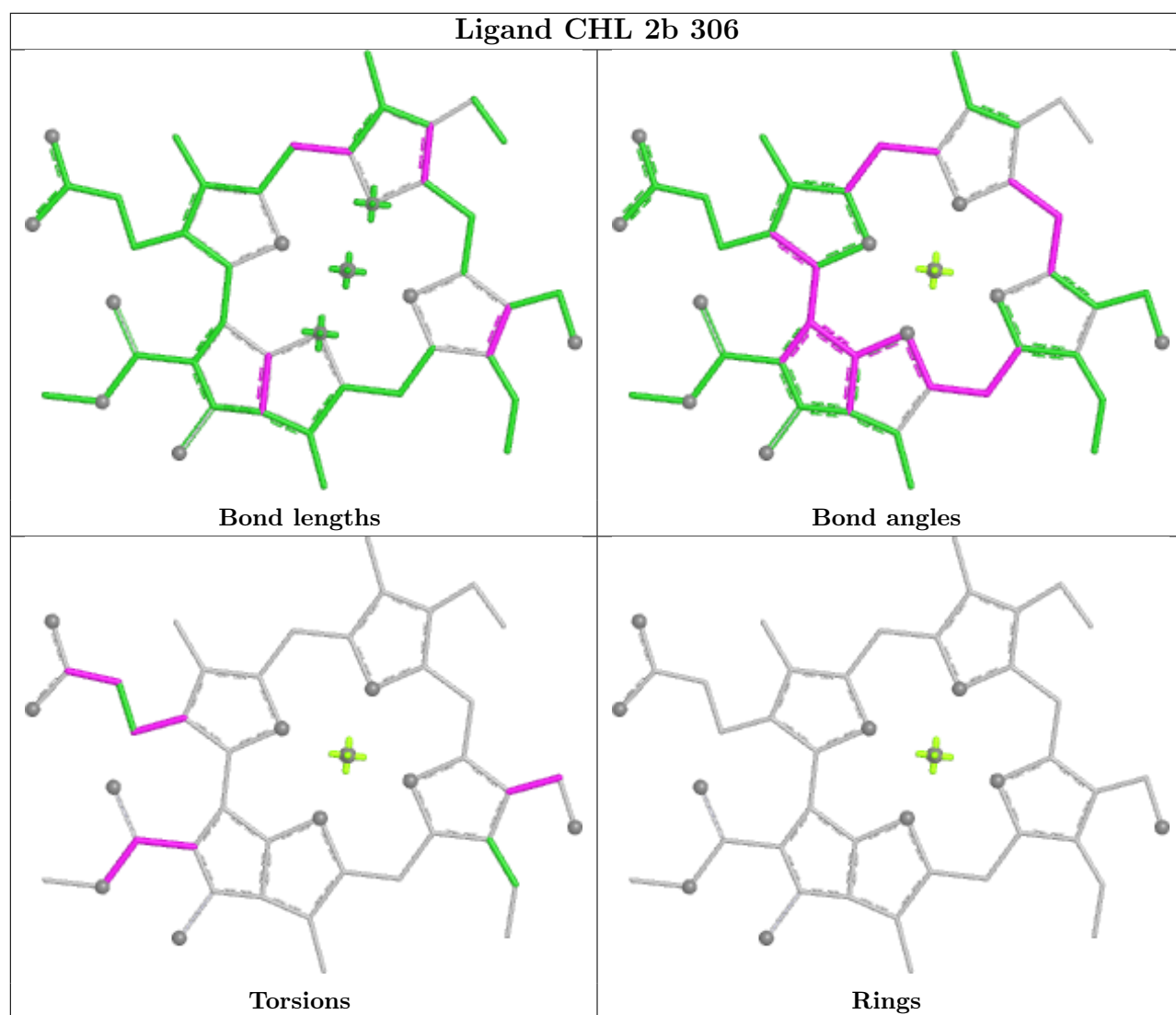


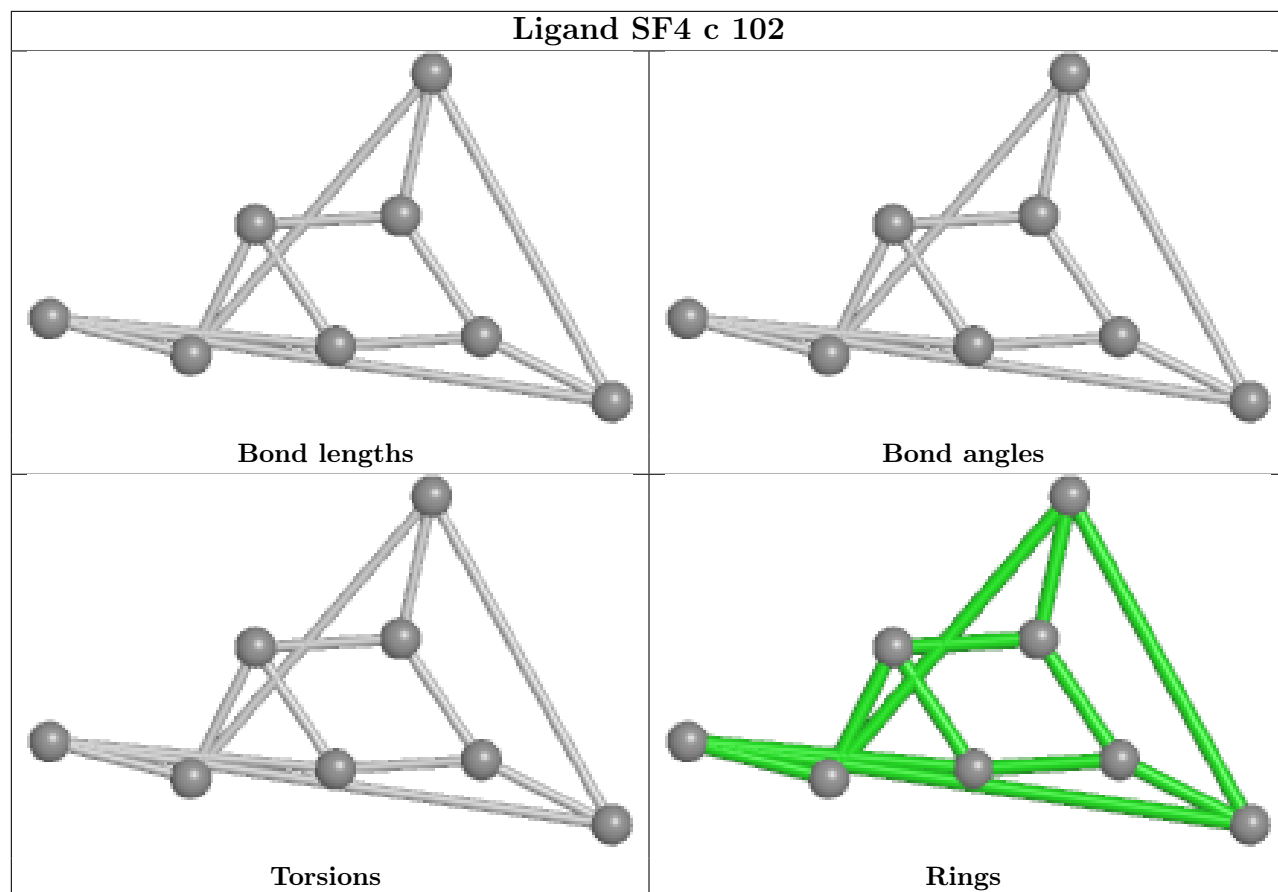


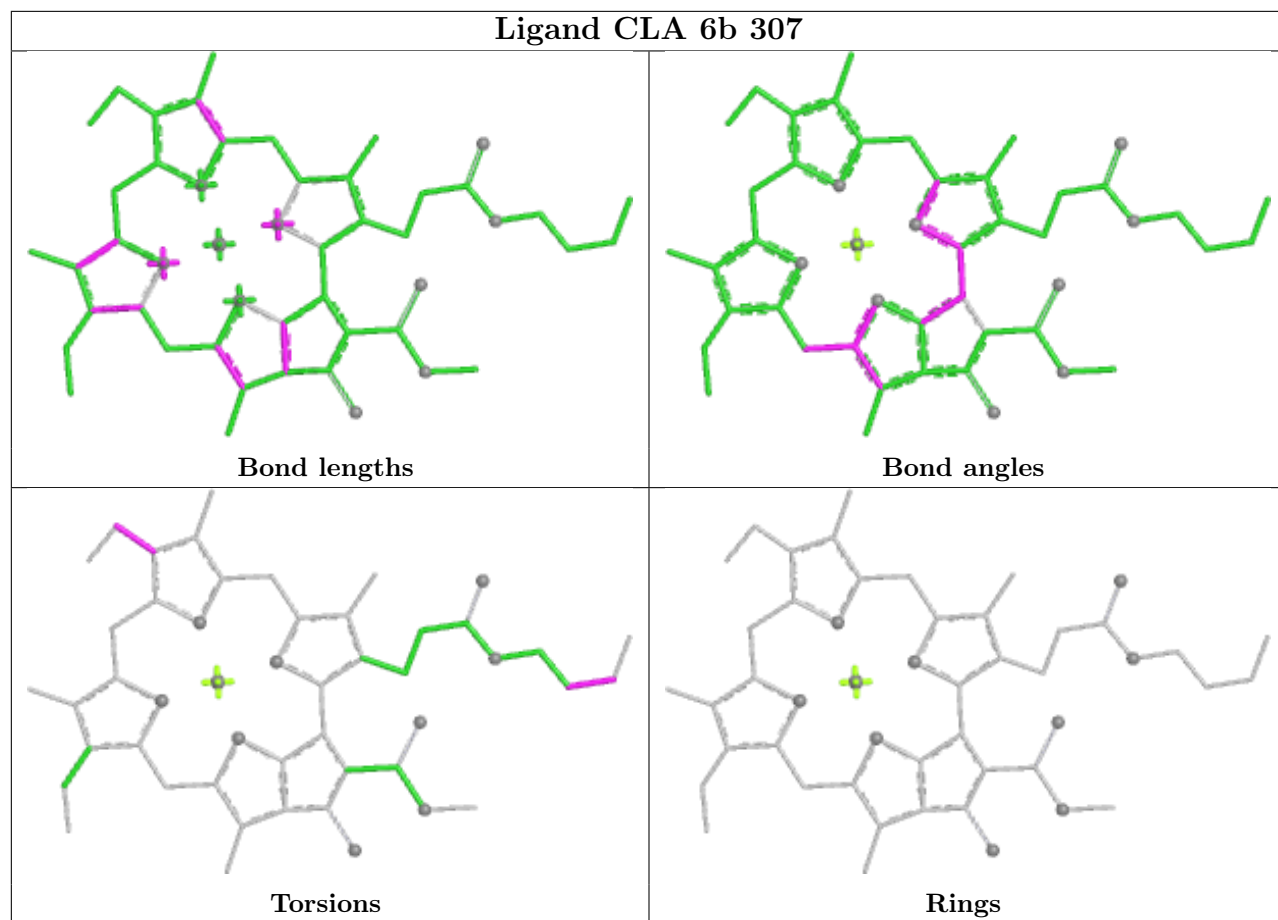




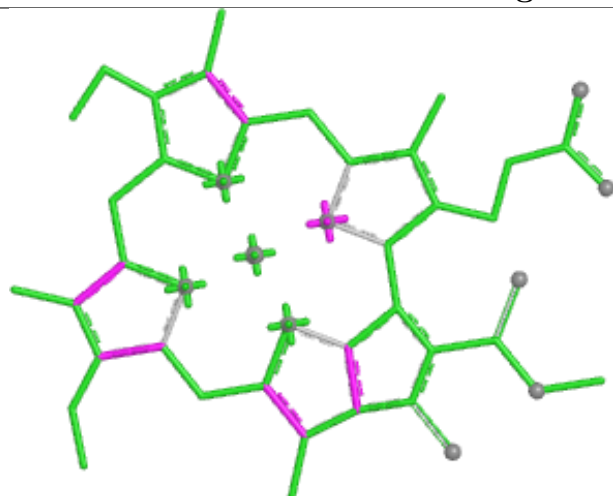




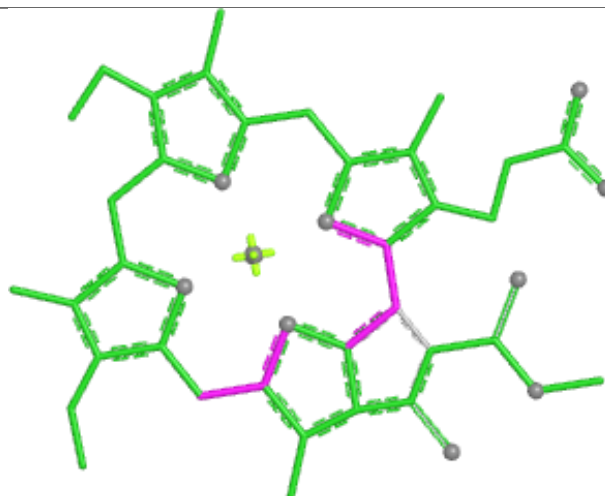




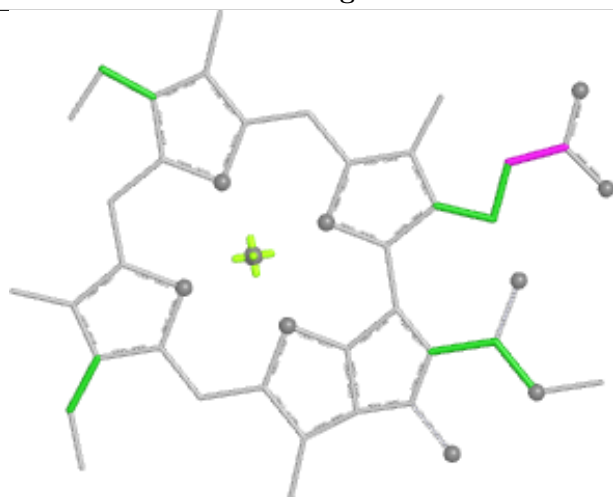
## Ligand CLA F 302



Bond lengths



Bond angles

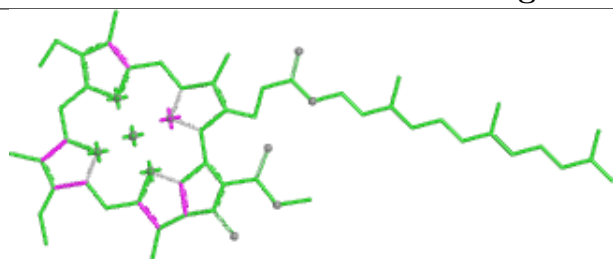


Torsions

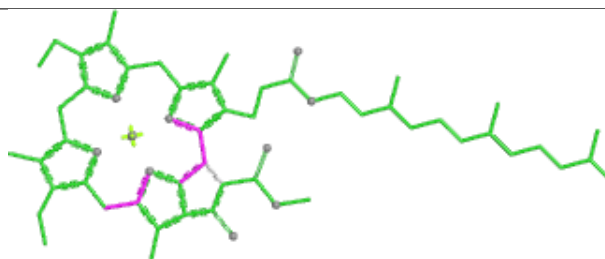


Rings

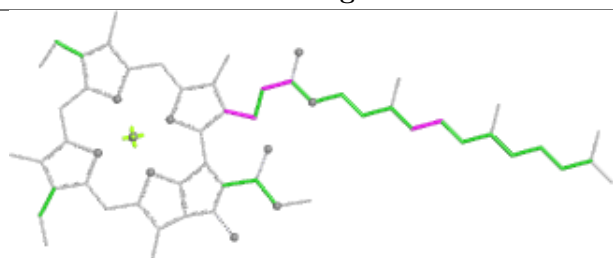
## Ligand CLA a 834



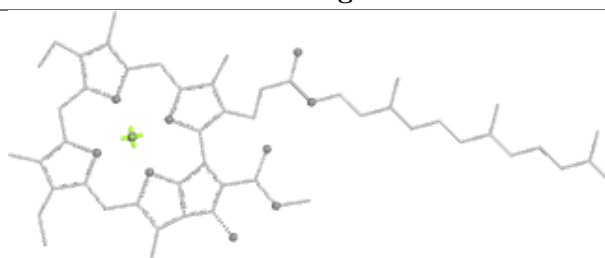
Bond lengths



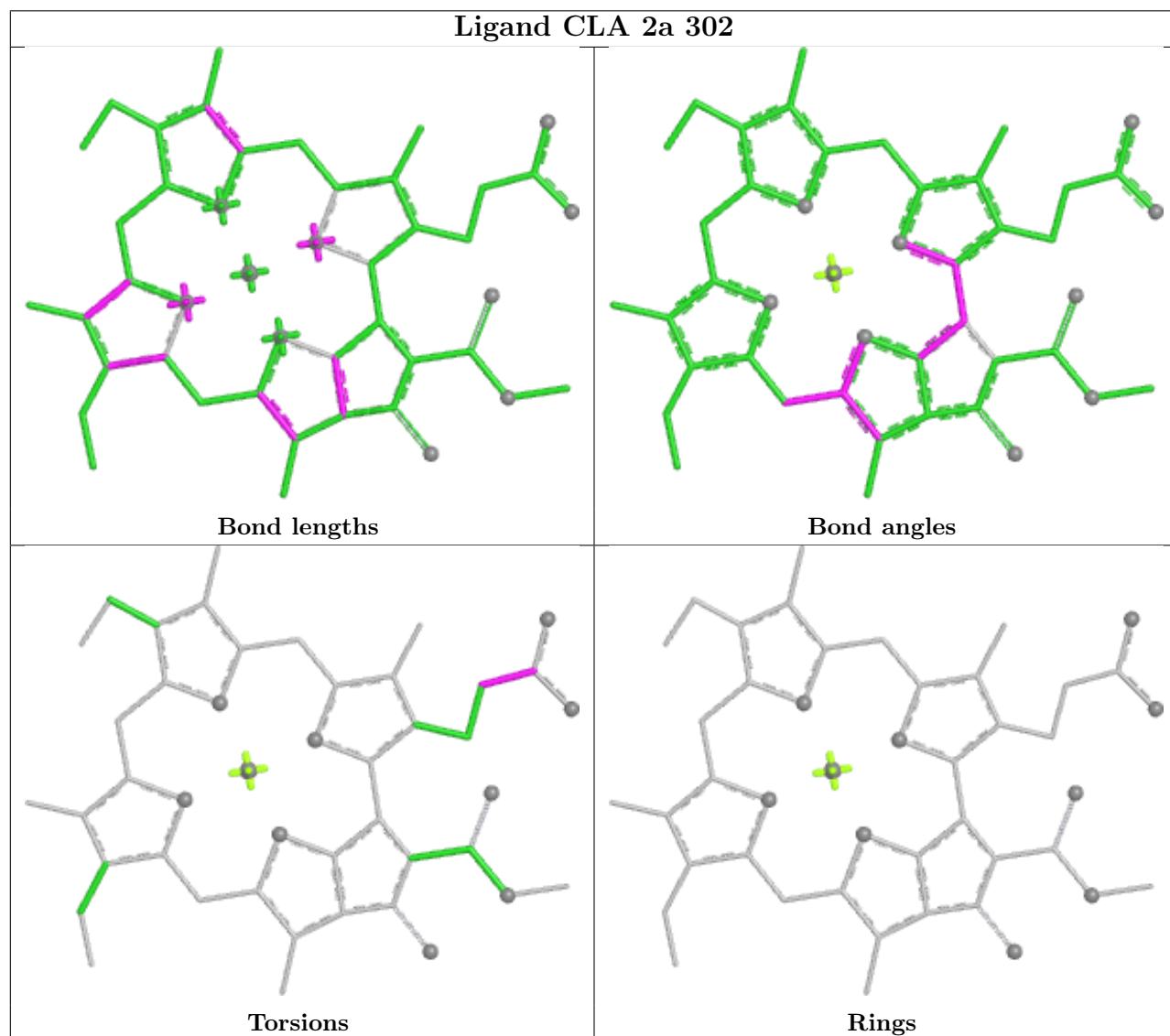
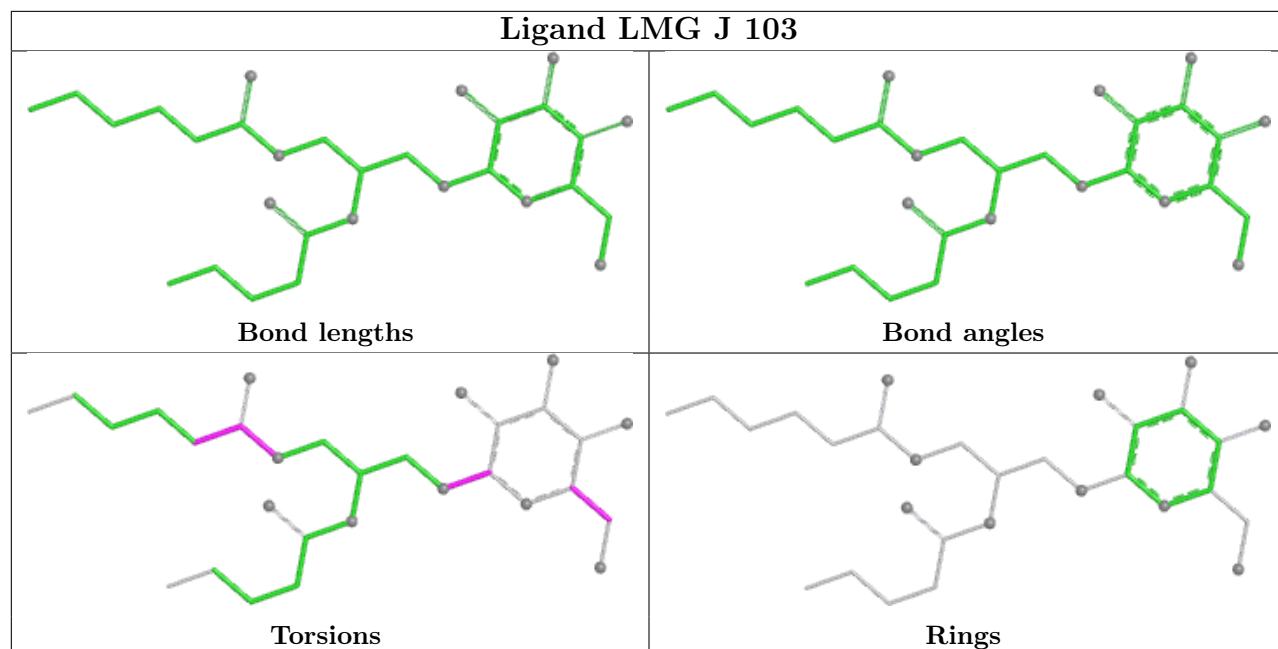
Bond angles



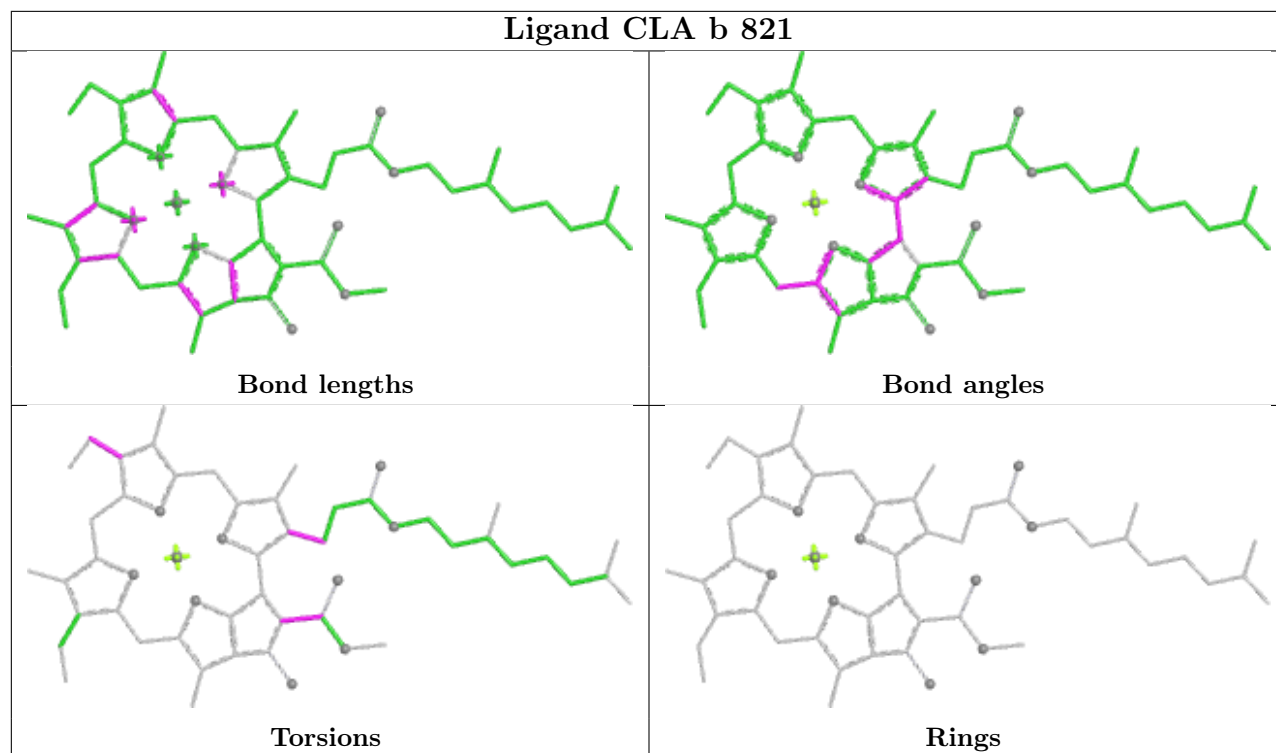
Torsions



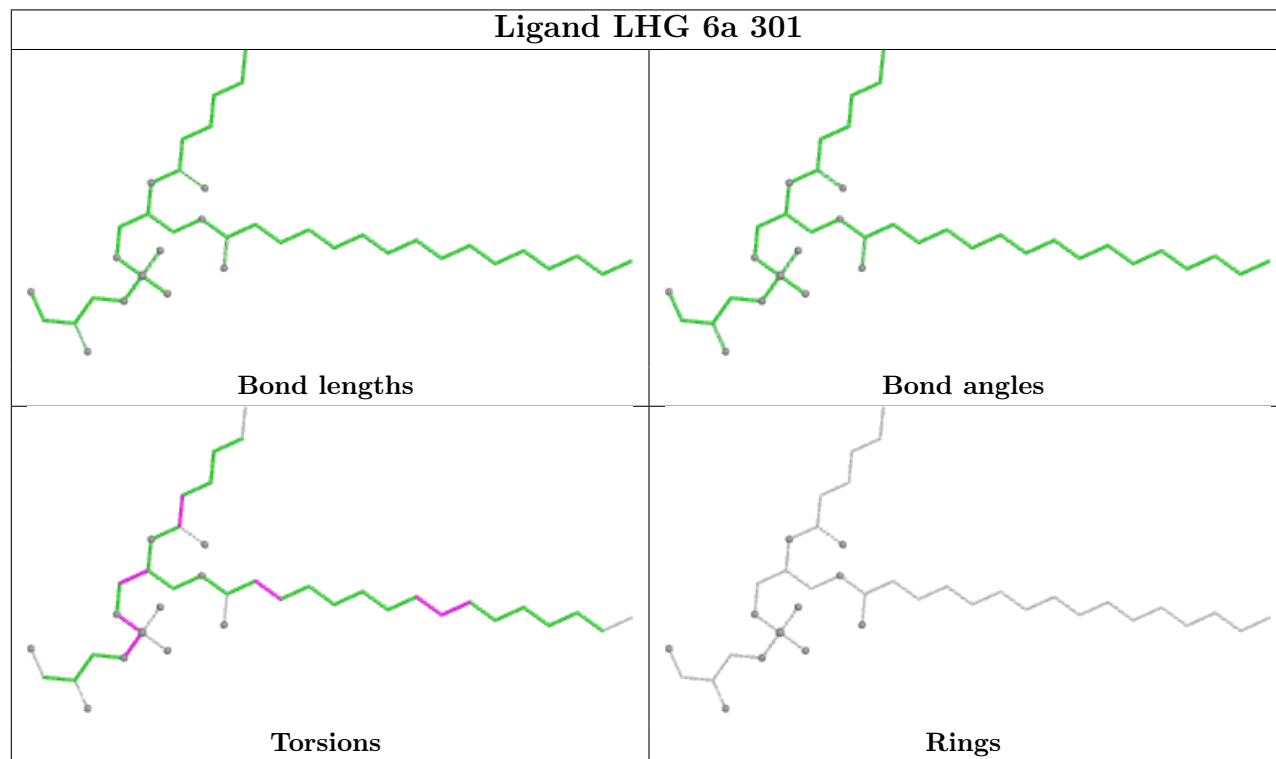
Rings

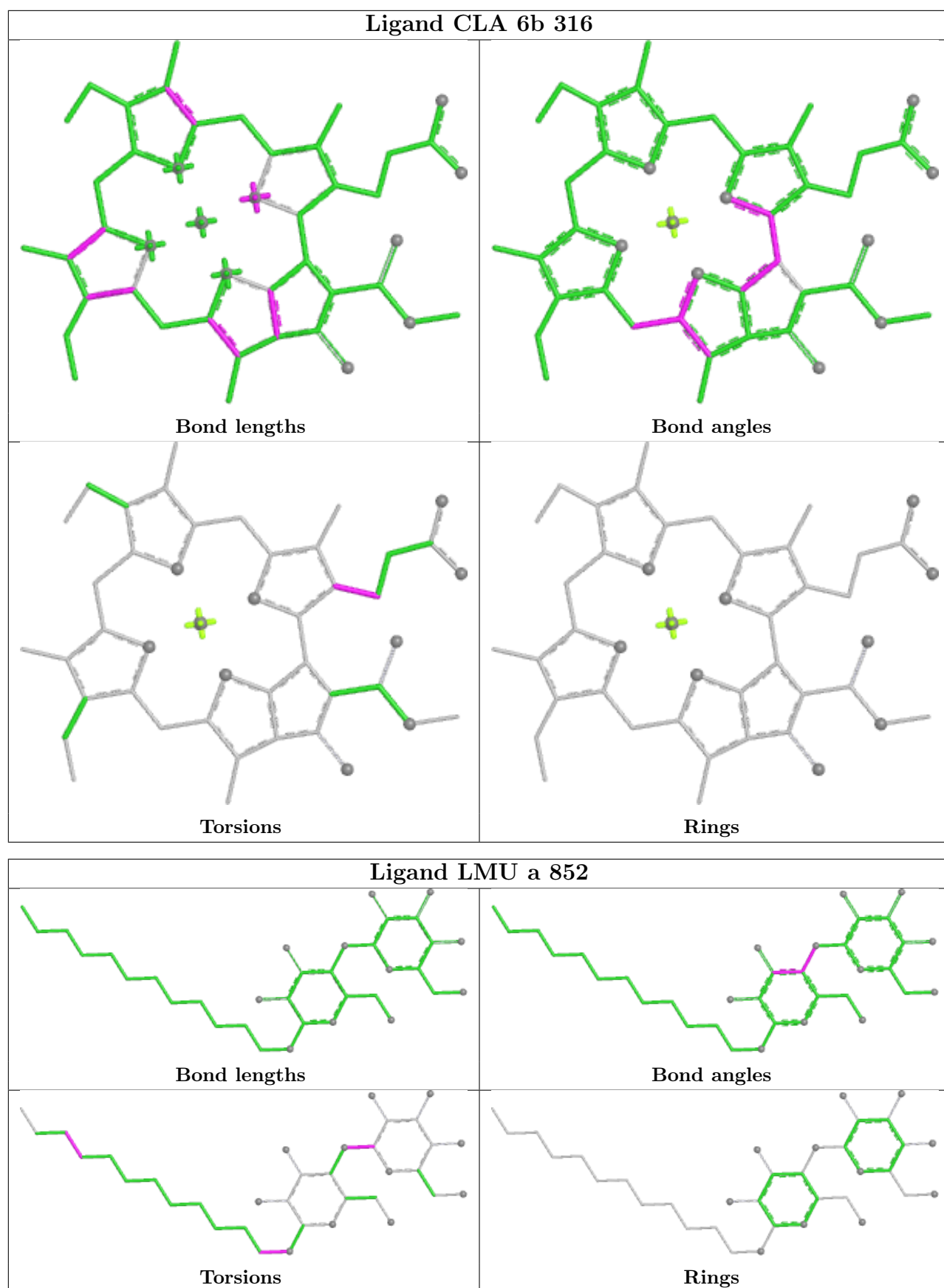


## Ligand CLA b 821

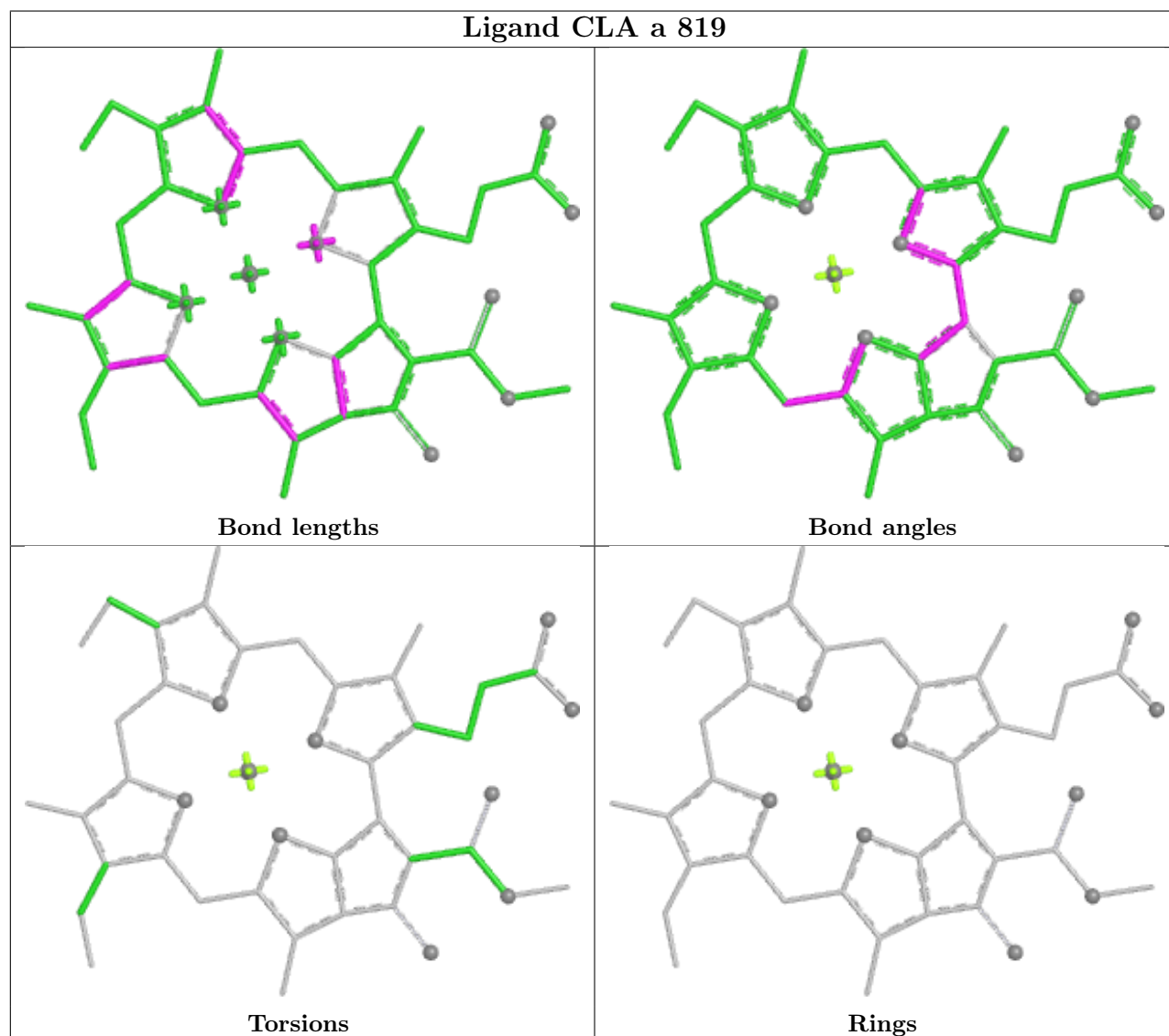
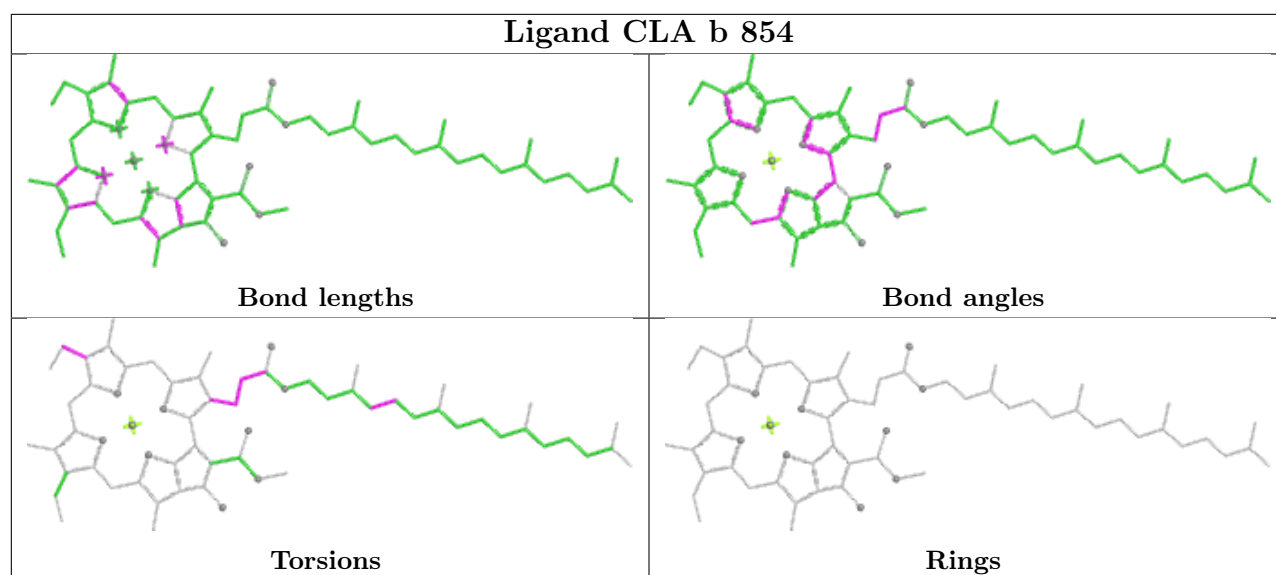


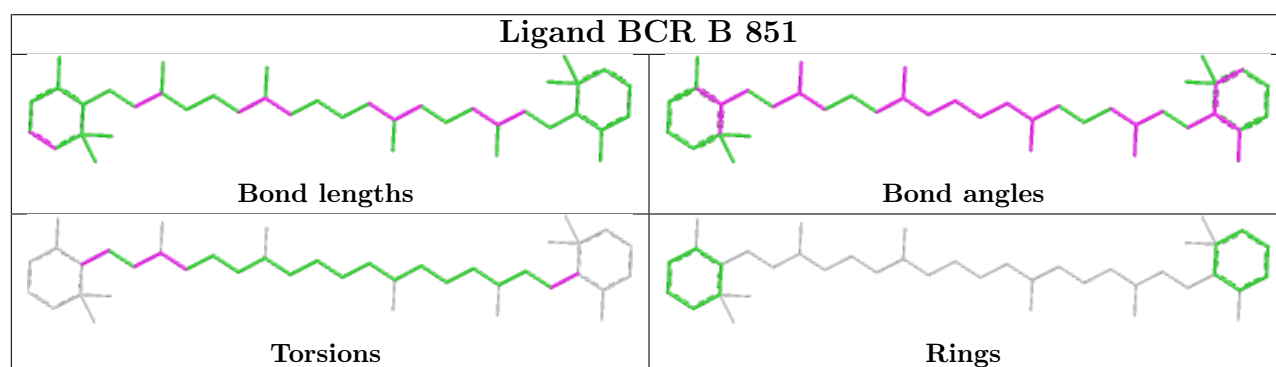
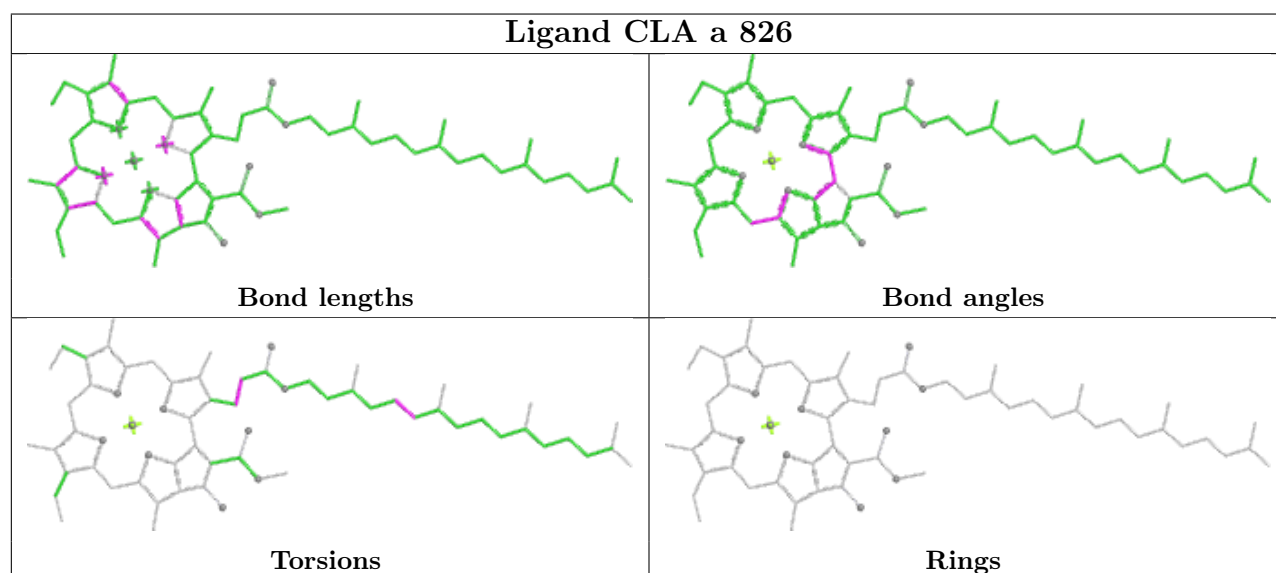
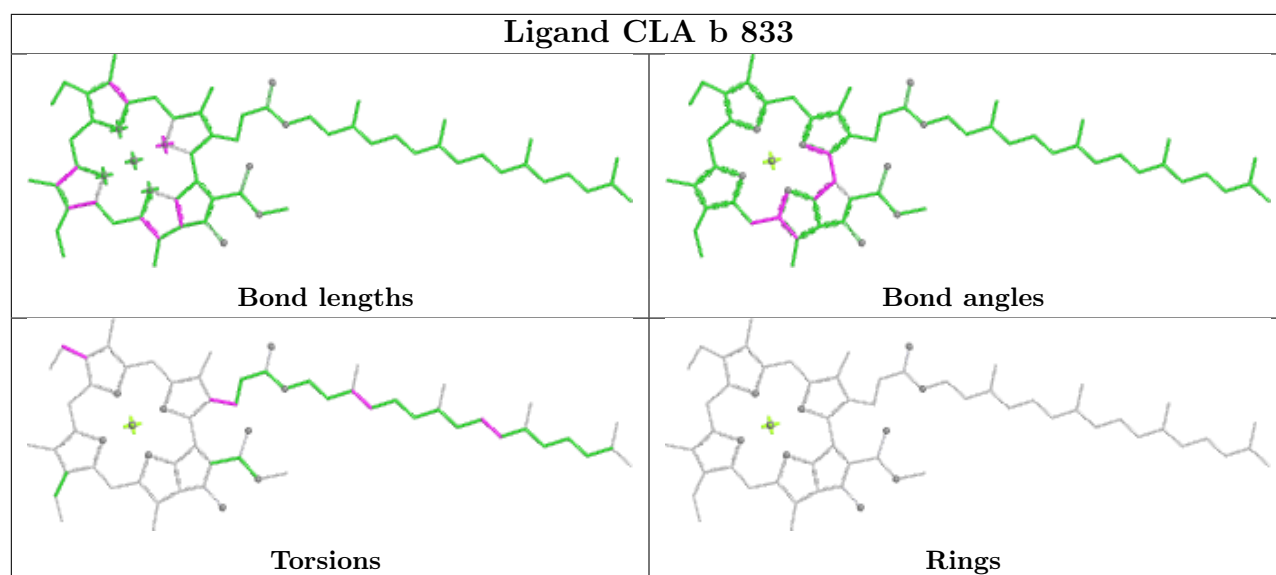
## Ligand LHG 6a 301

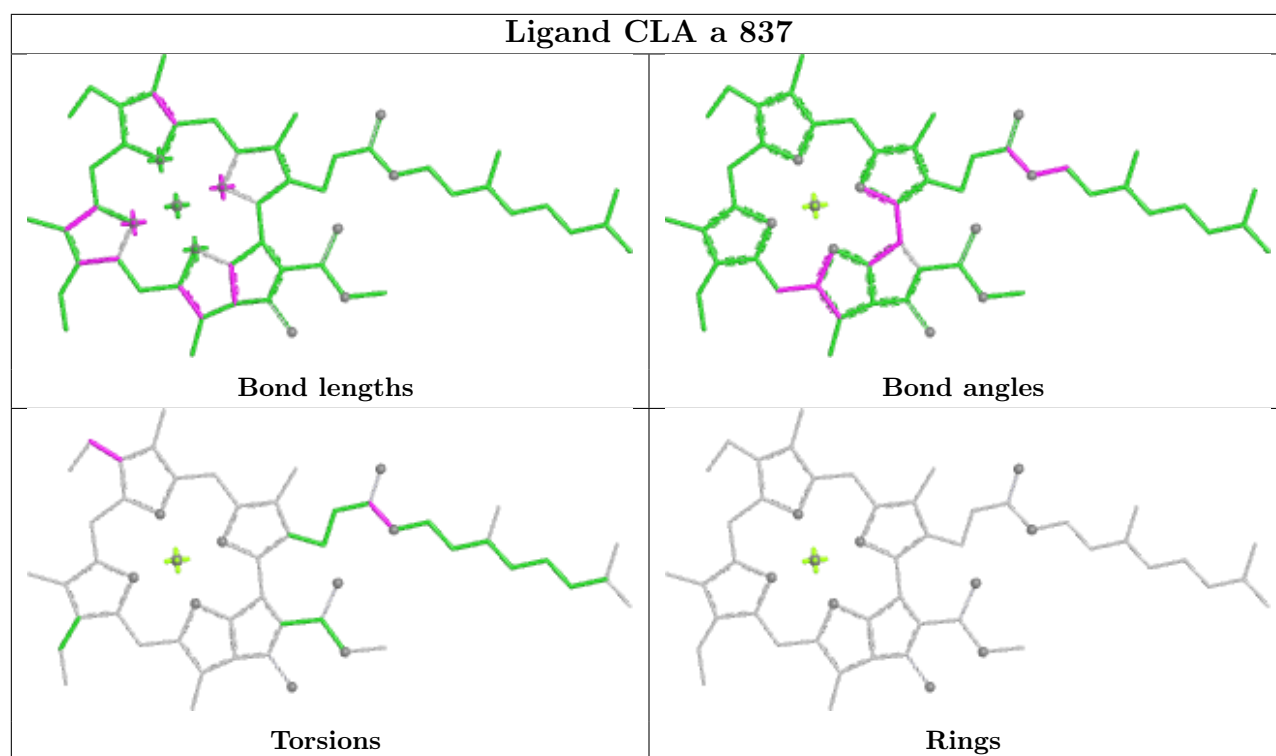


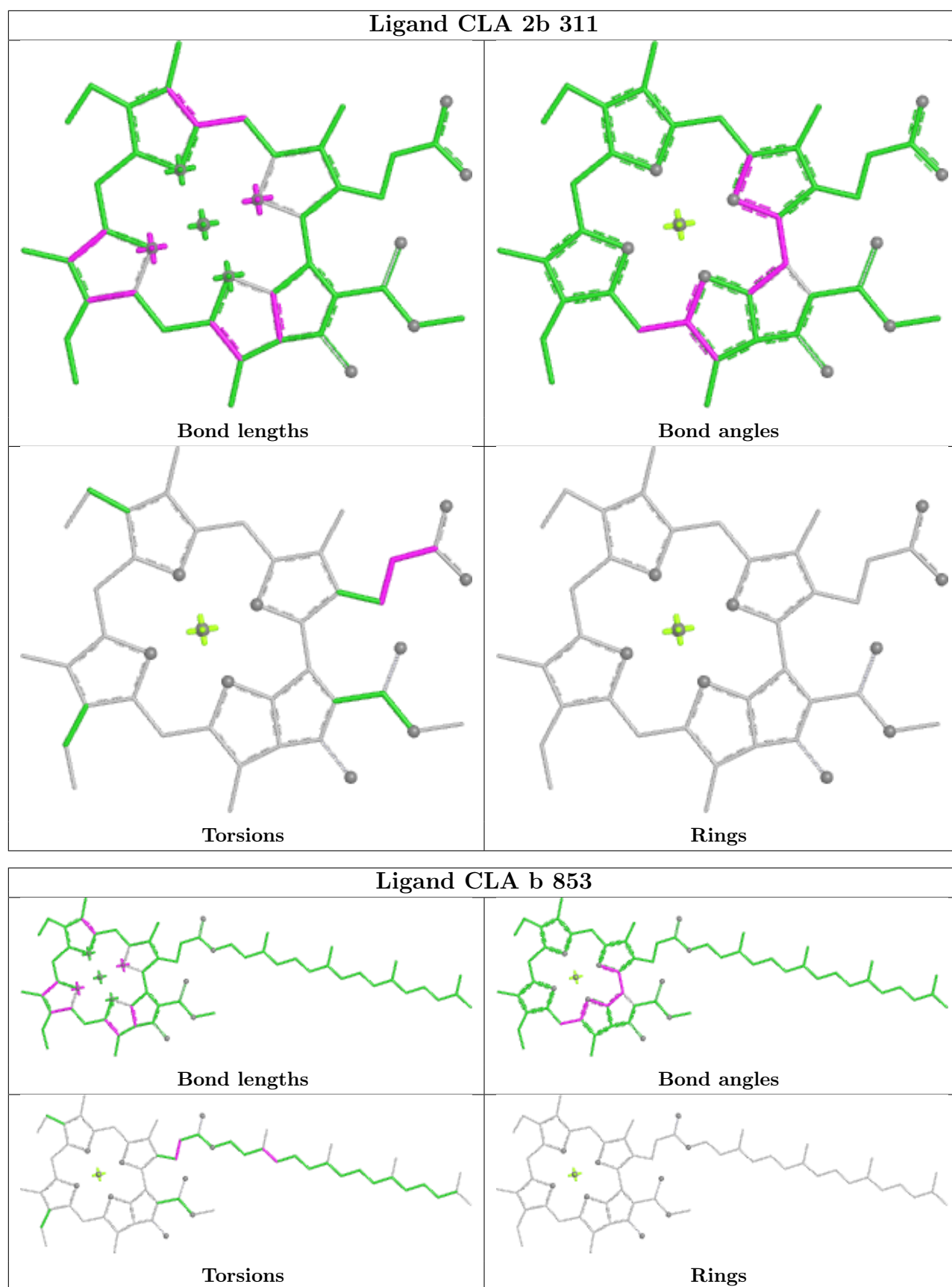


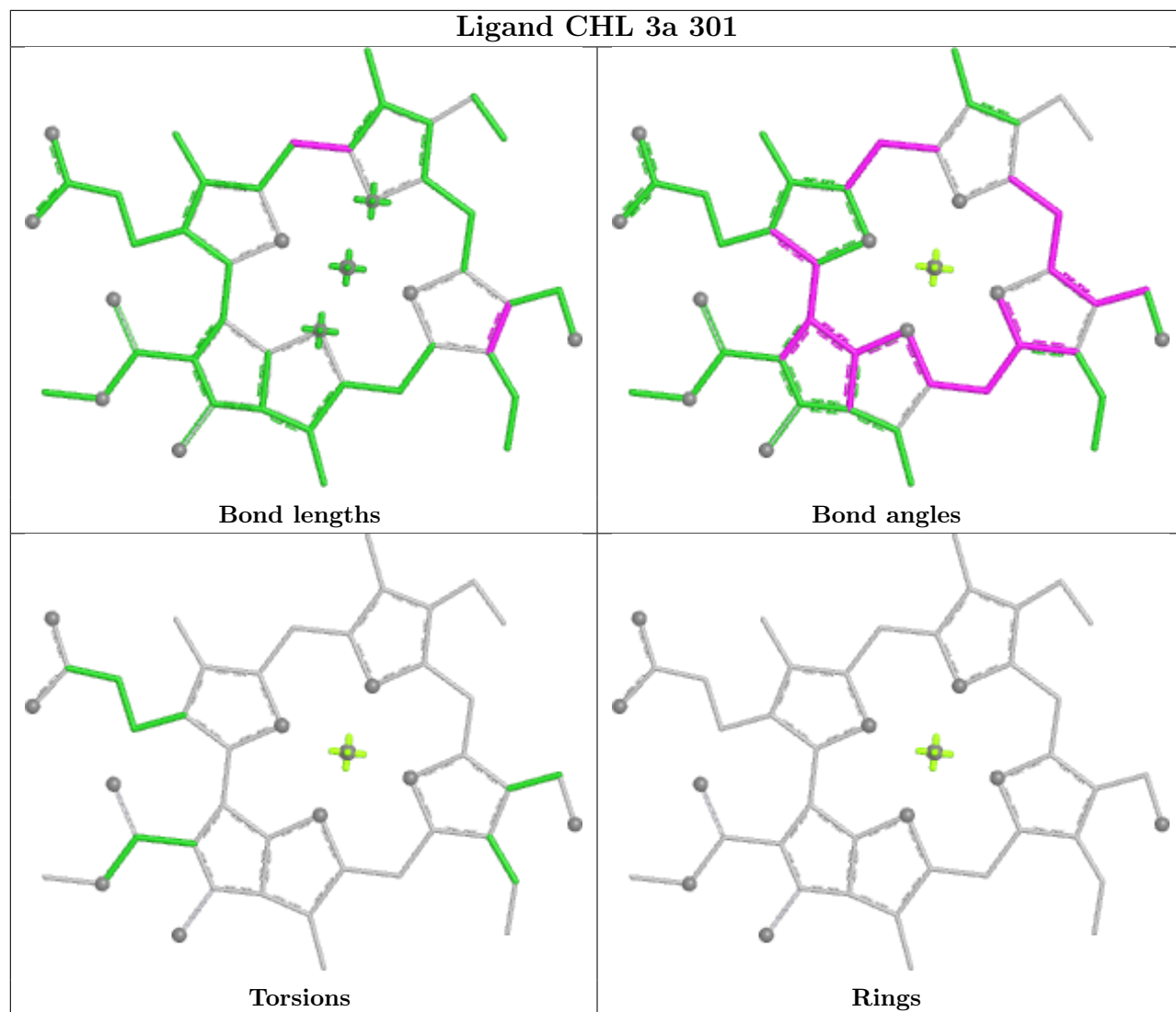


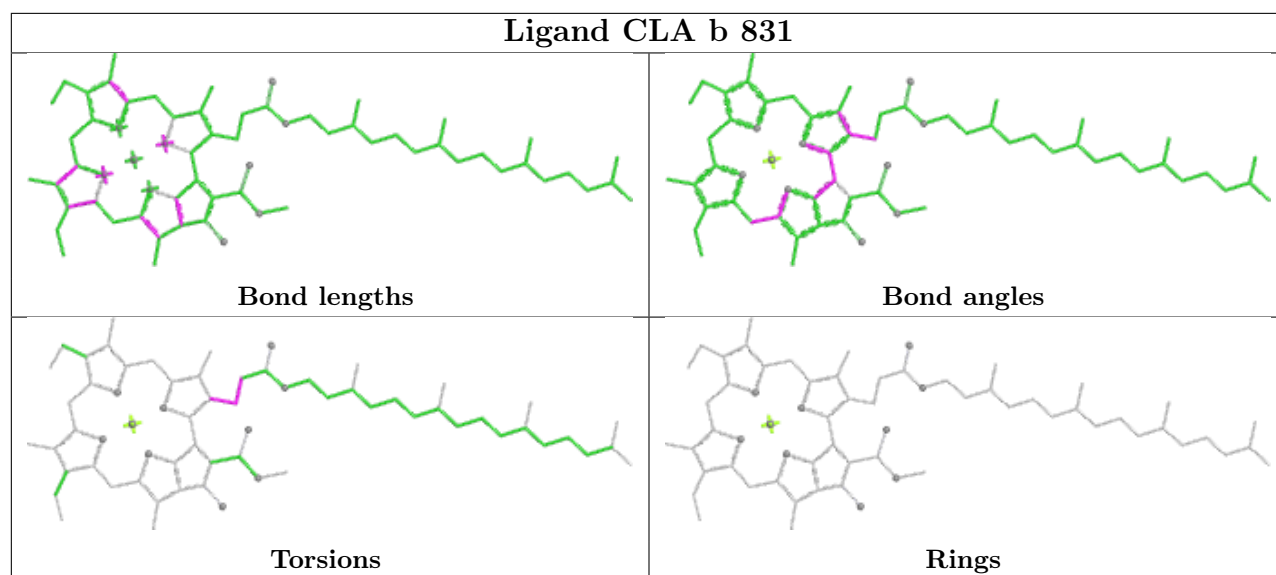
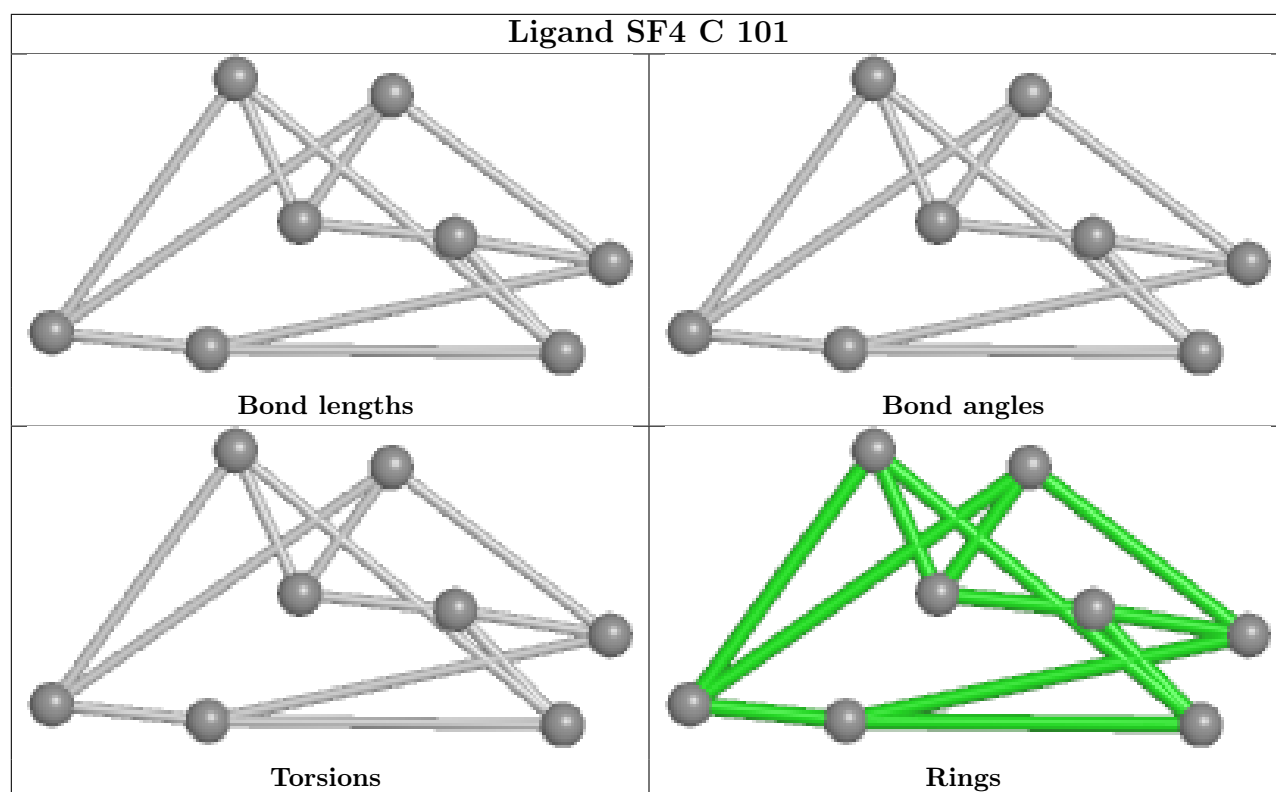


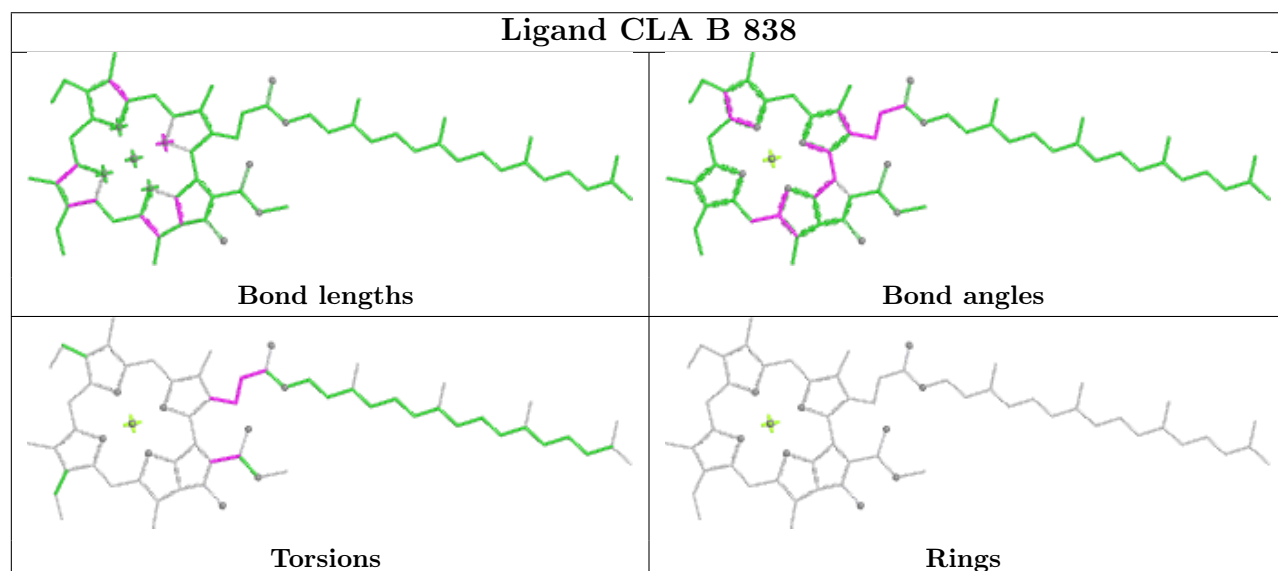
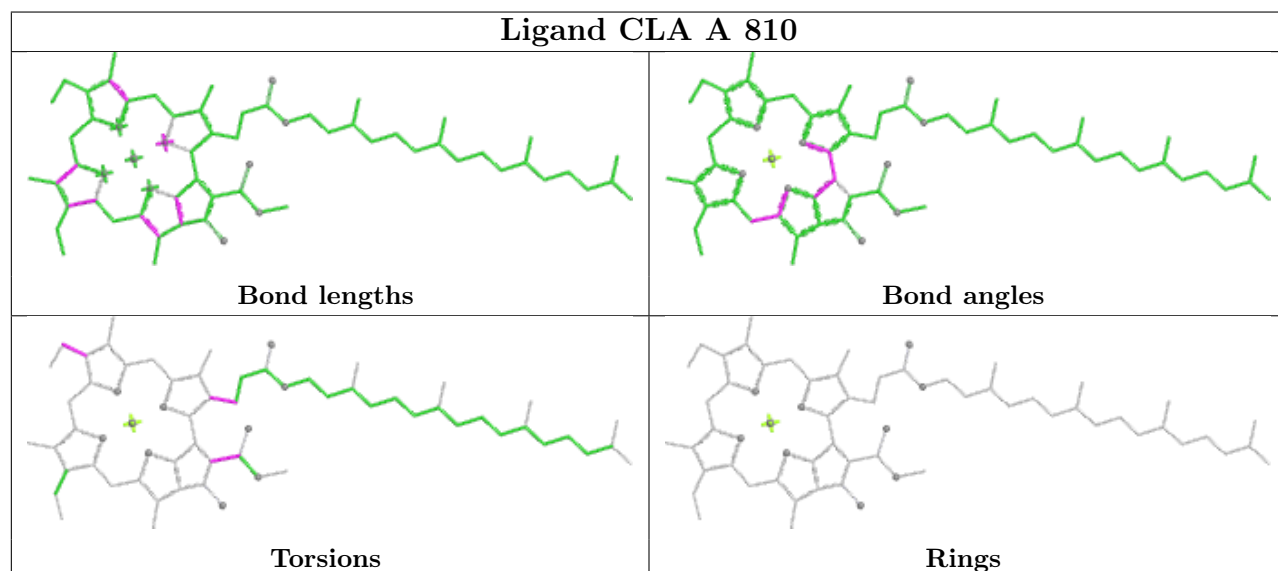
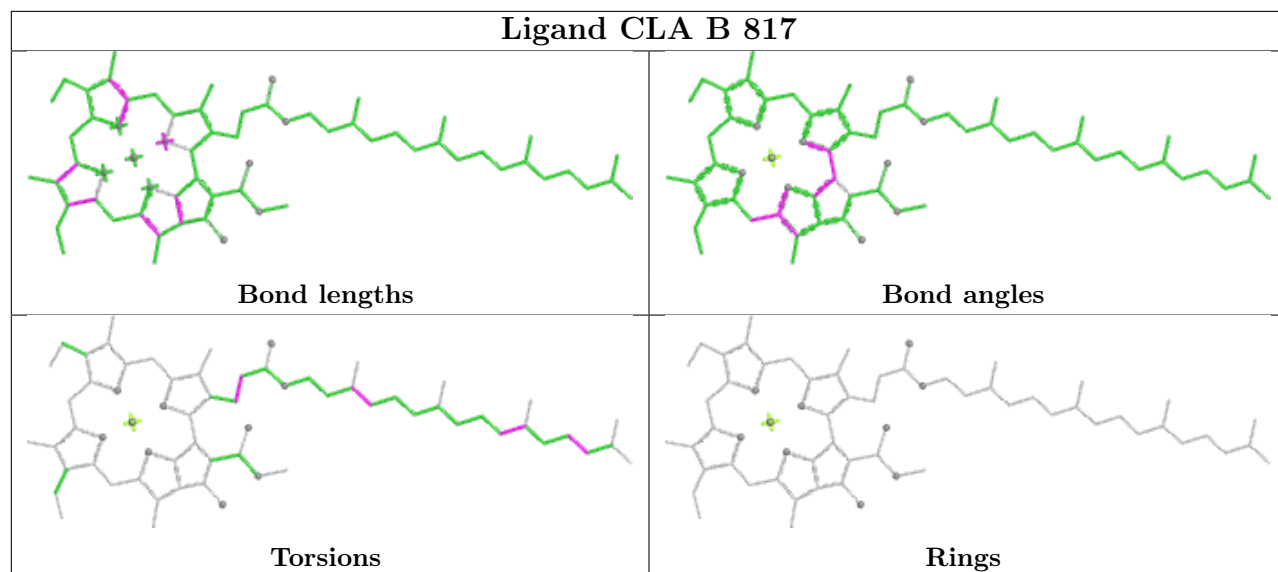


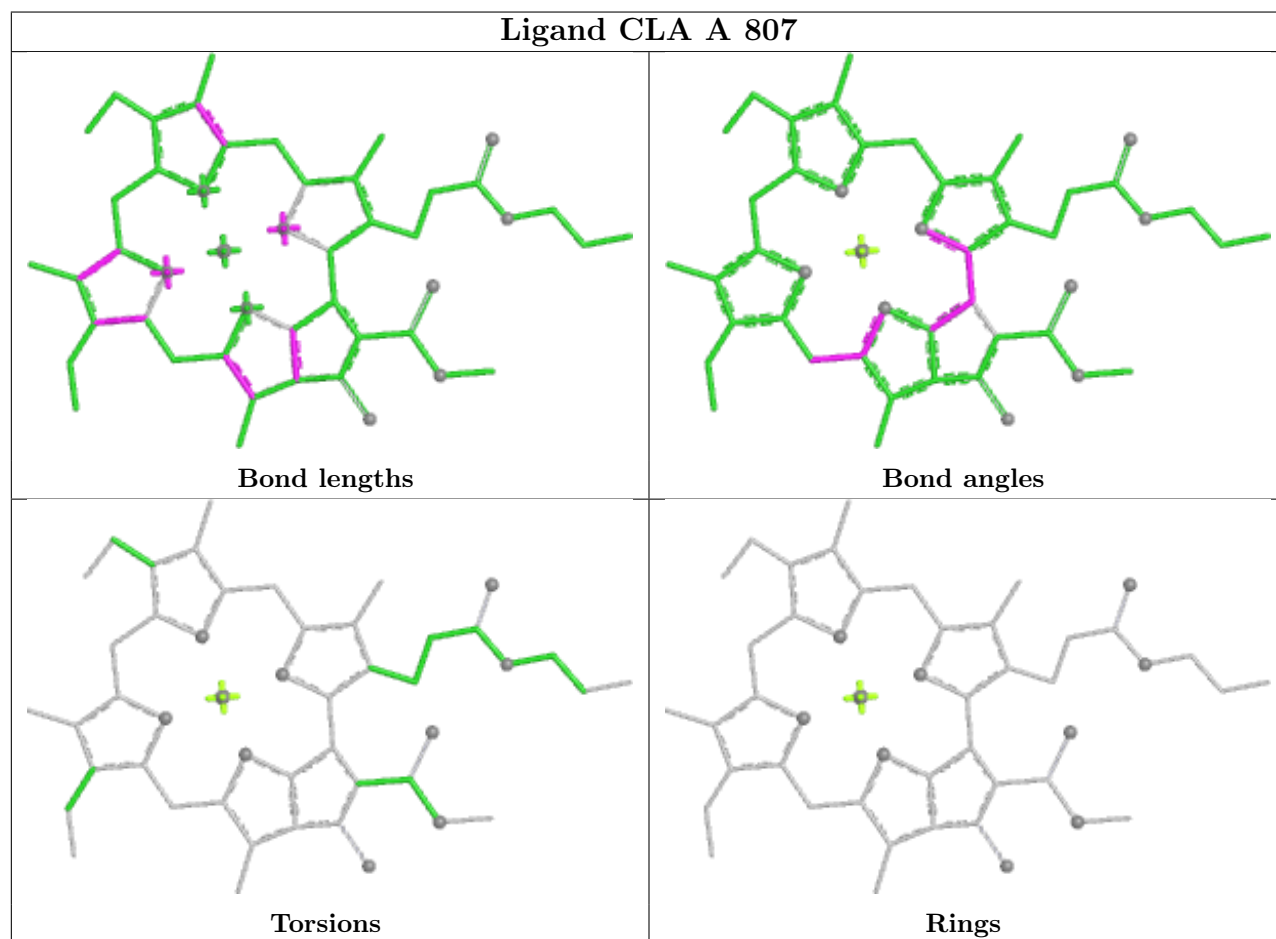
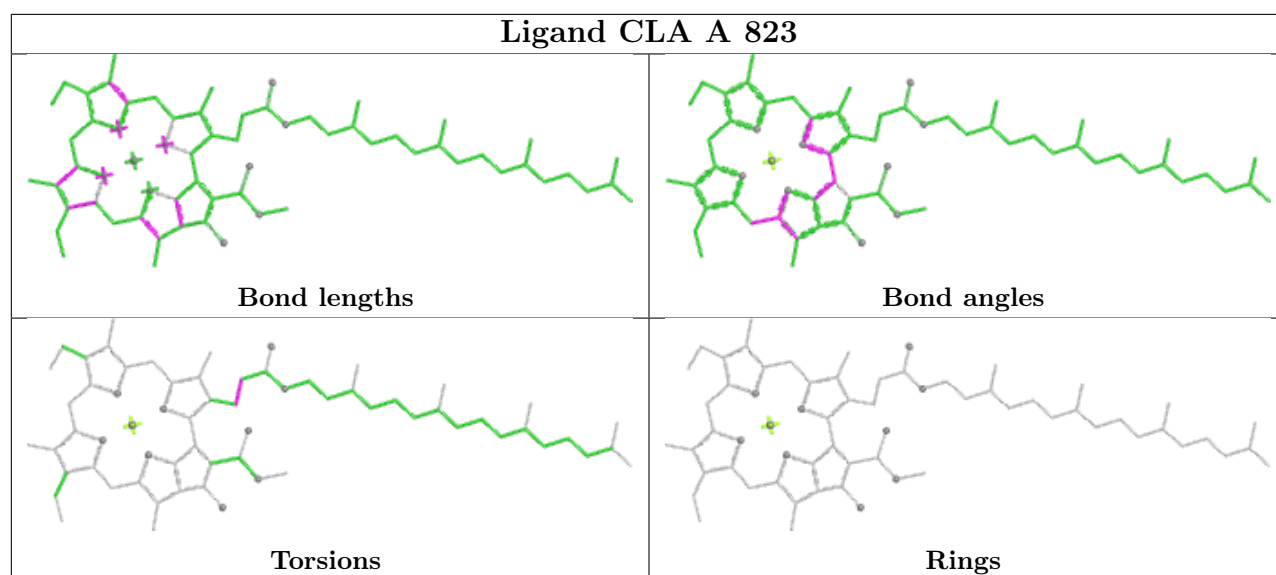




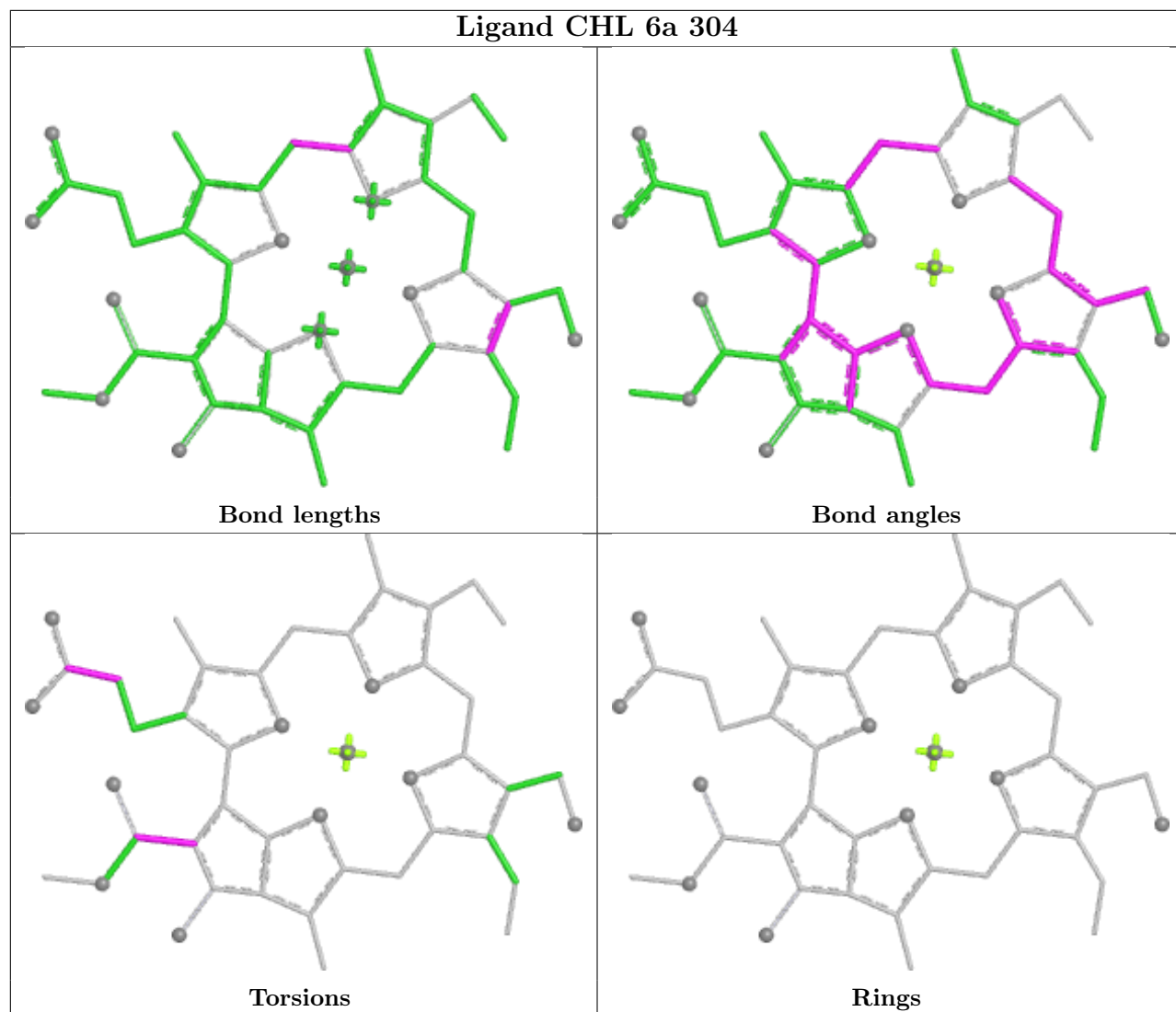




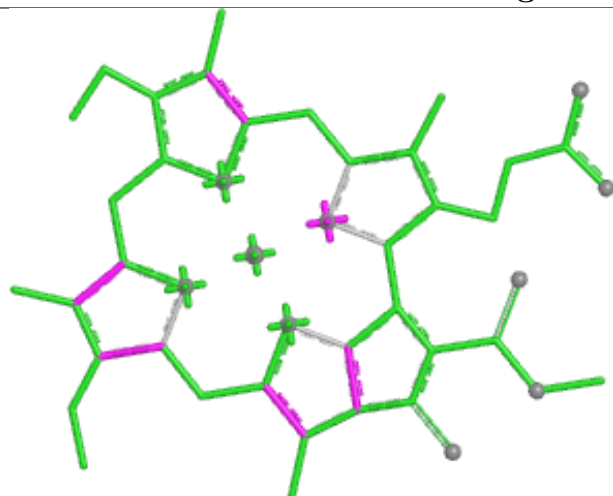




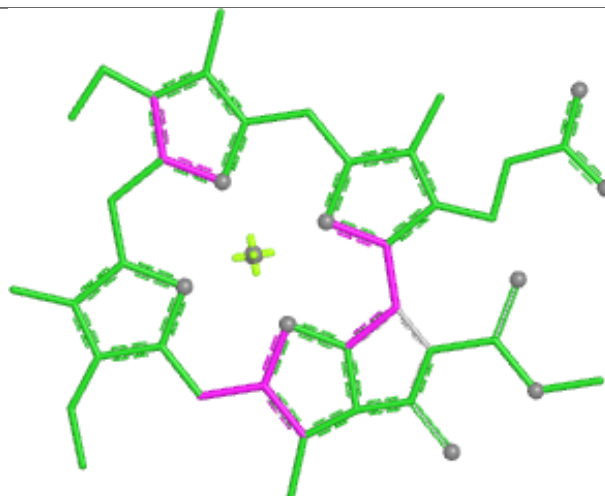




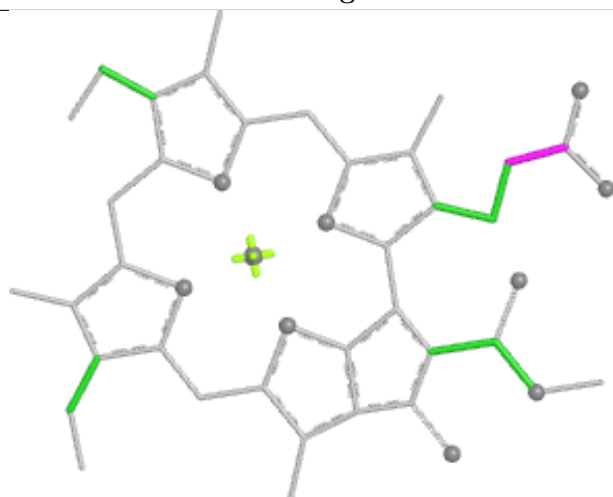
## Ligand CLA b 829



Bond lengths



Bond angles

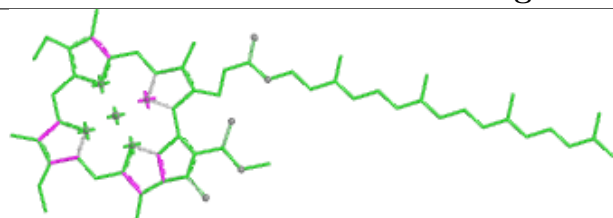


Torsions

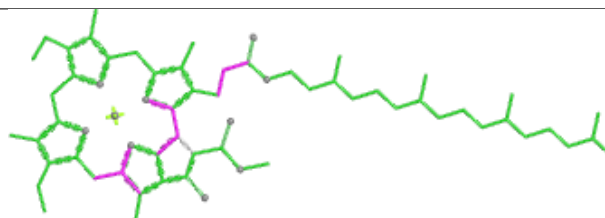


Rings

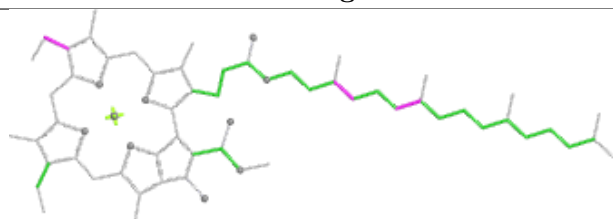
## Ligand CLA B 836



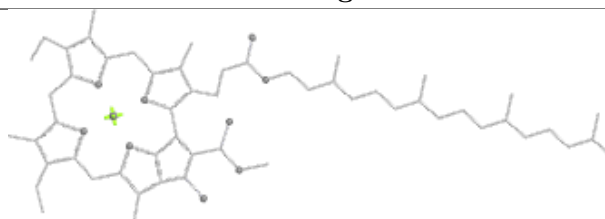
Bond lengths



Bond angles

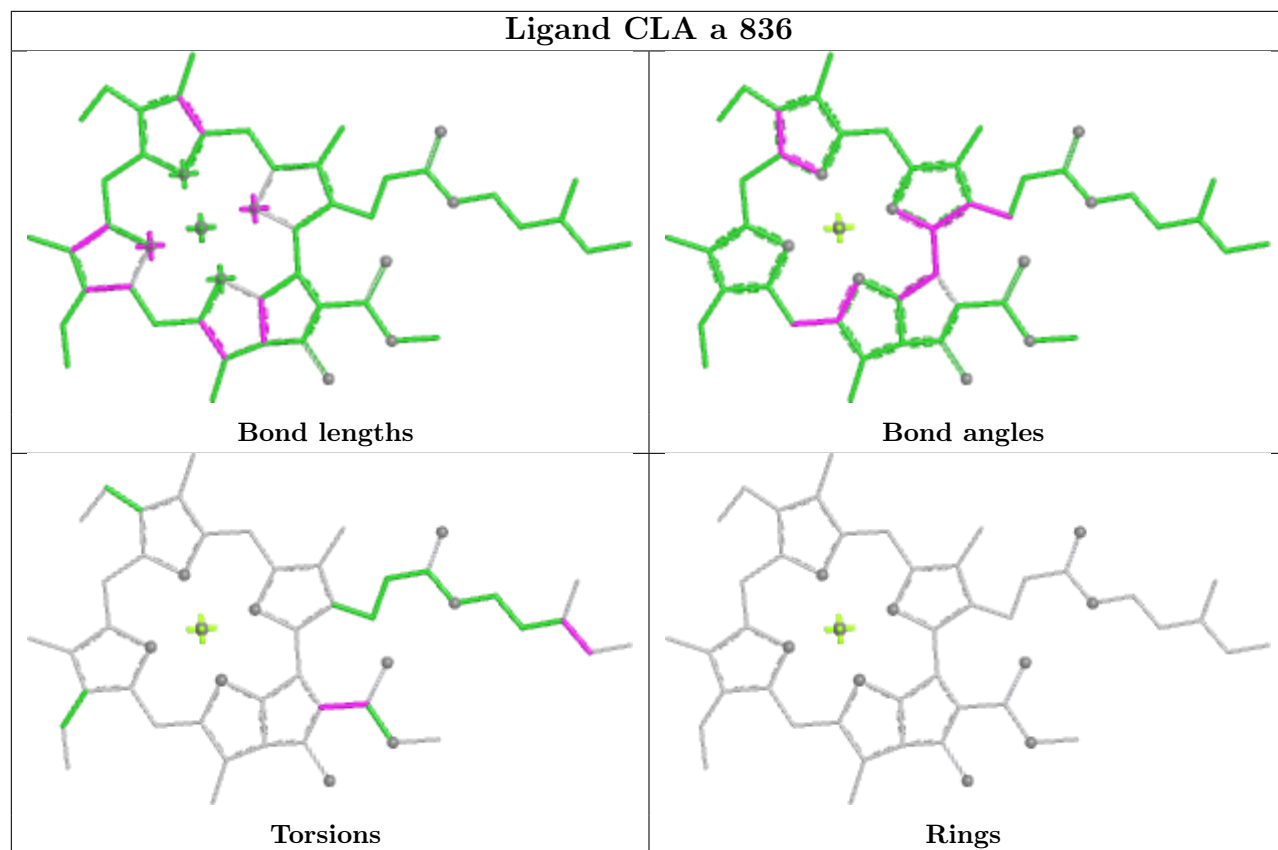


Torsions

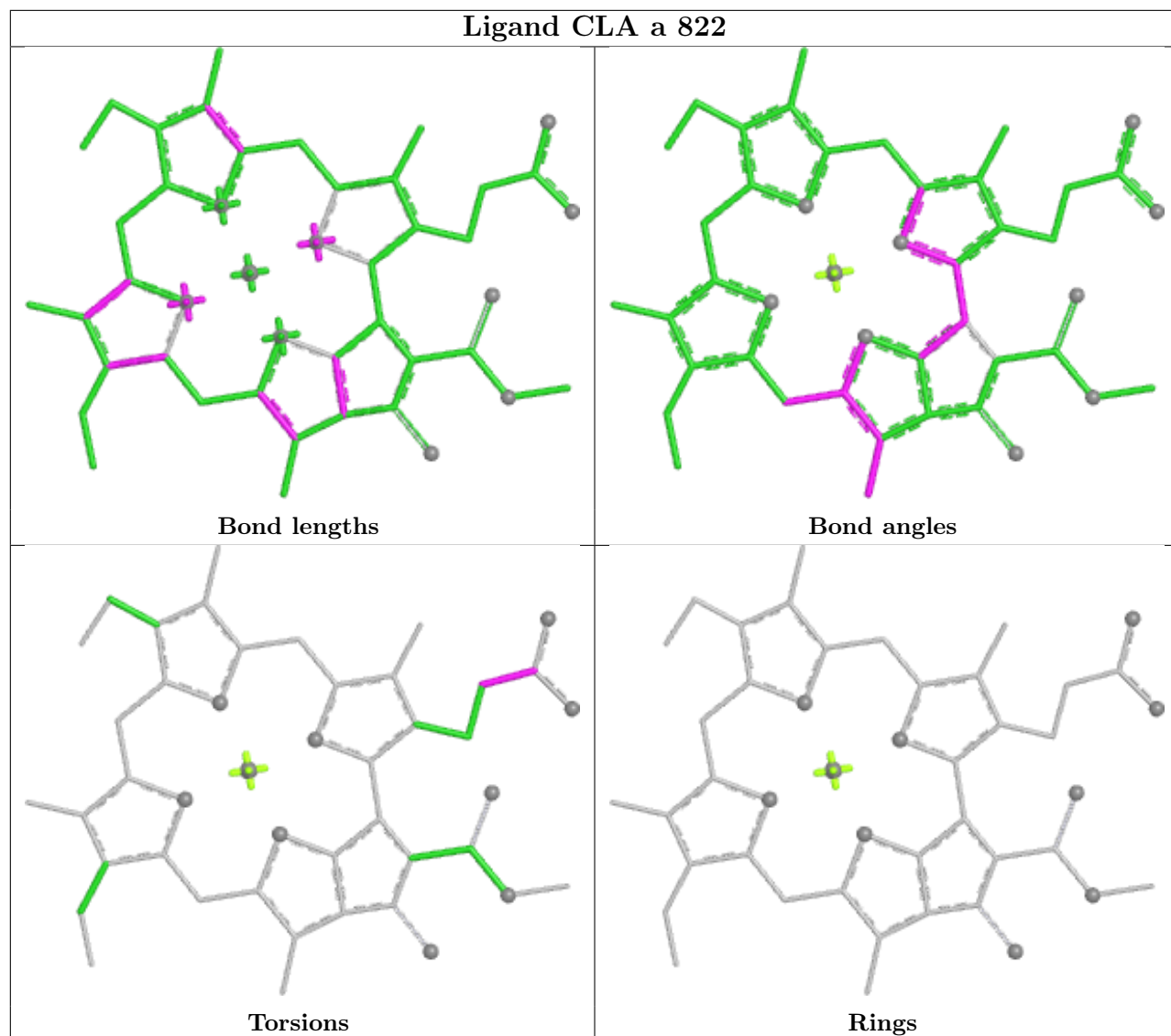


Rings

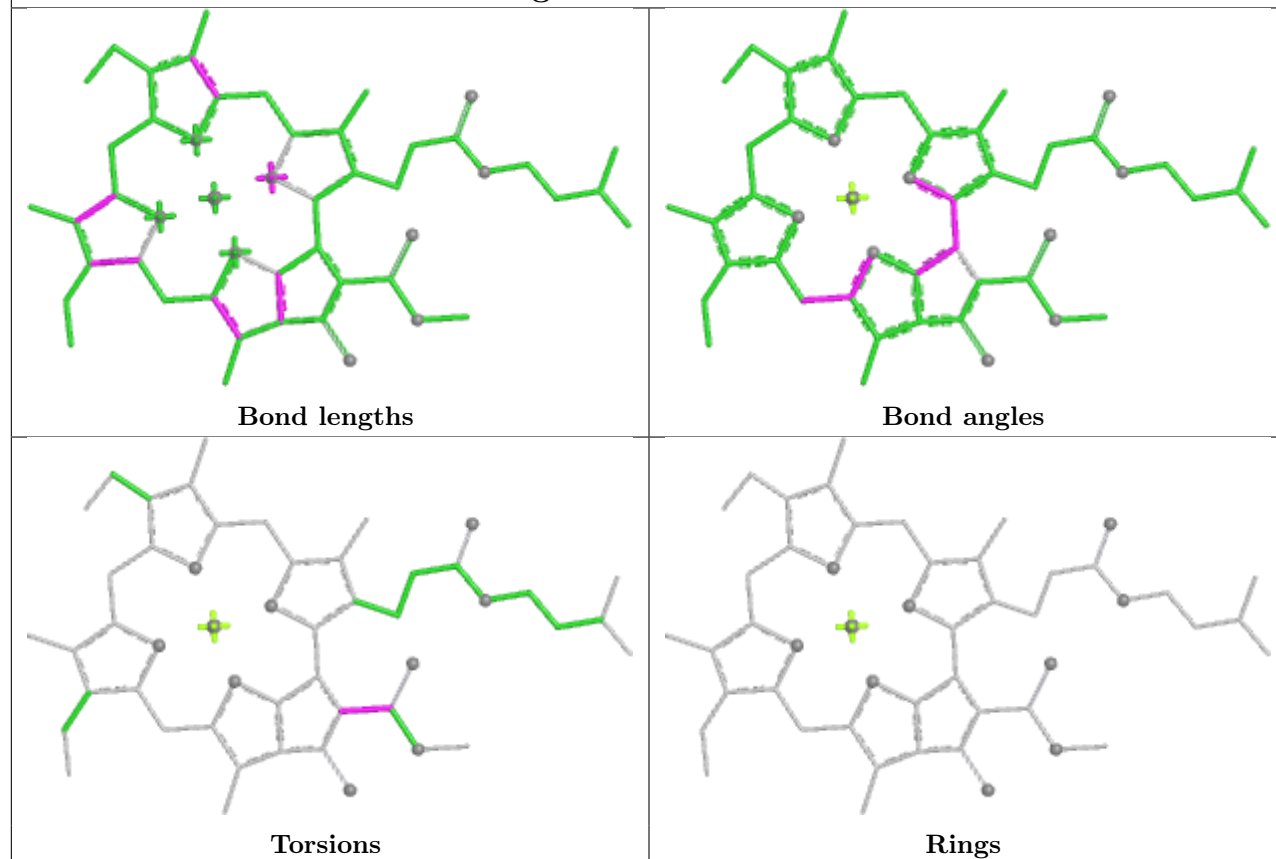
## Ligand CLA a 836



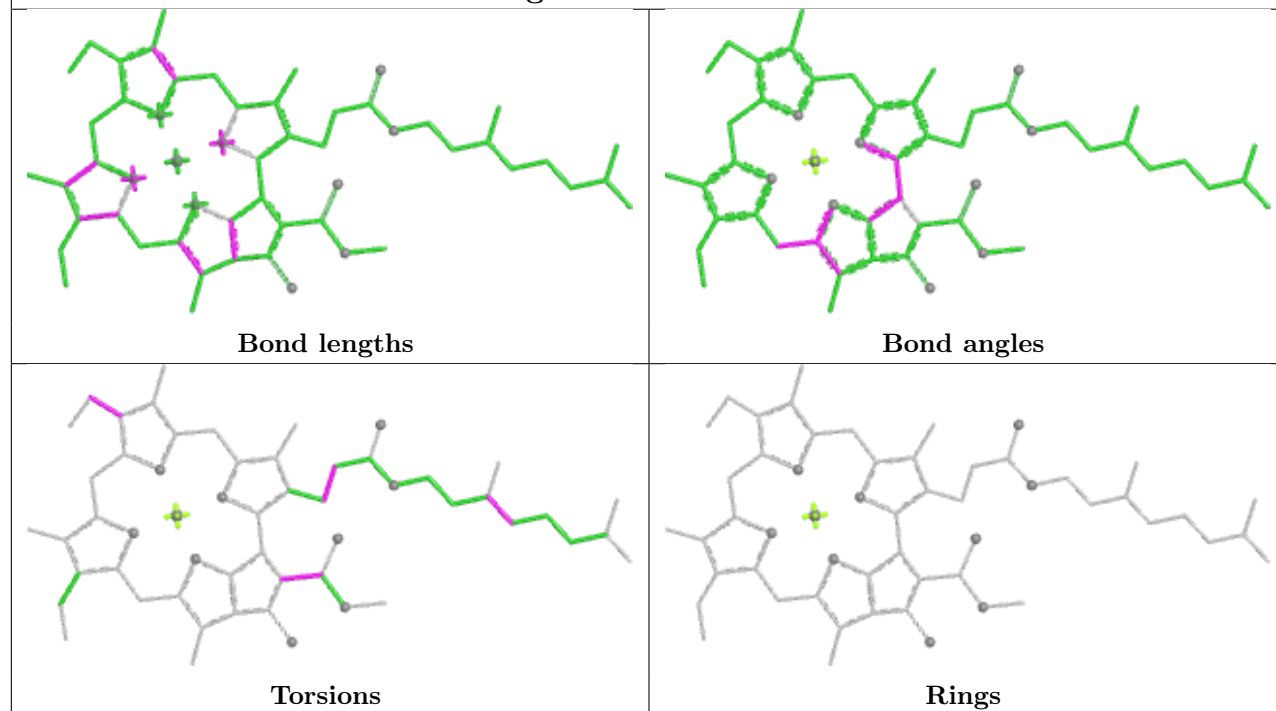
## Ligand CLA a 822

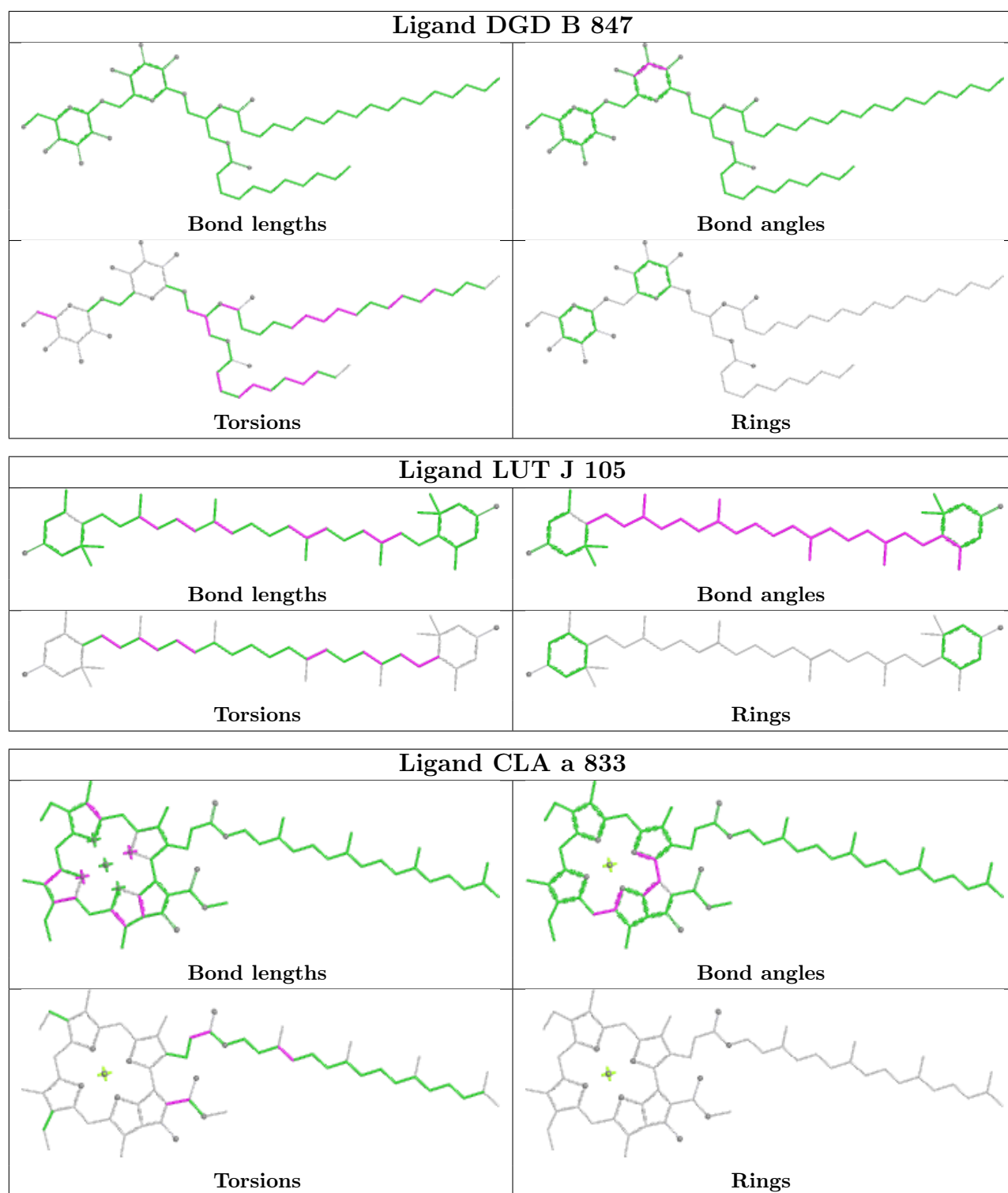


## Ligand CLA B 814

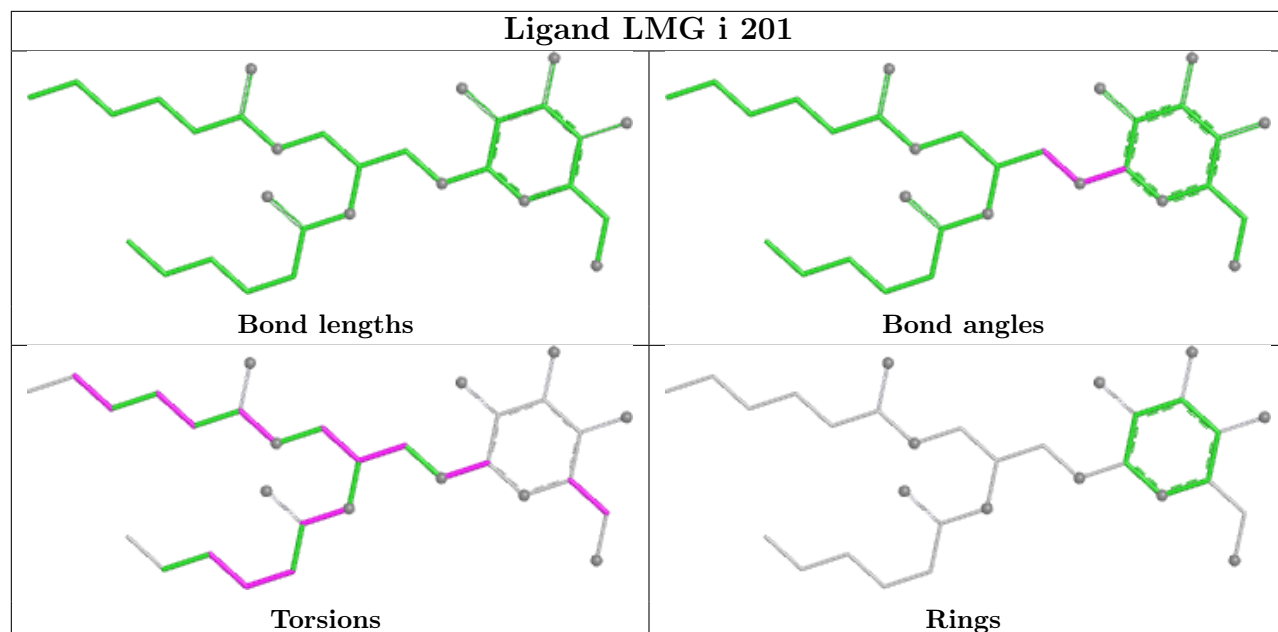


## Ligand CLA 2b 301

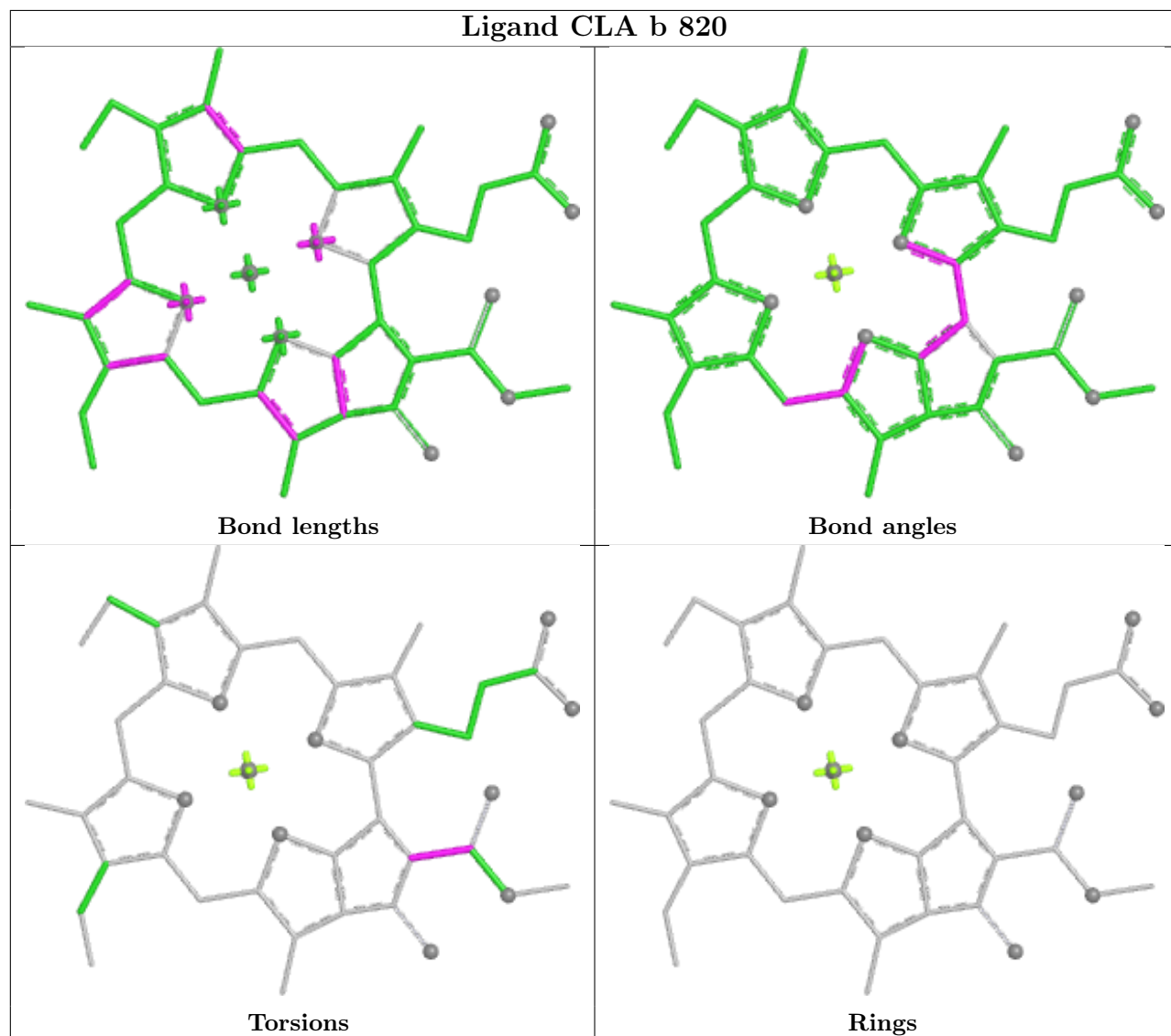


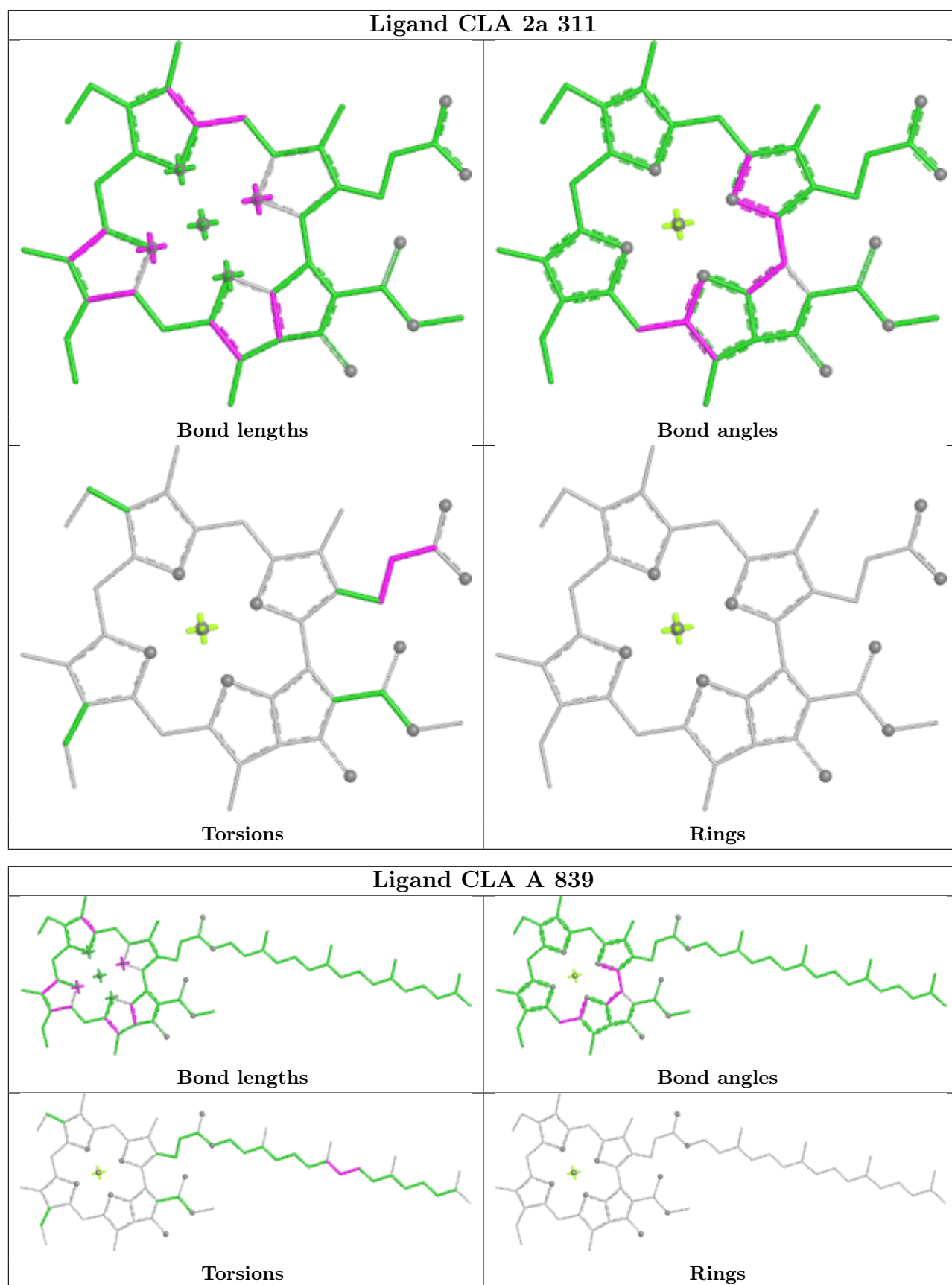


## Ligand LMG i 201



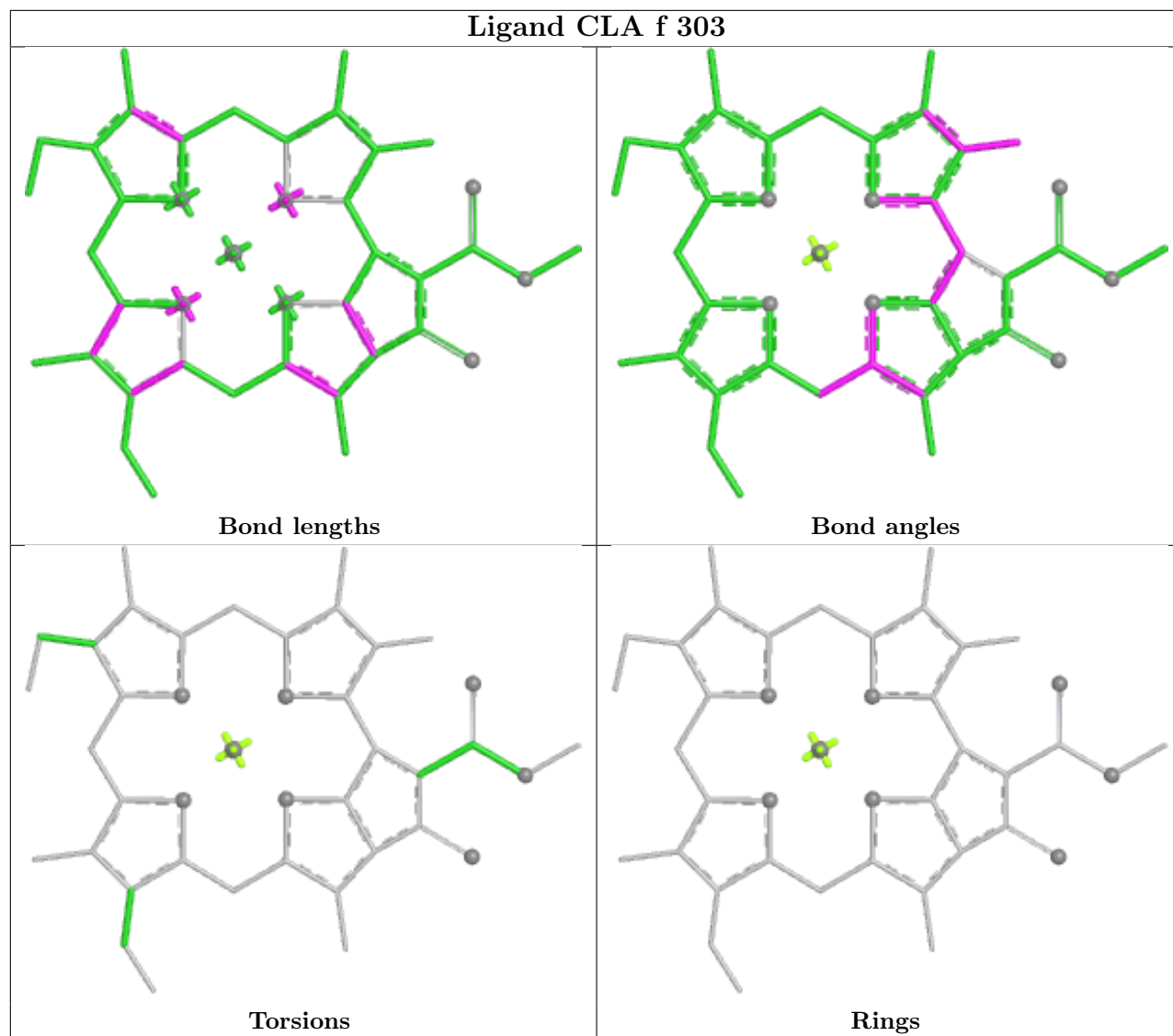
## Ligand CLA b 820



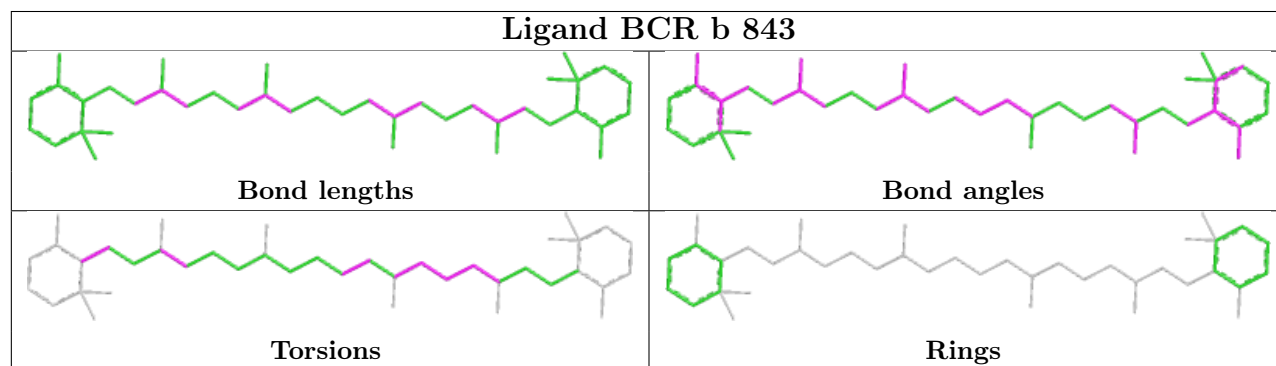


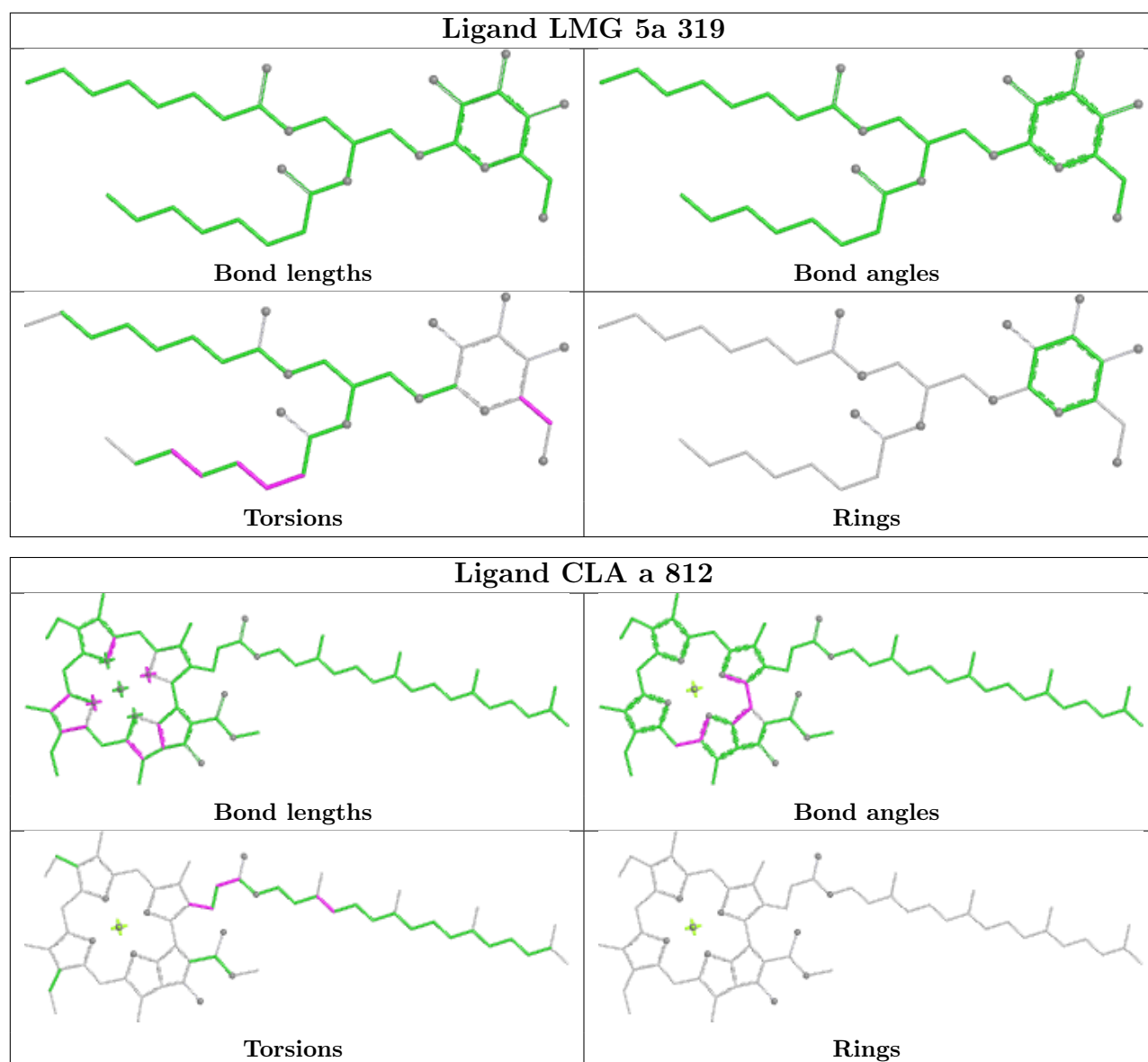


## Ligand CLA f 303

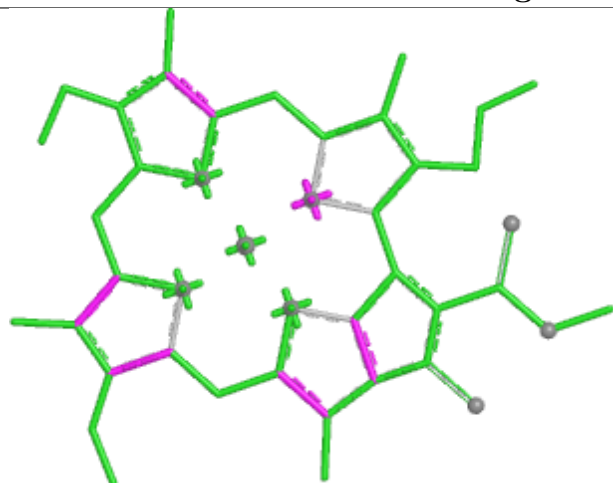


## Ligand BCR b 843

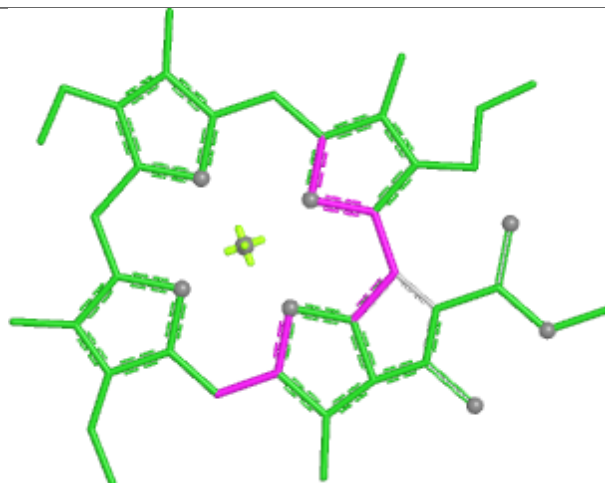




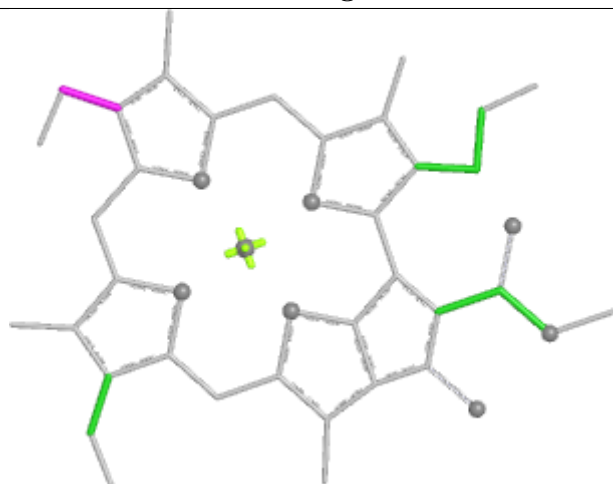
## Ligand CLA B 819



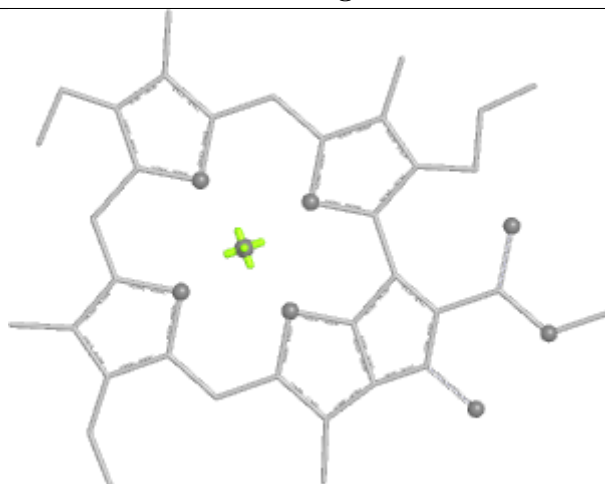
Bond lengths



Bond angles

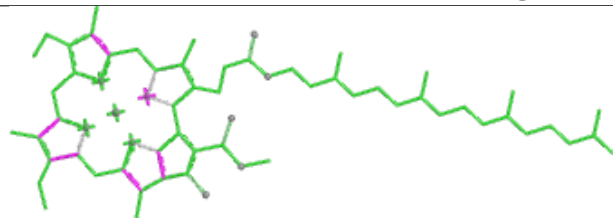


Torsions

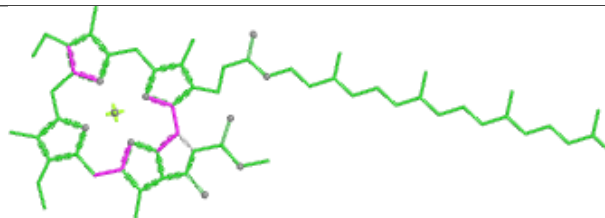


Rings

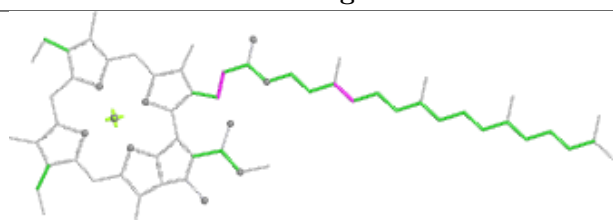
## Ligand CLA A 820



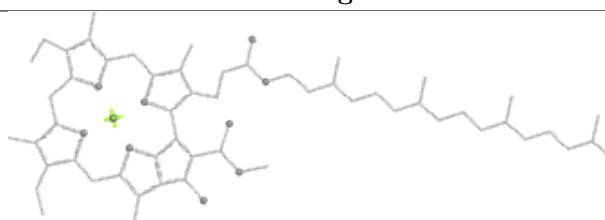
Bond lengths



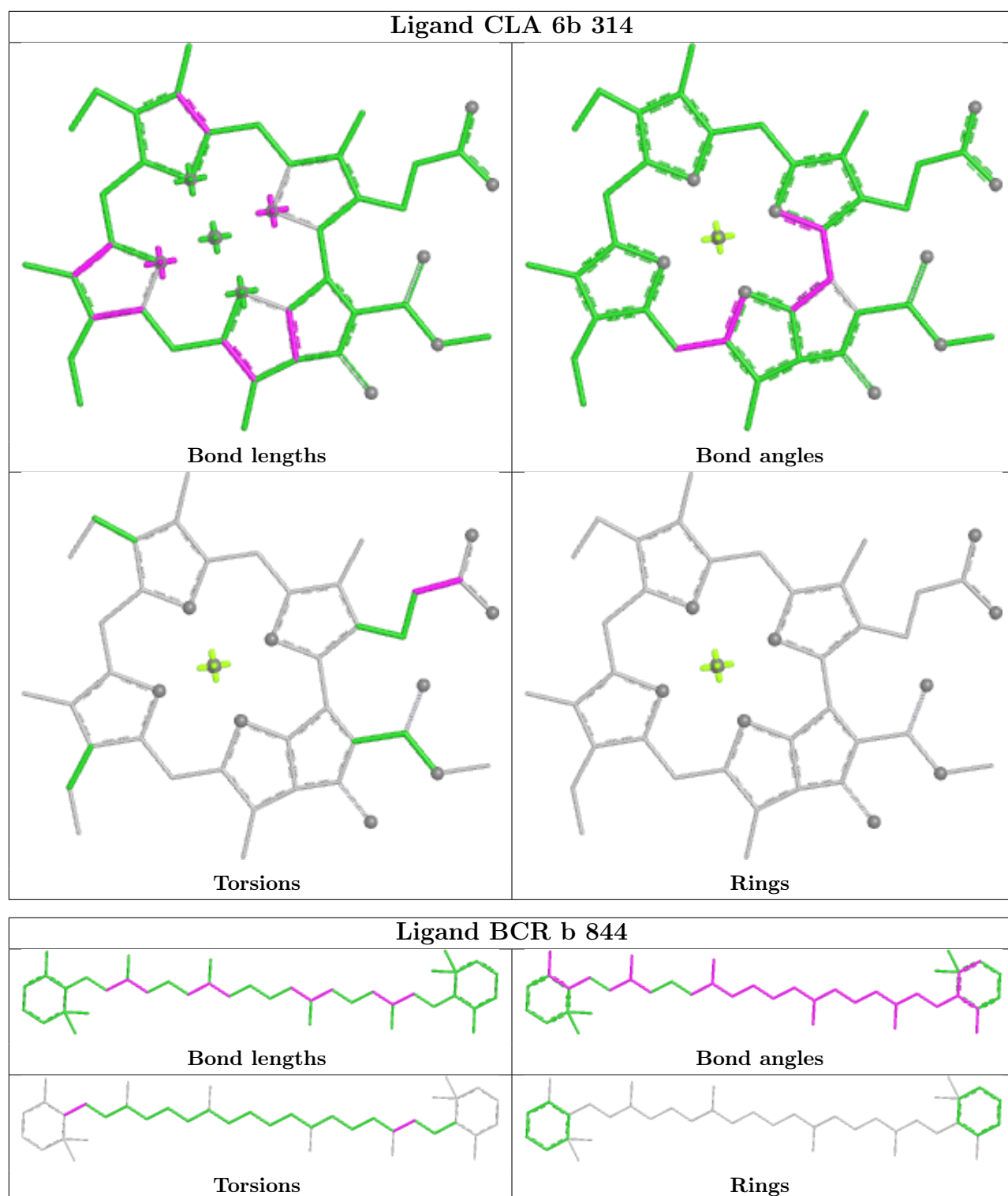
Bond angles

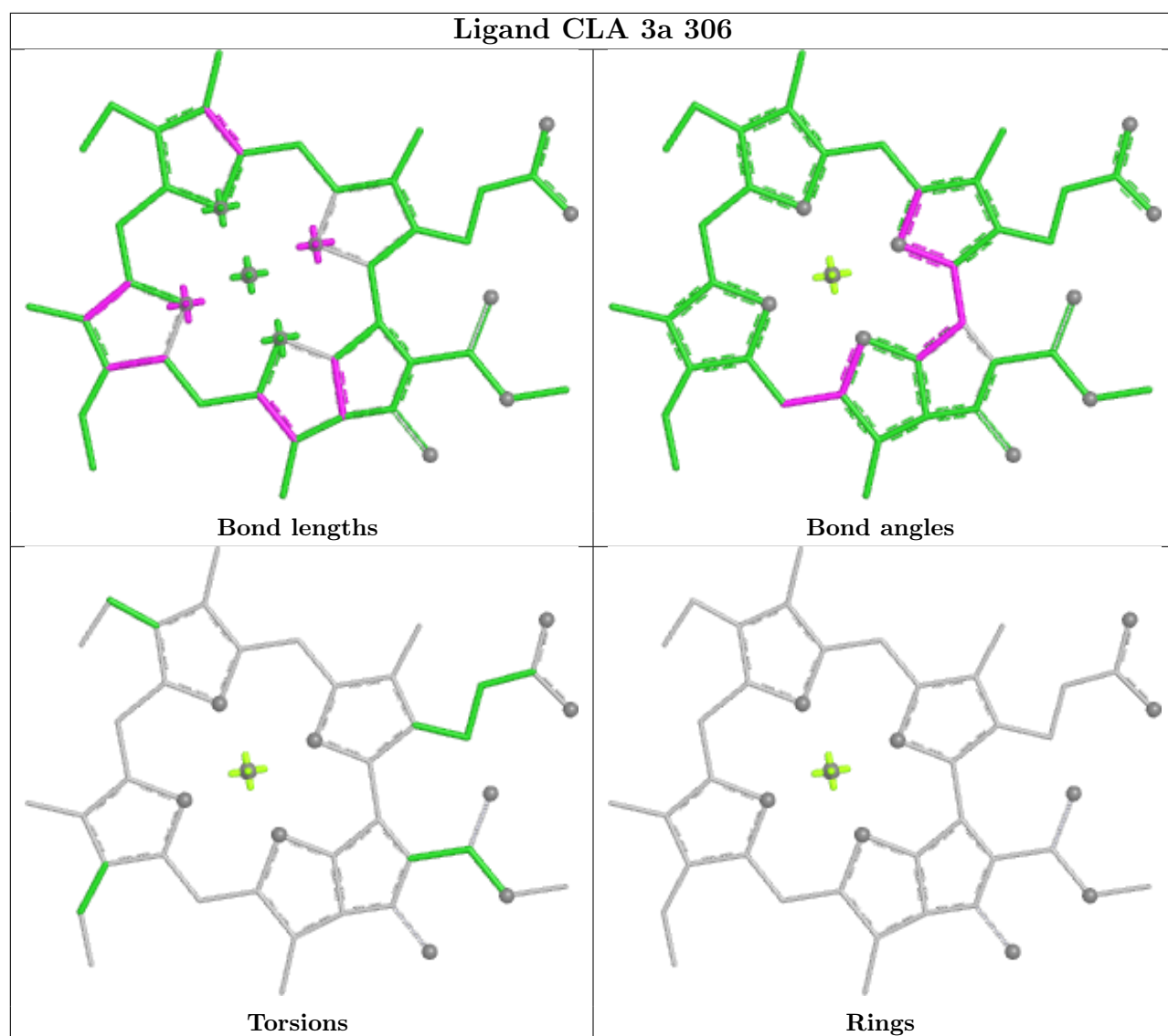


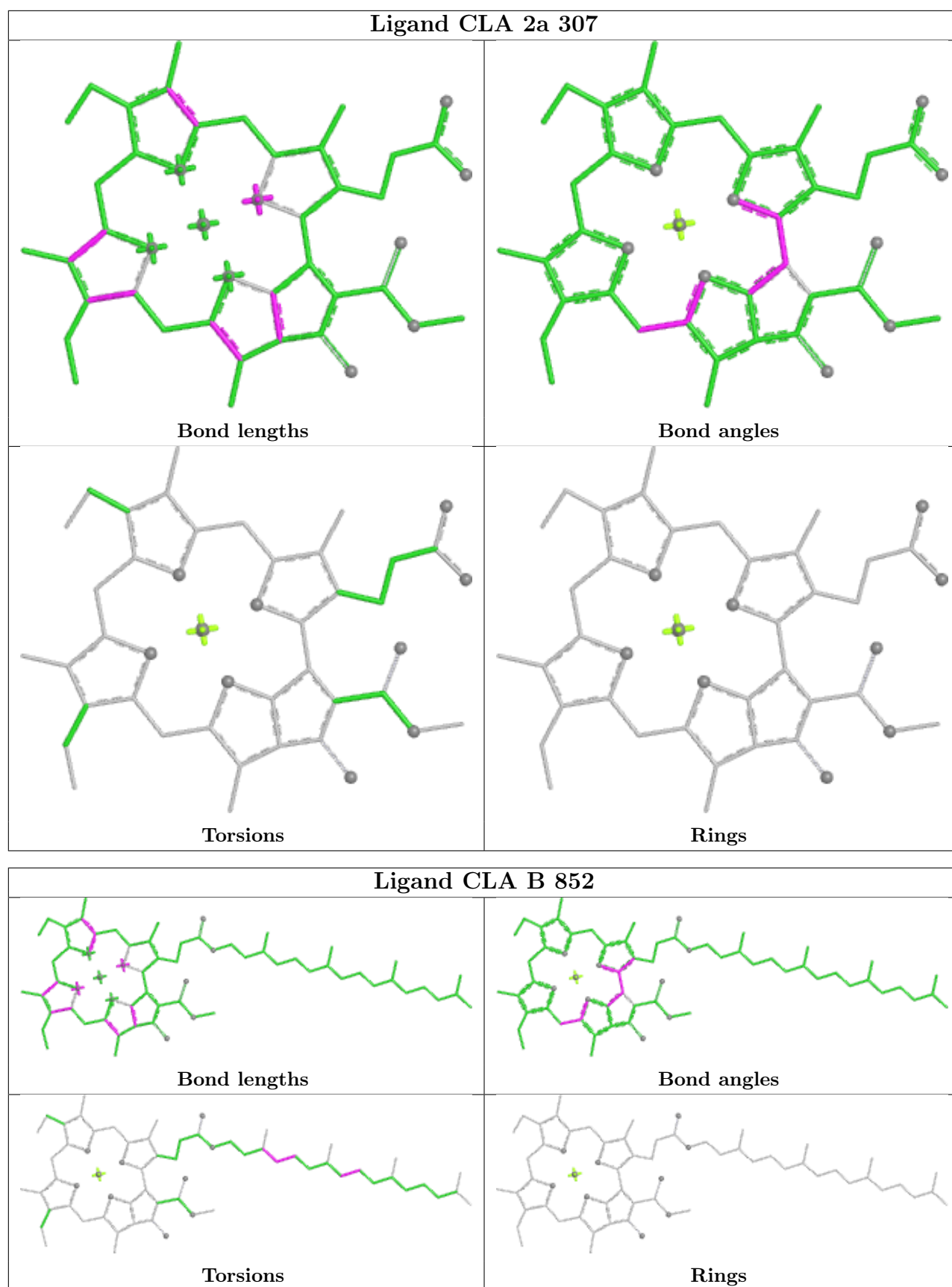
Torsions



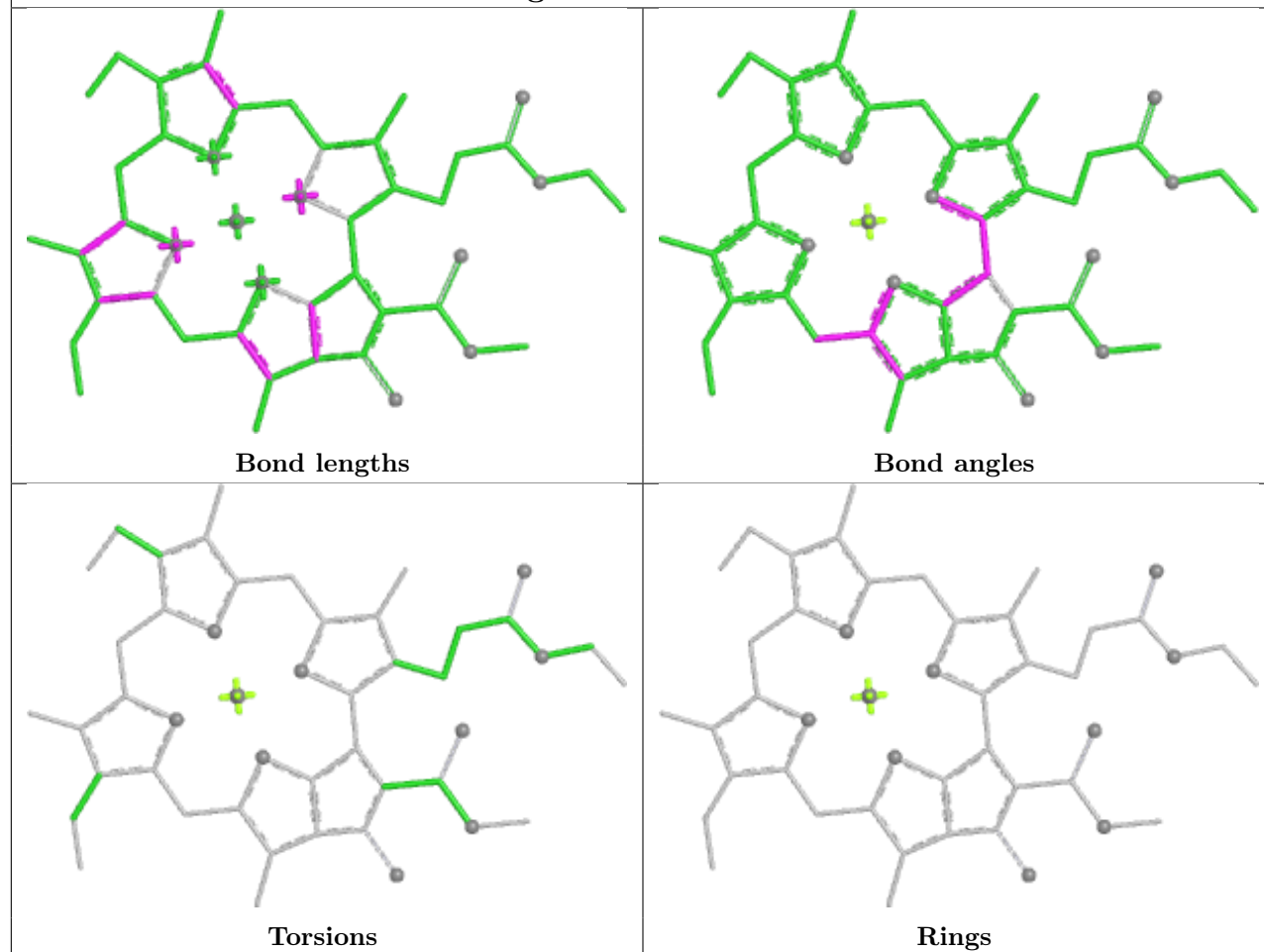
Rings



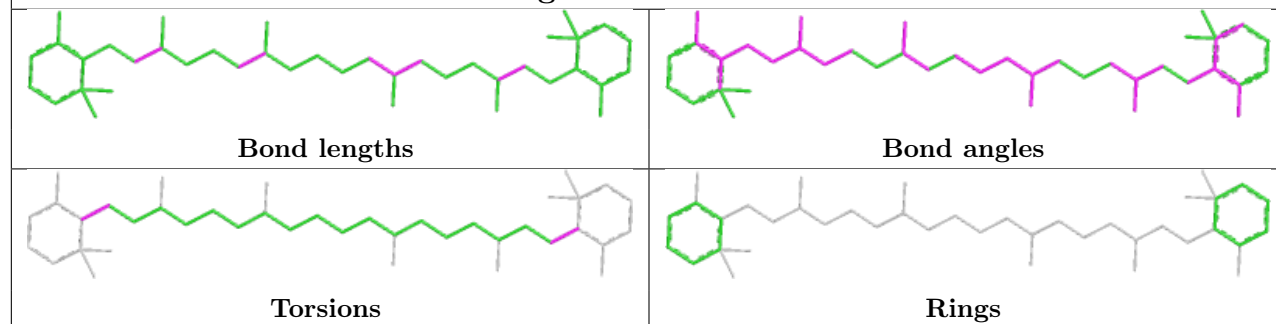


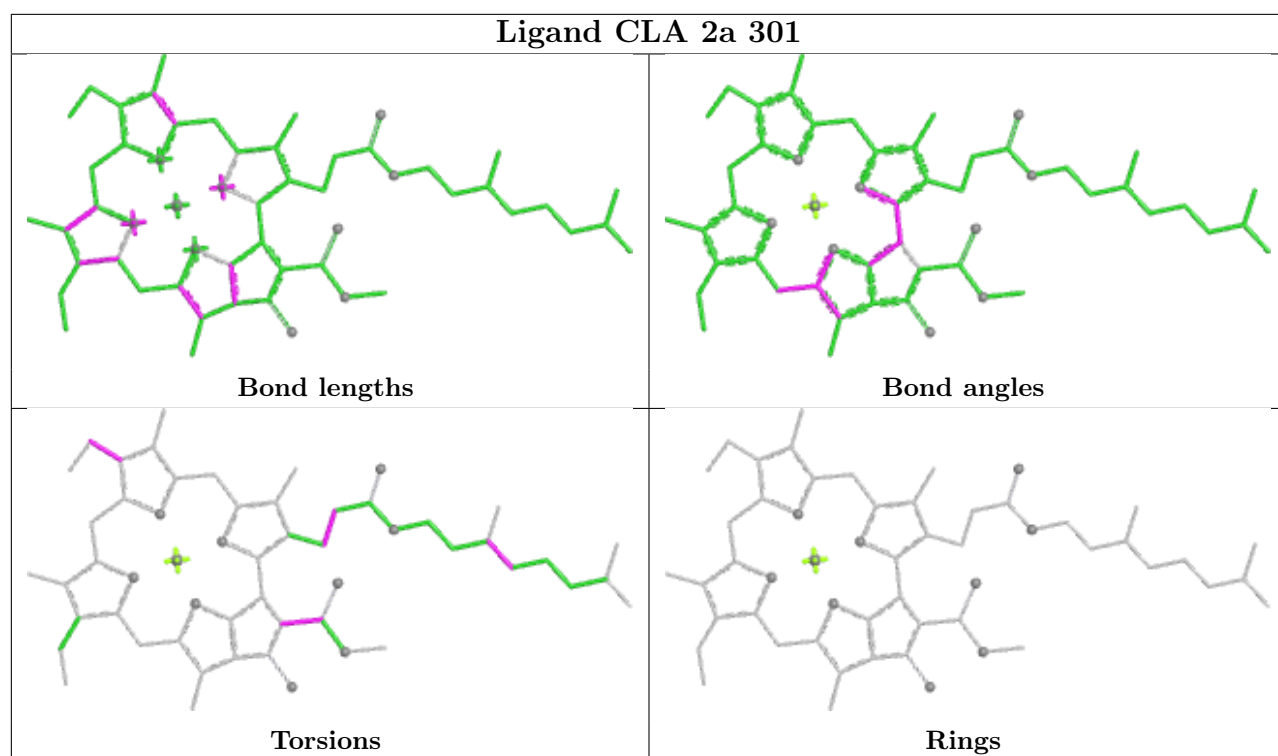


## Ligand CLA B 837

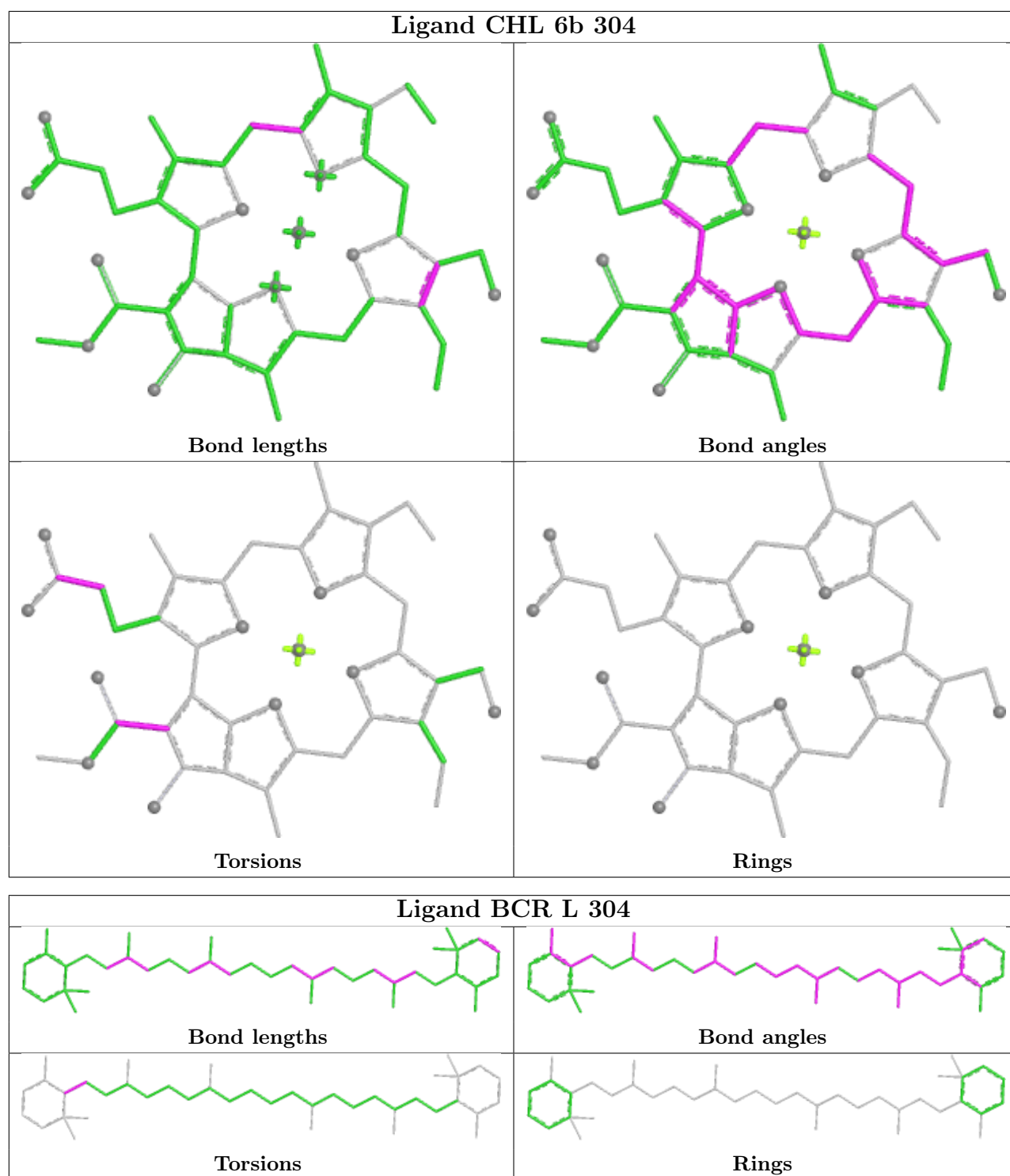


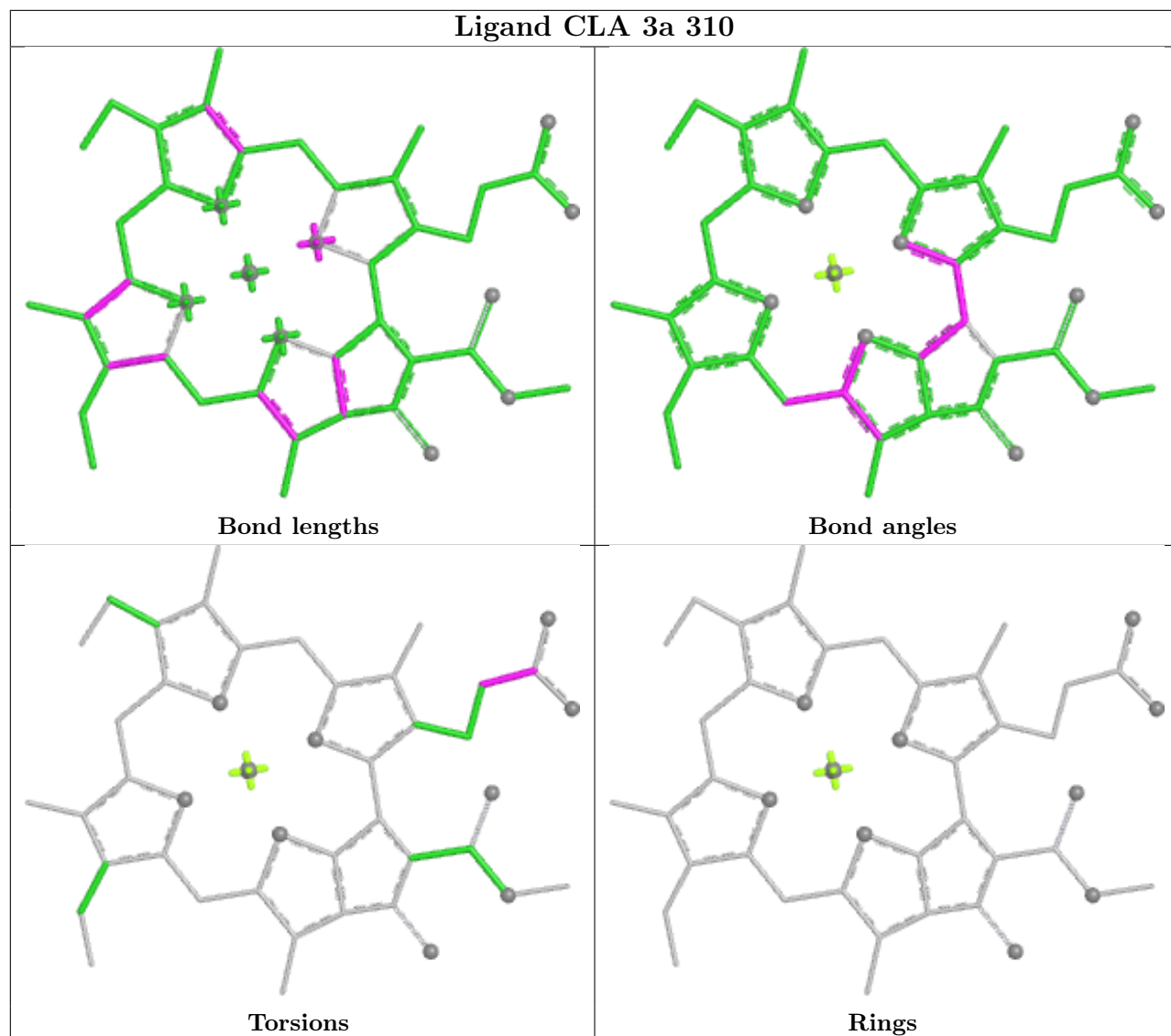
## Ligand BCR f 301

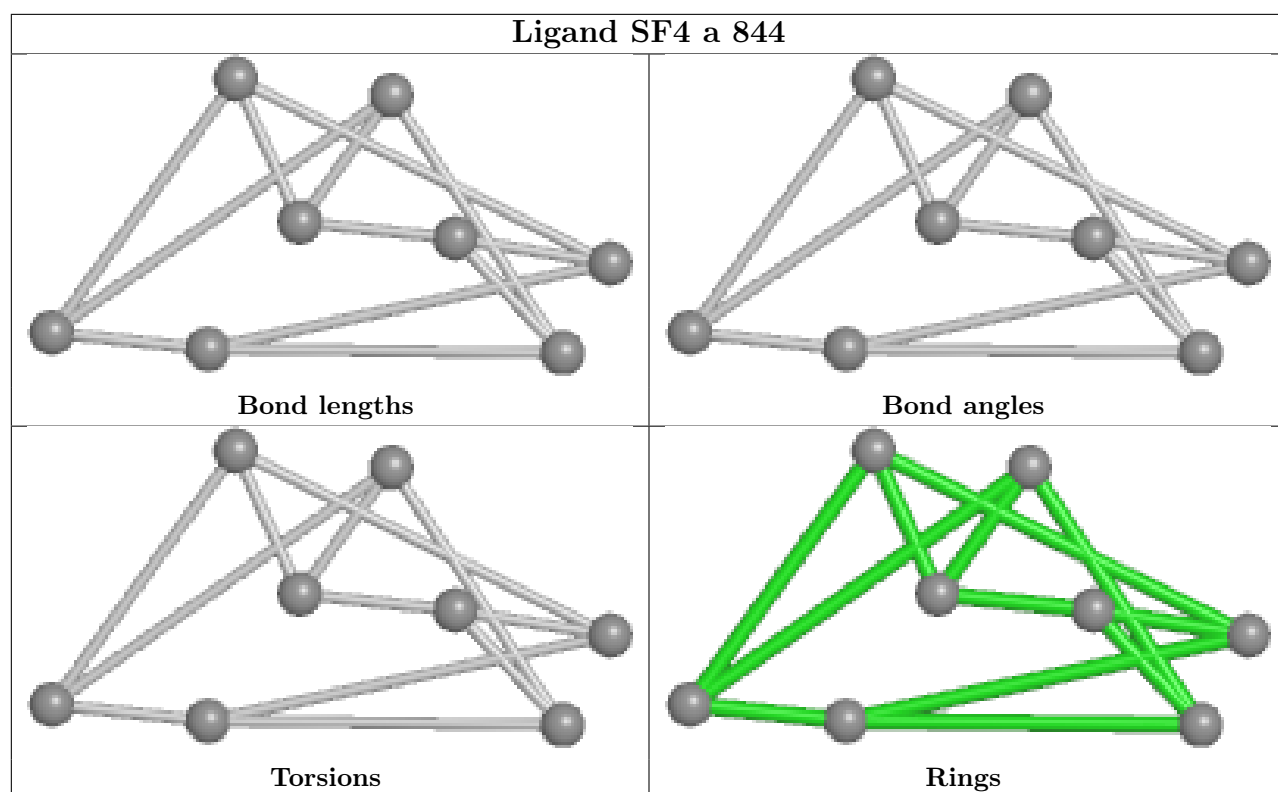


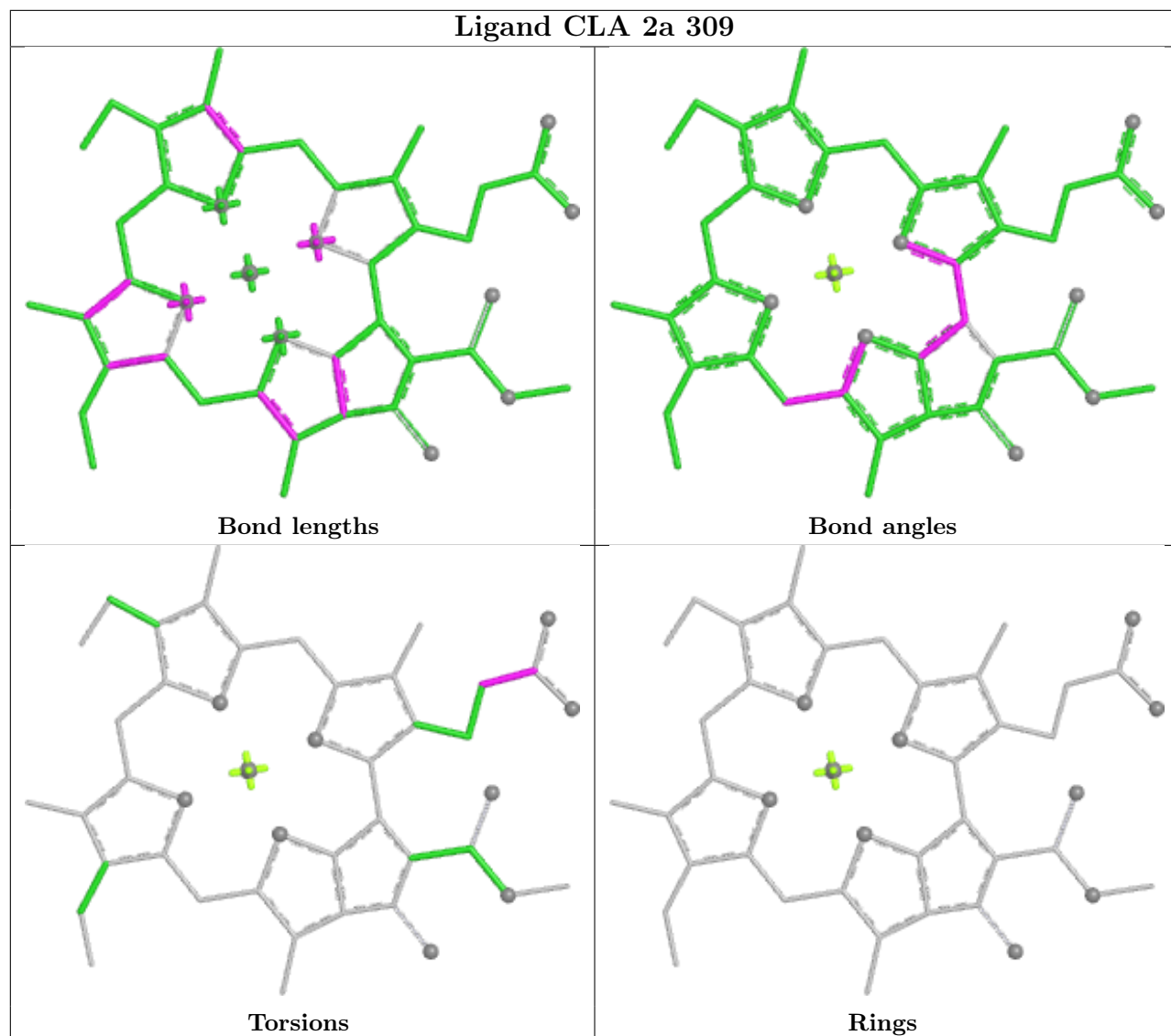


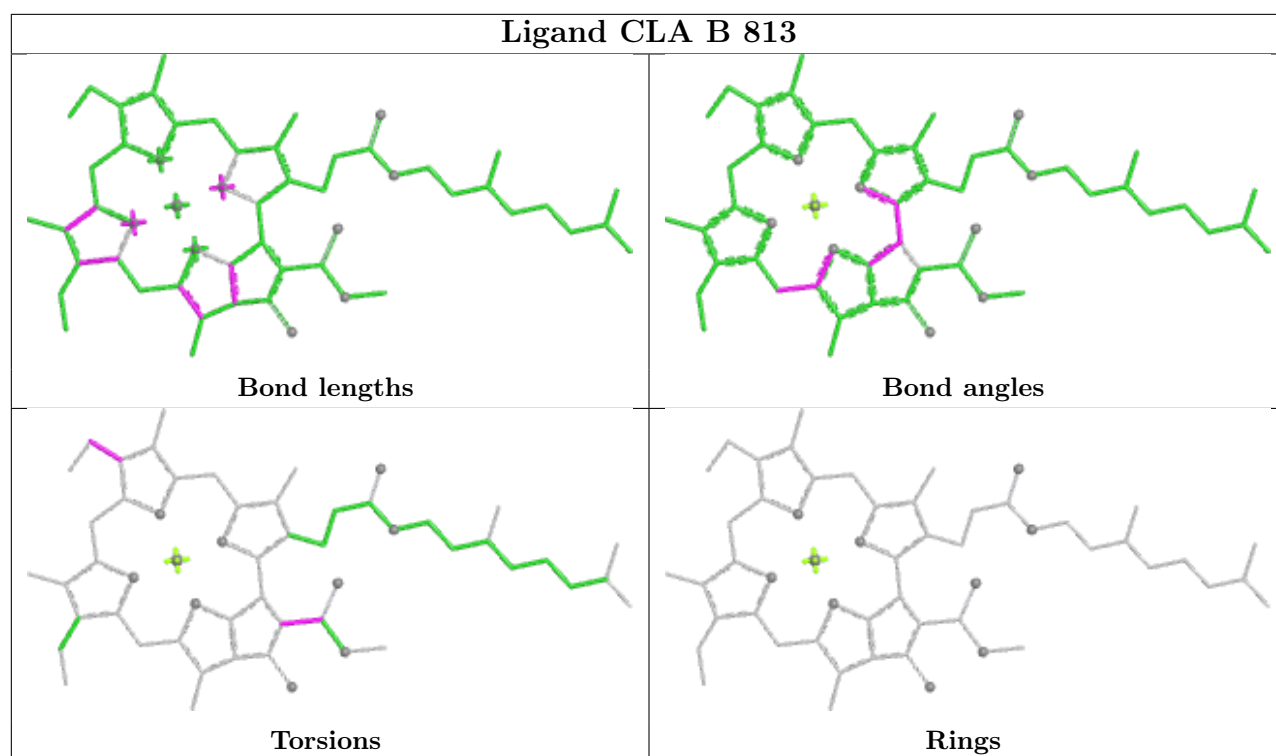


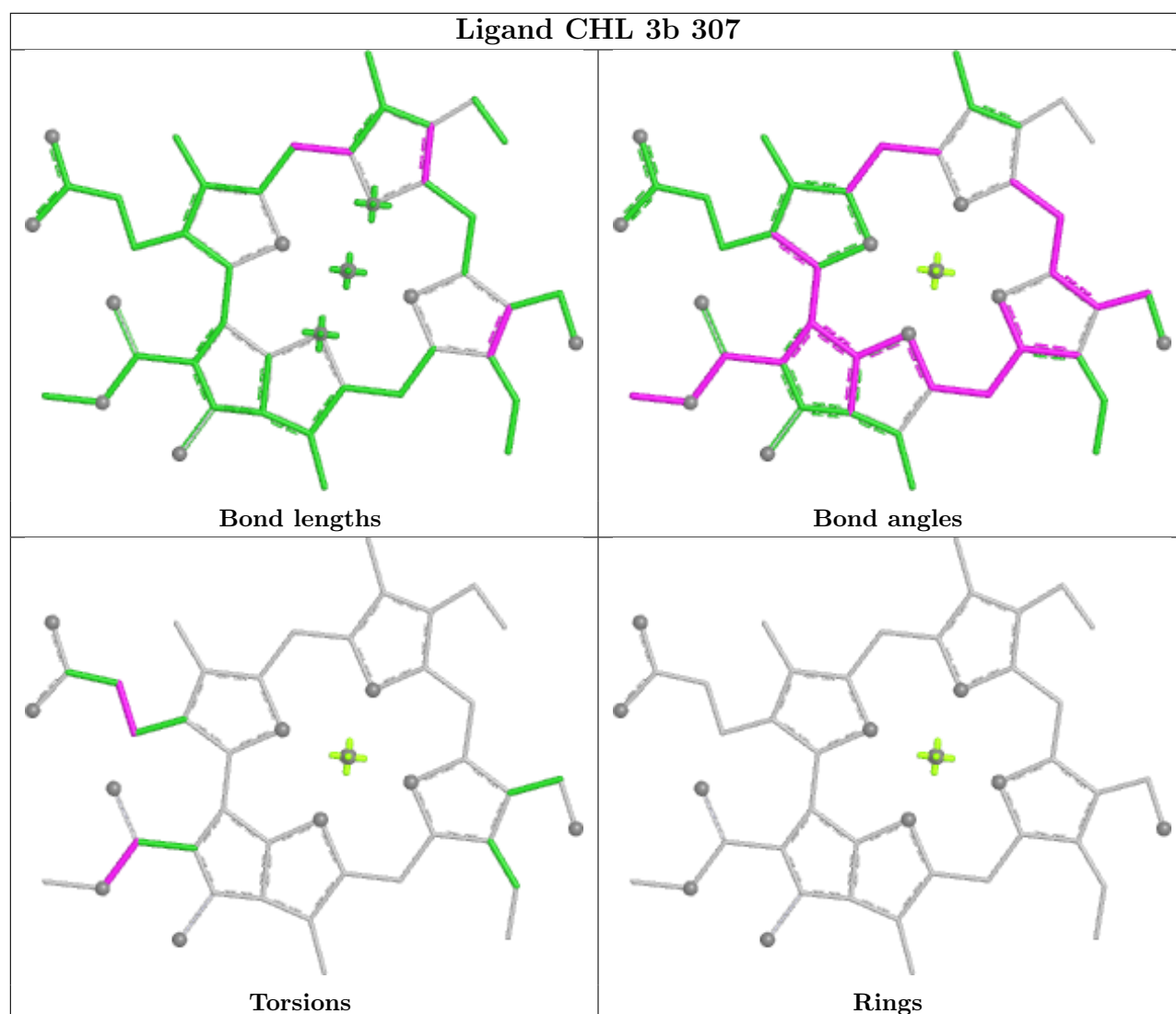




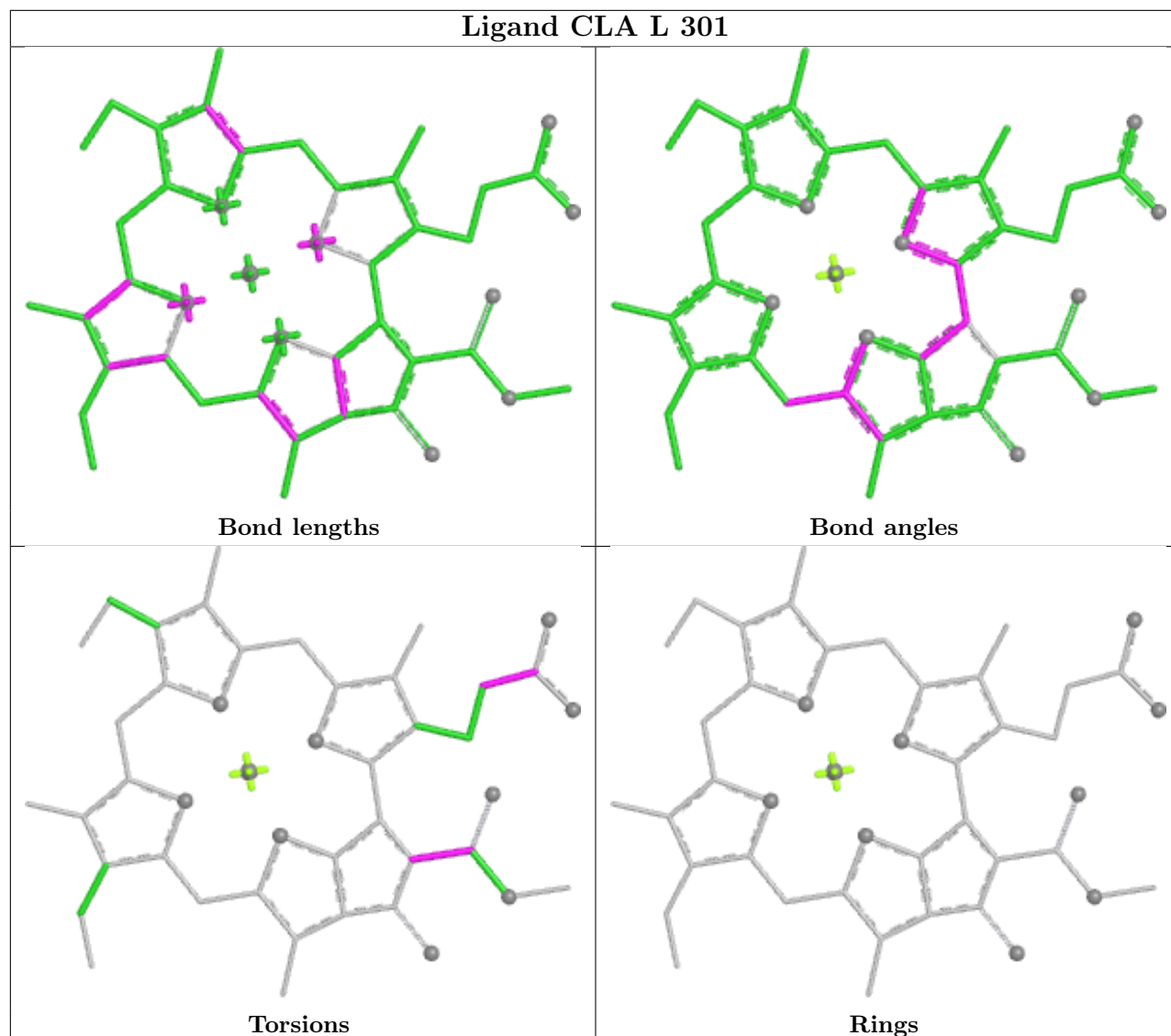




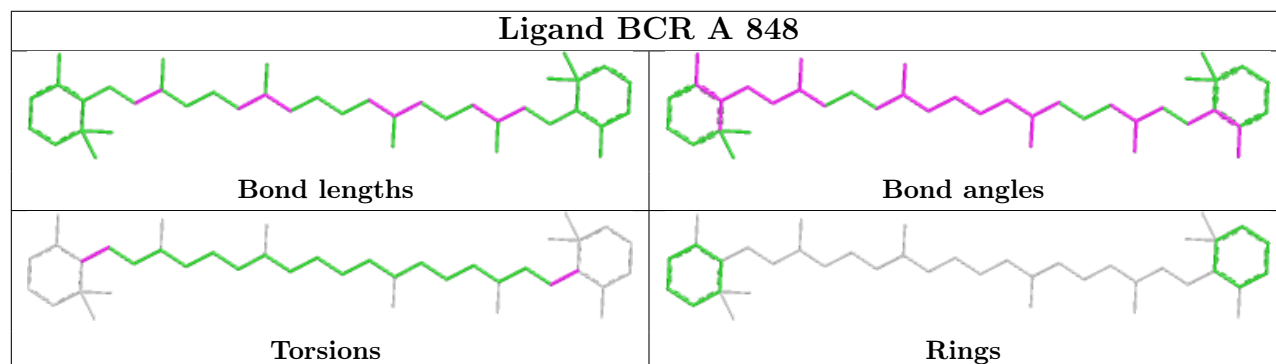


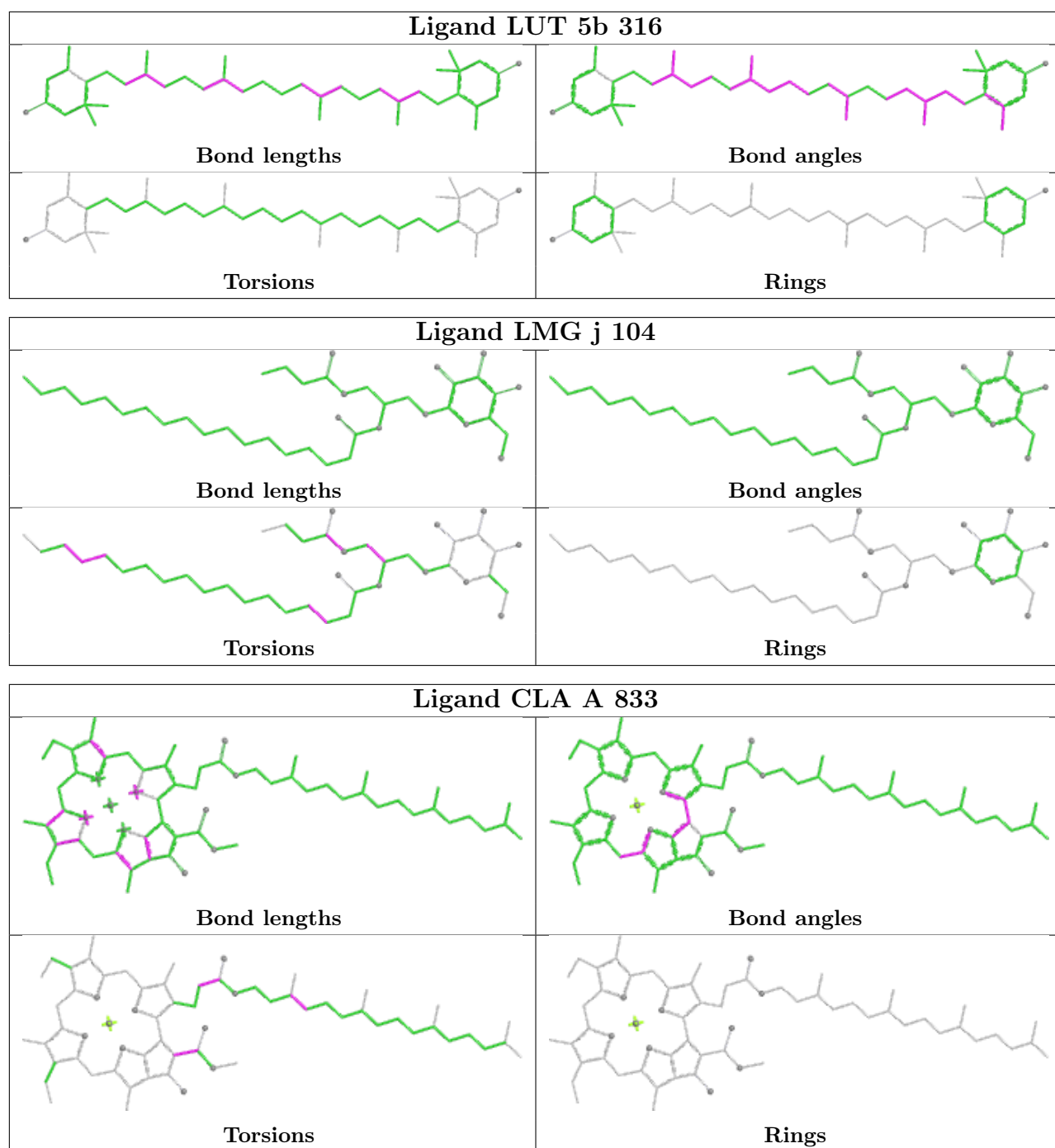


## Ligand CLA L 301

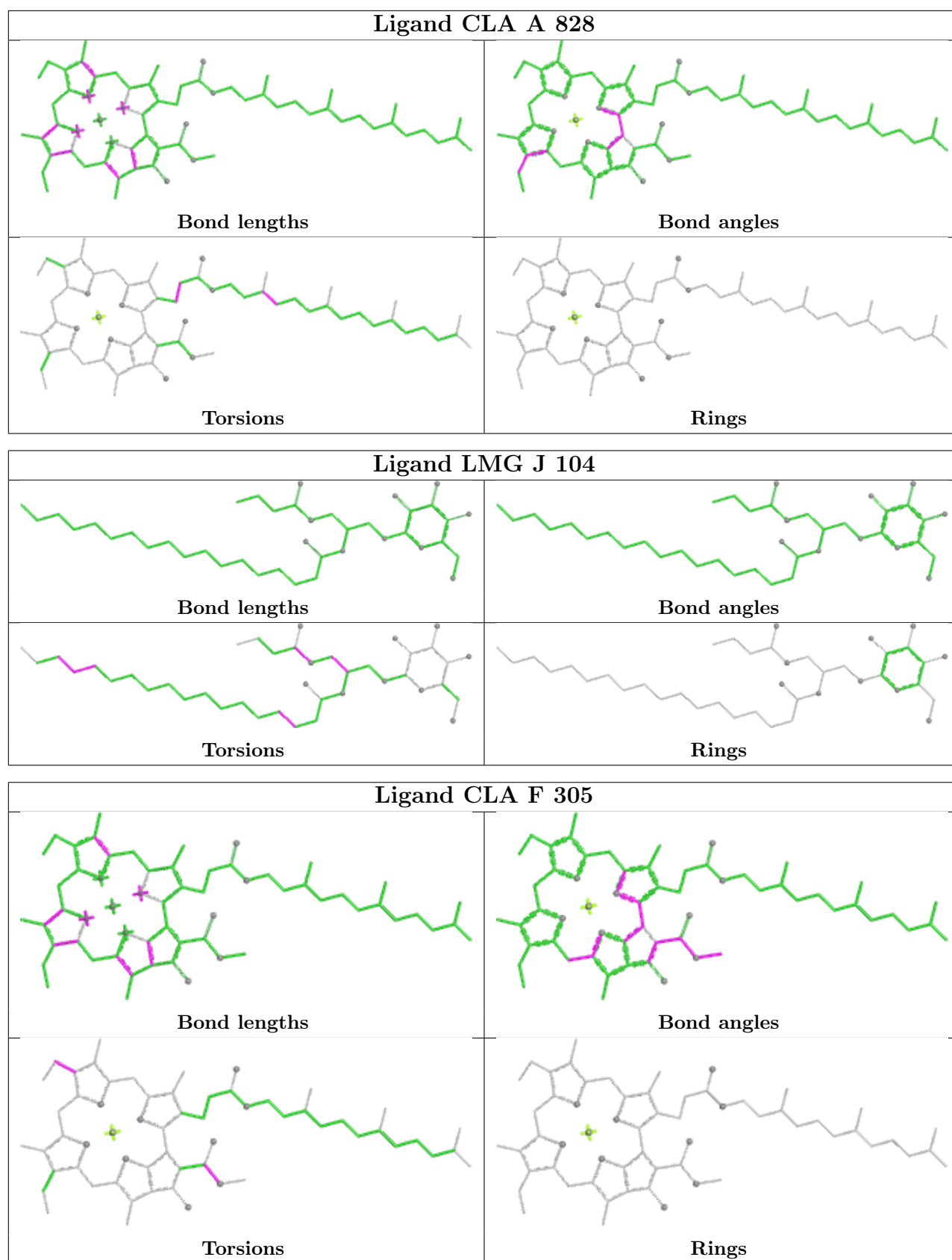


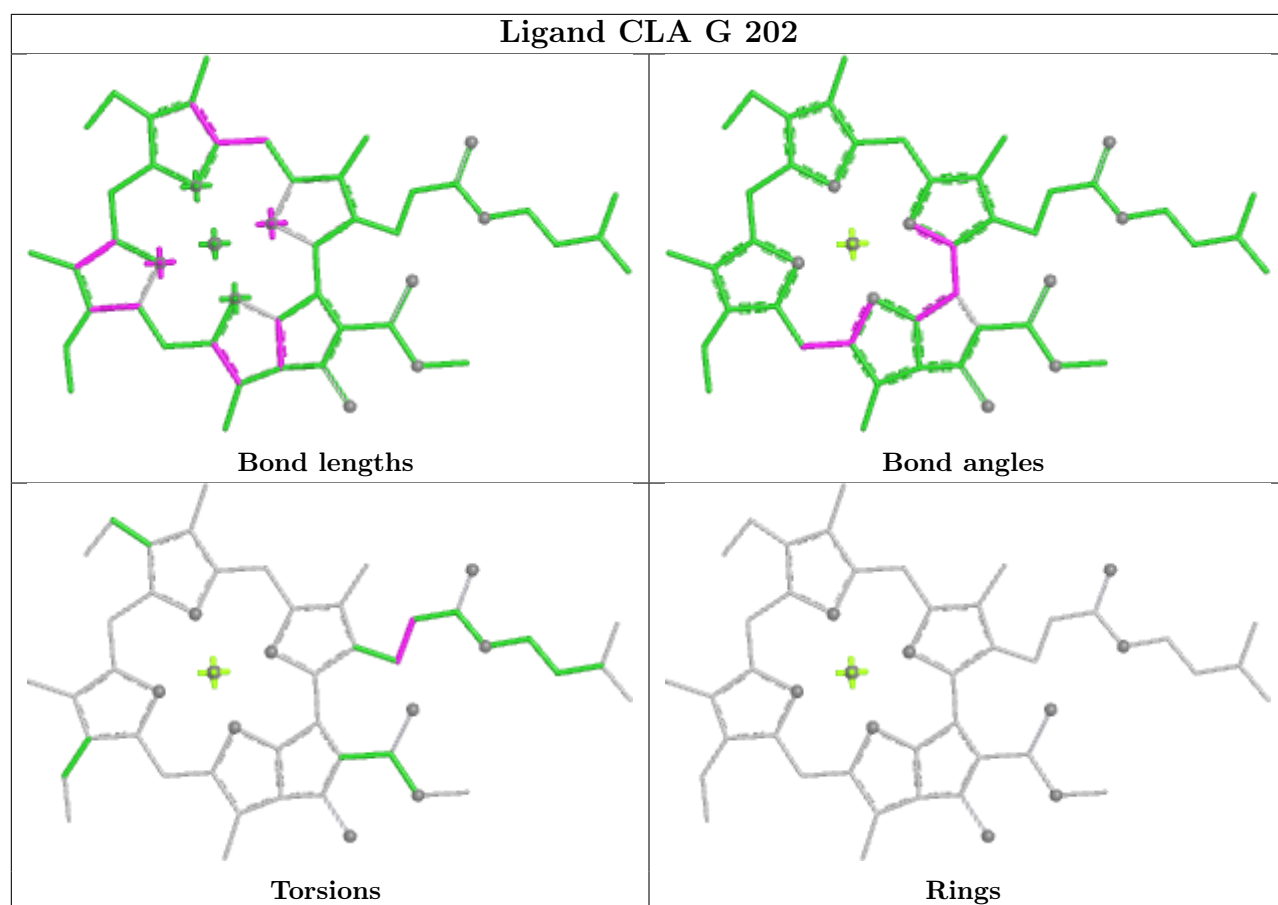
## Ligand BCR A 848

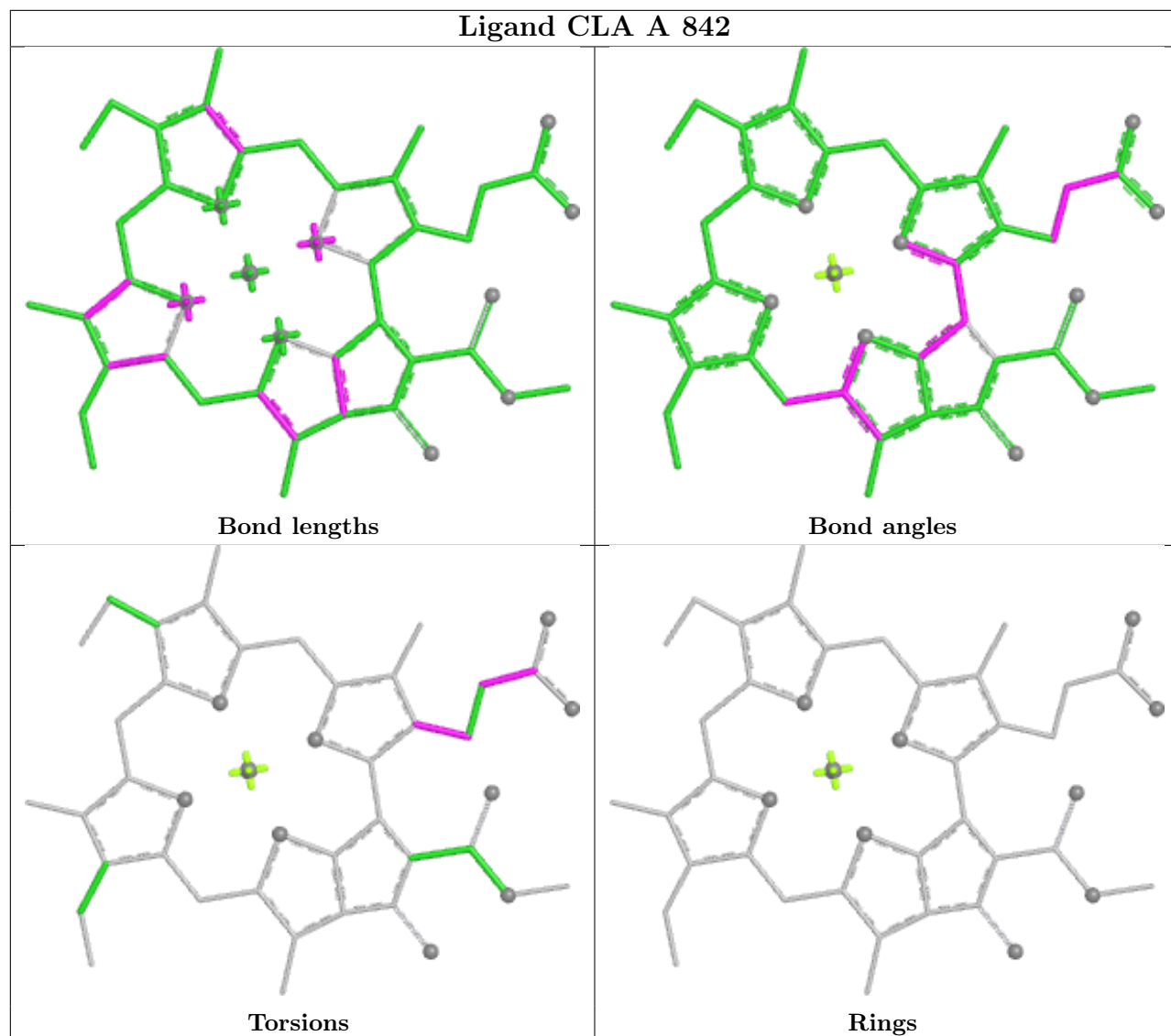


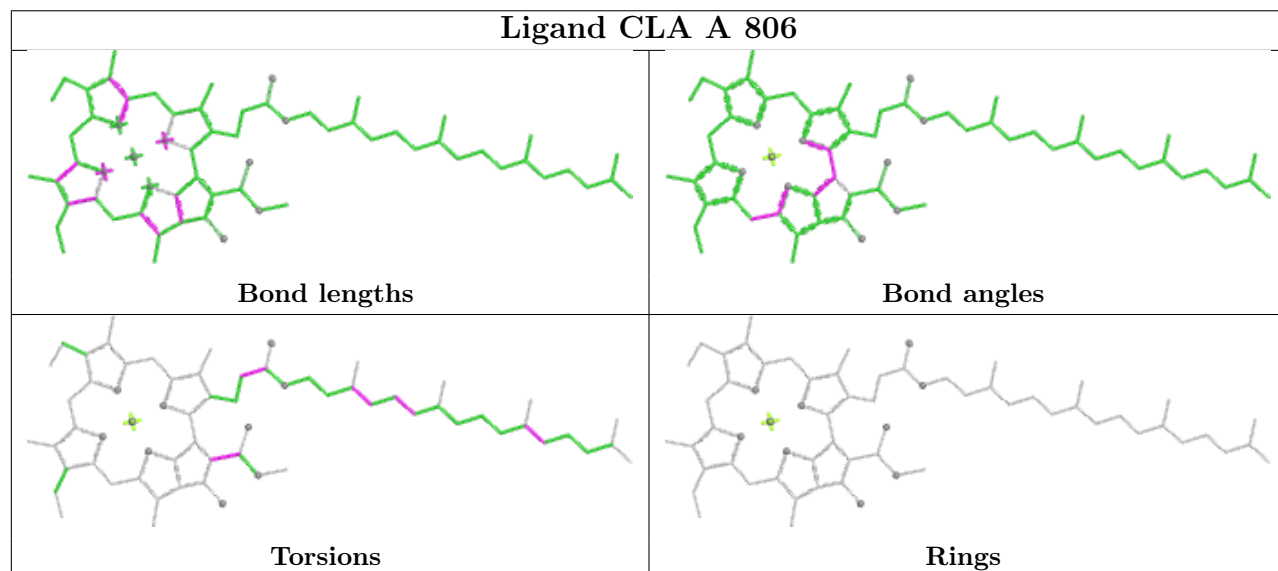
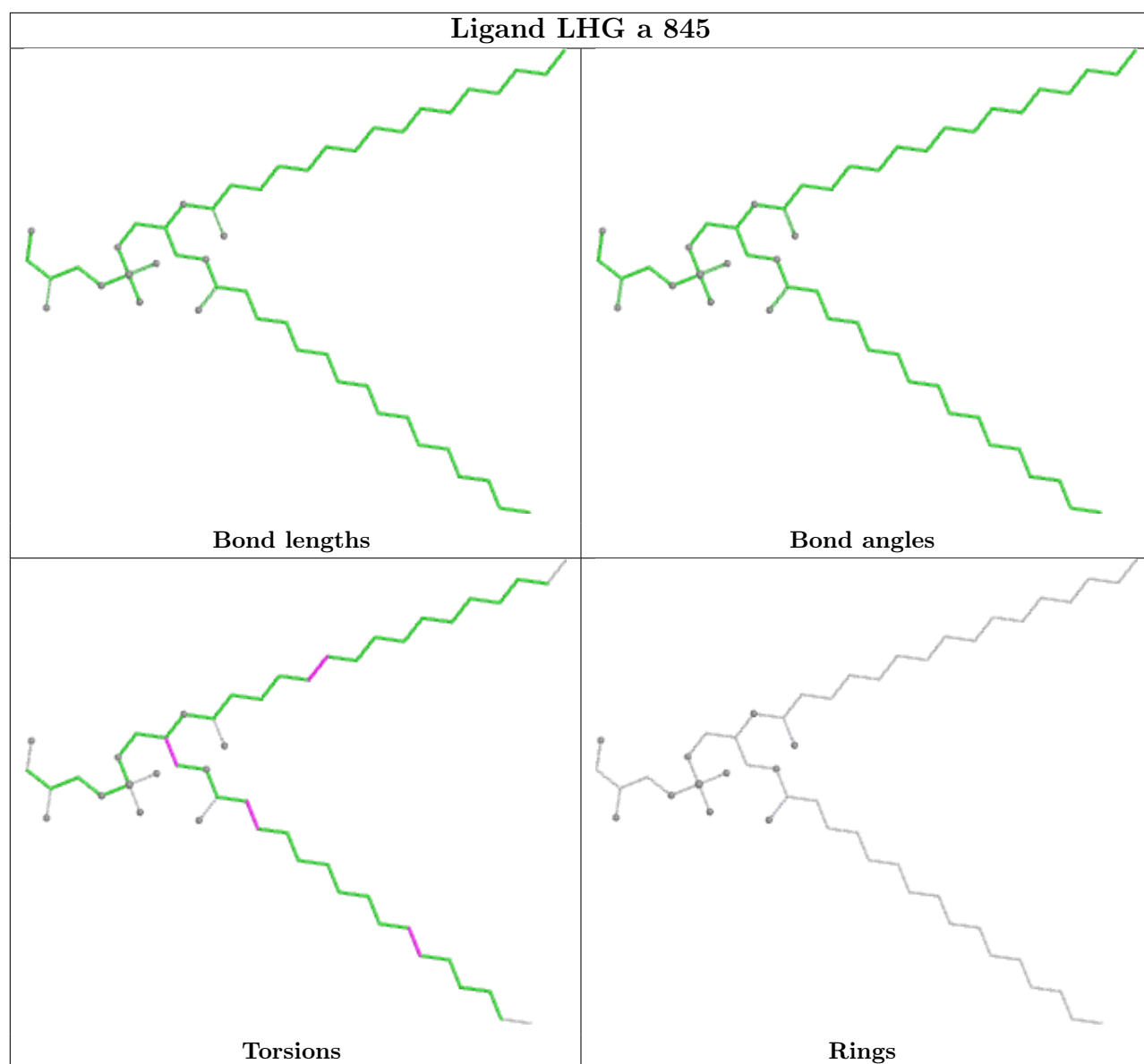


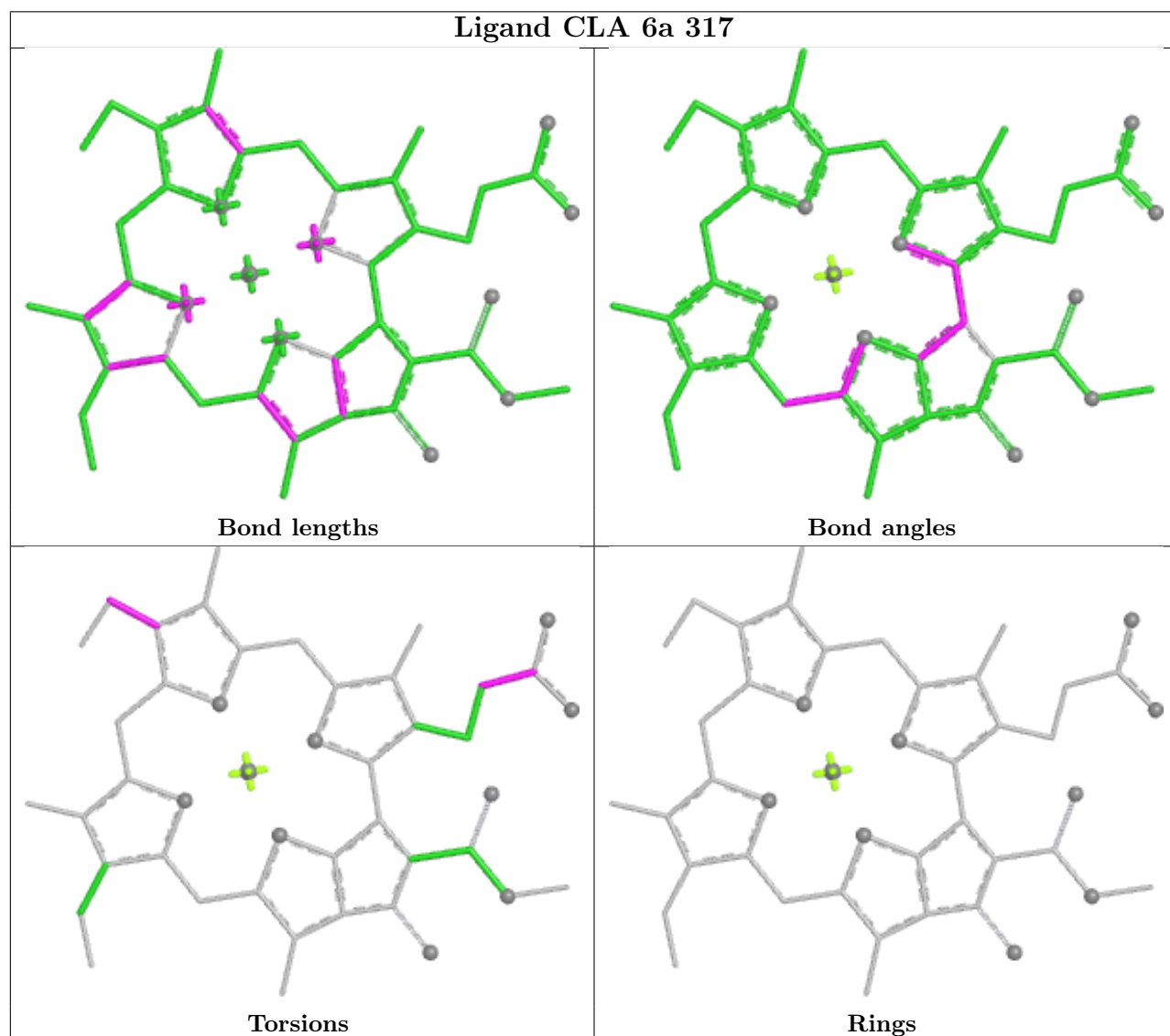
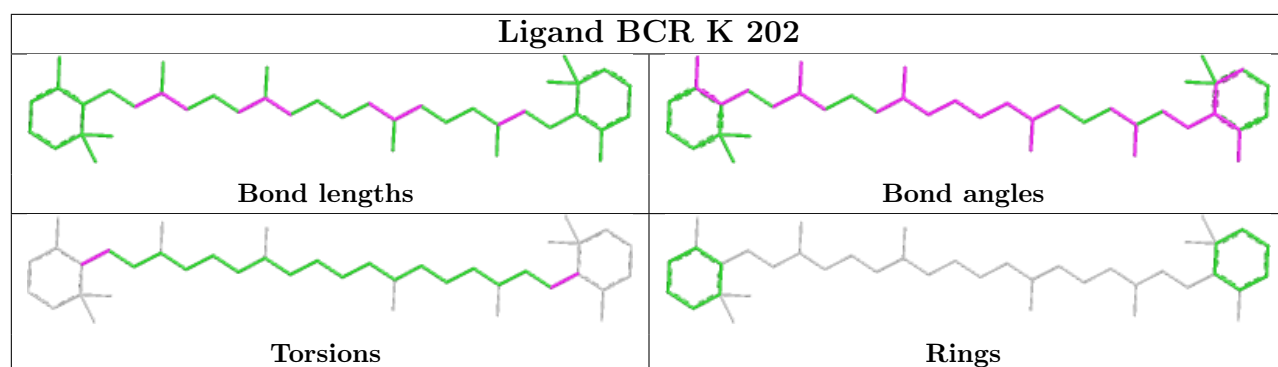


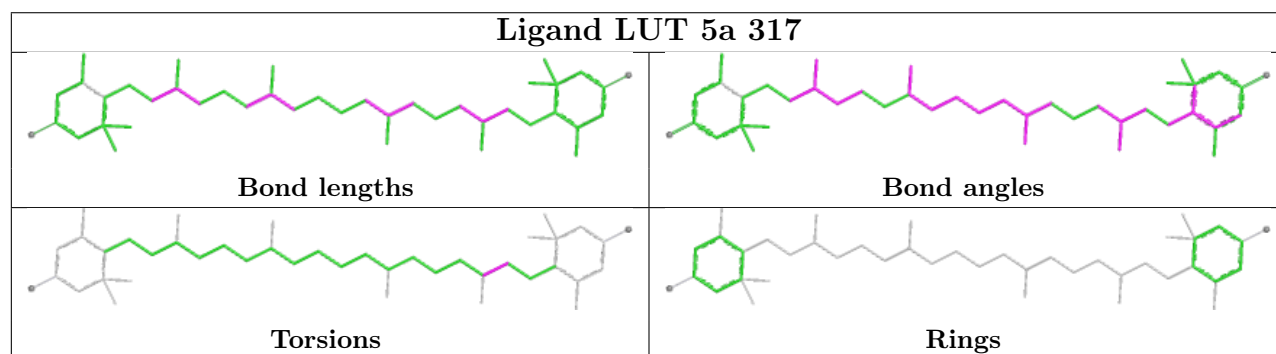
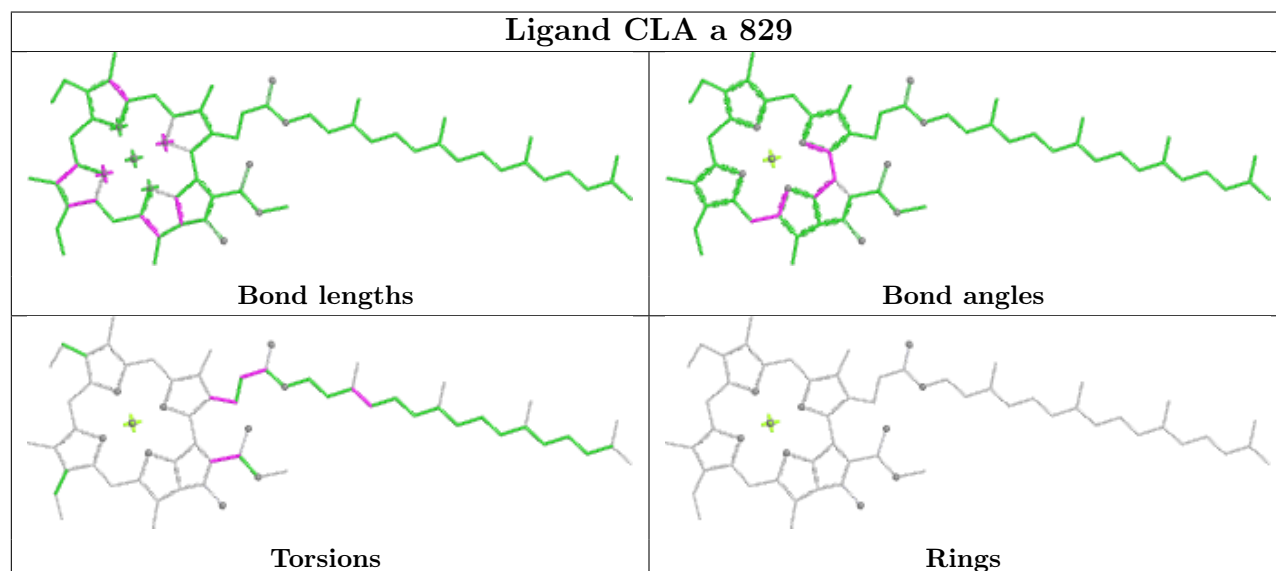
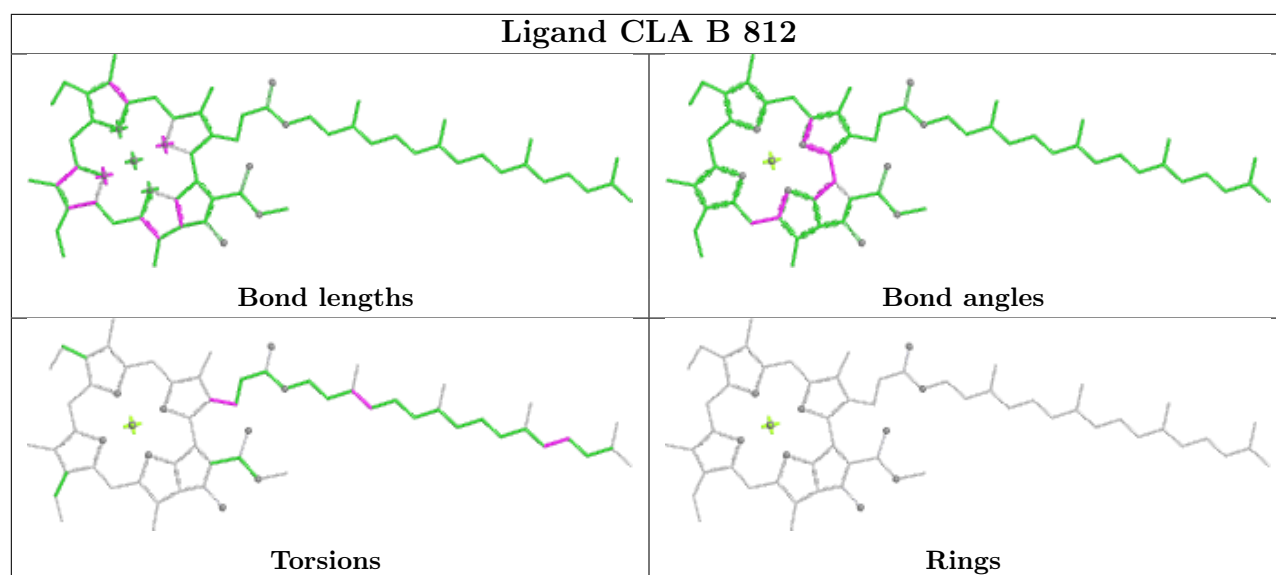


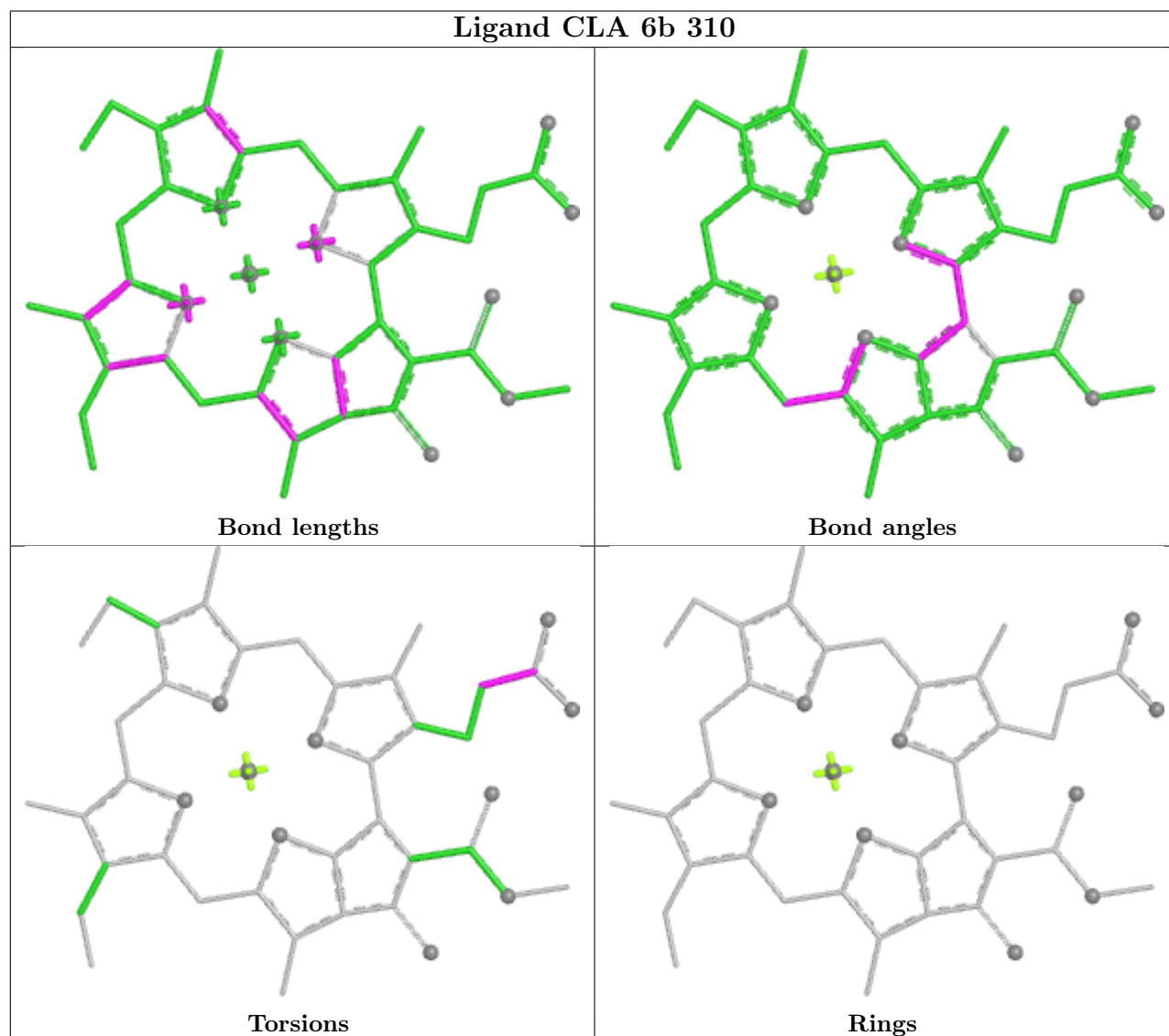
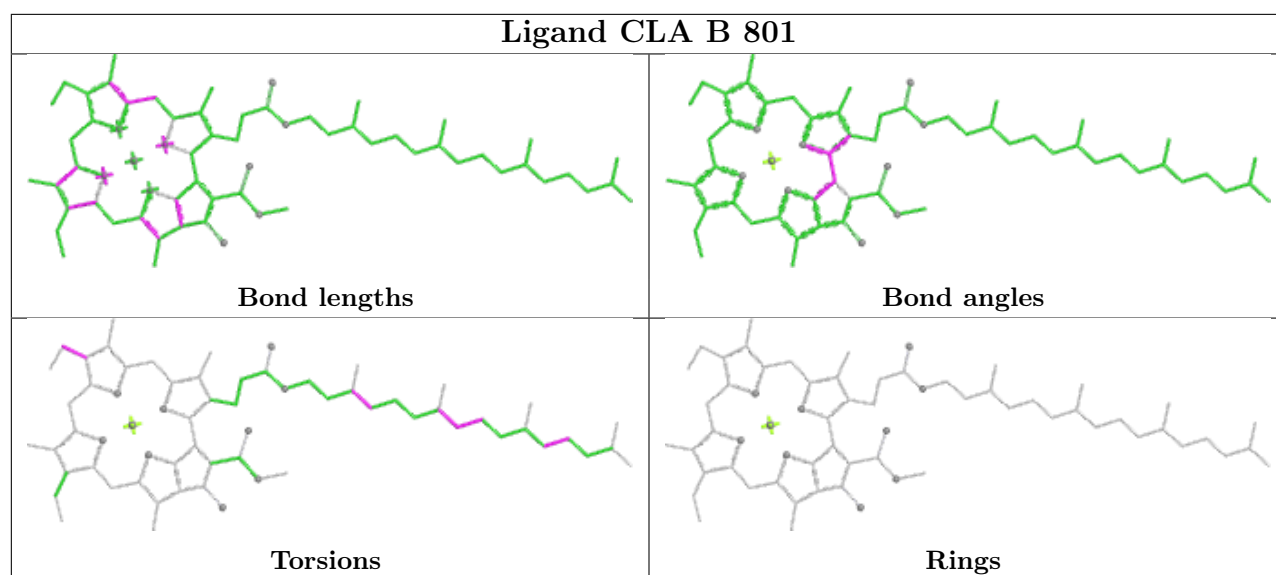


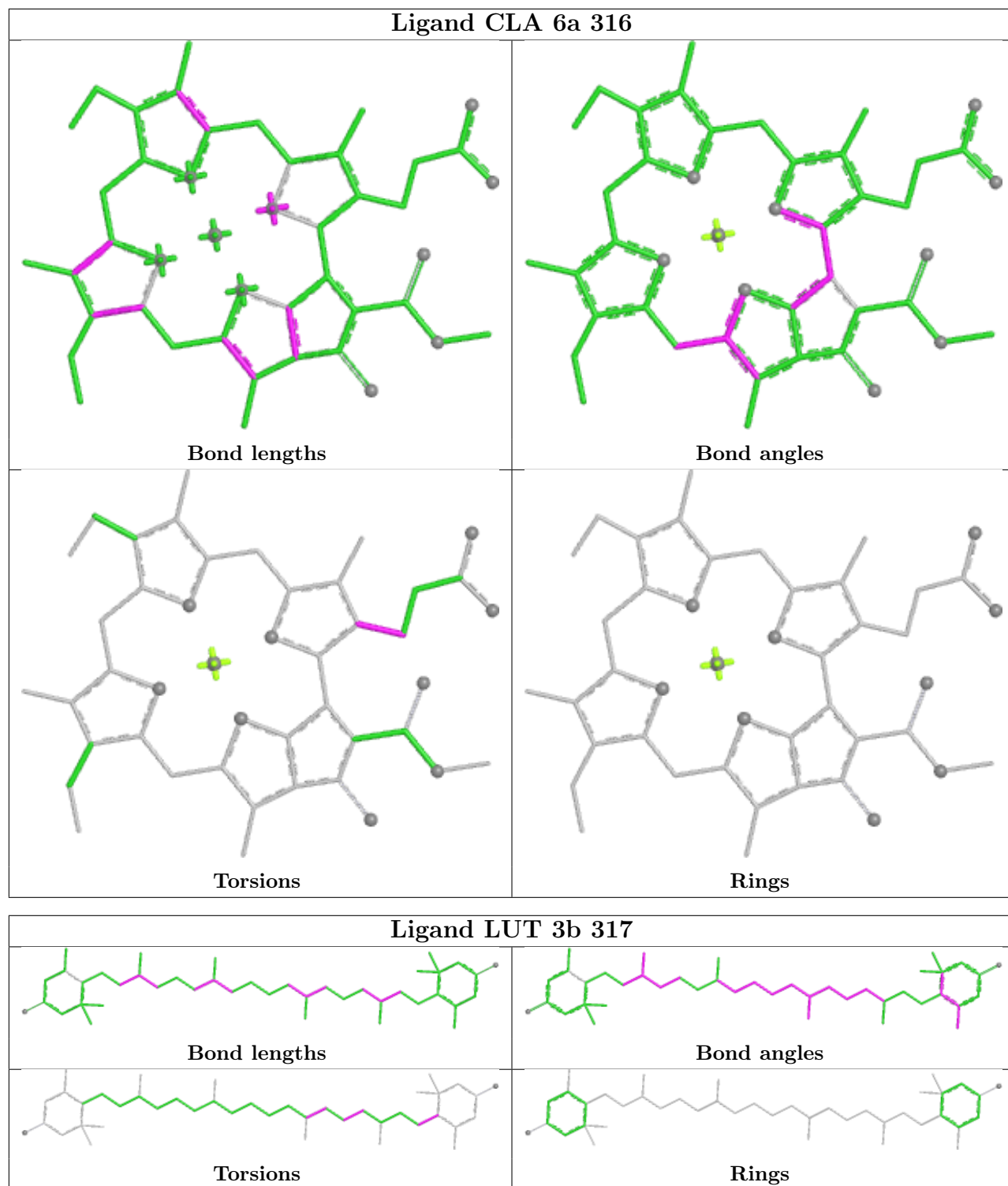




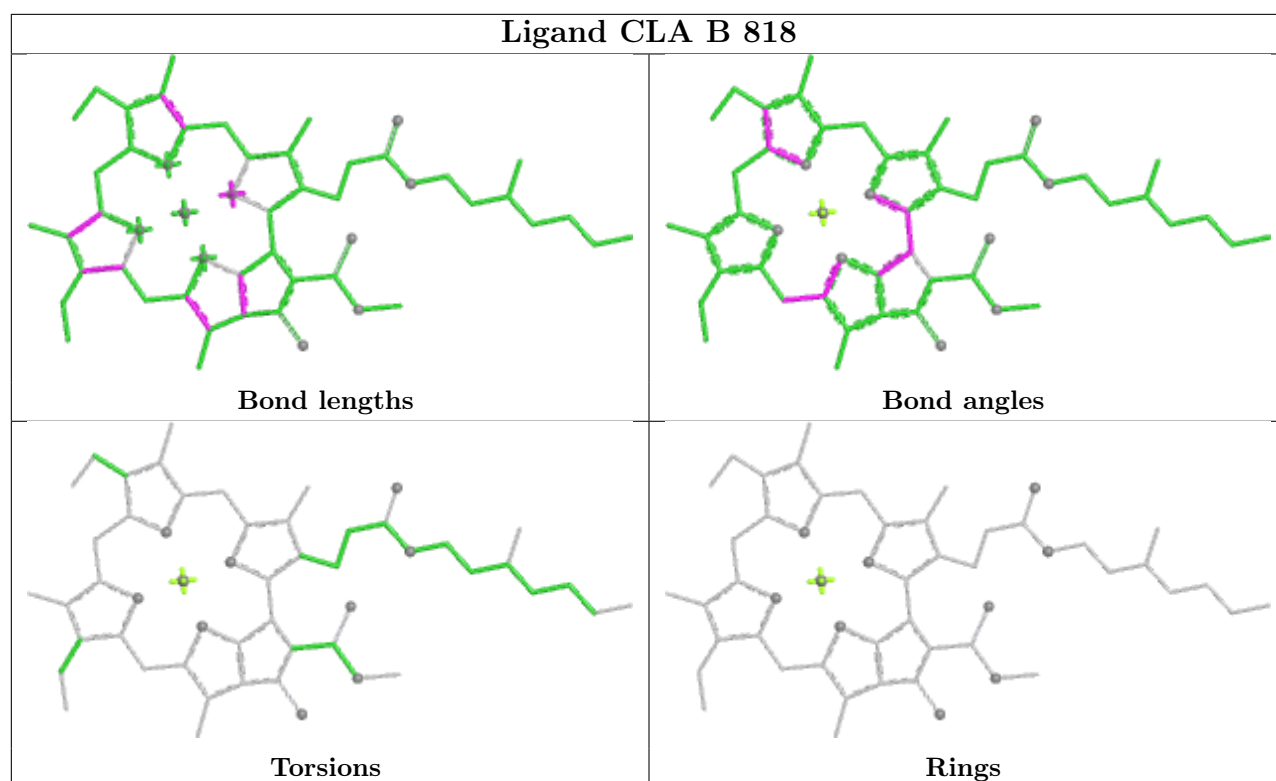


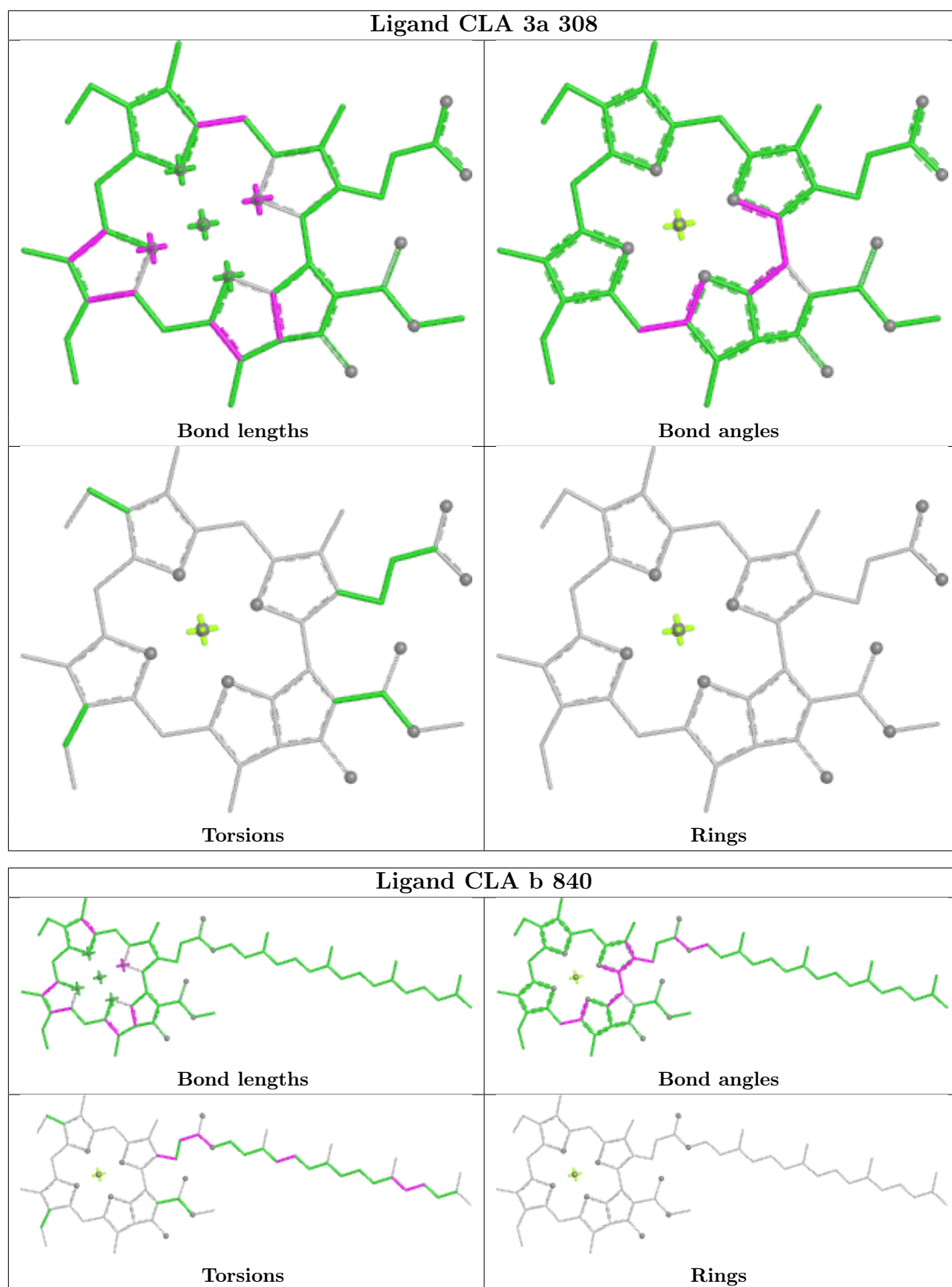


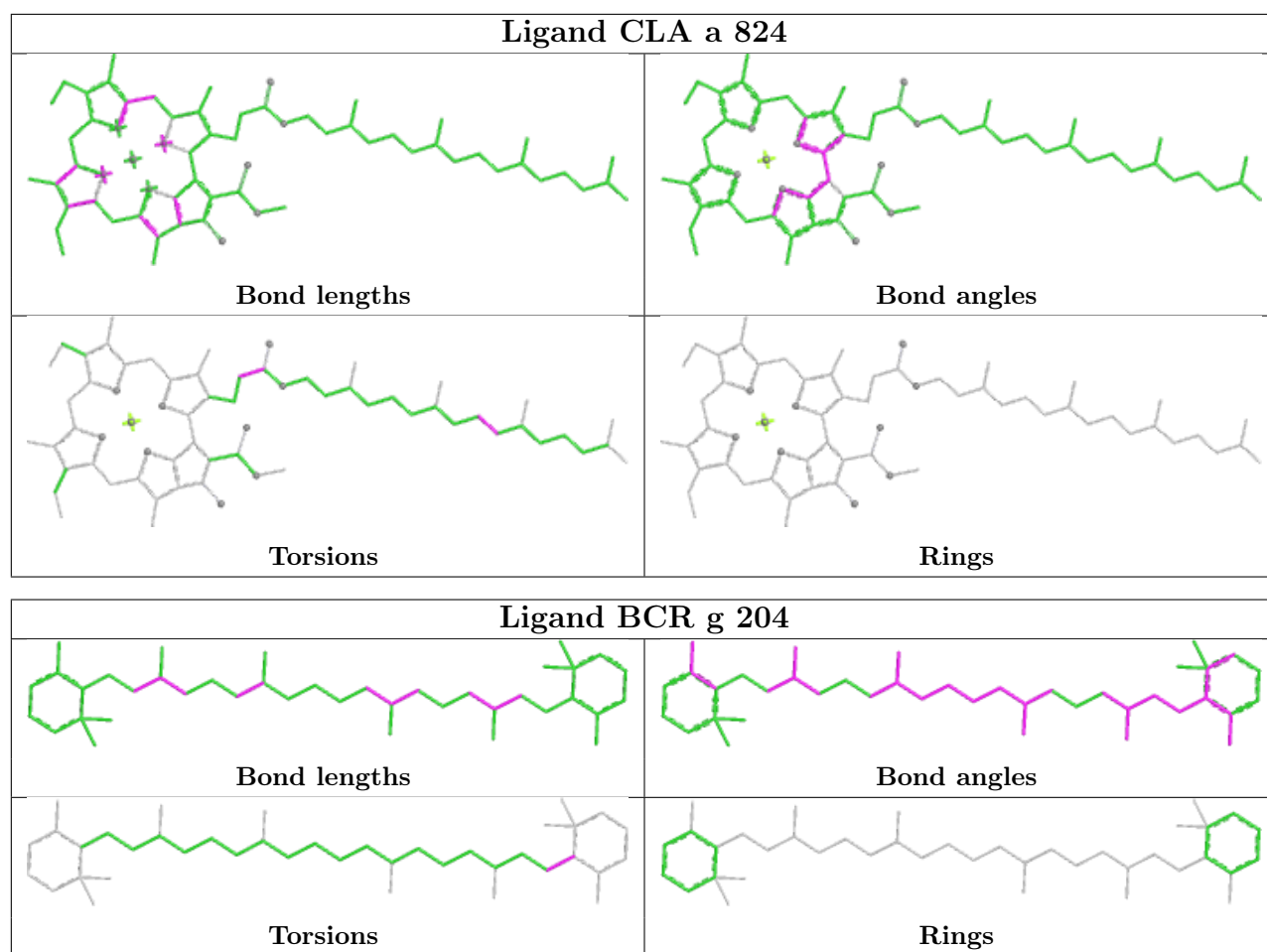


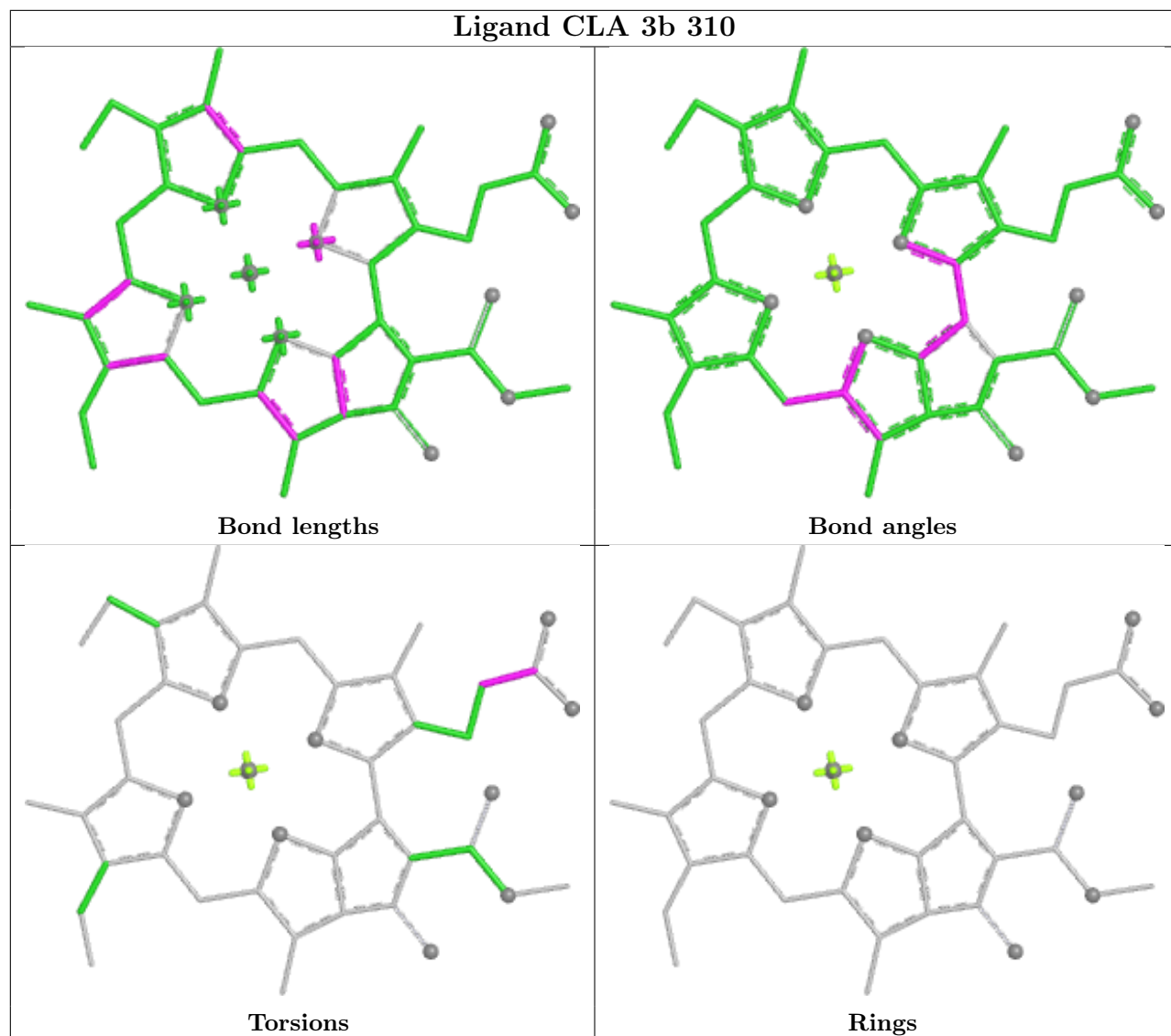


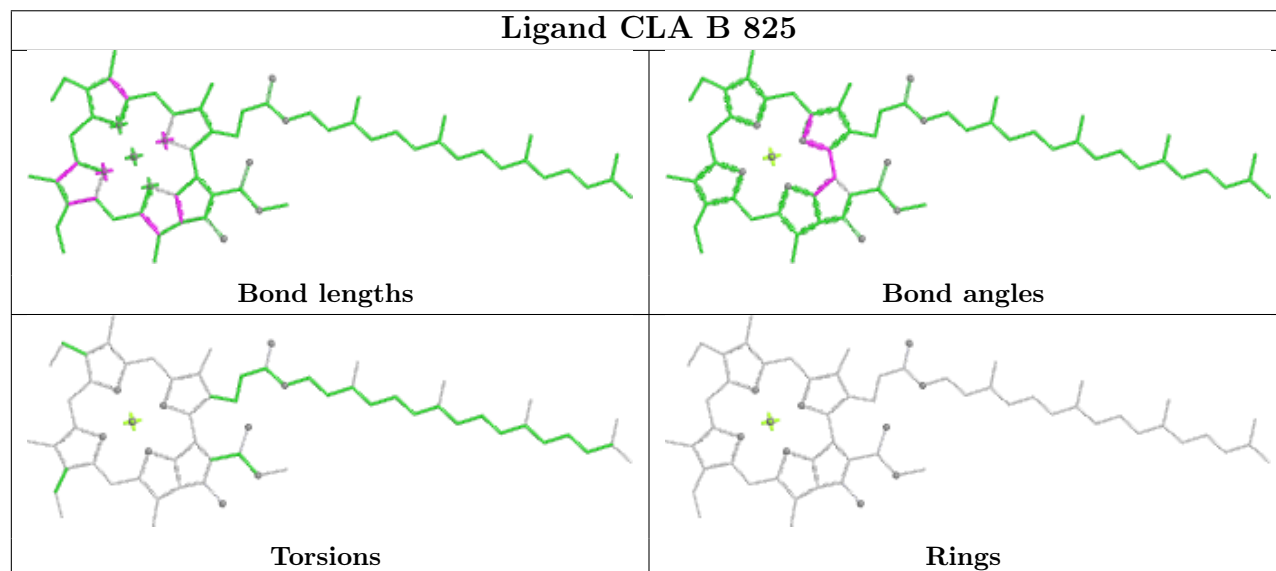
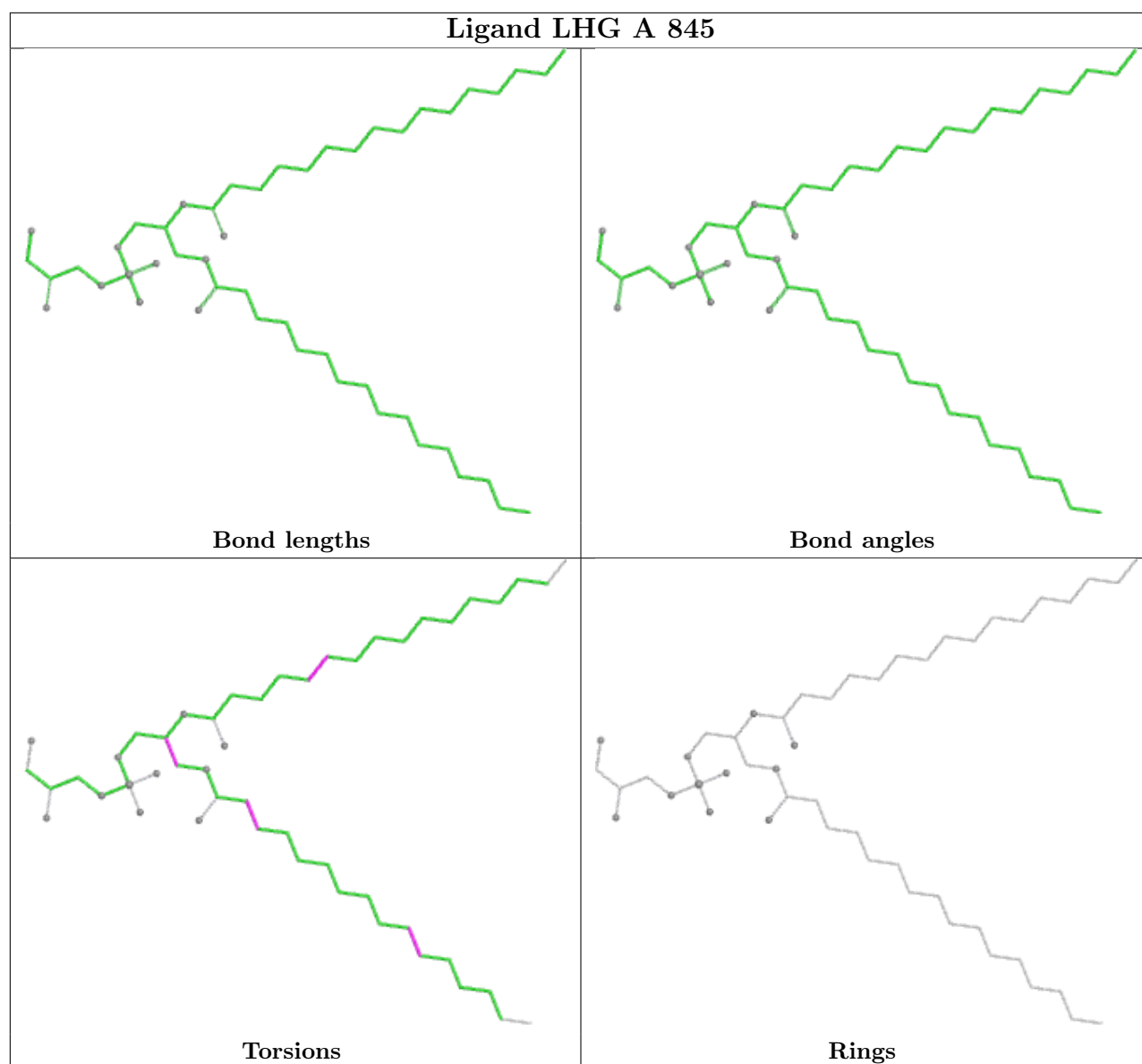


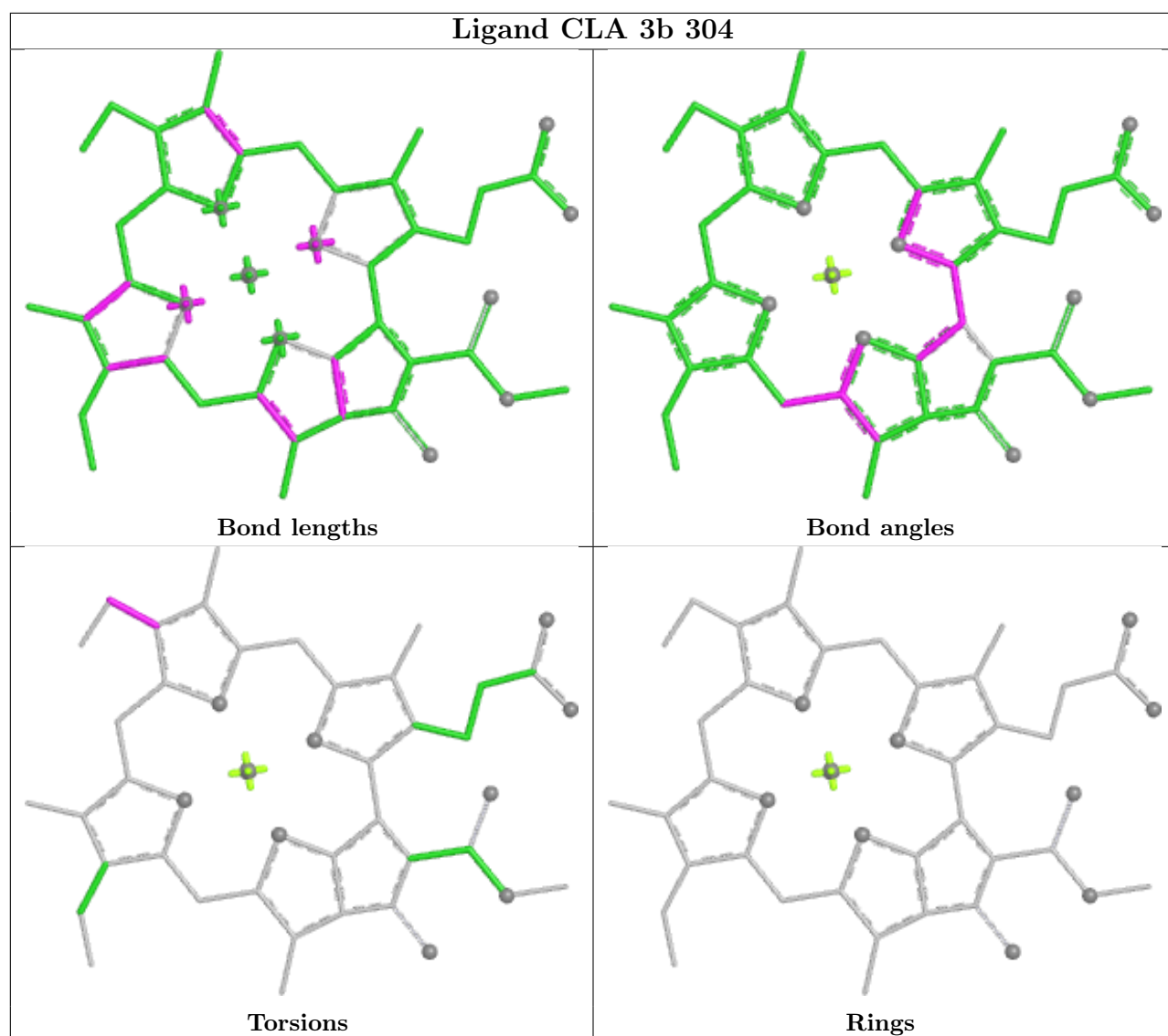












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

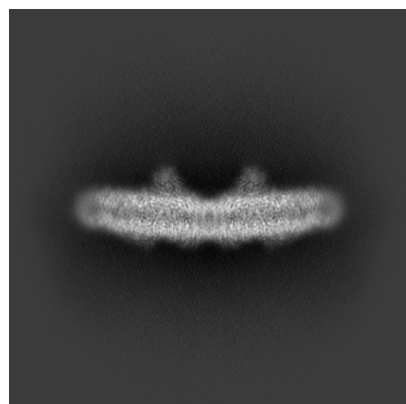
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63405. These allow visual inspection of the internal detail of the map and identification of artifacts.

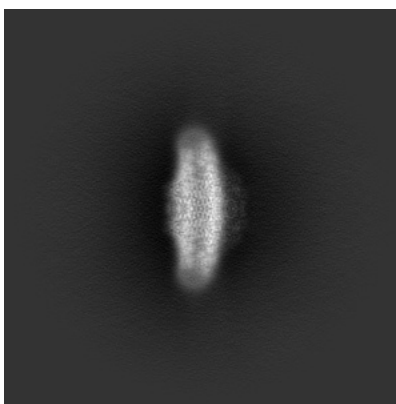
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

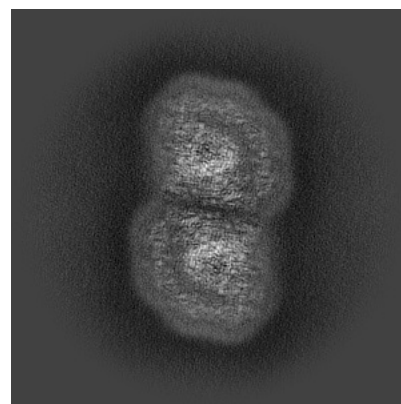
#### 6.1.1 Primary map



X

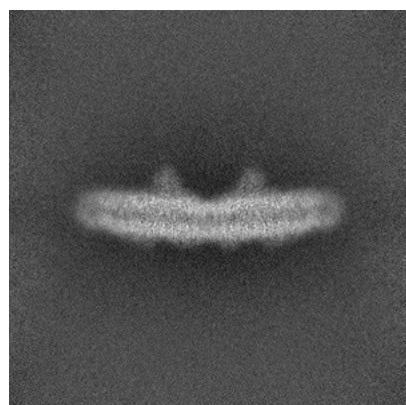


Y

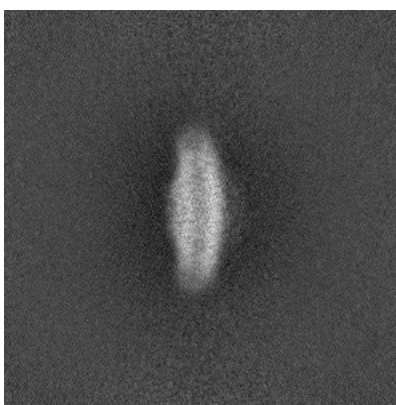


Z

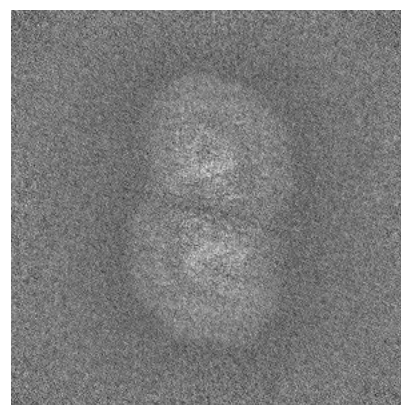
#### 6.1.2 Raw map



X



Y



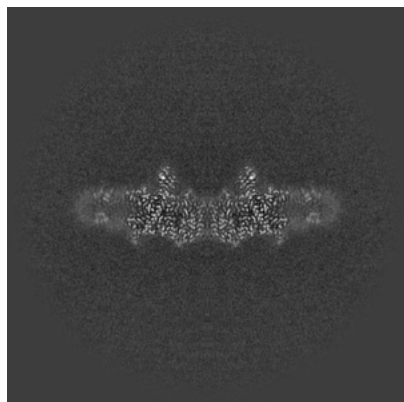
Z

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

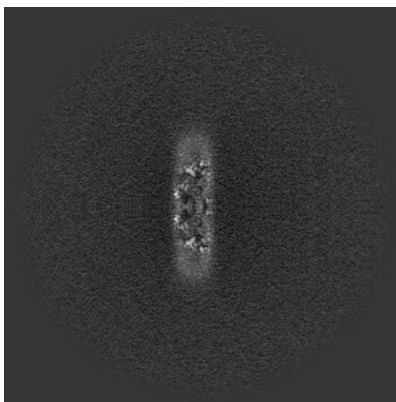


## 6.2 Central slices [i](#)

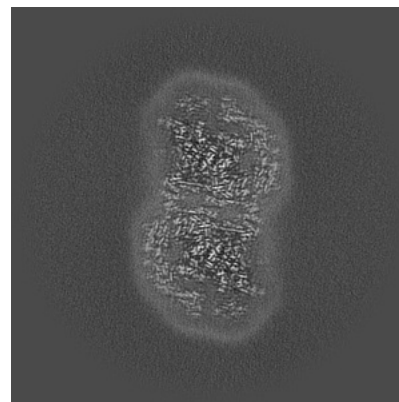
### 6.2.1 Primary map



X Index: 320

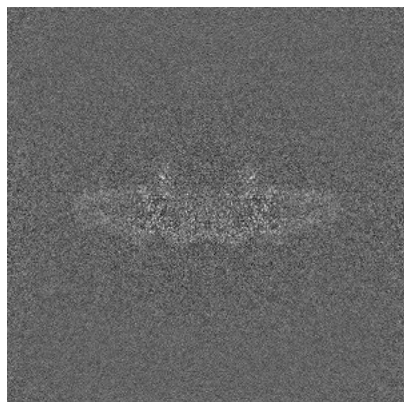


Y Index: 320

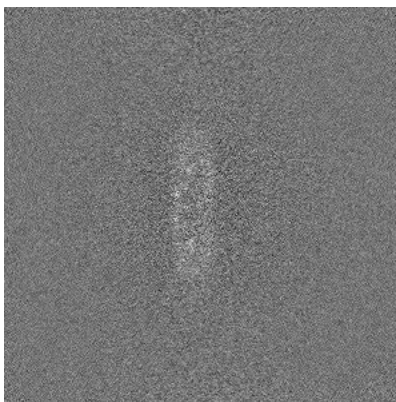


Z Index: 320

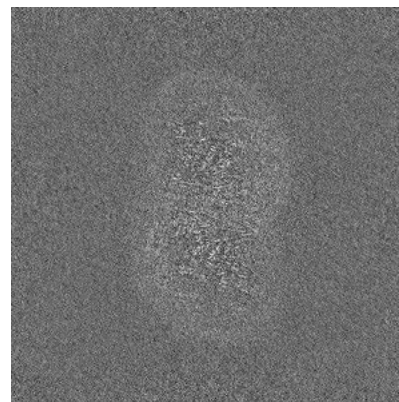
### 6.2.2 Raw map



X Index: 320



Y Index: 320



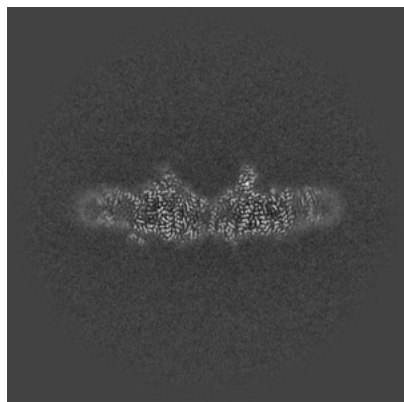
Z Index: 320

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

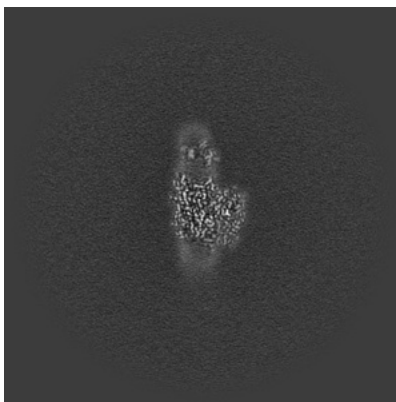


## 6.3 Largest variance slices [i](#)

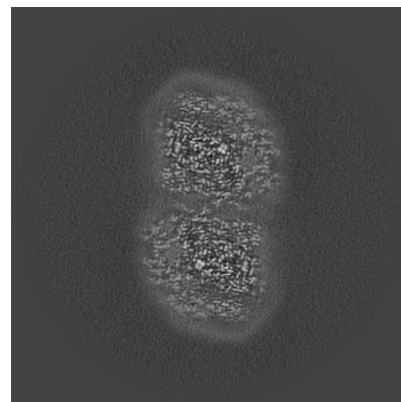
### 6.3.1 Primary map



X Index: 308

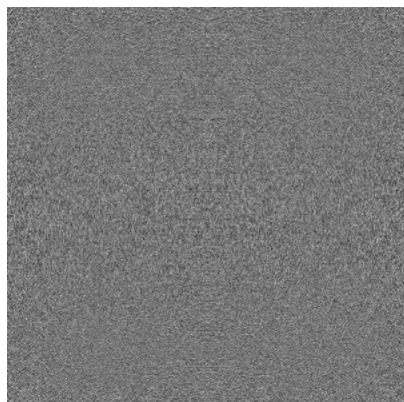


Y Index: 385

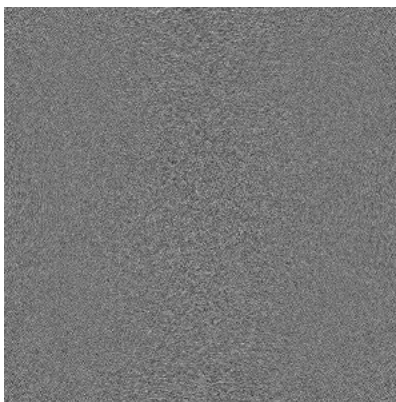


Z Index: 330

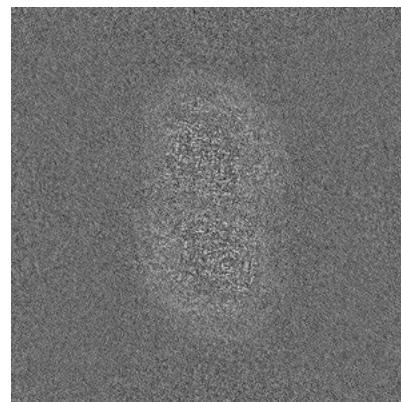
### 6.3.2 Raw map



X Index: 0



Y Index: 0

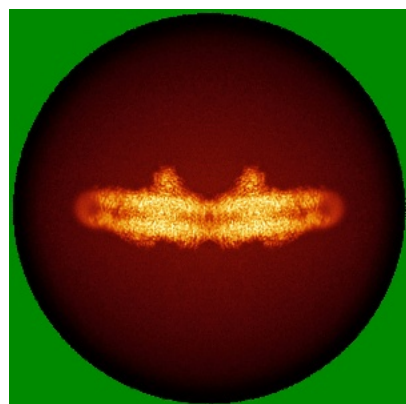


Z Index: 329

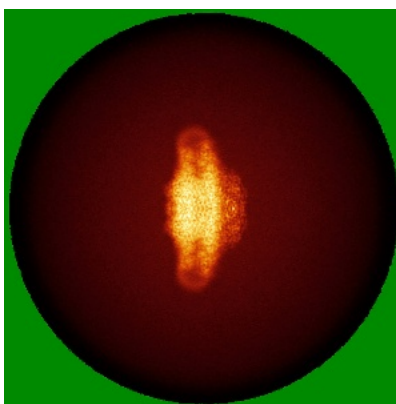
The images above show the largest variance slices of the map in three orthogonal directions.

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

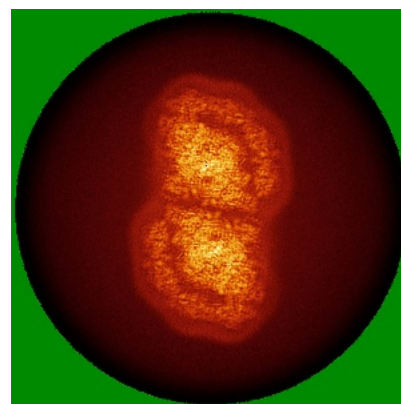
### 6.4.1 Primary map



X

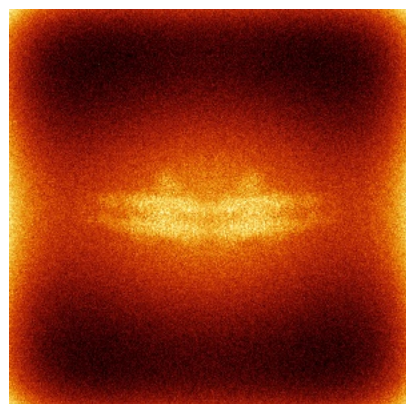


Y

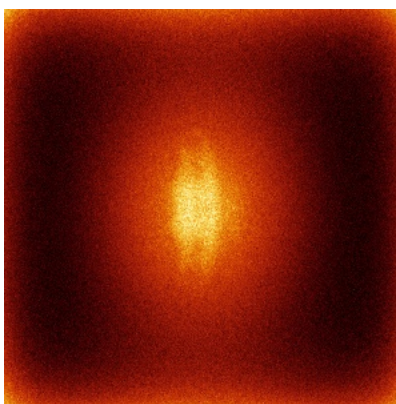


Z

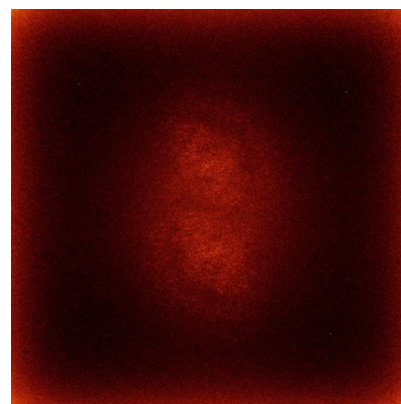
### 6.4.2 Raw map



X



Y

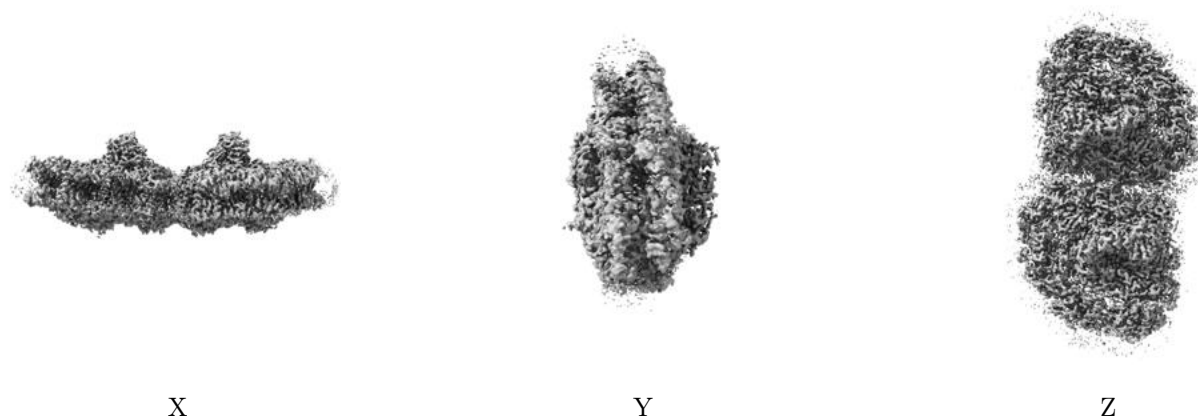


Z

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.

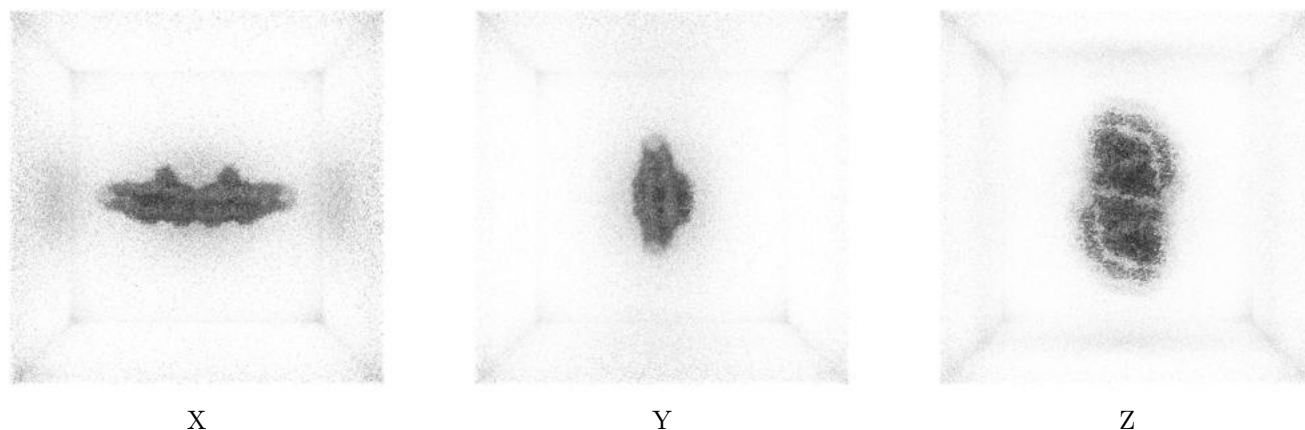
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



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

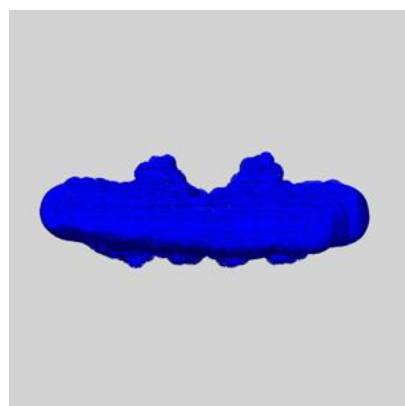
## 6.6 Mask visualisation [i](#)

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

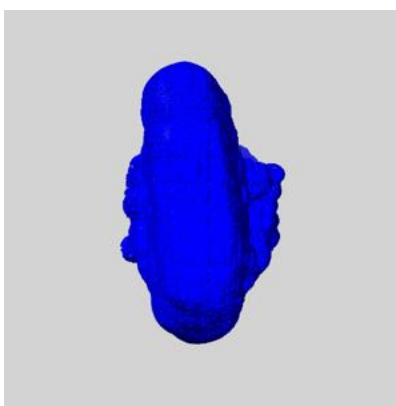
A mask typically either:

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

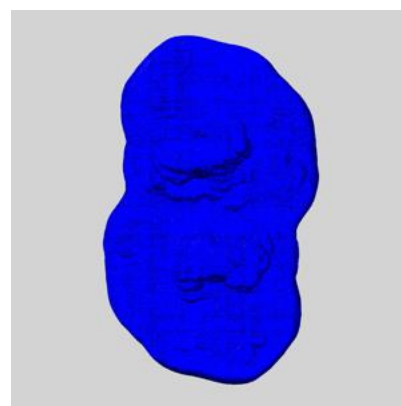
### 6.6.1 emd\_63405\_msk\_1.map [i](#)



X



Y

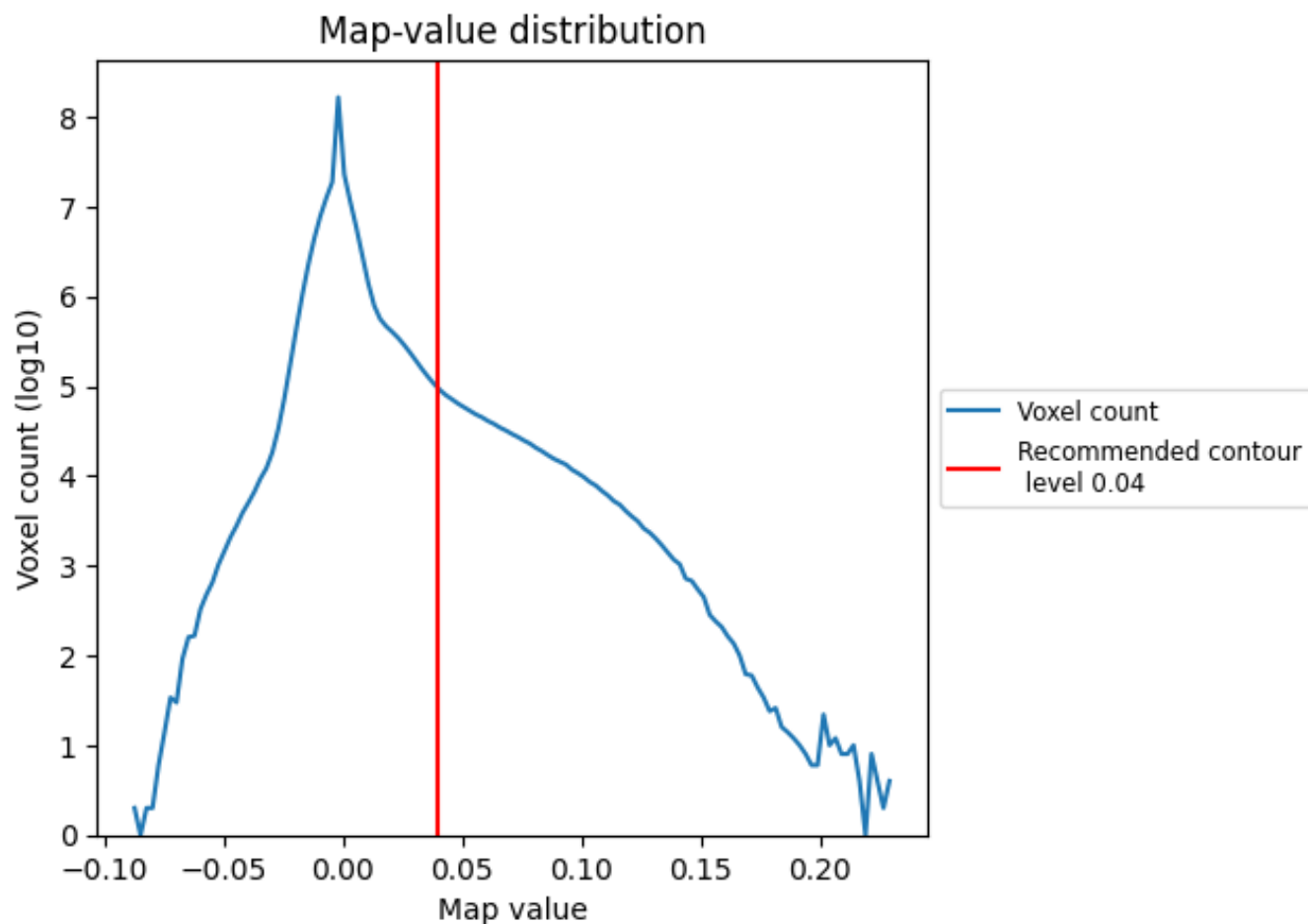


Z

## 7 Map analysis [i](#)

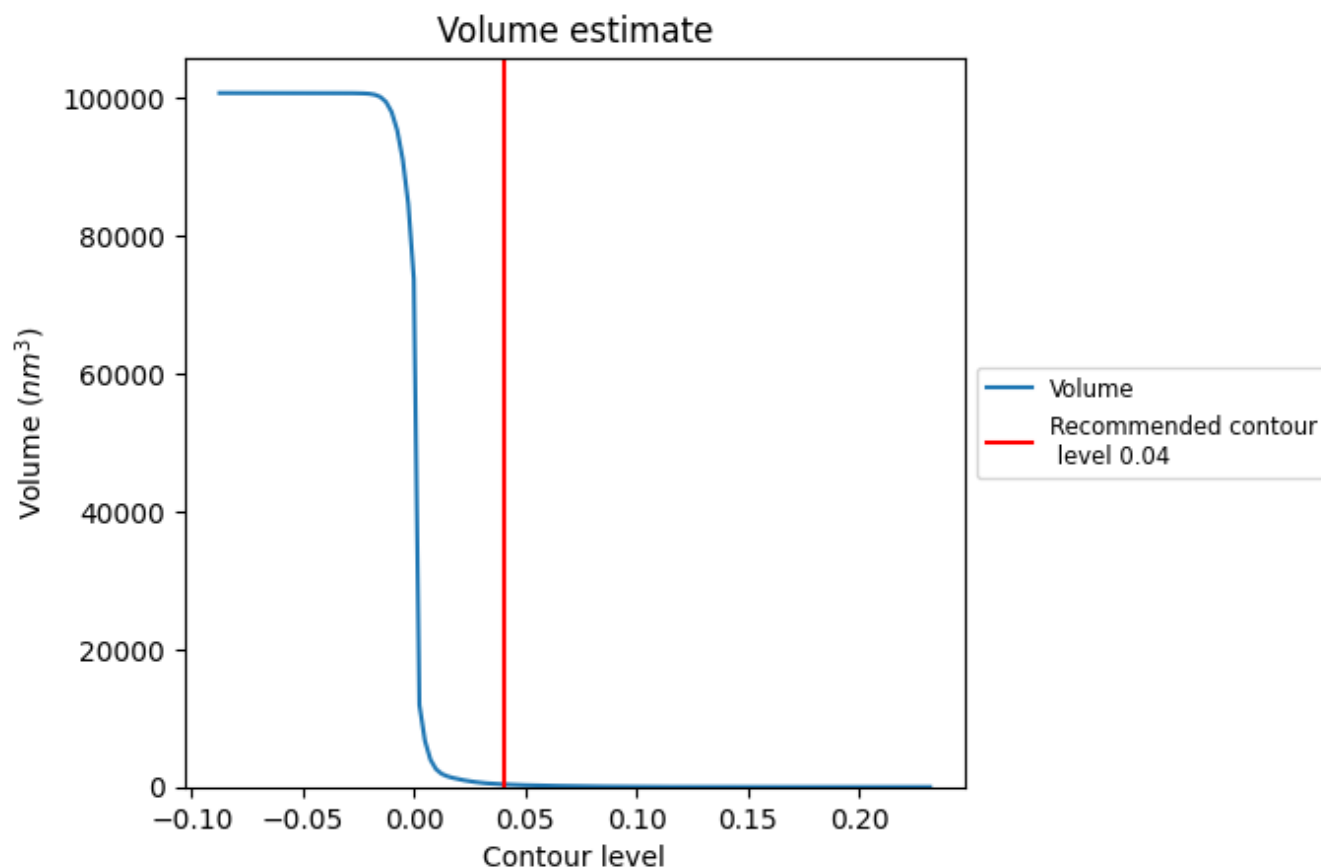
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

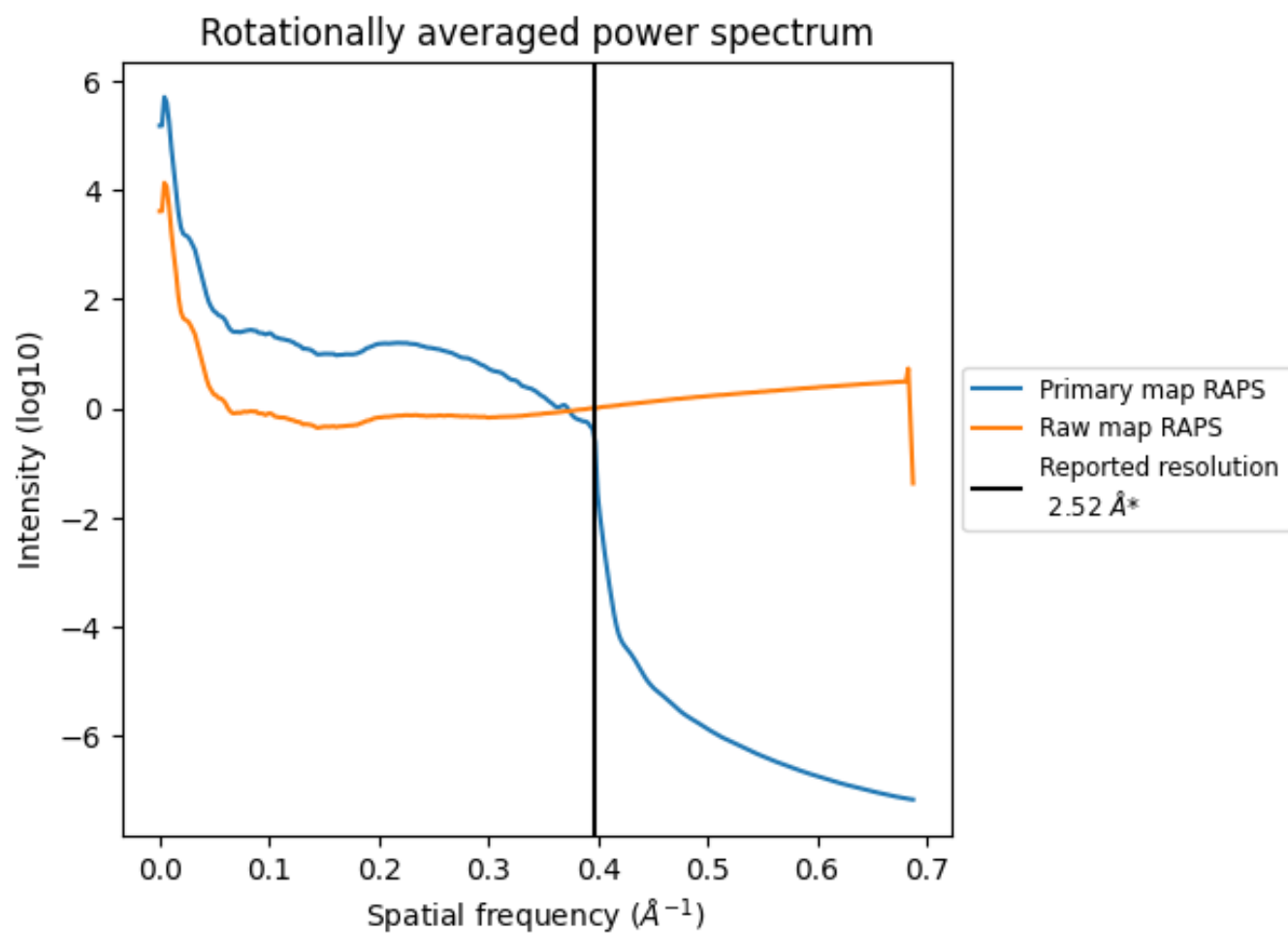


The volume at the recommended contour level is 380  $\text{nm}^3$ ; this corresponds to an approximate mass of 343 kDa.

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 ⓘ

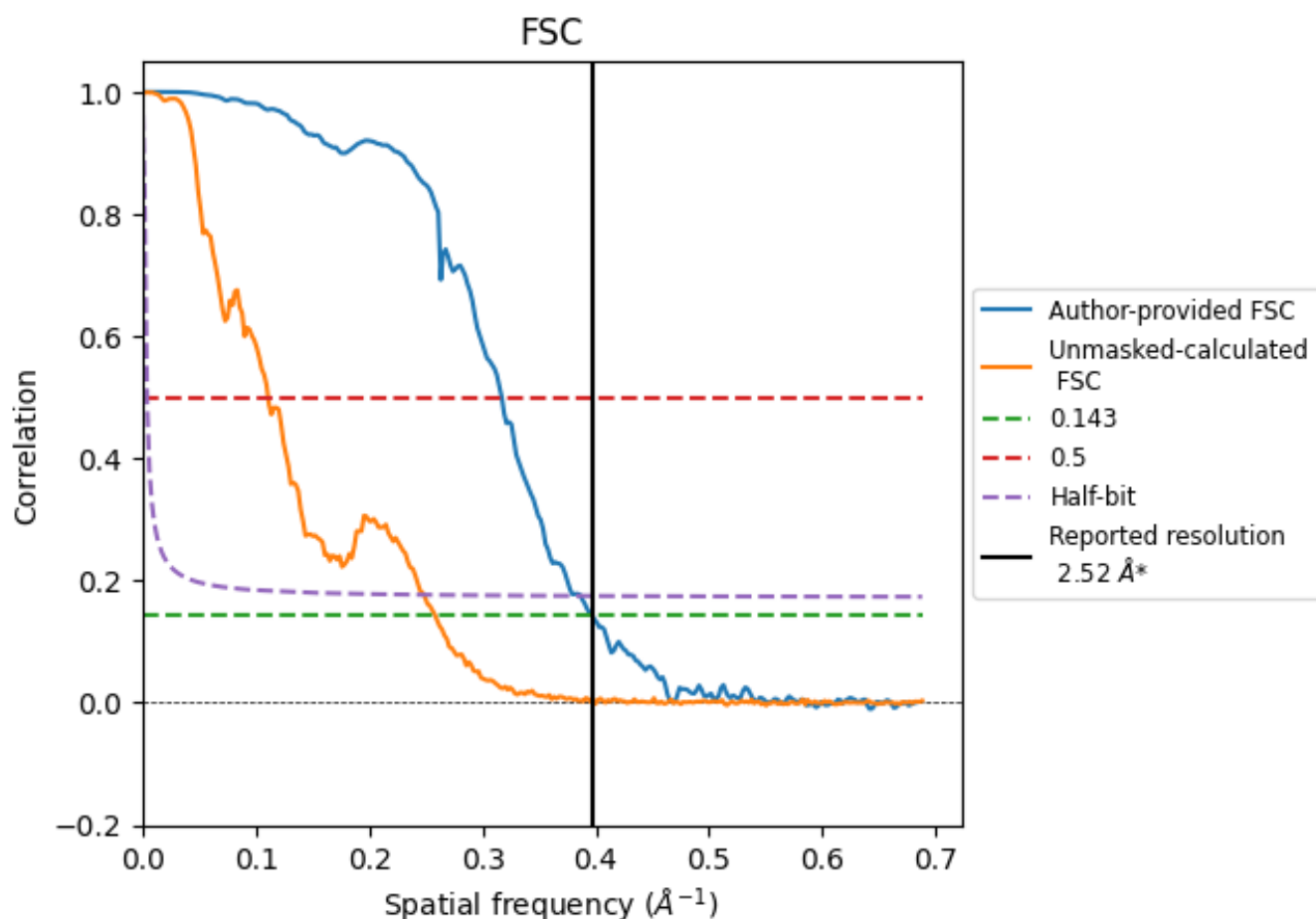


\*Reported resolution corresponds to spatial frequency of 0.397  $\text{\AA}^{-1}$

## 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 0.397  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

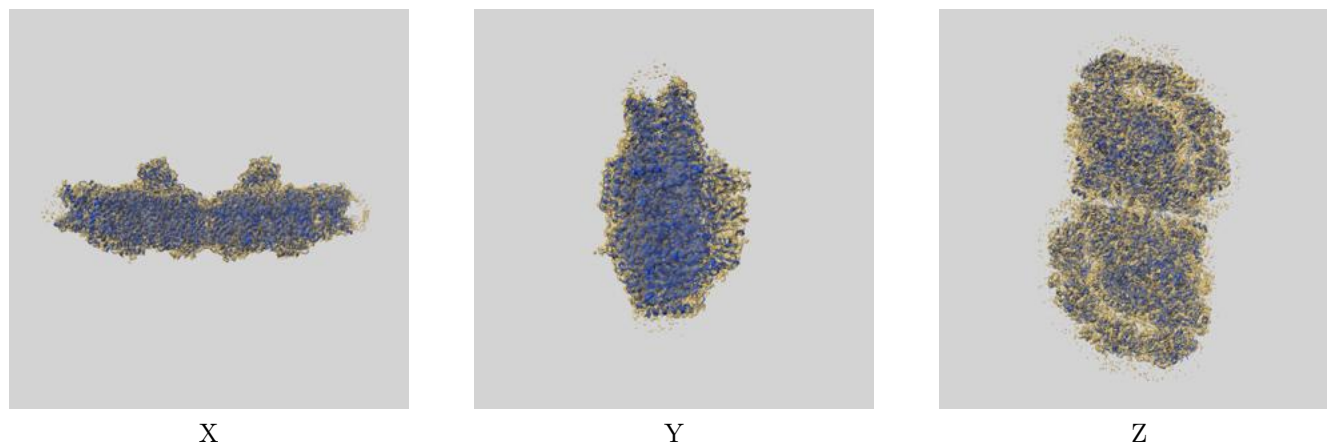
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.52	3.15	2.59
Unmasked-calculated*	3.87	9.01	4.03

\*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 3.87 differs from the reported value 2.52 by more than 10 %

## 9 Map-model fit [i](#)

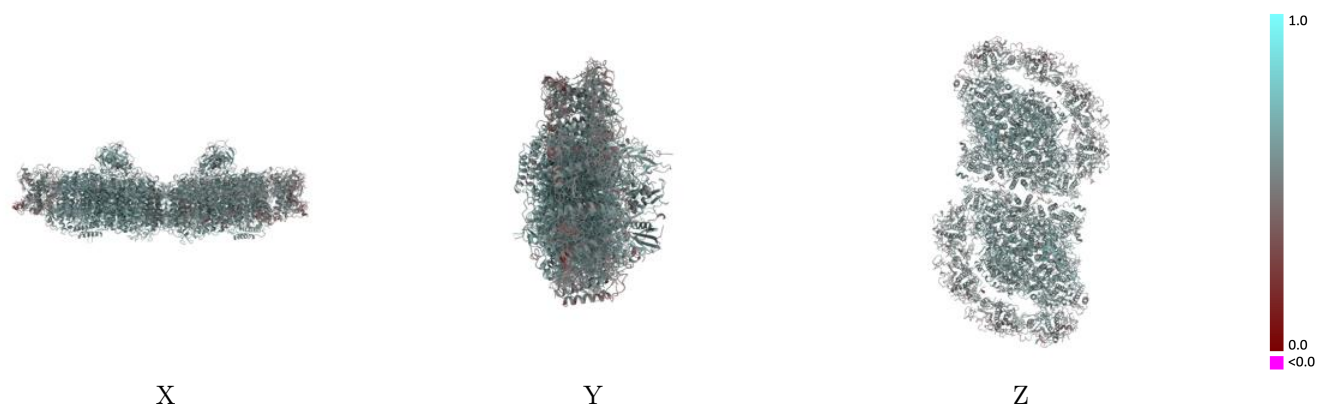
This section contains information regarding the fit between EMDB map EMD-63405 and PDB model 9LUU. Per-residue inclusion information can be found in section [3](#) on page [39](#).

### 9.1 Map-model overlay [i](#)



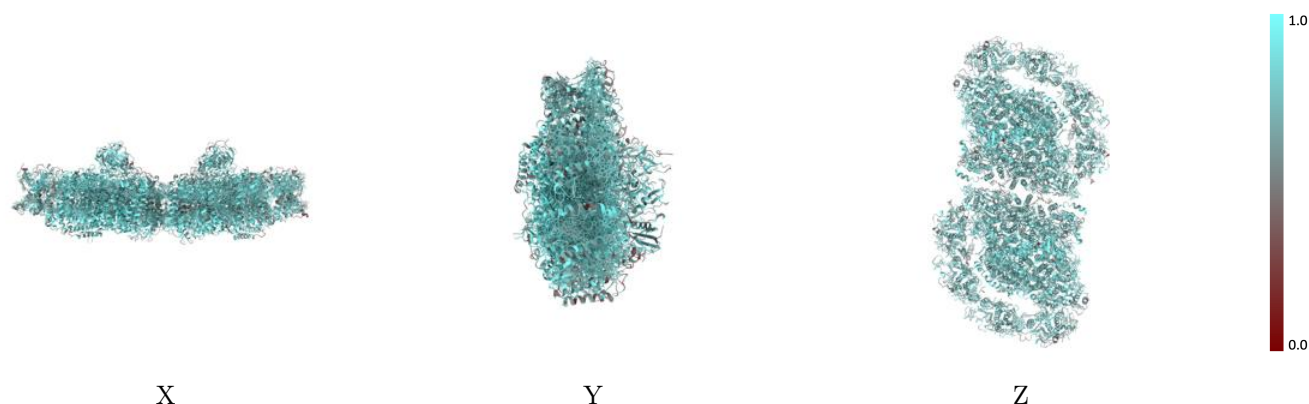
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



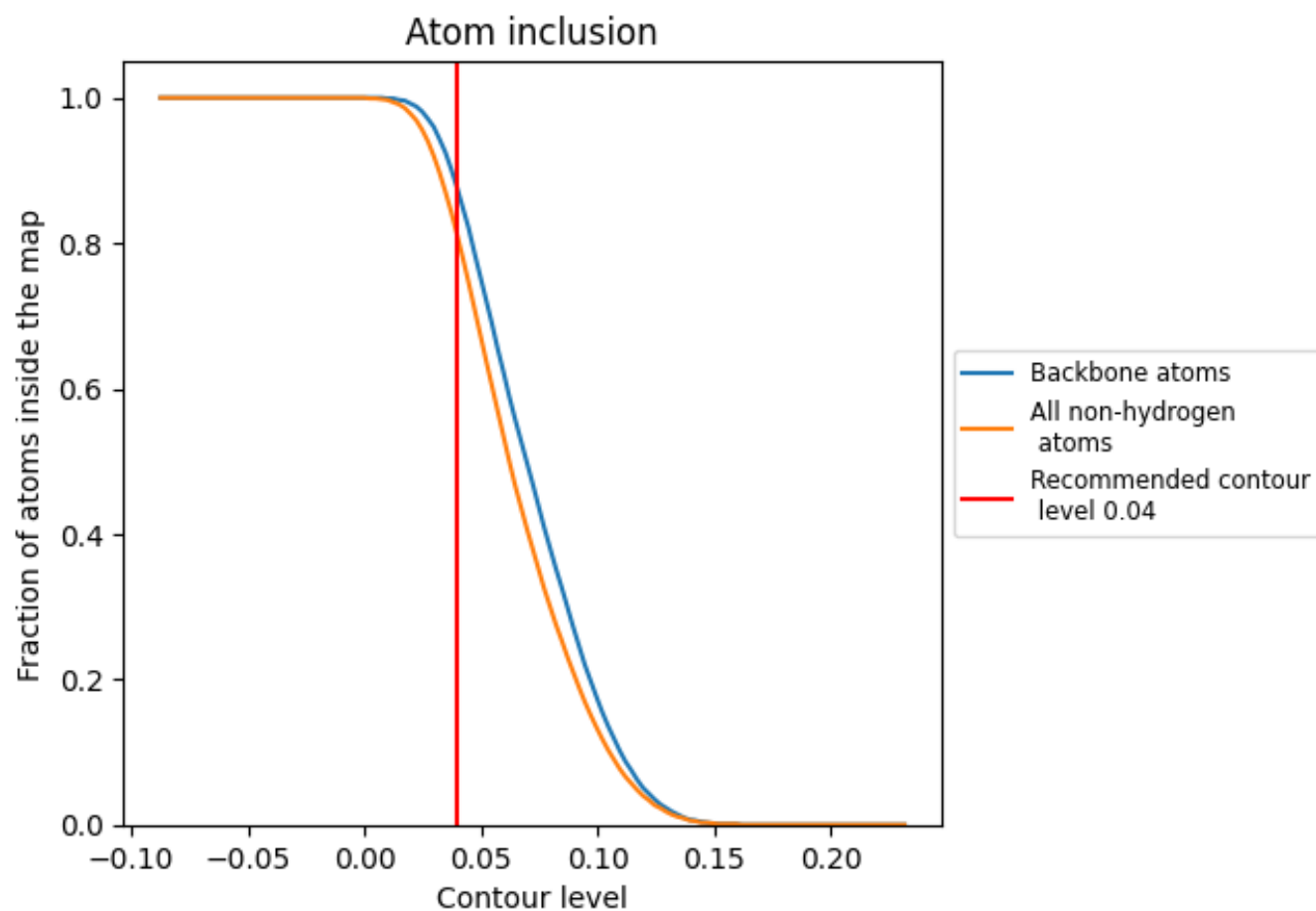
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.5640
2a	 0.7070	 0.4850
2b	 0.7070	 0.4870
3a	 0.6950	 0.4870
3b	 0.6940	 0.4880
5a	 0.7140	 0.4950
5b	 0.7150	 0.4950
6a	 0.7250	 0.5070
6b	 0.7260	 0.5080
A	 0.8850	 0.6030
B	 0.8810	 0.6040
C	 0.8490	 0.5870
D	 0.7440	 0.5700
E	 0.7300	 0.5650
F	 0.8140	 0.5760
G	 0.7850	 0.5660
H	 0.6830	 0.5330
I	 0.7670	 0.5560
J	 0.8440	 0.5740
K	 0.6270	 0.4780
L	 0.7730	 0.5640
M	 0.7350	 0.5420
a	 0.8850	 0.6030
b	 0.8810	 0.6040
c	 0.8480	 0.5880
d	 0.7440	 0.5710
e	 0.7320	 0.5630
f	 0.8120	 0.5750
g	 0.7830	 0.5670
h	 0.6850	 0.5350
i	 0.7670	 0.5520
j	 0.8460	 0.5740
k	 0.6270	 0.4800
l	 0.7740	 0.5650
m	 0.7350	 0.5450

