



## wwPDB EM Validation Summary Report ⓘ

Dec 26, 2024 – 10:04 AM EST

PDB ID : 6L4U  
EMDB ID : EMD-0835  
Title : Structure of the PSI-FCPI supercomplex from diatom  
Authors : Nagao, R.; Kato, K.; Miyazaki, N.; Akita, F.; Shen, J.R.  
Deposited on : 2019-10-21  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

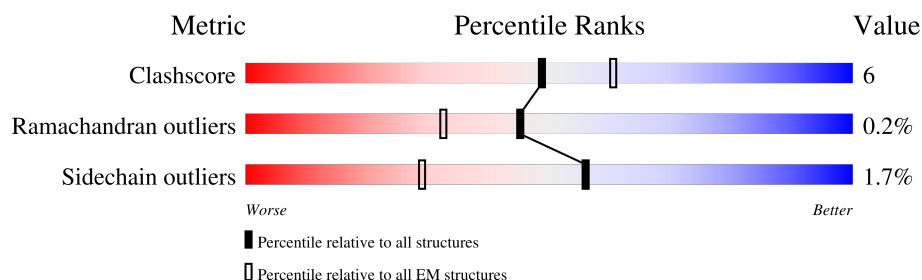
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	751	87% 11% .
2	B	733	90% 10%
3	C	81	83% 14% ...
4	D	139	82% 12% . 6%
5	E	67	85% . 10%
6	F	185	81% 6% 13%
7	I	36	94% . .
8	J	41	76% 24%

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Mol	Chain	Length	Quality of chain
9	L	151	
10	M	30	
11	1u	130	
12	2u	121	
13	1	227	
14	2	205	
15	3	200	
16	4	215	
17	5	266	
18	6	208	
19	7	296	
20	8	270	
21	9	214	
22	10	207	
23	11	229	
24	12	204	
25	13	244	
26	14	249	
27	15	281	
28	16	218	

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
29	CL0	A	801	X	-	-	-
30	CLA	1	301	X	-	-	-
30	CLA	1	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	1	303	X	-	-	-
30	CLA	1	304	X	-	-	-
30	CLA	1	305	X	-	-	-
30	CLA	10	303	X	-	-	-
30	CLA	10	304	X	-	-	-
30	CLA	10	305	X	-	-	-
30	CLA	10	307	X	-	-	-
30	CLA	10	308	X	-	-	-
30	CLA	10	309	X	-	-	-
30	CLA	11	304	X	-	-	-
30	CLA	11	306	X	-	-	-
30	CLA	11	308	X	-	-	-
30	CLA	11	310	X	-	-	-
30	CLA	12	303	X	-	-	-
30	CLA	12	304	X	-	-	-
30	CLA	12	306	X	-	-	-
30	CLA	12	307	X	-	-	-
30	CLA	12	308	X	-	-	-
30	CLA	12	312	X	-	-	-
30	CLA	12	321	X	-	-	-
30	CLA	13	301	X	-	-	-
30	CLA	13	302	X	-	-	-
30	CLA	13	307	X	-	-	-
30	CLA	13	309	X	-	-	-
30	CLA	14	302	X	-	-	-
30	CLA	14	303	X	-	-	-
30	CLA	14	304	X	-	-	-
30	CLA	14	305	X	-	-	-
30	CLA	14	309	X	-	-	-
30	CLA	14	310	X	-	-	-
30	CLA	14	313	X	-	-	-
30	CLA	15	303	X	-	-	-
30	CLA	15	304	X	-	-	-
30	CLA	15	305	X	-	-	-
30	CLA	15	306	X	-	-	-
30	CLA	15	307	X	-	-	-
30	CLA	15	308	X	-	-	-
30	CLA	15	310	X	-	-	-
30	CLA	15	311	X	-	-	-
30	CLA	15	312	X	-	-	-
30	CLA	16	302	X	-	-	-
30	CLA	16	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	16	305	X	-	-	-
30	CLA	16	306	X	-	-	-
30	CLA	16	307	X	-	-	-
30	CLA	16	308	X	-	-	-
30	CLA	16	310	X	-	-	-
30	CLA	2	301	X	-	-	-
30	CLA	2	304	X	-	-	-
30	CLA	2	305	X	-	-	-
30	CLA	2	307	X	-	-	-
30	CLA	2	309	X	-	-	-
30	CLA	2	310	X	-	-	-
30	CLA	2u	202	X	-	-	-
30	CLA	3	301	X	-	-	-
30	CLA	3	302	X	-	-	-
30	CLA	3	303	X	-	-	-
30	CLA	3	305	X	-	-	-
30	CLA	3	306	X	-	-	-
30	CLA	3	307	X	-	-	-
30	CLA	4	301	X	-	-	-
30	CLA	4	302	X	-	-	-
30	CLA	4	303	X	-	-	-
30	CLA	4	304	X	-	-	-
30	CLA	4	305	X	-	-	-
30	CLA	4	306	X	-	-	-
30	CLA	4	309	X	-	-	-
30	CLA	4	311	X	-	-	-
30	CLA	5	302	X	-	-	-
30	CLA	5	303	X	-	-	-
30	CLA	5	304	X	-	-	-
30	CLA	5	307	X	-	-	-
30	CLA	5	309	X	-	-	-
30	CLA	5	311	X	-	-	-
30	CLA	6	304	X	-	-	-
30	CLA	6	305	X	-	-	-
30	CLA	6	306	X	-	-	-
30	CLA	6	307	X	-	-	-
30	CLA	6	309	X	-	-	-
30	CLA	6	310	X	-	-	-
30	CLA	6	315	X	-	-	-
30	CLA	6	316	X	-	-	-
30	CLA	6	317	X	-	-	-
30	CLA	7	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	7	304	X	-	-	-
30	CLA	7	305	X	-	-	-
30	CLA	7	306	X	-	-	-
30	CLA	7	309	X	-	-	-
30	CLA	7	311	X	-	-	-
30	CLA	7	312	X	-	-	-
30	CLA	8	301	X	-	-	-
30	CLA	8	302	X	-	-	-
30	CLA	8	304	X	-	-	-
30	CLA	8	308	X	-	-	-
30	CLA	9	301	X	-	-	-
30	CLA	9	302	X	-	-	-
30	CLA	9	305	X	-	-	-
30	CLA	9	306	X	-	-	-
30	CLA	9	307	X	-	-	-
30	CLA	9	308	X	-	-	-
30	CLA	9	309	X	-	-	-
30	CLA	A	802	X	-	-	-
30	CLA	A	803	X	-	-	-
30	CLA	A	804	X	-	-	-
30	CLA	A	805	X	-	-	-
30	CLA	A	806	X	-	-	-
30	CLA	A	807	X	-	-	-
30	CLA	A	808	X	-	-	-
30	CLA	A	809	X	-	-	-
30	CLA	A	810	X	-	-	-
30	CLA	A	811	X	-	-	-
30	CLA	A	812	X	-	-	-
30	CLA	A	813	X	-	-	-
30	CLA	A	814	X	-	-	-
30	CLA	A	815	X	-	-	-
30	CLA	A	816	X	-	-	-
30	CLA	A	820	X	-	-	-
30	CLA	A	821	X	-	-	-
30	CLA	A	822	X	-	-	-
30	CLA	A	824	X	-	-	-
30	CLA	A	825	X	-	-	-
30	CLA	A	826	X	-	-	-
30	CLA	A	827	X	-	-	-
30	CLA	A	828	X	-	-	-
30	CLA	A	829	X	-	-	-
30	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	A	831	X	-	-	-
30	CLA	A	833	X	-	-	-
30	CLA	A	834	X	-	-	-
30	CLA	A	835	X	-	-	-
30	CLA	A	836	X	-	-	-
30	CLA	A	837	X	-	-	-
30	CLA	A	838	X	-	-	-
30	CLA	A	839	X	-	-	-
30	CLA	A	840	X	-	-	-
30	CLA	A	841	X	-	-	-
30	CLA	A	842	X	-	-	-
30	CLA	A	843	X	-	-	-
30	CLA	A	844	X	-	-	-
30	CLA	B	801	X	-	-	-
30	CLA	B	802	X	-	-	-
30	CLA	B	803	X	-	-	-
30	CLA	B	804	X	-	-	-
30	CLA	B	805	X	-	-	-
30	CLA	B	806	X	-	-	-
30	CLA	B	807	X	-	-	-
30	CLA	B	808	X	-	-	-
30	CLA	B	809	X	-	-	-
30	CLA	B	810	X	-	-	-
30	CLA	B	811	X	-	-	-
30	CLA	B	812	X	-	-	-
30	CLA	B	813	X	-	-	-
30	CLA	B	814	X	-	-	-
30	CLA	B	815	X	-	-	-
30	CLA	B	817	X	-	-	-
30	CLA	B	818	X	-	-	-
30	CLA	B	819	X	-	-	-
30	CLA	B	821	X	-	-	-
30	CLA	B	823	X	-	-	-
30	CLA	B	824	X	-	-	-
30	CLA	B	825	X	-	-	-
30	CLA	B	826	X	-	-	-
30	CLA	B	827	X	-	-	-
30	CLA	B	828	X	-	-	-
30	CLA	B	829	X	-	-	-
30	CLA	B	830	X	-	-	-
30	CLA	B	832	X	-	-	-
30	CLA	B	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	B	834	X	-	-	-
30	CLA	B	835	X	-	-	-
30	CLA	B	836	X	-	-	-
30	CLA	B	837	X	-	-	-
30	CLA	B	838	X	-	-	-
30	CLA	B	839	X	-	-	-
30	CLA	F	201	X	-	-	-
30	CLA	F	202	X	-	-	-
30	CLA	F	203	X	-	-	-
30	CLA	J	101	X	-	-	-
30	CLA	L	202	X	-	-	-
30	CLA	L	203	X	-	-	-

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 62199 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5841	3816	991	1005	29		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5801	3814	977	992	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	131	Total	C	N	O	S	0	0
			1037	663	177	194	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	60	Total	C	N	O	0	0
			478	302	86	90		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1257	806	213	234	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	35	Total	C	N	O	S	0	0
			273	190	37	44	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			344	236	50	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	137	Total	C	N	O	S	0	0
			1030	680	169	179	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			227	151	35	40	1		

- Molecule 11 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1u	130	Total	C	N	O		0	0
			650	390	130	130			

- Molecule 12 is a protein called Photosystem I reaction center subunit Psu28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2u	89	Total	C	N	O	S	0	0
			674	438	110	120	6		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhc15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	141	Total	C	N	O	S	0	0
			1086	692	184	201	9		

- Molecule 14 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhc8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	172	Total	C	N	O	S	0	0
			1310	846	216	238	10		

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	164	Total	C	N	O	S	0	0
			1275	825	213	232	5		

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	179	Total	C	N	O	S	0	0
			1368	878	227	250	13		

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	169	Total	C	N	O	S	0	0
			1304	834	222	236	12		

- Molecule 18 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	174	Total	C	N	O	S	0	0
			1354	884	216	246	8		

- Molecule 19 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	7	188	Total	C	N	O	S	0	0
			1416	894	240	266	16		

- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	8	213	Total	C	N	O	S	0	0
			1660	1075	274	302	9		

- Molecule 21 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	9	163	Total	C	N	O	S	0	0
			1267	816	211	233	7		

- Molecule 22 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	10	169	Total	C	N	O	S	0	0
			1302	849	212	233	8		

- Molecule 23 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	11	191	Total	C	N	O	S	0	0
			1479	958	243	270	8		

- Molecule 24 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	12	173	Total	C	N	O	S	0	0
			1274	814	209	243	8		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	13	150	Total	C	N	O	S	0	0
			1148	736	203	204	5		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	14	208	Total	C	N	O	S	0	0
			1609	1049	262	292	6		

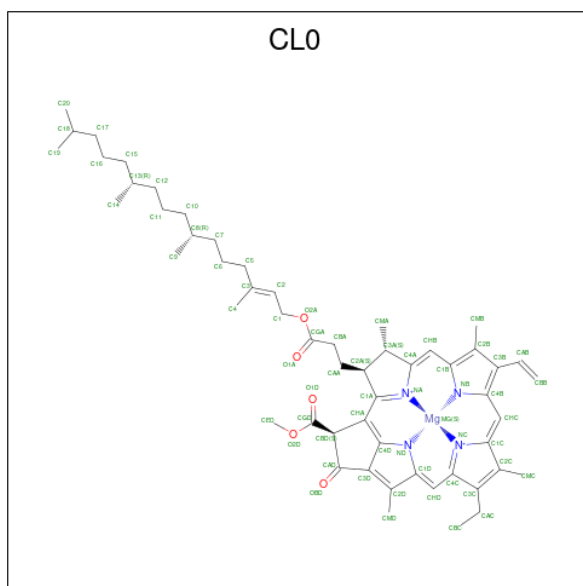
- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	15	211	Total	C	N	O	S	0	0
			1654	1077	273	298	6		

- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq5.

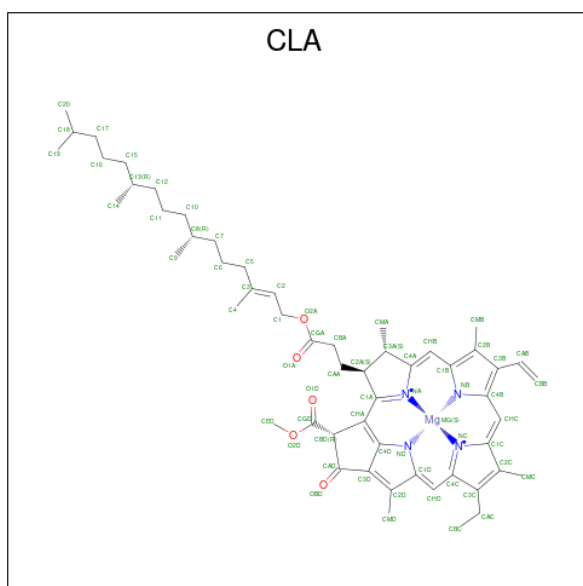
Mol	Chain	Residues	Atoms					AltConf	Trace
28	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 29 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

- Molecule 30 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

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Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
30	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	2u	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 49	C 39	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0

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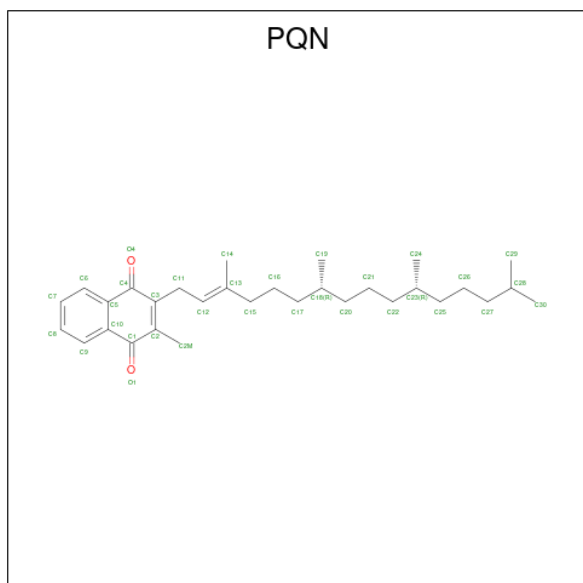
Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 57	C 47	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



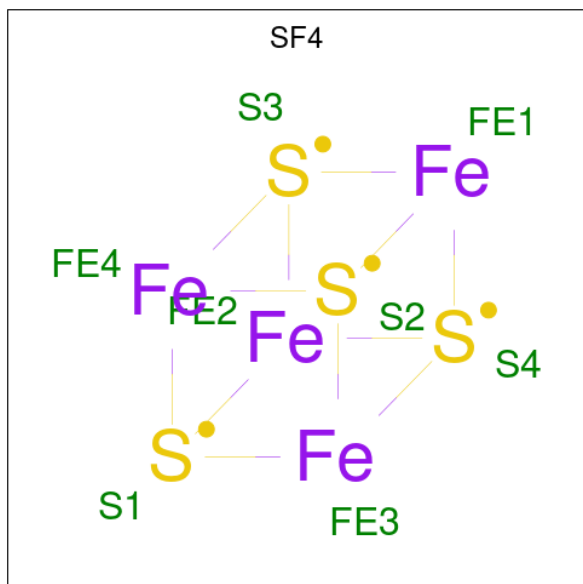
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			33	31	2	

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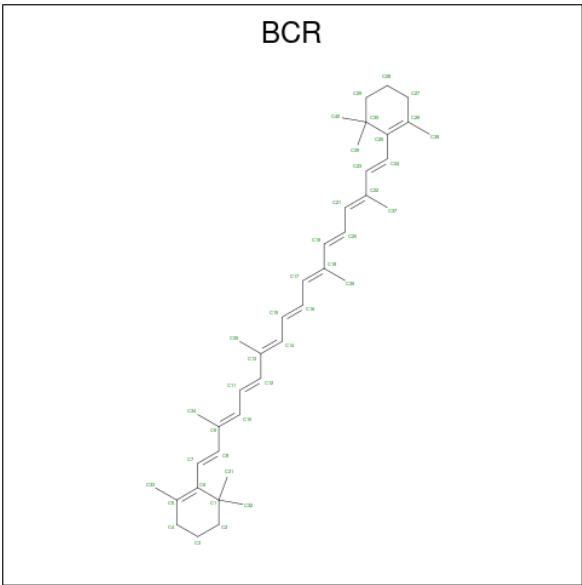
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			33	31	2	

- Molecule 32 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 33 is BETA-CAROTENE (three-letter code: BCR) (formula:  $\text{C}_{40}\text{H}_{56}$ ).



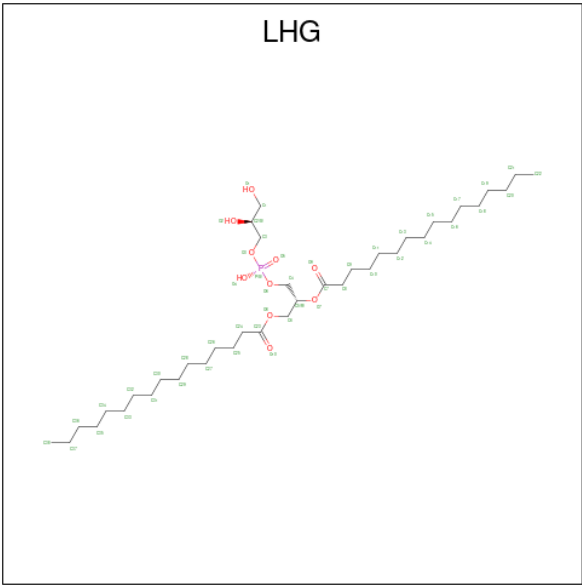
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	F	1	Total	C	0
			40	40	
33	I	1	Total	C	0
			40	40	
33	J	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
33	J	1	Total	C	0
			40	40	
33	L	1	Total	C	0
			40	40	
33	L	1	Total	C	0
			40	40	
33	L	1	Total	C	0
			40	40	
33	M	1	Total	C	0
			40	40	
33	2u	1	Total	C	0
			40	40	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



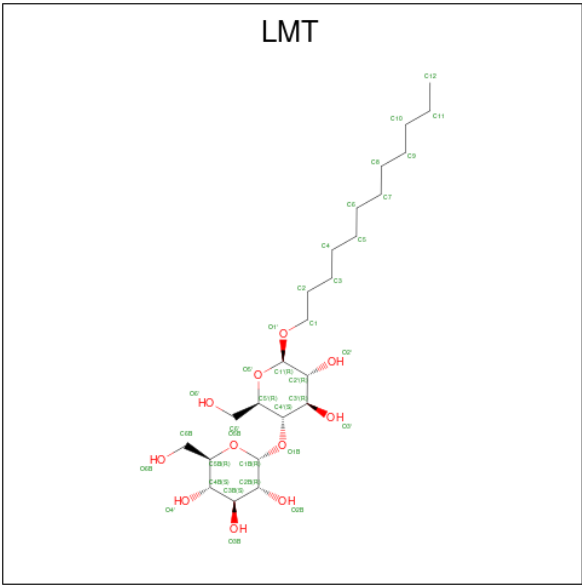
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			49	38	10	1	
34	A	1	Total	C	O	P	0
			27	16	10	1	
34	B	1	Total	C	O	P	0
			27	16	10	1	
34	2	1	Total	C	O	P	0
			27	16	10	1	
34	5	1	Total	C	O	P	0
			27	16	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	6	1	27	16	10	1	0
34	9	1	34	23	10	1	0

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



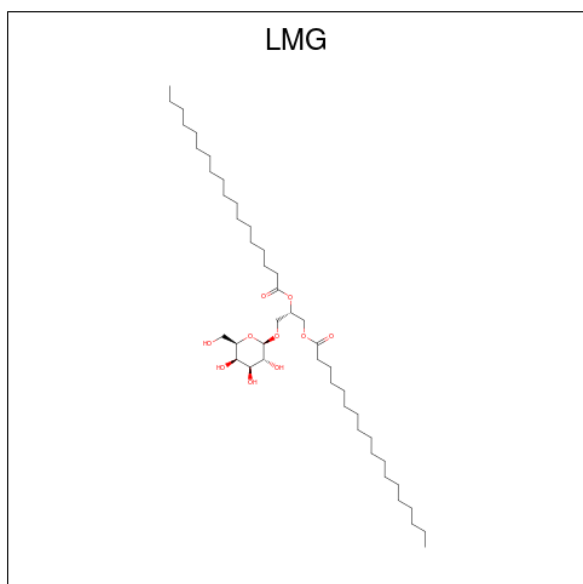
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	A	1	35	24	11	0
35	A	1	35	24	11	0
35	A	1	35	24	11	0
35	B	1	35	24	11	0
35	B	1	35	24	11	0
35	1	1	35	24	11	0
35	6	1	31	20	11	0
35	7	1	35	24	11	0
35	7	1	35	24	11	0

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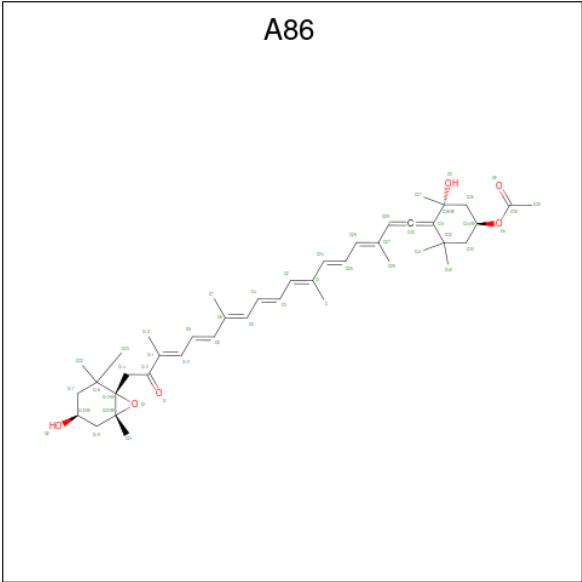
Mol	Chain	Residues	Atoms			AltConf
35	8	1	Total	C	O	0
			35	24	11	
35	9	1	Total	C	O	0
			32	21	11	
35	11	1	Total	C	O	0
			35	24	11	
35	11	1	Total	C	O	0
			35	24	11	
35	11	1	Total	C	O	0
			35	24	11	
35	11	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	12	1	Total	C	O	0
			35	24	11	
35	15	1	Total	C	O	0
			35	24	11	
35	16	1	Total	C	O	0
			35	24	11	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			34	24	10	
36	B	1	Total	C	O	0
			55	45	10	
36	B	1	Total	C	O	0
			43	33	10	
36	F	1	Total	C	O	0
			27	17	10	
36	2u	1	Total	C	O	0
			31	21	10	
36	3	1	Total	C	O	0
			37	27	10	
36	5	1	Total	C	O	0
			33	23	10	
36	6	1	Total	C	O	0
			33	23	10	
36	7	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			42	32	10	
36	8	1	Total	C	O	0
			29	19	10	
36	14	1	Total	C	O	0
			38	28	10	

- Molecule 37 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 (three-letter code: A86) (formula: C<sub>42</sub>H<sub>58</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			AltConf
37	2u	1	Total	C	O	0
			48	42	6	
37	2u	1	Total	C	O	0
			48	42	6	
37	1	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	3	1	Total	C	O	0
			48	42	6	
37	3	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	5	1	Total	C	O	0
			48	42	6	
37	5	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
37	5	1	Total	C	O	0
			48	42	6	
37	6	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	12	1	Total	C	O	0
			48	42	6	
37	12	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
37	13	1	Total	C	O	0
			45	40	5	
37	13	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	16	1	Total	C	O	0
			48	42	6	
37	16	1	Total	C	O	0
			48	42	6	

- Molecule 38 is Chlorophyll c1 (three-letter code: KC1) (formula:  $C_{35}H_{30}MgN_4O_5$ ).



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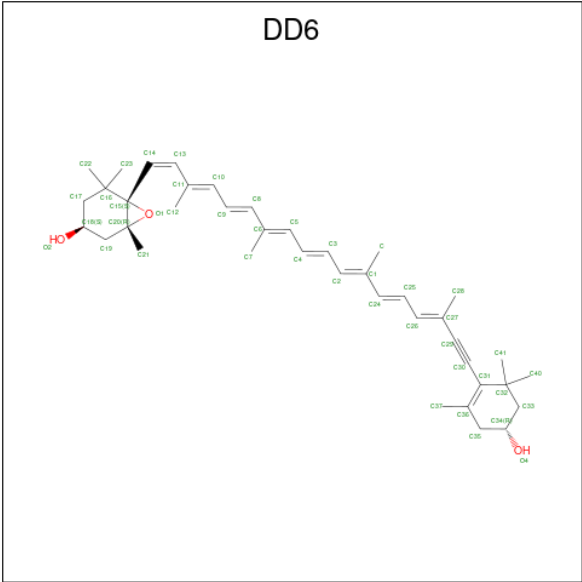
Mol	Chain	Residues	Atoms					AltConf
38	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
38	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	16	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 39 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	4	1	Total	C	O	0
			43	40	3	
39	4	1	Total	C	O	0
			43	40	3	
39	5	1	Total	C	O	0
			43	40	3	
39	5	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
39	6	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	8	1	Total	C	O	0
			43	40	3	
39	8	1	Total	C	O	0
			43	40	3	
39	9	1	Total	C	O	0
			43	40	3	
39	10	1	Total	C	O	0
			43	40	3	
39	10	1	Total	C	O	0
			43	40	3	
39	11	1	Total	C	O	0
			43	40	3	
39	12	1	Total	C	O	0
			43	40	3	
39	12	1	Total	C	O	0
			43	40	3	
39	13	1	Total	C	O	0
			43	40	3	
39	15	1	Total	C	O	0
			43	40	3	
39	15	1	Total	C	O	0
			43	40	3	
39	16	1	Total	C	O	0
			43	40	3	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	42	Total	O	0
			42	42	
40	B	53	Total	O	0
			53	53	

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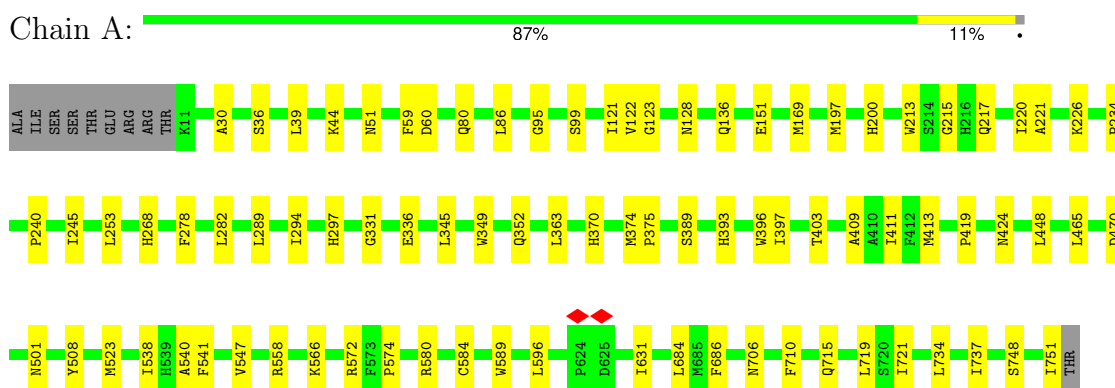
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Mol	Chain	Residues	Atoms		AltConf
40	C	15	Total 15	O 15	0
40	D	13	Total 13	O 13	0
40	E	3	Total 3	O 3	0
40	F	3	Total 3	O 3	0
40	I	1	Total 1	O 1	0
40	L	8	Total 8	O 8	0
40	1	1	Total 1	O 1	0
40	2	2	Total 2	O 2	0
40	3	1	Total 1	O 1	0
40	5	1	Total 1	O 1	0
40	6	2	Total 2	O 2	0
40	7	2	Total 2	O 2	0
40	8	4	Total 4	O 4	0
40	9	1	Total 1	O 1	0
40	10	1	Total 1	O 1	0
40	11	1	Total 1	O 1	0
40	12	2	Total 2	O 2	0

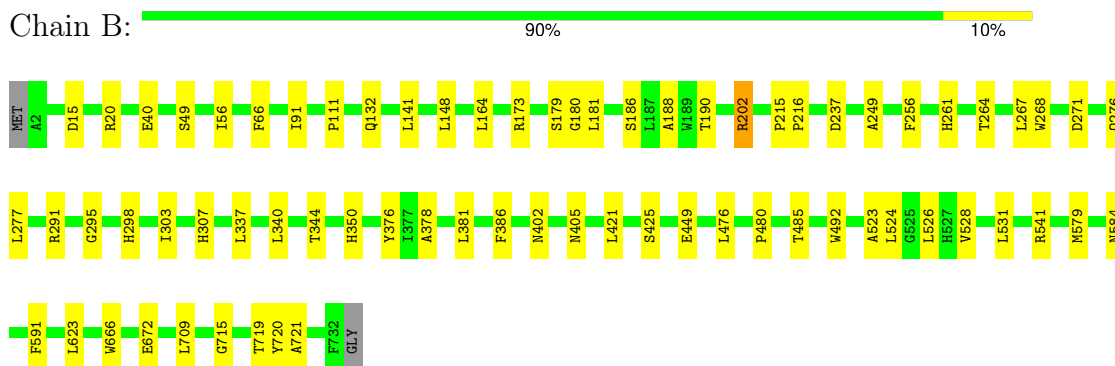
### 3 Residue-property plots [i](#)

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

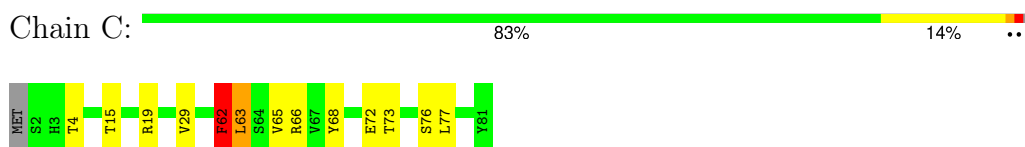
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



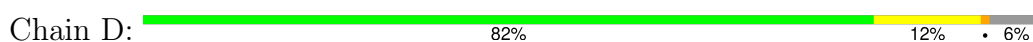
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II





- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 85% 10%



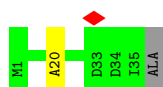
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 81% 6% 13%



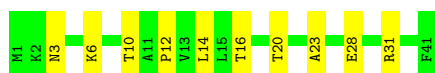
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 94% 1% 2%



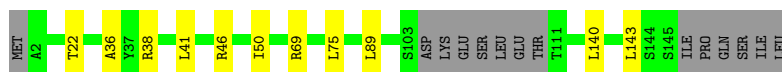
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 76% 24%



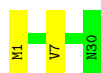
- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 83% 7% 9%



- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 93% 7%



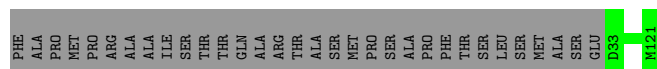
- Molecule 11: Unknown protein 1

Chain 1u: 5% 99% 1%



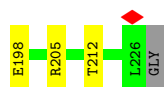
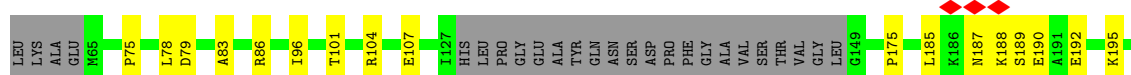
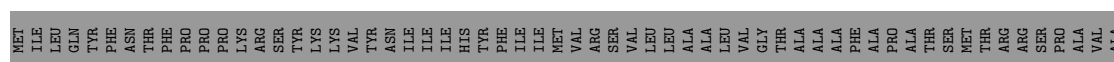
- Molecule 12: Photosystem I reaction center subunit Psa28

Chain 2u: 74% 26%



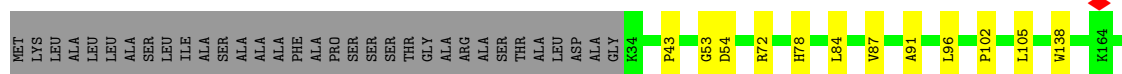
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcr15

Chain 1: 53% 9% 38%



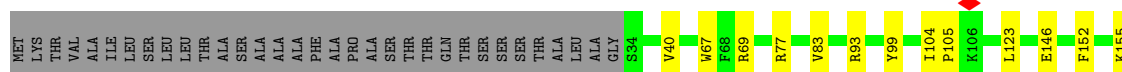
- Molecule 14: Fucoxanthin chlorophyll a/c-binding protein Lhcr8

Chain 2: 77% 7% 16%



- Molecule 15: Fucoxanthin chlorophyll a/c-binding protein Lhcr2

Chain 3: 74% 8% 18%



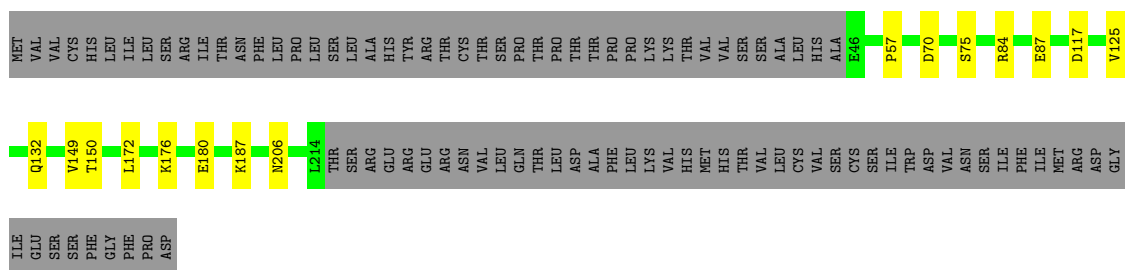
- Molecule 16: Fucoxanthin chlorophyll a/c-binding protein Lhcr9

Chain 4: 79% 5% 17%



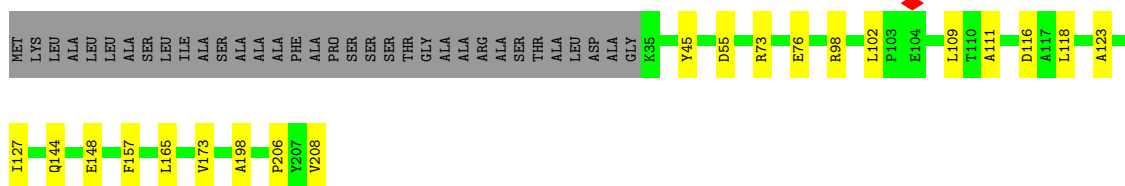
• Molecule 17: Fucoxanthin chlorophyll a/c-binding protein Lher11

Chain 5: 58% 6% 36%



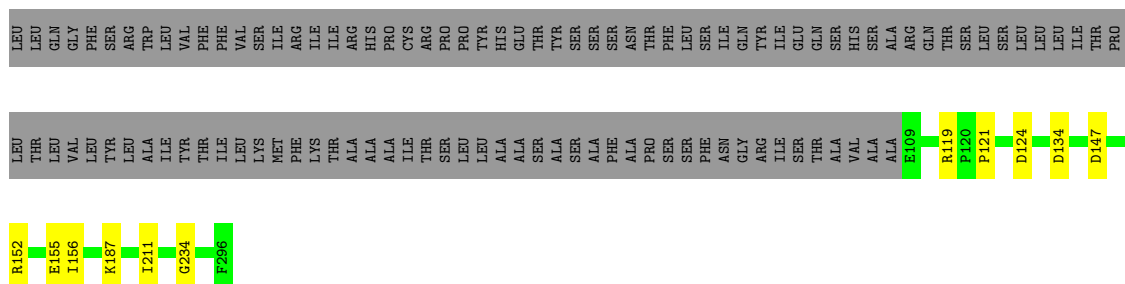
• Molecule 18: Fucoxanthin chlorophyll a/c-binding protein Lher12

Chain 6: 74% 10% 16%



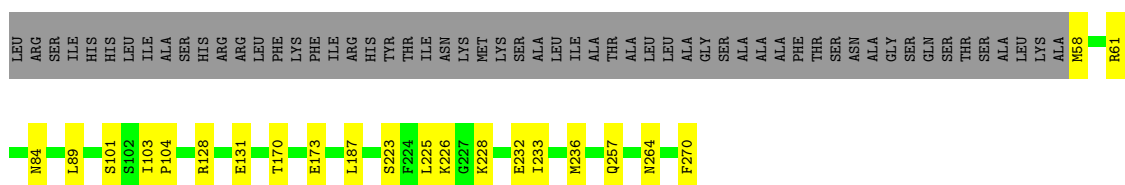
• Molecule 19: Fucoxanthin chlorophyll a/c-binding protein Lher10

Chain 7: 60% 36%

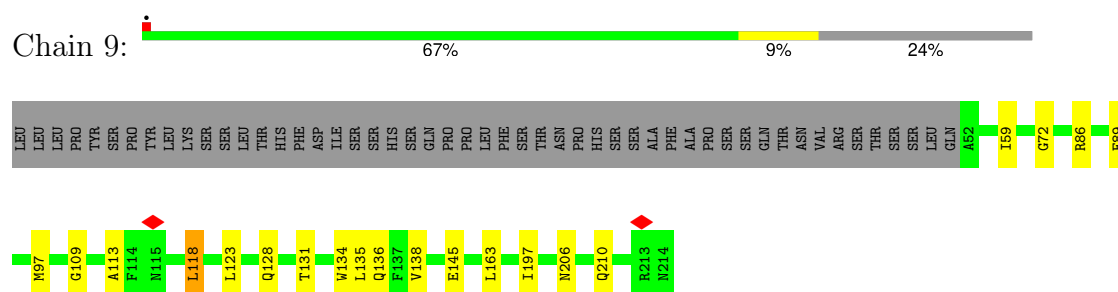


• Molecule 20: Fucoxanthin chlorophyll a/c-binding protein Lher4

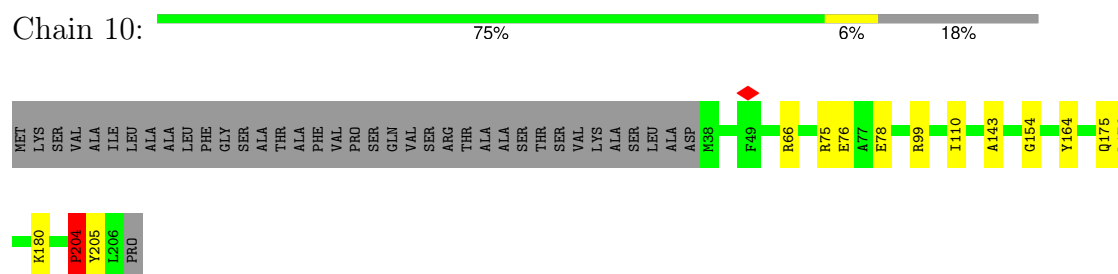
Chain 8: 71% 8% 21%



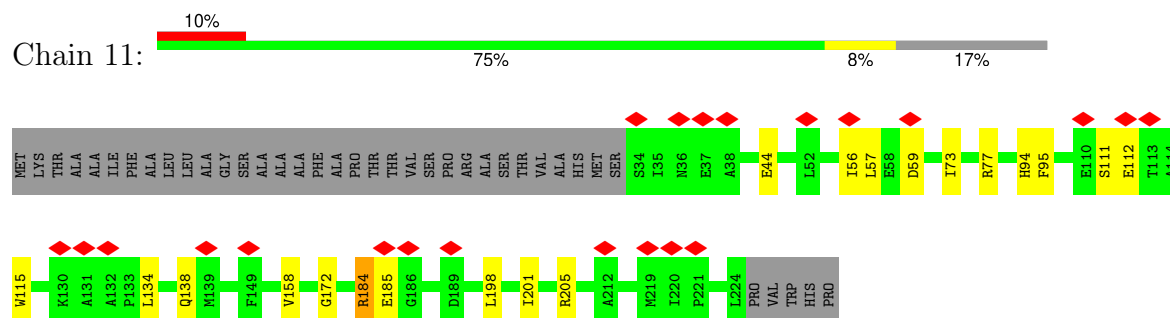
- Molecule 21: Fucoxanthin chlorophyll a/c-binding protein Lhcf6



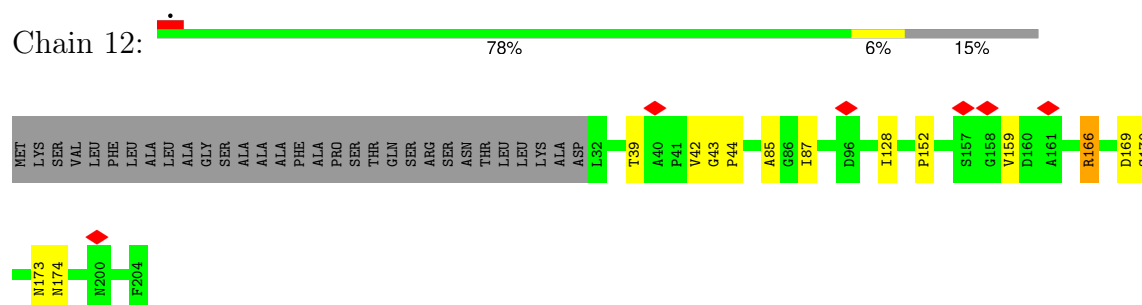
- Molecule 22: Fucoxanthin chlorophyll a/c-binding protein Lhcr3



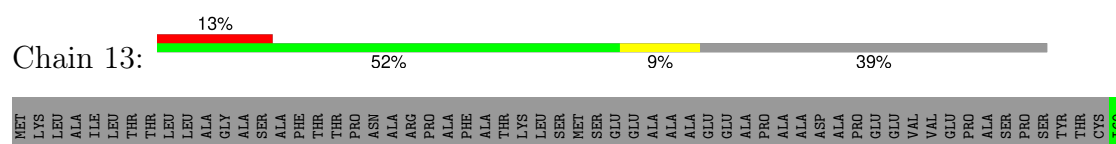
- Molecule 23: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

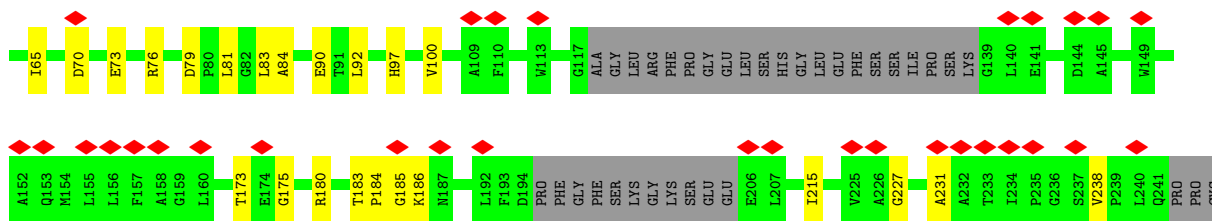


- Molecule 24: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

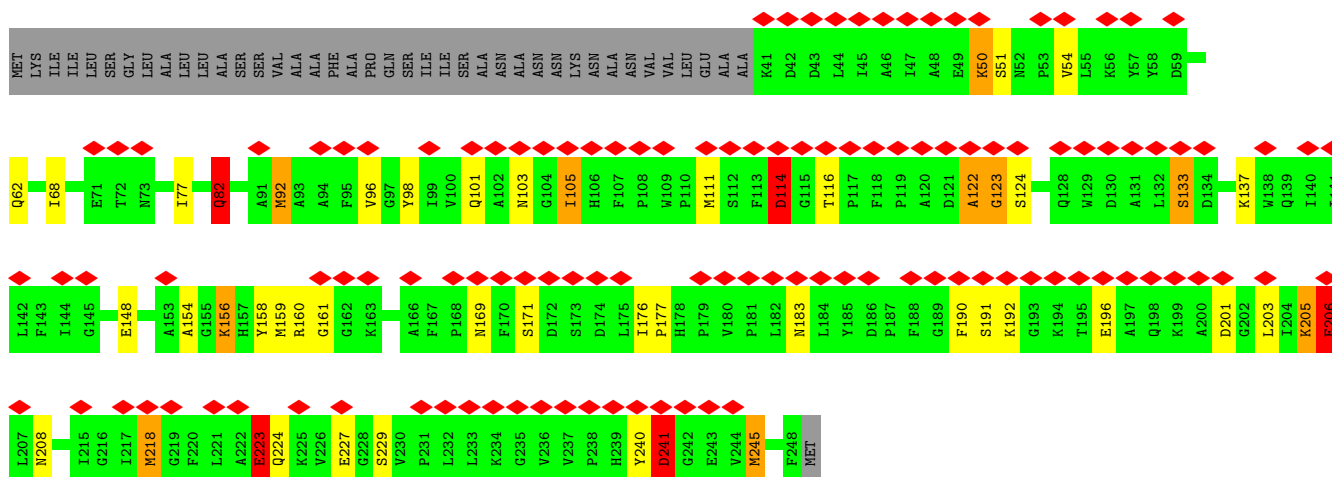


- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcq11

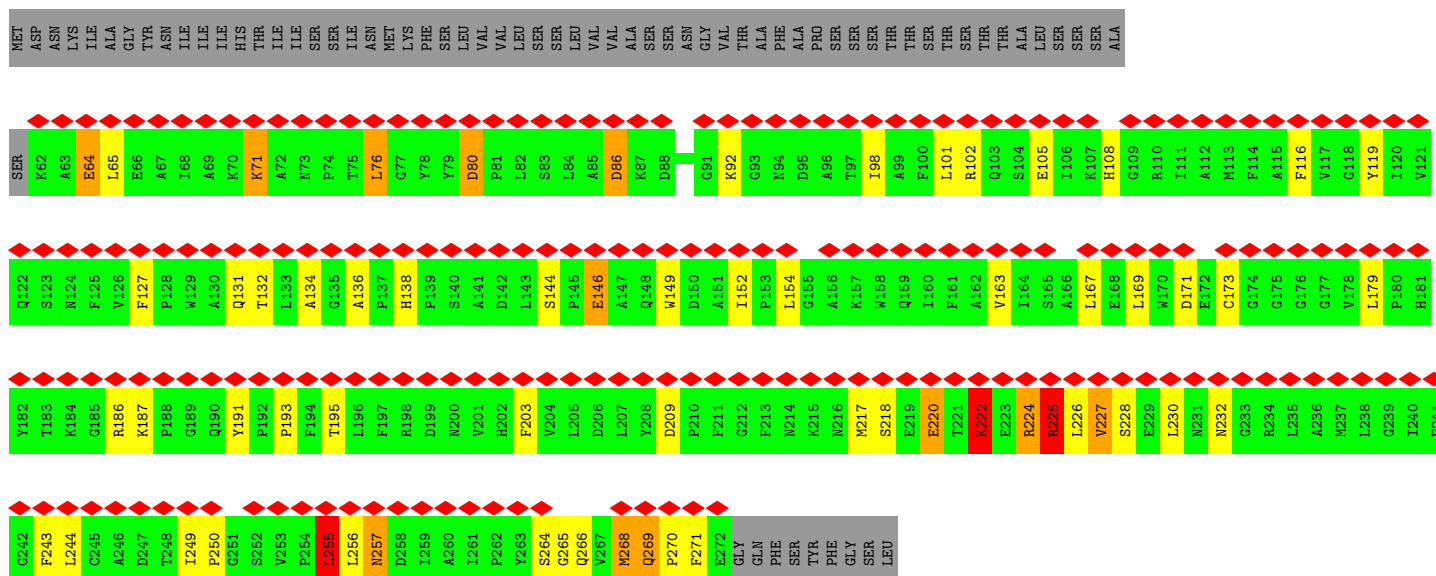
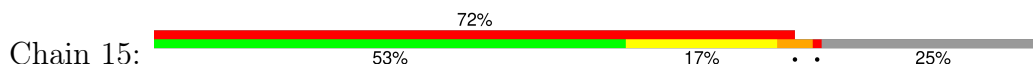




• Molecule 26: Fucoxanthin chlorophyll a/c-binding protein Lhcq10

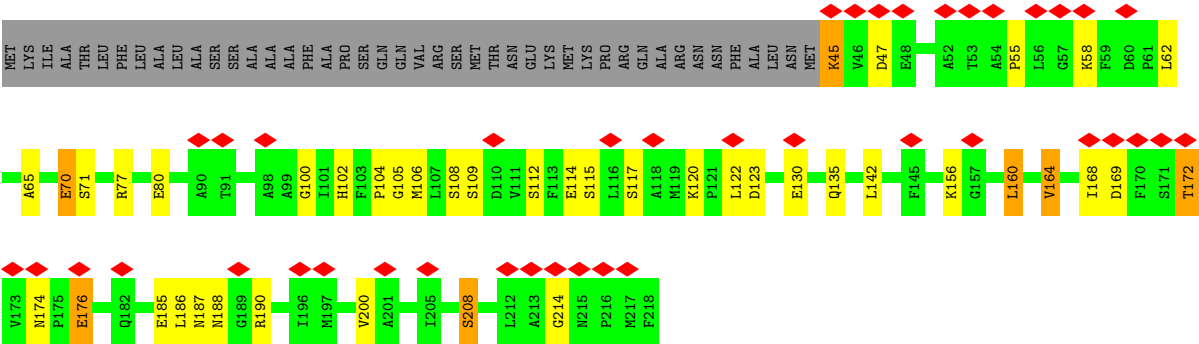


• Molecule 27: Fucoxanthin chlorophyll a/c-binding protein Lhcq8



• Molecule 28: Fucoxanthin chlorophyll a/c-binding protein Lhcq5





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470801	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.401	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	560.952, 560.952, 560.952	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, LHG, LMT, CLA, CL0, KC1, A86, SF4, DD6, PQN, BCR

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	0.39	0/6039	0.50	0/8220
2	B	0.38	0/6011	0.51	0/8209
3	C	0.44	0/609	0.63	1/826 (0.1%)
4	D	0.38	0/1064	0.62	0/1437
5	E	0.37	0/486	0.53	0/656
6	F	0.36	0/1287	0.50	0/1745
7	I	0.37	0/281	0.60	0/383
8	J	0.34	0/355	0.56	0/480
9	L	0.34	0/1054	0.49	0/1432
10	M	0.32	0/229	0.48	0/313
12	2u	0.32	0/696	0.45	0/948
13	1	0.30	0/1106	0.45	0/1490
14	2	0.35	0/1344	0.55	0/1818
15	3	0.32	0/1309	0.57	2/1767 (0.1%)
16	4	0.35	0/1404	0.51	0/1897
17	5	0.33	0/1336	0.52	0/1804
18	6	0.36	0/1391	0.48	0/1886
19	7	0.33	0/1445	0.48	0/1952
20	8	0.35	0/1706	0.49	0/2310
21	9	0.32	0/1302	0.54	1/1769 (0.1%)
22	10	0.32	0/1344	0.51	0/1824
23	11	0.30	0/1522	0.52	0/2070
24	12	0.32	0/1305	0.51	0/1776
25	13	0.31	0/1177	0.52	0/1592
26	14	0.55	4/1660 (0.2%)	1.29	23/2255 (1.0%)
27	15	0.61	2/1705 (0.1%)	1.46	33/2319 (1.4%)
28	16	0.48	1/1347 (0.1%)	0.98	12/1833 (0.7%)
All	All	0.38	7/40514 (0.0%)	0.65	72/55011 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
11	1u	0	1
16	4	0	1
21	9	0	2
22	10	0	1
26	14	0	7
27	15	0	8
28	16	0	1
All	All	0	22

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	15	146	GLU	CB-CG	-10.73	1.31	1.52
28	16	70	GLU	CB-CG	-7.53	1.37	1.52
26	14	50	LYS	CD-CE	-6.61	1.34	1.51
26	14	206	GLU	CG-CD	-5.84	1.43	1.51
27	15	224	ARG	CB-CG	-5.79	1.36	1.52

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	92	MET	CA-CB-CG	25.47	156.60	113.30
27	15	224	ARG	NE-CZ-NH1	-23.93	108.33	120.30
27	15	224	ARG	NE-CZ-NH2	22.70	131.65	120.30
27	15	146	GLU	CA-CB-CG	16.51	149.72	113.40
26	14	92	MET	CB-CG-SD	13.82	153.87	112.40

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1u	97	UNK	Peptide
16	4	145	HIS	Sidechain
21	9	109	GLY	Peptide
21	9	113	ALA	Peptide
4	D	91	GLU	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	5841	0	5666	71	0
2	B	5801	0	5614	50	0
3	C	599	0	579	6	0
4	D	1037	0	1023	10	0
5	E	478	0	473	2	0
6	F	1257	0	1259	11	0
7	I	273	0	285	1	0
8	J	344	0	351	10	0
9	L	1030	0	1063	11	0
10	M	227	0	247	2	0
11	1u	650	0	138	0	0
12	2u	674	0	658	0	0
13	1	1086	0	1089	13	0
14	2	1310	0	1287	13	0
15	3	1275	0	1239	9	0
16	4	1368	0	1344	8	0
17	5	1304	0	1286	10	0
18	6	1354	0	1328	13	0
19	7	1416	0	1379	8	0
20	8	1660	0	1625	16	0
21	9	1267	0	1210	12	0
22	10	1302	0	1274	8	0
23	11	1479	0	1452	16	0
24	12	1274	0	1267	10	0
25	13	1148	0	1130	16	0
26	14	1609	0	1568	22	0
27	15	1654	0	1613	21	0
28	16	1313	0	1309	22	0
29	A	65	0	72	3	0
30	1	390	0	425	12	0
30	10	435	0	465	7	0
30	11	315	0	337	11	0
30	12	566	0	604	12	0
30	13	350	0	354	11	0
30	14	468	0	400	8	0
30	15	685	0	589	16	0
30	16	478	0	429	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	2	620	0	649	16	0
30	2u	65	0	72	0	0
30	3	472	0	474	8	0
30	4	484	0	495	14	0
30	5	455	0	499	12	0
30	6	620	0	656	13	0
30	7	566	0	609	14	0
30	8	420	0	427	8	0
30	9	486	0	503	12	0
30	A	2614	0	2694	105	0
30	B	2465	0	2570	91	0
30	F	175	0	177	9	0
30	J	45	0	33	1	0
30	L	110	0	105	7	0
31	A	33	0	46	5	0
31	B	33	0	46	1	0
32	A	8	0	0	0	0
32	C	16	0	0	0	0
33	2u	40	0	56	0	0
33	A	200	0	280	13	0
33	B	240	0	336	12	0
33	F	40	0	56	3	0
33	I	40	0	56	2	0
33	J	80	0	112	7	0
33	L	120	0	168	10	0
33	M	40	0	56	3	0
34	2	27	0	24	0	0
34	5	27	0	24	1	0
34	6	27	0	24	0	0
34	9	34	0	38	0	0
34	A	76	0	98	2	0
34	B	27	0	24	0	0
35	1	35	0	46	0	0
35	11	140	0	184	5	0
35	12	140	0	184	4	0
35	15	35	0	46	0	0
35	16	35	0	46	0	0
35	6	31	0	35	2	0
35	7	70	0	91	2	0
35	8	35	0	46	0	0
35	9	32	0	37	0	0
35	A	105	0	138	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	70	0	92	0	0
36	14	38	0	46	2	0
36	2u	31	0	31	0	0
36	3	37	0	44	2	0
36	5	33	0	36	0	0
36	6	33	0	34	1	0
36	7	37	0	44	0	0
36	8	108	0	123	1	0
36	A	34	0	38	2	0
36	B	98	0	141	3	0
36	F	27	0	24	0	0
37	1	48	0	0	0	0
37	10	240	0	0	0	0
37	11	192	0	0	2	0
37	12	96	0	0	0	0
37	13	93	0	0	0	0
37	14	384	0	0	2	0
37	15	336	0	0	0	0
37	16	96	0	0	0	0
37	2	144	0	0	0	0
37	2u	96	0	0	0	0
37	3	96	0	0	0	0
37	4	192	0	0	1	0
37	5	144	0	0	1	0
37	6	48	0	0	0	0
37	7	144	0	0	1	0
37	8	96	0	0	1	0
37	9	144	0	0	1	0
38	1	90	0	0	0	0
38	10	135	0	0	0	0
38	11	180	0	0	0	0
38	12	180	0	0	1	0
38	13	270	0	0	0	0
38	14	135	0	0	0	0
38	16	90	0	0	1	0
38	2	135	0	0	0	0
38	3	135	0	0	1	0
38	4	135	0	0	1	0
38	5	180	0	0	2	0
38	6	180	0	0	0	0
38	7	90	0	0	0	0
38	8	315	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	9	180	0	0	0	0
39	1	43	0	0	0	0
39	10	86	0	0	1	0
39	11	43	0	0	0	0
39	12	86	0	0	0	0
39	13	43	0	0	1	0
39	15	86	0	0	0	0
39	16	43	0	0	0	0
39	2	129	0	0	0	0
39	3	129	0	0	0	0
39	4	86	0	0	0	0
39	5	86	0	0	0	0
39	6	172	0	0	3	0
39	7	172	0	0	0	0
39	8	86	0	0	0	0
39	9	43	0	0	0	0
40	1	1	0	0	0	0
40	10	1	0	0	0	0
40	11	1	0	0	0	0
40	12	2	0	0	0	0
40	2	2	0	0	0	0
40	3	1	0	0	0	0
40	5	1	0	0	0	0
40	6	2	0	0	0	0
40	7	2	0	0	0	0
40	8	4	0	0	0	0
40	9	1	0	0	0	0
40	A	42	0	0	2	0
40	B	53	0	0	0	0
40	C	15	0	0	0	0
40	D	13	0	0	0	0
40	E	3	0	0	0	0
40	F	3	0	0	0	0
40	I	1	0	0	0	0
40	L	8	0	0	0	0
All	All	62199	0	55344	644	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 6.

The worst 5 of 644 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)
26:14:101:GLN:OE1	30:14:303:CLA:NA	2.01	0.94
23:11:44:GLU:OE1	30:11:310:CLA:NC	2.10	0.84
25:13:73:GLU:OE1	30:13:307:CLA:NC	2.11	0.83
27:15:105:GLU:OE1	30:15:302:CLA:NB	2.21	0.74
30:B:815:CLA:HBB1	33:B:841:BCR:H333	1.74	0.70

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	739/751 (98%)	712 (96%)	25 (3%)	2 (0%)	37	51
2	B	729/733 (100%)	699 (96%)	29 (4%)	1 (0%)	48	65
3	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	4	4
4	D	129/139 (93%)	109 (84%)	18 (14%)	2 (2%)	8	11
5	E	58/67 (87%)	55 (95%)	3 (5%)	0	100	100
6	F	159/185 (86%)	152 (96%)	7 (4%)	0	100	100
7	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	L	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
12	2u	87/121 (72%)	87 (100%)	0	0	100	100
13	1	137/227 (60%)	130 (95%)	7 (5%)	0	100	100
14	2	170/205 (83%)	151 (89%)	19 (11%)	0	100	100
15	3	162/200 (81%)	151 (93%)	9 (6%)	2 (1%)	11	16
16	4	177/215 (82%)	167 (94%)	10 (6%)	0	100	100
17	5	167/266 (63%)	157 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	6	172/208 (83%)	167 (97%)	5 (3%)	0	100	100
19	7	186/296 (63%)	179 (96%)	7 (4%)	0	100	100
20	8	211/270 (78%)	203 (96%)	8 (4%)	0	100	100
21	9	161/214 (75%)	149 (92%)	12 (8%)	0	100	100
22	10	167/207 (81%)	157 (94%)	8 (5%)	2 (1%)	11	16
23	11	189/229 (82%)	173 (92%)	16 (8%)	0	100	100
24	12	171/204 (84%)	160 (94%)	11 (6%)	0	100	100
25	13	144/244 (59%)	133 (92%)	11 (8%)	0	100	100
26	14	206/249 (83%)	177 (86%)	29 (14%)	0	100	100
27	15	209/281 (74%)	171 (82%)	37 (18%)	1 (0%)	25	38
28	16	172/218 (79%)	157 (91%)	15 (9%)	0	100	100
All	All	5013/6068 (83%)	4694 (94%)	307 (6%)	12 (0%)	45	59

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
4	D	92	VAL
2	B	492	TRP
3	C	62	PHE
3	C	63	LEU

### 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	602/611 (98%)	601 (100%)	1 (0%)	92	97
2	B	592/593 (100%)	589 (100%)	3 (0%)	86	94
3	C	69/70 (99%)	66 (96%)	3 (4%)	25	42
4	D	111/119 (93%)	111 (100%)	0	100	100
5	E	51/58 (88%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	132/153 (86%)	132 (100%)	0	100	100
7	I	29/29 (100%)	29 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	L	107/121 (88%)	107 (100%)	0	100	100
10	M	24/24 (100%)	24 (100%)	0	100	100
12	2u	69/94 (73%)	69 (100%)	0	100	100
13	1	114/183 (62%)	113 (99%)	1 (1%)	75	88
14	2	134/154 (87%)	134 (100%)	0	100	100
15	3	128/154 (83%)	127 (99%)	1 (1%)	79	90
16	4	142/165 (86%)	142 (100%)	0	100	100
17	5	137/228 (60%)	136 (99%)	1 (1%)	81	91
18	6	140/160 (88%)	140 (100%)	0	100	100
19	7	143/236 (61%)	143 (100%)	0	100	100
20	8	171/215 (80%)	171 (100%)	0	100	100
21	9	126/175 (72%)	125 (99%)	1 (1%)	79	90
22	10	133/161 (83%)	133 (100%)	0	100	100
23	11	154/181 (85%)	153 (99%)	1 (1%)	84	92
24	12	136/159 (86%)	134 (98%)	2 (2%)	60	77
25	13	112/184 (61%)	111 (99%)	1 (1%)	75	88
26	14	166/196 (85%)	145 (87%)	21 (13%)	3	4
27	15	171/231 (74%)	151 (88%)	20 (12%)	4	6
28	16	139/174 (80%)	127 (91%)	12 (9%)	8	14
All	All	4069/4865 (84%)	4001 (98%)	68 (2%)	56	75

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	16	47	ASP
28	16	70	GLU
28	16	172	THR
26	14	156	LYS
26	14	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
22	10	175	GLN
28	16	177	GLN
22	10	201	HIS
26	14	183	ASN
2	B	632	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

427 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	$\# Z  > 2$
30	CLA	F	201	40	63,73,73	1.94	17 (26%)	74,113,113	2.56	27 (36%)
32	SF4	C	102	3	0,12,12	-	-	-		
38	KC1	6	308	18	48,53,53	3.10	21 (43%)	54,89,89	3.72	27 (50%)
39	DD6	12	315	30	40,45,45	5.50	23 (57%)	51,67,67	5.92	25 (49%)
30	CLA	B	837	40	63,73,73	1.96	16 (25%)	74,113,113	2.59	26 (35%)
30	CLA	7	311	19	63,73,73	2.00	16 (25%)	74,113,113	2.51	26 (35%)
30	CLA	4	303	16	63,73,73	2.00	15 (23%)	74,113,113	2.58	26 (35%)
39	DD6	15	319	30	40,45,45	5.65	24 (60%)	51,67,67	6.12	29 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	KC1	1	308	13	48,53,53	3.15	25 (52%)	54,89,89	3.69	27 (50%)
38	KC1	8	314	38,40	48,53,53	3.11	25 (52%)	54,89,89	3.57	29 (53%)
30	CLA	14	313	26	44,54,73	2.48	16 (36%)	51,90,113	3.17	27 (52%)
36	LMG	6	301	30	33,33,55	0.95	1 (3%)	41,41,63	1.22	4 (9%)
33	BCR	L	201	-	41,41,41	1.13	3 (7%)	56,56,56	1.33	6 (10%)
30	CLA	5	311	17,40	63,73,73	2.06	15 (23%)	74,113,113	2.70	27 (36%)
30	CLA	A	817	36,40	47,57,73	2.32	15 (31%)	53,93,113	3.04	23 (43%)
30	CLA	A	840	1	45,55,73	2.33	17 (37%)	52,91,113	3.18	26 (50%)
30	CLA	A	824	1	49,59,73	2.25	17 (34%)	56,96,113	3.04	27 (48%)
30	CLA	1	302	13,30	63,73,73	2.01	15 (23%)	74,113,113	2.61	26 (35%)
30	CLA	A	831	1	63,73,73	1.95	14 (22%)	74,113,113	2.76	28 (37%)
30	CLA	B	804	2	50,60,73	2.24	17 (34%)	57,97,113	3.00	29 (50%)
36	LMG	2u	204	12	31,31,55	1.11	3 (9%)	39,39,63	1.18	5 (12%)
37	A86	8	315	-	47,50,50	4.01	22 (46%)	51,76,76	7.00	20 (39%)
30	CLA	B	808	2	63,73,73	1.94	15 (23%)	74,113,113	2.68	28 (37%)
30	CLA	B	803	-	63,73,73	1.92	16 (25%)	74,113,113	2.57	27 (36%)
30	CLA	5	302	17	63,73,73	1.98	16 (25%)	74,113,113	2.58	28 (37%)
30	CLA	A	812	1,30	63,73,73	1.93	15 (23%)	74,113,113	2.67	26 (35%)
30	CLA	4	302	16	63,73,73	2.00	15 (23%)	74,113,113	2.54	25 (33%)
30	CLA	2	303	14	53,63,73	2.43	15 (28%)	62,101,113	2.78	28 (45%)
30	CLA	3	305	15	60,70,73	2.08	16 (26%)	70,109,113	2.65	30 (42%)
30	CLA	5	303	17	63,73,73	1.99	17 (26%)	74,113,113	2.54	27 (36%)
39	DD6	11	313	-	40,45,45	5.53	23 (57%)	51,67,67	5.92	29 (56%)
30	CLA	7	309	19	63,73,73	1.95	16 (25%)	74,113,113	2.56	25 (33%)
37	A86	11	301	-	47,50,50	4.30	23 (48%)	51,76,76	6.83	19 (37%)
38	KC1	4	310	16	48,53,53	3.15	25 (52%)	54,89,89	3.78	28 (51%)
39	DD6	10	314	-	40,45,45	5.49	24 (60%)	51,67,67	5.89	28 (54%)
30	CLA	A	813	1	63,73,73	2.02	15 (23%)	74,113,113	2.58	27 (36%)
30	CLA	2	301	2,14	63,73,73	1.94	15 (23%)	74,113,113	2.75	25 (33%)
30	CLA	B	832	37,40	63,73,73	2.02	16 (25%)	74,113,113	2.60	30 (40%)
37	A86	2	319	-	47,50,50	4.10	22 (46%)	51,76,76	6.21	19 (37%)
30	CLA	10	307	22	63,73,73	1.98	16 (25%)	74,113,113	2.52	27 (36%)
30	CLA	9	305	-	63,73,73	2.03	17 (26%)	74,113,113	2.77	31 (41%)
30	CLA	A	844	-	63,73,73	2.09	16 (25%)	74,113,113	2.53	29 (39%)
38	KC1	12	311	24	48,53,53	3.14	24 (50%)	54,89,89	3.78	32 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CLA	8	308	20	53,63,73	2.19	14 (26%)	62,101,113	2.83	27 (43%)
33	BCR	F	204	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	7 (12%)
36	LMG	3	317	-	37,37,55	0.97	2 (5%)	45,45,63	1.43	6 (13%)
30	CLA	3	310	15	43,53,73	2.44	16 (37%)	50,89,113	3.11	24 (48%)
38	KC1	10	310	22	48,53,53	3.11	25 (52%)	54,89,89	3.80	31 (57%)
30	CLA	2	307	14	63,73,73	1.98	15 (23%)	74,113,113	2.54	27 (36%)
37	A86	10	317	-	47,50,50	4.44	24 (51%)	51,76,76	6.74	14 (27%)
30	CLA	B	829	2	63,73,73	1.95	13 (20%)	74,113,113	2.57	25 (33%)
35	LMT	9	317	-	33,33,36	0.49	0	44,44,47	1.12	5 (11%)
38	KC1	9	311	21	48,53,53	3.16	24 (50%)	54,89,89	3.80	30 (55%)
37	A86	14	318	-	47,50,50	4.34	24 (51%)	51,76,76	7.05	16 (31%)
37	A86	12	316	-	47,50,50	4.32	25 (53%)	51,76,76	6.98	17 (33%)
30	CLA	6	307	39,18	63,73,73	2.01	15 (23%)	74,113,113	2.51	29 (39%)
30	CLA	15	309	27	63,73,73	2.11	16 (25%)	74,113,113	2.58	25 (33%)
30	CLA	15	312	27	43,53,73	2.50	15 (34%)	50,89,113	3.25	28 (56%)
39	DD6	2	316	-	40,45,45	5.41	24 (60%)	51,67,67	5.74	27 (52%)
35	LMT	11	317	-	36,36,36	0.43	0	47,47,47	0.90	2 (4%)
30	CLA	16	301	28	63,73,73	2.02	16 (25%)	74,113,113	2.65	26 (35%)
36	LMG	B	849	2	43,43,55	0.95	2 (4%)	51,51,63	1.18	4 (7%)
30	CLA	B	825	2	63,73,73	1.99	16 (25%)	74,113,113	2.69	29 (39%)
30	CLA	B	817	2	57,67,73	2.08	15 (26%)	66,105,113	2.84	26 (39%)
30	CLA	13	301	25	63,73,73	2.02	17 (26%)	74,113,113	2.72	25 (33%)
38	KC1	1	306	13	48,53,53	3.14	23 (47%)	54,89,89	3.71	30 (55%)
30	CLA	A	804	1	63,73,73	1.95	15 (23%)	74,113,113	2.65	28 (37%)
30	CLA	J	101	8	43,53,73	2.45	16 (37%)	50,89,113	3.02	24 (48%)
39	DD6	2	317	-	40,45,45	5.56	24 (60%)	51,67,67	5.58	27 (52%)
30	CLA	7	306	19	63,73,73	1.97	16 (25%)	74,113,113	2.52	28 (37%)
33	BCR	I	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.32	5 (8%)
30	CLA	A	806	1	63,73,73	1.98	16 (25%)	74,113,113	2.83	29 (39%)
30	CLA	B	801	2	63,73,73	1.88	16 (25%)	74,113,113	2.75	31 (41%)
37	A86	7	315	-	47,50,50	4.07	23 (48%)	51,76,76	6.41	18 (35%)
38	KC1	6	311	18	48,53,53	3.07	22 (45%)	54,89,89	3.85	29 (53%)
38	KC1	8	307	20	48,53,53	3.06	21 (43%)	54,89,89	3.77	29 (53%)
30	CLA	16	302	28	63,73,73	2.02	17 (26%)	74,113,113	2.60	27 (36%)
38	KC1	5	305	17	48,53,53	3.12	24 (50%)	54,89,89	3.69	28 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CLA	16	303	28	63,73,73	2.03	15 (23%)	74,113,113	2.75	27 (36%)
30	CLA	13	303	-	63,73,73	2.10	16 (25%)	74,113,113	2.67	29 (39%)
30	CLA	B	839	34	63,73,73	1.93	15 (23%)	74,113,113	2.77	27 (36%)
31	PQN	B	840	-	34,34,34	1.53	2 (5%)	43,45,45	1.15	5 (11%)
35	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.90	3 (6%)
30	CLA	10	304	22	63,73,73	2.03	16 (25%)	74,113,113	2.56	26 (35%)
30	CLA	7	303	19	63,73,73	1.96	14 (22%)	74,113,113	2.62	28 (37%)
33	BCR	B	843	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	6 (10%)
37	A86	11	315	-	47,50,50	4.23	24 (51%)	51,76,76	6.15	22 (43%)
38	KC1	7	308	40	48,53,53	3.13	23 (47%)	54,89,89	3.57	27 (50%)
30	CLA	16	310	28	43,53,73	2.51	17 (39%)	50,89,113	3.11	26 (52%)
36	LMG	F	205	-	27,27,55	1.01	1 (3%)	35,35,63	1.26	5 (14%)
37	A86	14	314	-	47,50,50	4.31	24 (51%)	51,76,76	6.93	22 (43%)
30	CLA	B	807	2	63,73,73	1.94	16 (25%)	74,113,113	2.67	27 (36%)
30	CLA	15	306	-	43,53,73	2.51	17 (39%)	50,89,113	3.20	24 (48%)
37	A86	14	315	26	47,50,50	4.22	24 (51%)	51,76,76	7.41	20 (39%)
33	BCR	A	851	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
30	CLA	B	824	40	63,73,73	2.01	15 (23%)	74,113,113	4.53	31 (41%)
30	CLA	A	825	1	57,67,73	2.10	16 (28%)	66,105,113	2.67	26 (39%)
37	A86	3	315	-	47,50,50	4.38	24 (51%)	51,76,76	6.83	16 (31%)
30	CLA	14	305	26	48,58,73	2.34	15 (31%)	56,95,113	2.92	26 (46%)
30	CLA	A	830	1	63,73,73	1.91	15 (23%)	74,113,113	2.53	30 (40%)
35	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.66	0
30	CLA	B	813	2	63,73,73	1.98	15 (23%)	74,113,113	2.58	28 (37%)
35	LMT	B	852	-	36,36,36	0.36	0	47,47,47	1.14	2 (4%)
37	A86	15	321	27	47,50,50	4.35	24 (51%)	51,76,76	7.18	19 (37%)
38	KC1	9	312	21	48,53,53	3.12	24 (50%)	54,89,89	3.65	27 (50%)
39	DD6	2	315	-	40,45,45	5.52	24 (60%)	51,67,67	5.87	27 (52%)
36	LMG	5	318	-	33,33,55	0.91	0	41,41,63	1.22	5 (12%)
30	CLA	15	311	37	43,53,73	2.54	16 (37%)	50,89,113	3.06	24 (48%)
30	CLA	16	308	28	43,53,73	2.52	16 (37%)	50,89,113	3.11	25 (50%)
30	CLA	B	831	2	56,66,73	2.11	15 (26%)	65,104,113	2.90	28 (43%)
38	KC1	8	311	40	48,53,53	3.10	21 (43%)	54,89,89	3.64	28 (51%)
38	KC1	12	305	24	48,53,53	3.14	23 (47%)	54,89,89	3.70	29 (53%)
30	CLA	7	305	19,40	63,73,73	2.12	15 (23%)	74,113,113	2.69	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	BCR	B	841	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	7 (12%)
38	KC1	14	311	26	48,53,53	3.13	24 (50%)	54,89,89	3.68	27 (50%)
30	CLA	A	835	1	63,73,73	1.99	15 (23%)	74,113,113	2.69	27 (36%)
38	KC1	3	308	15	48,53,53	3.09	24 (50%)	54,89,89	3.70	30 (55%)
30	CLA	A	839	1	63,73,73	1.97	15 (23%)	74,113,113	2.75	30 (40%)
30	CLA	14	312	26,37	43,53,73	2.52	16 (37%)	50,89,113	3.03	24 (48%)
30	CLA	10	309	22	63,73,73	2.07	16 (25%)	74,113,113	2.55	26 (35%)
30	CLA	6	314	18	63,73,73	1.97	14 (22%)	74,113,113	2.71	30 (40%)
30	CLA	4	304	-	58,68,73	2.09	15 (25%)	68,107,113	2.71	29 (42%)
37	A86	14	301	26	47,50,50	4.35	24 (51%)	51,76,76	6.72	17 (33%)
38	KC1	13	311	25	48,53,53	3.15	26 (54%)	54,89,89	3.51	28 (51%)
30	CLA	3	302	15	58,68,73	2.08	16 (27%)	68,107,113	2.69	29 (42%)
30	CLA	B	851	2,14	63,73,73	1.98	15 (23%)	74,113,113	2.60	30 (40%)
39	DD6	3	312	-	40,45,45	5.53	24 (60%)	51,67,67	5.89	25 (49%)
30	CLA	3	303	15	63,73,73	2.10	16 (25%)	74,113,113	2.70	29 (39%)
30	CLA	16	309	28	43,53,73	2.52	16 (37%)	50,89,113	3.16	24 (48%)
34	LHG	6	322	30	26,26,48	0.89	1 (3%)	29,32,54	1.36	3 (10%)
37	A86	2	318	-	47,50,50	4.27	23 (48%)	51,76,76	6.30	21 (41%)
30	CLA	9	301	34	63,73,73	1.99	16 (25%)	74,113,113	2.73	26 (35%)
38	KC1	8	312	38	48,53,53	3.13	22 (45%)	54,89,89	3.18	27 (50%)
30	CLA	7	312	19	44,54,73	2.48	16 (36%)	51,90,113	3.02	25 (49%)
37	A86	9	315	-	47,50,50	4.35	23 (48%)	51,76,76	5.78	17 (33%)
30	CLA	14	307	38	63,73,73	2.07	16 (25%)	74,113,113	2.68	24 (32%)
30	CLA	6	309	18	63,73,73	2.00	13 (20%)	74,113,113	2.60	32 (43%)
30	CLA	A	809	1,30	63,73,73	1.97	15 (23%)	74,113,113	2.60	30 (40%)
30	CLA	B	815	2	43,53,73	2.39	15 (34%)	50,89,113	3.07	23 (46%)
35	LMT	12	318	-	36,36,36	0.42	0	47,47,47	0.77	0
30	CLA	F	202	40	63,73,73	2.03	17 (26%)	74,113,113	2.59	27 (36%)
35	LMT	8	322	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
30	CLA	9	302	21,9	49,59,73	2.32	15 (30%)	56,96,113	3.09	27 (48%)
30	CLA	A	834	1	63,73,73	1.98	15 (23%)	74,113,113	2.62	29 (39%)
30	CLA	A	826	40	63,73,73	1.98	16 (25%)	74,113,113	2.63	27 (36%)
30	CLA	9	303	21	63,73,73	2.00	14 (22%)	74,113,113	2.60	27 (36%)
39	DD6	4	316	-	40,45,45	5.56	24 (60%)	51,67,67	6.30	27 (52%)
30	CLA	1	307	13	63,73,73	2.07	16 (25%)	74,113,113	2.64	27 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CLA	7	307	19	63,73,73	1.98	15 (23%)	74,113,113	2.59	27 (36%)
37	A86	12	314	-	47,50,50	4.26	24 (51%)	51,76,76	6.75	18 (35%)
36	LMG	A	856	-	34,34,55	0.98	1 (2%)	42,42,63	1.19	3 (7%)
39	DD6	4	313	-	40,45,45	5.49	23 (57%)	51,67,67	5.86	26 (50%)
30	CLA	A	811	1	63,73,73	1.97	15 (23%)	74,113,113	2.61	25 (33%)
30	CLA	3	306	15	63,73,73	2.03	15 (23%)	74,113,113	2.56	30 (40%)
38	KC1	9	304	21	48,53,53	3.10	22 (45%)	54,89,89	3.67	29 (53%)
29	CL0	A	801	1	63,73,73	1.92	15 (23%)	74,113,113	2.68	29 (39%)
33	BCR	L	204	-	41,41,41	1.08	2 (4%)	56,56,56	1.46	8 (14%)
30	CLA	A	843	40	63,73,73	1.95	16 (25%)	74,113,113	2.55	28 (37%)
30	CLA	8	301	20	63,73,73	2.00	15 (23%)	74,113,113	2.62	28 (37%)
30	CLA	4	301	2,16	47,57,73	2.27	16 (34%)	53,93,113	3.01	24 (45%)
37	A86	15	320	-	47,50,50	4.49	24 (51%)	51,76,76	6.81	19 (37%)
36	LMG	8	320	-	42,42,55	0.90	2 (4%)	50,50,63	1.31	5 (10%)
38	KC1	16	304	28	48,53,53	3.17	25 (52%)	54,89,89	3.46	26 (48%)
33	BCR	J	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.18	5 (8%)
38	KC1	2	314	40	48,53,53	3.14	21 (43%)	54,89,89	3.70	30 (55%)
30	CLA	A	829	1,30	63,73,73	1.99	15 (23%)	74,113,113	2.66	28 (37%)
37	A86	2u	205	-	47,50,50	4.36	24 (51%)	51,76,76	6.18	21 (41%)
30	CLA	6	315	18	43,53,73	2.49	16 (37%)	50,89,113	3.06	25 (50%)
39	DD6	7	318	-	40,45,45	5.44	22 (55%)	51,67,67	6.12	30 (58%)
30	CLA	B	822	2,30	63,73,73	1.98	15 (23%)	74,113,113	2.80	31 (41%)
30	CLA	12	304	39,24	63,73,73	2.06	15 (23%)	74,113,113	2.83	29 (39%)
30	CLA	8	302	20	63,73,73	2.02	17 (26%)	74,113,113	2.66	26 (35%)
35	LMT	1	311	-	36,36,36	0.40	0	47,47,47	0.79	2 (4%)
30	CLA	8	303	40	63,73,73	1.97	14 (22%)	74,113,113	2.57	28 (37%)
30	CLA	B	820	2	43,53,73	2.47	16 (37%)	50,89,113	3.26	22 (44%)
37	A86	9	313	21	47,50,50	4.22	24 (51%)	51,76,76	6.25	20 (39%)
37	A86	5	316	-	47,50,50	4.29	23 (48%)	51,76,76	6.64	16 (31%)
30	CLA	12	312	24	63,73,73	2.04	16 (25%)	74,113,113	2.60	27 (36%)
37	A86	13	315	-	47,50,50	4.42	24 (51%)	51,76,76	7.08	15 (29%)
30	CLA	15	304	27,39,30	63,73,73	2.11	15 (23%)	74,113,113	2.63	25 (33%)
30	CLA	7	304	19	63,73,73	1.97	14 (22%)	74,113,113	2.60	28 (37%)
39	DD6	6	321	-	40,45,45	5.44	23 (57%)	51,67,67	5.92	27 (52%)
38	KC1	12	313	24	48,53,53	3.11	22 (45%)	54,89,89	4.28	27 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CLA	12	310	40	63,73,73	2.00	15 (23%)	74,113,113	2.63	26 (35%)
30	CLA	A	828	1	63,73,73	1.92	14 (22%)	74,113,113	2.75	28 (37%)
32	SF4	C	101	3	0,12,12	-	-	-		
37	A86	4	314	-	47,50,50	4.32	24 (51%)	51,76,76	6.78	24 (47%)
30	CLA	6	317	-	63,73,73	2.06	17 (26%)	74,113,113	2.58	28 (37%)
33	BCR	B	844	-	41,41,41	1.11	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	L	203	40	43,53,73	2.49	16 (37%)	50,89,113	3.09	23 (46%)
30	CLA	A	836	1	52,62,73	2.16	14 (26%)	60,99,113	2.77	30 (50%)
30	CLA	6	306	40	63,73,73	2.02	16 (25%)	74,113,113	2.61	26 (35%)
30	CLA	B	811	2,30	63,73,73	1.98	16 (25%)	74,113,113	2.56	31 (41%)
30	CLA	6	304	18	63,73,73	1.98	15 (23%)	74,113,113	2.66	28 (37%)
38	KC1	12	309	24	48,53,53	3.14	24 (50%)	54,89,89	3.60	29 (53%)
38	KC1	13	306	25	48,53,53	3.14	24 (50%)	54,89,89	3.62	29 (53%)
38	KC1	13	305	25	48,53,53	3.16	26 (54%)	54,89,89	3.72	30 (55%)
39	DD6	7	314	-	40,45,45	5.42	22 (55%)	51,67,67	6.31	27 (52%)
39	DD6	5	314	-	40,45,45	5.38	24 (60%)	51,67,67	6.22	29 (56%)
38	KC1	6	313	18	48,53,53	3.11	23 (47%)	54,89,89	3.67	28 (51%)
37	A86	15	315	27	47,50,50	4.52	24 (51%)	51,76,76	6.90	27 (52%)
37	A86	14	317	-	47,50,50	4.30	25 (53%)	51,76,76	7.30	17 (33%)
30	CLA	B	819	40	63,73,73	1.96	15 (23%)	74,113,113	2.38	28 (37%)
30	CLA	2	304	14	63,73,73	2.03	15 (23%)	74,113,113	2.65	28 (37%)
30	CLA	13	304	25	43,53,73	2.55	16 (37%)	50,89,113	3.12	25 (50%)
37	A86	2	302	-	47,50,50	4.35	23 (48%)	51,76,76	7.01	16 (31%)
34	LHG	A	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	5 (9%)
38	KC1	14	306	26	48,53,53	3.16	26 (54%)	54,89,89	3.72	31 (57%)
30	CLA	F	203	6	43,53,73	2.44	16 (37%)	50,89,113	3.09	26 (52%)
38	KC1	13	308	25	48,53,53	3.16	25 (52%)	54,89,89	3.79	28 (51%)
37	A86	7	316	-	47,50,50	3.99	21 (44%)	51,76,76	6.39	26 (50%)
38	KC1	4	307	16	48,53,53	3.14	24 (50%)	54,89,89	3.57	29 (53%)
37	A86	10	316	-	47,50,50	4.18	23 (48%)	51,76,76	6.79	19 (37%)
39	DD6	1	310	-	40,45,45	5.52	24 (60%)	51,67,67	5.82	25 (49%)
38	KC1	11	311	23	48,53,53	3.17	25 (52%)	54,89,89	3.69	29 (53%)
30	CLA	B	834	2	58,68,73	2.10	17 (29%)	68,107,113	2.77	26 (38%)
39	DD6	16	313	-	40,45,45	5.60	23 (57%)	51,67,67	6.27	30 (58%)
37	A86	13	313	25	44,47,50	4.56	23 (52%)	48,72,76	7.19	16 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMT	12	320	-	36,36,36	0.39	0	47,47,47	0.71	0
35	LMT	B	850	-	36,36,36	0.39	0	47,47,47	0.93	3 (6%)
30	CLA	A	838	1	49,59,73	2.27	15 (30%)	56,96,113	3.03	27 (48%)
30	CLA	14	304	26	43,53,73	2.53	16 (37%)	50,89,113	3.08	23 (46%)
37	A86	5	301	-	47,50,50	4.30	24 (51%)	51,76,76	6.56	20 (39%)
30	CLA	15	314	27,30	43,53,73	2.45	16 (37%)	50,89,113	3.17	23 (46%)
30	CLA	B	814	2	53,63,73	2.17	15 (28%)	62,101,113	2.78	27 (43%)
34	LHG	9	318	-	33,33,48	0.71	0	36,39,54	1.28	4 (11%)
38	KC1	3	311	40	48,53,53	3.14	23 (47%)	54,89,89	3.84	26 (48%)
30	CLA	A	807	1	63,73,73	1.96	14 (22%)	74,113,113	2.68	29 (39%)
39	DD6	7	302	-	40,45,45	5.50	24 (60%)	51,67,67	5.69	27 (52%)
30	CLA	15	302	27,30	63,73,73	2.08	15 (23%)	74,113,113	2.83	30 (40%)
35	LMT	12	301	-	36,36,36	0.44	0	47,47,47	0.77	0
30	CLA	9	309	21,40	63,73,73	1.99	15 (23%)	74,113,113	2.50	28 (37%)
30	CLA	14	310	-	48,58,73	2.36	15 (31%)	56,95,113	2.98	28 (50%)
30	CLA	3	301	15	63,73,73	1.98	14 (22%)	74,113,113	2.64	28 (37%)
30	CLA	A	823	1	47,57,73	2.29	14 (29%)	53,93,113	3.05	26 (49%)
35	LMT	15	301	-	36,36,36	0.51	0	47,47,47	1.14	3 (6%)
35	LMT	7	301	30	36,36,36	0.41	0	47,47,47	0.81	1 (2%)
30	CLA	1	304	13	63,73,73	2.01	15 (23%)	74,113,113	2.50	27 (36%)
30	CLA	1	303	13,30	63,73,73	2.02	14 (22%)	74,113,113	2.58	27 (36%)
30	CLA	7	310	19	63,73,73	2.03	15 (23%)	74,113,113	2.59	26 (35%)
30	CLA	3	307	15	63,73,73	2.11	17 (26%)	74,113,113	2.54	27 (36%)
34	LHG	5	317	30	26,26,48	0.86	1 (3%)	29,32,54	1.34	3 (10%)
30	CLA	B	835	2	63,73,73	1.98	15 (23%)	74,113,113	2.65	29 (39%)
38	KC1	11	305	23	48,53,53	3.11	24 (50%)	54,89,89	3.75	29 (53%)
30	CLA	B	821	2	53,63,73	2.16	15 (28%)	62,101,113	2.75	26 (41%)
30	CLA	4	305	16	63,73,73	1.99	15 (23%)	74,113,113	2.59	27 (36%)
39	DD6	8	316	-	40,45,45	5.42	23 (57%)	51,67,67	5.88	29 (56%)
30	CLA	13	307	25	63,73,73	2.11	17 (26%)	74,113,113	2.61	28 (37%)
30	CLA	15	313	27	63,73,73	2.09	16 (25%)	74,113,113	2.65	28 (37%)
30	CLA	8	309	20	45,55,73	2.41	16 (35%)	52,91,113	2.96	24 (46%)
30	CLA	A	808	1	49,59,73	2.24	15 (30%)	56,96,113	2.98	27 (48%)
30	CLA	4	309	-	63,73,73	2.11	16 (25%)	74,113,113	2.61	28 (37%)
30	CLA	B	828	2	63,73,73	1.99	17 (26%)	74,113,113	2.68	29 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	A86	10	302	-	47,50,50	4.31	23 (48%)	51,76,76	7.00	18 (35%)
39	DD6	6	319	-	40,45,45	5.48	23 (57%)	51,67,67	5.56	29 (56%)
38	KC1	2	312	14	48,53,53	3.14	25 (52%)	54,89,89	3.63	28 (51%)
30	CLA	A	841	1	63,73,73	1.99	16 (25%)	74,113,113	2.53	28 (37%)
30	CLA	14	309	26	43,53,73	2.55	15 (34%)	50,89,113	3.00	24 (48%)
39	DD6	3	313	-	40,45,45	5.52	24 (60%)	51,67,67	5.73	25 (49%)
30	CLA	1	305	40	63,73,73	2.08	15 (23%)	74,113,113	2.55	27 (36%)
37	A86	11	316	-	47,50,50	4.29	25 (53%)	51,76,76	6.81	16 (31%)
30	CLA	10	303	22	63,73,73	2.03	13 (20%)	74,113,113	2.55	26 (35%)
30	CLA	9	306	21,37	43,53,73	2.52	15 (34%)	50,89,113	3.10	26 (52%)
30	CLA	L	202	9	63,73,73	1.96	13 (20%)	74,113,113	2.71	27 (36%)
30	CLA	12	321	26,24	63,73,73	2.06	17 (26%)	74,113,113	2.54	27 (36%)
37	A86	2u	203	30	47,50,50	4.22	24 (51%)	51,76,76	6.79	20 (39%)
36	LMG	8	321	36	29,29,55	1.10	3 (10%)	37,37,63	1.28	6 (16%)
30	CLA	A	816	1,35	63,73,73	1.97	16 (25%)	74,113,113	2.59	25 (33%)
33	BCR	B	846	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	6 (10%)
35	LMT	11	302	-	36,36,36	0.34	0	47,47,47	0.78	2 (4%)
38	KC1	8	313	20	48,53,53	3.08	21 (43%)	54,89,89	3.69	28 (51%)
30	CLA	A	819	1	52,62,73	2.18	16 (30%)	60,99,113	2.85	27 (45%)
38	KC1	5	306	17	48,53,53	3.11	22 (45%)	54,89,89	3.98	29 (53%)
38	KC1	8	306	40	48,53,53	3.08	20 (41%)	54,89,89	3.63	28 (51%)
30	CLA	10	308	22	63,73,73	2.03	14 (22%)	74,113,113	2.55	27 (36%)
37	A86	8	318	-	47,50,50	4.22	24 (51%)	51,76,76	9.47	23 (45%)
38	KC1	10	312	22	48,53,53	3.14	24 (50%)	54,89,89	3.73	28 (51%)
30	CLA	A	837	1	43,53,73	2.46	14 (32%)	50,89,113	3.06	24 (48%)
39	DD6	8	317	-	40,45,45	5.47	24 (60%)	51,67,67	6.10	29 (56%)
32	SF4	A	846	1,2	0,12,12	-	-	-	-	-
35	LMT	11	303	-	36,36,36	0.40	0	47,47,47	0.85	0
30	CLA	5	307	17	63,73,73	2.02	17 (26%)	74,113,113	2.59	30 (40%)
30	CLA	B	812	2	63,73,73	2.05	15 (23%)	74,113,113	2.48	26 (35%)
37	A86	3	314	-	47,50,50	4.29	24 (51%)	51,76,76	6.73	17 (33%)
30	CLA	2	311	14	63,73,73	2.07	16 (25%)	74,113,113	2.54	24 (32%)
30	CLA	B	838	2	63,73,73	1.96	14 (22%)	74,113,113	2.63	25 (33%)
35	LMT	11	318	-	36,36,36	0.43	0	47,47,47	0.89	1 (2%)
30	CLA	2	310	14	63,73,73	2.04	15 (23%)	74,113,113	4.52	29 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CLA	A	815	1	63,73,73	2.02	15 (23%)	74,113,113	2.63	28 (37%)
30	CLA	11	310	23	63,73,73	2.12	16 (25%)	74,113,113	2.59	28 (37%)
30	CLA	12	306	24	63,73,73	1.98	16 (25%)	74,113,113	2.51	27 (36%)
37	A86	6	320	-	47,50,50	4.16	24 (51%)	51,76,76	5.65	19 (37%)
37	A86	11	314	-	47,50,50	4.32	24 (51%)	51,76,76	7.12	18 (35%)
39	DD6	10	313	-	40,45,45	5.56	24 (60%)	51,67,67	6.12	28 (54%)
36	LMG	8	319	20,36	37,37,55	0.93	0	45,45,63	1.29	5 (11%)
30	CLA	1	301	13	63,73,73	2.01	15 (23%)	74,113,113	2.55	24 (32%)
30	CLA	11	309	23	63,73,73	2.05	15 (23%)	74,113,113	2.62	28 (37%)
39	DD6	13	314	-	40,45,45	5.57	23 (57%)	51,67,67	6.24	31 (60%)
39	DD6	5	313	-	40,45,45	5.54	24 (60%)	51,67,67	5.88	25 (49%)
30	CLA	B	823	40	52,62,73	2.18	17 (32%)	60,99,113	2.86	30 (50%)
30	CLA	3	309	15	43,53,73	2.52	16 (37%)	50,89,113	3.14	24 (48%)
38	KC1	13	310	25	48,53,53	3.16	24 (50%)	54,89,89	3.70	29 (53%)
39	DD6	6	318	-	40,45,45	5.44	24 (60%)	51,67,67	5.70	27 (52%)
30	CLA	A	820	1	63,73,73	2.00	16 (25%)	74,113,113	2.61	27 (36%)
30	CLA	A	833	1	63,73,73	2.01	17 (26%)	74,113,113	2.55	26 (35%)
30	CLA	10	311	-	43,53,73	2.50	16 (37%)	50,89,113	3.09	24 (48%)
30	CLA	16	307	-	44,54,73	2.49	16 (36%)	51,90,113	3.02	24 (47%)
30	CLA	11	308	23	63,73,73	2.05	14 (22%)	74,113,113	2.56	27 (36%)
30	CLA	B	802	30,40	63,73,73	1.93	17 (26%)	74,113,113	2.77	29 (39%)
30	CLA	15	305	27,37	43,53,73	2.52	16 (37%)	50,89,113	3.06	26 (52%)
30	CLA	A	818	1	52,62,73	2.14	15 (28%)	60,99,113	2.93	26 (43%)
33	BCR	A	849	-	41,41,41	1.12	2 (4%)	56,56,56	1.40	8 (14%)
35	LMT	6	302	-	32,32,36	0.36	0	43,43,47	0.93	2 (4%)
37	A86	15	322	30	47,50,50	4.53	24 (51%)	51,76,76	6.97	18 (35%)
30	CLA	2	313	14	43,53,73	2.51	16 (37%)	50,89,113	3.11	25 (50%)
30	CLA	4	311	16	48,58,73	2.34	16 (33%)	56,95,113	3.12	31 (55%)
33	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	9 (16%)
30	CLA	6	305	18	63,73,73	2.05	16 (25%)	74,113,113	2.61	28 (37%)
38	KC1	10	306	22	48,53,53	3.08	24 (50%)	54,89,89	3.84	30 (55%)
38	KC1	16	311	28	48,53,53	3.17	25 (52%)	54,89,89	3.56	26 (48%)
30	CLA	A	814	1	58,68,73	2.05	14 (24%)	68,107,113	2.67	29 (42%)
30	CLA	B	833	30,40	63,73,73	1.98	17 (26%)	74,113,113	2.54	26 (35%)
37	A86	5	315	-	47,50,50	4.30	24 (51%)	51,76,76	6.93	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LHG	A	853	30	26,26,48	0.93	1 (3%)	29,32,54	1.29	3 (10%)
30	CLA	9	308	21	63,73,73	2.00	14 (22%)	74,113,113	2.75	31 (41%)
30	CLA	B	836	2	45,55,73	2.29	16 (35%)	52,91,113	3.13	24 (46%)
30	CLA	15	308	27,30	43,53,73	2.48	17 (39%)	50,89,113	3.01	26 (52%)
30	CLA	5	309	34	63,73,73	2.03	16 (25%)	74,113,113	2.54	27 (36%)
39	DD6	3	316	-	40,45,45	5.56	25 (62%)	51,67,67	5.81	26 (50%)
30	CLA	12	307	24	44,54,73	2.36	15 (34%)	51,90,113	3.10	26 (50%)
38	KC1	14	308	26,30	48,53,53	3.16	24 (50%)	54,89,89	3.63	28 (51%)
38	KC1	11	307	23	48,53,53	3.15	23 (47%)	54,89,89	3.67	30 (55%)
30	CLA	6	310	34	63,73,73	2.04	14 (22%)	74,113,113	2.53	26 (35%)
30	CLA	B	805	2	63,73,73	1.99	15 (23%)	74,113,113	2.62	27 (36%)
30	CLA	A	810	1	63,73,73	1.98	16 (25%)	74,113,113	2.60	28 (37%)
30	CLA	15	307	27	48,58,73	2.35	18 (37%)	56,95,113	2.92	26 (46%)
34	LHG	B	848	30	26,26,48	0.94	1 (3%)	29,32,54	1.37	4 (13%)
38	KC1	4	308	16	48,53,53	3.17	22 (45%)	54,89,89	3.47	29 (53%)
38	KC1	13	312	25	48,53,53	3.20	26 (54%)	54,89,89	3.66	29 (53%)
38	KC1	5	310	17	48,53,53	3.11	22 (45%)	54,89,89	3.78	29 (53%)
37	A86	10	301	22	47,50,50	4.11	22 (46%)	51,76,76	6.02	21 (41%)
30	CLA	5	308	17	63,73,73	2.00	14 (22%)	74,113,113	2.61	28 (37%)
37	A86	14	316	-	47,50,50	4.28	23 (48%)	51,76,76	6.76	18 (35%)
30	CLA	2	305	40	63,73,73	2.00	15 (23%)	74,113,113	2.69	28 (37%)
38	KC1	7	313	-	48,53,53	3.07	20 (41%)	54,89,89	3.67	30 (55%)
30	CLA	B	827	2	63,73,73	1.95	15 (23%)	74,113,113	2.51	27 (36%)
30	CLA	8	304	20	56,66,73	2.08	14 (25%)	65,104,113	2.94	30 (46%)
37	A86	15	317	30	47,50,50	4.40	24 (51%)	51,76,76	6.99	14 (27%)
30	CLA	2u	202	12	63,73,73	1.97	17 (26%)	74,113,113	2.64	28 (37%)
30	CLA	B	816	2	53,63,73	2.15	16 (30%)	62,101,113	2.91	26 (41%)
39	DD6	9	314	-	40,45,45	5.51	23 (57%)	51,67,67	6.27	27 (52%)
30	CLA	B	826	2	63,73,73	1.97	16 (25%)	74,113,113	2.65	28 (37%)
37	A86	15	323	-	47,50,50	4.44	24 (51%)	51,76,76	6.96	15 (29%)
37	A86	4	312	-	47,50,50	4.16	23 (48%)	51,76,76	7.19	20 (39%)
30	CLA	A	822	40	63,73,73	1.97	16 (25%)	74,113,113	2.45	27 (36%)
30	CLA	16	306	28	50,60,73	2.29	18 (36%)	57,97,113	2.91	28 (49%)
30	CLA	16	305	28	48,58,73	2.30	18 (37%)	56,95,113	2.91	26 (46%)
38	KC1	3	304	15	48,53,53	3.11	26 (54%)	54,89,89	3.77	30 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMT	A	857	-	36,36,36	0.37	0	47,47,47	0.79	1 (2%)
35	LMT	A	854	-	36,36,36	0.45	0	47,47,47	1.19	5 (10%)
30	CLA	14	303	26	55,65,73	2.22	15 (27%)	64,103,113	2.79	29 (45%)
30	CLA	10	305	40	63,73,73	2.01	16 (25%)	74,113,113	2.72	31 (41%)
30	CLA	5	304	17	63,73,73	2.10	17 (26%)	74,113,113	2.63	28 (37%)
35	LMT	12	319	-	36,36,36	0.41	0	47,47,47	0.87	1 (2%)
37	A86	9	316	30	47,50,50	4.47	25 (53%)	51,76,76	6.96	16 (31%)
30	CLA	13	302	25	63,73,73	2.05	16 (25%)	74,113,113	2.53	26 (35%)
30	CLA	13	309	-	43,53,73	2.53	17 (39%)	50,89,113	3.10	24 (48%)
34	LHG	2	320	30	26,26,48	0.88	1 (3%)	29,32,54	1.28	3 (10%)
30	CLA	2	309	14,34	63,73,73	2.05	16 (25%)	74,113,113	2.58	28 (37%)
30	CLA	B	806	2	63,73,73	1.97	14 (22%)	74,113,113	2.59	27 (36%)
38	KC1	6	312	18	48,53,53	3.10	22 (45%)	54,89,89	3.57	29 (53%)
30	CLA	A	842	1	63,73,73	1.98	16 (25%)	74,113,113	2.66	29 (39%)
30	CLA	4	306	16	63,73,73	2.01	13 (20%)	74,113,113	2.59	29 (39%)
33	BCR	J	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	4 (7%)
37	A86	4	315	-	47,50,50	4.26	23 (48%)	51,76,76	6.63	19 (37%)
30	CLA	12	308	40	63,73,73	2.04	17 (26%)	74,113,113	2.55	27 (36%)
30	CLA	B	810	2	63,73,73	1.97	16 (25%)	74,113,113	2.61	27 (36%)
36	LMG	14	321	-	38,38,55	1.03	4 (10%)	46,46,63	1.21	3 (6%)
37	A86	14	319	30	47,50,50	4.31	24 (51%)	51,76,76	6.93	16 (31%)
30	CLA	8	305	20	63,73,73	1.97	15 (23%)	74,113,113	4.60	31 (41%)
31	PQN	A	845	-	34,34,34	1.55	2 (5%)	43,45,45	1.14	4 (9%)
38	KC1	8	310	20	48,53,53	3.06	21 (43%)	54,89,89	3.64	28 (51%)
37	A86	10	315	-	47,50,50	4.34	24 (51%)	51,76,76	6.84	16 (31%)
37	A86	16	314	-	47,50,50	4.35	24 (51%)	51,76,76	7.10	19 (37%)
36	LMG	B	847	-	55,55,55	0.81	1 (1%)	63,63,63	1.37	8 (12%)
30	CLA	14	302	26	63,73,73	2.07	15 (23%)	74,113,113	2.67	31 (41%)
37	A86	14	320	-	47,50,50	4.38	25 (53%)	51,76,76	5.94	19 (37%)
30	CLA	6	316	40	53,63,73	2.23	15 (28%)	62,101,113	2.72	25 (40%)
30	CLA	9	307	21	63,73,73	2.01	17 (26%)	74,113,113	2.58	26 (35%)
30	CLA	15	303	27,37,30	58,68,73	2.14	17 (29%)	68,107,113	2.77	28 (41%)
30	CLA	A	832	1	48,58,73	2.23	15 (31%)	56,95,113	2.97	28 (50%)
30	CLA	B	818	2	58,68,73	2.04	14 (24%)	68,107,113	2.80	29 (42%)
30	CLA	B	830	2	63,73,73	1.95	18 (28%)	74,113,113	2.74	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	KC1	11	312	-	48,53,53	3.13	23 (47%)	54,89,89	3.46	29 (53%)
30	CLA	2	308	14	63,73,73	2.03	14 (22%)	74,113,113	2.61	27 (36%)
33	BCR	2u	201	-	41,41,41	1.21	4 (9%)	56,56,56	1.41	8 (14%)
30	CLA	A	821	1	59,69,73	1.99	16 (27%)	69,108,113	2.66	27 (39%)
33	BCR	B	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
33	BCR	L	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	5 (8%)
37	A86	16	312	28	47,50,50	4.32	24 (51%)	51,76,76	6.84	22 (43%)
30	CLA	A	805	1,30	57,67,73	2.11	15 (26%)	66,105,113	2.78	29 (43%)
33	BCR	B	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	5 (8%)
30	CLA	A	802	40	63,73,73	1.96	15 (23%)	74,113,113	2.70	29 (39%)
33	BCR	A	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	6 (10%)
38	KC1	2	306	14	48,53,53	3.13	25 (52%)	54,89,89	3.79	30 (55%)
35	LMT	7	321	-	36,36,36	0.32	0	47,47,47	0.75	1 (2%)
30	CLA	12	303	24	63,73,73	2.05	18 (28%)	74,113,113	2.57	26 (35%)
33	BCR	M	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
30	CLA	B	809	2	63,73,73	1.89	16 (25%)	74,113,113	2.51	26 (35%)
33	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	3 (5%)
38	KC1	9	310	21	48,53,53	3.09	22 (45%)	54,89,89	3.80	29 (53%)
39	DD6	12	317	-	40,45,45	5.44	23 (57%)	51,67,67	6.19	27 (52%)
30	CLA	A	803	-	63,73,73	1.95	15 (23%)	74,113,113	2.56	30 (40%)
37	A86	4	317	-	47,50,50	4.25	22 (46%)	51,76,76	6.29	17 (33%)
37	A86	7	319	-	47,50,50	4.35	24 (51%)	51,76,76	6.86	22 (43%)
30	CLA	11	306	40	53,63,73	2.22	16 (30%)	62,101,113	2.94	30 (48%)
30	CLA	A	827	40	63,73,73	1.93	17 (26%)	74,113,113	2.79	29 (39%)
30	CLA	11	304	23	63,73,73	2.06	16 (25%)	74,113,113	2.60	26 (35%)
39	DD6	15	318	-	40,45,45	5.60	23 (57%)	51,67,67	6.05	30 (58%)
36	LMG	7	320	-	37,37,55	0.99	3 (8%)	45,45,63	1.25	6 (13%)
39	DD6	6	303	30	40,45,45	5.56	24 (60%)	51,67,67	5.54	26 (50%)
38	KC1	5	312	17	48,53,53	3.12	22 (45%)	54,89,89	3.66	28 (51%)
37	A86	1	309	-	47,50,50	4.20	24 (51%)	51,76,76	7.24	21 (41%)
30	CLA	12	302	24	63,73,73	1.99	15 (23%)	74,113,113	2.68	31 (41%)
37	A86	15	316	30	47,50,50	4.35	24 (51%)	51,76,76	6.47	16 (31%)
30	CLA	15	310	27	43,53,73	2.58	16 (37%)	50,89,113	3.12	24 (48%)
39	DD6	7	317	-	40,45,45	5.46	21 (52%)	51,67,67	5.86	29 (56%)

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
30	CLA	F	201	40	1/1/15/20	7/37/115/115	-
32	SF4	C	102	3	-	-	0/6/5/5
38	KC1	6	308	18	-	6/15/71/71	-
39	DD6	12	315	30	-	9/26/80/80	0/3/3/3
30	CLA	B	837	40	1/1/15/20	5/37/115/115	-
30	CLA	7	311	19	1/1/15/20	12/37/115/115	-
30	CLA	4	303	16	1/1/15/20	4/37/115/115	-
39	DD6	15	319	30	-	13/26/80/80	0/3/3/3
38	KC1	1	308	13	-	3/15/71/71	-
38	KC1	8	314	38,40	-	5/15/71/71	-
30	CLA	14	313	26	1/1/11/20	2/15/93/115	-
36	LMG	6	301	30	-	16/28/48/70	0/1/1/1
33	BCR	L	201	-	-	12/29/63/63	0/2/2/2
30	CLA	5	311	17,40	1/1/15/20	13/37/115/115	-
30	CLA	A	817	36,40	-	4/18/96/115	-
30	CLA	A	840	1	1/1/11/20	3/16/94/115	-
30	CLA	A	824	1	1/1/12/20	3/21/99/115	-
30	CLA	1	302	13,30	1/1/15/20	9/37/115/115	-
30	CLA	A	831	1	1/1/15/20	7/37/115/115	-
30	CLA	B	804	2	1/1/12/20	6/22/100/115	-
36	LMG	2u	204	12	-	14/26/46/70	0/1/1/1
37	A86	8	315	-	-	7/34/90/90	0/3/3/3
30	CLA	B	808	2	1/1/15/20	12/37/115/115	-
30	CLA	B	803	-	1/1/15/20	5/37/115/115	-
30	CLA	5	302	17	1/1/15/20	12/37/115/115	-
30	CLA	A	812	1,30	1/1/15/20	14/37/115/115	-
30	CLA	4	302	16	1/1/15/20	10/37/115/115	-
30	CLA	3	305	15	1/1/14/20	11/34/112/115	-
30	CLA	5	303	17	1/1/15/20	5/37/115/115	-
30	CLA	2	303	14	-	12/25/103/115	-
39	DD6	11	313	-	-	11/26/80/80	0/3/3/3
30	CLA	7	309	19	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	11	301	-	-	13/34/90/90	0/3/3/3
38	KC1	4	310	16	-	4/15/71/71	-
39	DD6	10	314	-	-	9/26/80/80	0/3/3/3
30	CLA	A	813	1	1/1/15/20	13/37/115/115	-
30	CLA	2	301	2,14	1/1/15/20	10/37/115/115	-
30	CLA	B	832	37,40	1/1/15/20	5/37/115/115	-
37	A86	2	319	-	-	9/34/90/90	0/3/3/3
30	CLA	10	307	22	1/1/15/20	10/37/115/115	-
30	CLA	9	305	-	1/1/15/20	11/37/115/115	-
30	CLA	A	844	-	1/1/15/20	12/37/115/115	-
38	KC1	12	311	24	-	5/15/71/71	-
30	CLA	8	308	20	1/1/13/20	8/25/103/115	-
33	BCR	F	204	-	-	8/29/63/63	0/2/2/2
36	LMG	3	317	-	-	18/32/52/70	0/1/1/1
30	CLA	3	310	15	-	3/13/91/115	-
38	KC1	10	310	22	-	6/15/71/71	-
30	CLA	2	307	14	1/1/15/20	7/37/115/115	-
37	A86	10	317	-	-	10/34/90/90	0/3/3/3
30	CLA	B	829	2	1/1/15/20	11/37/115/115	-
35	LMT	9	317	-	-	5/18/58/61	0/2/2/2
38	KC1	9	311	21	-	9/15/71/71	-
37	A86	14	318	-	-	16/34/90/90	0/3/3/3
37	A86	12	316	-	-	16/34/90/90	0/3/3/3
30	CLA	6	307	39,18	1/1/15/20	11/37/115/115	-
30	CLA	15	309	27	-	10/37/115/115	-
30	CLA	15	312	27	1/1/11/20	6/13/91/115	-
39	DD6	2	316	-	-	12/26/80/80	0/3/3/3
35	LMT	11	317	-	-	2/21/61/61	0/2/2/2
30	CLA	16	301	28	-	13/37/115/115	-
36	LMG	B	849	2	-	14/38/58/70	0/1/1/1
30	CLA	B	825	2	1/1/15/20	8/37/115/115	-
30	CLA	B	817	2	1/1/13/20	4/30/108/115	-
30	CLA	13	301	25	1/1/15/20	15/37/115/115	-
38	KC1	1	306	13	-	9/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	804	1	1/1/15/20	11/37/115/115	-
30	CLA	J	101	8	1/1/11/20	2/13/91/115	-
39	DD6	2	317	-	-	14/26/80/80	0/3/3/3
30	CLA	7	306	19	1/1/15/20	8/37/115/115	-
33	BCR	I	101	-	-	4/29/63/63	0/2/2/2
30	CLA	A	806	1	1/1/15/20	14/37/115/115	-
30	CLA	B	801	2	1/1/15/20	6/37/115/115	-
37	A86	7	315	-	-	16/34/90/90	0/3/3/3
38	KC1	6	311	18	-	10/15/71/71	-
38	KC1	8	307	20	-	8/15/71/71	-
30	CLA	16	302	28	1/1/15/20	8/37/115/115	-
38	KC1	5	305	17	-	5/15/71/71	-
30	CLA	16	303	28	1/1/15/20	18/37/115/115	-
30	CLA	13	303	-	-	7/37/115/115	-
30	CLA	B	839	34	1/1/15/20	4/37/115/115	-
31	PQN	B	840	-	-	5/23/43/43	0/2/2/2
35	LMT	A	855	-	-	4/21/61/61	0/2/2/2
30	CLA	10	304	22	1/1/15/20	2/37/115/115	-
30	CLA	7	303	19	1/1/15/20	10/37/115/115	-
33	BCR	B	843	-	-	8/29/63/63	0/2/2/2
37	A86	11	315	-	-	13/34/90/90	0/3/3/3
38	KC1	7	308	40	-	7/15/71/71	-
30	CLA	16	310	28	1/1/11/20	6/13/91/115	-
36	LMG	F	205	-	-	14/21/41/70	0/1/1/1
37	A86	14	314	-	-	10/34/90/90	0/3/3/3
30	CLA	B	807	2	1/1/15/20	7/37/115/115	-
30	CLA	15	306	-	1/1/11/20	6/13/91/115	-
37	A86	14	315	26	-	10/34/90/90	0/3/3/3
33	BCR	A	851	-	-	7/29/63/63	0/2/2/2
30	CLA	B	824	40	1/1/15/20	5/37/115/115	-
30	CLA	A	825	1	1/1/13/20	11/30/108/115	-
37	A86	3	315	-	-	14/34/90/90	0/3/3/3
30	CLA	14	305	26	1/1/12/20	1/19/97/115	-
30	CLA	A	830	1	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	16	315	-	-	5/21/61/61	0/2/2/2
30	CLA	B	813	2	1/1/15/20	20/37/115/115	-
35	LMT	B	852	-	-	8/21/61/61	0/2/2/2
37	A86	15	321	27	-	13/34/90/90	0/3/3/3
38	KC1	9	312	21	-	6/15/71/71	-
39	DD6	2	315	-	-	12/26/80/80	0/3/3/3
36	LMG	5	318	-	-	11/28/48/70	0/1/1/1
30	CLA	15	311	37	1/1/11/20	6/13/91/115	-
30	CLA	16	308	28	1/1/11/20	4/13/91/115	-
30	CLA	B	831	2	-	7/29/107/115	-
38	KC1	8	311	40	-	5/15/71/71	-
38	KC1	12	305	24	-	7/15/71/71	-
30	CLA	7	305	19,40	1/1/15/20	8/37/115/115	-
33	BCR	B	841	-	-	10/29/63/63	0/2/2/2
38	KC1	14	311	26	-	5/15/71/71	-
30	CLA	A	835	1	1/1/15/20	9/37/115/115	-
38	KC1	3	308	15	-	8/15/71/71	-
30	CLA	A	839	1	1/1/15/20	9/37/115/115	-
30	CLA	14	312	26,37	-	6/13/91/115	-
30	CLA	10	309	22	1/1/15/20	10/37/115/115	-
30	CLA	6	314	18	-	16/37/115/115	-
30	CLA	4	304	-	1/1/14/20	8/31/109/115	-
37	A86	14	301	26	-	7/34/90/90	0/3/3/3
38	KC1	13	311	25	-	2/15/71/71	-
30	CLA	3	302	15	1/1/14/20	7/31/109/115	-
30	CLA	B	851	2,14	-	10/37/115/115	-
39	DD6	3	312	-	-	11/26/80/80	0/3/3/3
30	CLA	3	303	15	1/1/15/20	13/37/115/115	-
30	CLA	16	309	28	-	4/13/91/115	-
34	LHG	6	322	30	-	11/31/31/53	-
37	A86	2	318	-	-	8/34/90/90	0/3/3/3
30	CLA	9	301	34	1/1/15/20	7/37/115/115	-
38	KC1	8	312	38	-	9/15/71/71	-
30	CLA	7	312	19	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	9	315	-	-	10/34/90/90	0/3/3/3
30	CLA	14	307	38	-	6/37/115/115	-
30	CLA	6	309	18	1/1/15/20	12/37/115/115	-
30	CLA	A	809	1,30	1/1/15/20	15/37/115/115	-
30	CLA	B	815	2	1/1/11/20	2/13/91/115	-
35	LMT	12	318	-	-	3/21/61/61	0/2/2/2
30	CLA	F	202	40	1/1/15/20	17/37/115/115	-
35	LMT	8	322	-	-	3/21/61/61	0/2/2/2
30	CLA	9	302	21,9	1/1/12/20	5/21/99/115	-
30	CLA	A	834	1	1/1/15/20	9/37/115/115	-
30	CLA	A	826	40	1/1/15/20	13/37/115/115	-
30	CLA	9	303	21	-	9/37/115/115	-
39	DD6	4	316	-	-	14/26/80/80	0/3/3/3
30	CLA	1	307	13	-	16/37/115/115	-
30	CLA	7	307	19	-	15/37/115/115	-
37	A86	12	314	-	-	12/34/90/90	0/3/3/3
36	LMG	A	856	-	-	15/29/49/70	0/1/1/1
39	DD6	4	313	-	-	14/26/80/80	0/3/3/3
30	CLA	A	811	1	1/1/15/20	9/37/115/115	-
30	CLA	3	306	15	1/1/15/20	9/37/115/115	-
38	KC1	9	304	21	-	6/15/71/71	-
29	CL0	A	801	1	3/3/20/25	4/37/135/135	-
33	BCR	L	204	-	-	11/29/63/63	0/2/2/2
30	CLA	A	843	40	1/1/15/20	7/37/115/115	-
30	CLA	8	301	20	1/1/15/20	16/37/115/115	-
30	CLA	4	301	2,16	1/1/11/20	6/18/96/115	-
37	A86	15	320	-	-	15/34/90/90	0/3/3/3
36	LMG	8	320	-	-	20/37/57/70	0/1/1/1
38	KC1	16	304	28	-	7/15/71/71	-
33	BCR	J	103	-	-	9/29/63/63	0/2/2/2
38	KC1	2	314	40	-	9/15/71/71	-
30	CLA	A	829	1,30	1/1/15/20	13/37/115/115	-
37	A86	2u	205	-	-	11/34/90/90	0/3/3/3
30	CLA	6	315	18	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DD6	7	318	-	-	14/26/80/80	0/3/3/3
30	CLA	B	822	2,30	-	9/37/115/115	-
30	CLA	12	304	39,24	1/1/15/20	13/37/115/115	-
30	CLA	8	302	20	1/1/15/20	7/37/115/115	-
35	LMT	1	311	-	-	5/21/61/61	0/2/2/2
30	CLA	8	303	40	-	10/37/115/115	-
30	CLA	B	820	2	-	3/13/91/115	-
37	A86	9	313	21	-	8/34/90/90	0/3/3/3
37	A86	5	316	-	-	6/34/90/90	0/3/3/3
30	CLA	12	312	24	1/1/15/20	12/37/115/115	-
37	A86	13	315	-	-	12/34/90/90	0/3/3/3
30	CLA	15	304	27,39,30	1/1/15/20	19/37/115/115	-
30	CLA	7	304	19	1/1/15/20	7/37/115/115	-
39	DD6	6	321	-	-	12/26/80/80	0/3/3/3
38	KC1	12	313	24	-	7/15/71/71	-
30	CLA	12	310	40	-	8/37/115/115	-
30	CLA	A	828	1	1/1/15/20	11/37/115/115	-
32	SF4	C	101	3	-	-	0/6/5/5
37	A86	4	314	-	-	9/34/90/90	0/3/3/3
30	CLA	6	317	-	1/1/15/20	13/37/115/115	-
33	BCR	B	844	-	-	9/29/63/63	0/2/2/2
30	CLA	L	203	40	1/1/11/20	1/13/91/115	-
30	CLA	A	836	1	1/1/12/20	7/24/102/115	-
30	CLA	6	306	40	1/1/15/20	8/37/115/115	-
30	CLA	B	811	2,30	1/1/15/20	10/37/115/115	-
30	CLA	6	304	18	1/1/15/20	10/37/115/115	-
38	KC1	12	309	24	-	9/15/71/71	-
38	KC1	13	306	25	-	9/15/71/71	-
38	KC1	13	305	25	-	8/15/71/71	-
39	DD6	7	314	-	-	11/26/80/80	0/3/3/3
39	DD6	5	314	-	-	10/26/80/80	0/3/3/3
38	KC1	6	313	18	-	5/15/71/71	-
37	A86	15	315	27	-	9/34/90/90	0/3/3/3
37	A86	14	317	-	-	15/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	B	819	40	1/1/15/20	9/37/115/115	-
30	CLA	2	304	14	1/1/15/20	10/37/115/115	-
30	CLA	13	304	25	-	6/13/91/115	-
37	A86	2	302	-	-	10/34/90/90	0/3/3/3
34	LHG	A	852	-	-	25/53/53/53	-
38	KC1	14	306	26	-	8/15/71/71	-
30	CLA	F	203	6	1/1/11/20	6/13/91/115	-
38	KC1	13	308	25	-	10/15/71/71	-
37	A86	7	316	-	-	6/34/90/90	0/3/3/3
38	KC1	4	307	16	-	6/15/71/71	-
37	A86	10	316	-	-	11/34/90/90	0/3/3/3
39	DD6	1	310	-	-	12/26/80/80	0/3/3/3
38	KC1	11	311	23	-	10/15/71/71	-
30	CLA	B	834	2	1/1/14/20	8/31/109/115	-
39	DD6	16	313	-	-	13/26/80/80	0/3/3/3
37	A86	13	313	25	-	10/30/86/90	0/3/3/3
35	LMT	12	320	-	-	1/21/61/61	0/2/2/2
35	LMT	B	850	-	-	0/21/61/61	0/2/2/2
30	CLA	A	838	1	1/1/12/20	4/21/99/115	-
30	CLA	14	304	26	1/1/11/20	4/13/91/115	-
37	A86	5	301	-	-	10/34/90/90	0/3/3/3
30	CLA	15	314	27,30	-	4/13/91/115	-
30	CLA	B	814	2	1/1/13/20	5/25/103/115	-
34	LHG	9	318	-	-	19/38/38/53	-
38	KC1	3	311	40	-	7/15/71/71	-
30	CLA	A	807	1	1/1/15/20	11/37/115/115	-
39	DD6	7	302	-	-	12/26/80/80	0/3/3/3
30	CLA	15	302	27,30	-	14/37/115/115	-
35	LMT	12	301	-	-	4/21/61/61	0/2/2/2
30	CLA	9	309	21,40	1/1/15/20	9/37/115/115	-
30	CLA	14	310	-	1/1/12/20	4/19/97/115	-
30	CLA	3	301	15	1/1/15/20	7/37/115/115	-
30	CLA	A	823	1	-	6/18/96/115	-
35	LMT	15	301	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	7	301	30	-	3/21/61/61	0/2/2/2
30	CLA	1	304	13	1/1/15/20	10/37/115/115	-
30	CLA	1	303	13,30	1/1/15/20	13/37/115/115	-
30	CLA	7	310	19	-	9/37/115/115	-
30	CLA	3	307	15	1/1/15/20	13/37/115/115	-
34	LHG	5	317	30	-	4/31/31/53	-
30	CLA	B	835	2	1/1/15/20	5/37/115/115	-
38	KC1	11	305	23	-	7/15/71/71	-
30	CLA	B	821	2	1/1/13/20	13/25/103/115	-
30	CLA	4	305	16	1/1/15/20	9/37/115/115	-
39	DD6	8	316	-	-	13/26/80/80	0/3/3/3
30	CLA	13	307	25	1/1/15/20	6/37/115/115	-
30	CLA	15	313	27	-	10/37/115/115	-
30	CLA	8	309	20	-	3/16/94/115	-
30	CLA	A	808	1	1/1/12/20	3/21/99/115	-
30	CLA	4	309	-	1/1/15/20	8/37/115/115	-
30	CLA	B	828	2	1/1/15/20	13/37/115/115	-
37	A86	10	302	-	-	12/34/90/90	0/3/3/3
39	DD6	6	319	-	-	11/26/80/80	0/3/3/3
38	KC1	2	312	14	-	4/15/71/71	-
30	CLA	A	841	1	1/1/15/20	8/37/115/115	-
30	CLA	14	309	26	1/1/11/20	3/13/91/115	-
39	DD6	3	313	-	-	9/26/80/80	0/3/3/3
30	CLA	1	305	40	1/1/15/20	8/37/115/115	-
37	A86	11	316	-	-	13/34/90/90	0/3/3/3
30	CLA	10	303	22	1/1/15/20	12/37/115/115	-
30	CLA	9	306	21,37	1/1/11/20	5/13/91/115	-
30	CLA	L	202	9	1/1/15/20	7/37/115/115	-
30	CLA	12	321	26,24	1/1/15/20	3/37/115/115	-
37	A86	2u	203	30	-	14/34/90/90	0/3/3/3
36	LMG	8	321	36	-	5/24/44/70	0/1/1/1
30	CLA	A	816	1,35	1/1/15/20	17/37/115/115	-
33	BCR	B	846	-	-	7/29/63/63	0/2/2/2
35	LMT	11	302	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	8	313	20	-	5/15/71/71	-
30	CLA	A	819	1	-	6/24/102/115	-
38	KC1	5	306	17	-	10/15/71/71	-
38	KC1	8	306	40	-	8/15/71/71	-
30	CLA	10	308	22	1/1/15/20	11/37/115/115	-
37	A86	8	318	-	-	11/34/90/90	0/3/3/3
38	KC1	10	312	22	-	5/15/71/71	-
30	CLA	A	837	1	1/1/11/20	4/13/91/115	-
39	DD6	8	317	-	-	10/26/80/80	0/3/3/3
35	LMT	11	303	-	-	11/21/61/61	0/2/2/2
32	SF4	A	846	1,2	-	-	0/6/5/5
30	CLA	5	307	17	1/1/15/20	13/37/115/115	-
30	CLA	B	812	2	1/1/15/20	7/37/115/115	-
37	A86	3	314	-	-	8/34/90/90	0/3/3/3
30	CLA	2	311	14	-	9/37/115/115	-
30	CLA	B	838	2	1/1/15/20	15/37/115/115	-
35	LMT	11	318	-	-	1/21/61/61	0/2/2/2
30	CLA	2	310	14	1/1/15/20	6/37/115/115	-
30	CLA	A	815	1	1/1/15/20	7/37/115/115	-
30	CLA	11	310	23	1/1/15/20	15/37/115/115	-
30	CLA	12	306	24	1/1/15/20	5/37/115/115	-
37	A86	6	320	-	-	9/34/90/90	0/3/3/3
37	A86	11	314	-	-	12/34/90/90	0/3/3/3
39	DD6	10	313	-	-	11/26/80/80	0/3/3/3
36	LMG	8	319	20,36	-	17/32/52/70	0/1/1/1
30	CLA	1	301	13	1/1/15/20	13/37/115/115	-
30	CLA	11	309	23	-	15/37/115/115	-
39	DD6	13	314	-	-	13/26/80/80	0/3/3/3
39	DD6	5	313	-	-	9/26/80/80	0/3/3/3
30	CLA	B	823	40	1/1/12/20	3/24/102/115	-
30	CLA	3	309	15	-	4/13/91/115	-
38	KC1	13	310	25	-	5/15/71/71	-
39	DD6	6	318	-	-	11/26/80/80	0/3/3/3
30	CLA	A	820	1	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	833	1	1/1/15/20	13/37/115/115	-
30	CLA	16	307	-	1/1/11/20	3/15/93/115	-
30	CLA	10	311	-	-	6/13/91/115	-
30	CLA	11	308	23	1/1/15/20	10/37/115/115	-
30	CLA	B	802	30,40	1/1/15/20	9/37/115/115	-
30	CLA	15	305	27,37	1/1/11/20	8/13/91/115	-
30	CLA	A	818	1	-	6/24/102/115	-
33	BCR	A	849	-	-	10/29/63/63	0/2/2/2
35	LMT	6	302	-	-	2/17/57/61	0/2/2/2
37	A86	15	322	30	-	15/34/90/90	0/3/3/3
30	CLA	2	313	14	-	3/13/91/115	-
30	CLA	4	311	16	1/1/12/20	0/19/97/115	-
33	BCR	A	850	-	-	11/29/63/63	0/2/2/2
30	CLA	6	305	18	1/1/15/20	5/37/115/115	-
38	KC1	10	306	22	-	8/15/71/71	-
38	KC1	16	311	28	-	6/15/71/71	-
30	CLA	A	814	1	1/1/14/20	9/31/109/115	-
30	CLA	B	833	30,40	1/1/15/20	11/37/115/115	-
37	A86	5	315	-	-	6/34/90/90	0/3/3/3
34	LHG	A	853	30	-	8/31/31/53	-
30	CLA	9	308	21	1/1/15/20	13/37/115/115	-
30	CLA	B	836	2	1/1/11/20	2/16/94/115	-
30	CLA	15	308	27,30	1/1/11/20	8/13/91/115	-
30	CLA	5	309	34	1/1/15/20	9/37/115/115	-
39	DD6	3	316	-	-	12/26/80/80	0/3/3/3
30	CLA	12	307	24	1/1/11/20	4/15/93/115	-
38	KC1	14	308	26,30	-	9/15/71/71	-
38	KC1	11	307	23	-	10/15/71/71	-
30	CLA	6	310	34	1/1/15/20	8/37/115/115	-
30	CLA	B	805	2	1/1/15/20	9/37/115/115	-
30	CLA	A	810	1	1/1/15/20	11/37/115/115	-
30	CLA	15	307	27	1/1/12/20	6/19/97/115	-
34	LHG	B	848	30	-	18/31/31/53	-
38	KC1	4	308	16	-	2/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	13	312	25	-	6/15/71/71	-
38	KC1	5	310	17	-	6/15/71/71	-
37	A86	10	301	22	-	6/34/90/90	0/3/3/3
30	CLA	5	308	17	-	13/37/115/115	-
37	A86	14	316	-	-	10/34/90/90	0/3/3/3
30	CLA	2	305	40	1/1/15/20	10/37/115/115	-
38	KC1	7	313	-	-	4/15/71/71	-
30	CLA	B	827	2	1/1/15/20	5/37/115/115	-
30	CLA	8	304	20	1/1/13/20	8/29/107/115	-
37	A86	15	317	30	-	15/34/90/90	0/3/3/3
30	CLA	2u	202	12	1/1/15/20	13/37/115/115	-
30	CLA	B	816	2	-	7/25/103/115	-
39	DD6	9	314	-	-	12/26/80/80	0/3/3/3
30	CLA	B	826	2	1/1/15/20	14/37/115/115	-
37	A86	15	323	-	-	16/34/90/90	0/3/3/3
37	A86	4	312	-	-	9/34/90/90	0/3/3/3
30	CLA	A	822	40	1/1/15/20	7/37/115/115	-
30	CLA	16	306	28	1/1/12/20	13/22/100/115	-
30	CLA	16	305	28	1/1/12/20	2/19/97/115	-
38	KC1	3	304	15	-	5/15/71/71	-
35	LMT	A	857	-	-	2/21/61/61	0/2/2/2
35	LMT	A	854	-	-	16/21/61/61	0/2/2/2
30	CLA	14	303	26	1/1/13/20	8/28/106/115	-
30	CLA	10	305	40	1/1/15/20	9/37/115/115	-
30	CLA	5	304	17	1/1/15/20	11/37/115/115	-
35	LMT	12	319	-	-	0/21/61/61	0/2/2/2
37	A86	9	316	30	-	9/34/90/90	0/3/3/3
30	CLA	13	302	25	1/1/15/20	14/37/115/115	-
30	CLA	13	309	-	1/1/11/20	7/13/91/115	-
34	LHG	2	320	30	-	12/31/31/53	-
30	CLA	2	309	14,34	1/1/15/20	9/37/115/115	-
30	CLA	B	806	2	1/1/15/20	7/37/115/115	-
38	KC1	6	312	18	-	5/15/71/71	-
30	CLA	A	842	1	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	4	306	16	1/1/15/20	10/37/115/115	-
33	BCR	J	102	-	-	10/29/63/63	0/2/2/2
37	A86	4	315	-	-	5/34/90/90	0/3/3/3
30	CLA	12	308	40	1/1/15/20	11/37/115/115	-
30	CLA	B	810	2	1/1/15/20	7/37/115/115	-
36	LMG	14	321	-	-	13/33/53/70	0/1/1/1
37	A86	14	319	30	-	10/34/90/90	0/3/3/3
30	CLA	8	305	20	-	13/37/115/115	-
31	PQN	A	845	-	-	6/23/43/43	0/2/2/2
38	KC1	8	310	20	-	8/15/71/71	-
37	A86	10	315	-	-	13/34/90/90	0/3/3/3
37	A86	16	314	-	-	10/34/90/90	0/3/3/3
36	LMG	B	847	-	-	25/50/70/70	0/1/1/1
30	CLA	14	302	26	1/1/15/20	10/37/115/115	-
37	A86	14	320	-	-	10/34/90/90	0/3/3/3
30	CLA	6	316	40	1/1/13/20	7/25/103/115	-
30	CLA	9	307	21	1/1/15/20	9/37/115/115	-
30	CLA	15	303	27,37,30	1/1/14/20	8/31/109/115	-
30	CLA	A	832	1	-	4/19/97/115	-
30	CLA	B	818	2	1/1/14/20	5/31/109/115	-
30	CLA	B	830	2	1/1/15/20	10/37/115/115	-
38	KC1	11	312	-	-	5/15/71/71	-
30	CLA	2	308	14	-	8/37/115/115	-
33	BCR	2u	201	-	-	11/29/63/63	0/2/2/2
30	CLA	A	821	1	1/1/14/20	9/33/111/115	-
33	BCR	B	842	-	-	8/29/63/63	0/2/2/2
33	BCR	L	205	-	-	8/29/63/63	0/2/2/2
37	A86	16	312	28	-	14/34/90/90	0/3/3/3
30	CLA	A	805	1,30	1/1/13/20	9/30/108/115	-
33	BCR	B	845	-	-	11/29/63/63	0/2/2/2
30	CLA	A	802	40	1/1/15/20	7/37/115/115	-
33	BCR	A	847	-	-	10/29/63/63	0/2/2/2
38	KC1	2	306	14	-	5/15/71/71	-
35	LMT	7	321	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	12	303	24	1/1/15/20	6/37/115/115	-
33	BCR	M	101	-	-	10/29/63/63	0/2/2/2
30	CLA	B	809	2	1/1/15/20	10/37/115/115	-
33	BCR	A	848	-	-	10/29/63/63	0/2/2/2
38	KC1	9	310	21	-	6/15/71/71	-
39	DD6	12	317	-	-	13/26/80/80	0/3/3/3
30	CLA	A	803	-	1/1/15/20	7/37/115/115	-
37	A86	4	317	-	-	5/34/90/90	0/3/3/3
37	A86	7	319	-	-	10/34/90/90	0/3/3/3
30	CLA	11	306	40	1/1/13/20	8/25/103/115	-
30	CLA	A	827	40	1/1/15/20	3/37/115/115	-
30	CLA	11	304	23	1/1/15/20	9/37/115/115	-
39	DD6	15	318	-	-	13/26/80/80	0/3/3/3
36	LMG	7	320	-	-	14/32/52/70	0/1/1/1
39	DD6	6	303	30	-	10/26/80/80	0/3/3/3
38	KC1	5	312	17	-	6/15/71/71	-
37	A86	1	309	-	-	7/34/90/90	0/3/3/3
30	CLA	12	302	24	-	13/37/115/115	-
37	A86	15	316	30	-	13/34/90/90	0/3/3/3
30	CLA	15	310	27	1/1/11/20	6/13/91/115	-
39	DD6	7	317	-	-	10/26/80/80	0/3/3/3

The worst 5 of 6801 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	322	A86	C14-C13	16.41	1.69	1.51
37	15	315	A86	C14-C13	16.01	1.69	1.51
37	9	313	A86	C14-C13	15.74	1.68	1.51
37	16	314	A86	C14-C13	15.70	1.68	1.51
37	10	317	A86	C14-C13	15.54	1.68	1.51

The worst 5 of 9694 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	14	315	A86	O1-C20-C19	46.49	157.06	113.49
37	14	317	A86	O1-C20-C19	45.77	156.39	113.49
37	15	321	A86	O1-C20-C19	45.61	156.24	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	8	318	A86	O1-C20-C19	45.45	156.09	113.49
37	4	312	A86	O1-C20-C19	45.21	155.87	113.49

5 of 185 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	801	CL0	NA
29	A	801	CL0	NC
29	A	801	CL0	ND
30	A	802	CLA	ND
30	A	803	CLA	ND

5 of 3749 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	804	CLA	C3A-C2A-CAA-CBA
30	A	806	CLA	C1A-C2A-CAA-CBA
30	A	806	CLA	C3A-C2A-CAA-CBA
30	A	807	CLA	C1A-C2A-CAA-CBA
30	A	807	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

235 monomers are involved in 440 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	F	201	CLA	6	0
30	B	837	CLA	2	0
30	7	311	CLA	2	0
36	6	301	LMG	1	0
33	L	201	BCR	2	0
30	A	817	CLA	3	0
30	A	840	CLA	1	0
30	A	824	CLA	1	0
30	1	302	CLA	3	0
30	A	831	CLA	5	0
30	B	804	CLA	2	0
37	8	315	A86	1	0
30	B	808	CLA	2	0
30	B	803	CLA	1	0
30	5	302	CLA	3	0
30	A	812	CLA	4	0
30	4	302	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	2	303	CLA	4	0
30	3	305	CLA	1	0
30	5	303	CLA	4	0
30	7	309	CLA	6	0
38	4	310	KC1	1	0
30	A	813	CLA	3	0
30	2	301	CLA	1	0
30	10	307	CLA	1	0
30	9	305	CLA	2	0
30	A	844	CLA	1	0
30	8	308	CLA	1	0
33	F	204	BCR	3	0
36	3	317	LMG	2	0
30	3	310	CLA	2	0
30	2	307	CLA	3	0
30	6	307	CLA	1	0
30	15	309	CLA	2	0
35	11	317	LMT	2	0
30	16	301	CLA	6	0
36	B	849	LMG	1	0
30	B	825	CLA	1	0
30	B	817	CLA	5	0
30	13	301	CLA	5	0
30	A	804	CLA	4	0
30	J	101	CLA	1	0
30	7	306	CLA	3	0
33	I	101	BCR	2	0
30	A	806	CLA	5	0
30	B	801	CLA	4	0
37	7	315	A86	1	0
30	16	302	CLA	1	0
30	16	303	CLA	1	0
30	B	839	CLA	3	0
31	B	840	PQN	1	0
35	A	855	LMT	2	0
30	10	304	CLA	1	0
30	7	303	CLA	1	0
33	B	843	BCR	2	0
37	11	315	A86	1	0
30	16	310	CLA	1	0
30	B	807	CLA	2	0
33	A	851	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	824	CLA	3	0
30	14	305	CLA	1	0
30	A	830	CLA	4	0
30	B	813	CLA	7	0
30	B	831	CLA	2	0
33	B	841	BCR	1	0
30	A	835	CLA	2	0
30	A	839	CLA	6	0
30	14	312	CLA	1	0
30	10	309	CLA	2	0
30	6	314	CLA	2	0
30	3	302	CLA	1	0
30	B	851	CLA	1	0
30	3	303	CLA	2	0
30	16	309	CLA	1	0
30	9	301	CLA	1	0
30	14	307	CLA	1	0
30	6	309	CLA	3	0
30	A	809	CLA	1	0
30	B	815	CLA	2	0
30	F	202	CLA	3	0
30	9	302	CLA	1	0
30	A	834	CLA	2	0
30	A	826	CLA	4	0
30	1	307	CLA	2	0
30	7	307	CLA	2	0
36	A	856	LMG	2	0
30	A	811	CLA	3	0
30	3	306	CLA	2	0
29	A	801	CL0	3	0
33	L	204	BCR	4	0
30	A	843	CLA	2	0
30	8	301	CLA	1	0
30	4	301	CLA	3	0
38	16	304	KC1	1	0
33	J	103	BCR	4	0
30	A	829	CLA	10	0
30	B	822	CLA	2	0
30	8	302	CLA	2	0
30	8	303	CLA	2	0
30	B	820	CLA	2	0
30	12	312	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	15	304	CLA	2	0
30	7	304	CLA	1	0
39	6	321	DD6	1	0
30	12	310	CLA	2	0
30	A	828	CLA	2	0
33	B	844	BCR	2	0
30	L	203	CLA	2	0
30	A	836	CLA	3	0
30	6	306	CLA	2	0
30	B	811	CLA	4	0
38	12	309	KC1	1	0
37	14	317	A86	1	0
30	B	819	CLA	2	0
30	2	304	CLA	1	0
34	A	852	LHG	1	0
30	B	834	CLA	2	0
35	12	320	LMT	1	0
30	A	838	CLA	1	0
30	A	807	CLA	2	0
30	15	302	CLA	4	0
35	12	301	LMT	2	0
30	3	301	CLA	1	0
30	A	823	CLA	1	0
35	7	301	LMT	1	0
30	1	304	CLA	2	0
30	1	303	CLA	3	0
34	5	317	LHG	1	0
30	B	835	CLA	4	0
30	B	821	CLA	2	0
30	4	305	CLA	1	0
30	13	307	CLA	4	0
30	15	313	CLA	4	0
30	4	309	CLA	1	0
30	B	828	CLA	5	0
39	6	319	DD6	1	0
30	A	841	CLA	2	0
37	11	316	A86	1	0
30	10	303	CLA	3	0
30	9	306	CLA	2	0
30	L	202	CLA	5	0
30	12	321	CLA	2	0
36	8	321	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	816	CLA	4	0
33	B	846	BCR	4	0
30	A	819	CLA	3	0
30	10	308	CLA	1	0
30	A	837	CLA	1	0
35	11	303	LMT	1	0
30	5	307	CLA	2	0
30	B	812	CLA	2	0
30	2	311	CLA	1	0
30	B	838	CLA	7	0
35	11	318	LMT	2	0
30	2	310	CLA	1	0
30	11	310	CLA	4	0
39	10	313	DD6	1	0
36	8	319	LMG	1	0
30	1	301	CLA	2	0
39	13	314	DD6	1	0
30	B	823	CLA	1	0
39	6	318	DD6	1	0
30	A	820	CLA	6	0
30	A	833	CLA	6	0
30	16	307	CLA	2	0
30	11	308	CLA	2	0
30	B	802	CLA	2	0
30	A	818	CLA	1	0
33	A	849	BCR	4	0
35	6	302	LMT	2	0
30	4	311	CLA	2	0
33	A	850	BCR	2	0
30	A	814	CLA	3	0
30	B	833	CLA	1	0
37	5	315	A86	1	0
34	A	853	LHG	1	0
30	9	308	CLA	2	0
30	B	836	CLA	4	0
30	15	308	CLA	1	0
30	B	805	CLA	2	0
30	A	810	CLA	5	0
30	15	307	CLA	1	0
38	5	310	KC1	1	0
30	5	308	CLA	2	0
30	2	305	CLA	2	0

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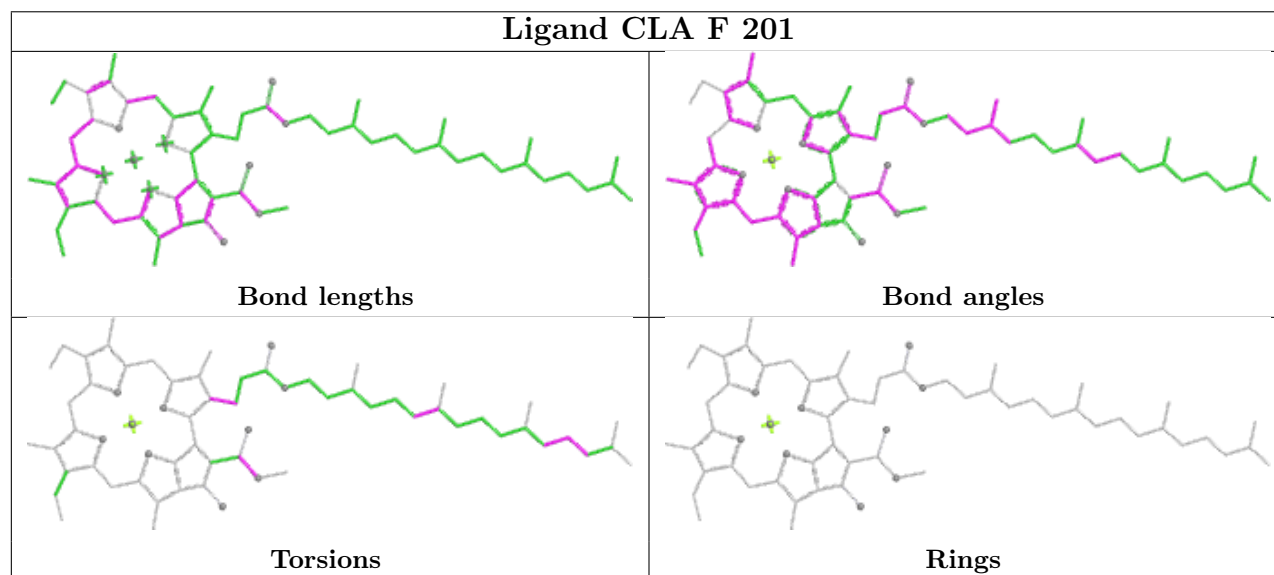
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	827	CLA	5	0
30	B	816	CLA	2	0
30	B	826	CLA	5	0
30	A	822	CLA	3	0
30	16	306	CLA	1	0
38	3	304	KC1	1	0
35	A	857	LMT	1	0
30	14	303	CLA	3	0
30	10	305	CLA	1	0
30	5	304	CLA	2	0
35	12	319	LMT	1	0
37	9	316	A86	1	0
30	13	302	CLA	3	0
30	2	309	CLA	2	0
30	B	806	CLA	7	0
30	A	842	CLA	4	0
30	4	306	CLA	6	0
33	J	102	BCR	3	0
37	4	315	A86	1	0
30	12	308	CLA	4	0
36	14	321	LMG	2	0
30	8	305	CLA	2	0
31	A	845	PQN	5	0
36	B	847	LMG	2	0
30	14	302	CLA	2	0
37	14	320	A86	1	0
30	6	316	CLA	5	0
30	9	307	CLA	4	0
30	15	303	CLA	3	0
30	A	832	CLA	1	0
30	B	818	CLA	1	0
30	B	830	CLA	2	0
30	2	308	CLA	1	0
30	A	821	CLA	2	0
33	B	842	BCR	1	0
33	L	205	BCR	4	0
30	A	805	CLA	3	0
33	B	845	BCR	2	0
30	A	802	CLA	3	0
33	A	847	BCR	3	0
35	7	321	LMT	1	0
30	12	303	CLA	2	0

*Continued on next page...*

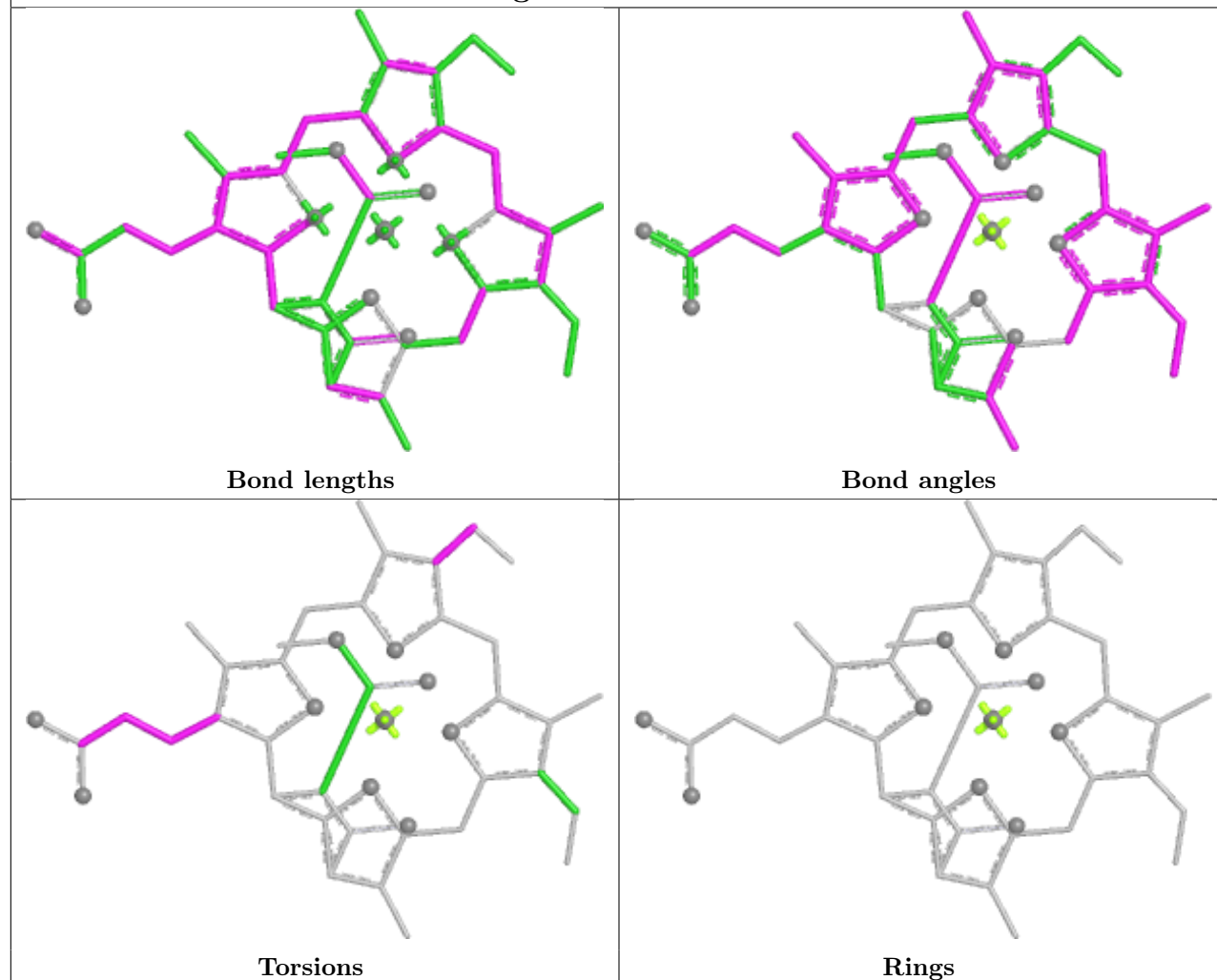
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	M	101	BCR	3	0
30	B	809	CLA	7	0
33	A	848	BCR	2	0
30	A	803	CLA	2	0
30	11	306	CLA	2	0
30	11	304	CLA	3	0
38	5	312	KC1	1	0
30	12	302	CLA	1	0

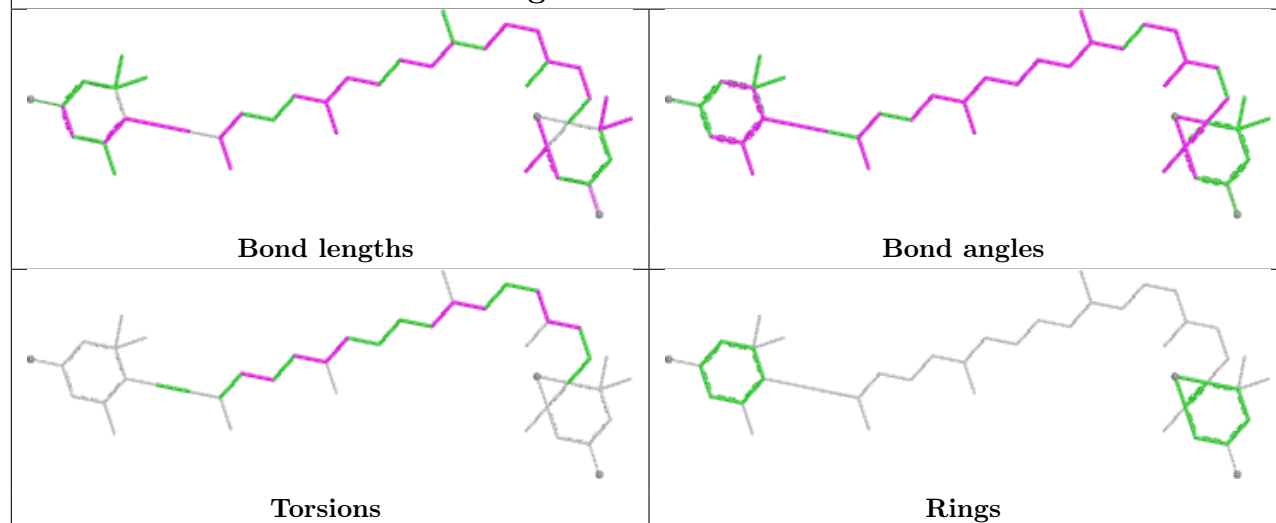
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

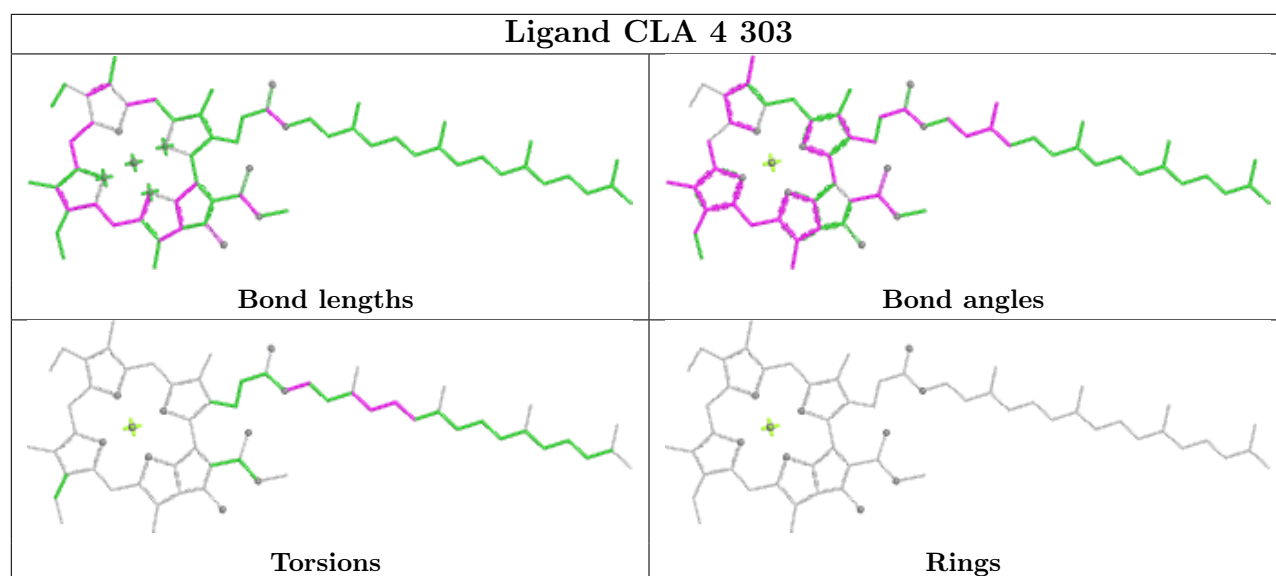
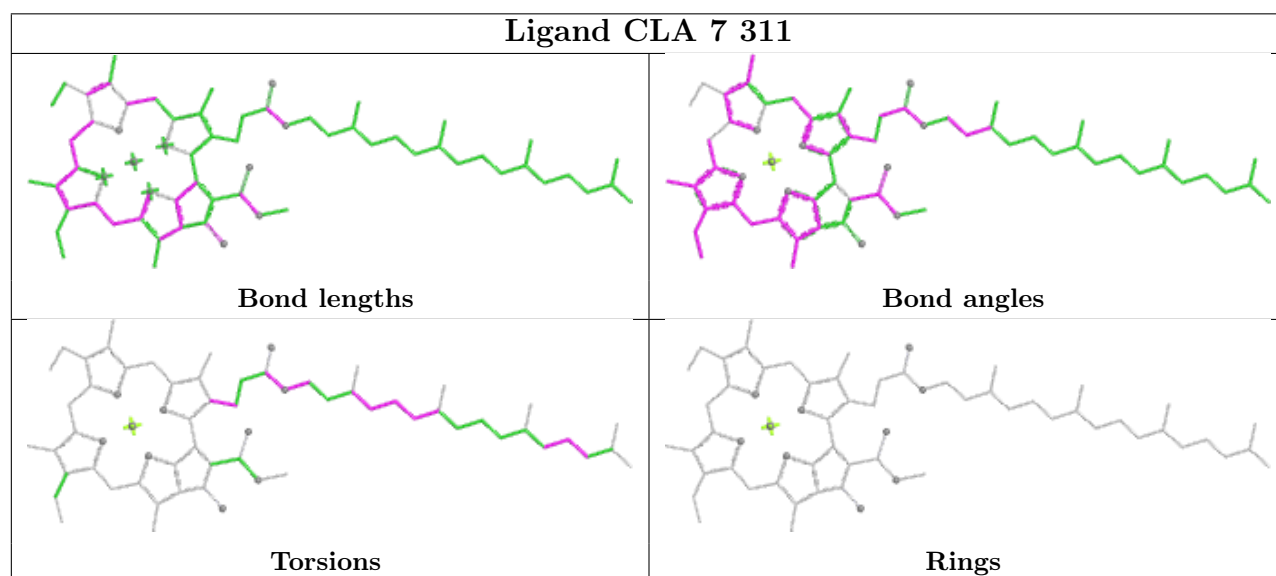
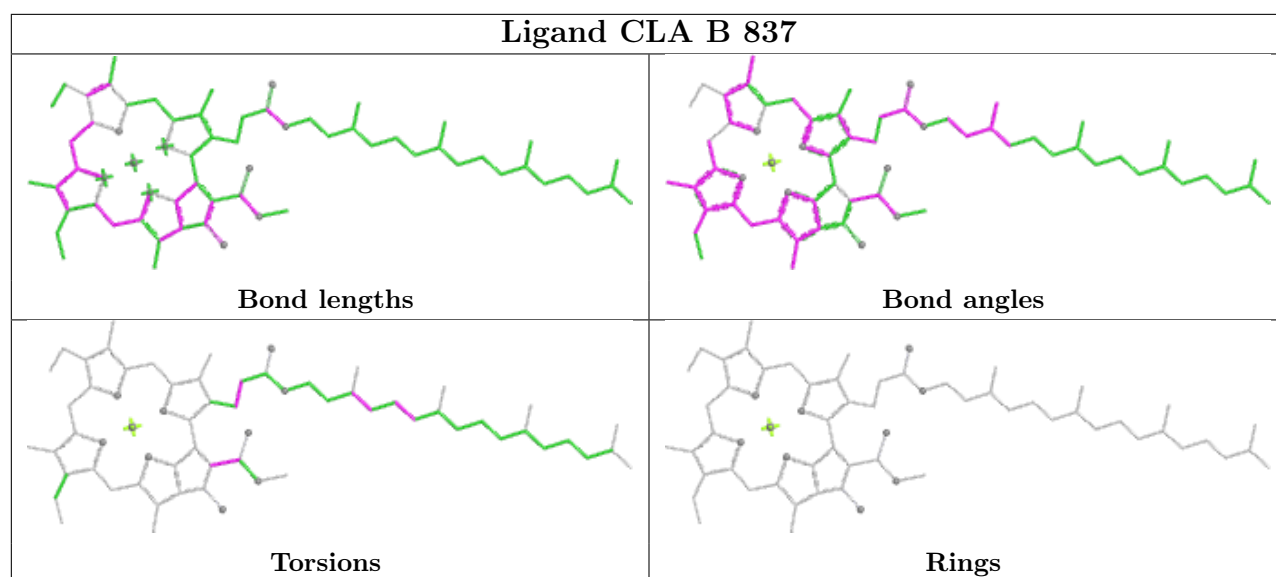


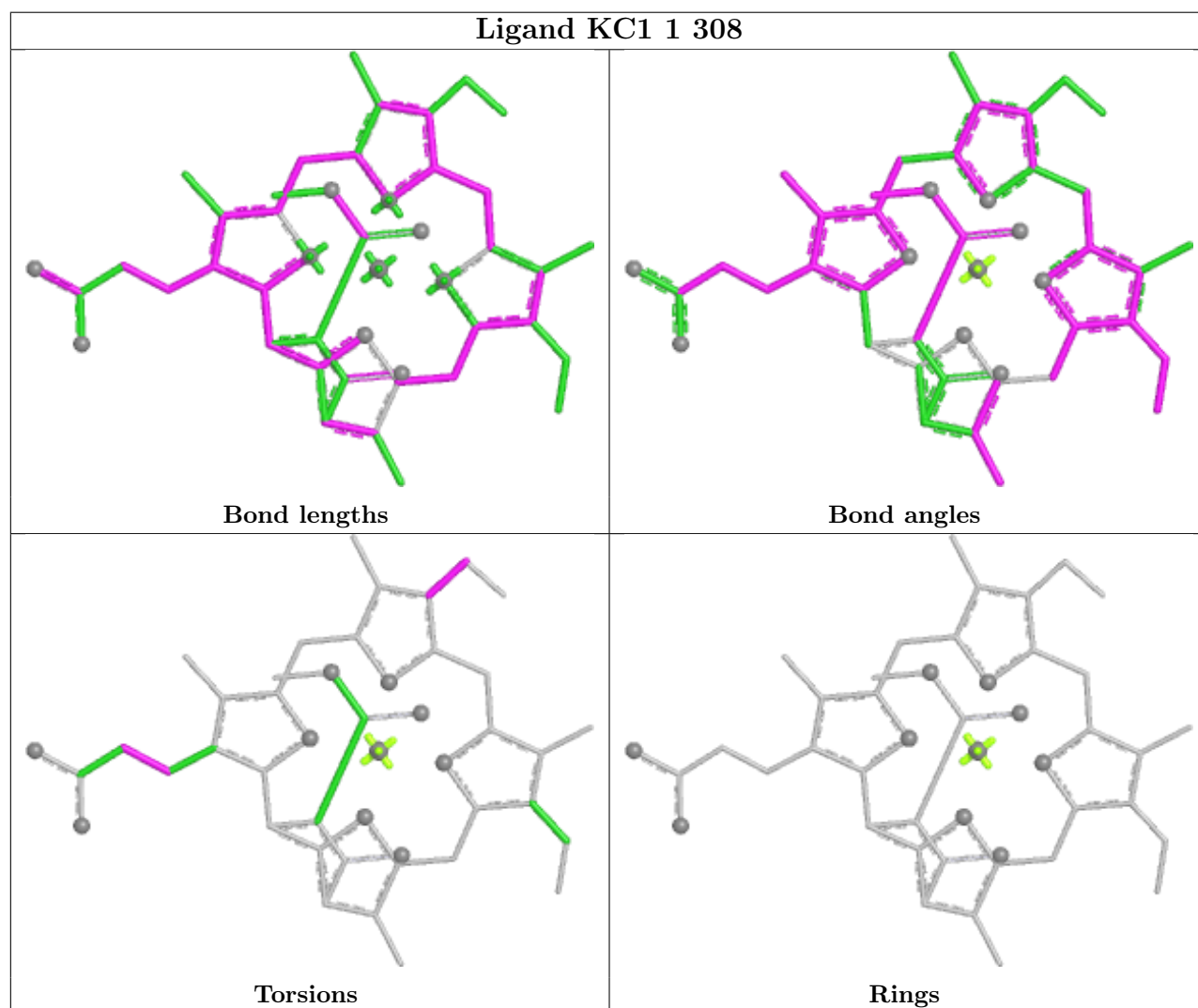
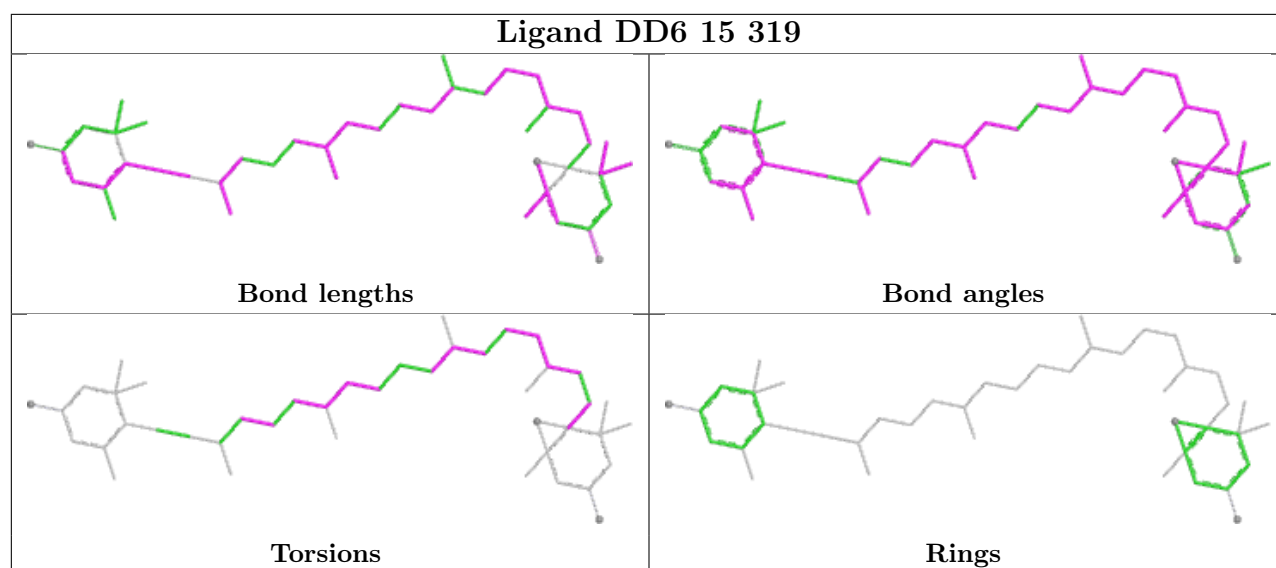
## Ligand KC1 6 308



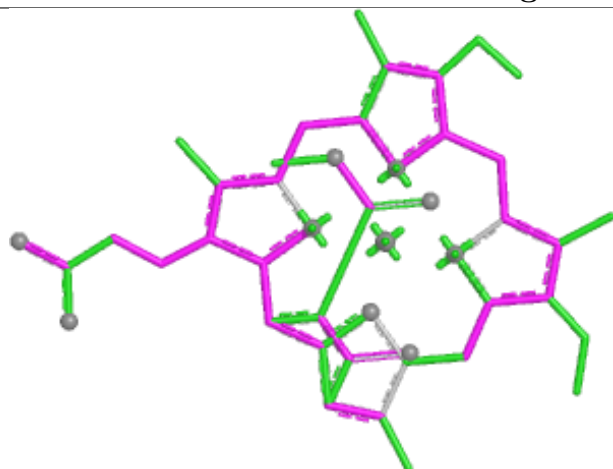
## Ligand DD6 12 315



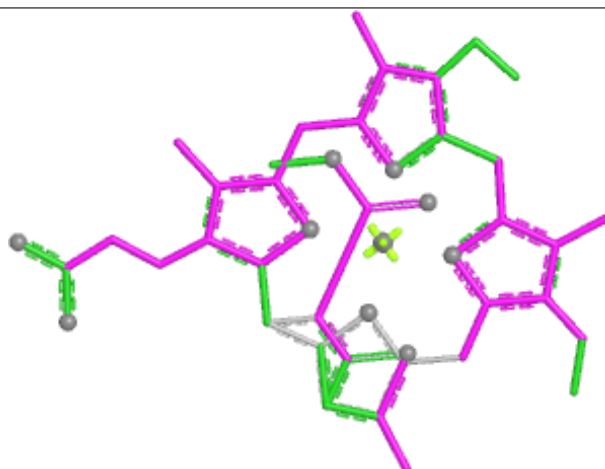




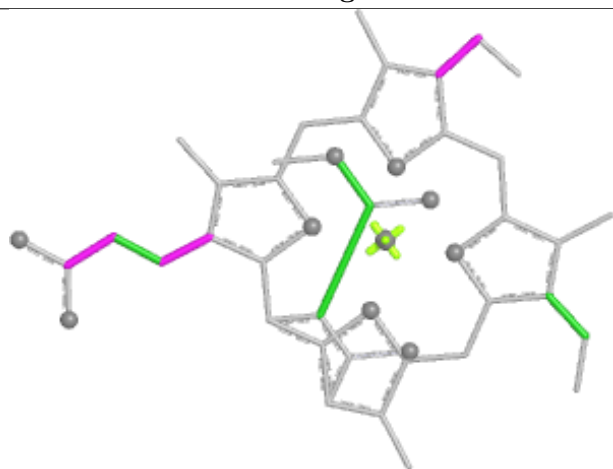
## Ligand KC1 8 314



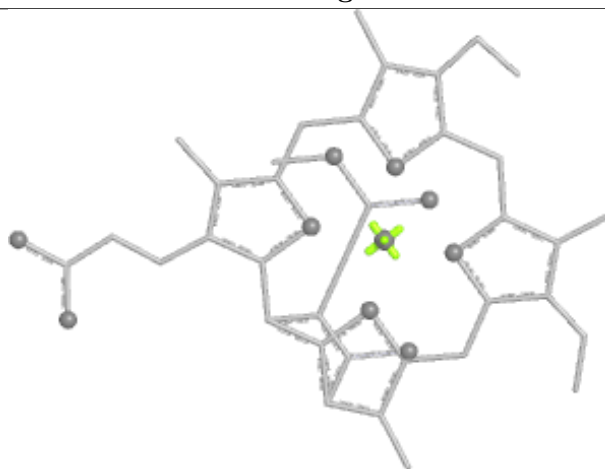
Bond lengths



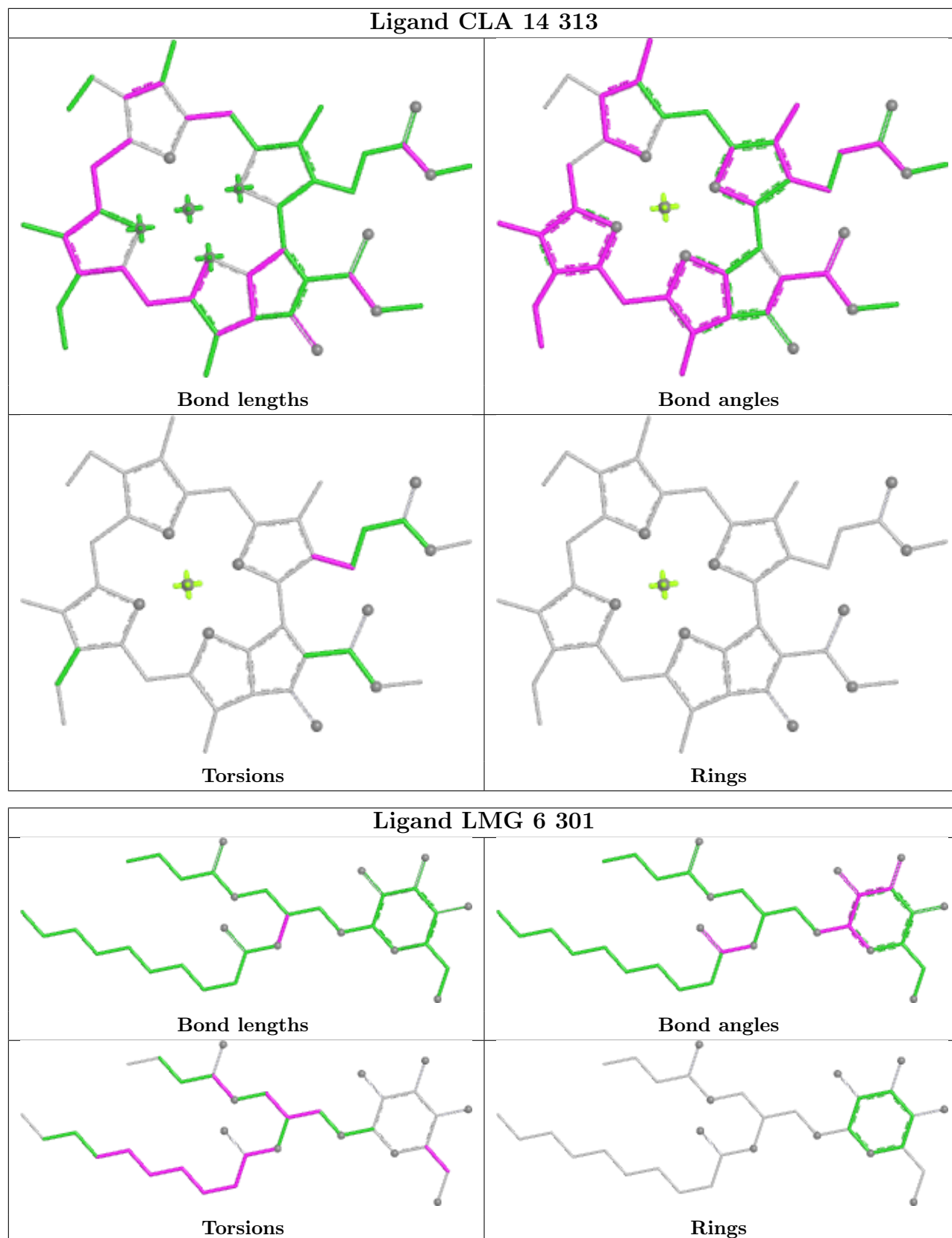
Bond angles

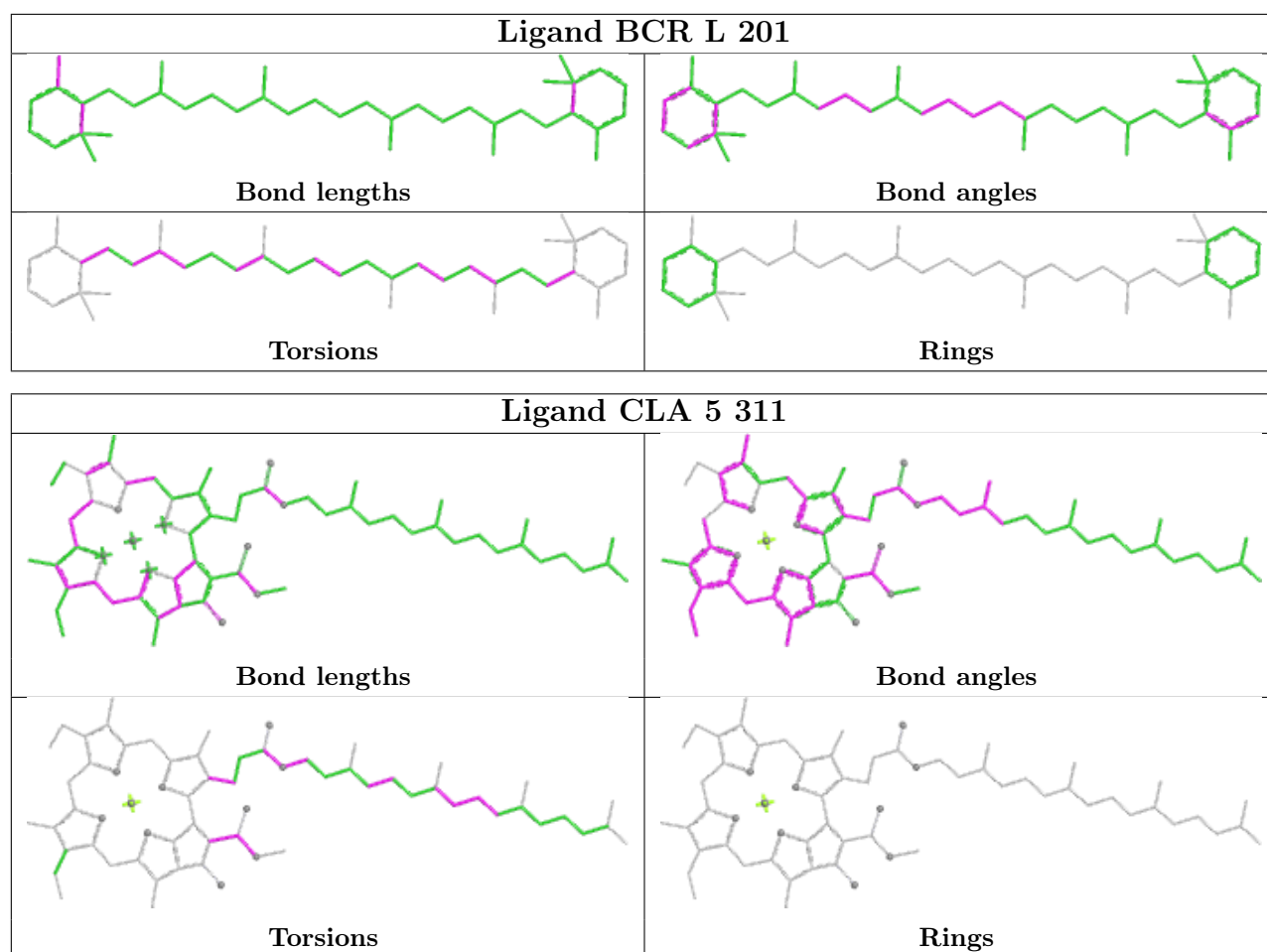


Torsions

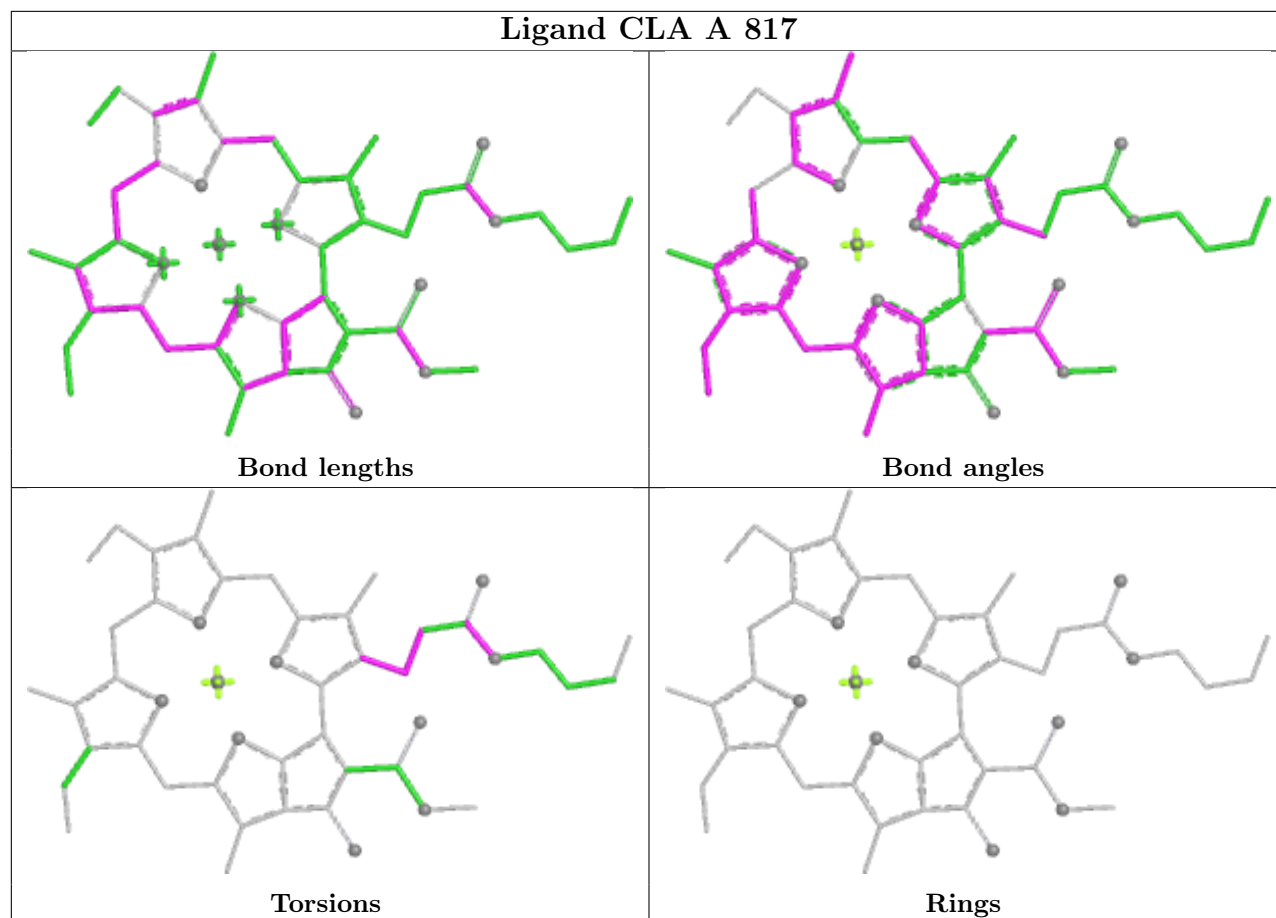


Rings

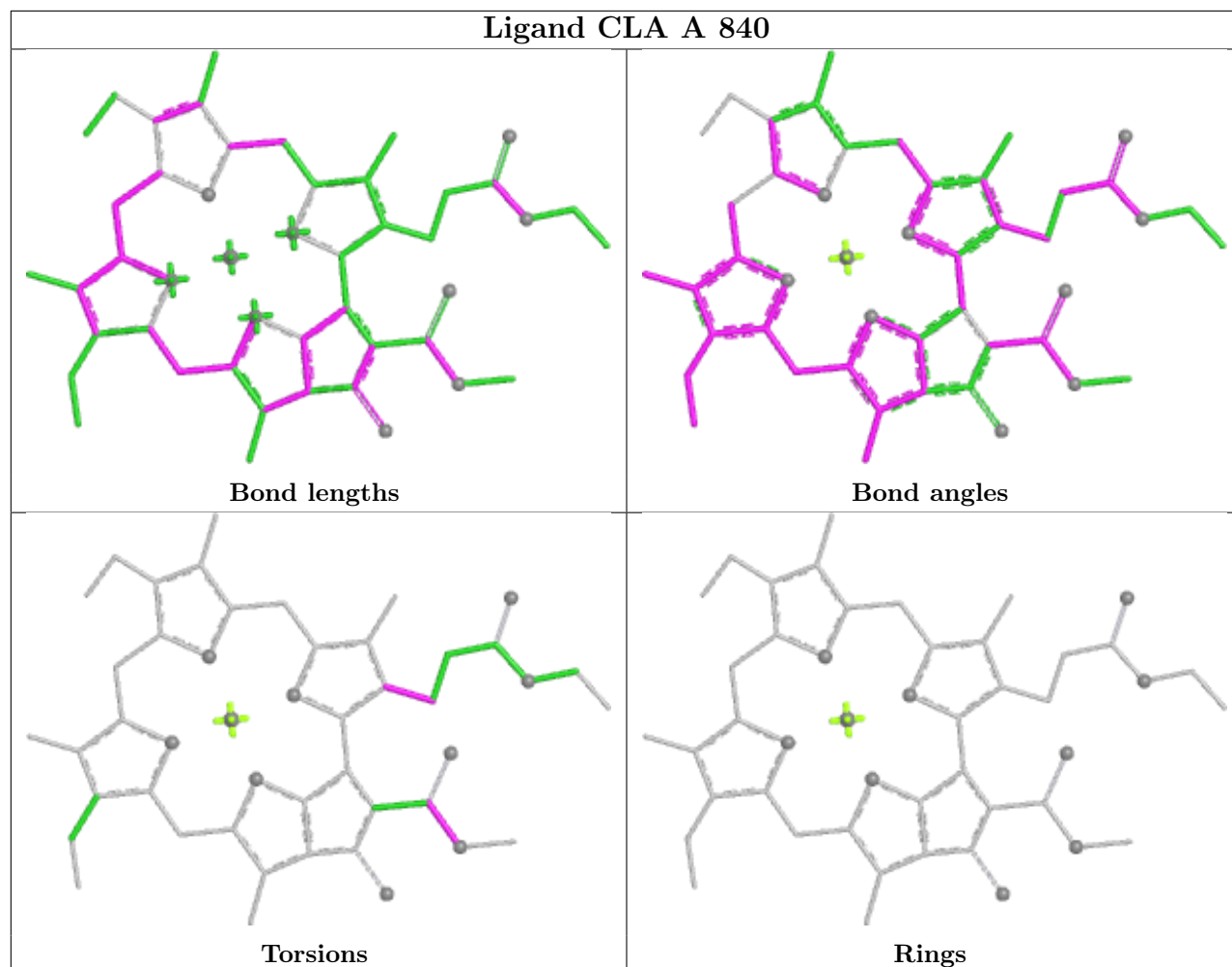


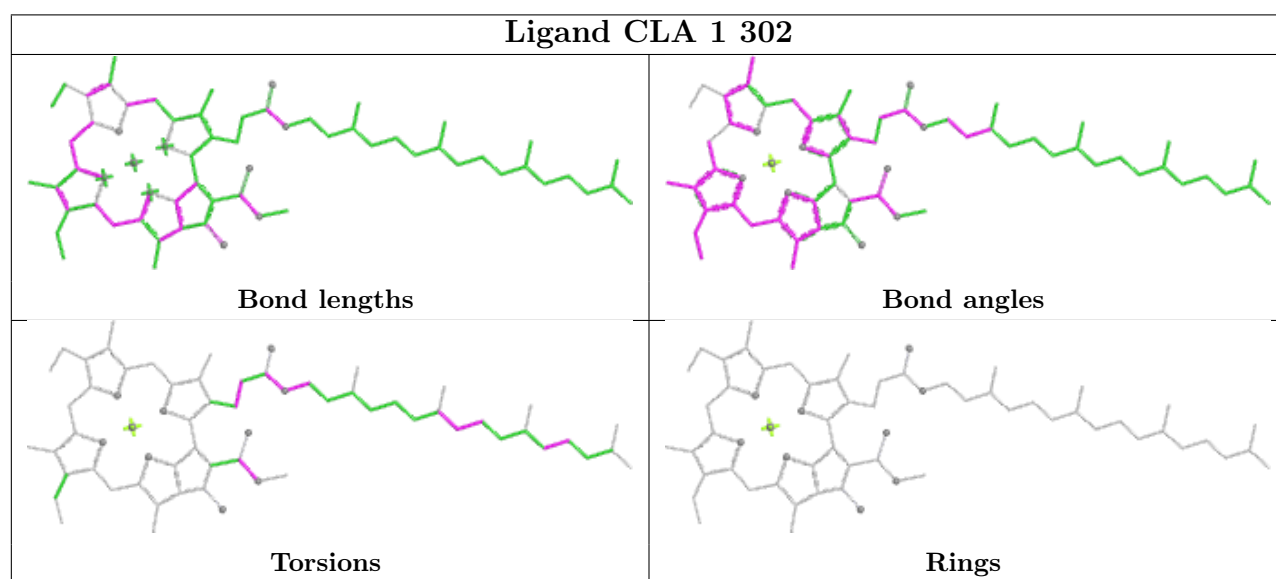
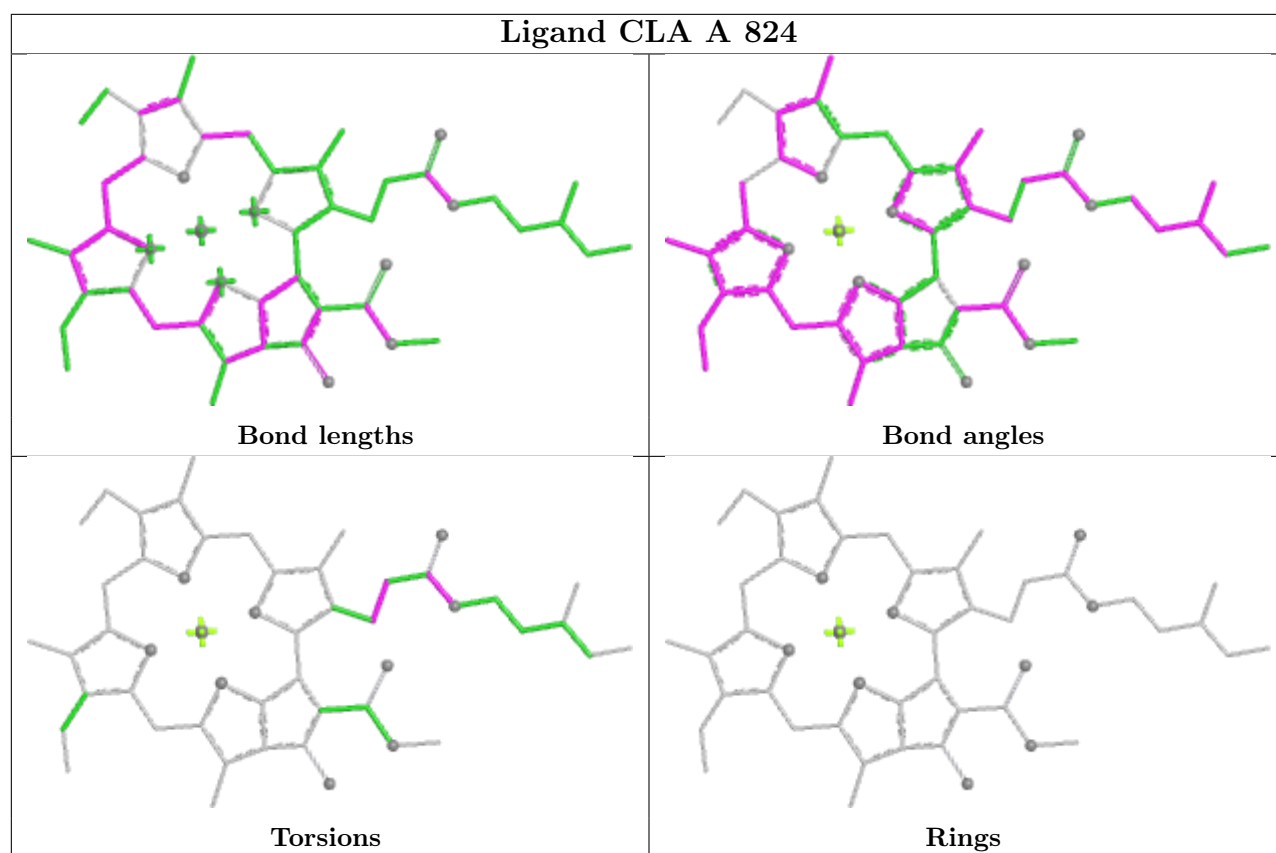


## Ligand CLA A 817

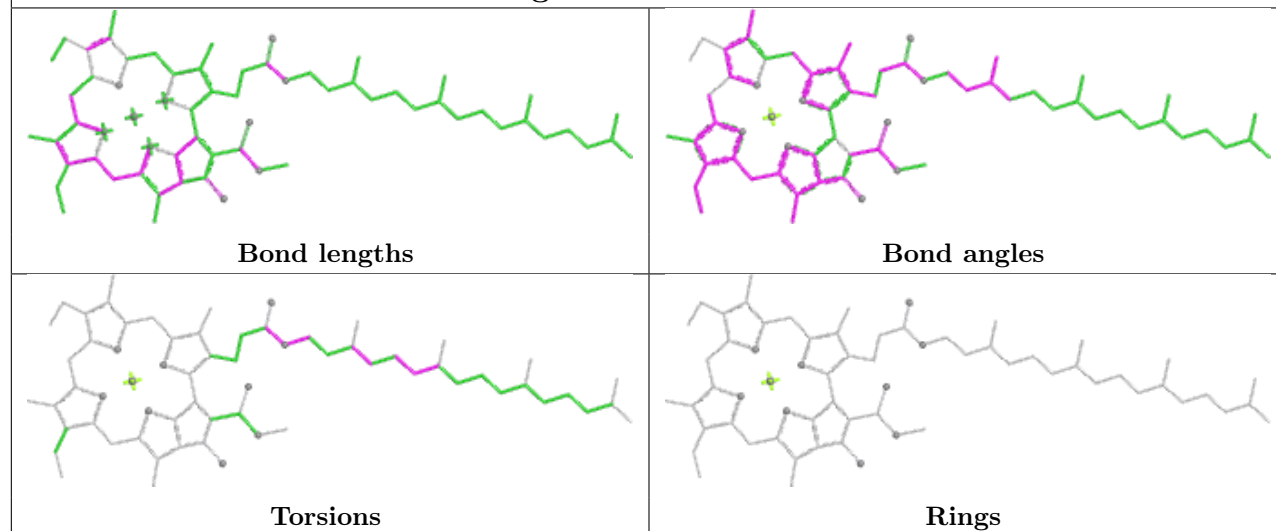


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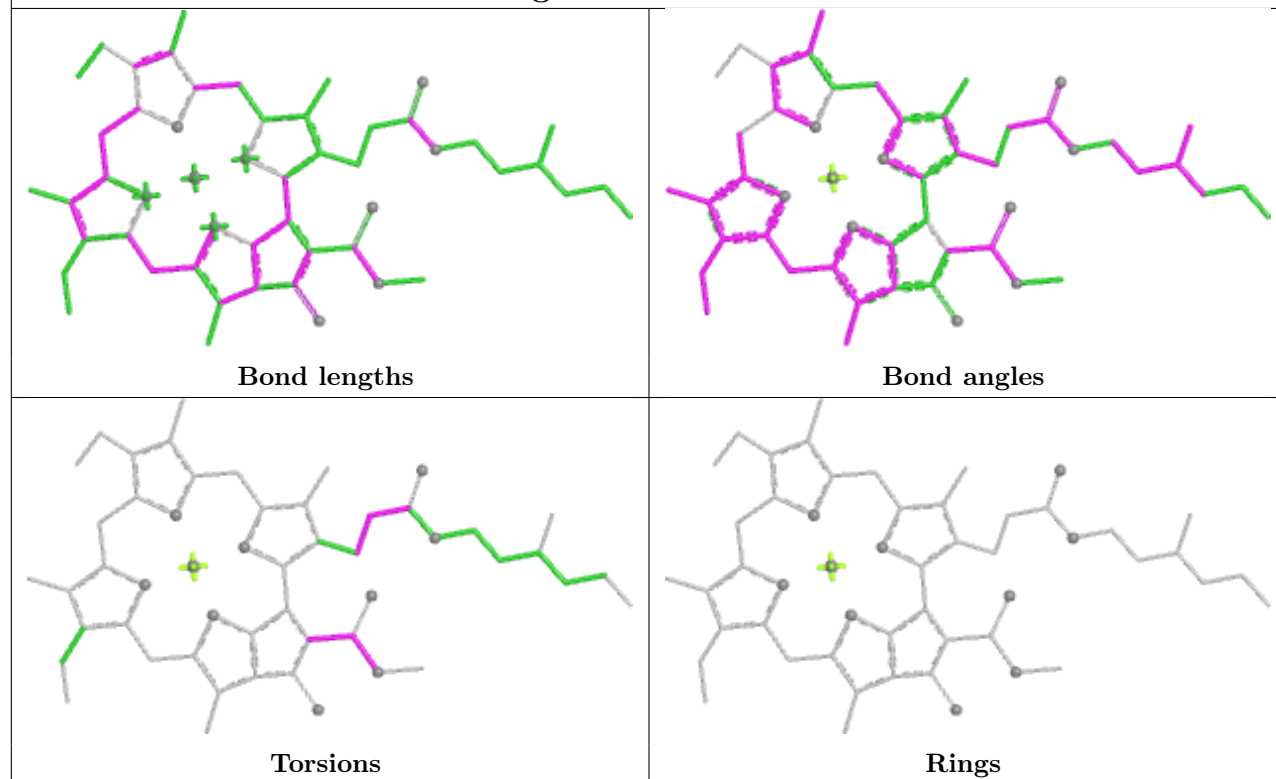


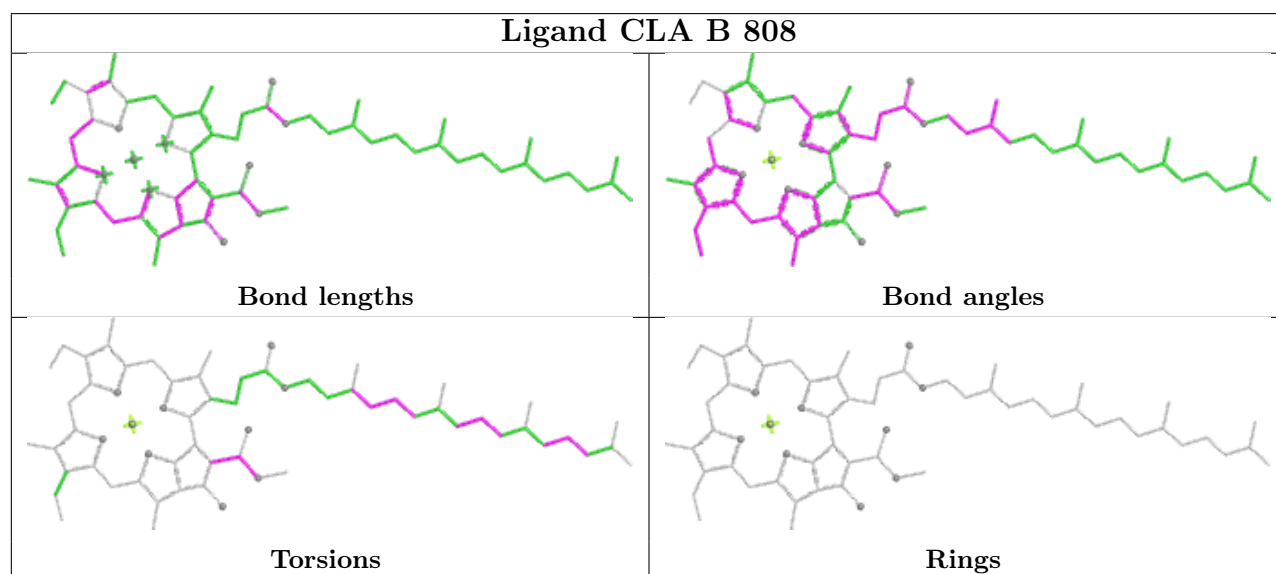
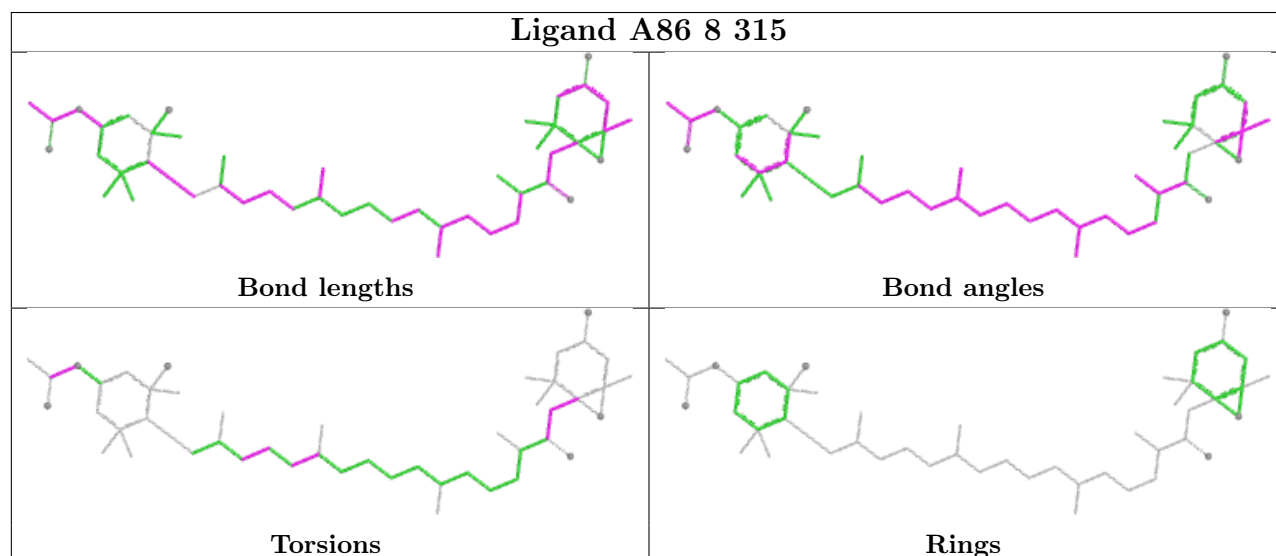
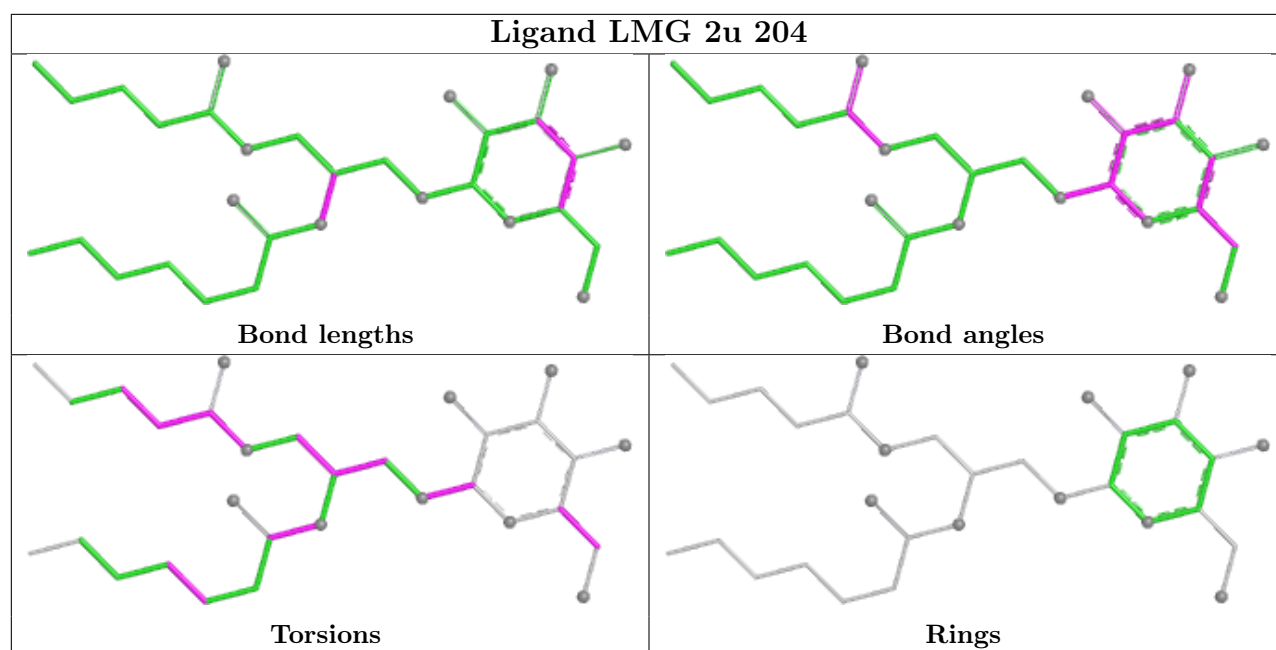


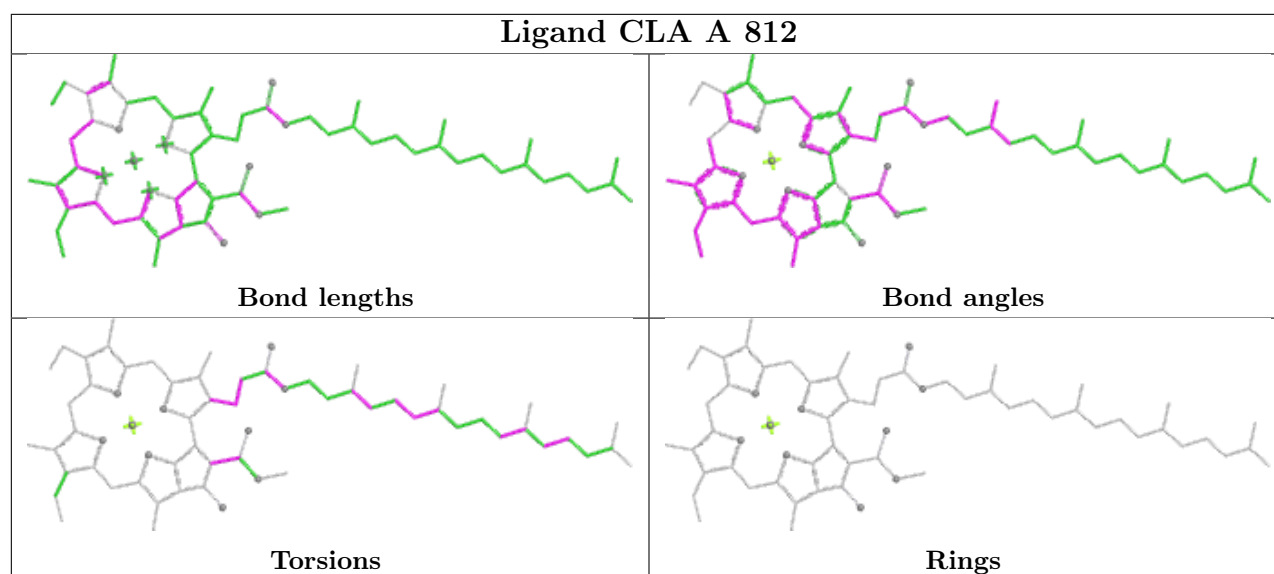
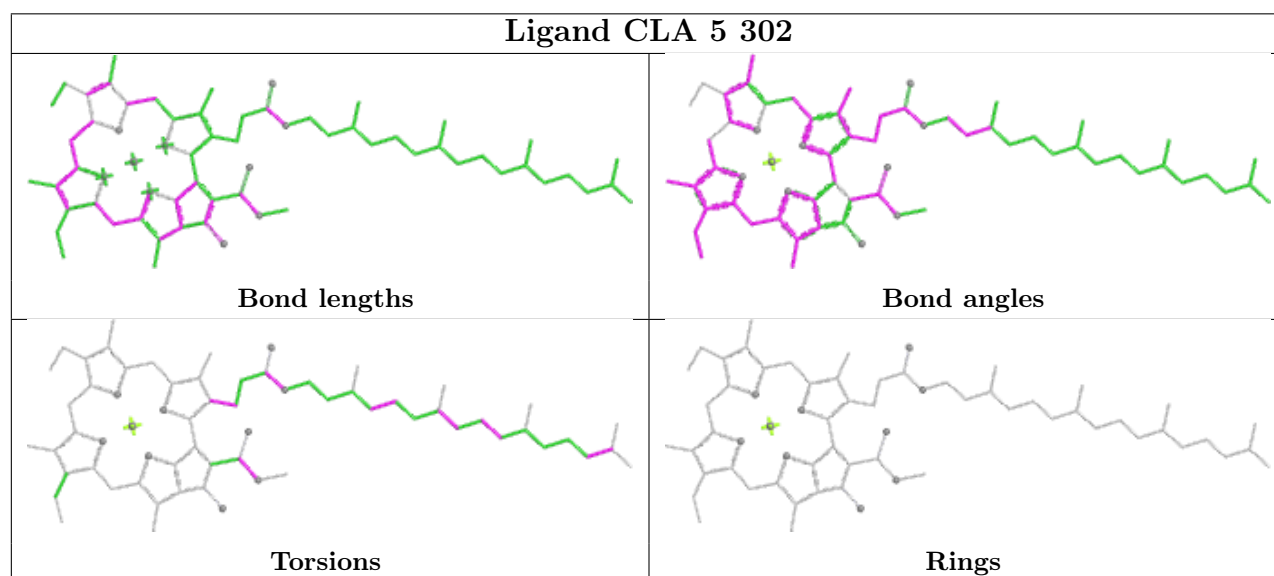
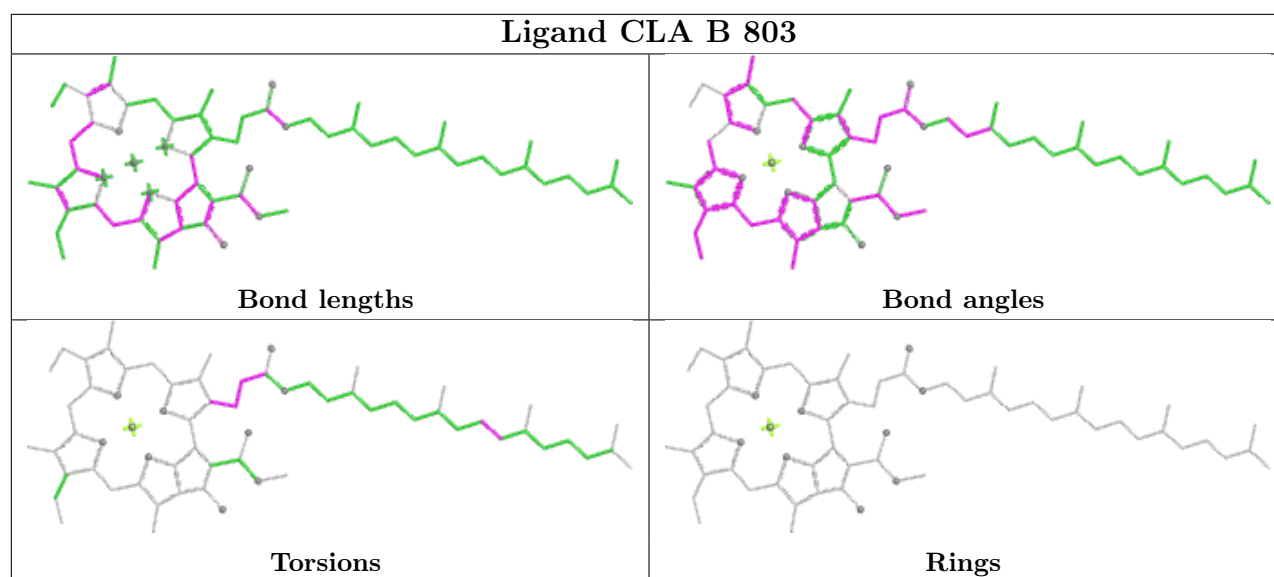
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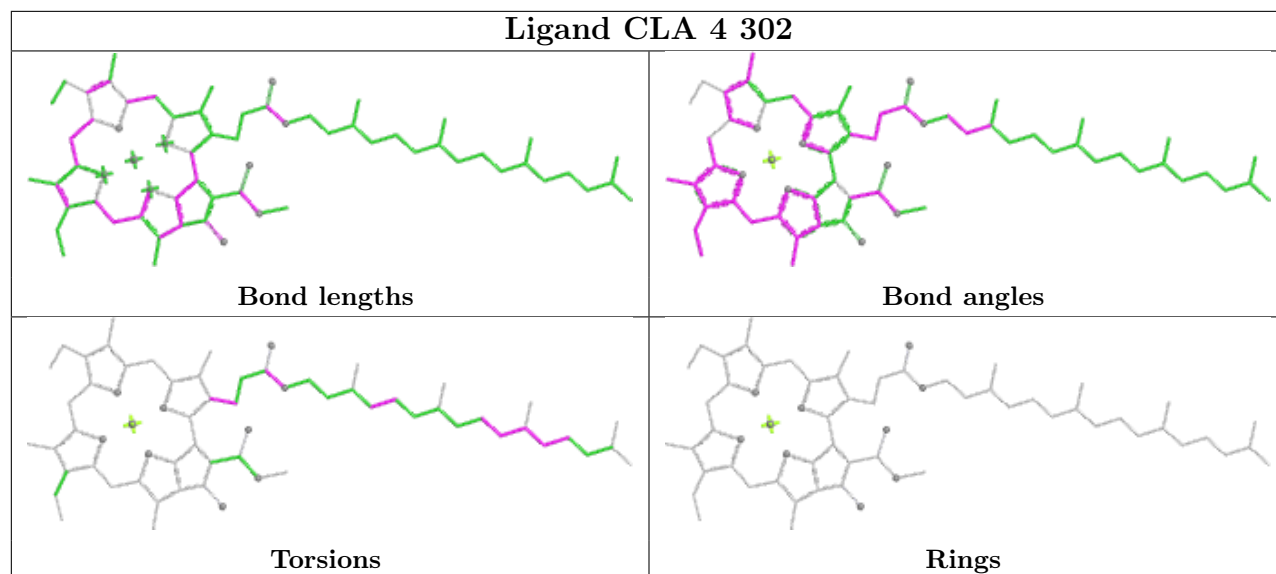
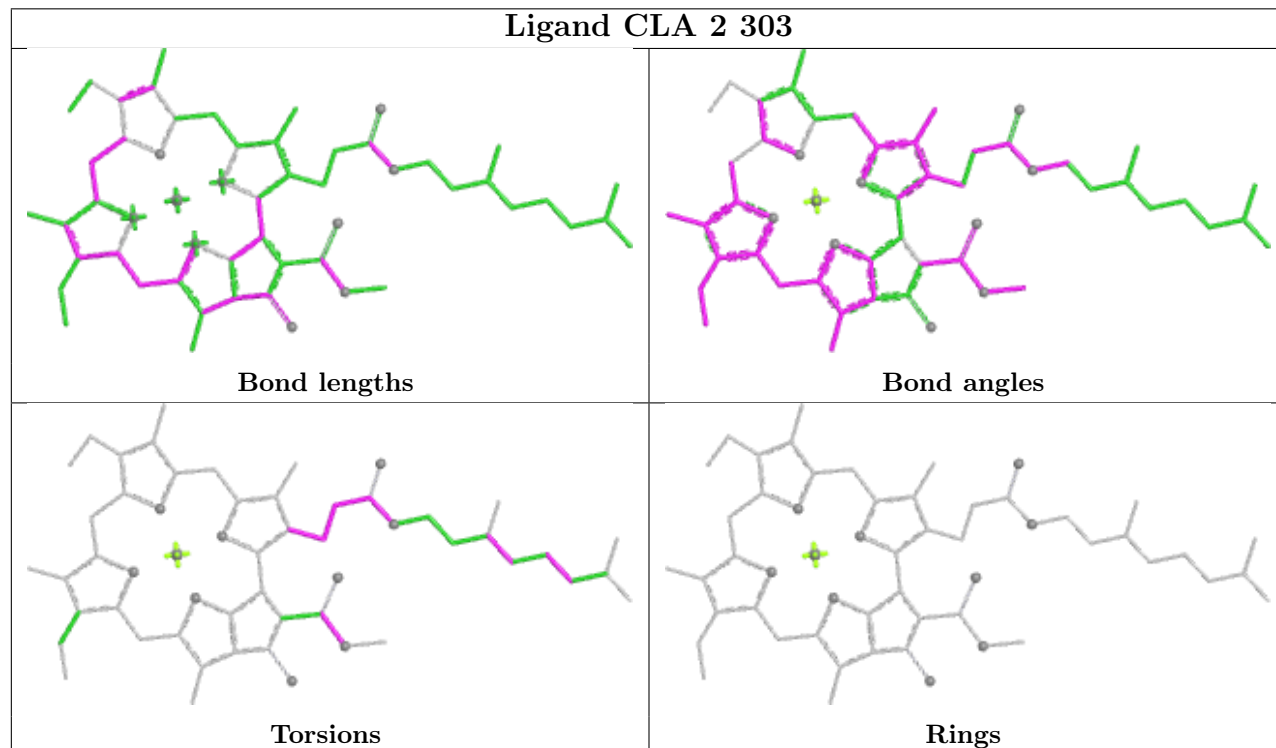


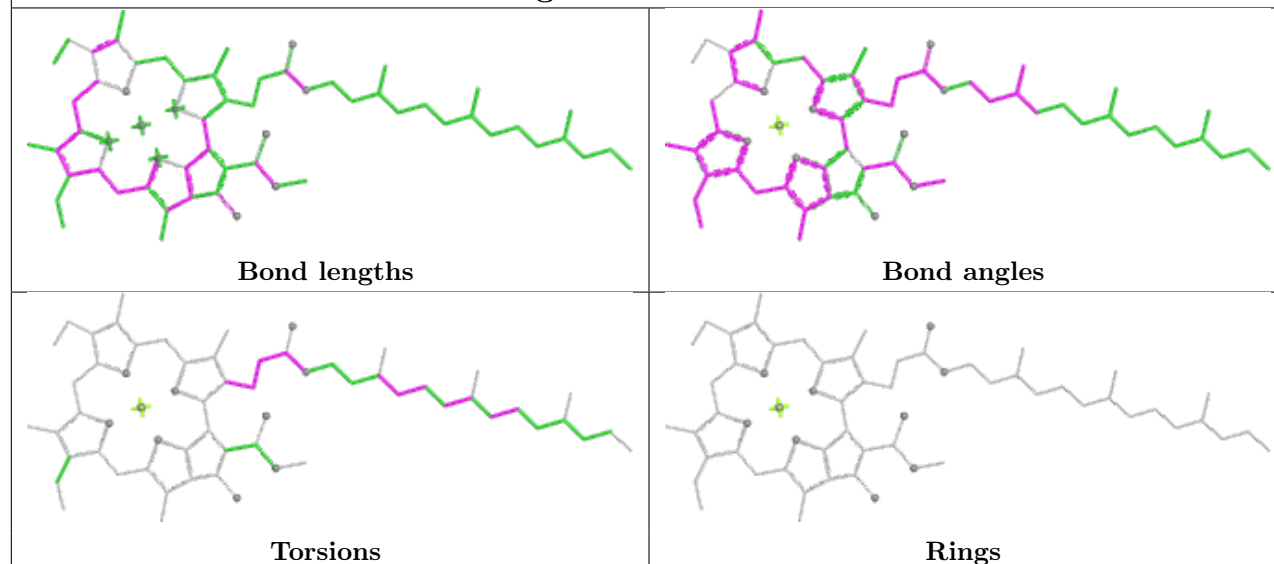
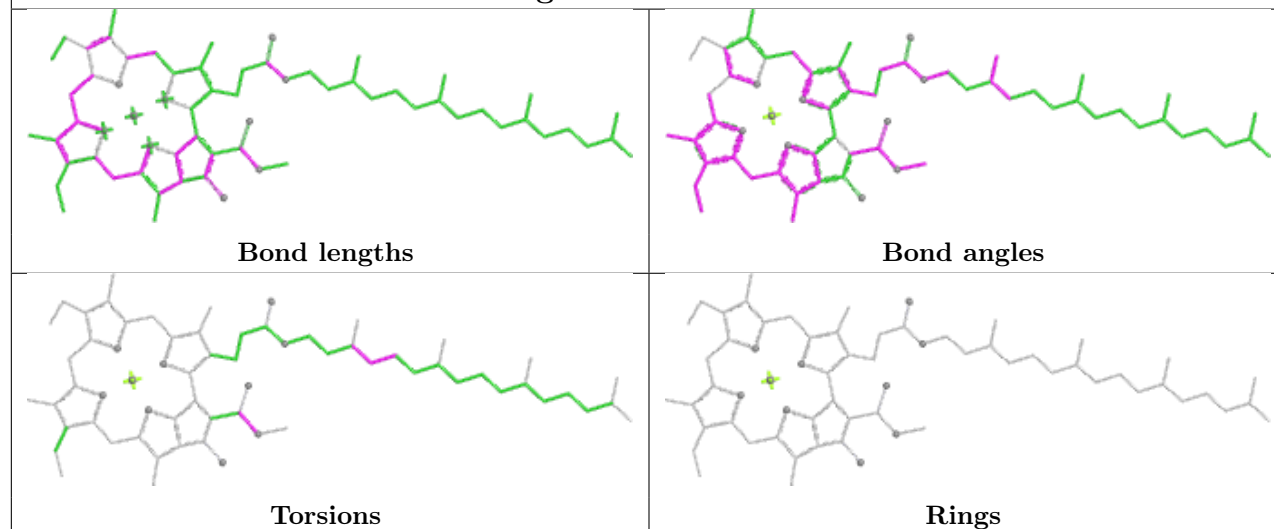
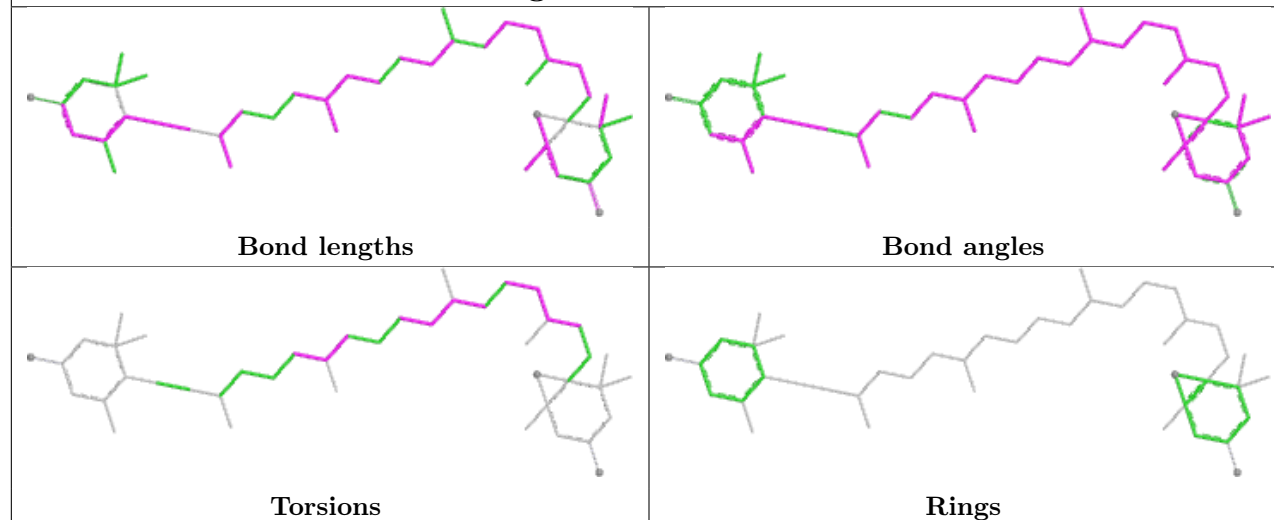
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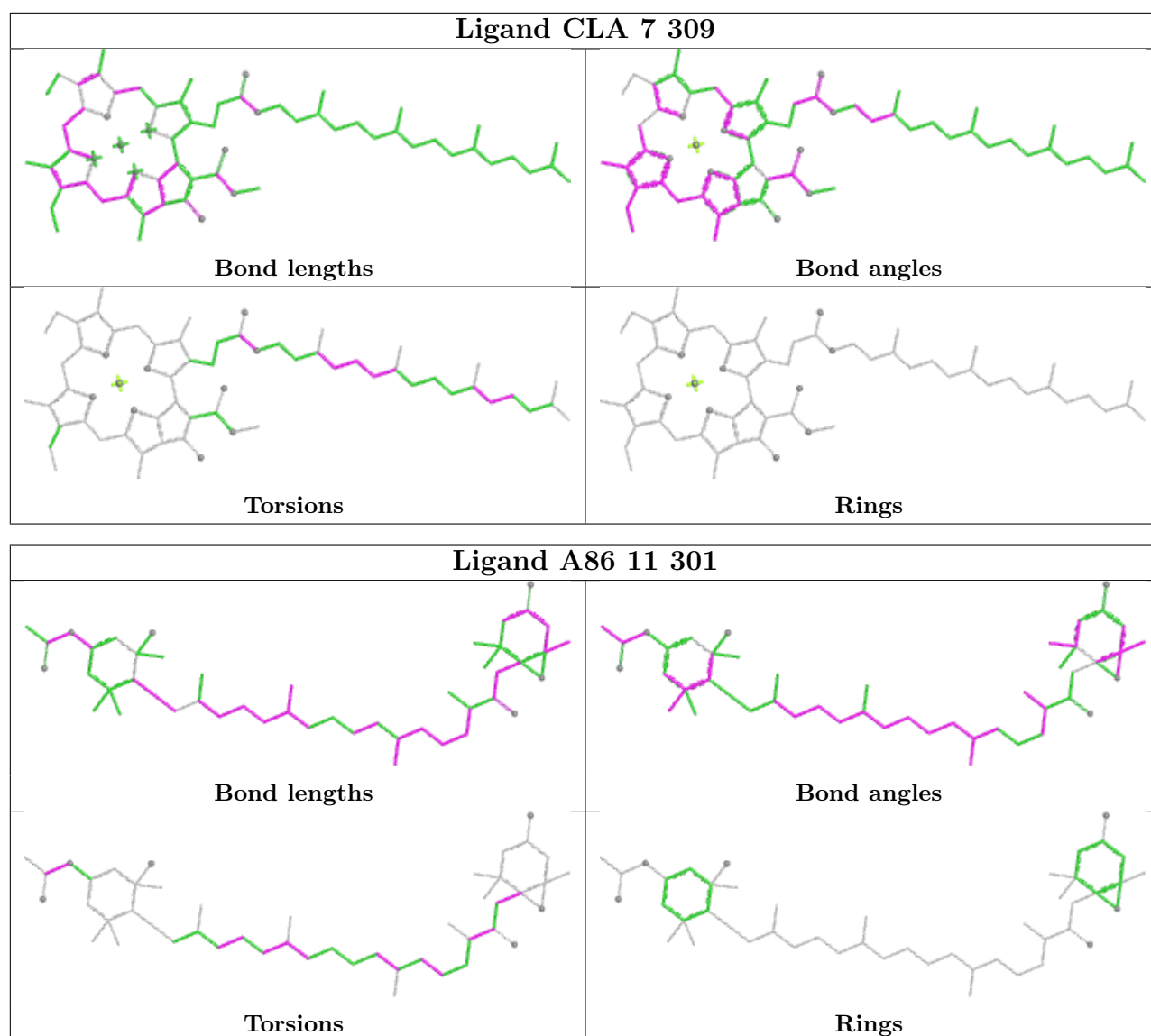




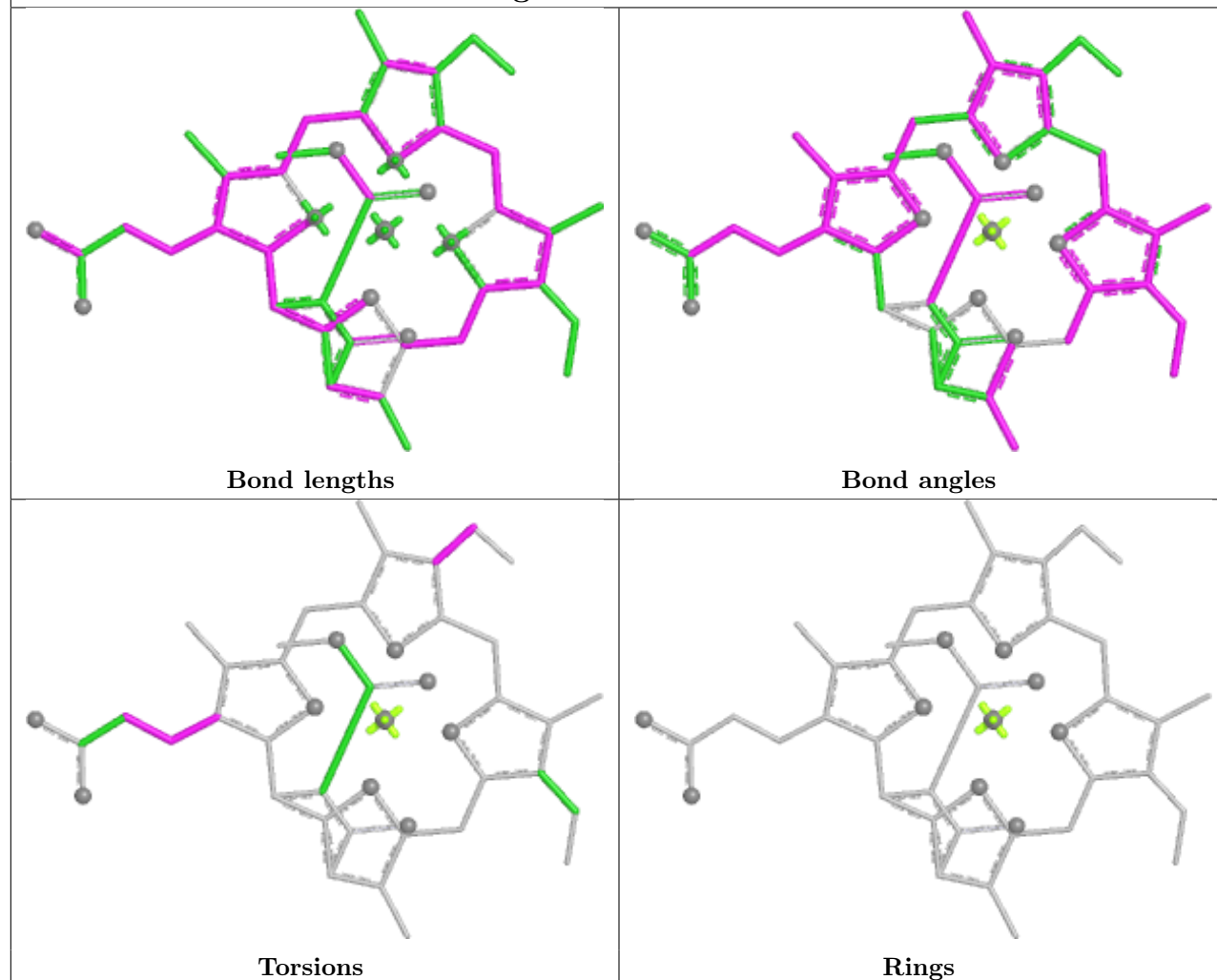


**Ligand CLA 4 302****Ligand CLA 2 303**

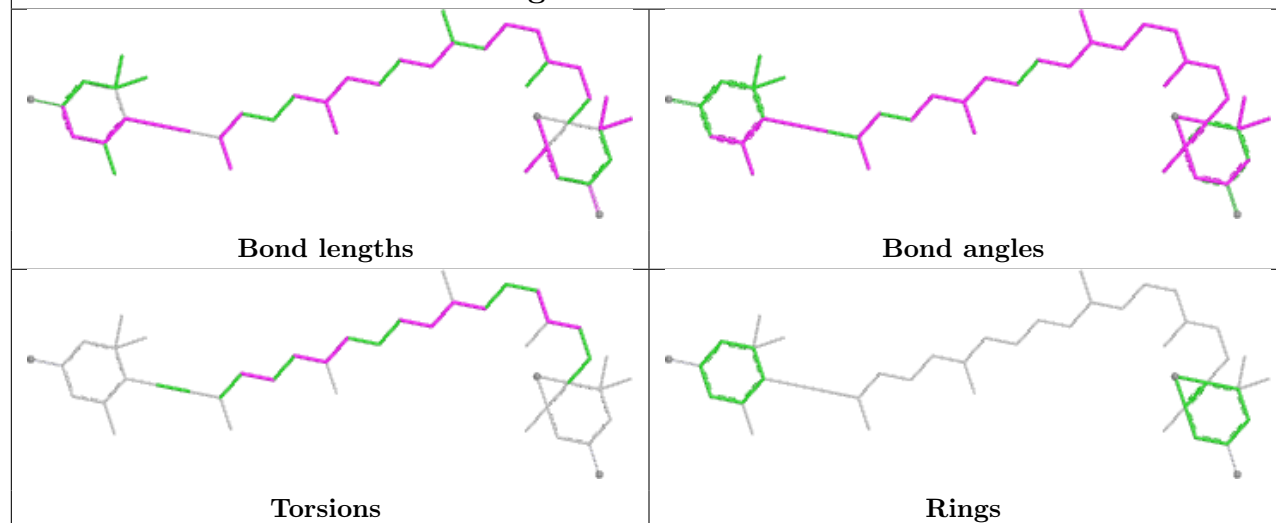
**Ligand CLA 3 305****Ligand CLA 5 303****Ligand DD6 11 313**

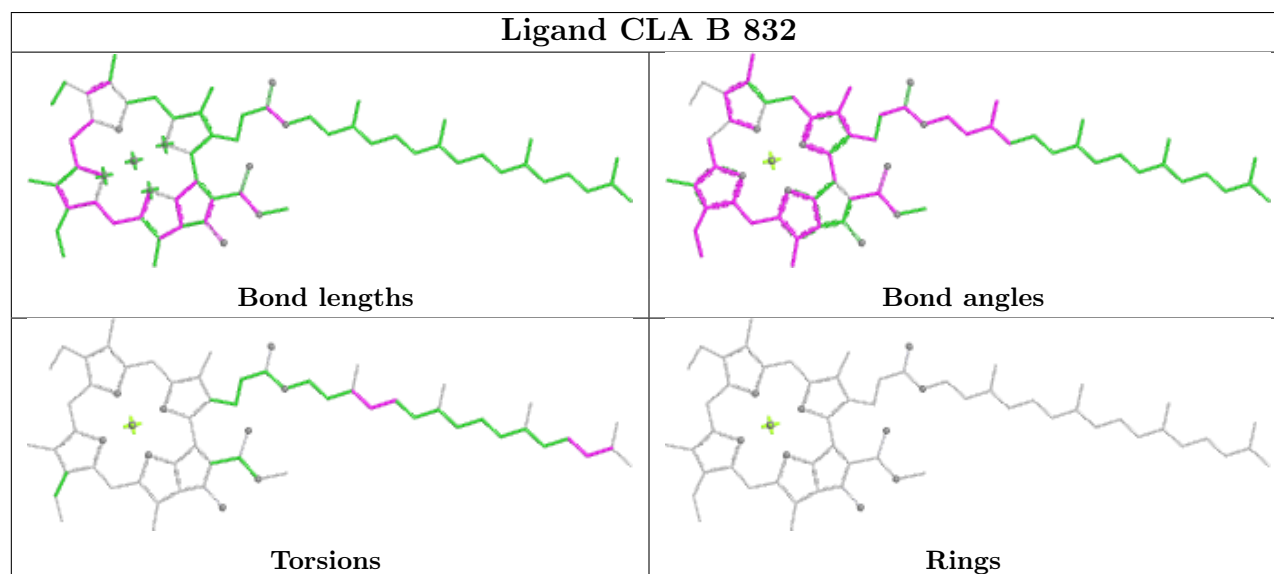
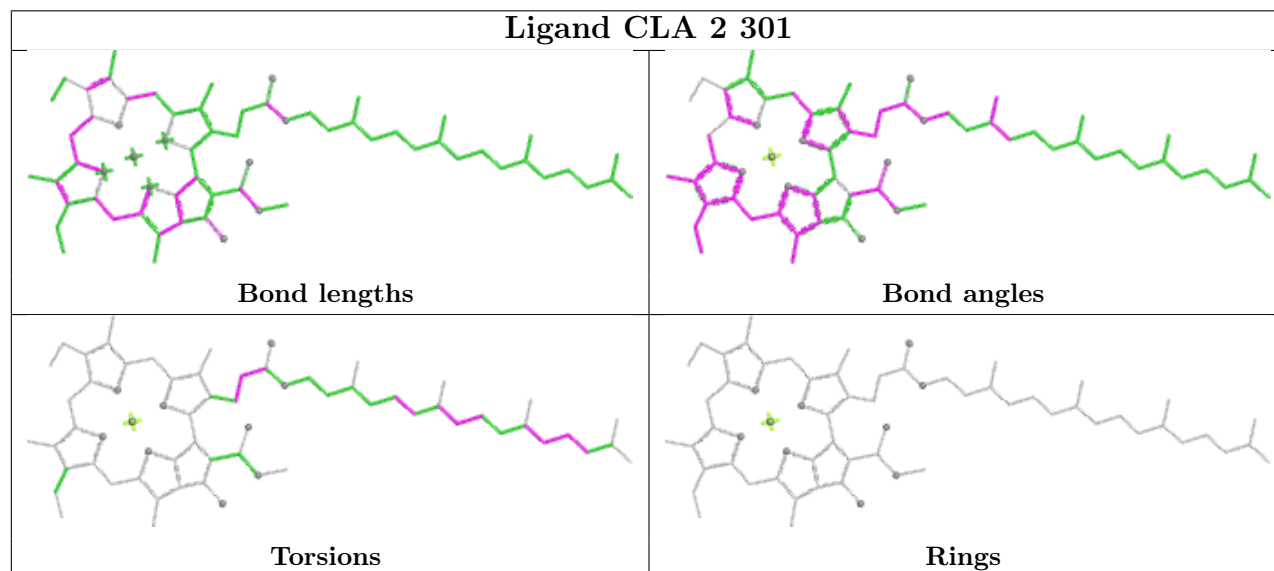
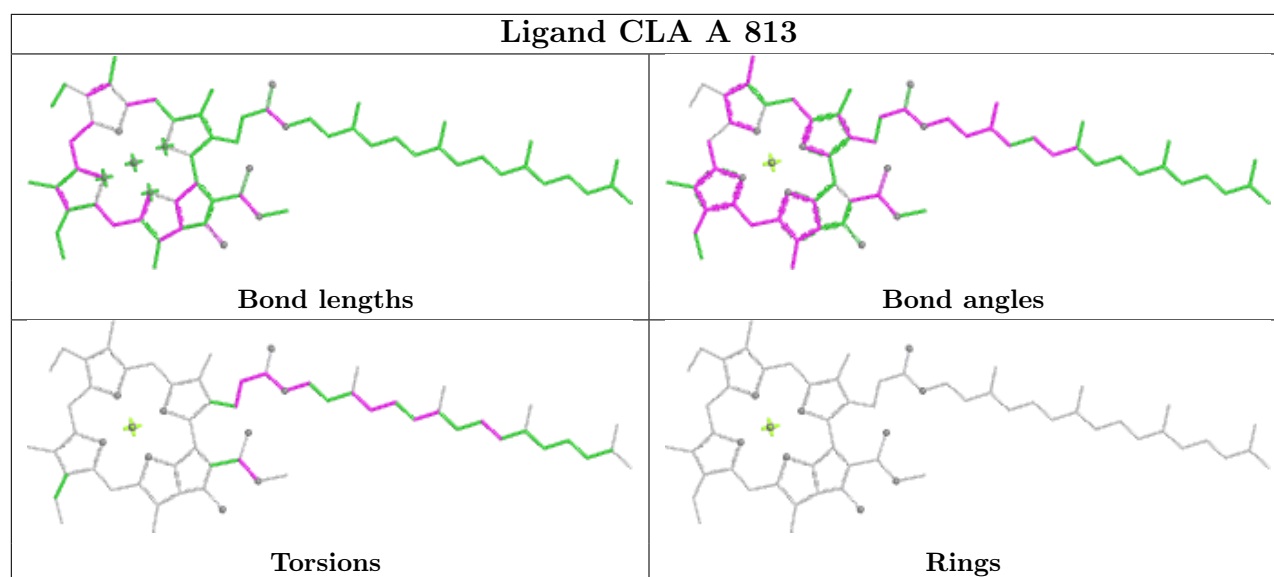


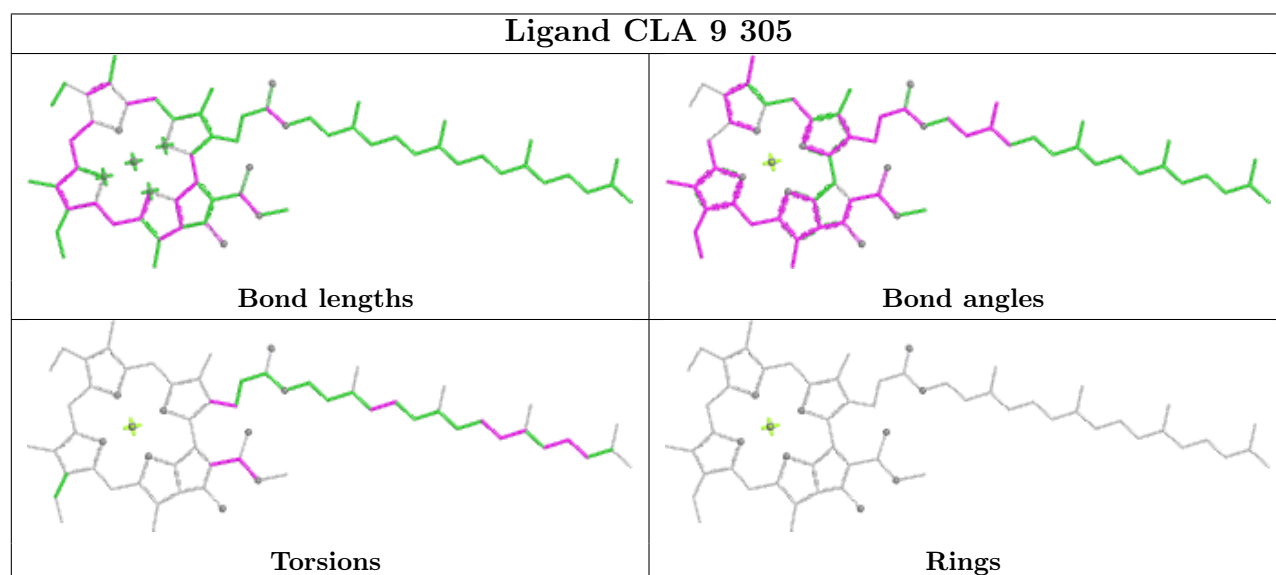
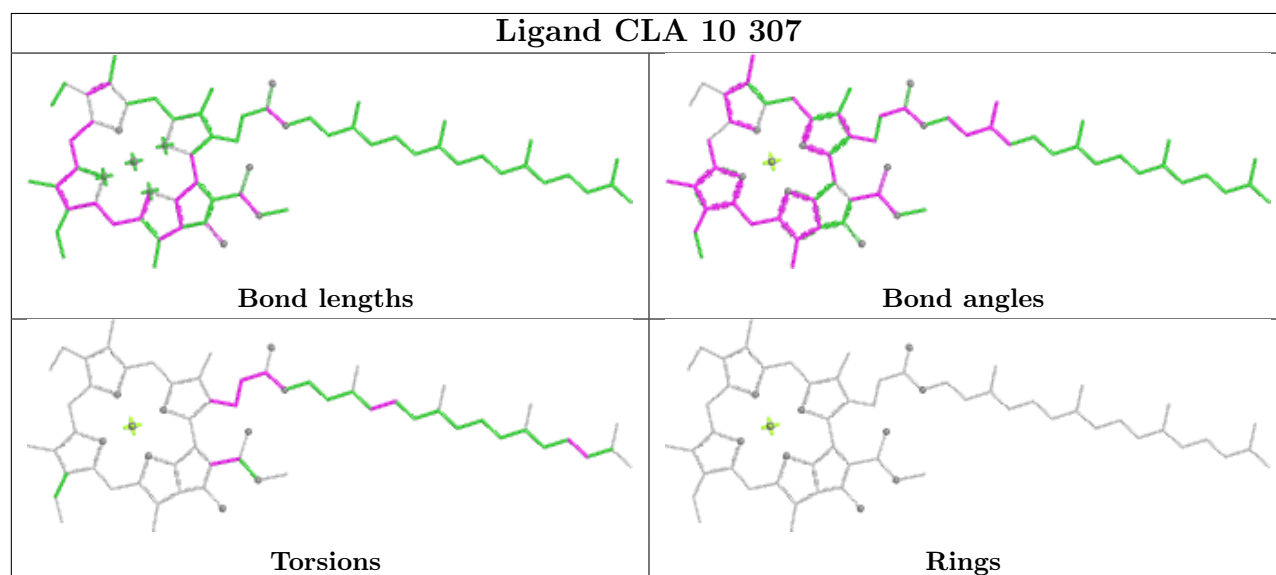
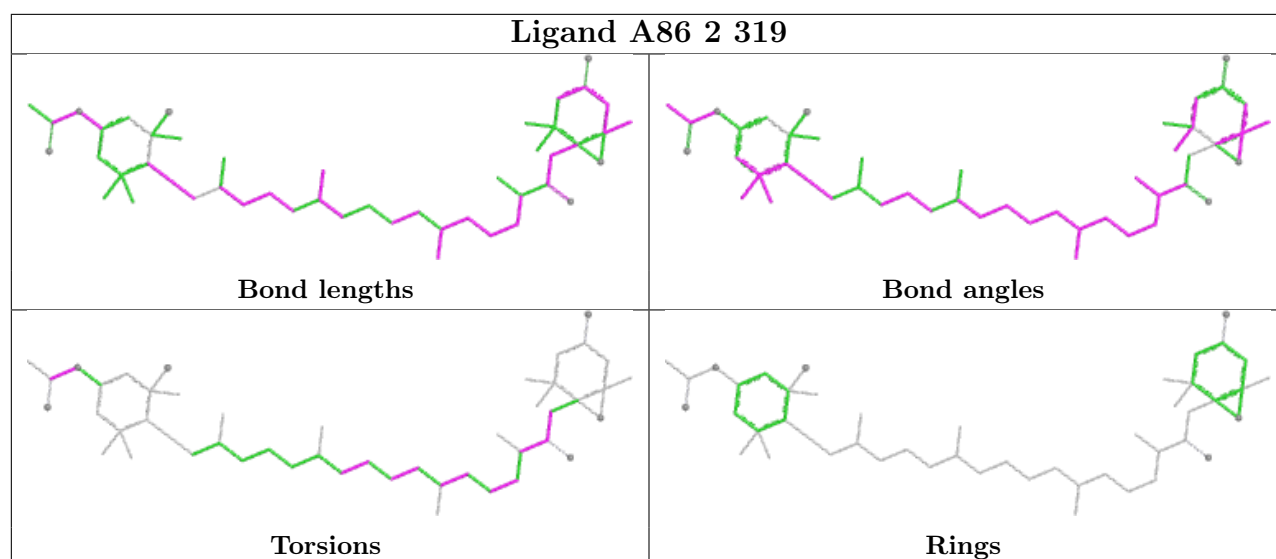
## Ligand KC1 4 310



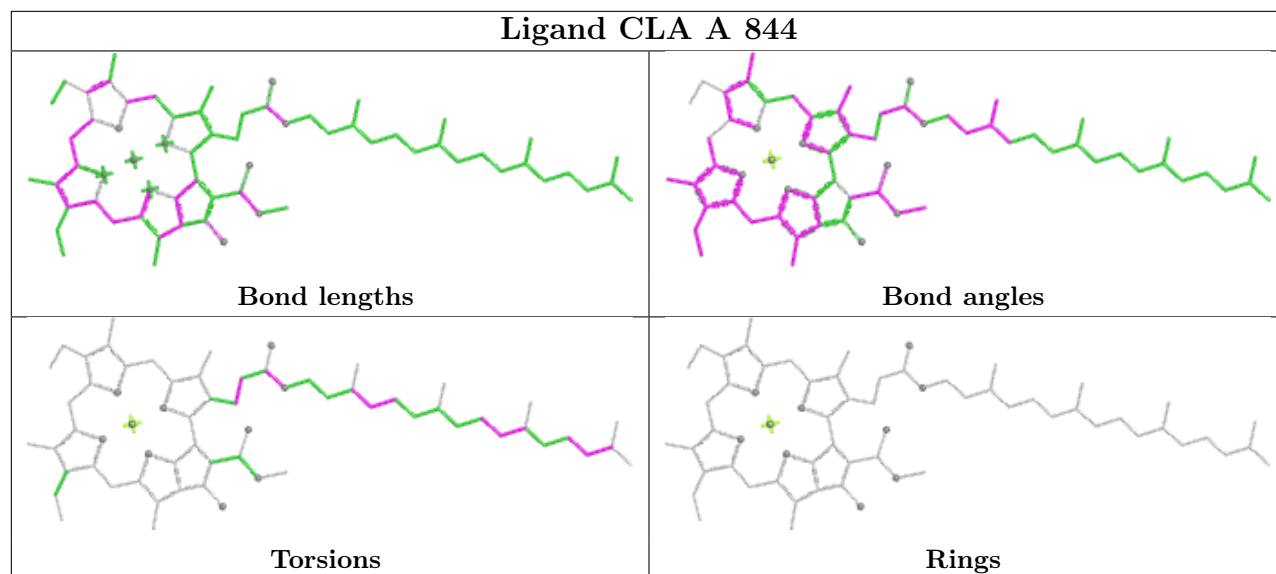
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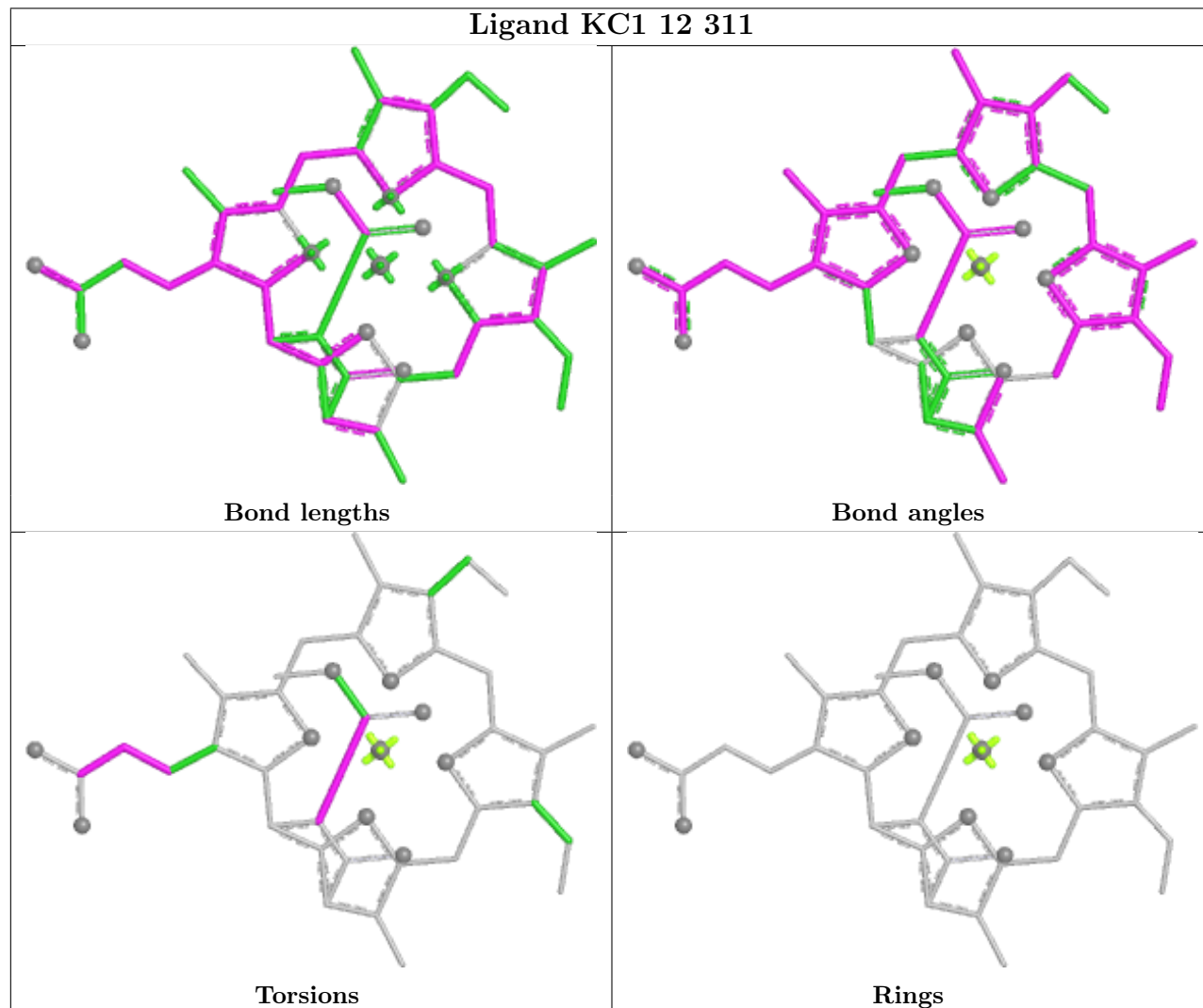


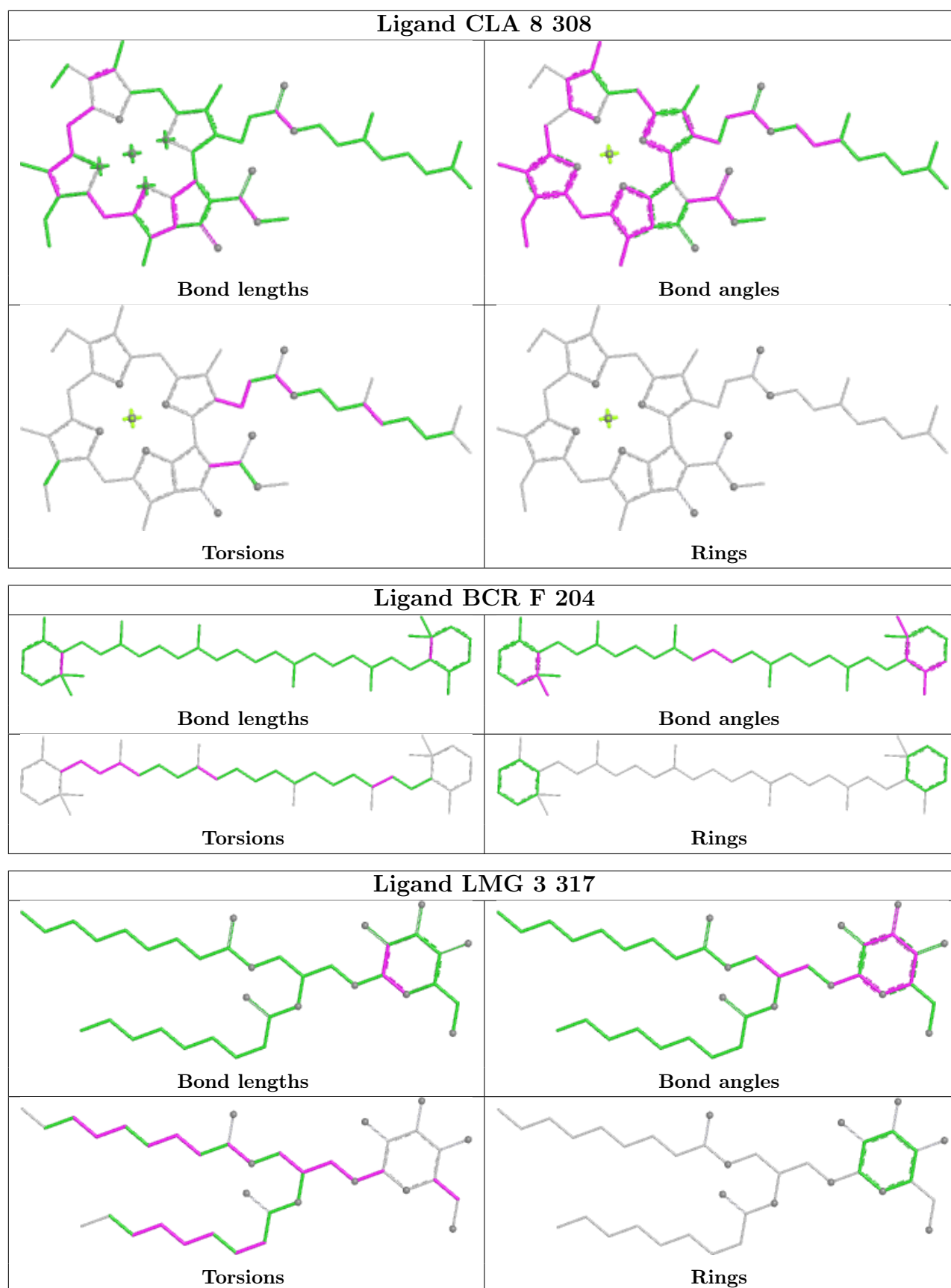


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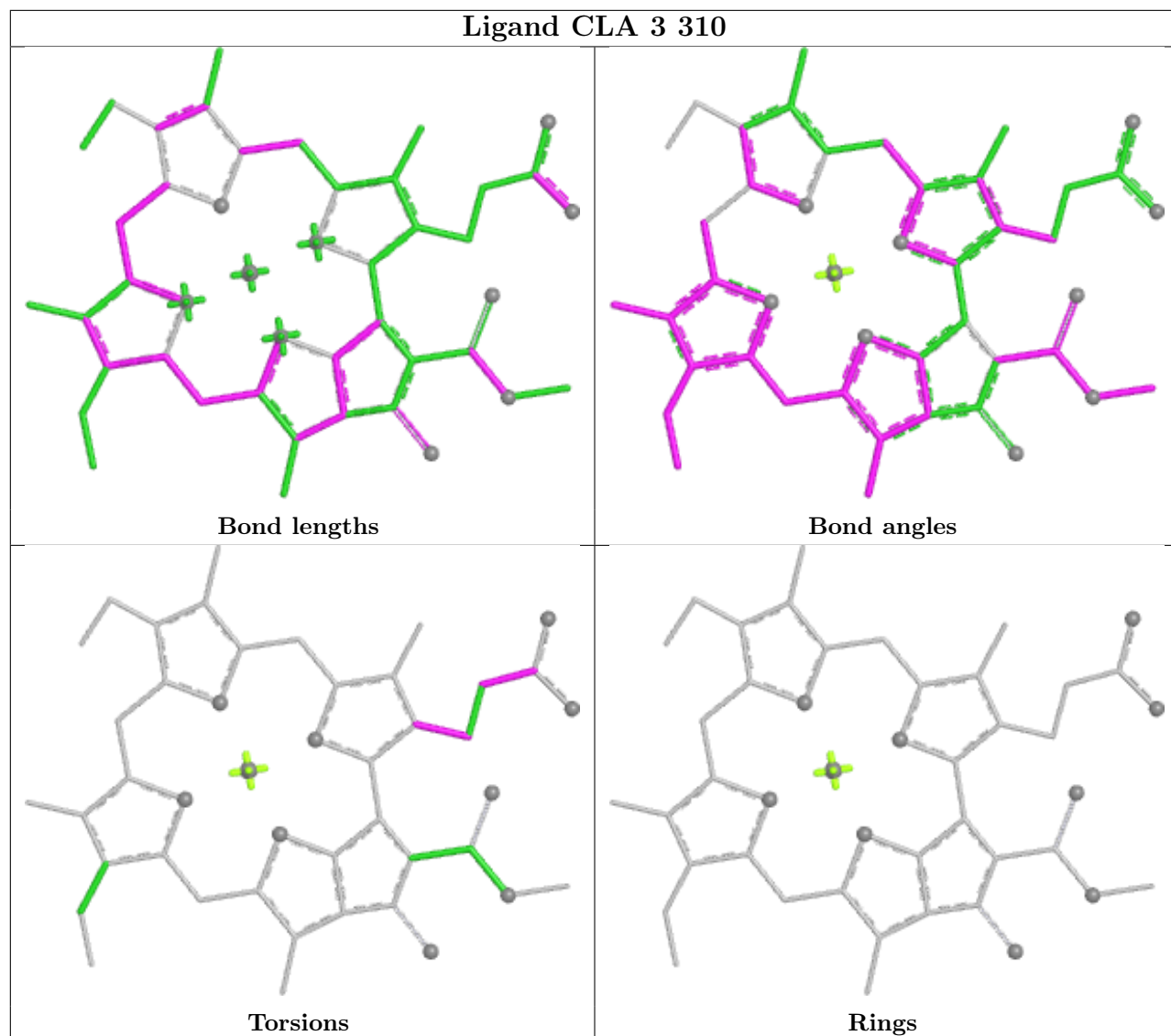


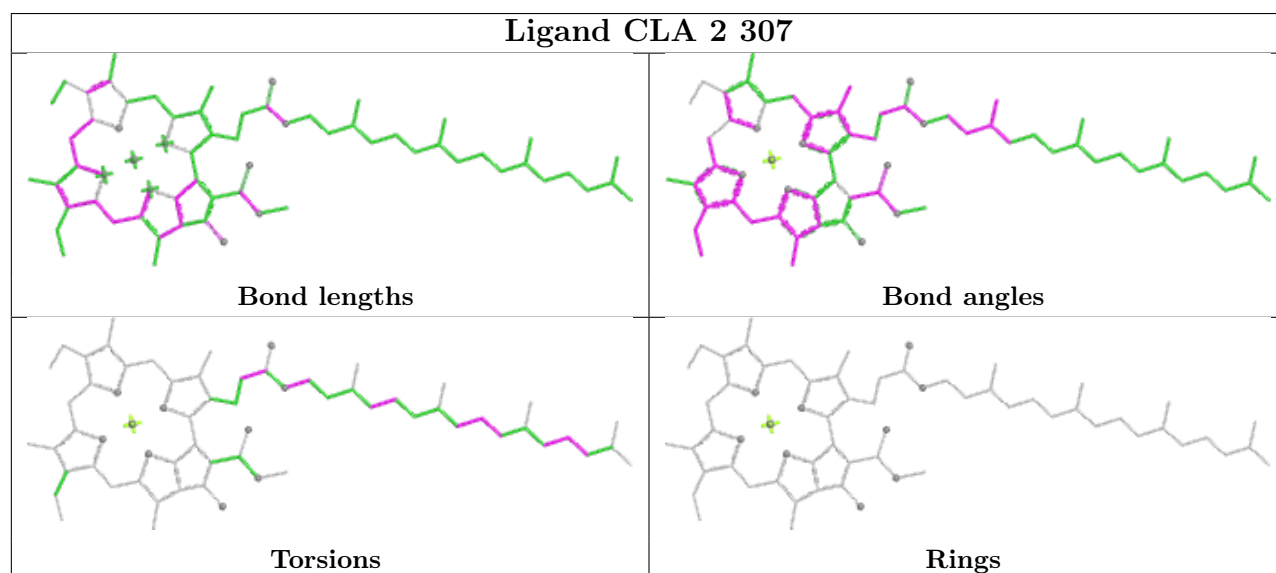
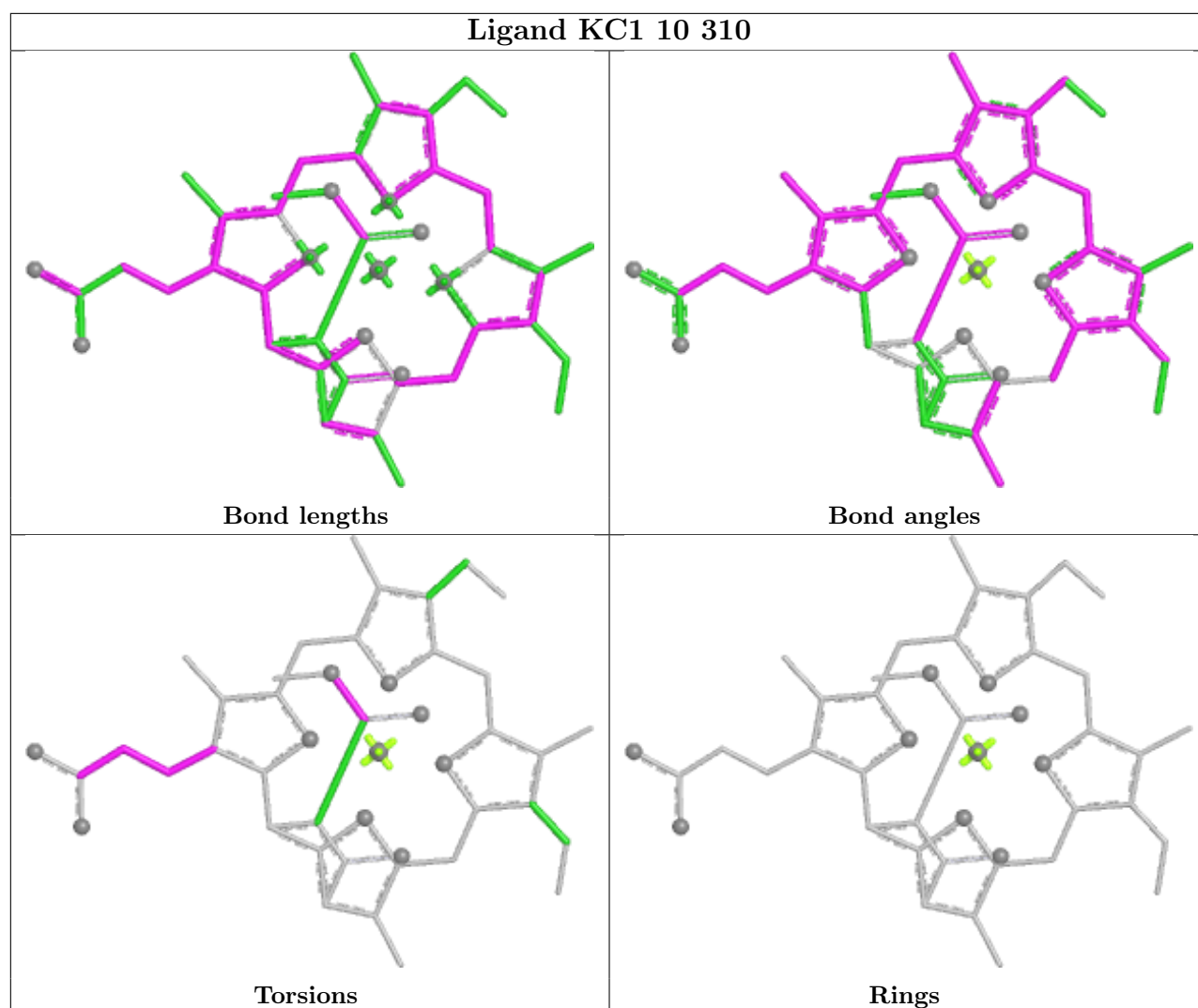
## Ligand KC1 12 311

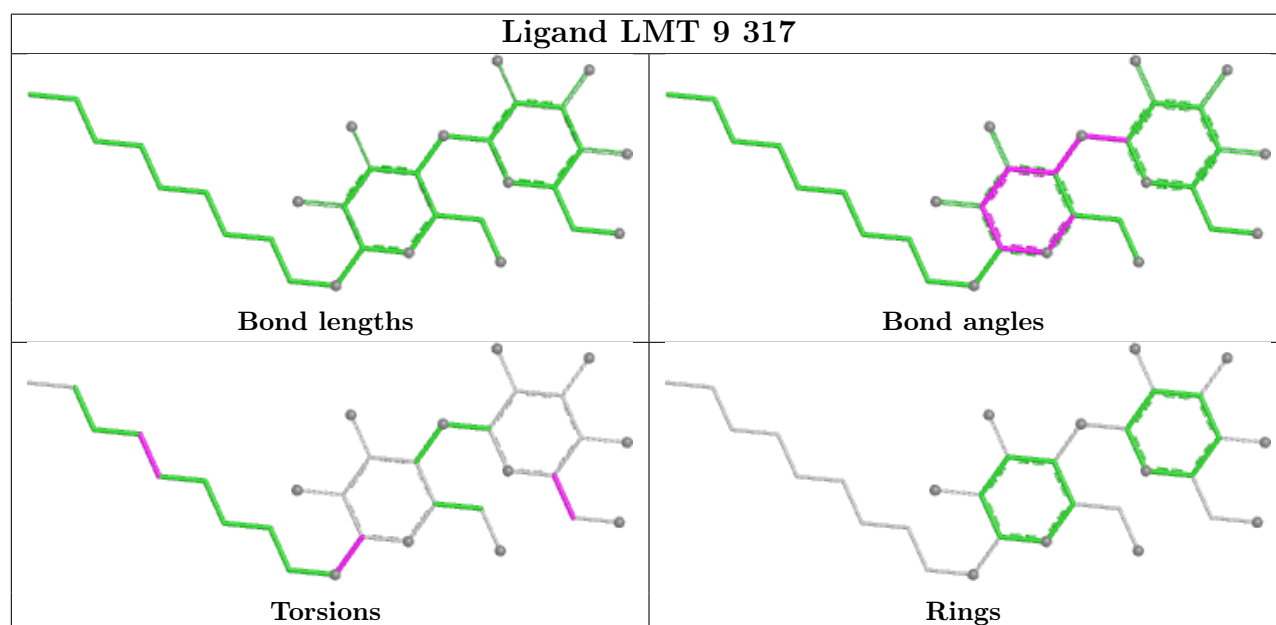
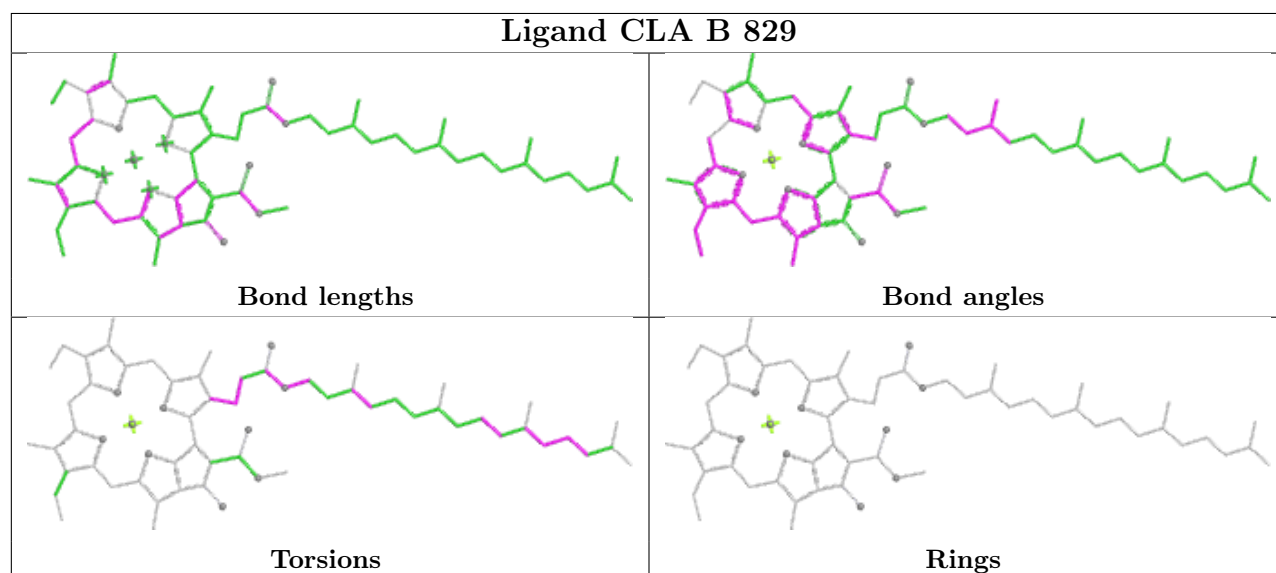
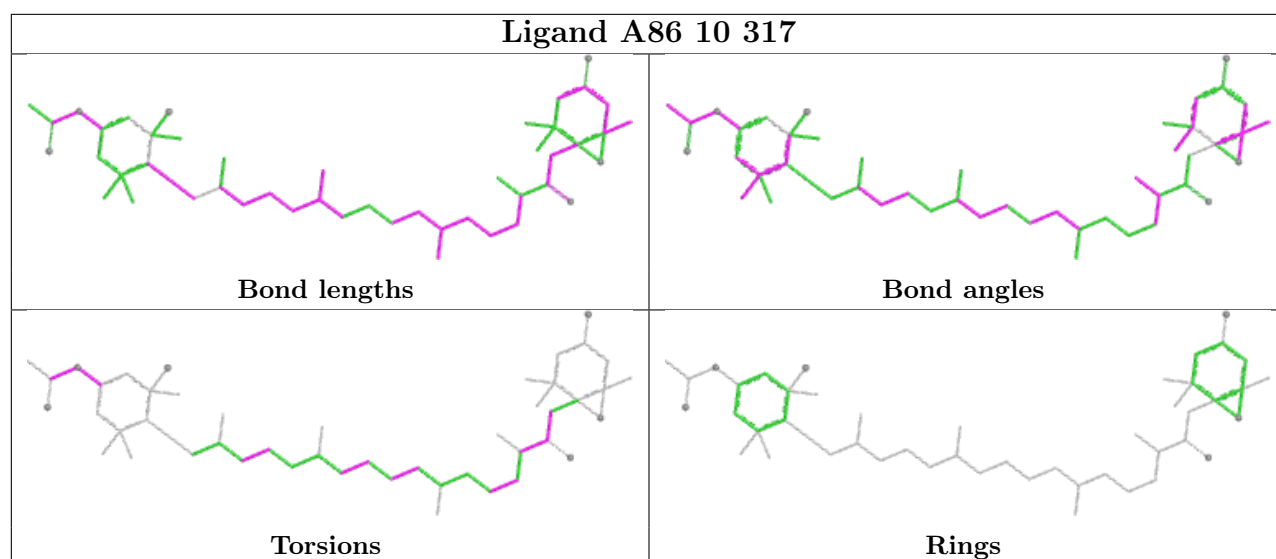




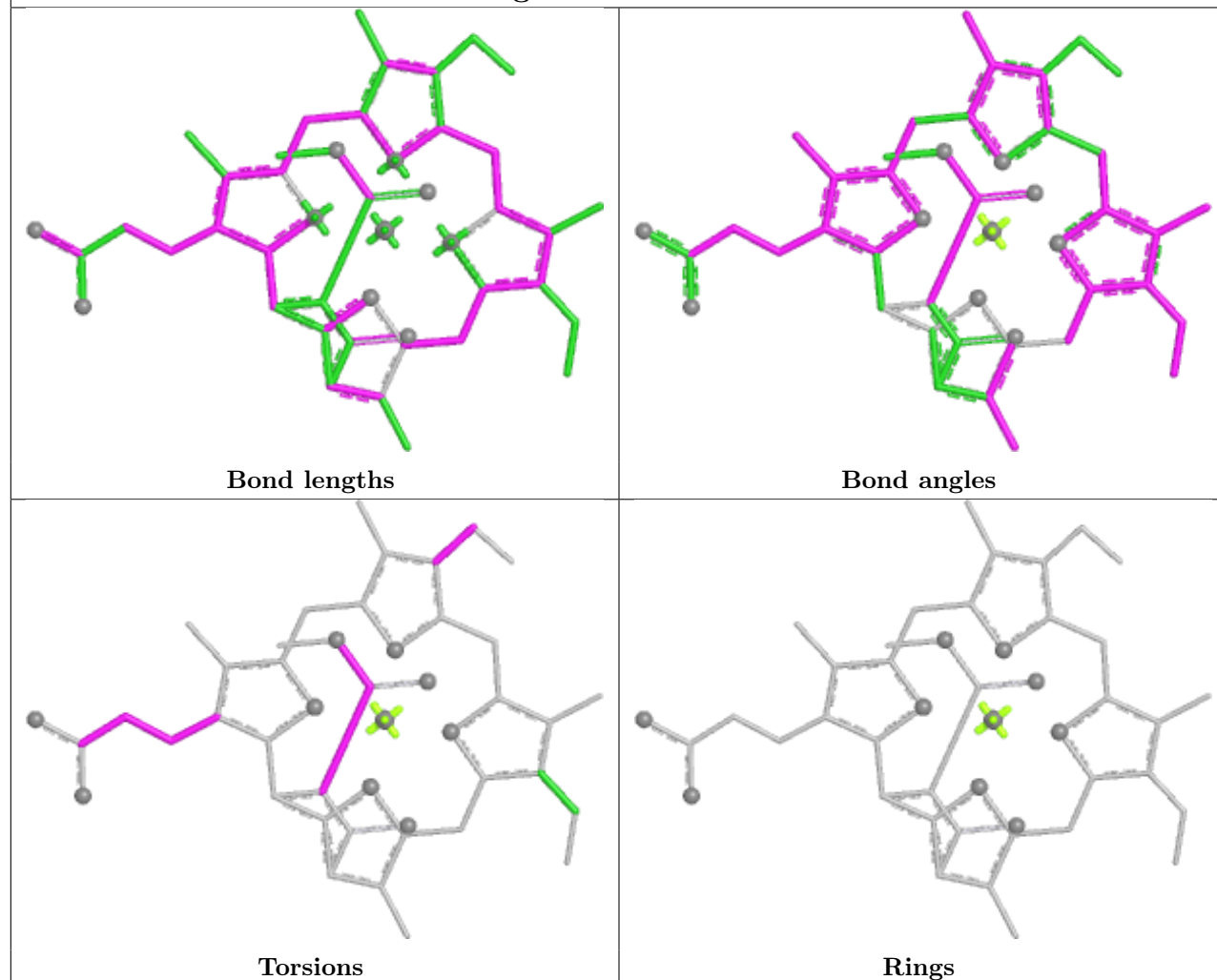
## Ligand CLA 3 310



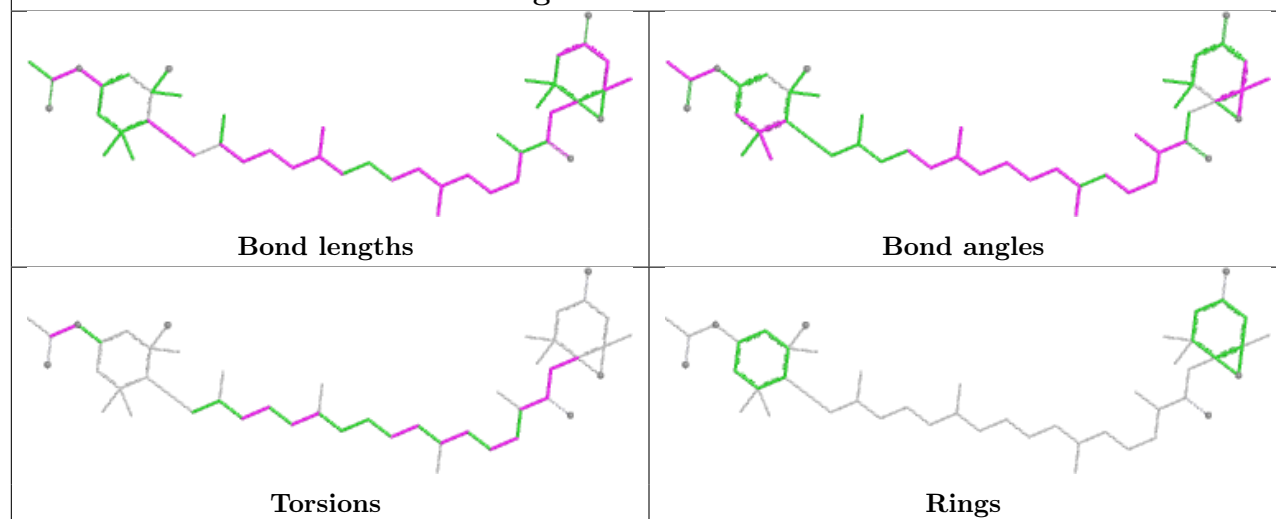


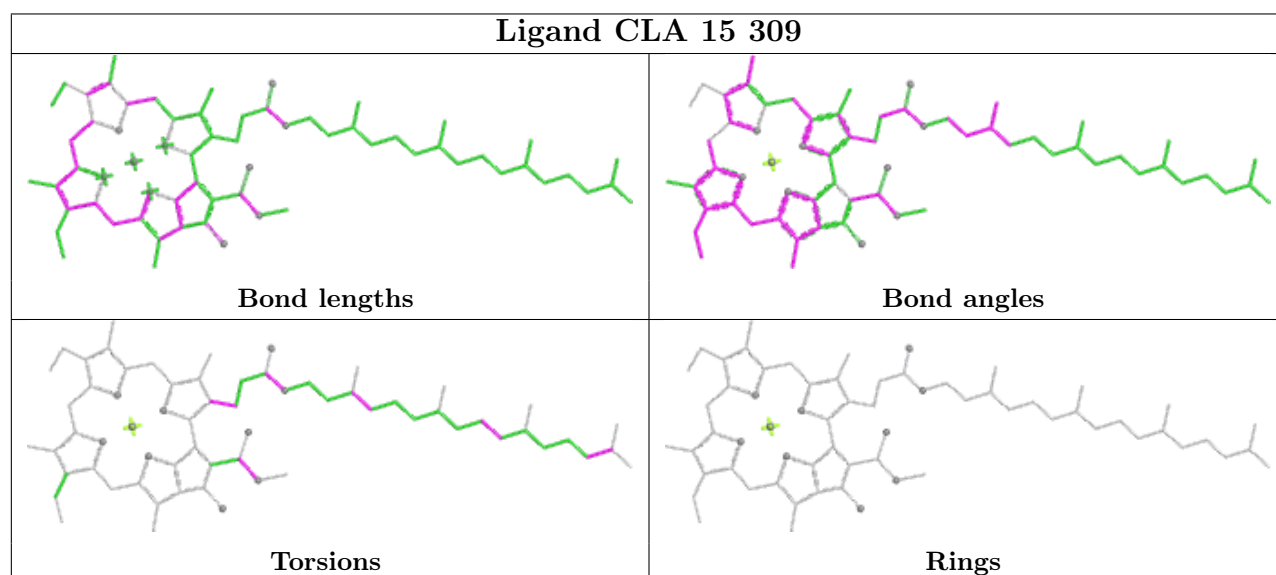
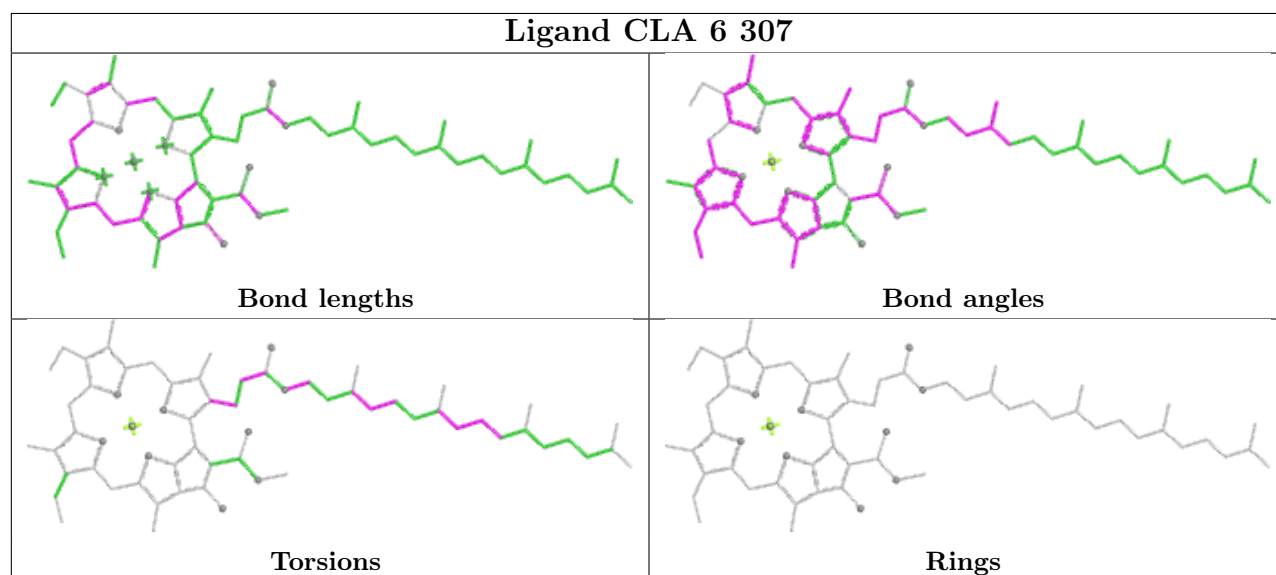
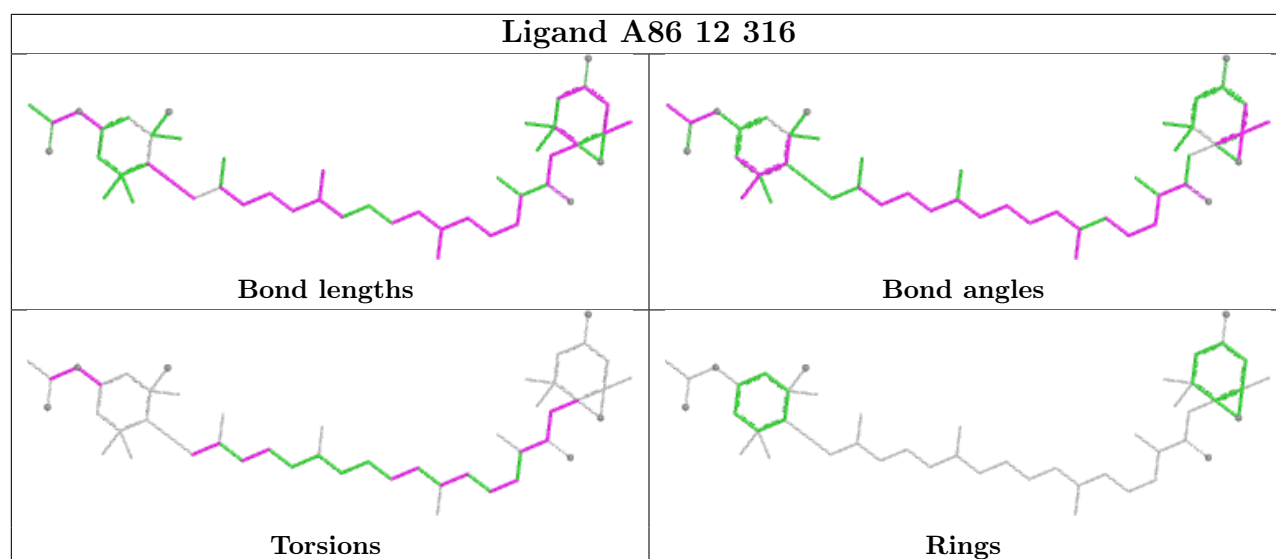


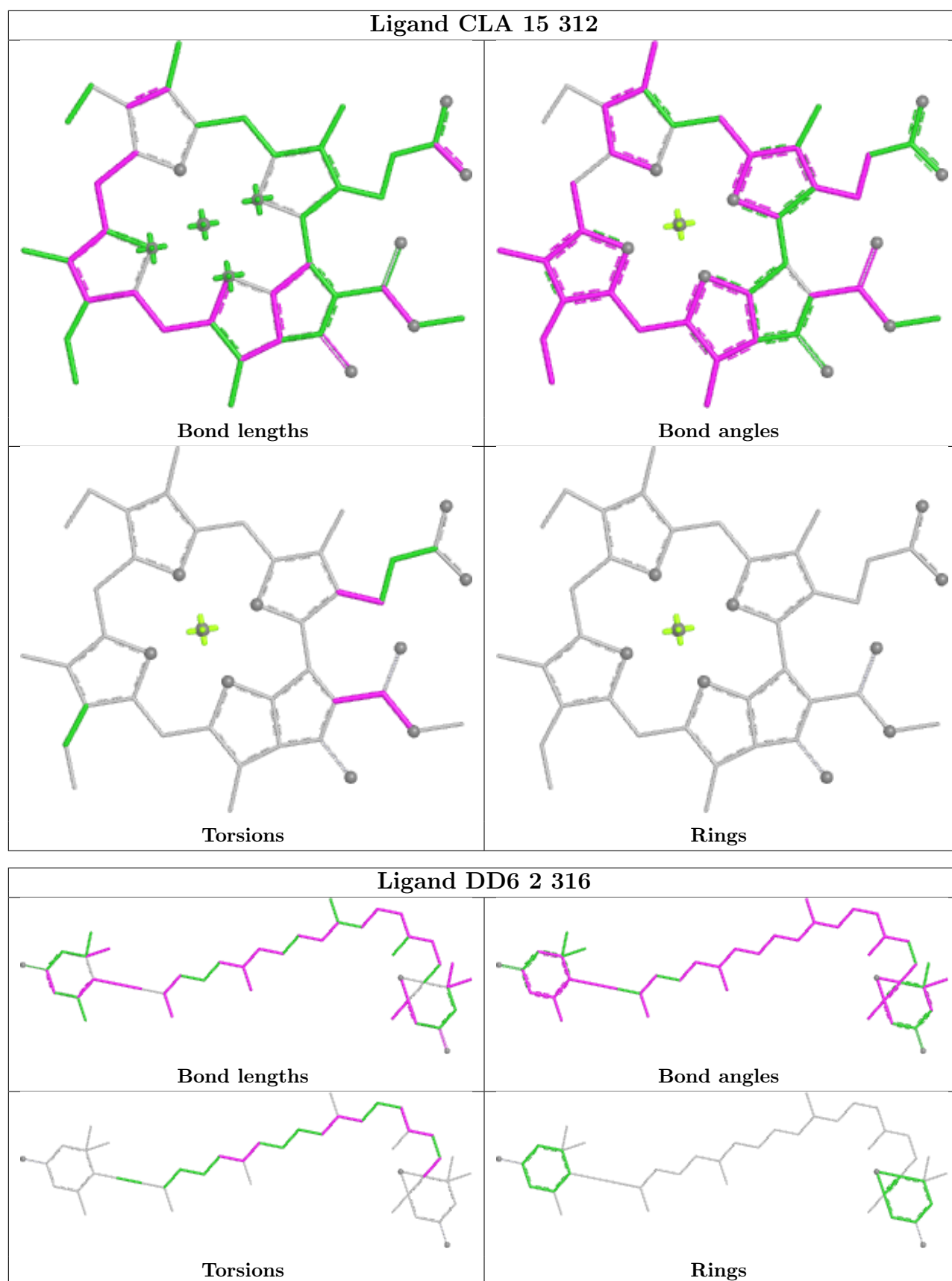
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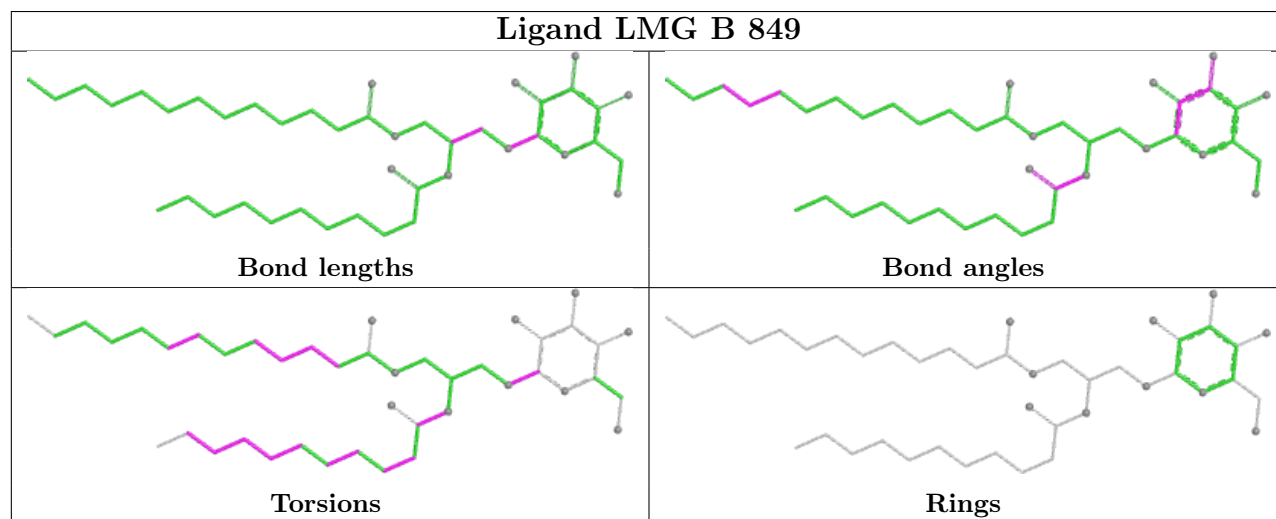
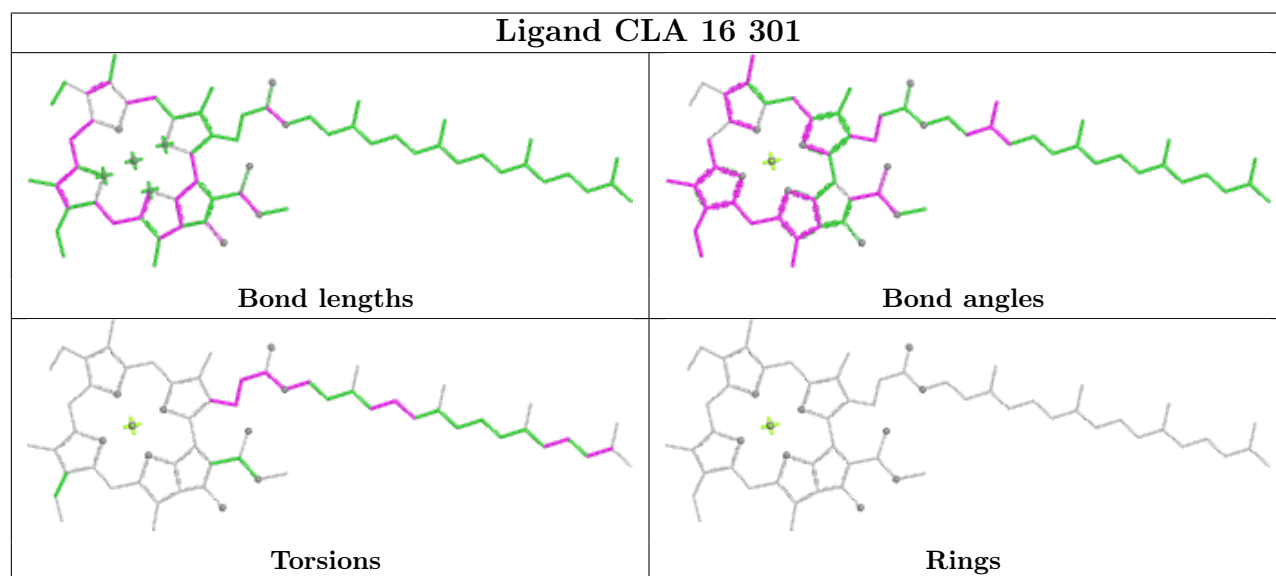
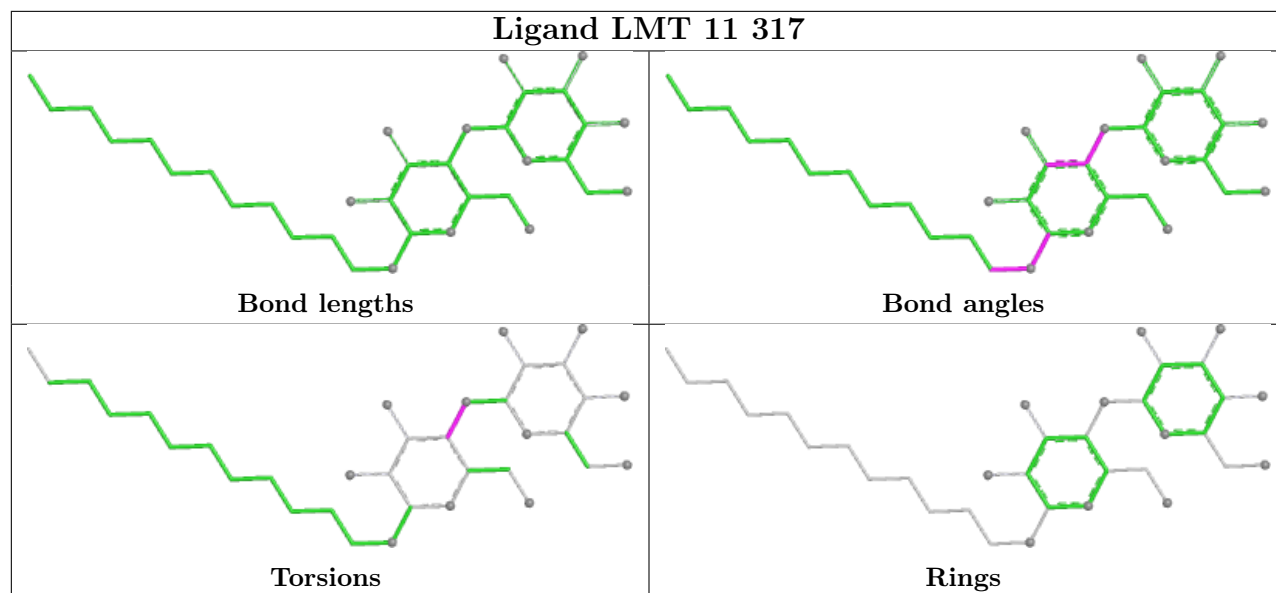


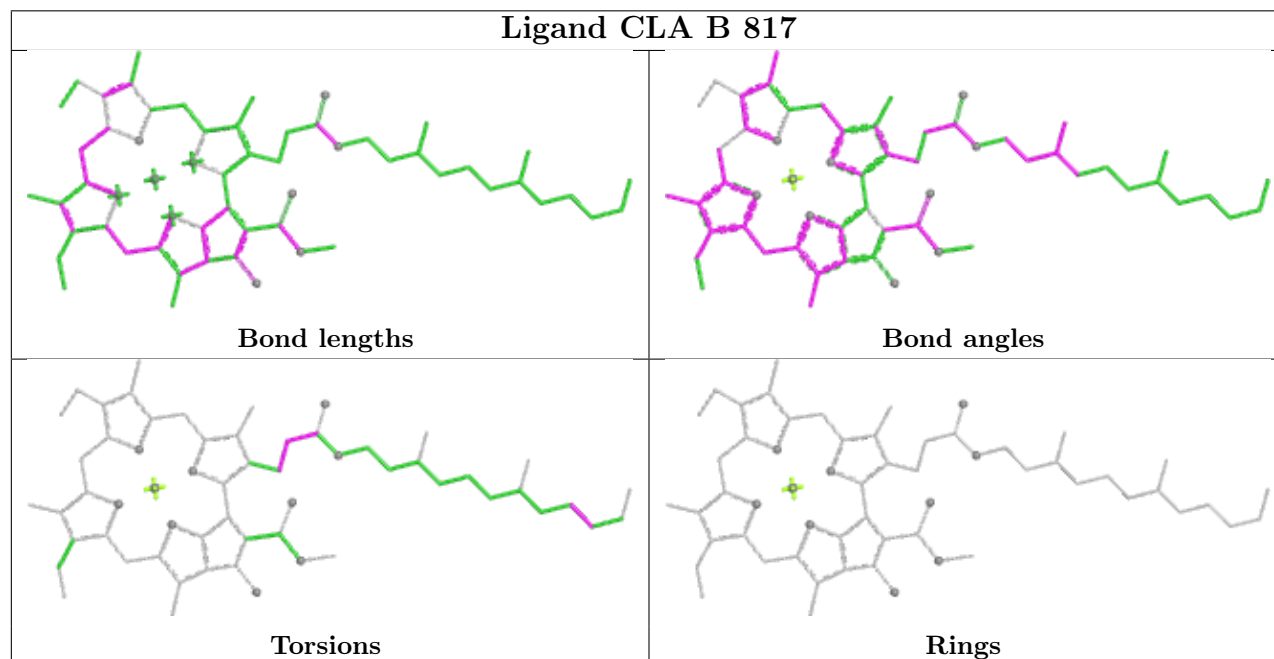
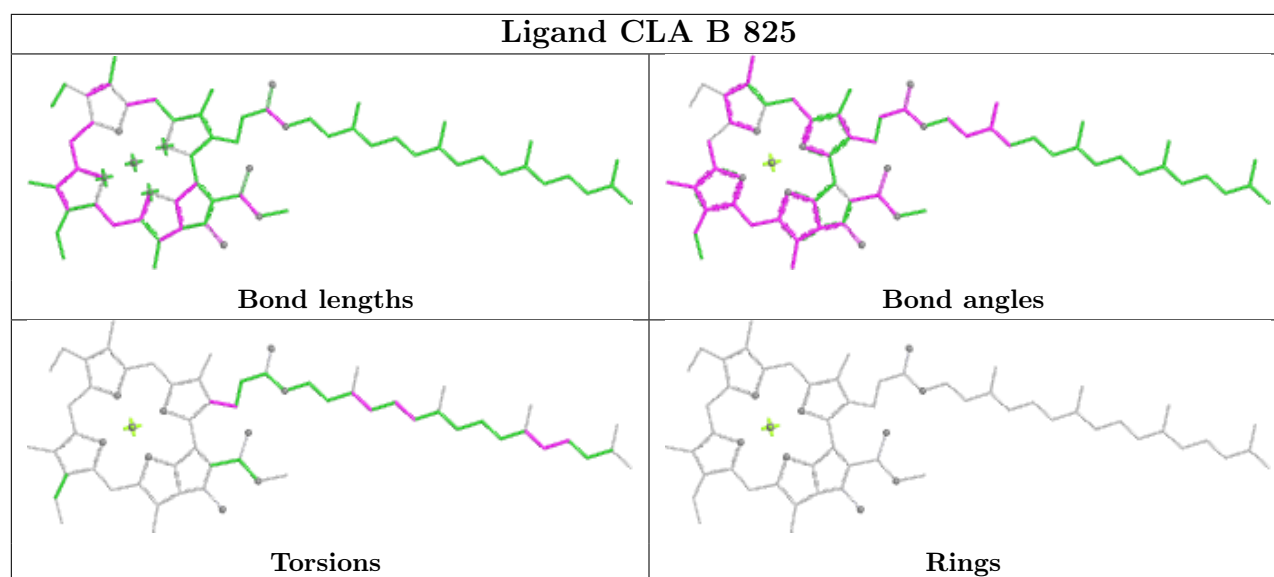
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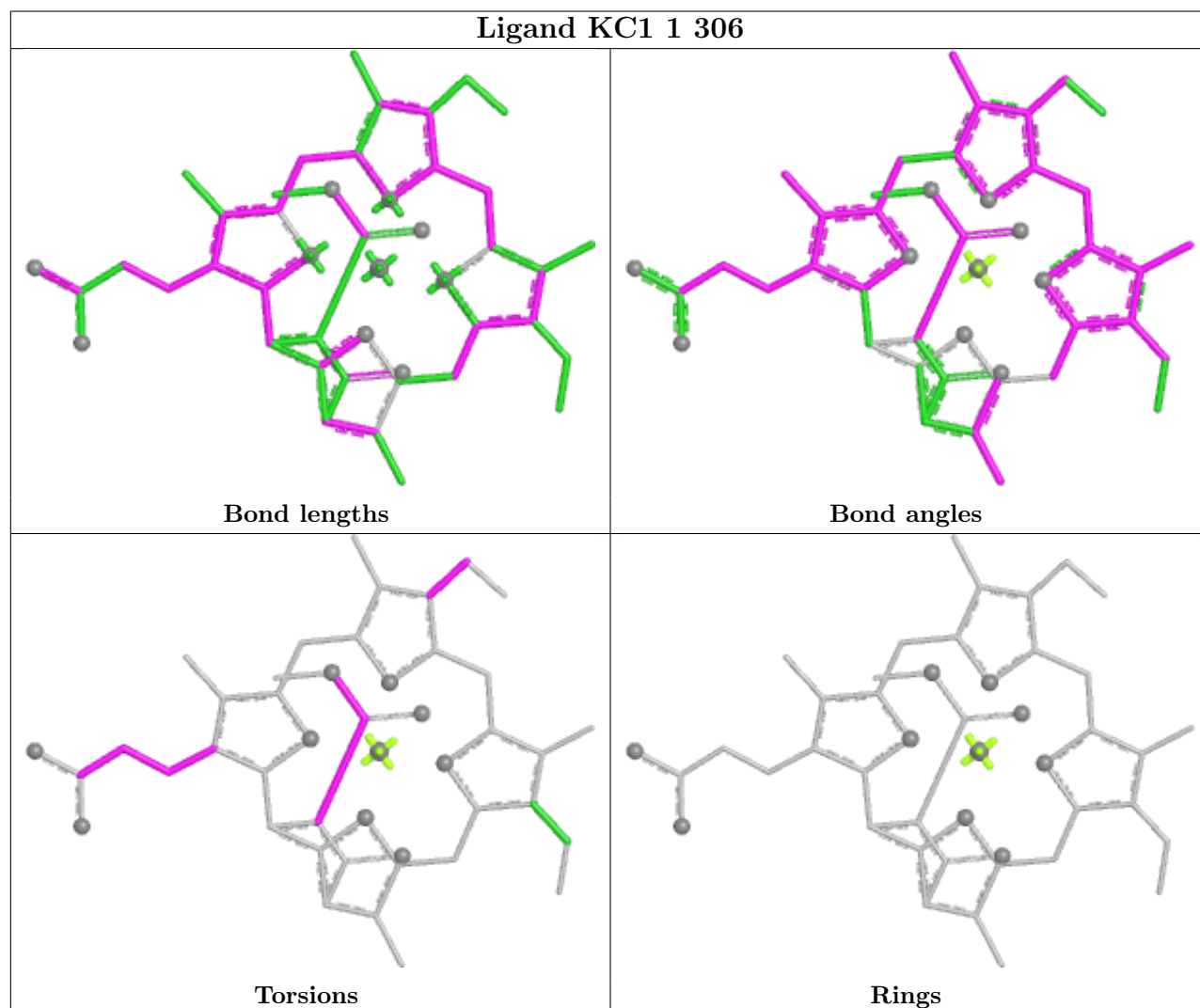
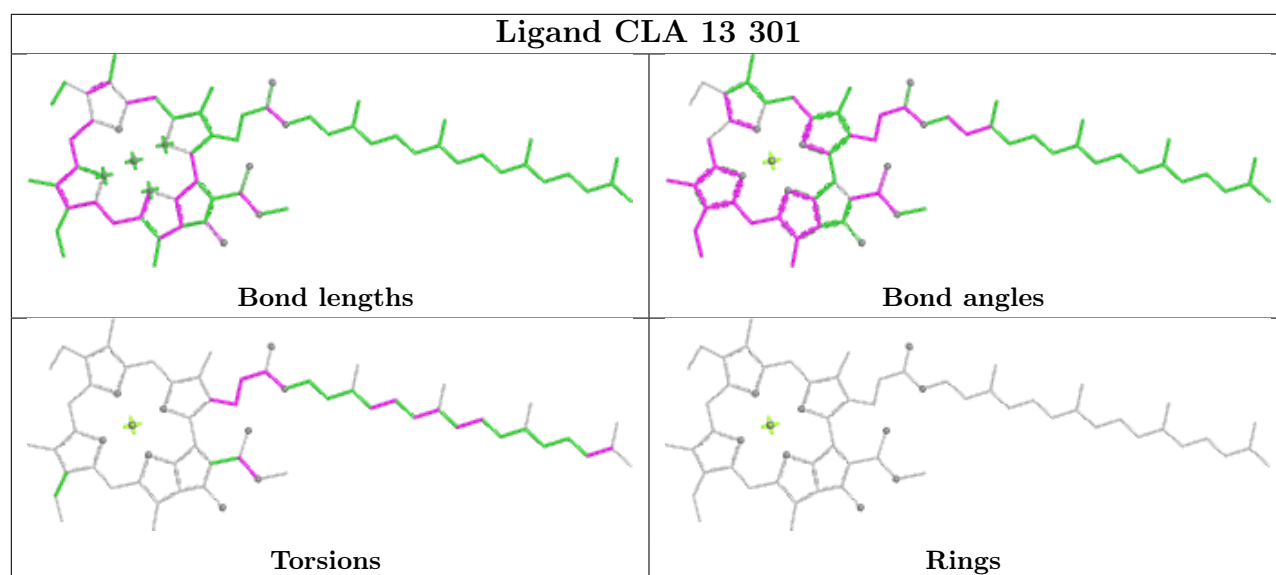




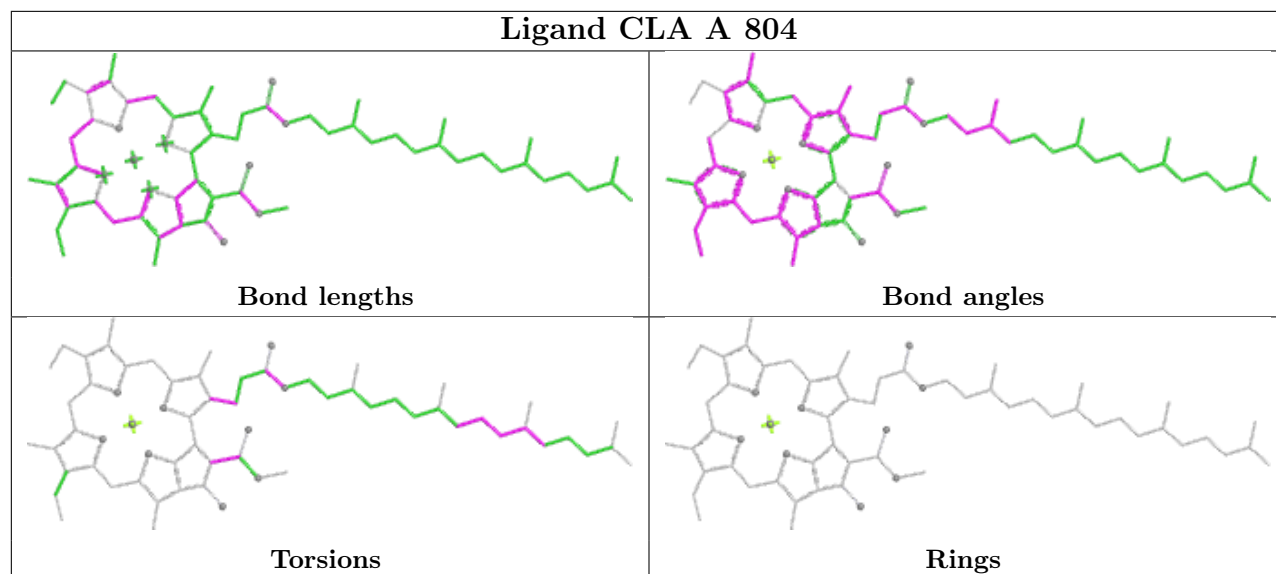




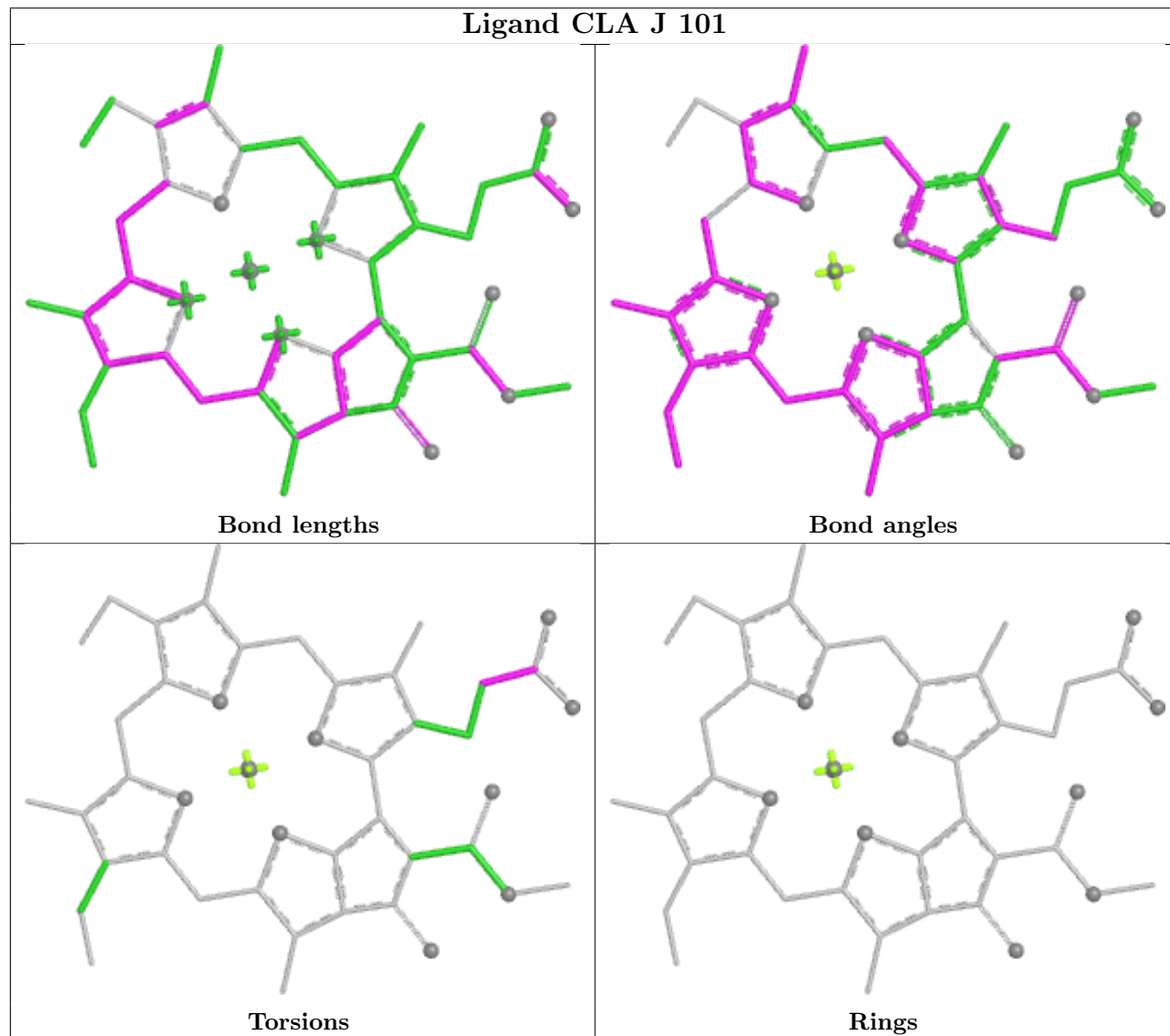


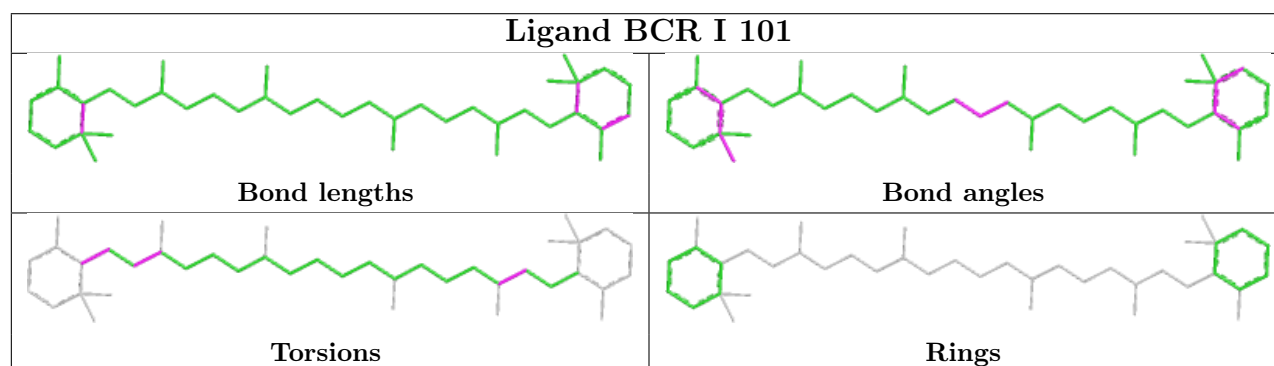
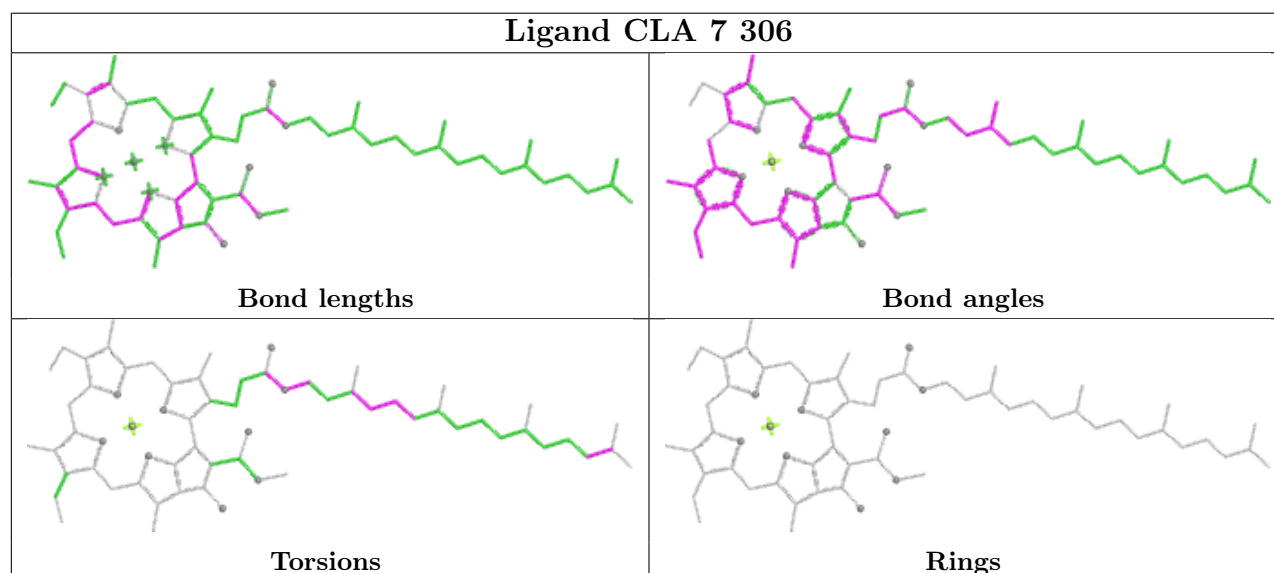
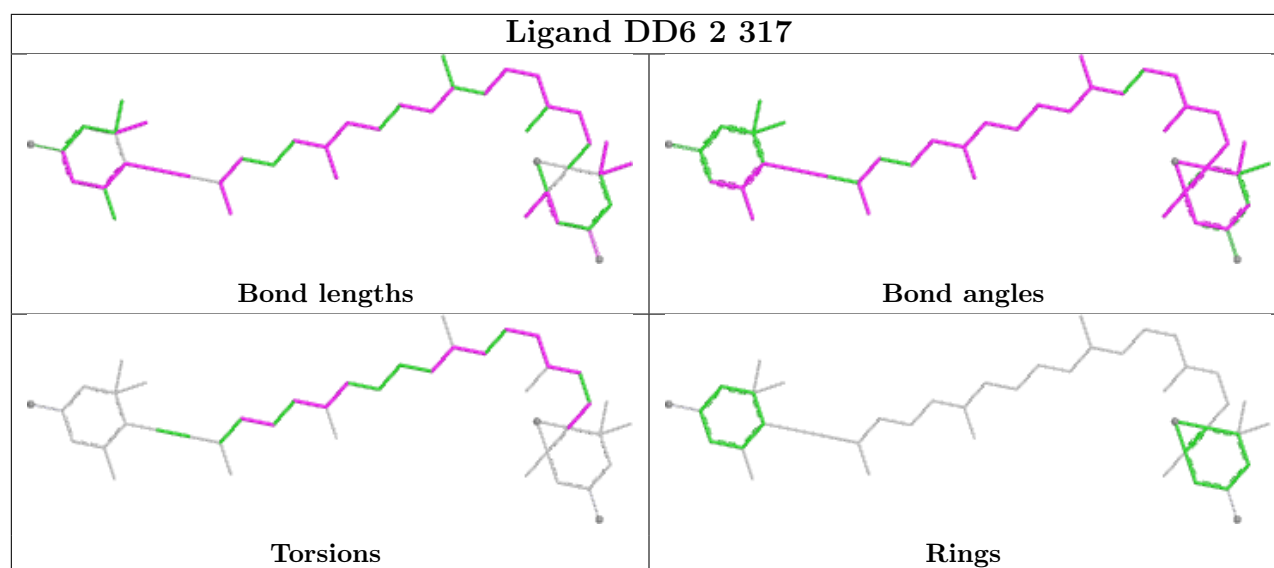


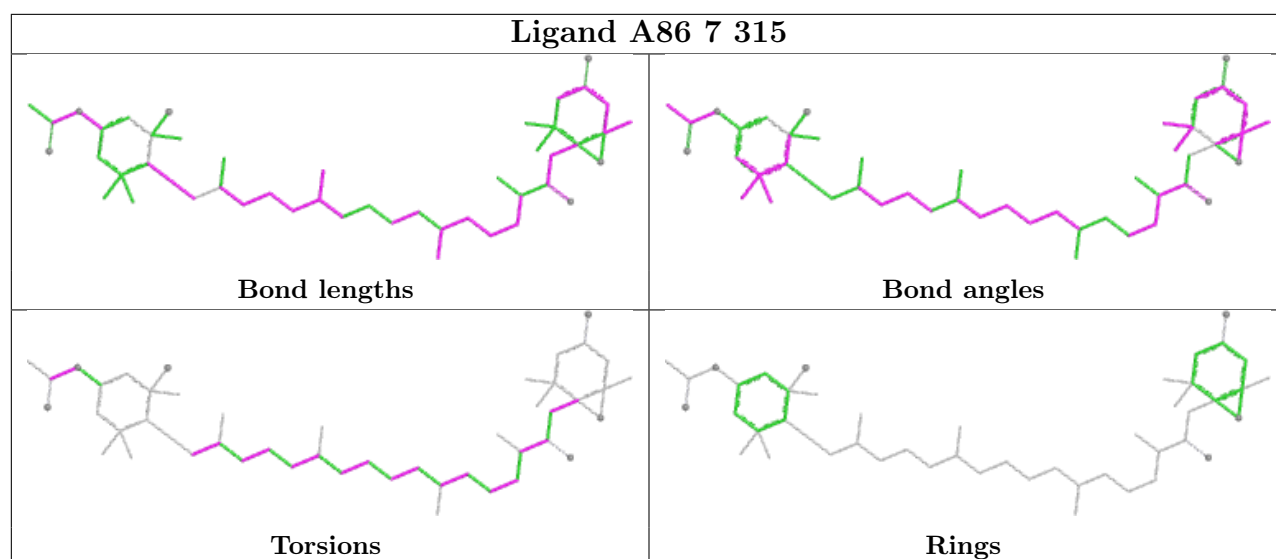
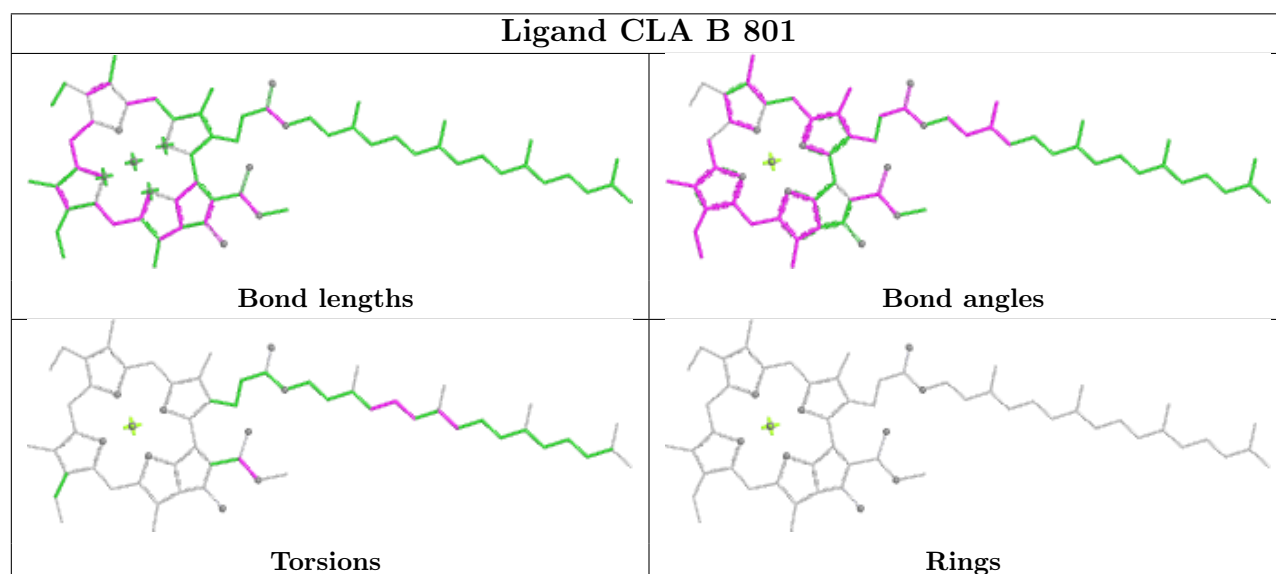
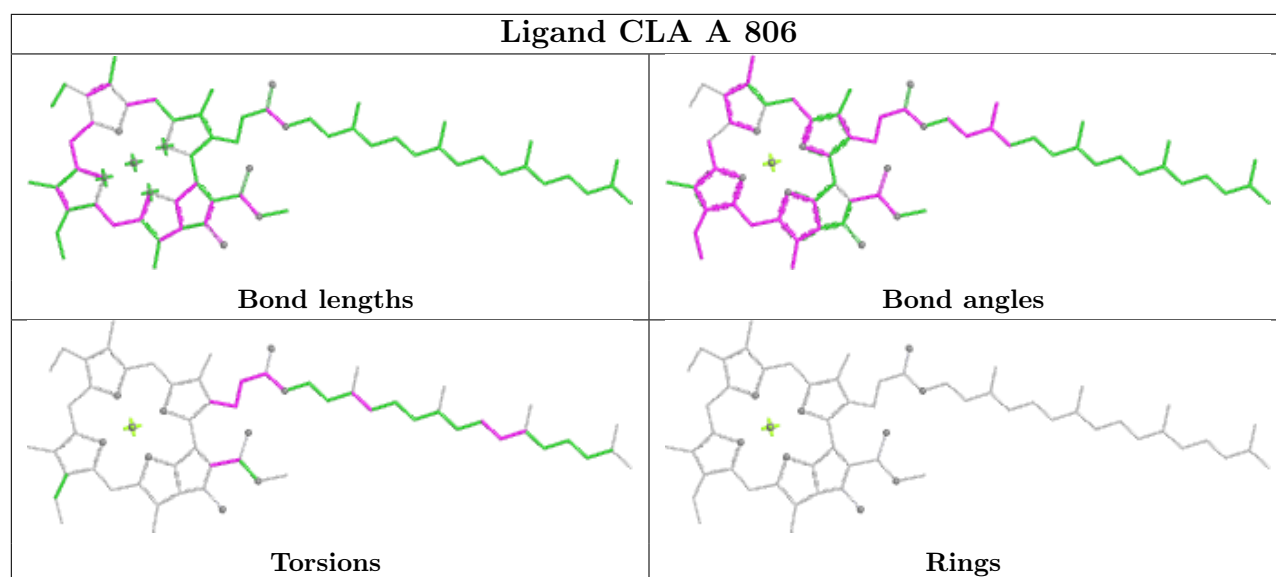
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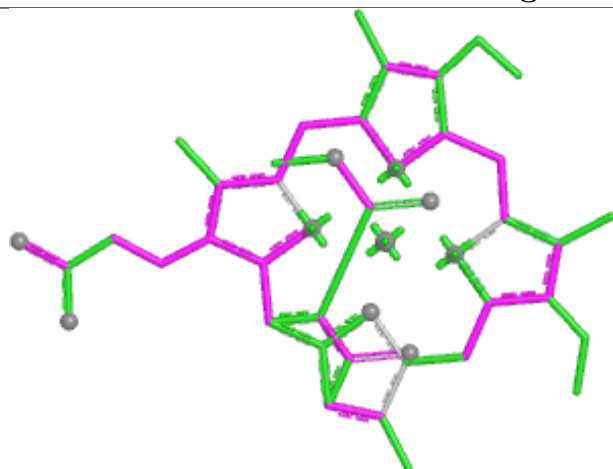
## Ligand CLA J 101



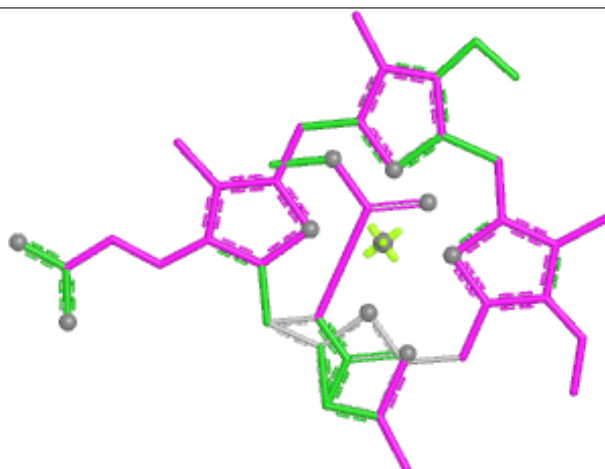




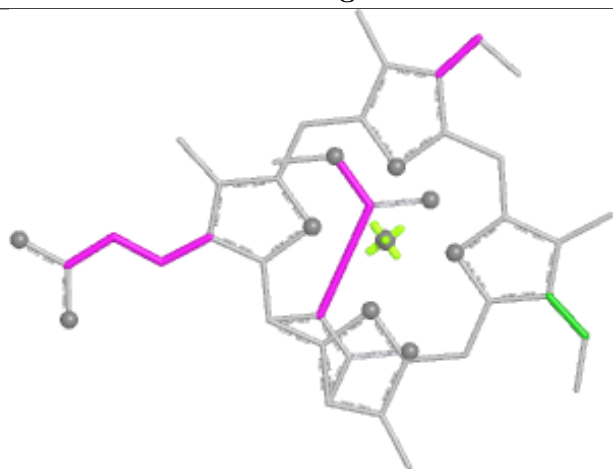
## Ligand KC1 6 311



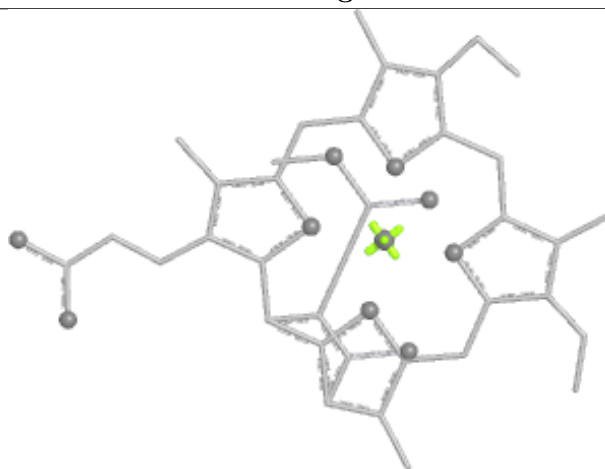
Bond lengths



Bond angles

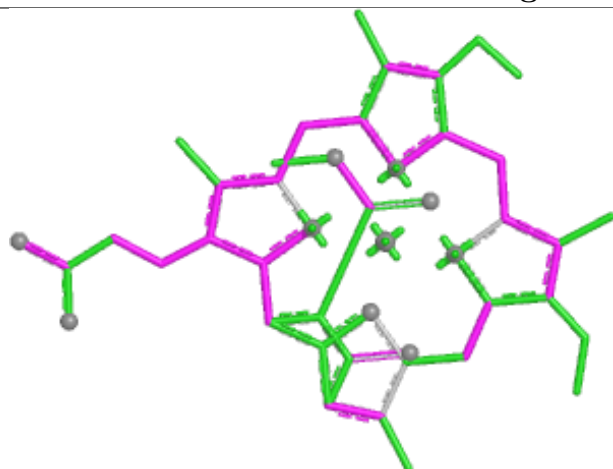


Torsions

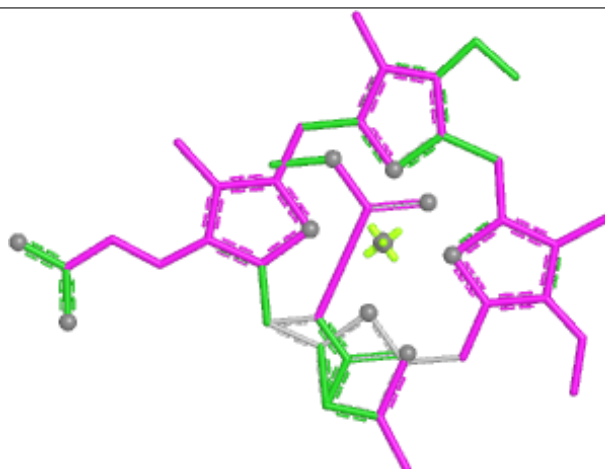


Rings

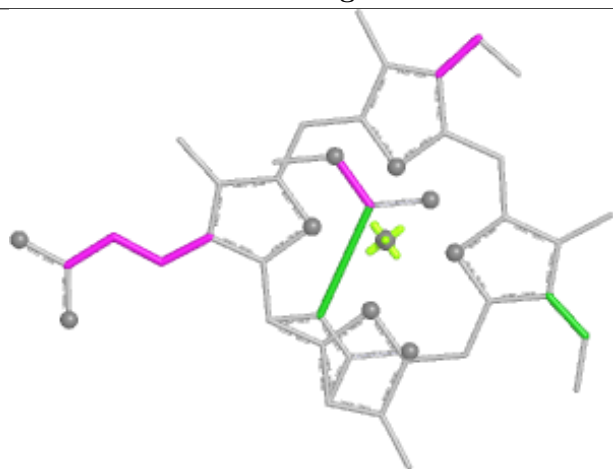
## Ligand KC1 8 307



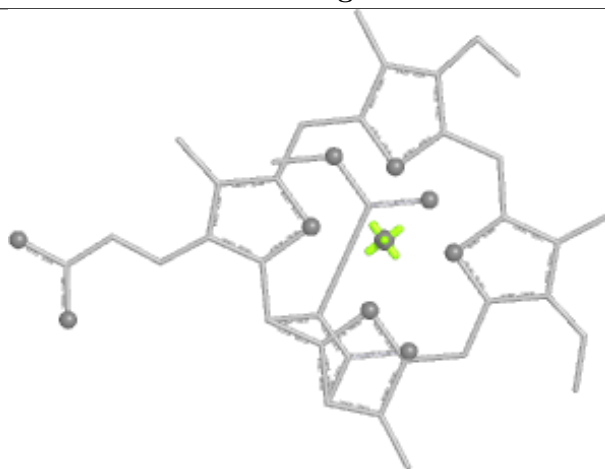
Bond lengths



Bond angles

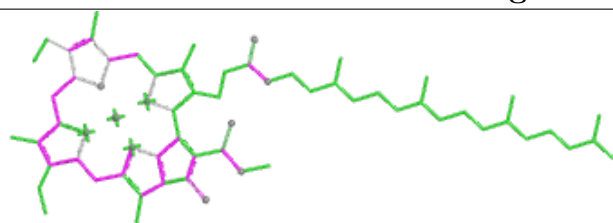


Torsions

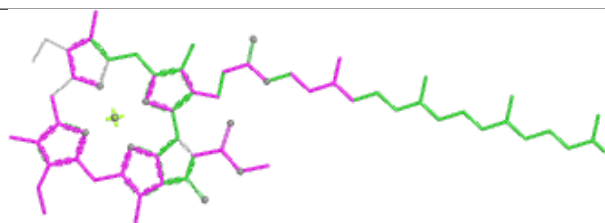


Rings

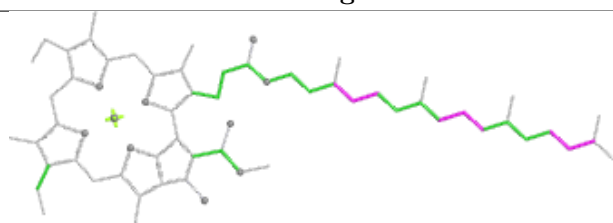
## Ligand CLA 16 302



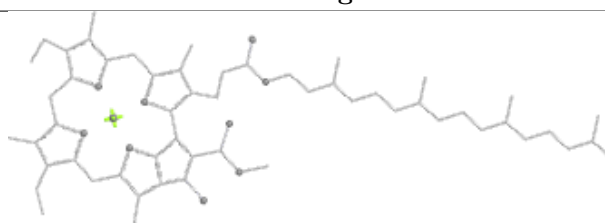
Bond lengths



Bond angles

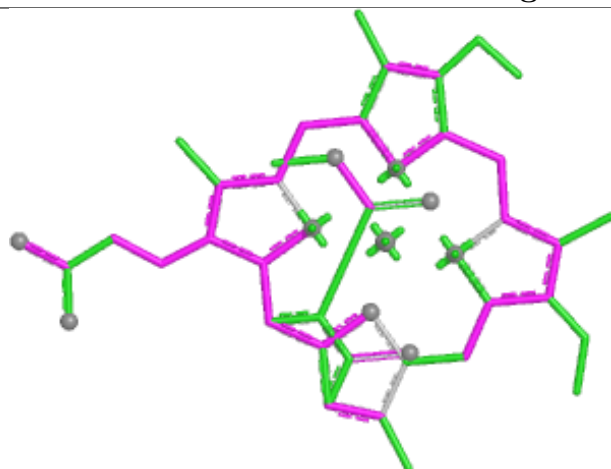


Torsions

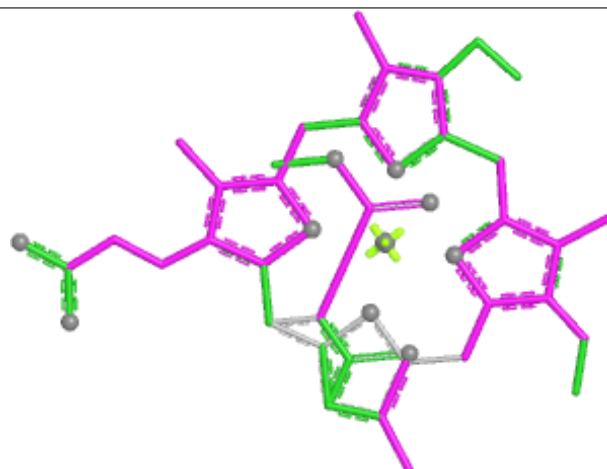


Rings

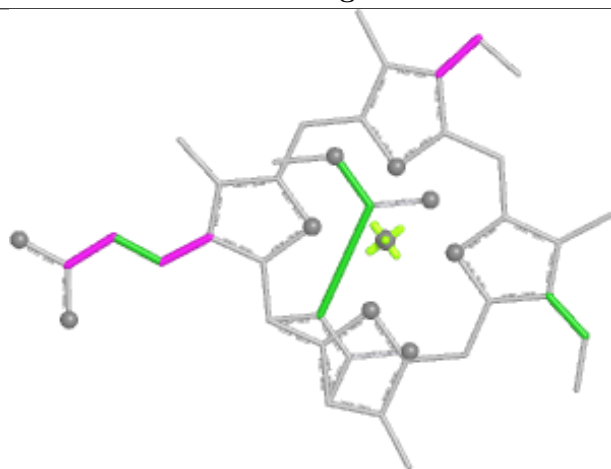
## Ligand KC1 5 305



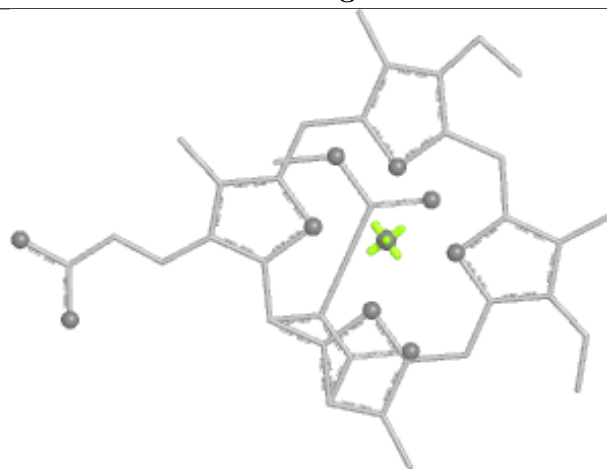
Bond lengths



Bond angles

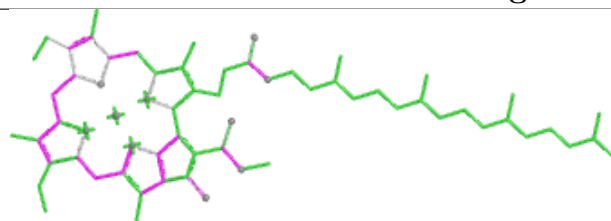


Torsions

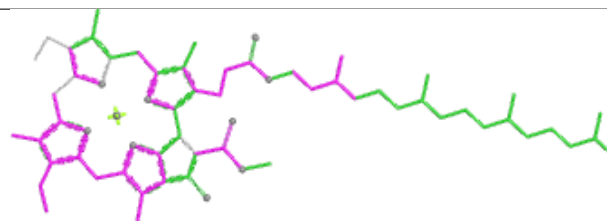


Rings

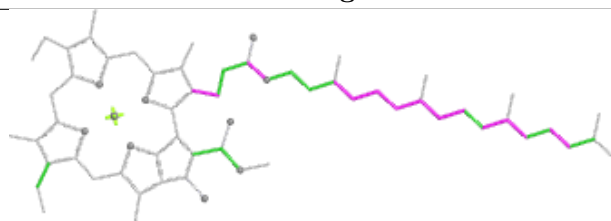
## Ligand CLA 16 303



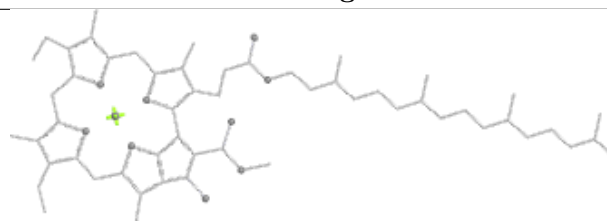
Bond lengths



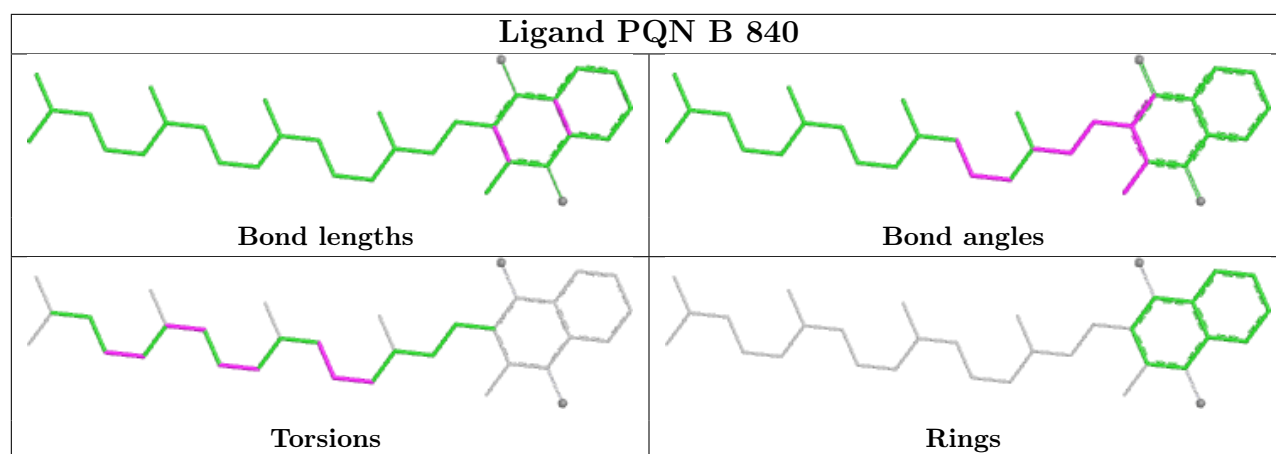
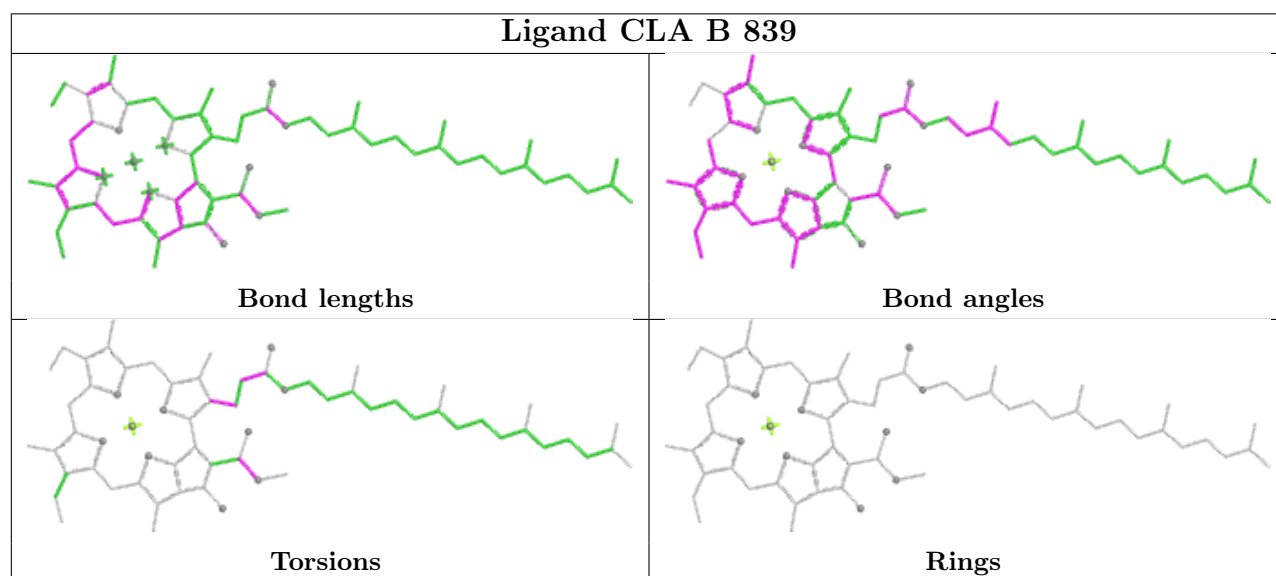
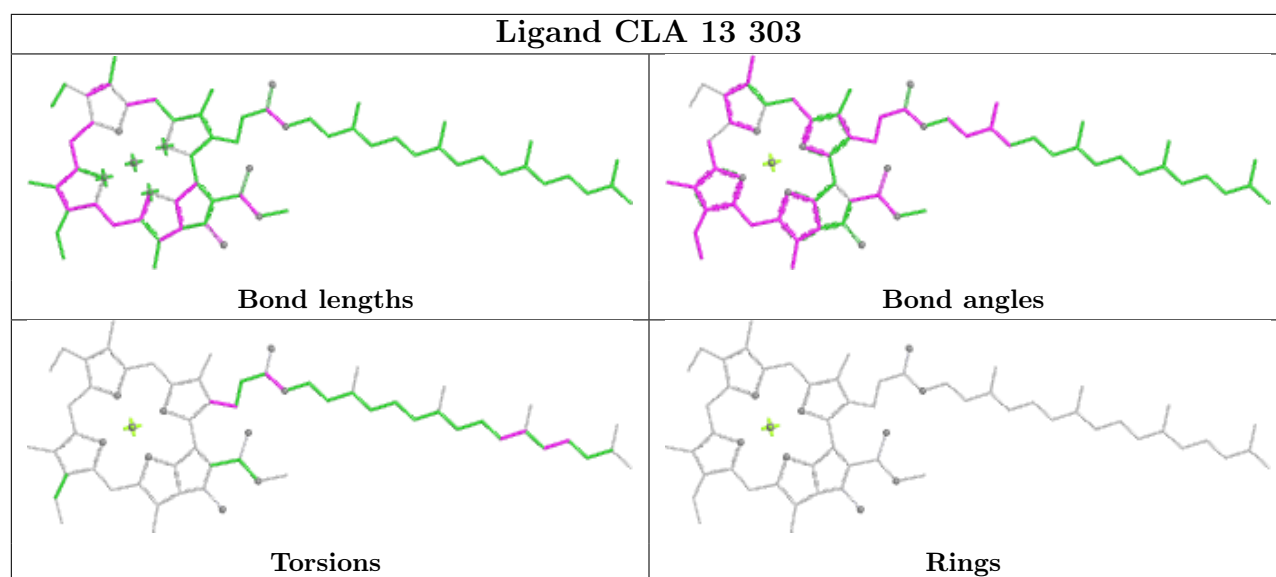
Bond angles

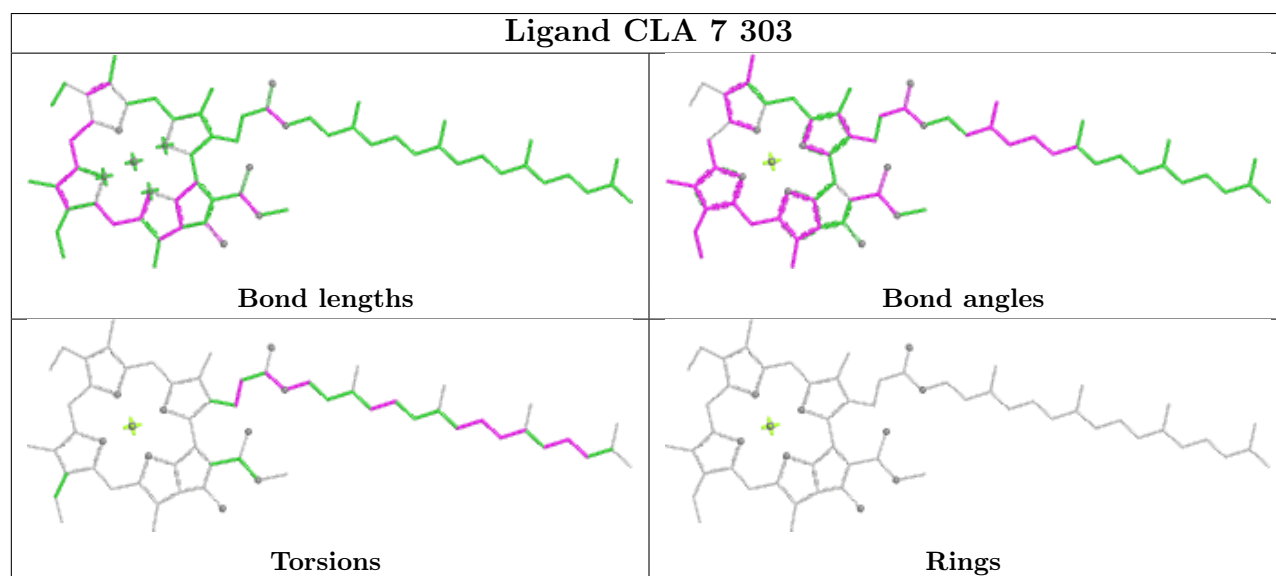
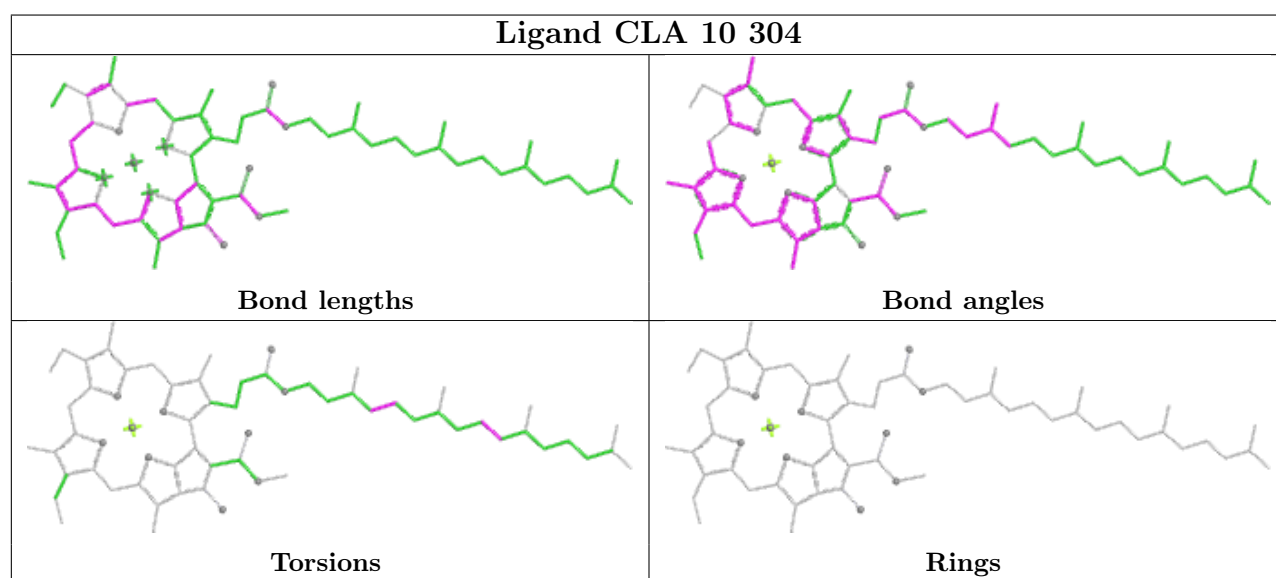
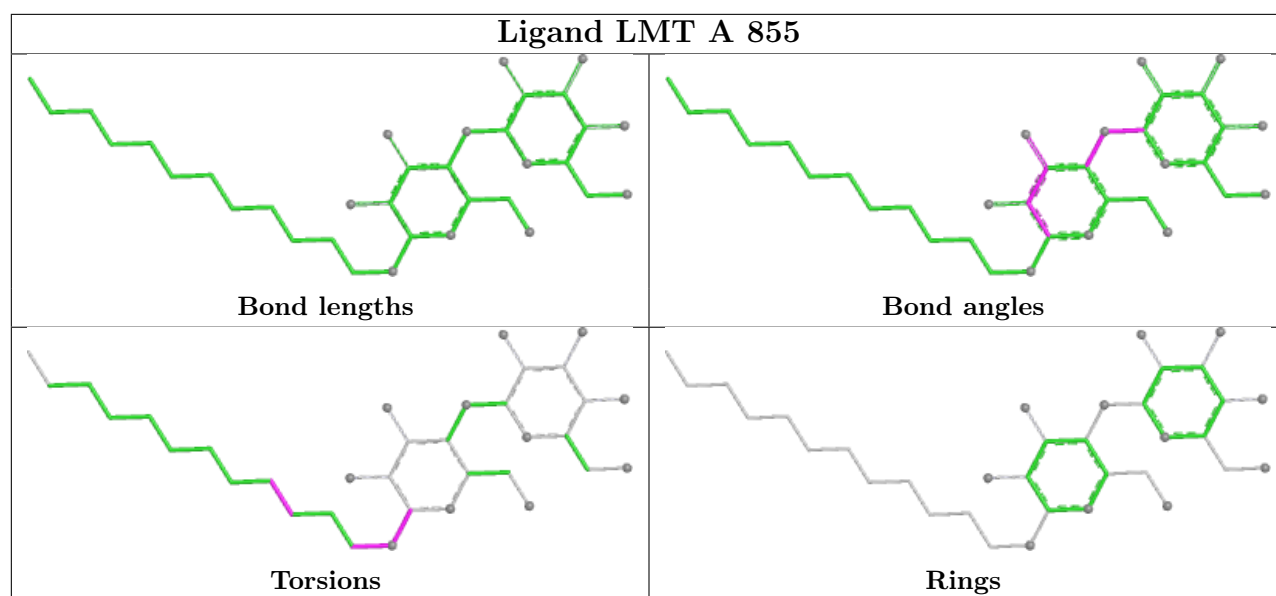


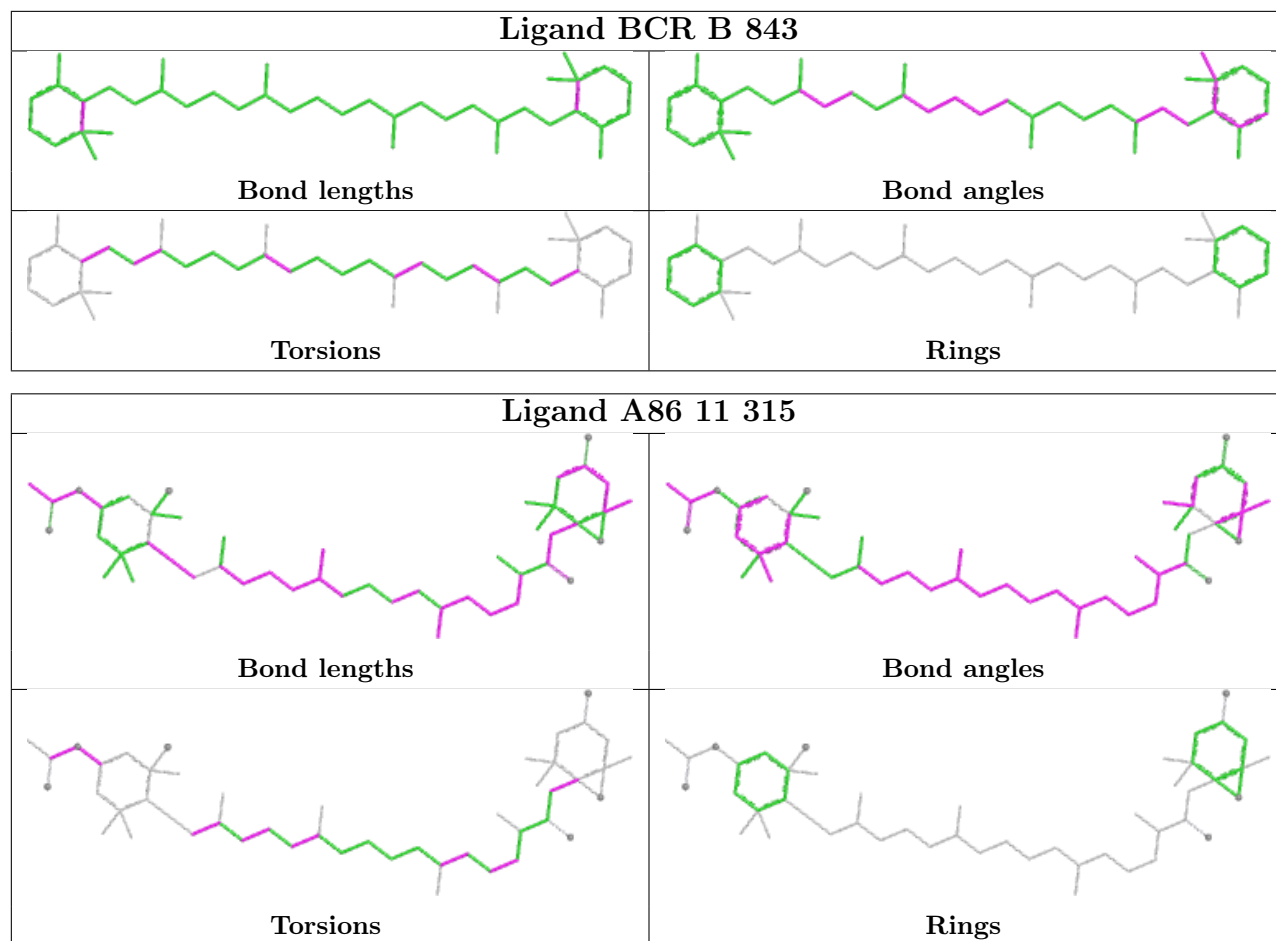
Torsions



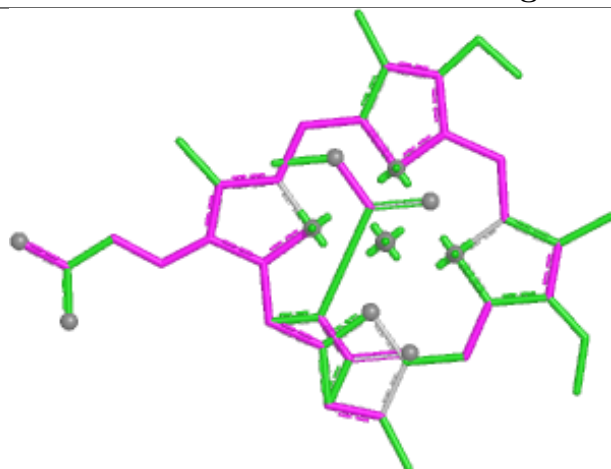
Rings



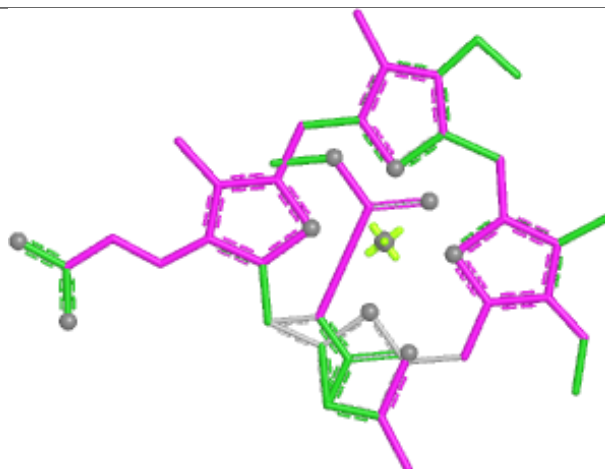




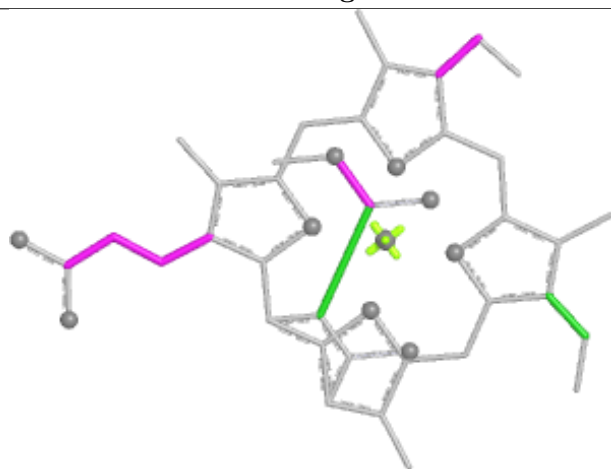
## Ligand KC1 7 308



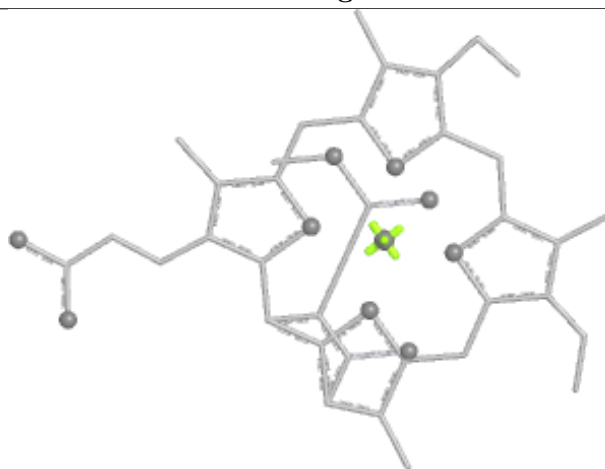
Bond lengths



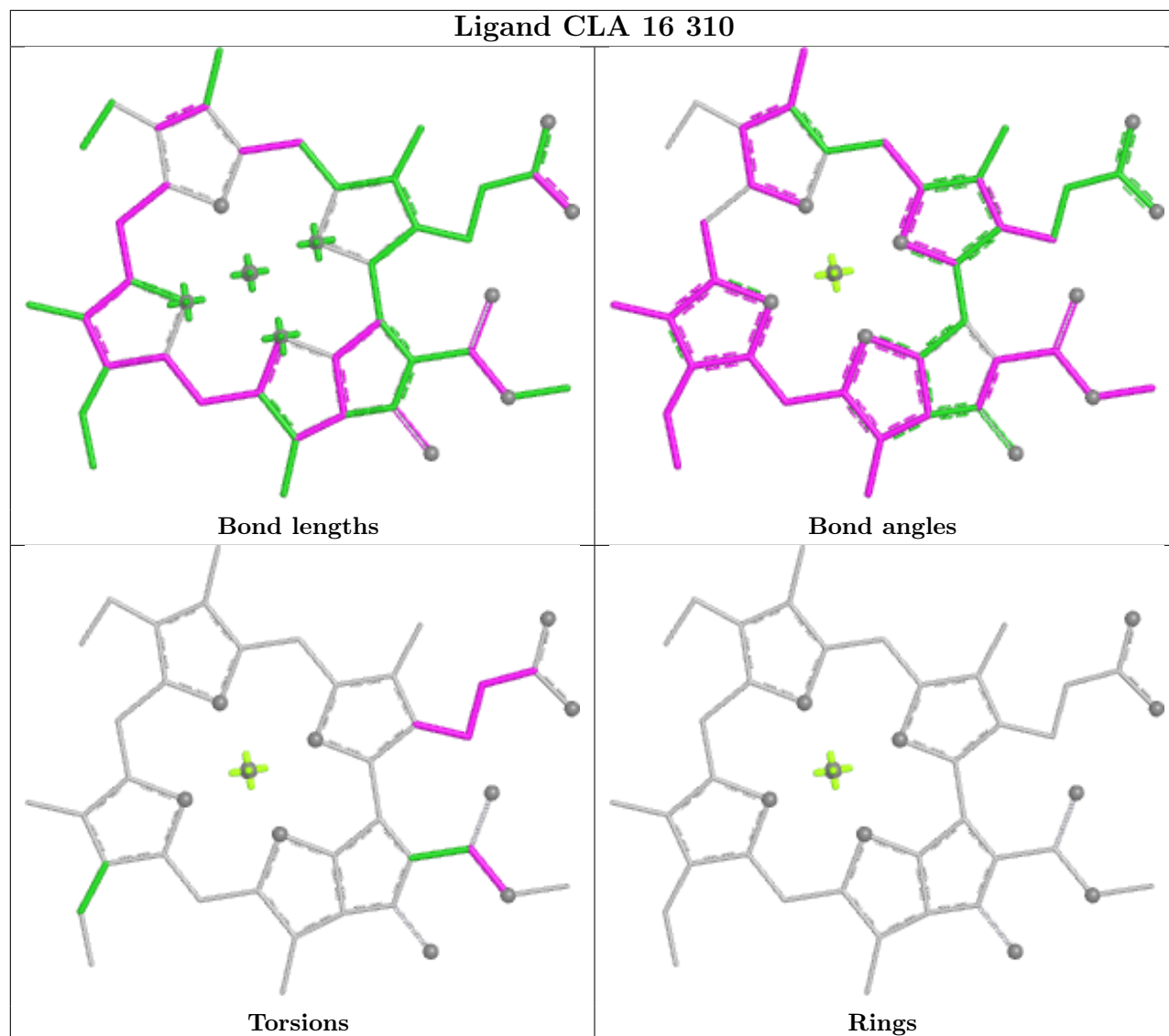
Bond angles

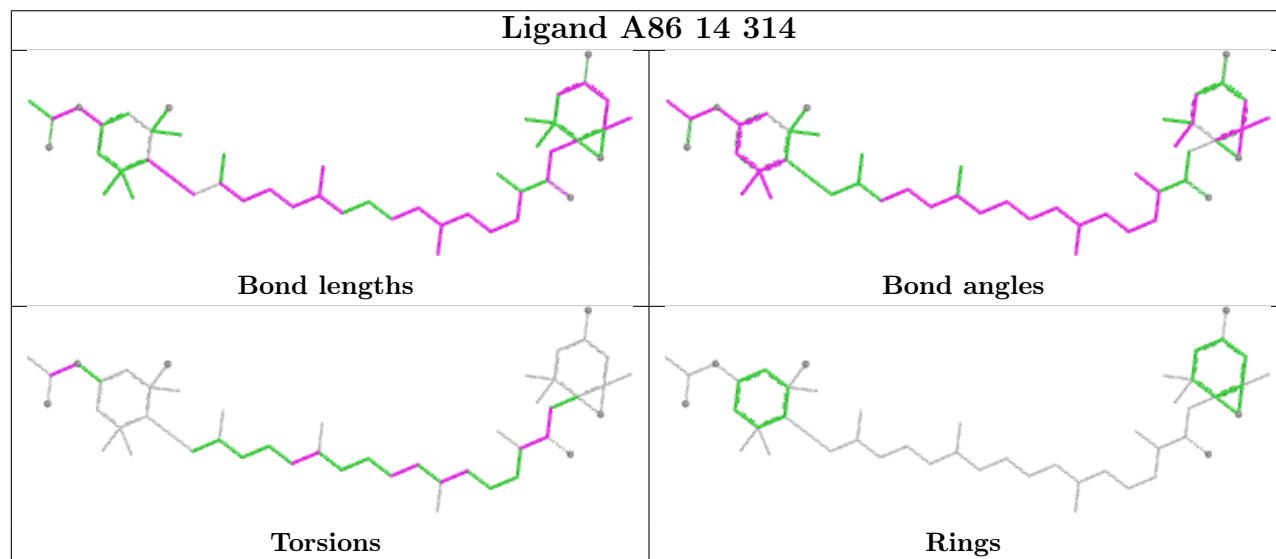
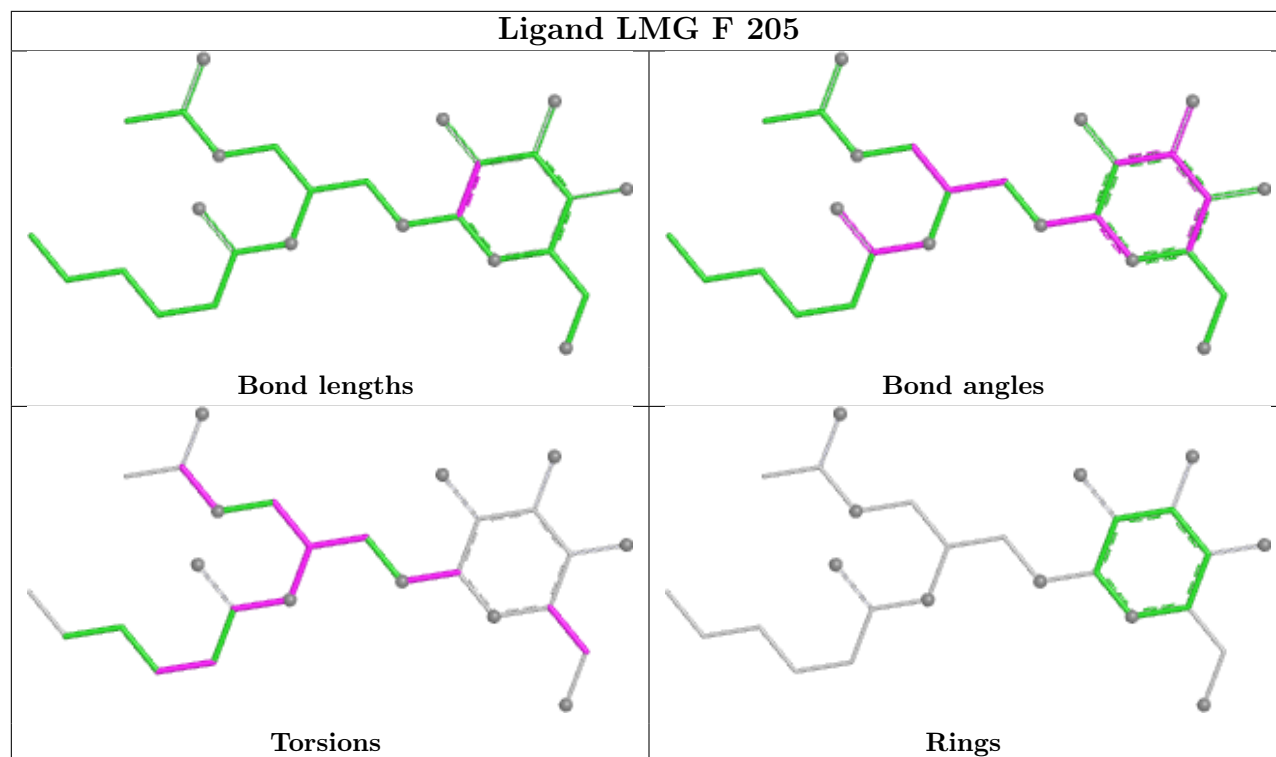


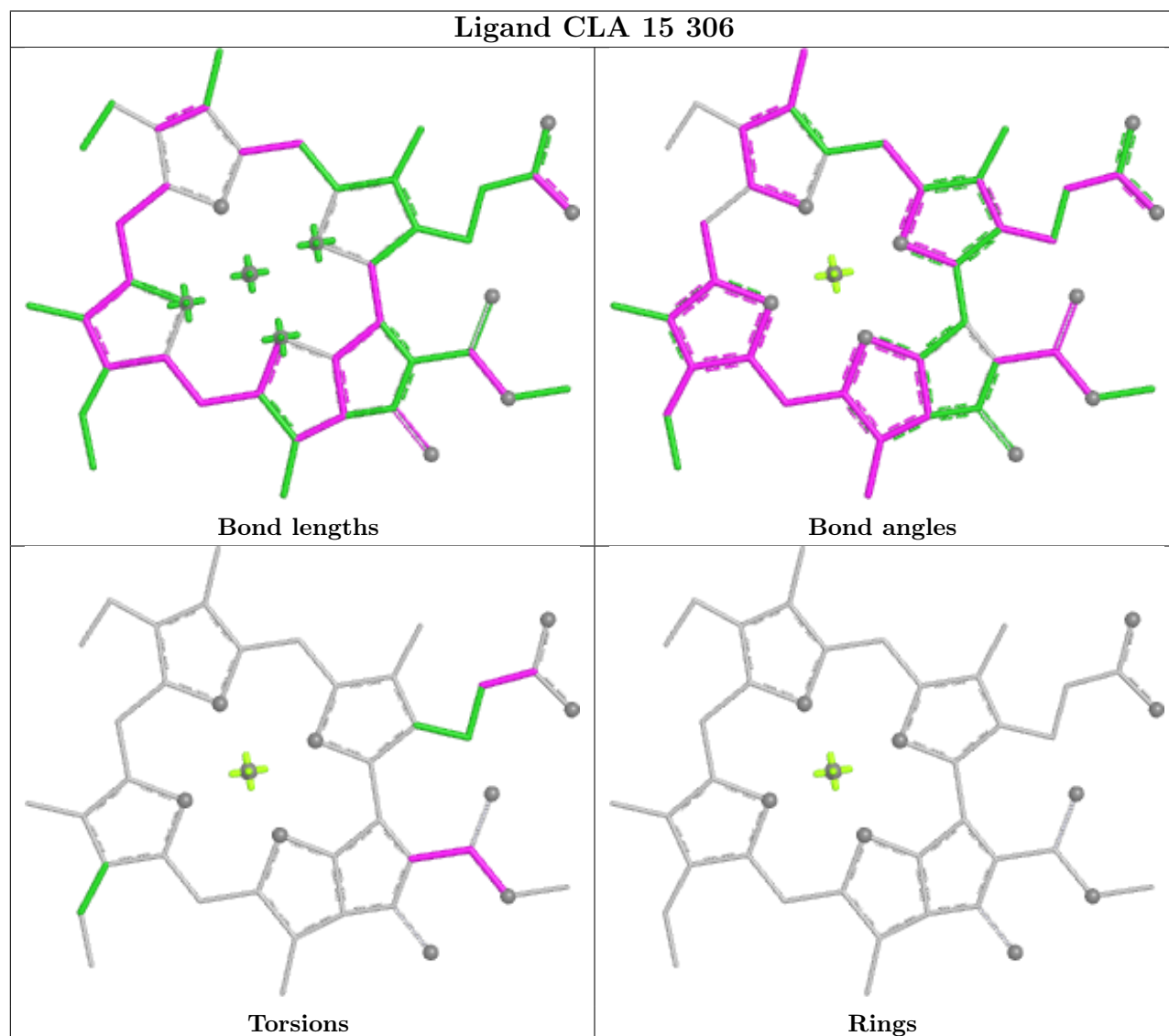
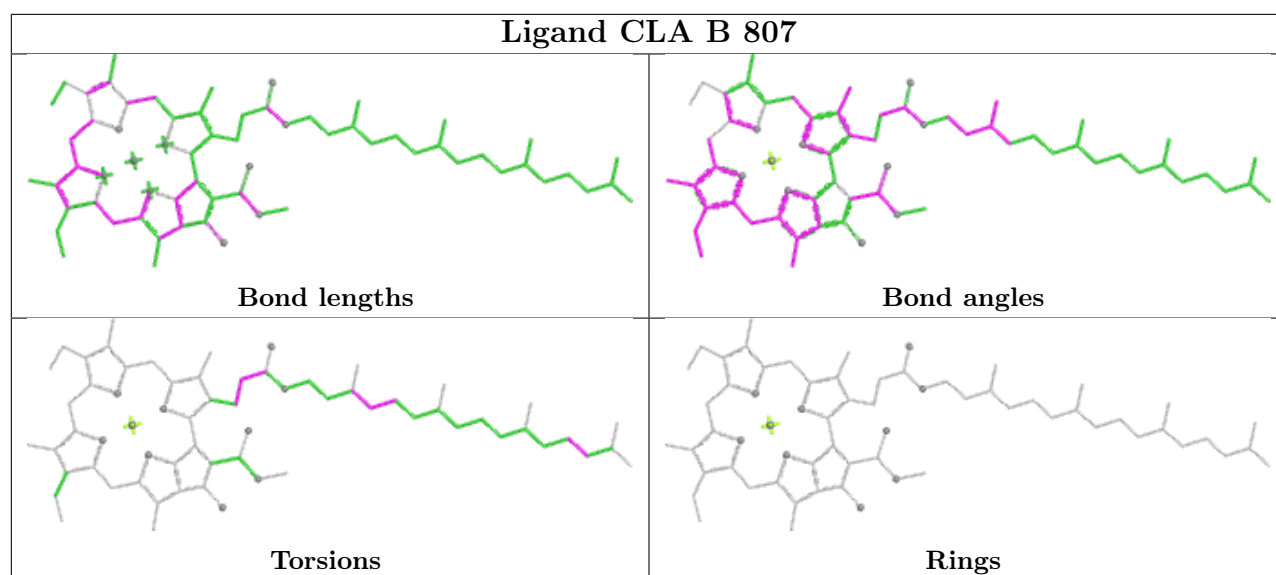
Torsions

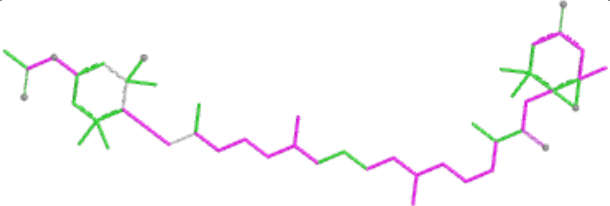
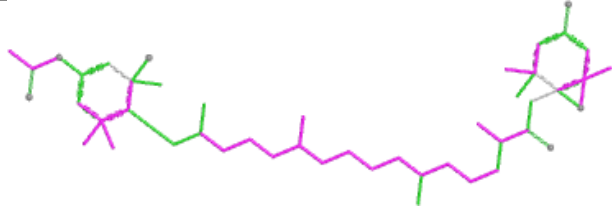
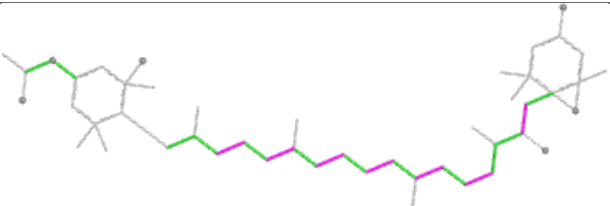
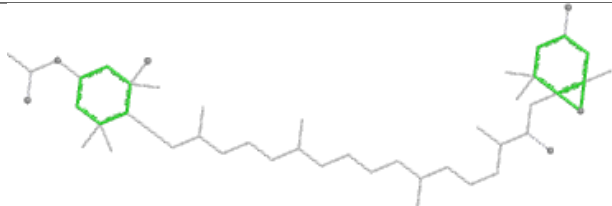
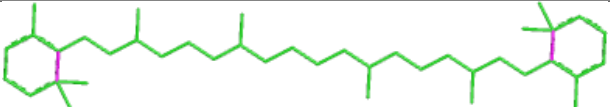
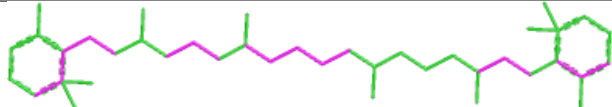
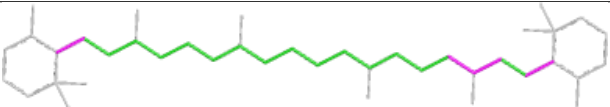
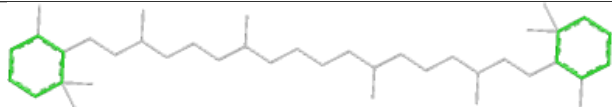
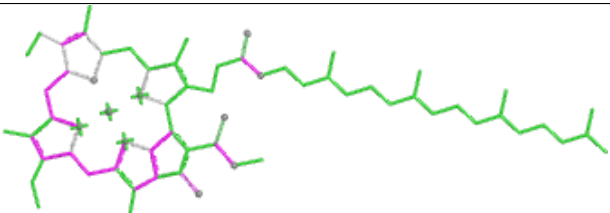
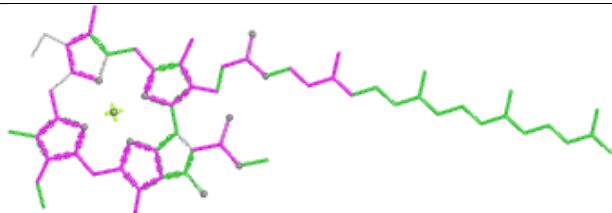
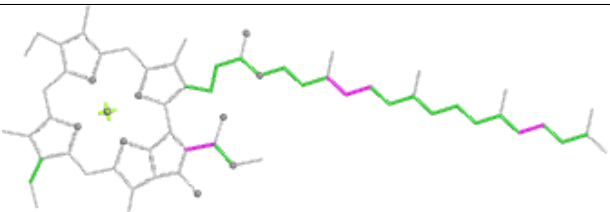
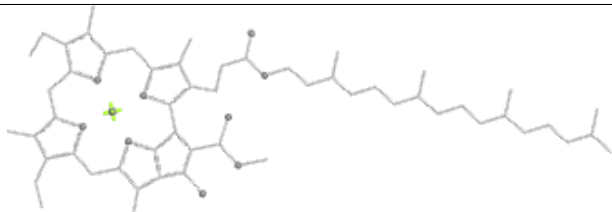


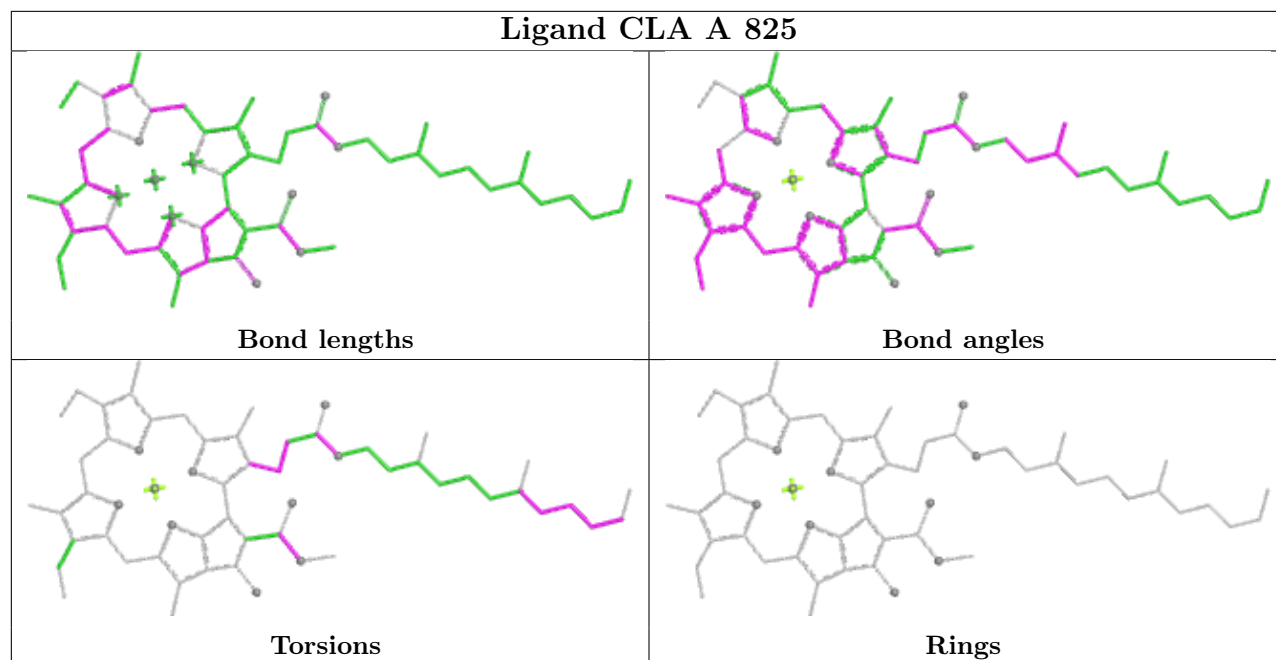
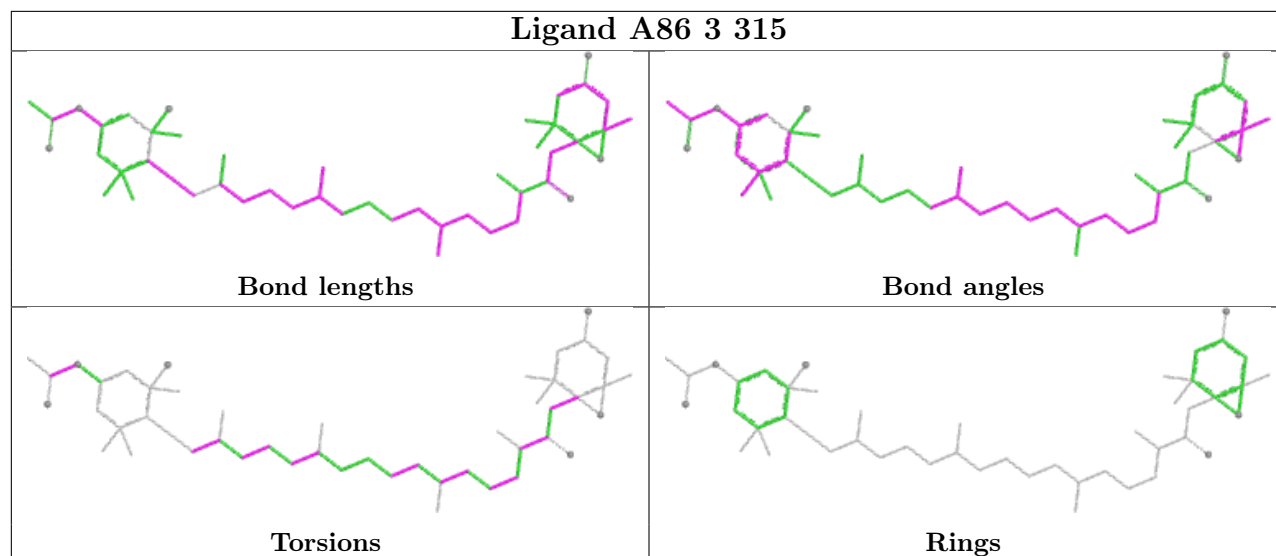
Rings

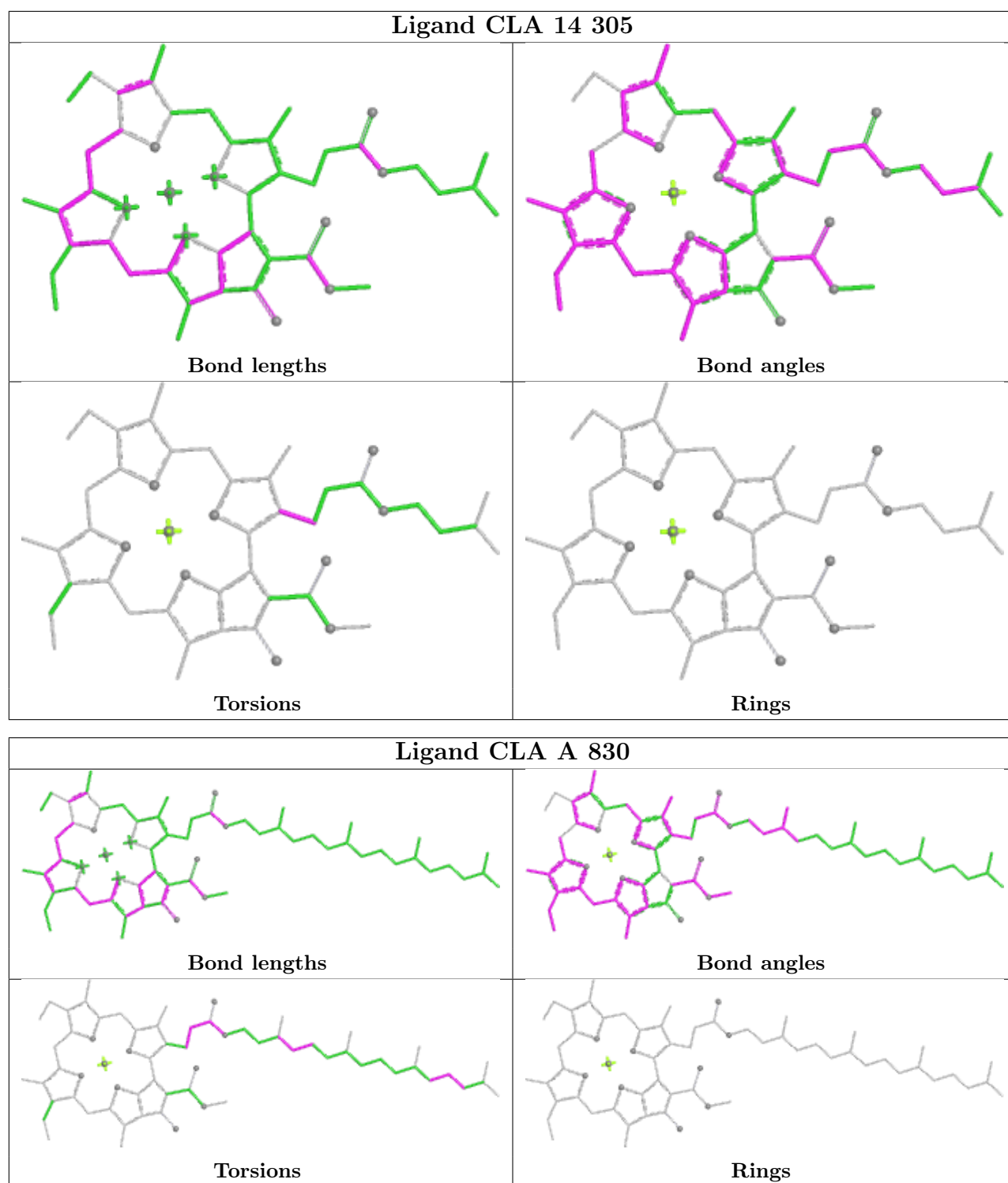


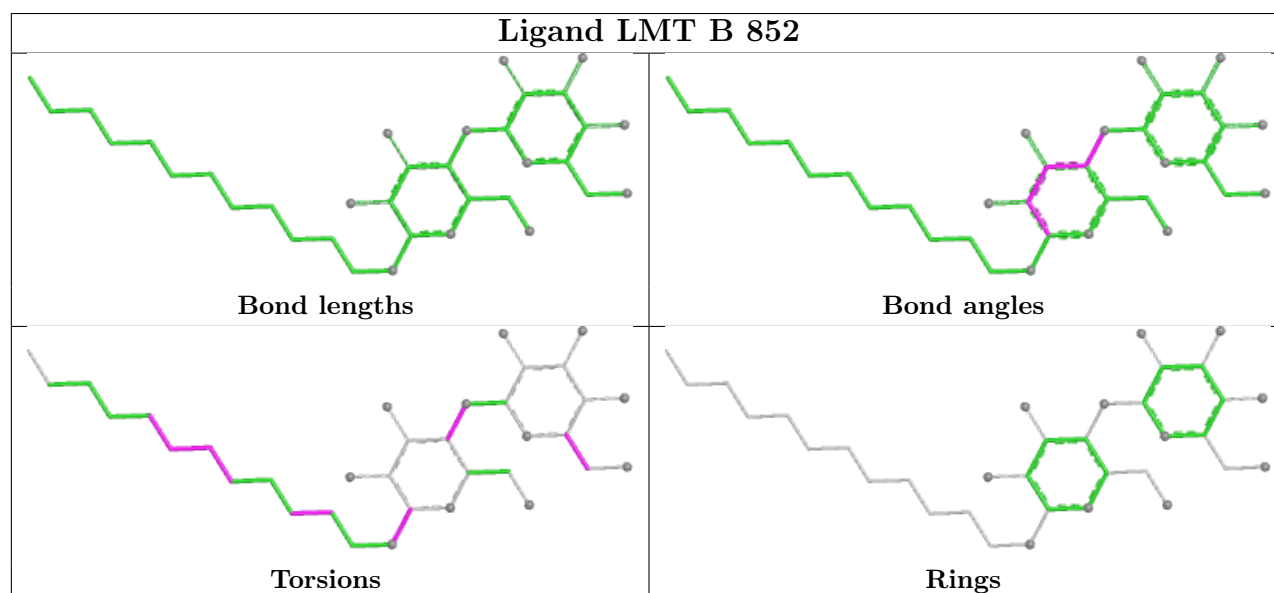
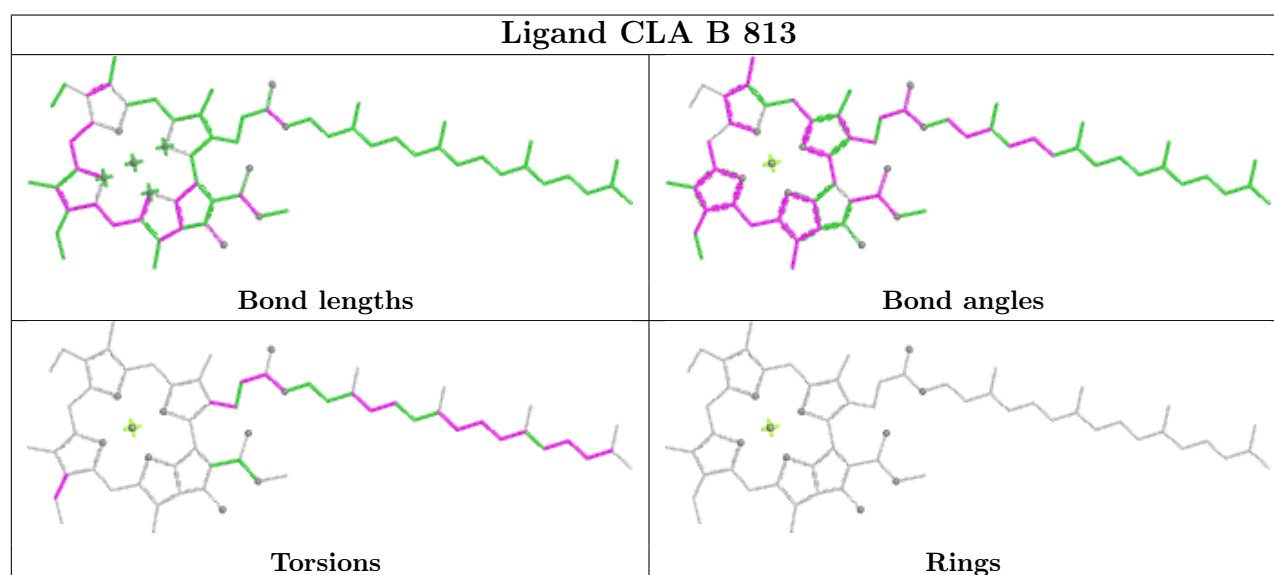
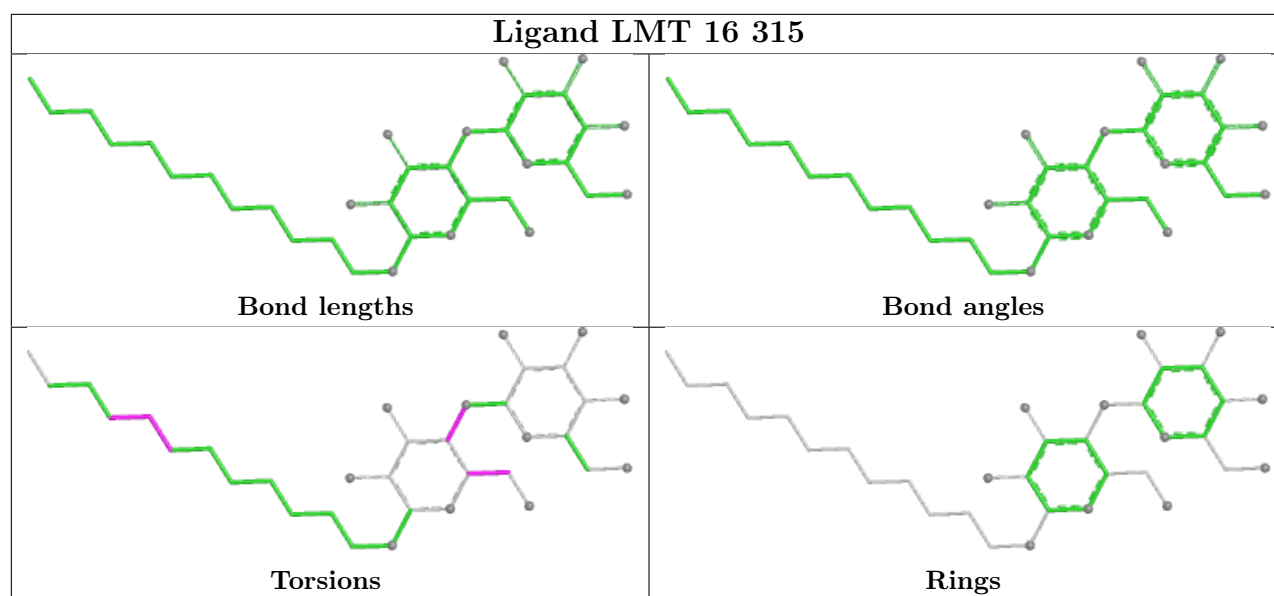


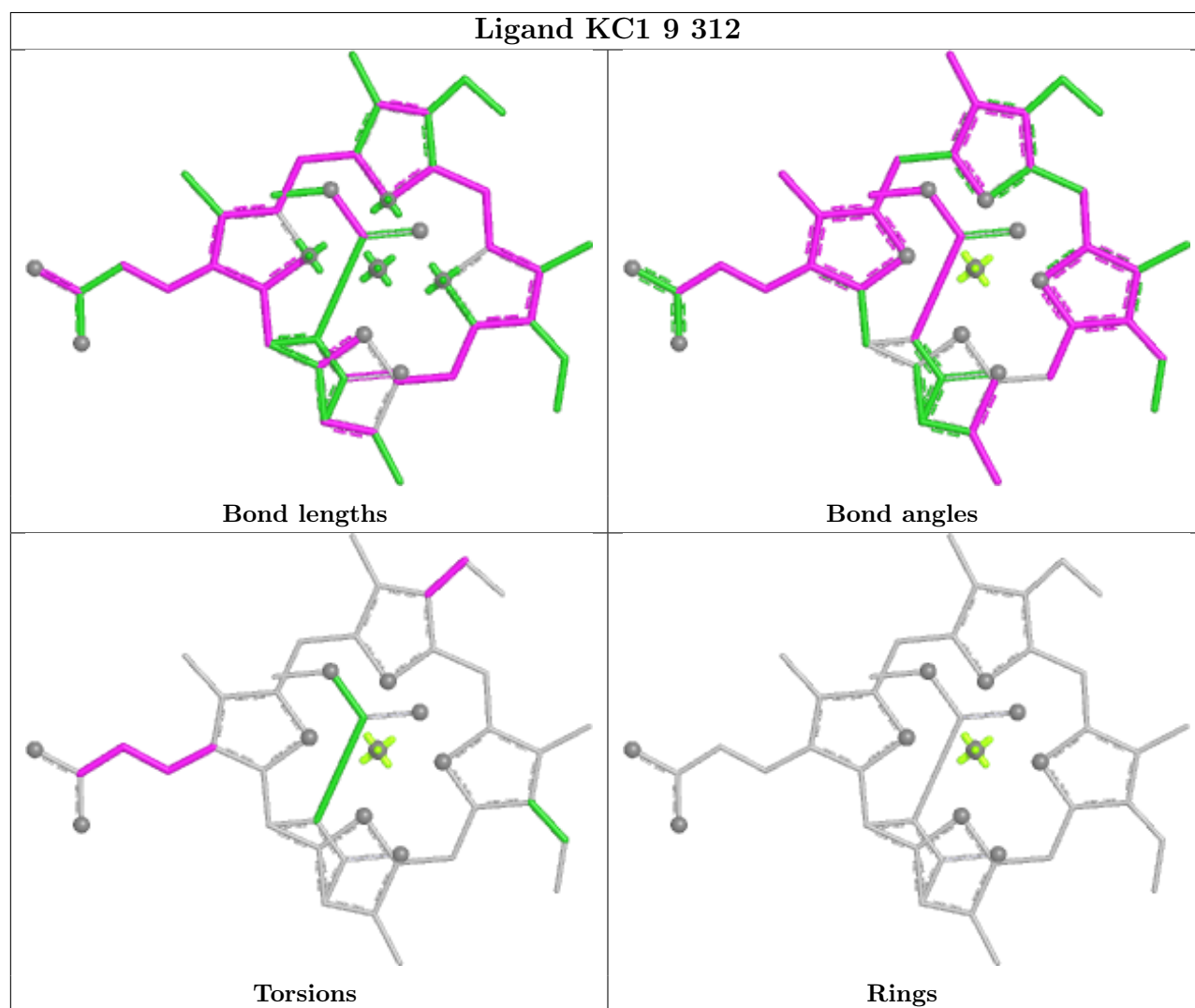
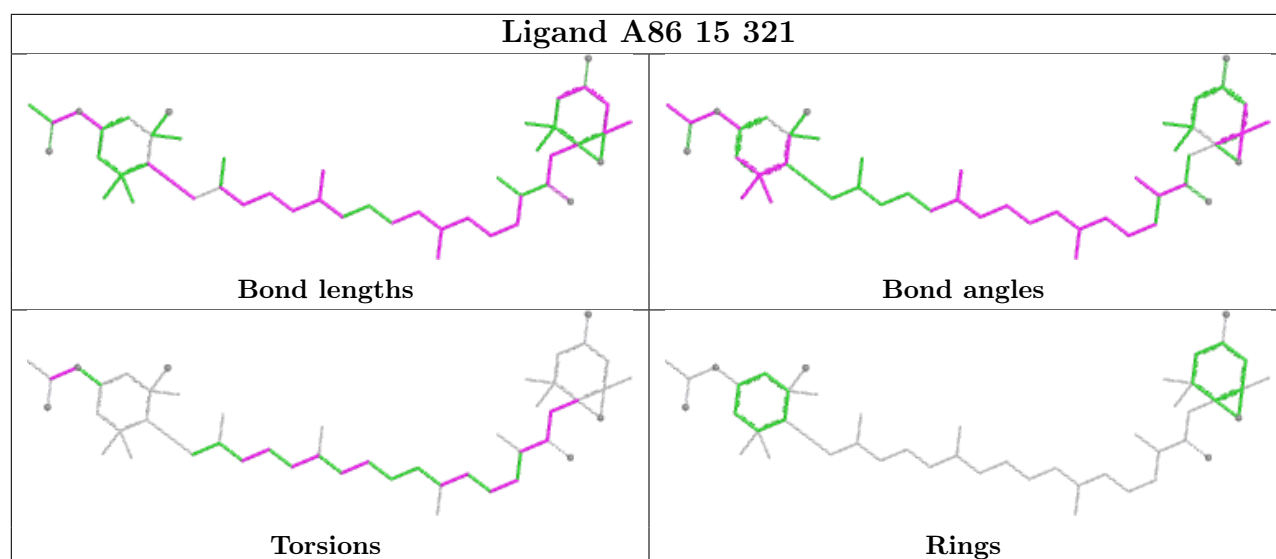


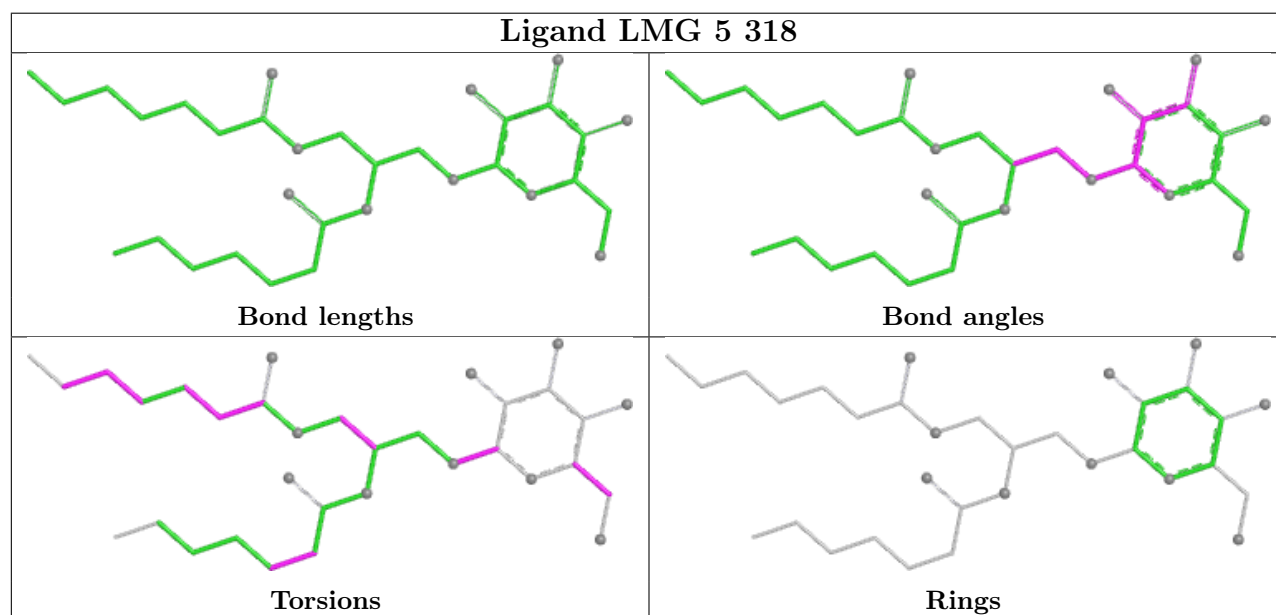
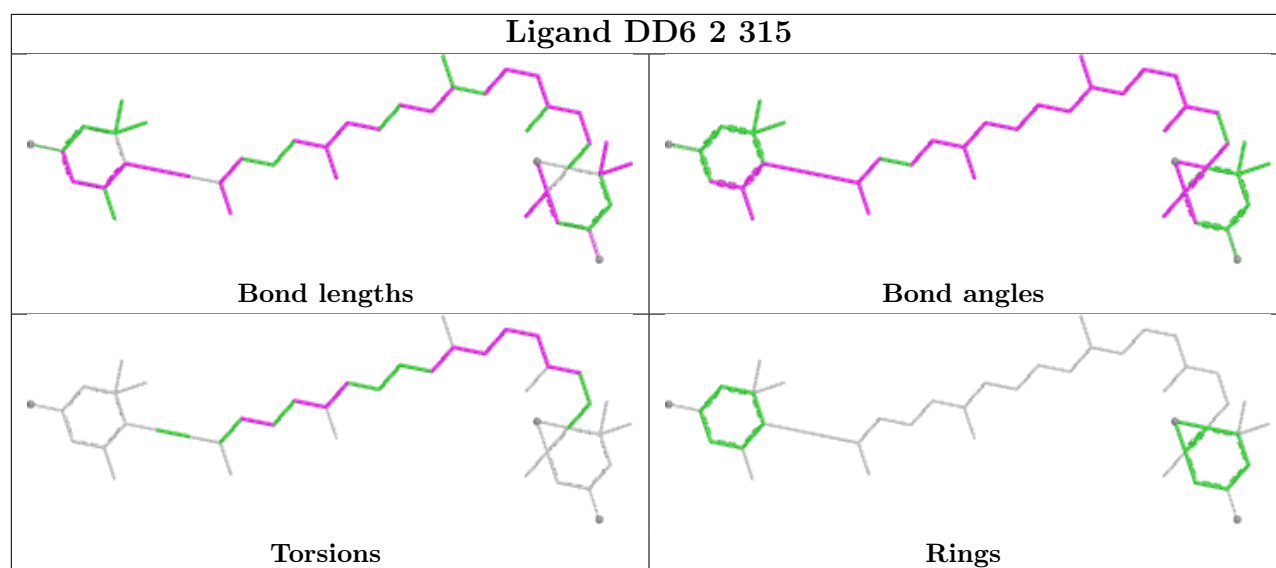
Ligand A86 14 315	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 851	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 824	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

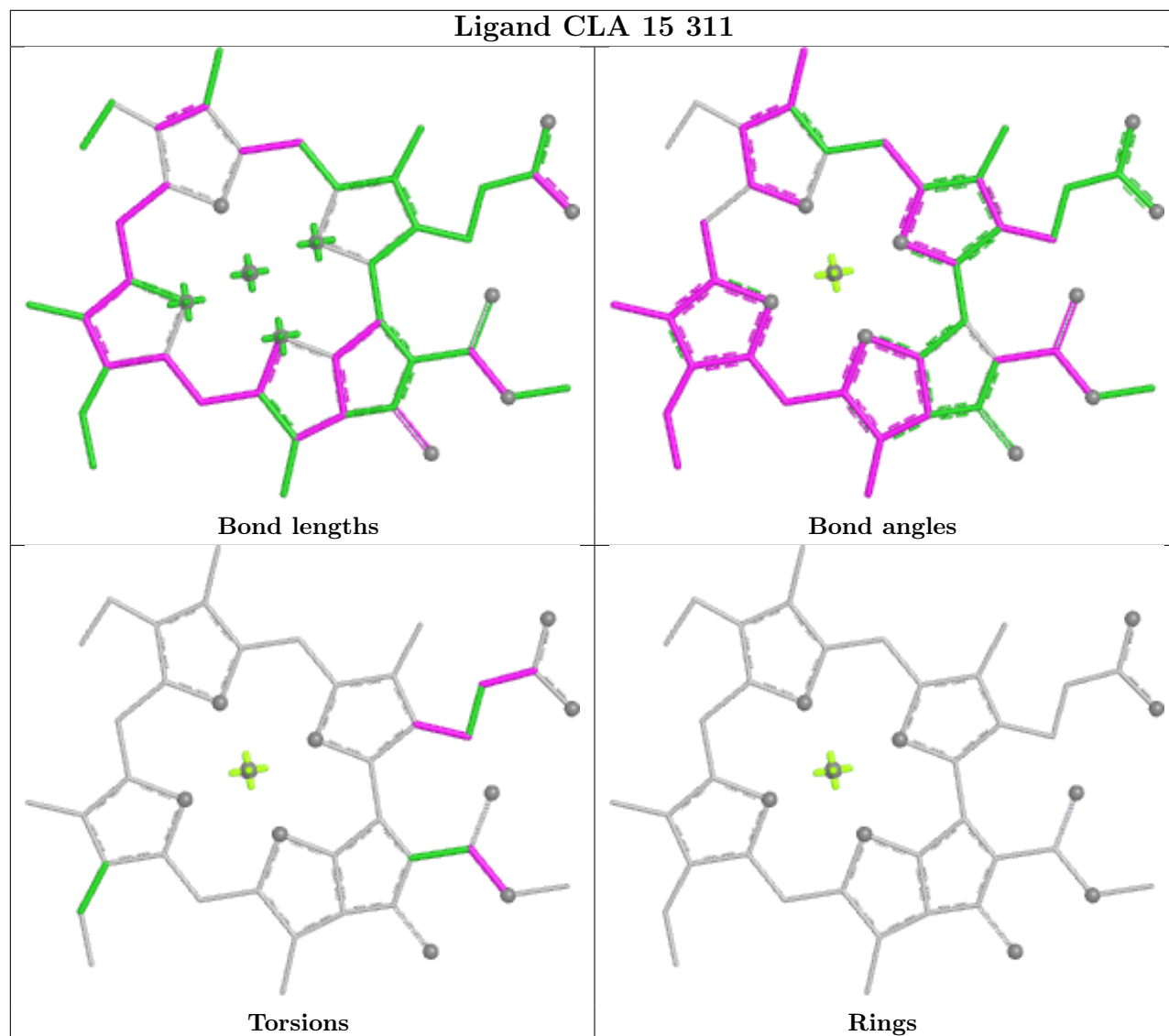
**Ligand CLA A 825****Ligand A86 3 315**

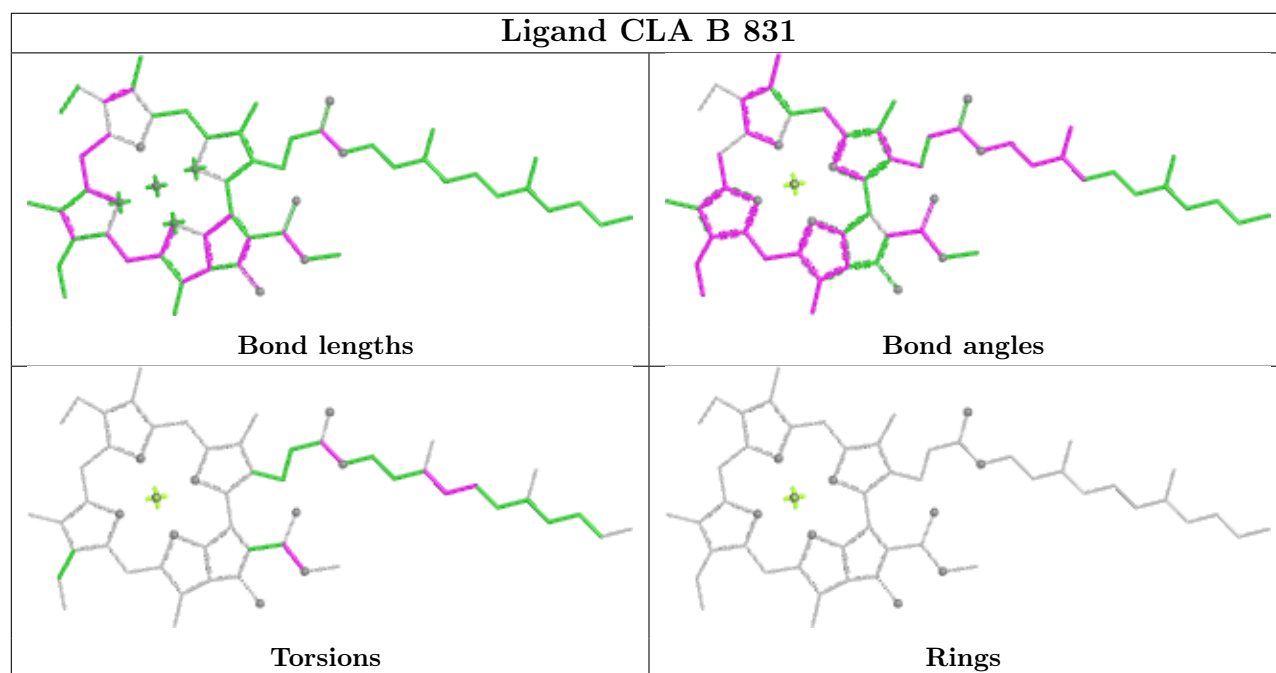
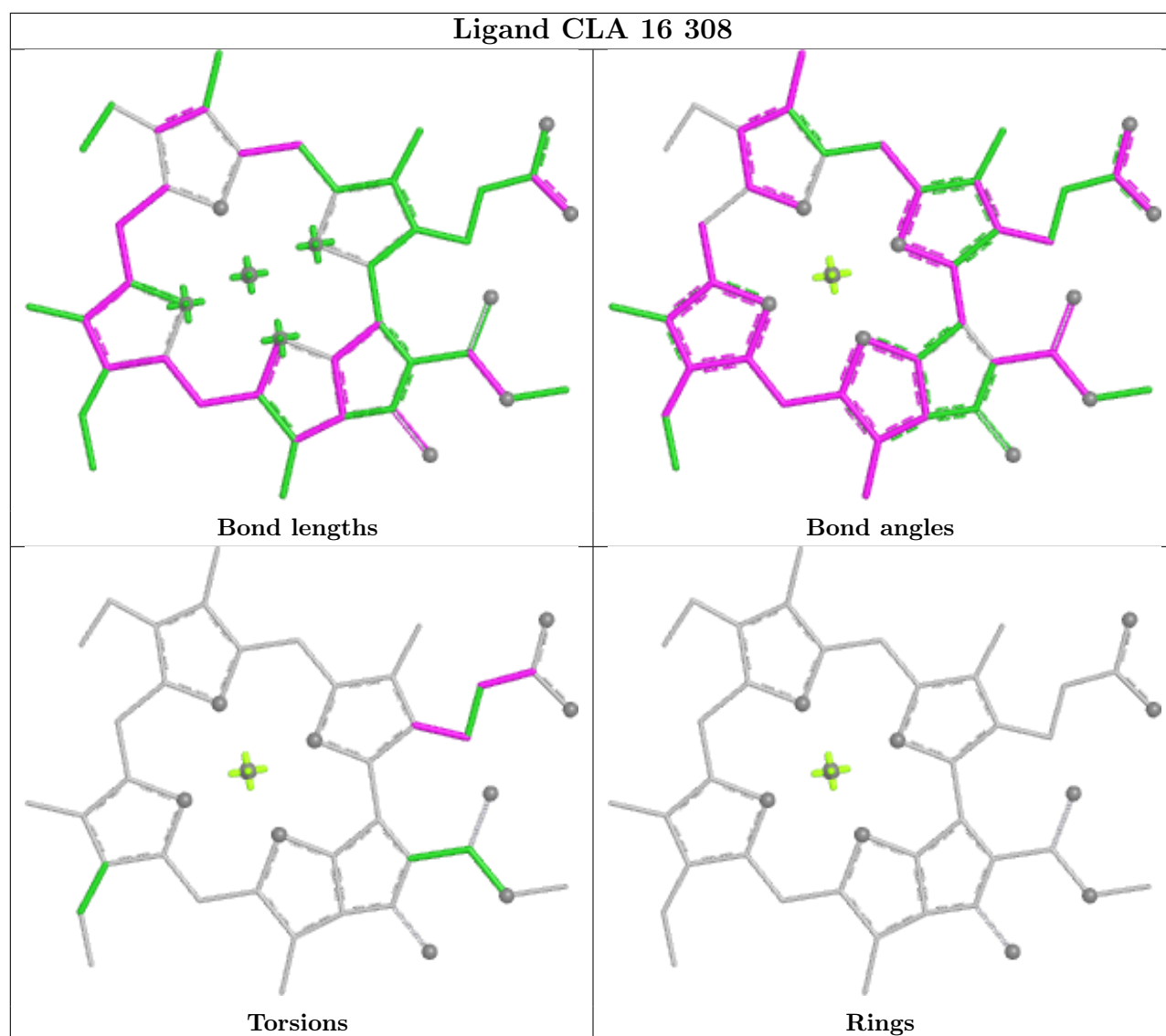




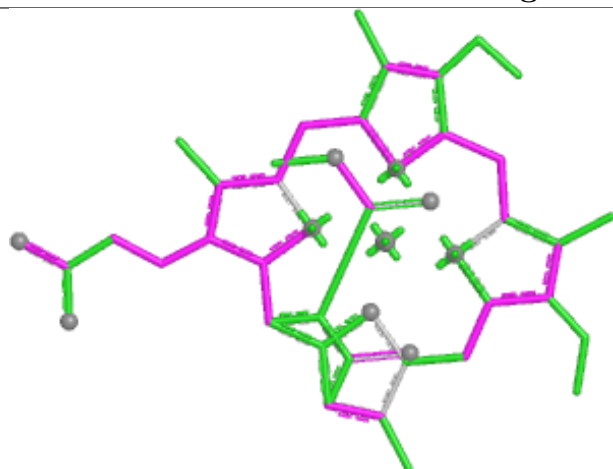




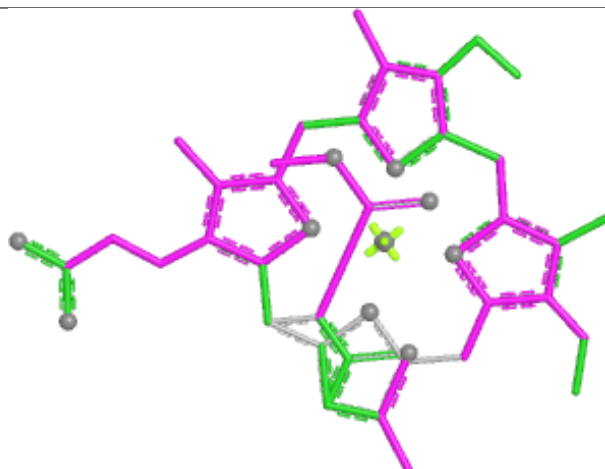




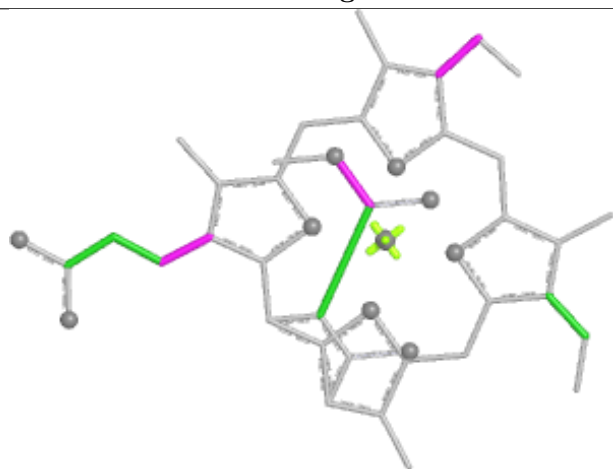
## Ligand KC1 8 311



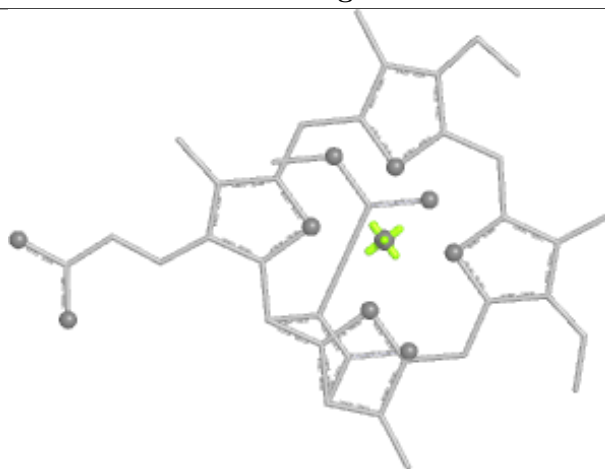
Bond lengths



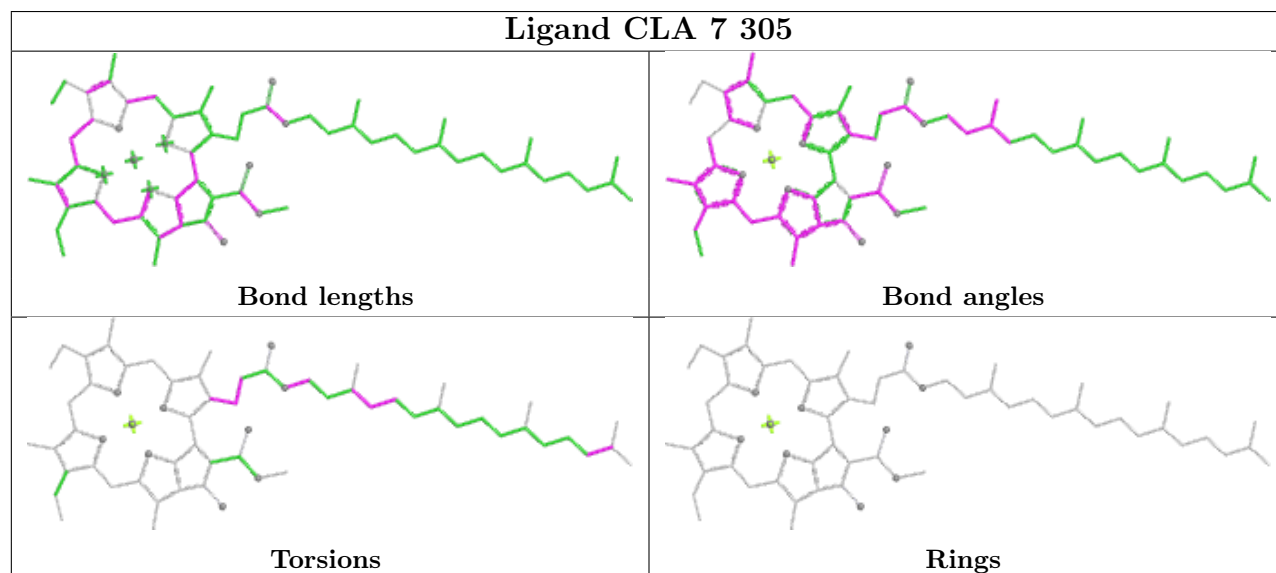
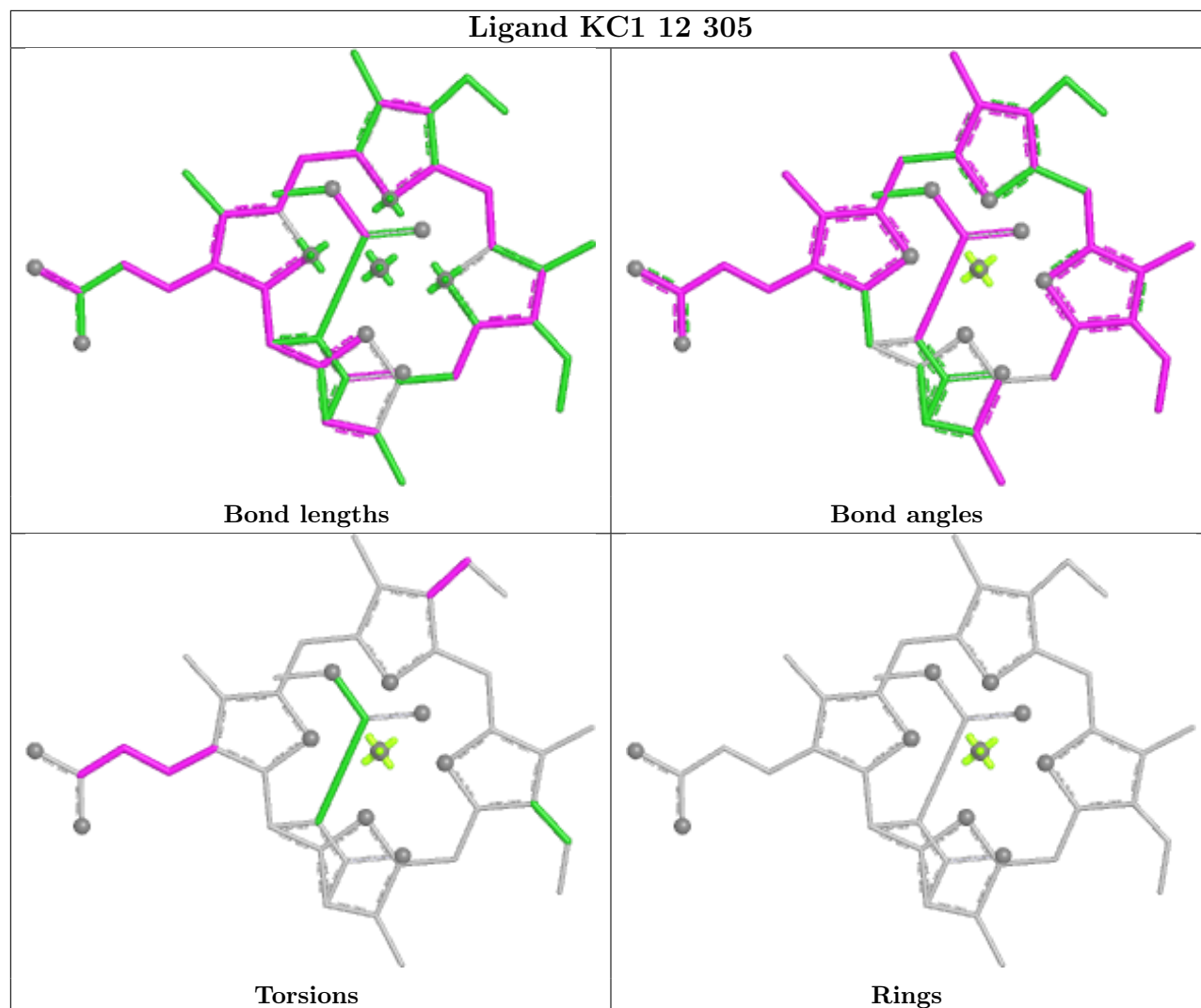
Bond angles

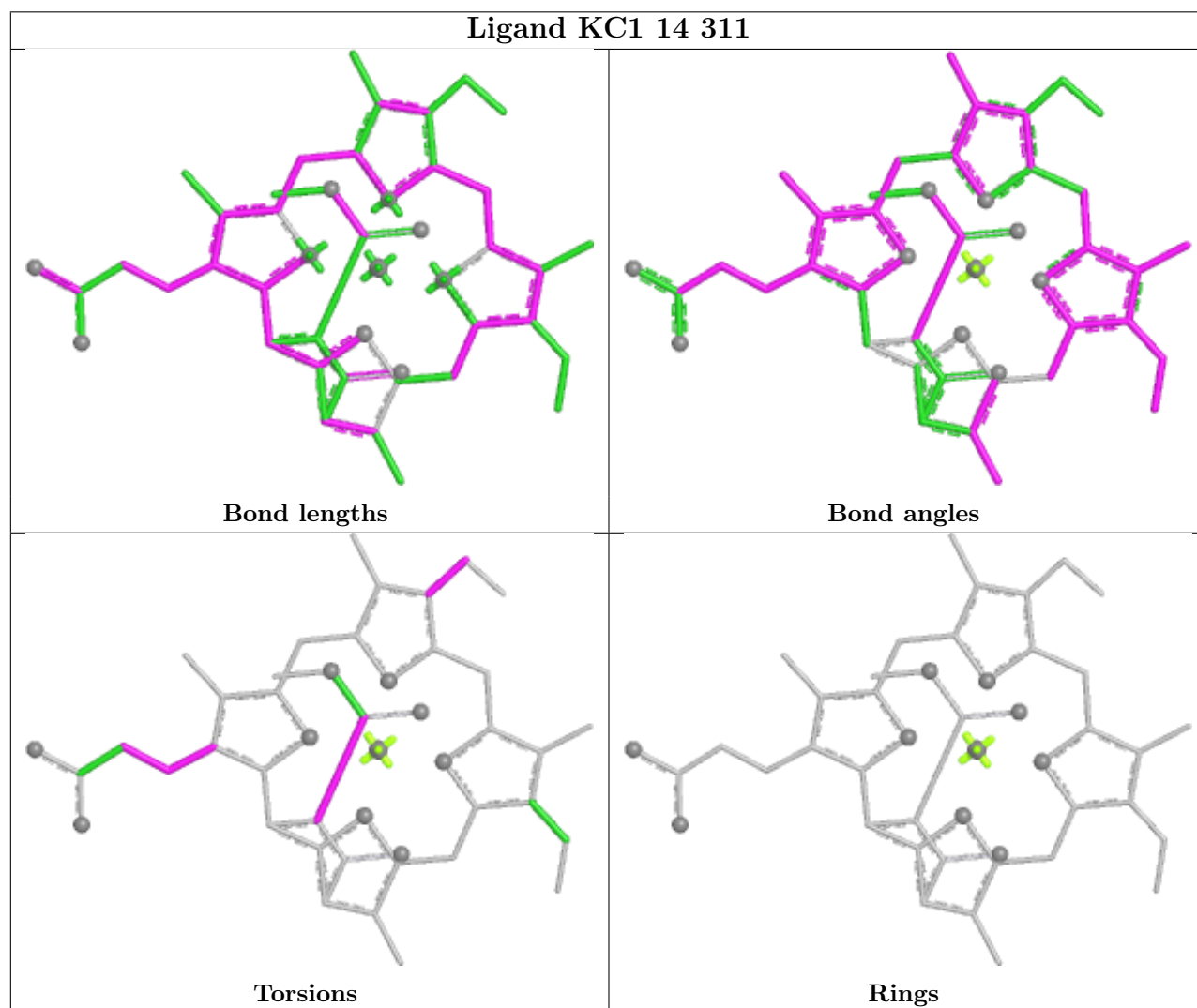
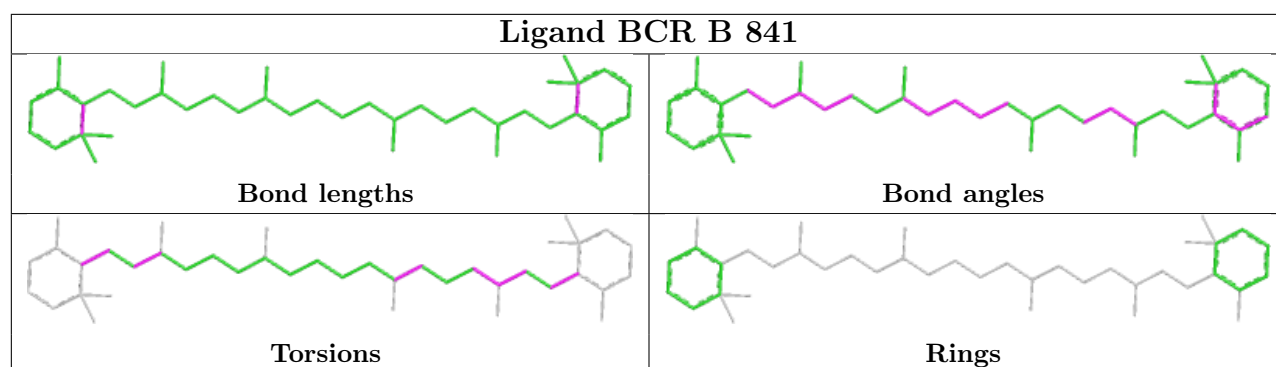


Torsions

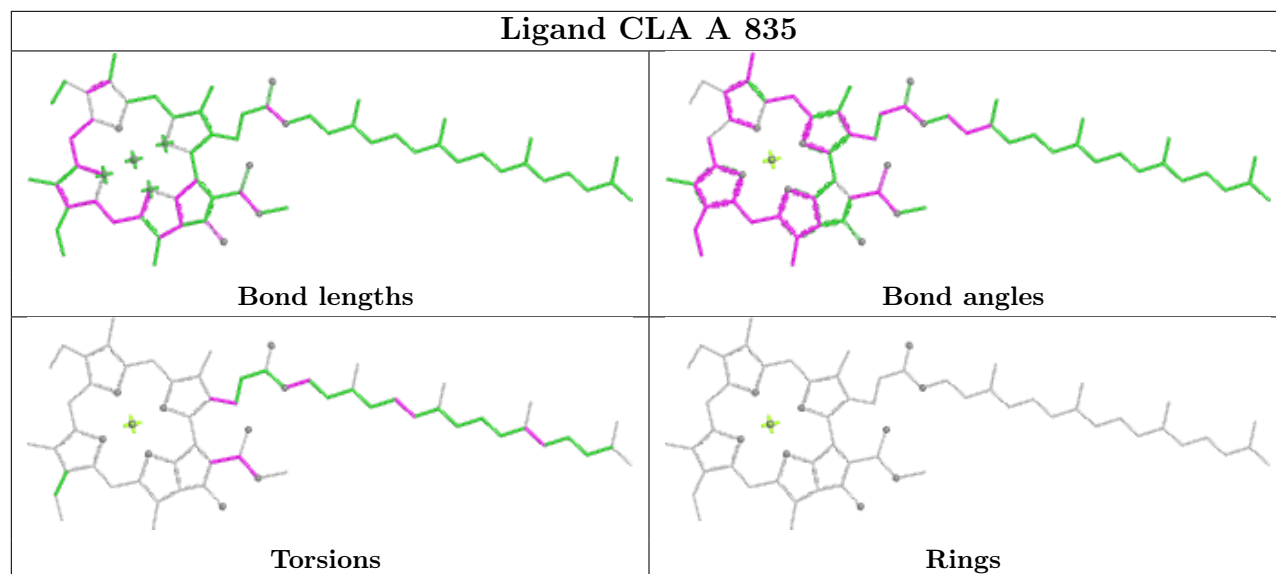


Rings

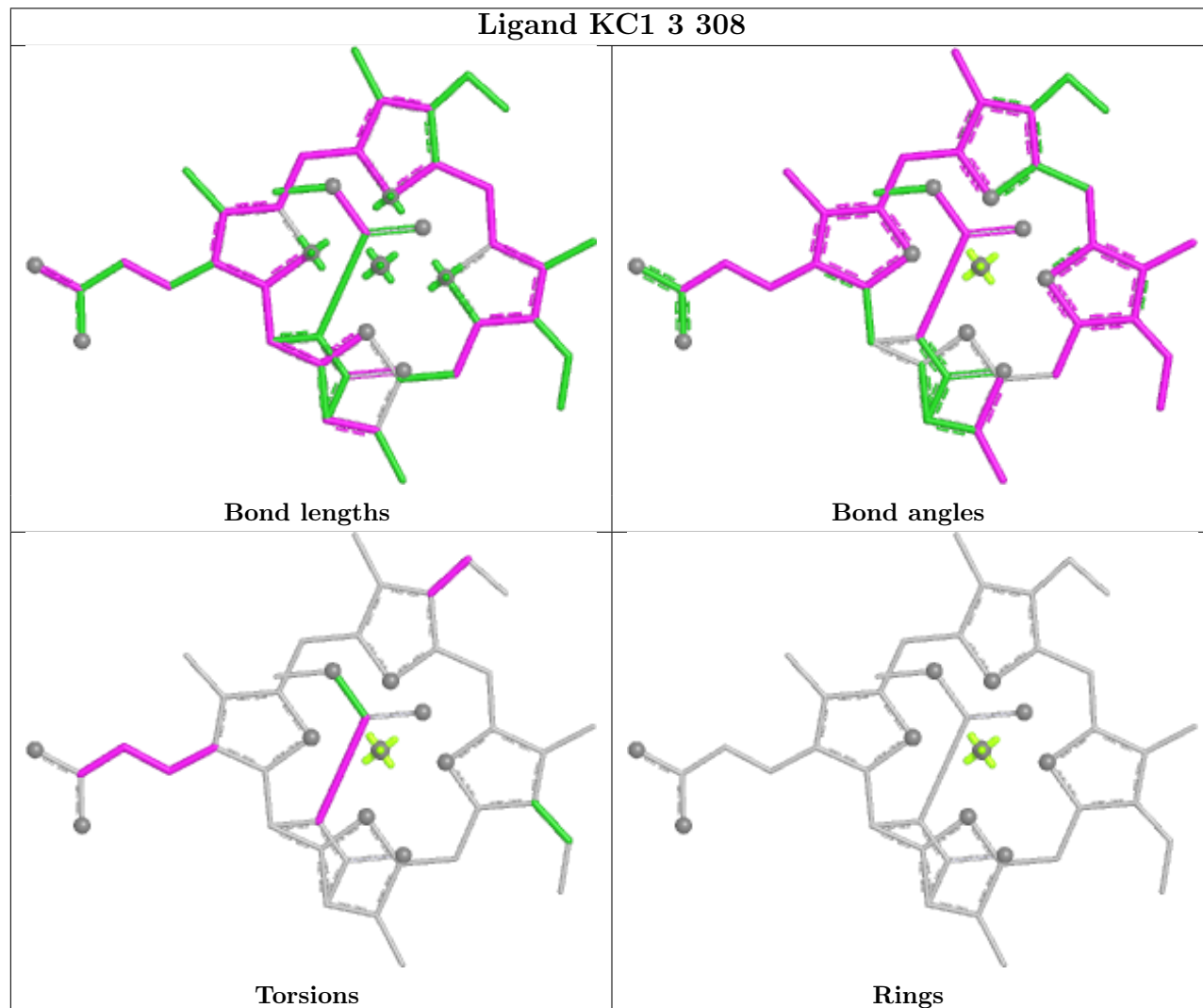


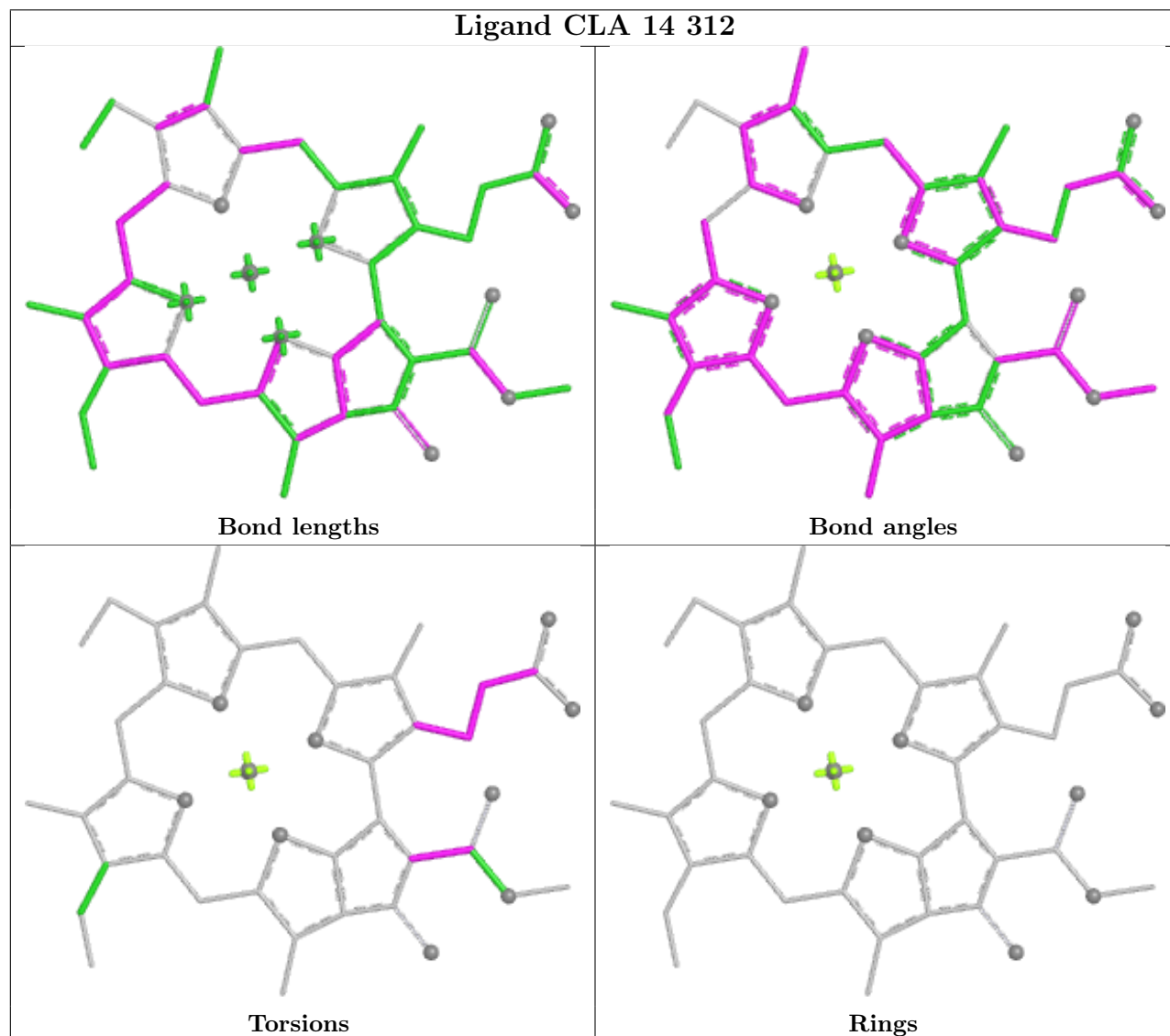
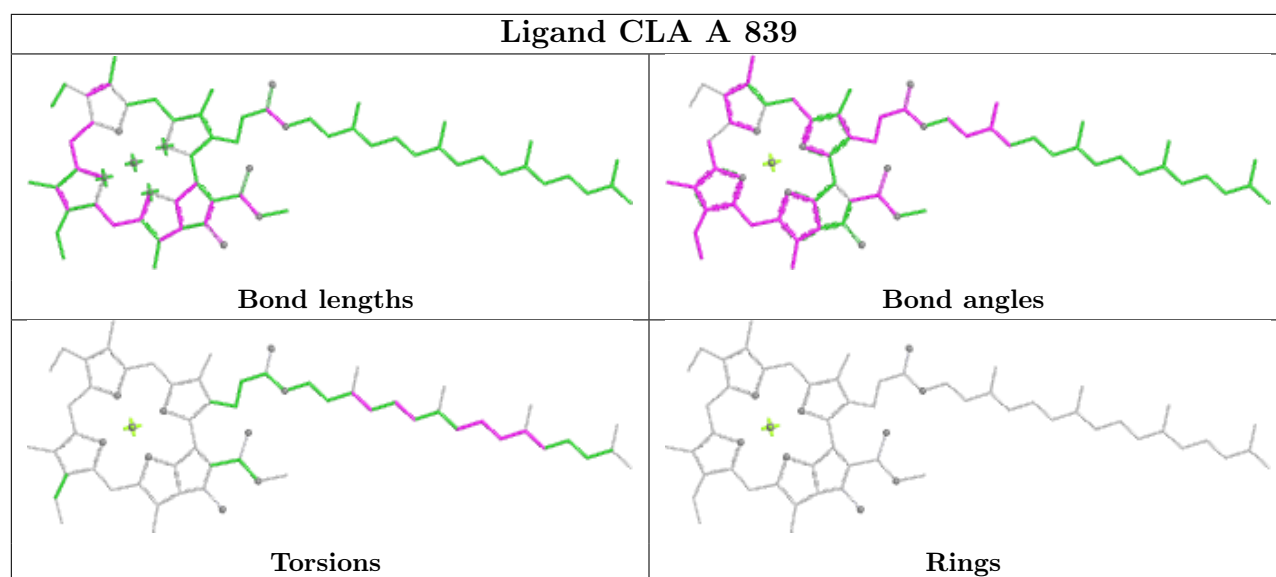


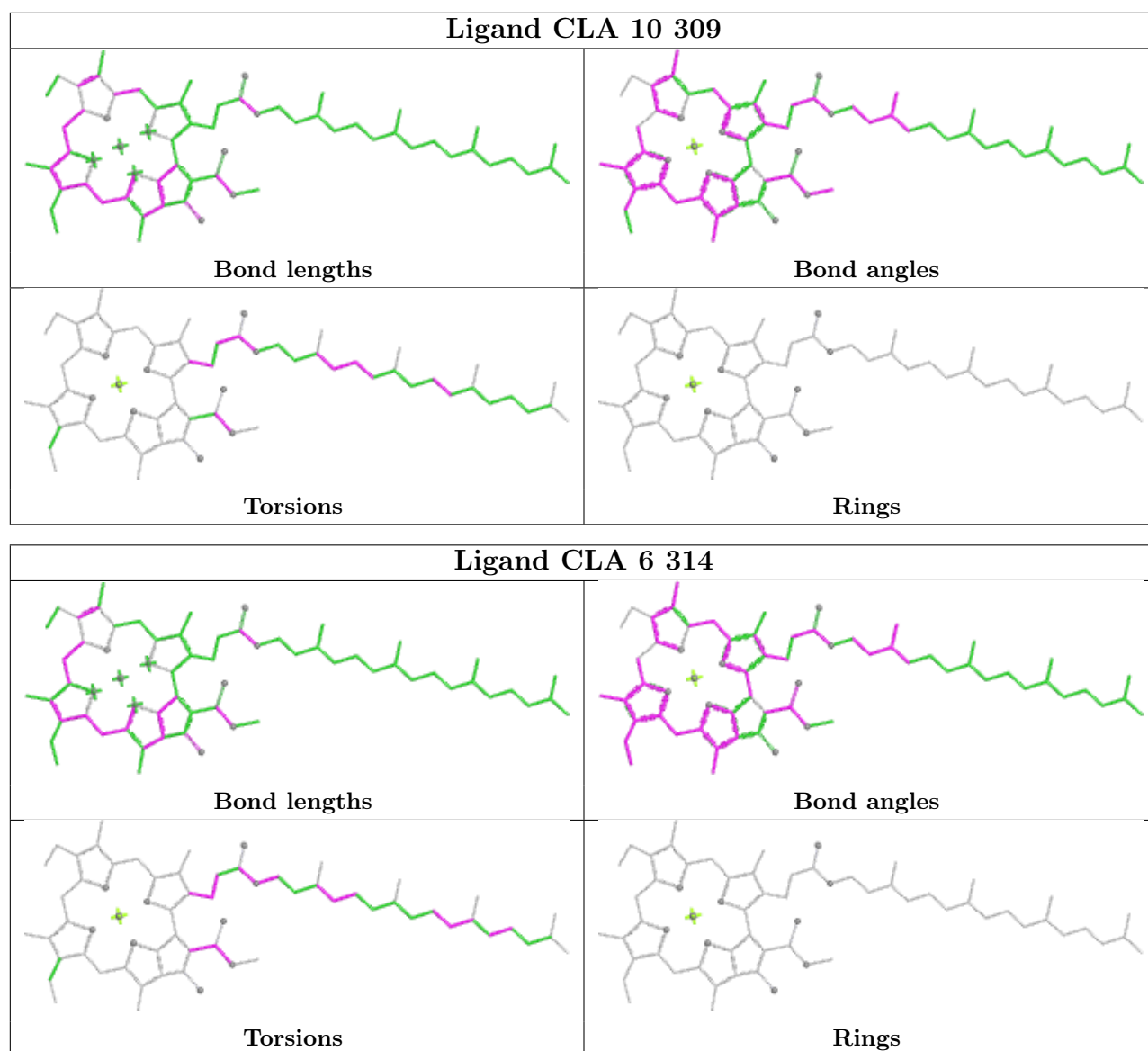
## Ligand CLA A 835

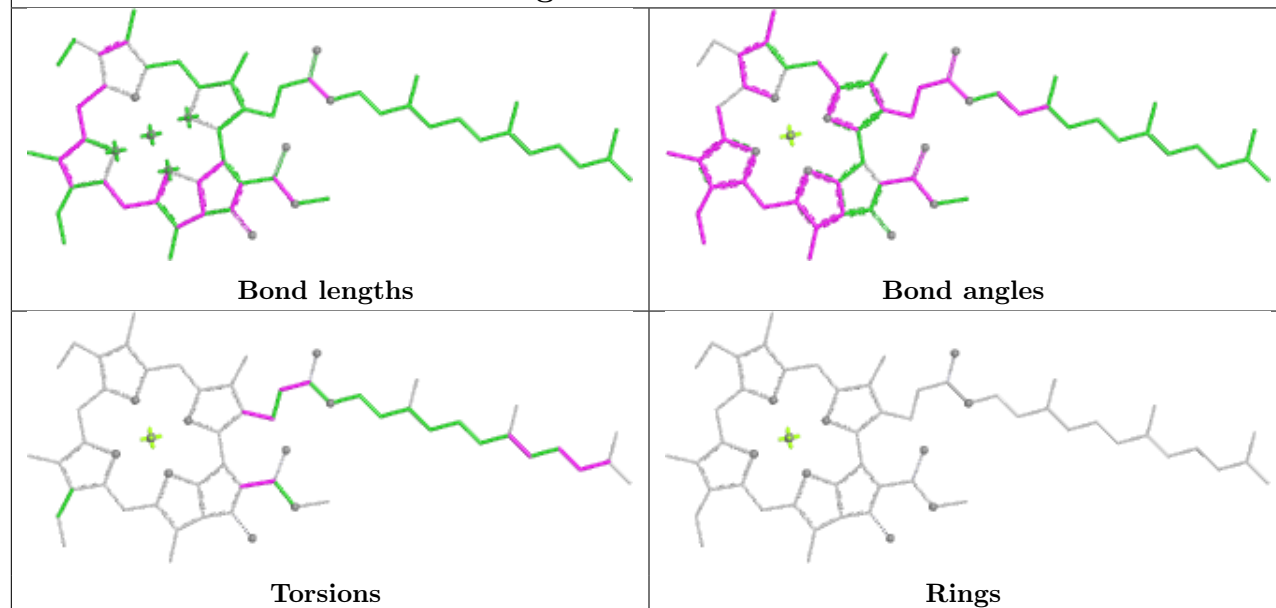
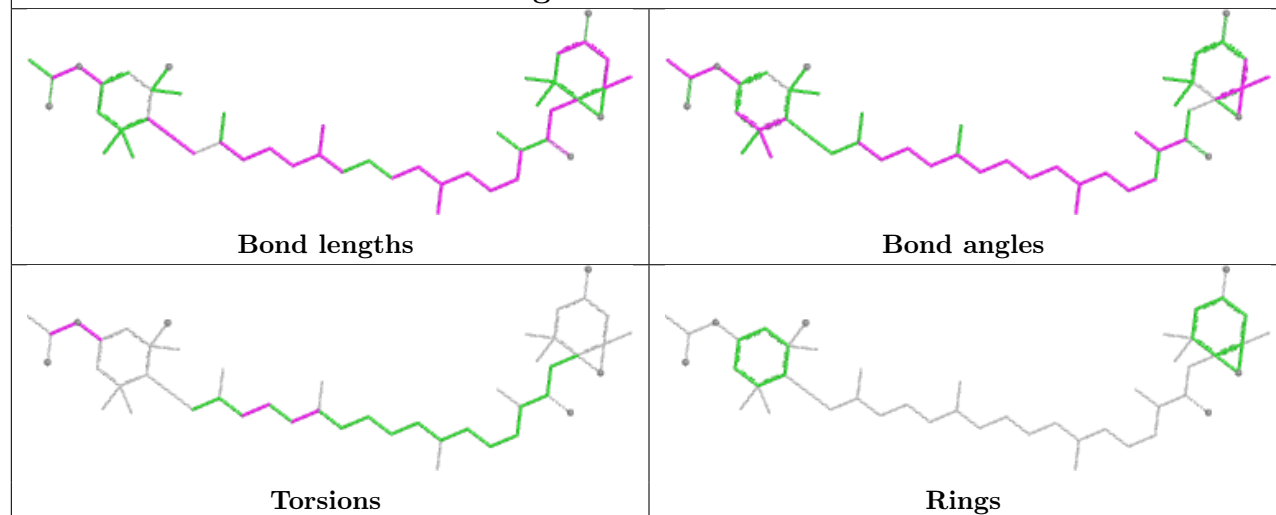


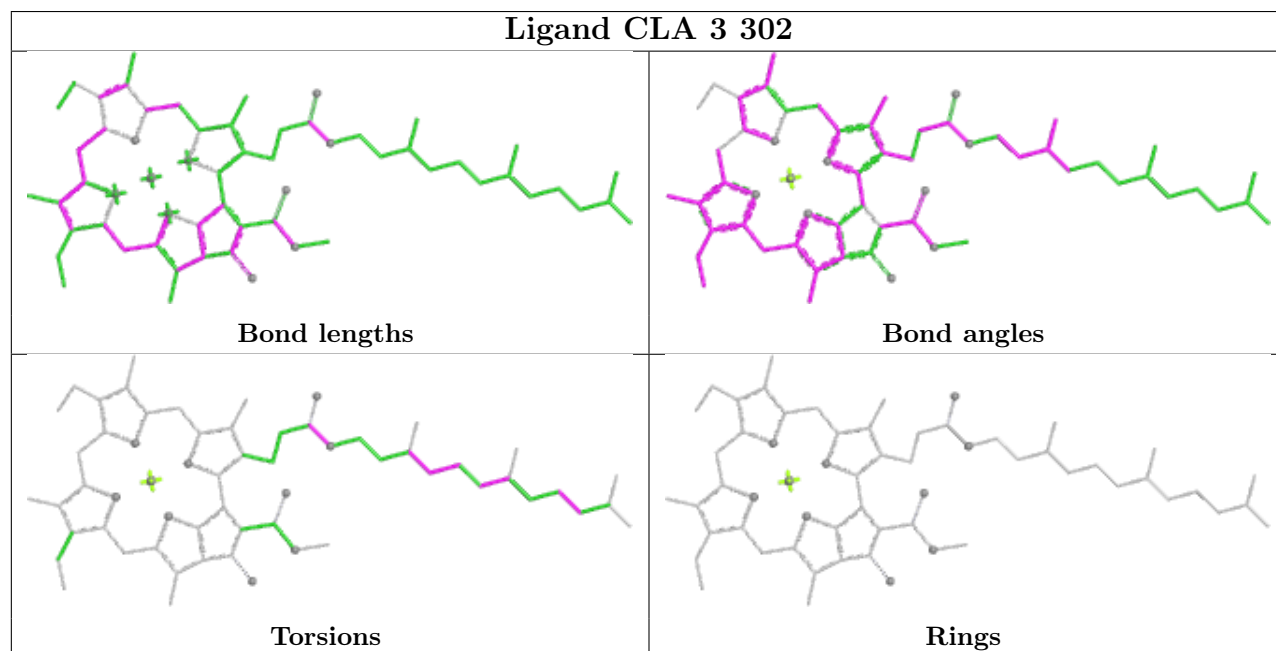
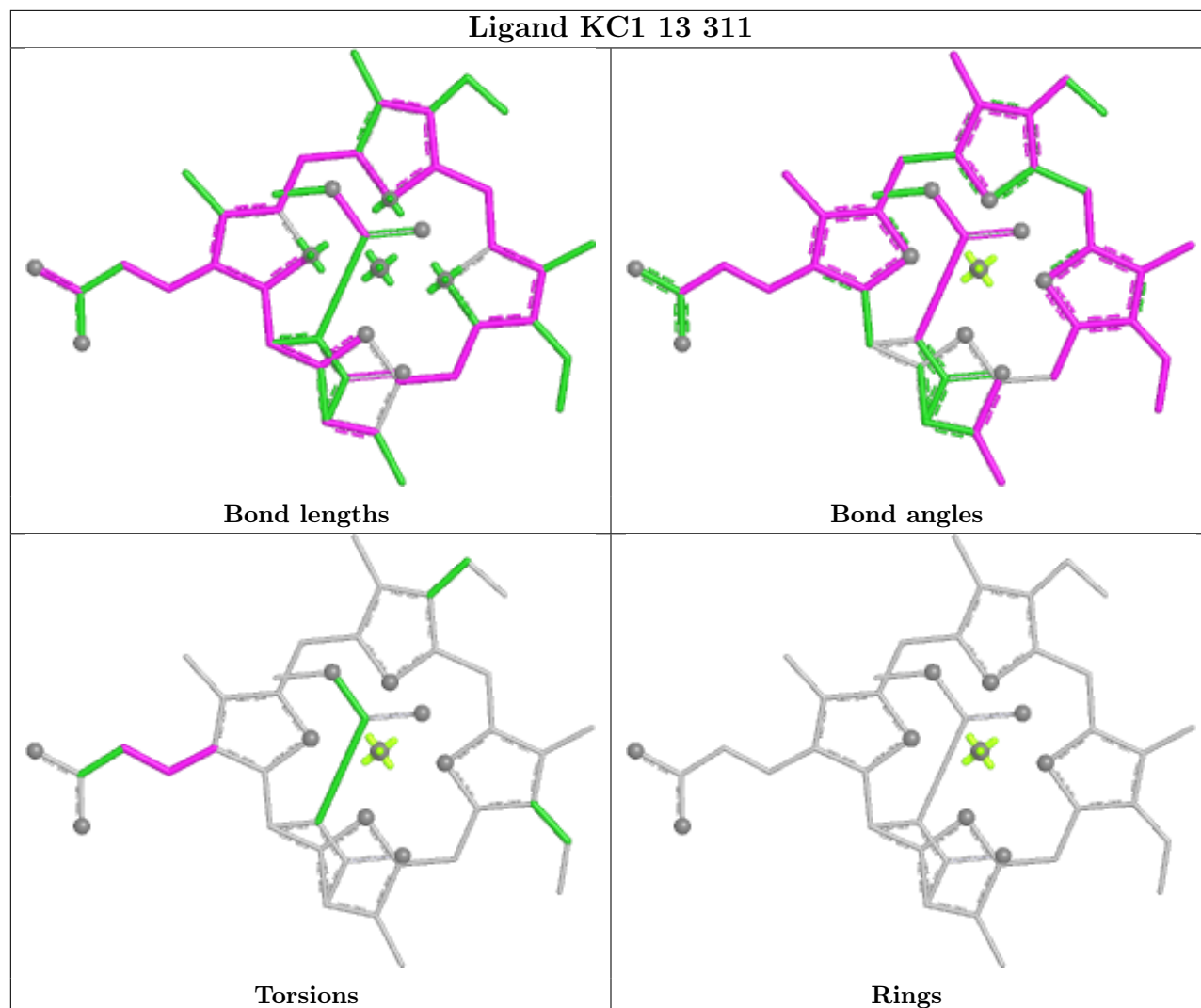
## Ligand KC1 3 308

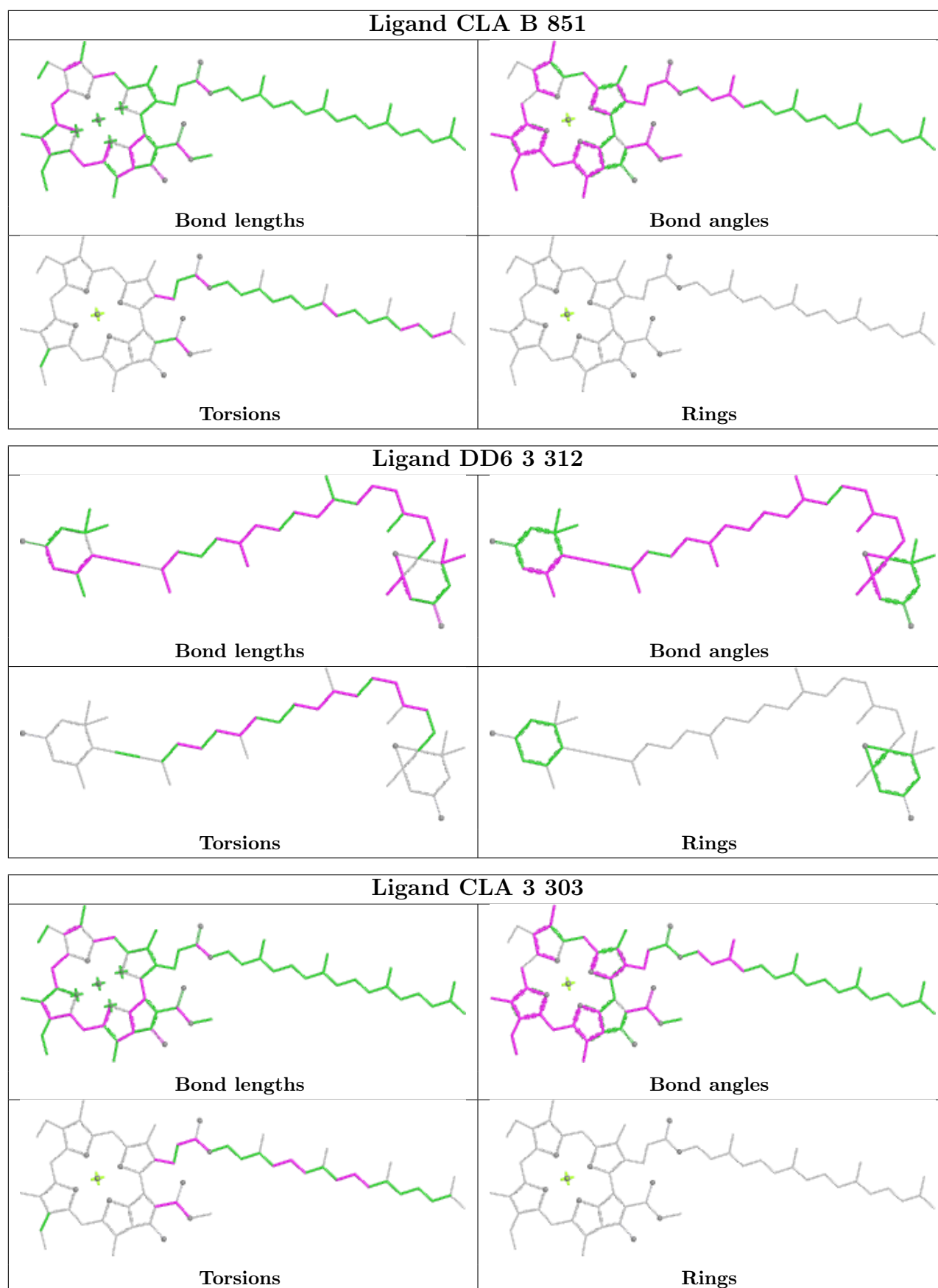


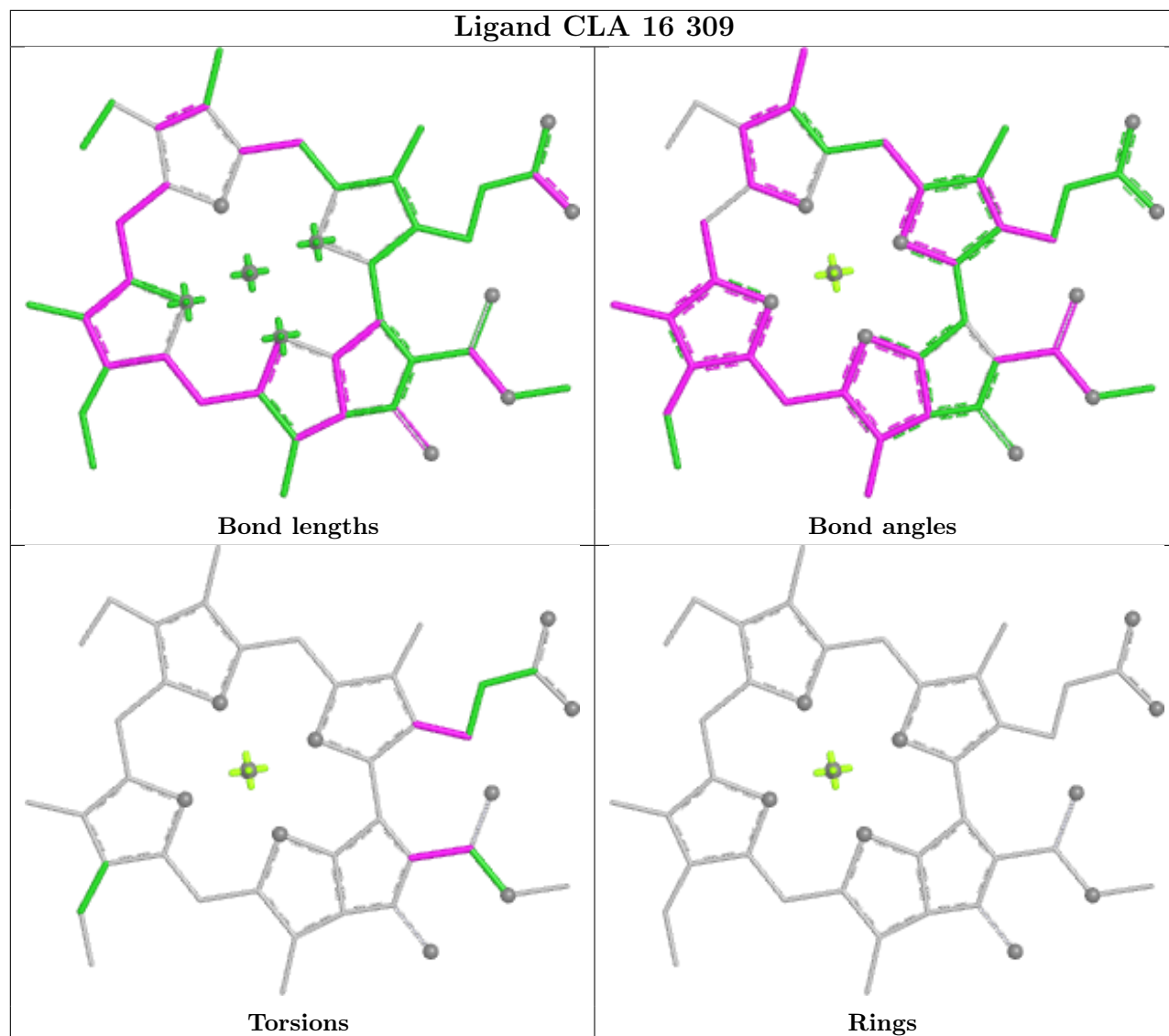


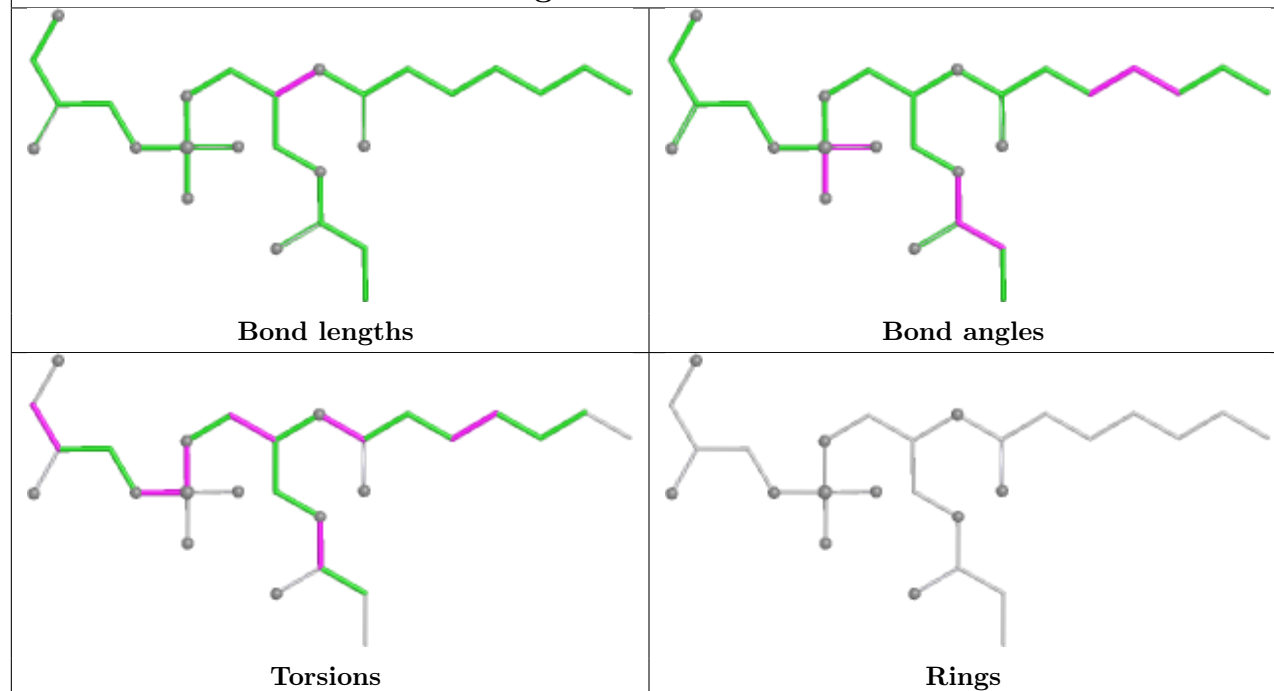
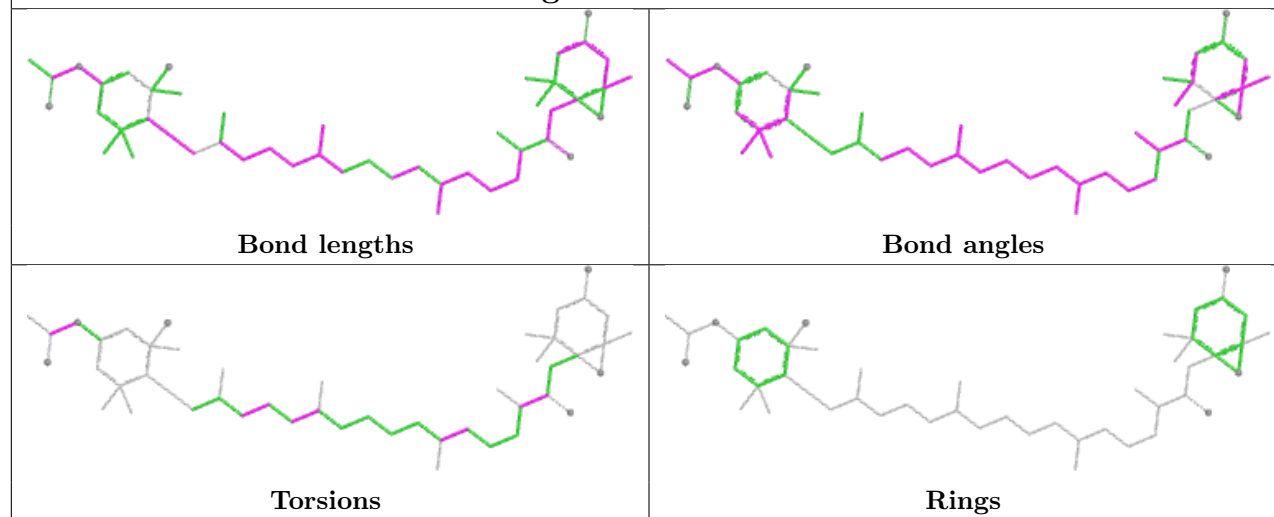


**Ligand CLA 4 304****Ligand A86 14 301**

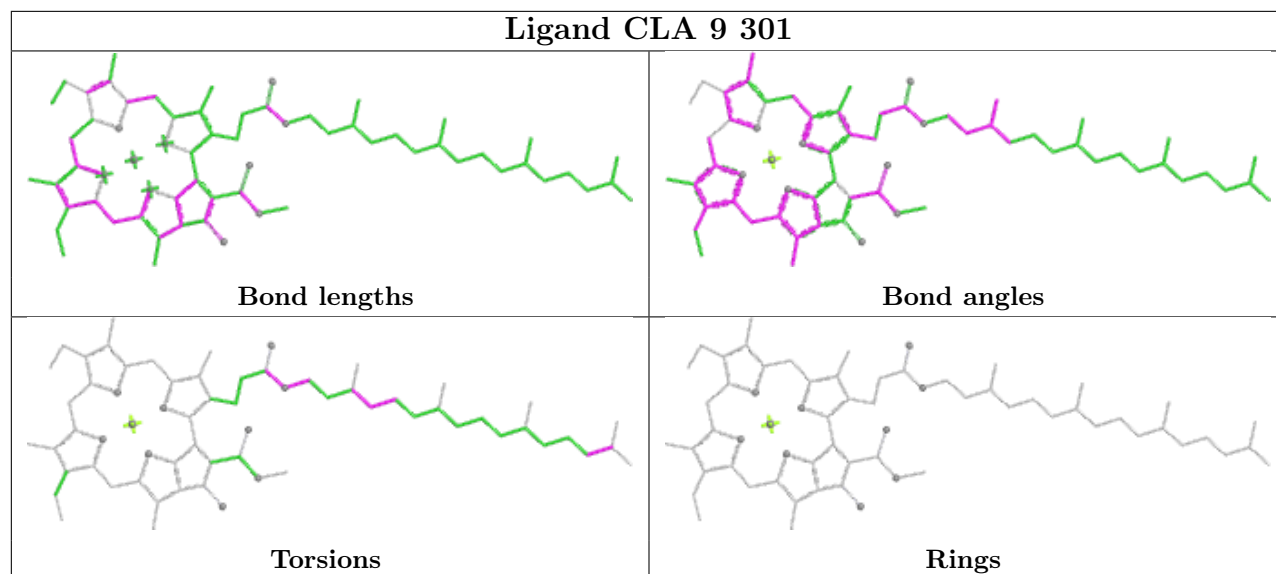




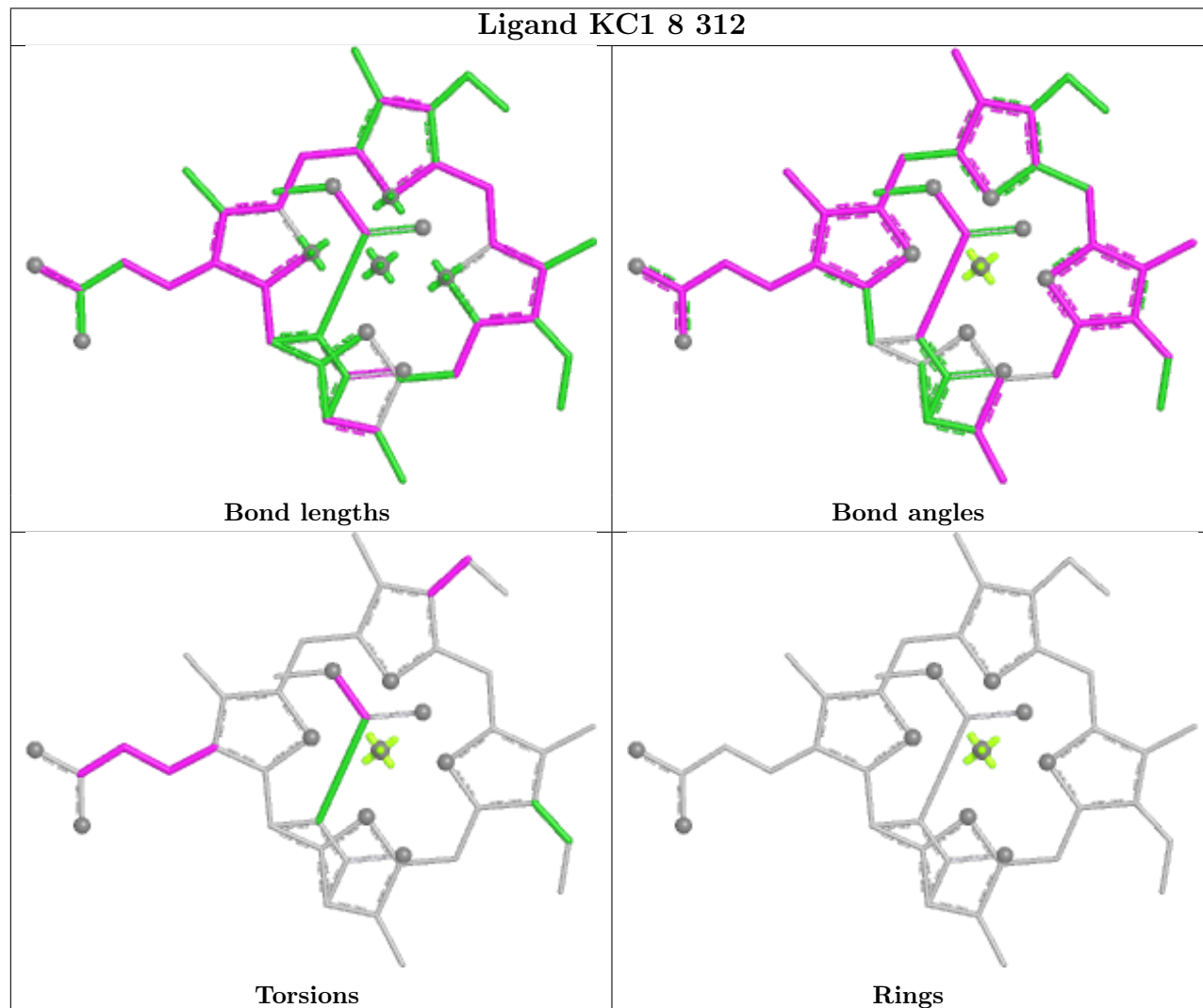


**Ligand LHG 6 322****Ligand A86 2 318**

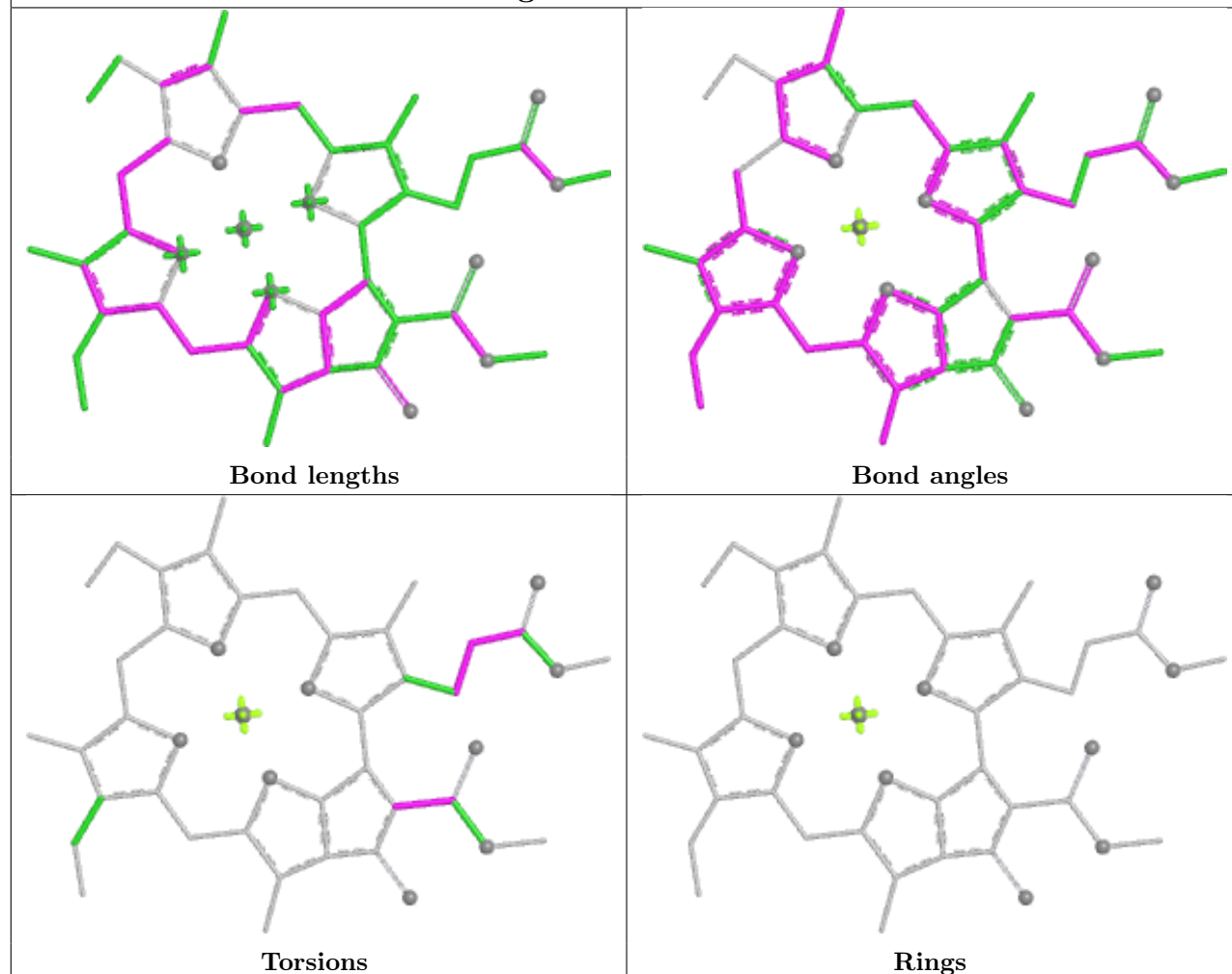
## Ligand CLA 9 301



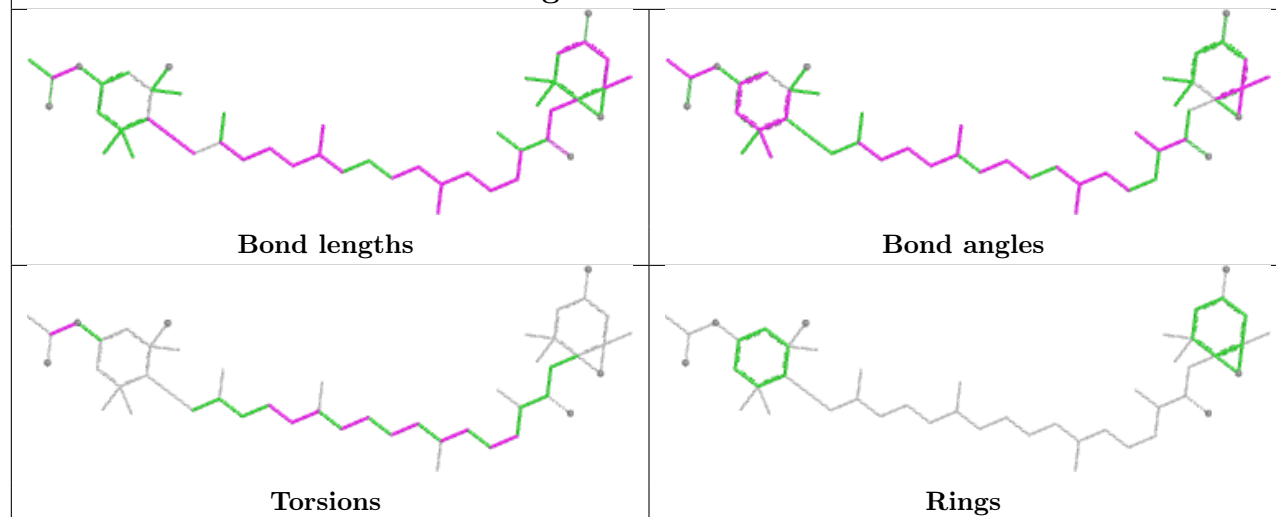
## Ligand KC1 8 312

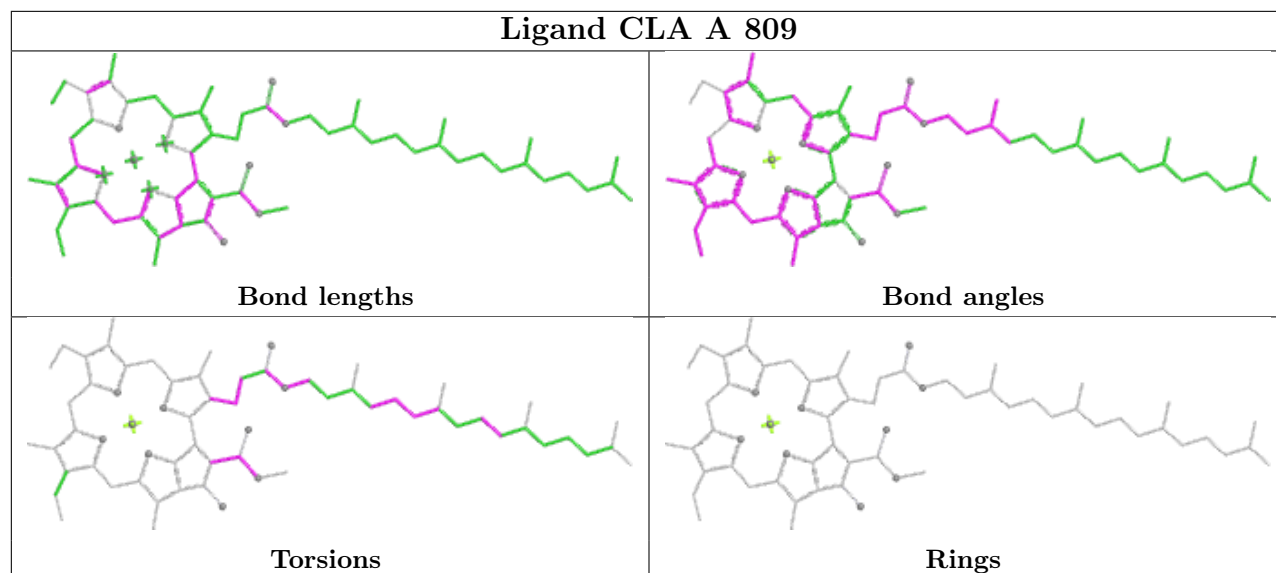
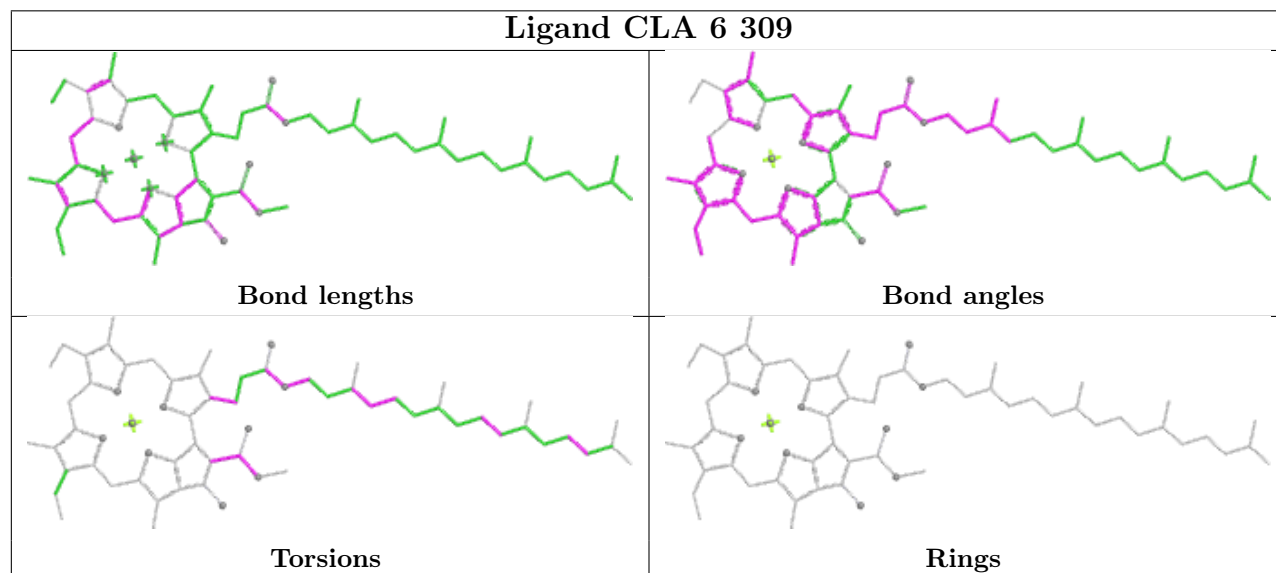
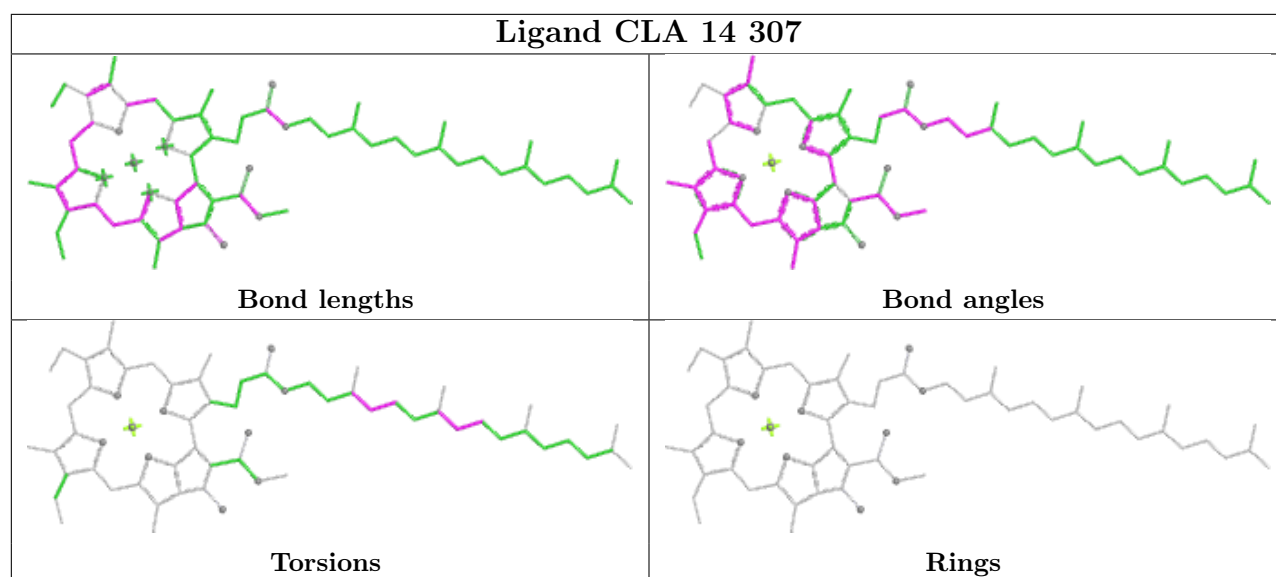


## Ligand CLA 7 312

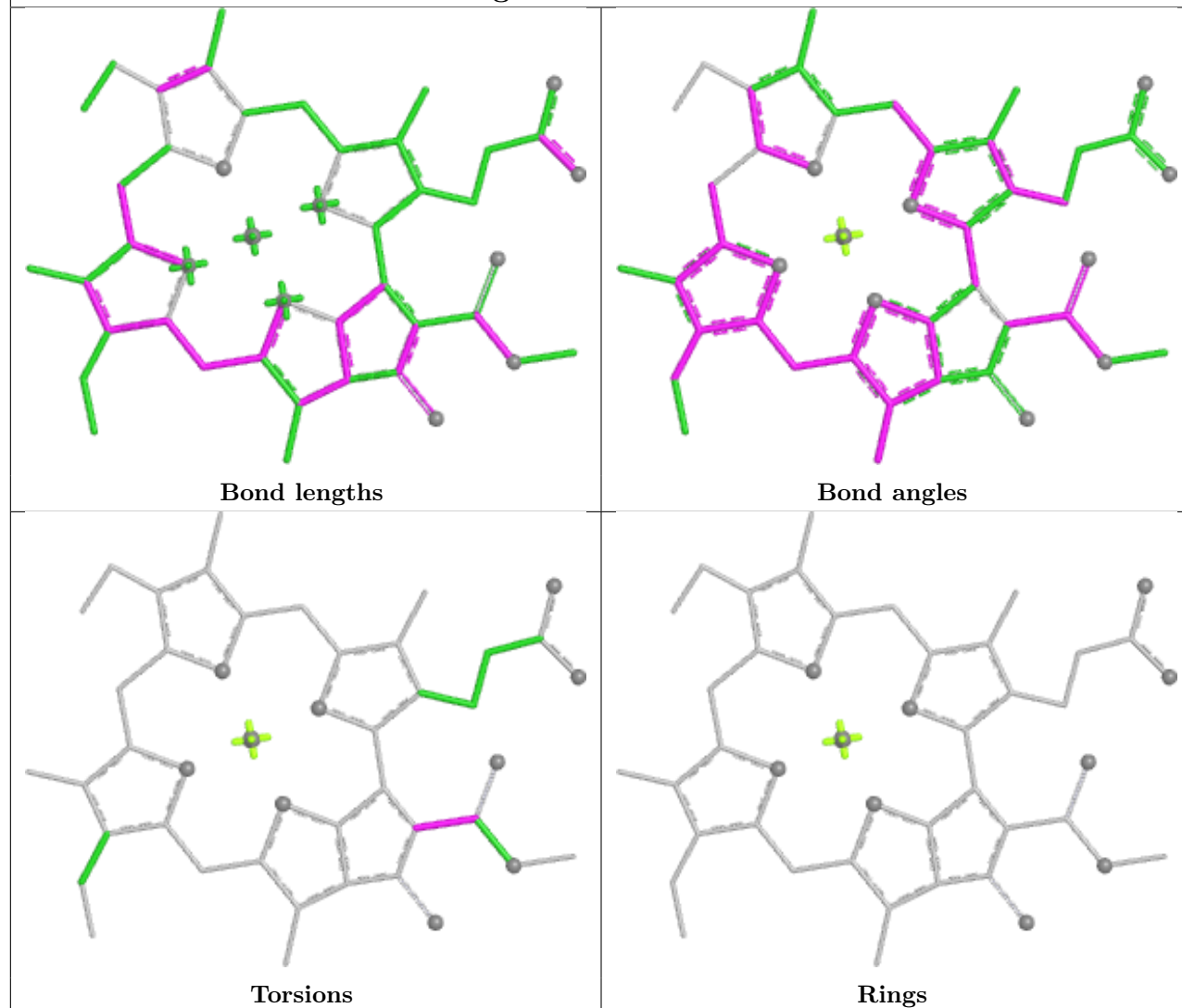


## Ligand A86 9 315

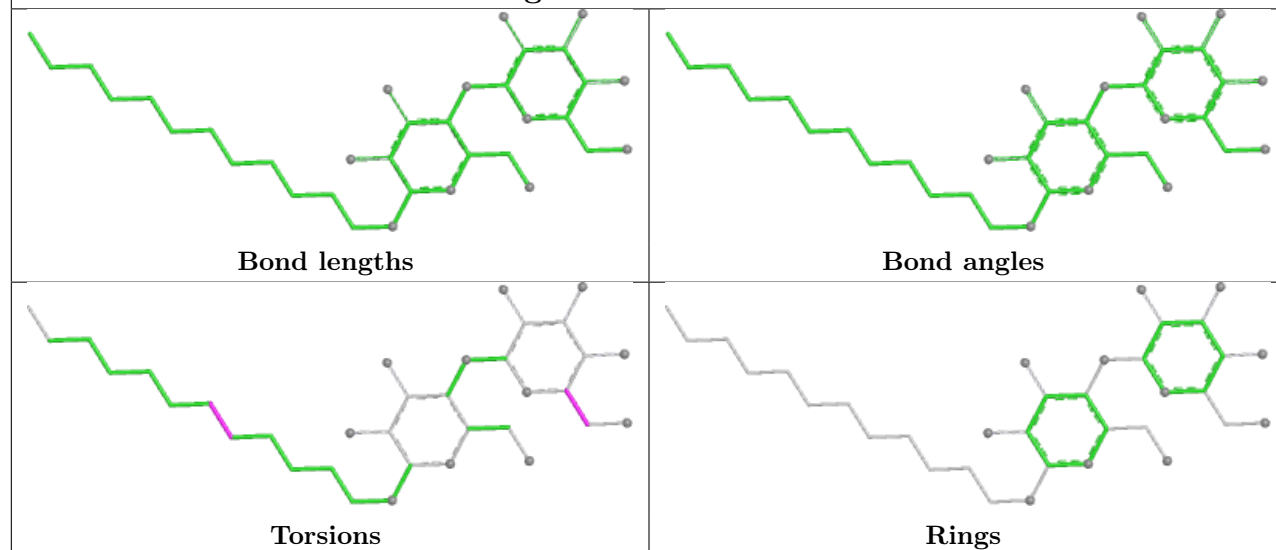


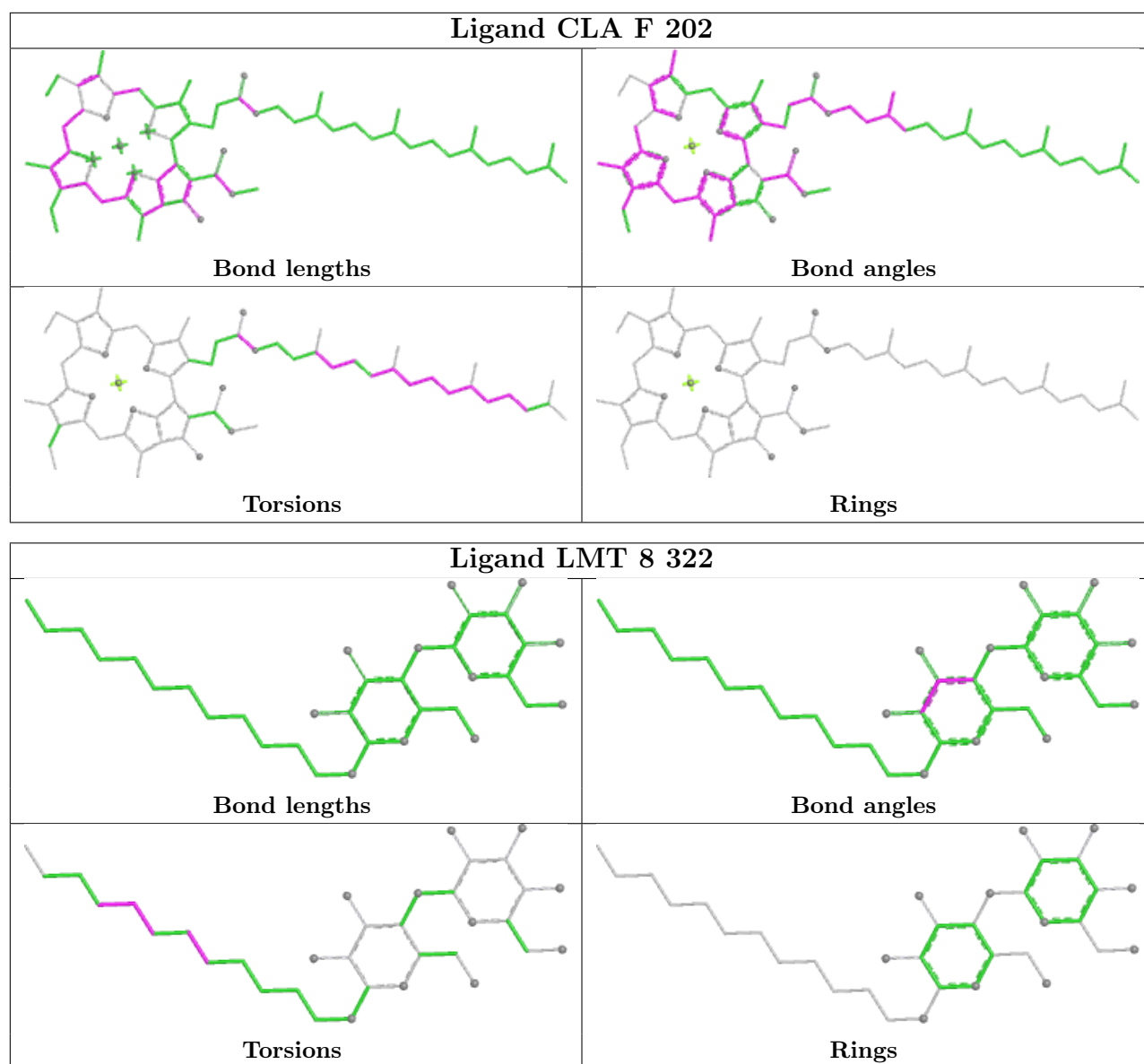


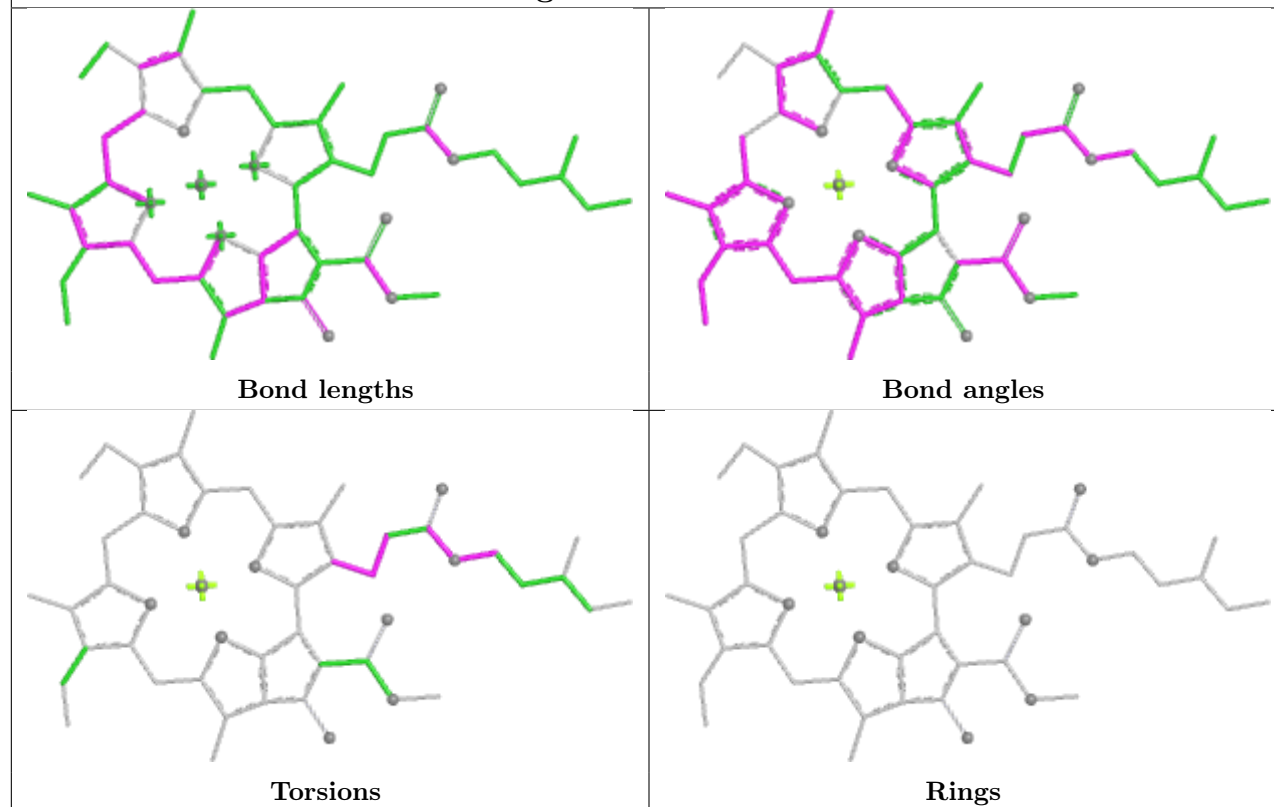
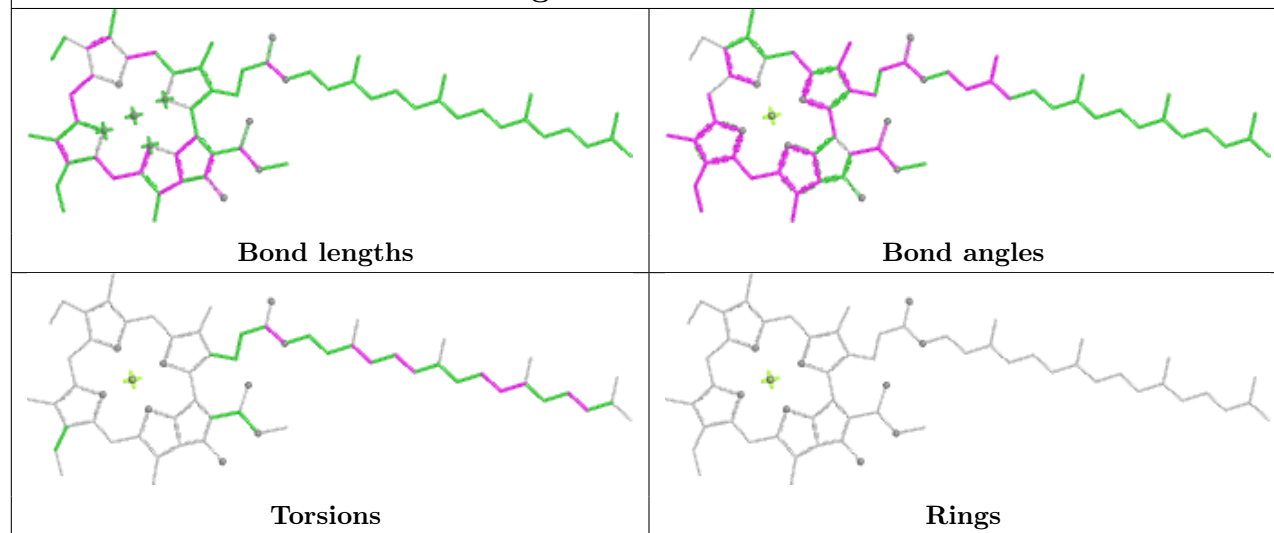
## Ligand CLA B 815

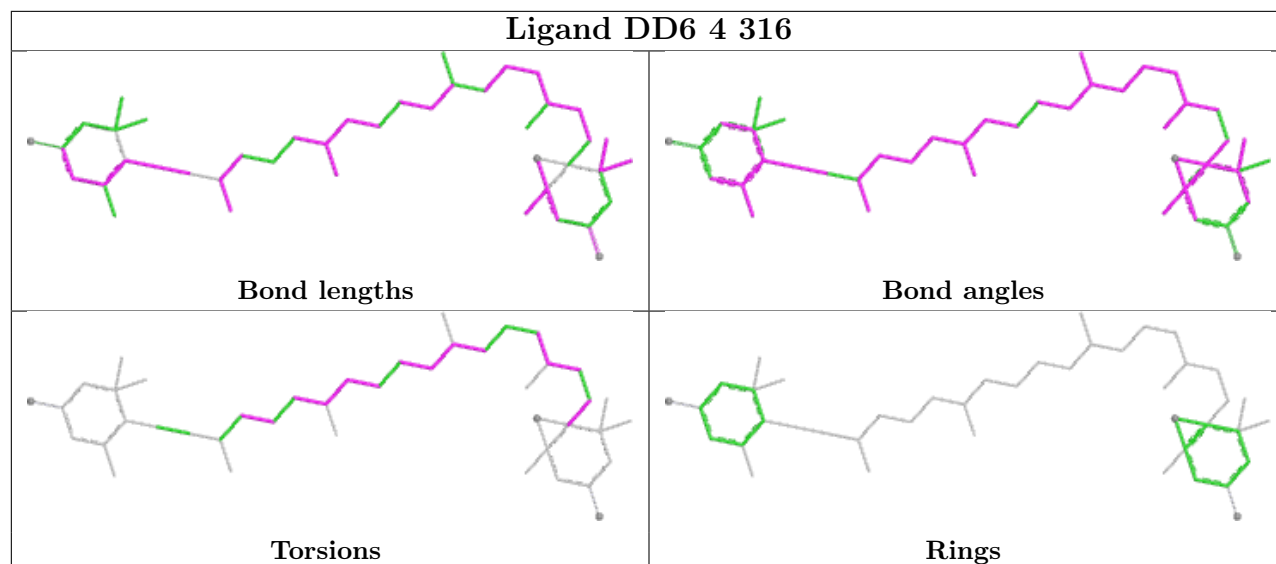
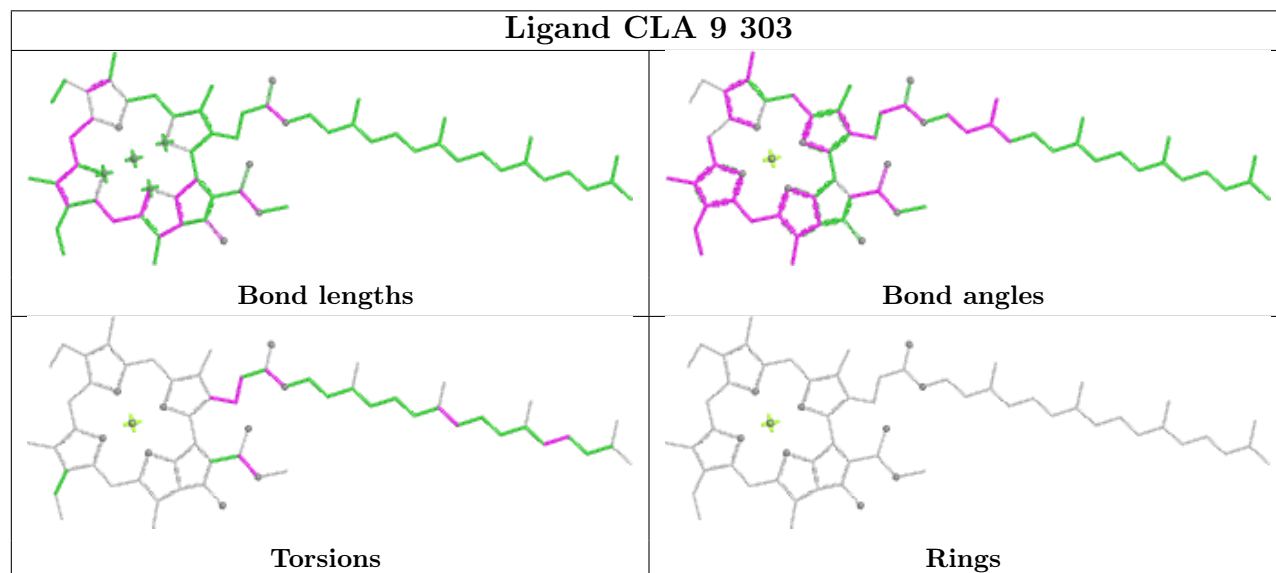
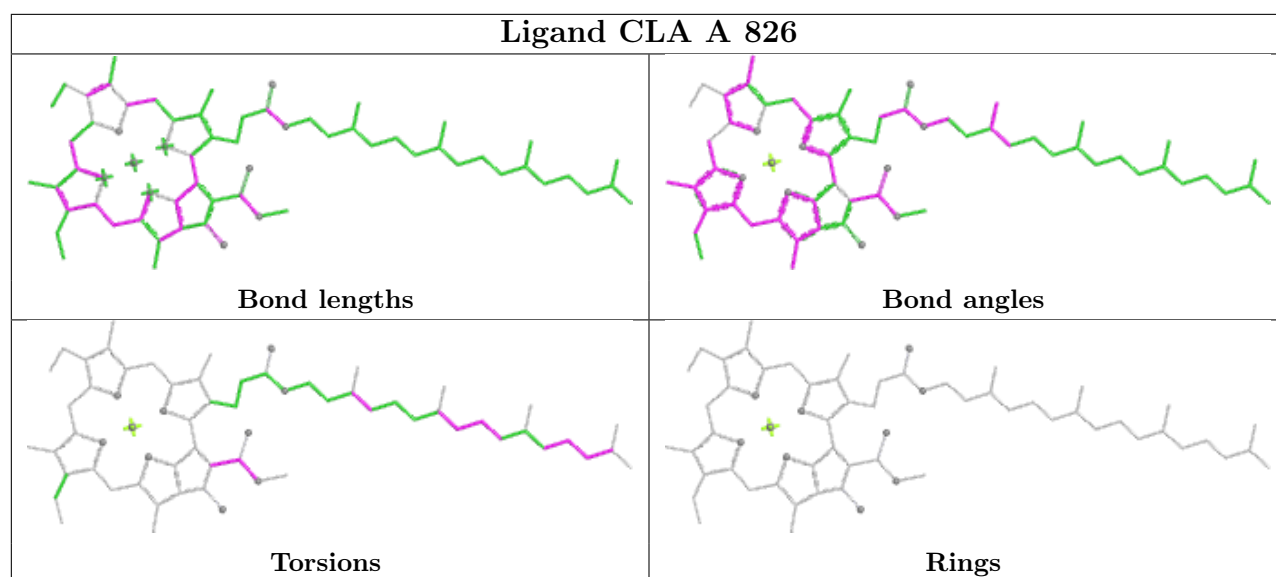


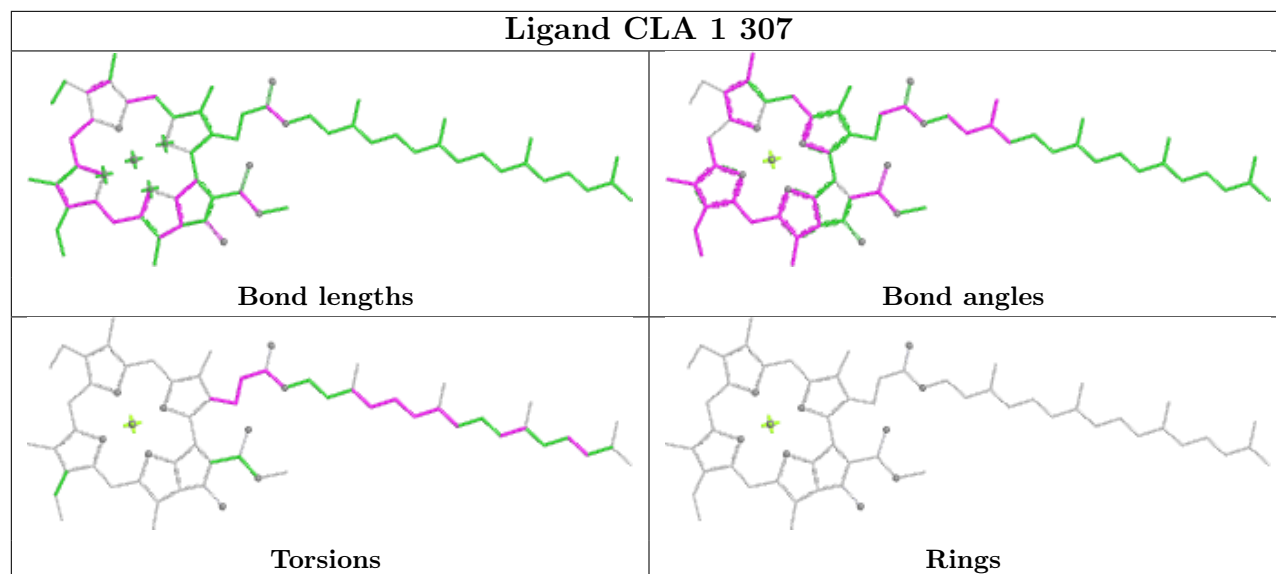
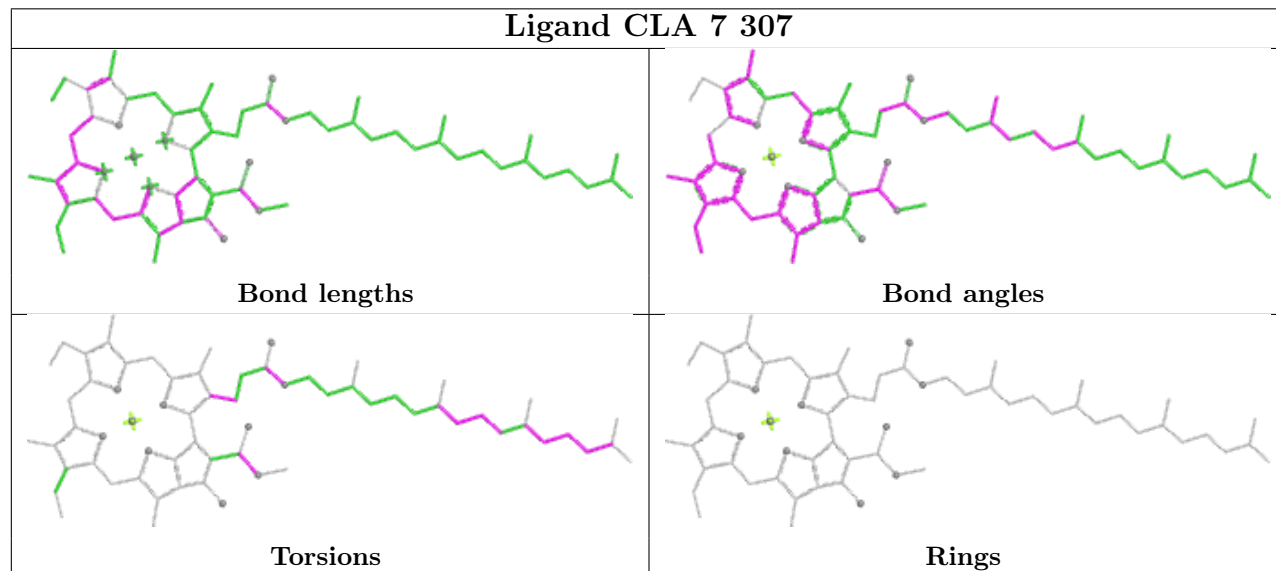
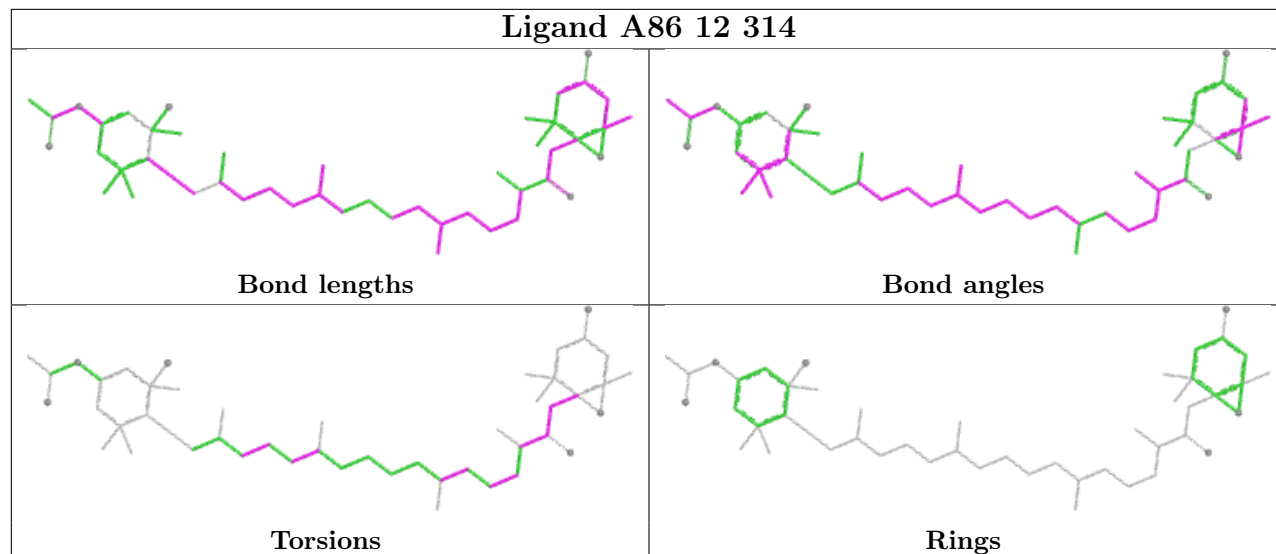
## Ligand LMT 12 318

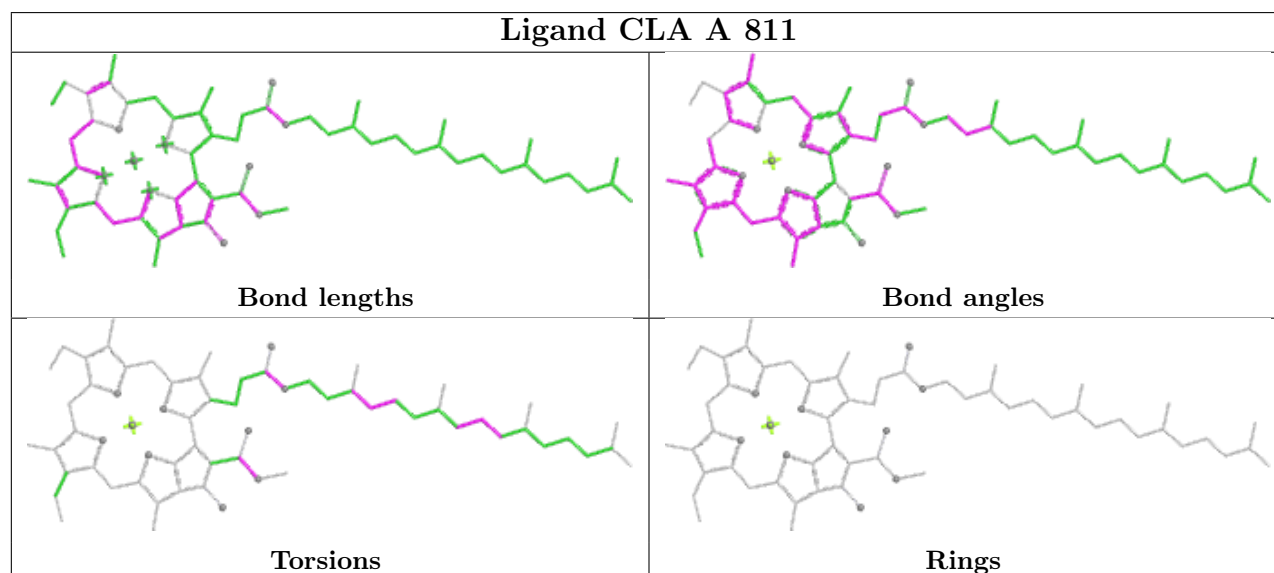
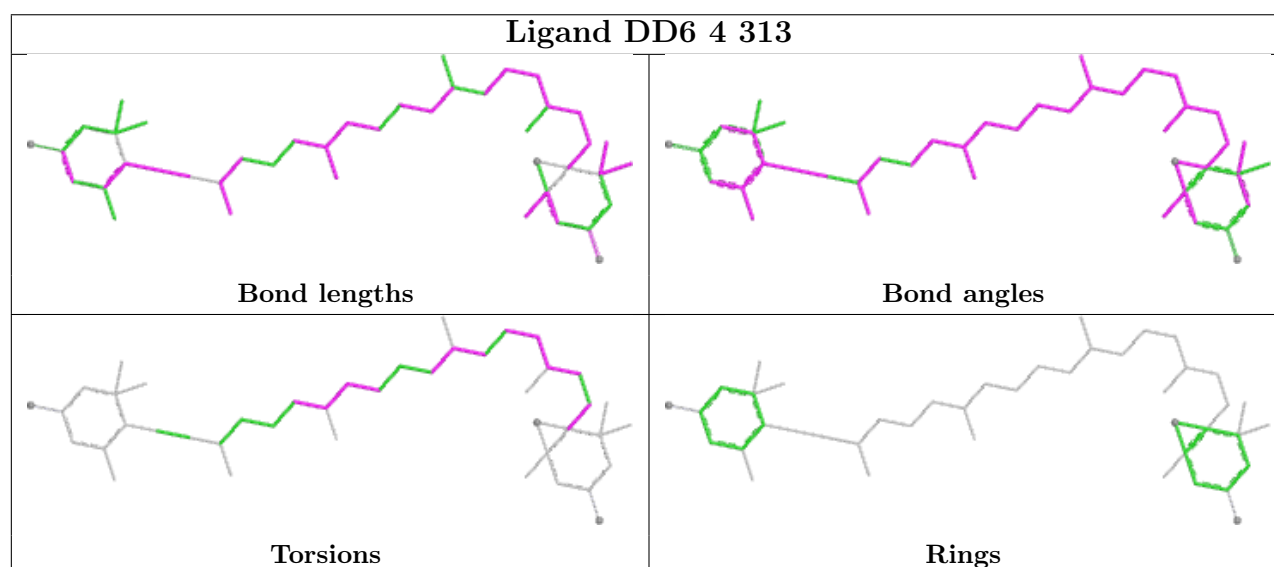
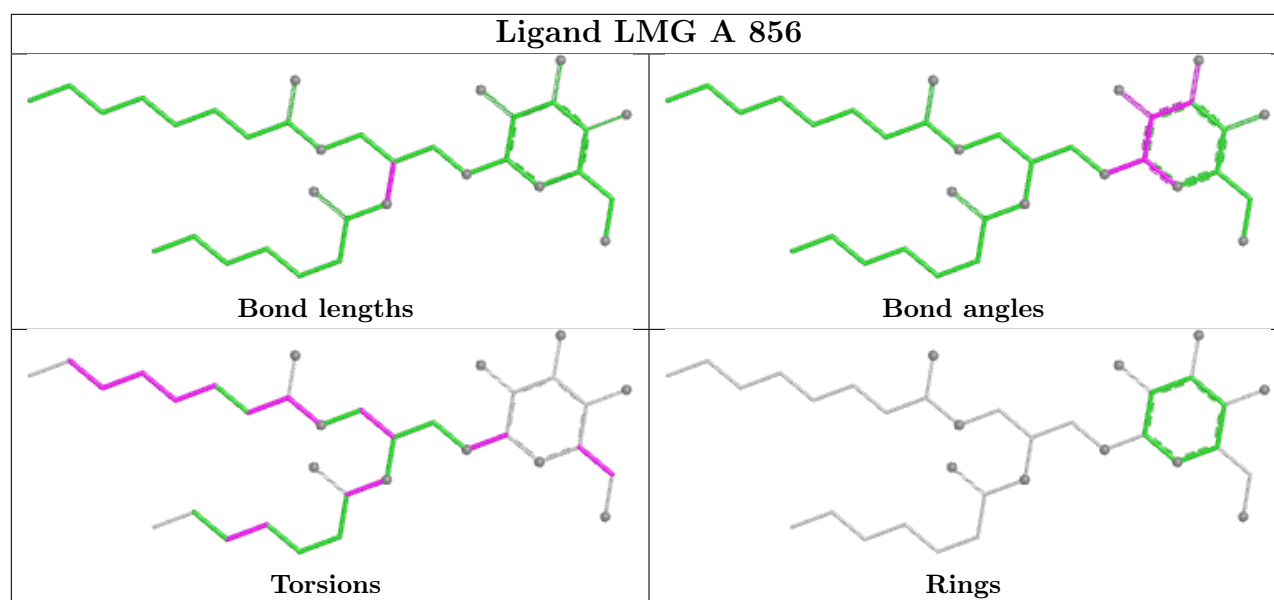




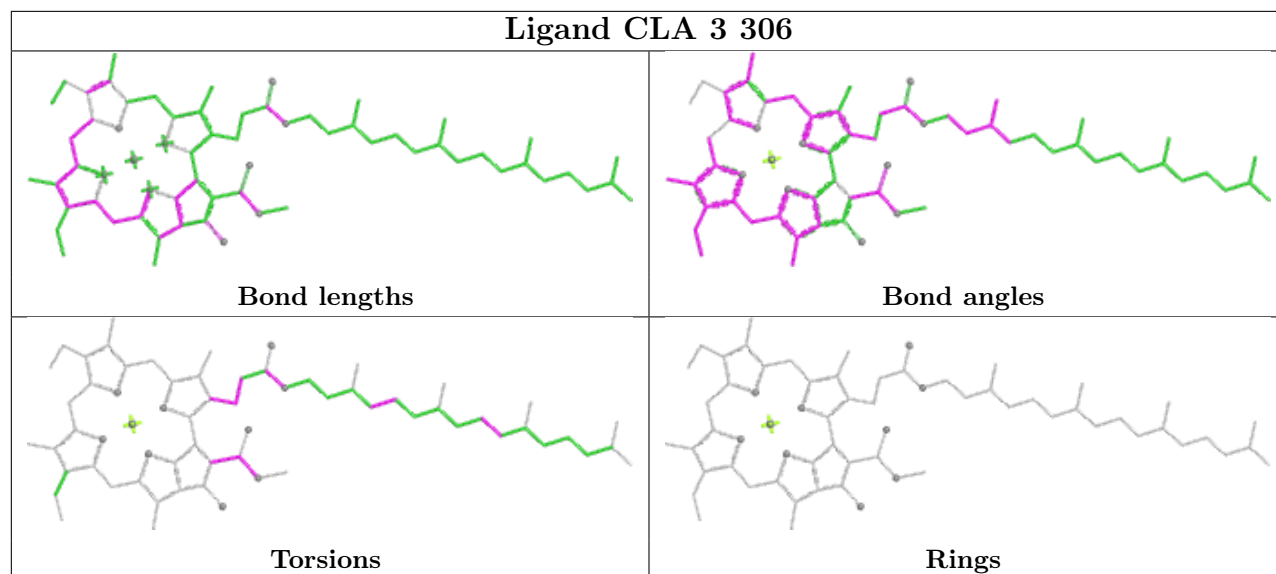
**Ligand CLA 9 302****Ligand CLA A 834**



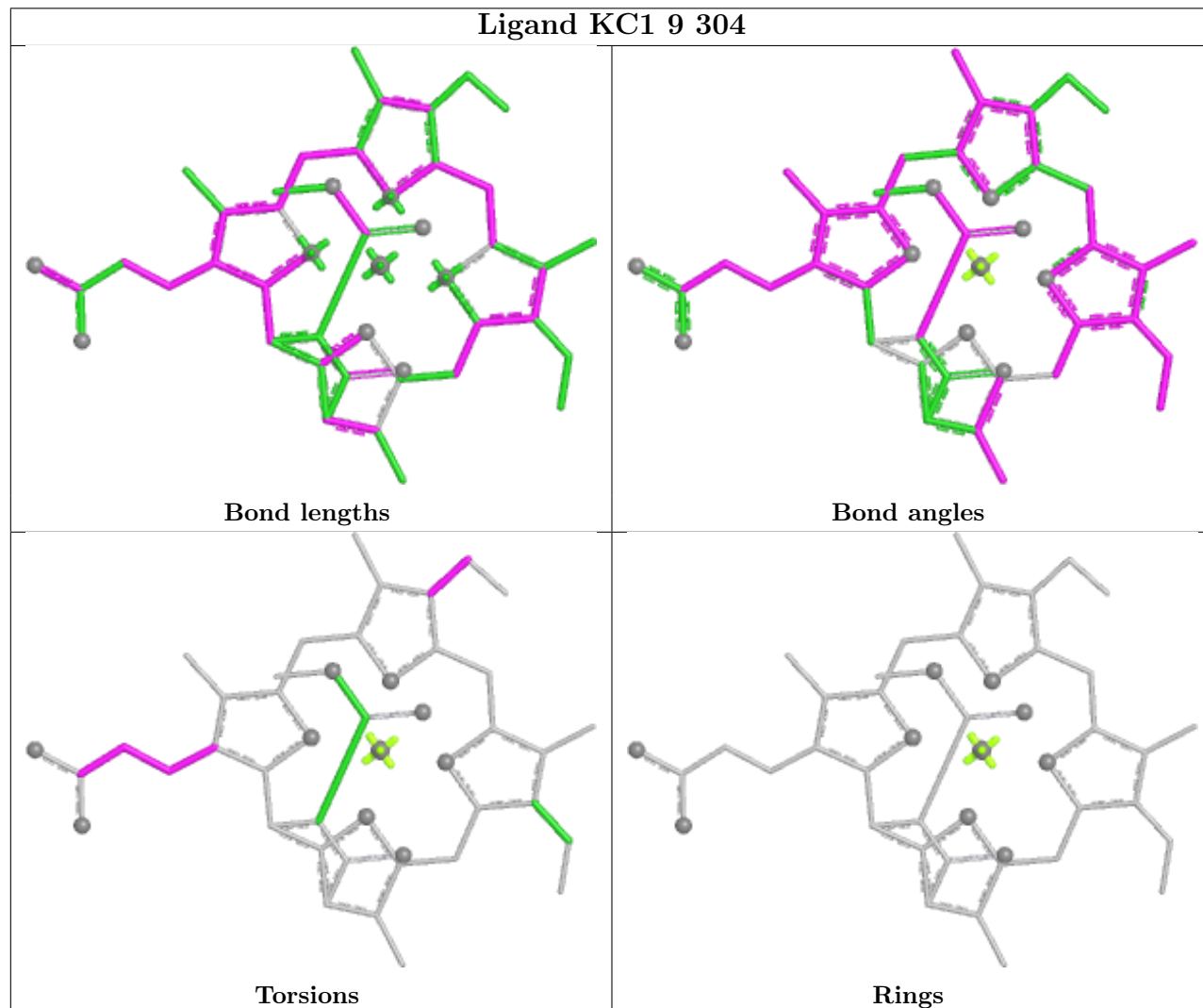
**Ligand CLA 1 307****Ligand CLA 7 307****Ligand A86 12 314**

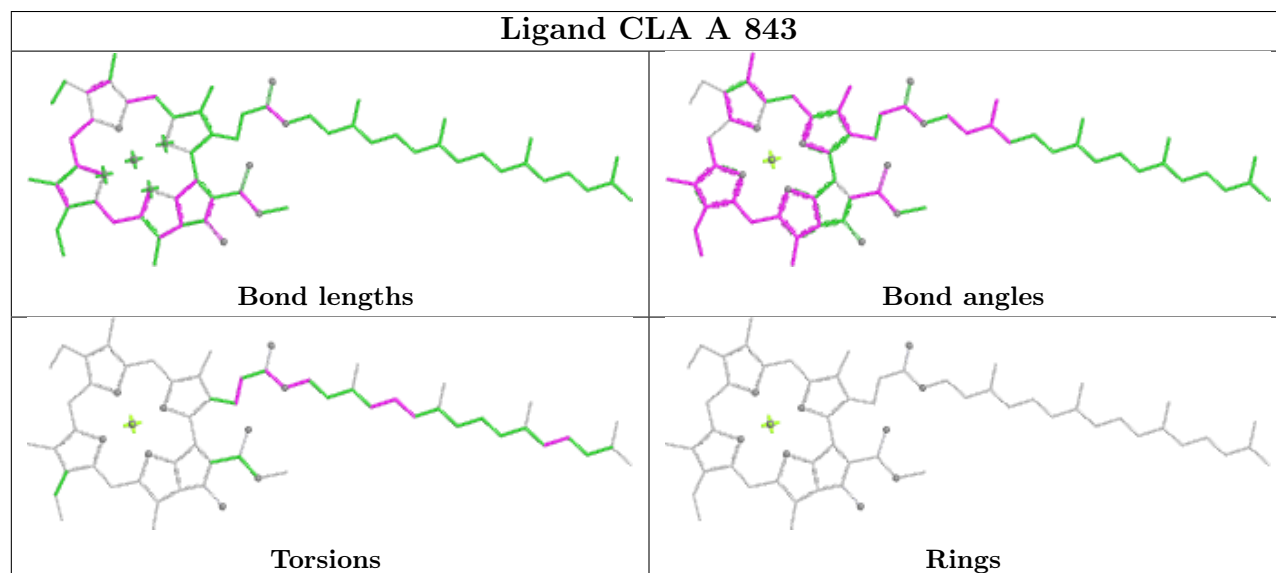
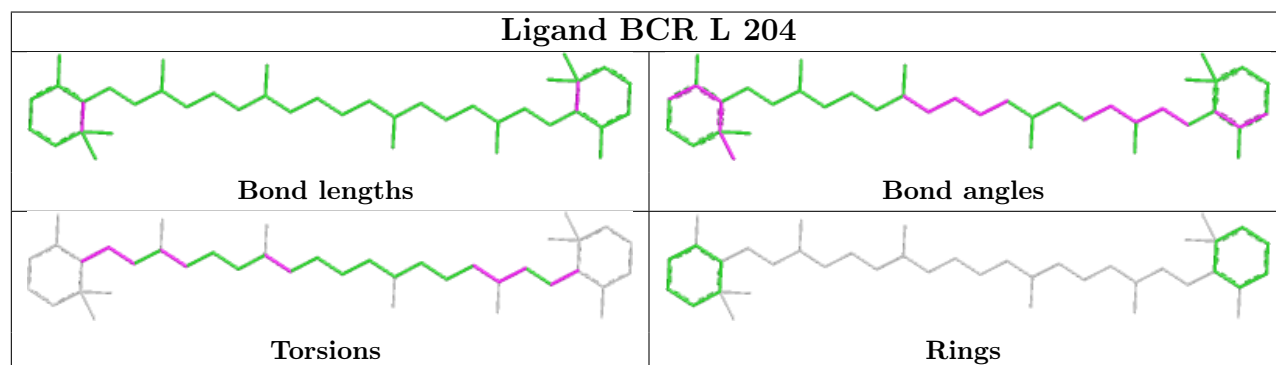
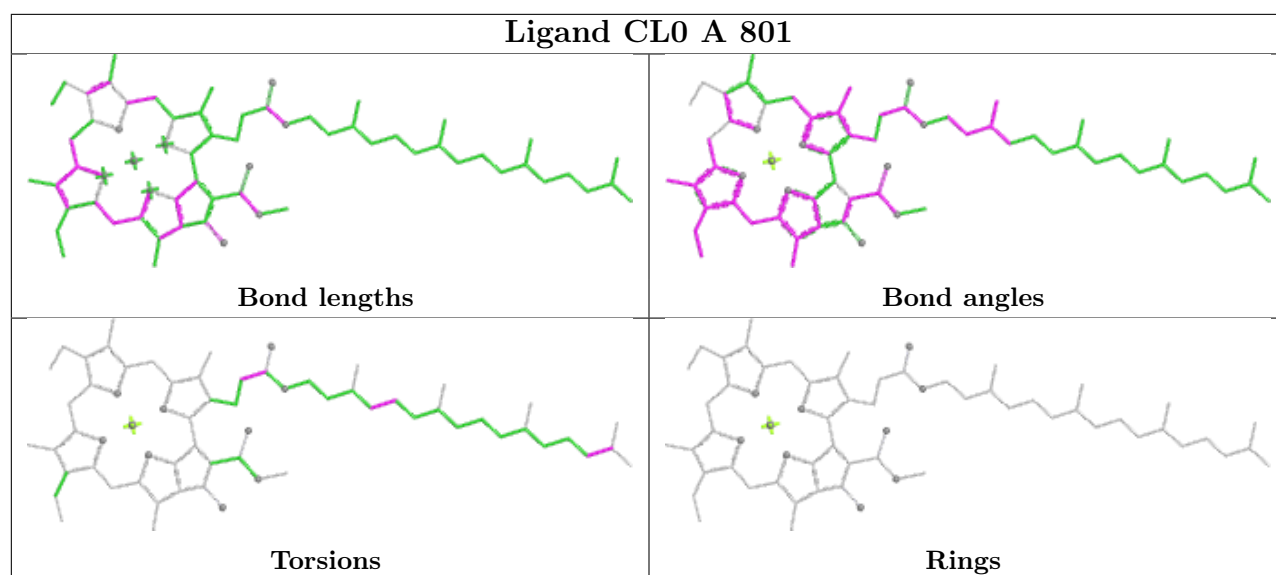


## Ligand CLA 3 306

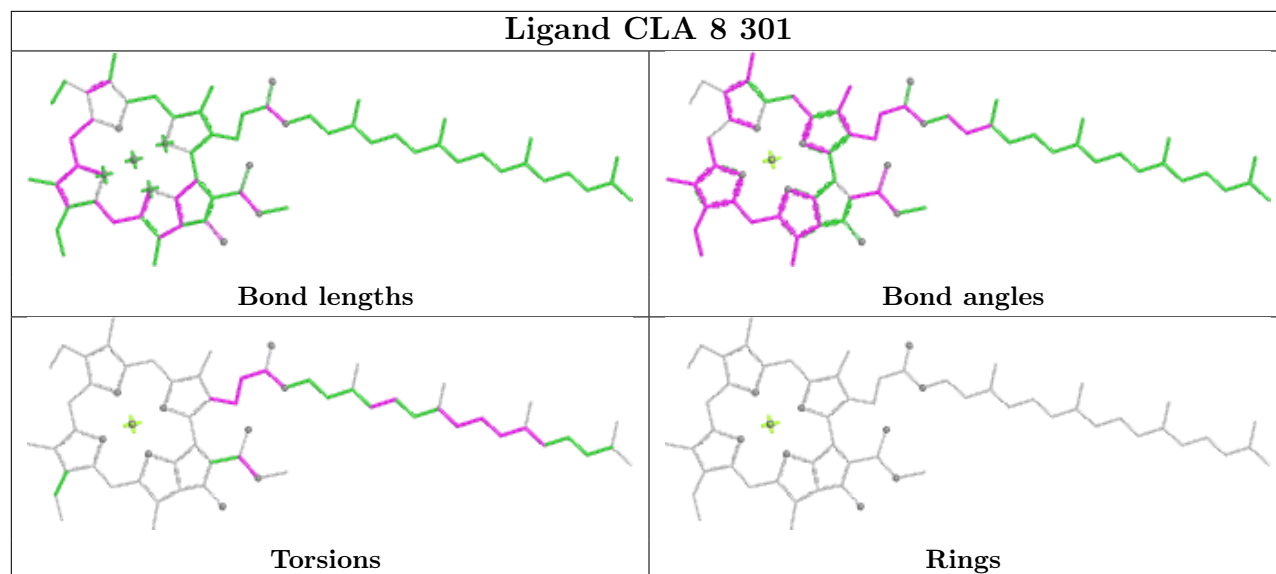


## Ligand KC1 9 304

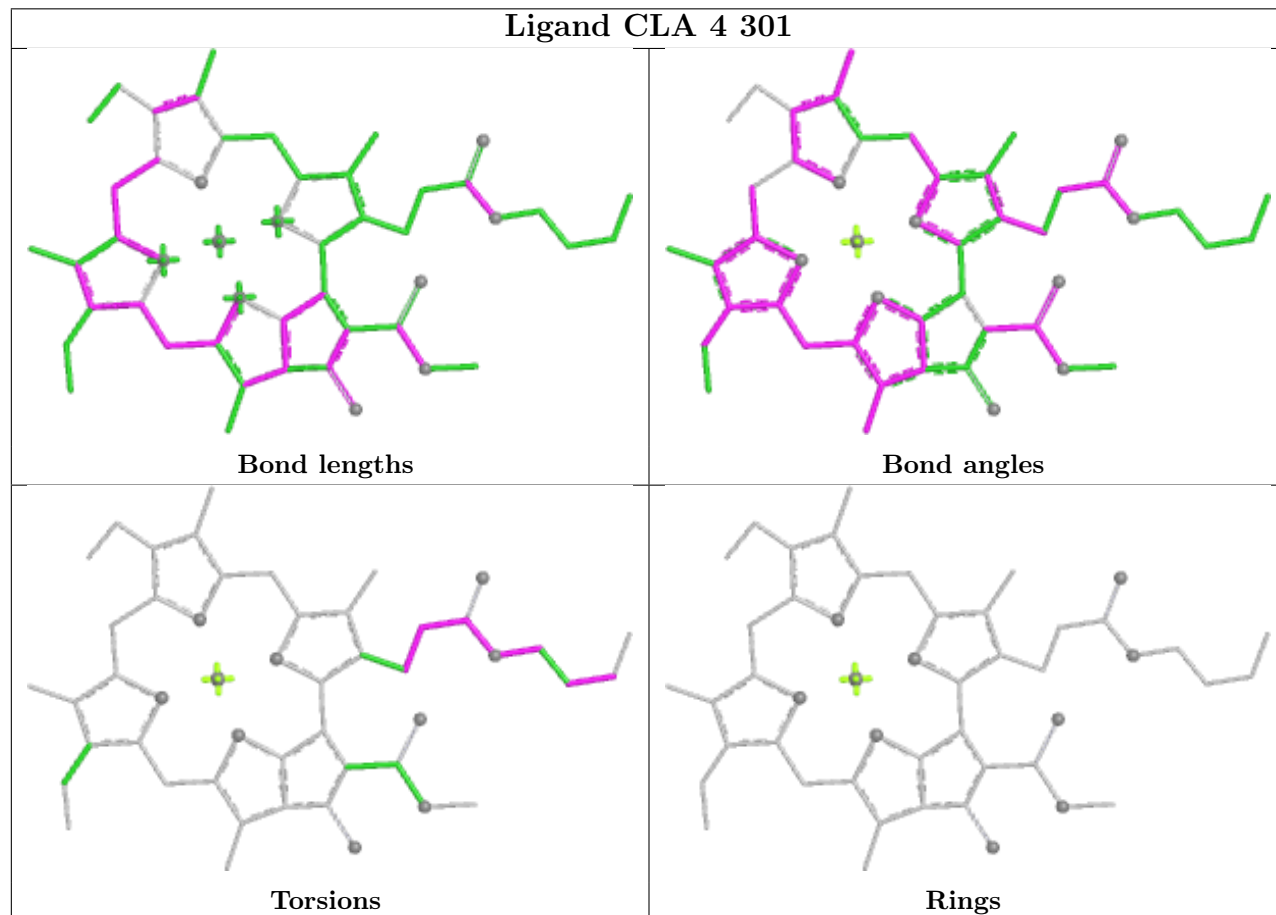


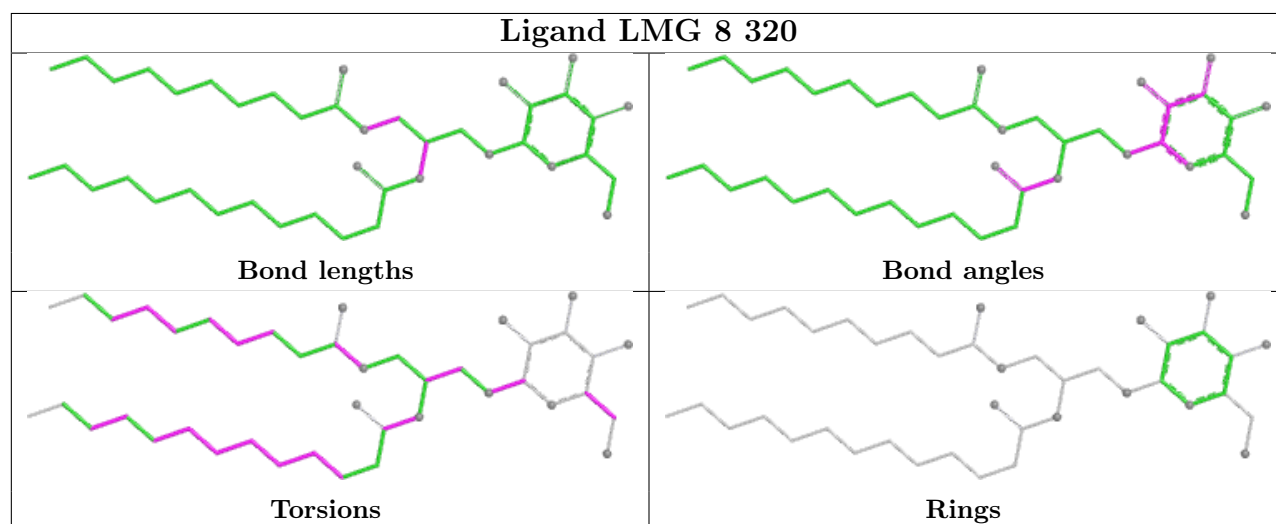
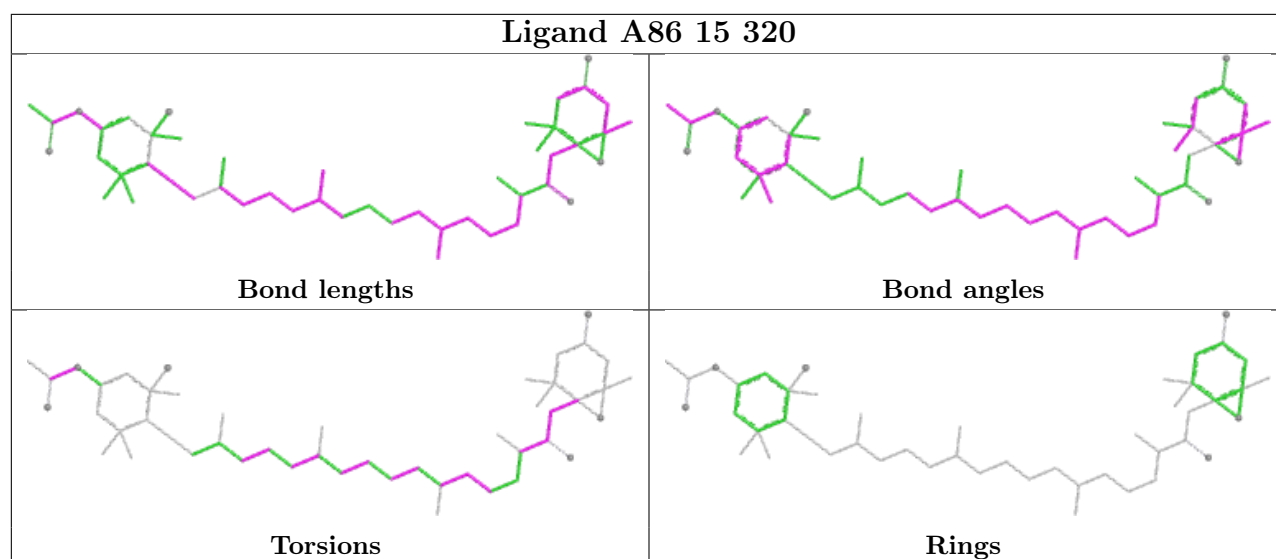


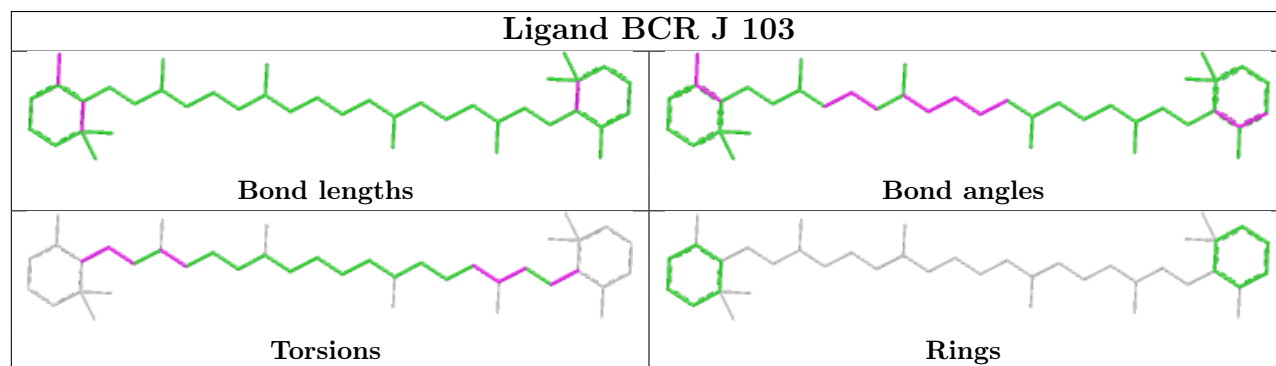
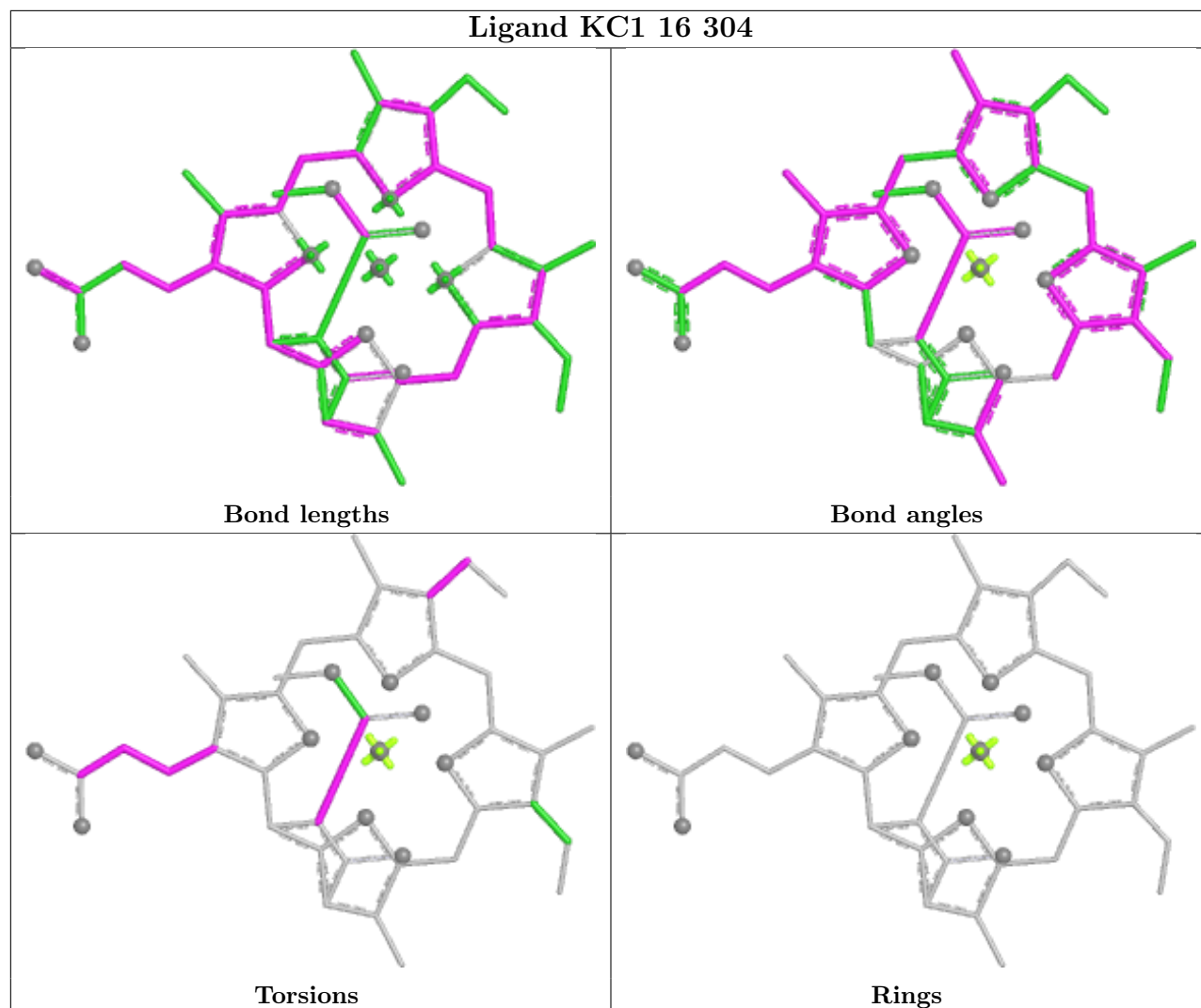
## Ligand CLA 8 301



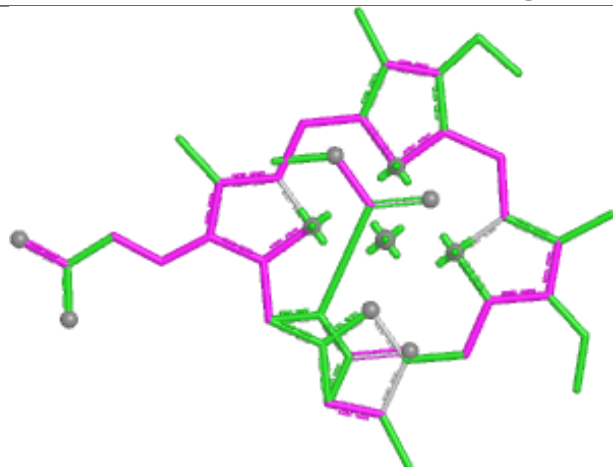
## Ligand CLA 4 301



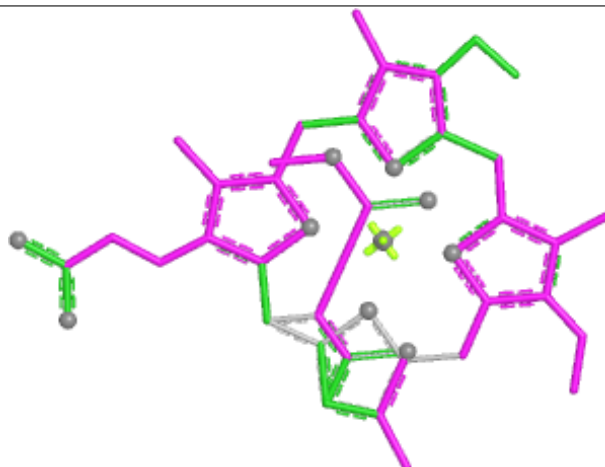




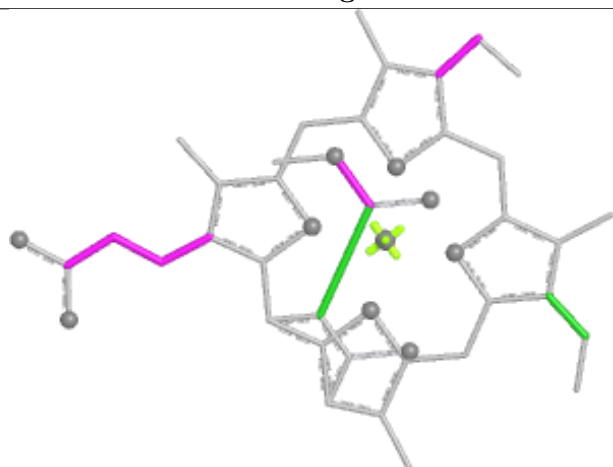
## Ligand KC1 2 314



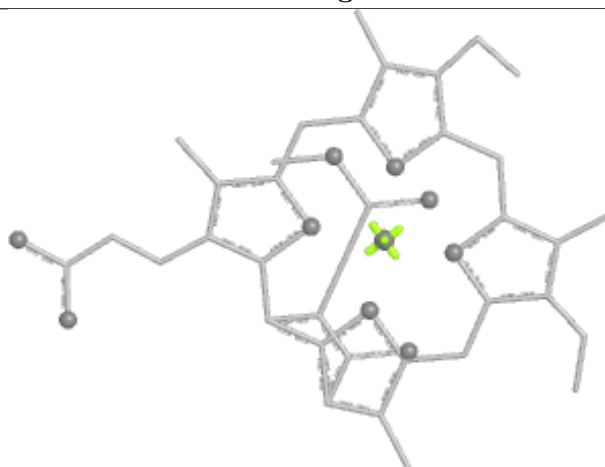
Bond lengths



Bond angles

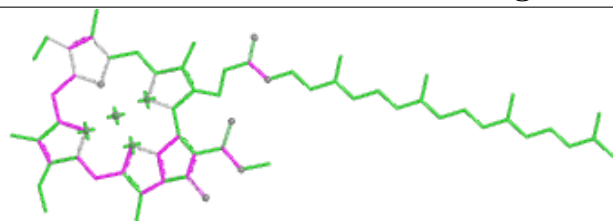


Torsions

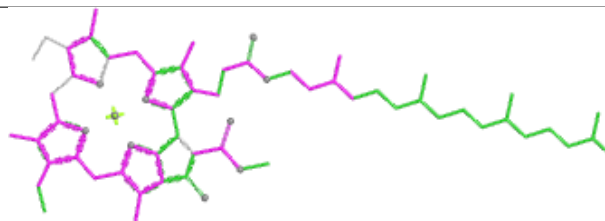


Rings

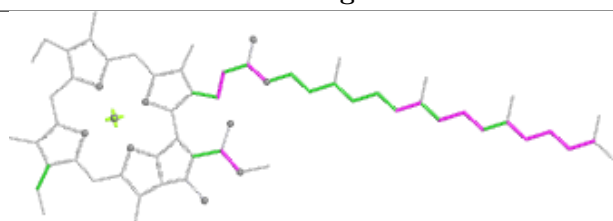
## Ligand CLA A 829



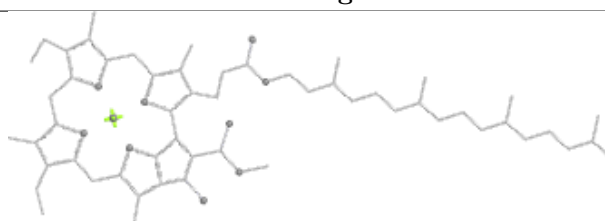
Bond lengths



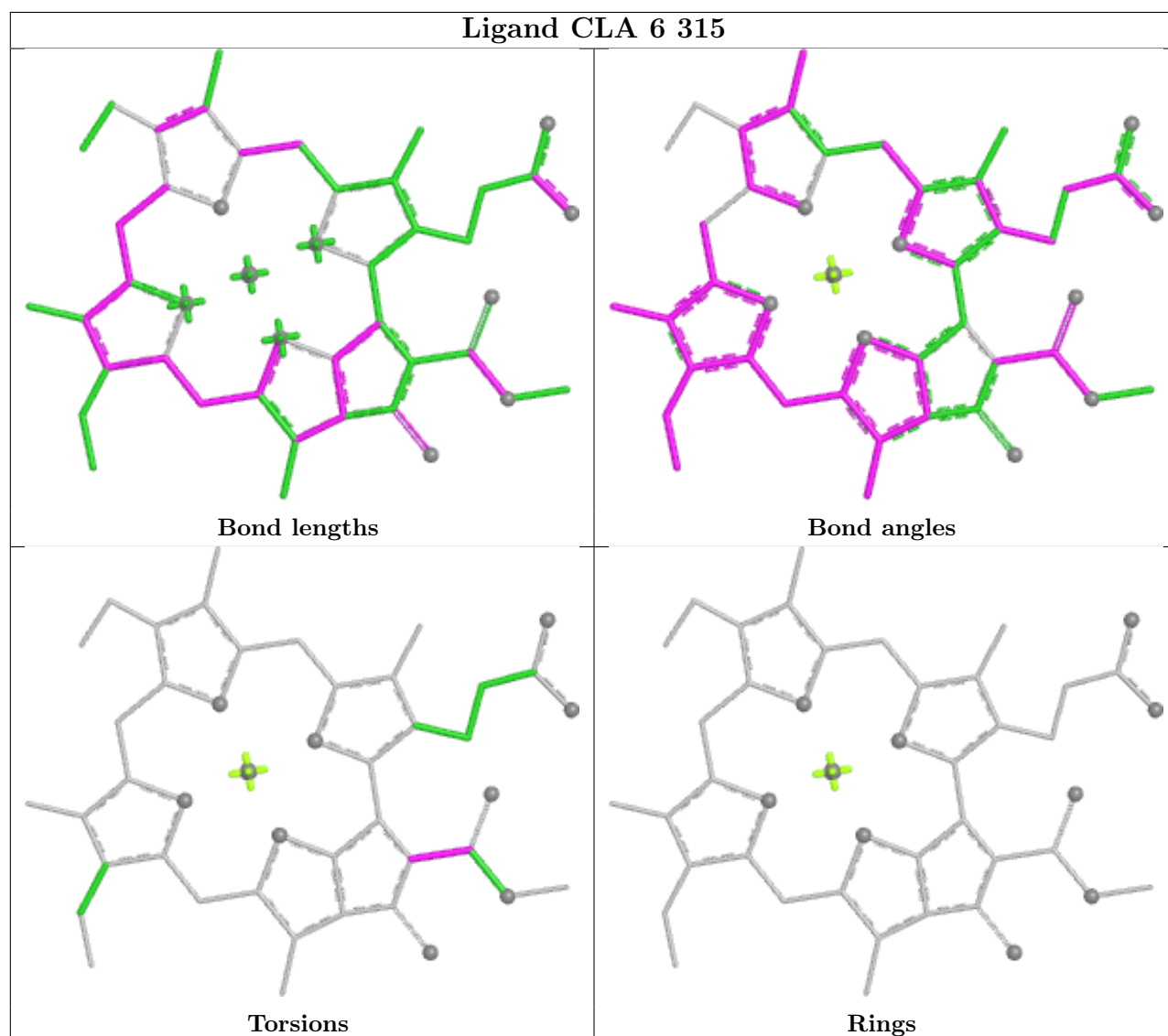
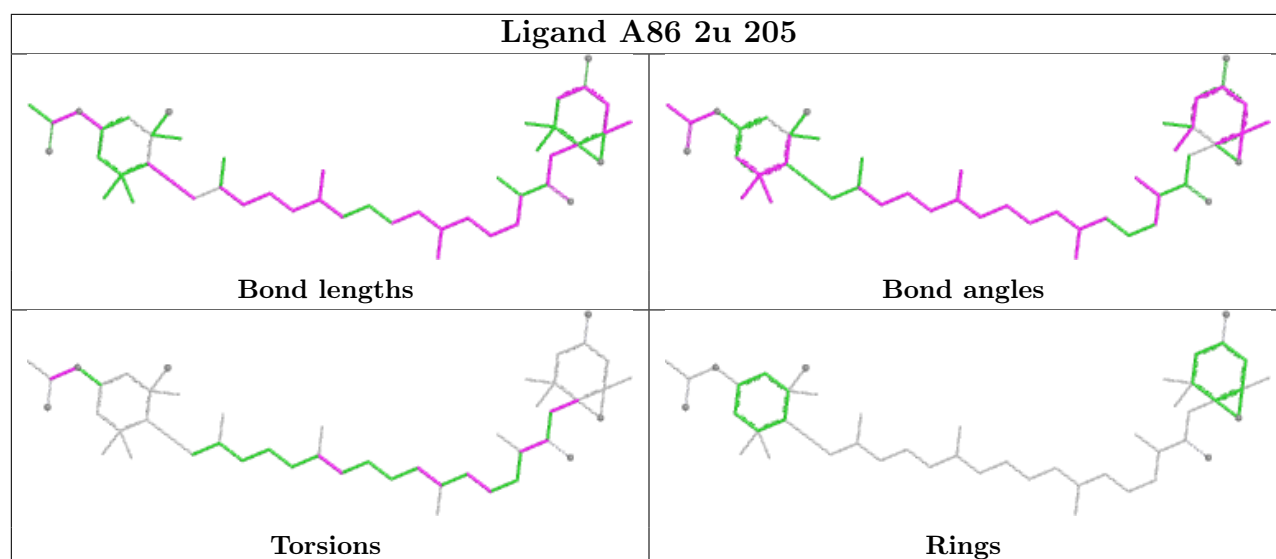
Bond angles

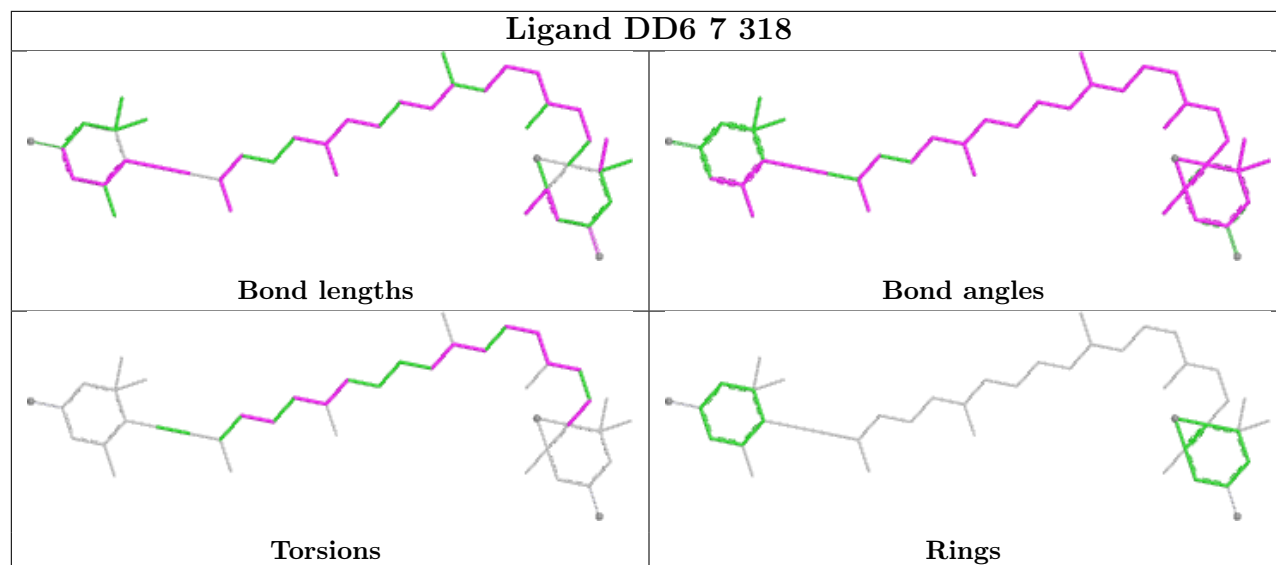
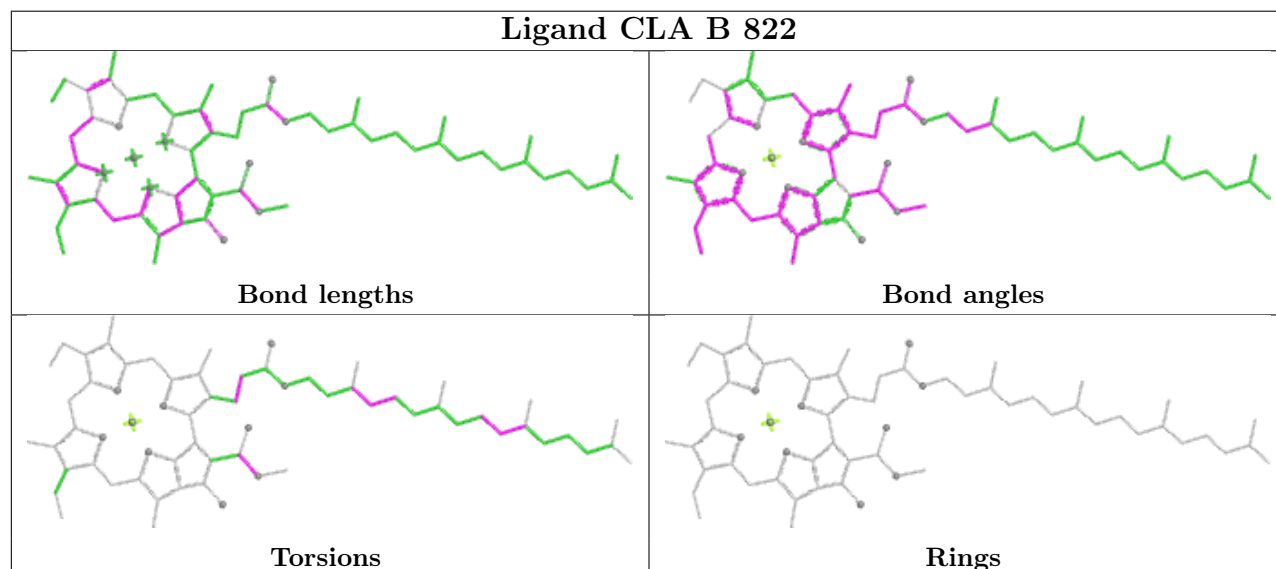
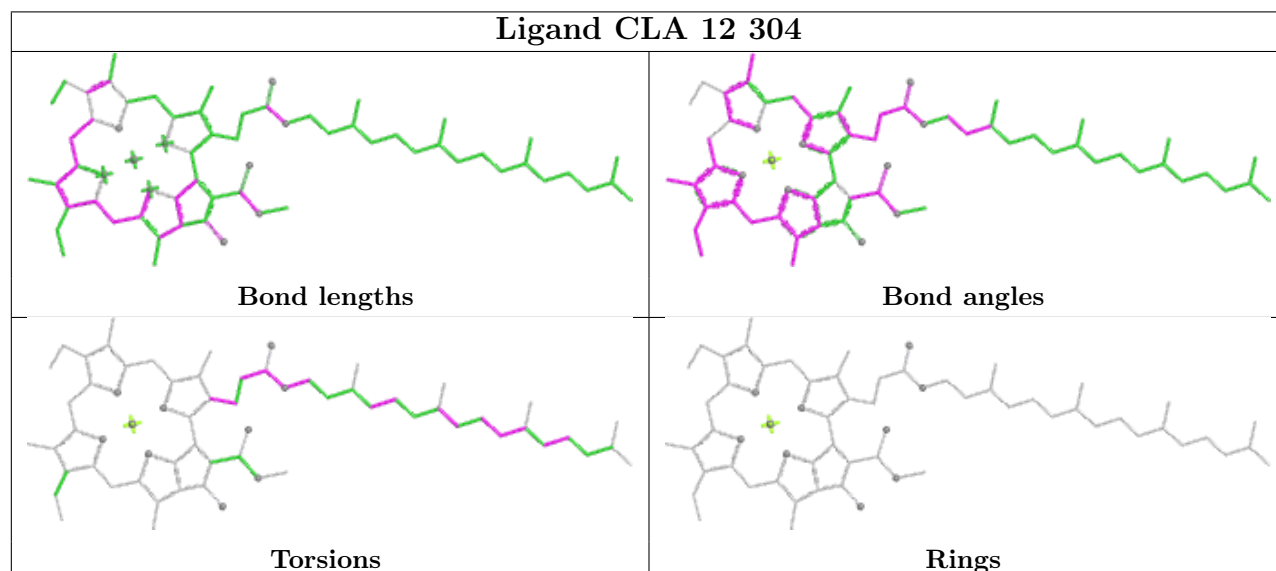


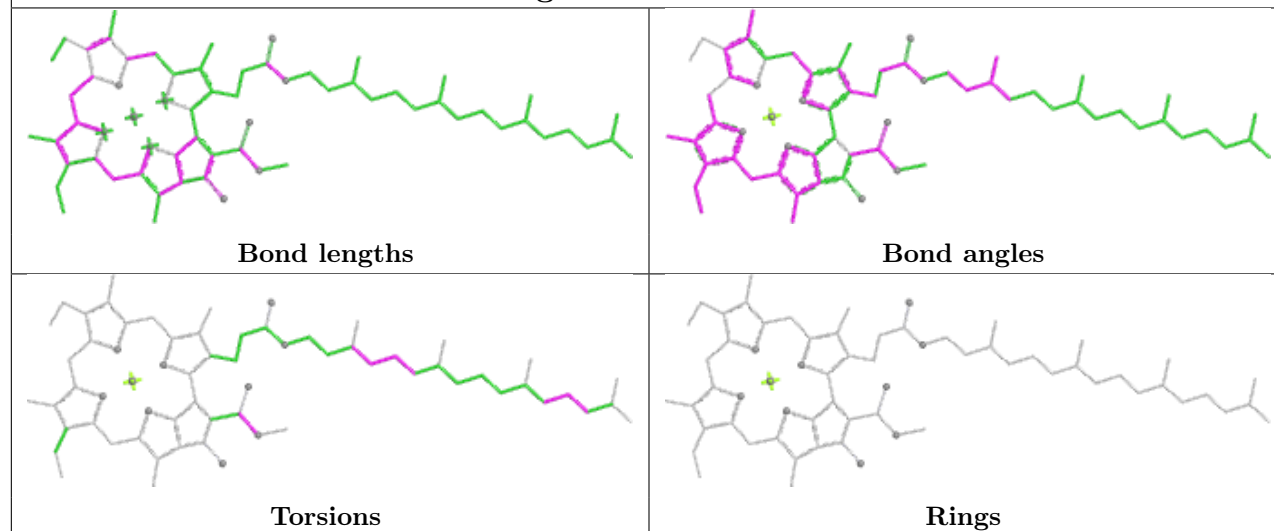
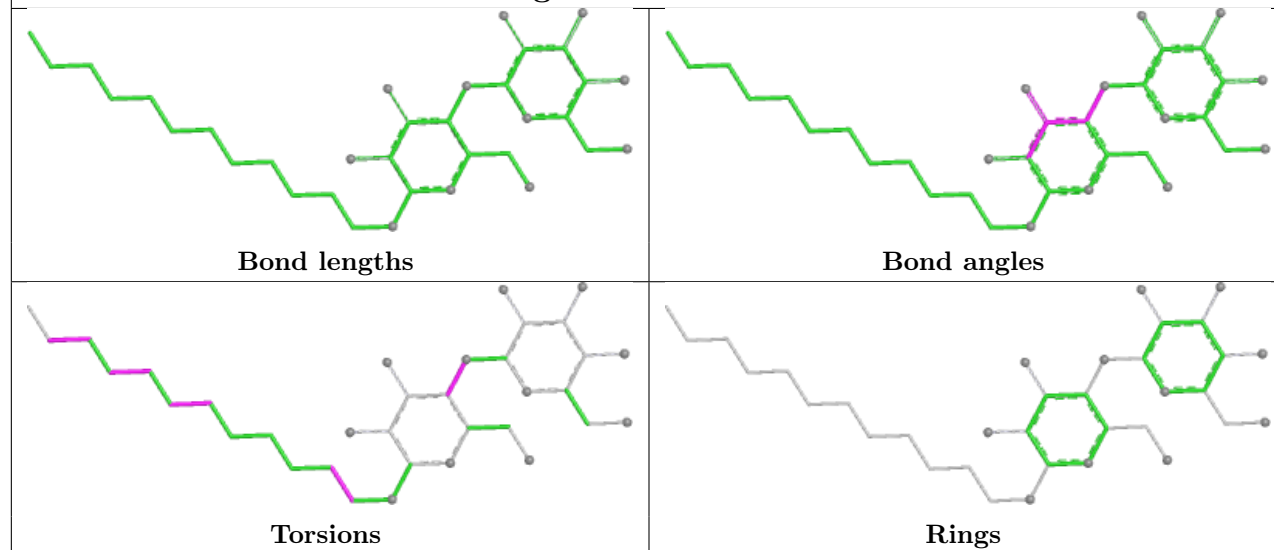
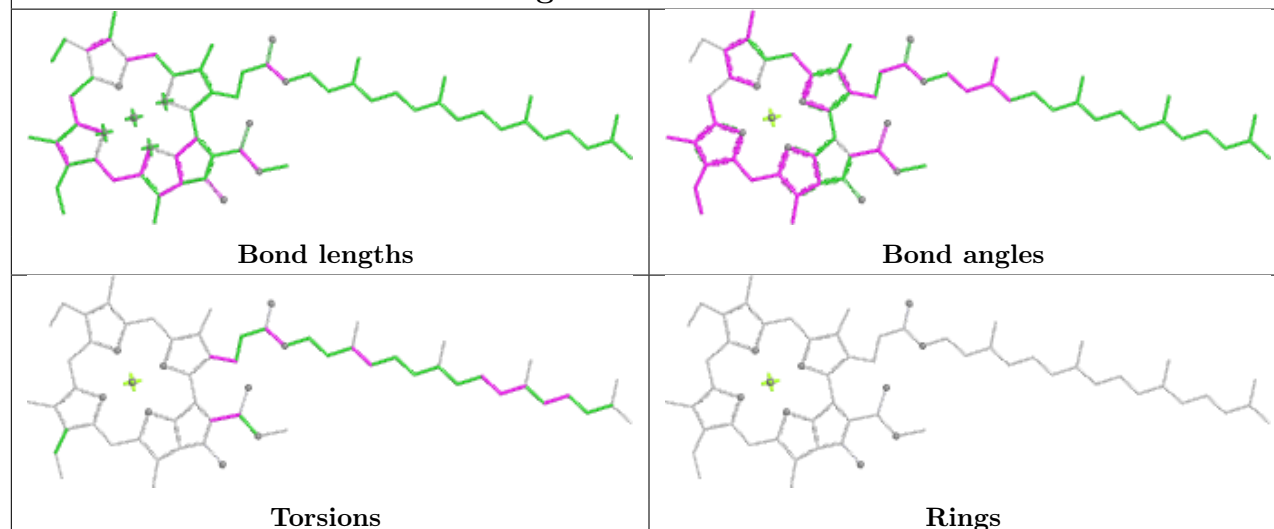
Torsions



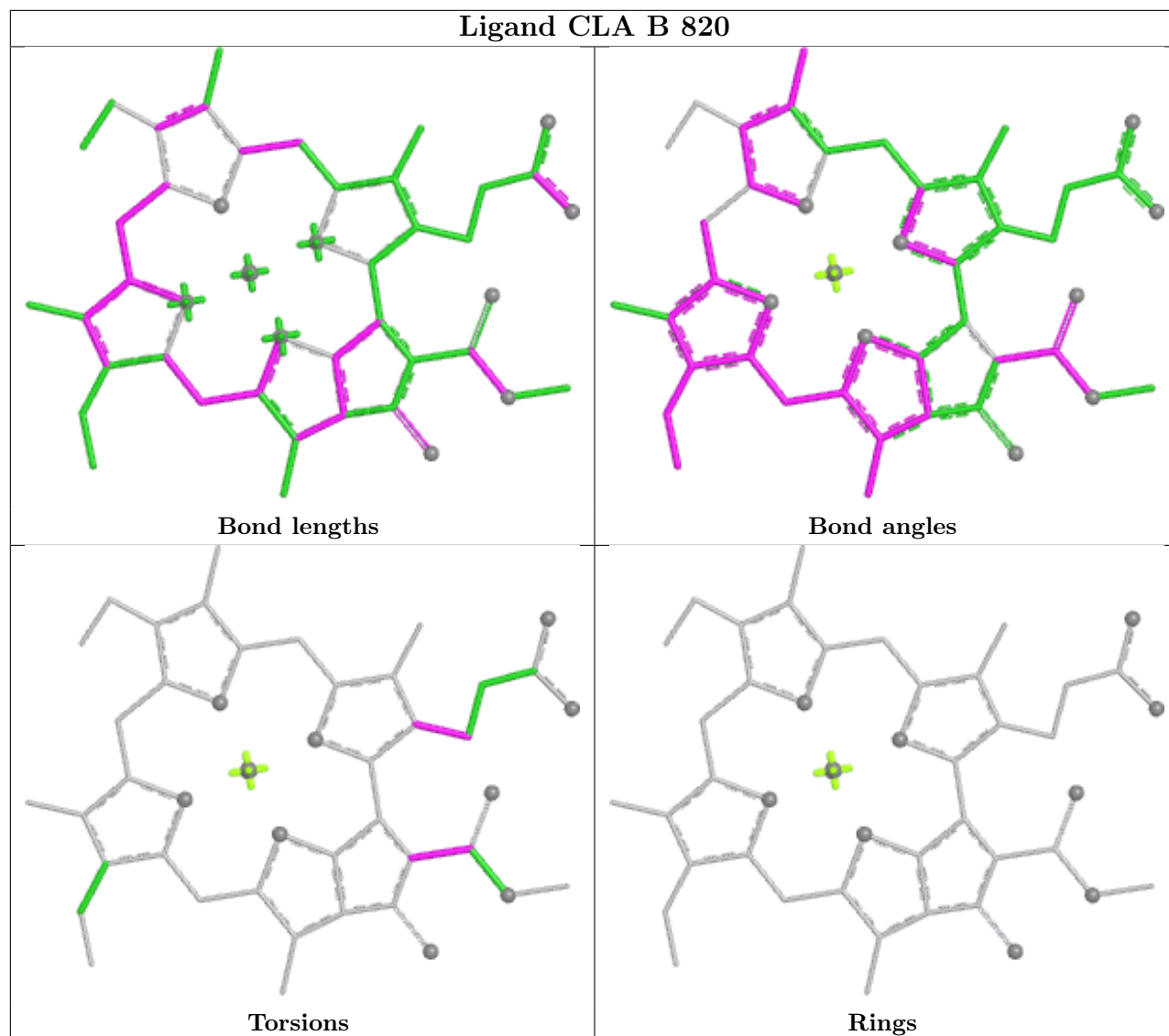
Rings



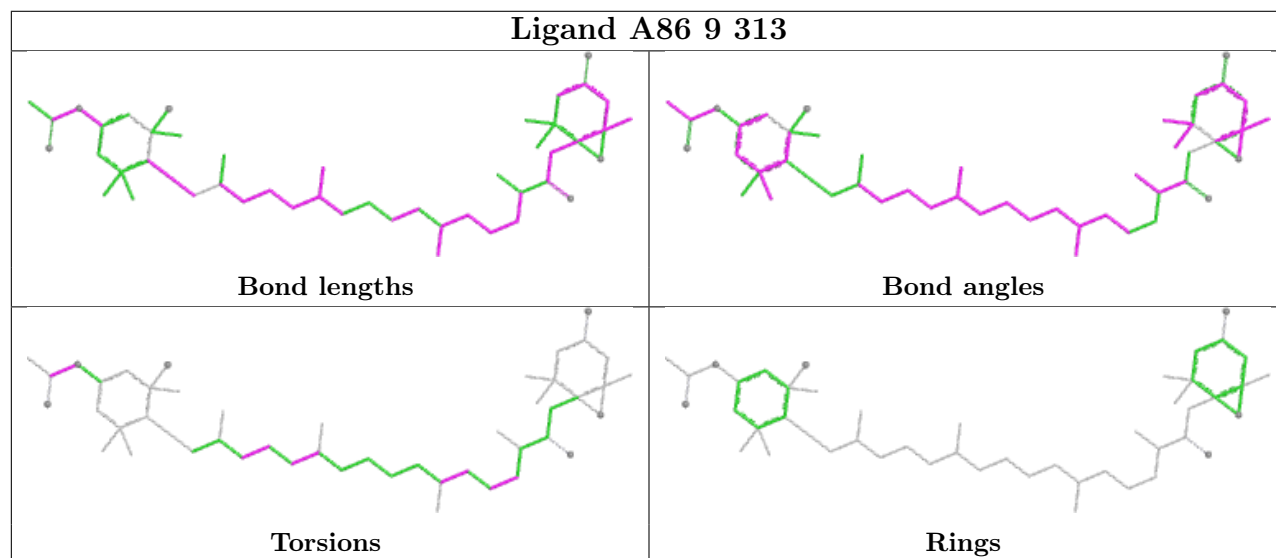
**Ligand DD6 7 318****Ligand CLA B 822****Ligand CLA 12 304**

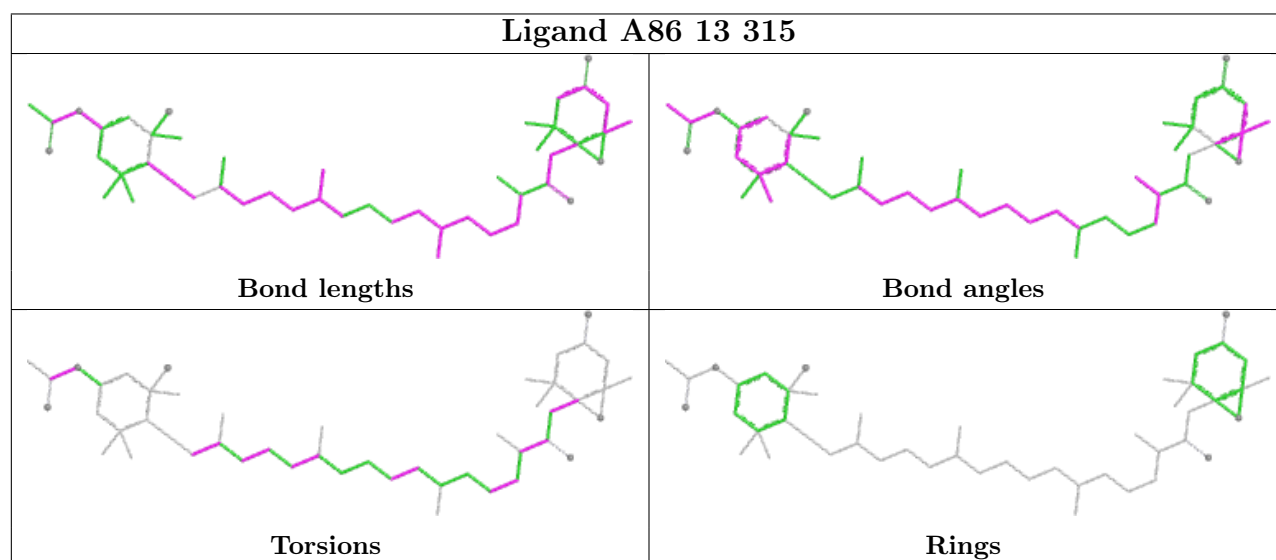
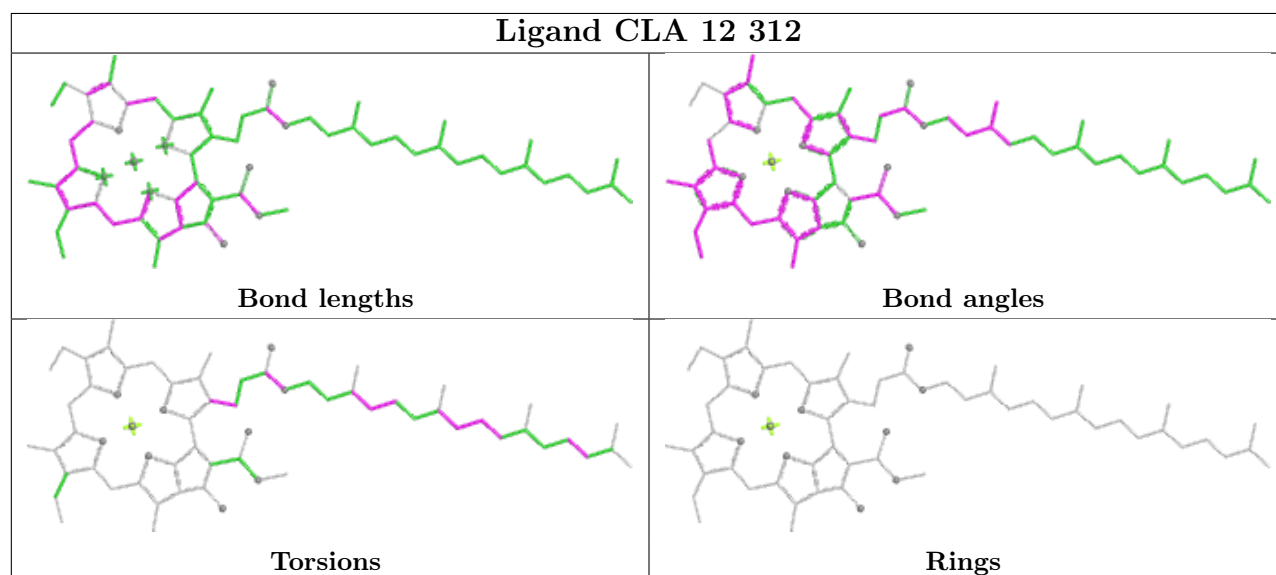
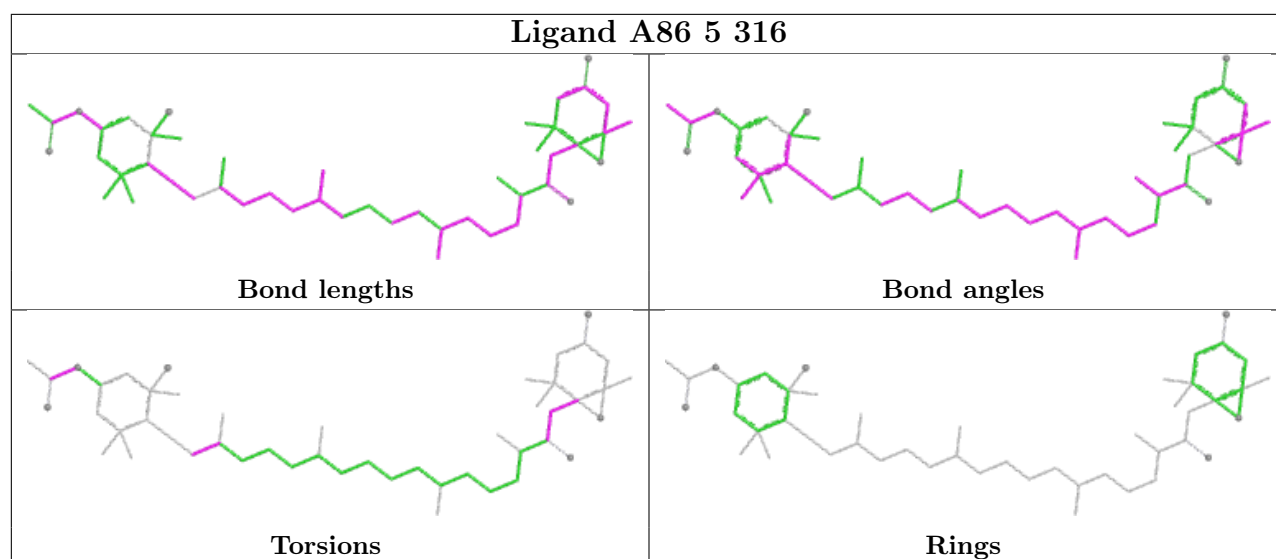
**Ligand CLA 8 302****Ligand LMT 1 311****Ligand CLA 8 303**

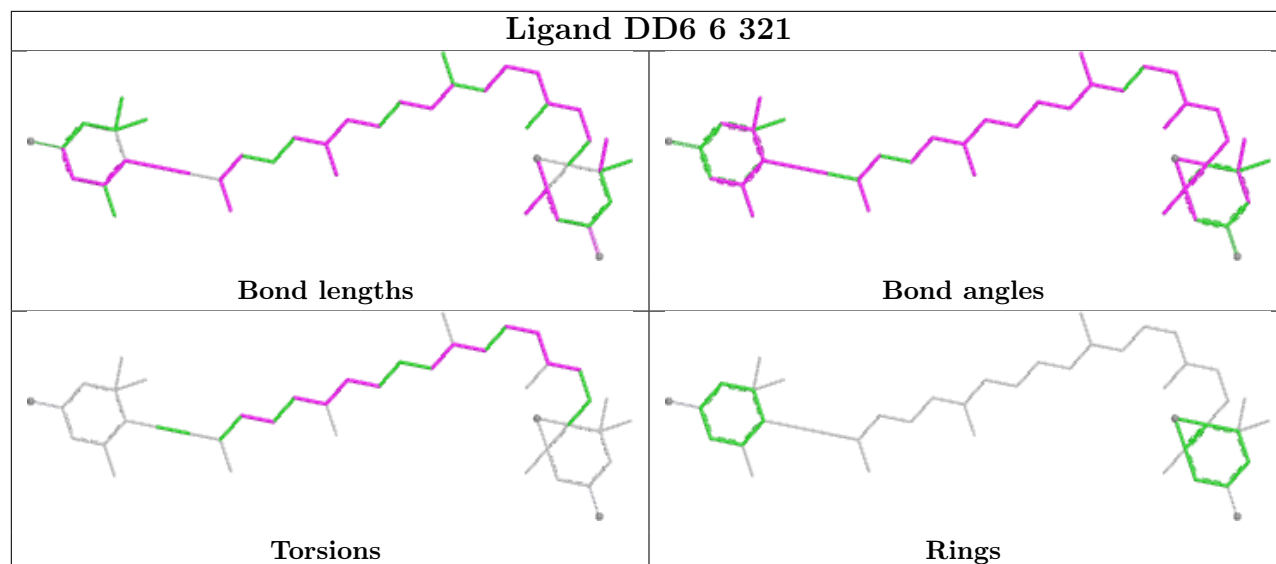
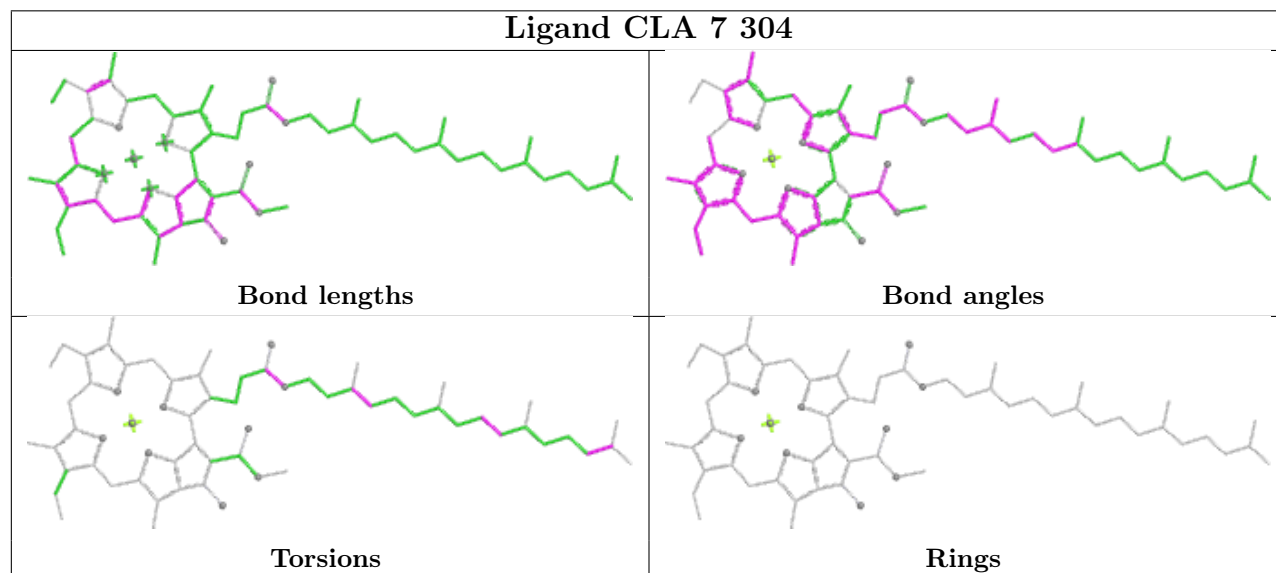
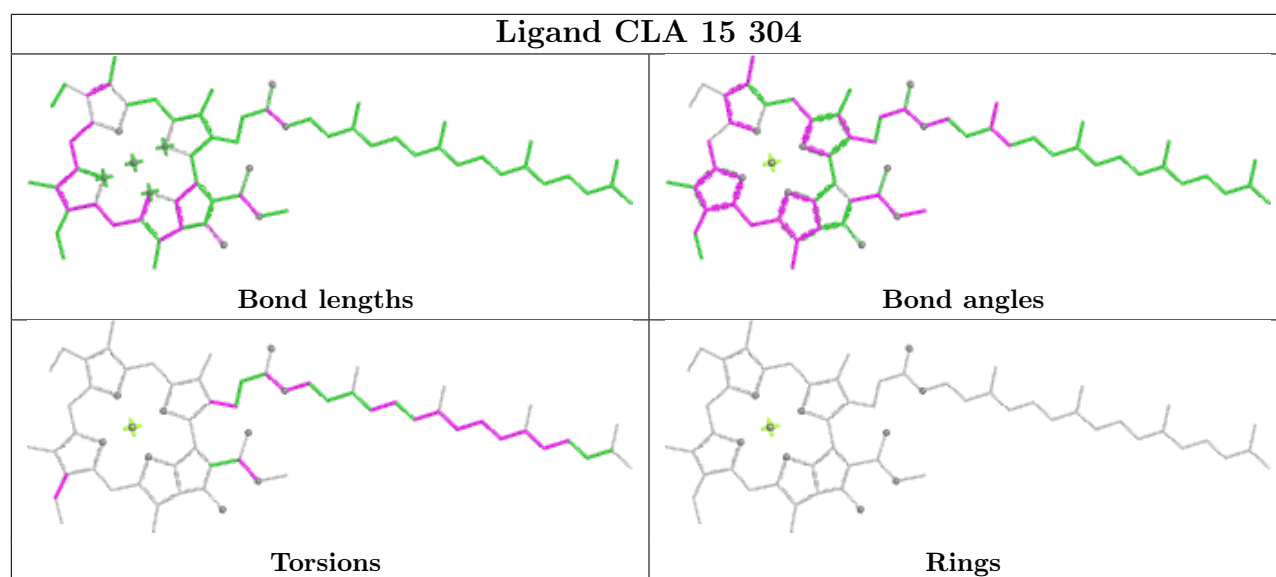
## Ligand CLA B 820

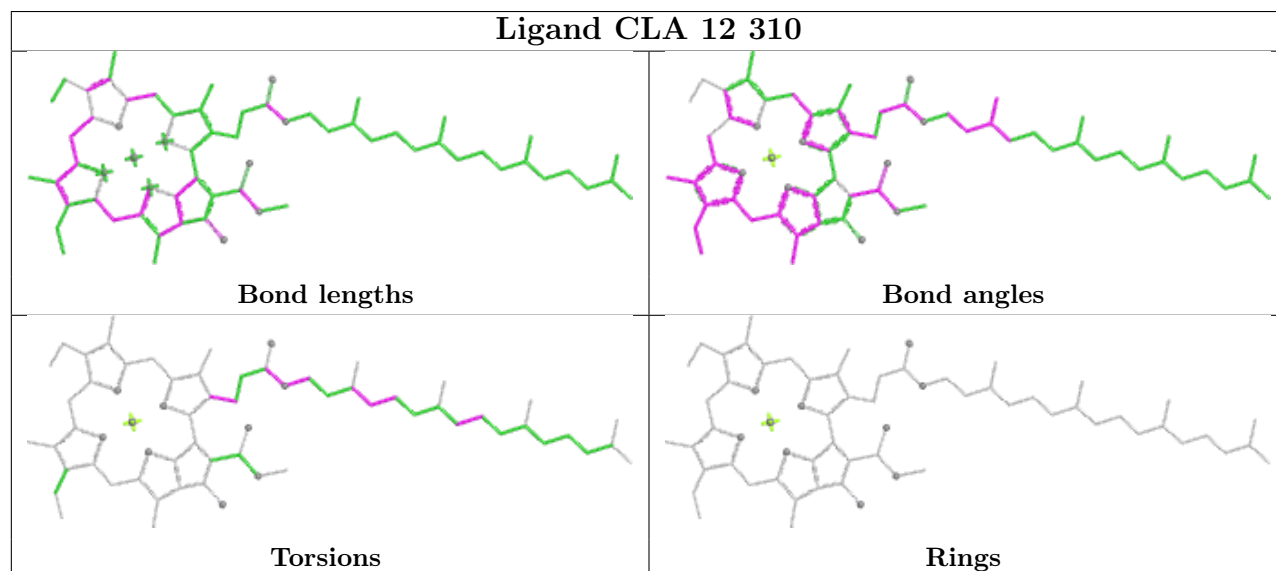
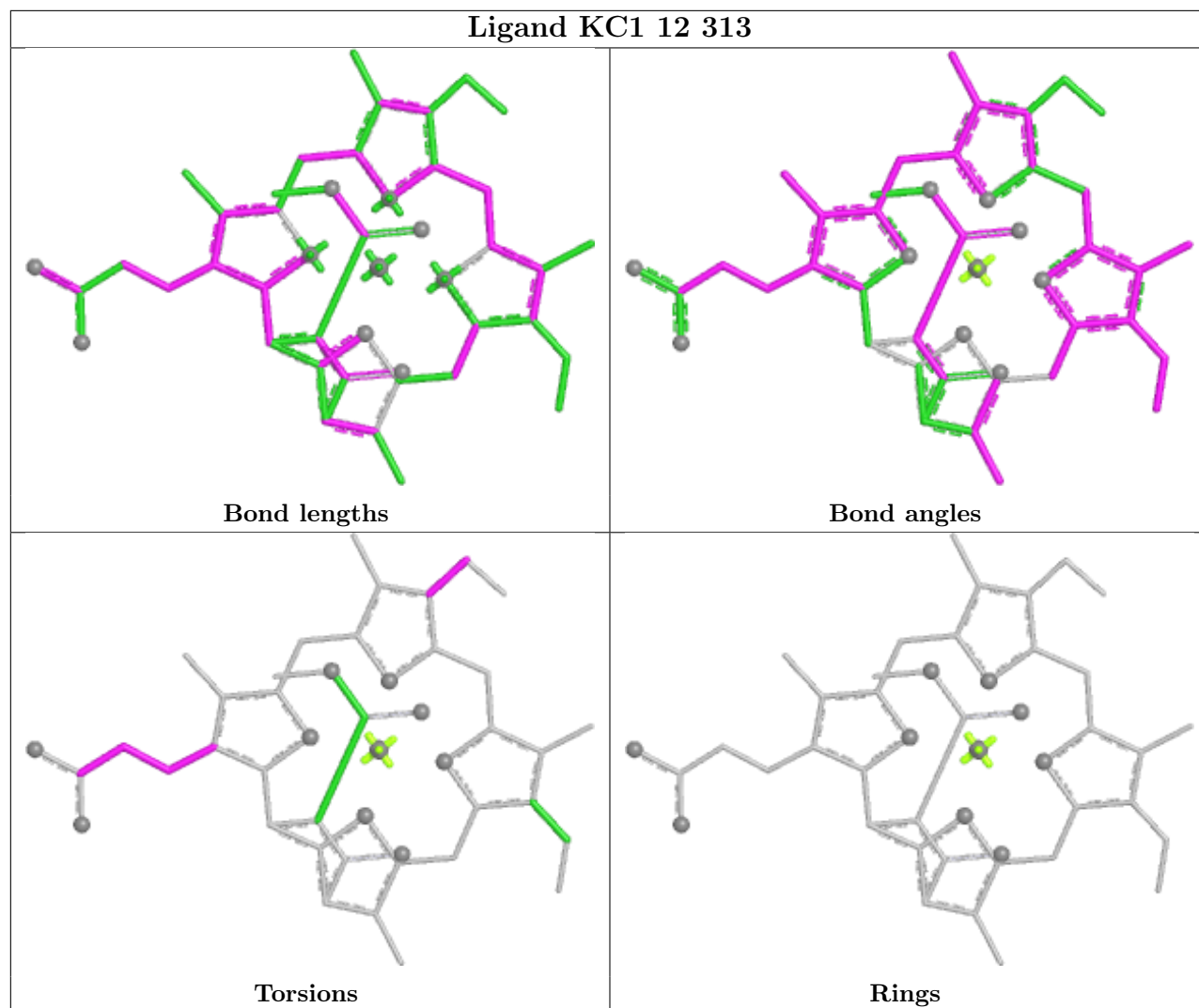


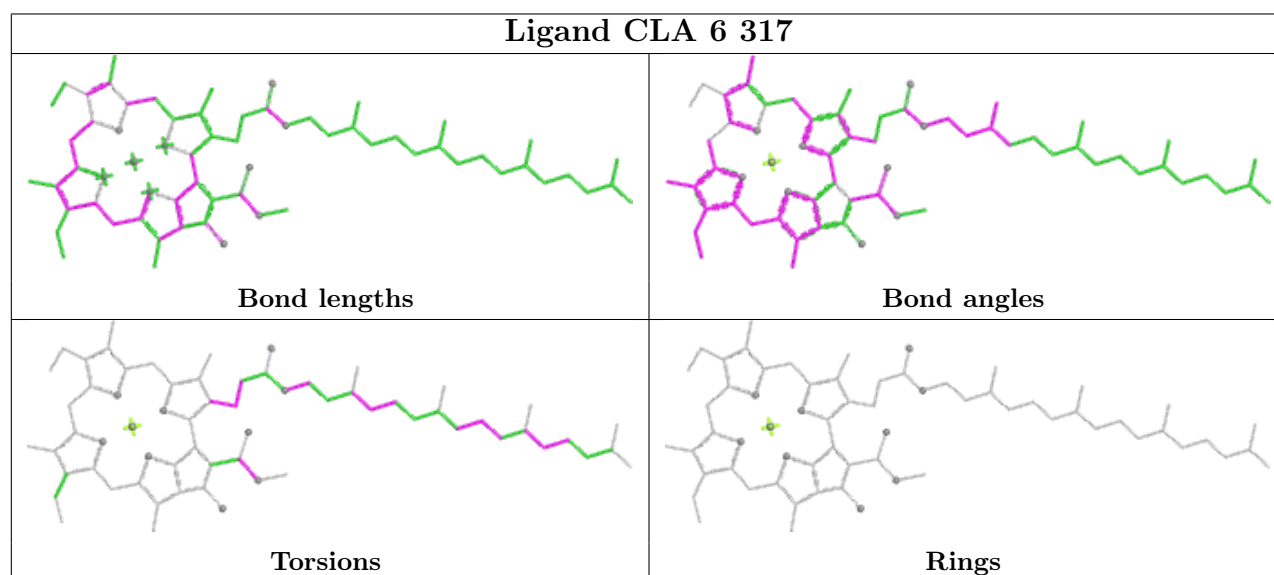
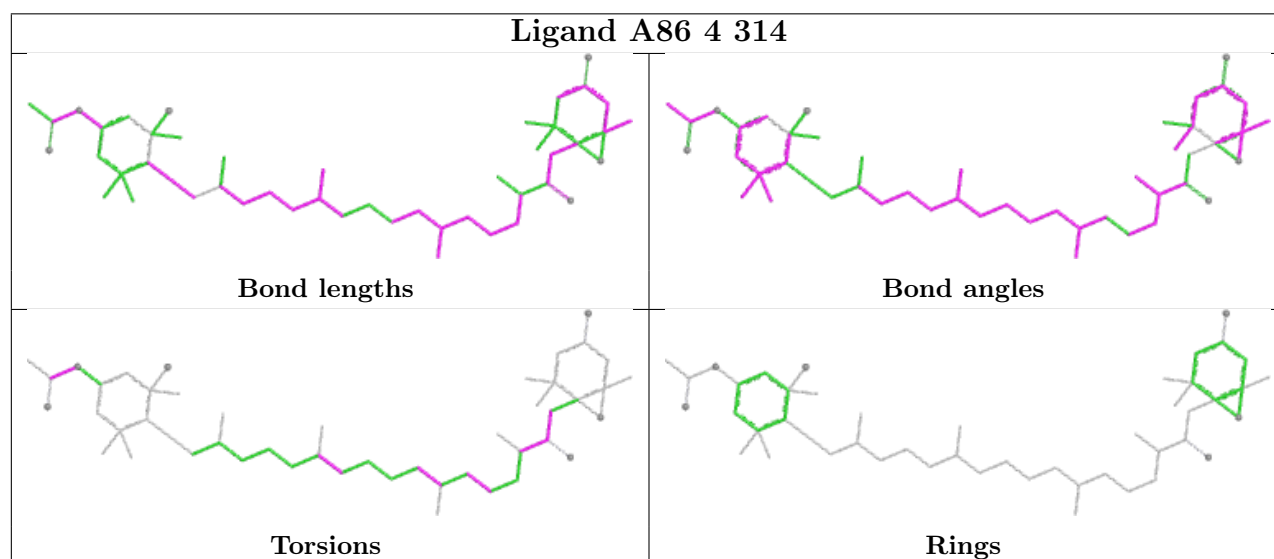
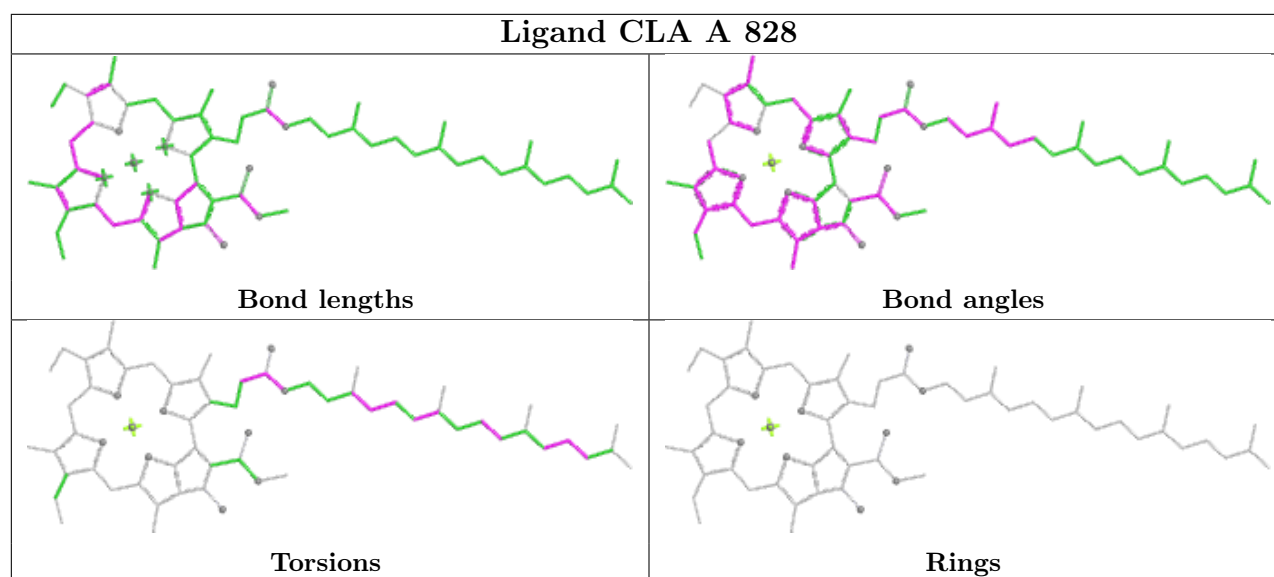
## Ligand A86 9 313

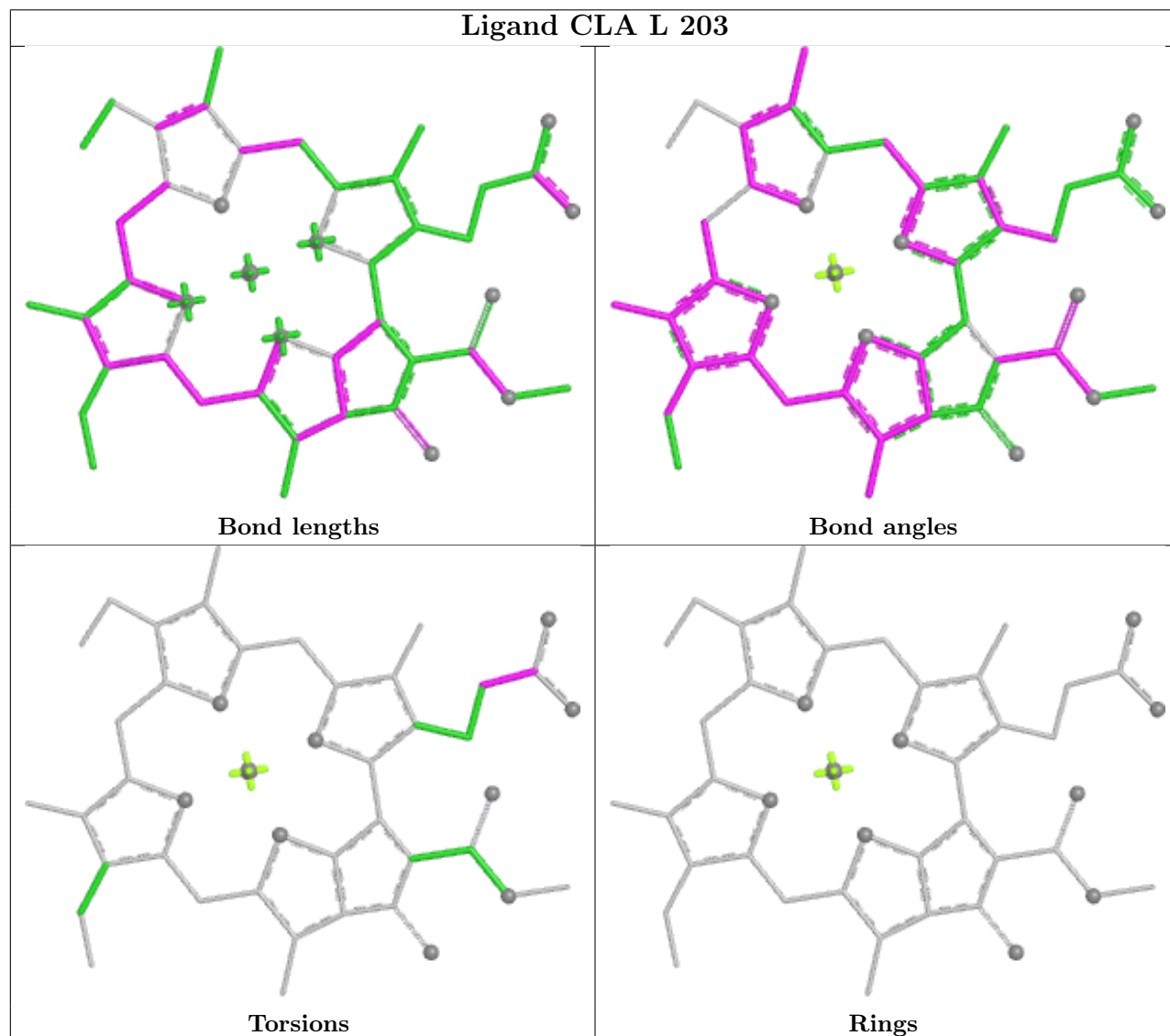
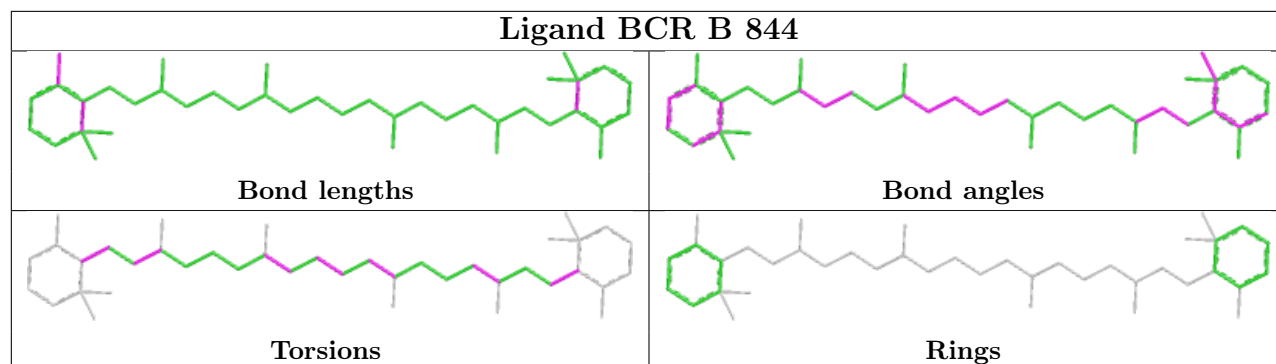


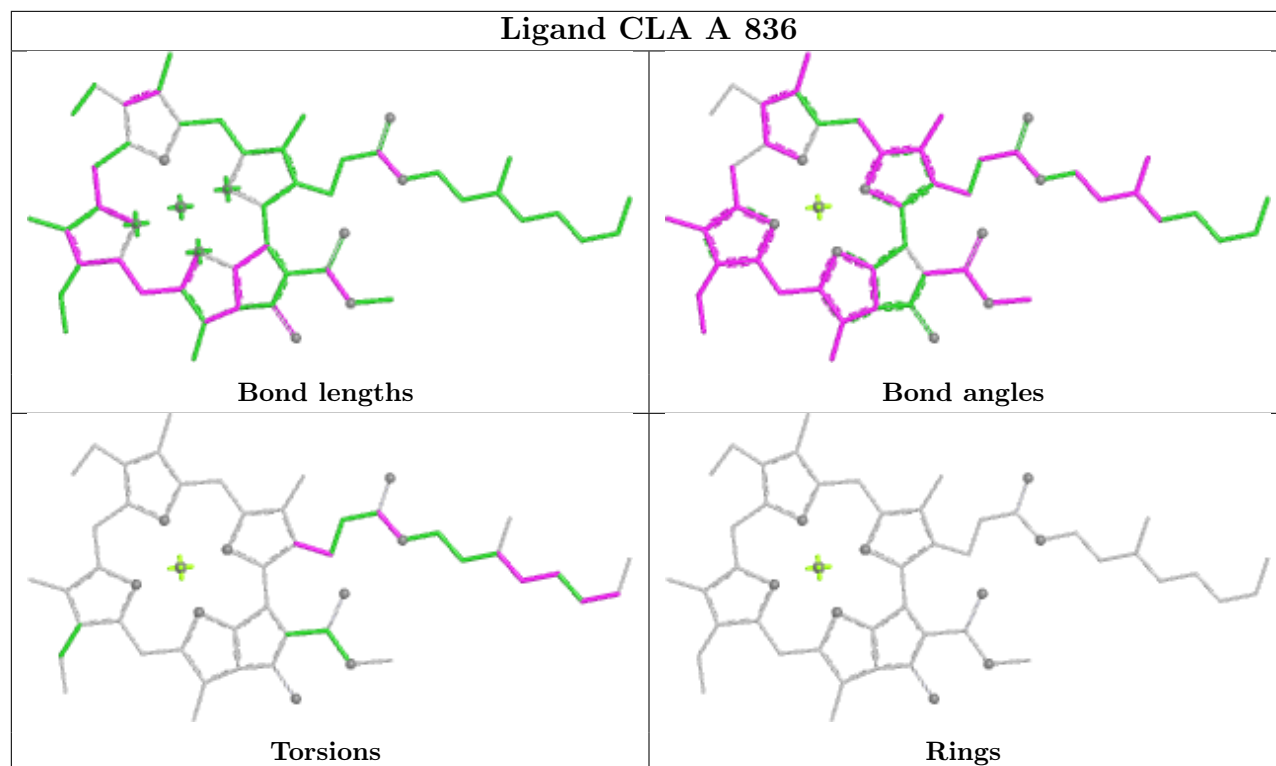
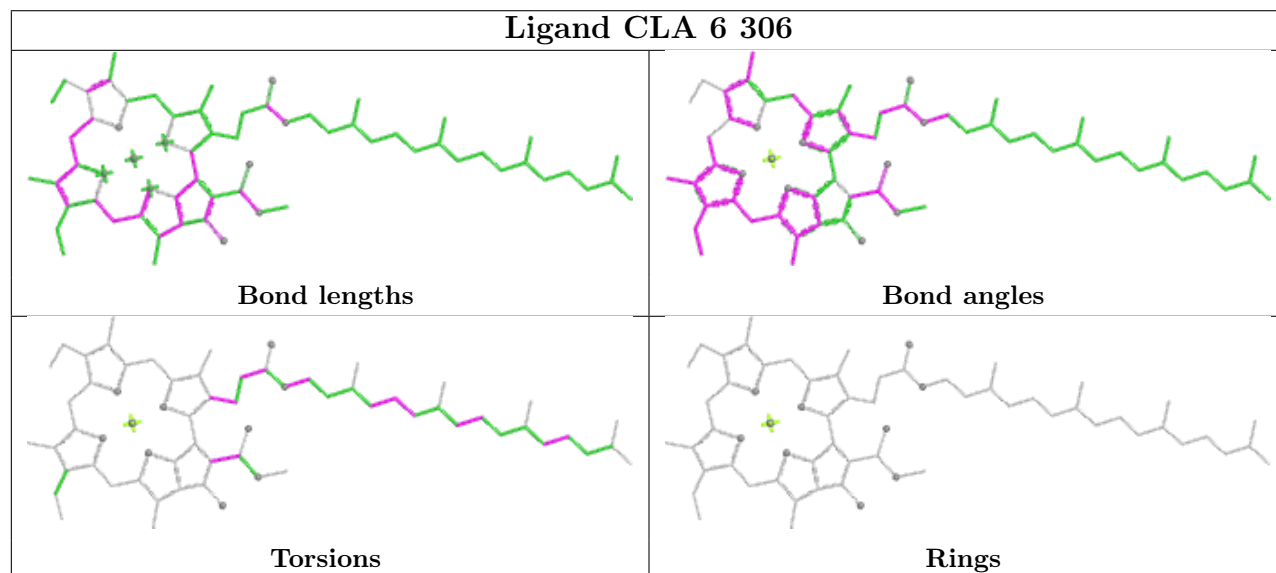


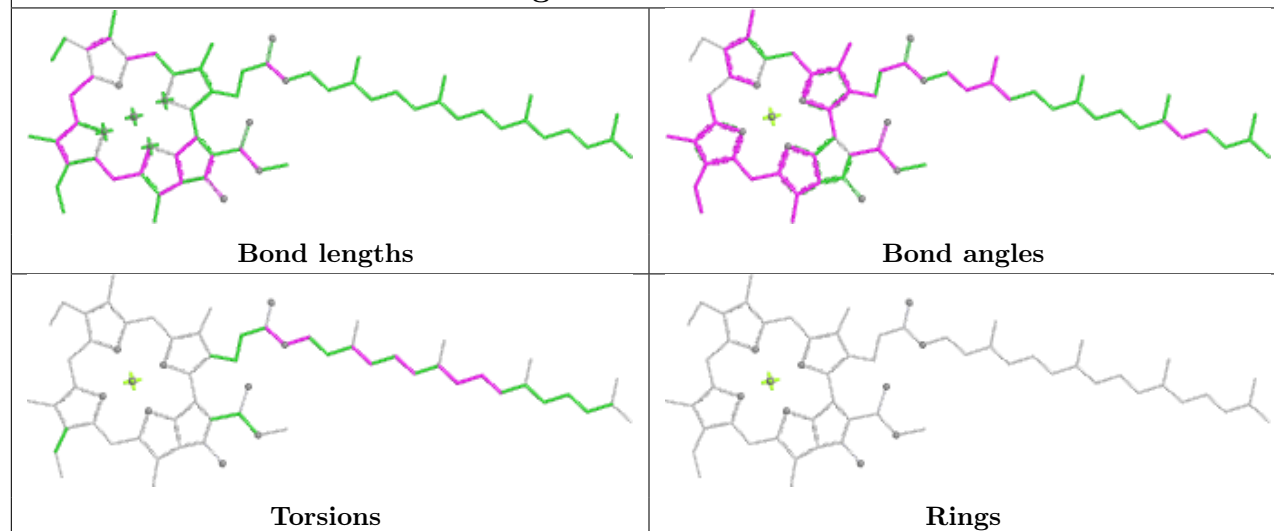
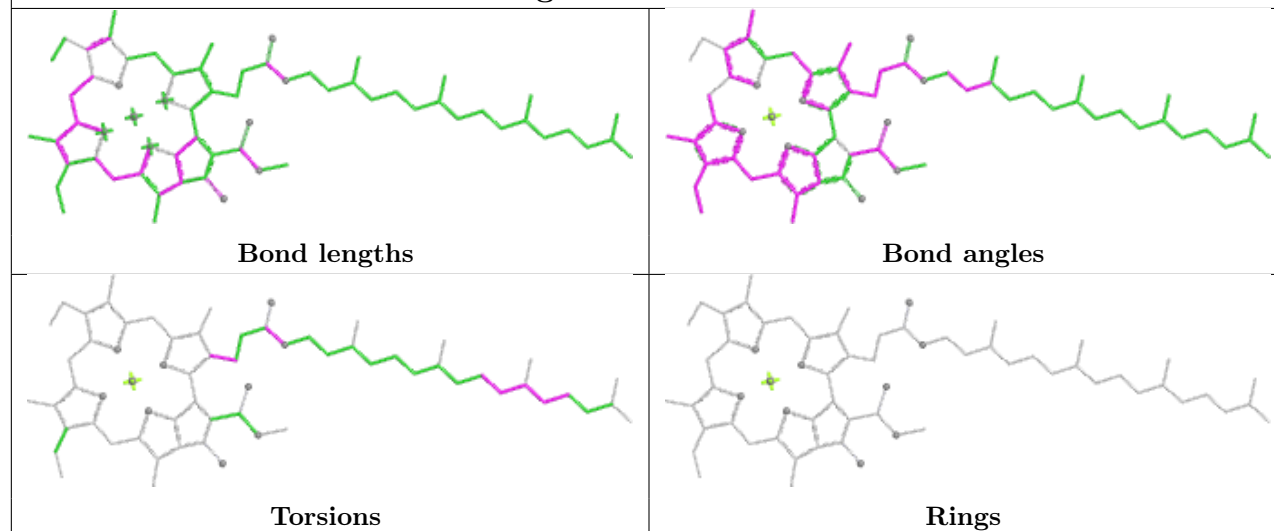


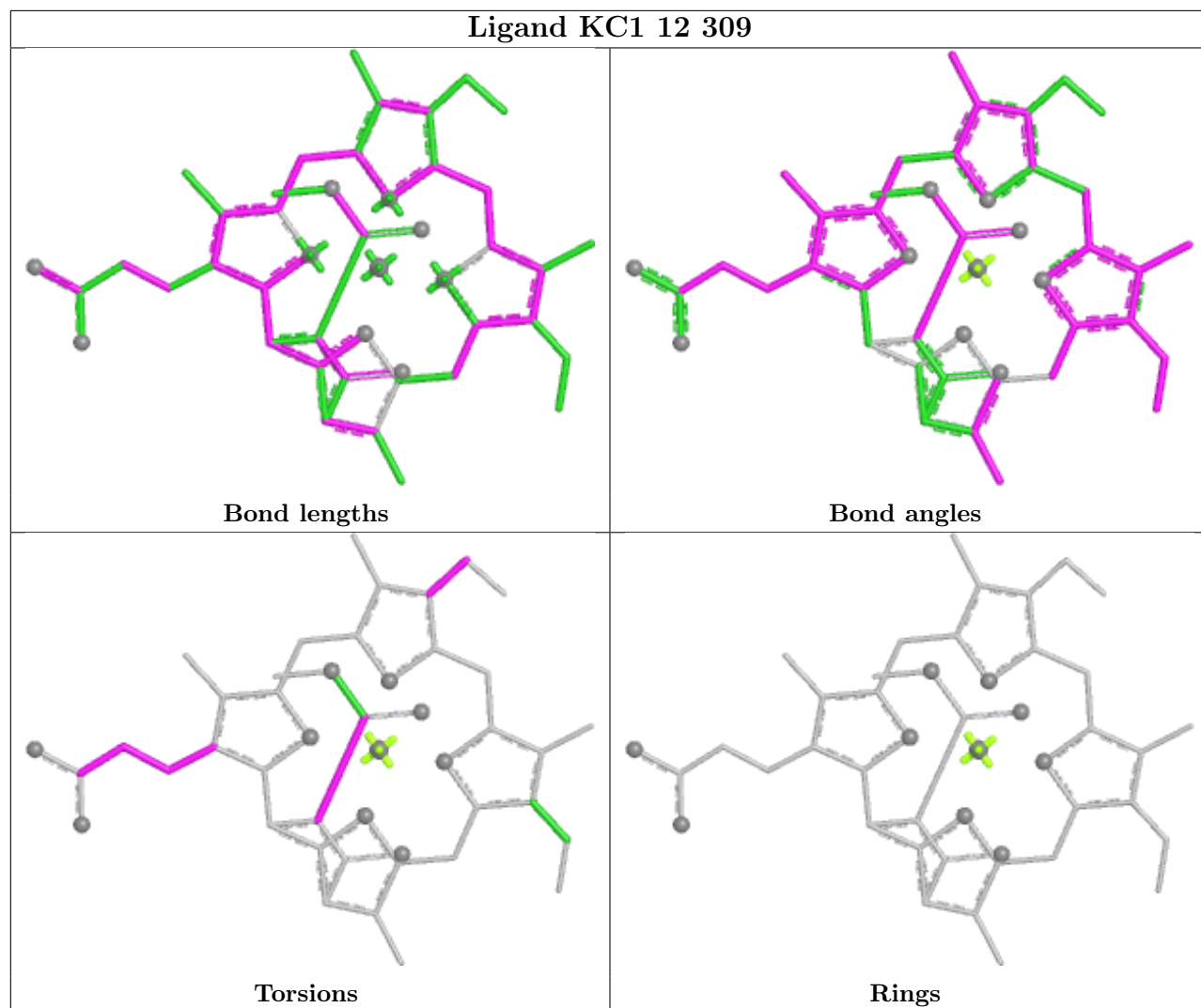


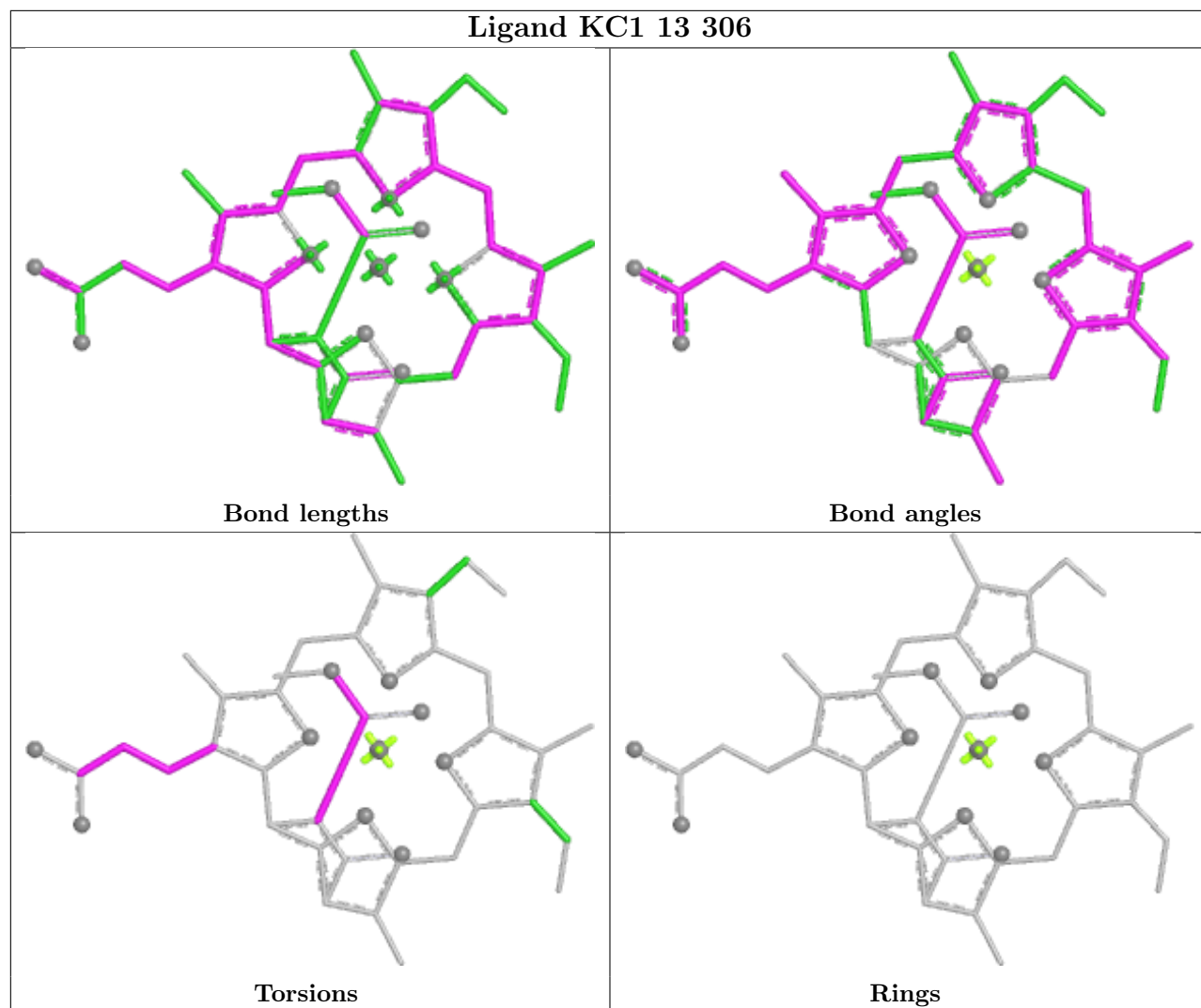


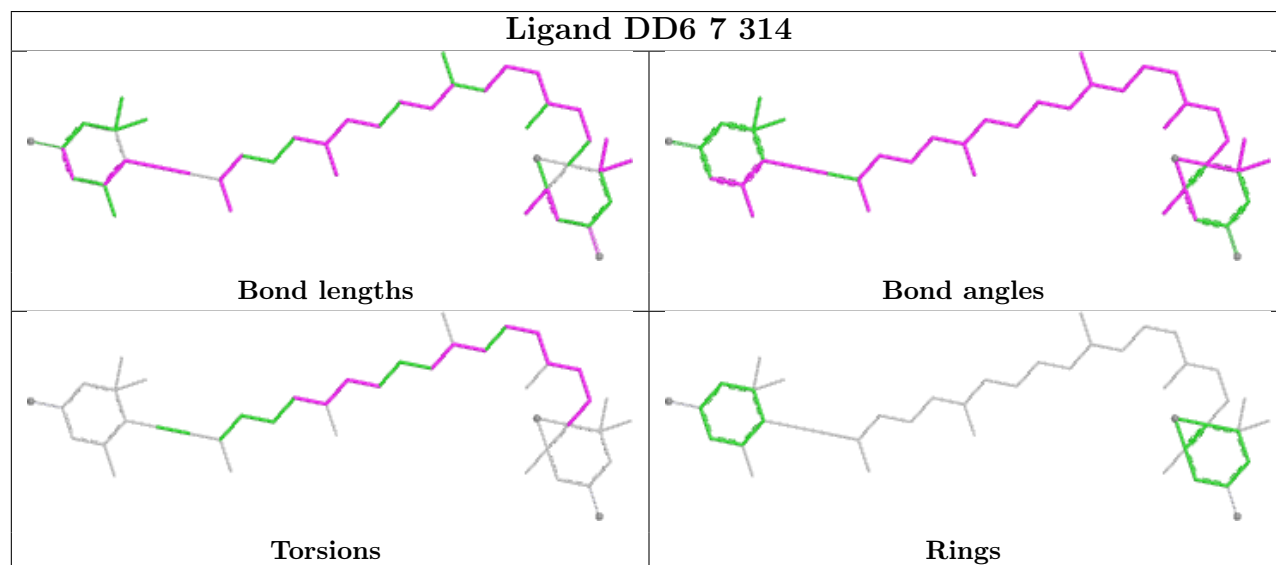
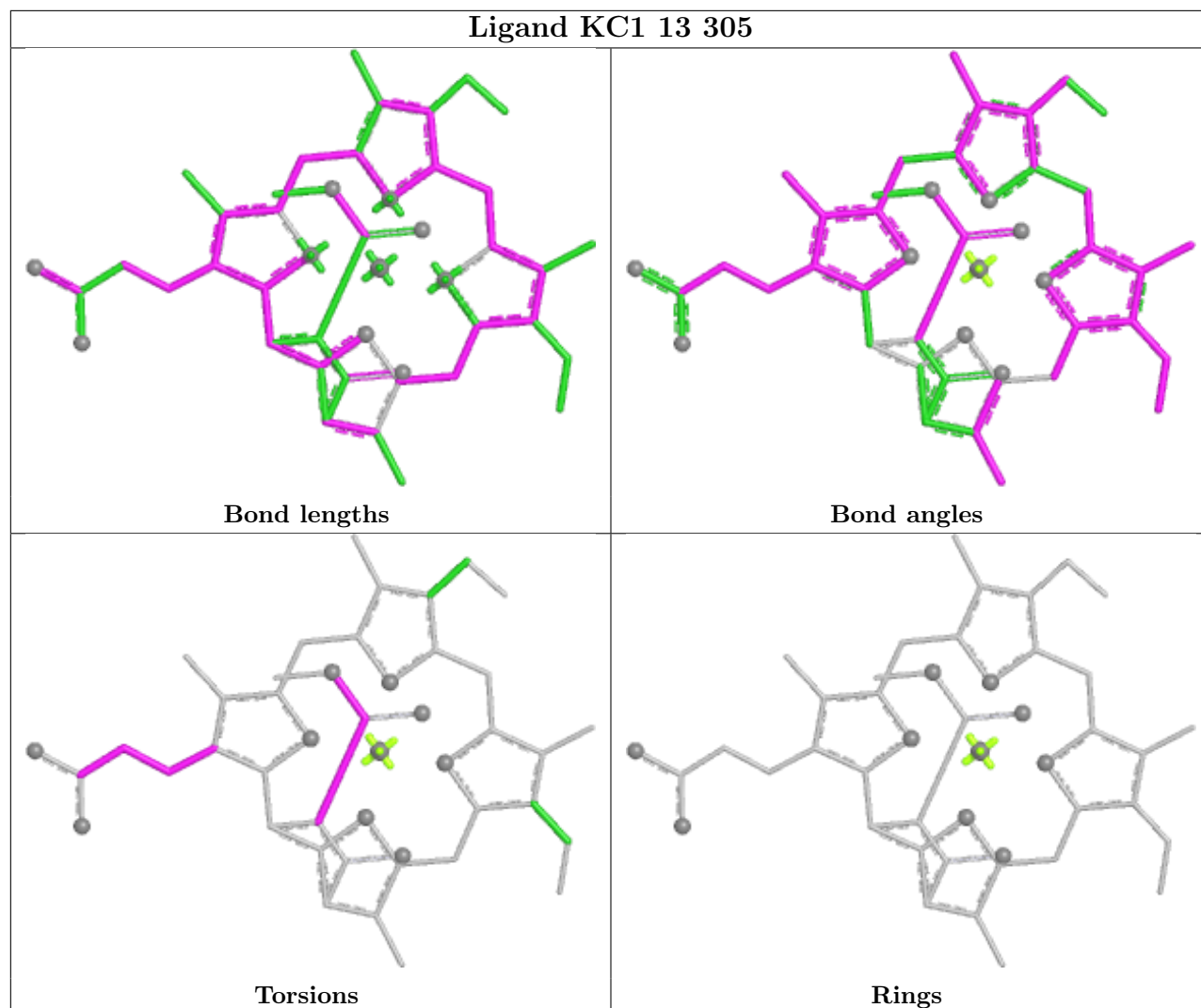


**Ligand CLA A 836****Ligand CLA 6 306**

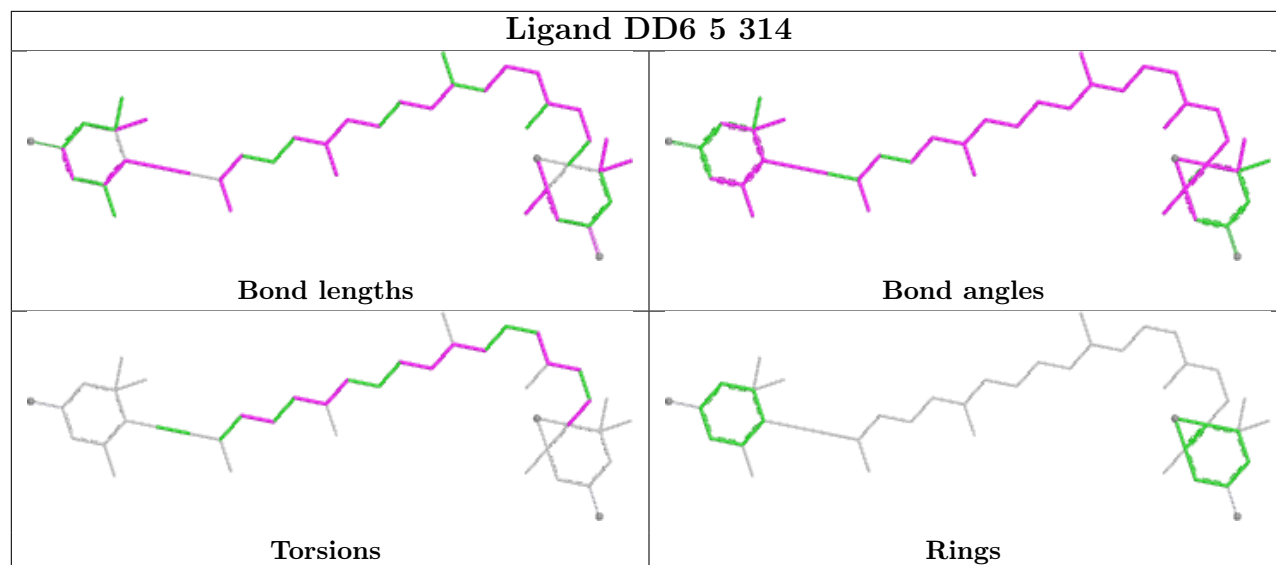
**Ligand CLA B 811****Ligand CLA 6 304**



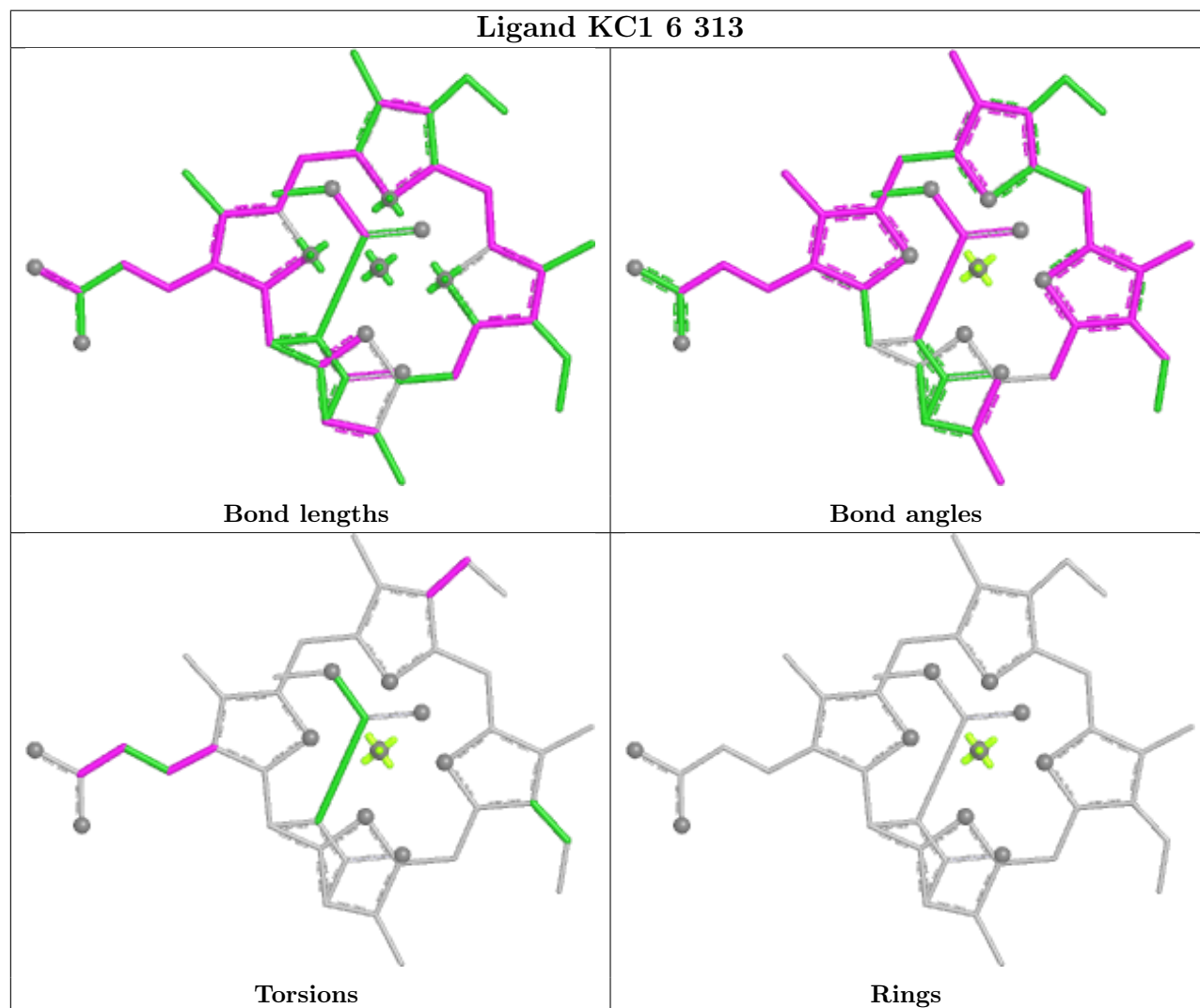


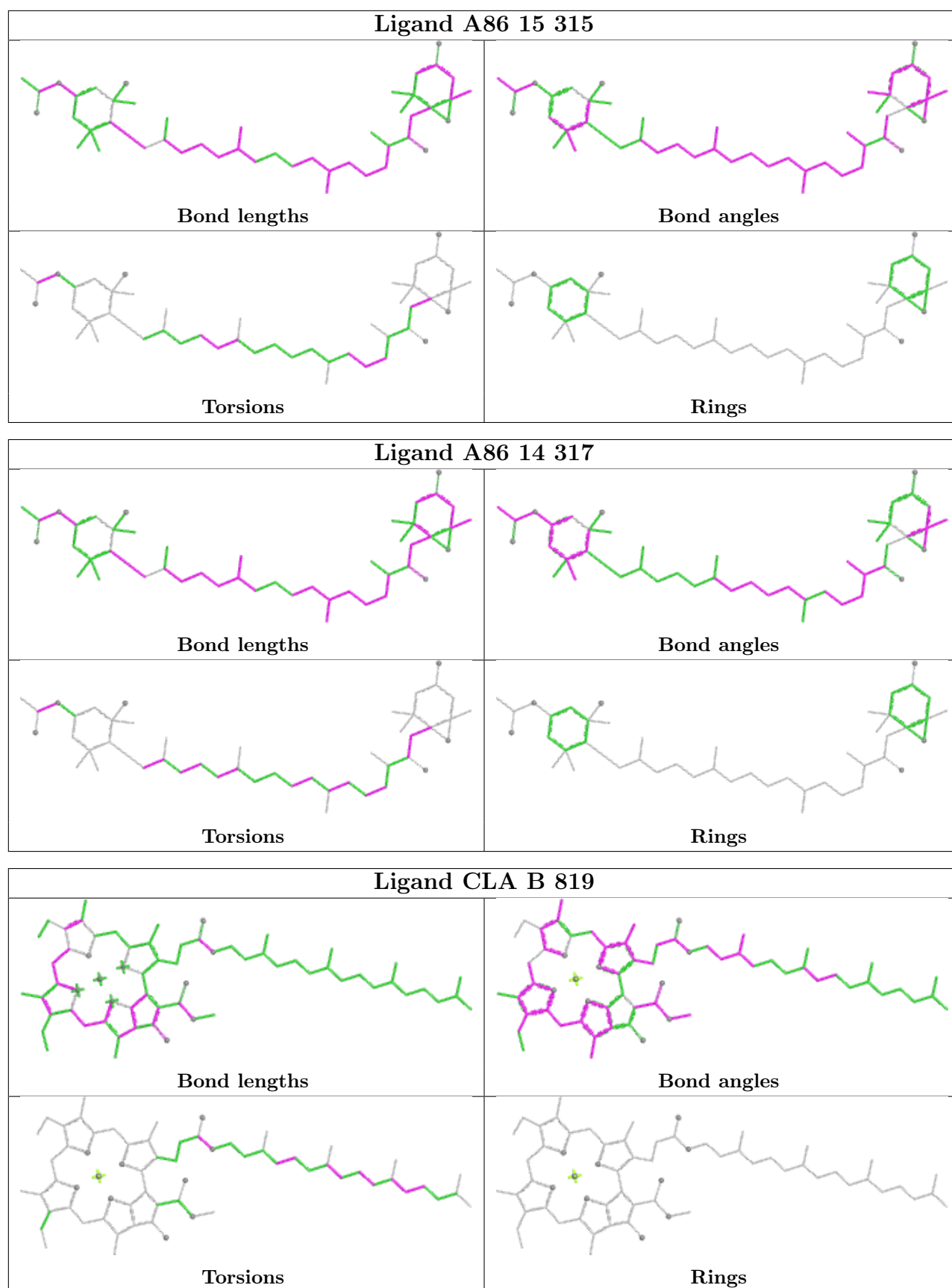


## Ligand DD6 5 314

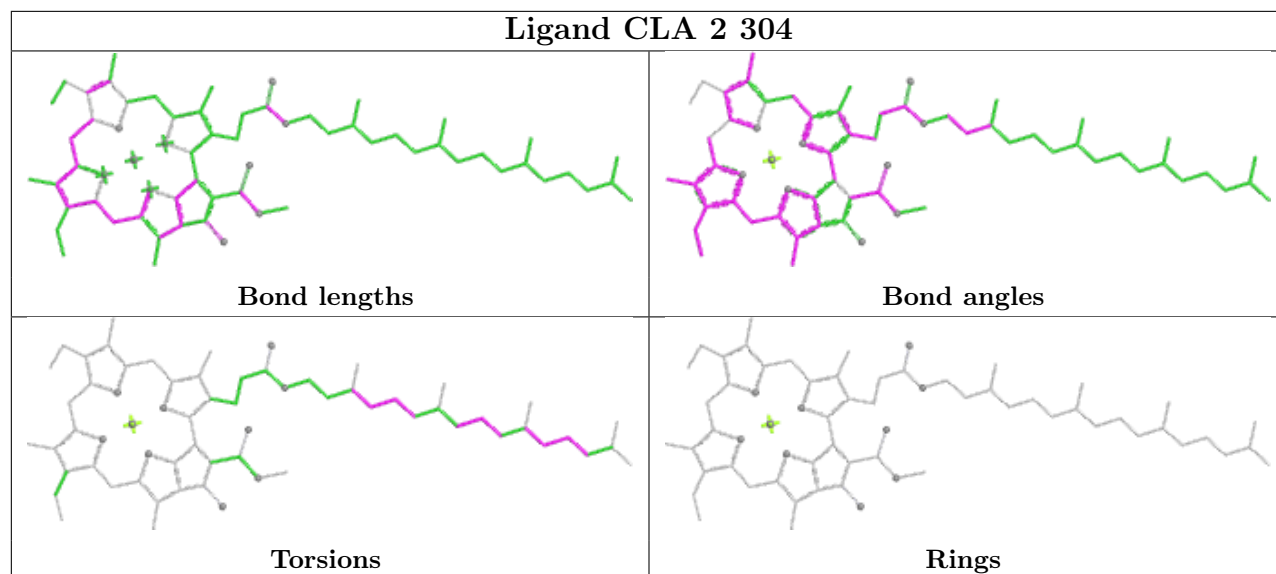


## Ligand KC1 6 313

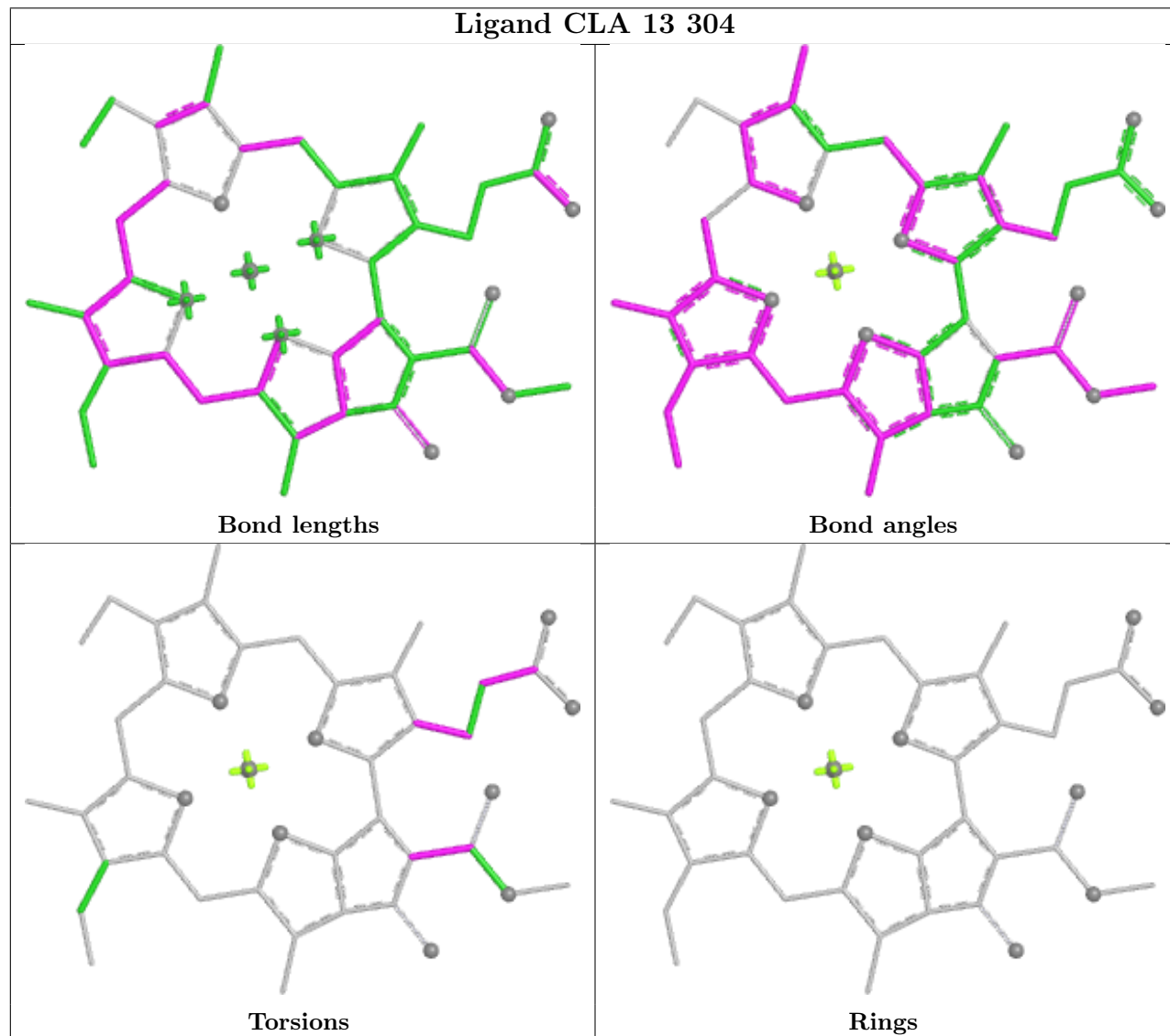


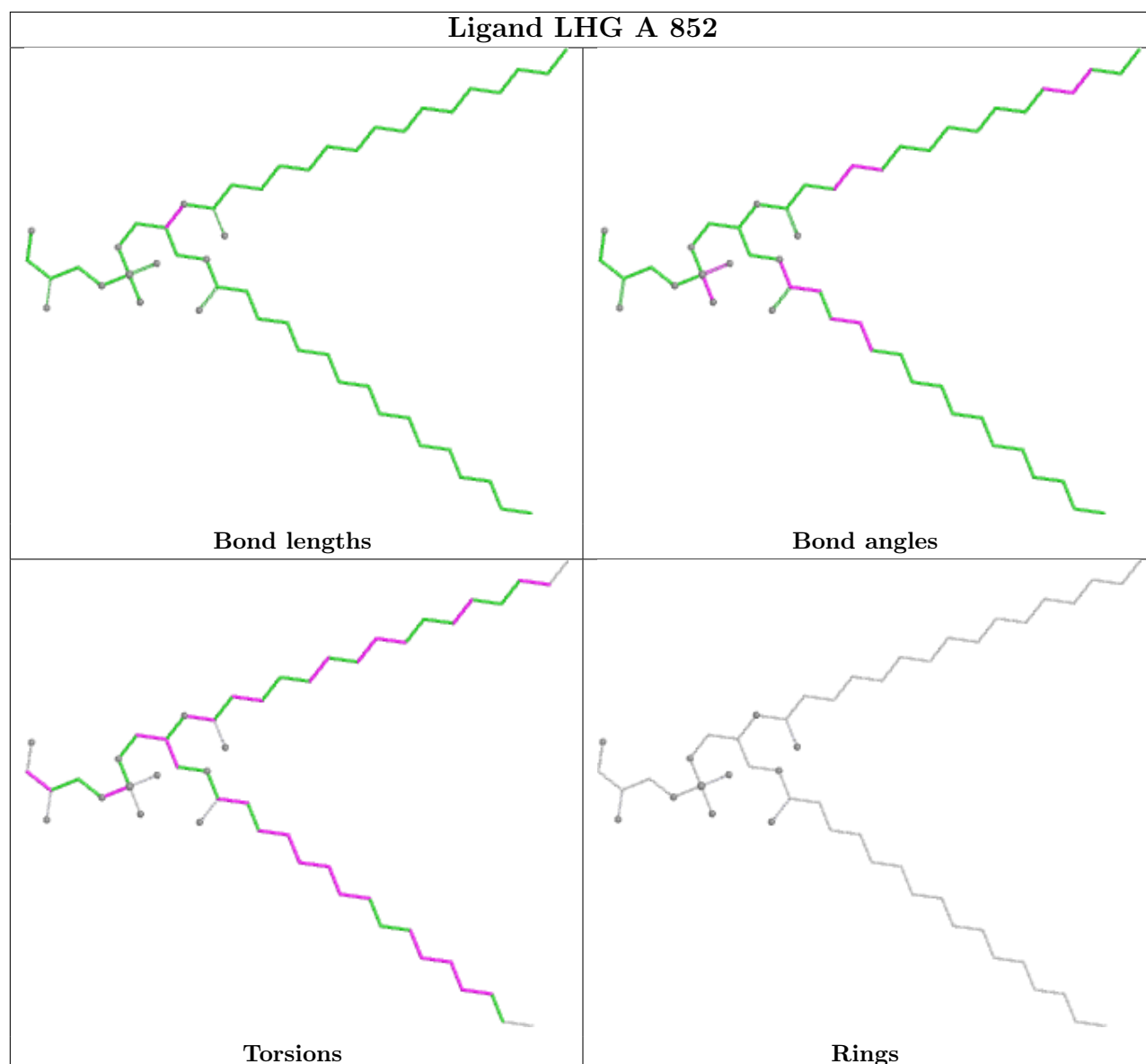
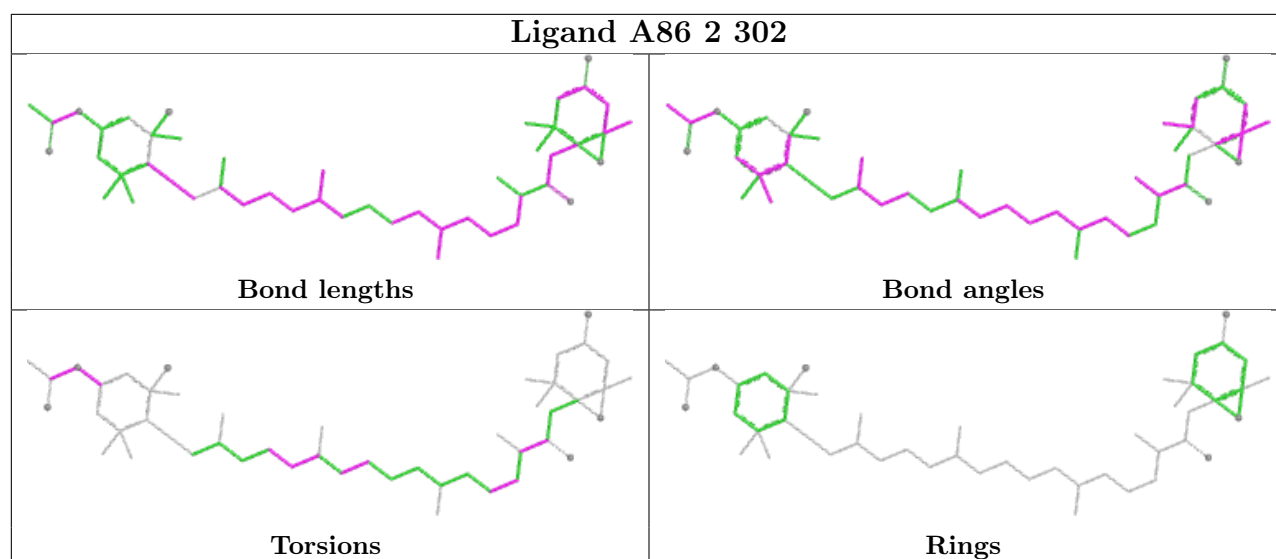


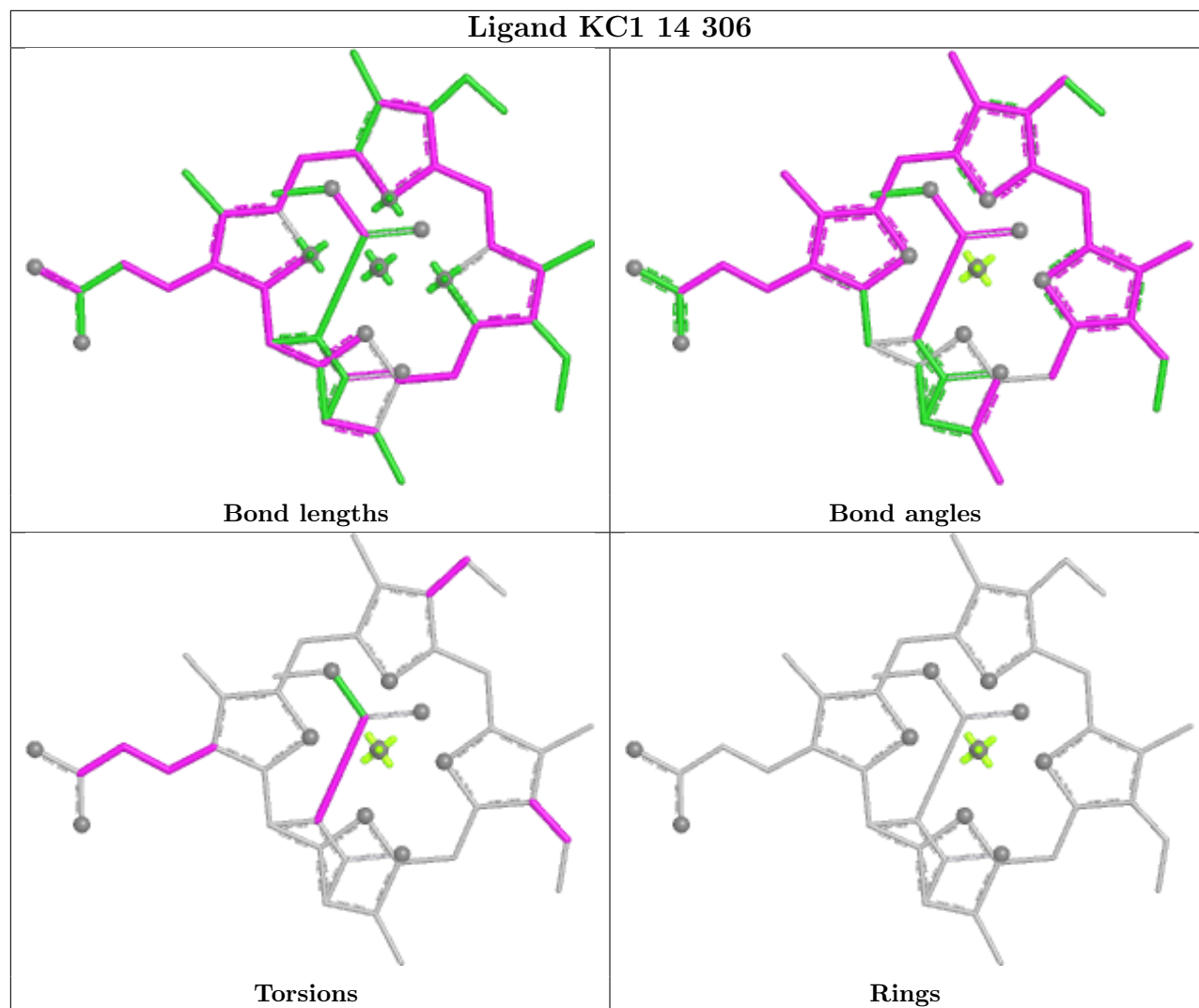
## Ligand CLA 2 304



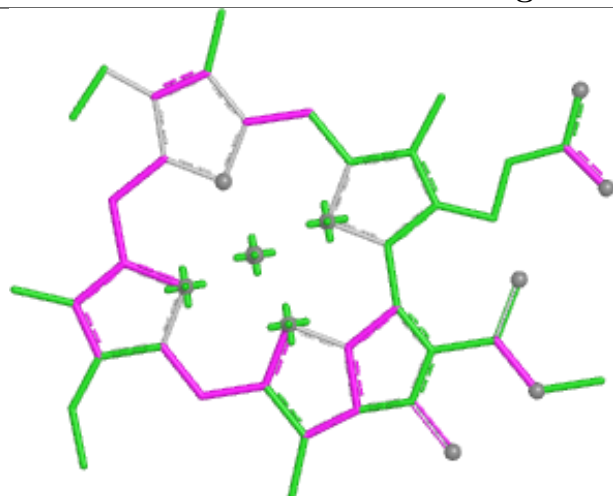
## Ligand CLA 13 304



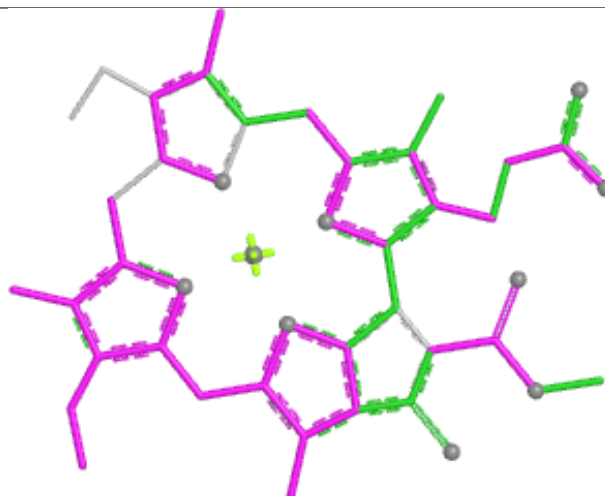




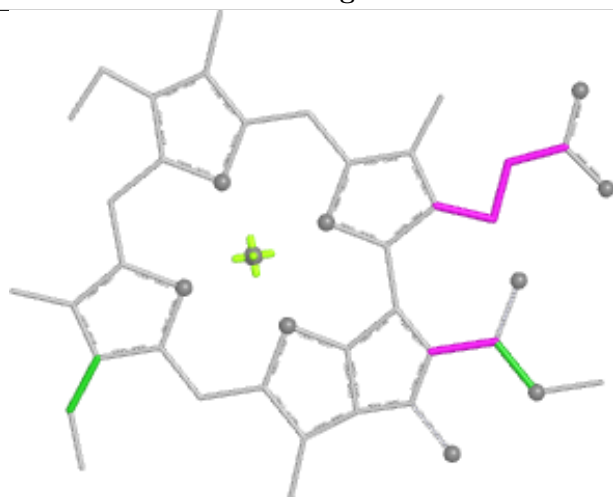
## Ligand CLA F 203



Bond lengths



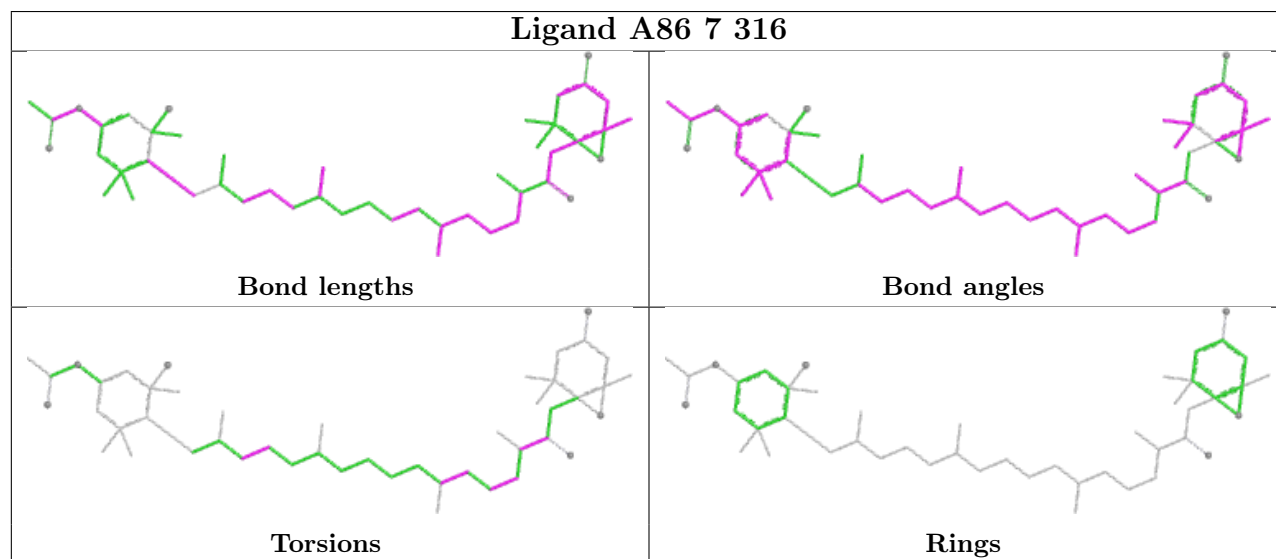
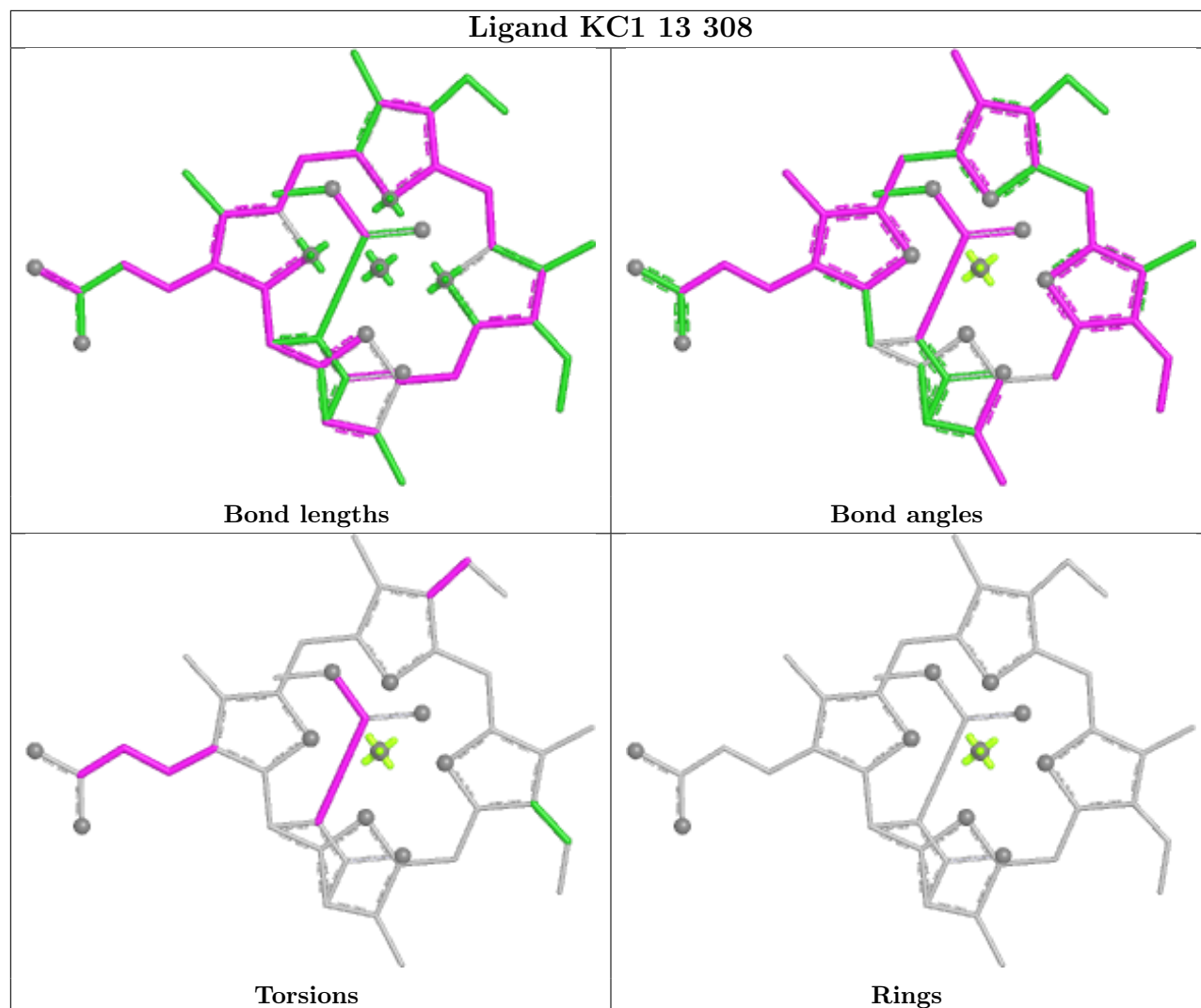
Bond angles



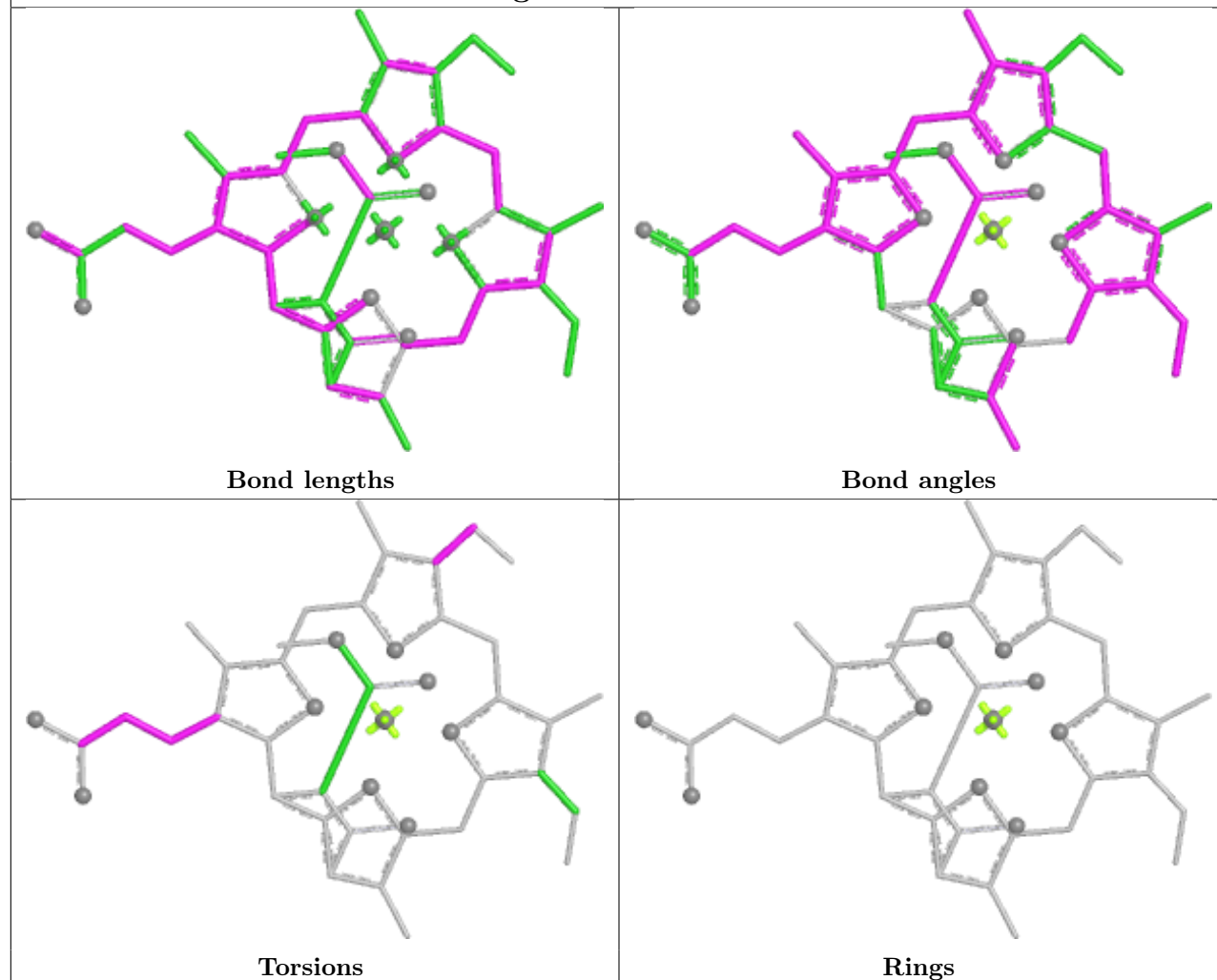
Torsions



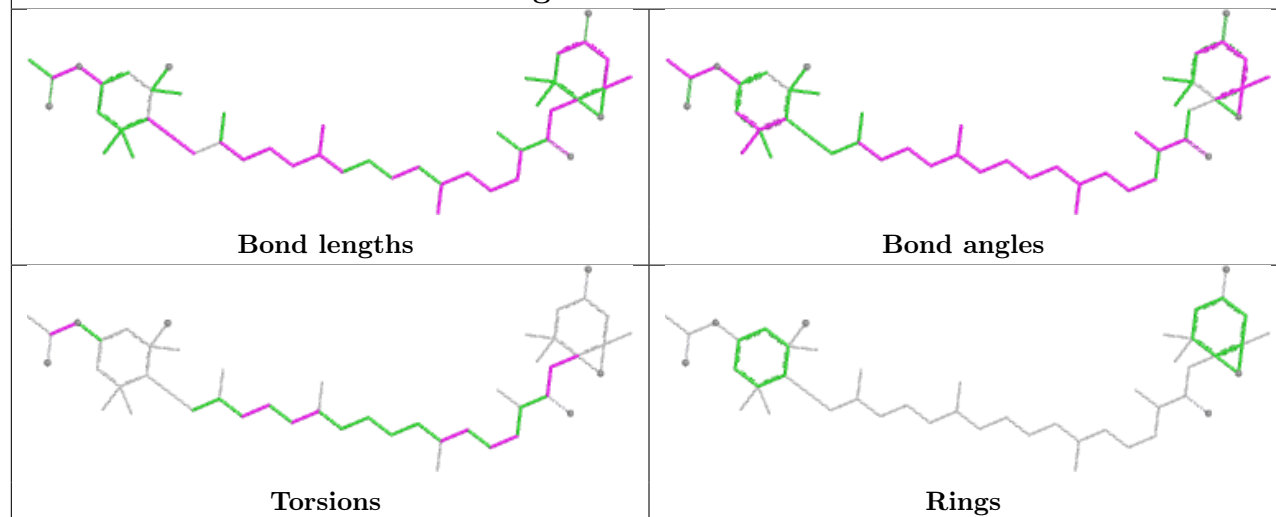
Rings

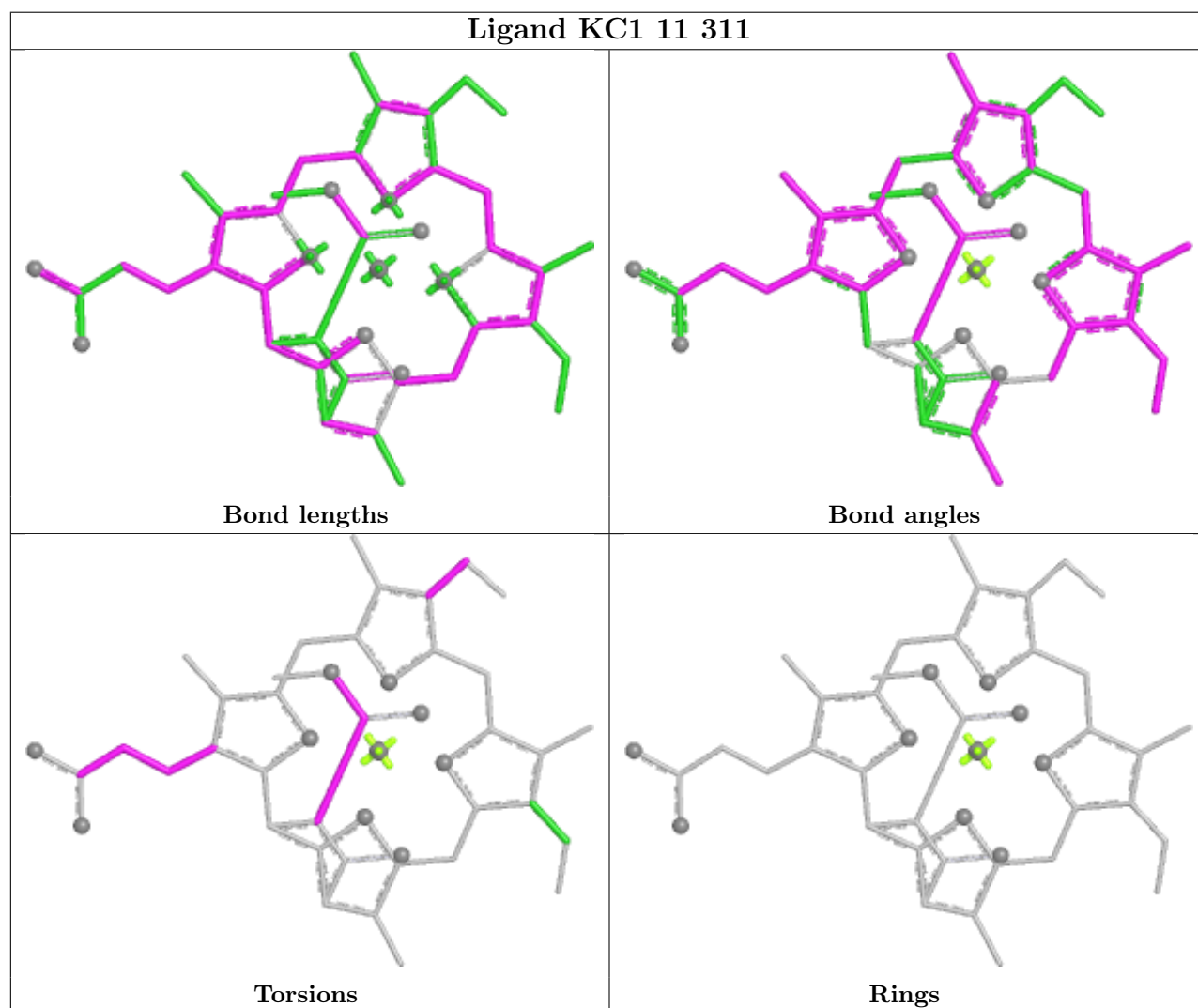
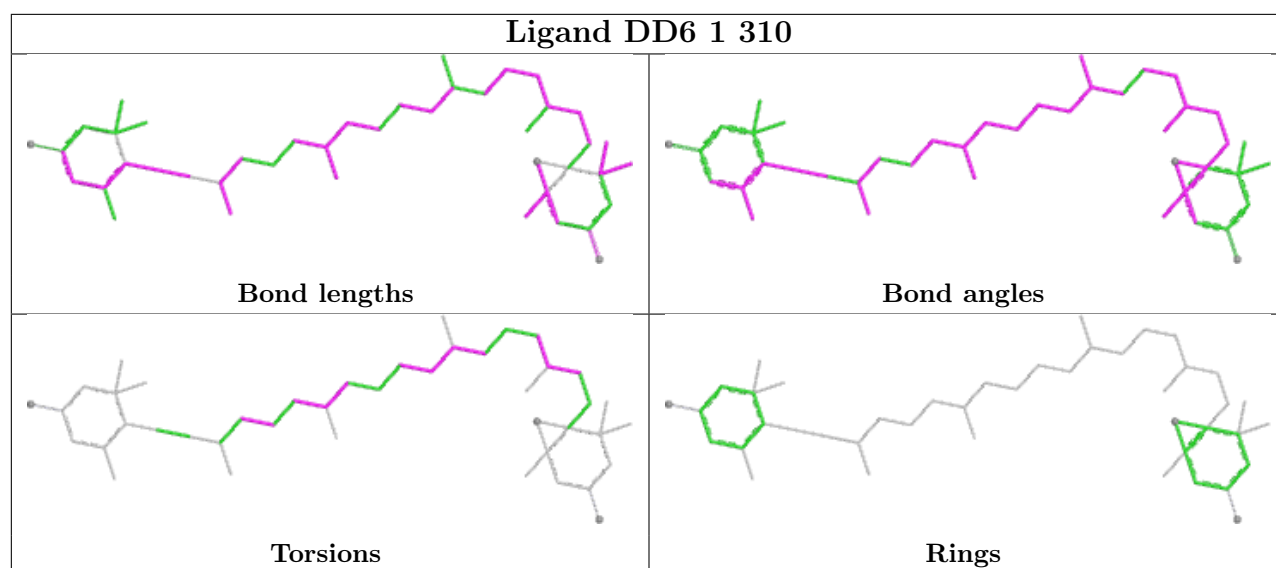


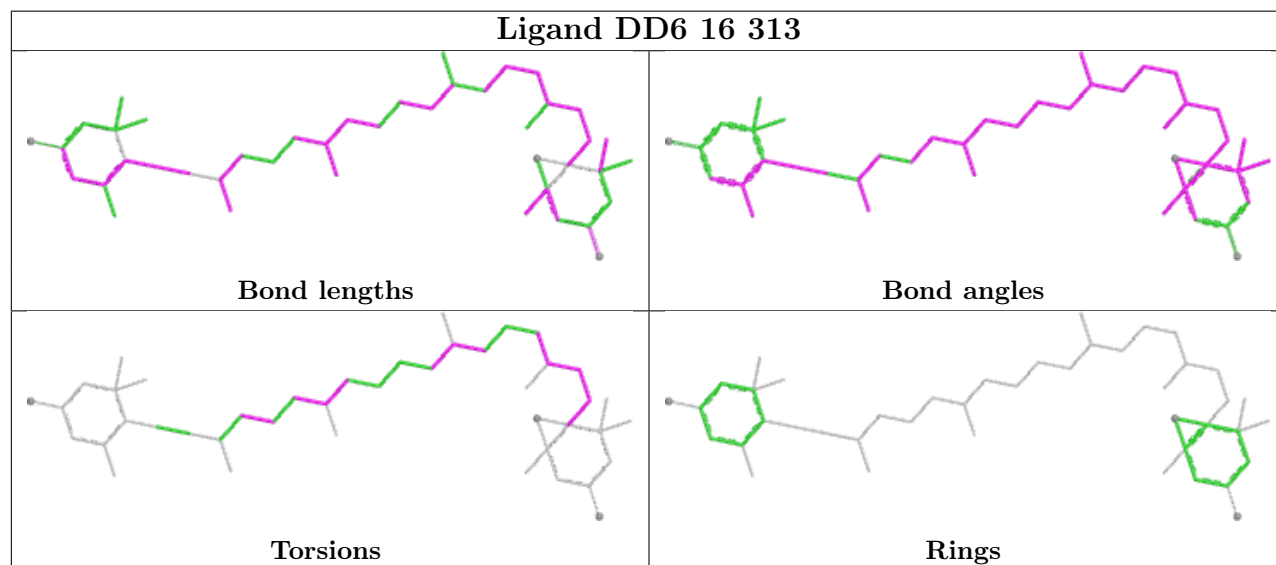
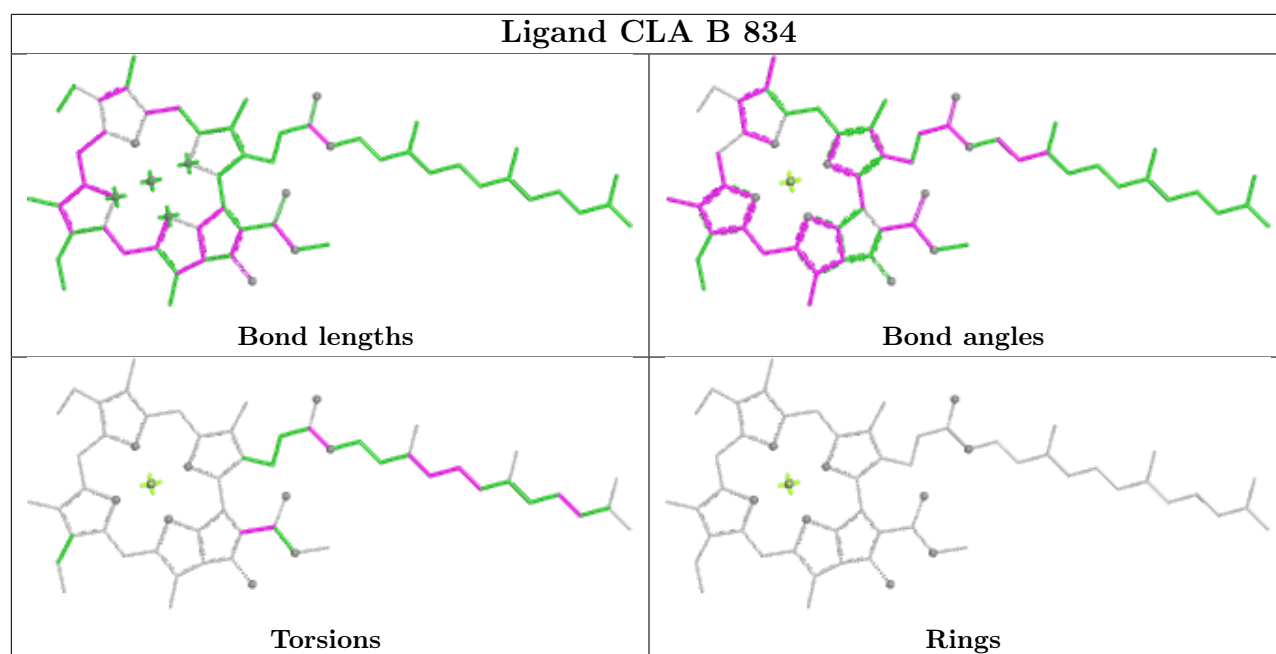
## Ligand KC1 4 307

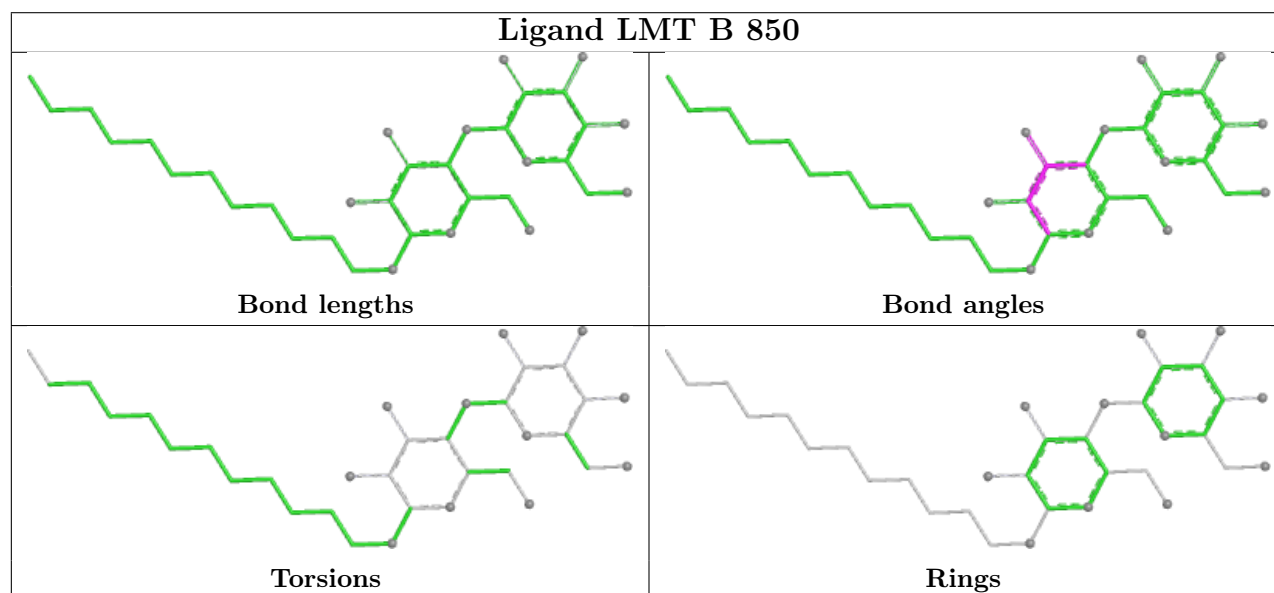
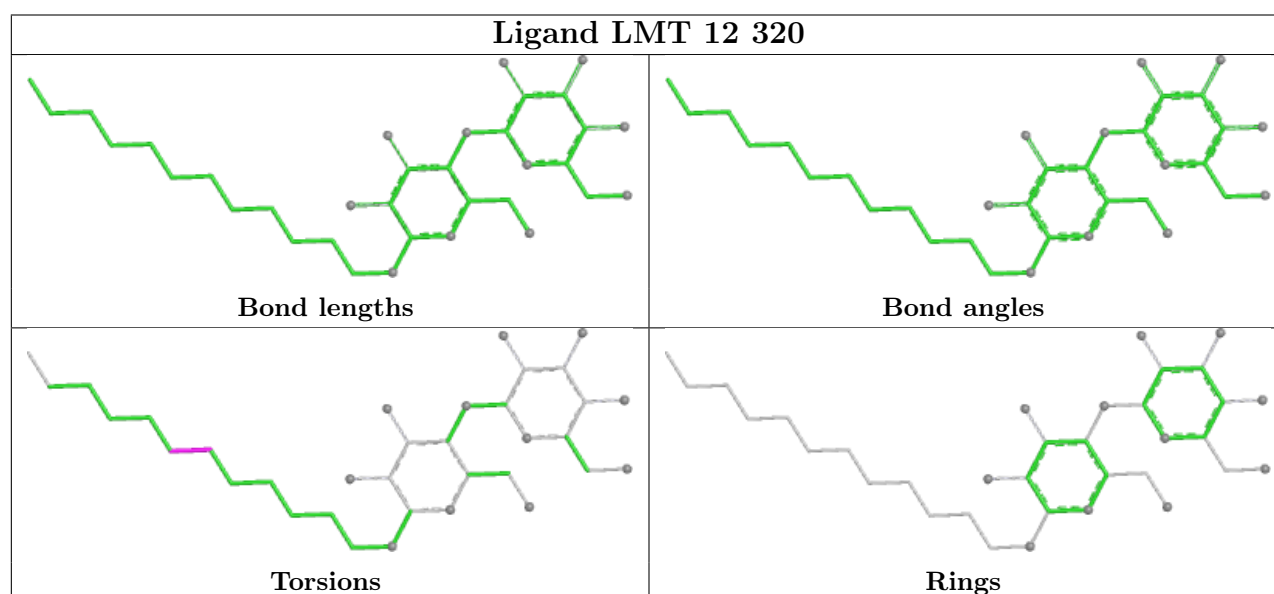
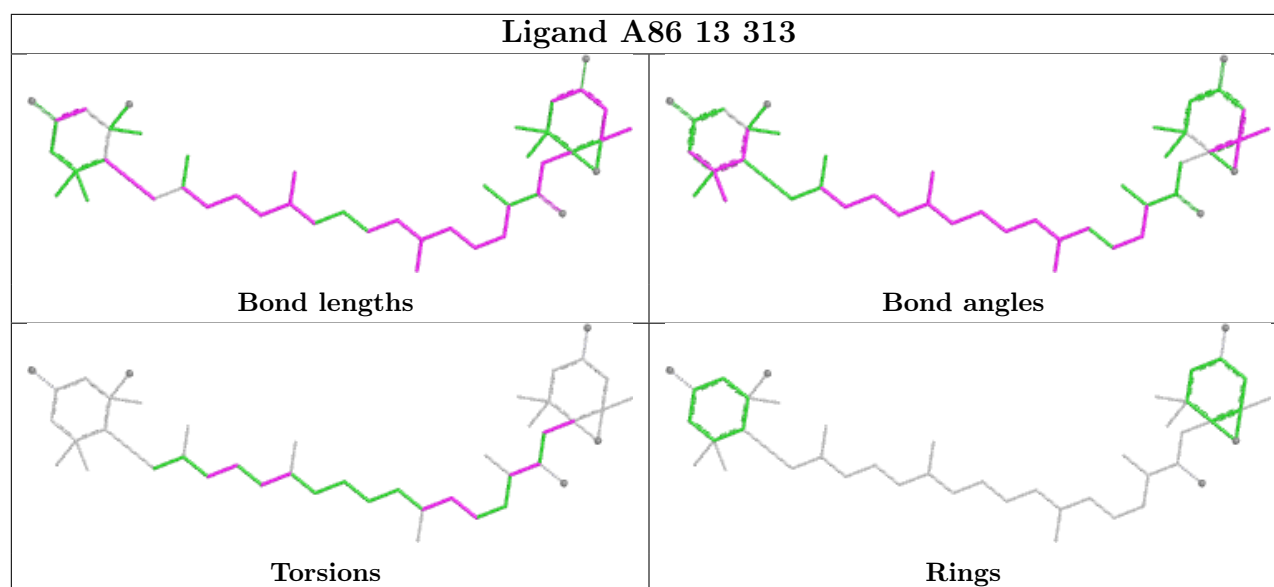


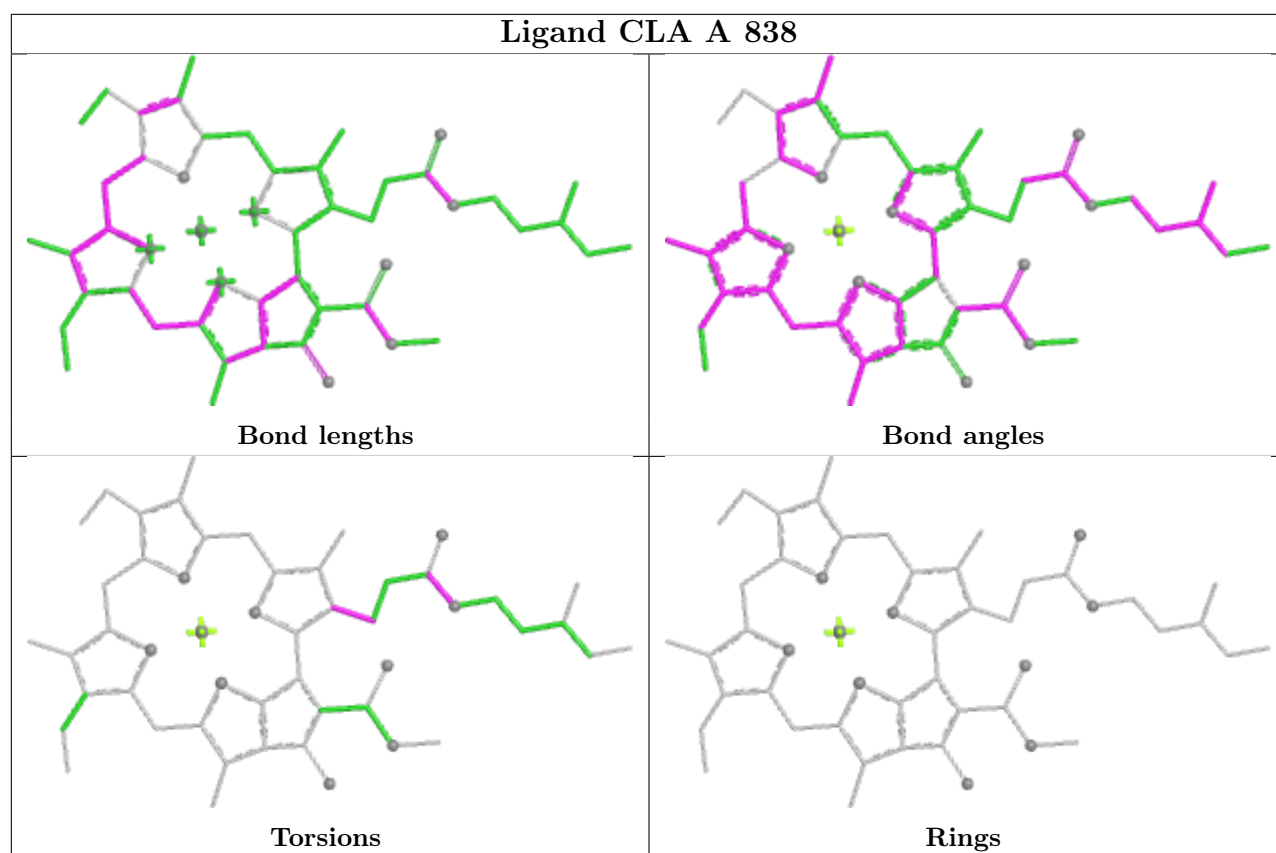
## Ligand A86 10 316

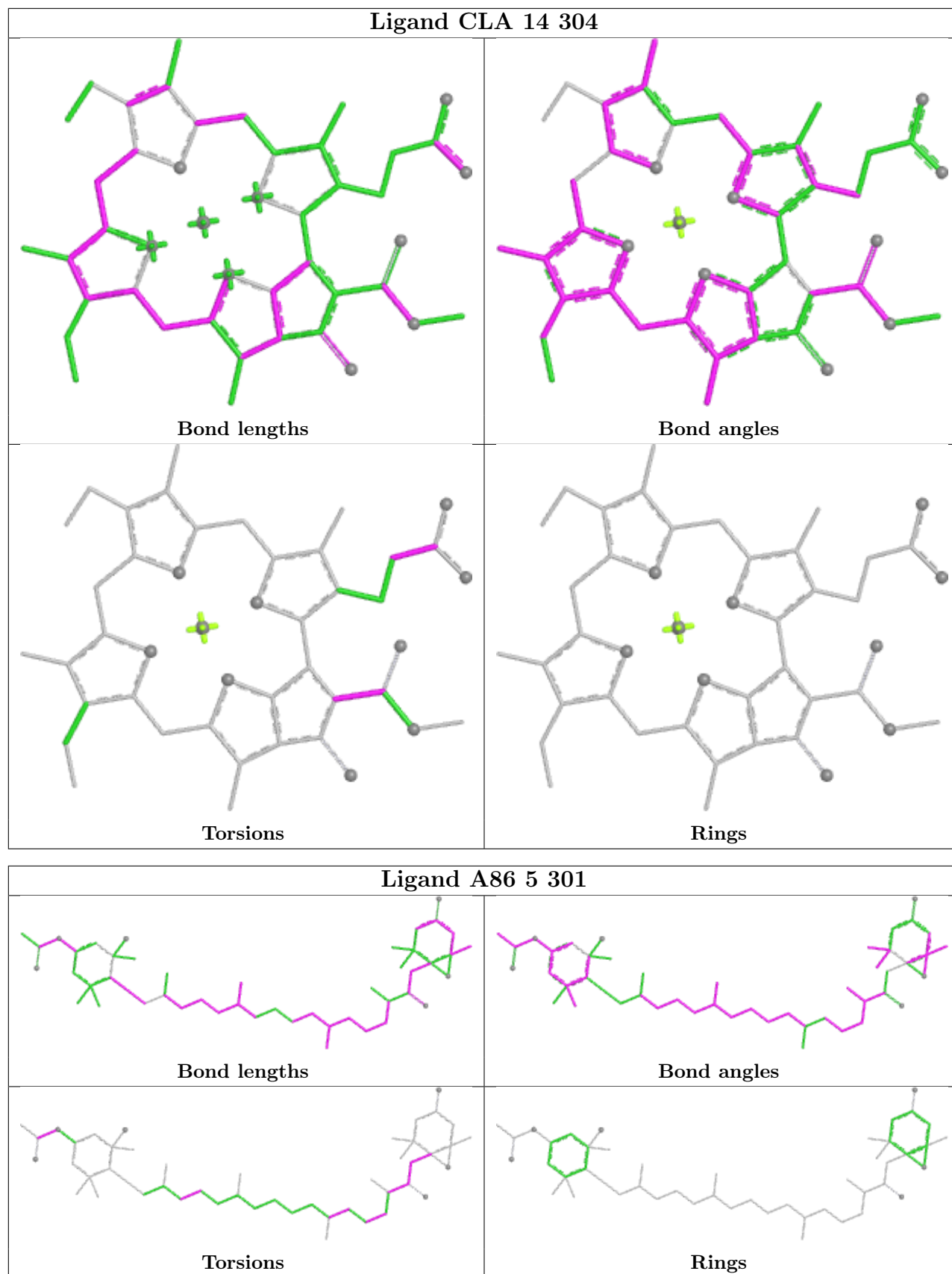


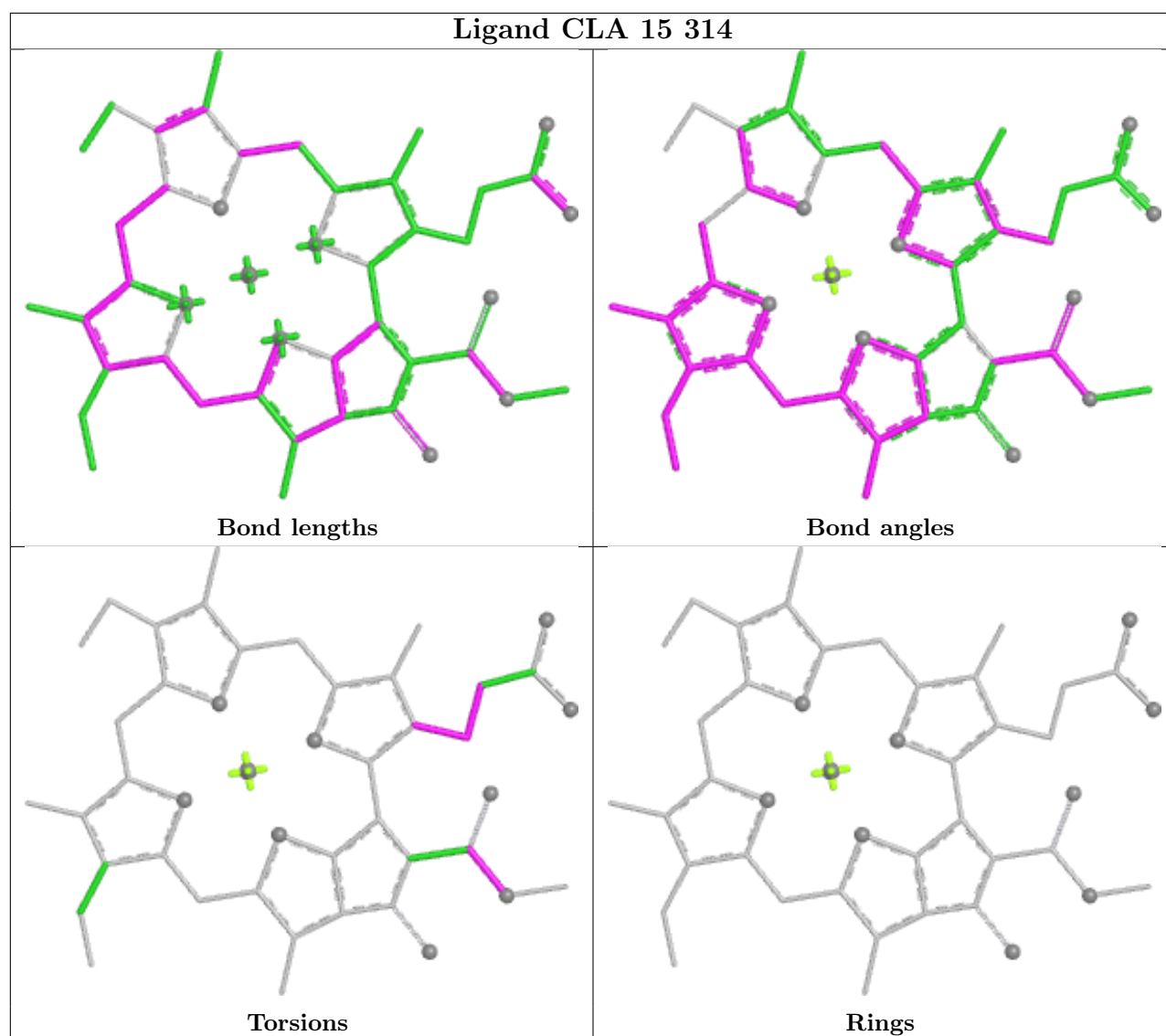


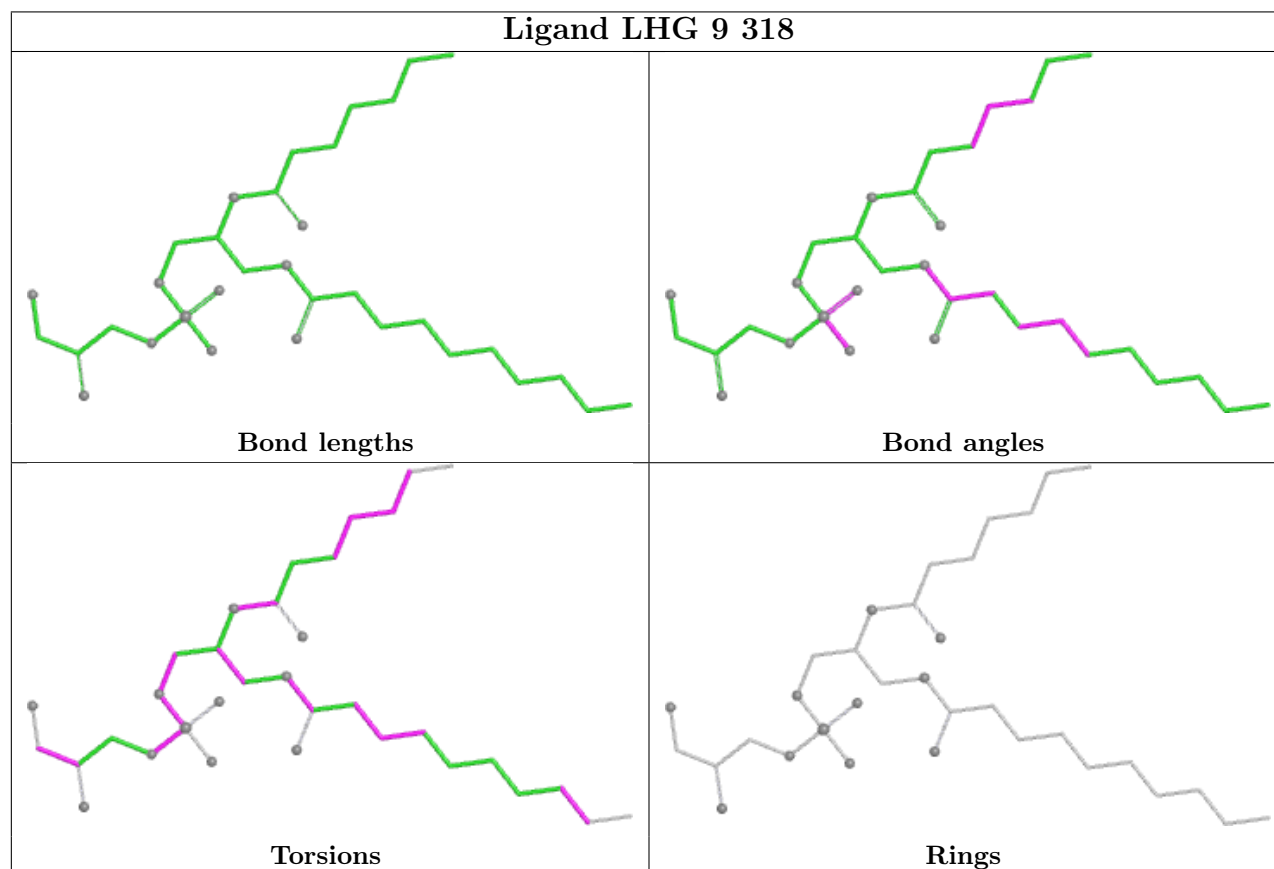
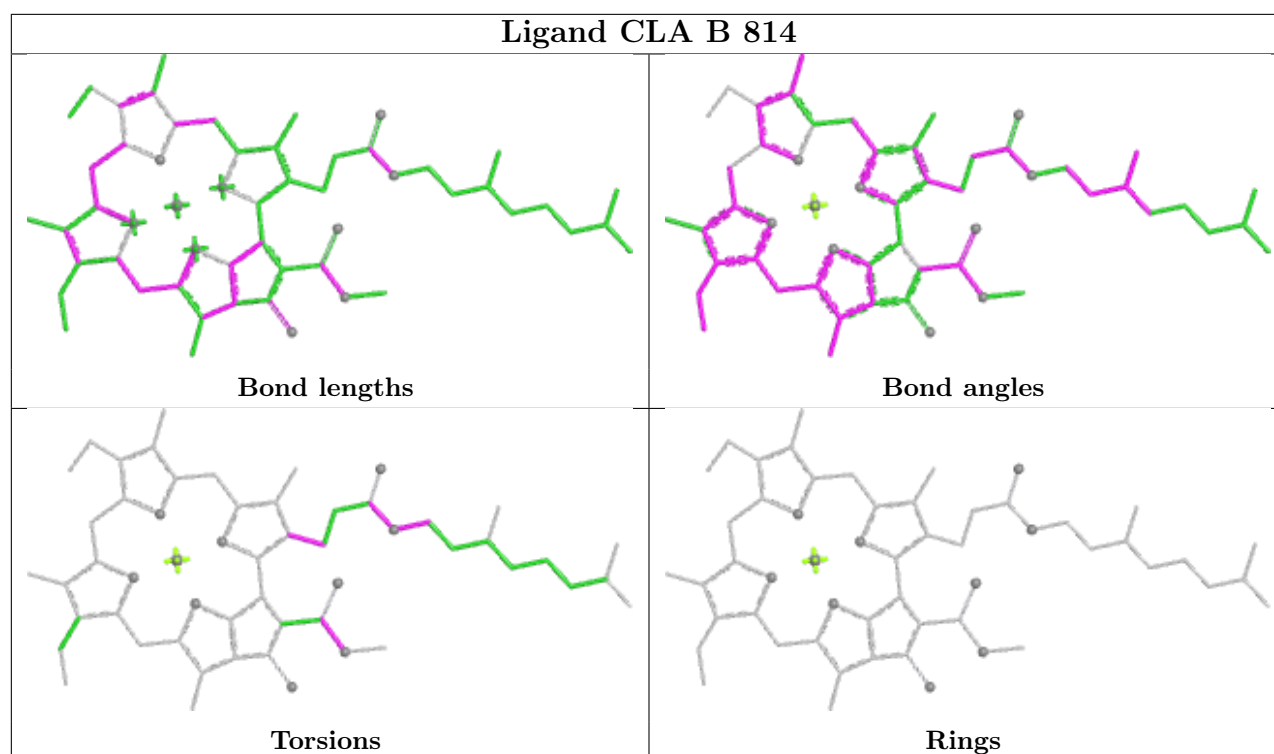




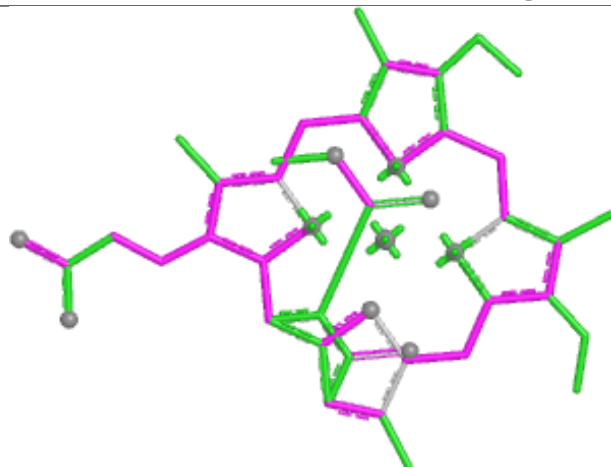




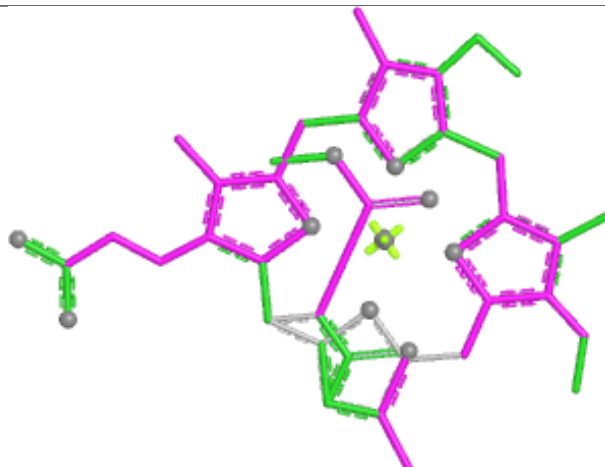




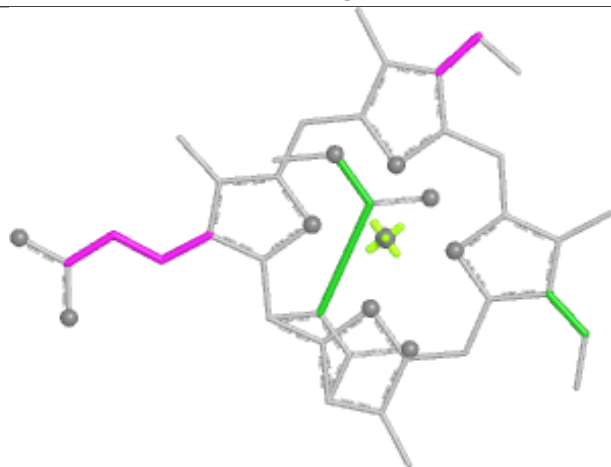
## Ligand KC1 3 311



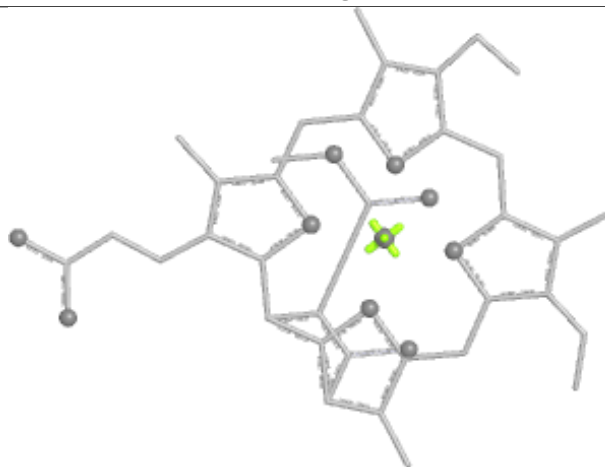
Bond lengths



Bond angles

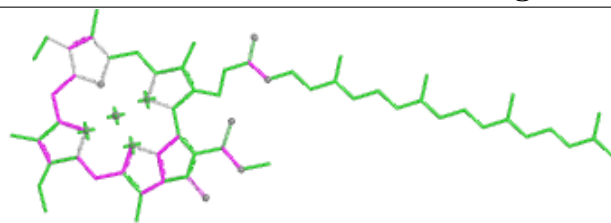


Torsions

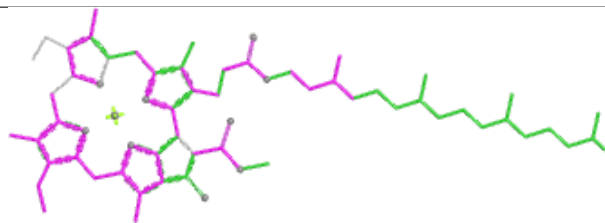


Rings

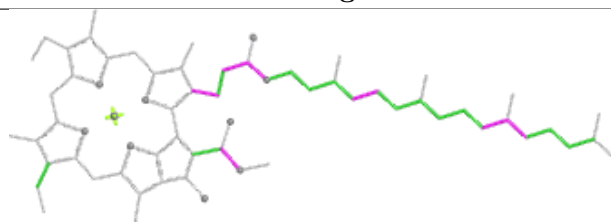
## Ligand CLA A 807



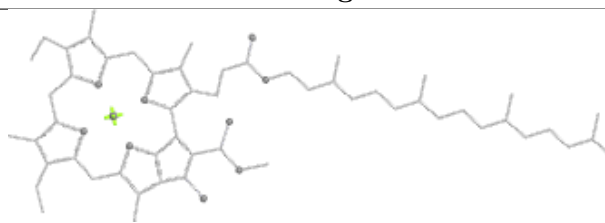
Bond lengths



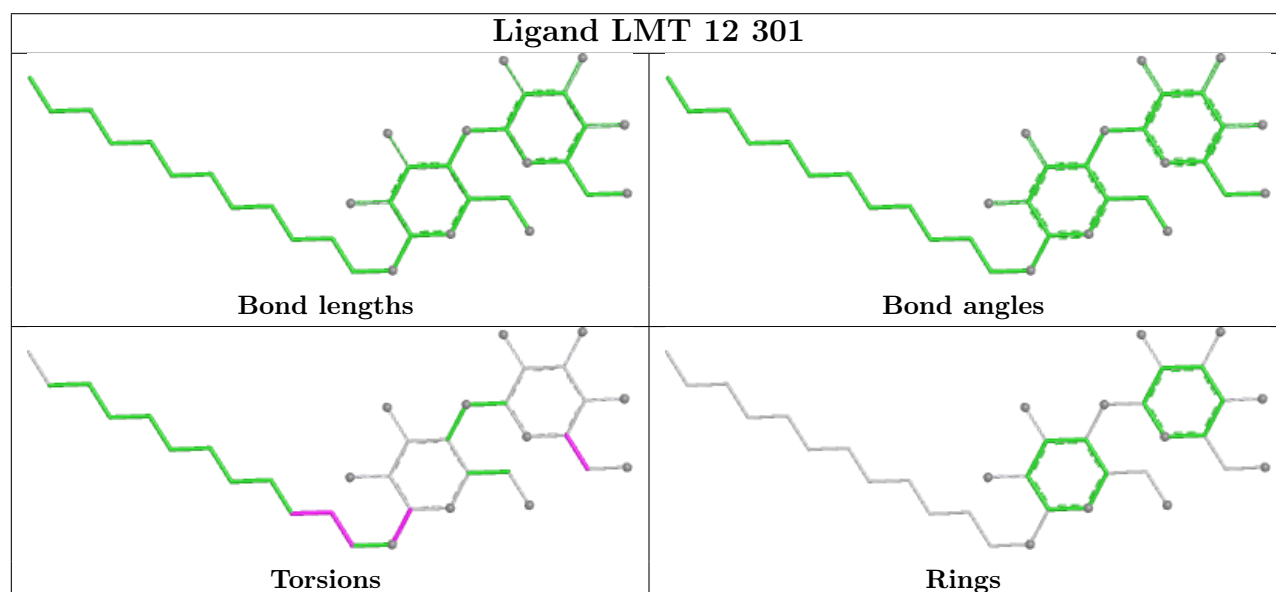
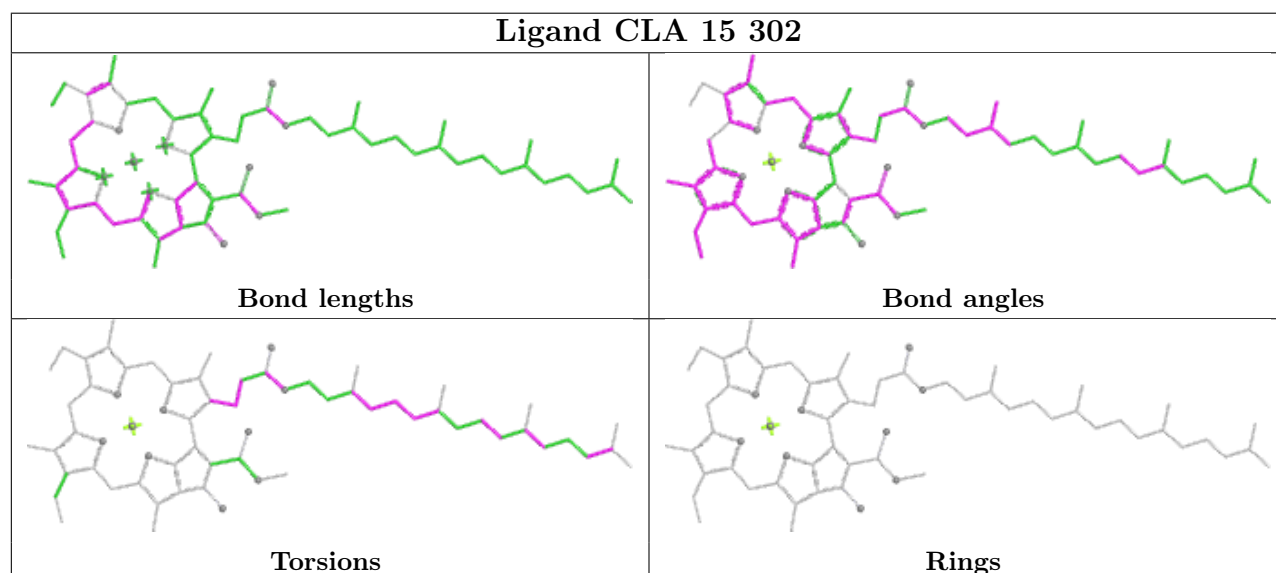
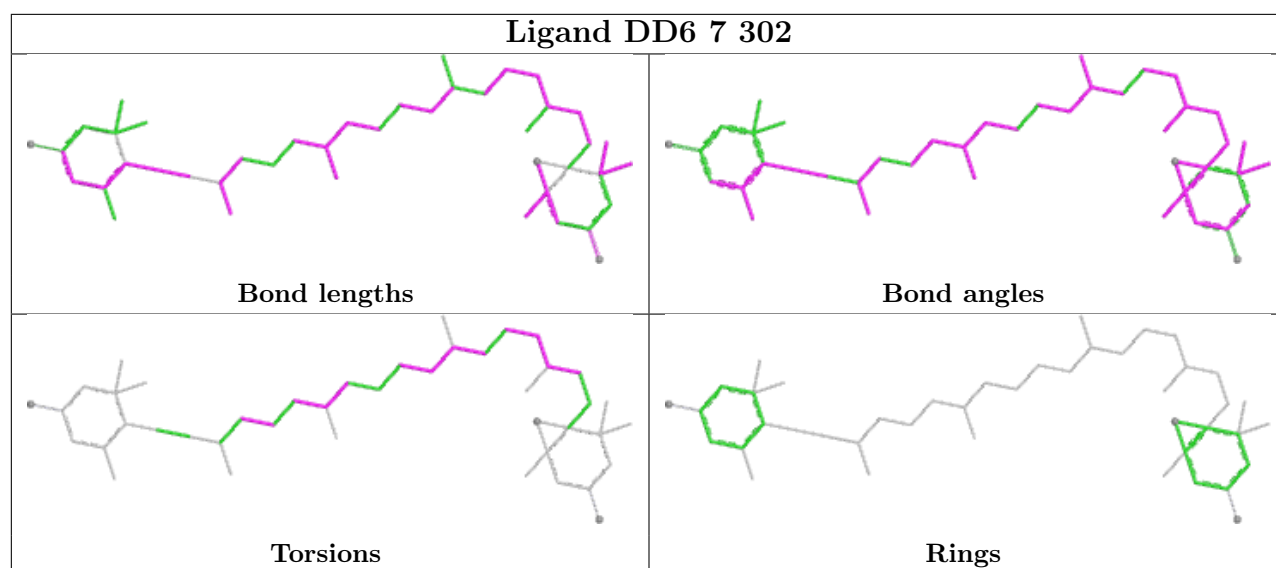
Bond angles



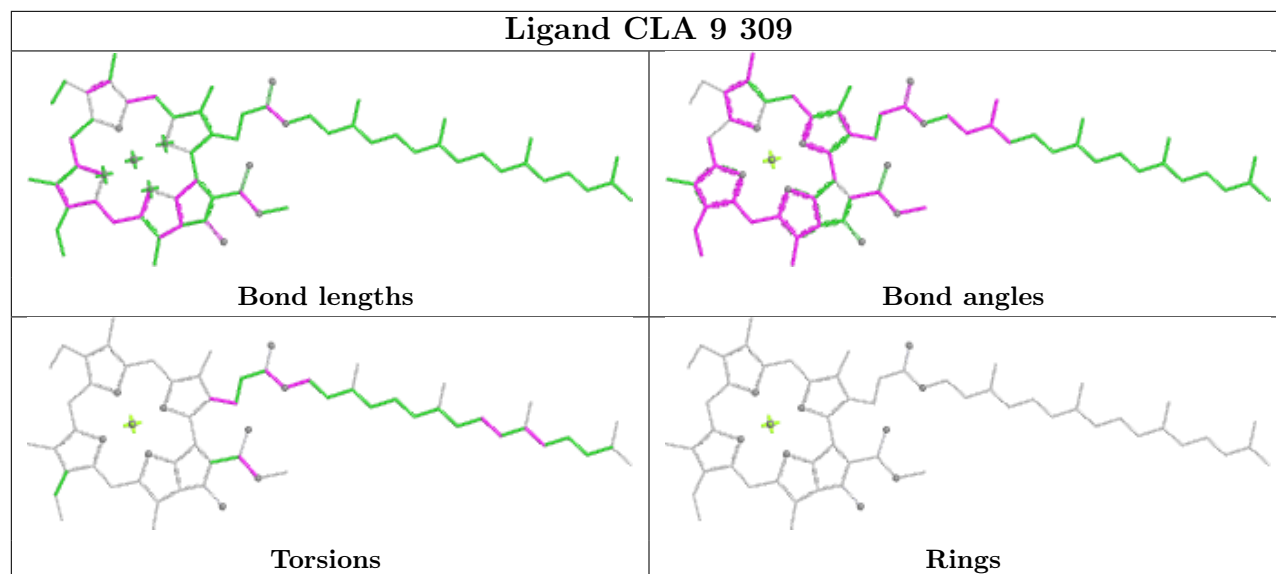
Torsions



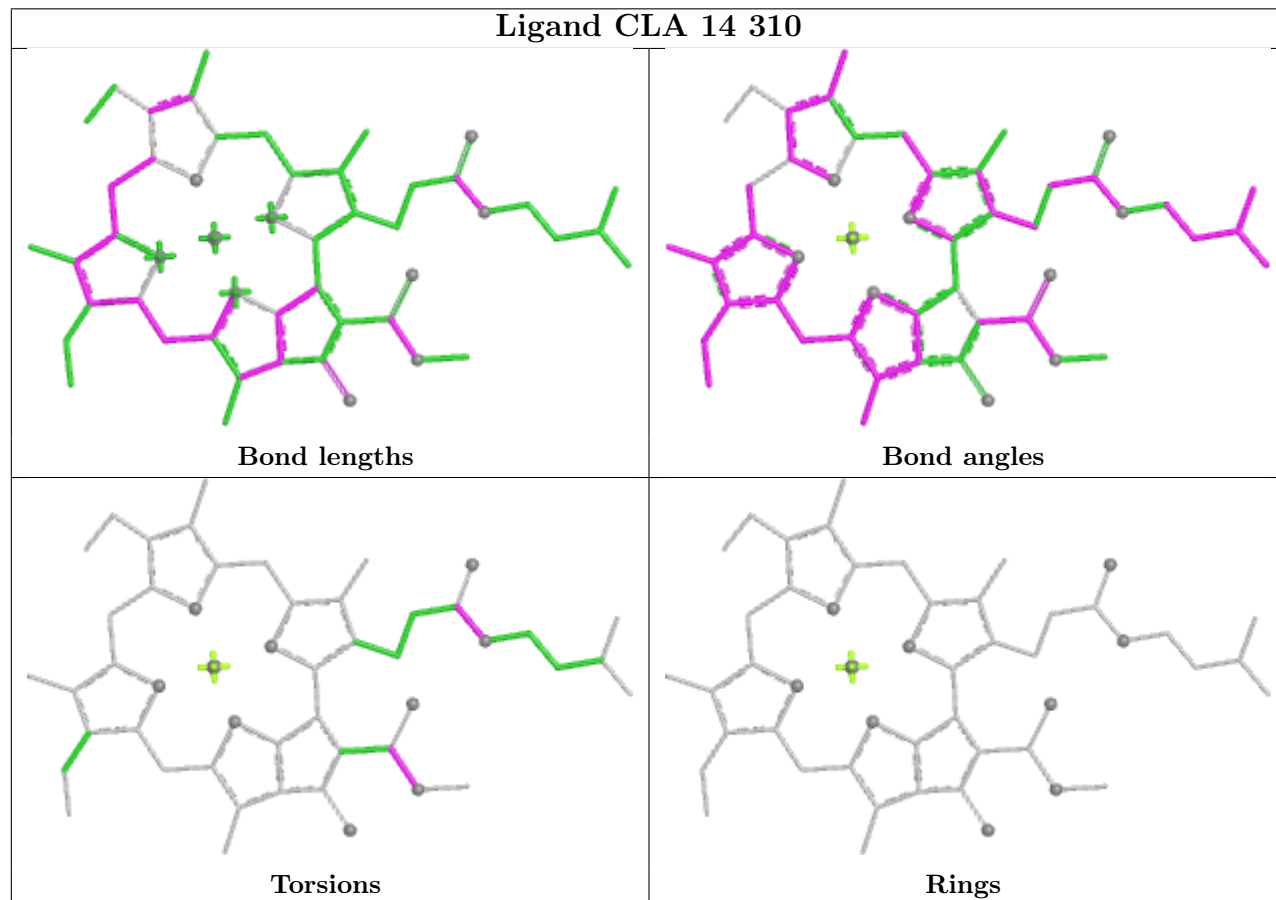
Rings

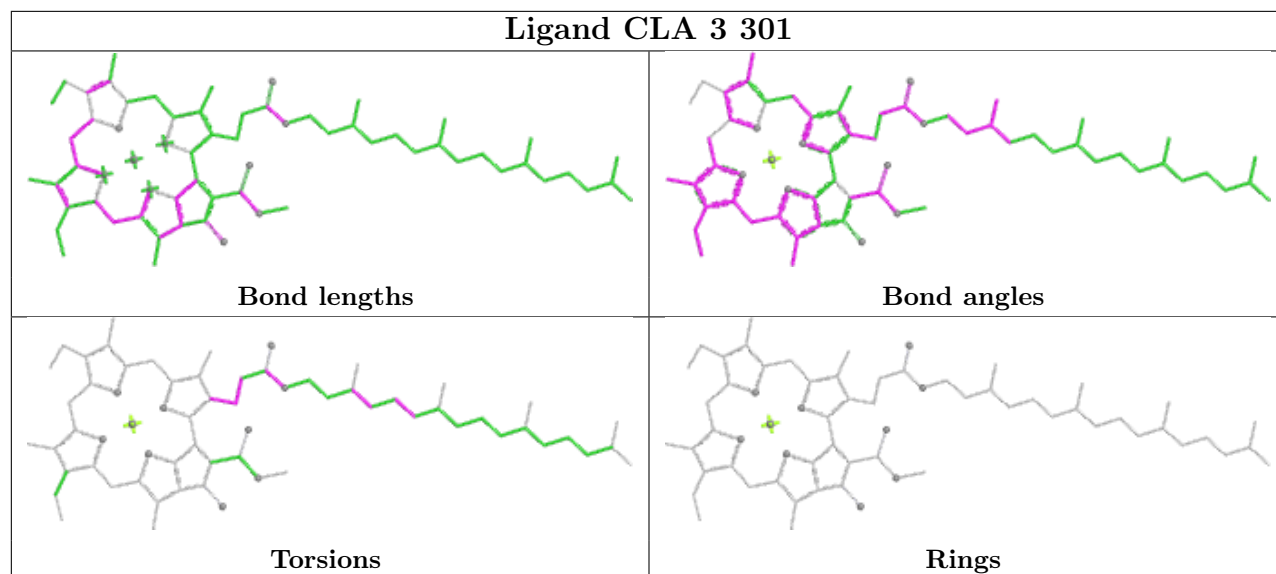
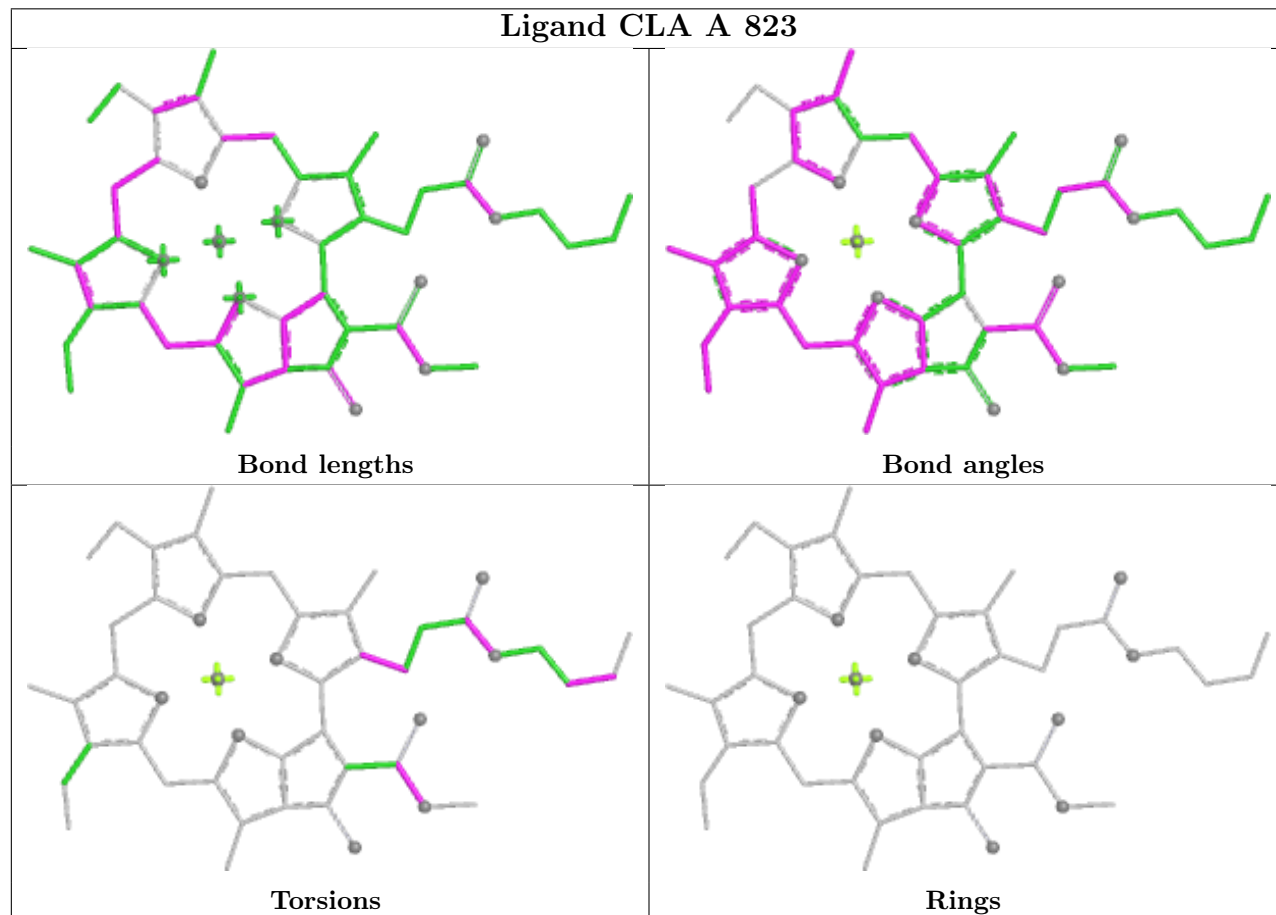


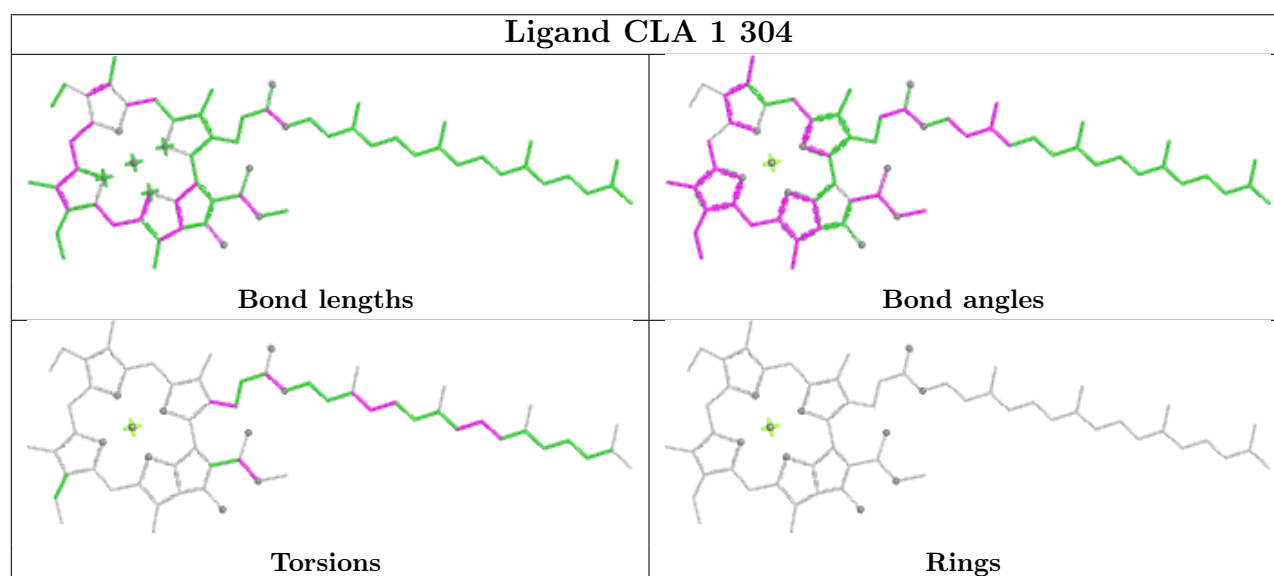
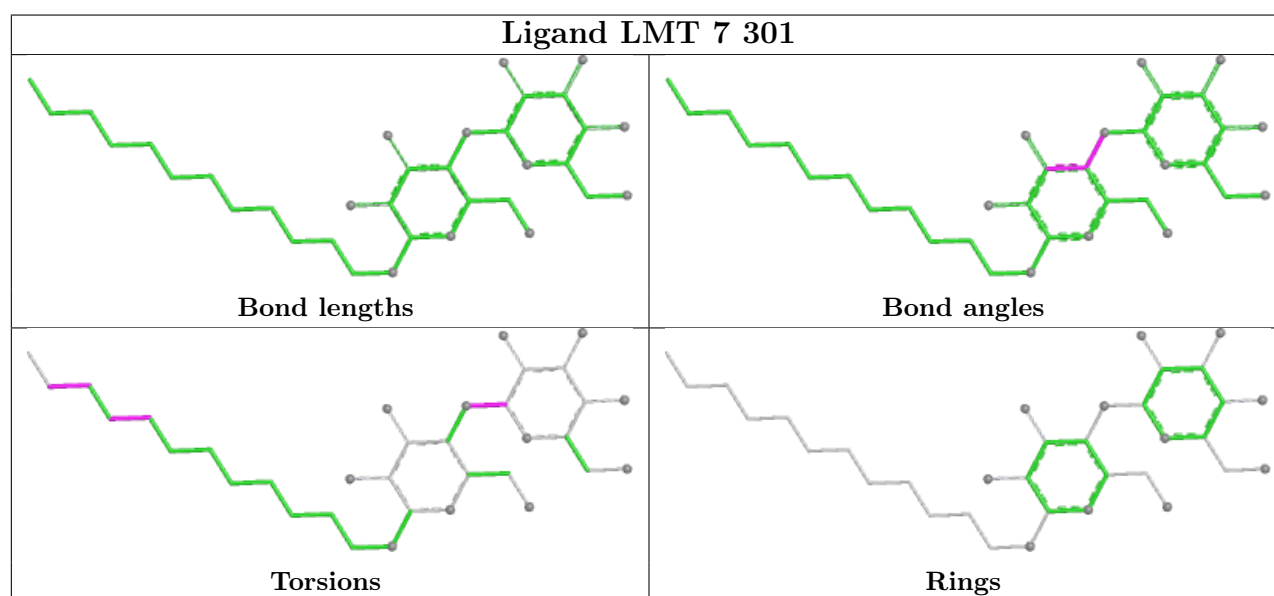
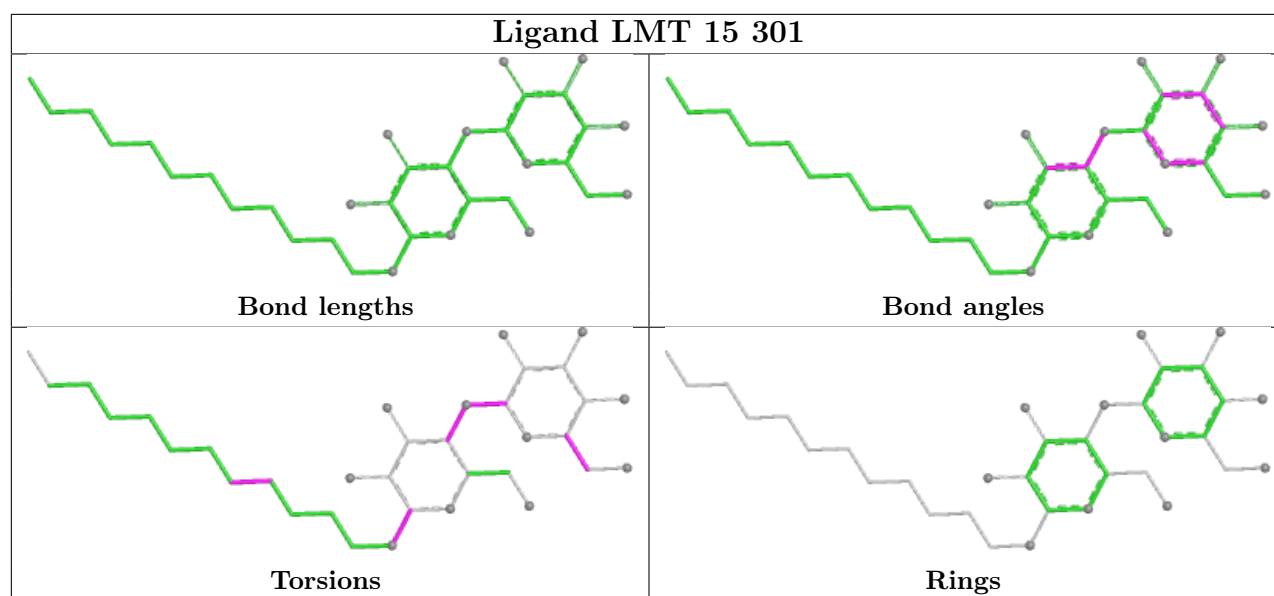
## Ligand CLA 9 309

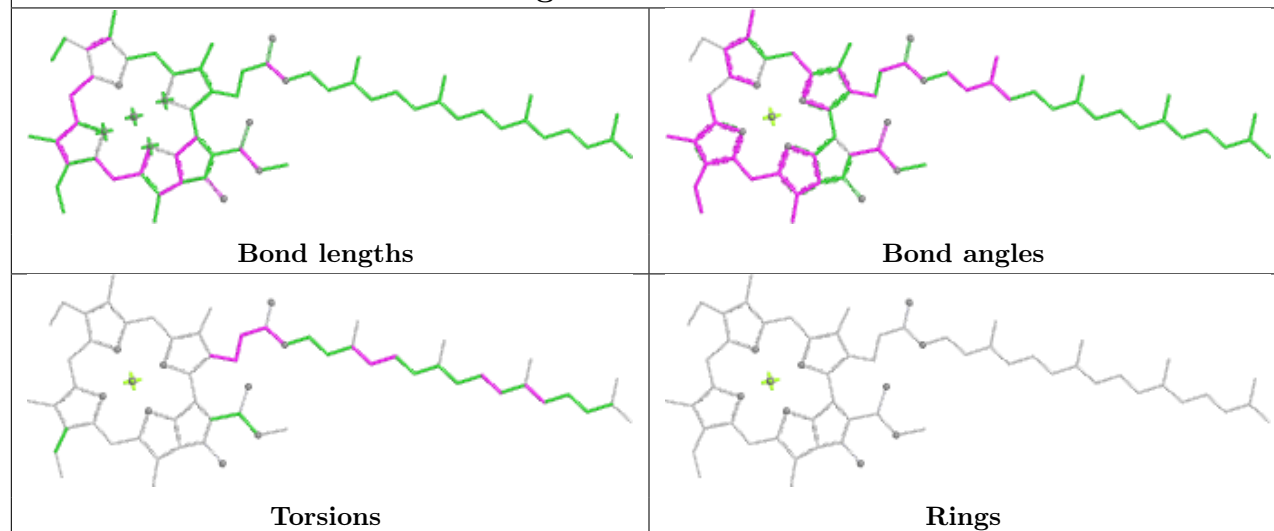
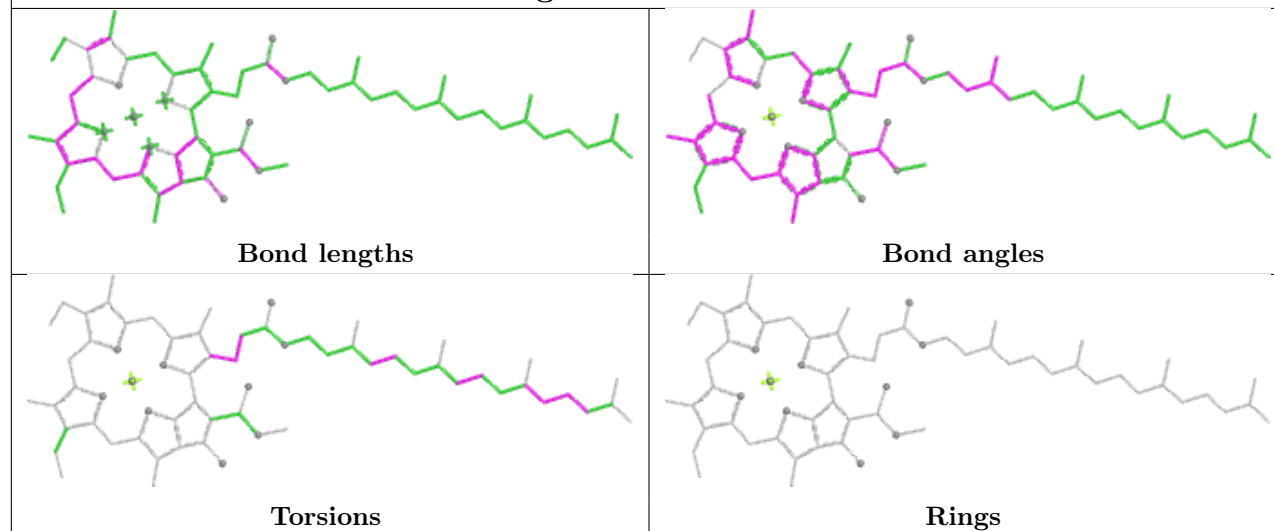
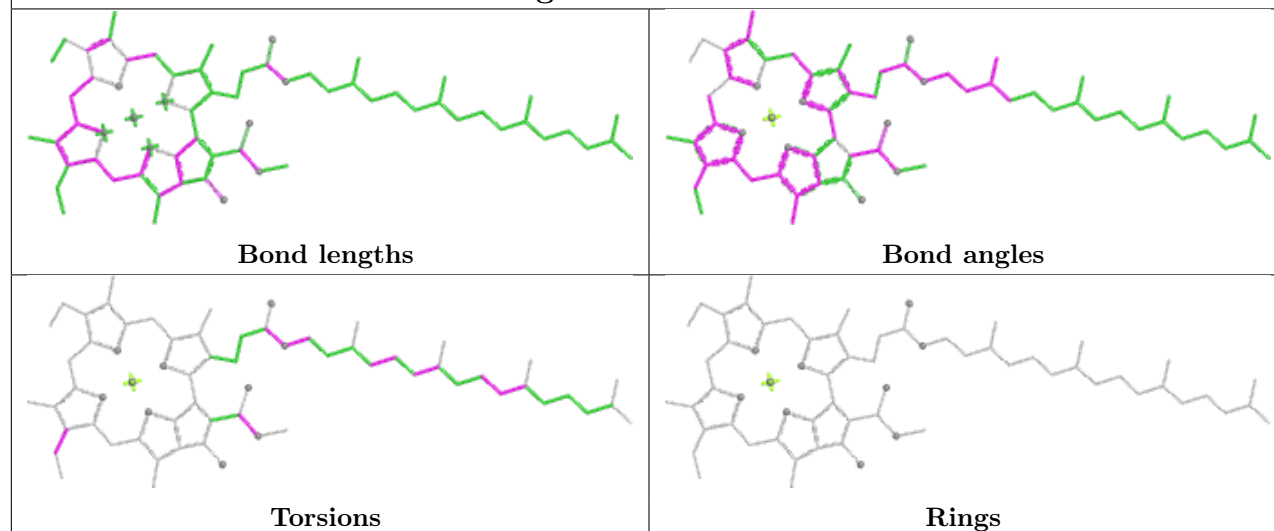


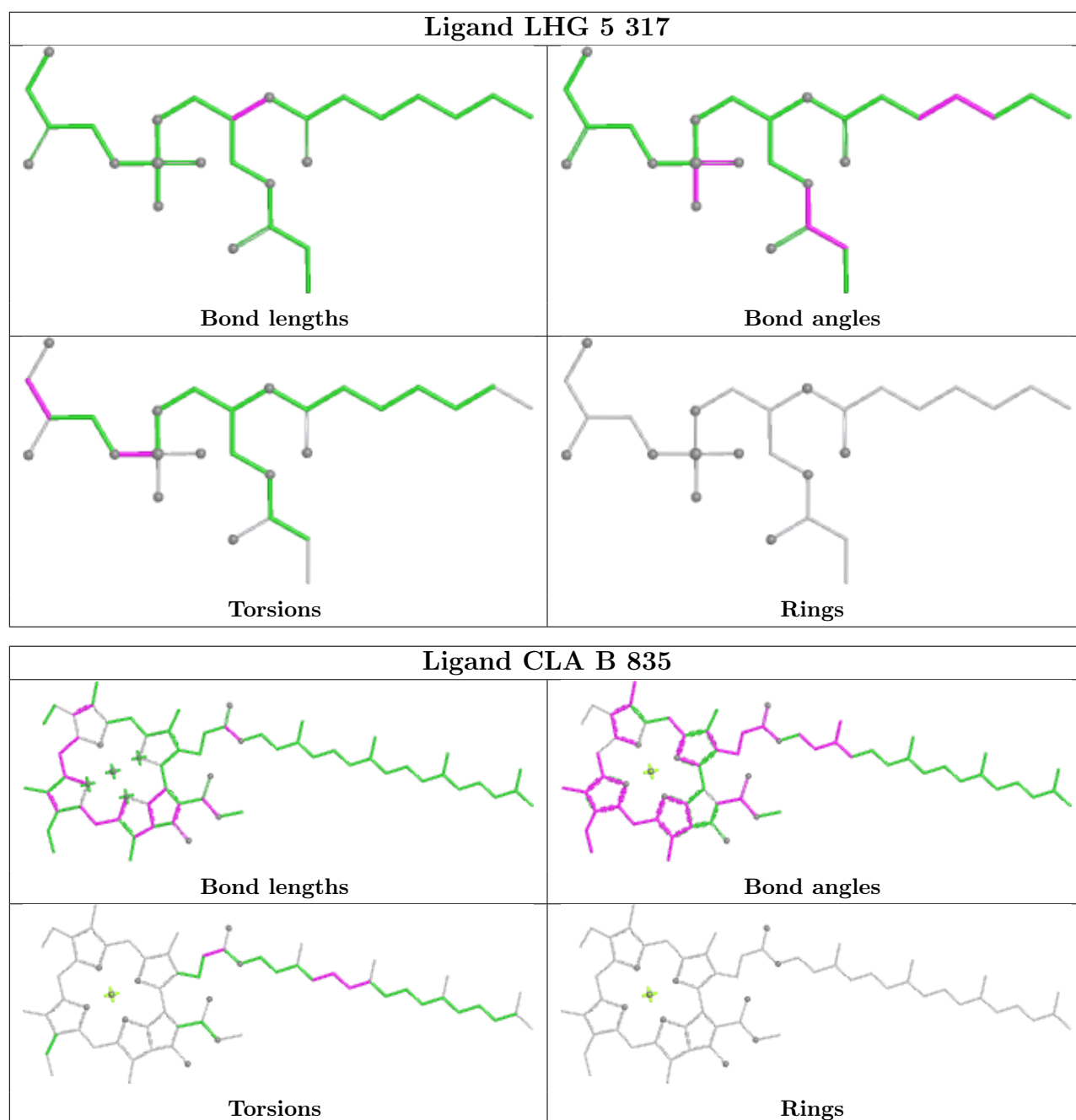
## Ligand CLA 14 310

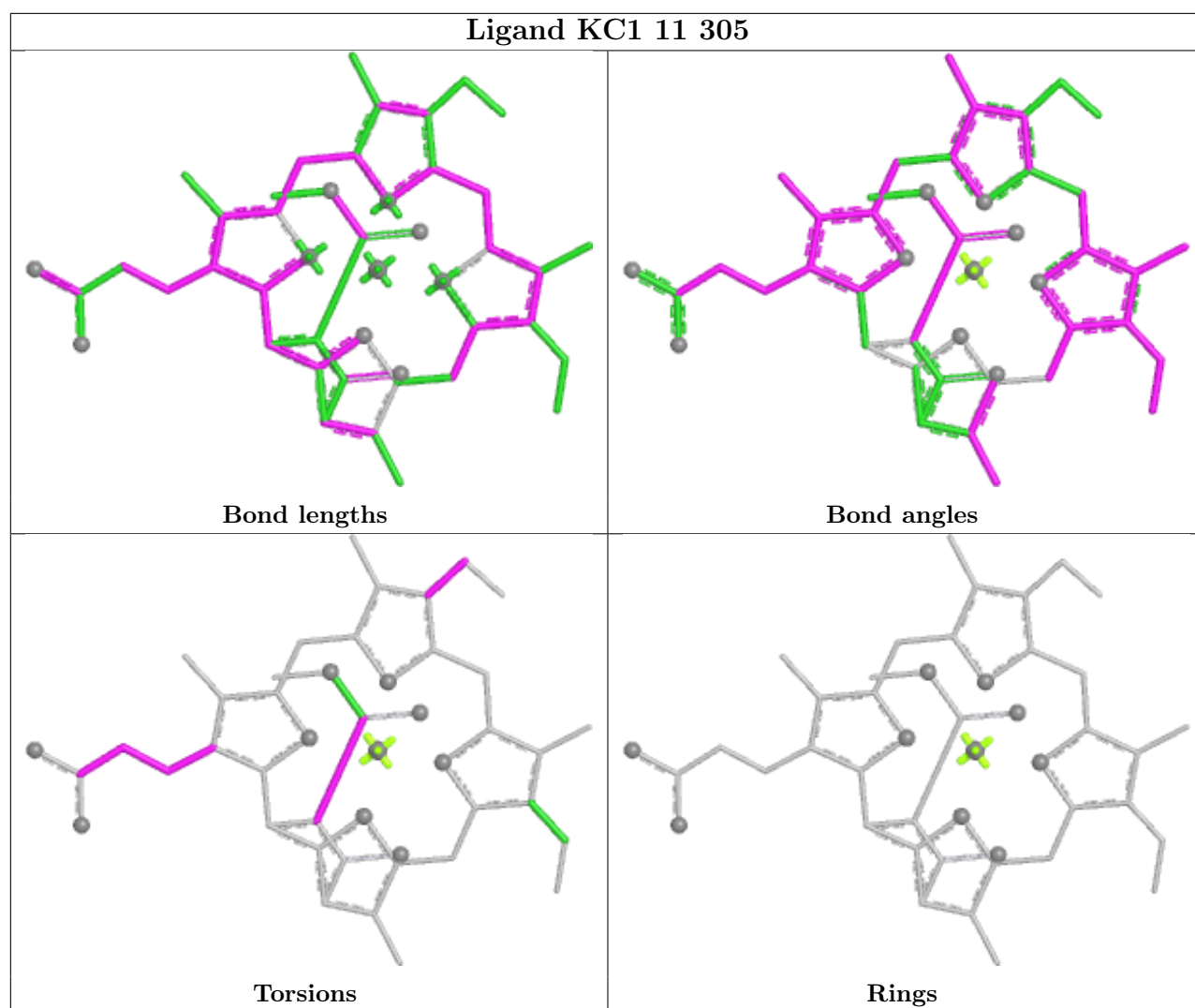


**Ligand CLA 3 301****Ligand CLA A 823**

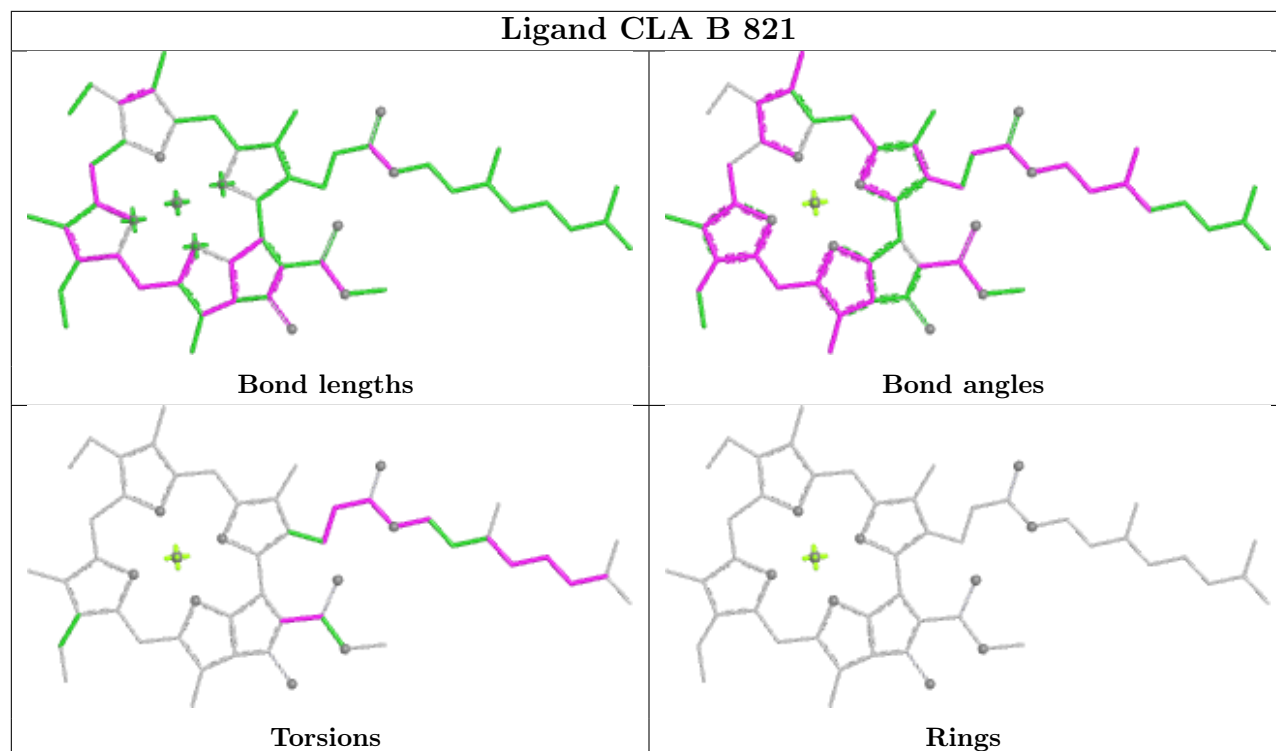


**Ligand CLA 1 303****Ligand CLA 7 310****Ligand CLA 3 307**

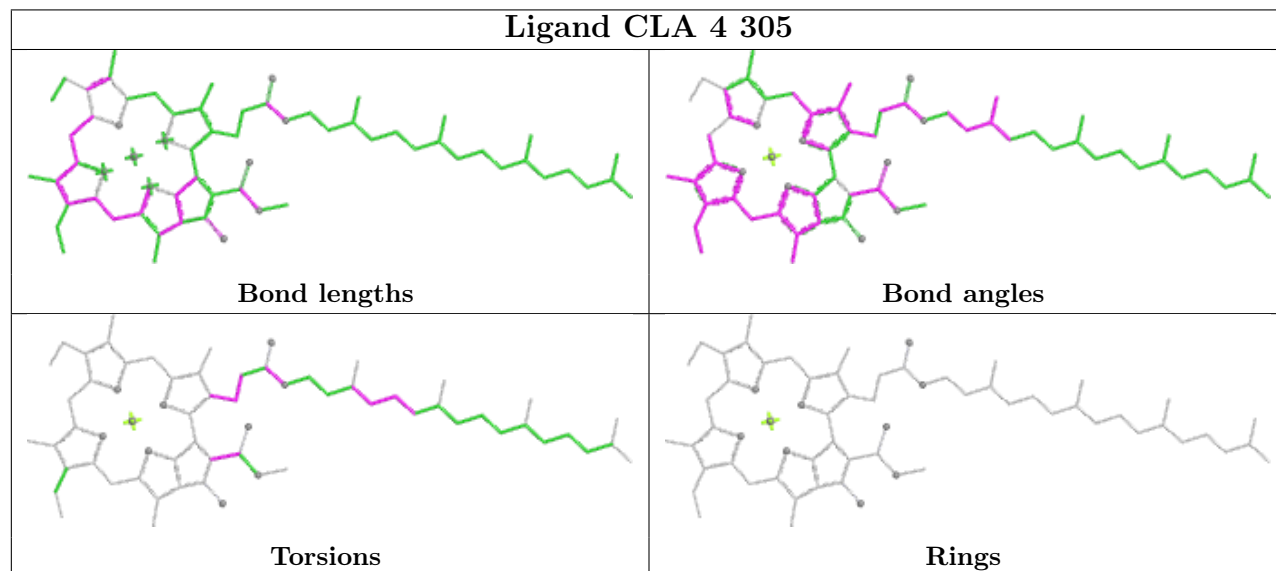


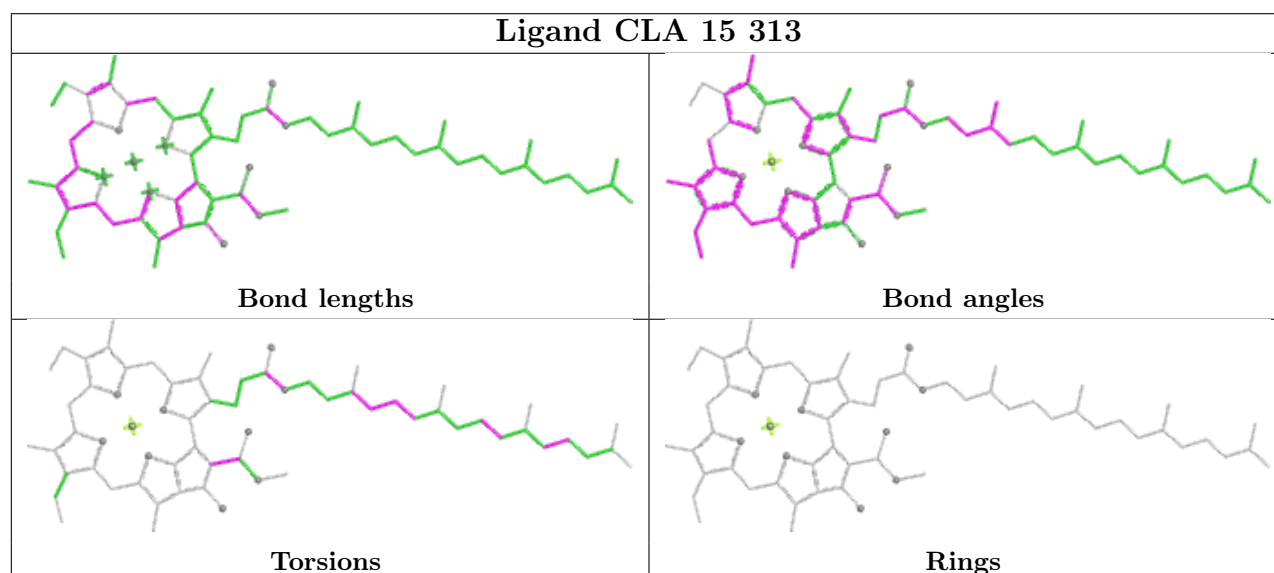
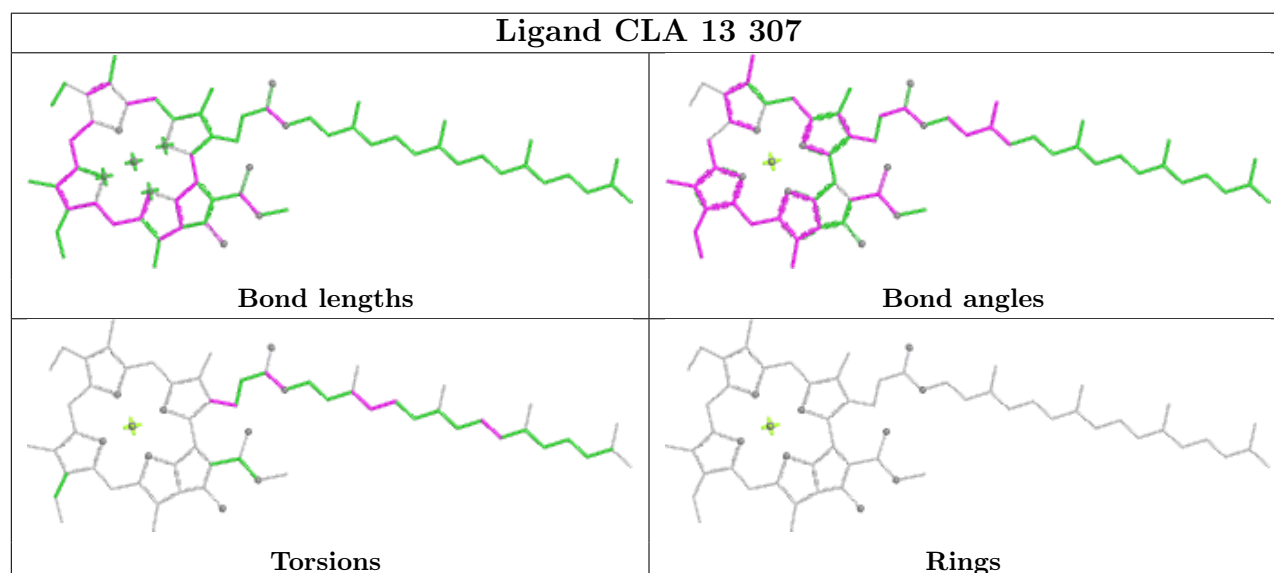
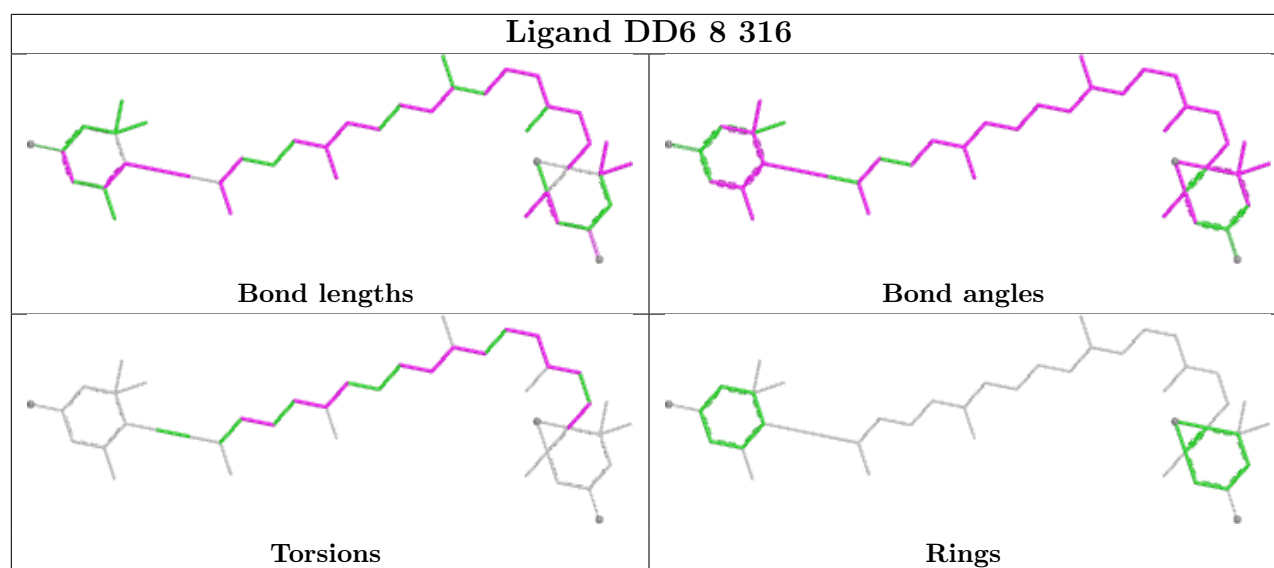


## Ligand CLA B 821

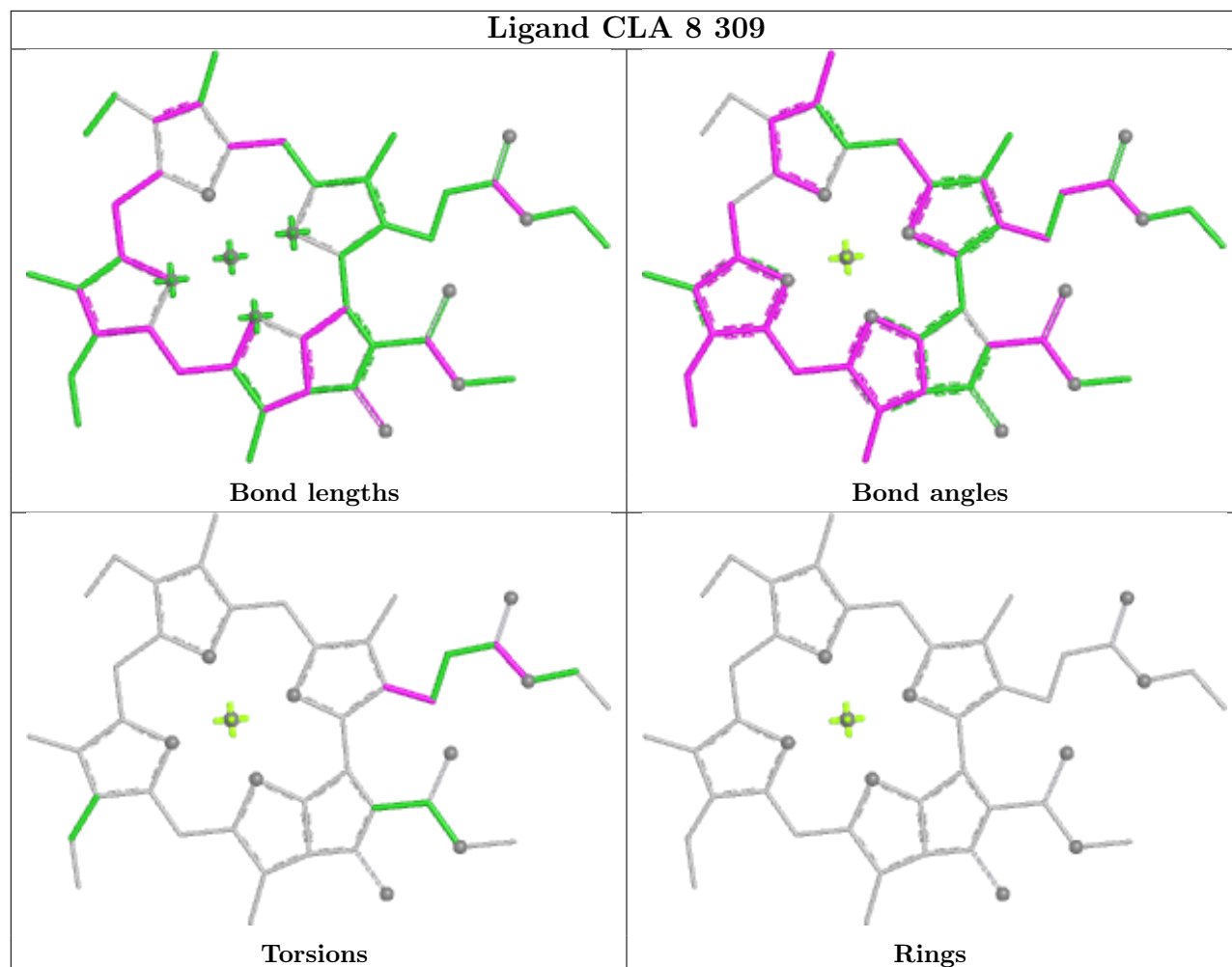


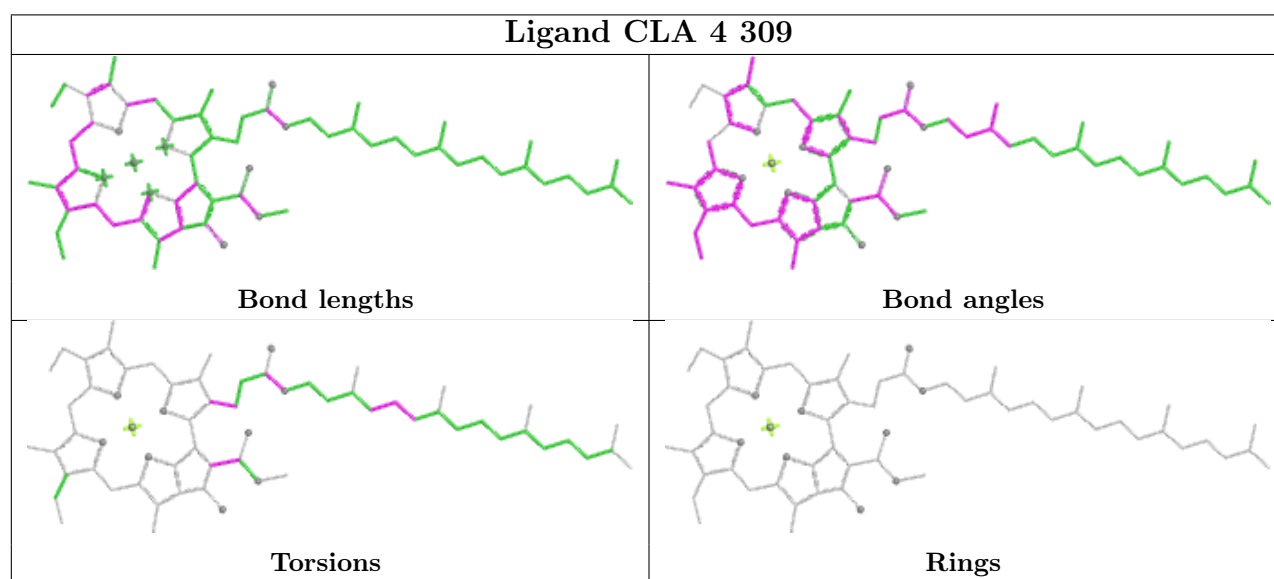
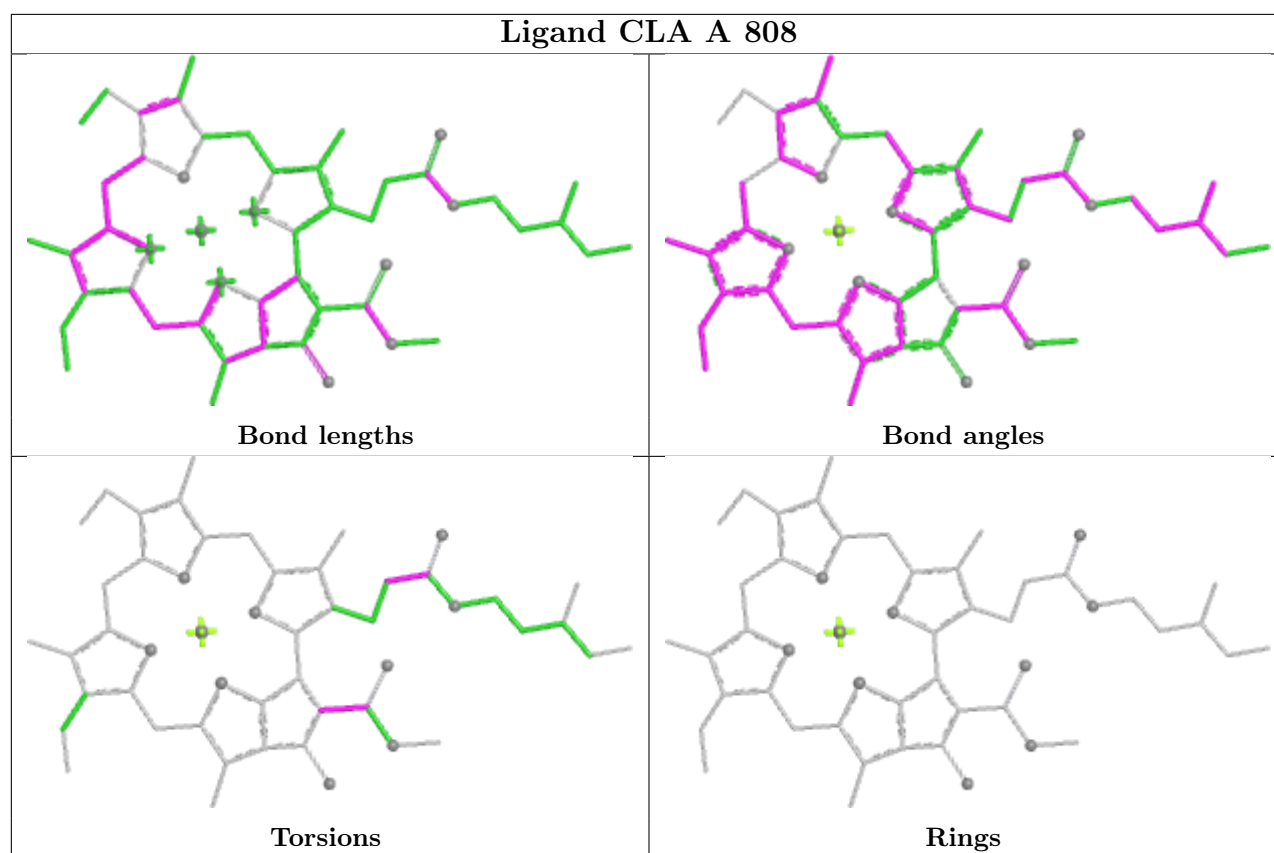
## Ligand CLA 4 305

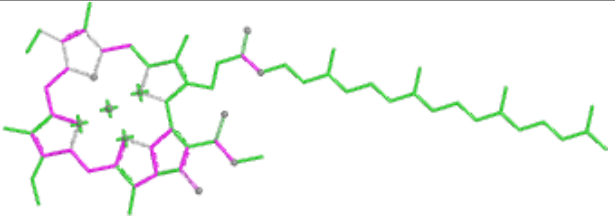
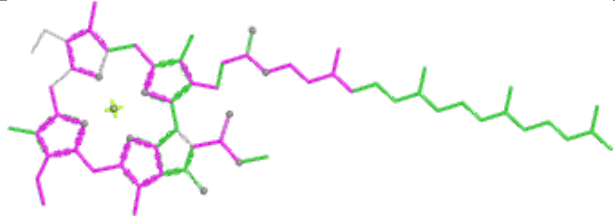
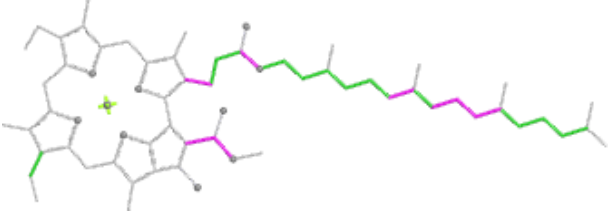
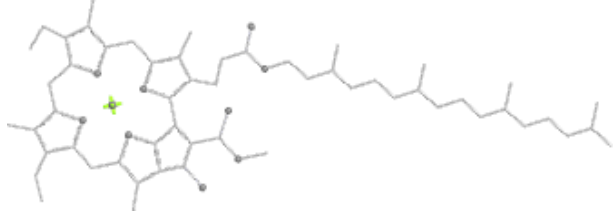
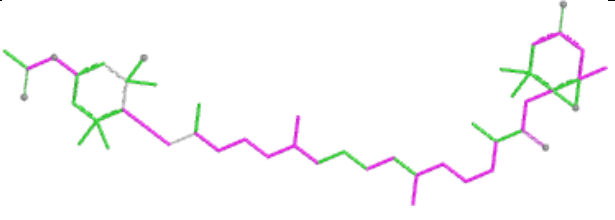
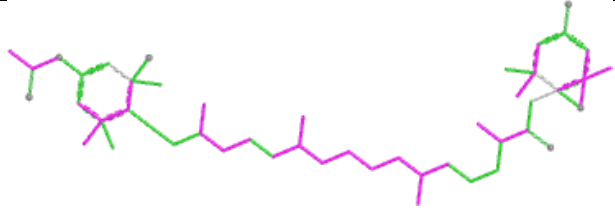
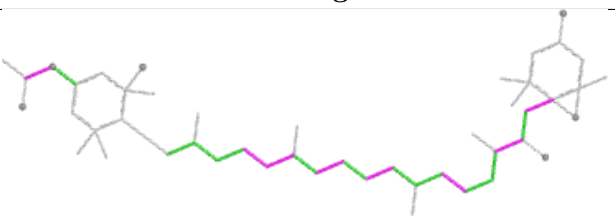
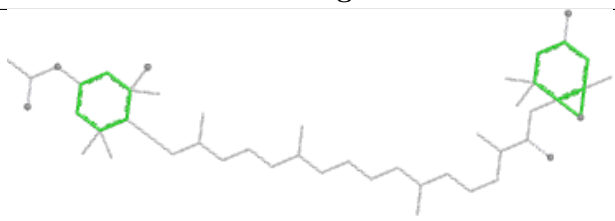
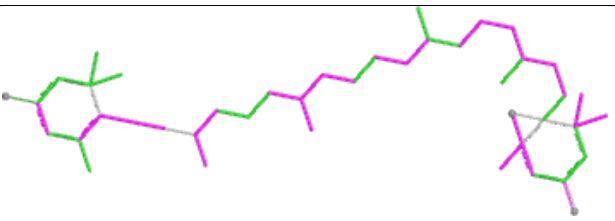
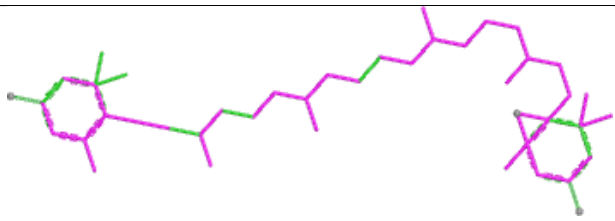
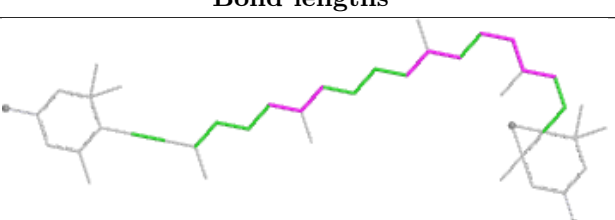
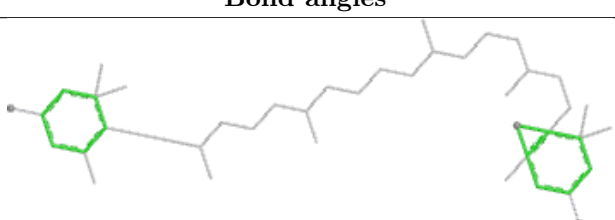




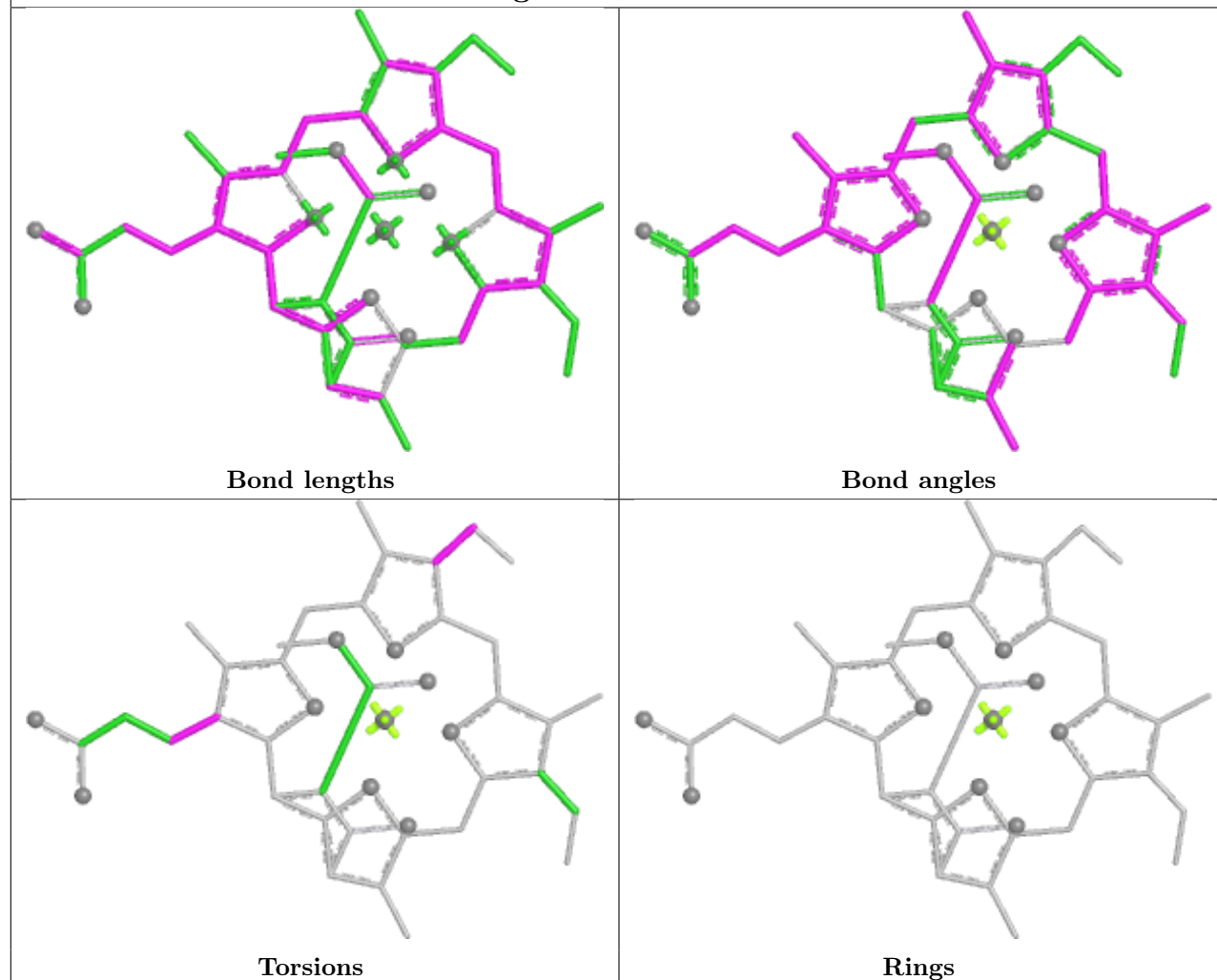
## Ligand CLA 8 309



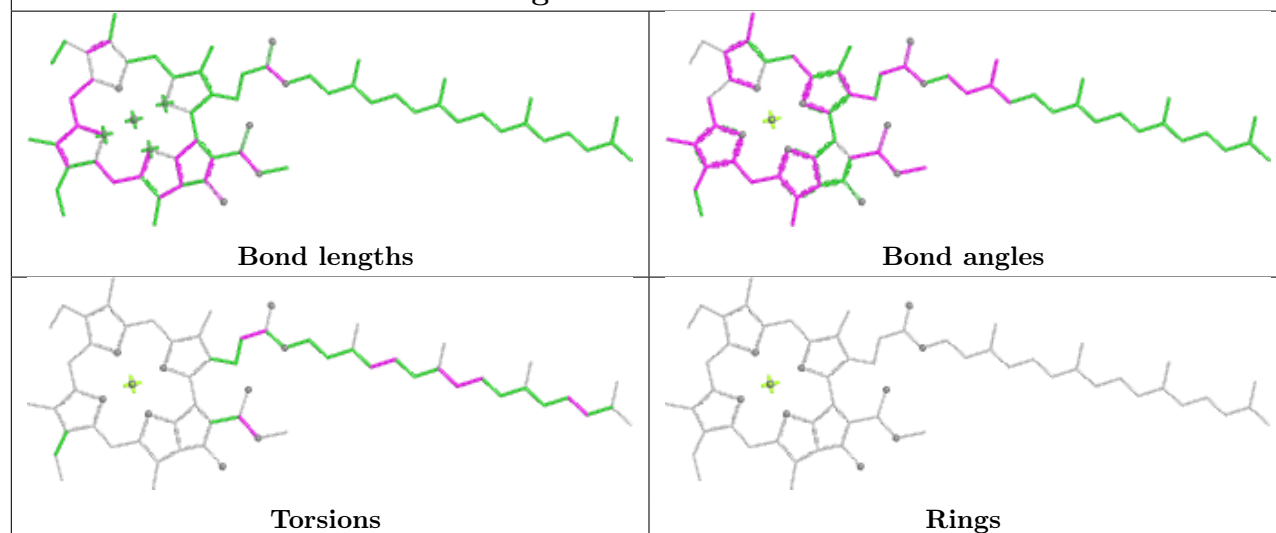


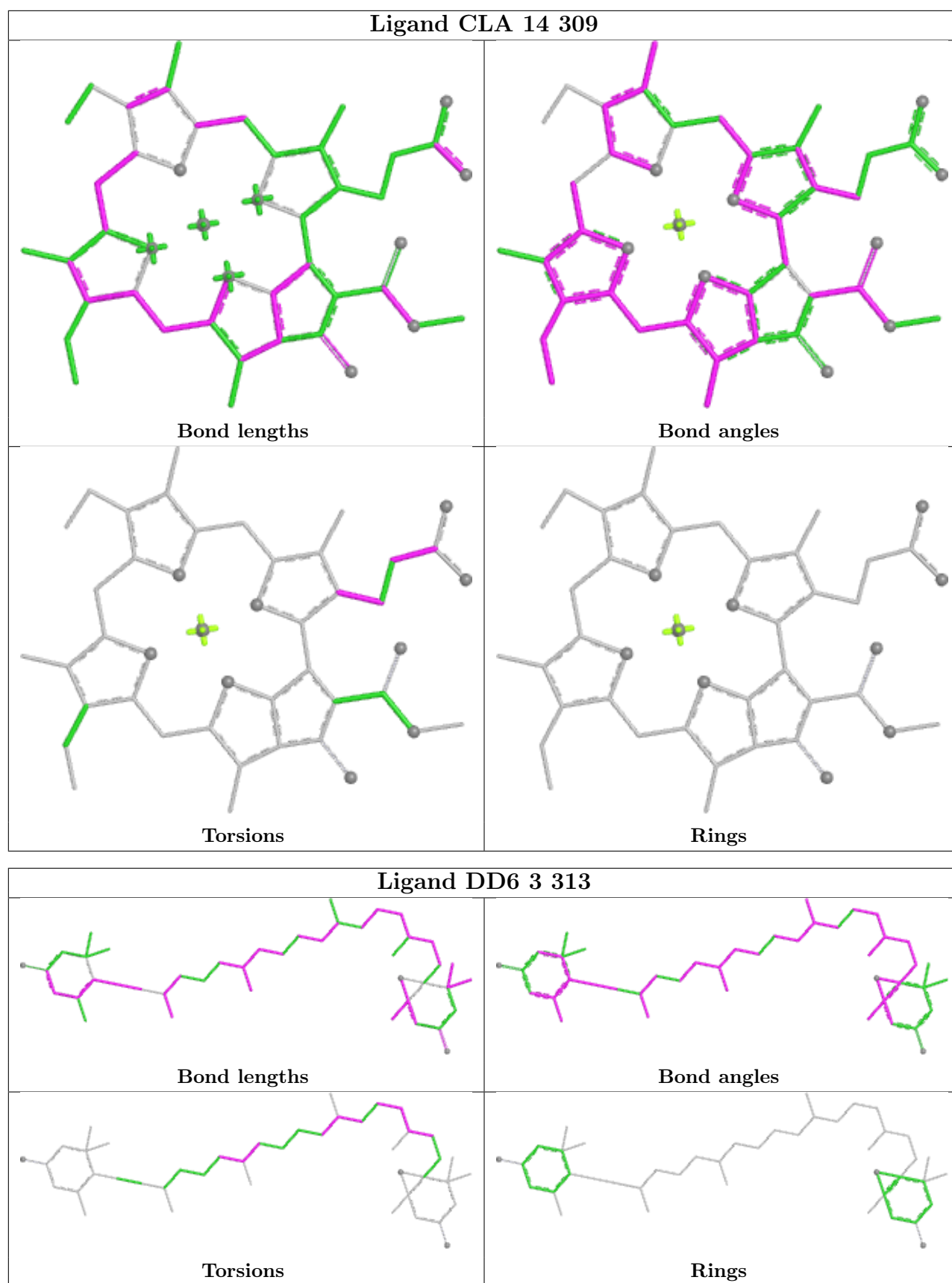
Ligand CLA B 828	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand A86 10 302	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DD6 6 319	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

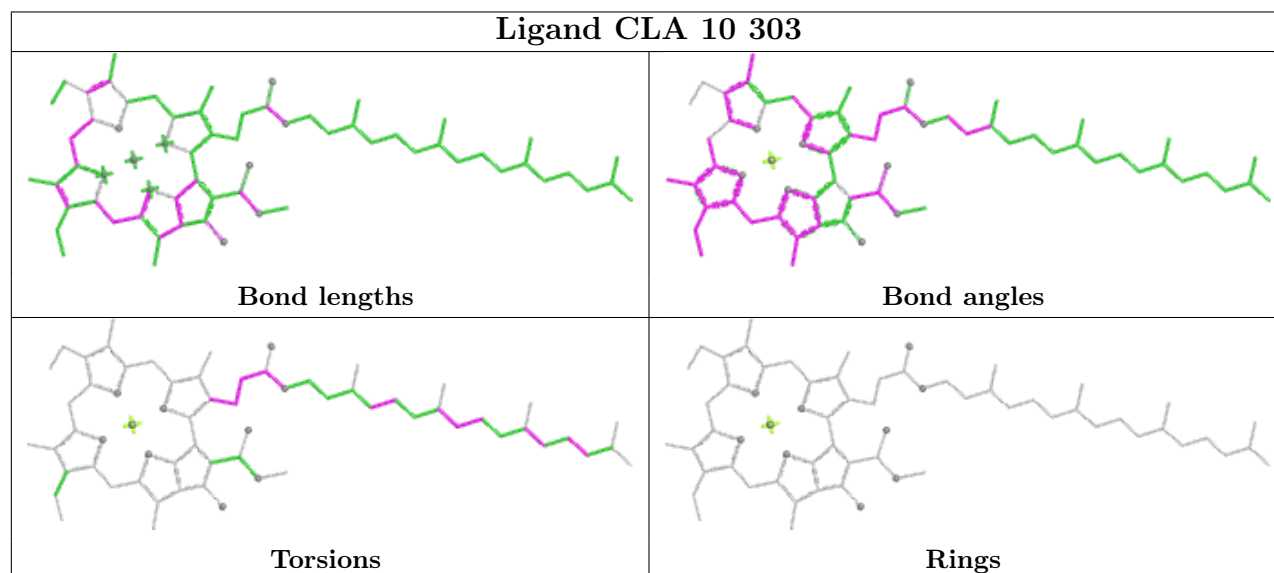
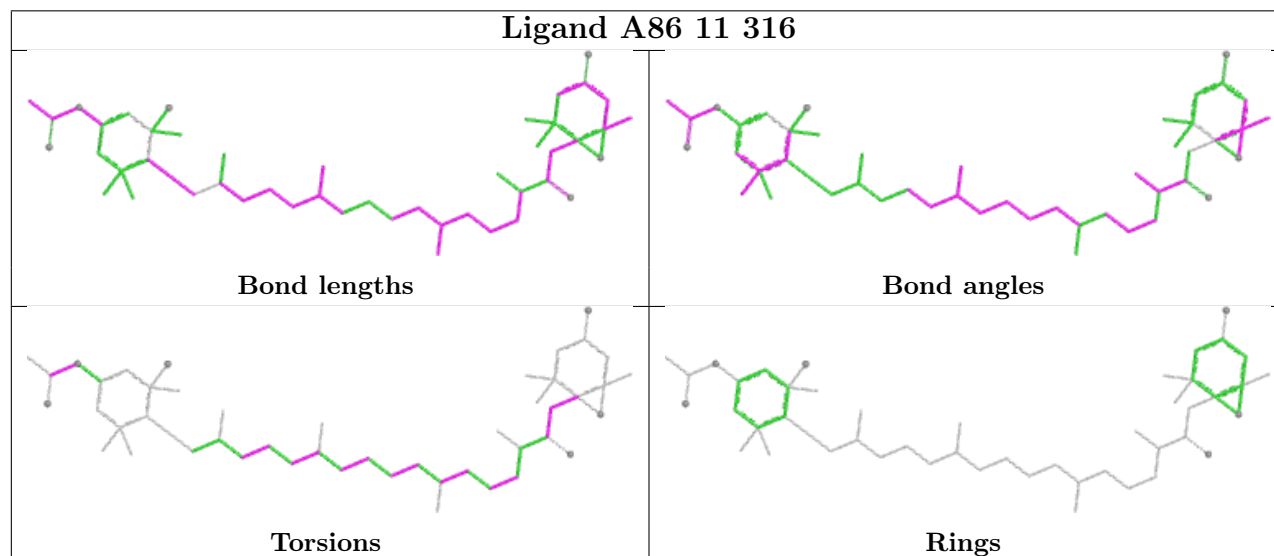
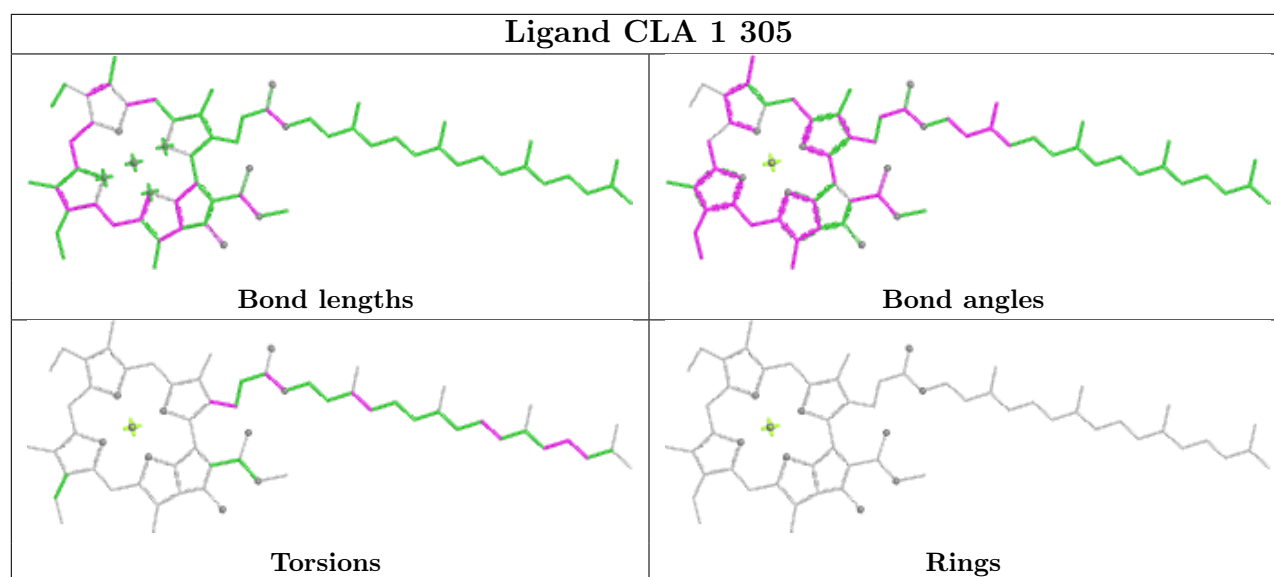
## Ligand KC1 2 312



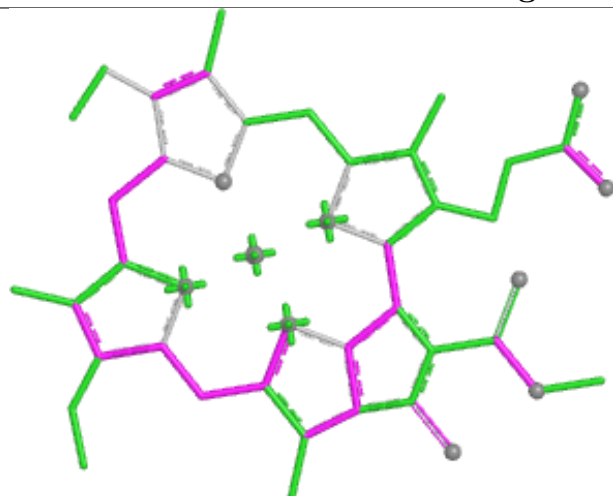
## Ligand CLA A 841



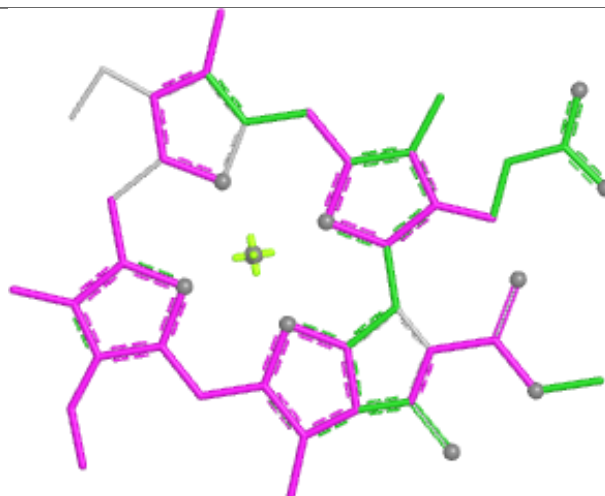




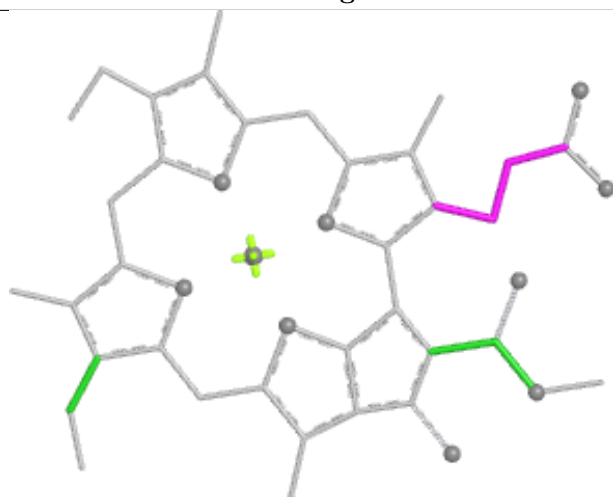
## Ligand CLA 9 306



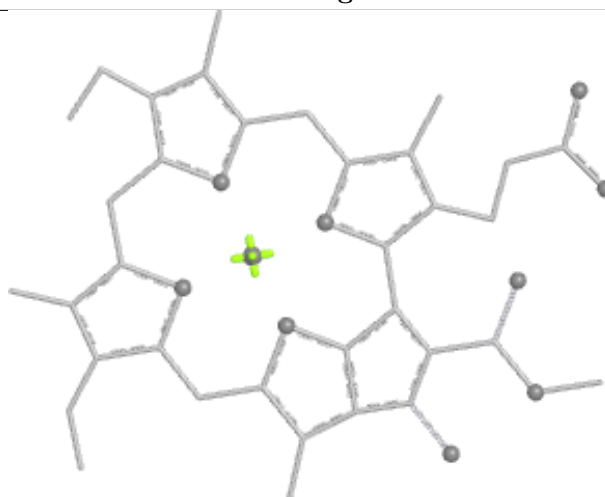
Bond lengths



Bond angles

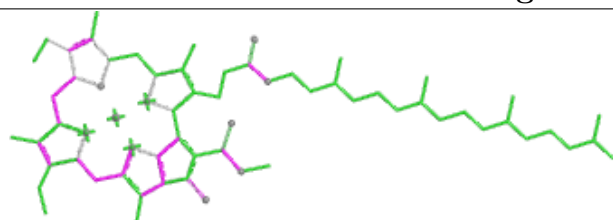


Torsions

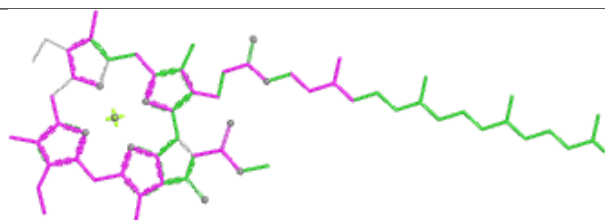


Rings

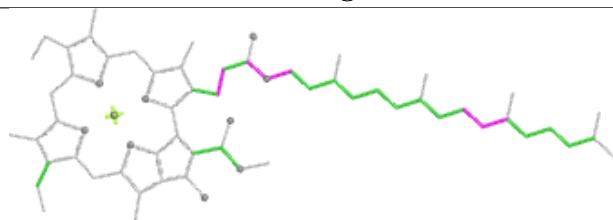
## Ligand CLA L 202



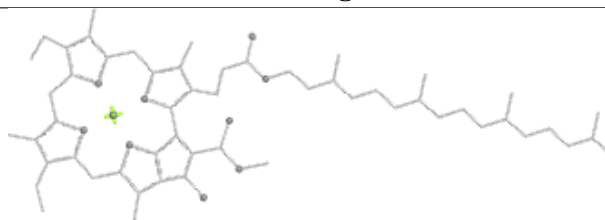
Bond lengths



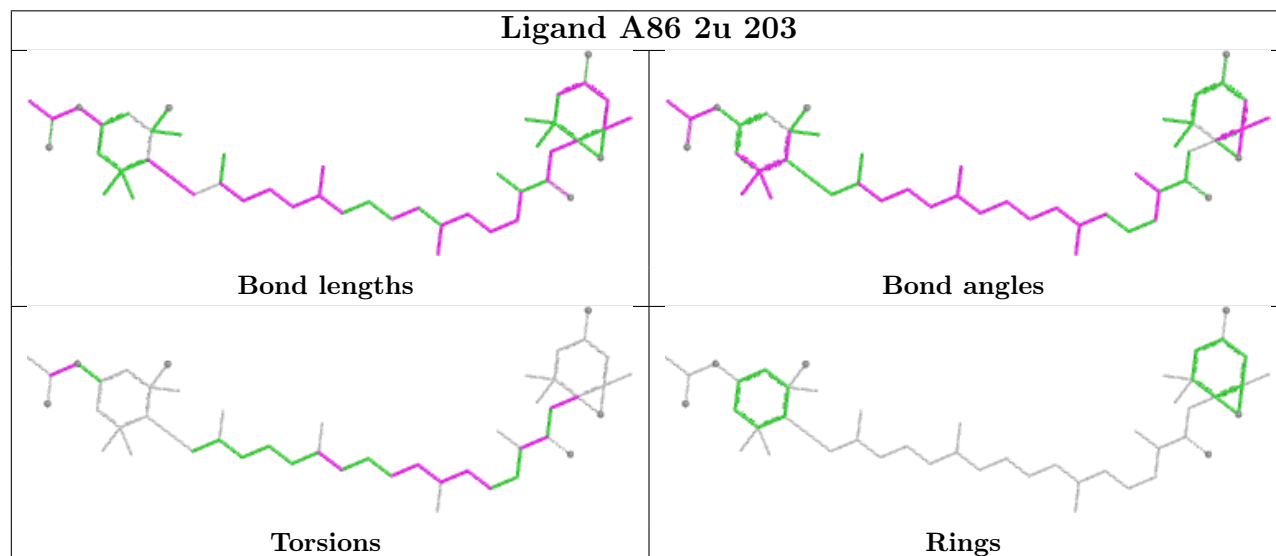
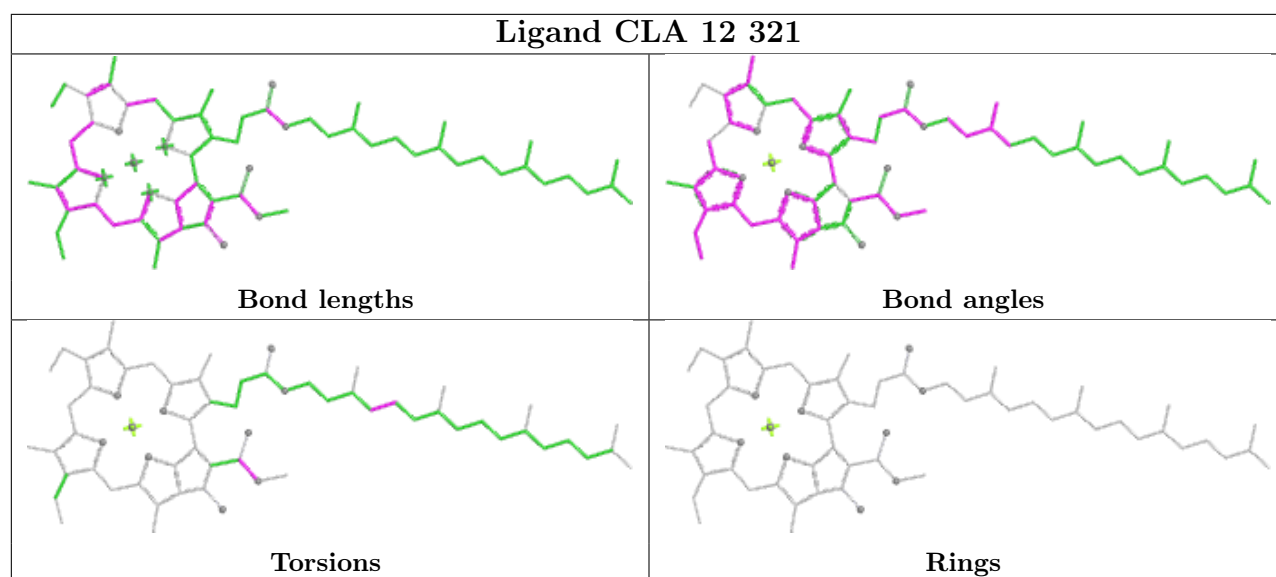
Bond angles

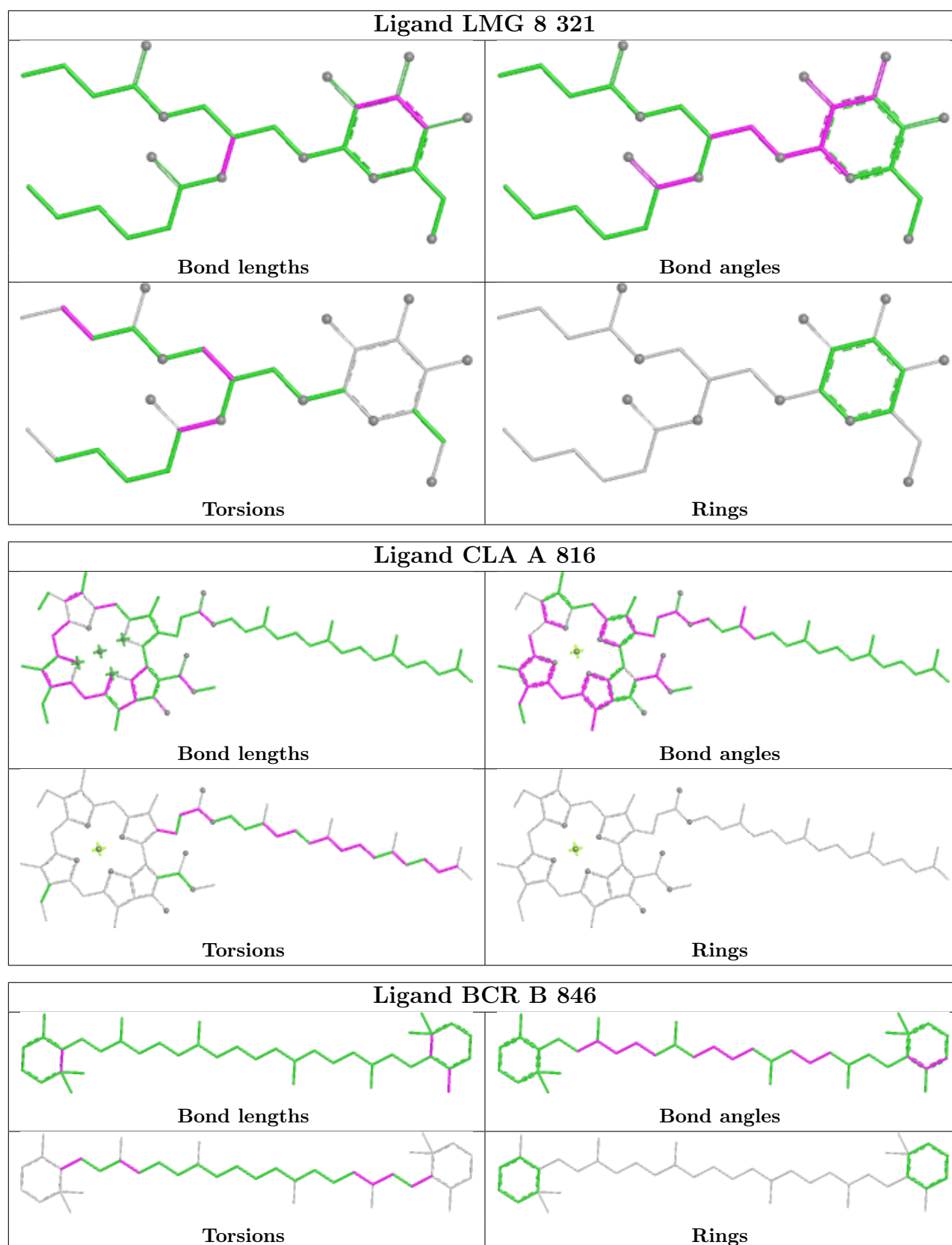


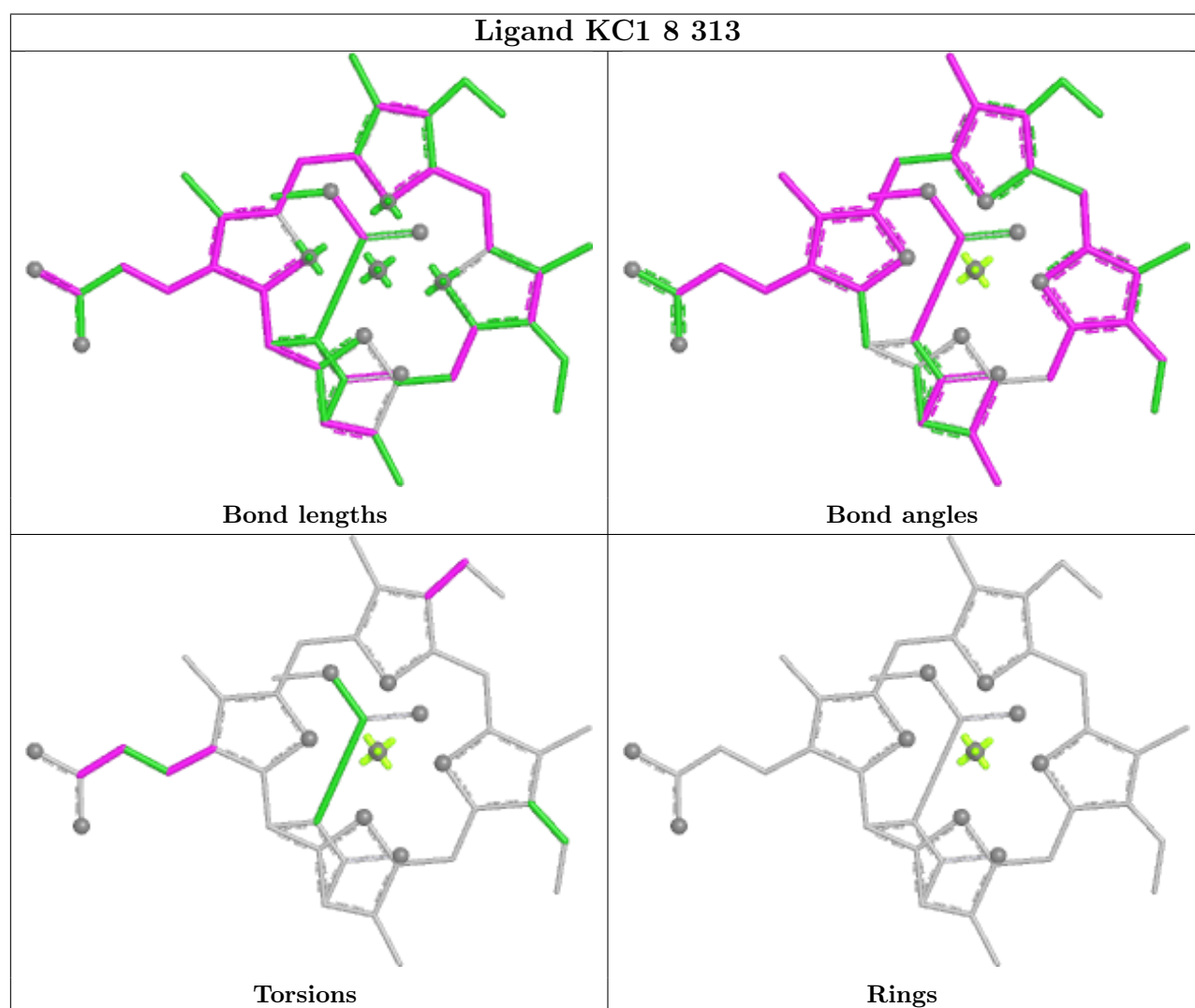
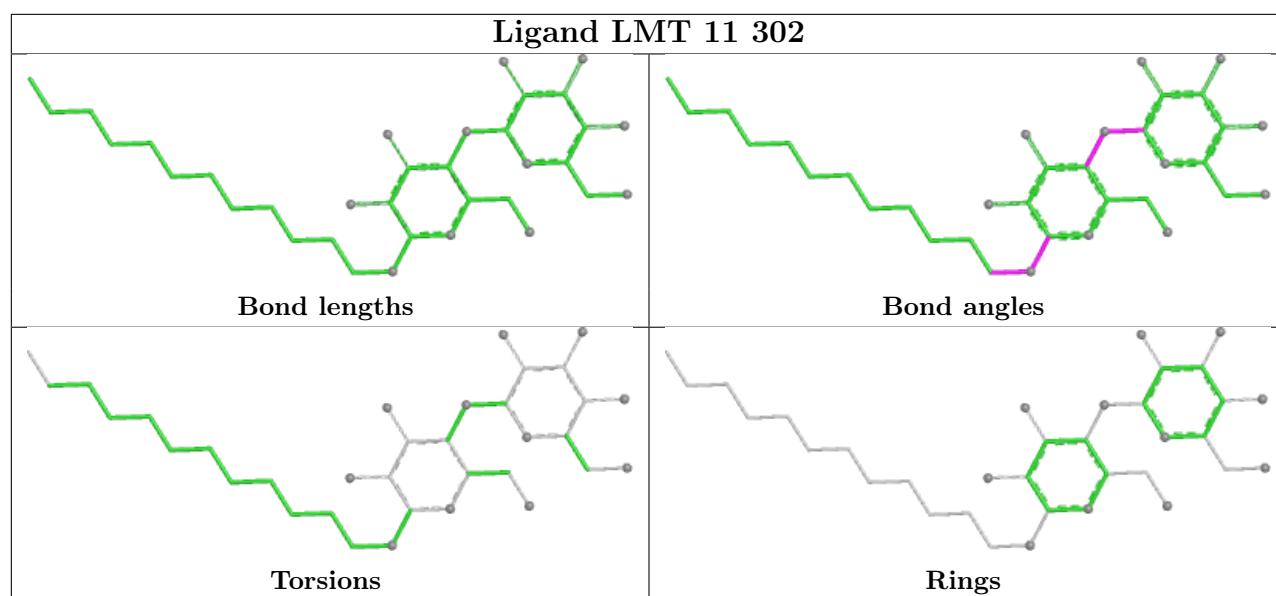
Torsions

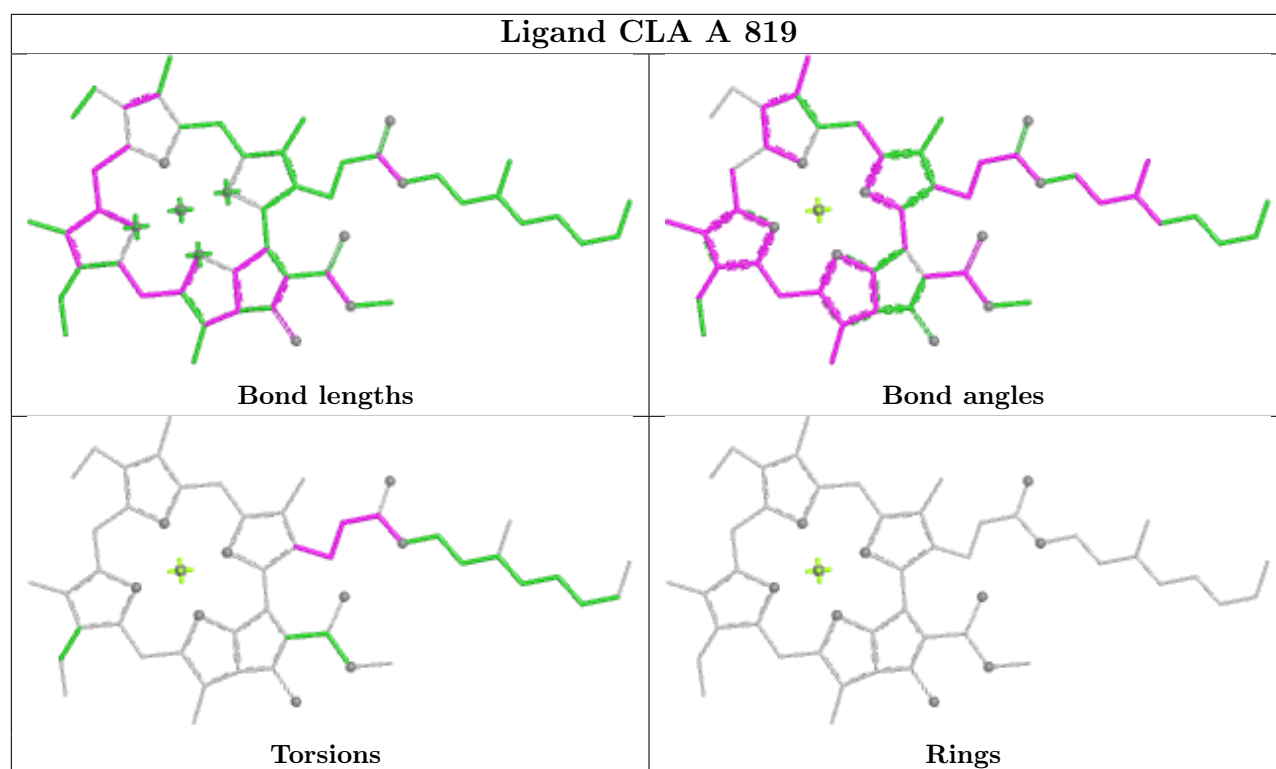


Rings

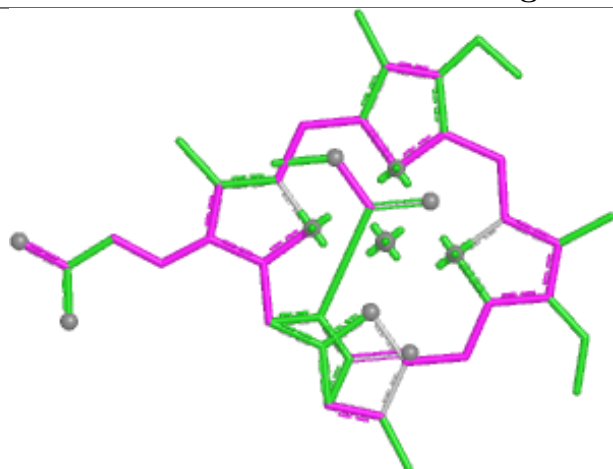




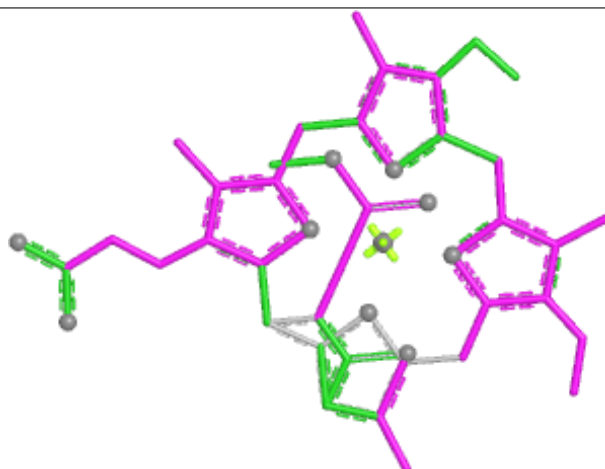




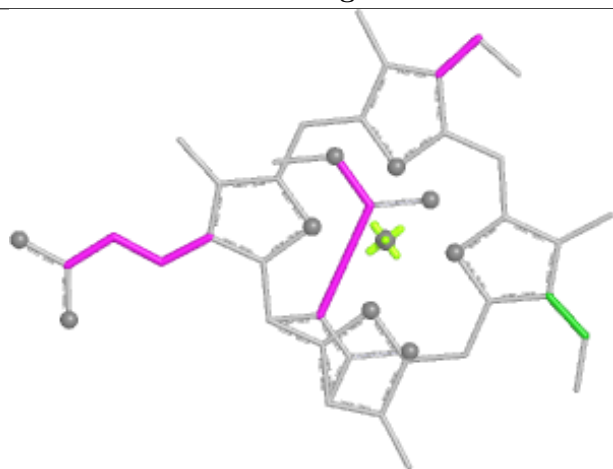
## Ligand KC1 5 306



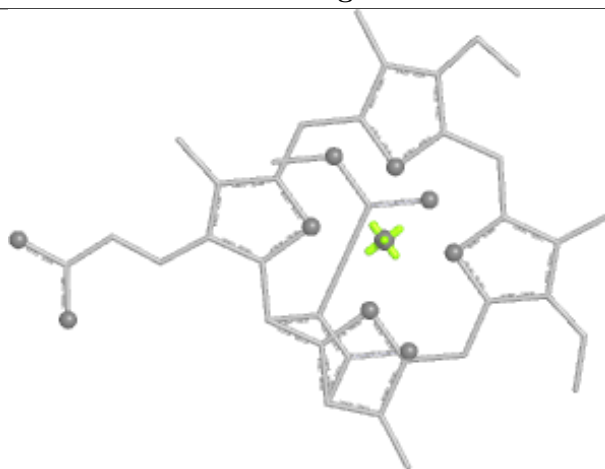
Bond lengths



Bond angles

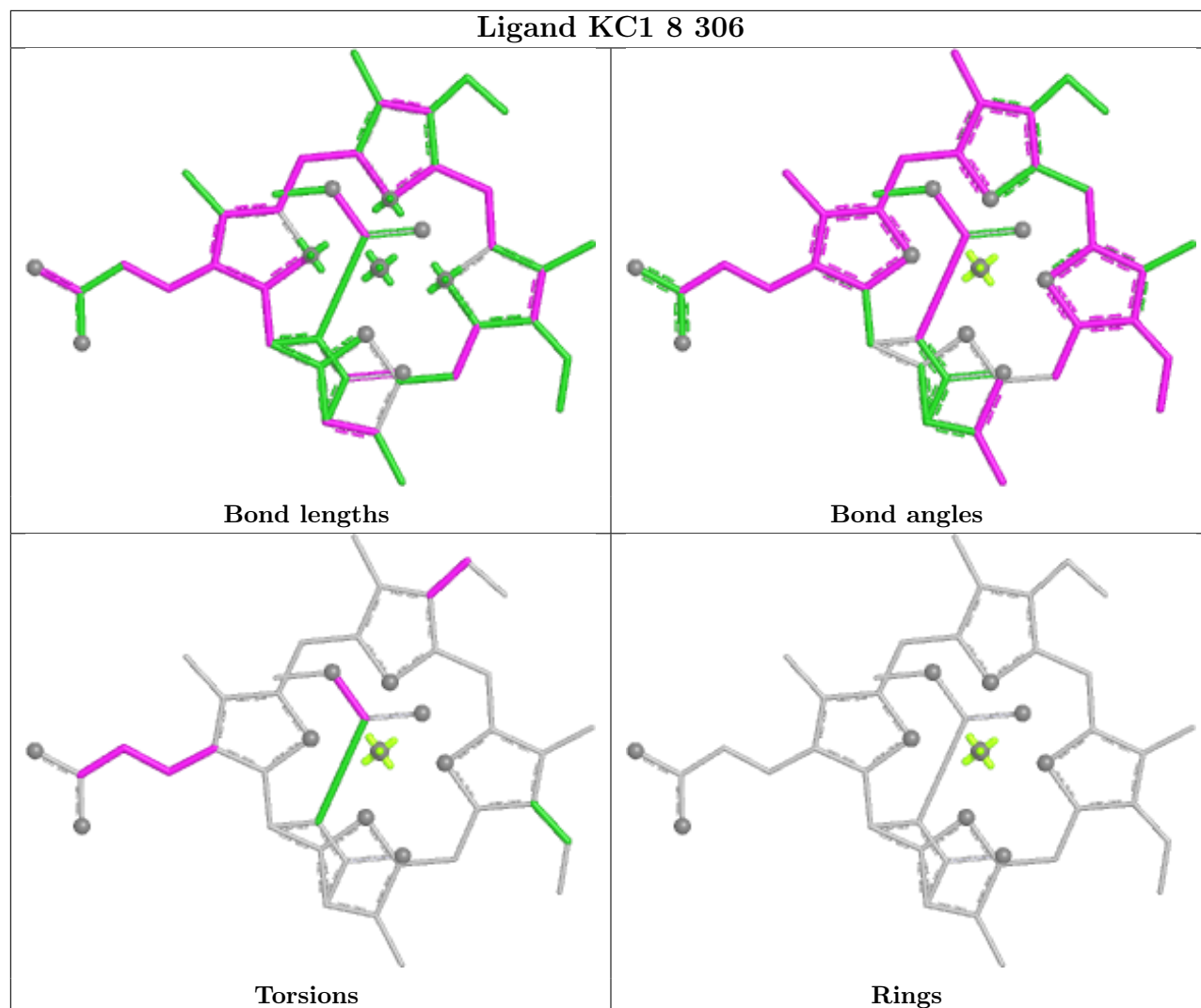


Torsions

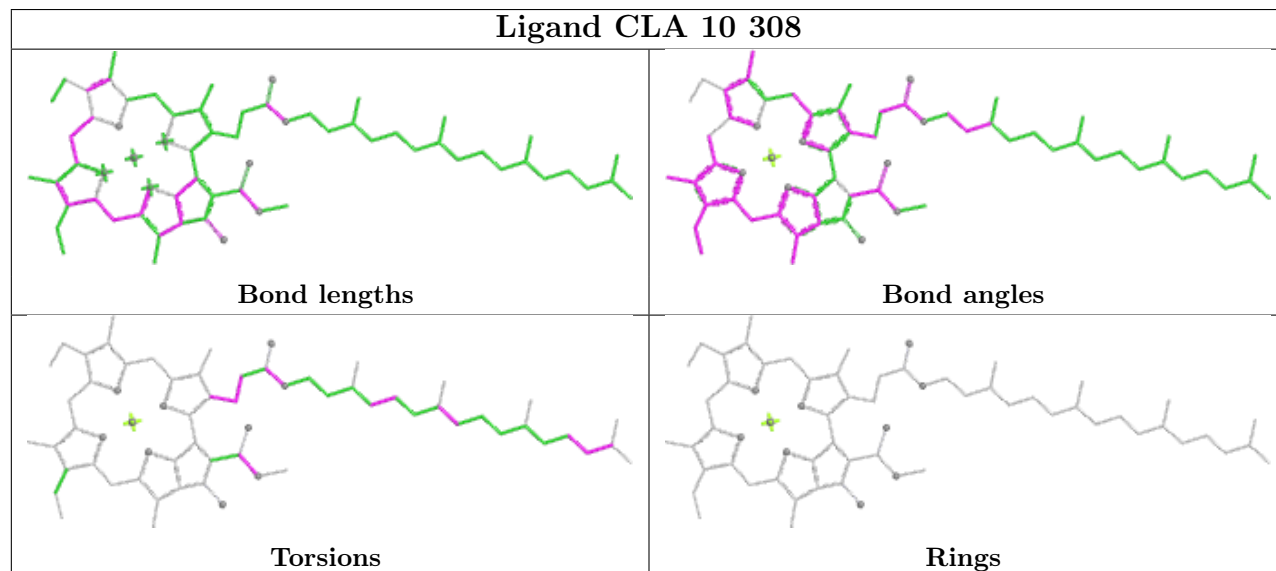


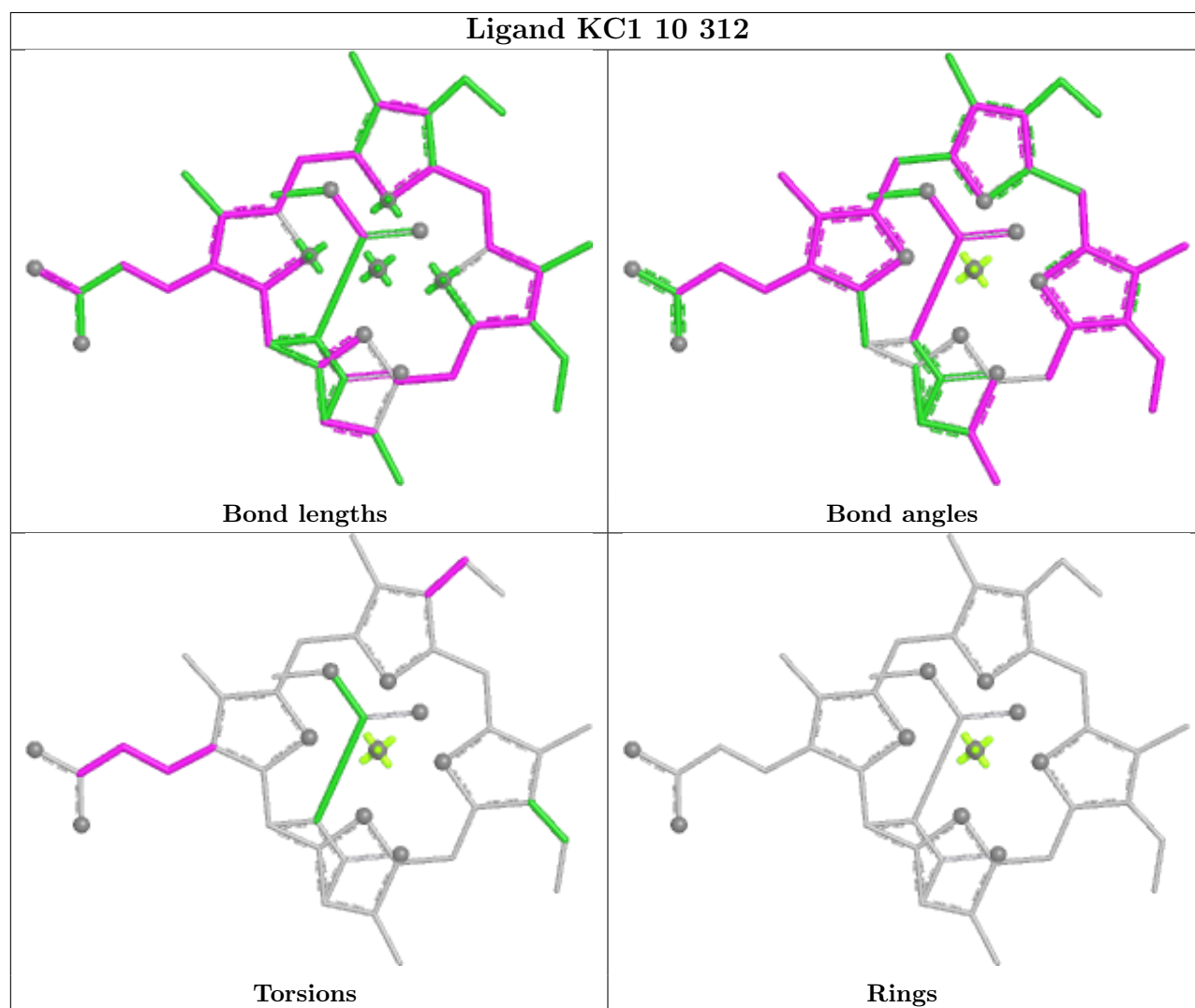
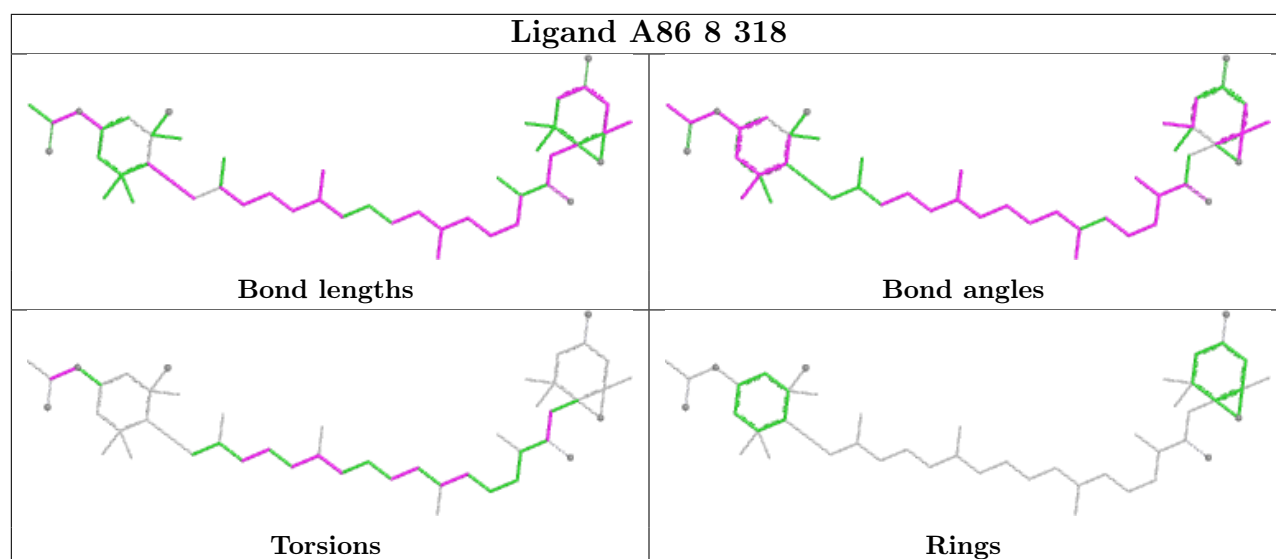
Rings

## Ligand KC1 8 306

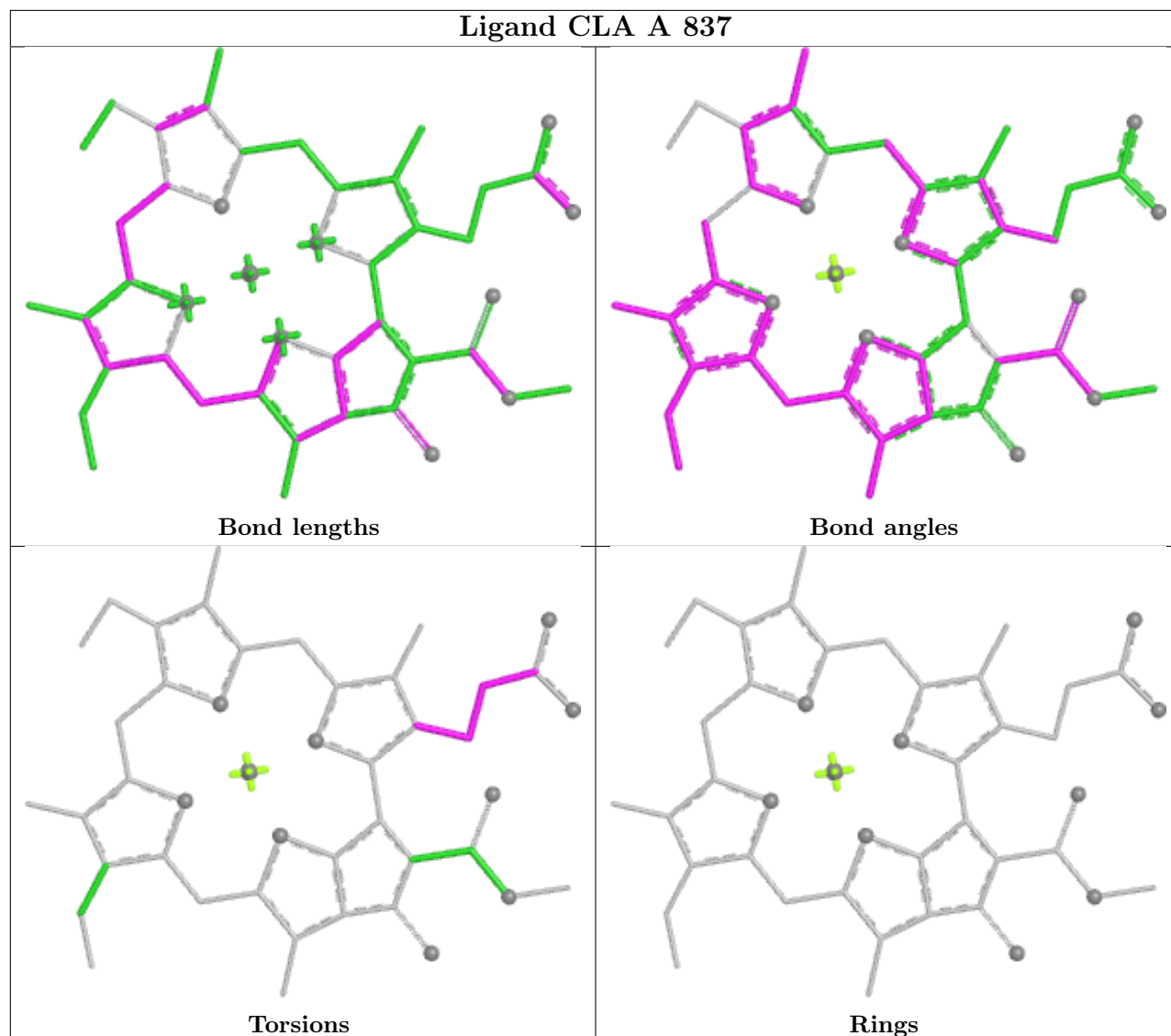


## Ligand CLA 10 308

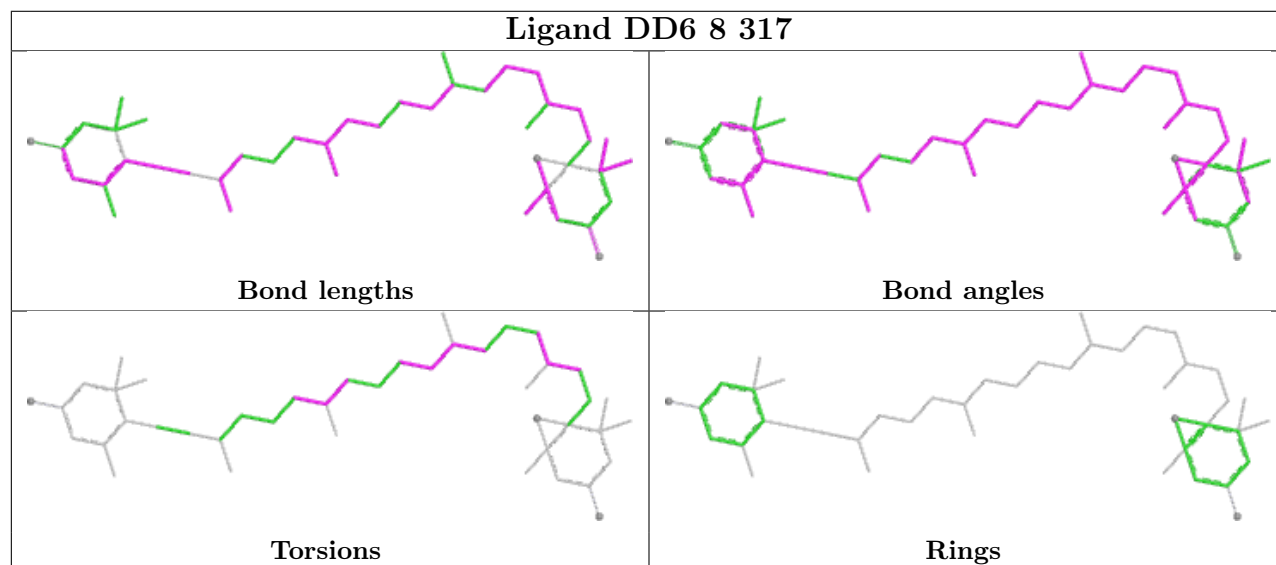


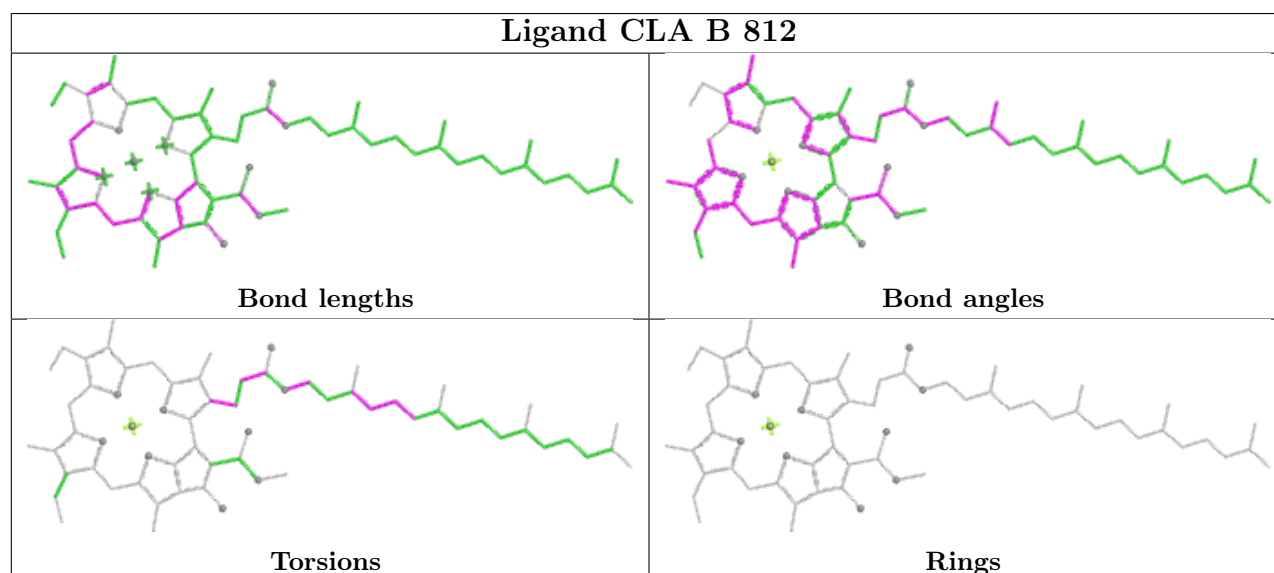
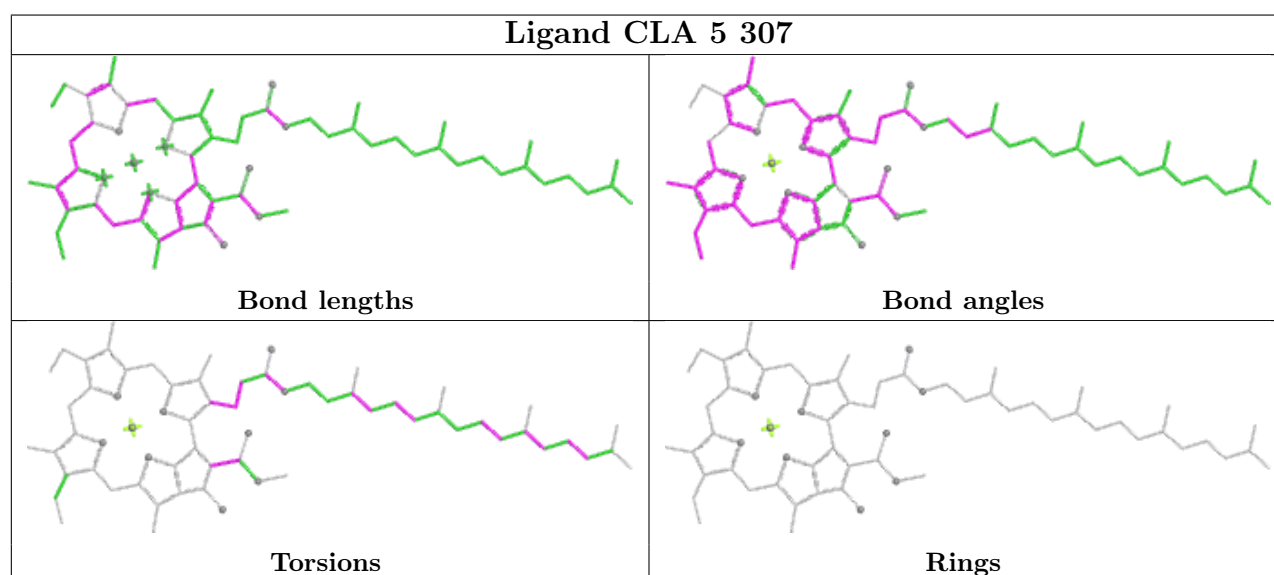
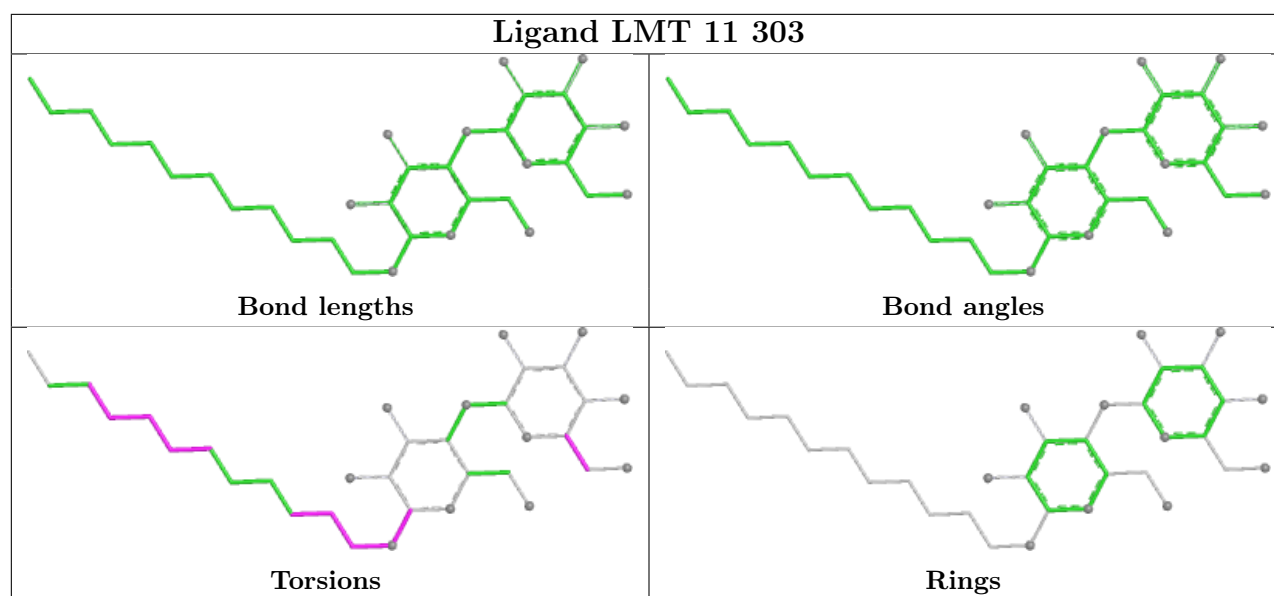


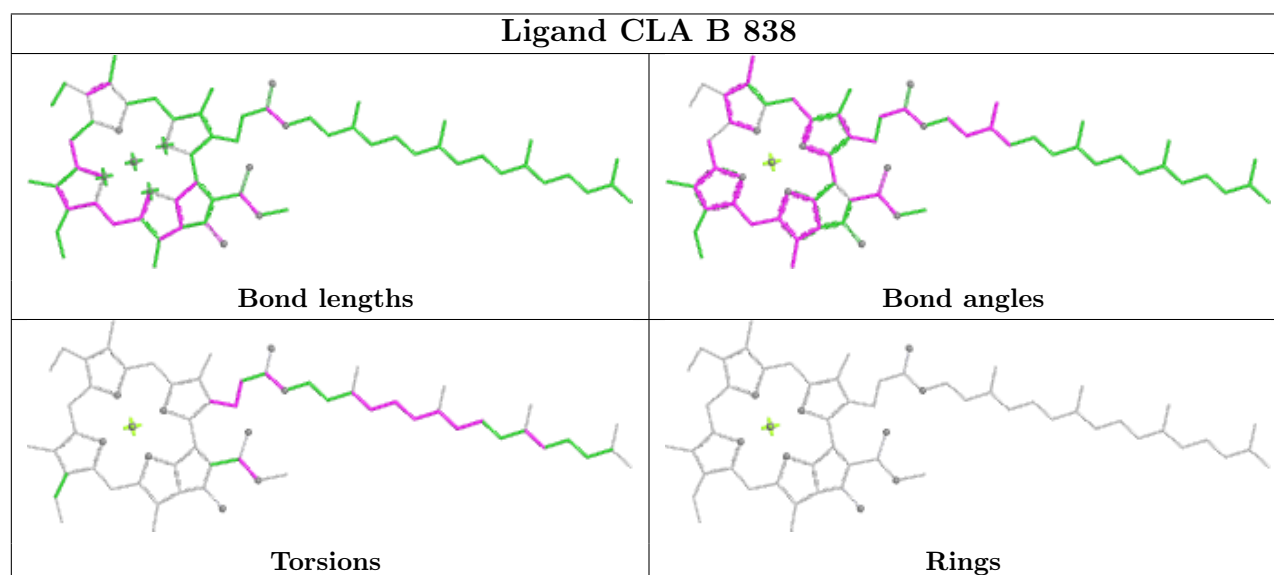
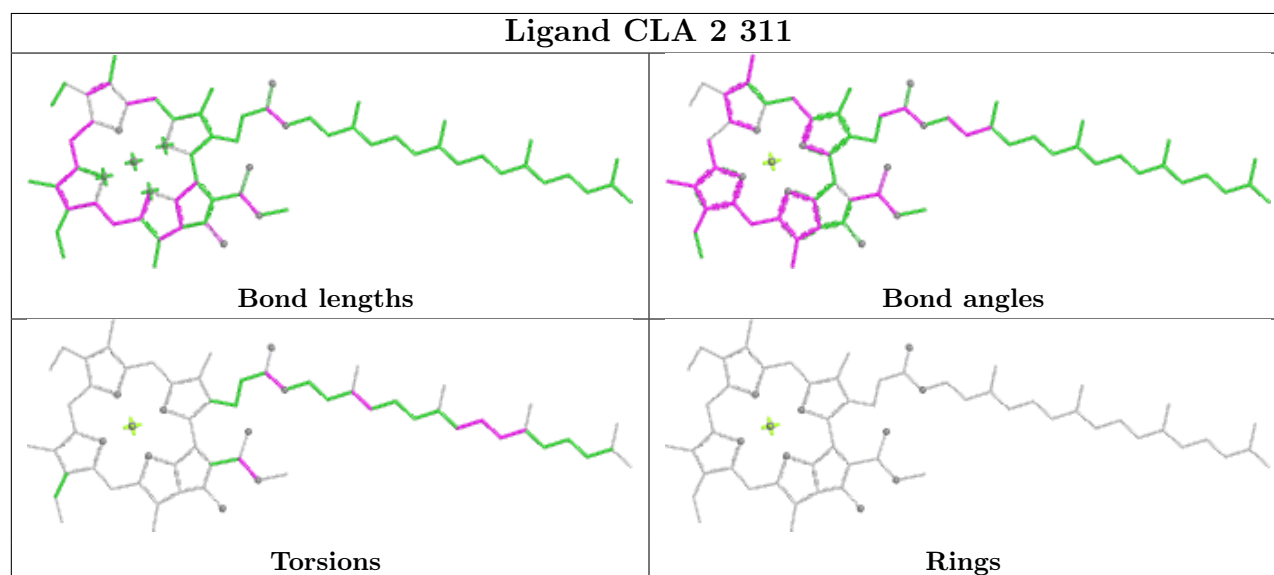
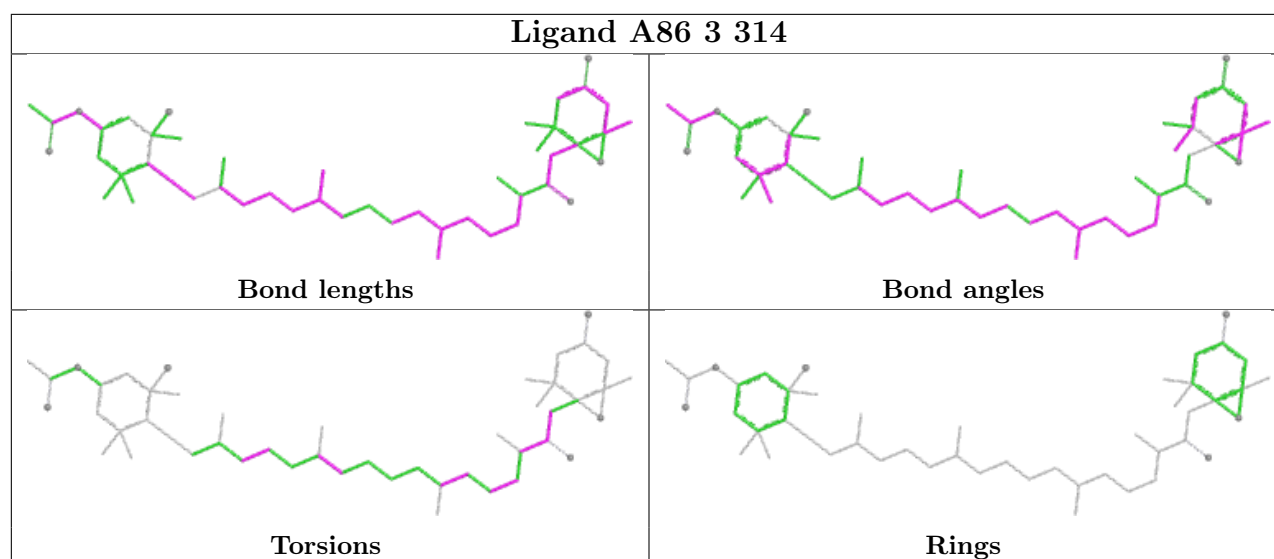
## Ligand CLA A 837

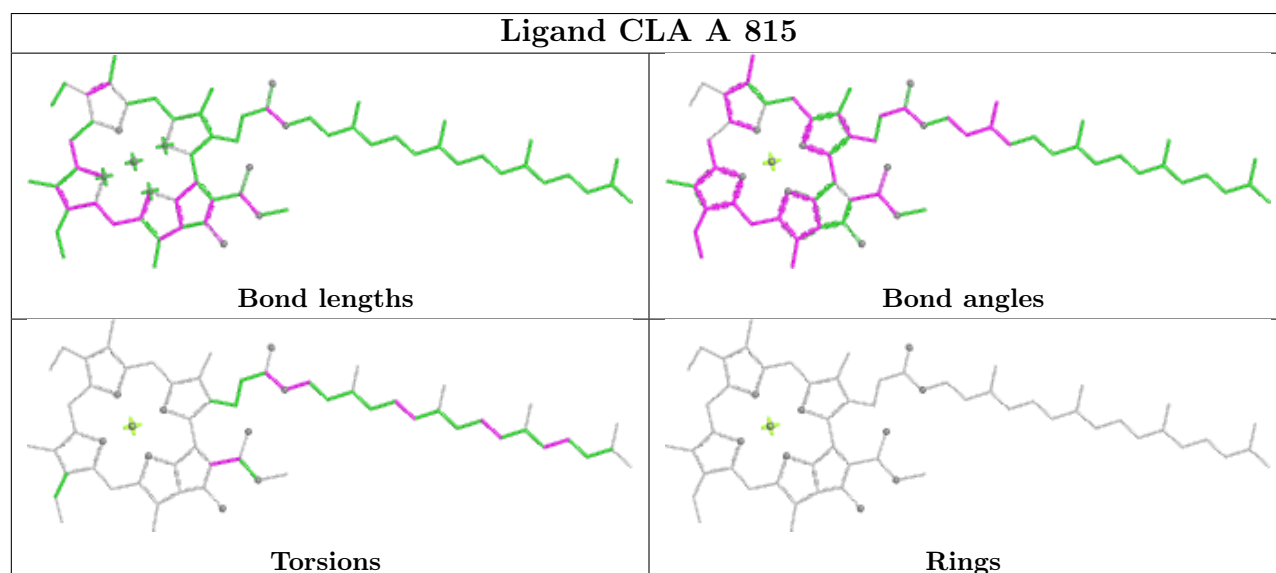
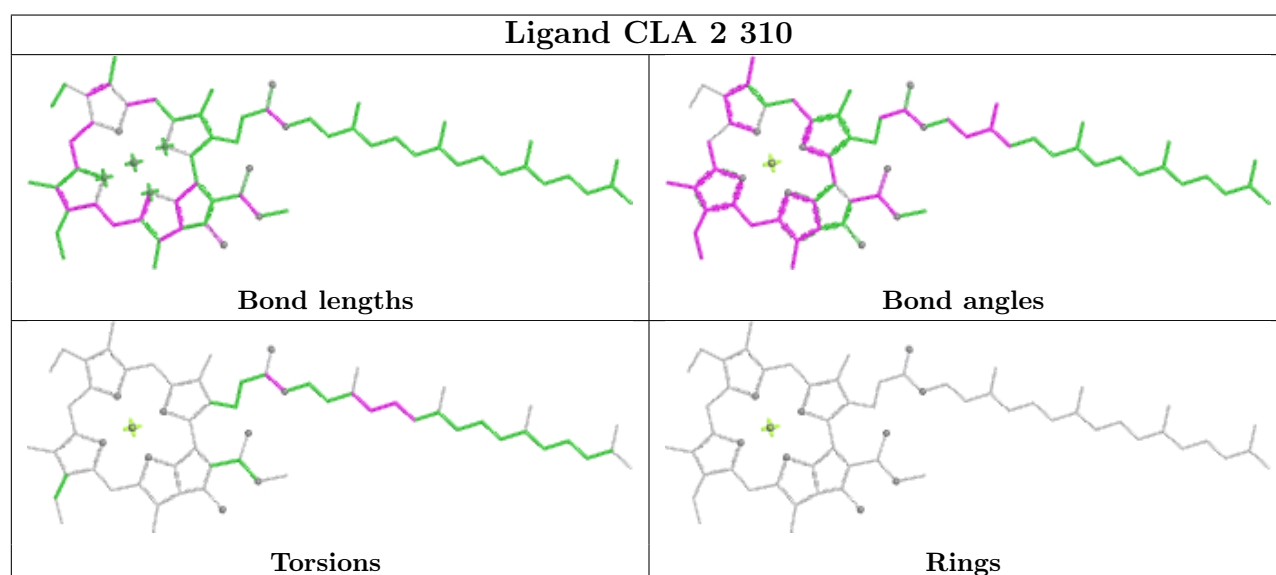
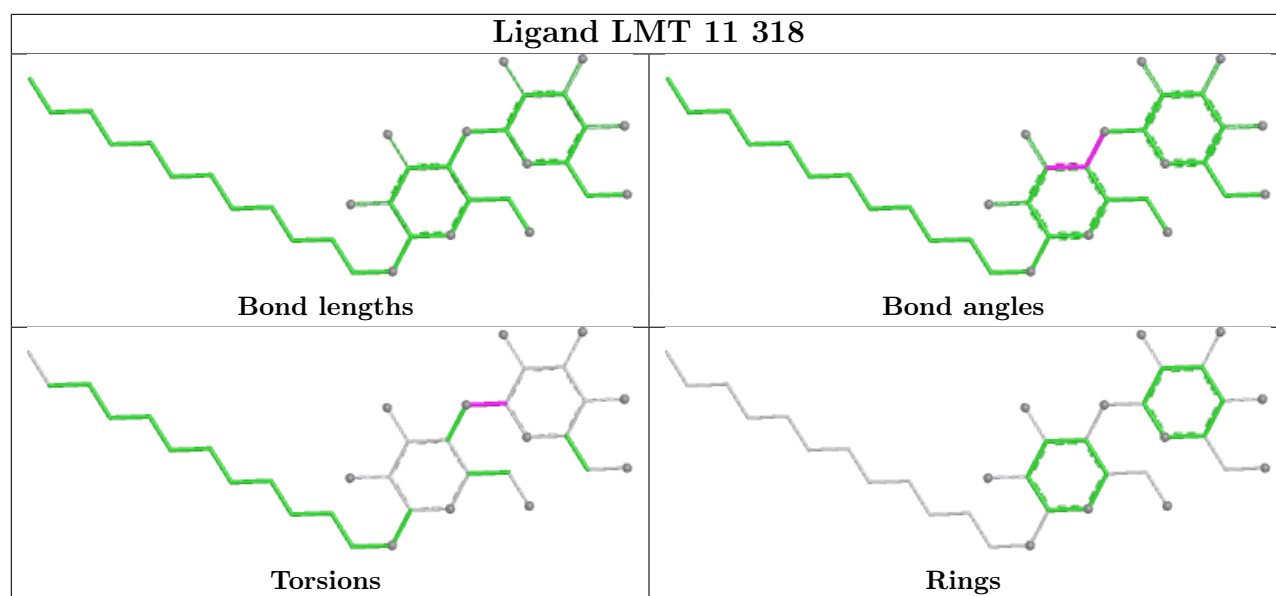


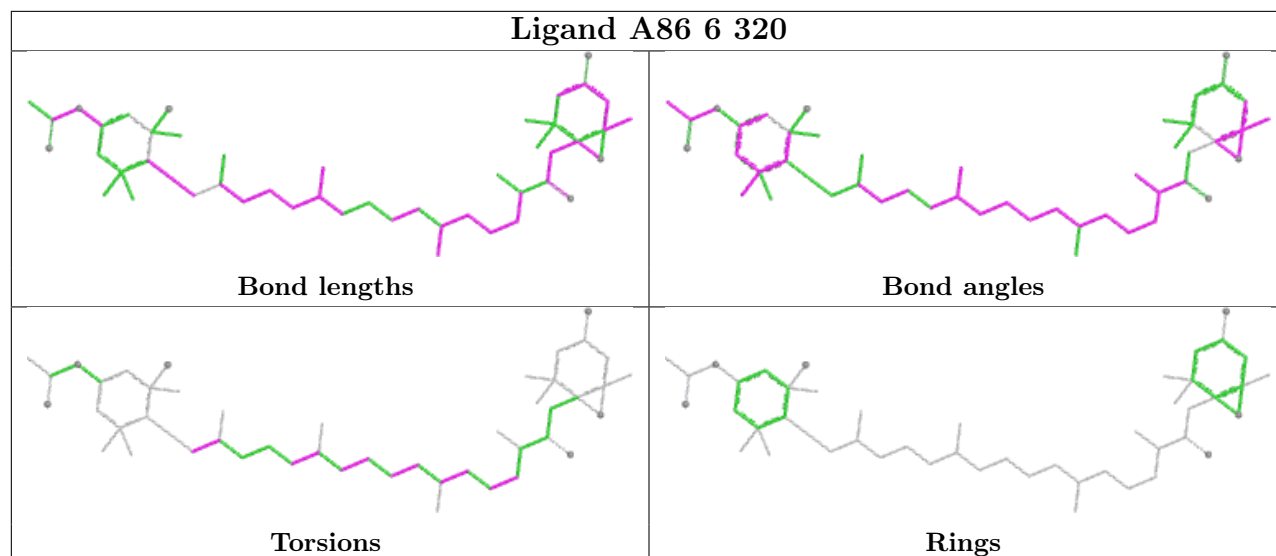
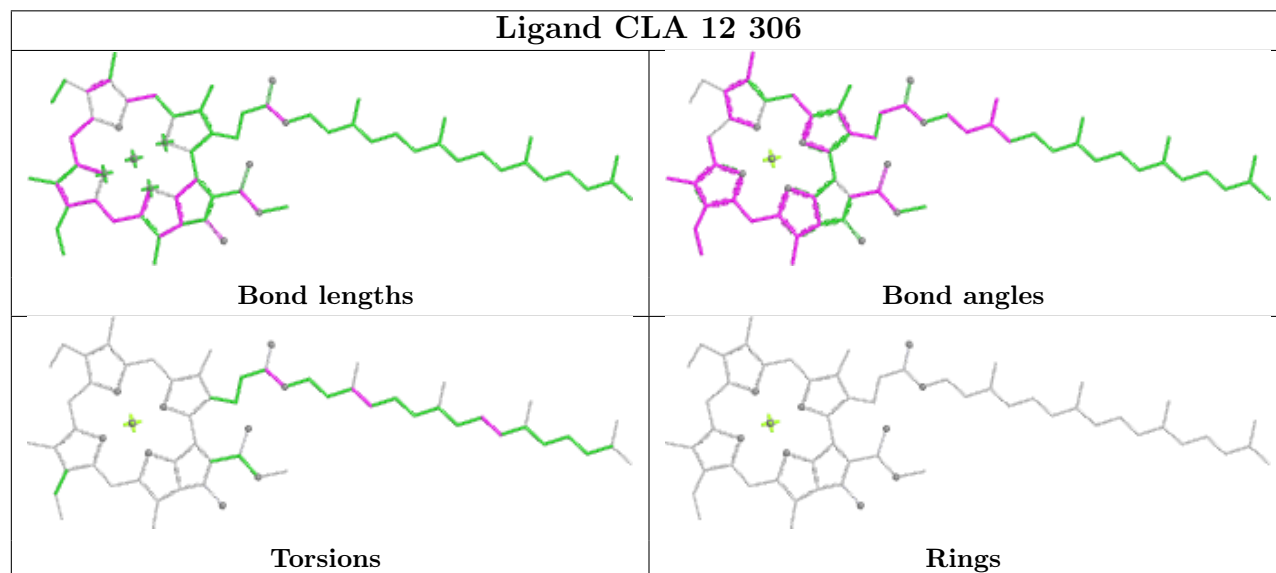
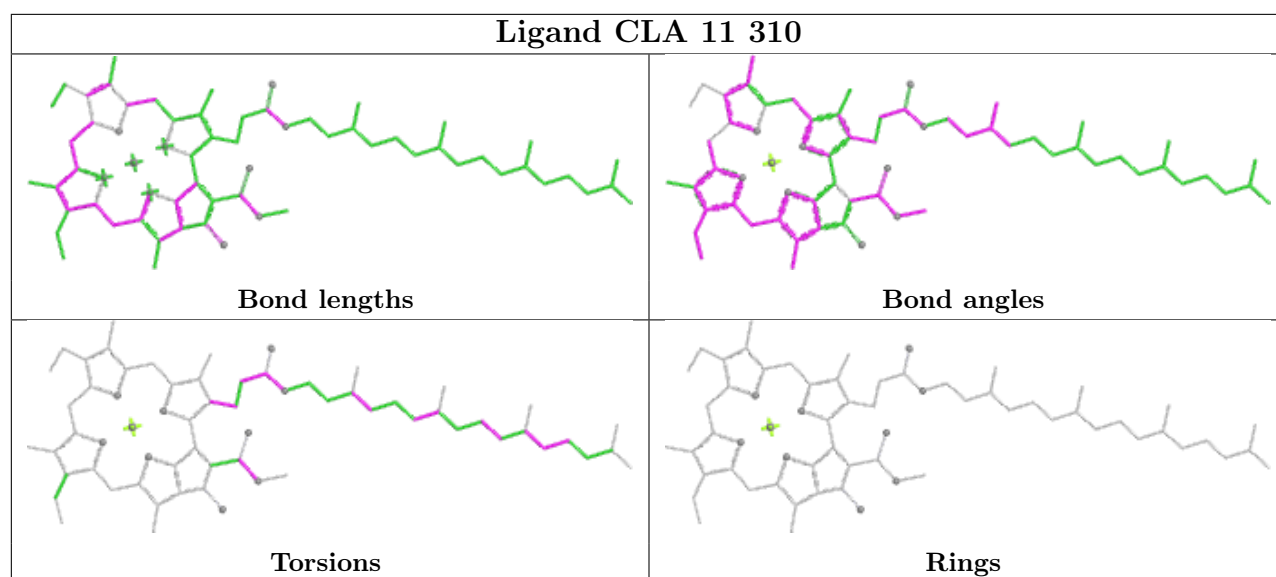
## Ligand DD6 8 317

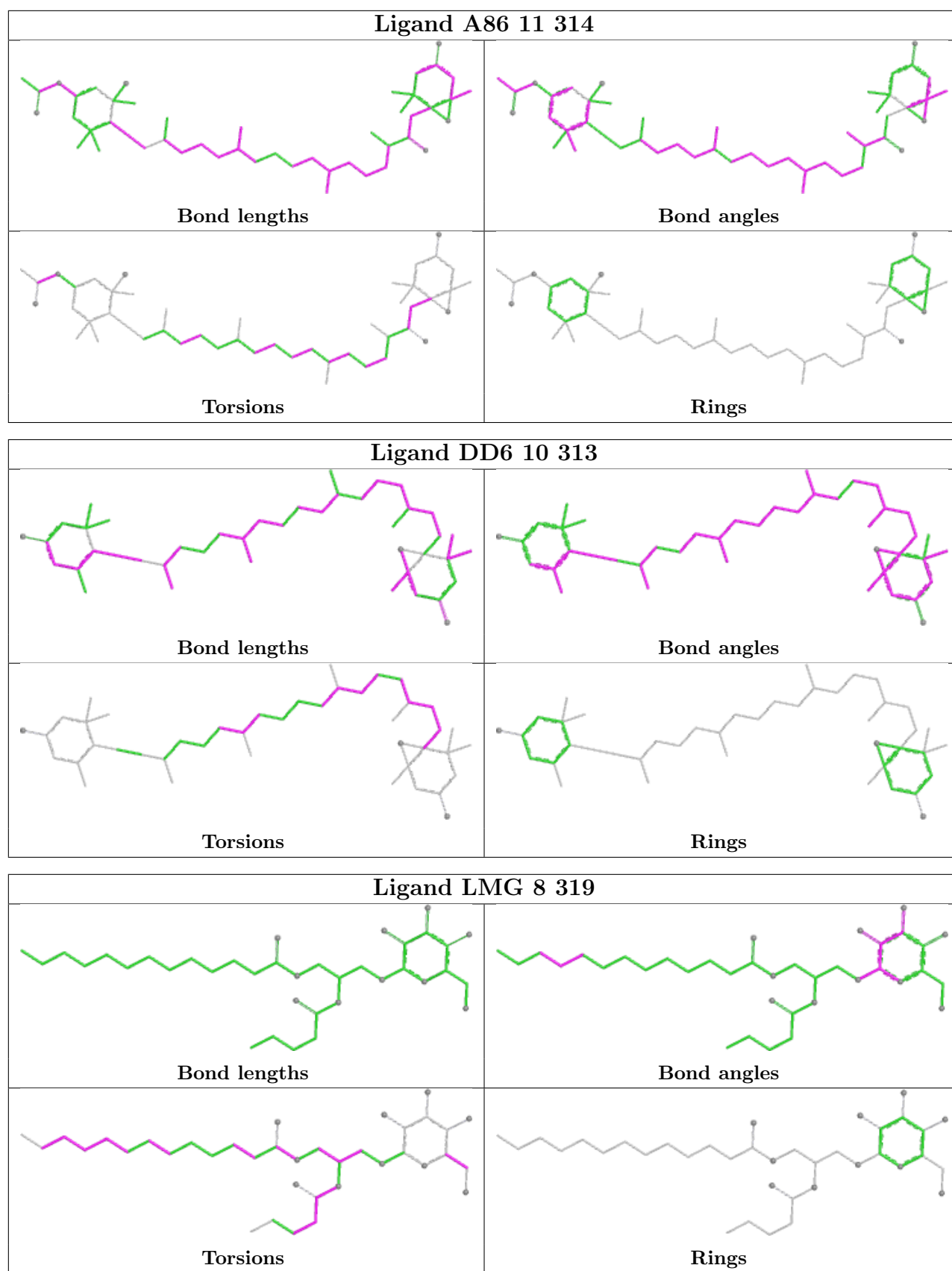


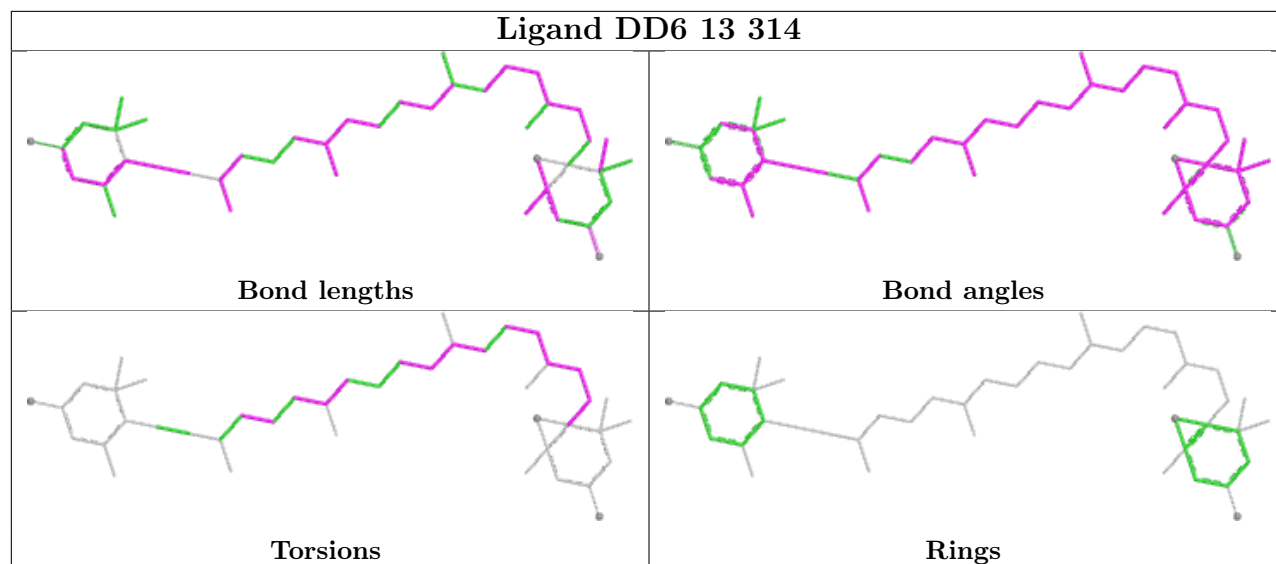
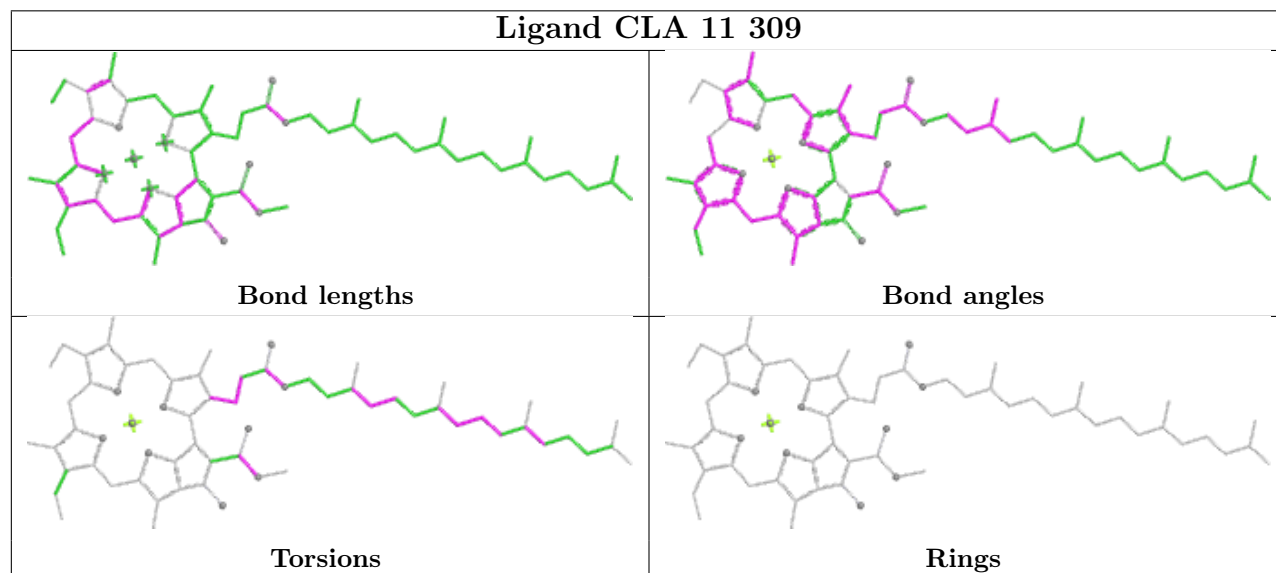
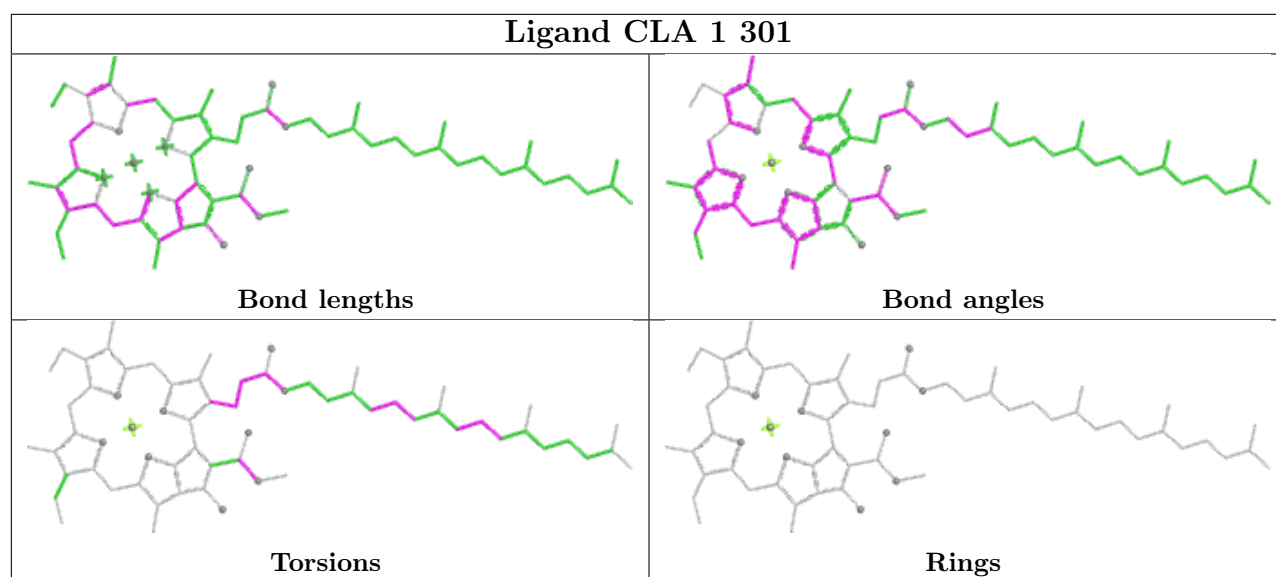


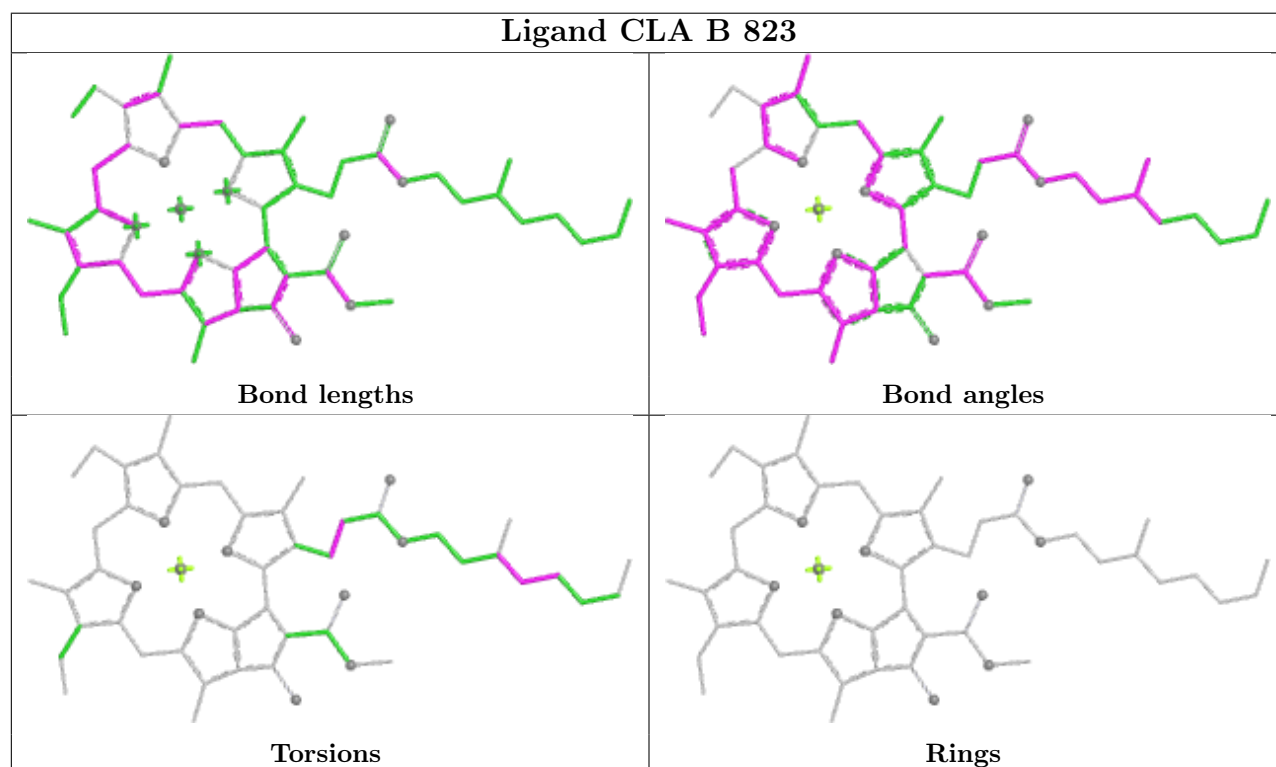
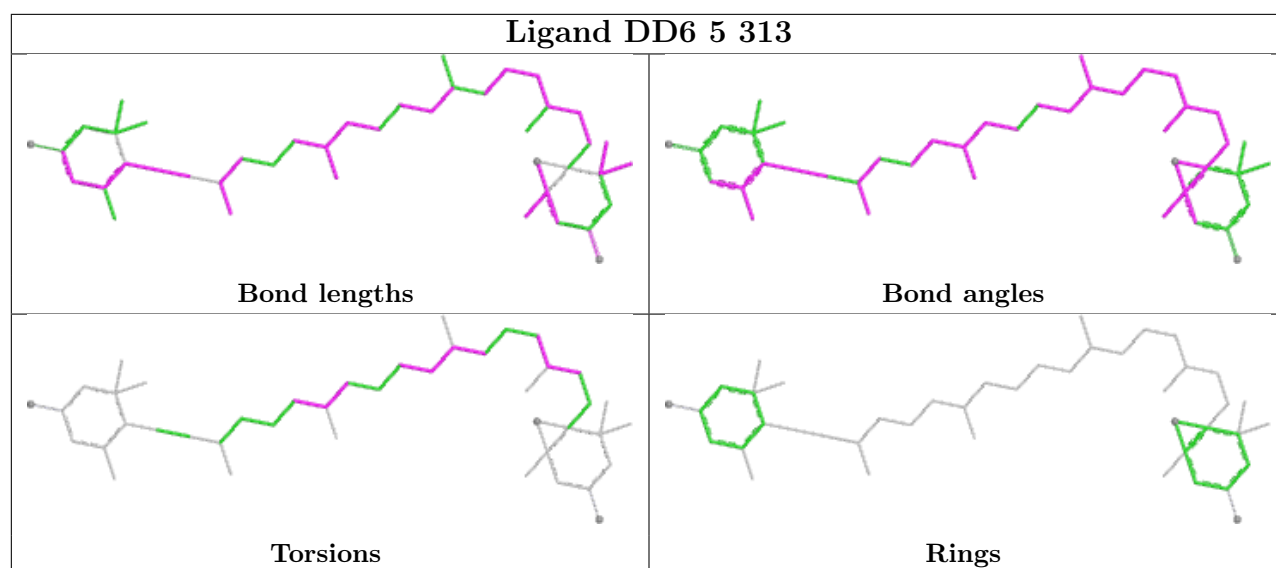




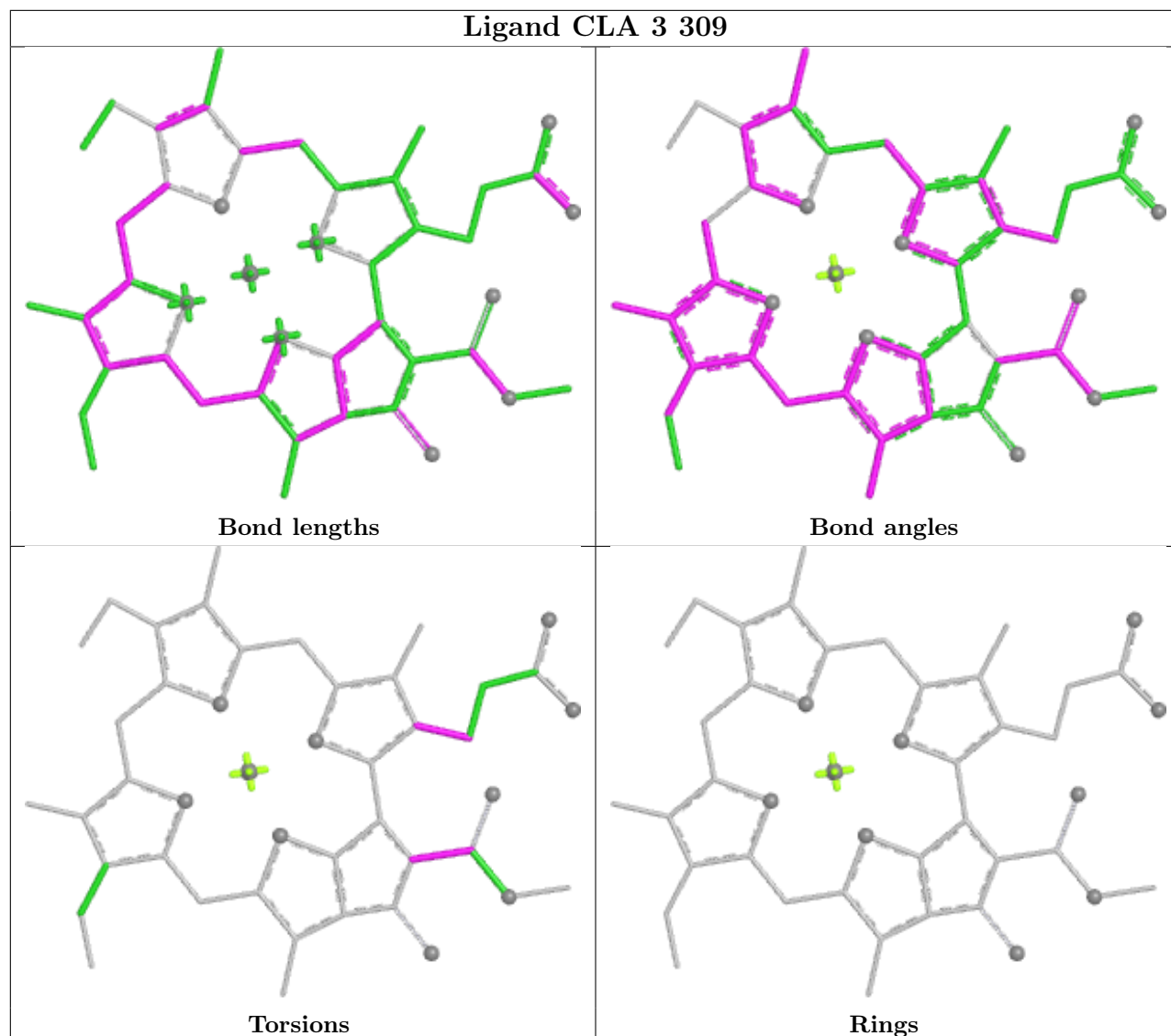


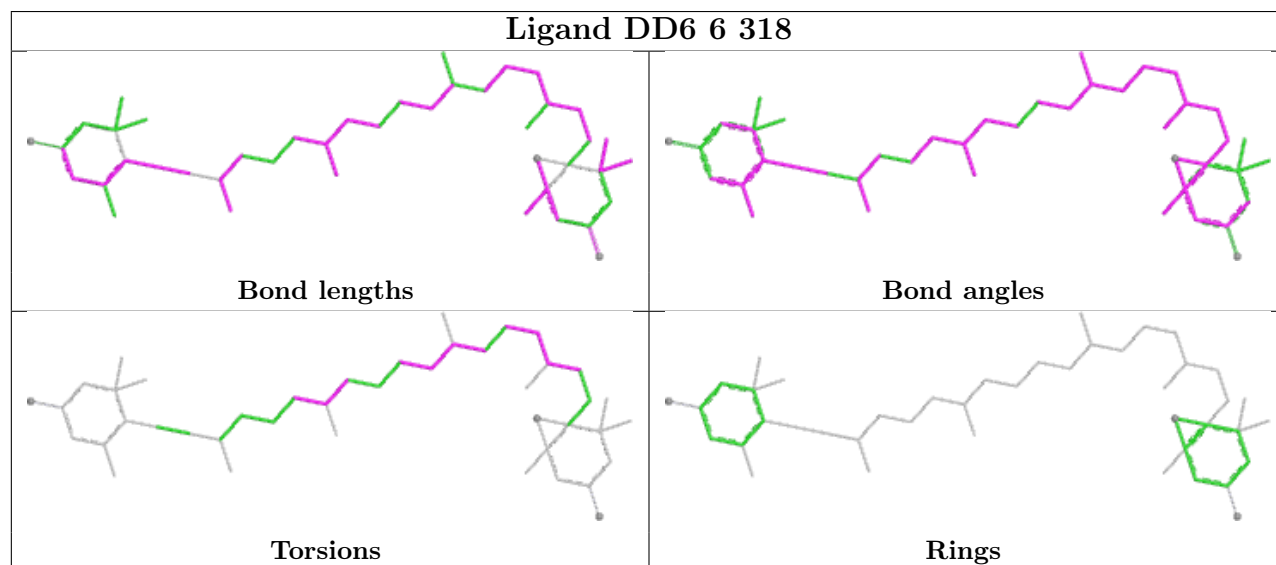
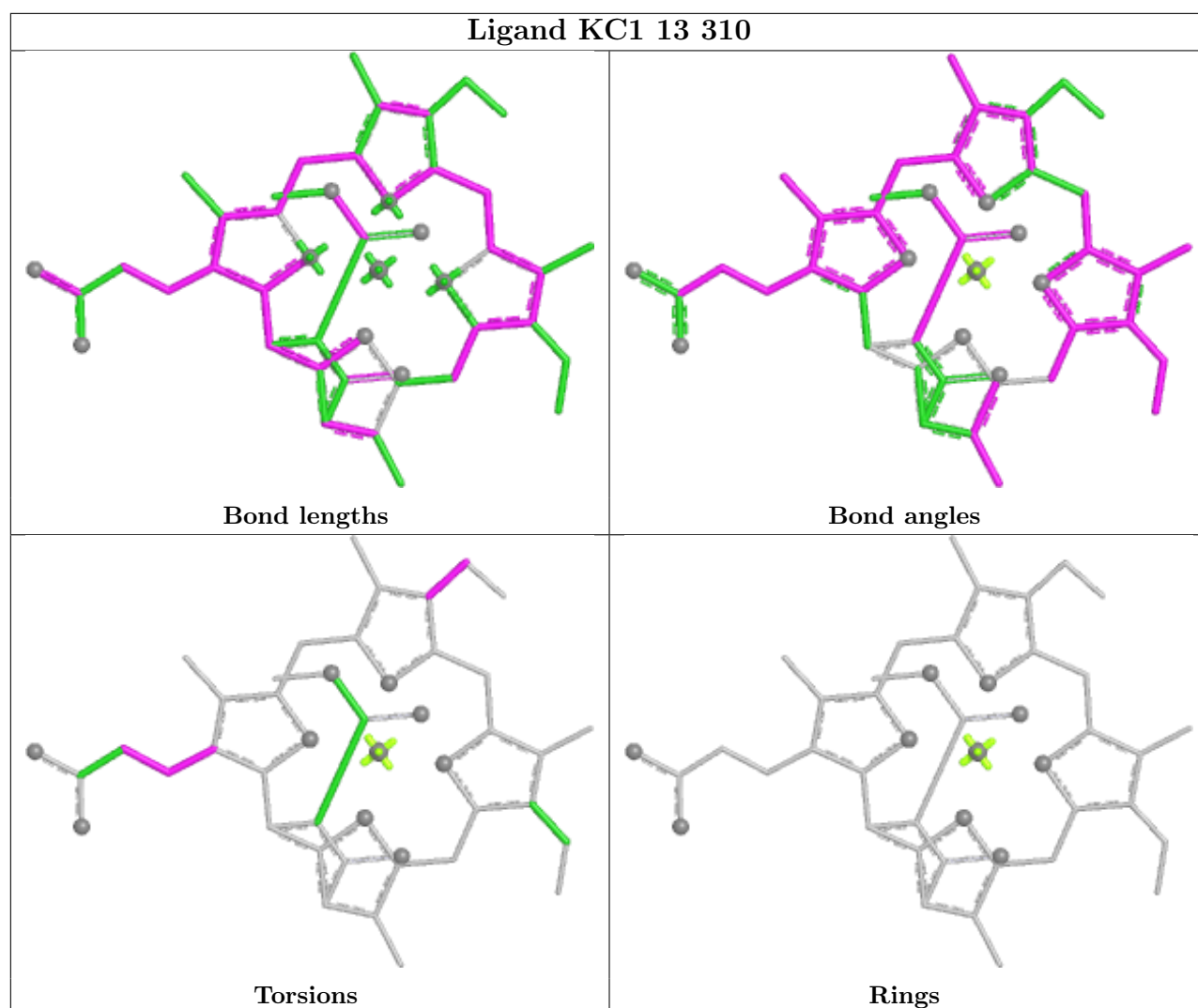


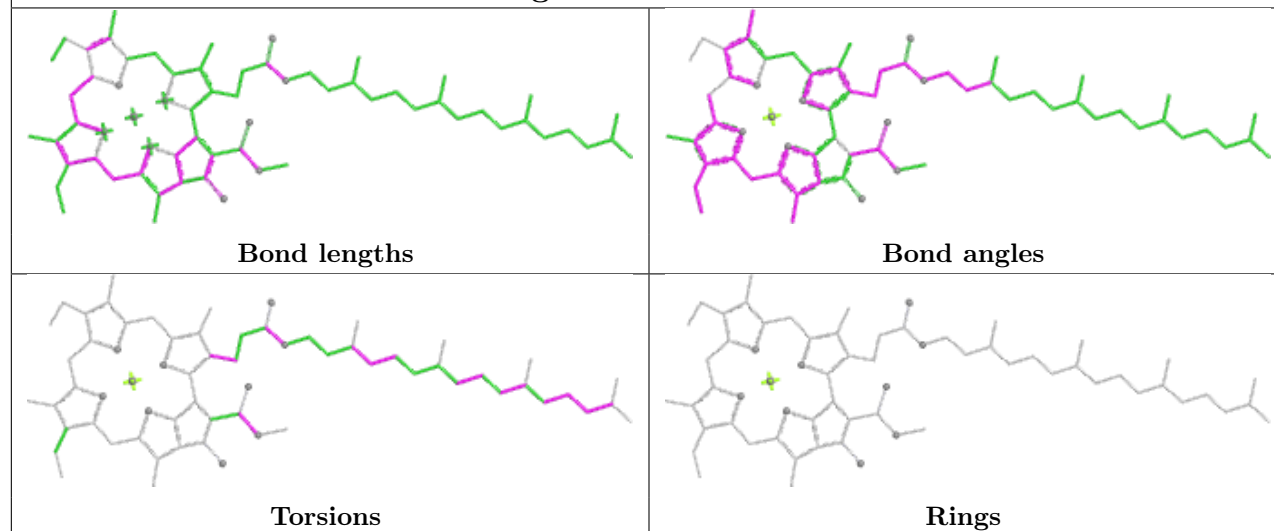
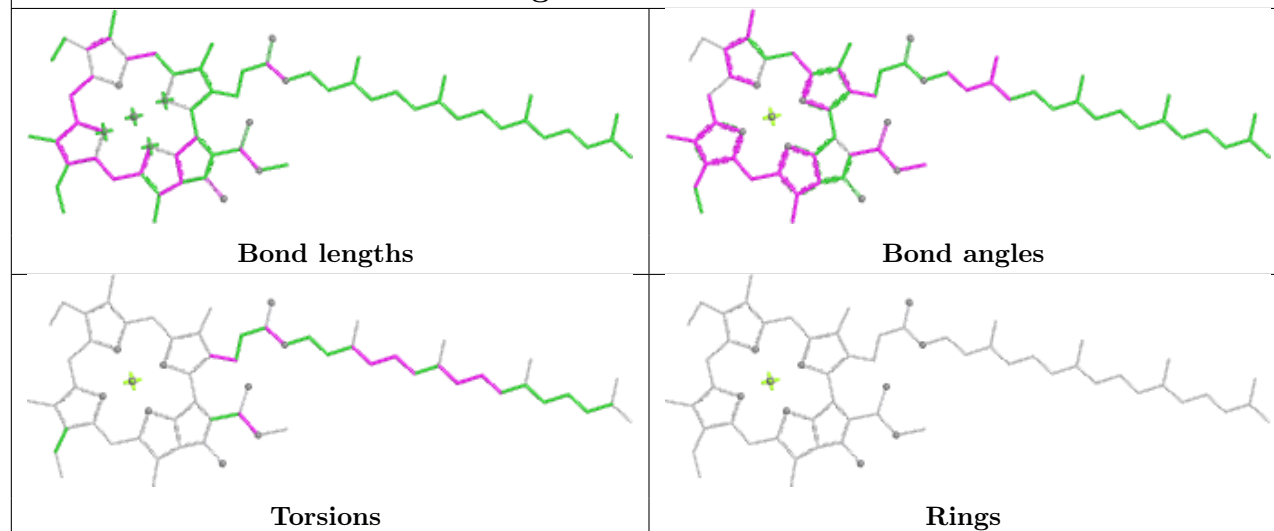


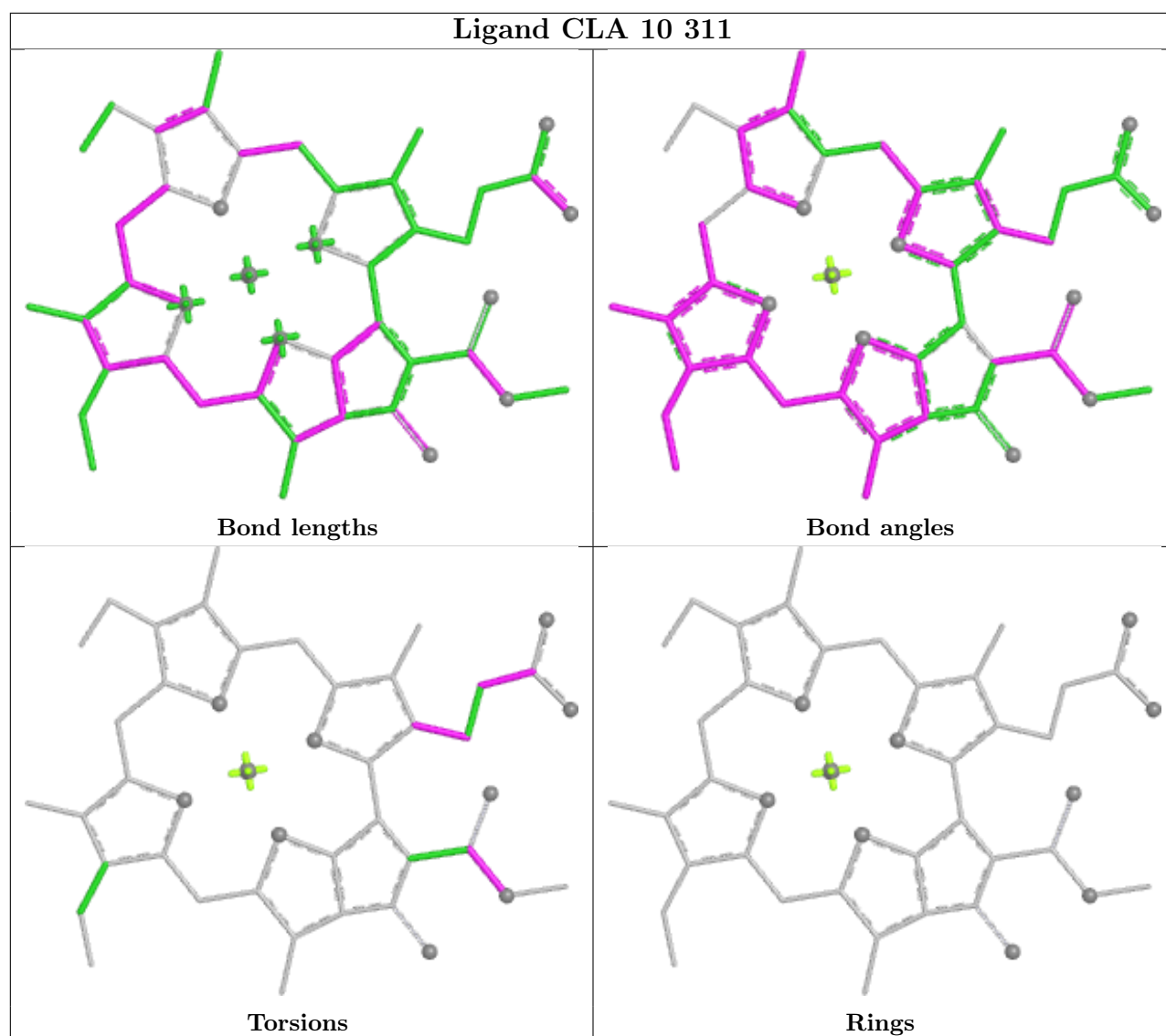


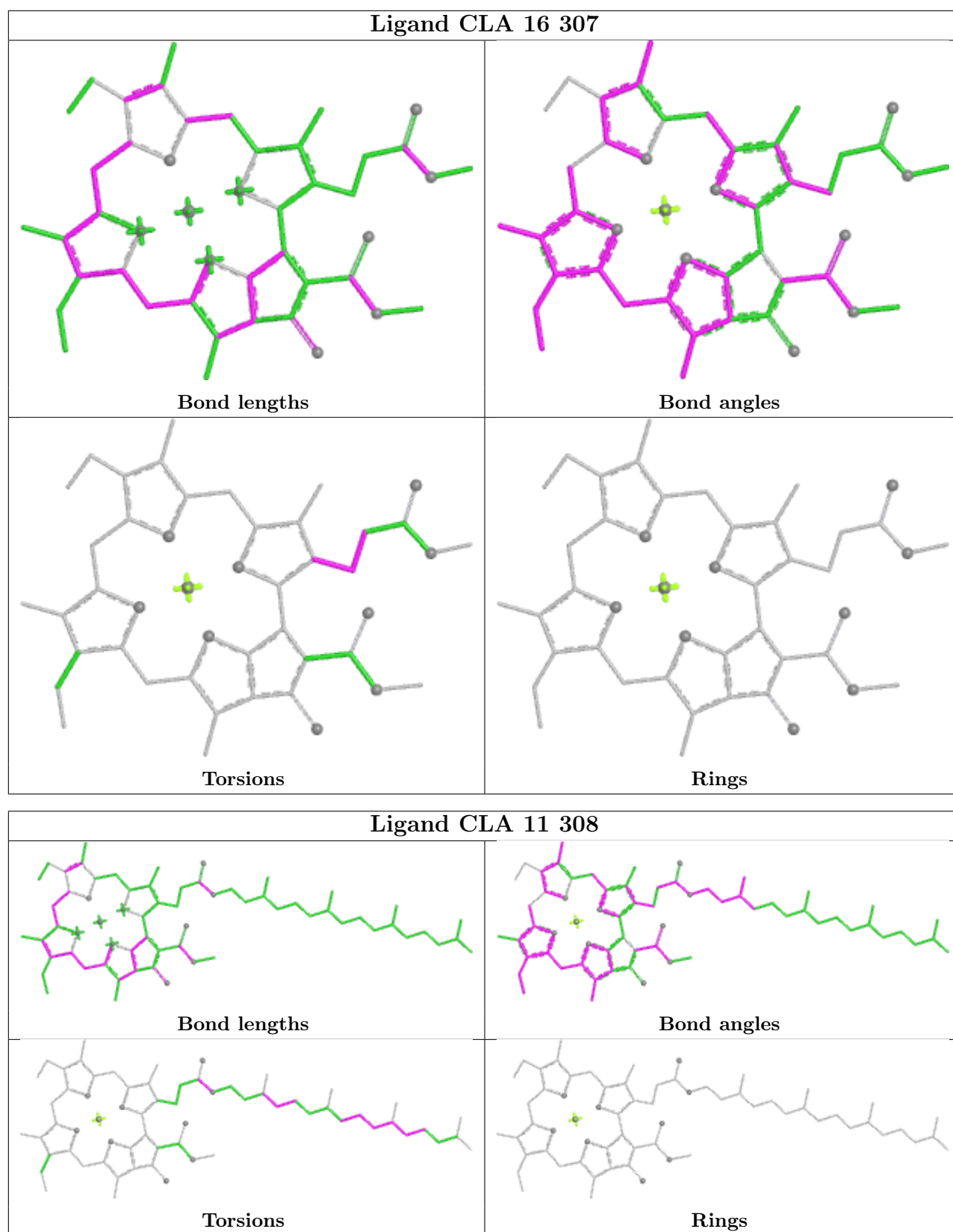
## Ligand CLA 3 309



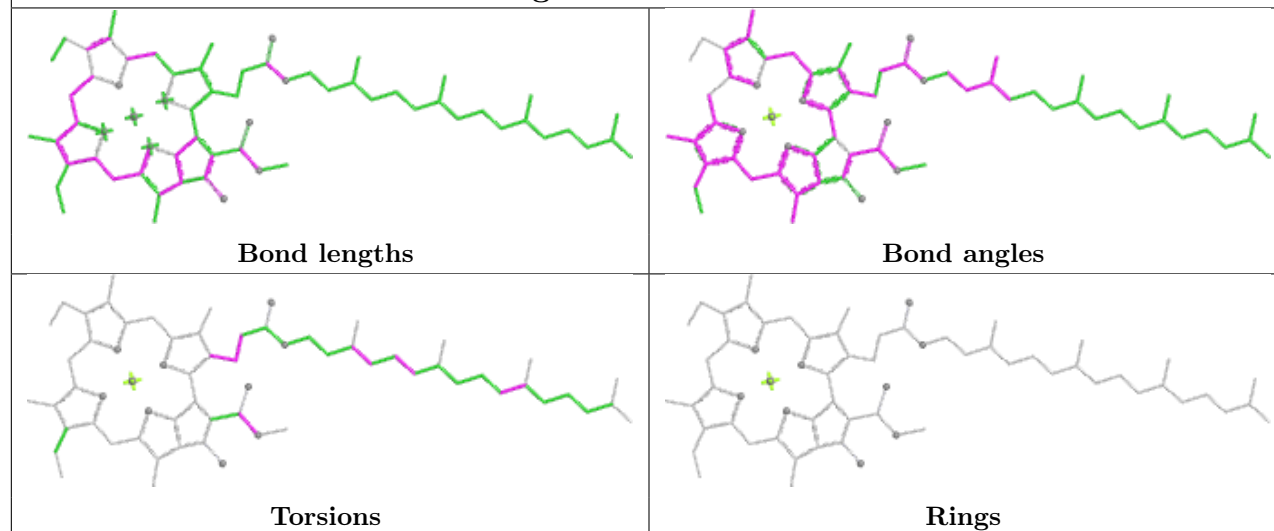


**Ligand CLA A 820****Ligand CLA A 833**

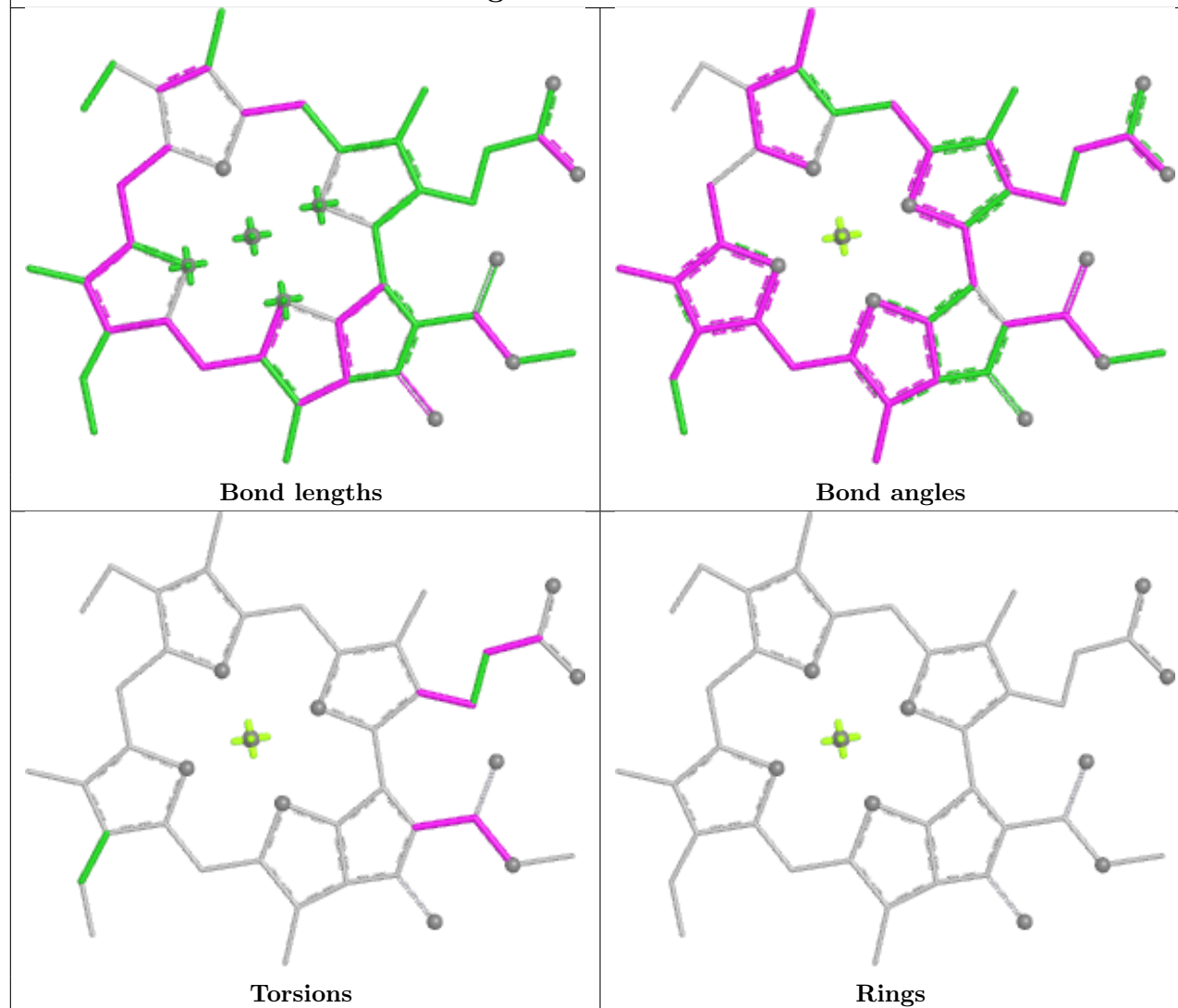


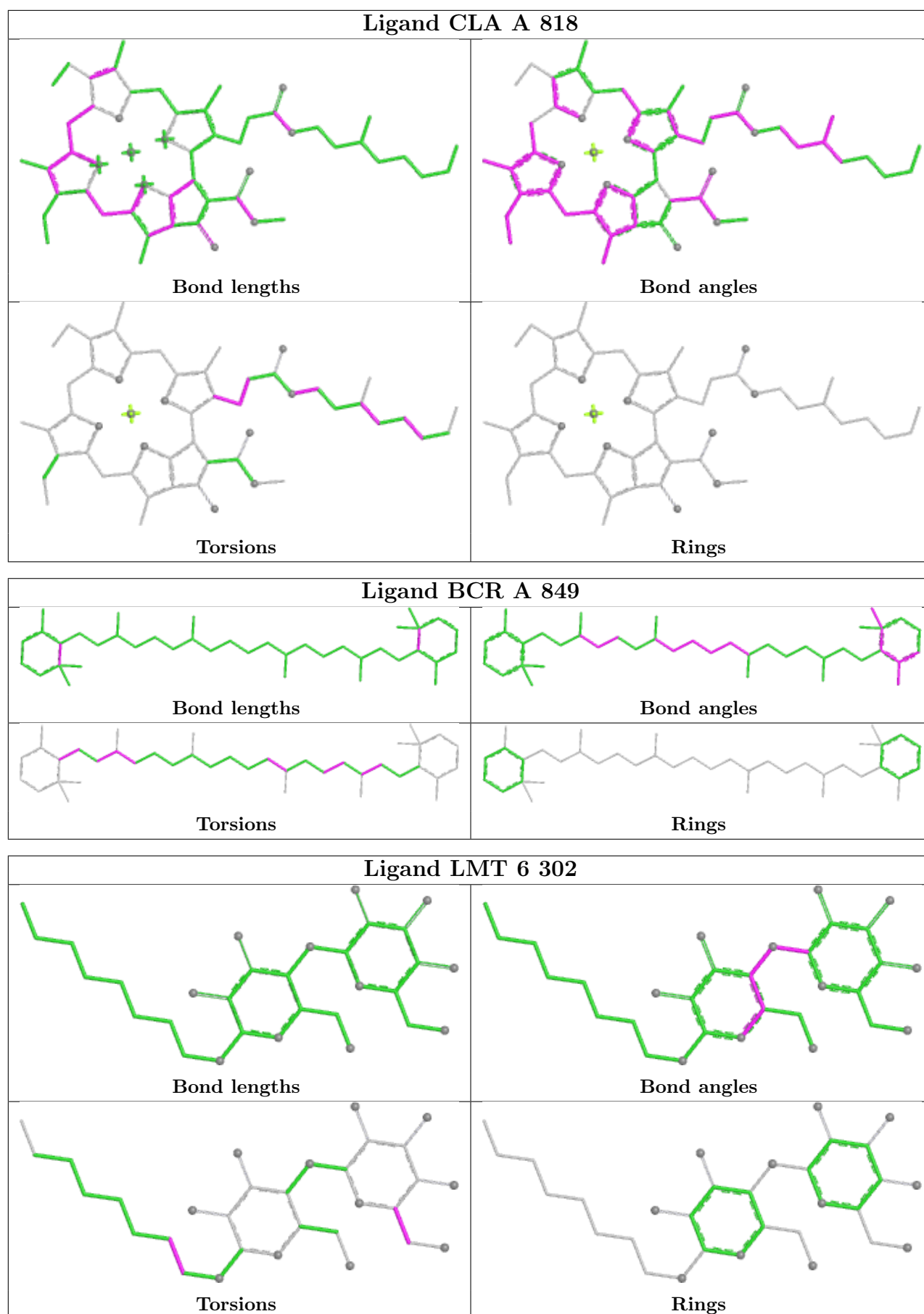


## Ligand CLA B 802

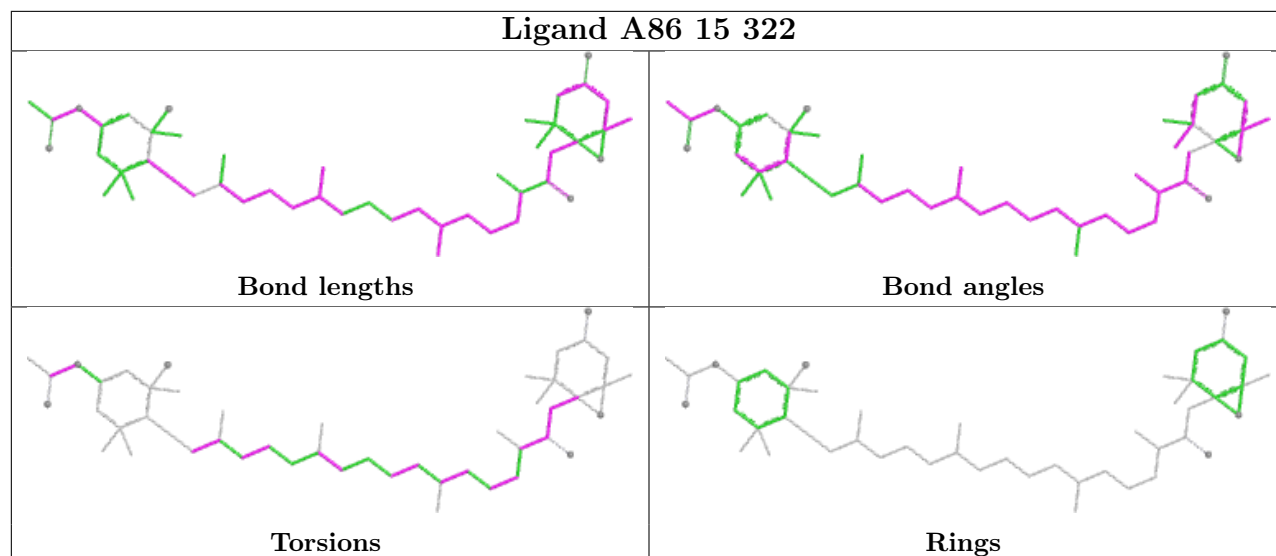


## Ligand CLA 15 305

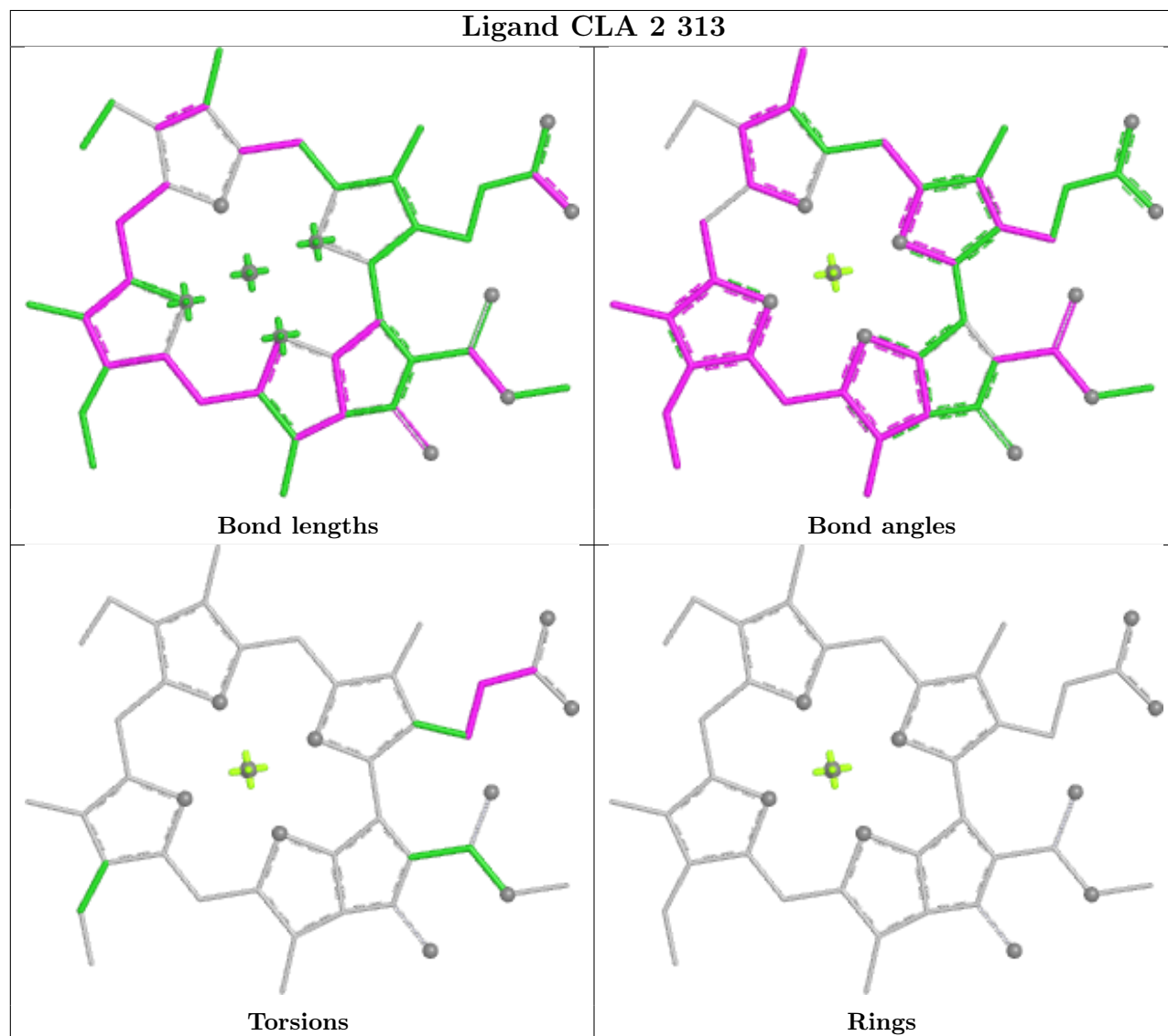


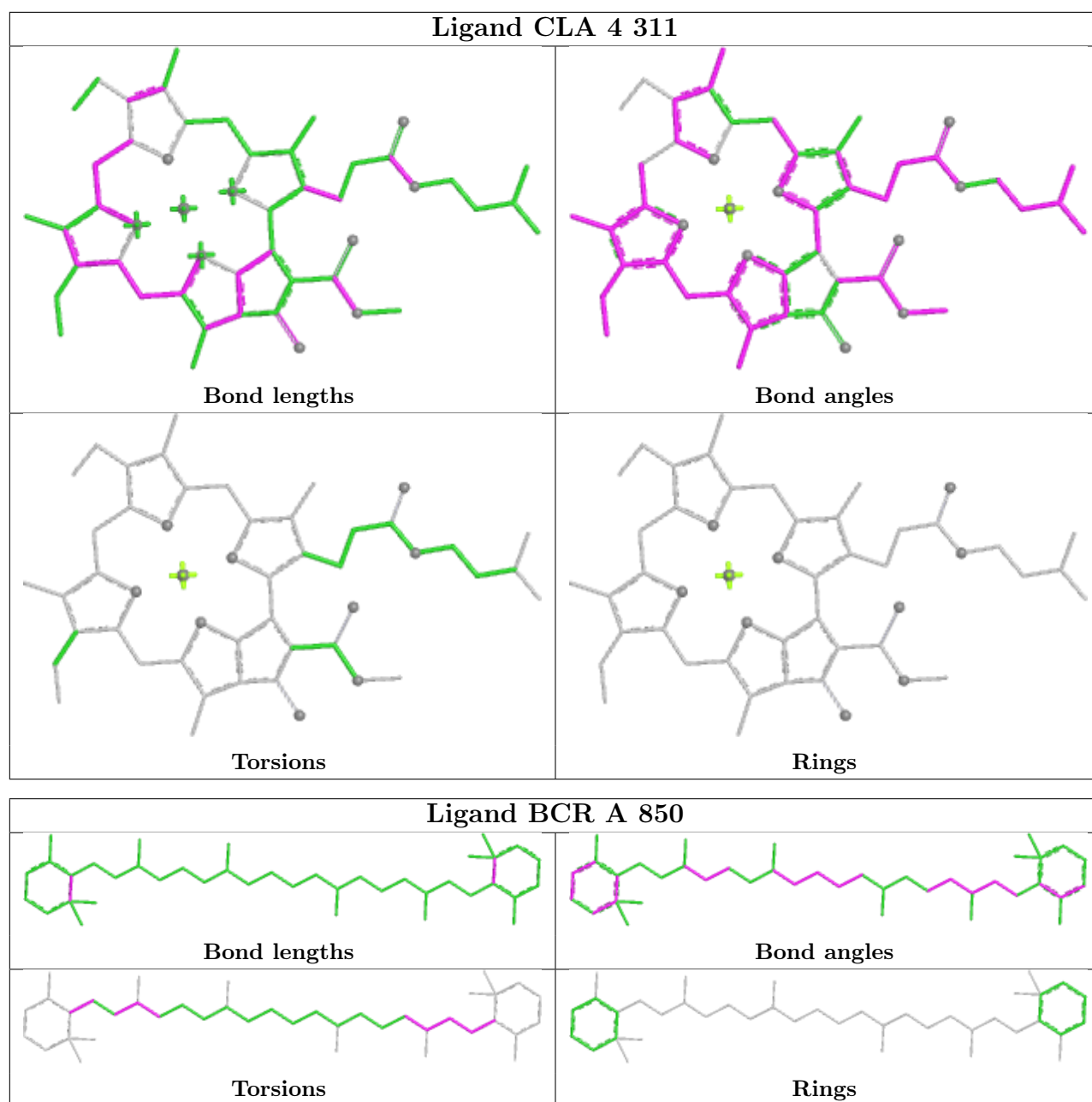


## Ligand A86 15 322

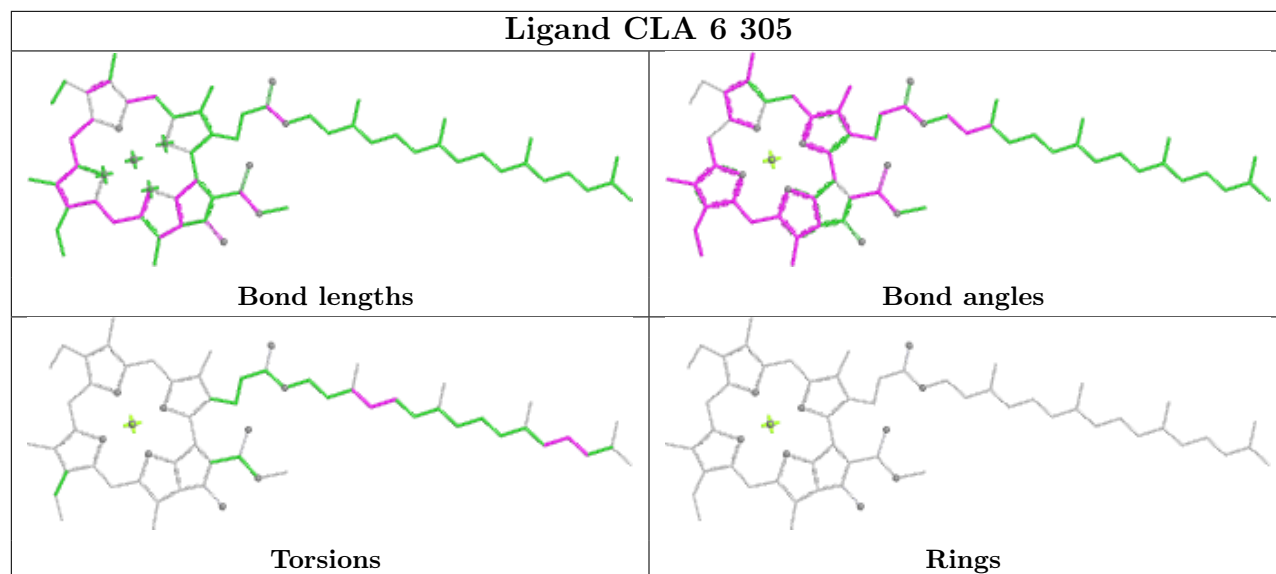


## Ligand CLA 2 313

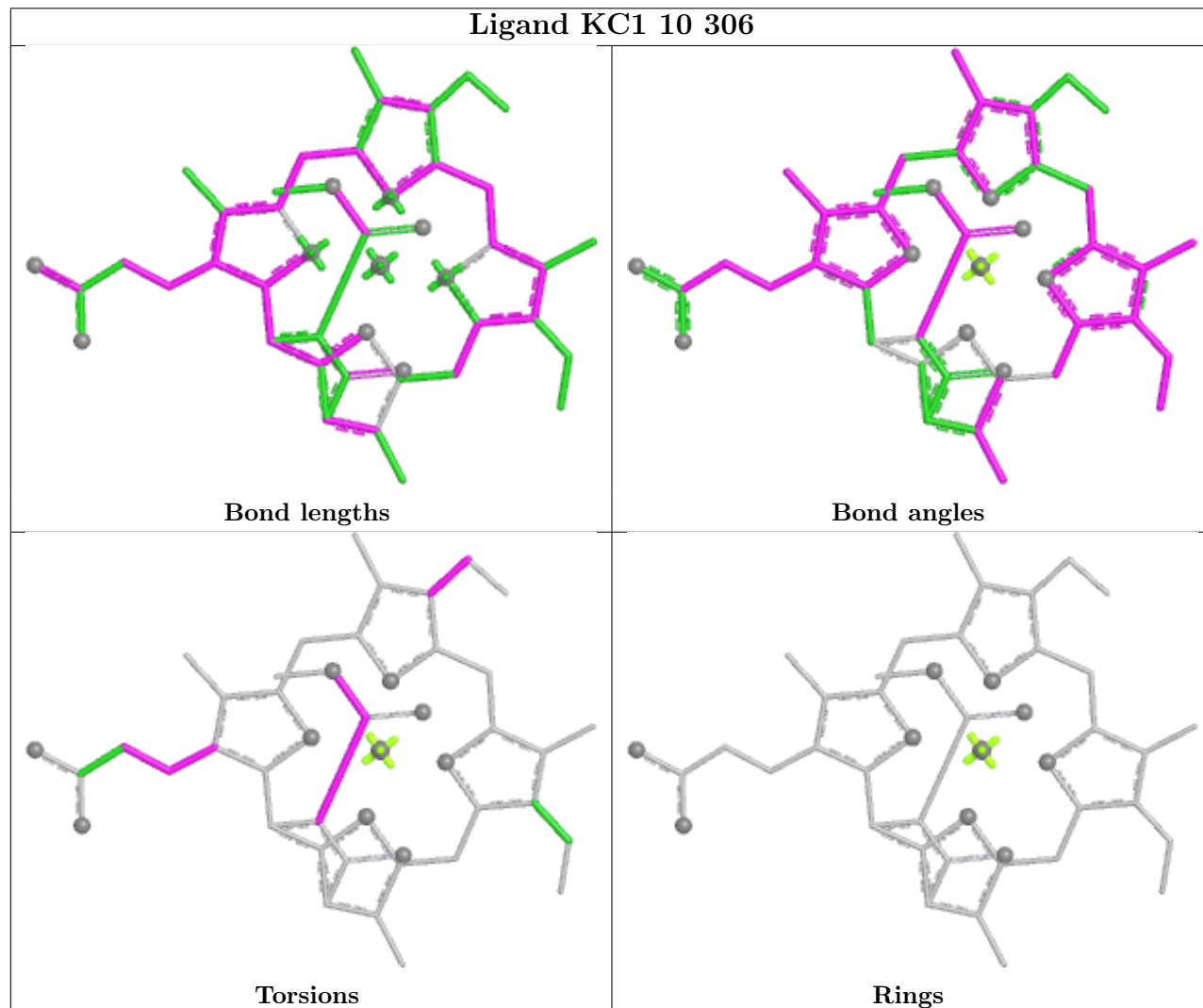


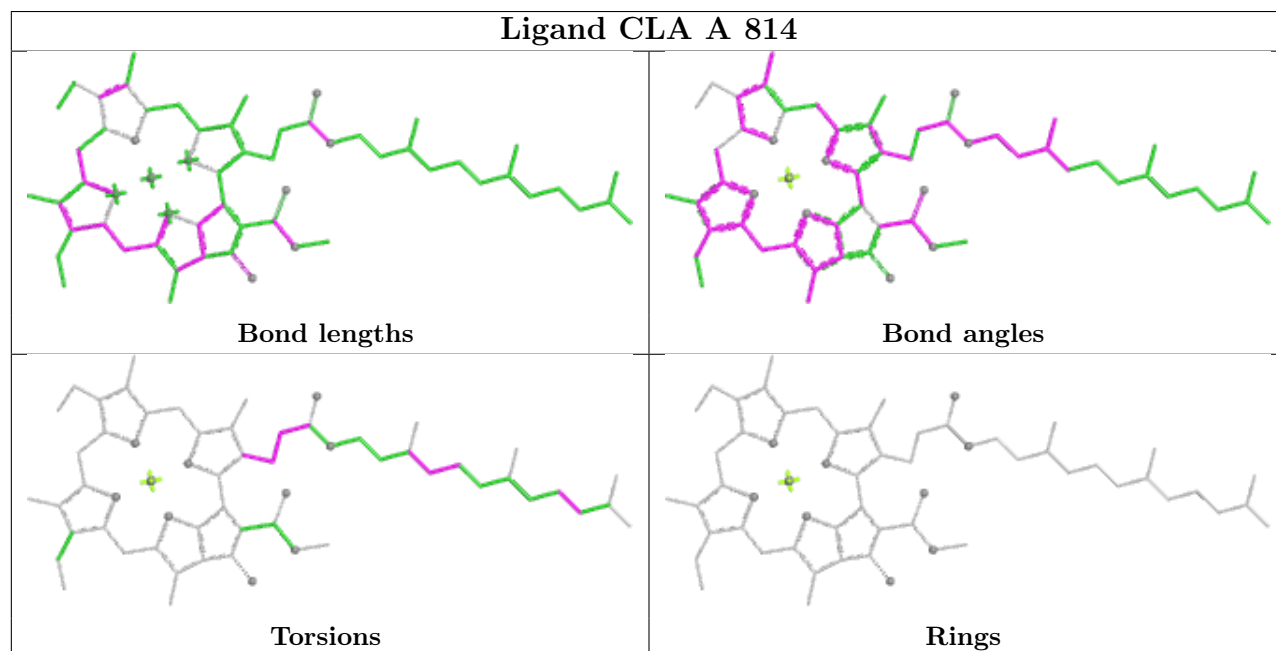
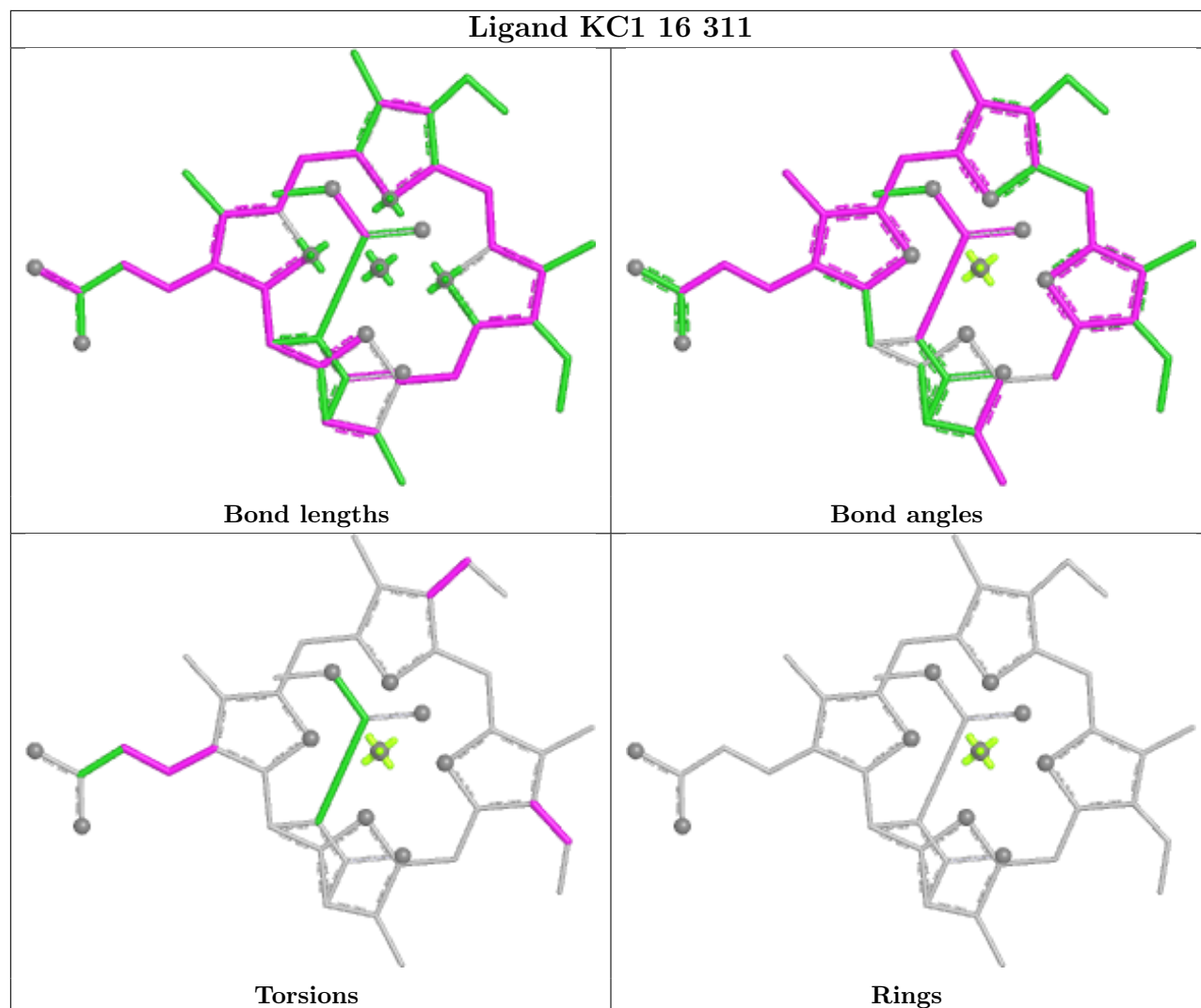


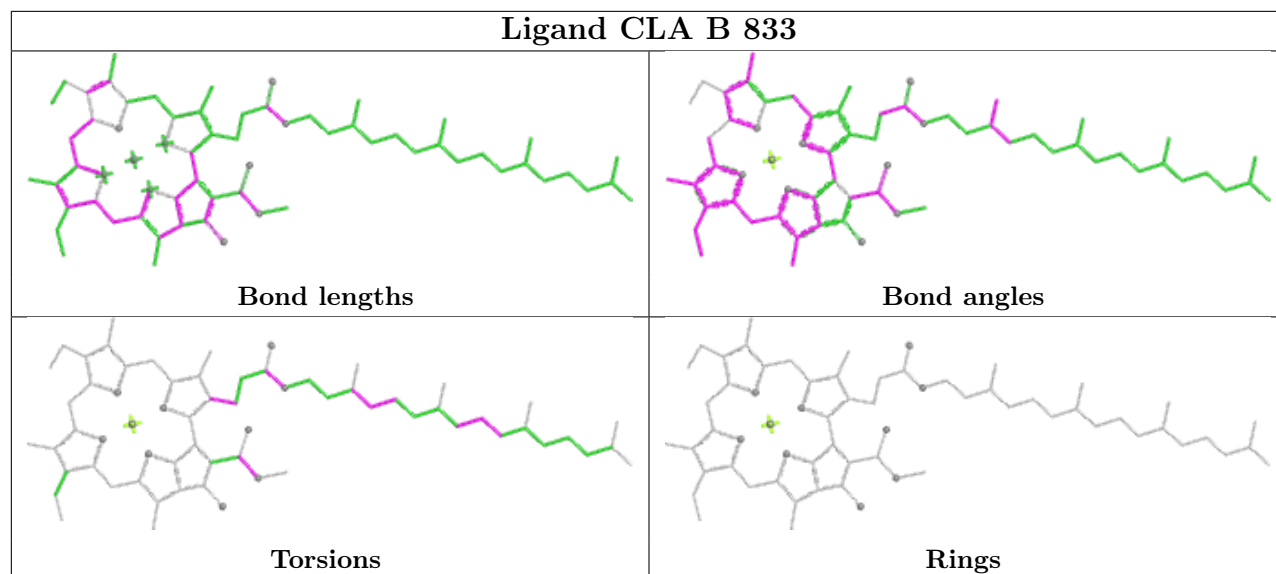
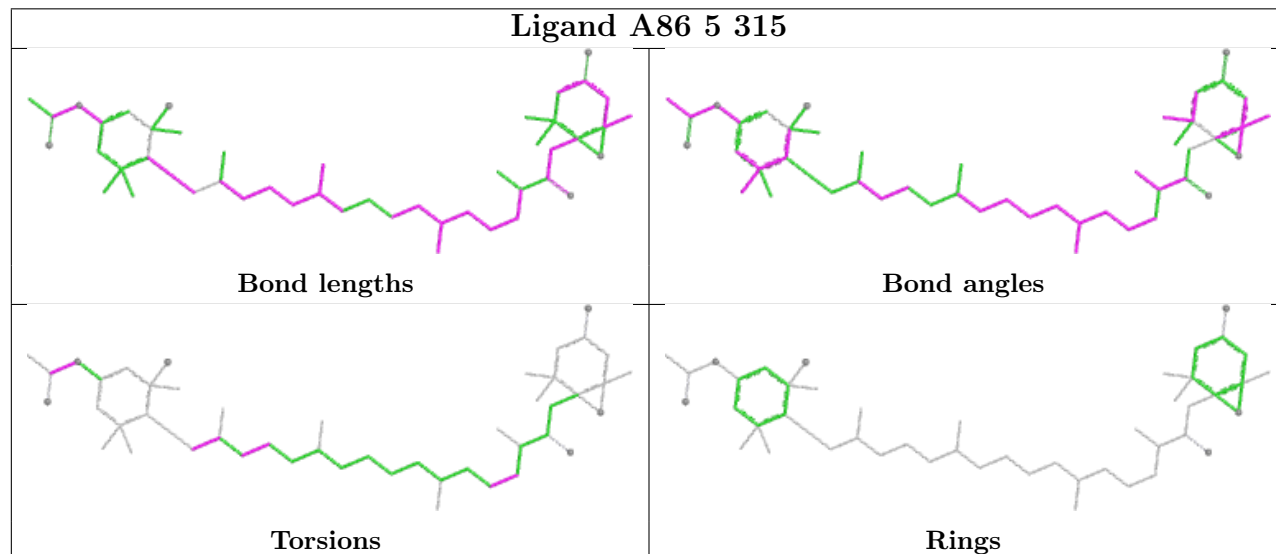
## Ligand CLA 6 305

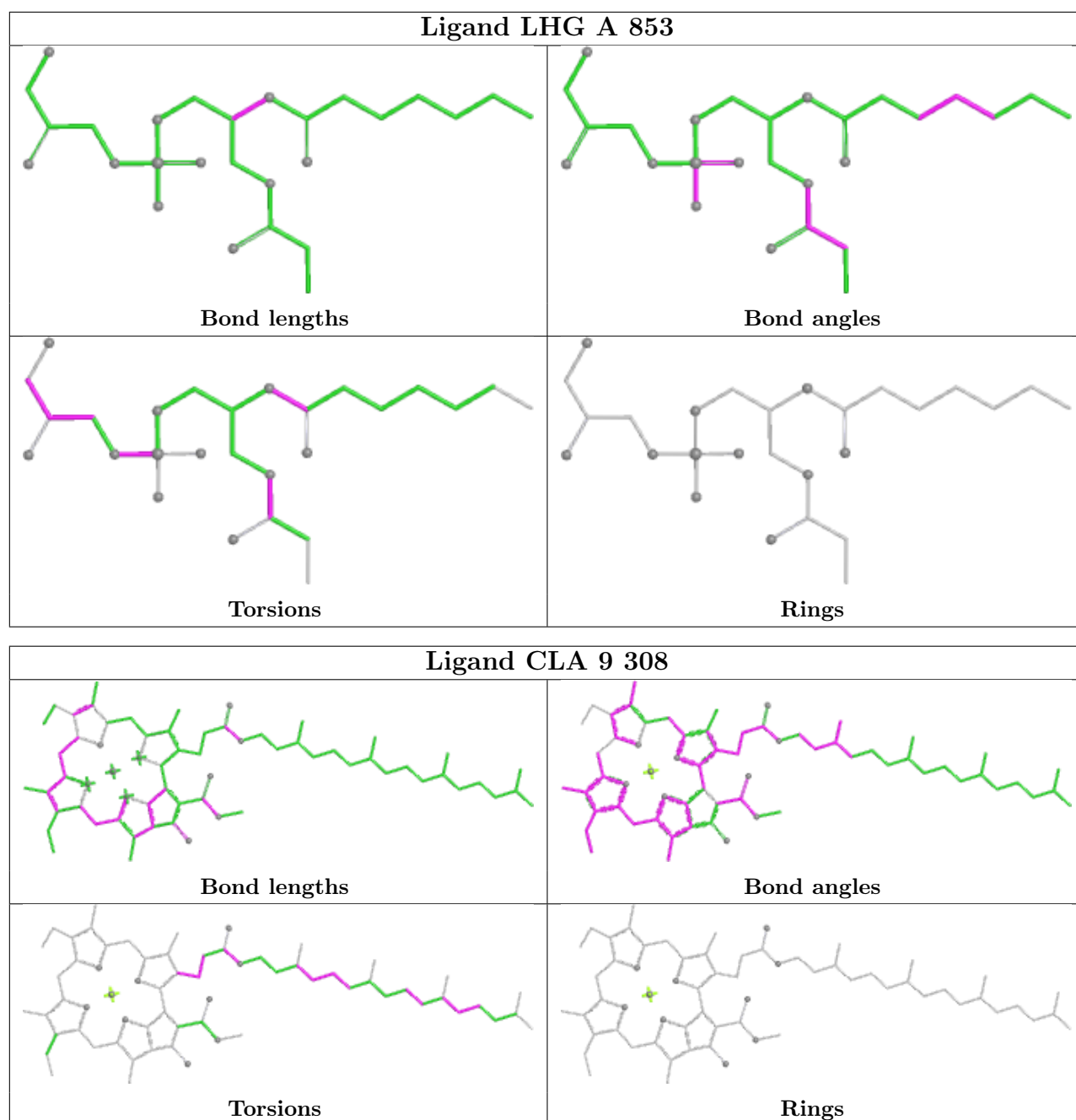


## Ligand KC1 10 306

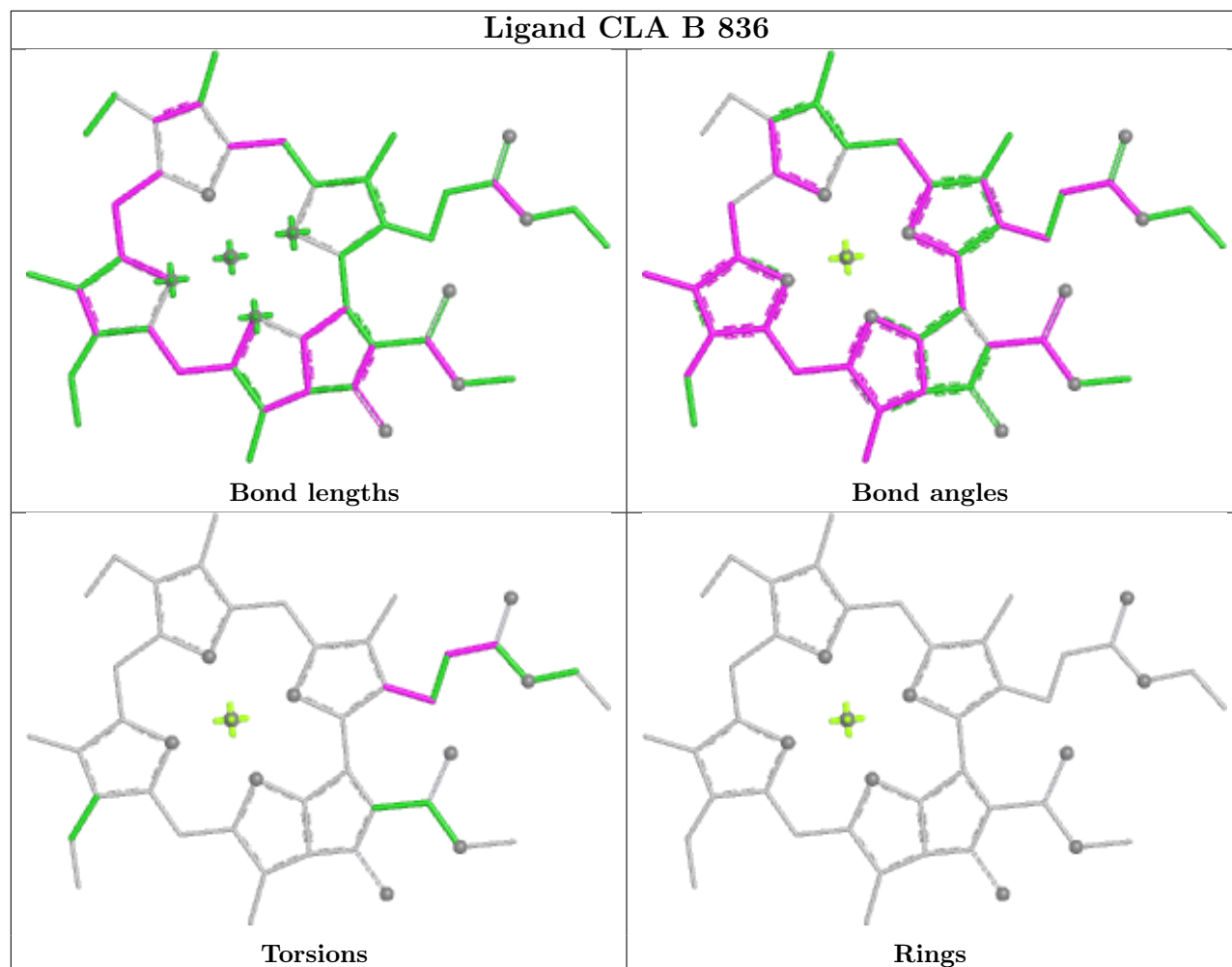


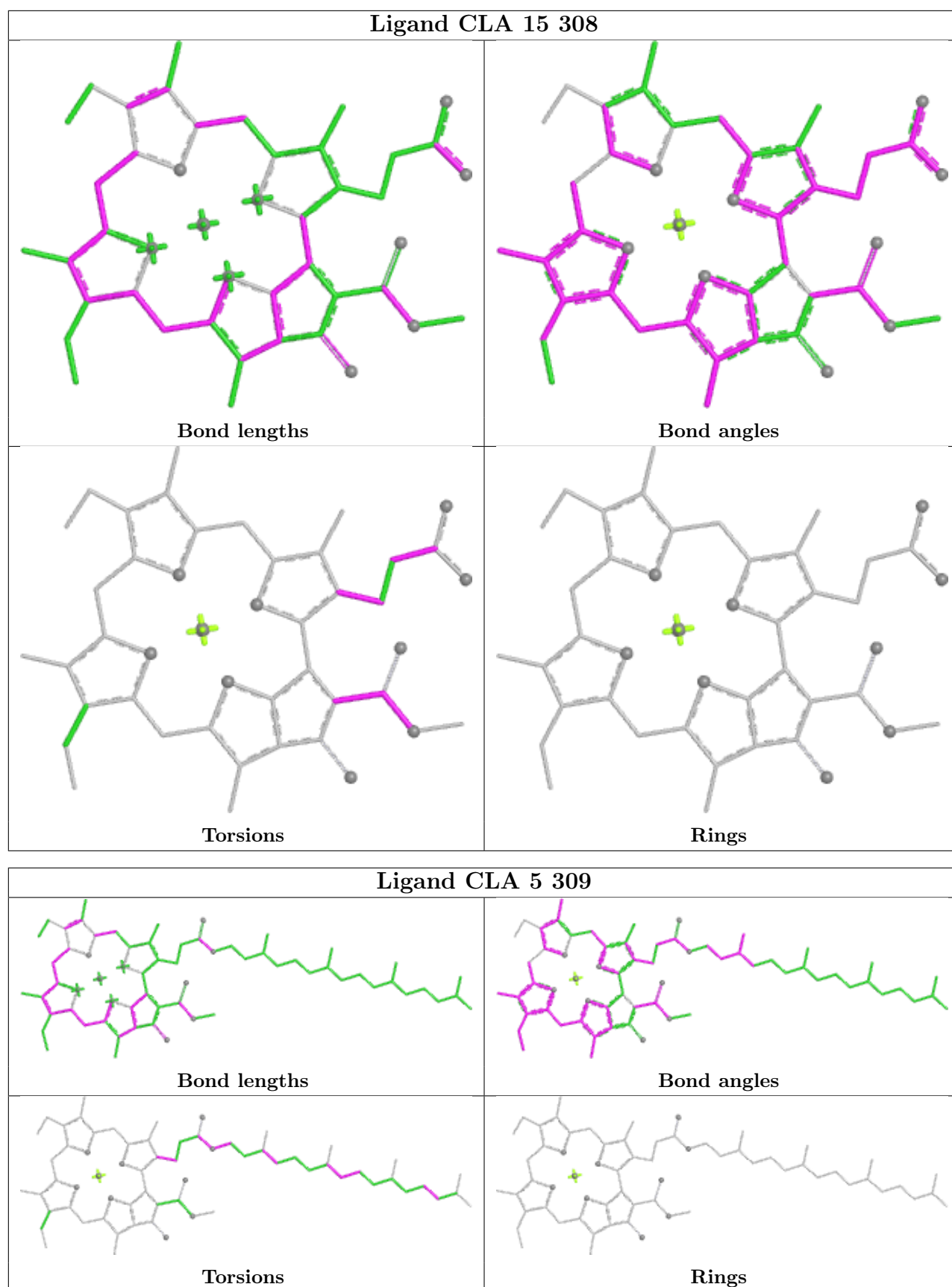


**Ligand CLA B 833****Ligand A86 5 315**

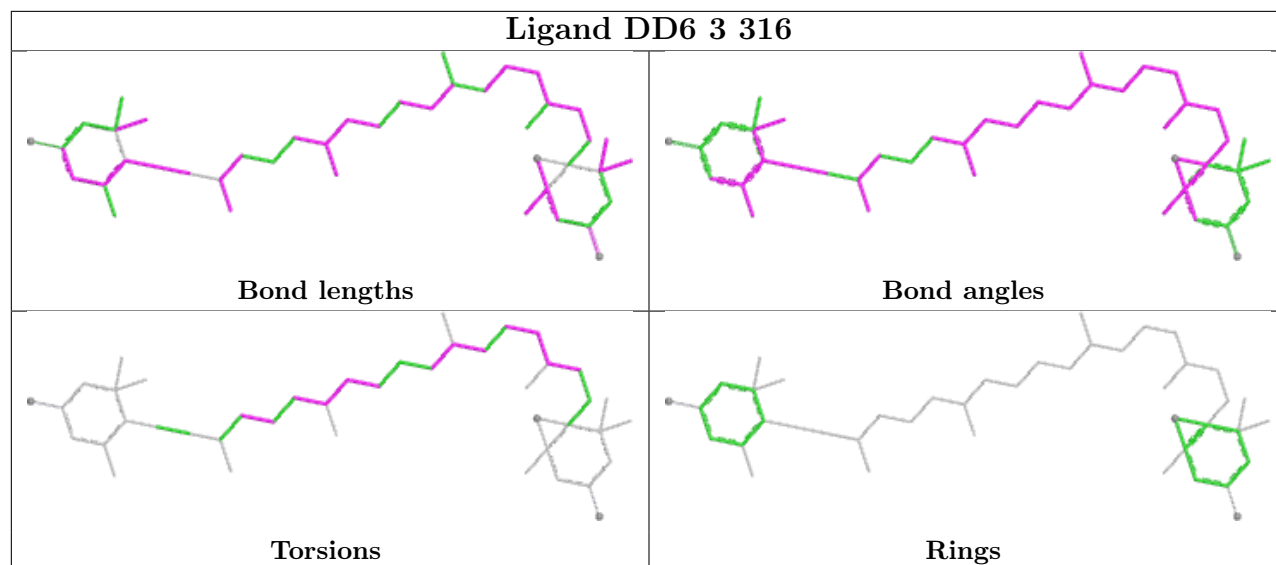


## Ligand CLA B 836

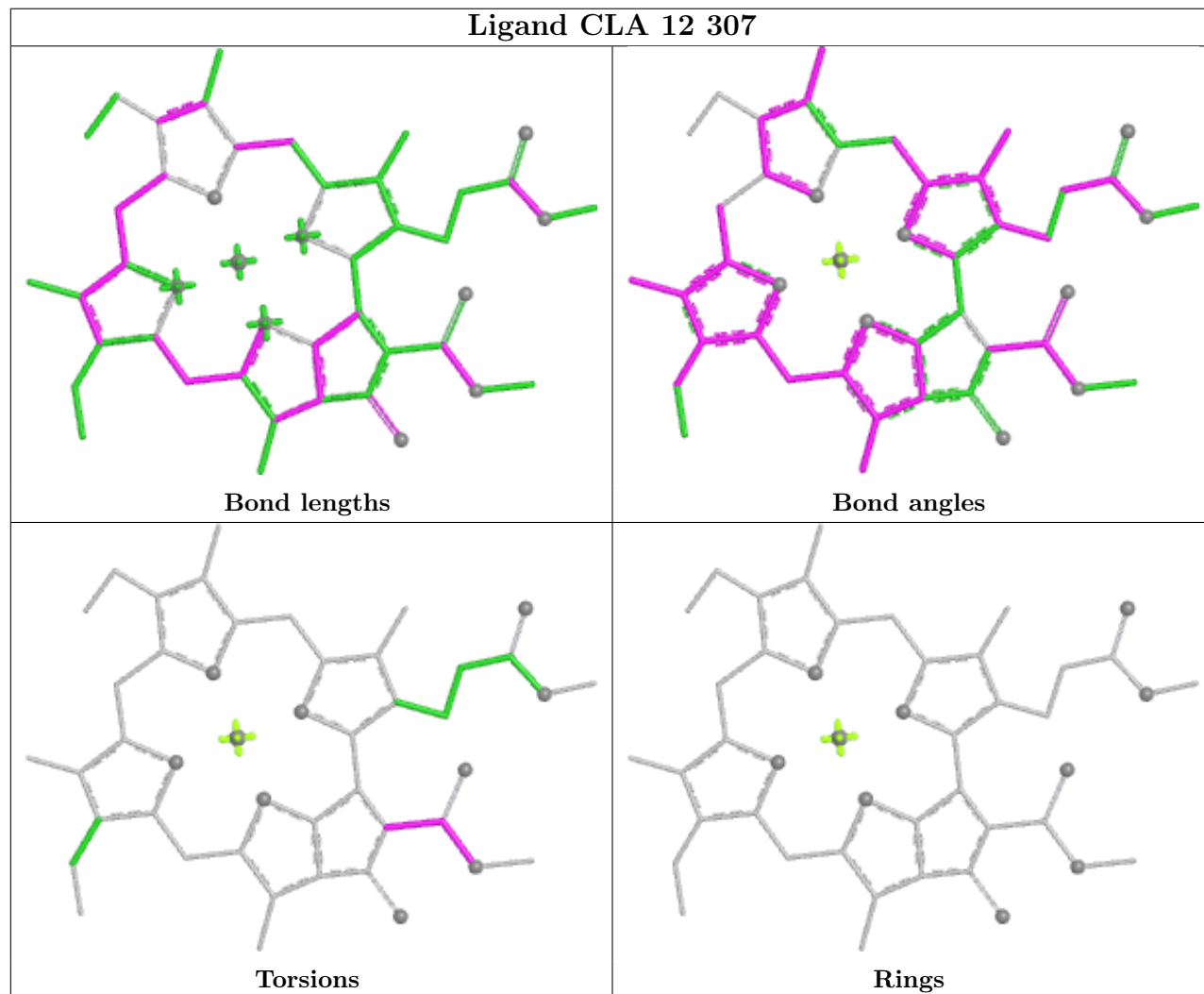


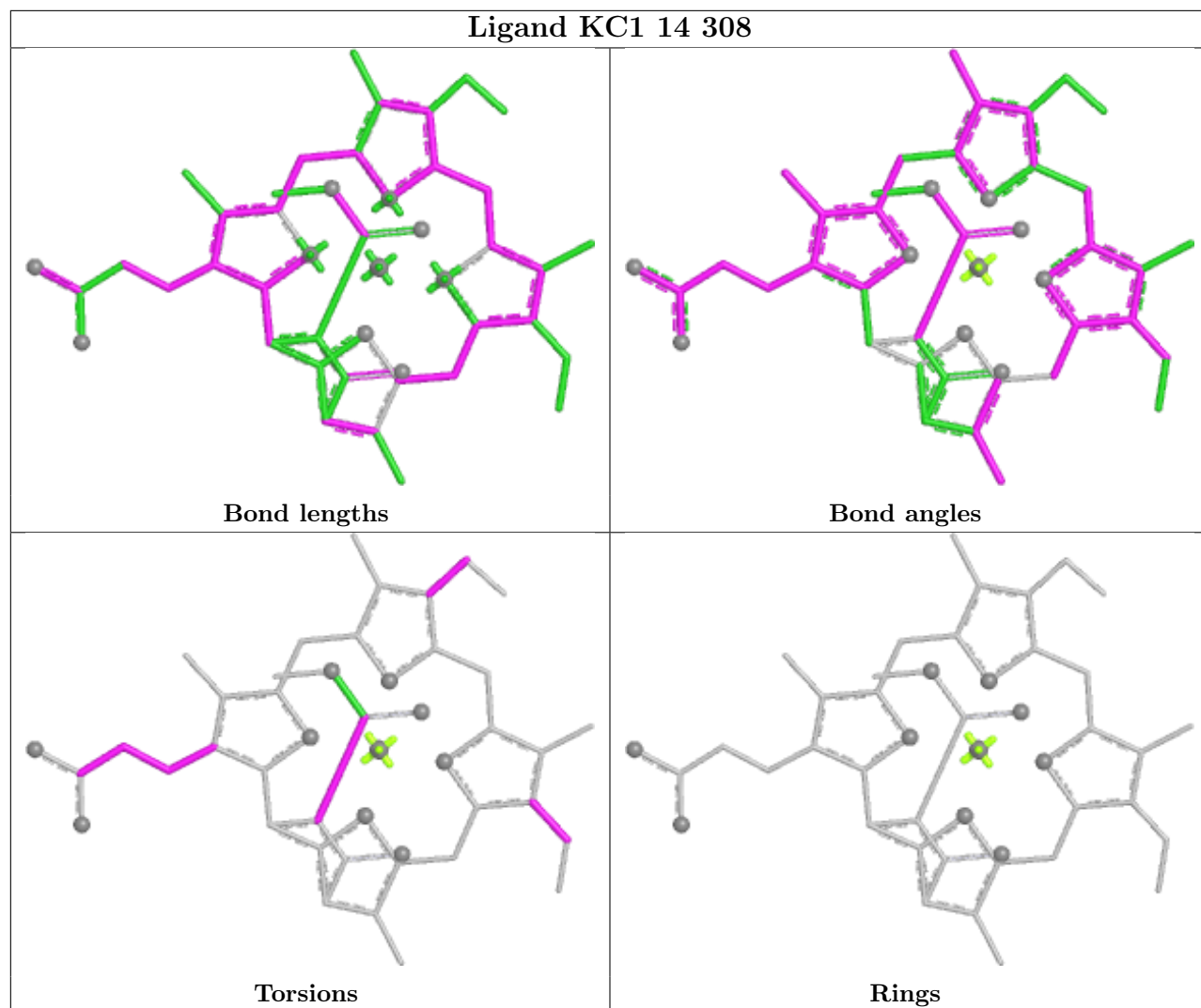


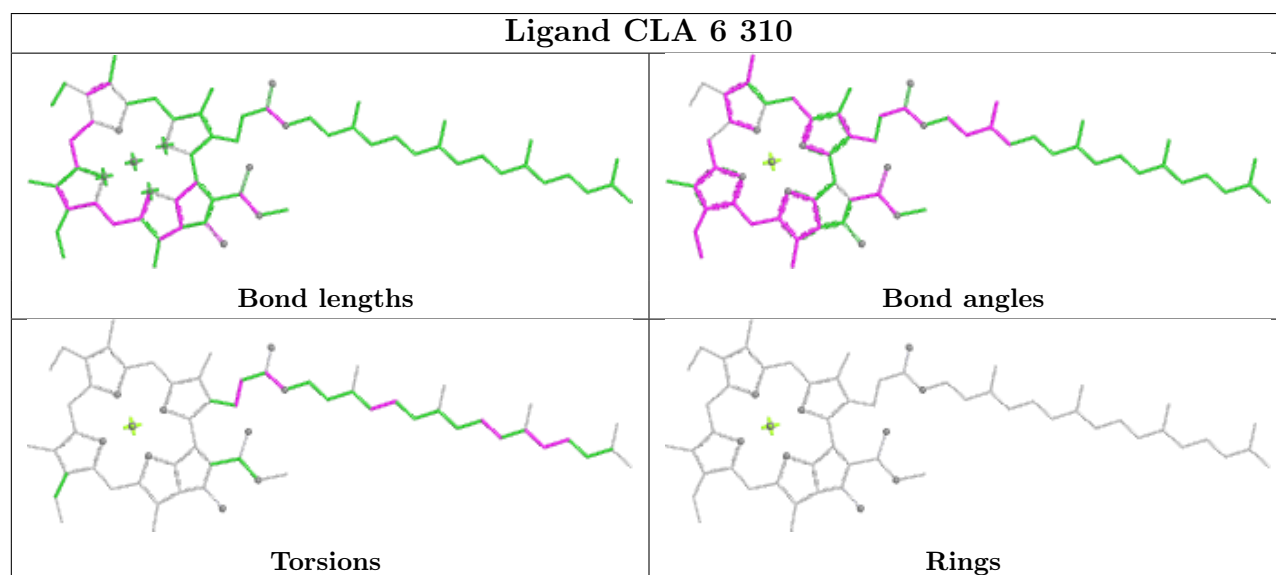
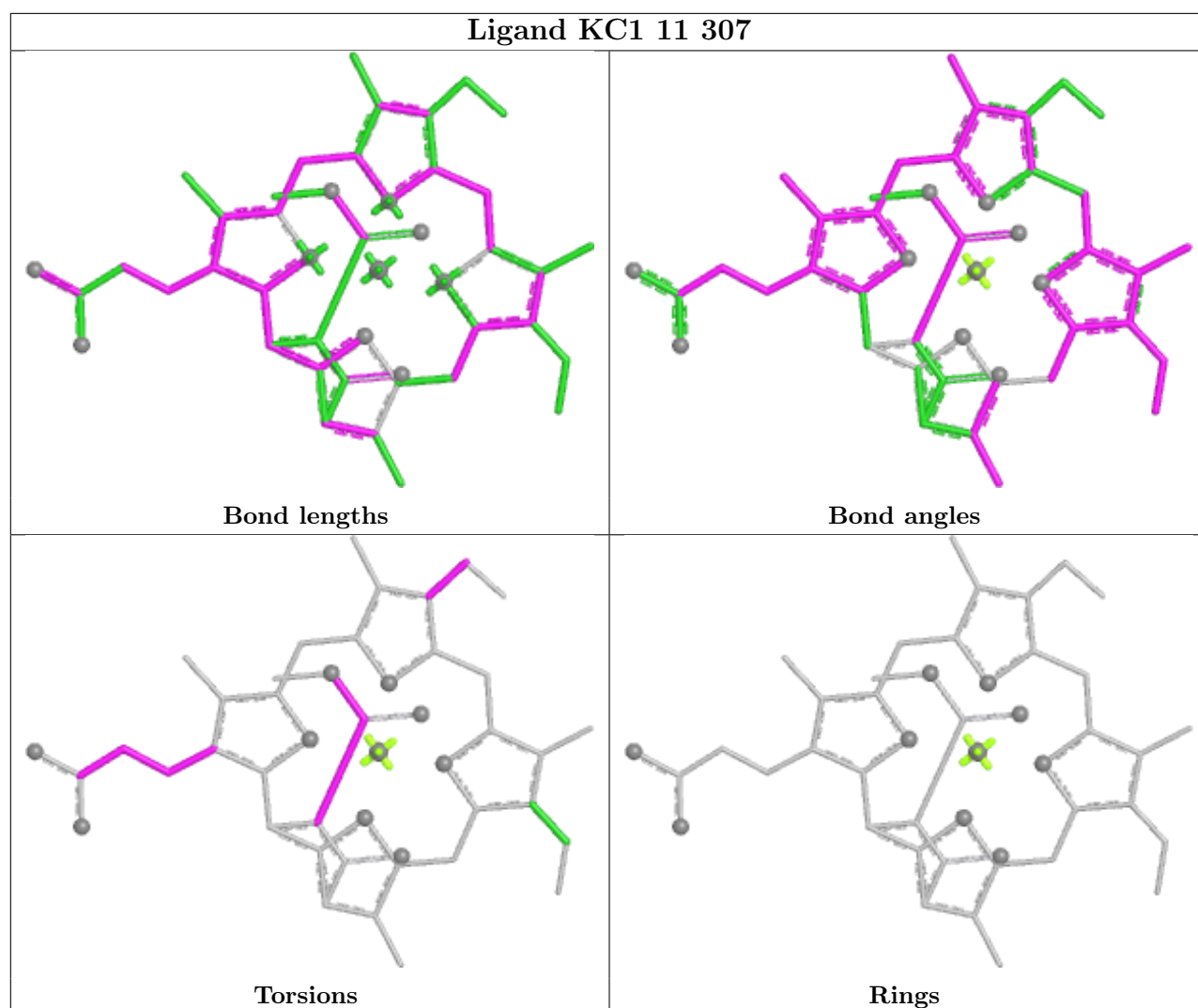
## Ligand DD6 3 316

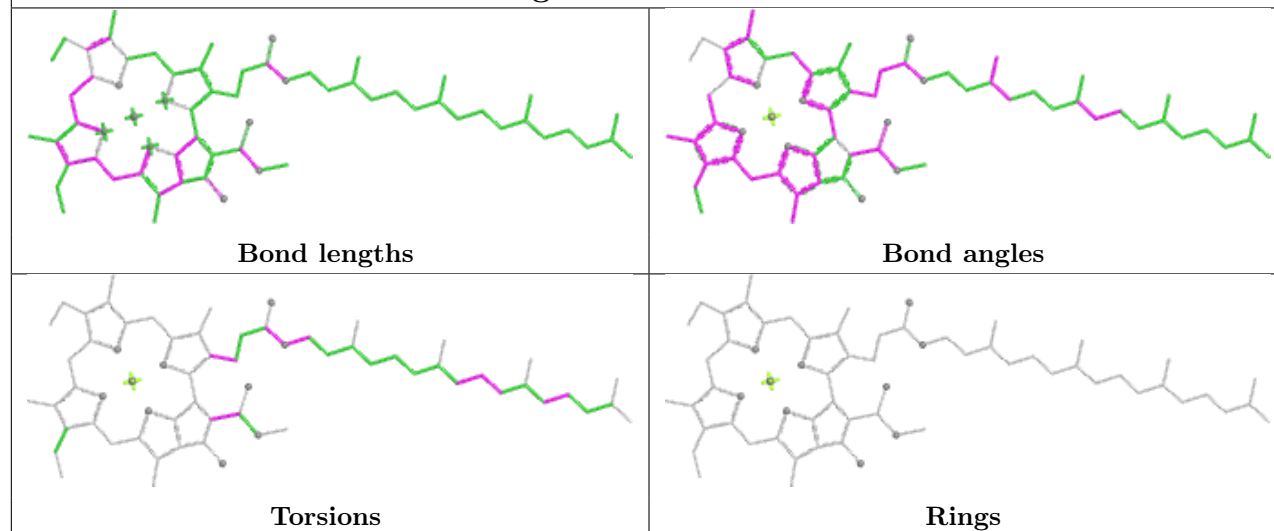
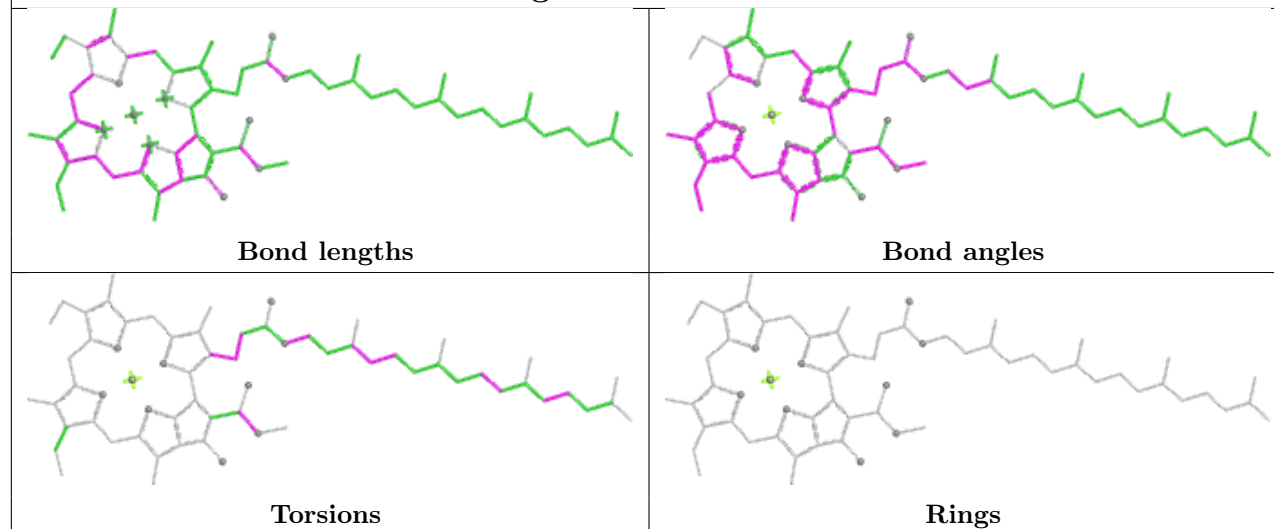


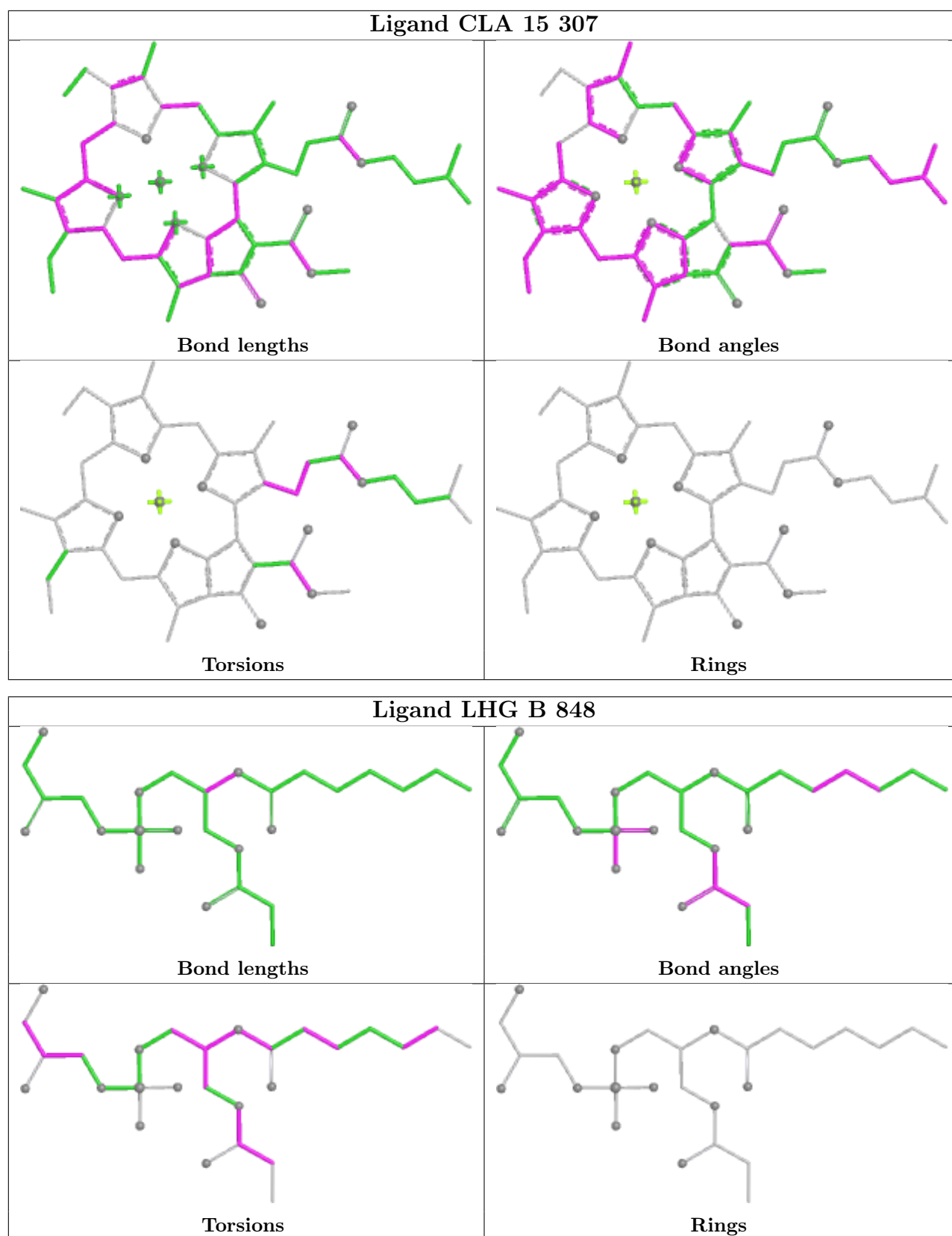
## Ligand CLA 12 307



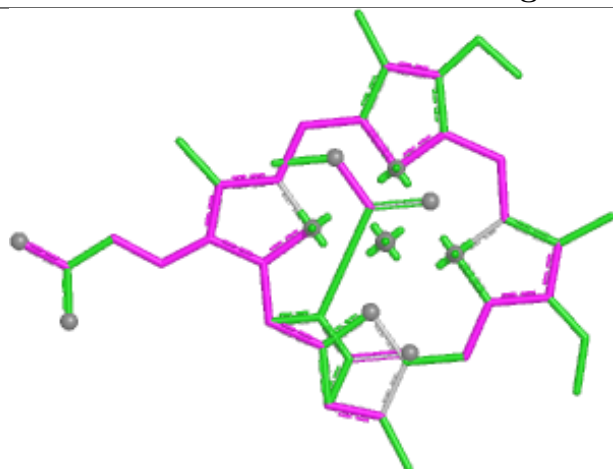




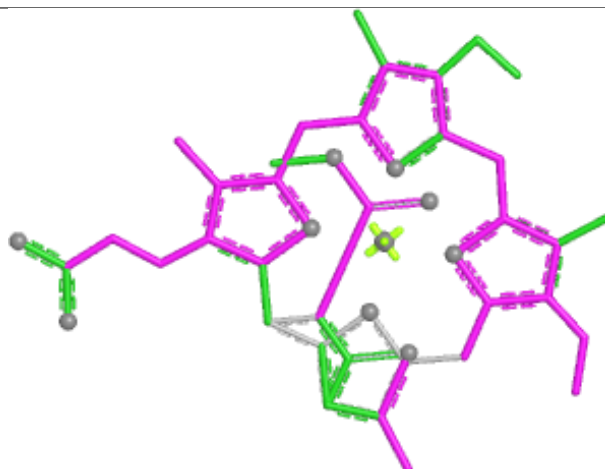
**Ligand CLA B 805****Ligand CLA A 810**



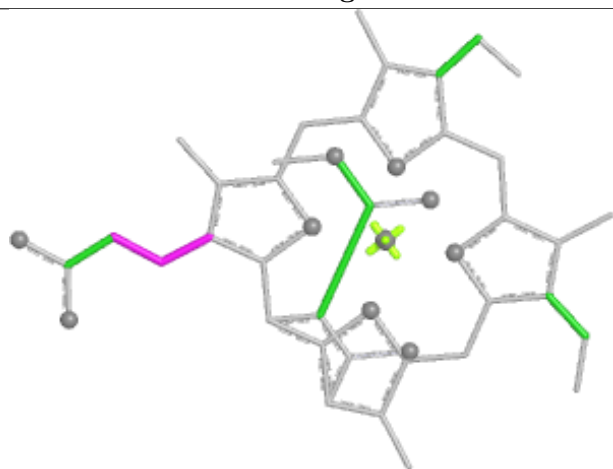
## Ligand KC1 4 308



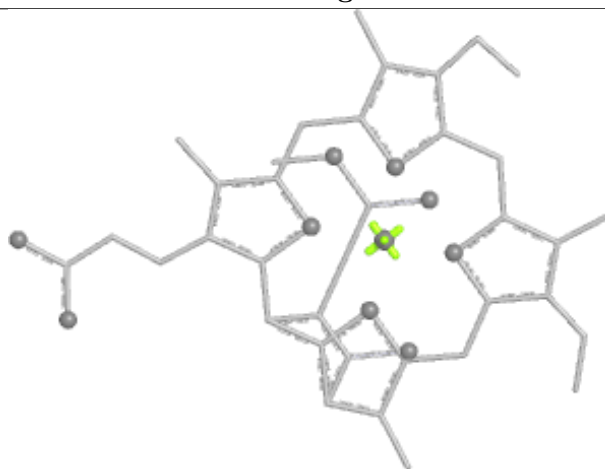
Bond lengths



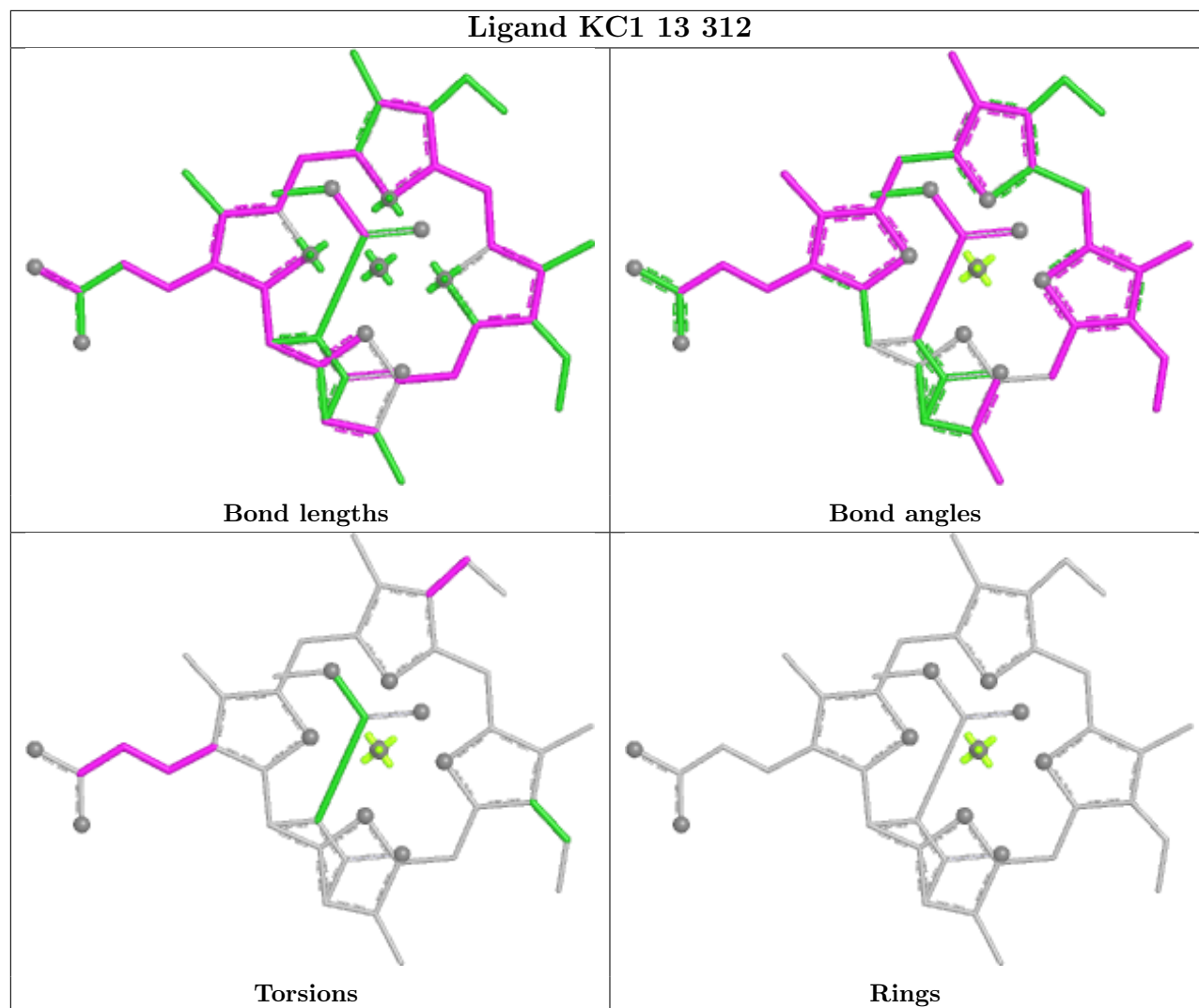
Bond angles



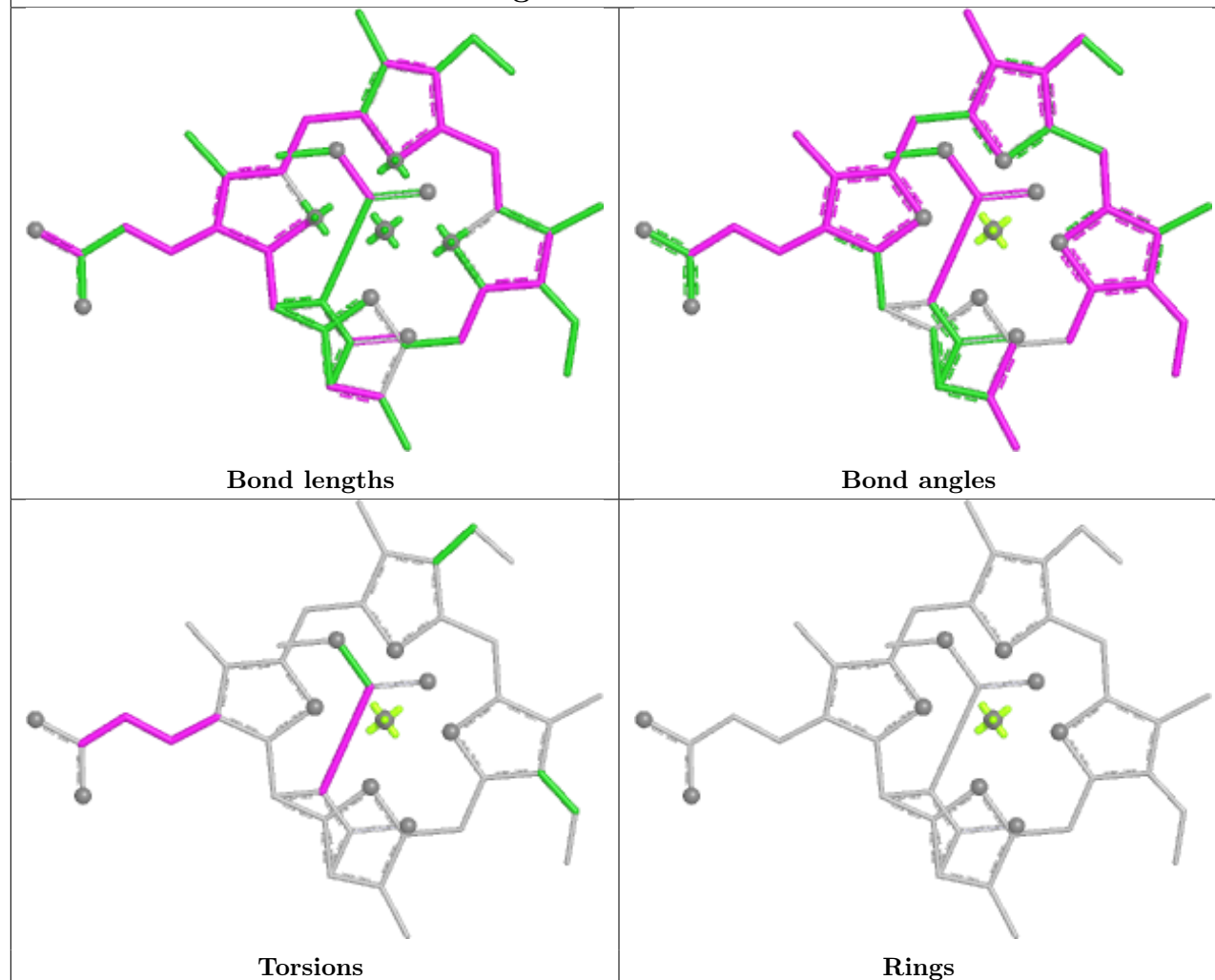
Torsions



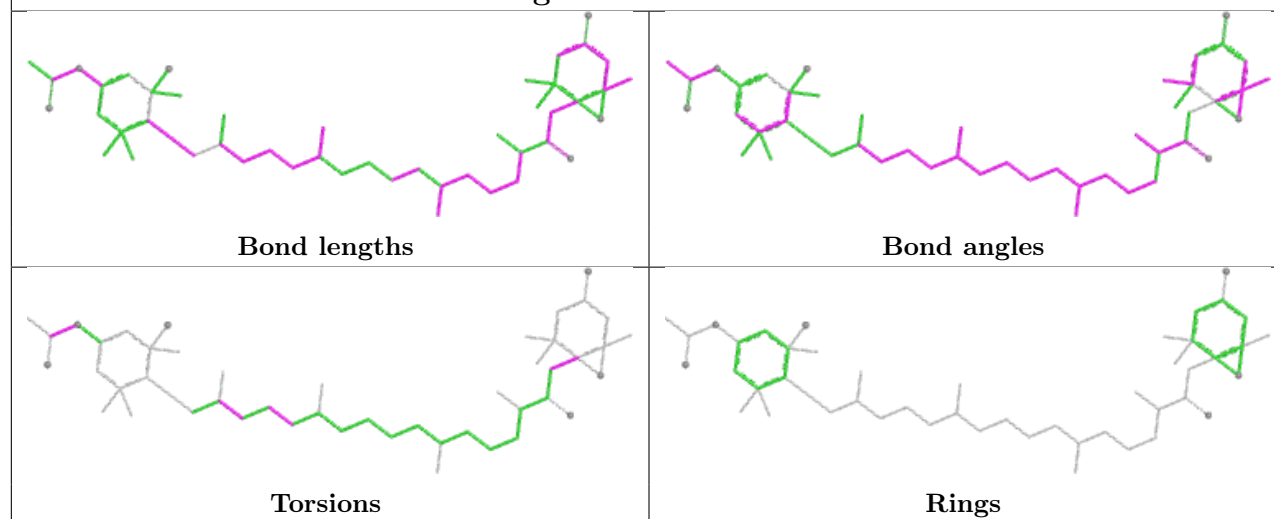
Rings

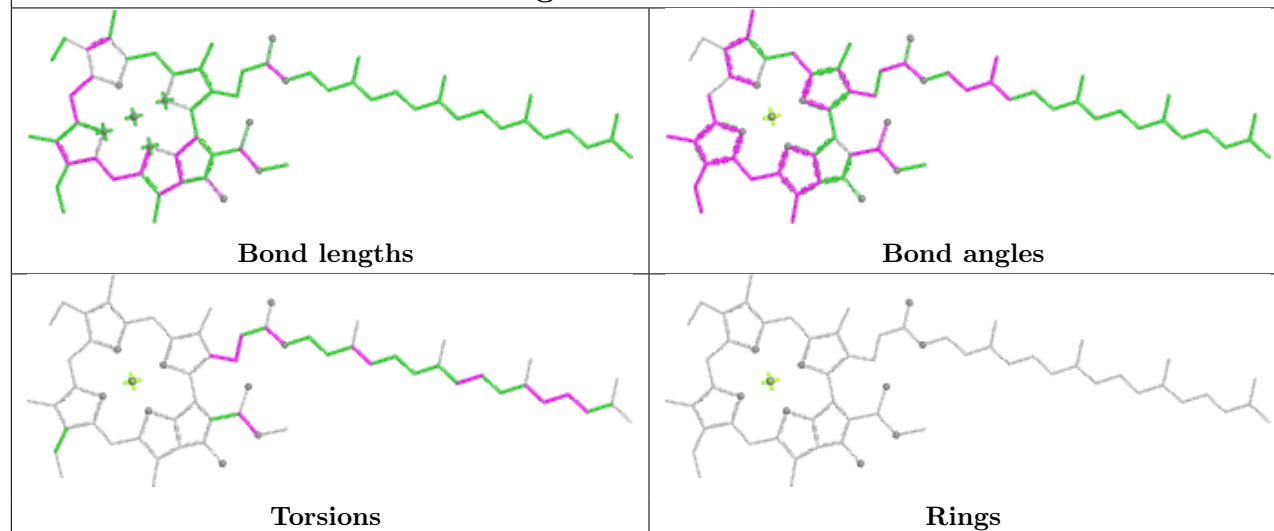
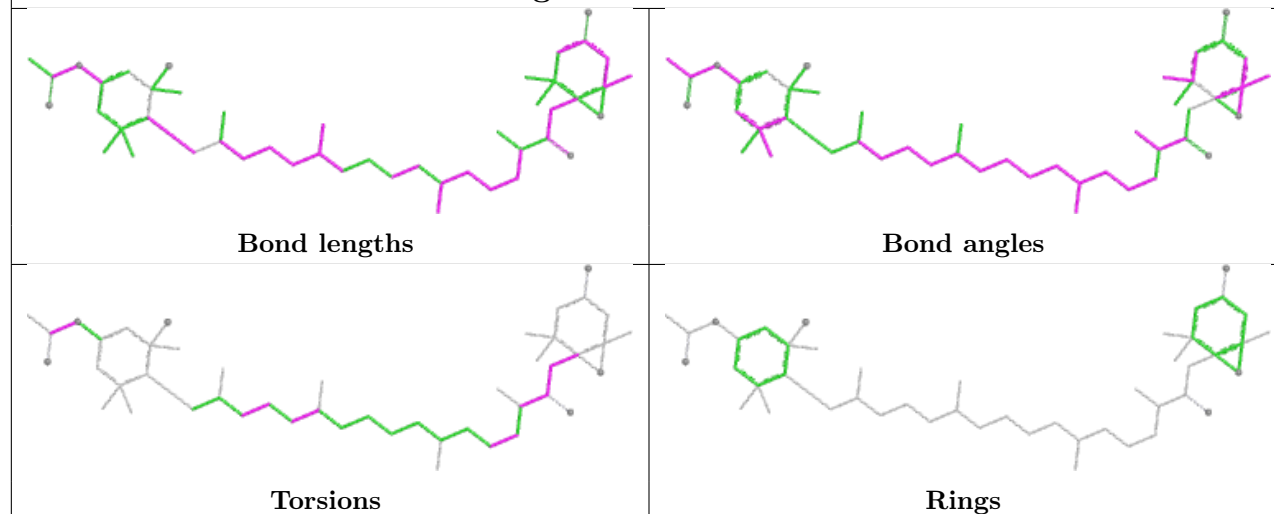
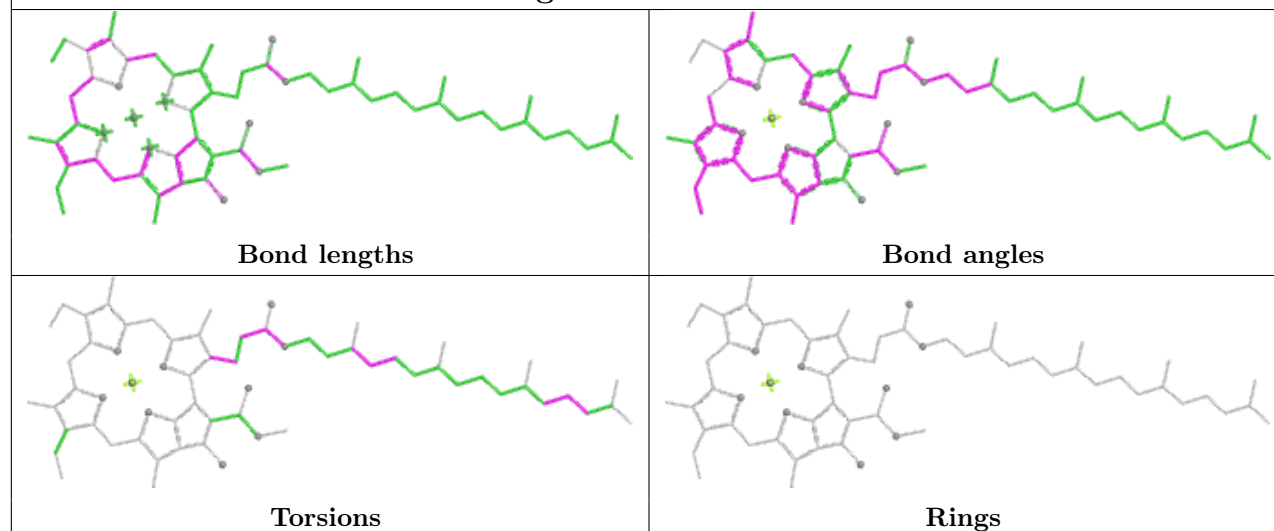


## Ligand KC1 5 310

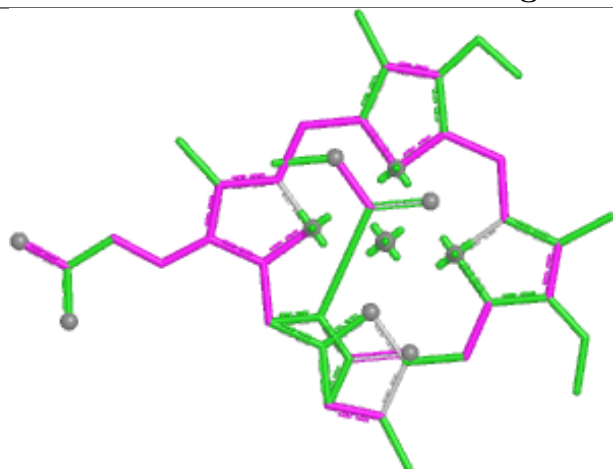


## Ligand A86 10 301

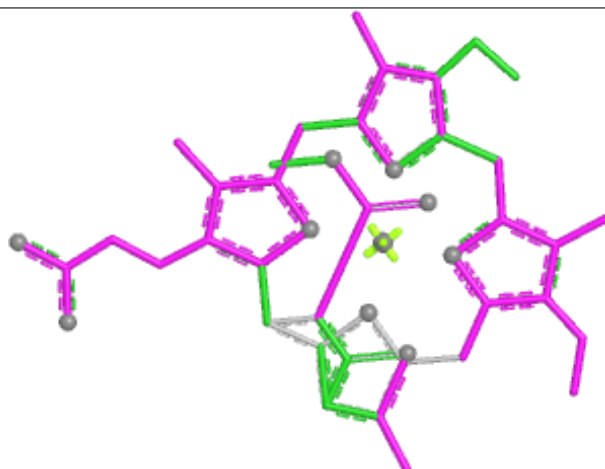


**Ligand CLA 5 308****Ligand A86 14 316****Ligand CLA 2 305**

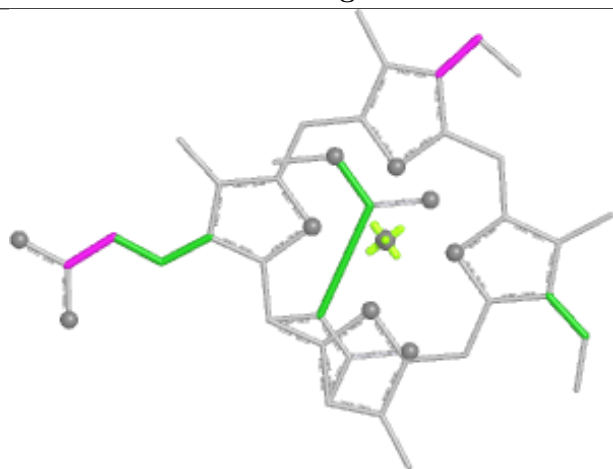
## Ligand KC1 7 313



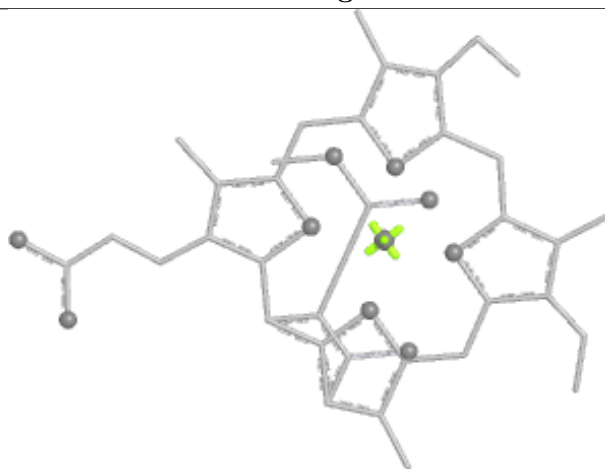
Bond lengths



Bond angles

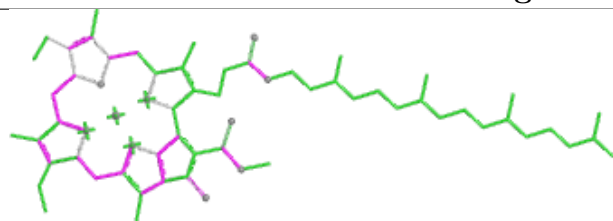


Torsions

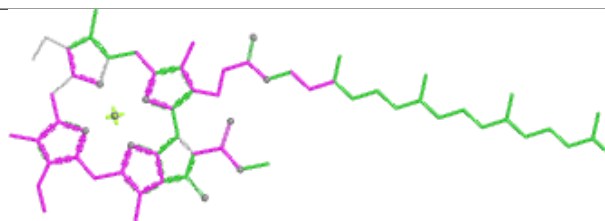


Rings

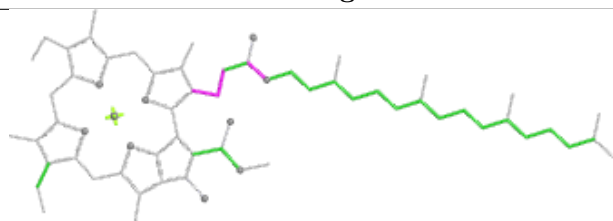
## Ligand CLA B 827



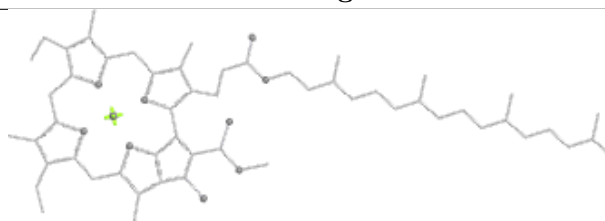
Bond lengths



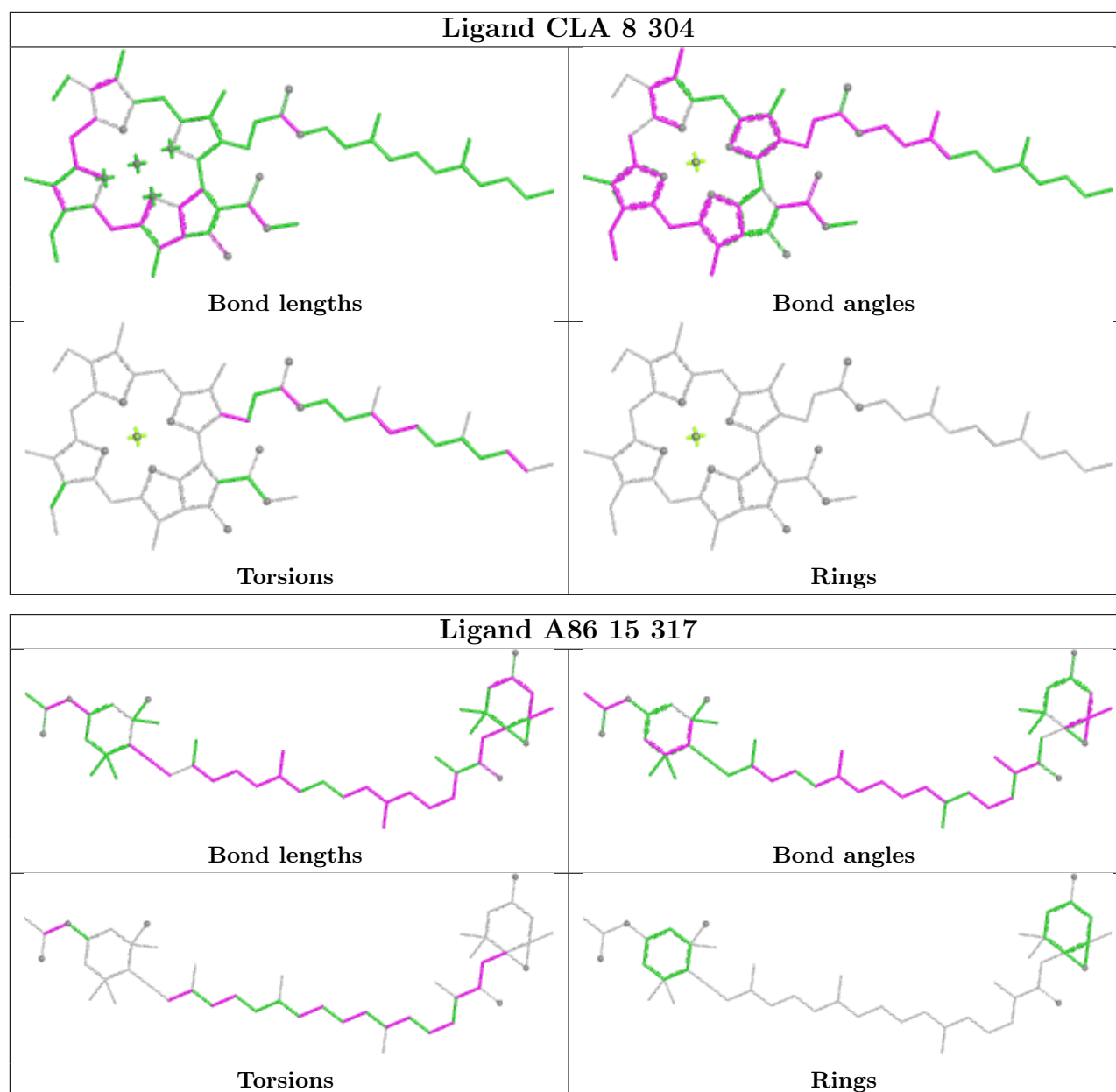
Bond angles

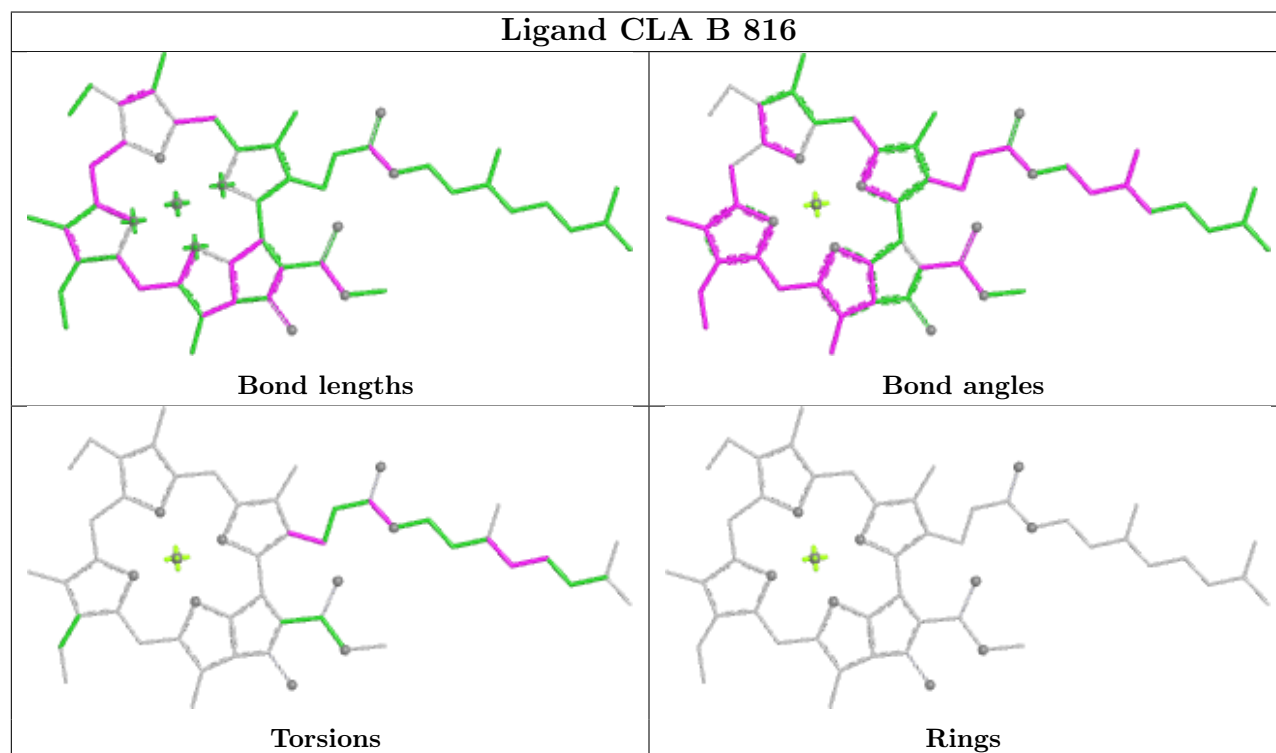
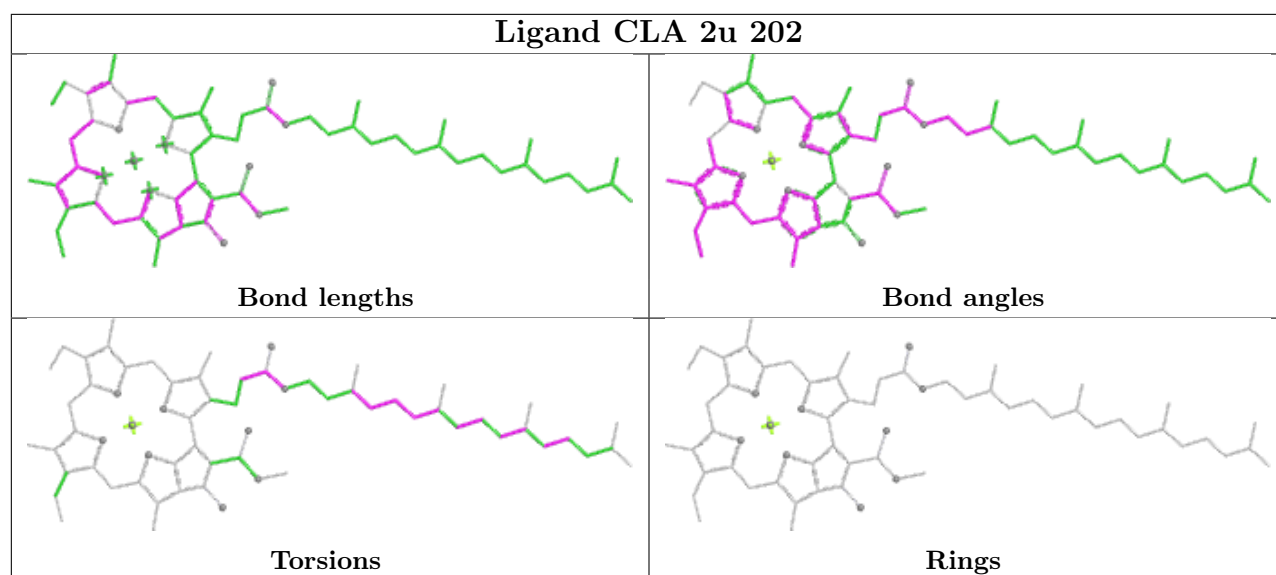


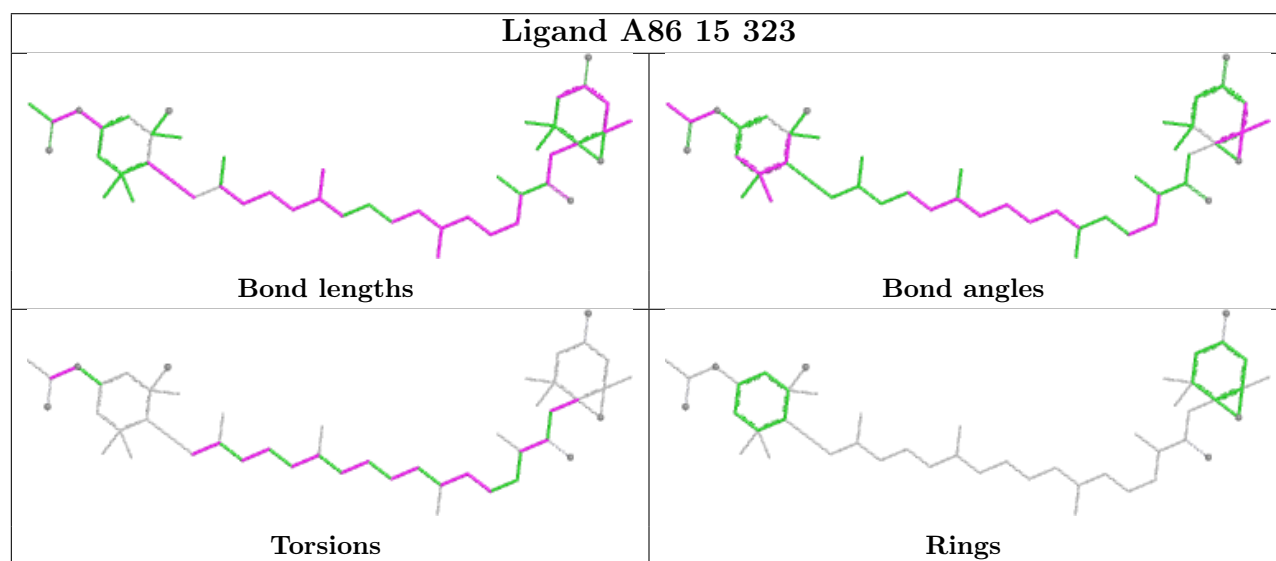
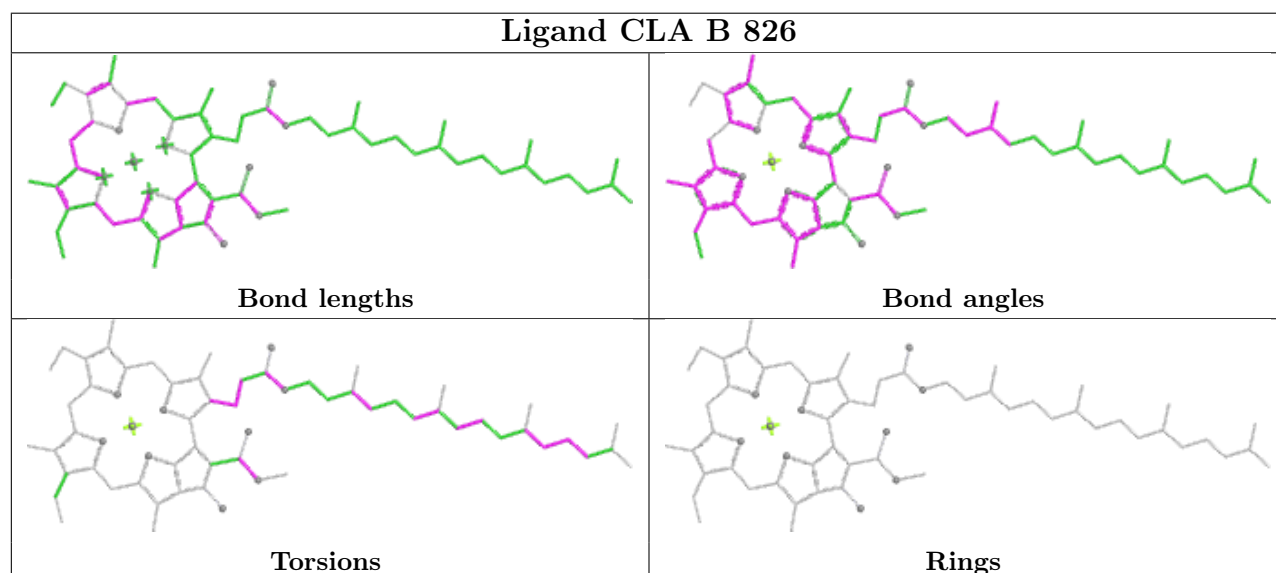
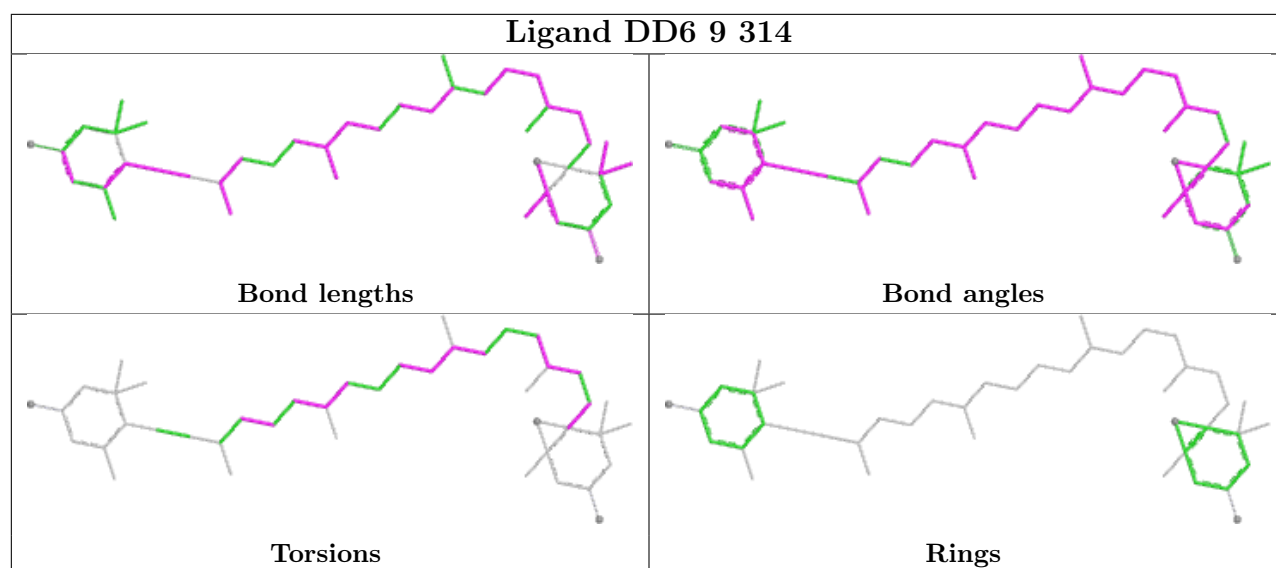
Torsions

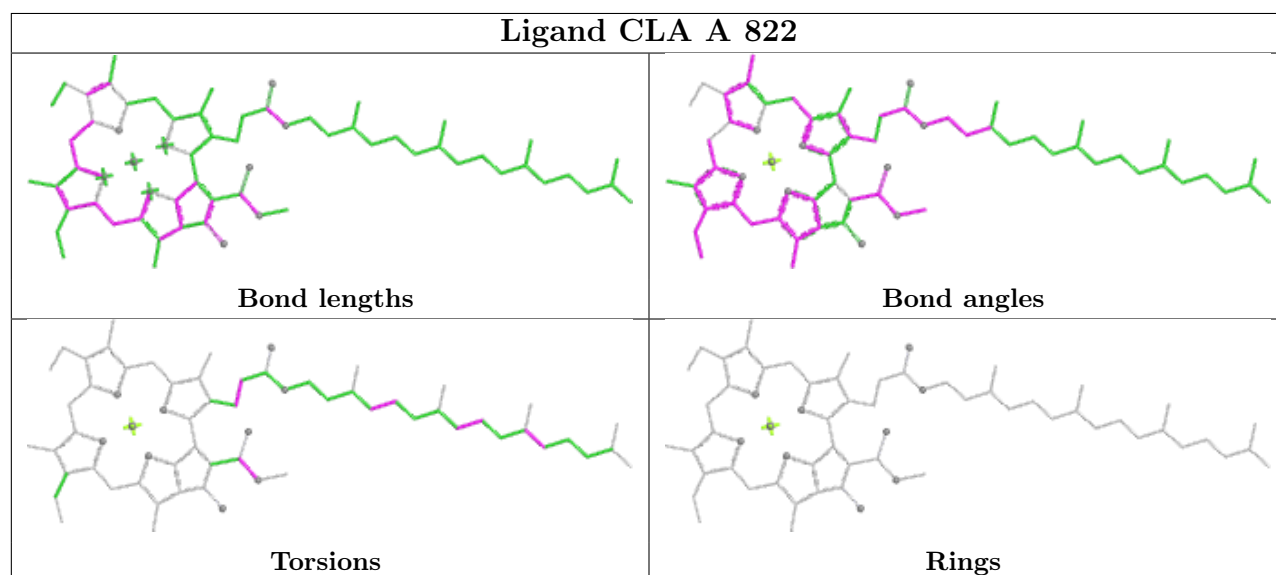
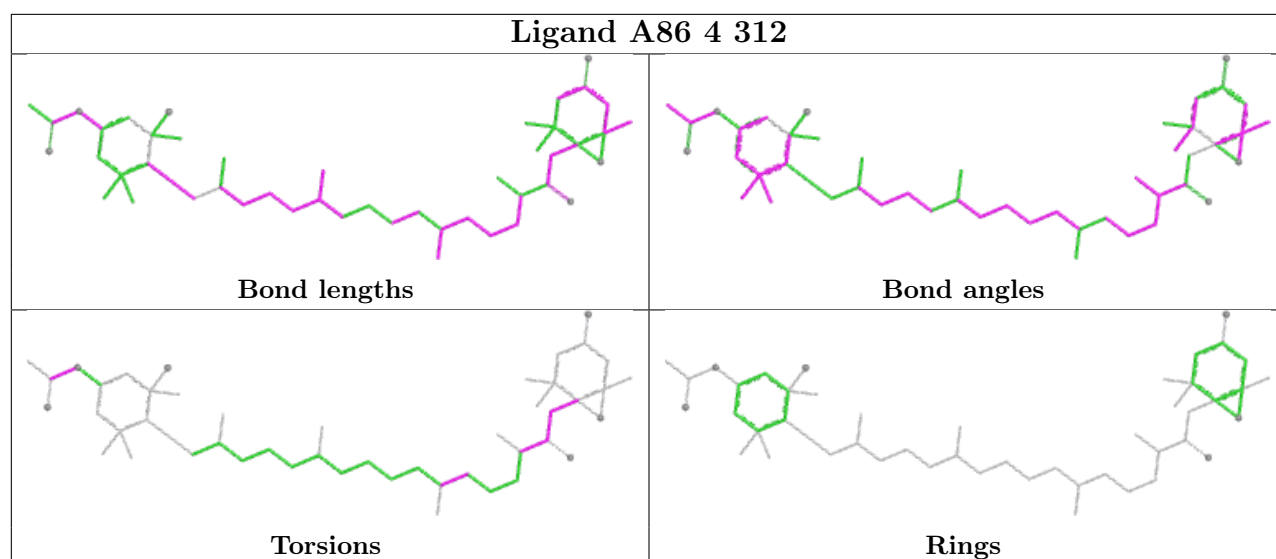


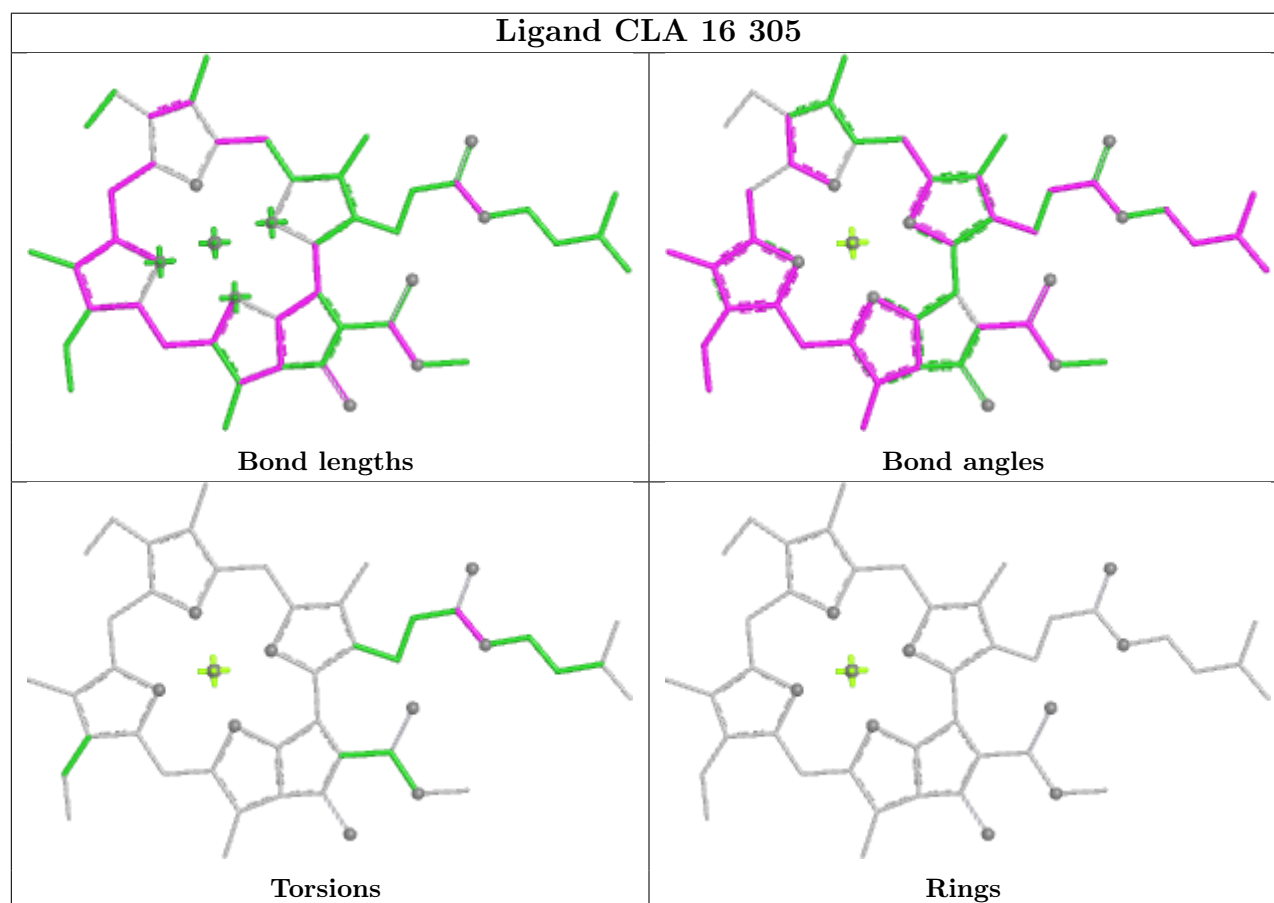
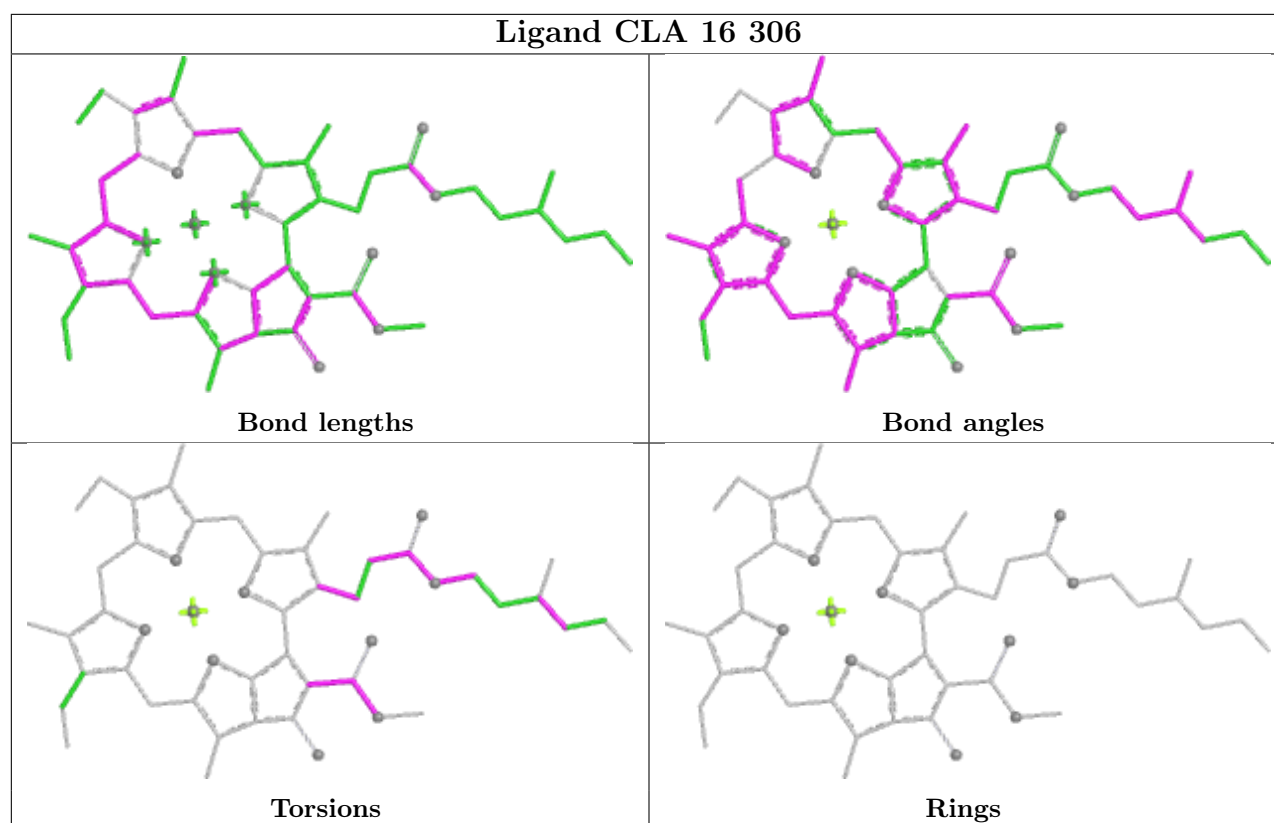
Rings



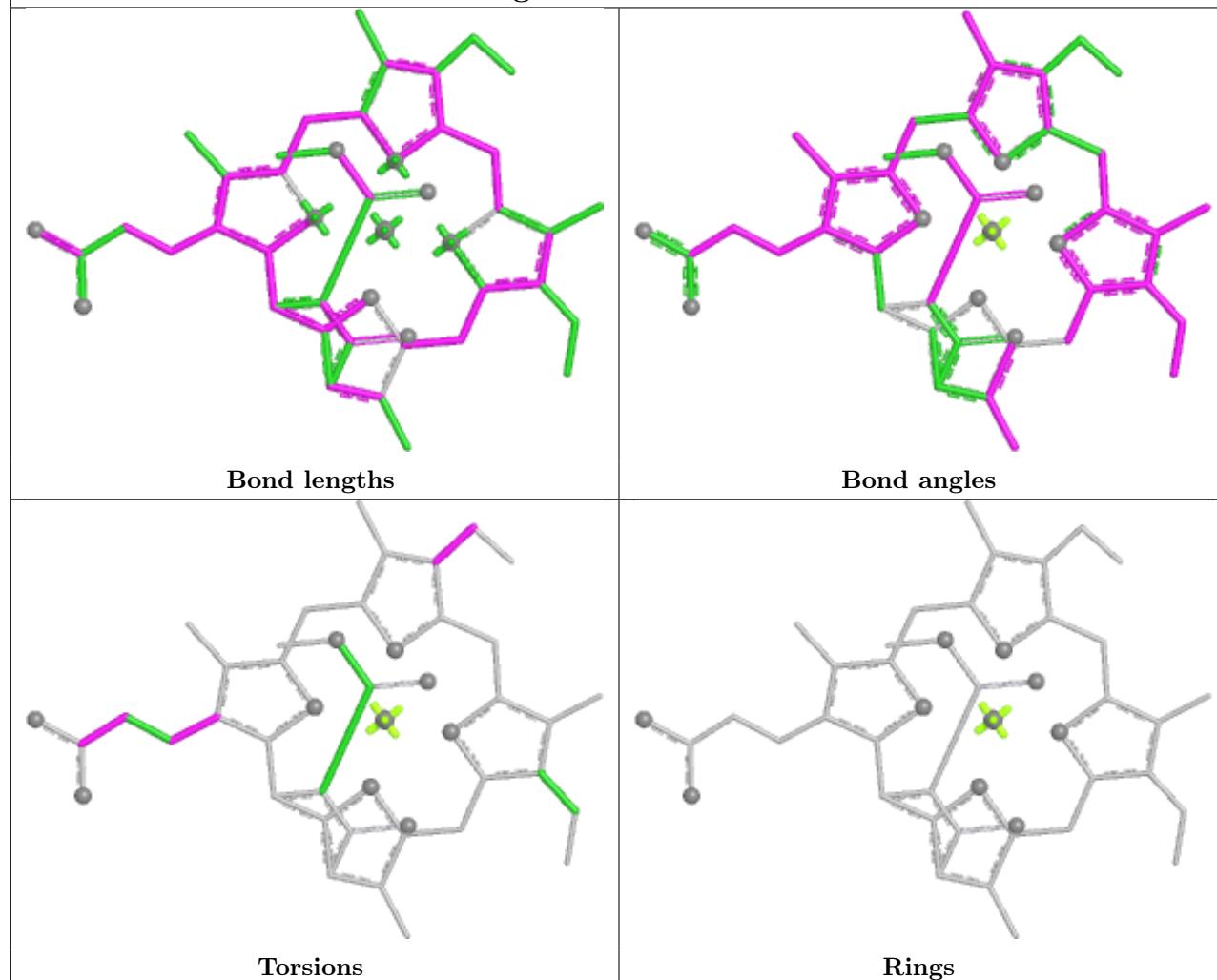




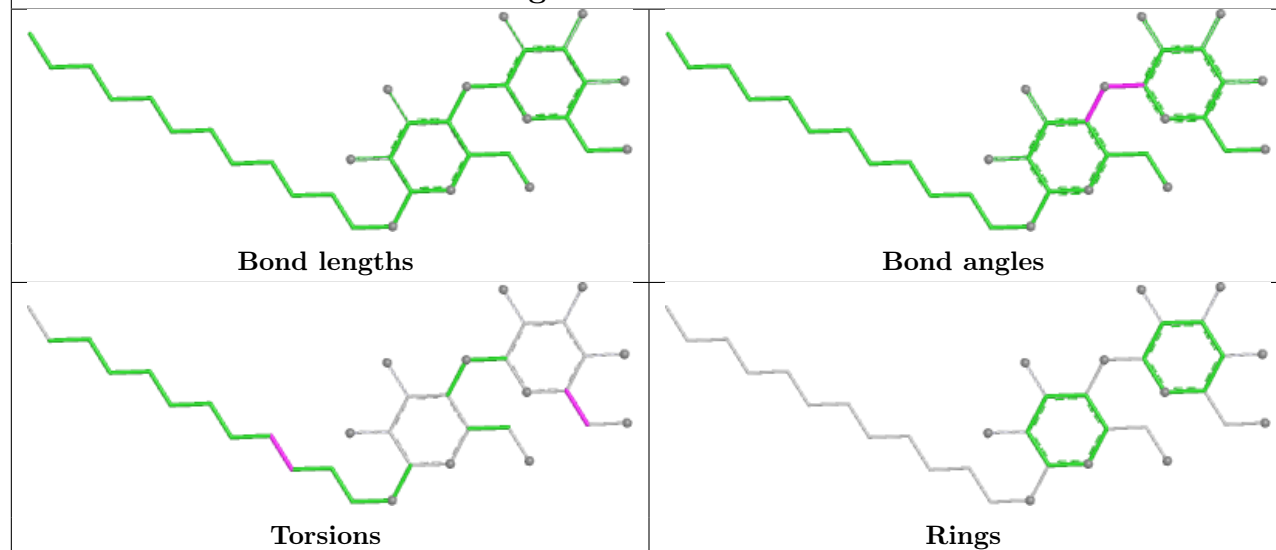


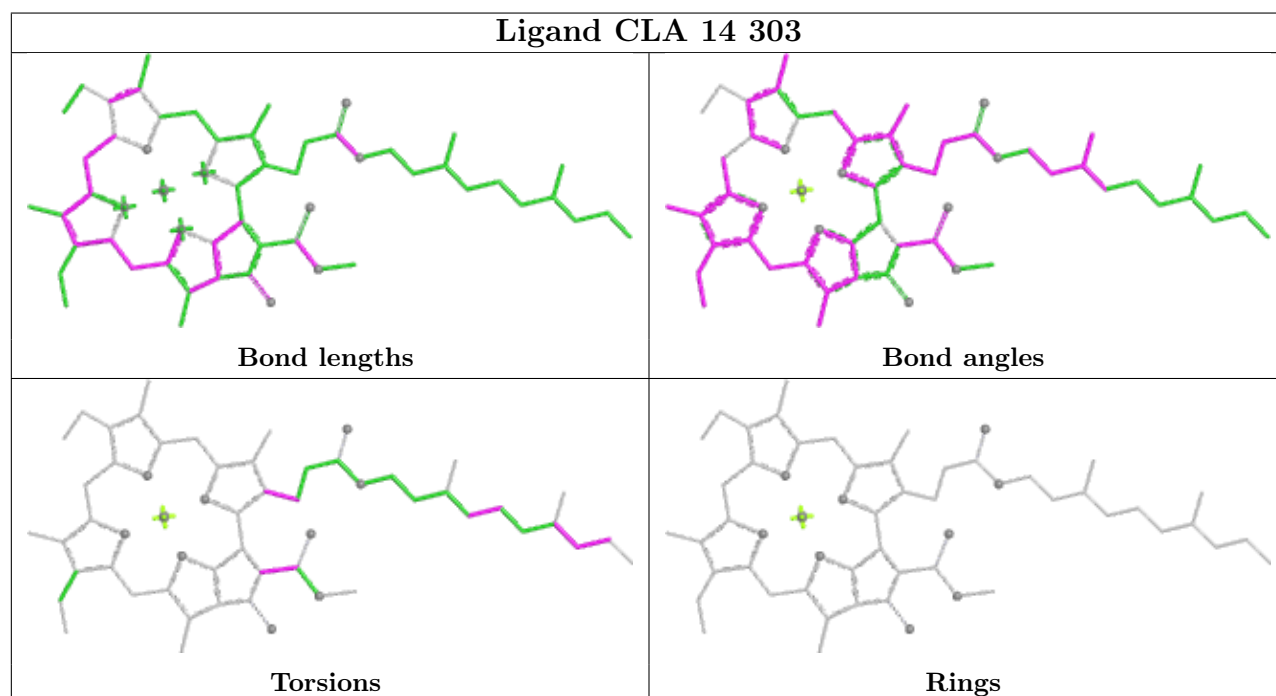
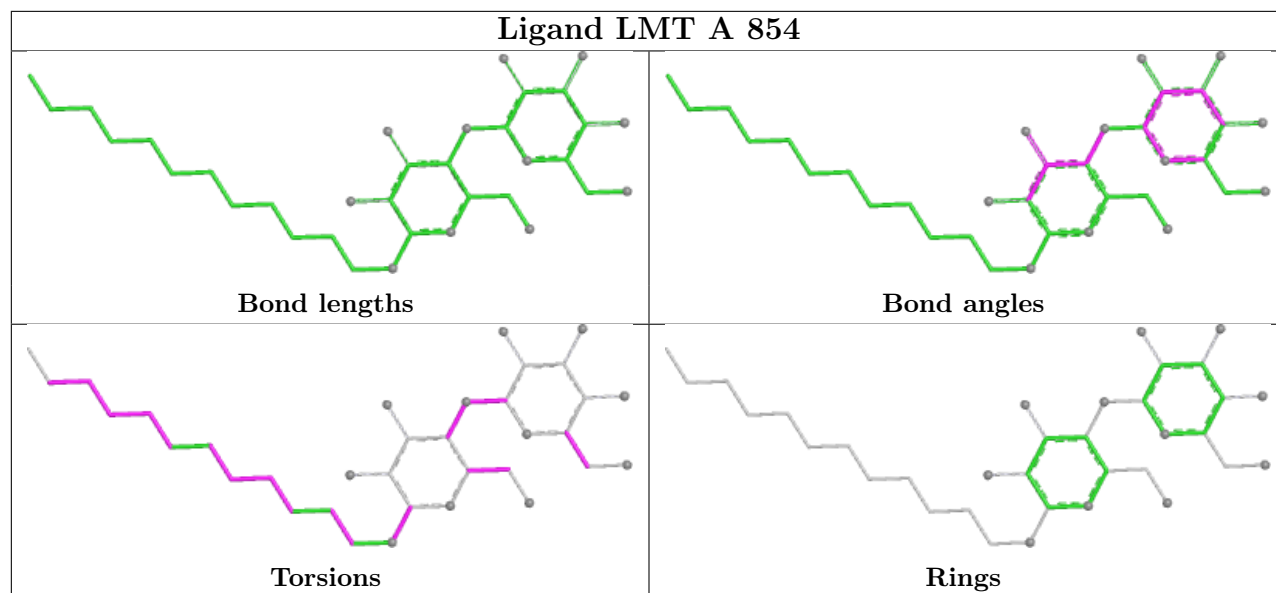


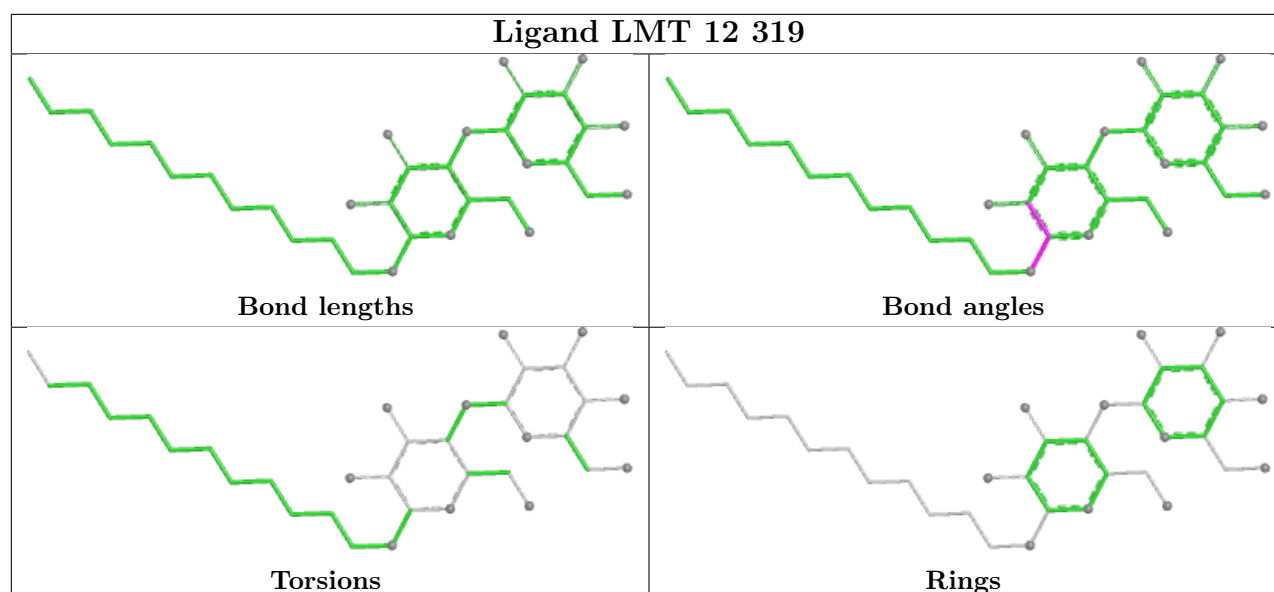
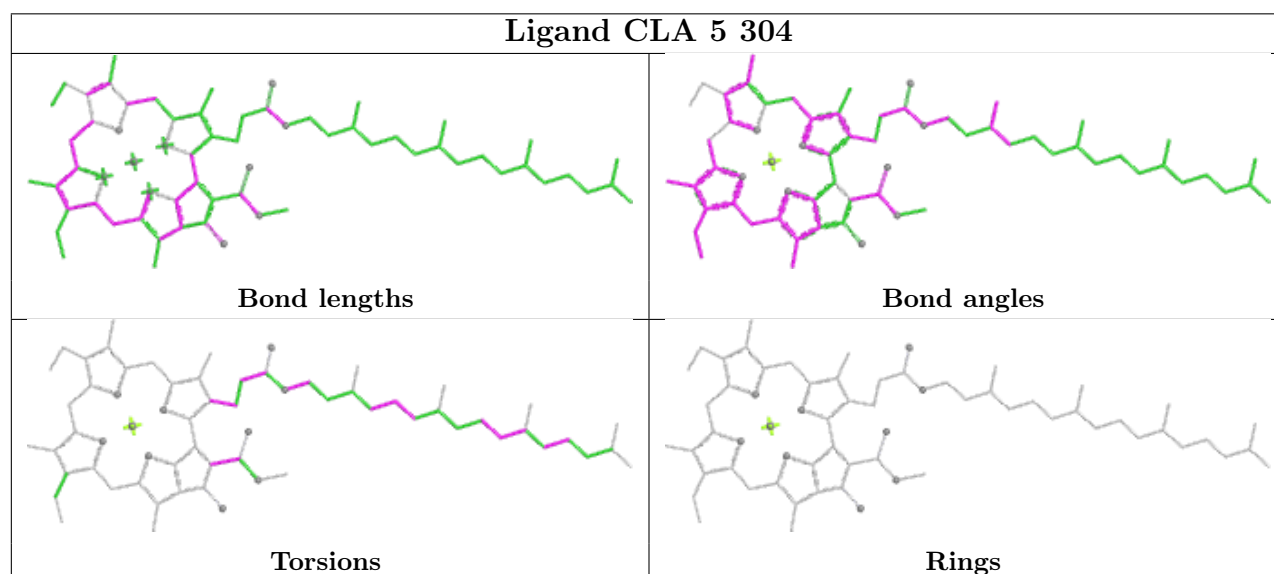
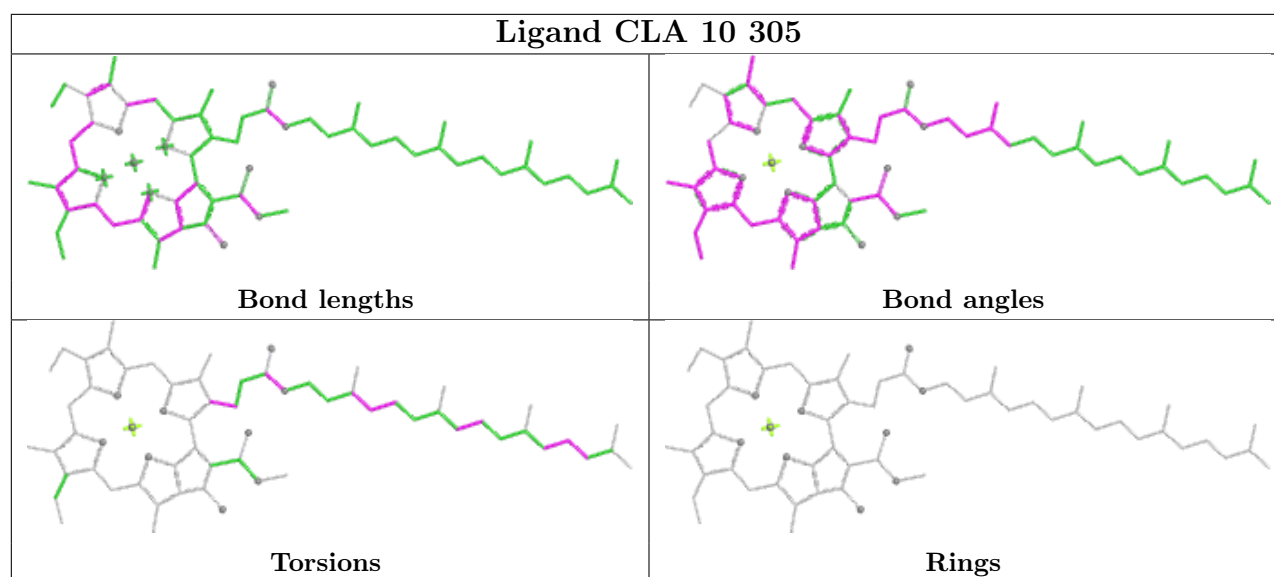
## Ligand KC1 3 304

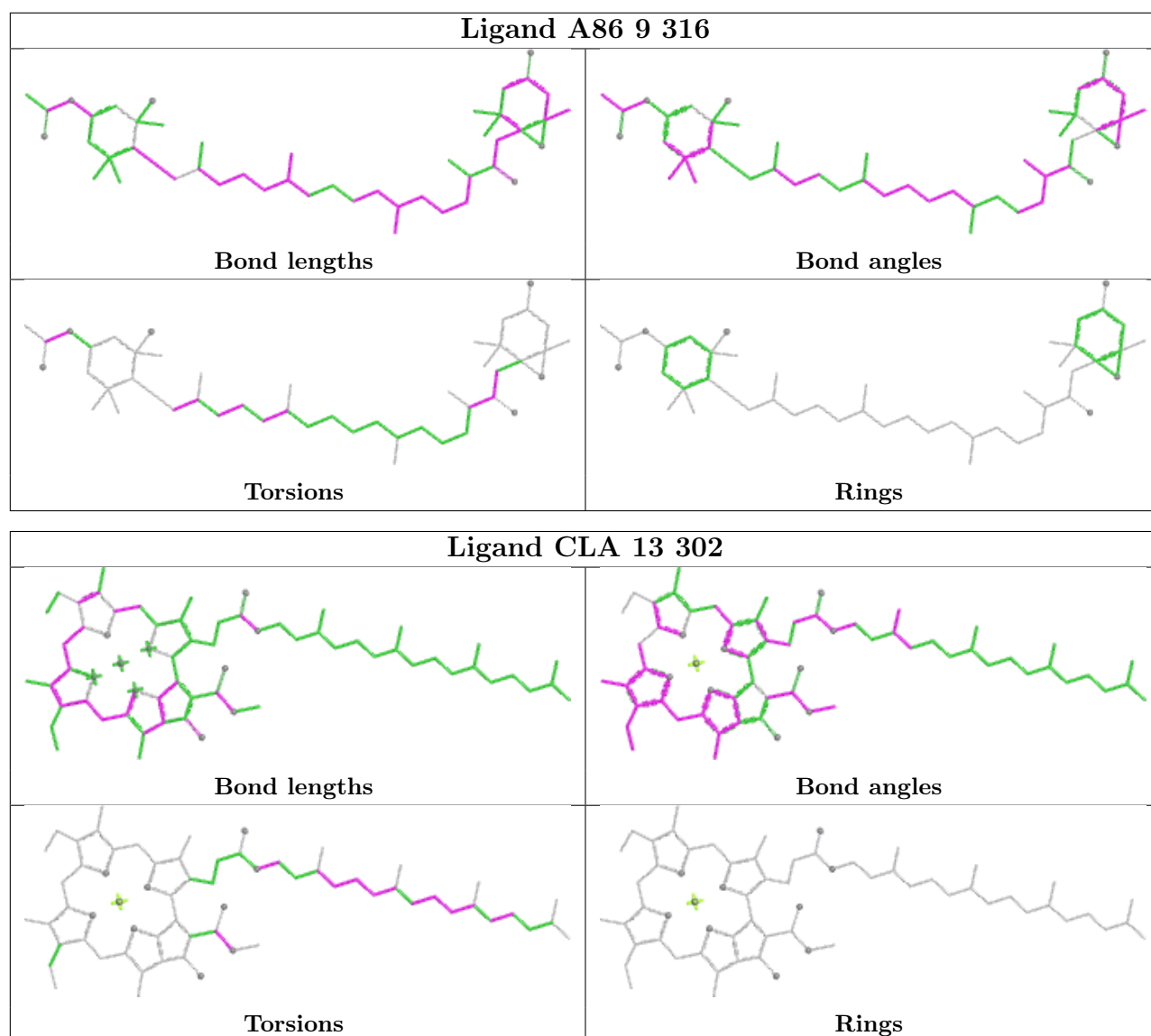


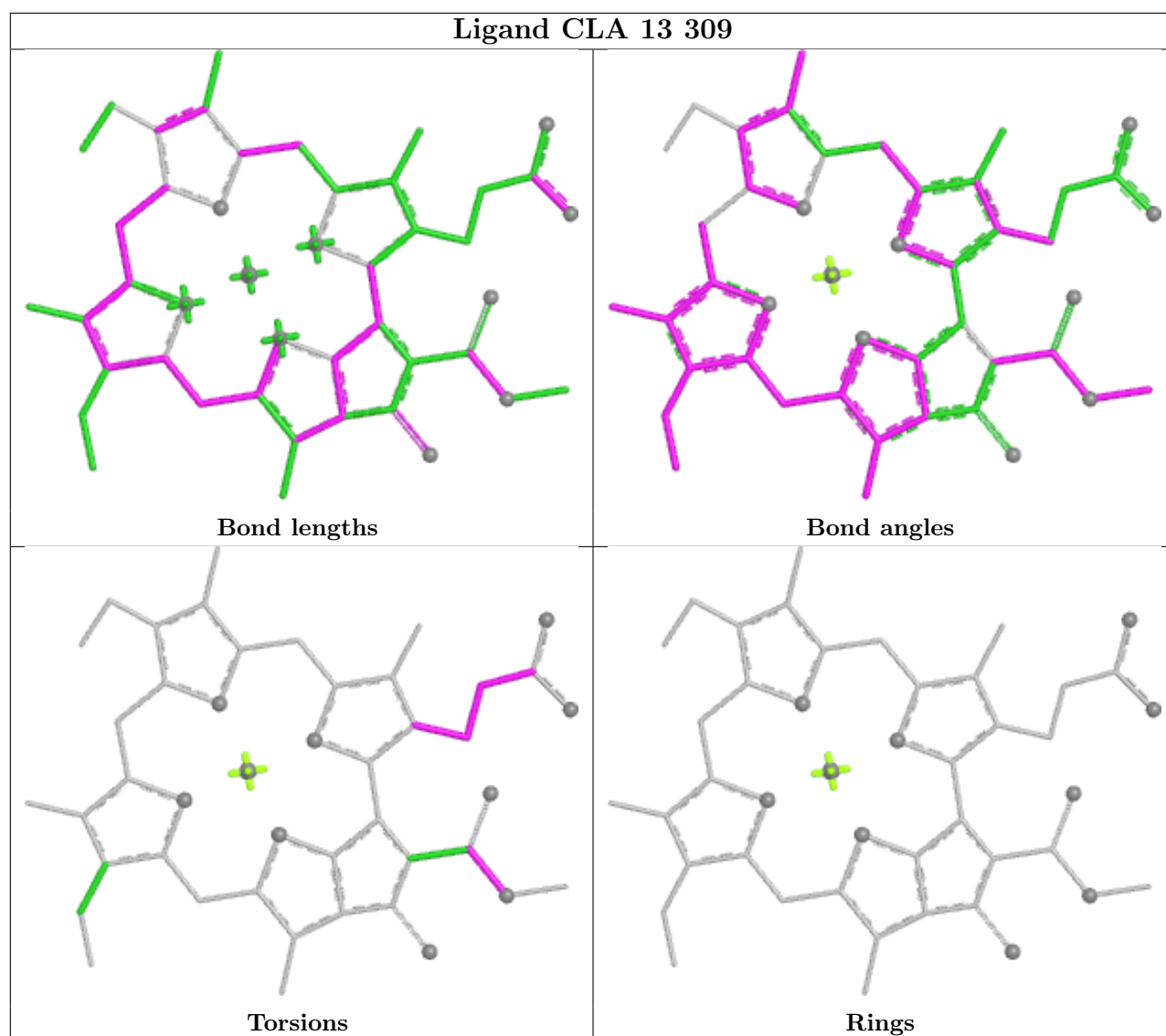
## Ligand LMT A 857

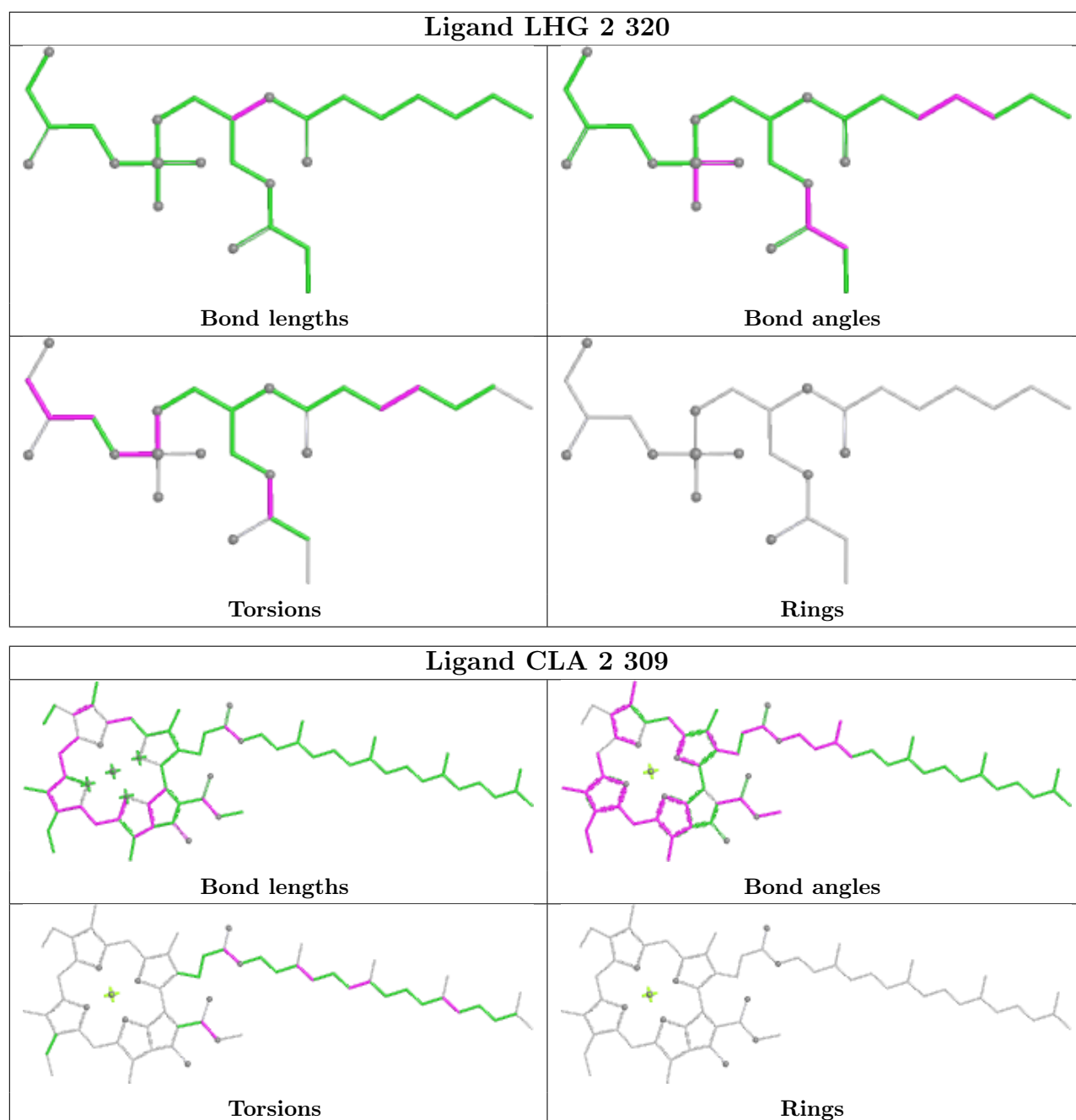




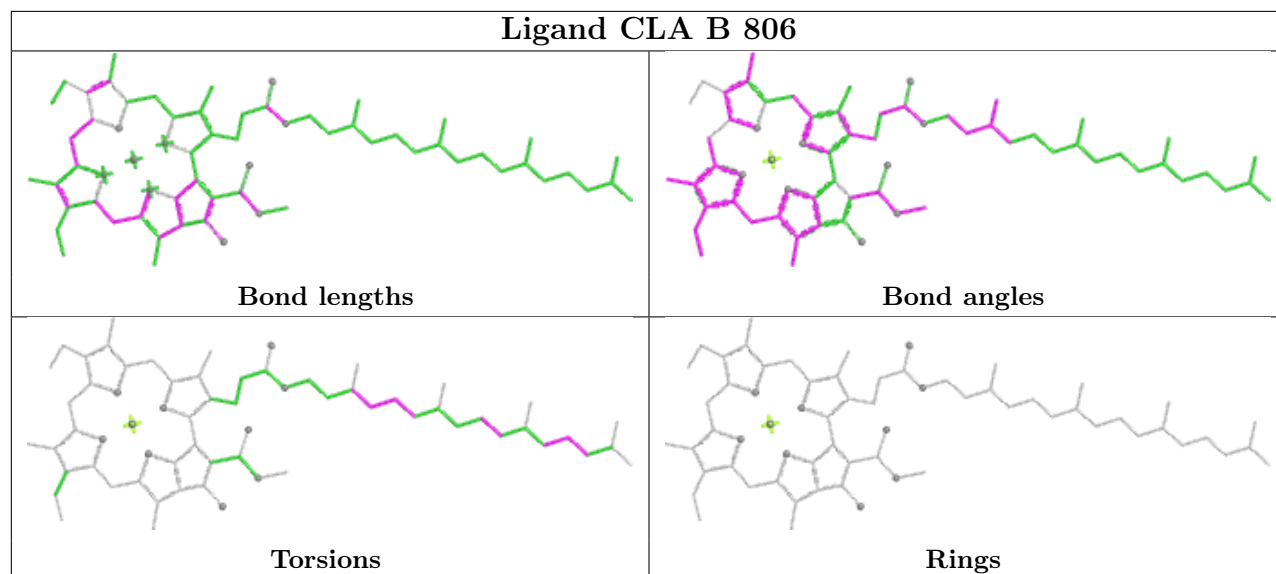




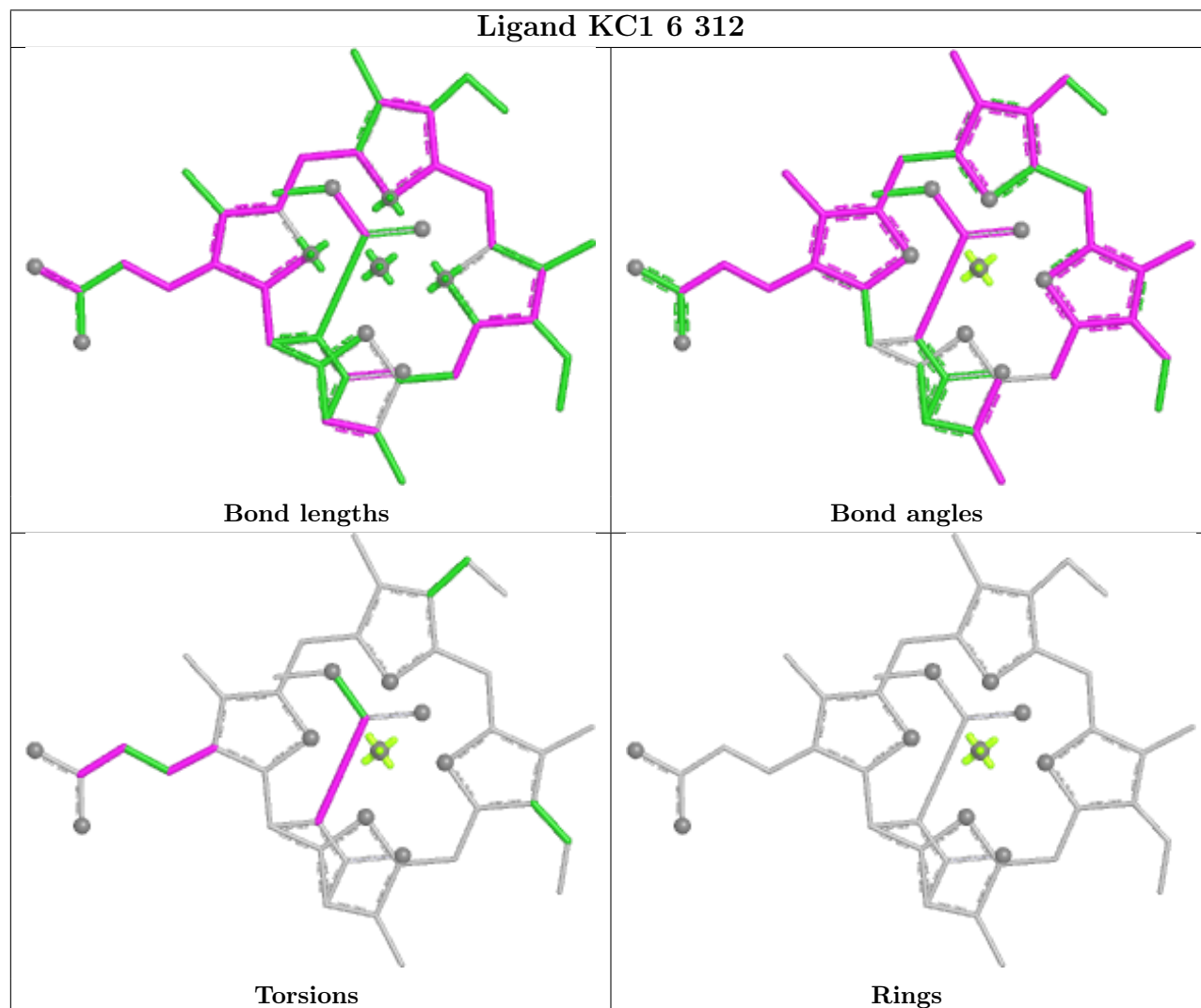


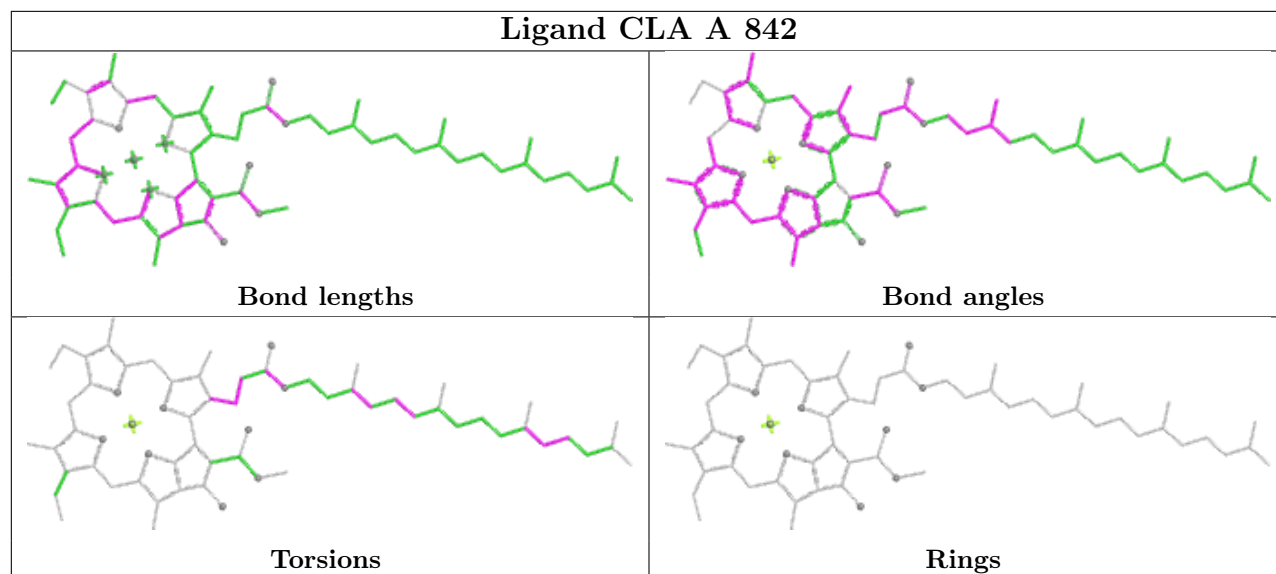
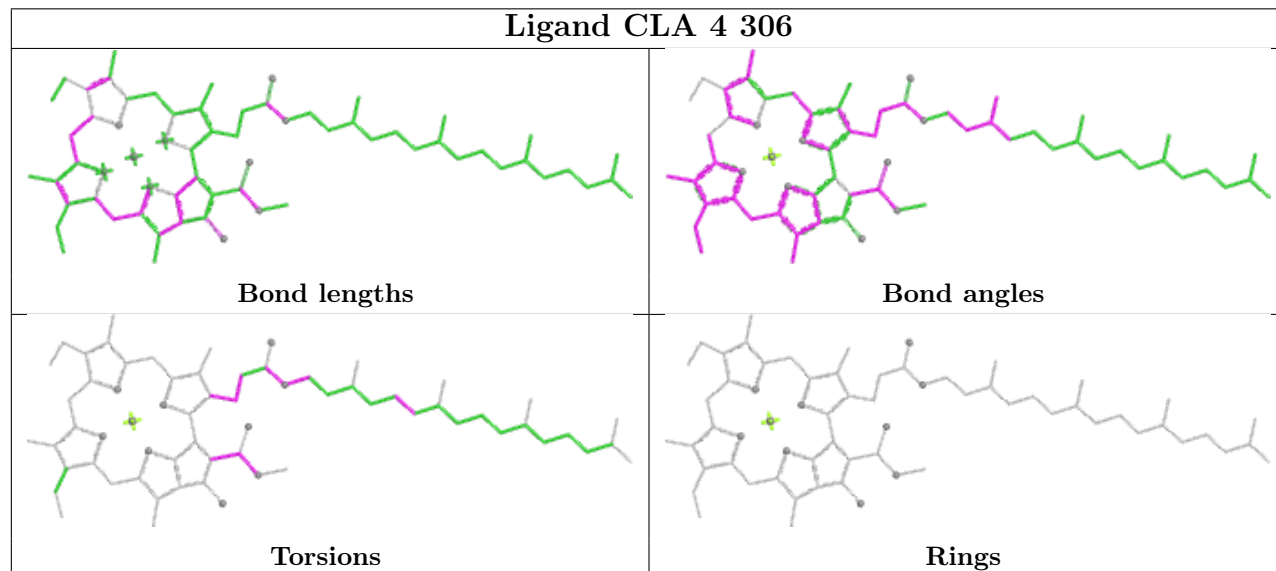
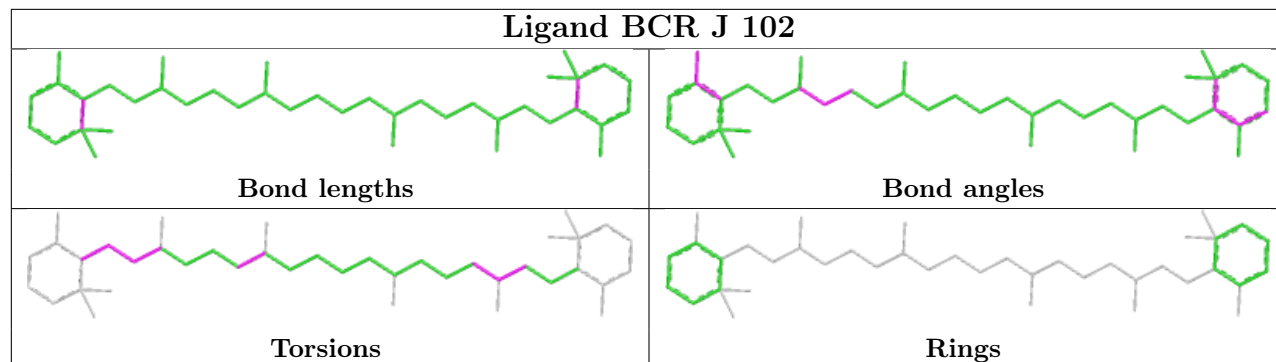


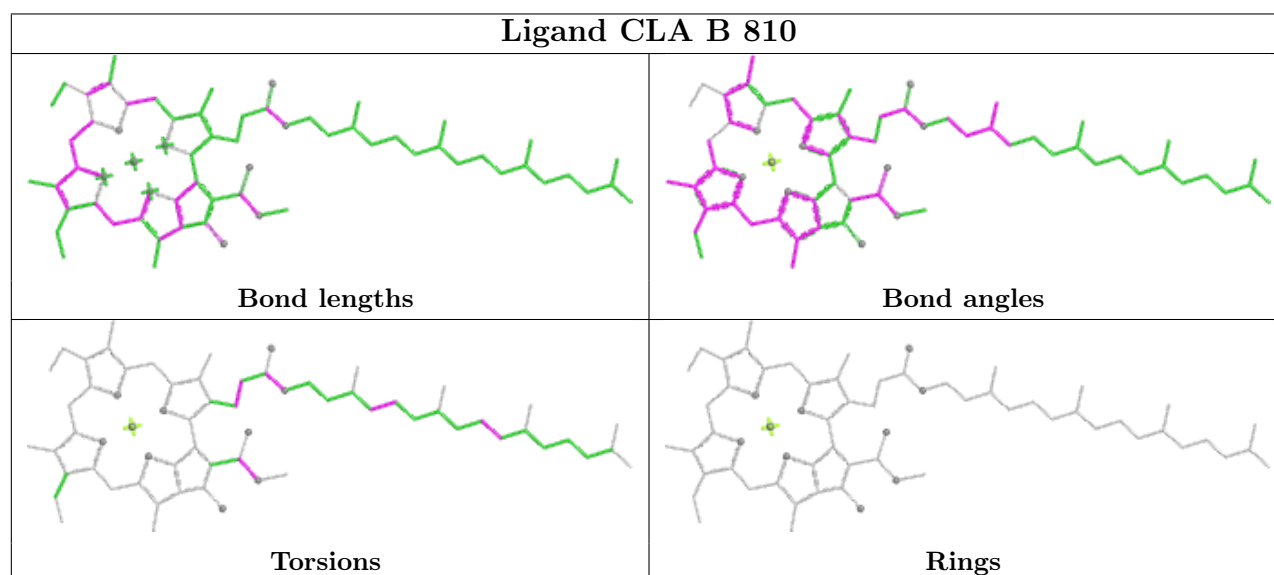
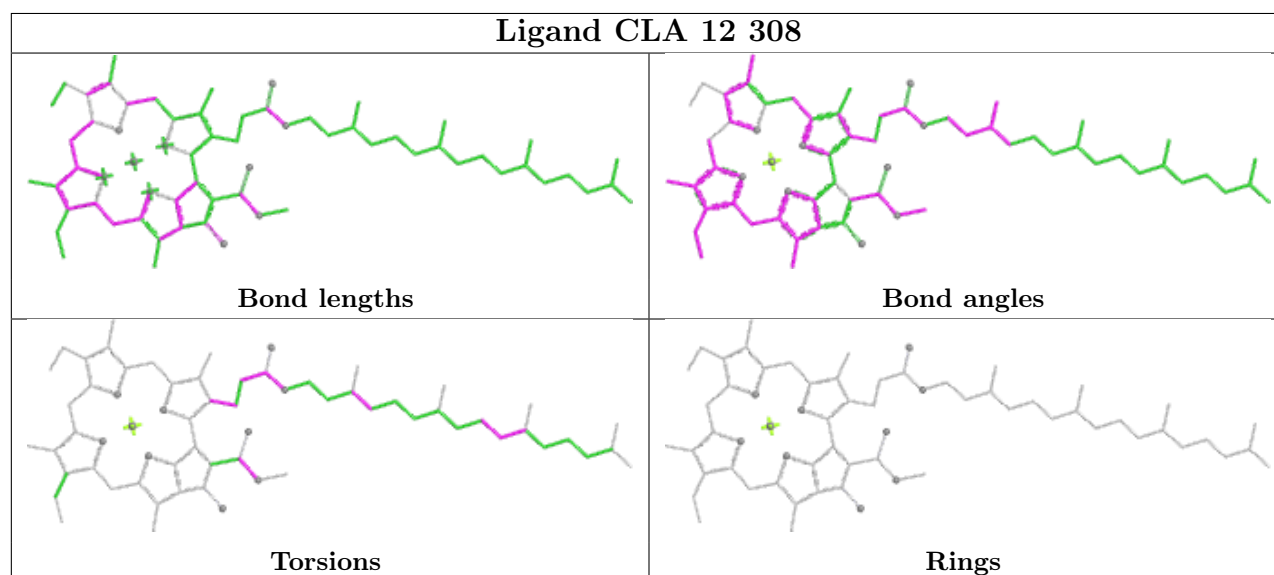
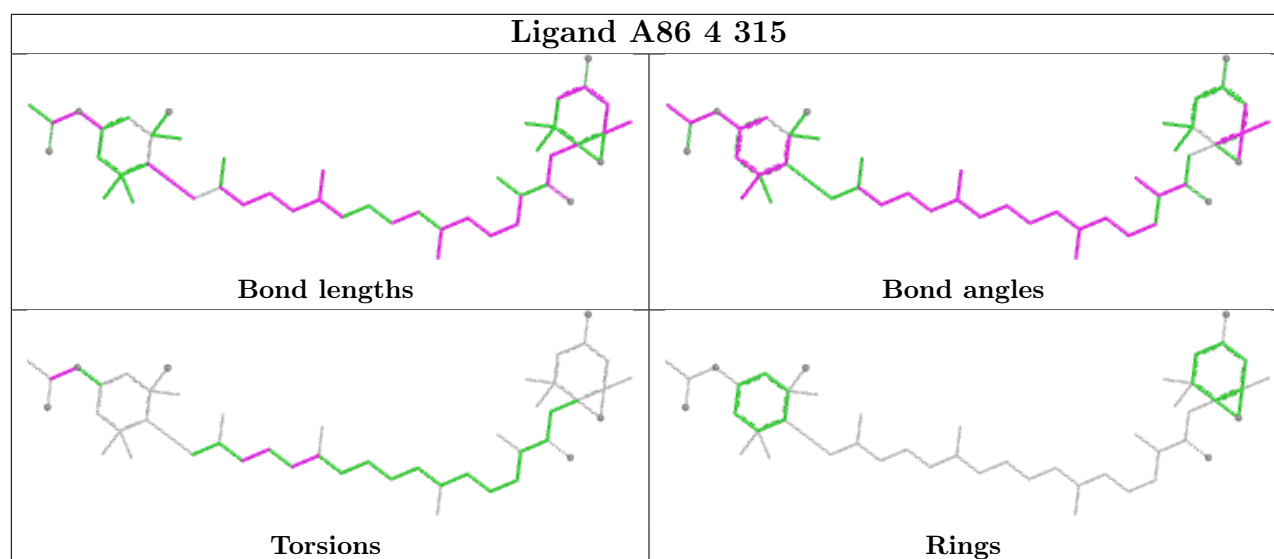
## Ligand CLA B 806

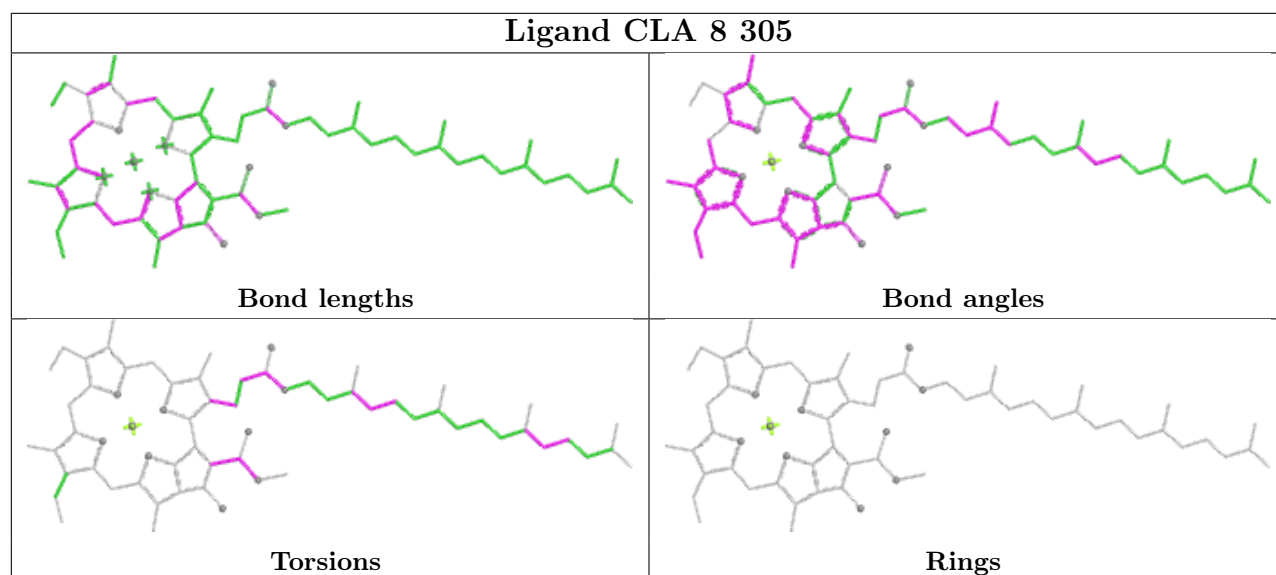
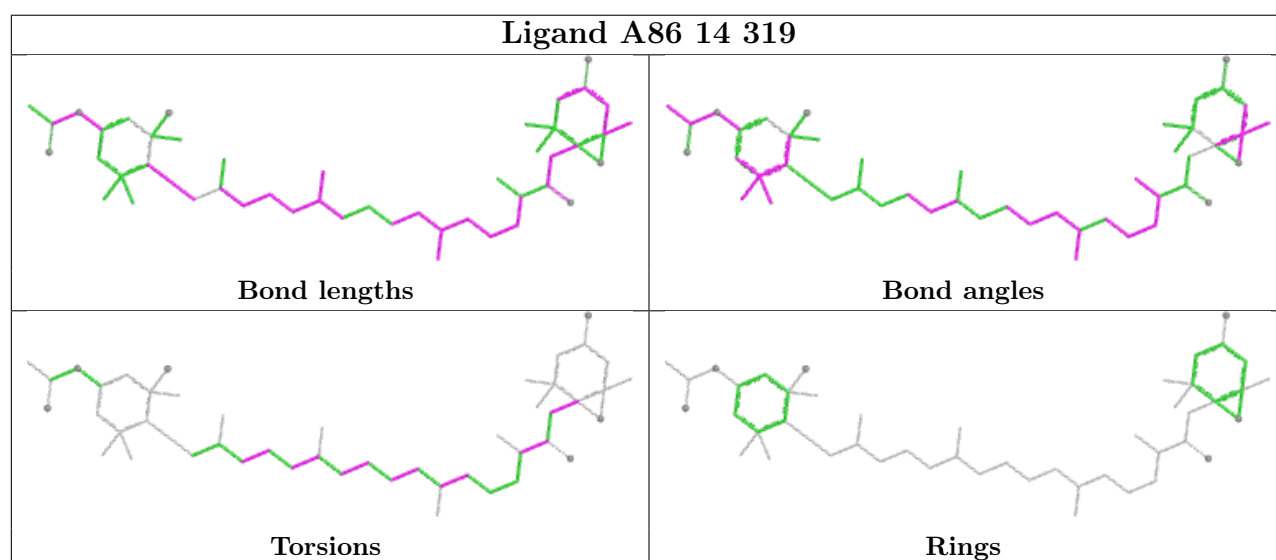
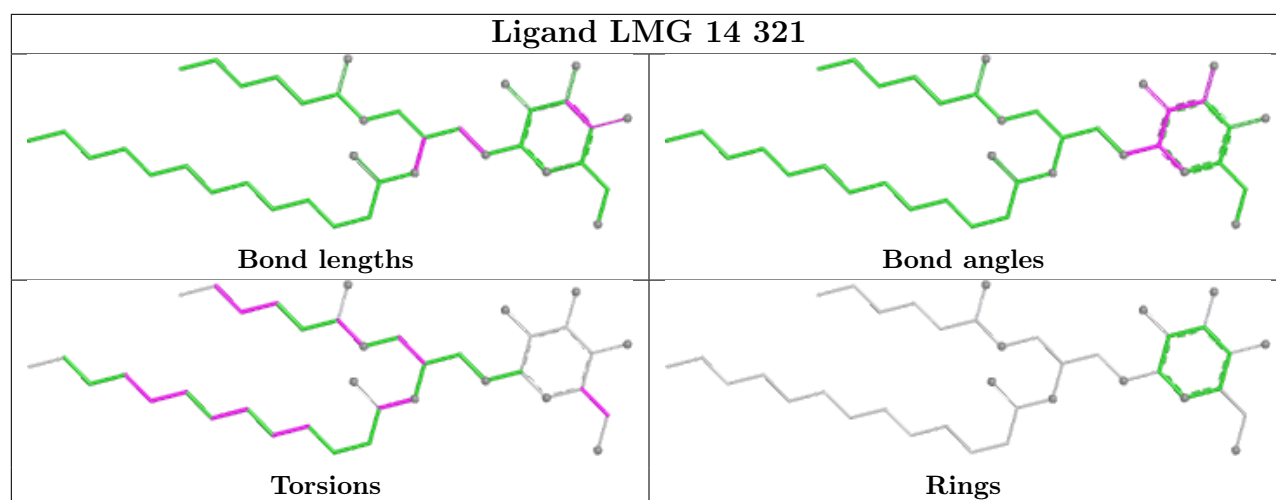


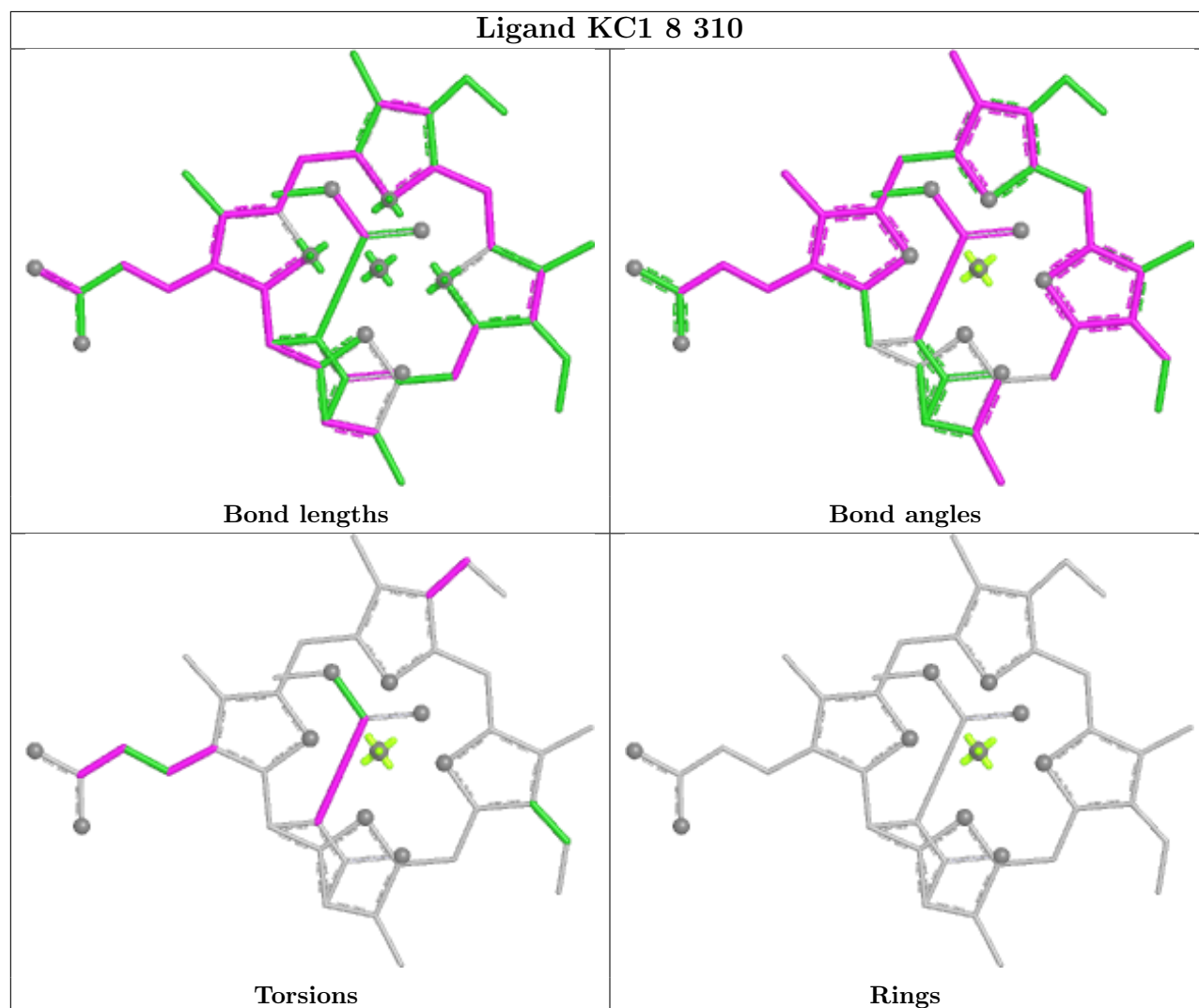
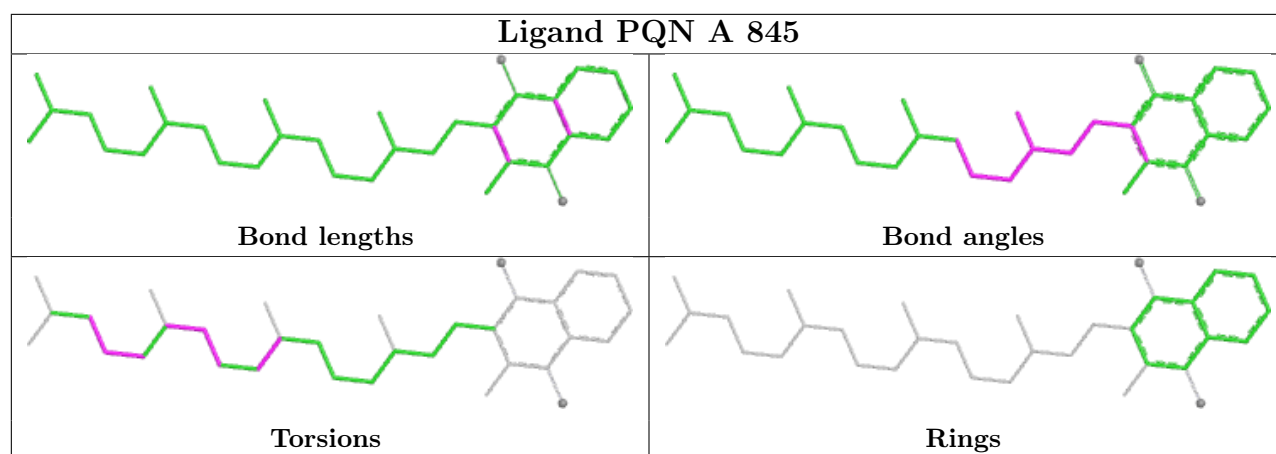
## Ligand KC1 6 312

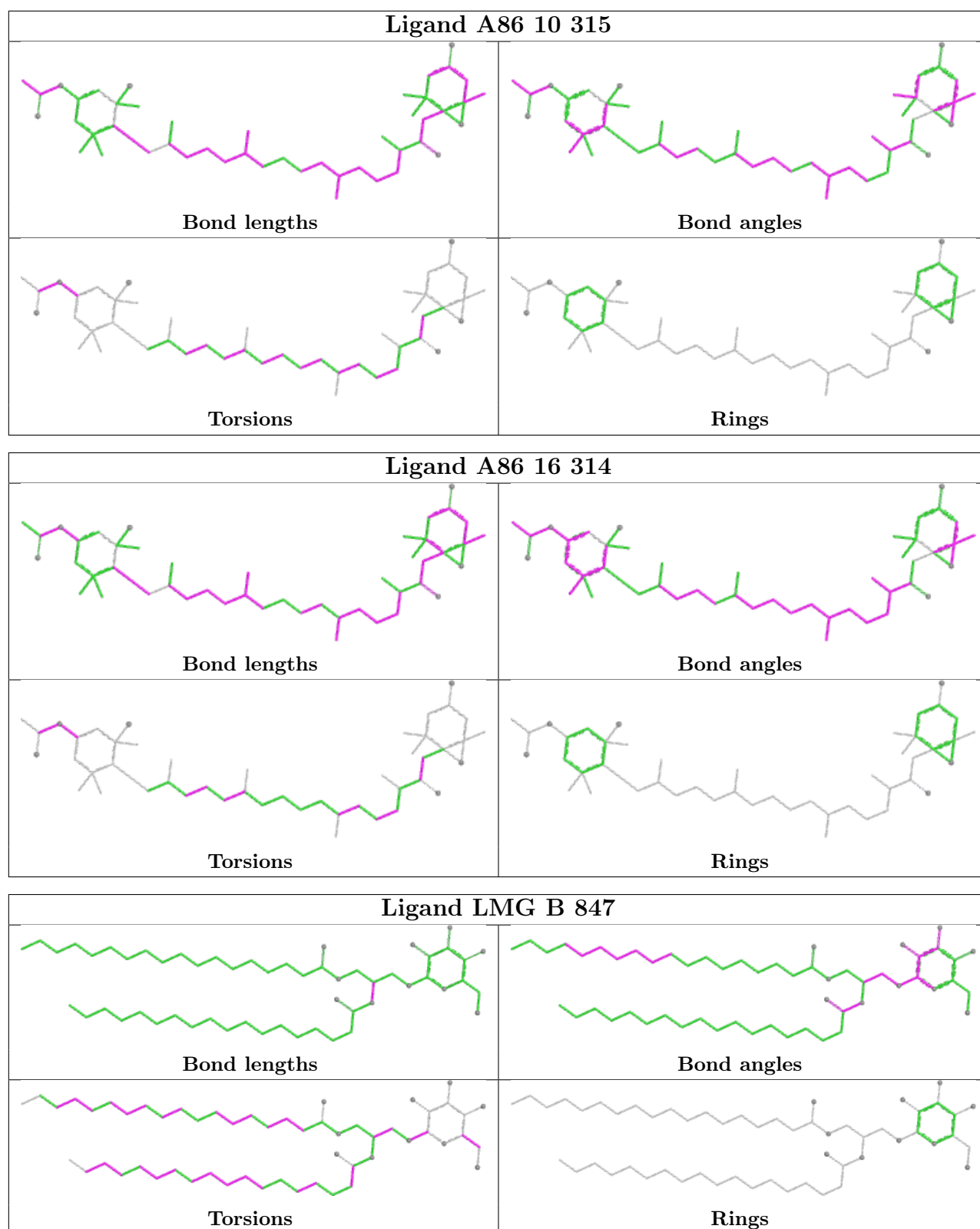


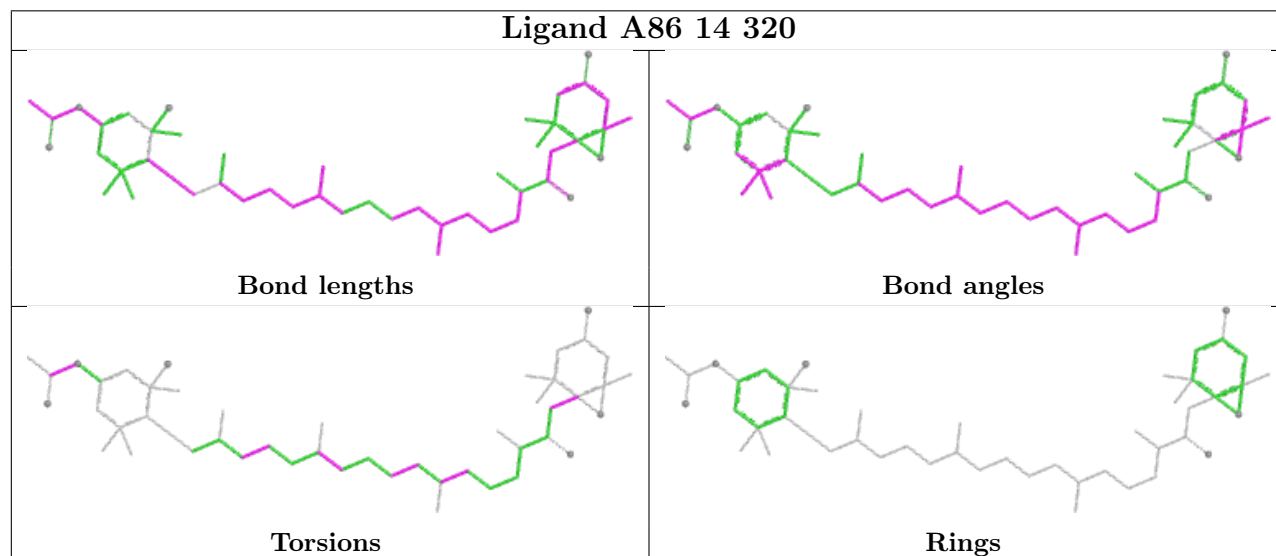
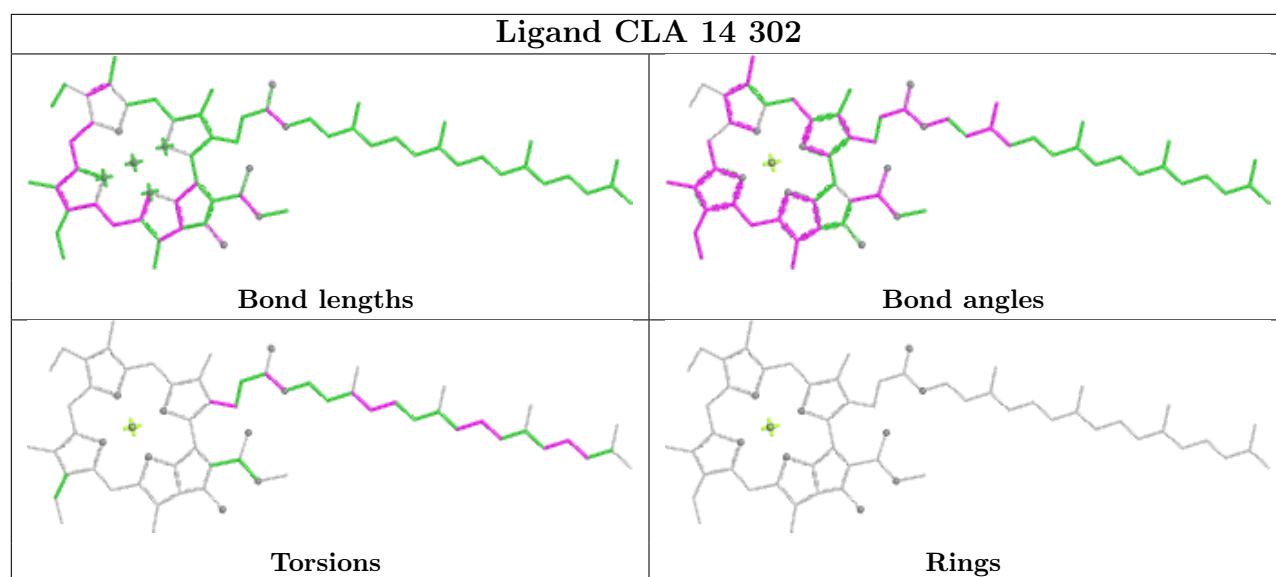
**Ligand CLA A 842****Ligand CLA 4 306****Ligand BCR J 102**

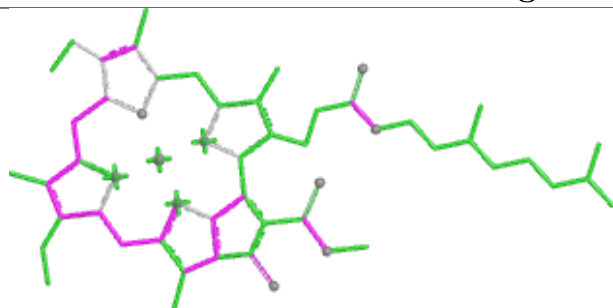




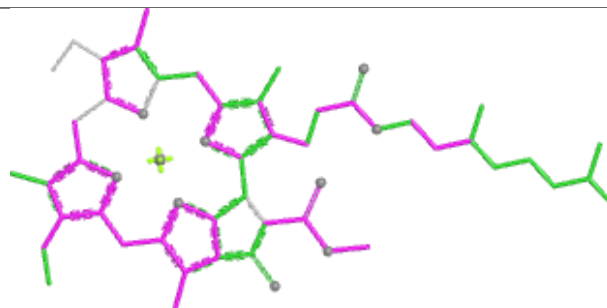




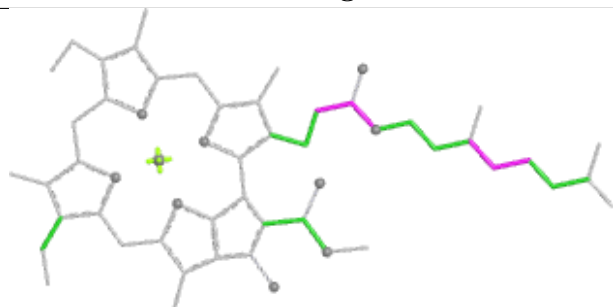


**Ligand CLA 6 316**

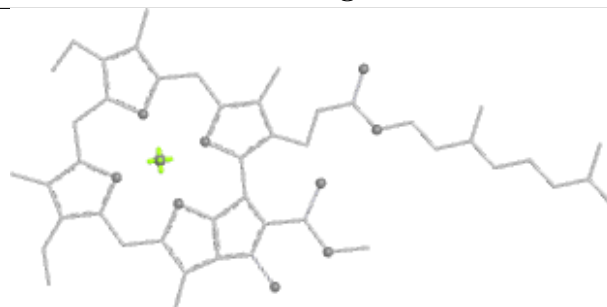
Bond lengths



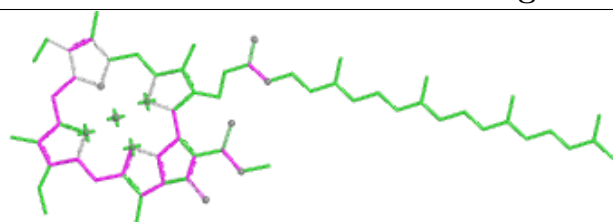
Bond angles



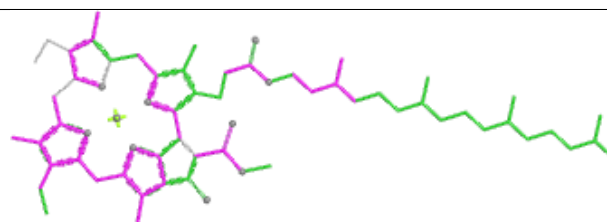
Torsions



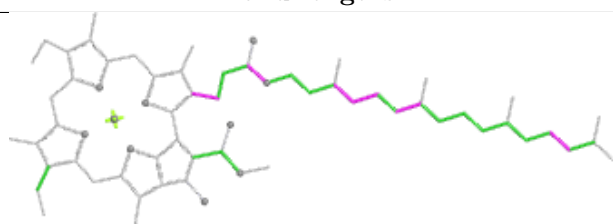
Rings

**Ligand CLA 9 307**

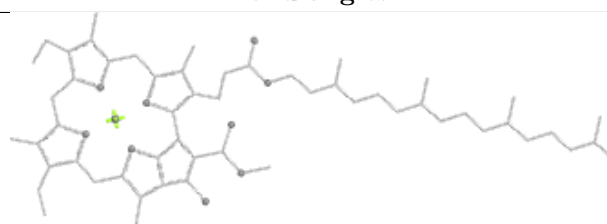
Bond lengths



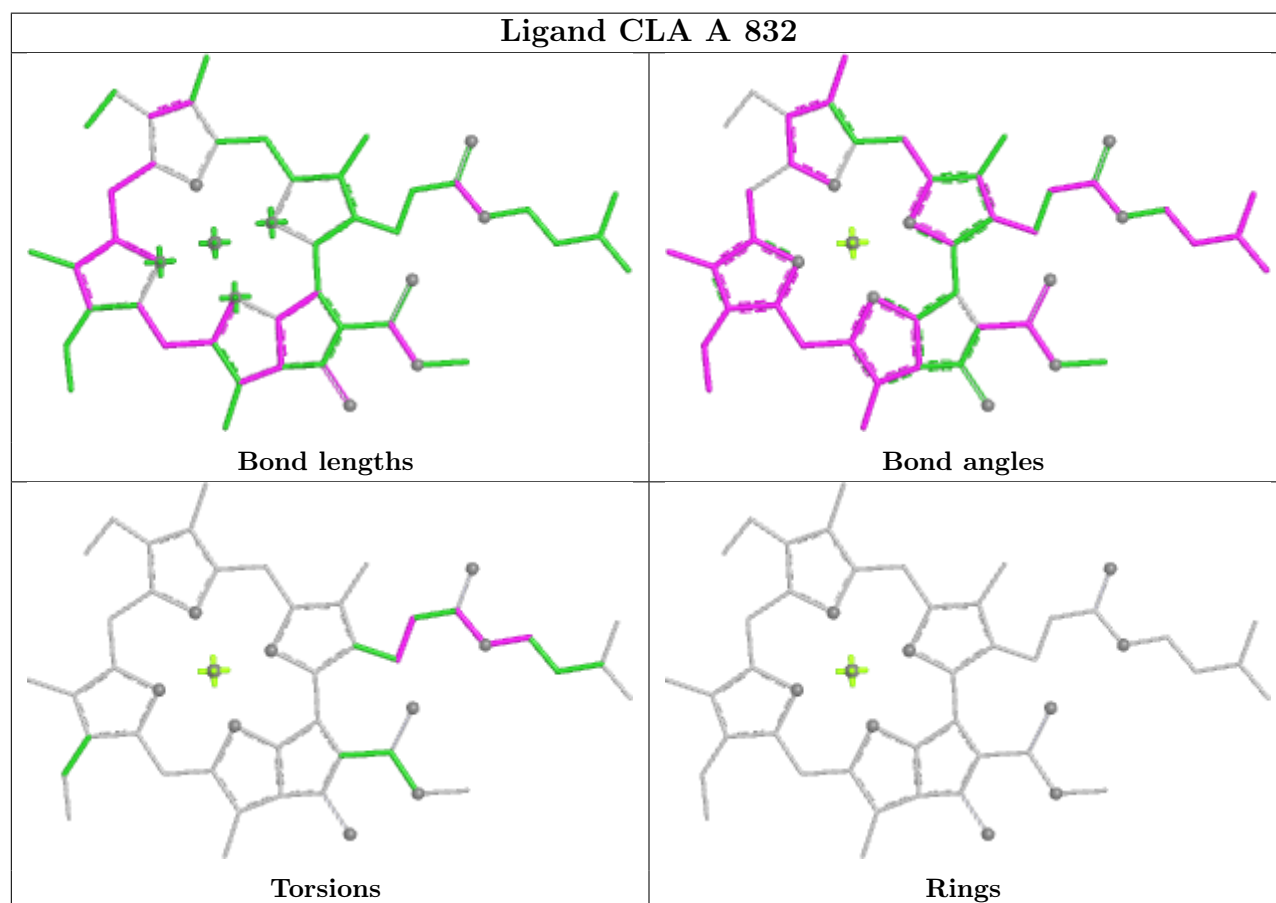
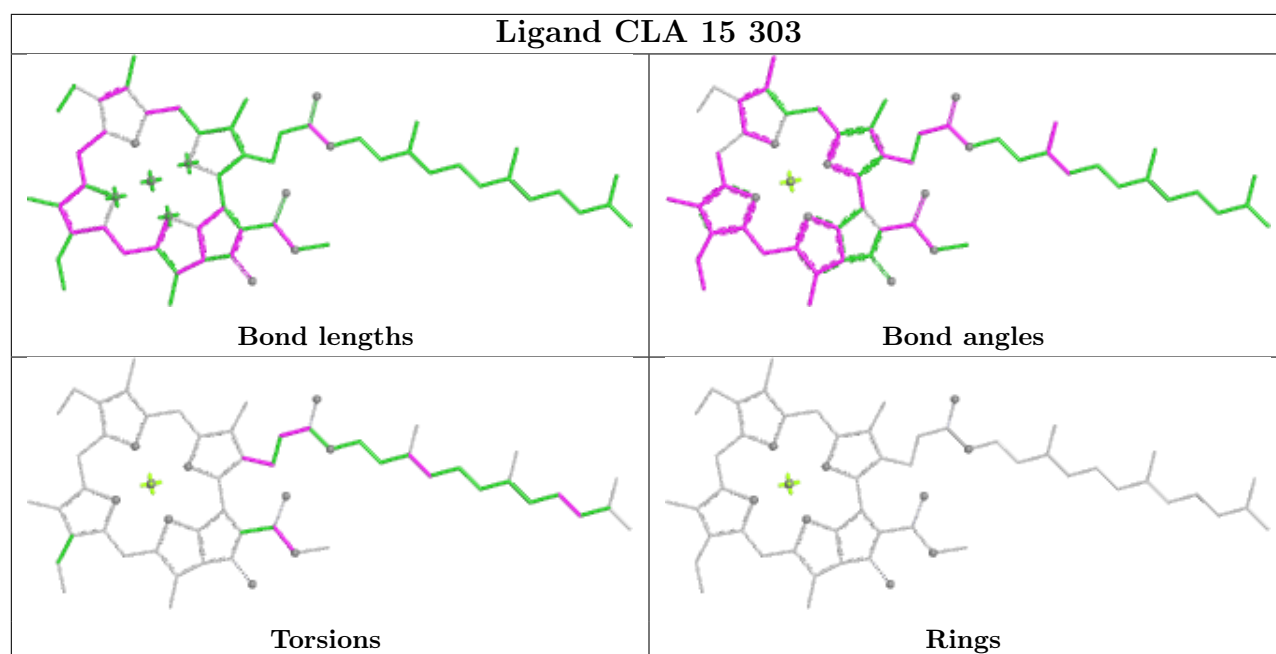
Bond angles

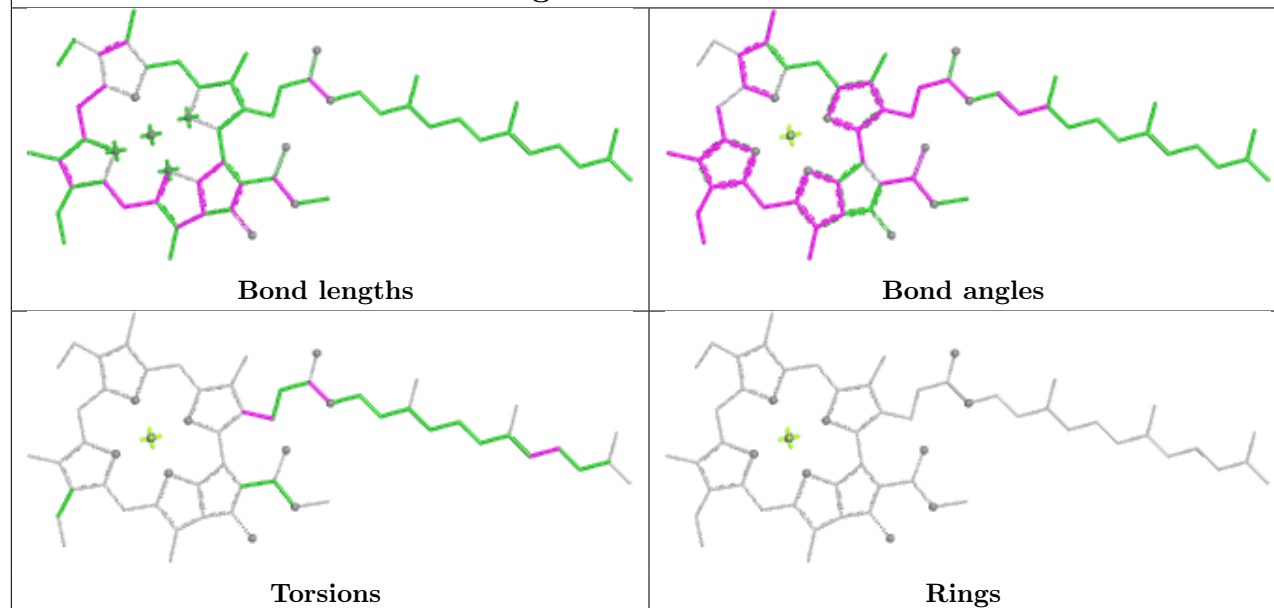
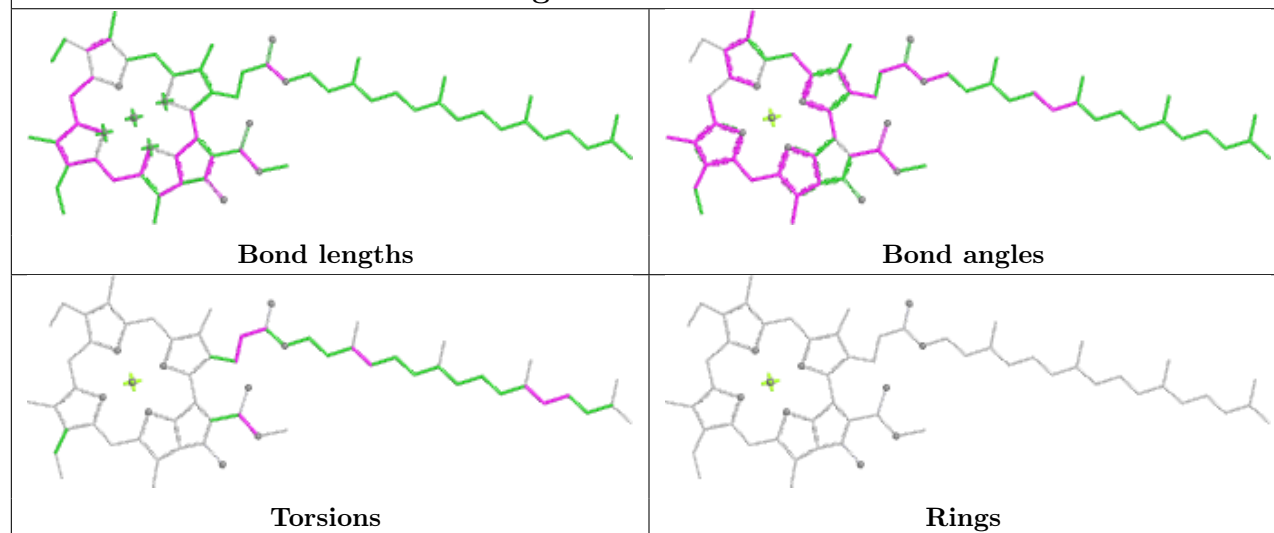


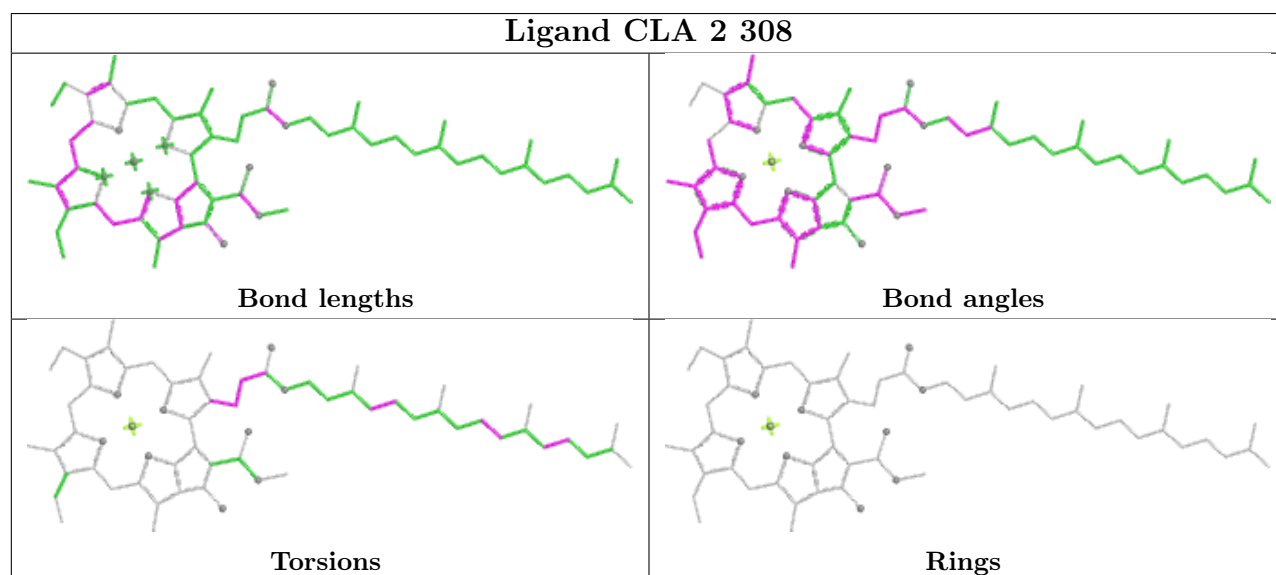
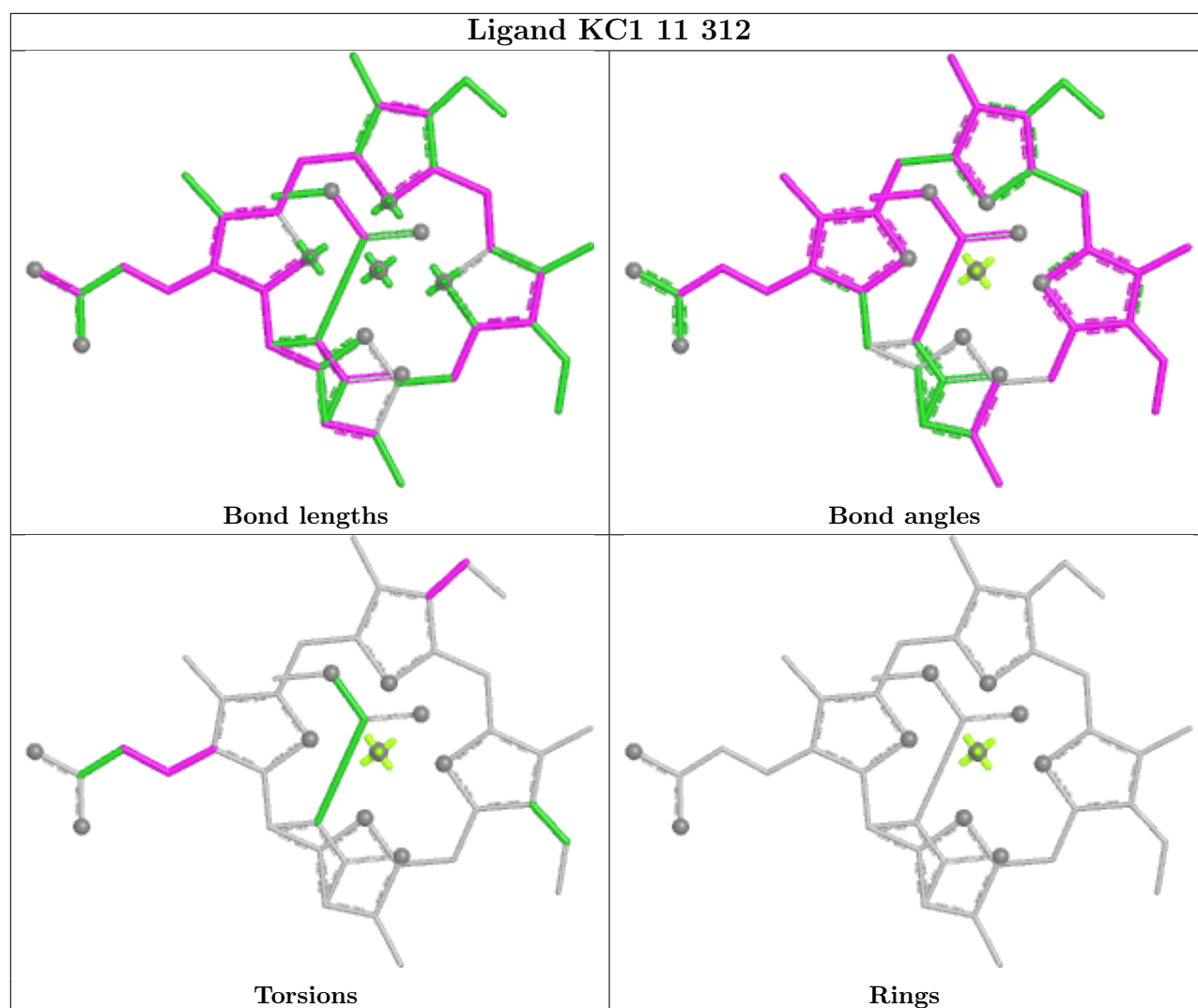
Torsions

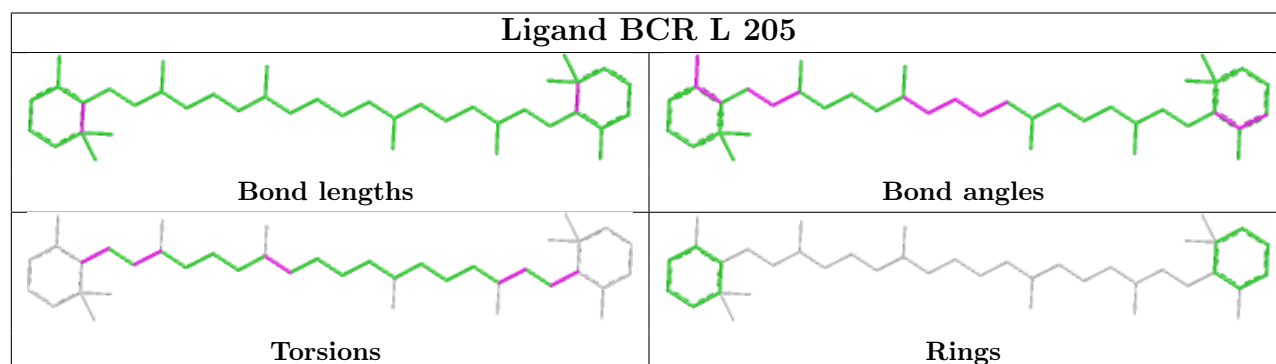
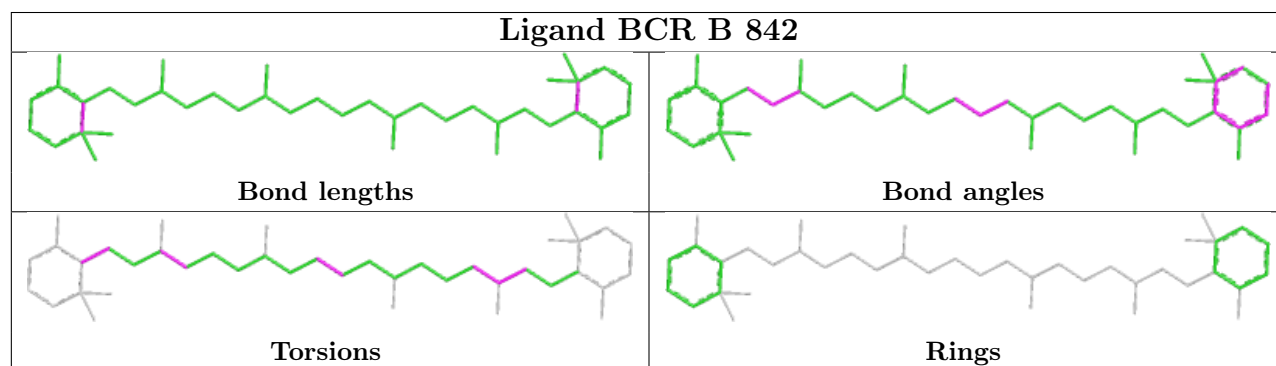
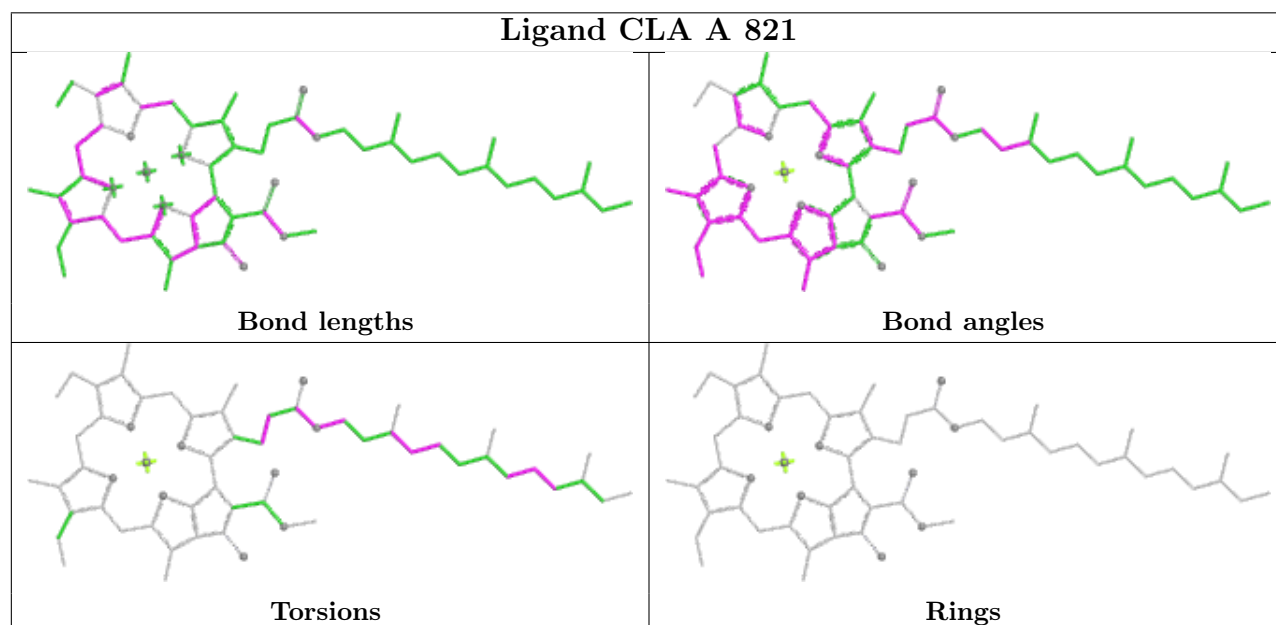
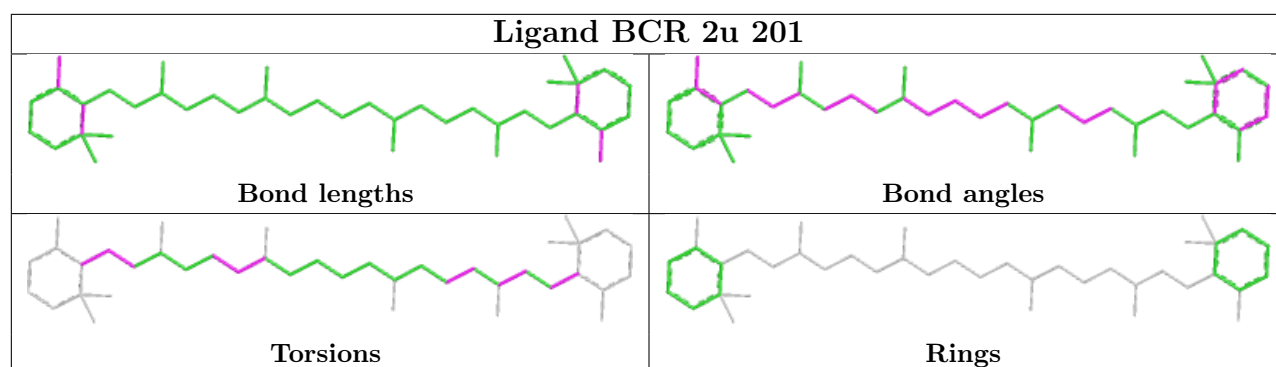


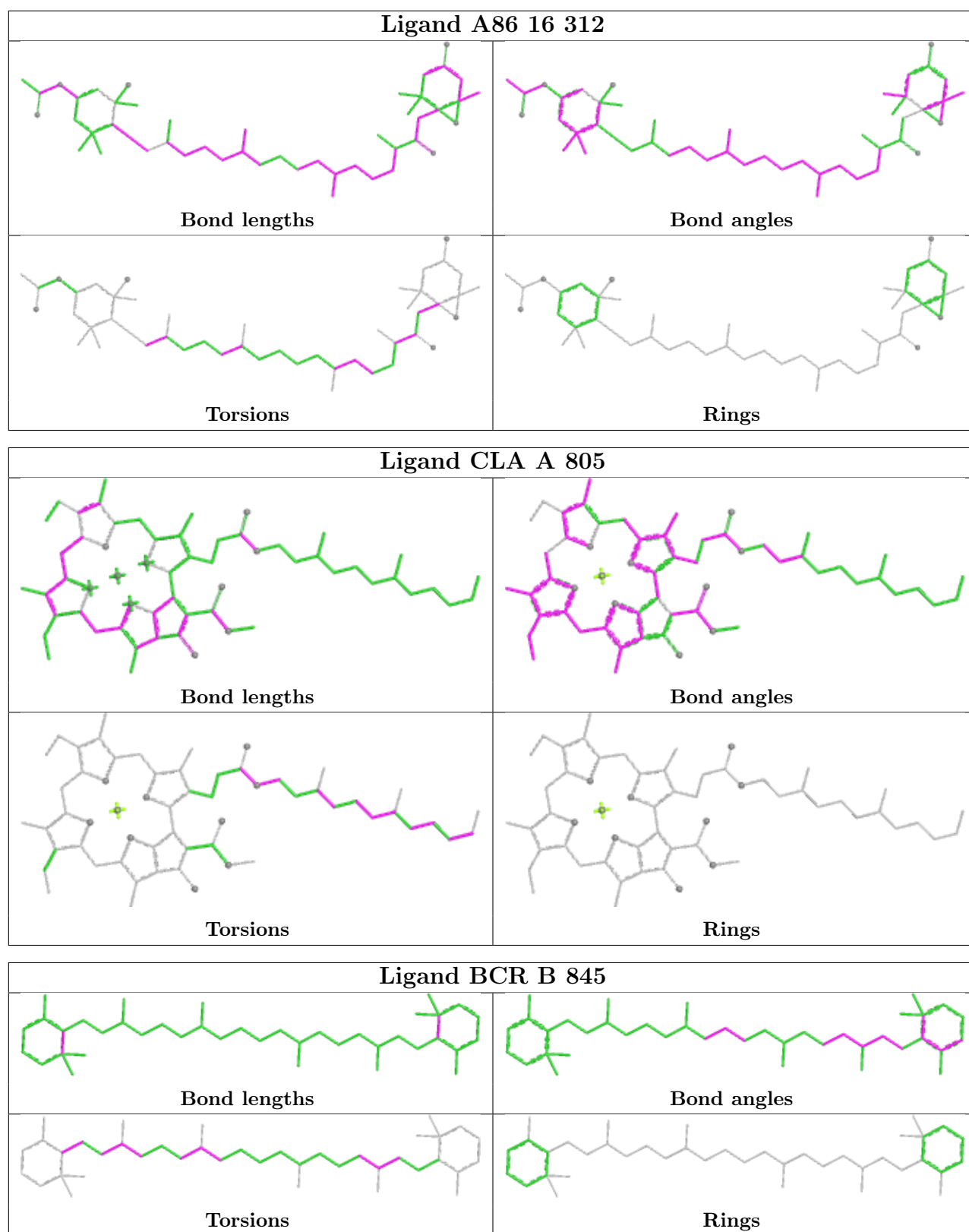
Rings

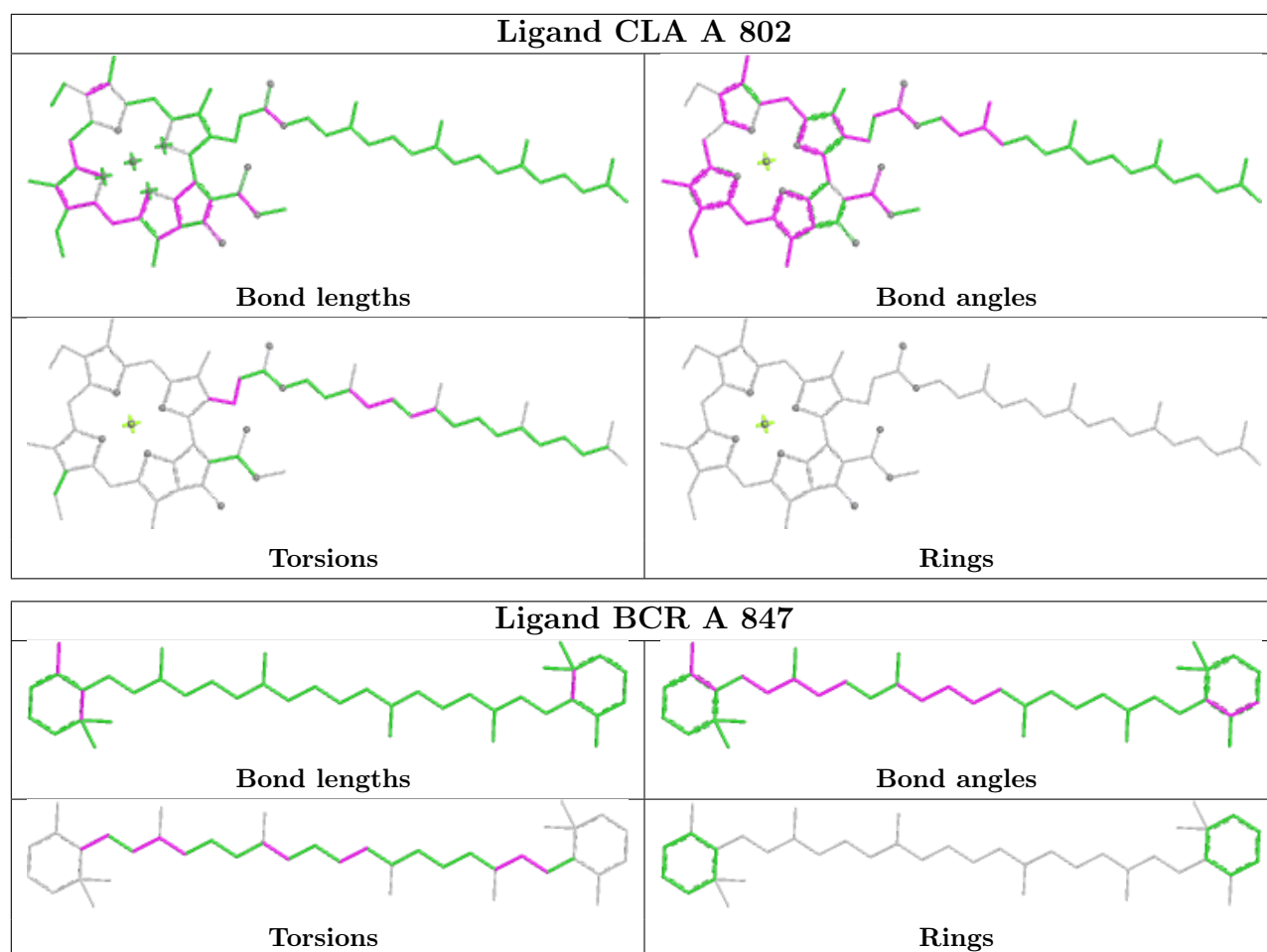


**Ligand CLA B 818****Ligand CLA B 830**

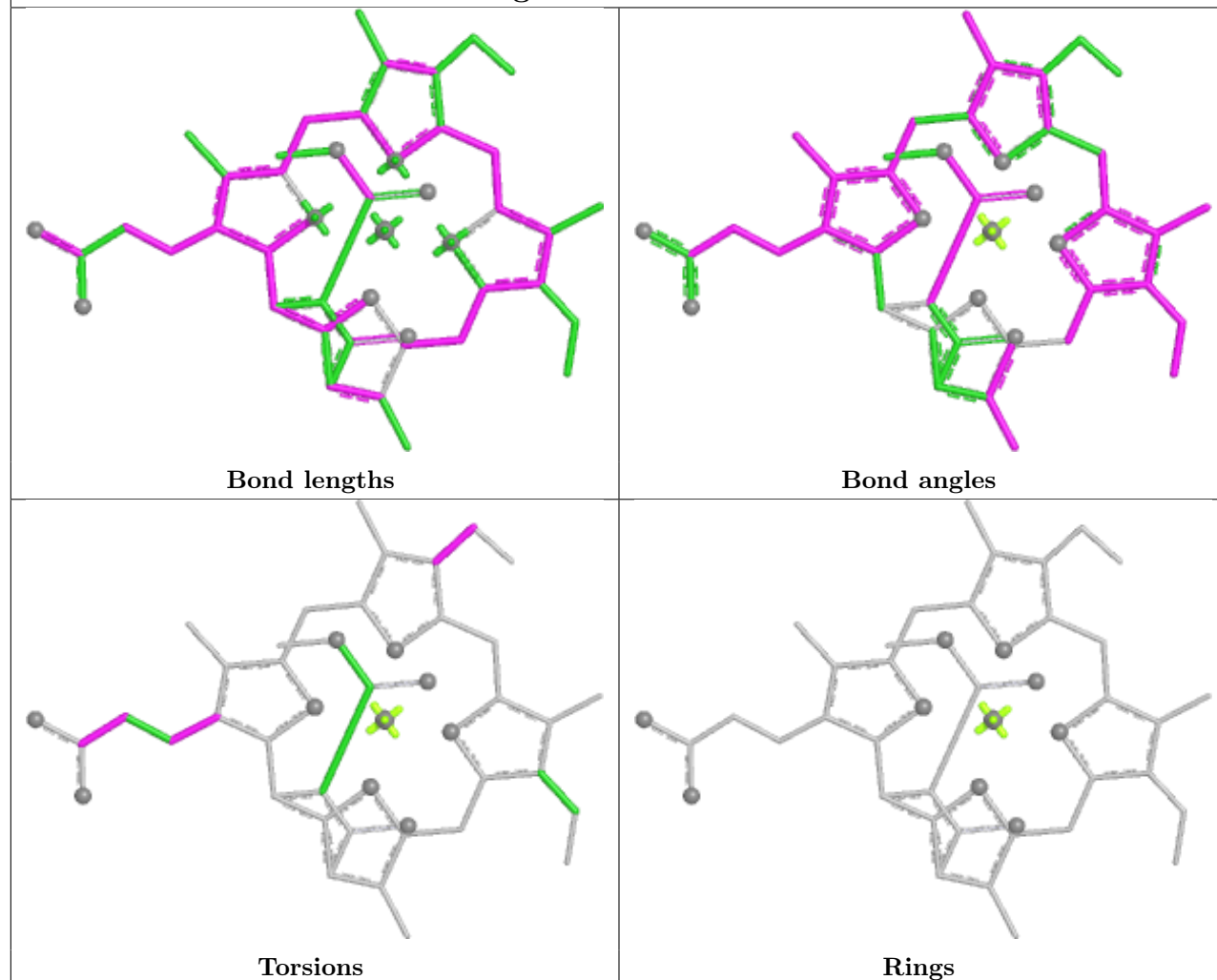




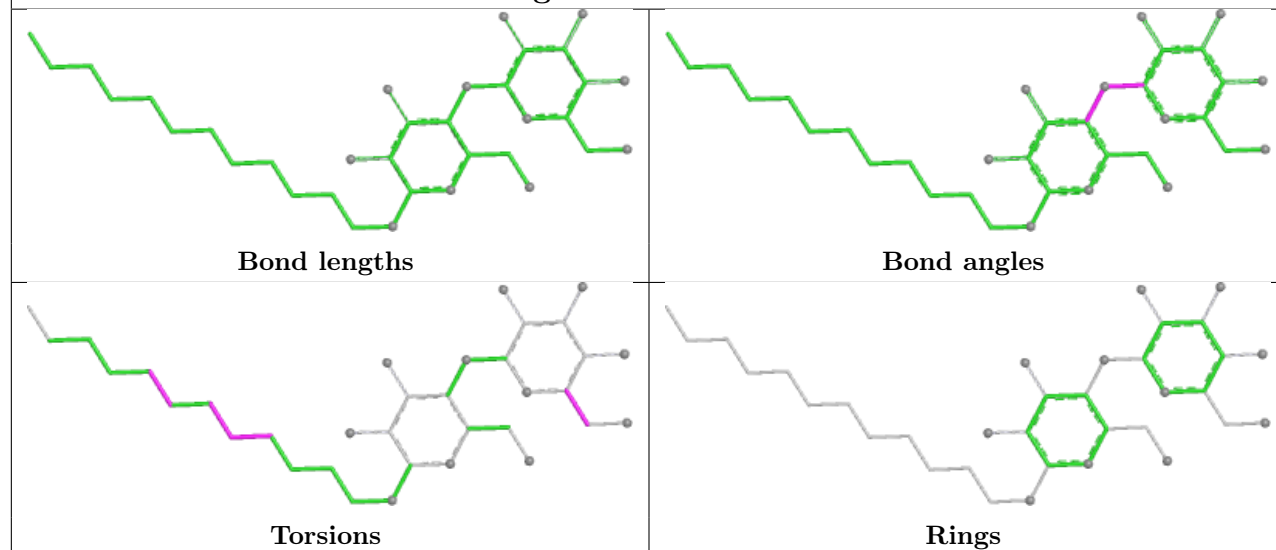


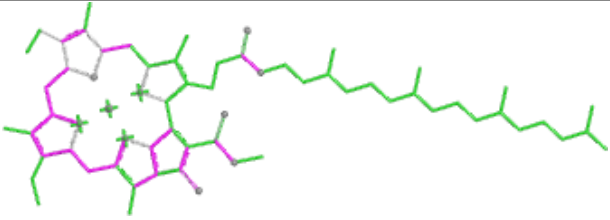
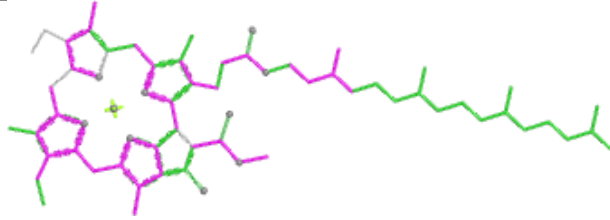
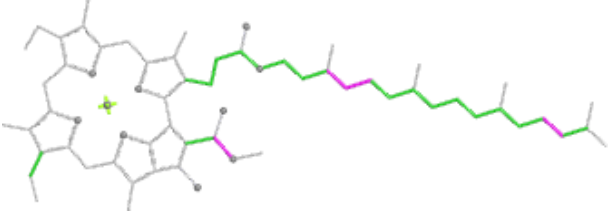
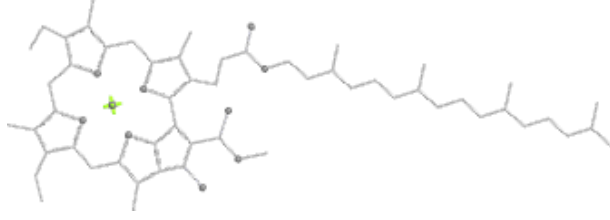
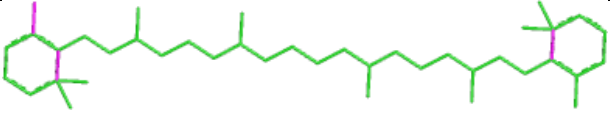
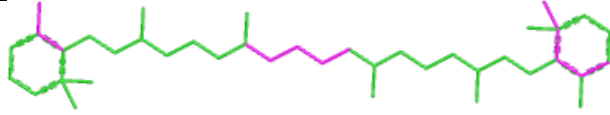
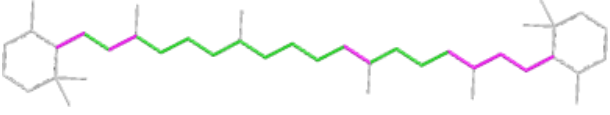
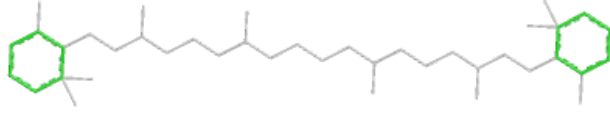
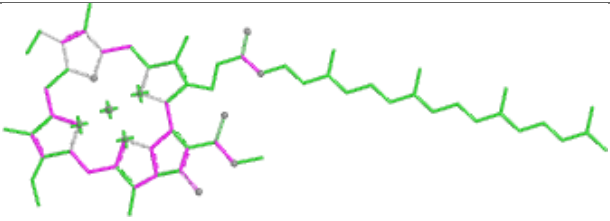
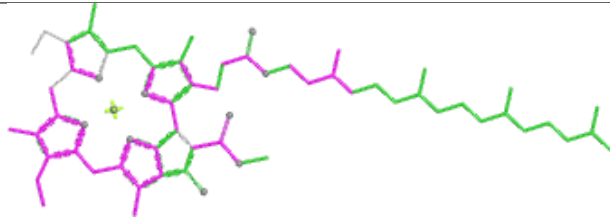
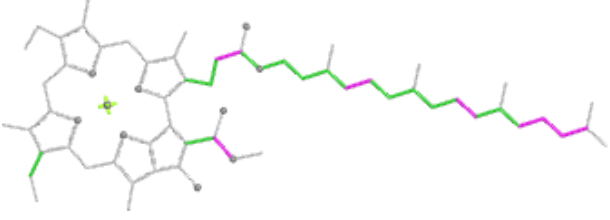
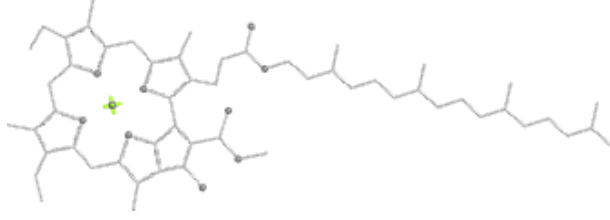


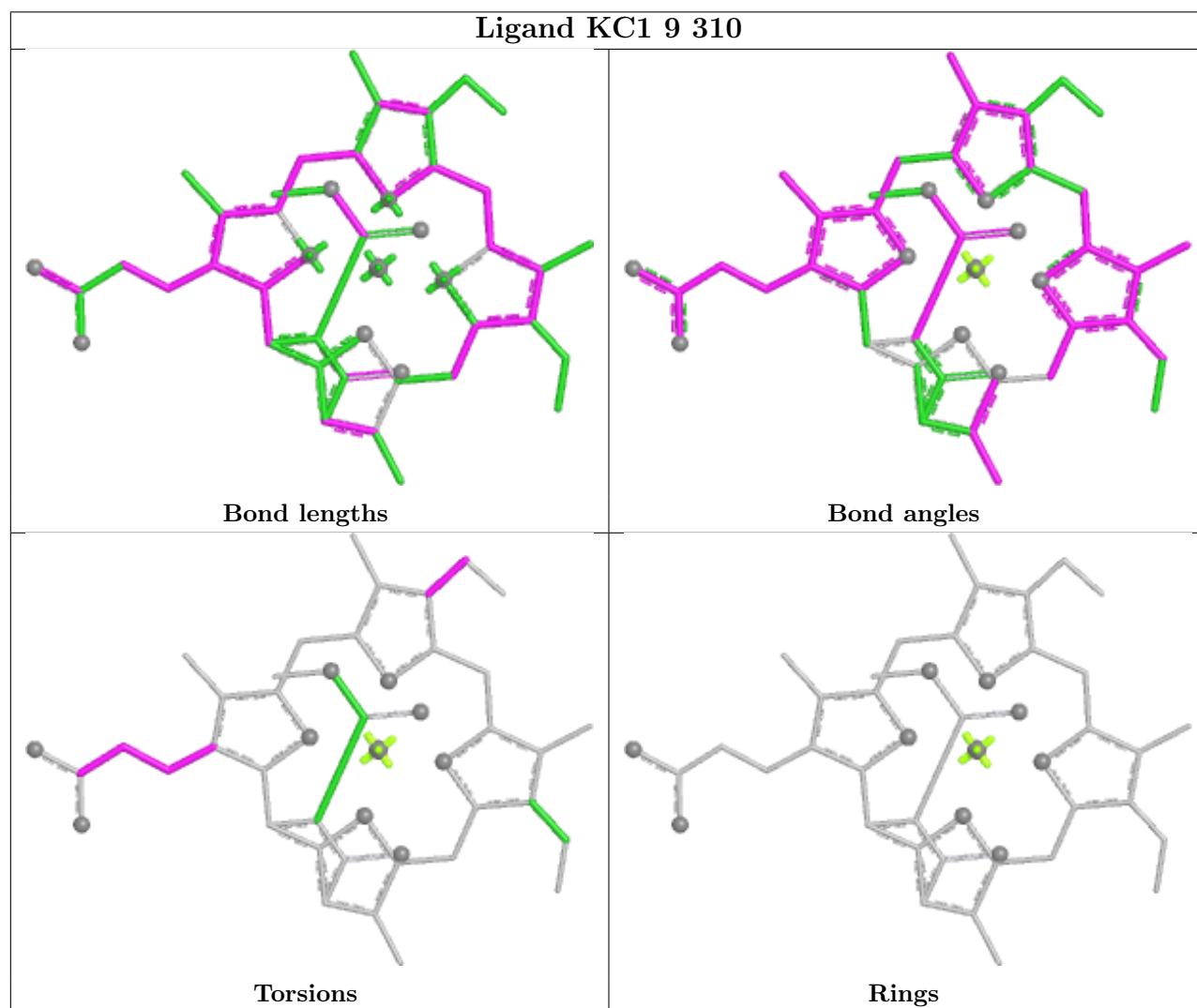
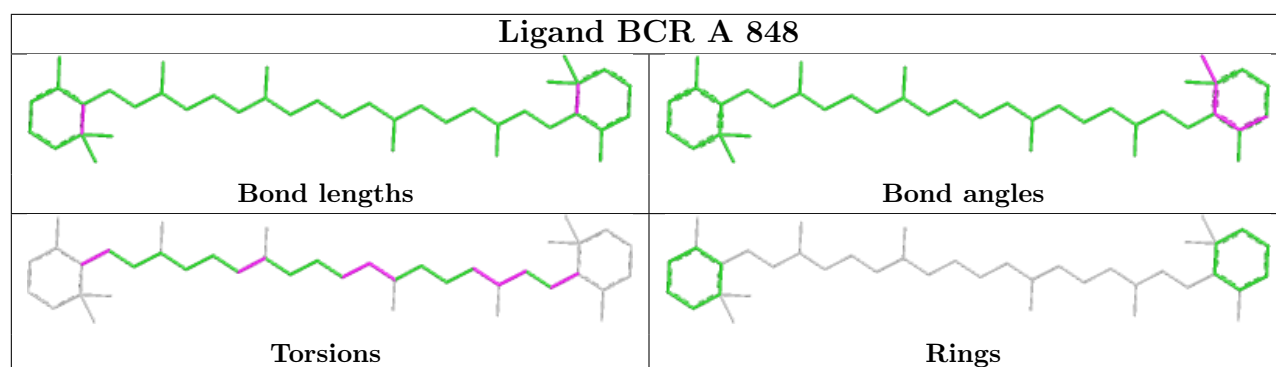
## Ligand KC1 2 306

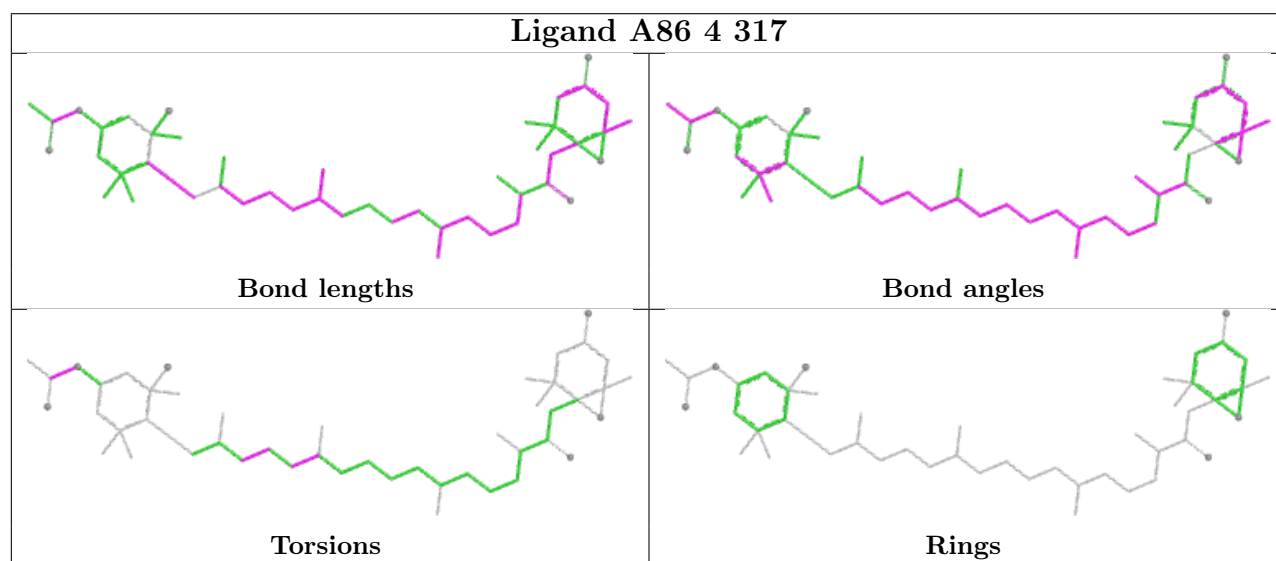
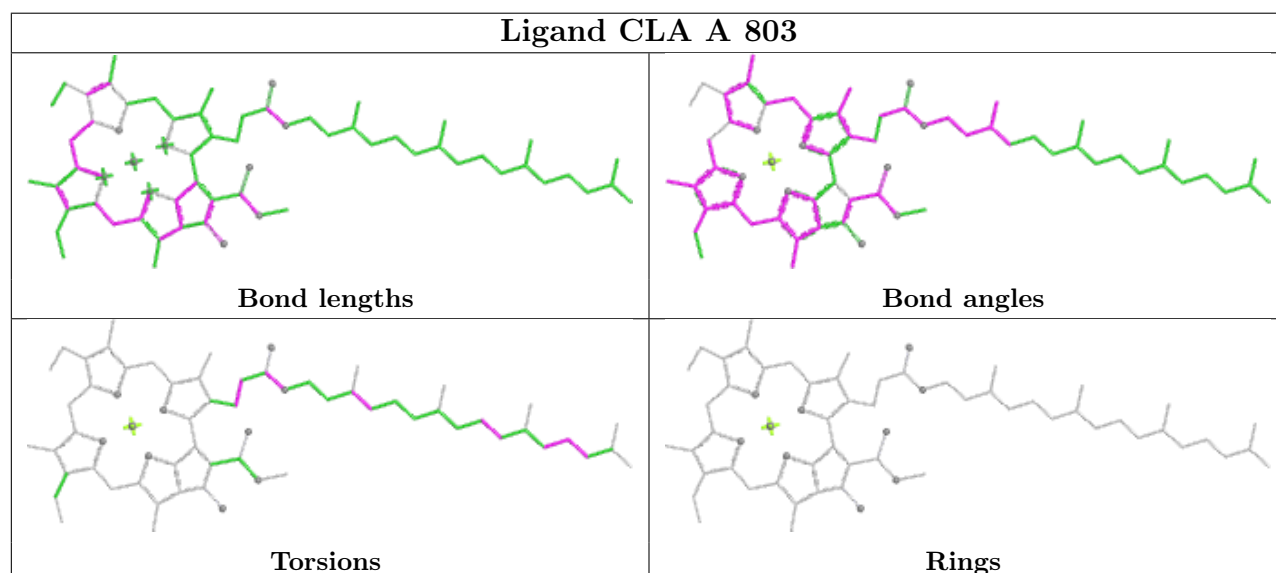
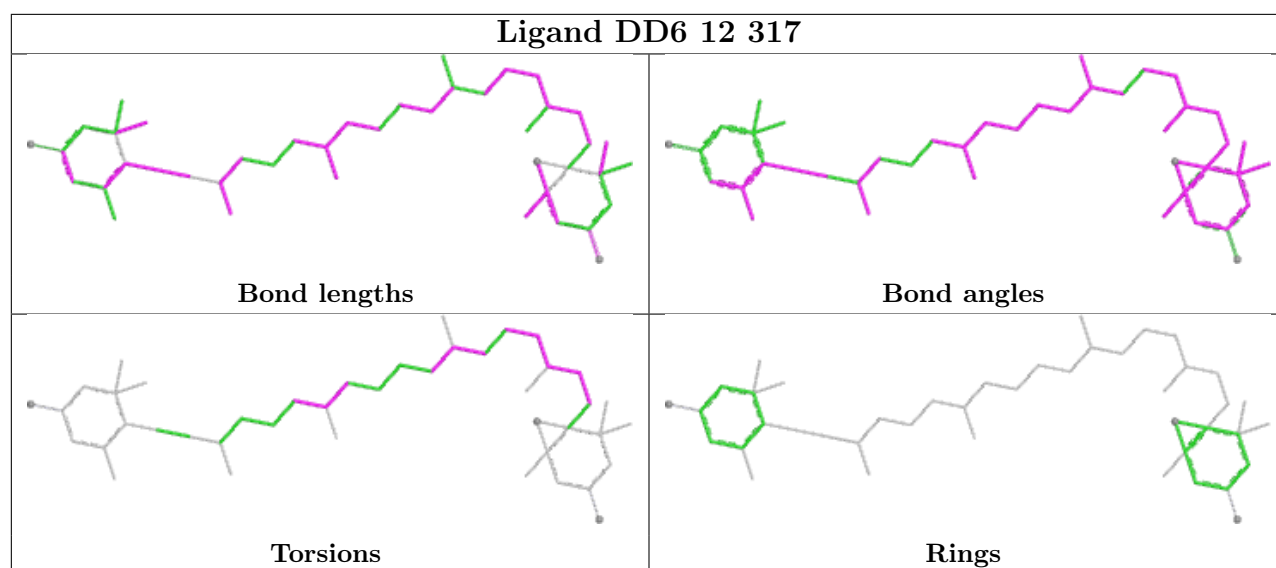


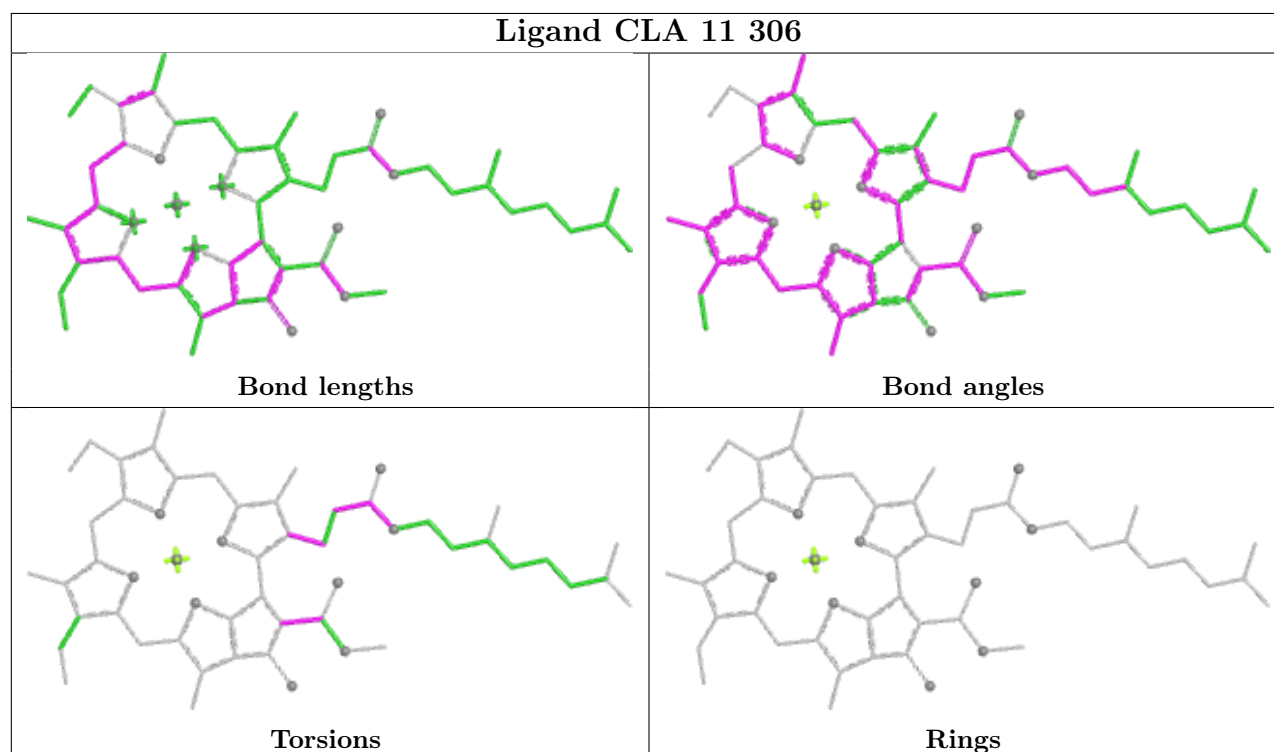
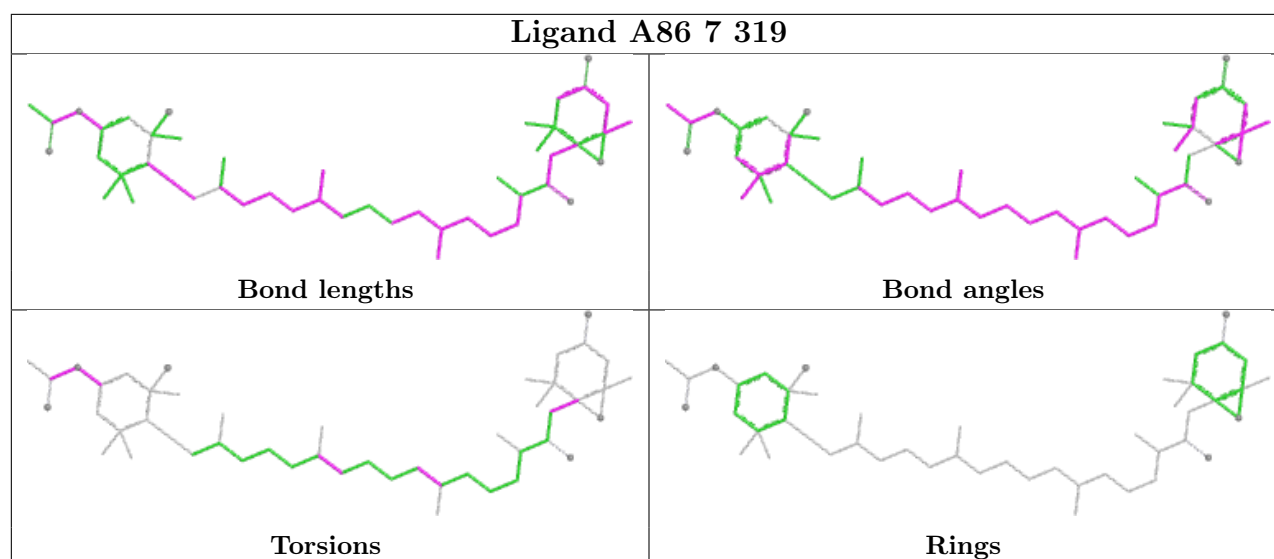
## Ligand LMT 7 321

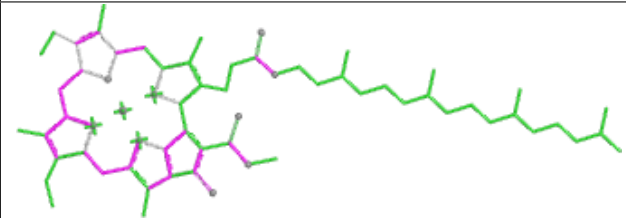
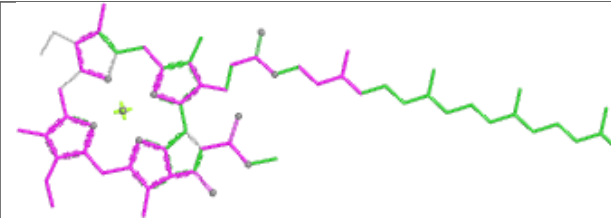
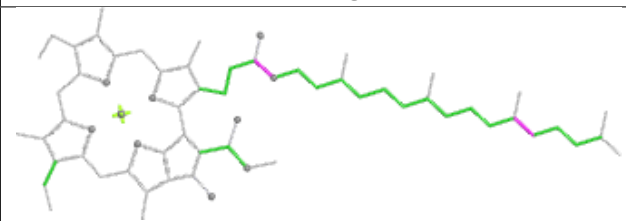
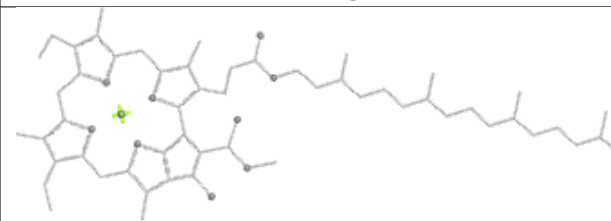


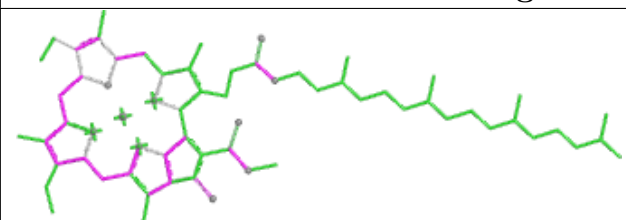
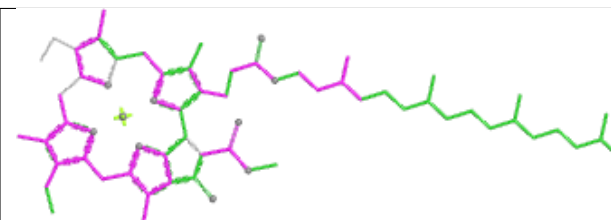
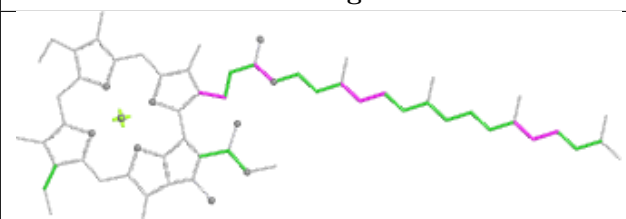
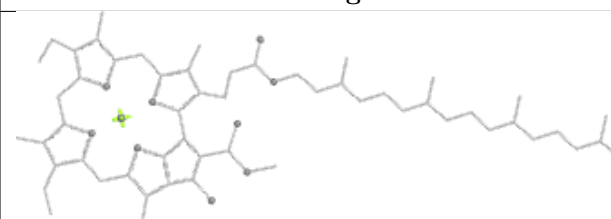
Ligand CLA 12 303	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR M 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 809	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

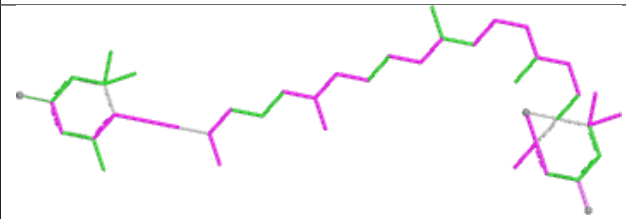
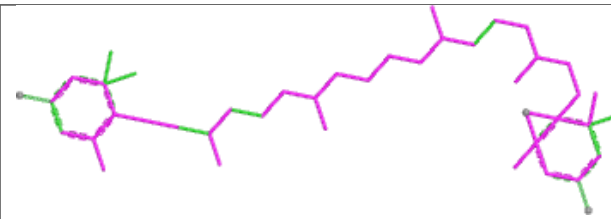
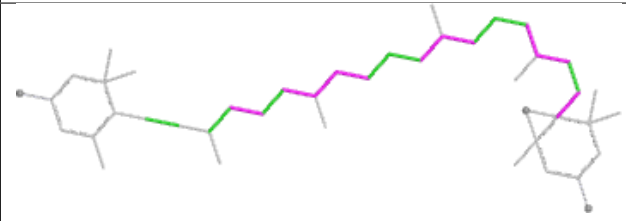
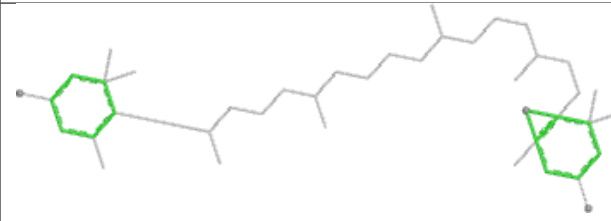


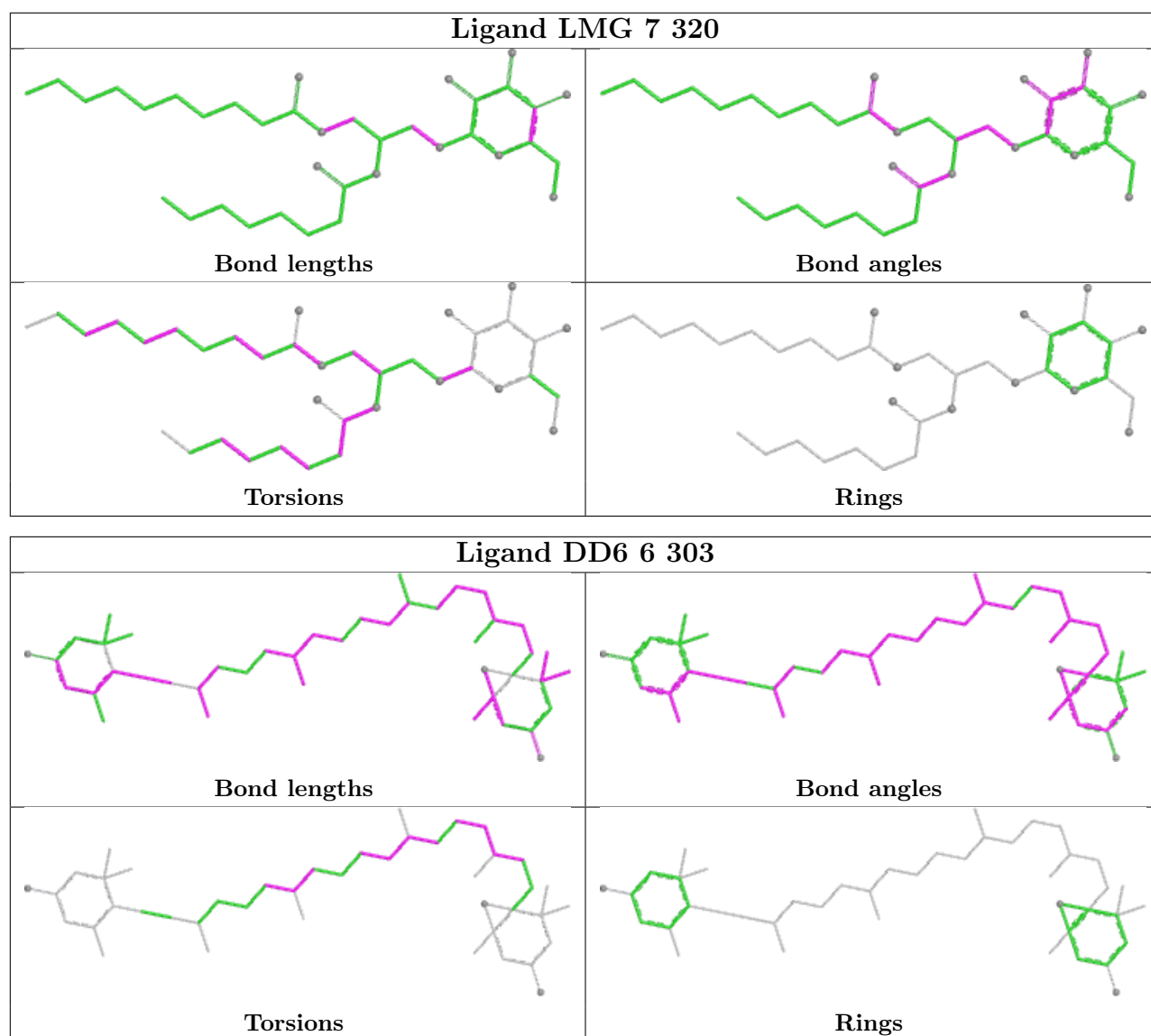




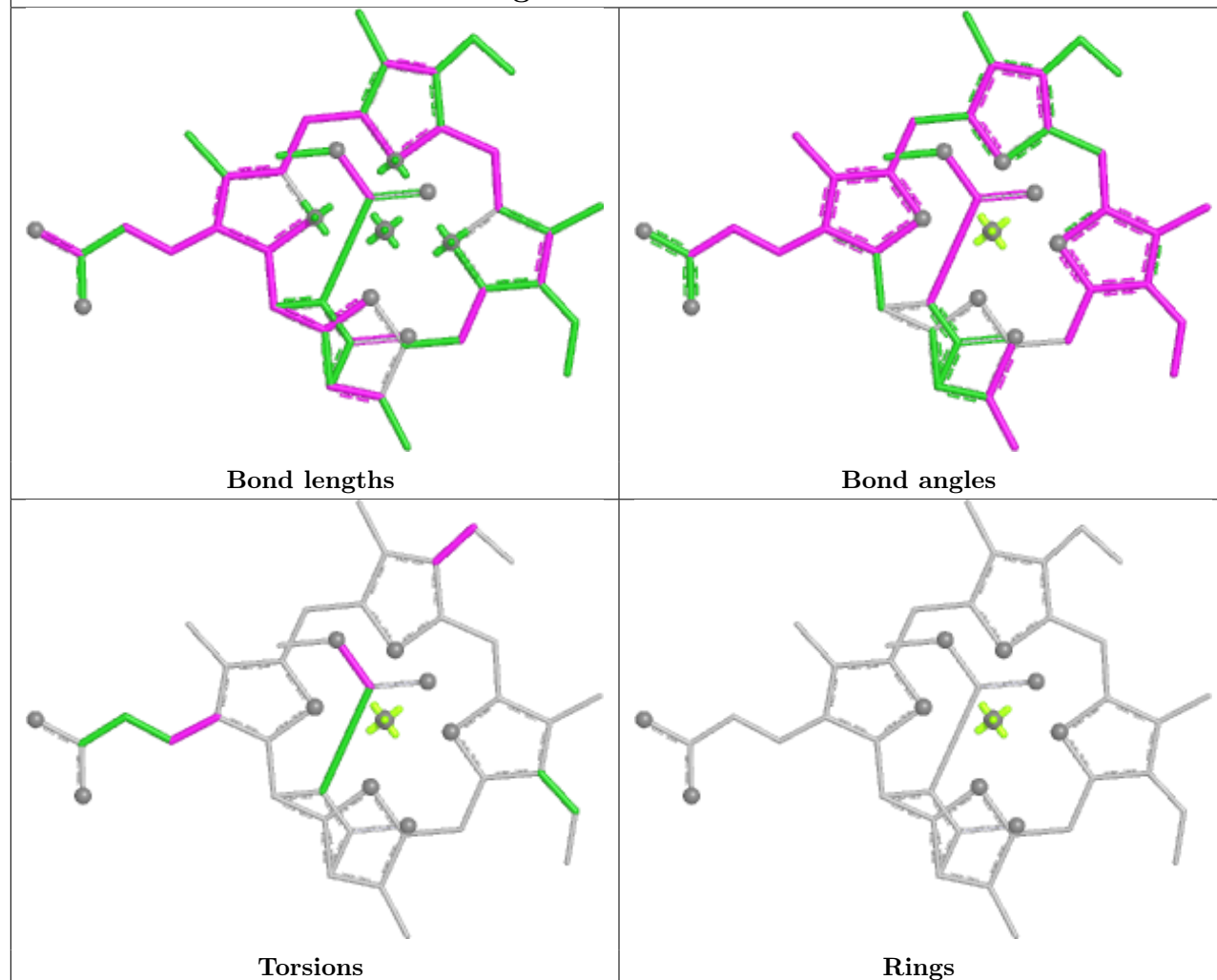
Ligand CLA A 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 11 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

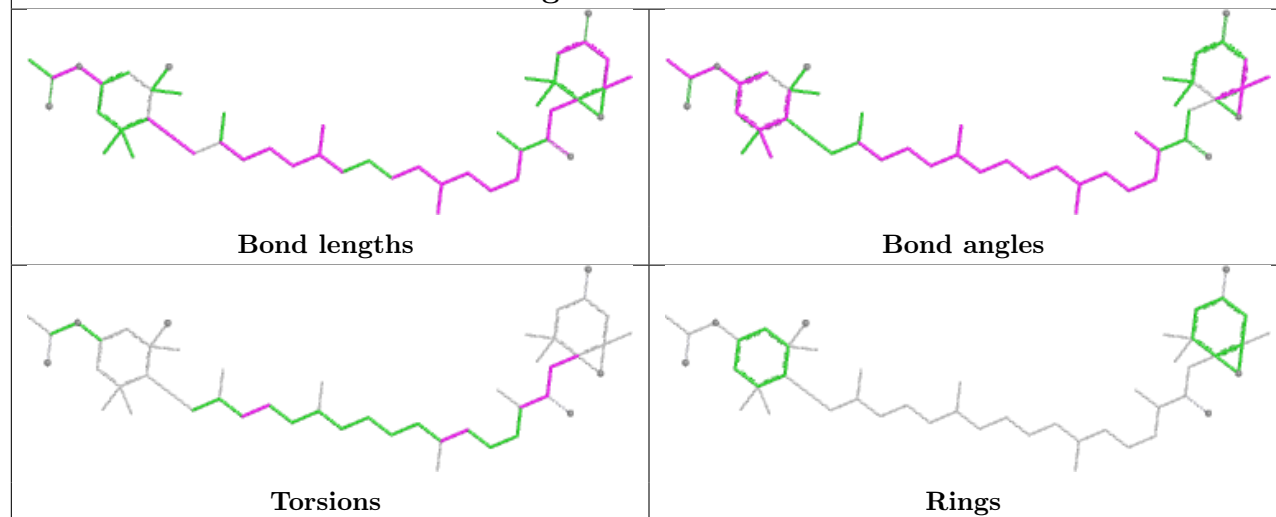
Ligand DD6 15 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

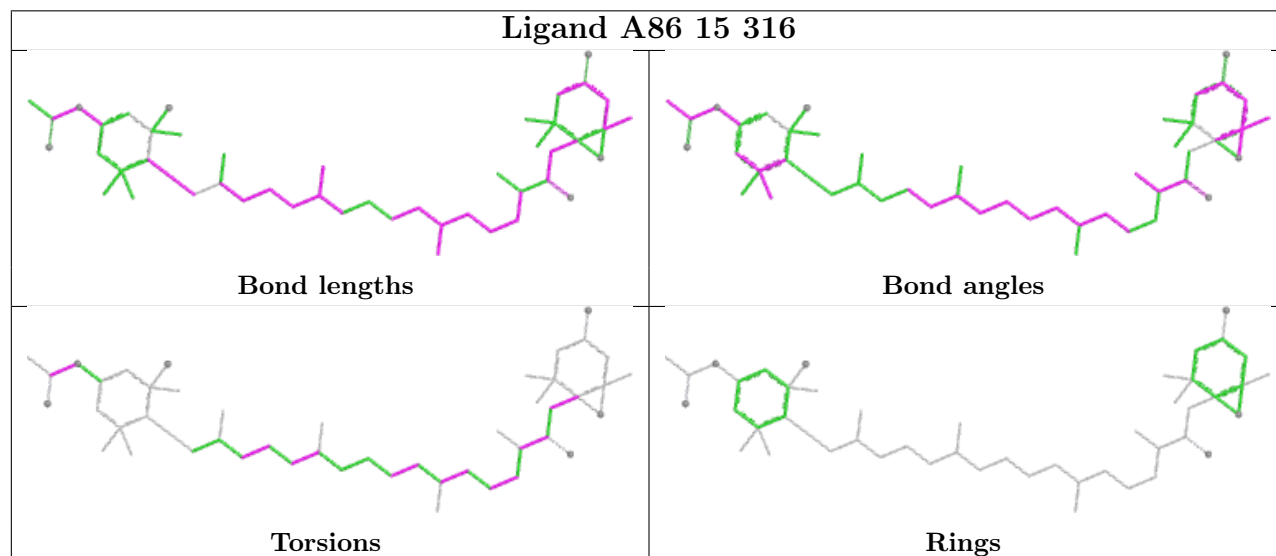
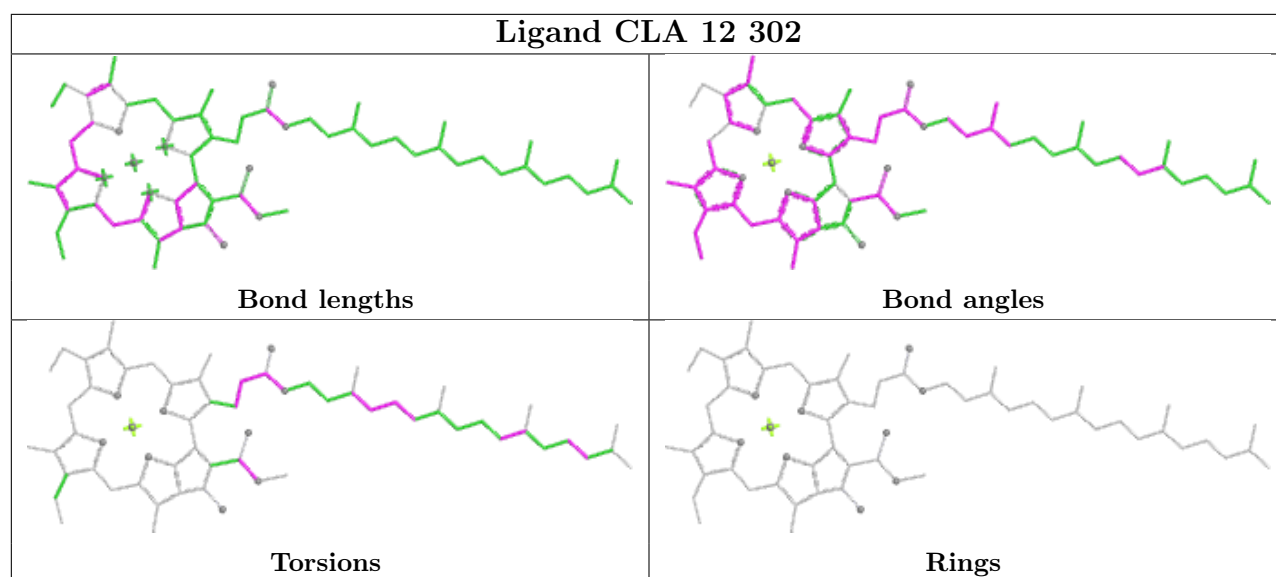


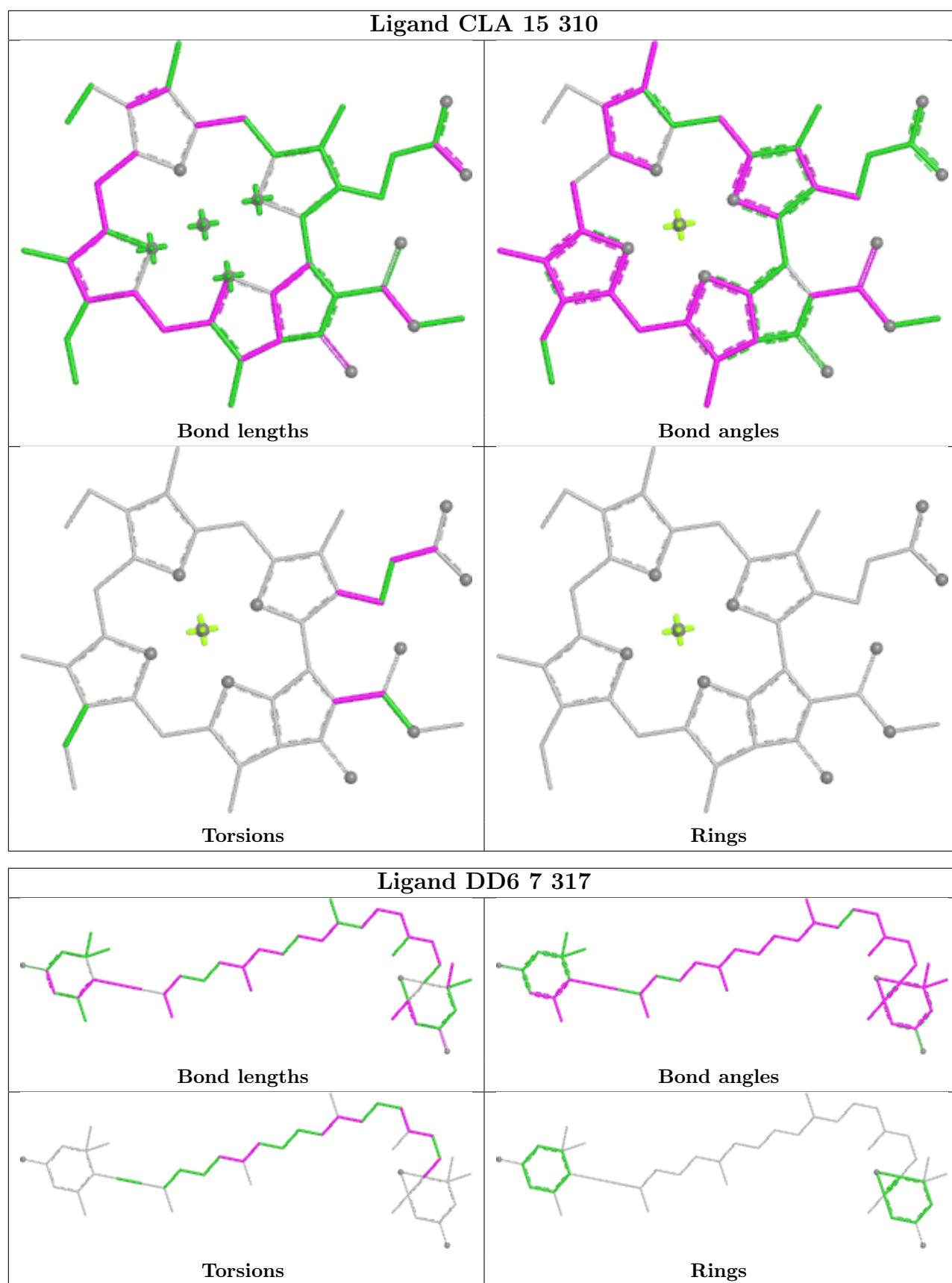
## Ligand KC1 5 312



## Ligand A86 1 309







## 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-0835. These allow visual inspection of the internal detail of the map and identification of artifacts.

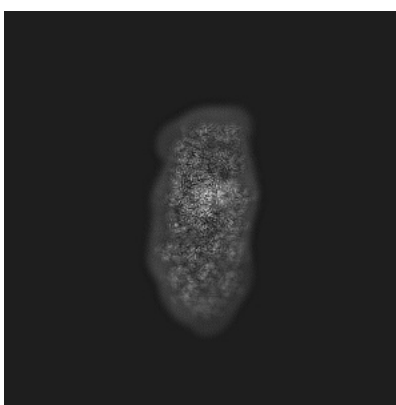
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

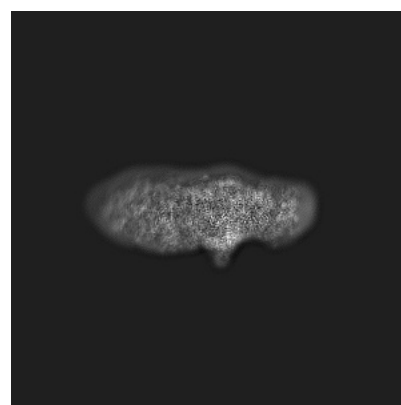
#### 6.1.1 Primary map



X



Y

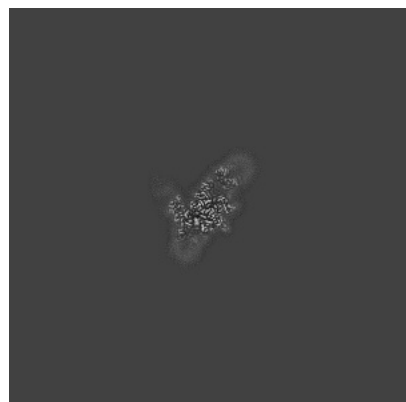


Z

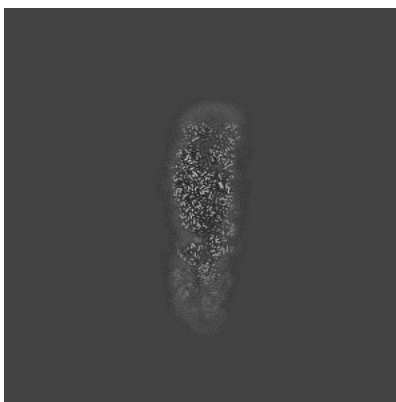
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

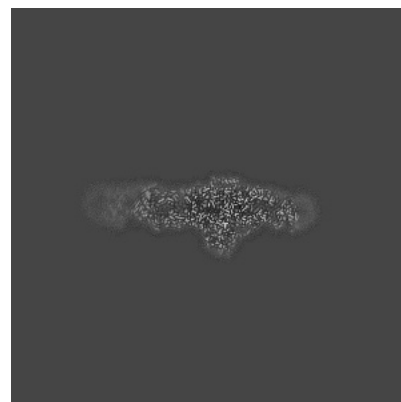
#### 6.2.1 Primary map



X Index: 252



Y Index: 252

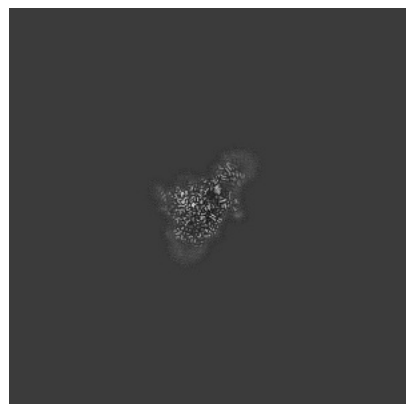


Z Index: 252

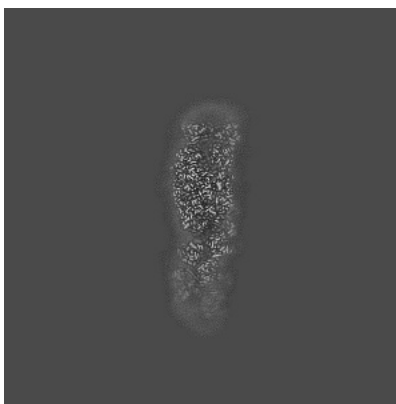
The images above show central slices of the map in three orthogonal directions.

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

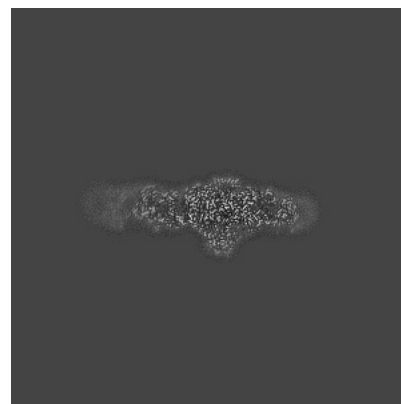
### 6.3.1 Primary map



X Index: 273



Y Index: 251

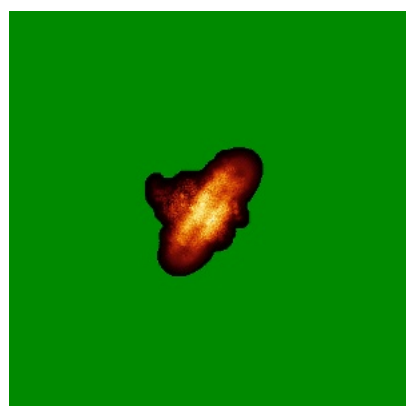


Z Index: 250

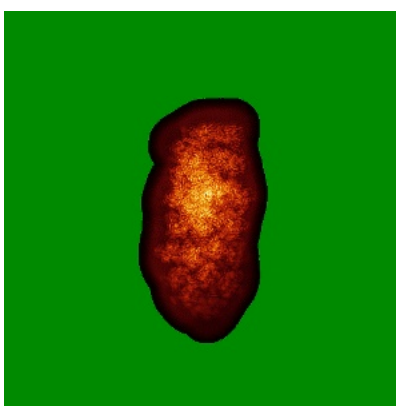
The images above show the largest variance slices of the map in three orthogonal directions.

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

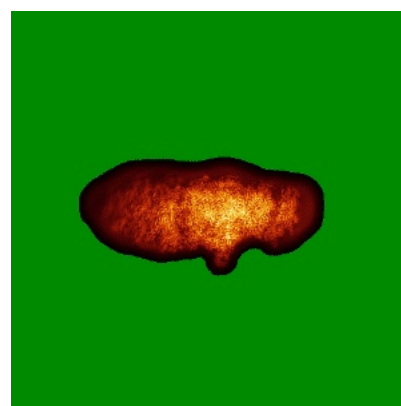
### 6.4.1 Primary map



X



Y

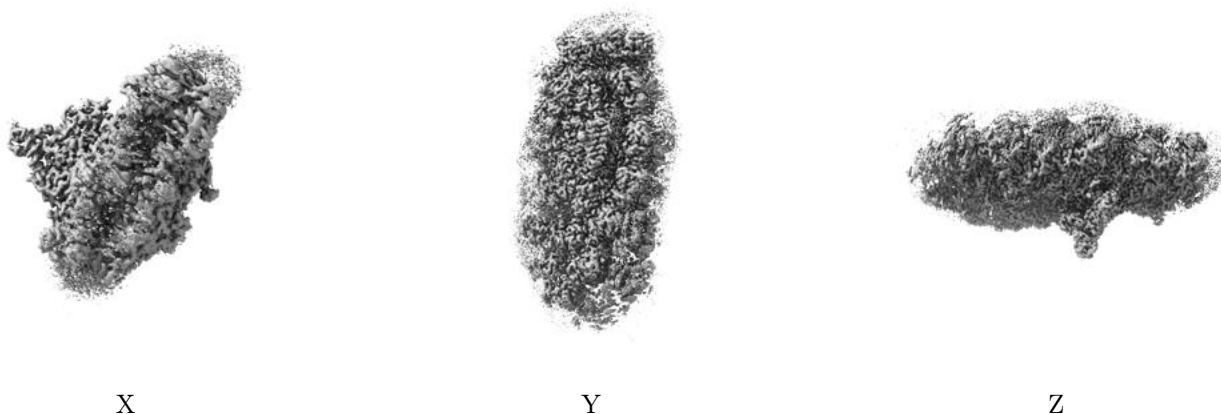


Z

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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

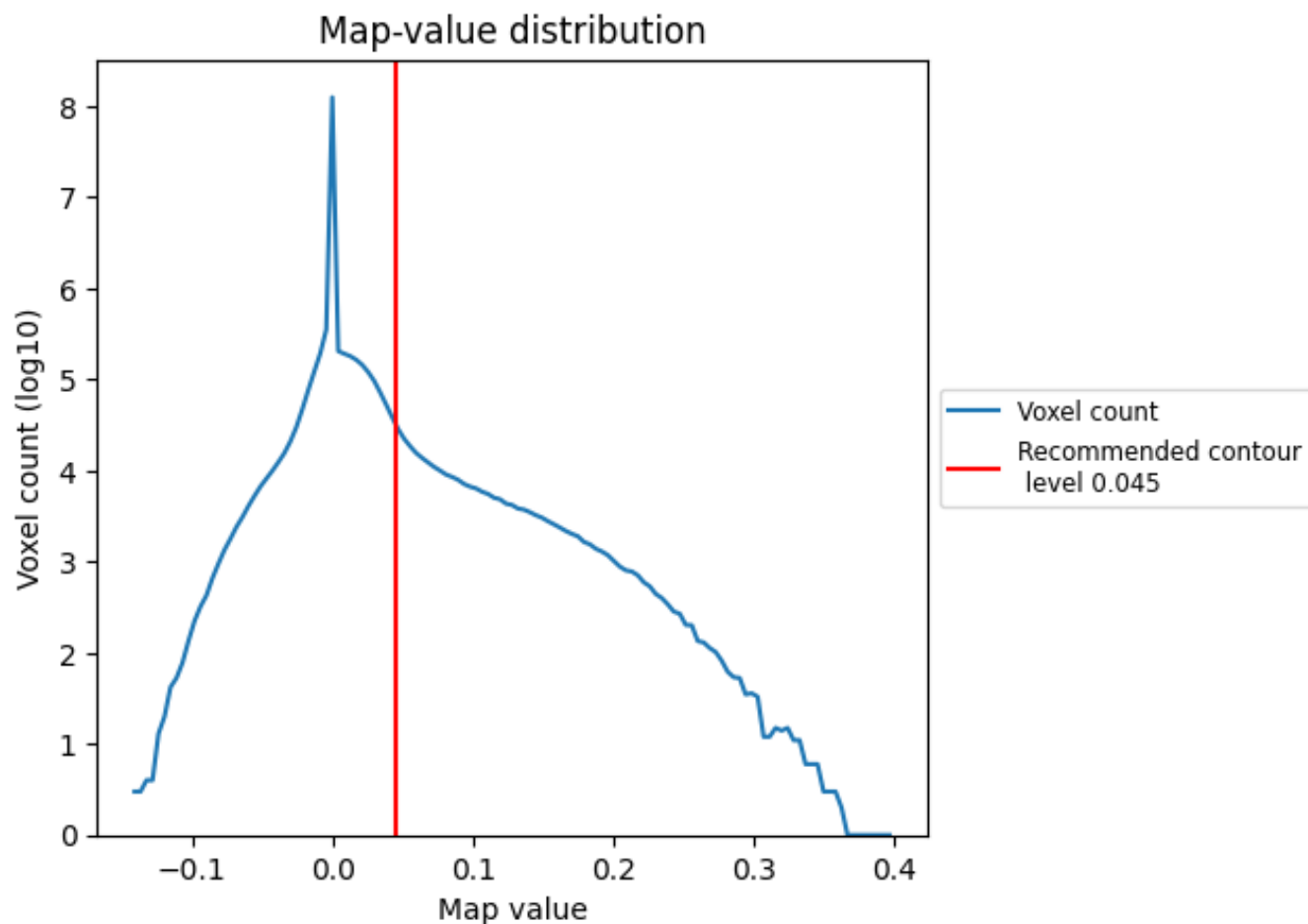
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

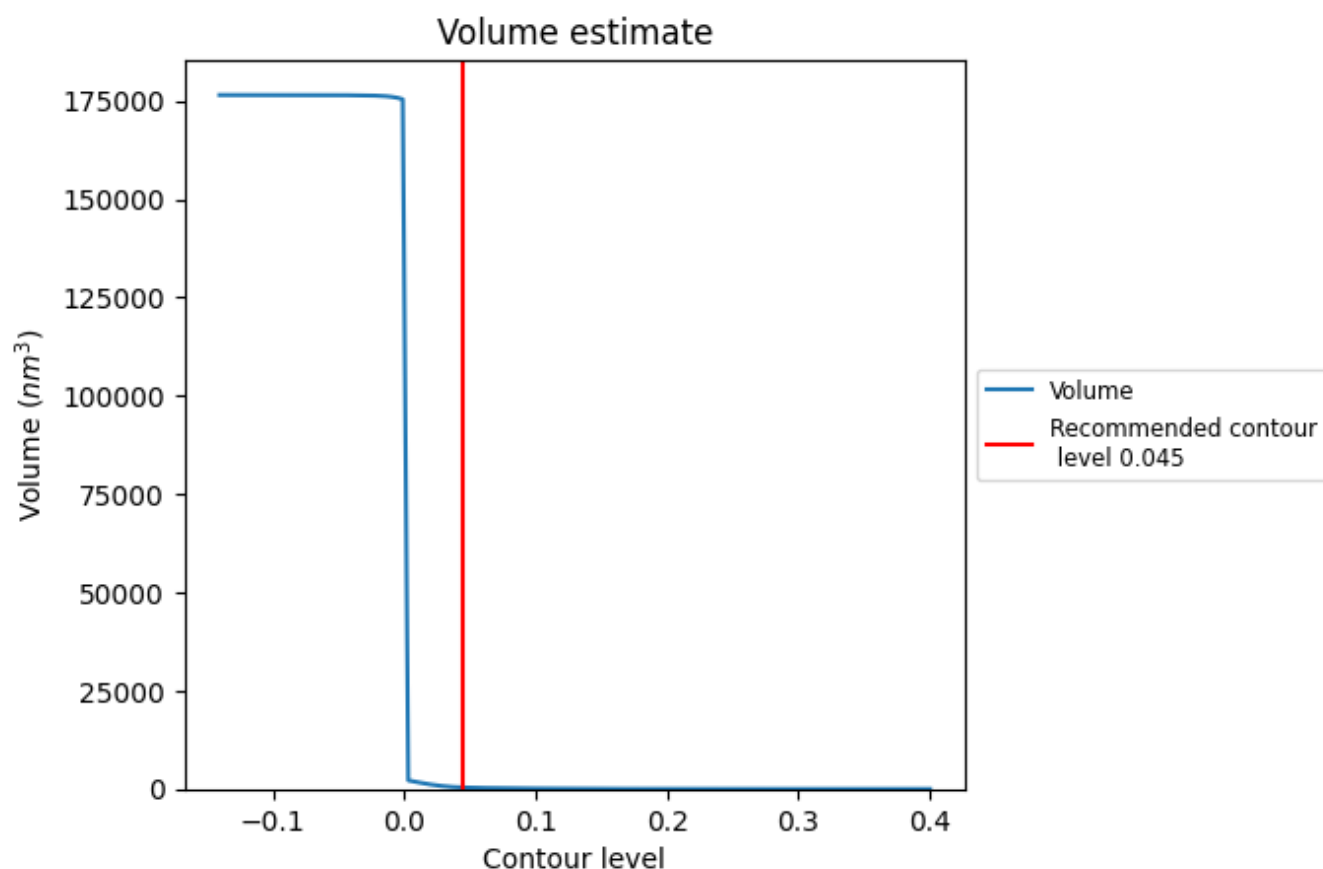
This section contains the results of statistical analysis of the map.

### 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.

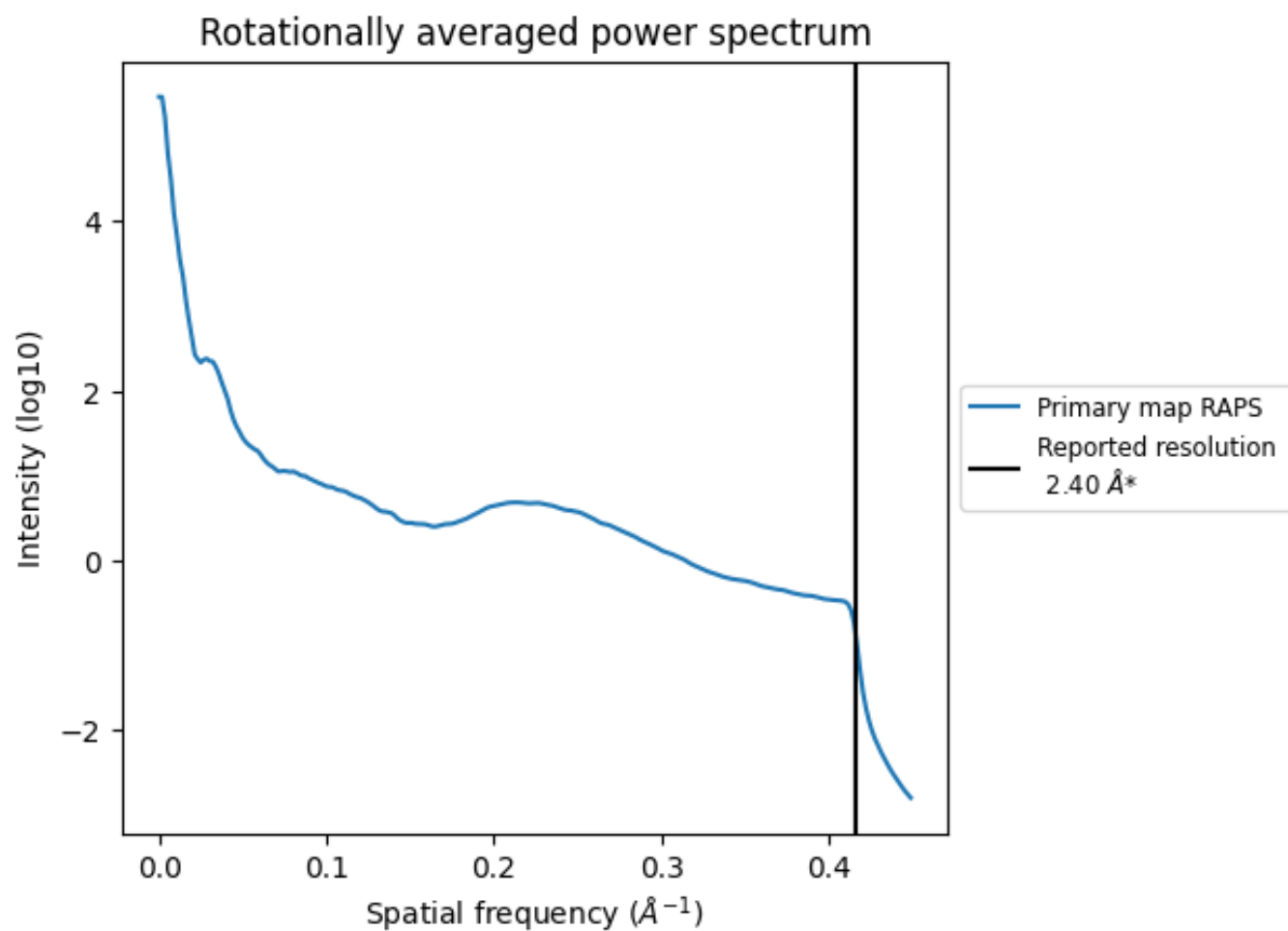
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370  $\text{nm}^3$ ; this corresponds to an approximate mass of 334 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 ⓘ

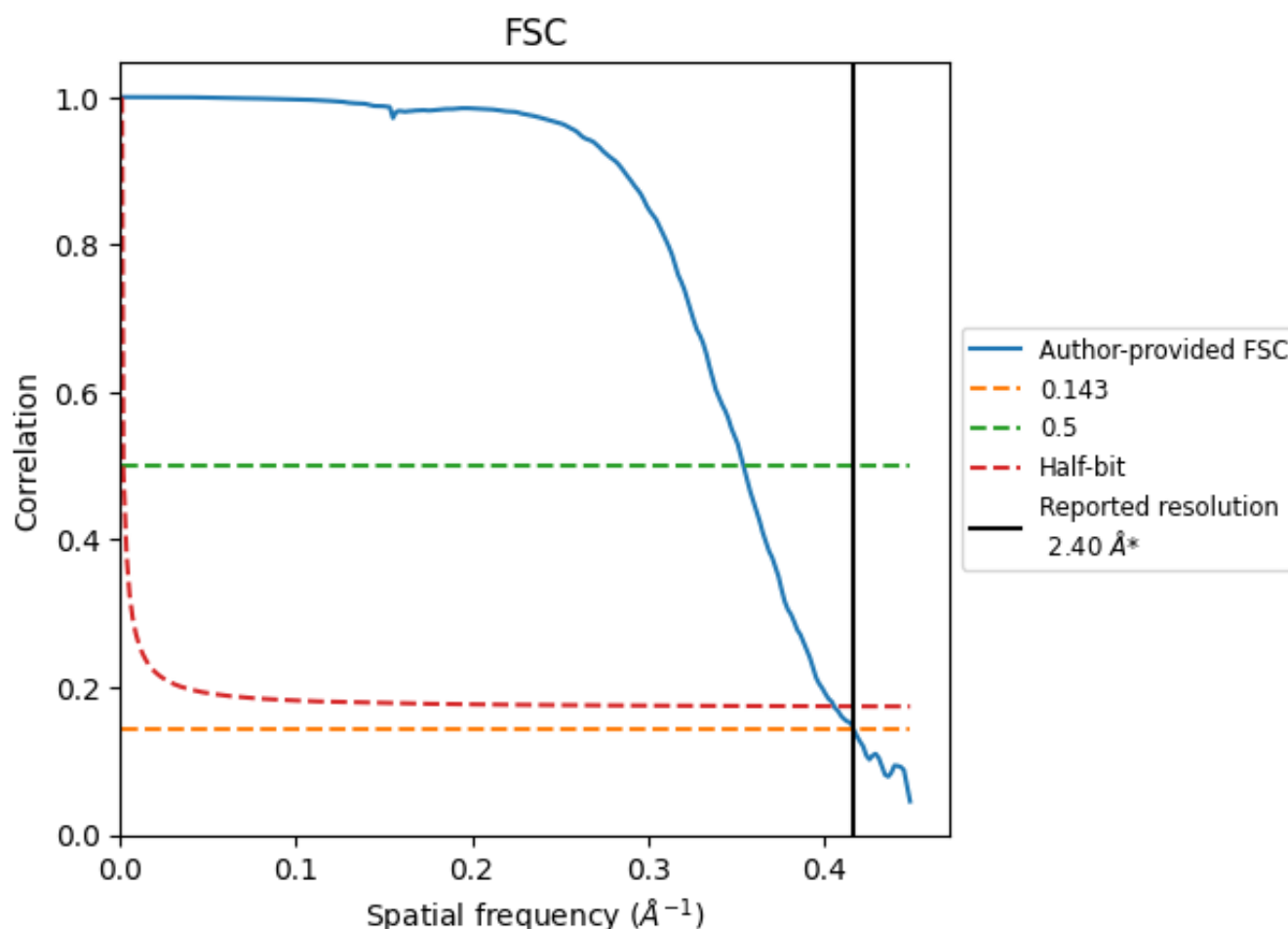


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

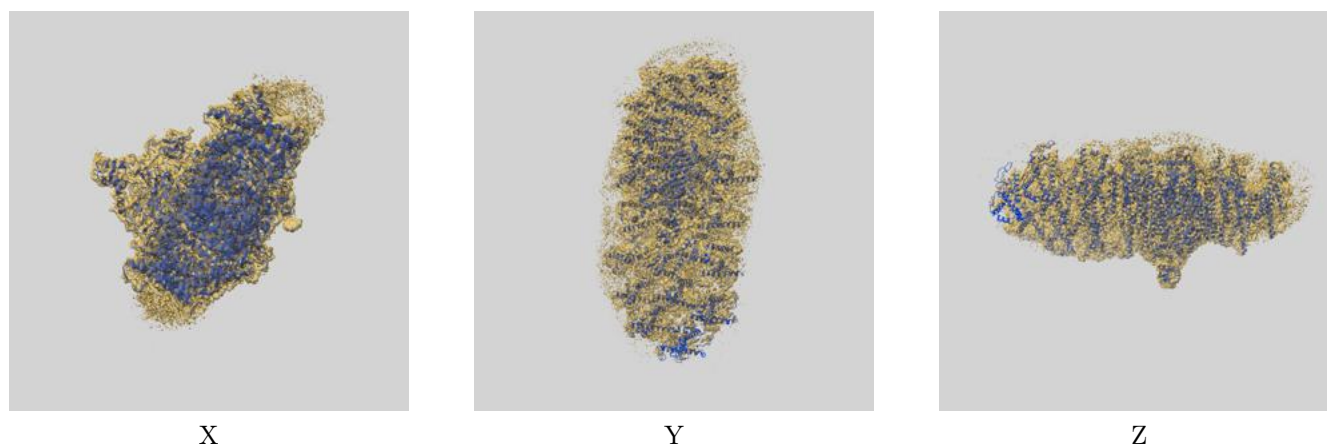
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.82	2.46
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

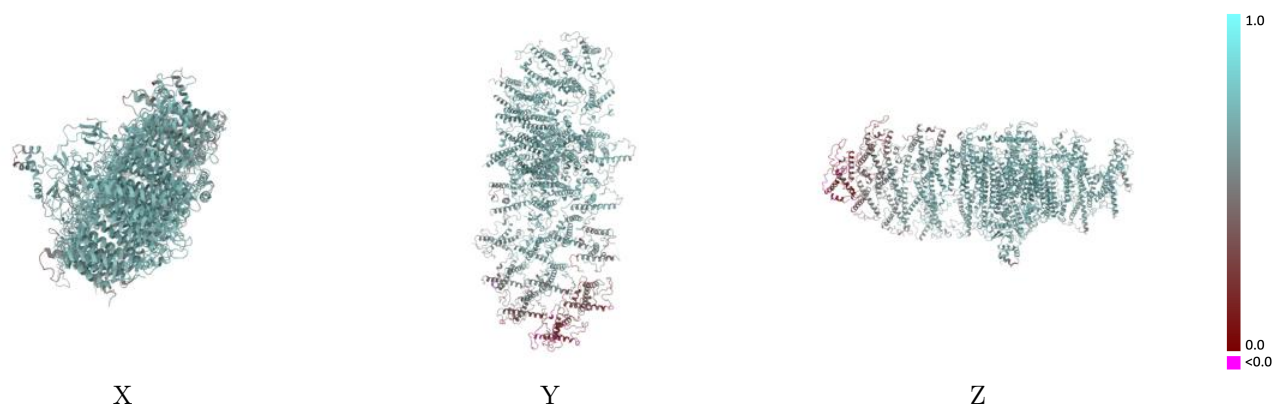
This section contains information regarding the fit between EMDB map EMD-0835 and PDB model 6L4U. Per-residue inclusion information can be found in section [3](#) on page [40](#).

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



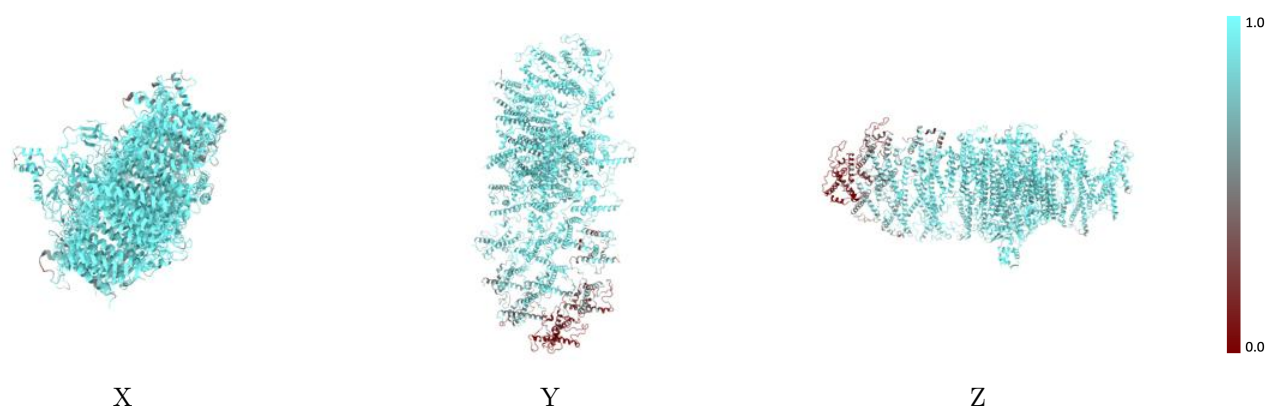
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



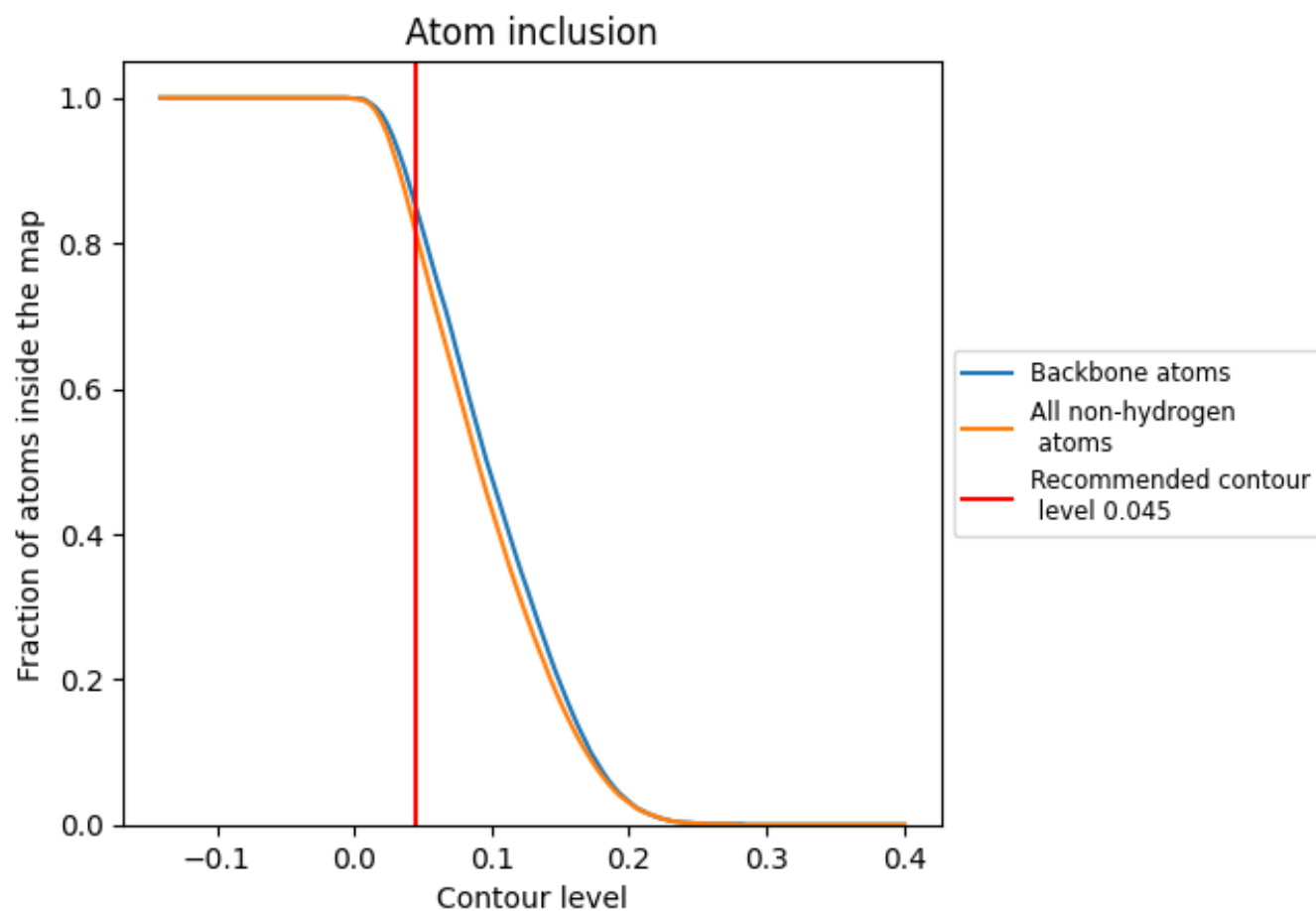
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).



























































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.5870
1	 0.8160	 0.5890
10	 0.8010	 0.5590
11	 0.6960	 0.5050
12	 0.7640	 0.5640
13	 0.6120	 0.4800
14	 0.3760	 0.3440
15	 0.1110	 0.2110
16	 0.5790	 0.4140
1u	 0.9010	 0.5810
2	 0.8680	 0.6050
2u	 0.9370	 0.6560
3	 0.8200	 0.5840
4	 0.8600	 0.6130
5	 0.8460	 0.6020
6	 0.8750	 0.6140
7	 0.8830	 0.6270
8	 0.9030	 0.6360
9	 0.8260	 0.5850
A	 0.9420	 0.6770
B	 0.9490	 0.6780
C	 0.9800	 0.6770
D	 0.9540	 0.6510
E	 0.9330	 0.6710
F	 0.9250	 0.6620
I	 0.9070	 0.6480
J	 0.9410	 0.6590
L	 0.9540	 0.6600
M	 0.9200	 0.6500

