



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 02:19 AM JST

PDB ID : 6LY5 / pdb_00006ly5
EMDB ID : EMD-30012
Title : Organization and energy transfer in a huge diatom PSI-FCPI supercomplex
Authors : Xiong, P.; Caizhe, X.
Deposited on : 2020-02-13
Resolution : 2.38 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

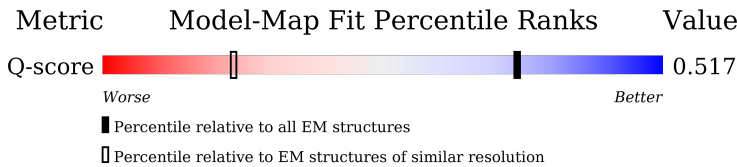
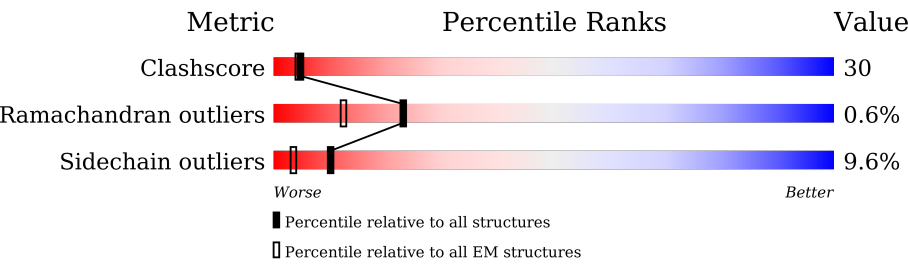
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.38 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	4811 (1.88 - 2.88)

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

Mol	Chain	Length	Quality of chain
1	A	168	65%31%.
2	B	223	38%17%.41%
3	C	198	58%20%5%18%
4	D	207	56%20%7%17%

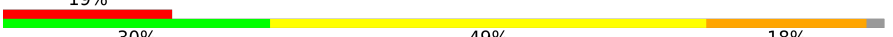
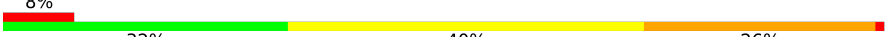
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Mol	Chain	Length	Quality of chain
5	E	222	
6	F	215	
7	G	245	
8	H	203	
9	I	195	
10	J	200	
11	K	207	
12	L	229	
13	M	306	
14	N	219	
15	O	205	
15	P	205	
15	Q	205	
16	R	246	
17	S	254	
18	T	207	
19	W	198	
19	X	198	
20	a	743	
21	b	733	
22	c	80	
23	d	132	
24	e	63	
25	f	162	
26	i	40	

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Mol	Chain	Length	Quality of chain
27	j	42	
28	l	172	
29	m	29	
30	g	134	
31	h	139	
32	U	160	
33	V	179	

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
34	DD6	L	305	-	-	X	-
34	DD6	W	204	-	-	X	-
34	DD6	W	205	-	-	X	-
35	A86	Q	316	-	-	X	-
35	A86	S	304	-	-	X	-
35	A86	V	301	-	-	X	-
35	A86	X	314	-	-	X	-
36	CLA	A	306	X	-	-	-
36	CLA	C	207	X	-	-	-
36	CLA	D	309	X	-	-	-
36	CLA	E	313	X	-	-	-
36	CLA	E	315	X	-	X	-
36	CLA	F	317	X	-	X	-
36	CLA	G	315	X	-	X	-
36	CLA	I	305	X	-	-	-
36	CLA	I	306	X	-	-	-
36	CLA	I	308	X	-	X	-
36	CLA	K	307	X	-	-	-
36	CLA	K	310	X	-	X	-
36	CLA	L	308	X	-	X	-
36	CLA	O	316	X	-	X	-
36	CLA	Q	314	-	-	X	-
36	CLA	U	306	X	-	X	-
36	CLA	V	305	-	-	X	-
36	CLA	V	306	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	V	314	X	-	X	-
36	CLA	W	212	-	-	X	-
36	CLA	X	315	-	-	X	-
36	CLA	a	802	X	-	-	-
36	CLA	a	806	X	-	-	-
36	CLA	a	816	X	-	X	-
36	CLA	a	823	X	-	-	-
36	CLA	a	825	X	-	-	-
36	CLA	a	848	X	-	-	-
36	CLA	b	816	X	-	-	-
36	CLA	b	817	X	-	-	-
36	CLA	b	836	X	-	-	-
36	CLA	f	803	X	-	-	-
36	CLA	f	804	X	-	-	-
36	CLA	j	102	X	-	-	-
36	CLA	l	205	X	-	-	-
39	LMT	F	321	-	-	X	-
39	LMT	h	205	-	-	X	-
41	LHG	E	322	-	-	X	-
41	LHG	f	808	-	-	X	-
41	LHG	i	104	-	-	X	-
42	LMG	J	318	-	-	X	-
42	LMG	V	316	-	-	X	-
42	LMG	j	105	-	-	X	-

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 81344 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 FCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	168	Total	C	N	O	S	0	0
			1287	825	213	237	12		

- Molecule 2 is a protein called FCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1013	662	166	176	9		

- Molecule 3 is a protein called FCPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	163	Total	C	N	O	S	0	0
			1247	796	210	232	9		

- Molecule 4 is a protein called FCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	172	Total	C	N	O	S	0	0
			1337	870	214	245	8		

- Molecule 5 is a protein called FCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	188	Total	C	N	O	S	0	0
			1411	891	240	265	15		

- Molecule 6 is a protein called FCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	180	Total	C	N	O	S	0	0
			1375	880	230	253	12		

- Molecule 7 is a protein called FCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	214	Total	C	N	O	S	0	0
			1668	1079	276	305	8		

- Molecule 8 is a protein called FCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	170	Total	C	N	O	S	0	0
			1291	832	213	236	10		

- Molecule 9 is a protein called FCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	161	Total	C	N	O	S	0	0
			1250	807	208	228	7		

- Molecule 10 is a protein called FCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1301	843	217	236	5		

- Molecule 11 is a protein called FCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	169	Total	C	N	O	S	0	0
			1304	850	214	232	8		

- Molecule 12 is a protein called FCPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	196	Total	C	N	O	S	0	0
			1523	989	250	276	8		

- Molecule 13 is a protein called FCPI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	187	Total	C	N	O	S	0	0
			1423	914	248	255	6		

- Molecule 14 is a protein called FCPI-21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	219	Total	C	N	O	S	0	0
			1716	1119	282	309	6		

- Molecule 15 is a protein called FCPI.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		
15	P	173	Total	C	N	O	S	0	0
			1296	834	213	241	8		
15	Q	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		

- Molecule 16 is a protein called FCPI-24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	211	Total	C	N	O	S	0	0
			1628	1061	266	294	7		

- Molecule 17 is a protein called FCPI-23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	220	Total	C	N	O	S	0	0
			1722	1122	283	311	6		

- Molecule 18 is a protein called FCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	172	Total	C	N	O	S	0	0
			1326	848	226	247	5		

- Molecule 19 is a protein called FCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	160	Total	C	N	O	S	0	0
			1239	799	203	233	4		
19	X	161	Total	C	N	O	S	1	0
			1253	808	207	234	4		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	742	Total	C	N	O	S	0	0
			5858	3826	991	1013	28		

- Molecule 21 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	732	Total	C	N	O	S	1	0
			5820	3828	980	994	18		

- Molecule 22 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	80	Total	C	N	O	S	0	0
			597	368	104	114	11		

- Molecule 23 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	132	Total	C	N	O	S	1	0
			1056	681	186	186	3		

- Molecule 24 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	63	Total	C	N	O	0	0
			507	321	90	96		

- Molecule 25 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	162	Total	C	N	O	S	0	0
			1223	789	211	220	3		

- Molecule 26 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	i	33	Total	C	N	O	S	0	0
			256	176	40	38	2		

- Molecule 27 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	41	Total	C	N	O	S	0	0
			324	219	50	54	1		

- Molecule 28 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	l	144	Total	C	N	O	S	0	0
			1094	726	178	187	3		

- Molecule 29 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	m	28	Total	C	N	O	S	0	0
			198	130	32	34	2		

- Molecule 30 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	134	Total	C	N	O	S	0	0
			670	402	134	134			

- Molecule 31 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	89	Total	C	N	O	S	0	0
			676	440	110	120	6		

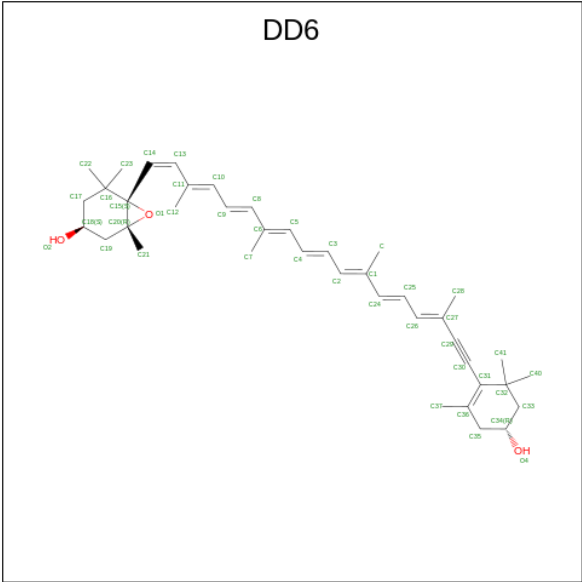
- Molecule 32 is a protein called FCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	156	Total	C	N	O	S	0	0
			1194	766	199	221	8		

- Molecule 33 is a protein called FCPI-19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	179	Total	C	N	O	S	0	0
			1361	871	234	252	4		

- Molecule 34 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃).



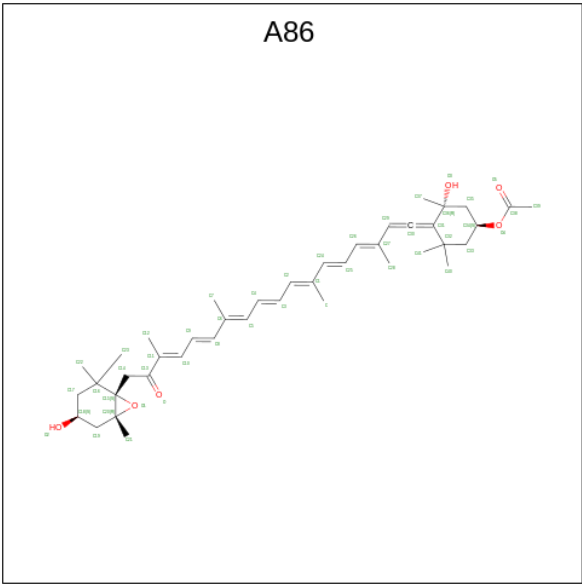
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	C	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
34	F	1	Total 43	C 40	O 3	0
34	G	1	Total 43	C 40	O 3	0
34	H	1	Total 43	C 40	O 3	0
34	H	1	Total 43	C 40	O 3	0
34	I	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	L	1	Total 43	C 40	O 3	0
34	M	1	Total 43	C 40	O 3	0
34	O	1	Total 43	C 40	O 3	0
34	P	1	Total 43	C 40	O 3	0
34	Q	1	Total 43	C 40	O 3	0
34	R	1	Total 43	C 40	O 3	0
34	R	1	Total 43	C 40	O 3	0
34	S	1	Total 43	C 40	O 3	0
34	S	1	Total 43	C 40	O 3	0
34	W	1	Total 43	C 40	O 3	0
34	W	1	Total 43	C 40	O 3	0
34	a	1	Total 43	C 40	O 3	0
34	j	1	Total 43	C 40	O 3	0

- Molecule 35 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	42	6	
35	A	1	Total	C	O	0
			48	42	6	
35	B	1	Total	C	O	0
			48	42	6	
35	B	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	D	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	H	1	Total	C	O	0
			48	42	6	
35	H	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	K	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	

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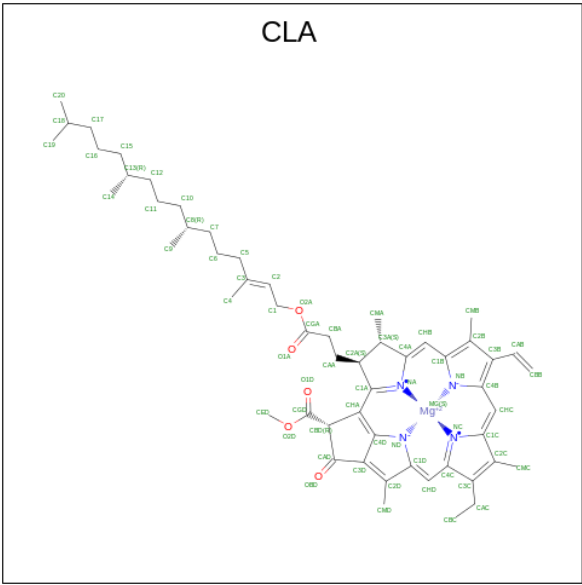
Mol	Chain	Residues	Atoms			AltConf
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	W	1	Total	C	O	0
			48	42	6	
35	W	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	h	1	Total	C	O	0
			48	42	6	
35	h	1	Total	C	O	0
			48	42	6	
35	U	1	Total	C	O	0
			48	42	6	
35	U	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	U	1	Total	C	O	0
			48	42	6	
35	U	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	

- Molecule 36 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	C	1	Total 43	C 35	Mg 1	N 4	O 3	0
36	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	D	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	D	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	D	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	E	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	F	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	F	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	H	1	Total 48	C 38	Mg 1	N 4	O 5	0
36	H	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	H	1	Total 64	C 54	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	I	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	I	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	J	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	J	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	K	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	K	1	Total 59	C 49	Mg 1	N 4	O 5	0
36	K	1	Total 62	C 52	Mg 1	N 4	O 5	0
36	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	M	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	M	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	M	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	N	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
36	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	N	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	N	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
36	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	N	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	O	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	O	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	O	1	Total 40	C 32	Mg 1	N 4	O 3	0
36	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	P	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	P	1	Total 51	C 41	Mg 1	N 4	O 5	0
36	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 45	C 37	Mg 1	N 4	O 3	0
36	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	T	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	W	1	Total 48	C 38	Mg 1	N 4	O 5	0
36	W	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	W	1	Total 57	C 47	Mg 1	N 4	O 5	0
36	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	W	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	W	1	Total 48	C 38	Mg 1	N 4	O 5	0
36	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	W	1	Total 43	C 35	Mg 1	N 4	O 3	0
36	X	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	X	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	X	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	X	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	X	1	Total 41	C 33	Mg 1	N 4	O 3	0

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

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Mol	Chain	Residues	Atoms					AltConf
36	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
36	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
36	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
36	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	b	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	f	1	Total 52	C 42	Mg 1	N 4	O 5	0

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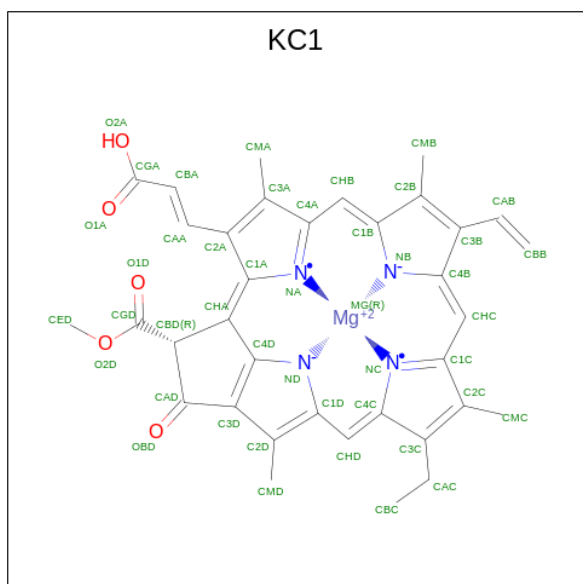
Mol	Chain	Residues	Atoms					AltConf
36	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	V	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	V	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 37 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



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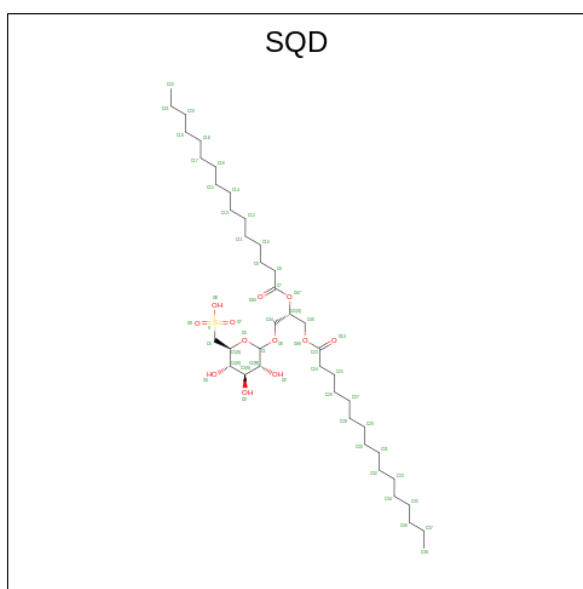
Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

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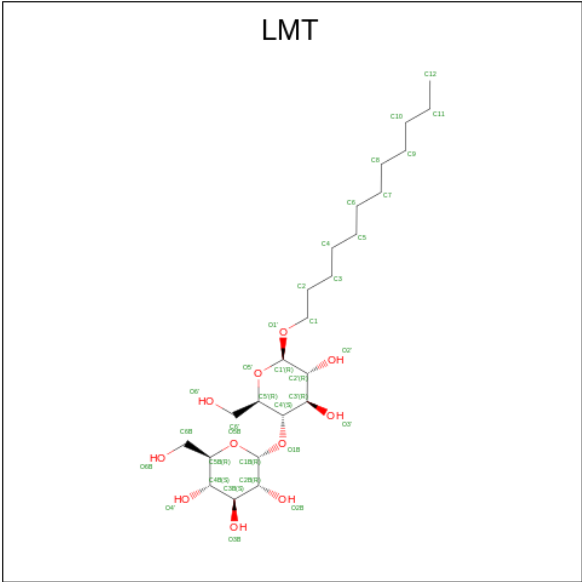
Mol	Chain	Residues	Atoms					AltConf
37	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	O	S	0
			28	15	12	1	
38	b	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 39 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



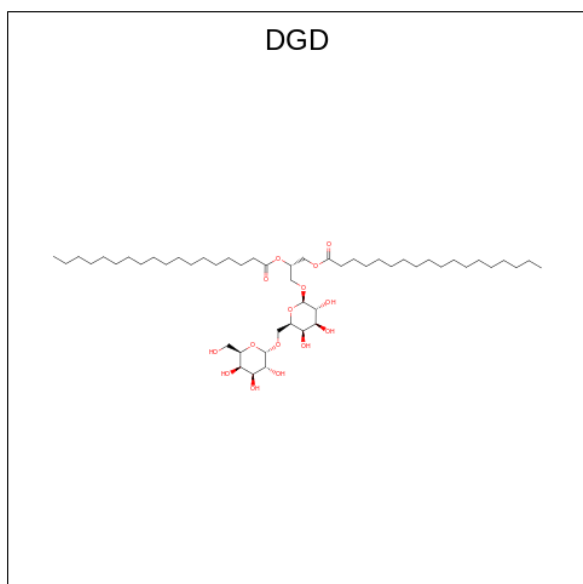
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			35	24	11	
39	B	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			23	17	6	
39	E	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			33	22	11	
39	G	1	Total	C	O	0
			35	24	11	
39	G	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	K	1	Total	C	O	0
			31	20	11	
39	K	1	Total	C	O	0
			35	24	11	
39	L	1	Total	C	O	0
			35	24	11	

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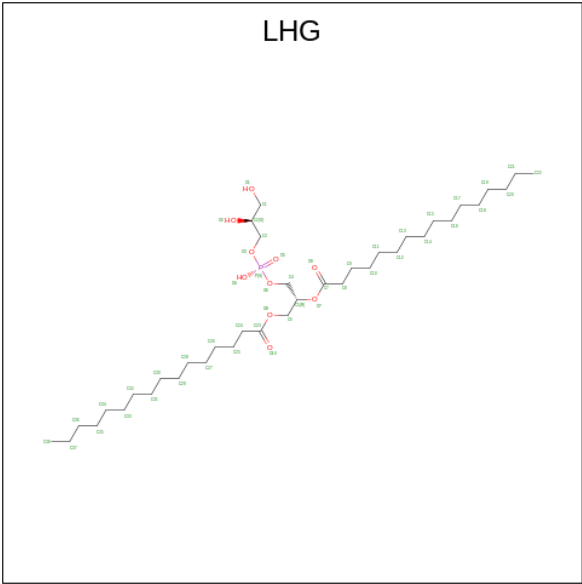
Mol	Chain	Residues	Atoms			AltConf
39	L	1	Total	C	O	0
			31	20	11	
39	P	1	Total	C	O	0
			23	17	6	
39	P	1	Total	C	O	0
			23	17	6	
39	a	1	Total	C	O	0
			35	24	11	
39	a	1	Total	C	O	0
			32	21	11	
39	a	1	Total	C	O	0
			35	24	11	
39	b	1	Total	C	O	0
			35	24	11	
39	b	1	Total	C	O	0
			24	19	5	
39	f	1	Total	C	O	0
			24	18	6	
39	h	1	Total	C	O	0
			35	24	11	
39	U	1	Total	C	O	0
			35	24	11	
39	U	1	Total	C	O	0
			35	24	11	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	C	O	0
			57	42	15	
40	L	1	Total	C	O	0
			47	32	15	
40	b	1	Total	C	O	0
			60	45	15	

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



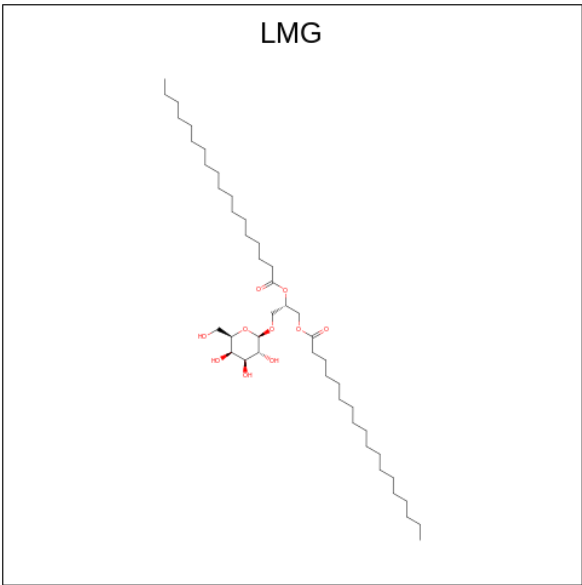
Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total	C	O	P	0
			46	35	10	1	
41	D	1	Total	C	O	P	0
			49	38	10	1	
41	E	1	Total	C	O	P	0
			49	38	10	1	
41	F	1	Total	C	O	P	0
			33	24	8	1	
41	F	1	Total	C	O	P	0
			41	30	10	1	
41	G	1	Total	C	O	P	0
			49	38	10	1	
41	G	1	Total	C	O	P	0
			40	29	10	1	
41	G	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
41	I	1	Total	C	O	P	0
			49	38	10	1	
41	O	1	Total	C	O	P	0
			42	31	10	1	
41	O	1	Total	C	O	P	0
			49	38	10	1	
41	Q	1	Total	C	O	P	0
			49	38	10	1	
41	R	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			48	37	10	1	
41	a	1	Total	C	O	P	0
			27	16	10	1	
41	a	1	Total	C	O	P	0
			47	36	10	1	
41	b	1	Total	C	O	P	0
			49	38	10	1	
41	f	1	Total	C	O	P	0
			49	38	10	1	
41	f	1	Total	C	O	P	0
			42	31	10	1	
41	i	1	Total	C	O	P	0
			46	35	10	1	
41	j	1	Total	C	O	P	0
			49	38	10	1	
41	l	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



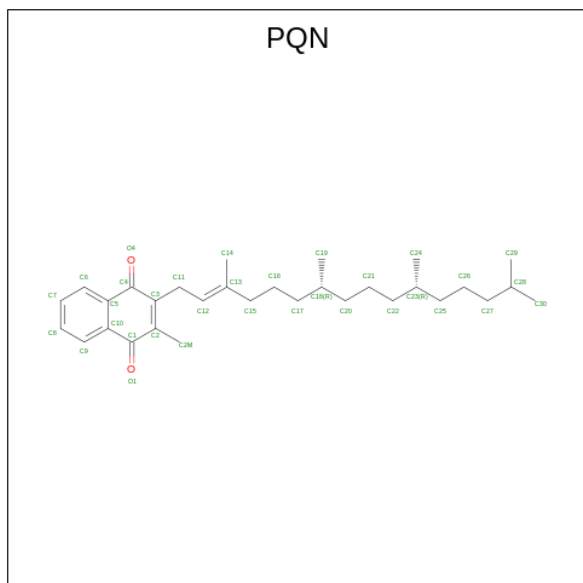
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			46	36	10	
42	D	1	Total	C	O	0
			37	27	10	
42	E	1	Total	C	O	0
			46	36	10	
42	E	1	Total	C	O	0
			40	30	10	
42	G	1	Total	C	O	0
			55	45	10	
42	G	1	Total	C	O	0
			55	45	10	
42	I	1	Total	C	O	0
			55	45	10	
42	J	1	Total	C	O	0
			55	45	10	
42	J	1	Total	C	O	0
			44	34	10	
42	L	1	Total	C	O	0
			33	23	10	
42	a	1	Total	C	O	0
			54	44	10	
42	j	1	Total	C	O	0
			52	42	10	
42	m	1	Total	C	O	0
			37	27	10	
42	h	1	Total	C	O	0
			45	35	10	

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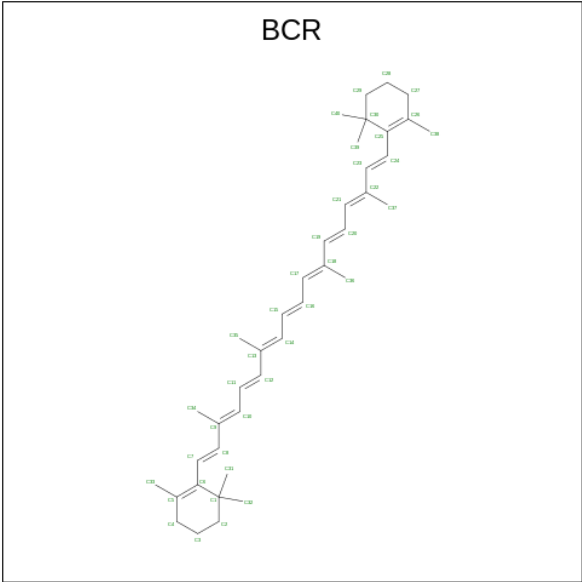
Mol	Chain	Residues	Atoms			AltConf
42	V	1	Total	C	O	0
			46	36	10	
42	V	1	Total	C	O	0
			46	36	10	

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 44 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



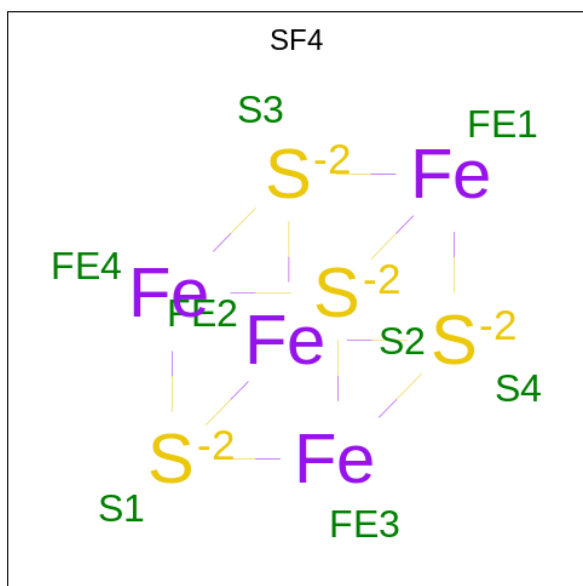
Mol	Chain	Residues	Atoms	AltConf
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	i	1	Total C 40 40	0
44	i	1	Total C 40 40	0
44	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
44	l	1	Total C 40 40	0
44	l	1	Total C 40 40	0
44	m	1	Total C 40 40	0
44	h	1	Total C 40 40	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
45	b	1	Total Fe S 8 4 4	0
45	c	1	Total Fe S 8 4 4	0
45	c	1	Total Fe S 8 4 4	0

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	AltConf
46	a	64	Total O 64 64	0
46	b	72	Total O 72 72	0

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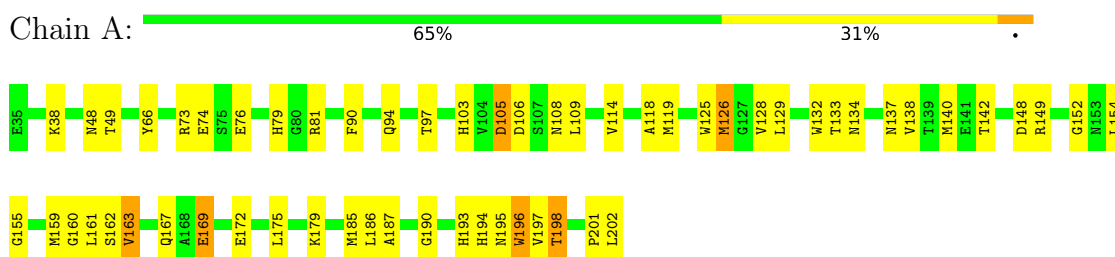
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Mol	Chain	Residues	Atoms		AltConf
46	c	7	Total 7	O 7	0
46	d	4	Total 4	O 4	0
46	f	2	Total 2	O 2	0
46	j	1	Total 1	O 1	0
46	l	3	Total 3	O 3	0

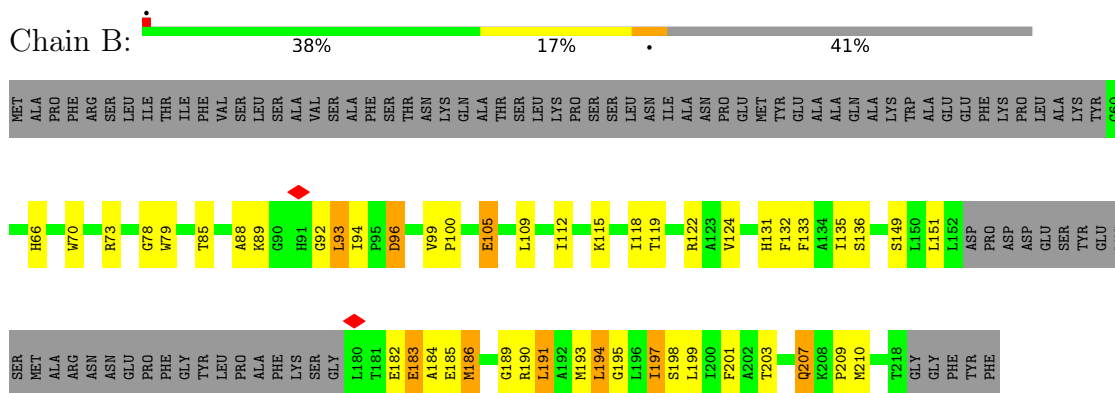
3 Residue-property plots

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

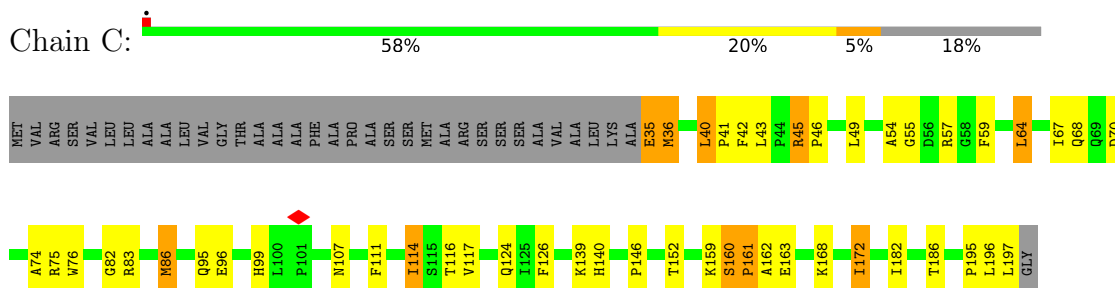
• Molecule 1: FCPI-7



• Molecule 2: FCPI-1

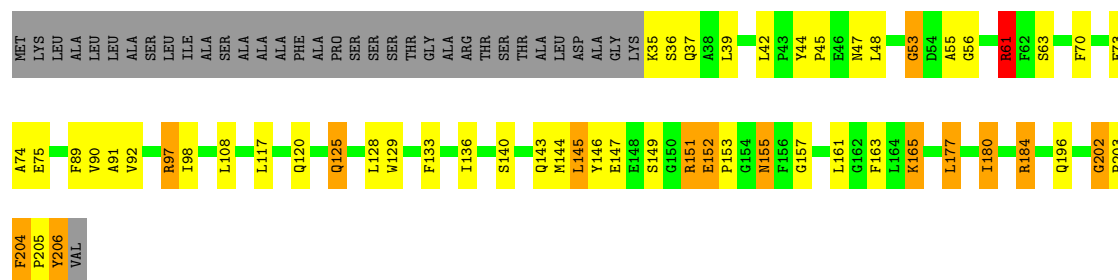


• Molecule 3: FCPI-11



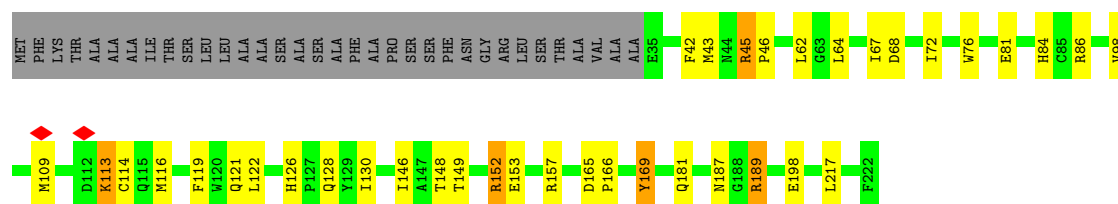
• Molecule 4: FCPI-6





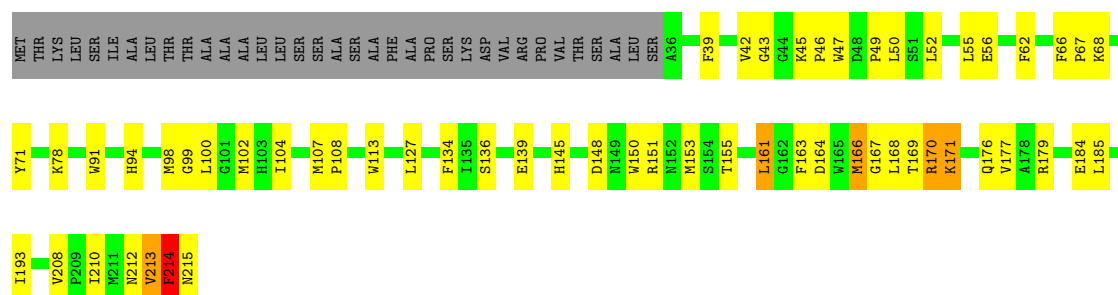
• Molecule 5: FCPI-5

Chain E: 68% 15% 15%



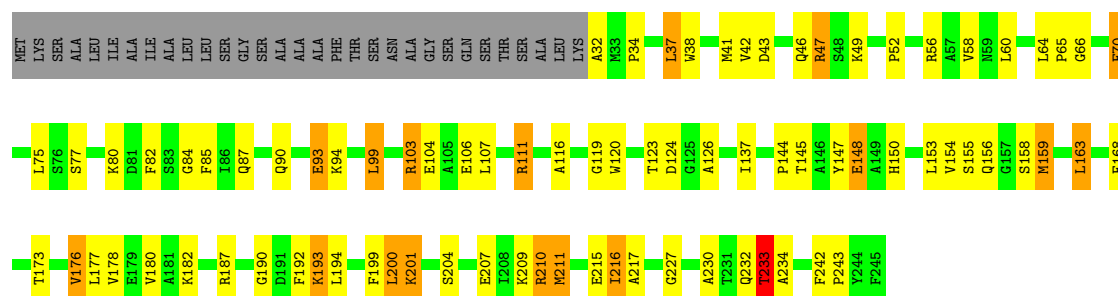
• Molecule 6: FCPI-8

Chain F: 57% 24% 16%



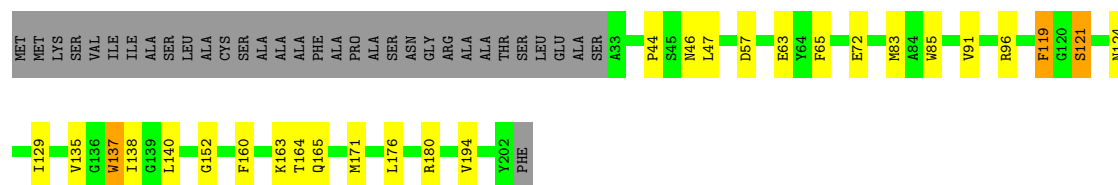
• Molecule 7: FCPI-4

Chain G: 53% 27% 7% 13%

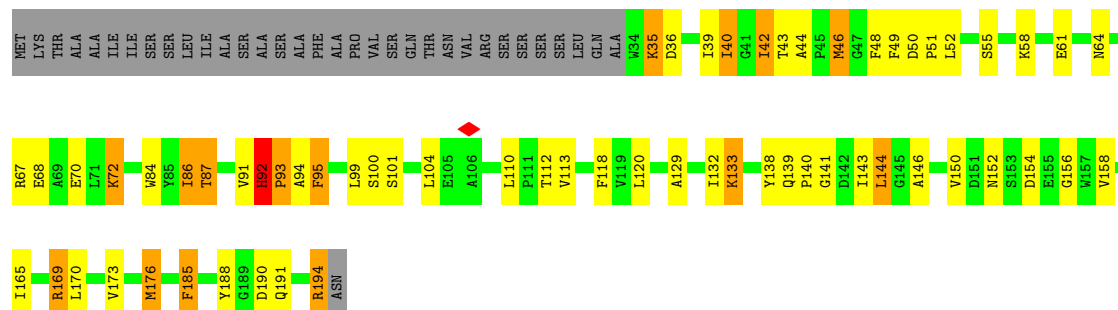


• Molecule 8: FCPI-10

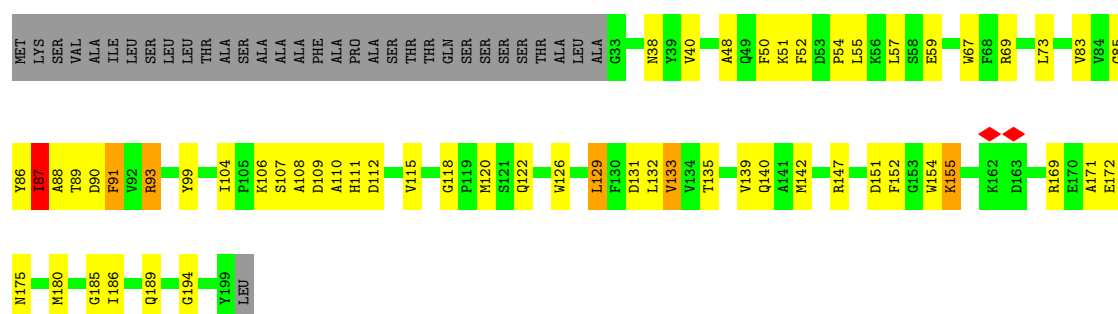
Chain H: 70% 12% 16%



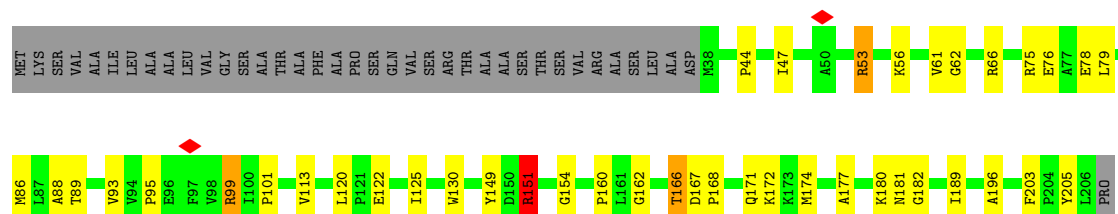
- Molecule 9: FCPI-3



- Molecule 10: FCPI-9

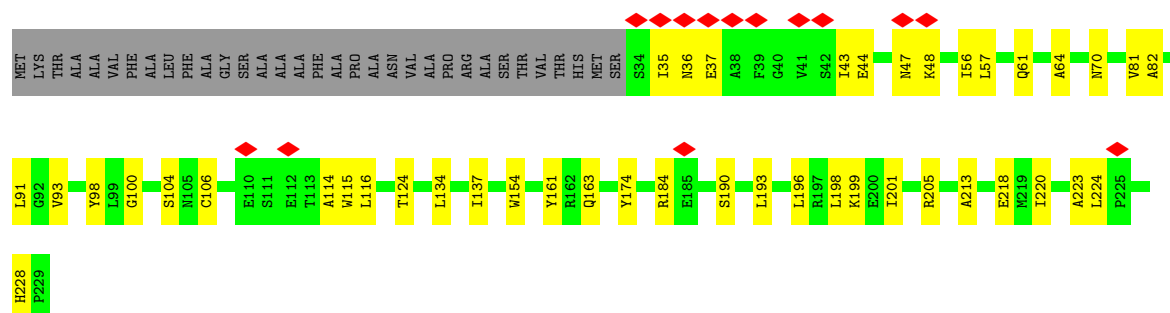


- Molecule 11: FCPI-13



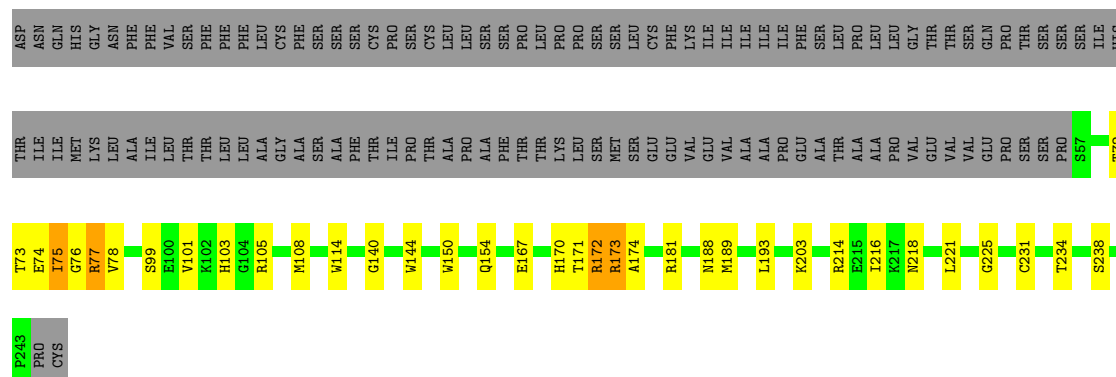
- Molecule 12: FCPI-14





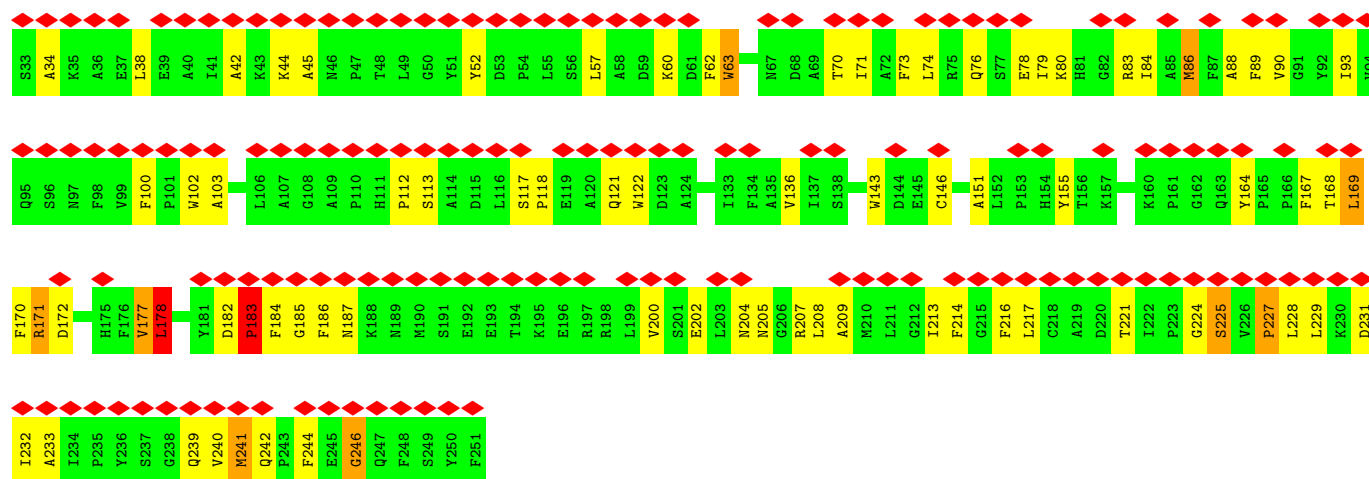
• Molecule 13: FCPI-16

Chain M: 49% 10% 39%



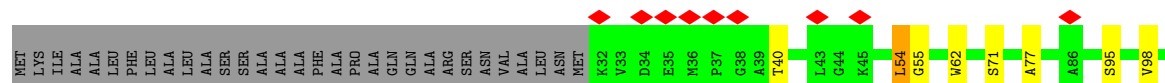
• Molecule 14: FCPI-21

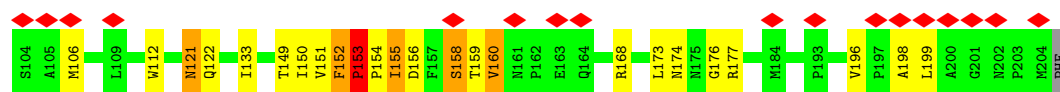
Chain N: 71% 63% 32%



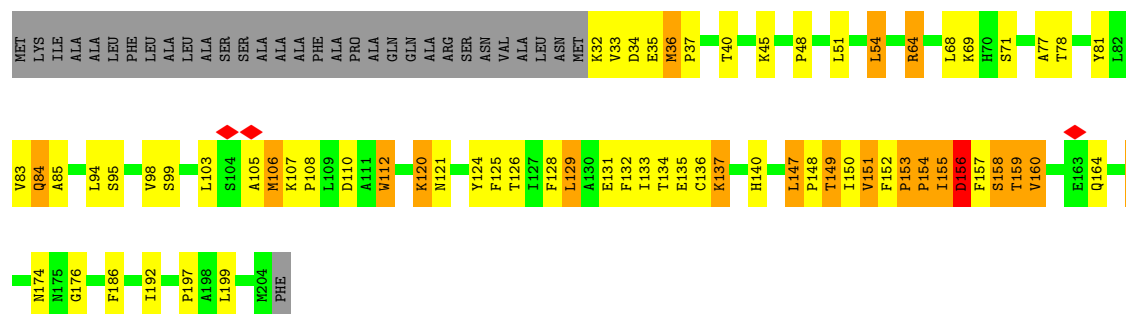
• Molecule 15: FCPI

Chain O: 13% 69% 12% 16%

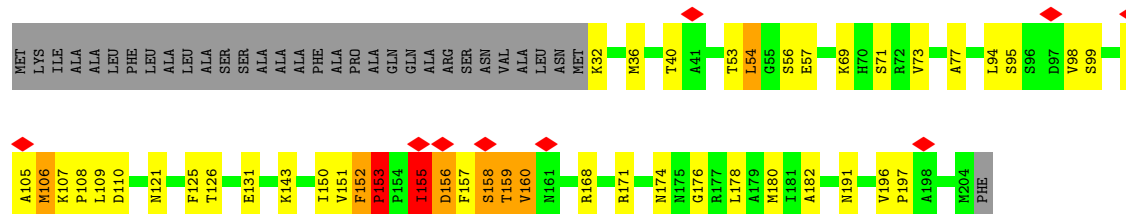




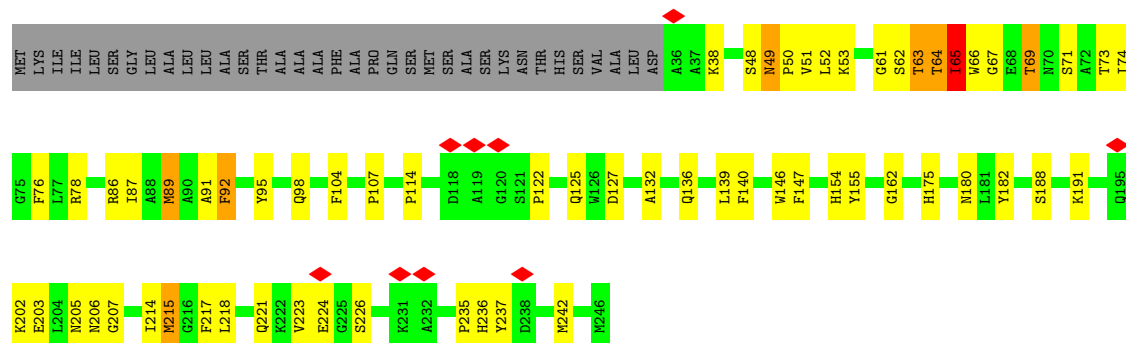
• Molecule 15: FCPI



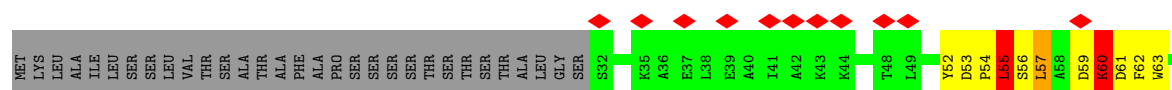
• Molecule 15: FCPI

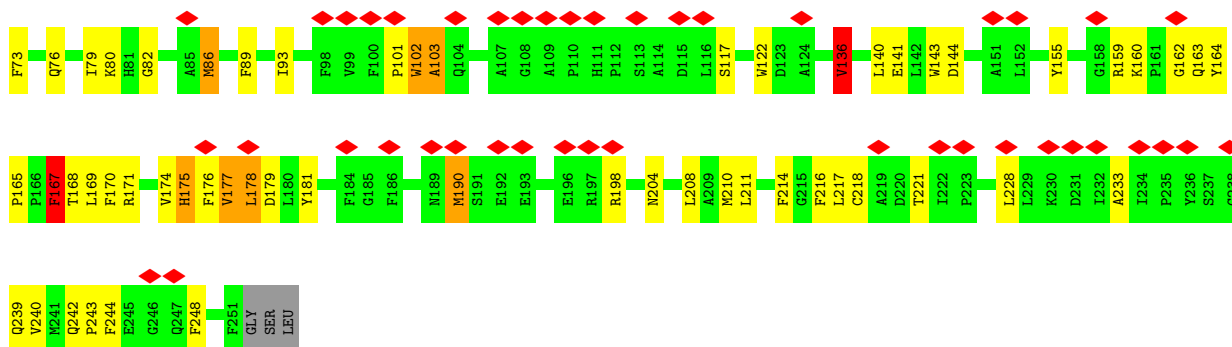


• Molecule 16: FCPI-24

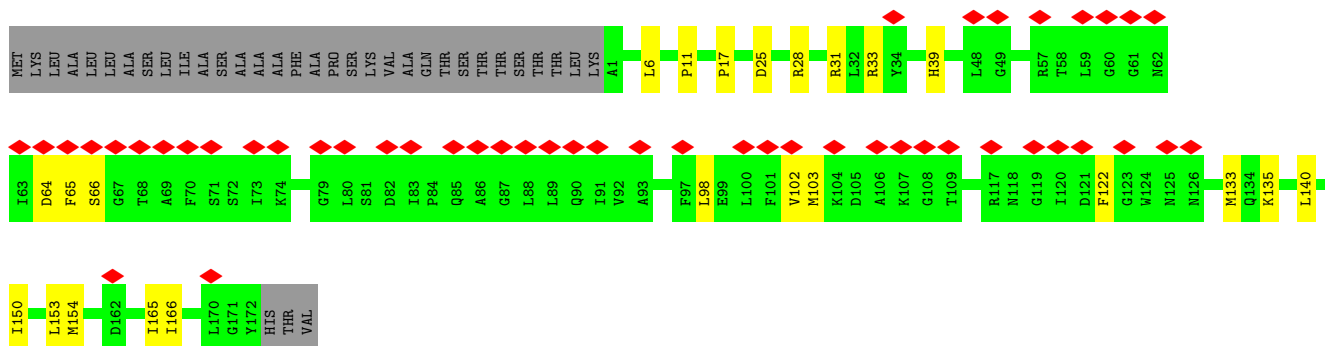


• Molecule 17: FCPI-23

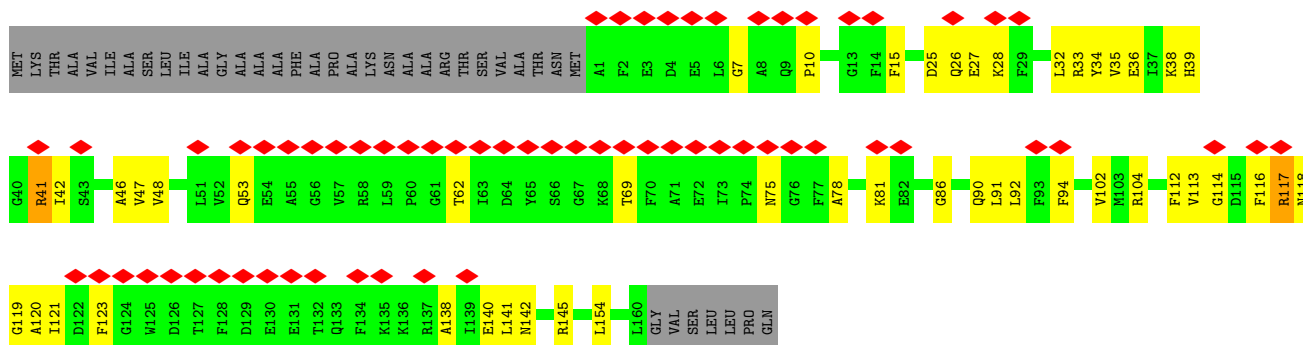




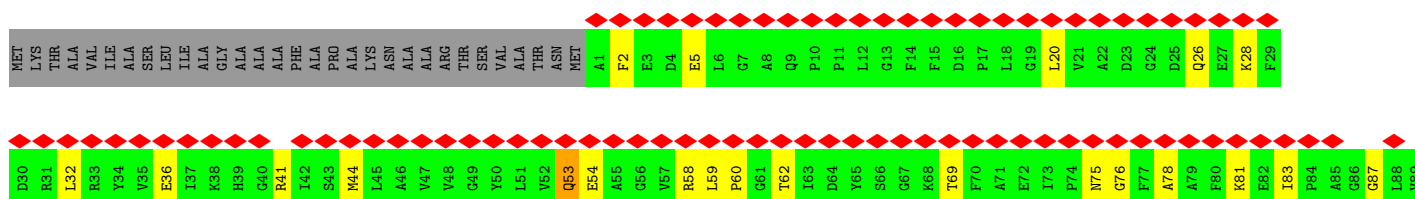
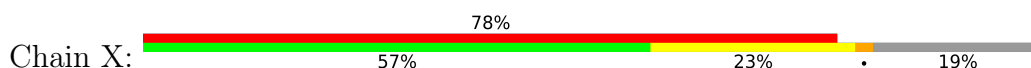
• Molecule 18: FCPI-12

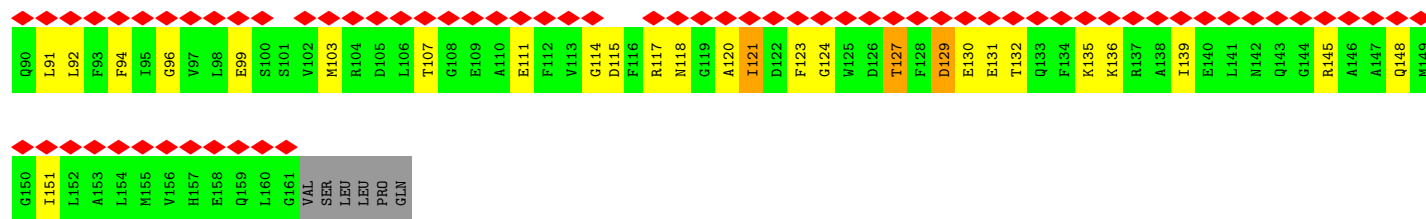


• Molecule 19: FCPI-17



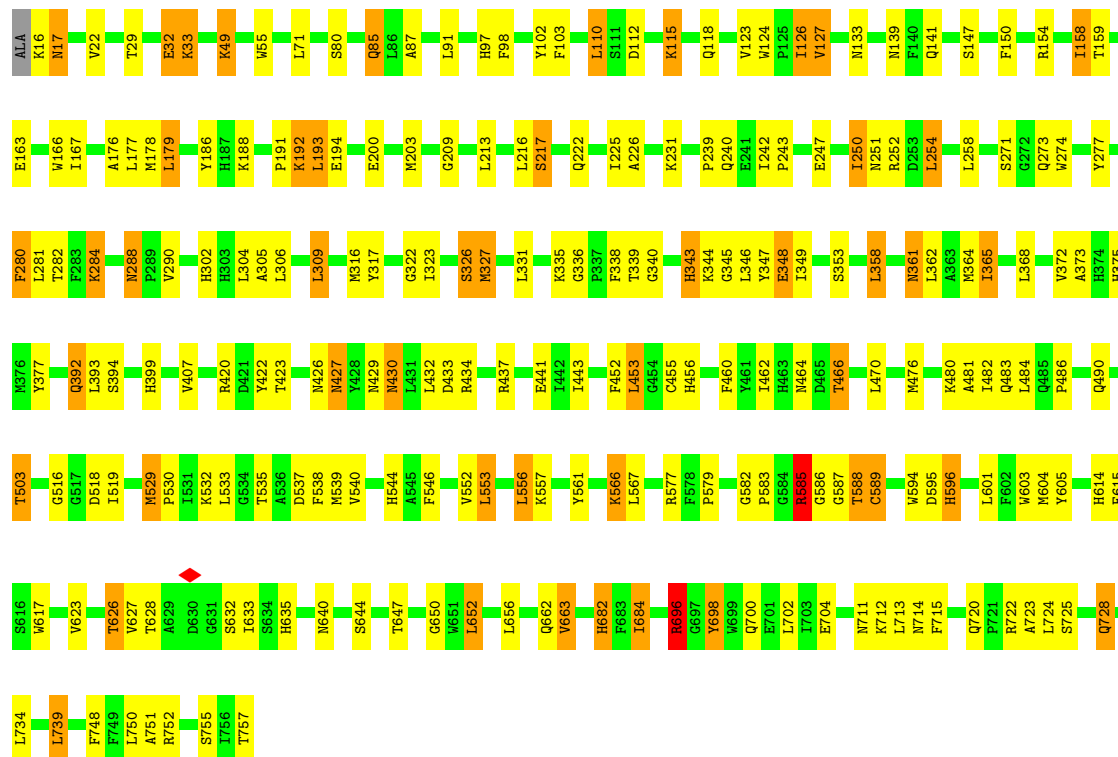
• Molecule 19: FCPI-17





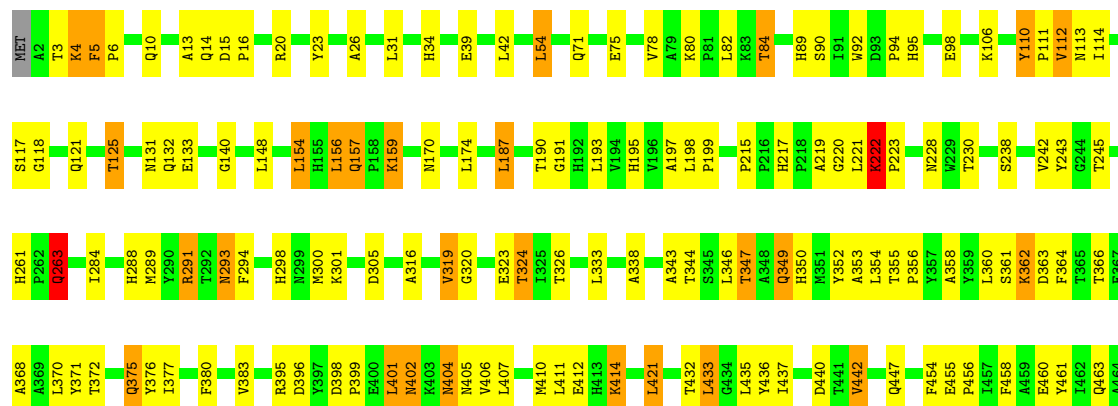
• Molecule 20: PsaA

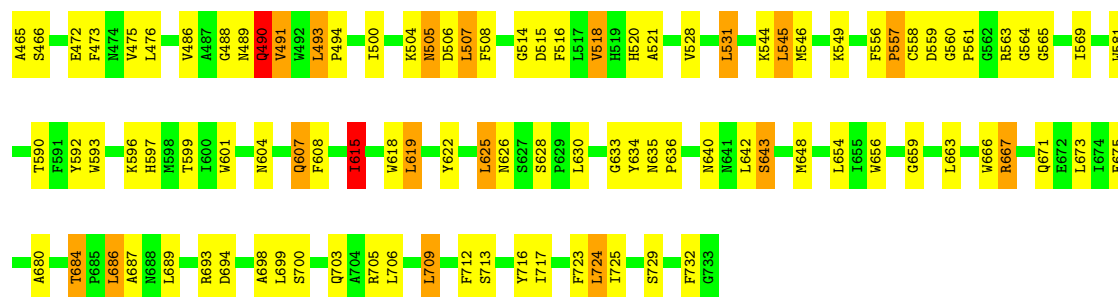
Chain a: 69% 24% 6%



• Molecule 21: PsaB

Chain b: 66% 27% 6%

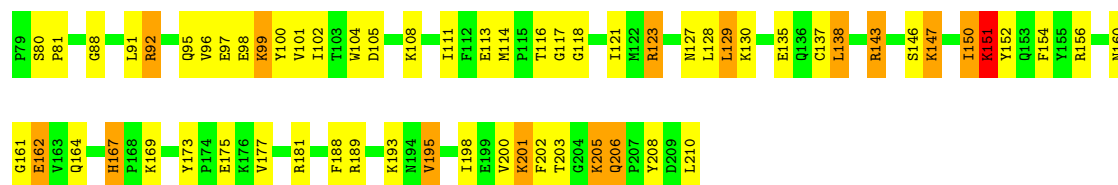




• Molecule 22: PsaC



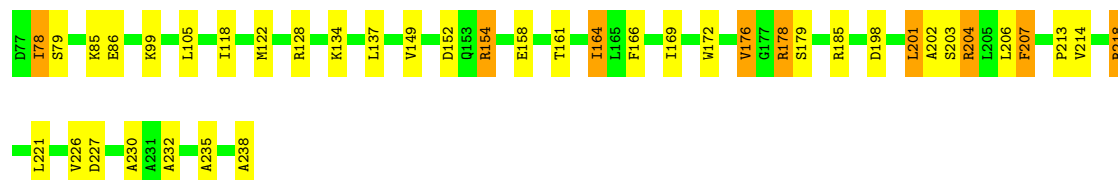
• Molecule 23: PsaD



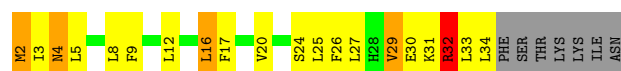
• Molecule 24: PsaE



• Molecule 25: PsaF



• Molecule 26: PsaI



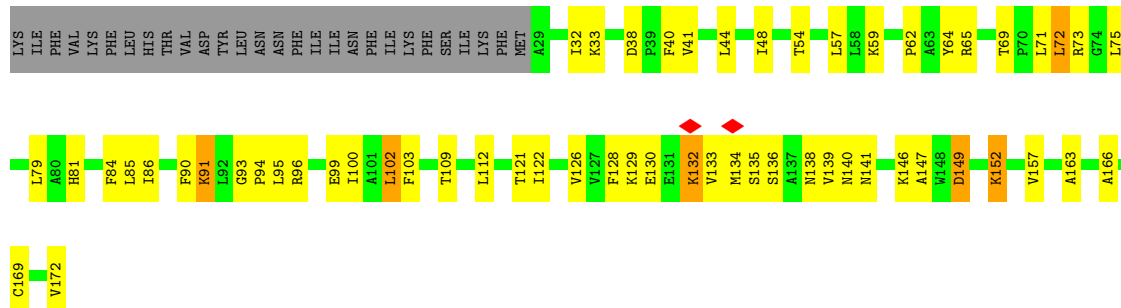
- Molecule 27: PsaJ

Chain j:  43% 38% 17% .



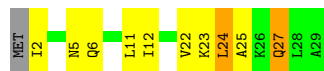
- Molecule 28: PsaL

Chain l:  49% 31% . 16%



- Molecule 29: PsaM

Chain m:  62% 28% 7% .



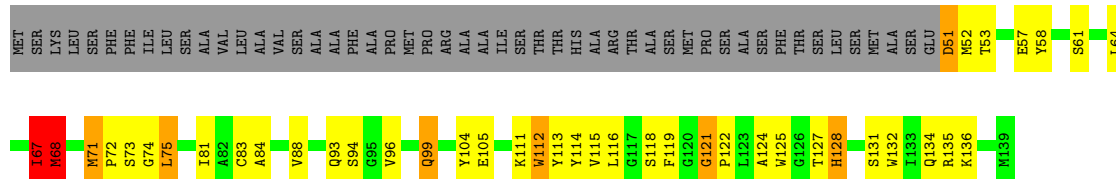
- Molecule 30: PsaS

Chain g:  90% 10%



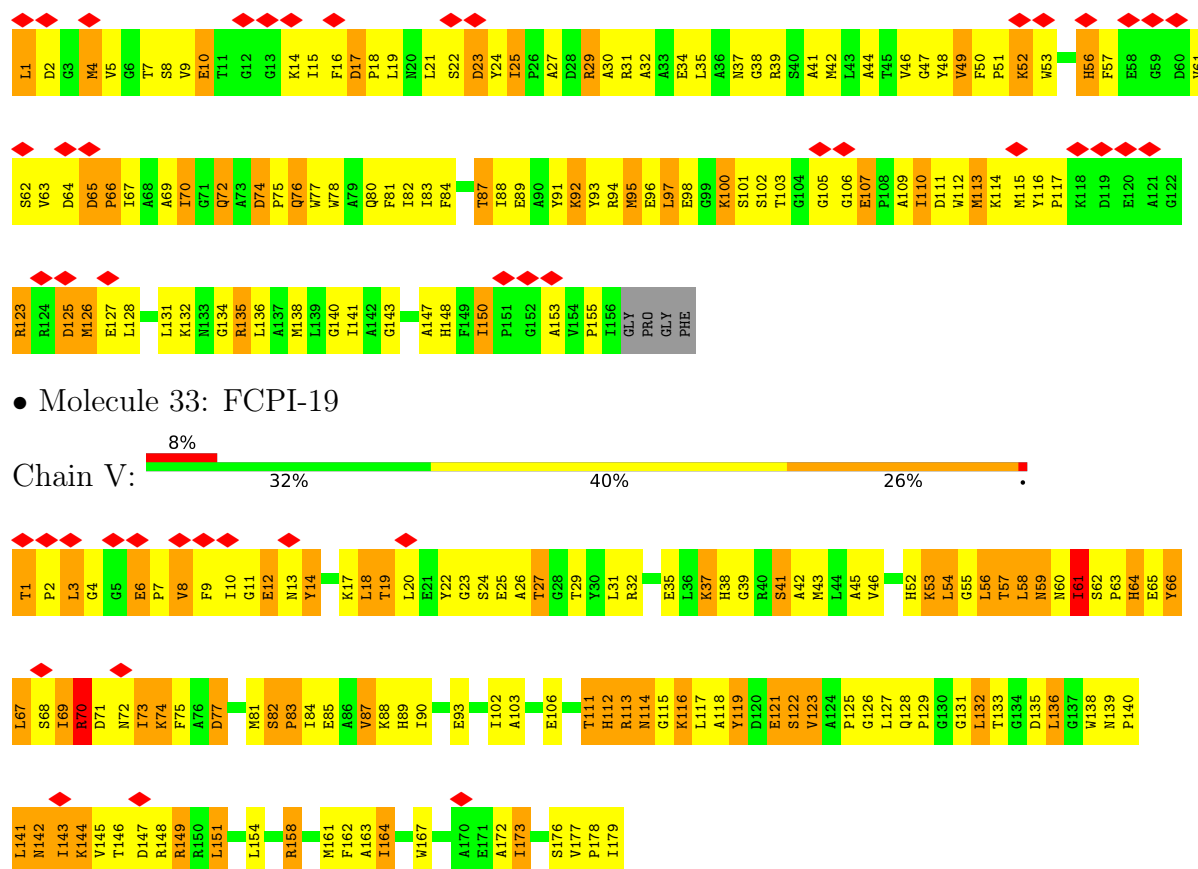
- Molecule 31: PsaR

Chain h:  33% 24% 5% . 36%



- Molecule 32: FCPI-2

Chain U:  19% 30% 49% 18% .



• Molecule 33: FCPI-19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	164480	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	567.32, 567.32, 567.32	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, SF4, BCR, DD6, DGD, LMT, A86, LHG, LMG, SQD, KC1, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/1319	0.80	0/1786
2	B	0.87	2/1039 (0.2%)	1.16	11/1412 (0.8%)
3	C	0.41	0/1275	0.77	3/1726 (0.2%)
4	D	0.49	0/1373	0.84	5/1860 (0.3%)
5	E	0.48	0/1439	0.70	1/1944 (0.1%)
6	F	0.43	0/1411	0.84	5/1908 (0.3%)
7	G	0.45	0/1714	0.79	2/2321 (0.1%)
8	H	0.48	0/1326	0.80	1/1798 (0.1%)
9	I	0.44	0/1285	1.00	6/1746 (0.3%)
10	J	0.50	1/1339 (0.1%)	0.94	4/1811 (0.2%)
11	K	0.49	0/1346	0.84	4/1826 (0.2%)
12	L	0.45	0/1571	0.71	0/2141
13	M	0.40	0/1464	0.74	3/1982 (0.2%)
14	N	0.48	0/1770	1.01	7/2405 (0.3%)
15	O	0.47	0/1335	0.92	7/1817 (0.4%)
15	P	0.47	1/1329 (0.1%)	1.31	11/1810 (0.6%)
15	Q	0.48	0/1335	0.92	8/1817 (0.4%)
16	R	0.35	0/1680	0.72	1/2282 (0.0%)
17	S	0.40	0/1776	0.89	3/2413 (0.1%)
18	T	0.34	0/1353	0.62	0/1823
19	W	0.48	1/1265 (0.1%)	0.85	3/1707 (0.2%)
19	X	0.50	2/1282 (0.2%)	0.93	7/1729 (0.4%)
20	a	0.47	0/6053	0.80	19/8238 (0.2%)
21	b	0.48	2/6031 (0.0%)	0.85	20/8231 (0.2%)
22	c	0.45	0/607	0.82	2/822 (0.2%)
23	d	4.08	2/1086 (0.2%)	1.45	9/1461 (0.6%)
24	e	0.40	0/517	0.58	0/701
25	f	0.47	0/1248	0.75	2/1687 (0.1%)
26	i	0.60	0/262	1.24	2/356 (0.6%)
27	j	0.57	0/333	0.82	1/455 (0.2%)
28	l	0.48	0/1121	0.83	2/1520 (0.1%)
29	m	0.57	0/198	0.82	0/269

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	h	0.49	0/698	1.08	10/951 (1.1%)
32	U	0.59	0/1225	2.00	10/1657 (0.6%)
33	V	0.38	0/1393	0.88	5/1894 (0.3%)
All	All	0.76	11/51798 (0.0%)	0.92	174/70306 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	2
14	N	0	7
15	O	0	1
15	P	0	1
15	Q	0	1
17	S	0	2
19	W	0	3
23	d	0	5
30	g	0	1
33	V	0	1
All	All	0	25

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	151[A]	LYS	CA-C	94.74	2.66	1.52
23	d	151[B]	LYS	CA-C	94.74	2.66	1.52
2	B	186	MET	C-N	22.66	1.54	1.33
15	P	156	ASP	C-N	9.60	1.48	1.33
2	B	183	GLU	C-N	-8.62	1.21	1.33

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	65	ASP	CA-C-N	48.07	179.93	119.84
32	U	65	ASP	C-N-CA	48.07	179.93	119.84
23	d	151[A]	LYS	CB-CA-C	-26.47	64.81	109.80
23	d	151[B]	LYS	CB-CA-C	-26.47	64.81	109.80
15	P	156	ASP	O-C-N	-23.88	90.36	123.07

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	91	PHE	Mainchain
12	L	228	HIS	Peptide
12	L	47	ASN	Peptide
14	N	112	PRO	Peptide
14	N	172	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1287	0	1265	83	0
2	B	1013	0	1016	100	0
3	C	1247	0	1240	72	0
4	D	1337	0	1310	69	0
5	E	1411	0	1376	46	0
6	F	1375	0	1345	82	0
7	G	1668	0	1631	110	0
8	H	1291	0	1258	47	0
9	I	1250	0	1196	79	0
10	J	1301	0	1256	66	0
11	K	1304	0	1281	48	0
12	L	1523	0	1488	71	0
13	M	1423	0	1397	37	0
14	N	1716	0	1658	139	0
15	O	1302	0	1296	64	0
15	P	1296	0	1291	125	0
15	Q	1302	0	1300	115	0
16	R	1628	0	1588	115	0
17	S	1722	0	1670	149	0
18	T	1326	0	1304	18	0
19	W	1239	0	1208	55	0
19	X	1253	0	1232	91	0
20	a	5858	0	5689	242	0
21	b	5820	0	5647	269	0
22	c	597	0	583	29	0
23	d	1056	0	1074	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	e	507	0	504	23	0
25	f	1223	0	1238	79	0
26	i	256	0	284	29	0
27	j	324	0	338	48	0
28	l	1094	0	1129	55	0
29	m	198	0	213	27	0
30	g	670	0	143	23	0
31	h	676	0	662	75	0
32	U	1194	0	1160	221	0
33	V	1361	0	1354	361	0
34	A	129	0	0	14	0
34	B	86	0	0	15	0
34	C	43	0	0	4	0
34	D	172	0	0	19	0
34	E	172	0	0	12	0
34	F	43	0	0	3	0
34	G	43	0	0	2	0
34	H	86	0	0	6	0
34	I	43	0	0	6	0
34	J	43	0	0	4	0
34	K	86	0	0	8	0
34	L	43	0	0	25	0
34	M	43	0	0	18	0
34	O	43	0	0	6	0
34	P	43	0	0	6	0
34	Q	43	0	0	19	0
34	R	86	0	0	16	0
34	S	86	0	0	3	0
34	W	86	0	0	45	0
34	a	43	0	0	1	0
34	j	43	0	0	4	0
35	A	96	0	0	3	0
35	B	96	0	0	19	0
35	C	144	0	0	16	0
35	D	48	0	0	6	0
35	E	144	0	0	18	0
35	F	288	0	0	12	0
35	G	192	0	0	9	0
35	H	96	0	0	7	0
35	I	144	0	0	21	0
35	J	240	0	0	29	0
35	K	192	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	L	240	0	0	14	0
35	M	192	0	0	12	0
35	N	336	0	0	55	0
35	O	240	0	0	27	0
35	P	192	0	0	6	0
35	Q	192	0	0	42	0
35	R	336	0	0	10	0
35	S	288	0	0	27	0
35	T	336	0	0	9	0
35	U	192	0	0	35	0
35	V	192	0	0	46	0
35	W	96	0	0	1	0
35	X	288	0	0	27	0
35	h	96	0	0	9	0
36	A	517	0	509	59	0
36	B	329	0	299	34	0
36	C	516	0	513	41	0
36	D	618	0	591	45	0
36	E	550	0	576	54	0
36	F	452	0	431	57	0
36	G	556	0	526	75	0
36	H	760	0	747	60	0
36	I	555	0	520	91	0
36	J	562	0	540	30	0
36	K	529	0	532	61	0
36	L	527	0	523	54	0
36	M	525	0	462	38	0
36	N	601	0	503	65	0
36	O	506	0	492	34	0
36	P	686	0	666	50	0
36	Q	458	0	441	78	0
36	R	661	0	616	25	0
36	S	658	0	611	46	0
36	T	408	0	409	27	0
36	U	449	0	427	96	0
36	V	545	0	565	145	0
36	W	629	0	552	49	0
36	X	368	0	273	36	0
36	a	2437	0	2463	146	0
36	b	2337	0	2371	117	0
36	f	247	0	259	39	0
36	h	65	0	72	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	i	65	0	71	3	0
36	j	172	0	172	31	0
36	l	294	0	291	24	0
37	A	45	0	0	4	0
37	B	45	0	0	2	0
37	C	45	0	0	1	0
37	D	45	0	0	0	0
37	E	45	0	0	2	0
37	F	90	0	0	20	0
37	G	135	0	0	8	0
37	H	45	0	0	0	0
37	J	45	0	0	0	0
37	K	45	0	0	9	0
37	L	90	0	0	11	0
37	M	135	0	0	7	0
37	N	45	0	0	0	0
37	O	90	0	0	13	0
37	P	90	0	0	2	0
37	Q	90	0	0	16	0
37	R	45	0	0	0	0
37	S	45	0	0	4	0
37	T	90	0	0	18	0
37	U	45	0	0	0	0
37	V	45	0	0	1	0
37	W	90	0	0	14	0
37	X	45	0	0	0	0
38	A	28	0	19	7	0
38	b	46	0	56	10	0
39	B	70	0	92	20	0
39	E	93	0	118	25	0
39	F	68	0	85	35	0
39	G	70	0	90	14	0
39	I	70	0	92	22	0
39	K	66	0	81	14	0
39	L	66	0	77	10	0
39	P	46	0	60	8	0
39	U	70	0	92	27	0
39	a	102	0	129	25	0
39	b	59	0	78	25	0
39	f	24	0	35	2	0
39	h	35	0	43	21	0
40	C	57	0	75	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	L	47	0	52	20	0
40	b	60	0	81	4	0
41	D	95	0	137	28	0
41	E	49	0	74	24	0
41	F	74	0	97	5	0
41	G	136	0	194	27	0
41	I	49	0	74	10	0
41	O	91	0	129	14	0
41	Q	49	0	72	19	0
41	R	49	0	74	14	0
41	a	122	0	160	20	0
41	b	49	0	74	18	0
41	f	91	0	129	41	0
41	i	46	0	65	28	0
41	j	49	0	74	14	0
41	l	48	0	69	17	0
42	D	83	0	109	17	0
42	E	86	0	112	25	0
42	G	110	0	172	22	0
42	I	55	0	86	14	0
42	J	99	0	147	36	0
42	L	33	0	36	10	0
42	V	92	0	130	41	0
42	a	54	0	81	20	0
42	h	45	0	63	7	0
42	j	52	0	77	26	0
42	m	37	0	43	9	0
43	a	33	0	46	3	0
43	b	33	0	46	3	0
44	a	160	0	224	13	0
44	b	200	0	280	14	0
44	f	80	0	112	3	0
44	h	40	0	56	4	0
44	i	80	0	112	9	0
44	j	40	0	56	1	0
44	l	80	0	112	5	0
44	m	40	0	56	11	0
45	b	8	0	0	1	0
45	c	16	0	0	0	0
46	a	64	0	0	7	0
46	b	72	0	0	13	0
46	c	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	d	4	0	0	0	0
46	f	2	0	0	0	0
46	j	1	0	0	0	0
46	l	3	0	0	3	0
All	All	81344	0	72580	4619	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 30.

The worst 5 of 4619 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)
33:V:140:PRO:CB	35:V:303:A86:C39	1.75	1.63
32:U:42:MET:HB3	35:U:304:A86:C	1.26	1.62
36:Q:314:CLA:HED3	36:Q:314:CLA:C1A	1.29	1.59
33:V:69:ILE:CG2	36:V:309:CLA:CGA	1.75	1.59
5:E:128:GLN:HG3	34:E:301:DD6:C23	1.32	1.56

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	A	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	10	14
2	B	128/223 (57%)	121 (94%)	7 (6%)	0	100	100
3	C	161/198 (81%)	150 (93%)	9 (6%)	2 (1%)	10	14
4	D	170/207 (82%)	160 (94%)	9 (5%)	1 (1%)	21	30
5	E	186/222 (84%)	178 (96%)	8 (4%)	0	100	100
6	F	178/215 (83%)	165 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	212/245 (86%)	197 (93%)	14 (7%)	1 (0%)	24	34
8	H	168/203 (83%)	151 (90%)	17 (10%)	0	100	100
9	I	159/195 (82%)	146 (92%)	13 (8%)	0	100	100
10	J	165/200 (82%)	145 (88%)	17 (10%)	3 (2%)	6	8
11	K	167/207 (81%)	152 (91%)	15 (9%)	0	100	100
12	L	194/229 (85%)	176 (91%)	18 (9%)	0	100	100
13	M	185/306 (60%)	169 (91%)	15 (8%)	1 (0%)	24	34
14	N	217/219 (99%)	174 (80%)	40 (18%)	3 (1%)	9	11
15	O	171/205 (83%)	147 (86%)	21 (12%)	3 (2%)	6	8
15	P	171/205 (83%)	153 (90%)	16 (9%)	2 (1%)	10	14
15	Q	171/205 (83%)	150 (88%)	19 (11%)	2 (1%)	10	14
16	R	209/246 (85%)	182 (87%)	25 (12%)	2 (1%)	12	17
17	S	218/254 (86%)	184 (84%)	29 (13%)	5 (2%)	5	5
18	T	170/207 (82%)	164 (96%)	6 (4%)	0	100	100
19	W	158/198 (80%)	133 (84%)	25 (16%)	0	100	100
19	X	160/198 (81%)	146 (91%)	13 (8%)	1 (1%)	21	30
20	a	740/743 (100%)	713 (96%)	26 (4%)	1 (0%)	48	62
21	b	731/733 (100%)	699 (96%)	31 (4%)	1 (0%)	48	62
22	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
23	d	131/132 (99%)	125 (95%)	6 (5%)	0	100	100
24	e	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
25	f	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
26	i	31/40 (78%)	31 (100%)	0	0	100	100
27	j	39/42 (93%)	37 (95%)	1 (3%)	1 (3%)	4	4
28	l	142/172 (83%)	131 (92%)	11 (8%)	0	100	100
29	m	26/29 (90%)	26 (100%)	0	0	100	100
31	h	87/139 (63%)	87 (100%)	0	0	100	100
32	U	154/160 (96%)	123 (80%)	26 (17%)	5 (3%)	3	2
33	V	177/179 (99%)	152 (86%)	20 (11%)	5 (3%)	4	3
All	All	6441/7429 (87%)	5903 (92%)	497 (8%)	41 (1%)	23	30

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	87	ILE
15	O	153	PRO
15	O	155	ILE
15	Q	153	PRO
17	S	103	ALA

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	A	137/137 (100%)	128 (93%)	9 (7%)	15	24
2	B	105/180 (58%)	98 (93%)	7 (7%)	15	23
3	C	131/153 (86%)	122 (93%)	9 (7%)	14	22
4	D	140/163 (86%)	125 (89%)	15 (11%)	6	8
5	E	142/164 (87%)	136 (96%)	6 (4%)	26	42
6	F	142/169 (84%)	135 (95%)	7 (5%)	22	36
7	G	172/193 (89%)	146 (85%)	26 (15%)	3	3
8	H	131/154 (85%)	129 (98%)	2 (2%)	57	75
9	I	124/152 (82%)	101 (82%)	23 (18%)	1	2
10	J	130/154 (84%)	122 (94%)	8 (6%)	16	26
11	K	133/160 (83%)	130 (98%)	3 (2%)	44	64
12	L	159/180 (88%)	159 (100%)	0	100	100
13	M	142/247 (58%)	135 (95%)	7 (5%)	22	36
14	N	176/176 (100%)	170 (97%)	6 (3%)	32	51
15	O	138/159 (87%)	134 (97%)	4 (3%)	37	57
15	P	137/159 (86%)	120 (88%)	17 (12%)	4	6
15	Q	138/159 (87%)	133 (96%)	5 (4%)	31	49
16	R	167/193 (86%)	160 (96%)	7 (4%)	26	42
17	S	177/204 (87%)	169 (96%)	8 (4%)	24	39
18	T	136/163 (83%)	135 (99%)	1 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	W	125/151 (83%)	125 (100%)	0	100	100
19	X	127/151 (84%)	125 (98%)	2 (2%)	55	74
20	a	606/606 (100%)	543 (90%)	63 (10%)	7	9
21	b	593/593 (100%)	517 (87%)	76 (13%)	4	5
22	c	67/69 (97%)	59 (88%)	8 (12%)	5	6
23	d	111/111 (100%)	88 (79%)	23 (21%)	1	1
24	e	55/55 (100%)	51 (93%)	4 (7%)	13	20
25	f	119/125 (95%)	105 (88%)	14 (12%)	5	6
26	i	29/36 (81%)	20 (69%)	9 (31%)	0	0
27	j	34/35 (97%)	29 (85%)	5 (15%)	3	3
28	l	114/143 (80%)	98 (86%)	16 (14%)	3	4
29	m	20/23 (87%)	17 (85%)	3 (15%)	3	3
31	h	70/109 (64%)	54 (77%)	16 (23%)	1	1
32	U	119/121 (98%)	82 (69%)	37 (31%)	0	0
33	V	137/137 (100%)	83 (61%)	54 (39%)	0	0
All	All	5183/5884 (88%)	4683 (90%)	500 (10%)	10	11

5 of 500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	a	728	GLN
32	U	127	GLU
21	b	491	VAL
32	U	114	LYS
33	V	74	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
21	b	404	ASN
33	V	89	HIS
21	b	520	HIS
25	f	155	HIS
15	O	84	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

589 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$
35	A86	O	305	-	44,50,50	1.42	4 (9%)	51,76,76	1.95	16 (31%)
36	CLA	O	314	-	45,49,73	1.51	9 (20%)	54,84,113	1.72	8 (14%)
36	CLA	J	310	-	69,73,73	1.21	10 (14%)	83,113,113	1.36	7 (8%)
36	CLA	a	824	-	69,73,73	1.29	12 (17%)	83,113,113	1.80	19 (22%)
35	A86	K	302	-	44,50,50	1.38	4 (9%)	51,76,76	3.29	20 (39%)
36	CLA	N	311	14	50,54,73	1.45	7 (14%)	60,90,113	1.72	8 (13%)
36	CLA	S	311	35	50,54,73	1.50	10 (20%)	60,90,113	1.55	9 (15%)
36	CLA	M	312	13,36	51,55,73	1.46	9 (17%)	61,91,113	1.58	8 (13%)
36	CLA	T	309	18	69,73,73	1.23	9 (13%)	83,113,113	1.41	8 (9%)
36	CLA	K	310	-	66,70,73	1.97	19 (28%)	79,109,113	2.81	29 (36%)
44	BCR	b	844	-	41,41,41	1.11	3 (7%)	56,56,56	1.31	5 (8%)
36	CLA	G	307	-	45,50,73	2.21	14 (31%)	53,85,113	3.15	17 (32%)
34	DD6	O	304	-	39,45,45	1.90	3 (7%)	52,67,67	2.00	14 (26%)
36	CLA	I	309	9	50,54,73	1.44	8 (16%)	60,90,113	1.92	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DD6	D	303	-	39,45,45	2.97	8 (20%)	52,67,67	2.65	18 (34%)
36	CLA	C	206	-	65,69,73	1.27	8 (12%)	78,108,113	1.38	5 (6%)
36	CLA	L	308	-	65,69,73	1.92	14 (21%)	78,108,113	2.83	22 (28%)
35	A86	E	305	5	44,50,50	1.23	4 (9%)	51,76,76	2.04	14 (27%)
36	CLA	V	308	-	69,73,73	1.23	10 (14%)	83,113,113	1.37	10 (12%)
41	LHG	D	319	42	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
35	A86	G	306	-	44,50,50	1.21	4 (9%)	51,76,76	2.34	18 (35%)
36	CLA	b	810	21	69,73,73	1.18	9 (13%)	83,113,113	1.32	6 (7%)
34	DD6	H	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.97	12 (23%)
36	CLA	b	812	21	69,73,73	1.23	10 (14%)	83,113,113	1.48	14 (16%)
36	CLA	b	841	41	69,73,73	1.32	12 (17%)	83,113,113	1.82	16 (19%)
35	A86	C	203	-	44,50,50	1.24	4 (9%)	51,76,76	2.07	16 (31%)
36	CLA	S	315	17	47,51,73	1.51	8 (17%)	56,86,113	1.97	10 (17%)
37	KC1	T	310	18	49,53,53	4.55	27 (55%)	63,89,89	6.90	40 (63%)
36	CLA	O	308	15	69,73,73	1.26	9 (13%)	83,113,113	1.43	7 (8%)
36	CLA	F	316	6	45,49,73	1.48	10 (22%)	54,84,113	1.50	7 (12%)
36	CLA	L	311	-	69,73,73	1.25	11 (15%)	83,113,113	1.34	10 (12%)
36	CLA	X	309	19	48,53,73	1.52	8 (16%)	57,89,113	1.66	10 (17%)
34	DD6	J	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.87	12 (23%)
42	LMG	I	315	-	55,55,55	0.89	2 (3%)	63,63,63	1.00	3 (4%)
36	CLA	S	309	-	65,69,73	1.30	11 (16%)	78,108,113	1.30	8 (10%)
36	CLA	b	818	21	59,63,73	1.34	8 (13%)	71,101,113	1.65	13 (18%)
37	KC1	X	311	-	49,53,53	2.86	19 (38%)	63,89,89	4.42	36 (57%)
41	LHG	G	301	-	48,48,48	0.77	2 (4%)	51,54,54	1.28	6 (11%)
44	BCR	h	201	-	41,41,41	1.26	5 (12%)	56,56,56	1.42	10 (17%)
36	CLA	W	208	-	49,53,73	1.48	10 (20%)	59,89,113	1.48	4 (6%)
36	CLA	Q	310	15	69,73,73	2.74	17 (24%)	83,113,113	2.82	23 (27%)
35	A86	K	306	11	44,50,50	1.22	3 (6%)	51,76,76	3.50	21 (41%)
36	CLA	H	317	8	69,73,73	1.25	10 (14%)	83,113,113	1.30	6 (7%)
36	CLA	N	309	14	55,59,73	1.41	8 (14%)	66,96,113	1.74	8 (12%)
35	A86	X	305	-	44,50,50	1.29	4 (9%)	51,76,76	3.04	18 (35%)
41	LHG	O	318	15	48,48,48	0.88	3 (6%)	51,54,54	1.22	4 (7%)
35	A86	S	305	-	44,50,50	1.27	3 (6%)	51,76,76	2.95	20 (39%)
39	LMT	E	323	-	36,36,36	0.35	0	47,47,47	0.82	1 (2%)
34	DD6	H	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.92	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	b	801	46	69,73,73	1.29	12 (17%)	83,113,113	1.39	10 (12%)
36	CLA	b	808	21	69,73,73	1.21	10 (14%)	83,113,113	1.40	8 (9%)
36	CLA	J	308	-	65,69,73	1.27	9 (13%)	78,108,113	1.63	10 (12%)
36	CLA	A	305	1	53,57,73	1.41	9 (16%)	62,93,113	1.42	6 (9%)
41	LHG	F	319	-	40,40,48	1.03	2 (5%)	43,46,54	1.10	3 (6%)
35	A86	C	204	-	44,50,50	1.84	14 (31%)	51,76,76	2.68	16 (31%)
36	CLA	b	825	-	69,73,73	1.24	11 (15%)	83,113,113	1.43	9 (10%)
37	KC1	L	317	-	49,53,53	2.75	19 (38%)	63,89,89	4.79	38 (60%)
36	CLA	S	312	17	69,73,73	1.27	9 (13%)	83,113,113	1.37	10 (12%)
35	A86	P	306	-	44,50,50	1.22	3 (6%)	51,76,76	1.89	13 (25%)
36	CLA	j	106	27	46,50,73	1.46	10 (21%)	55,85,113	1.59	7 (12%)
37	KC1	J	314	-	49,53,53	2.70	18 (36%)	63,89,89	5.38	38 (60%)
39	LMT	E	321	-	23,23,36	0.45	0	28,28,47	0.59	0
36	CLA	a	834	20	49,53,73	1.47	9 (18%)	59,89,113	1.56	7 (11%)
36	CLA	J	313	-	69,73,73	1.24	10 (14%)	83,113,113	1.37	7 (8%)
45	SF4	c	101	22	0,12,12	-	-	-	-	-
37	KC1	Q	311	15	49,53,53	2.88	19 (38%)	63,89,89	6.04	39 (61%)
34	DD6	a	849	-	39,45,45	2.01	3 (7%)	52,67,67	1.84	13 (25%)
39	LMT	f	807	-	24,24,36	0.43	0	29,29,47	0.58	0
36	CLA	D	310	-	69,73,73	1.18	8 (11%)	83,113,113	1.45	9 (10%)
36	CLA	b	813	21	58,62,73	1.40	13 (22%)	73,100,113	1.40	10 (13%)
35	A86	K	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.26	13 (25%)
35	A86	F	304	36	44,50,50	1.25	4 (9%)	51,76,76	2.03	13 (25%)
36	CLA	D	308	-	69,73,73	1.27	11 (15%)	83,113,113	1.54	13 (15%)
34	DD6	I	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	15 (28%)
36	CLA	W	206	19	65,69,73	1.26	6 (9%)	78,108,113	1.47	6 (7%)
36	CLA	B	308	2	69,73,73	1.28	9 (13%)	83,113,113	1.47	12 (14%)
36	CLA	O	316	-	69,73,73	1.84	15 (21%)	83,113,113	2.88	27 (32%)
36	CLA	K	307	-	65,69,73	1.92	15 (23%)	78,108,113	2.89	22 (28%)
36	CLA	P	318	-	55,59,73	1.41	9 (16%)	66,96,113	1.45	6 (9%)
36	CLA	H	312	8	69,73,73	1.23	11 (15%)	83,113,113	1.48	11 (13%)
35	A86	R	302	16	44,50,50	1.38	5 (11%)	51,76,76	2.80	15 (29%)
35	A86	G	304	-	44,50,50	1.43	5 (11%)	51,76,76	3.69	25 (49%)
36	CLA	D	313	-	69,73,73	1.20	11 (15%)	83,113,113	1.51	12 (14%)
36	CLA	D	316	-	56,60,73	1.37	9 (16%)	67,97,113	1.69	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	E	315	-	69,73,73	1.96	20 (28%)	83,113,113	2.88	28 (33%)
35	A86	S	303	17	44,50,50	1.32	5 (11%)	51,76,76	3.30	22 (43%)
36	CLA	E	310	-	69,73,73	1.29	8 (11%)	83,113,113	1.43	10 (12%)
39	LMT	E	320	-	36,36,36	0.37	0	47,47,47	0.67	0
36	CLA	S	321	-	56,60,73	1.38	9 (16%)	67,97,113	1.64	8 (11%)
36	CLA	P	301	15	69,73,73	1.23	11 (15%)	83,113,113	1.45	8 (9%)
36	CLA	a	822	-	55,59,73	1.60	11 (20%)	66,96,113	2.18	18 (27%)
36	CLA	H	316	-	69,73,73	1.23	10 (14%)	83,113,113	1.38	5 (6%)
36	CLA	A	309	1	50,54,73	1.45	9 (18%)	60,90,113	1.48	5 (8%)
44	BCR	a	844	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	5 (8%)
34	DD6	W	205	-	39,45,45	1.99	3 (7%)	52,67,67	2.03	15 (28%)
36	CLA	a	838	20	69,73,73	1.21	10 (14%)	83,113,113	1.36	8 (9%)
35	A86	E	307	36	44,50,50	1.24	4 (9%)	51,76,76	2.07	12 (23%)
36	CLA	H	309	8	69,73,73	1.24	9 (13%)	83,113,113	1.35	6 (7%)
36	CLA	W	212	19	69,73,73	1.29	9 (13%)	83,113,113	1.64	11 (13%)
36	CLA	a	810	36,20	66,70,73	1.21	9 (13%)	79,109,113	1.43	6 (7%)
34	DD6	D	301	-	39,45,45	2.01	3 (7%)	52,67,67	1.99	13 (25%)
36	CLA	R	314	16	50,54,73	1.48	9 (18%)	60,90,113	1.75	9 (15%)
42	LMG	J	318	-	55,55,55	0.89	2 (3%)	63,63,63	1.02	3 (4%)
41	LHG	R	323	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	S	320	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	7 (8%)
36	CLA	Q	307	15	54,58,73	1.40	10 (18%)	63,94,113	1.46	5 (7%)
35	A86	A	302	-	44,50,50	1.61	6 (13%)	51,76,76	4.76	25 (49%)
36	CLA	a	814	20	54,58,73	1.40	11 (20%)	65,95,113	1.72	7 (10%)
35	A86	L	307	-	44,50,50	1.24	4 (9%)	51,76,76	1.93	11 (21%)
35	A86	F	305	-	44,50,50	1.35	6 (13%)	51,76,76	2.84	20 (39%)
41	LHG	f	808	25	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)
35	A86	L	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.01	14 (27%)
35	A86	I	302	-	44,50,50	1.30	4 (9%)	51,76,76	2.66	17 (33%)
36	CLA	b	837	21	69,73,73	1.21	10 (14%)	83,113,113	1.46	12 (14%)
37	KC1	M	313	13,36	49,53,53	2.71	19 (38%)	63,89,89	5.30	40 (63%)
36	CLA	a	839	46	69,73,73	1.21	10 (14%)	83,113,113	1.37	8 (9%)
36	CLA	P	302	-	46,50,73	1.47	9 (19%)	55,85,113	1.68	8 (14%)
37	KC1	T	315	-	49,53,53	2.75	18 (36%)	63,89,89	5.01	36 (57%)
35	A86	T	301	36	44,50,50	1.25	4 (9%)	51,76,76	2.07	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	W	201	19	52,56,73	1.43	8 (15%)	62,92,113	1.43	5 (8%)
36	CLA	b	839	-	69,73,73	1.21	10 (14%)	83,113,113	1.43	8 (9%)
36	CLA	b	820	21	64,68,73	1.30	11 (17%)	77,107,113	1.34	7 (9%)
36	CLA	a	817	20	69,73,73	1.26	10 (14%)	83,113,113	1.61	15 (18%)
35	A86	A	316	-	44,50,50	1.23	4 (9%)	51,76,76	2.16	16 (31%)
36	CLA	D	311	4	50,54,73	1.43	9 (18%)	60,90,113	1.48	5 (8%)
35	A86	T	305	18	44,50,50	1.48	5 (11%)	51,76,76	3.68	22 (43%)
37	KC1	V	312	33	49,53,53	2.86	20 (40%)	63,89,89	4.75	36 (57%)
36	CLA	a	837	20	69,73,73	1.20	9 (13%)	83,113,113	1.40	8 (9%)
34	DD6	L	305	-	39,45,45	2.04	3 (7%)	52,67,67	2.00	15 (28%)
36	CLA	C	205	-	47,51,73	1.45	9 (19%)	56,86,113	1.56	9 (16%)
42	LMG	D	321	-	37,37,55	1.08	2 (5%)	45,45,63	1.02	2 (4%)
35	A86	N	320	-	44,50,50	1.38	6 (13%)	51,76,76	3.30	24 (47%)
36	CLA	J	311	-	50,54,73	1.47	10 (20%)	60,90,113	1.48	7 (11%)
34	DD6	A	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	12 (23%)
36	CLA	I	305	-	65,69,73	1.86	13 (20%)	78,108,113	1.63	11 (14%)
37	KC1	K	314	11	49,53,53	2.65	18 (36%)	63,89,89	5.06	38 (60%)
36	CLA	F	314	35,6	69,73,73	1.23	11 (15%)	83,113,113	1.45	8 (9%)
36	CLA	J	307	10	65,69,73	1.27	10 (15%)	78,108,113	1.45	12 (15%)
37	KC1	O	315	15	49,53,53	2.88	19 (38%)	63,89,89	6.04	39 (61%)
35	A86	Q	316	15,36	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
36	CLA	R	311	16	69,73,73	1.23	9 (13%)	83,113,113	1.36	8 (9%)
37	KC1	L	315	35,12	49,53,53	2.80	18 (36%)	63,89,89	5.32	39 (61%)
36	CLA	H	310	8	50,54,73	1.74	12 (24%)	60,90,113	2.66	19 (31%)
36	CLA	U	307	-	54,58,73	1.38	10 (18%)	65,95,113	1.39	4 (6%)
35	A86	W	203	36	44,50,50	1.37	4 (9%)	51,76,76	2.83	20 (39%)
36	CLA	E	308	5	53,57,73	1.39	11 (20%)	62,93,113	1.52	8 (12%)
36	CLA	a	801	20	69,73,73	1.30	9 (13%)	83,113,113	1.53	13 (15%)
36	CLA	V	305	35	65,69,73	1.38	7 (10%)	78,108,113	1.45	9 (11%)
35	A86	U	301	-	44,50,50	1.37	3 (6%)	51,76,76	3.80	25 (49%)
36	CLA	U	305	-	65,69,73	1.29	8 (12%)	78,108,113	1.34	5 (6%)
36	CLA	i	102	26	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
36	CLA	b	814	21	59,63,73	1.32	10 (16%)	71,101,113	1.38	6 (8%)
36	CLA	E	316	-	69,73,73	1.24	8 (11%)	83,113,113	1.54	10 (12%)
36	CLA	N	313	14	45,49,73	1.58	8 (17%)	54,84,113	1.78	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	LMG	D	320	41	46,46,55	0.98	2 (4%)	54,54,63	1.03	3 (5%)
36	CLA	B	311	2	59,63,73	1.35	7 (11%)	71,101,113	1.68	12 (16%)
36	CLA	b	822	21	50,54,73	1.43	10 (20%)	60,90,113	1.50	8 (13%)
36	CLA	A	313	-	45,49,73	1.51	9 (20%)	54,84,113	1.71	7 (12%)
39	LMT	U	315	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
37	KC1	M	317	-	49,53,53	2.75	20 (40%)	63,89,89	4.78	38 (60%)
36	CLA	R	315	-	69,73,73	1.23	9 (13%)	83,113,113	1.35	5 (6%)
36	CLA	W	210	-	50,54,73	1.46	8 (16%)	60,90,113	1.87	15 (25%)
36	CLA	K	308	-	69,73,73	1.24	9 (13%)	83,113,113	1.38	9 (10%)
36	CLA	N	317	14	58,62,73	1.39	9 (15%)	69,99,113	1.51	10 (14%)
36	CLA	G	316	-	53,57,73	1.40	10 (18%)	62,93,113	1.49	5 (8%)
35	A86	Q	303	-	44,50,50	1.33	5 (11%)	51,76,76	2.05	15 (29%)
44	BCR	a	847	-	41,41,41	1.23	4 (9%)	56,56,56	1.25	5 (8%)
37	KC1	Q	313	-	49,53,53	2.89	19 (38%)	63,89,89	6.04	39 (61%)
36	CLA	A	306	-	65,69,73	1.94	18 (27%)	78,108,113	2.78	29 (37%)
36	CLA	a	813	20	49,53,73	1.50	11 (22%)	59,89,113	1.75	11 (18%)
42	LMG	h	206	-	45,45,55	0.99	2 (4%)	53,53,63	1.03	3 (5%)
35	A86	M	304	-	44,50,50	1.23	3 (6%)	51,76,76	2.06	14 (27%)
35	A86	R	309	-	44,50,50	1.23	4 (9%)	51,76,76	2.84	16 (31%)
36	CLA	j	101	27,1	69,73,73	1.24	10 (14%)	83,113,113	1.27	7 (8%)
36	CLA	a	809	-	60,64,73	1.29	10 (16%)	72,102,113	1.41	8 (11%)
36	CLA	W	207	34	69,73,73	1.25	8 (11%)	83,113,113	1.42	8 (9%)
34	DD6	D	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.63	9 (17%)
39	LMT	K	318	-	36,36,36	0.41	0	47,47,47	0.72	1 (2%)
40	DGD	L	302	42	48,48,67	0.98	2 (4%)	62,62,81	1.05	4 (6%)
36	CLA	C	208	3	69,73,73	1.25	10 (14%)	83,113,113	1.36	8 (9%)
36	CLA	a	802	-	69,73,73	1.34	8 (11%)	83,113,113	1.83	14 (16%)
41	LHG	Q	315	36	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	R	320	16	49,53,73	1.51	11 (22%)	59,89,113	1.71	13 (22%)
34	DD6	E	304	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	10 (19%)
36	CLA	B	309	2	56,60,73	1.78	11 (19%)	67,97,113	2.23	20 (29%)
36	CLA	b	823	21	59,63,73	1.30	10 (16%)	71,101,113	1.45	7 (9%)
45	SF4	c	102	-	0,12,12	-	-	-	-	-
39	LMT	I	317	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
36	CLA	a	803	36,20	59,63,73	1.32	11 (18%)	71,101,113	1.55	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A86	X	302	35	44,50,50	1.22	4 (9%)	51,76,76	2.97	18 (35%)
36	CLA	W	211	19	69,73,73	1.24	8 (11%)	83,113,113	1.50	9 (10%)
41	LHG	I	316	-	48,48,48	0.95	2 (4%)	51,54,54	1.00	2 (3%)
37	KC1	S	316	-	49,53,53	2.83	20 (40%)	63,89,89	5.25	40 (63%)
36	CLA	E	317	-	50,54,73	1.47	8 (16%)	60,90,113	1.44	6 (10%)
36	CLA	B	305	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	10 (12%)
41	LHG	i	104	-	45,45,48	0.98	2 (4%)	48,51,54	1.03	2 (4%)
36	CLA	I	307	9	58,62,73	1.33	11 (18%)	69,99,113	1.49	9 (13%)
37	KC1	R	317	-	49,53,53	2.71	19 (38%)	63,89,89	5.25	38 (60%)
35	A86	U	302	-	44,50,50	1.33	4 (9%)	51,76,76	3.12	22 (43%)
42	LMG	G	325	-	55,55,55	0.89	2 (3%)	63,63,63	1.01	3 (4%)
45	SF4	b	803	20,21	0,12,12	-	-	-	-	-
35	A86	F	302	-	44,50,50	1.24	4 (9%)	51,76,76	1.92	11 (21%)
35	A86	R	301	-	44,50,50	1.47	4 (9%)	51,76,76	3.48	24 (47%)
35	A86	N	305	-	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
36	CLA	M	310	13,35	50,54,73	2.12	9 (18%)	60,90,113	1.96	13 (21%)
36	CLA	L	312	12	50,54,73	1.46	9 (18%)	60,90,113	1.77	8 (13%)
36	CLA	a	811	20	58,62,73	1.34	9 (15%)	69,99,113	1.44	6 (8%)
35	A86	F	307	-	44,50,50	1.31	3 (6%)	51,76,76	3.94	22 (43%)
34	DD6	Q	302	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
41	LHG	a	850	-	46,46,48	0.96	2 (4%)	49,52,54	1.04	3 (6%)
36	CLA	a	836	-	69,73,73	1.17	10 (14%)	83,113,113	1.56	10 (12%)
36	CLA	S	310	17	69,73,73	1.24	10 (14%)	83,113,113	1.60	13 (15%)
36	CLA	Q	305	-	65,69,73	1.28	9 (13%)	78,108,113	1.37	5 (6%)
37	KC1	W	213	-	49,53,53	2.86	20 (40%)	63,89,89	4.90	35 (55%)
42	LMG	j	105	-	52,52,55	0.91	2 (3%)	60,60,63	1.00	3 (5%)
36	CLA	W	218	19	47,51,73	1.49	10 (21%)	56,86,113	1.64	8 (14%)
36	CLA	M	307	-	69,73,73	1.25	12 (17%)	83,113,113	1.46	9 (10%)
36	CLA	U	313	-	45,49,73	1.51	7 (15%)	54,84,113	1.70	9 (16%)
35	A86	R	304	36,16	44,50,50	1.30	3 (6%)	51,76,76	2.95	17 (33%)
36	CLA	F	313	-	56,60,73	1.34	9 (16%)	67,97,113	1.46	8 (11%)
35	A86	J	303	-	44,50,50	1.41	4 (9%)	51,76,76	2.80	20 (39%)
36	CLA	S	317	-	45,49,73	1.52	8 (17%)	54,84,113	1.55	6 (11%)
36	CLA	U	308	32,35	60,64,73	1.35	8 (13%)	72,102,113	1.63	8 (11%)
36	CLA	V	307	-	55,59,73	1.42	9 (16%)	66,96,113	1.38	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	LHG	F	318	-	32,32,48	0.88	1 (3%)	36,37,54	1.72	6 (16%)
39	LMT	b	851	-	24,24,36	0.42	0	29,29,47	0.81	0
36	CLA	a	816	20	69,73,73	1.56	9 (13%)	83,113,113	2.07	18 (21%)
35	A86	P	304	-	44,50,50	1.33	5 (11%)	51,76,76	2.74	17 (33%)
35	A86	J	302	-	44,50,50	1.26	4 (9%)	51,76,76	2.08	12 (23%)
36	CLA	P	310	15,41	69,73,73	1.25	9 (13%)	83,113,113	1.35	6 (7%)
36	CLA	a	831	-	69,73,73	1.25	10 (14%)	83,113,113	1.27	10 (12%)
36	CLA	b	831	21	54,58,73	1.42	11 (20%)	65,95,113	1.55	8 (12%)
36	CLA	R	312	16	69,73,73	1.25	9 (13%)	83,113,113	1.51	10 (12%)
36	CLA	F	312	-	69,73,73	1.23	9 (13%)	83,113,113	1.33	7 (8%)
35	A86	P	303	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)
34	DD6	E	306	-	39,45,45	2.03	3 (7%)	52,67,67	2.04	10 (19%)
36	CLA	G	314	7	45,49,73	1.48	9 (20%)	54,84,113	1.70	8 (14%)
36	CLA	D	306	4	49,53,73	1.53	11 (22%)	59,89,113	1.65	9 (15%)
39	LMT	G	323	-	36,36,36	0.39	0	47,47,47	0.82	0
36	CLA	X	310	19	45,49,73	1.55	8 (17%)	54,84,113	2.03	9 (16%)
35	A86	I	304	-	44,50,50	1.47	4 (9%)	51,76,76	3.38	21 (41%)
36	CLA	G	319	7	54,58,73	2.01	18 (33%)	65,95,113	4.02	30 (46%)
35	A86	S	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
36	CLA	O	311	-	62,66,73	1.29	9 (14%)	74,104,113	1.37	5 (6%)
44	BCR	b	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.26	7 (12%)
36	CLA	a	805	20	69,73,73	1.23	11 (15%)	83,113,113	1.35	9 (10%)
36	CLA	H	306	-	65,69,73	1.27	10 (15%)	78,108,113	1.34	5 (6%)
35	A86	Q	304	-	44,50,50	1.39	6 (13%)	51,76,76	3.30	24 (47%)
35	A86	M	302	-	44,50,50	1.29	4 (9%)	51,76,76	2.78	16 (31%)
36	CLA	I	313	-	45,49,73	1.49	10 (22%)	54,84,113	1.58	6 (11%)
37	KC1	F	315	-	49,53,53	2.67	17 (34%)	63,89,89	5.79	37 (58%)
42	LMG	E	318	-	46,46,55	0.98	2 (4%)	54,54,63	1.06	2 (3%)
36	CLA	I	306	9	69,73,73	1.67	15 (21%)	83,113,113	2.48	24 (28%)
35	A86	T	306	-	44,50,50	1.23	4 (9%)	51,76,76	2.88	18 (35%)
36	CLA	F	310	6	60,64,73	1.30	10 (16%)	72,102,113	1.50	13 (18%)
36	CLA	C	214	-	45,49,73	1.48	10 (22%)	54,84,113	1.60	8 (14%)
42	LMG	V	315	-	46,46,55	0.98	2 (4%)	54,54,63	4.29	4 (7%)
36	CLA	a	841	41	56,60,73	1.41	10 (17%)	67,97,113	1.55	9 (13%)
39	LMT	h	205	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LMT	b	848	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
36	CLA	f	805	25	56,60,73	1.34	10 (17%)	67,97,113	1.52	8 (11%)
36	CLA	J	316	10	50,54,73	1.45	9 (18%)	60,90,113	1.73	10 (16%)
36	CLA	l	202	28,21	69,73,73	1.26	11 (15%)	83,113,113	1.33	9 (10%)
39	LMT	B	312	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
44	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	3 (5%)
36	CLA	b	832	21	53,57,73	1.33	11 (20%)	62,93,113	1.55	8 (12%)
41	LHG	f	809	-	41,41,48	1.01	2 (4%)	44,47,54	1.09	3 (6%)
34	DD6	E	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.93	10 (19%)
44	BCR	l	207	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	8 (14%)
36	CLA	B	307	-	50,54,73	1.45	8 (16%)	60,90,113	1.52	7 (11%)
36	CLA	S	319	17	69,73,73	1.28	10 (14%)	83,113,113	1.48	9 (10%)
36	CLA	F	311	-	56,60,73	1.36	9 (16%)	67,97,113	1.53	6 (8%)
36	CLA	T	312	18	50,54,73	1.46	8 (16%)	60,90,113	1.64	10 (16%)
35	A86	V	303	35	44,50,50	1.28	4 (9%)	51,76,76	3.25	22 (43%)
36	CLA	L	309	12	69,73,73	1.23	10 (14%)	83,113,113	1.34	9 (10%)
36	CLA	A	307	-	64,68,73	1.27	10 (15%)	77,107,113	1.38	9 (11%)
35	A86	O	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.07	14 (27%)
36	CLA	l	204	28	53,57,73	2.03	16 (30%)	62,93,113	2.45	20 (32%)
44	BCR	b	846	-	41,41,41	1.15	4 (9%)	56,56,56	1.44	10 (17%)
36	CLA	X	306	-	65,69,73	1.31	7 (10%)	78,108,113	1.37	6 (7%)
36	CLA	P	313	-	69,73,73	1.23	9 (13%)	83,113,113	1.32	4 (4%)
35	A86	L	319	-	44,50,50	1.43	6 (13%)	51,76,76	3.47	24 (47%)
37	KC1	G	317	-	49,53,53	2.71	20 (40%)	63,89,89	4.44	38 (60%)
36	CLA	R	313	-	69,73,73	1.23	11 (15%)	83,113,113	1.25	8 (9%)
36	CLA	R	322	16	56,60,73	1.42	10 (17%)	67,97,113	1.66	10 (14%)
36	CLA	P	308	-	65,69,73	1.28	9 (13%)	78,108,113	1.38	5 (6%)
36	CLA	V	306	33	69,73,73	1.30	8 (11%)	83,113,113	1.50	12 (14%)
36	CLA	a	807	20	69,73,73	1.20	11 (15%)	83,113,113	1.49	12 (14%)
36	CLA	J	317	10	51,55,73	1.42	10 (19%)	61,91,113	1.42	5 (8%)
36	CLA	a	832	-	69,73,73	1.22	9 (13%)	83,113,113	1.52	12 (14%)
36	CLA	b	826	46,21	68,72,73	1.33	12 (17%)	81,111,113	2.00	17 (20%)
44	BCR	i	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.32	7 (12%)
37	KC1	C	213	3	49,53,53	2.74	18 (36%)	63,89,89	4.34	34 (53%)
36	CLA	P	316	-	45,49,73	1.51	9 (20%)	54,84,113	1.73	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	Q	308	-	69,73,73	1.24	10 (14%)	83,113,113	1.42	10 (12%)
37	KC1	F	308	6	49,53,53	2.73	20 (40%)	63,89,89	5.24	36 (57%)
36	CLA	C	209	-	69,73,73	1.26	10 (14%)	83,113,113	1.40	9 (10%)
36	CLA	X	308	19	51,55,73	2.57	11 (21%)	61,91,113	2.62	20 (32%)
36	CLA	f	804	46	69,73,73	1.99	19 (27%)	83,113,113	3.08	32 (38%)
39	LMT	a	854	-	36,36,36	0.40	0	47,47,47	0.75	0
34	DD6	R	308	-	39,45,45	2.02	3 (7%)	52,67,67	2.12	13 (25%)
35	A86	K	303	-	44,50,50	1.31	4 (9%)	51,76,76	2.80	17 (33%)
36	CLA	X	313	19	46,50,73	2.14	12 (26%)	55,85,113	4.04	20 (36%)
44	BCR	b	845	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	8 (14%)
36	CLA	O	312	-	43,48,73	1.79	12 (27%)	52,82,113	1.53	10 (19%)
44	BCR	a	845	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	5 (8%)
36	CLA	N	318	-	51,55,73	1.44	9 (17%)	61,91,113	1.68	9 (14%)
36	CLA	H	318	-	54,58,73	1.42	12 (22%)	65,95,113	1.51	8 (12%)
37	KC1	B	310	2	49,53,53	2.88	20 (40%)	63,89,89	4.55	36 (57%)
36	CLA	M	309	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	6 (7%)
44	BCR	i	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	7 (12%)
36	CLA	a	808	20	69,73,73	1.23	11 (15%)	83,113,113	1.41	9 (10%)
36	CLA	b	811	21	69,73,73	1.24	10 (14%)	83,113,113	1.52	8 (9%)
35	A86	X	301	-	44,50,50	1.55	5 (11%)	51,76,76	3.61	28 (54%)
36	CLA	M	306	13,37	59,63,73	1.33	9 (15%)	71,101,113	1.58	10 (14%)
36	CLA	I	308	9	69,73,73	1.88	17 (24%)	83,113,113	2.71	24 (28%)
36	CLA	C	207	-	69,73,73	1.98	17 (24%)	83,113,113	2.97	26 (31%)
36	CLA	b	824	21	57,61,73	2.02	17 (29%)	68,98,113	2.57	25 (36%)
36	CLA	F	317	6	60,64,73	1.97	16 (26%)	72,102,113	2.65	24 (33%)
36	CLA	a	804	20	69,73,73	1.25	10 (14%)	83,113,113	1.42	12 (14%)
44	BCR	f	801	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
39	LMT	B	313	-	36,36,36	0.43	0	47,47,47	0.73	1 (2%)
36	CLA	b	829	21	69,73,73	1.25	11 (15%)	83,113,113	1.31	6 (7%)
36	CLA	O	306	-	65,69,73	1.28	9 (13%)	78,108,113	1.37	5 (6%)
39	LMT	I	318	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
36	CLA	E	311	5	69,73,73	1.23	10 (14%)	83,113,113	1.33	7 (8%)
36	CLA	a	818	20	69,73,73	1.25	8 (11%)	83,113,113	1.54	11 (13%)
36	CLA	Q	314	-	69,73,73	1.27	8 (11%)	83,113,113	3.97	14 (16%)
37	KC1	U	312	32,35	49,53,53	2.95	21 (42%)	63,89,89	4.31	34 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	b	807	21	49,53,73	1.42	11 (22%)	59,89,113	1.57	8 (13%)
39	LMT	a	851	-	36,36,36	0.43	0	47,47,47	0.74	1 (2%)
34	DD6	S	307	-	39,45,45	2.03	3 (7%)	52,67,67	2.07	15 (28%)
35	A86	R	306	-	44,50,50	1.34	4 (9%)	51,76,76	2.91	16 (31%)
36	CLA	J	309	10	69,73,73	1.25	10 (14%)	83,113,113	1.26	8 (9%)
36	CLA	N	308	14	69,73,73	1.40	8 (11%)	83,113,113	1.80	20 (24%)
36	CLA	G	311	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	8 (9%)
41	LHG	a	843	36	26,26,48	1.24	2 (7%)	29,32,54	1.31	2 (6%)
42	LMG	G	324	-	55,55,55	0.90	2 (3%)	63,63,63	1.00	3 (4%)
41	LHG	b	850	36	48,48,48	0.92	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	b	836	21	62,66,73	2.02	15 (24%)	74,104,113	3.01	24 (32%)
35	A86	F	301	-	44,50,50	1.24	4 (9%)	51,76,76	2.32	16 (31%)
34	DD6	A	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.86	9 (17%)
36	CLA	K	316	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
37	KC1	O	313	15	49,53,53	2.88	20 (40%)	63,89,89	6.04	39 (61%)
35	A86	X	303	36	44,50,50	1.47	5 (11%)	51,76,76	3.76	24 (47%)
35	A86	G	302	-	44,50,50	1.18	3 (6%)	51,76,76	1.92	13 (25%)
41	LHG	G	321	36	46,46,48	0.96	2 (4%)	49,52,54	1.06	2 (4%)
37	KC1	M	318	-	49,53,53	4.98	26 (53%)	63,89,89	7.21	36 (57%)
35	A86	V	301	35	44,50,50	1.23	4 (9%)	51,76,76	2.22	16 (31%)
36	CLA	G	310	7	69,73,73	1.23	12 (17%)	83,113,113	1.26	8 (9%)
36	CLA	a	819	-	49,53,73	1.50	12 (24%)	59,89,113	2.16	8 (13%)
39	LMT	U	314	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
36	CLA	P	309	41	69,73,73	1.24	11 (15%)	83,113,113	1.37	7 (8%)
36	CLA	V	314	-	69,73,73	1.97	16 (23%)	83,113,113	2.90	24 (28%)
38	SQD	A	315	-	27,28,54	1.50	4 (14%)	36,39,65	1.29	5 (13%)
36	CLA	a	823	-	59,63,73	1.71	13 (22%)	71,101,113	2.27	21 (29%)
36	CLA	b	830	21	69,73,73	1.29	10 (14%)	83,113,113	1.66	13 (15%)
44	BCR	b	843	-	41,41,41	1.18	3 (7%)	56,56,56	1.18	5 (8%)
36	CLA	a	812	20	69,73,73	1.23	10 (14%)	83,113,113	1.40	8 (9%)
36	CLA	a	821	20	53,57,73	1.38	11 (20%)	62,93,113	1.53	7 (11%)
37	KC1	H	313	-	49,53,53	2.65	21 (42%)	63,89,89	4.55	36 (57%)
35	A86	h	204	-	44,50,50	1.23	4 (9%)	51,76,76	2.14	11 (21%)
39	LMT	G	322	-	36,36,36	0.39	0	47,47,47	0.69	0
36	CLA	G	315	7	60,64,73	1.92	15 (25%)	72,102,113	2.85	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	X	307	35,19	54,58,73	1.49	9 (16%)	65,95,113	1.76	12 (18%)
36	CLA	G	313	7	69,73,73	1.36	9 (13%)	83,113,113	1.85	16 (19%)
35	A86	G	305	-	44,50,50	1.23	3 (6%)	51,76,76	2.23	15 (29%)
35	A86	P	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.05	13 (25%)
35	A86	I	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.39	18 (35%)
36	CLA	P	311	-	69,73,73	1.24	10 (14%)	83,113,113	1.42	10 (12%)
36	CLA	a	848	36	69,73,73	1.55	14 (20%)	83,113,113	1.90	18 (21%)
36	CLA	S	318	-	46,50,73	1.48	6 (13%)	55,85,113	1.60	6 (10%)
36	CLA	b	821	46	69,73,73	1.22	10 (14%)	83,113,113	1.42	8 (9%)
42	LMG	m	102	-	37,37,55	1.08	2 (5%)	45,45,63	1.08	3 (6%)
36	CLA	Q	309	15	50,54,73	1.46	9 (18%)	60,90,113	1.60	8 (13%)
36	CLA	b	840	21	69,73,73	1.23	11 (15%)	83,113,113	1.48	12 (14%)
36	CLA	K	313	-	69,73,73	1.30	13 (18%)	83,113,113	1.48	11 (13%)
36	CLA	F	309	-	69,73,73	1.25	10 (14%)	83,113,113	1.43	12 (14%)
39	LMT	L	318	-	32,32,36	0.45	0	43,43,47	0.79	1 (2%)
36	CLA	G	312	7	62,66,73	1.28	11 (17%)	74,104,113	1.47	6 (8%)
35	A86	J	305	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	15 (29%)
36	CLA	N	310	14	45,49,73	1.73	10 (22%)	54,84,113	2.52	18 (33%)
36	CLA	b	805	36,21	69,73,73	1.27	10 (14%)	83,113,113	1.30	13 (15%)
39	LMT	F	321	-	34,34,36	0.65	0	45,45,47	1.61	6 (13%)
44	BCR	f	806	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	7 (12%)
36	CLA	E	312	-	69,73,73	1.24	11 (15%)	83,113,113	1.44	10 (12%)
36	CLA	L	316	-	45,49,73	1.53	7 (15%)	54,84,113	1.58	6 (11%)
36	CLA	T	308	18	65,69,73	1.28	7 (10%)	78,108,113	1.43	7 (8%)
35	A86	E	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.19	13 (25%)
42	LMG	a	852	-	54,54,55	0.90	2 (3%)	62,62,63	1.03	3 (4%)
37	KC1	G	318	-	49,53,53	2.74	20 (40%)	63,89,89	4.46	41 (65%)
36	CLA	M	314	-	45,49,73	1.51	9 (20%)	54,84,113	1.56	6 (11%)
43	PQN	b	842	-	34,34,34	1.56	2 (5%)	42,45,45	1.19	4 (9%)
37	KC1	P	315	35	49,53,53	2.88	20 (40%)	63,89,89	6.04	39 (61%)
36	CLA	T	316	-	45,49,73	1.52	9 (20%)	54,84,113	1.55	7 (12%)
44	BCR	j	107	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	7 (12%)
36	CLA	H	308	8	67,72,73	1.27	12 (17%)	80,112,113	1.33	11 (13%)
36	CLA	R	310	-	65,69,73	1.28	10 (15%)	78,108,113	1.39	7 (8%)
36	CLA	a	828	-	69,73,73	1.21	9 (13%)	83,113,113	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	P	314	-	64,68,73	1.43	11 (17%)	77,107,113	1.67	16 (20%)
41	LHG	j	104	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	D	312	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
36	CLA	b	802	20	69,73,73	1.22	10 (14%)	83,113,113	1.38	8 (9%)
38	SQD	b	804	-	45,46,54	1.27	4 (8%)	54,57,65	1.21	4 (7%)
36	CLA	b	819	-	63,67,73	1.33	8 (12%)	75,105,113	1.89	17 (22%)
36	CLA	K	312	-	69,73,73	1.21	10 (14%)	83,113,113	1.33	6 (7%)
39	LMT	K	317	-	32,32,36	0.43	0	43,43,47	0.70	0
37	KC1	W	217	-	49,53,53	2.87	18 (36%)	63,89,89	4.42	37 (58%)
35	A86	S	302	-	44,50,50	1.20	3 (6%)	51,76,76	2.68	15 (29%)
36	CLA	I	314	-	45,49,73	1.50	8 (17%)	54,84,113	1.63	8 (14%)
41	LHG	G	320	-	39,39,48	1.04	2 (5%)	42,45,54	1.11	3 (7%)
44	BCR	m	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.34	7 (12%)
36	CLA	R	321	16	69,73,73	1.27	9 (13%)	83,113,113	1.44	10 (12%)
34	DD6	A	301	-	39,45,45	2.04	3 (7%)	52,67,67	2.08	15 (28%)
35	A86	T	302	18	44,50,50	1.24	3 (6%)	51,76,76	2.85	21 (41%)
36	CLA	b	838	21	51,55,73	1.37	10 (19%)	61,91,113	1.44	7 (11%)
34	DD6	P	305	-	39,45,45	2.02	3 (7%)	52,67,67	2.06	16 (30%)
36	CLA	D	315	-	45,49,73	1.47	10 (22%)	54,84,113	1.80	9 (16%)
36	CLA	K	311	11	50,54,73	1.46	9 (18%)	60,90,113	1.51	8 (13%)
36	CLA	b	827	-	69,73,73	1.33	10 (14%)	83,113,113	1.40	9 (10%)
35	A86	R	305	-	44,50,50	1.22	4 (9%)	51,76,76	1.81	11 (21%)
35	A86	B	301	-	44,50,50	1.23	4 (9%)	51,76,76	1.98	13 (25%)
37	KC1	G	308	-	49,53,53	2.71	20 (40%)	63,89,89	4.85	38 (60%)
36	CLA	a	830	20	54,58,73	1.71	13 (24%)	65,95,113	3.30	20 (30%)
36	CLA	N	319	14	46,50,73	3.35	13 (28%)	55,85,113	5.74	32 (58%)
35	A86	O	303	-	44,50,50	1.34	5 (11%)	51,76,76	2.73	17 (33%)
36	CLA	C	210	3	50,54,73	1.49	9 (18%)	60,90,113	1.55	7 (11%)
36	CLA	W	216	35,19	49,53,73	1.95	10 (20%)	59,89,113	3.01	15 (25%)
44	BCR	l	203	-	41,41,41	1.23	4 (9%)	56,56,56	1.21	5 (8%)
39	LMT	L	303	-	36,36,36	1.33	6 (16%)	47,47,47	0.96	1 (2%)
36	CLA	b	817	21	63,67,73	1.73	14 (22%)	75,105,113	2.17	18 (24%)
36	CLA	b	809	21	69,73,73	1.22	11 (15%)	83,113,113	1.30	6 (7%)
42	LMG	J	319	-	44,44,55	0.99	2 (4%)	52,52,63	1.11	3 (5%)
36	CLA	A	314	1	69,73,73	1.32	8 (11%)	83,113,113	1.81	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A86	Q	301	-	44,50,50	1.33	5 (11%)	51,76,76	2.73	17 (33%)
36	CLA	D	309	4	59,63,73	2.08	18 (30%)	71,101,113	3.19	29 (40%)
35	A86	V	302	-	44,50,50	1.32	4 (9%)	51,76,76	2.92	21 (41%)
36	CLA	K	309	11	63,67,73	1.31	10 (15%)	75,105,113	1.34	7 (9%)
36	CLA	N	307	-	65,69,73	1.29	8 (12%)	78,108,113	1.34	4 (5%)
36	CLA	b	835	-	49,53,73	1.45	10 (20%)	59,89,113	1.64	9 (15%)
36	CLA	a	827	20	66,70,73	1.28	10 (15%)	79,109,113	1.51	10 (12%)
34	DD6	F	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	14 (26%)
35	A86	H	301	-	44,50,50	1.29	3 (6%)	51,76,76	4.88	20 (39%)
36	CLA	b	833	21	62,66,73	1.31	10 (16%)	74,104,113	1.57	11 (14%)
36	CLA	J	315	10	45,49,73	1.51	9 (20%)	54,84,113	1.64	7 (12%)
36	CLA	E	314	-	69,73,73	1.21	11 (15%)	83,113,113	1.51	13 (15%)
34	DD6	B	304	-	39,45,45	2.01	3 (7%)	52,67,67	2.14	16 (30%)
35	A86	X	304	19	44,50,50	1.34	4 (9%)	51,76,76	3.26	20 (39%)
35	A86	M	301	-	44,50,50	1.36	4 (9%)	51,76,76	3.39	22 (43%)
36	CLA	M	308	-	56,60,73	1.39	11 (19%)	67,97,113	1.60	8 (11%)
36	CLA	V	313	33	69,73,73	1.27	10 (14%)	83,113,113	1.26	7 (8%)
36	CLA	D	307	41	65,69,73	1.25	9 (13%)	78,108,113	1.60	16 (20%)
41	LHG	l	208	-	47,47,48	0.95	2 (4%)	50,53,54	1.02	3 (6%)
36	CLA	a	815	46	49,53,73	1.46	9 (18%)	59,89,113	1.53	5 (8%)
36	CLA	L	314	12	69,73,73	1.23	9 (13%)	83,113,113	1.45	10 (12%)
35	A86	V	304	-	44,50,50	1.48	6 (13%)	51,76,76	3.49	18 (35%)
36	CLA	M	316	36	46,50,73	1.47	9 (19%)	55,85,113	1.47	4 (7%)
36	CLA	W	209	19	61,65,73	1.35	10 (16%)	73,103,113	1.41	11 (15%)
35	A86	U	304	32,37	44,50,50	1.21	3 (6%)	51,76,76	2.34	19 (37%)
34	DD6	S	306	-	39,45,45	1.96	3 (7%)	52,67,67	2.00	13 (25%)
36	CLA	Q	312	-	45,49,73	1.52	9 (20%)	54,84,113	1.73	8 (14%)
36	CLA	a	826	20	69,73,73	1.23	10 (14%)	83,113,113	1.51	9 (10%)
36	CLA	H	307	8	64,68,73	1.37	9 (14%)	77,107,113	1.87	20 (25%)
35	A86	S	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.13	16 (31%)
35	A86	F	306	-	44,50,50	1.26	4 (9%)	51,76,76	2.04	13 (25%)
41	LHG	O	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.08	3 (6%)
35	A86	L	306	37	44,50,50	1.24	3 (6%)	51,76,76	2.98	19 (37%)
35	A86	T	307	-	44,50,50	1.24	3 (6%)	51,76,76	3.14	21 (41%)
36	CLA	R	316	-	50,54,73	1.49	11 (22%)	60,90,113	1.96	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A86	C	202	36,3	44,50,50	1.40	5 (11%)	51,76,76	3.09	17 (33%)
36	CLA	b	828	21	69,73,73	1.30	10 (14%)	83,113,113	1.43	13 (15%)
36	CLA	T	311	18	69,73,73	1.28	10 (14%)	83,113,113	1.93	14 (16%)
36	CLA	b	815	21	69,73,73	1.27	11 (15%)	83,113,113	1.36	7 (8%)
41	LHG	D	318	36	45,45,48	0.30	0	48,51,54	0.39	0
36	CLA	L	320	12	69,73,73	1.23	9 (13%)	83,113,113	1.32	5 (6%)
36	CLA	H	311	-	69,73,73	1.18	10 (14%)	83,113,113	1.43	9 (10%)
36	CLA	b	816	21	64,68,73	1.99	17 (26%)	77,107,113	1.92	18 (23%)
36	CLA	U	306	32	69,73,73	1.92	17 (24%)	83,113,113	2.65	25 (30%)
35	A86	O	302	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)
36	CLA	L	310	-	58,62,73	1.38	9 (15%)	69,99,113	1.31	5 (7%)
34	DD6	G	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	10 (19%)
34	DD6	j	103	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	12 (23%)
39	LMT	F	320	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
36	CLA	I	311	9	69,73,73	1.20	10 (14%)	83,113,113	1.49	10 (12%)
36	CLA	a	806	-	69,73,73	1.46	10 (14%)	83,113,113	1.97	19 (22%)
35	A86	B	303	-	44,50,50	1.30	3 (6%)	51,76,76	4.01	27 (52%)
36	CLA	Q	306	-	69,73,73	1.23	11 (15%)	83,113,113	1.37	7 (8%)
41	LHG	E	322	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
40	DGD	C	215	-	58,58,67	0.90	2 (3%)	72,72,81	0.96	3 (4%)
34	DD6	D	304	-	39,45,45	1.97	3 (7%)	52,67,67	1.91	12 (23%)
36	CLA	l	206	46	54,58,73	1.36	10 (18%)	65,95,113	1.48	7 (10%)
35	A86	S	308	37	44,50,50	1.23	4 (9%)	51,76,76	2.12	16 (31%)
36	CLA	U	311	32	69,73,73	1.27	11 (15%)	83,113,113	1.53	13 (15%)
36	CLA	T	314	-	69,73,73	1.22	8 (11%)	83,113,113	1.53	11 (13%)
34	DD6	B	302	-	39,45,45	2.01	3 (7%)	52,67,67	2.07	16 (30%)
36	CLA	H	315	8	69,73,73	1.26	10 (14%)	83,113,113	1.53	13 (15%)
35	A86	J	306	-	44,50,50	1.25	3 (6%)	51,76,76	1.96	11 (21%)
35	A86	N	304	-	44,50,50	2.90	7 (15%)	51,76,76	7.45	18 (35%)
36	CLA	S	314	17	69,73,73	1.32	11 (15%)	83,113,113	1.46	11 (13%)
36	CLA	A	308	-	69,73,73	1.22	9 (13%)	83,113,113	1.44	10 (12%)
34	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	13 (25%)
34	DD6	M	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.96	11 (21%)
36	CLA	b	806	-	69,73,73	1.28	9 (13%)	83,113,113	1.60	13 (15%)
36	CLA	V	311	33	69,73,73	1.24	10 (14%)	83,113,113	1.62	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	KC1	D	314	4	49,53,53	2.66	18 (36%)	63,89,89	4.84	39 (61%)
36	CLA	a	825	-	69,73,73	1.38	11 (15%)	83,113,113	1.73	12 (14%)
36	CLA	S	313	-	50,54,73	1.45	7 (14%)	60,90,113	1.81	12 (20%)
36	CLA	B	306	-	50,54,73	1.42	8 (16%)	60,90,113	1.61	6 (10%)
40	DGD	b	849	-	61,61,67	1.05	7 (11%)	75,75,81	1.49	11 (14%)
37	KC1	N	314	14	49,53,53	2.87	22 (44%)	63,89,89	4.43	37 (58%)
35	A86	N	303	-	44,50,50	1.31	5 (11%)	51,76,76	3.31	22 (43%)
35	A86	U	303	36	44,50,50	1.23	4 (9%)	51,76,76	2.00	14 (27%)
36	CLA	f	803	-	69,73,73	1.81	17 (24%)	83,113,113	2.56	27 (32%)
36	CLA	J	312	10	69,73,73	1.21	10 (14%)	83,113,113	1.41	8 (9%)
36	CLA	a	835	20	55,59,73	1.41	11 (20%)	66,96,113	1.43	8 (12%)
35	A86	N	306	-	44,50,50	1.22	3 (6%)	51,76,76	2.83	16 (31%)
34	DD6	W	204	36	39,45,45	2.04	3 (7%)	52,67,67	2.01	13 (25%)
36	CLA	H	314	-	45,49,73	1.49	11 (24%)	54,84,113	1.72	8 (14%)
36	CLA	X	312	-	45,49,73	1.52	9 (20%)	54,84,113	1.71	8 (14%)
36	CLA	C	211	-	69,73,73	1.24	11 (15%)	83,113,113	1.36	7 (8%)
36	CLA	a	833	20	54,58,73	1.37	10 (18%)	65,95,113	1.64	8 (12%)
35	A86	h	202	-	44,50,50	1.24	4 (9%)	51,76,76	1.74	10 (19%)
36	CLA	H	305	8	52,56,73	1.44	8 (15%)	62,92,113	1.48	7 (11%)
35	A86	R	303	-	44,50,50	1.36	5 (11%)	51,76,76	3.63	21 (41%)
36	CLA	X	315	-	45,49,73	1.53	7 (15%)	54,84,113	1.58	9 (16%)
37	KC1	A	312	1	49,53,53	2.73	18 (36%)	63,89,89	6.28	44 (69%)
37	KC1	E	309	-	49,53,53	2.70	19 (38%)	63,89,89	4.86	41 (65%)
42	LMG	L	321	40	33,33,55	1.13	2 (6%)	41,41,63	1.15	3 (7%)
36	CLA	W	214	19	45,49,73	1.66	8 (17%)	54,84,113	1.82	13 (24%)
36	CLA	N	315	-	45,49,73	1.54	7 (15%)	54,84,113	1.73	12 (22%)
41	LHG	a	842	-	47,47,48	0.76	1 (2%)	50,53,54	1.27	4 (8%)
36	CLA	a	820	-	69,73,73	1.22	11 (15%)	83,113,113	1.40	11 (13%)
42	LMG	E	319	-	40,40,55	1.04	2 (5%)	48,48,63	1.11	3 (6%)
36	CLA	W	215	-	52,56,73	1.63	10 (19%)	62,92,113	1.42	8 (12%)
36	CLA	h	203	31	69,73,73	1.21	10 (14%)	83,113,113	1.47	9 (10%)
36	CLA	P	312	15	50,54,73	1.45	9 (18%)	60,90,113	1.58	8 (13%)
36	CLA	M	311	13,35	69,73,73	1.25	9 (13%)	83,113,113	1.27	4 (4%)
36	CLA	I	312	9	56,60,73	1.41	9 (16%)	67,97,113	1.42	6 (8%)
35	A86	L	304	-	44,50,50	1.39	4 (9%)	51,76,76	2.99	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	R	318	35	45,49,73	1.53	9 (20%)	54,84,113	1.57	9 (16%)
35	A86	O	319	36,35	44,50,50	1.28	5 (11%)	51,76,76	2.93	18 (35%)
35	A86	T	303	-	44,50,50	1.22	4 (9%)	51,76,76	3.14	21 (41%)
35	A86	D	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.08	11 (21%)
36	CLA	O	307	-	69,73,73	1.24	11 (15%)	83,113,113	1.36	7 (8%)
35	A86	W	202	36,19	44,50,50	1.50	6 (13%)	51,76,76	3.63	29 (56%)
35	A86	T	304	-	44,50,50	1.11	3 (6%)	51,76,76	1.69	11 (21%)
36	CLA	A	310	-	69,73,73	1.23	11 (15%)	83,113,113	1.36	8 (9%)
36	CLA	I	310	35	69,73,73	1.22	10 (14%)	83,113,113	1.38	8 (9%)
34	DD6	C	201	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	13 (25%)
36	CLA	l	205	-	69,73,73	1.54	14 (20%)	83,113,113	2.13	17 (20%)
36	CLA	l	201	-	69,73,73	1.23	10 (14%)	83,113,113	1.44	12 (14%)
36	CLA	P	319	-	64,68,73	1.97	13 (20%)	77,107,113	2.21	16 (20%)
36	CLA	E	313	-	69,73,73	1.77	16 (23%)	83,113,113	2.40	24 (28%)
43	PQN	a	840	-	34,34,34	1.58	2 (5%)	42,45,45	1.15	4 (9%)
36	CLA	f	802	21	69,73,73	1.28	10 (14%)	83,113,113	1.42	8 (9%)
36	CLA	R	319	16	49,53,73	1.47	9 (18%)	59,89,113	1.83	12 (20%)
36	CLA	j	102	-	69,73,73	1.63	13 (18%)	83,113,113	2.19	18 (21%)
36	CLA	G	309	7	69,73,73	1.21	12 (17%)	83,113,113	1.80	14 (16%)
36	CLA	N	316	14	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
35	A86	H	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.31	17 (33%)
36	CLA	b	834	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
36	CLA	V	310	33	69,73,73	1.23	9 (13%)	83,113,113	1.32	5 (6%)
36	CLA	U	310	-	69,73,73	1.25	8 (11%)	83,113,113	1.53	12 (14%)
36	CLA	A	311	-	69,73,73	1.23	10 (14%)	83,113,113	1.36	6 (7%)
39	LMT	a	853	-	33,33,36	0.42	0	44,44,47	0.74	1 (2%)
39	LMT	P	321	-	23,23,36	0.43	0	28,28,47	0.61	0
36	CLA	M	315	13	51,55,73	1.44	10 (19%)	61,91,113	1.58	6 (9%)
36	CLA	L	313	-	69,73,73	1.20	8 (11%)	83,113,113	1.43	8 (9%)
34	DD6	K	305	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	14 (26%)
42	LMG	V	316	-	46,46,55	0.98	2 (4%)	54,54,63	1.04	3 (5%)
36	CLA	D	317	-	62,66,73	1.30	10 (16%)	74,104,113	1.40	6 (8%)
37	KC1	P	317	15	49,53,53	2.60	19 (38%)	63,89,89	5.00	37 (58%)
36	CLA	N	312	-	51,55,73	1.37	8 (15%)	61,91,113	1.49	4 (6%)
35	A86	X	314	19	44,50,50	1.26	4 (9%)	51,76,76	2.07	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	O	310	15	50,54,73	1.45	9 (18%)	60,90,113	1.59	8 (13%)
36	CLA	K	315	-	45,49,73	1.51	10 (22%)	54,84,113	1.62	7 (12%)
35	A86	N	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.68	15 (29%)
39	LMT	P	320	-	23,23,36	0.43	0	28,28,47	0.62	0
35	A86	N	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
36	CLA	O	309	-	69,73,73	1.25	11 (15%)	83,113,113	1.42	11 (13%)
36	CLA	a	829	20	69,73,73	1.27	9 (13%)	83,113,113	1.62	14 (16%)
36	CLA	C	212	35	69,73,73	1.22	11 (15%)	83,113,113	1.54	13 (15%)
35	A86	J	301	-	44,50,50	1.26	4 (9%)	51,76,76	2.23	18 (35%)
35	A86	M	305	-	44,50,50	1.34	4 (9%)	51,76,76	2.88	15 (29%)
34	DD6	E	303	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	10 (19%)
34	DD6	R	307	-	39,45,45	2.00	2 (5%)	52,67,67	2.11	15 (28%)
36	CLA	T	313	18	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
36	CLA	V	309	33	47,51,73	1.45	8 (17%)	56,86,113	1.89	11 (19%)
36	CLA	U	309	32	50,54,73	1.52	7 (14%)	60,90,113	1.71	10 (16%)

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
35	A86	O	305	-	-	14/34/90/90	0/3/3/3
36	CLA	O	314	-	-	5/10/86/115	-
36	CLA	J	310	-	-	11/39/115/115	-
36	CLA	a	824	-	-	11/39/115/115	-
35	A86	K	302	-	-	8/34/90/90	0/3/3/3
36	CLA	N	311	14	-	6/17/93/115	-
36	CLA	S	311	35	-	4/17/93/115	-
36	CLA	M	312	13,36	-	12/18/94/115	-
36	CLA	T	309	18	-	20/39/115/115	-
36	CLA	K	310	-	1/1/14/20	16/36/112/115	-
44	BCR	b	844	-	-	6/29/63/63	0/2/2/2
36	CLA	G	307	-	-	2/11/87/115	-
34	DD6	O	304	-	-	5/26/80/80	0/3/3/3
36	CLA	I	309	9	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	D	303	-	-	9/26/80/80	0/3/3/3
36	CLA	C	206	-	-	17/35/111/115	-
36	CLA	L	308	-	1/1/14/20	22/35/111/115	-
35	A86	E	305	5	-	5/34/90/90	0/3/3/3
36	CLA	V	308	-	-	18/39/115/115	-
41	LHG	D	319	42	-	30/53/53/53	-
35	A86	G	306	-	-	6/34/90/90	1/3/3/3
36	CLA	b	810	21	-	10/39/115/115	-
34	DD6	H	303	-	-	6/26/80/80	0/3/3/3
36	CLA	b	812	21	-	6/39/115/115	-
36	CLA	b	841	41	-	9/39/115/115	-
35	A86	C	203	-	-	8/34/90/90	1/3/3/3
36	CLA	S	315	17	-	5/13/89/115	-
37	KC1	T	310	18	-	11/15/71/71	-
36	CLA	O	308	15	-	15/39/115/115	-
36	CLA	F	316	6	-	3/10/86/115	-
36	CLA	L	311	-	-	14/39/115/115	-
36	CLA	X	309	19	-	8/15/91/115	-
34	DD6	J	304	-	-	5/26/80/80	0/3/3/3
42	LMG	I	315	-	-	32/50/70/70	0/1/1/1
36	CLA	S	309	-	-	10/35/111/115	-
36	CLA	b	818	21	-	4/27/103/115	-
37	KC1	X	311	-	-	3/15/71/71	-
41	LHG	G	301	-	-	24/53/53/53	-
44	BCR	h	201	-	-	9/29/63/63	0/2/2/2
36	CLA	W	208	-	-	7/15/91/115	-
36	CLA	Q	310	15	-	22/39/115/115	-
35	A86	K	306	11	-	8/34/90/90	0/3/3/3
36	CLA	H	317	8	-	10/39/115/115	-
36	CLA	N	309	14	-	8/23/99/115	-
35	A86	X	305	-	-	8/34/90/90	0/3/3/3
41	LHG	O	318	15	-	30/53/53/53	-
35	A86	S	305	-	-	9/34/90/90	0/3/3/3
39	LMT	E	323	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	H	302	-	-	2/26/80/80	0/3/3/3
36	CLA	b	801	46	-	8/39/115/115	-
36	CLA	b	808	21	-	14/39/115/115	-
36	CLA	J	308	-	-	14/35/111/115	-
36	CLA	A	305	1	-	6/20/96/115	-
41	LHG	F	319	-	-	33/45/45/53	-
35	A86	C	204	-	-	12/34/90/90	0/3/3/3
36	CLA	b	825	-	-	13/39/115/115	-
37	KC1	L	317	-	-	3/15/71/71	-
36	CLA	S	312	17	-	17/39/115/115	-
35	A86	P	306	-	-	3/34/90/90	0/3/3/3
36	CLA	j	106	27	-	8/12/88/115	-
37	KC1	J	314	-	-	4/15/71/71	-
39	LMT	E	321	-	-	9/15/35/61	0/1/1/2
36	CLA	a	834	20	-	7/15/91/115	-
36	CLA	J	313	-	-	15/39/115/115	-
45	SF4	c	101	22	-	-	0/6/5/5
37	KC1	Q	311	15	-	2/15/71/71	-
34	DD6	a	849	-	-	6/26/80/80	0/3/3/3
39	LMT	f	807	-	-	7/15/35/61	0/1/1/2
36	CLA	D	310	-	-	9/39/115/115	-
36	CLA	b	813	21	-	3/25/101/115	-
35	A86	K	301	-	-	6/34/90/90	1/3/3/3
35	A86	F	304	36	-	4/34/90/90	0/3/3/3
36	CLA	D	308	-	-	16/39/115/115	-
34	DD6	I	303	-	-	4/26/80/80	0/3/3/3
36	CLA	W	206	19	-	10/35/111/115	-
36	CLA	O	316	-	1/1/15/20	28/39/115/115	-
36	CLA	B	308	2	-	14/39/115/115	-
36	CLA	K	307	-	1/1/14/20	21/35/111/115	-
36	CLA	P	318	-	-	8/23/99/115	-
36	CLA	H	312	8	-	17/39/115/115	-
35	A86	R	302	16	-	6/34/90/90	0/3/3/3
35	A86	G	304	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	D	313	-	-	8/39/115/115	-
36	CLA	D	316	-	-	11/24/100/115	-
36	CLA	E	315	-	1/1/15/20	16/39/115/115	-
35	A86	S	303	17	-	4/34/90/90	0/3/3/3
36	CLA	E	310	-	-	7/39/115/115	-
39	LMT	E	320	-	-	13/21/61/61	0/2/2/2
36	CLA	S	321	-	-	12/24/100/115	-
36	CLA	P	301	15	-	18/39/115/115	-
36	CLA	a	822	-	-	4/23/99/115	-
36	CLA	H	316	-	-	18/39/115/115	-
36	CLA	A	309	1	-	9/17/93/115	-
44	BCR	a	844	-	-	6/29/63/63	0/2/2/2
34	DD6	W	205	-	-	8/26/80/80	0/3/3/3
36	CLA	a	838	20	-	8/39/115/115	-
35	A86	E	307	36	-	3/34/90/90	0/3/3/3
36	CLA	H	309	8	-	17/39/115/115	-
36	CLA	W	212	19	-	15/39/115/115	-
36	CLA	a	810	36,20	-	17/36/112/115	-
34	DD6	D	301	-	-	11/26/80/80	0/3/3/3
36	CLA	R	314	16	-	11/17/93/115	-
42	LMG	J	318	-	-	28/50/70/70	0/1/1/1
41	LHG	R	323	-	-	29/53/53/53	-
36	CLA	S	320	-	-	18/39/115/115	-
36	CLA	Q	307	15	-	6/21/97/115	-
35	A86	A	302	-	-	9/34/90/90	0/3/3/3
36	CLA	a	814	20	-	4/21/97/115	-
35	A86	L	307	-	-	8/34/90/90	1/3/3/3
35	A86	F	305	-	-	8/34/90/90	0/3/3/3
41	LHG	f	808	25	-	29/53/53/53	-
35	A86	L	301	-	-	5/34/90/90	1/3/3/3
35	A86	I	302	-	-	7/34/90/90	0/3/3/3
36	CLA	b	837	21	-	8/39/115/115	-
37	KC1	M	313	13,36	-	5/15/71/71	-
36	CLA	a	839	46	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	P	302	-	-	5/12/88/115	-
37	KC1	T	315	-	-	7/15/71/71	-
35	A86	T	301	36	-	4/34/90/90	1/3/3/3
36	CLA	W	201	19	-	4/19/95/115	-
36	CLA	b	839	-	-	6/39/115/115	-
36	CLA	b	820	21	-	17/33/109/115	-
36	CLA	a	817	20	-	17/39/115/115	-
35	A86	A	316	-	-	9/34/90/90	0/3/3/3
36	CLA	D	311	4	-	7/17/93/115	-
35	A86	T	305	18	-	7/34/90/90	0/3/3/3
37	KC1	V	312	33	-	7/15/71/71	-
36	CLA	a	837	20	-	10/39/115/115	-
34	DD6	L	305	-	-	7/26/80/80	0/3/3/3
36	CLA	C	205	-	-	4/13/89/115	-
42	LMG	D	321	-	-	21/32/52/70	0/1/1/1
35	A86	N	320	-	-	10/34/90/90	0/3/3/3
36	CLA	J	311	-	-	5/17/93/115	-
34	DD6	A	304	-	-	4/26/80/80	0/3/3/3
36	CLA	I	305	-	1/1/14/20	10/35/111/115	-
37	KC1	K	314	11	-	5/15/71/71	-
36	CLA	F	314	35,6	-	16/39/115/115	-
36	CLA	J	307	10	-	11/35/111/115	-
37	KC1	O	315	15	-	2/15/71/71	-
35	A86	Q	316	15,36	-	2/34/90/90	0/3/3/3
36	CLA	R	311	16	-	13/39/115/115	-
37	KC1	L	315	35,12	-	6/15/71/71	-
36	CLA	H	310	8	-	7/17/93/115	-
36	CLA	U	307	-	-	3/21/97/115	-
35	A86	W	203	36	-	6/34/90/90	0/3/3/3
36	CLA	E	308	5	-	10/20/96/115	-
36	CLA	a	801	20	-	12/39/115/115	-
36	CLA	V	305	35	-	13/35/111/115	-
35	A86	U	301	-	-	8/34/90/90	0/3/3/3
36	CLA	U	305	-	-	13/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	i	102	26	-	20/39/115/115	-
36	CLA	b	814	21	-	5/27/103/115	-
36	CLA	E	316	-	-	19/39/115/115	-
36	CLA	N	313	14	-	2/10/86/115	-
42	LMG	D	320	41	-	24/41/61/70	0/1/1/1
36	CLA	B	311	2	-	13/27/103/115	-
36	CLA	b	822	21	-	7/17/93/115	-
36	CLA	A	313	-	-	4/10/86/115	-
39	LMT	U	315	-	-	17/21/61/61	0/2/2/2
37	KC1	M	317	-	-	3/15/71/71	-
36	CLA	R	315	-	-	13/39/115/115	-
36	CLA	W	210	-	-	9/17/93/115	-
36	CLA	K	308	-	-	11/39/115/115	-
36	CLA	N	317	14	-	10/26/102/115	-
36	CLA	G	316	-	-	10/20/96/115	-
35	A86	Q	303	-	-	8/34/90/90	0/3/3/3
44	BCR	a	847	-	-	6/29/63/63	0/2/2/2
37	KC1	Q	313	-	-	2/15/71/71	-
36	CLA	A	306	-	1/1/14/20	19/35/111/115	-
36	CLA	a	813	20	-	2/15/91/115	-
42	LMG	h	206	-	-	24/40/60/70	0/1/1/1
35	A86	M	304	-	-	14/34/90/90	0/3/3/3
35	A86	R	309	-	-	8/34/90/90	0/3/3/3
36	CLA	j	101	27,1	-	19/39/115/115	-
36	CLA	a	809	-	-	11/29/105/115	-
36	CLA	W	207	34	-	17/39/115/115	-
34	DD6	D	305	-	-	3/26/80/80	0/3/3/3
39	LMT	K	318	-	-	12/21/61/61	0/2/2/2
40	DGD	L	302	42	-	21/36/76/95	0/2/2/2
36	CLA	C	208	3	-	19/39/115/115	-
36	CLA	a	802	-	1/1/15/20	11/39/115/115	-
41	LHG	Q	315	36	-	33/53/53/53	-
36	CLA	R	320	16	-	5/15/91/115	-
34	DD6	E	304	-	-	4/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	B	309	2	-	6/24/100/115	-
36	CLA	b	823	21	-	4/27/103/115	-
45	SF4	c	102	-	-	-	0/6/5/5
39	LMT	I	317	-	-	13/21/61/61	0/2/2/2
36	CLA	a	803	36,20	-	5/27/103/115	-
35	A86	X	302	35	-	6/34/90/90	0/3/3/3
36	CLA	W	211	19	-	10/39/115/115	-
41	LHG	I	316	-	-	30/53/53/53	-
37	KC1	S	316	-	-	6/15/71/71	-
36	CLA	E	317	-	-	7/17/93/115	-
36	CLA	B	305	2	-	24/39/115/115	-
41	LHG	i	104	-	-	29/50/50/53	-
36	CLA	I	307	9	-	4/26/102/115	-
37	KC1	R	317	-	-	3/15/71/71	-
35	A86	U	302	-	-	9/34/90/90	0/3/3/3
42	LMG	G	325	-	-	27/50/70/70	0/1/1/1
45	SF4	b	803	20,21	-	-	0/6/5/5
35	A86	F	302	-	-	8/34/90/90	0/3/3/3
35	A86	R	301	-	-	9/34/90/90	0/3/3/3
35	A86	N	305	-	-	2/34/90/90	0/3/3/3
36	CLA	M	310	13,35	-	7/17/93/115	-
36	CLA	L	312	12	-	8/17/93/115	-
36	CLA	a	811	20	-	6/26/102/115	-
35	A86	F	307	-	-	6/34/90/90	0/3/3/3
34	DD6	Q	302	-	-	8/26/80/80	0/3/3/3
41	LHG	a	850	-	-	36/51/51/53	-
36	CLA	a	836	-	-	11/39/115/115	-
36	CLA	S	310	17	-	16/39/115/115	-
36	CLA	Q	305	-	-	11/35/111/115	-
37	KC1	W	213	-	-	5/15/71/71	-
42	LMG	j	105	-	-	31/47/67/70	0/1/1/1
36	CLA	W	218	19	-	9/13/89/115	-
36	CLA	M	307	-	-	12/39/115/115	-
36	CLA	U	313	-	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	R	304	36,16	-	8/34/90/90	0/3/3/3
36	CLA	F	313	-	-	8/24/100/115	-
35	A86	J	303	-	-	7/34/90/90	0/3/3/3
36	CLA	S	317	-	-	5/10/86/115	-
36	CLA	U	308	32,35	-	12/29/105/115	-
36	CLA	V	307	-	-	7/23/99/115	-
41	LHG	F	318	-	-	15/34/34/53	-
39	LMT	b	851	-	-	7/15/35/61	0/1/1/2
36	CLA	a	816	20	1/1/15/20	21/39/115/115	-
35	A86	P	304	-	-	6/34/90/90	0/3/3/3
35	A86	J	302	-	-	5/34/90/90	1/3/3/3
36	CLA	P	310	15,41	-	13/39/115/115	-
36	CLA	a	831	-	-	16/39/115/115	-
36	CLA	b	831	21	-	9/21/97/115	-
36	CLA	R	312	16	-	14/39/115/115	-
36	CLA	F	312	-	-	22/39/115/115	-
35	A86	P	303	-	-	9/34/90/90	0/3/3/3
34	DD6	E	306	-	-	4/26/80/80	0/3/3/3
36	CLA	G	314	7	-	4/10/86/115	-
36	CLA	D	306	4	-	6/15/91/115	-
39	LMT	G	323	-	-	16/21/61/61	0/2/2/2
36	CLA	X	310	19	-	4/10/86/115	-
35	A86	I	304	-	-	9/34/90/90	0/3/3/3
36	CLA	G	319	7	-	8/21/97/115	-
35	A86	S	301	-	-	8/34/90/90	0/3/3/3
36	CLA	O	311	-	-	9/31/107/115	-
44	BCR	b	847	-	-	8/29/63/63	0/2/2/2
36	CLA	a	805	20	-	18/39/115/115	-
36	CLA	H	306	-	-	8/35/111/115	-
35	A86	Q	304	-	-	10/34/90/90	0/3/3/3
35	A86	M	302	-	-	7/34/90/90	0/3/3/3
36	CLA	I	313	-	-	5/10/86/115	-
37	KC1	F	315	-	-	3/15/71/71	-
42	LMG	E	318	-	-	24/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	I	306	9	1/1/15/20	15/39/115/115	-
35	A86	T	306	-	-	6/34/90/90	0/3/3/3
36	CLA	F	310	6	-	10/29/105/115	-
36	CLA	C	214	-	-	4/10/86/115	-
42	LMG	V	315	-	-	24/41/61/70	0/1/1/1
36	CLA	a	841	41	-	7/24/100/115	-
39	LMT	h	205	-	-	10/21/61/61	0/2/2/2
39	LMT	b	848	-	-	12/21/61/61	0/2/2/2
36	CLA	f	805	25	-	9/24/100/115	-
36	CLA	J	316	10	-	8/17/93/115	-
36	CLA	l	202	28,21	-	13/39/115/115	-
39	LMT	B	312	-	-	14/21/61/61	0/2/2/2
44	BCR	a	846	-	-	7/29/63/63	0/2/2/2
36	CLA	b	832	21	-	4/20/96/115	-
41	LHG	f	809	-	-	28/46/46/53	-
34	DD6	E	301	-	-	4/26/80/80	0/3/3/3
44	BCR	l	207	-	-	7/29/63/63	0/2/2/2
36	CLA	B	307	-	-	7/17/93/115	-
36	CLA	S	319	17	-	8/39/115/115	-
36	CLA	F	311	-	-	10/24/100/115	-
36	CLA	T	312	18	-	7/17/93/115	-
35	A86	V	303	35	-	8/34/90/90	0/3/3/3
36	CLA	L	309	12	-	12/39/115/115	-
36	CLA	A	307	-	-	10/33/109/115	-
35	A86	O	301	-	-	4/34/90/90	0/3/3/3
36	CLA	l	204	28	-	8/20/96/115	-
44	BCR	b	846	-	-	8/29/63/63	0/2/2/2
36	CLA	X	306	-	-	11/35/111/115	-
36	CLA	P	313	-	-	12/39/115/115	-
35	A86	L	319	-	-	9/34/90/90	0/3/3/3
37	KC1	G	317	-	-	6/15/71/71	-
36	CLA	R	313	-	-	15/39/115/115	-
36	CLA	R	322	16	-	13/24/100/115	-
36	CLA	P	308	-	-	11/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	V	306	33	-	19/39/115/115	-
36	CLA	a	807	20	-	13/39/115/115	-
36	CLA	J	317	10	-	5/18/94/115	-
36	CLA	a	832	-	-	16/39/115/115	-
36	CLA	b	826	46,21	-	11/38/114/115	-
44	BCR	i	103	-	-	11/29/63/63	0/2/2/2
37	KC1	C	213	3	-	6/15/71/71	-
36	CLA	P	316	-	-	5/10/86/115	-
36	CLA	Q	308	-	-	20/39/115/115	-
37	KC1	F	308	6	-	7/15/71/71	-
36	CLA	C	209	-	-	12/39/115/115	-
36	CLA	X	308	19	-	12/18/94/115	-
36	CLA	f	804	46	1/1/15/20	10/39/115/115	-
39	LMT	a	854	-	-	16/21/61/61	0/2/2/2
34	DD6	R	308	-	-	10/26/80/80	0/3/3/3
35	A86	K	303	-	-	5/34/90/90	0/3/3/3
36	CLA	X	313	19	-	6/12/88/115	-
44	BCR	b	845	-	-	7/29/63/63	0/2/2/2
36	CLA	O	312	-	-	6/10/82/115	-
44	BCR	a	845	-	-	9/29/63/63	0/2/2/2
36	CLA	N	318	-	-	7/18/94/115	-
36	CLA	H	318	-	-	10/21/97/115	-
37	KC1	B	310	2	-	3/15/71/71	-
36	CLA	M	309	-	-	15/39/115/115	-
44	BCR	i	101	-	-	2/29/63/63	0/2/2/2
36	CLA	a	808	20	-	11/39/115/115	-
36	CLA	b	811	21	-	12/39/115/115	-
35	A86	X	301	-	-	8/34/90/90	0/3/3/3
36	CLA	M	306	13,37	-	10/27/103/115	-
36	CLA	I	308	9	1/1/15/20	19/39/115/115	-
36	CLA	C	207	-	1/1/15/20	16/39/115/115	-
36	CLA	b	824	21	-	14/25/101/115	-
36	CLA	F	317	6	1/1/13/20	10/29/105/115	-
36	CLA	a	804	20	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	BCR	f	801	-	-	9/29/63/63	0/2/2/2
39	LMT	B	313	-	-	16/21/61/61	0/2/2/2
36	CLA	b	829	21	-	11/39/115/115	-
36	CLA	O	306	-	-	11/35/111/115	-
39	LMT	I	318	-	-	17/21/61/61	0/2/2/2
36	CLA	E	311	5	-	16/39/115/115	-
36	CLA	a	818	20	-	14/39/115/115	-
36	CLA	Q	314	-	-	22/39/115/115	-
37	KC1	U	312	32,35	-	4/15/71/71	-
36	CLA	b	807	21	-	3/15/91/115	-
39	LMT	a	851	-	-	15/21/61/61	0/2/2/2
34	DD6	S	307	-	-	6/26/80/80	0/3/3/3
35	A86	R	306	-	-	8/34/90/90	0/3/3/3
36	CLA	J	309	10	-	10/39/115/115	-
36	CLA	N	308	14	-	17/39/115/115	-
36	CLA	G	311	-	-	17/39/115/115	-
41	LHG	a	843	36	-	10/31/31/53	-
42	LMG	G	324	-	-	31/50/70/70	0/1/1/1
41	LHG	b	850	36	-	27/53/53/53	-
36	CLA	b	836	21	1/1/13/20	9/31/107/115	-
35	A86	F	301	-	-	4/34/90/90	0/3/3/3
34	DD6	A	303	-	-	5/26/80/80	0/3/3/3
36	CLA	K	316	-	-	12/39/115/115	-
37	KC1	O	313	15	-	2/15/71/71	-
35	A86	X	303	36	-	9/34/90/90	0/3/3/3
35	A86	G	302	-	-	7/34/90/90	0/3/3/3
41	LHG	G	321	36	-	27/51/51/53	-
37	KC1	M	318	-	-	10/15/71/71	-
35	A86	V	301	35	-	10/34/90/90	1/3/3/3
36	CLA	G	310	7	-	5/39/115/115	-
36	CLA	a	819	-	-	5/15/91/115	-
39	LMT	U	314	-	-	14/21/61/61	0/2/2/2
36	CLA	V	314	-	1/1/15/20	17/39/115/115	-
36	CLA	P	309	41	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	A	315	-	-	11/22/42/69	0/1/1/1
36	CLA	a	823	-	1/1/13/20	12/27/103/115	-
36	CLA	b	830	21	-	5/39/115/115	-
44	BCR	b	843	-	-	9/29/63/63	0/2/2/2
36	CLA	a	812	20	-	14/39/115/115	-
36	CLA	a	821	20	-	4/20/96/115	-
37	KC1	H	313	-	-	6/15/71/71	-
35	A86	h	204	-	-	1/34/90/90	0/3/3/3
39	LMT	G	322	-	-	17/21/61/61	0/2/2/2
36	CLA	G	315	7	1/1/13/20	11/29/105/115	-
36	CLA	X	307	35,19	-	6/21/97/115	-
36	CLA	G	313	7	-	18/39/115/115	-
35	A86	G	305	-	-	4/34/90/90	0/3/3/3
35	A86	P	307	-	-	2/34/90/90	0/3/3/3
35	A86	I	301	-	-	10/34/90/90	0/3/3/3
36	CLA	P	311	-	-	19/39/115/115	-
36	CLA	a	848	36	1/1/15/20	13/39/115/115	-
36	CLA	S	318	-	-	9/12/88/115	-
36	CLA	b	821	46	-	13/39/115/115	-
42	LMG	m	102	-	-	14/32/52/70	0/1/1/1
36	CLA	Q	309	15	-	9/17/93/115	-
36	CLA	b	840	21	-	12/39/115/115	-
36	CLA	K	313	-	-	13/39/115/115	-
36	CLA	F	309	-	-	13/39/115/115	-
39	LMT	L	318	-	-	13/17/57/61	0/2/2/2
36	CLA	G	312	7	-	6/31/107/115	-
35	A86	J	305	-	-	6/34/90/90	0/3/3/3
36	CLA	N	310	14	-	1/10/86/115	-
36	CLA	b	805	36,21	-	18/39/115/115	-
39	LMT	F	321	-	-	11/19/59/61	0/2/2/2
44	BCR	f	806	-	-	9/29/63/63	0/2/2/2
36	CLA	E	312	-	-	15/39/115/115	-
36	CLA	L	316	-	-	3/10/86/115	-
36	CLA	T	308	18	-	10/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	E	302	-	-	4/34/90/90	0/3/3/3
42	LMG	a	852	-	-	26/49/69/70	0/1/1/1
37	KC1	G	318	-	-	5/15/71/71	-
36	CLA	M	314	-	-	4/10/86/115	-
43	PQN	b	842	-	-	11/23/43/43	0/2/2/2
37	KC1	P	315	35	-	2/15/71/71	-
36	CLA	T	316	-	-	2/10/86/115	-
44	BCR	j	107	-	-	5/29/63/63	0/2/2/2
36	CLA	H	308	8	-	15/37/113/115	-
36	CLA	R	310	-	-	18/35/111/115	-
36	CLA	a	828	-	-	20/39/115/115	-
36	CLA	P	314	-	-	23/33/109/115	-
41	LHG	j	104	-	-	32/53/53/53	-
36	CLA	D	312	-	-	13/39/115/115	-
36	CLA	b	802	20	-	11/39/115/115	-
38	SQD	b	804	-	-	23/41/61/69	0/1/1/1
36	CLA	b	819	-	-	7/32/108/115	-
36	CLA	K	312	-	-	7/39/115/115	-
39	LMT	K	317	-	-	14/17/57/61	0/2/2/2
37	KC1	W	217	-	-	4/15/71/71	-
35	A86	S	302	-	-	6/34/90/90	0/3/3/3
36	CLA	I	314	-	-	2/10/86/115	-
41	LHG	G	320	-	-	18/44/44/53	-
44	BCR	m	101	-	-	9/29/63/63	0/2/2/2
36	CLA	R	321	16	-	9/39/115/115	-
34	DD6	A	301	-	-	7/26/80/80	0/3/3/3
35	A86	T	302	18	-	7/34/90/90	0/3/3/3
36	CLA	b	838	21	-	3/18/94/115	-
34	DD6	P	305	-	-	2/26/80/80	0/3/3/3
36	CLA	D	315	-	-	2/10/86/115	-
36	CLA	K	311	11	-	8/17/93/115	-
36	CLA	b	827	-	-	10/39/115/115	-
35	A86	R	305	-	-	5/34/90/90	0/3/3/3
35	A86	B	301	-	-	10/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC1	G	308	-	-	5/15/71/71	-
36	CLA	a	830	20	-	12/21/97/115	-
36	CLA	N	319	14	-	5/12/88/115	-
35	A86	O	303	-	-	6/34/90/90	0/3/3/3
36	CLA	C	210	3	-	6/17/93/115	-
36	CLA	W	216	35,19	-	5/15/91/115	-
44	BCR	l	203	-	-	10/29/63/63	0/2/2/2
39	LMT	L	303	-	-	10/21/61/61	0/2/2/2
36	CLA	b	817	21	1/1/13/20	9/32/108/115	-
36	CLA	b	809	21	-	18/39/115/115	-
42	LMG	J	319	-	-	23/39/59/70	0/1/1/1
36	CLA	A	314	1	-	22/39/115/115	-
35	A86	Q	301	-	-	6/34/90/90	0/3/3/3
36	CLA	D	309	4	1/1/13/20	8/27/103/115	-
35	A86	V	302	-	-	5/34/90/90	0/3/3/3
36	CLA	K	309	11	-	14/32/108/115	-
36	CLA	N	307	-	-	9/35/111/115	-
36	CLA	b	835	-	-	5/15/91/115	-
36	CLA	a	827	20	-	14/36/112/115	-
34	DD6	F	303	-	-	8/26/80/80	0/3/3/3
35	A86	H	301	-	-	5/34/90/90	0/3/3/3
36	CLA	b	833	21	-	11/31/107/115	-
36	CLA	J	315	10	-	2/10/86/115	-
36	CLA	E	314	-	-	8/39/115/115	-
34	DD6	B	304	-	-	2/26/80/80	0/3/3/3
35	A86	X	304	19	-	7/34/90/90	0/3/3/3
35	A86	M	301	-	-	8/34/90/90	0/3/3/3
36	CLA	M	308	-	-	7/24/100/115	-
36	CLA	V	313	33	-	15/39/115/115	-
36	CLA	D	307	41	-	19/35/111/115	-
41	LHG	l	208	-	-	34/52/52/53	-
36	CLA	a	815	46	-	5/15/91/115	-
36	CLA	L	314	12	-	19/39/115/115	-
35	A86	V	304	-	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	M	316	36	-	6/12/88/115	-
36	CLA	W	209	19	-	15/30/106/115	-
35	A86	U	304	32,37	-	11/34/90/90	0/3/3/3
34	DD6	S	306	-	-	5/26/80/80	0/3/3/3
36	CLA	Q	312	-	-	5/10/86/115	-
36	CLA	a	826	20	-	12/39/115/115	-
36	CLA	H	307	8	-	5/33/109/115	-
35	A86	S	304	-	-	9/34/90/90	0/3/3/3
35	A86	F	306	-	-	0/34/90/90	1/3/3/3
41	LHG	O	317	-	-	33/46/46/53	-
35	A86	L	306	37	-	10/34/90/90	0/3/3/3
35	A86	T	307	-	-	9/34/90/90	0/3/3/3
36	CLA	R	316	-	-	8/17/93/115	-
35	A86	C	202	36,3	-	8/34/90/90	0/3/3/3
36	CLA	b	828	21	-	14/39/115/115	-
36	CLA	T	311	18	-	13/39/115/115	-
36	CLA	b	815	21	-	19/39/115/115	-
41	LHG	D	318	36	-	30/50/50/53	-
36	CLA	L	320	12	-	11/39/115/115	-
36	CLA	U	306	32	1/1/15/20	20/39/115/115	-
36	CLA	b	816	21	1/1/14/20	17/33/109/115	-
36	CLA	H	311	-	-	9/39/115/115	-
35	A86	O	302	-	-	9/34/90/90	0/3/3/3
36	CLA	L	310	-	-	4/26/102/115	-
34	DD6	G	303	-	-	4/26/80/80	0/3/3/3
34	DD6	j	103	-	-	9/26/80/80	0/3/3/3
39	LMT	F	320	-	-	12/21/61/61	0/2/2/2
36	CLA	I	311	9	-	17/39/115/115	-
36	CLA	a	806	-	1/1/15/20	12/39/115/115	-
35	A86	B	303	-	-	13/34/90/90	0/3/3/3
36	CLA	Q	306	-	-	14/39/115/115	-
41	LHG	E	322	-	-	28/53/53/53	-
40	DGD	C	215	-	-	31/46/86/95	0/2/2/2
34	DD6	D	304	-	-	8/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	I	206	46	-	6/21/97/115	-
35	A86	S	308	37	-	12/34/90/90	0/3/3/3
36	CLA	U	311	32	-	21/39/115/115	-
36	CLA	T	314	-	-	15/39/115/115	-
34	DD6	B	302	-	-	4/26/80/80	0/3/3/3
36	CLA	H	315	8	-	15/39/115/115	-
35	A86	J	306	-	-	10/34/90/90	0/3/3/3
35	A86	N	304	-	-	8/34/90/90	0/3/3/3
36	CLA	S	314	17	-	11/39/115/115	-
36	CLA	A	308	-	-	13/39/115/115	-
34	DD6	K	304	-	-	2/26/80/80	0/3/3/3
34	DD6	M	303	-	-	3/26/80/80	0/3/3/3
36	CLA	b	806	-	-	14/39/115/115	-
36	CLA	V	311	33	-	13/39/115/115	-
37	KC1	D	314	4	-	5/15/71/71	-
36	CLA	a	825	-	1/1/15/20	15/39/115/115	-
36	CLA	S	313	-	-	8/17/93/115	-
36	CLA	B	306	-	-	6/17/93/115	-
40	DGD	b	849	-	-	21/49/89/95	0/2/2/2
37	KC1	N	314	14	-	7/15/71/71	-
35	A86	N	303	-	-	4/34/90/90	0/3/3/3
35	A86	U	303	36	-	17/34/90/90	0/3/3/3
36	CLA	f	803	-	1/1/15/20	13/39/115/115	-
36	CLA	J	312	10	-	10/39/115/115	-
36	CLA	a	835	20	-	2/23/99/115	-
35	A86	N	306	-	-	8/34/90/90	0/3/3/3
34	DD6	W	204	36	-	7/26/80/80	0/3/3/3
36	CLA	H	314	-	-	3/10/86/115	-
36	CLA	X	312	-	-	3/10/86/115	-
36	CLA	C	211	-	-	13/39/115/115	-
36	CLA	a	833	20	-	4/21/97/115	-
35	A86	h	202	-	-	3/34/90/90	1/3/3/3
36	CLA	H	305	8	-	8/19/95/115	-
35	A86	R	303	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	X	315	-	-	3/10/86/115	-
37	KC1	A	312	1	-	2/15/71/71	-
37	KC1	E	309	-	-	5/15/71/71	-
42	LMG	L	321	40	-	15/28/48/70	0/1/1/1
36	CLA	W	214	19	-	5/10/86/115	-
36	CLA	N	315	-	-	0/10/86/115	-
41	LHG	a	842	-	-	24/52/52/53	-
36	CLA	a	820	-	-	11/39/115/115	-
42	LMG	E	319	-	-	23/35/55/70	0/1/1/1
36	CLA	W	215	-	-	6/19/95/115	-
36	CLA	h	203	31	-	20/39/115/115	-
36	CLA	P	312	15	-	9/17/93/115	-
36	CLA	M	311	13,35	-	10/39/115/115	-
36	CLA	I	312	9	-	4/24/100/115	-
35	A86	L	304	-	-	6/34/90/90	0/3/3/3
36	CLA	R	318	35	-	4/10/86/115	-
35	A86	O	319	36,35	-	8/34/90/90	0/3/3/3
35	A86	T	303	-	-	6/34/90/90	0/3/3/3
35	A86	D	302	-	-	7/34/90/90	0/3/3/3
36	CLA	O	307	-	-	14/39/115/115	-
35	A86	W	202	36,19	-	8/34/90/90	0/3/3/3
35	A86	T	304	-	-	0/34/90/90	0/3/3/3
36	CLA	A	310	-	-	11/39/115/115	-
36	CLA	I	310	35	-	11/39/115/115	-
36	CLA	l	205	-	1/1/15/20	14/39/115/115	-
34	DD6	C	201	-	-	7/26/80/80	0/3/3/3
36	CLA	l	201	-	-	16/39/115/115	-
36	CLA	P	319	-	-	16/33/109/115	-
36	CLA	E	313	-	1/1/15/20	10/39/115/115	-
43	PQN	a	840	-	-	7/23/43/43	0/2/2/2
36	CLA	j	102	-	1/1/15/20	13/39/115/115	-
36	CLA	R	319	16	-	7/15/91/115	-
36	CLA	f	802	21	-	16/39/115/115	-
36	CLA	G	309	7	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	N	316	14	-	13/39/115/115	-
35	A86	H	304	-	-	8/34/90/90	0/3/3/3
36	CLA	b	834	-	-	10/39/115/115	-
36	CLA	V	310	33	-	8/39/115/115	-
36	CLA	U	310	-	-	19/39/115/115	-
36	CLA	A	311	-	-	20/39/115/115	-
39	LMT	a	853	-	-	10/18/58/61	0/2/2/2
39	LMT	P	321	-	-	10/14/34/61	0/1/1/2
36	CLA	M	315	13	-	8/18/94/115	-
36	CLA	L	313	-	-	8/39/115/115	-
34	DD6	K	305	-	-	0/26/80/80	0/3/3/3
42	LMG	V	316	-	-	24/41/61/70	0/1/1/1
36	CLA	D	317	-	-	12/31/107/115	-
37	KC1	P	317	15	-	4/15/71/71	-
36	CLA	N	312	-	-	9/18/94/115	-
35	A86	X	314	19	-	3/34/90/90	1/3/3/3
36	CLA	O	310	15	-	9/17/93/115	-
36	CLA	K	315	-	-	3/10/86/115	-
35	A86	N	302	-	-	6/34/90/90	0/3/3/3
39	LMT	P	320	-	-	8/14/34/61	0/1/1/2
35	A86	N	301	-	-	8/34/90/90	0/3/3/3
36	CLA	O	309	-	-	19/39/115/115	-
36	CLA	a	829	20	-	13/39/115/115	-
36	CLA	C	212	35	-	25/39/115/115	-
35	A86	J	301	-	-	11/34/90/90	0/3/3/3
35	A86	M	305	-	-	8/34/90/90	0/3/3/3
34	DD6	E	303	-	-	7/26/80/80	0/3/3/3
34	DD6	R	307	-	-	11/26/80/80	0/3/3/3
36	CLA	T	313	18	-	8/39/115/115	-
36	CLA	V	309	33	-	4/13/89/115	-
36	CLA	U	309	32	-	6/17/93/115	-

The worst 5 of 4701 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	318	KC1	C4C-NC	17.10	1.63	1.37
36	Q	310	CLA	CAA-C2A	15.78	1.83	1.54
37	M	318	KC1	C1A-NA	15.77	1.68	1.38
37	T	310	KC1	C1A-NA	14.39	1.66	1.38
37	T	310	KC1	C4C-NC	13.45	1.57	1.37

The worst 5 of 7313 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	N	304	A86	O1-C20-C21	-47.08	58.64	115.06
36	Q	314	CLA	C4-C3-C5	-24.40	74.22	115.27
37	M	318	KC1	C1D-ND-C4D	-22.78	90.15	106.33
42	V	315	LMG	O7-C10-C11	22.29	159.53	111.50
35	A	302	A86	C33-C32-C31	-21.39	88.43	109.21

5 of 29 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	A	306	CLA	C8
36	C	207	CLA	C8
36	D	309	CLA	C8
36	E	313	CLA	C8
36	E	315	CLA	C8

5 of 6194 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	301	DD6	C10-C11-C13-C14
34	A	301	DD6	C12-C11-C13-C14
34	A	301	DD6	C13-C14-C15-C20
34	A	301	DD6	C13-C14-C15-O1
34	A	303	DD6	C10-C11-C13-C14

5 of 11 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	V	301	A86	C31-C32-C33-C34-C35-C36
35	J	302	A86	C31-C32-C33-C34-C35-C36
35	K	301	A86	C31-C32-C33-C34-C35-C36
35	G	306	A86	C31-C32-C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
35	T	301	A86	C31-C32-C33-C34-C35-C36

498 monomers are involved in 2732 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	O	305	A86	13	0
36	J	310	CLA	4	0
36	a	824	CLA	2	0
36	S	311	CLA	8	0
36	M	312	CLA	3	0
36	T	309	CLA	4	0
36	K	310	CLA	21	0
44	b	844	BCR	2	0
36	G	307	CLA	12	0
34	O	304	DD6	6	0
36	I	309	CLA	17	0
34	D	303	DD6	5	0
36	C	206	CLA	3	0
36	L	308	CLA	36	0
35	E	305	A86	4	0
36	V	308	CLA	12	0
41	D	319	LHG	12	0
35	G	306	A86	4	0
36	b	810	CLA	2	0
34	H	303	DD6	5	0
36	b	812	CLA	2	0
36	b	841	CLA	7	0
35	C	203	A86	12	0
36	S	315	CLA	15	0
37	T	310	KC1	17	0
36	O	308	CLA	6	0
36	F	316	CLA	3	0
36	L	311	CLA	2	0
36	X	309	CLA	2	0
34	J	304	DD6	4	0
42	I	315	LMG	14	0
36	S	309	CLA	5	0
36	b	818	CLA	3	0
41	G	301	LHG	3	0
44	h	201	BCR	4	0
36	W	208	CLA	1	0
36	Q	310	CLA	9	0
36	H	317	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	N	309	CLA	6	0
35	X	305	A86	2	0
41	O	318	LHG	6	0
39	E	323	LMT	5	0
34	H	302	DD6	1	0
36	b	801	CLA	1	0
36	b	808	CLA	1	0
36	J	308	CLA	8	0
36	A	305	CLA	4	0
41	F	319	LHG	4	0
35	C	204	A86	4	0
36	b	825	CLA	3	0
37	L	317	KC1	2	0
36	S	312	CLA	3	0
35	P	306	A86	4	0
36	j	106	CLA	1	0
39	E	321	LMT	8	0
36	a	834	CLA	2	0
36	J	313	CLA	5	0
37	Q	311	KC1	8	0
34	a	849	DD6	1	0
39	f	807	LMT	2	0
36	D	310	CLA	1	0
36	b	813	CLA	1	0
35	K	301	A86	4	0
36	D	308	CLA	6	0
34	I	303	DD6	6	0
36	W	206	CLA	1	0
36	B	308	CLA	7	0
36	O	316	CLA	22	0
36	K	307	CLA	15	0
36	P	318	CLA	1	0
36	H	312	CLA	2	0
36	D	313	CLA	3	0
36	D	316	CLA	1	0
36	E	315	CLA	29	0
36	E	310	CLA	1	0
39	E	320	LMT	16	0
36	S	321	CLA	7	0
36	P	301	CLA	9	0
36	a	822	CLA	3	0
36	H	316	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	309	CLA	6	0
44	a	844	BCR	7	0
34	W	205	DD6	23	0
36	a	838	CLA	1	0
35	E	307	A86	14	0
36	W	212	CLA	23	0
36	a	810	CLA	4	0
34	D	301	DD6	12	0
36	R	314	CLA	3	0
42	J	318	LMG	24	0
41	R	323	LHG	14	0
36	S	320	CLA	2	0
36	Q	307	CLA	5	0
35	A	302	A86	1	0
35	L	307	A86	8	0
41	f	808	LHG	23	0
35	L	301	A86	5	0
35	I	302	A86	17	0
36	b	837	CLA	2	0
37	M	313	KC1	1	0
36	a	839	CLA	1	0
36	P	302	CLA	6	0
37	T	315	KC1	1	0
35	T	301	A86	2	0
36	W	201	CLA	1	0
36	b	839	CLA	1	0
36	b	820	CLA	6	0
36	a	817	CLA	3	0
35	A	316	A86	2	0
36	D	311	CLA	5	0
37	V	312	KC1	1	0
34	L	305	DD6	25	0
36	C	205	CLA	14	0
42	D	321	LMG	5	0
36	J	311	CLA	3	0
34	A	304	DD6	2	0
36	I	305	CLA	5	0
37	K	314	KC1	9	0
36	F	314	CLA	6	0
36	J	307	CLA	1	0
37	O	315	KC1	12	0
35	Q	316	A86	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	R	311	CLA	1	0
37	L	315	KC1	9	0
36	H	310	CLA	9	0
36	U	307	CLA	11	0
35	W	203	A86	1	0
36	E	308	CLA	3	0
36	a	801	CLA	6	0
36	V	305	CLA	32	0
35	U	301	A86	1	0
36	U	305	CLA	3	0
36	i	102	CLA	3	0
36	b	814	CLA	2	0
36	E	316	CLA	3	0
36	N	313	CLA	5	0
42	D	320	LMG	12	0
36	B	311	CLA	7	0
36	b	822	CLA	2	0
36	A	313	CLA	3	0
39	U	315	LMT	17	0
36	K	308	CLA	2	0
36	N	317	CLA	3	0
36	G	316	CLA	3	0
35	Q	303	A86	14	0
44	a	847	BCR	1	0
37	Q	313	KC1	8	0
36	A	306	CLA	17	0
36	a	813	CLA	12	0
42	h	206	LMG	7	0
35	M	304	A86	12	0
36	j	101	CLA	11	0
36	a	809	CLA	5	0
36	W	207	CLA	8	0
39	K	318	LMT	8	0
40	L	302	DGD	20	0
36	C	208	CLA	5	0
36	a	802	CLA	4	0
41	Q	315	LHG	19	0
36	R	320	CLA	7	0
36	B	309	CLA	16	0
36	b	823	CLA	11	0
39	I	317	LMT	15	0
36	a	803	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	X	302	A86	1	0
36	W	211	CLA	1	0
41	I	316	LHG	10	0
37	S	316	KC1	4	0
36	E	317	CLA	1	0
36	B	305	CLA	3	0
41	i	104	LHG	28	0
36	I	307	CLA	6	0
35	U	302	A86	4	0
42	G	325	LMG	14	0
45	b	803	SF4	1	0
35	F	302	A86	2	0
35	N	305	A86	20	0
36	M	310	CLA	1	0
36	L	312	CLA	1	0
36	a	811	CLA	3	0
34	Q	302	DD6	19	0
41	a	850	LHG	15	0
36	a	836	CLA	6	0
36	Q	305	CLA	4	0
42	j	105	LMG	26	0
36	W	218	CLA	4	0
36	M	307	CLA	18	0
36	U	313	CLA	1	0
35	R	304	A86	2	0
36	F	313	CLA	6	0
36	U	308	CLA	19	0
36	V	307	CLA	1	0
41	F	318	LHG	1	0
39	b	851	LMT	20	0
36	a	816	CLA	30	0
35	J	302	A86	3	0
36	P	310	CLA	2	0
36	a	831	CLA	1	0
36	b	831	CLA	2	0
36	F	312	CLA	6	0
34	E	306	DD6	4	0
36	G	314	CLA	1	0
36	D	306	CLA	5	0
39	G	323	LMT	4	0
36	X	310	CLA	3	0
36	G	319	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	O	311	CLA	3	0
44	b	847	BCR	1	0
36	a	805	CLA	1	0
35	Q	304	A86	1	0
36	I	313	CLA	2	0
37	F	315	KC1	5	0
42	E	318	LMG	19	0
36	I	306	CLA	14	0
35	T	306	A86	1	0
42	V	315	LMG	14	0
36	a	841	CLA	3	0
39	h	205	LMT	21	0
39	b	848	LMT	5	0
36	f	805	CLA	20	0
36	l	202	CLA	8	0
39	B	312	LMT	15	0
44	a	846	BCR	2	0
41	f	809	LHG	20	0
34	E	301	DD6	4	0
44	l	207	BCR	4	0
36	B	307	CLA	1	0
36	S	319	CLA	2	0
36	F	311	CLA	2	0
36	T	312	CLA	1	0
35	V	303	A86	13	0
36	L	309	CLA	10	0
36	A	307	CLA	3	0
35	O	301	A86	13	0
36	l	204	CLA	6	0
44	b	846	BCR	4	0
36	P	313	CLA	7	0
37	G	317	KC1	6	0
36	R	313	CLA	2	0
36	R	322	CLA	1	0
36	P	308	CLA	1	0
36	V	306	CLA	22	0
36	a	807	CLA	1	0
36	J	317	CLA	1	0
36	a	832	CLA	3	0
36	b	826	CLA	1	0
44	i	103	BCR	5	0
37	C	213	KC1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	P	316	CLA	4	0
36	Q	308	CLA	7	0
37	F	308	KC1	15	0
36	C	209	CLA	1	0
36	X	308	CLA	4	0
36	f	804	CLA	12	0
39	a	854	LMT	5	0
34	R	308	DD6	5	0
35	K	303	A86	2	0
44	b	845	BCR	1	0
36	O	312	CLA	2	0
44	a	845	BCR	3	0
36	N	318	CLA	15	0
36	H	318	CLA	4	0
37	B	310	KC1	2	0
36	M	309	CLA	8	0
44	i	101	BCR	4	0
36	a	808	CLA	7	0
36	b	811	CLA	1	0
36	M	306	CLA	1	0
36	I	308	CLA	29	0
36	C	207	CLA	7	0
36	b	824	CLA	4	0
36	F	317	CLA	29	0
36	a	804	CLA	3	0
44	f	801	BCR	2	0
39	B	313	LMT	5	0
36	b	829	CLA	3	0
36	O	306	CLA	1	0
39	I	318	LMT	7	0
36	E	311	CLA	6	0
36	a	818	CLA	3	0
36	Q	314	CLA	50	0
36	b	807	CLA	4	0
39	a	851	LMT	8	0
34	S	307	DD6	1	0
36	J	309	CLA	2	0
36	N	308	CLA	4	0
36	G	311	CLA	11	0
41	a	843	LHG	5	0
42	G	324	LMG	17	0
41	b	850	LHG	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	b	836	CLA	20	0
35	F	301	A86	10	0
34	A	303	DD6	4	0
36	K	316	CLA	3	0
37	O	313	KC1	1	0
35	G	302	A86	2	0
41	G	321	LHG	10	0
37	M	318	KC1	6	0
35	V	301	A86	27	0
36	G	310	CLA	1	0
36	a	819	CLA	10	0
39	U	314	LMT	15	0
36	P	309	CLA	2	0
36	V	314	CLA	31	0
38	A	315	SQD	7	0
36	a	823	CLA	1	0
36	b	830	CLA	1	0
44	b	843	BCR	6	0
36	a	812	CLA	1	0
36	a	821	CLA	2	0
35	h	204	A86	4	0
39	G	322	LMT	10	0
36	G	315	CLA	24	0
36	X	307	CLA	3	0
36	G	313	CLA	18	0
35	G	305	A86	3	0
35	P	307	A86	2	0
35	I	301	A86	4	0
36	a	848	CLA	10	0
36	S	318	CLA	3	0
36	b	821	CLA	1	0
42	m	102	LMG	9	0
36	b	840	CLA	3	0
36	K	313	CLA	6	0
36	F	309	CLA	5	0
39	L	318	LMT	9	0
35	J	305	A86	6	0
36	N	310	CLA	6	0
36	b	805	CLA	2	0
39	F	321	LMT	25	0
44	f	806	BCR	1	0
36	E	312	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	T	308	CLA	3	0
42	a	852	LMG	20	0
43	b	842	PQN	3	0
37	P	315	KC1	2	0
36	T	316	CLA	1	0
44	j	107	BCR	1	0
36	H	308	CLA	19	0
36	R	310	CLA	9	0
36	a	828	CLA	1	0
36	P	314	CLA	5	0
41	j	104	LHG	14	0
36	D	312	CLA	2	0
36	b	802	CLA	3	0
38	b	804	SQD	10	0
36	b	819	CLA	3	0
36	K	312	CLA	3	0
39	K	317	LMT	6	0
37	W	217	KC1	14	0
35	S	302	A86	1	0
36	I	314	CLA	2	0
41	G	320	LHG	14	0
44	m	101	BCR	11	0
36	R	321	CLA	2	0
34	A	301	DD6	8	0
36	b	838	CLA	1	0
34	P	305	DD6	6	0
36	D	315	CLA	1	0
36	K	311	CLA	5	0
35	R	305	A86	7	0
35	B	301	A86	11	0
37	G	308	KC1	2	0
36	a	830	CLA	4	0
36	N	319	CLA	14	0
36	C	210	CLA	6	0
36	W	216	CLA	1	0
44	l	203	BCR	1	0
39	L	303	LMT	1	0
36	b	817	CLA	6	0
36	b	809	CLA	2	0
42	J	319	LMG	12	0
36	A	314	CLA	20	0
36	D	309	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	K	309	CLA	6	0
36	a	827	CLA	2	0
34	F	303	DD6	3	0
36	b	833	CLA	8	0
36	J	315	CLA	3	0
36	E	314	CLA	4	0
34	B	304	DD6	10	0
36	V	313	CLA	12	0
36	D	307	CLA	12	0
41	l	208	LHG	17	0
36	a	815	CLA	3	0
36	L	314	CLA	2	0
35	V	304	A86	6	0
36	M	316	CLA	3	0
36	W	209	CLA	7	0
35	U	304	A86	15	0
34	S	306	DD6	2	0
36	a	826	CLA	2	0
36	H	307	CLA	10	0
35	S	304	A86	21	0
41	O	317	LHG	8	0
36	R	316	CLA	1	0
36	b	828	CLA	4	0
36	T	311	CLA	4	0
36	b	815	CLA	2	0
41	D	318	LHG	16	0
36	L	320	CLA	2	0
36	H	311	CLA	3	0
36	b	816	CLA	9	0
36	U	306	CLA	31	0
36	L	310	CLA	1	0
34	G	303	DD6	2	0
34	j	103	DD6	4	0
39	F	320	LMT	19	0
36	I	311	CLA	1	0
36	a	806	CLA	19	0
35	B	303	A86	8	0
36	Q	306	CLA	3	0
41	E	322	LHG	24	0
40	C	215	DGD	19	0
34	D	304	DD6	2	0
36	l	206	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	S	308	A86	5	0
36	U	311	CLA	16	0
36	T	314	CLA	1	0
34	B	302	DD6	5	0
36	H	315	CLA	3	0
35	J	306	A86	6	0
35	N	304	A86	14	0
36	S	314	CLA	3	0
36	A	308	CLA	2	0
34	K	304	DD6	4	0
34	M	303	DD6	18	0
36	b	806	CLA	2	0
36	V	311	CLA	16	0
36	a	825	CLA	2	0
36	S	313	CLA	1	0
40	b	849	DGD	4	0
35	N	303	A86	15	0
35	U	303	A86	15	0
36	f	803	CLA	3	0
36	J	312	CLA	5	0
36	a	835	CLA	1	0
35	N	306	A86	1	0
34	W	204	DD6	22	0
36	H	314	CLA	6	0
36	C	211	CLA	1	0
36	a	833	CLA	2	0
35	h	202	A86	5	0
36	H	305	CLA	2	0
35	R	303	A86	1	0
36	X	315	CLA	24	0
37	A	312	KC1	4	0
37	E	309	KC1	2	0
42	L	321	LMG	10	0
36	N	315	CLA	1	0
42	E	319	LMG	6	0
36	W	215	CLA	3	0
36	h	203	CLA	11	0
36	M	311	CLA	3	0
36	I	312	CLA	16	0
35	L	304	A86	1	0
35	O	319	A86	1	0
35	T	303	A86	1	0

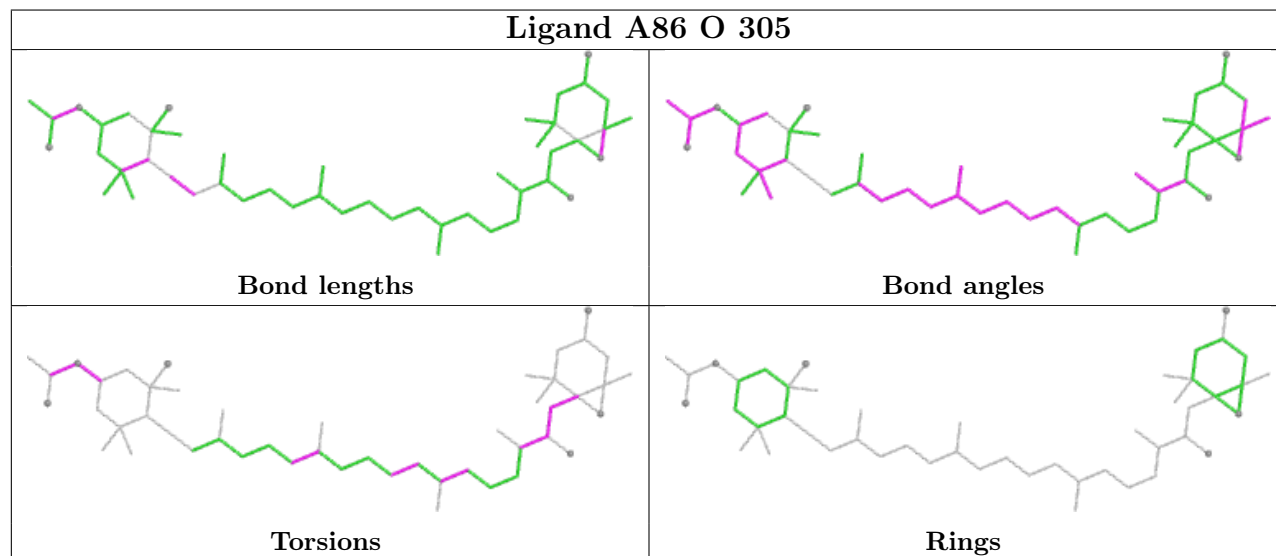
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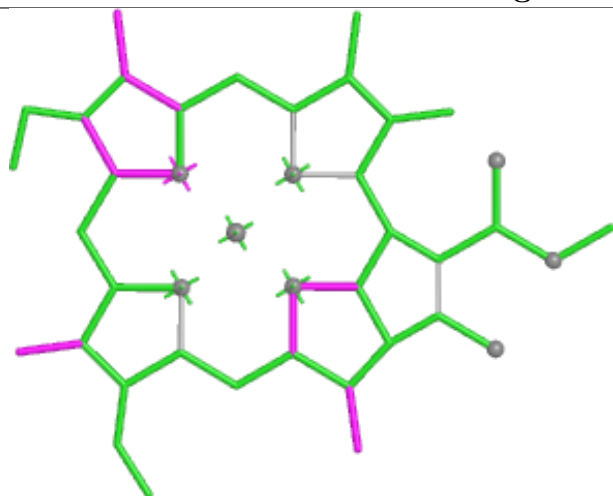
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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35	T	304	A86	5	0
36	A	310	CLA	1	0
36	I	310	CLA	4	0
34	C	201	DD6	4	0
36	l	205	CLA	3	0
36	l	201	CLA	6	0
36	P	319	CLA	13	0
36	E	313	CLA	7	0
43	a	840	PQN	3	0
36	f	802	CLA	4	0
36	j	102	CLA	19	0
36	G	309	CLA	4	0
36	N	316	CLA	6	0
35	H	304	A86	7	0
36	b	834	CLA	3	0
36	V	310	CLA	15	0
36	U	310	CLA	15	0
36	A	311	CLA	3	0
39	a	853	LMT	12	0
39	P	321	LMT	2	0
36	M	315	CLA	2	0
34	K	305	DD6	4	0
42	V	316	LMG	28	0
36	D	317	CLA	1	0
36	N	312	CLA	6	0
35	X	314	A86	24	0
36	K	315	CLA	2	0
35	N	302	A86	4	0
39	P	320	LMT	6	0
35	N	301	A86	2	0
36	O	309	CLA	8	0
36	a	829	CLA	1	0
36	C	212	CLA	6	0
35	J	301	A86	14	0
34	E	303	DD6	4	0
34	R	307	DD6	11	0
36	T	313	CLA	13	0
36	V	309	CLA	7	0
36	U	309	CLA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

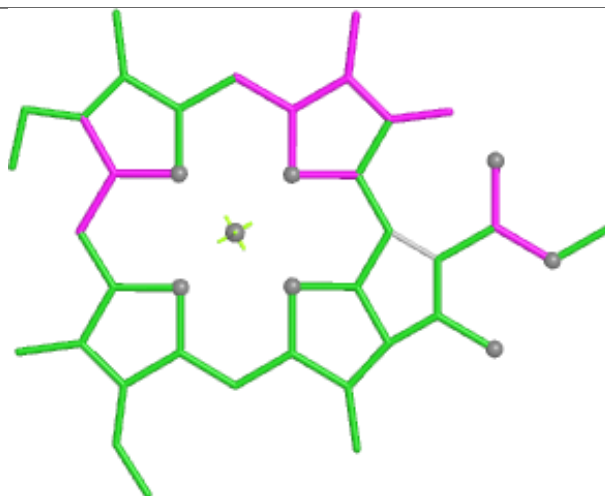
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



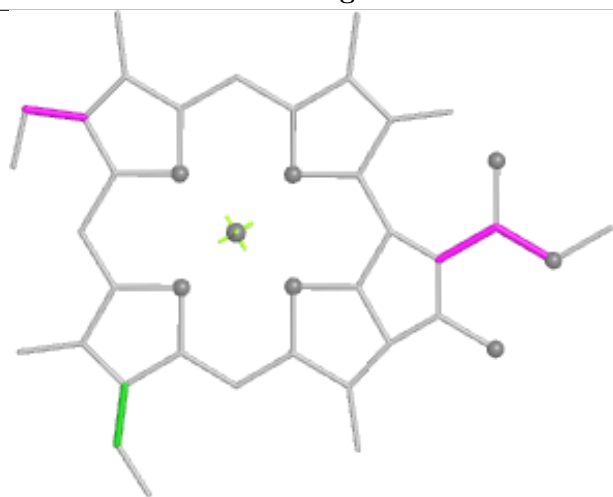
Ligand CLA O 314



Bond lengths



Bond angles

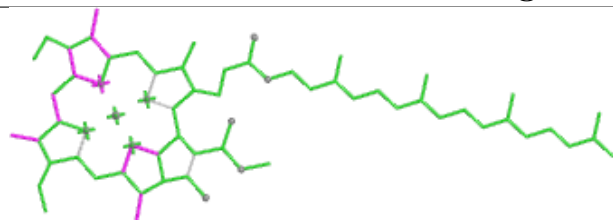


Torsions

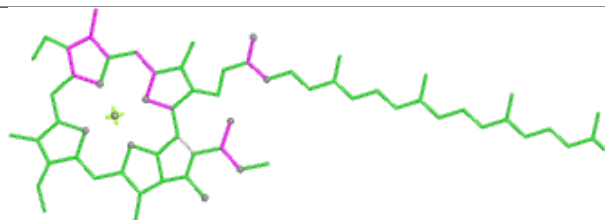


Rings

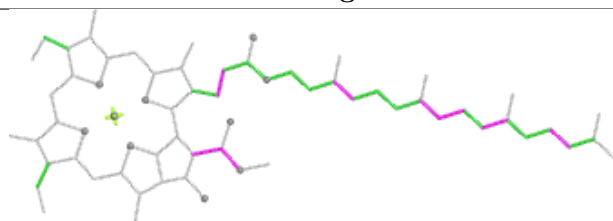
Ligand CLA J 310



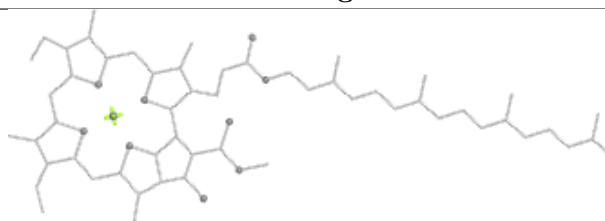
Bond lengths



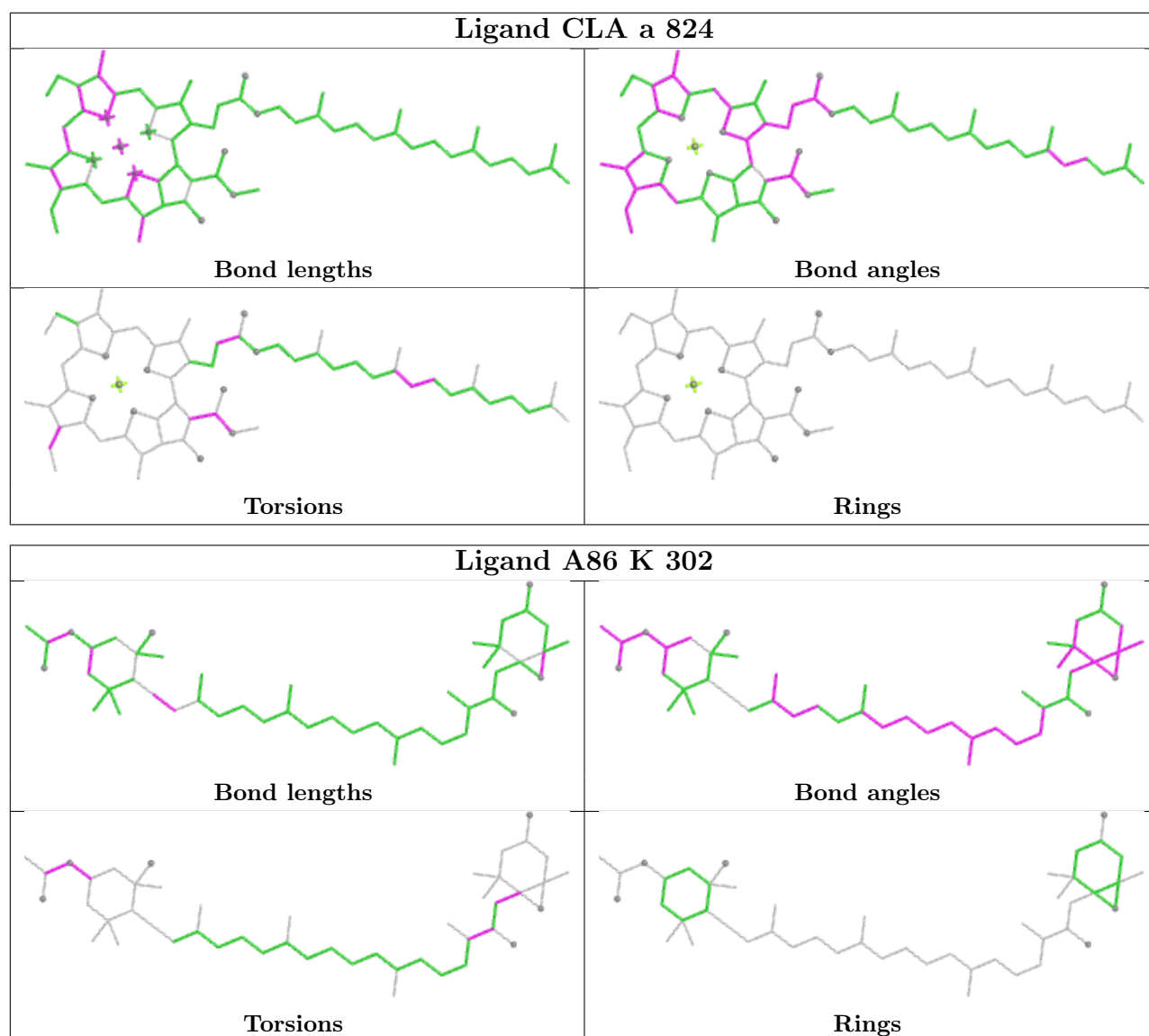
Bond angles

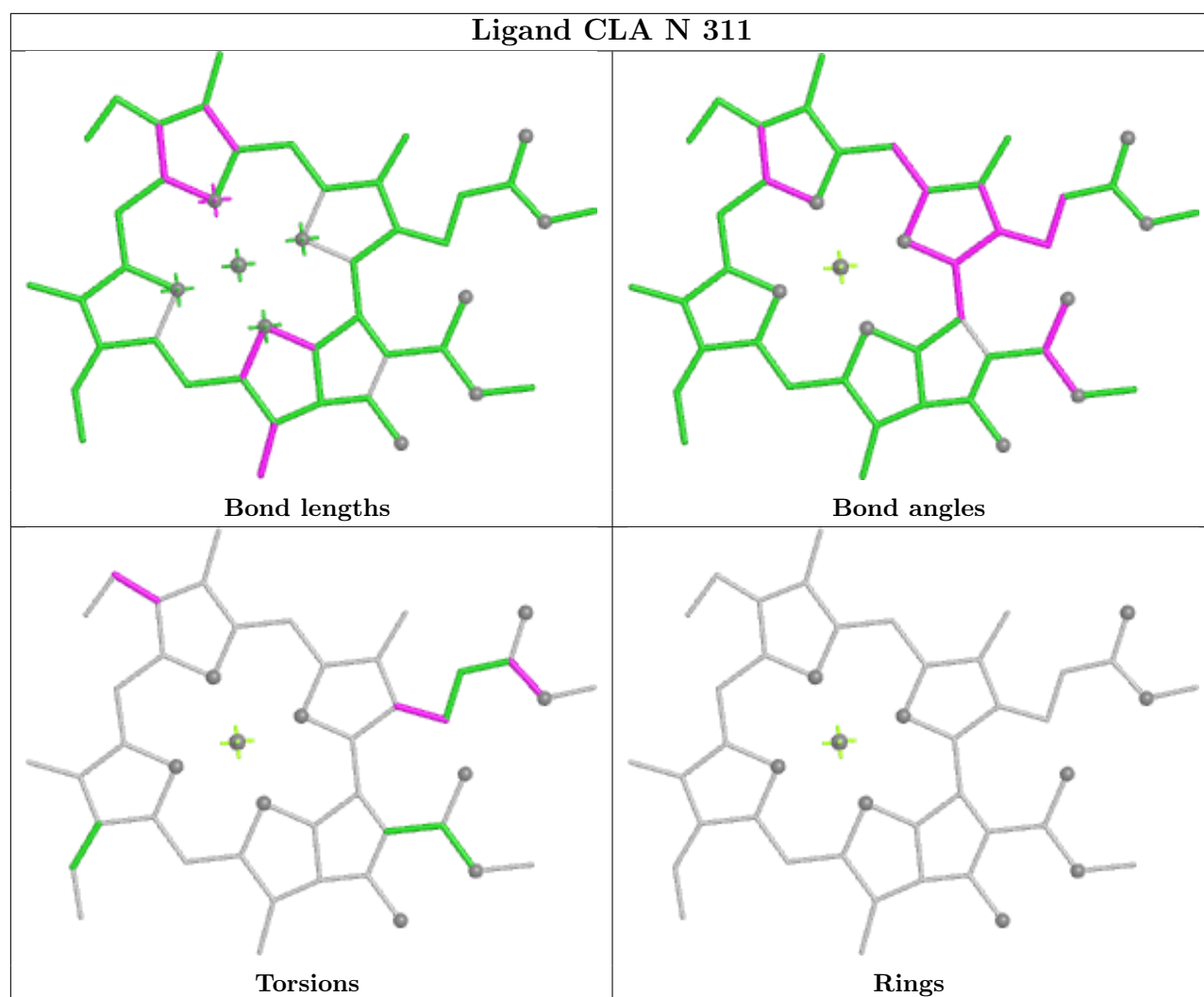


Torsions

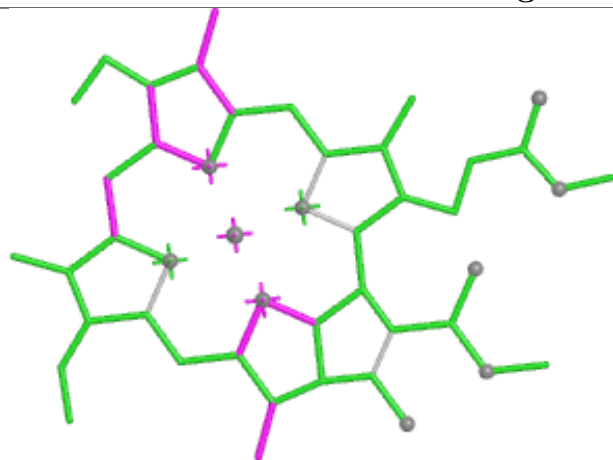


Rings

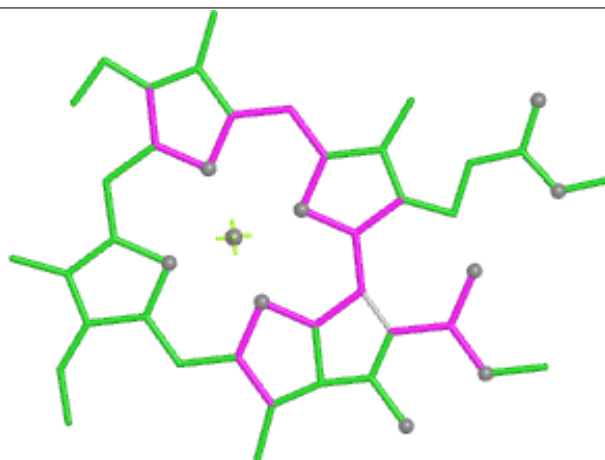




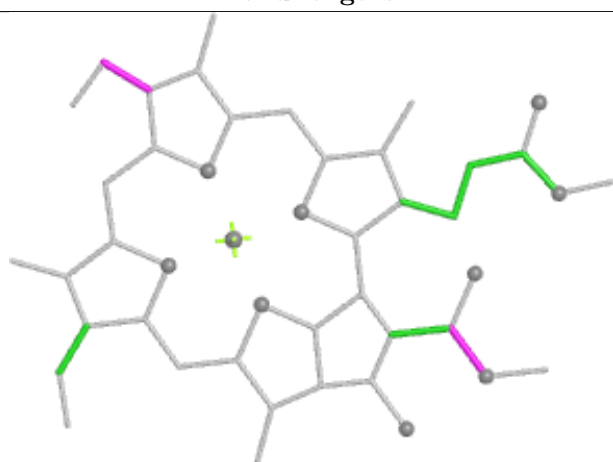
Ligand CLA S 311



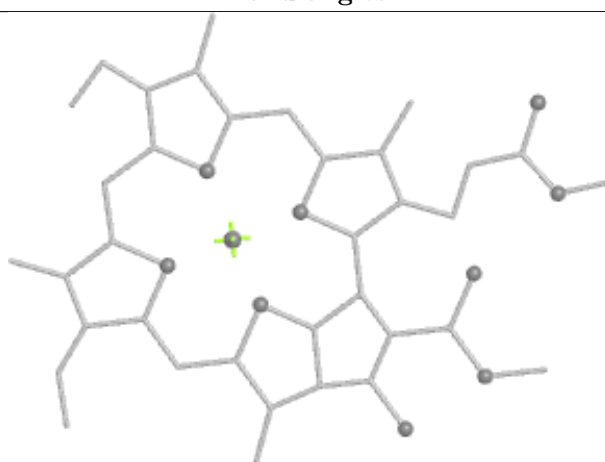
Bond lengths



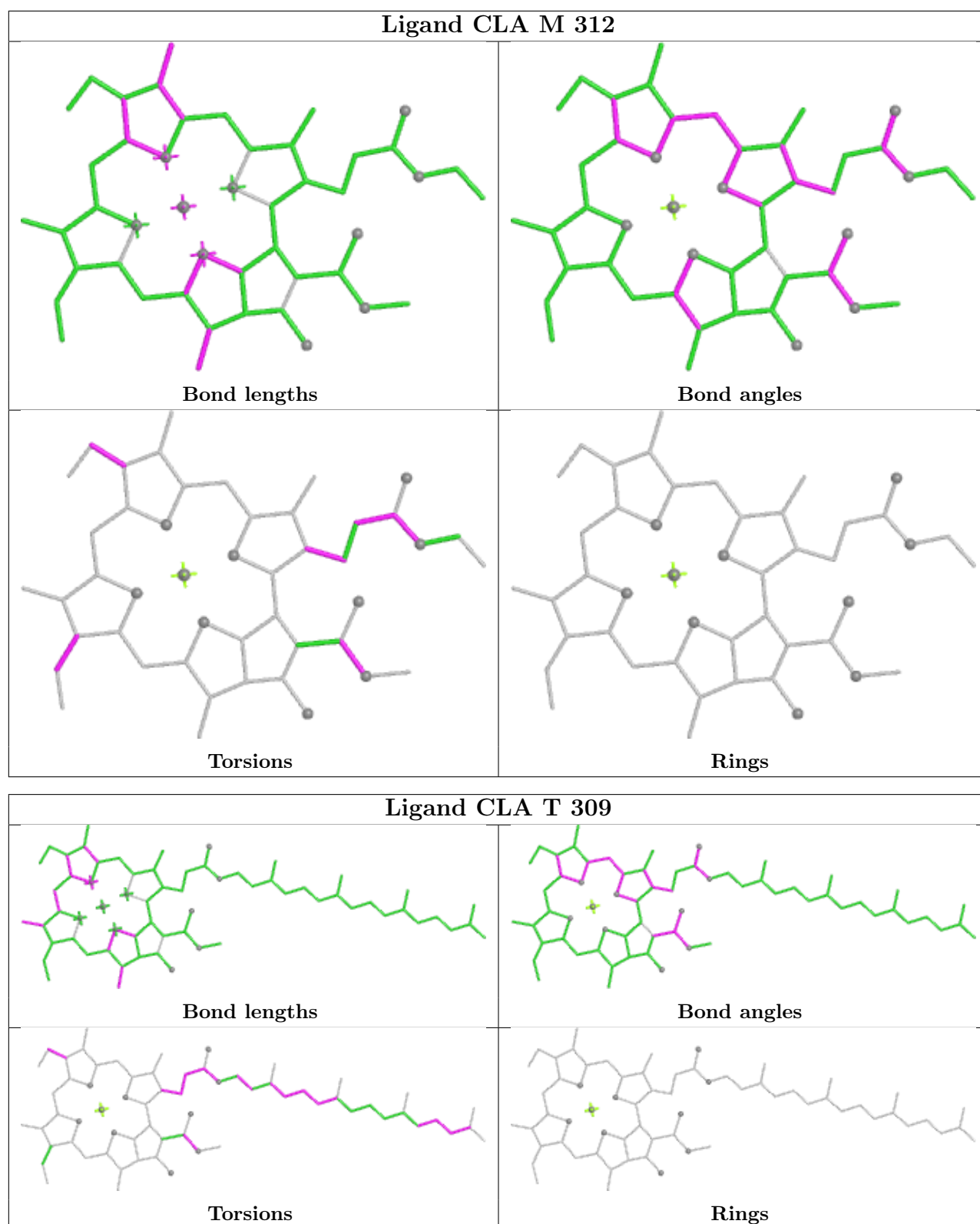
Bond angles

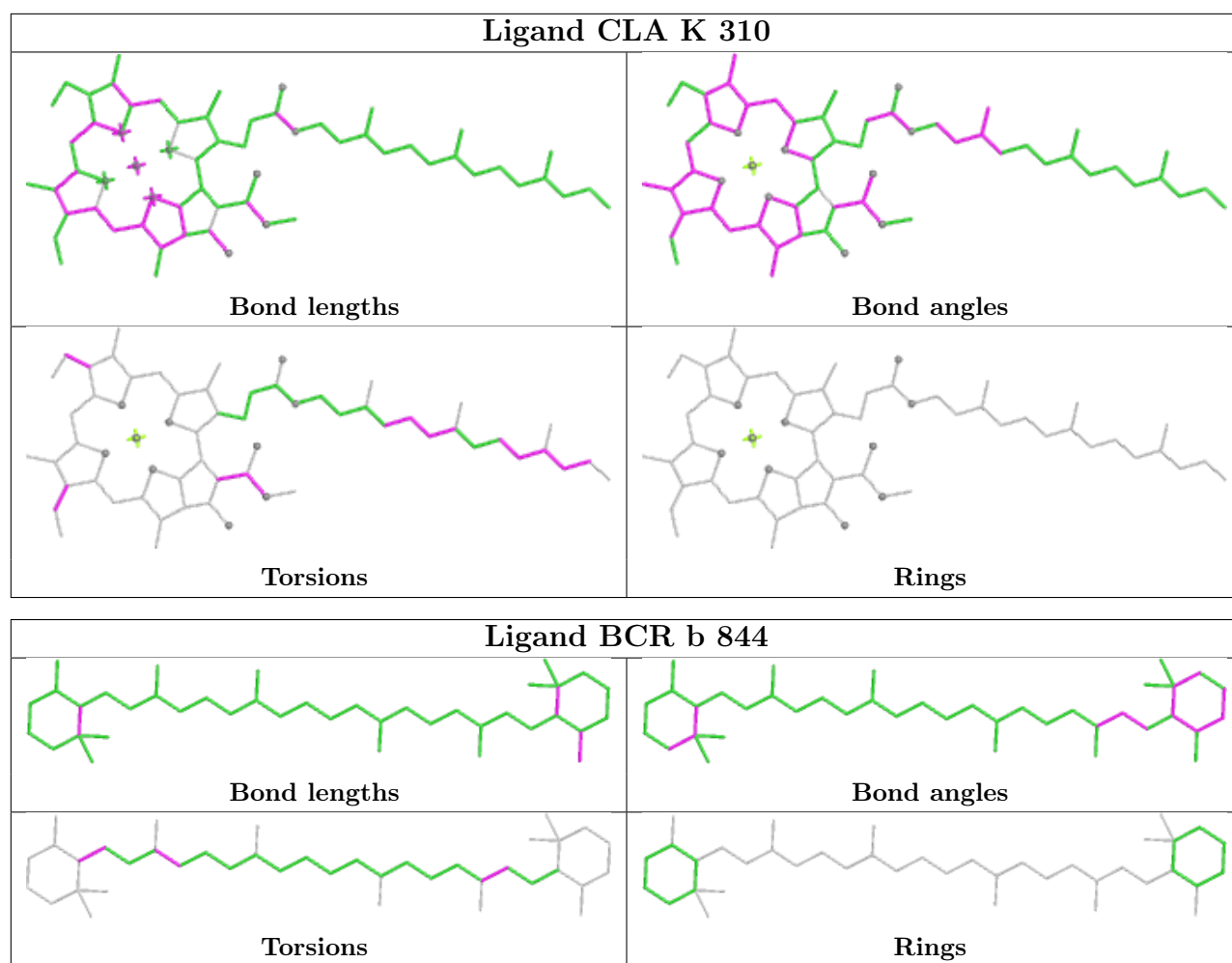


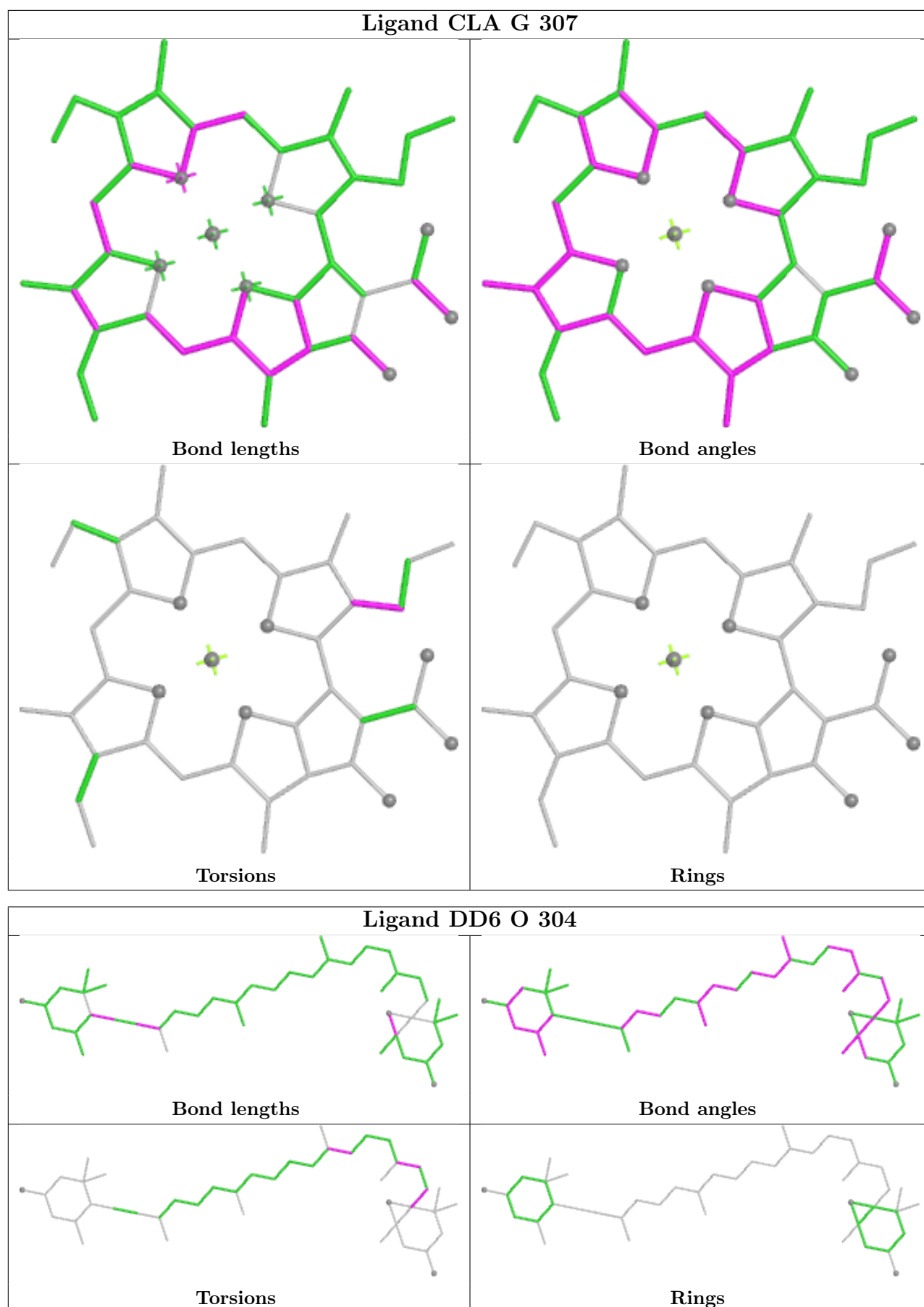
Torsions



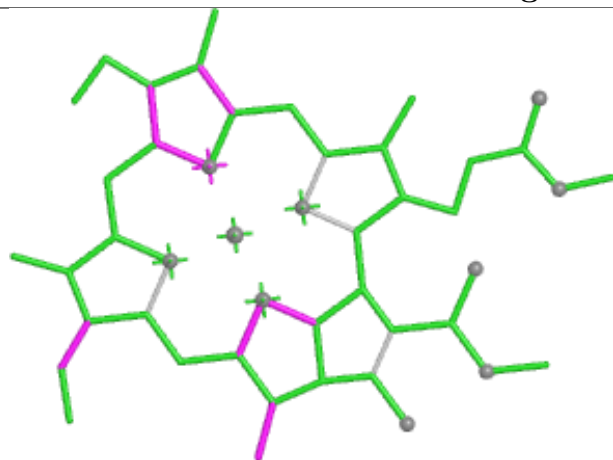
Rings



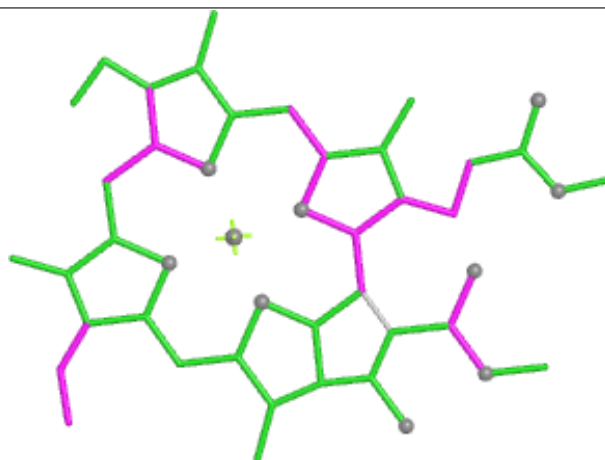




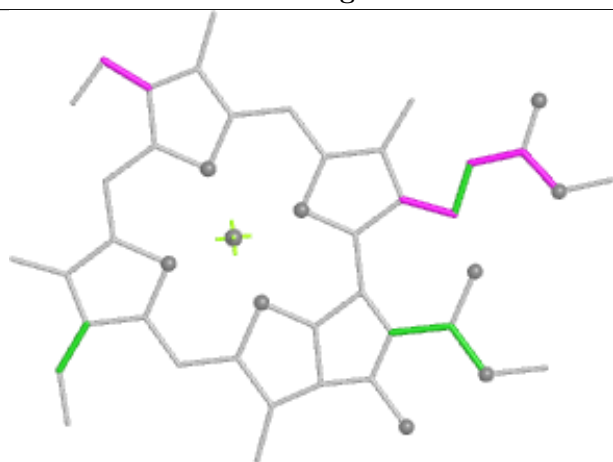
Ligand CLA I 309



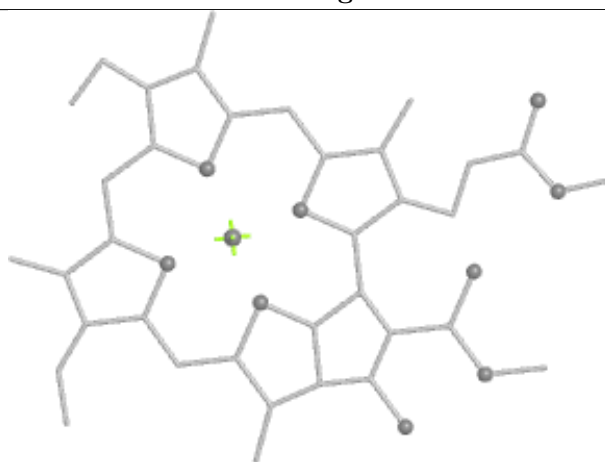
Bond lengths



Bond angles

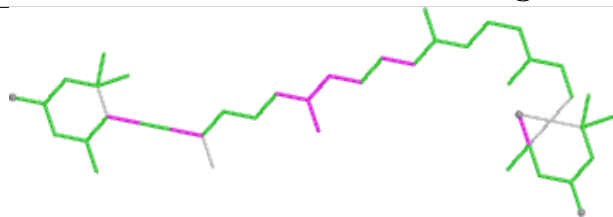


Torsions

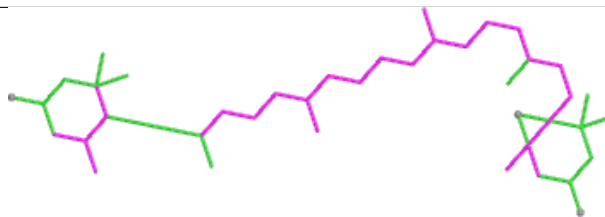


Rings

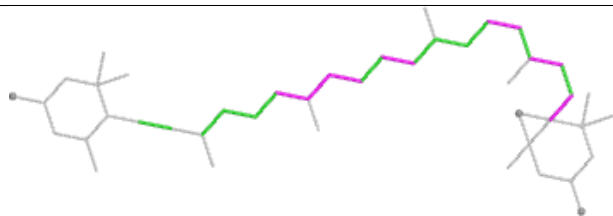
Ligand DD6 D 303



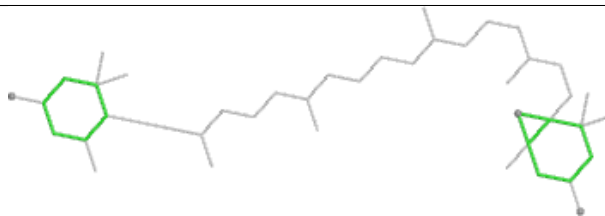
Bond lengths



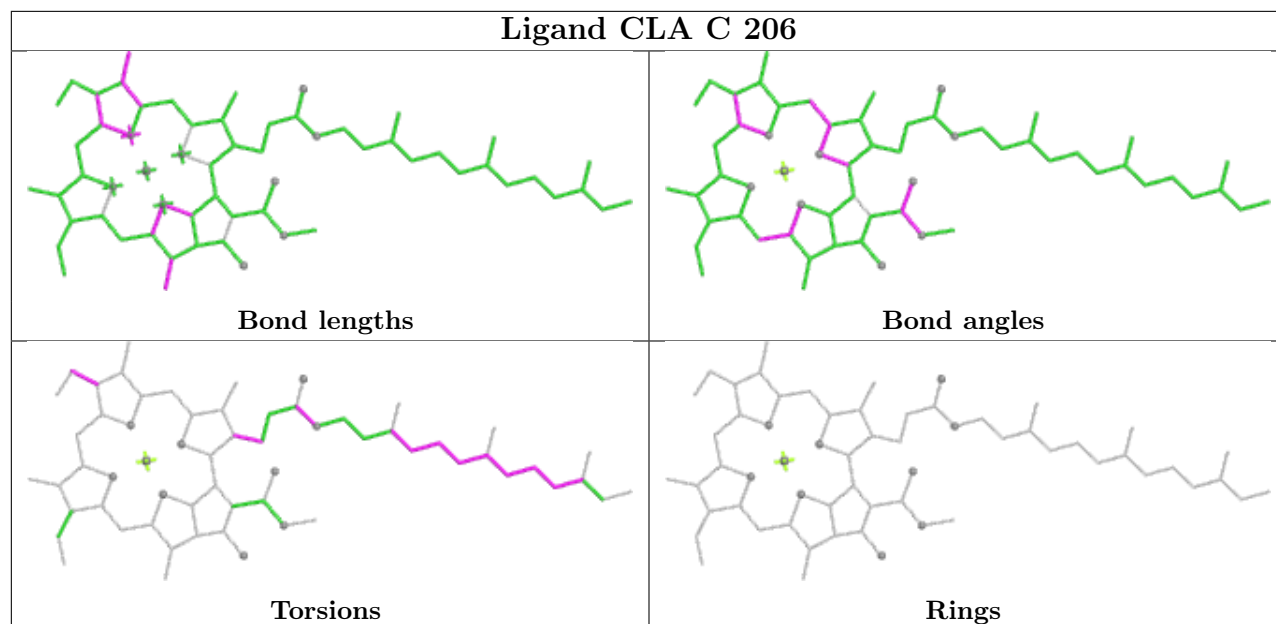
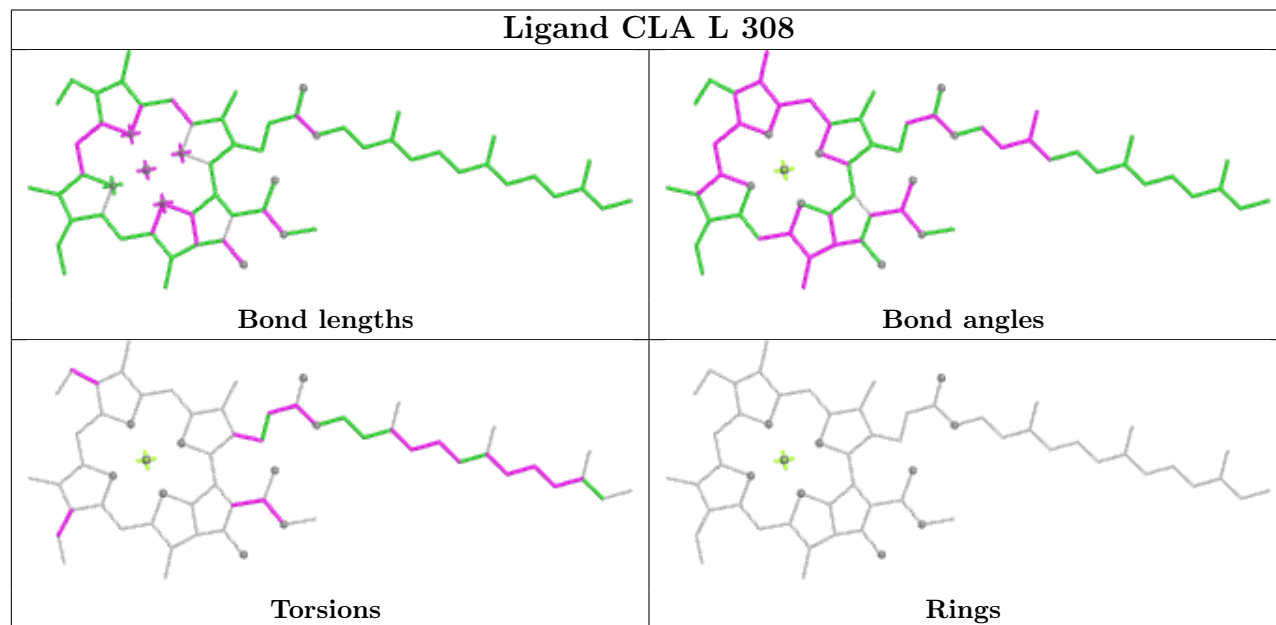
Bond angles

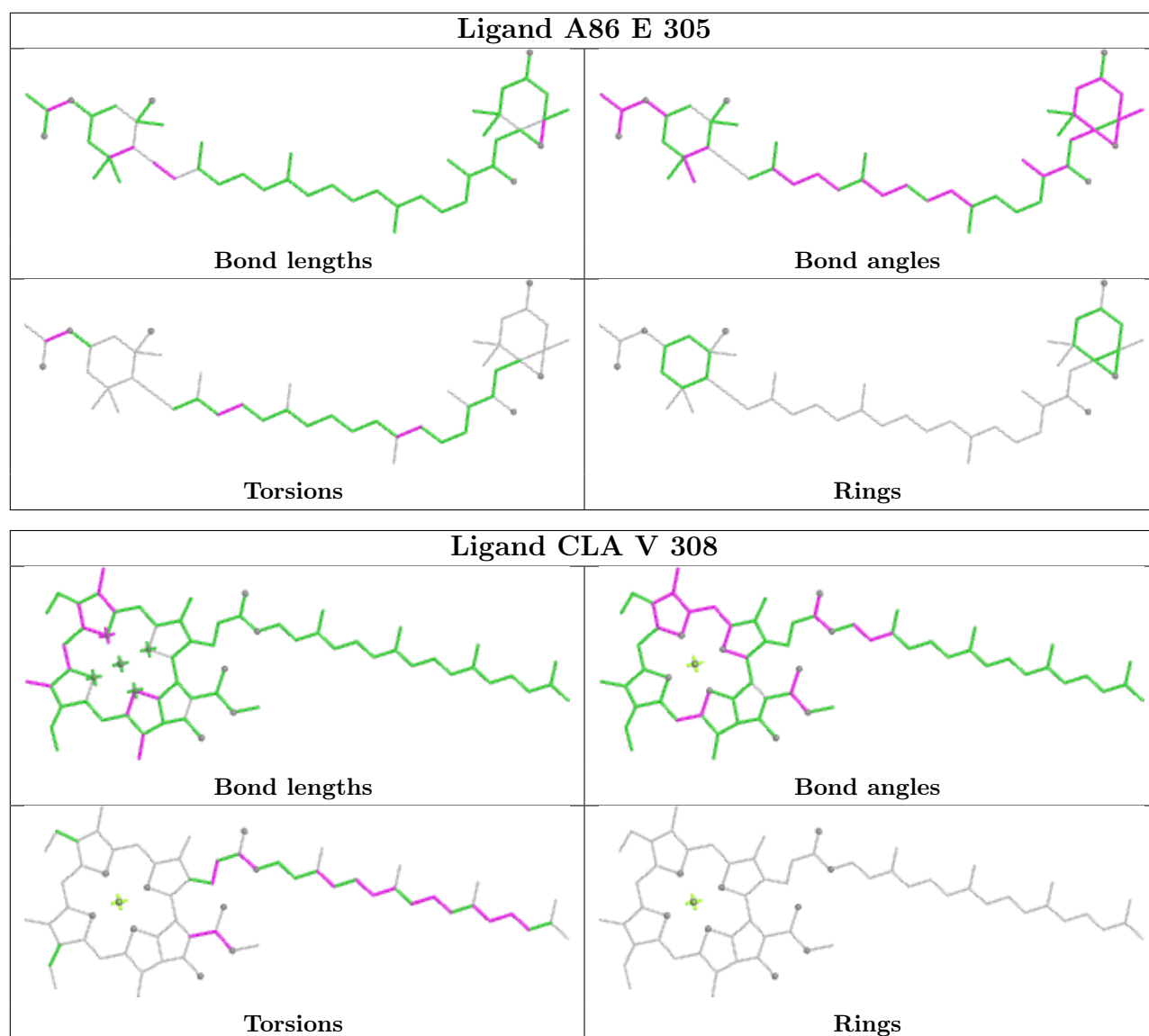


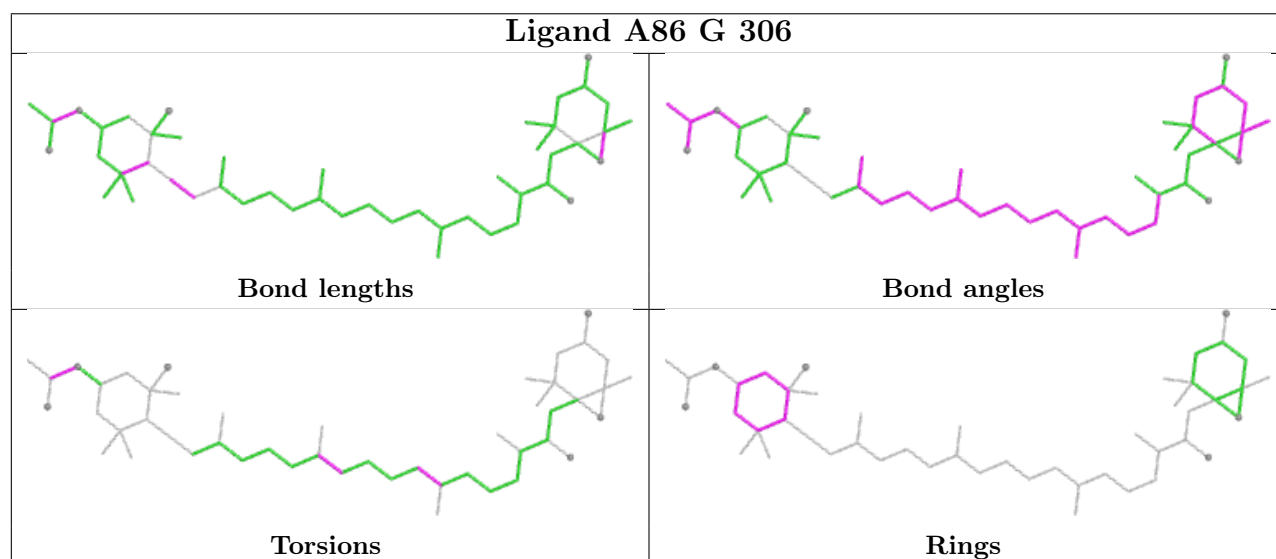
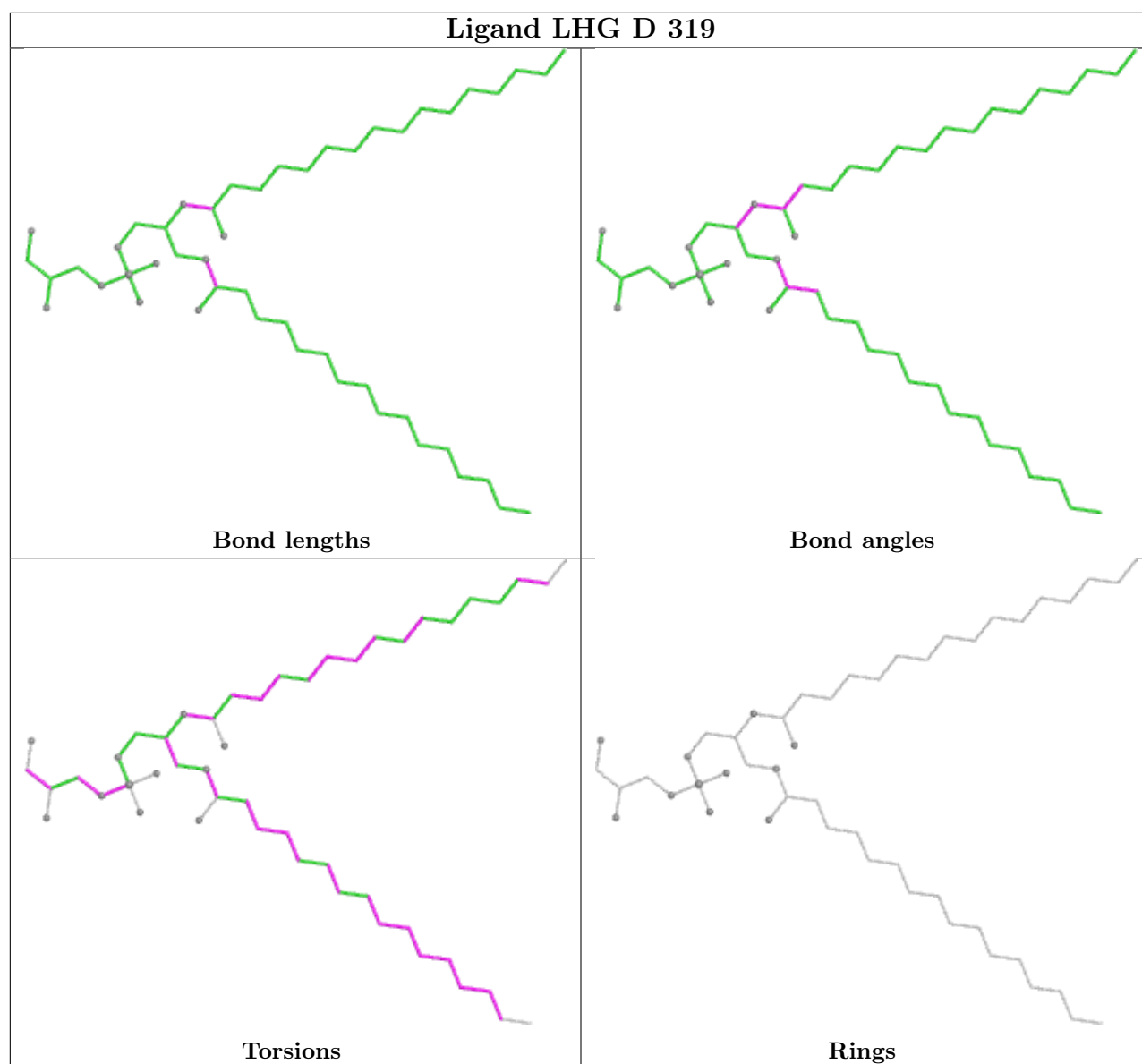
Torsions

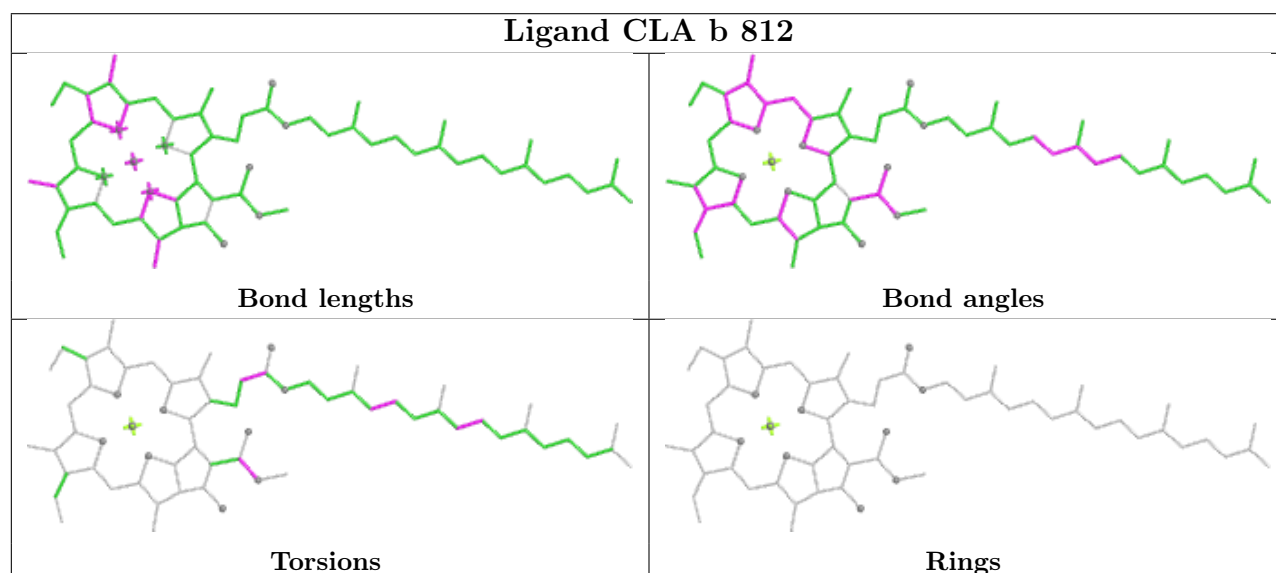
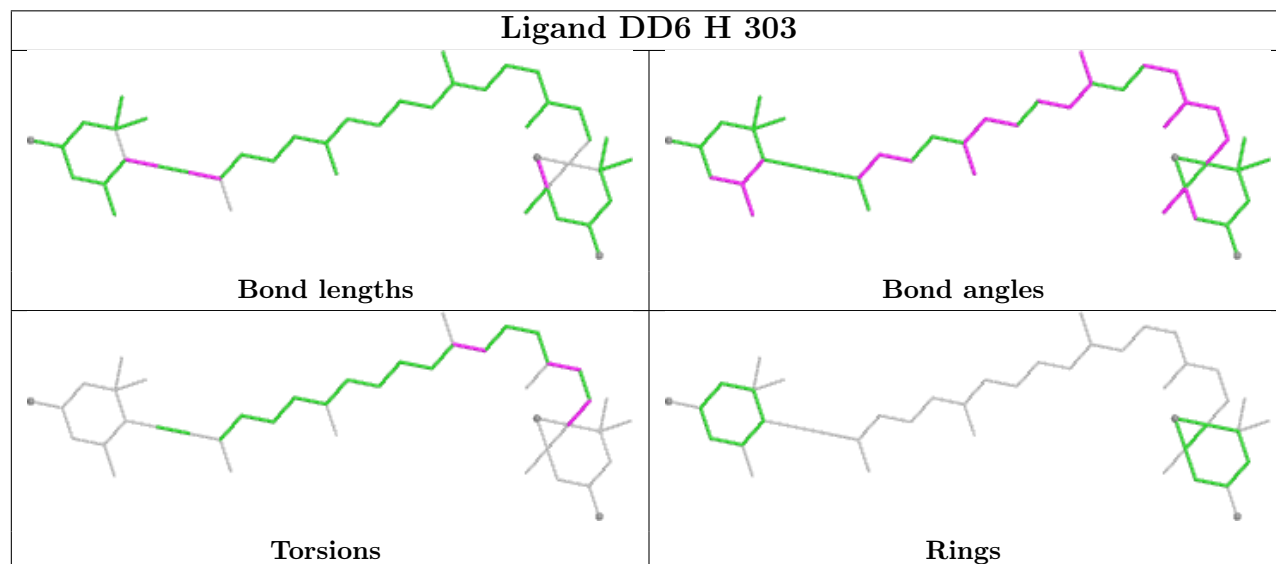
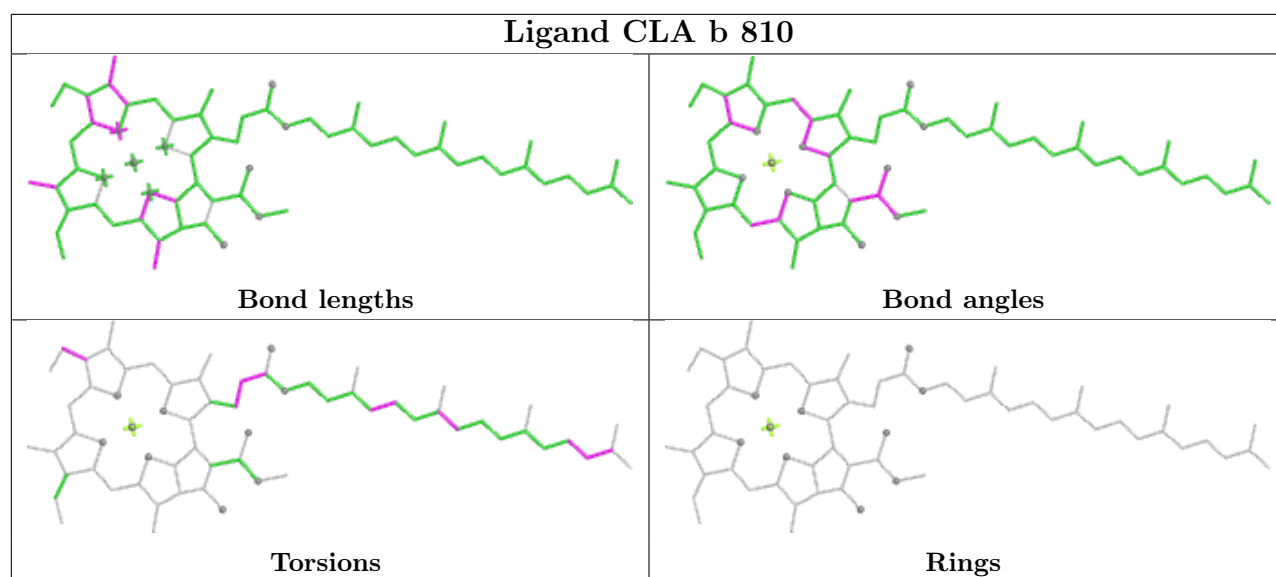


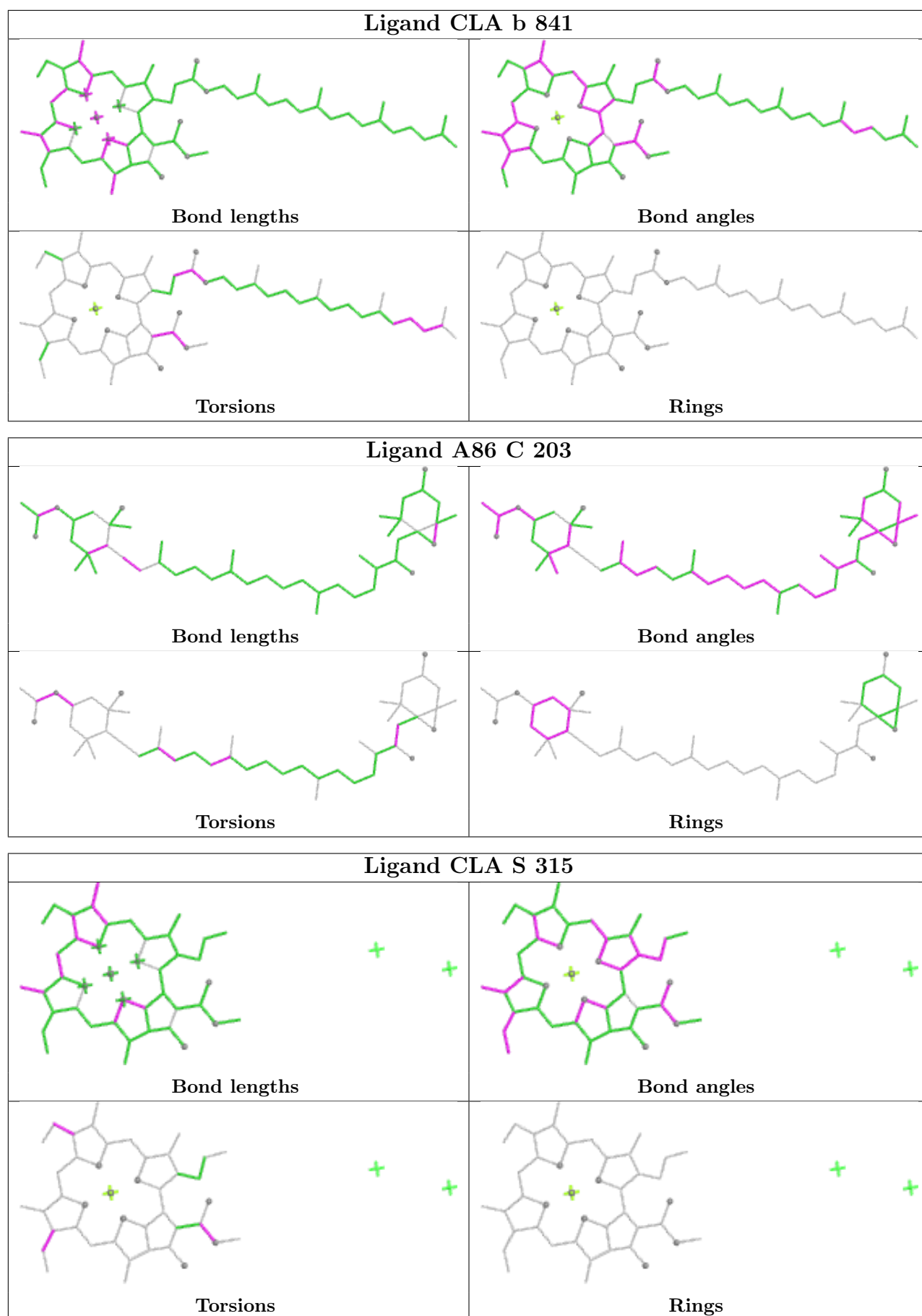
Rings

Ligand CLA C 206**Ligand CLA L 308**

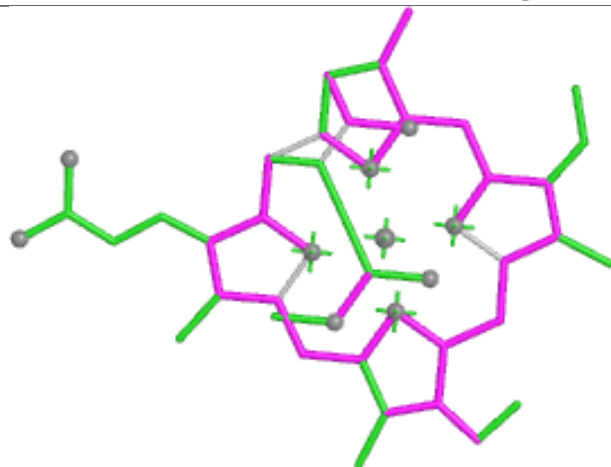




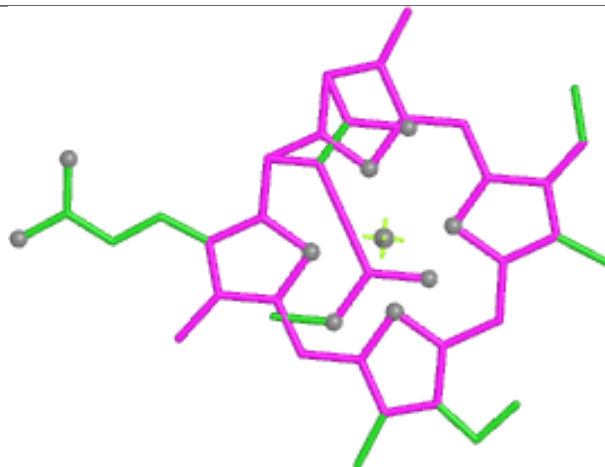




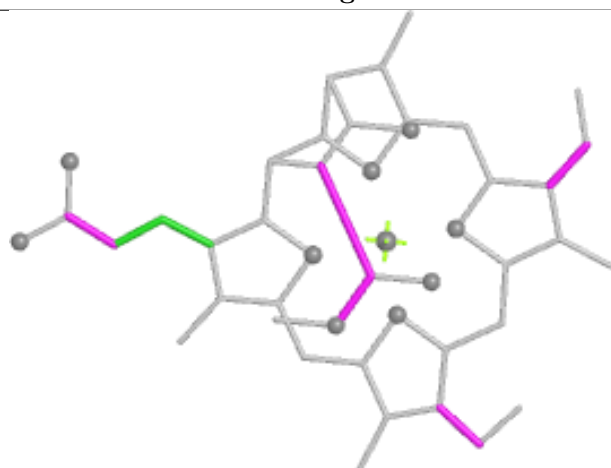
Ligand KC1 T 310



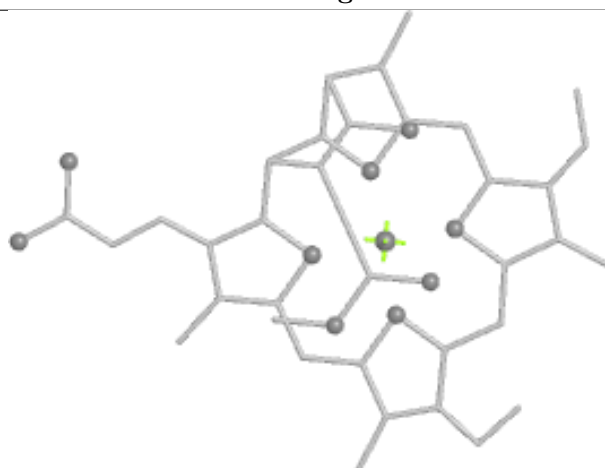
Bond lengths



Bond angles

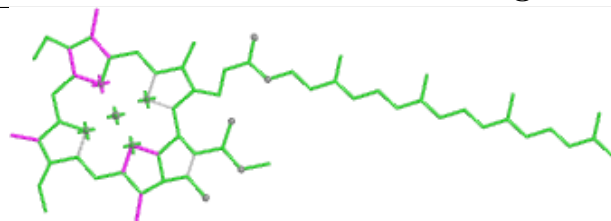


Torsions

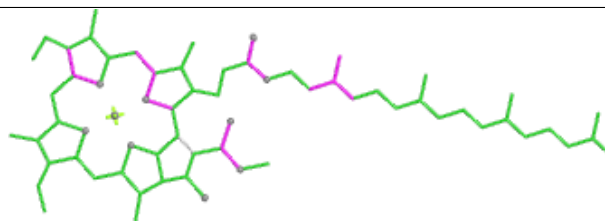


Rings

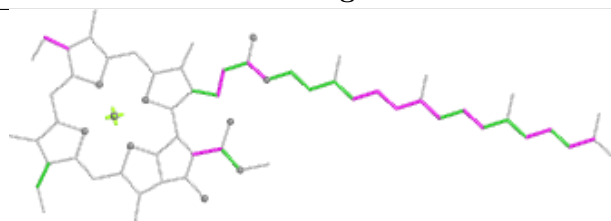
Ligand CLA O 308



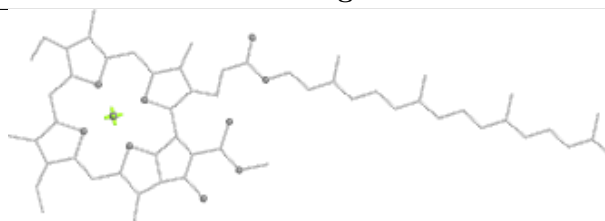
Bond lengths



Bond angles

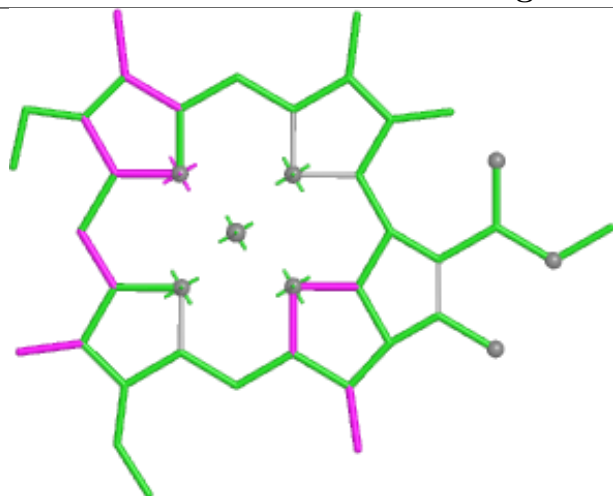


Torsions



Rings

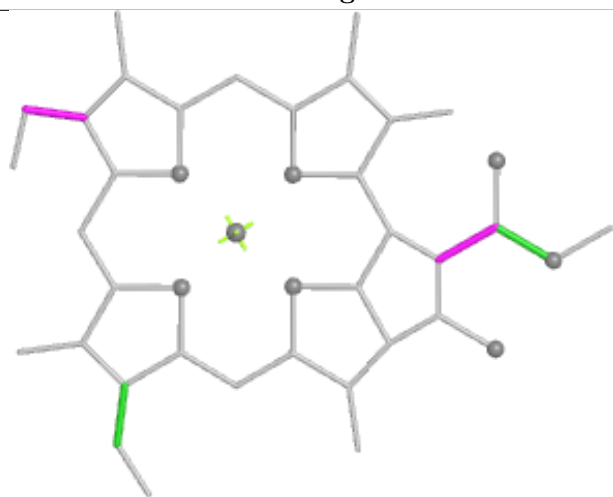
Ligand CLA F 316



Bond lengths



Bond angles

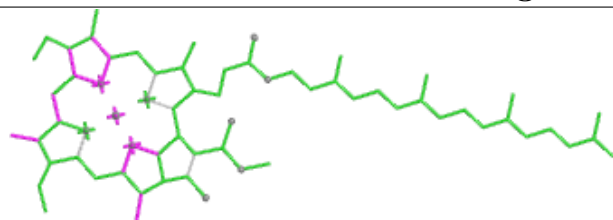


Torsions

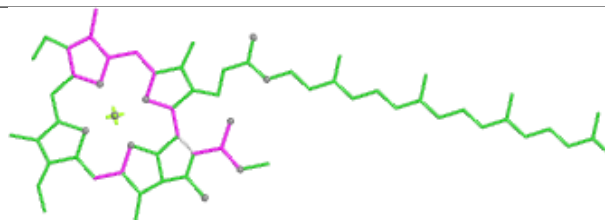


Rings

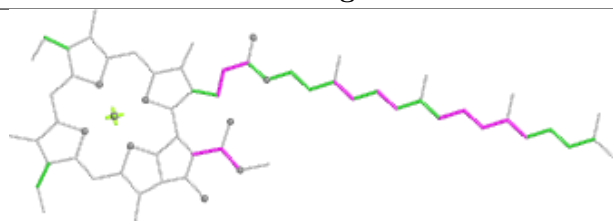
Ligand CLA L 311



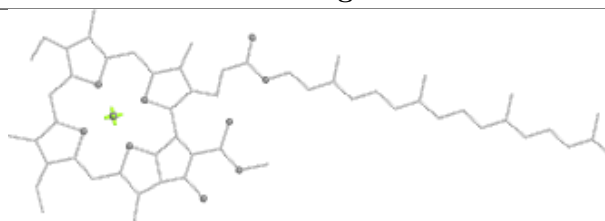
Bond lengths



Bond angles

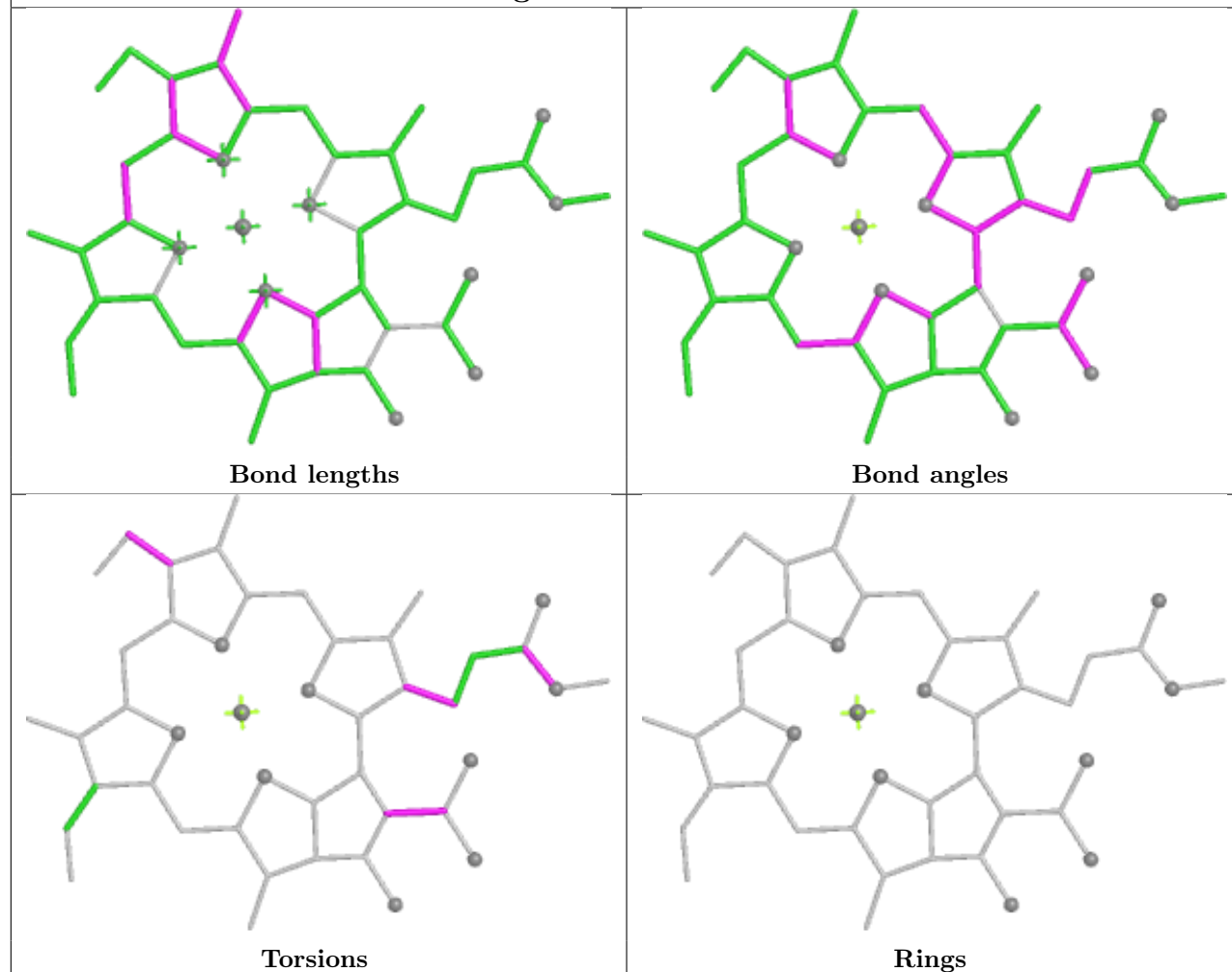


Torsions

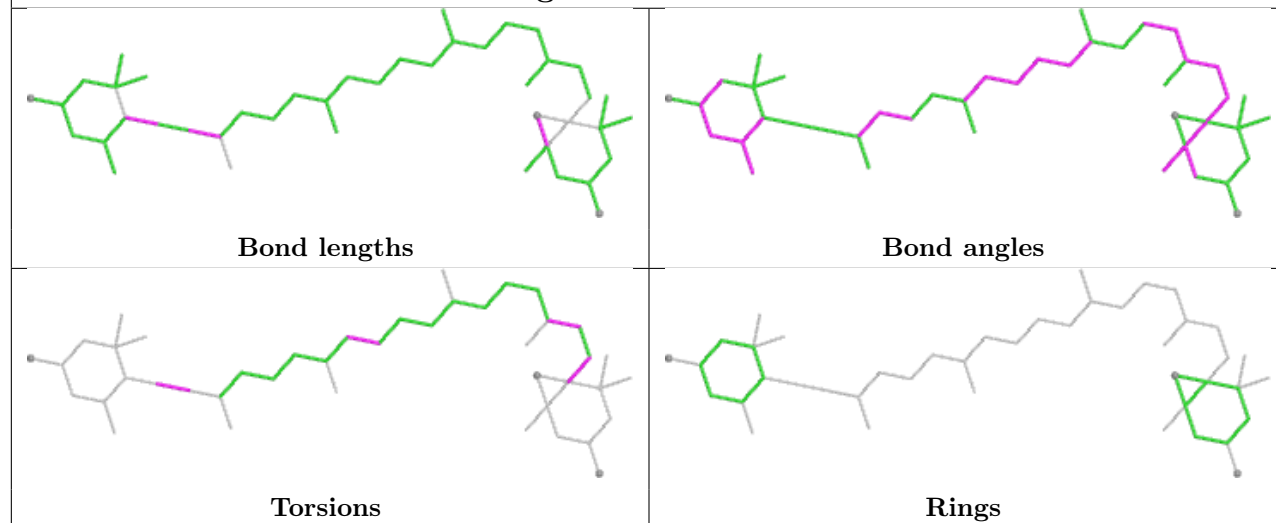


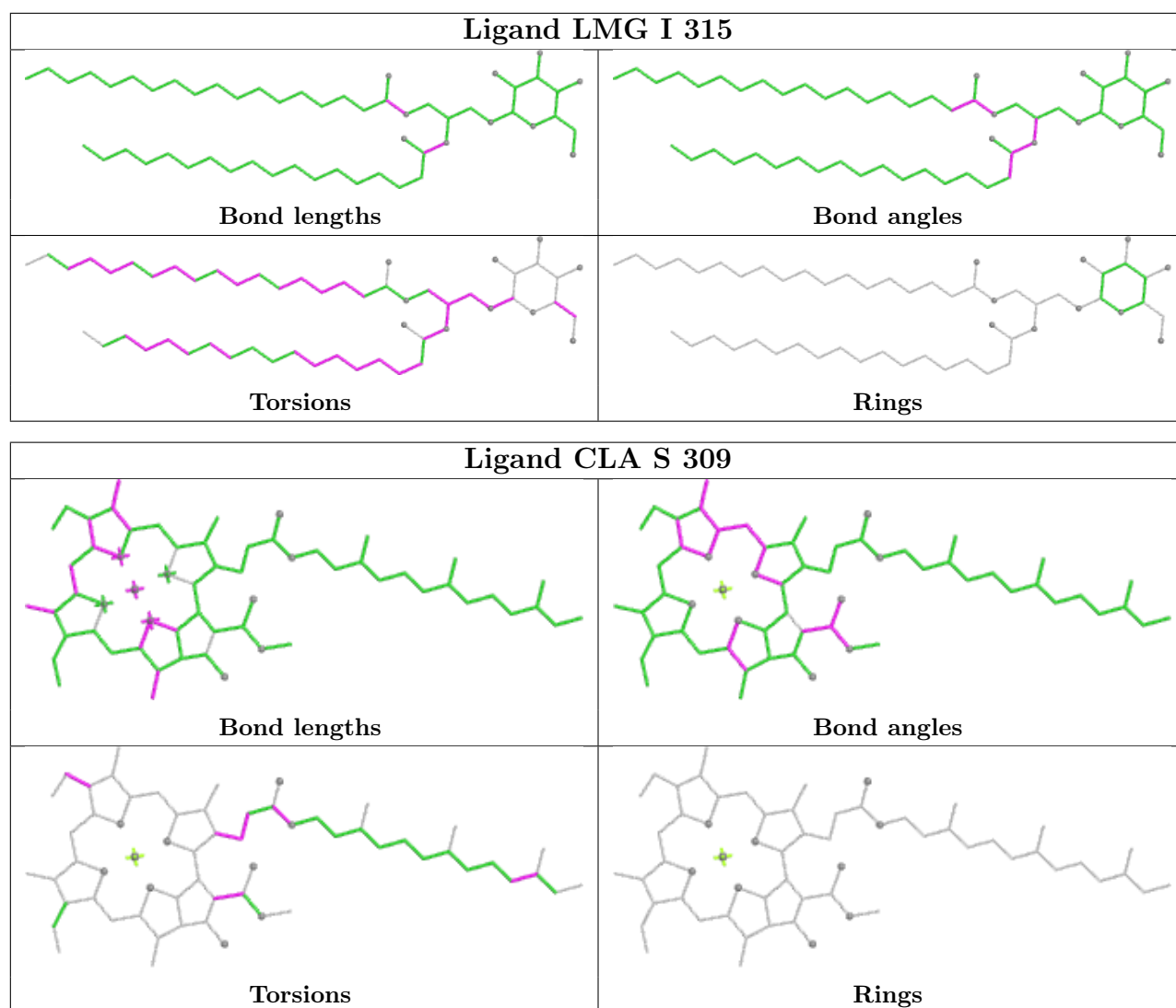
Rings

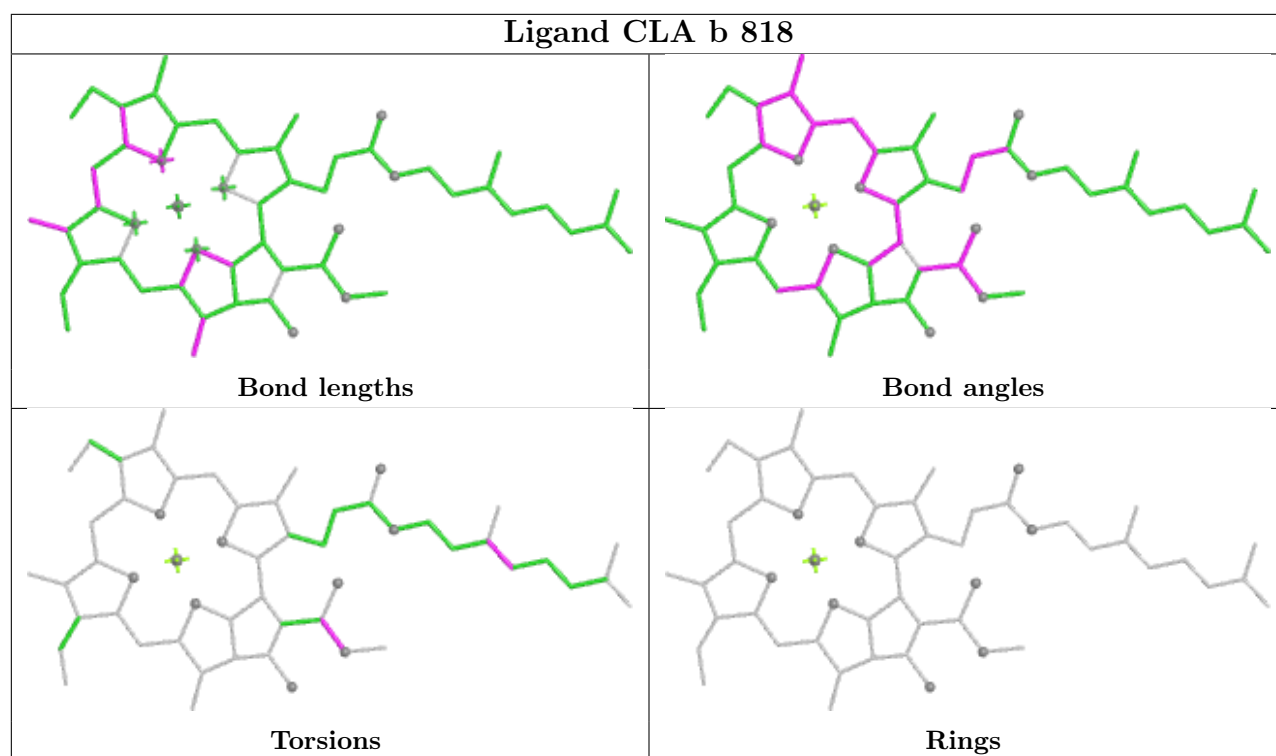
Ligand CLA X 309



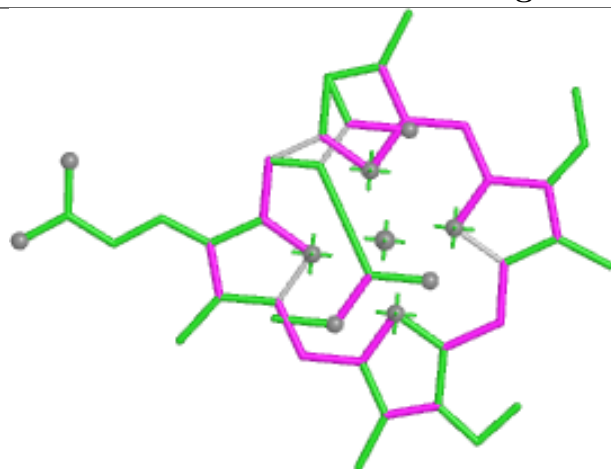
Ligand DD6 J 304



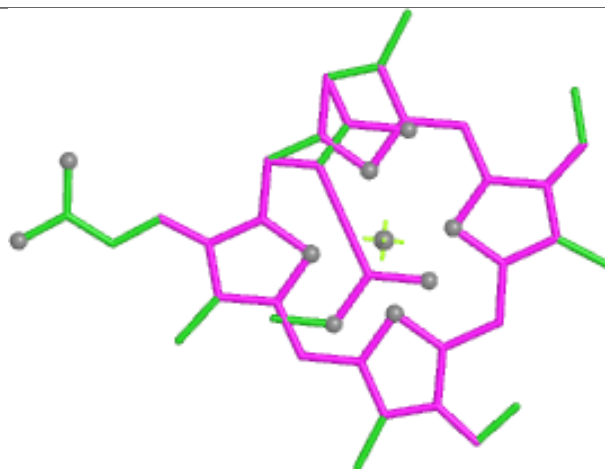




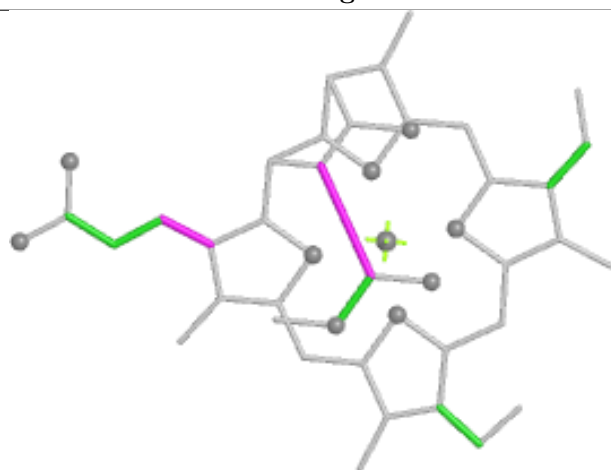
Ligand KC1 X 311



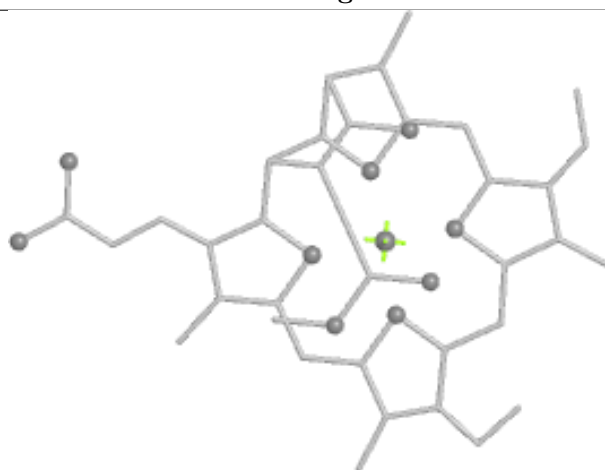
Bond lengths



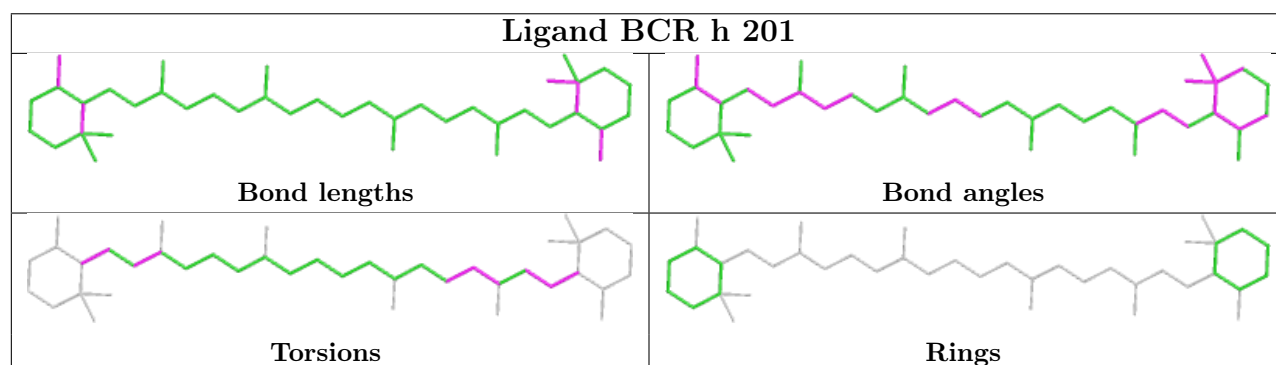
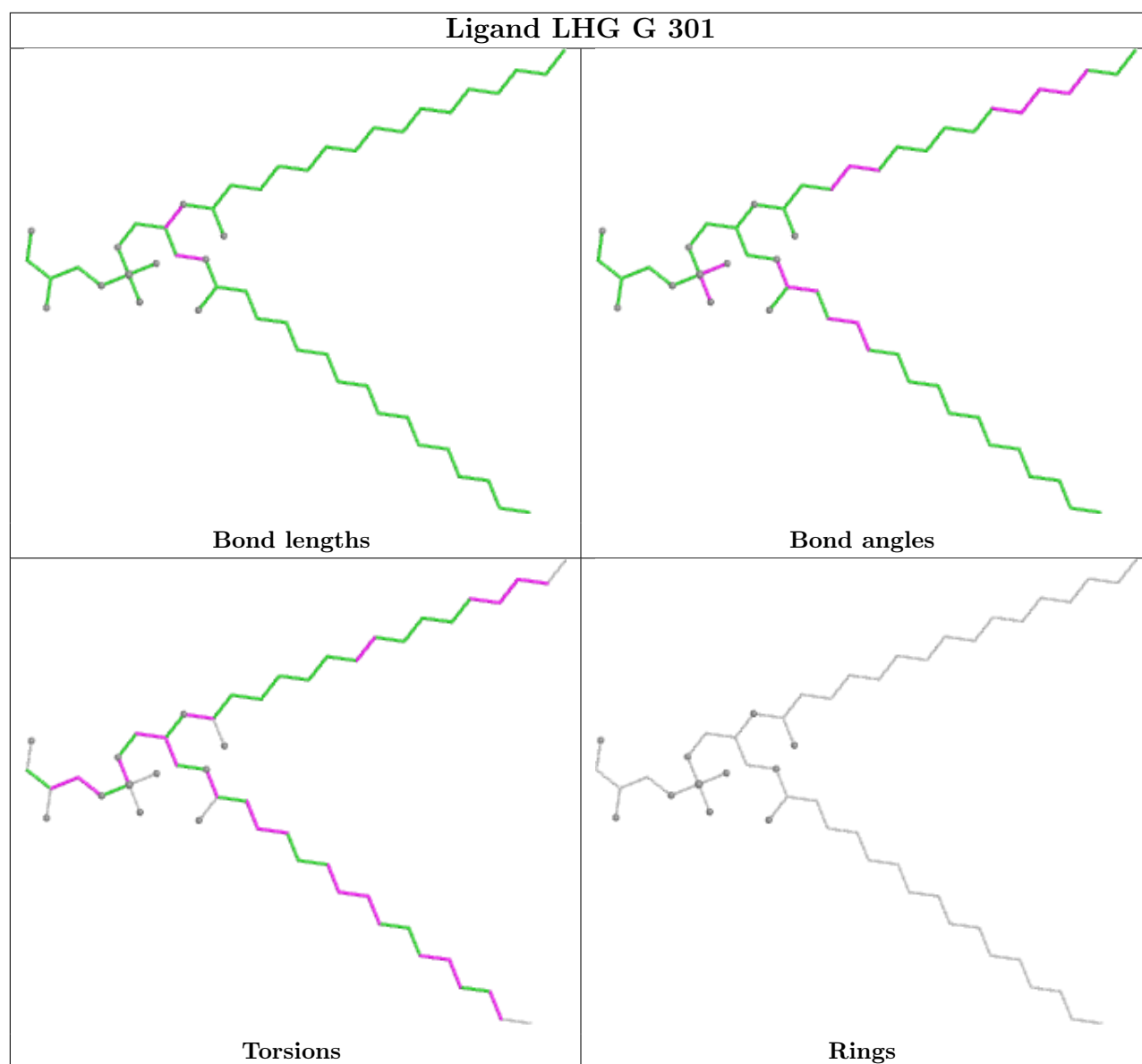
Bond angles

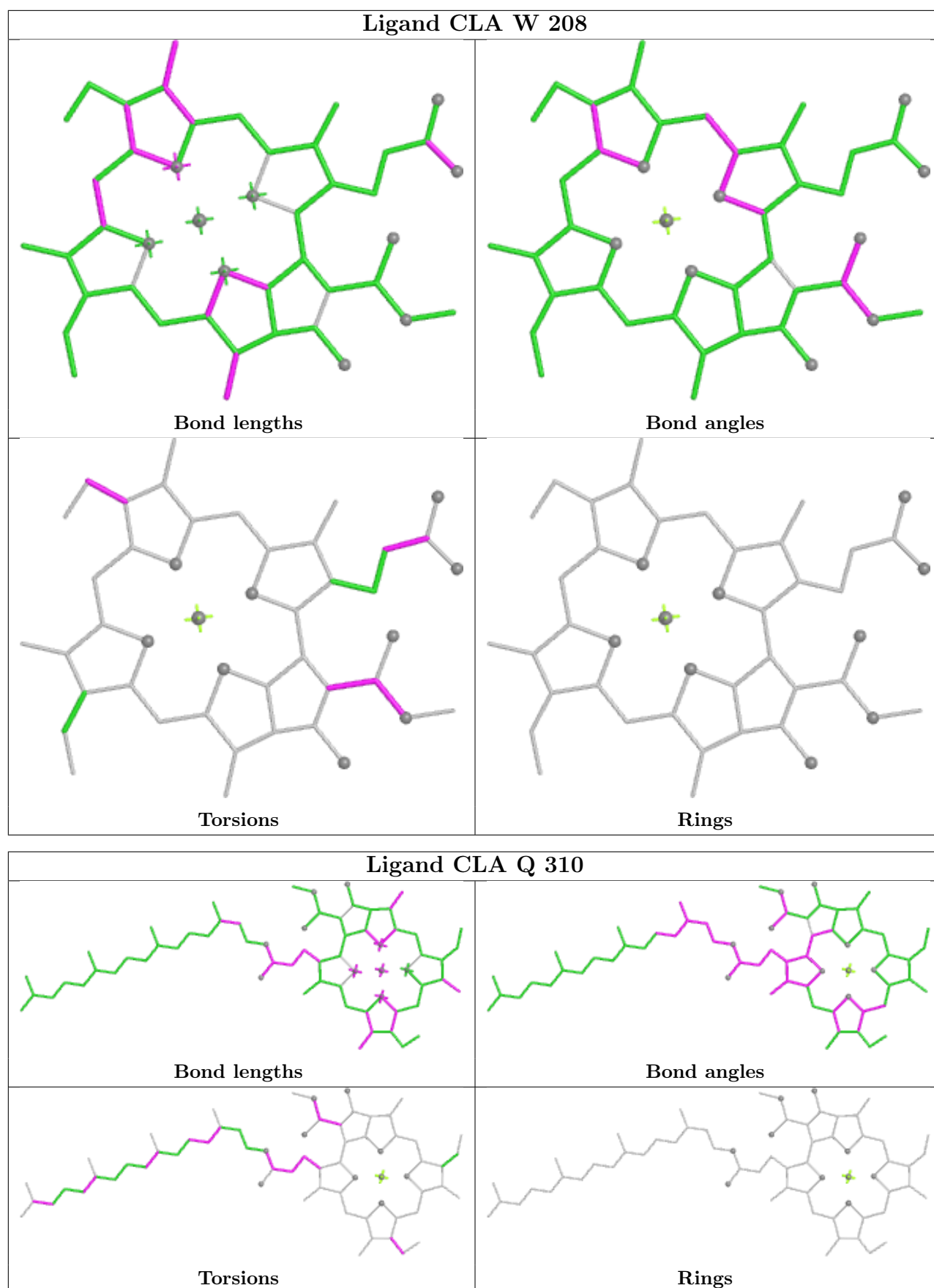


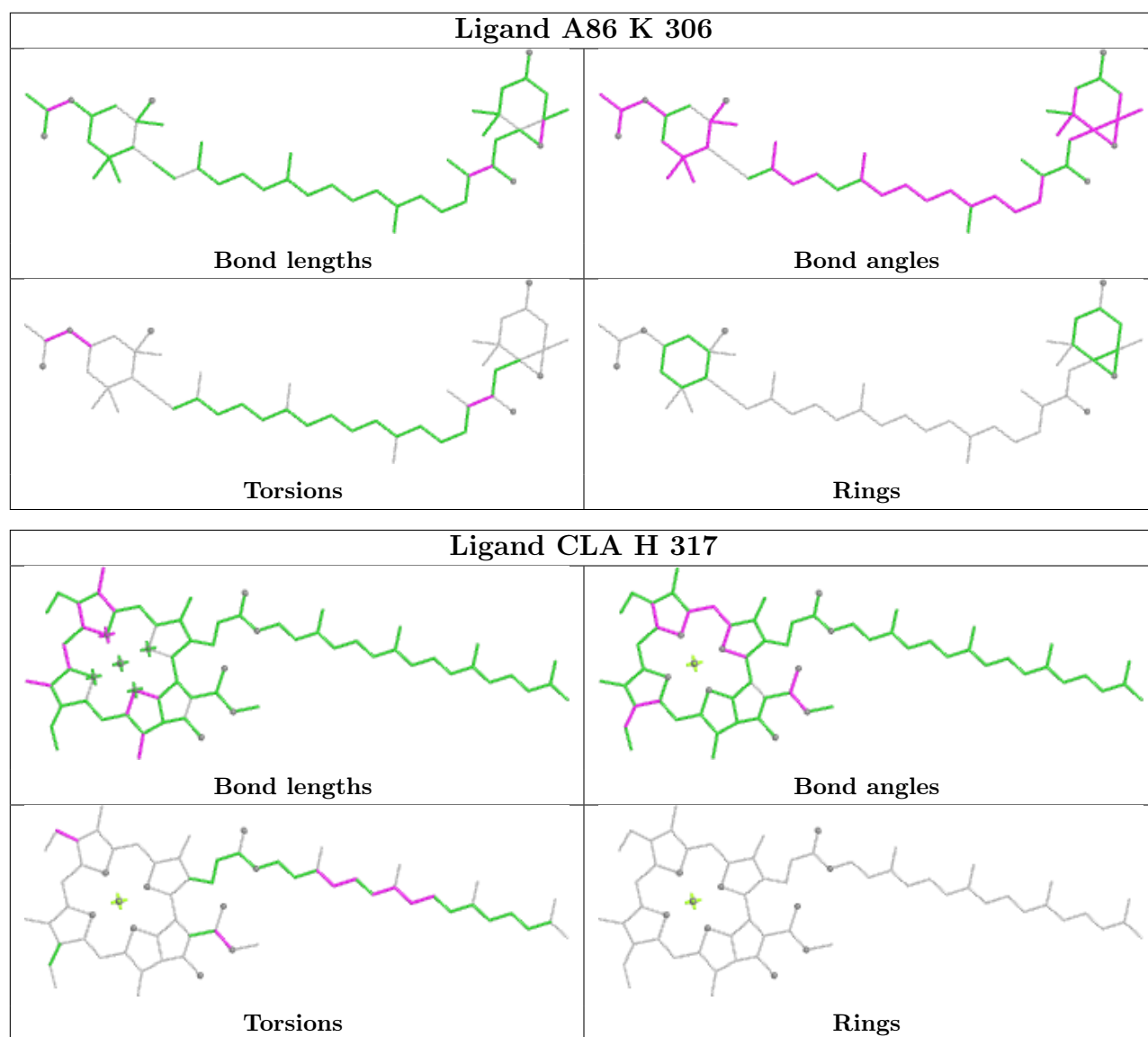
Torsions

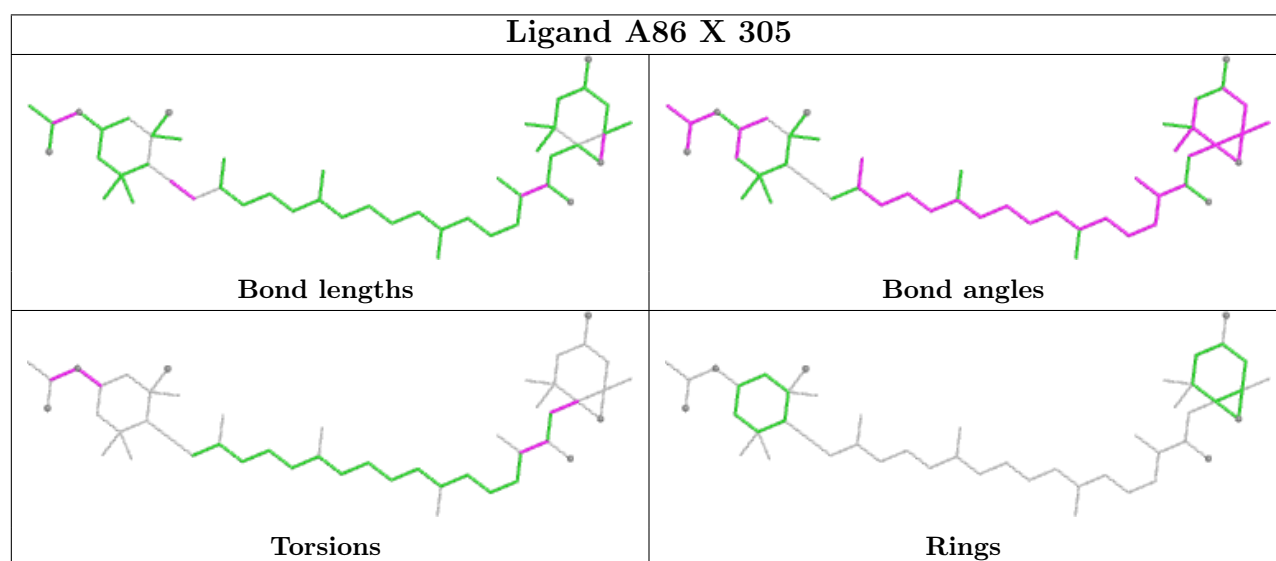
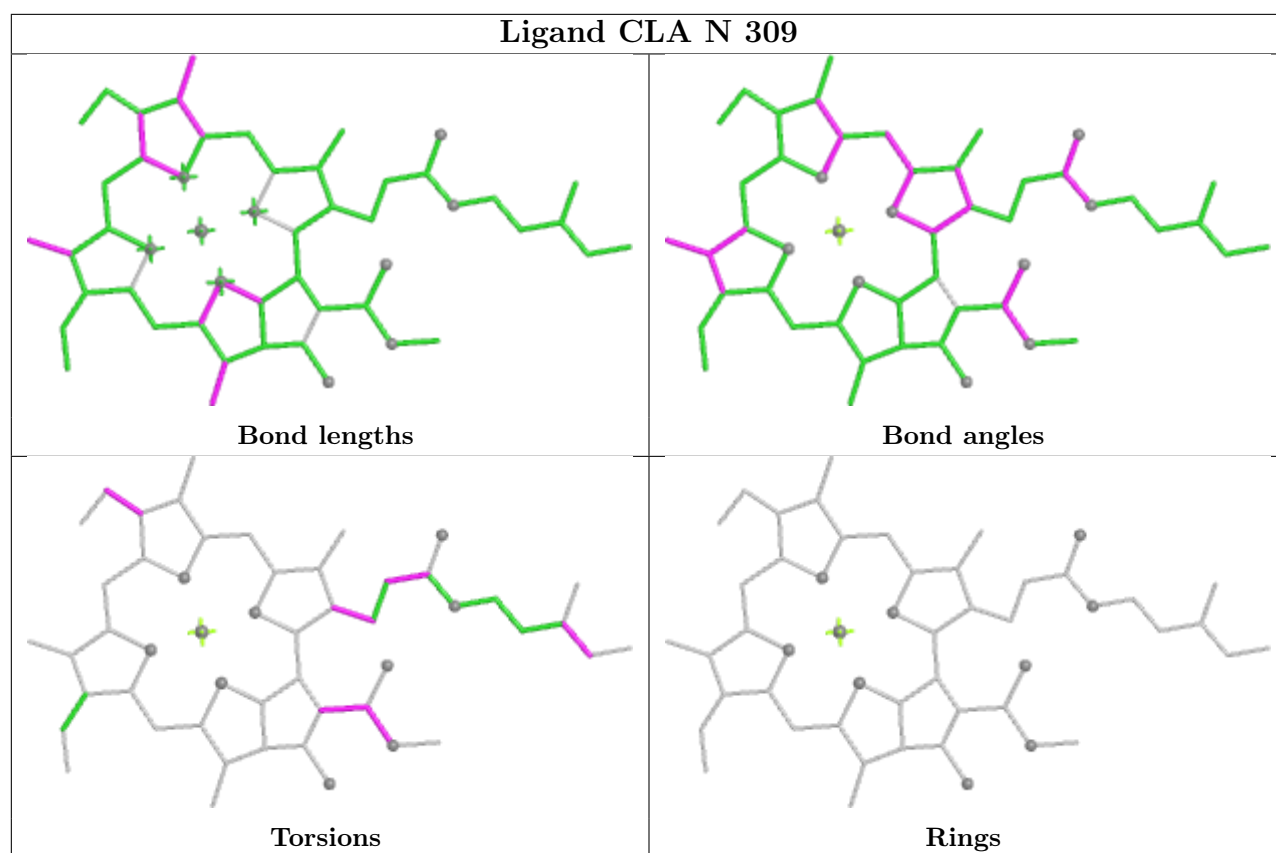


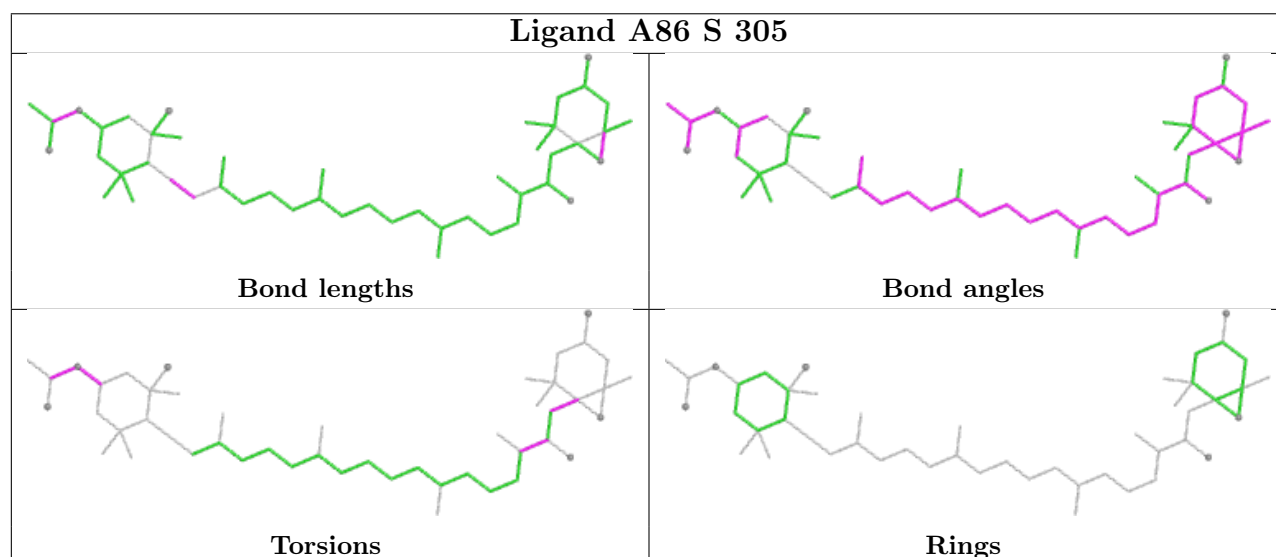
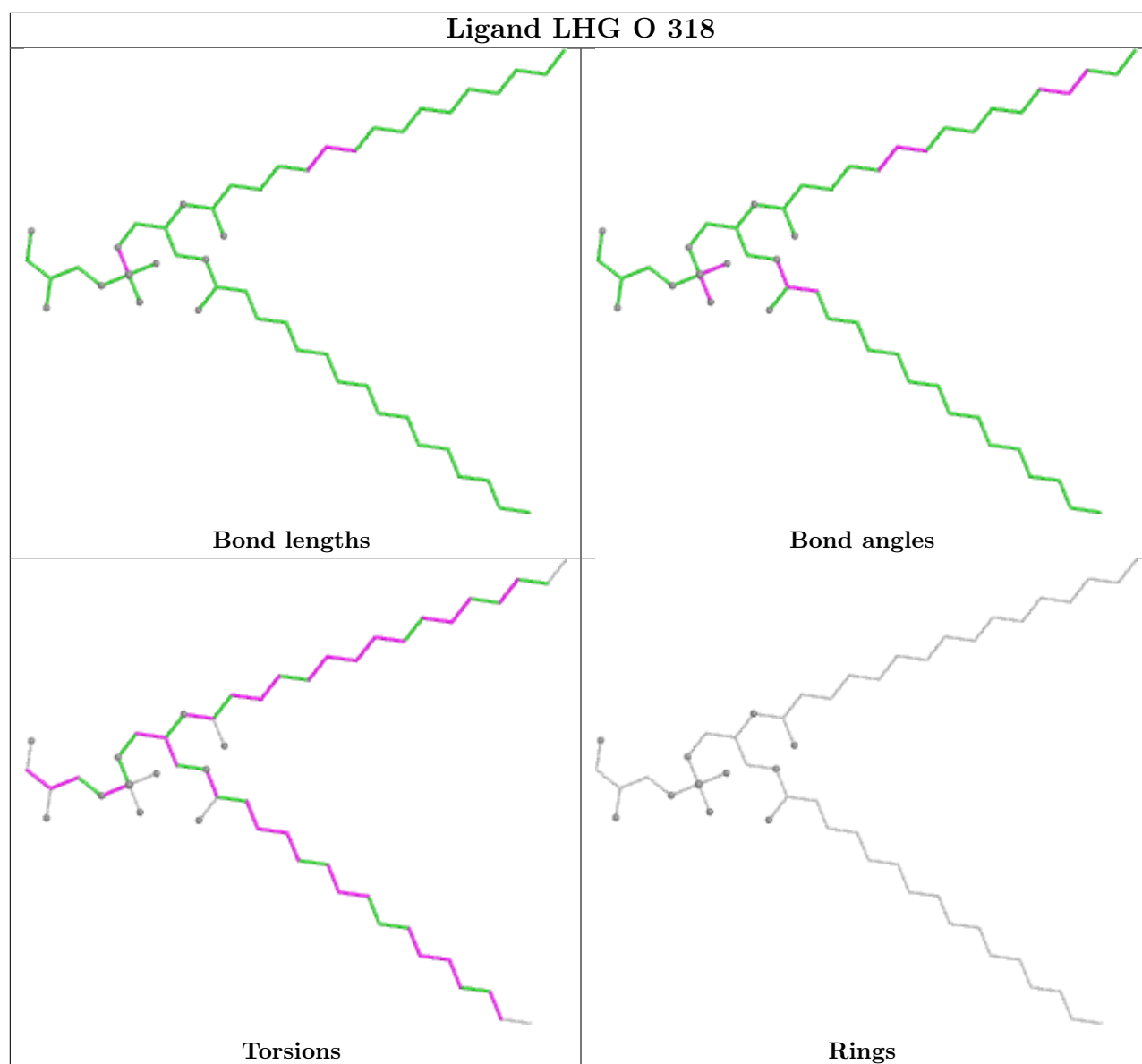
Rings

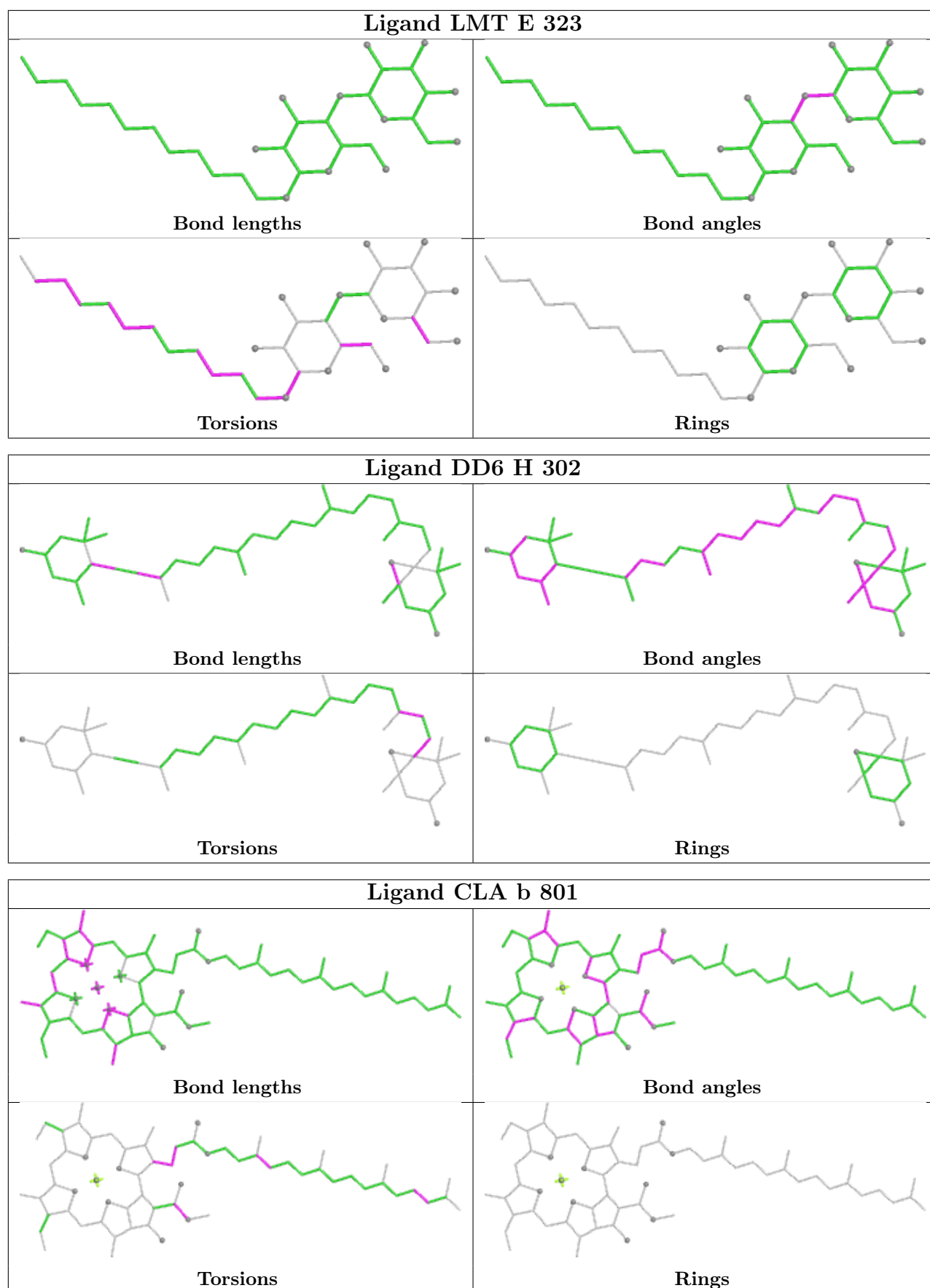


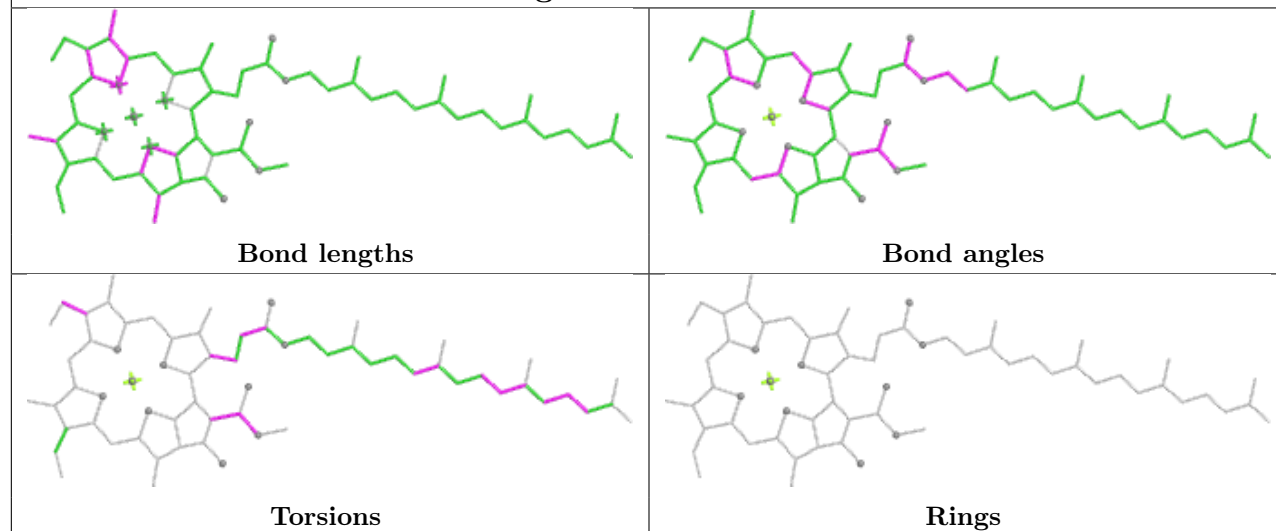
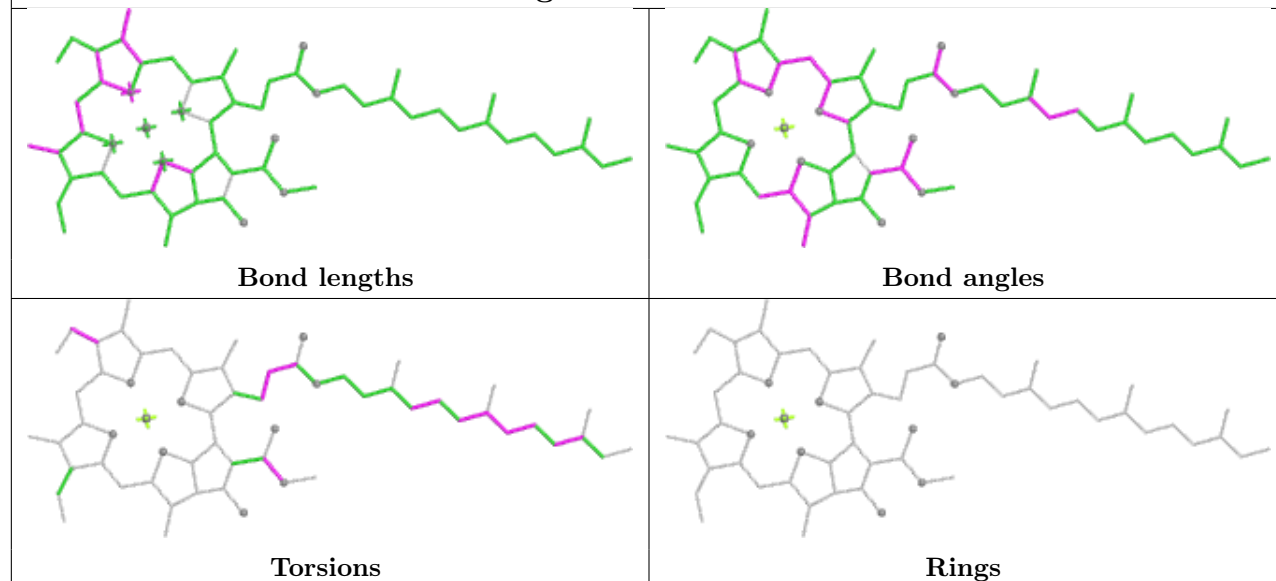




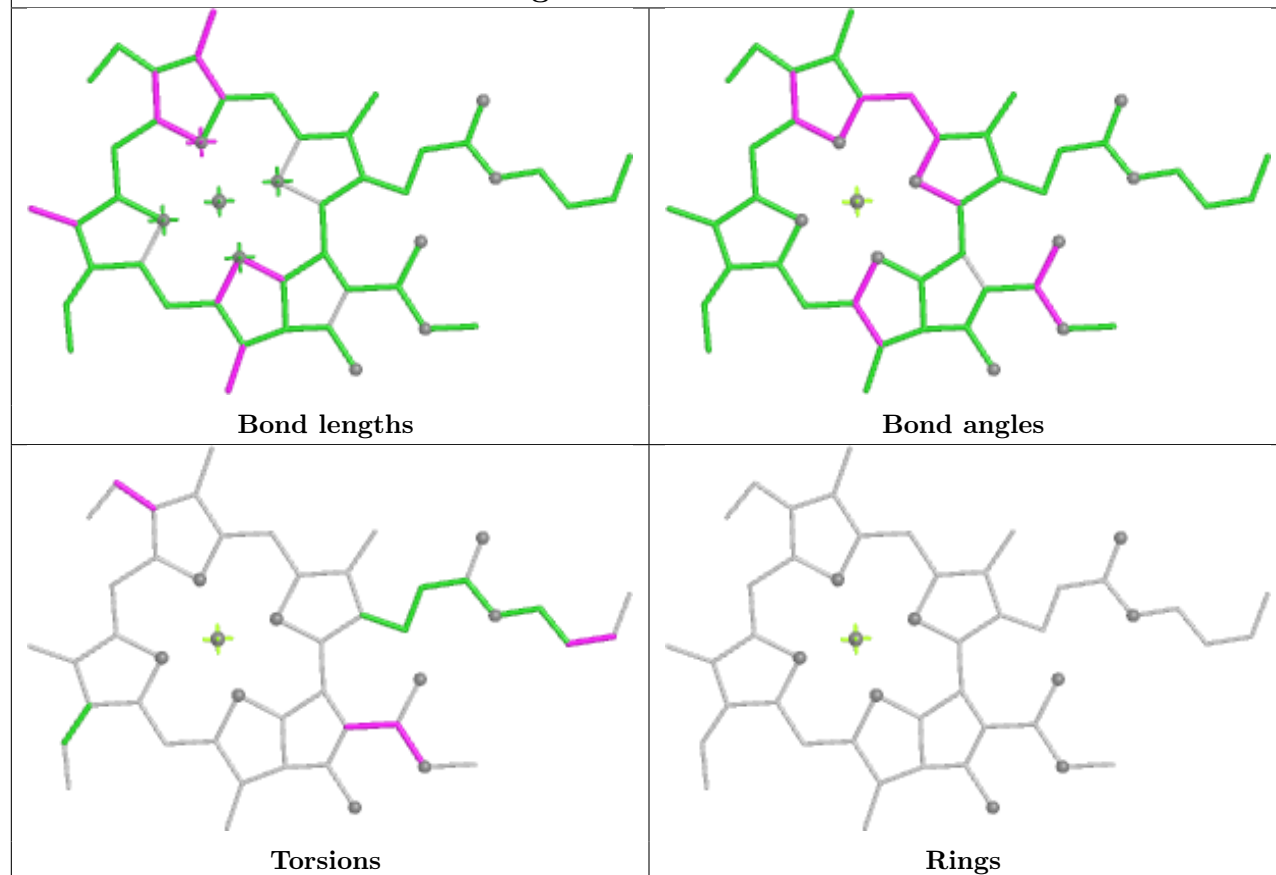




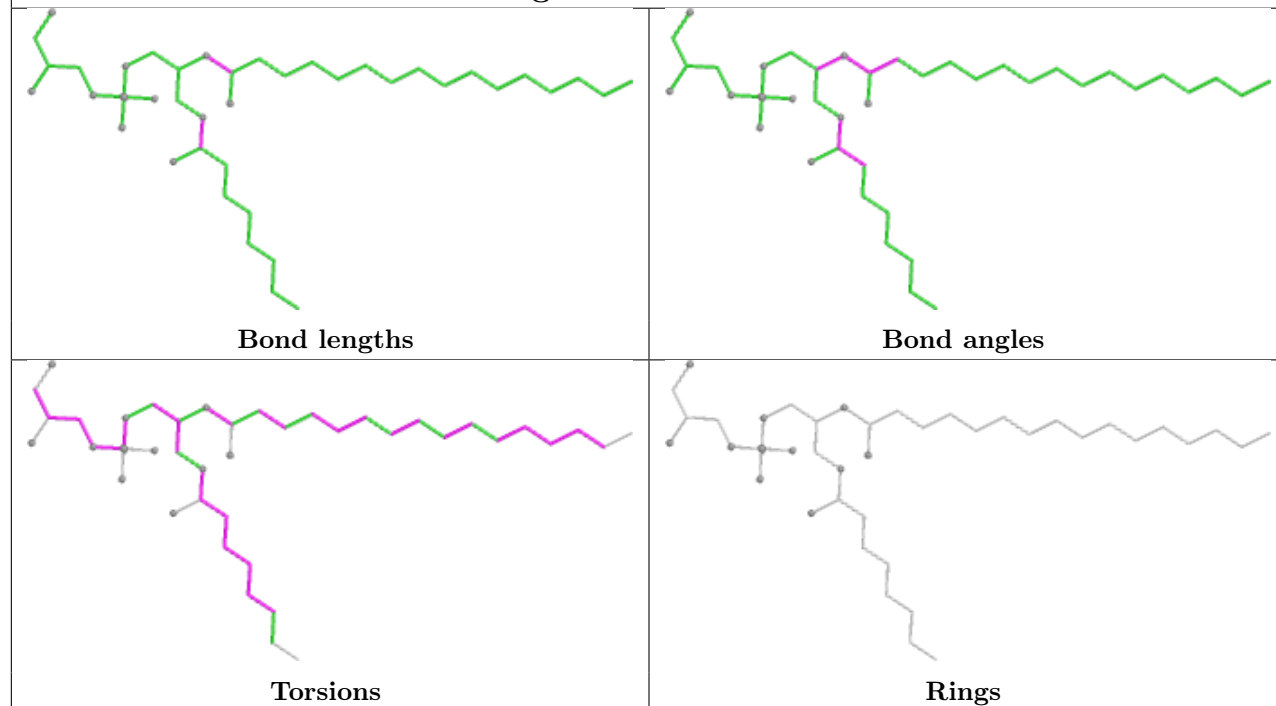


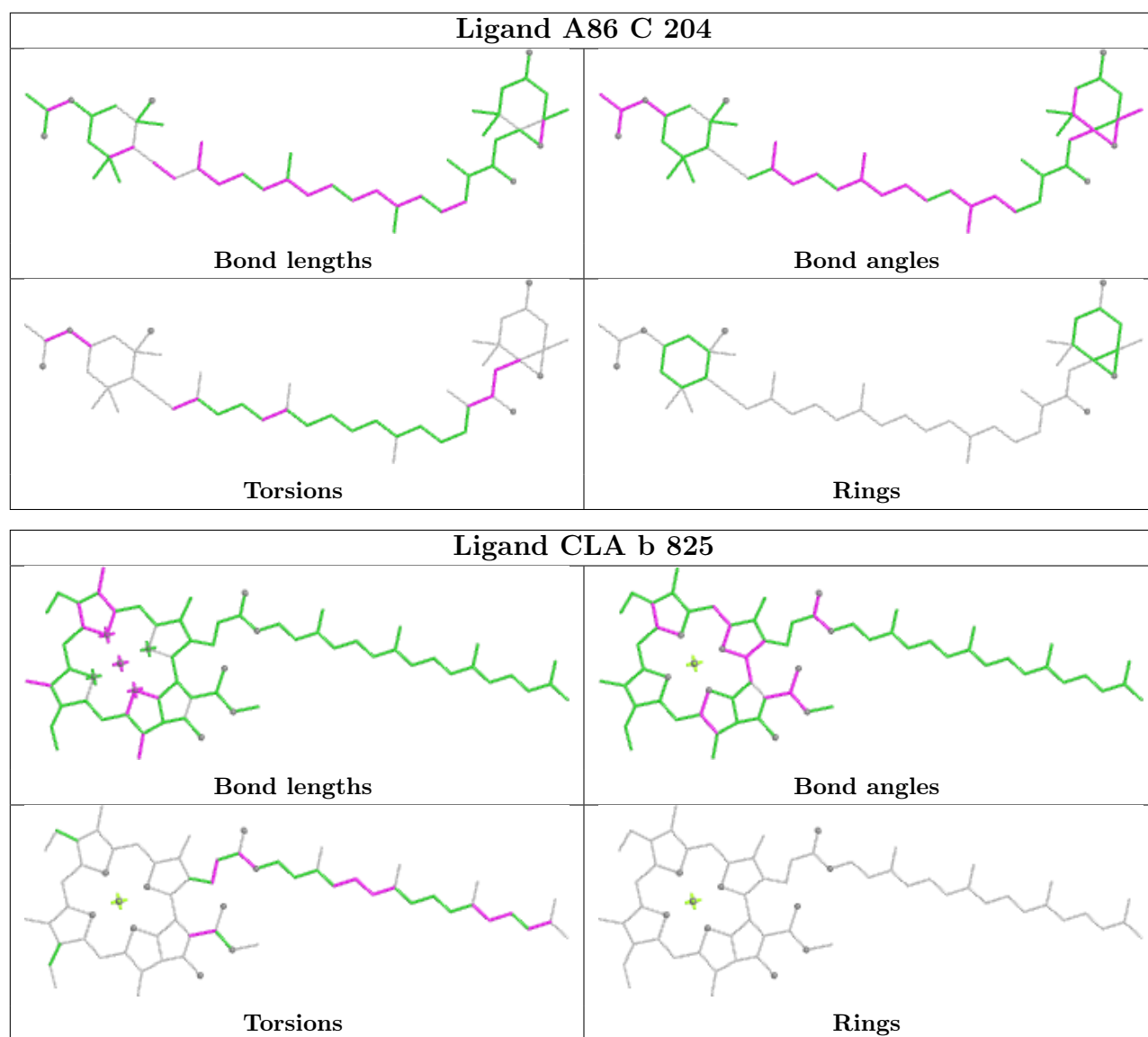
Ligand CLA b 808**Ligand CLA J 308**

Ligand CLA A 305

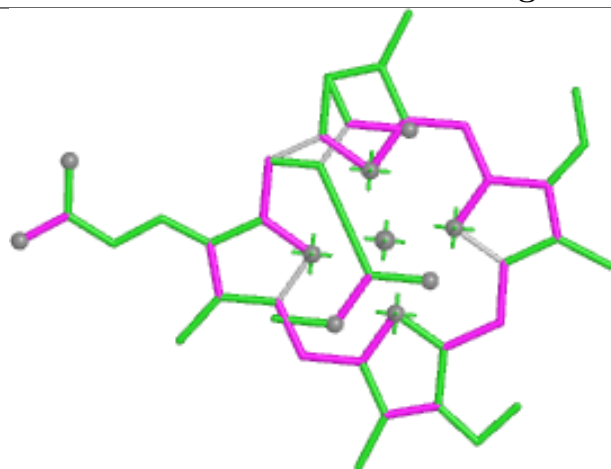


Ligand LHG F 319

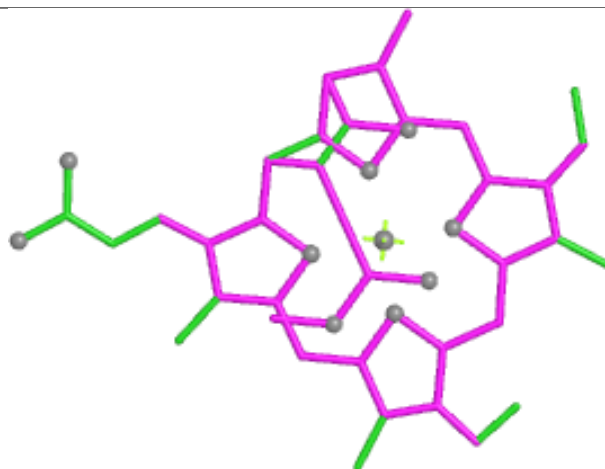




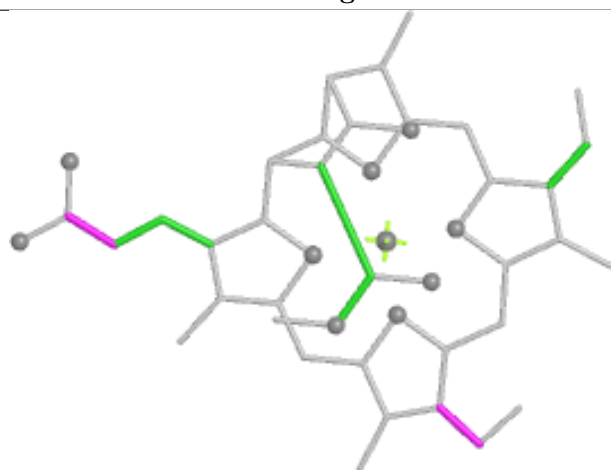
Ligand KC1 L 317



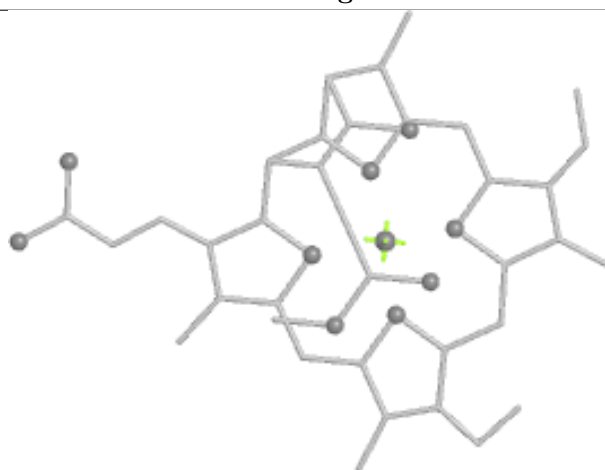
Bond lengths



Bond angles

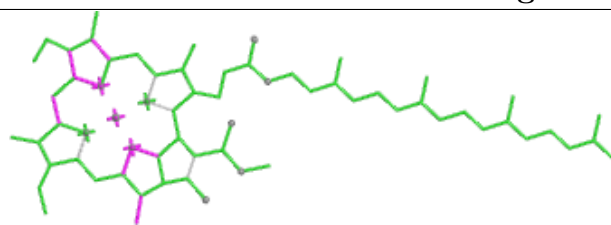


Torsions

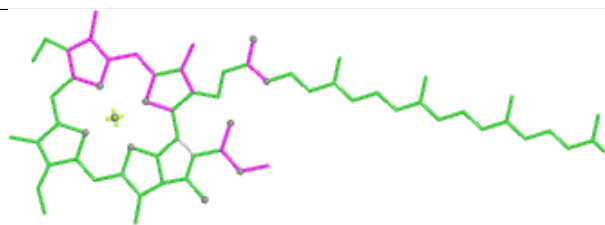


Rings

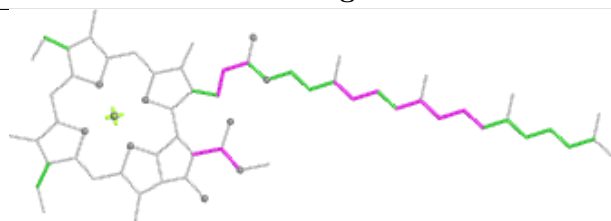
Ligand CLA S 312



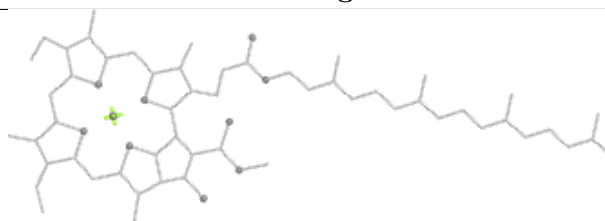
Bond lengths



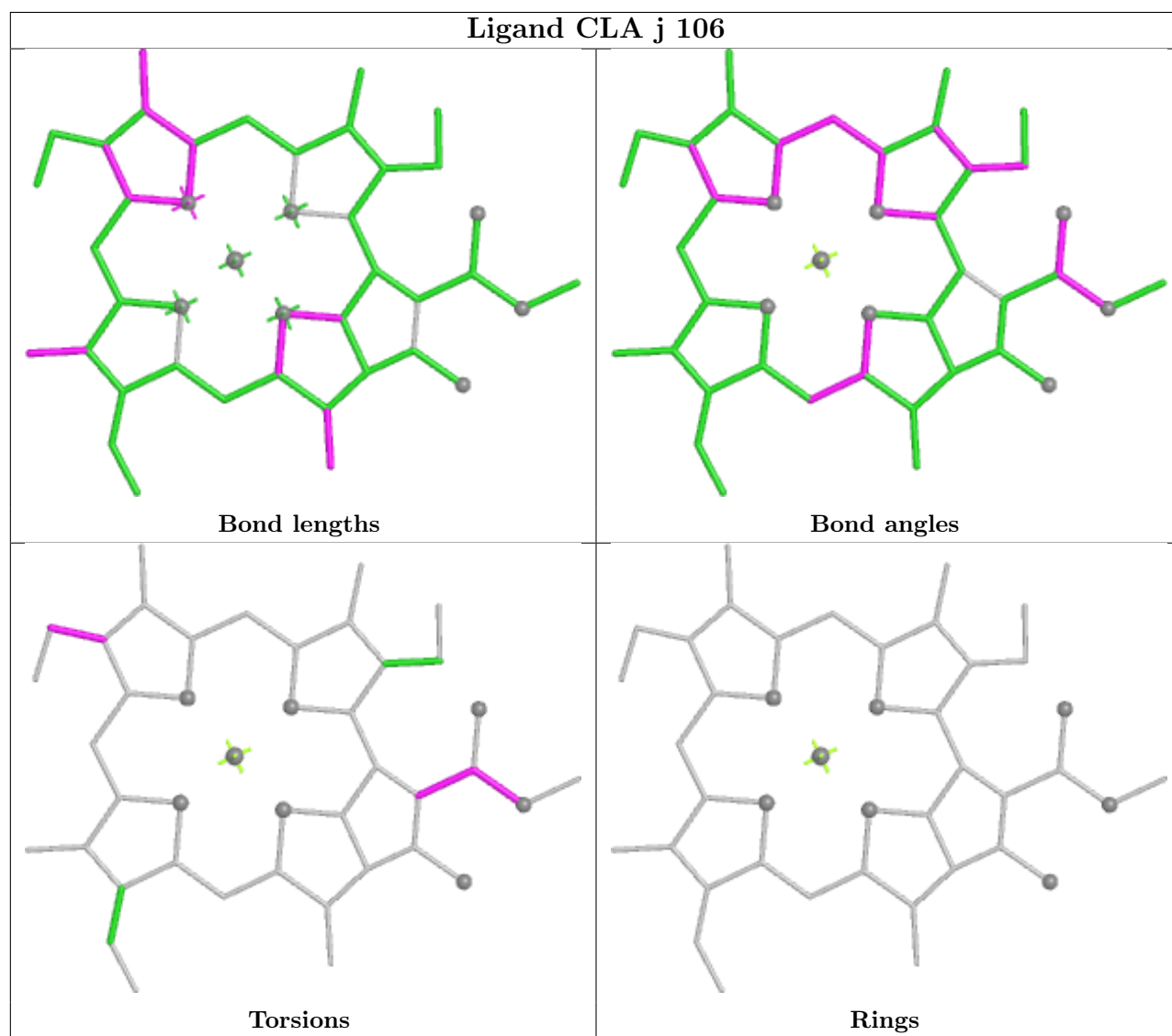
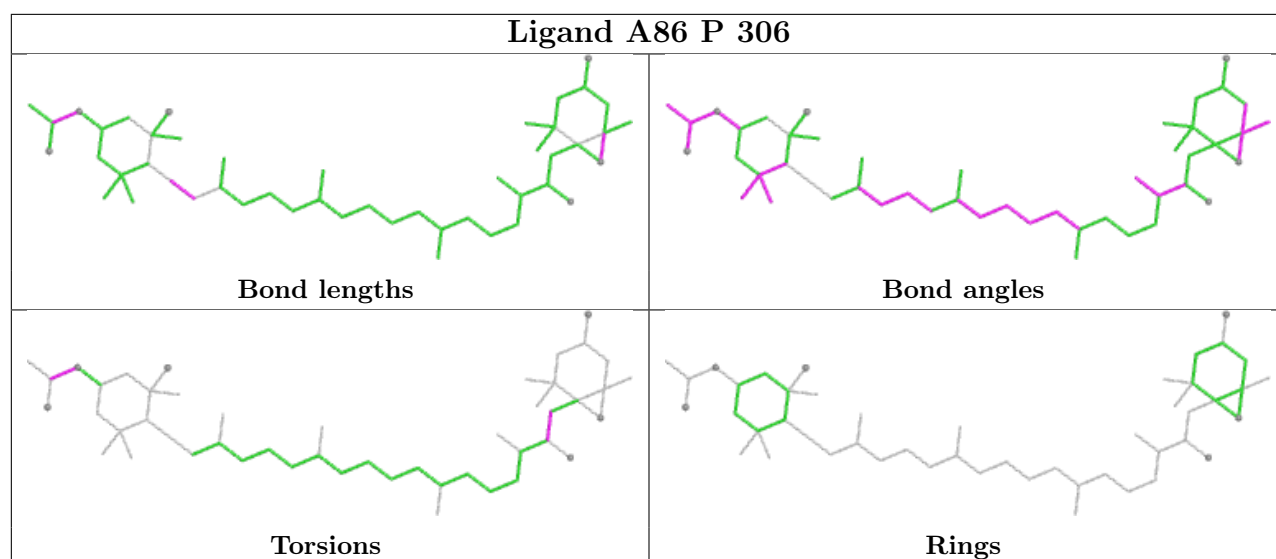
Bond angles



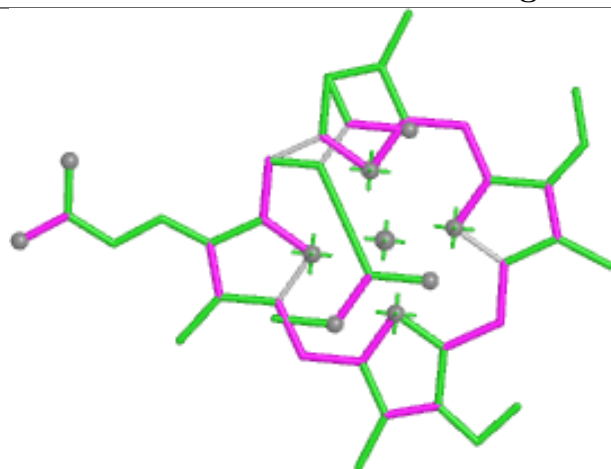
Torsions



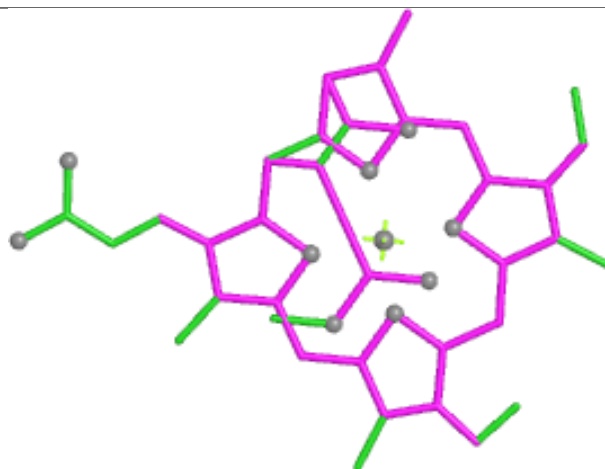
Rings



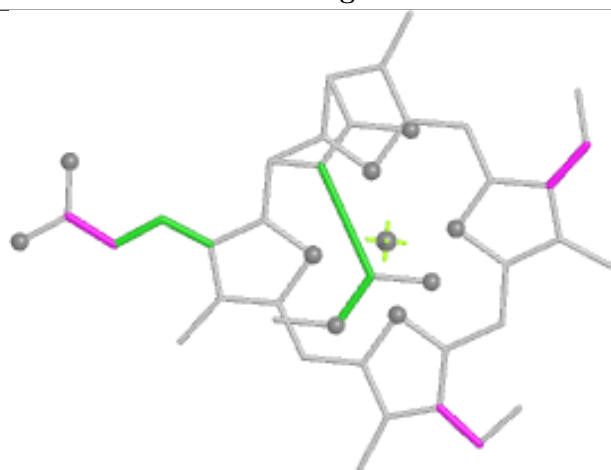
Ligand KC1 J 314



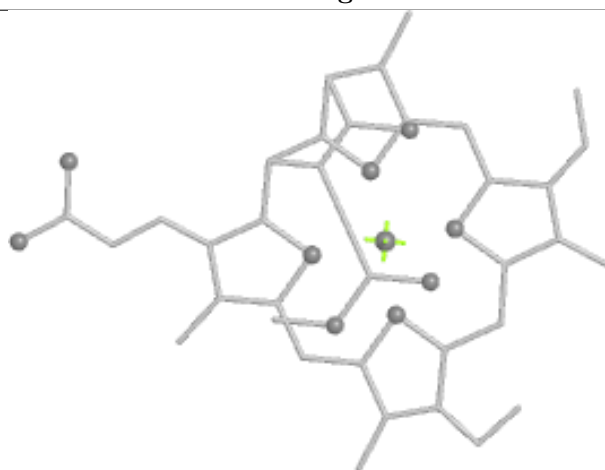
Bond lengths



Bond angles

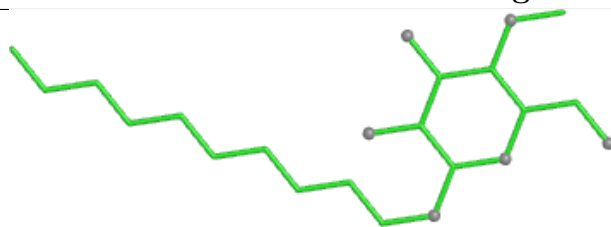


Torsions

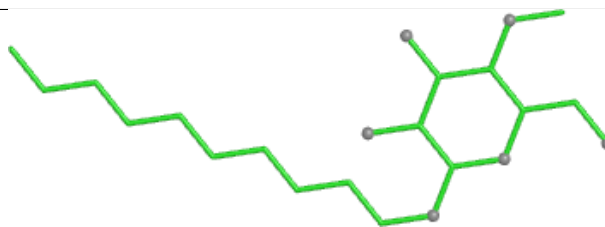


Rings

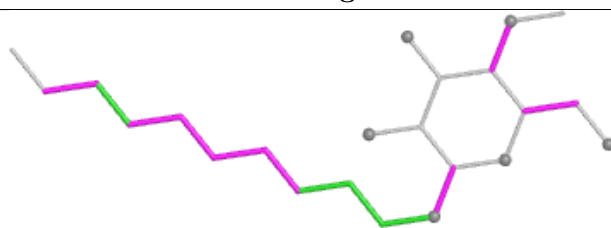
Ligand LMT E 321



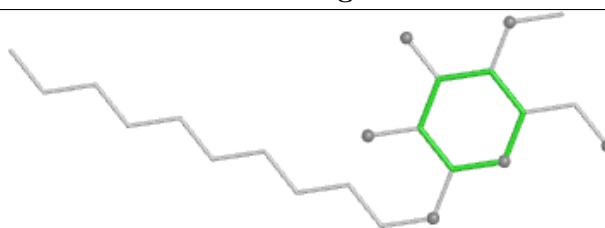
Bond lengths



Bond angles

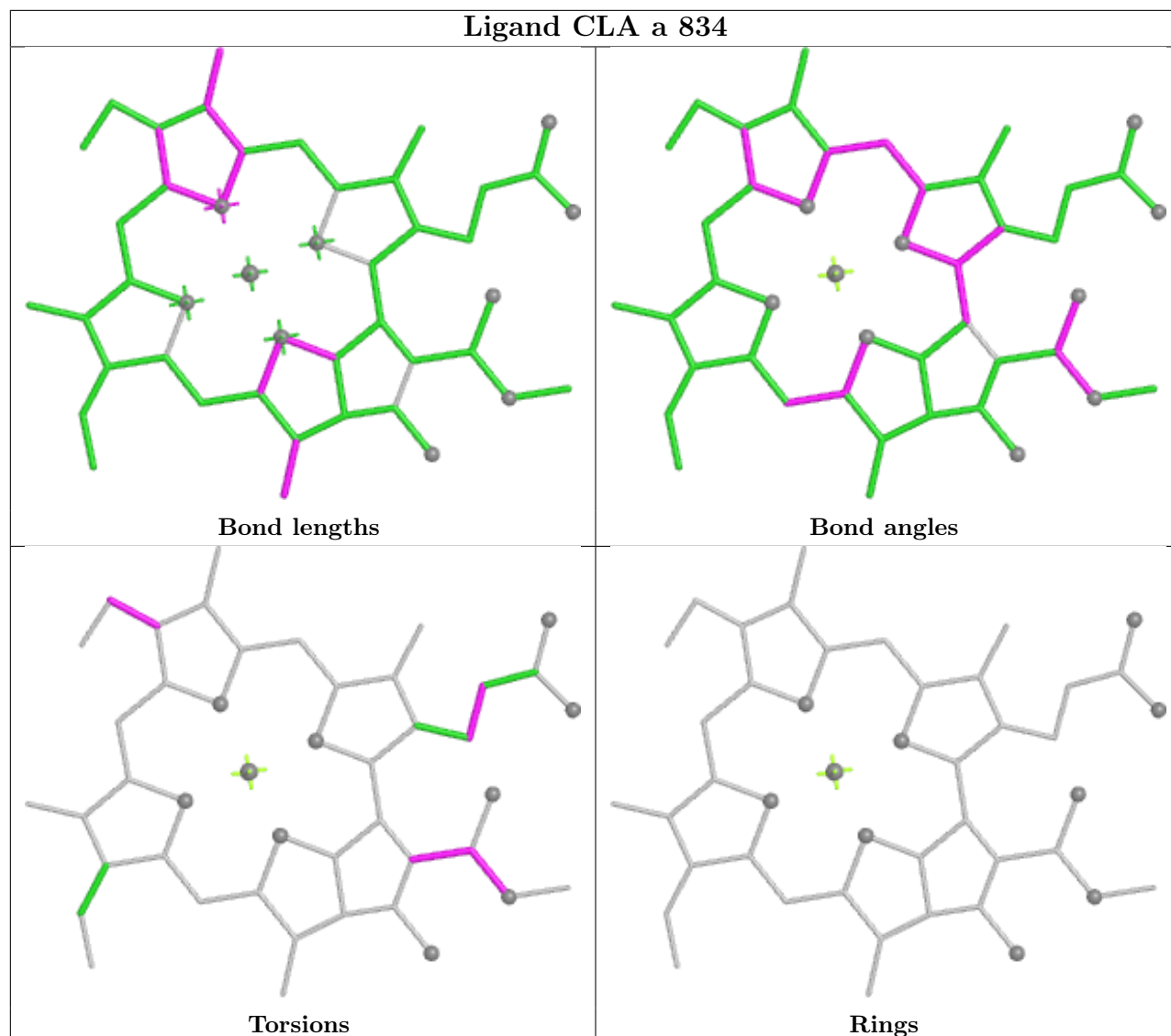


Torsions

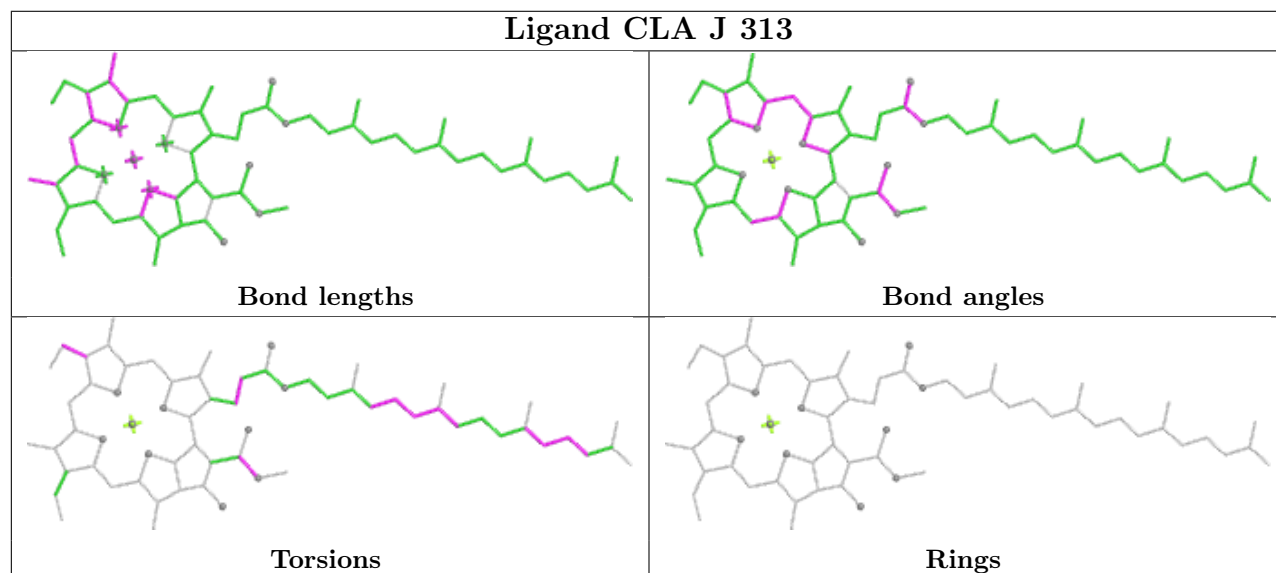


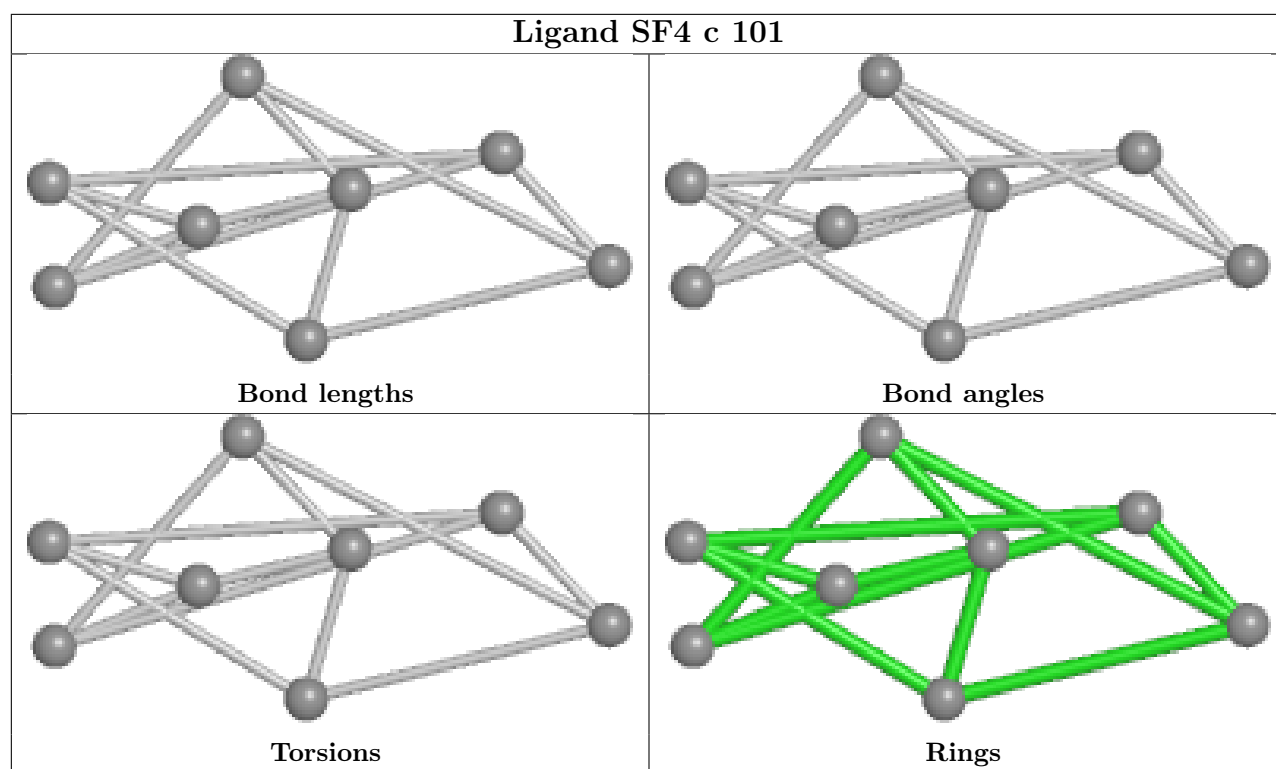
Rings

Ligand CLA a 834

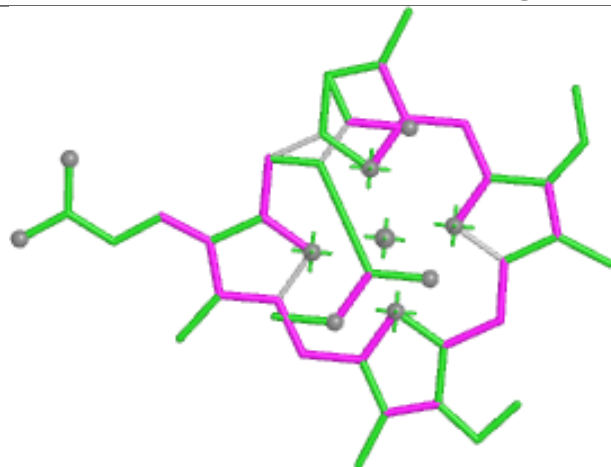


Ligand CLA J 313

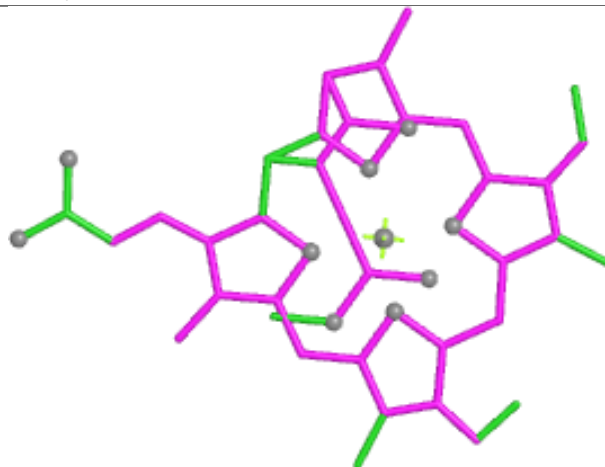




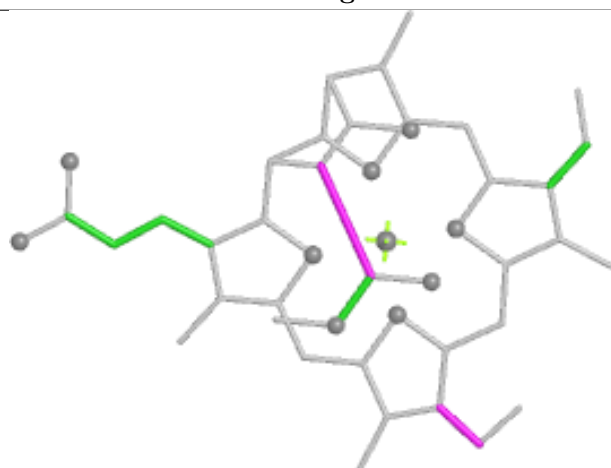
Ligand KC1 Q 311



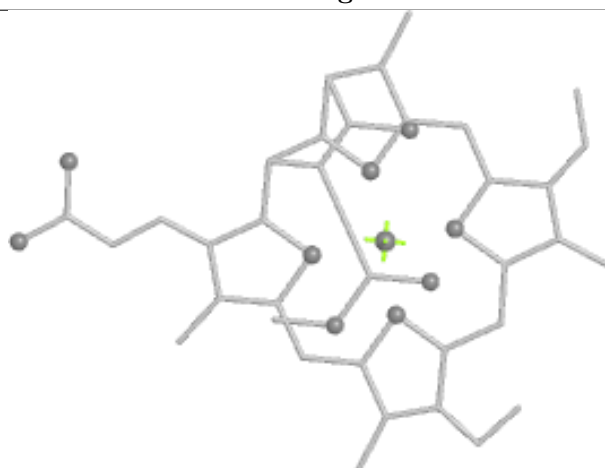
Bond lengths



Bond angles



Torsions

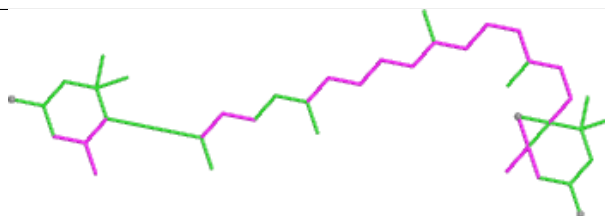


Rings

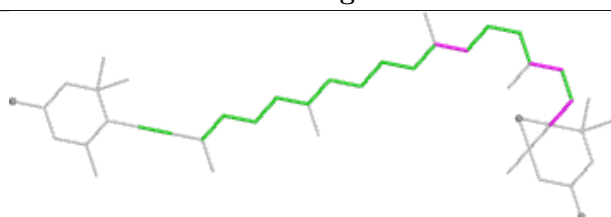
Ligand DD6 a 849



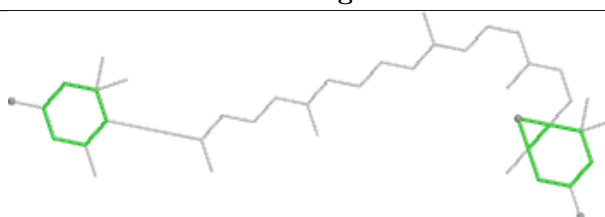
Bond lengths



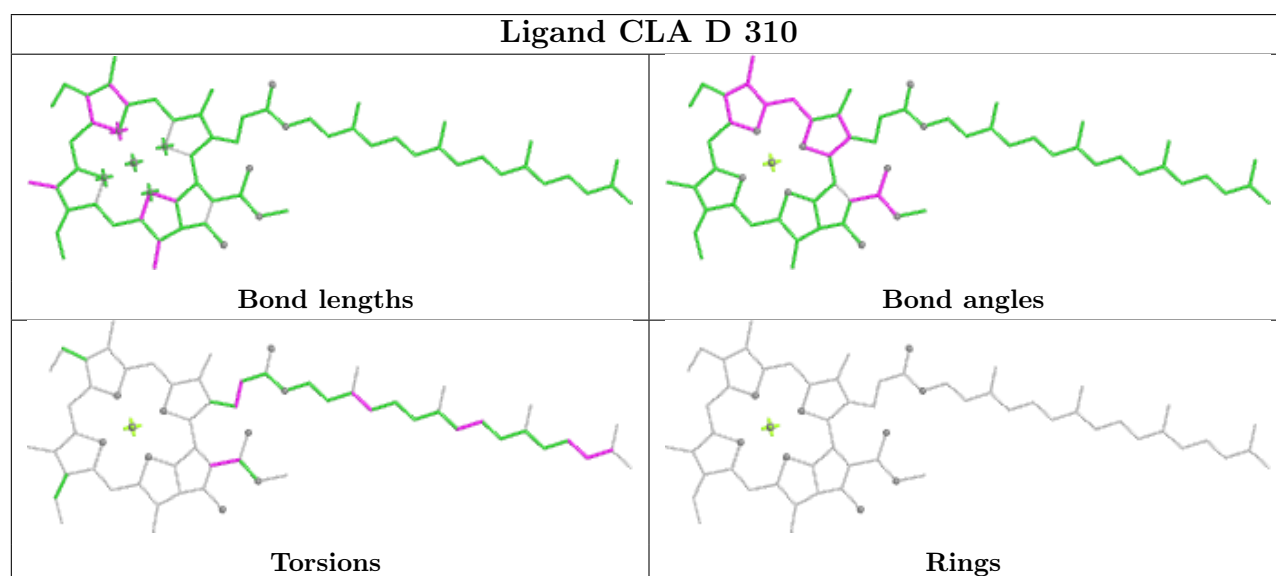
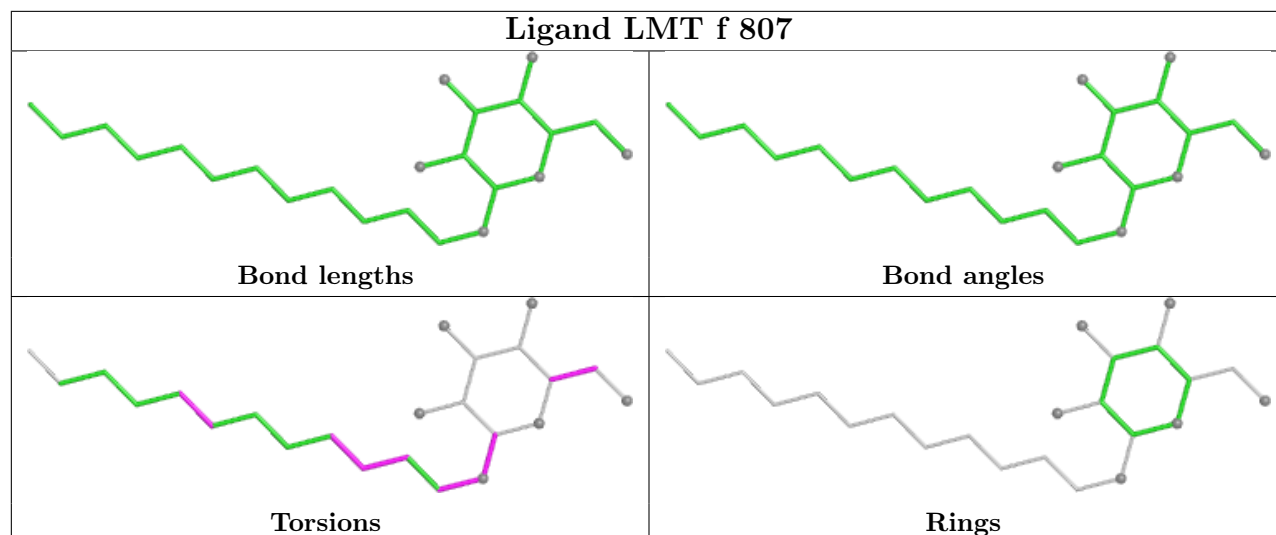
Bond angles



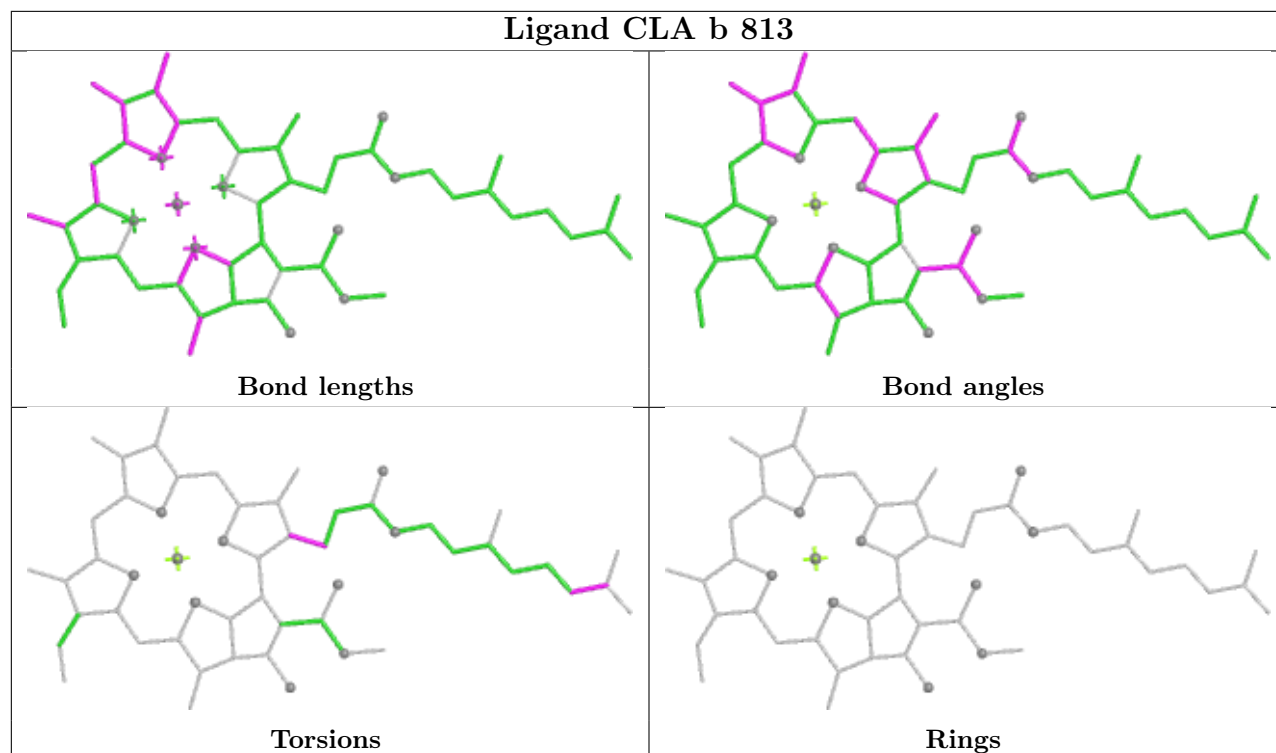
Torsions



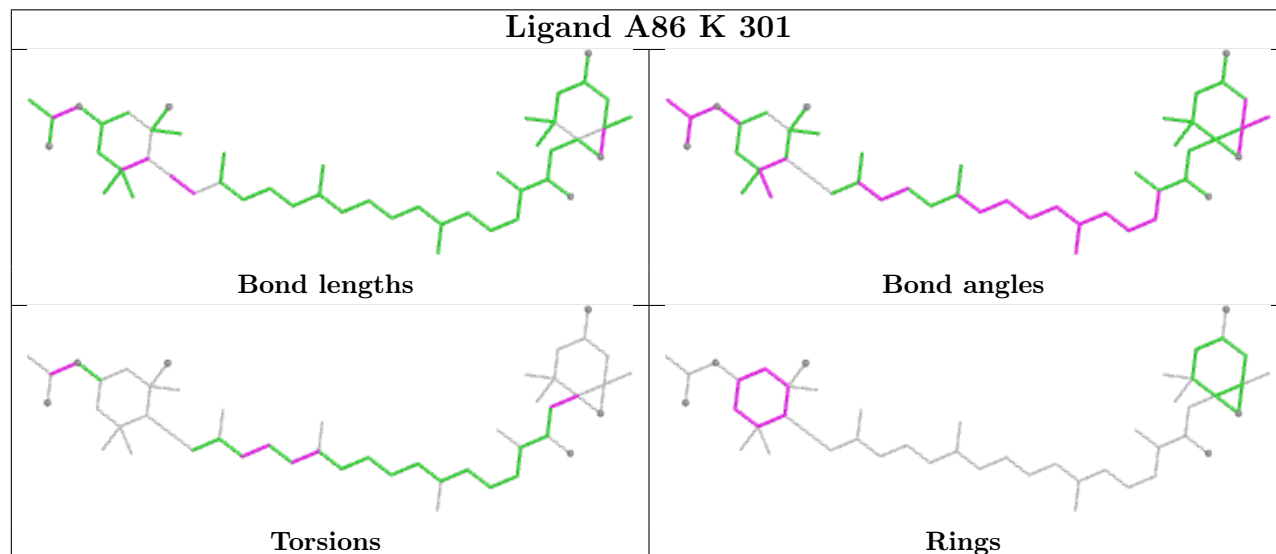
Rings

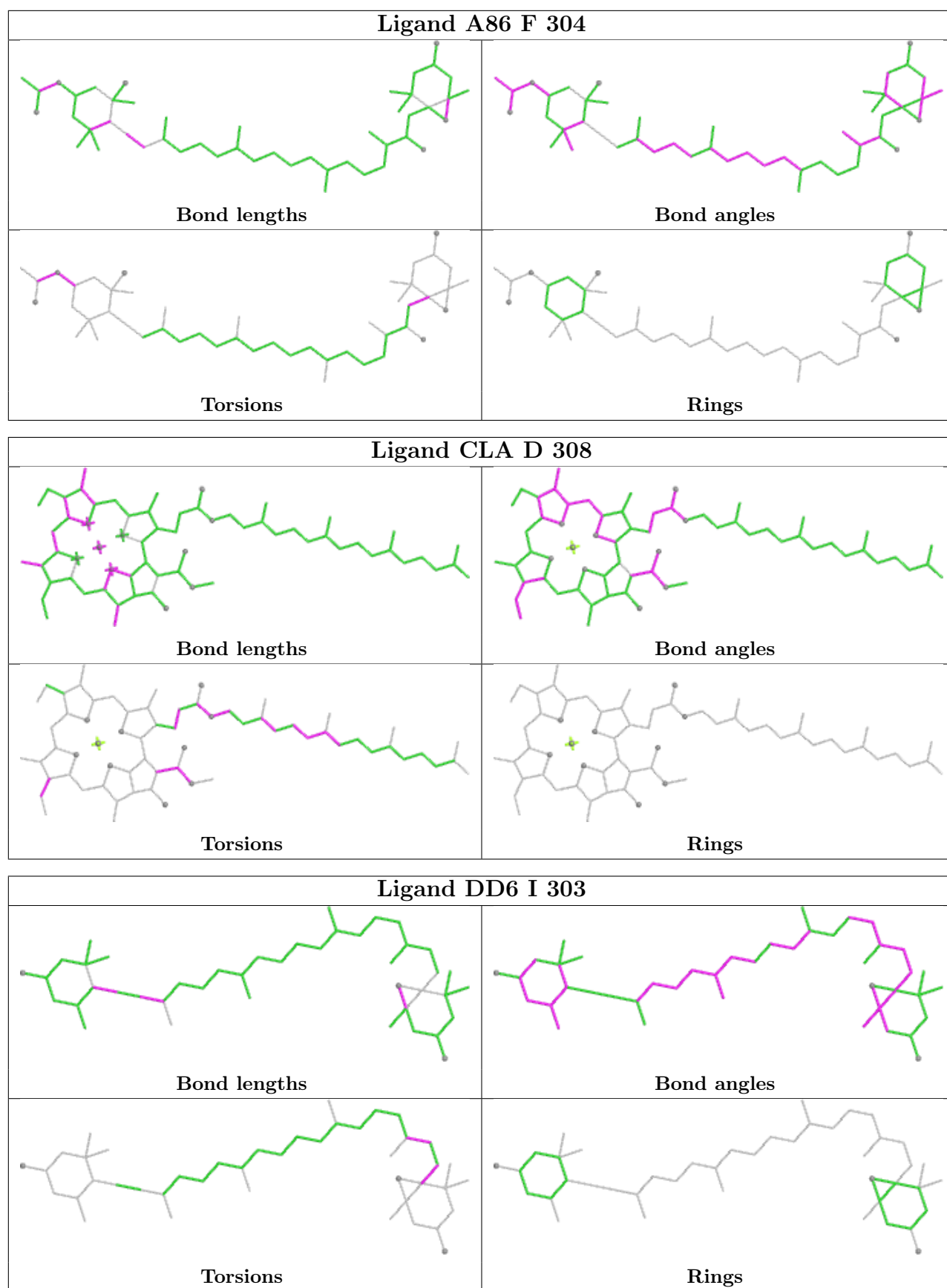


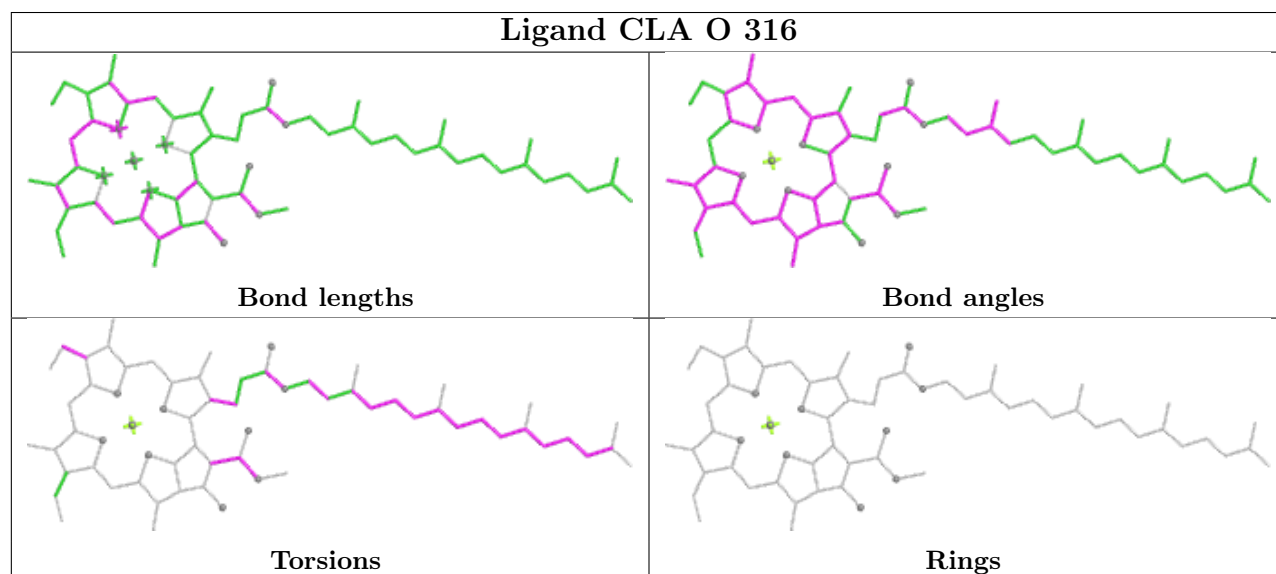
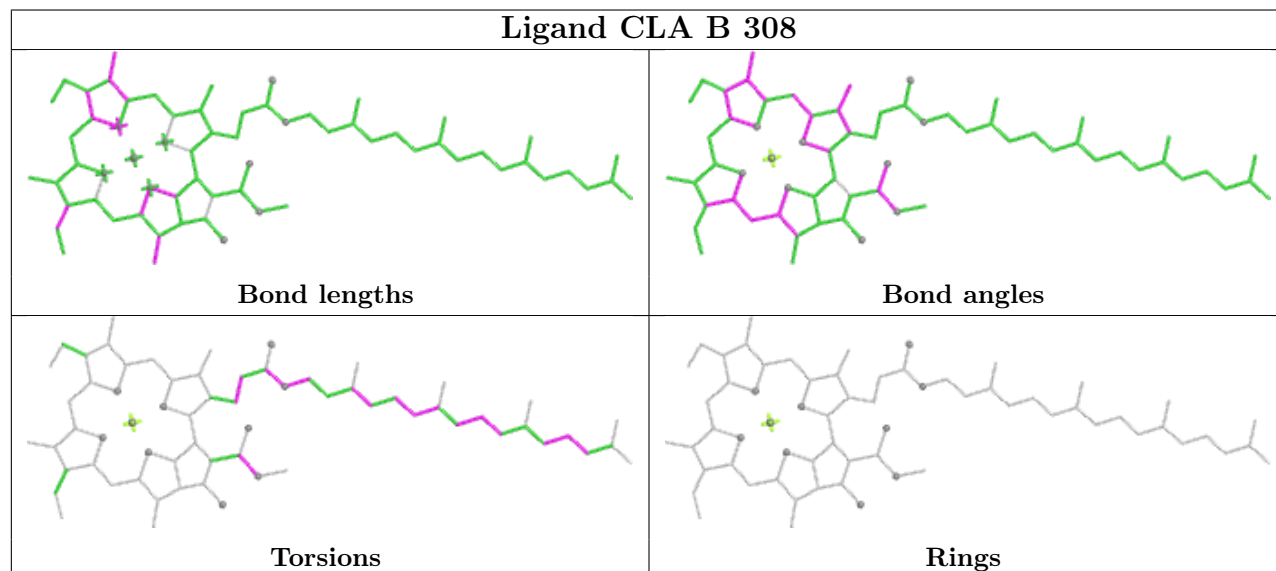
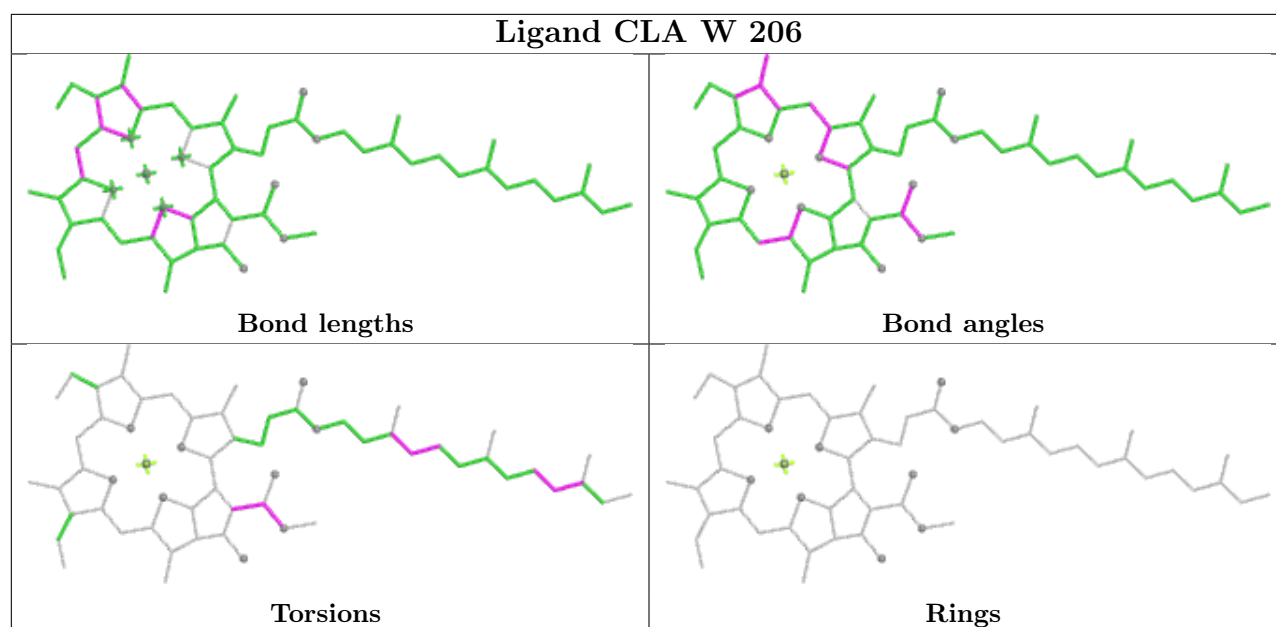
Ligand CLA b 813



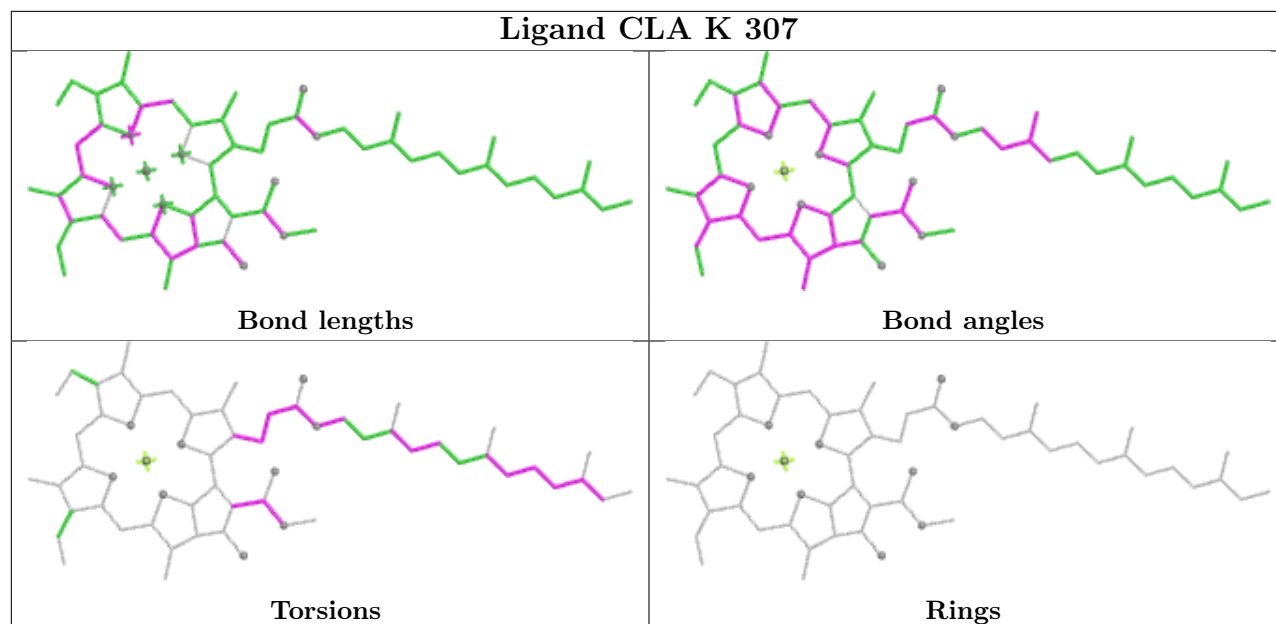
Ligand A86 K 301



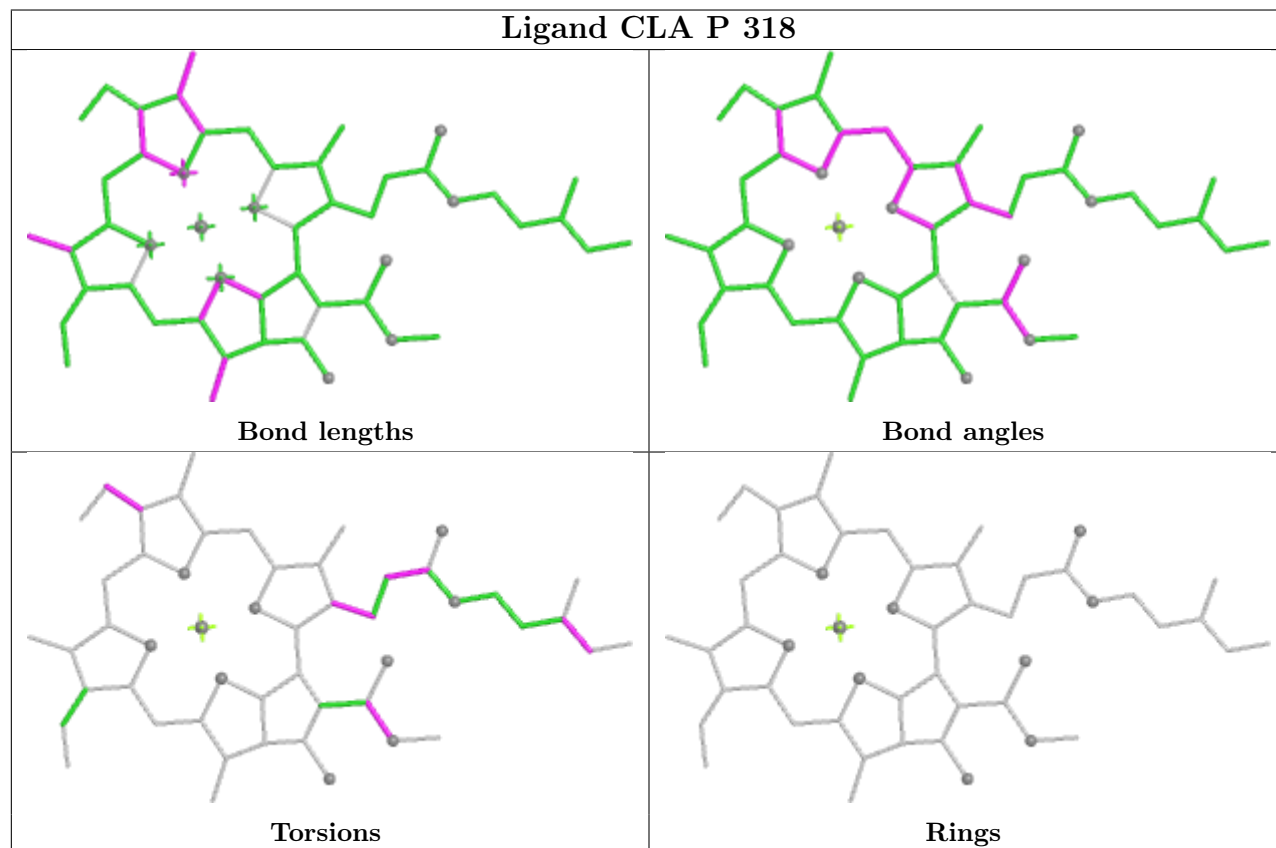


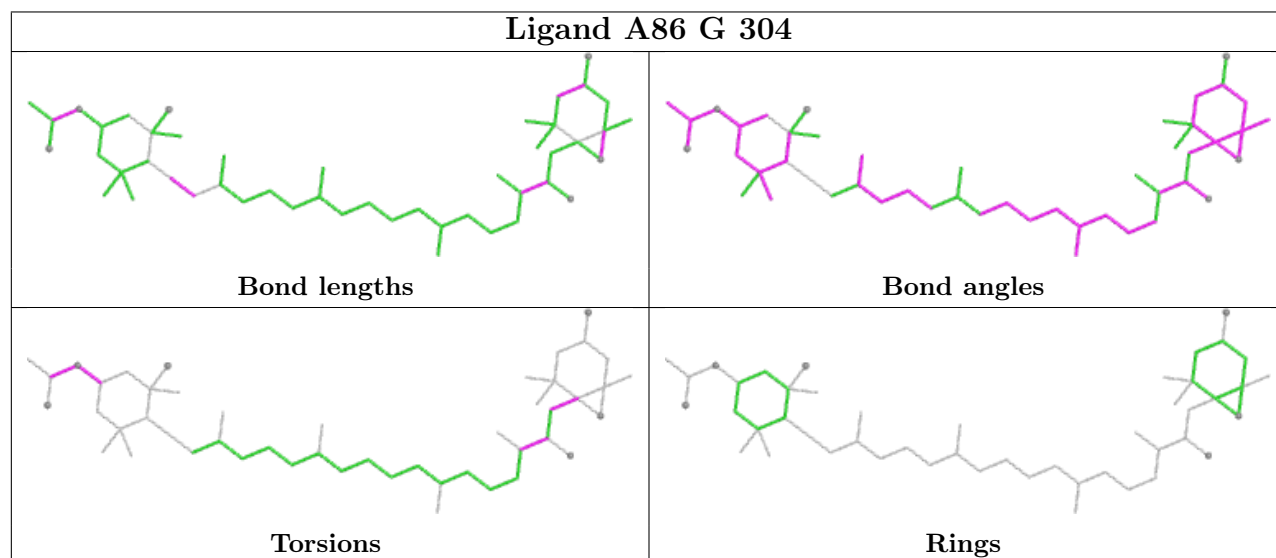
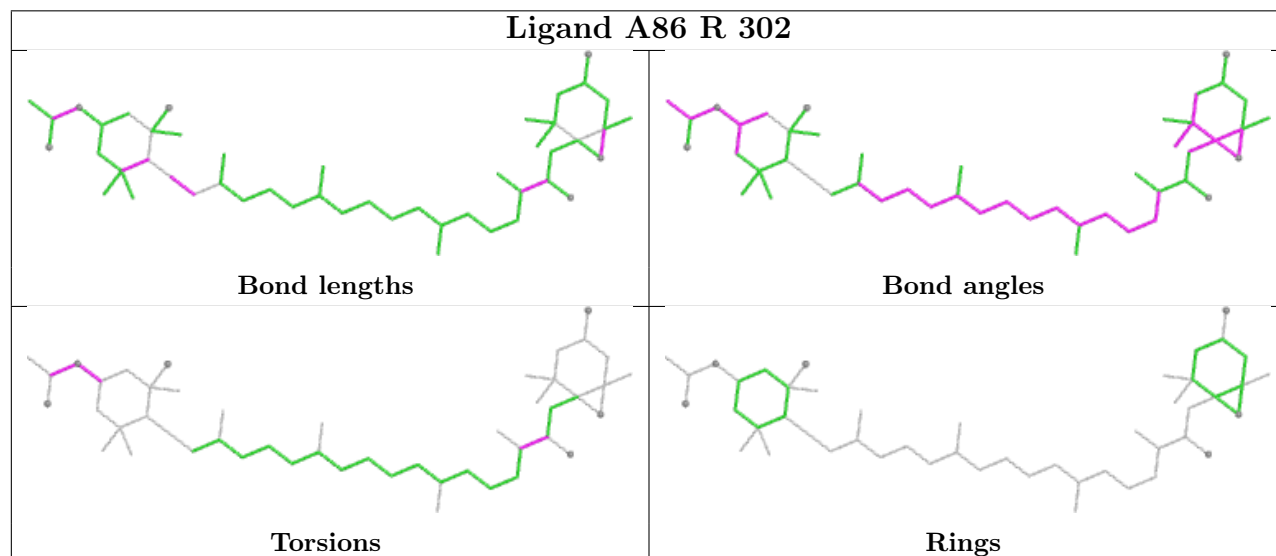
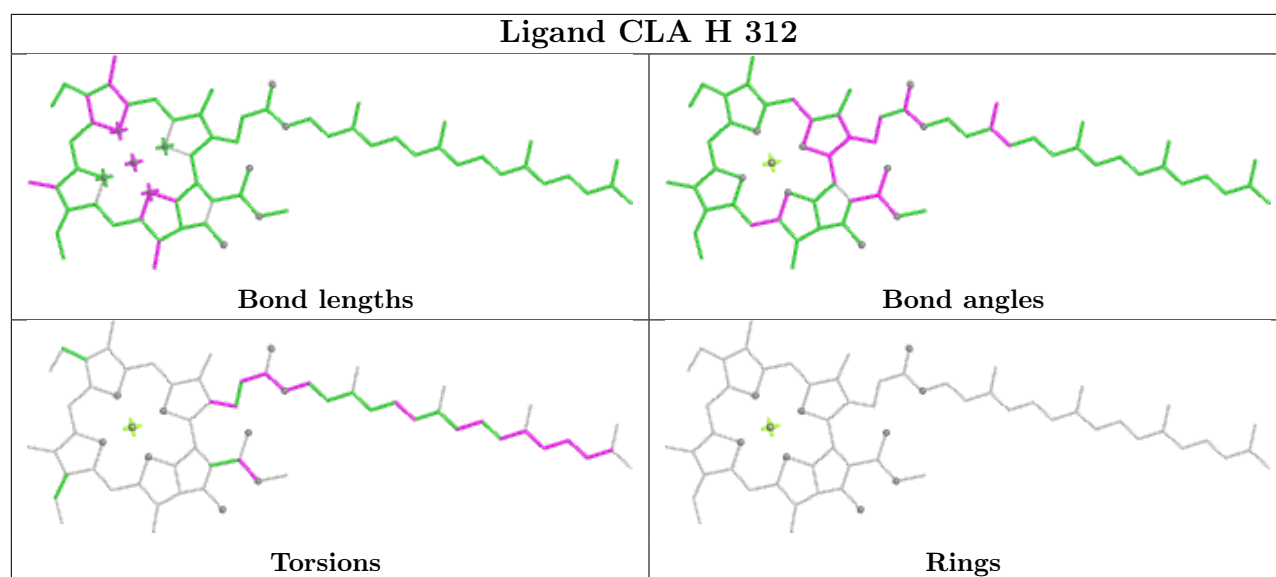


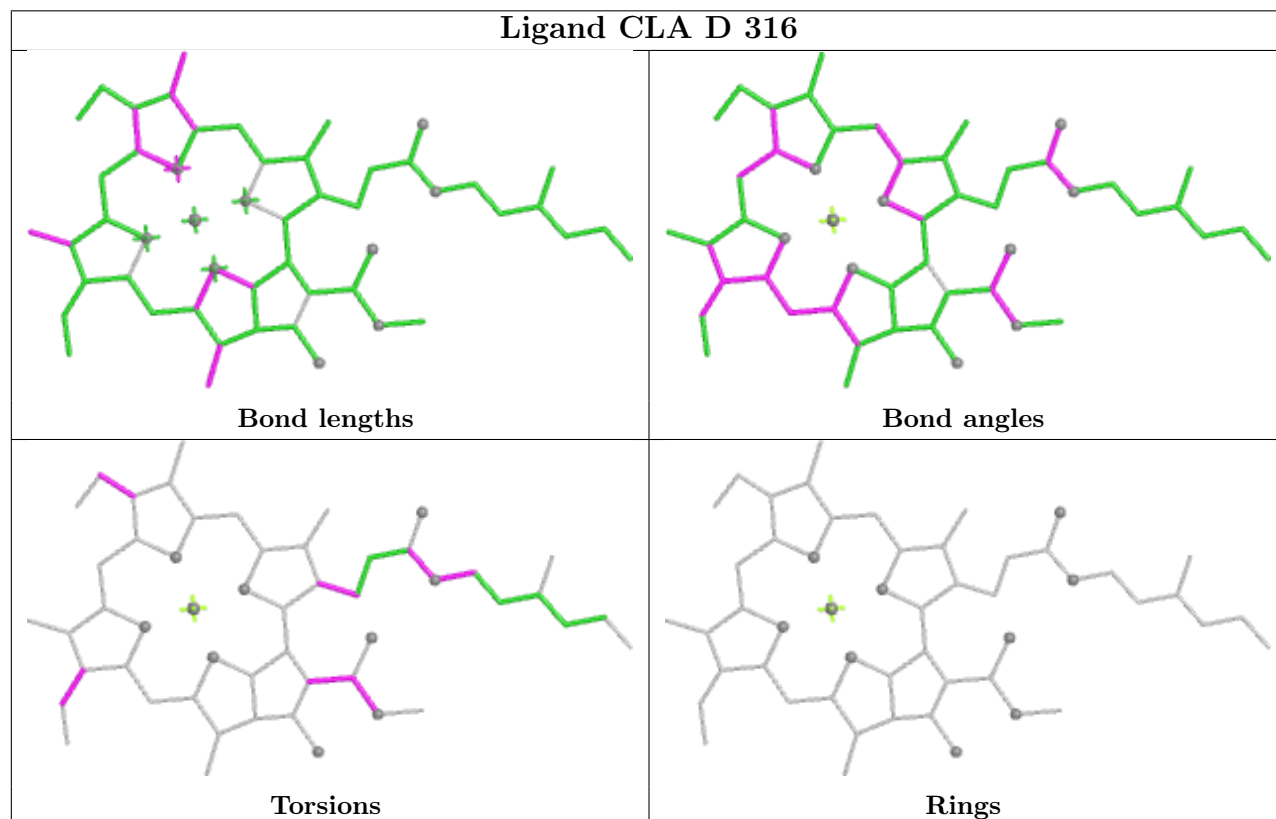
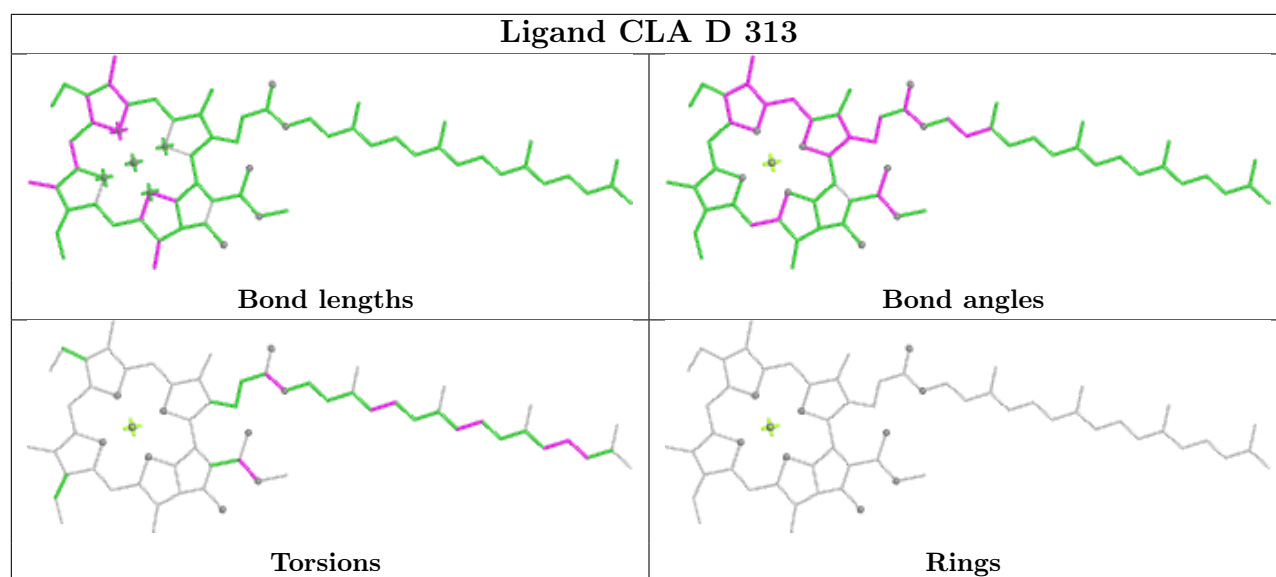
Ligand CLA K 307

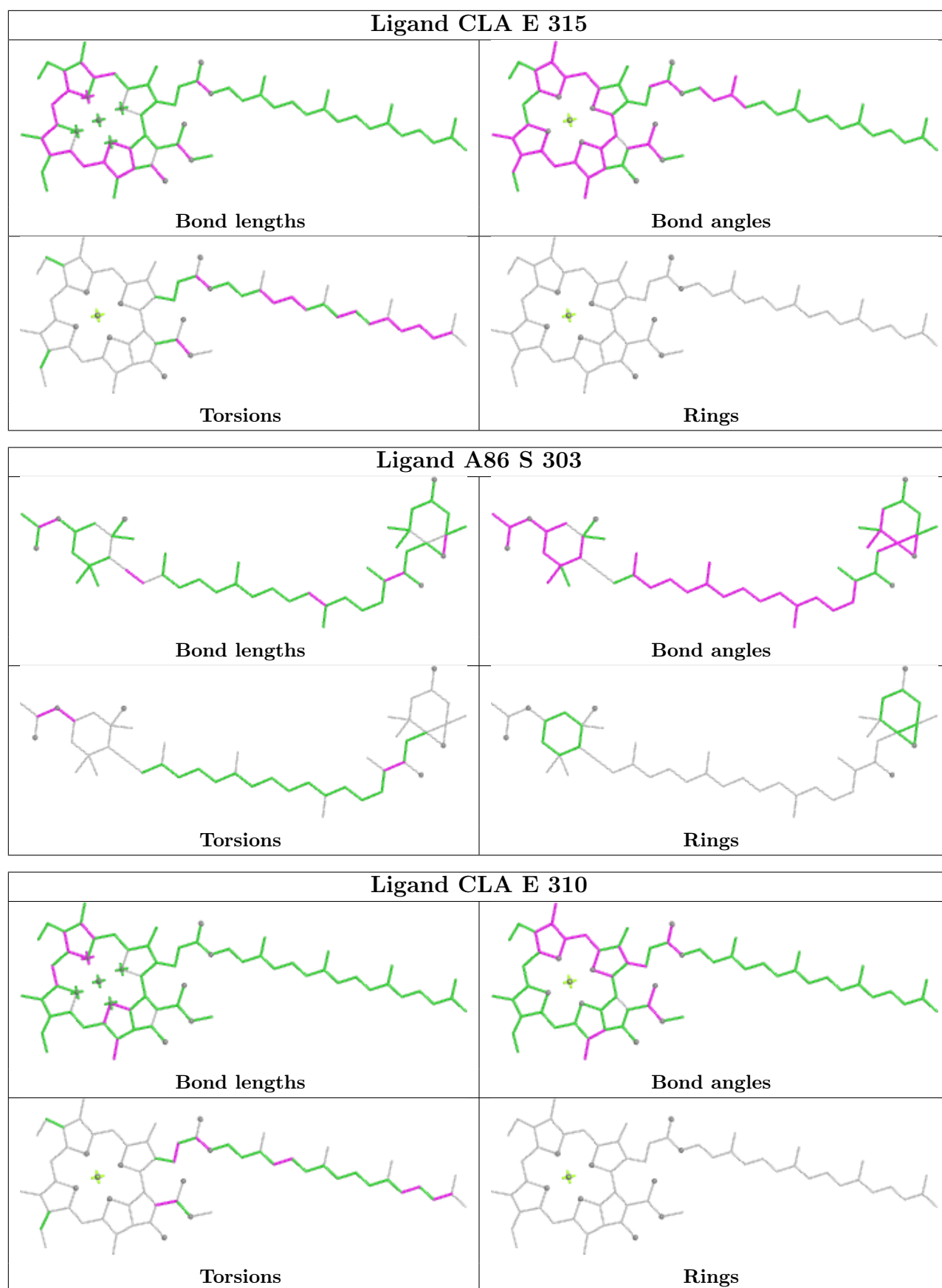


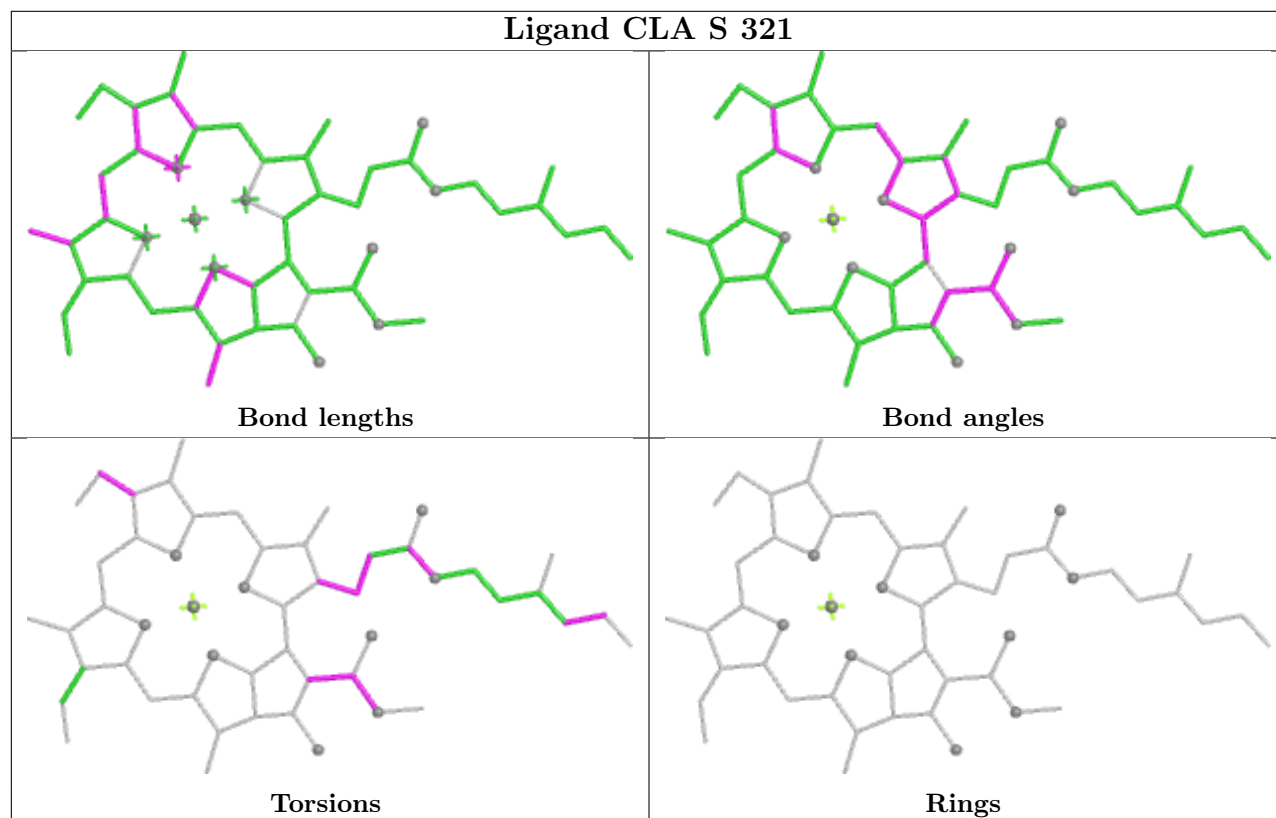
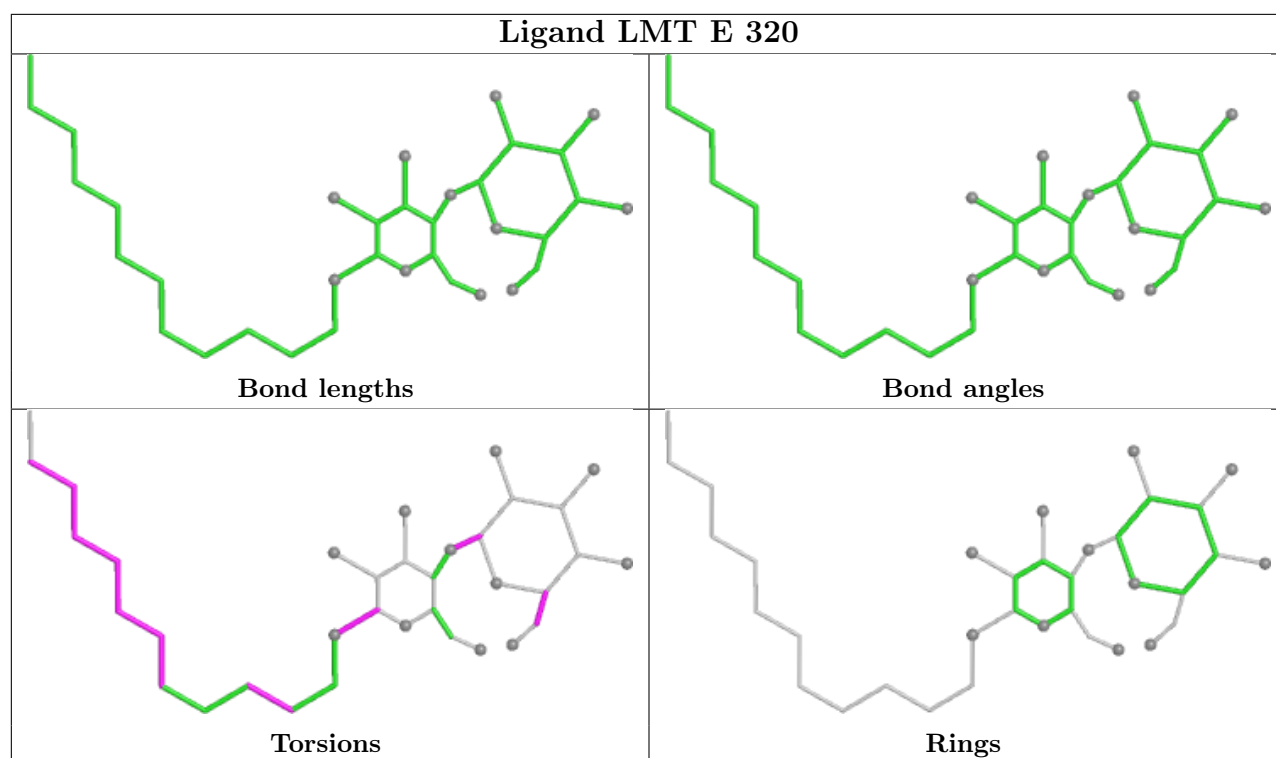
Ligand CLA P 318



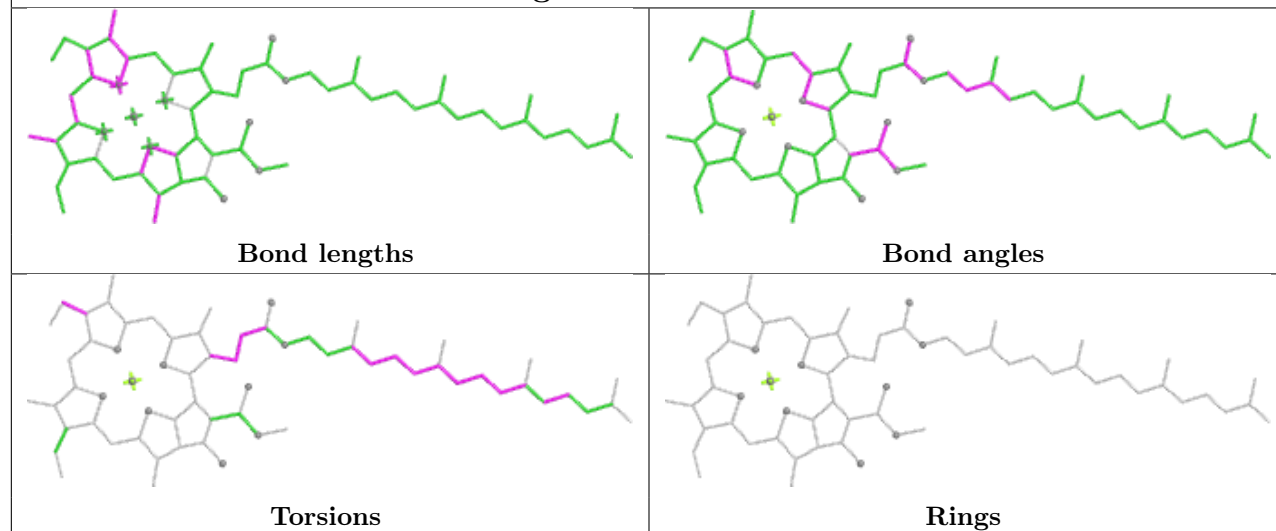




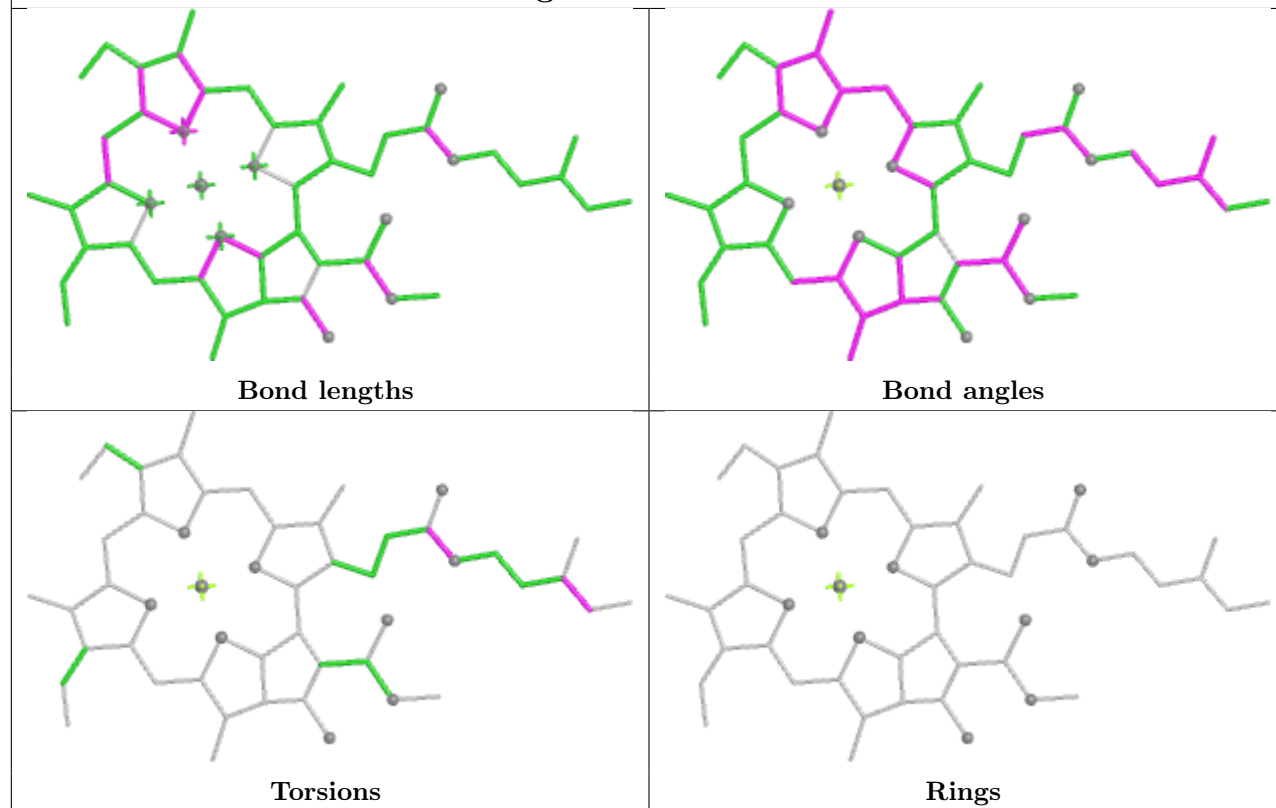




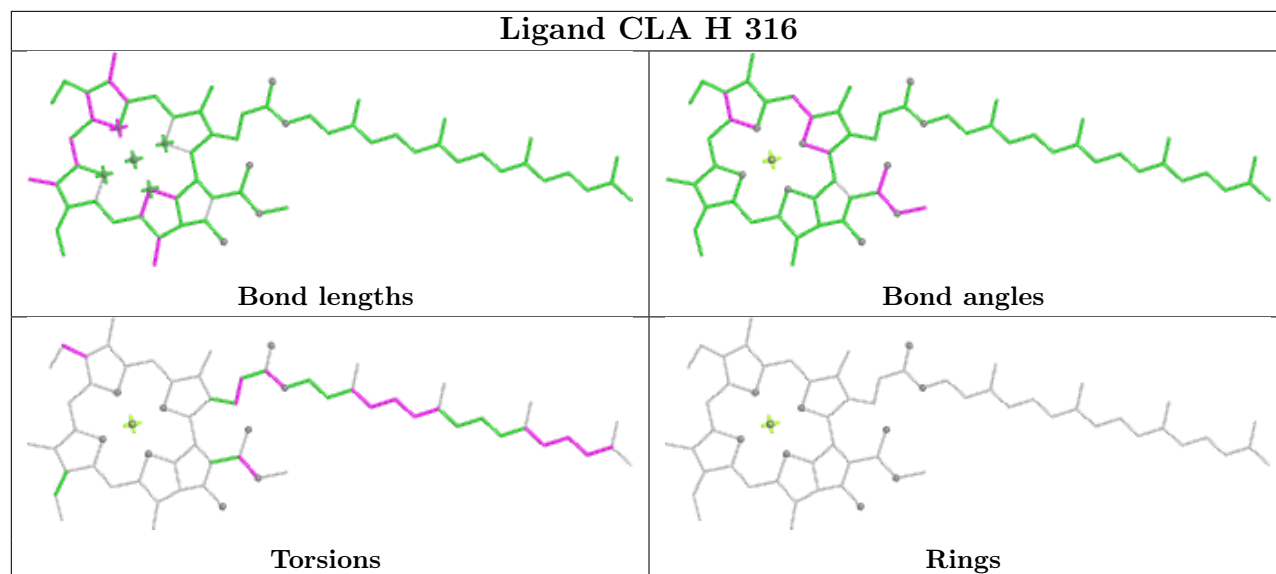
Ligand CLA P 301



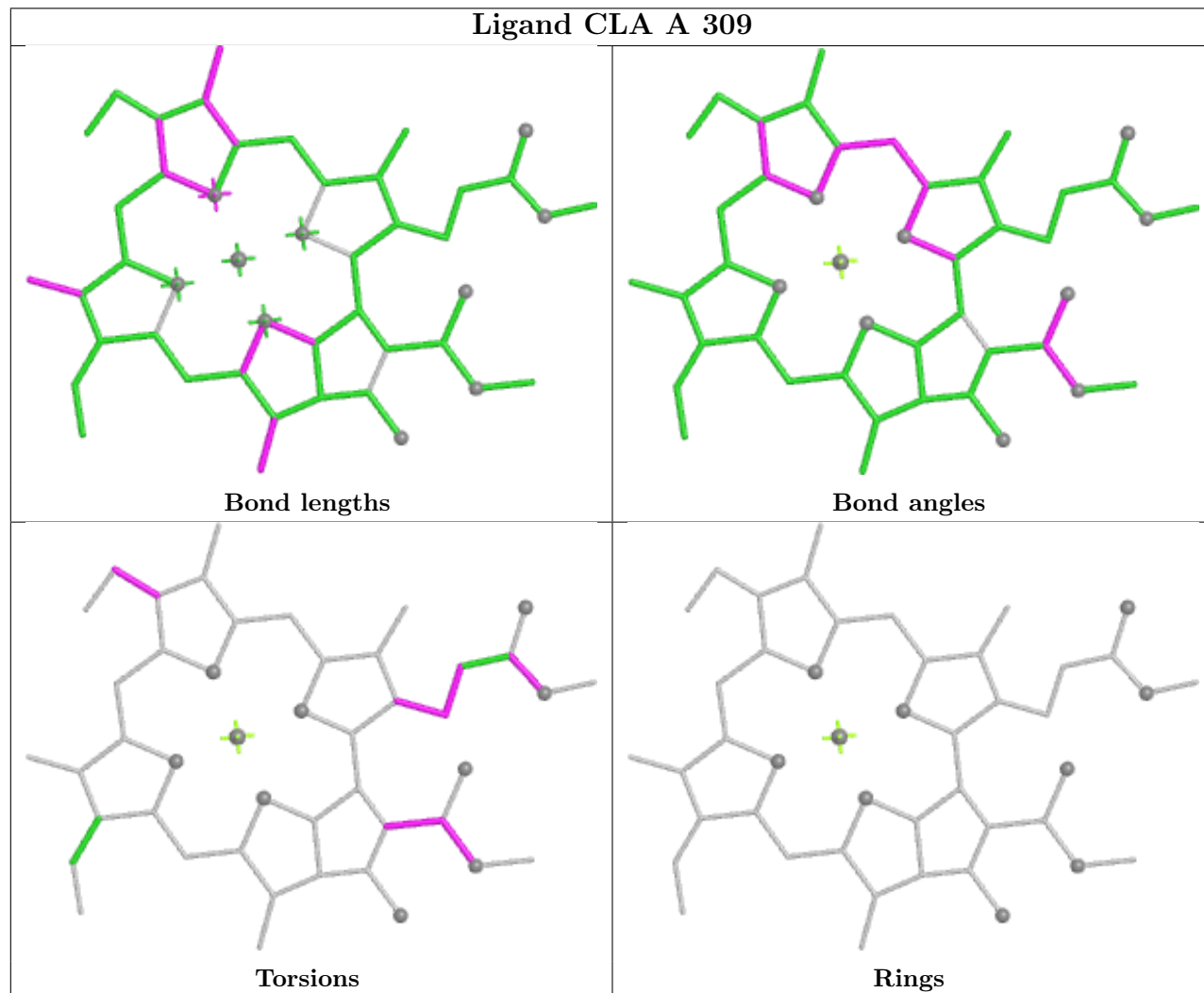
Ligand CLA a 822

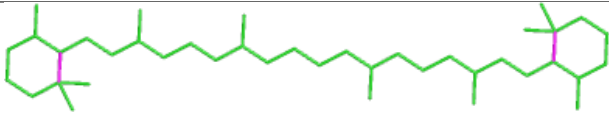
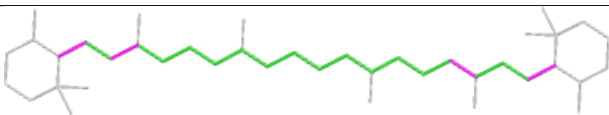
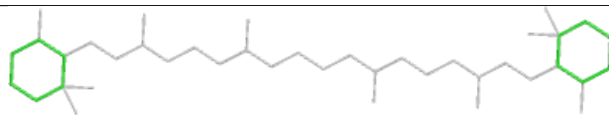


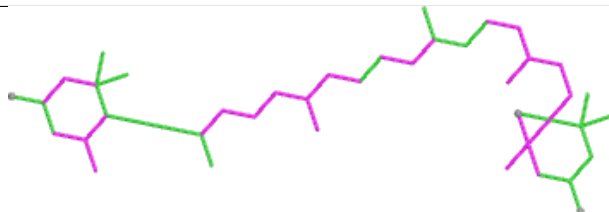
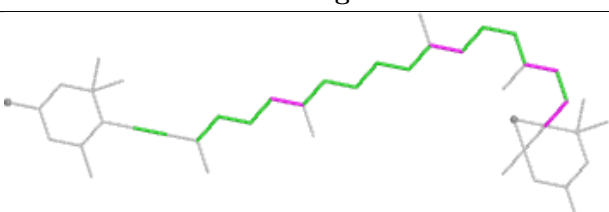
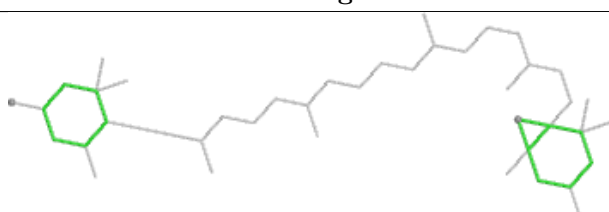
Ligand CLA H 316

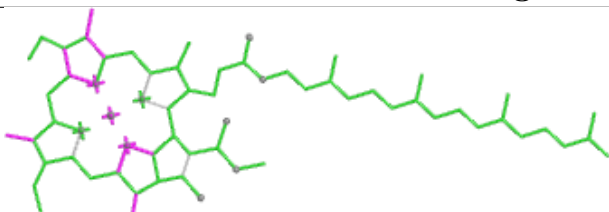
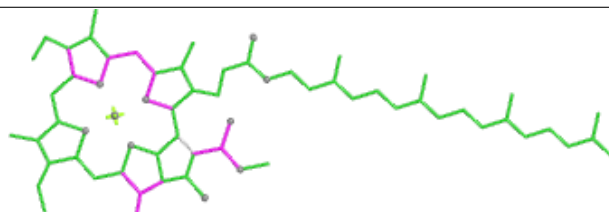
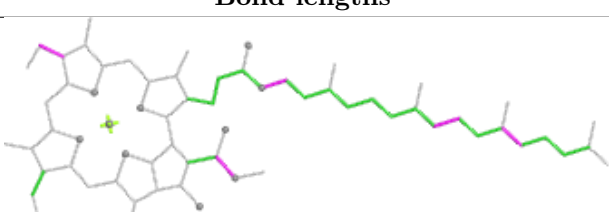
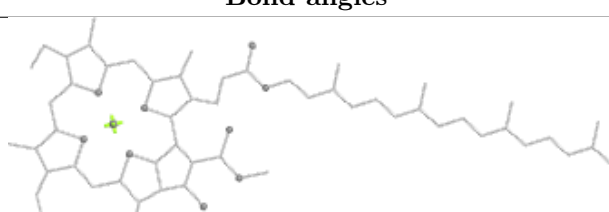


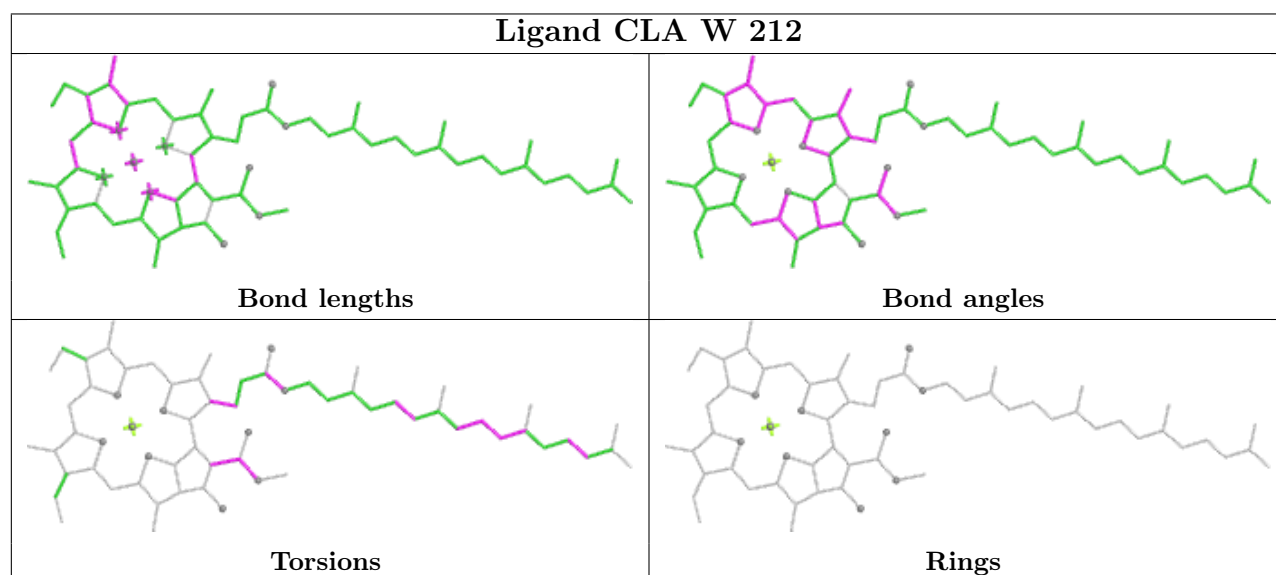
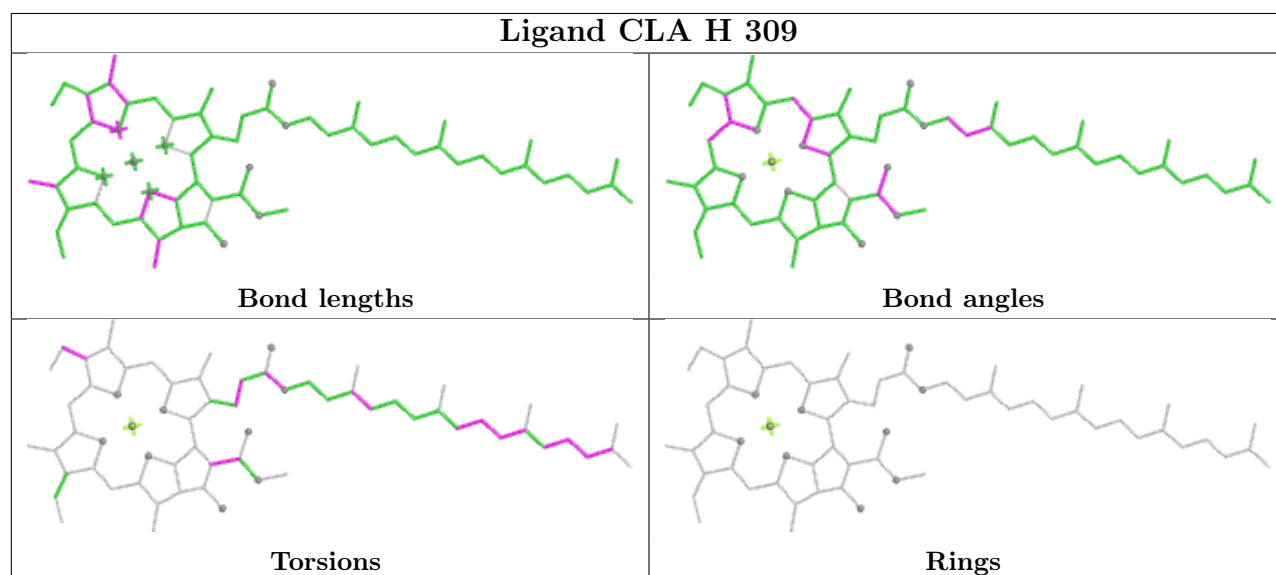
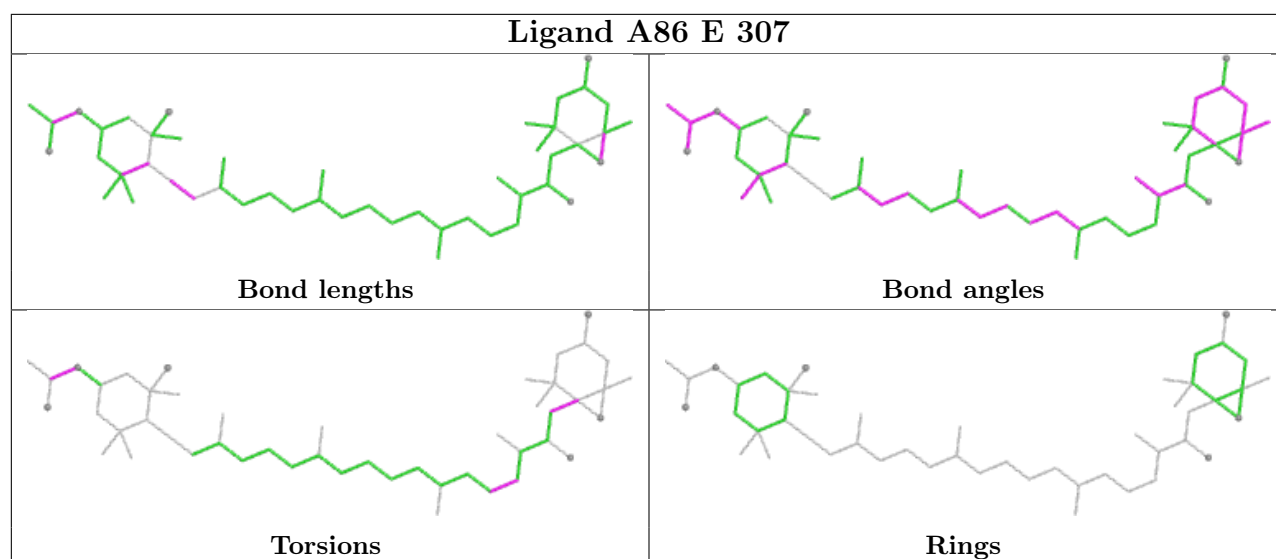
Ligand CLA A 309

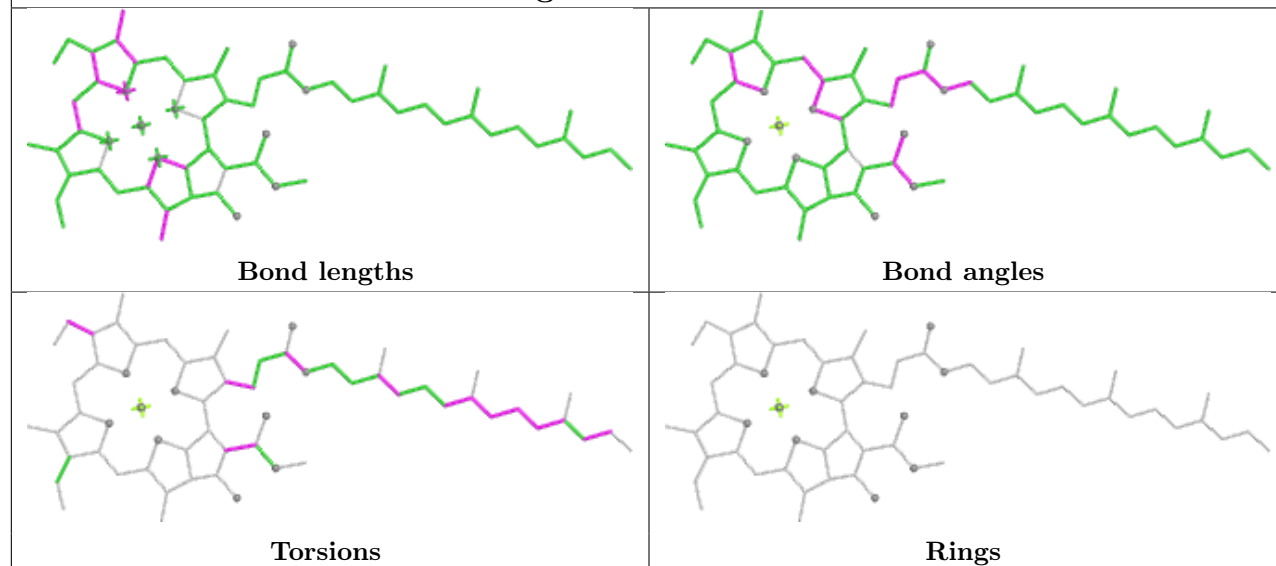
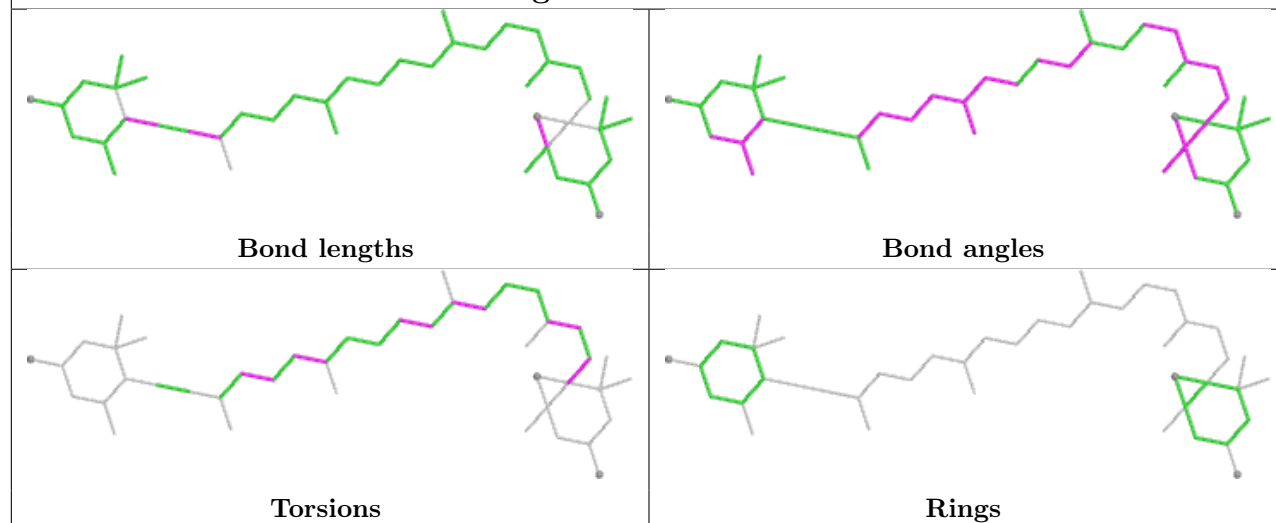


Ligand BCR a 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

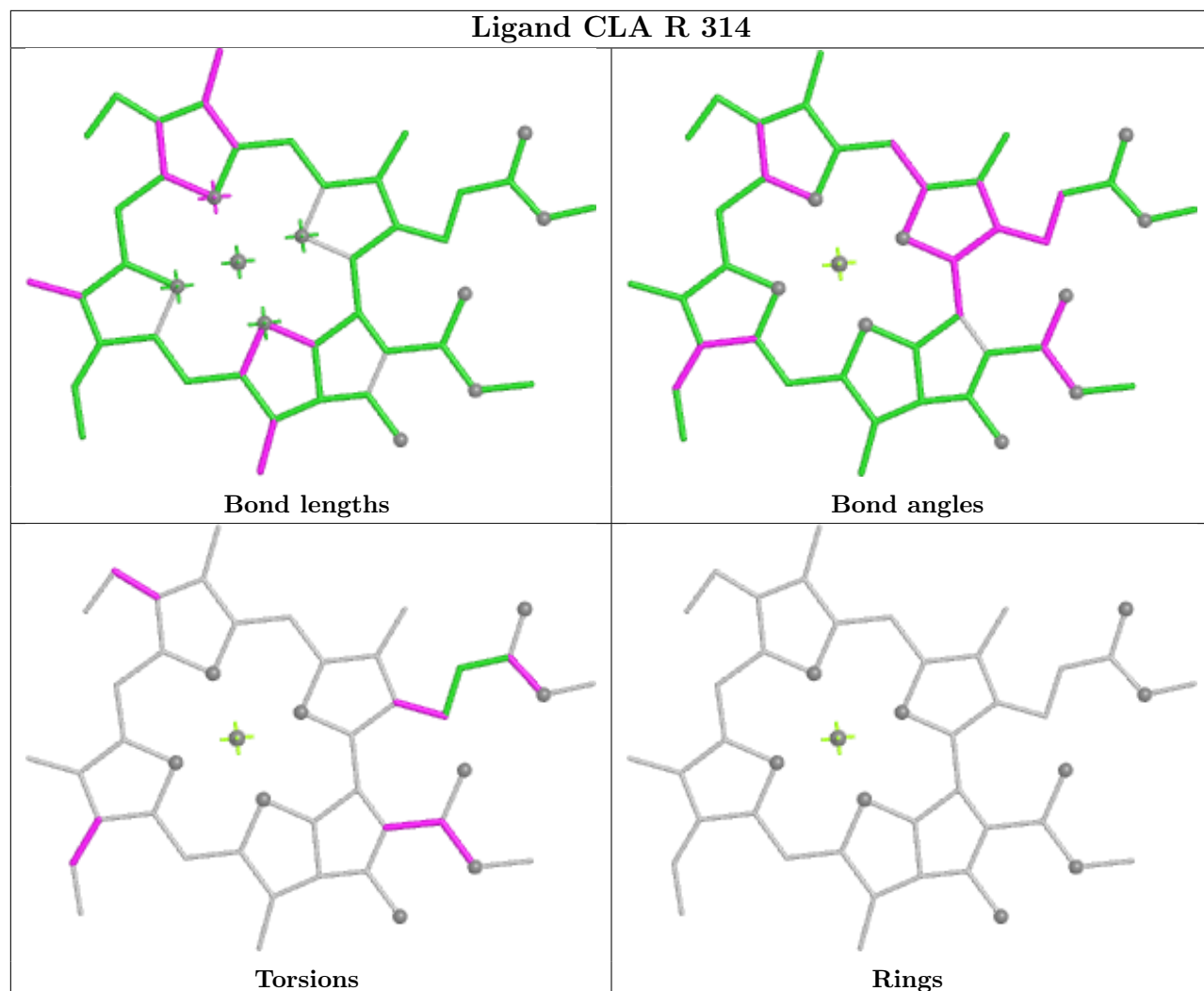
Ligand DD6 W 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

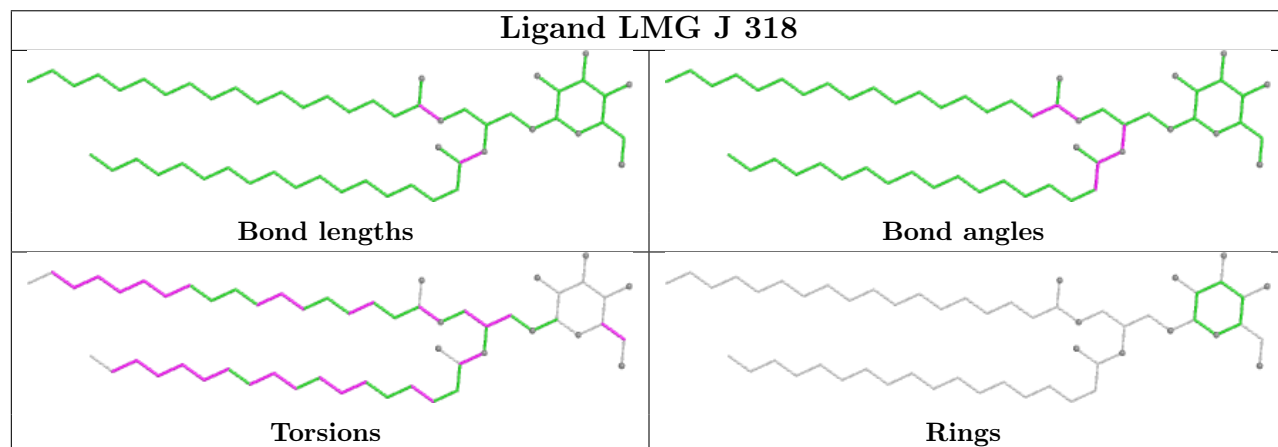


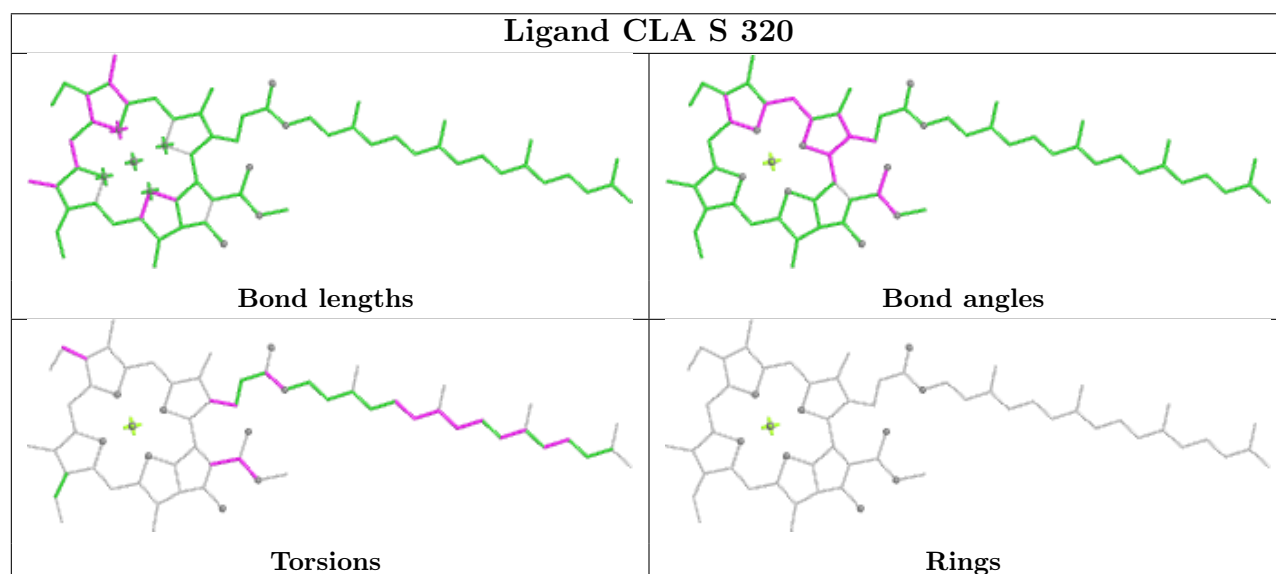
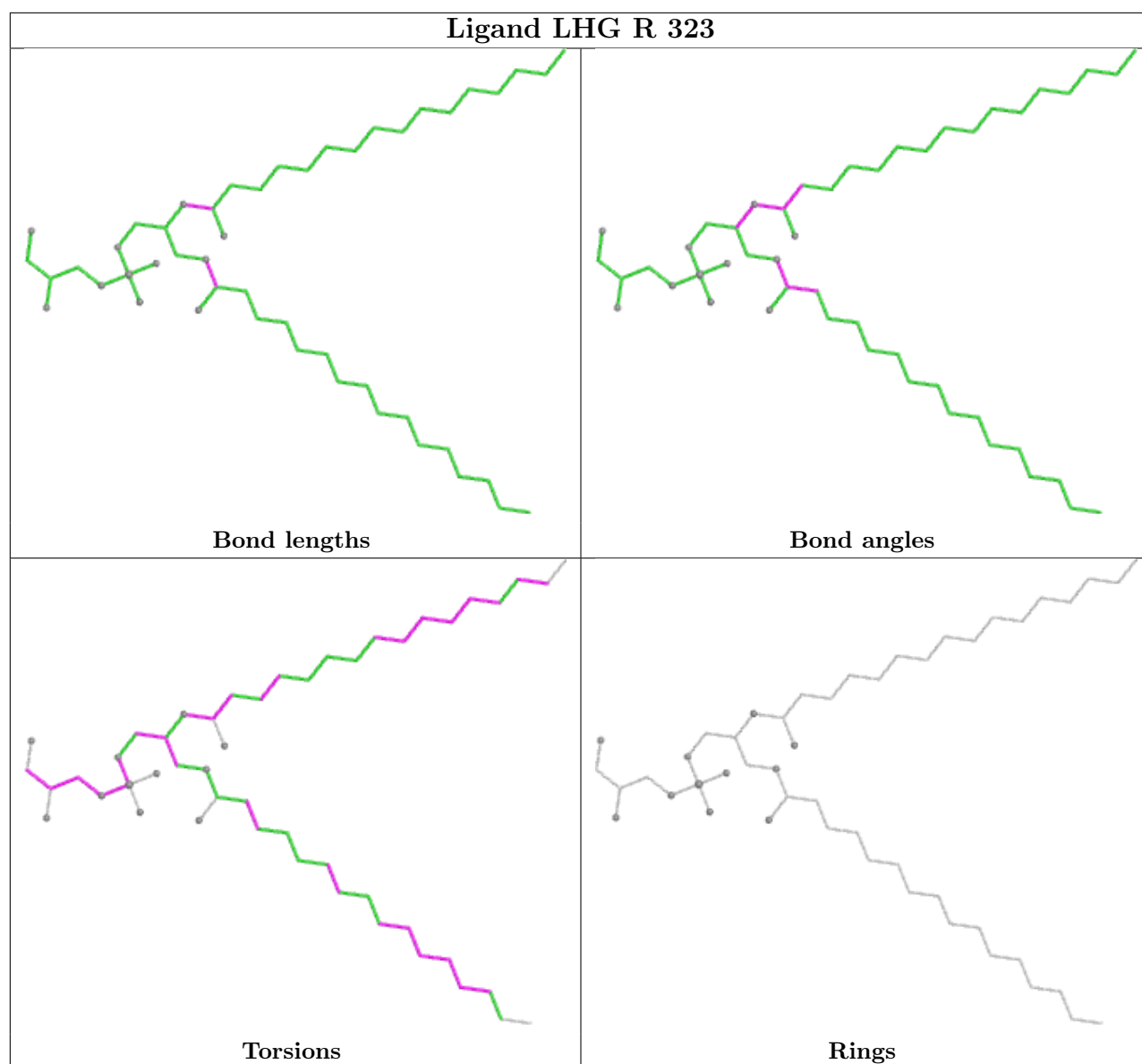
Ligand CLA a 810**Ligand DD6 D 301**

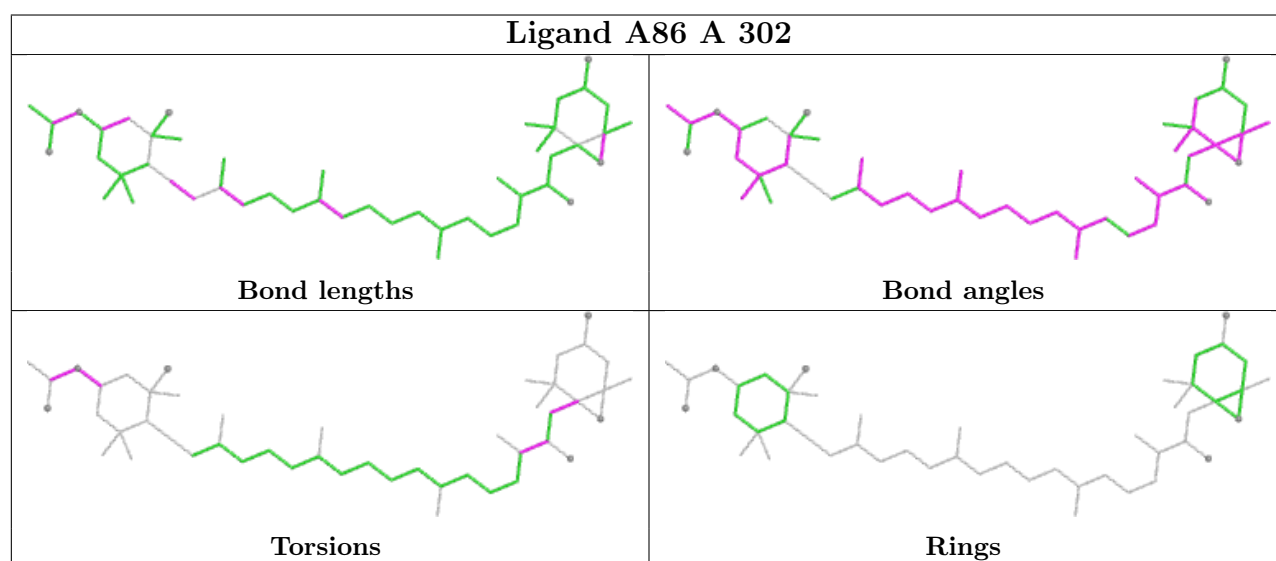
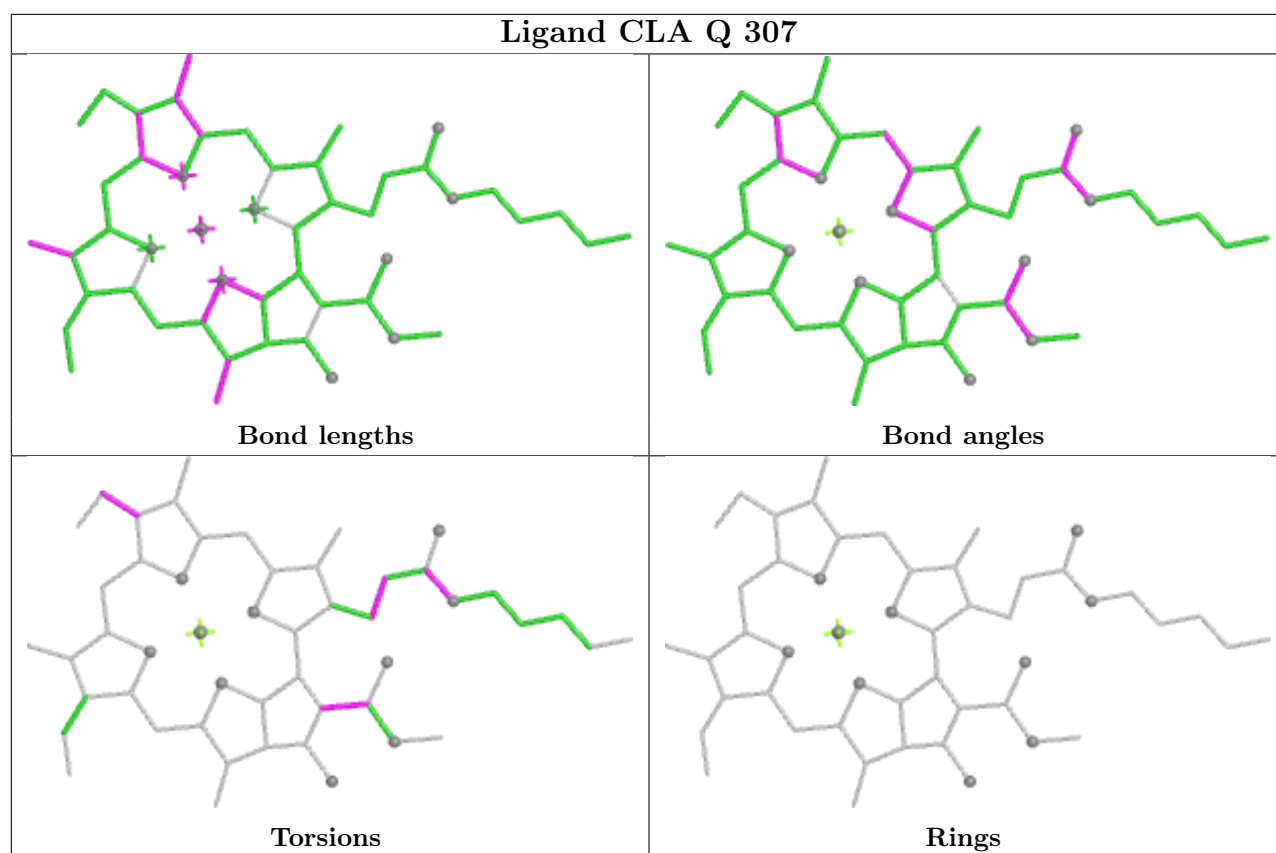
Ligand CLA R 314



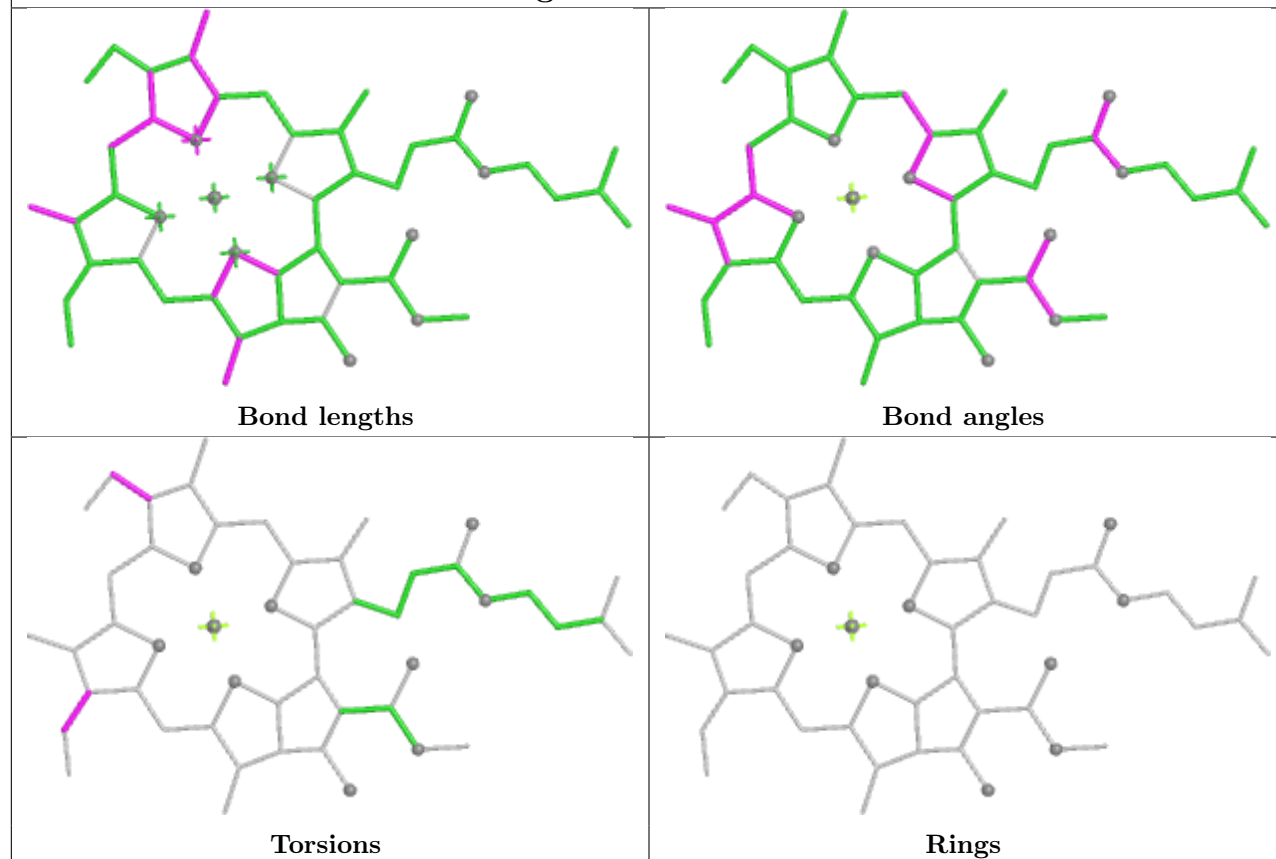
Ligand LMG J 318



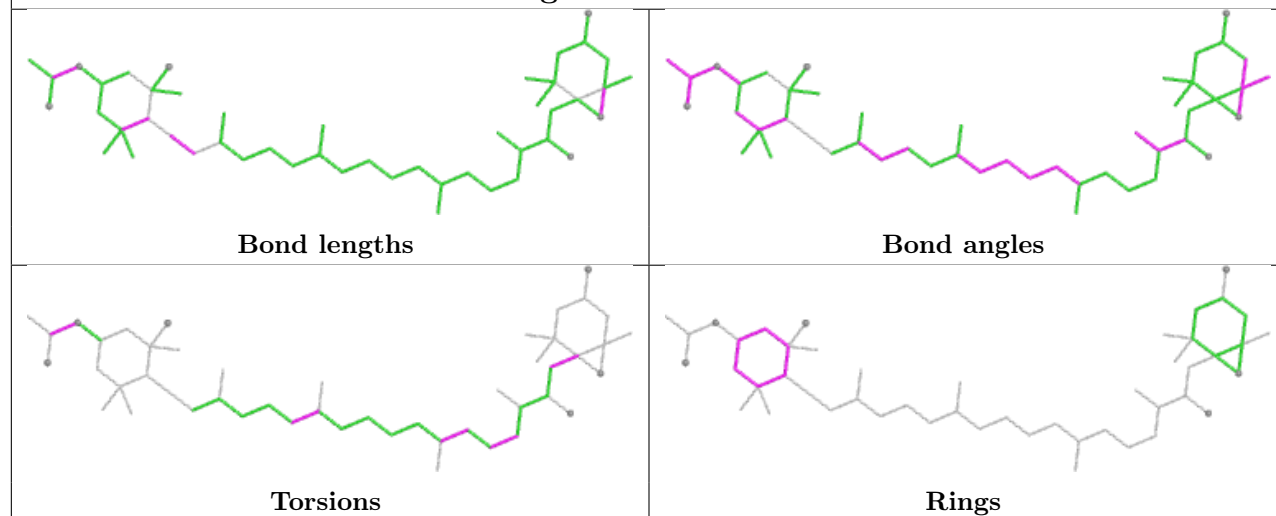


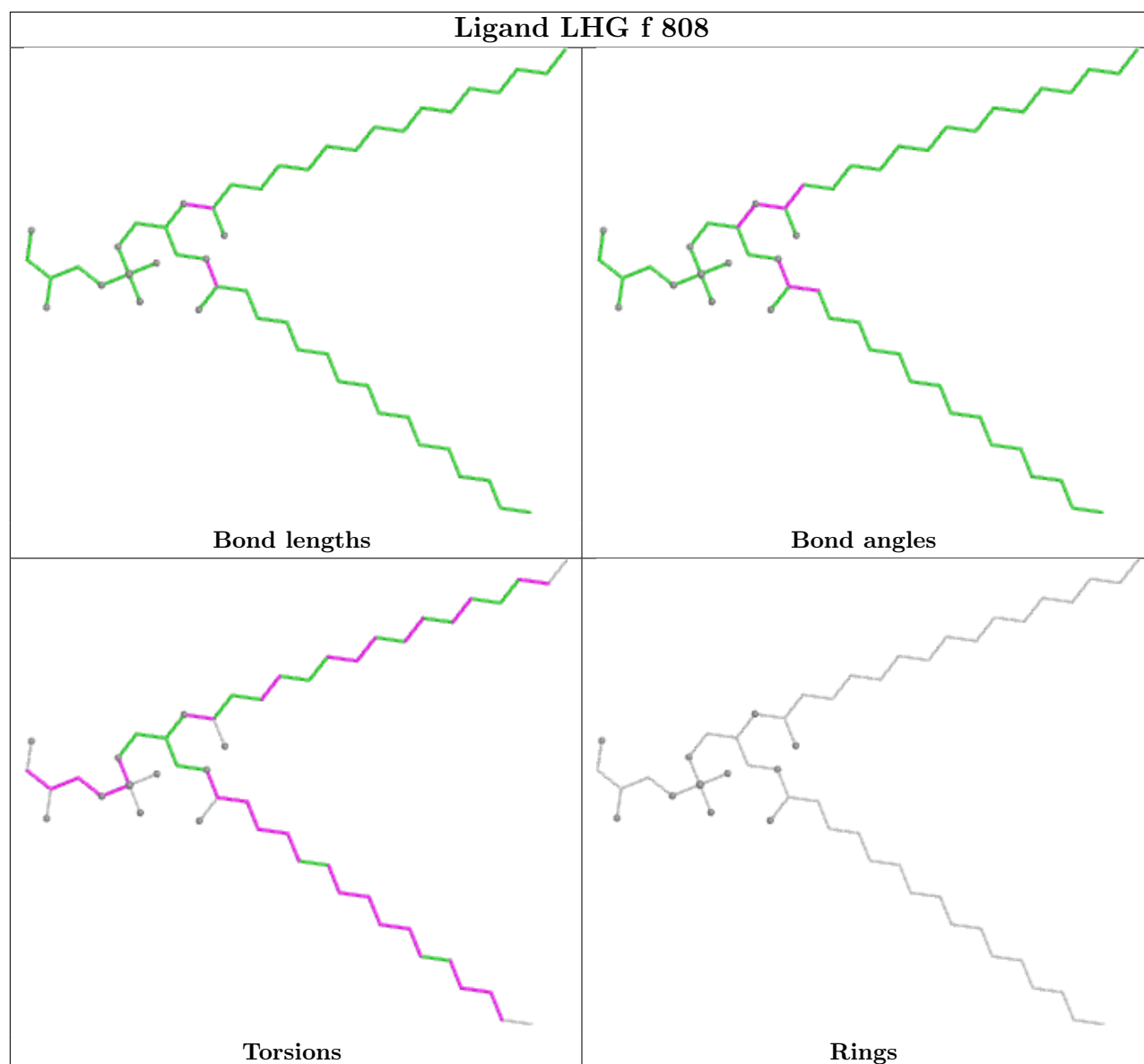
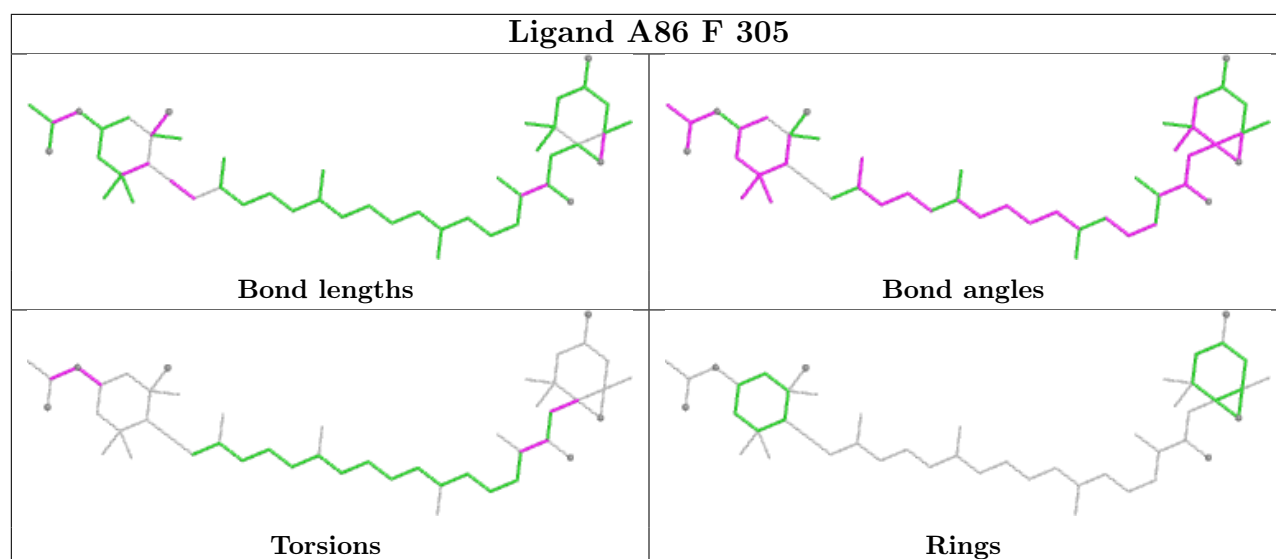


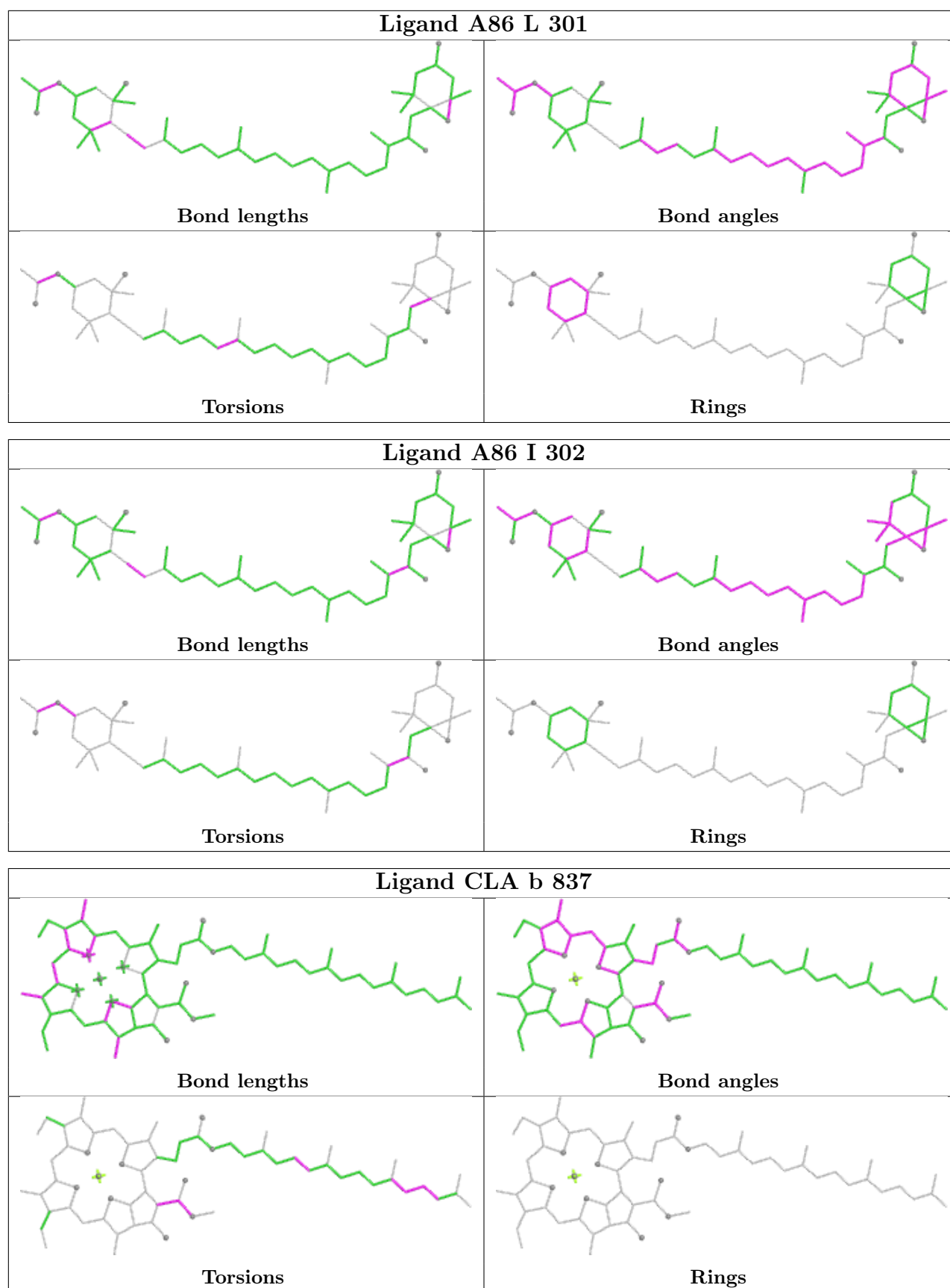
Ligand CLA a 814

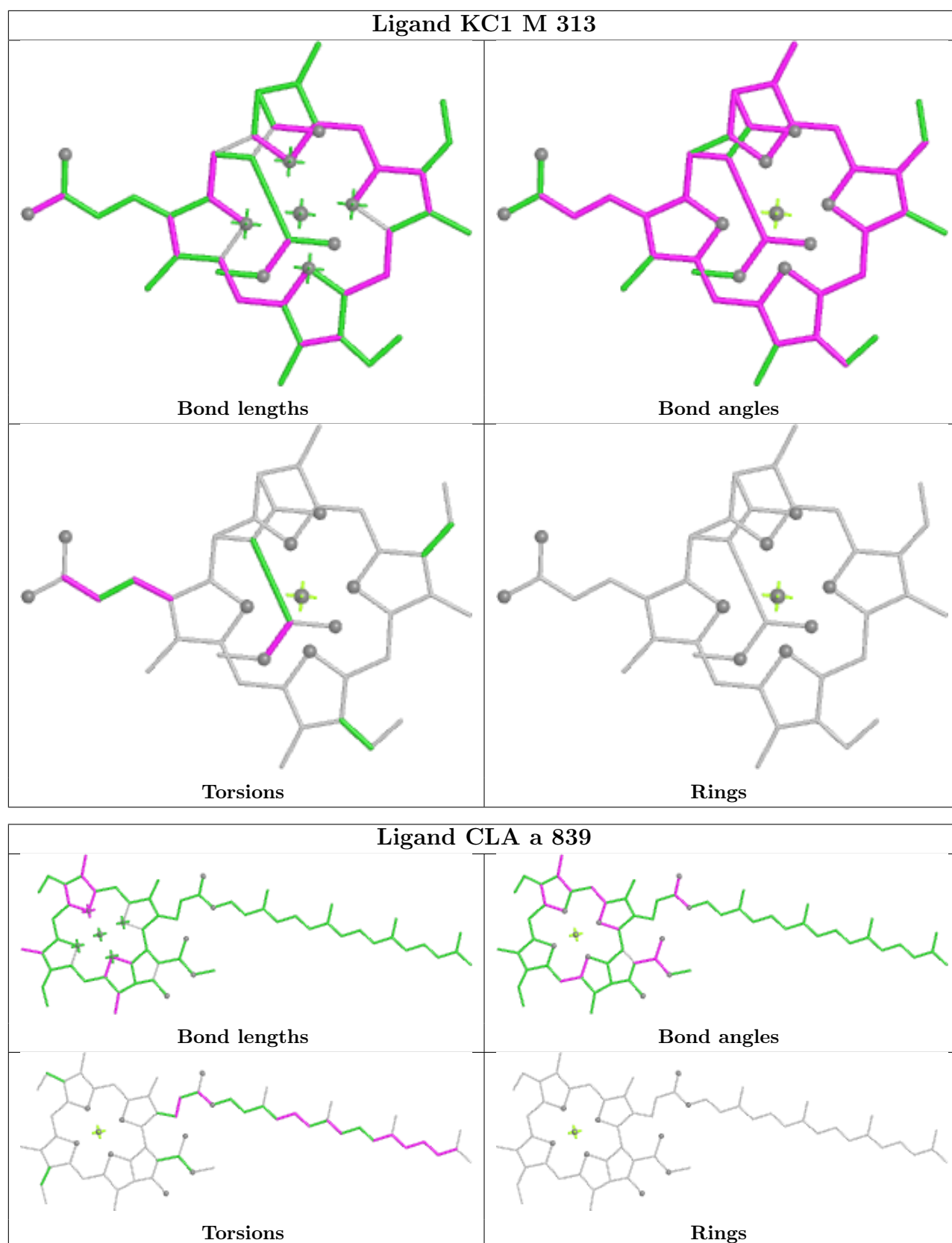


Ligand A86 L 307

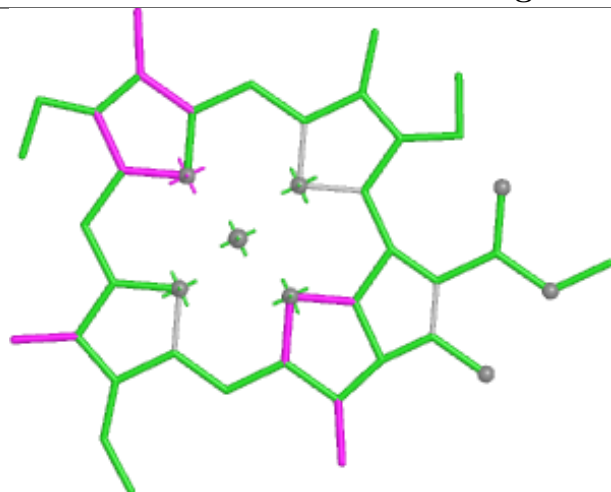




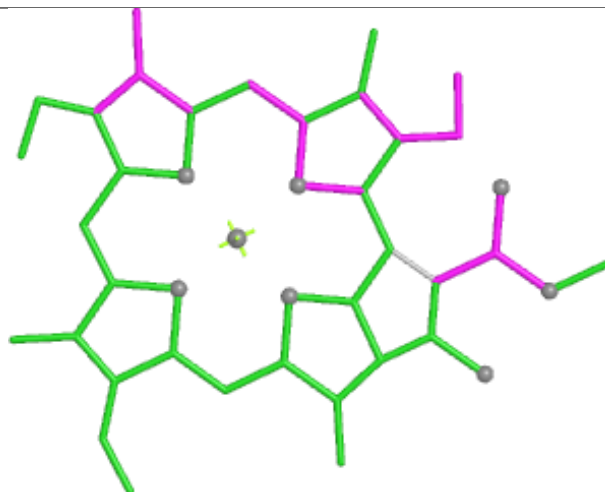




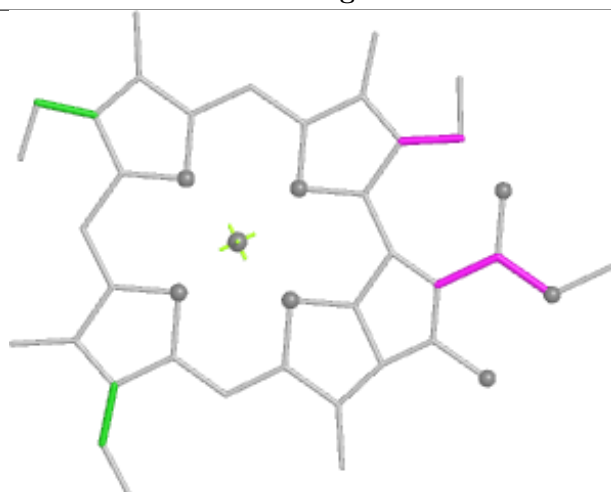
Ligand CLA P 302



Bond lengths



Bond angles

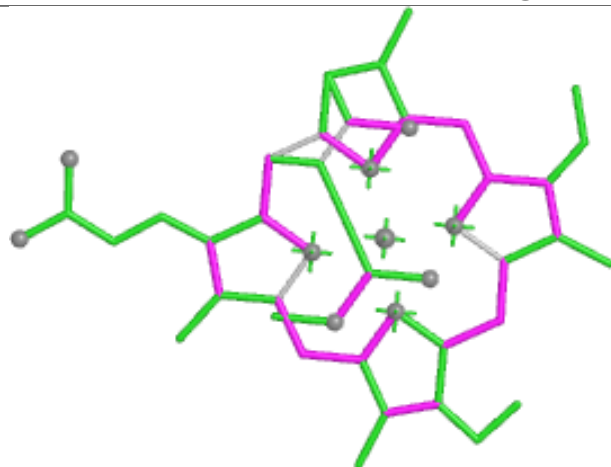


Torsions

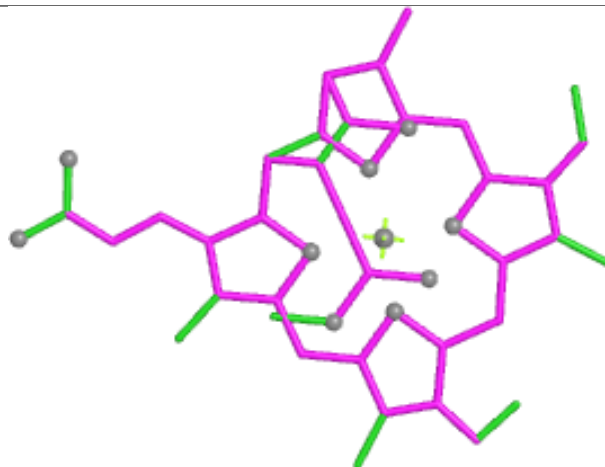


Rings

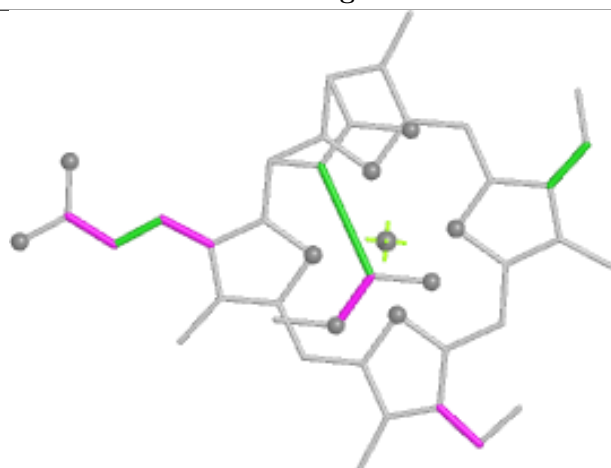
Ligand KC1 T 315



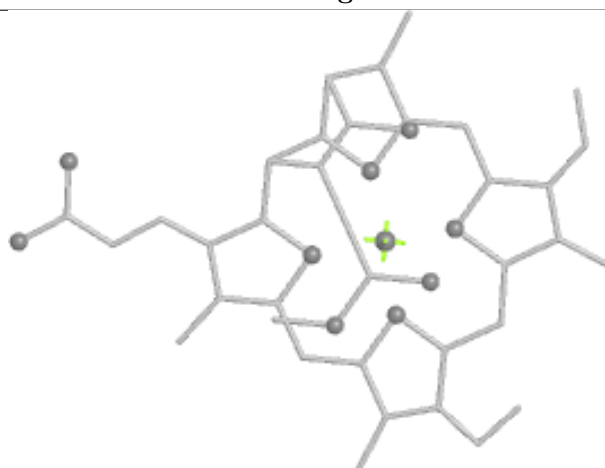
Bond lengths



Bond angles

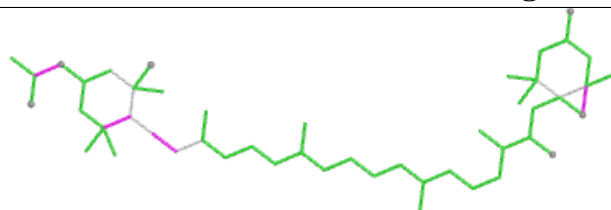


Torsions

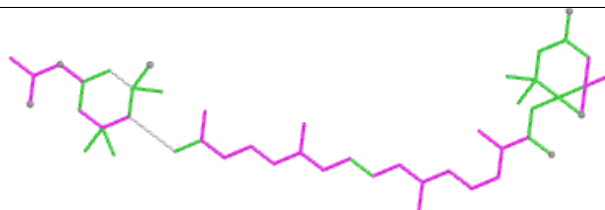


Rings

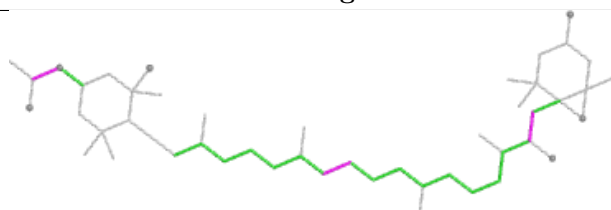
Ligand A86 T 301



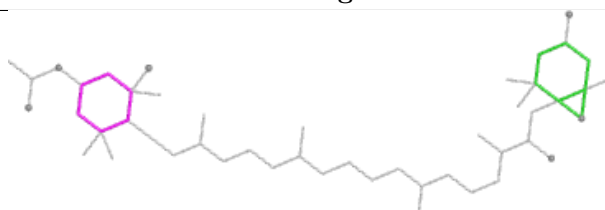
Bond lengths



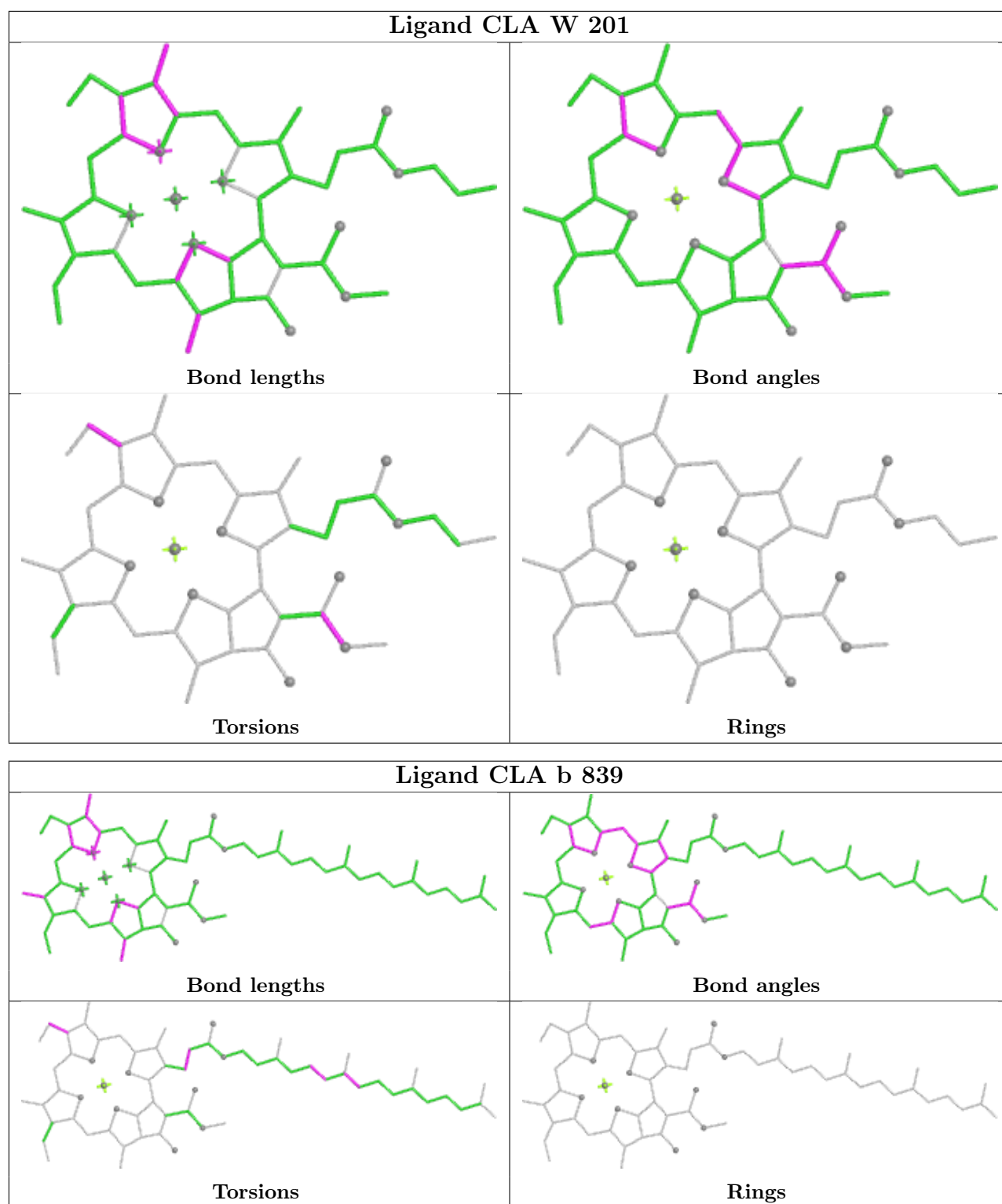
Bond angles

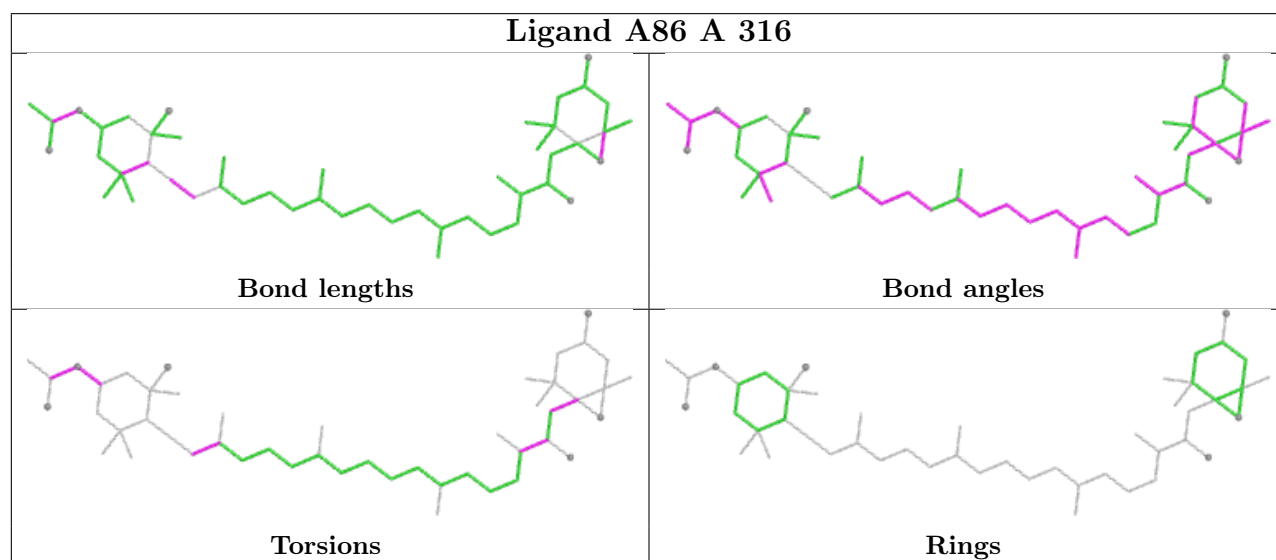
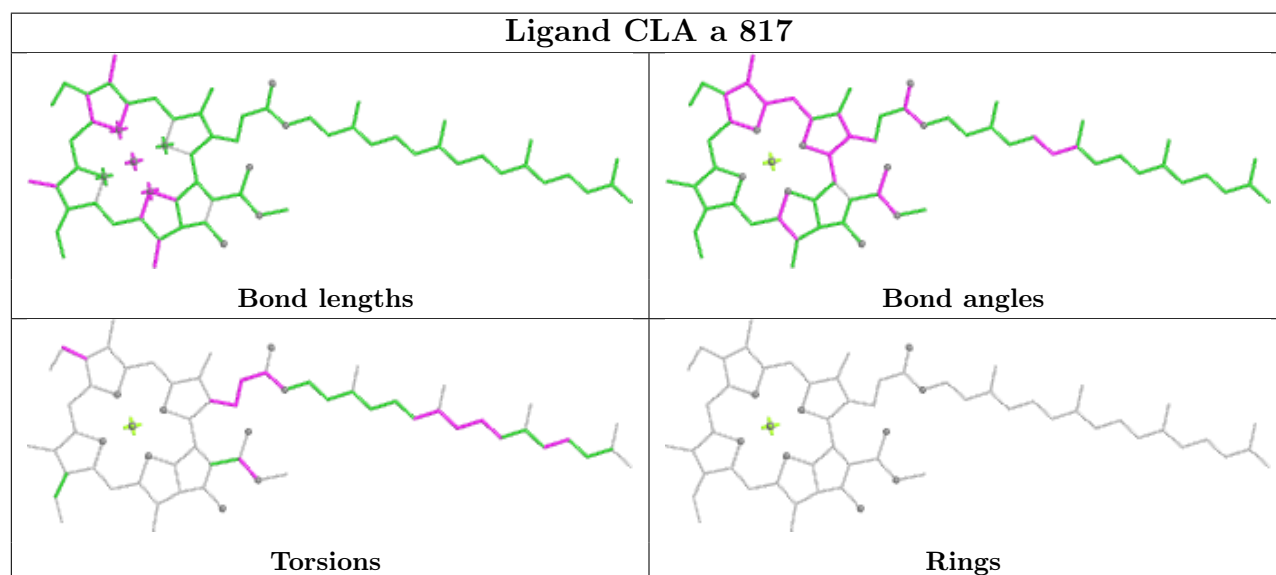
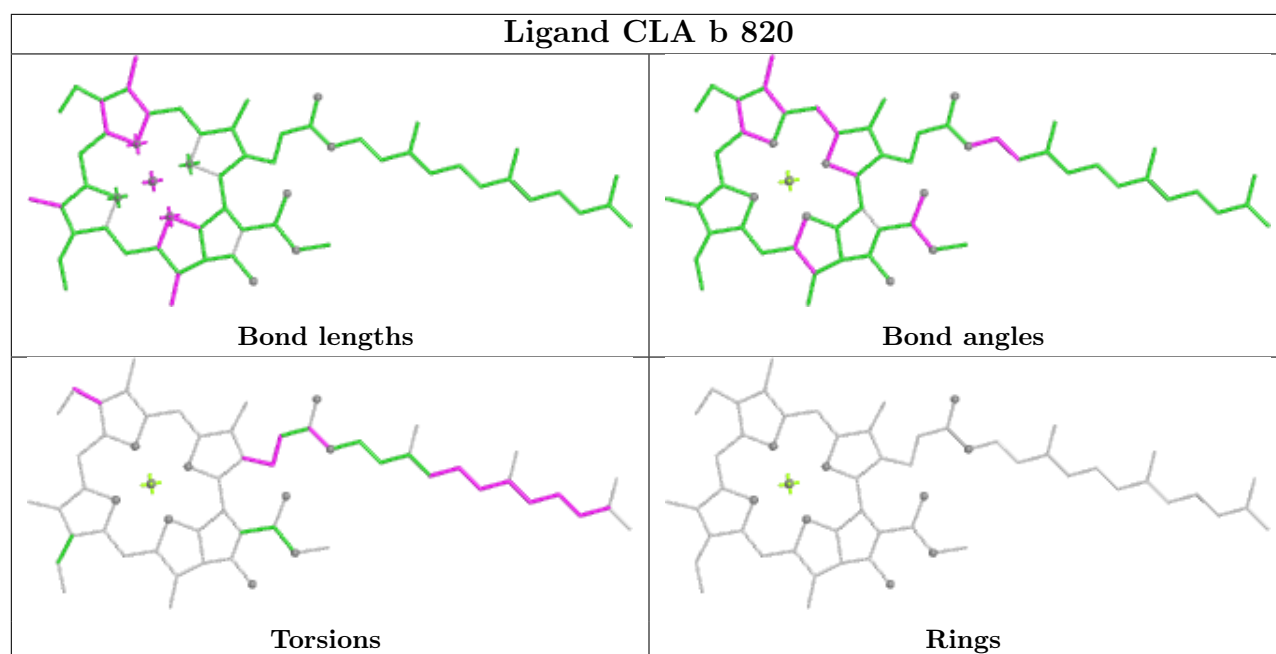


Torsions

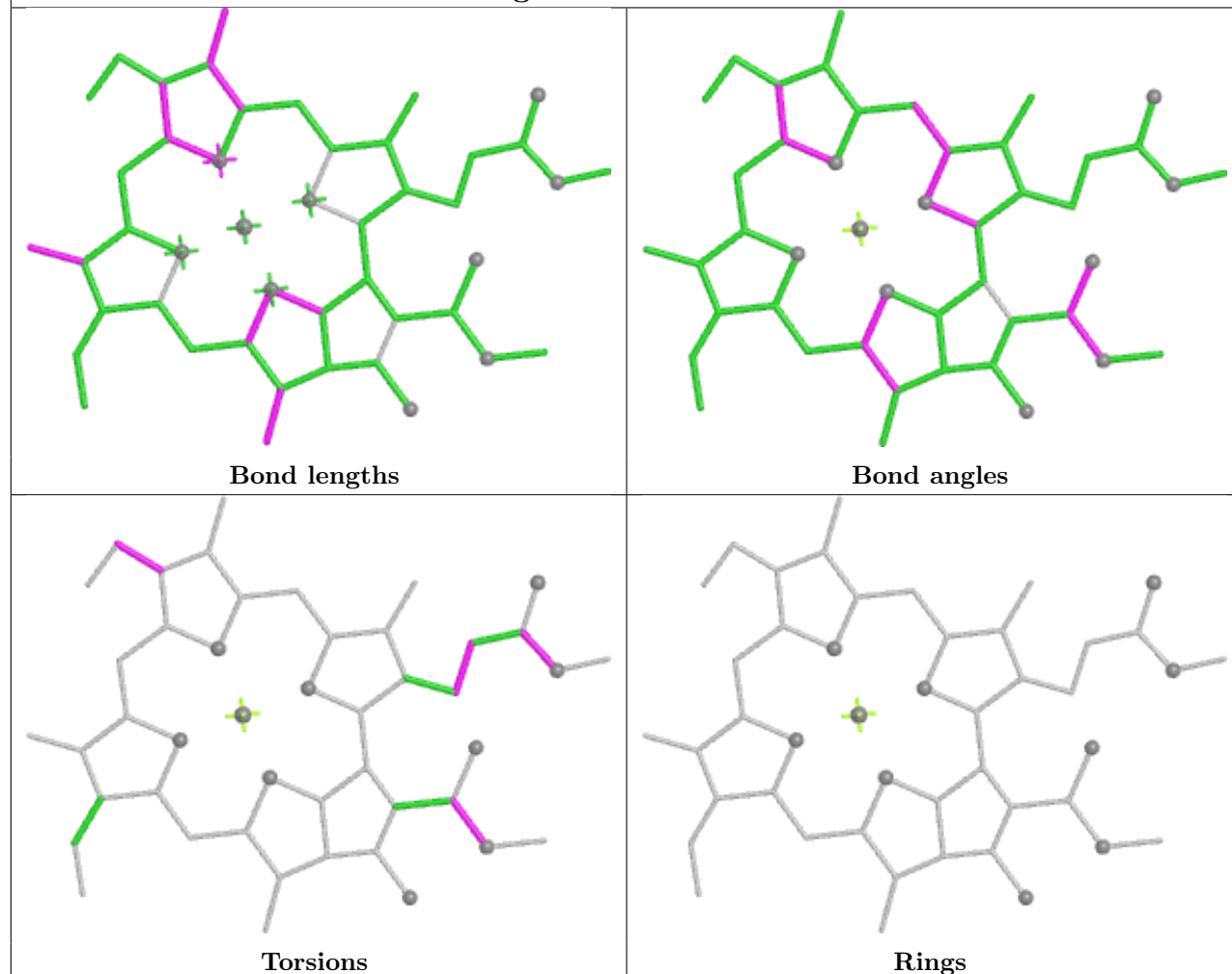


Rings

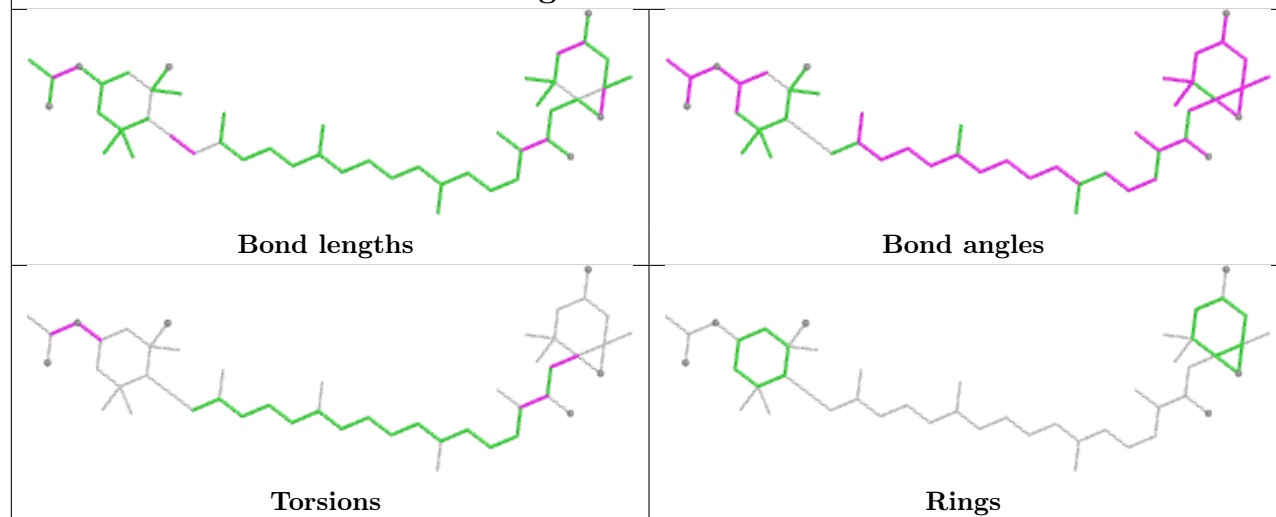




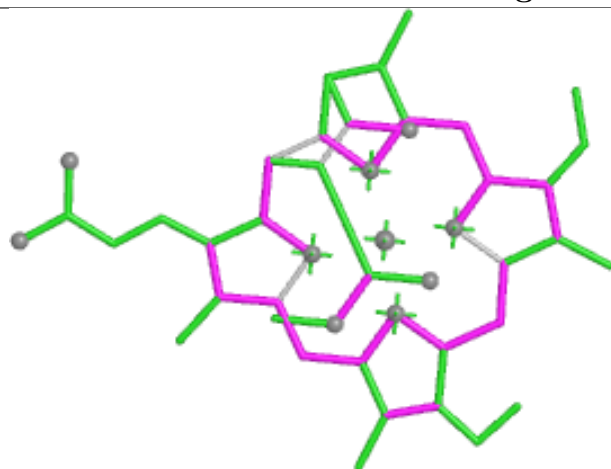
Ligand CLA D 311



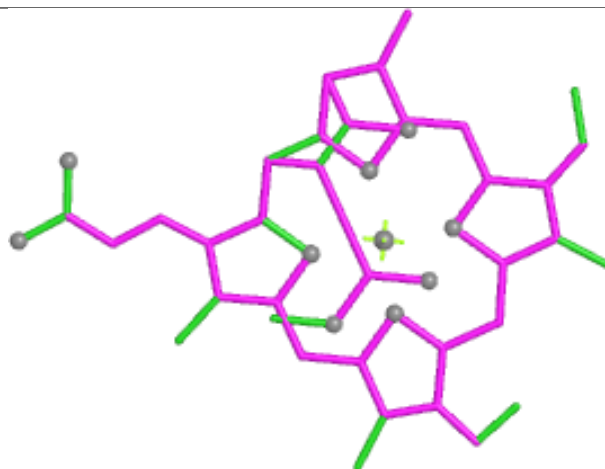
Ligand A86 T 305



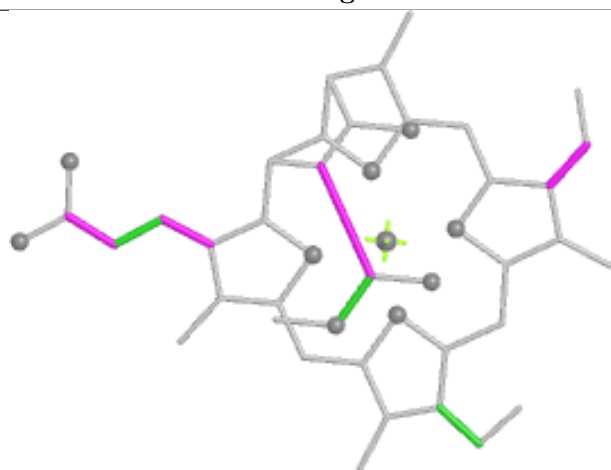
Ligand KC1 V 312



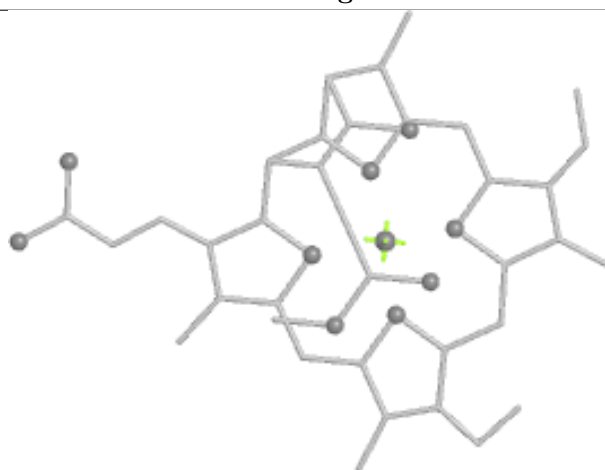
Bond lengths



Bond angles

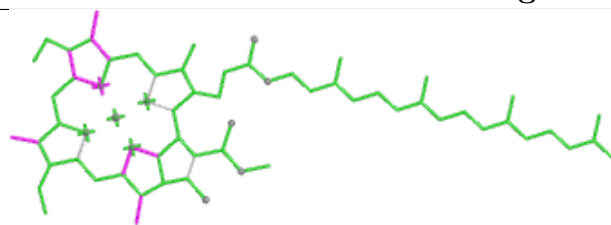


Torsions

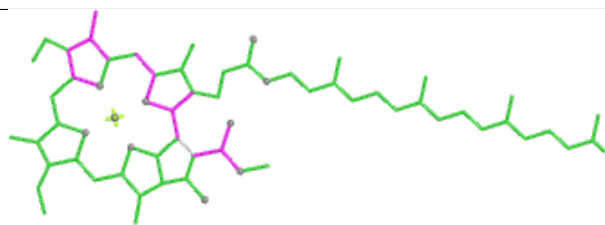


Rings

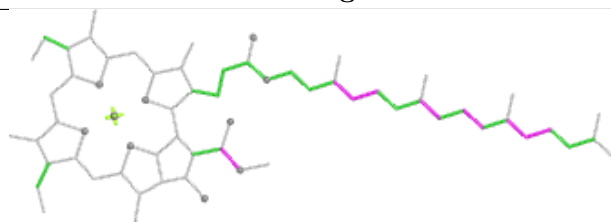
Ligand CLA a 837



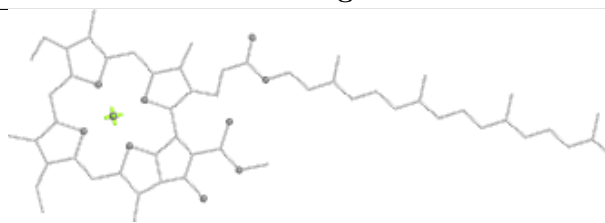
Bond lengths



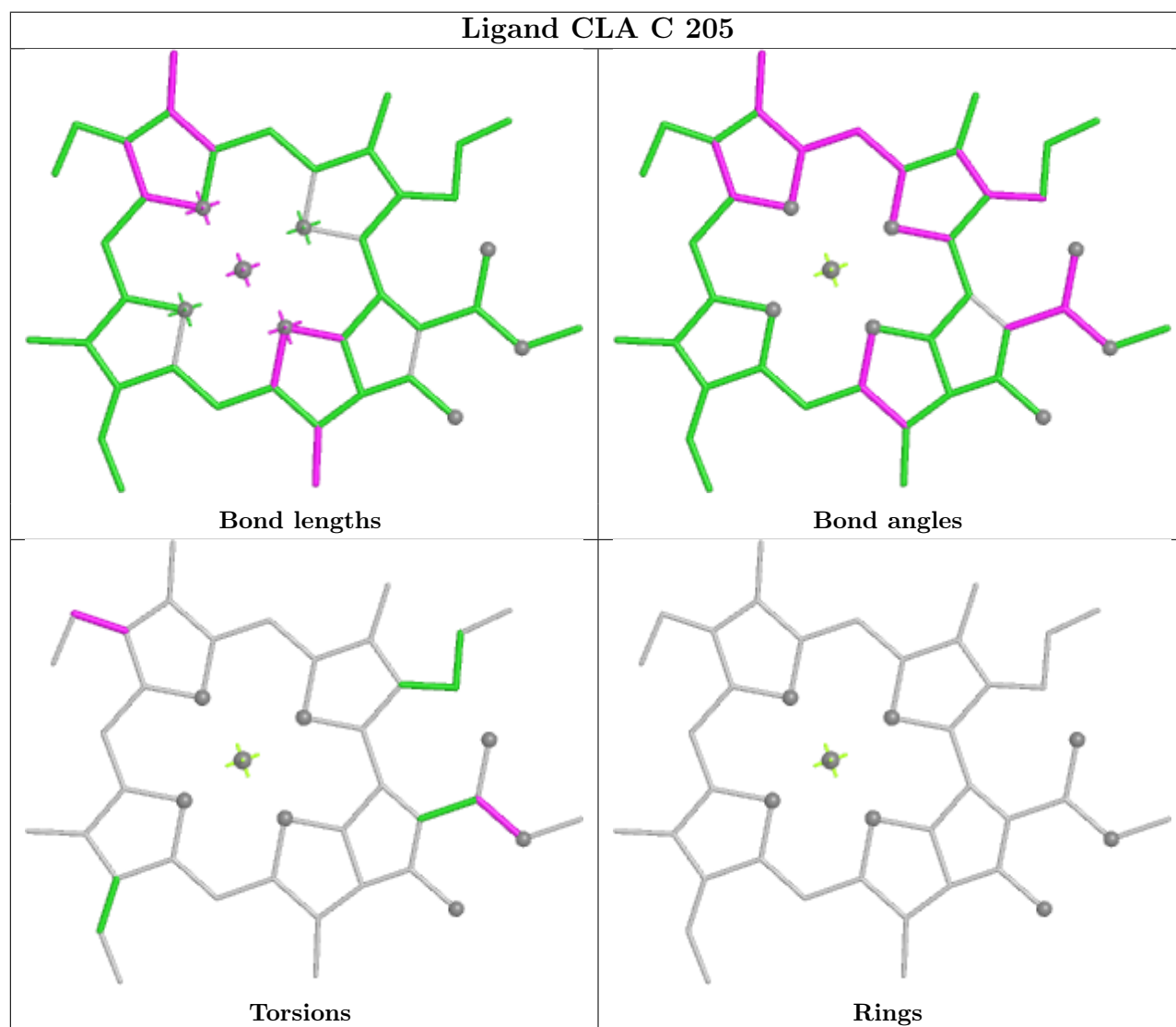
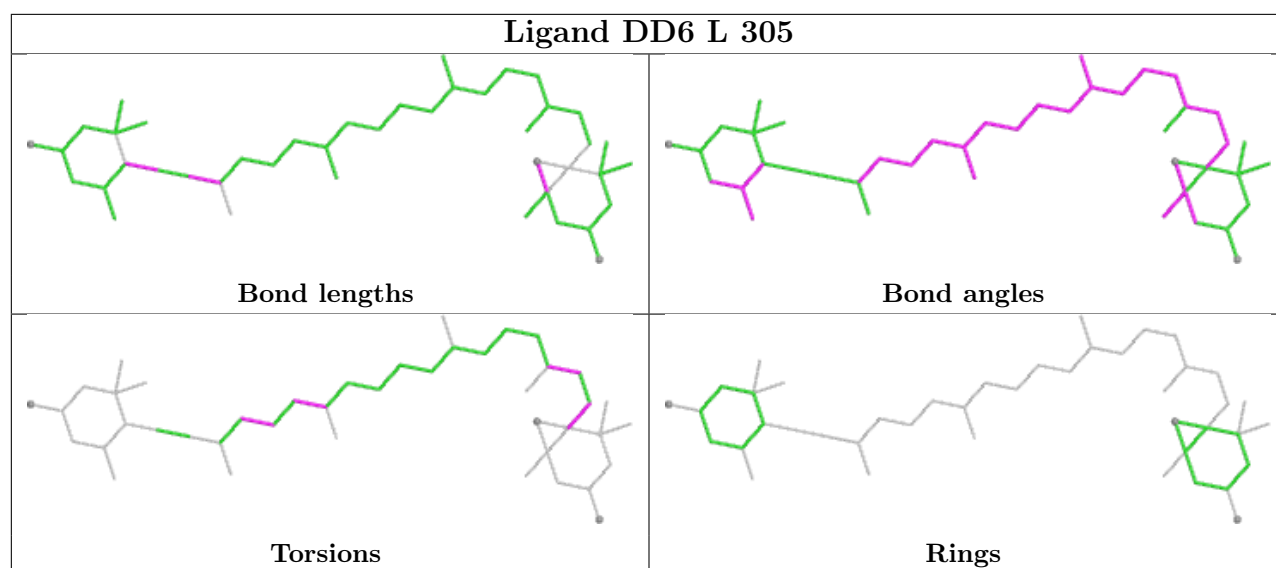
Bond angles

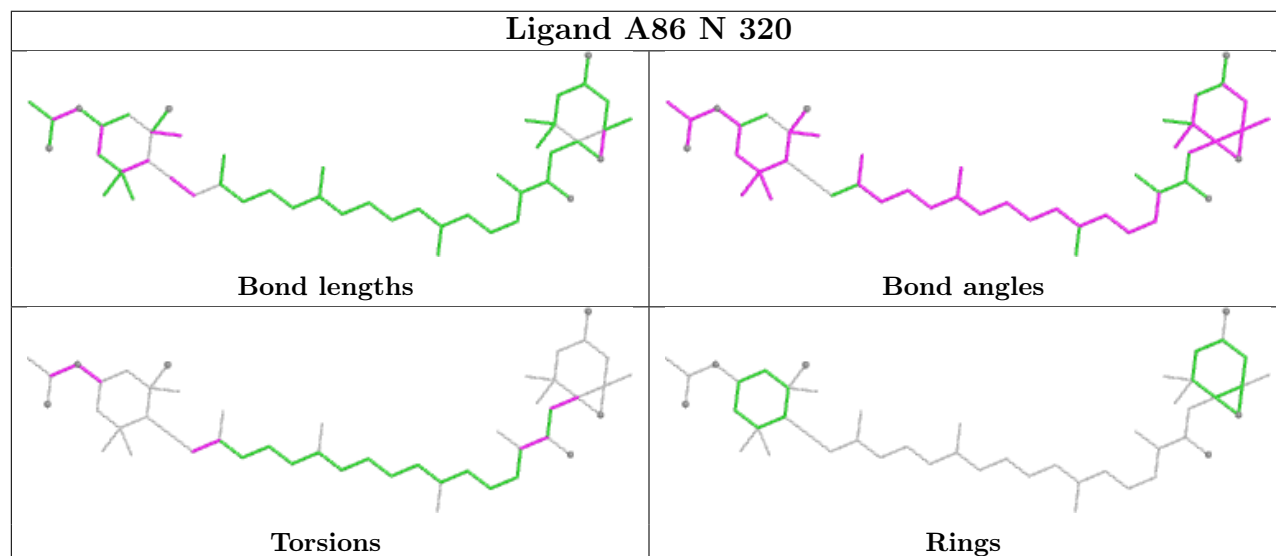
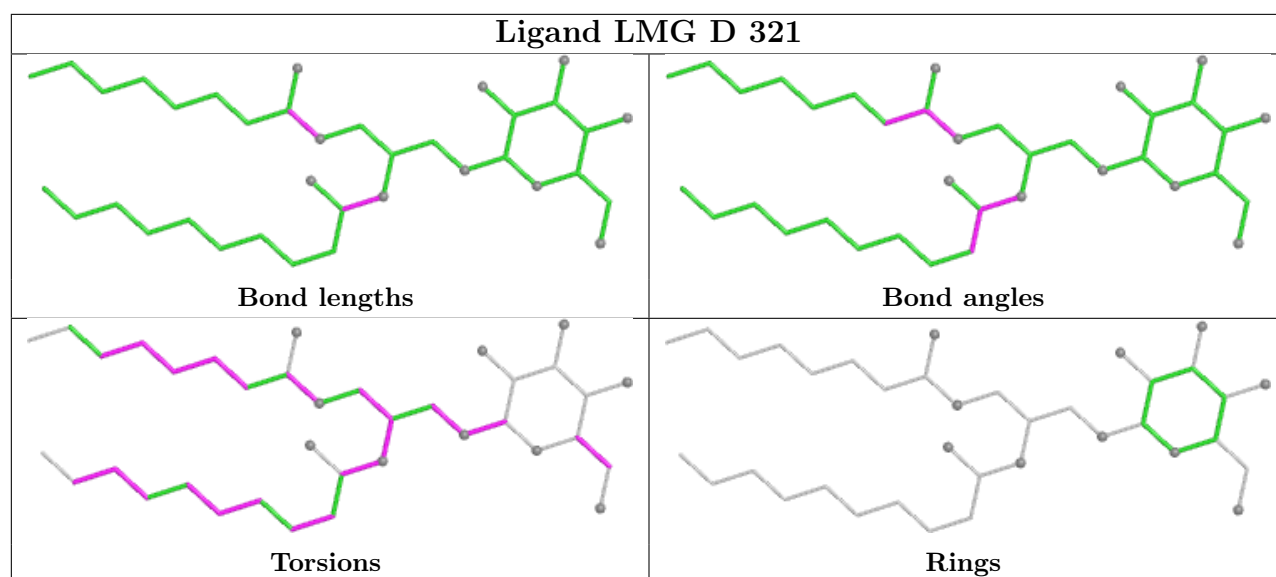


Torsions

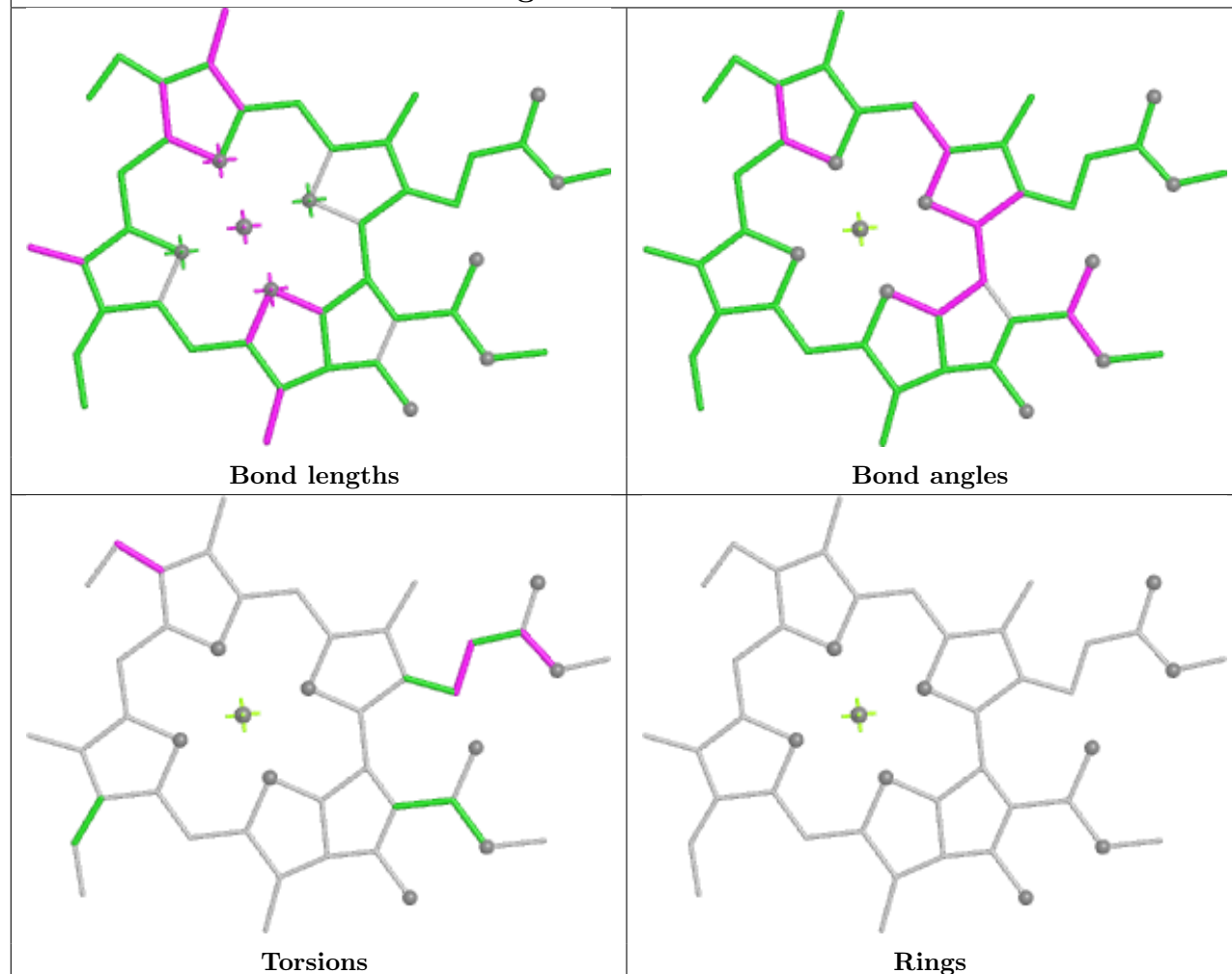


Rings

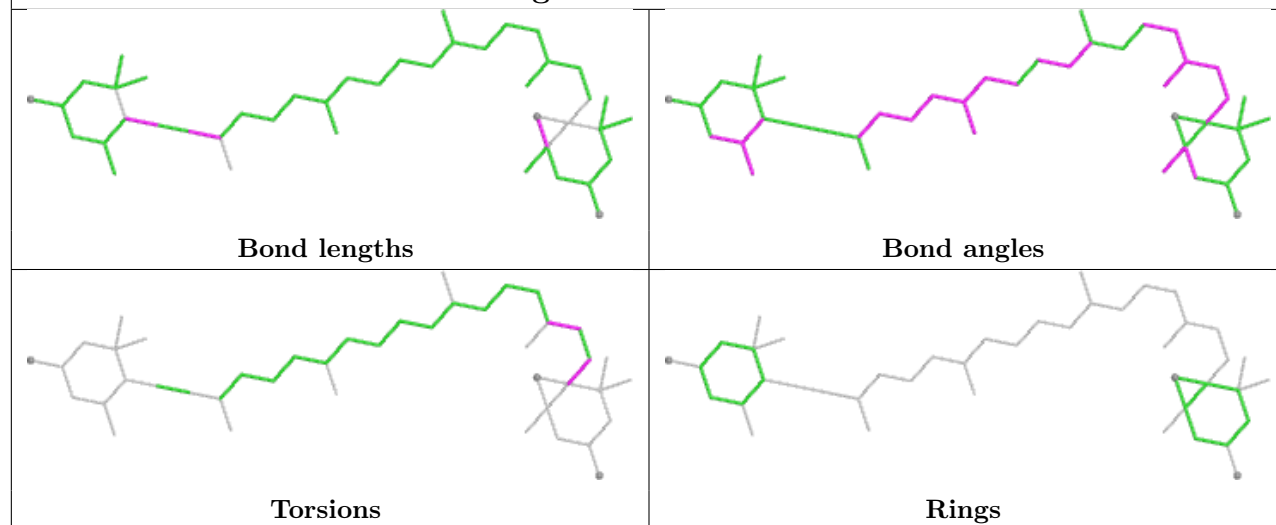




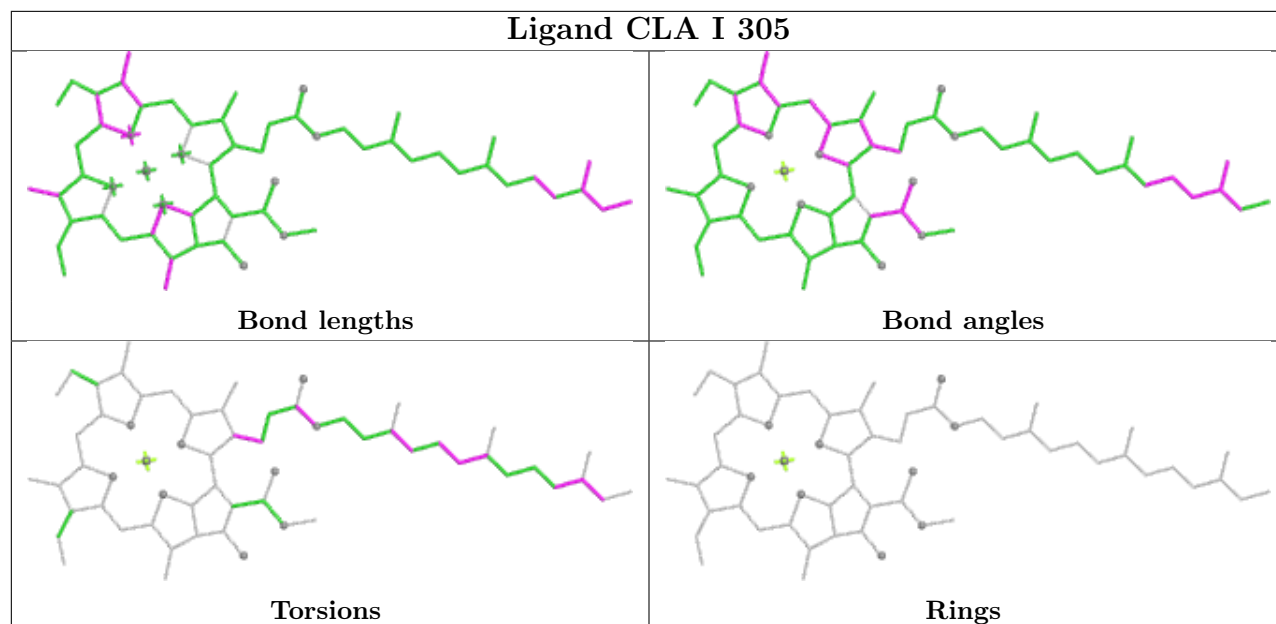
Ligand CLA J 311



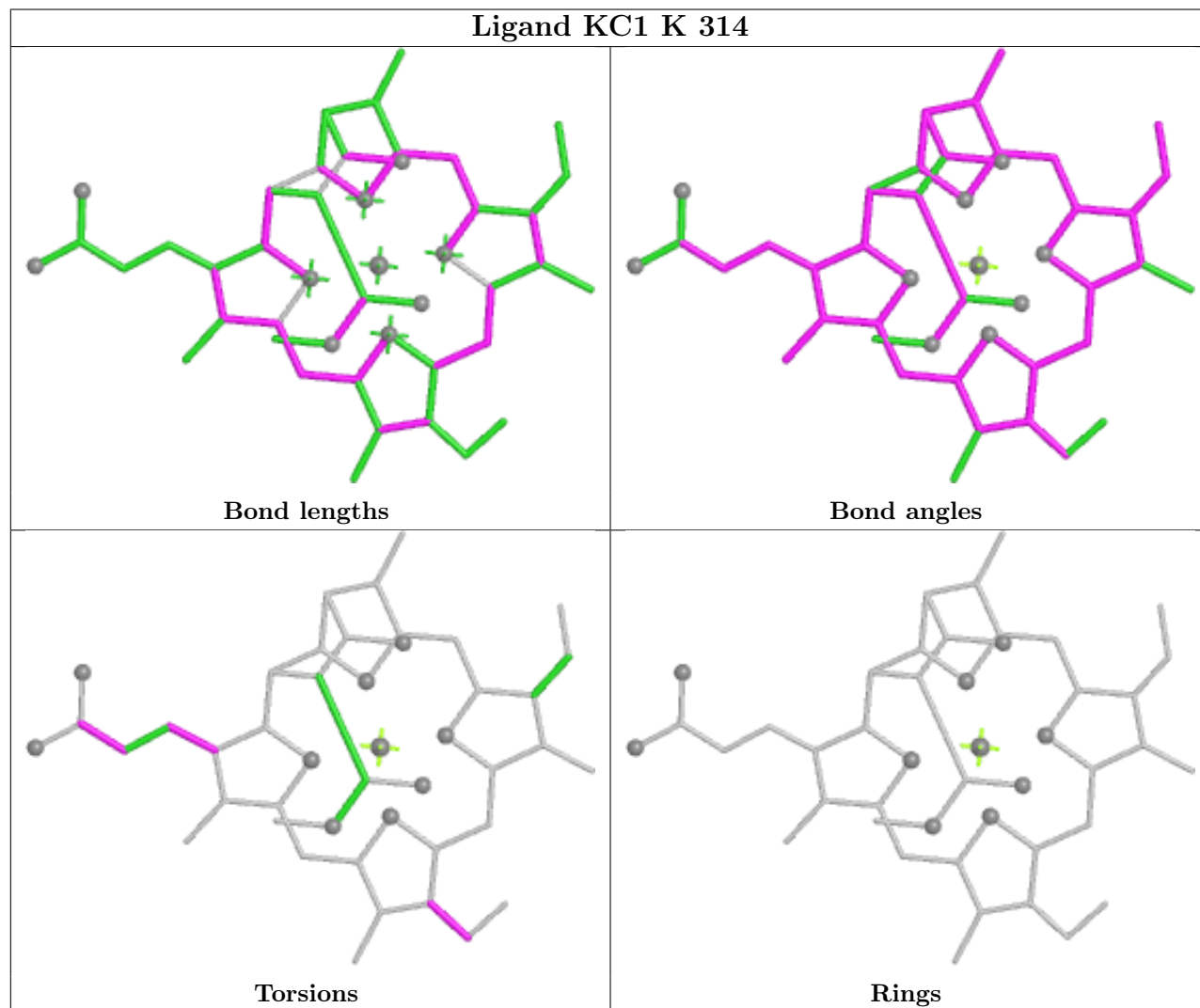
Ligand DD6 A 304

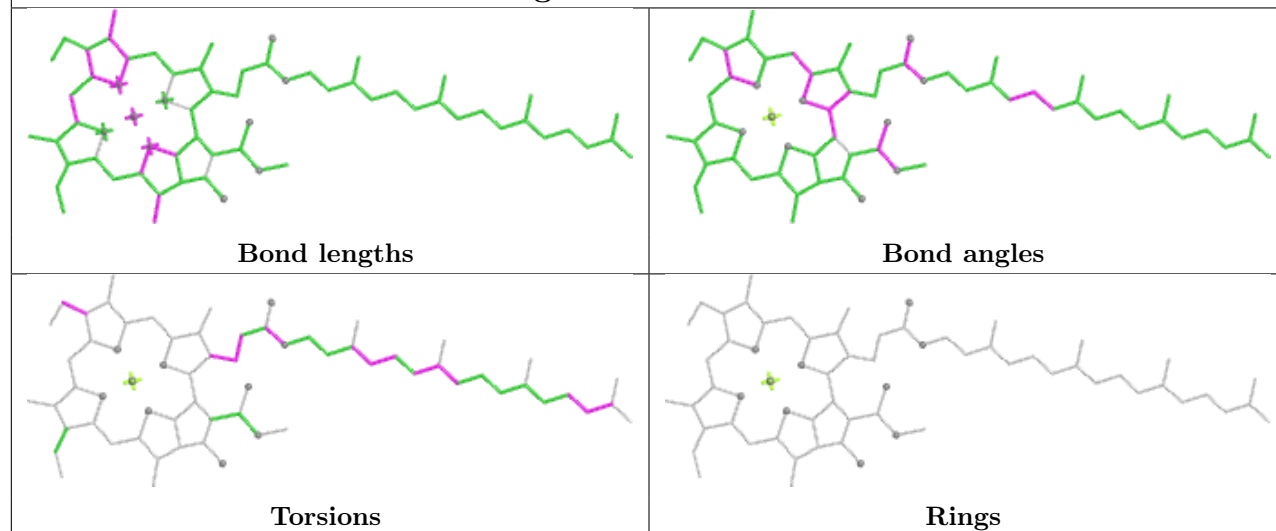
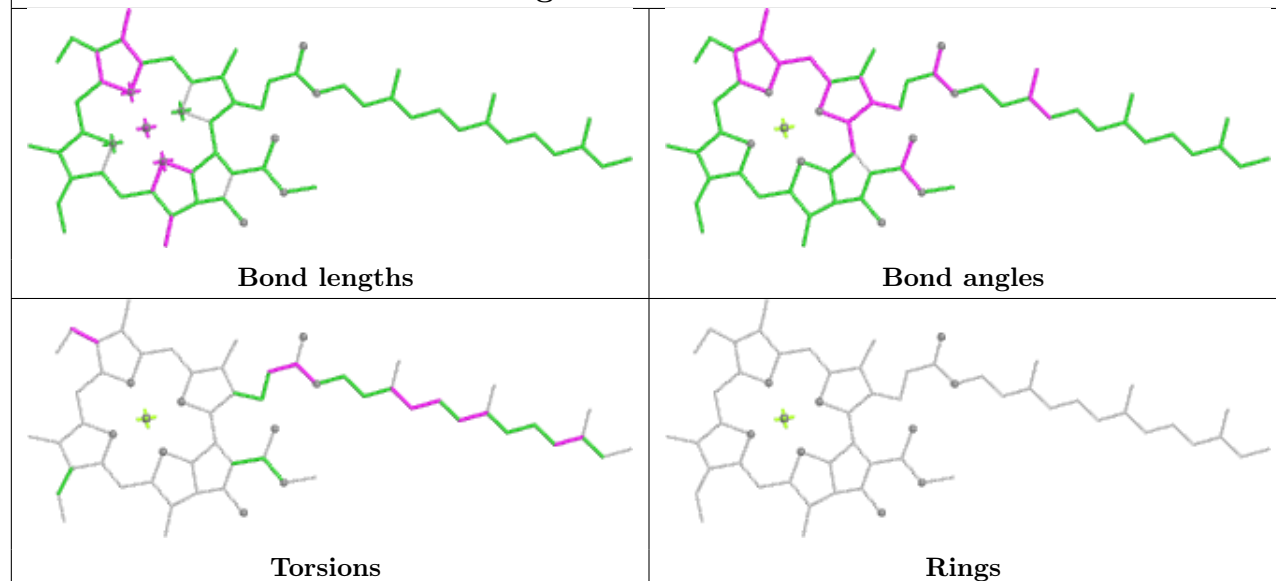


Ligand CLA I 305

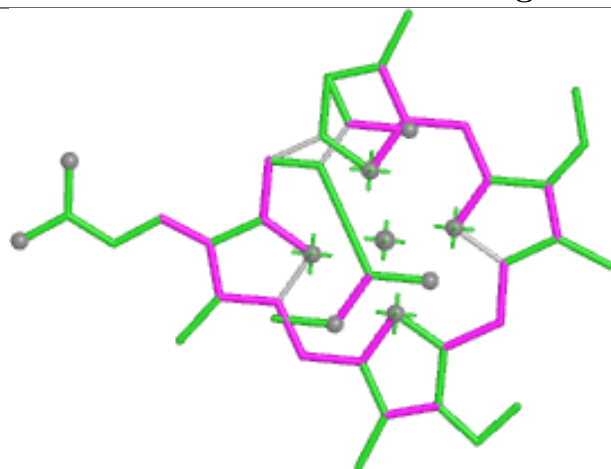


Ligand KC1 K 314

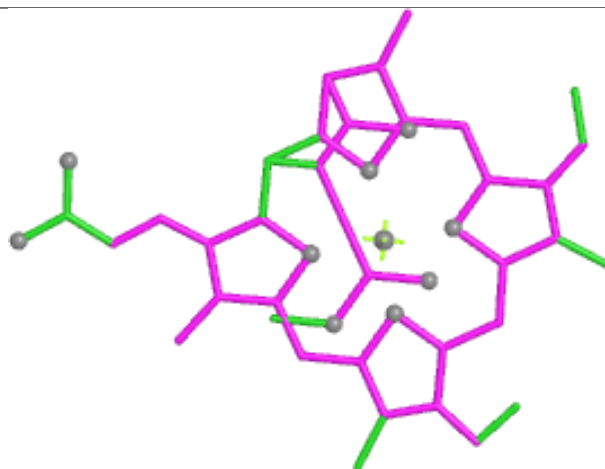


Ligand CLA F 314**Ligand CLA J 307**

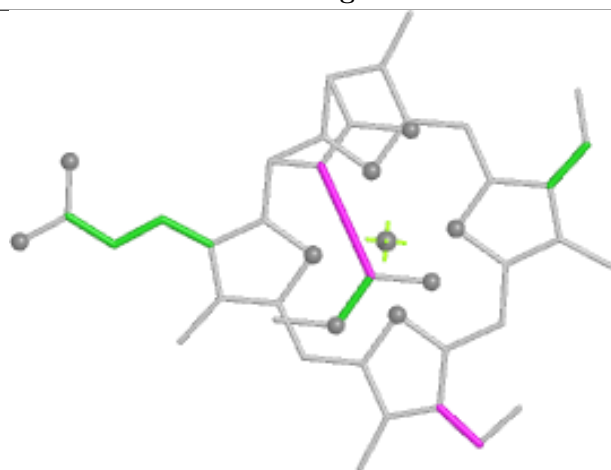
Ligand KC1 O 315



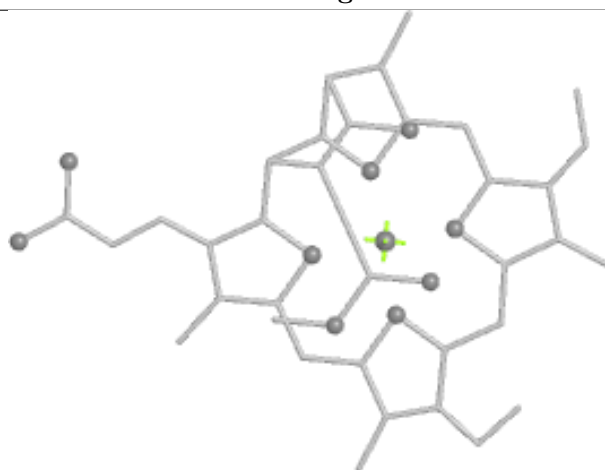
Bond lengths



Bond angles

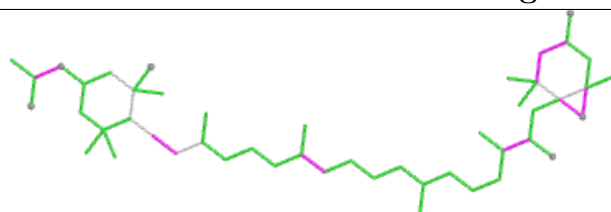


Torsions

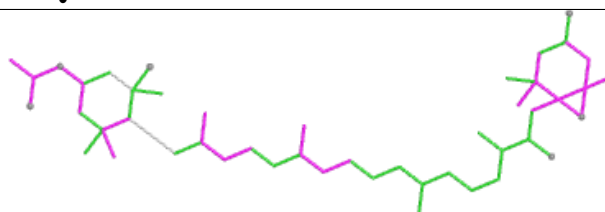


Rings

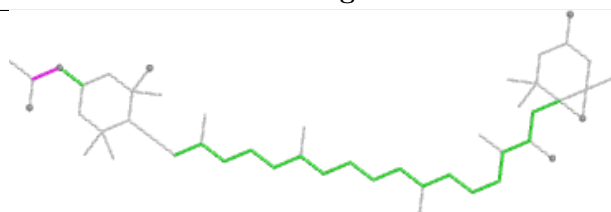
Ligand A86 Q 316



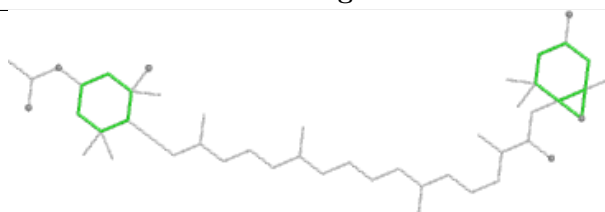
Bond lengths



Bond angles

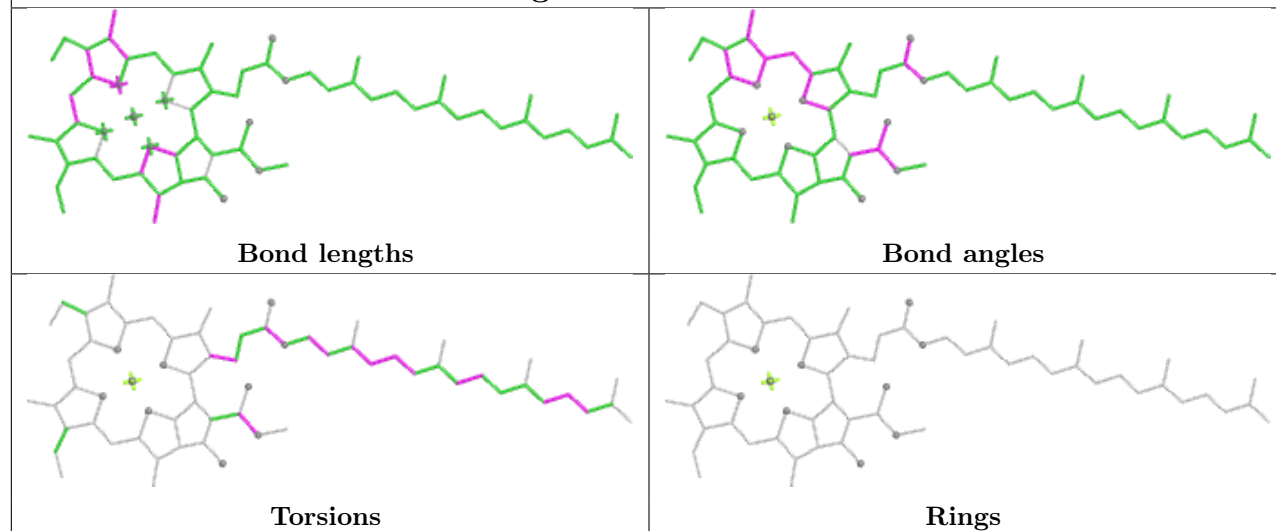


Torsions

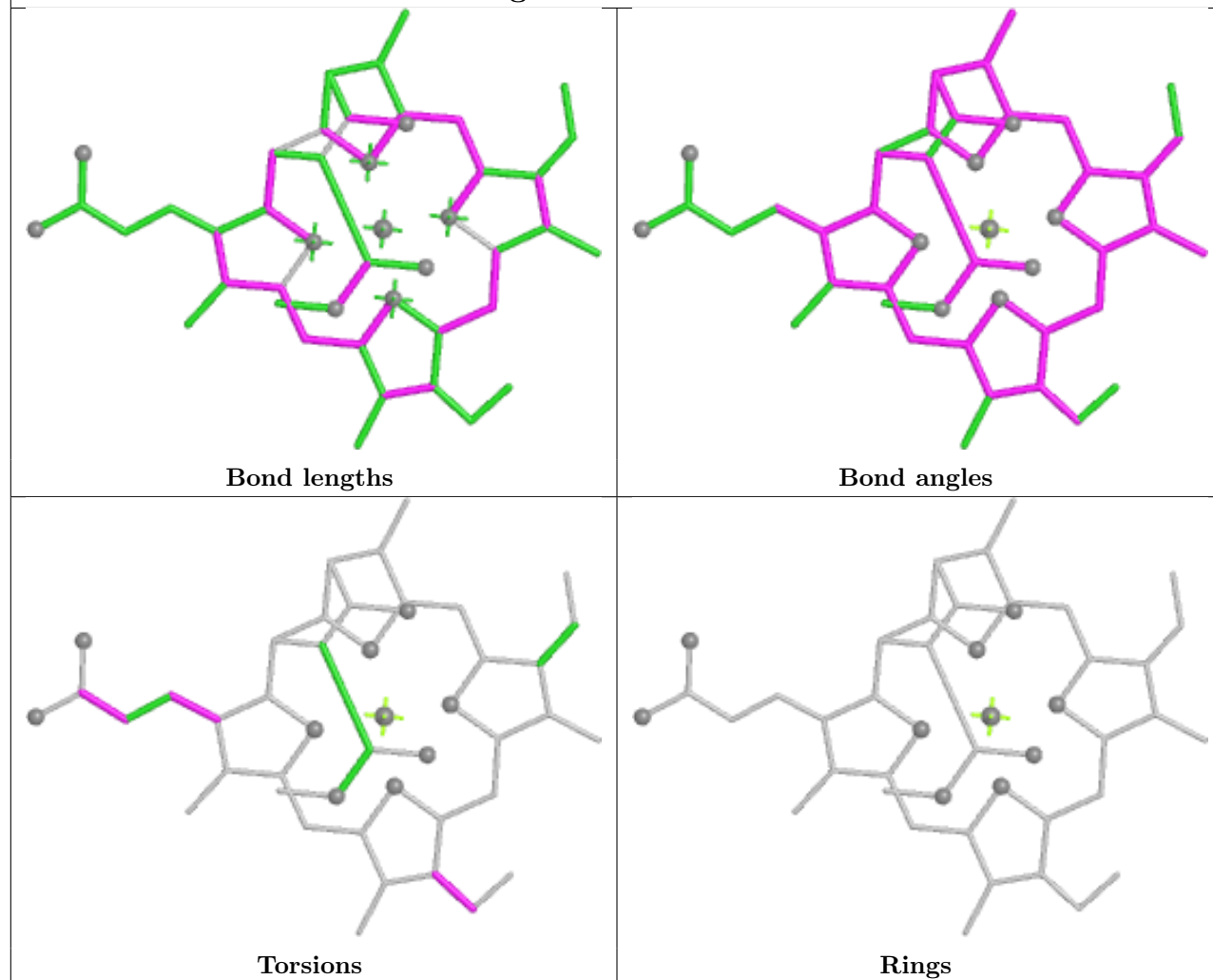


Rings

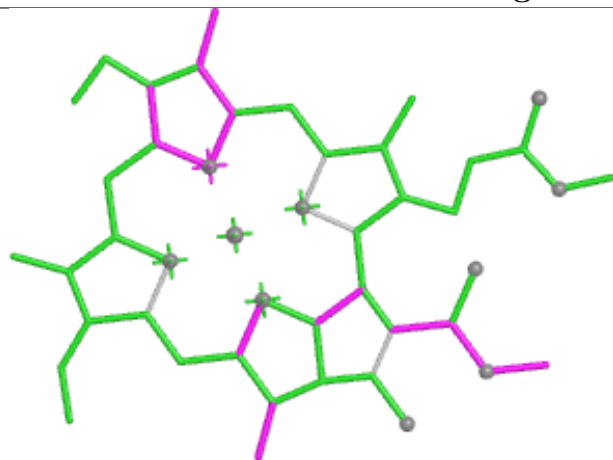
Ligand CLA R 311



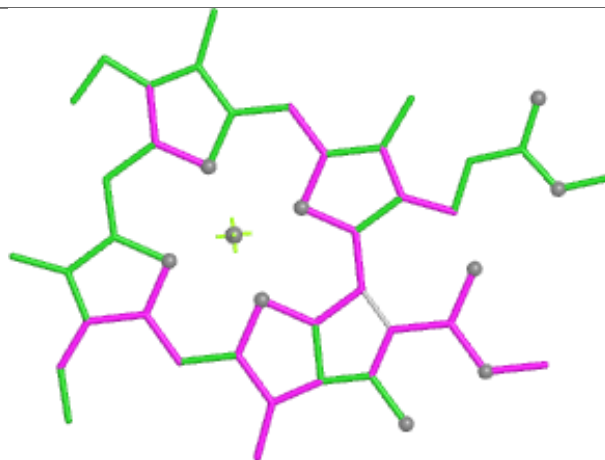
Ligand KC1 L 315



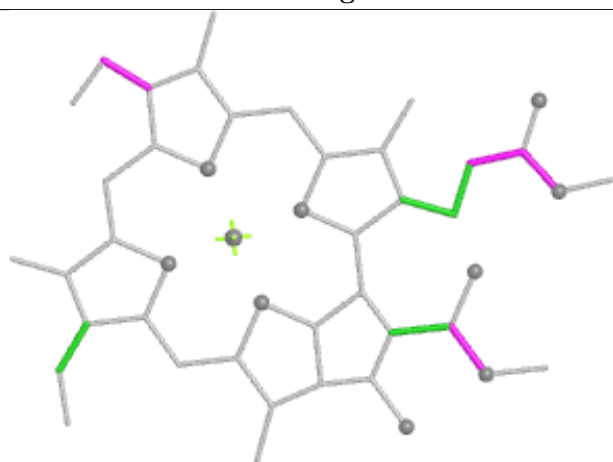
Ligand CLA H 310



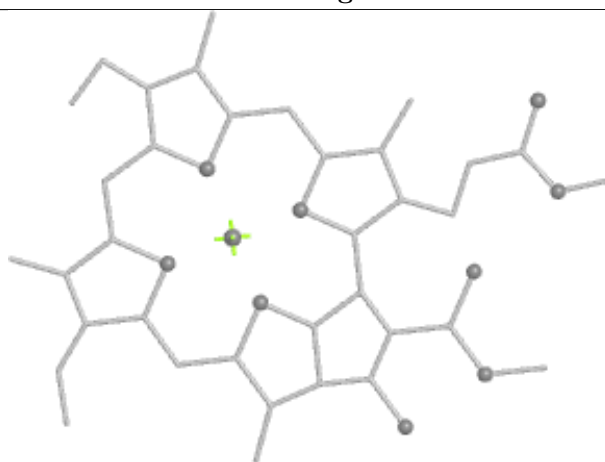
Bond lengths



Bond angles

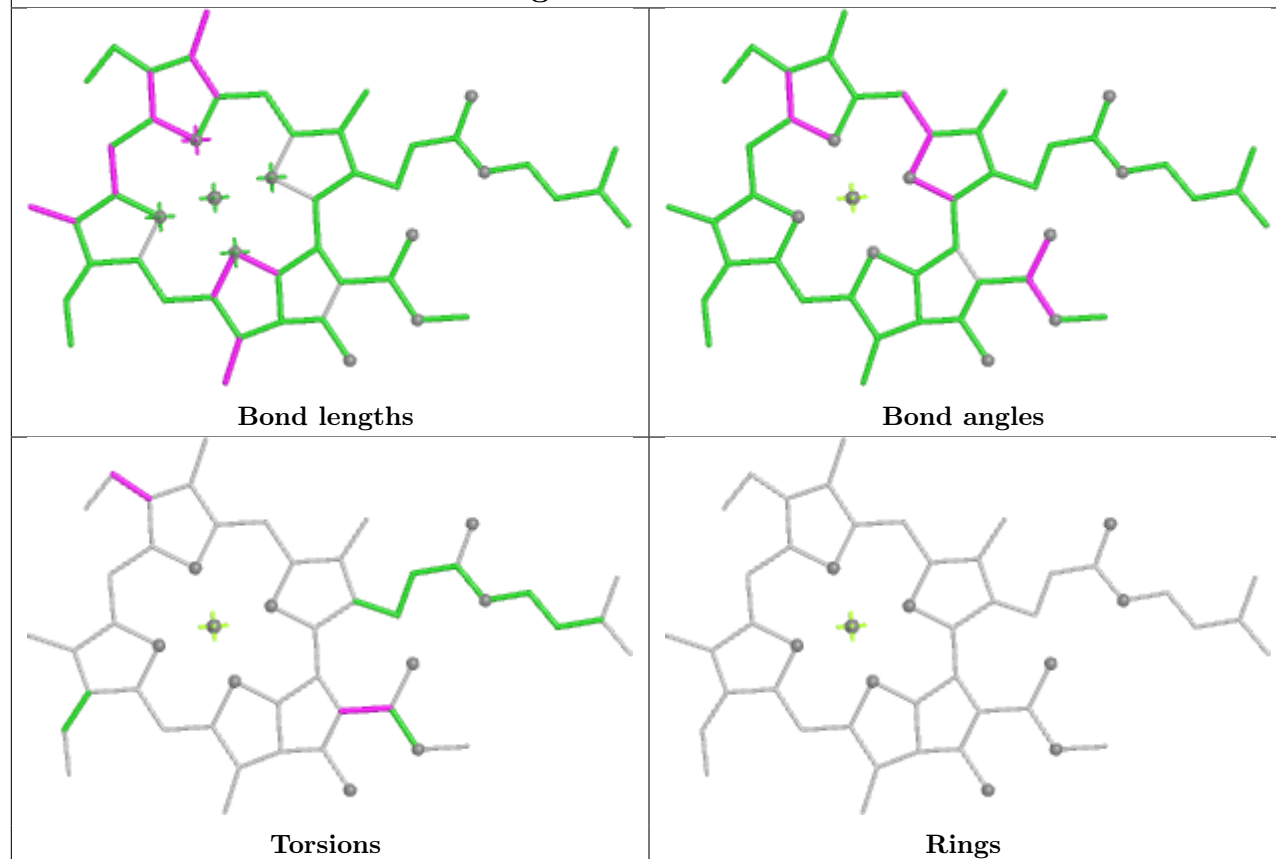


Torsions

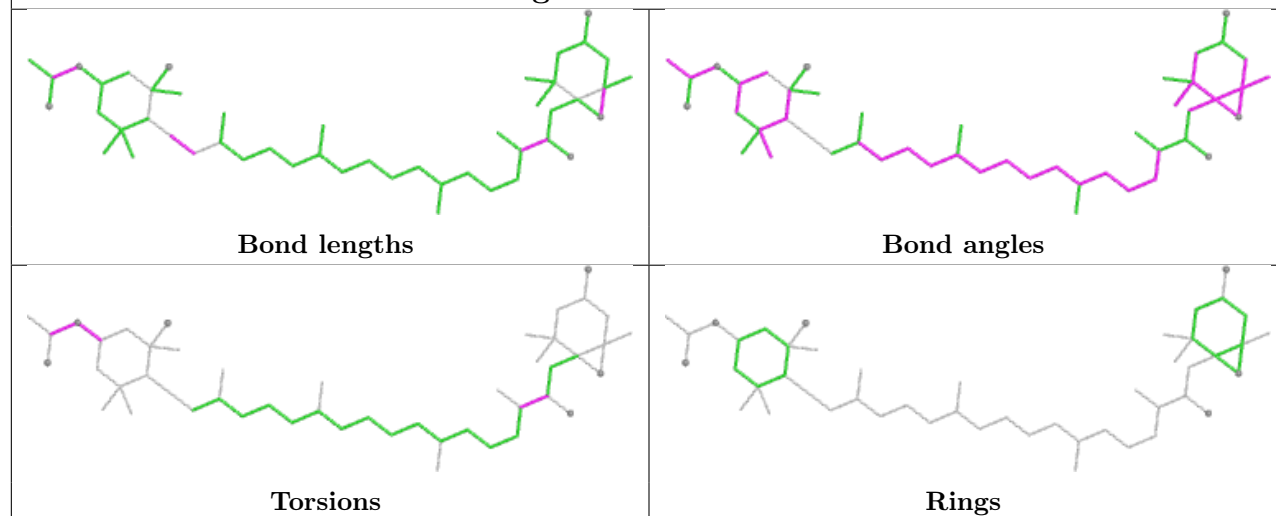


Rings

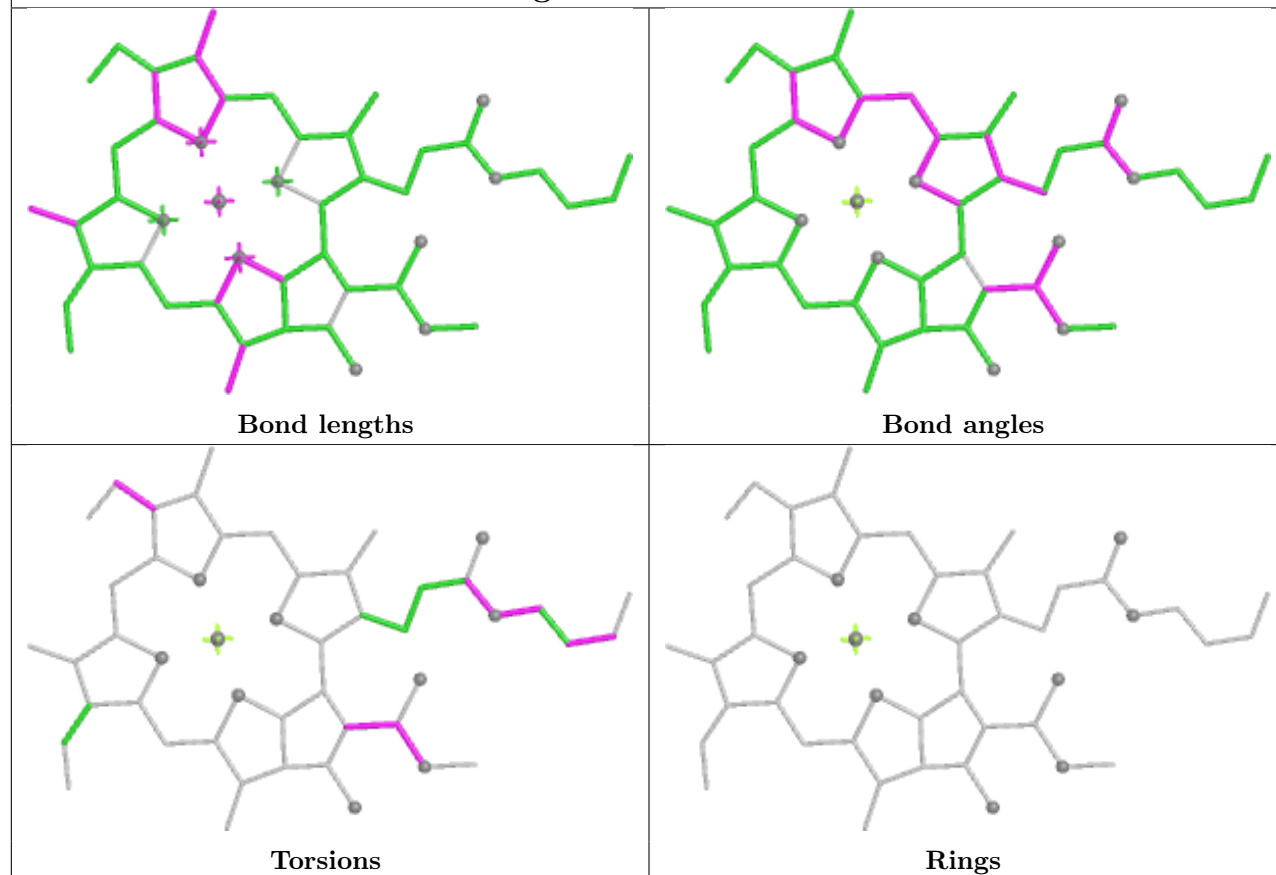
Ligand CLA U 307



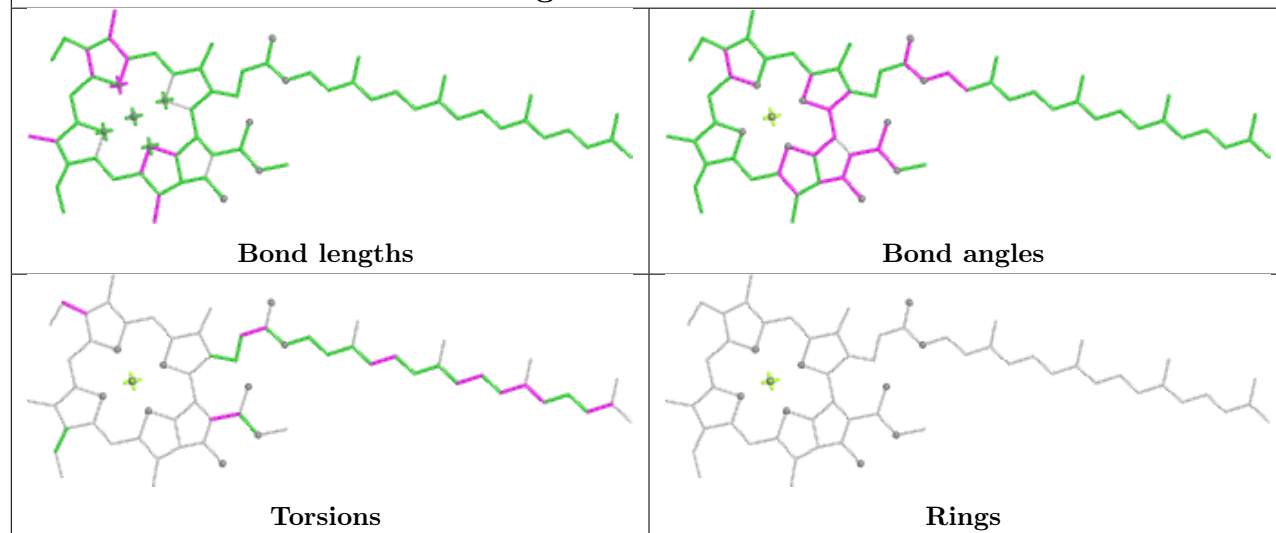
Ligand A86 W 203

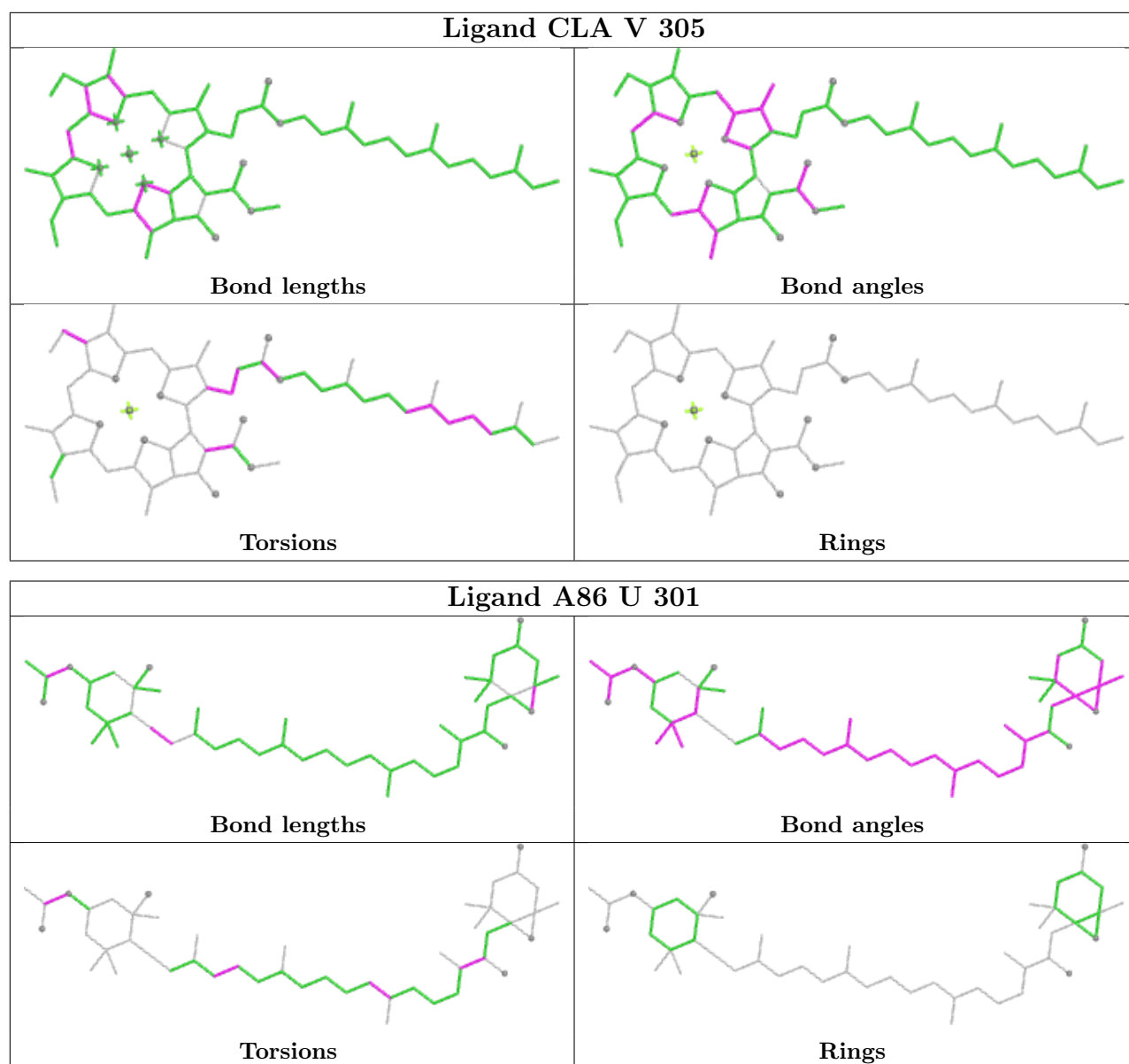


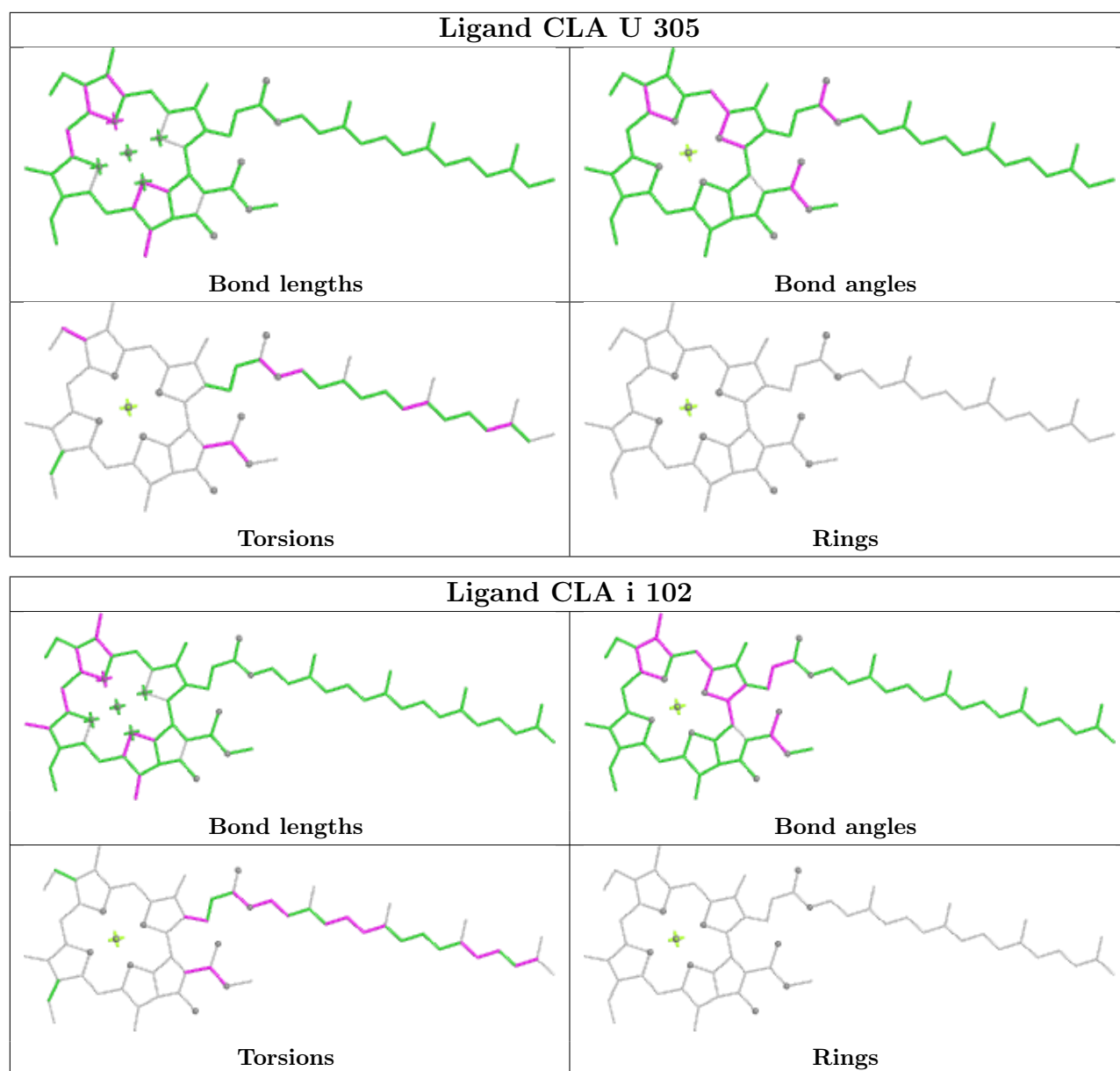
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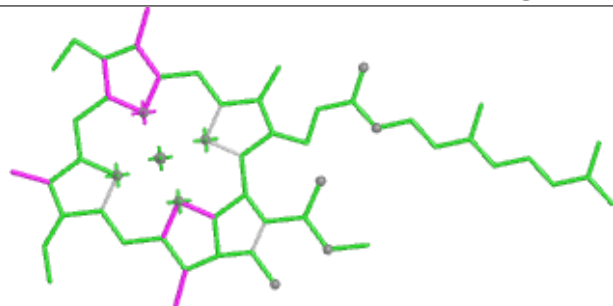


Ligand CLA a 801

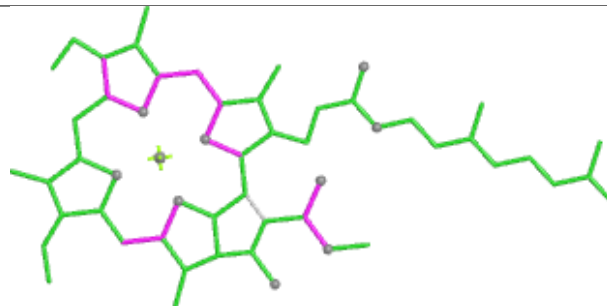




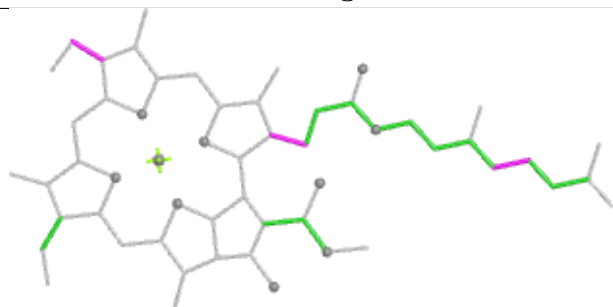


Ligand CLA b 814

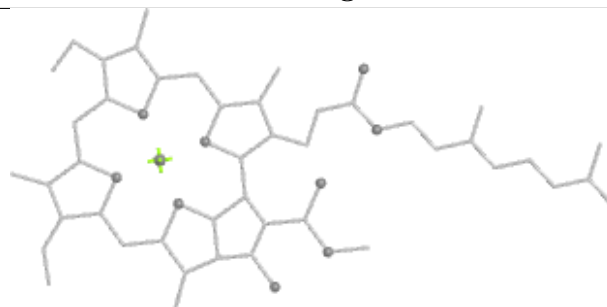
Bond lengths



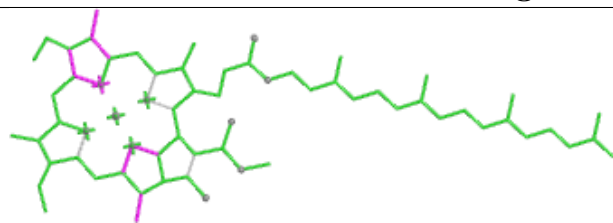
Bond angles



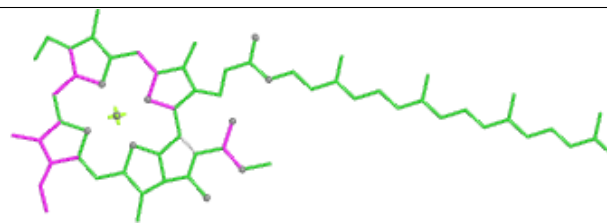
Torsions



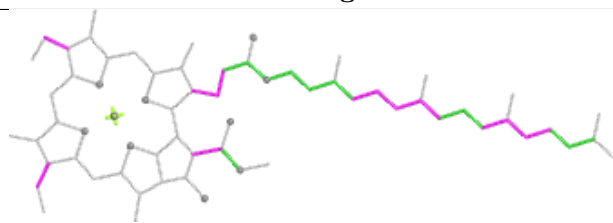
Rings

Ligand CLA E 316

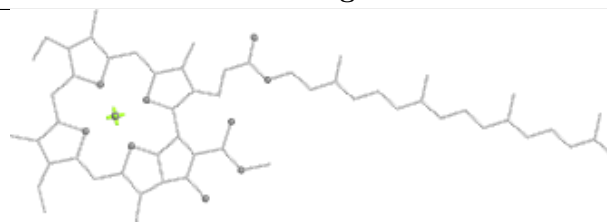
Bond lengths



Bond angles

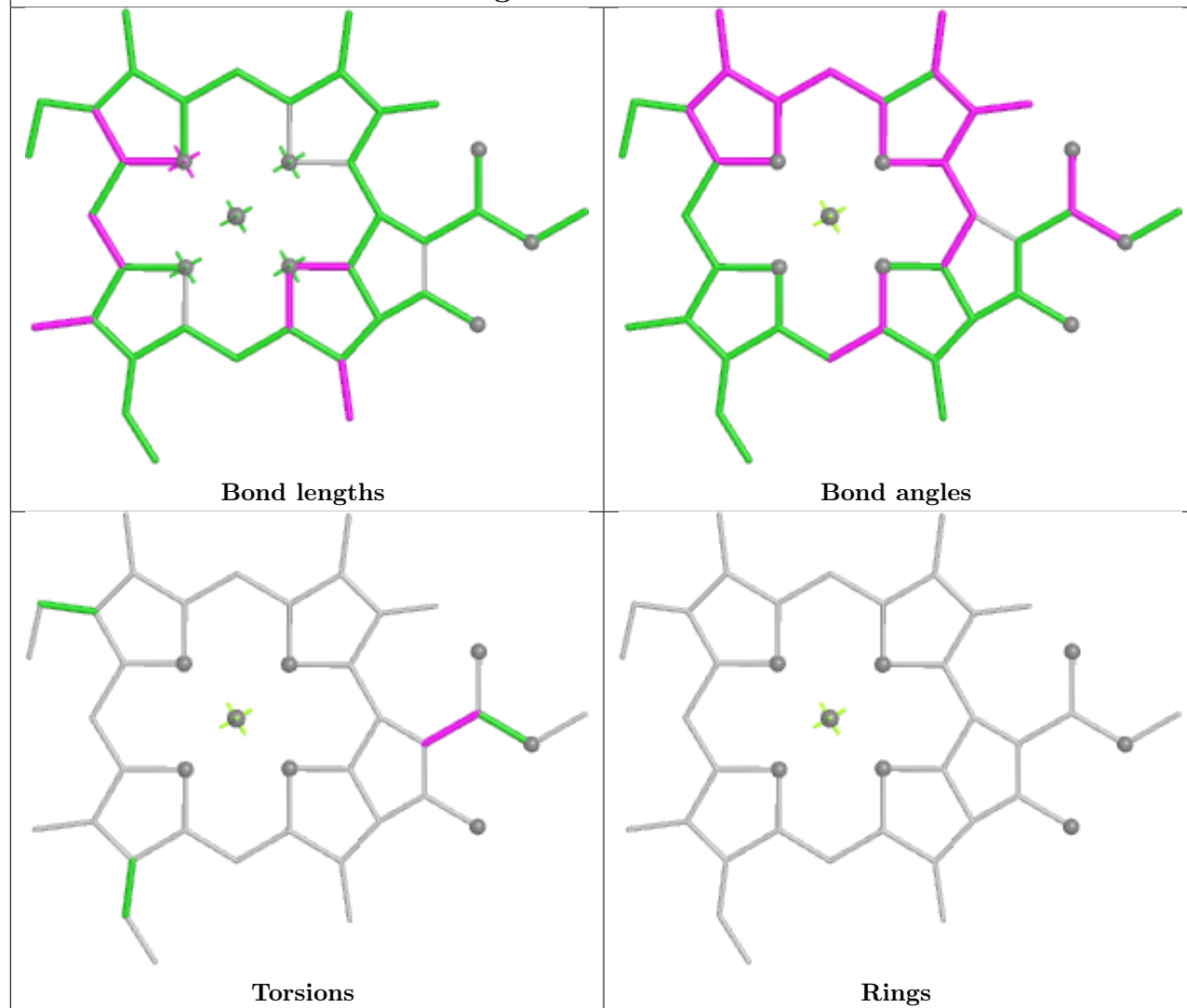


Torsions

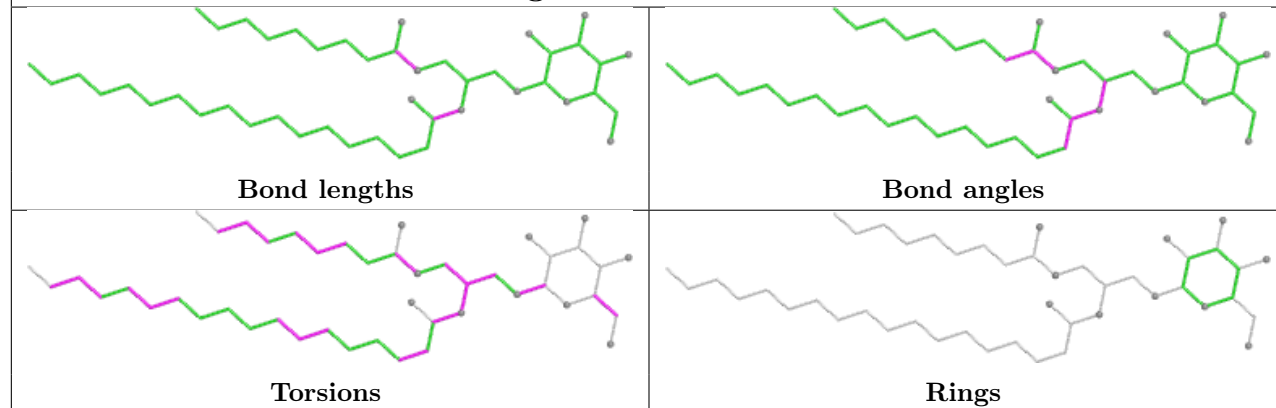


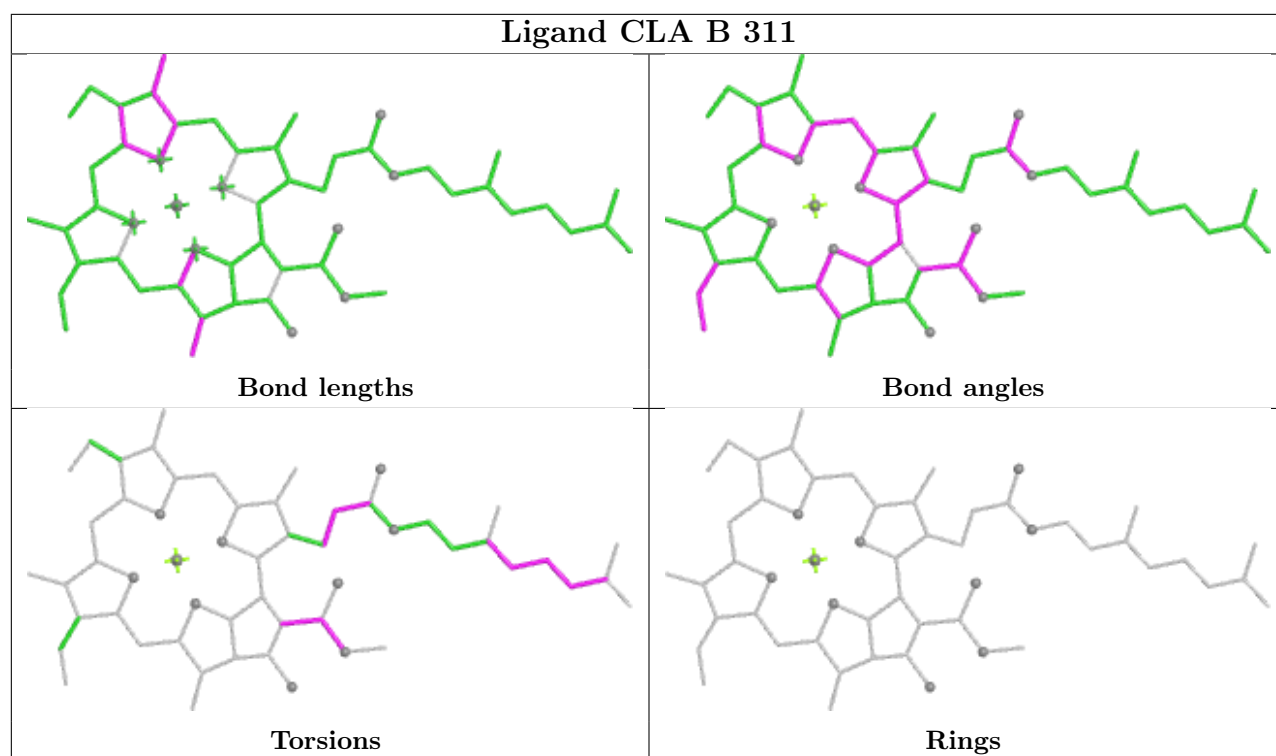
Rings

Ligand CLA N 313

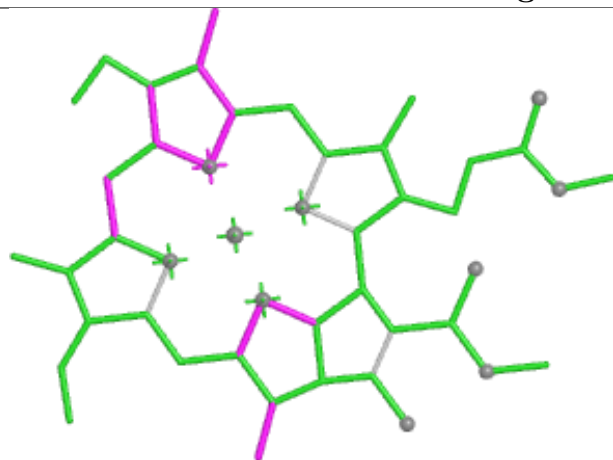


Ligand LMG D 320

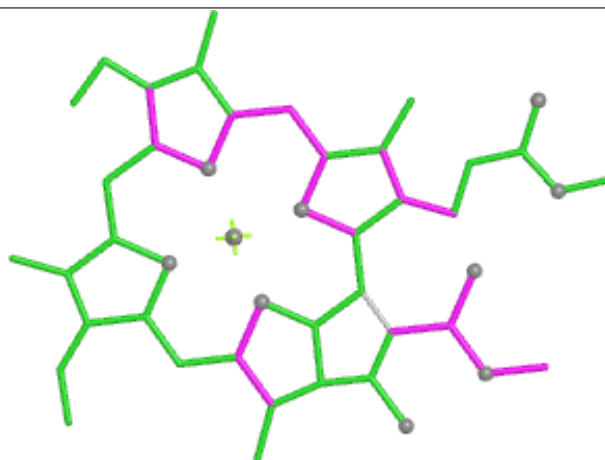




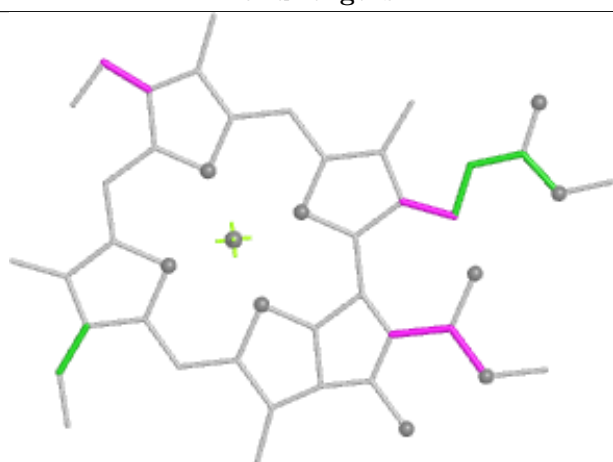
Ligand CLA b 822



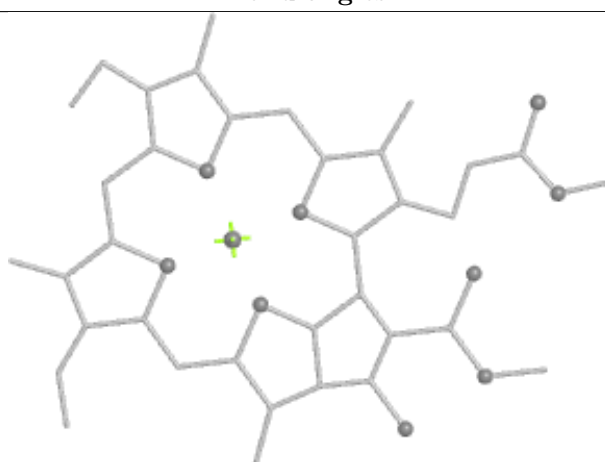
Bond lengths



Bond angles

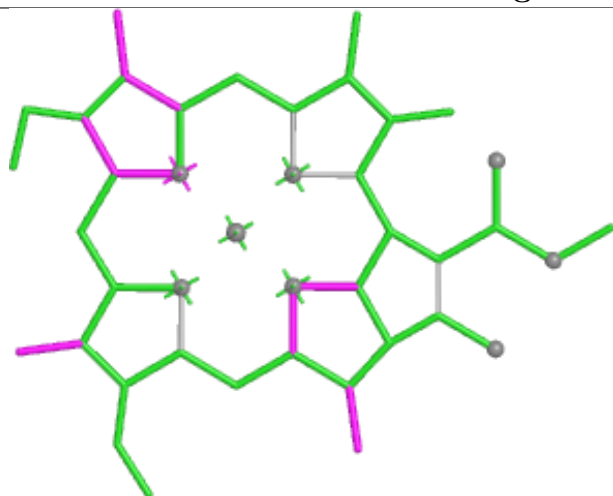


Torsions

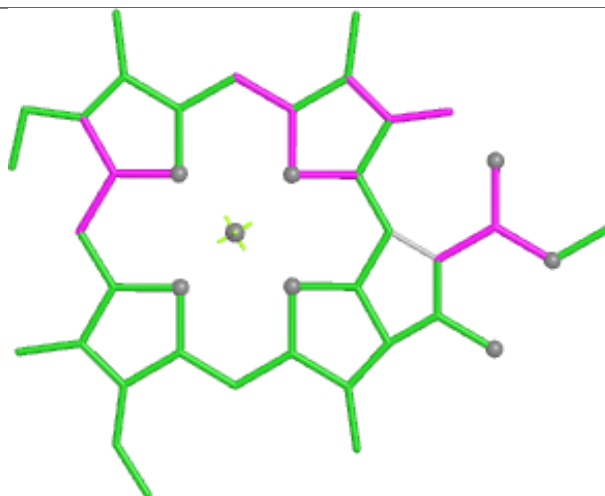


Rings

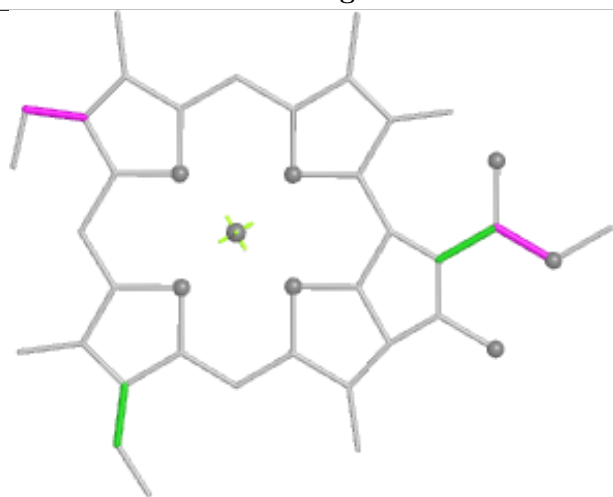
Ligand CLA A 313



Bond lengths



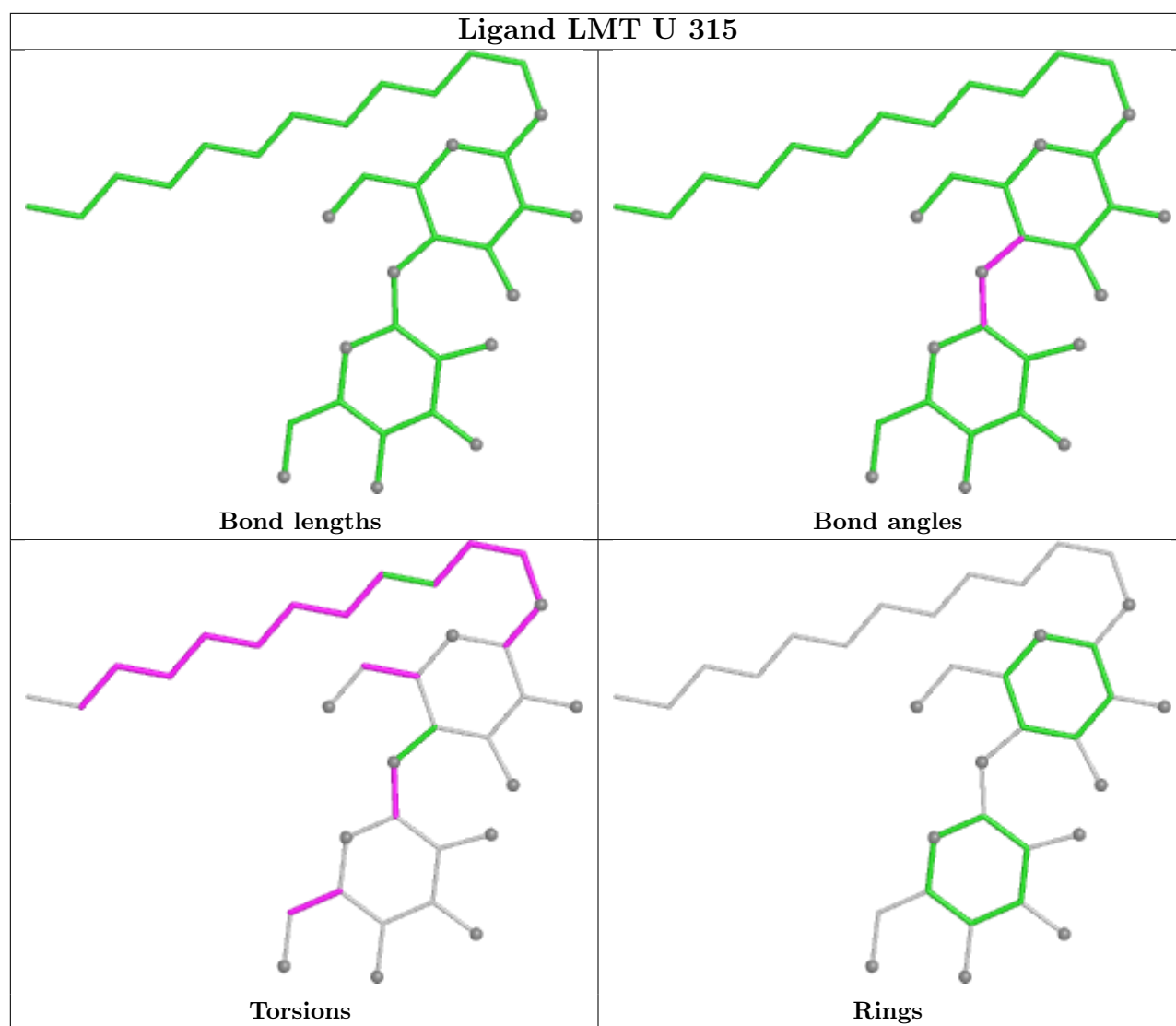
Bond angles

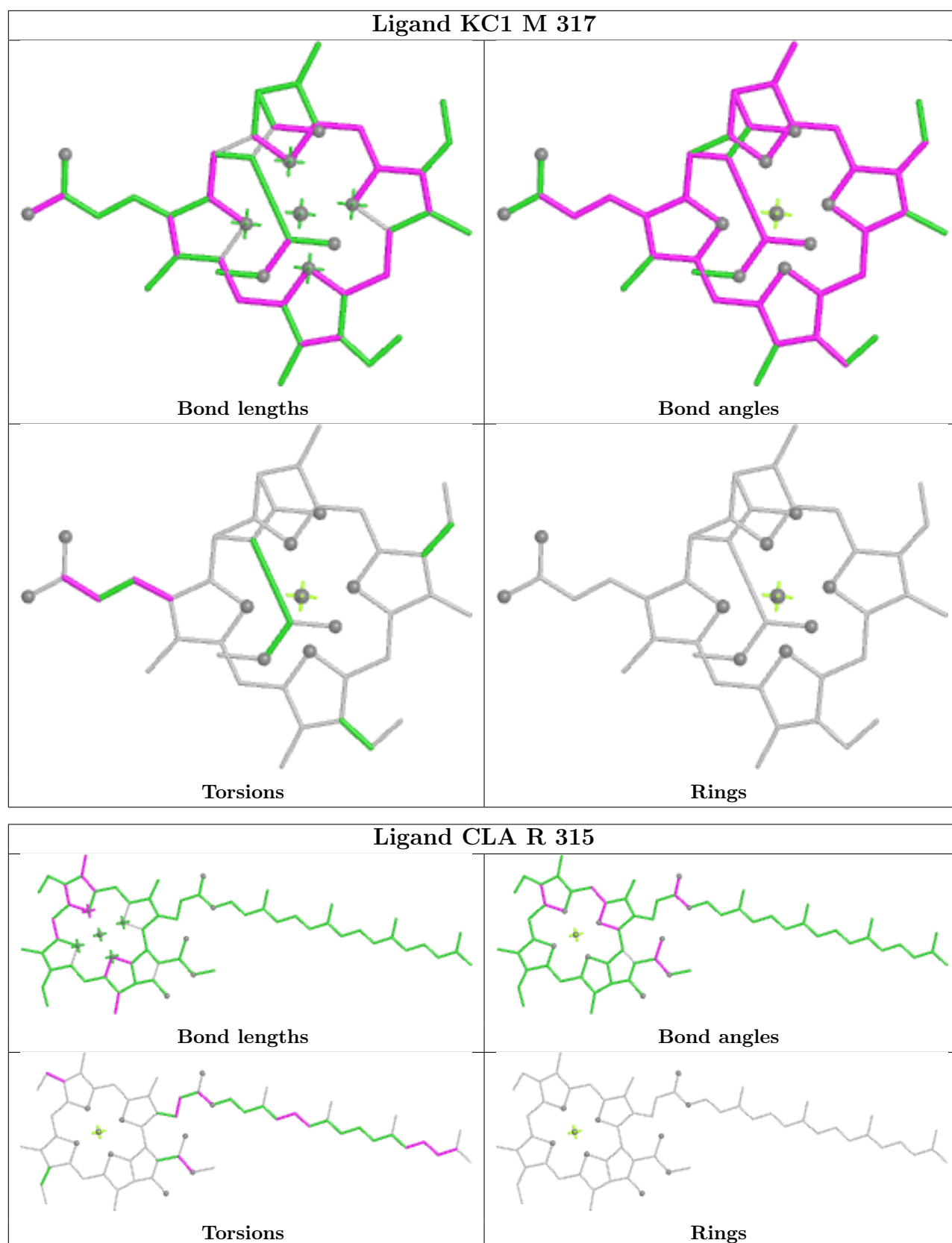


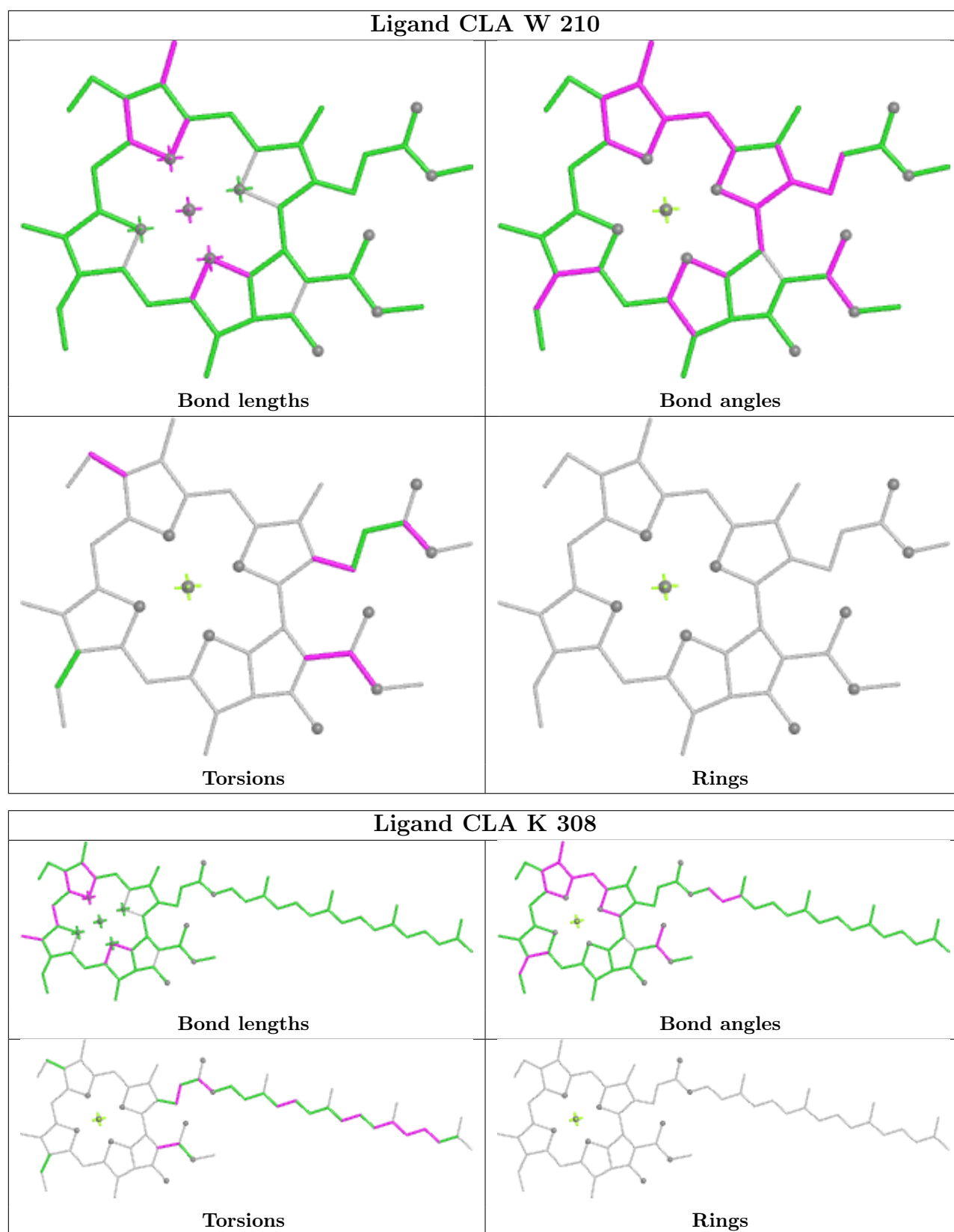
Torsions



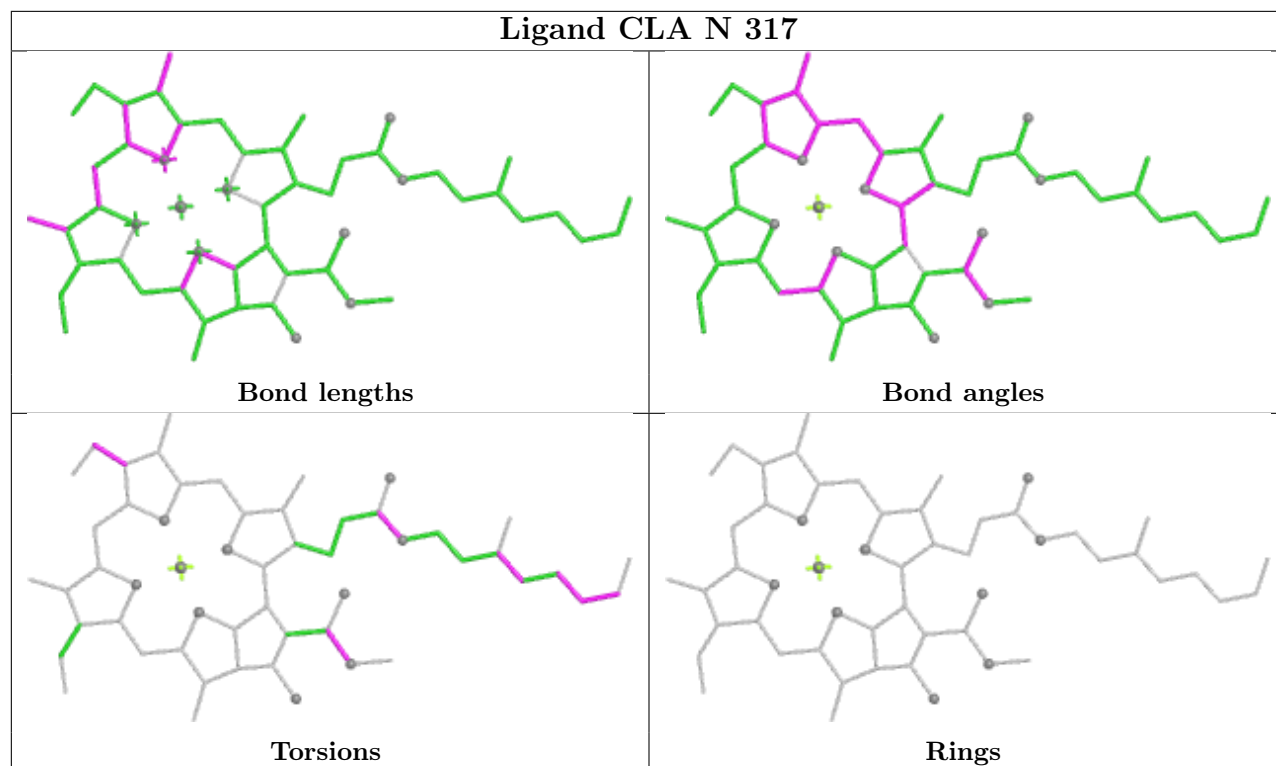
Rings



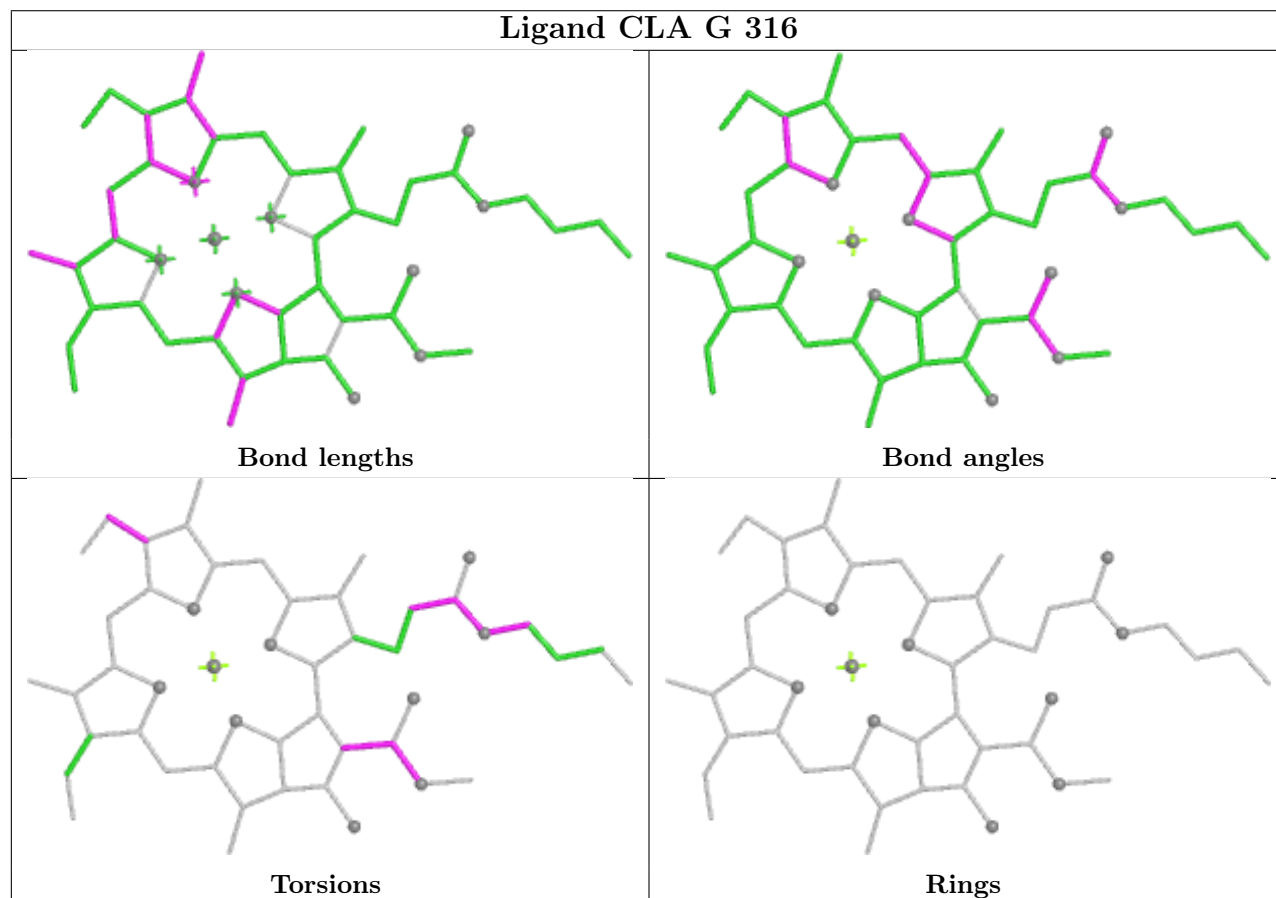


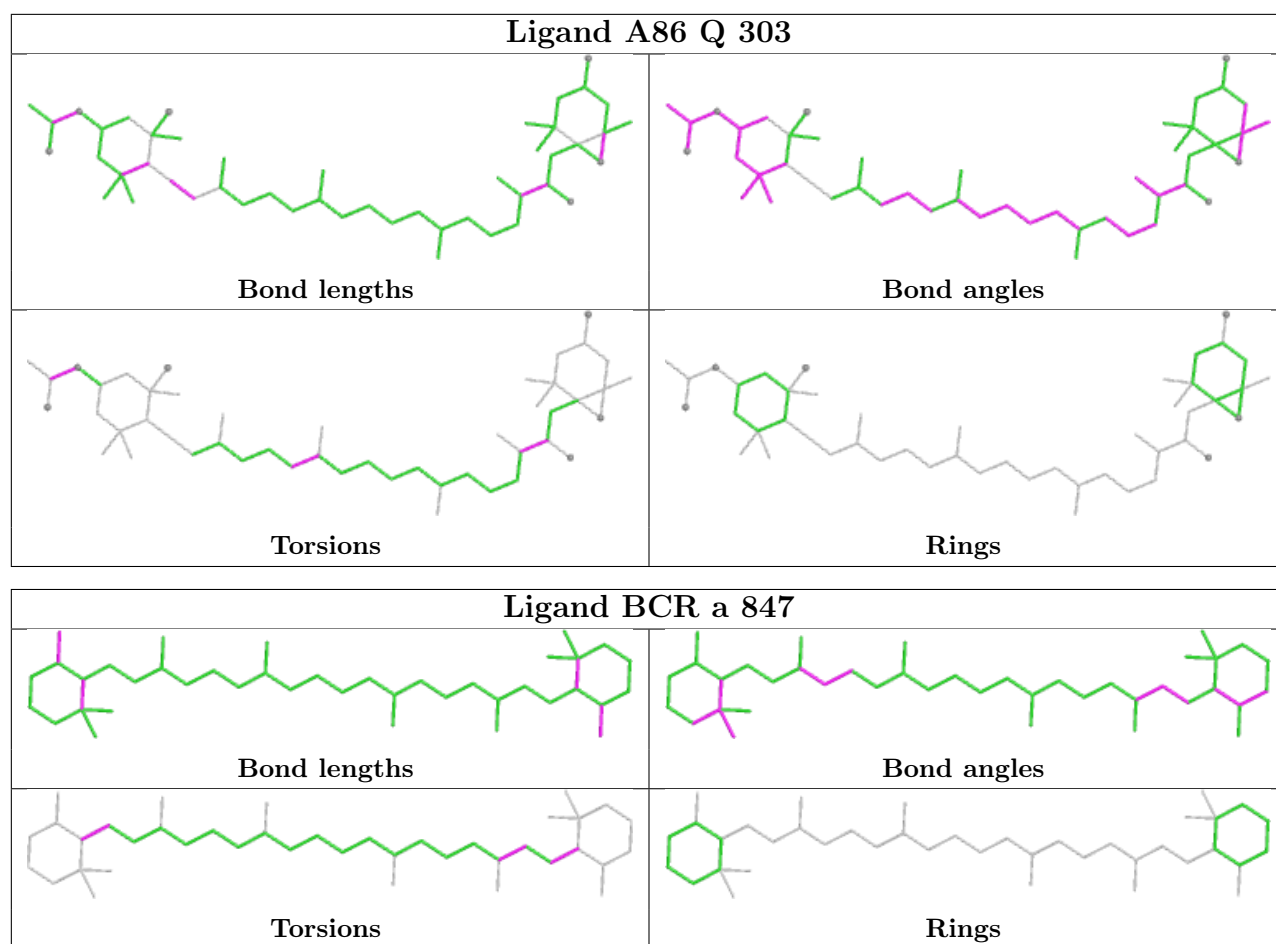


Ligand CLA N 317

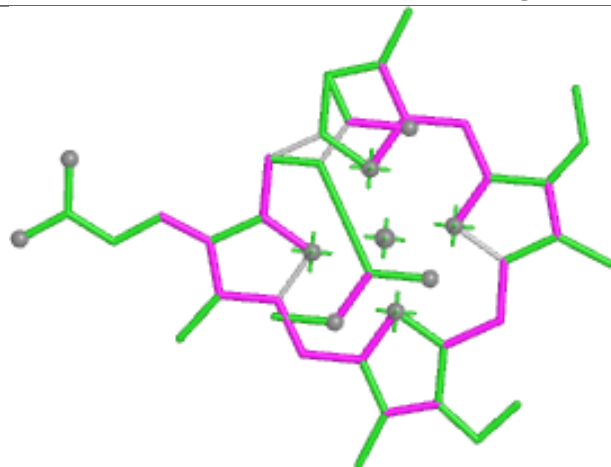


Ligand CLA G 316

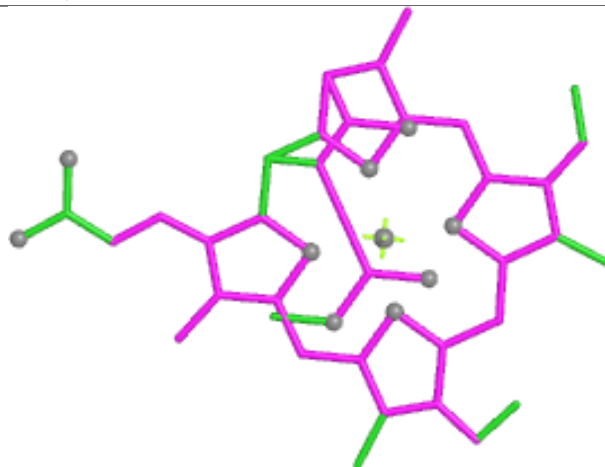




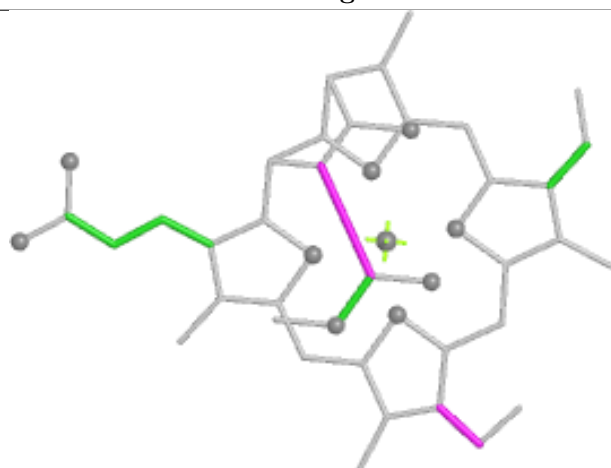
Ligand KC1 Q 313



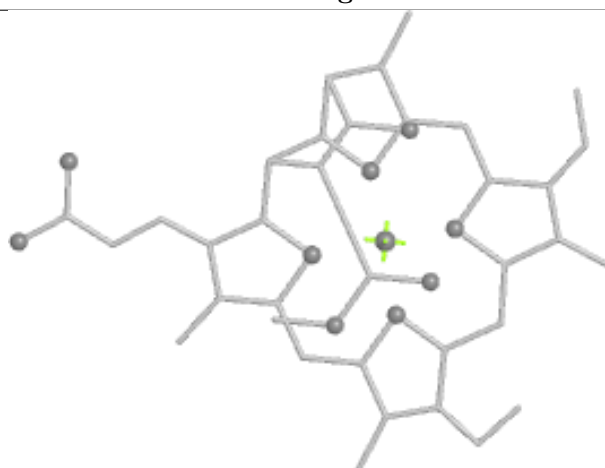
Bond lengths



Bond angles

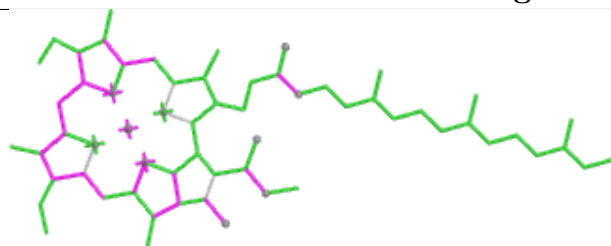


Torsions

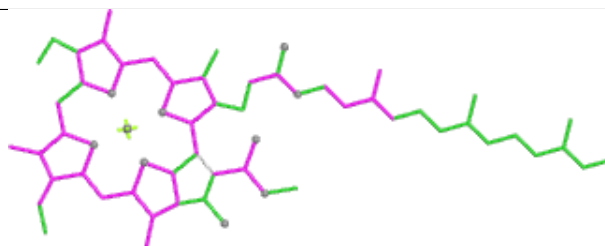


Rings

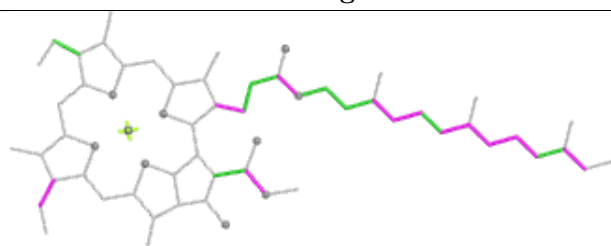
Ligand CLA A 306



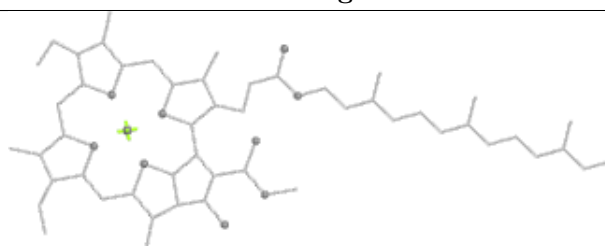
Bond lengths



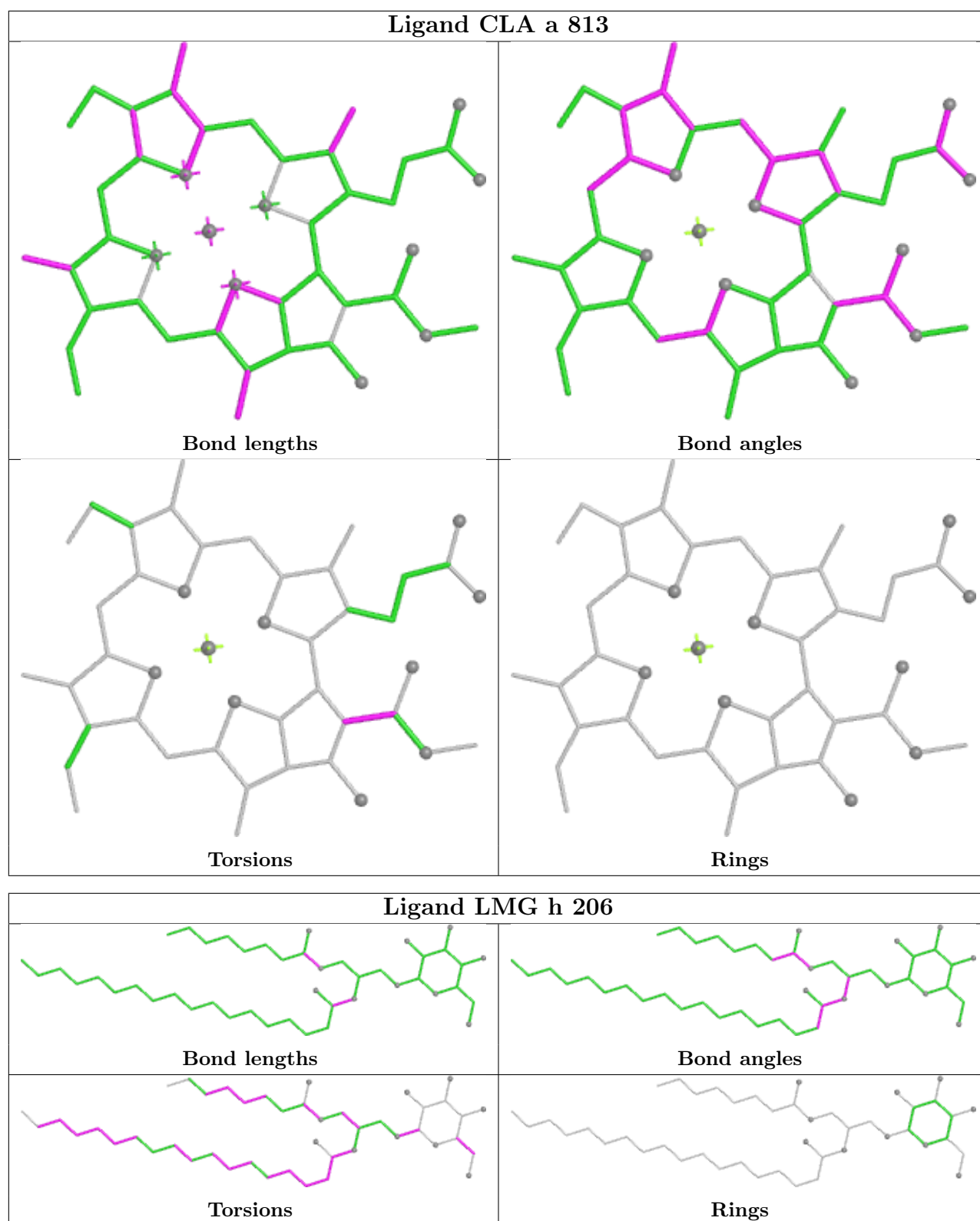
Bond angles

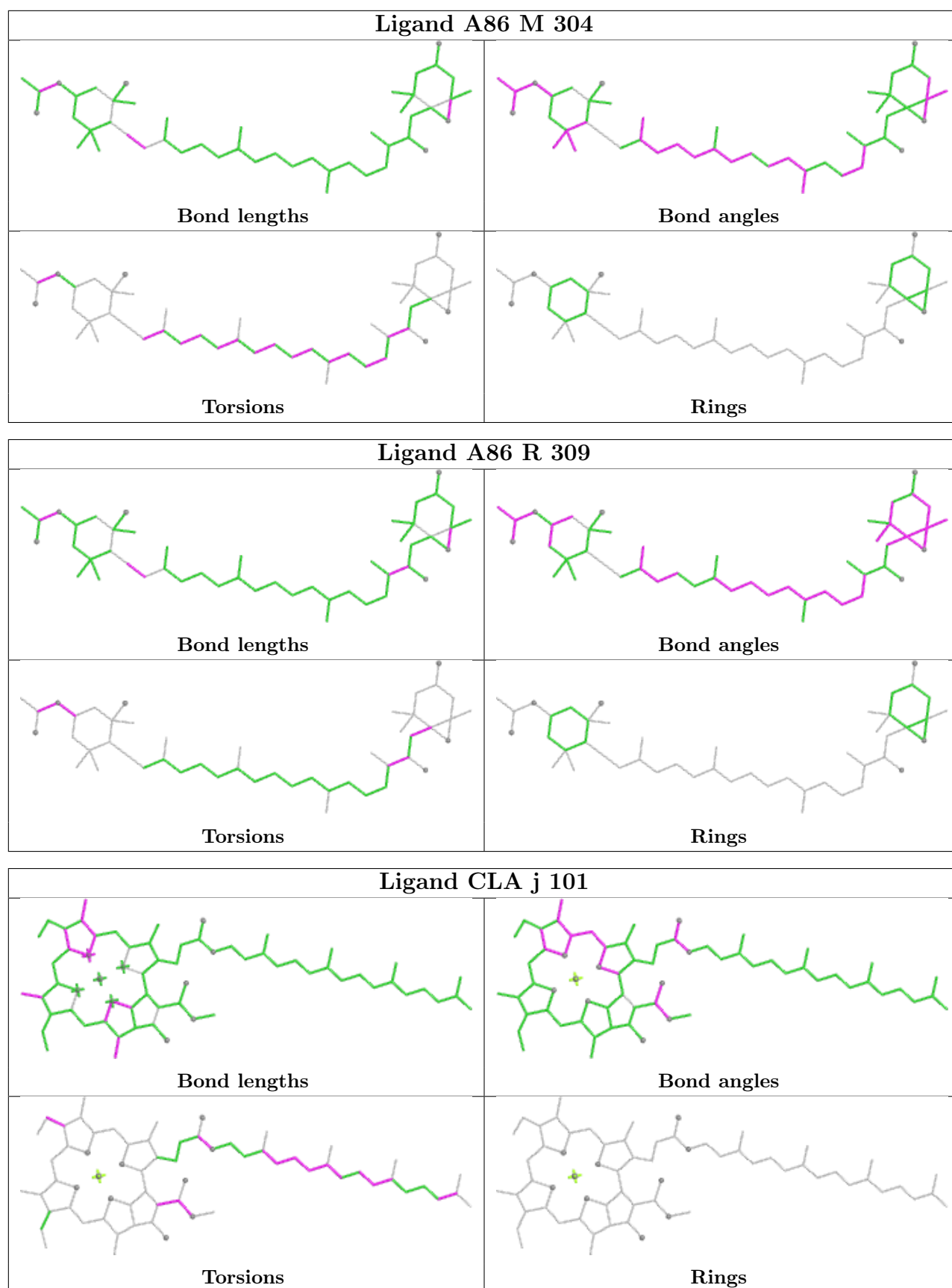


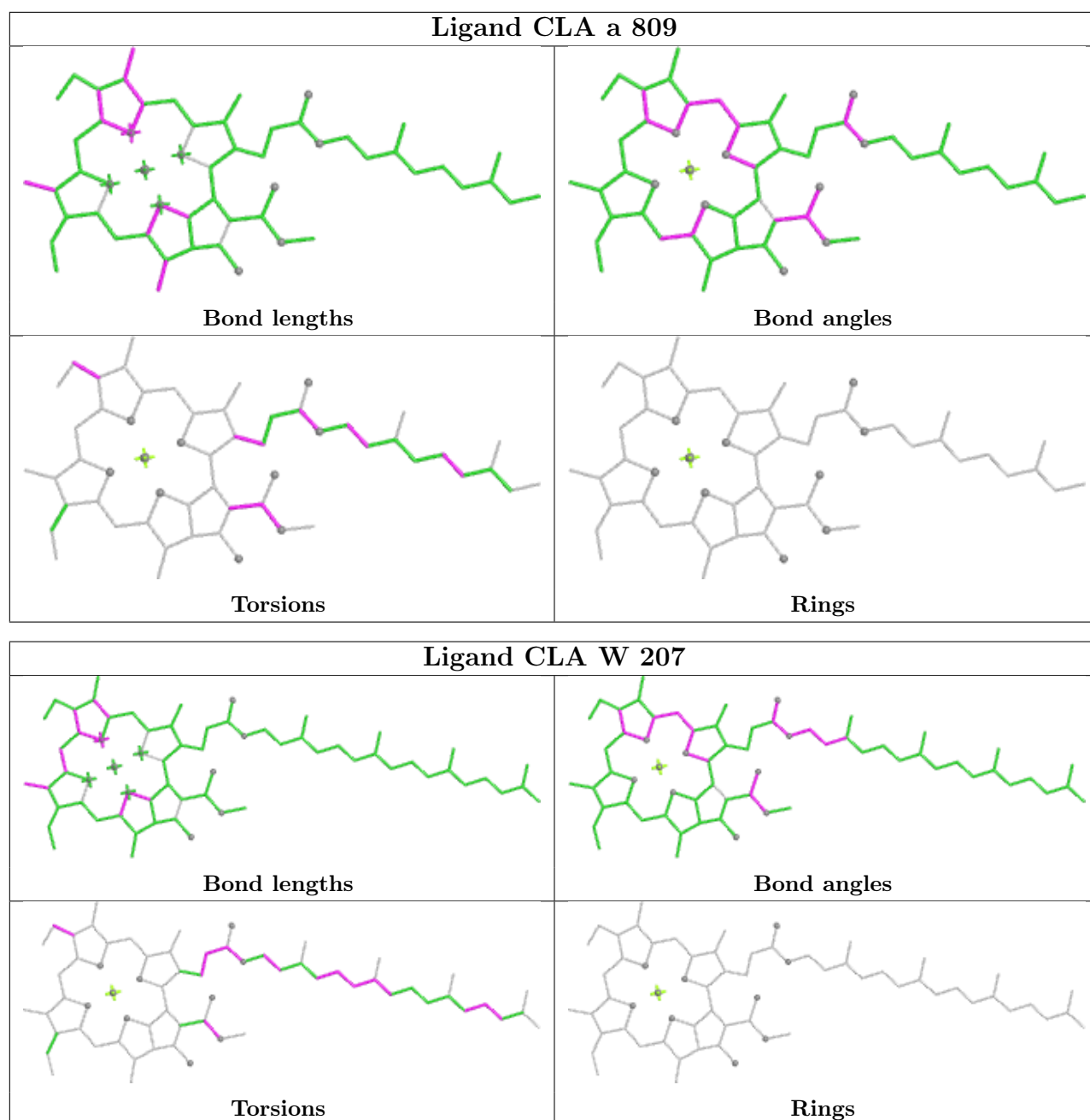
Torsions

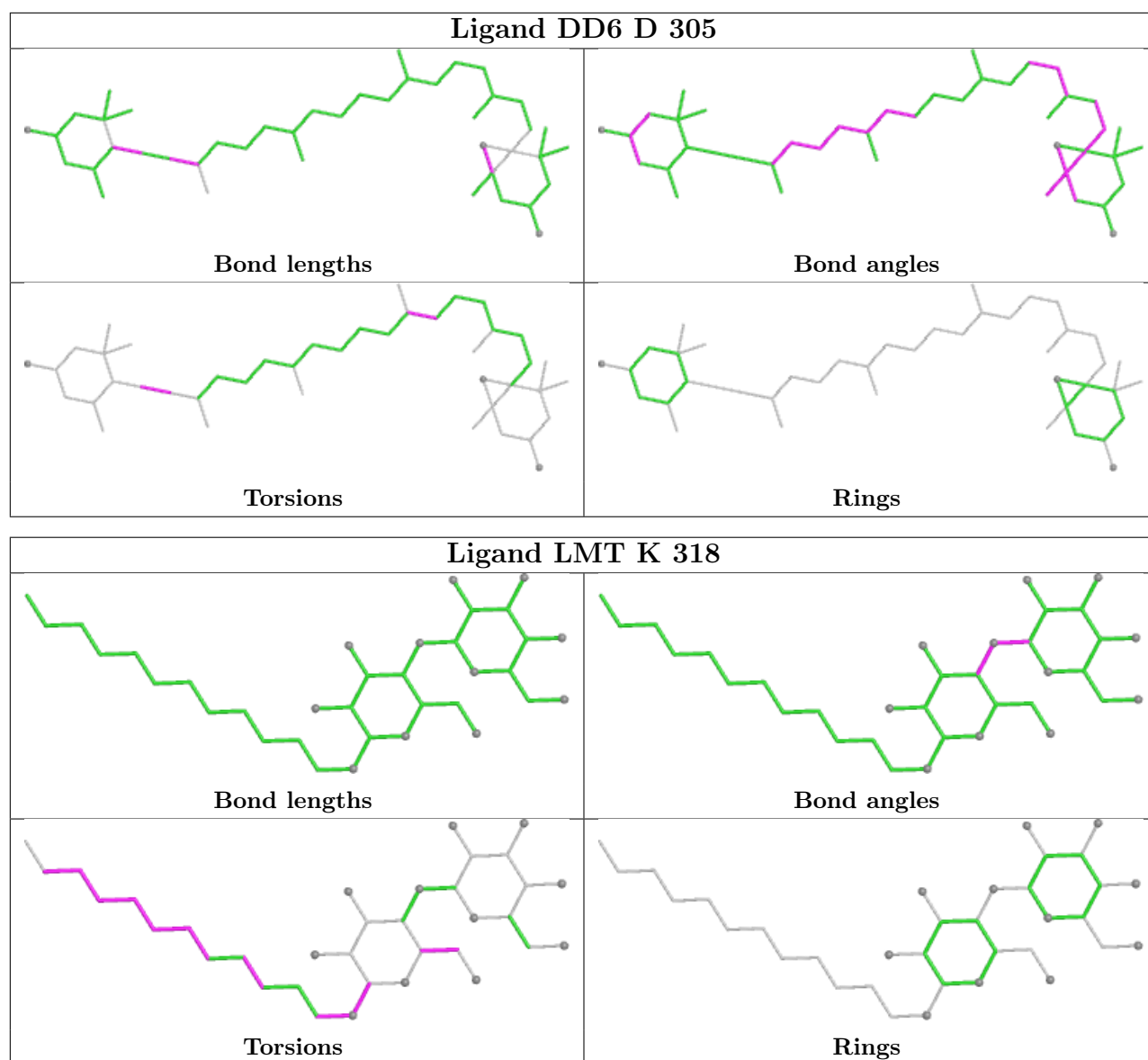


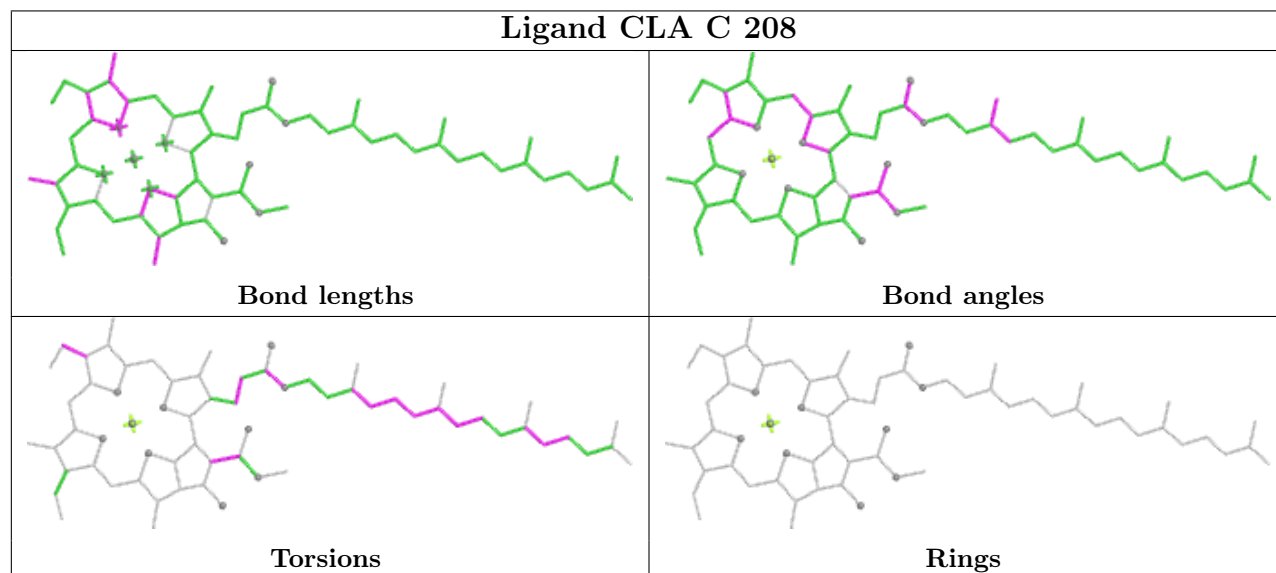
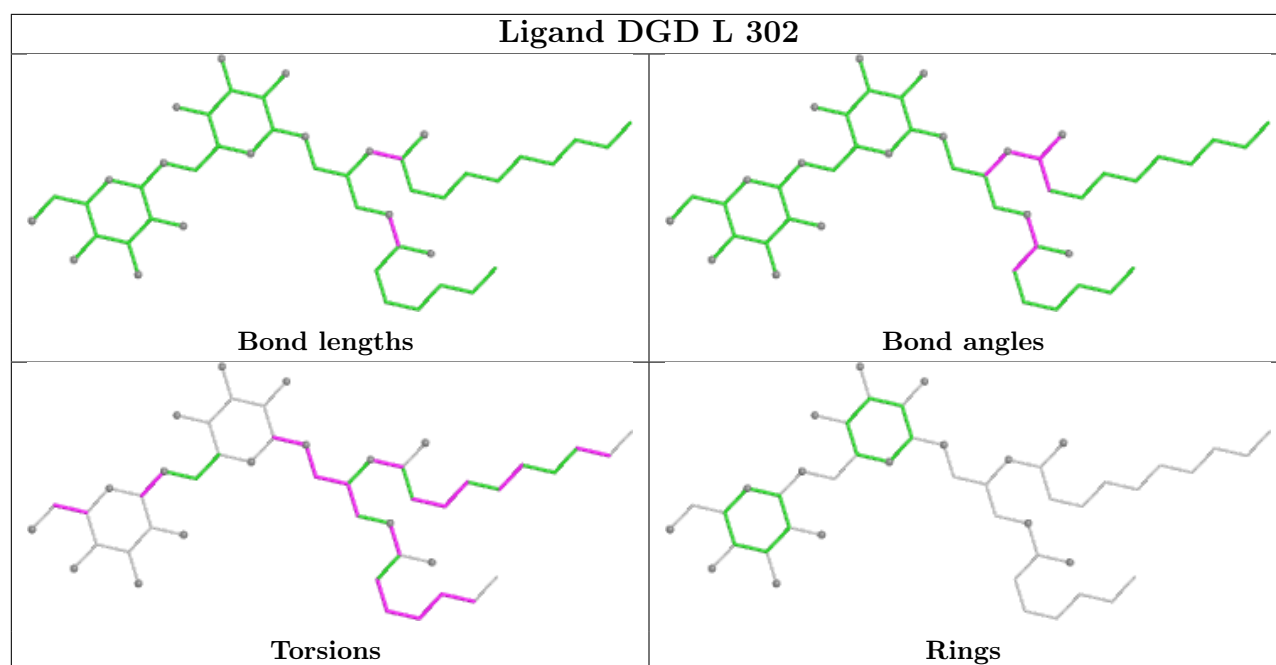
Rings

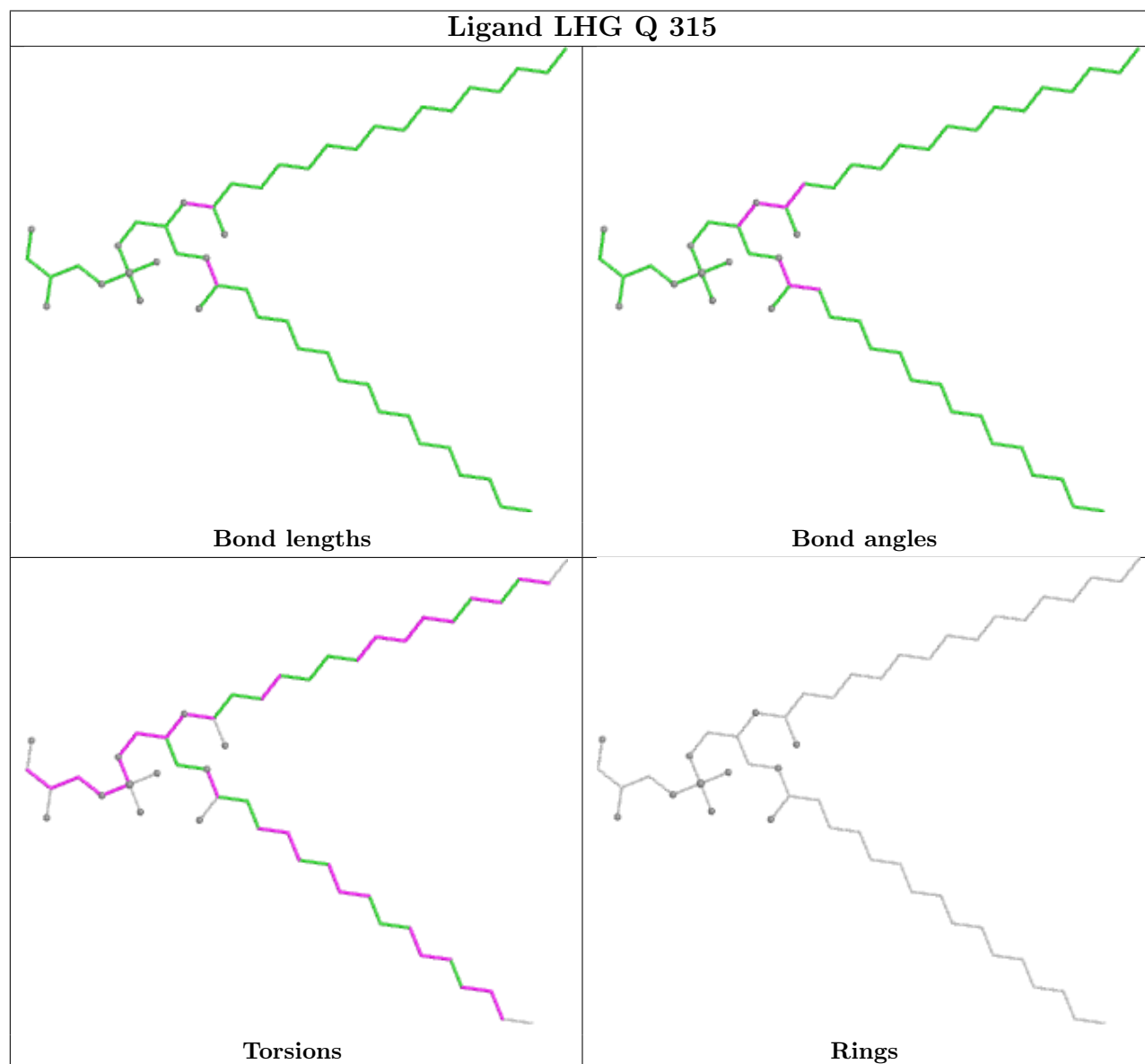
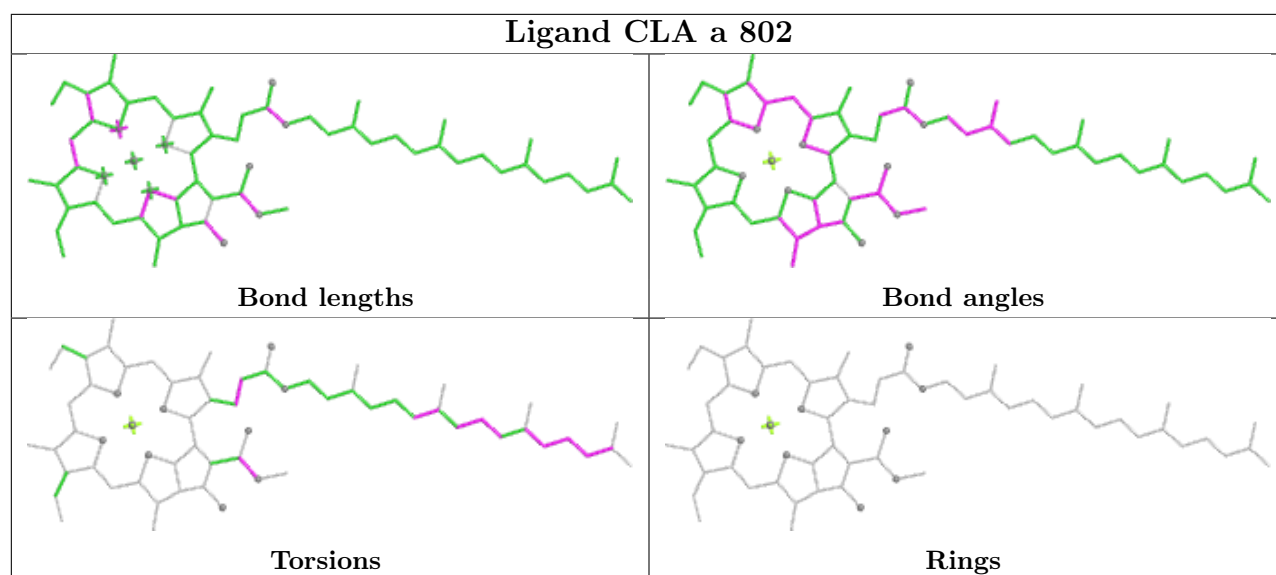


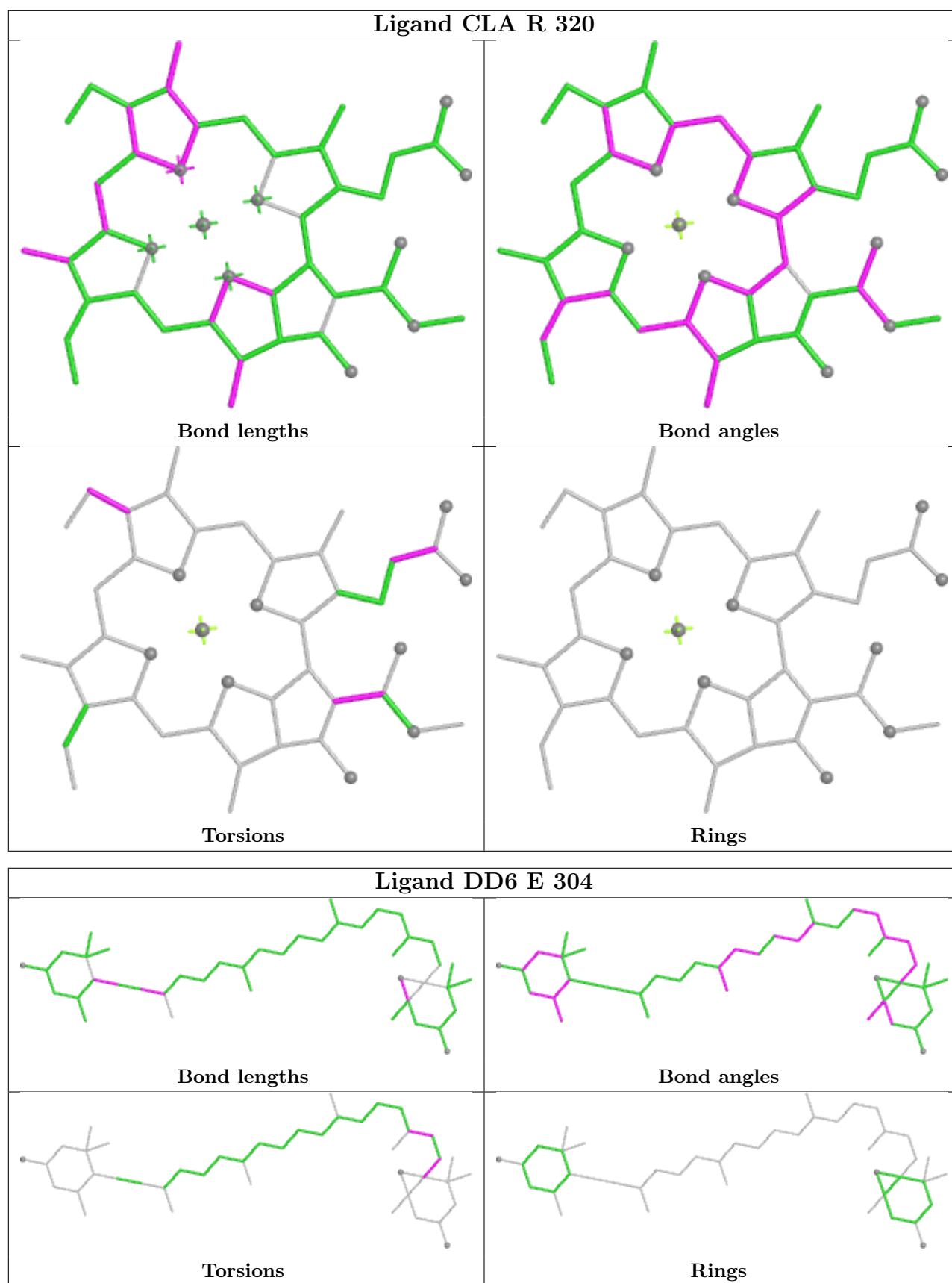


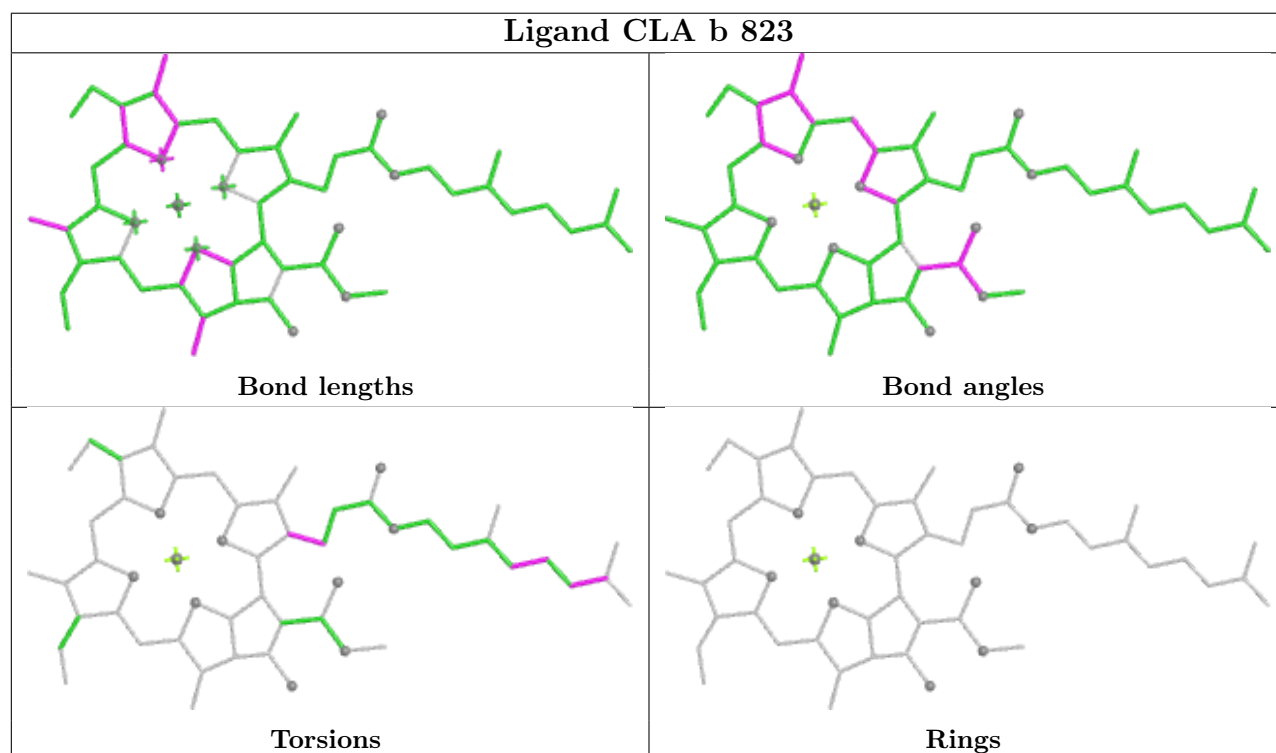
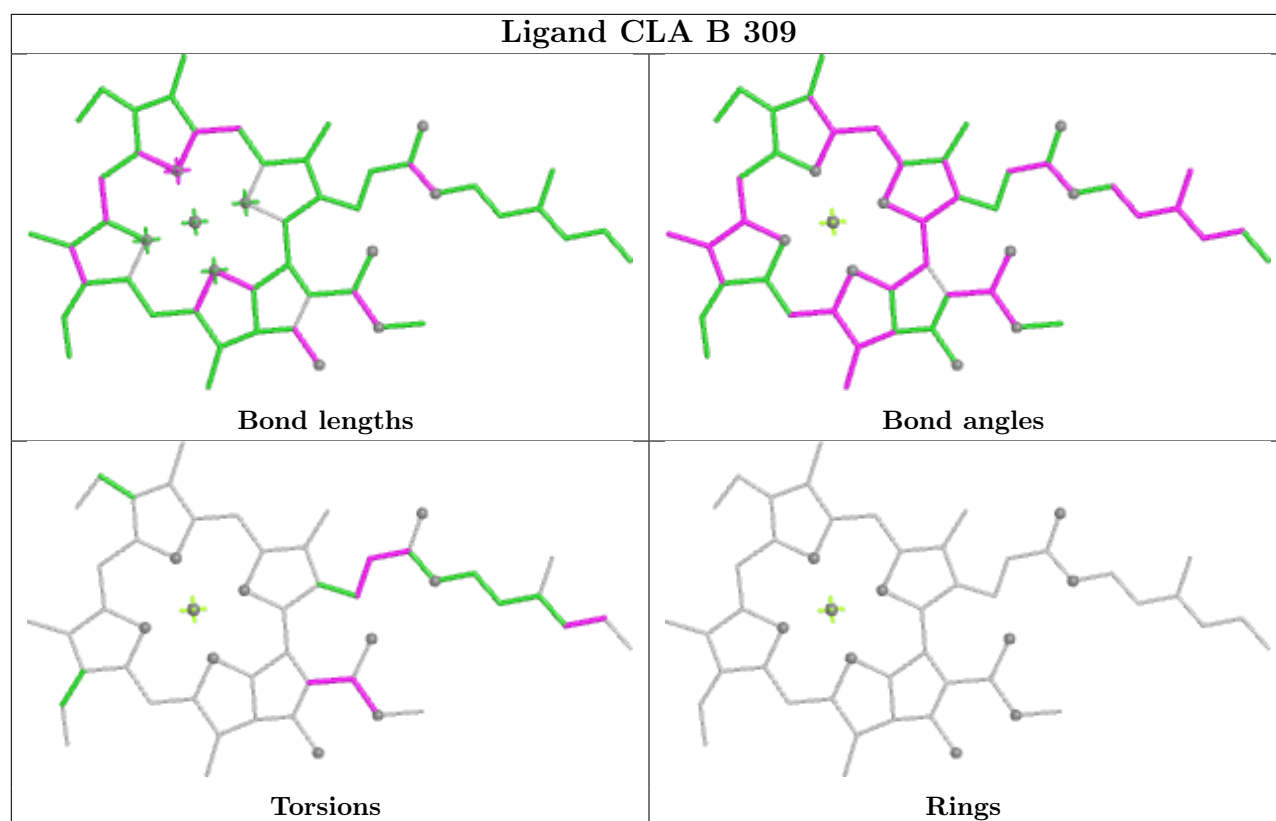


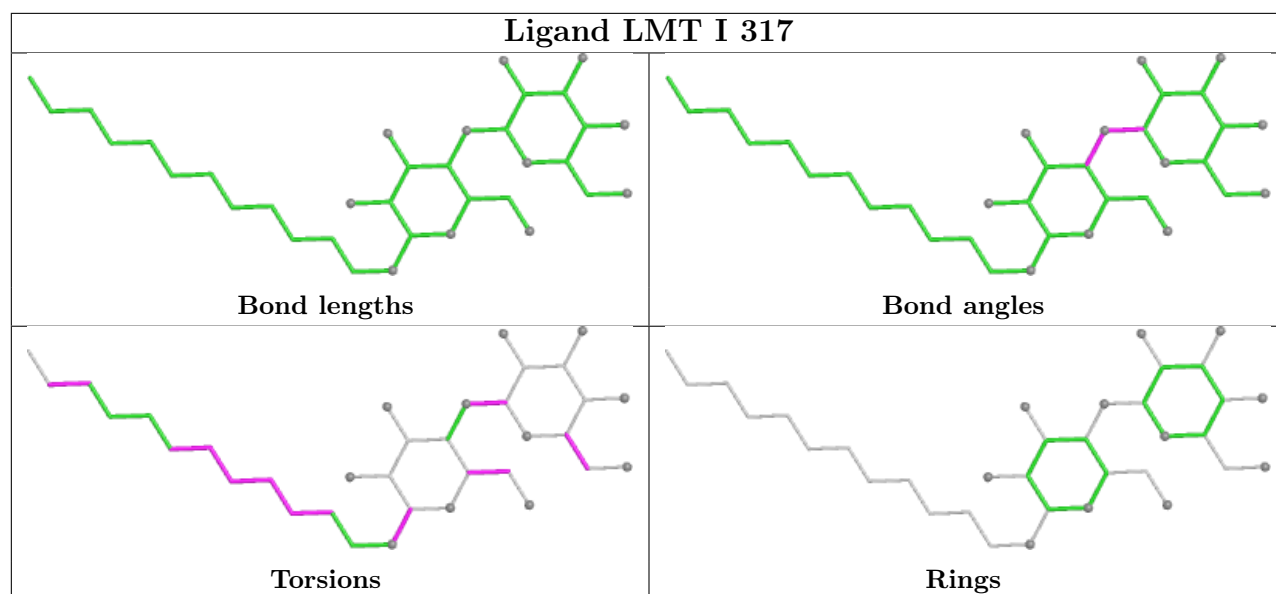
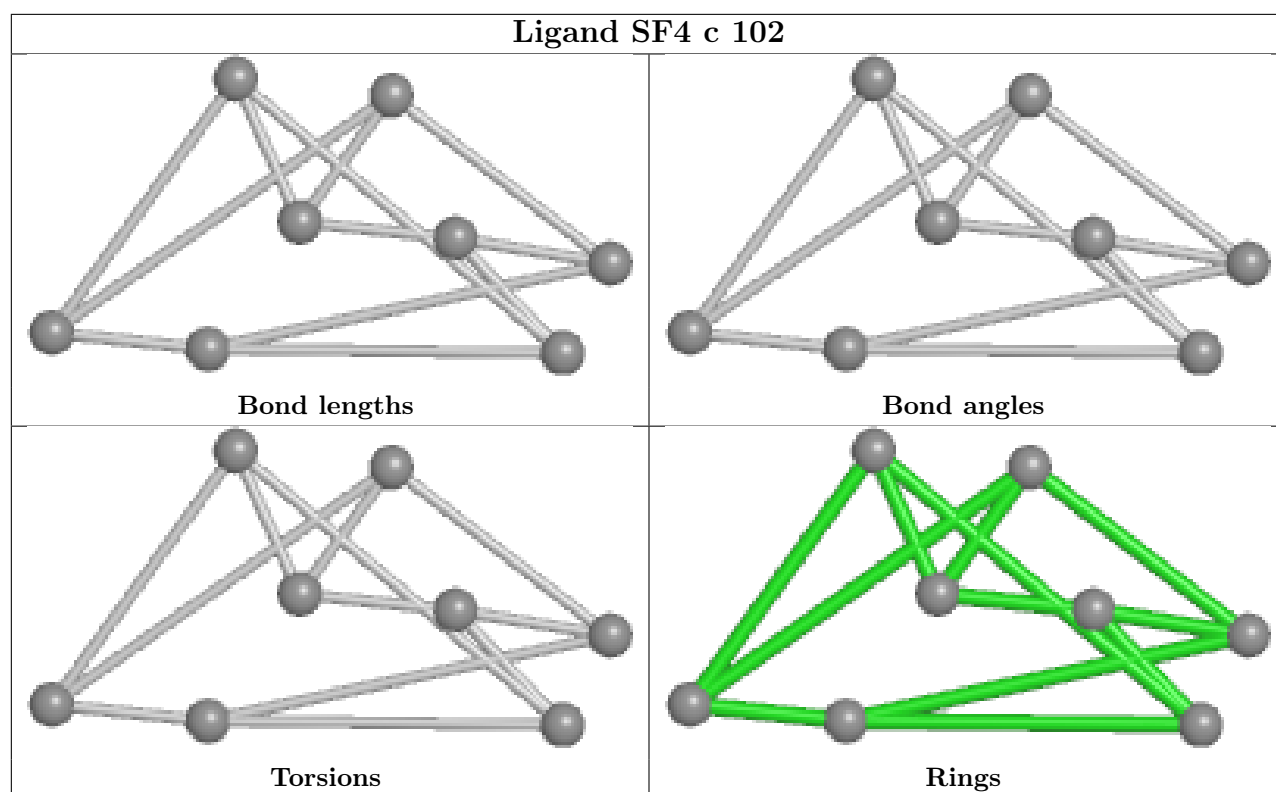


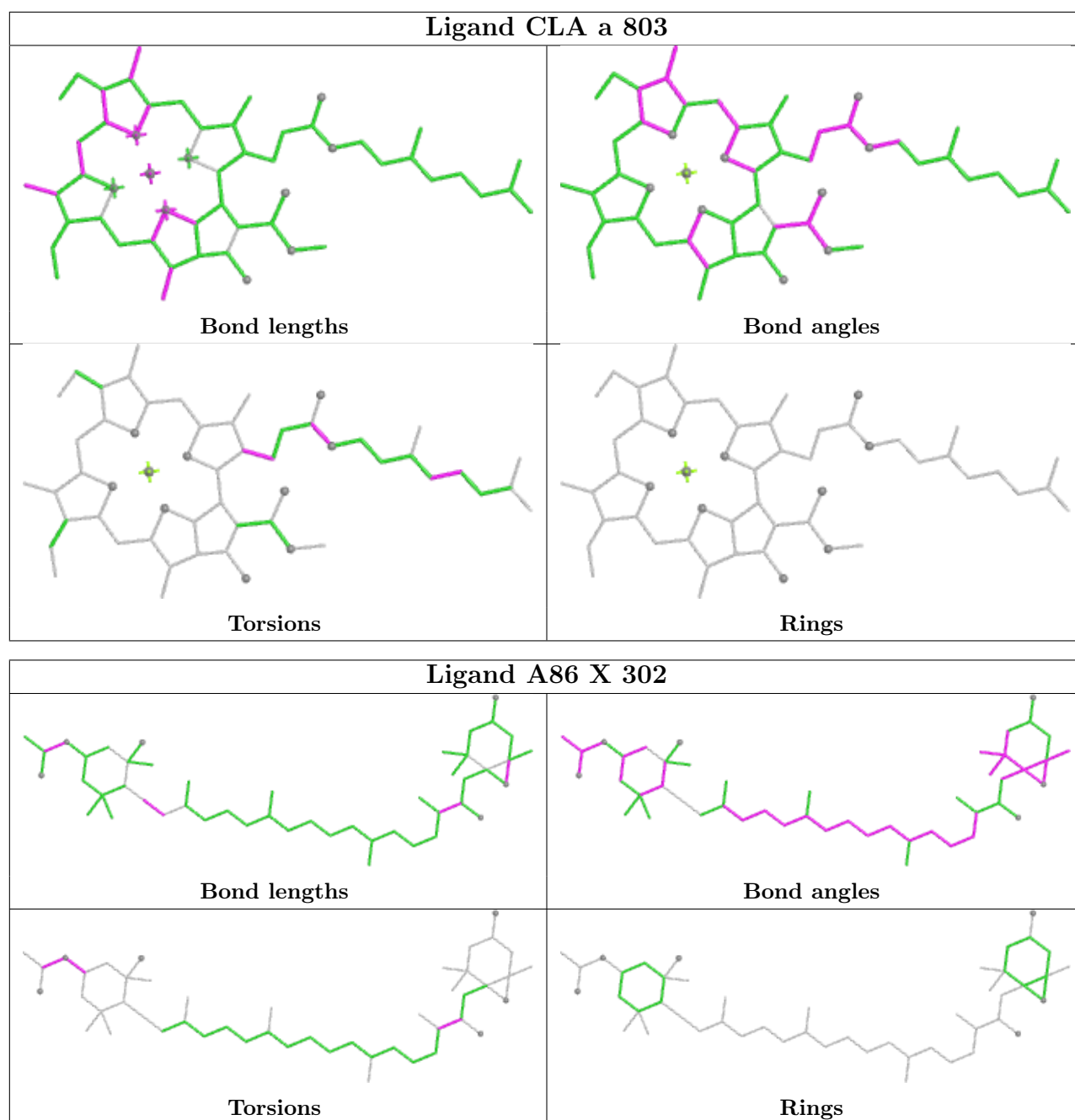


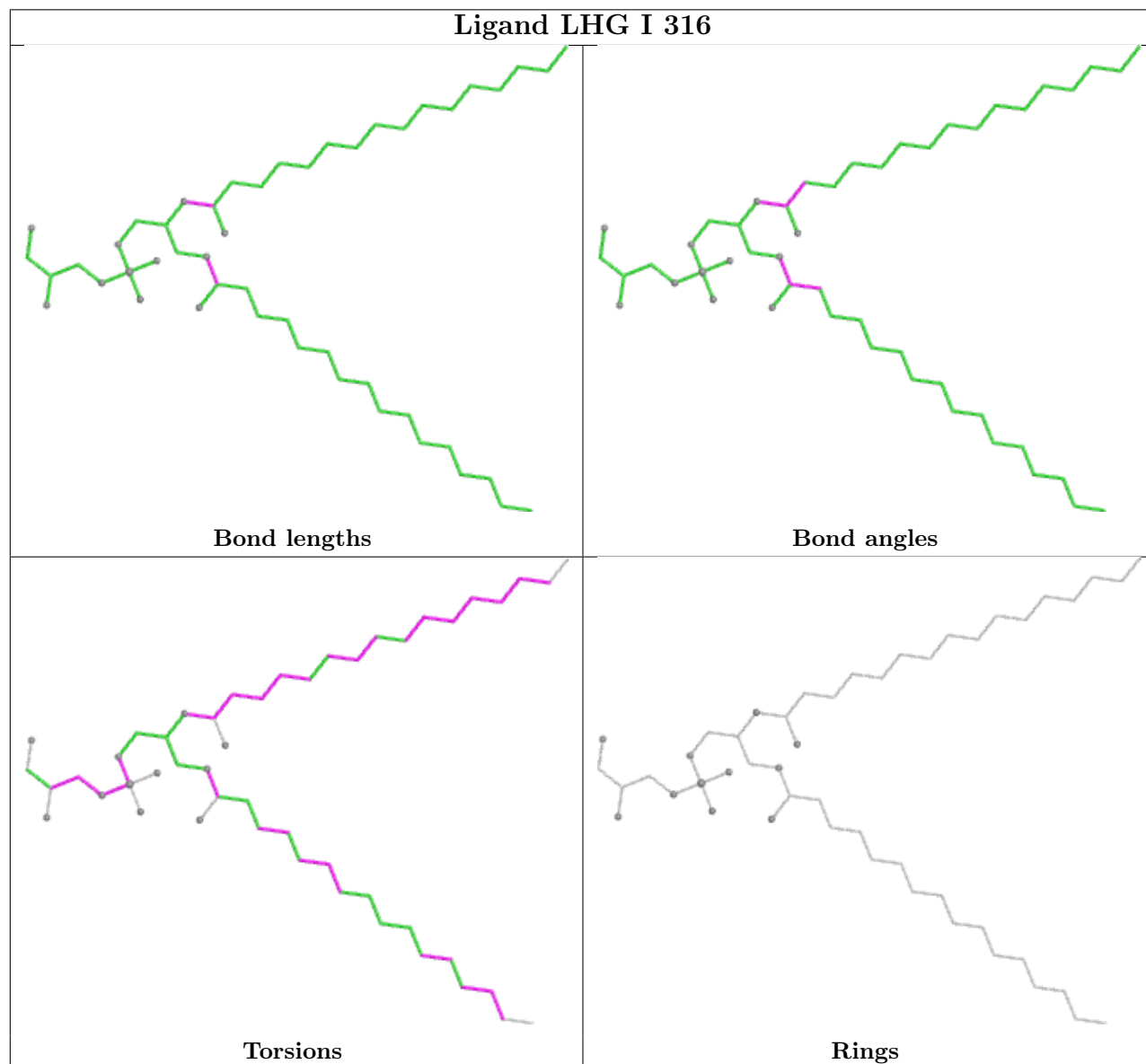
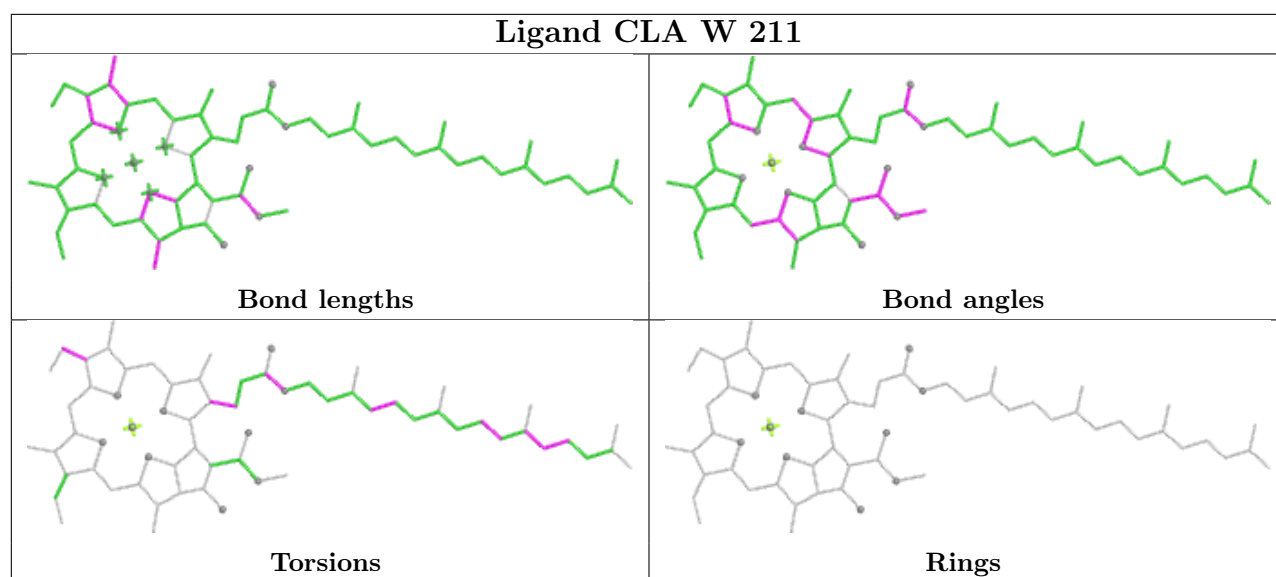




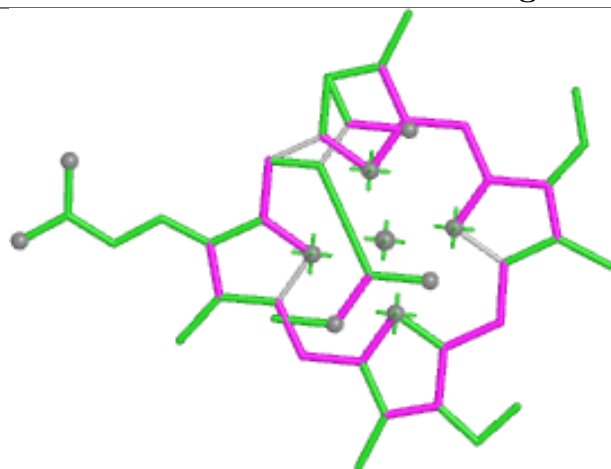




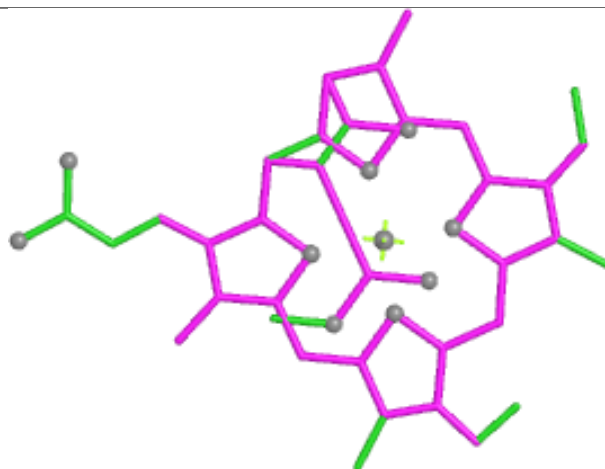




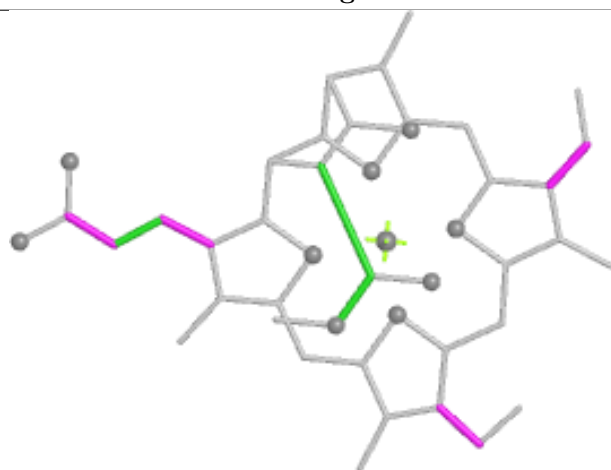
Ligand KC1 S 316



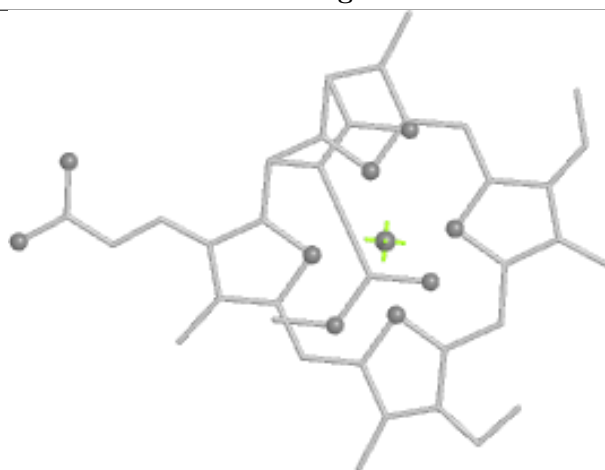
Bond lengths



Bond angles

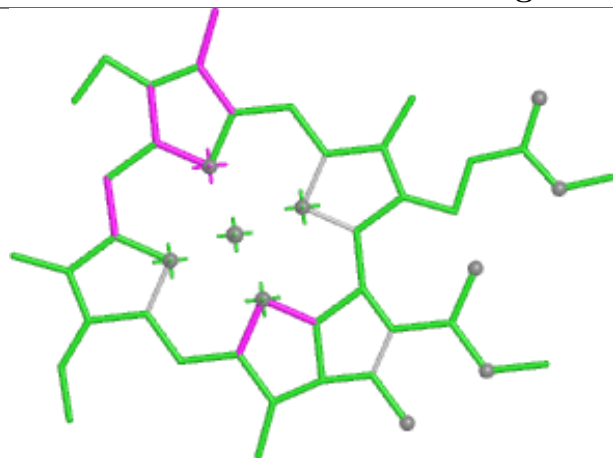


Torsions

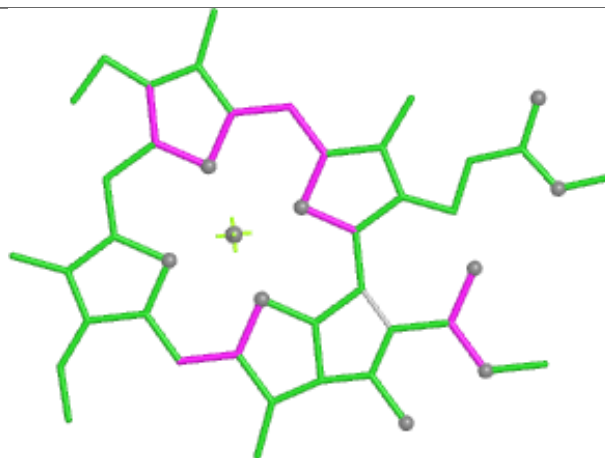


Rings

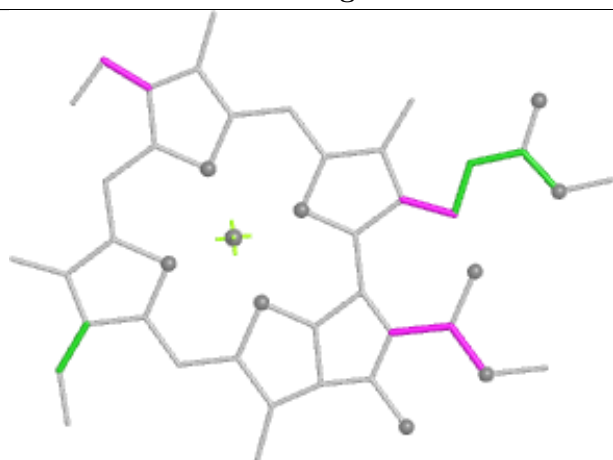
Ligand CLA E 317



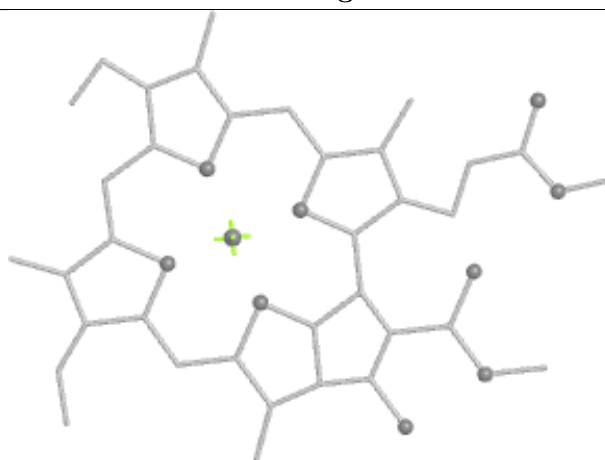
Bond lengths



Bond angles

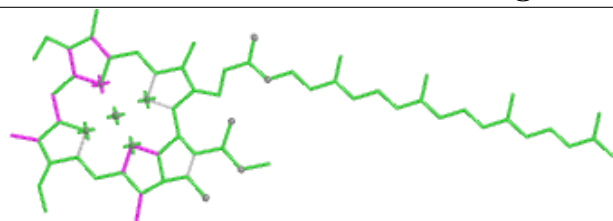


Torsions

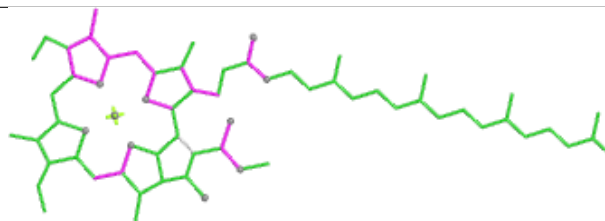


Rings

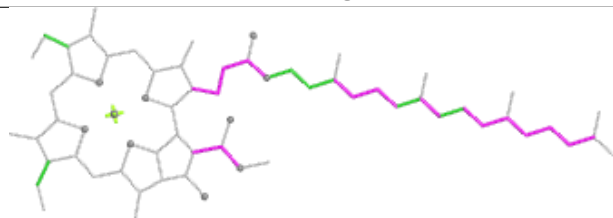
Ligand CLA B 305



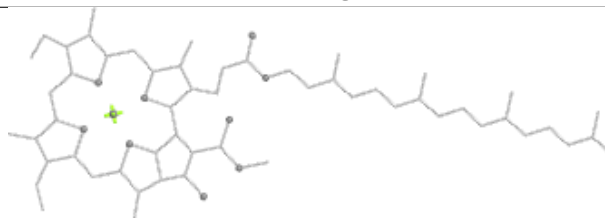
Bond lengths



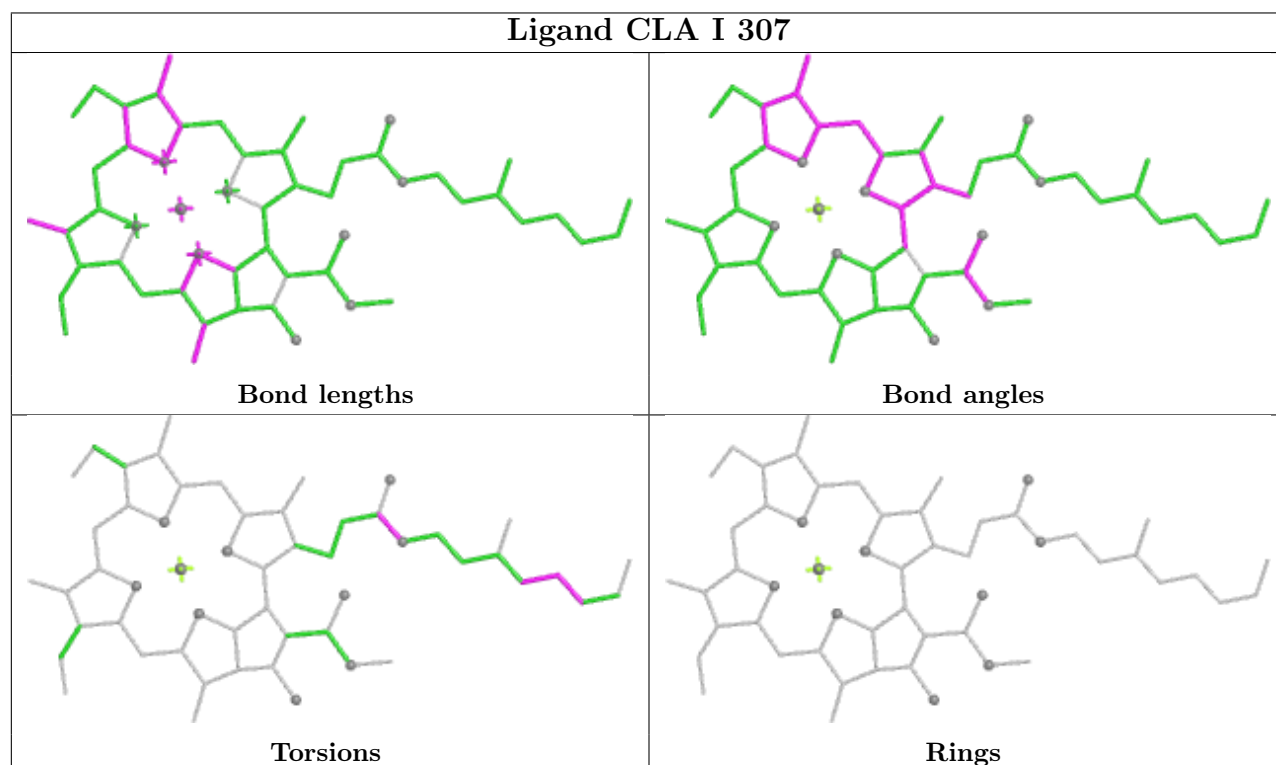
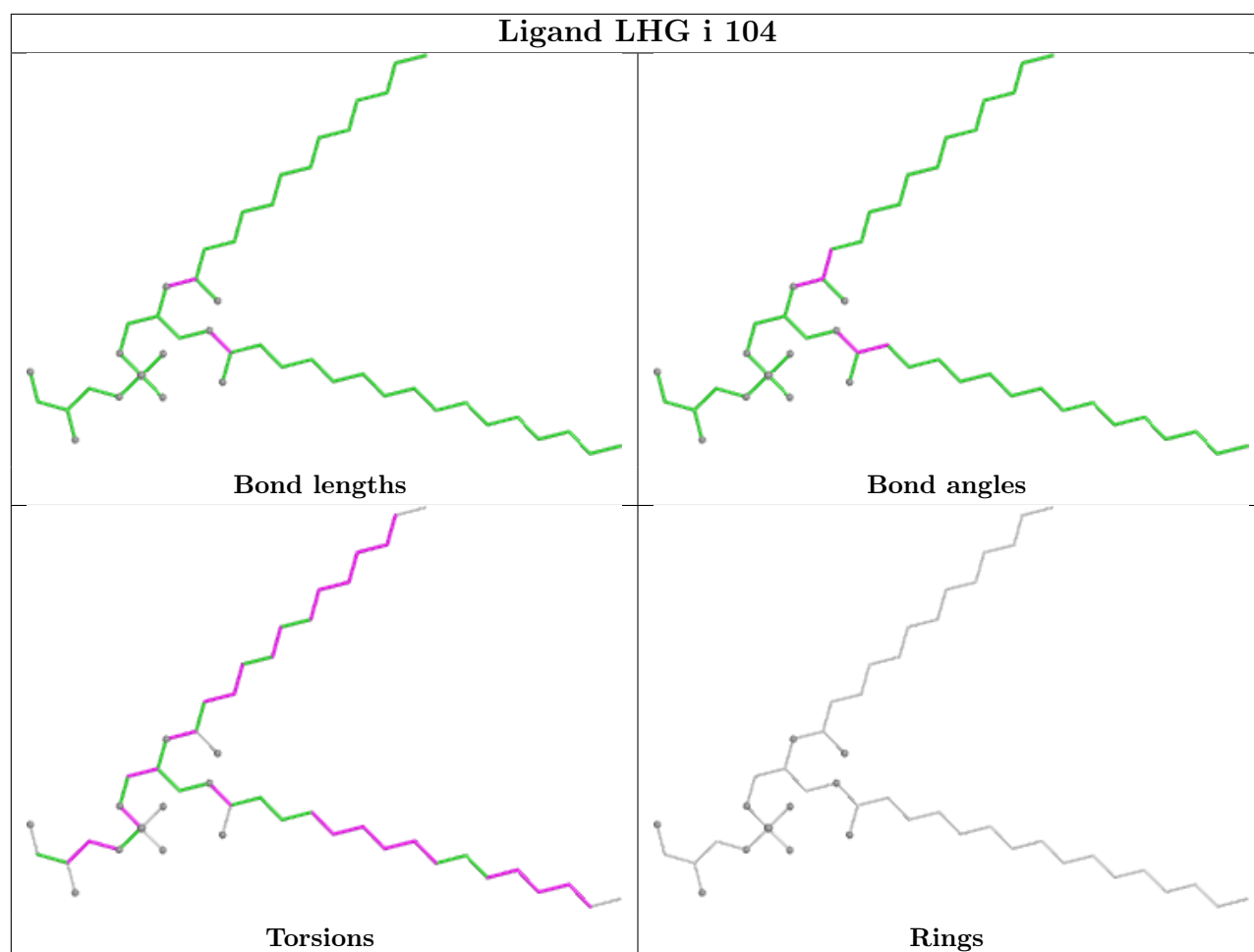
Bond angles



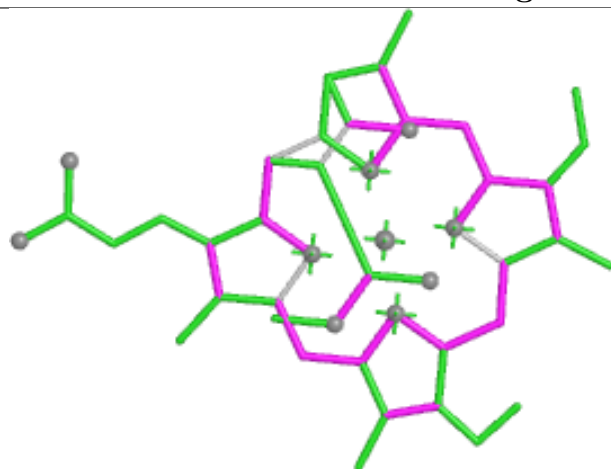
Torsions



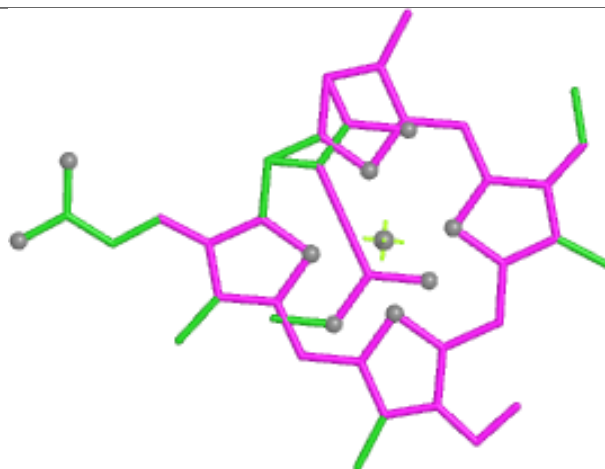
Rings



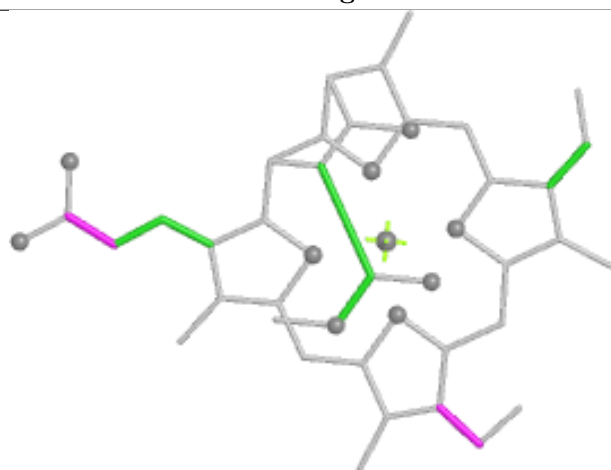
Ligand KC1 R 317



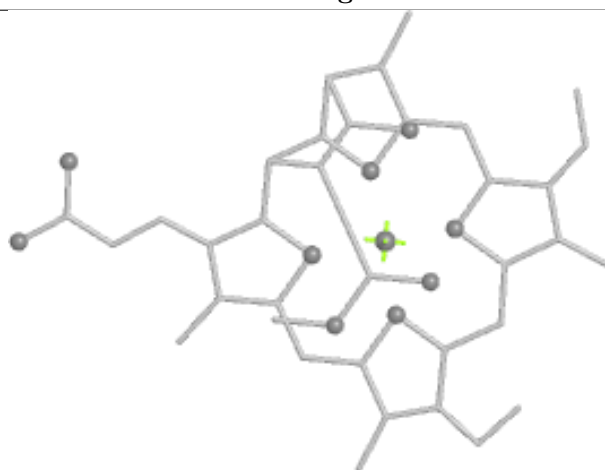
Bond lengths



Bond angles

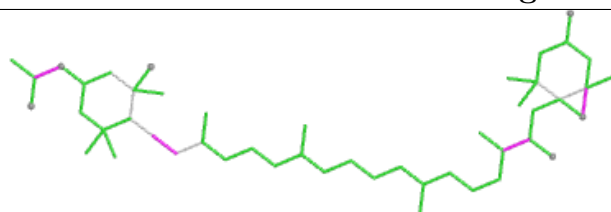


Torsions

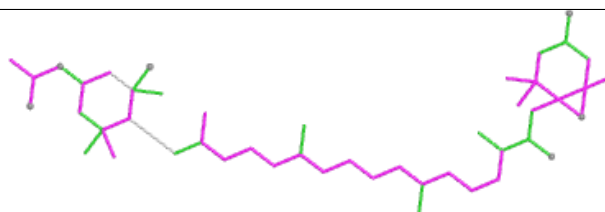


Rings

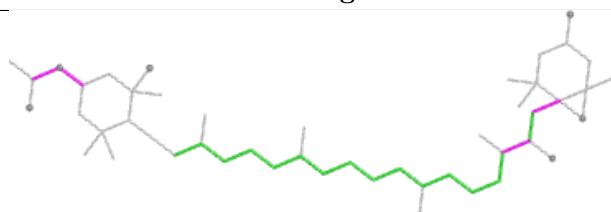
Ligand A86 U 302



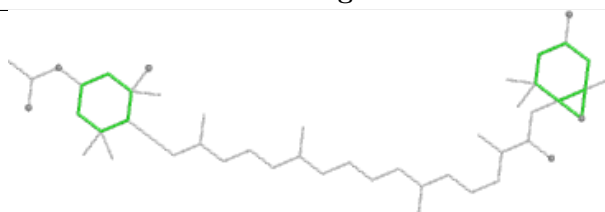
Bond lengths



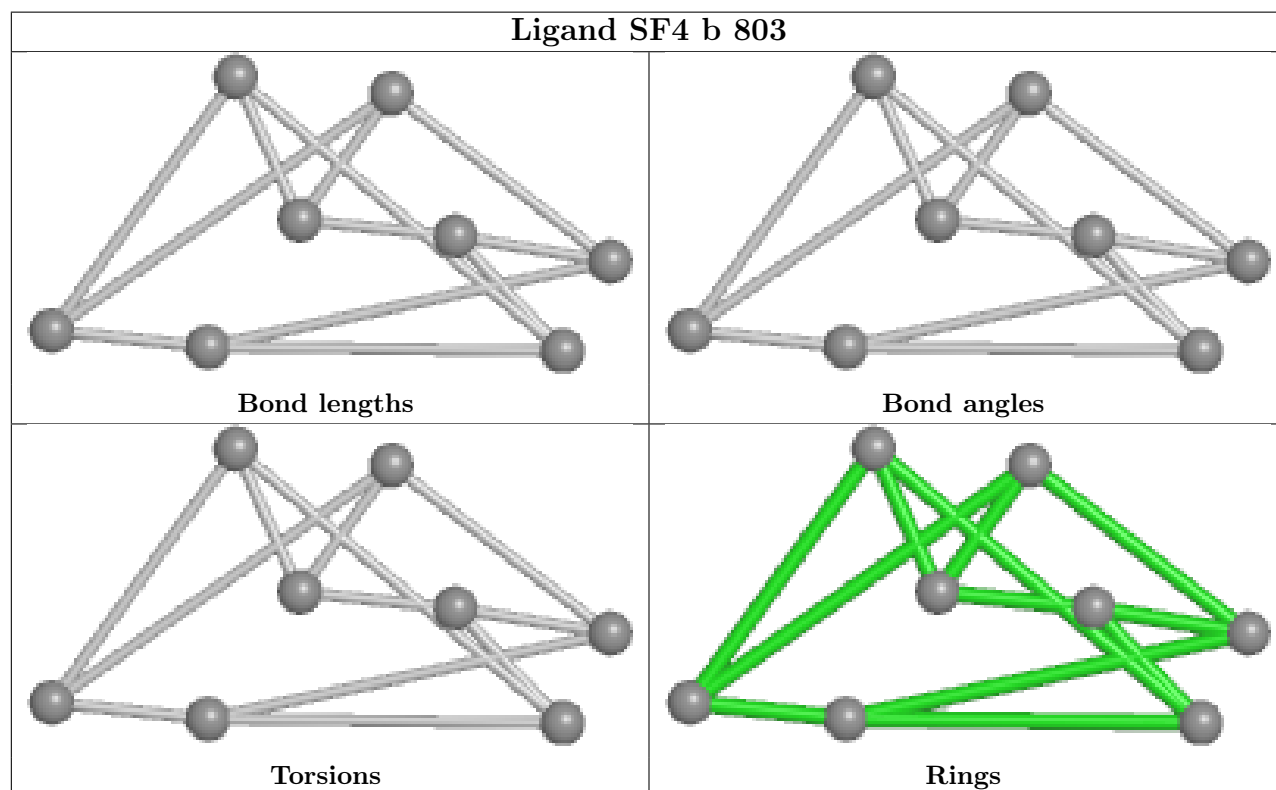
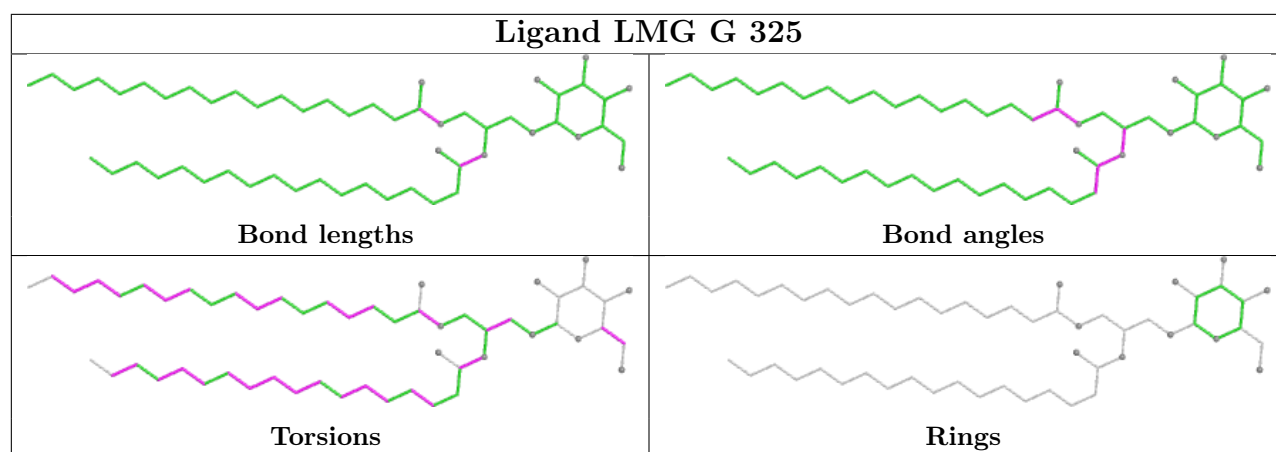
Bond angles

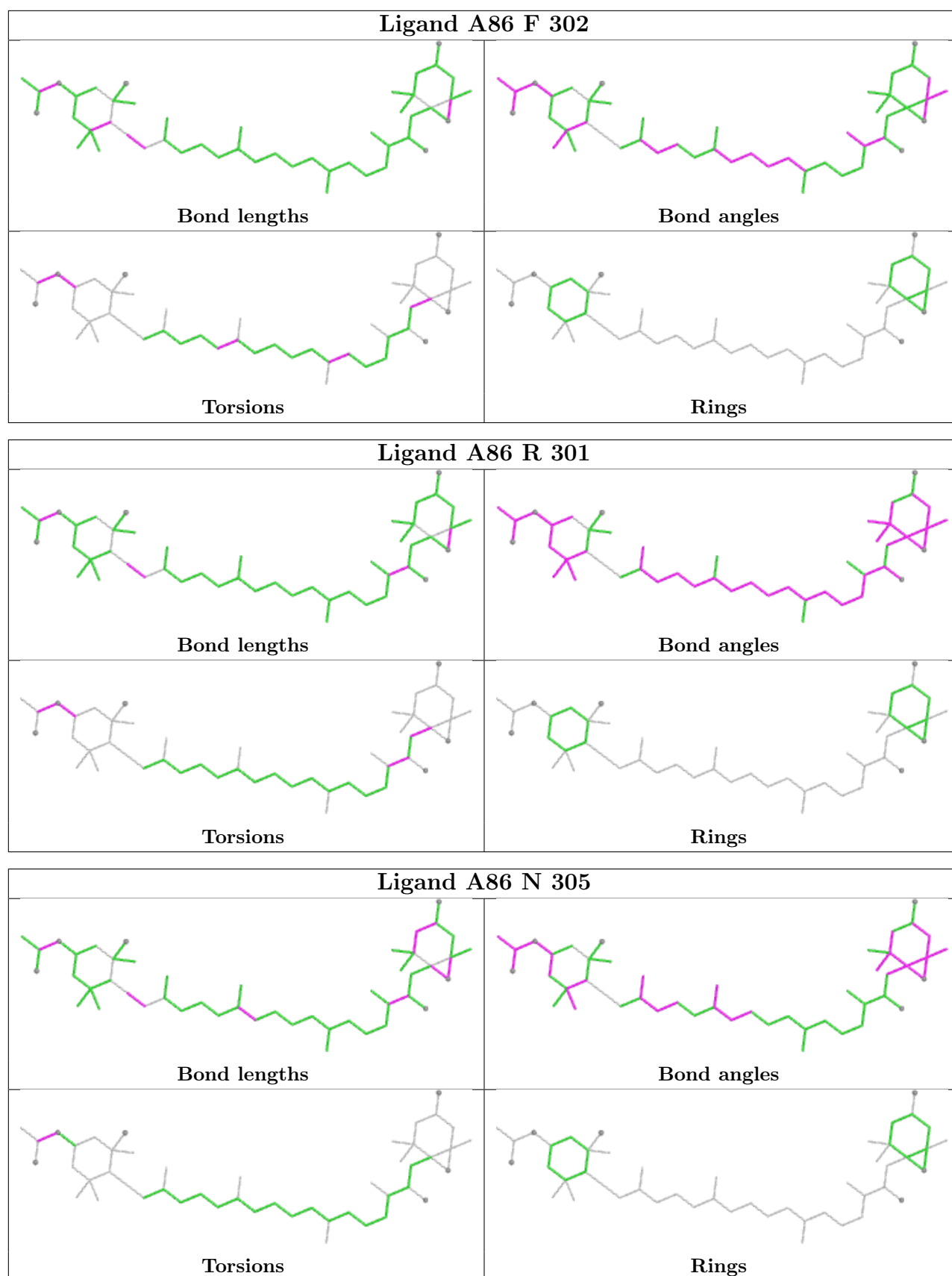


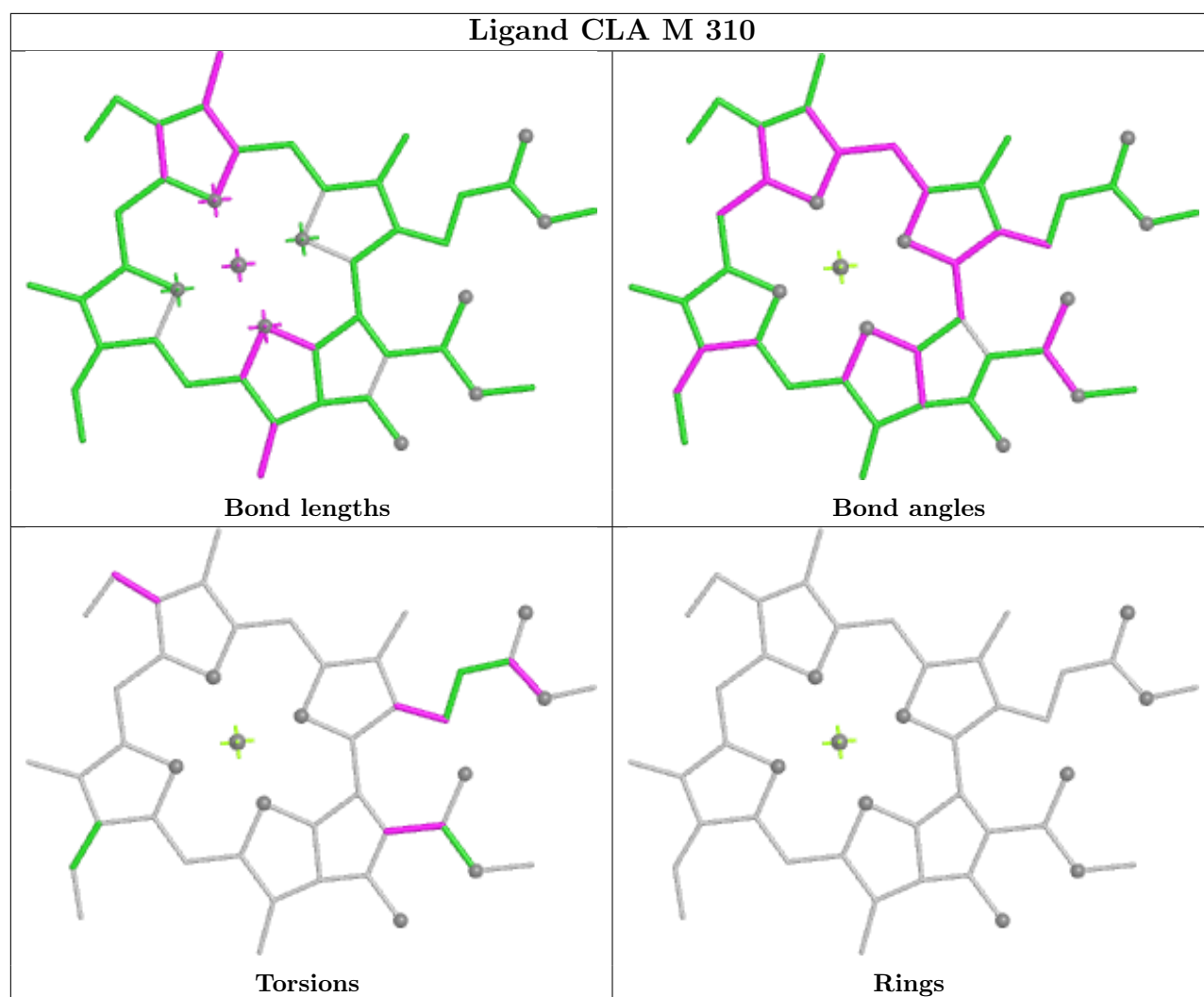
Torsions



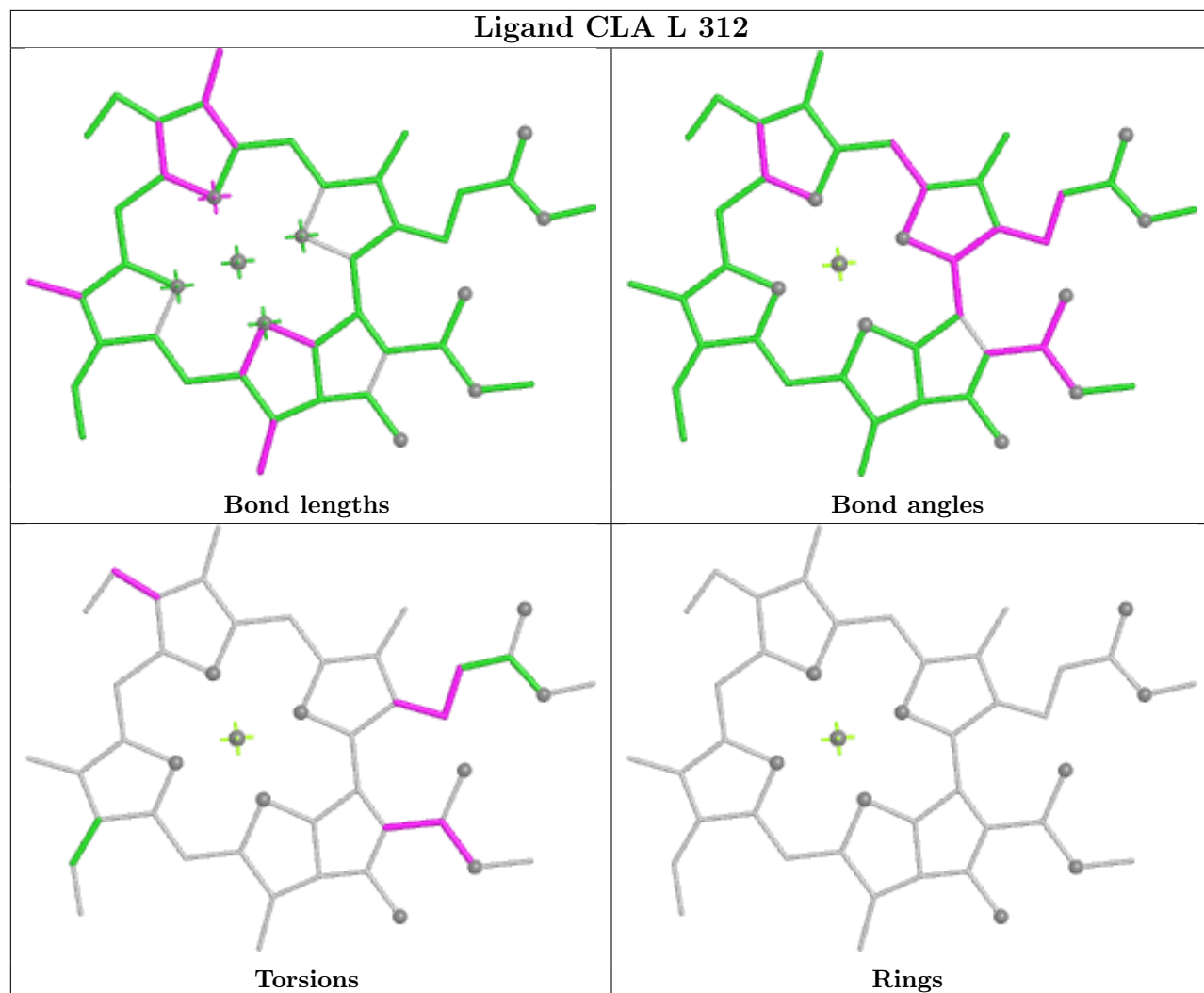
Rings

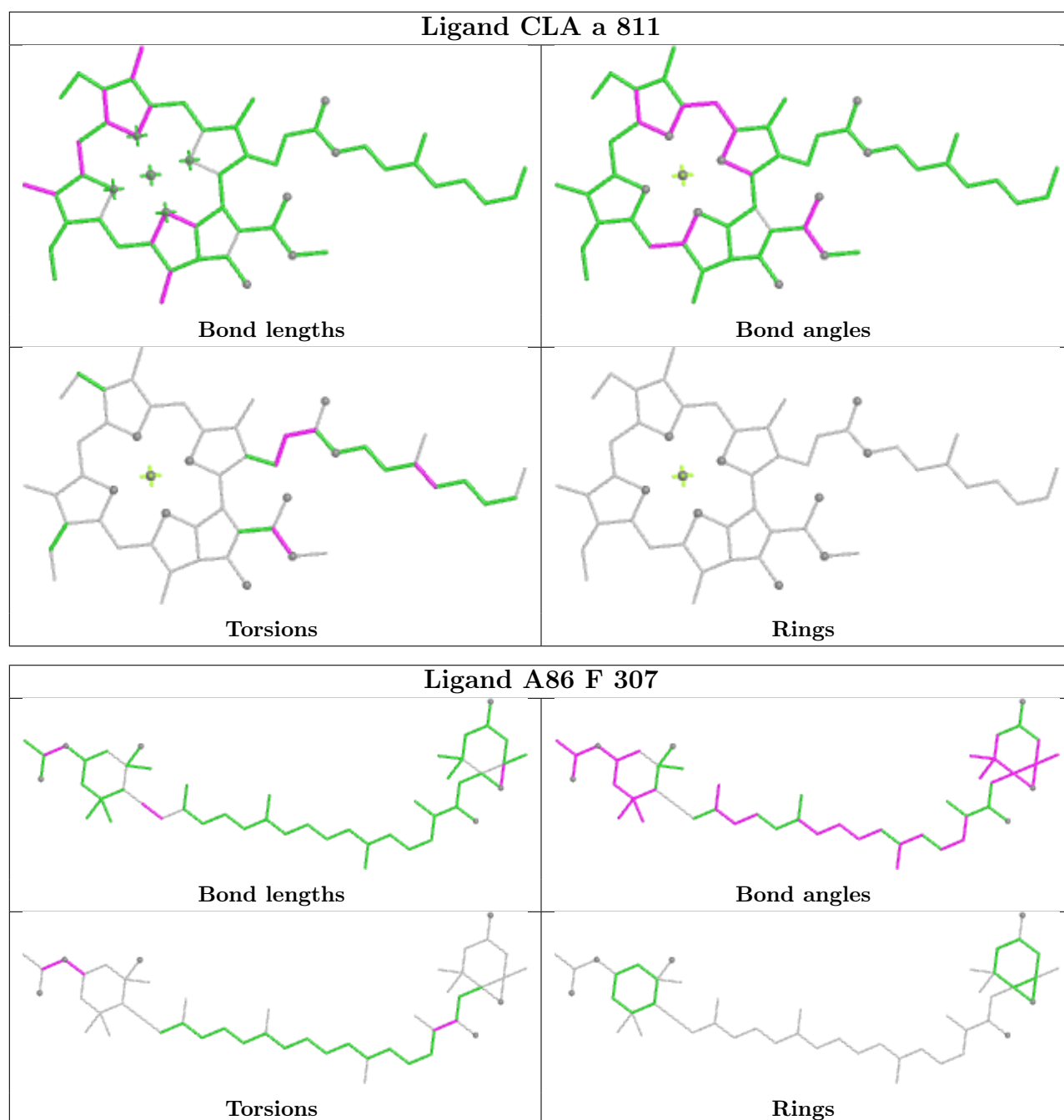


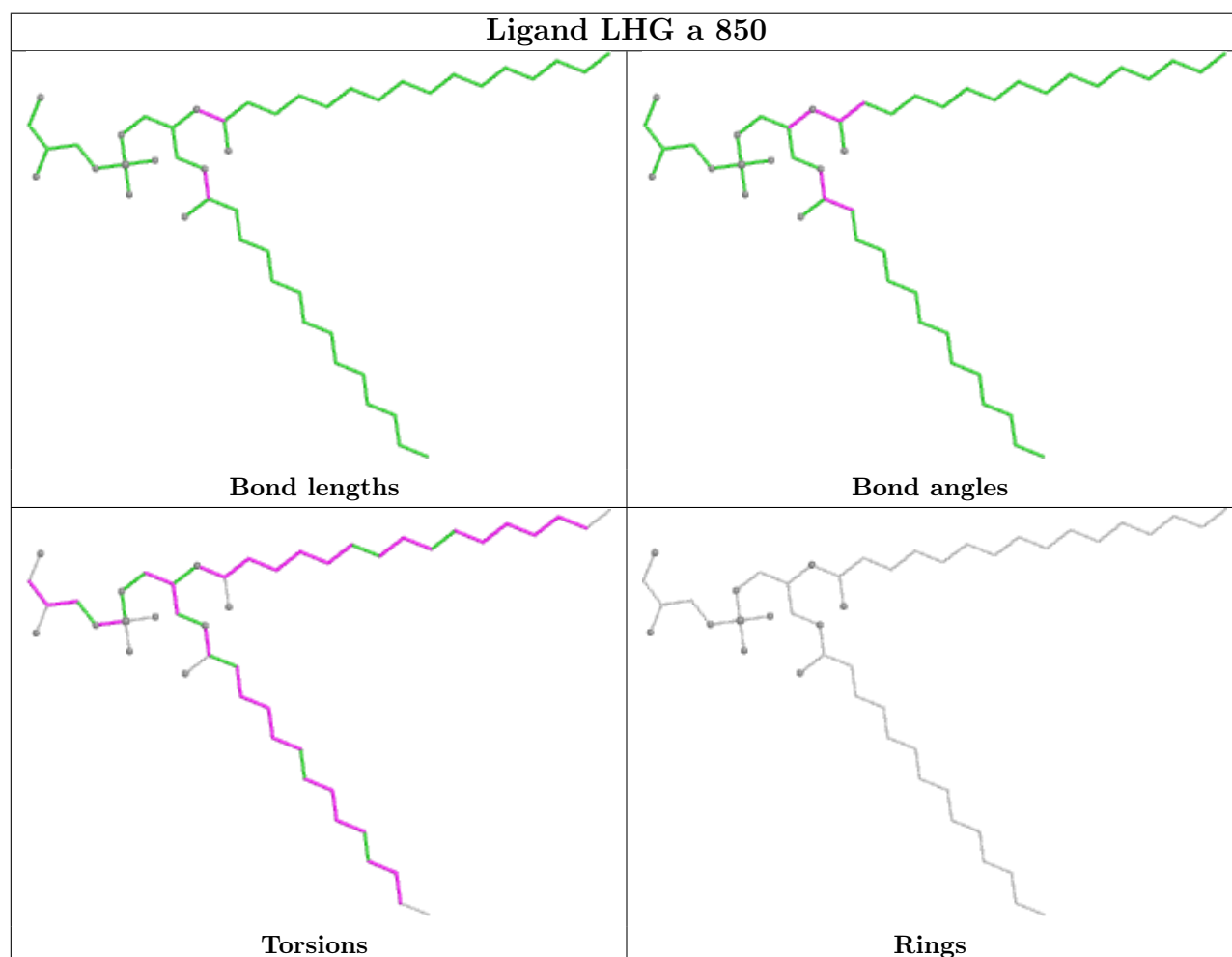
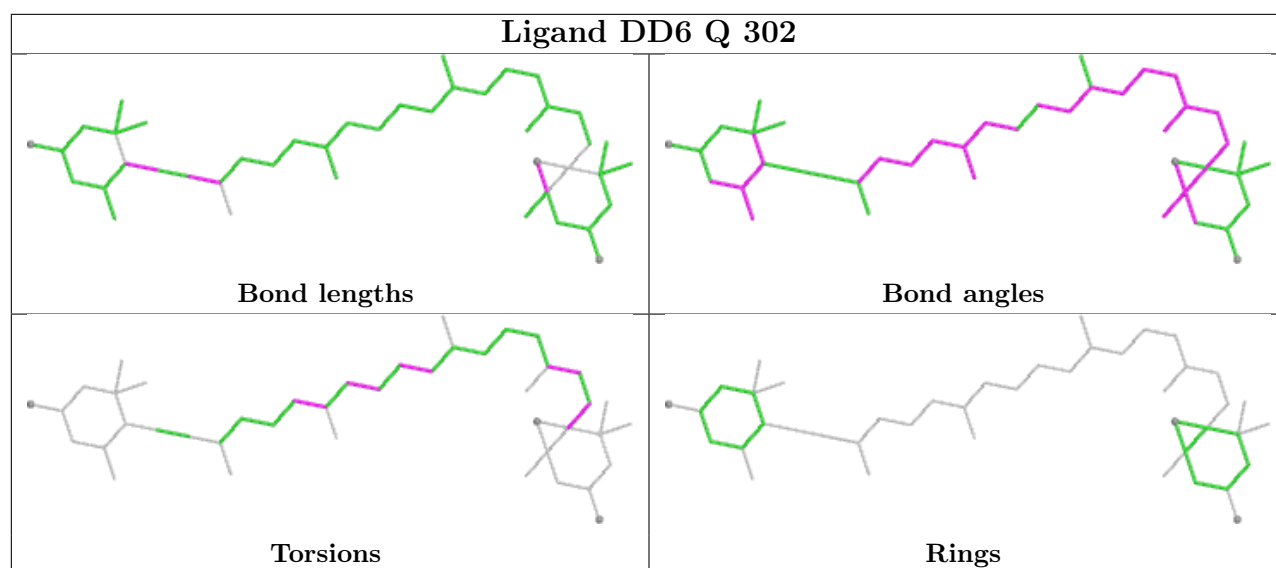


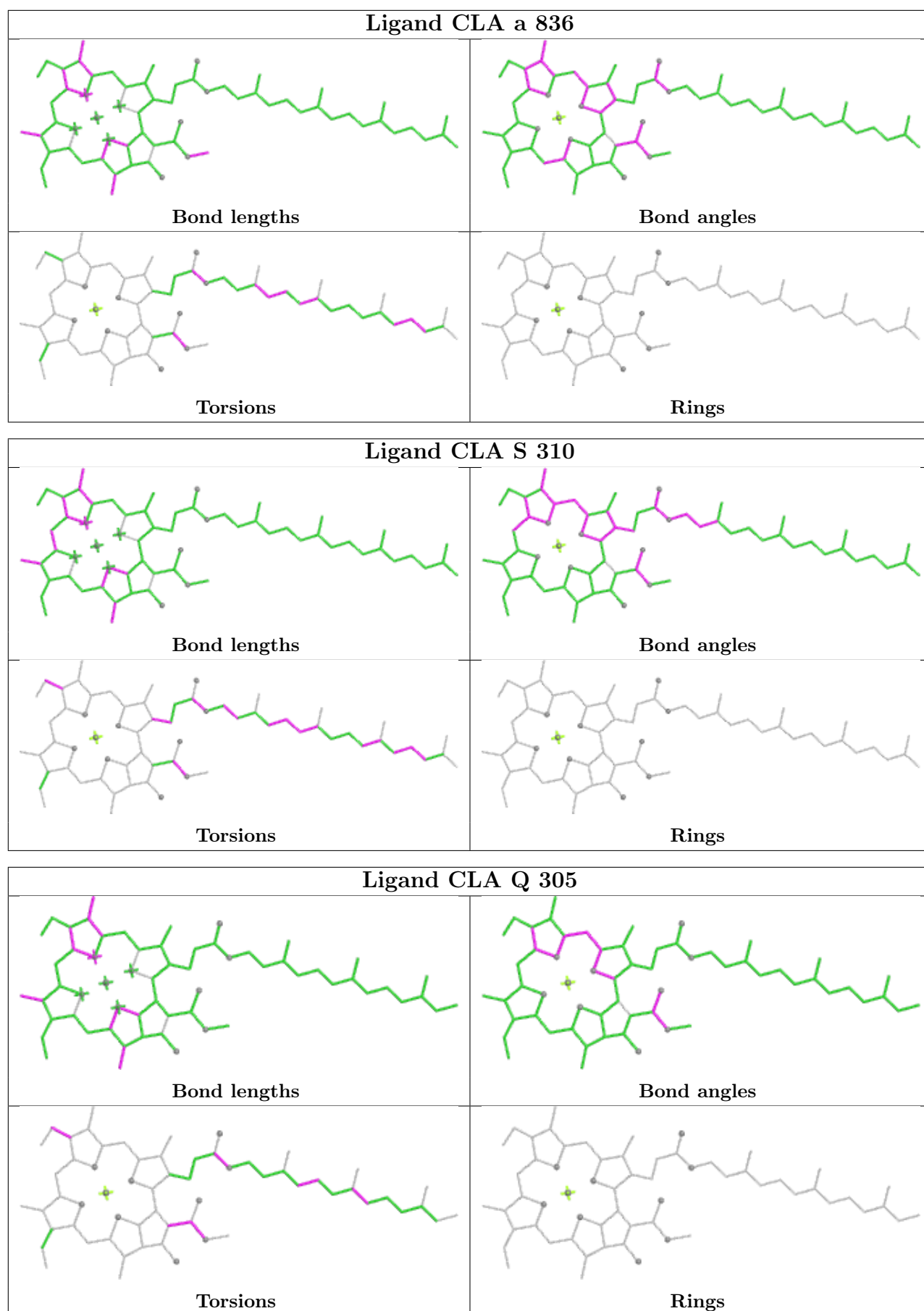


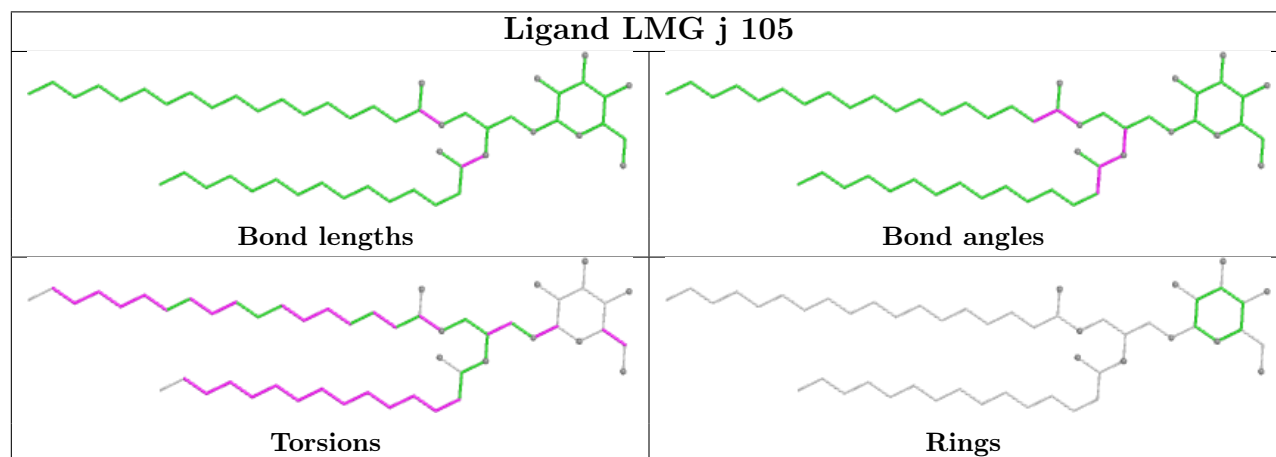
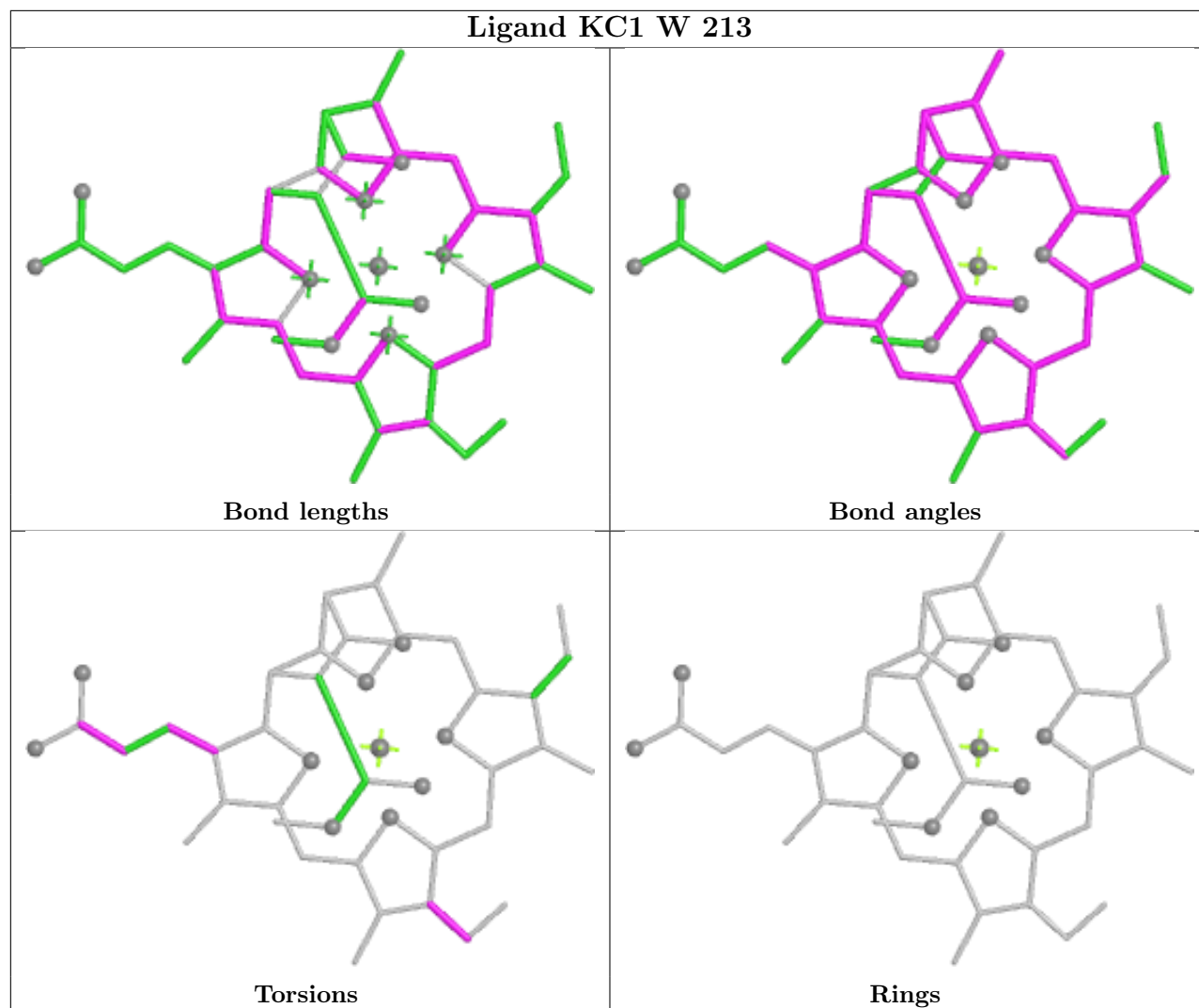
Ligand CLA L 312

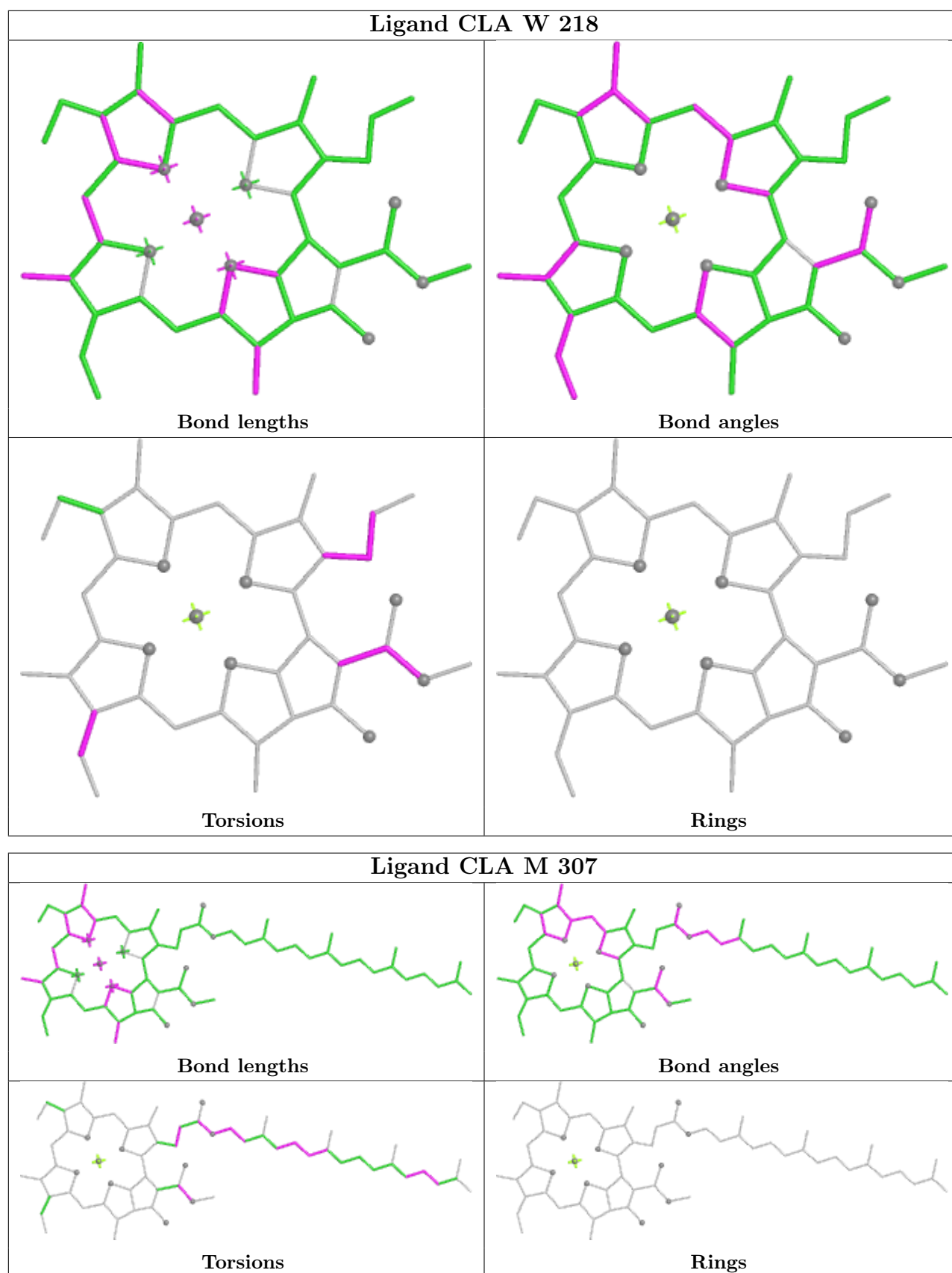




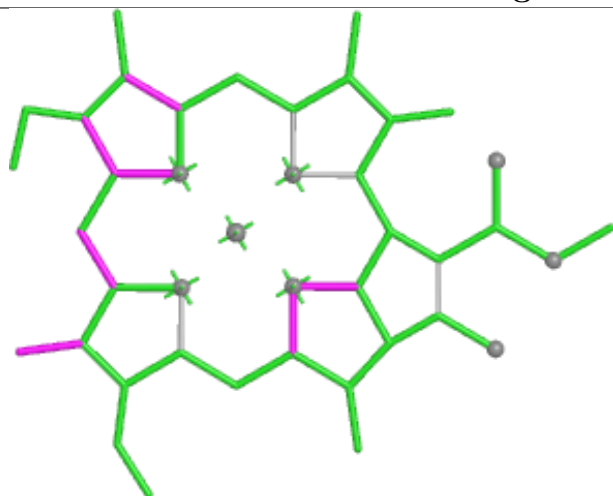




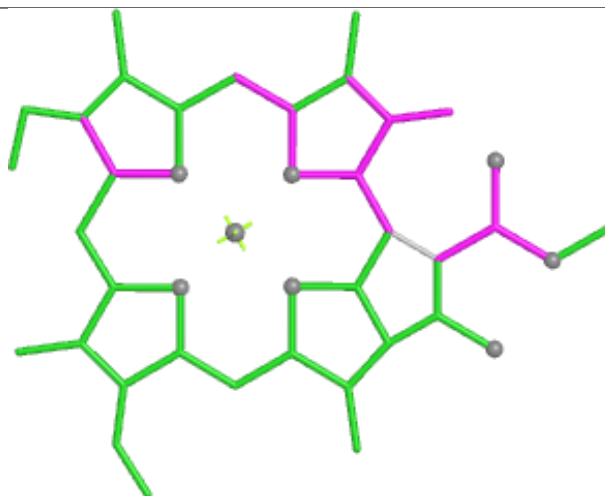




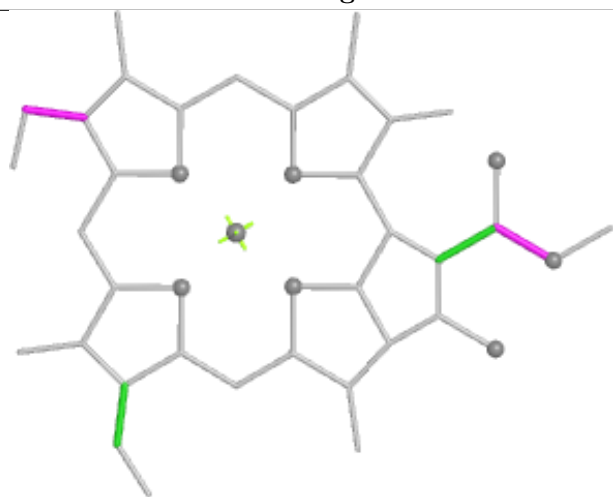
Ligand CLA U 313



Bond lengths



Bond angles

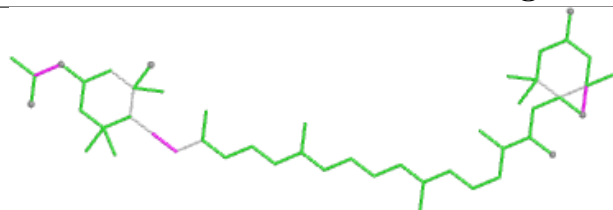


Torsions

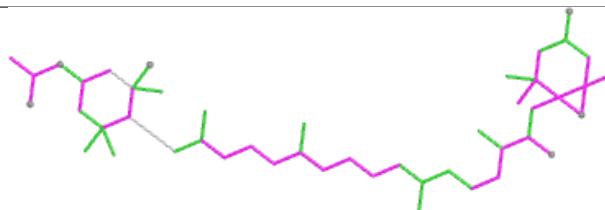


Rings

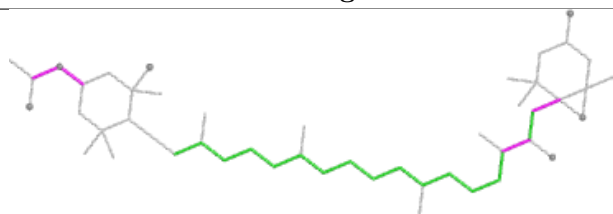
Ligand A86 R 304



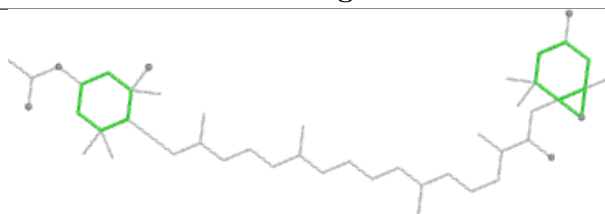
Bond lengths



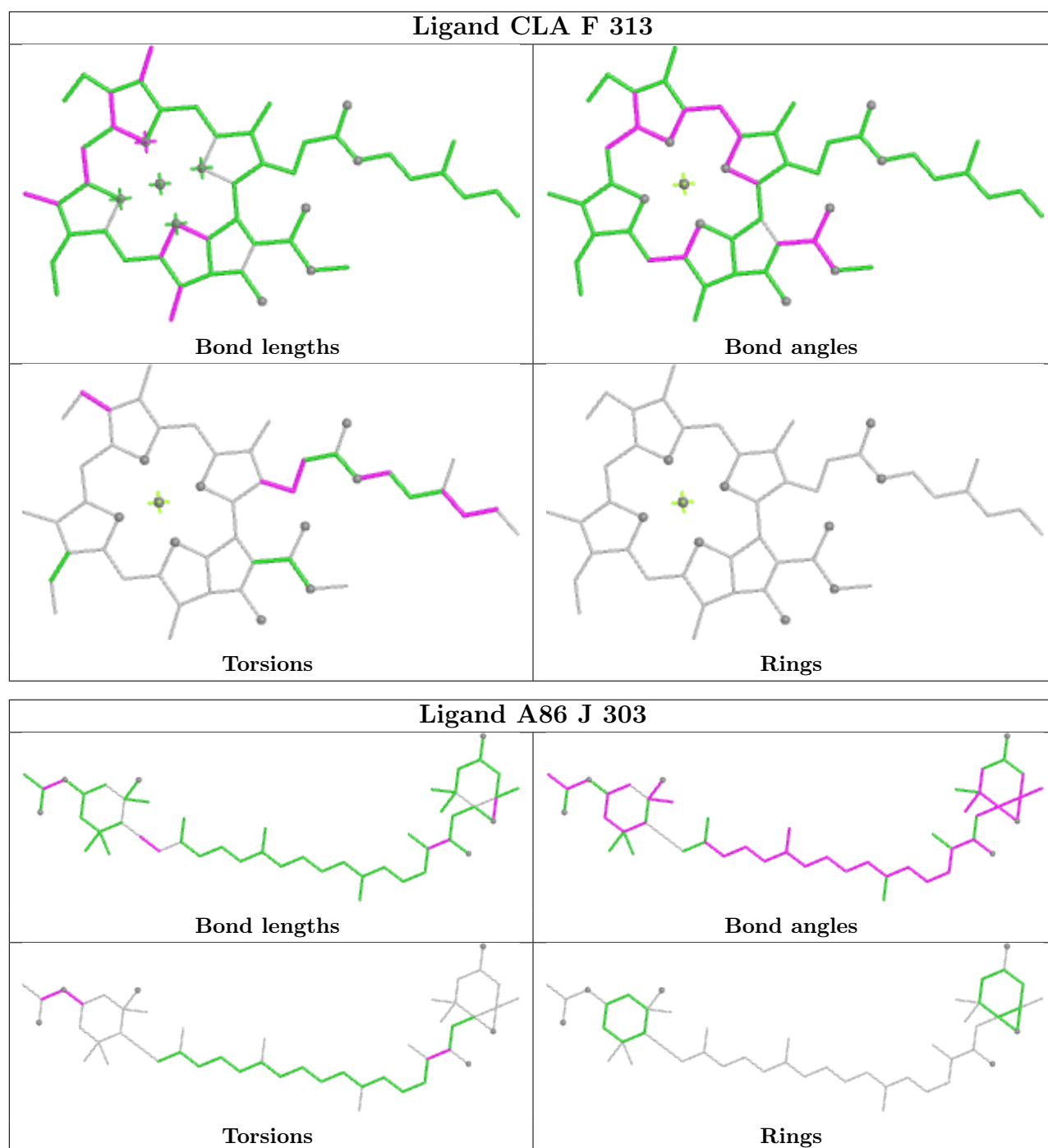
Bond angles



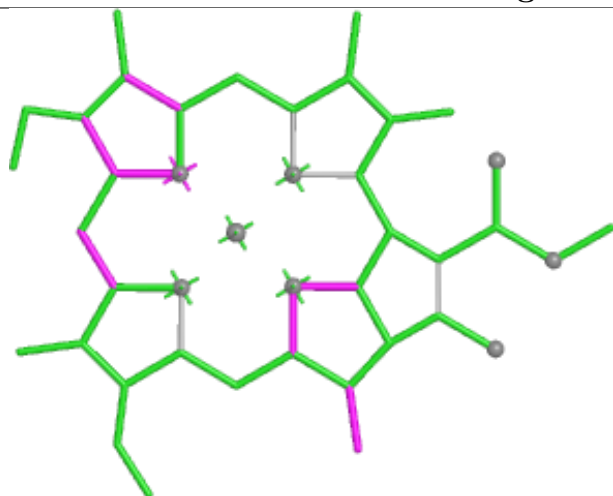
Torsions



Rings



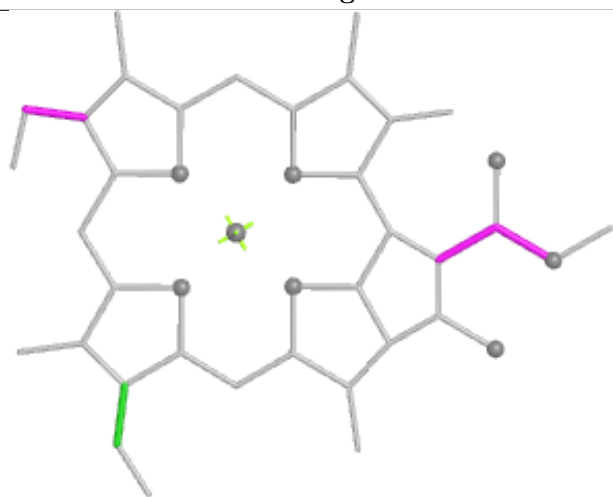
Ligand CLA S 317



Bond lengths



Bond angles

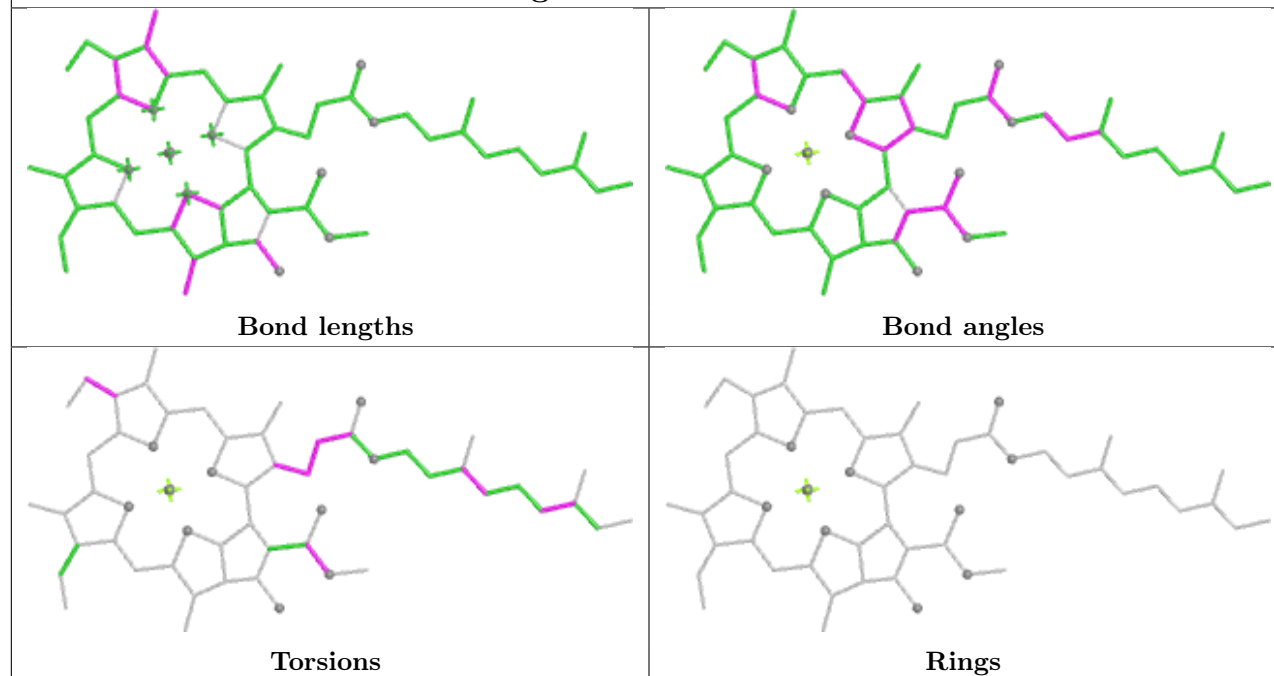


Torsions

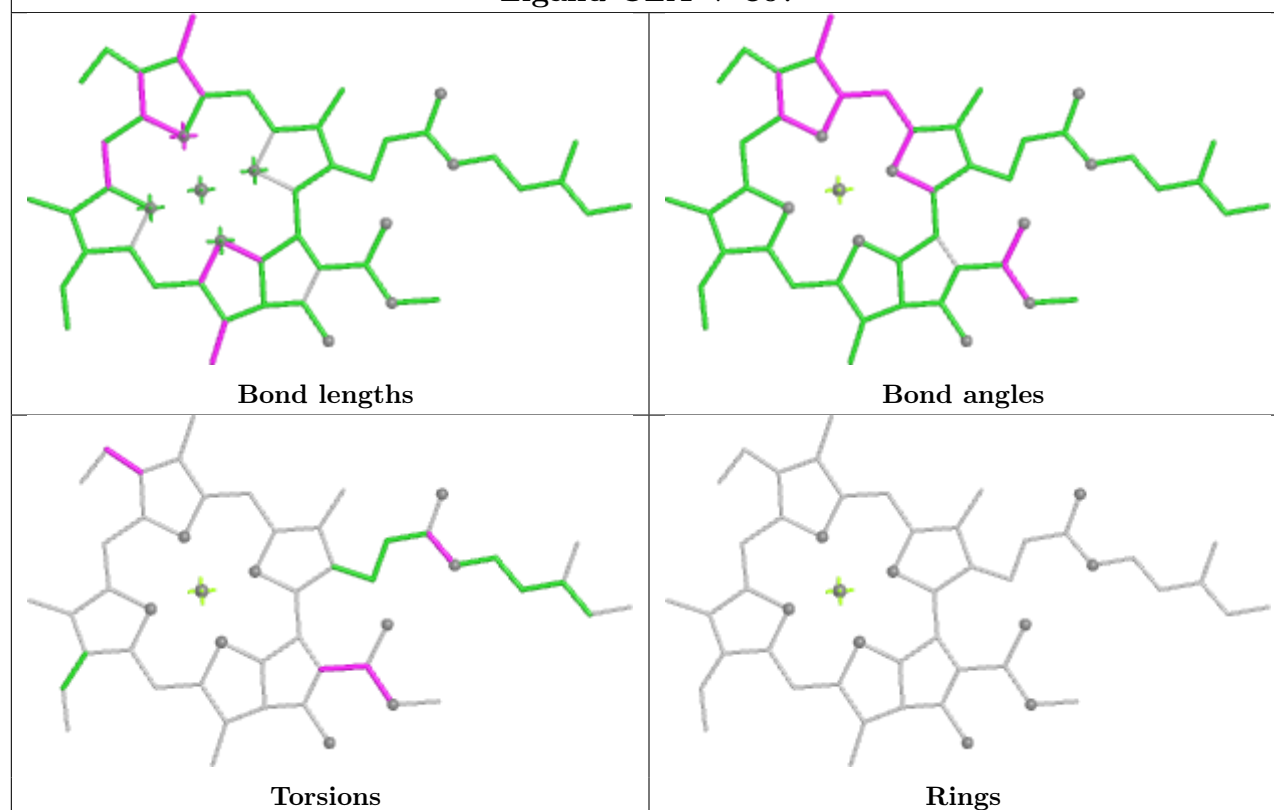


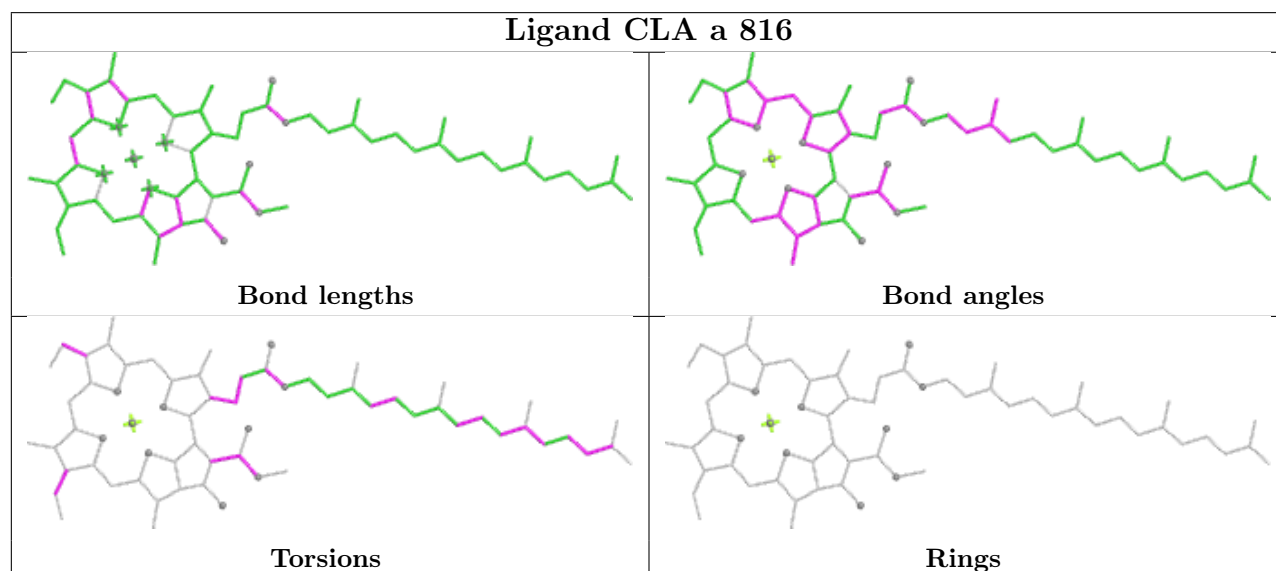
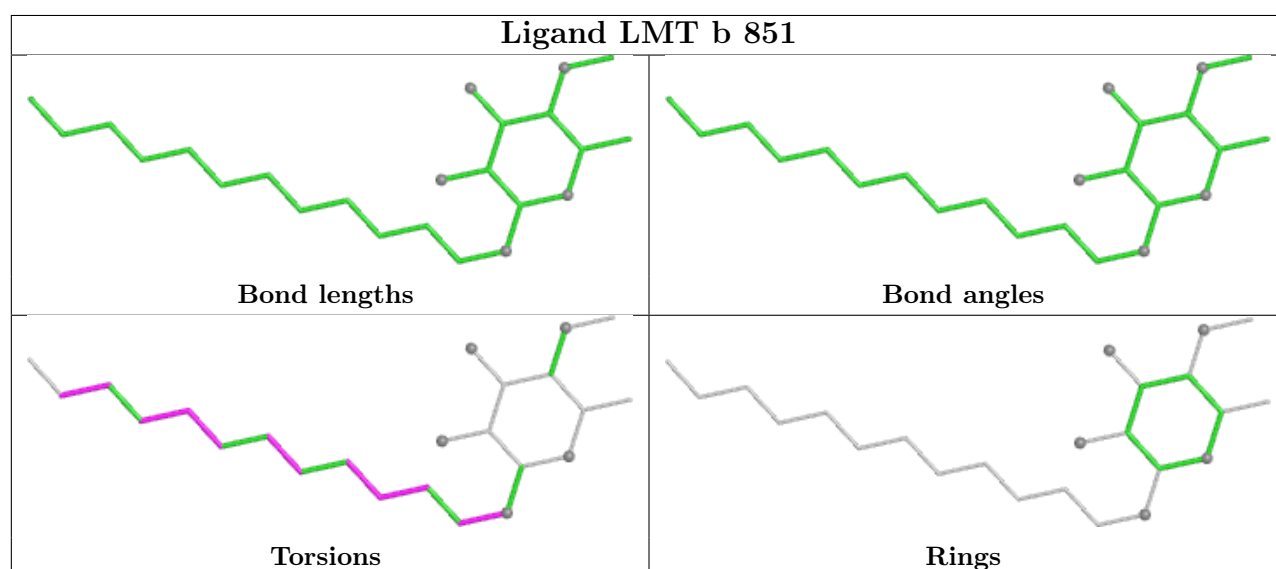
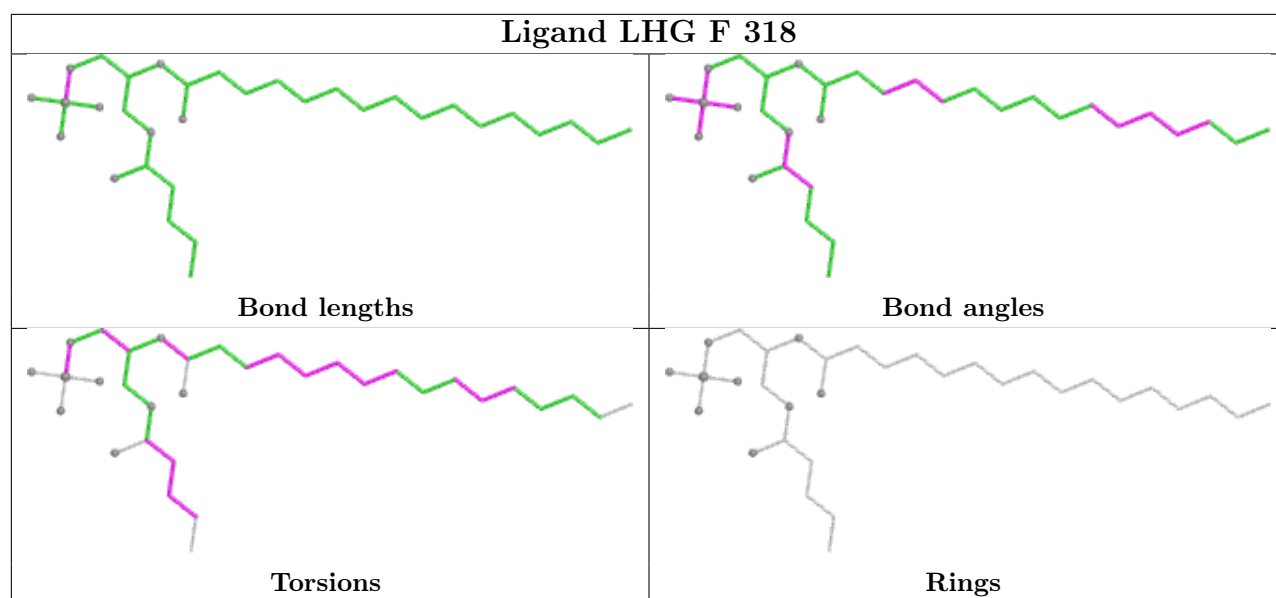
Rings

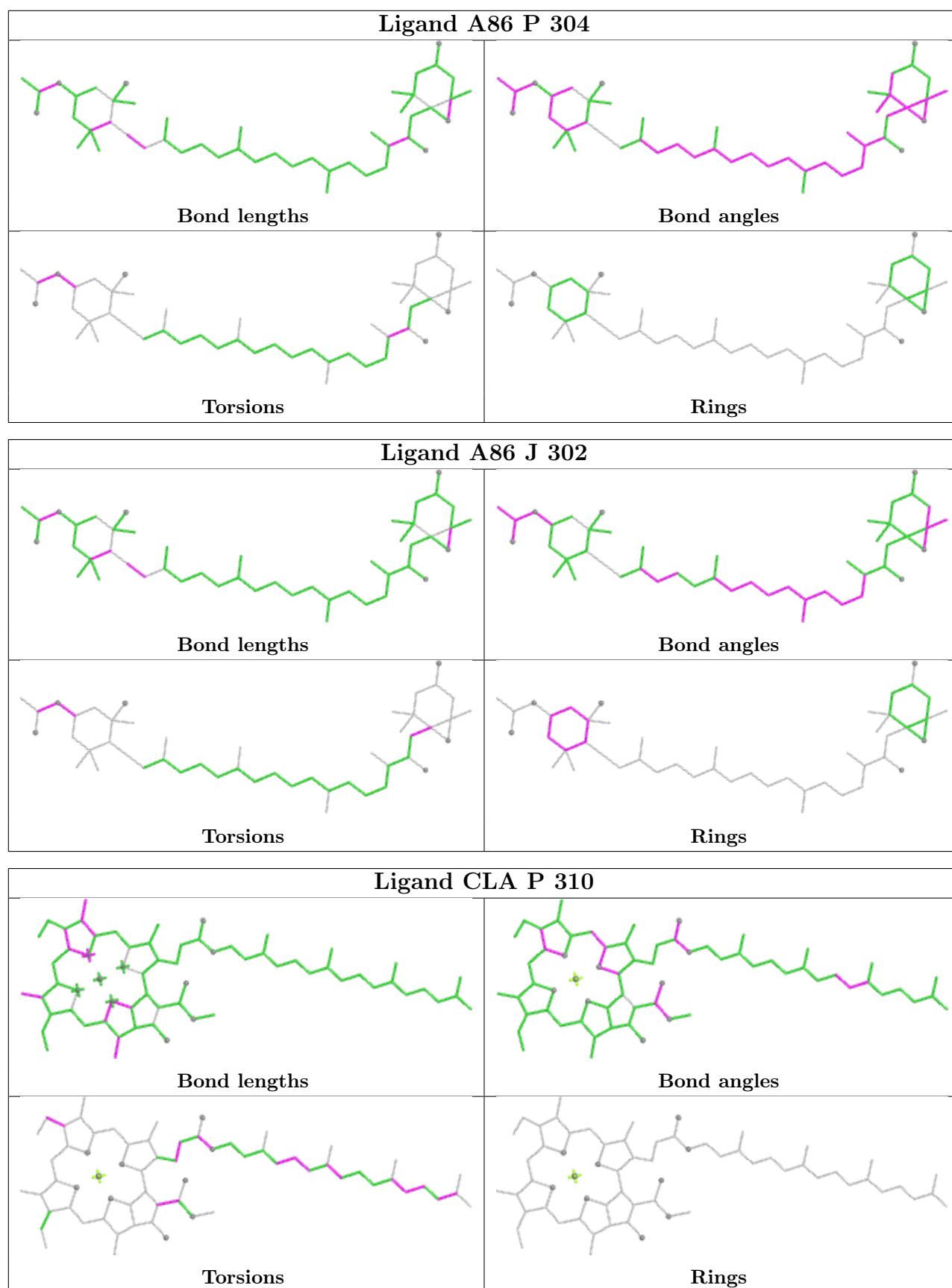
Ligand CLA U 308

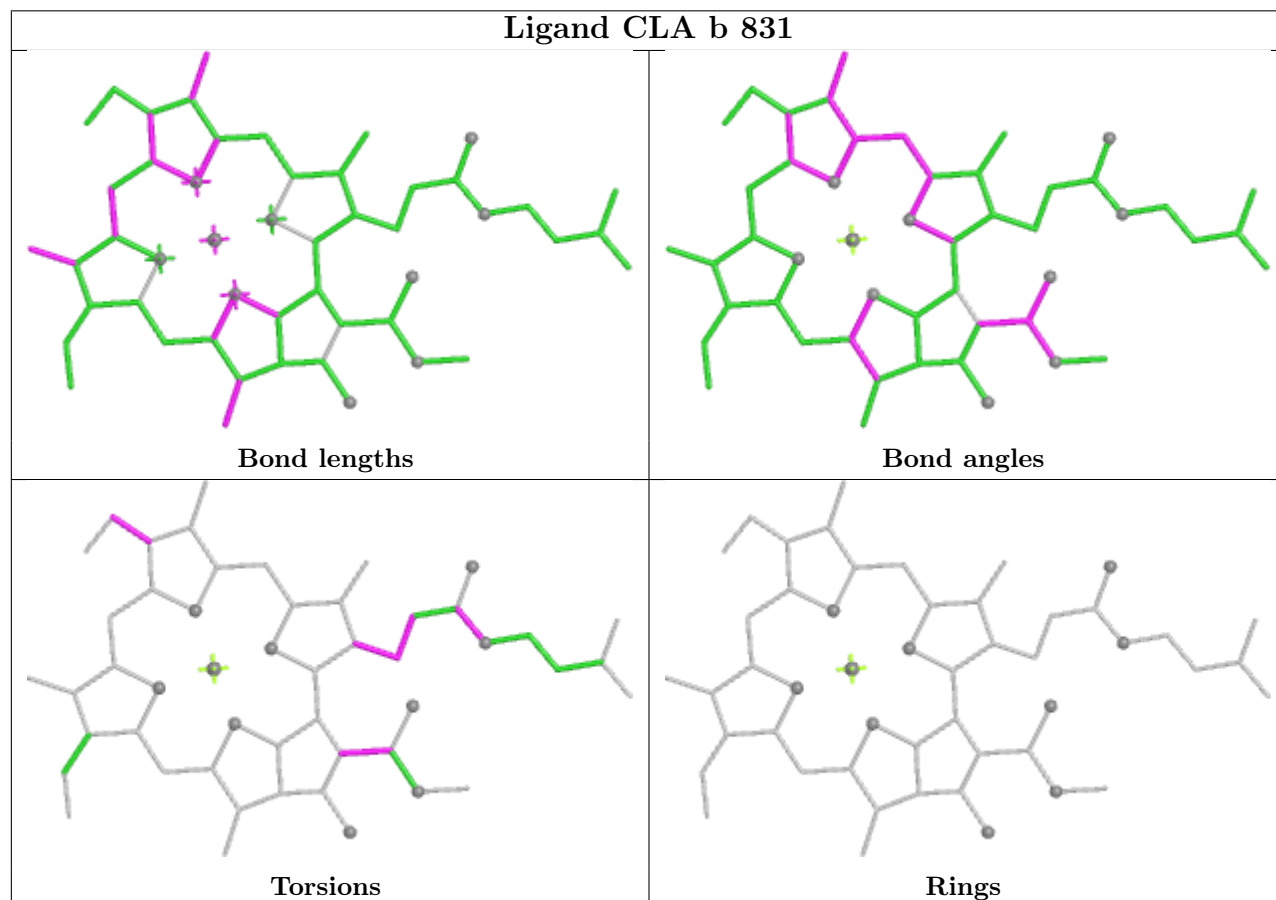
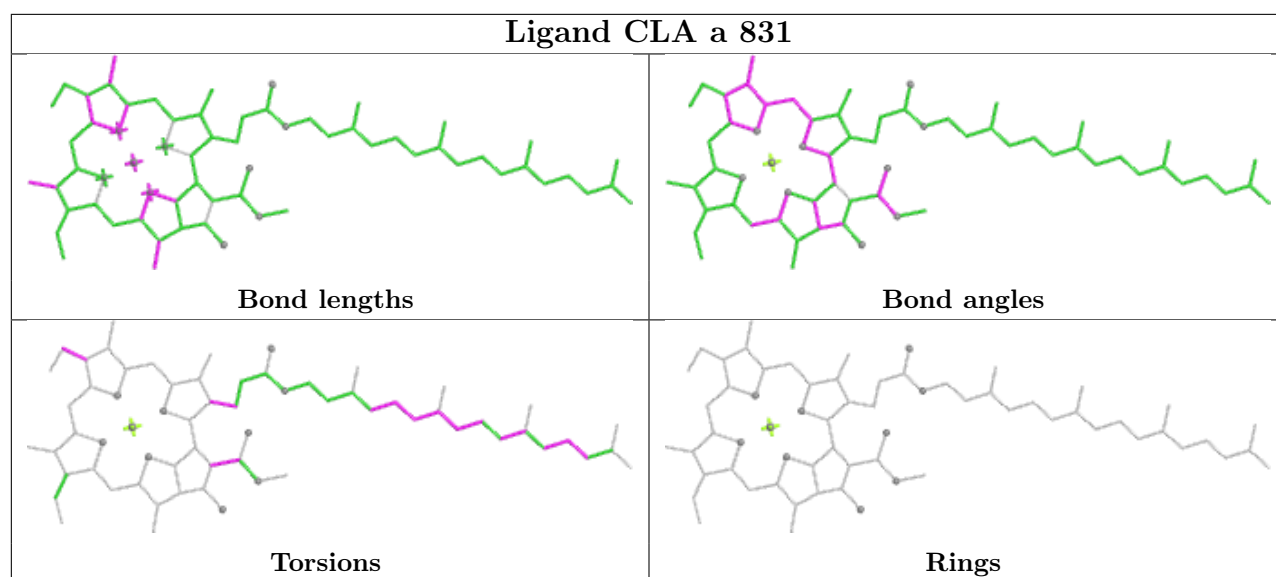


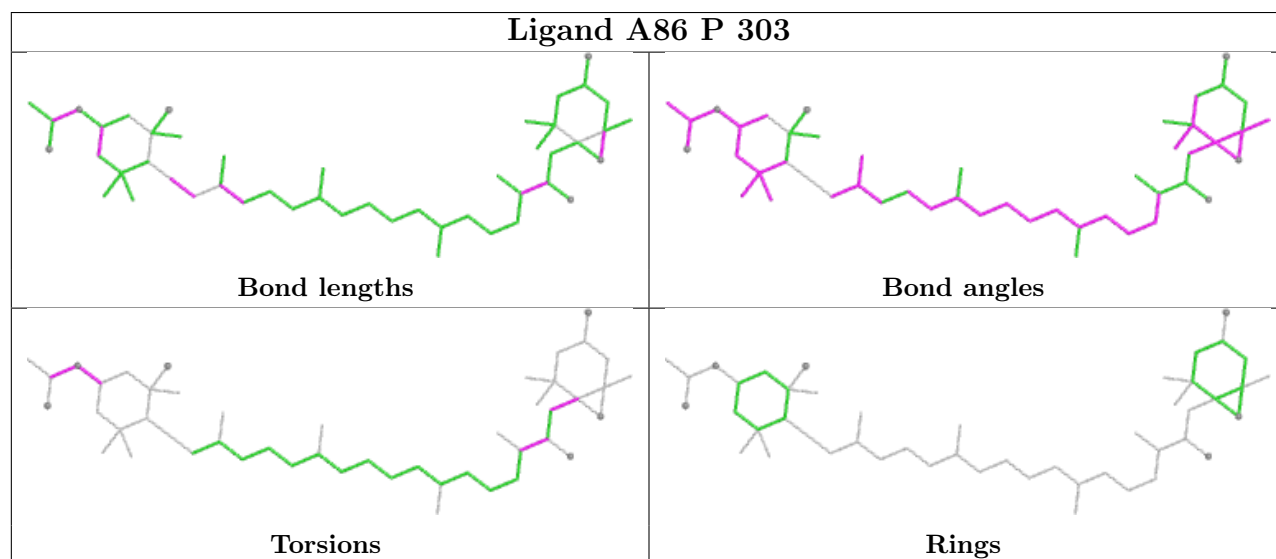
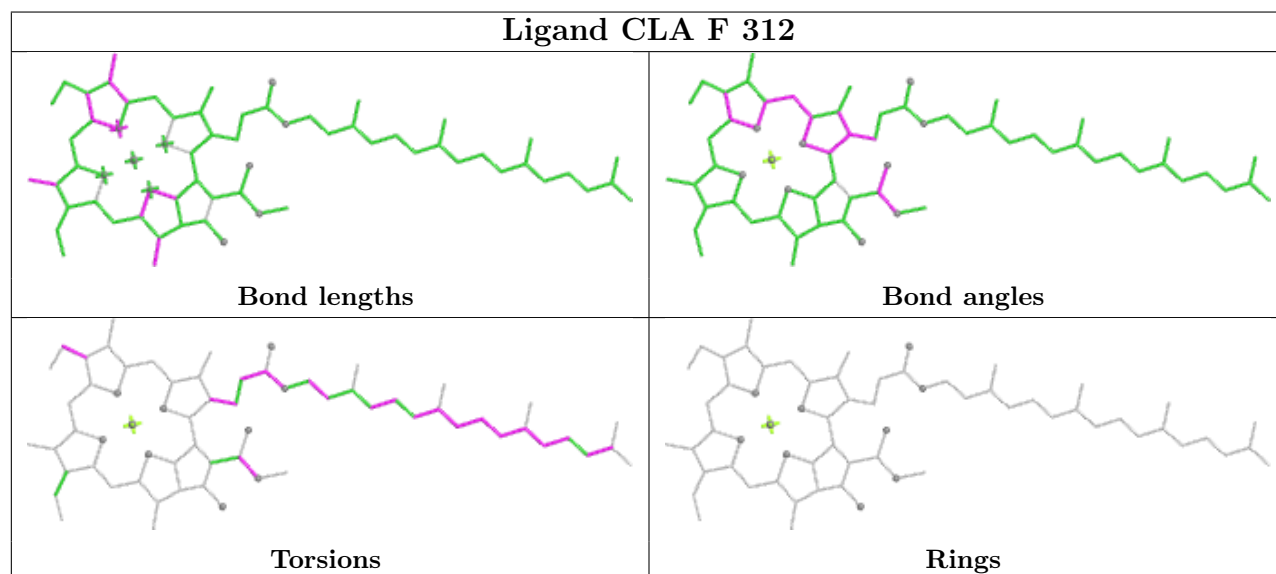
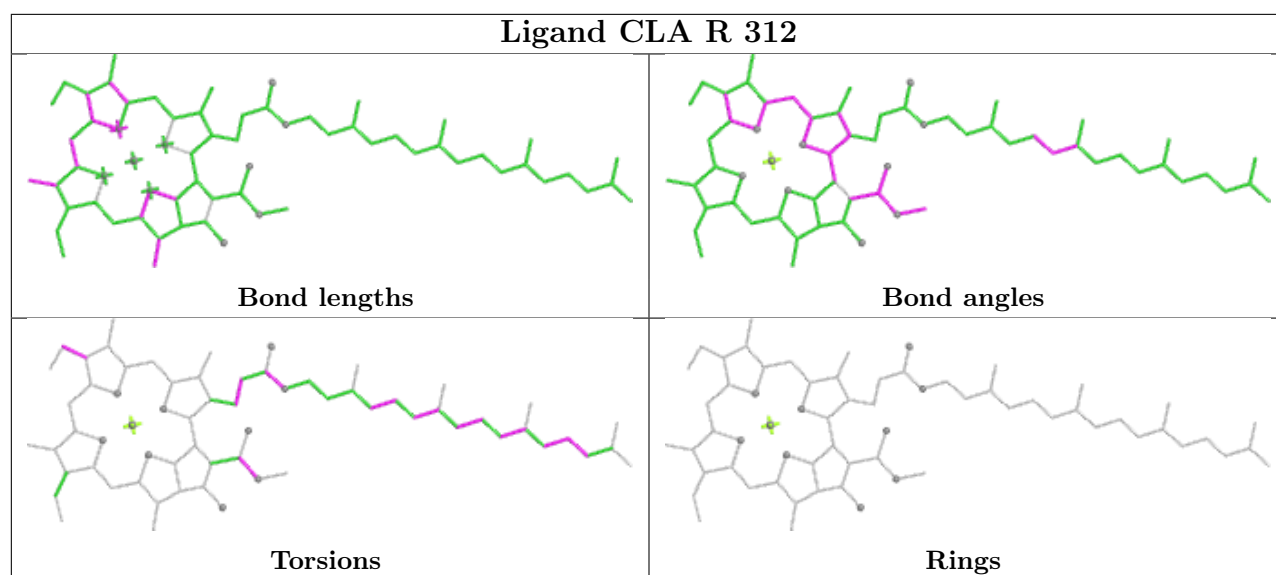
Ligand CLA V 307

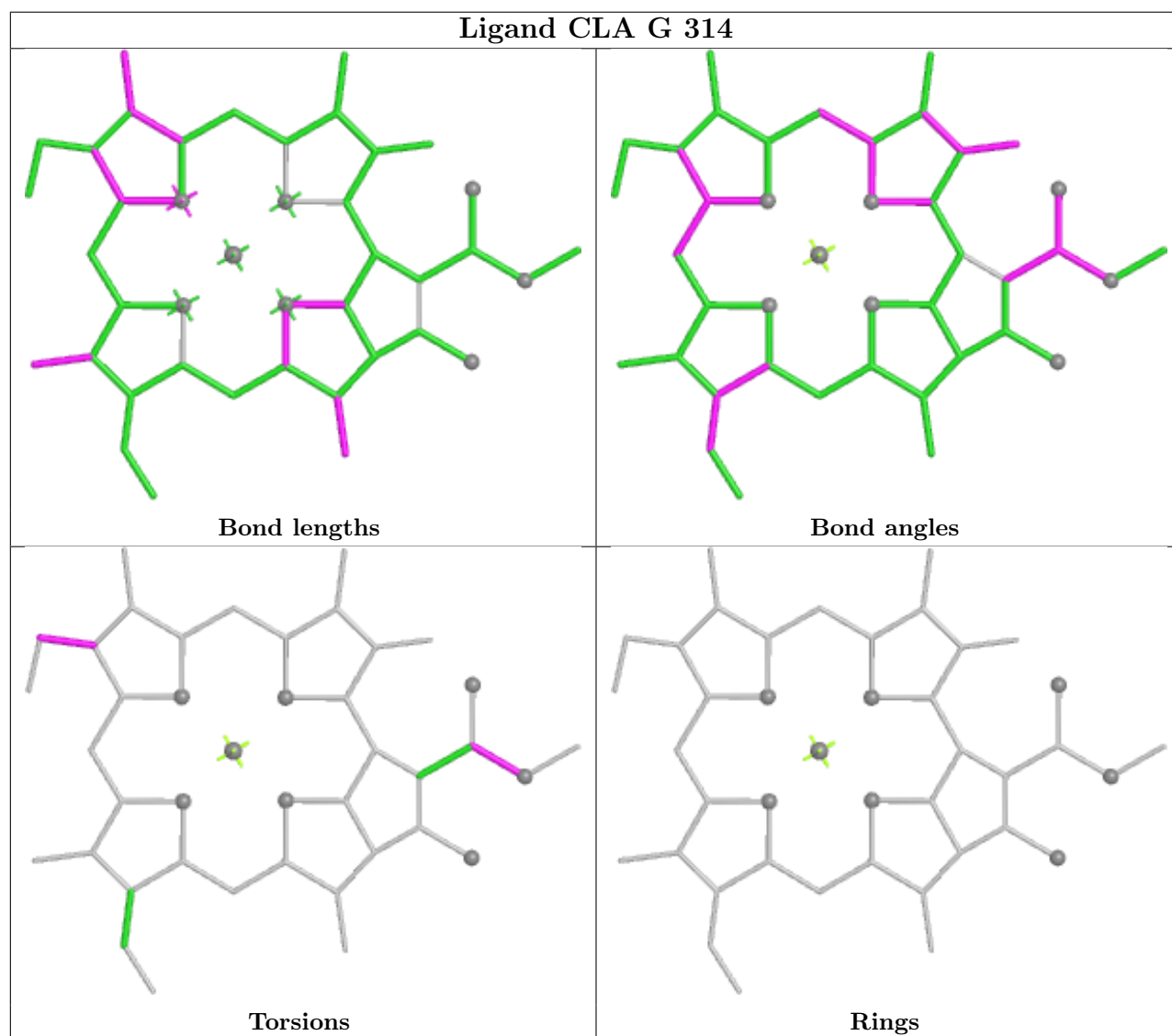
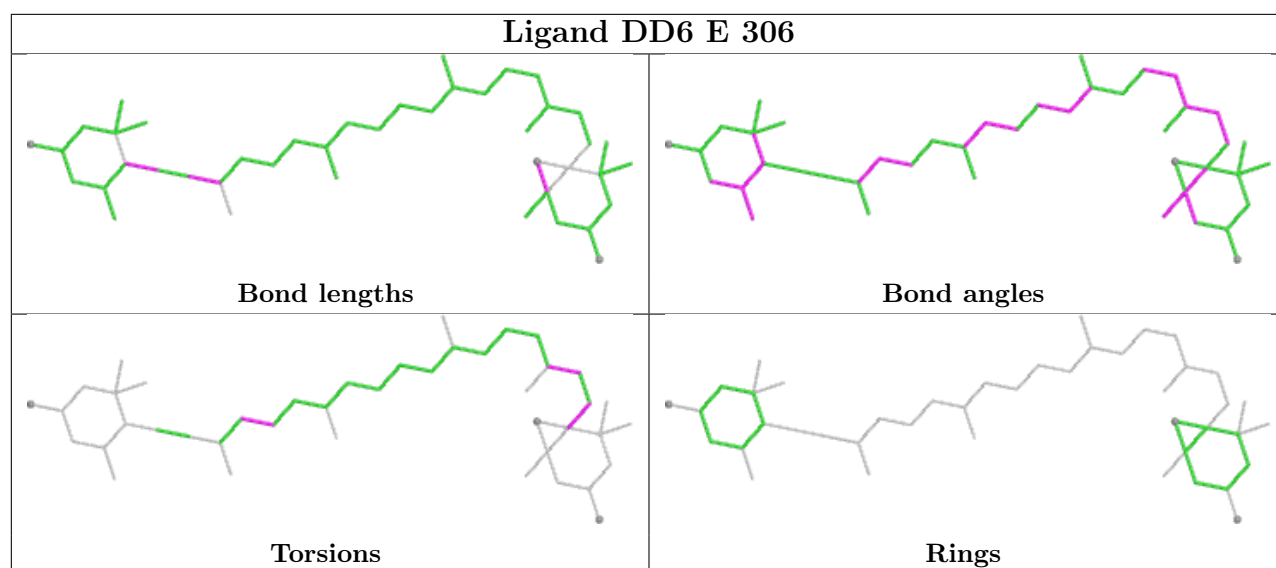


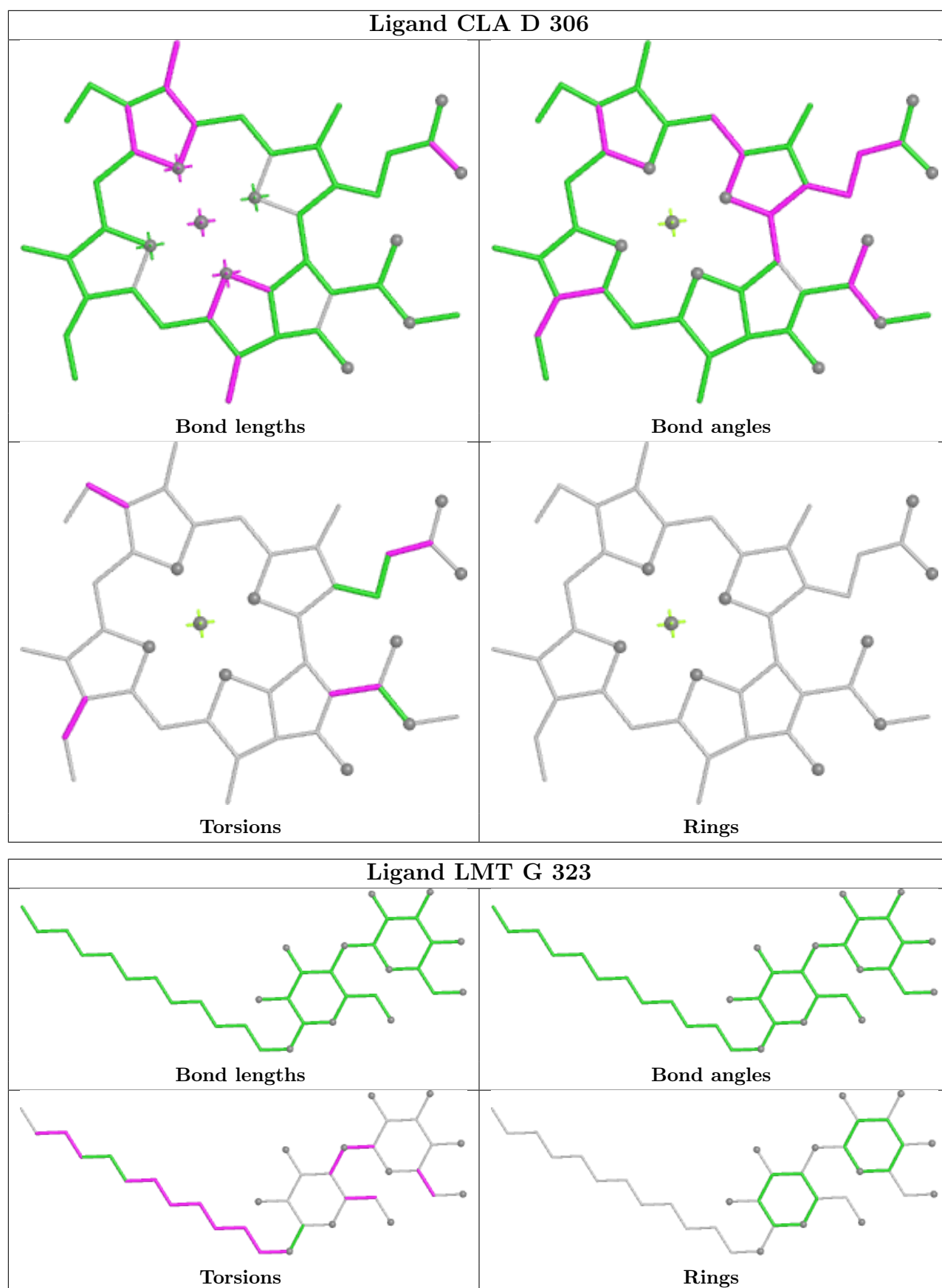




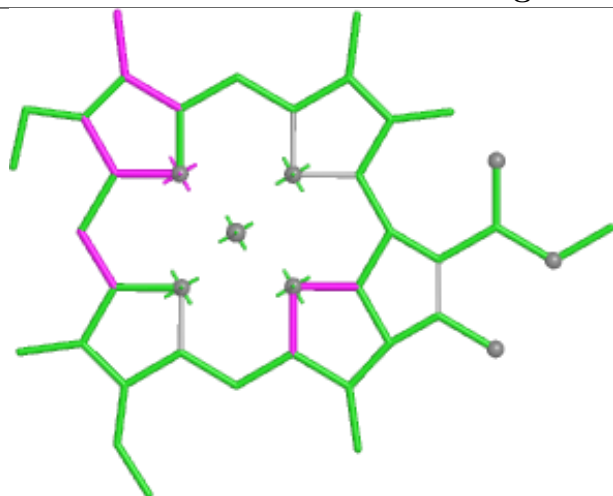








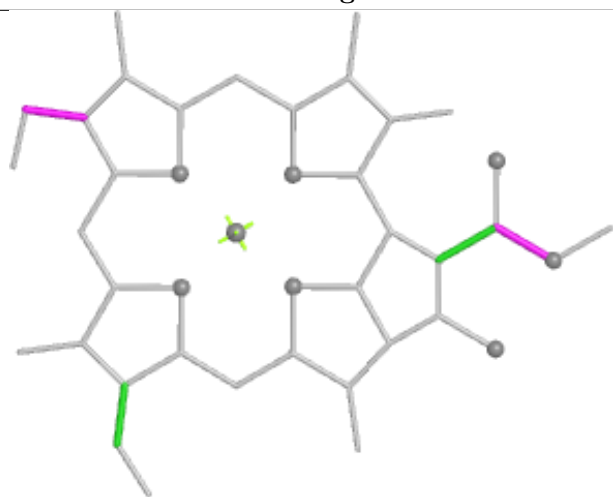
Ligand CLA X 310



Bond lengths



Bond angles

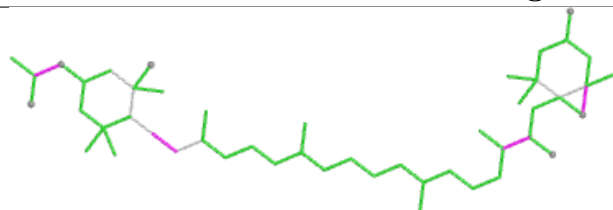


Torsions

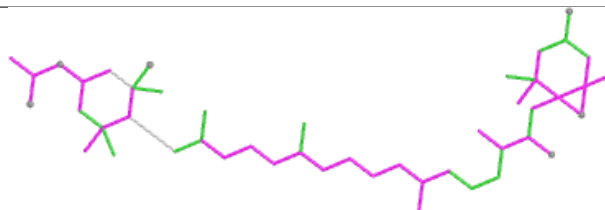


Rings

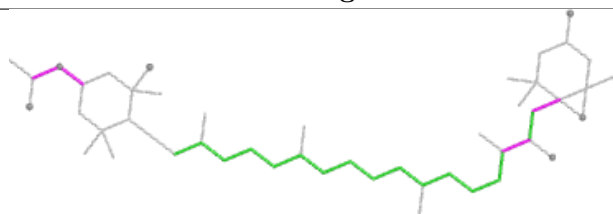
Ligand A86 I 304



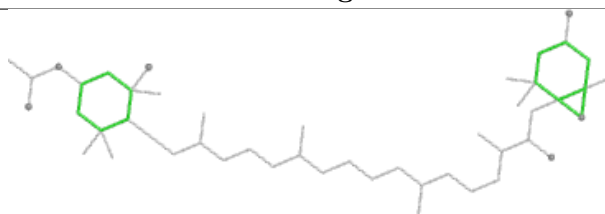
Bond lengths



Bond angles

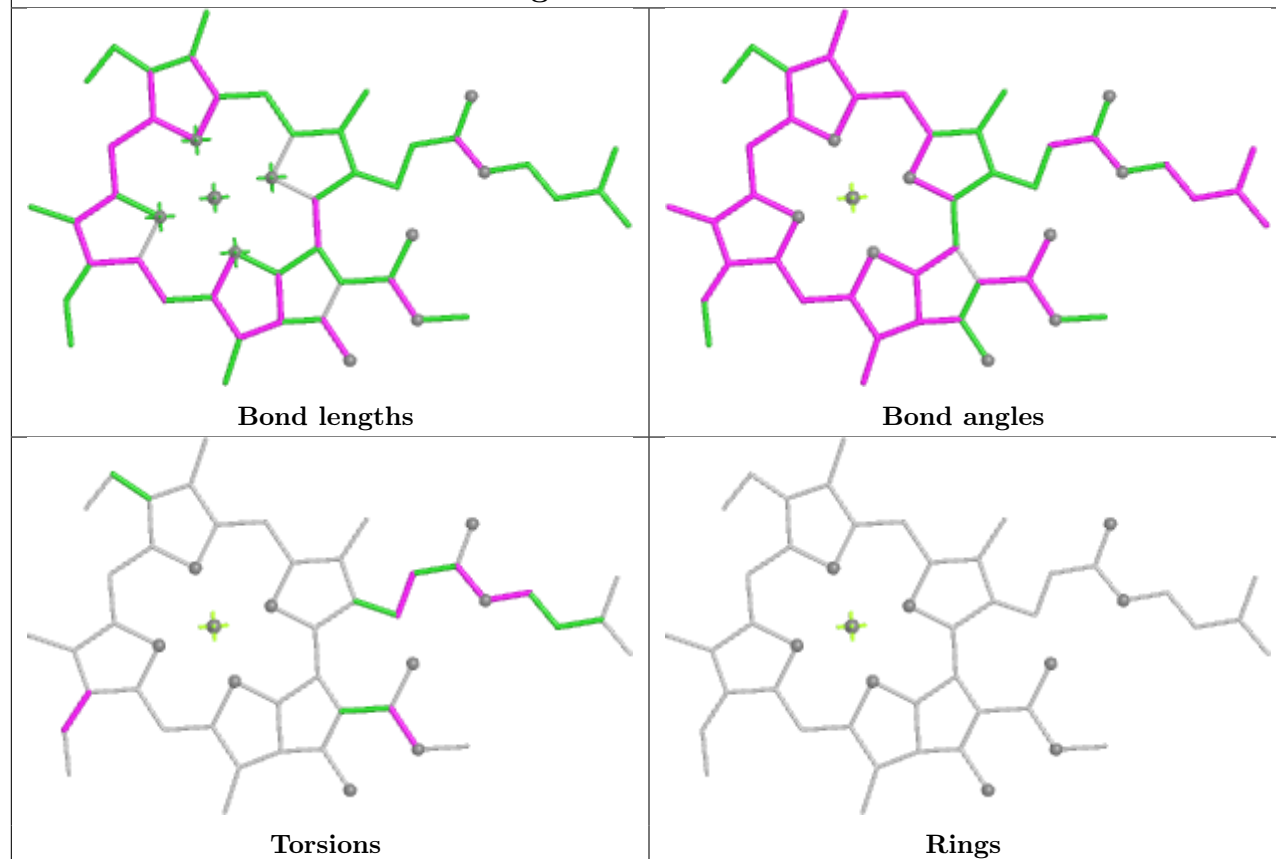


Torsions

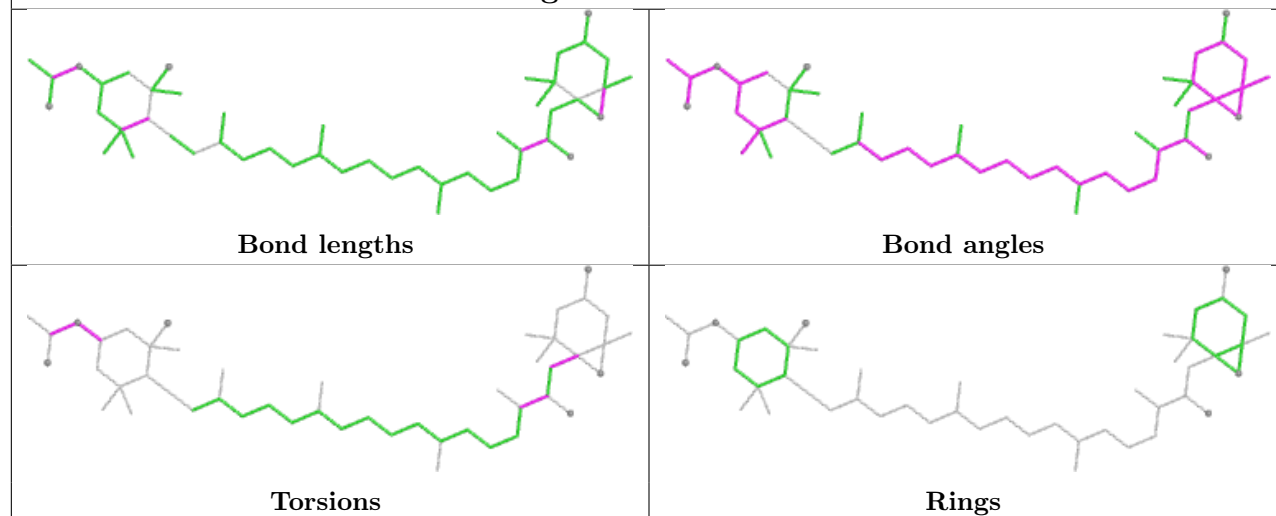


Rings

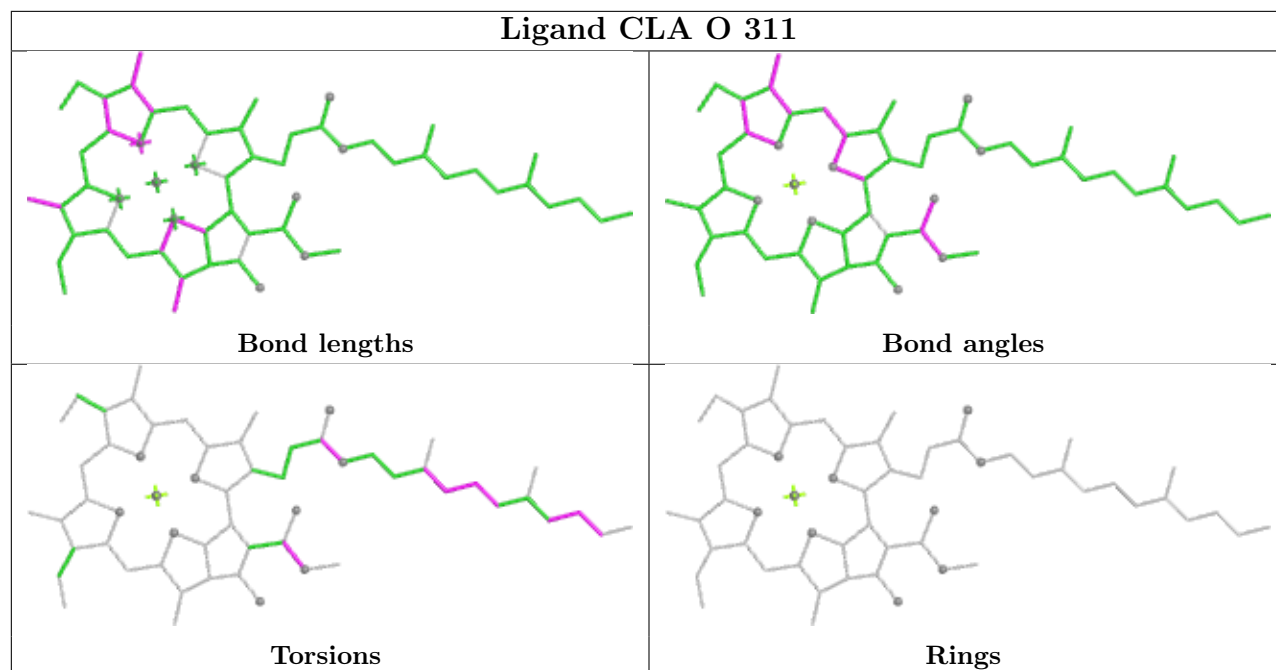
Ligand CLA G 319



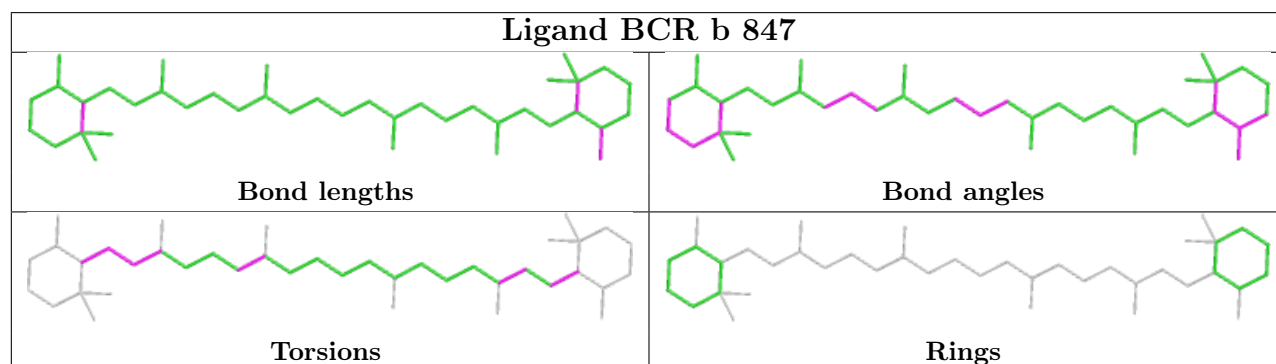
Ligand A86 S 301



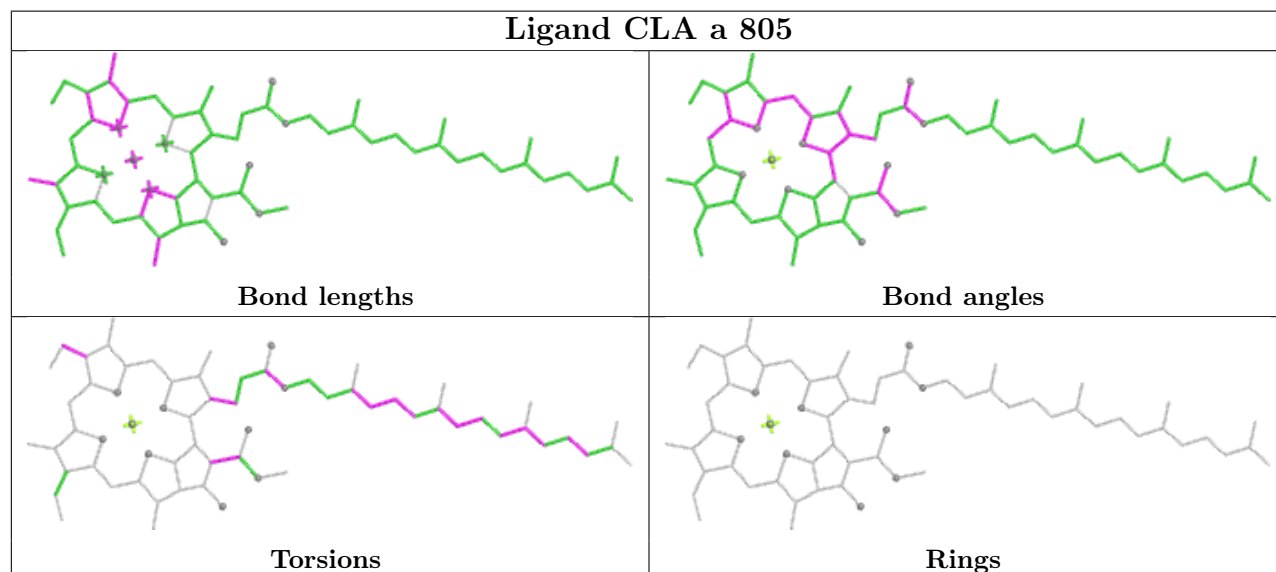
Ligand CLA O 311

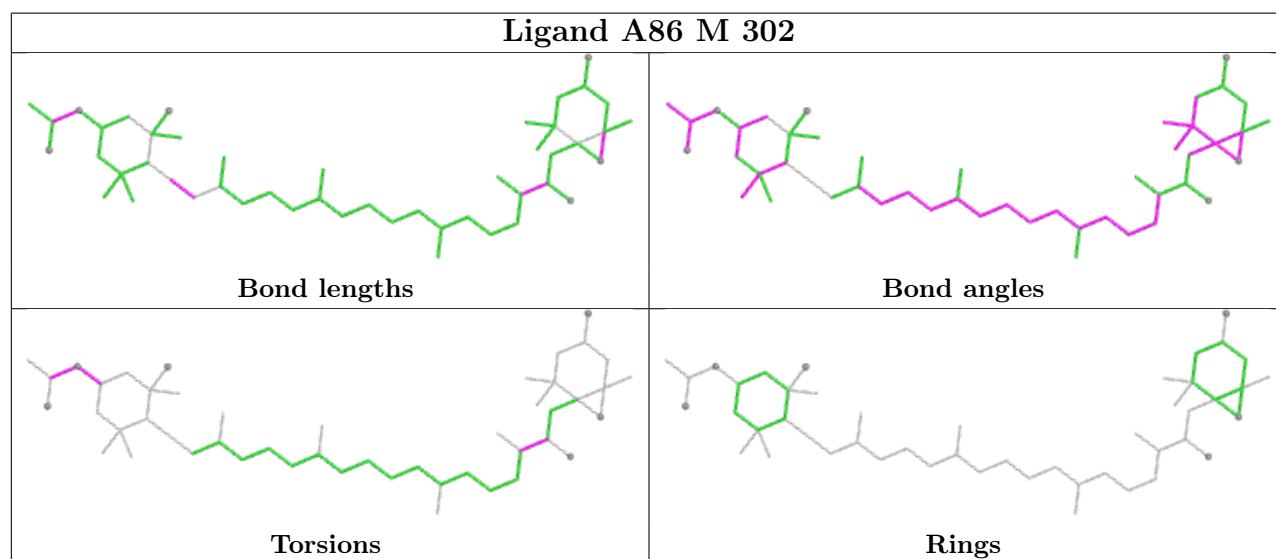
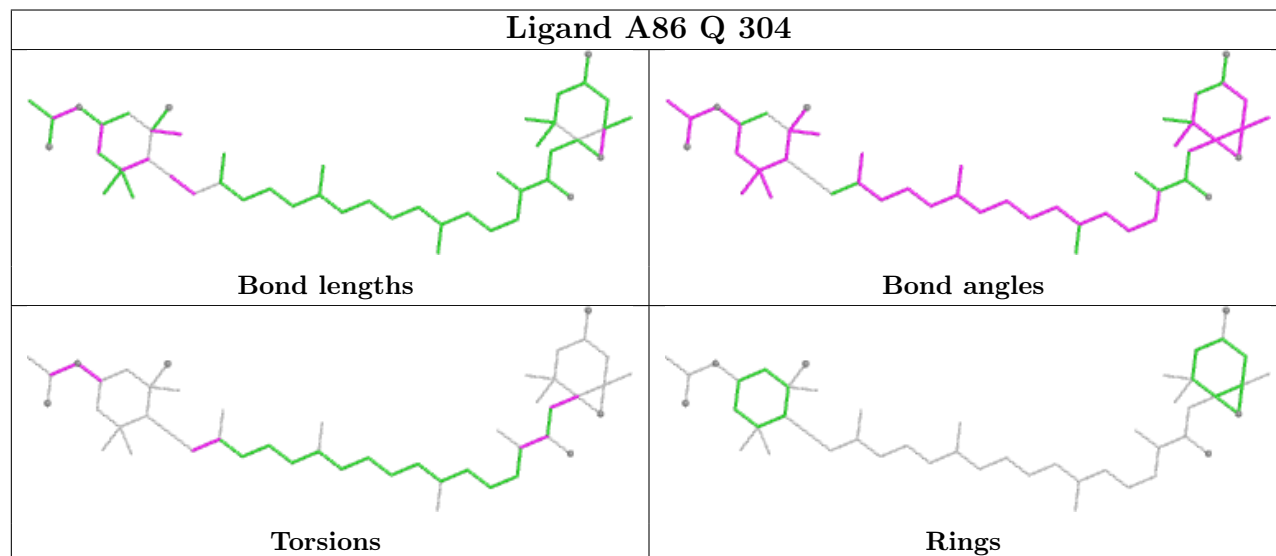
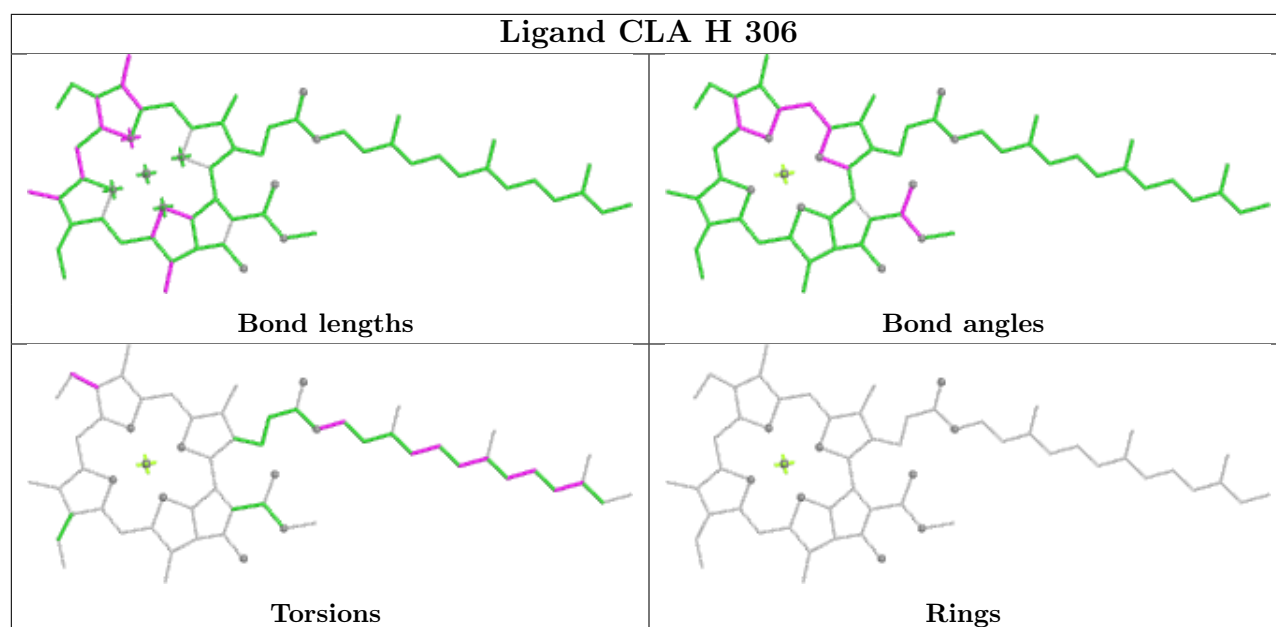


Ligand BCR b 847

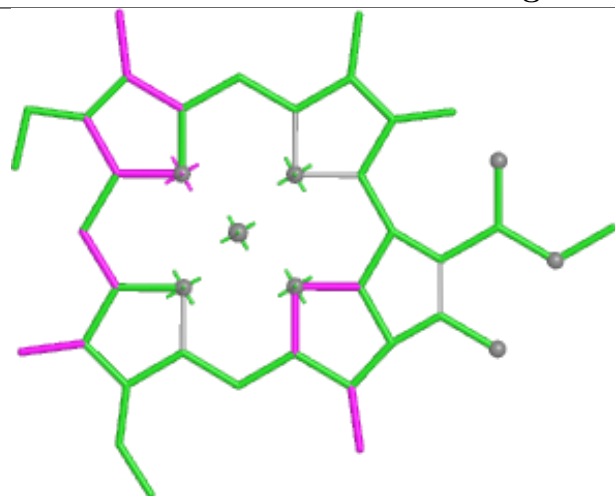


Ligand CLA a 805

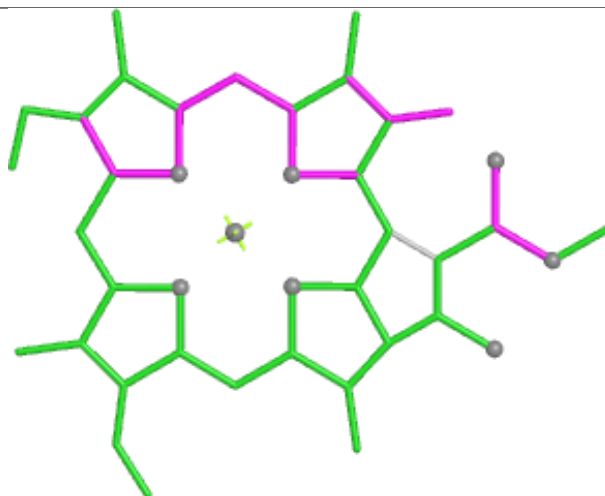




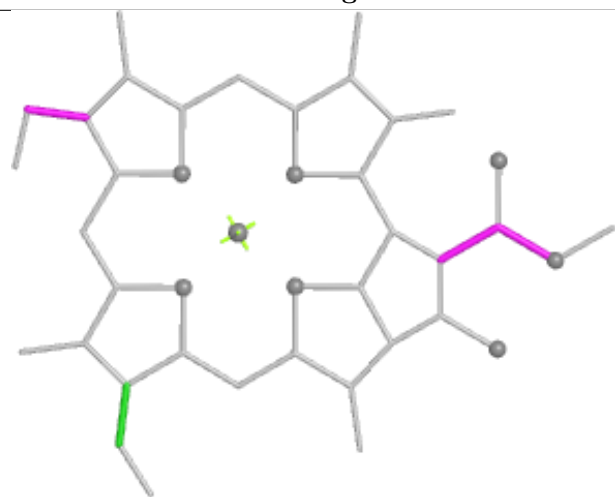
Ligand CLA I 313



Bond lengths



Bond angles

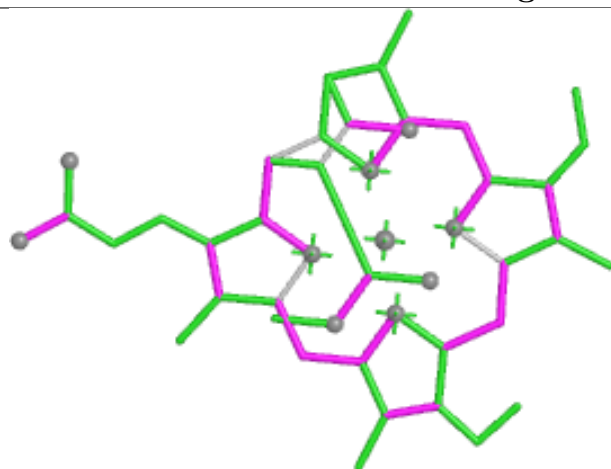


Torsions

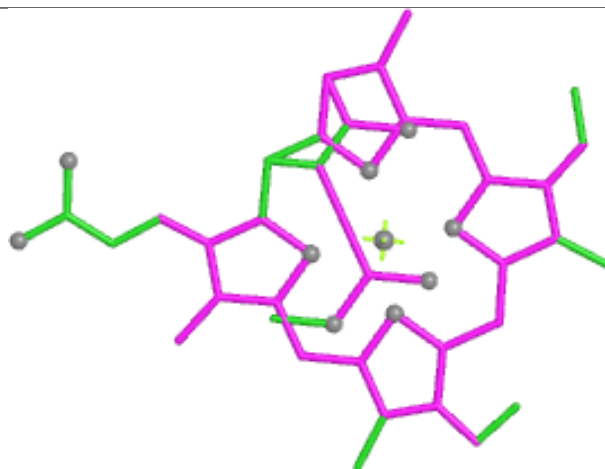


Rings

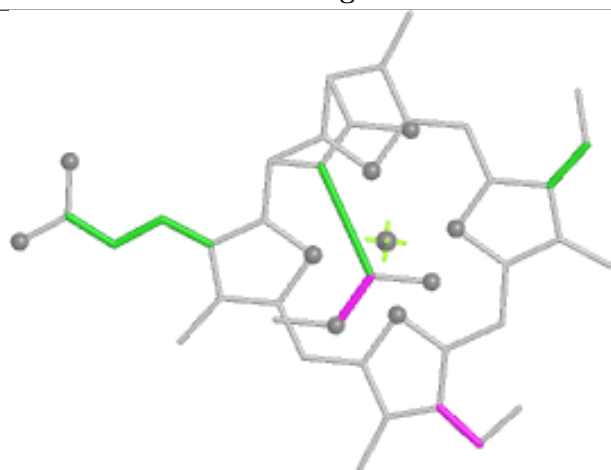
Ligand KC1 F 315



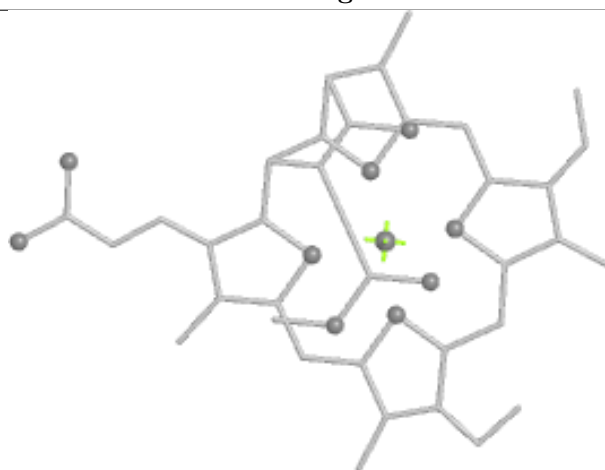
Bond lengths



Bond angles

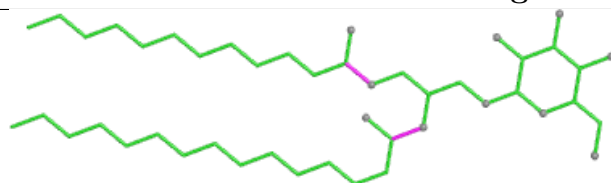


Torsions

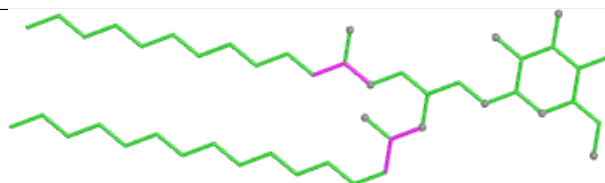


Rings

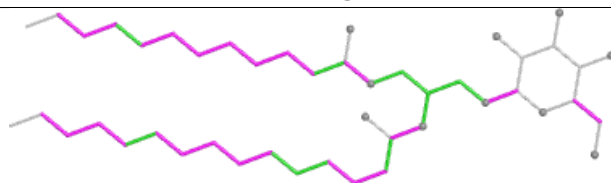
Ligand LMG E 318



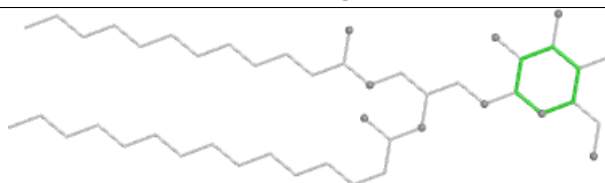
Bond lengths



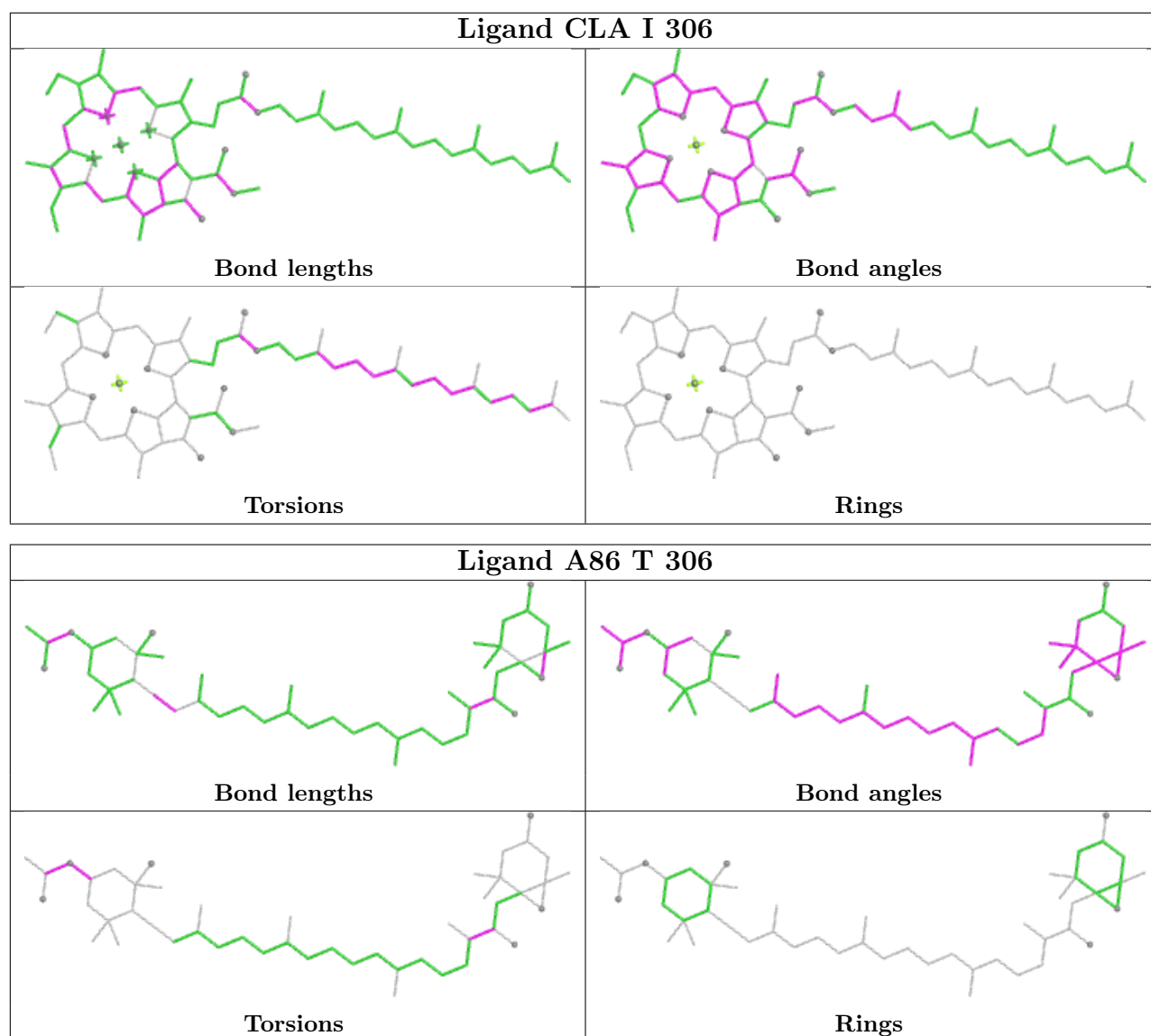
Bond angles

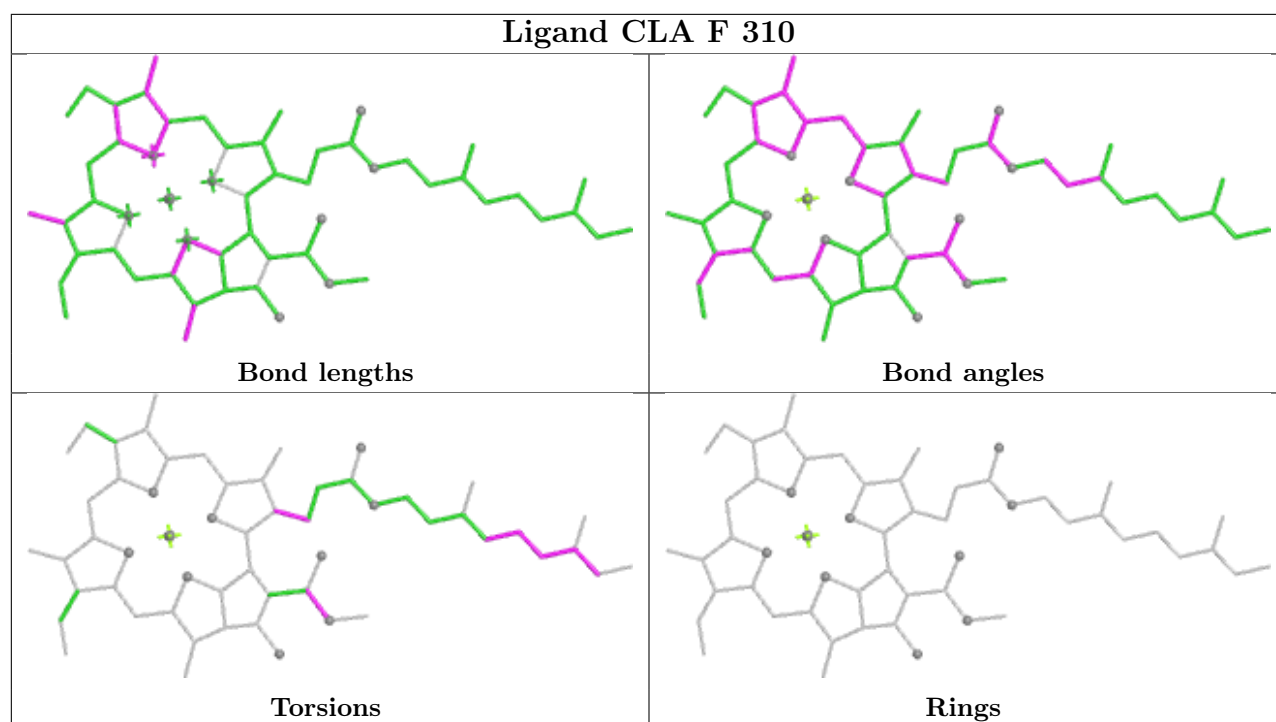


Torsions

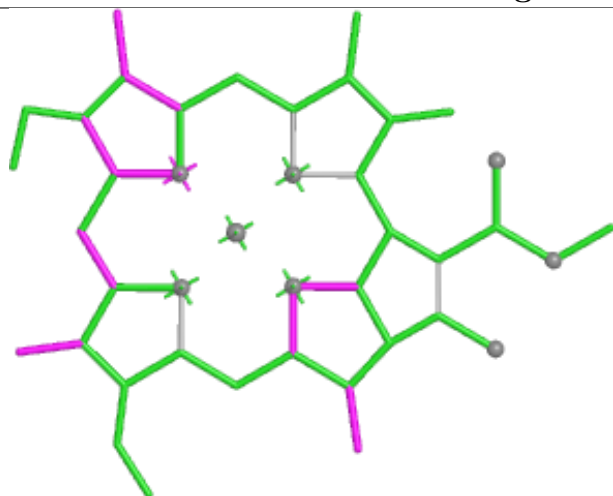


Rings





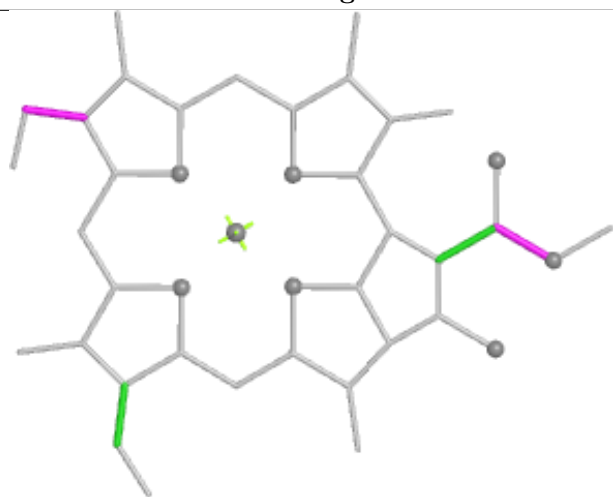
Ligand CLA C 214



Bond lengths



Bond angles

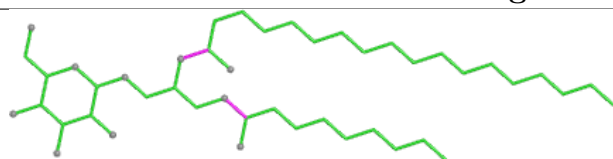


Torsions

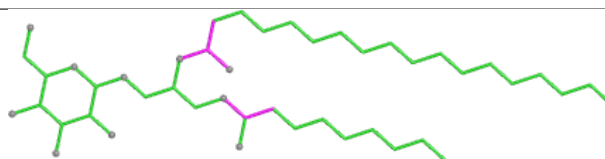


Rings

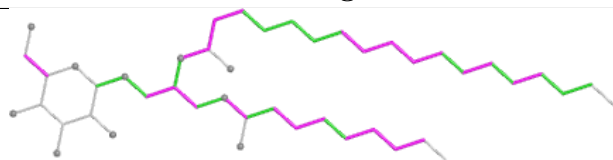
Ligand LMG V 315



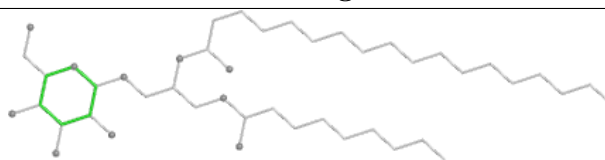
Bond lengths



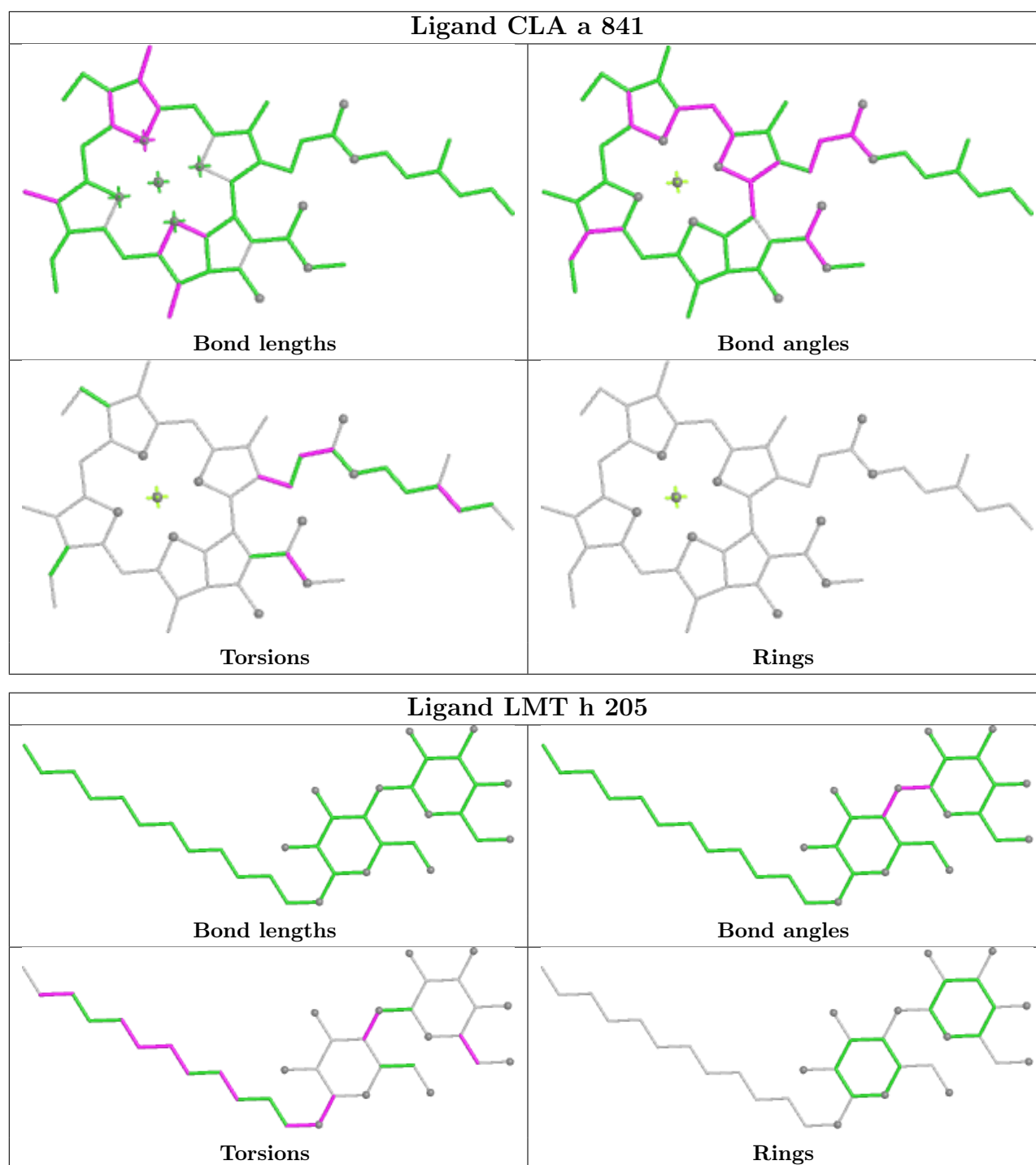
Bond angles

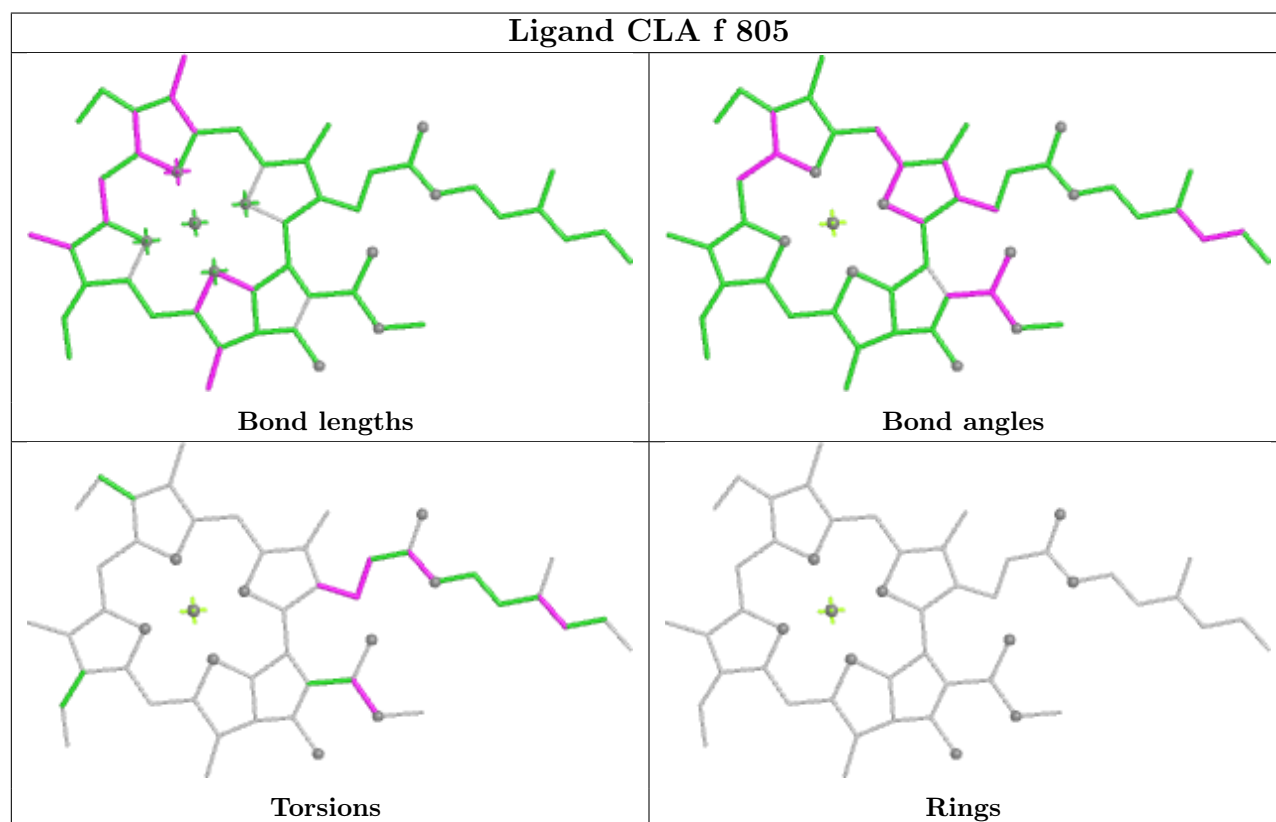
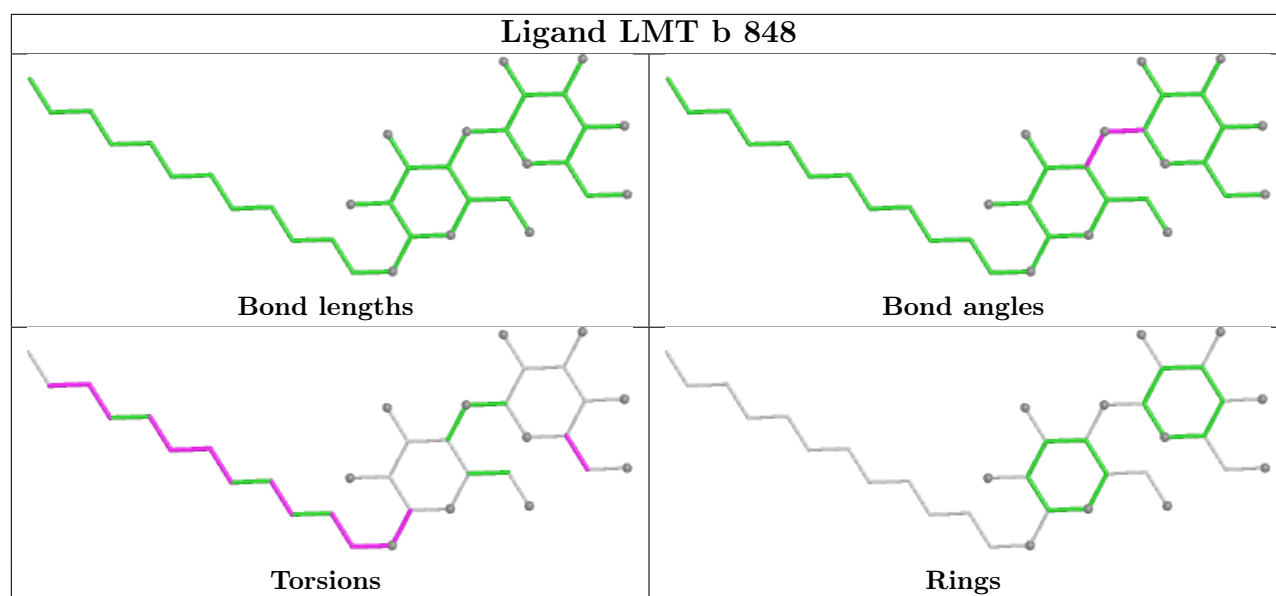


Torsions

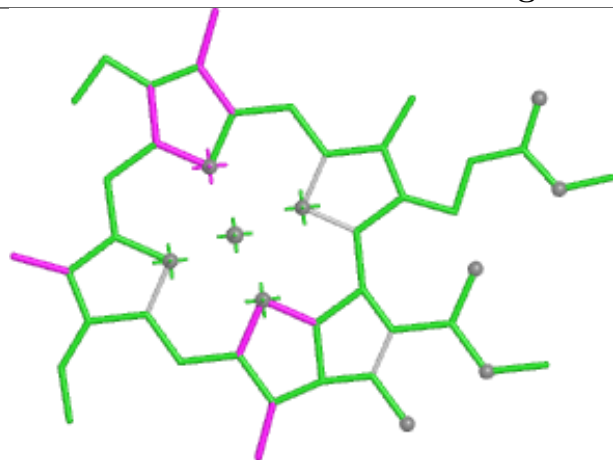


Rings

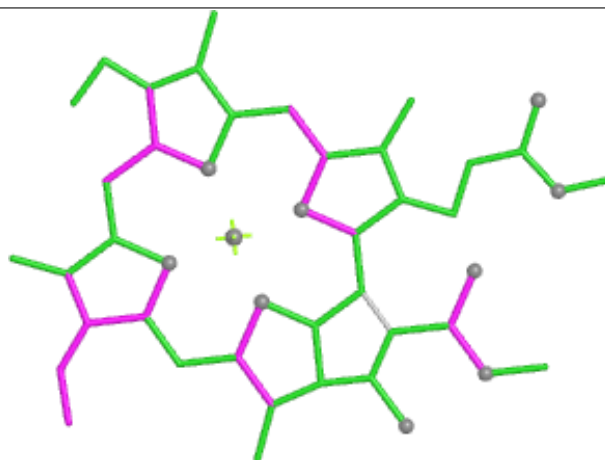




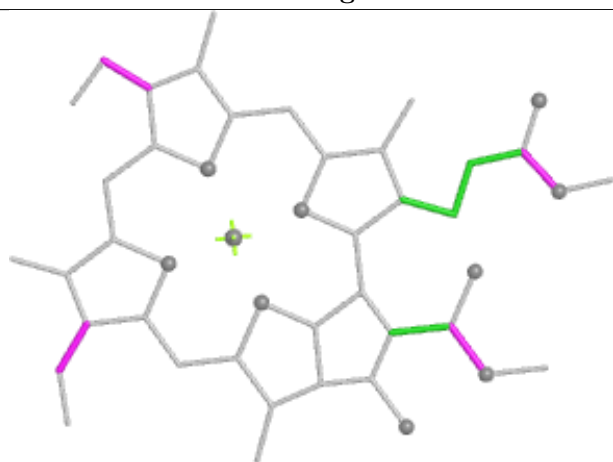
Ligand CLA J 316



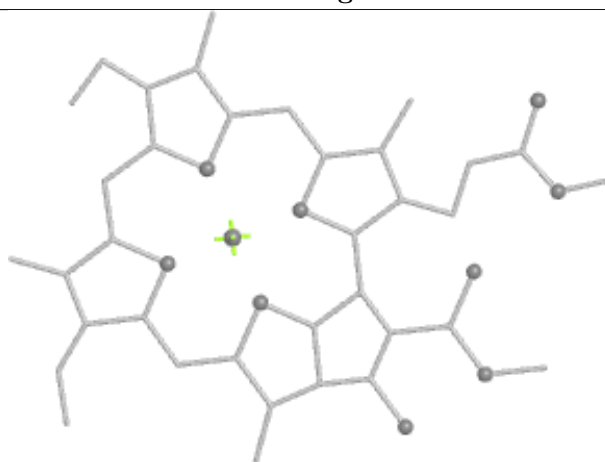
Bond lengths



Bond angles

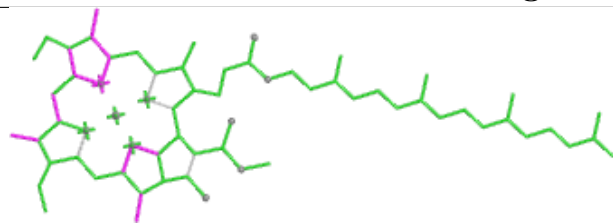


Torsions

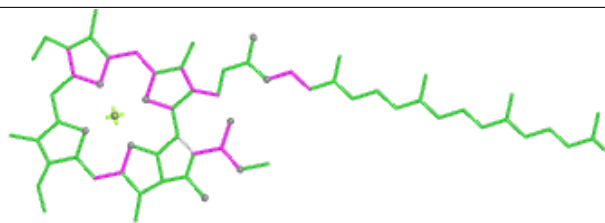


Rings

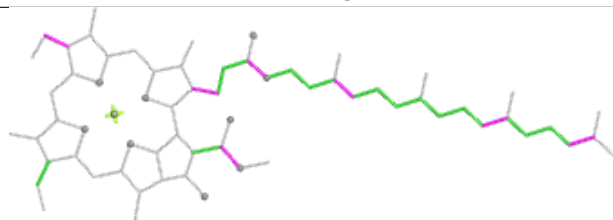
Ligand CLA I 202



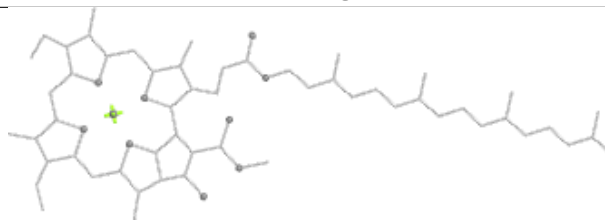
Bond lengths



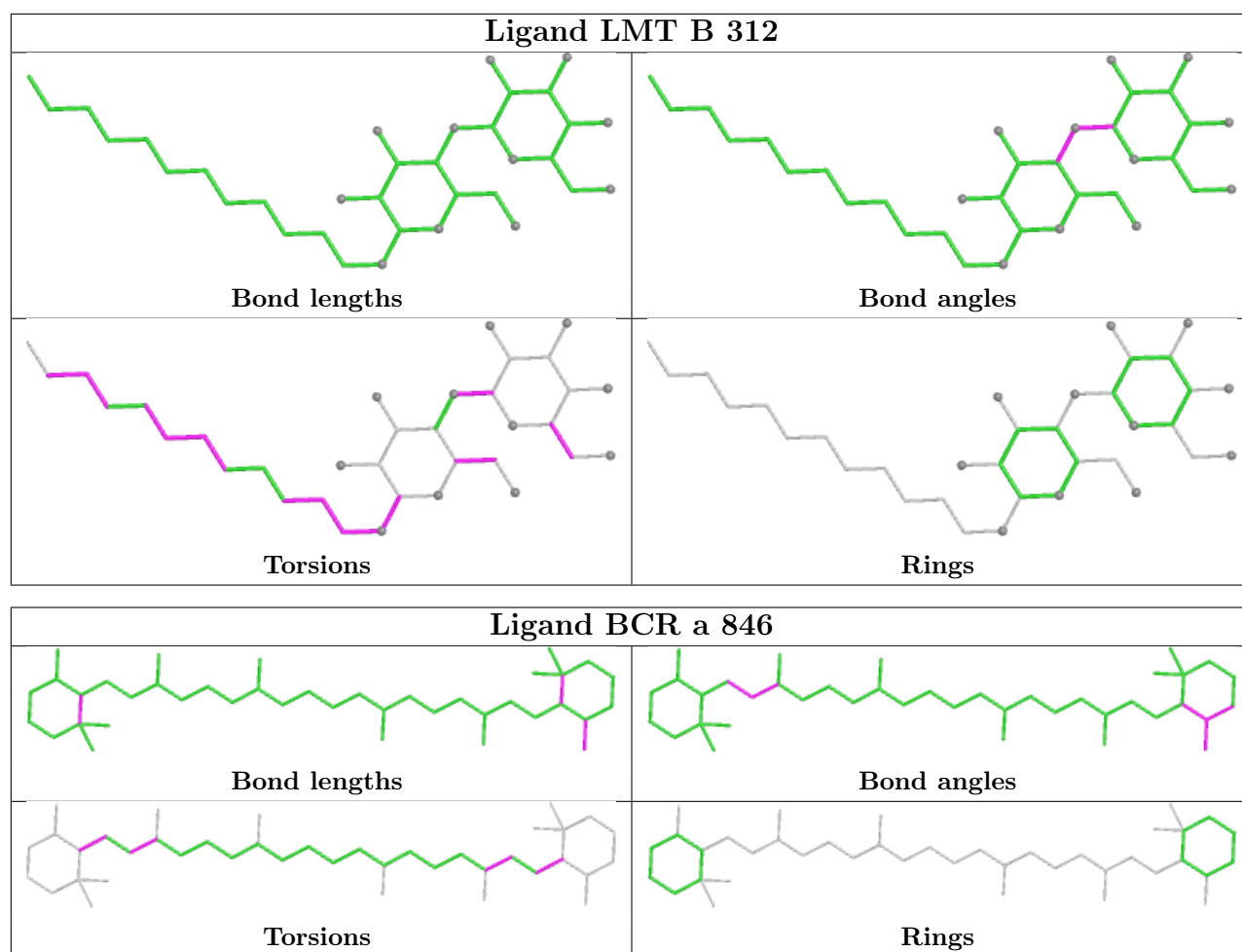
Bond angles



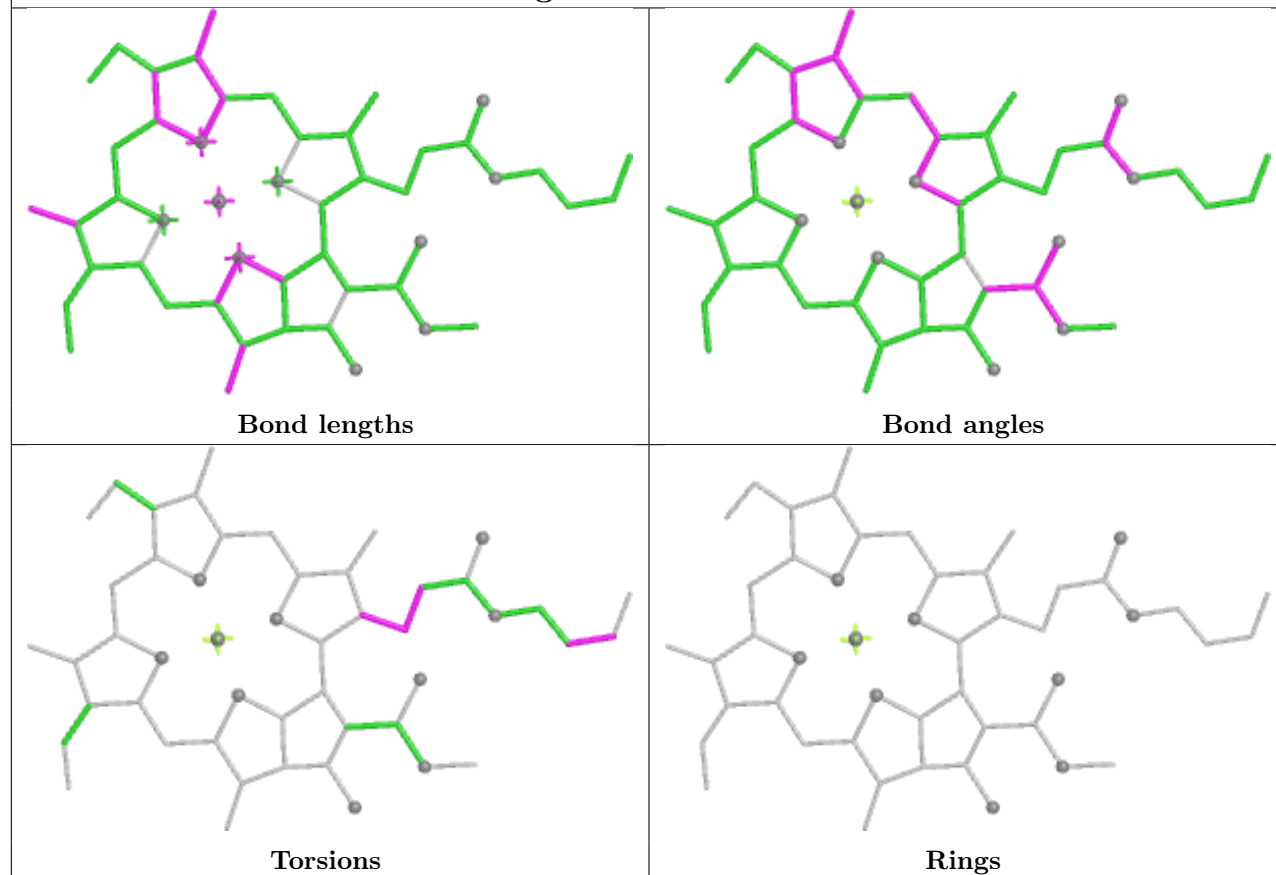
Torsions



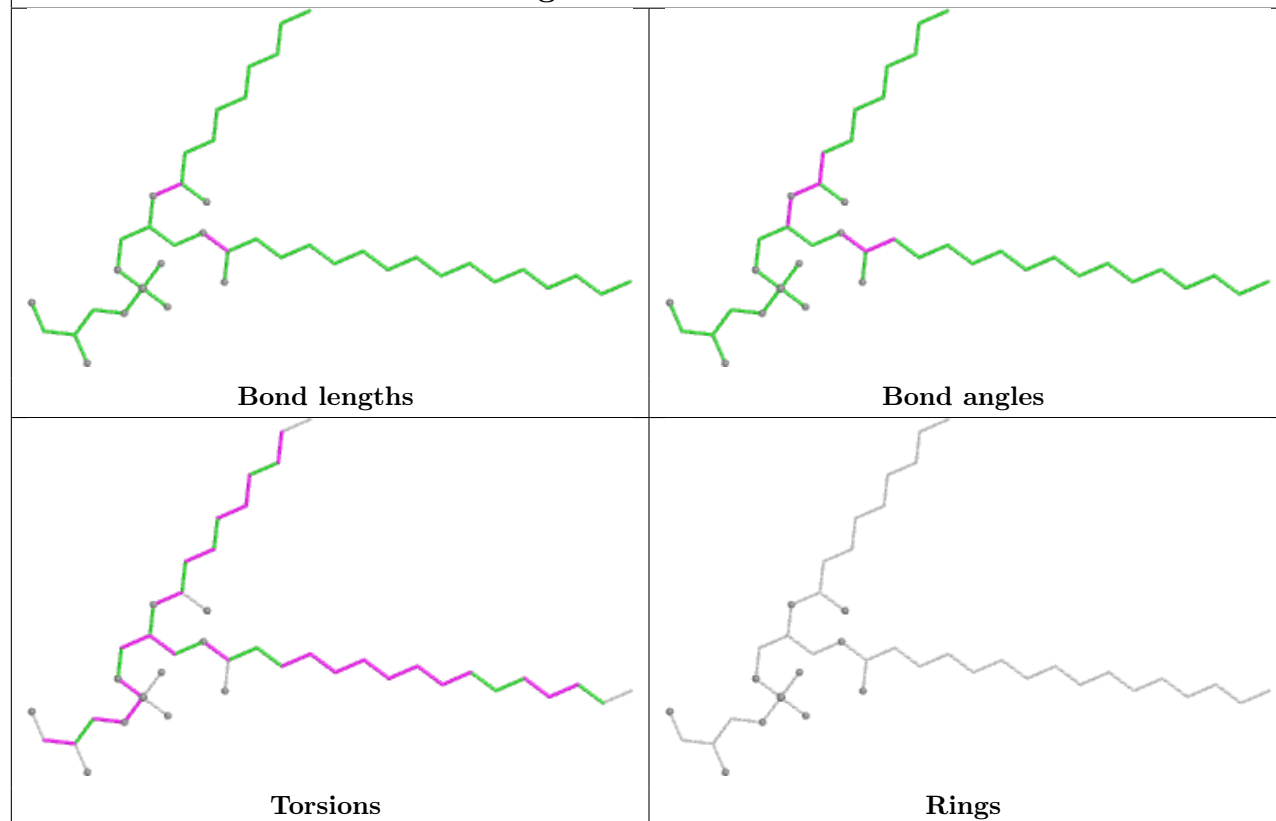
Rings

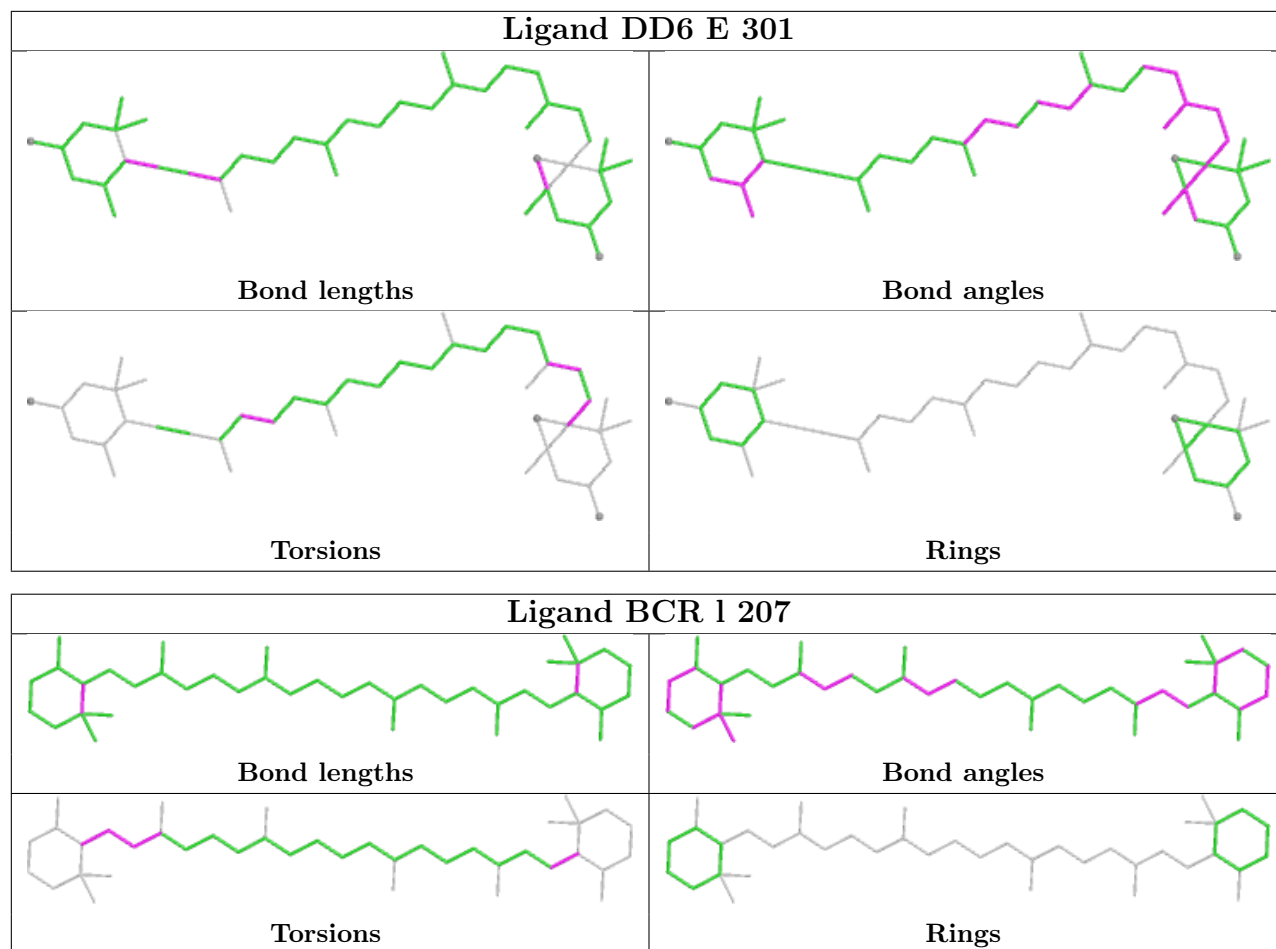


Ligand CLA b 832

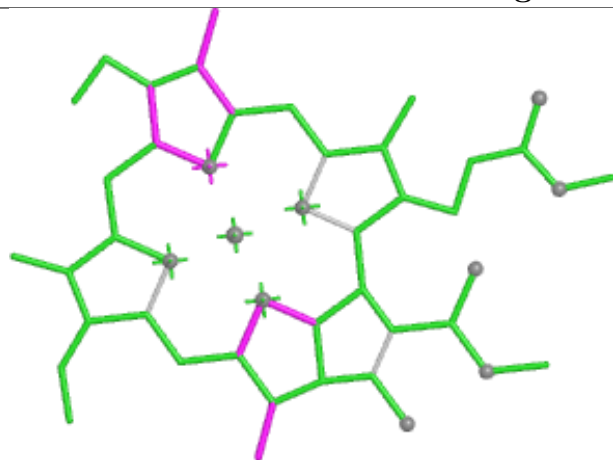


Ligand LHG f 809

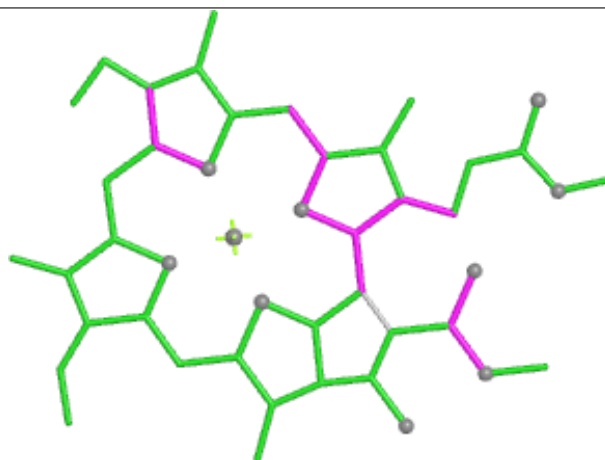




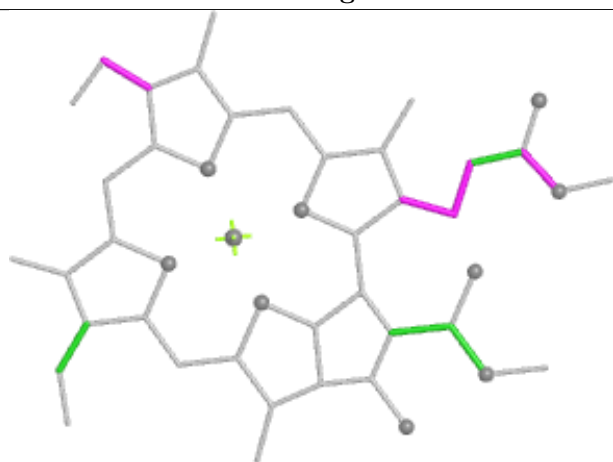
Ligand CLA B 307



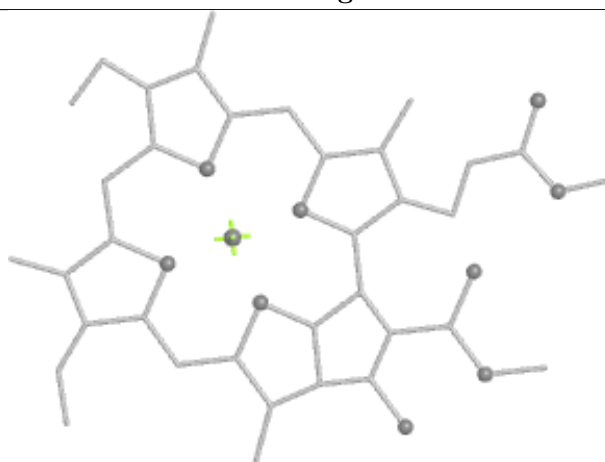
Bond lengths



Bond angles

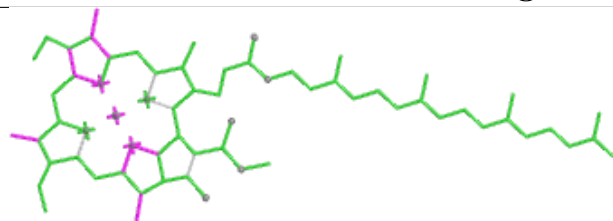


Torsions

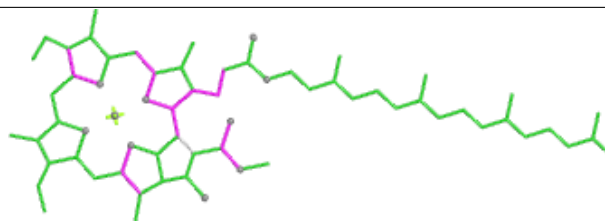


Rings

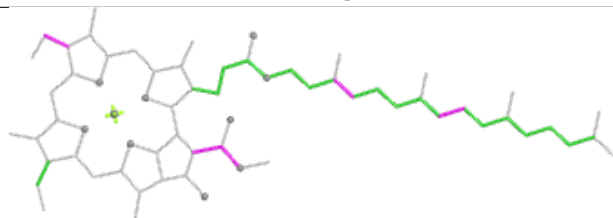
Ligand CLA S 319



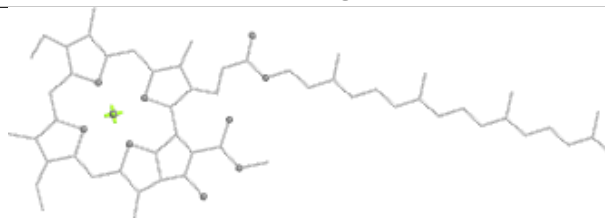
Bond lengths



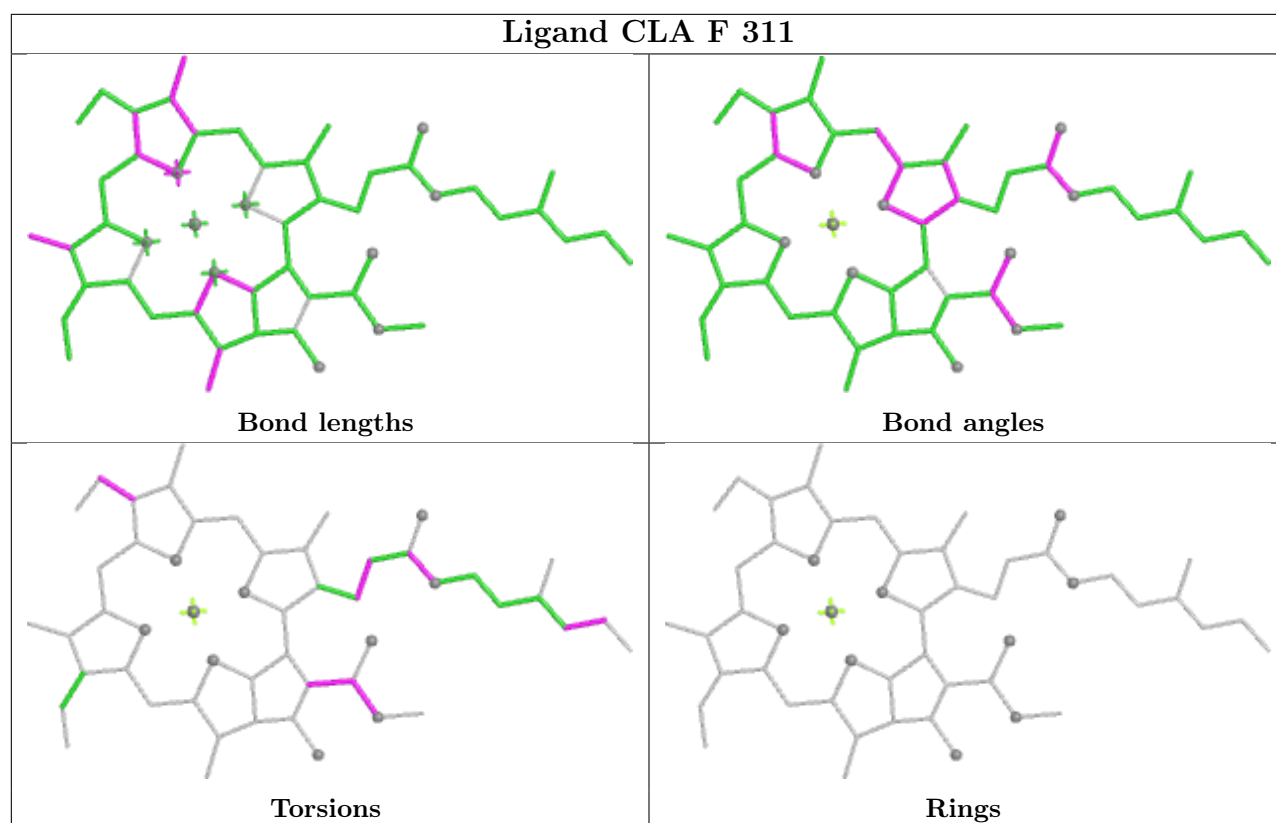
Bond angles



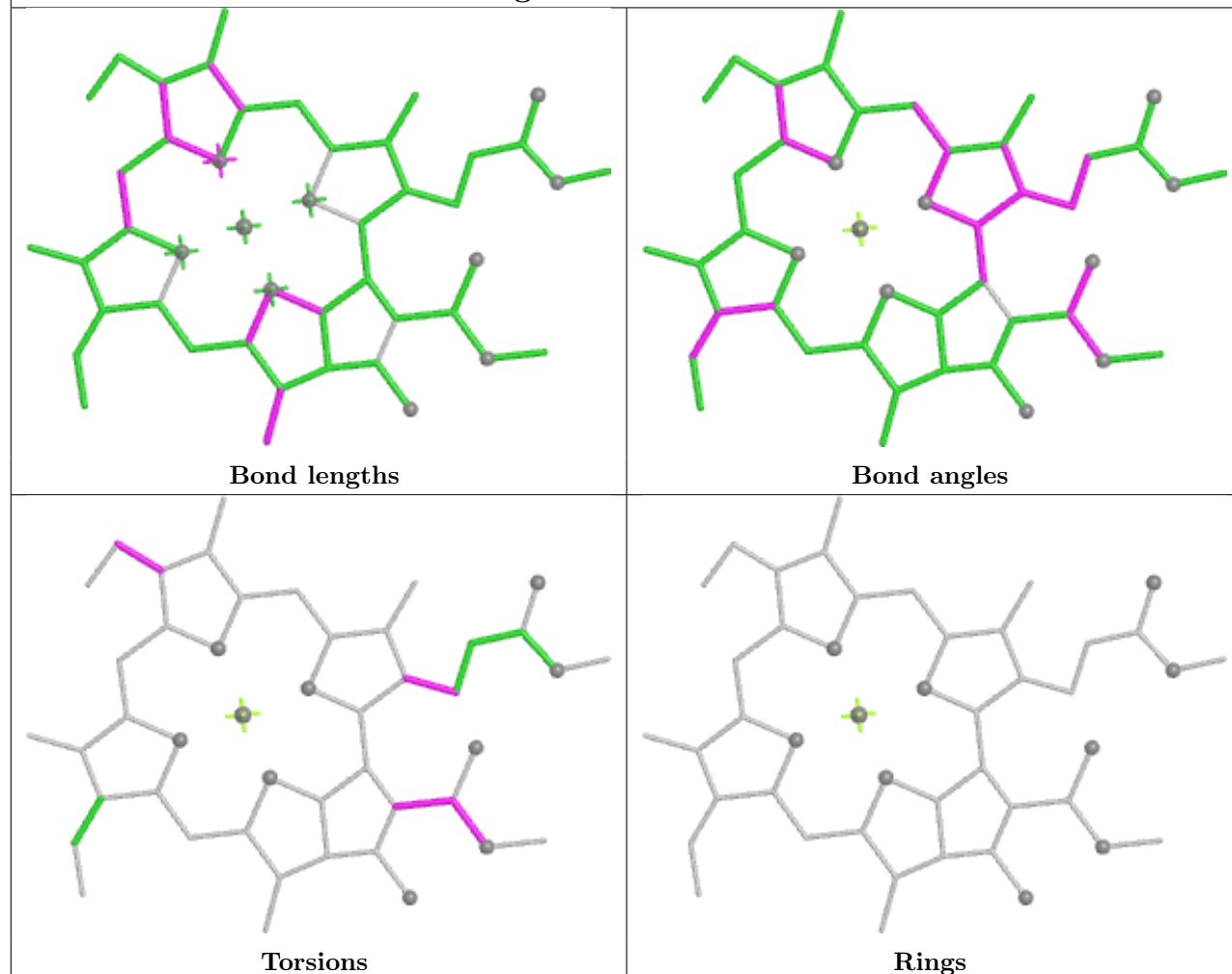
Torsions



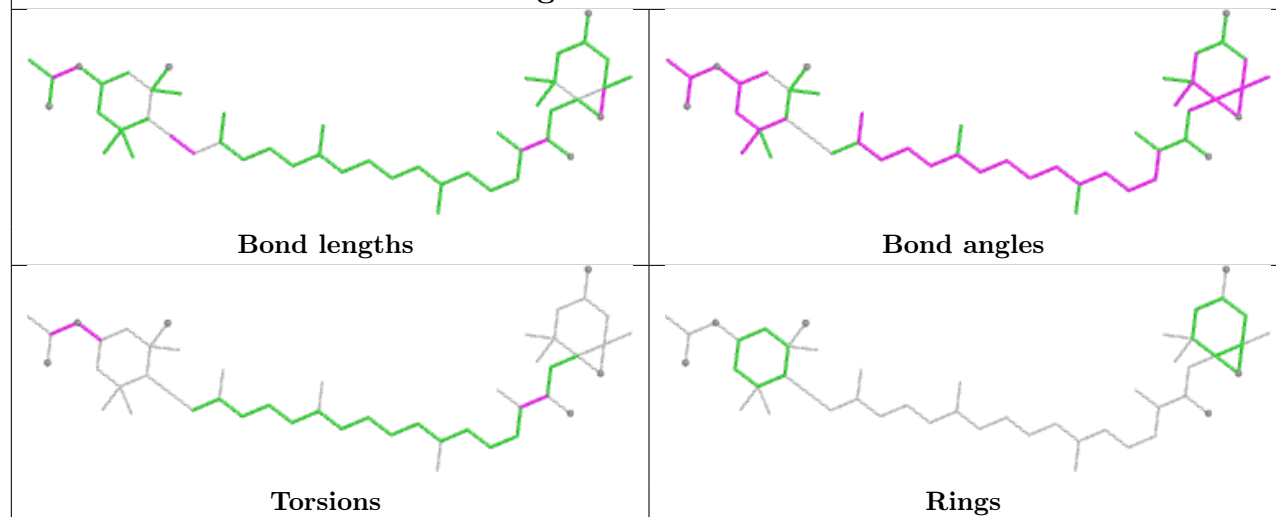
Rings

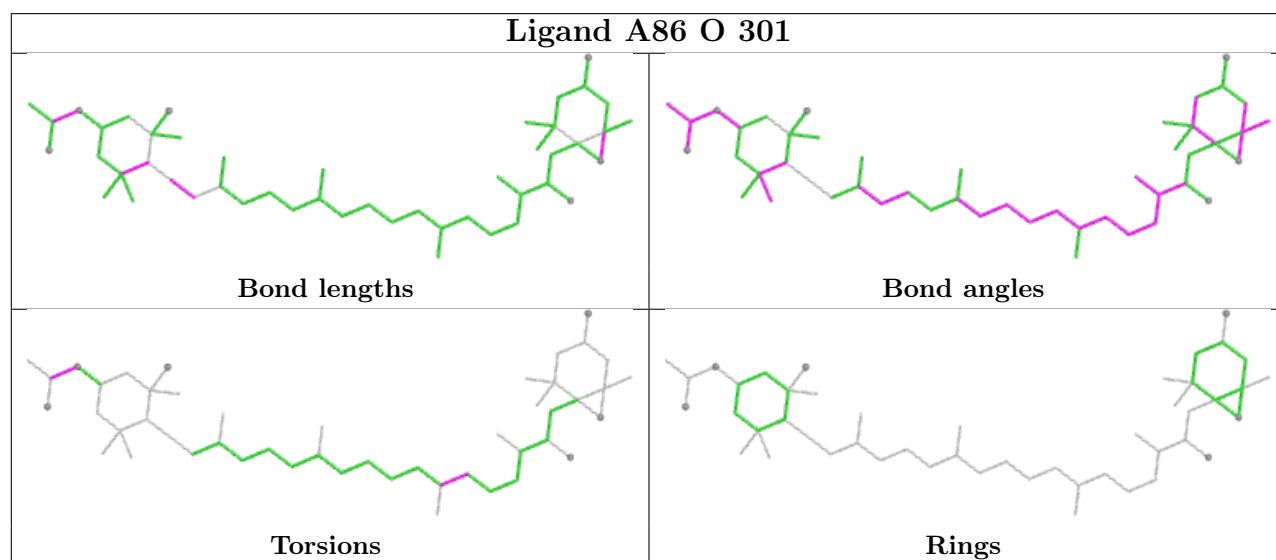
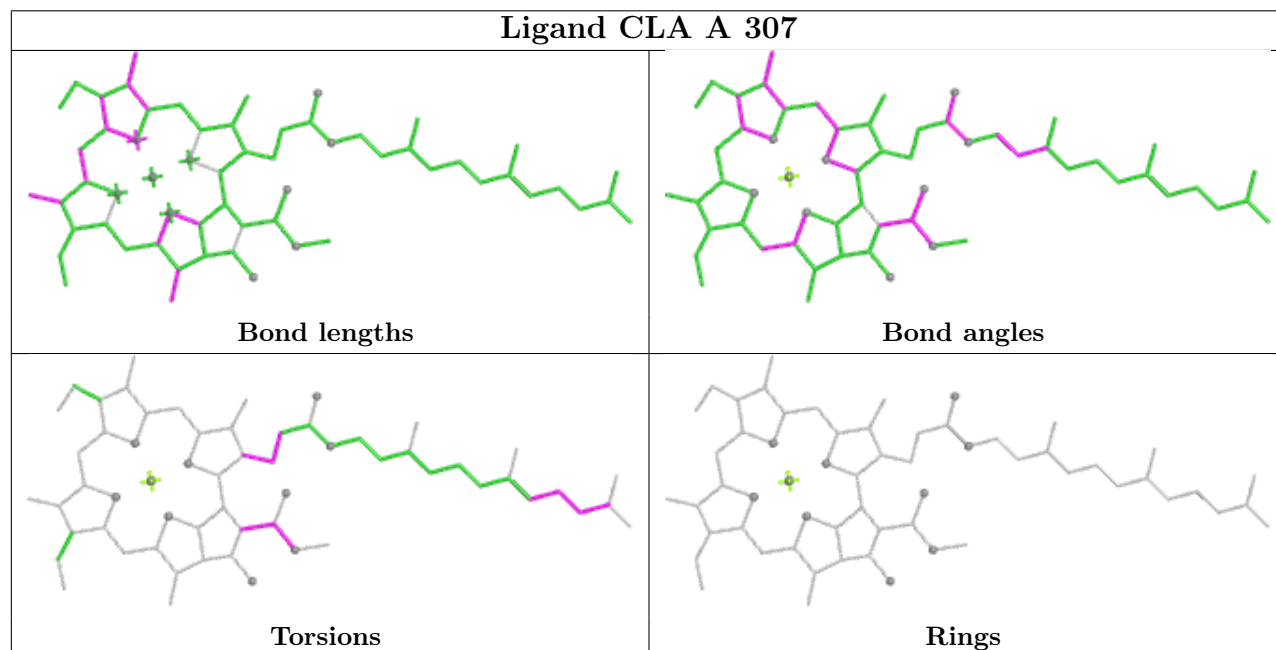
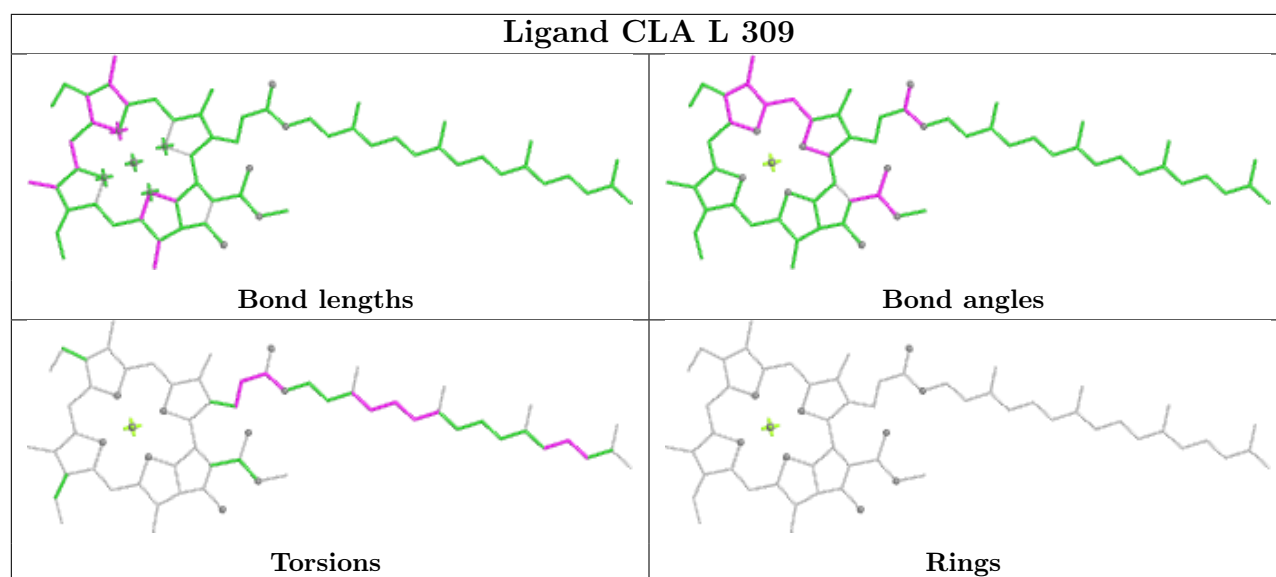


Ligand CLA T 312

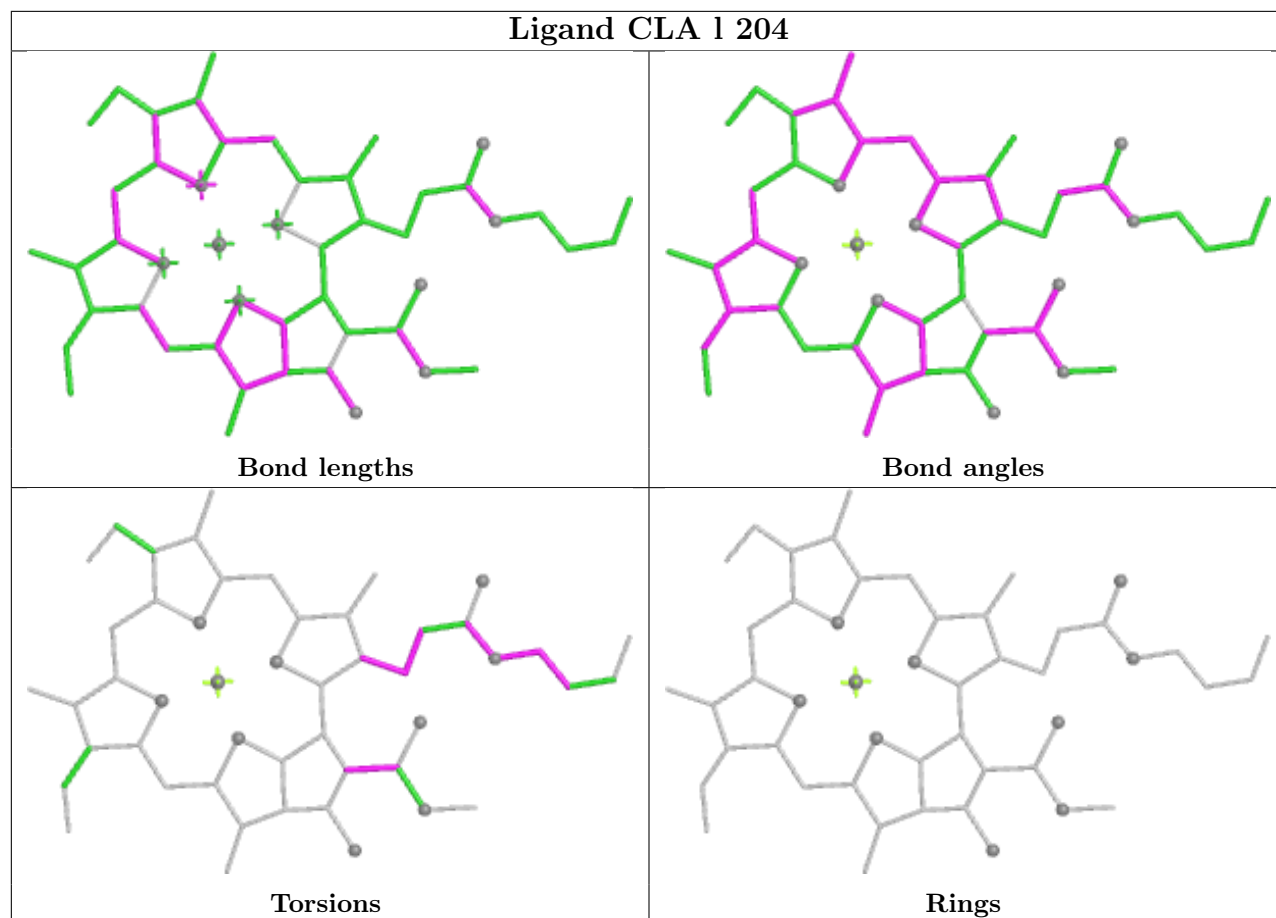


Ligand A86 V 303

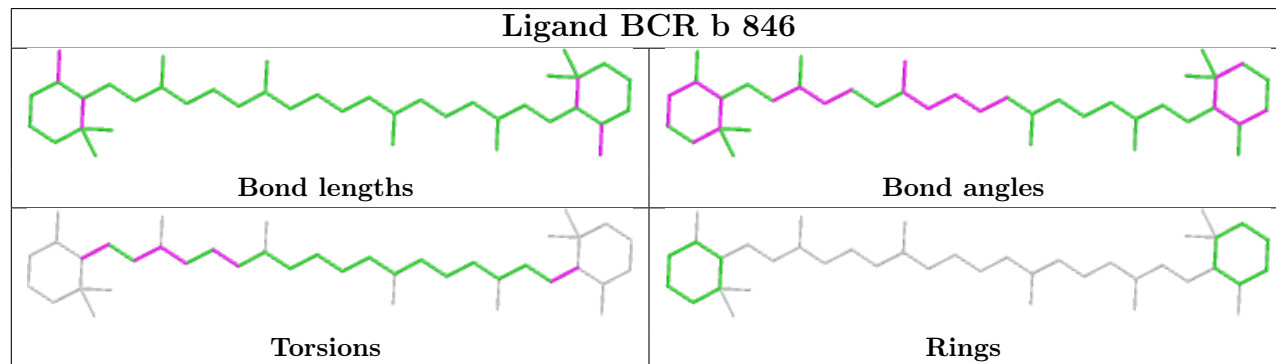


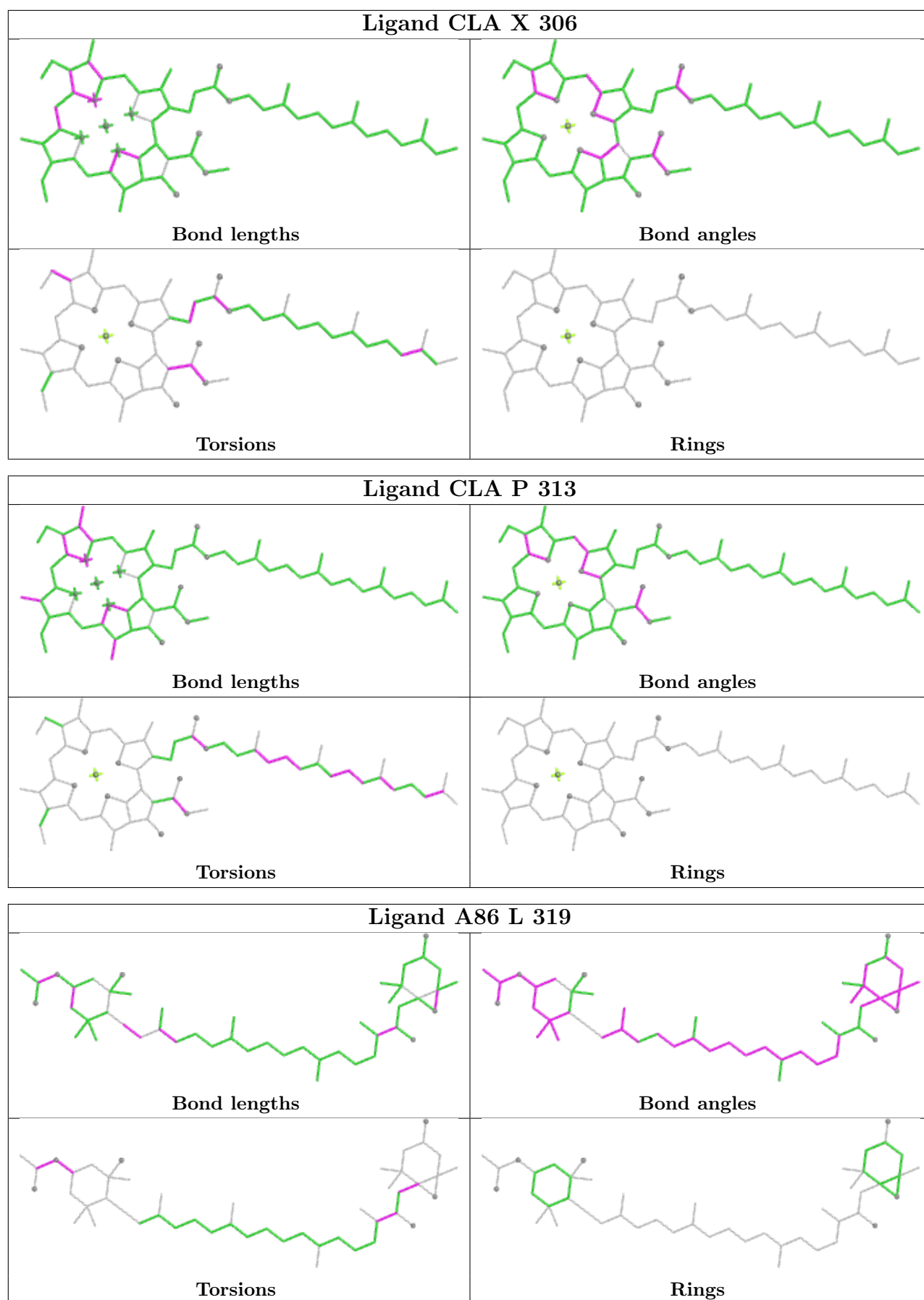


Ligand CLA l 204

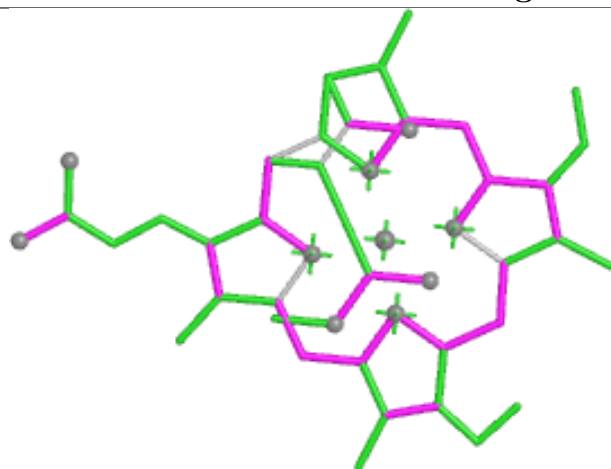


Ligand BCR b 846

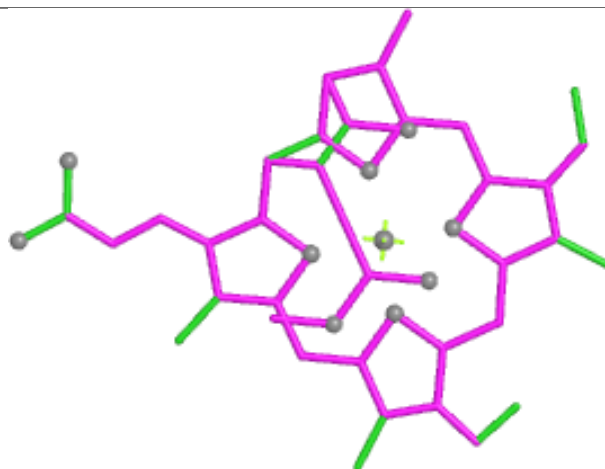




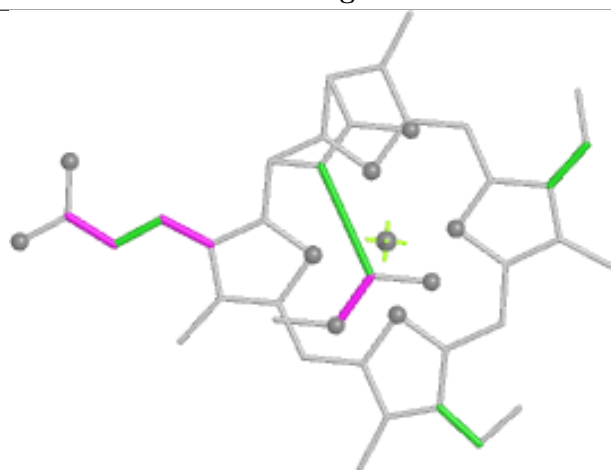
Ligand KC1 G 317



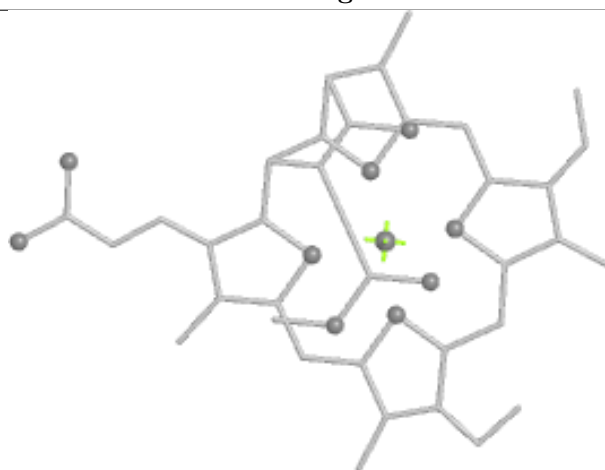
Bond lengths



Bond angles

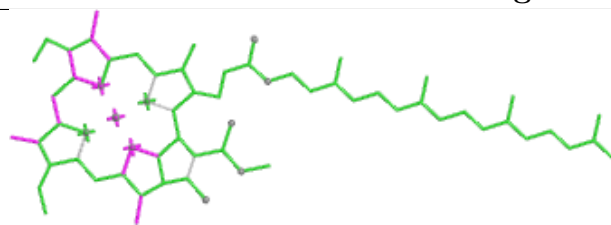


Torsions

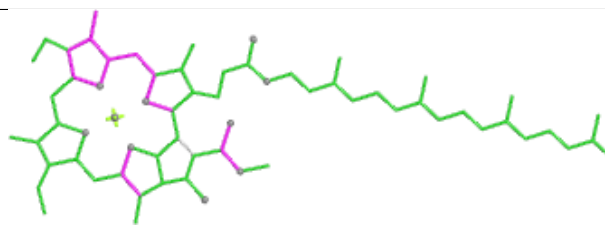


Rings

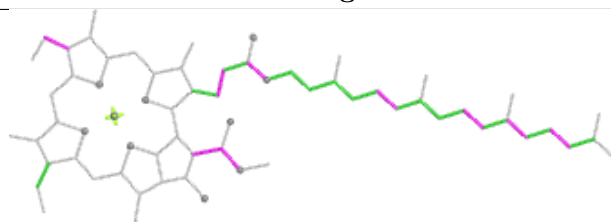
Ligand CLA R 313



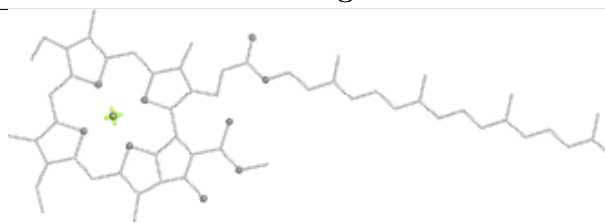
Bond lengths



Bond angles

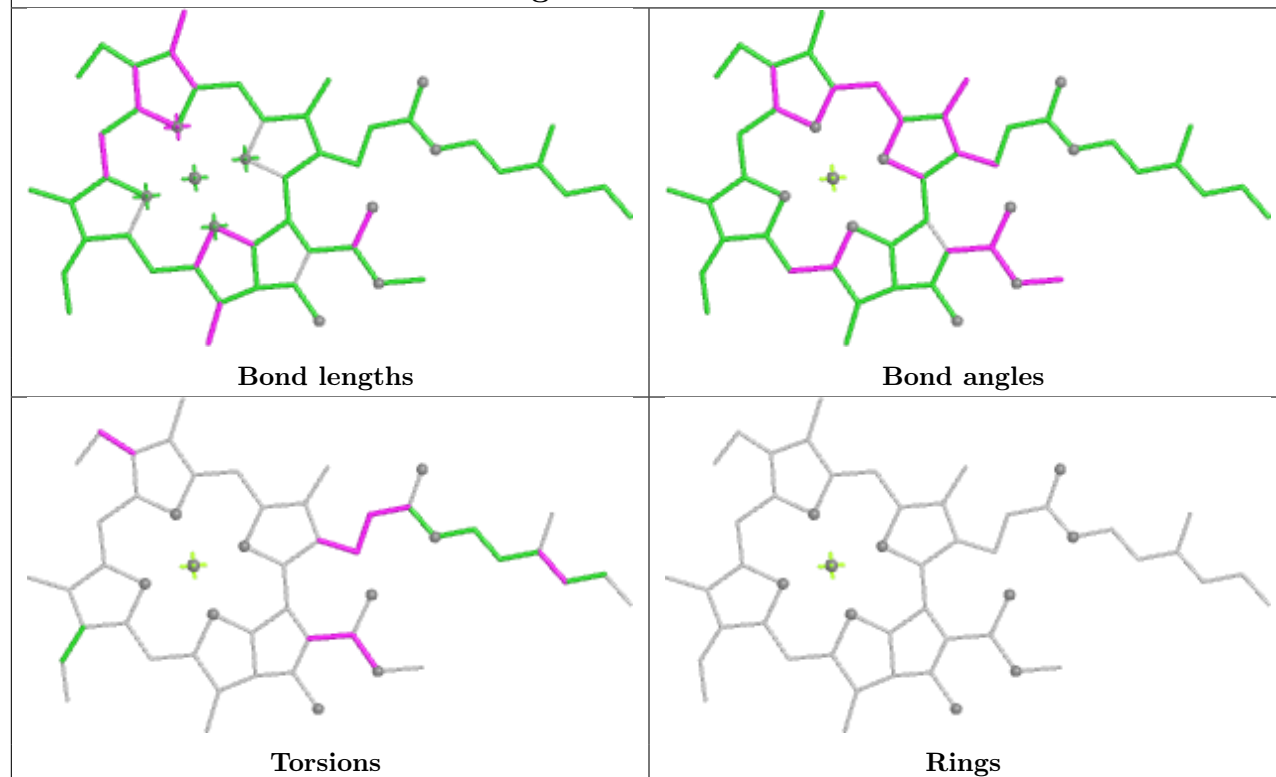


Torsions

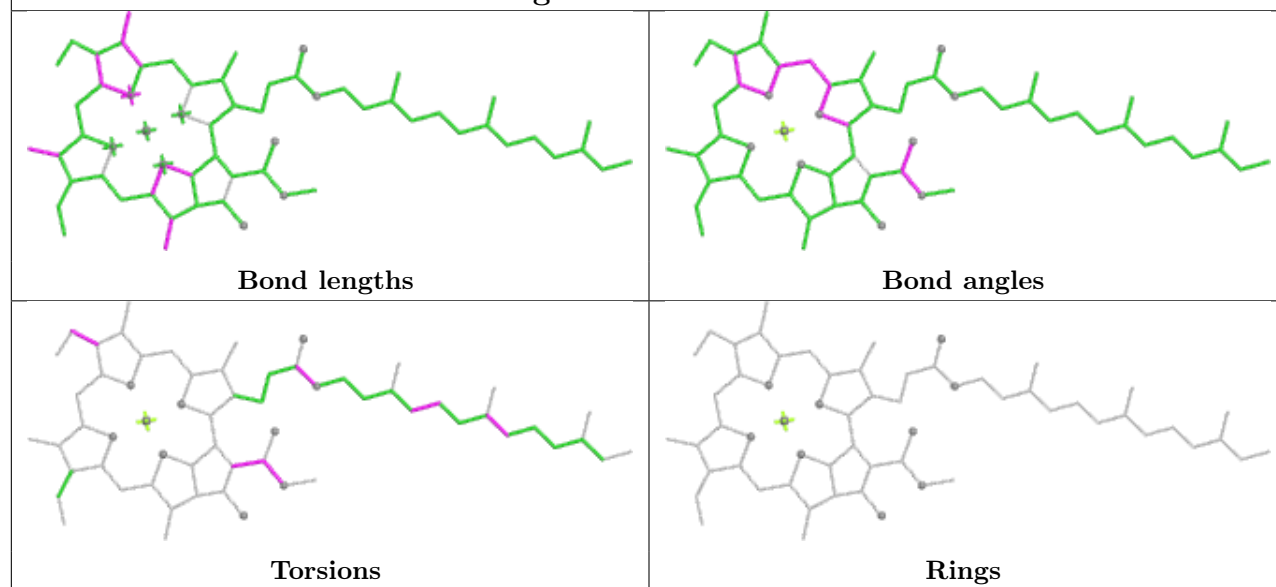


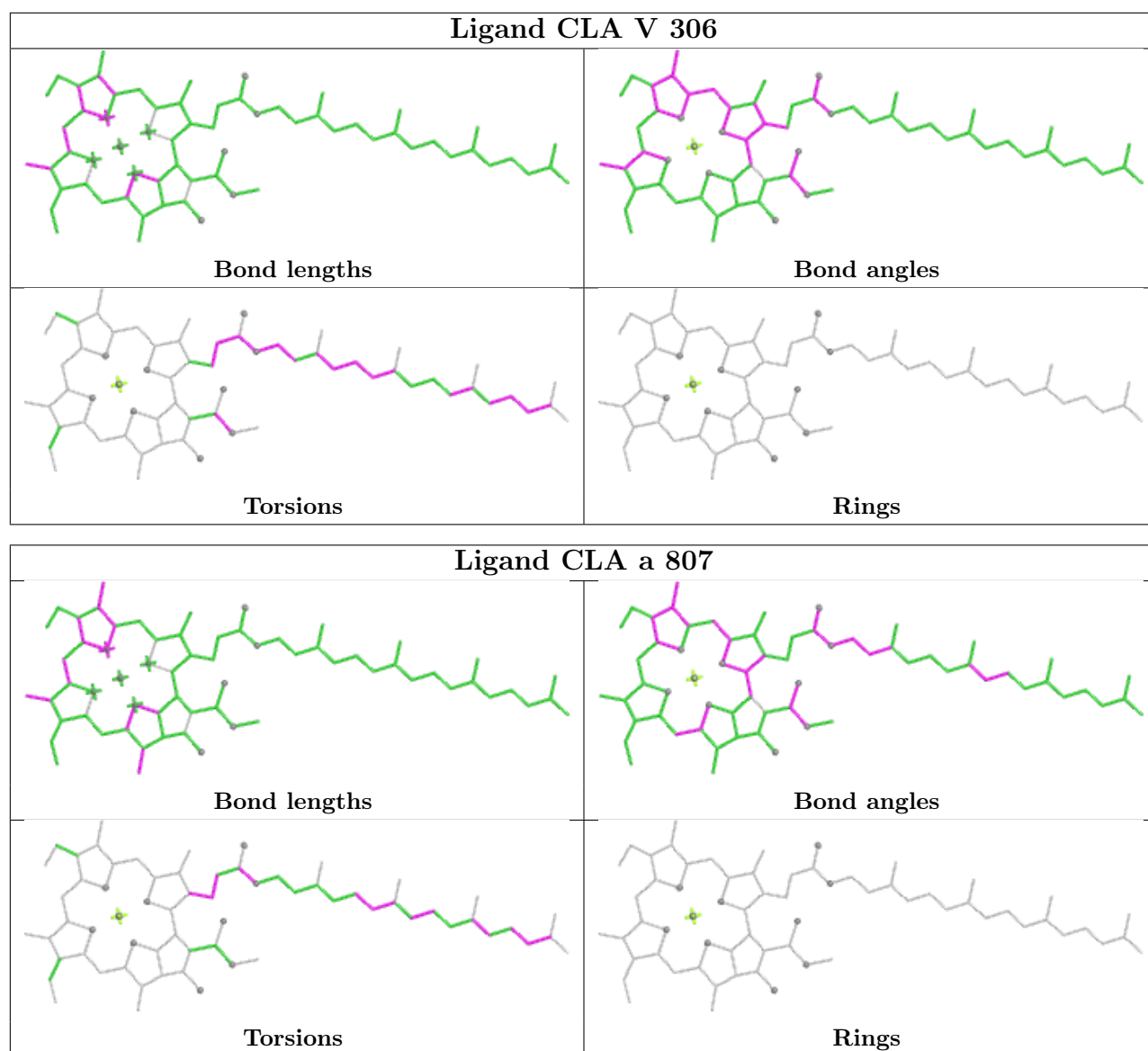
Rings

Ligand CLA R 322

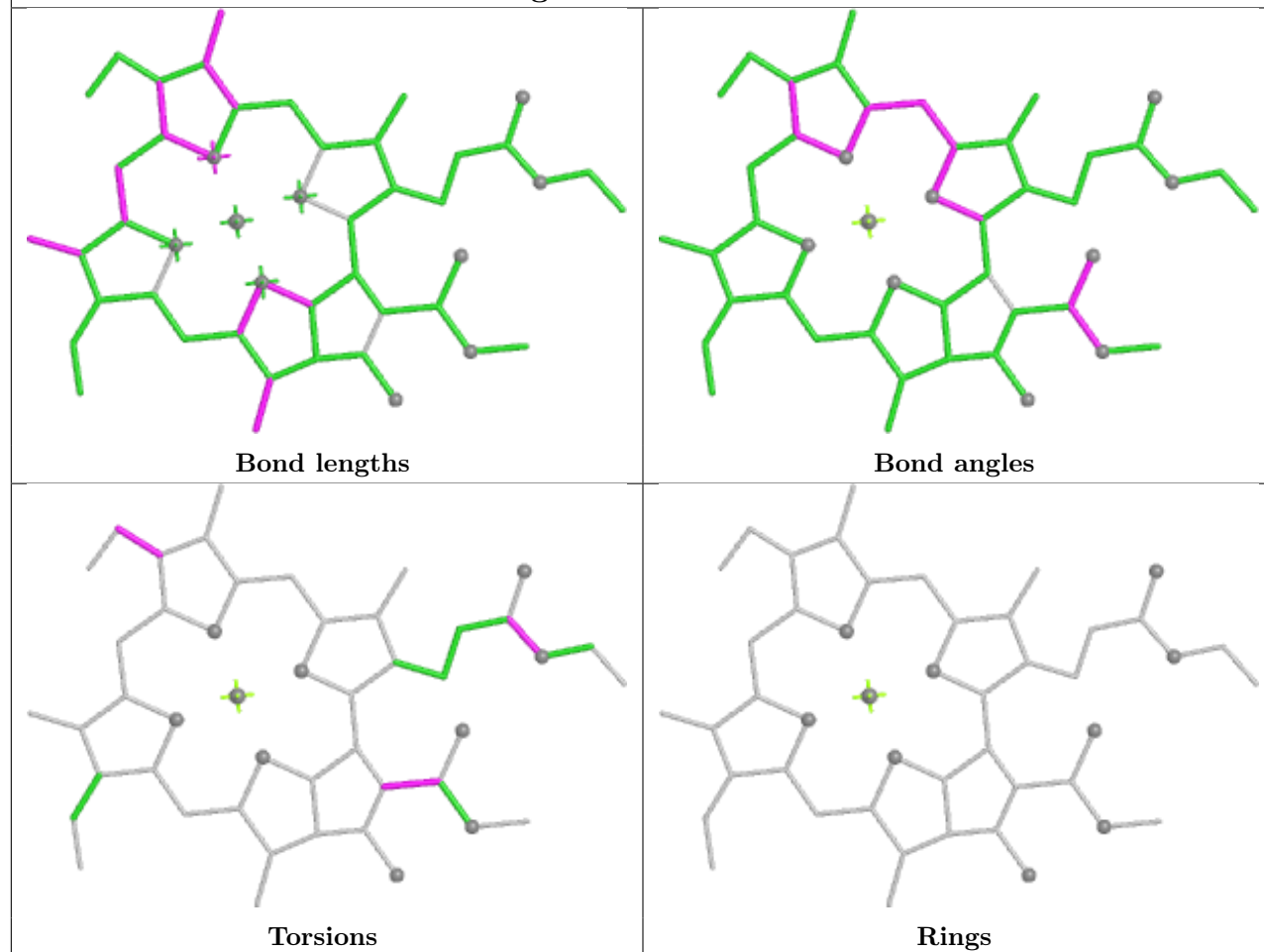


Ligand CLA P 308

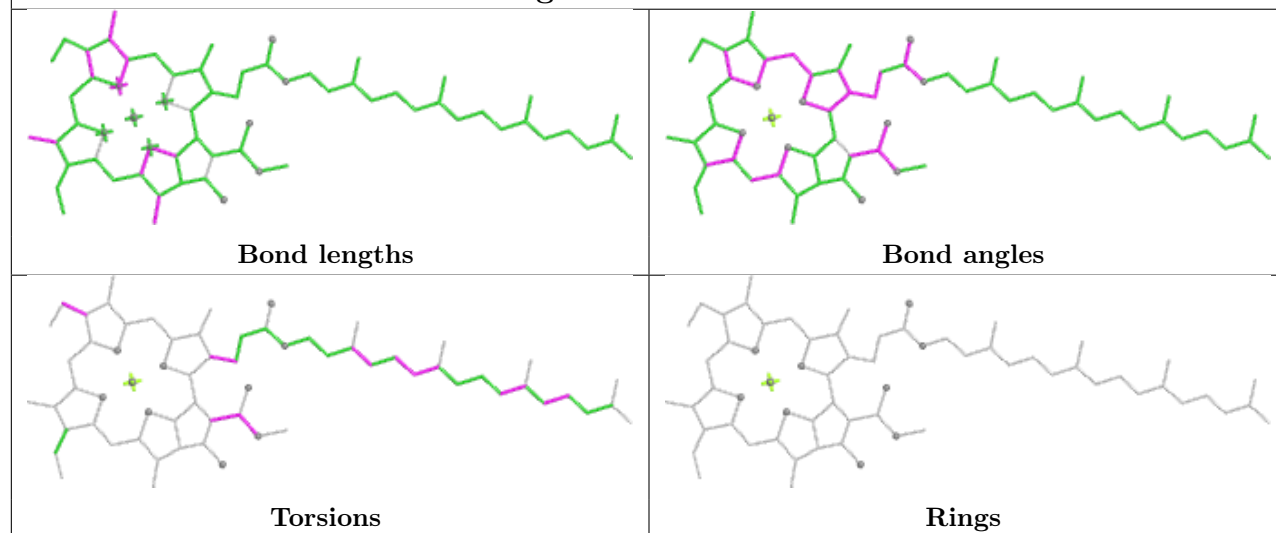


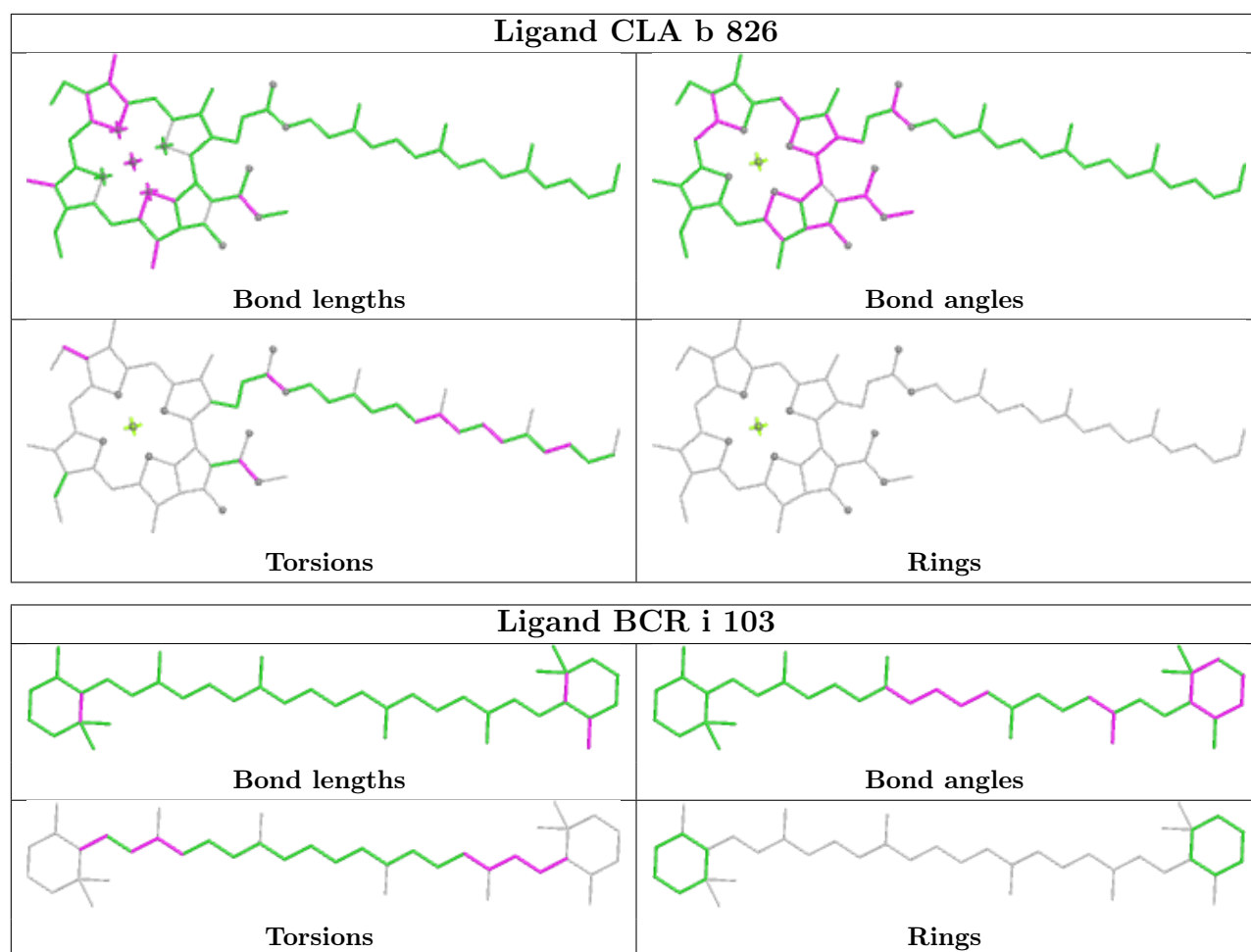


Ligand CLA J 317

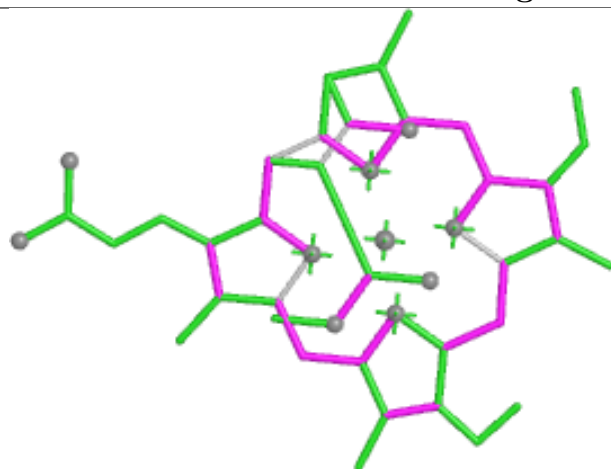


Ligand CLA a 832

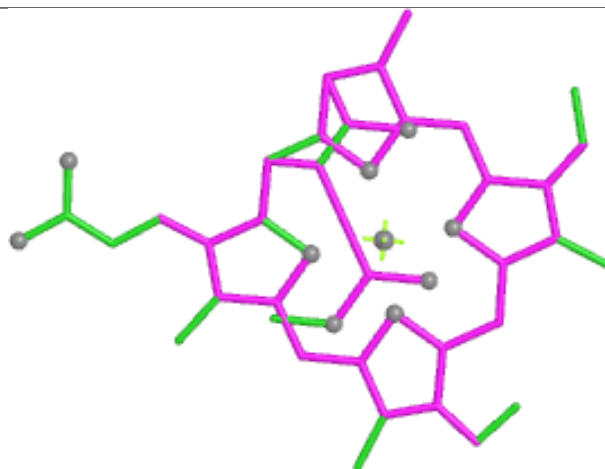




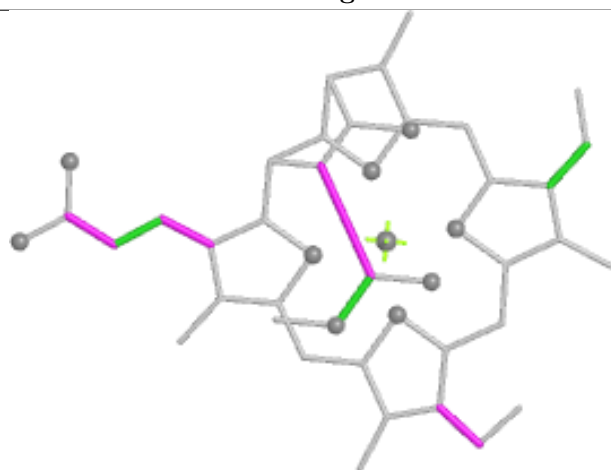
Ligand KC1 C 213



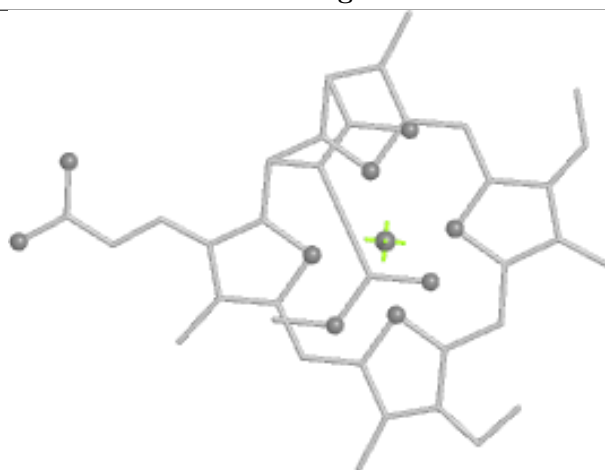
Bond lengths



Bond angles

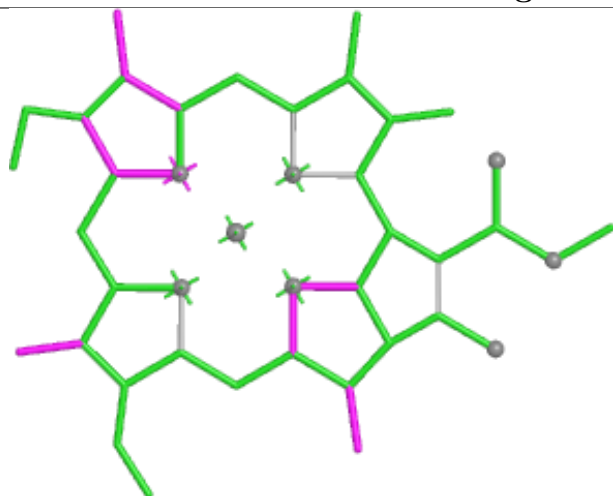


Torsions

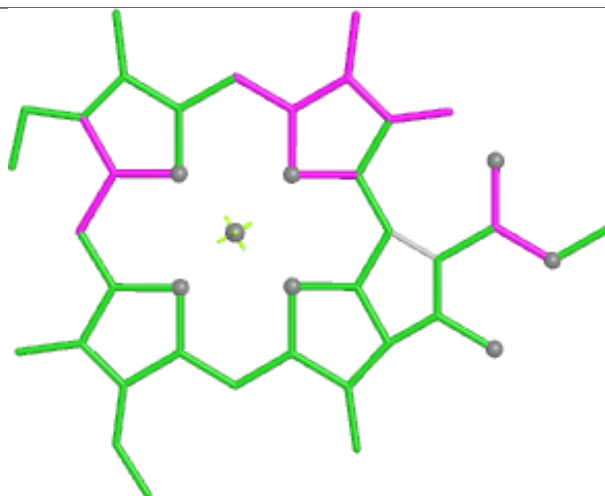


Rings

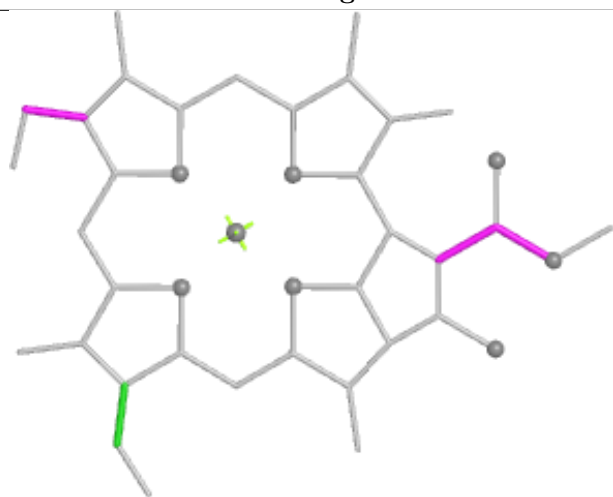
Ligand CLA P 316



Bond lengths



Bond angles

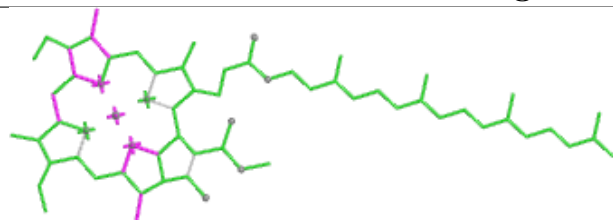


Torsions

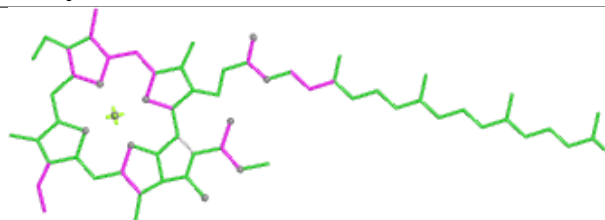


Rings

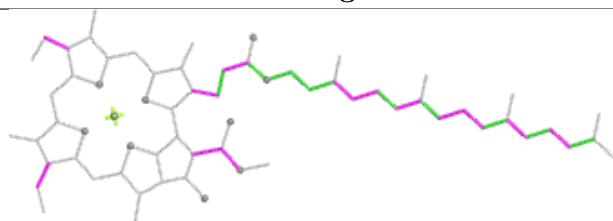
Ligand CLA Q 308



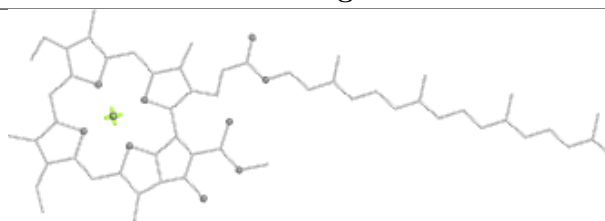
Bond lengths



Bond angles

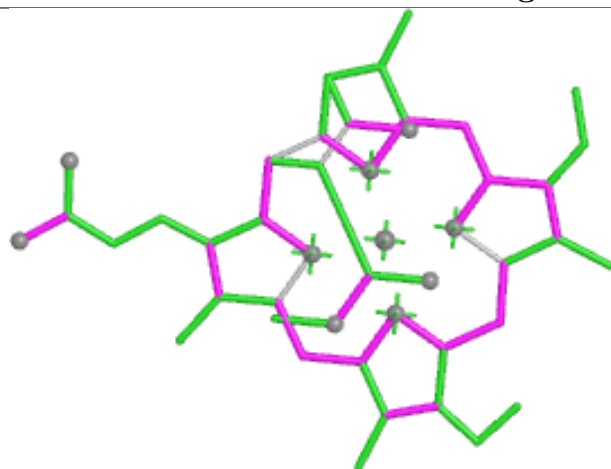


Torsions

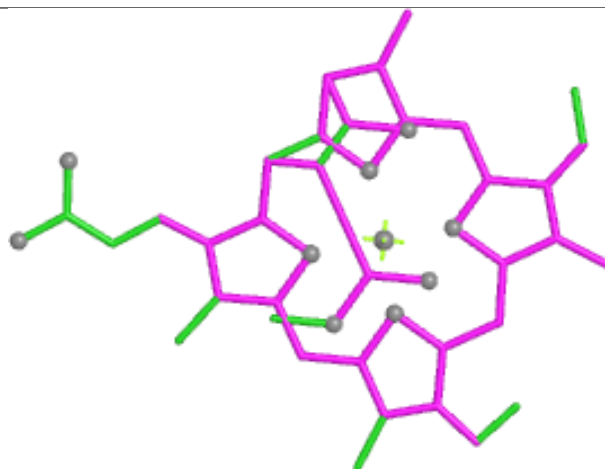


Rings

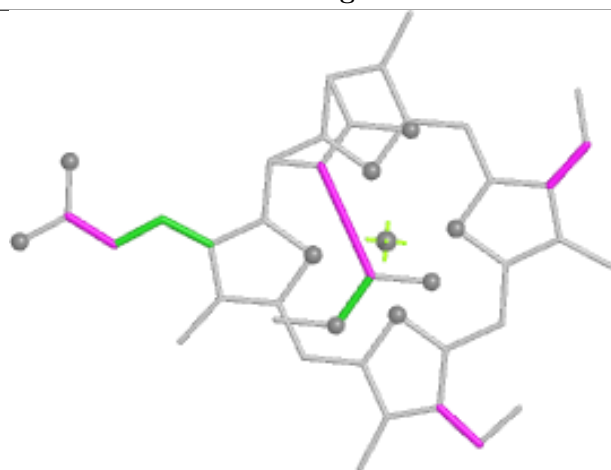
Ligand KC1 F 308



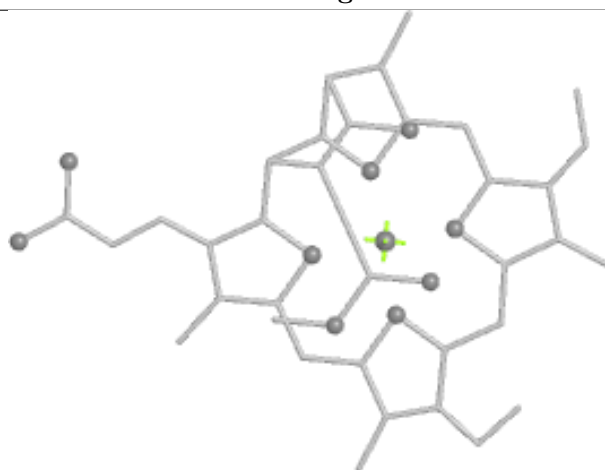
Bond lengths



Bond angles

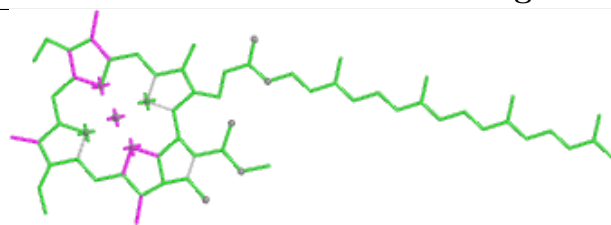


Torsions

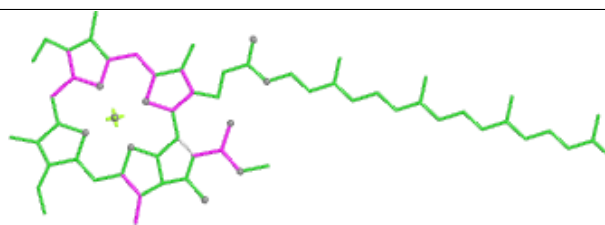


Rings

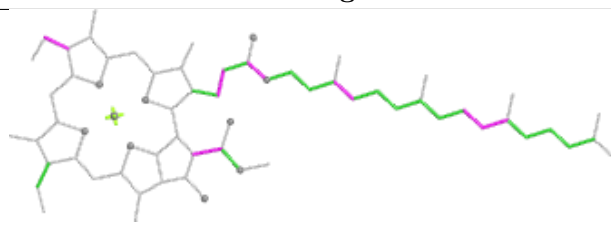
Ligand CLA C 209



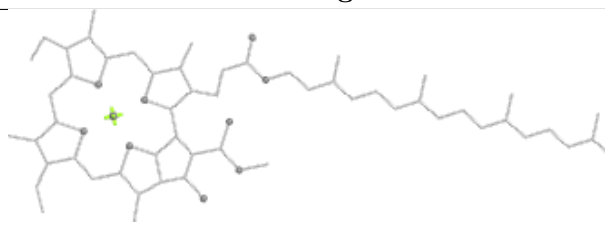
Bond lengths



Bond angles

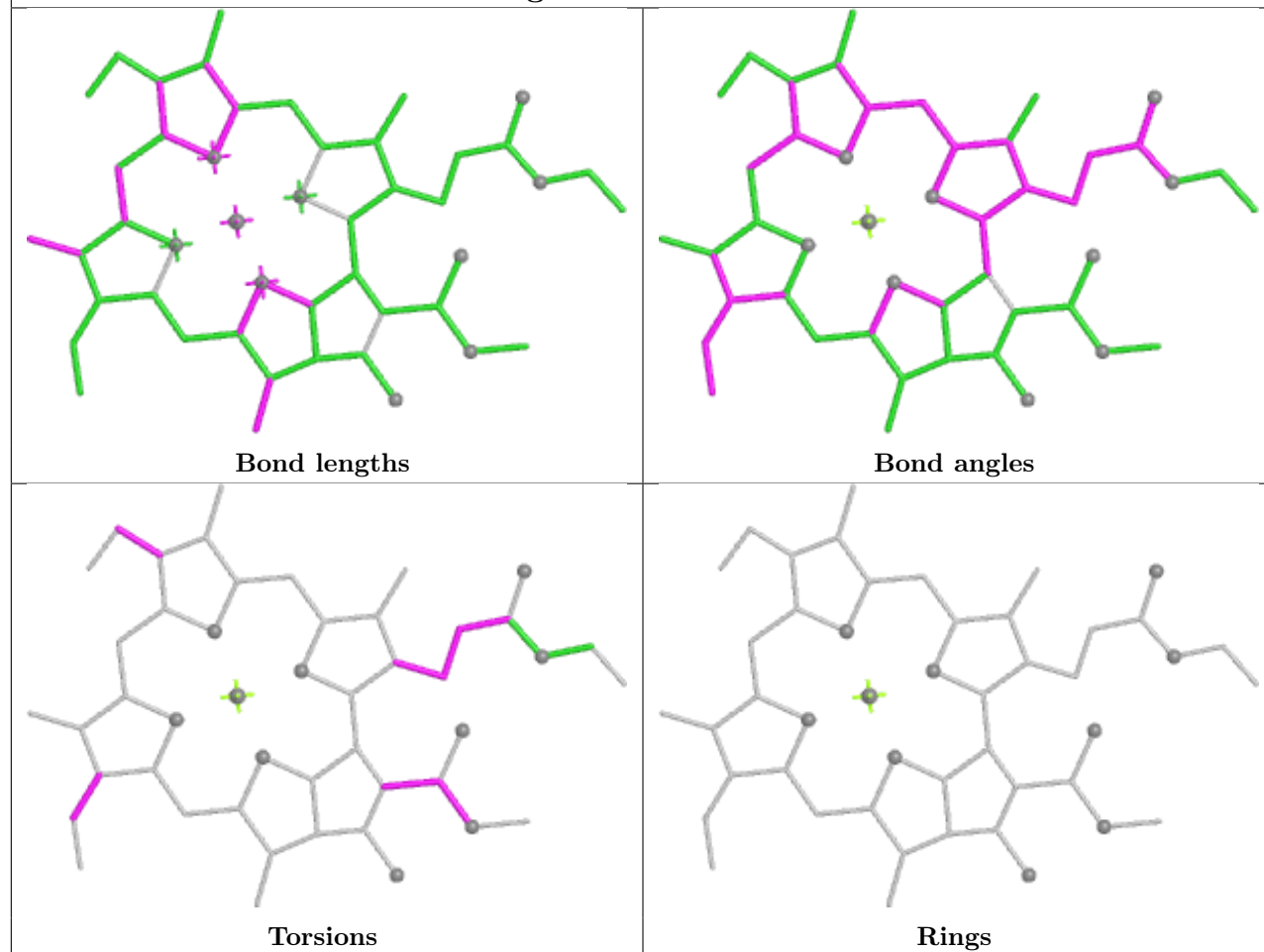


Torsions

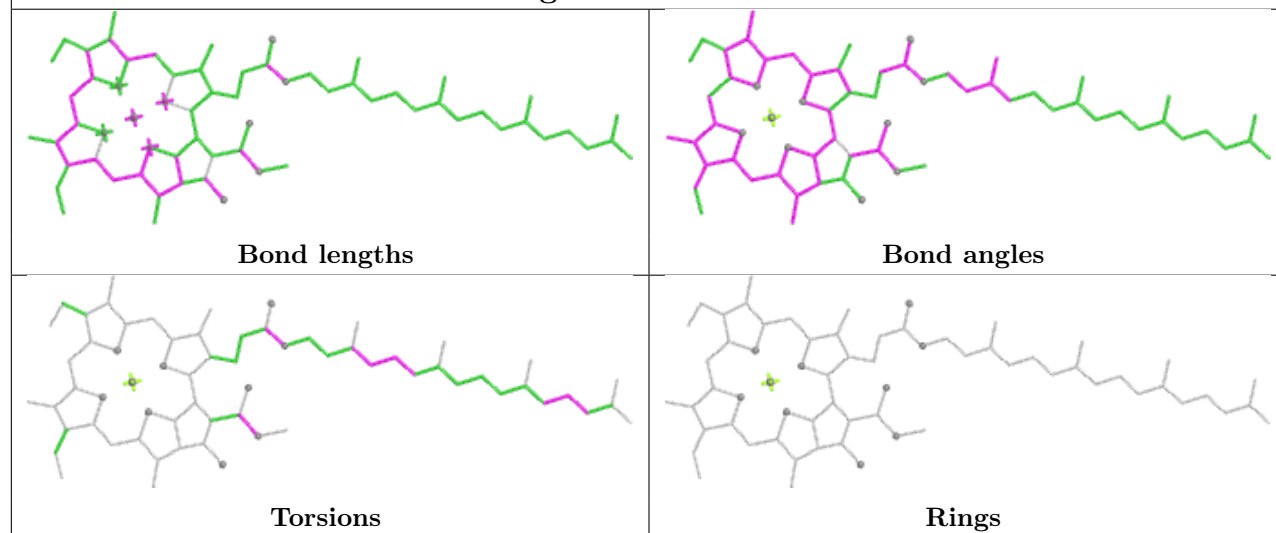


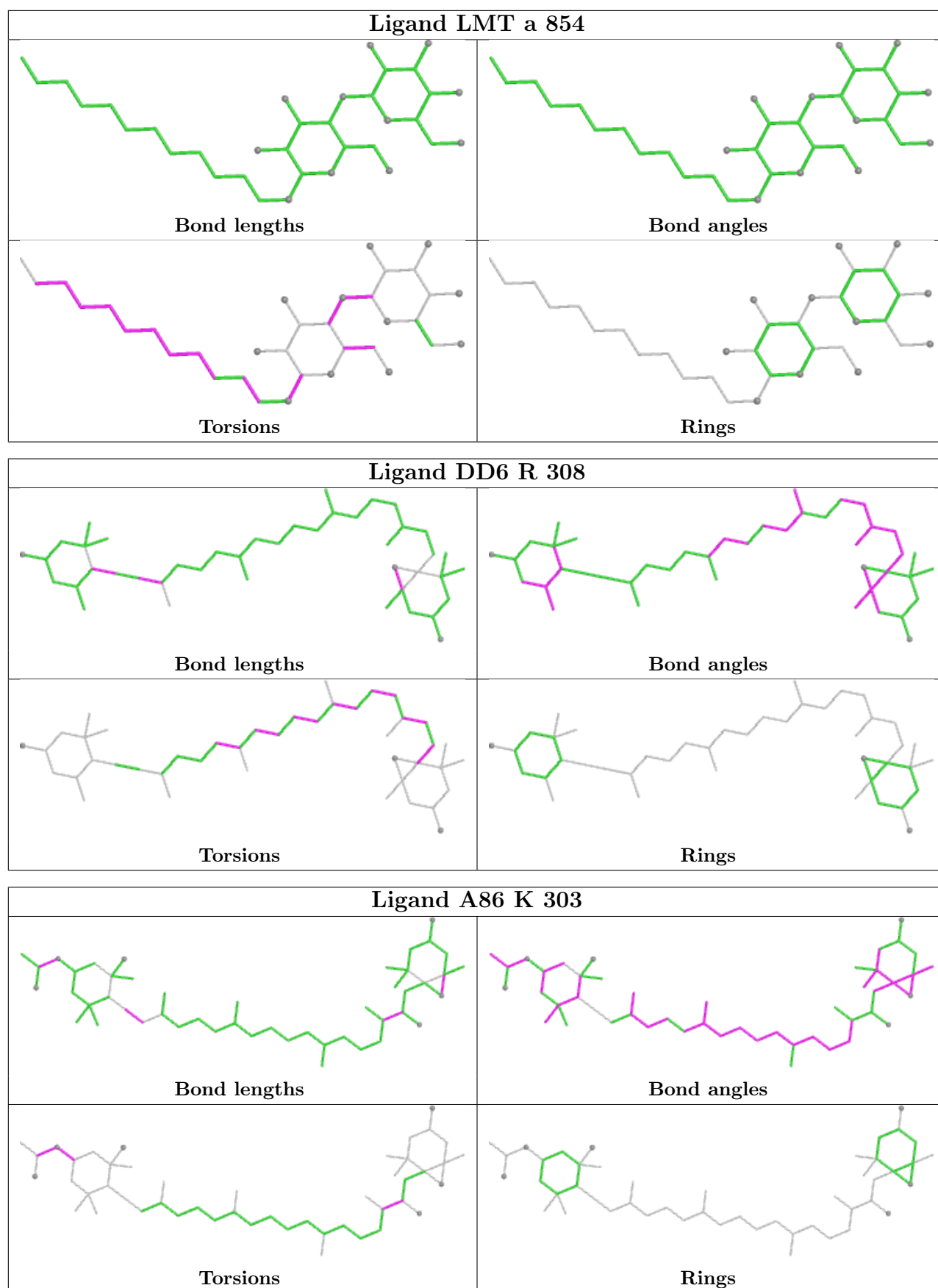
Rings

Ligand CLA X 308

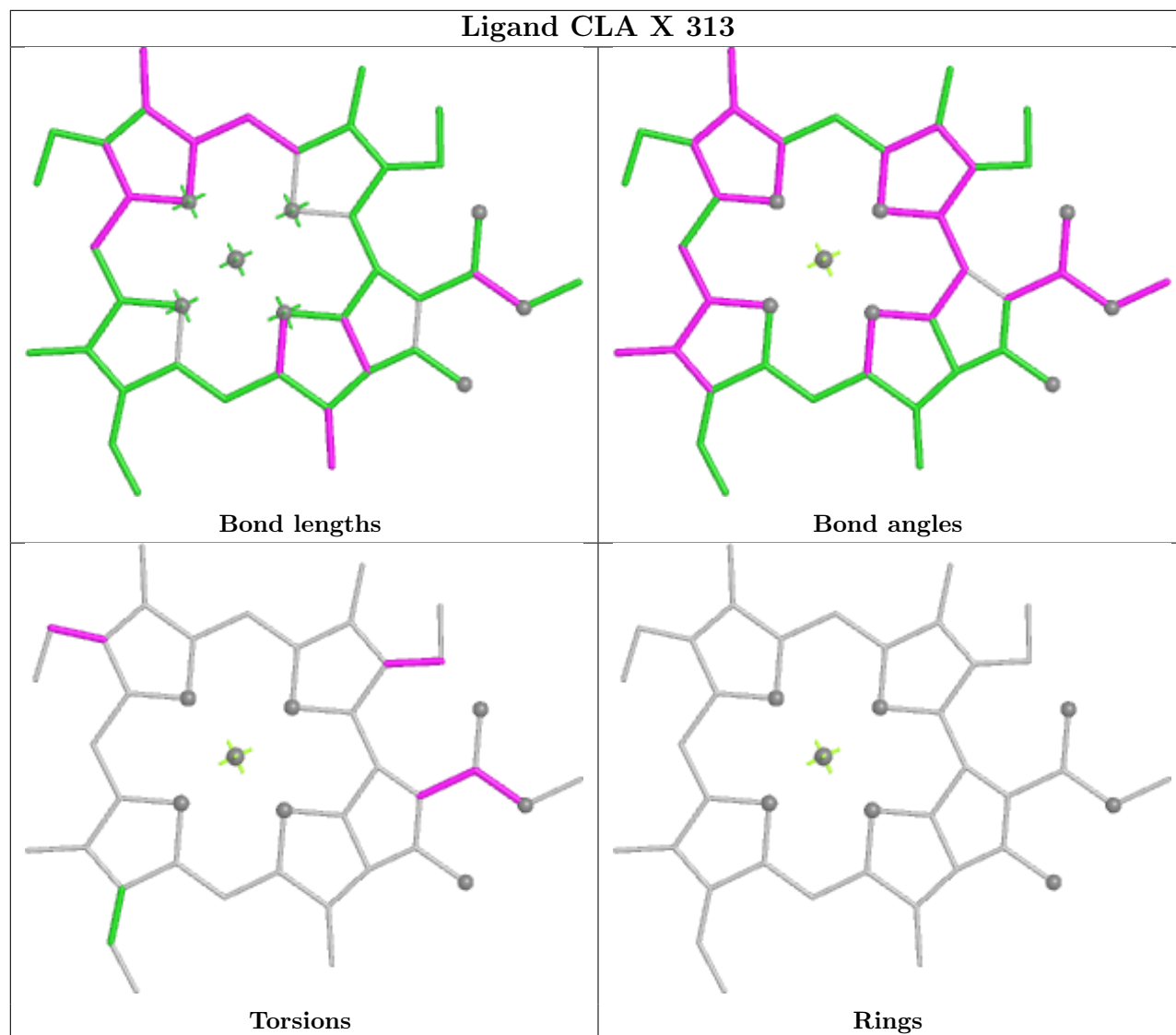


Ligand CLA f 804

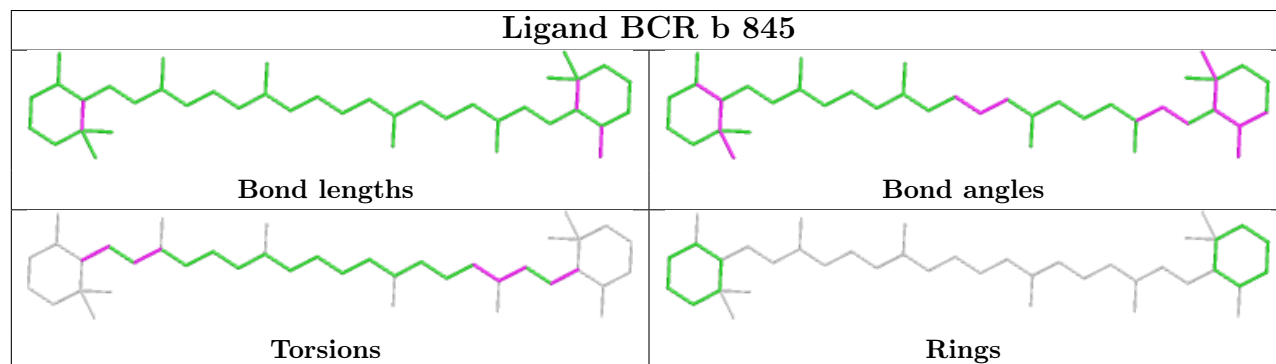




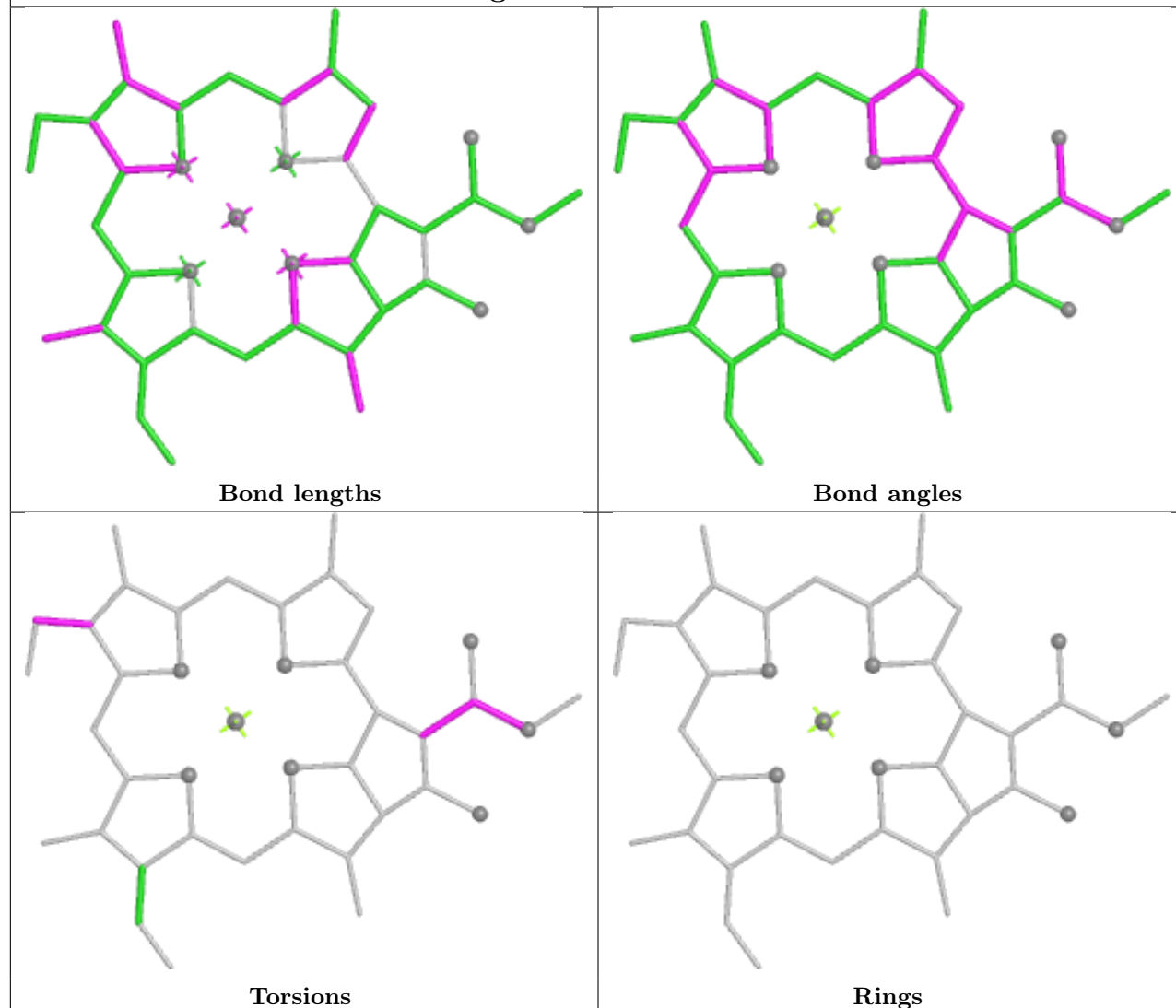
Ligand CLA X 313



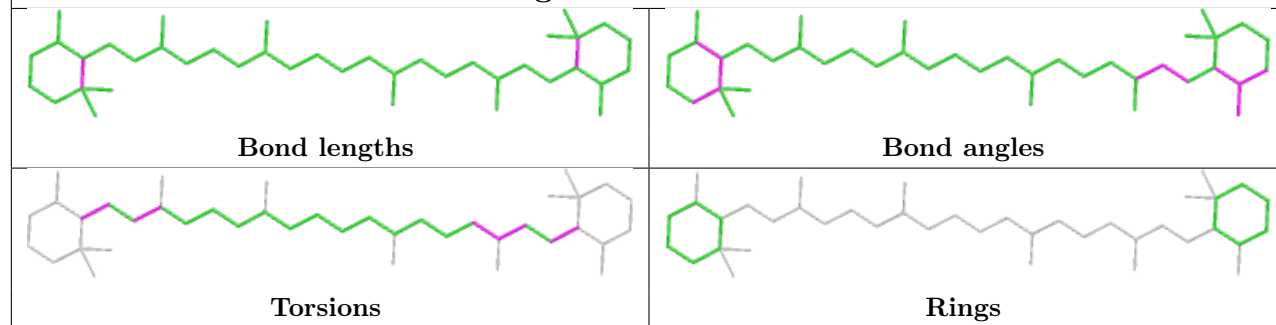
Ligand BCR b 845



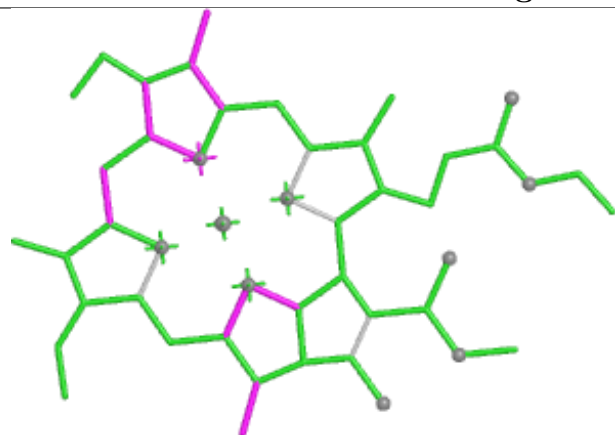
Ligand CLA O 312



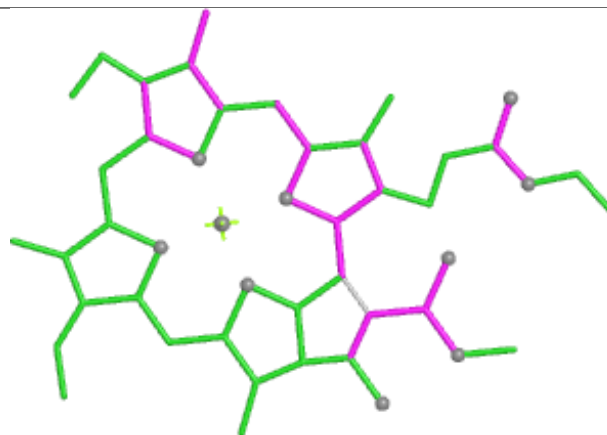
Ligand BCR a 845



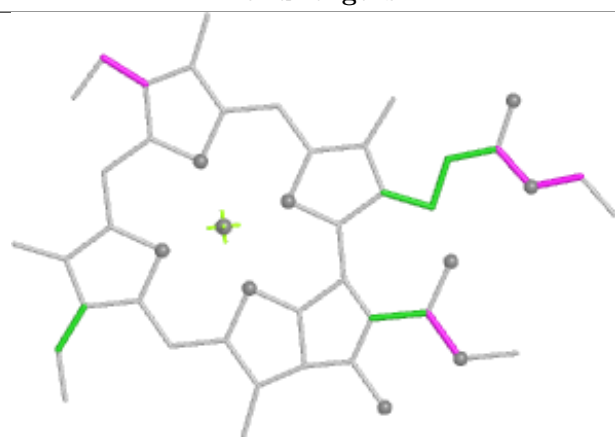
Ligand CLA N 318



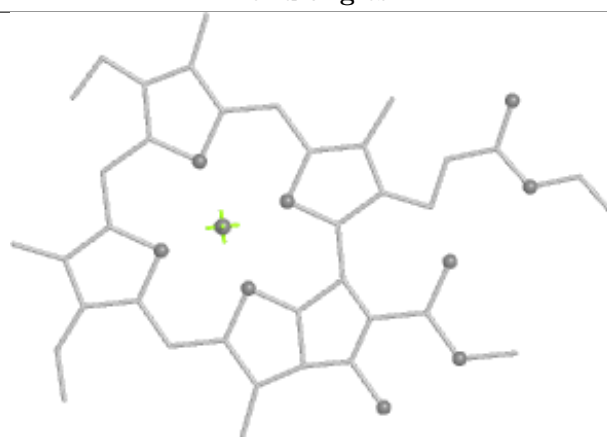
Bond lengths



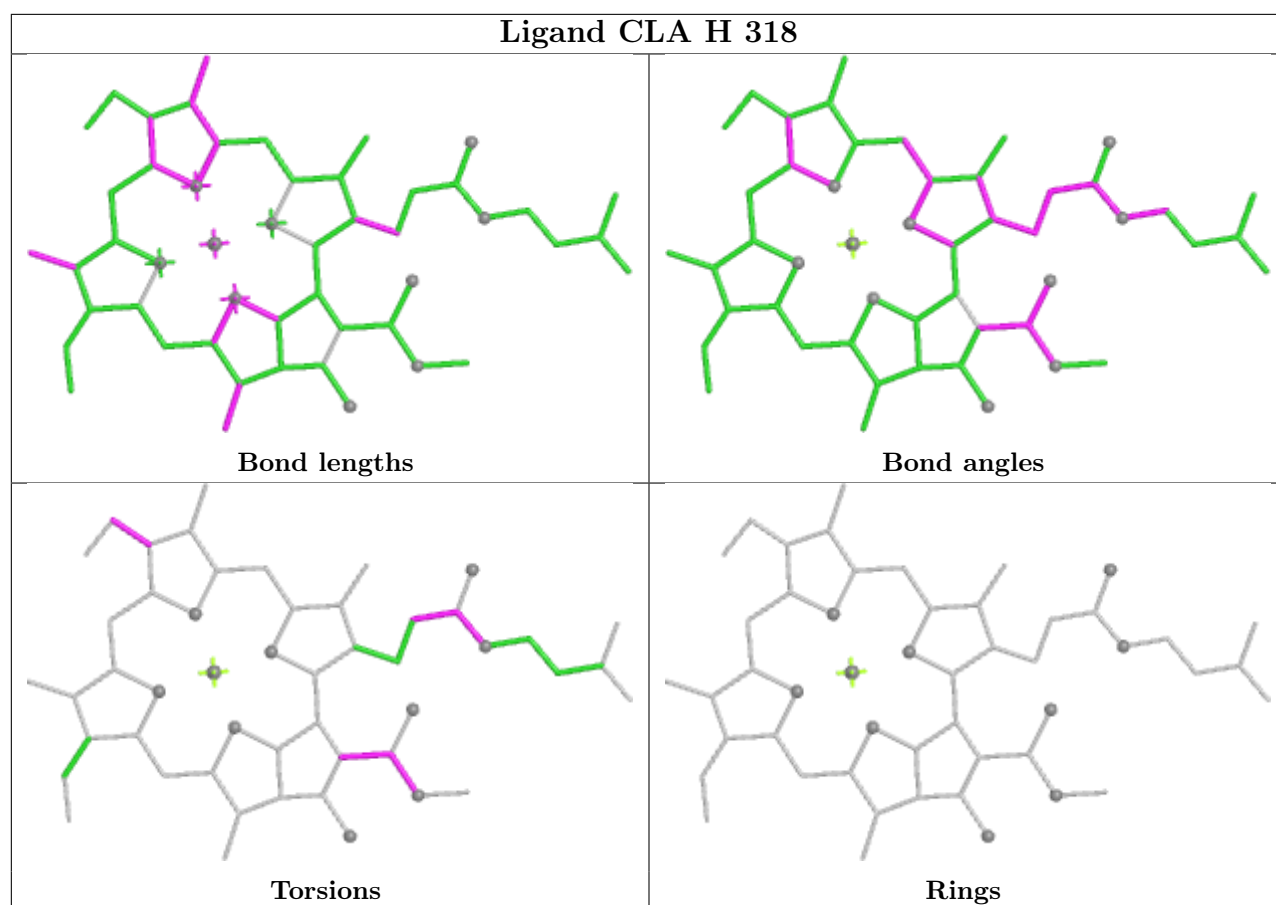
Bond angles



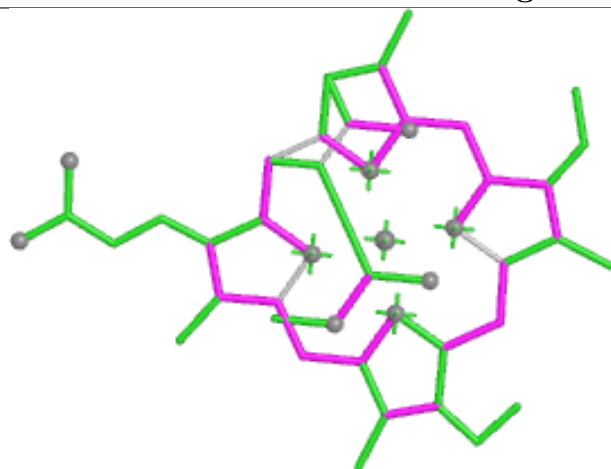
Torsions



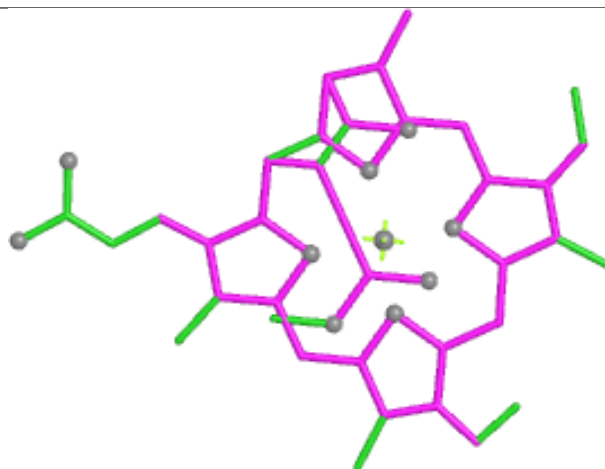
Rings



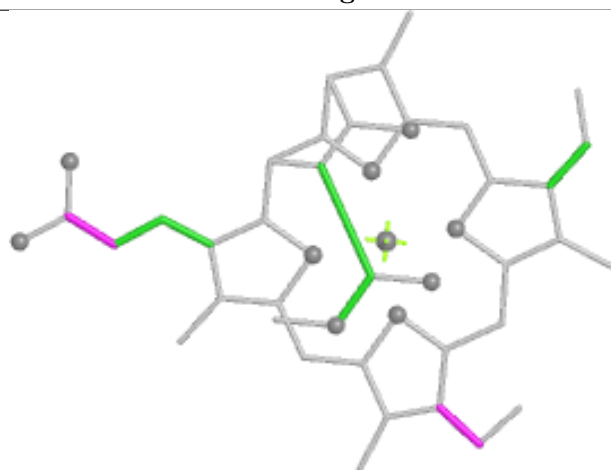
Ligand KC1 B 310



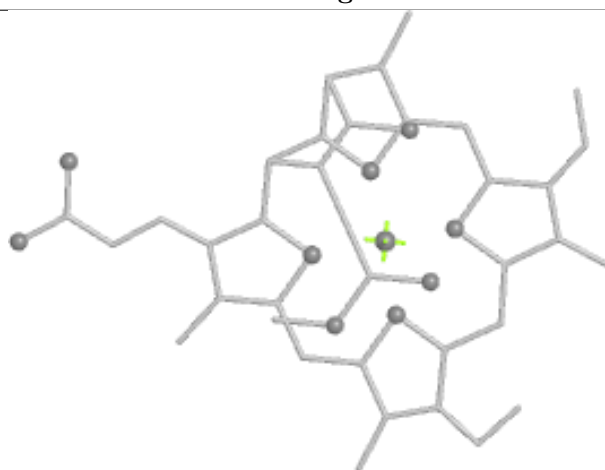
Bond lengths



Bond angles

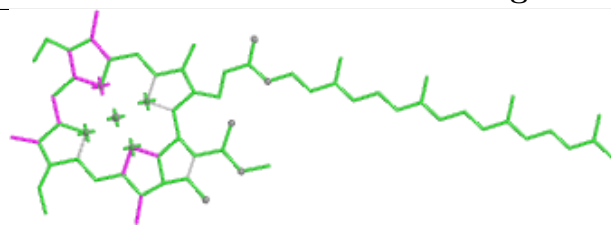


Torsions

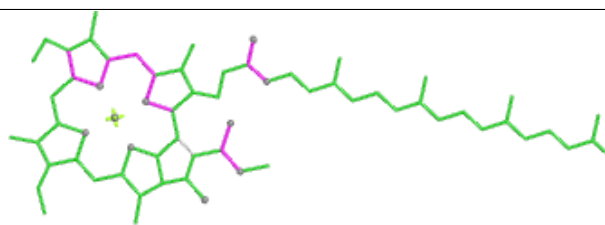


Rings

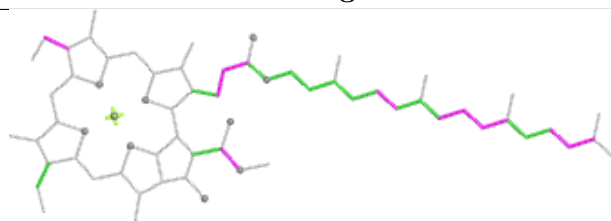
Ligand CLA M 309



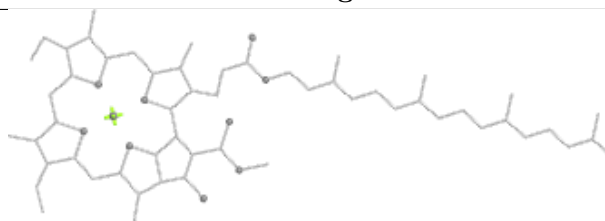
Bond lengths



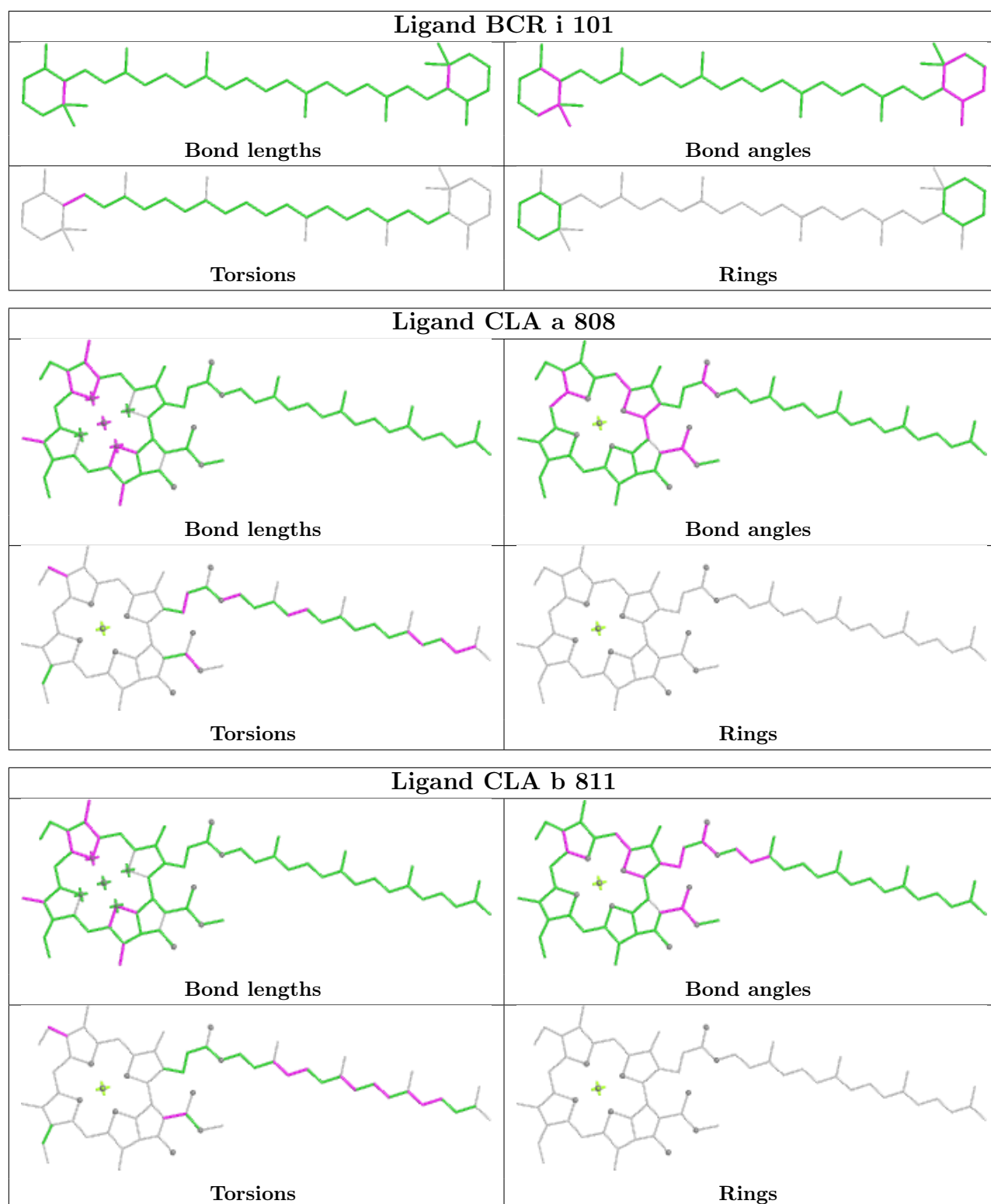
Bond angles

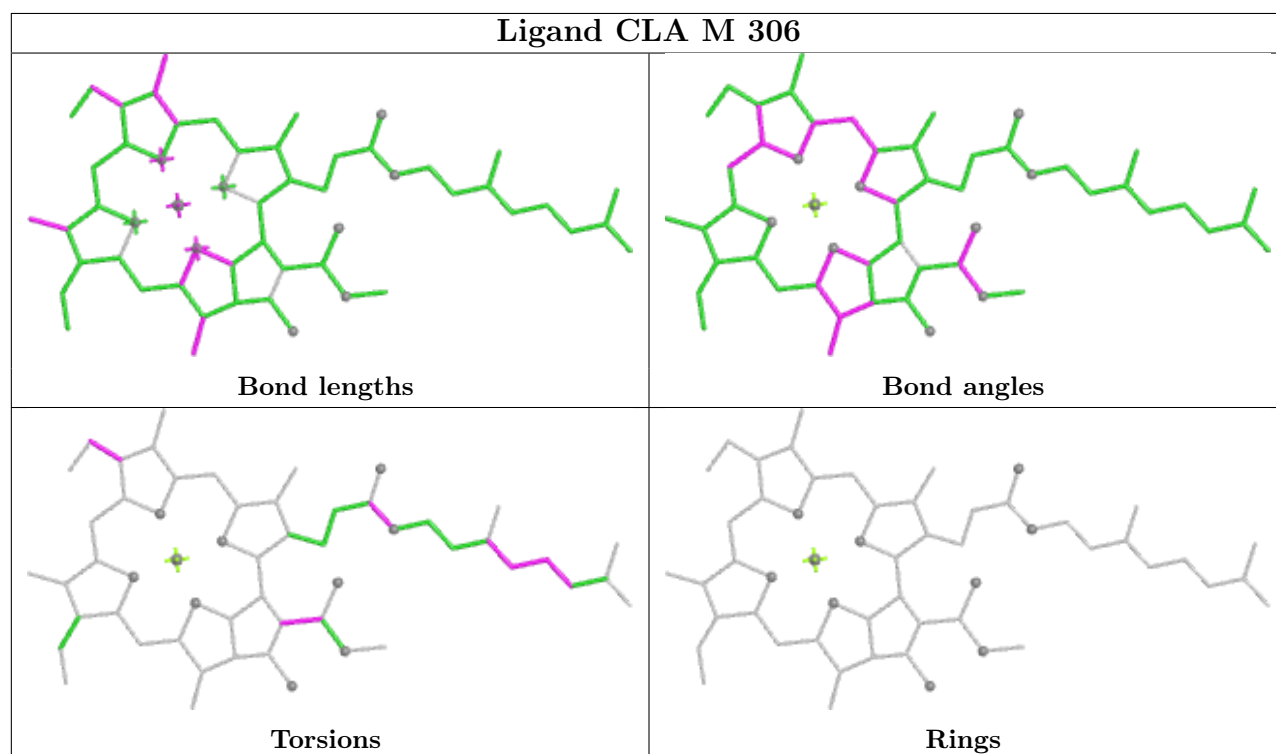
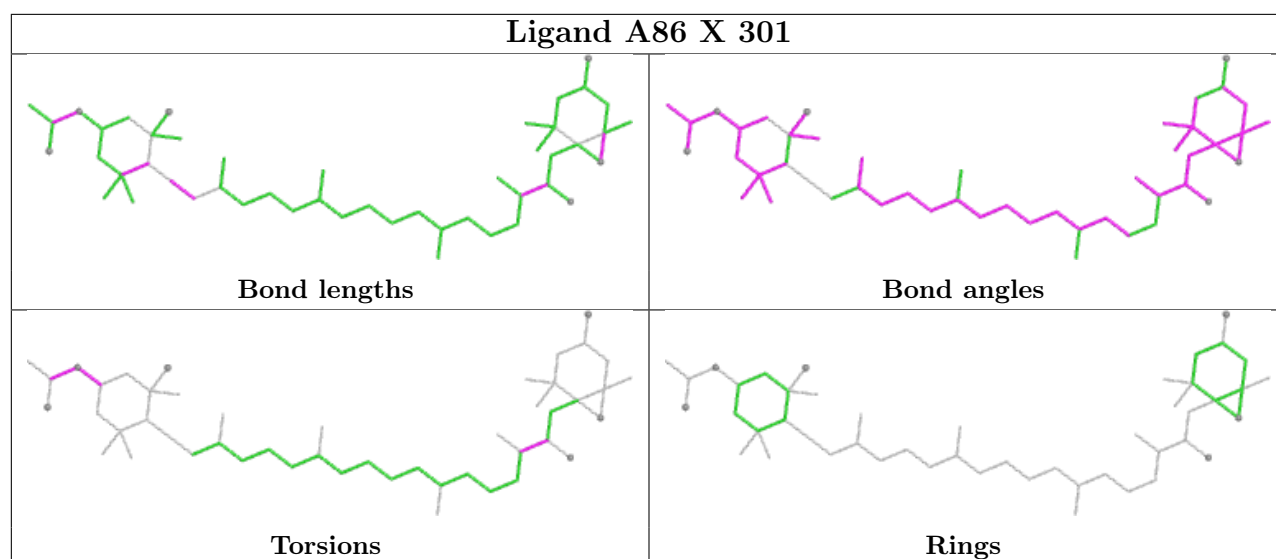


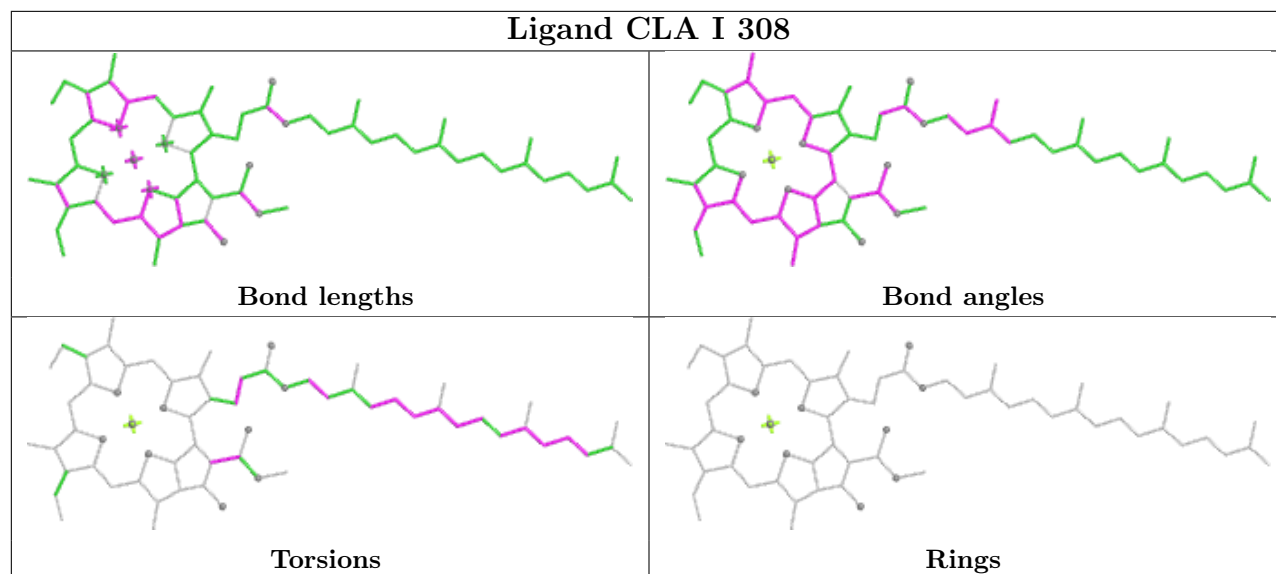
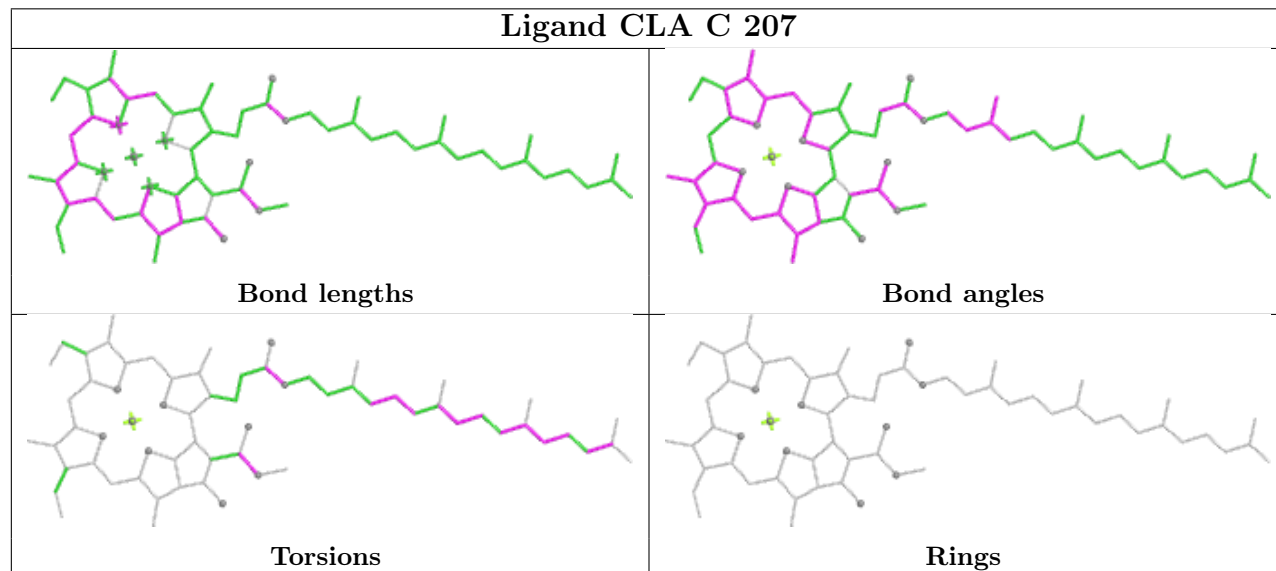
Torsions



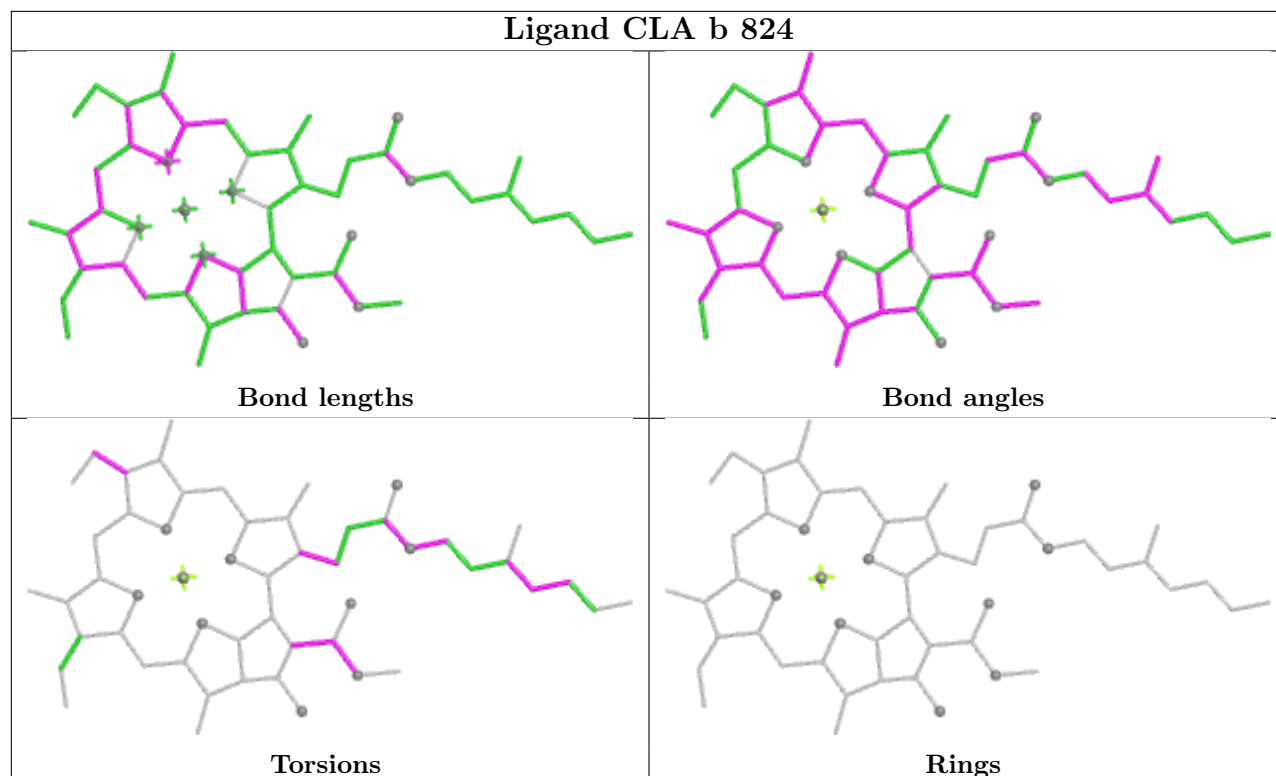
Rings



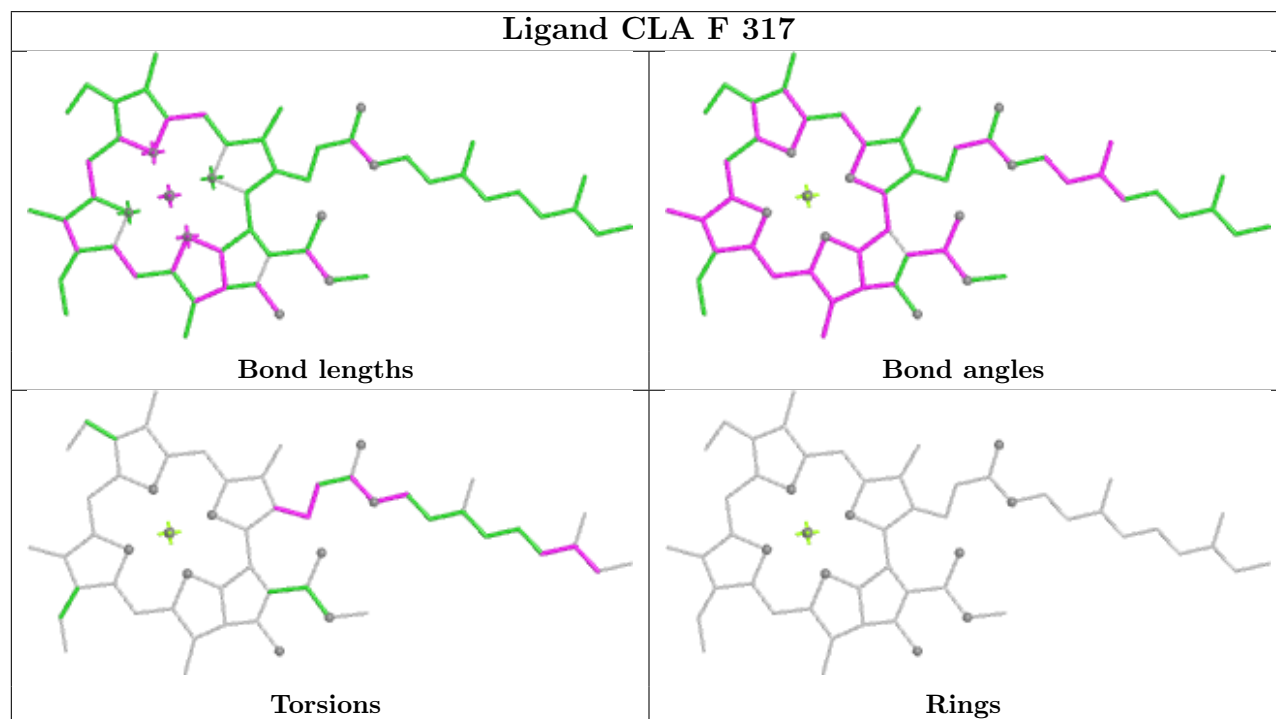


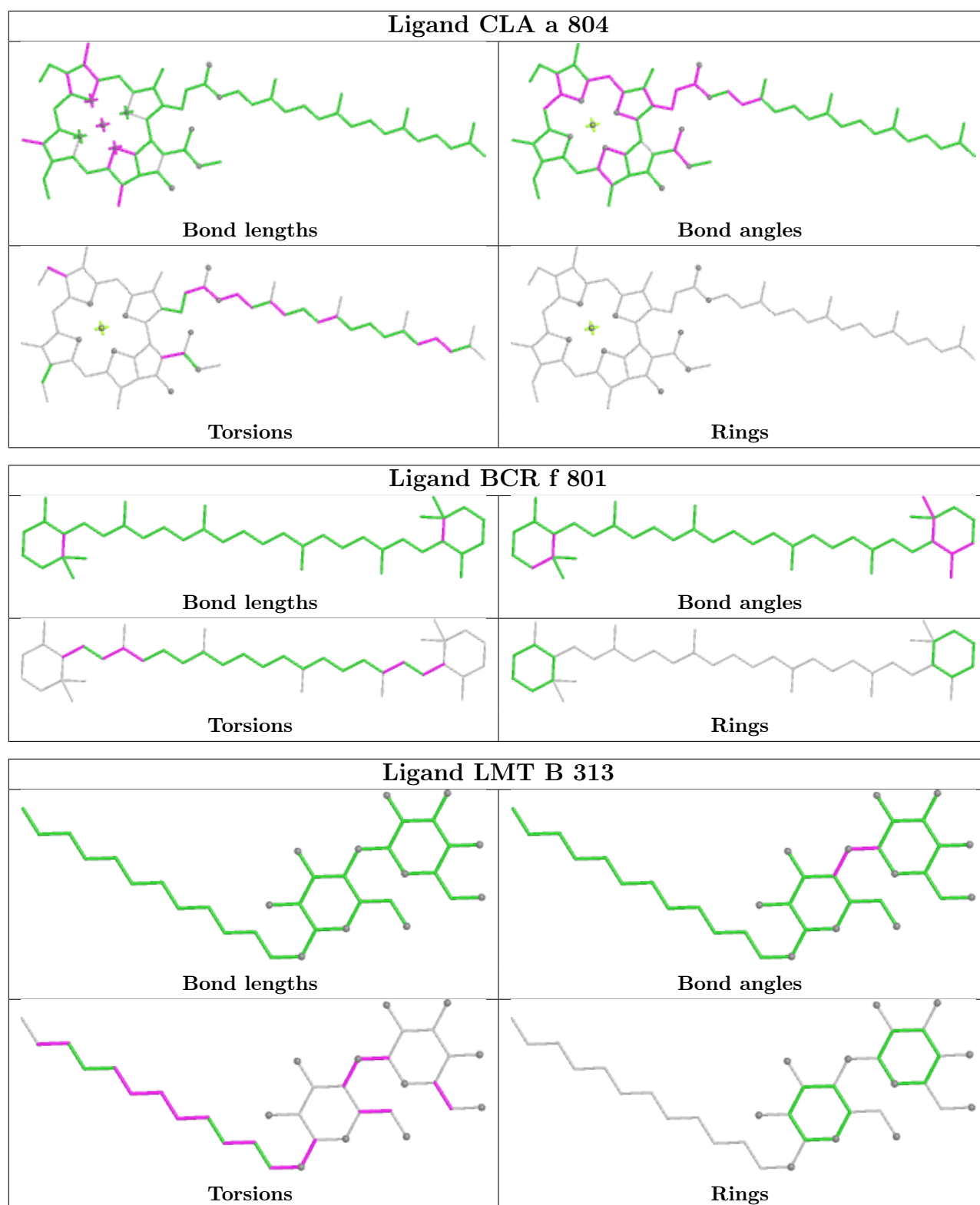
Ligand CLA I 308**Ligand CLA C 207**

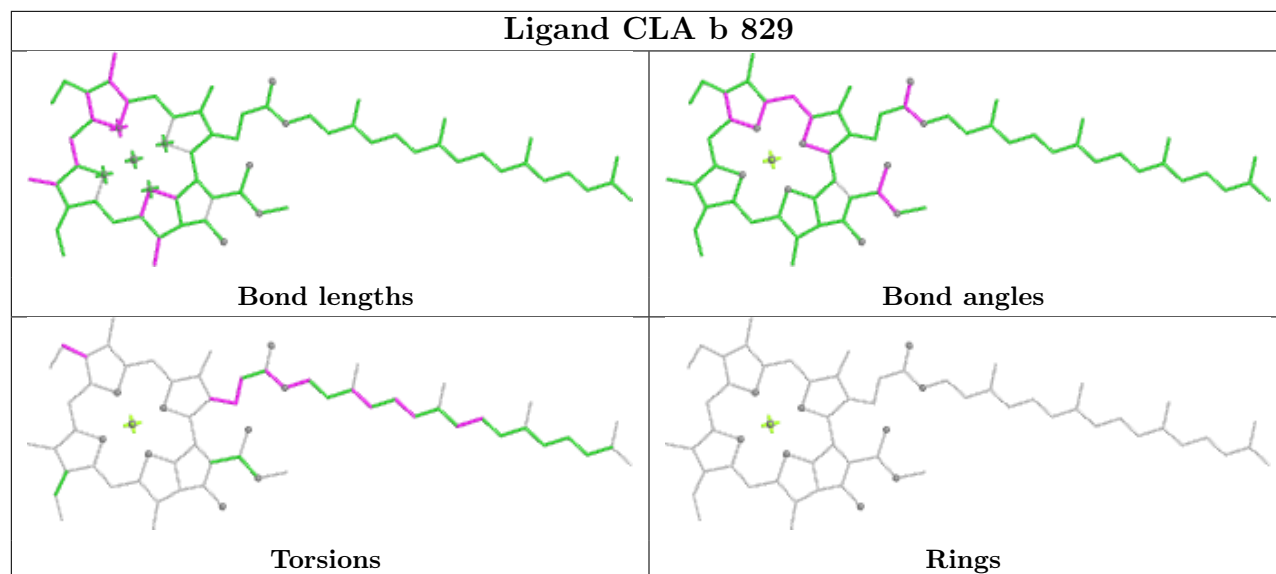
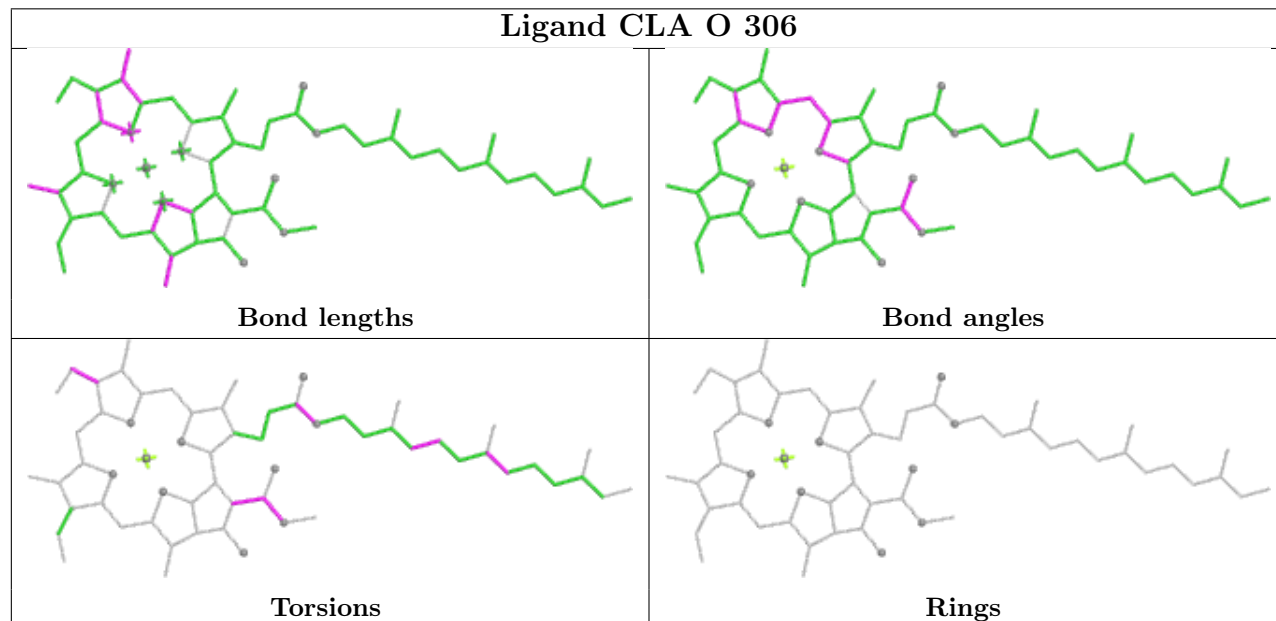
Ligand CLA b 824

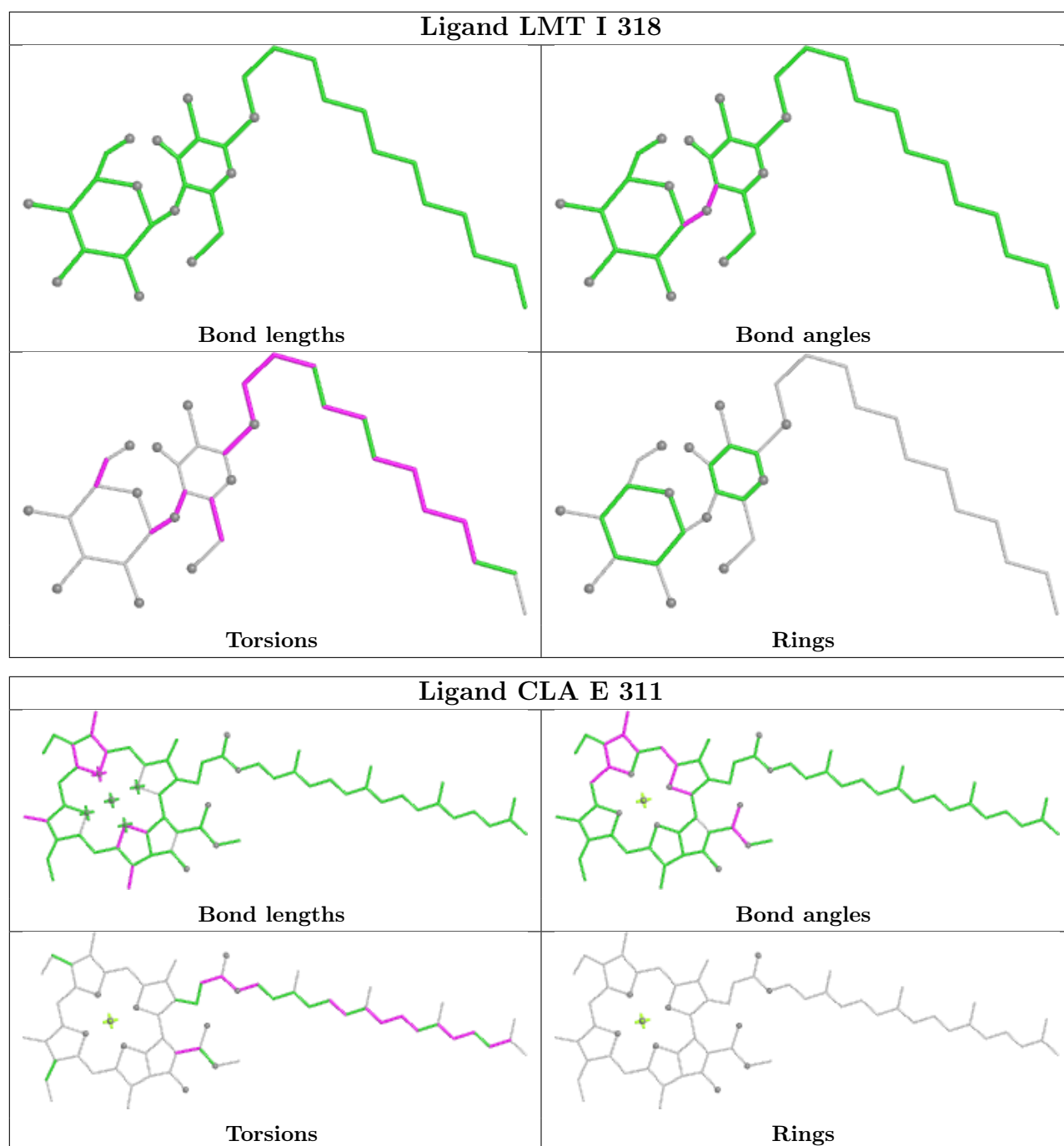


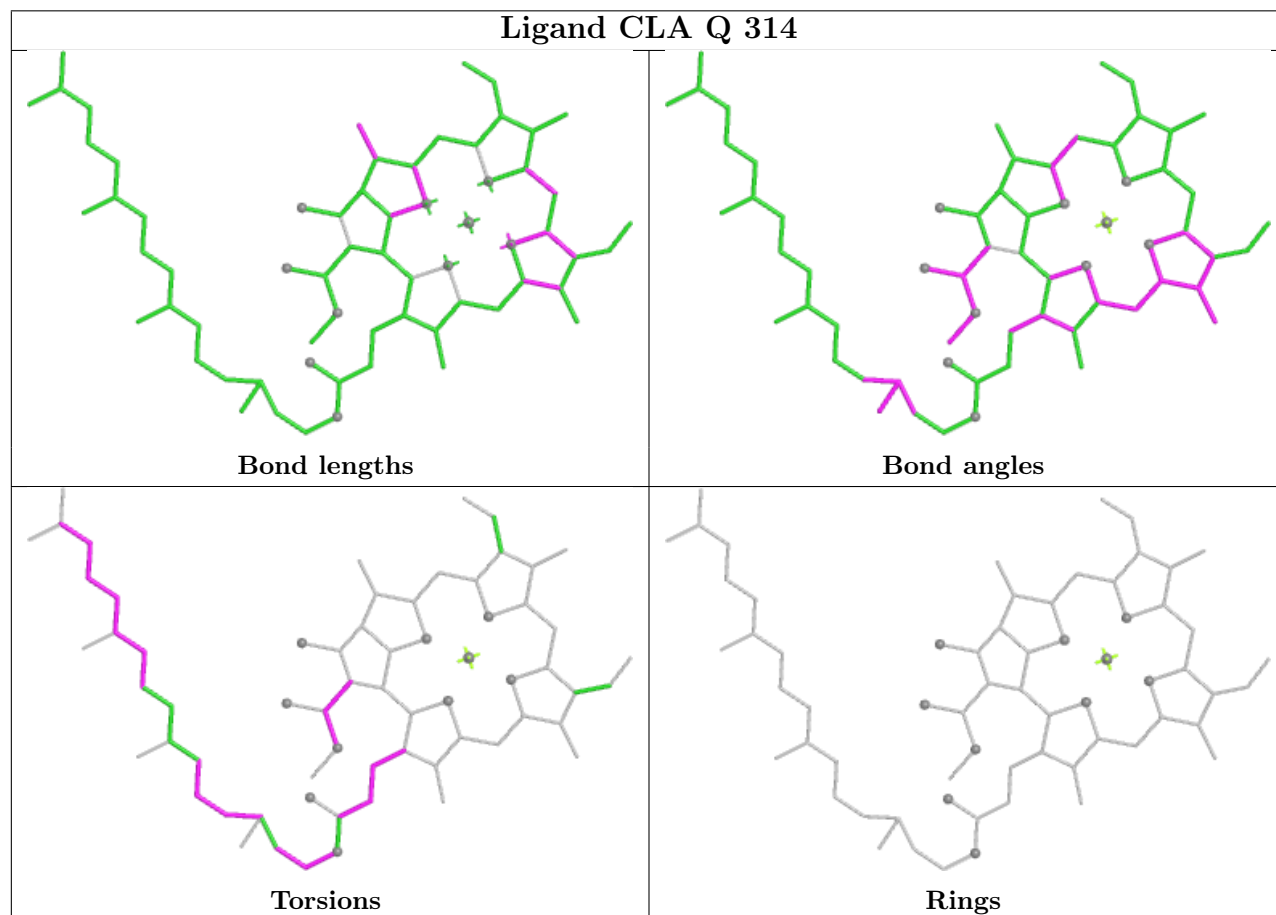
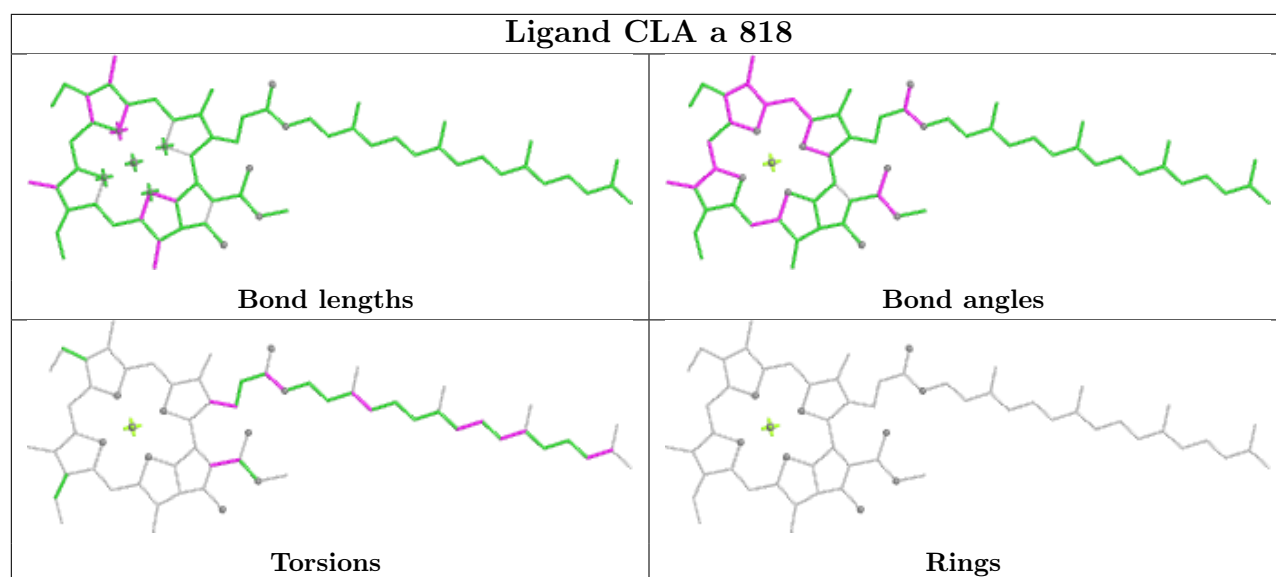
Ligand CLA F 317



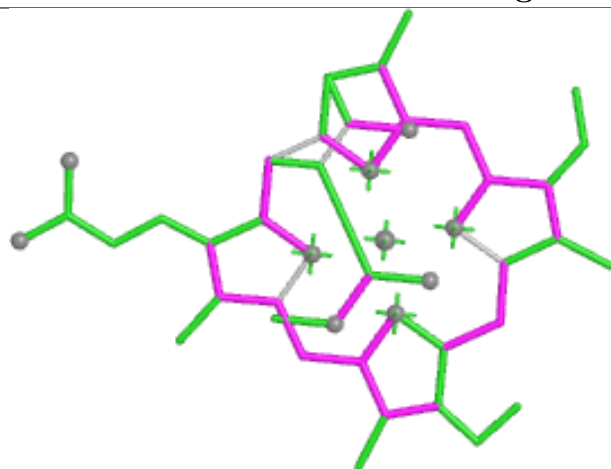


Ligand CLA b 829**Ligand CLA O 306**

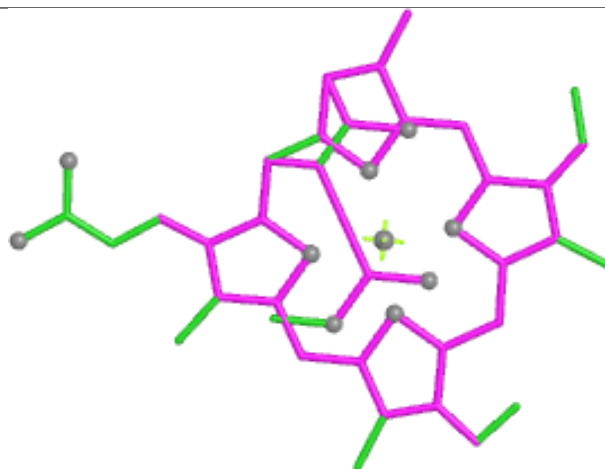




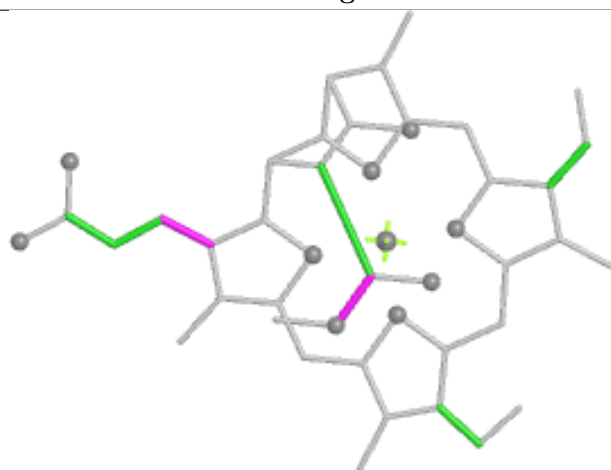
Ligand KC1 U 312



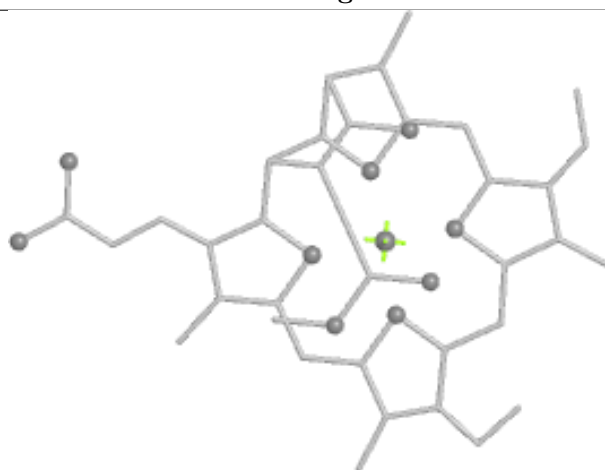
Bond lengths



Bond angles

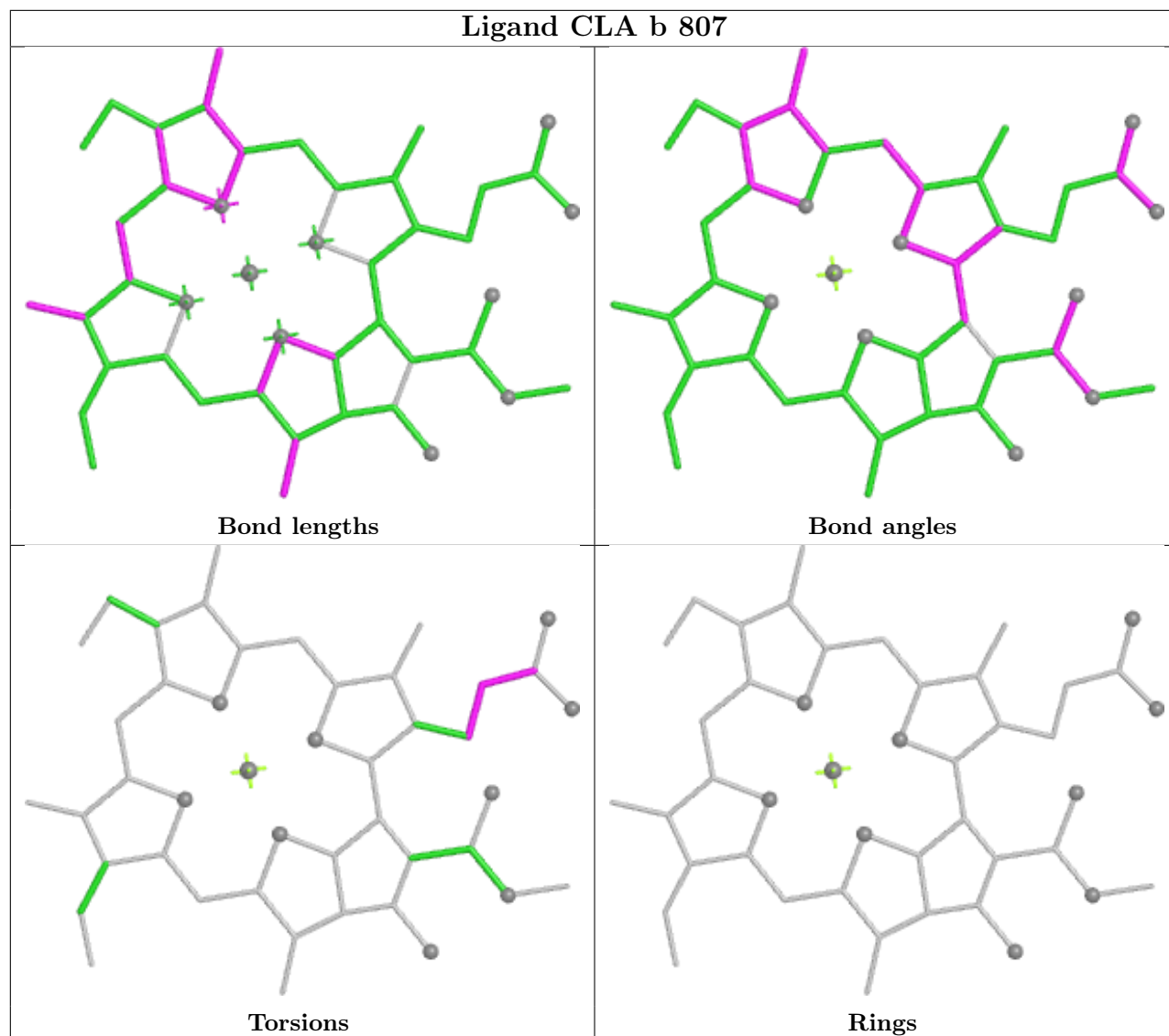


Torsions

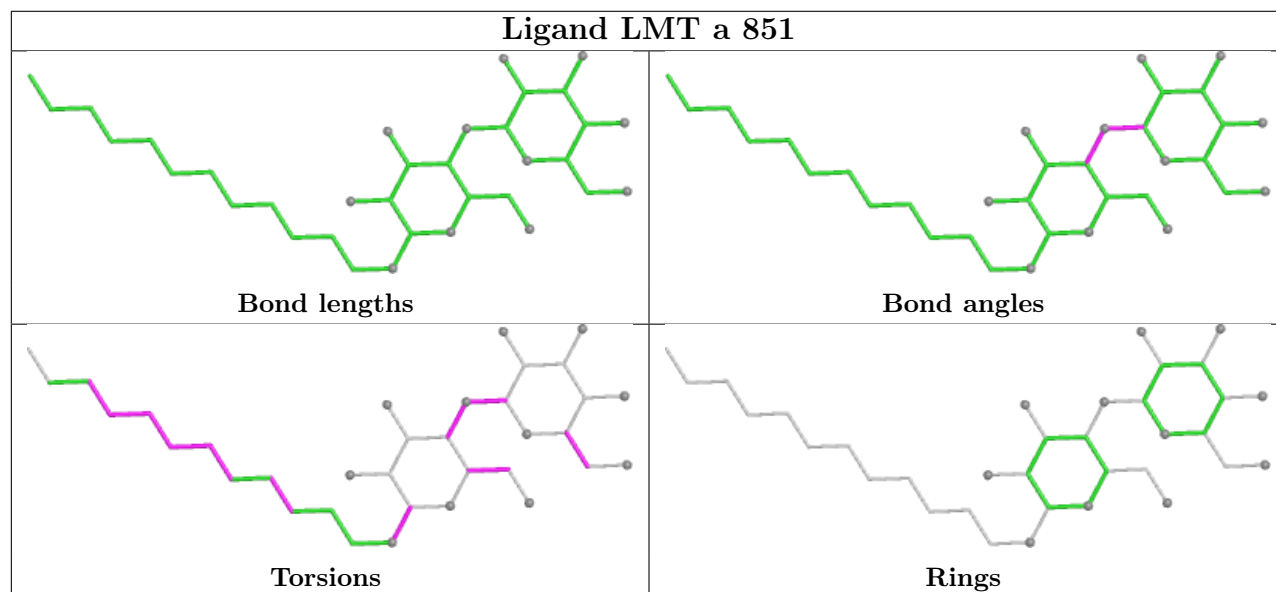


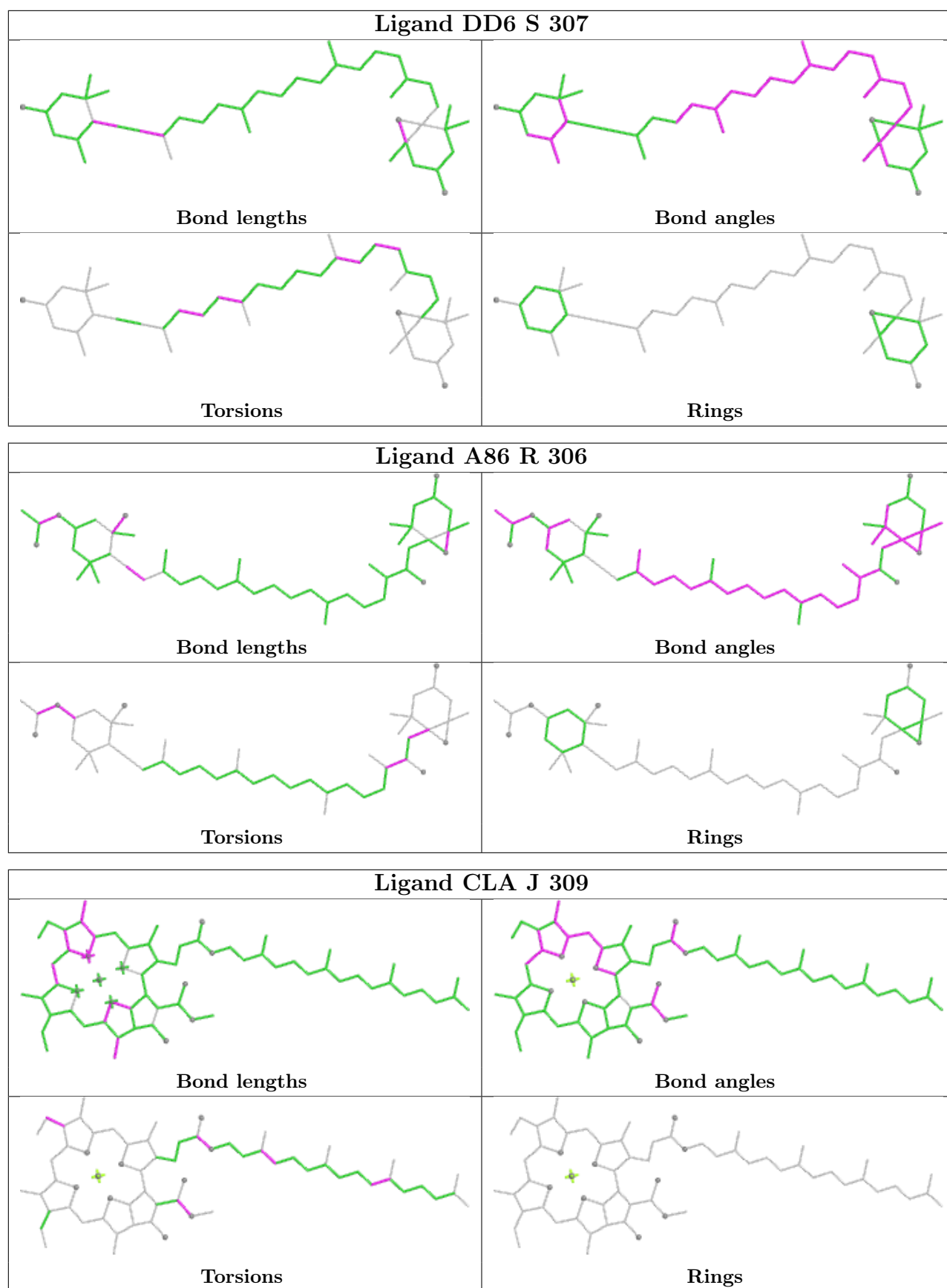
Rings

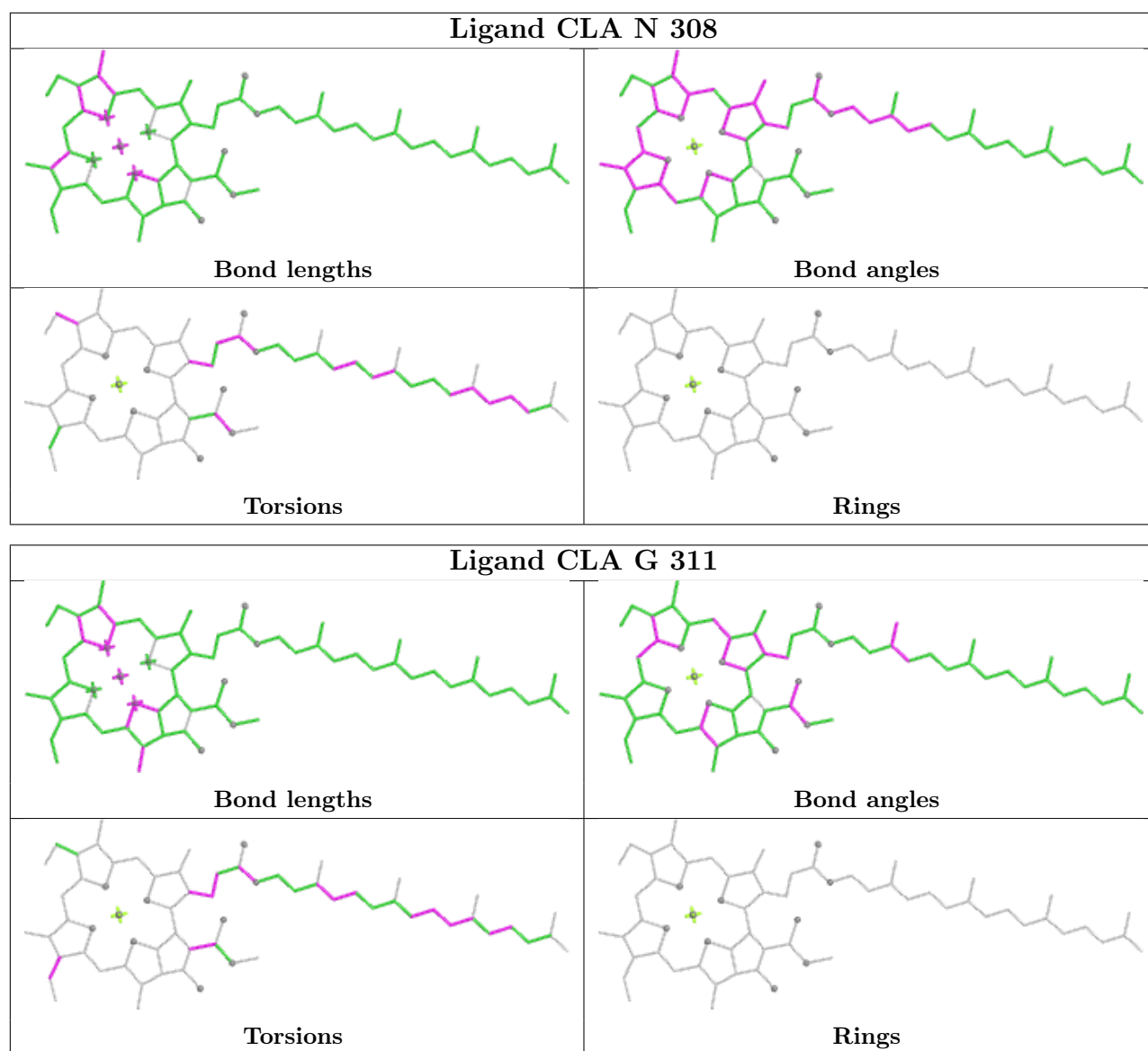
Ligand CLA b 807

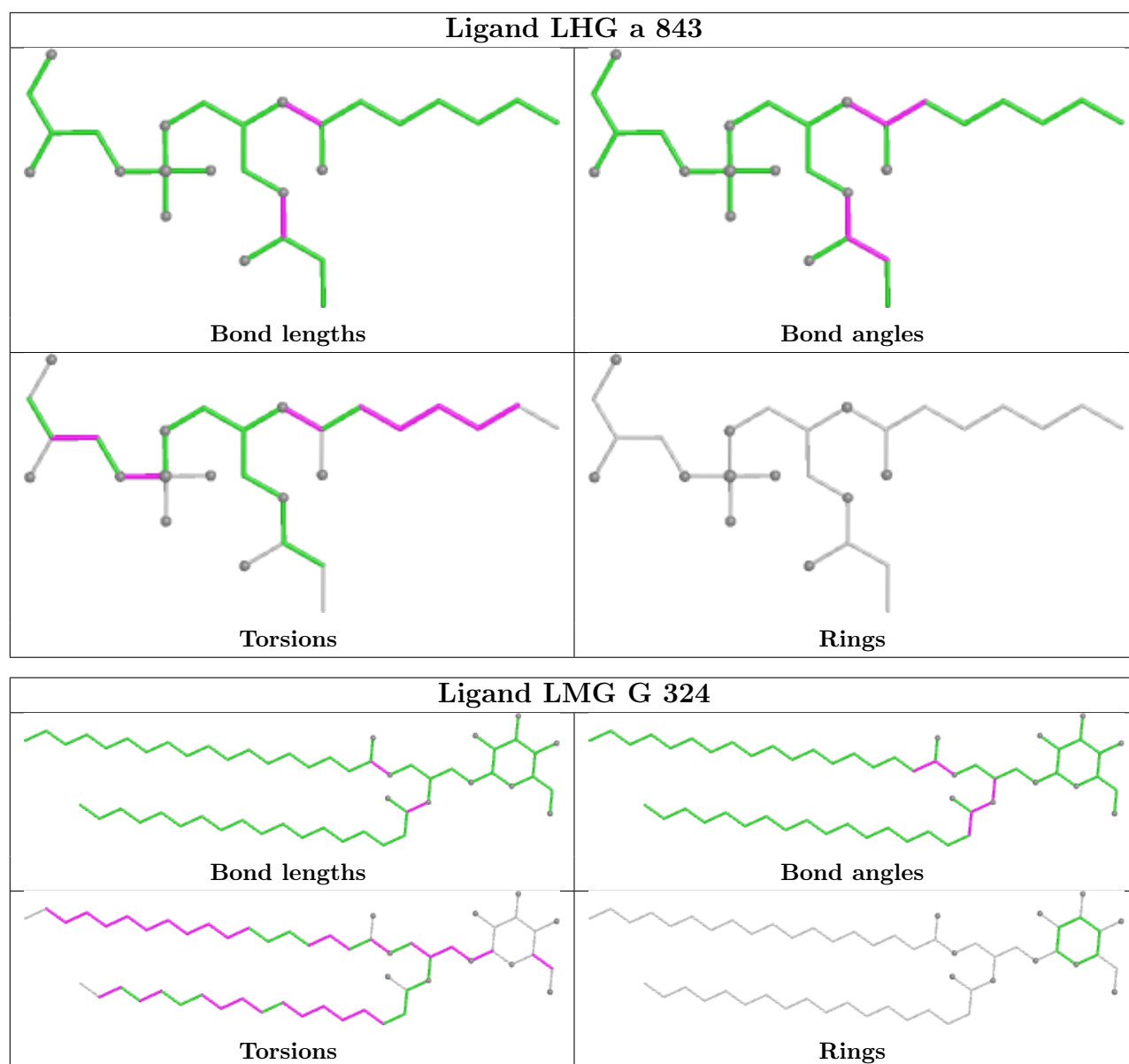


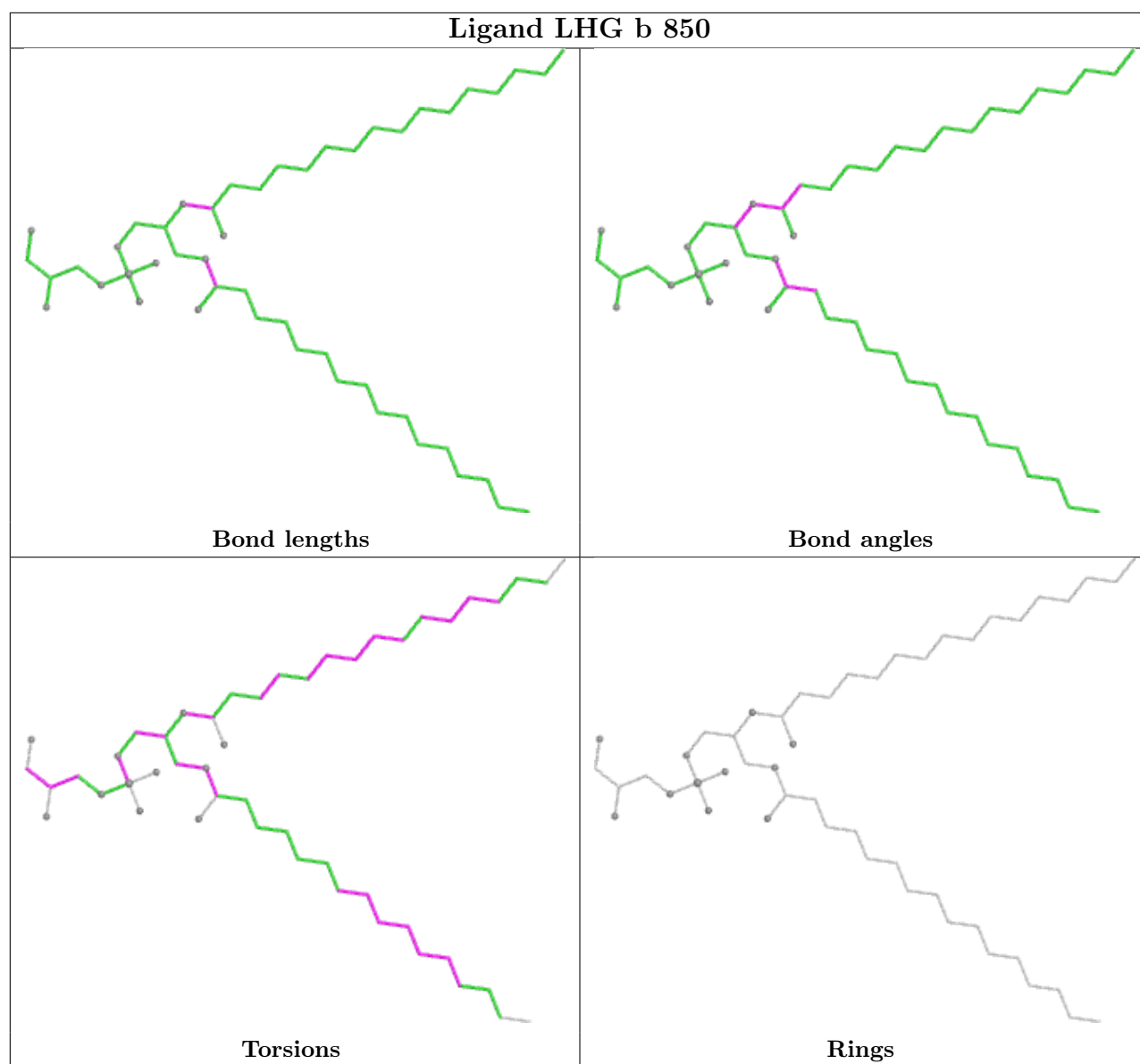
Ligand LMT a 851

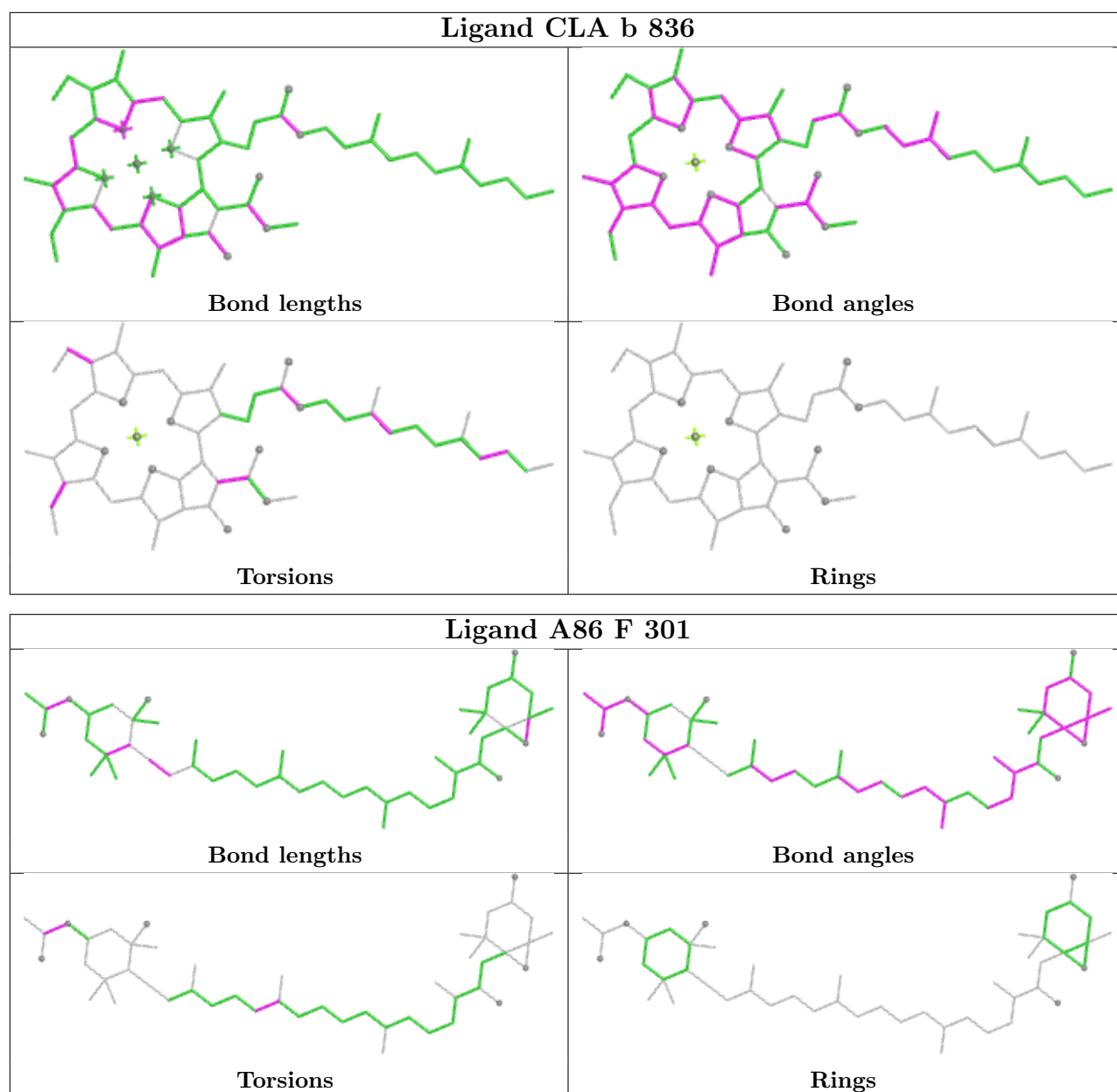


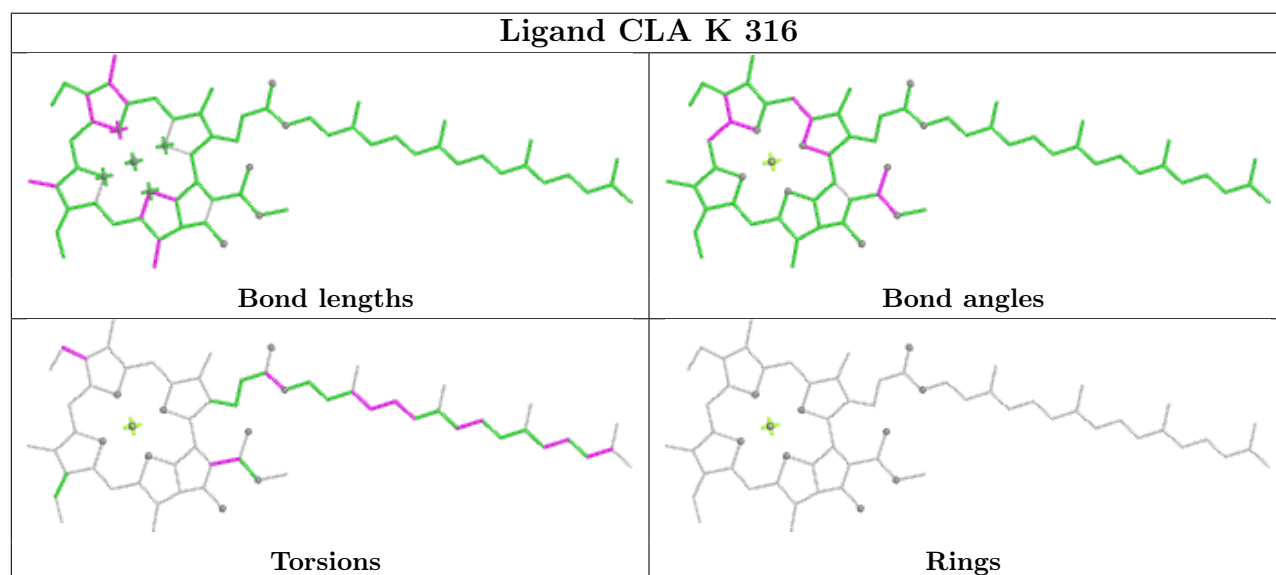
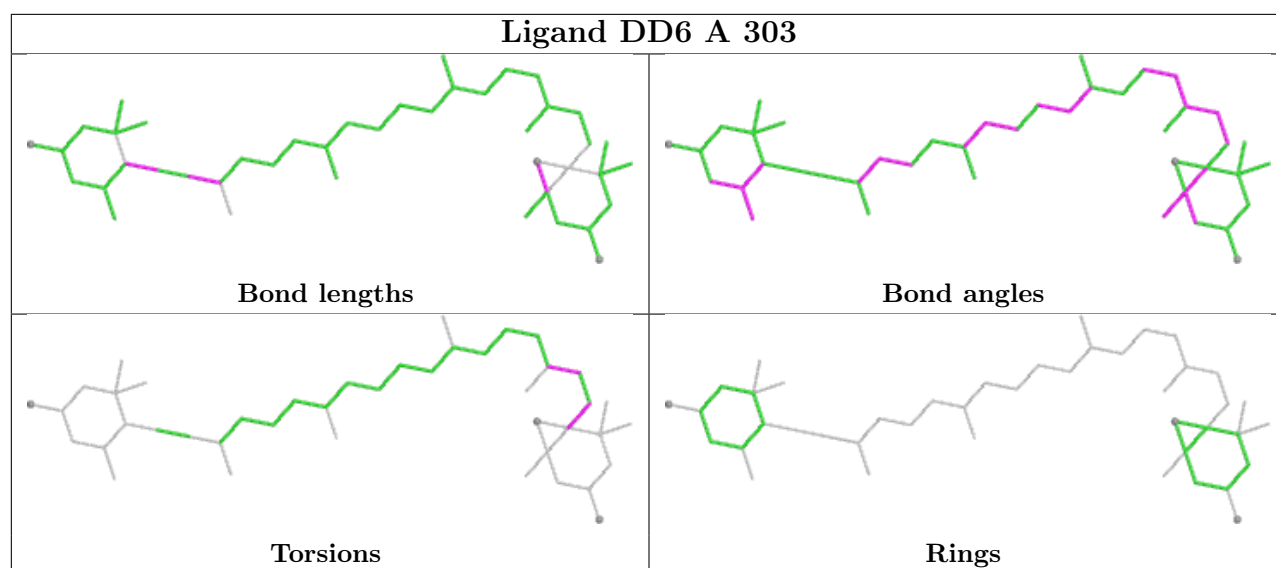




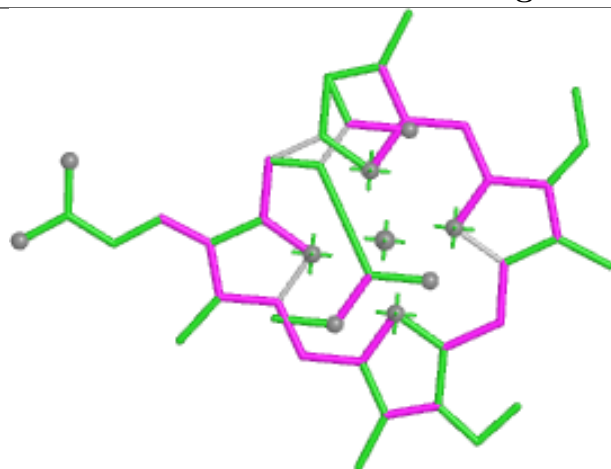




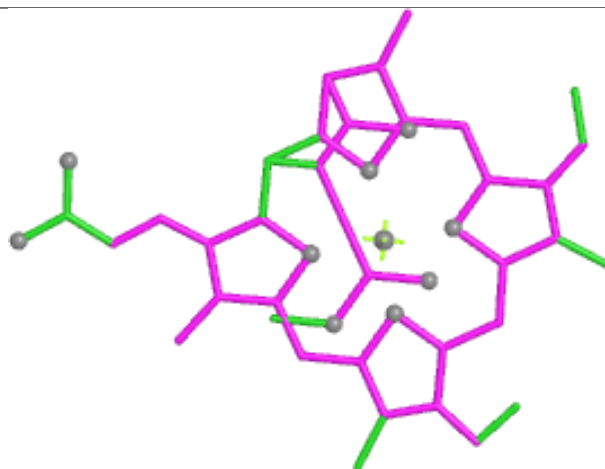




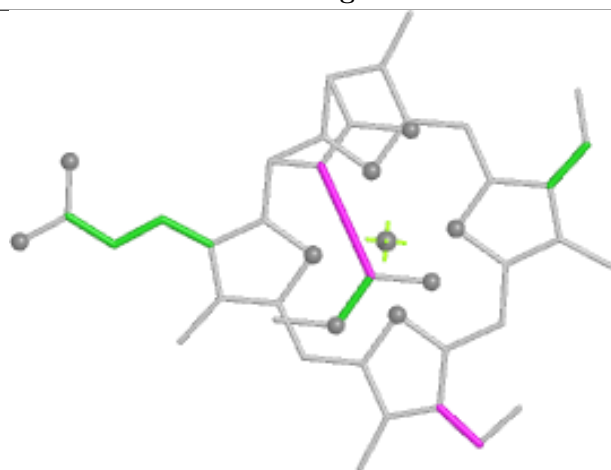
Ligand KC1 O 313



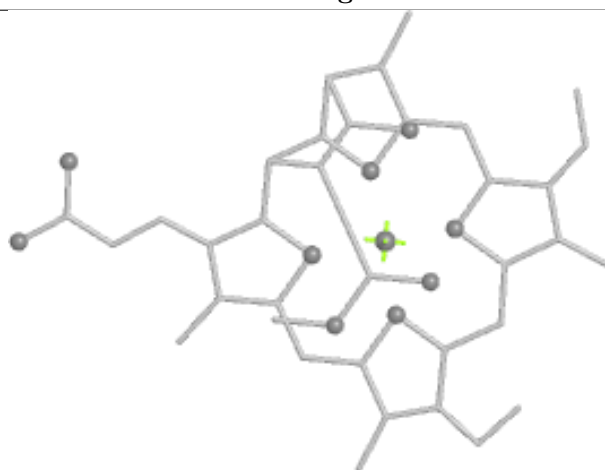
Bond lengths



Bond angles

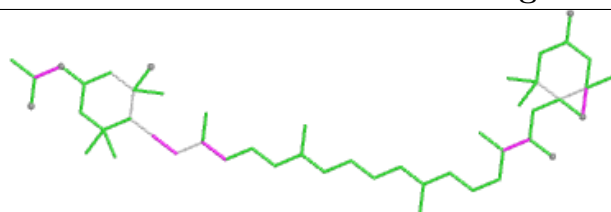


Torsions

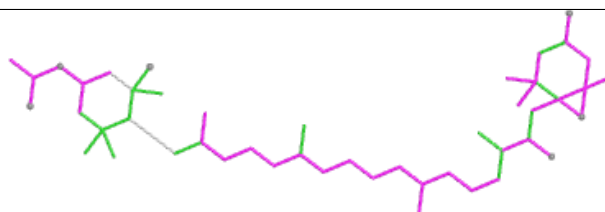


Rings

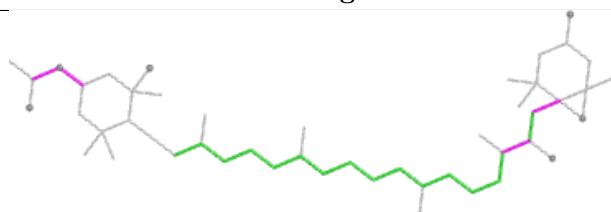
Ligand A86 X 303



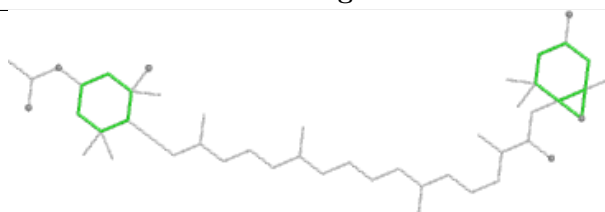
Bond lengths



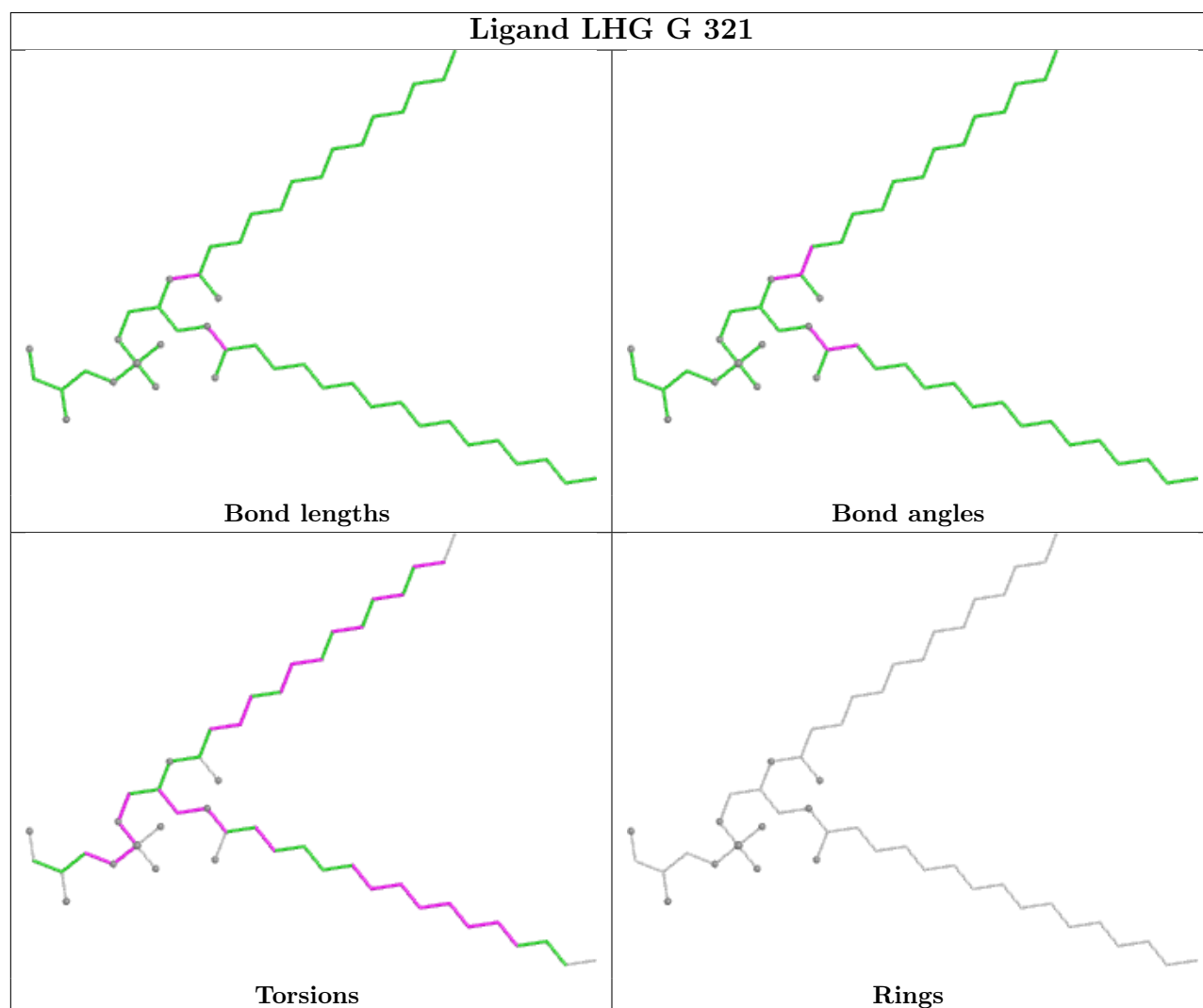
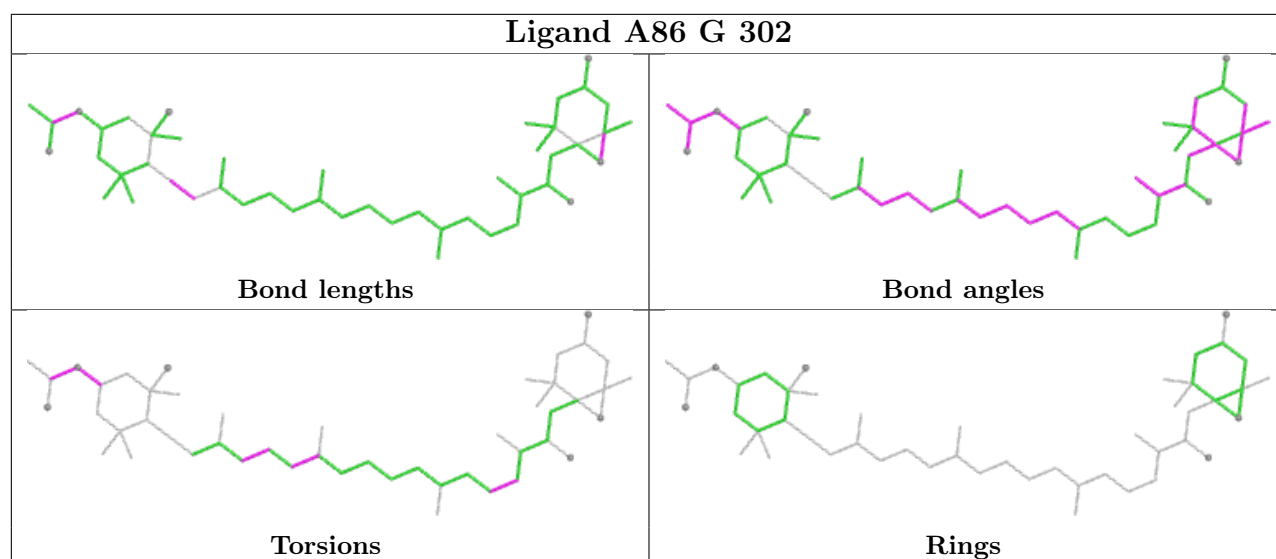
Bond angles

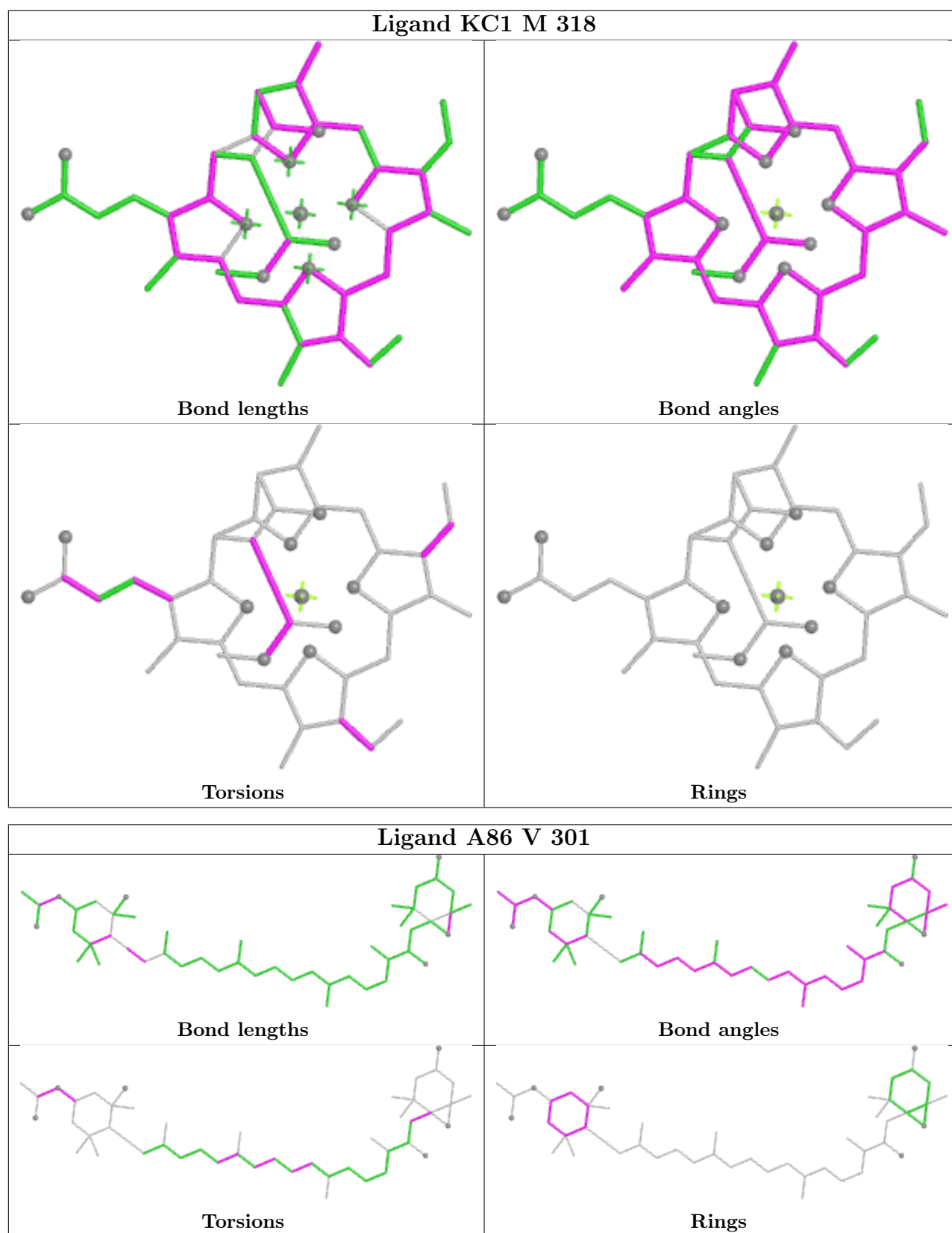


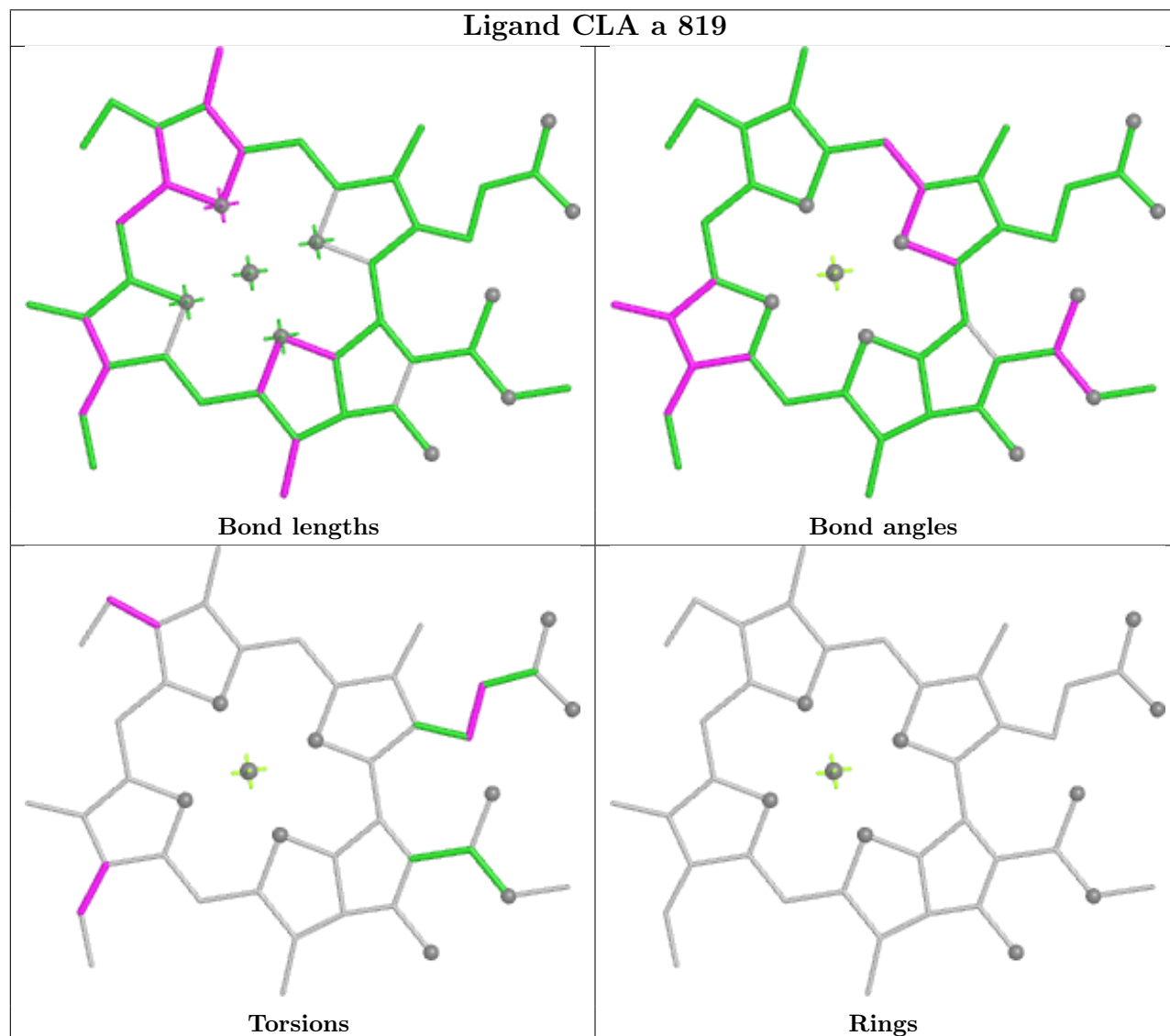
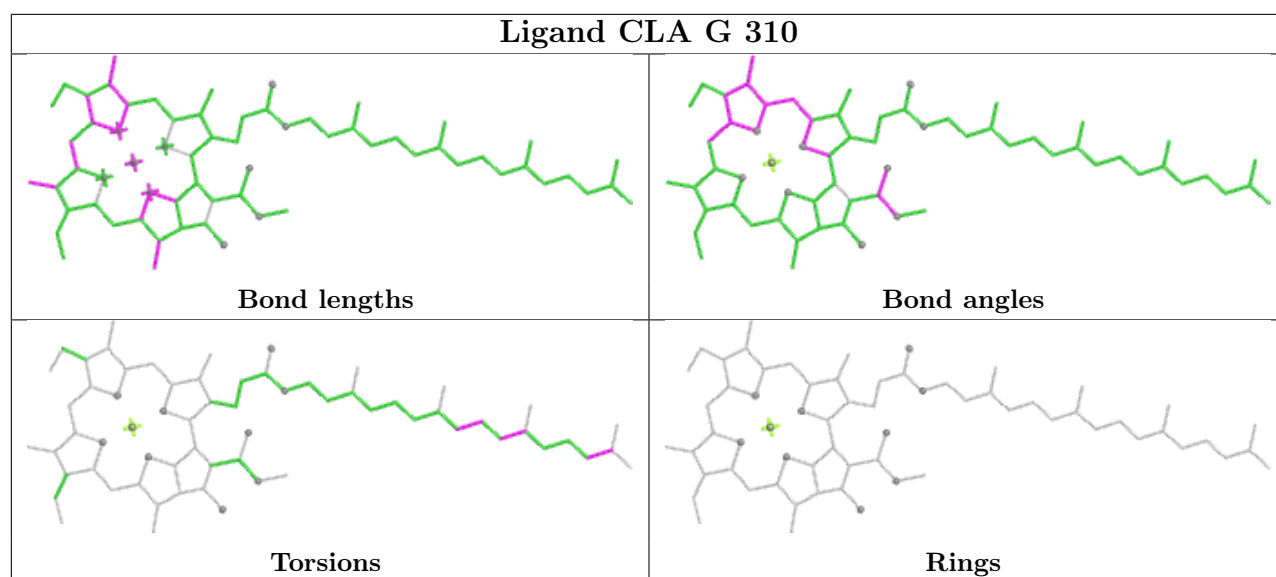
Torsions

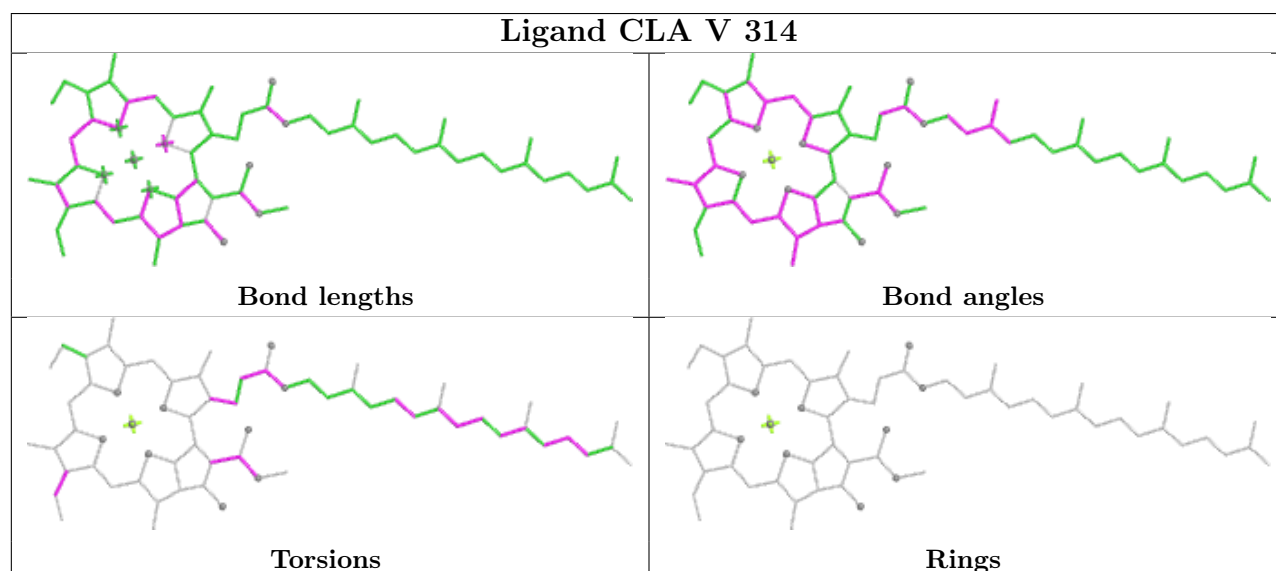
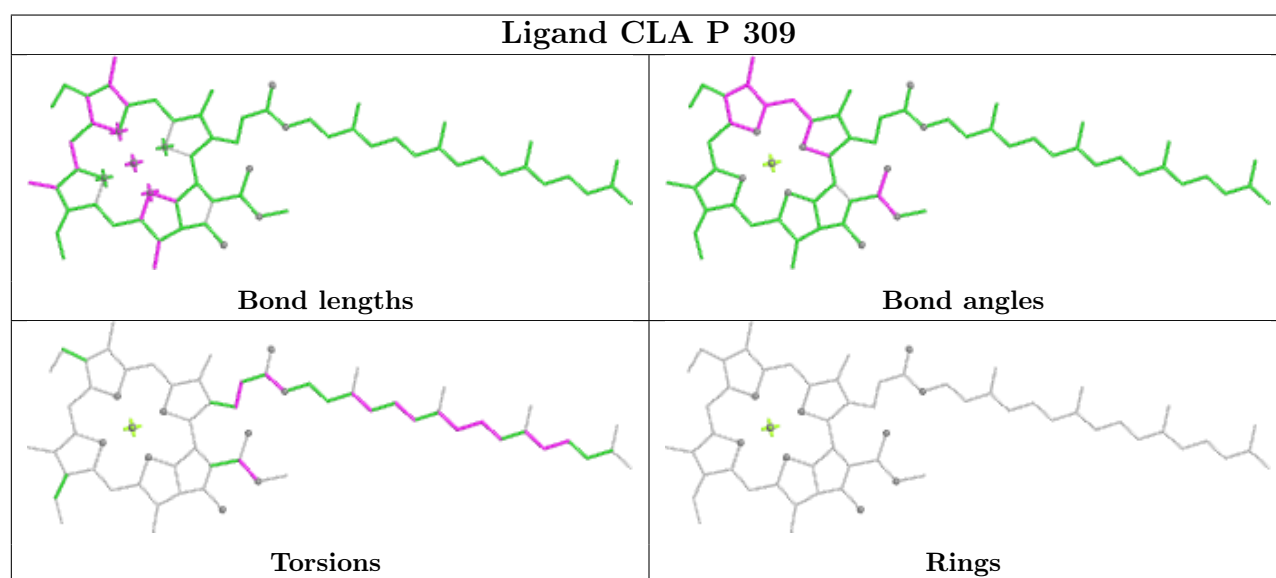
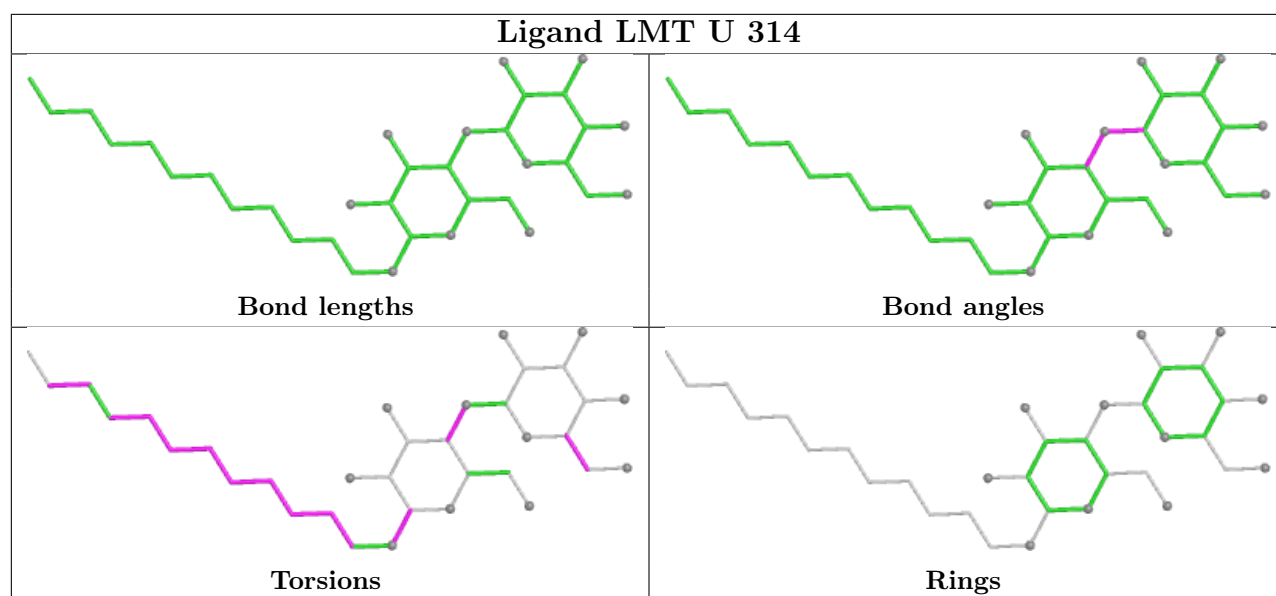


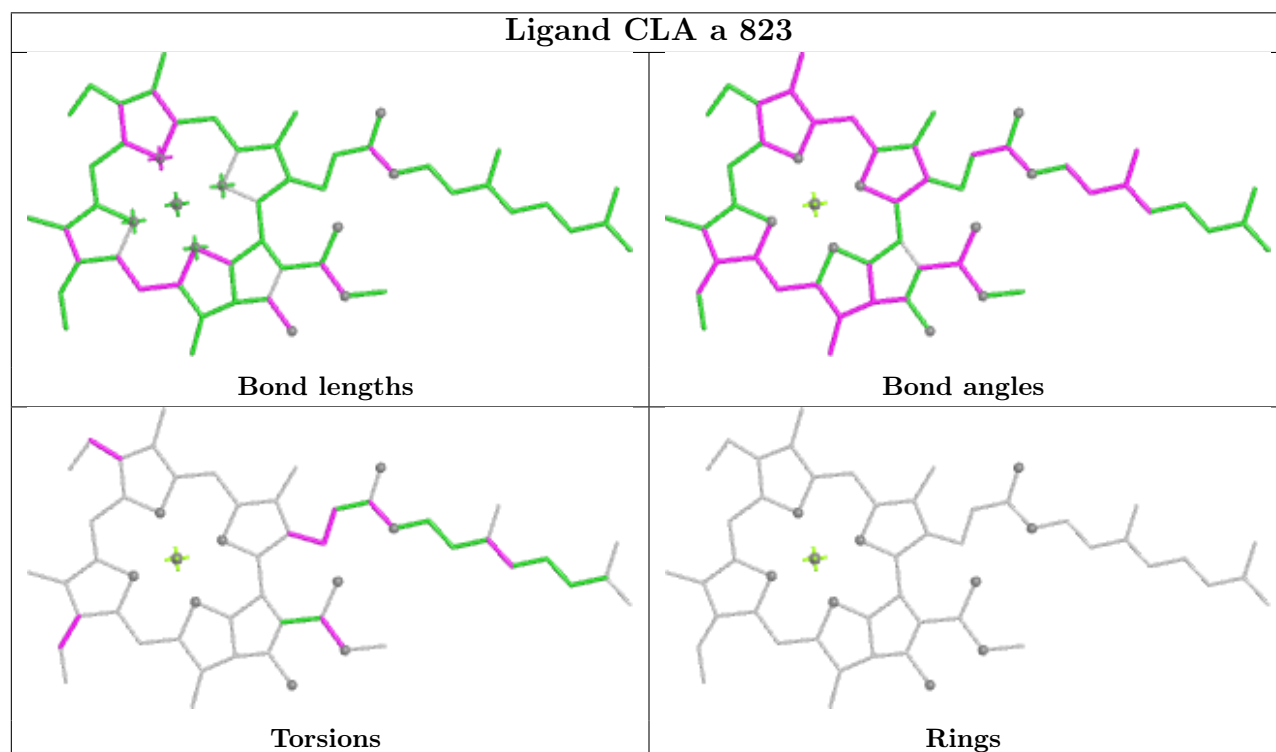
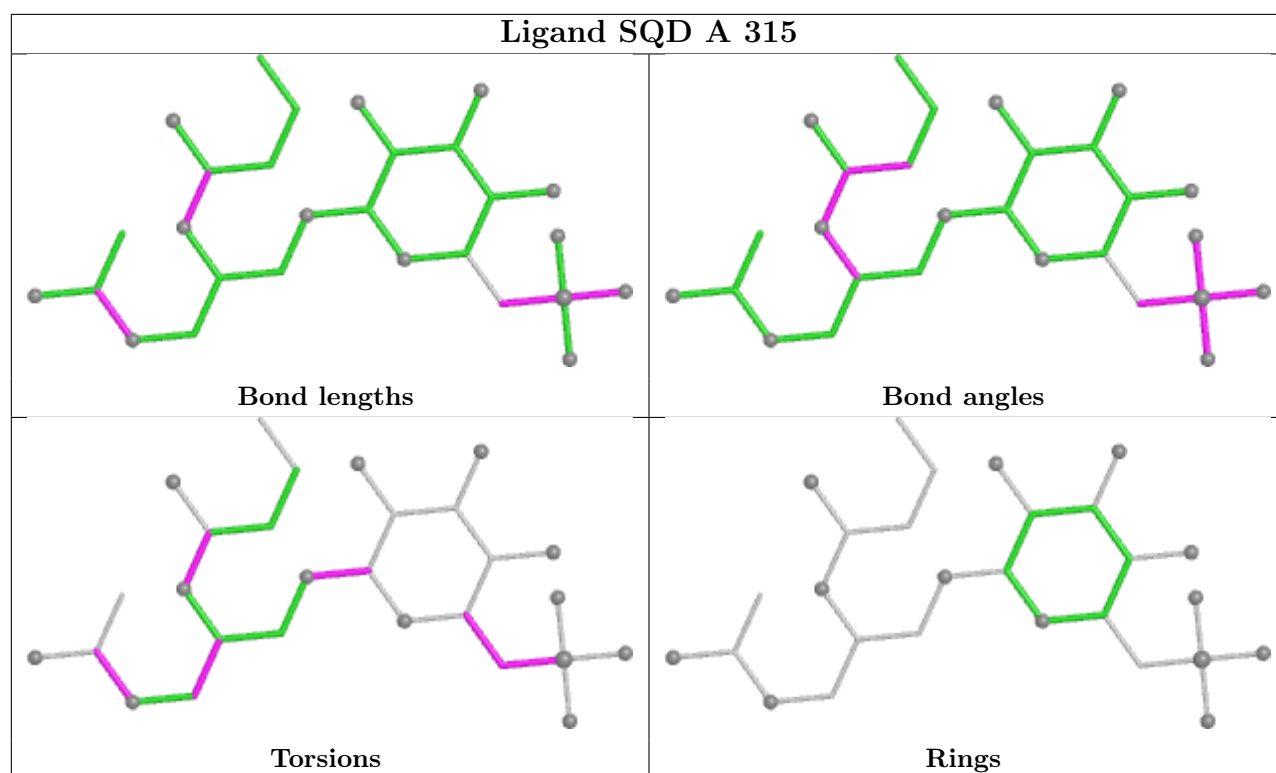
Rings

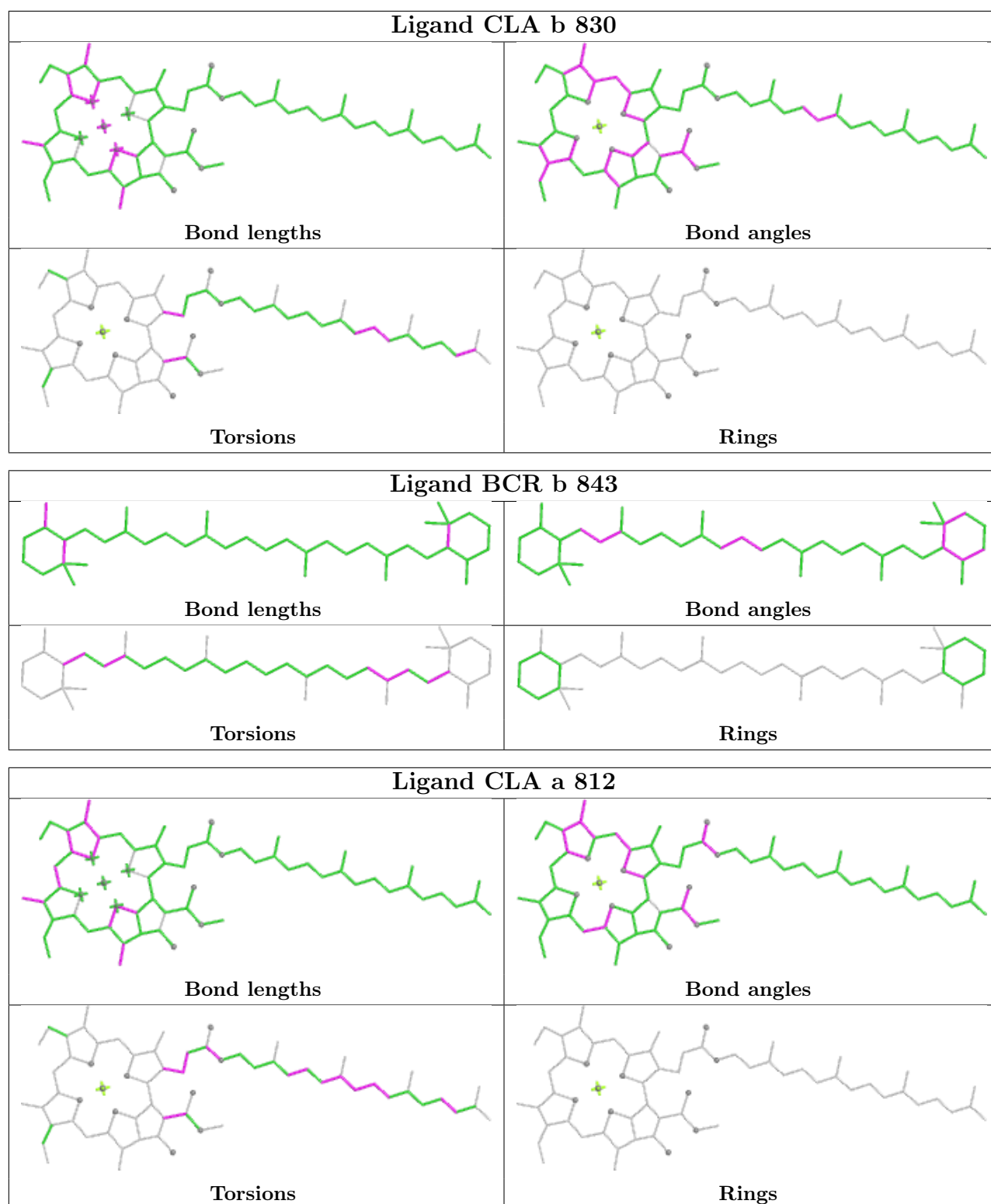


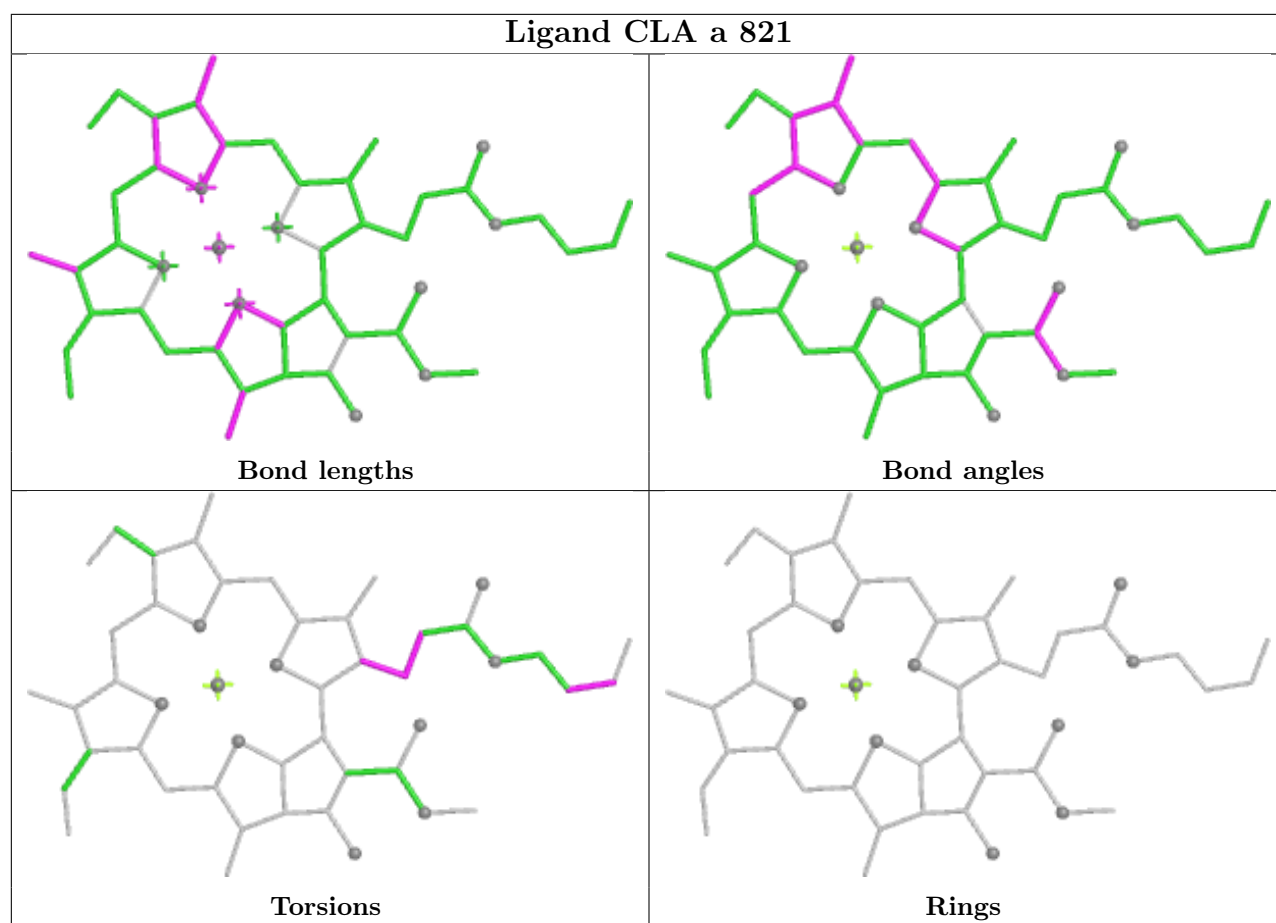




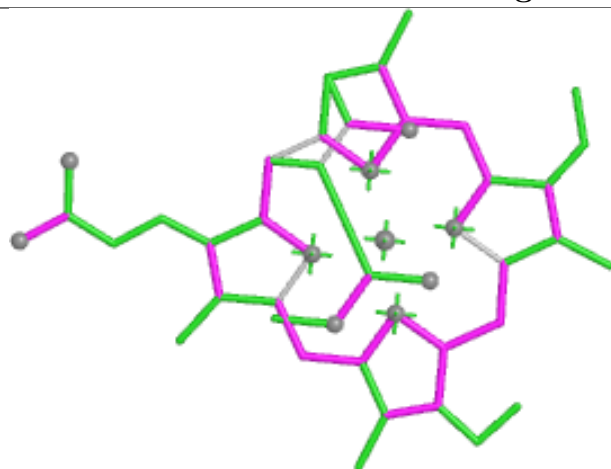




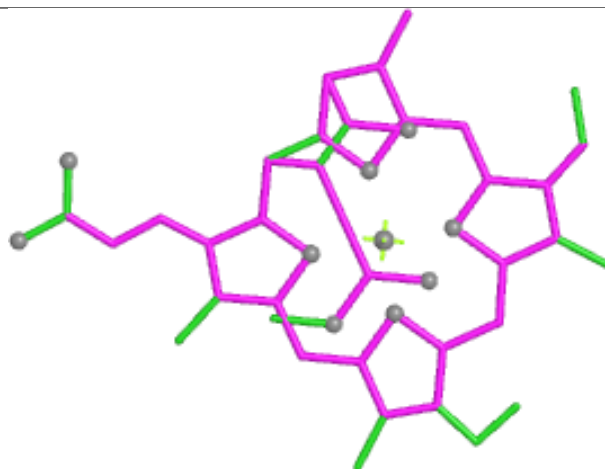




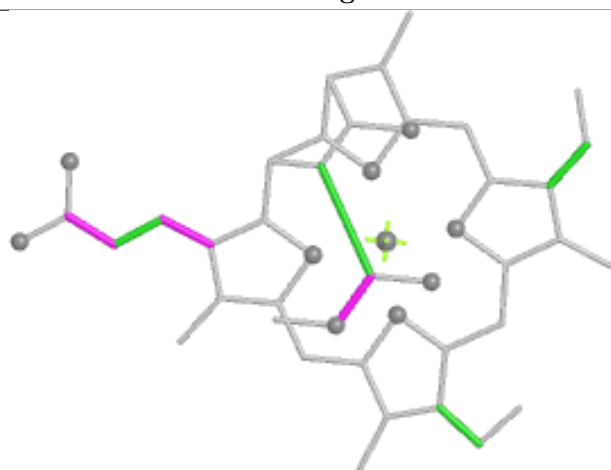
Ligand KC1 H 313



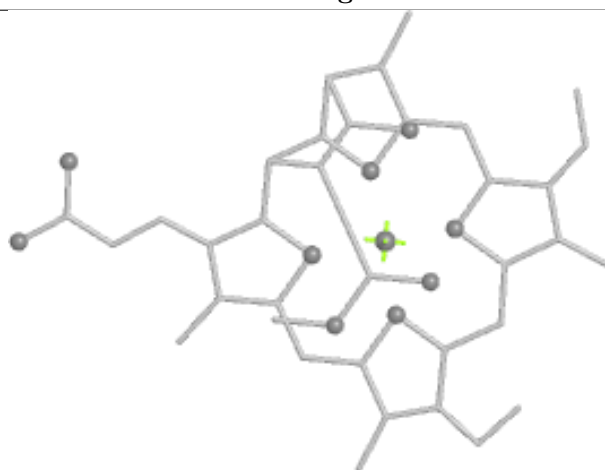
Bond lengths



Bond angles

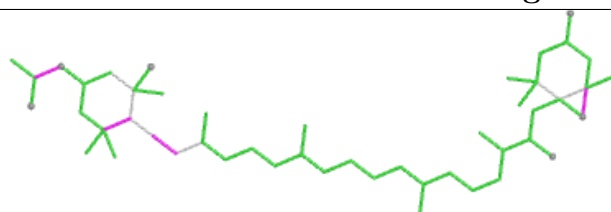


Torsions

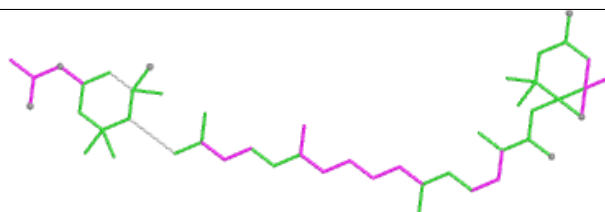


Rings

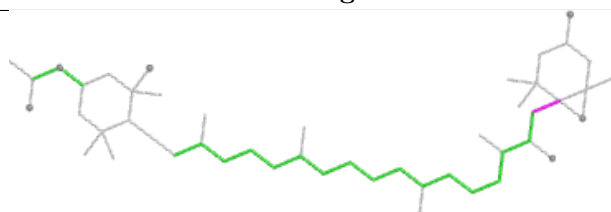
Ligand A86 h 204



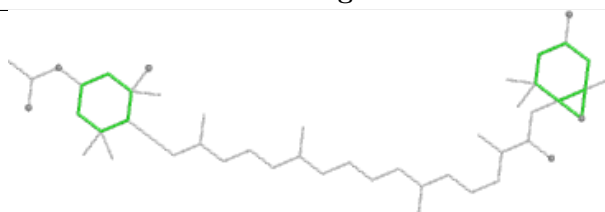
Bond lengths



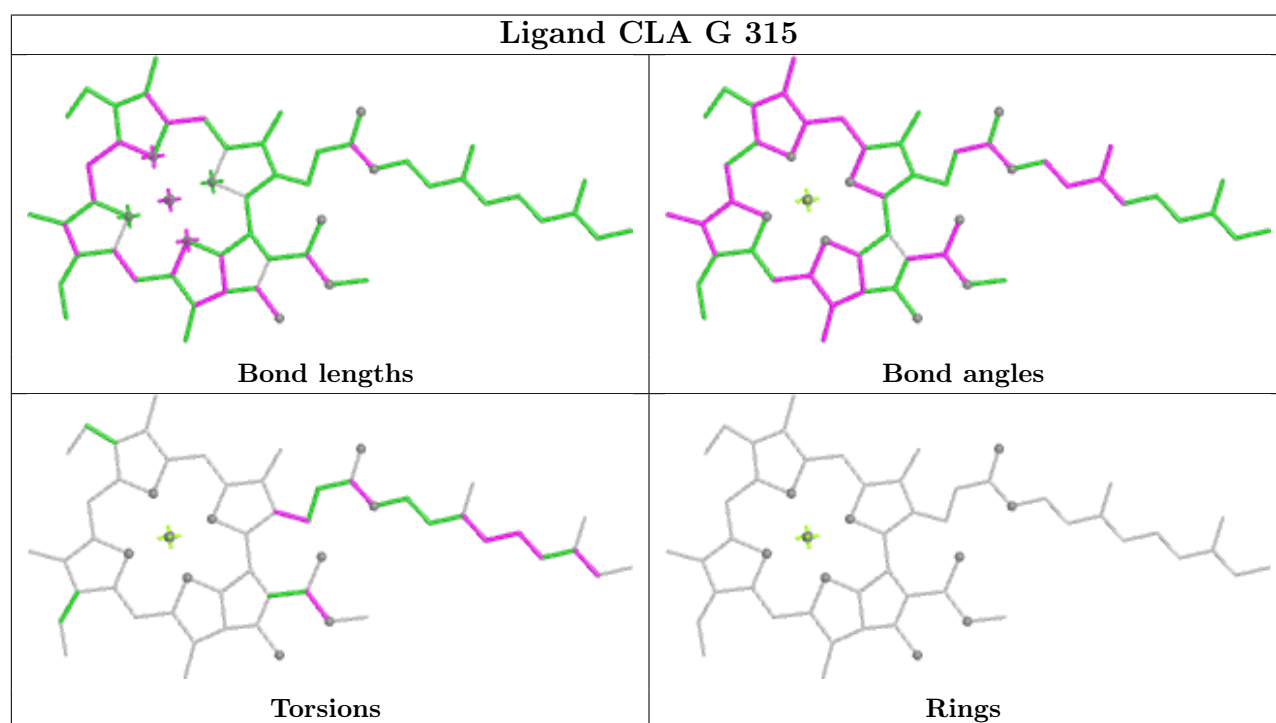
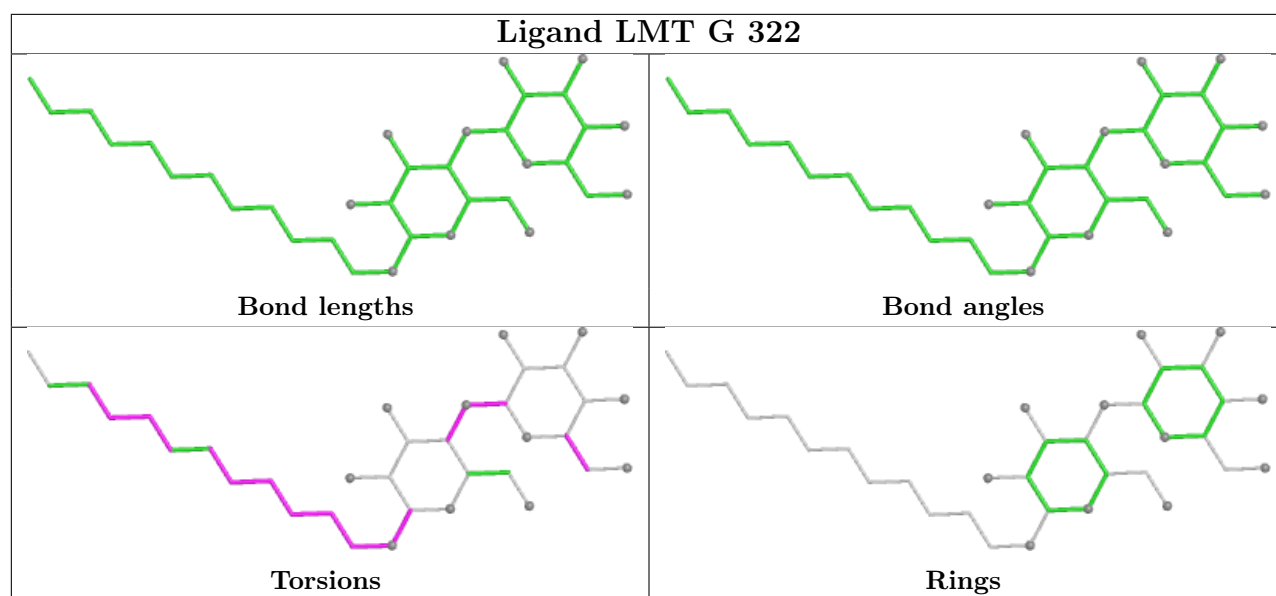
Bond angles



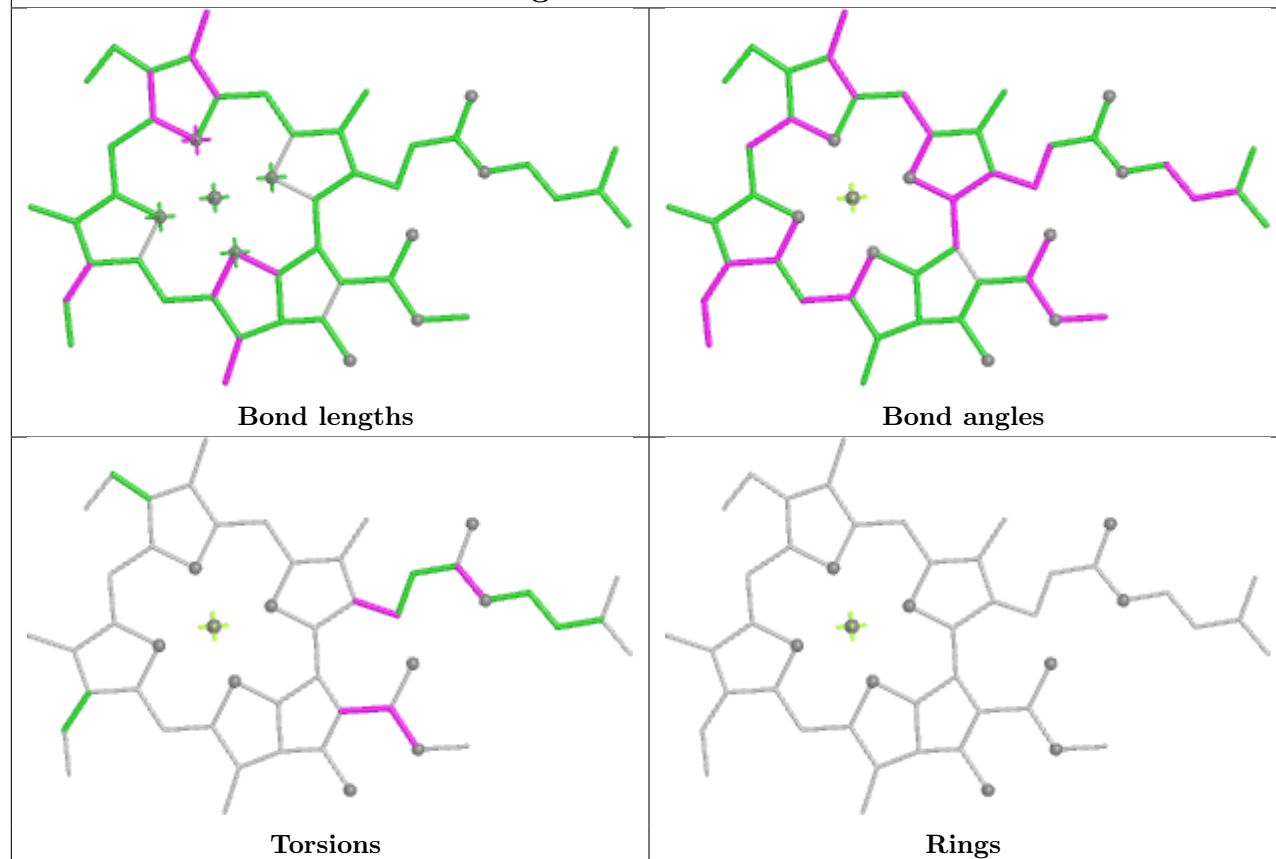
Torsions



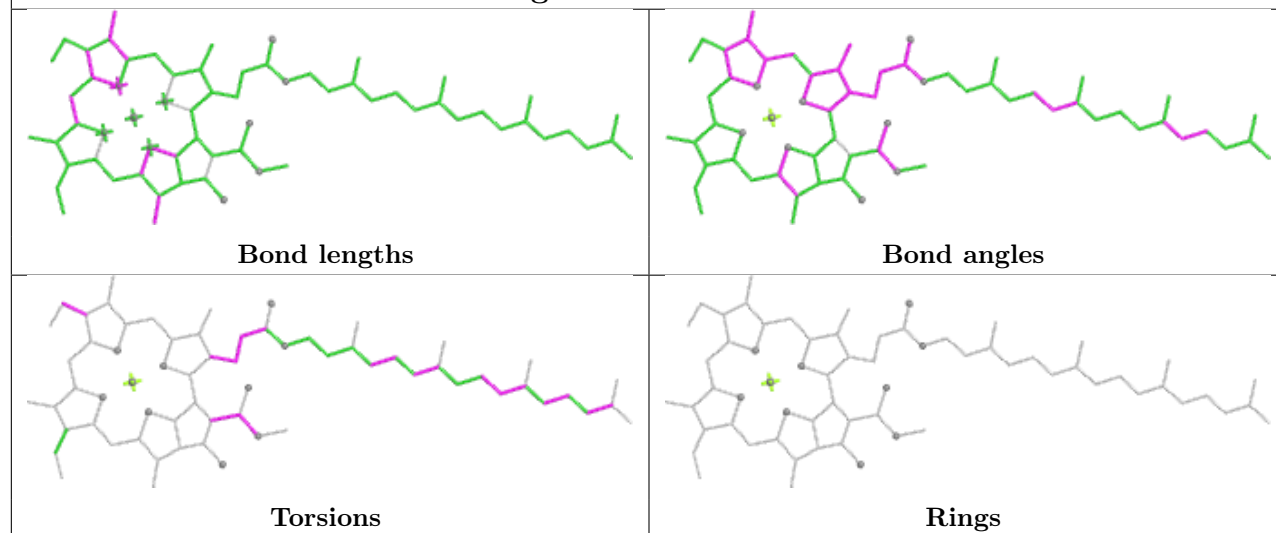
Rings

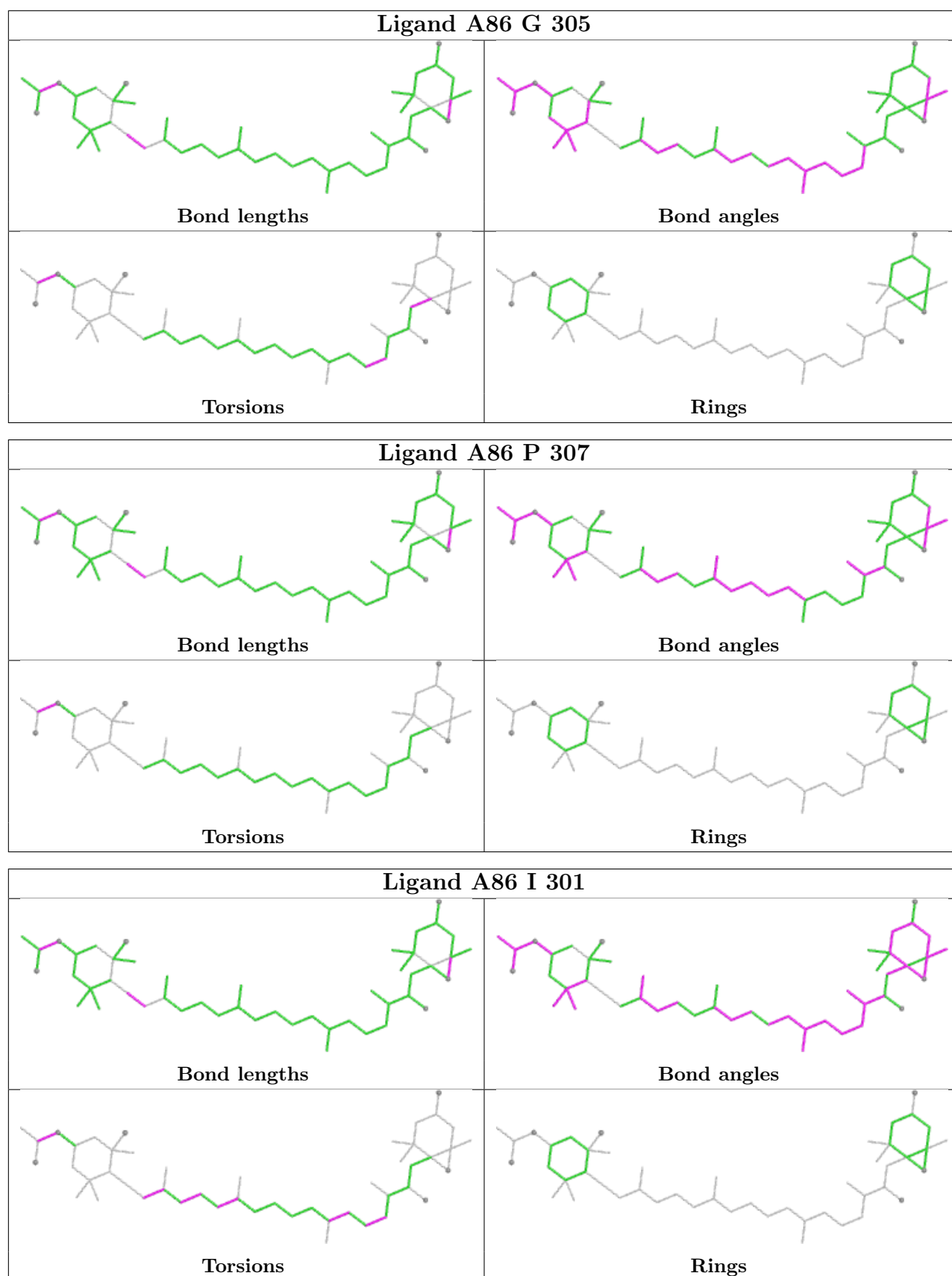


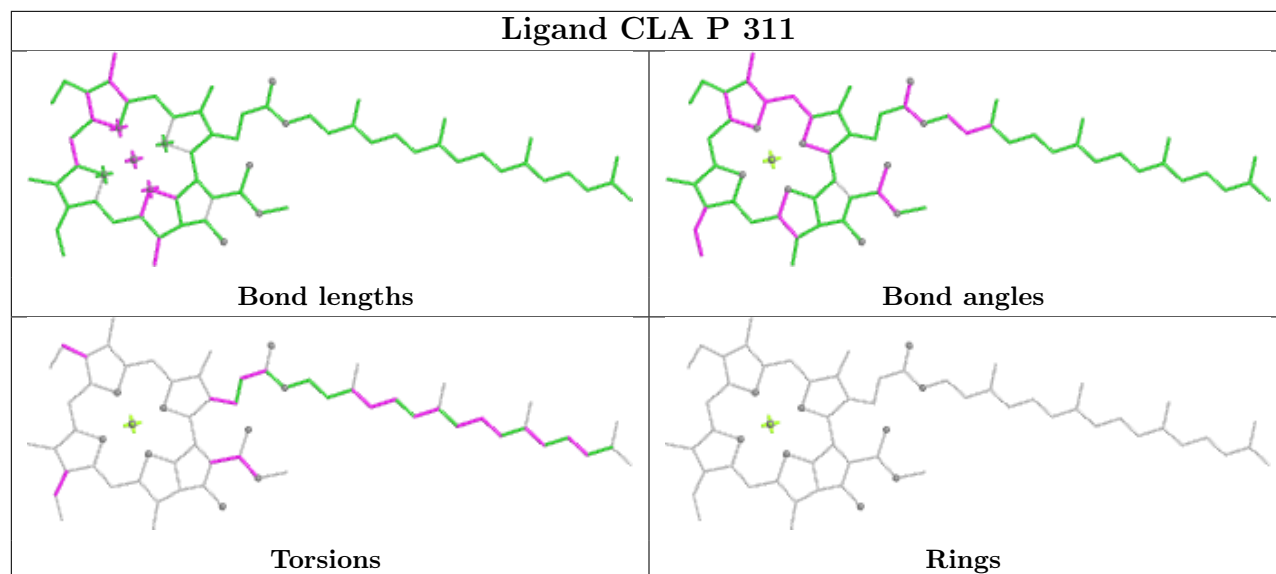
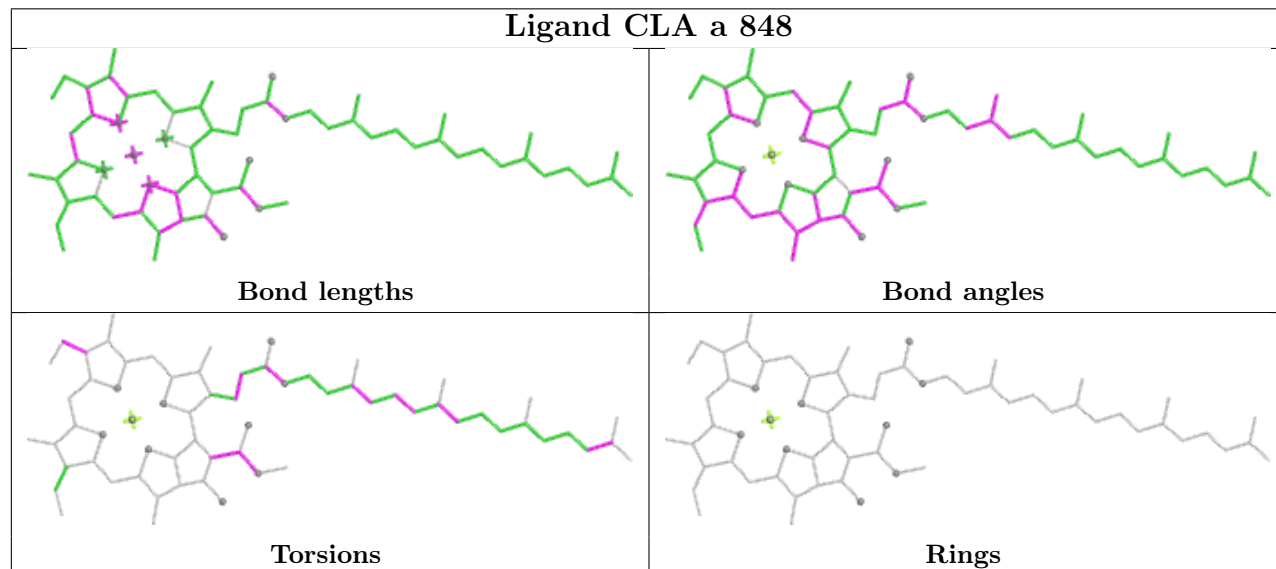
Ligand CLA X 307



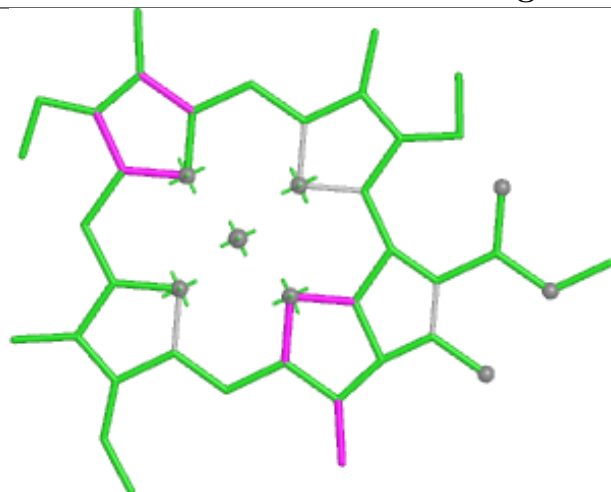
Ligand CLA G 313



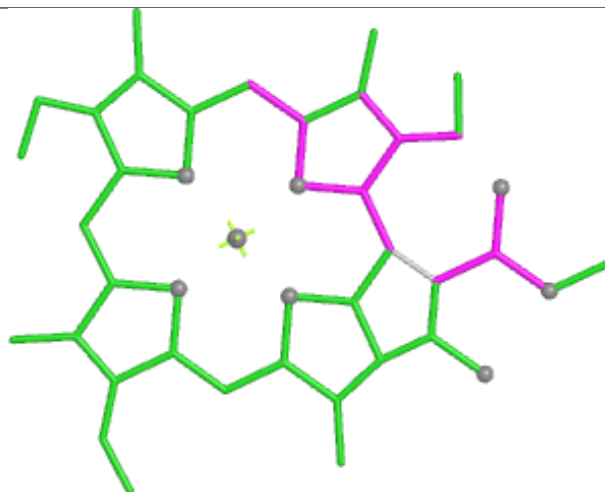


Ligand CLA P 311**Ligand CLA a 848**

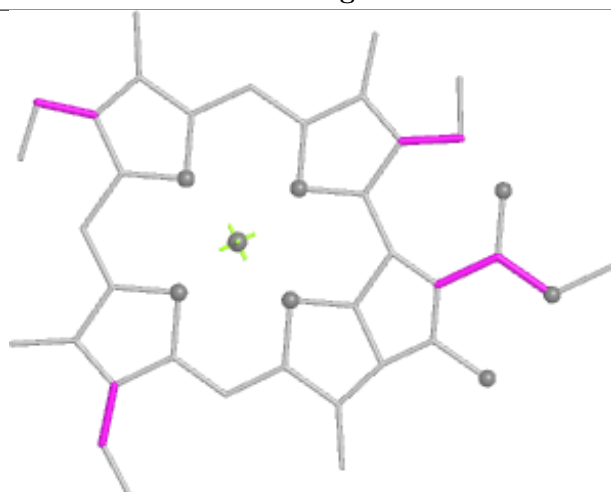
Ligand CLA S 318



Bond lengths



Bond angles

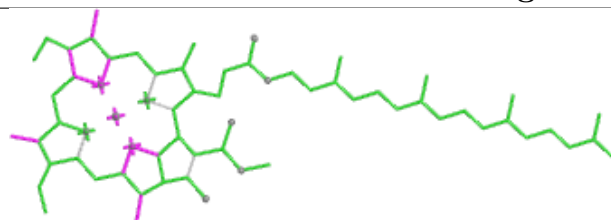


Torsions

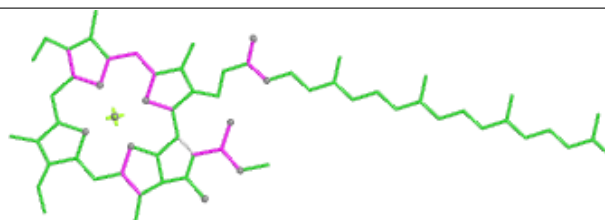


Rings

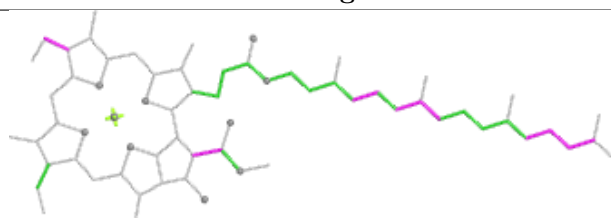
Ligand CLA b 821



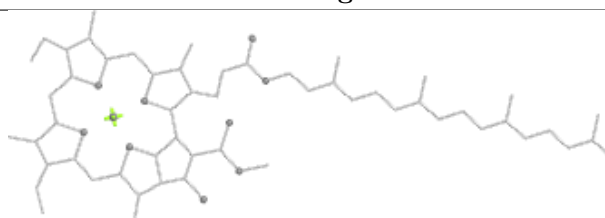
Bond lengths



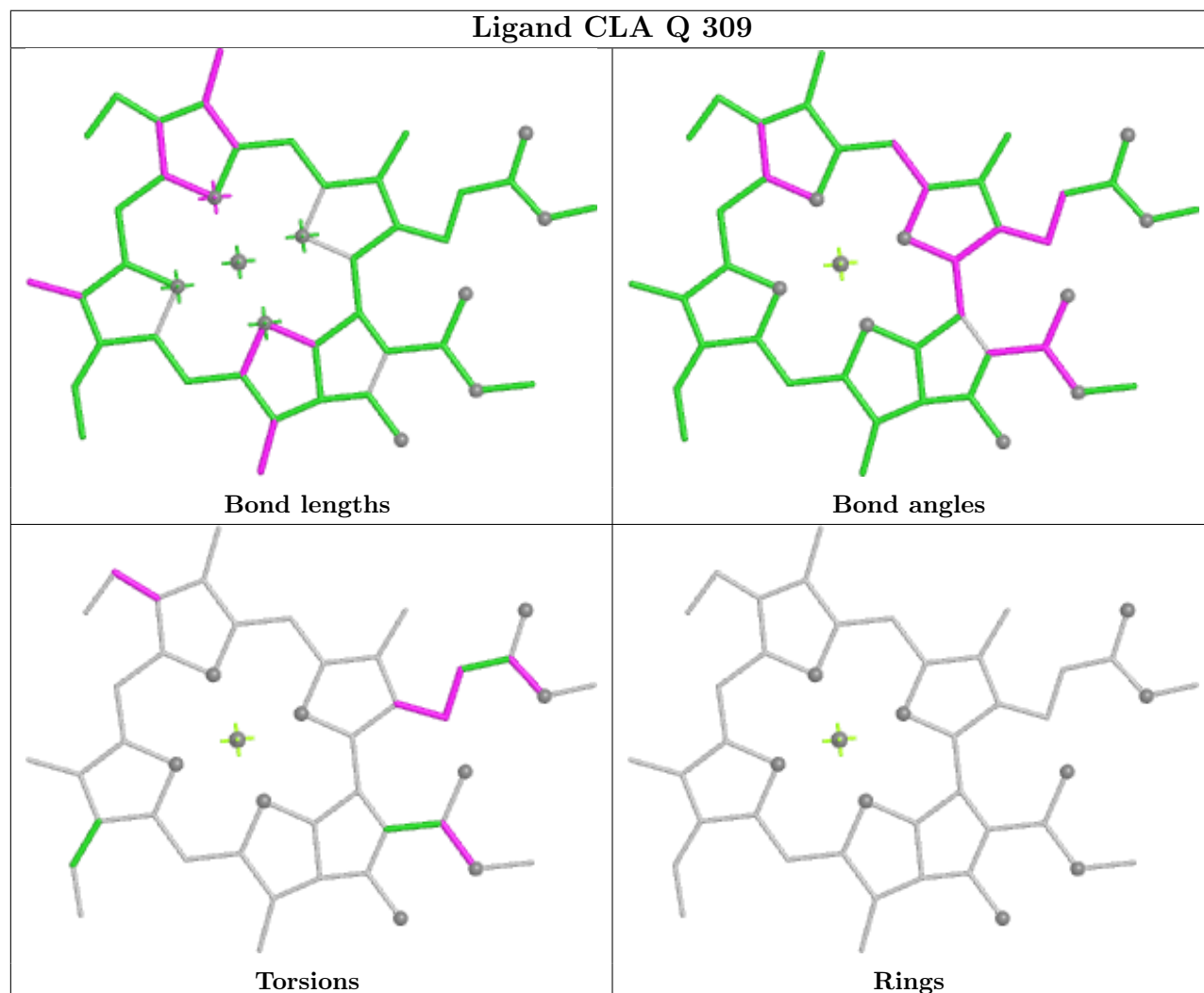
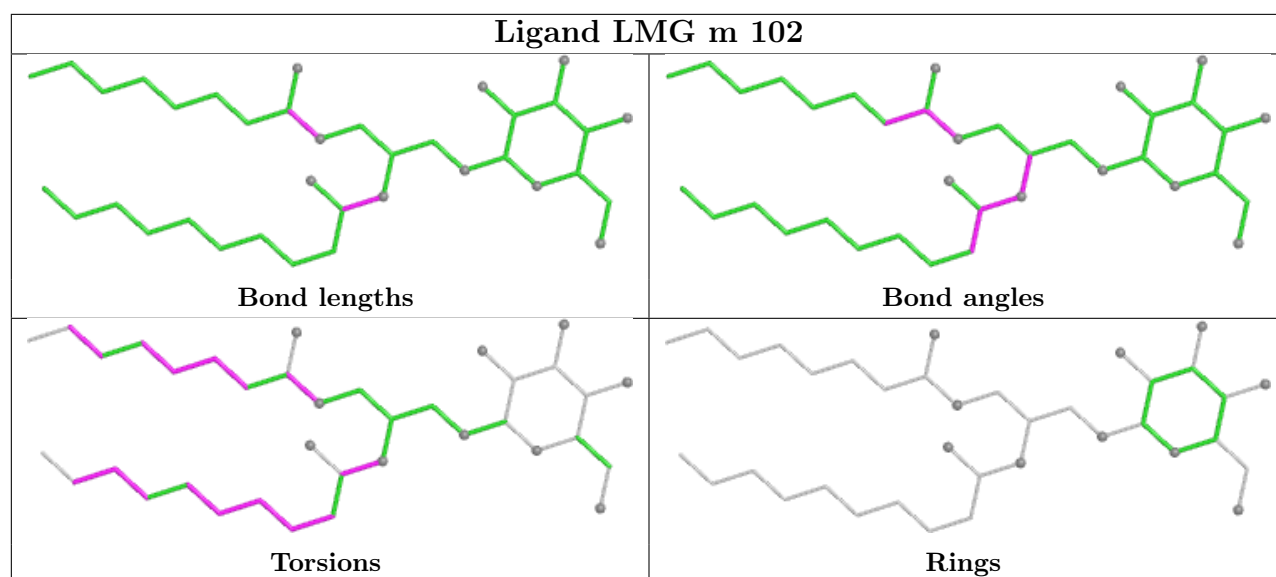
Bond angles

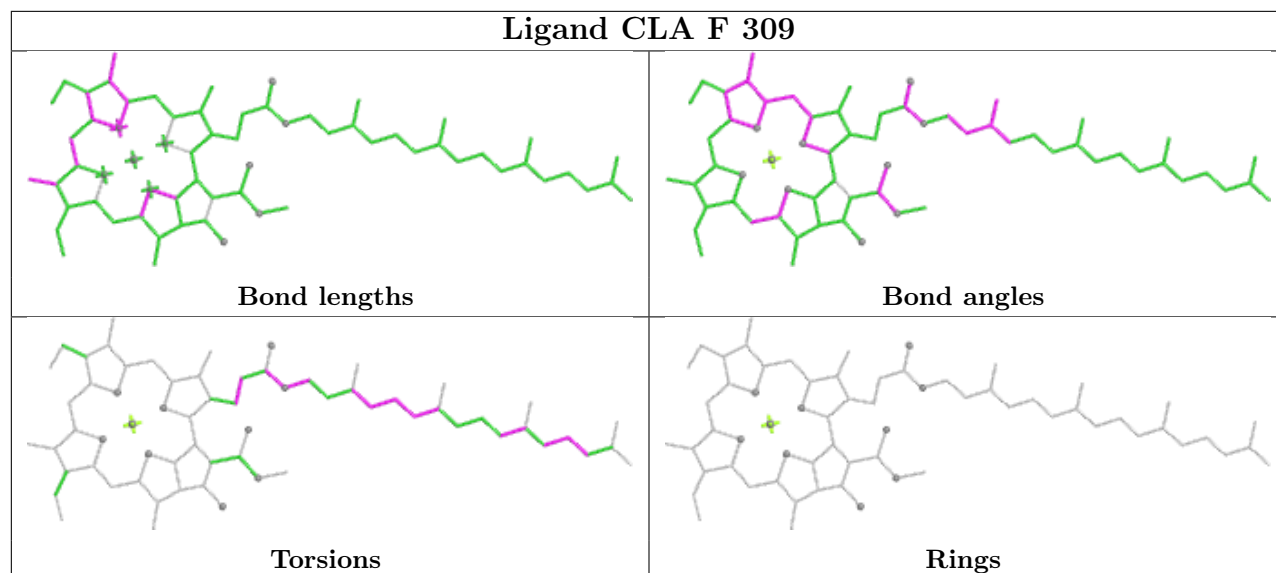
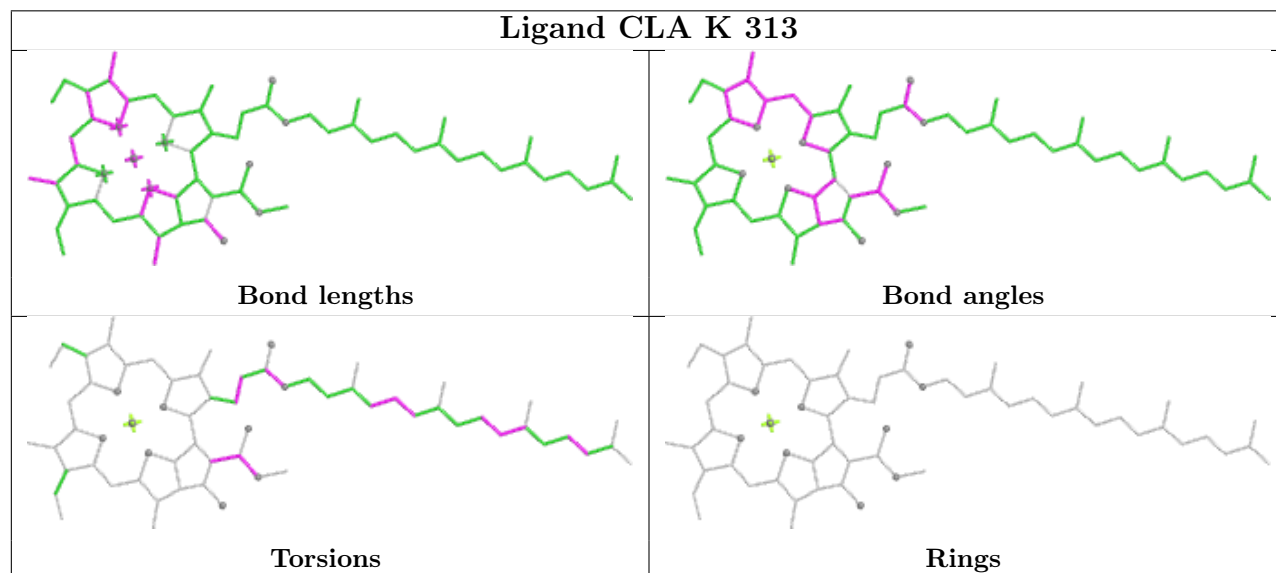
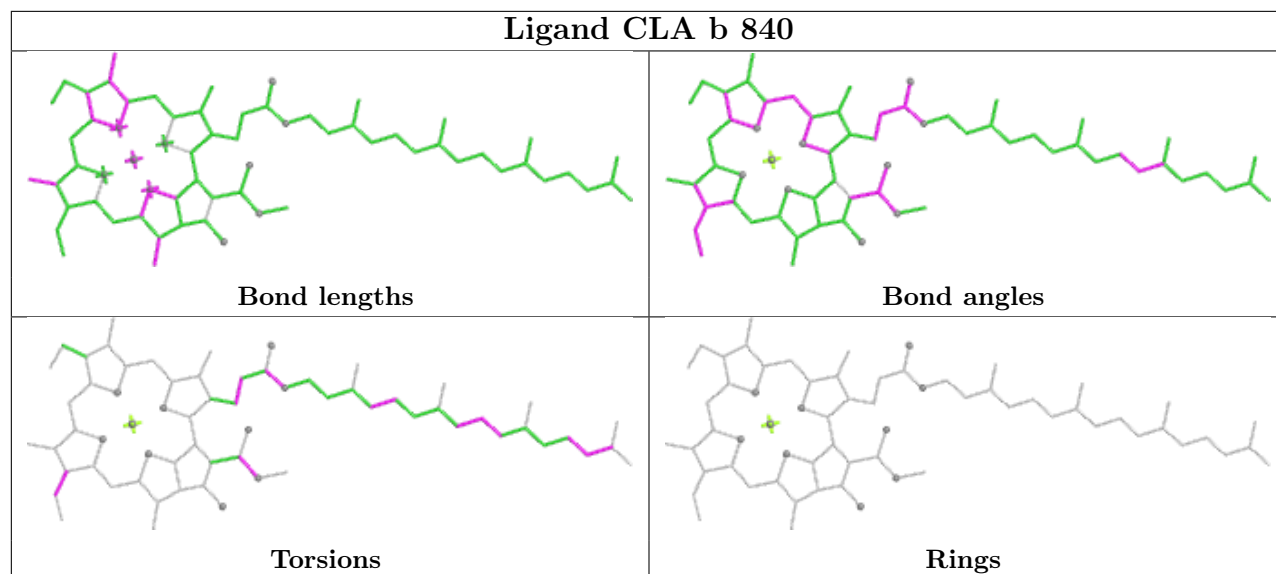


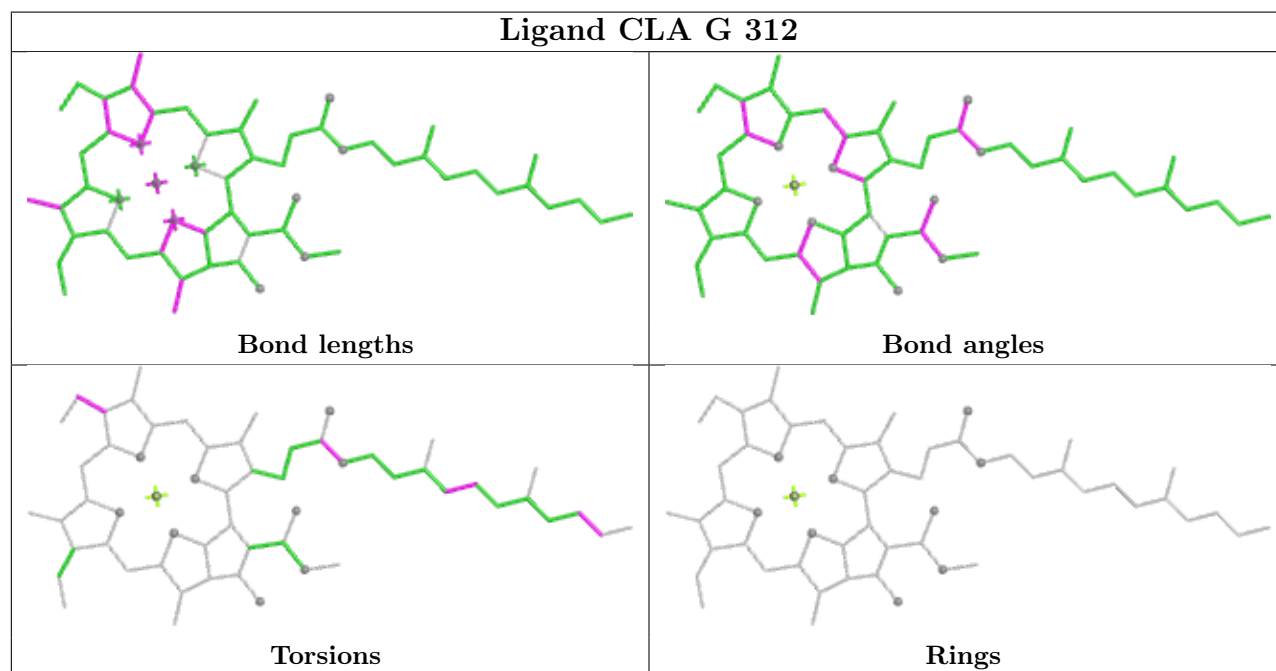
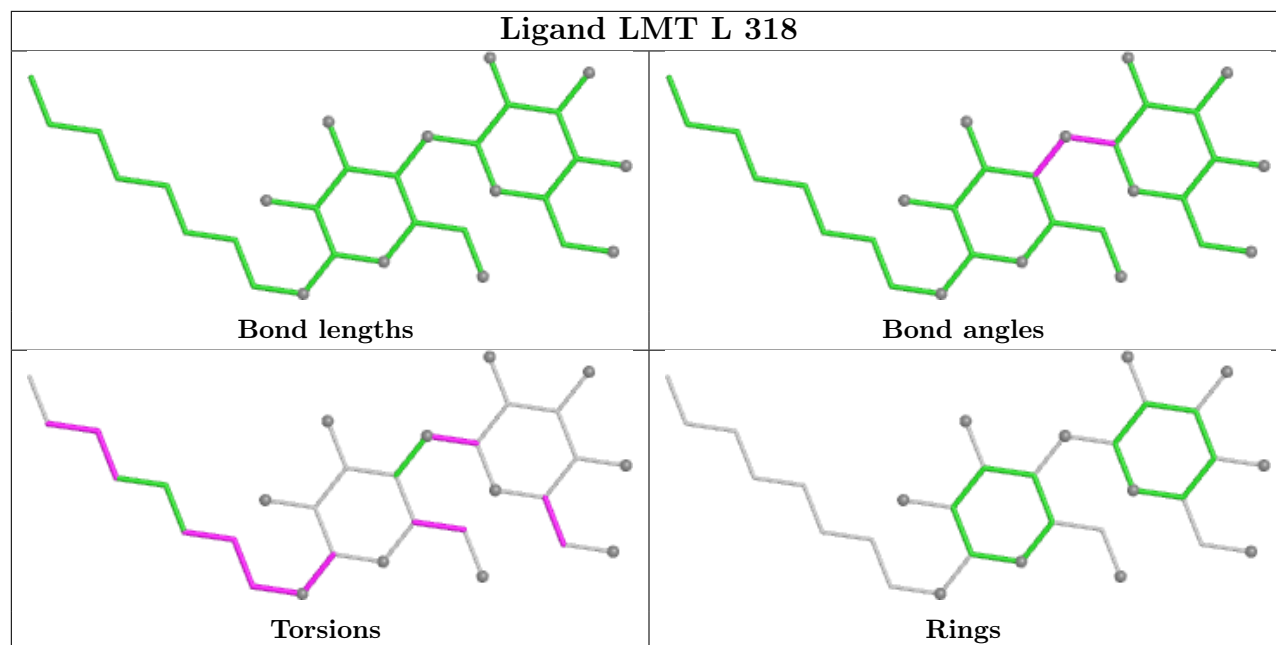
Torsions

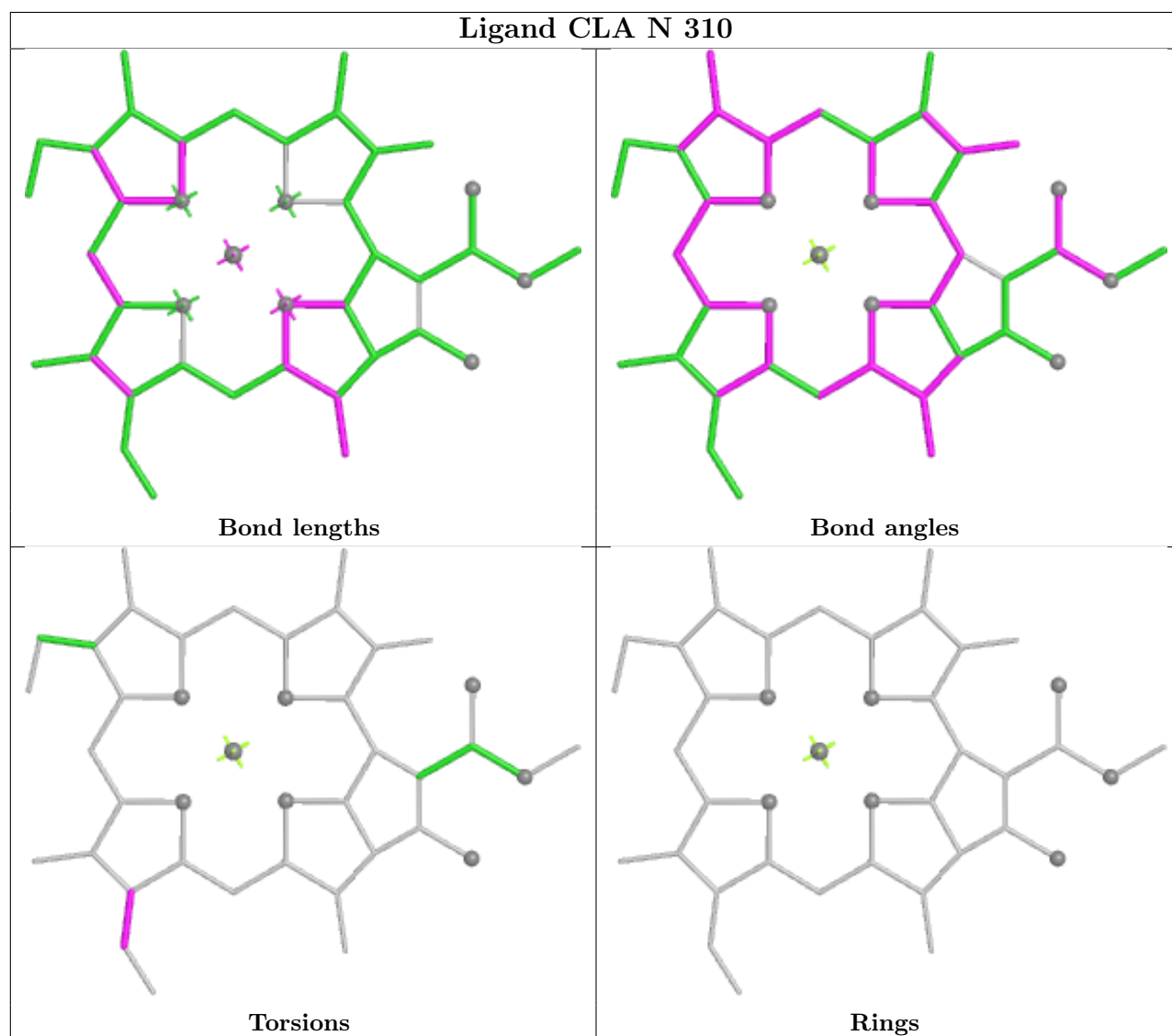
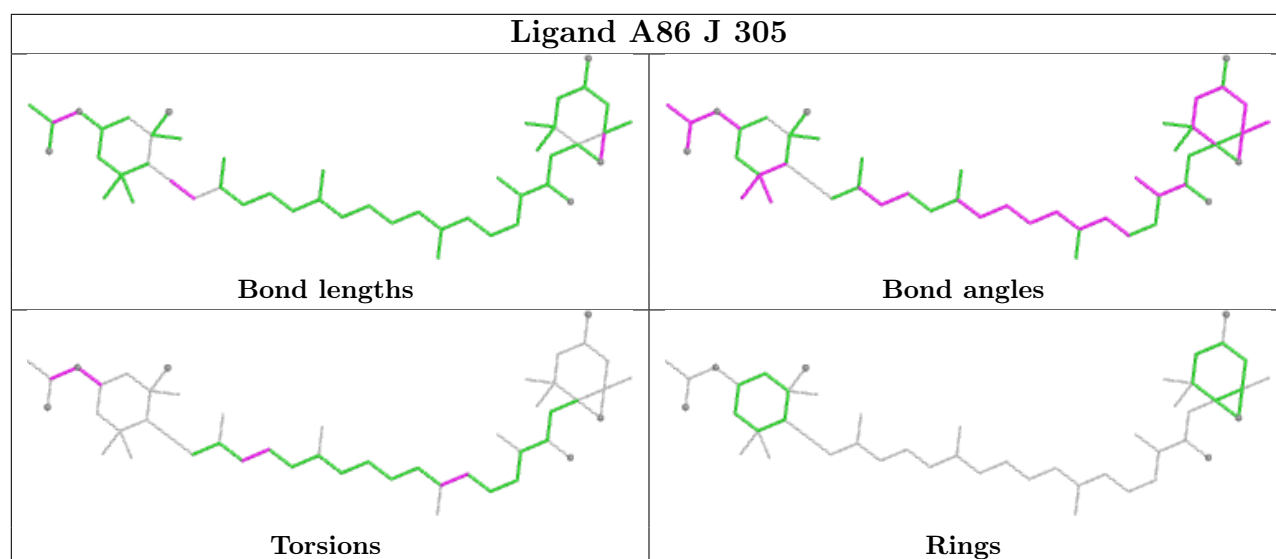


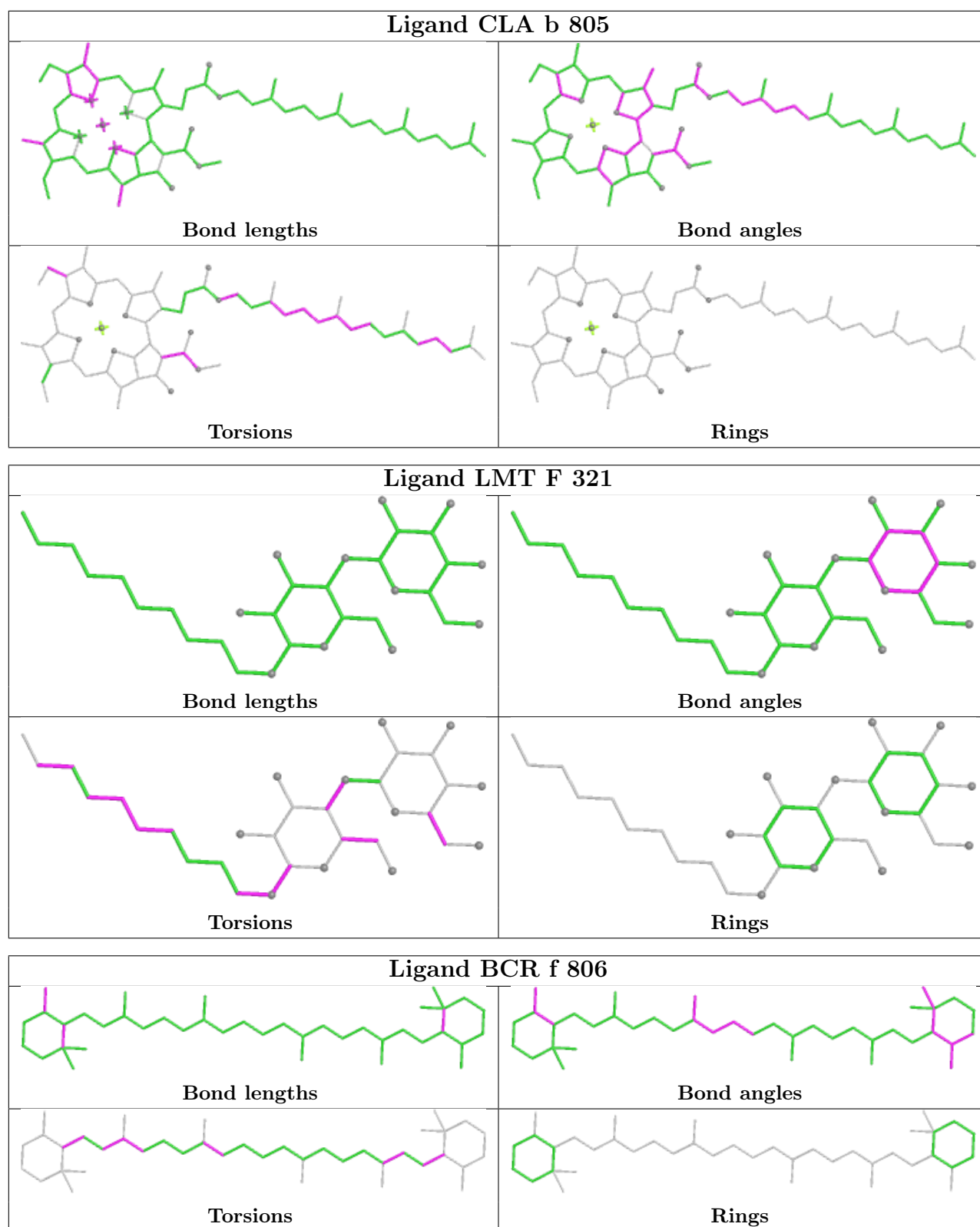
Rings

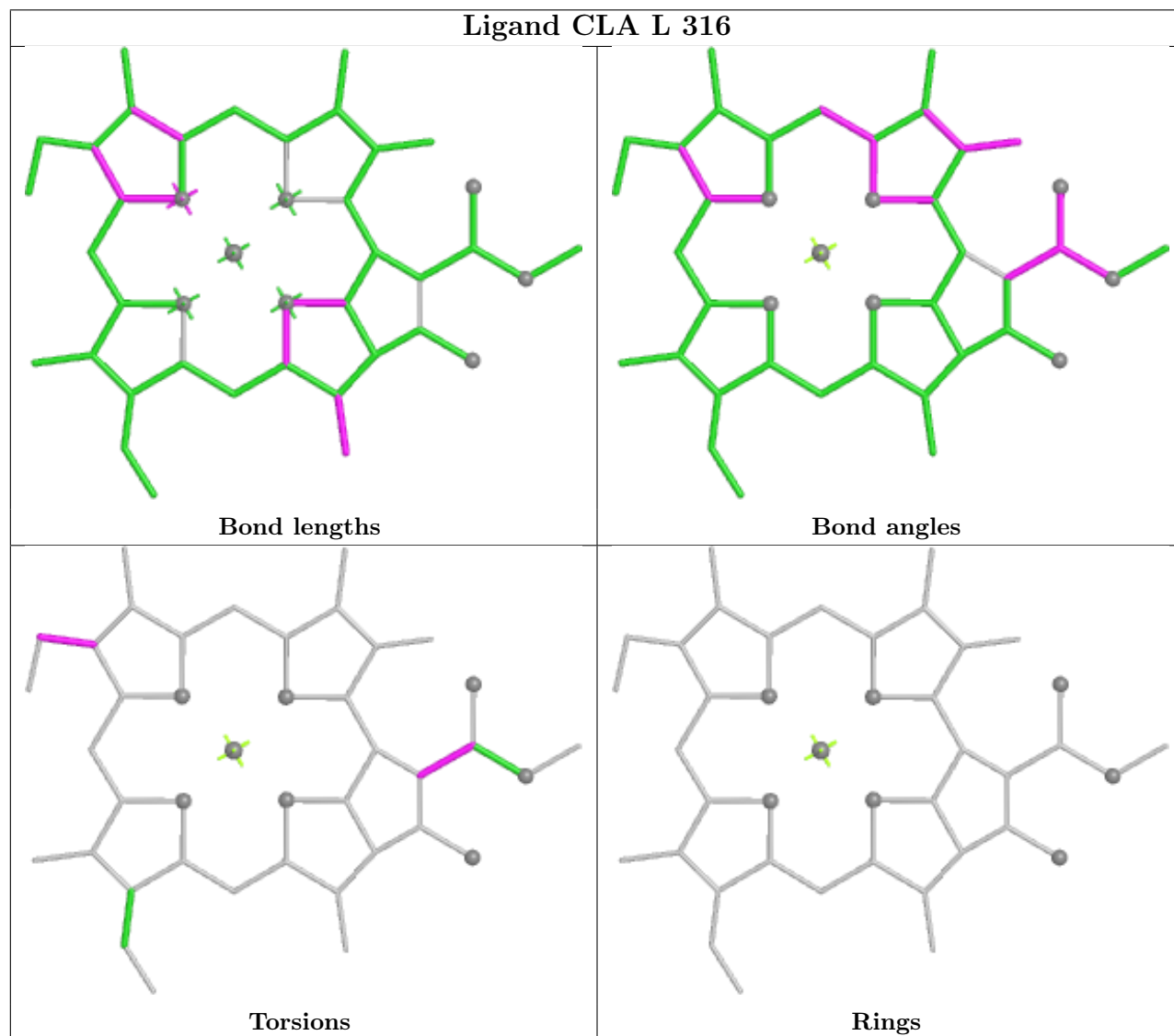
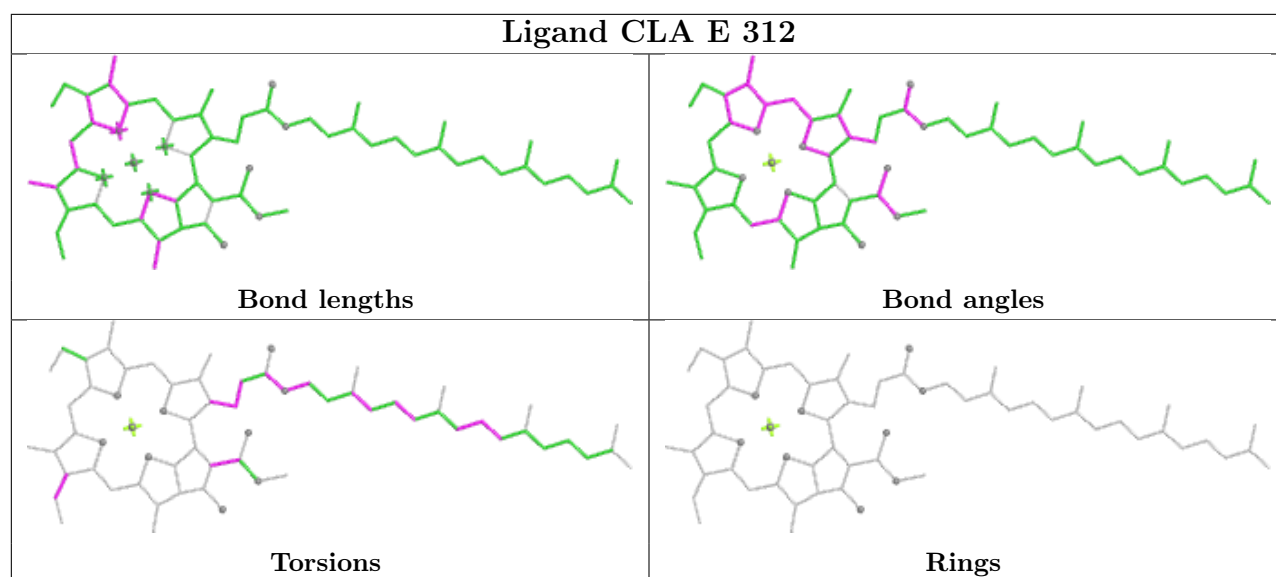


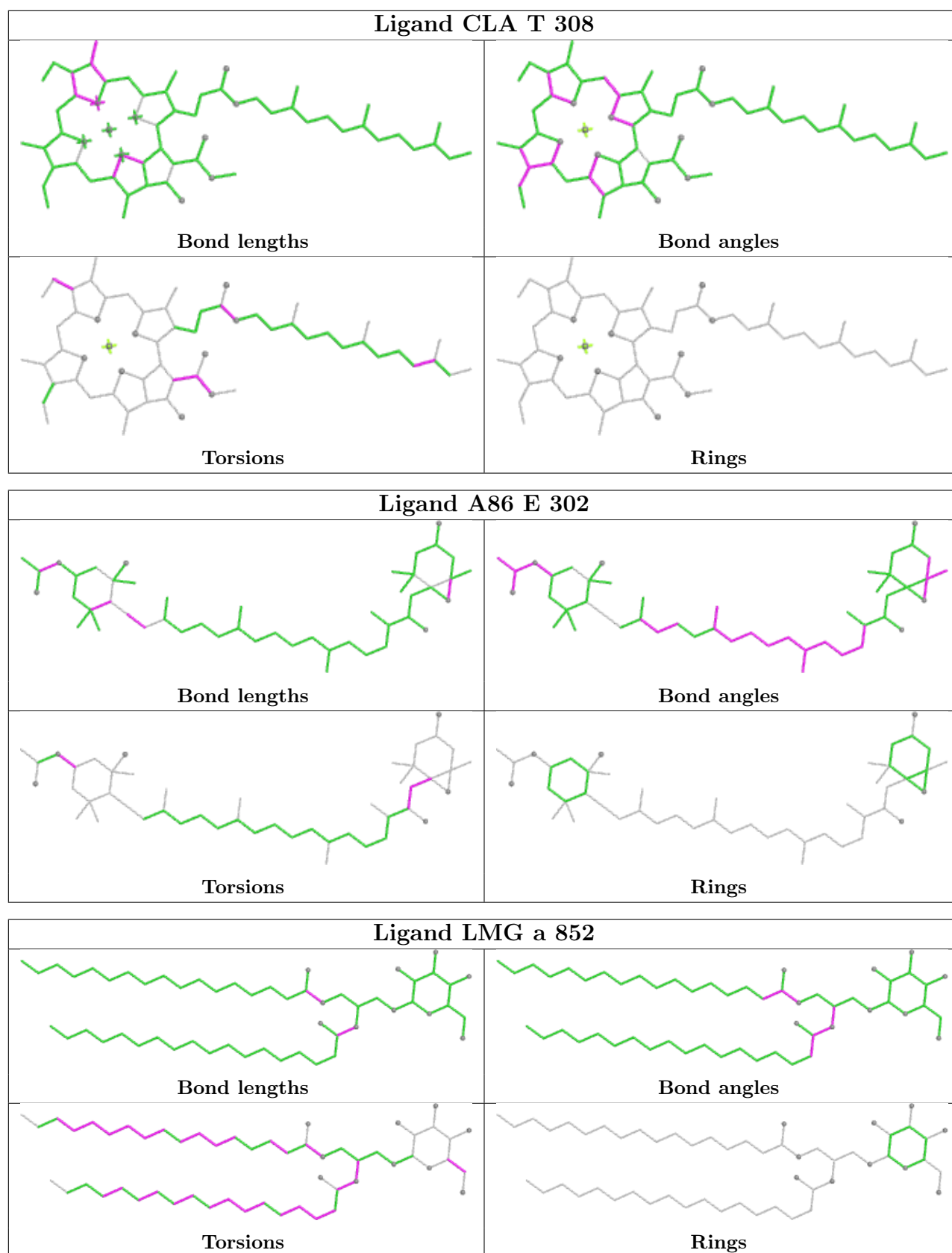




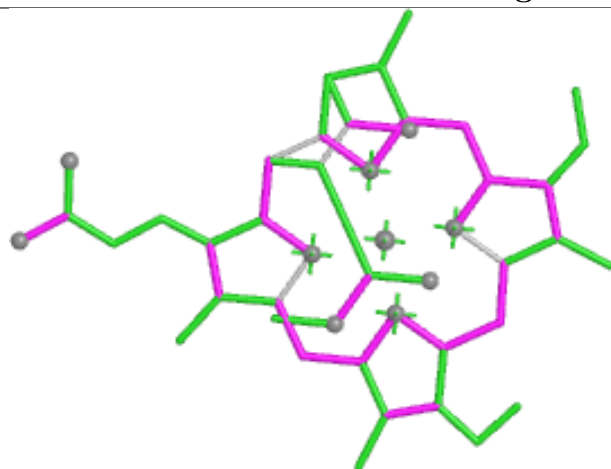




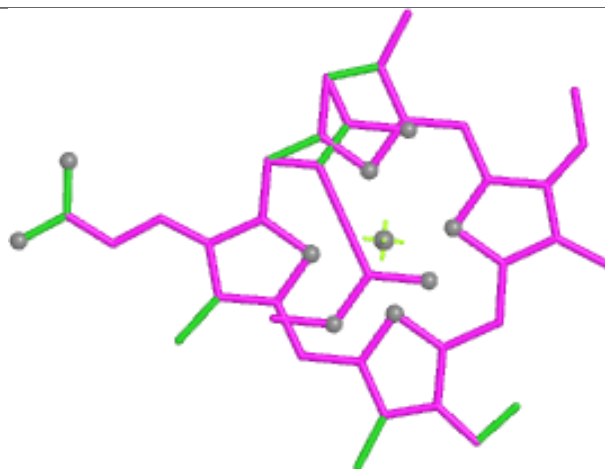




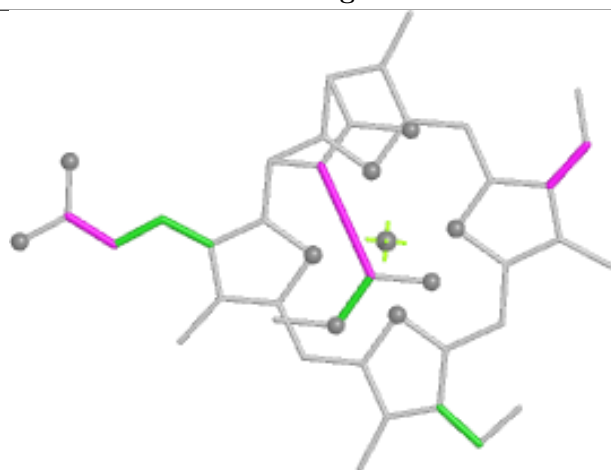
Ligand KC1 G 318



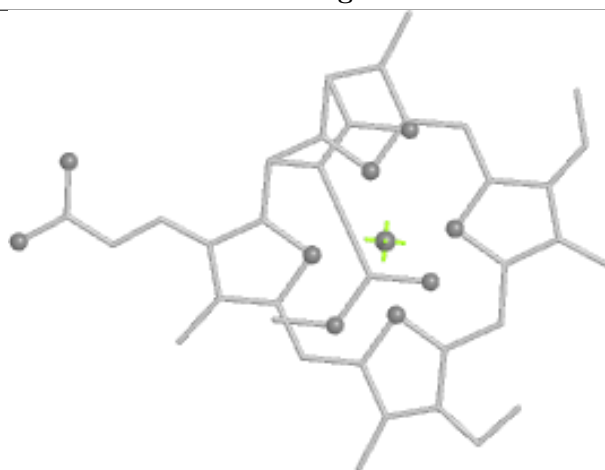
Bond lengths



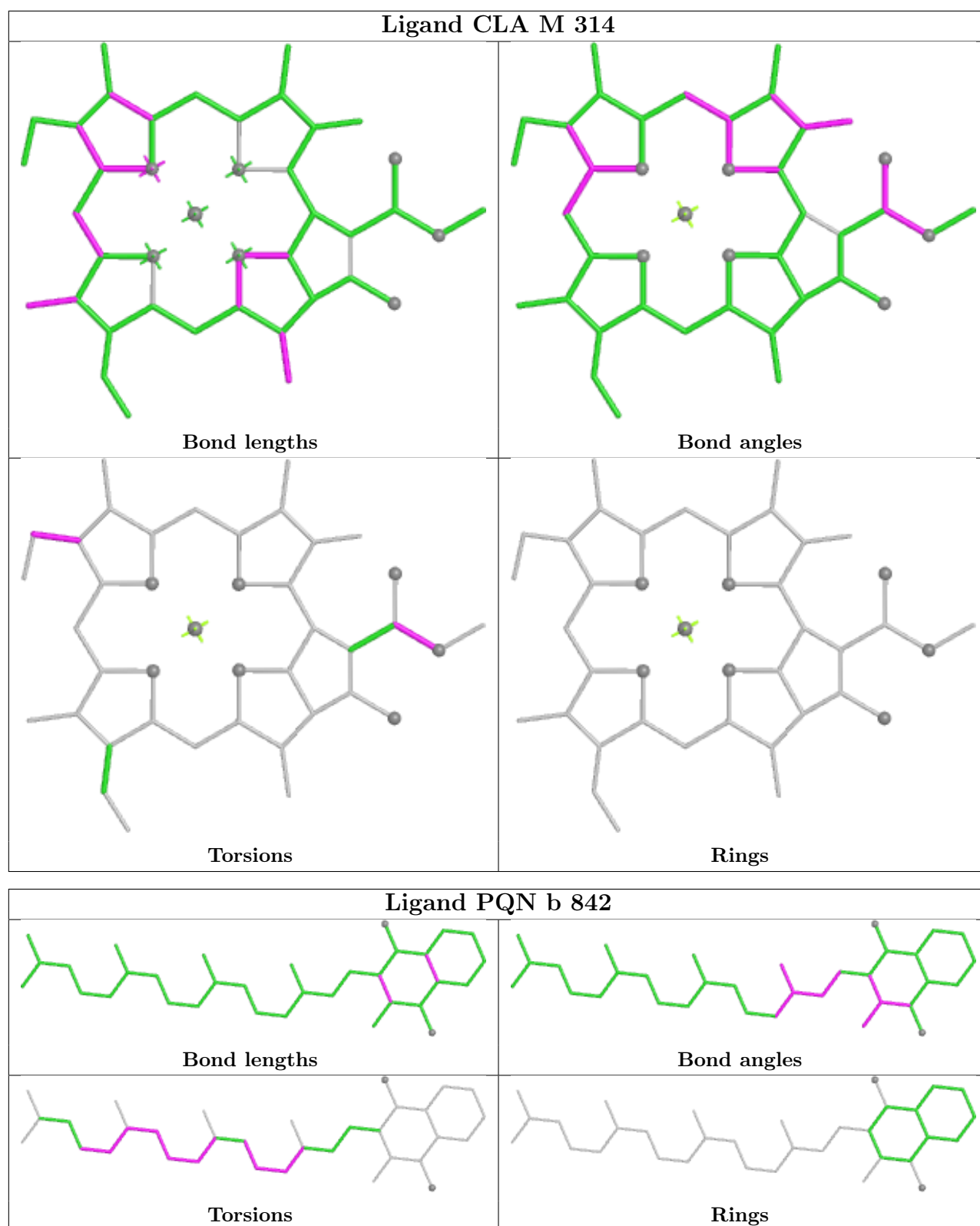
Bond angles



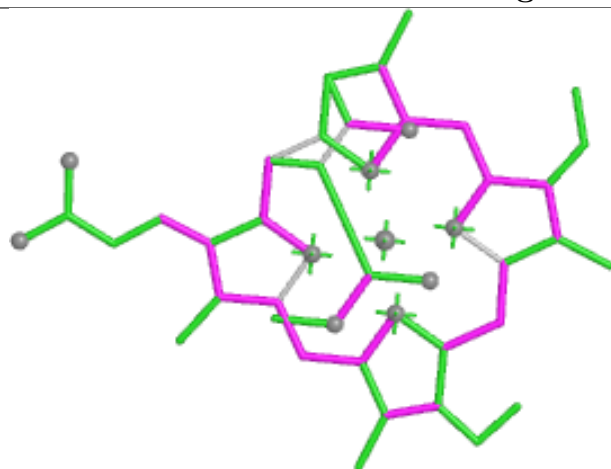
Torsions



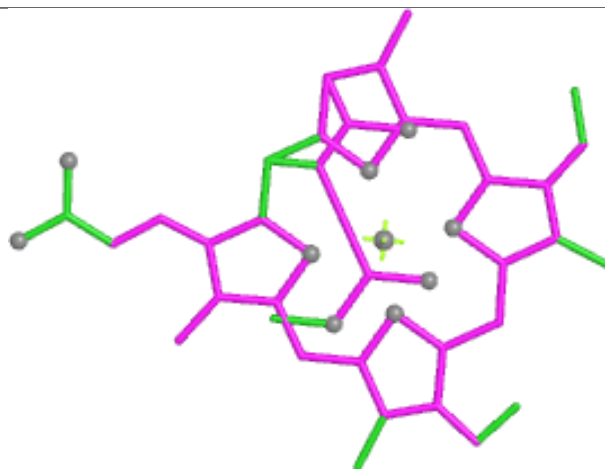
Rings



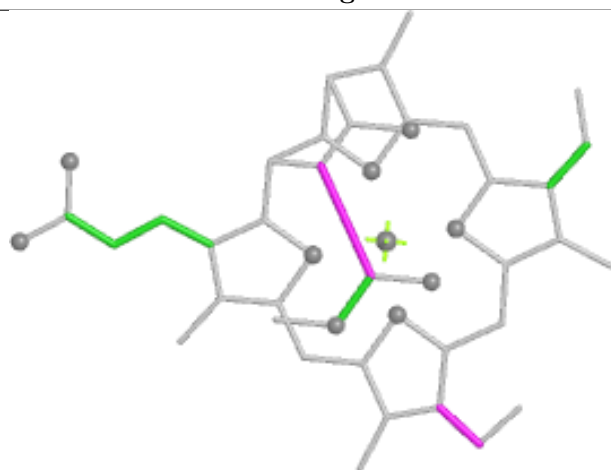
Ligand KC1 P 315



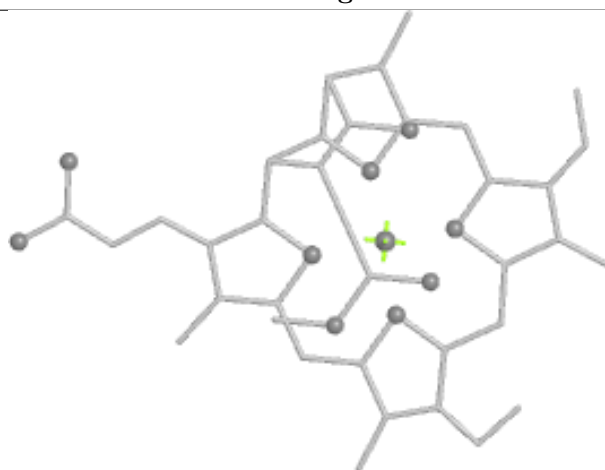
Bond lengths



Bond angles

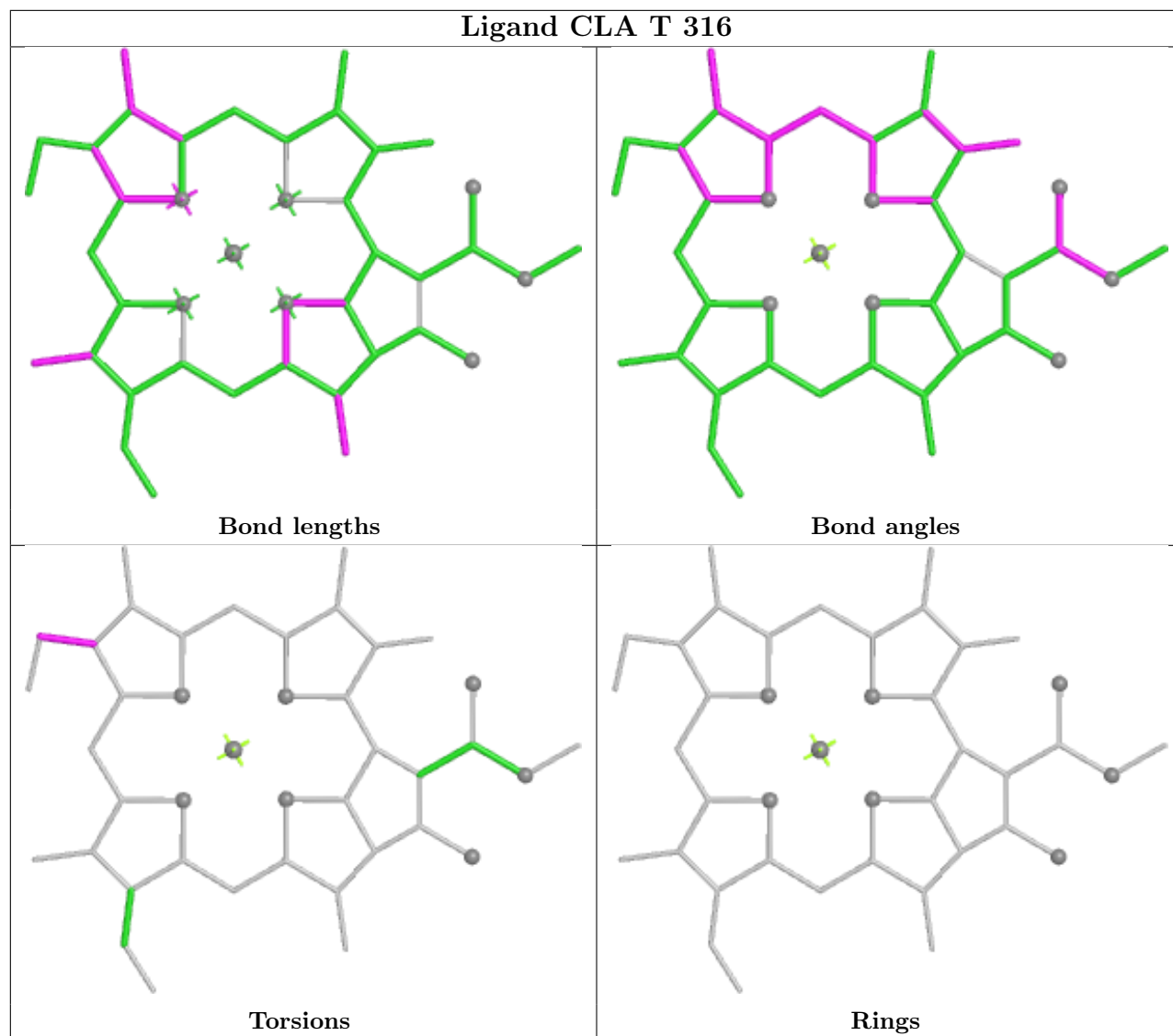


Torsions

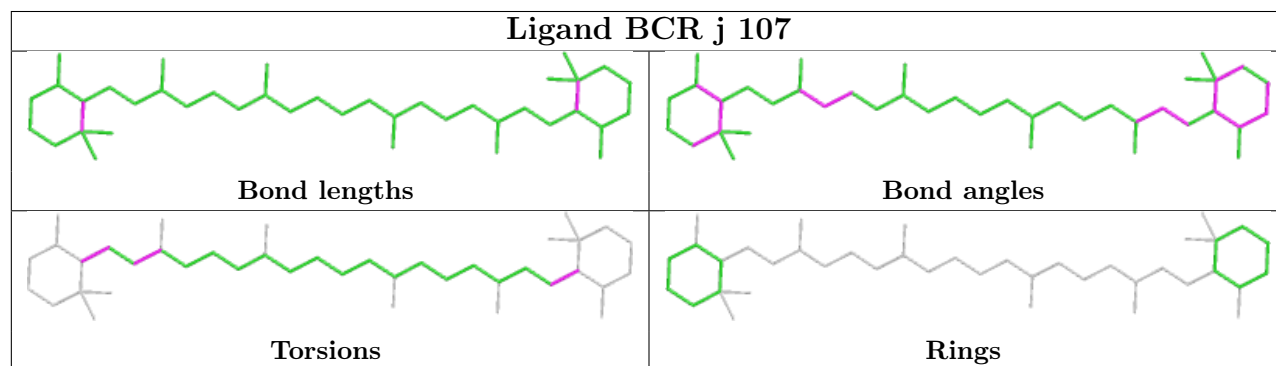


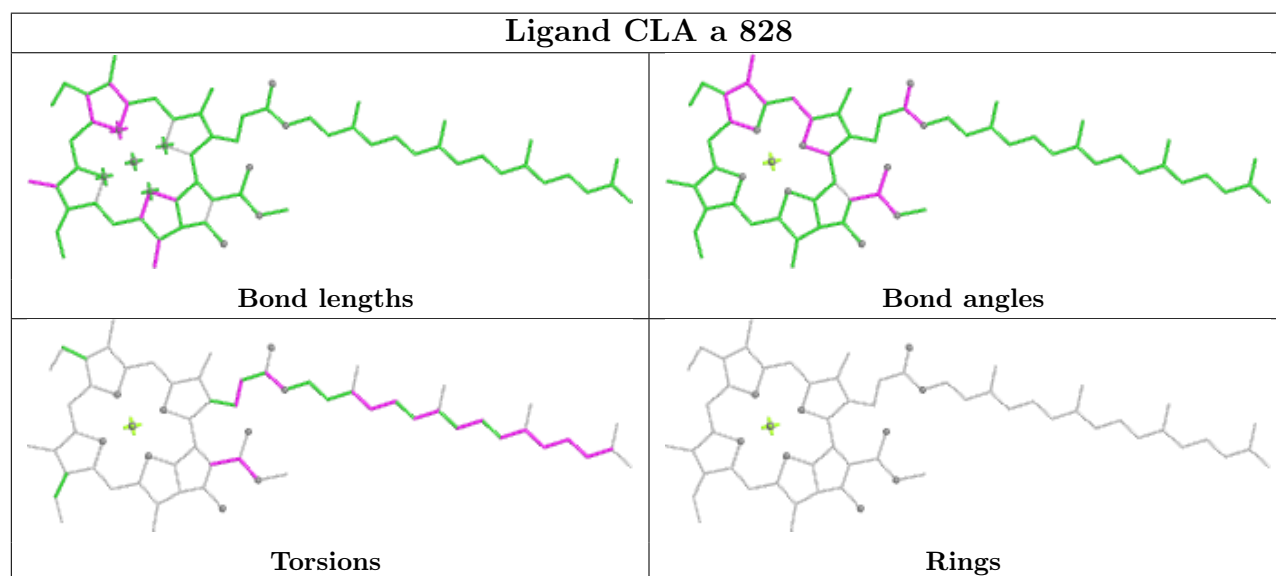
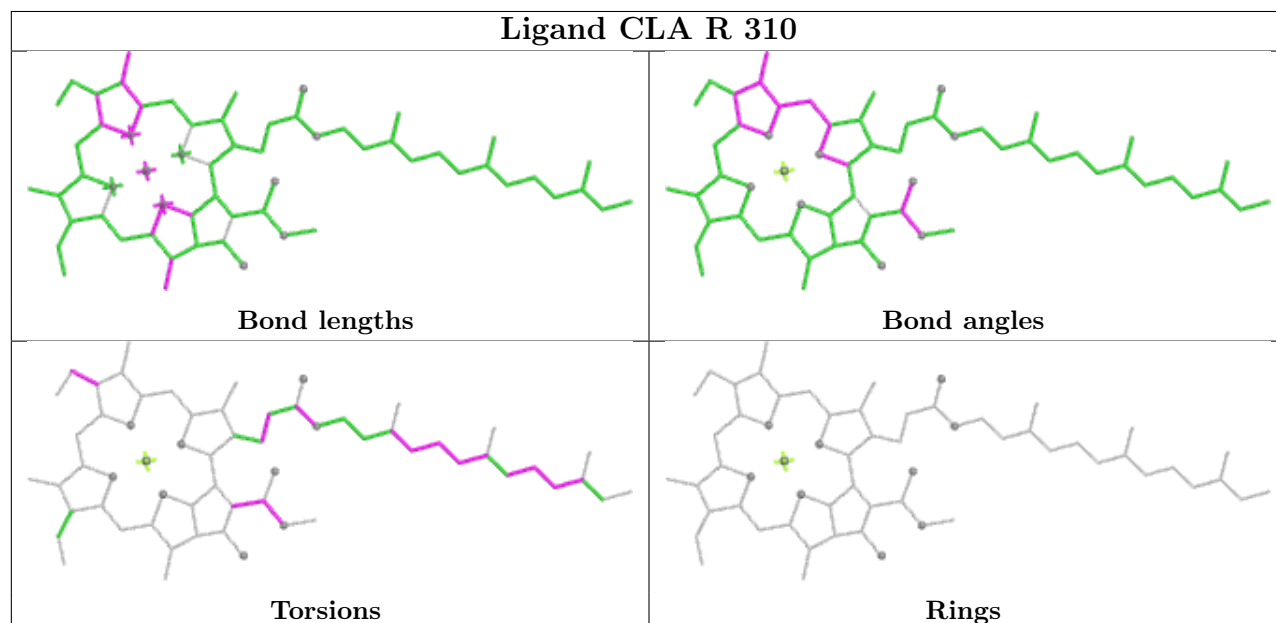
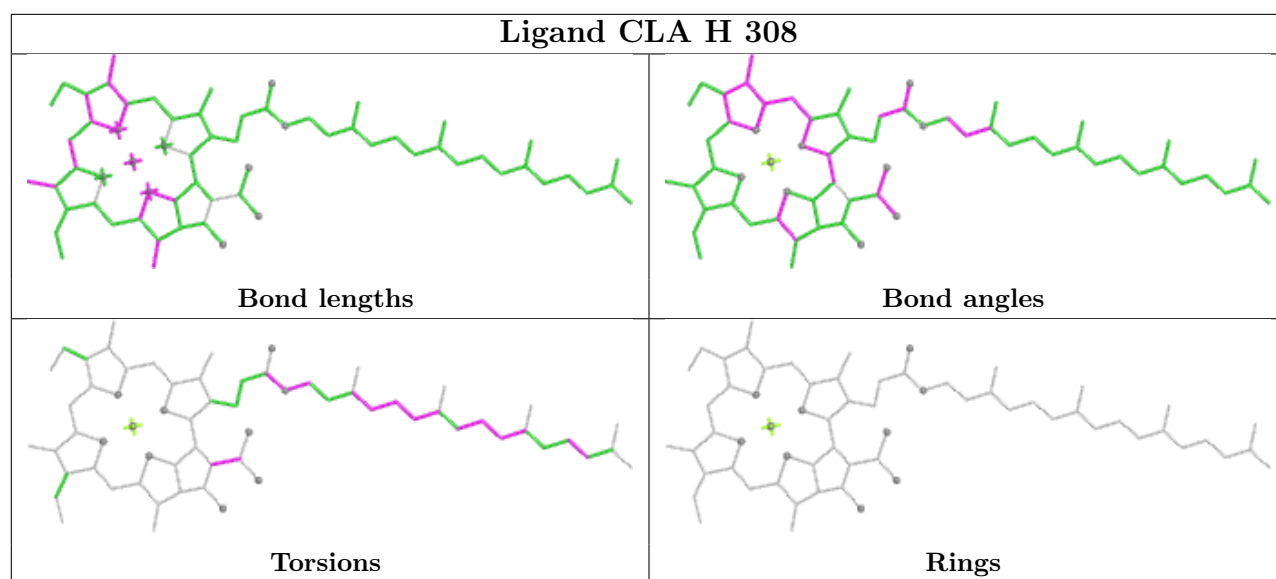
Rings

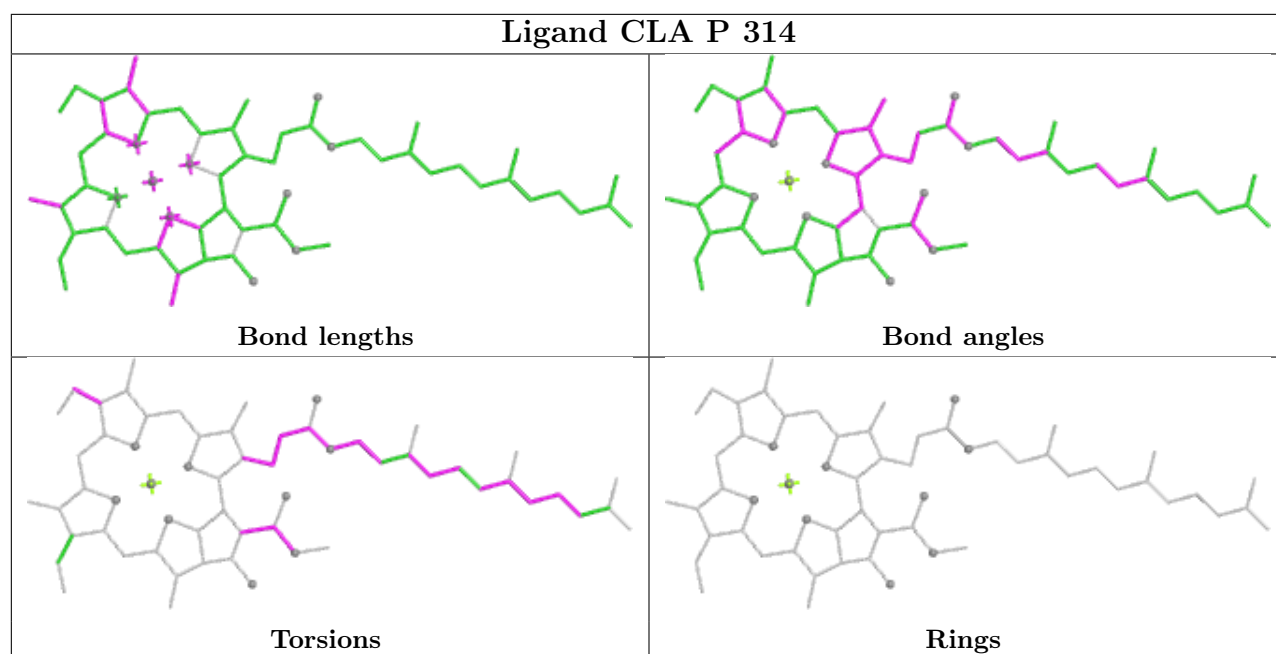
Ligand CLA T 316

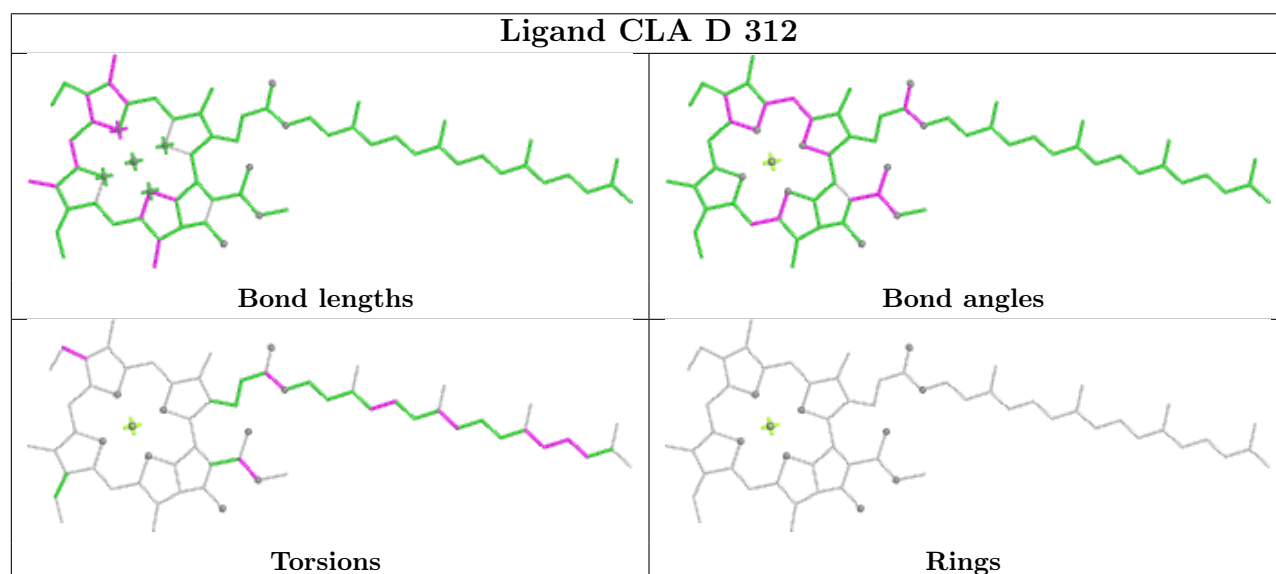
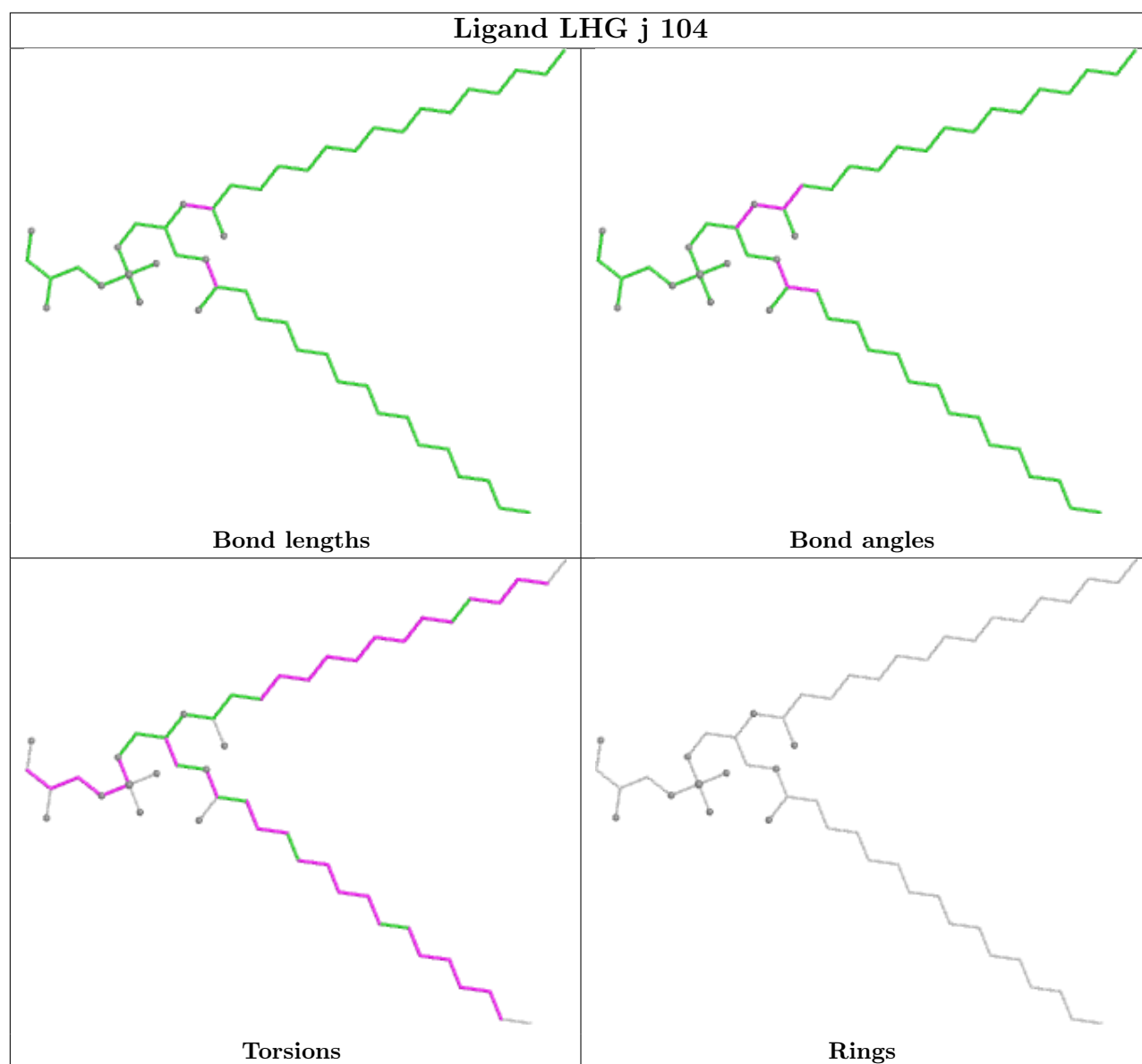


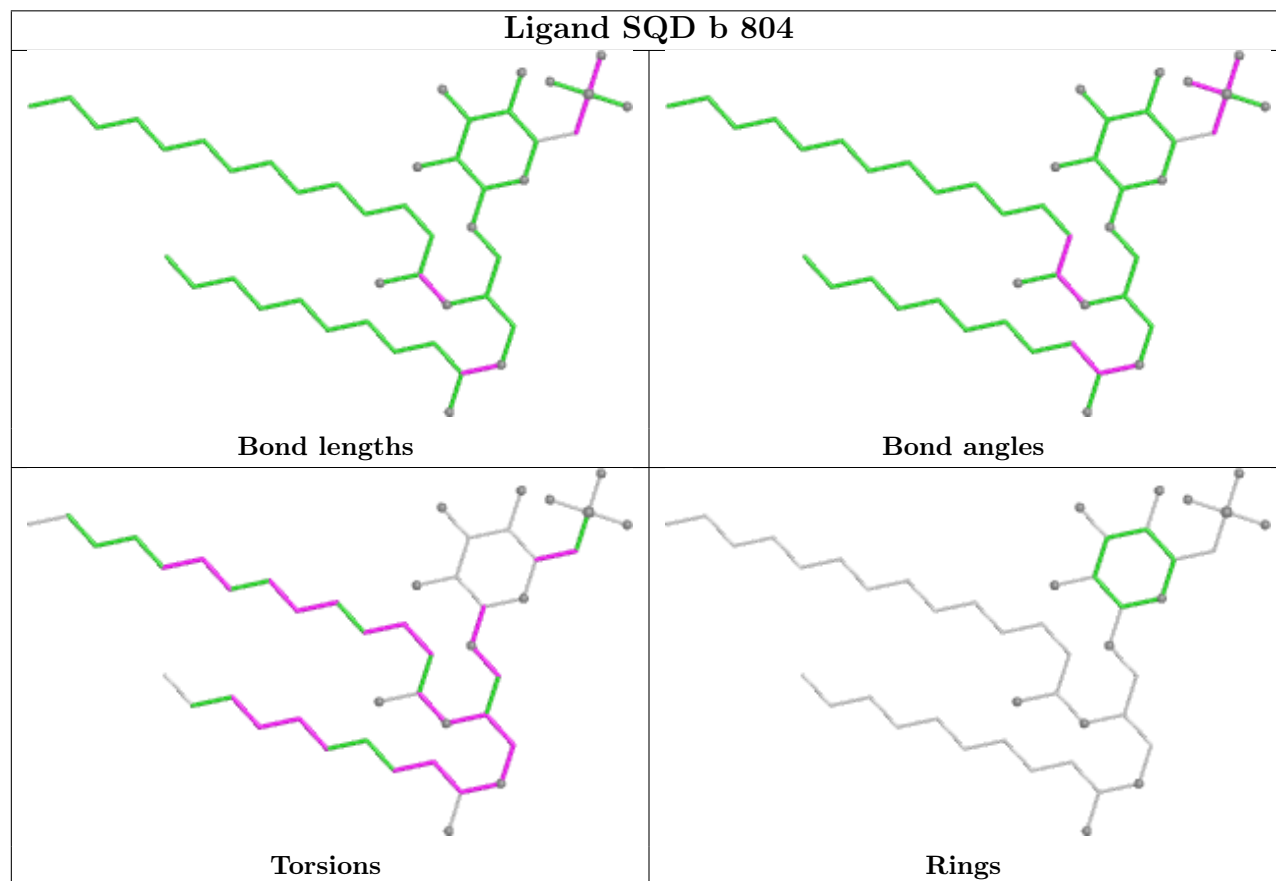
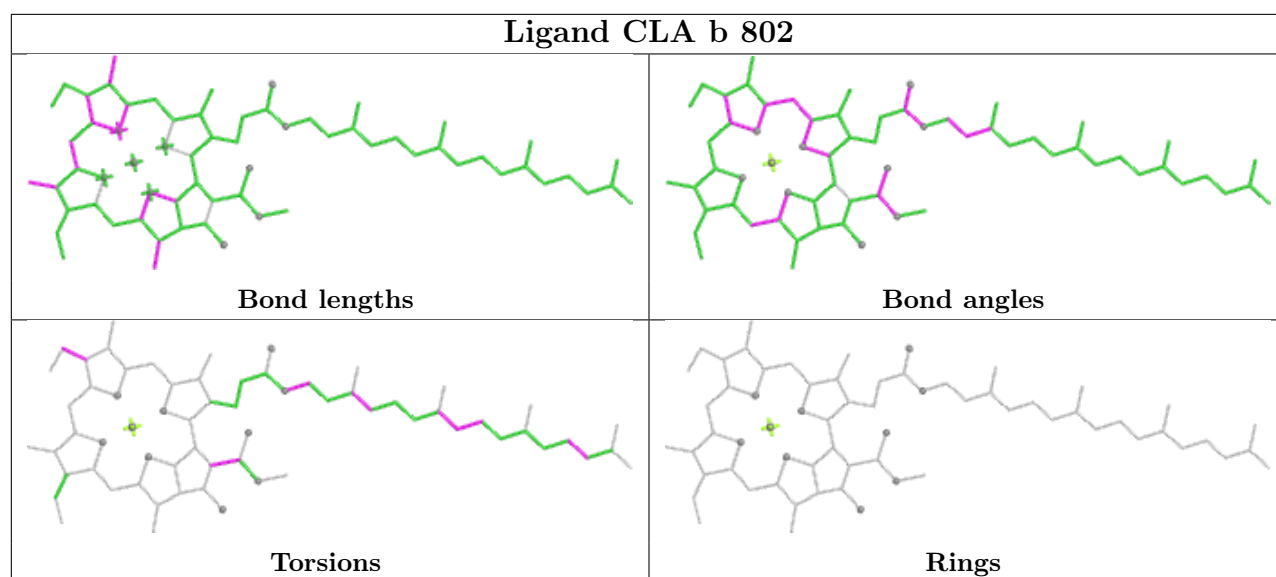
Ligand BCR j 107

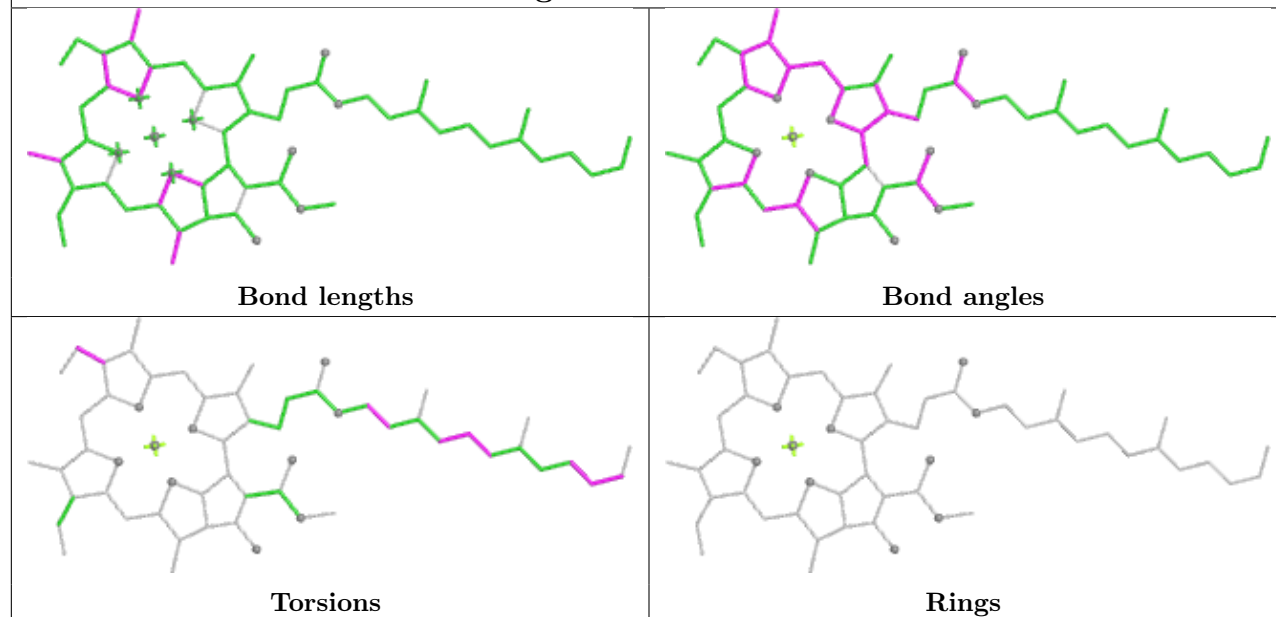
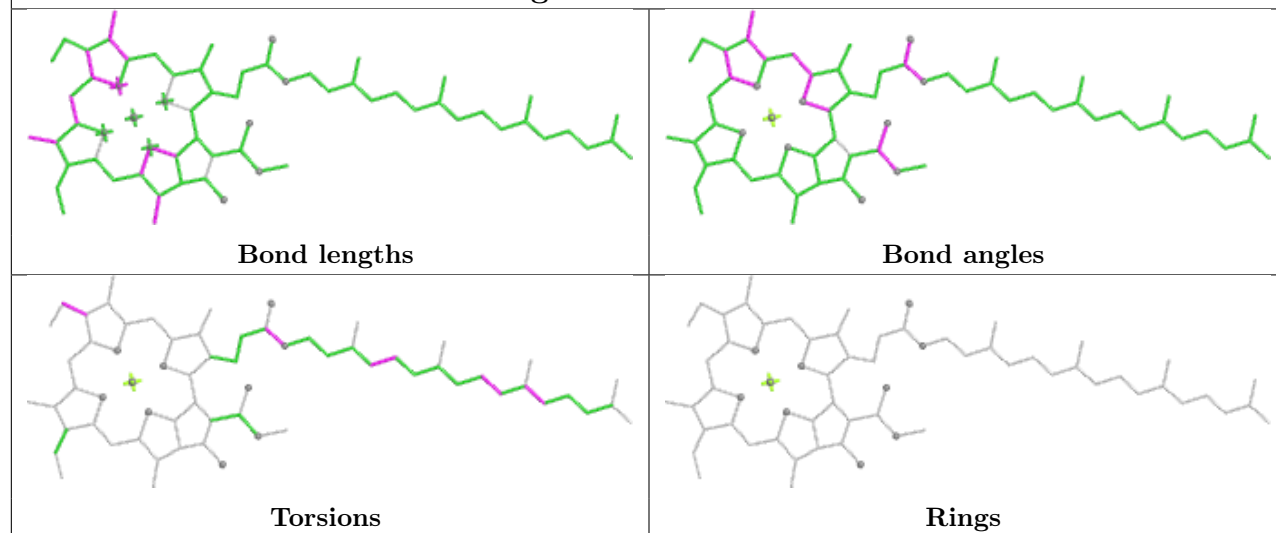


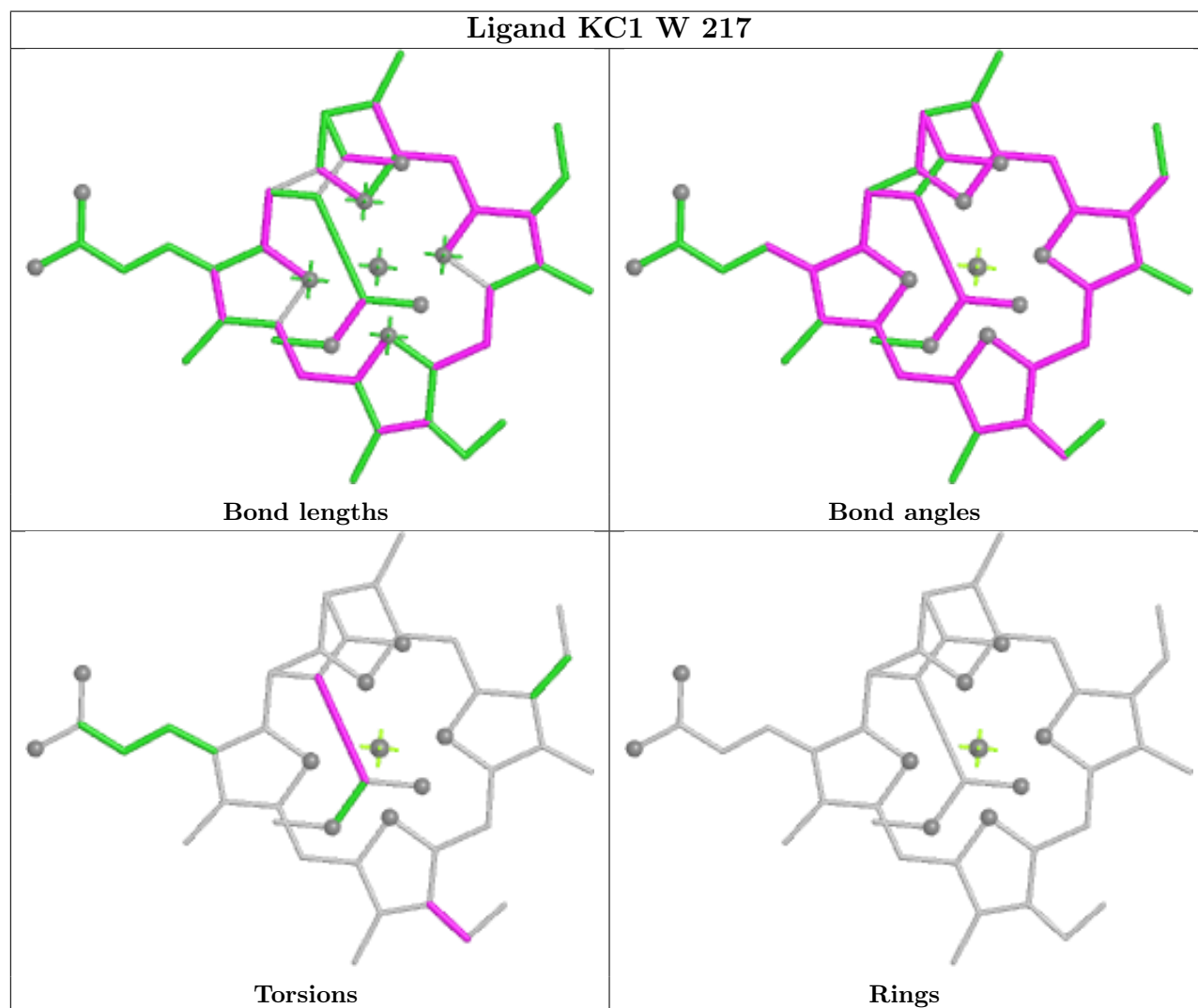
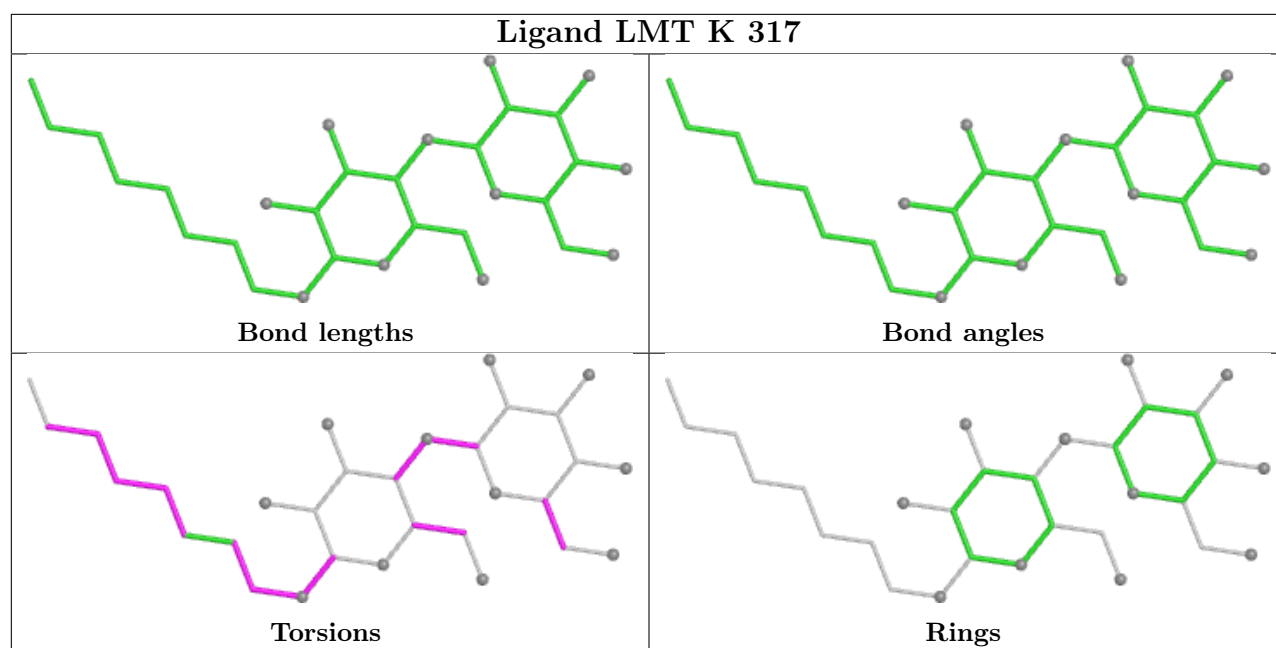


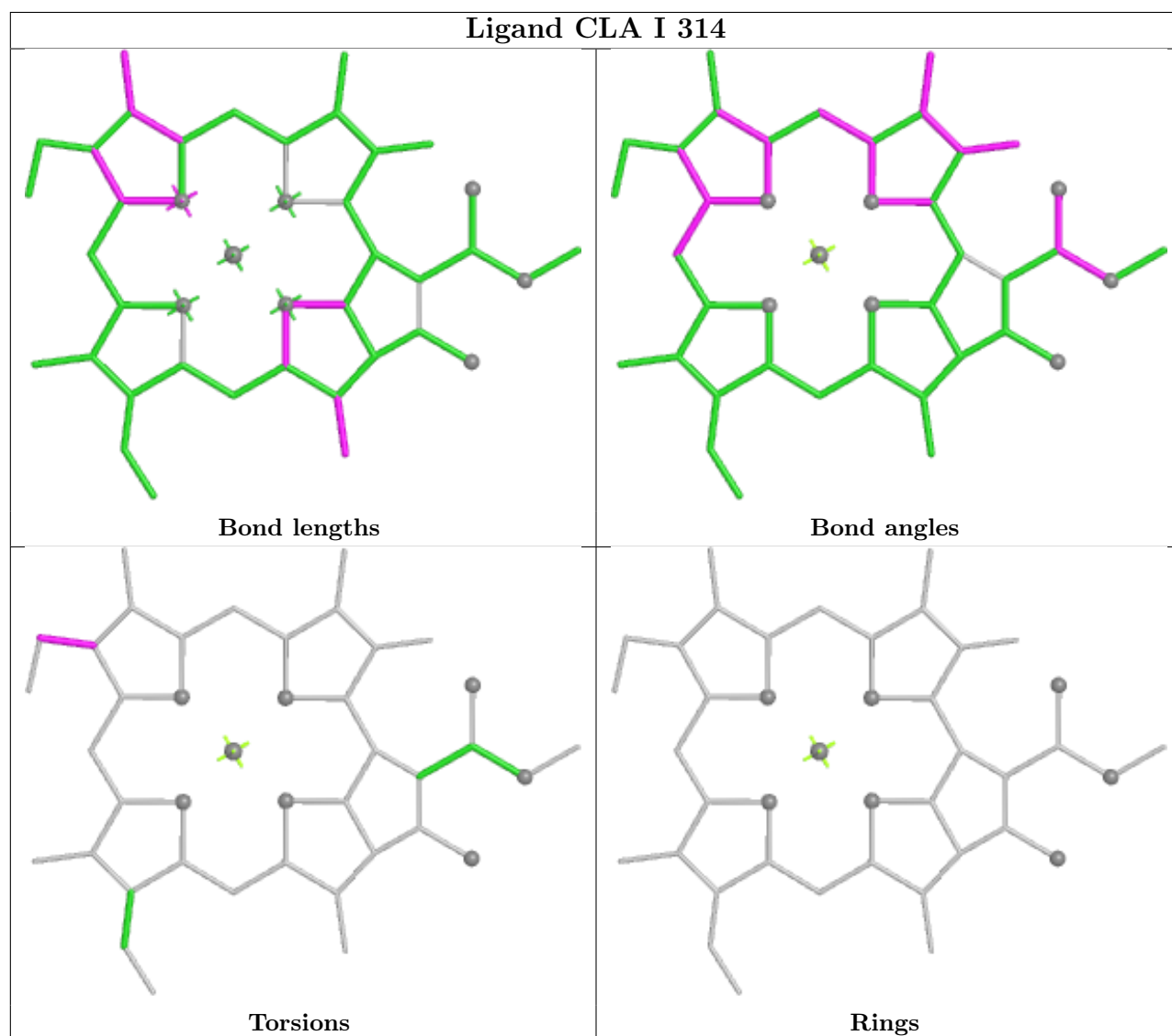
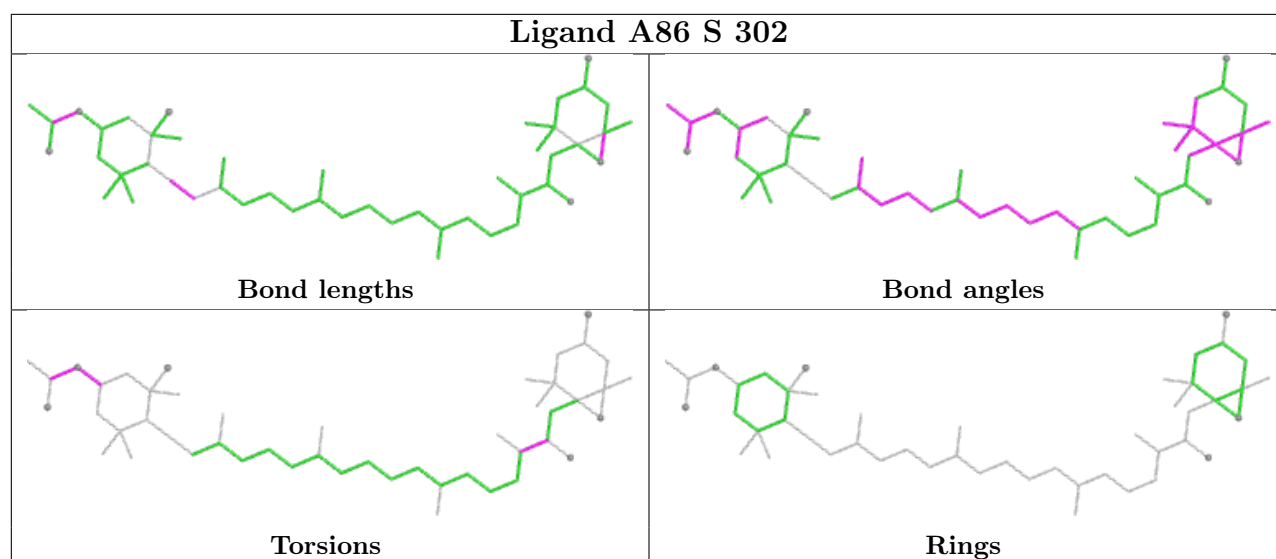


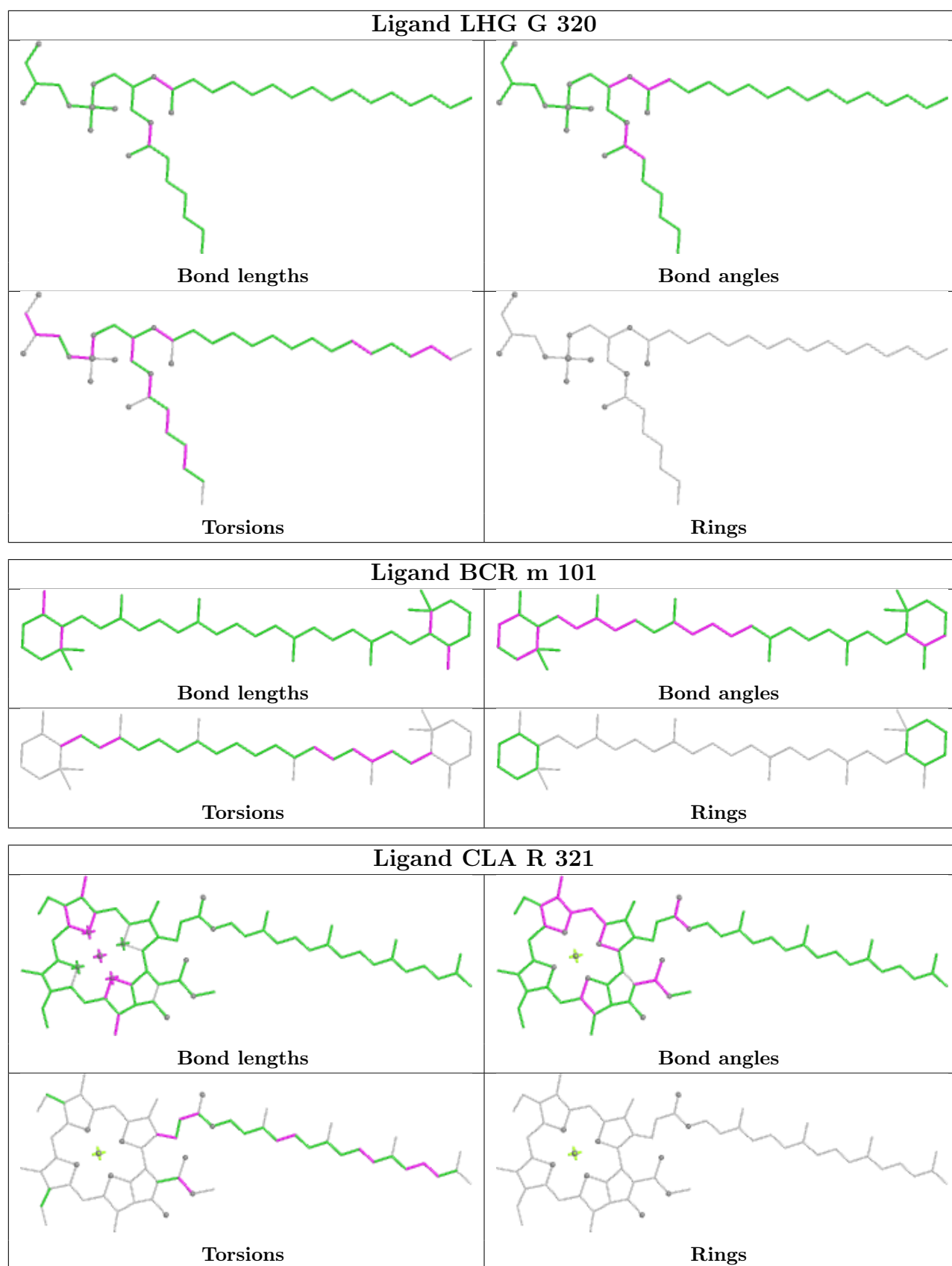


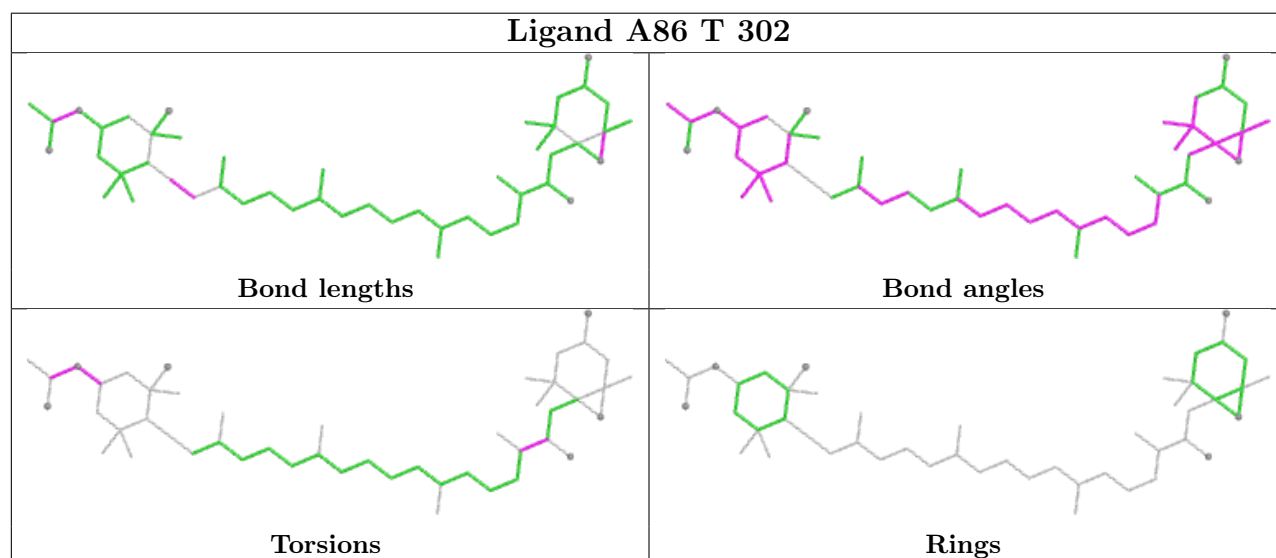
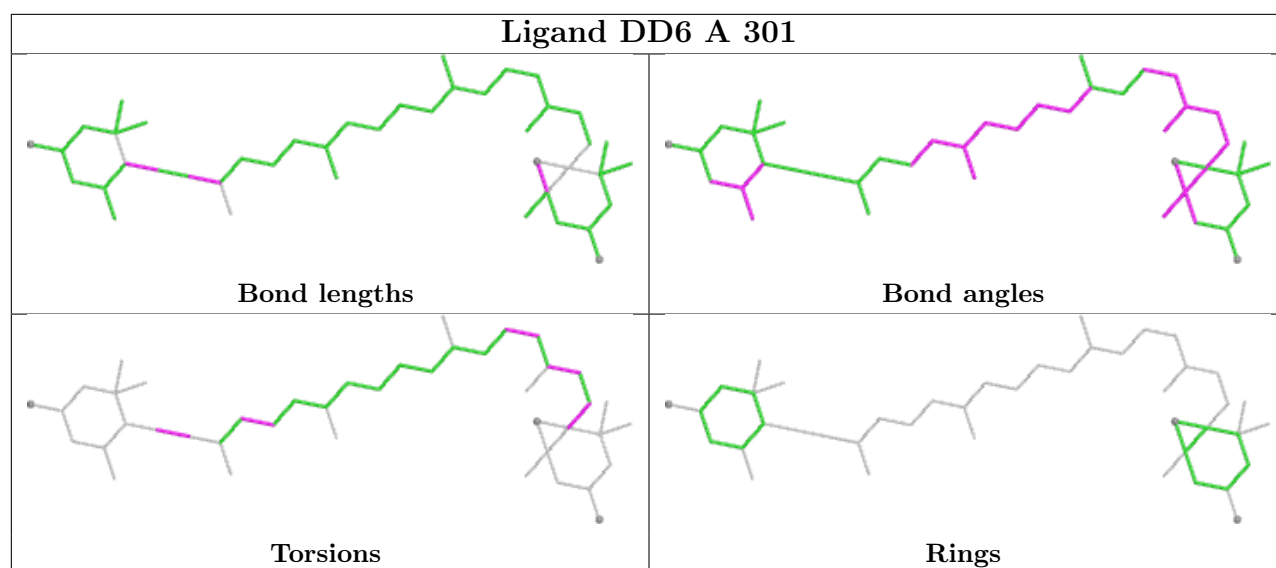


Ligand CLA b 819**Ligand CLA K 312**

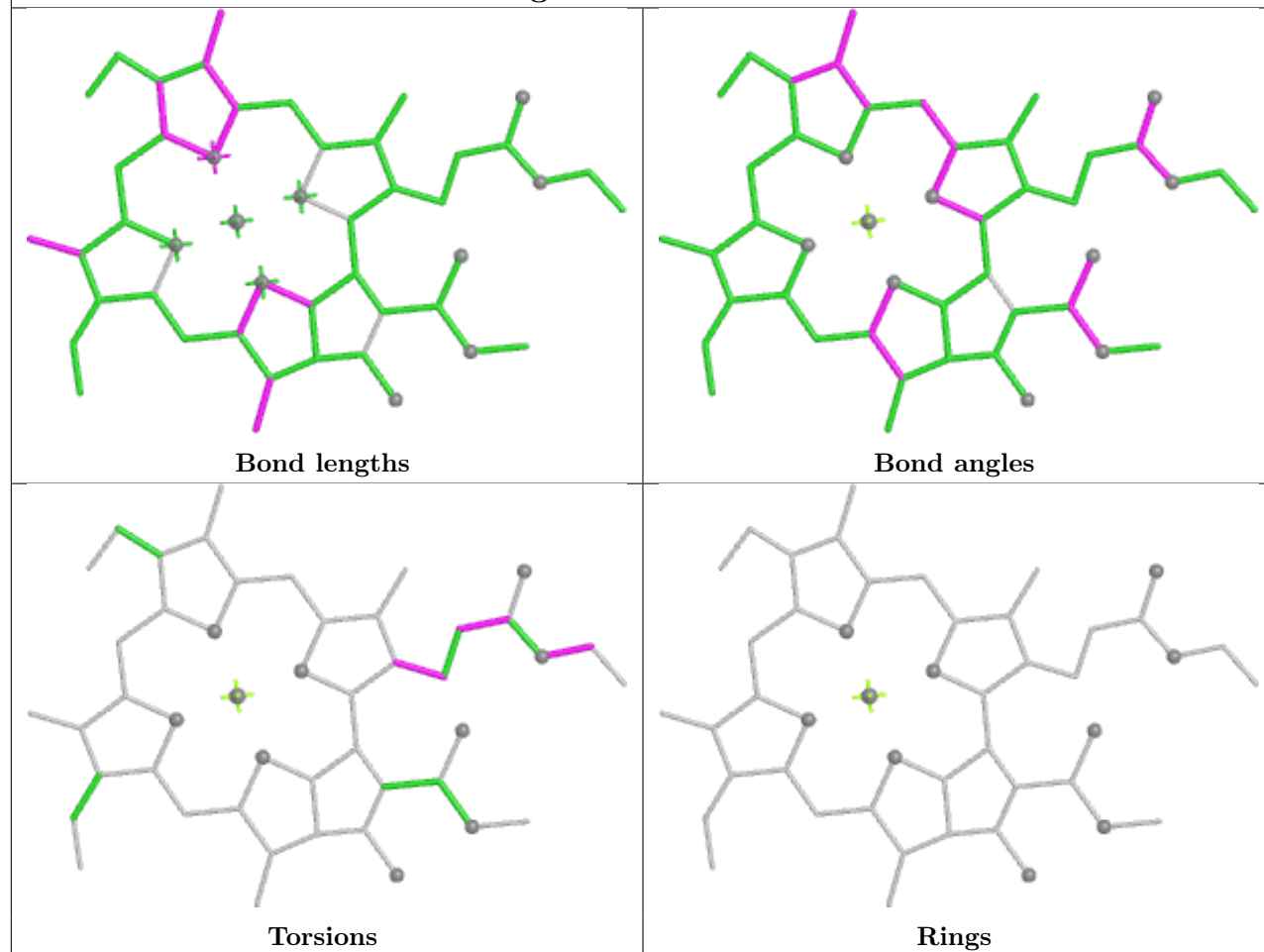




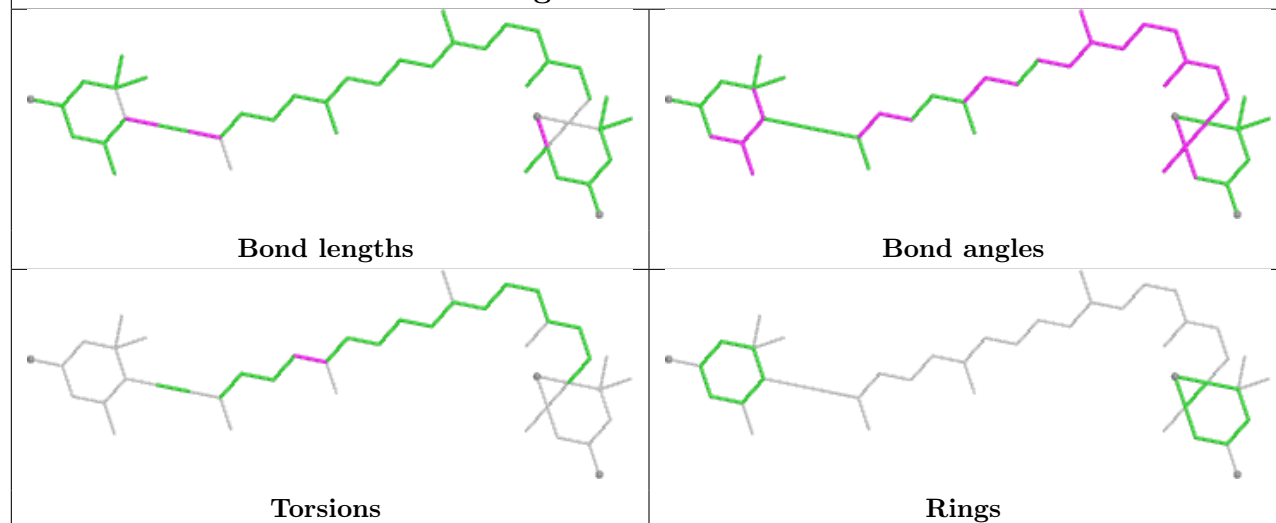




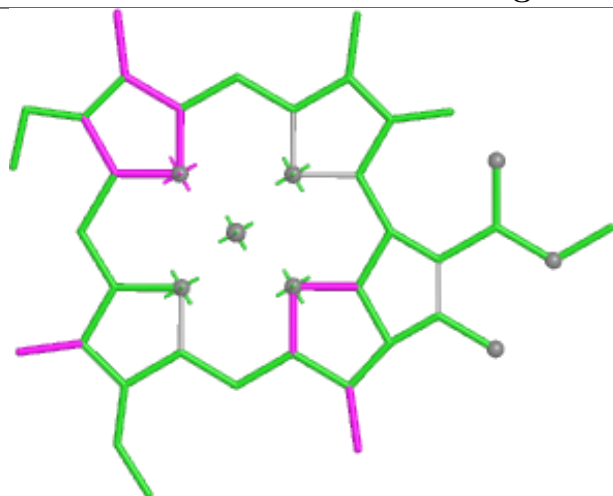
Ligand CLA b 838



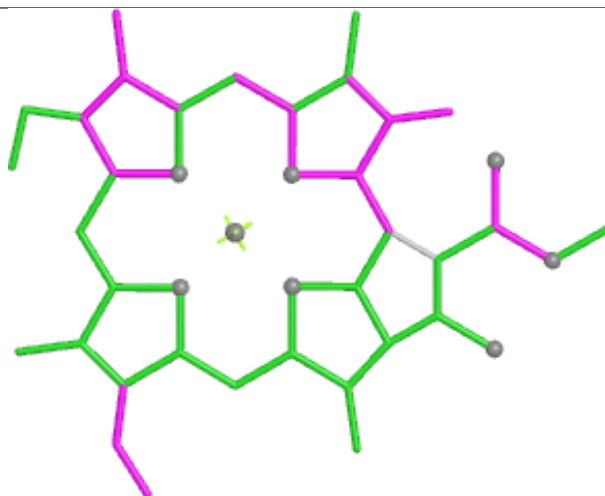
Ligand DD6 P 305



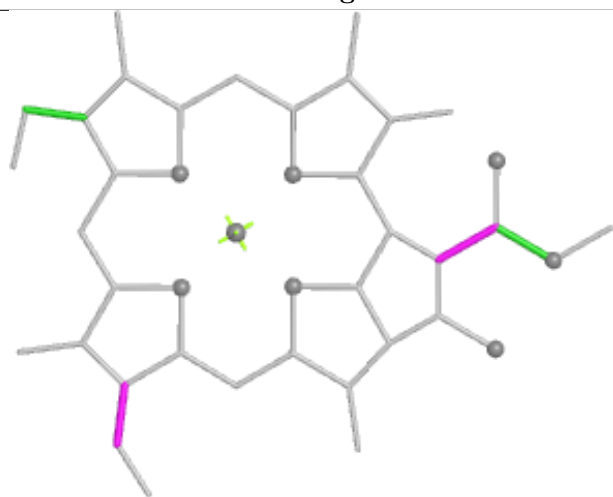
Ligand CLA D 315



Bond lengths



Bond angles

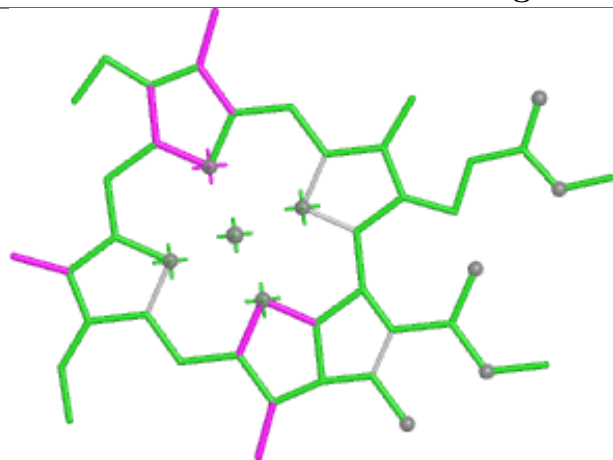


Torsions

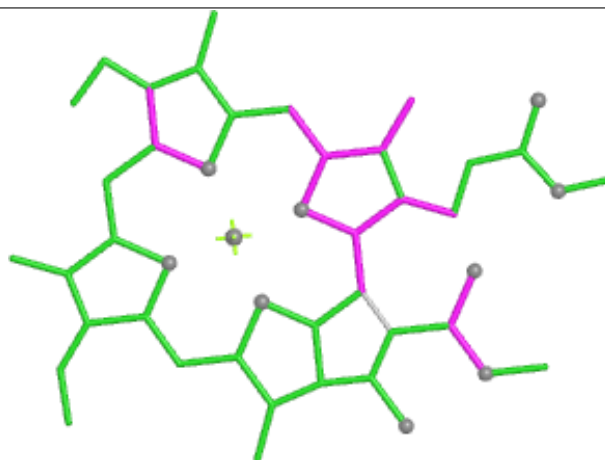


Rings

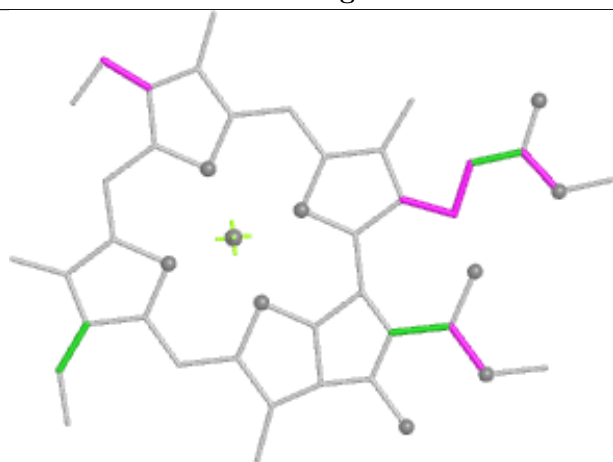
Ligand CLA K 311



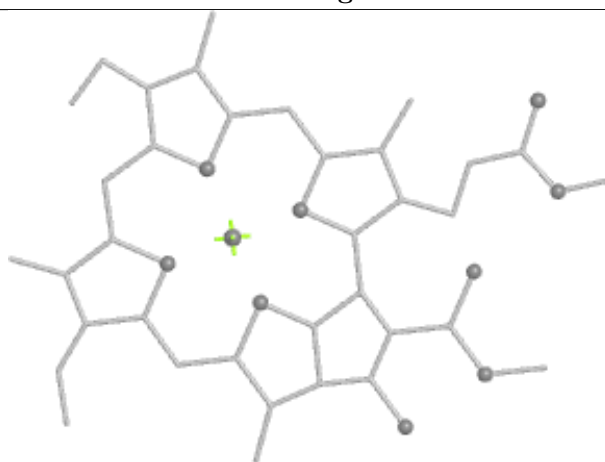
Bond lengths



Bond angles

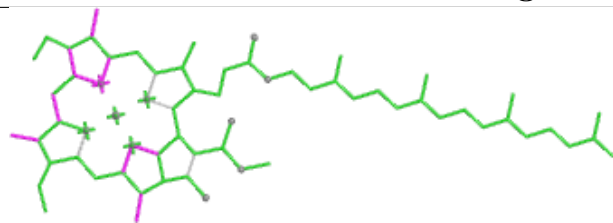


Torsions

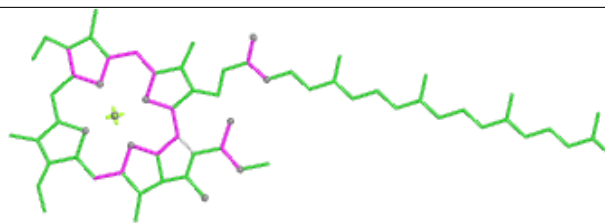


Rings

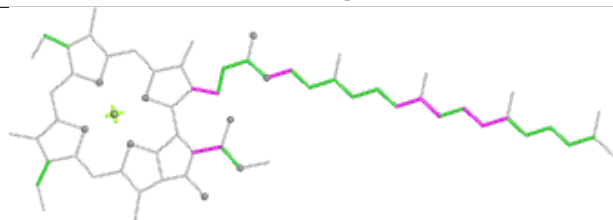
Ligand CLA b 827



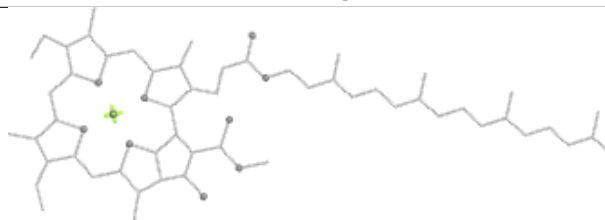
Bond lengths



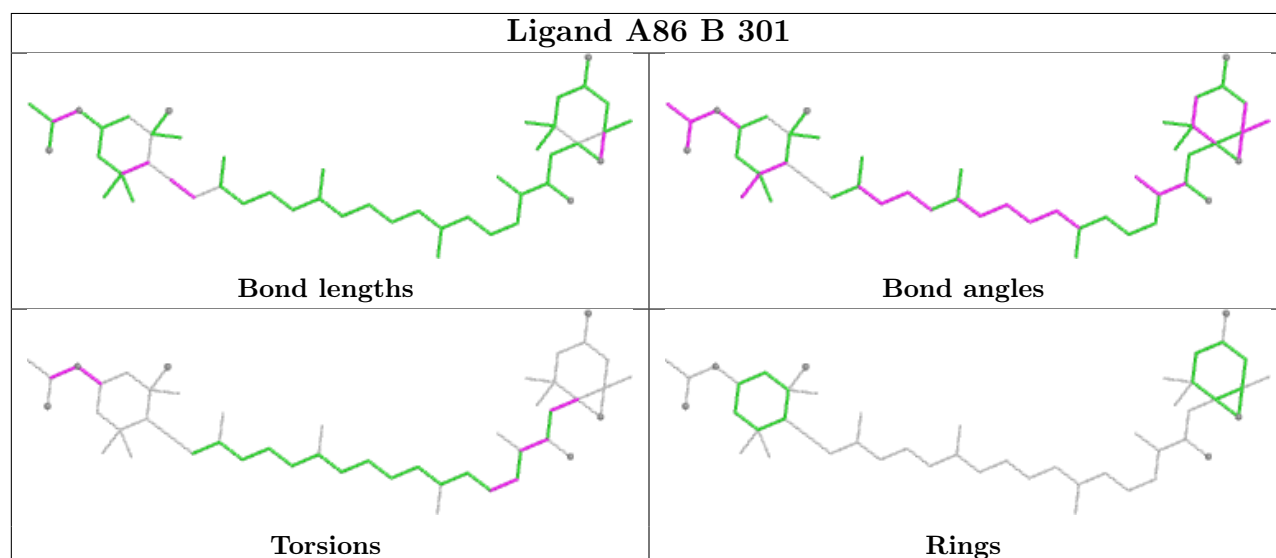
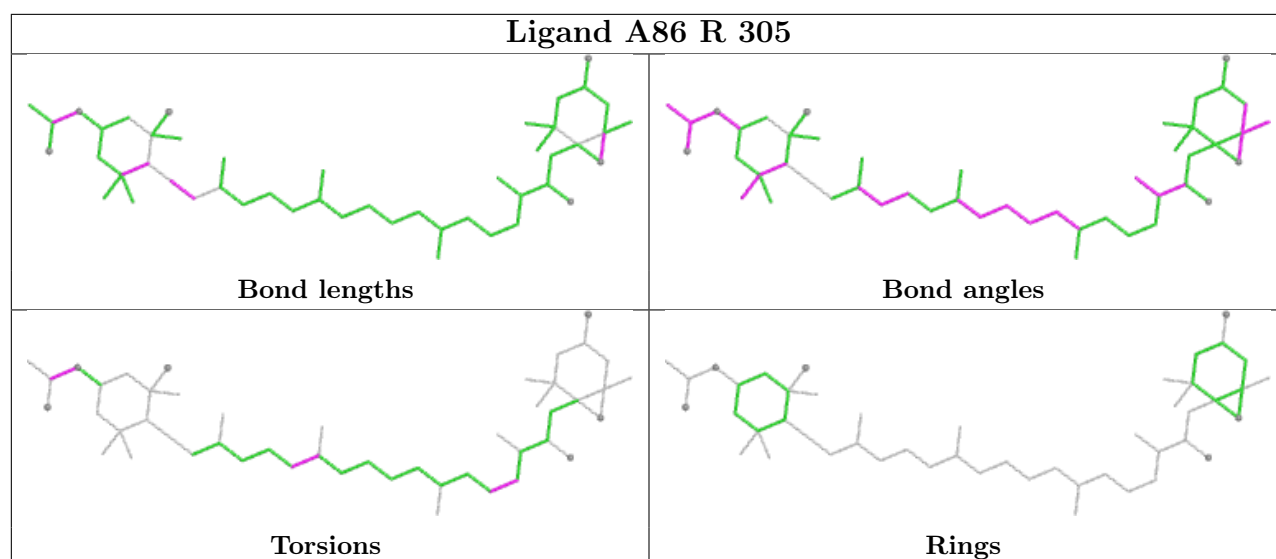
Bond angles



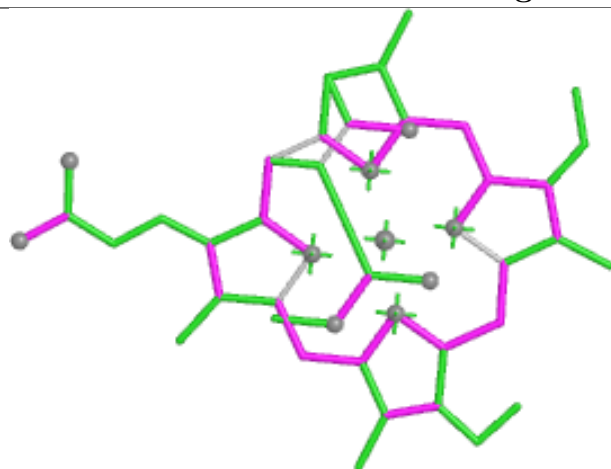
Torsions



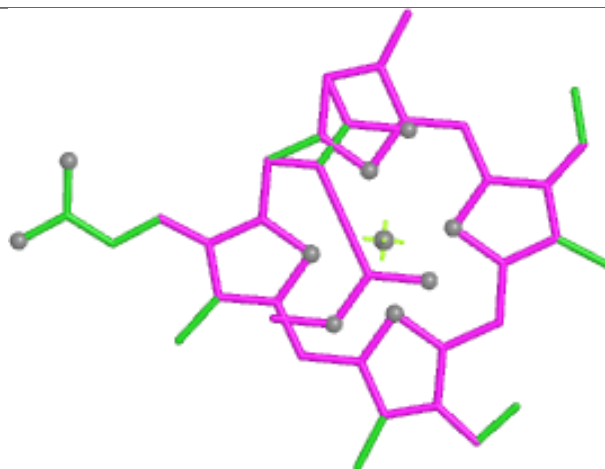
Rings



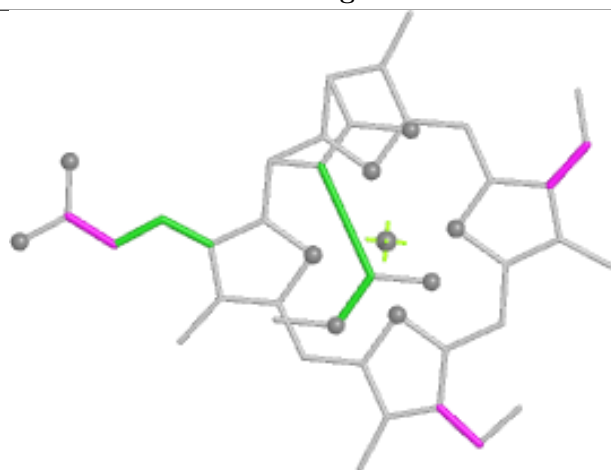
Ligand KC1 G 308



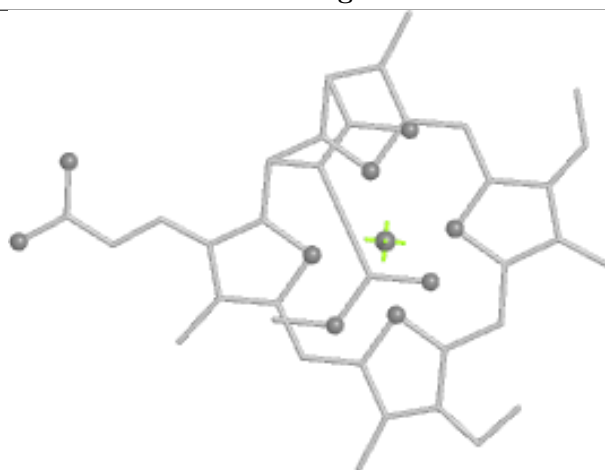
Bond lengths



Bond angles

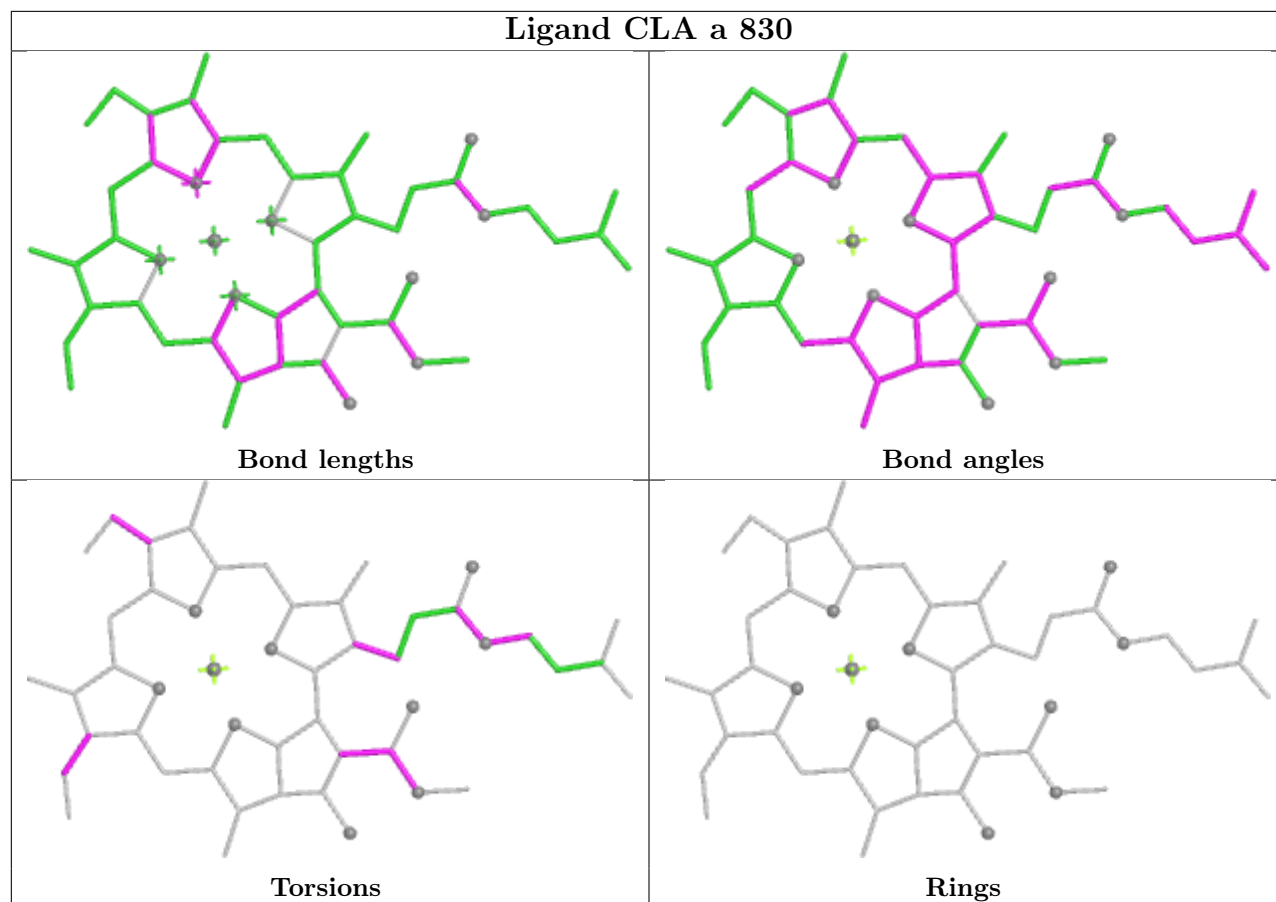


Torsions

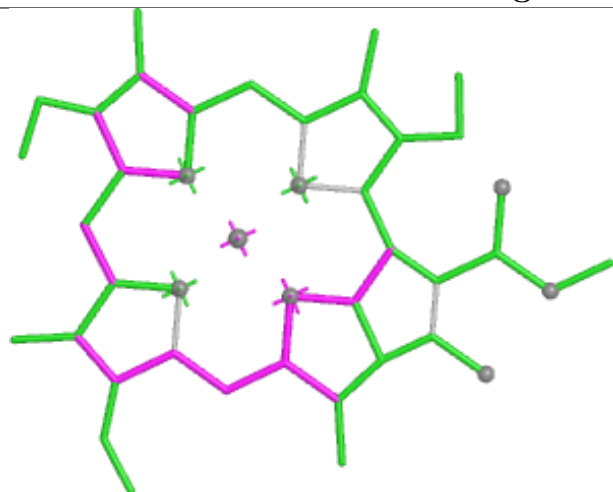


Rings

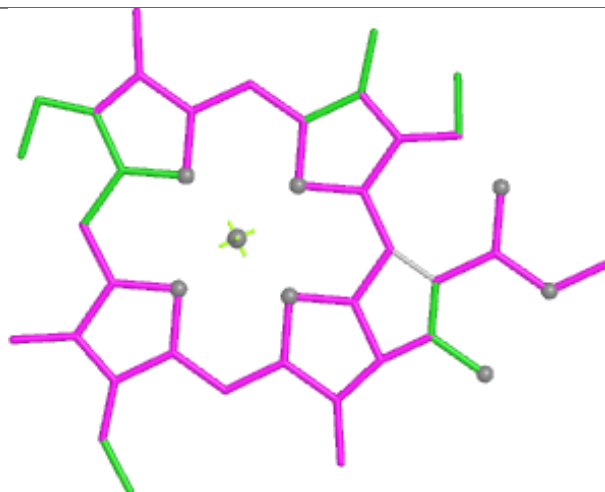
Ligand CLA a 830



Ligand CLA N 319



Bond lengths



Bond angles

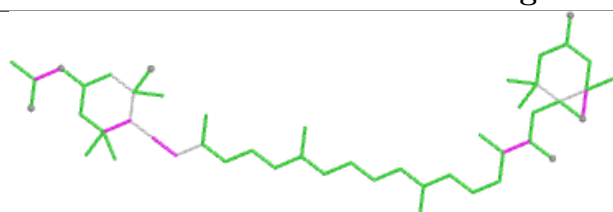


Torsions

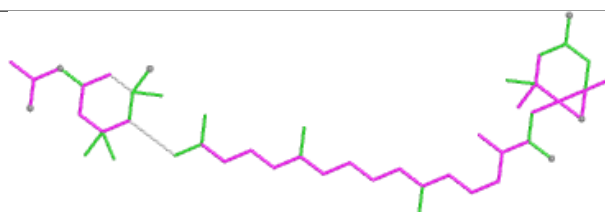


Rings

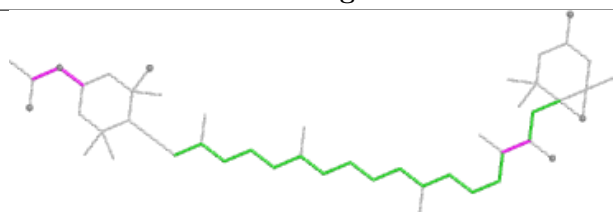
Ligand A86 O 303



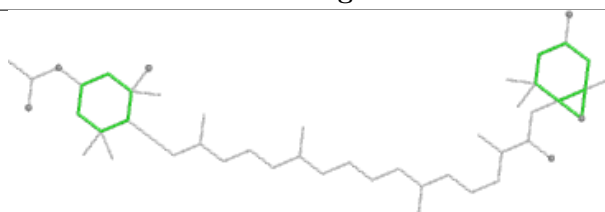
Bond lengths



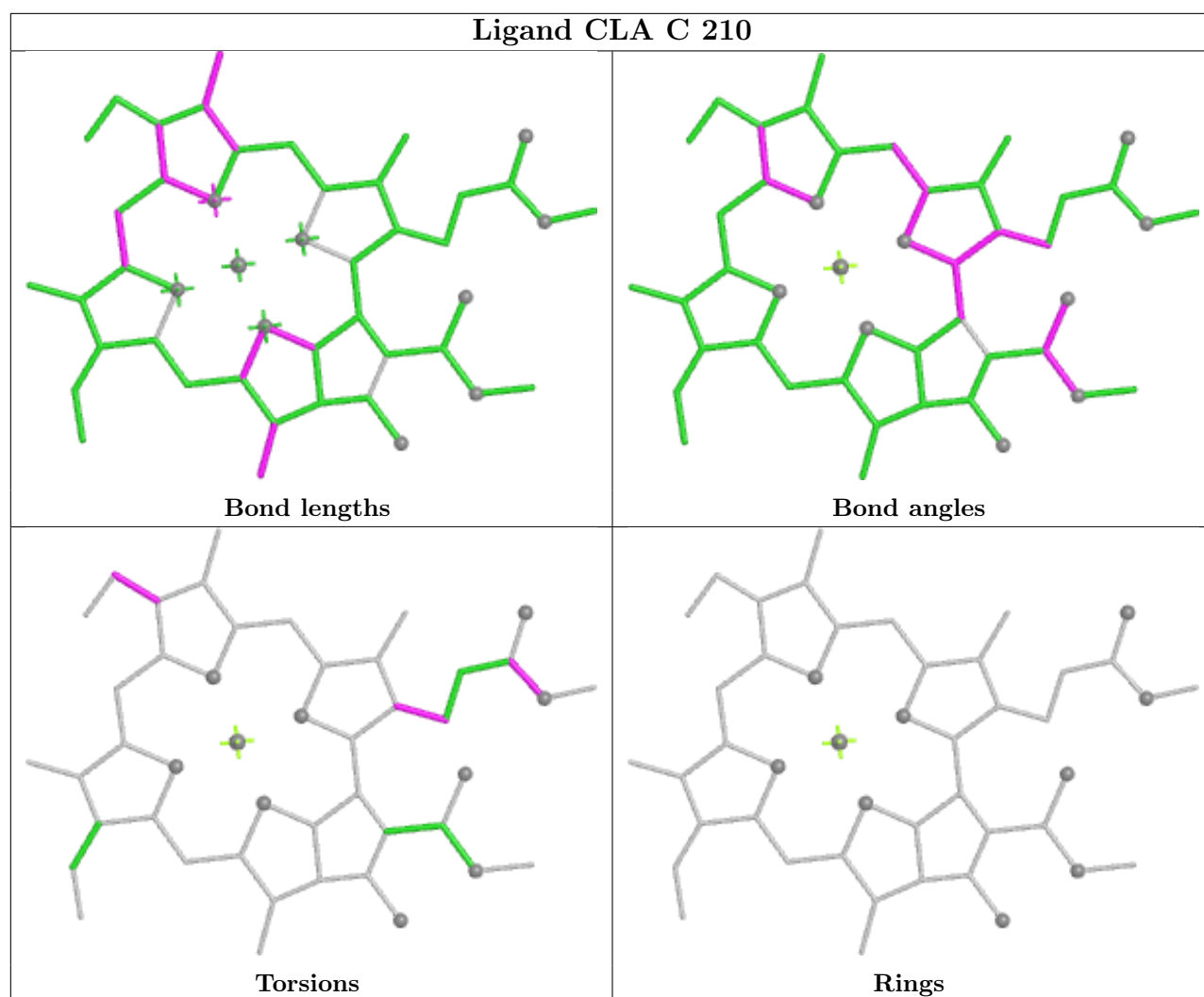
Bond angles

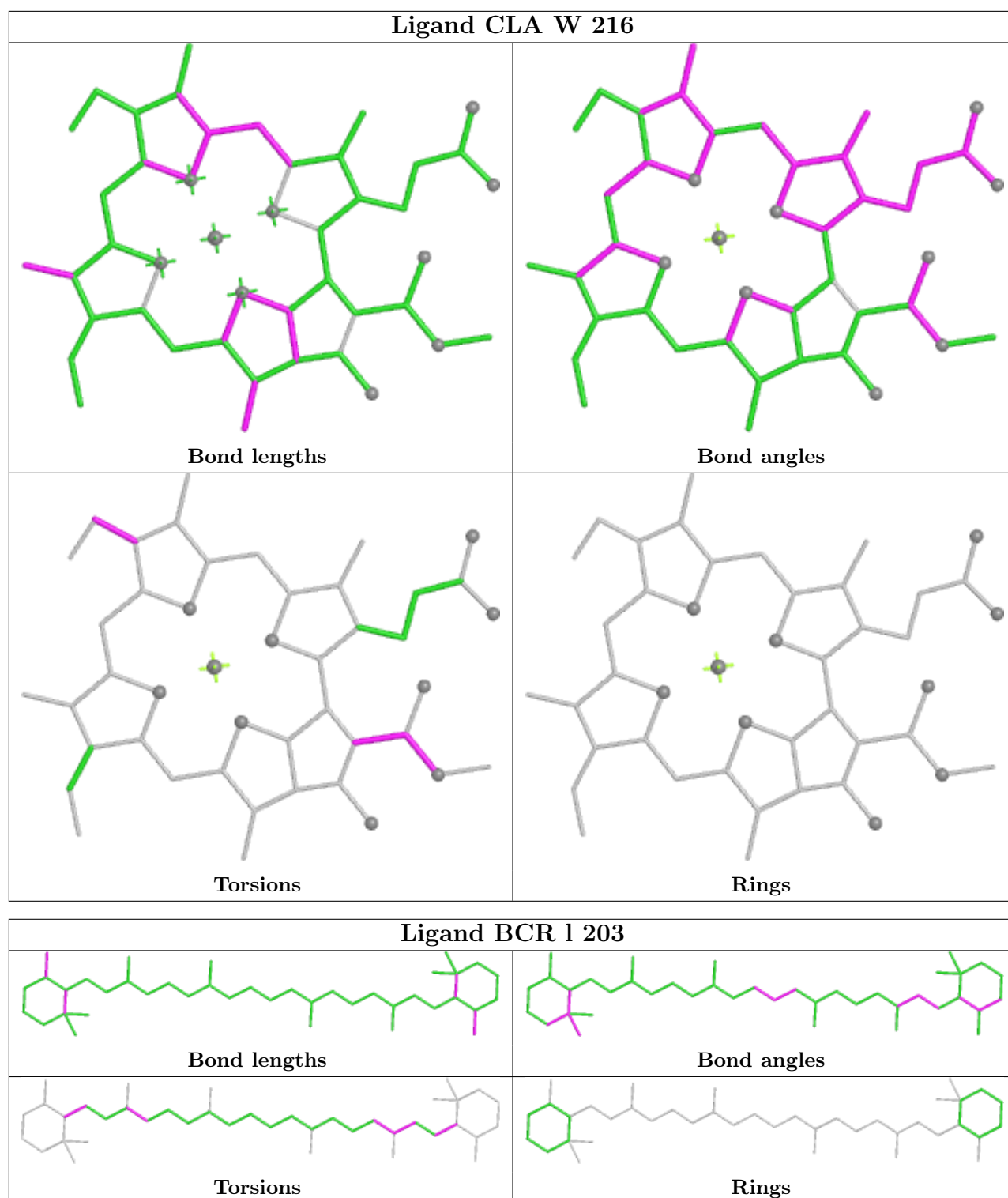


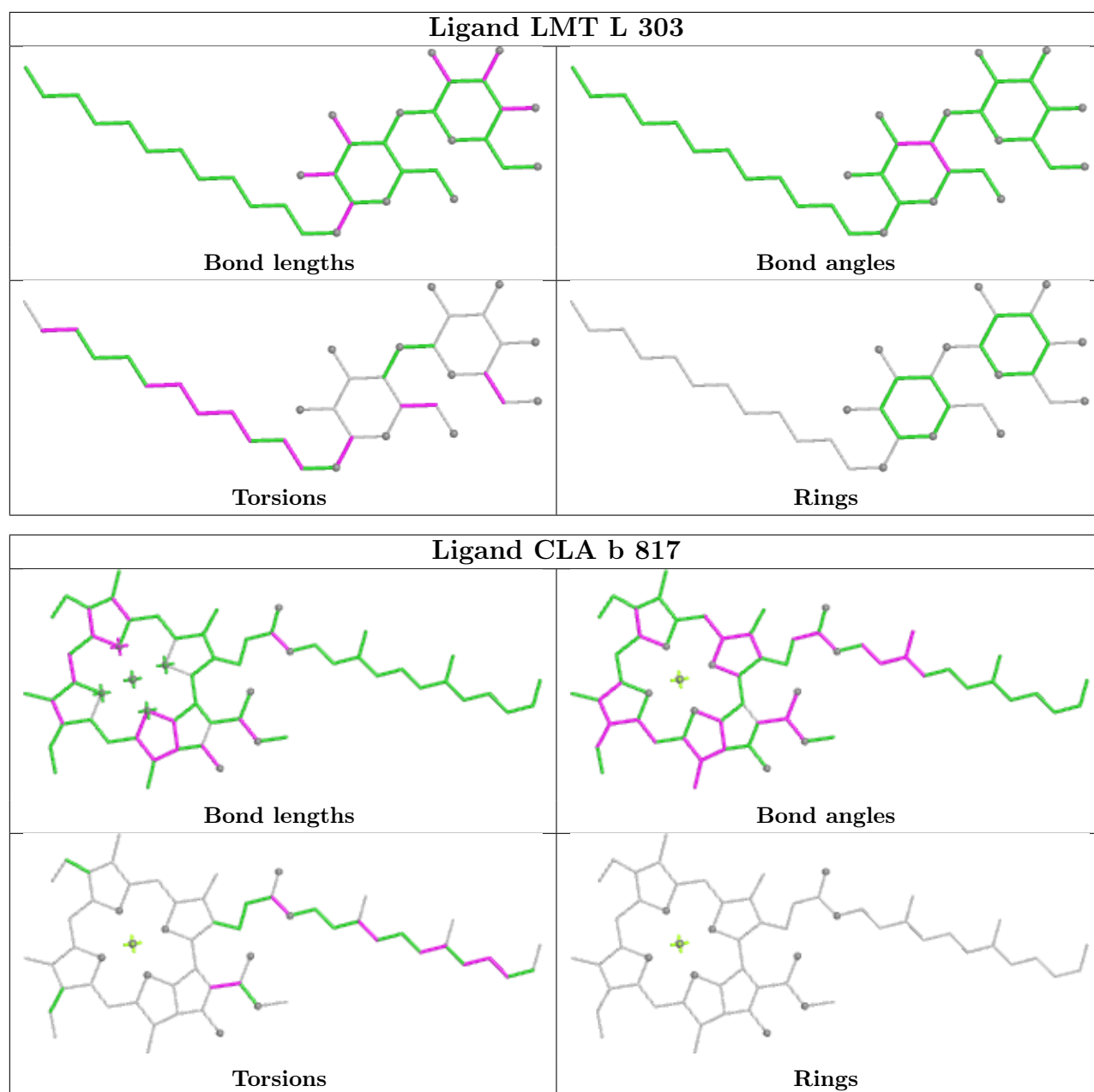
Torsions

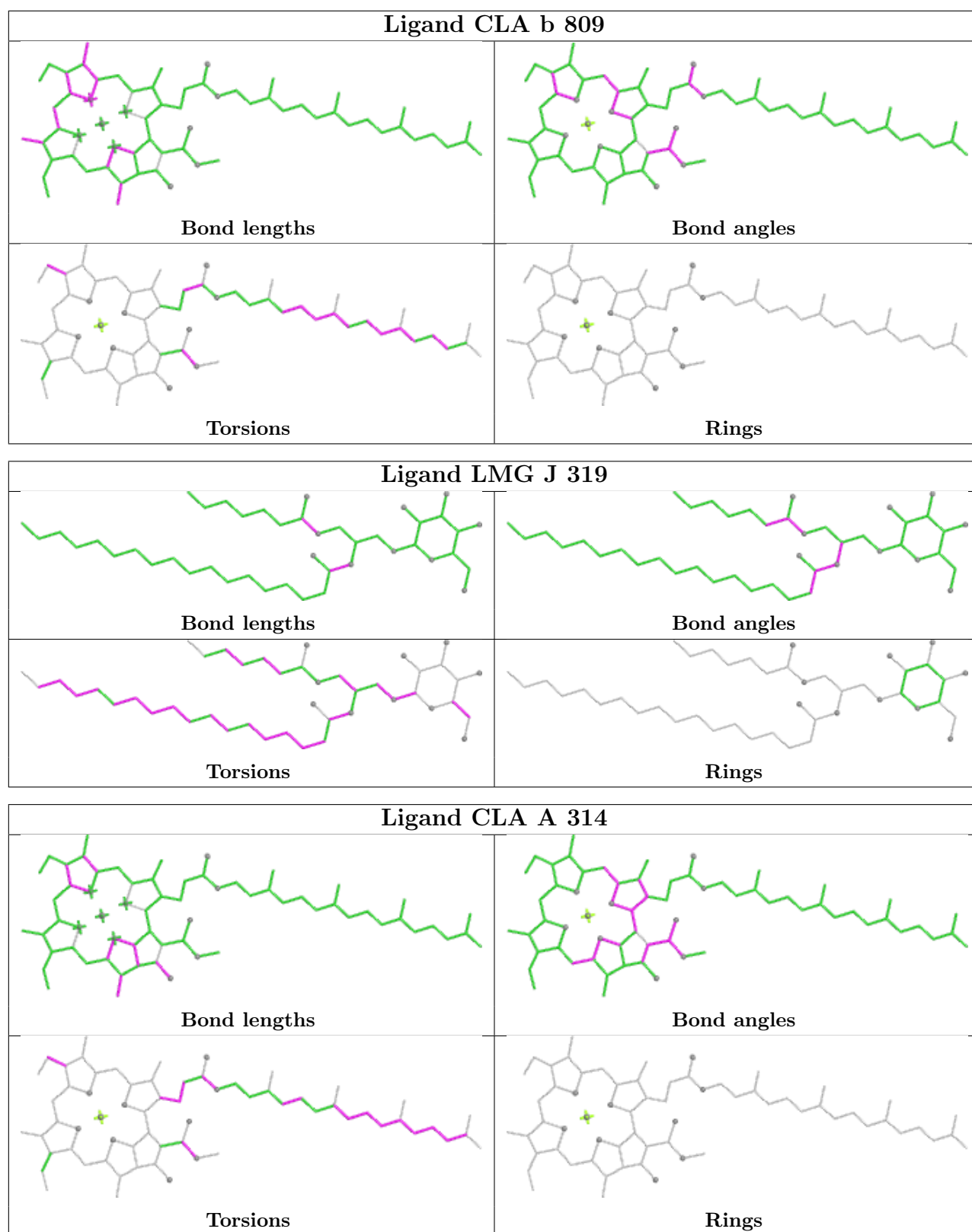


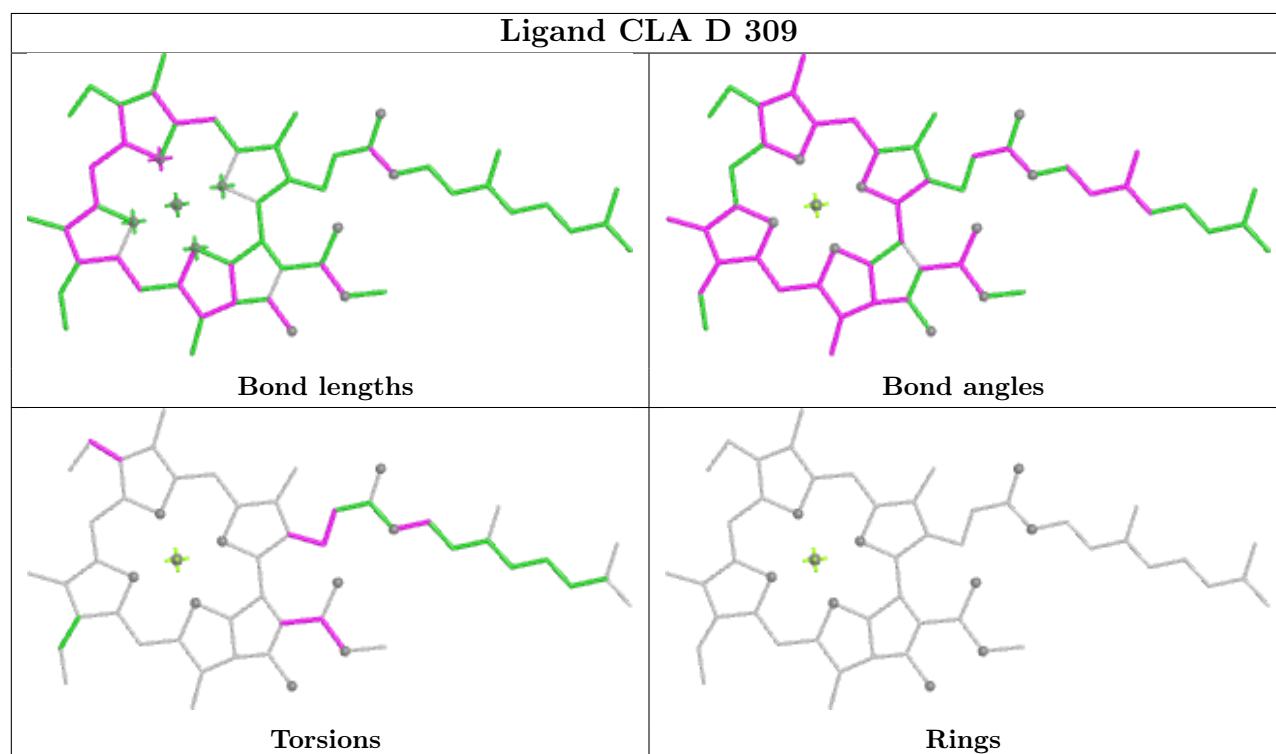
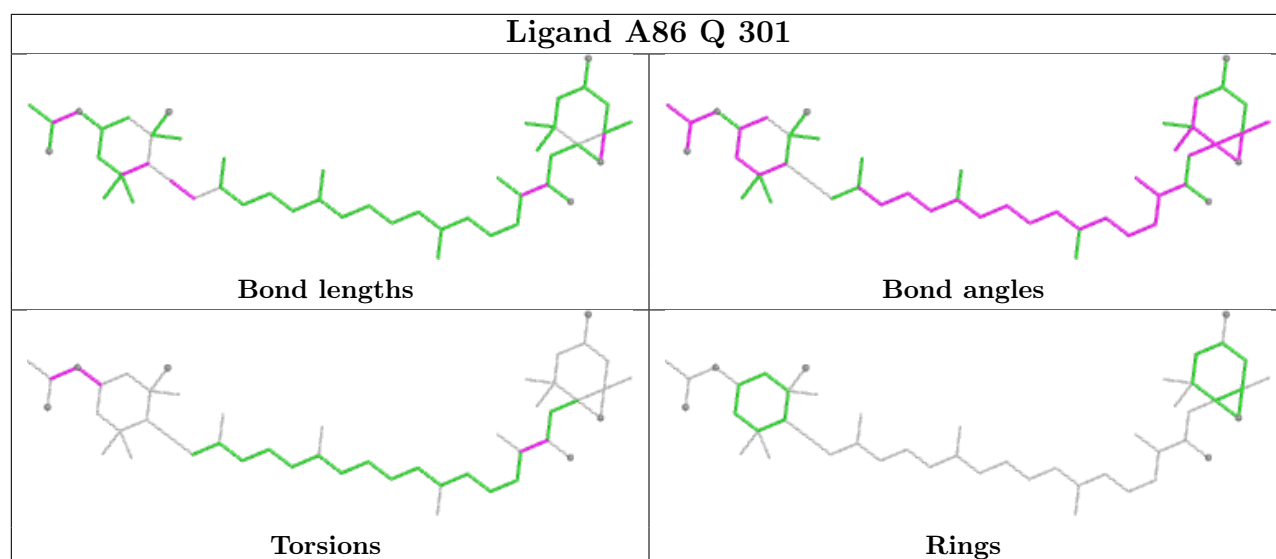
Rings

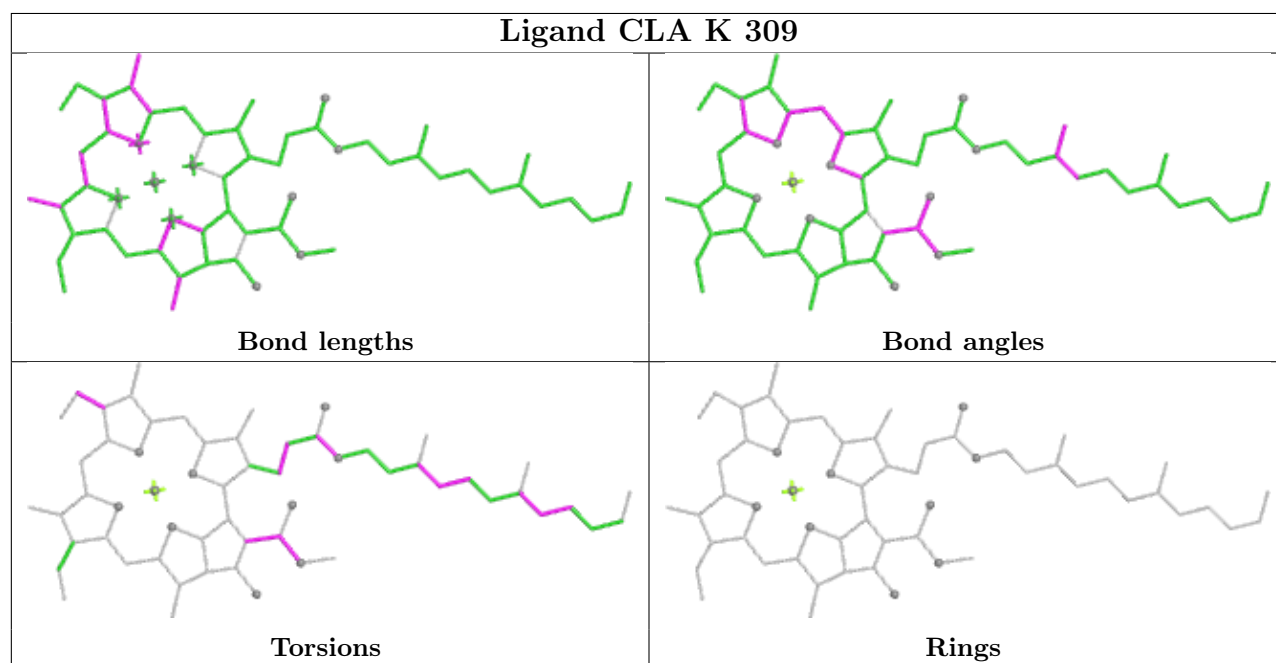
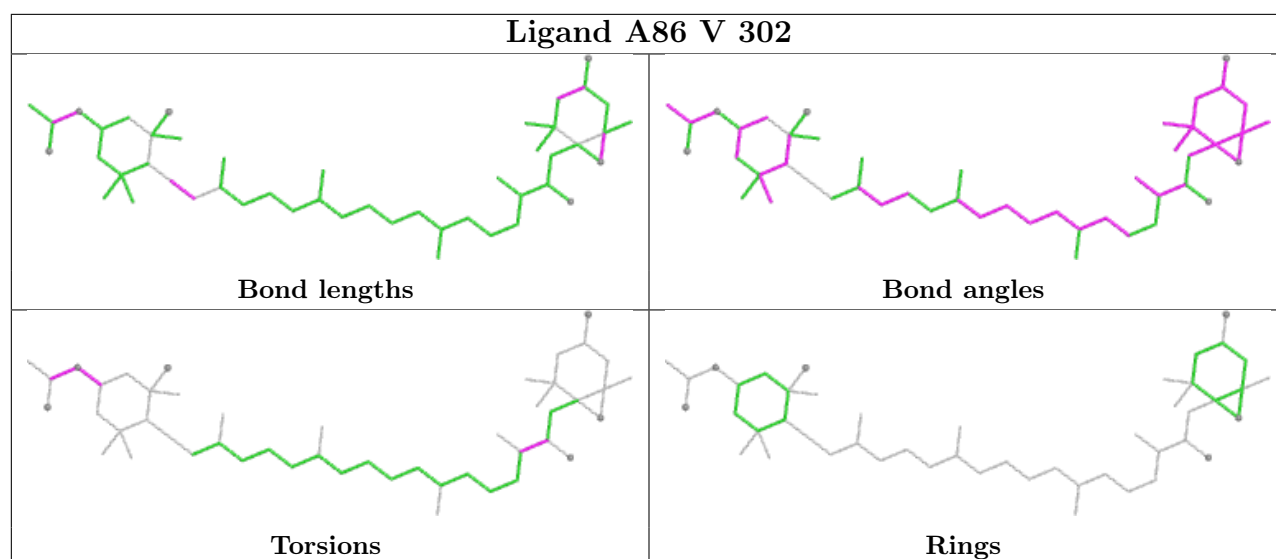


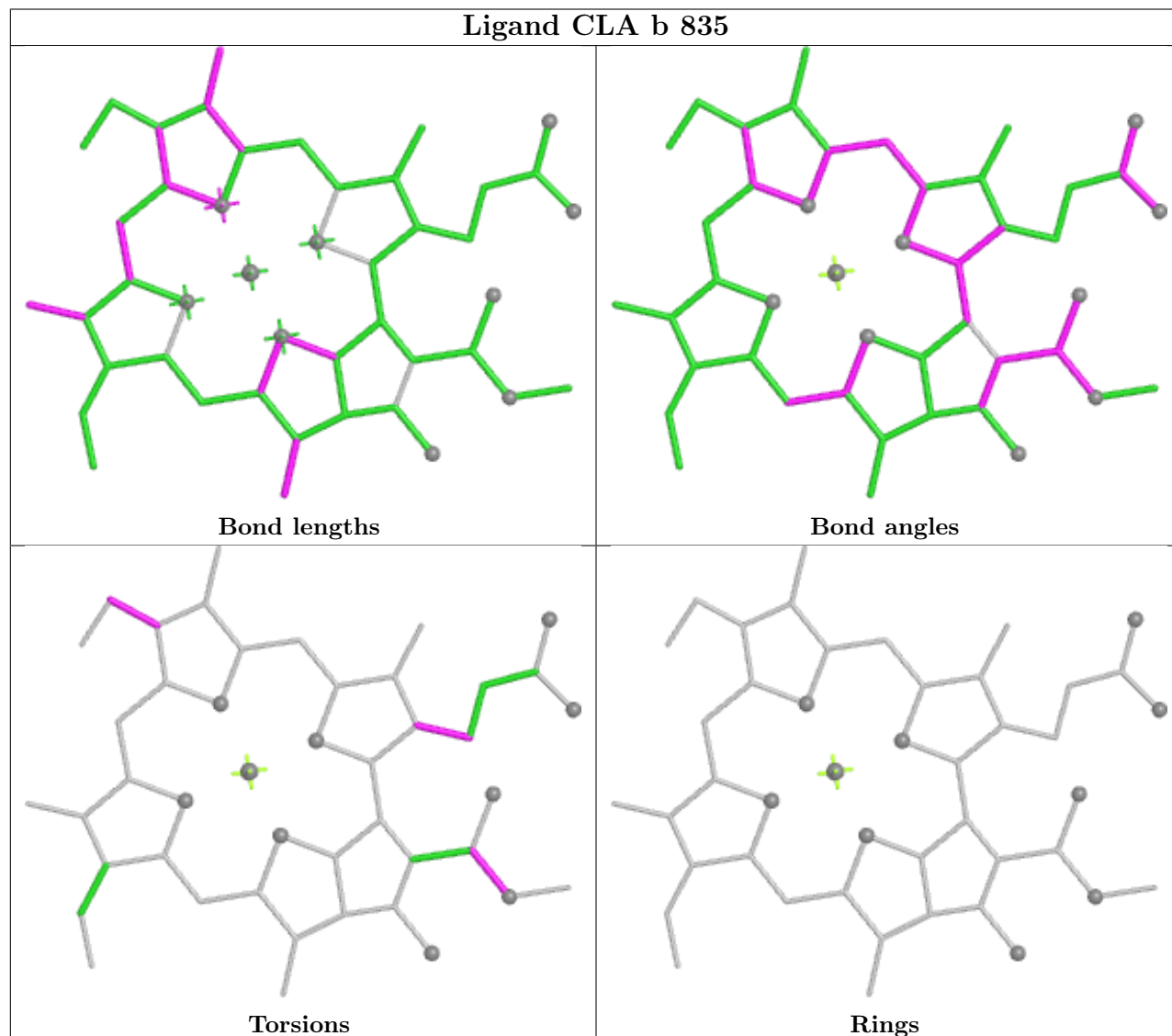
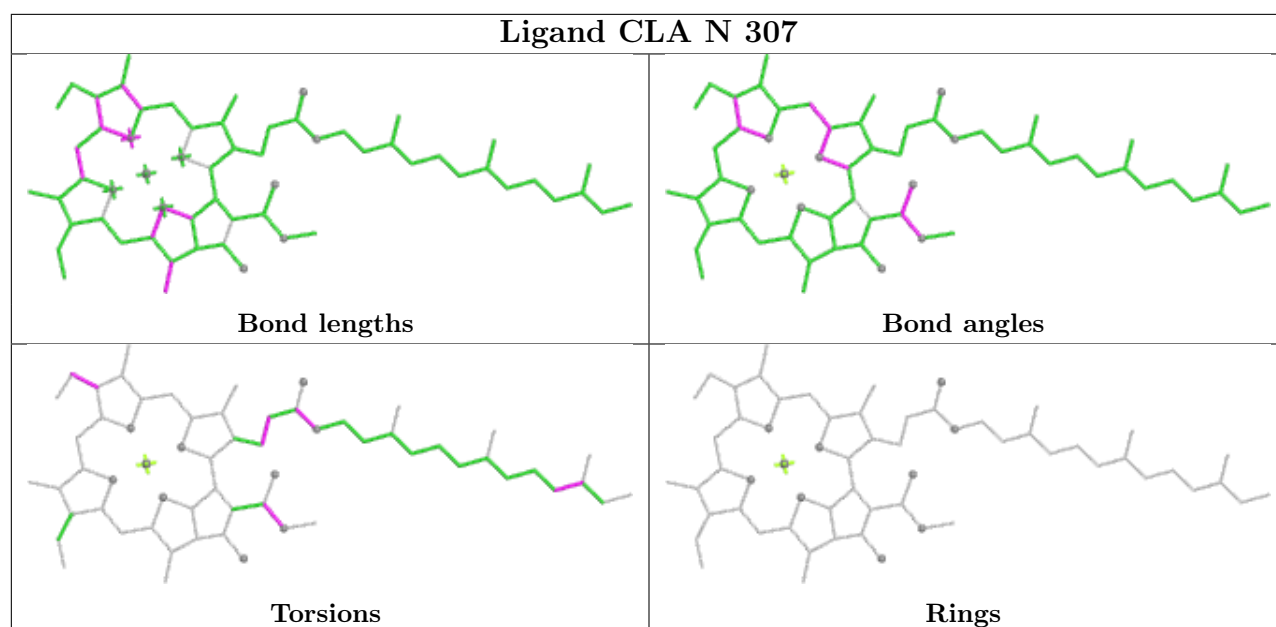


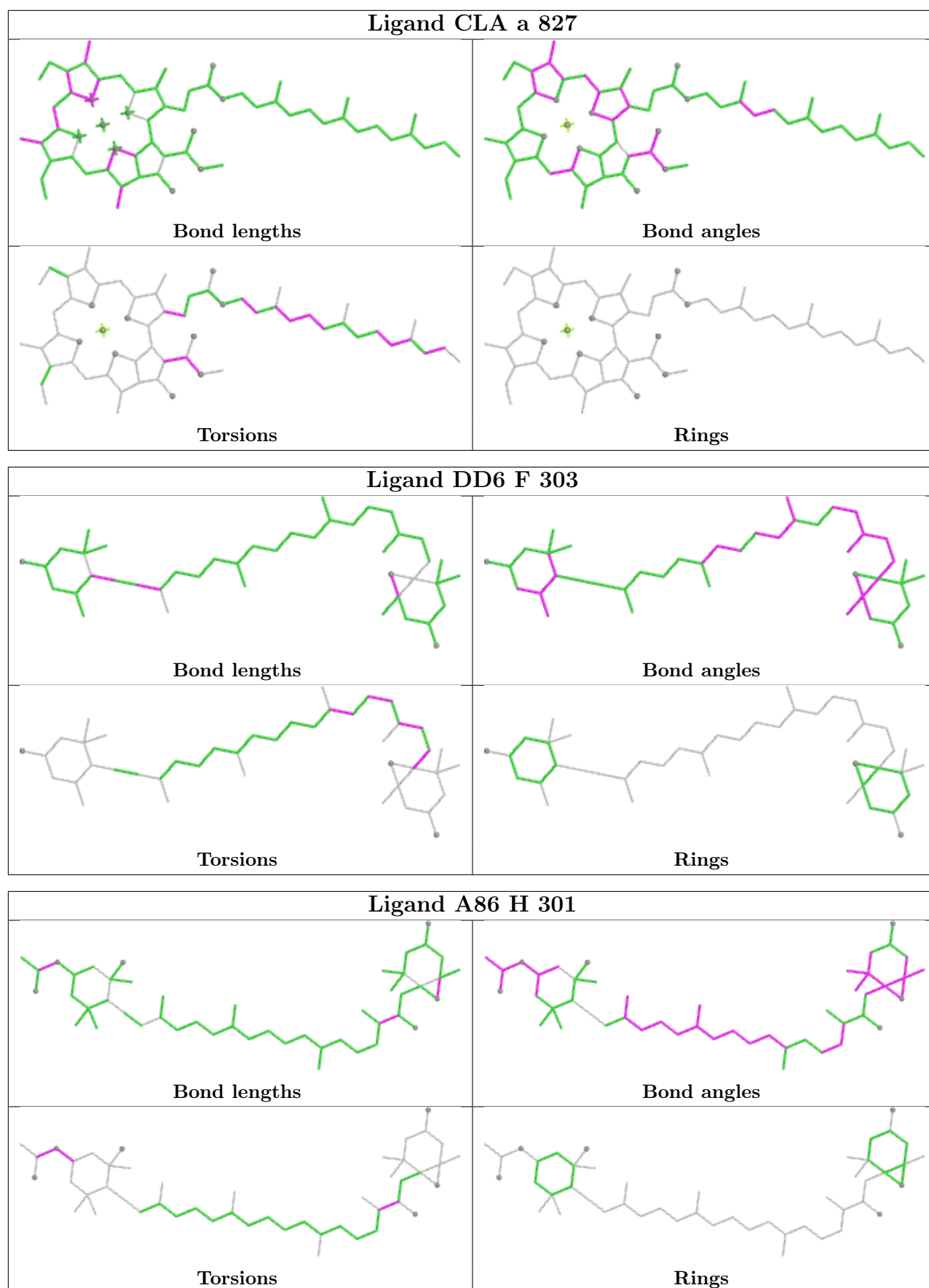




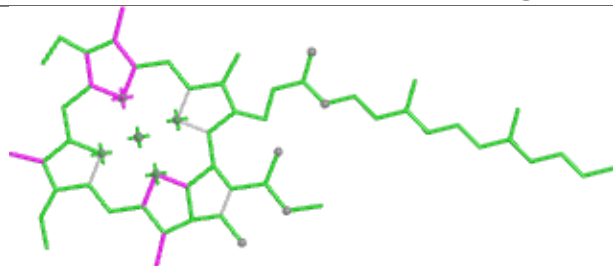




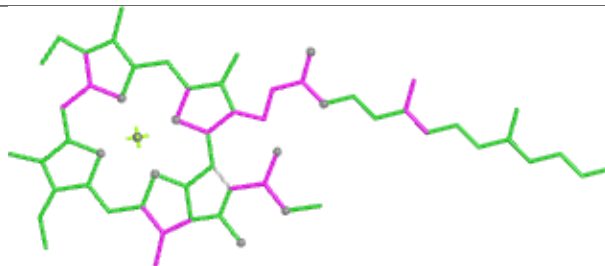




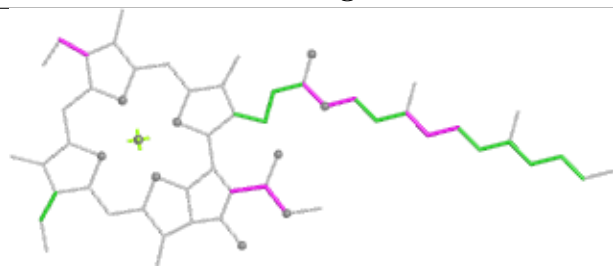
Ligand CLA b 833



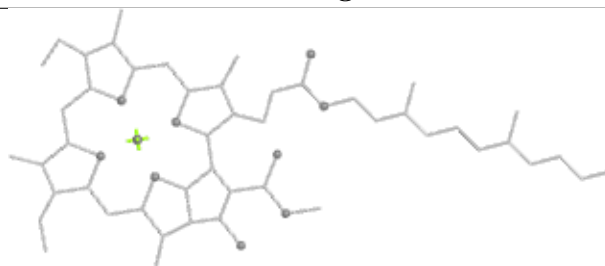
Bond lengths



Bond angles

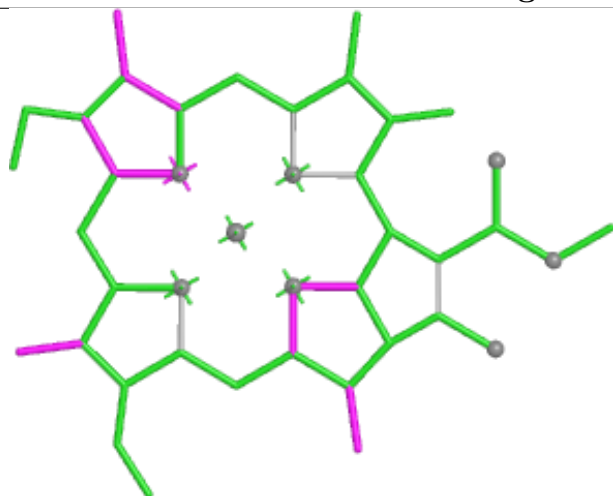


Torsions

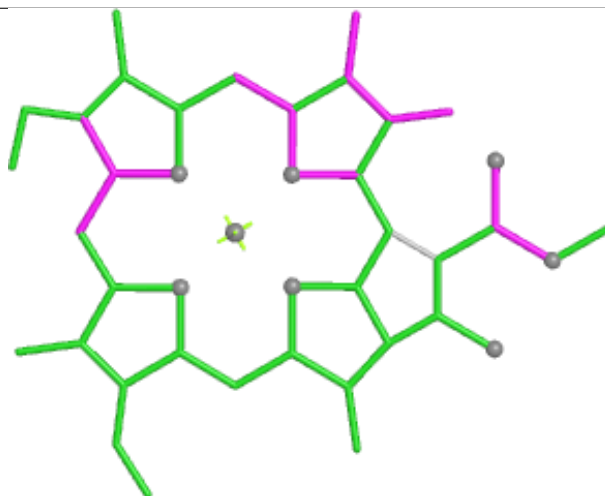


Rings

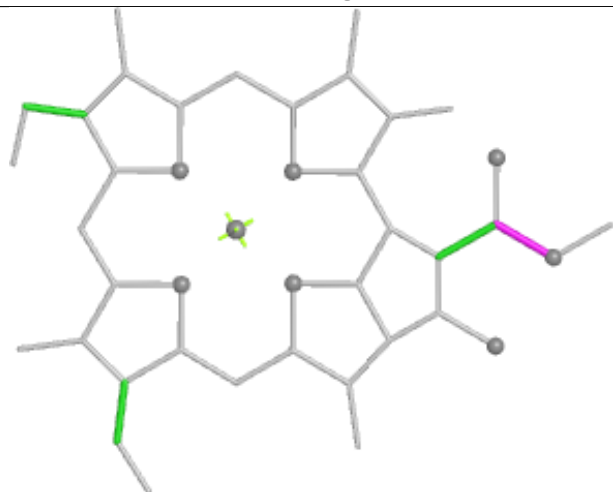
Ligand CLA J 315



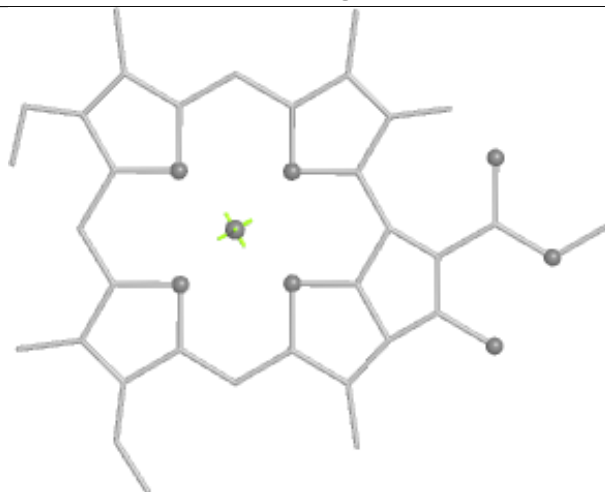
Bond lengths



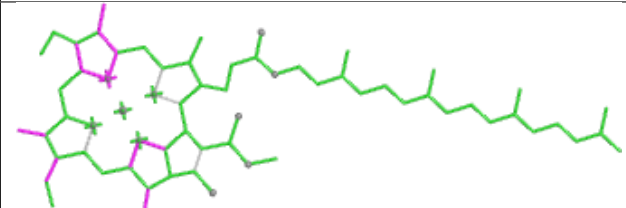
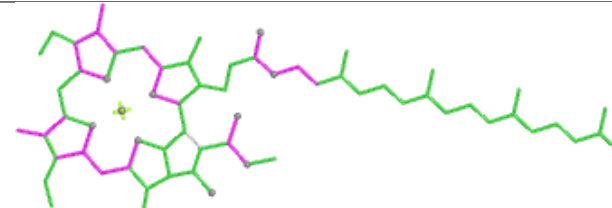
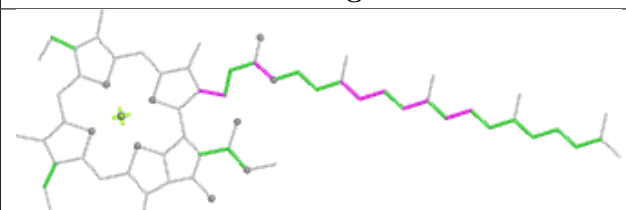
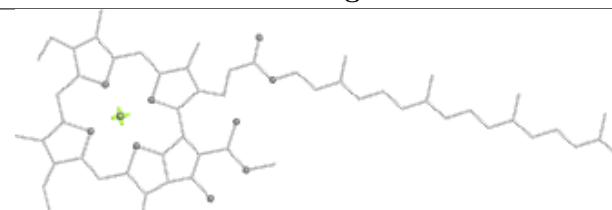
Bond angles

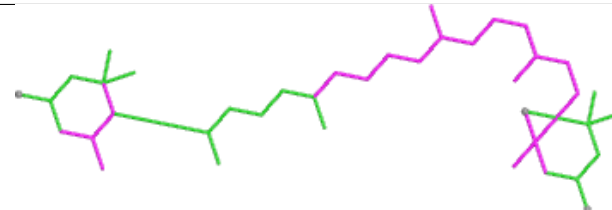
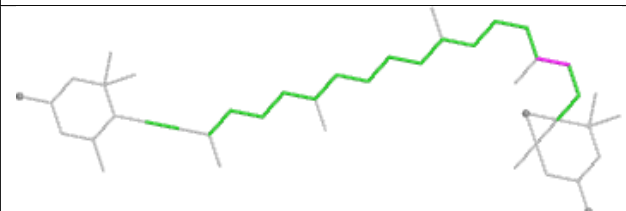
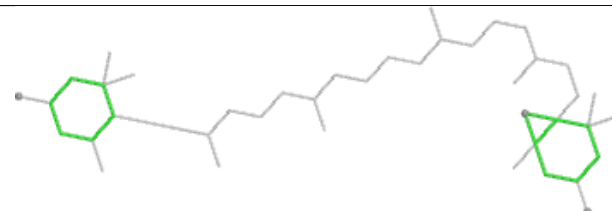


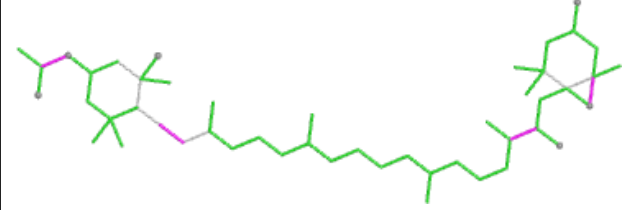
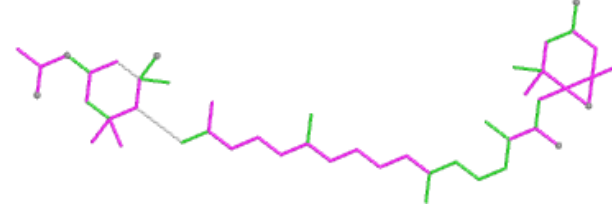
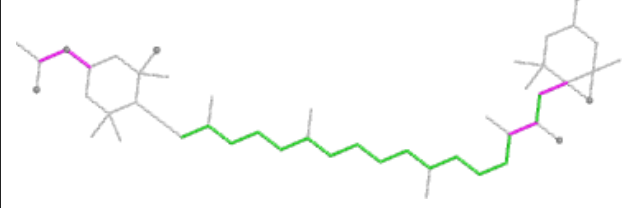
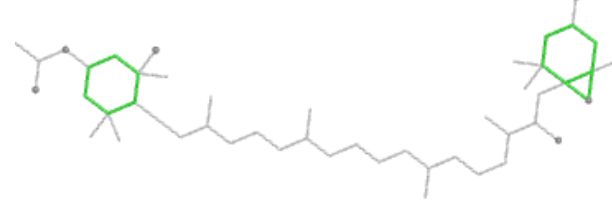
Torsions

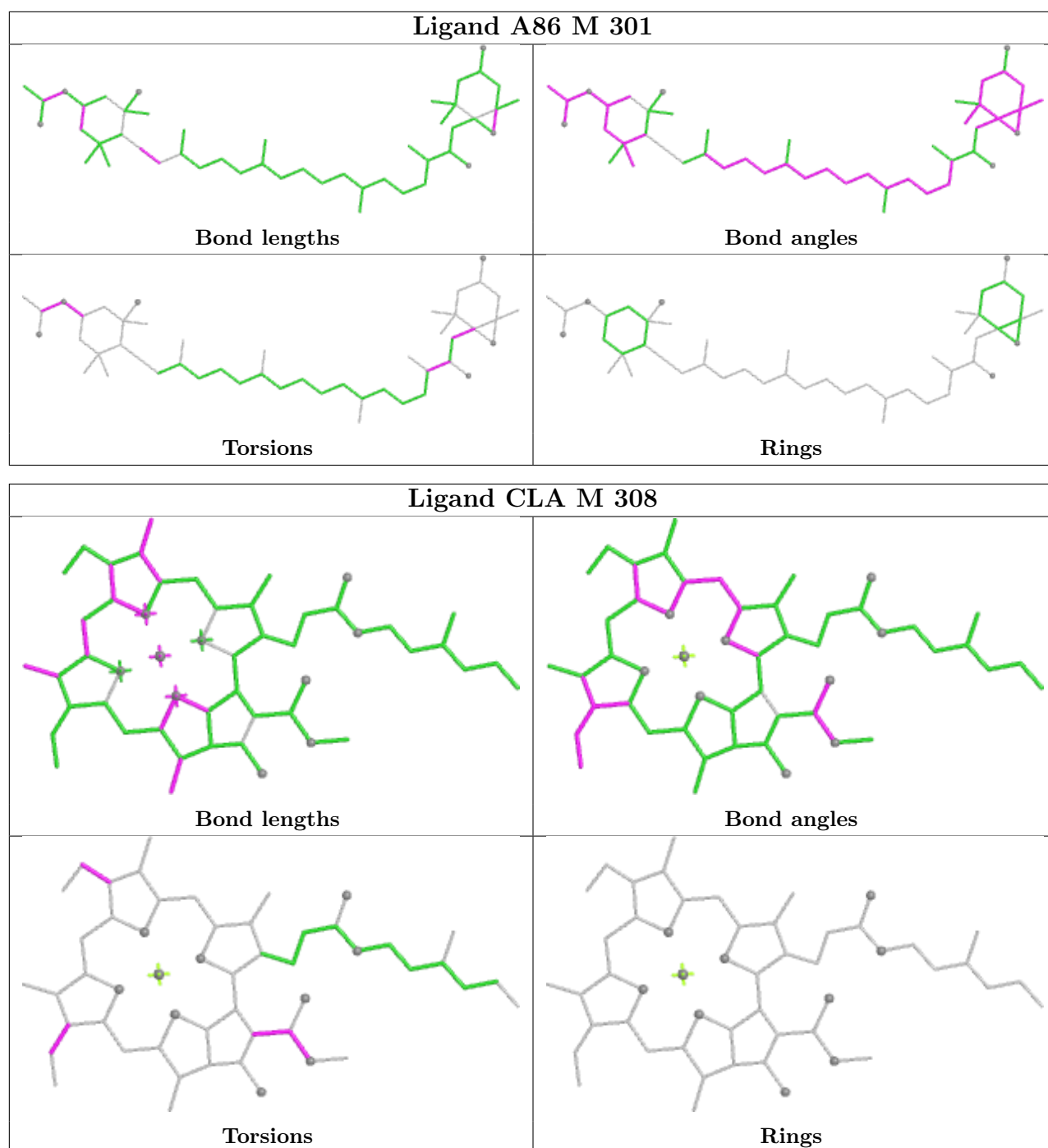


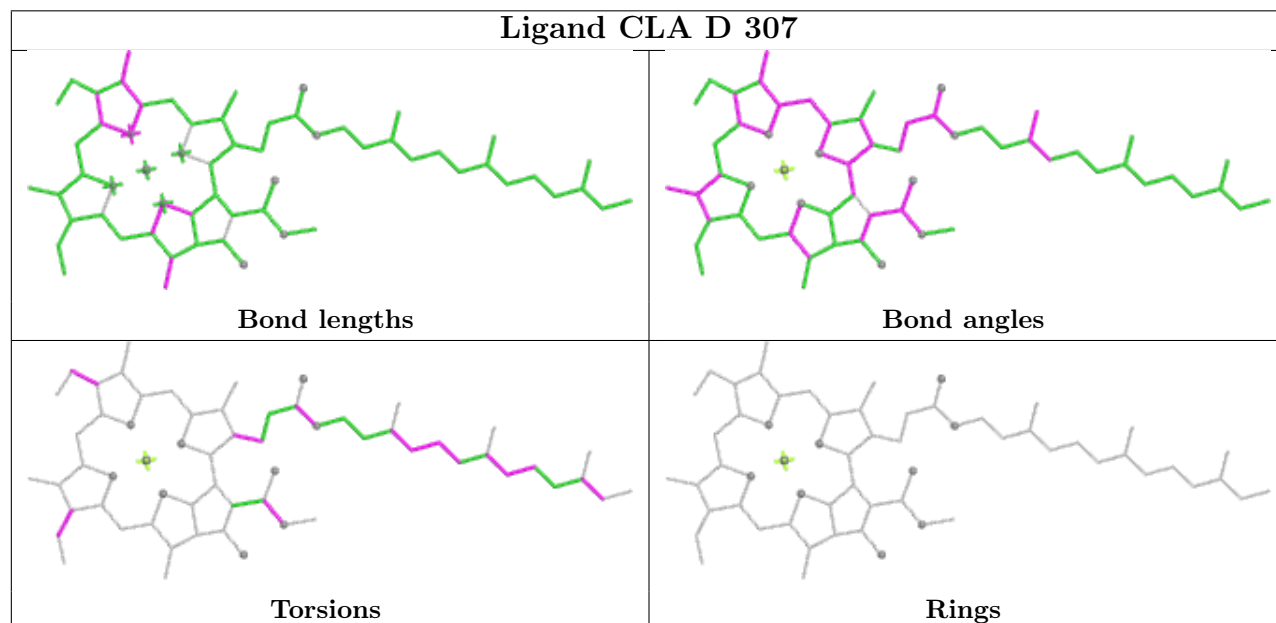
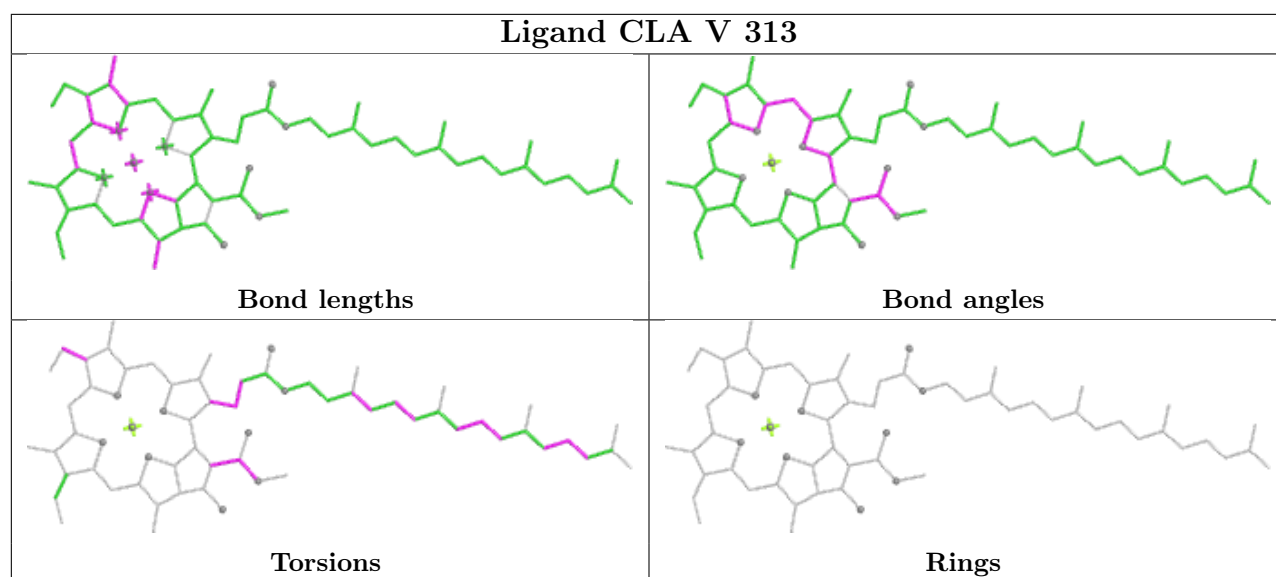
Rings

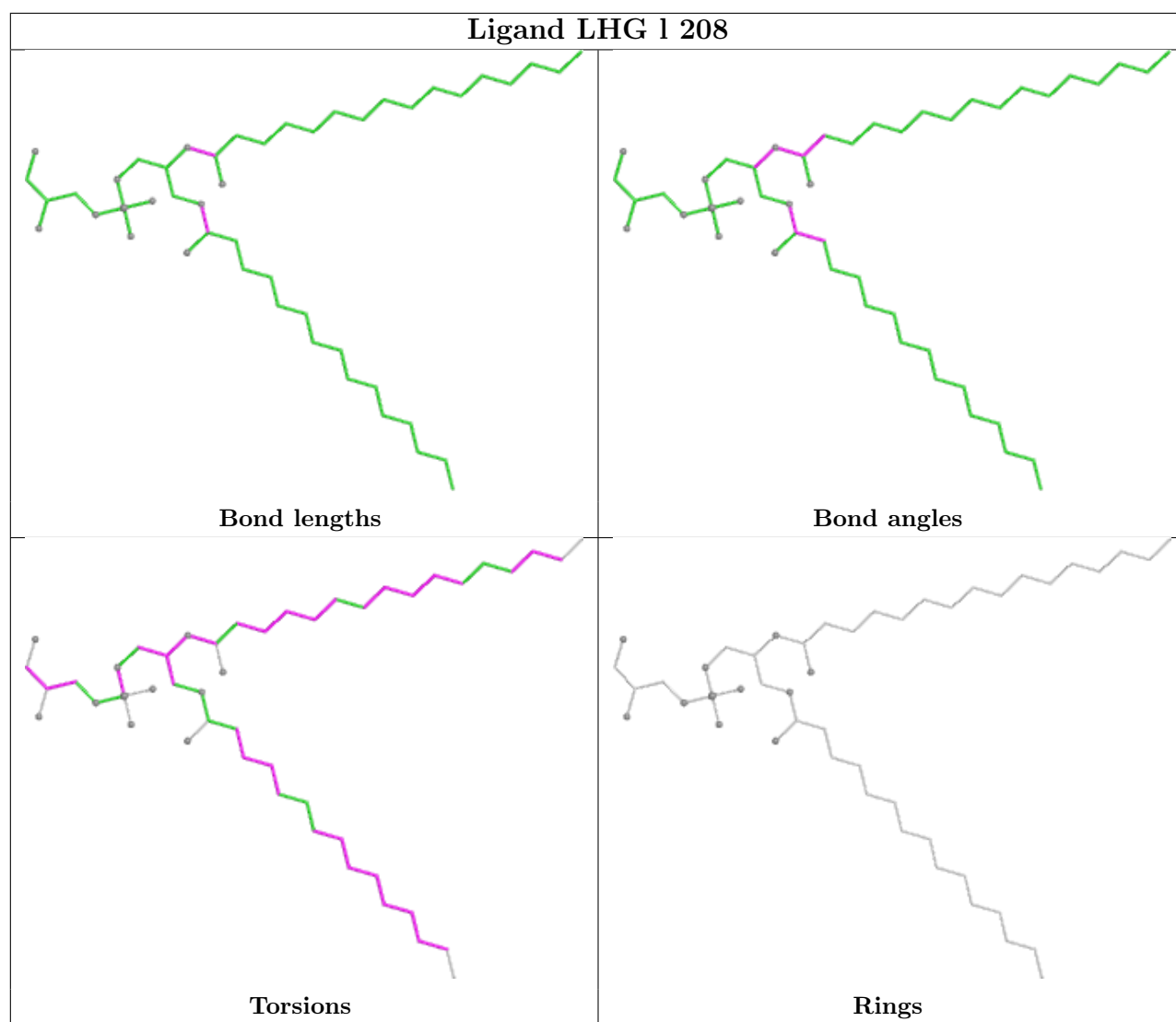
Ligand CLA E 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 B 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

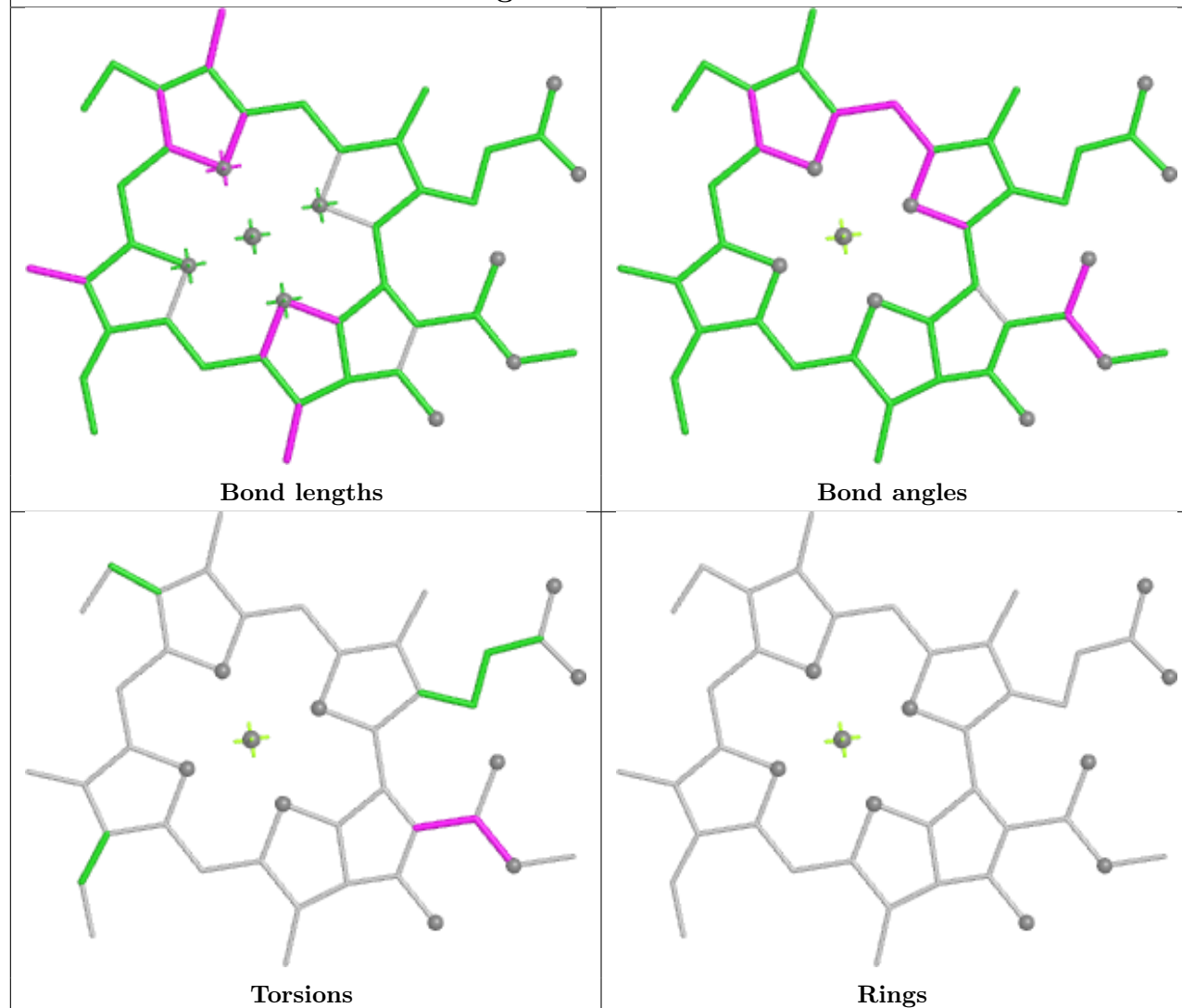
Ligand A86 X 304	
	
Bond lengths	Bond angles
	
Torsions	Rings



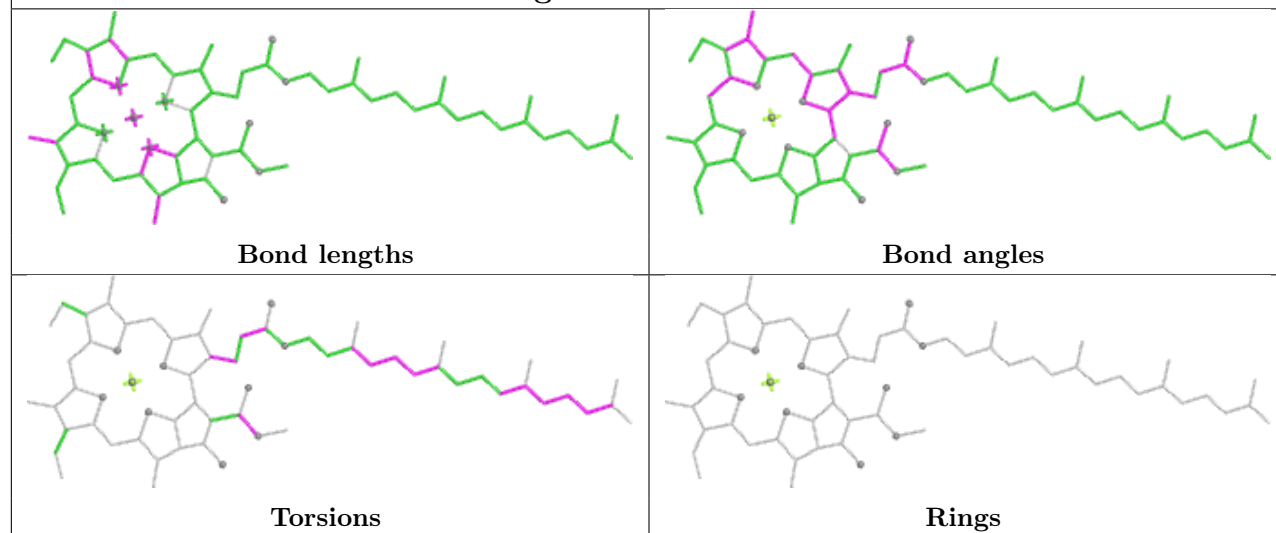


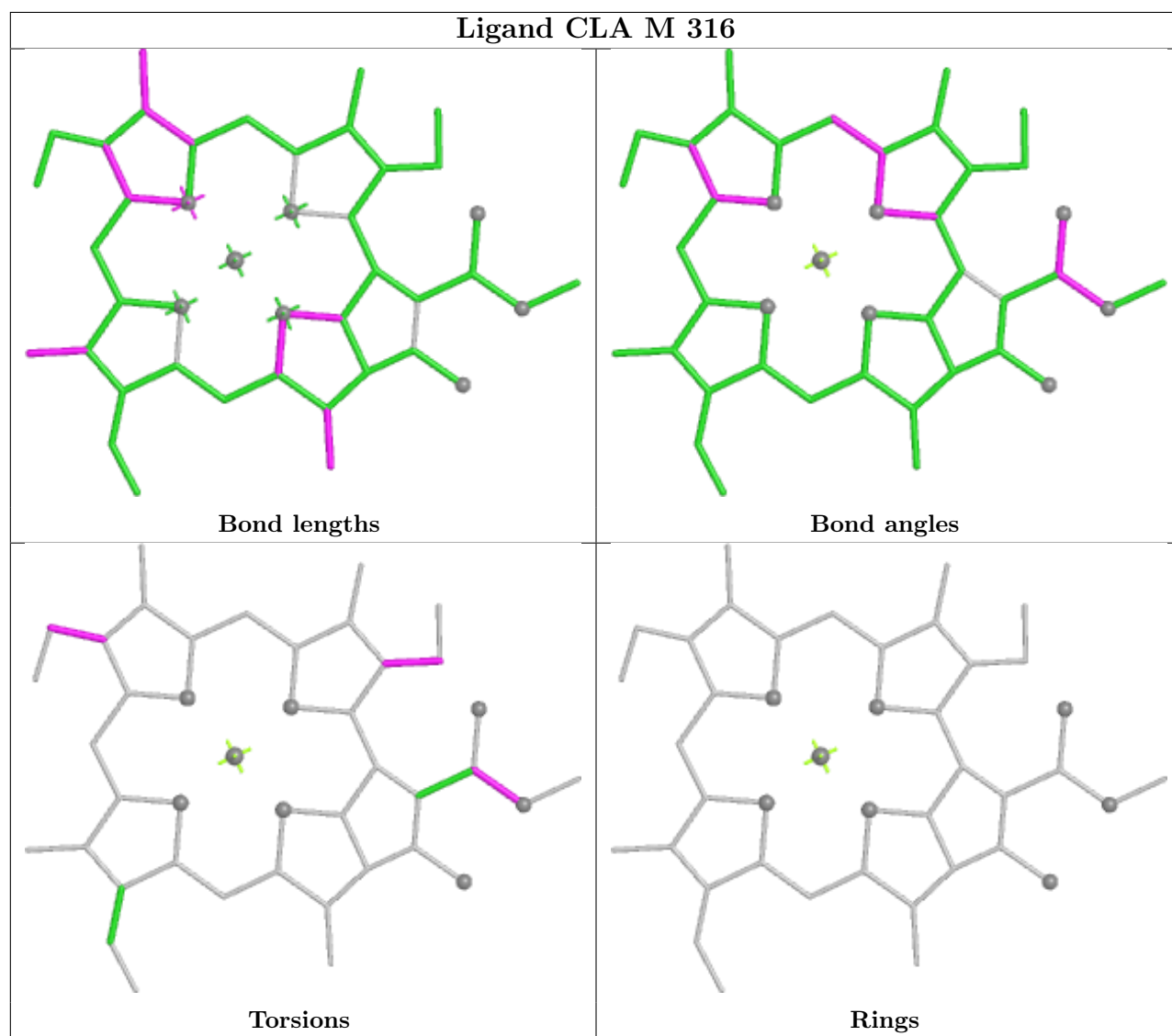
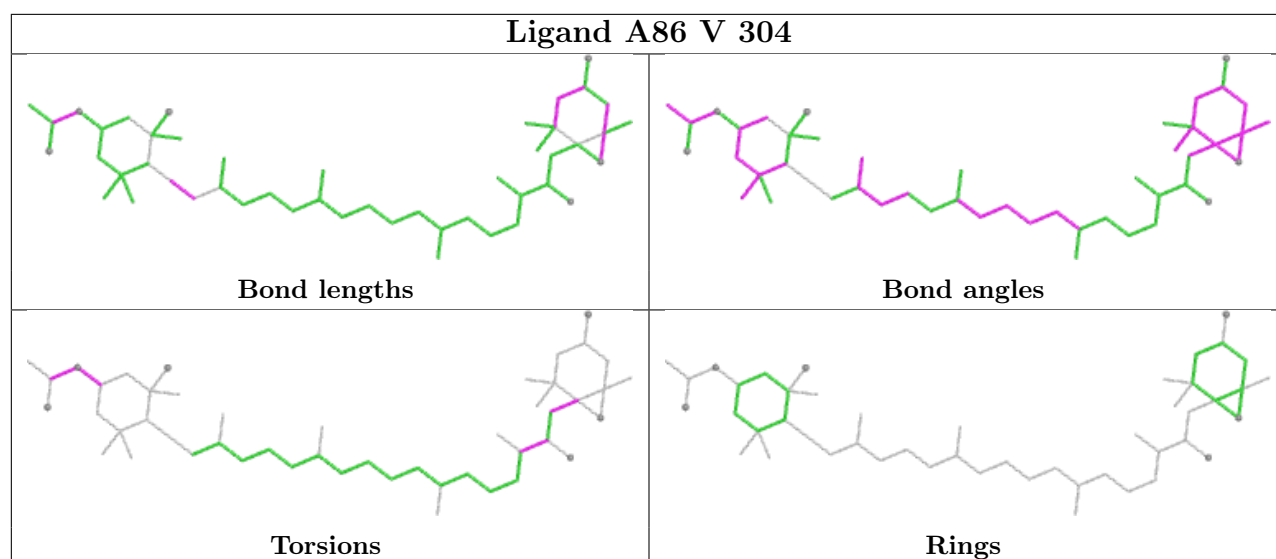


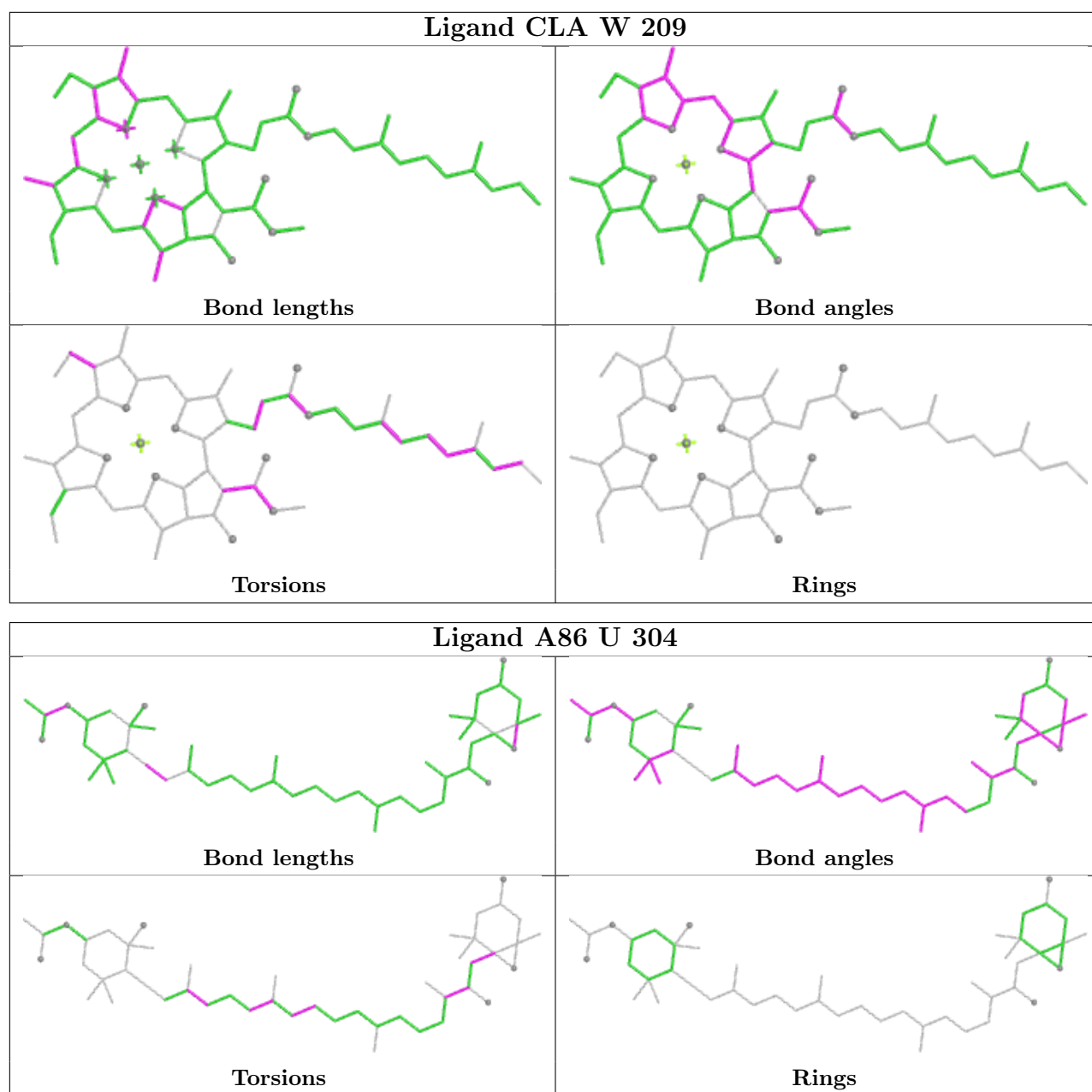
Ligand CLA a 815

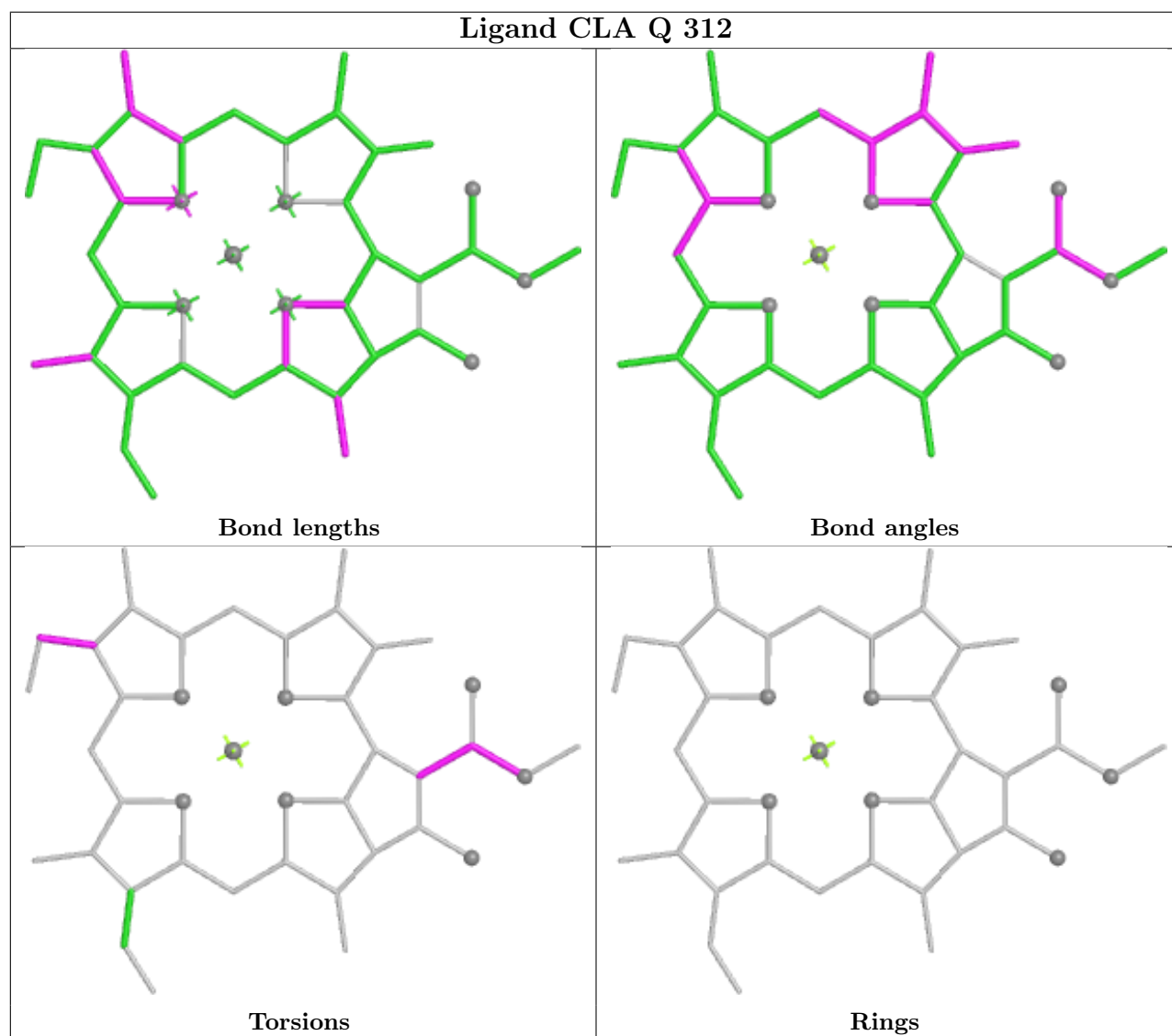
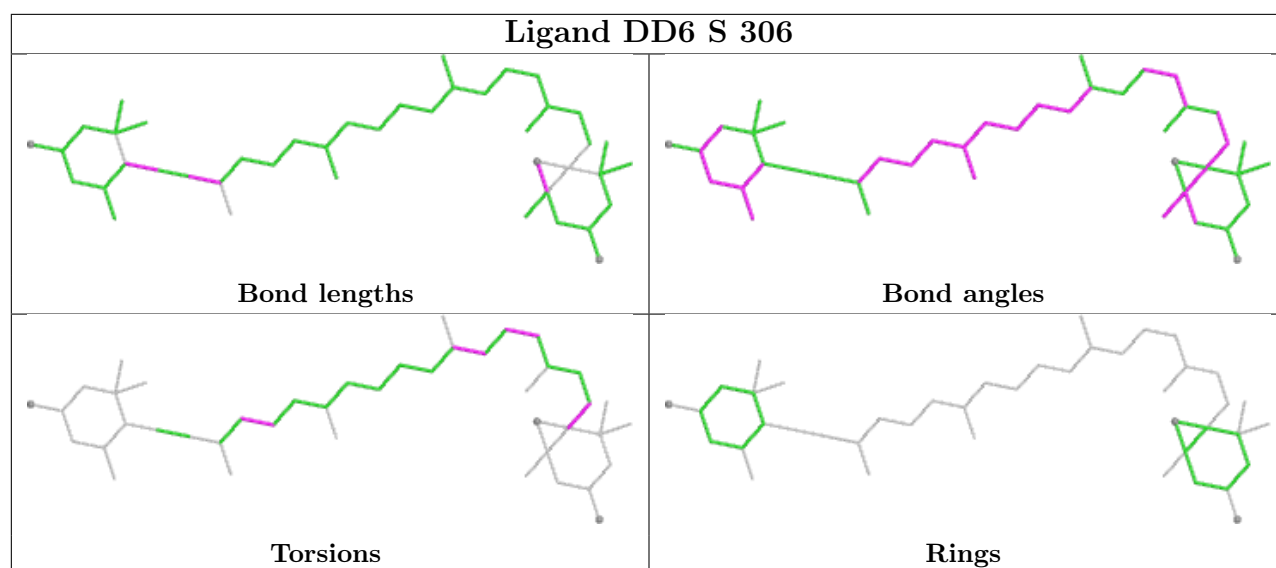


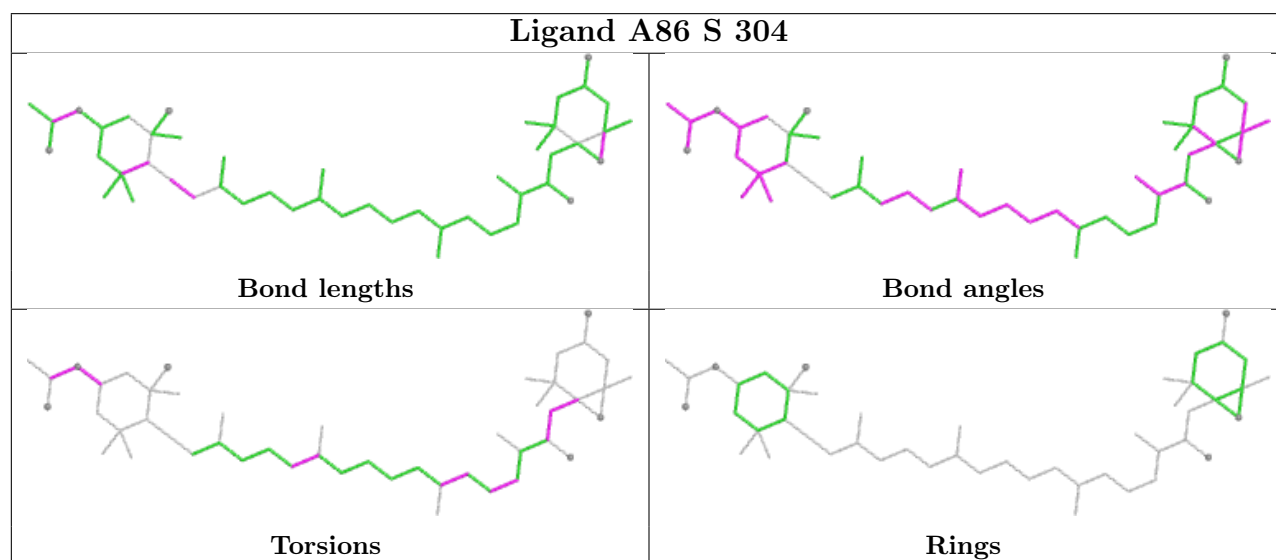
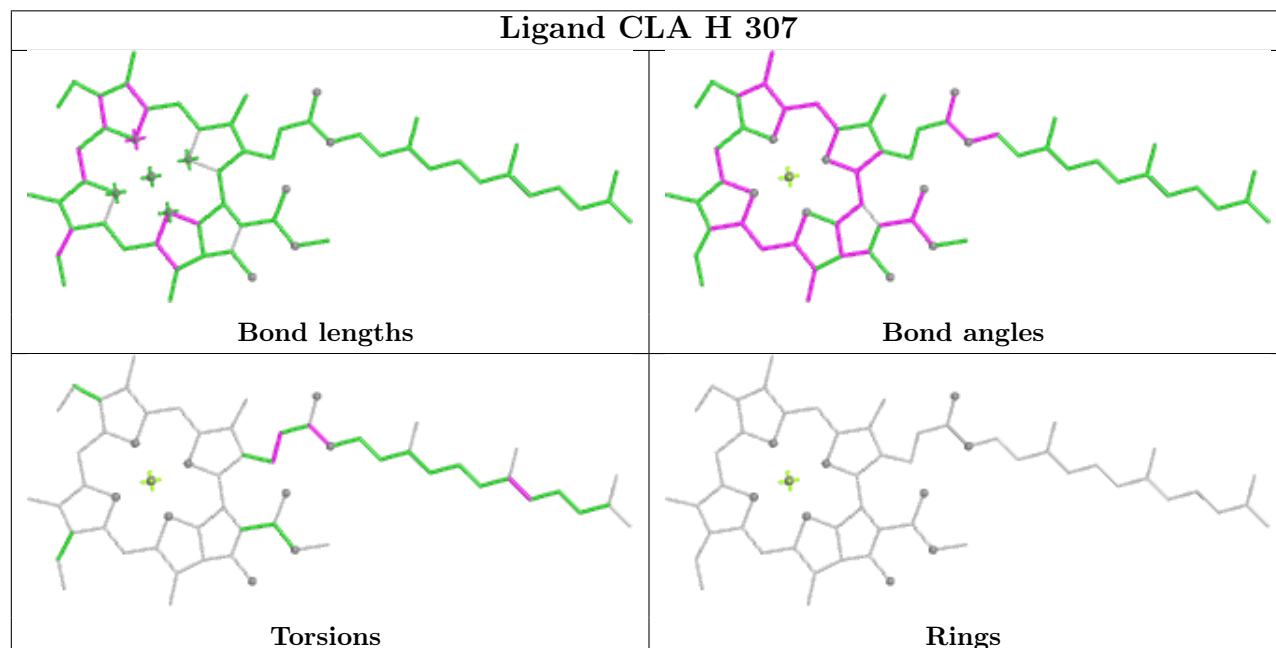
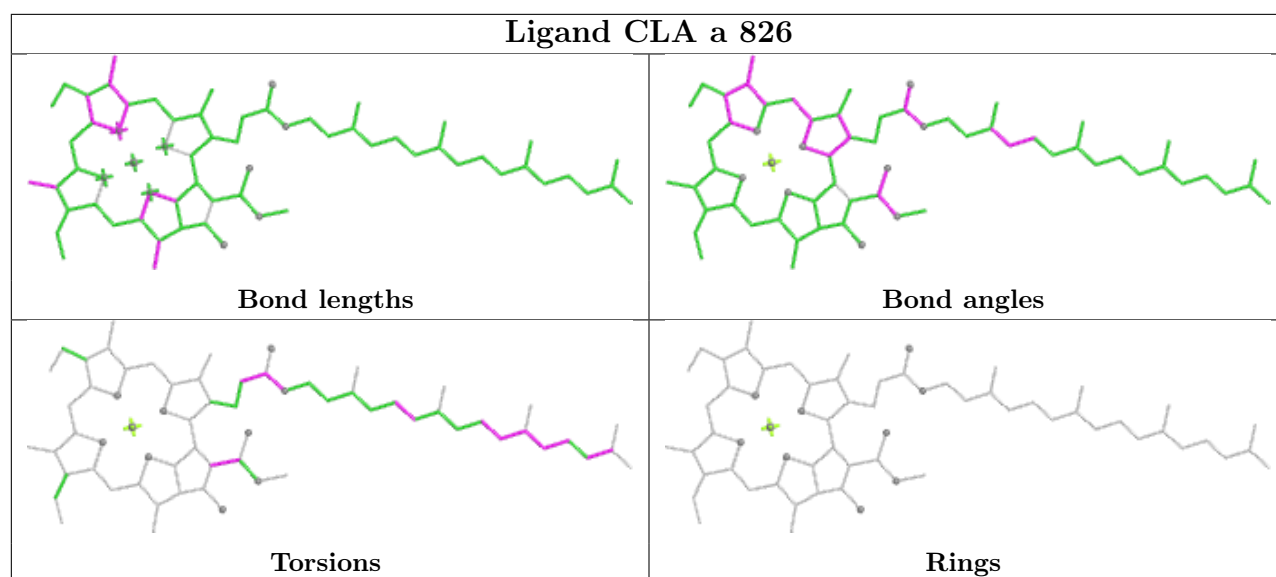
Ligand CLA L 314

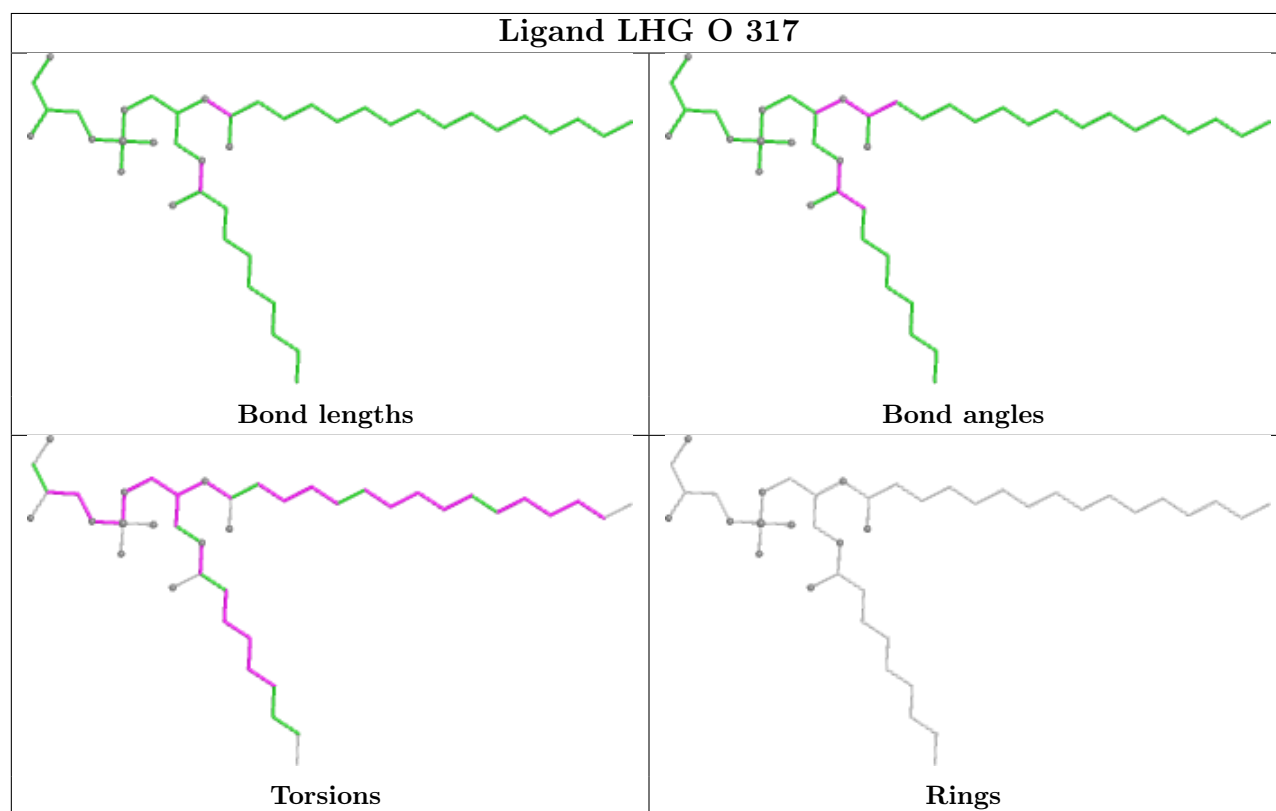
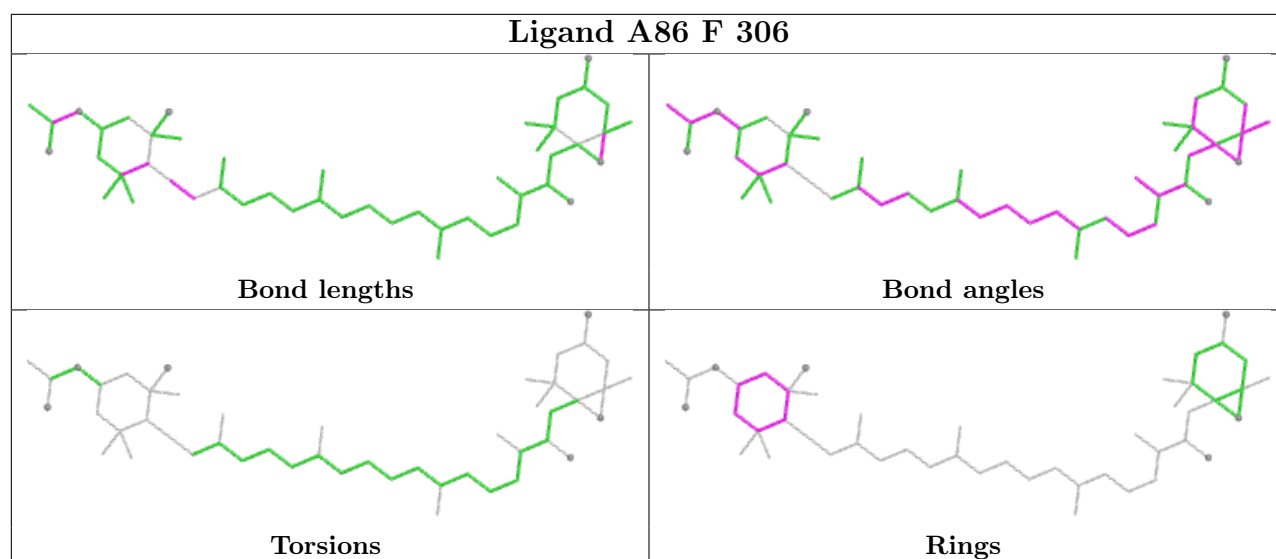


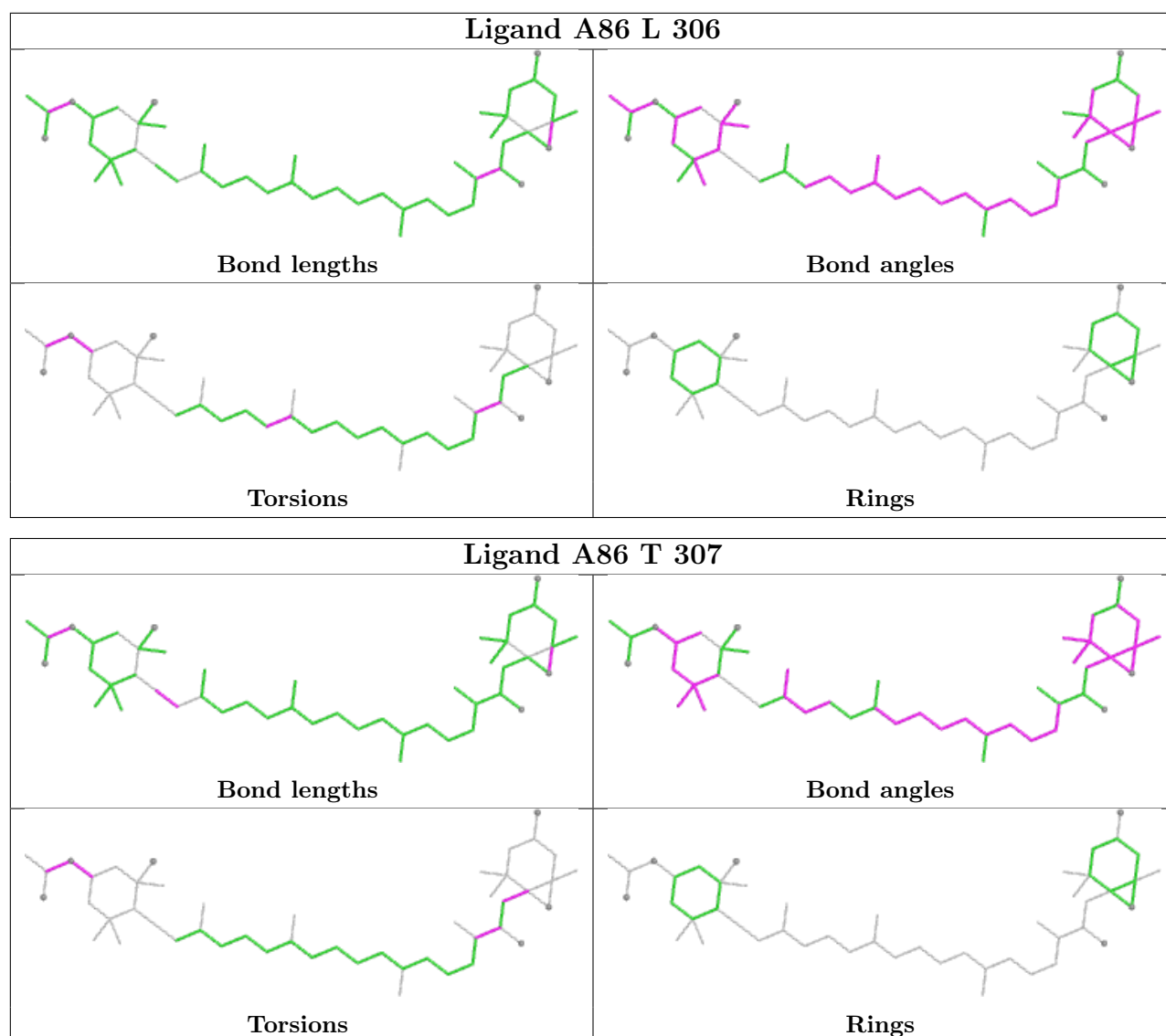




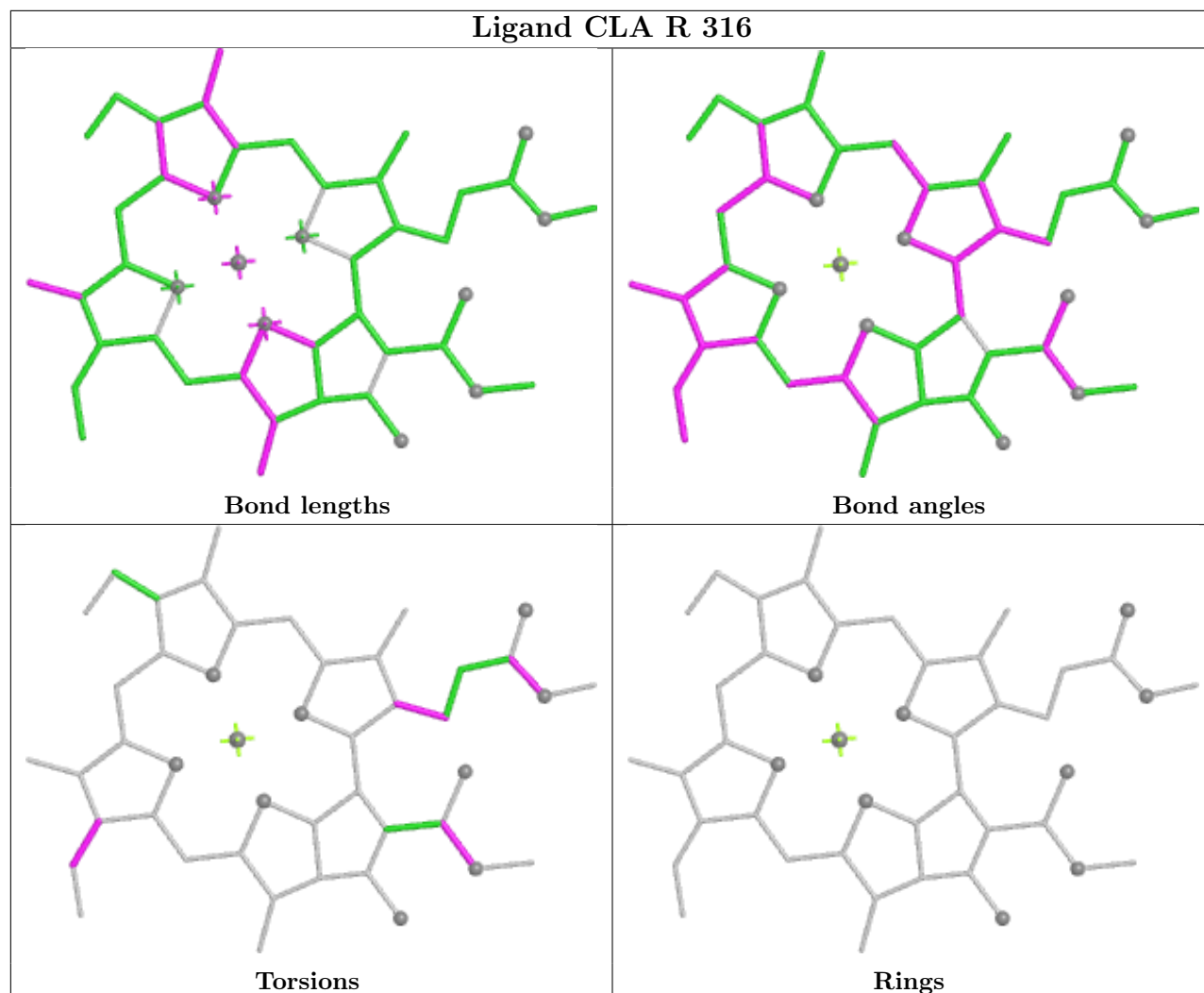




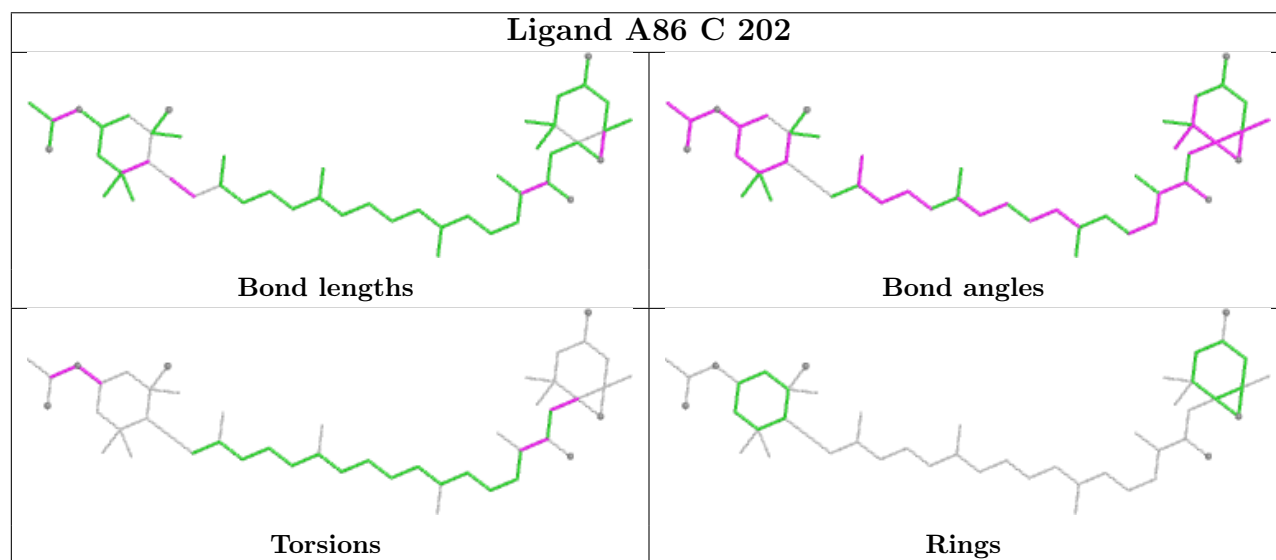


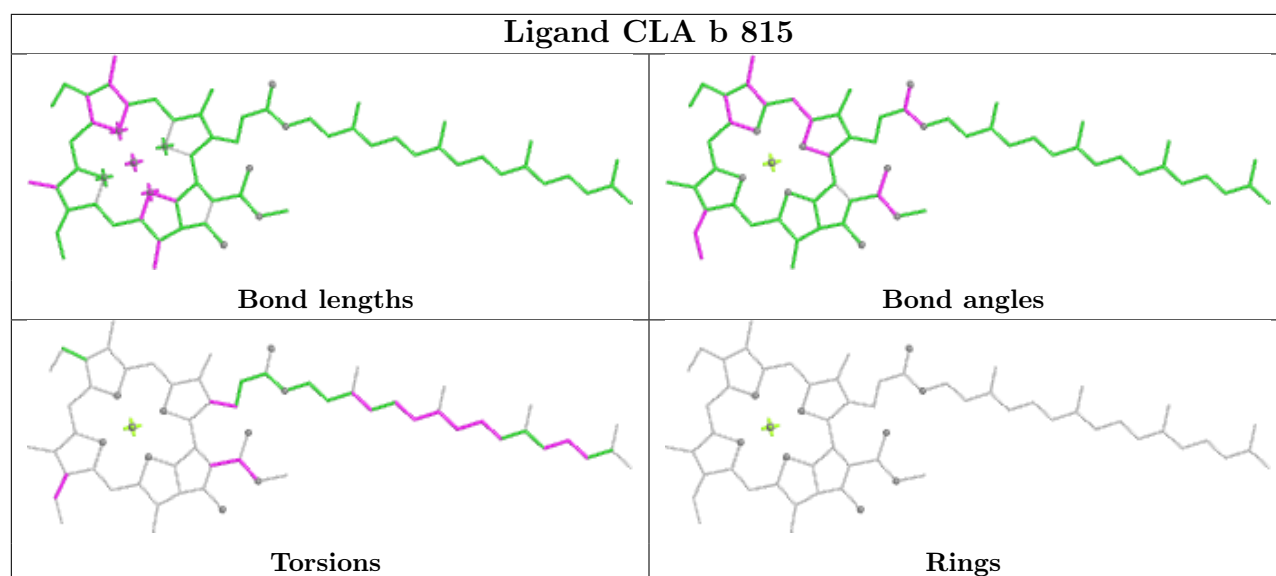
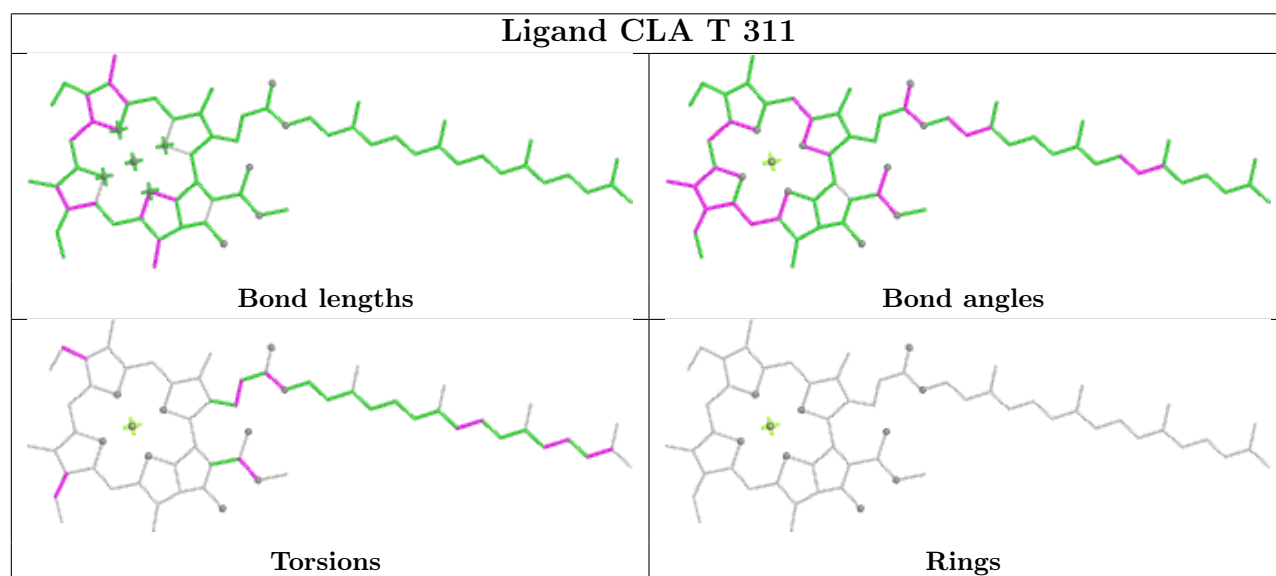
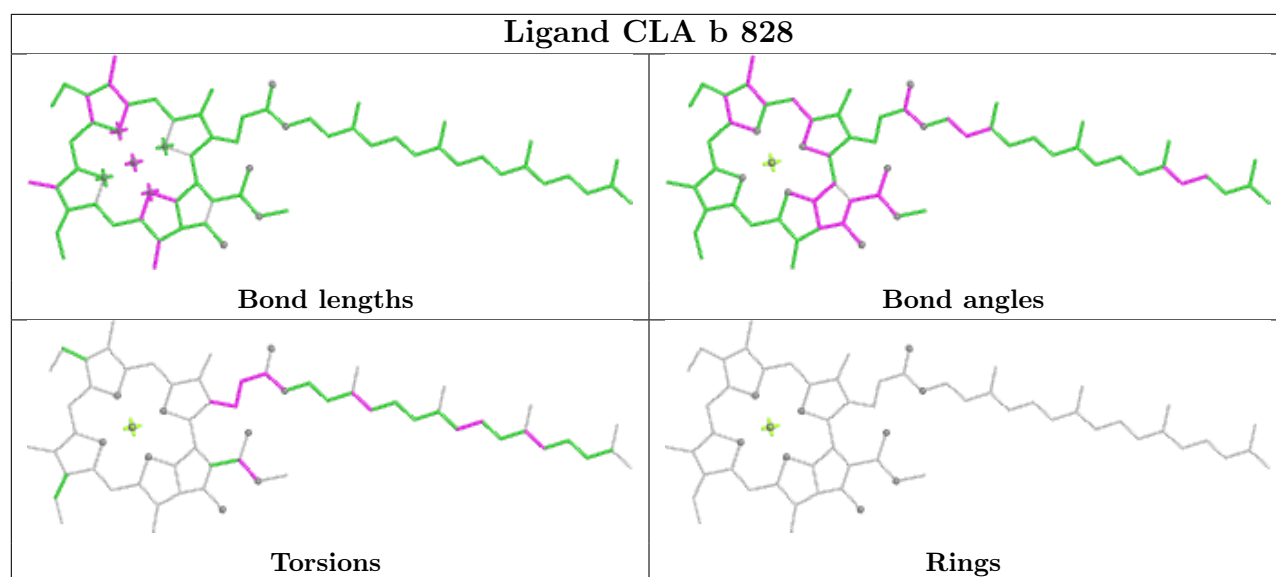


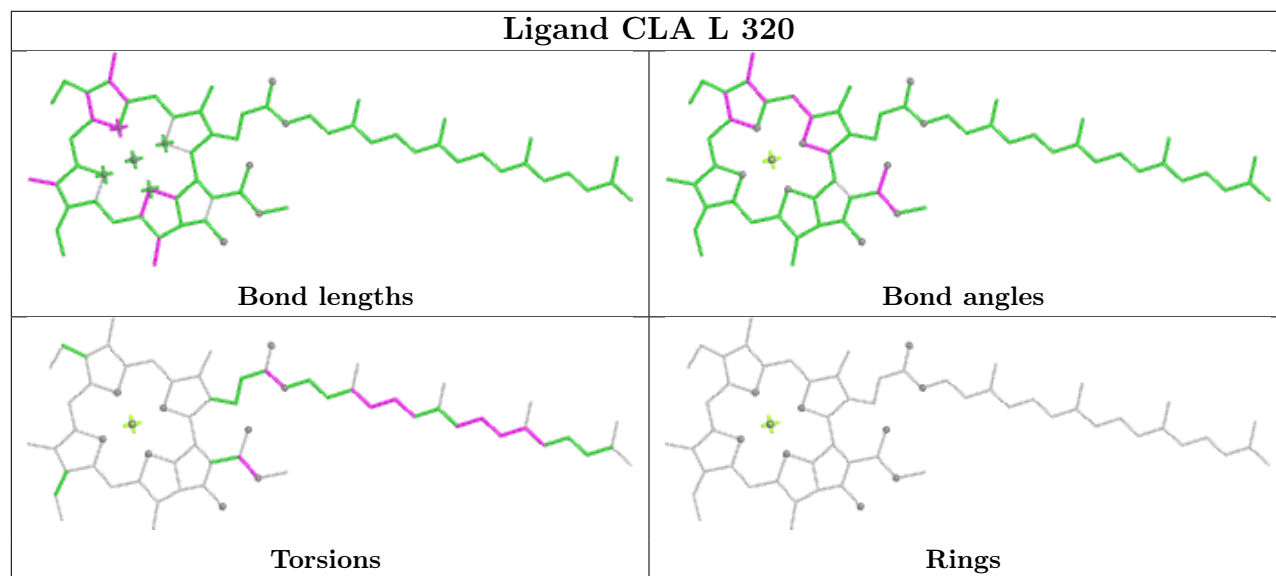
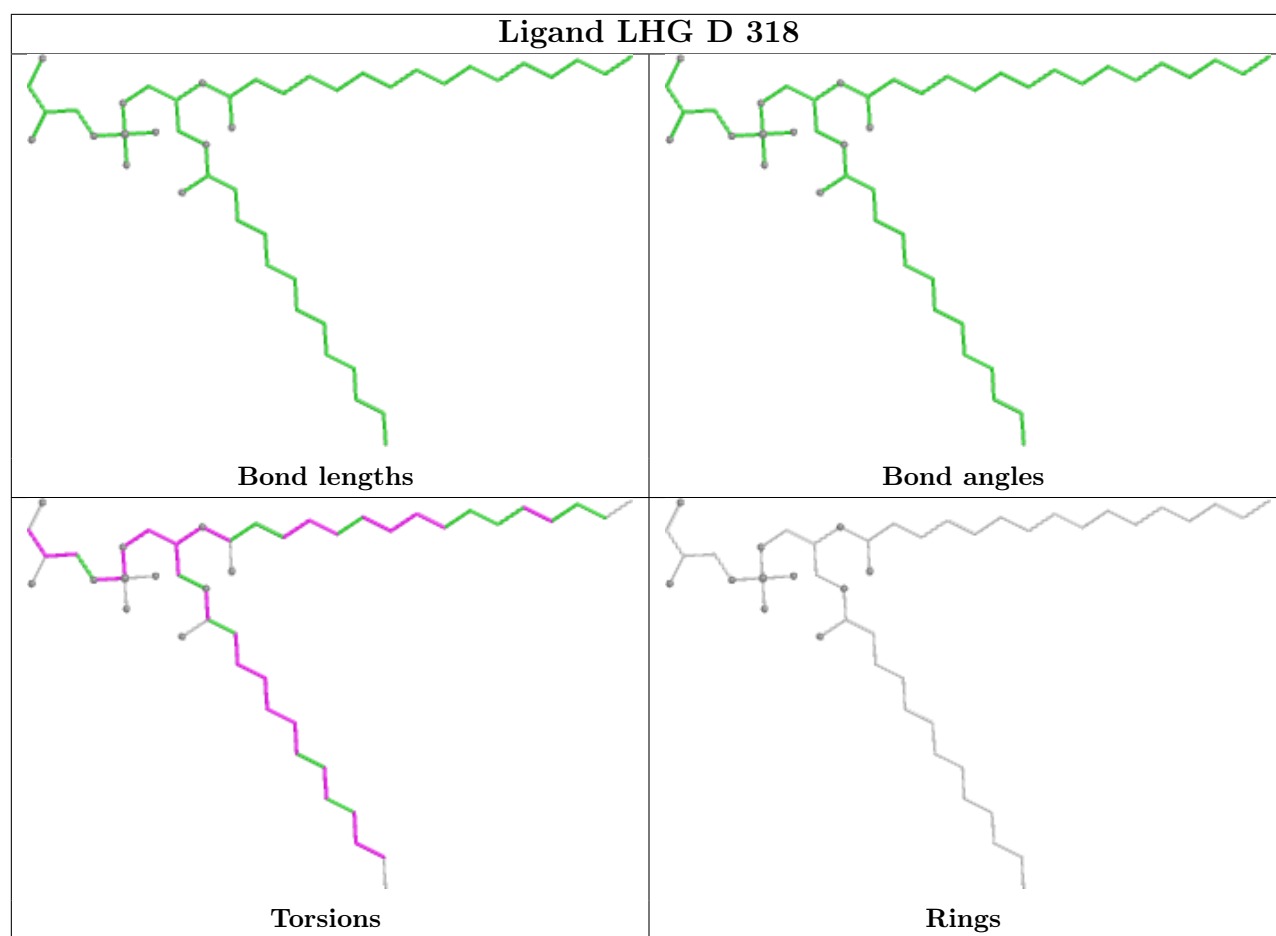
Ligand CLA R 316

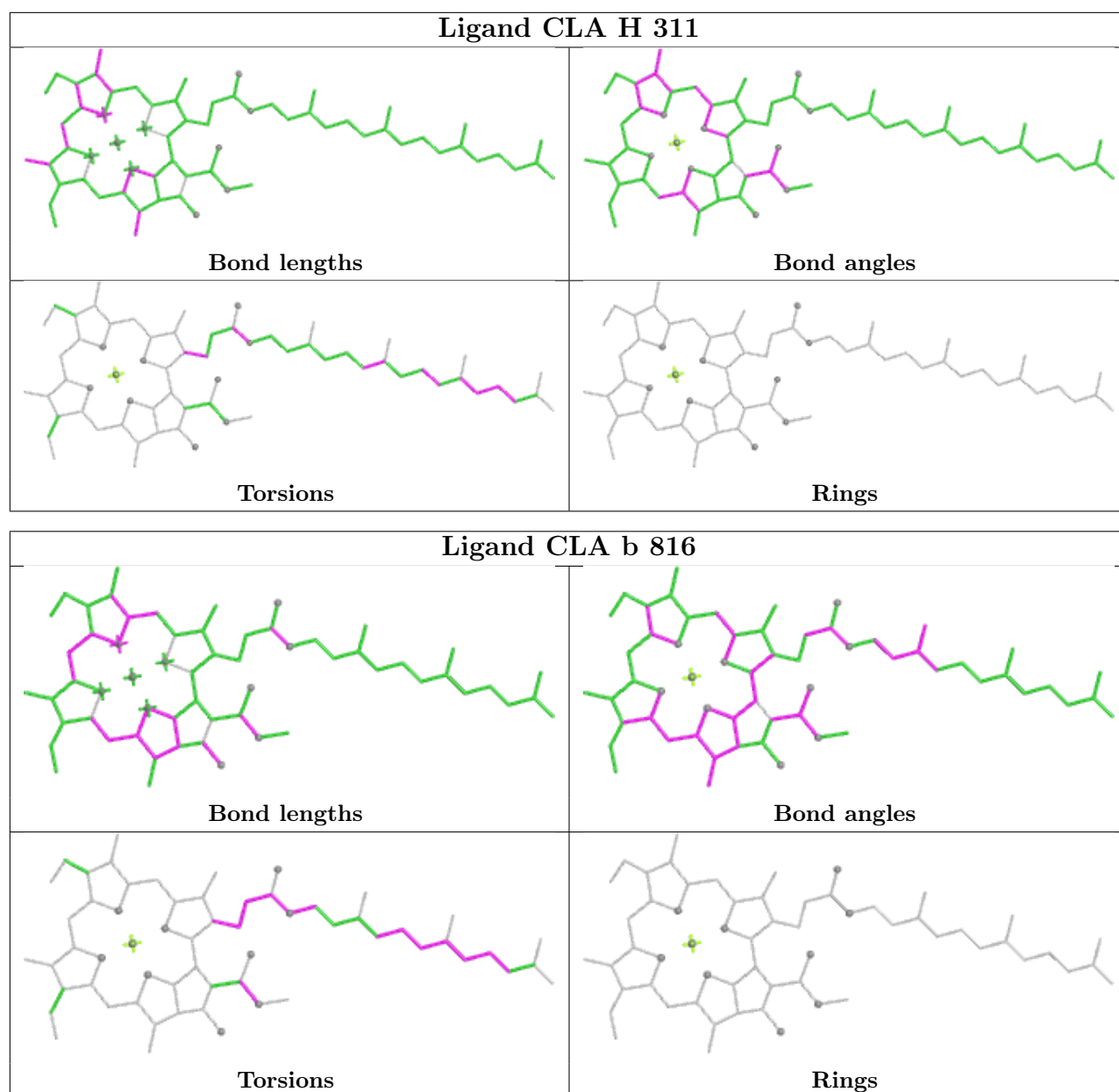


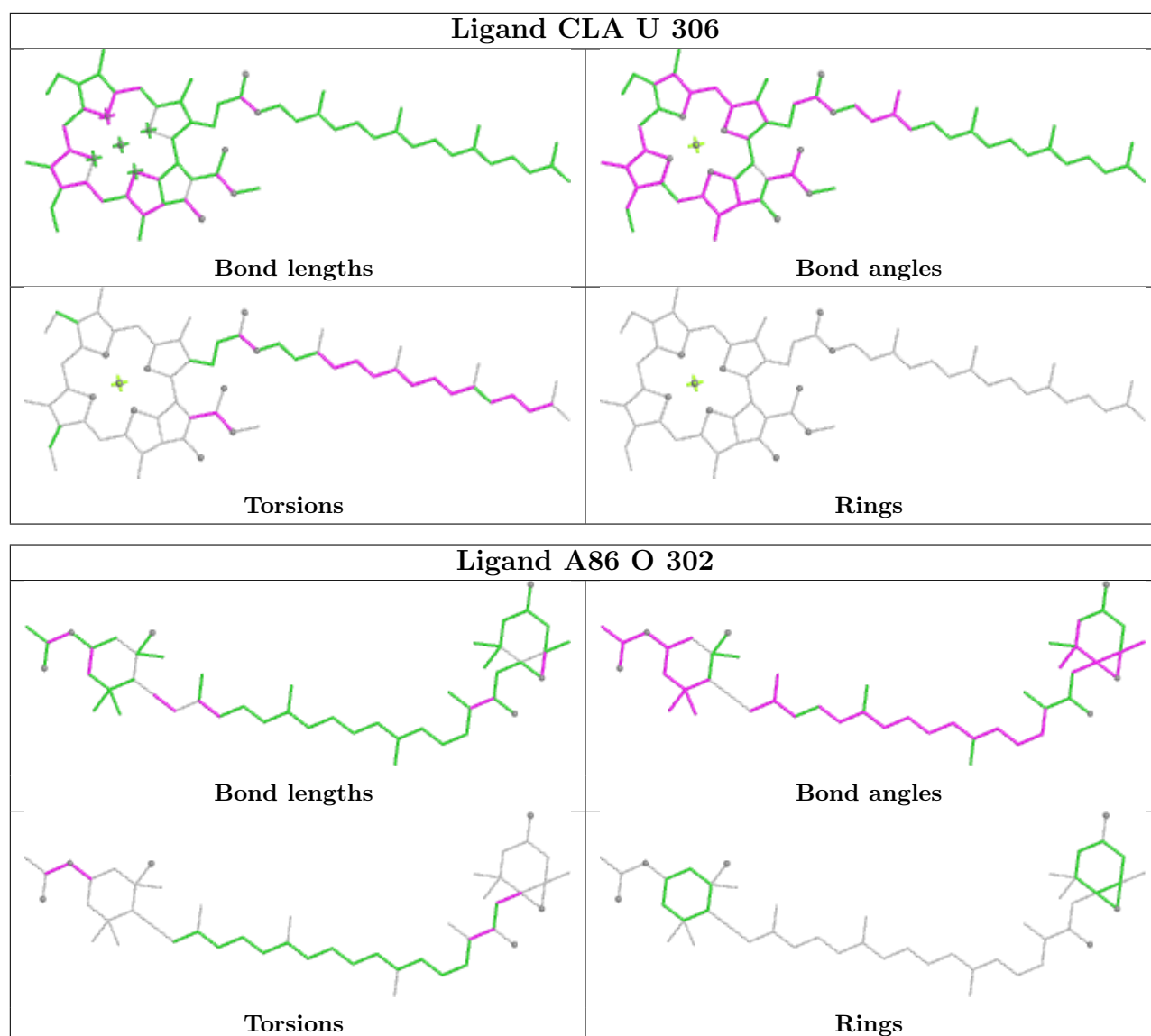
Ligand A86 C 202

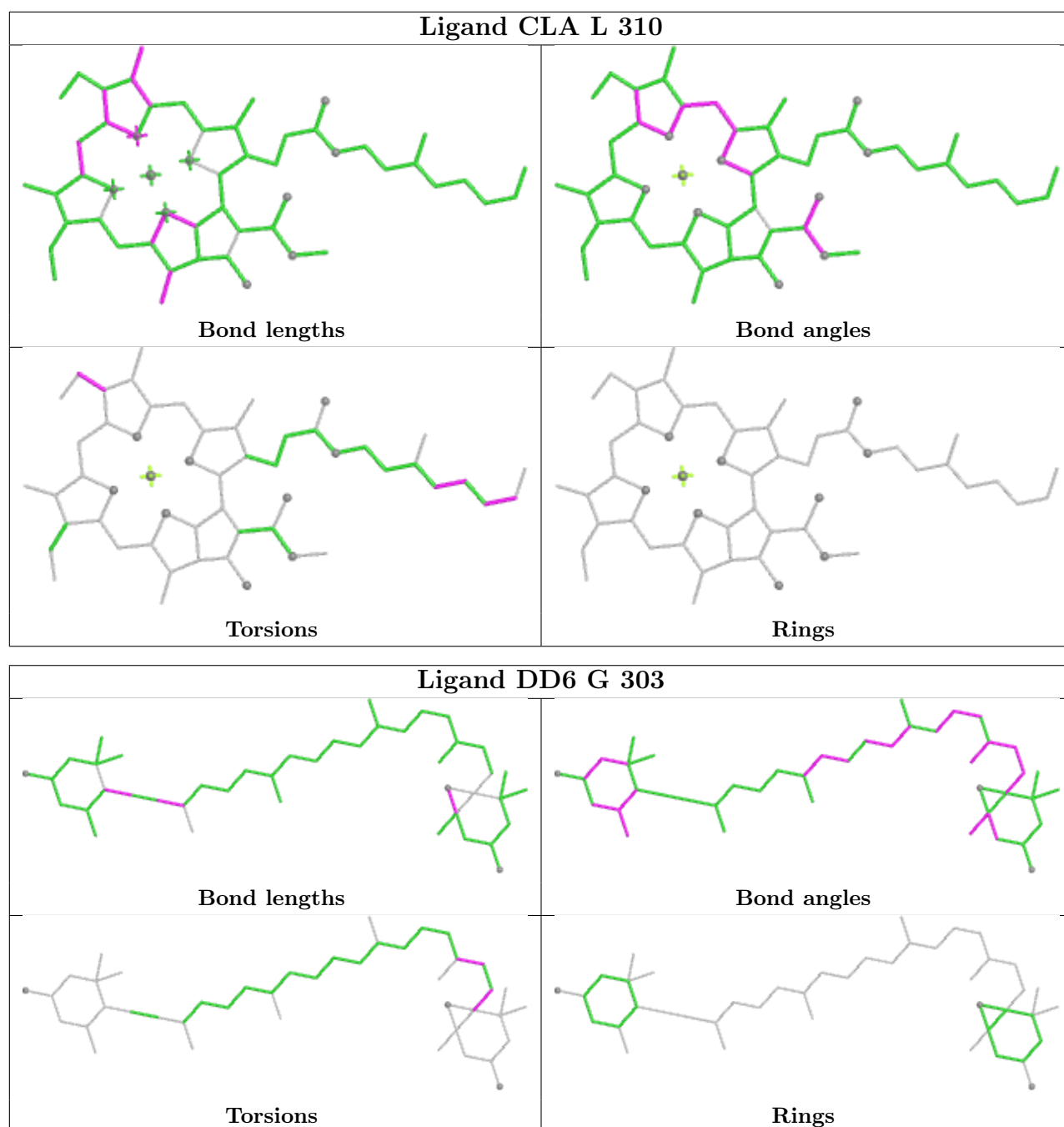


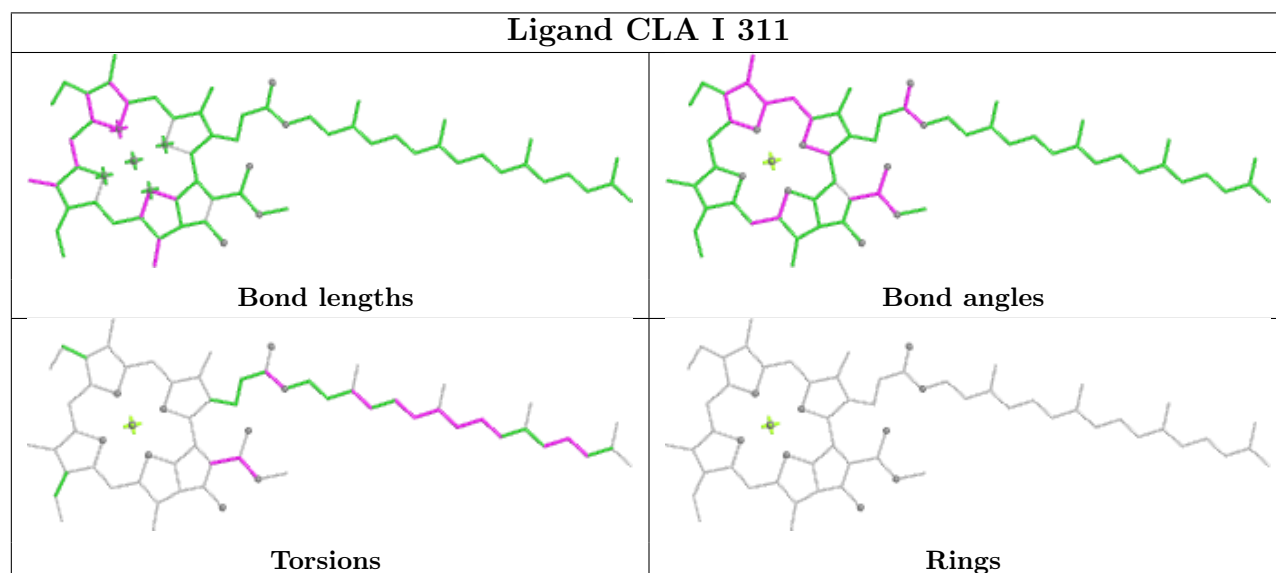
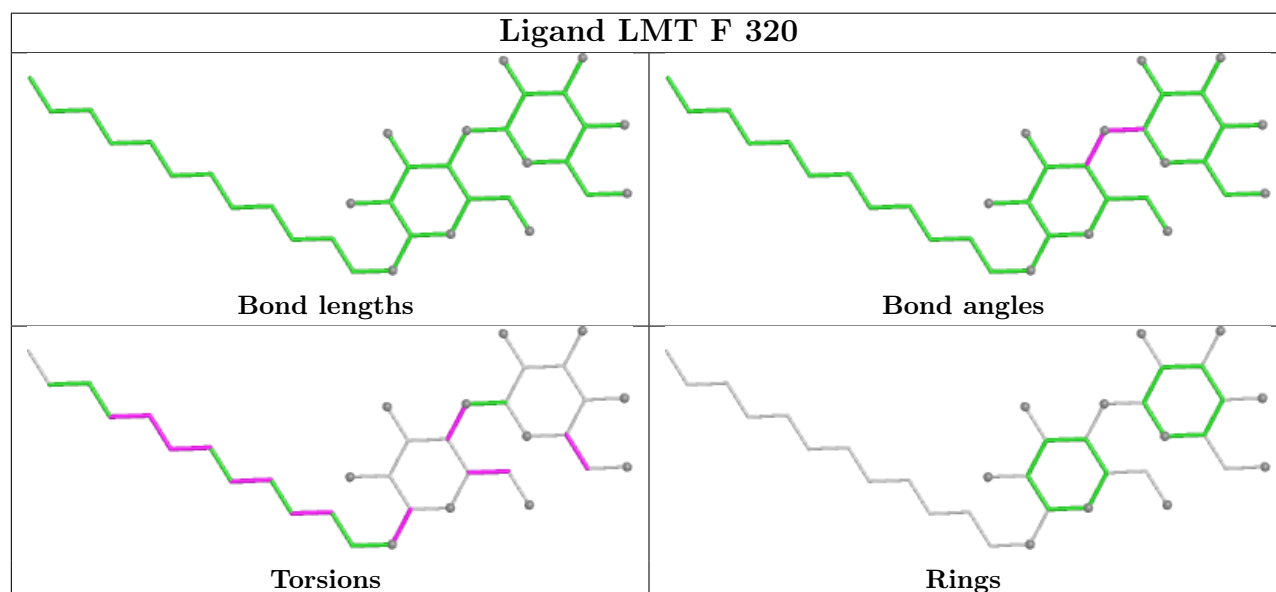
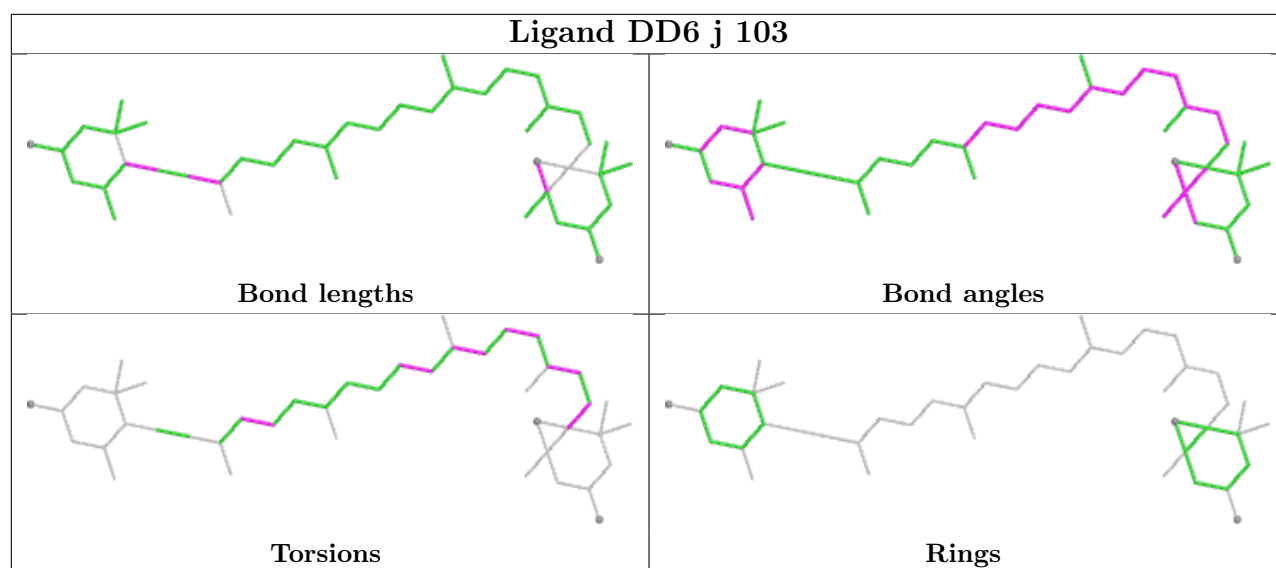


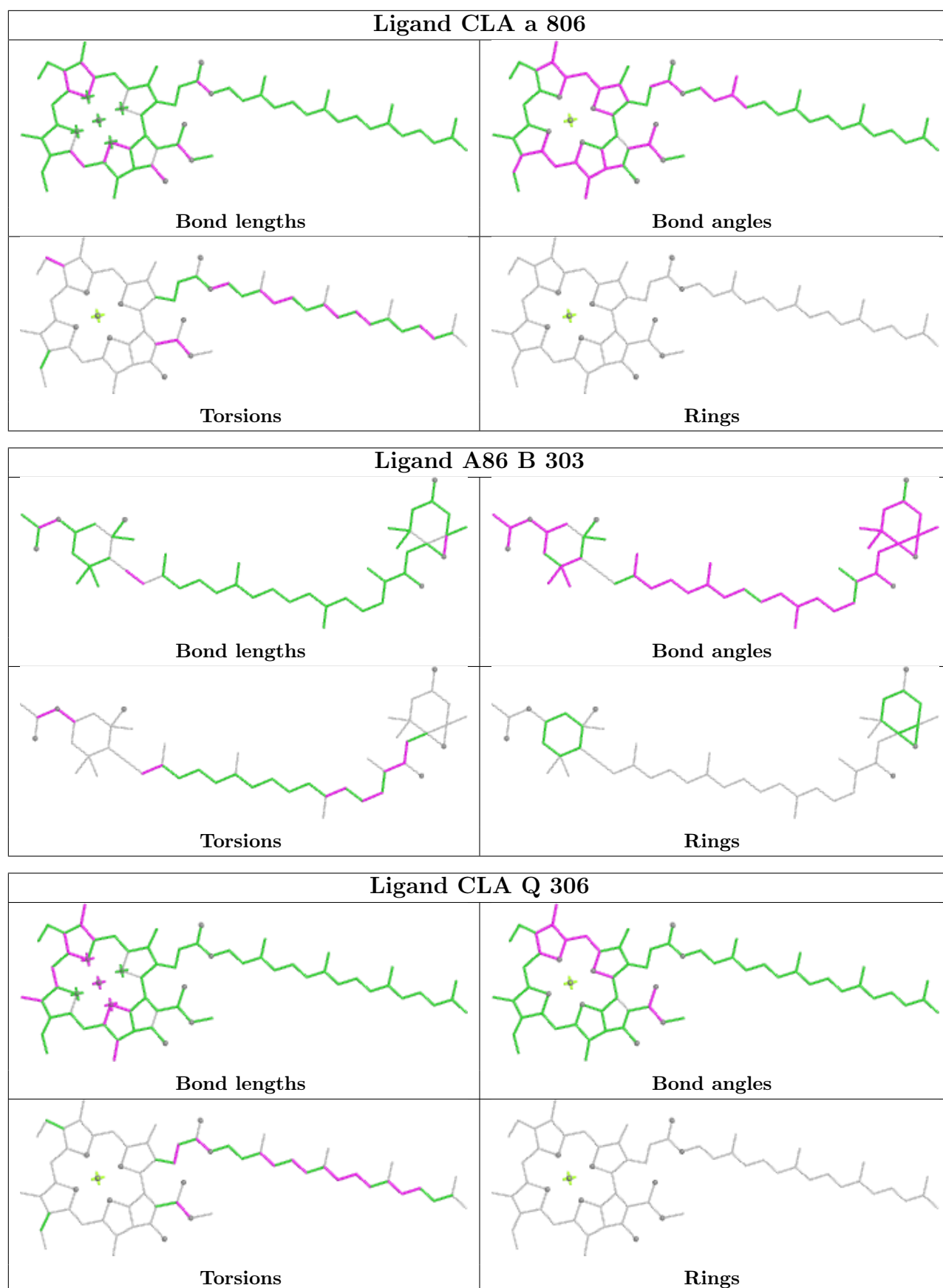


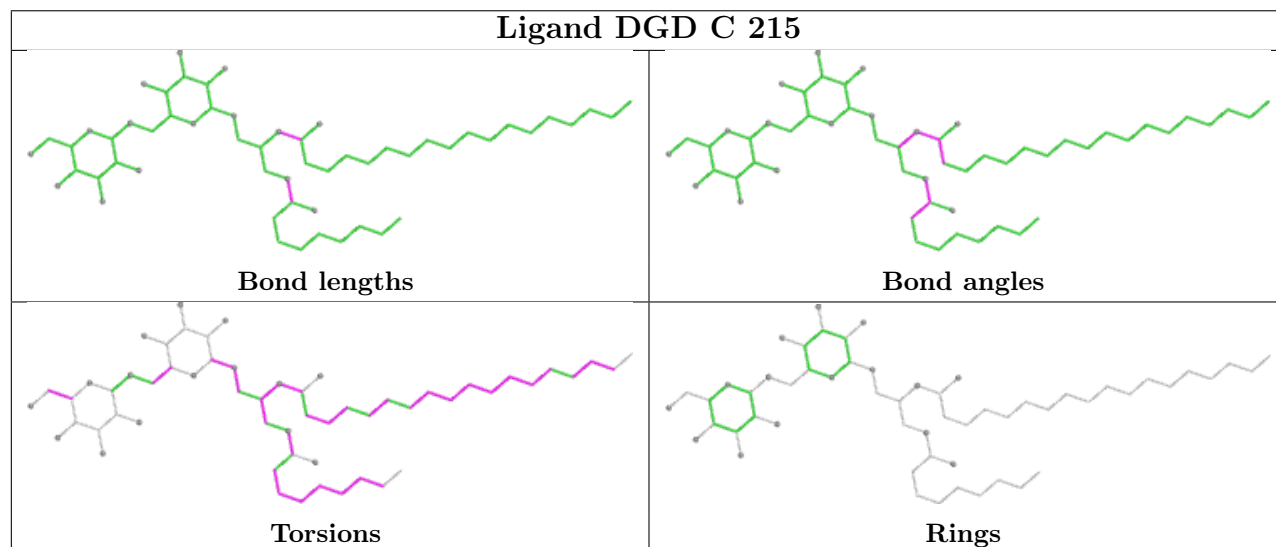
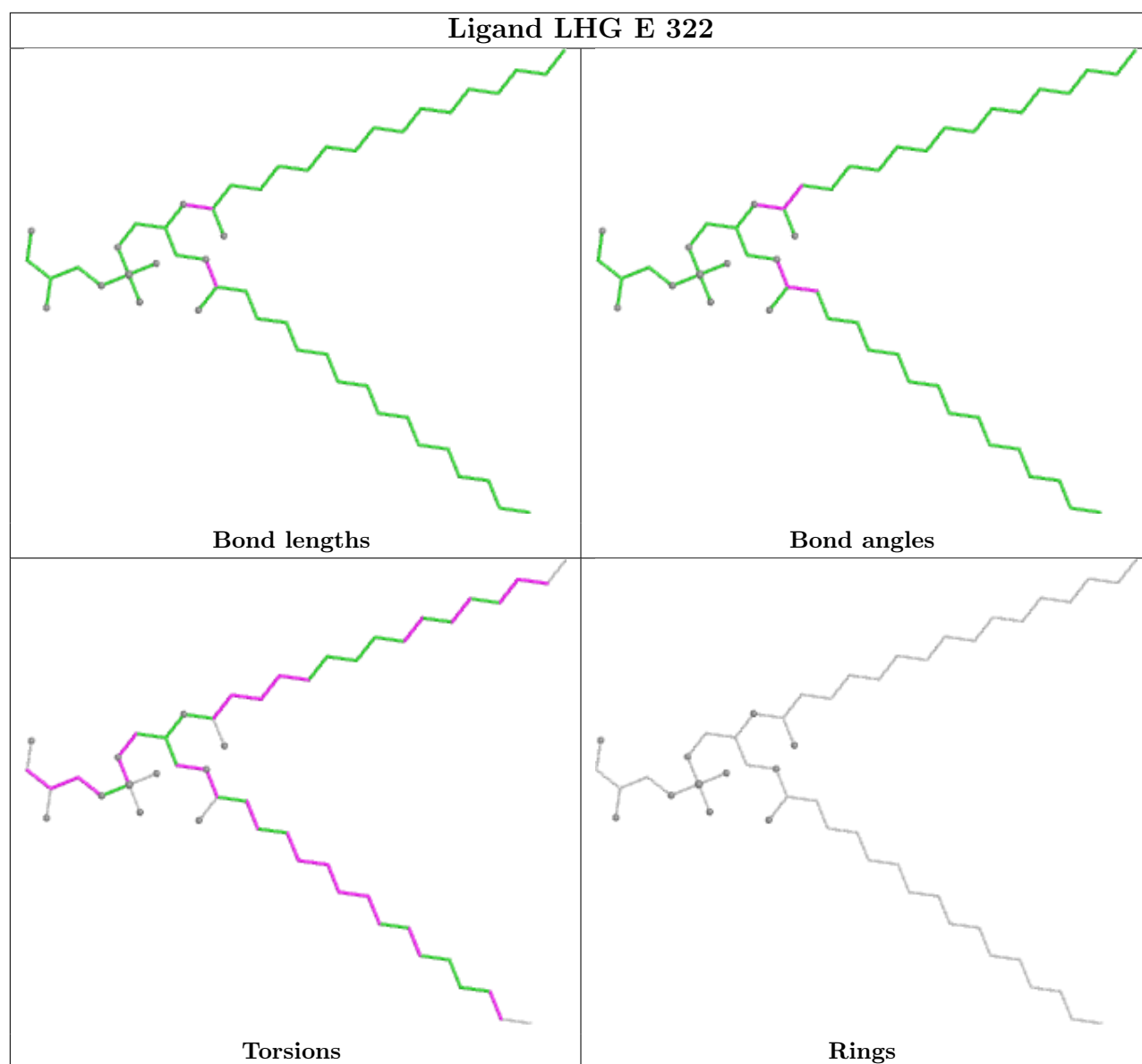


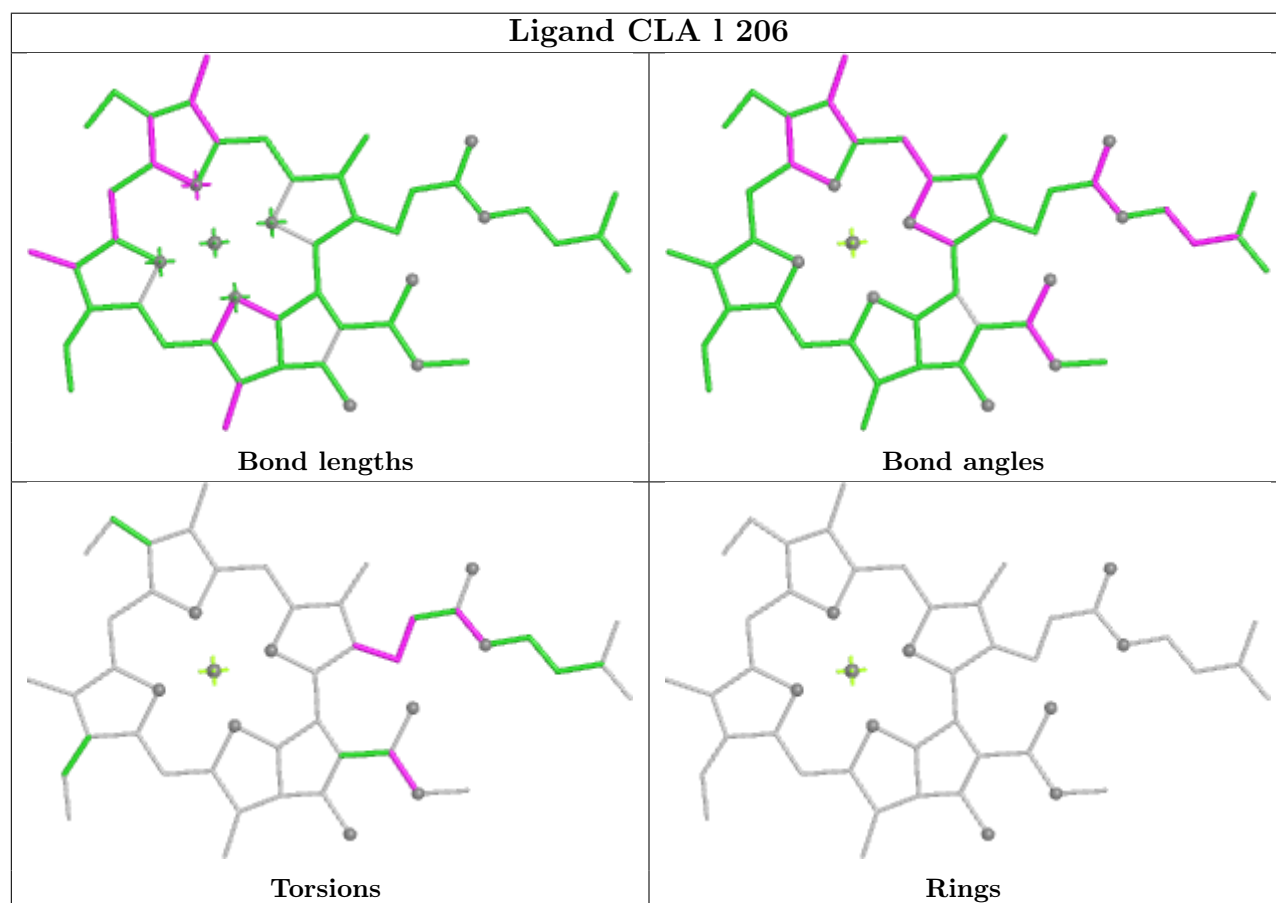
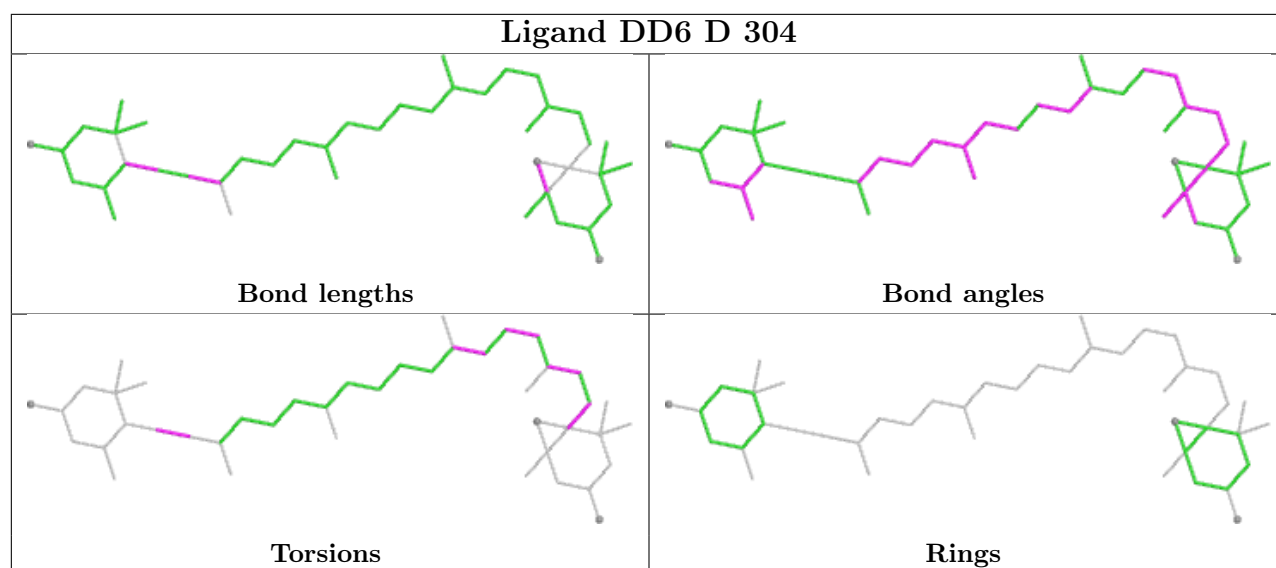


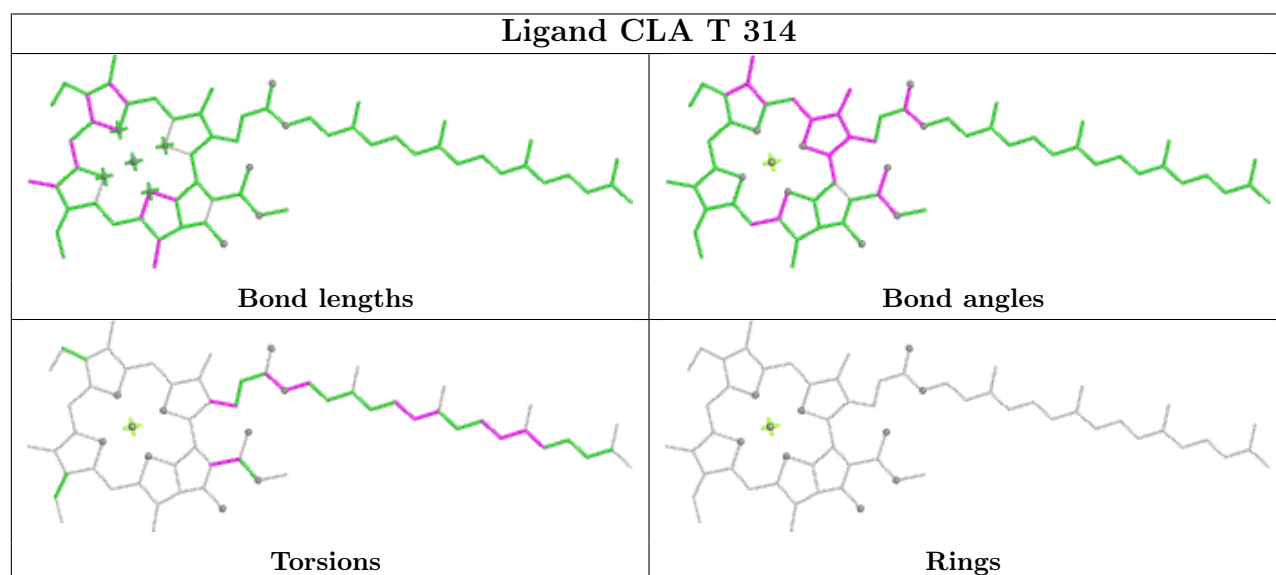
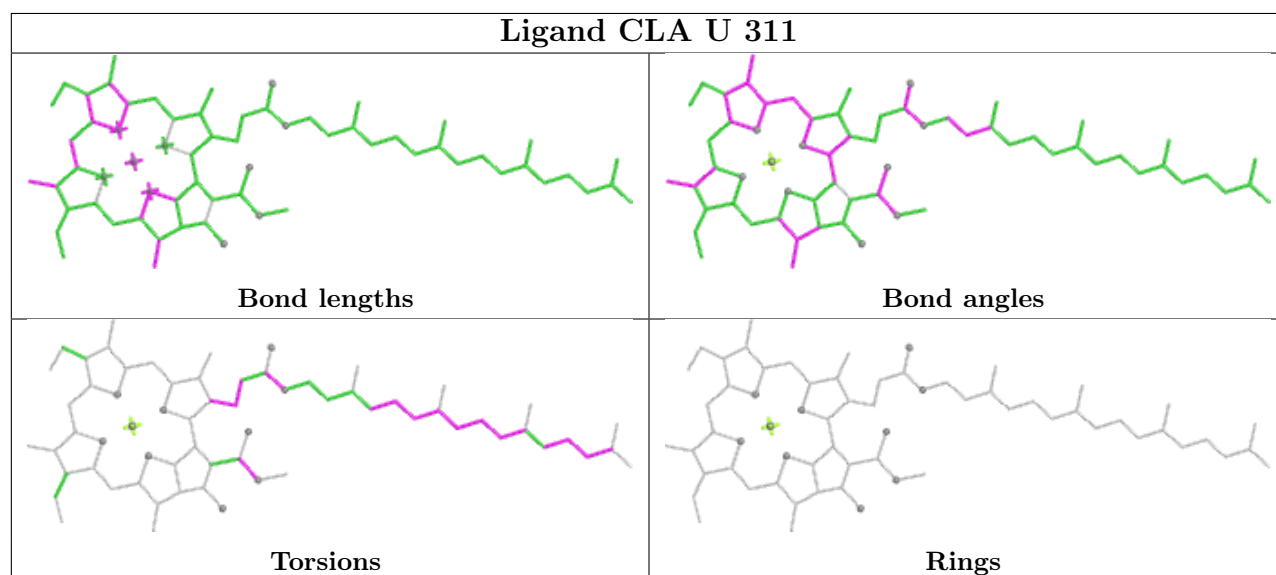
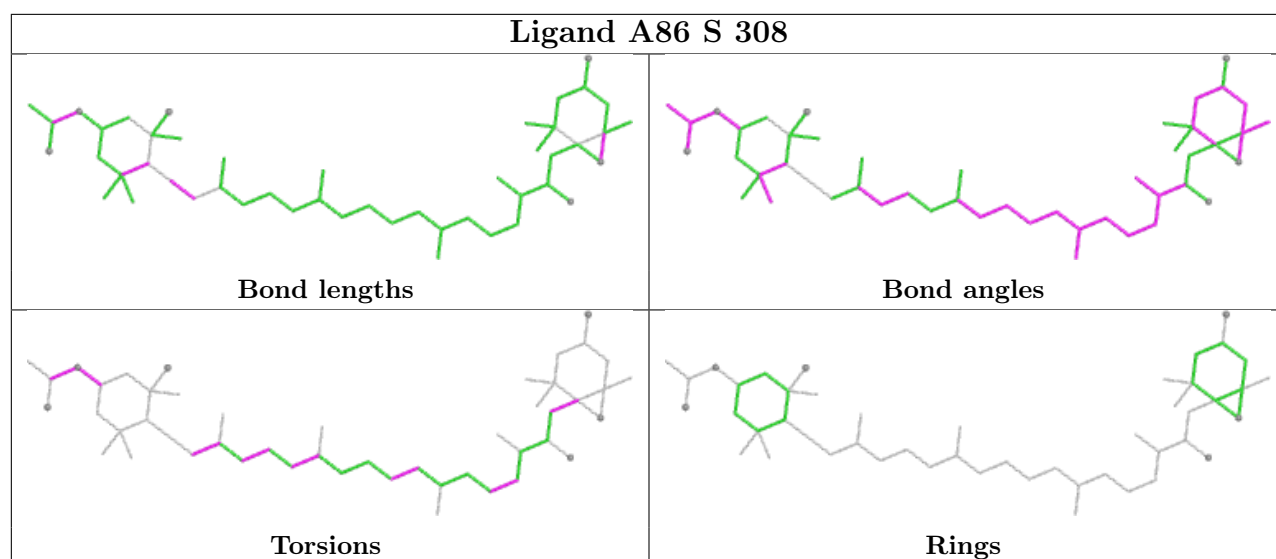




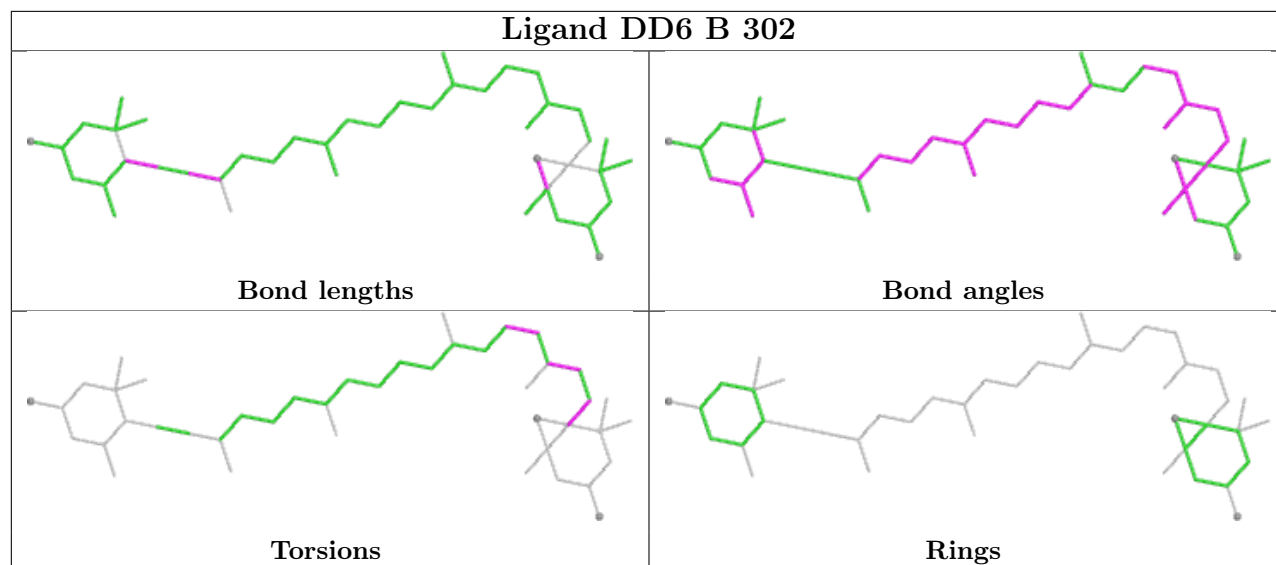




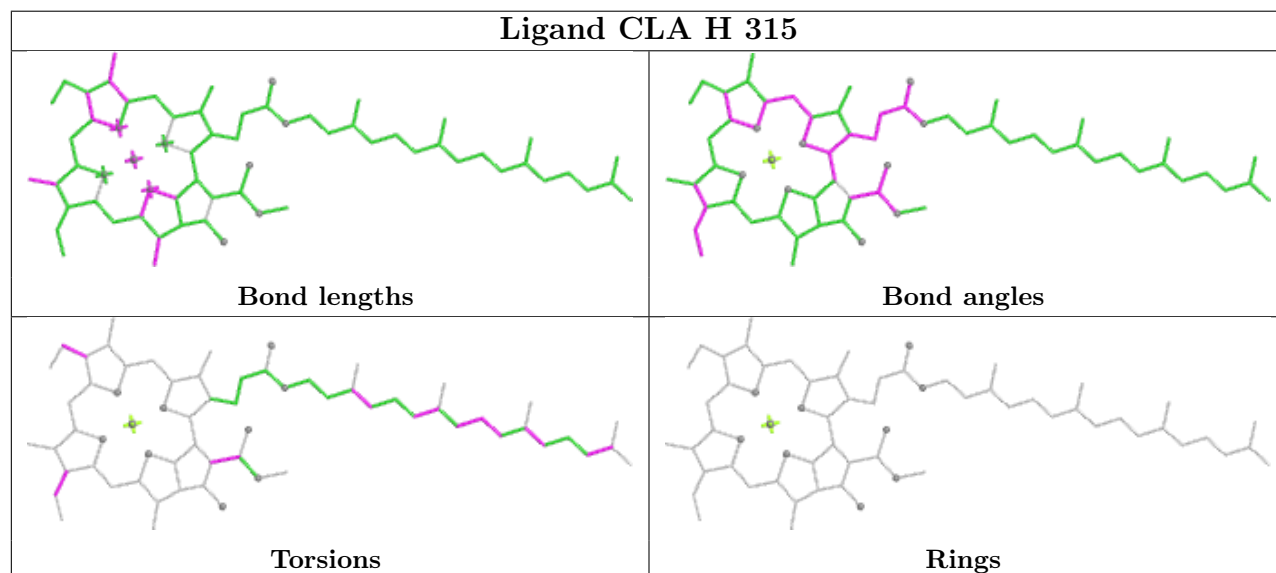




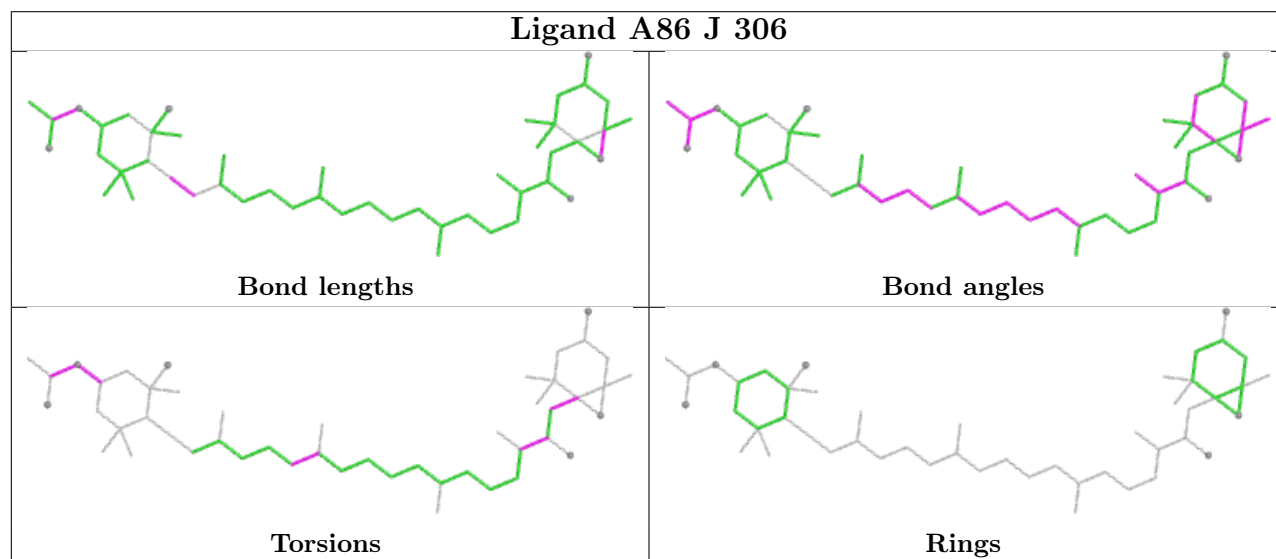
Ligand DD6 B 302

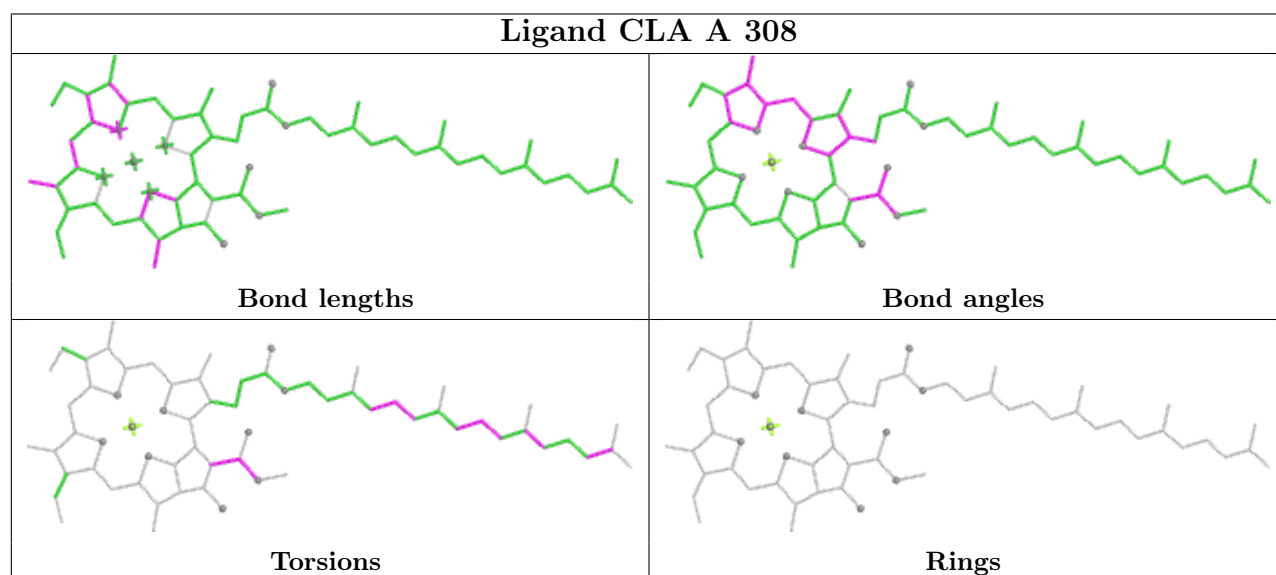
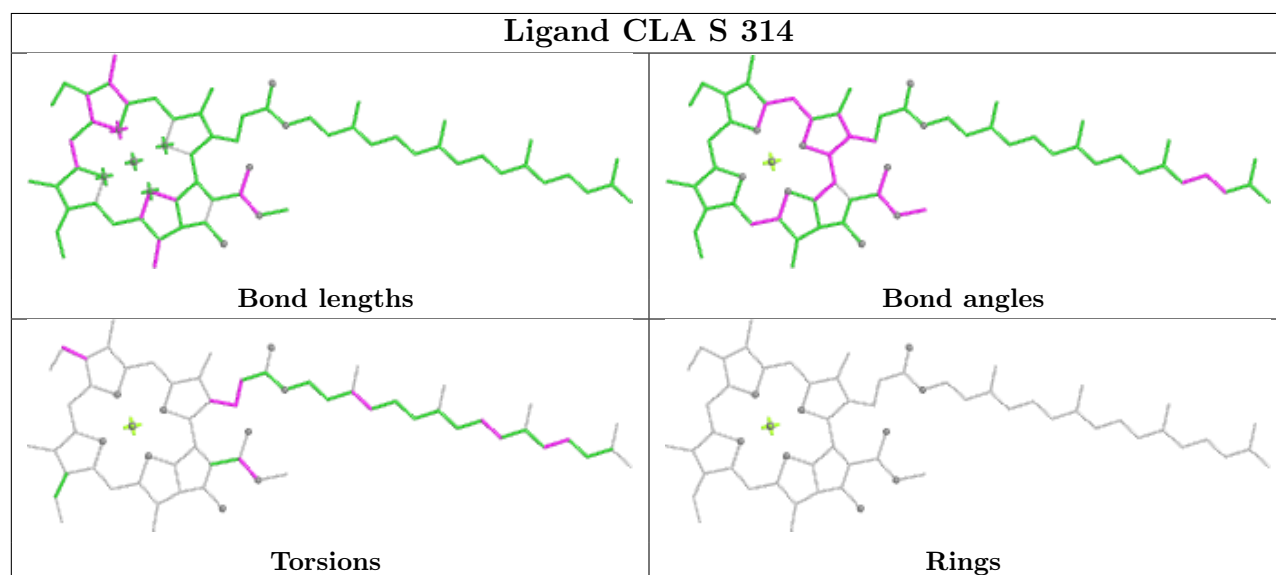
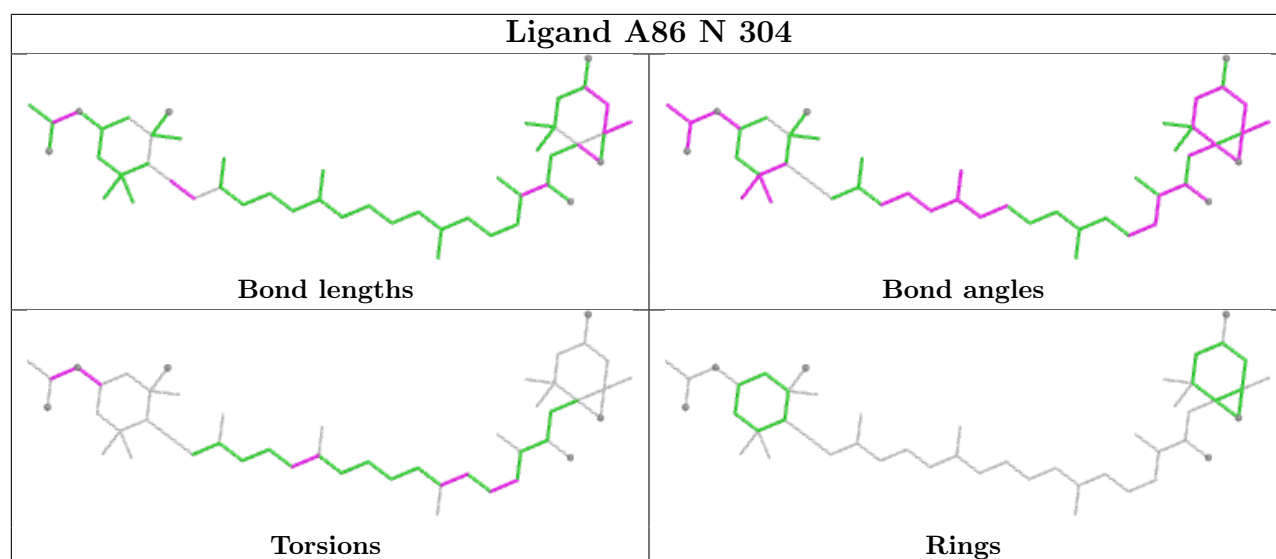


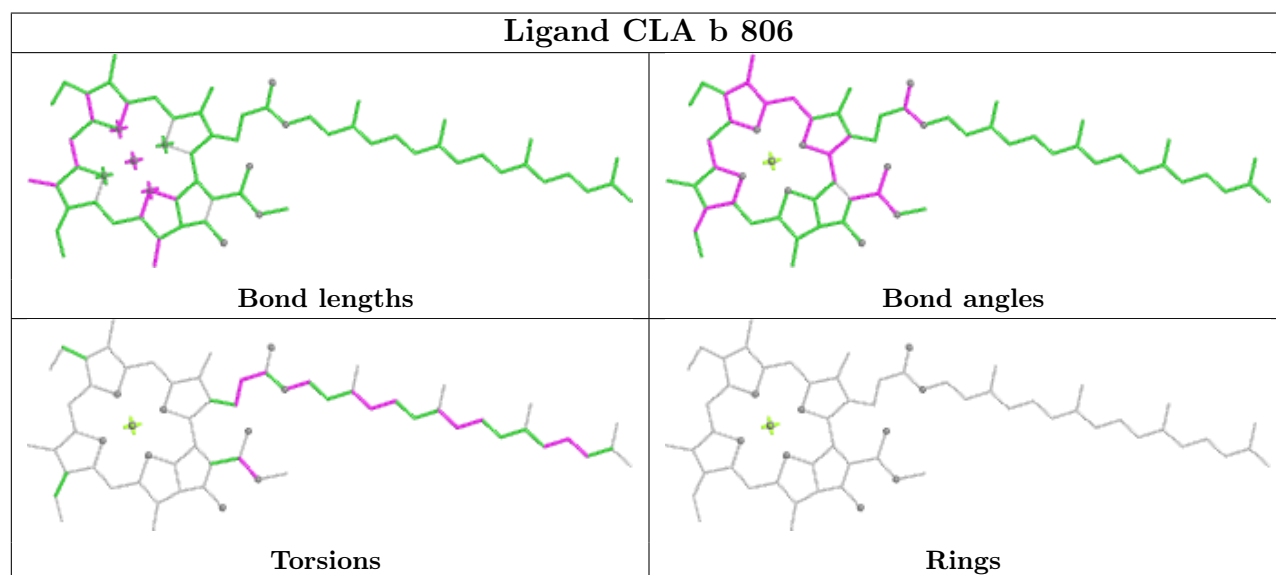
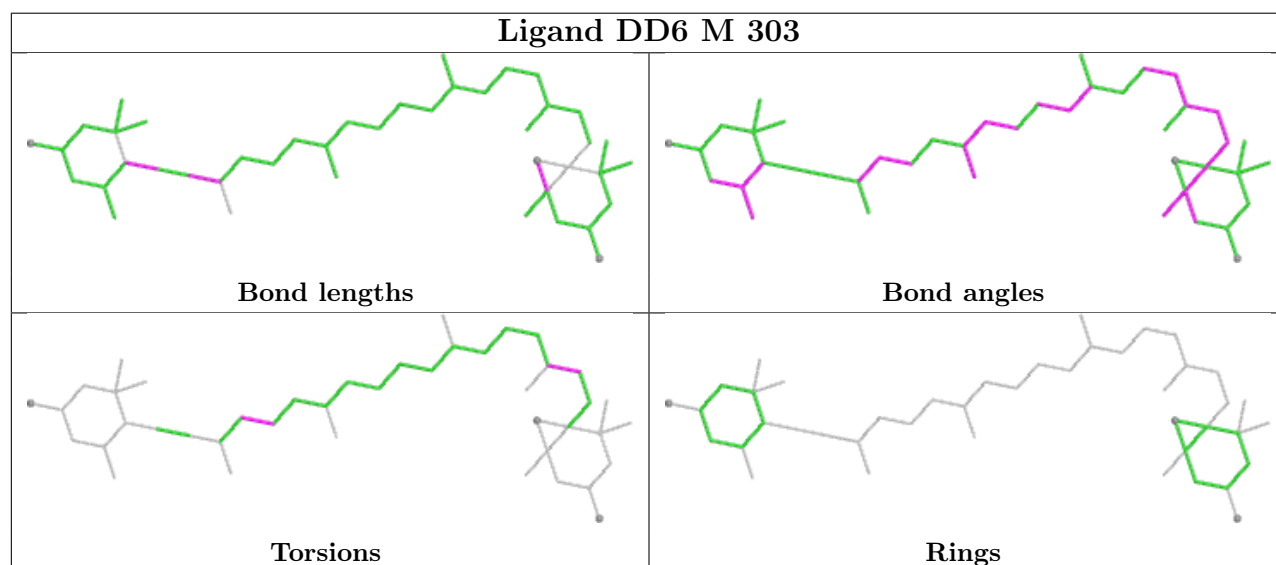
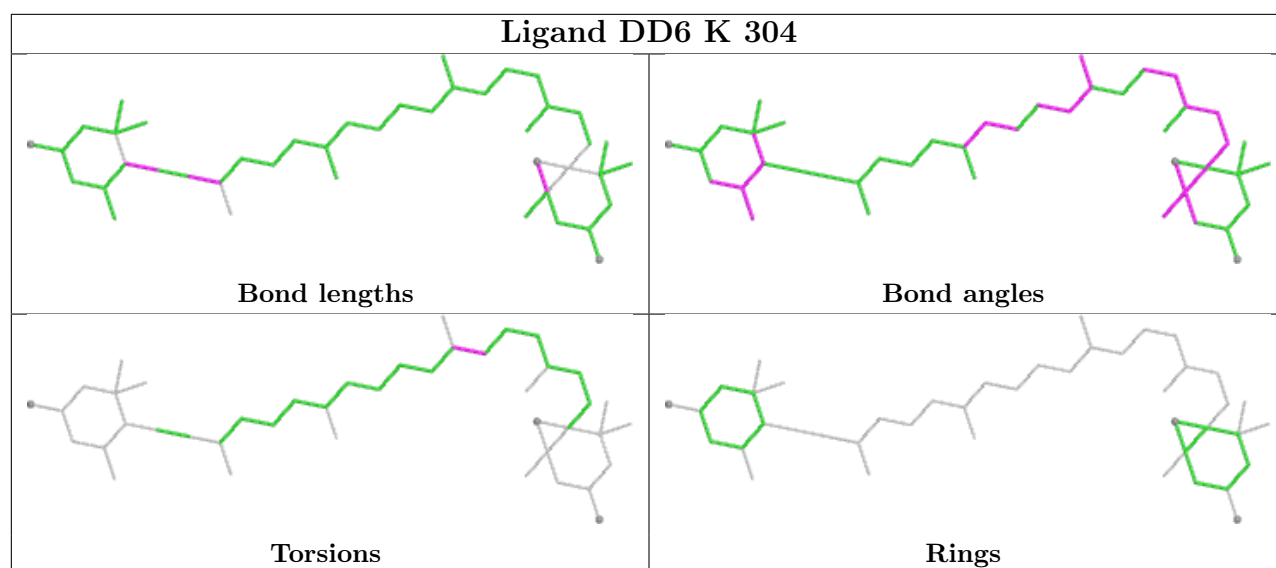
Ligand CLA H 315



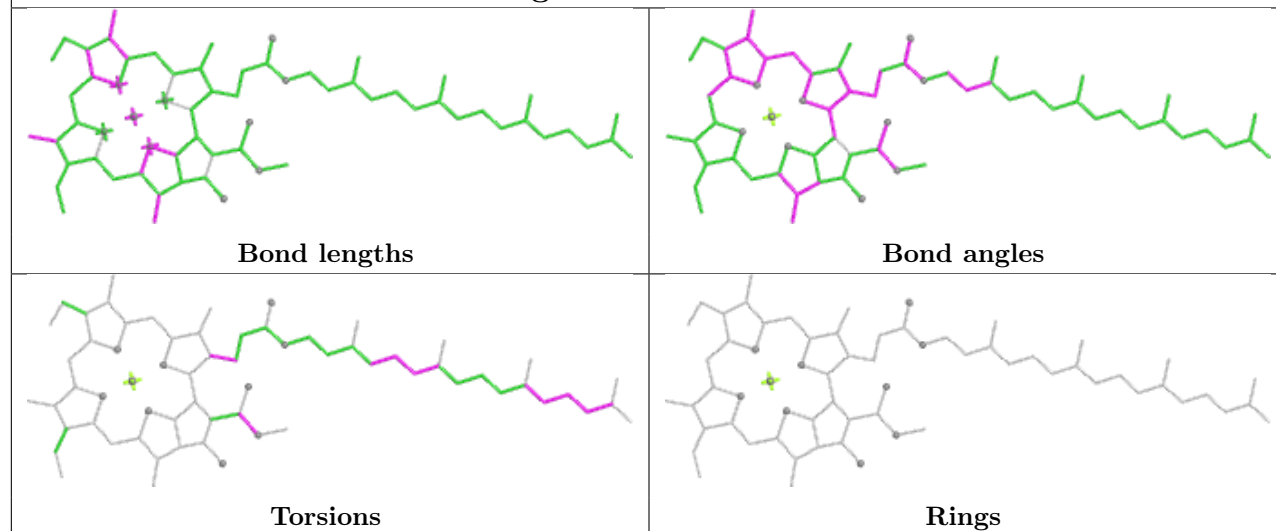
Ligand A86 J 306



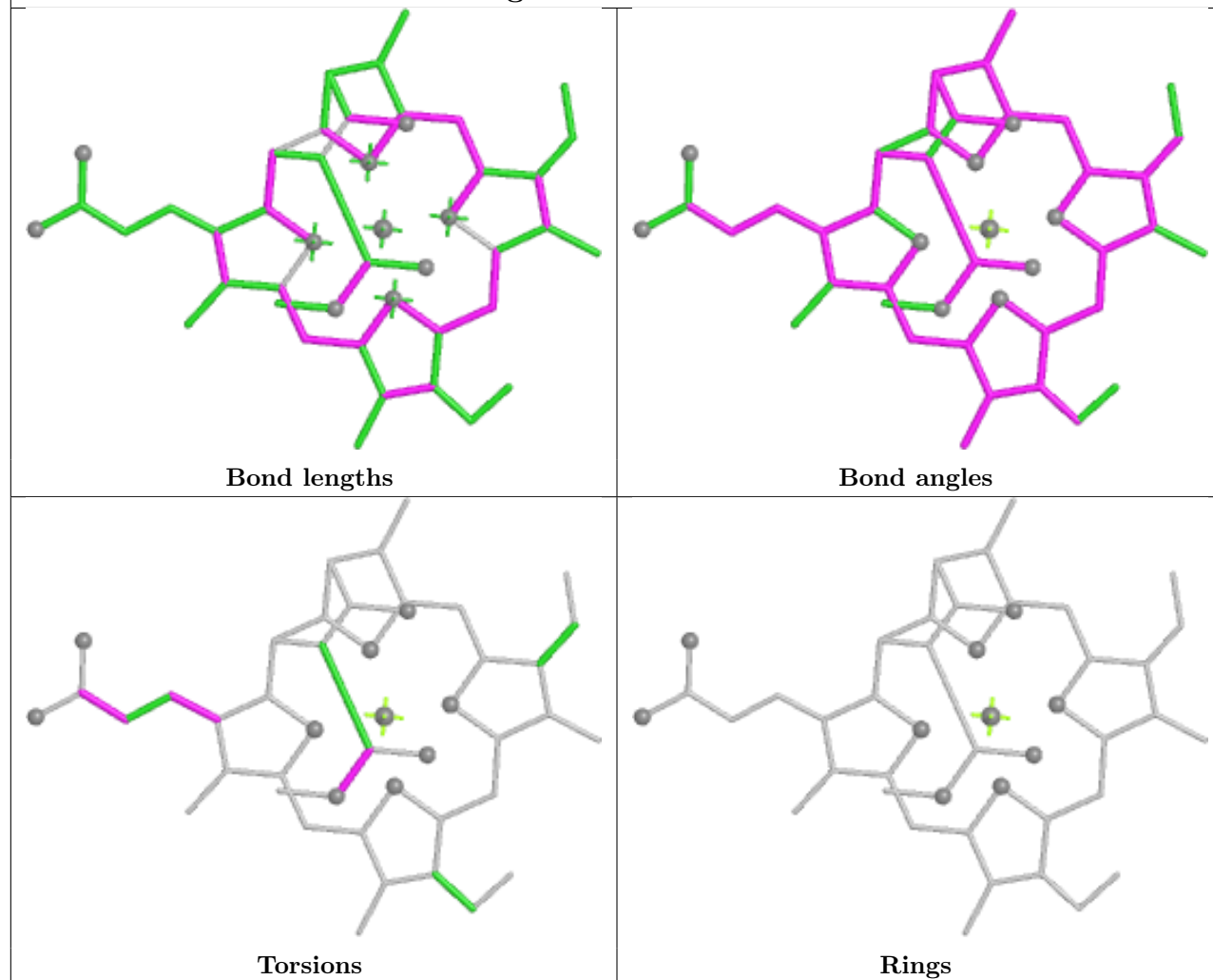




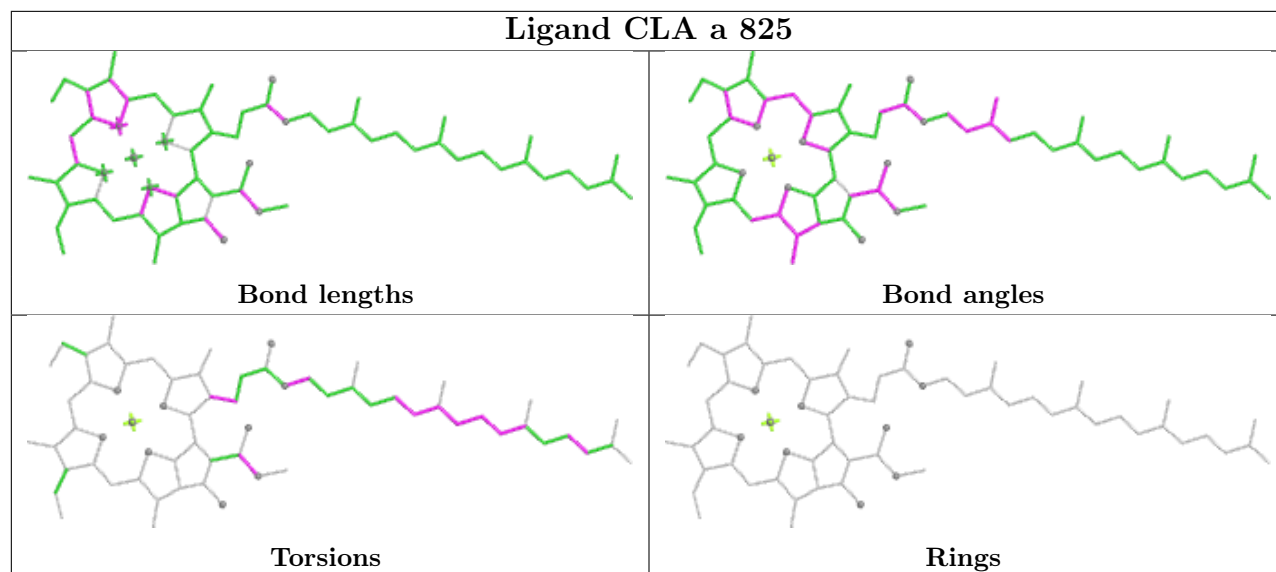
Ligand CLA V 311



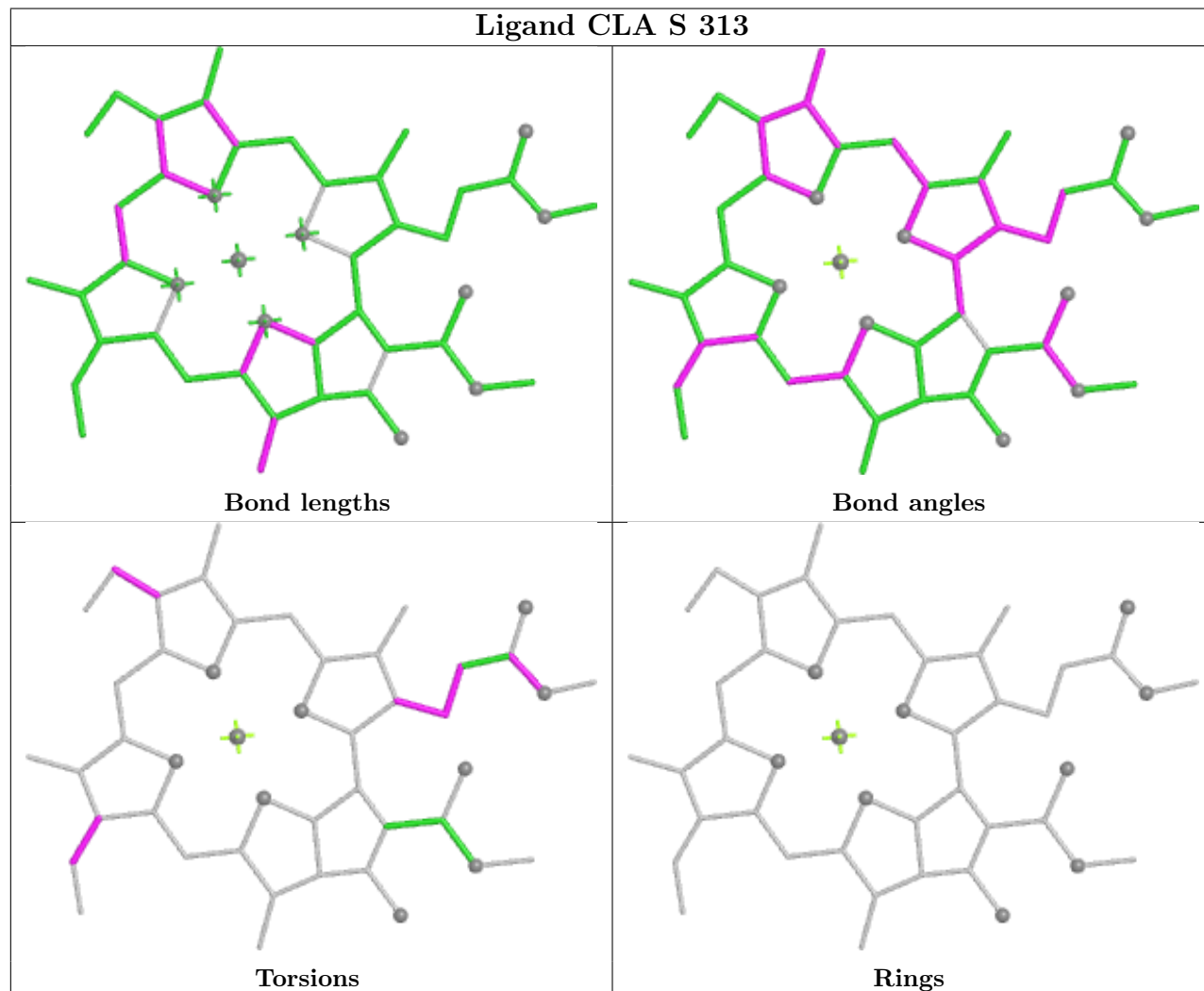
Ligand KC1 D 314



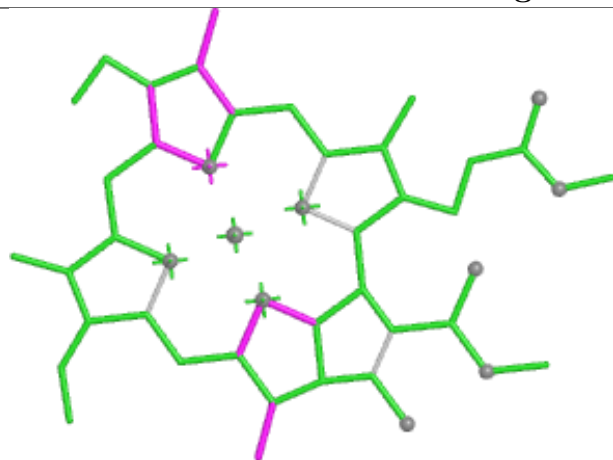
Ligand CLA a 825



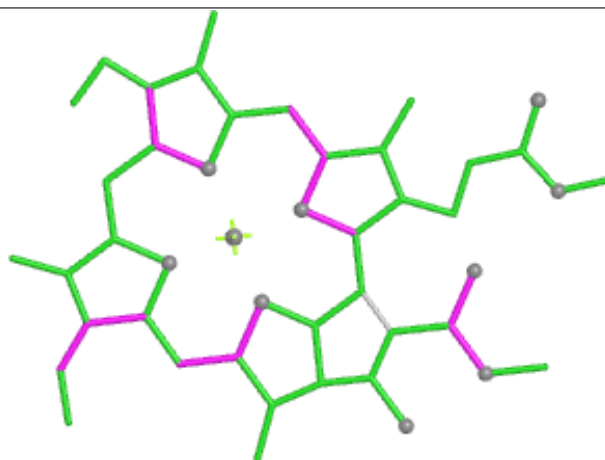
Ligand CLA S 313



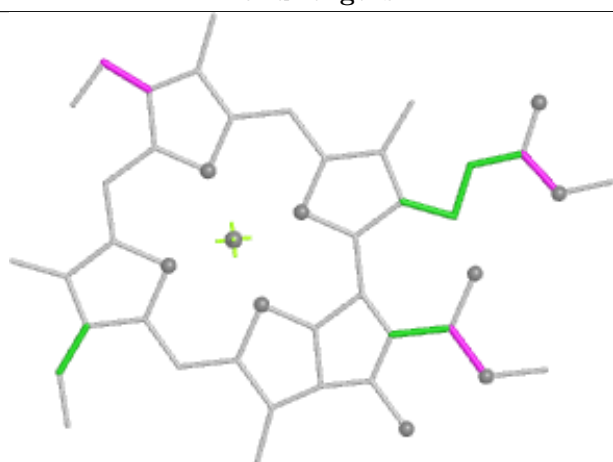
Ligand CLA B 306



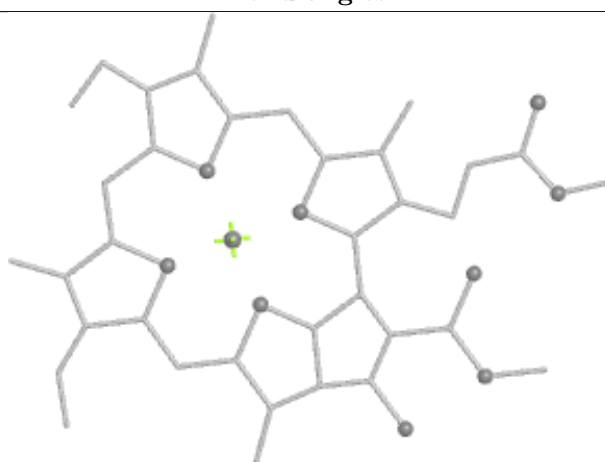
Bond lengths



Bond angles

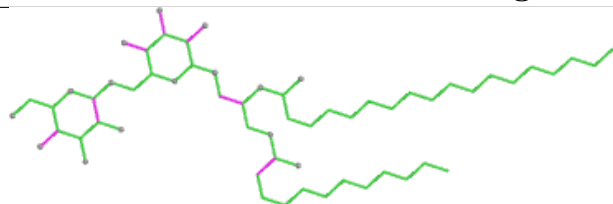


Torsions

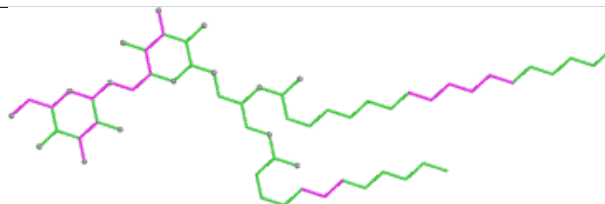


Rings

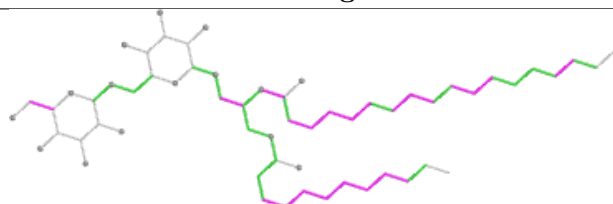
Ligand DGD b 849



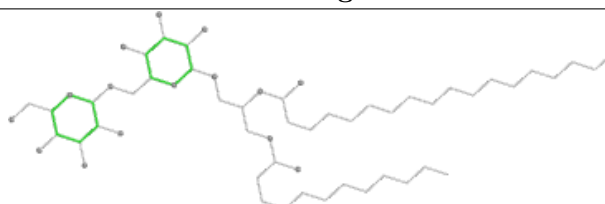
Bond lengths



Bond angles

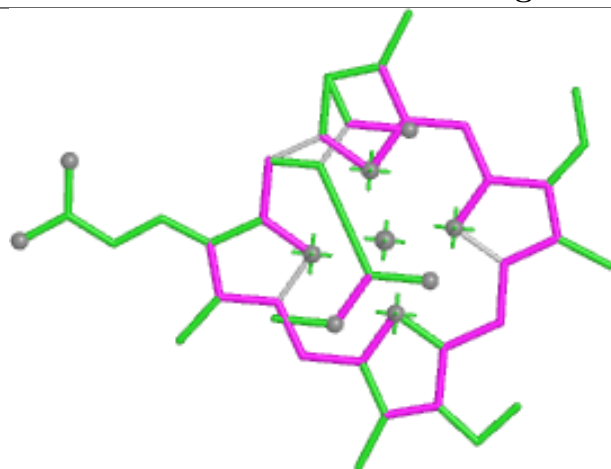


Torsions

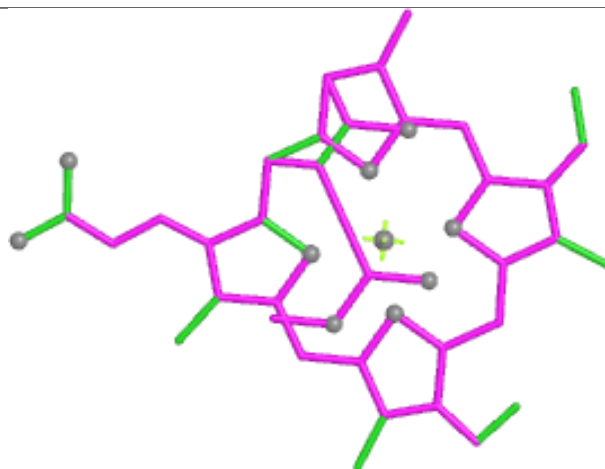


Rings

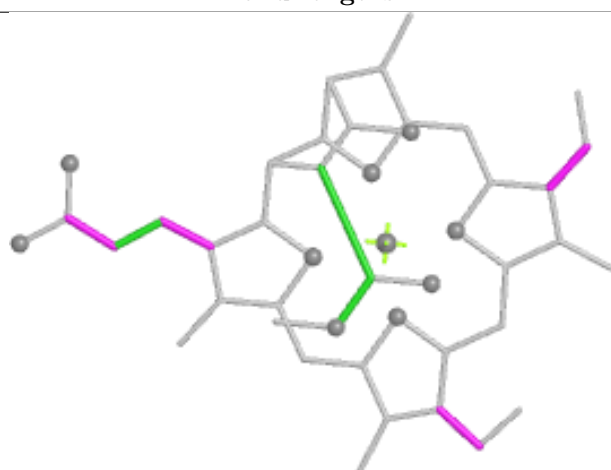
Ligand KC1 N 314



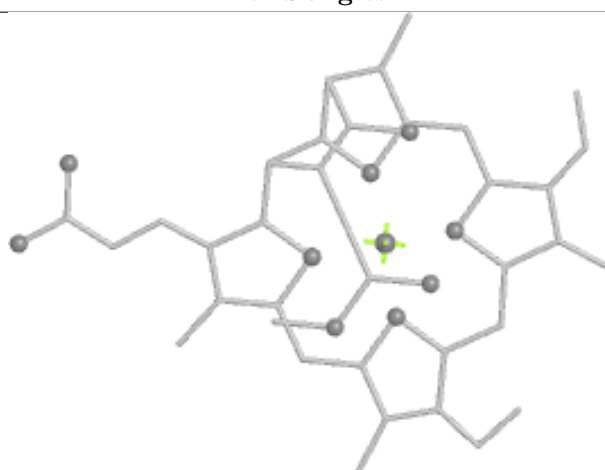
Bond lengths



Bond angles

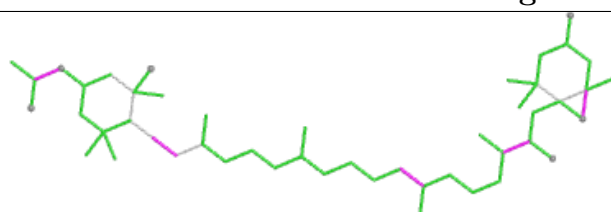


Torsions

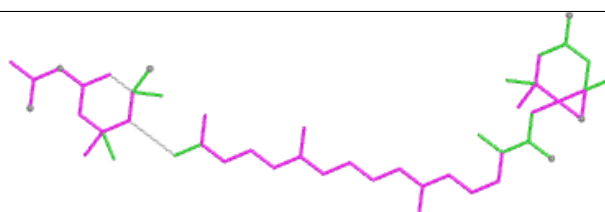


Rings

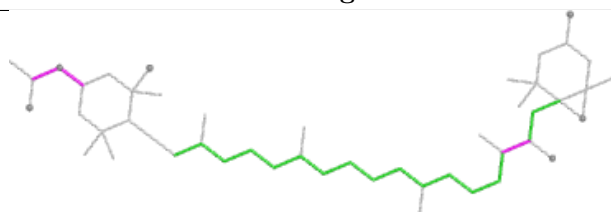
Ligand A86 N 303



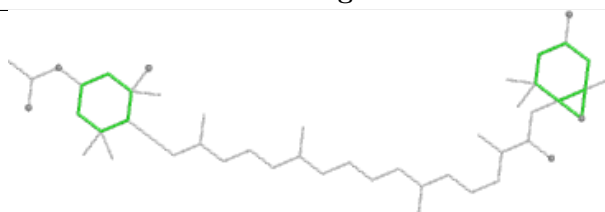
Bond lengths



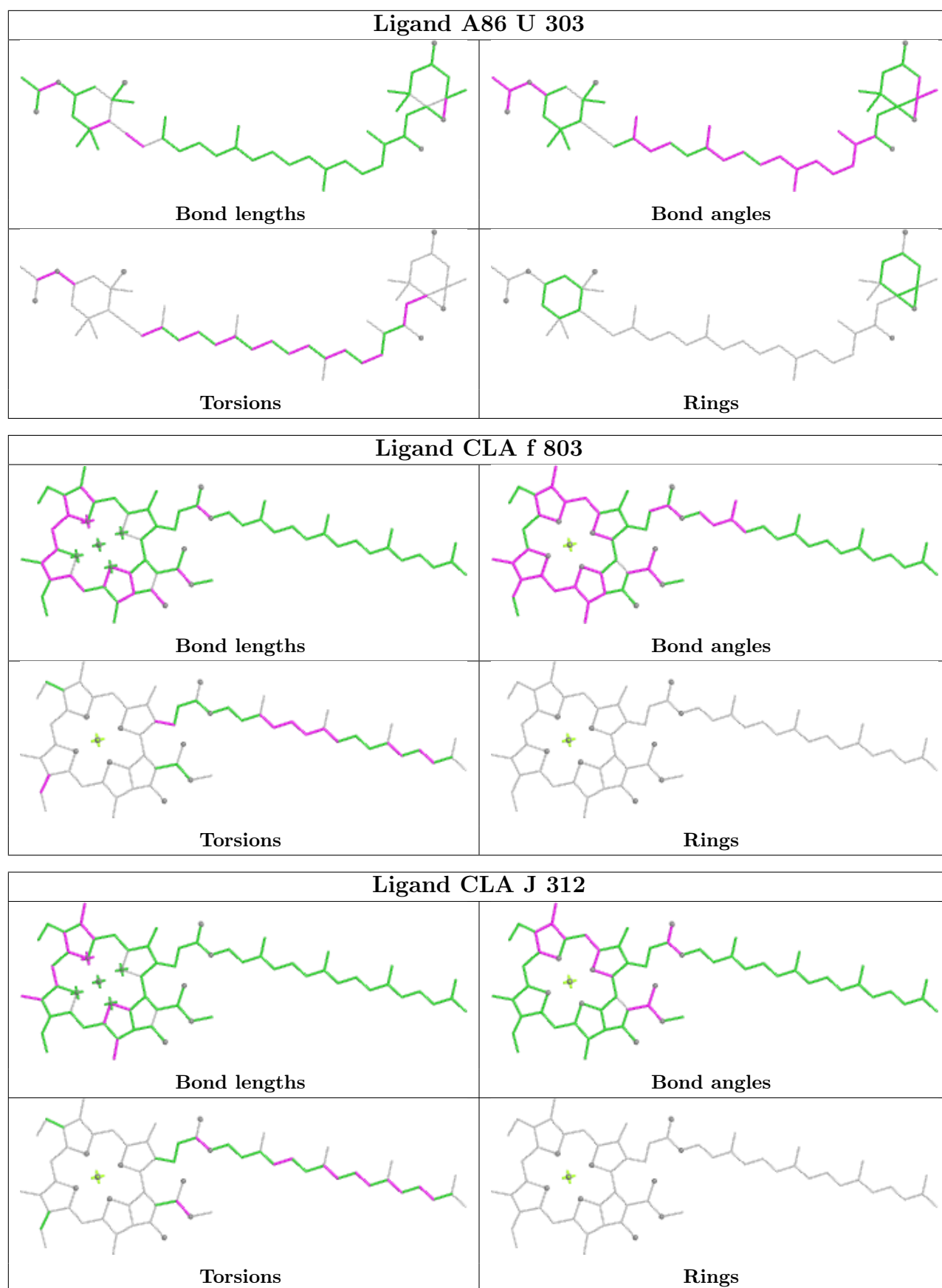
Bond angles

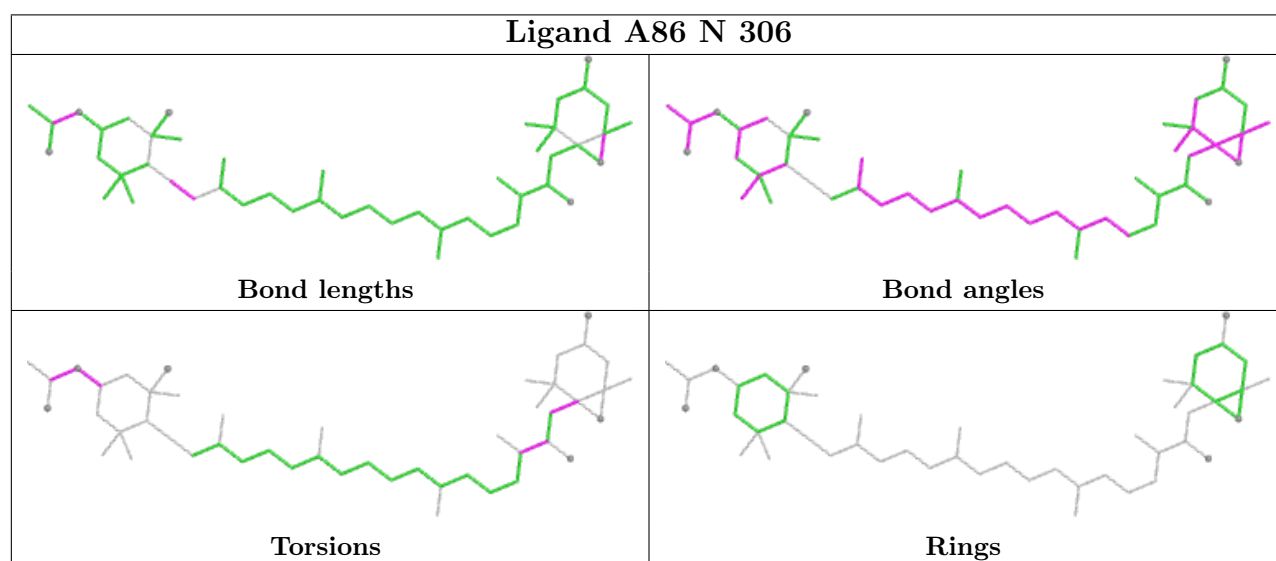
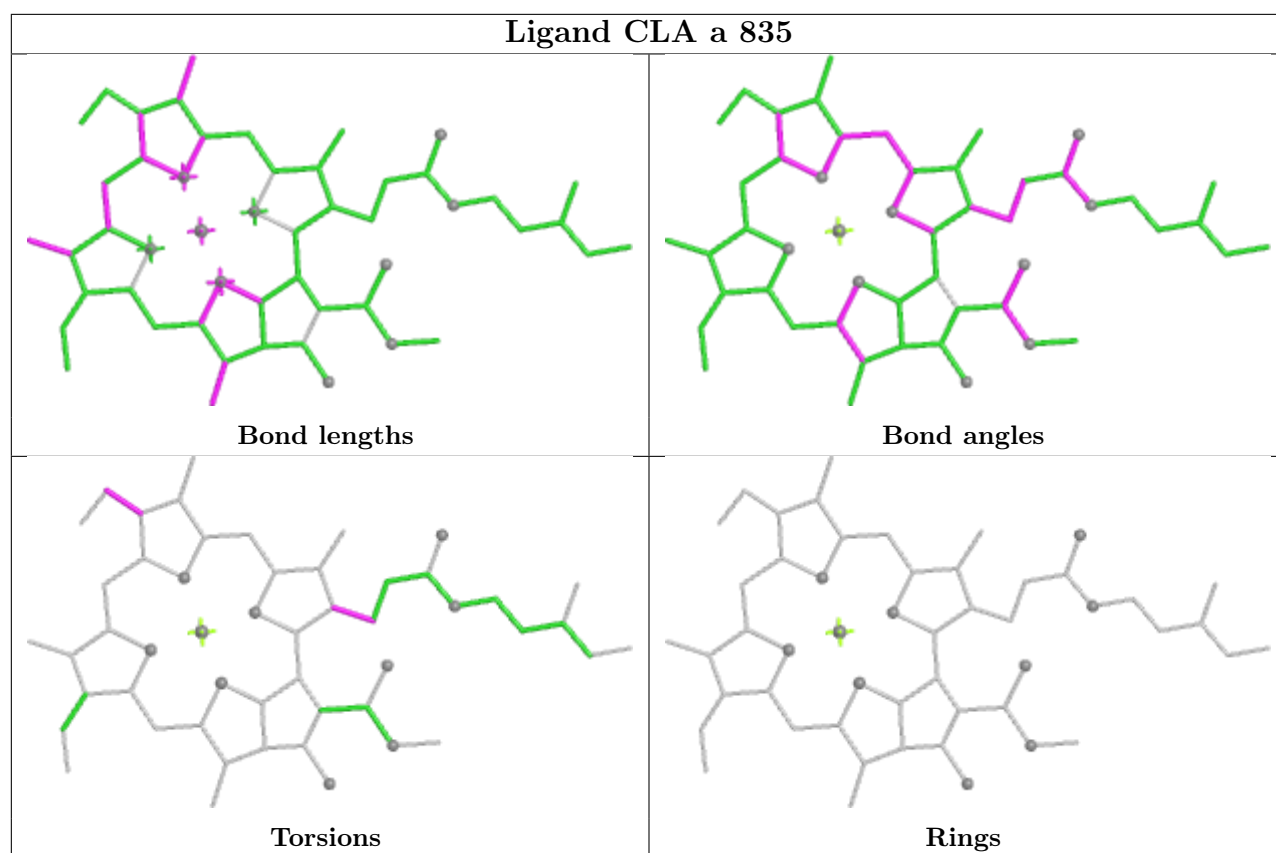


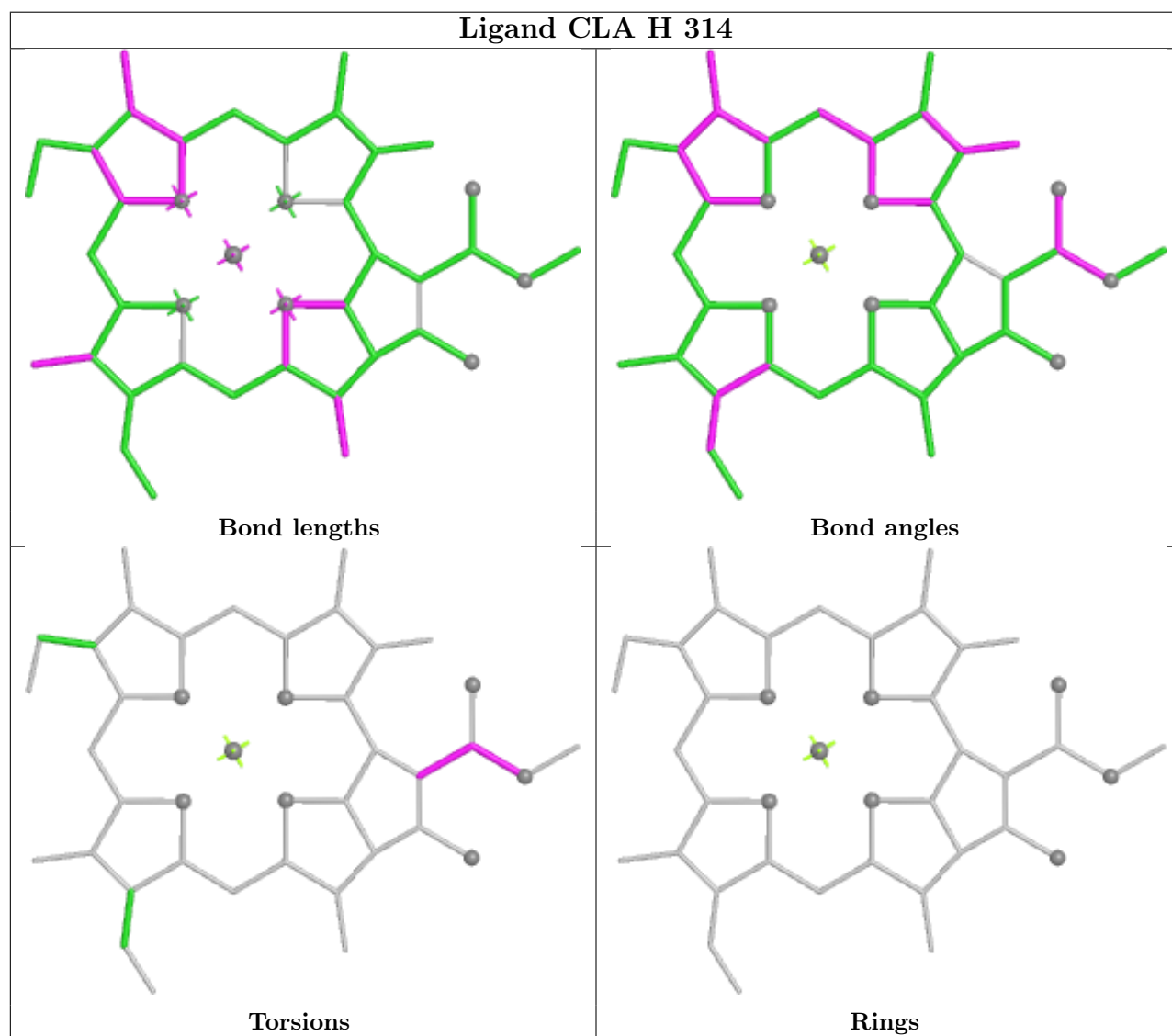
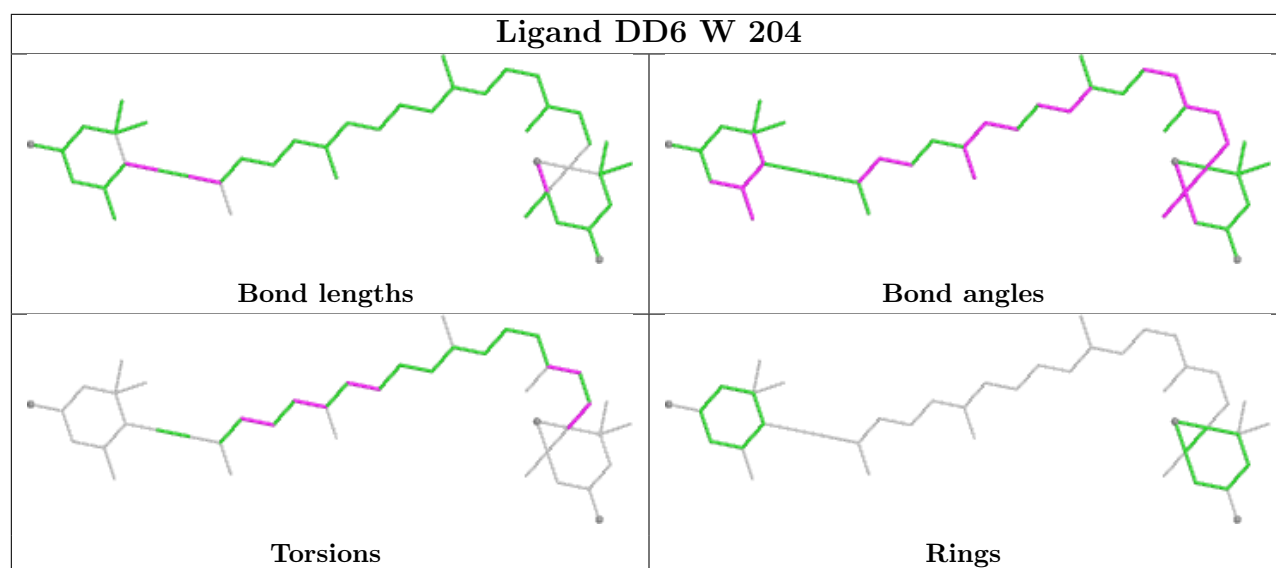
Torsions



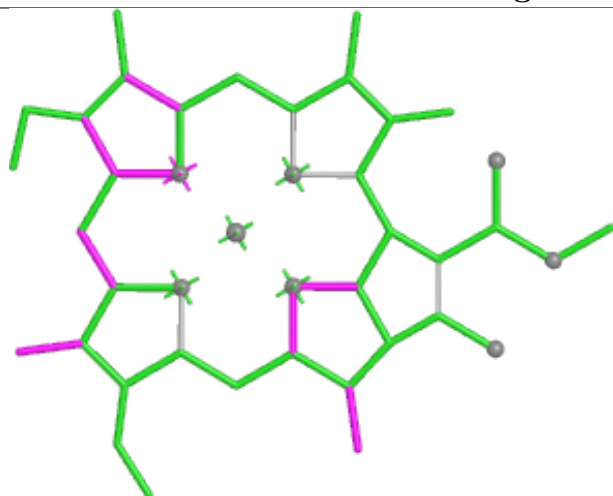
Rings



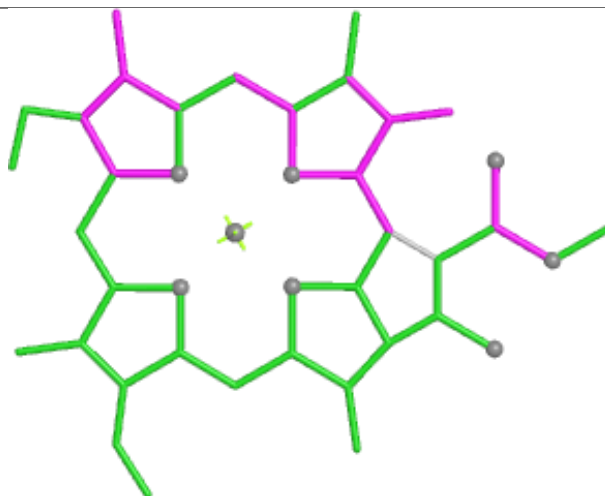




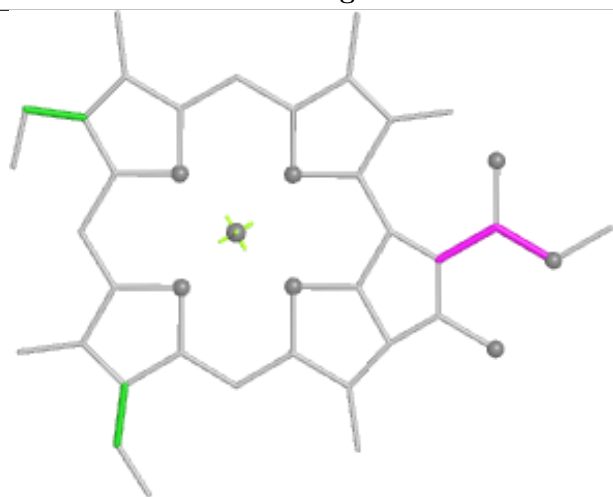
Ligand CLA X 312



Bond lengths



Bond angles

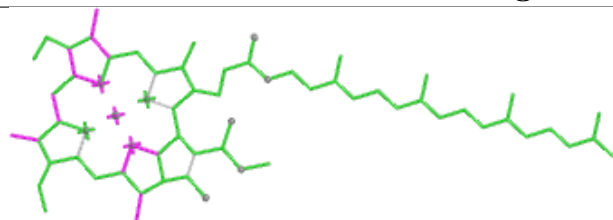


Torsions

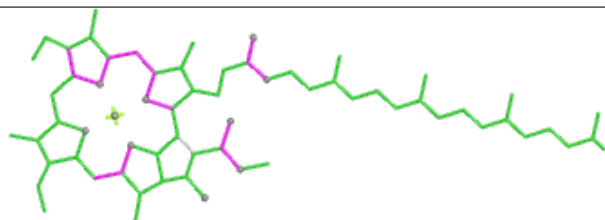


Rings

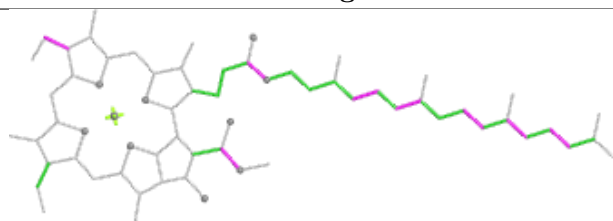
Ligand CLA C 211



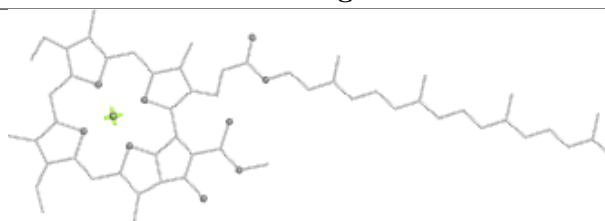
Bond lengths



Bond angles

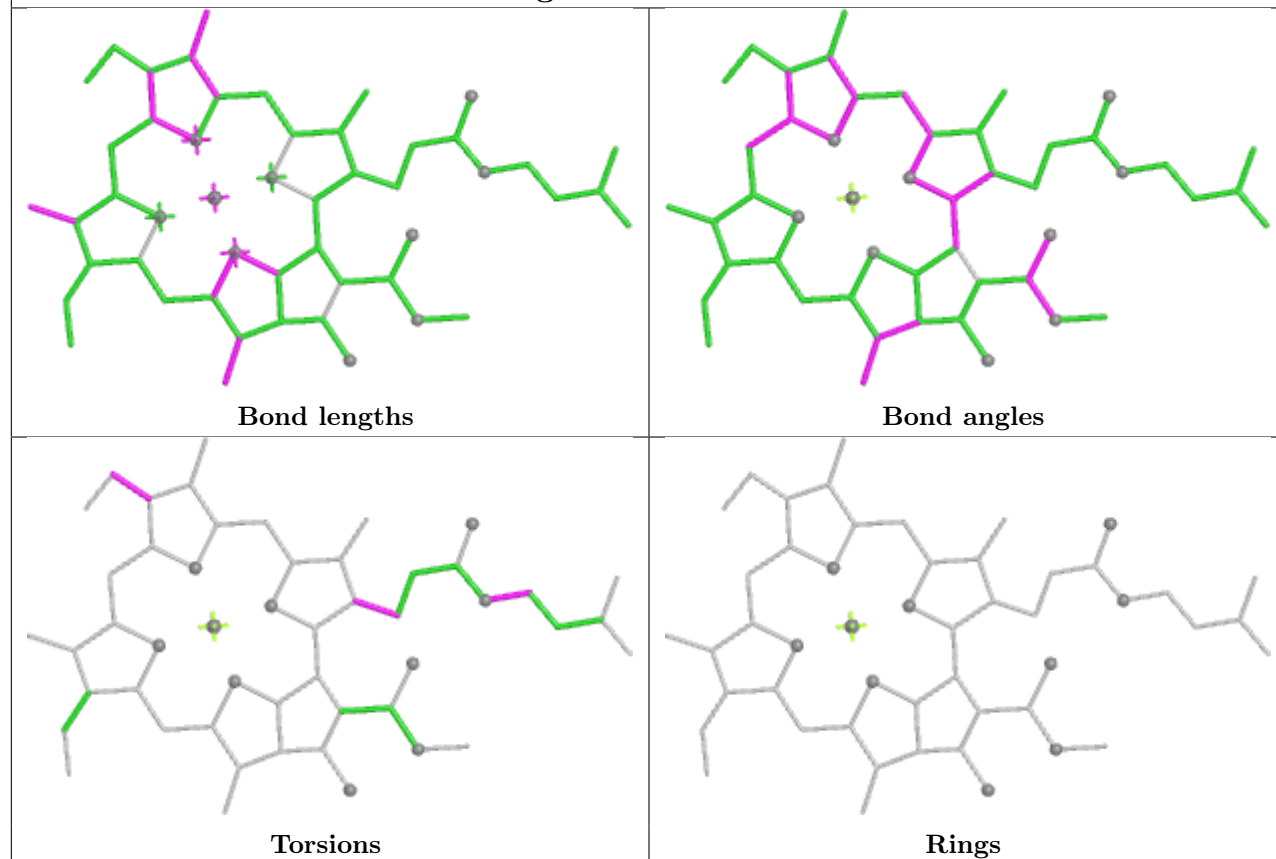


Torsions

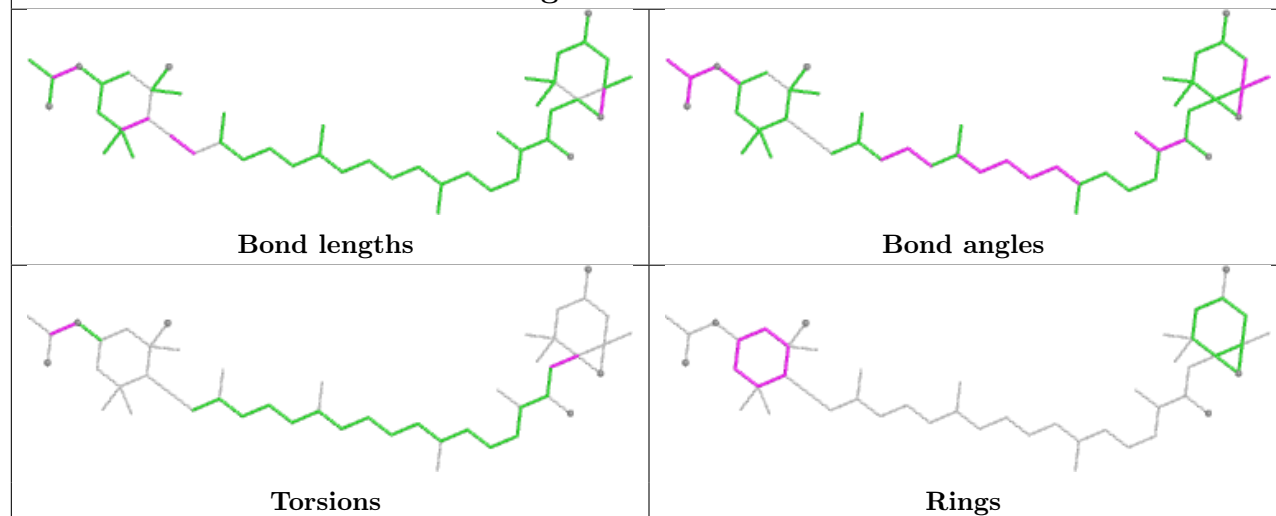


Rings

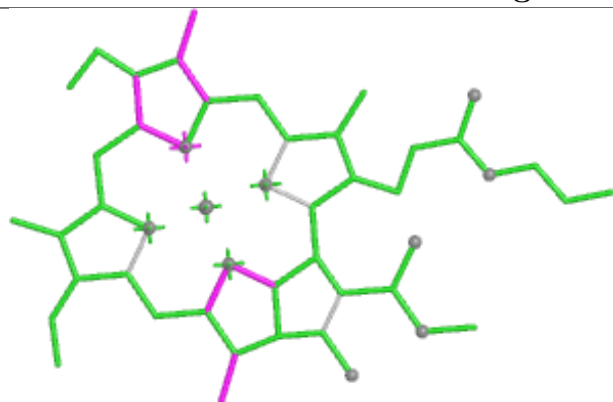
Ligand CLA a 833



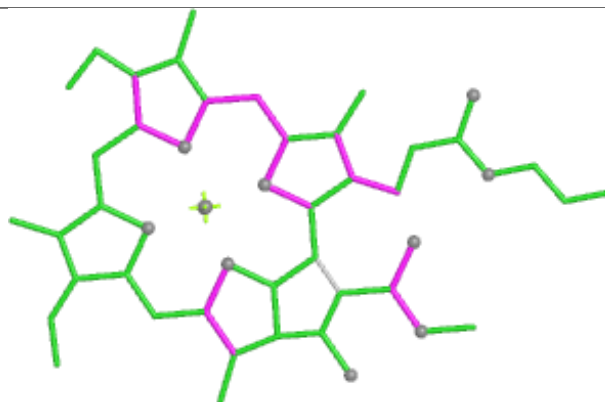
Ligand A86 h 202



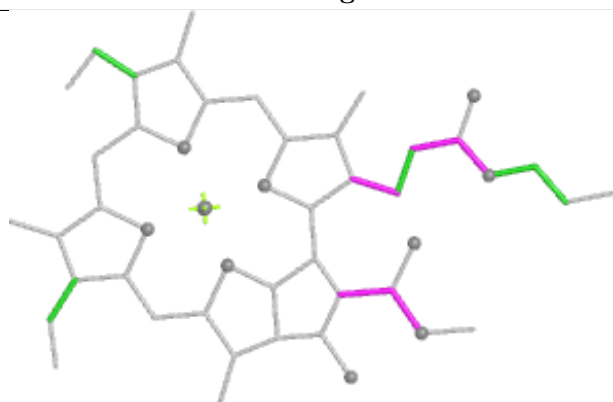
Ligand CLA H 305



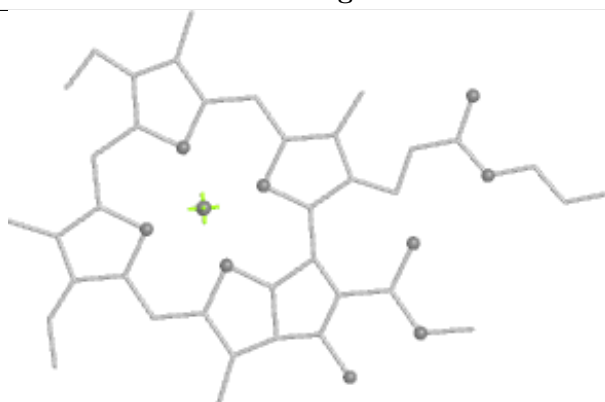
Bond lengths



Bond angles

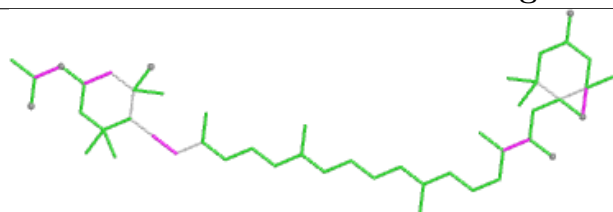


Torsions

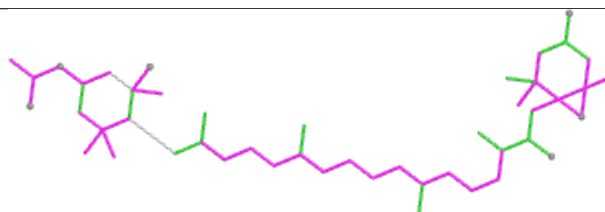


Rings

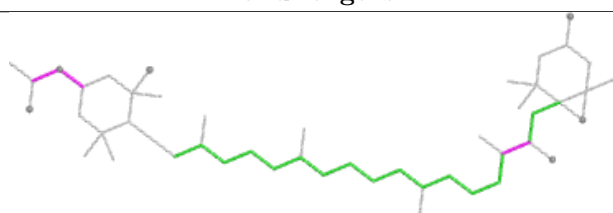
Ligand A86 R 303



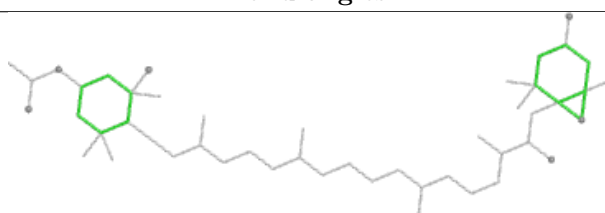
Bond lengths



Bond angles

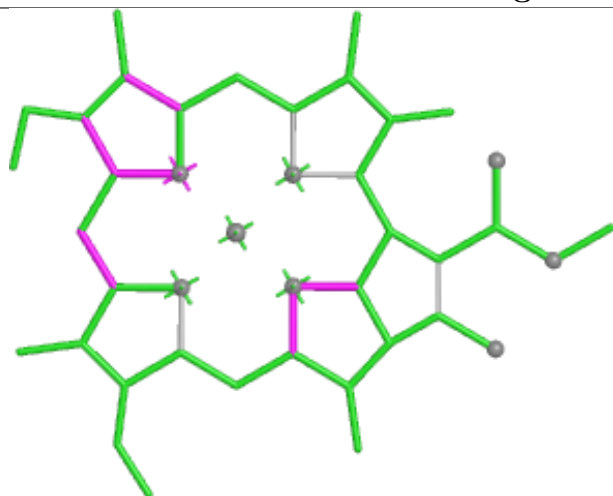


Torsions

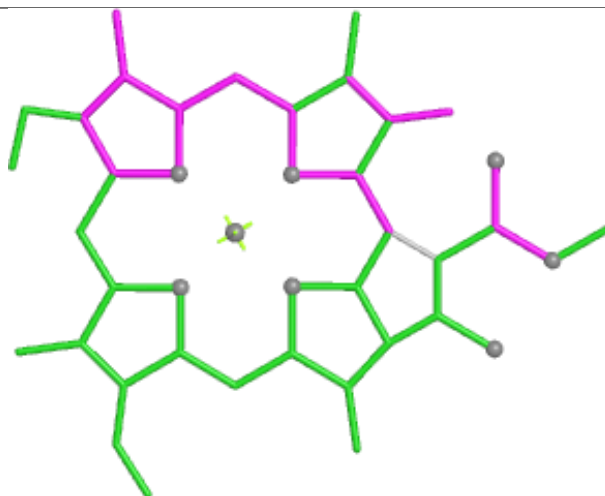


Rings

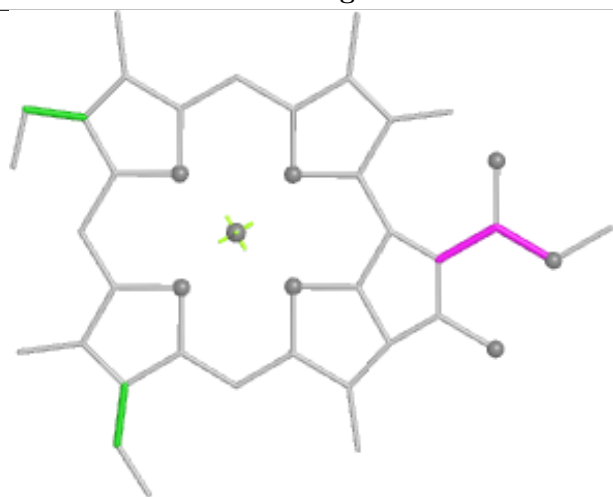
Ligand CLA X 315



Bond lengths



Bond angles

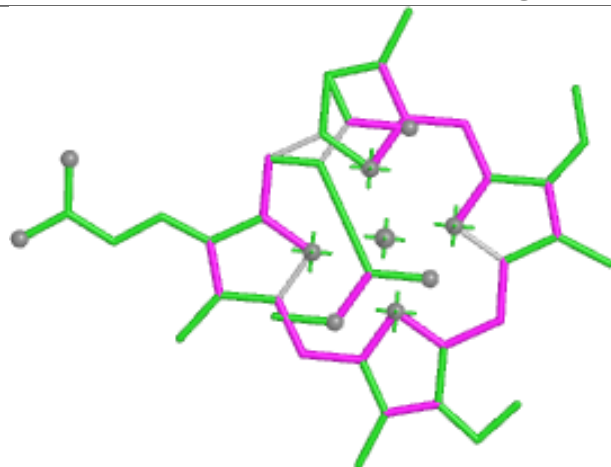


Torsions

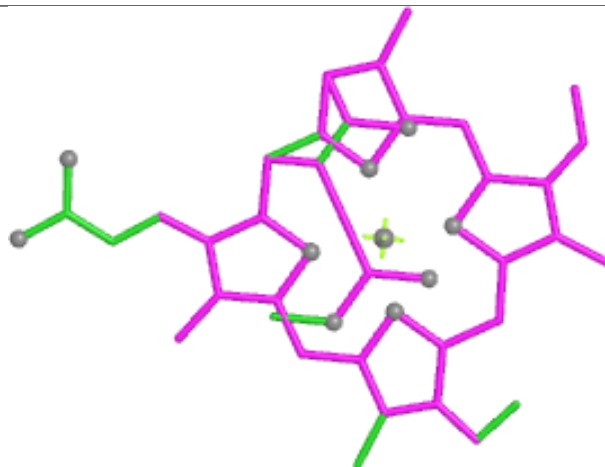


Rings

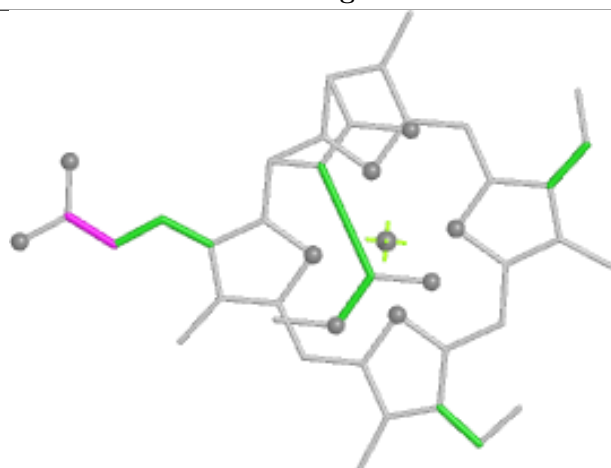
Ligand KC1 A 312



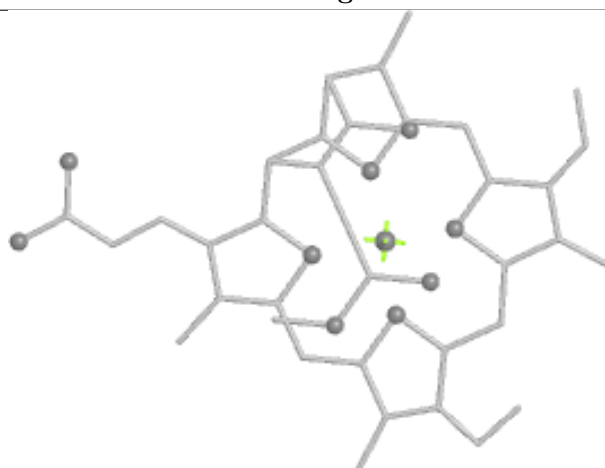
Bond lengths



Bond angles

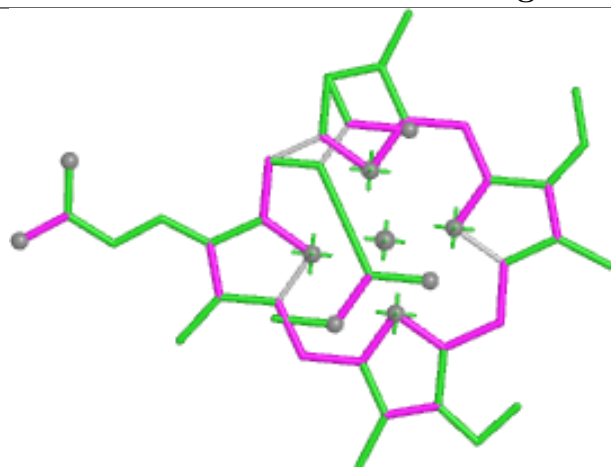


Torsions

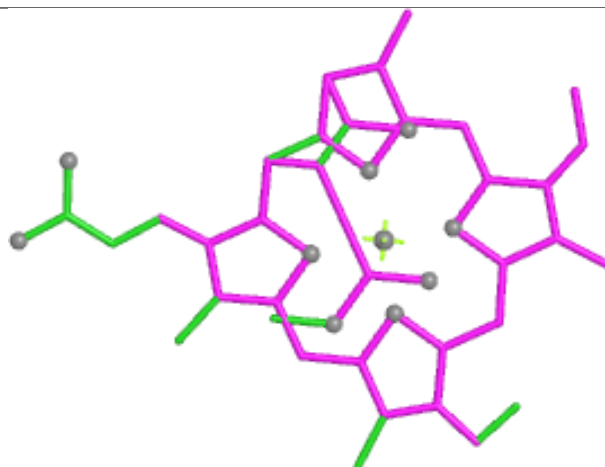


Rings

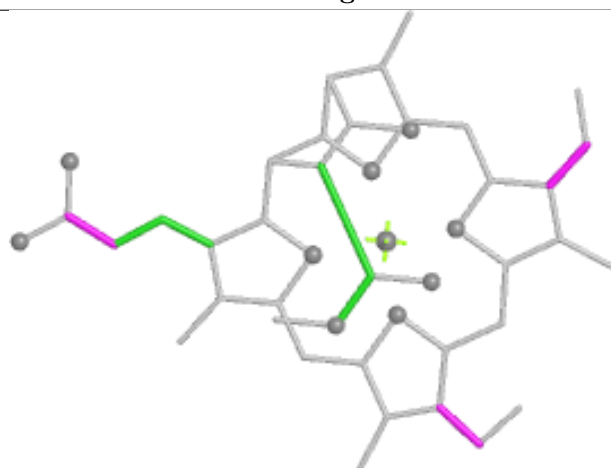
Ligand KC1 E 309



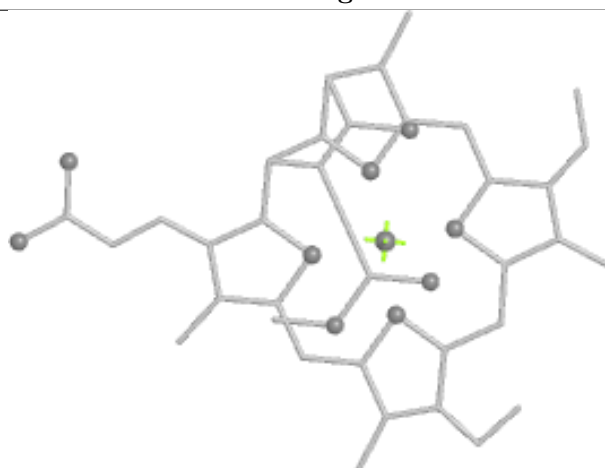
Bond lengths



Bond angles

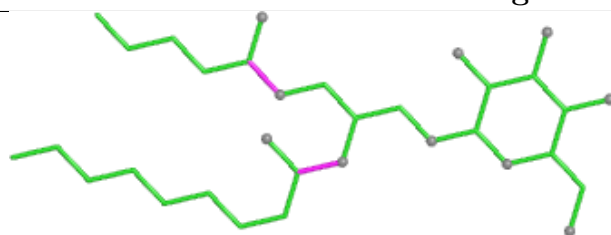


Torsions

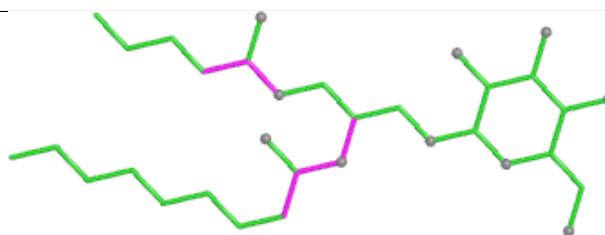


Rings

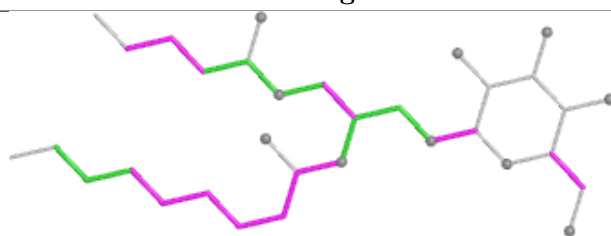
Ligand LMG L 321



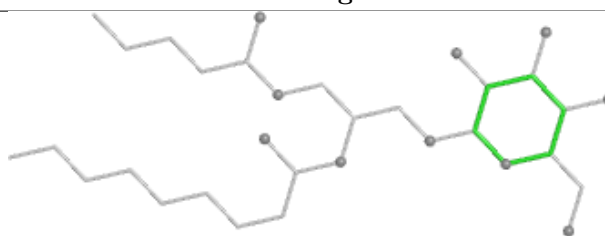
Bond lengths



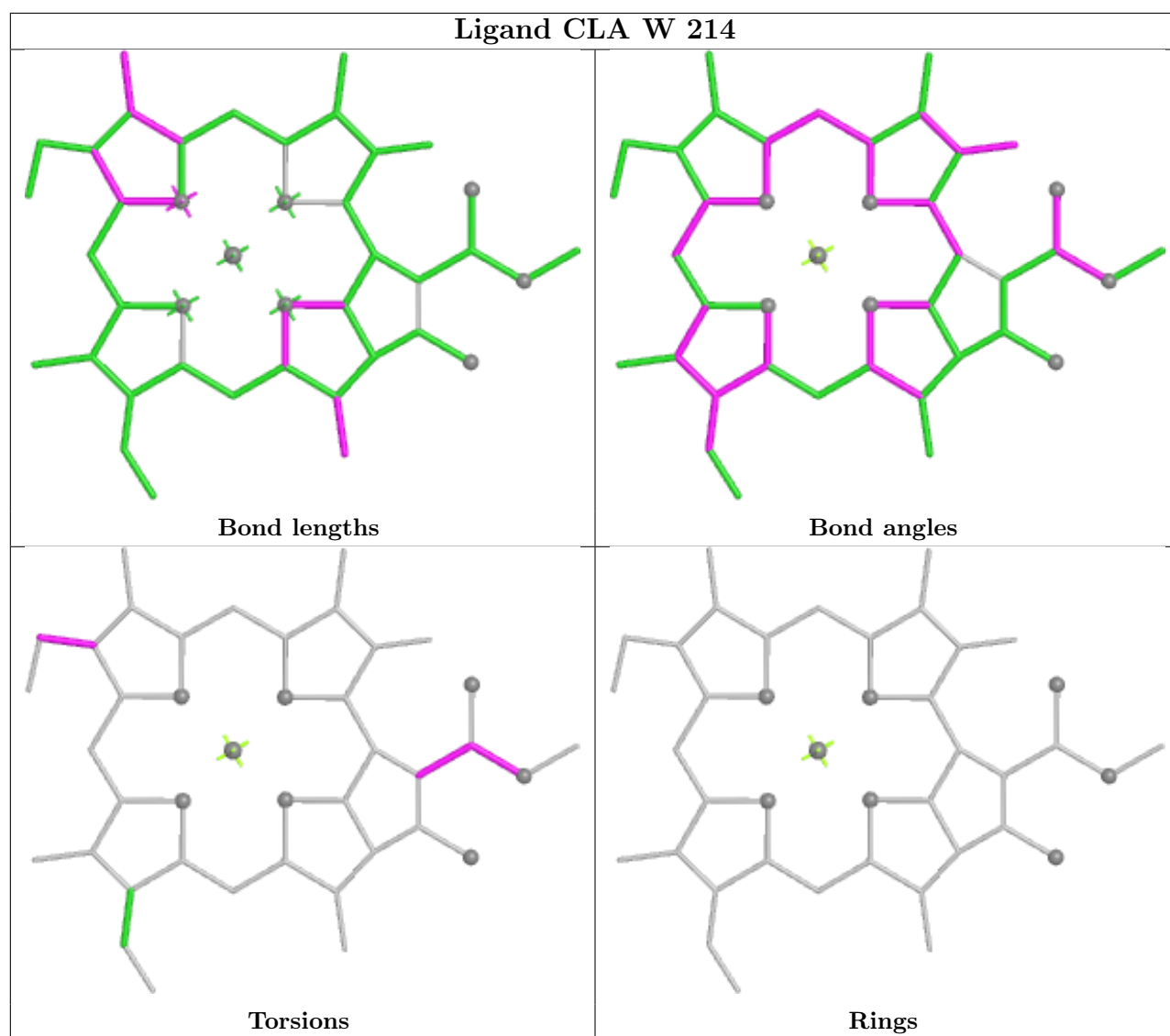
Bond angles



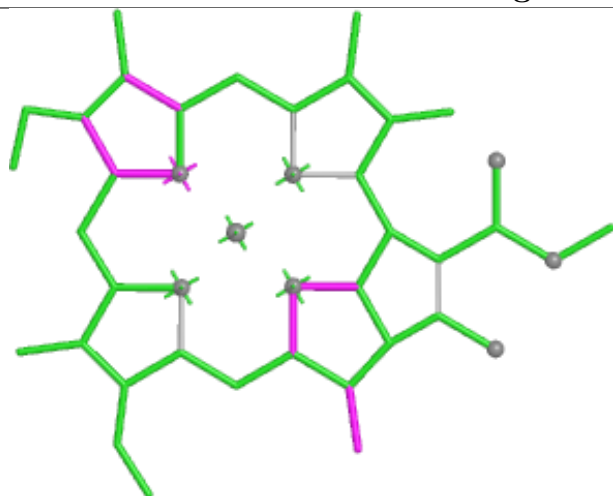
Torsions



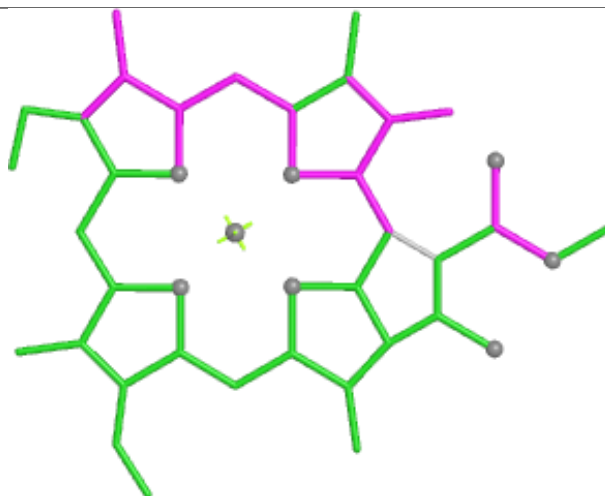
Rings



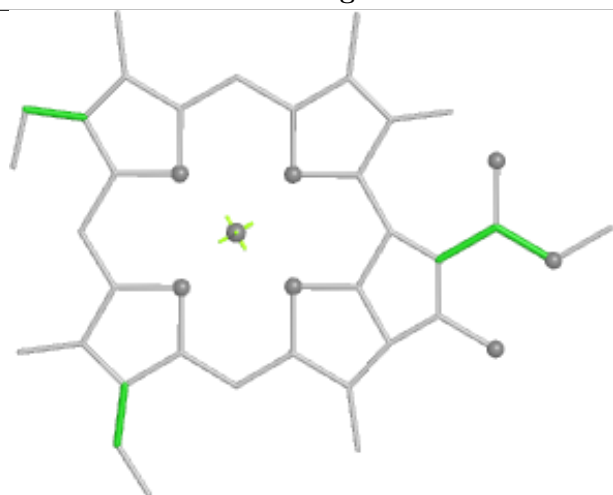
Ligand CLA N 315



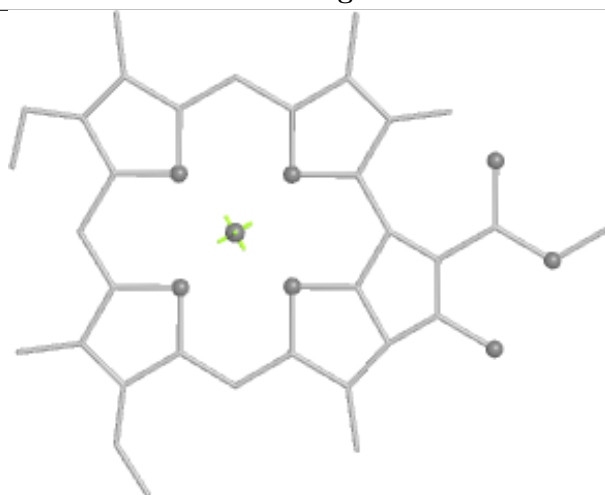
Bond lengths



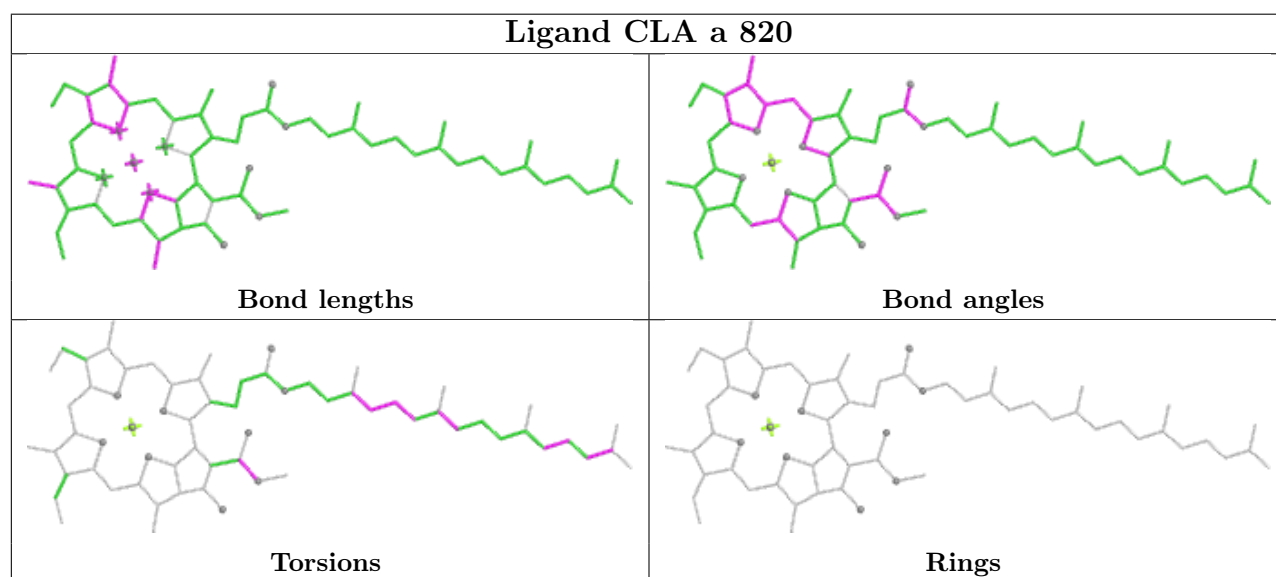
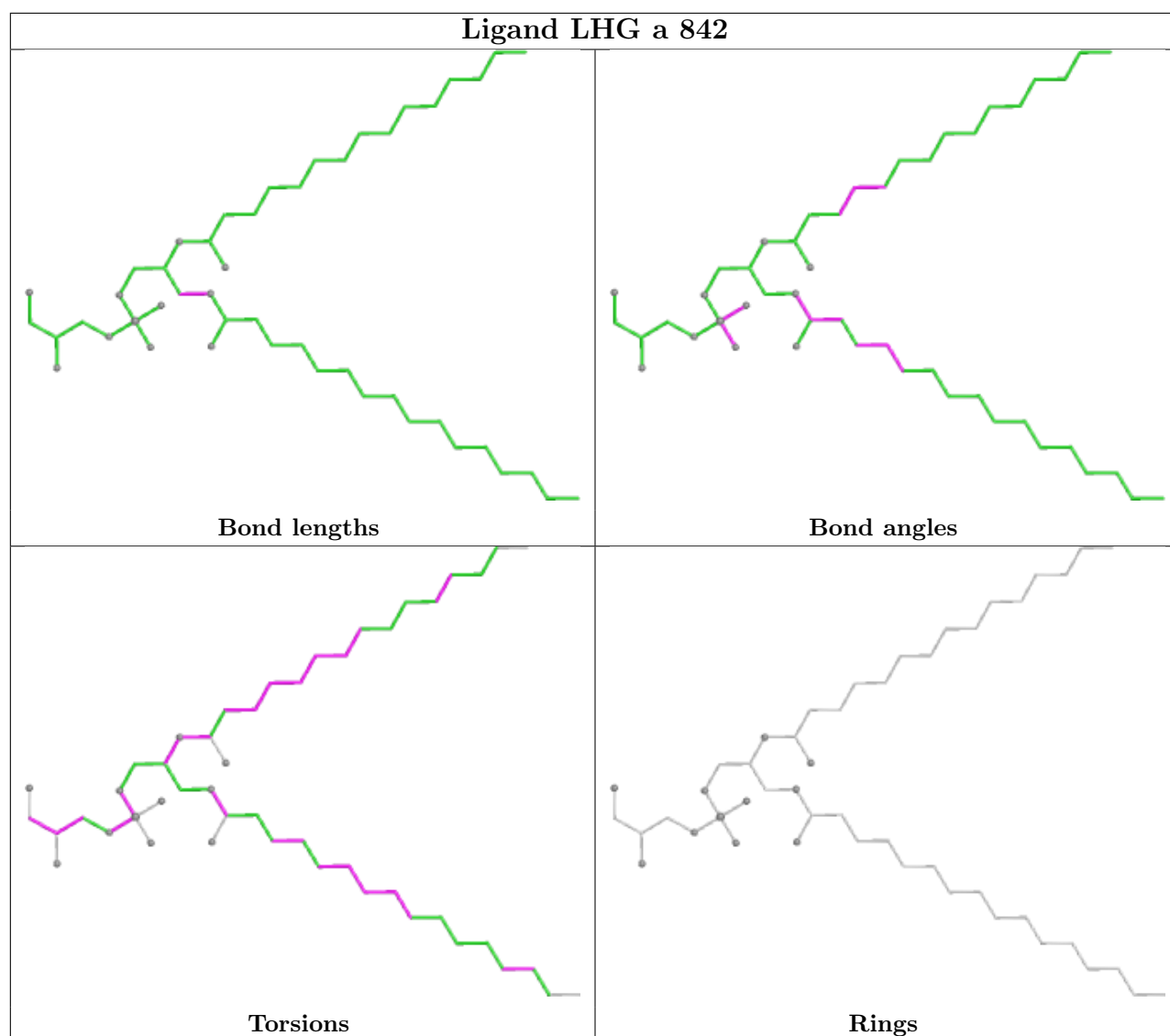
Bond angles

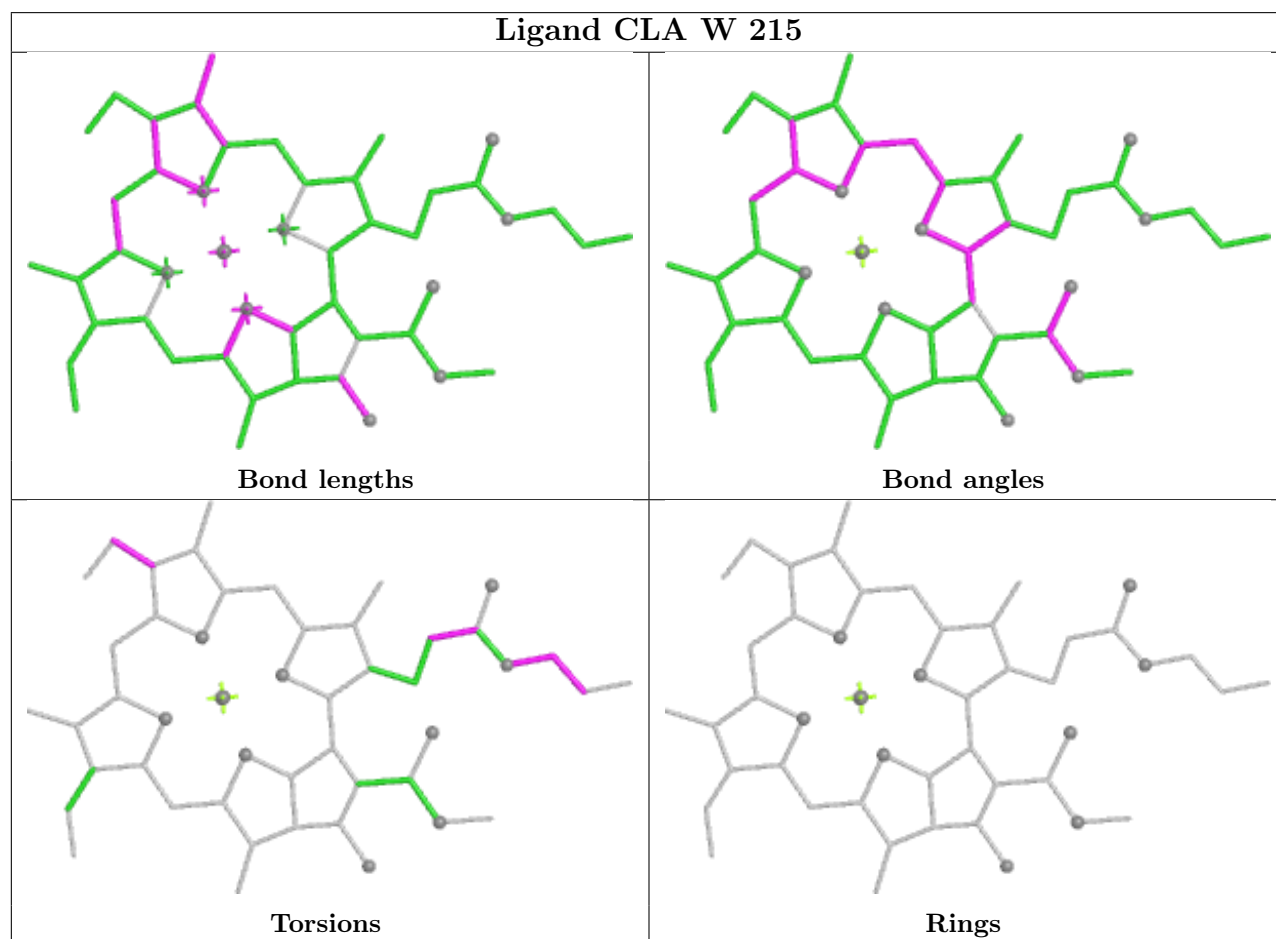
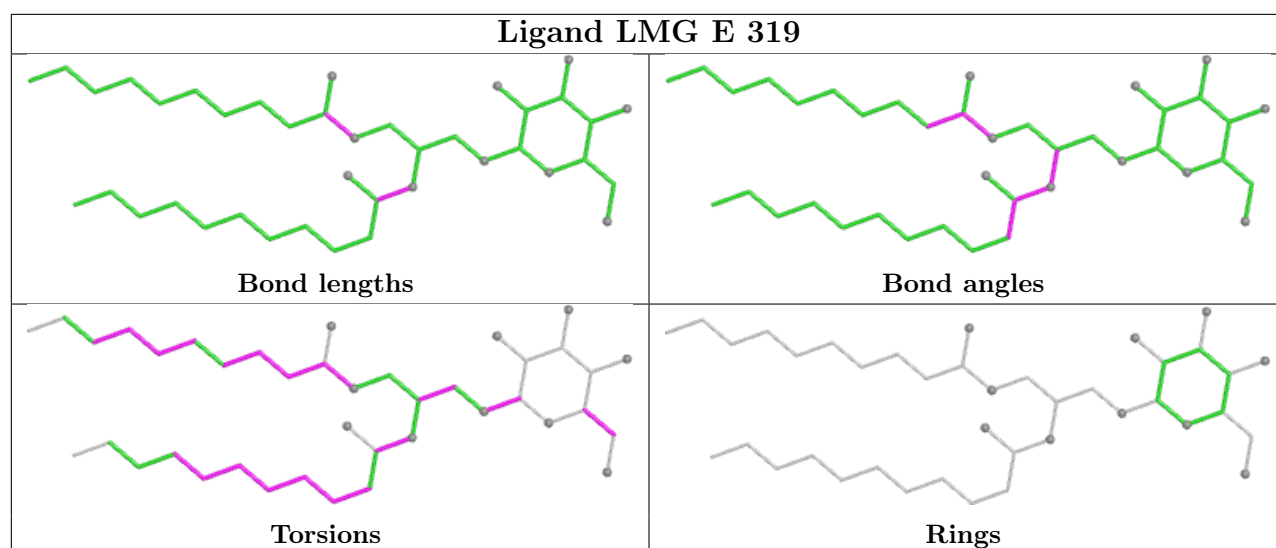


Torsions

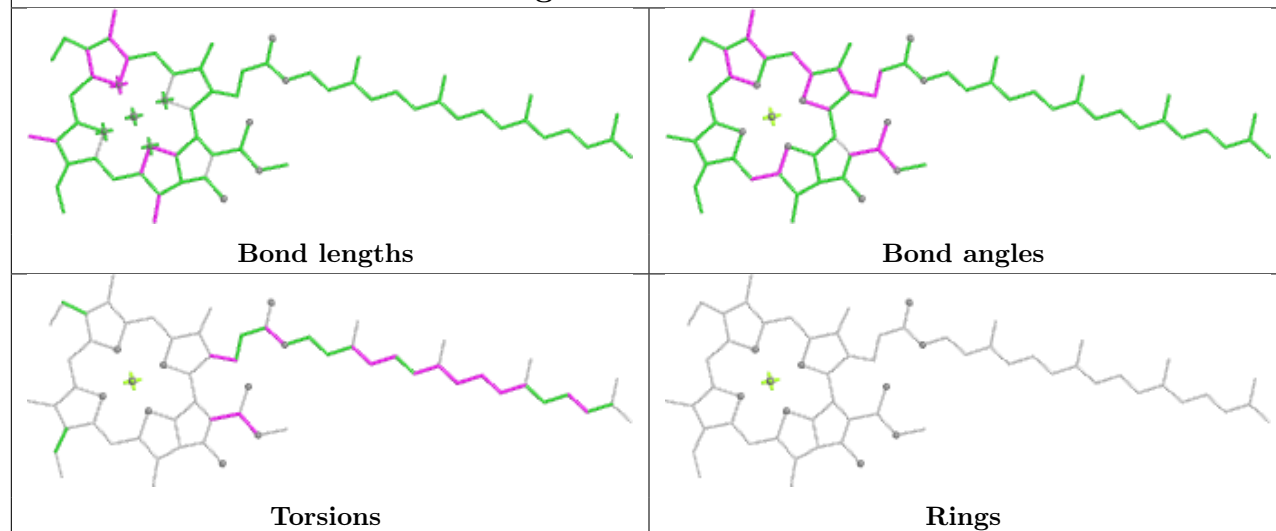


Rings

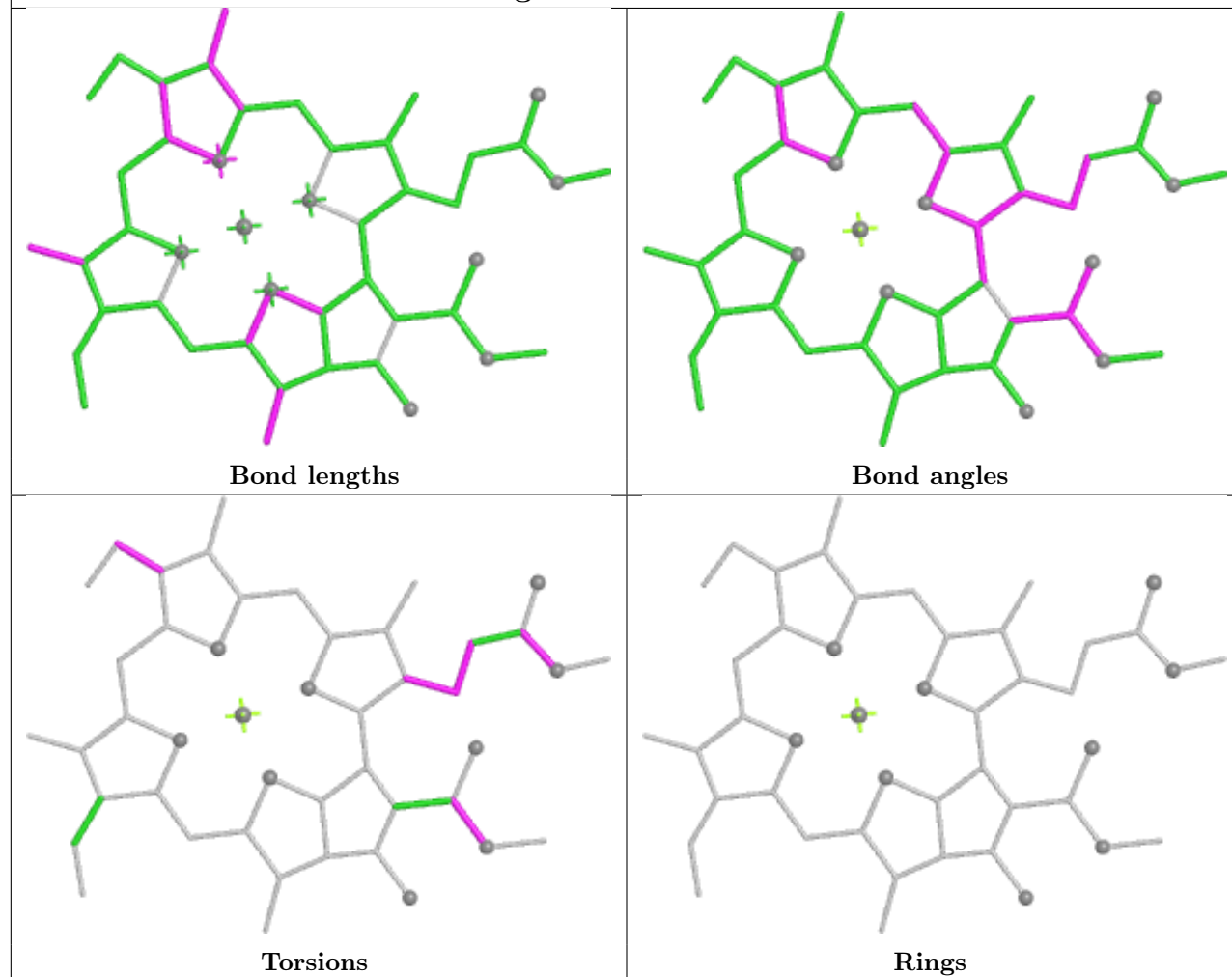


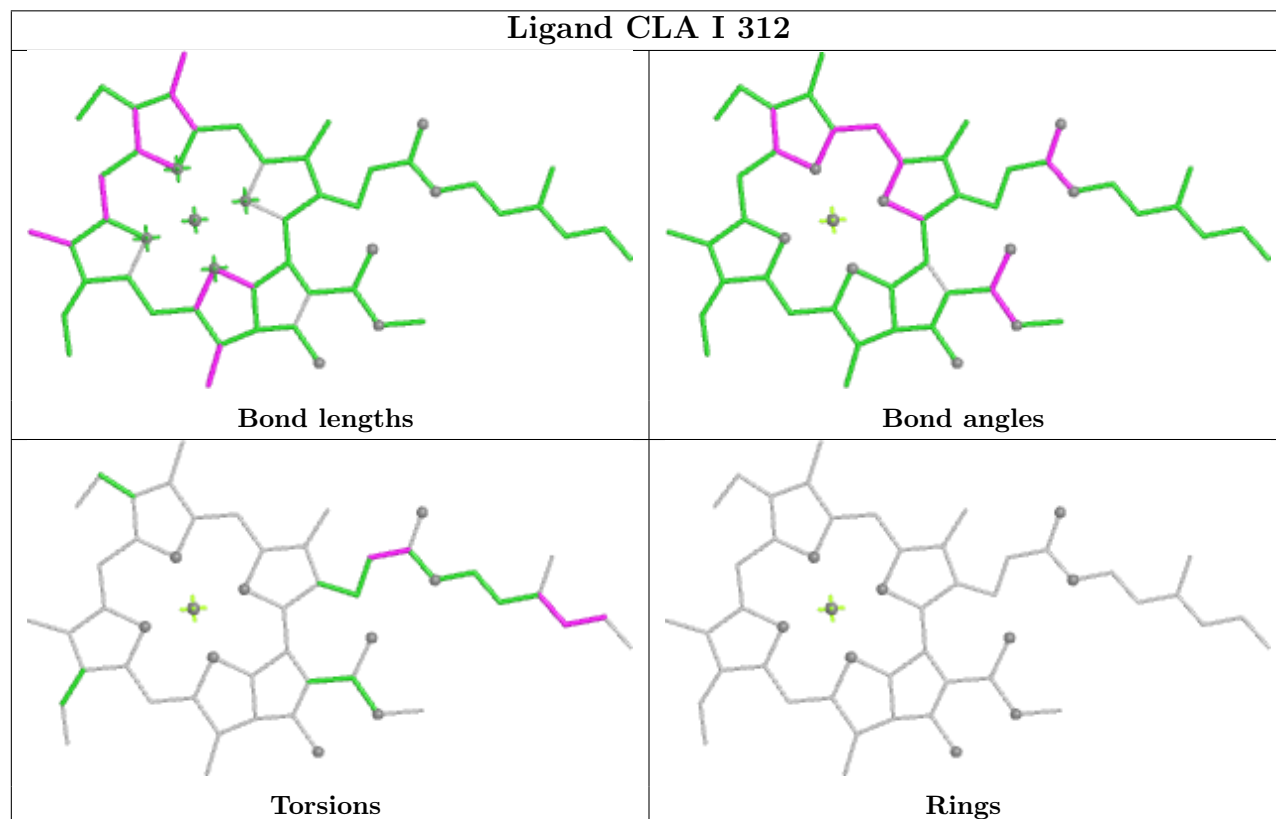
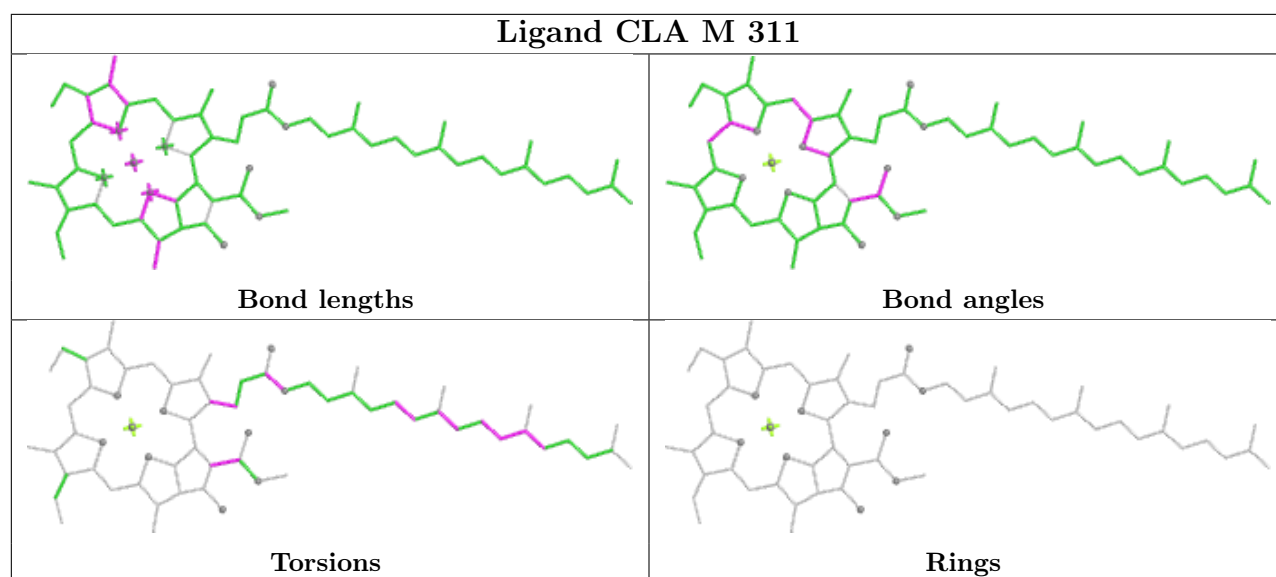


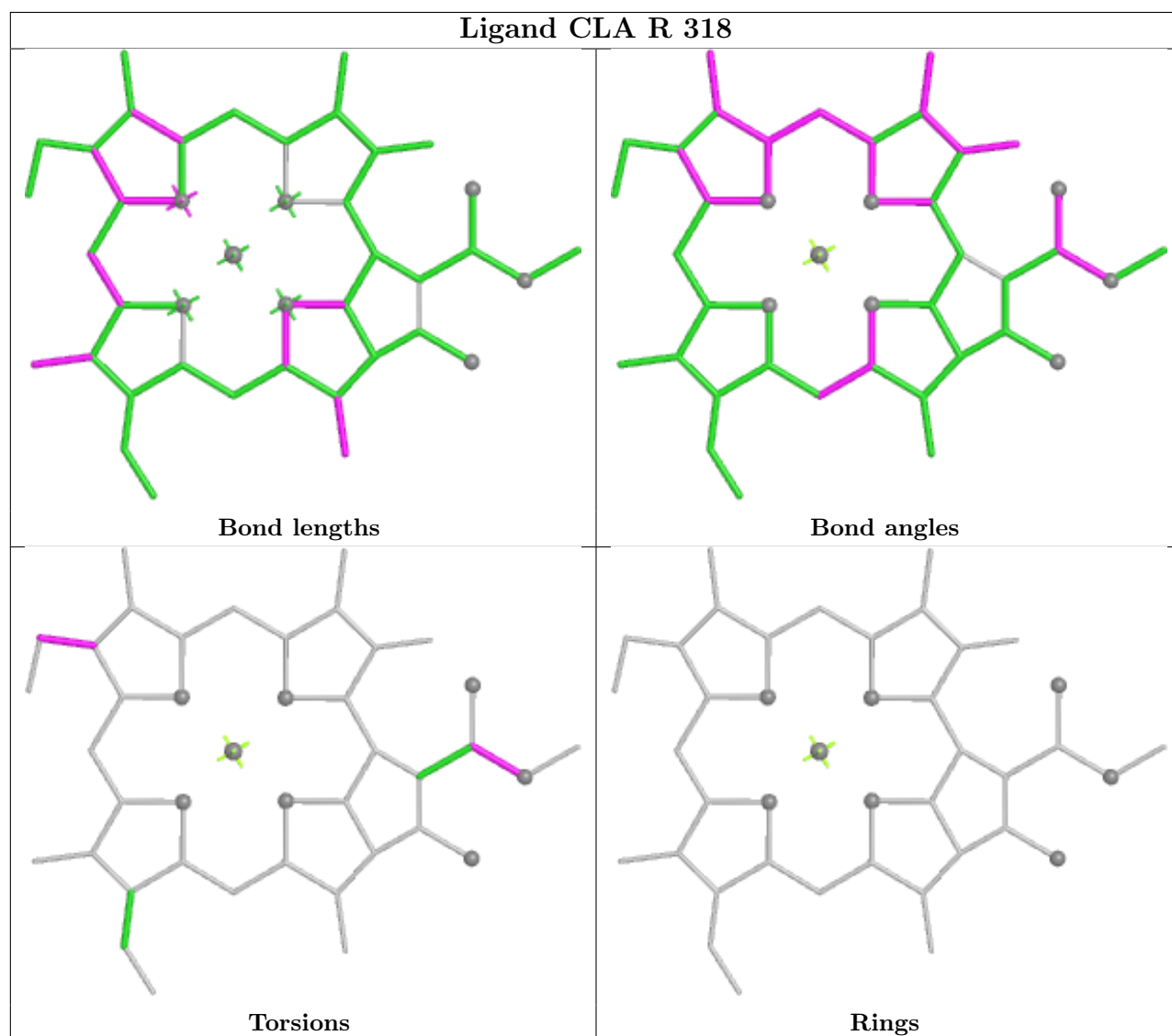
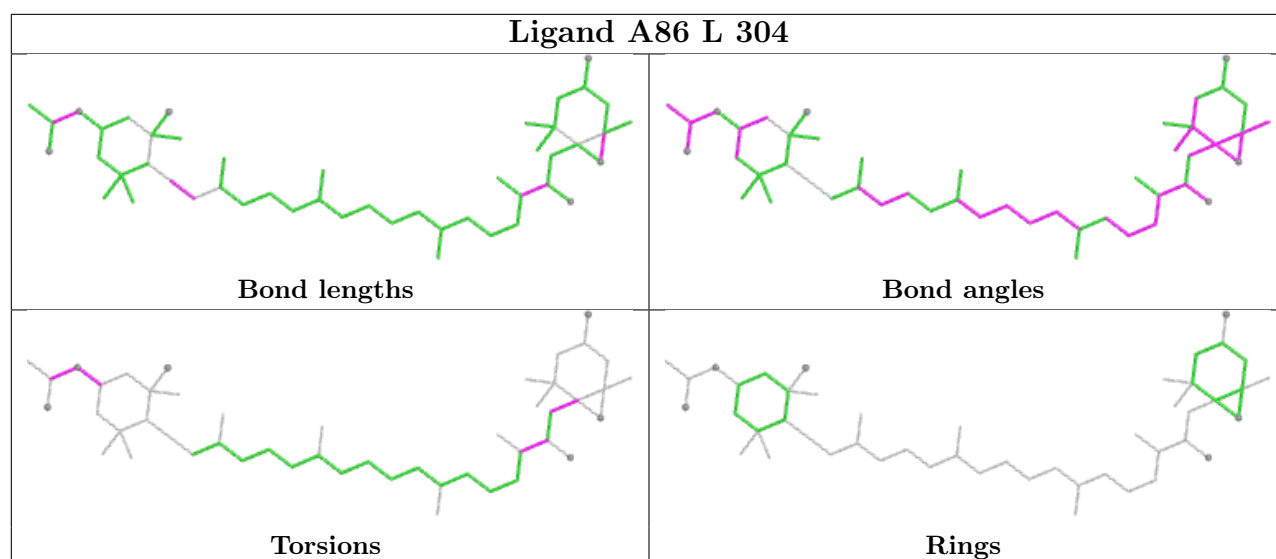
Ligand CLA h 203

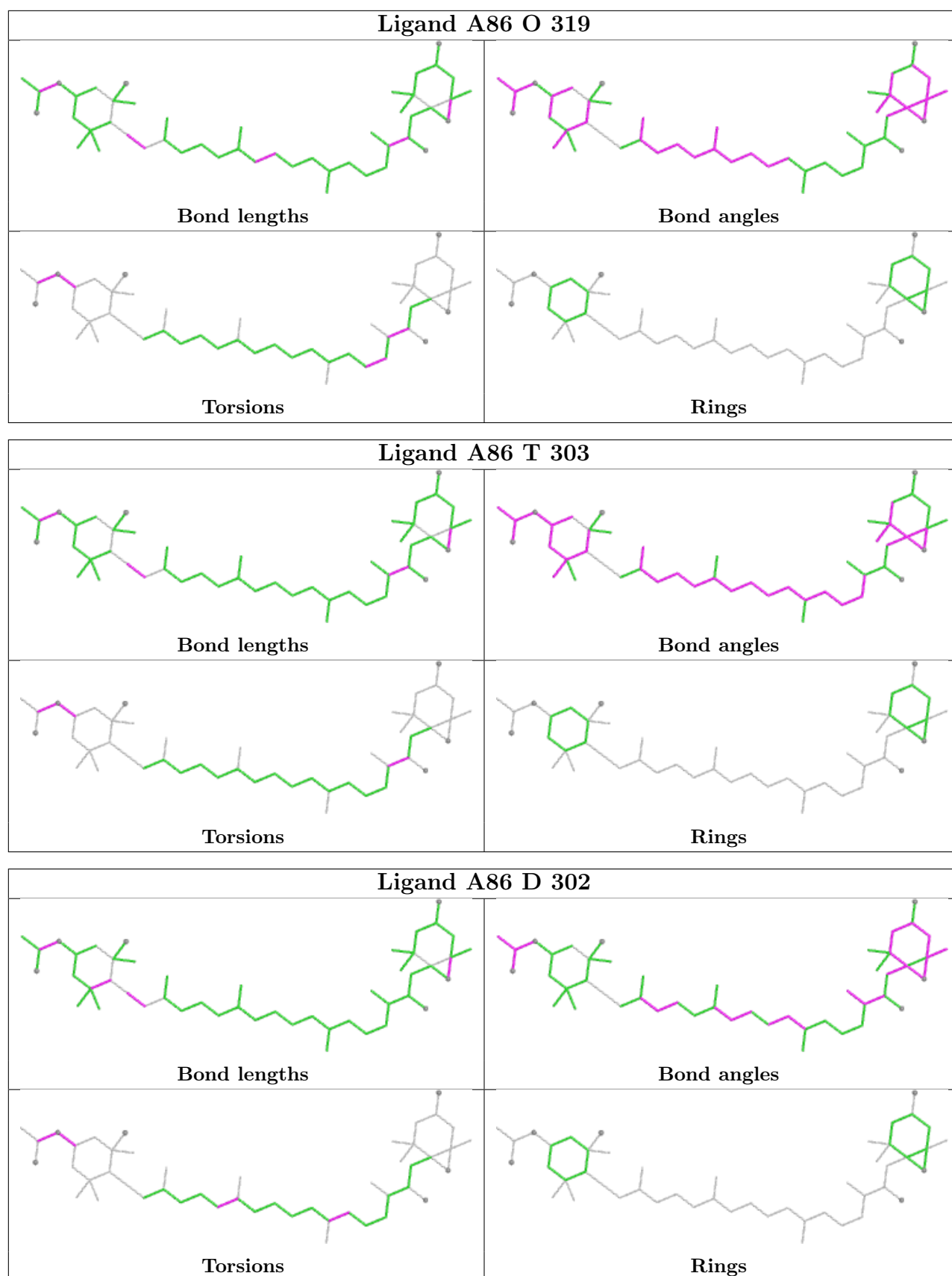


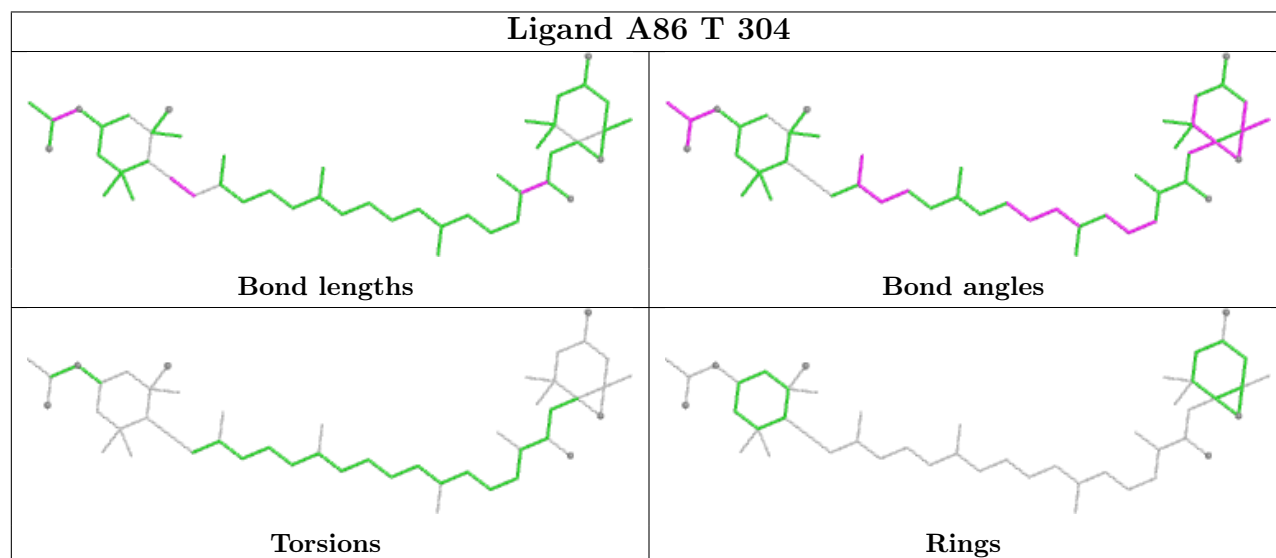
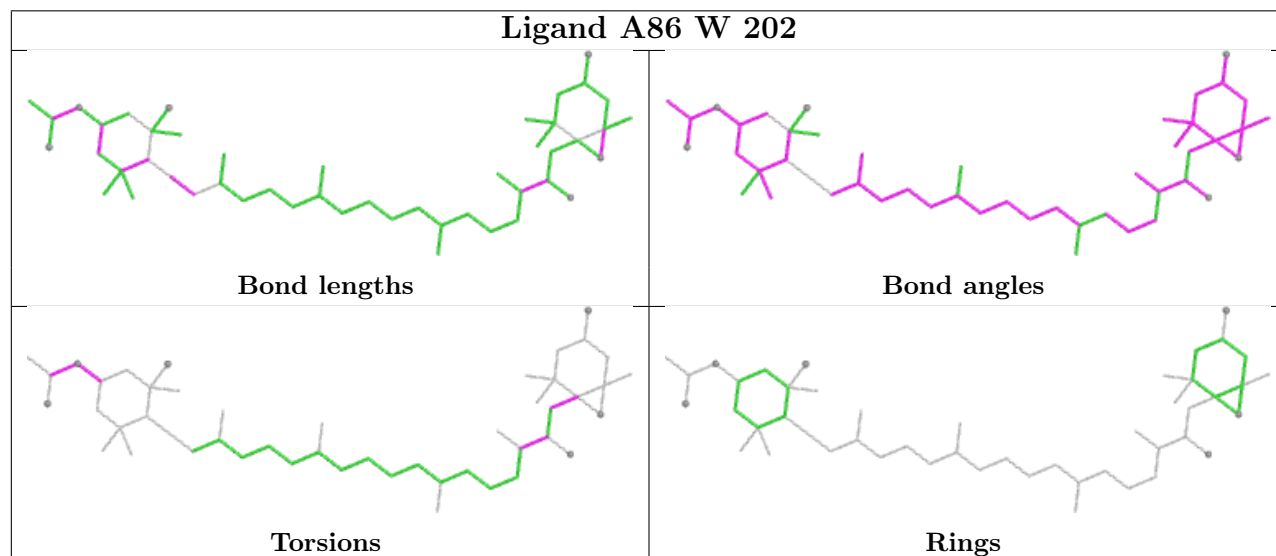
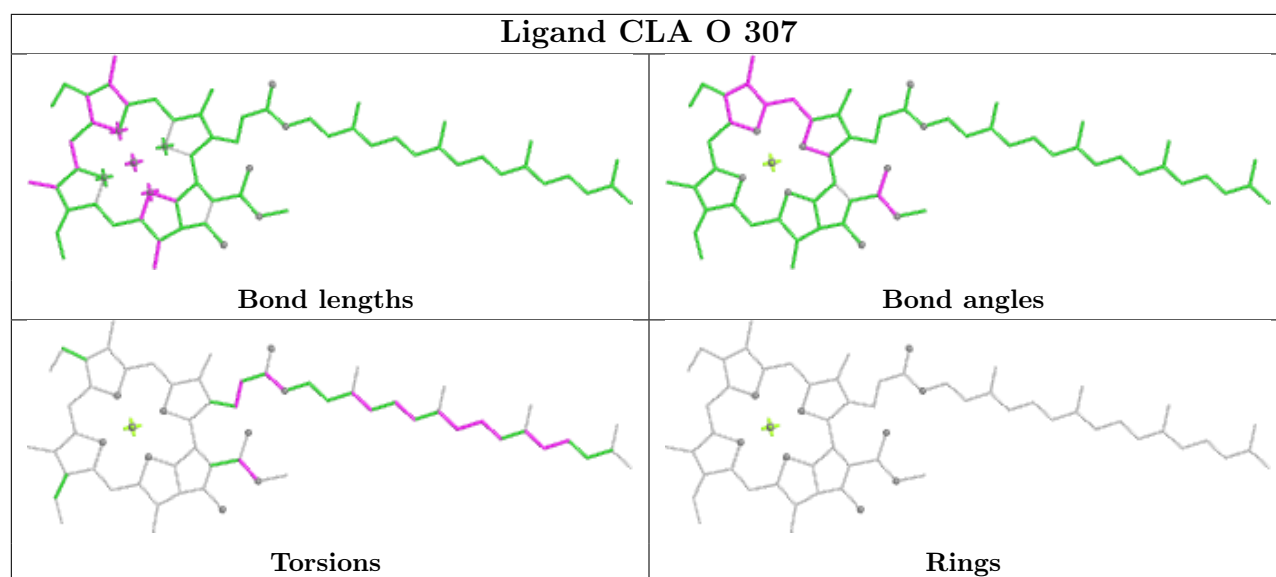
Ligand CLA P 312

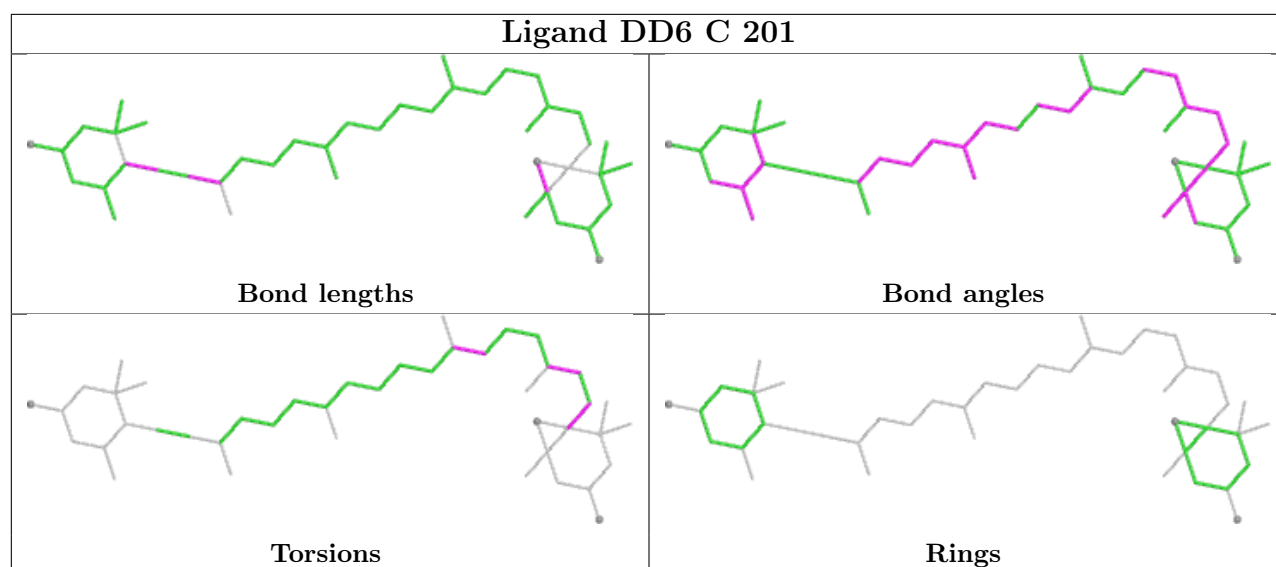
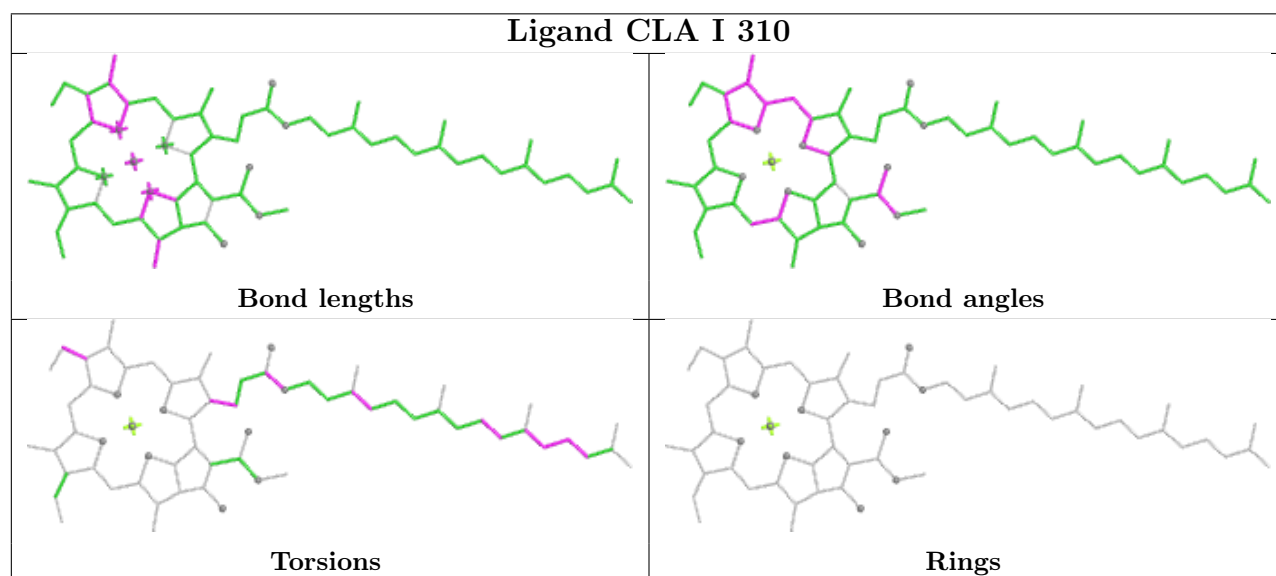
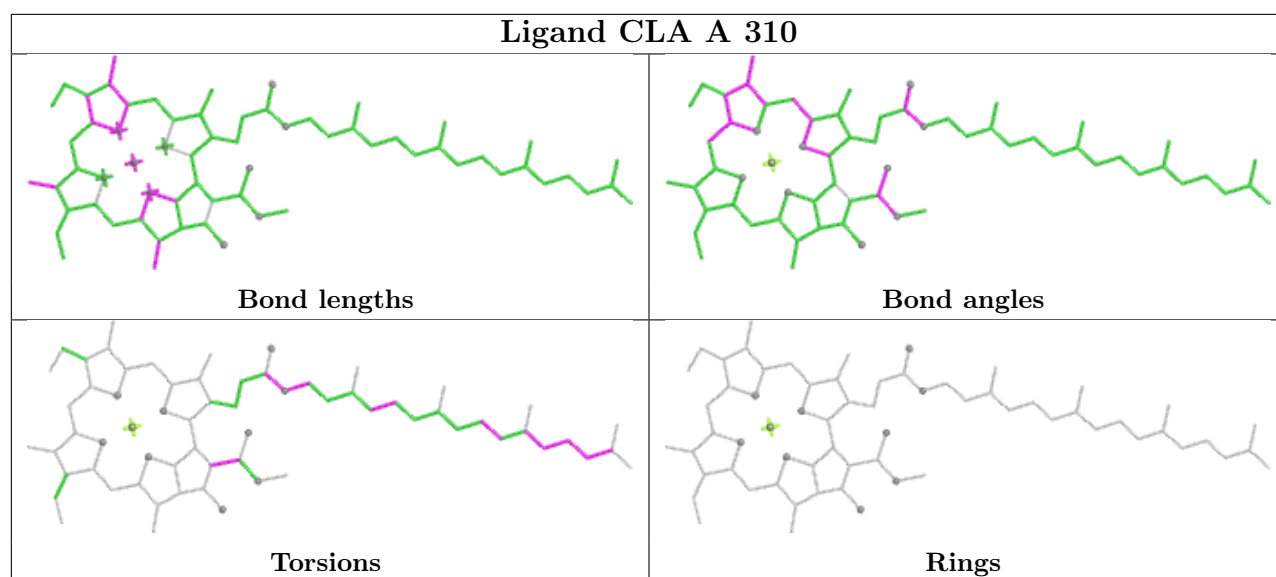


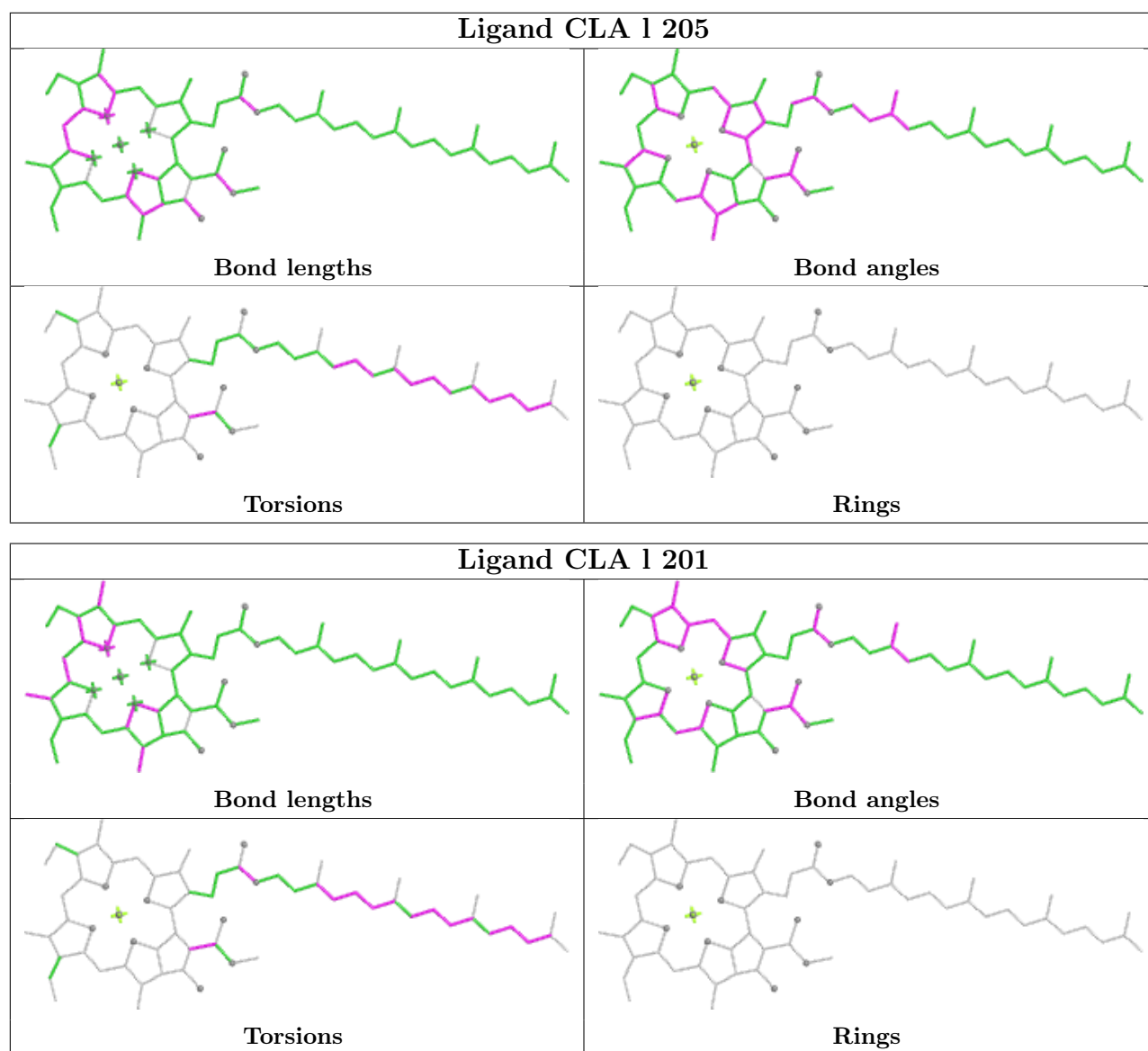


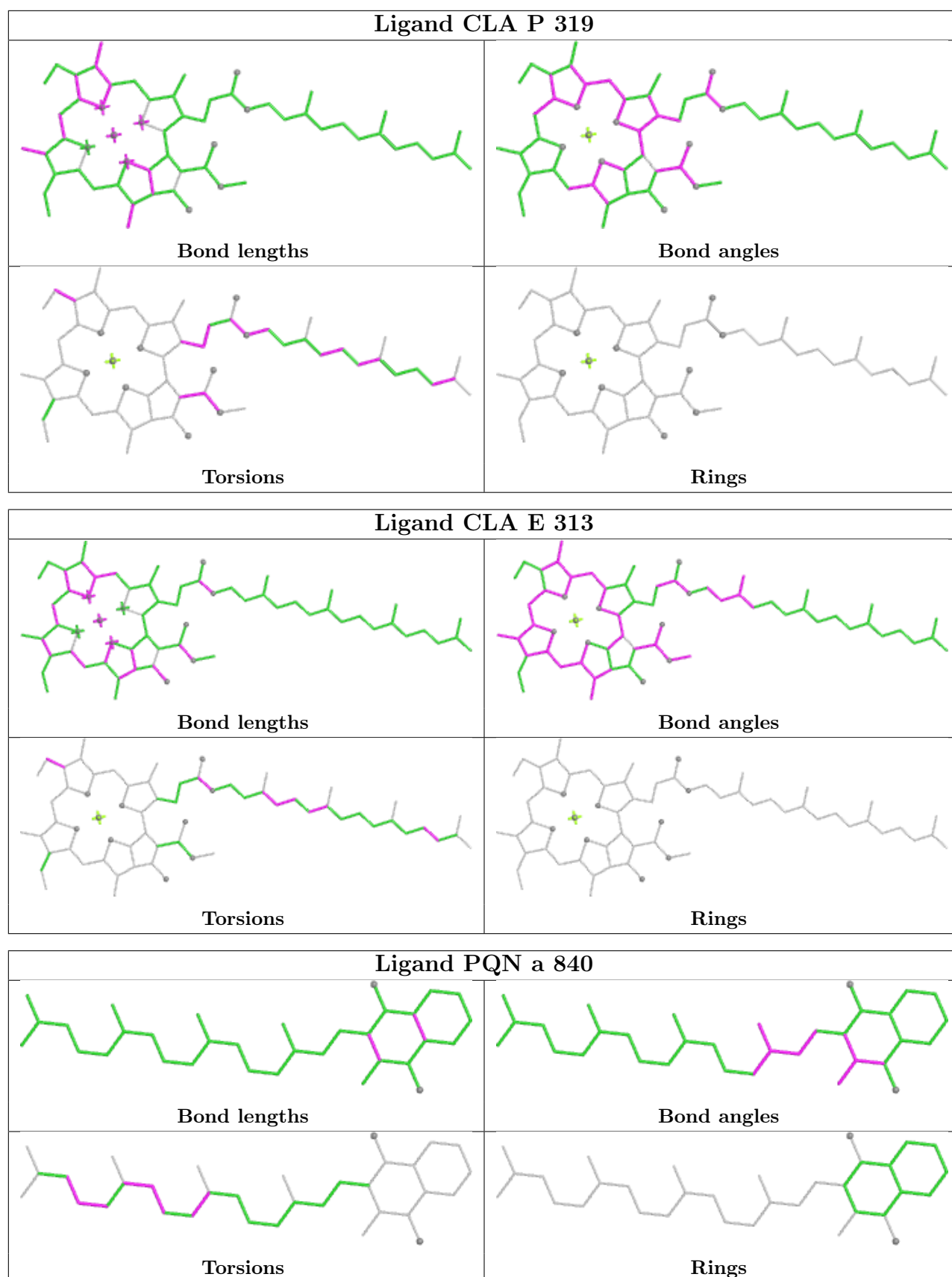




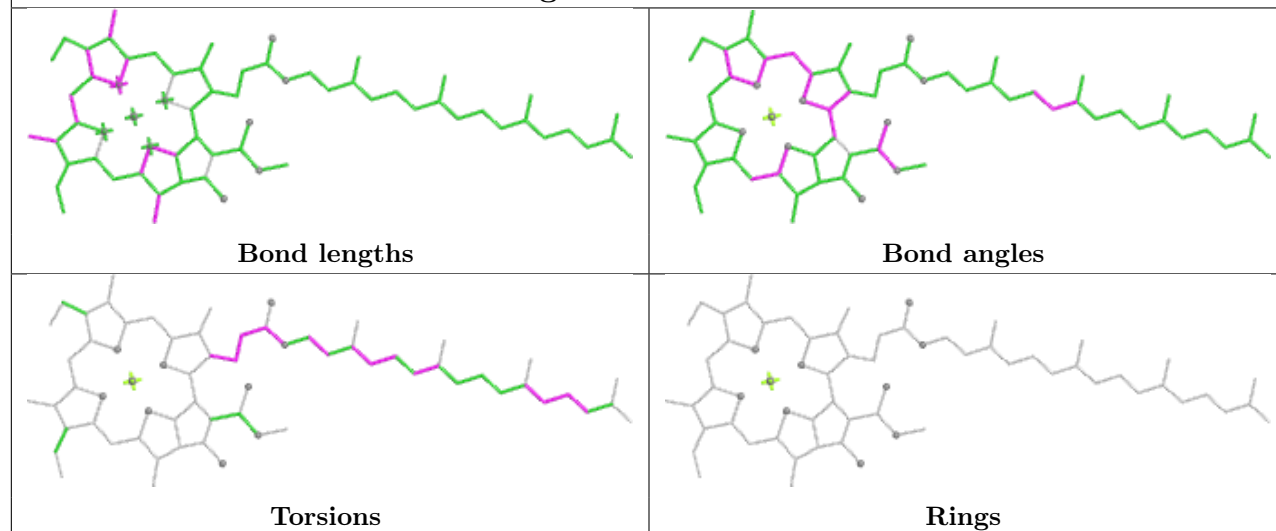




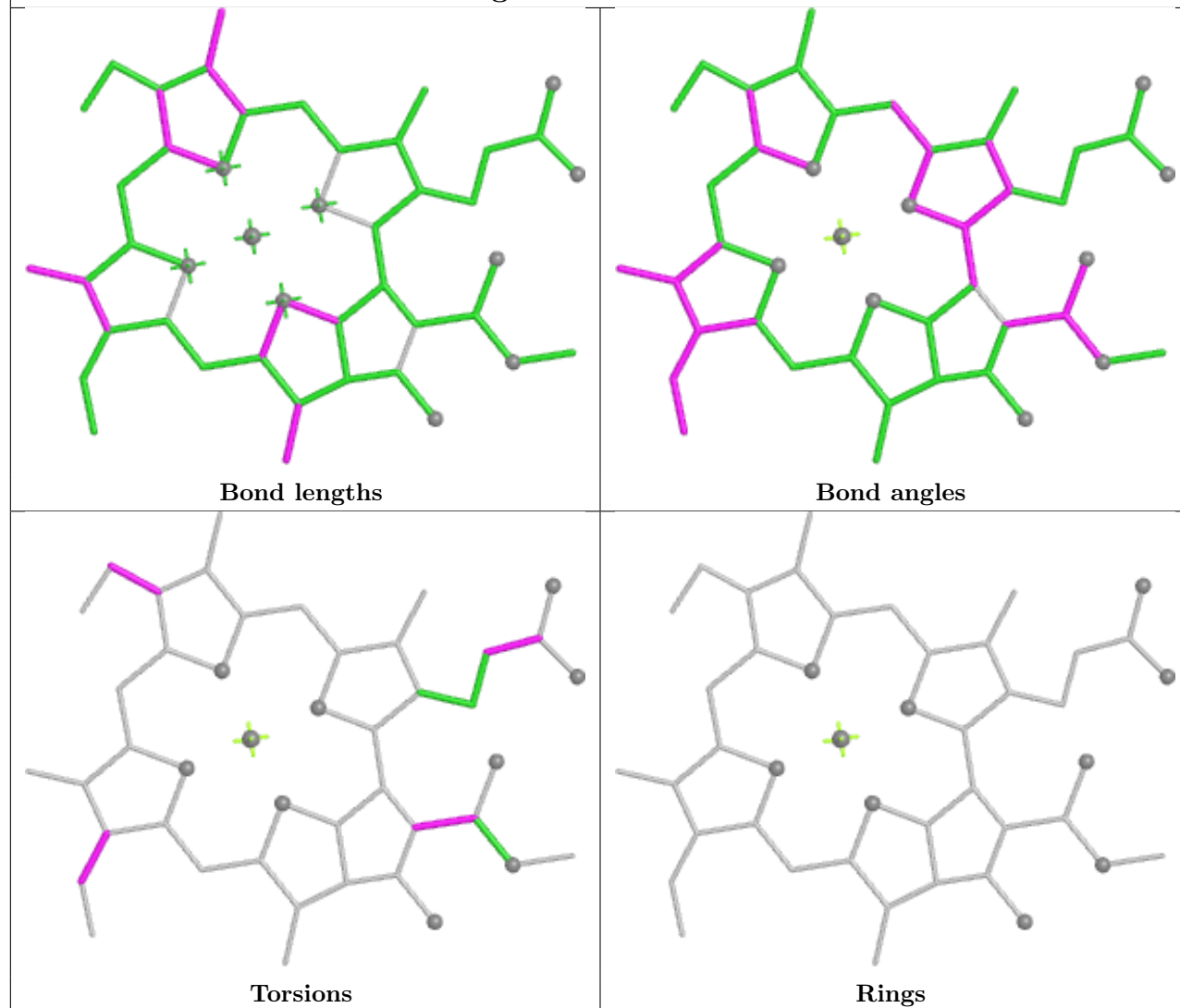


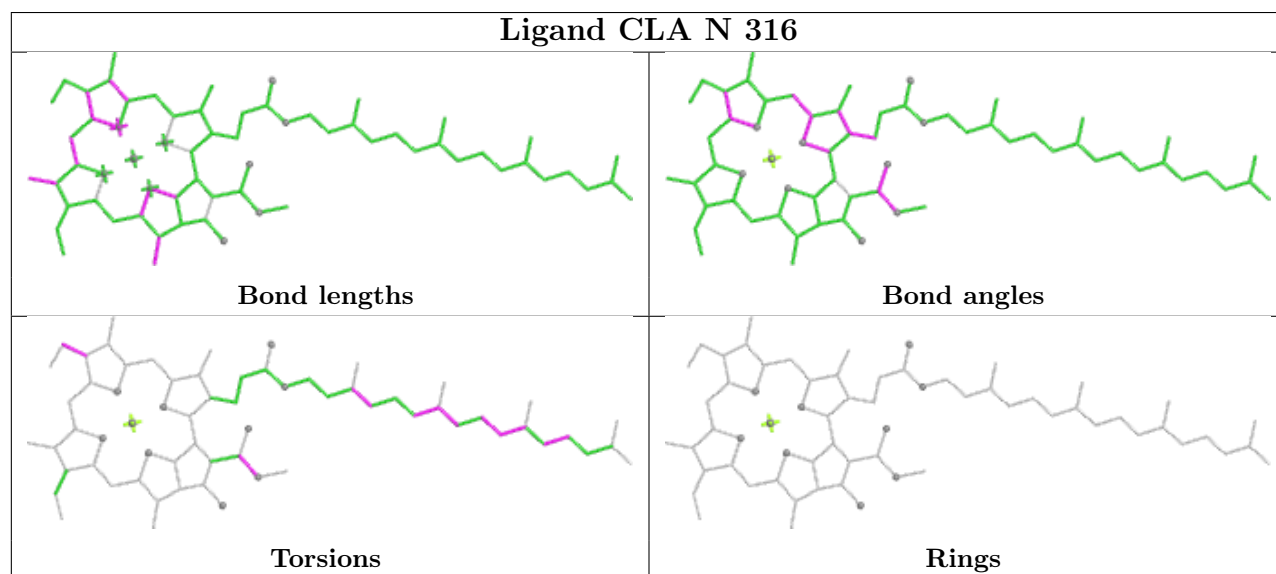
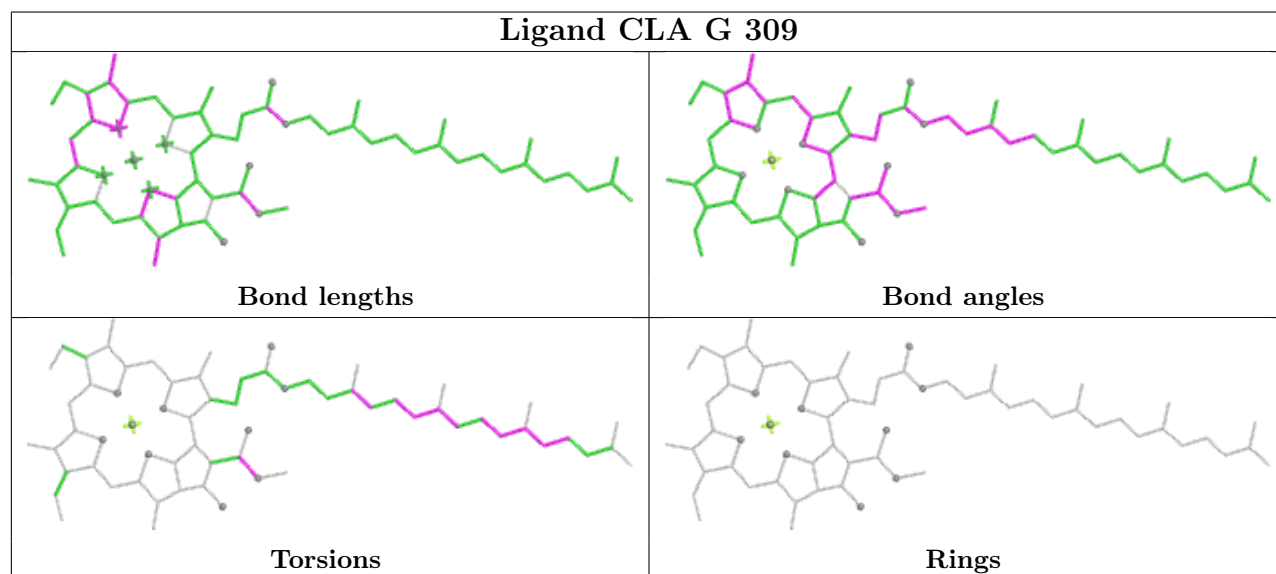
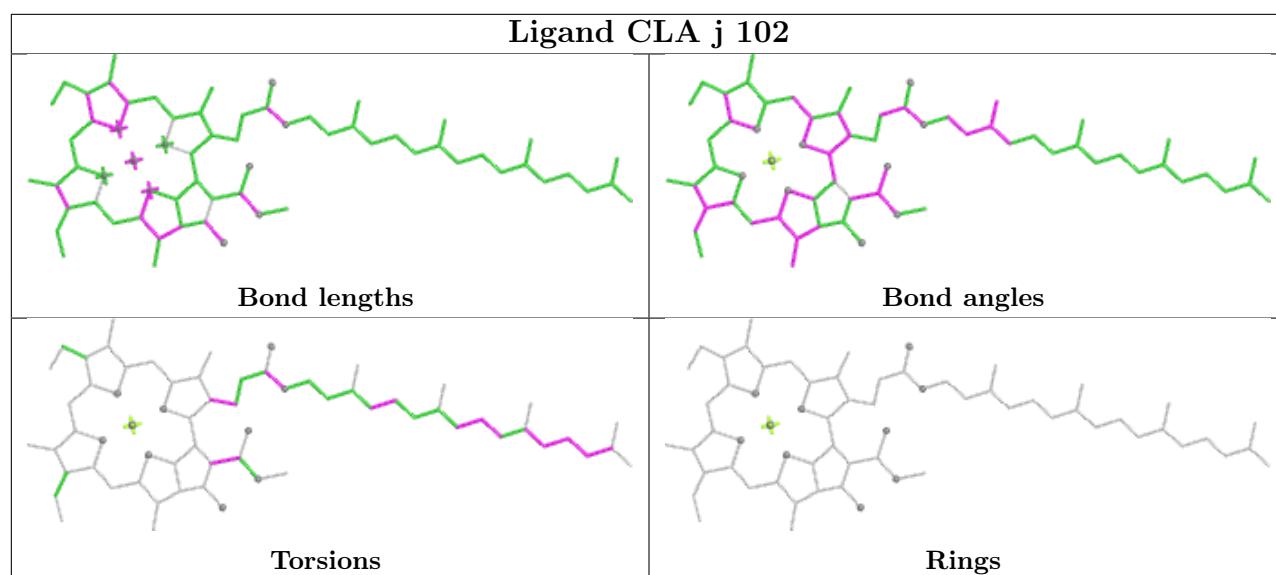


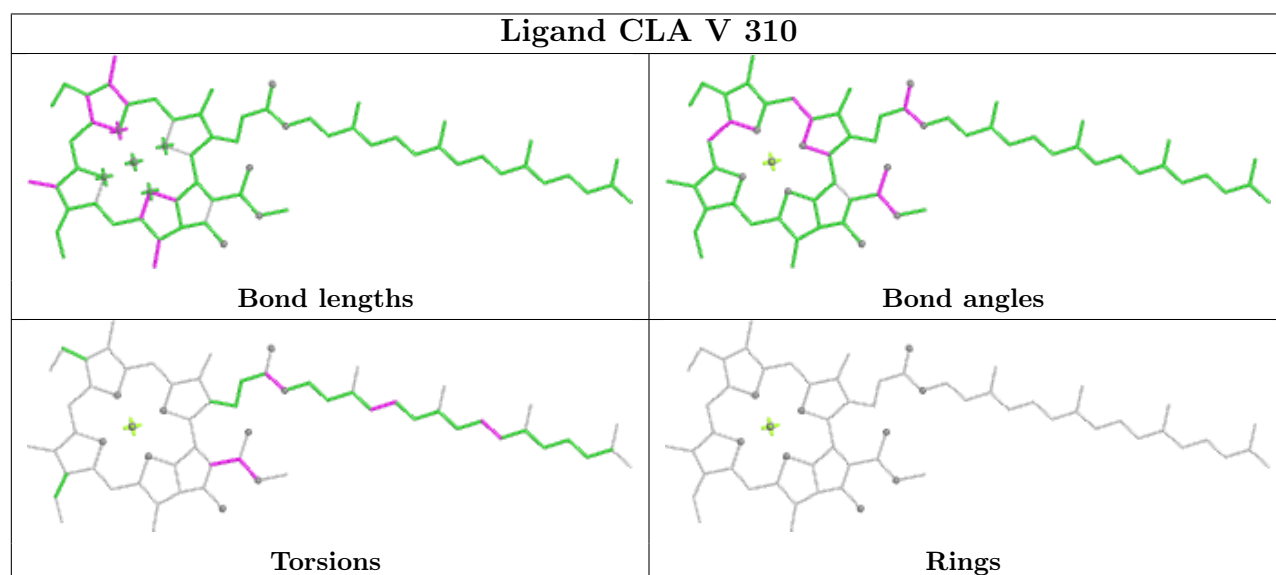
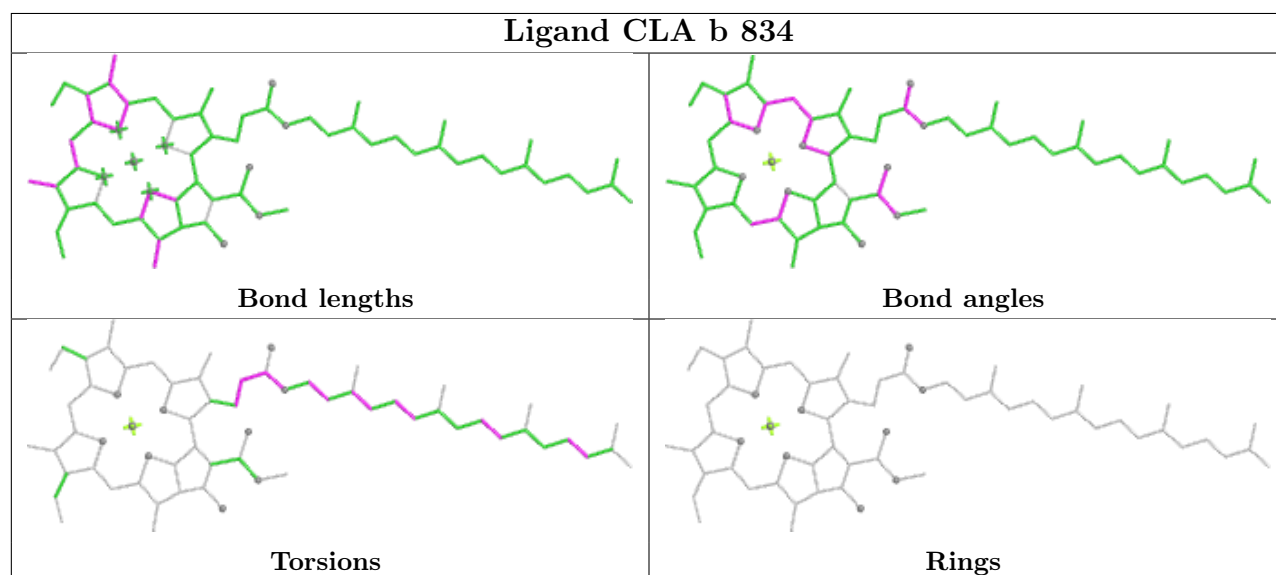
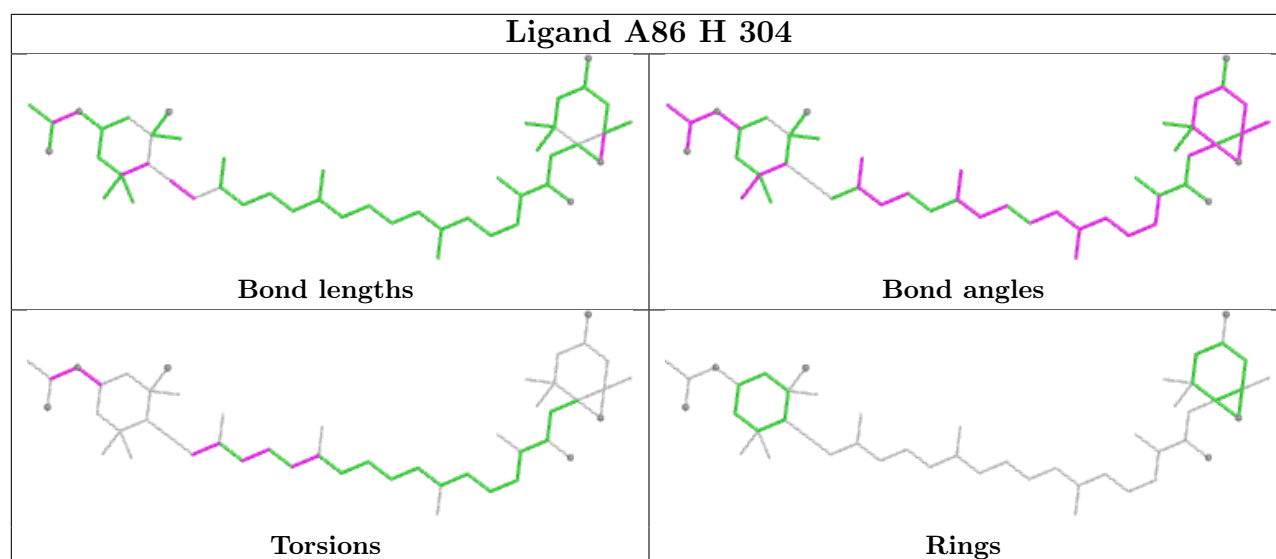
Ligand CLA f 802

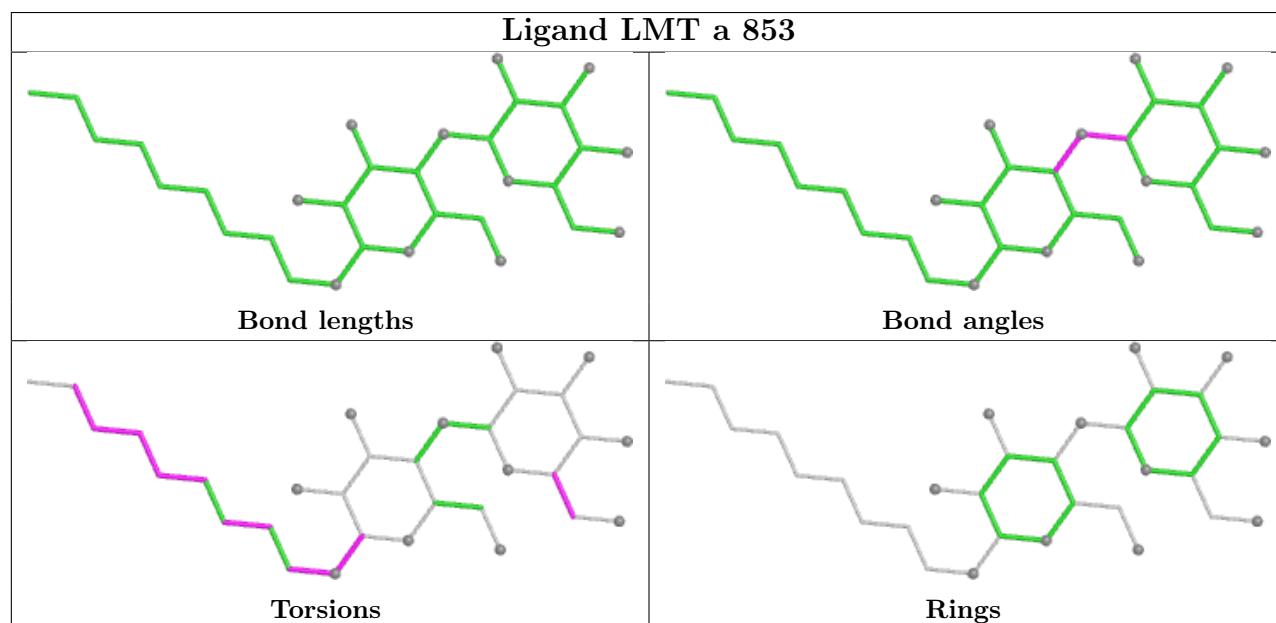
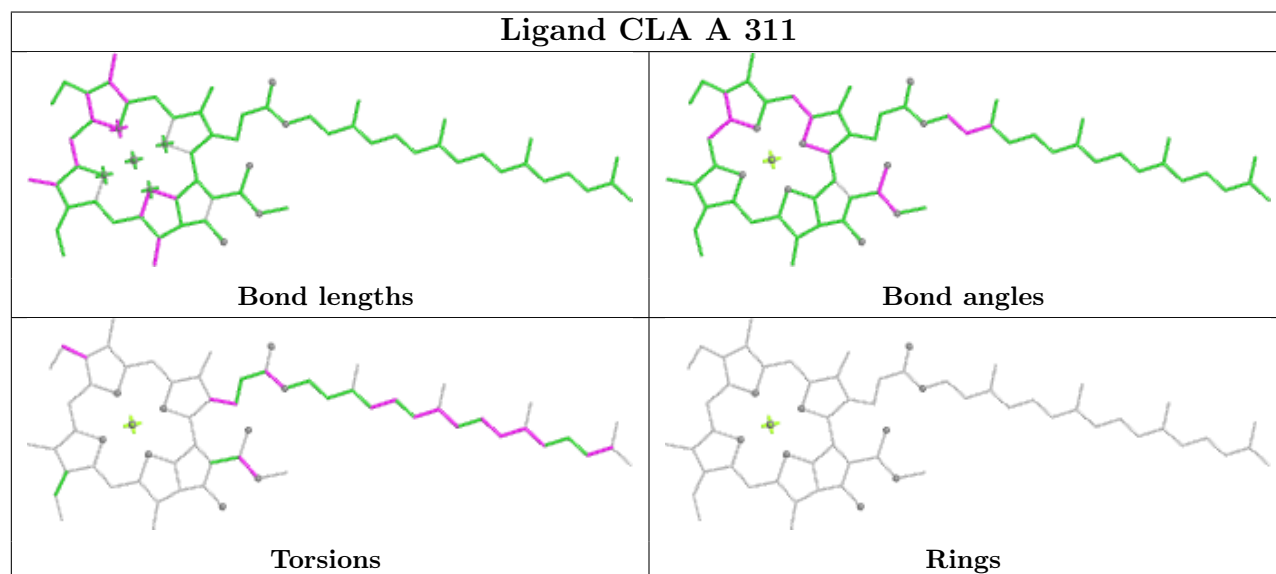
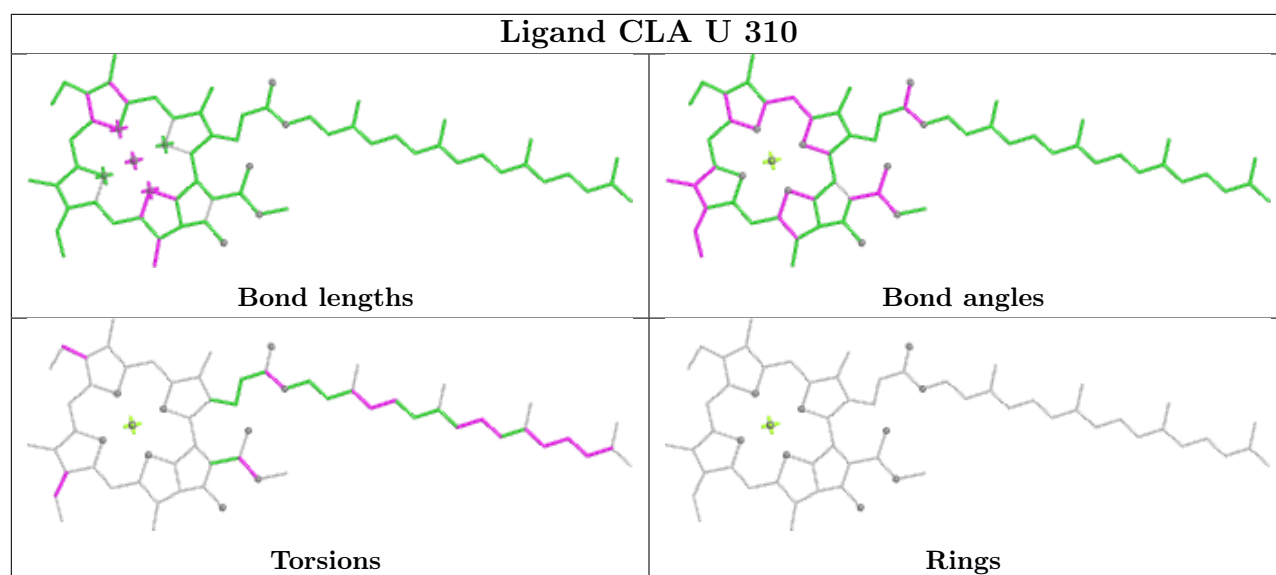


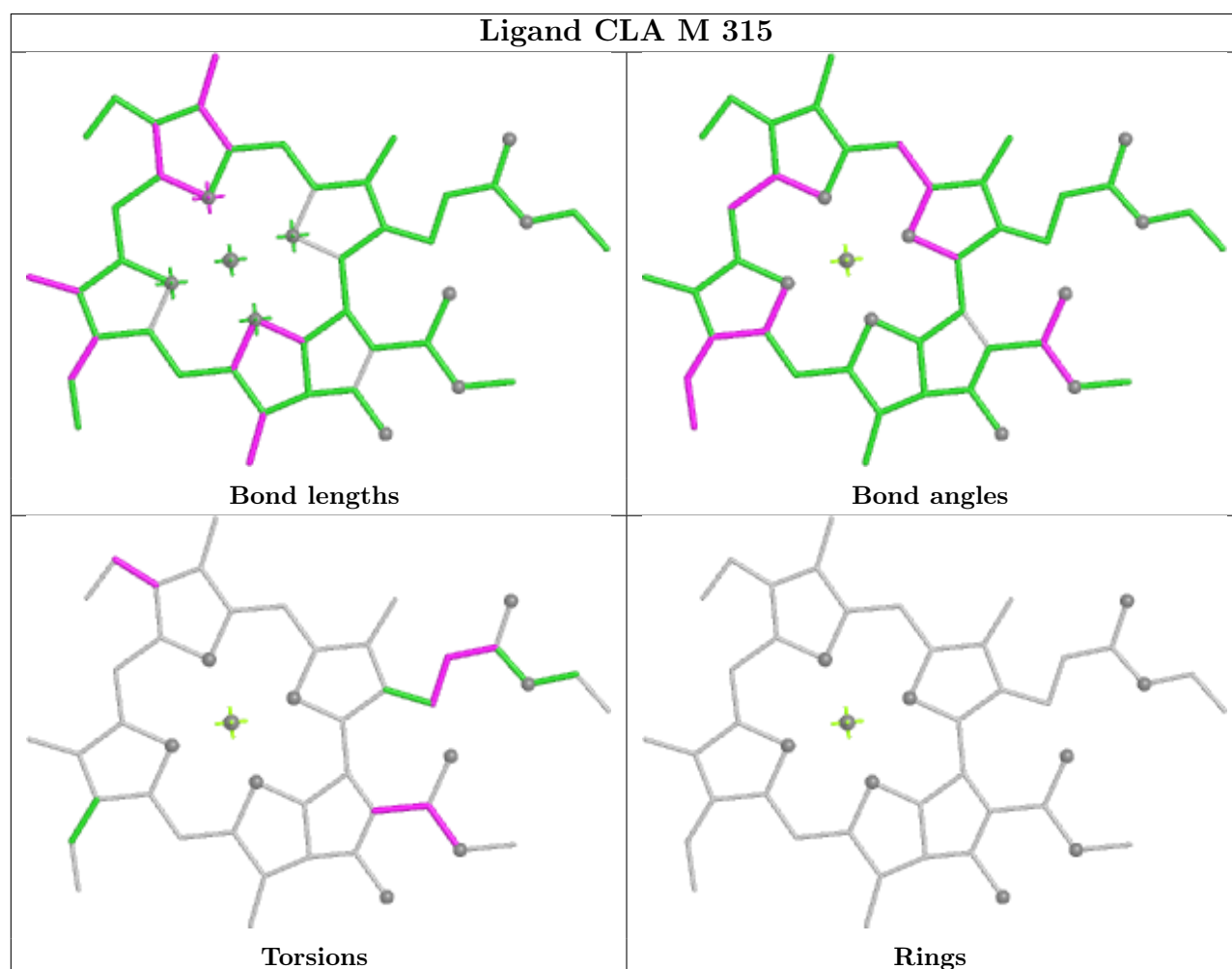
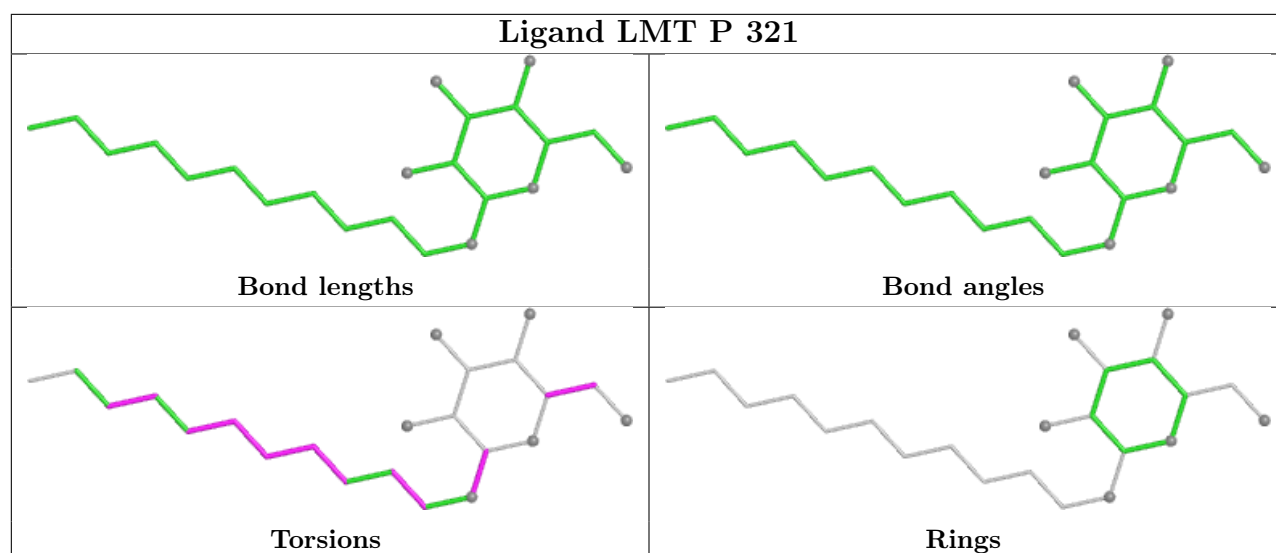
Ligand CLA R 319

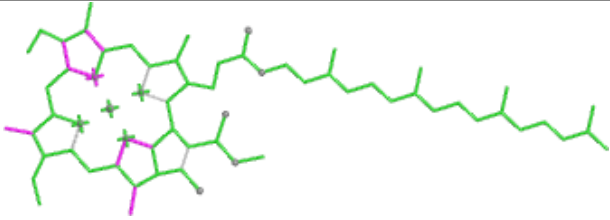
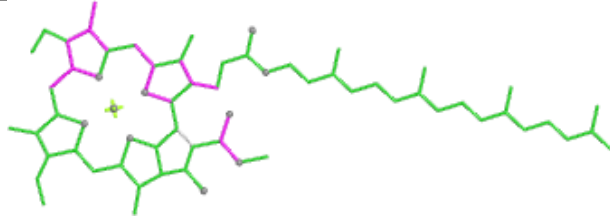
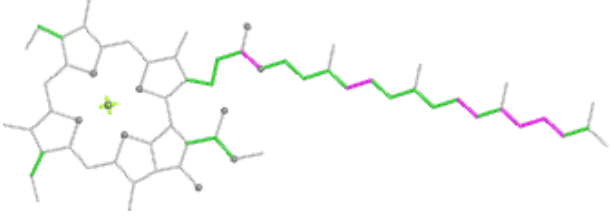
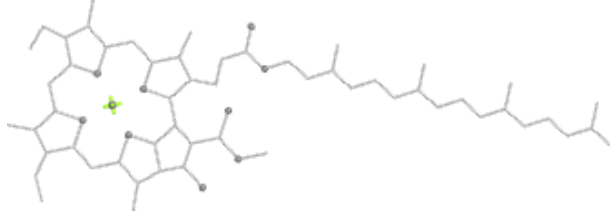
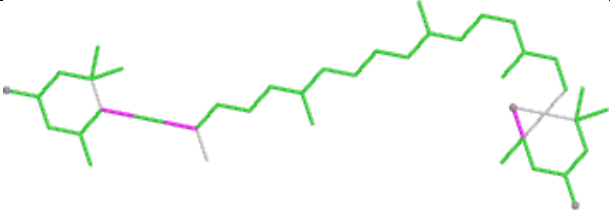
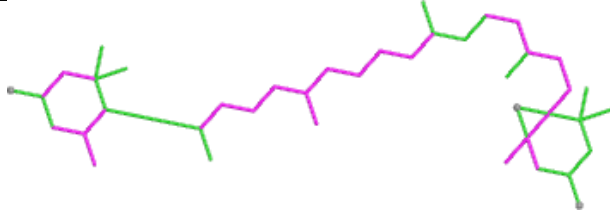
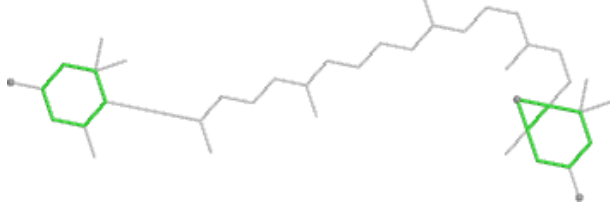
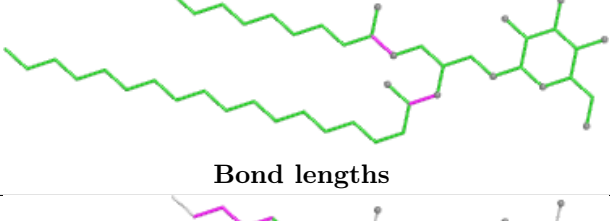
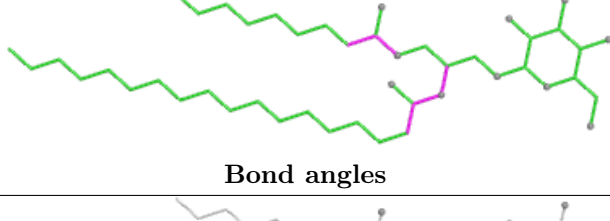
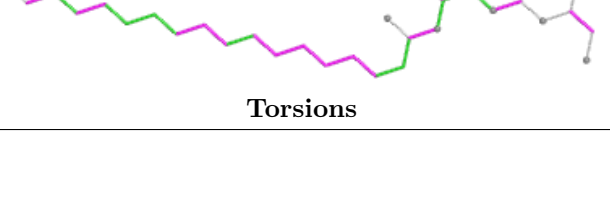




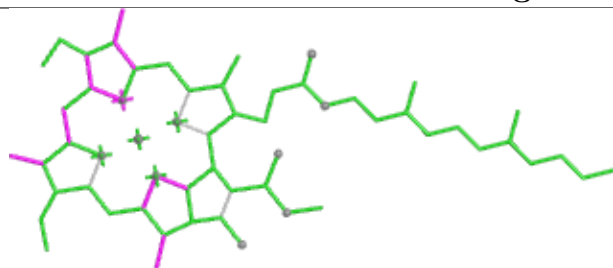




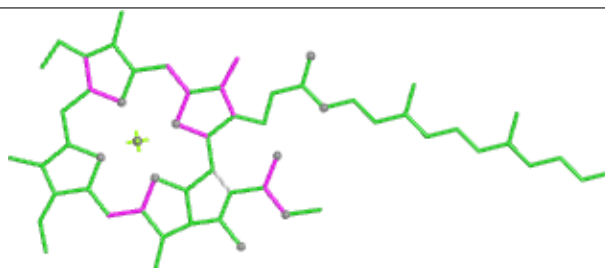


Ligand CLA L 313	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DD6 K 305	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG V 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

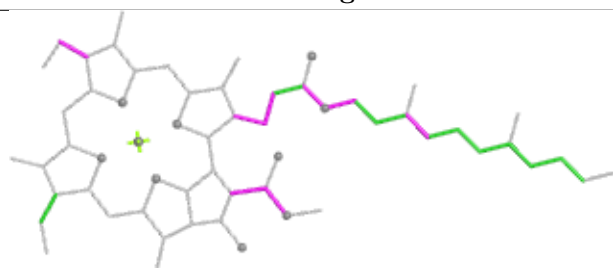
Ligand CLA D 317



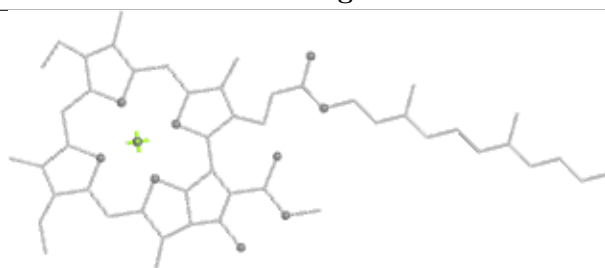
Bond lengths



Bond angles

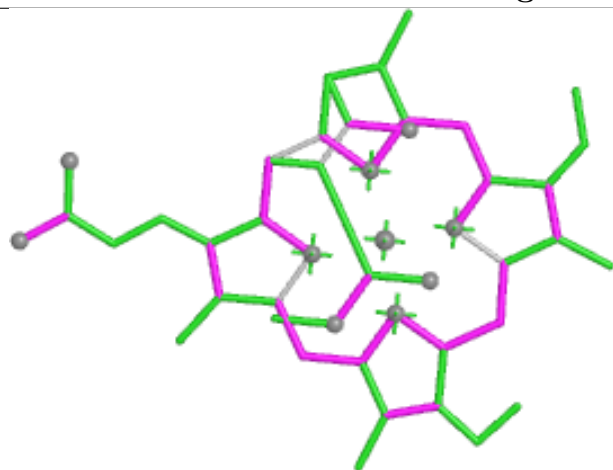


Torsions

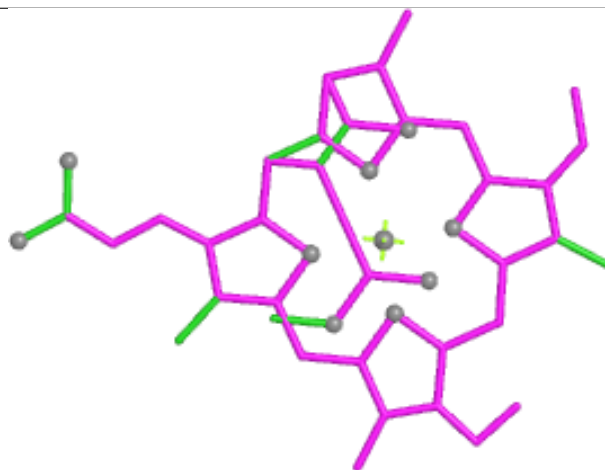


Rings

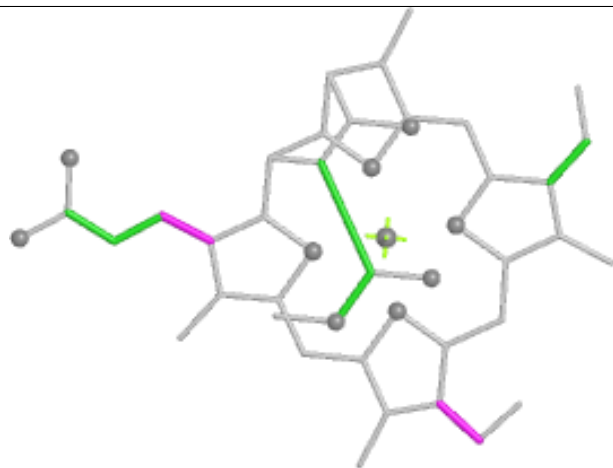
Ligand KC1 P 317



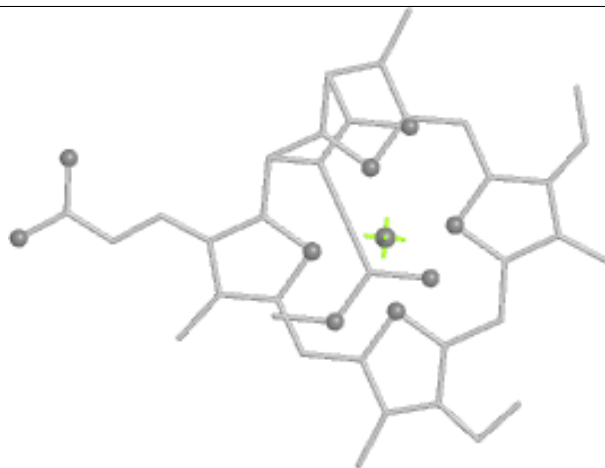
Bond lengths



Bond angles

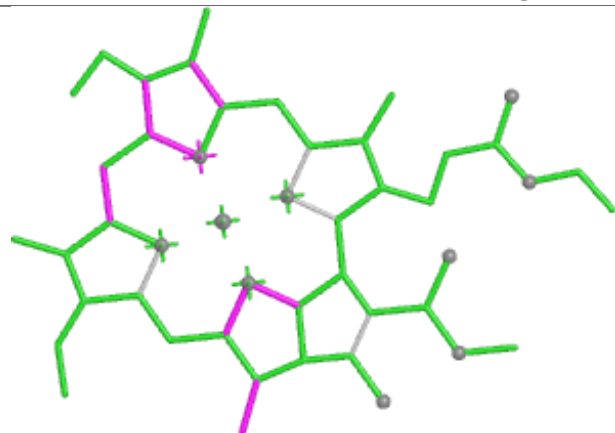


Torsions

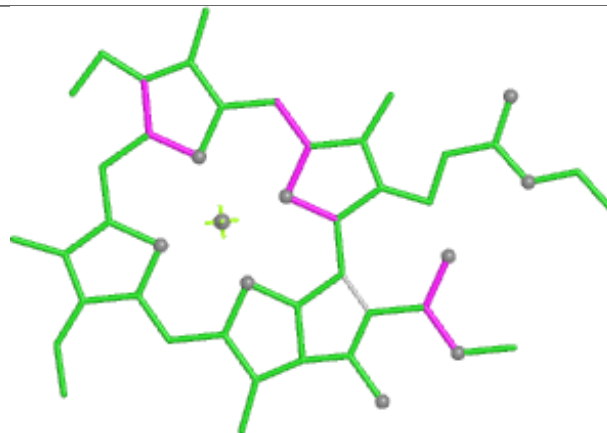


Rings

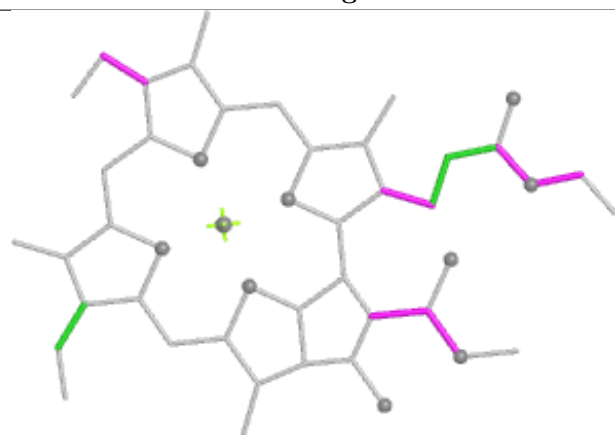
Ligand CLA N 312



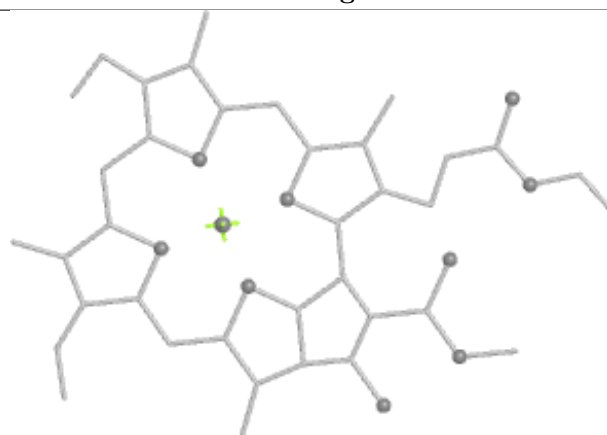
Bond lengths



Bond angles

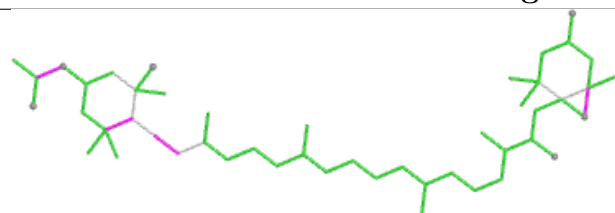


Torsions

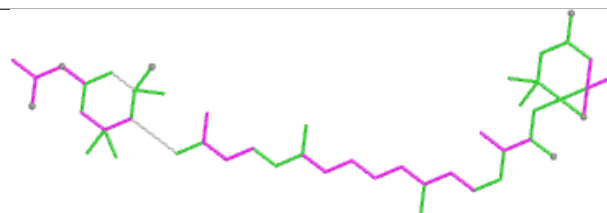


Rings

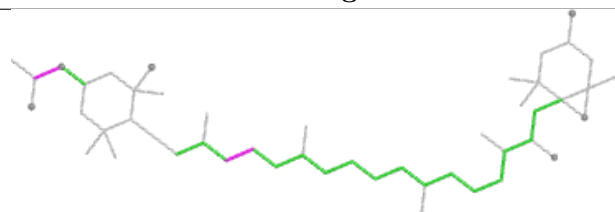
Ligand A86 X 314



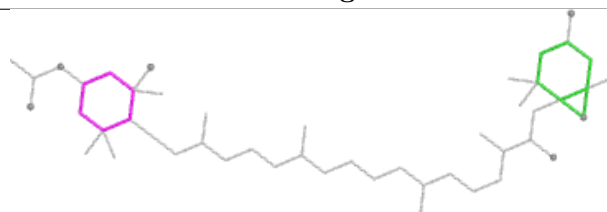
Bond lengths



Bond angles

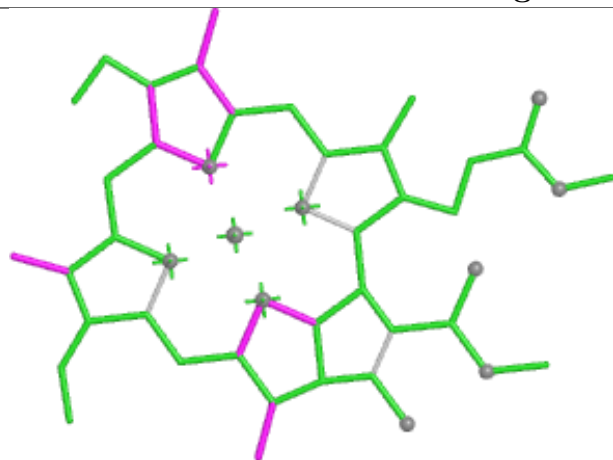


Torsions

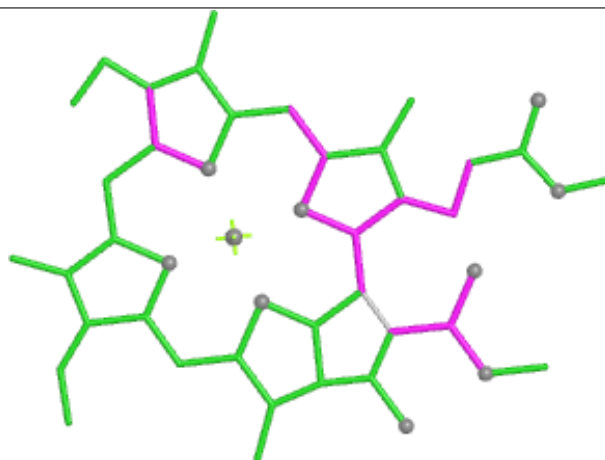


Rings

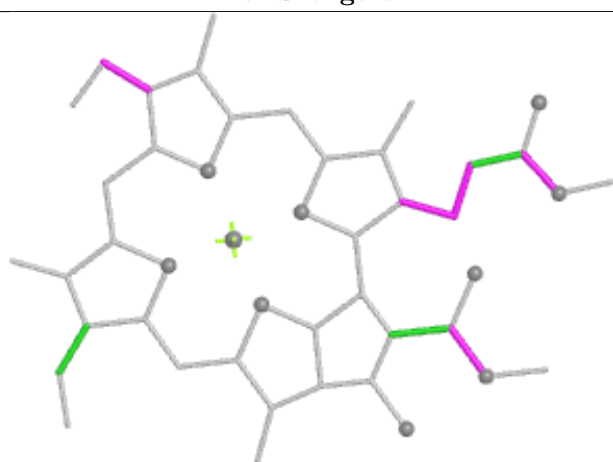
Ligand CLA O 310



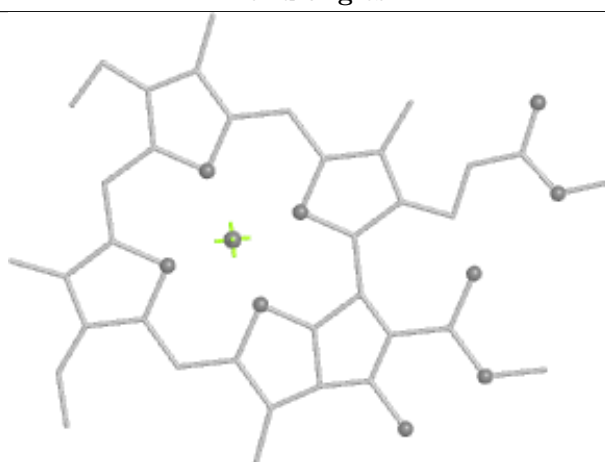
Bond lengths



Bond angles

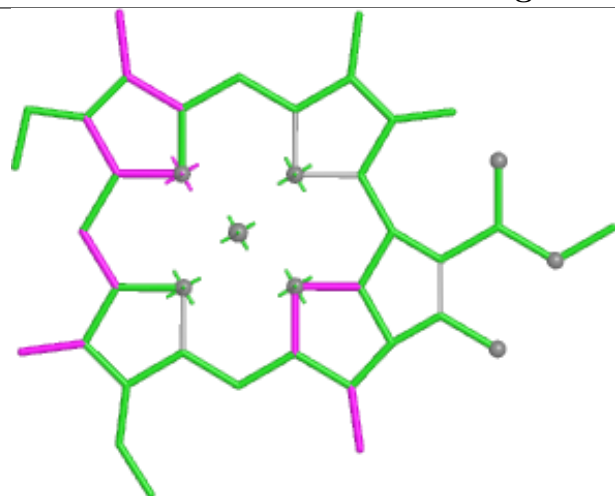


Torsions

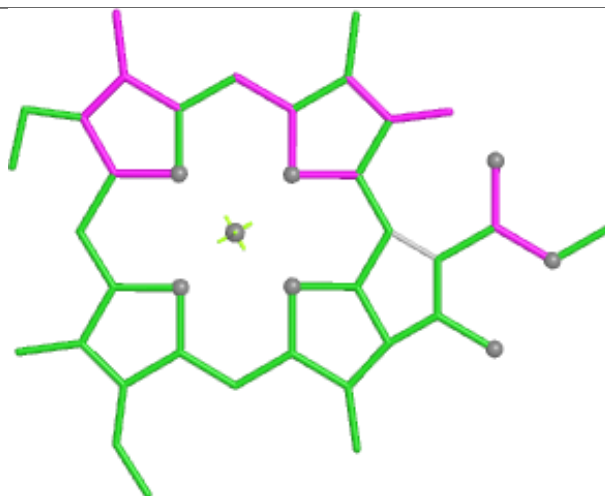


Rings

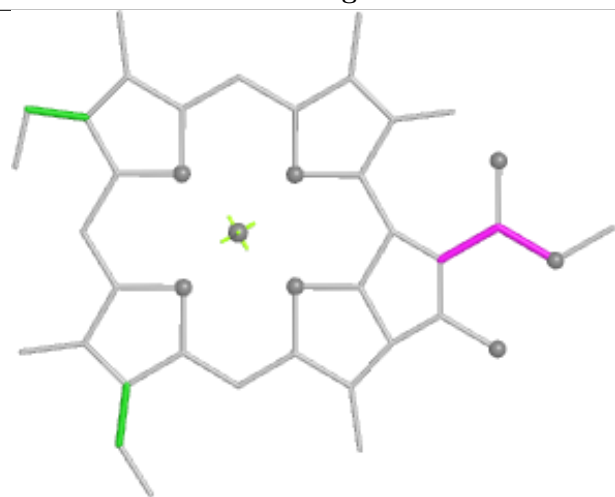
Ligand CLA K 315



Bond lengths



Bond angles

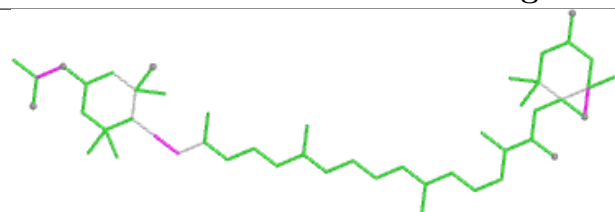


Torsions

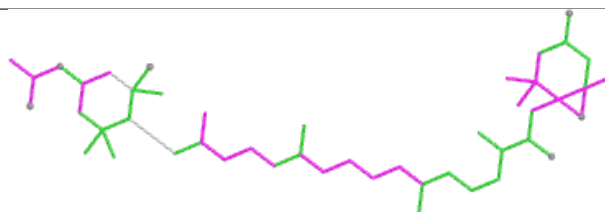


Rings

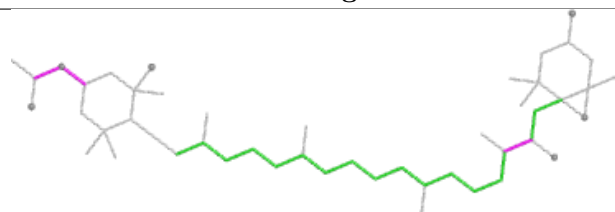
Ligand A86 N 302



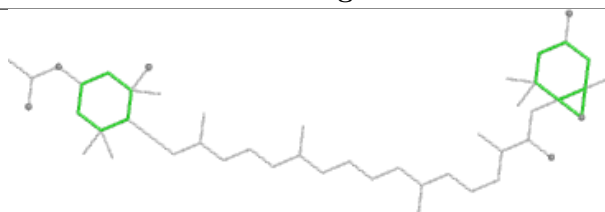
Bond lengths



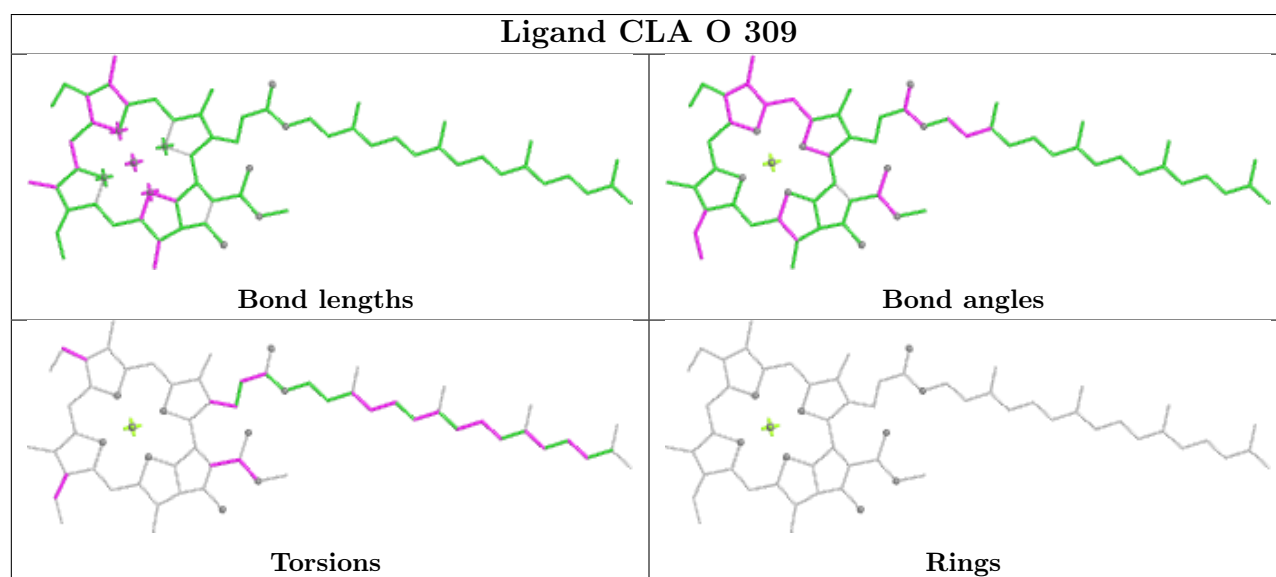
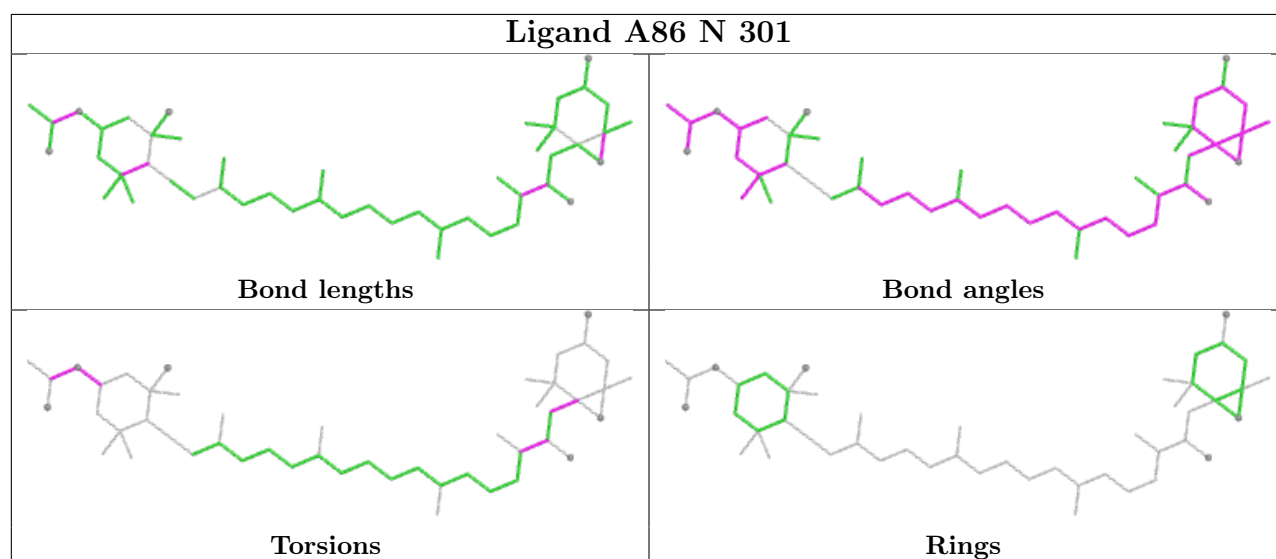
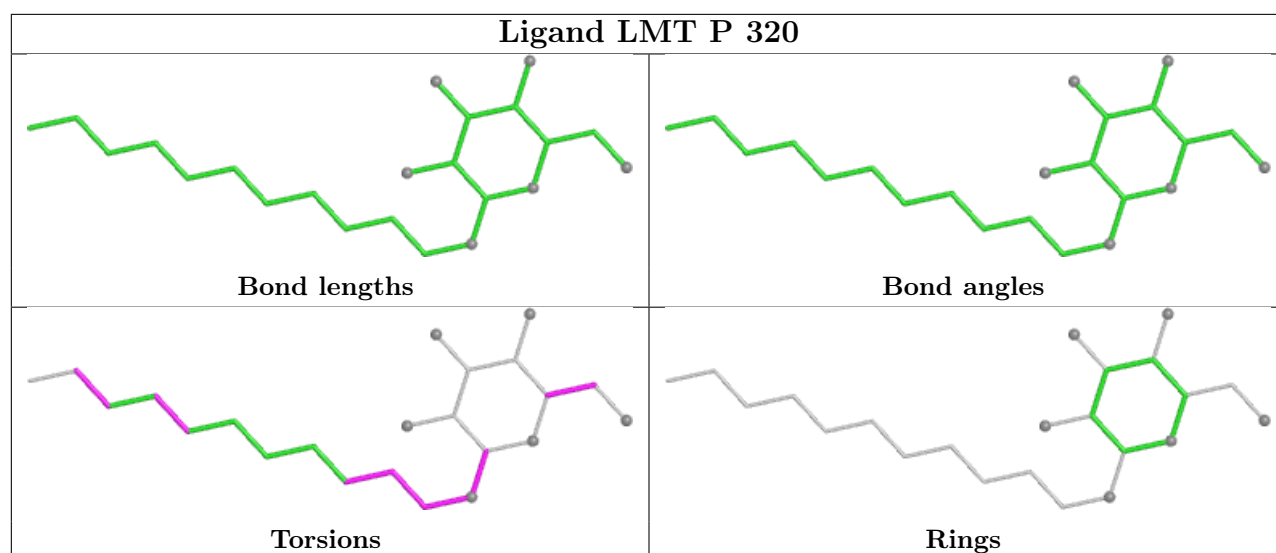
Bond angles

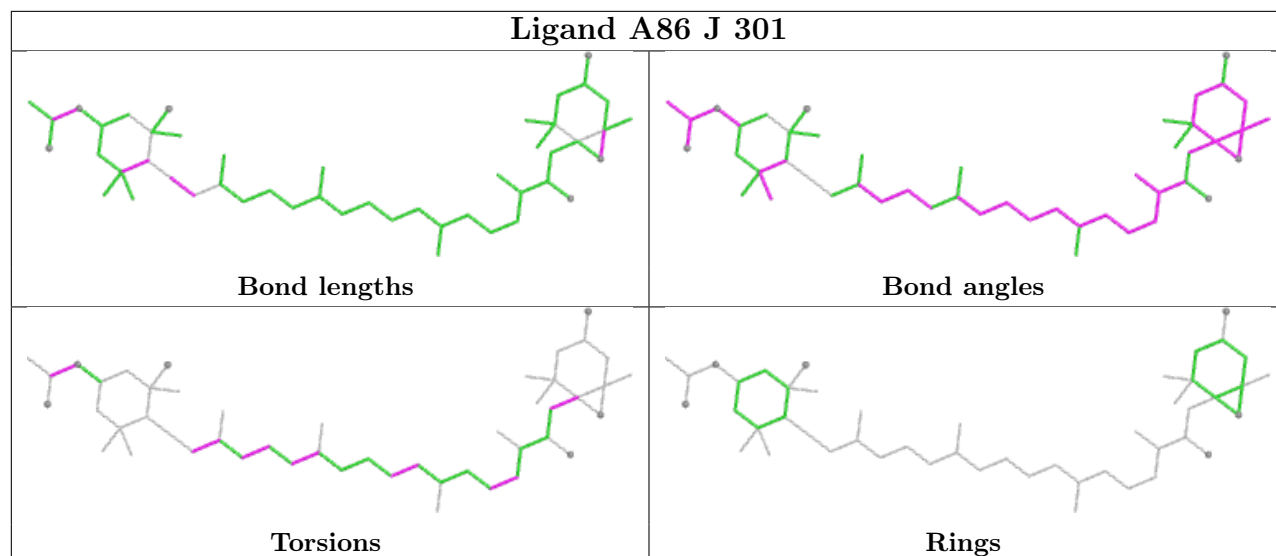
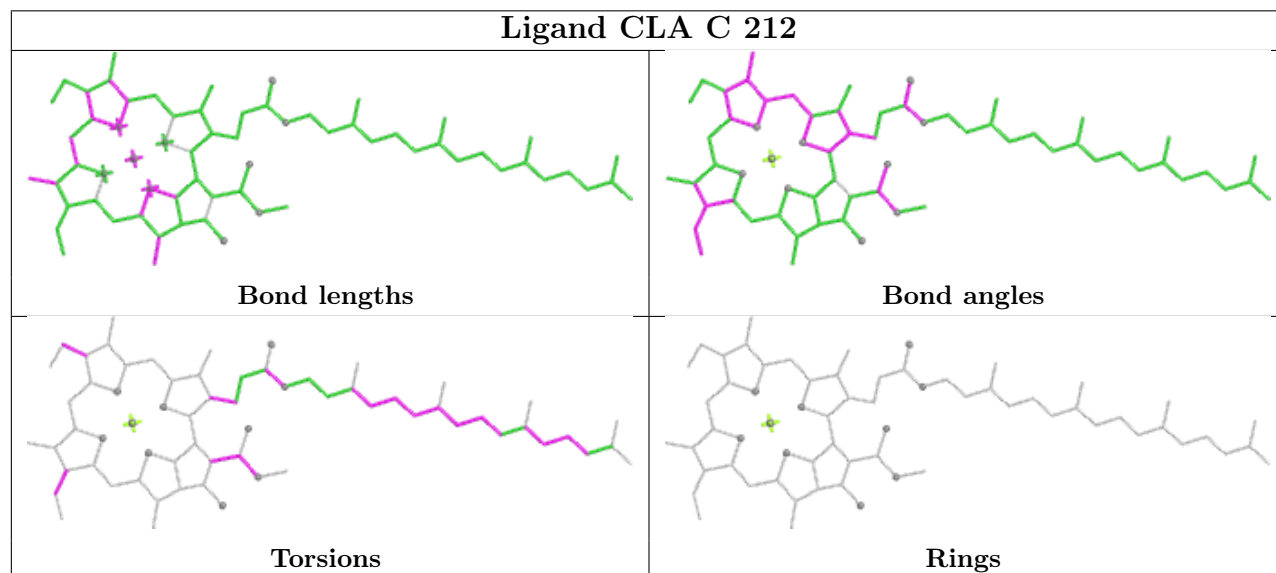
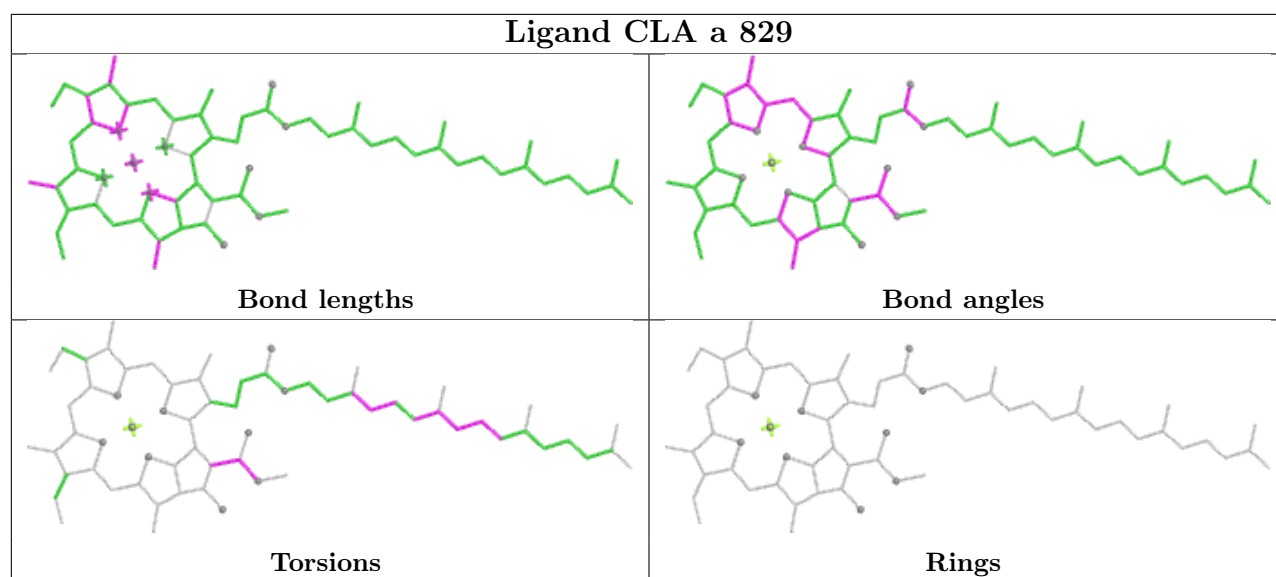


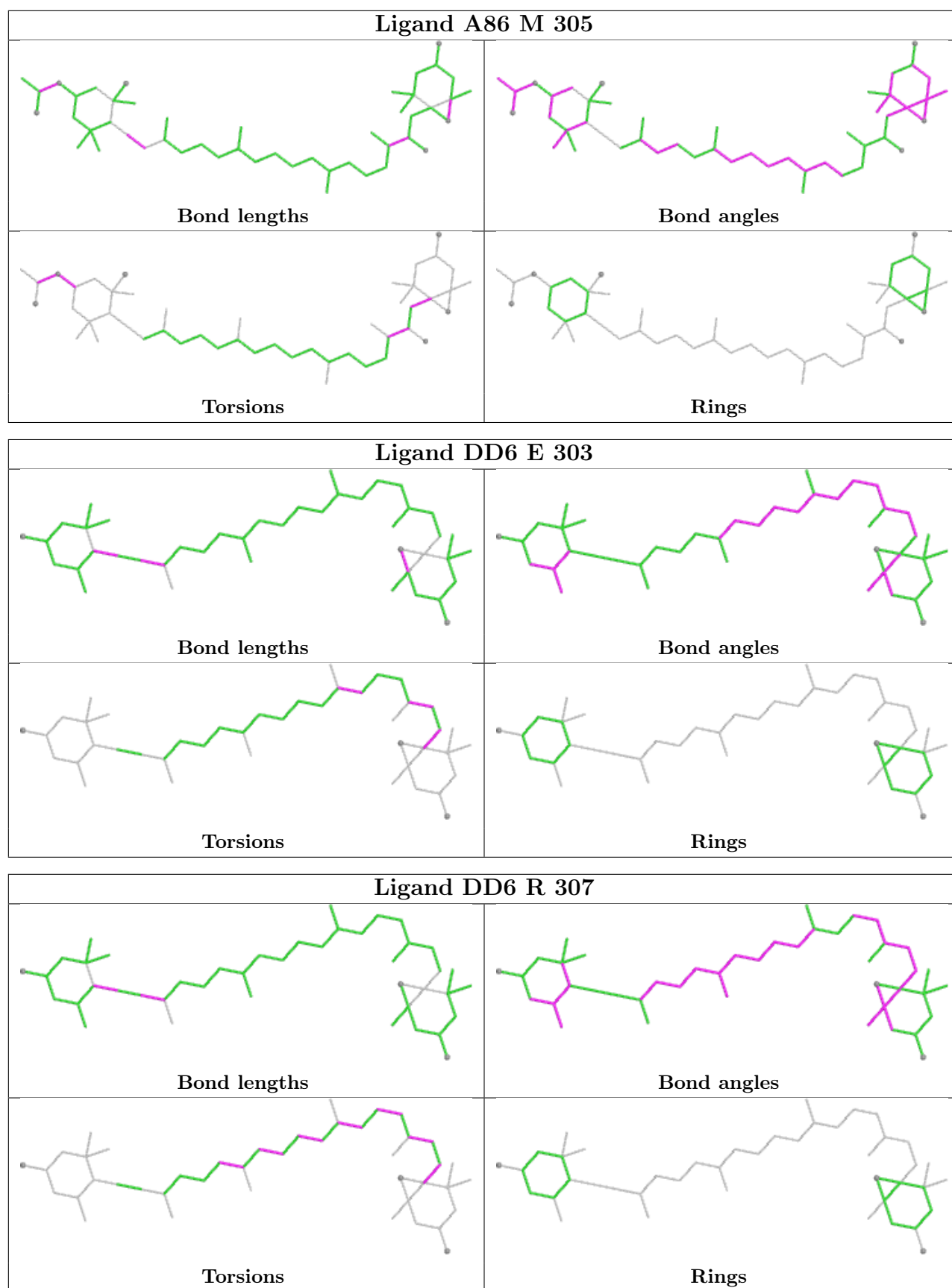
Torsions

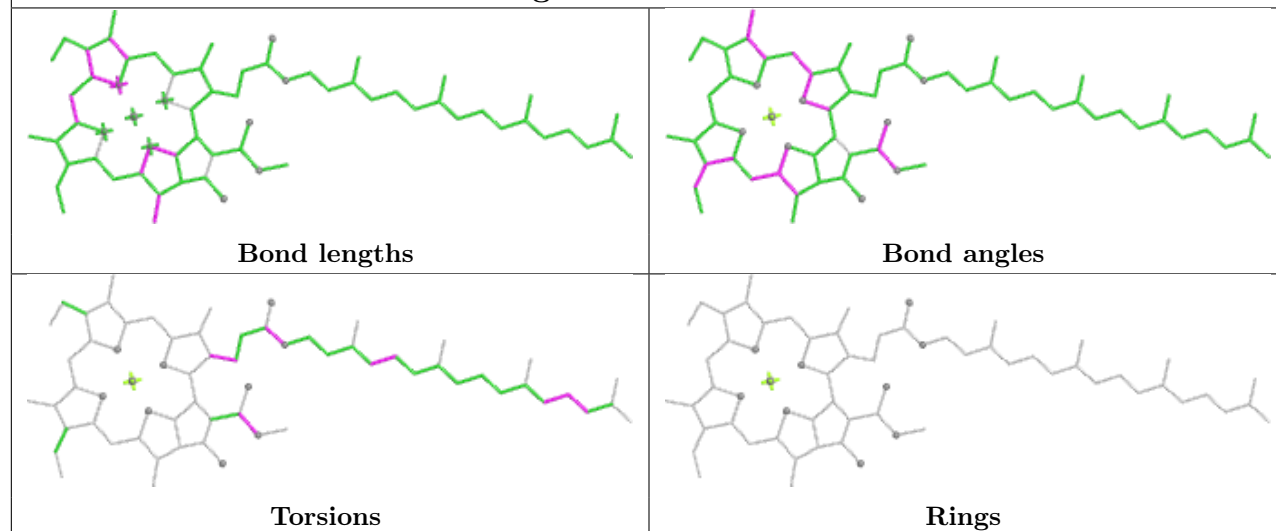
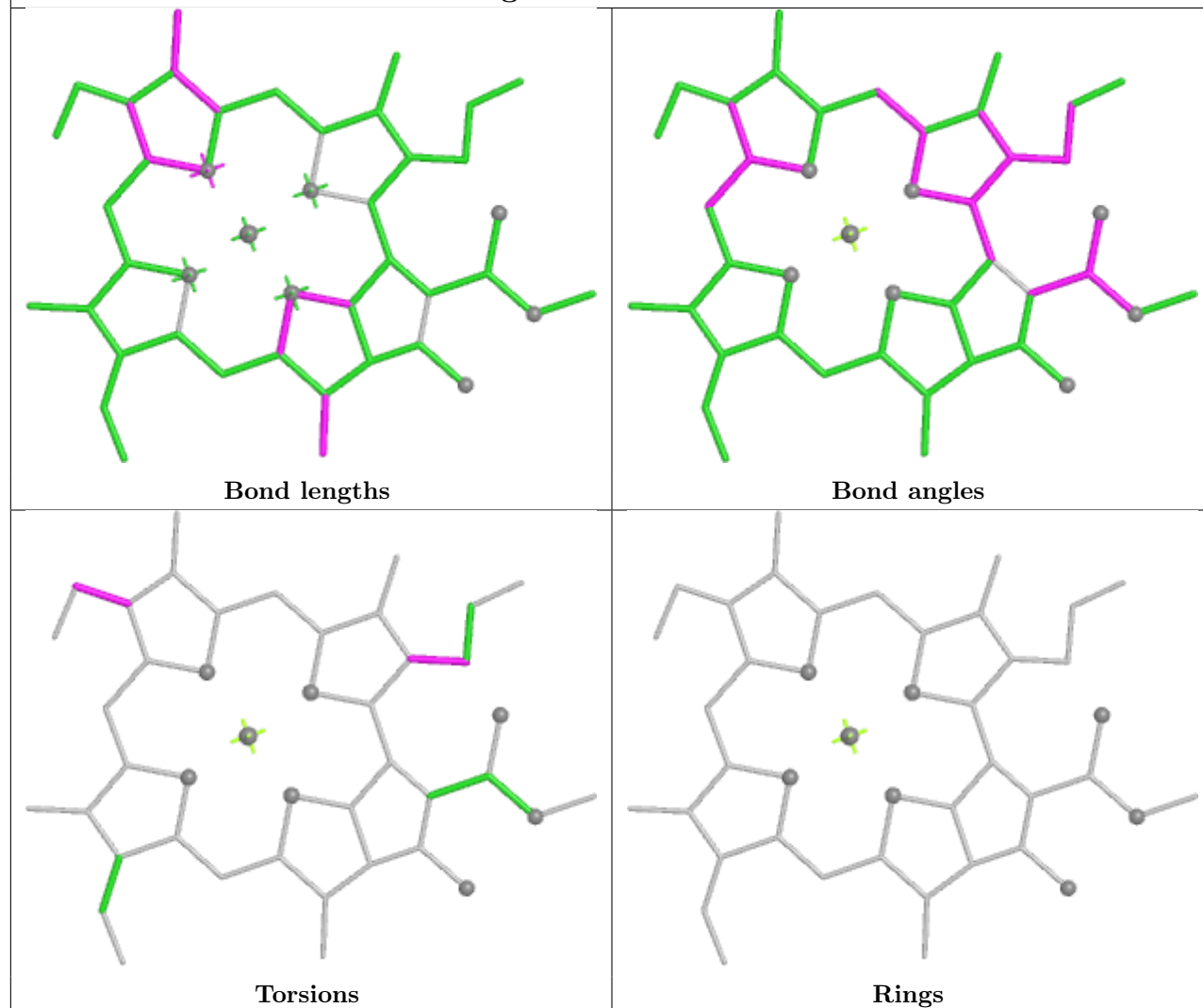


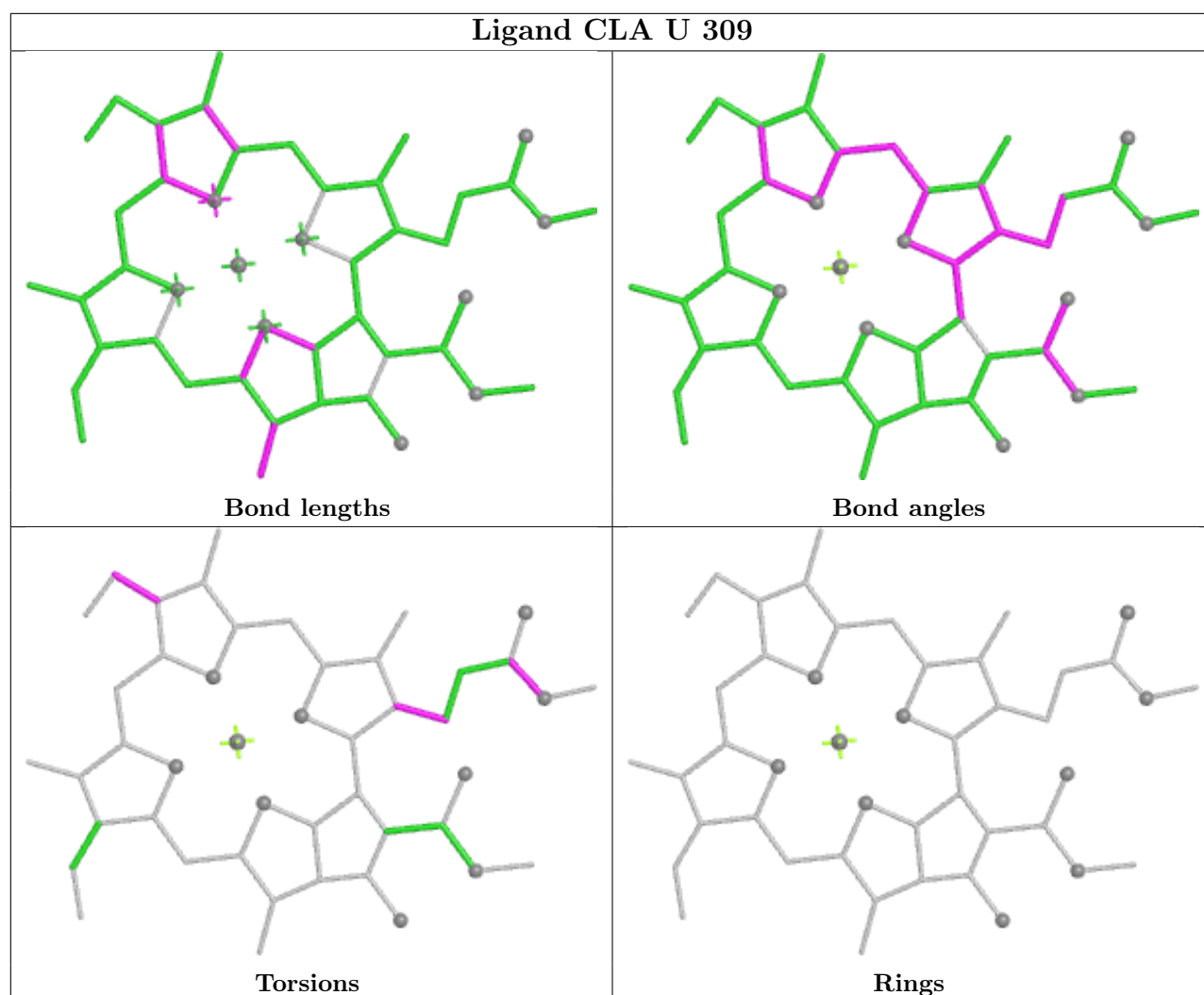
Rings







Ligand CLA T 313**Ligand CLA V 309**



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.

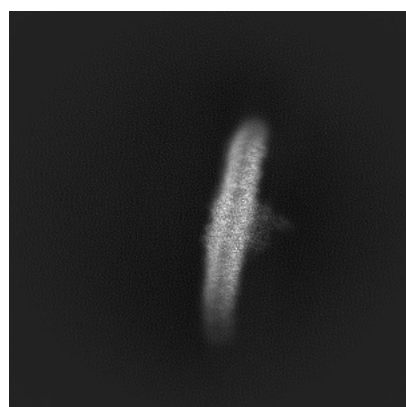
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30012. These allow visual inspection of the internal detail of the map and identification of artifacts.

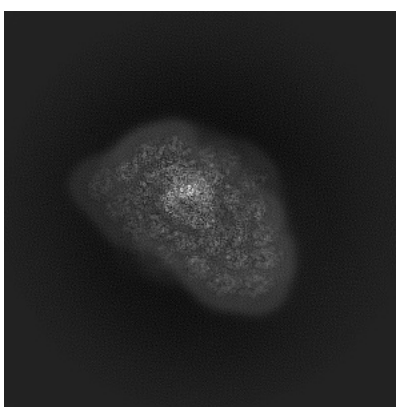
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

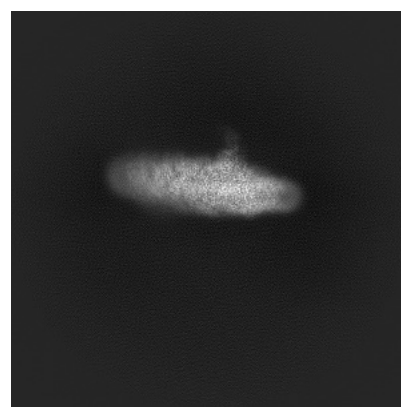
6.1.1 Primary map



X



Y

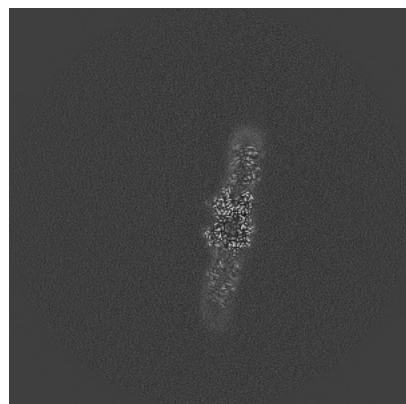


Z

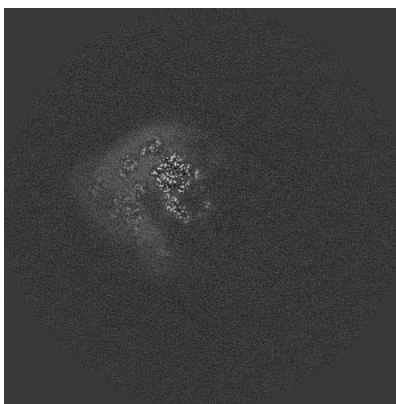
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

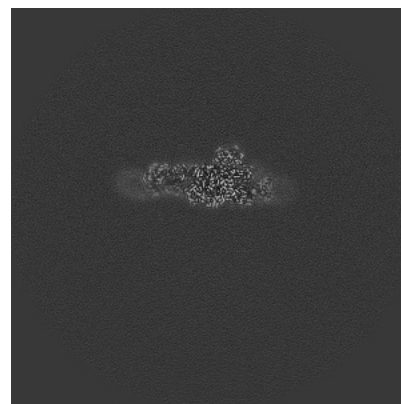
6.2.1 Primary map



X Index: 260



Y Index: 260



Z Index: 260

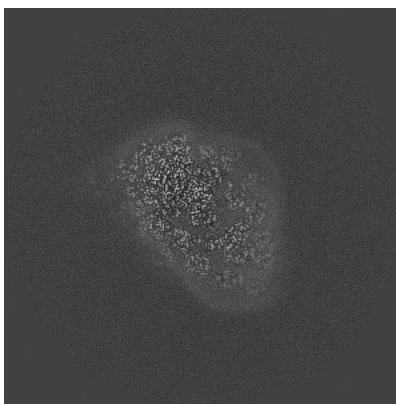
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

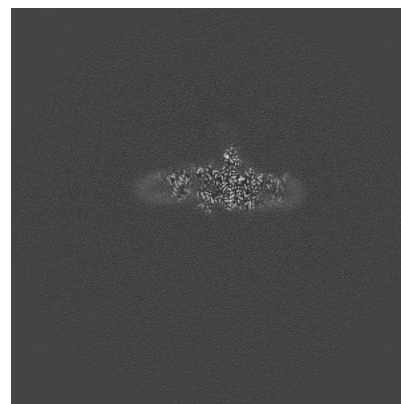
6.3.1 Primary map



X Index: 278



Y Index: 294

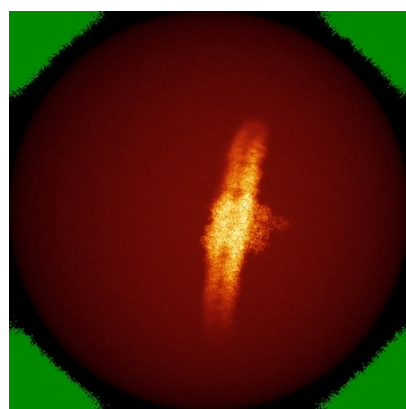


Z Index: 231

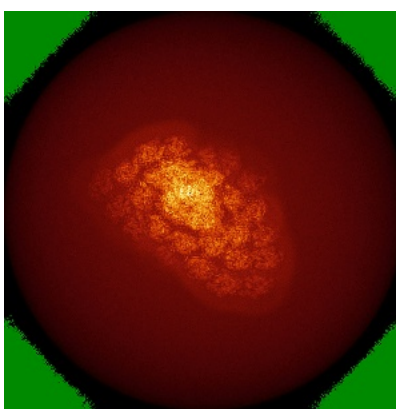
The images above show the largest variance slices of the map in three orthogonal directions.

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

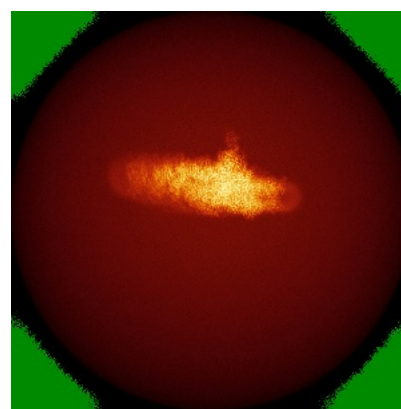
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

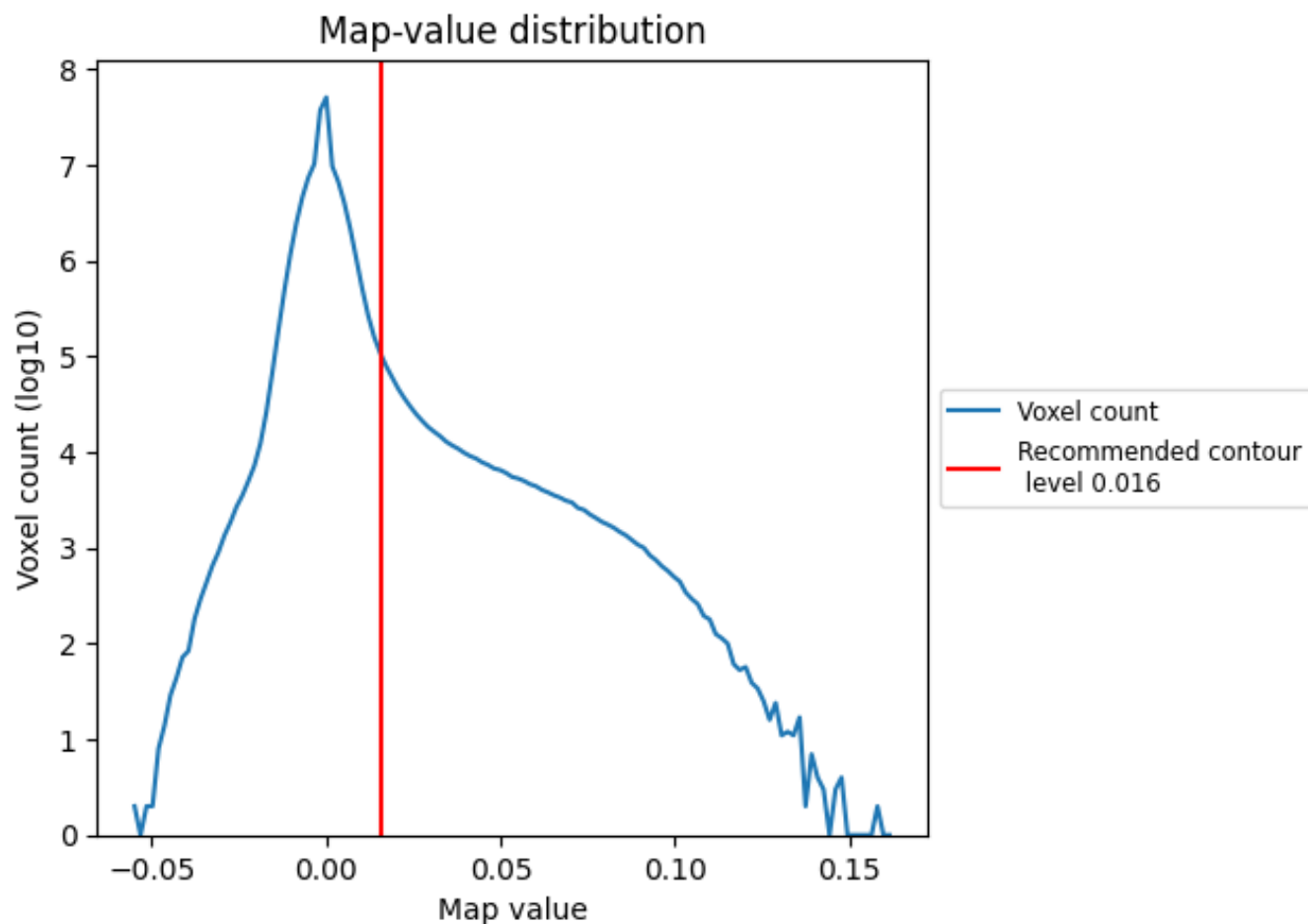
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

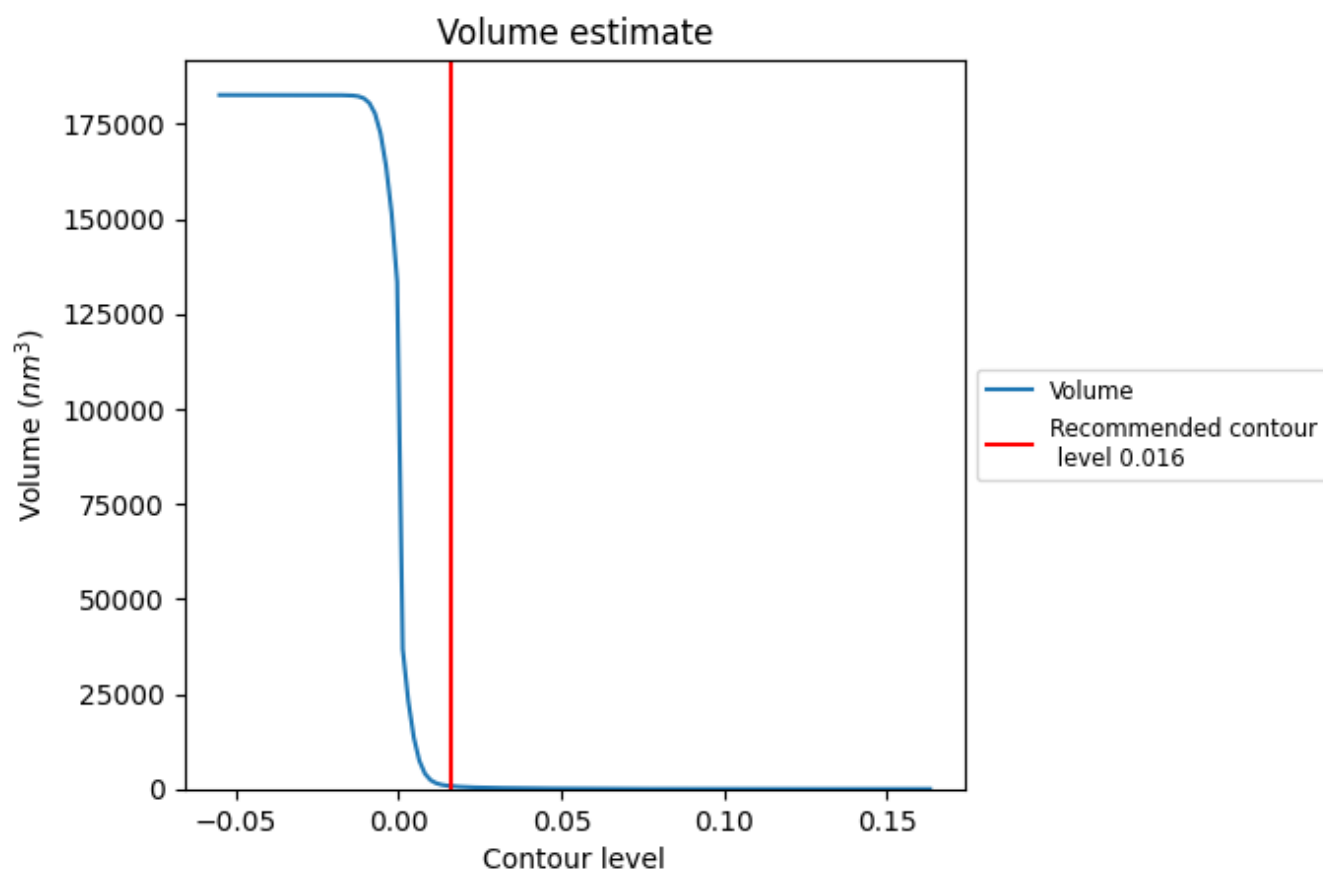
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

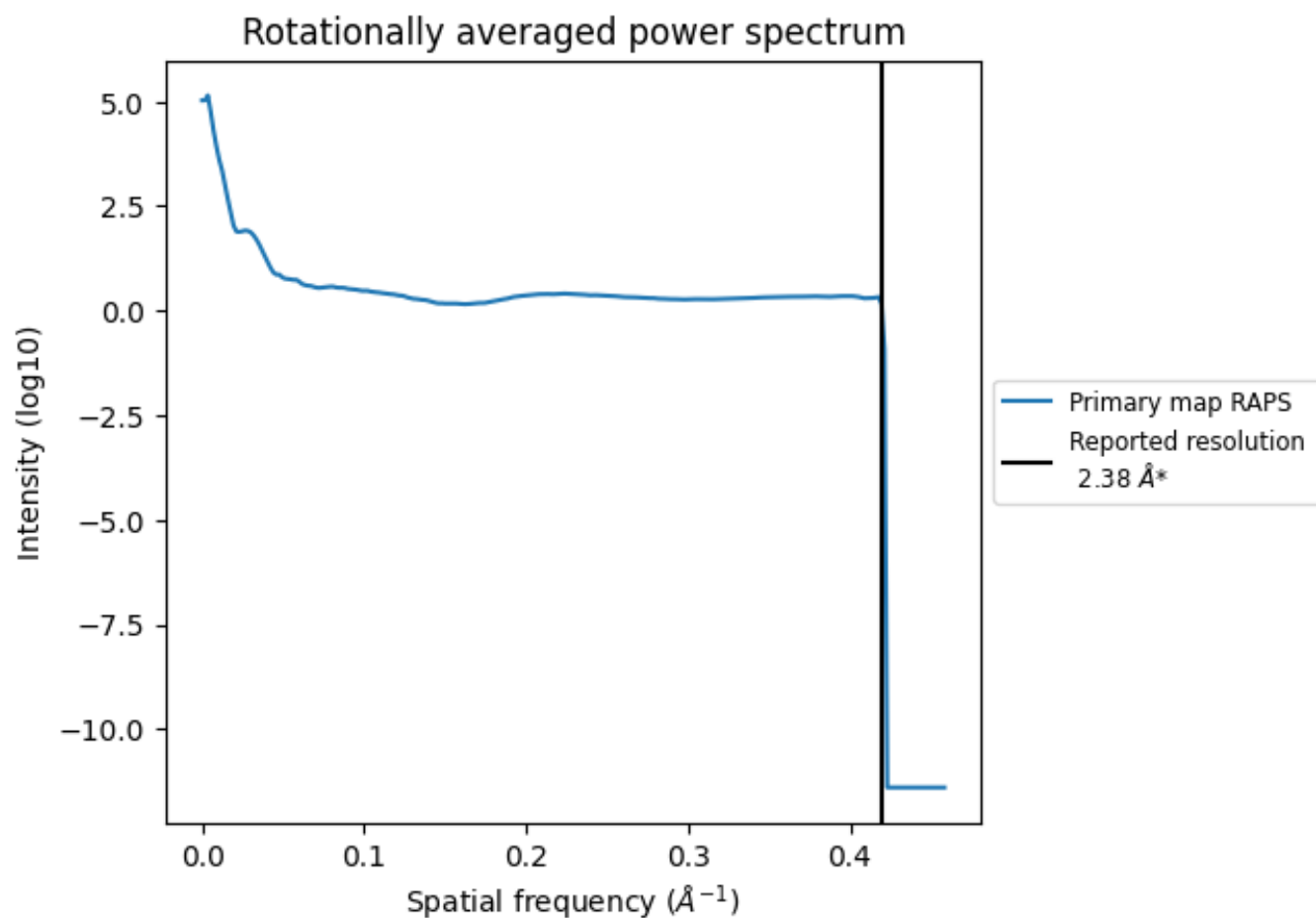
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778 nm^3 ; this corresponds to an approximate mass of 703 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 0.420 Å⁻¹

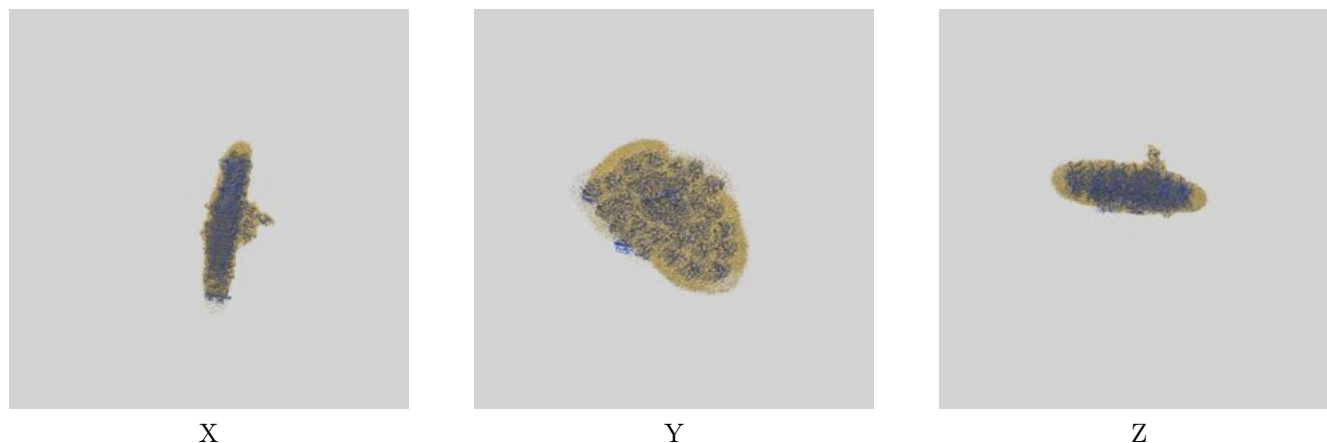
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

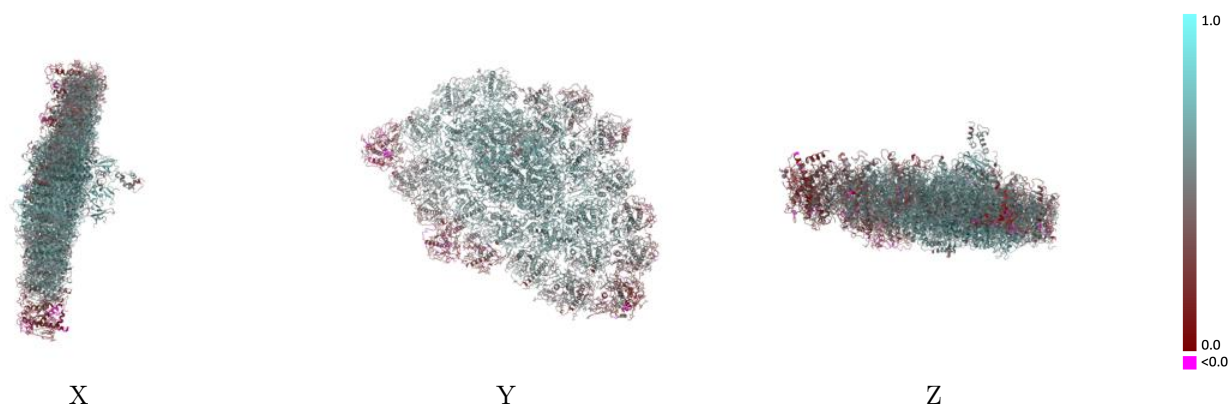
This section contains information regarding the fit between EMDB map EMD-30012 and PDB model 6LY5. Per-residue inclusion information can be found in [section 3](#) on [page 46](#).

9.1 Map-model overlay [i](#)



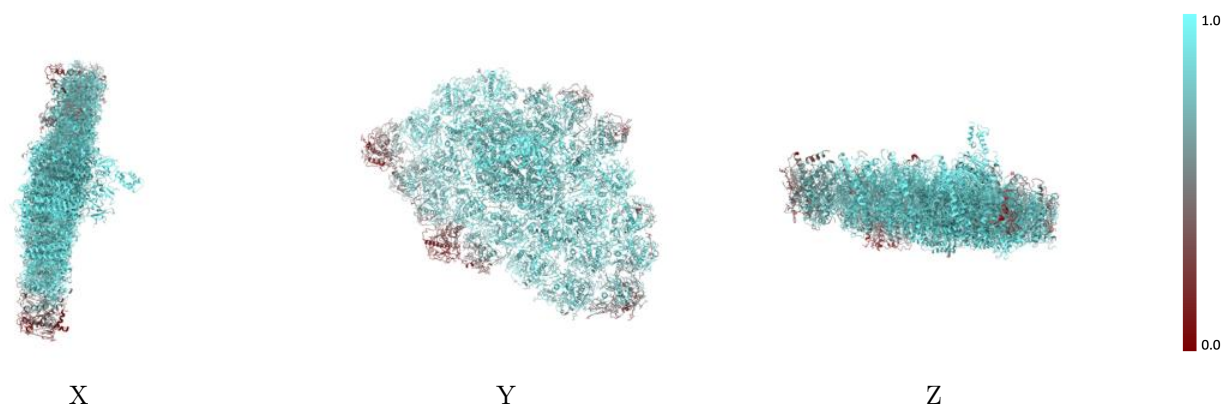
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



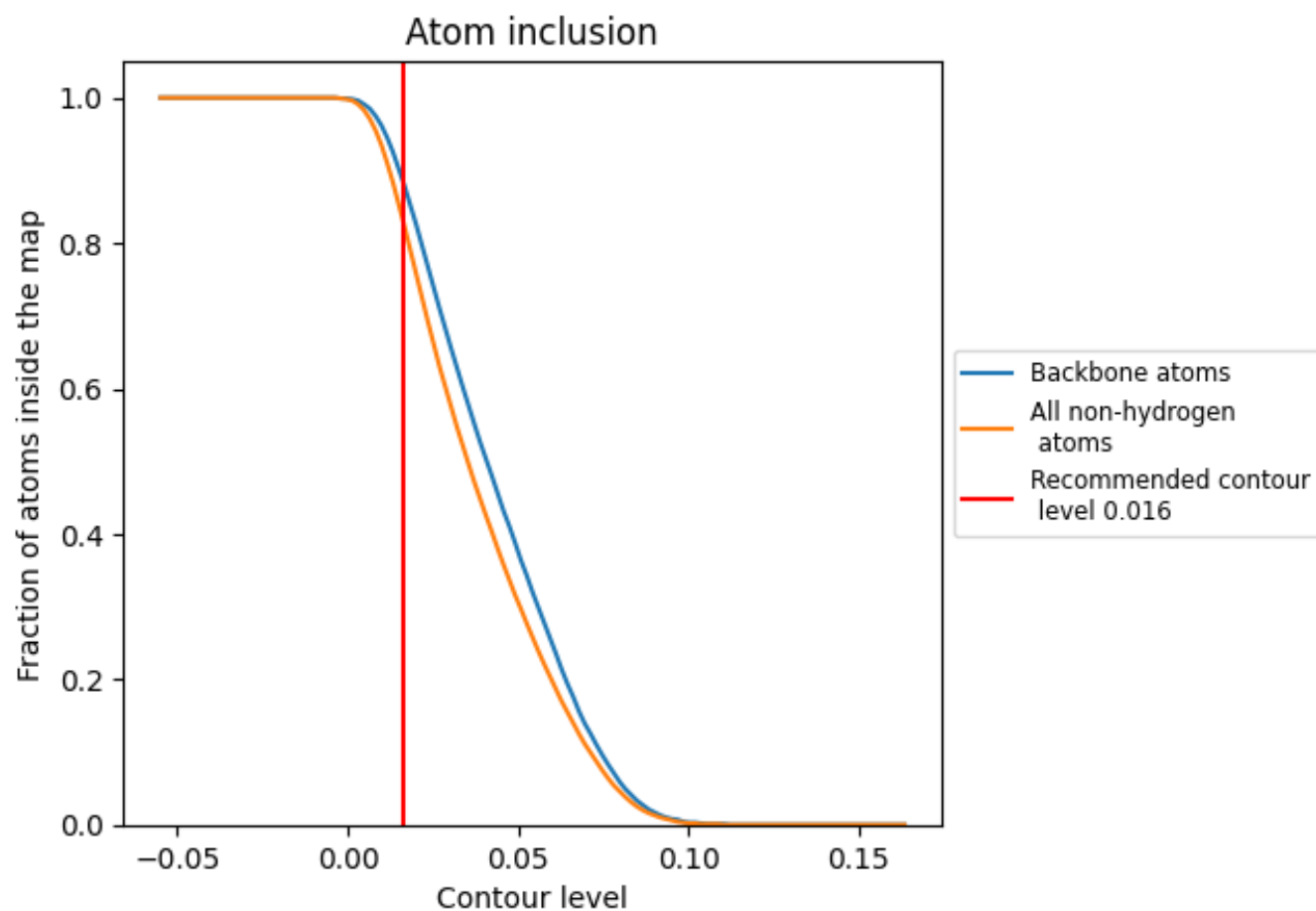
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.5170
A	 0.9410	 0.5810
B	 0.8370	 0.4930
C	 0.8980	 0.5340
D	 0.9340	 0.5870
E	 0.9530	 0.6050
F	 0.9430	 0.5960
G	 0.9570	 0.6150
H	 0.8900	 0.5450
I	 0.9240	 0.5640
J	 0.9060	 0.5400
K	 0.8890	 0.5170
L	 0.8050	 0.4220
M	 0.8700	 0.4820
N	 0.3040	 0.1740
O	 0.6670	 0.4100
P	 0.8980	 0.5260
Q	 0.7760	 0.3880
R	 0.7930	 0.4220
S	 0.5670	 0.2610
T	 0.6280	 0.3920
U	 0.6600	 0.3880
V	 0.7550	 0.4470
W	 0.4970	 0.2640
X	 0.1530	 0.1400
a	 0.9830	 0.6690
b	 0.9910	 0.6730
c	 0.9770	 0.6620
d	 0.9460	 0.6200
e	 0.9210	 0.5940
f	 0.9320	 0.6150
g	 0.8870	 0.4480
h	 0.9690	 0.6040
i	 0.9430	 0.6250
j	 0.9380	 0.6250



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Chain	Atom inclusion	Q-score
l	 0.9580	 0.6310
m	 0.9420	 0.6140