



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:25 AM UTC

PDB ID : 8JW0 / pdb_00008jw0
EMDB ID : EMD-36678
Title : PSI-AcpPCI supercomplex from Amphidinium carterae
Authors : Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on : 2023-06-28
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

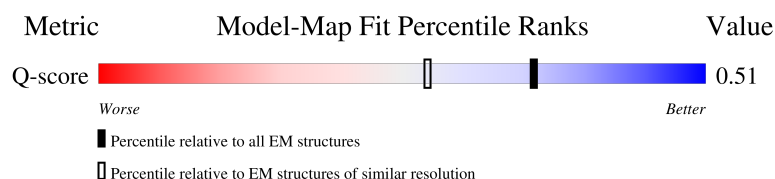
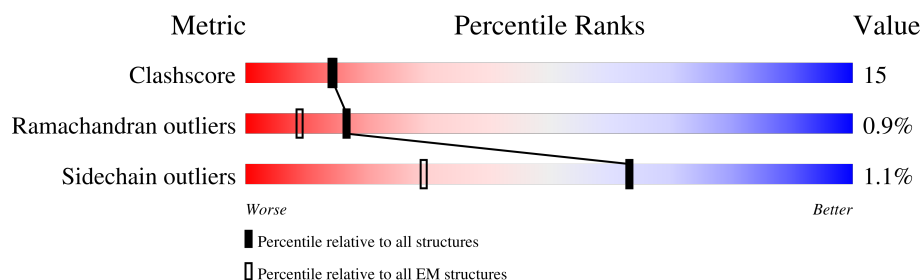
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



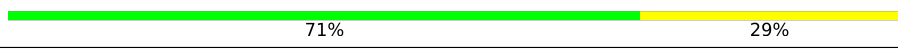
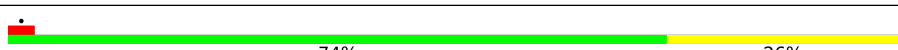
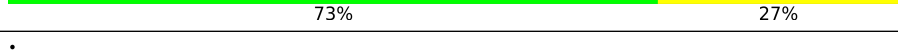
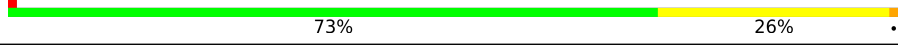
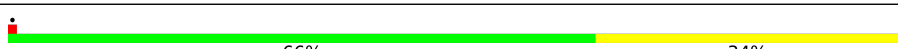
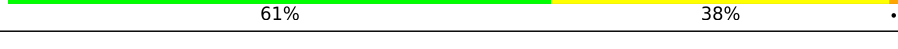
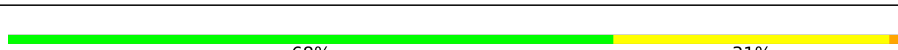
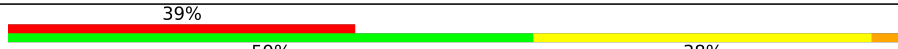
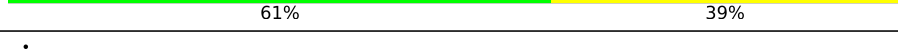
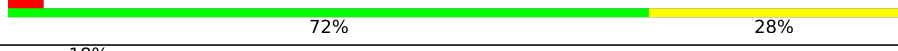
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	a	645	5% 74% 26%
2	b	617	70% 30%
3	c	86	76% 23% .
4	d	257	75% 25%

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Mol	Chain	Length	Quality of chain
5	e	74	
6	f	185	
7	h	132	
8	i	126	
9	j	70	
10	l	253	
11	m	89	
12	A	180	
13	G	215	
14	I	194	
15	K	172	
16	F	176	
17	J	165	
18	M	168	
19	L	185	
20	D	160	
21	B	172	
22	H	160	
23	N	160	
24	O	161	
25	C	160	
25	T	160	
26	Q	162	
27	P	160	
28	E	142	

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	CLA	A	206	X	-	-	-
29	CLA	A	207	X	-	-	-
29	CLA	A	208	X	-	-	-
29	CLA	A	209	X	-	-	-
29	CLA	A	210	X	-	-	-
29	CLA	A	211	X	-	-	-
29	CLA	A	212	X	-	-	-
29	CLA	A	214	X	-	-	-
29	CLA	A	215	X	-	-	-
29	CLA	A	216	X	-	-	-
29	CLA	A	217	X	-	-	-
29	CLA	A	218	X	-	-	-
29	CLA	B	306	X	-	-	-
29	CLA	B	307	X	-	-	-
29	CLA	B	308	X	-	-	-
29	CLA	B	309	X	-	-	-
29	CLA	B	310	X	-	-	-
29	CLA	B	311	X	-	-	-
29	CLA	B	312	X	-	-	-
29	CLA	B	314	X	-	-	-
29	CLA	B	315	X	-	-	-
29	CLA	B	316	X	-	-	-
29	CLA	C	308	X	-	-	-
29	CLA	C	309	X	-	-	-
29	CLA	C	311	X	-	-	-
29	CLA	C	313	X	-	-	-
29	CLA	C	314	X	-	-	-
29	CLA	C	316	X	-	-	-
29	CLA	D	308	X	-	-	-
29	CLA	D	309	X	-	-	-
29	CLA	D	311	X	-	-	-
29	CLA	D	312	X	-	-	-
29	CLA	D	313	X	-	-	-
29	CLA	D	314	X	-	-	-
29	CLA	D	316	X	-	-	-
29	CLA	E	305	X	-	-	-
29	CLA	E	306	X	-	-	-
29	CLA	E	308	X	-	-	-
29	CLA	E	309	X	-	-	-
29	CLA	E	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	E	311	X	-	-	-
29	CLA	E	313	X	-	-	-
29	CLA	E	315	X	-	-	-
29	CLA	F	307	X	-	-	-
29	CLA	F	308	X	-	-	-
29	CLA	F	310	X	-	-	-
29	CLA	F	311	X	-	-	-
29	CLA	F	312	X	-	-	-
29	CLA	F	313	X	-	-	-
29	CLA	F	315	X	-	-	-
29	CLA	F	316	X	-	-	-
29	CLA	G	301	X	-	-	-
29	CLA	G	302	X	-	-	-
29	CLA	G	304	X	-	-	-
29	CLA	G	311	X	-	-	-
29	CLA	G	312	X	-	-	-
29	CLA	G	313	X	-	-	-
29	CLA	G	314	X	-	-	-
29	CLA	G	316	X	-	-	-
29	CLA	G	317	X	-	-	-
29	CLA	G	319	X	-	-	-
29	CLA	H	307	X	-	-	-
29	CLA	H	308	X	-	-	-
29	CLA	H	310	X	-	-	-
29	CLA	H	312	X	-	-	-
29	CLA	H	313	X	-	-	-
29	CLA	H	315	X	-	-	-
29	CLA	I	201	X	-	-	-
29	CLA	I	207	X	-	-	-
29	CLA	I	208	X	-	-	-
29	CLA	I	209	X	-	-	-
29	CLA	I	210	X	-	-	-
29	CLA	I	211	X	-	-	-
29	CLA	I	212	X	-	-	-
29	CLA	I	213	X	-	-	-
29	CLA	I	214	X	-	-	-
29	CLA	I	216	X	-	-	-
29	CLA	I	217	X	-	-	-
29	CLA	J	305	X	-	-	-
29	CLA	J	306	X	-	-	-
29	CLA	J	307	X	-	-	-
29	CLA	J	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	J	309	X	-	-	-
29	CLA	J	310	X	-	-	-
29	CLA	J	311	X	-	-	-
29	CLA	J	313	X	-	-	-
29	CLA	K	207	X	-	-	-
29	CLA	K	208	X	-	-	-
29	CLA	K	209	X	-	-	-
29	CLA	K	210	X	-	-	-
29	CLA	K	211	X	-	-	-
29	CLA	K	212	X	-	-	-
29	CLA	K	213	X	-	-	-
29	CLA	K	214	X	-	-	-
29	CLA	K	216	X	-	-	-
29	CLA	K	217	X	-	-	-
29	CLA	K	218	X	-	-	-
29	CLA	L	307	X	-	-	-
29	CLA	L	308	X	-	-	-
29	CLA	L	309	X	-	-	-
29	CLA	L	310	X	-	-	-
29	CLA	L	311	X	-	-	-
29	CLA	L	312	X	-	-	-
29	CLA	L	313	X	-	-	-
29	CLA	L	315	X	-	-	-
29	CLA	L	316	X	-	-	-
29	CLA	L	317	X	-	-	-
29	CLA	M	306	X	-	-	-
29	CLA	M	307	X	-	-	-
29	CLA	M	308	X	-	-	-
29	CLA	M	309	X	-	-	-
29	CLA	M	310	X	-	-	-
29	CLA	M	311	X	-	-	-
29	CLA	M	313	X	-	-	-
29	CLA	M	314	X	-	-	-
29	CLA	M	315	X	-	-	-
29	CLA	N	308	X	-	-	-
29	CLA	N	309	X	-	-	-
29	CLA	N	311	X	-	-	-
29	CLA	N	313	X	-	-	-
29	CLA	N	314	X	-	-	-
29	CLA	N	316	X	-	-	-
29	CLA	O	308	X	-	-	-
29	CLA	O	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	O	313	X	-	-	-
29	CLA	O	316	X	-	-	-
29	CLA	P	209	X	-	-	-
29	CLA	P	210	X	-	-	-
29	CLA	P	212	X	-	-	-
29	CLA	P	214	X	-	-	-
29	CLA	P	215	X	-	-	-
29	CLA	P	217	X	-	-	-
29	CLA	Q	307	X	-	-	-
29	CLA	Q	308	X	-	-	-
29	CLA	Q	310	X	-	-	-
29	CLA	Q	312	X	-	-	-
29	CLA	Q	313	X	-	-	-
29	CLA	Q	315	X	-	-	-
29	CLA	T	308	X	-	-	-
29	CLA	T	309	X	-	-	-
29	CLA	T	311	X	-	-	-
29	CLA	T	313	X	-	-	-
29	CLA	T	314	X	-	-	-
29	CLA	T	316	X	-	-	-
29	CLA	a	801	X	-	-	-
29	CLA	a	802	X	-	-	-
29	CLA	a	803	X	-	-	-
29	CLA	a	804	X	-	-	-
29	CLA	a	805	X	-	-	-
29	CLA	a	806	X	-	-	-
29	CLA	a	807	X	-	-	-
29	CLA	a	808	X	-	-	-
29	CLA	a	809	X	-	-	-
29	CLA	a	810	X	-	-	-
29	CLA	a	811	X	-	-	-
29	CLA	a	812	X	-	-	-
29	CLA	a	813	X	-	-	-
29	CLA	a	814	X	-	-	-
29	CLA	a	815	X	-	-	-
29	CLA	a	816	X	-	-	-
29	CLA	a	817	X	-	-	-
29	CLA	a	818	X	-	-	-
29	CLA	a	819	X	-	-	-
29	CLA	a	820	X	-	-	-
29	CLA	a	821	X	-	-	-
29	CLA	a	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	a	823	X	-	-	-
29	CLA	a	824	X	-	-	-
29	CLA	a	825	X	-	-	-
29	CLA	a	826	X	-	-	-
29	CLA	a	827	X	-	-	-
29	CLA	a	828	X	-	-	-
29	CLA	a	829	X	-	-	-
29	CLA	a	830	X	-	-	-
29	CLA	a	831	X	-	-	-
29	CLA	a	837	X	-	-	-
29	CLA	b	701	X	-	-	-
29	CLA	b	702	X	-	-	-
29	CLA	b	703	X	-	-	-
29	CLA	b	704	X	-	-	-
29	CLA	b	705	X	-	-	-
29	CLA	b	706	X	-	-	-
29	CLA	b	707	X	-	-	-
29	CLA	b	708	X	-	-	-
29	CLA	b	709	X	-	-	-
29	CLA	b	710	X	-	-	-
29	CLA	b	711	X	-	-	-
29	CLA	b	712	X	-	-	-
29	CLA	b	713	X	-	-	-
29	CLA	b	714	X	-	-	-
29	CLA	b	715	X	-	-	-
29	CLA	b	716	X	-	-	-
29	CLA	b	717	X	-	-	-
29	CLA	b	718	X	-	-	-
29	CLA	b	719	X	-	-	-
29	CLA	b	720	X	-	-	-
29	CLA	b	721	X	-	-	-
29	CLA	b	722	X	-	-	-
29	CLA	b	723	X	-	-	-
29	CLA	b	724	X	-	-	-
29	CLA	b	725	X	-	-	-
29	CLA	b	726	X	-	-	-
29	CLA	b	731	X	-	-	-
29	CLA	b	736	X	-	-	-
29	CLA	f	802	X	-	-	-
29	CLA	f	803	X	-	-	-
29	CLA	f	805	X	-	-	-
29	CLA	h	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	i	201	X	-	-	-
29	CLA	i	202	X	-	-	-
29	CLA	i	203	X	-	-	-
29	CLA	j	104	X	-	-	-
29	CLA	l	501	X	-	-	-
29	CLA	l	502	X	-	-	-
29	CLA	l	503	X	-	-	-
29	CLA	l	504	X	-	-	-
29	CLA	l	505	X	-	-	-
29	CLA	l	508	X	-	-	-
29	CLA	l	509	X	-	-	-
29	CLA	l	510	X	-	-	-
33	SF4	a	836	-	-	X	-
33	SF4	c	102	-	-	X	-

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 63119 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	645	Total	C	N	O	S	0	0
			4980	3267	825	874	14		

- Molecule 2 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	617	Total	C	N	O	S	0	0
			4813	3185	765	848	15		

- Molecule 3 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	86	Total	C	N	O	S	0	0
			647	401	109	128	9		

- Molecule 4 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	257	Total	C	N	O	S	0	0
			1985	1259	340	375	11		

- Molecule 5 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	74	Total	C	N	O	0	0
			607	392	102	113		

- Molecule 6 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	185	Total	C	N	O	S	0	0
			1455	926	257	263	9		

- Molecule 7 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	132	Total	C	N	O	S	0	0
			1056	693	167	191	5		

- Molecule 8 is a protein called Photosystem I Psal.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	126	Total	C	N	O	S	0	0
			1001	651	164	183	3		

- Molecule 9 is a protein called Photosystem I Psaj.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	70	Total	C	N	O	S	0	0
			549	362	86	100	1		

- Molecule 10 is a protein called Photosystem I Psal.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	253	Total	C	N	O	S	0	0
			1961	1274	321	355	11		

- Molecule 11 is a protein called Photosystem I Psam.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	89	Total	C	N	O	S	0	0
			679	438	109	131	1		

- Molecule 12 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	180	Total	C	N	O	S	0	0
			1358	882	221	245	10		

- Molecule 13 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	215	Total	C	N	O	S	0	0
			1675	1086	278	299	12		

- Molecule 14 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	194	Total	C	N	O	S	0	0
			1455	946	244	253	12		

- Molecule 15 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	172	Total	C	N	O	S	0	0
			1325	857	222	234	12		

- Molecule 16 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	176	Total	C	N	O	S	0	0
			1356	869	226	249	12		

- Molecule 17 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	165	Total	C	N	O	S	0	0
			1282	828	207	239	8		

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	168	Total	C	N	O	S	0	0
			1346	885	224	232	5		

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	185	Total	C	N	O	S	0	0
			1453	942	242	263	6		

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	160	Total	C	N	O	S	0	0
			1198	761	200	230	7		

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	172	Total	C	N	O	S	0	0
			1371	888	226	245	12		

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	160	Total	C	N	O	S	0	0
			1202	769	198	228	7		

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	160	Total	C	N	O	S	0	0
			1203	767	200	229	7		

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	161	Total	C	N	O	S	0	0
			1226	789	204	226	7		

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	159	Total	C	N	O	S	0	0
			1189	756	199	226	8		
25	C	160	Total	C	N	O	S	0	0
			1200	765	200	227	8		

- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	162	Total	C	N	O	S	0	0
			1219	787	204	219	9		

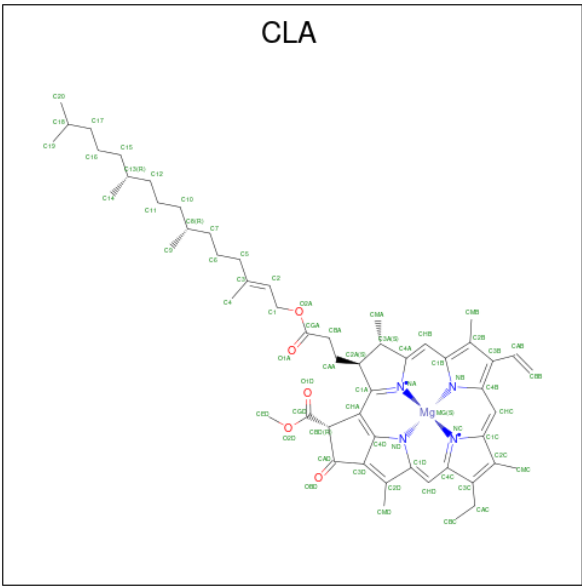
- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	160	Total	C	N	O	S	0	0
			1218	778	204	228	8		

- Molecule 28 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	142	Total	C	N	O	S	0	0
			1071	684	178	201	8		

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
29	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	j	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	l	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	G	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	I	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	I	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	I	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	I	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	K	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	K	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	K	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	J	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	J	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	J	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	M	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	M	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	M	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	M	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	M	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	M	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	L	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	L	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	L	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	L	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	B	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	N	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	T	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	T	1	Total 46	C 36	Mg 1	N 4	O 5	0

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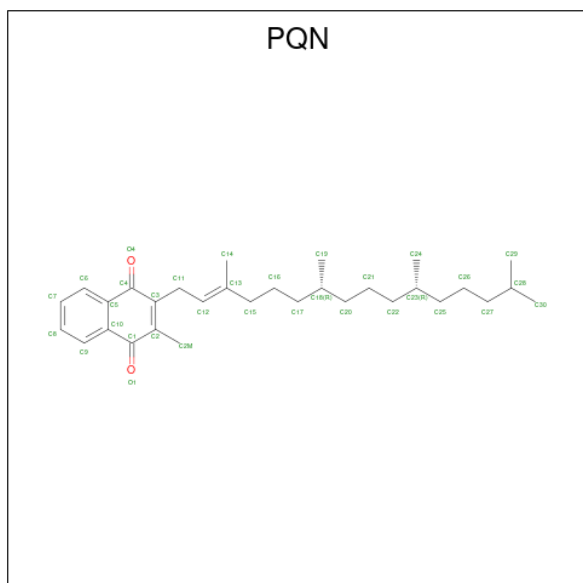
Mol	Chain	Residues	Atoms					AltConf
29	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	T	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	Q	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	P	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	P	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	P	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	P	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	E	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	E	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



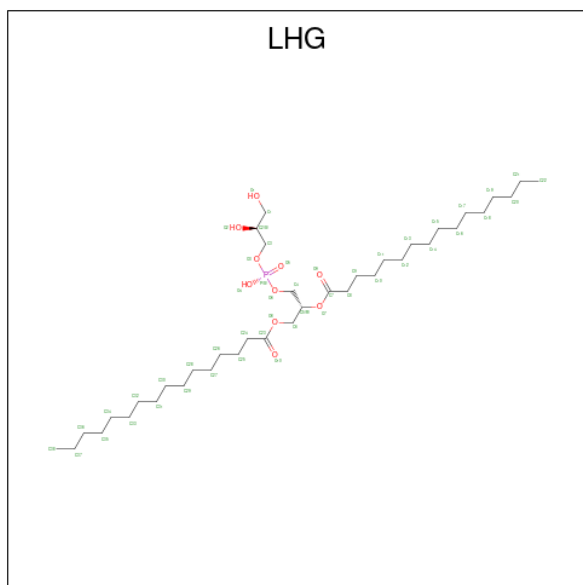
Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			33	31	2	

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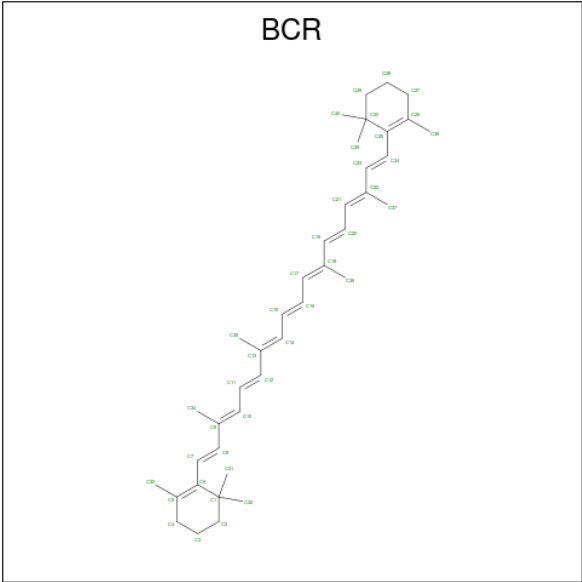
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	b	1	33	31	2	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



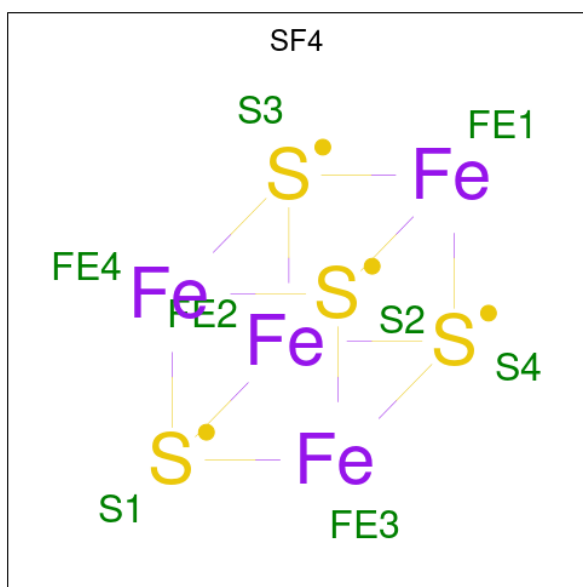
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	a	1	48	37	10	1	0

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



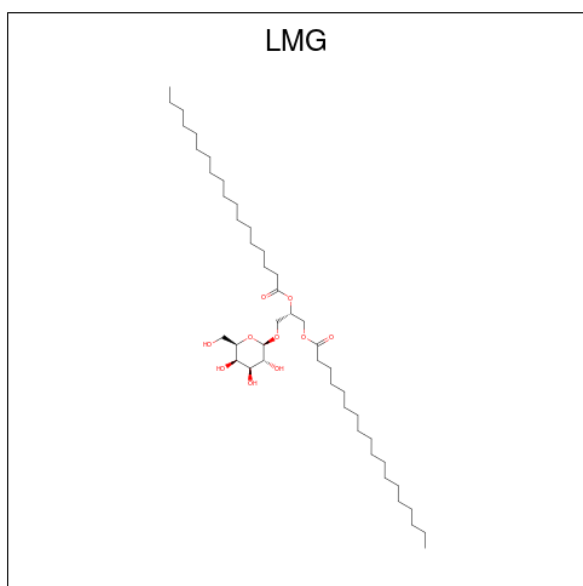
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C 40 40	0

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



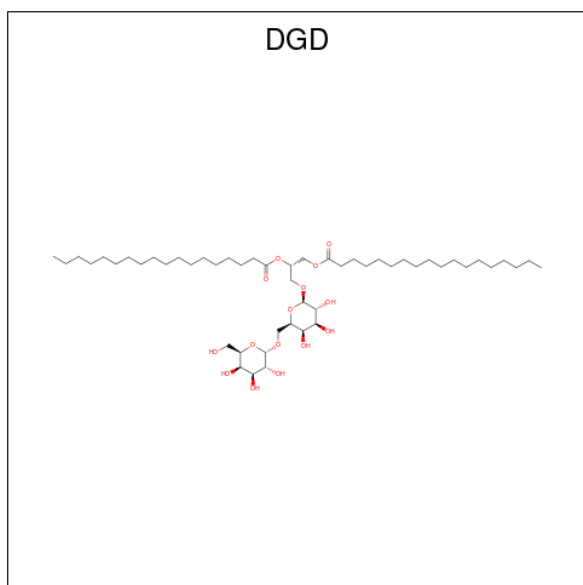
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	Fe	S	0
			8	4	4	
33	c	1	Total	Fe	S	0
			8	4	4	
33	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



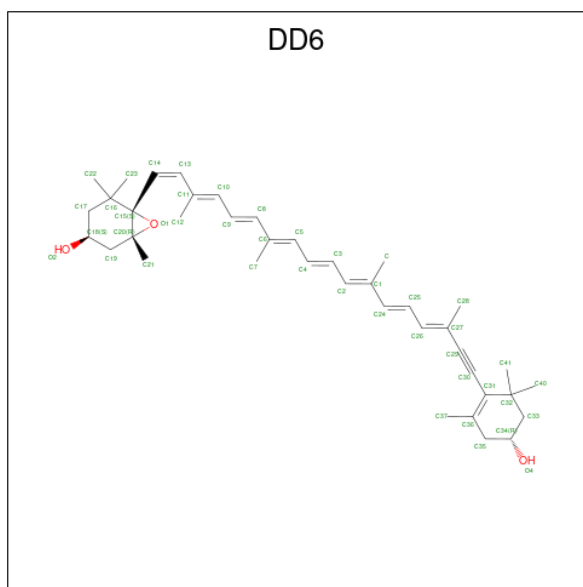
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			44	34	10	
34	b	1	Total	C	O	0
			40	30	10	
34	h	1	Total	C	O	0
			28	18	10	
34	j	1	Total	C	O	0
			43	33	10	
34	A	1	Total	C	O	0
			37	27	10	
34	K	1	Total	C	O	0
			43	33	10	
34	K	1	Total	C	O	0
			35	25	10	
34	K	1	Total	C	O	0
			36	26	10	
34	P	1	Total	C	O	0
			27	17	10	
34	E	1	Total	C	O	0
			32	22	10	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	b	1	Total	C	O	0
			57	42	15	
35	h	1	Total	C	O	0
			54	39	15	
35	j	1	Total	C	O	0
			43	28	15	
35	j	1	Total	C	O	0
			41	26	15	
35	j	1	Total	C	O	0
			49	34	15	
35	m	1	Total	C	O	0
			66	51	15	
35	G	1	Total	C	O	0
			45	30	15	
35	B	1	Total	C	O	0
			45	30	15	

- Molecule 36 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	h	1	Total	C	O	0
			43	40	3	
36	m	1	Total	C	O	0
			43	40	3	
36	A	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total 43	C 40	O 3	0
36	A	1	Total 43	C 40	O 3	0
36	G	1	Total 43	C 40	O 3	0
36	G	1	Total 43	C 40	O 3	0
36	G	1	Total 43	C 40	O 3	0
36	G	1	Total 43	C 40	O 3	0
36	I	1	Total 43	C 40	O 3	0
36	I	1	Total 43	C 40	O 3	0
36	I	1	Total 43	C 40	O 3	0
36	I	1	Total 43	C 40	O 3	0
36	I	1	Total 43	C 40	O 3	0
36	K	1	Total 43	C 40	O 3	0
36	K	1	Total 43	C 40	O 3	0
36	K	1	Total 43	C 40	O 3	0
36	K	1	Total 43	C 40	O 3	0
36	K	1	Total 43	C 40	O 3	0
36	K	1	Total 43	C 40	O 3	0
36	F	1	Total 43	C 40	O 3	0
36	F	1	Total 43	C 40	O 3	0
36	J	1	Total 43	C 40	O 3	0
36	J	1	Total 43	C 40	O 3	0

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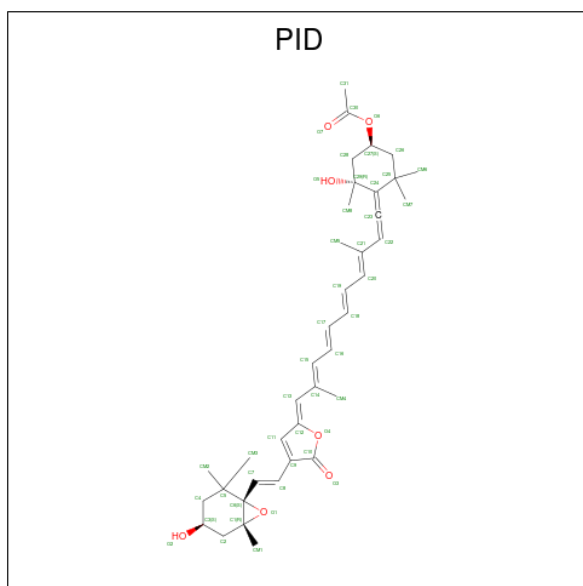
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	J	1	43	40	3	0
36	M	1	43	40	3	0
36	M	1	43	40	3	0
36	M	1	43	40	3	0
36	M	1	43	40	3	0
36	L	1	43	40	3	0
36	L	1	43	40	3	0
36	L	1	43	40	3	0
36	L	1	43	40	3	0
36	D	1	43	40	3	0
36	D	1	43	40	3	0
36	B	1	42	39	3	0
36	B	1	43	40	3	0
36	B	1	43	40	3	0
36	B	1	43	40	3	0
36	B	1	43	40	3	0
36	B	1	43	40	3	0
36	H	1	43	40	3	0
36	N	1	43	40	3	0
36	O	1	43	40	3	0
36	T	1	43	40	3	0
36	Q	1	43	40	3	0

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Mol	Chain	Residues	Atoms			AltConf
36	C	1	Total	C	O	0
			43	40	3	
36	P	1	Total	C	O	0
			43	40	3	
36	E	1	Total	C	O	0
			43	40	3	
36	E	1	Total	C	O	0
			43	40	3	

- Molecule 37 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	h	1	Total	C	O	0
			46	39	7	
37	j	1	Total	C	O	0
			46	39	7	
37	G	1	Total	C	O	0
			46	39	7	
37	G	1	Total	C	O	0
			46	39	7	
37	G	1	Total	C	O	0
			46	39	7	
37	F	1	Total	C	O	0
			46	39	7	
37	F	1	Total	C	O	0
			46	39	7	

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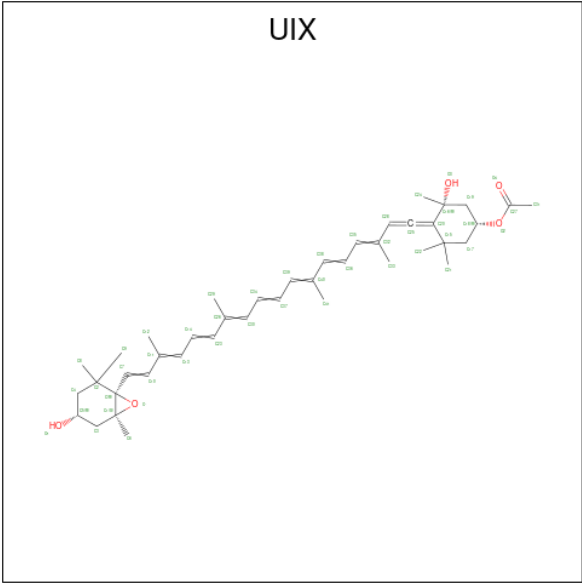
Mol	Chain	Residues	Atoms			AltConf
37	F	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	N	1	Total 46	C 39	O 7	0
37	N	1	Total 46	C 39	O 7	0
37	N	1	Total 46	C 39	O 7	0
37	N	1	Total 46	C 39	O 7	0
37	N	1	Total 46	C 39	O 7	0
37	O	1	Total 46	C 39	O 7	0
37	O	1	Total 46	C 39	O 7	0
37	O	1	Total 46	C 39	O 7	0
37	O	1	Total 46	C 39	O 7	0
37	O	1	Total 46	C 39	O 7	0

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Mol	Chain	Residues	Atoms			AltConf
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	E	1	Total	C	O	0
			46	39	7	

- Molecule 38 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			47	42	5	
38	F	1	Total	C	O	0
			47	42	5	
38	J	1	Total	C	O	0
			47	42	5	
38	L	1	Total	C	O	0
			47	42	5	
38	B	1	Total	C	O	0
			47	42	5	
38	N	1	Total	C	O	0
			47	42	5	
38	O	1	Total	C	O	0
			47	42	5	
38	T	1	Total	C	O	0
			47	42	5	
38	Q	1	Total	C	O	0
			47	42	5	
38	C	1	Total	C	O	0
			47	42	5	
38	P	1	Total	C	O	0
			47	42	5	

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Mol	Chain	Residues	Atoms			AltConf
38	E	1	Total	C	O	0
			47	42	5	

- # KC1

Mol	Chain	Residues	Atoms					AltConf
39	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	M	1	Total 45	C 35	Mg 1	N 4	O 5	0



WORLD WIDE
PDB
PROTEIN DATA BANK

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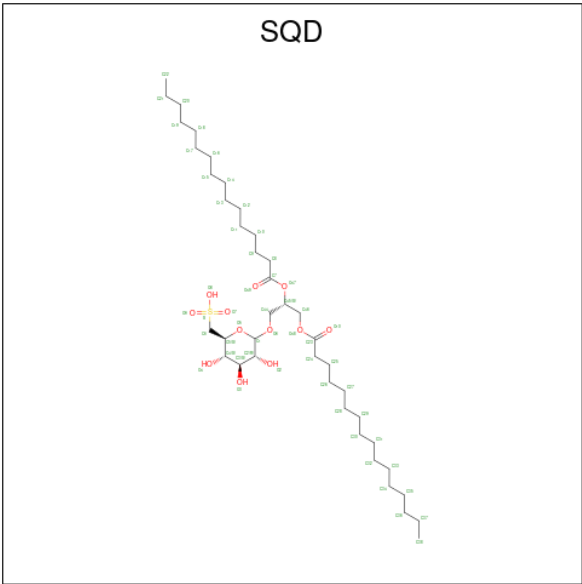
Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).

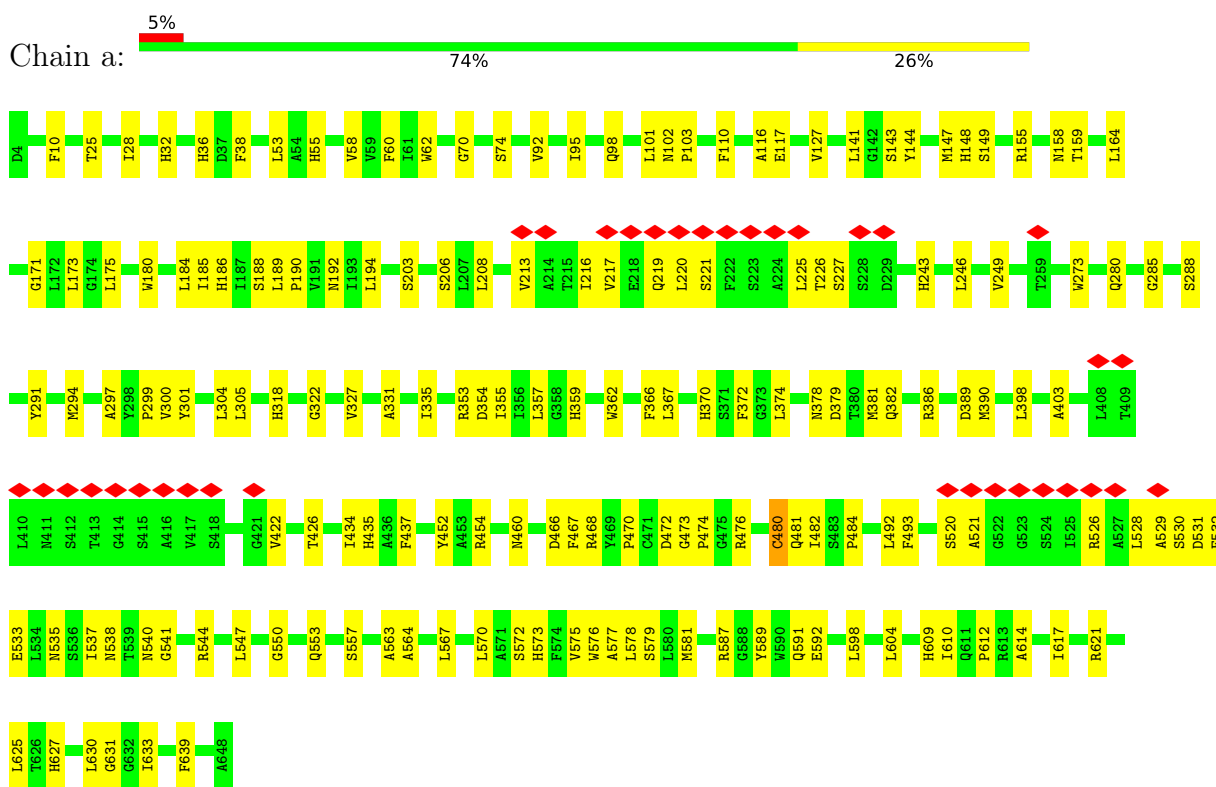


Mol	Chain	Residues	Atoms				AltConf
40	J	1	Total	C	O	S	0
			45	32	12	1	
40	B	1	Total	C	O	S	0
			42	29	12	1	

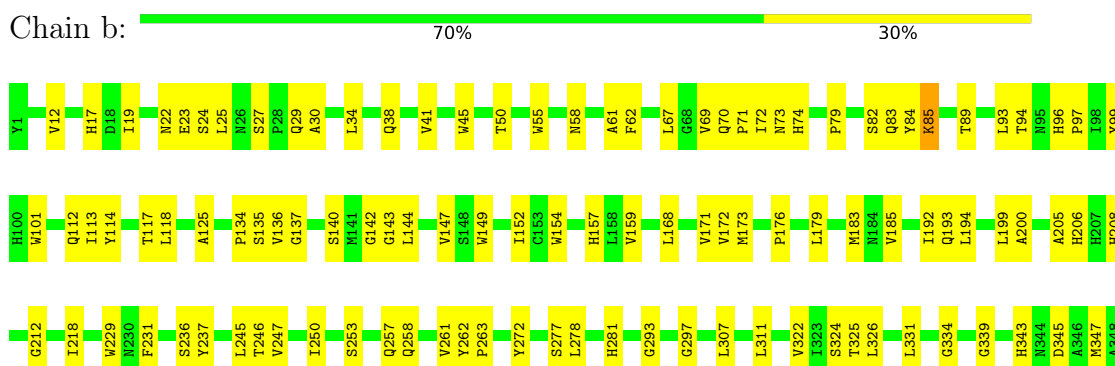
3 Residue-property plots

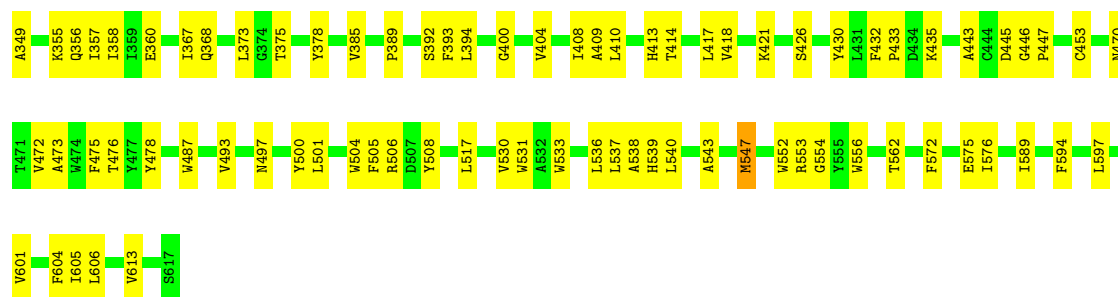
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Photosystem I PsaA



• Molecule 2: Photosystem I PsbB





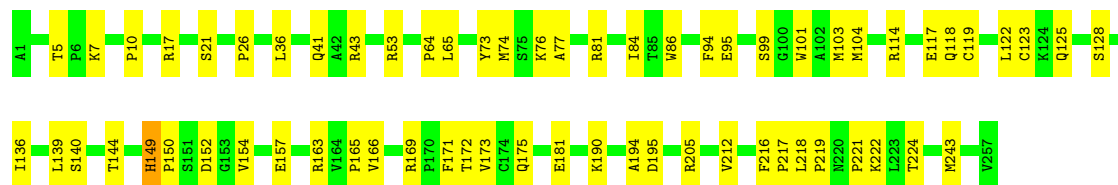
• Molecule 3: Photosystem I Psac

Chain c: 76% 23% .



• Molecule 4: Photosystem I Psad

Chain d: 75% 25%



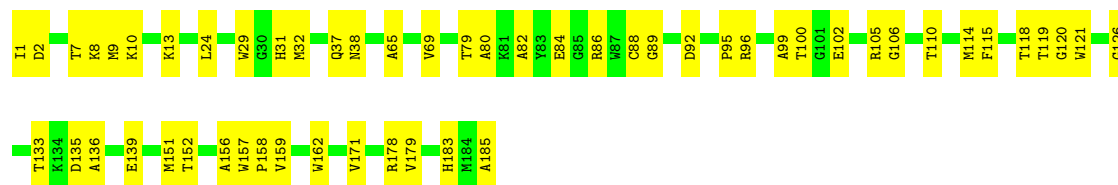
• Molecule 5: Photosystem I Psae

Chain e: 81% 19%



• Molecule 6: Photosystem I Psaf

Chain f: 71% 29%

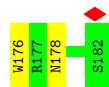


• Molecule 7: Photosystem I Psar

Chain h: 80% 15% 5%



• Molecule 8: Photosystem I Psal



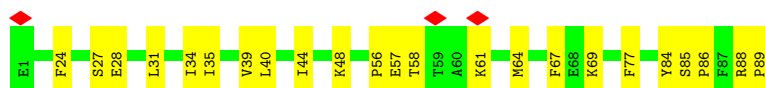
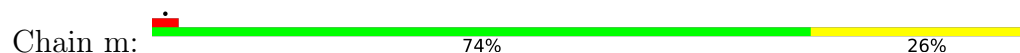
• Molecule 9: Photosystem I Psaj



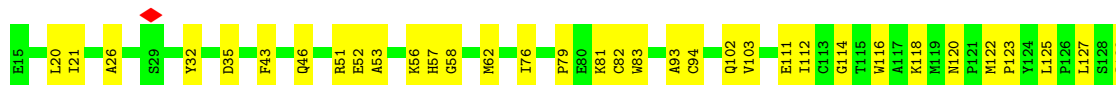
• Molecule 10: Photosystem I Psal



• Molecule 11: Photosystem I Psam

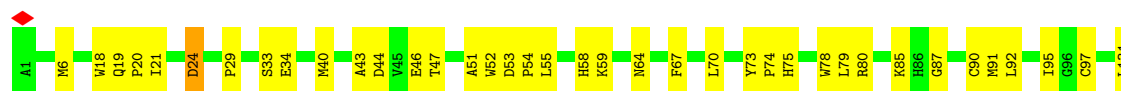


• Molecule 12: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

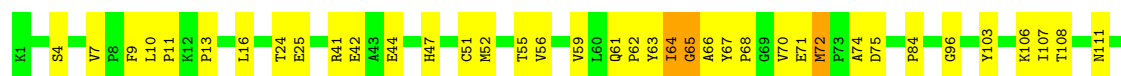




- Molecule 13: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8



- Molecule 14: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



- Molecule 15: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6

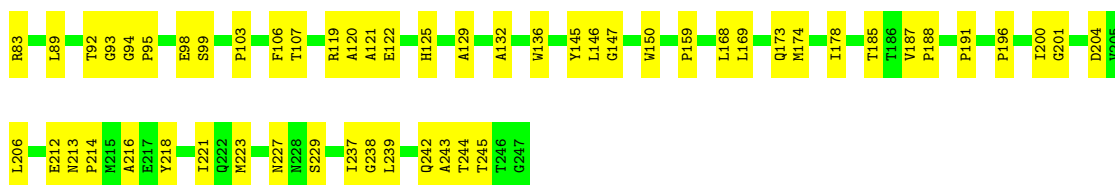


- Molecule 16: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2

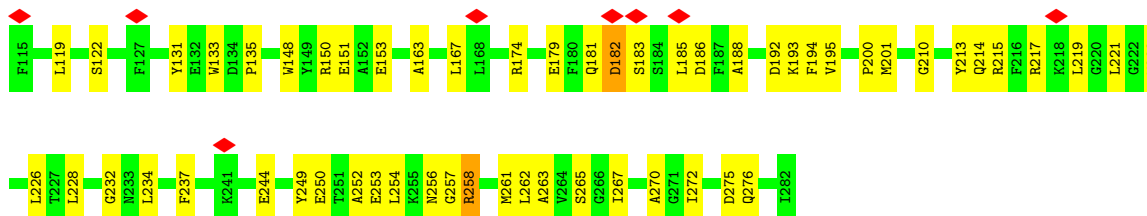


- Molecule 17: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3

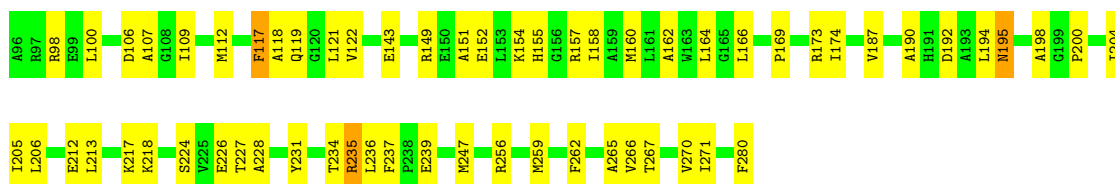




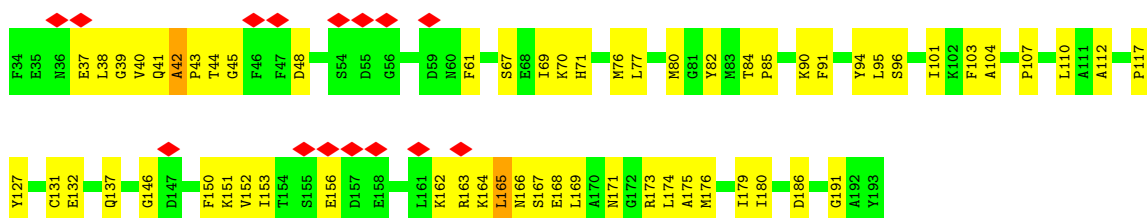
- Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4



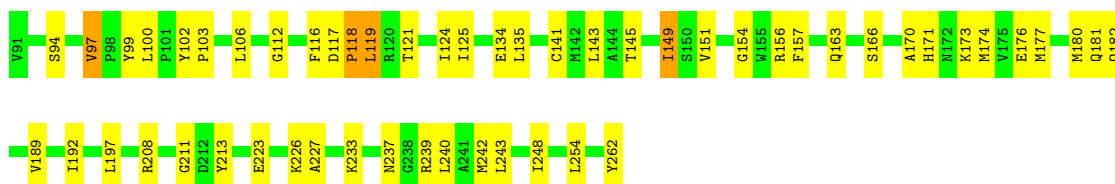
- Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



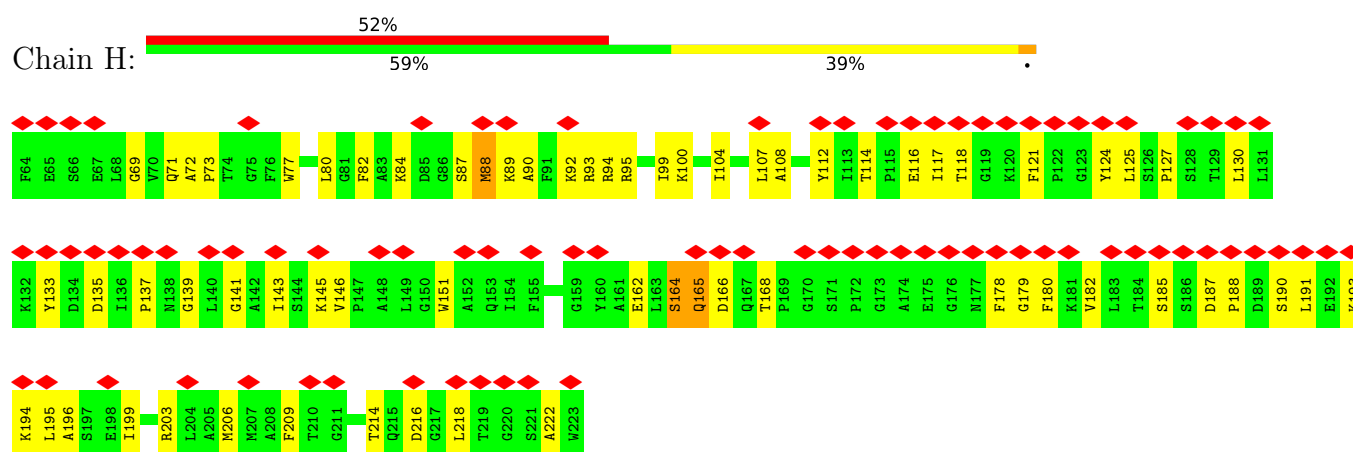
- Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9



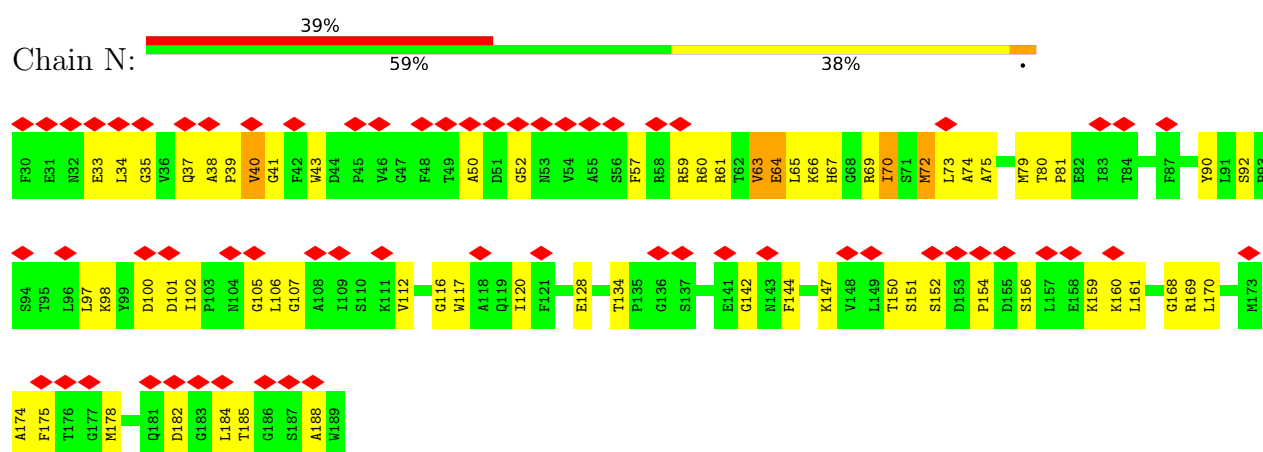
- Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11



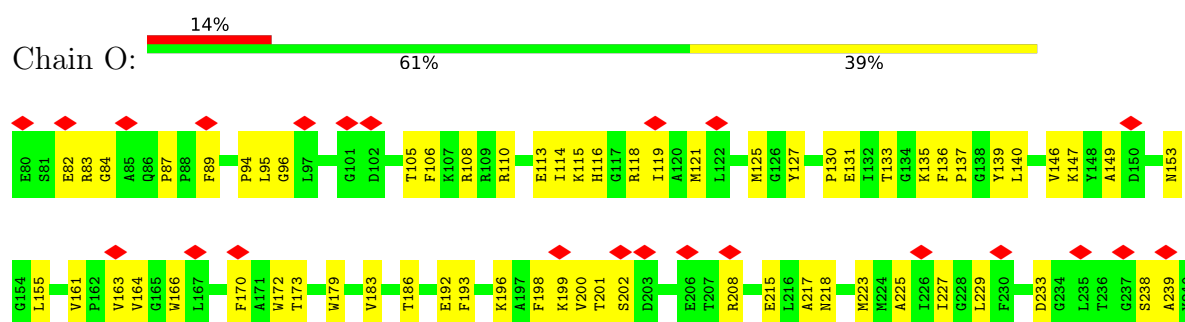
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



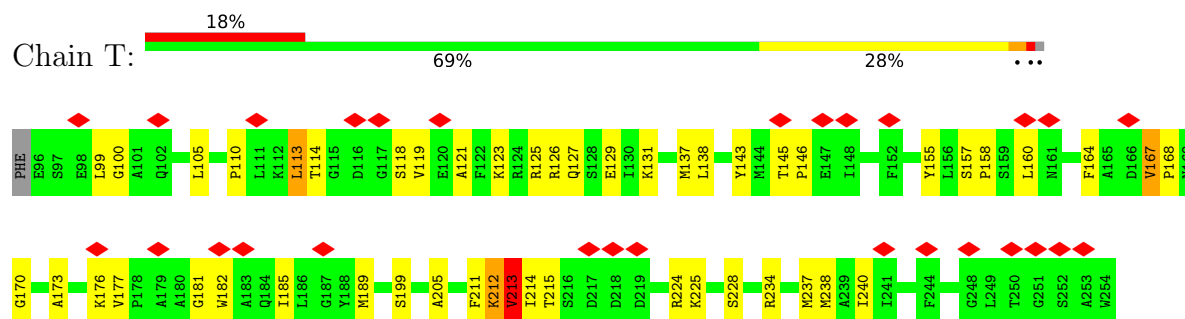
• Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13



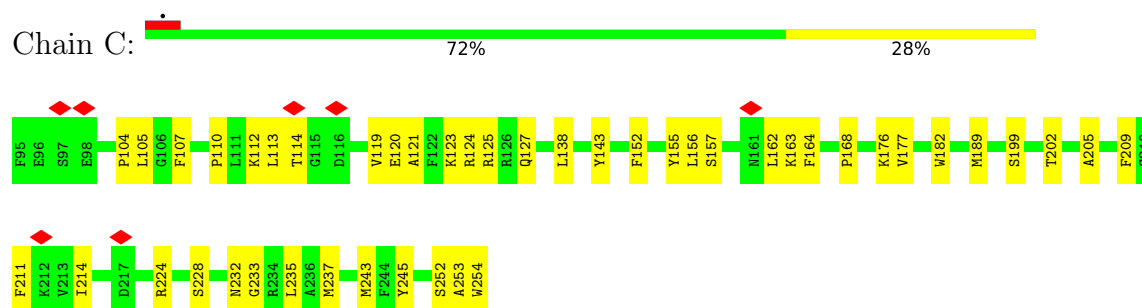
• Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15



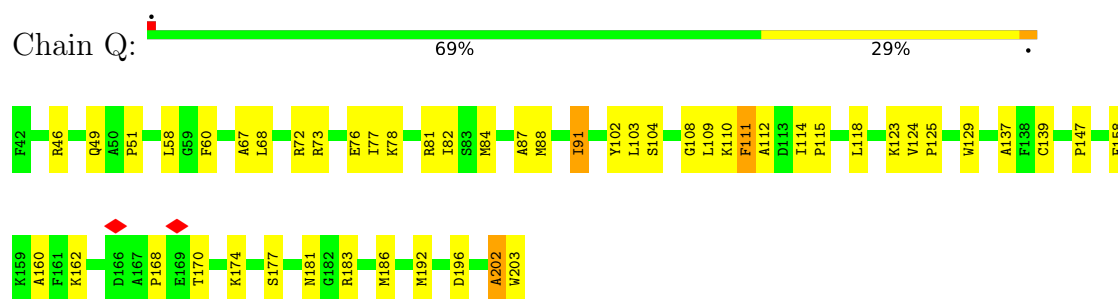
• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16



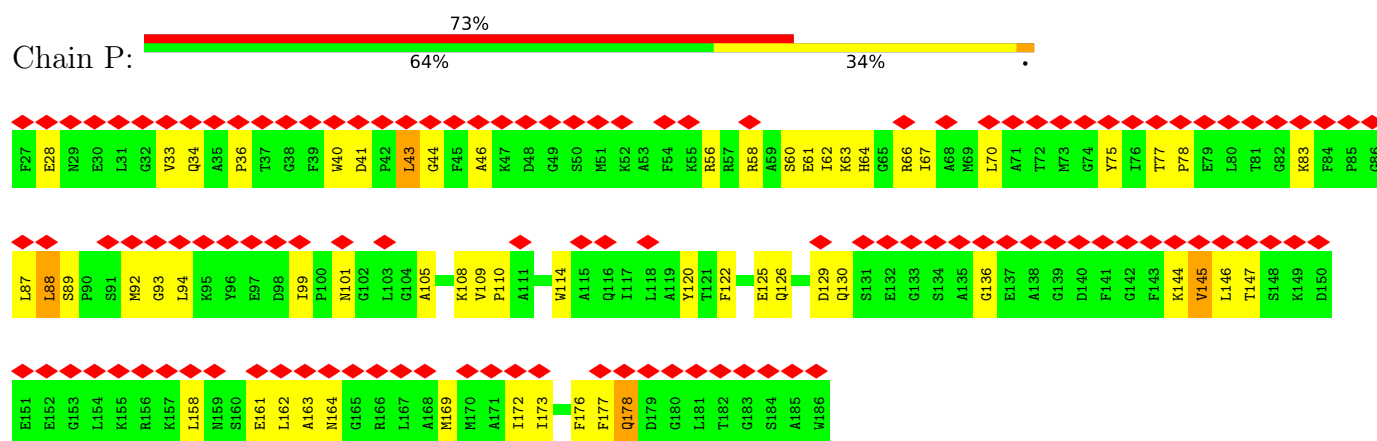
- Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16



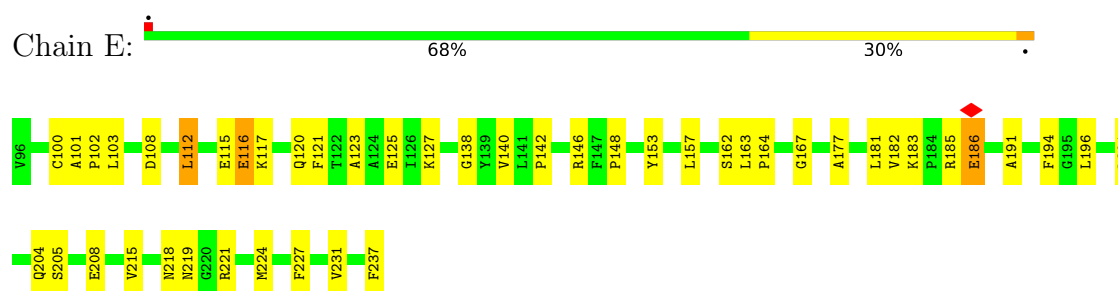
- Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17



- Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14



- Molecule 28: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	356838	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)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.883	Depositor
Minimum map value	-0.563	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.22	Depositor
Map size ($\text{\AA}$)	665.6, 665.6, 665.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	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: CLA, DD6, PQN, KC1, UIX, SF4, DGD, LHG, PID, LMG, SQD, 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	0.30	1/5133 (0.0%)	0.36	0/7019
2	b	0.31	0/4968	0.39	0/6804
3	c	0.20	0/657	0.28	0/897
4	d	0.20	0/2034	0.34	0/2766
5	e	0.16	0/624	0.23	0/851
6	f	0.16	0/1484	0.26	0/1998
7	h	0.28	0/1089	0.43	0/1479
8	i	0.26	0/1030	0.45	0/1394
9	j	0.42	0/566	0.51	0/774
10	l	0.16	0/2014	0.29	0/2737
11	m	0.26	0/694	0.43	0/939
12	A	0.18	0/1395	0.31	0/1892
13	G	0.19	0/1730	0.32	0/2348
14	I	0.28	0/1499	0.42	0/2037
15	K	0.19	0/1358	0.30	0/1838
16	F	0.21	0/1395	0.45	0/1886
17	J	0.18	0/1317	0.38	0/1795
18	M	0.16	0/1395	0.45	0/1888
19	L	0.18	0/1490	0.42	0/2021
20	D	0.19	0/1223	0.46	2/1650 (0.1%)
21	B	0.28	0/1404	0.42	2/1891 (0.1%)
22	H	0.18	0/1232	0.39	0/1665
23	N	0.19	0/1233	0.45	0/1671
24	O	0.20	0/1260	0.45	0/1709
25	C	0.14	0/1226	0.33	0/1653
25	T	0.15	0/1214	0.37	0/1637
26	Q	0.18	0/1251	0.41	0/1690
27	P	0.17	0/1245	0.39	0/1673
28	E	0.19	0/1093	0.44	0/1473
All	All	0.23	1/44253 (0.0%)	0.38	4/60075 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	589	TYR	N-CA	-5.09	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	119	LEU	N-CA-C	-7.66	100.82	111.39
20	D	42	ALA	CA-C-N	-6.56	114.14	120.83
20	D	42	ALA	C-N-CA	-6.56	114.14	120.83
21	B	118	PRO	N-CA-C	-5.14	101.88	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	4980	0	4912	140	0
2	b	4813	0	4698	164	0
3	c	647	0	628	22	0
4	d	1985	0	1951	54	0
5	e	607	0	582	8	0
6	f	1455	0	1492	43	0
7	h	1056	0	1035	38	0
8	i	1001	0	999	33	0
9	j	549	0	546	20	0
10	l	1961	0	1942	68	0
11	m	679	0	685	28	0
12	A	1358	0	1328	37	0
13	G	1675	0	1614	49	0
14	I	1455	0	1392	45	0
15	K	1325	0	1317	54	0
16	F	1356	0	1315	66	0
17	J	1282	0	1255	45	0
18	M	1346	0	1263	43	0
19	L	1453	0	1423	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	1198	0	1176	52	0
21	B	1371	0	1372	45	0
22	H	1202	0	1182	58	0
23	N	1203	0	1172	56	0
24	O	1226	0	1200	65	0
25	C	1200	0	1185	43	0
25	T	1189	0	1176	43	0
26	Q	1219	0	1210	49	0
27	P	1218	0	1202	51	0
28	E	1071	0	1050	41	0
29	A	616	0	527	19	0
29	B	527	0	473	17	0
29	C	297	0	245	17	0
29	D	318	0	231	20	0
29	E	494	0	461	28	0
29	F	358	0	256	22	0
29	G	565	0	536	30	0
29	H	297	0	245	16	0
29	I	602	0	547	28	0
29	J	400	0	331	18	0
29	K	541	0	431	28	0
29	L	506	0	414	22	0
29	M	435	0	337	16	0
29	N	297	0	245	16	0
29	O	297	0	245	20	0
29	P	297	0	245	20	0
29	Q	311	0	276	19	0
29	T	273	0	198	18	0
29	a	1841	0	1790	120	0
29	b	1676	0	1696	119	0
29	f	152	0	125	8	0
29	h	60	0	59	7	0
29	i	185	0	193	19	0
29	j	52	0	43	0	0
29	l	447	0	438	35	0
30	a	33	0	46	6	0
30	b	33	0	46	3	0
31	a	48	0	69	5	0
32	a	120	0	168	16	0
32	b	120	0	168	19	0
32	f	80	0	112	13	0
32	i	40	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	l	80	0	112	8	0
32	m	40	0	56	8	0
33	a	8	0	0	2	0
33	c	16	0	0	3	0
34	A	37	0	44	2	0
34	E	32	0	34	6	0
34	K	114	0	138	7	0
34	P	27	0	24	1	0
34	b	130	0	170	13	0
34	h	28	0	26	2	0
34	j	43	0	56	3	0
35	B	45	0	48	0	0
35	G	45	0	48	2	0
35	b	57	0	72	2	0
35	h	54	0	69	9	0
35	j	133	0	140	9	0
35	m	66	0	96	5	0
36	A	129	0	0	2	0
36	B	214	0	0	8	0
36	C	43	0	0	1	0
36	D	86	0	0	3	0
36	E	86	0	0	0	0
36	F	86	0	0	2	0
36	G	172	0	0	4	0
36	H	43	0	0	0	0
36	I	215	0	0	4	0
36	J	129	0	0	5	0
36	K	258	0	0	4	0
36	L	172	0	0	2	0
36	M	172	0	0	6	0
36	N	43	0	0	1	0
36	O	43	0	0	2	0
36	P	43	0	0	1	0
36	Q	43	0	0	0	0
36	T	43	0	0	1	0
36	h	43	0	0	0	0
36	m	43	0	0	0	0
37	C	230	0	250	21	0
37	D	230	0	250	20	0
37	E	46	0	50	7	0
37	F	138	0	150	19	0
37	G	138	0	150	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	H	230	0	250	23	0
37	N	230	0	250	21	0
37	O	230	0	250	24	0
37	P	230	0	250	22	0
37	Q	184	0	200	17	0
37	T	276	0	300	20	0
37	h	46	0	50	1	0
37	j	46	0	50	5	0
38	A	47	0	0	0	0
38	B	47	0	0	1	0
38	C	47	0	0	0	0
38	E	47	0	0	1	0
38	F	47	0	0	2	0
38	J	47	0	0	1	0
38	L	47	0	0	0	0
38	N	47	0	0	0	0
38	O	47	0	0	0	0
38	P	47	0	0	0	0
38	Q	47	0	0	0	0
38	T	47	0	0	0	0
39	A	90	0	0	0	0
39	B	45	0	0	0	0
39	C	135	0	0	1	0
39	D	90	0	0	2	0
39	E	90	0	0	2	0
39	F	90	0	0	0	0
39	G	90	0	0	2	0
39	H	135	0	0	2	0
39	I	45	0	0	1	0
39	J	45	0	0	0	0
39	K	45	0	0	0	0
39	L	90	0	0	0	0
39	M	90	0	0	0	0
39	N	135	0	0	5	0
39	O	135	0	0	0	0
39	P	135	0	0	2	0
39	Q	135	0	0	2	0
39	T	135	0	0	0	0
40	B	42	0	48	3	0
40	J	45	0	54	7	0
All	All	63119	0	57239	1854	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 15.

The worst 5 of 1854 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)
37:F:304:PID:HM11	37:F:304:PID:H8	1.33	1.09
37:H:306:PID:HM11	37:H:306:PID:H8	1.45	0.96
7:h:38:ARG:H	7:h:39:PRO:HD2	1.31	0.95
16:F:183:ALA:HB1	37:F:304:PID:H8	1.52	0.91
37:Q:304:PID:H20	29:Q:313:CLA:HAB	1.55	0.87

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	643/645 (100%)	594 (92%)	47 (7%)	2 (0%)	36	65
2	b	615/617 (100%)	581 (94%)	34 (6%)	0	100	100
3	c	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
4	d	255/257 (99%)	239 (94%)	15 (6%)	1 (0%)	30	59
5	e	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
6	f	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
7	h	130/132 (98%)	121 (93%)	6 (5%)	3 (2%)	5	19
8	i	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
9	j	68/70 (97%)	60 (88%)	8 (12%)	0	100	100
10	l	251/253 (99%)	231 (92%)	20 (8%)	0	100	100
11	m	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
12	A	178/180 (99%)	163 (92%)	15 (8%)	0	100	100
13	G	213/215 (99%)	189 (89%)	23 (11%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	I	192/194 (99%)	165 (86%)	21 (11%)	6 (3%)	3	14
15	K	170/172 (99%)	153 (90%)	16 (9%)	1 (1%)	21	51
16	F	174/176 (99%)	154 (88%)	19 (11%)	1 (1%)	21	51
17	J	163/165 (99%)	144 (88%)	18 (11%)	1 (1%)	21	51
18	M	166/168 (99%)	134 (81%)	26 (16%)	6 (4%)	2	11
19	L	183/185 (99%)	152 (83%)	26 (14%)	5 (3%)	4	16
20	D	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	21	51
21	B	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
22	H	158/160 (99%)	135 (85%)	19 (12%)	4 (2%)	4	17
23	N	158/160 (99%)	126 (80%)	31 (20%)	1 (1%)	21	51
24	O	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	6	23
25	C	158/160 (99%)	146 (92%)	11 (7%)	1 (1%)	21	51
25	T	157/160 (98%)	142 (90%)	11 (7%)	4 (2%)	4	17
26	Q	160/162 (99%)	138 (86%)	20 (12%)	2 (1%)	9	32
27	P	158/160 (99%)	139 (88%)	16 (10%)	3 (2%)	6	23
28	E	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	5	21
All	All	5527/5586 (99%)	4986 (90%)	492 (9%)	49 (1%)	16	41

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	520	SER
4	d	149	HIS
14	I	116	SER
14	I	135	LYS
14	I	186	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	531/535 (99%)	527 (99%)	4 (1%)	73	90
2	b	502/504 (100%)	495 (99%)	7 (1%)	59	85
3	c	73/74 (99%)	72 (99%)	1 (1%)	59	85
4	d	213/222 (96%)	213 (100%)	0	100	100
5	e	65/66 (98%)	65 (100%)	0	100	100
6	f	151/151 (100%)	150 (99%)	1 (1%)	76	92
7	h	109/109 (100%)	105 (96%)	4 (4%)	30	64
8	i	106/106 (100%)	104 (98%)	2 (2%)	50	79
9	j	60/60 (100%)	58 (97%)	2 (3%)	33	67
10	l	200/203 (98%)	200 (100%)	0	100	100
11	m	72/72 (100%)	72 (100%)	0	100	100
12	A	136/141 (96%)	136 (100%)	0	100	100
13	G	171/171 (100%)	169 (99%)	2 (1%)	63	86
14	I	141/156 (90%)	137 (97%)	4 (3%)	38	72
15	K	133/138 (96%)	133 (100%)	0	100	100
16	F	140/140 (100%)	138 (99%)	2 (1%)	59	85
17	J	136/136 (100%)	135 (99%)	1 (1%)	76	92
18	M	128/128 (100%)	126 (98%)	2 (2%)	55	83
19	L	145/145 (100%)	145 (100%)	0	100	100
20	D	123/123 (100%)	120 (98%)	3 (2%)	43	75
21	B	146/146 (100%)	144 (99%)	2 (1%)	59	85
22	H	123/123 (100%)	122 (99%)	1 (1%)	73	90
23	N	124/124 (100%)	119 (96%)	5 (4%)	28	62
24	O	124/124 (100%)	123 (99%)	1 (1%)	73	90
25	C	121/121 (100%)	121 (100%)	0	100	100
25	T	120/121 (99%)	118 (98%)	2 (2%)	53	82
26	Q	120/120 (100%)	119 (99%)	1 (1%)	73	90
27	P	123/123 (100%)	121 (98%)	2 (2%)	55	83
28	E	108/108 (100%)	107 (99%)	1 (1%)	70	90
All	All	4444/4490 (99%)	4394 (99%)	50 (1%)	63	88

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	F	170	LEU
21	B	97	VAL
28	E	112	LEU
17	J	229	SER
20	D	41	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
18	M	276	GLN
22	H	71	GLN
21	B	251	GLN
23	N	133	GLN
12	A	24	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

411 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
39	KC1	D	315	-	49,53,53	1.36	5 (10%)	61,89,89	1.73	11 (18%)
29	CLA	C	311	-	55,59,73	1.30	9 (16%)	64,96,113	1.40	5 (7%)
38	UIX	T	306	-	43,49,49	1.41	5 (11%)	53,74,74	2.80	22 (41%)
36	DD6	L	304	-	40,45,45	1.56	2 (5%)	51,67,67	1.97	16 (31%)
29	CLA	N	311	-	55,59,73	1.30	7 (12%)	64,96,113	1.38	5 (7%)
36	DD6	J	303	-	40,45,45	1.65	2 (5%)	51,67,67	2.10	17 (33%)
29	CLA	M	314	-	56,60,73	1.29	9 (16%)	65,97,113	1.32	5 (7%)
37	PID	N	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.43	5 (9%)
38	UIX	P	207	-	43,49,49	1.41	4 (9%)	53,74,74	2.59	19 (35%)
37	PID	O	307	-	43,49,49	1.25	3 (6%)	52,76,76	1.40	8 (15%)
37	PID	Q	303	-	43,49,49	1.27	3 (6%)	52,76,76	1.42	7 (13%)
29	CLA	G	311	13	55,59,73	1.29	8 (14%)	64,96,113	1.38	4 (6%)
36	DD6	B	301	-	39,44,45	1.57	2 (5%)	49,65,67	1.98	16 (32%)
29	CLA	D	312	20	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
36	DD6	G	307	-	40,45,45	2.35	8 (20%)	51,67,67	2.49	19 (37%)
36	DD6	I	205	-	40,45,45	2.09	4 (10%)	51,67,67	2.30	17 (33%)
29	CLA	a	804	-	59,63,73	1.26	9 (15%)	70,101,113	1.42	7 (10%)
37	PID	T	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	5 (9%)
29	CLA	a	828	-	50,54,73	1.36	9 (18%)	59,90,113	1.41	4 (6%)
39	KC1	P	211	-	49,53,53	1.34	6 (12%)	61,89,89	1.72	13 (21%)
36	DD6	Q	302	-	40,45,45	1.54	2 (5%)	51,67,67	1.84	13 (25%)
29	CLA	a	837	-	59,63,73	1.25	9 (15%)	70,101,113	1.29	6 (8%)
32	BCR	m	103	-	41,41,41	0.79	2 (4%)	56,56,56	2.37	17 (30%)
29	CLA	A	206	39	49,53,73	1.38	8 (16%)	58,89,113	1.48	5 (8%)
34	LMG	K	219	-	35,35,55	0.92	1 (2%)	43,43,63	1.20	4 (9%)
36	DD6	I	206	-	40,45,45	1.55	2 (5%)	51,67,67	1.88	16 (31%)
39	KC1	E	312	28	49,53,53	1.38	7 (14%)	61,89,89	1.71	14 (22%)
37	PID	O	305	-	43,49,49	1.25	3 (6%)	52,76,76	1.79	8 (15%)
29	CLA	Q	313	-	51,55,73	1.34	9 (17%)	60,91,113	1.41	5 (8%)
29	CLA	J	307	-	50,54,73	1.34	9 (18%)	59,90,113	1.38	4 (6%)
29	CLA	L	313	-	57,61,73	1.26	9 (15%)	67,98,113	1.37	5 (7%)
36	DD6	G	305	-	40,45,45	1.80	4 (10%)	51,67,67	2.97	16 (31%)
29	CLA	b	726	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
35	DGD	j	103	-	44,44,67	1.00	2 (4%)	58,58,81	1.33	8 (13%)
36	DD6	O	303	-	40,45,45	1.68	3 (7%)	51,67,67	2.15	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	SF4	c	101	3	0,12,12	-	-	-		
29	CLA	I	209	-	64,68,73	1.20	9 (14%)	76,107,113	5.01	8 (10%)
34	LMG	b	732	-	44,44,55	0.80	1 (2%)	52,52,63	1.33	6 (11%)
29	CLA	O	309	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
37	PID	P	205	-	43,49,49	1.24	3 (6%)	52,76,76	1.48	7 (13%)
29	CLA	a	801	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
39	KC1	O	310	-	49,53,53	1.36	7 (14%)	61,89,89	1.73	12 (19%)
39	KC1	F	314	-	49,53,53	1.36	7 (14%)	61,89,89	1.74	13 (21%)
29	CLA	b	713	-	57,61,73	1.29	8 (14%)	67,98,113	1.34	6 (8%)
38	UIX	C	306	-	43,49,49	1.40	5 (11%)	53,74,74	2.54	20 (37%)
29	CLA	B	311	21	55,59,73	1.30	9 (16%)	64,96,113	1.38	5 (7%)
29	CLA	K	208	-	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
29	CLA	M	310	18	52,56,73	1.33	9 (17%)	61,92,113	1.38	6 (9%)
36	DD6	P	204	-	40,45,45	1.53	2 (5%)	51,67,67	2.18	14 (27%)
29	CLA	H	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.45	5 (9%)
38	UIX	B	304	-	43,49,49	1.40	4 (9%)	53,74,74	2.41	18 (33%)
29	CLA	K	207	15	53,57,73	1.32	9 (16%)	61,93,113	1.40	5 (8%)
36	DD6	I	203	-	40,45,45	1.83	4 (10%)	51,67,67	2.33	17 (33%)
29	CLA	a	825	-	69,73,73	1.17	8 (11%)	82,113,113	1.36	8 (9%)
39	KC1	P	216	-	49,53,53	1.35	5 (10%)	61,89,89	1.72	12 (19%)
29	CLA	H	308	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
36	DD6	L	305	-	40,45,45	1.58	2 (5%)	51,67,67	1.98	16 (31%)
29	CLA	L	309	-	59,63,73	1.25	9 (15%)	70,101,113	1.33	6 (8%)
36	DD6	N	303	-	40,45,45	1.52	2 (5%)	51,67,67	1.73	13 (25%)
35	DGD	m	102	-	67,67,67	0.83	2 (2%)	81,81,81	0.92	4 (4%)
29	CLA	M	315	-	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
36	DD6	L	303	-	40,45,45	1.62	2 (5%)	51,67,67	1.76	15 (29%)
29	CLA	I	217	-	59,63,73	1.25	8 (13%)	70,101,113	1.32	6 (8%)
29	CLA	G	301	-	53,57,73	1.31	9 (16%)	61,93,113	1.38	6 (9%)
29	CLA	J	306	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
37	PID	h	204	-	43,49,49	1.27	3 (6%)	52,76,76	1.36	7 (13%)
29	CLA	a	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	5 (8%)
29	CLA	a	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	9 (10%)
37	PID	P	208	-	43,49,49	1.23	4 (9%)	52,76,76	2.33	7 (13%)
29	CLA	A	207	-	59,63,73	1.26	9 (15%)	70,101,113	1.33	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	G	312	13	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
36	DD6	K	204	-	40,45,45	1.65	2 (5%)	51,67,67	1.98	17 (33%)
29	CLA	a	817	-	49,53,73	1.39	9 (18%)	58,89,113	1.40	4 (6%)
39	KC1	O	315	-	49,53,53	1.36	5 (10%)	61,89,89	1.74	14 (22%)
29	CLA	I	208	-	50,54,73	1.35	9 (18%)	59,90,113	5.66	6 (10%)
29	CLA	i	202	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	6 (7%)
29	CLA	N	314	-	51,55,73	1.34	9 (17%)	60,91,113	1.43	7 (11%)
37	PID	P	206	-	43,49,49	1.24	4 (9%)	52,76,76	1.76	10 (19%)
29	CLA	Q	308	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
29	CLA	K	211	-	59,63,73	1.24	9 (15%)	70,101,113	1.37	7 (10%)
37	PID	P	203	-	43,49,49	1.27	3 (6%)	52,76,76	1.42	9 (17%)
39	KC1	H	309	-	49,53,53	1.35	6 (12%)	61,89,89	1.74	13 (21%)
29	CLA	B	307	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
37	PID	H	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.56	5 (9%)
39	KC1	E	307	-	49,53,53	1.37	7 (14%)	61,89,89	1.76	13 (21%)
36	DD6	K	221	-	40,45,45	1.67	3 (7%)	51,67,67	2.17	16 (31%)
29	CLA	b	704	-	69,73,73	1.16	9 (13%)	82,113,113	3.89	7 (8%)
29	CLA	E	305	-	65,69,73	1.22	8 (12%)	77,108,113	1.34	5 (6%)
35	DGD	j	106	-	50,50,67	0.97	2 (4%)	64,64,81	1.05	4 (6%)
29	CLA	L	310	-	59,63,73	1.26	9 (15%)	70,101,113	1.35	6 (8%)
35	DGD	b	733	-	58,58,67	0.95	4 (6%)	72,72,81	1.26	7 (9%)
36	DD6	E	302	-	40,45,45	1.65	2 (5%)	51,67,67	2.27	16 (31%)
34	LMG	j	102	-	43,43,55	0.77	1 (2%)	51,51,63	1.30	5 (9%)
29	CLA	J	313	-	45,49,73	1.41	9 (20%)	54,84,113	1.49	5 (9%)
29	CLA	F	307	-	50,54,73	1.35	8 (16%)	59,90,113	1.41	5 (8%)
29	CLA	T	311	-	50,54,73	1.36	7 (14%)	59,90,113	1.40	4 (6%)
29	CLA	M	309	-	50,54,73	1.38	9 (18%)	59,90,113	1.36	5 (8%)
38	UIX	O	306	-	43,49,49	1.38	4 (9%)	53,74,74	2.69	19 (35%)
29	CLA	E	313	-	45,49,73	1.42	7 (15%)	54,84,113	1.46	5 (9%)
35	DGD	j	105	-	42,42,67	1.04	2 (4%)	56,56,81	1.08	5 (8%)
29	CLA	a	826	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
36	DD6	M	303	-	40,45,45	1.65	3 (7%)	51,67,67	2.10	12 (23%)
39	KC1	F	309	-	49,53,53	1.37	6 (12%)	61,89,89	1.77	13 (21%)
29	CLA	a	823	-	62,66,73	1.21	9 (14%)	73,104,113	1.30	7 (9%)
32	BCR	b	729	-	41,41,41	0.73	1 (2%)	56,56,56	1.90	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	K	217	-	50,54,73	1.36	9 (18%)	59,90,113	1.41	4 (6%)
34	LMG	P	201	-	27,27,55	0.98	0	35,35,63	1.29	6 (17%)
32	BCR	l	507	-	41,41,41	0.71	0	56,56,56	1.99	17 (30%)
29	CLA	A	210	12	50,54,73	1.36	9 (18%)	59,90,113	1.33	4 (6%)
32	BCR	a	838	-	41,41,41	0.70	0	56,56,56	2.14	19 (33%)
29	CLA	I	214	-	59,63,73	1.24	9 (15%)	70,101,113	1.33	5 (7%)
29	CLA	a	811	-	60,64,73	1.26	9 (15%)	71,102,113	1.31	5 (7%)
29	CLA	N	308	-	51,55,73	1.36	8 (15%)	60,91,113	1.39	5 (8%)
29	CLA	b	725	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
37	PID	Q	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.52	8 (15%)
29	CLA	B	309	-	59,63,73	1.25	8 (13%)	70,101,113	1.34	6 (8%)
29	CLA	H	312	22	50,54,73	1.35	6 (12%)	59,90,113	1.40	6 (10%)
29	CLA	a	819	-	61,65,73	1.23	9 (14%)	72,103,113	1.30	6 (8%)
36	DD6	B	303	-	40,45,45	1.58	2 (5%)	51,67,67	1.77	13 (25%)
29	CLA	b	702	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
29	CLA	A	217	-	55,59,73	1.30	9 (16%)	64,96,113	1.38	7 (10%)
39	KC1	T	315	25	49,53,53	1.36	5 (10%)	61,89,89	1.72	13 (21%)
29	CLA	M	308	-	52,56,73	1.33	9 (17%)	61,92,113	1.38	4 (6%)
29	CLA	b	701	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
36	DD6	H	303	-	40,45,45	1.50	2 (5%)	51,67,67	1.94	13 (25%)
29	CLA	a	827	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
29	CLA	b	736	-	69,73,73	1.16	9 (13%)	82,113,113	6.00	10 (12%)
29	CLA	G	304	-	63,67,73	1.21	9 (14%)	74,105,113	1.40	5 (6%)
29	CLA	a	820	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	5 (6%)
29	CLA	L	315	-	45,49,73	1.42	9 (20%)	54,84,113	1.48	5 (9%)
29	CLA	h	201	-	64,68,73	1.20	9 (14%)	76,107,113	1.31	7 (9%)
29	CLA	C	308	-	51,55,73	1.34	9 (17%)	60,91,113	1.38	5 (8%)
29	CLA	a	806	1	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
36	DD6	K	206	-	40,45,45	1.57	2 (5%)	51,67,67	2.01	15 (29%)
37	PID	O	302	-	43,49,49	1.27	3 (6%)	52,76,76	1.38	8 (15%)
29	CLA	F	308	-	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
36	DD6	B	302	-	40,45,45	1.57	2 (5%)	51,67,67	1.92	15 (29%)
29	CLA	f	802	-	50,54,73	1.34	9 (18%)	59,90,113	1.38	4 (6%)
37	PID	j	101	-	43,49,49	1.27	3 (6%)	52,76,76	1.50	12 (23%)
29	CLA	I	212	-	59,63,73	1.26	9 (15%)	70,101,113	6.47	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	Q	312	-	50,54,73	1.35	9 (18%)	59,90,113	1.40	5 (8%)
37	PID	E	301	-	43,49,49	1.25	4 (9%)	52,76,76	1.90	11 (21%)
37	PID	H	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.94	10 (19%)
37	PID	C	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.39	7 (13%)
29	CLA	I	210	-	59,63,73	1.25	9 (15%)	70,101,113	1.33	5 (7%)
29	CLA	b	731	-	60,64,73	1.24	9 (15%)	71,102,113	1.34	6 (8%)
29	CLA	J	308	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	7 (9%)
37	PID	N	302	-	43,49,49	1.28	3 (6%)	52,76,76	1.39	7 (13%)
29	CLA	E	314	28	52,56,73	1.34	9 (17%)	61,92,113	1.36	5 (8%)
36	DD6	A	202	-	40,45,45	1.53	2 (5%)	51,67,67	1.79	13 (25%)
29	CLA	a	810	1	59,63,73	1.26	9 (15%)	70,101,113	1.36	6 (8%)
29	CLA	H	313	-	51,55,73	1.34	9 (17%)	60,91,113	1.48	5 (8%)
29	CLA	D	308	-	51,55,73	1.35	7 (13%)	60,91,113	1.40	5 (8%)
29	CLA	F	315	-	45,49,73	1.42	8 (17%)	54,84,113	1.53	6 (11%)
38	UIX	F	305	-	43,49,49	1.38	4 (9%)	53,74,74	2.75	19 (35%)
29	CLA	O	313	24	50,54,73	1.35	8 (16%)	59,90,113	1.40	6 (10%)
29	CLA	a	813	-	55,59,73	1.32	9 (16%)	64,96,113	1.37	6 (9%)
29	CLA	E	310	28	50,54,73	1.35	7 (14%)	59,90,113	1.39	5 (8%)
29	CLA	b	714	-	68,72,73	1.16	9 (13%)	80,111,113	1.28	7 (8%)
29	CLA	b	724	-	51,55,73	1.33	9 (17%)	60,91,113	1.40	6 (10%)
39	KC1	N	315	-	49,53,53	1.35	5 (10%)	61,89,89	1.71	13 (21%)
36	DD6	D	304	-	40,45,45	1.65	3 (7%)	51,67,67	2.11	13 (25%)
36	DD6	M	301	-	40,45,45	1.56	2 (5%)	51,67,67	1.84	16 (31%)
37	PID	T	302	-	43,49,49	1.26	4 (9%)	52,76,76	1.51	9 (17%)
29	CLA	j	104	29	56,60,73	1.28	9 (16%)	65,97,113	1.42	5 (7%)
29	CLA	F	313	16	50,54,73	1.36	9 (18%)	59,90,113	1.43	4 (6%)
29	CLA	Q	315	-	45,49,73	1.42	9 (20%)	54,84,113	1.51	5 (9%)
29	CLA	A	216	-	45,49,73	1.41	9 (20%)	54,84,113	1.48	5 (9%)
29	CLA	K	218	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
29	CLA	b	703	-	69,73,73	1.16	9 (13%)	82,113,113	1.18	5 (6%)
29	CLA	i	201	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
29	CLA	N	309	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	5 (6%)
29	CLA	a	805	-	59,63,73	1.25	9 (15%)	70,101,113	1.36	5 (7%)
29	CLA	G	317	-	57,61,73	1.28	9 (15%)	67,98,113	1.33	6 (8%)
32	BCR	b	728	-	41,41,41	0.77	1 (2%)	56,56,56	2.05	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	T	316	-	45,49,73	1.43	7 (15%)	54,84,113	1.49	5 (9%)
29	CLA	f	803	6	50,54,73	1.35	9 (18%)	59,90,113	1.40	4 (6%)
32	BCR	f	804	-	41,41,41	0.71	0	56,56,56	1.98	15 (26%)
29	CLA	F	311	-	50,54,73	1.34	9 (18%)	59,90,113	1.44	4 (6%)
39	KC1	C	315	25	49,53,53	1.38	5 (10%)	61,89,89	1.73	13 (21%)
37	PID	D	305	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	8 (15%)
34	LMG	K	220	-	36,36,55	0.86	1 (2%)	44,44,63	1.24	4 (9%)
29	CLA	a	822	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
38	UIX	Q	305	-	43,49,49	1.38	5 (11%)	53,74,74	2.79	20 (37%)
33	SF4	c	102	3	0,12,12	-	-	-	-	-
29	CLA	b	712	-	69,73,73	1.16	9 (13%)	82,113,113	3.75	8 (9%)
29	CLA	i	203	-	59,63,73	1.24	9 (15%)	70,101,113	1.37	7 (10%)
29	CLA	b	707	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
29	CLA	A	215	-	51,55,73	1.35	9 (17%)	60,91,113	1.41	5 (8%)
29	CLA	P	210	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
36	DD6	L	301	-	40,45,45	1.54	2 (5%)	51,67,67	1.93	13 (25%)
39	KC1	G	315	-	49,53,53	1.45	7 (14%)	61,89,89	1.85	13 (21%)
39	KC1	Q	309	-	49,53,53	1.36	5 (10%)	61,89,89	1.75	13 (21%)
29	CLA	b	715	-	50,54,73	1.35	9 (18%)	59,90,113	1.39	5 (8%)
29	CLA	N	316	-	45,49,73	1.43	8 (17%)	54,84,113	1.48	5 (9%)
29	CLA	G	316	-	69,73,73	1.18	9 (13%)	82,113,113	4.82	8 (9%)
33	SF4	a	836	2,1	0,12,12	-	-	-	-	-
37	PID	H	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	6 (11%)
29	CLA	a	814	-	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
40	SQD	J	314	-	43,45,54	0.43	1 (2%)	53,56,65	0.59	1 (1%)
29	CLA	T	308	-	51,55,73	1.35	8 (15%)	60,91,113	1.38	5 (8%)
39	KC1	M	305	-	49,53,53	1.37	6 (12%)	61,89,89	1.77	15 (24%)
39	KC1	P	213	27	49,53,53	1.39	5 (10%)	61,89,89	1.72	13 (21%)
29	CLA	B	312	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
29	CLA	b	716	-	57,61,73	1.26	9 (15%)	67,98,113	1.33	8 (11%)
29	CLA	b	722	-	62,66,73	1.22	9 (14%)	73,104,113	1.35	6 (8%)
29	CLA	H	310	-	55,59,73	1.32	8 (14%)	64,96,113	1.39	6 (9%)
29	CLA	D	309	-	50,54,73	1.36	8 (16%)	59,90,113	1.40	4 (6%)
29	CLA	C	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.54	5 (9%)
29	CLA	a	812	-	64,68,73	1.19	9 (14%)	76,107,113	1.34	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	717	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	6 (7%)
37	PID	Q	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.40	6 (11%)
37	PID	C	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.39	6 (11%)
29	CLA	G	319	13	45,49,73	1.41	8 (17%)	54,84,113	1.49	5 (9%)
36	DD6	I	202	-	40,45,45	1.56	2 (5%)	51,67,67	1.93	15 (29%)
37	PID	T	305	-	43,49,49	1.24	3 (6%)	52,76,76	1.47	7 (13%)
39	KC1	L	306	29	49,53,53	1.35	6 (12%)	61,89,89	1.74	15 (24%)
29	CLA	M	313	-	45,49,73	1.42	9 (20%)	54,84,113	1.51	5 (9%)
36	DD6	G	306	-	40,45,45	1.66	3 (7%)	51,67,67	2.21	15 (29%)
29	CLA	N	313	23	50,54,73	1.35	7 (14%)	59,90,113	4.61	9 (15%)
29	CLA	T	314	-	51,55,73	1.34	8 (15%)	60,91,113	1.46	9 (15%)
29	CLA	I	211	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	8 (9%)
35	DGD	h	203	-	55,55,67	0.91	2 (3%)	69,69,81	0.99	5 (7%)
29	CLA	D	311	-	50,54,73	1.35	9 (18%)	59,90,113	1.41	4 (6%)
29	CLA	H	307	-	51,55,73	1.35	8 (15%)	60,91,113	1.38	5 (8%)
29	CLA	D	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.52	5 (9%)
36	DD6	J	302	-	40,45,45	1.62	2 (5%)	51,67,67	2.22	17 (33%)
37	PID	F	302	-	43,49,49	1.25	3 (6%)	52,76,76	1.61	6 (11%)
39	KC1	D	310	-	49,53,53	1.36	6 (12%)	61,89,89	1.74	13 (21%)
29	CLA	a	830	-	60,64,73	1.24	8 (13%)	71,102,113	5.17	9 (12%)
29	CLA	l	505	-	69,73,73	1.18	9 (13%)	82,113,113	1.25	4 (4%)
39	KC1	L	314	-	49,53,53	1.36	7 (14%)	61,89,89	1.72	14 (22%)
36	DD6	F	301	-	40,45,45	1.66	4 (10%)	51,67,67	2.00	16 (31%)
34	LMG	h	205	-	28,28,55	1.02	1 (3%)	36,36,63	1.28	4 (11%)
29	CLA	C	313	25	50,54,73	1.35	9 (18%)	59,90,113	1.39	4 (6%)
29	CLA	E	311	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
32	BCR	a	835	-	41,41,41	0.75	0	56,56,56	2.12	16 (28%)
40	SQD	B	317	-	40,42,54	0.45	1 (2%)	50,53,65	0.49	0
29	CLA	C	309	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	4 (4%)
37	PID	H	302	-	43,49,49	1.27	3 (6%)	52,76,76	1.39	8 (15%)
36	DD6	A	204	-	40,45,45	1.56	2 (5%)	51,67,67	1.89	16 (31%)
37	PID	O	301	-	43,49,49	1.22	3 (6%)	52,76,76	1.55	6 (11%)
29	CLA	l	510	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	5 (8%)
29	CLA	B	316	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
34	LMG	b	734	-	40,40,55	0.81	1 (2%)	48,48,63	1.29	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PID	T	307	-	43,49,49	1.24	3 (6%)	52,76,76	1.55	9 (17%)
29	CLA	K	209	-	58,62,73	1.27	9 (15%)	68,99,113	1.35	6 (8%)
34	LMG	A	219	-	37,37,55	0.84	1 (2%)	45,45,63	1.31	6 (13%)
29	CLA	A	209	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
29	CLA	C	314	-	51,55,73	1.34	8 (15%)	60,91,113	1.46	6 (10%)
36	DD6	M	302	-	40,45,45	1.65	3 (7%)	51,67,67	2.07	15 (29%)
39	KC1	H	311	-	49,53,53	1.36	6 (12%)	61,89,89	1.70	13 (21%)
37	PID	G	309	-	43,49,49	1.25	3 (6%)	52,76,76	1.38	6 (11%)
29	CLA	L	316	-	56,60,73	1.31	9 (16%)	65,97,113	1.35	6 (9%)
29	CLA	P	214	27	50,54,73	1.37	8 (16%)	59,90,113	1.41	4 (6%)
37	PID	C	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.90	10 (19%)
29	CLA	a	816	-	50,54,73	1.35	9 (18%)	59,90,113	1.40	4 (6%)
36	DD6	D	301	-	40,45,45	1.62	2 (5%)	51,67,67	2.11	15 (29%)
29	CLA	l	509	-	45,49,73	1.40	9 (20%)	54,84,113	1.45	7 (12%)
37	PID	N	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.29	5 (9%)
29	CLA	K	216	-	45,49,73	1.41	9 (20%)	54,84,113	1.54	5 (9%)
29	CLA	b	708	2	56,60,73	1.30	9 (16%)	65,97,113	1.39	6 (9%)
39	KC1	C	310	-	49,53,53	1.38	6 (12%)	61,89,89	1.77	13 (21%)
37	PID	D	306	-	43,49,49	1.27	3 (6%)	52,76,76	1.41	9 (17%)
37	PID	F	304	-	43,49,49	1.59	4 (9%)	52,76,76	1.47	8 (15%)
39	KC1	Q	314	26	49,53,53	1.37	6 (12%)	61,89,89	1.76	12 (19%)
36	DD6	F	303	-	40,45,45	1.66	2 (5%)	51,67,67	2.04	12 (23%)
29	CLA	L	312	-	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
36	DD6	C	303	-	40,45,45	1.63	2 (5%)	51,67,67	2.04	14 (27%)
29	CLA	b	718	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
29	CLA	I	207	14	53,57,73	1.31	9 (16%)	61,93,113	1.43	5 (8%)
29	CLA	I	216	-	56,60,73	1.29	9 (16%)	65,97,113	1.44	7 (10%)
29	CLA	Q	310	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
37	PID	C	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.53	6 (11%)
29	CLA	a	821	-	51,55,73	1.35	8 (15%)	60,91,113	1.38	5 (8%)
29	CLA	B	314	21	45,49,73	1.40	9 (20%)	54,84,113	1.53	5 (9%)
29	CLA	K	210	-	54,58,73	1.30	7 (12%)	64,95,113	1.41	7 (10%)
29	CLA	f	805	-	64,68,73	1.21	8 (12%)	76,107,113	1.27	5 (6%)
29	CLA	G	313	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	5 (7%)
37	PID	O	304	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	K	201	-	43,43,55	0.79	1 (2%)	51,51,63	1.33	6 (11%)
29	CLA	B	310	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
37	PID	Q	306	-	43,49,49	1.24	3 (6%)	52,76,76	1.46	6 (11%)
29	CLA	a	808	-	55,59,73	1.31	9 (16%)	64,96,113	1.40	5 (7%)
29	CLA	E	308	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
29	CLA	A	208	-	59,63,73	1.24	9 (15%)	70,101,113	1.34	7 (10%)
34	LMG	b	730	-	46,46,55	0.81	2 (4%)	54,54,63	1.32	5 (9%)
37	PID	G	310	-	43,49,49	1.26	3 (6%)	52,76,76	1.39	7 (13%)
29	CLA	J	311	-	57,61,73	1.27	9 (15%)	67,98,113	1.36	5 (7%)
36	DD6	K	205	-	40,45,45	1.59	2 (5%)	51,67,67	1.87	16 (31%)
29	CLA	b	723	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	7 (8%)
39	KC1	A	205	29	49,53,53	1.36	6 (12%)	61,89,89	1.74	15 (24%)
29	CLA	B	315	-	50,54,73	1.36	9 (18%)	59,90,113	1.42	5 (8%)
36	DD6	G	308	-	40,45,45	1.56	1 (2%)	51,67,67	2.07	14 (27%)
39	KC1	C	312	-	49,53,53	1.38	6 (12%)	61,89,89	1.77	14 (22%)
39	KC1	G	318	-	49,53,53	1.36	6 (12%)	61,89,89	1.69	12 (19%)
37	PID	C	307	-	43,49,49	1.24	3 (6%)	52,76,76	1.49	7 (13%)
29	CLA	M	307	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	5 (7%)
36	DD6	K	203	-	40,45,45	1.64	3 (7%)	51,67,67	1.89	14 (27%)
36	DD6	h	202	-	40,45,45	1.76	4 (10%)	51,67,67	2.25	18 (35%)
32	BCR	i	204	-	41,41,41	0.70	0	56,56,56	2.37	14 (25%)
39	KC1	J	312	17	49,53,53	1.36	6 (12%)	61,89,89	1.74	13 (21%)
29	CLA	b	706	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	5 (6%)
29	CLA	K	214	-	59,63,73	1.26	9 (15%)	70,101,113	1.33	6 (8%)
37	PID	N	307	-	43,49,49	1.25	4 (9%)	52,76,76	1.59	10 (19%)
36	DD6	B	319	-	40,45,45	1.62	2 (5%)	51,67,67	2.24	17 (33%)
29	CLA	P	212	-	55,59,73	1.31	7 (12%)	64,96,113	1.38	5 (7%)
32	BCR	b	735	-	41,41,41	0.73	0	56,56,56	2.05	19 (33%)
29	CLA	a	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
29	CLA	b	720	-	69,73,73	1.18	9 (13%)	82,113,113	1.25	4 (4%)
36	DD6	I	204	-	40,45,45	1.78	4 (10%)	51,67,67	2.11	15 (29%)
35	DGD	B	318	-	46,46,67	1.01	2 (4%)	60,60,81	1.33	10 (16%)
29	CLA	O	308	-	51,55,73	1.37	8 (15%)	60,91,113	1.40	5 (8%)
39	KC1	M	312	-	49,53,53	1.36	6 (12%)	61,89,89	1.76	13 (21%)
29	CLA	A	218	12	64,68,73	1.20	9 (14%)	76,107,113	1.32	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	J	310	-	51,55,73	1.34	9 (17%)	60,91,113	1.41	7 (11%)
37	PID	P	202	-	43,49,49	1.22	3 (6%)	52,76,76	1.32	8 (15%)
29	CLA	D	313	20	49,53,73	1.38	9 (18%)	58,89,113	1.41	4 (6%)
29	CLA	A	214	12	45,49,73	1.41	9 (20%)	54,84,113	1.47	5 (9%)
29	CLA	O	311	-	55,59,73	1.31	9 (16%)	64,96,113	1.37	4 (6%)
39	KC1	H	314	-	49,53,53	1.35	5 (10%)	61,89,89	1.73	13 (21%)
29	CLA	L	308	-	57,61,73	1.28	9 (15%)	67,98,113	5.33	7 (10%)
29	CLA	b	721	-	62,66,73	1.23	9 (14%)	73,104,113	1.37	7 (9%)
29	CLA	a	809	1	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
29	CLA	l	508	-	45,49,73	1.40	9 (20%)	54,84,113	1.46	5 (9%)
37	PID	T	304	-	43,49,49	1.22	3 (6%)	52,76,76	1.39	5 (9%)
29	CLA	l	502	10	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
30	PQN	b	727	-	34,34,34	1.57	2 (5%)	43,45,45	1.25	4 (9%)
39	KC1	N	310	-	49,53,53	1.36	6 (12%)	61,89,89	1.73	12 (19%)
38	UIX	E	304	-	43,49,49	1.42	5 (11%)	53,74,74	2.41	19 (35%)
29	CLA	F	310	-	50,54,73	1.34	9 (18%)	59,90,113	1.47	5 (8%)
29	CLA	I	201	29	49,53,73	1.38	9 (18%)	58,89,113	1.45	4 (6%)
29	CLA	a	824	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
38	UIX	J	304	-	43,49,49	1.40	4 (9%)	53,74,74	2.29	14 (26%)
38	UIX	A	203	-	43,49,49	1.40	5 (11%)	53,74,74	2.35	21 (39%)
29	CLA	T	309	25	50,54,73	1.34	9 (18%)	59,90,113	1.41	5 (8%)
29	CLA	O	314	-	51,55,73	1.37	9 (17%)	60,91,113	1.43	8 (13%)
36	DD6	J	301	-	40,45,45	1.60	2 (5%)	51,67,67	2.26	16 (31%)
36	DD6	T	303	-	40,45,45	1.53	2 (5%)	51,67,67	1.97	14 (27%)
29	CLA	I	213	14	69,73,73	1.17	9 (13%)	82,113,113	3.76	9 (10%)
29	CLA	P	217	-	45,49,73	1.43	7 (15%)	54,84,113	1.55	5 (9%)
38	UIX	N	306	-	43,49,49	1.40	5 (11%)	53,74,74	2.57	16 (30%)
29	CLA	P	209	-	51,55,73	1.36	8 (15%)	60,91,113	1.38	5 (8%)
29	CLA	F	316	16	45,49,73	1.41	9 (20%)	54,84,113	1.50	5 (9%)
29	CLA	b	711	-	62,66,73	1.22	9 (14%)	73,104,113	1.33	5 (6%)
29	CLA	l	501	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	6 (7%)
37	PID	F	306	-	43,49,49	1.27	3 (6%)	52,76,76	1.43	7 (13%)
29	CLA	L	311	19	50,54,73	1.36	8 (16%)	59,90,113	1.34	4 (6%)
29	CLA	a	803	-	69,73,73	1.17	9 (13%)	82,113,113	1.20	5 (6%)
39	KC1	Q	311	-	49,53,53	1.42	7 (14%)	61,89,89	1.82	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCR	l	506	-	41,41,41	0.68	0	56,56,56	1.94	15 (26%)
29	CLA	E	306	28	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
29	CLA	A	212	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	5 (7%)
29	CLA	b	710	-	50,54,73	1.34	9 (18%)	59,90,113	1.36	4 (6%)
29	CLA	L	317	-	50,54,73	1.35	9 (18%)	59,90,113	1.41	4 (6%)
29	CLA	F	312	16	50,54,73	1.35	8 (16%)	59,90,113	1.38	4 (6%)
37	PID	G	303	-	43,49,49	1.28	3 (6%)	52,76,76	1.31	7 (13%)
29	CLA	a	818	-	51,55,73	1.34	9 (17%)	60,91,113	1.38	5 (8%)
37	PID	N	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.46	7 (13%)
29	CLA	K	212	-	56,60,73	1.31	9 (16%)	65,97,113	1.35	5 (7%)
36	DD6	M	304	-	40,45,45	1.59	2 (5%)	51,67,67	1.74	14 (27%)
39	KC1	T	310	-	49,53,53	1.38	5 (10%)	61,89,89	1.71	13 (21%)
32	BCR	a	834	-	41,41,41	0.70	0	56,56,56	2.05	14 (25%)
29	CLA	a	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
37	PID	T	317	-	43,49,49	1.26	3 (6%)	52,76,76	1.62	9 (17%)
29	CLA	G	302	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
37	PID	D	303	-	43,49,49	1.29	3 (6%)	52,76,76	1.54	11 (21%)
39	KC1	O	312	-	49,53,53	1.40	6 (12%)	61,89,89	1.90	14 (22%)
30	PQN	a	832	-	34,34,34	1.55	2 (5%)	43,45,45	1.30	6 (13%)
29	CLA	D	314	-	51,55,73	1.35	9 (17%)	60,91,113	1.46	6 (10%)
29	CLA	b	719	-	54,58,73	1.31	9 (16%)	64,95,113	1.40	8 (12%)
31	LHG	a	833	-	47,47,48	0.28	0	50,53,54	0.31	0
29	CLA	L	307	39	54,58,73	1.31	9 (16%)	64,95,113	5.47	8 (12%)
32	BCR	f	801	-	41,41,41	0.71	0	56,56,56	2.02	15 (26%)
39	KC1	N	312	23	49,53,53	1.36	5 (10%)	61,89,89	1.72	14 (22%)
29	CLA	J	305	-	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
29	CLA	Q	307	-	51,55,73	1.35	9 (17%)	60,91,113	1.38	5 (8%)
39	KC1	T	312	-	49,53,53	1.36	6 (12%)	61,89,89	1.77	12 (19%)
29	CLA	b	705	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	5 (6%)
29	CLA	J	309	17	50,54,73	1.35	8 (16%)	59,90,113	1.45	4 (6%)
39	KC1	A	213	-	49,53,53	1.36	6 (12%)	61,89,89	1.72	13 (21%)
29	CLA	B	308	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	7 (8%)
29	CLA	B	306	21	53,57,73	1.32	9 (16%)	61,93,113	1.40	5 (8%)
29	CLA	O	316	-	45,49,73	1.43	8 (17%)	54,84,113	1.48	5 (9%)
29	CLA	T	313	-	50,54,73	1.37	8 (16%)	59,90,113	1.39	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	E	309	-	50,54,73	1.36	8 (16%)	59,90,113	1.42	4 (6%)
36	DD6	m	101	-	40,45,45	1.57	2 (5%)	51,67,67	2.03	16 (31%)
38	UIX	L	302	-	43,49,49	1.37	4 (9%)	53,74,74	2.38	18 (33%)
36	DD6	B	305	-	40,45,45	1.56	2 (5%)	51,67,67	1.91	16 (31%)
36	DD6	E	303	-	40,45,45	1.58	2 (5%)	51,67,67	1.78	12 (23%)
36	DD6	K	202	-	40,45,45	1.67	2 (5%)	51,67,67	2.99	15 (29%)
36	DD6	A	201	-	40,45,45	1.56	2 (5%)	51,67,67	2.04	16 (31%)
34	LMG	E	316	-	32,32,55	0.99	2 (6%)	40,40,63	1.28	2 (5%)
29	CLA	l	503	10	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
37	PID	D	307	-	43,49,49	1.23	3 (6%)	52,76,76	1.53	7 (13%)
29	CLA	P	215	-	51,55,73	1.36	8 (15%)	60,91,113	1.54	7 (11%)
29	CLA	A	211	-	59,63,73	1.24	9 (15%)	70,101,113	1.30	7 (10%)
29	CLA	M	306	-	57,61,73	1.28	8 (14%)	67,98,113	1.37	6 (8%)
29	CLA	K	213	-	52,56,73	1.33	9 (17%)	61,92,113	1.36	5 (8%)
29	CLA	a	831	-	69,73,73	1.16	9 (13%)	82,113,113	4.83	9 (10%)
37	PID	H	306	-	43,49,49	1.27	4 (9%)	52,76,76	1.37	5 (9%)
35	DGD	G	320	-	46,46,67	1.02	2 (4%)	60,60,81	0.98	3 (5%)
37	PID	D	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.39	5 (9%)
29	CLA	b	709	-	64,68,73	1.20	9 (14%)	76,107,113	1.31	6 (7%)
29	CLA	l	504	-	69,73,73	1.16	9 (13%)	82,113,113	3.77	10 (12%)
29	CLA	M	311	-	50,54,73	1.36	9 (18%)	59,90,113	1.38	5 (8%)
29	CLA	G	314	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	6 (7%)
39	KC1	K	215	-	49,53,53	1.39	7 (14%)	61,89,89	1.77	14 (22%)
39	KC1	B	313	21	49,53,53	1.36	7 (14%)	61,89,89	1.73	13 (21%)
29	CLA	E	315	-	61,65,73	1.24	8 (13%)	72,103,113	1.33	6 (8%)
39	KC1	I	215	14	49,53,53	1.36	7 (14%)	61,89,89	1.74	14 (22%)

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
39	KC1	D	315	-	-	6/15/71/71	-
29	CLA	C	311	-	1/1/12/20	5/23/99/115	-
38	UIX	T	306	-	-	4/31/87/87	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DD6	L	304	-	-	2/26/80/80	0/3/3/3
29	CLA	N	311	-	1/1/12/20	4/23/99/115	-
36	DD6	J	303	-	-	2/26/80/80	0/3/3/3
29	CLA	M	314	-	1/1/12/20	7/24/100/115	-
37	PID	N	301	-	-	4/24/93/93	0/4/4/4
38	UIX	P	207	-	-	6/31/87/87	0/3/3/3
37	PID	O	307	-	-	4/24/93/93	0/4/4/4
37	PID	Q	303	-	-	0/24/93/93	0/4/4/4
29	CLA	G	311	13	1/1/12/20	9/23/99/115	-
36	DD6	B	301	-	-	4/24/78/80	0/3/3/3
29	CLA	D	312	20	1/1/11/20	7/17/93/115	-
36	DD6	G	307	-	-	2/26/80/80	0/3/3/3
36	DD6	I	205	-	-	6/26/80/80	0/3/3/3
29	CLA	a	804	-	1/1/13/20	1/27/103/115	-
37	PID	T	301	-	-	2/24/93/93	0/4/4/4
29	CLA	a	828	-	1/1/11/20	8/17/93/115	-
39	KC1	P	211	-	-	8/15/71/71	-
36	DD6	Q	302	-	-	1/26/80/80	0/3/3/3
29	CLA	a	837	-	1/1/13/20	11/27/103/115	-
32	BCR	m	103	-	-	5/29/63/63	0/2/2/2
29	CLA	A	206	39	1/1/11/20	4/15/91/115	-
34	LMG	K	219	-	-	17/30/50/70	0/1/1/1
36	DD6	I	206	-	-	2/26/80/80	0/3/3/3
39	KC1	E	312	28	-	6/15/71/71	-
37	PID	O	305	-	-	7/24/93/93	0/4/4/4
29	CLA	Q	313	-	1/1/11/20	6/18/94/115	-
29	CLA	J	307	-	1/1/11/20	3/17/93/115	-
29	CLA	L	313	-	1/1/12/20	6/25/101/115	-
36	DD6	G	305	-	-	7/26/80/80	0/3/3/3
29	CLA	b	726	-	1/1/15/20	7/39/115/115	-
35	DGD	j	103	-	-	10/32/72/95	0/2/2/2
36	DD6	O	303	-	-	4/26/80/80	0/3/3/3
33	SF4	c	101	3	-	-	0/6/5/5
29	CLA	I	209	-	1/1/14/20	13/33/109/115	-
34	LMG	b	732	-	-	20/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	O	309	-	-	8/39/115/115	-
37	PID	P	205	-	-	1/24/93/93	0/4/4/4
29	CLA	a	801	-	1/1/15/20	10/39/115/115	-
39	KC1	O	310	-	-	6/15/71/71	-
39	KC1	F	314	-	-	6/15/71/71	-
29	CLA	b	713	-	1/1/12/20	6/25/101/115	-
38	UIX	C	306	-	-	6/31/87/87	0/3/3/3
29	CLA	B	311	21	1/1/12/20	4/23/99/115	-
29	CLA	K	208	-	1/1/11/20	2/17/93/115	-
29	CLA	M	310	18	1/1/11/20	5/19/95/115	-
36	DD6	P	204	-	-	2/26/80/80	0/3/3/3
29	CLA	H	315	-	1/1/10/20	4/10/86/115	-
38	UIX	B	304	-	-	2/31/87/87	0/3/3/3
29	CLA	K	207	15	1/1/11/20	6/20/96/115	-
36	DD6	I	203	-	-	7/26/80/80	0/3/3/3
29	CLA	a	825	-	1/1/15/20	13/39/115/115	-
39	KC1	P	216	-	-	6/15/71/71	-
29	CLA	H	308	-	1/1/15/20	9/39/115/115	-
36	DD6	L	305	-	-	4/26/80/80	0/3/3/3
29	CLA	L	309	-	1/1/13/20	2/27/103/115	-
36	DD6	N	303	-	-	1/26/80/80	0/3/3/3
35	DGD	m	102	-	-	7/55/95/95	0/2/2/2
29	CLA	M	315	-	1/1/11/20	5/17/93/115	-
36	DD6	L	303	-	-	0/26/80/80	0/3/3/3
29	CLA	I	217	-	1/1/13/20	10/27/103/115	-
29	CLA	G	301	-	1/1/11/20	5/20/96/115	-
29	CLA	J	306	-	1/1/15/20	16/39/115/115	-
37	PID	h	204	-	-	2/24/93/93	1/4/4/4
29	CLA	a	815	-	1/1/11/20	4/15/91/115	-
29	CLA	a	802	-	1/1/15/20	9/39/115/115	-
37	PID	P	208	-	-	5/24/93/93	0/4/4/4
29	CLA	A	207	-	1/1/13/20	5/27/103/115	-
29	CLA	G	312	13	1/1/15/20	16/39/115/115	-
36	DD6	K	204	-	-	5/26/80/80	0/3/3/3
29	CLA	a	817	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	KC1	O	315	-	-	9/15/71/71	-
29	CLA	I	208	-	1/1/11/20	9/17/93/115	-
29	CLA	i	202	-	1/1/15/20	12/39/115/115	-
29	CLA	N	314	-	1/1/11/20	7/18/94/115	-
37	PID	P	206	-	-	9/24/93/93	0/4/4/4
29	CLA	Q	308	-	1/1/15/20	17/39/115/115	-
29	CLA	K	211	-	1/1/13/20	5/27/103/115	-
37	PID	P	203	-	-	3/24/93/93	0/4/4/4
39	KC1	H	309	-	-	9/15/71/71	-
29	CLA	B	307	-	1/1/11/20	4/15/91/115	-
37	PID	H	304	-	-	0/24/93/93	0/4/4/4
39	KC1	E	307	-	-	6/15/71/71	-
36	DD6	K	221	-	-	5/26/80/80	0/3/3/3
29	CLA	b	704	-	1/1/15/20	12/39/115/115	-
29	CLA	E	305	-	1/1/14/20	11/35/111/115	-
35	DGD	j	106	-	-	15/38/78/95	0/2/2/2
29	CLA	L	310	-	1/1/13/20	5/27/103/115	-
35	DGD	b	733	-	-	24/46/86/95	0/2/2/2
36	DD6	E	302	-	-	2/26/80/80	0/3/3/3
34	LMG	j	102	-	-	23/38/58/70	0/1/1/1
29	CLA	J	313	-	1/1/10/20	2/10/86/115	-
29	CLA	F	307	-	1/1/11/20	3/17/93/115	-
29	CLA	T	311	-	1/1/11/20	7/17/93/115	-
29	CLA	M	309	-	1/1/11/20	6/17/93/115	-
38	UIX	O	306	-	-	7/31/87/87	0/3/3/3
29	CLA	E	313	-	1/1/10/20	0/10/86/115	-
35	DGD	j	105	-	-	1/30/70/95	0/2/2/2
29	CLA	a	826	-	1/1/15/20	11/39/115/115	-
36	DD6	M	303	-	-	6/26/80/80	0/3/3/3
39	KC1	F	309	-	-	7/15/71/71	-
29	CLA	a	823	-	1/1/13/20	9/31/107/115	-
32	BCR	b	729	-	-	5/29/63/63	0/2/2/2
29	CLA	K	217	-	1/1/11/20	6/17/93/115	-
34	LMG	P	201	-	-	6/22/42/70	0/1/1/1
32	BCR	l	507	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	210	12	1/1/11/20	6/17/93/115	-
32	BCR	a	838	-	-	6/29/63/63	0/2/2/2
29	CLA	I	214	-	1/1/13/20	4/27/103/115	-
29	CLA	a	811	-	1/1/13/20	9/29/105/115	-
29	CLA	N	308	-	1/1/11/20	6/18/94/115	-
29	CLA	b	725	-	1/1/15/20	9/39/115/115	-
37	PID	Q	304	-	-	2/24/93/93	0/4/4/4
29	CLA	B	309	-	1/1/13/20	6/27/103/115	-
29	CLA	H	312	22	1/1/11/20	5/17/93/115	-
29	CLA	a	819	-	1/1/13/20	6/30/106/115	-
36	DD6	B	303	-	-	0/26/80/80	0/3/3/3
29	CLA	b	702	-	1/1/15/20	14/39/115/115	-
29	CLA	A	217	-	1/1/12/20	6/23/99/115	-
39	KC1	T	315	25	-	6/15/71/71	-
29	CLA	M	308	-	1/1/11/20	7/19/95/115	-
29	CLA	b	701	-	1/1/15/20	11/39/115/115	-
36	DD6	H	303	-	-	1/26/80/80	0/3/3/3
29	CLA	a	827	-	1/1/15/20	10/39/115/115	-
29	CLA	b	736	-	1/1/15/20	18/39/115/115	-
29	CLA	G	304	-	1/1/13/20	12/32/108/115	-
29	CLA	a	820	-	1/1/15/20	12/39/115/115	-
29	CLA	L	315	-	1/1/10/20	4/10/86/115	-
29	CLA	h	201	-	1/1/14/20	6/33/109/115	-
29	CLA	C	308	-	1/1/11/20	6/18/94/115	-
29	CLA	a	806	1	1/1/15/20	15/39/115/115	-
36	DD6	K	206	-	-	1/26/80/80	0/3/3/3
37	PID	O	302	-	-	2/24/93/93	0/4/4/4
29	CLA	F	308	-	1/1/11/20	3/17/93/115	-
36	DD6	B	302	-	-	2/26/80/80	0/3/3/3
29	CLA	f	802	-	1/1/11/20	4/17/93/115	-
37	PID	j	101	-	-	2/24/93/93	0/4/4/4
29	CLA	I	212	-	1/1/13/20	13/27/103/115	-
29	CLA	Q	312	-	1/1/11/20	5/17/93/115	-
37	PID	E	301	-	-	5/24/93/93	0/4/4/4
37	PID	H	305	-	-	3/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	C	302	-	-	2/24/93/93	0/4/4/4
29	CLA	I	210	-	1/1/13/20	6/27/103/115	-
29	CLA	b	731	-	1/1/13/20	3/29/105/115	-
29	CLA	J	308	-	1/1/13/20	9/29/105/115	-
37	PID	N	302	-	-	2/24/93/93	0/4/4/4
29	CLA	E	314	28	-	3/19/95/115	-
36	DD6	A	202	-	-	1/26/80/80	0/3/3/3
29	CLA	a	810	1	1/1/13/20	9/27/103/115	-
29	CLA	H	313	-	1/1/11/20	7/18/94/115	-
29	CLA	D	308	-	1/1/11/20	5/18/94/115	-
29	CLA	F	315	-	1/1/10/20	2/10/86/115	-
38	UIX	F	305	-	-	12/31/87/87	0/3/3/3
29	CLA	O	313	24	1/1/11/20	4/17/93/115	-
29	CLA	a	813	-	1/1/12/20	12/23/99/115	-
29	CLA	E	310	28	1/1/11/20	4/17/93/115	-
29	CLA	b	714	-	1/1/14/20	6/38/114/115	-
29	CLA	b	724	-	1/1/11/20	2/18/94/115	-
39	KC1	N	315	-	-	9/15/71/71	-
36	DD6	D	304	-	-	6/26/80/80	0/3/3/3
36	DD6	M	301	-	-	2/26/80/80	0/3/3/3
37	PID	T	302	-	-	2/24/93/93	0/4/4/4
29	CLA	j	104	29	1/1/12/20	4/24/100/115	-
29	CLA	F	313	16	1/1/11/20	8/17/93/115	-
29	CLA	Q	315	-	1/1/10/20	4/10/86/115	-
29	CLA	A	216	-	1/1/10/20	2/10/86/115	-
29	CLA	K	218	-	1/1/11/20	8/15/91/115	-
29	CLA	b	703	-	1/1/15/20	12/39/115/115	-
29	CLA	i	201	-	1/1/15/20	12/39/115/115	-
29	CLA	N	309	-	1/1/15/20	14/39/115/115	-
29	CLA	a	805	-	1/1/13/20	6/27/103/115	-
29	CLA	G	317	-	1/1/12/20	8/25/101/115	-
32	BCR	b	728	-	-	5/29/63/63	0/2/2/2
29	CLA	T	316	-	1/1/10/20	4/10/86/115	-
29	CLA	f	803	6	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	f	804	-	-	2/29/63/63	0/2/2/2
29	CLA	F	311	-	1/1/11/20	4/17/93/115	-
39	KC1	C	315	25	-	8/15/71/71	-
37	PID	D	305	-	-	5/24/93/93	0/4/4/4
34	LMG	K	220	-	-	13/31/51/70	0/1/1/1
29	CLA	a	822	-	1/1/15/20	7/39/115/115	-
38	UIX	Q	305	-	-	4/31/87/87	0/3/3/3
33	SF4	c	102	3	-	-	0/6/5/5
29	CLA	b	712	-	1/1/15/20	10/39/115/115	-
29	CLA	i	203	-	1/1/13/20	13/27/103/115	-
29	CLA	b	707	-	1/1/15/20	13/39/115/115	-
29	CLA	A	215	-	1/1/11/20	5/18/94/115	-
29	CLA	P	210	-	1/1/15/20	9/39/115/115	-
36	DD6	L	301	-	-	4/26/80/80	0/3/3/3
39	KC1	G	315	-	-	5/15/71/71	-
39	KC1	Q	309	-	-	5/15/71/71	-
29	CLA	b	715	-	1/1/11/20	8/17/93/115	-
29	CLA	N	316	-	1/1/10/20	4/10/86/115	-
29	CLA	G	316	-	1/1/15/20	10/39/115/115	-
33	SF4	a	836	2,1	-	-	0/6/5/5
37	PID	H	301	-	-	2/24/93/93	0/4/4/4
29	CLA	a	814	-	1/1/11/20	4/17/93/115	-
40	SQD	J	314	-	-	10/40/60/69	0/1/1/1
29	CLA	T	308	-	1/1/11/20	4/18/94/115	-
39	KC1	M	305	-	-	4/15/71/71	-
39	KC1	P	213	27	-	6/15/71/71	-
29	CLA	B	312	-	1/1/15/20	10/39/115/115	-
29	CLA	b	716	-	1/1/12/20	7/25/101/115	-
29	CLA	b	722	-	1/1/13/20	8/31/107/115	-
29	CLA	H	310	-	1/1/12/20	9/23/99/115	-
29	CLA	D	309	-	1/1/11/20	2/17/93/115	-
29	CLA	C	316	-	1/1/10/20	4/10/86/115	-
29	CLA	a	812	-	1/1/14/20	15/33/109/115	-
29	CLA	b	717	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	Q	301	-	-	2/24/93/93	0/4/4/4
37	PID	C	304	-	-	3/24/93/93	0/4/4/4
29	CLA	G	319	13	1/1/10/20	2/10/86/115	-
36	DD6	I	202	-	-	4/26/80/80	0/3/3/3
37	PID	T	305	-	-	0/24/93/93	0/4/4/4
39	KC1	L	306	29	-	5/15/71/71	-
29	CLA	M	313	-	1/1/10/20	4/10/86/115	-
36	DD6	G	306	-	-	1/26/80/80	0/3/3/3
29	CLA	N	313	23	1/1/11/20	8/17/93/115	-
29	CLA	T	314	-	1/1/11/20	7/18/94/115	-
29	CLA	I	211	-	1/1/15/20	8/39/115/115	-
35	DGD	h	203	-	-	8/43/83/95	0/2/2/2
29	CLA	D	311	-	1/1/11/20	11/17/93/115	-
29	CLA	H	307	-	1/1/11/20	5/18/94/115	-
29	CLA	D	316	-	1/1/10/20	4/10/86/115	-
36	DD6	J	302	-	-	2/26/80/80	0/3/3/3
37	PID	F	302	-	-	3/24/93/93	0/4/4/4
39	KC1	D	310	-	-	5/15/71/71	-
29	CLA	a	830	-	1/1/13/20	6/29/105/115	-
29	CLA	l	505	-	1/1/15/20	11/39/115/115	-
39	KC1	L	314	-	-	6/15/71/71	-
36	DD6	F	301	-	-	8/26/80/80	0/3/3/3
34	LMG	h	205	-	-	4/23/43/70	0/1/1/1
29	CLA	C	313	25	1/1/11/20	7/17/93/115	-
29	CLA	E	311	-	1/1/15/20	11/39/115/115	-
32	BCR	a	835	-	-	2/29/63/63	0/2/2/2
40	SQD	B	317	-	-	4/37/57/69	0/1/1/1
29	CLA	C	309	-	1/1/15/20	6/39/115/115	-
37	PID	H	302	-	-	2/24/93/93	0/4/4/4
36	DD6	A	204	-	-	2/26/80/80	0/3/3/3
37	PID	O	301	-	-	3/24/93/93	0/4/4/4
29	CLA	l	510	-	1/1/11/20	7/15/91/115	-
29	CLA	B	316	-	1/1/11/20	6/15/91/115	-
34	LMG	b	734	-	-	10/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	T	307	-	-	4/24/93/93	0/4/4/4
29	CLA	K	209	-	1/1/12/20	8/26/102/115	-
34	LMG	A	219	-	-	17/32/52/70	0/1/1/1
29	CLA	A	209	-	1/1/15/20	18/39/115/115	-
29	CLA	C	314	-	1/1/11/20	7/18/94/115	-
36	DD6	M	302	-	-	1/26/80/80	0/3/3/3
39	KC1	H	311	-	-	6/15/71/71	-
37	PID	G	309	-	-	2/24/93/93	0/4/4/4
29	CLA	L	316	-	1/1/12/20	11/24/100/115	-
29	CLA	P	214	27	1/1/11/20	9/17/93/115	-
37	PID	C	305	-	-	9/24/93/93	0/4/4/4
29	CLA	a	816	-	1/1/11/20	8/17/93/115	-
36	DD6	D	301	-	-	7/26/80/80	0/3/3/3
29	CLA	l	509	-	1/1/10/20	0/10/86/115	-
37	PID	N	305	-	-	19/24/93/93	0/4/4/4
29	CLA	K	216	-	1/1/10/20	4/10/86/115	-
29	CLA	b	708	2	1/1/12/20	4/24/100/115	-
39	KC1	C	310	-	-	7/15/71/71	-
37	PID	D	306	-	-	3/24/93/93	0/4/4/4
37	PID	F	304	-	-	14/24/93/93	1/4/4/4
39	KC1	Q	314	26	-	8/15/71/71	-
36	DD6	F	303	-	-	0/26/80/80	0/3/3/3
29	CLA	L	312	-	1/1/13/20	10/27/103/115	-
36	DD6	C	303	-	-	0/26/80/80	0/3/3/3
29	CLA	b	718	-	1/1/15/20	13/39/115/115	-
29	CLA	I	207	14	1/1/11/20	7/20/96/115	-
29	CLA	I	216	-	1/1/12/20	4/24/100/115	-
29	CLA	Q	310	-	1/1/15/20	14/39/115/115	-
37	PID	C	301	-	-	4/24/93/93	0/4/4/4
29	CLA	a	821	-	1/1/11/20	8/18/94/115	-
29	CLA	B	314	21	1/1/10/20	4/10/86/115	-
29	CLA	K	210	-	1/1/12/20	5/21/97/115	-
29	CLA	f	805	-	1/1/14/20	10/33/109/115	-
29	CLA	G	313	-	1/1/13/20	3/27/103/115	-
37	PID	O	304	-	-	3/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	K	201	-	-	17/38/58/70	0/1/1/1
29	CLA	B	310	-	1/1/15/20	14/39/115/115	-
37	PID	Q	306	-	-	4/24/93/93	0/4/4/4
29	CLA	a	808	-	1/1/12/20	5/23/99/115	-
29	CLA	E	308	-	1/1/15/20	10/39/115/115	-
29	CLA	A	208	-	1/1/13/20	3/27/103/115	-
34	LMG	b	730	-	-	19/41/61/70	0/1/1/1
37	PID	G	310	-	-	2/24/93/93	0/4/4/4
29	CLA	J	311	-	1/1/12/20	8/25/101/115	-
36	DD6	K	205	-	-	1/26/80/80	0/3/3/3
29	CLA	b	723	-	1/1/15/20	5/39/115/115	-
39	KC1	A	205	29	-	7/15/71/71	-
29	CLA	B	315	-	1/1/11/20	3/17/93/115	-
36	DD6	G	308	-	-	1/26/80/80	0/3/3/3
39	KC1	C	312	-	-	8/15/71/71	-
39	KC1	G	318	-	-	6/15/71/71	-
37	PID	C	307	-	-	2/24/93/93	0/4/4/4
29	CLA	M	307	-	1/1/13/20	5/27/103/115	-
36	DD6	K	203	-	-	6/26/80/80	0/3/3/3
36	DD6	h	202	-	-	2/26/80/80	0/3/3/3
32	BCR	i	204	-	-	4/29/63/63	0/2/2/2
39	KC1	J	312	17	-	5/15/71/71	-
29	CLA	b	706	-	1/1/15/20	11/39/115/115	-
29	CLA	K	214	-	1/1/13/20	7/27/103/115	-
37	PID	N	307	-	-	6/24/93/93	0/4/4/4
36	DD6	B	319	-	-	9/26/80/80	0/3/3/3
29	CLA	P	212	-	1/1/12/20	9/23/99/115	-
32	BCR	b	735	-	-	4/29/63/63	0/2/2/2
29	CLA	a	829	-	1/1/15/20	16/39/115/115	-
29	CLA	b	720	-	1/1/15/20	13/39/115/115	-
36	DD6	I	204	-	-	3/26/80/80	0/3/3/3
35	DGD	B	318	-	-	9/34/74/95	0/2/2/2
29	CLA	O	308	-	1/1/11/20	6/18/94/115	-
39	KC1	M	312	-	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	218	12	1/1/14/20	8/33/109/115	-
29	CLA	J	310	-	1/1/11/20	6/18/94/115	-
37	PID	P	202	-	-	4/24/93/93	0/4/4/4
29	CLA	D	313	20	1/1/11/20	3/15/91/115	-
29	CLA	A	214	12	1/1/10/20	4/10/86/115	-
29	CLA	O	311	-	1/1/12/20	4/23/99/115	-
39	KC1	H	314	-	-	6/15/71/71	-
29	CLA	L	308	-	1/1/12/20	8/25/101/115	-
29	CLA	b	721	-	1/1/13/20	10/31/107/115	-
29	CLA	a	809	1	1/1/15/20	15/39/115/115	-
29	CLA	l	508	-	1/1/10/20	0/10/86/115	-
37	PID	T	304	-	-	1/24/93/93	0/4/4/4
29	CLA	l	502	10	1/1/15/20	15/39/115/115	-
30	PQN	b	727	-	-	4/23/43/43	0/2/2/2
39	KC1	N	310	-	-	7/15/71/71	-
38	UIX	E	304	-	-	2/31/87/87	0/3/3/3
29	CLA	F	310	-	1/1/11/20	8/17/93/115	-
29	CLA	I	201	29	1/1/11/20	3/15/91/115	-
29	CLA	a	824	-	1/1/15/20	8/39/115/115	-
38	UIX	J	304	-	-	4/31/87/87	0/3/3/3
38	UIX	A	203	-	-	4/31/87/87	0/3/3/3
29	CLA	T	309	25	1/1/11/20	3/17/93/115	-
29	CLA	O	314	-	-	6/18/94/115	-
36	DD6	J	301	-	-	2/26/80/80	0/3/3/3
36	DD6	T	303	-	-	7/26/80/80	0/3/3/3
29	CLA	I	213	14	1/1/15/20	14/39/115/115	-
29	CLA	P	217	-	1/1/10/20	2/10/86/115	-
38	UIX	N	306	-	-	9/31/87/87	0/3/3/3
29	CLA	P	209	-	1/1/11/20	7/18/94/115	-
29	CLA	F	316	16	1/1/10/20	2/10/86/115	-
29	CLA	b	711	-	1/1/13/20	11/31/107/115	-
29	CLA	l	501	-	1/1/14/20	11/33/109/115	-
37	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	CLA	L	311	19	1/1/11/20	6/17/93/115	-
29	CLA	a	803	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	KC1	Q	311	-	-	5/15/71/71	-
32	BCR	l	506	-	-	9/29/63/63	0/2/2/2
29	CLA	E	306	28	1/1/15/20	16/39/115/115	-
29	CLA	A	212	-	1/1/13/20	10/27/103/115	-
29	CLA	b	710	-	1/1/11/20	8/17/93/115	-
29	CLA	L	317	-	1/1/11/20	7/17/93/115	-
29	CLA	F	312	16	1/1/11/20	5/17/93/115	-
37	PID	G	303	-	-	6/24/93/93	0/4/4/4
29	CLA	a	818	-	1/1/11/20	6/18/94/115	-
37	PID	N	304	-	-	1/24/93/93	0/4/4/4
29	CLA	K	212	-	1/1/12/20	7/24/100/115	-
36	DD6	M	304	-	-	3/26/80/80	0/3/3/3
39	KC1	T	310	-	-	6/15/71/71	-
32	BCR	a	834	-	-	0/29/63/63	0/2/2/2
29	CLA	a	807	-	1/1/15/20	14/39/115/115	-
37	PID	T	317	-	-	11/24/93/93	1/4/4/4
29	CLA	G	302	-	1/1/15/20	14/39/115/115	-
37	PID	D	303	-	-	1/24/93/93	0/4/4/4
39	KC1	O	312	-	-	3/15/71/71	-
30	PQN	a	832	-	-	6/23/43/43	0/2/2/2
29	CLA	D	314	-	1/1/11/20	6/18/94/115	-
29	CLA	b	719	-	1/1/12/20	10/21/97/115	-
31	LHG	a	833	-	-	7/52/52/53	-
29	CLA	L	307	39	1/1/12/20	12/21/97/115	-
32	BCR	f	801	-	-	5/29/63/63	0/2/2/2
39	KC1	N	312	23	-	6/15/71/71	-
29	CLA	J	305	-	1/1/11/20	4/17/93/115	-
29	CLA	Q	307	-	1/1/11/20	2/18/94/115	-
39	KC1	T	312	-	-	4/15/71/71	-
29	CLA	b	705	-	1/1/15/20	11/39/115/115	-
29	CLA	J	309	17	1/1/11/20	5/17/93/115	-
39	KC1	A	213	-	-	5/15/71/71	-
29	CLA	B	308	-	1/1/15/20	12/39/115/115	-
29	CLA	B	306	21	1/1/11/20	5/20/96/115	-
29	CLA	O	316	-	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	T	313	-	1/1/11/20	5/17/93/115	-
29	CLA	E	309	-	1/1/11/20	8/17/93/115	-
36	DD6	m	101	-	-	0/26/80/80	0/3/3/3
38	UIX	L	302	-	-	2/31/87/87	0/3/3/3
36	DD6	B	305	-	-	2/26/80/80	0/3/3/3
36	DD6	E	303	-	-	1/26/80/80	0/3/3/3
36	DD6	K	202	-	-	8/26/80/80	0/3/3/3
36	DD6	A	201	-	-	3/26/80/80	0/3/3/3
34	LMG	E	316	-	-	10/27/47/70	0/1/1/1
29	CLA	l	503	10	1/1/15/20	17/39/115/115	-
37	PID	D	307	-	-	4/24/93/93	0/4/4/4
29	CLA	P	215	-	1/1/11/20	8/18/94/115	-
29	CLA	A	211	-	1/1/13/20	5/27/103/115	-
29	CLA	M	306	-	1/1/12/20	5/25/101/115	-
29	CLA	K	213	-	1/1/11/20	7/19/95/115	-
29	CLA	a	831	-	1/1/15/20	11/39/115/115	-
37	PID	H	306	-	-	4/24/93/93	0/4/4/4
35	DGD	G	320	-	-	9/34/74/95	0/2/2/2
37	PID	D	302	-	-	1/24/93/93	0/4/4/4
29	CLA	b	709	-	1/1/14/20	16/33/109/115	-
29	CLA	l	504	-	1/1/15/20	10/39/115/115	-
29	CLA	M	311	-	1/1/11/20	6/17/93/115	-
29	CLA	G	314	-	1/1/14/20	9/33/109/115	-
39	KC1	K	215	-	-	7/15/71/71	-
39	KC1	B	313	21	-	7/15/71/71	-
29	CLA	E	315	-	1/1/13/20	7/30/106/115	-
39	KC1	I	215	14	-	11/15/71/71	-

The worst 5 of 2538 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	307	DD6	C30-C31	-9.31	1.24	1.42
36	I	203	DD6	C30-C31	-9.07	1.24	1.42
36	G	305	DD6	C30-C31	-8.84	1.25	1.42
36	K	202	DD6	C30-C31	-8.83	1.25	1.42
36	J	303	DD6	C30-C31	-8.78	1.25	1.42

The worst 5 of 3397 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	308	CLA	O2D-CGD-CBD	27.01	158.46	111.23
29	b	736	CLA	O2D-CGD-CBD	27.00	158.43	111.23
29	I	209	CLA	O2D-CGD-CBD	26.93	158.31	111.23
29	I	212	CLA	O2D-CGD-CBD	26.75	157.99	111.23
29	a	831	CLA	O2D-CGD-CBD	26.70	157.91	111.23

5 of 220 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	a	801	CLA	ND
29	a	802	CLA	ND
29	a	803	CLA	ND
29	a	804	CLA	ND
29	a	805	CLA	ND

5 of 2645 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	a	801	CLA	CBD-CGD-O2D-CED
29	a	805	CLA	C1A-C2A-CAA-CBA
29	a	805	CLA	C3A-C2A-CAA-CBA
29	a	805	CLA	CBD-CGD-O2D-CED
29	a	807	CLA	C1A-C2A-CAA-CBA

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	h	204	PID	C24-C25-C26-C27-C28-C29
37	T	317	PID	C24-C25-C26-C27-C28-C29
37	F	304	PID	C24-C25-C26-C27-C28-C29

331 monomers are involved in 958 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	D	315	KC1	2	0
29	C	311	CLA	2	0
29	N	311	CLA	1	0
36	J	303	DD6	1	0
29	M	314	CLA	1	0
37	N	301	PID	2	0
37	O	307	PID	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	Q	303	PID	2	0
36	B	301	DD6	2	0
29	D	312	CLA	4	0
36	G	307	DD6	3	0
36	I	205	DD6	3	0
29	a	804	CLA	6	0
37	T	301	PID	4	0
29	a	828	CLA	4	0
39	P	211	KC1	1	0
29	a	837	CLA	5	0
32	m	103	BCR	8	0
29	A	206	CLA	2	0
34	K	219	LMG	2	0
36	I	206	DD6	1	0
37	O	305	PID	7	0
29	Q	313	CLA	4	0
29	J	307	CLA	2	0
29	L	313	CLA	4	0
36	G	305	DD6	1	0
29	b	726	CLA	6	0
35	j	103	DGD	2	0
36	O	303	DD6	2	0
29	I	209	CLA	4	0
34	b	732	LMG	6	0
29	O	309	CLA	6	0
37	P	205	PID	3	0
29	a	801	CLA	4	0
29	b	713	CLA	1	0
36	P	204	DD6	1	0
29	H	315	CLA	2	0
38	B	304	UIX	1	0
29	a	825	CLA	4	0
39	P	216	KC1	1	0
29	H	308	CLA	5	0
36	L	305	DD6	1	0
36	N	303	DD6	1	0
35	m	102	DGD	5	0
29	M	315	CLA	1	0
29	I	217	CLA	4	0
29	G	301	CLA	2	0
29	J	306	CLA	5	0
37	h	204	PID	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	815	CLA	1	0
29	a	802	CLA	4	0
37	P	208	PID	3	0
29	A	207	CLA	1	0
29	G	312	CLA	4	0
36	K	204	DD6	2	0
29	a	817	CLA	1	0
29	I	208	CLA	1	0
29	i	202	CLA	8	0
29	N	314	CLA	5	0
37	P	206	PID	9	0
29	Q	308	CLA	4	0
29	K	211	CLA	3	0
37	P	203	PID	5	0
39	H	309	KC1	1	0
29	B	307	CLA	2	0
37	H	304	PID	4	0
39	E	307	KC1	2	0
36	K	221	DD6	2	0
29	b	704	CLA	2	0
29	E	305	CLA	6	0
35	j	106	DGD	4	0
29	L	310	CLA	3	0
35	b	733	DGD	2	0
34	j	102	LMG	3	0
29	J	313	CLA	1	0
29	F	307	CLA	3	0
29	T	311	CLA	1	0
29	M	309	CLA	2	0
29	E	313	CLA	2	0
35	j	105	DGD	4	0
29	a	826	CLA	5	0
36	M	303	DD6	1	0
29	a	823	CLA	5	0
32	b	729	BCR	5	0
29	K	217	CLA	1	0
34	P	201	LMG	1	0
32	l	507	BCR	4	0
32	a	838	BCR	5	0
29	I	214	CLA	4	0
29	a	811	CLA	2	0
29	N	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	b	725	CLA	3	0
37	Q	304	PID	5	0
29	B	309	CLA	1	0
29	H	312	CLA	2	0
29	a	819	CLA	4	0
36	B	303	DD6	1	0
29	b	702	CLA	11	0
29	A	217	CLA	2	0
29	M	308	CLA	1	0
29	b	701	CLA	5	0
29	a	827	CLA	4	0
29	b	736	CLA	4	0
29	G	304	CLA	7	0
29	a	820	CLA	4	0
29	L	315	CLA	2	0
29	h	201	CLA	7	0
29	C	308	CLA	2	0
29	a	806	CLA	11	0
37	O	302	PID	8	0
29	F	308	CLA	1	0
29	f	802	CLA	1	0
37	j	101	PID	5	0
29	I	212	CLA	3	0
29	Q	312	CLA	3	0
37	E	301	PID	7	0
37	H	305	PID	7	0
37	C	302	PID	4	0
29	I	210	CLA	3	0
29	b	731	CLA	2	0
37	N	302	PID	4	0
29	E	314	CLA	1	0
36	A	202	DD6	1	0
29	a	810	CLA	7	0
29	H	313	CLA	4	0
29	D	308	CLA	1	0
29	F	315	CLA	1	0
38	F	305	UIX	2	0
29	O	313	CLA	3	0
29	a	813	CLA	2	0
29	E	310	CLA	1	0
29	b	714	CLA	4	0
29	b	724	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	N	315	KC1	3	0
36	D	304	DD6	3	0
36	M	301	DD6	1	0
37	T	302	PID	4	0
29	F	313	CLA	4	0
29	Q	315	CLA	2	0
29	A	216	CLA	2	0
29	K	218	CLA	3	0
29	b	703	CLA	7	0
29	i	201	CLA	6	0
29	N	309	CLA	8	0
29	a	805	CLA	2	0
29	G	317	CLA	2	0
32	b	728	BCR	6	0
29	T	316	CLA	3	0
29	f	803	CLA	2	0
32	f	804	BCR	5	0
29	F	311	CLA	4	0
37	D	305	PID	5	0
34	K	220	LMG	1	0
29	a	822	CLA	2	0
33	c	102	SF4	3	0
29	b	712	CLA	5	0
29	i	203	CLA	5	0
29	b	707	CLA	7	0
29	A	215	CLA	2	0
29	P	210	CLA	7	0
36	L	301	DD6	1	0
39	G	315	KC1	1	0
29	b	715	CLA	4	0
29	G	316	CLA	1	0
33	a	836	SF4	2	0
37	H	301	PID	4	0
29	a	814	CLA	1	0
40	J	314	SQD	7	0
29	B	312	CLA	2	0
29	b	716	CLA	5	0
29	b	722	CLA	2	0
29	H	310	CLA	3	0
29	D	309	CLA	2	0
29	C	316	CLA	3	0
29	a	812	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	b	717	CLA	5	0
37	Q	301	PID	5	0
37	C	304	PID	4	0
37	T	305	PID	5	0
29	M	313	CLA	1	0
29	N	313	CLA	1	0
29	T	314	CLA	8	0
29	I	211	CLA	3	0
35	h	203	DGD	9	0
29	D	311	CLA	1	0
29	D	316	CLA	1	0
36	J	302	DD6	4	0
37	F	302	PID	1	0
29	a	830	CLA	1	0
29	l	505	CLA	6	0
34	h	205	LMG	2	0
29	C	313	CLA	1	0
29	E	311	CLA	3	0
32	a	835	BCR	4	0
40	B	317	SQD	3	0
29	C	309	CLA	3	0
37	H	302	PID	3	0
36	A	204	DD6	1	0
37	O	301	PID	2	0
29	l	510	CLA	3	0
29	B	316	CLA	1	0
34	b	734	LMG	1	0
37	T	307	PID	3	0
29	K	209	CLA	2	0
34	A	219	LMG	2	0
29	A	209	CLA	1	0
29	C	314	CLA	6	0
36	M	302	DD6	3	0
37	G	309	PID	2	0
29	L	316	CLA	4	0
29	P	214	CLA	2	0
37	C	305	PID	10	0
29	a	816	CLA	1	0
29	l	509	CLA	2	0
37	N	305	PID	7	0
29	b	708	CLA	3	0
39	C	310	KC1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	D	306	PID	3	0
37	F	304	PID	15	0
39	Q	314	KC1	2	0
36	F	303	DD6	2	0
29	L	312	CLA	4	0
36	C	303	DD6	1	0
29	b	718	CLA	5	0
29	I	207	CLA	2	0
29	I	216	CLA	2	0
29	Q	310	CLA	3	0
37	C	301	PID	2	0
29	a	821	CLA	3	0
29	K	210	CLA	4	0
29	f	805	CLA	5	0
29	G	313	CLA	1	0
37	O	304	PID	3	0
34	K	201	LMG	4	0
29	B	310	CLA	5	0
37	Q	306	PID	5	0
29	a	808	CLA	3	0
29	E	308	CLA	3	0
29	A	208	CLA	2	0
34	b	730	LMG	6	0
37	G	310	PID	3	0
29	J	311	CLA	2	0
29	b	723	CLA	6	0
29	B	315	CLA	1	0
39	G	318	KC1	1	0
37	C	307	PID	3	0
29	M	307	CLA	2	0
32	i	204	BCR	7	0
29	b	706	CLA	3	0
29	K	214	CLA	7	0
37	N	307	PID	6	0
36	B	319	DD6	4	0
29	P	212	CLA	2	0
32	b	735	BCR	8	0
29	a	829	CLA	5	0
29	b	720	CLA	5	0
29	A	218	CLA	2	0
29	J	310	CLA	3	0
37	P	202	PID	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	313	CLA	2	0
29	A	214	CLA	2	0
39	H	314	KC1	1	0
29	L	308	CLA	2	0
29	b	721	CLA	5	0
29	a	809	CLA	6	0
37	T	304	PID	4	0
29	l	502	CLA	1	0
30	b	727	PQN	3	0
39	N	310	KC1	2	0
38	E	304	UIX	1	0
29	F	310	CLA	5	0
29	a	824	CLA	10	0
38	J	304	UIX	1	0
29	T	309	CLA	4	0
29	O	314	CLA	10	0
36	T	303	DD6	1	0
29	I	213	CLA	3	0
29	P	217	CLA	2	0
29	P	209	CLA	2	0
29	b	711	CLA	6	0
29	l	501	CLA	9	0
37	F	306	PID	5	0
29	L	311	CLA	1	0
29	a	803	CLA	8	0
32	l	506	BCR	4	0
29	E	306	CLA	9	0
29	A	212	CLA	3	0
29	L	317	CLA	1	0
29	F	312	CLA	4	0
37	G	303	PID	3	0
29	a	818	CLA	1	0
37	N	304	PID	2	0
29	K	212	CLA	4	0
36	M	304	DD6	1	0
32	a	834	BCR	8	0
29	a	807	CLA	7	0
37	T	317	PID	3	0
29	G	302	CLA	9	0
37	D	303	PID	10	0
30	a	832	PQN	6	0
29	D	314	CLA	9	0

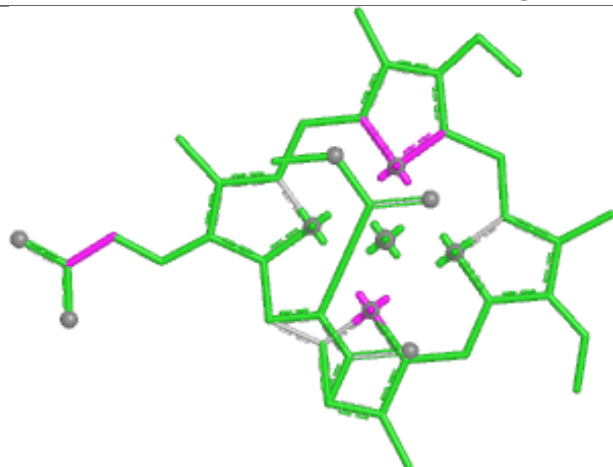
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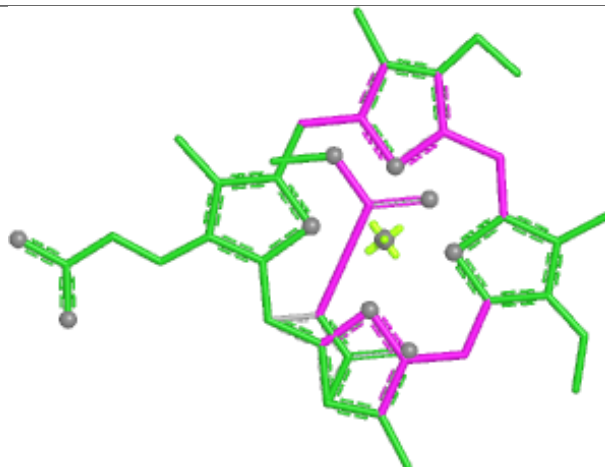
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	b	719	CLA	10	0
31	a	833	LHG	5	0
29	L	307	CLA	1	0
32	f	801	BCR	8	0
29	J	305	CLA	1	0
29	Q	307	CLA	3	0
29	b	705	CLA	9	0
29	J	309	CLA	5	0
29	B	308	CLA	5	0
29	B	306	CLA	1	0
29	O	316	CLA	1	0
29	T	313	CLA	2	0
36	B	305	DD6	1	0
34	E	316	LMG	6	0
29	l	503	CLA	6	0
37	D	307	PID	2	0
29	P	215	CLA	5	0
29	A	211	CLA	2	0
29	M	306	CLA	1	0
29	K	213	CLA	6	0
29	a	831	CLA	4	0
37	H	306	PID	7	0
35	G	320	DGD	2	0
37	D	302	PID	1	0
29	b	709	CLA	3	0
29	l	504	CLA	10	0
29	M	311	CLA	8	0
29	G	314	CLA	4	0
29	E	315	CLA	5	0
39	I	215	KC1	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.

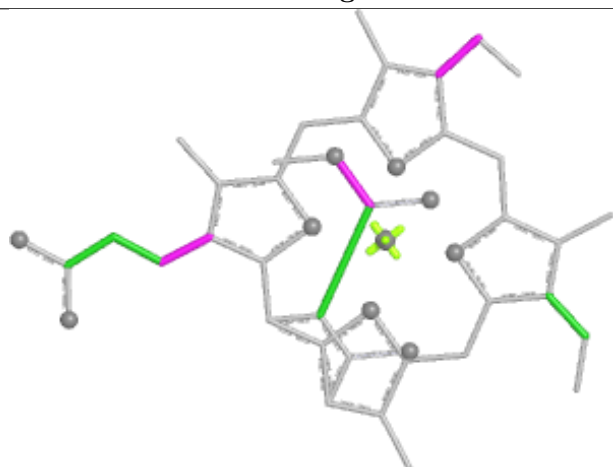
Ligand KC1 D 315



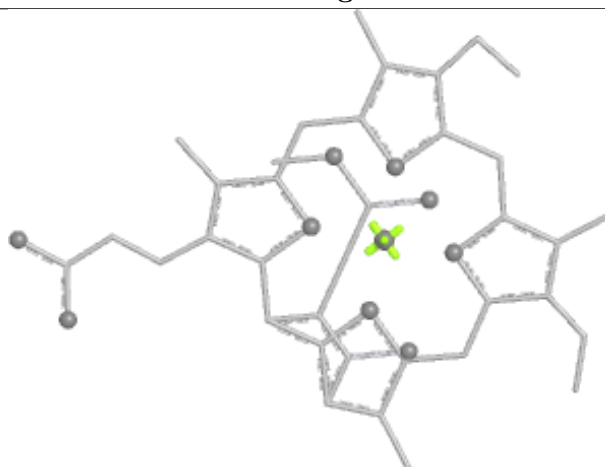
Bond lengths



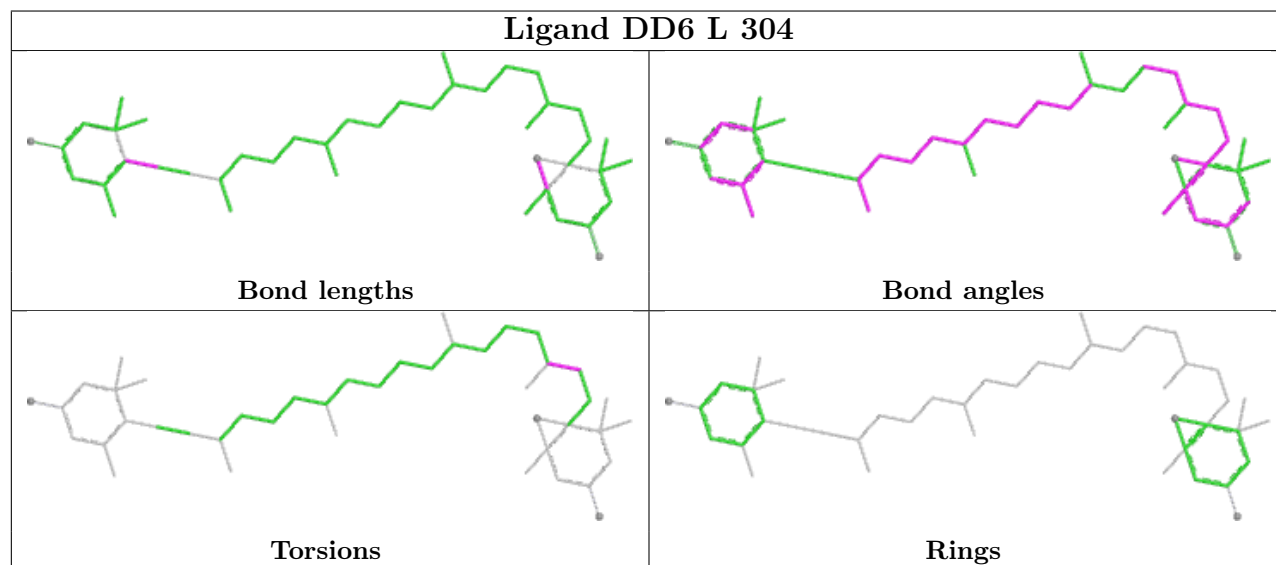
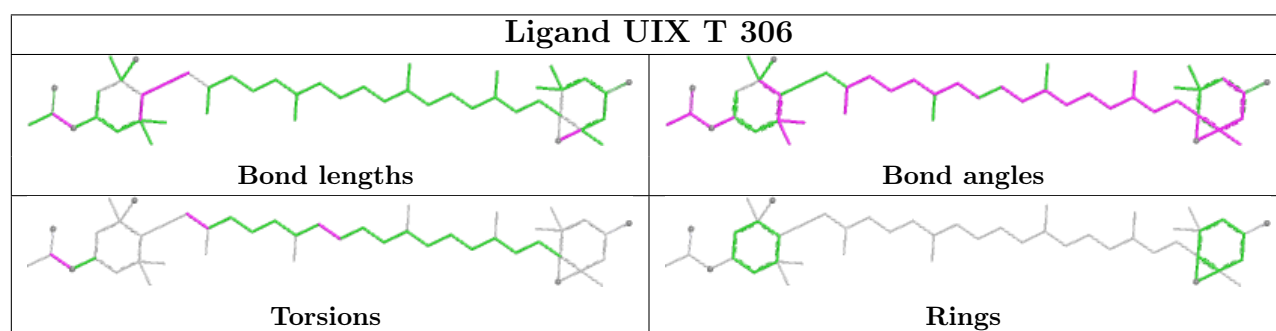
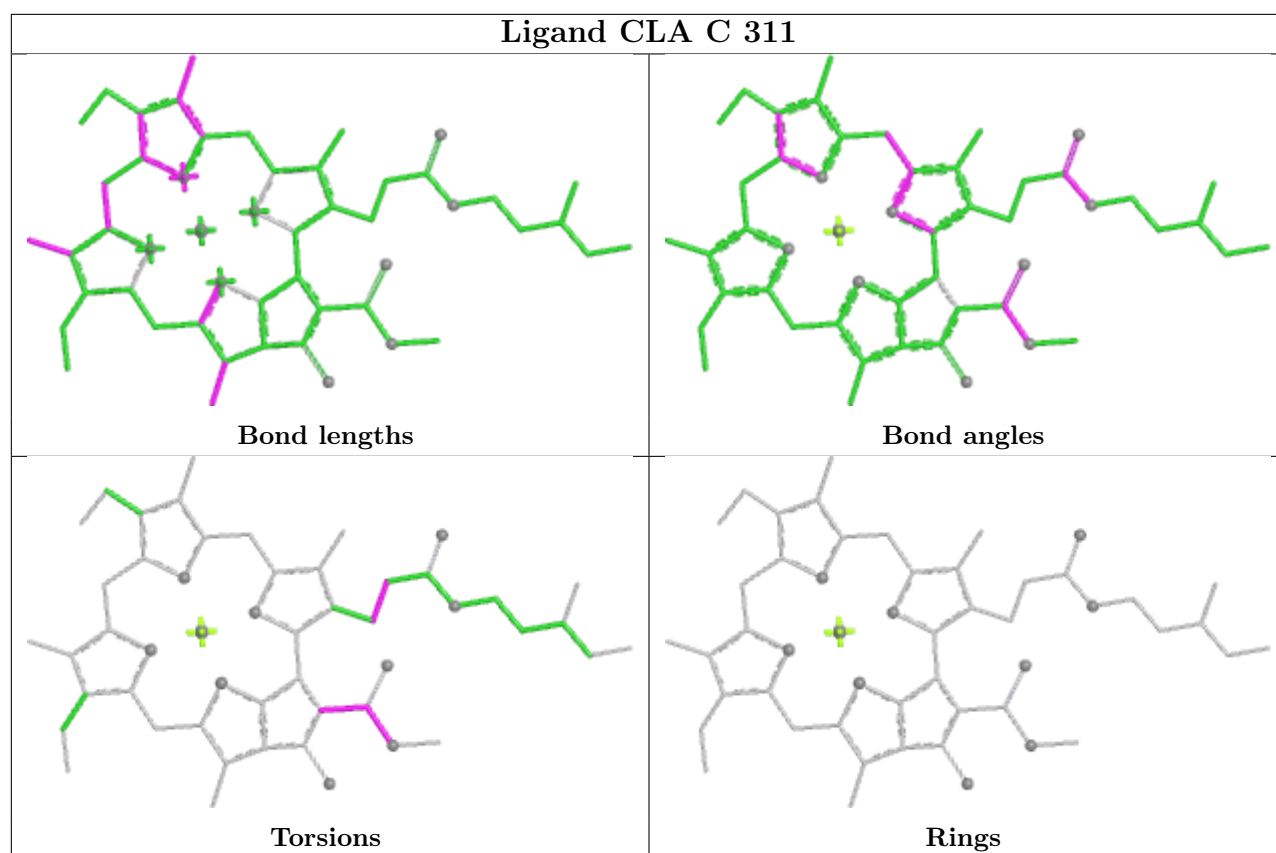
Bond angles

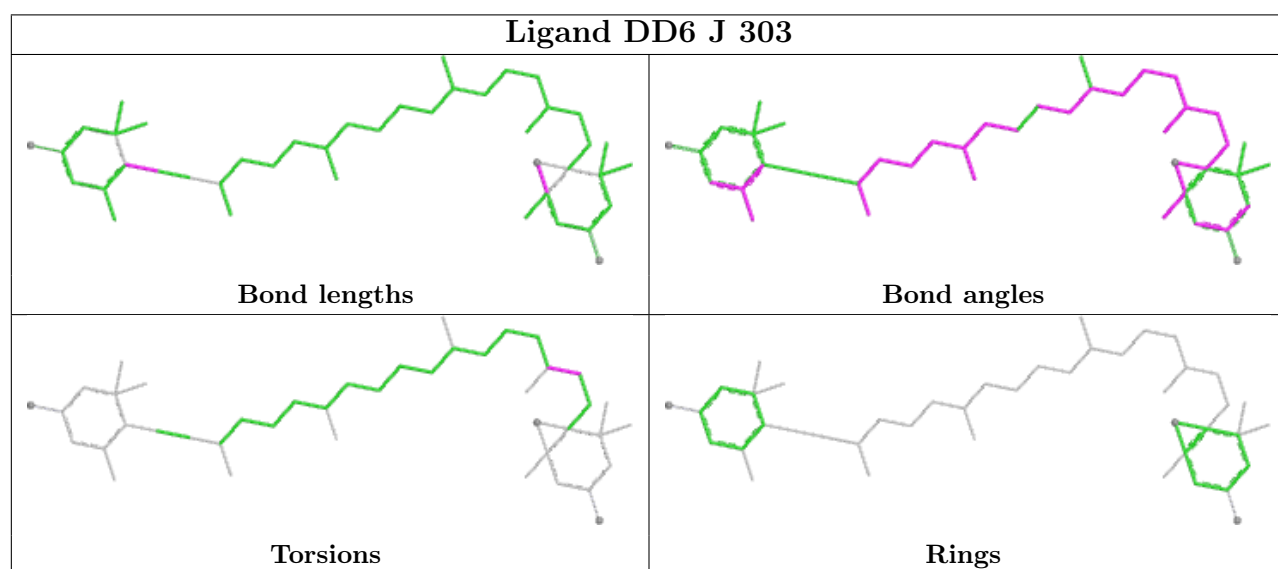
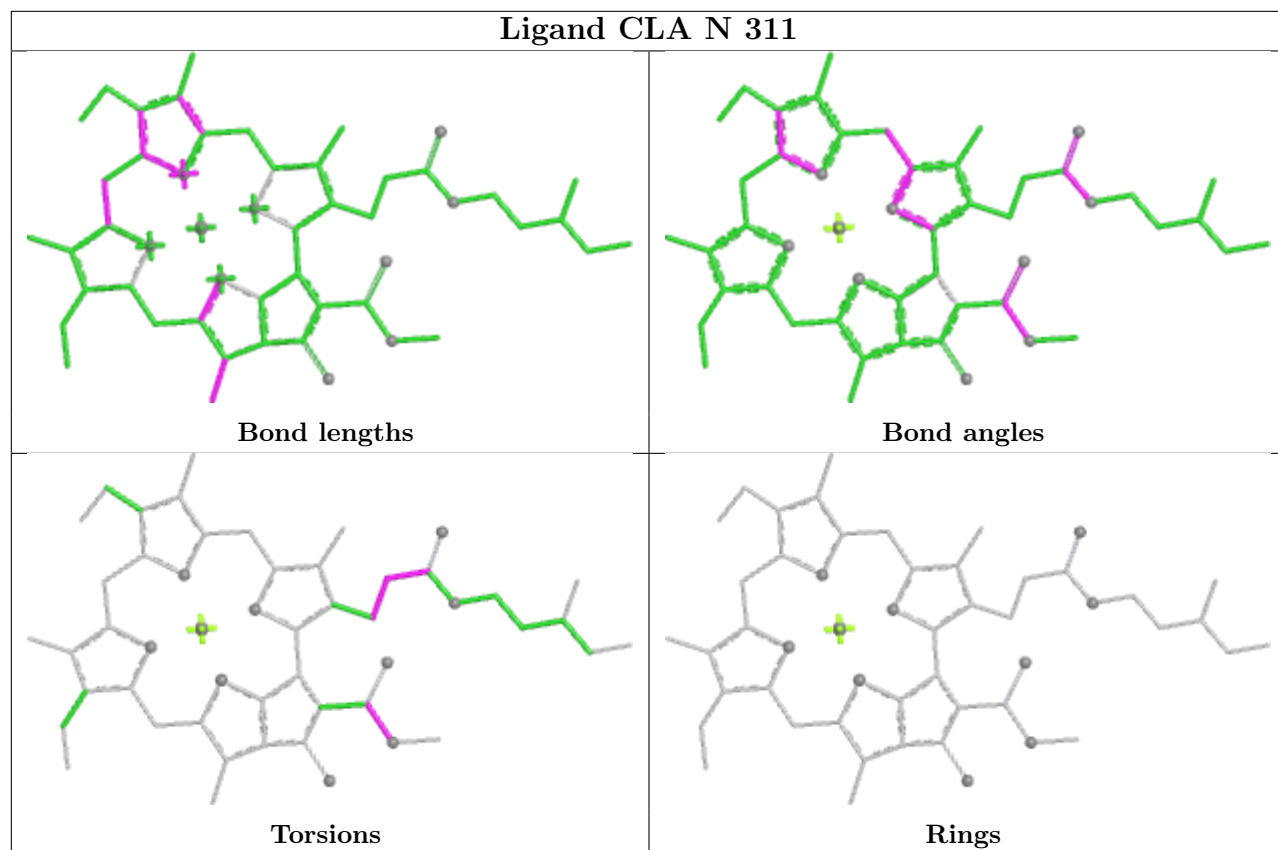


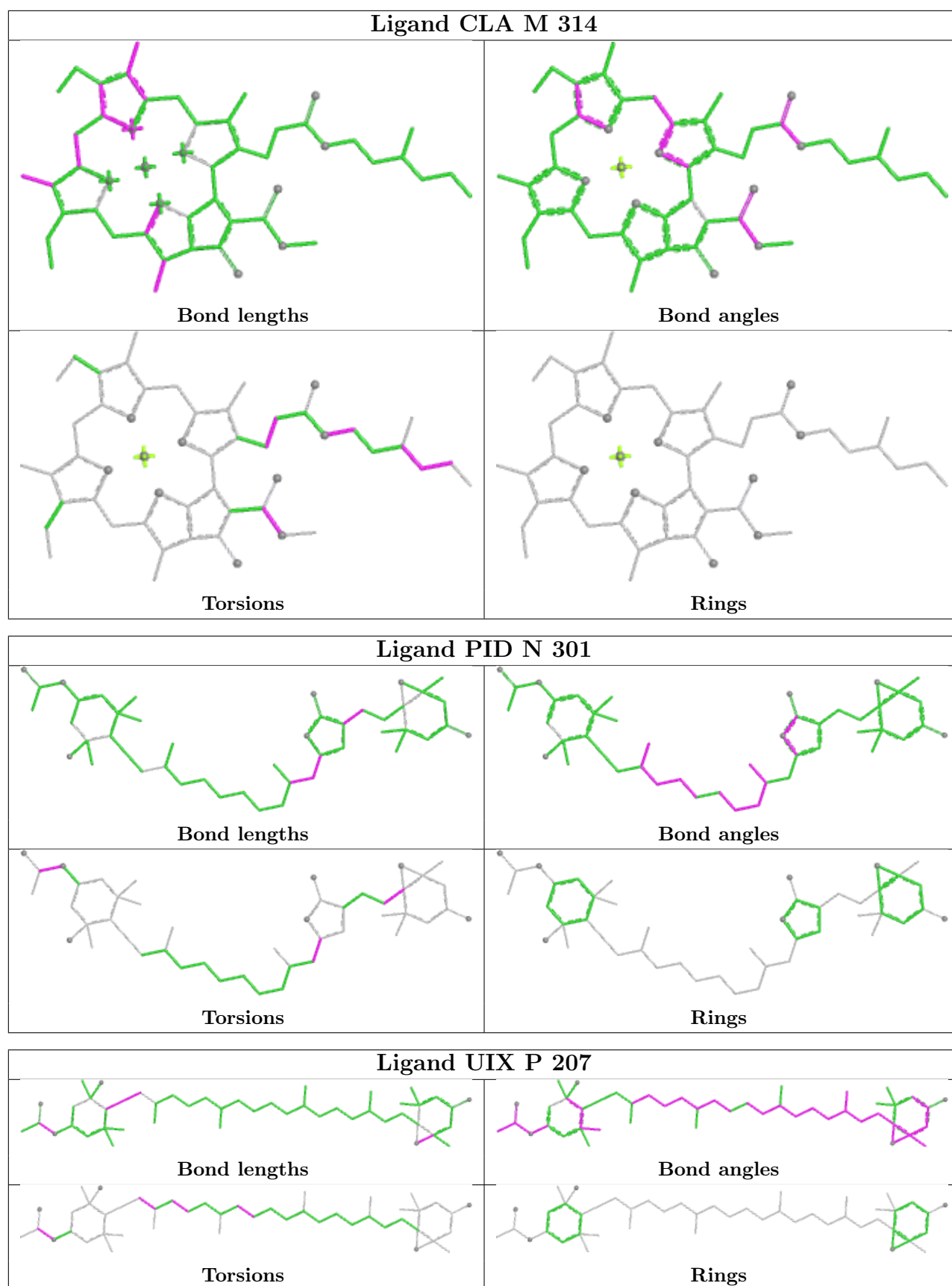
Torsions

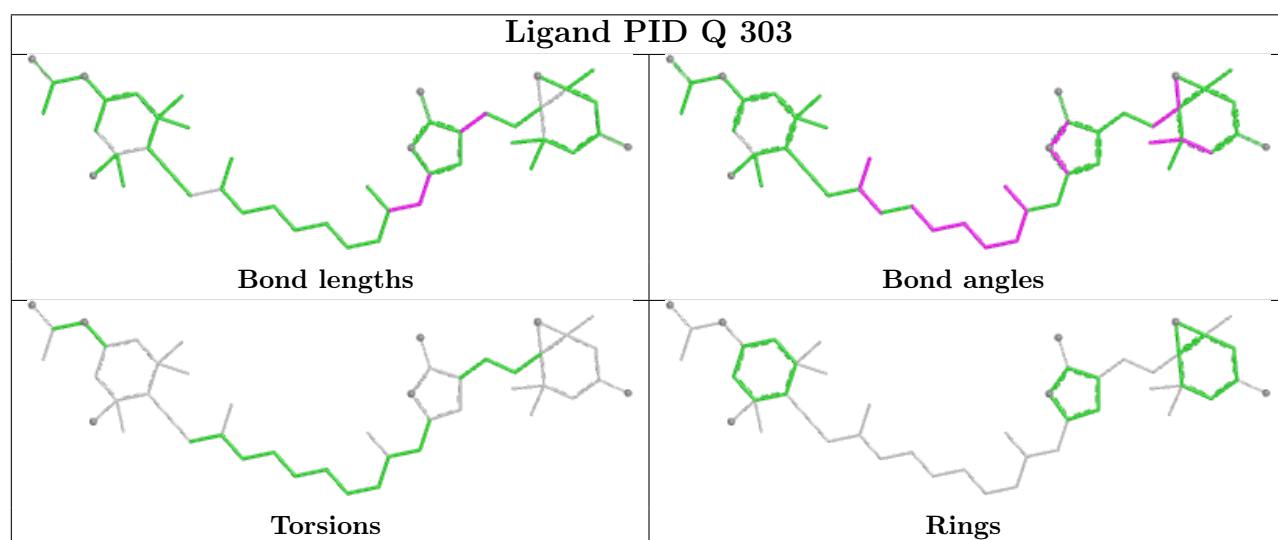
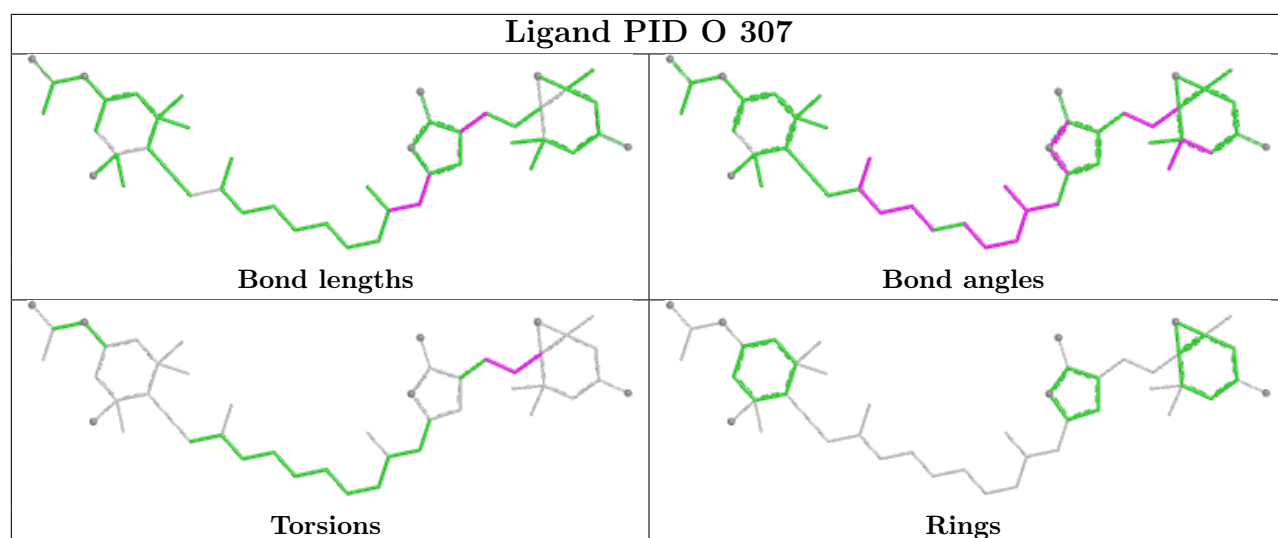


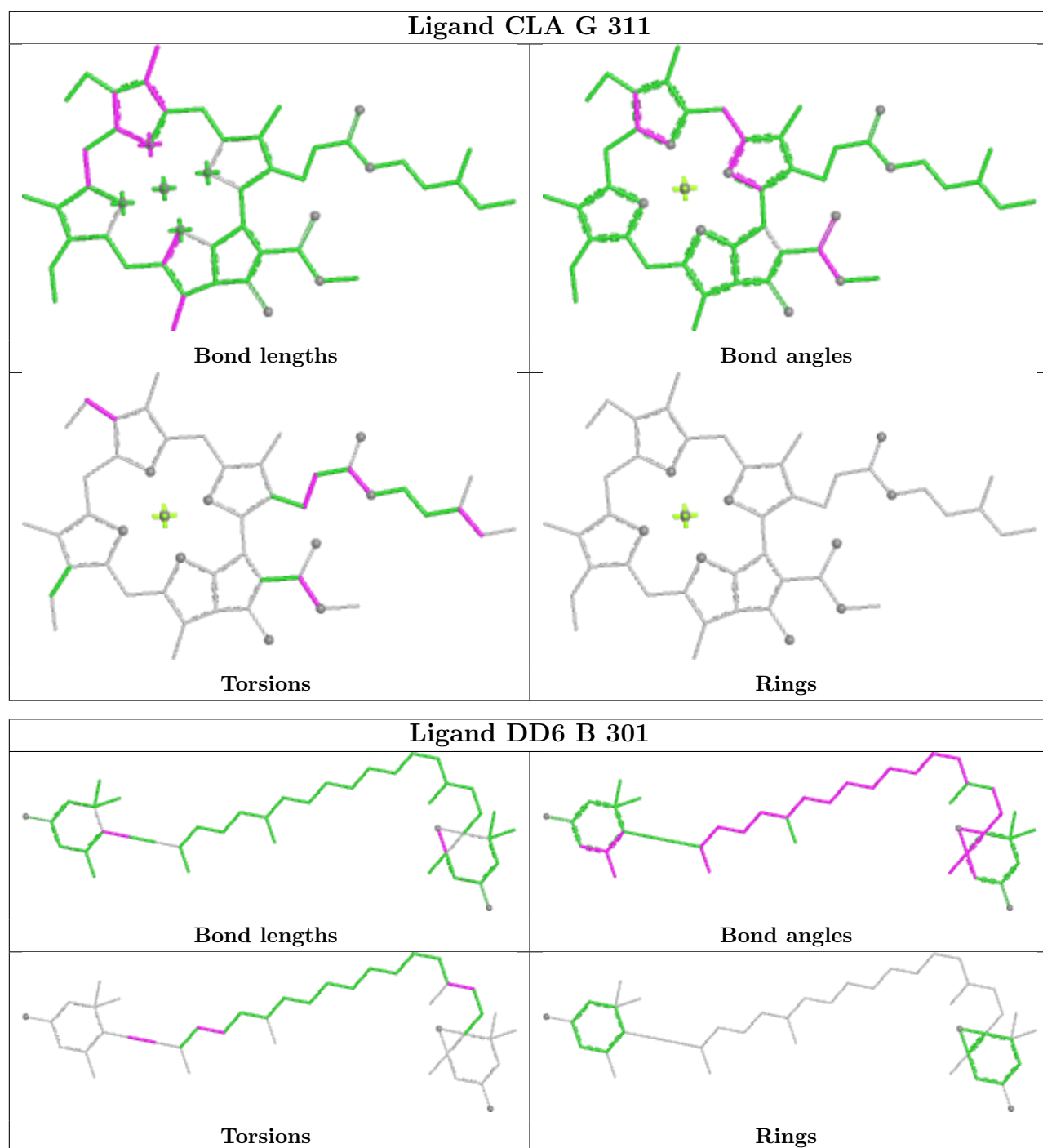
Rings



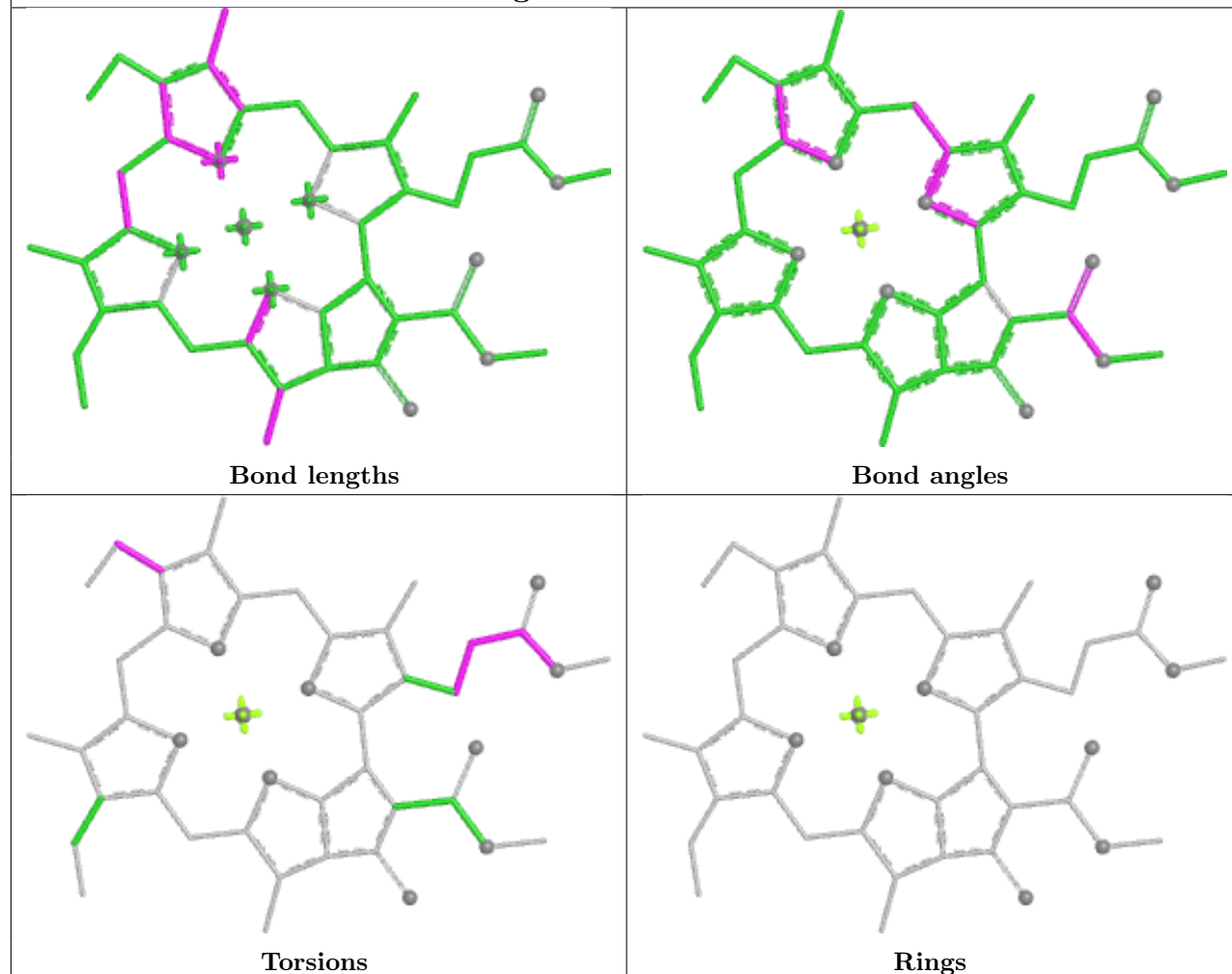




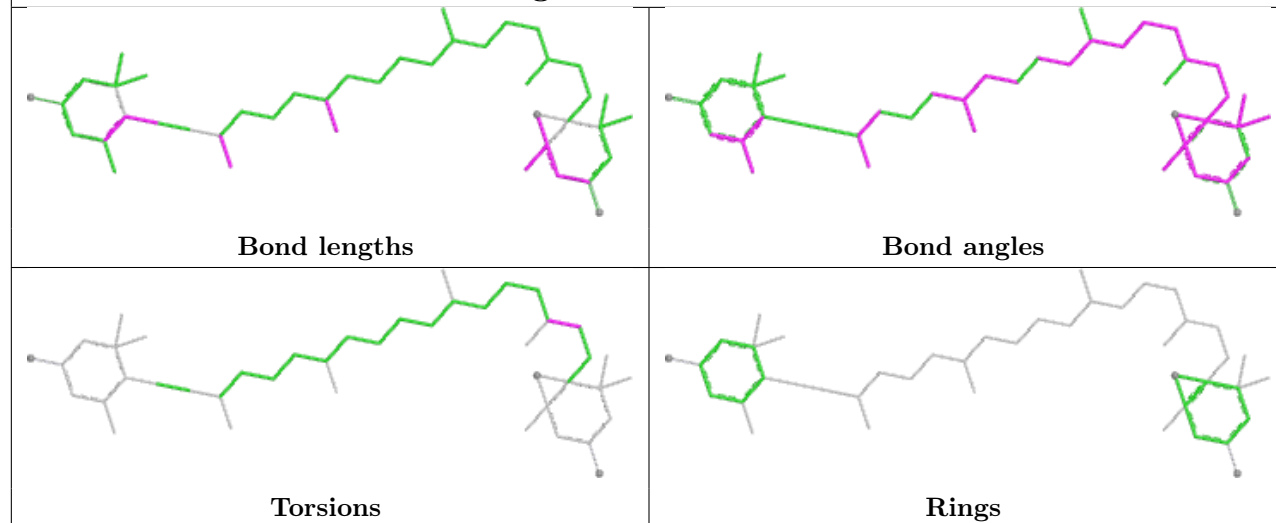


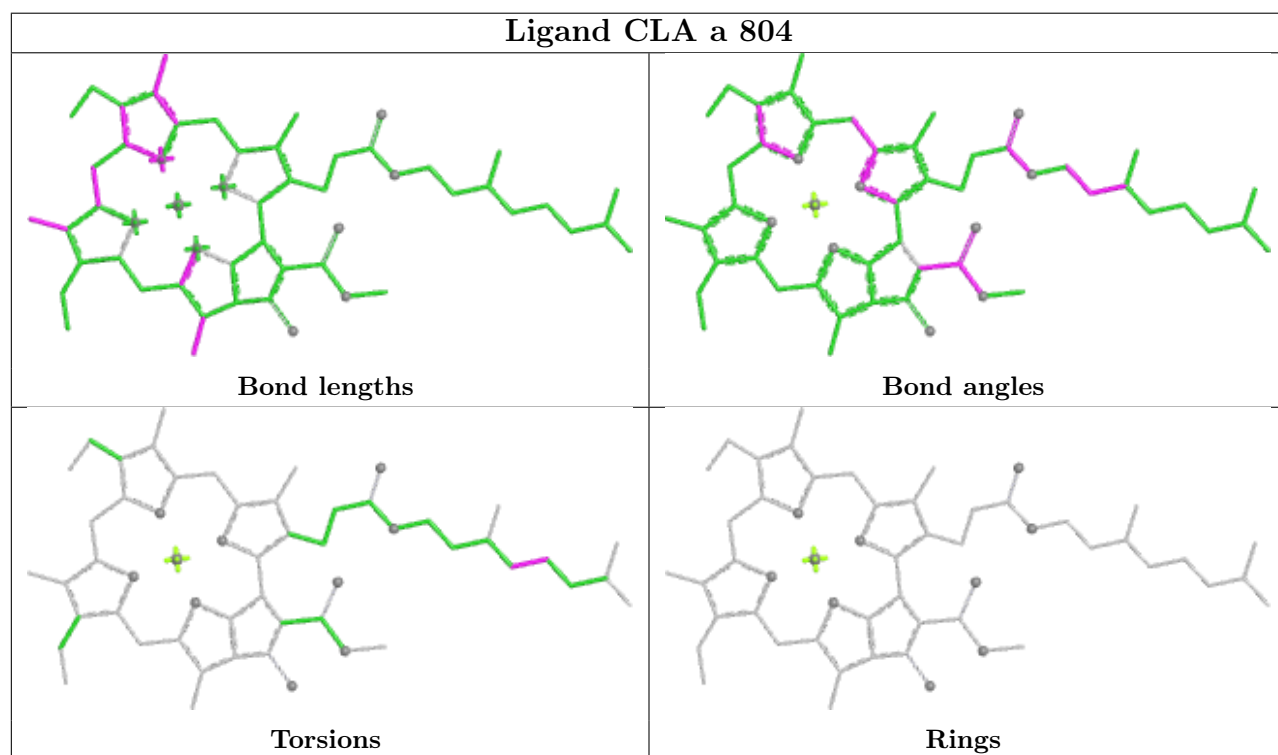
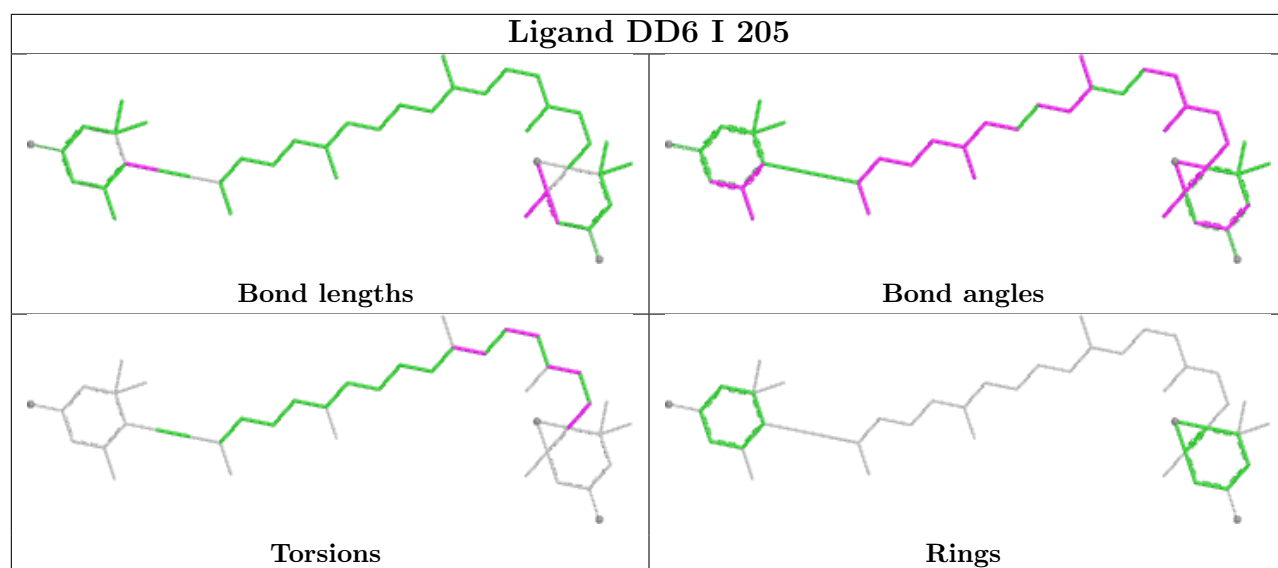


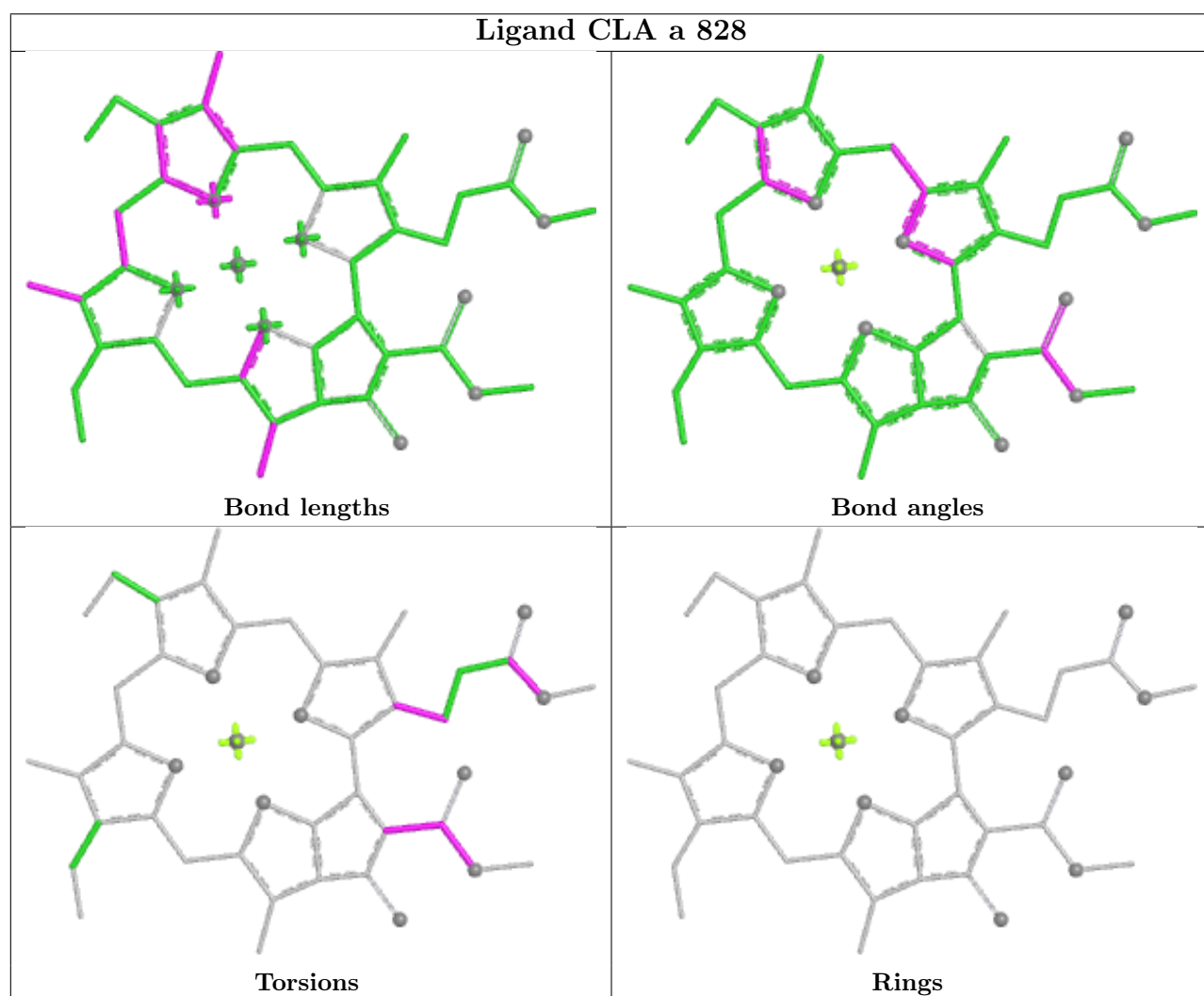
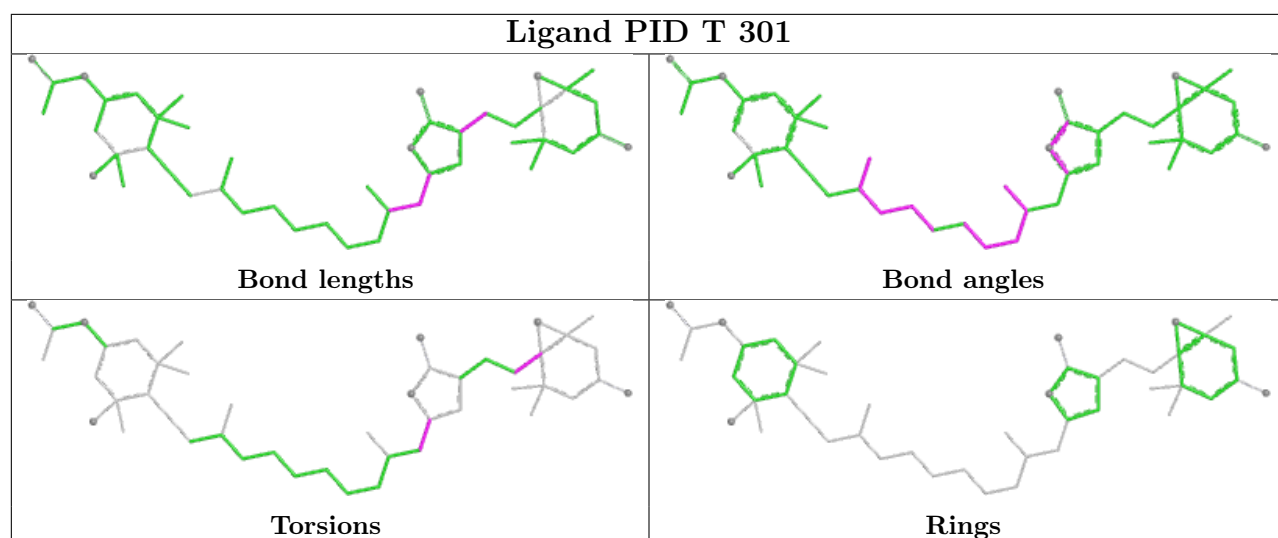
Ligand CLA D 312



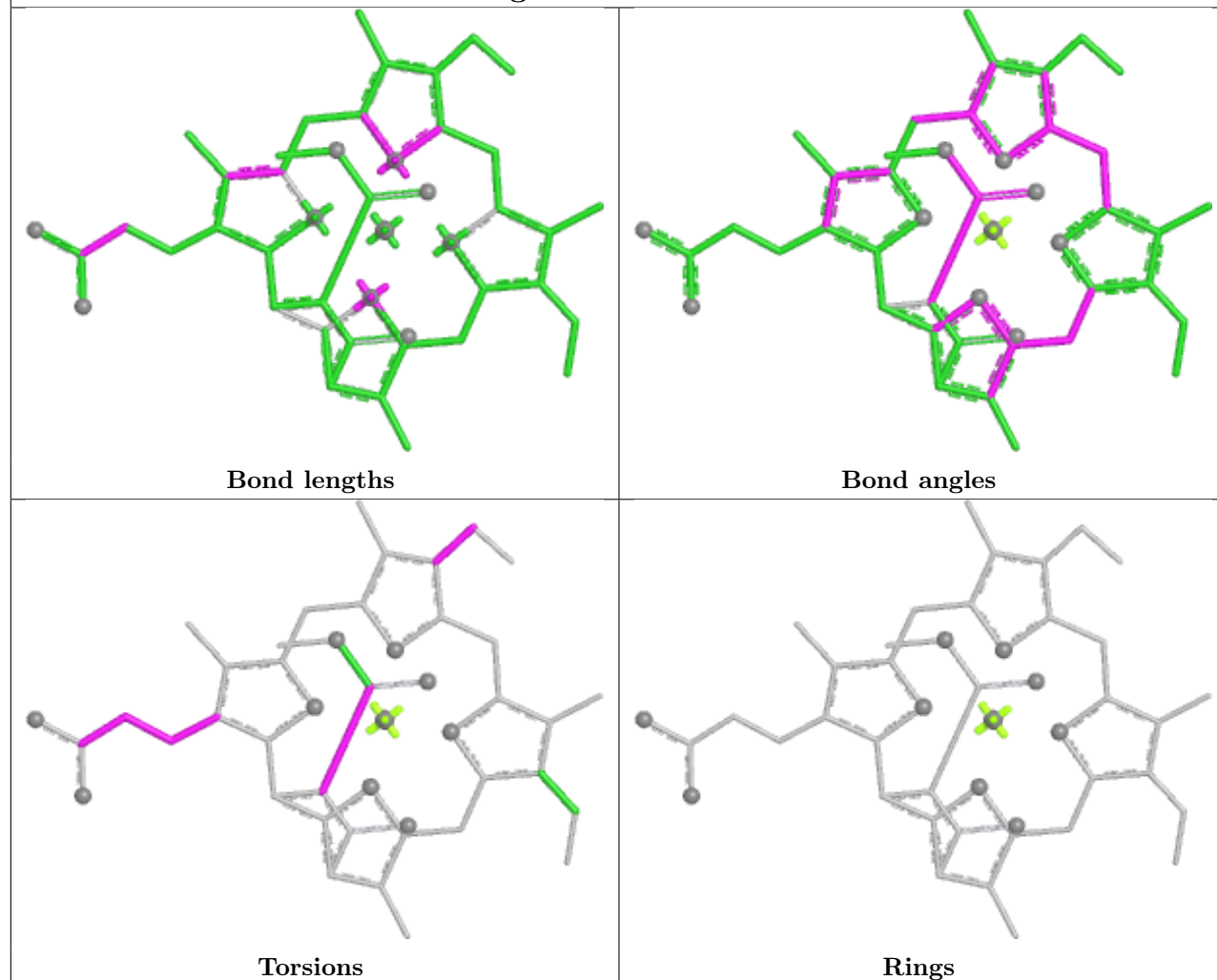
Ligand DD6 G 307



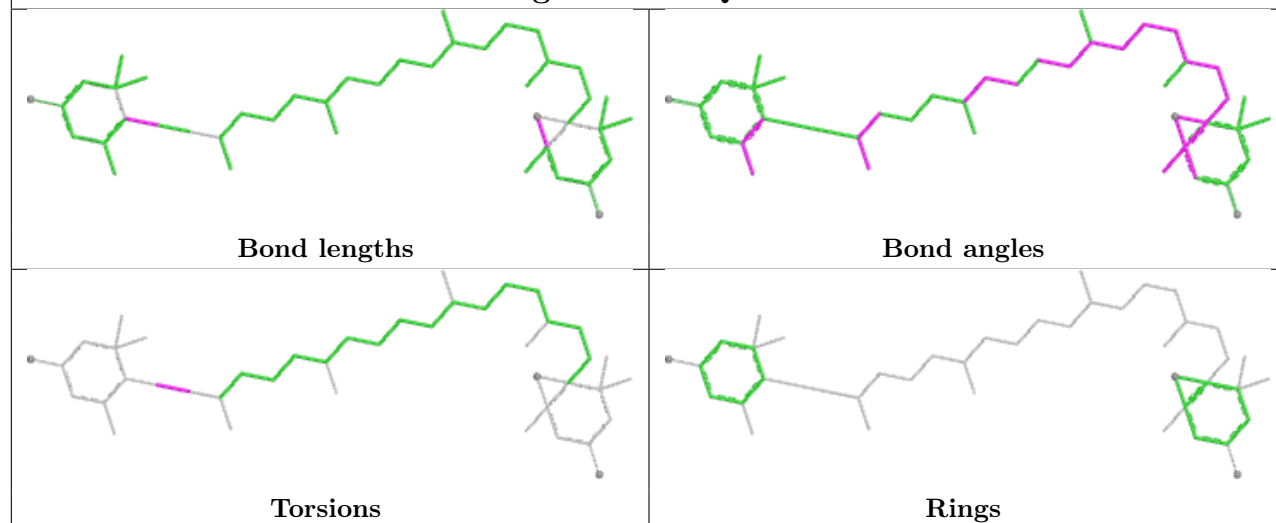


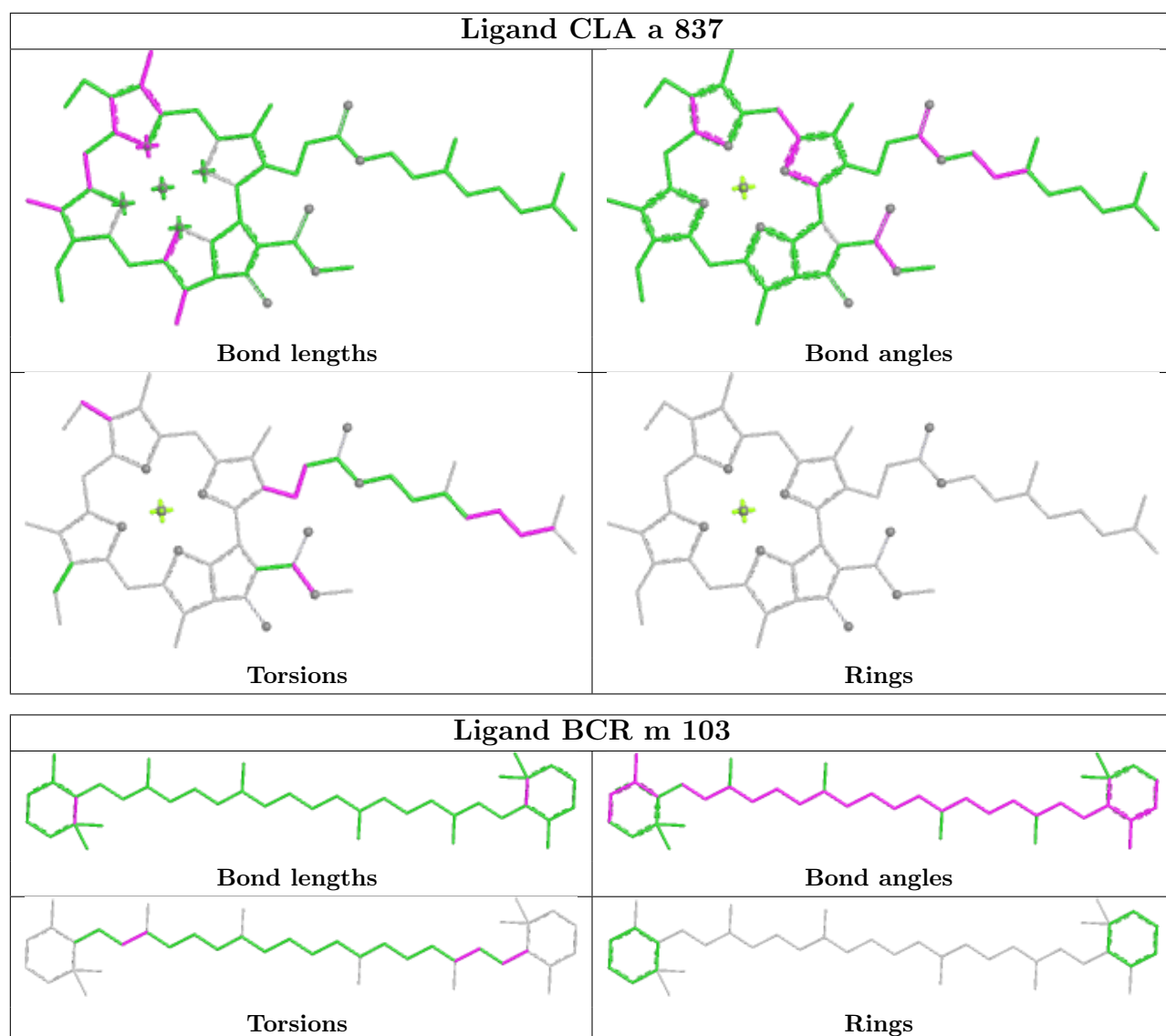


Ligand KC1 P 211

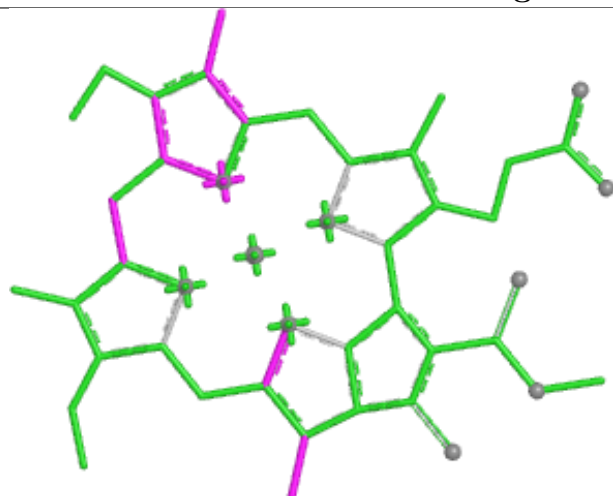


Ligand DD6 Q 302

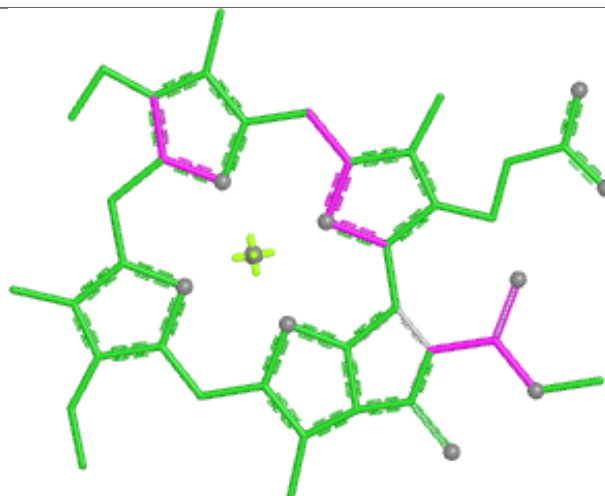




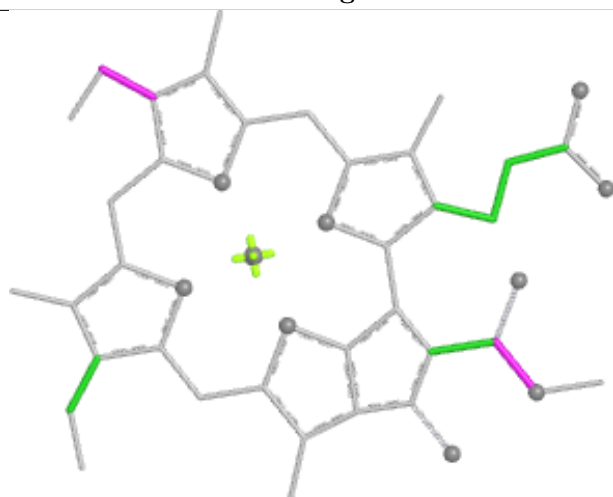
Ligand CLA A 206



Bond lengths



Bond angles

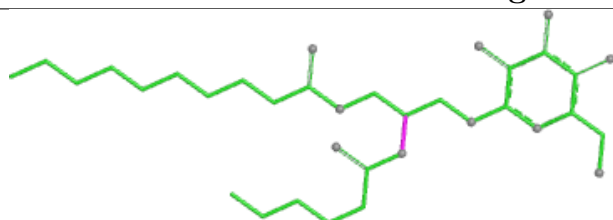


Torsions

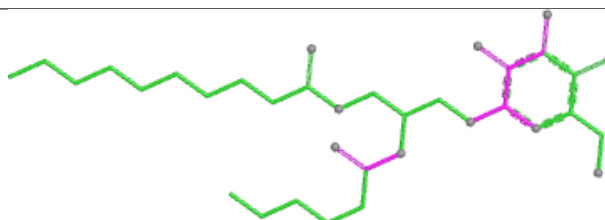


Rings

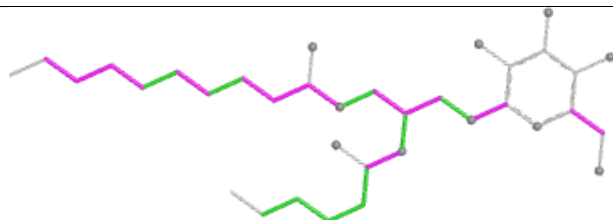
Ligand LMG K 219



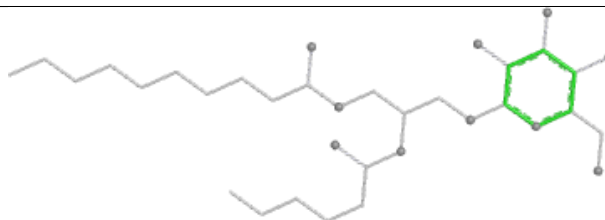
Bond lengths



Bond angles

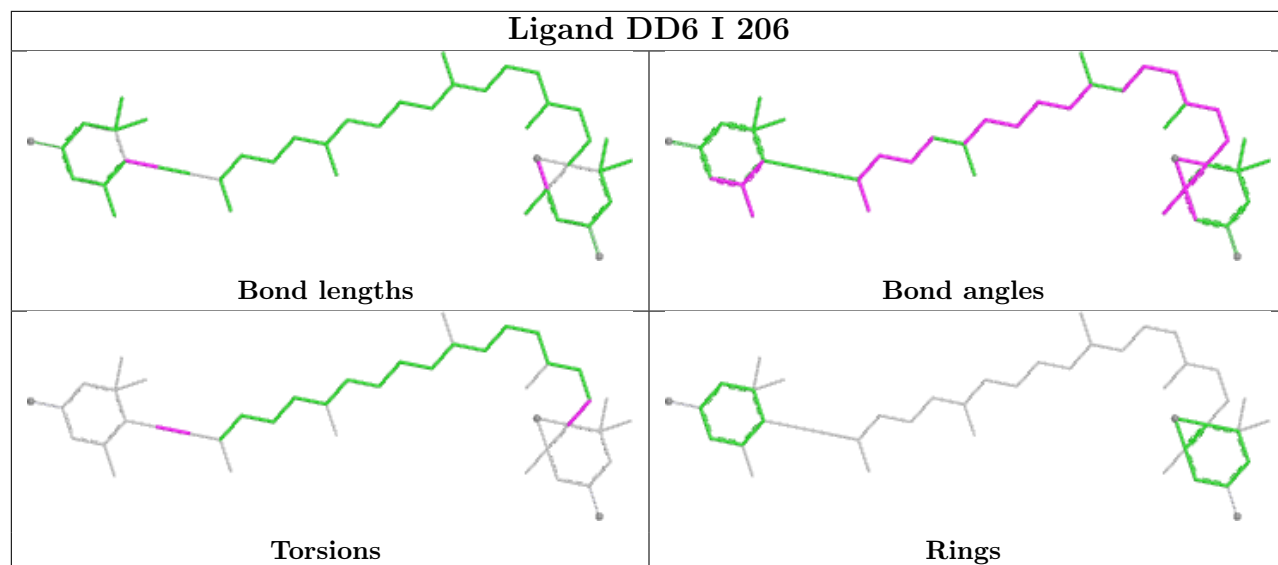


Torsions

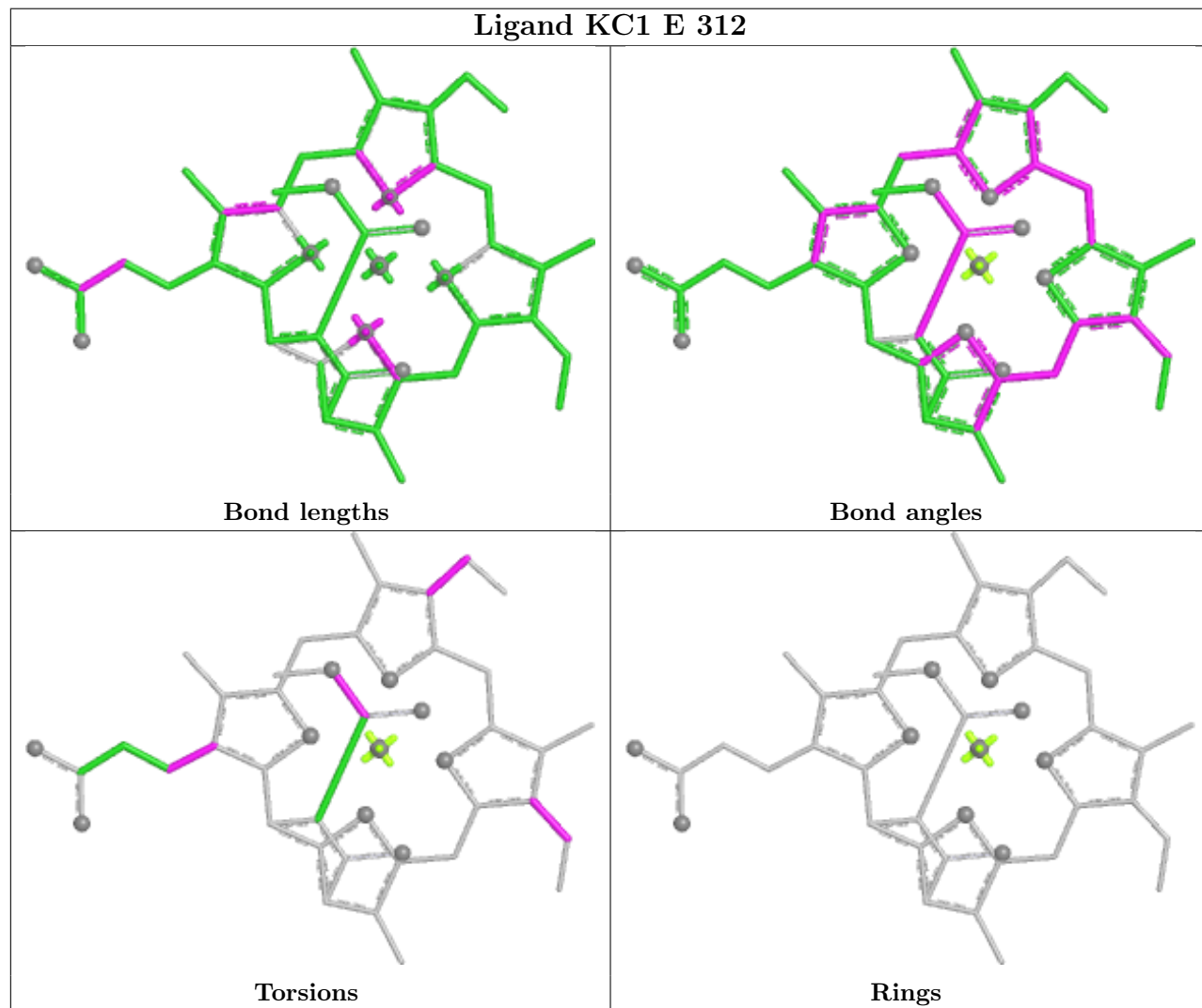


Rings

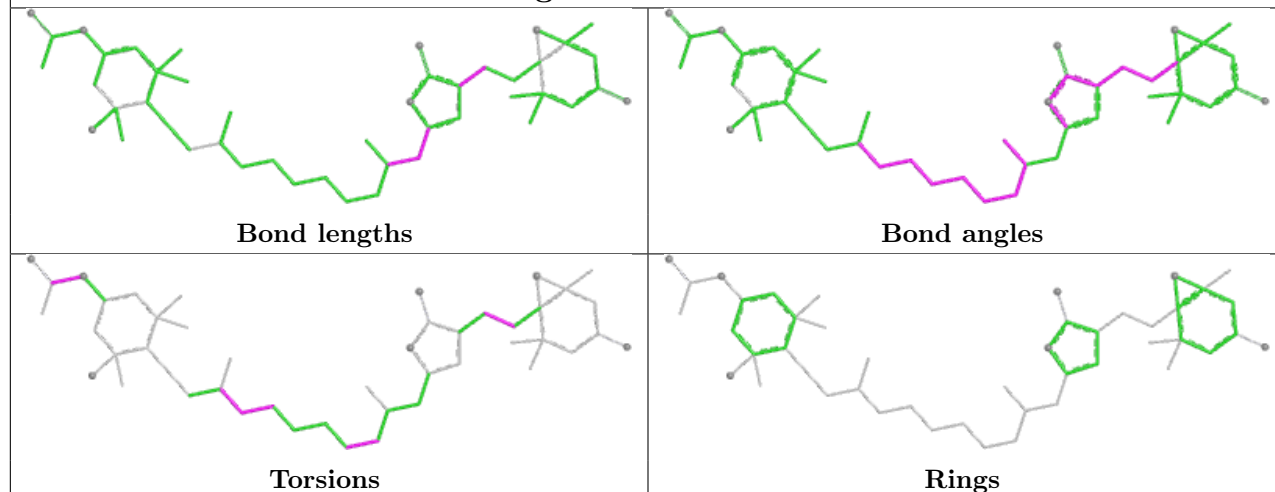
Ligand DD6 I 206



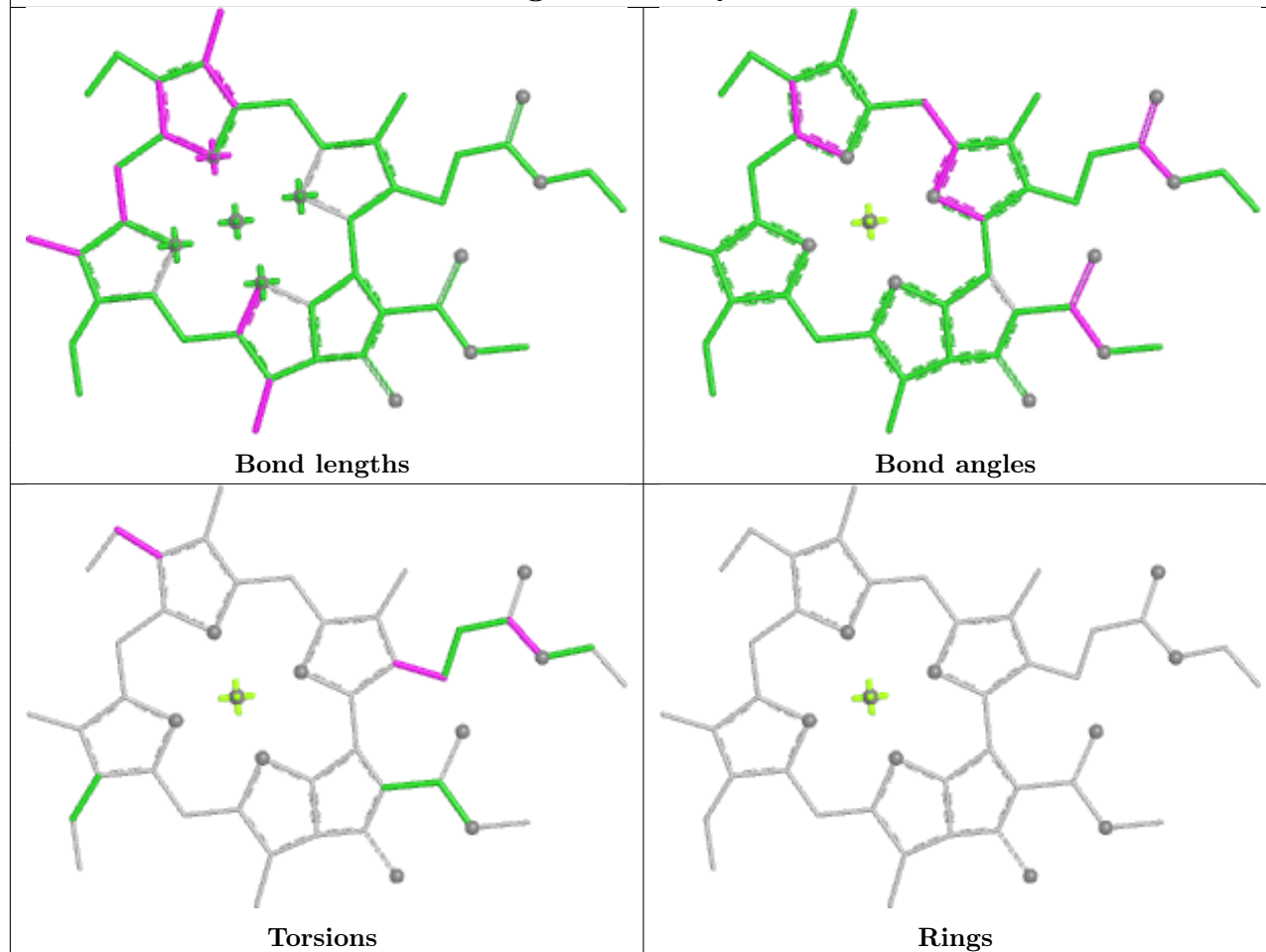
Ligand KC1 E 312



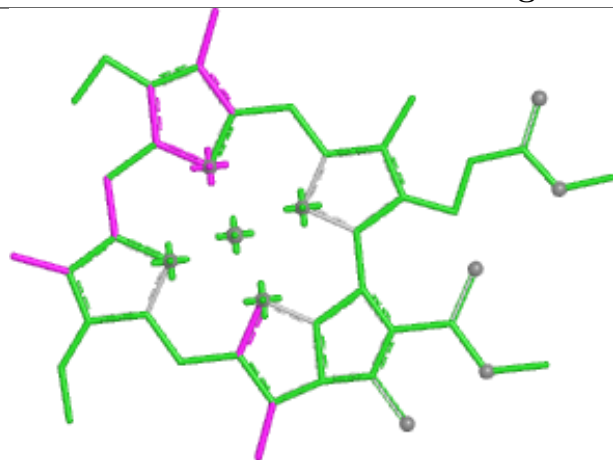
Ligand PID O 305



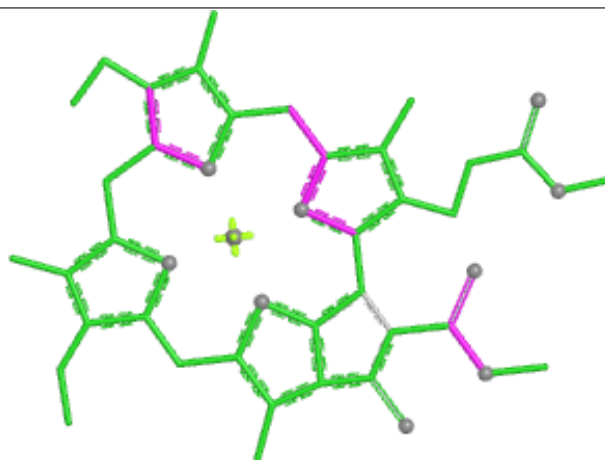
Ligand CLA Q 313



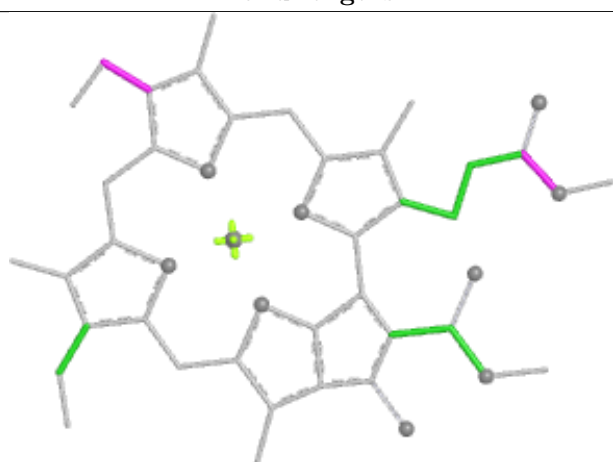
Ligand CLA J 307



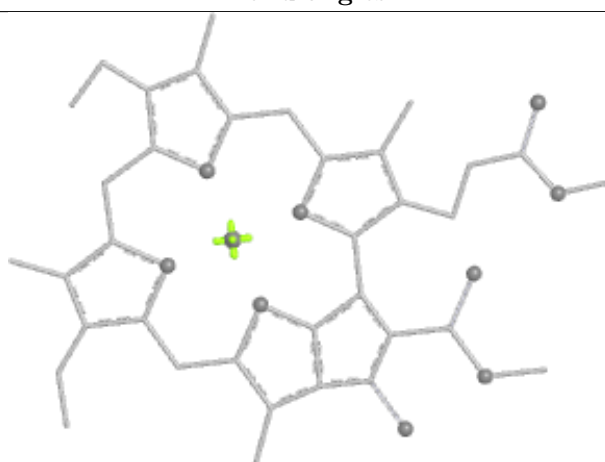
Bond lengths



Bond angles

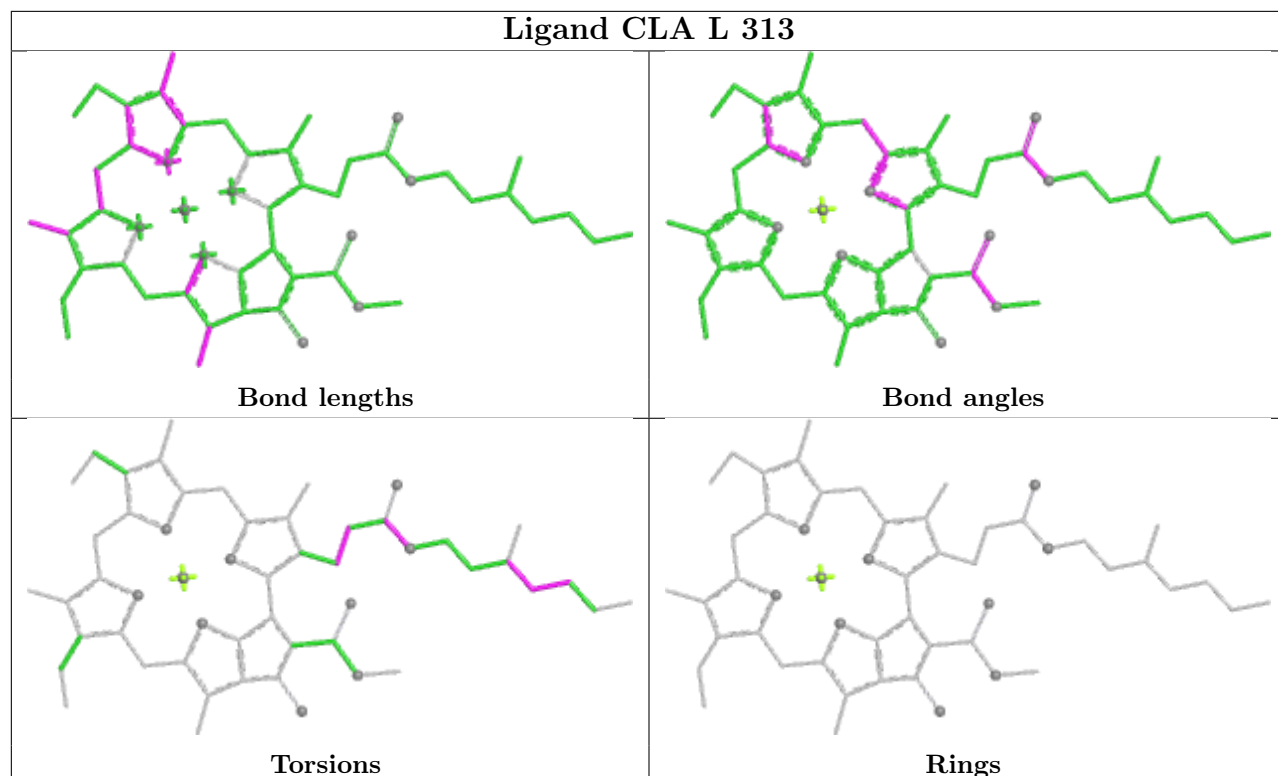


Torsions

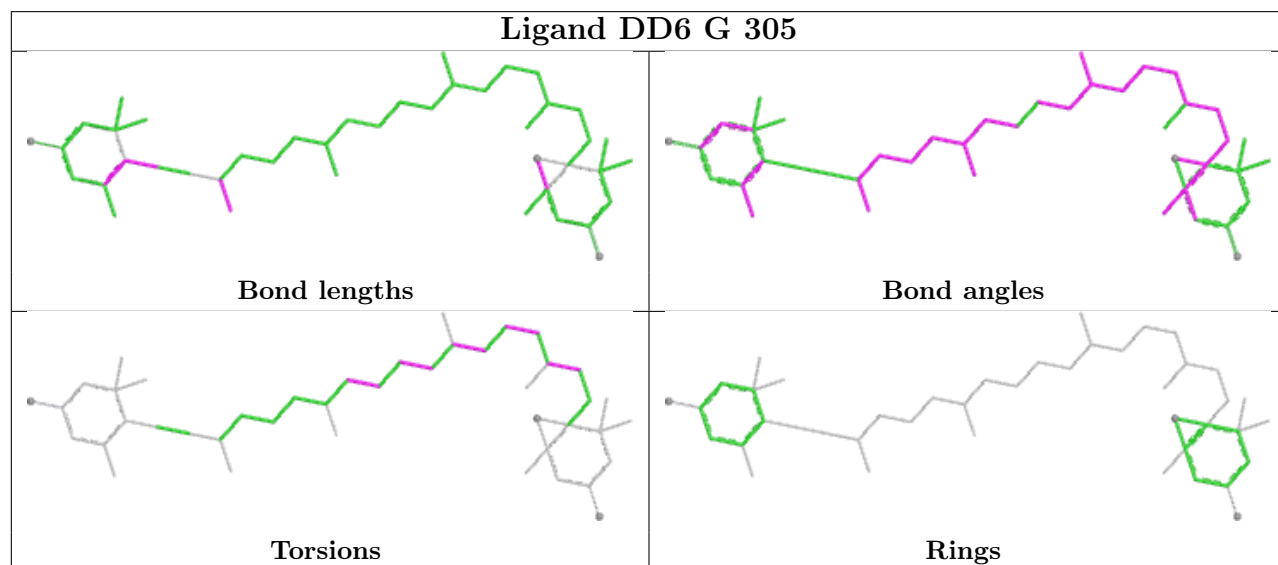


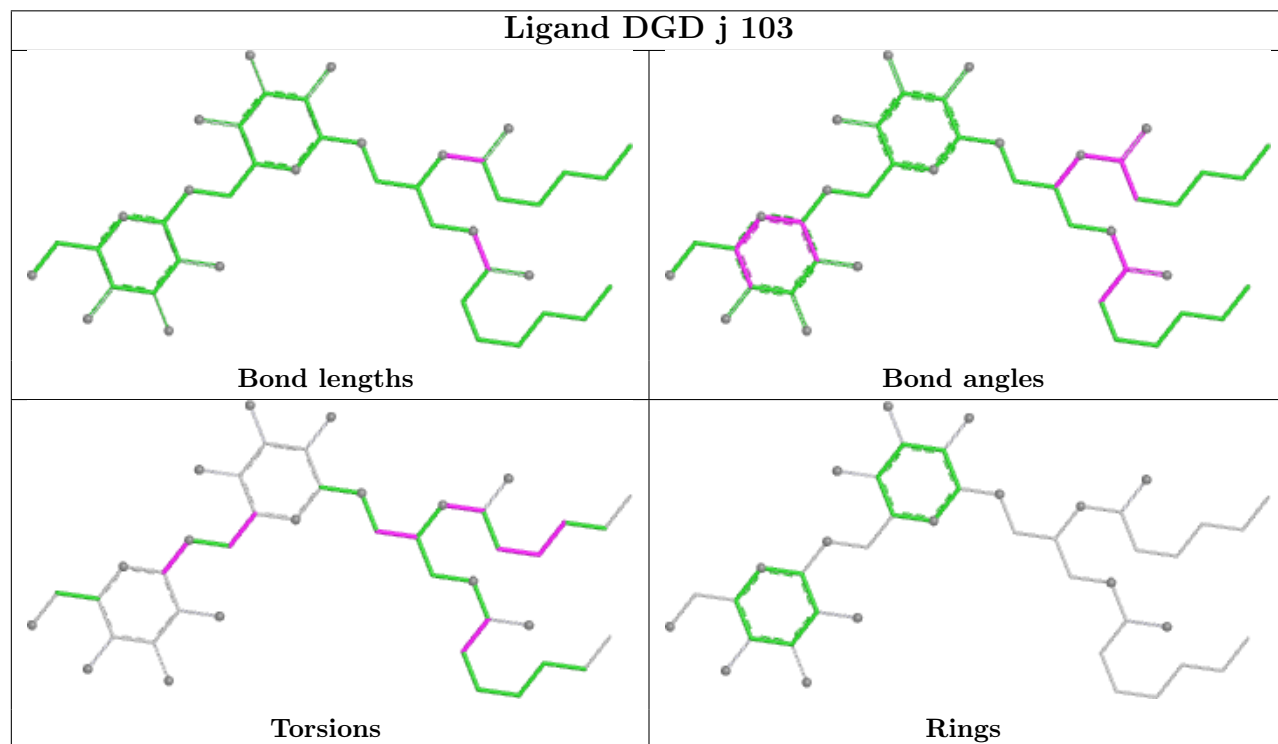
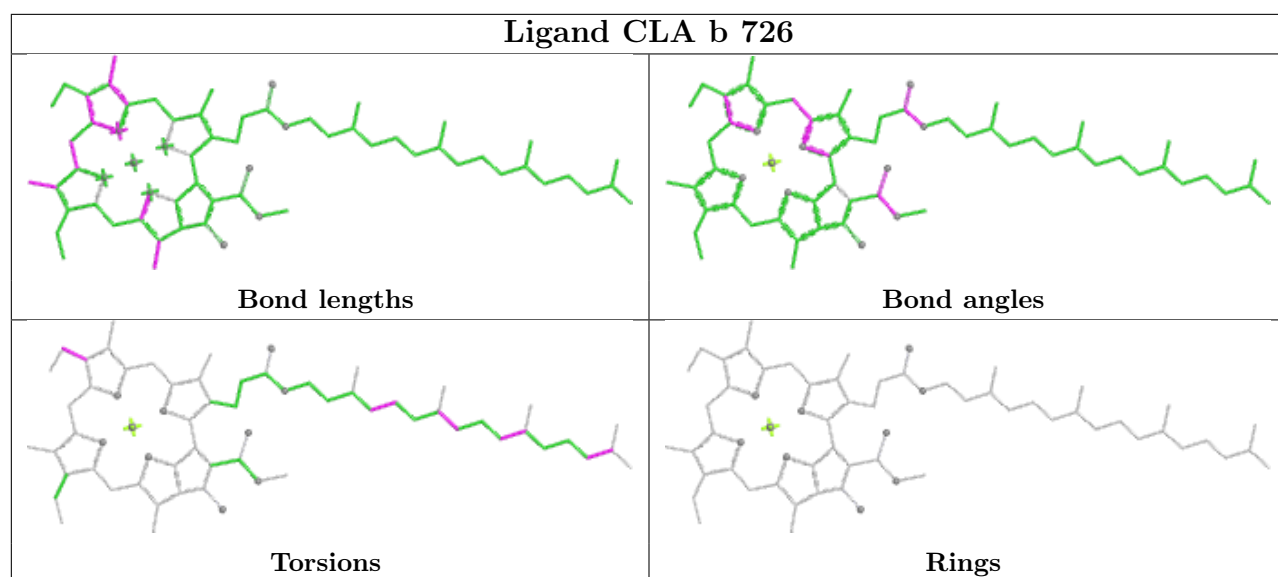
Rings

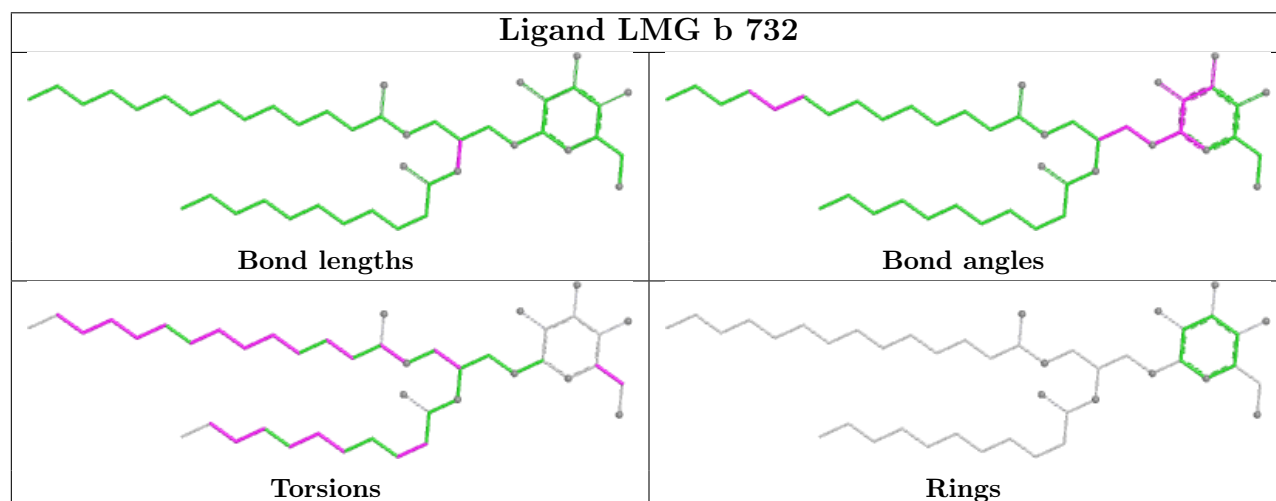
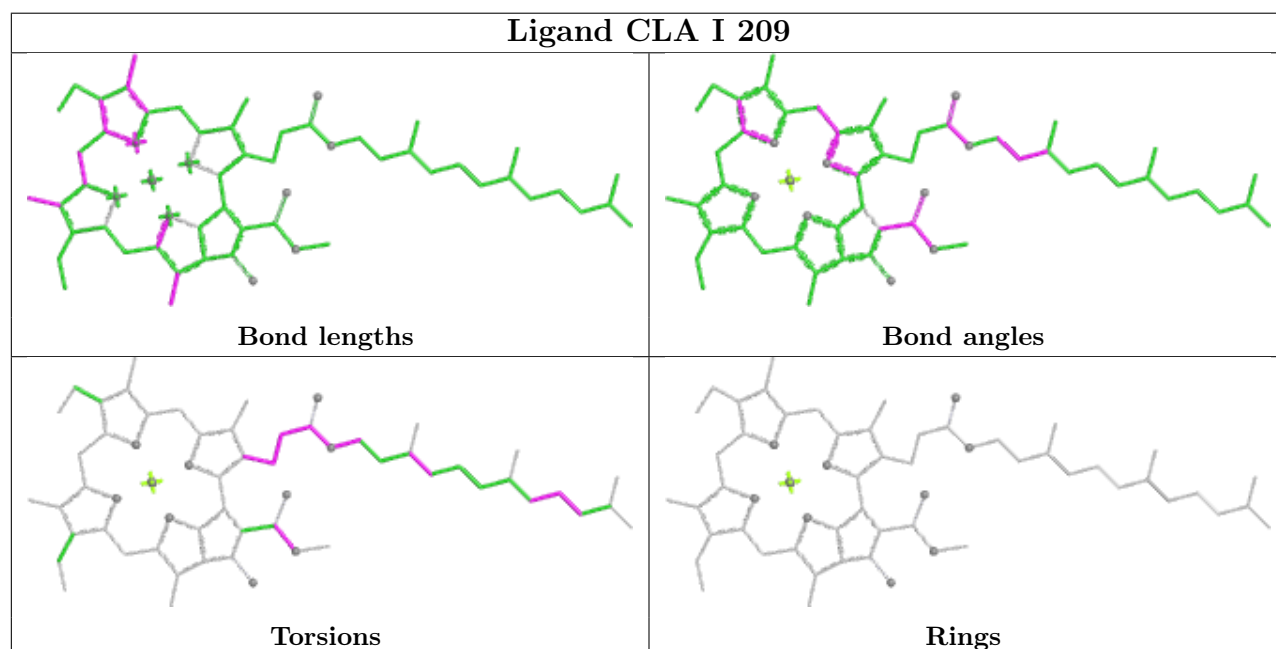
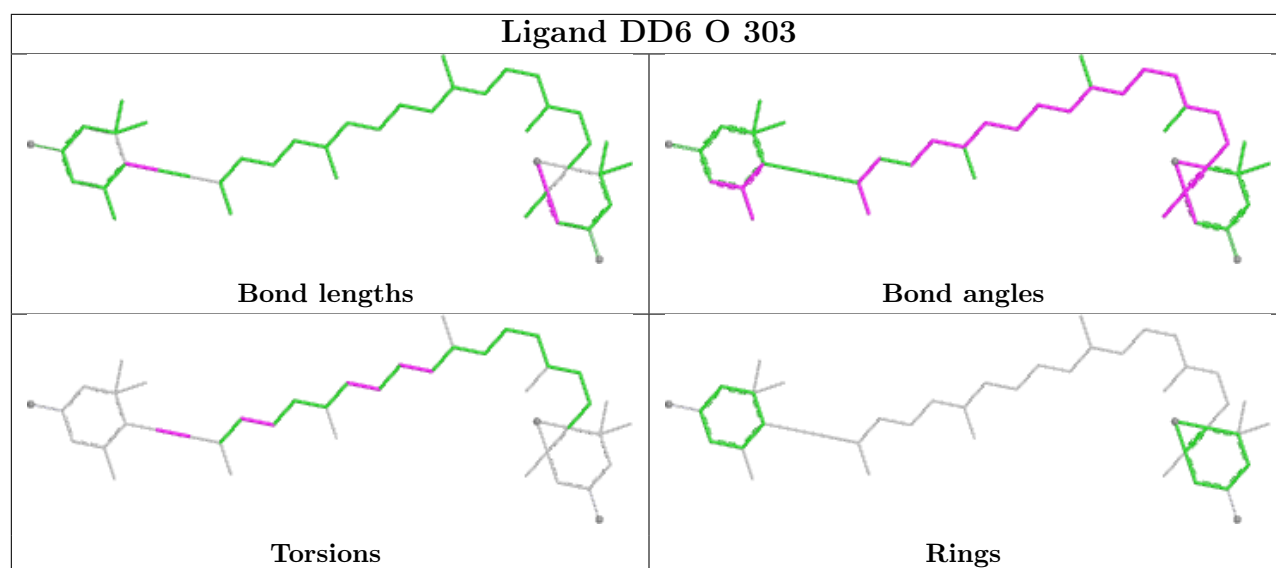
Ligand CLA L 313

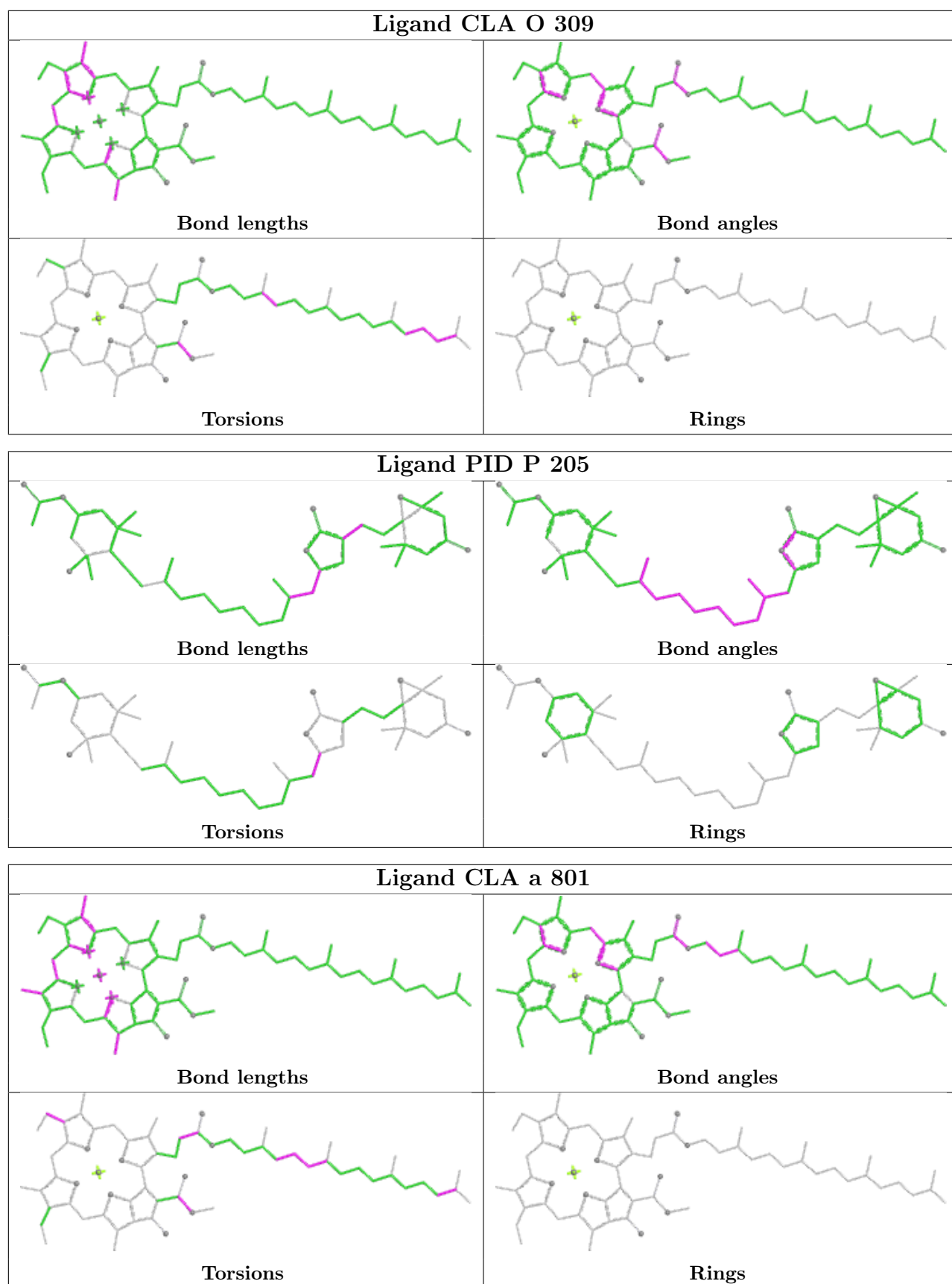


Ligand DD6 G 305

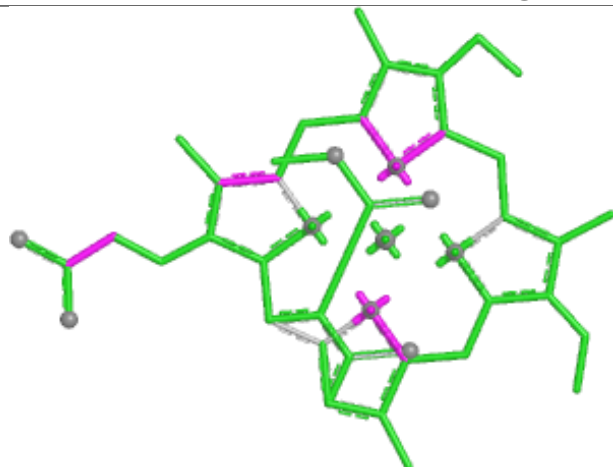




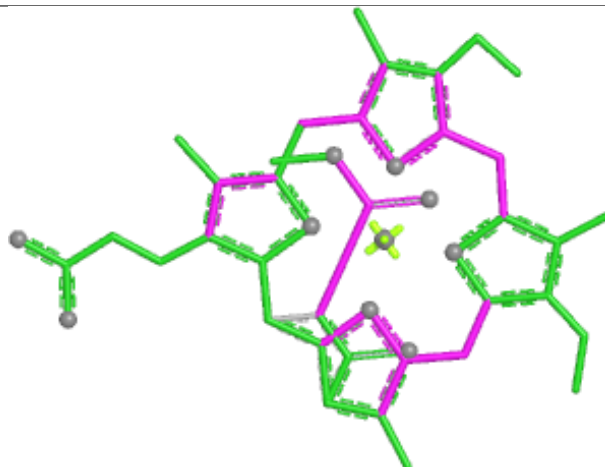




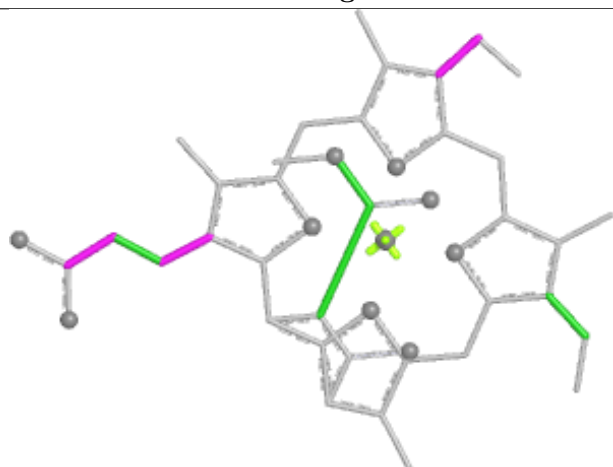
Ligand KC1 O 310



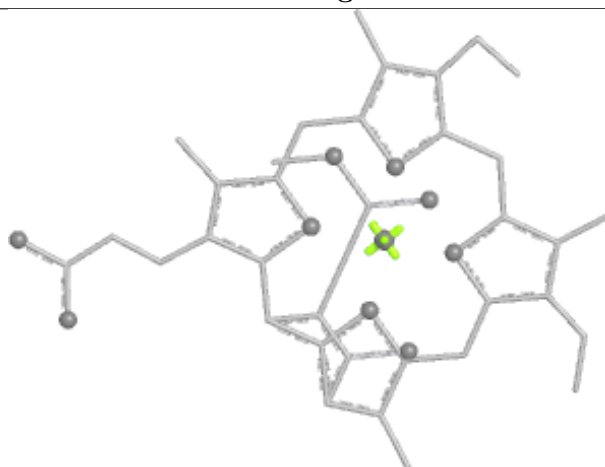
Bond lengths



Bond angles

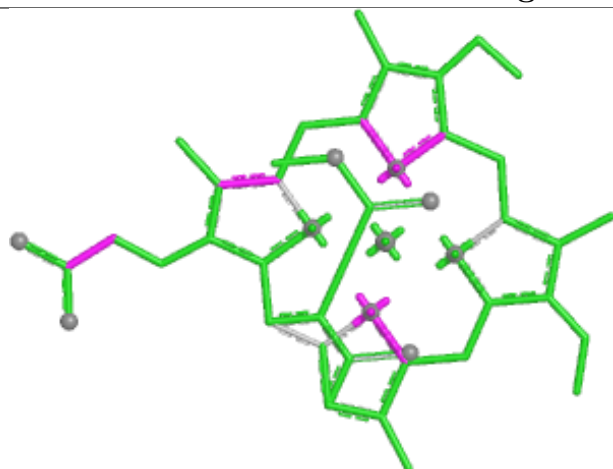


Torsions

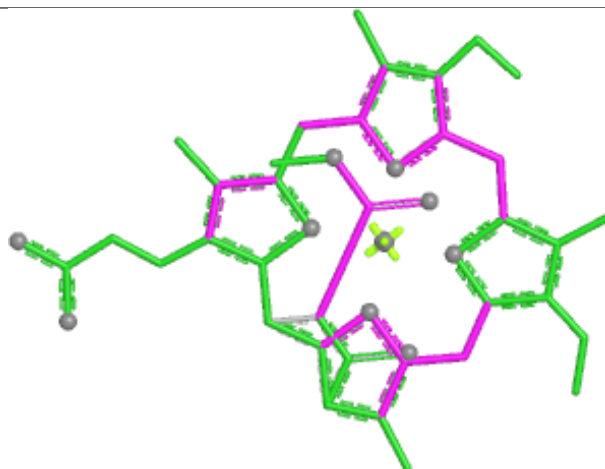


Rings

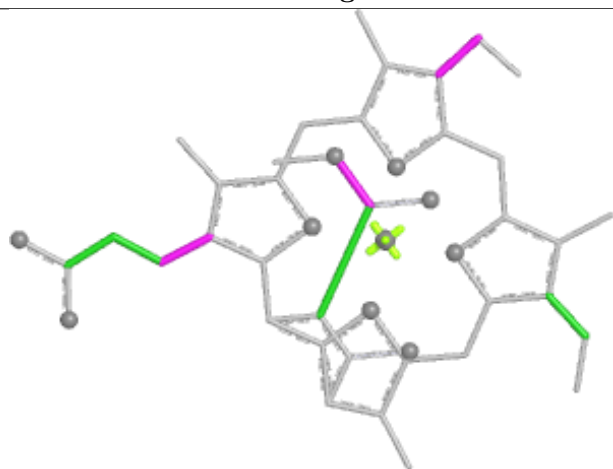
Ligand KC1 F 314



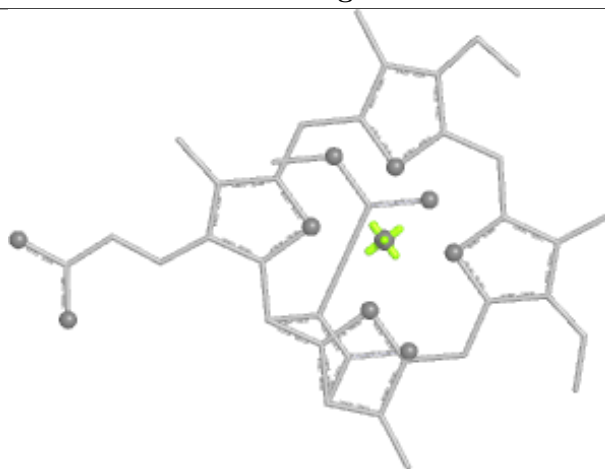
Bond lengths



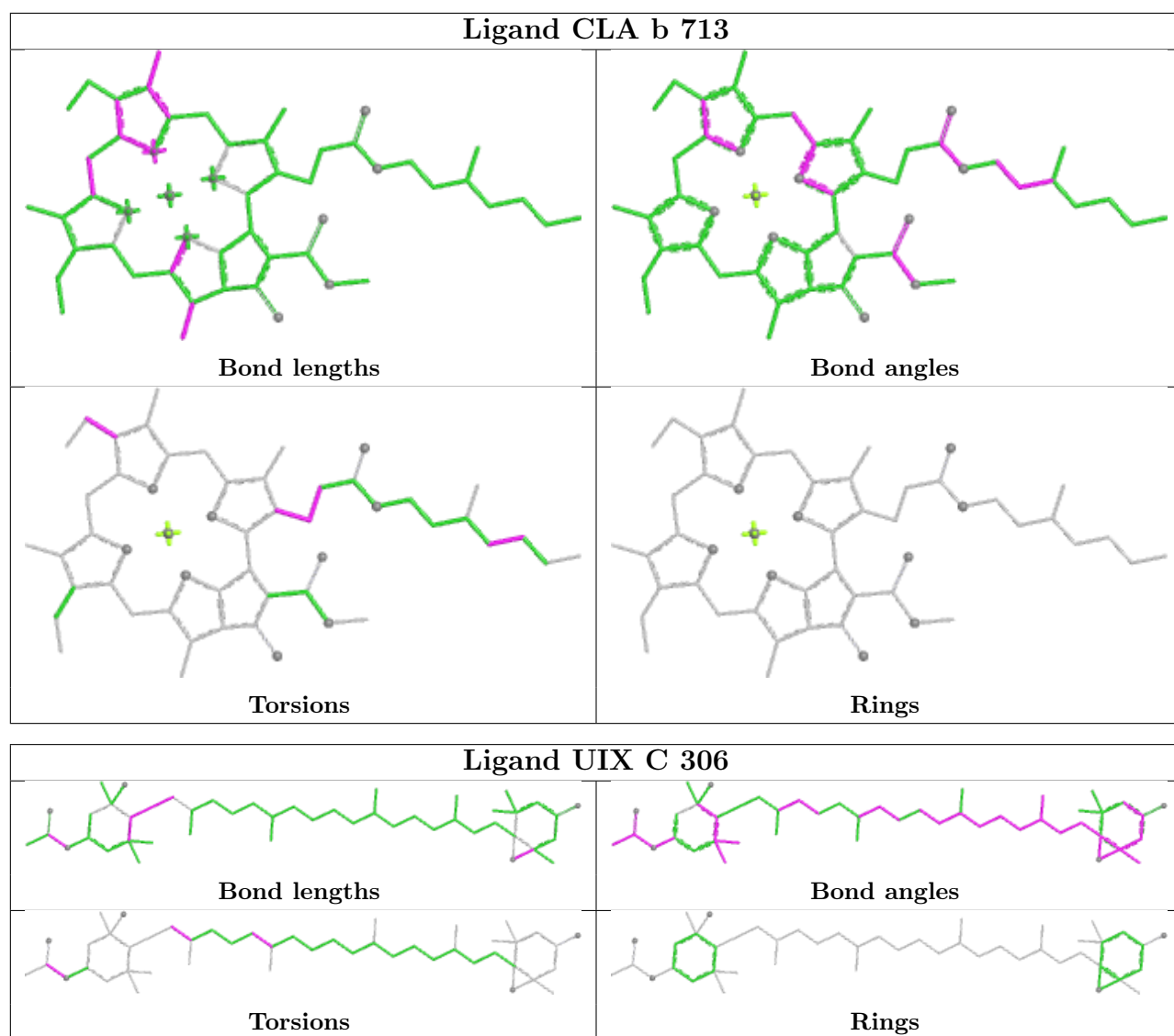
Bond angles

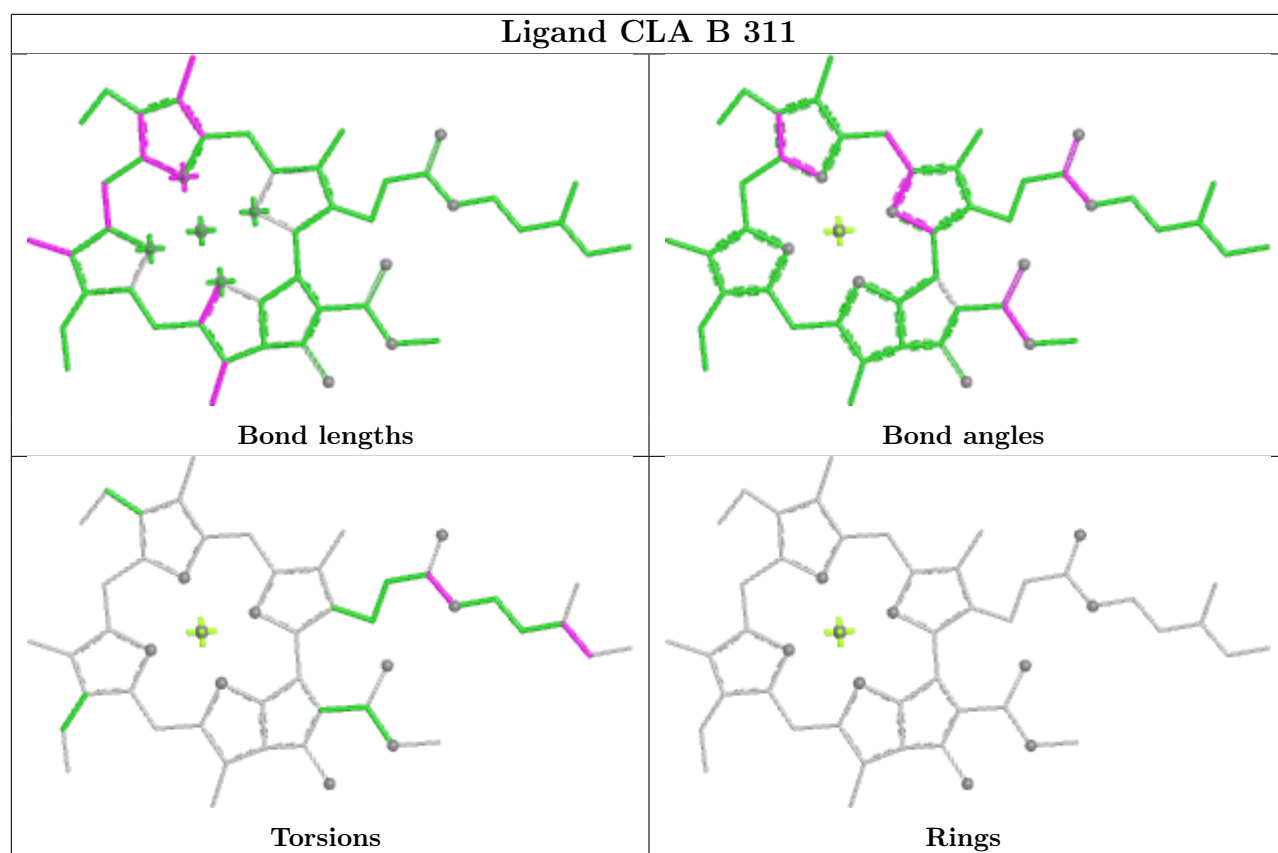


Torsions

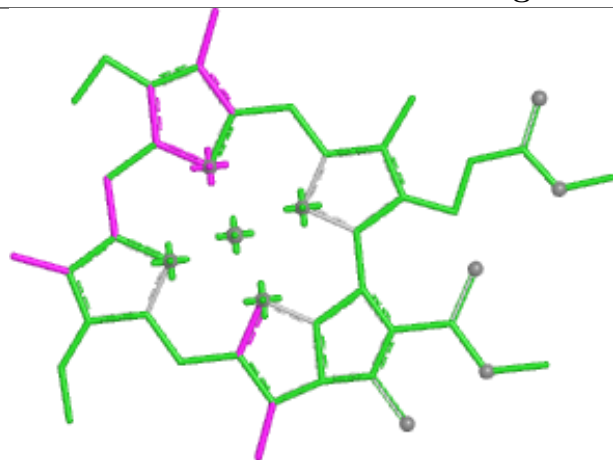


Rings

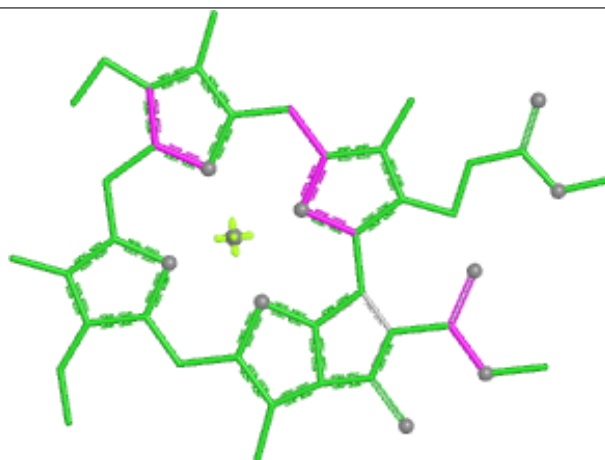




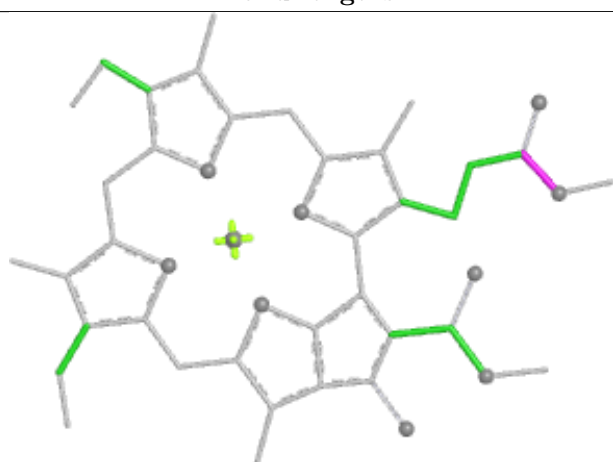
Ligand CLA K 208



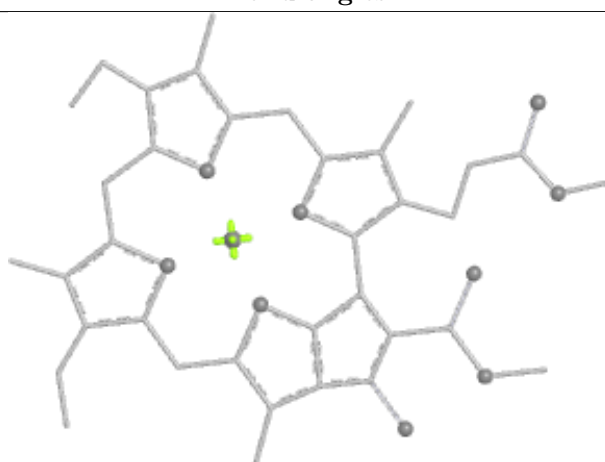
Bond lengths



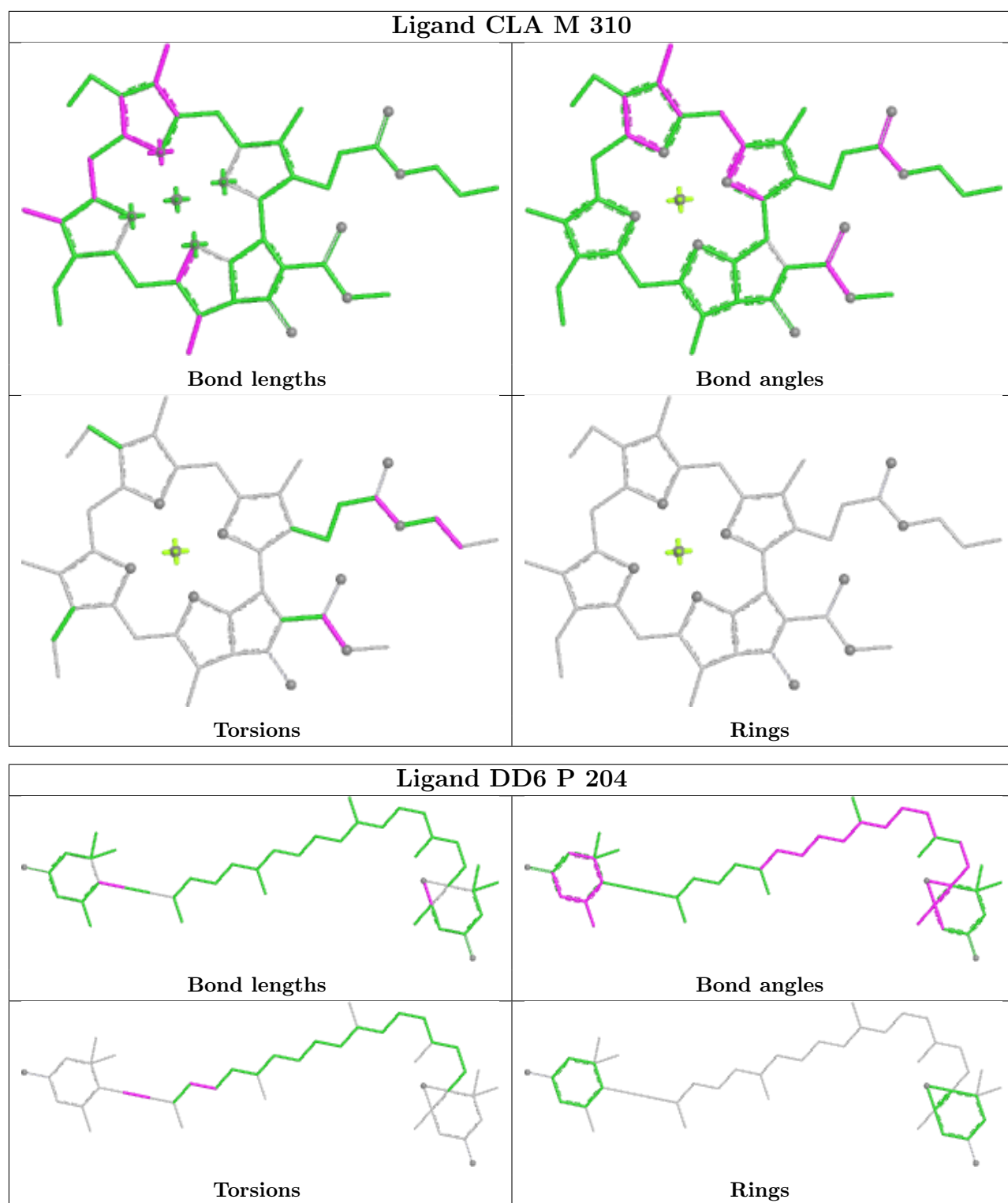
Bond angles



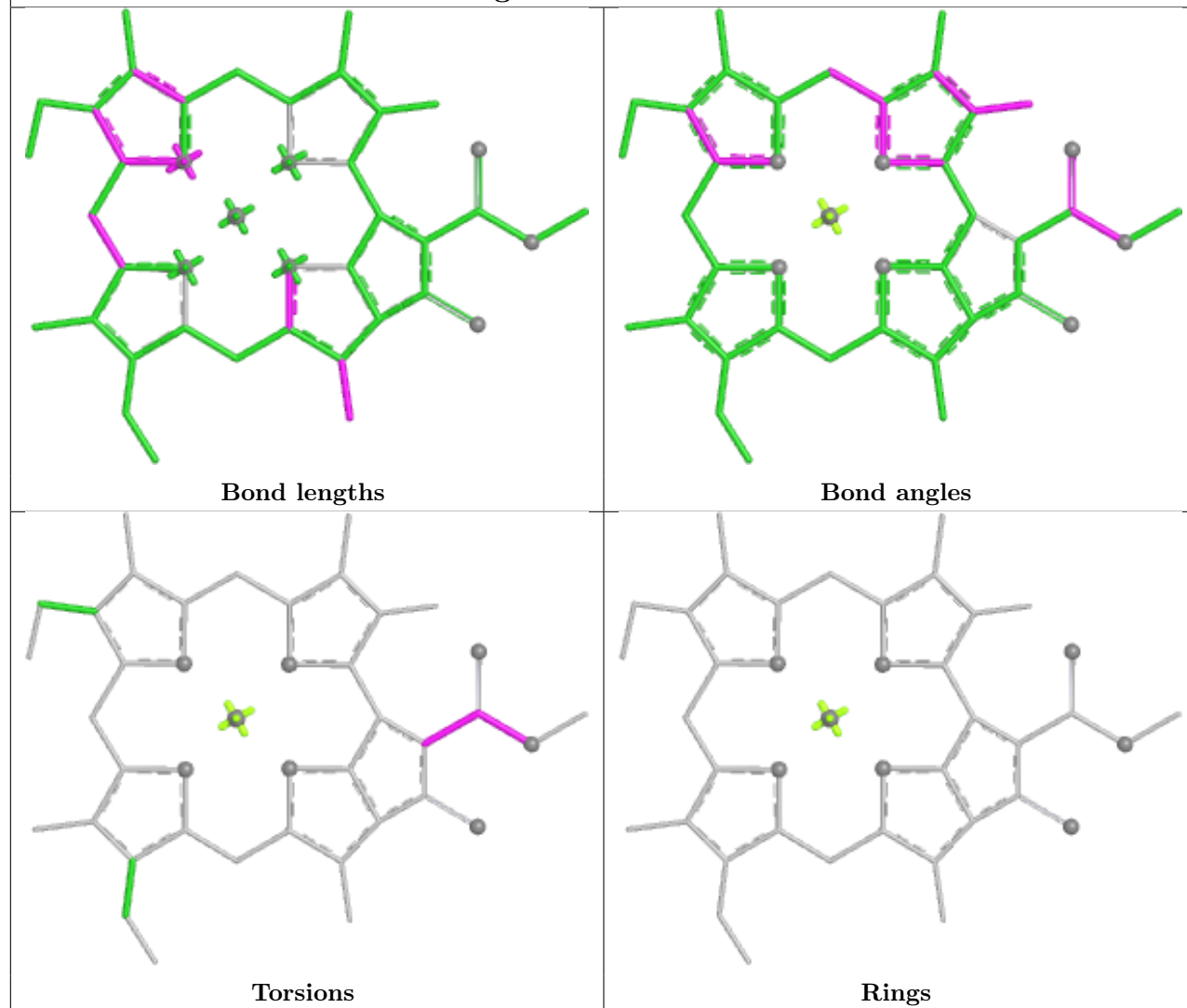
Torsions



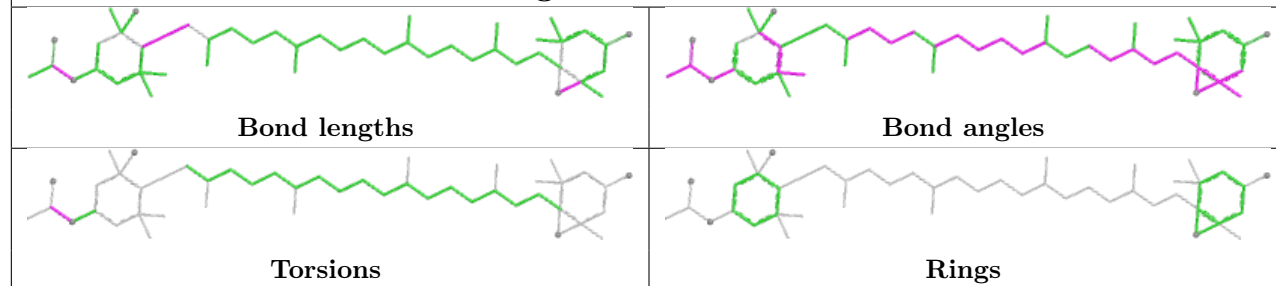
Rings



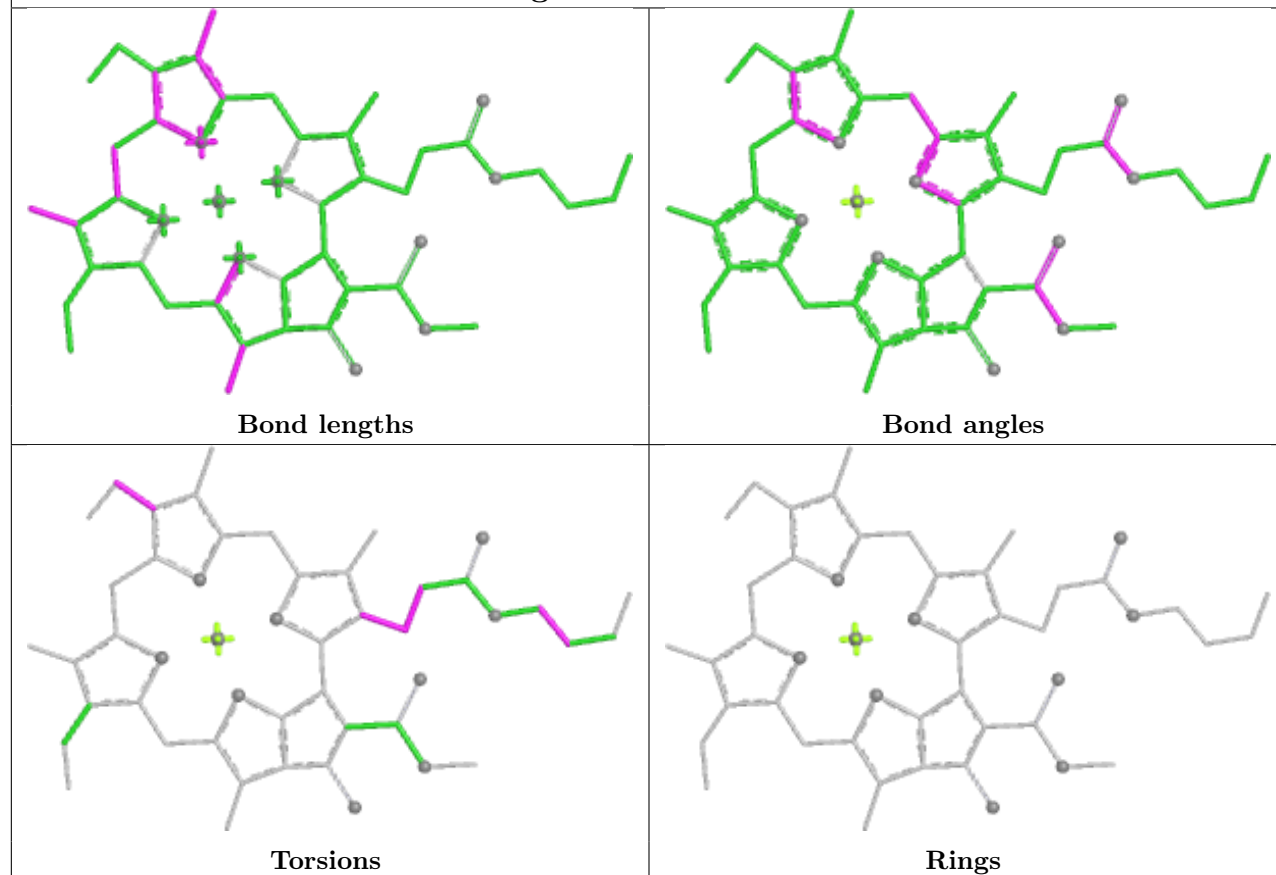
Ligand CLA H 315



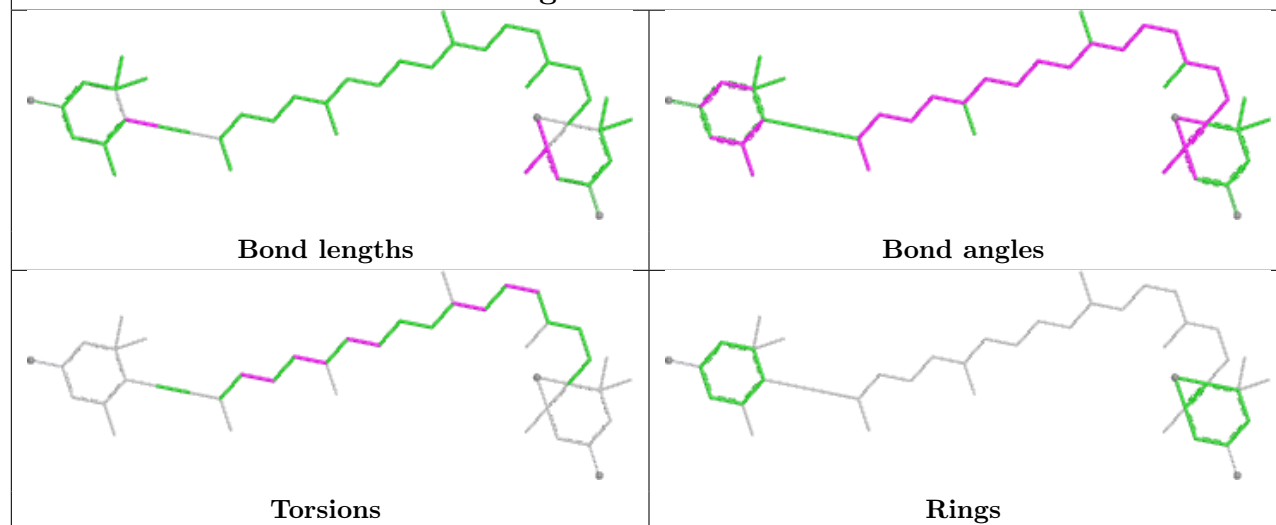
Ligand UIX B 304



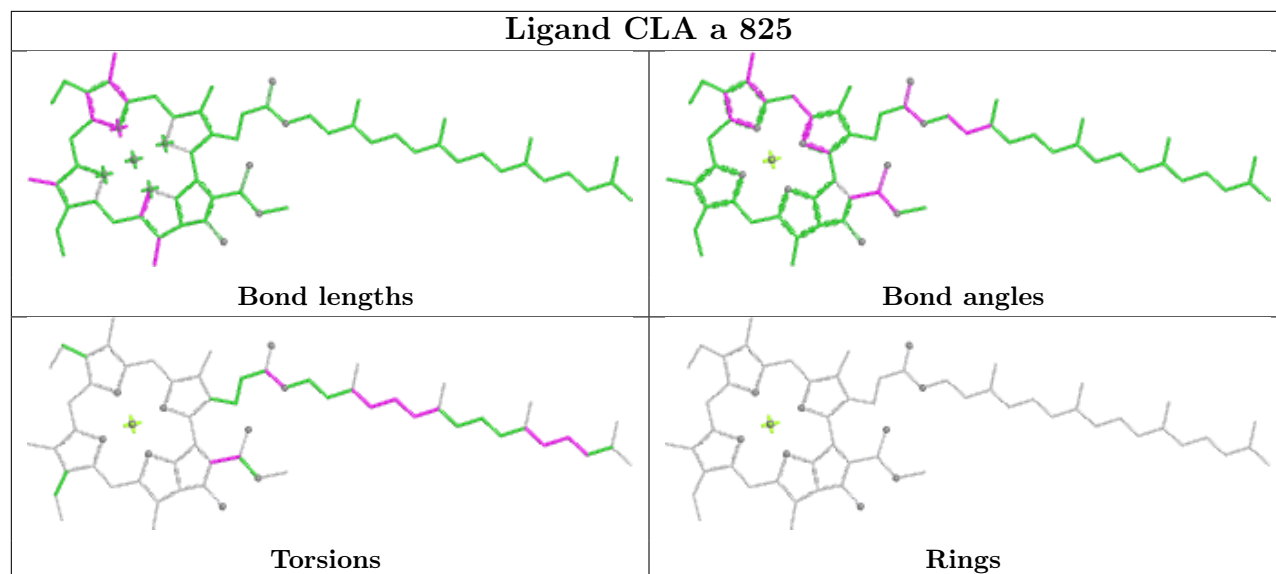
Ligand CLA K 207



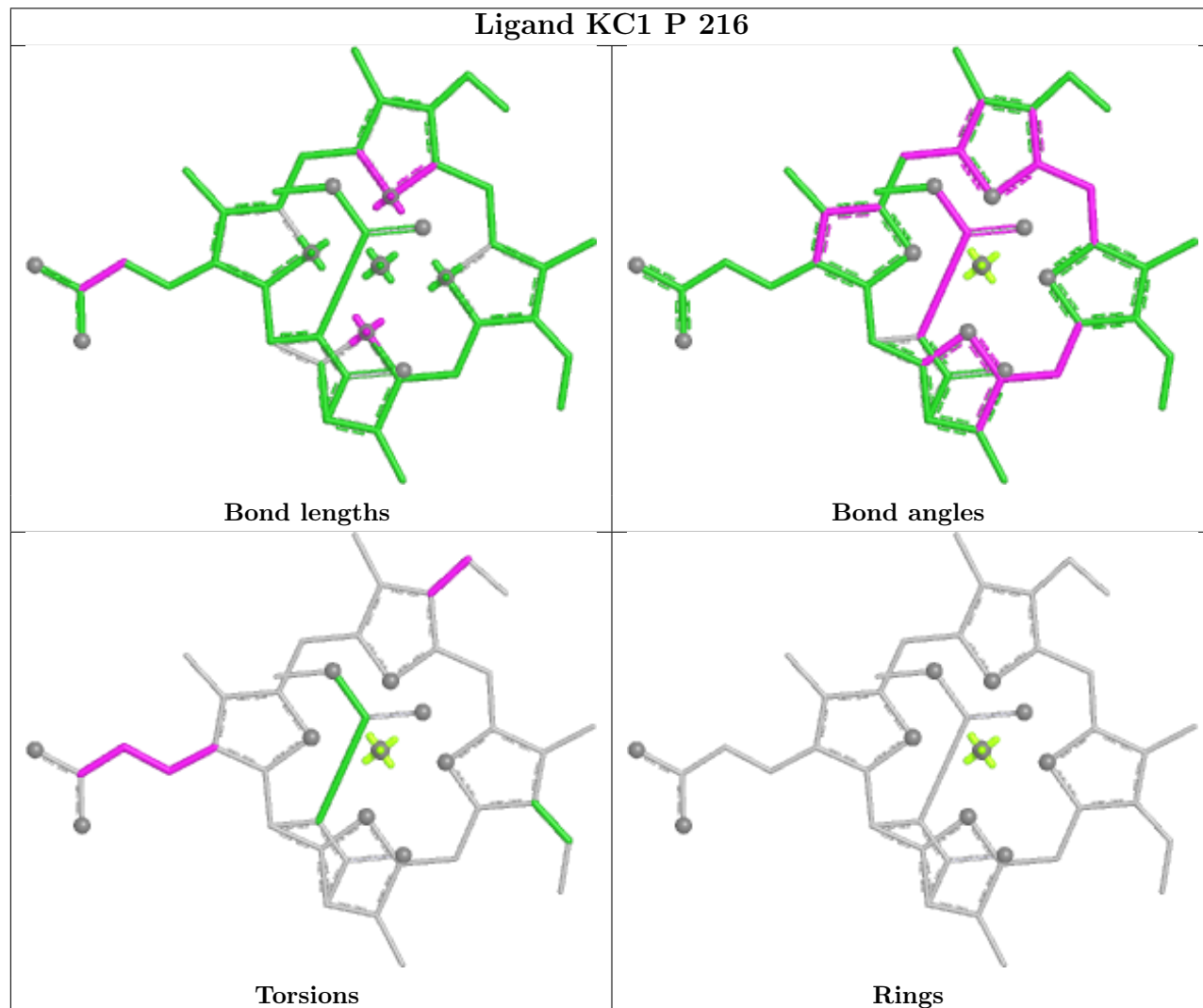
Ligand DD6 I 203

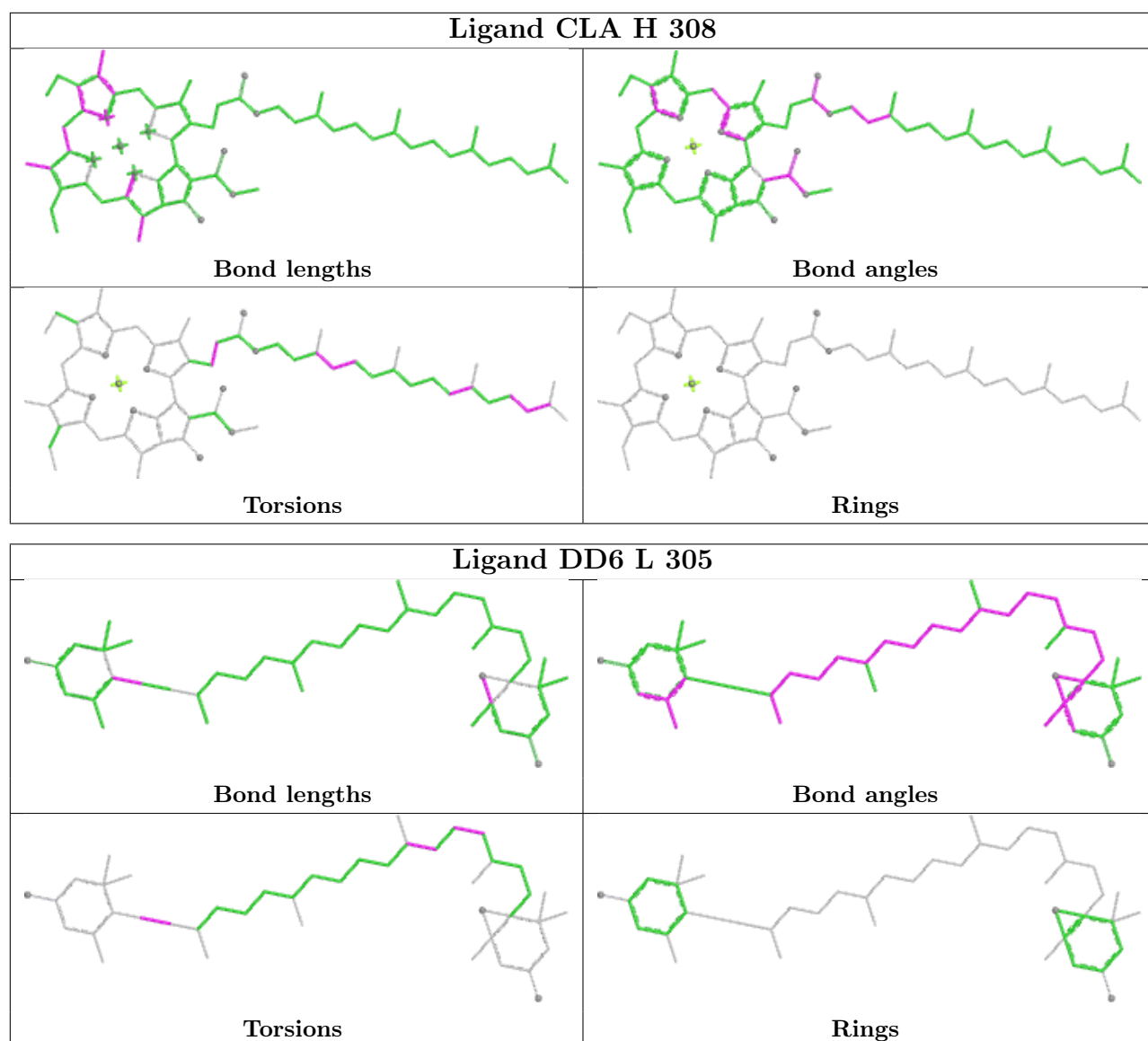


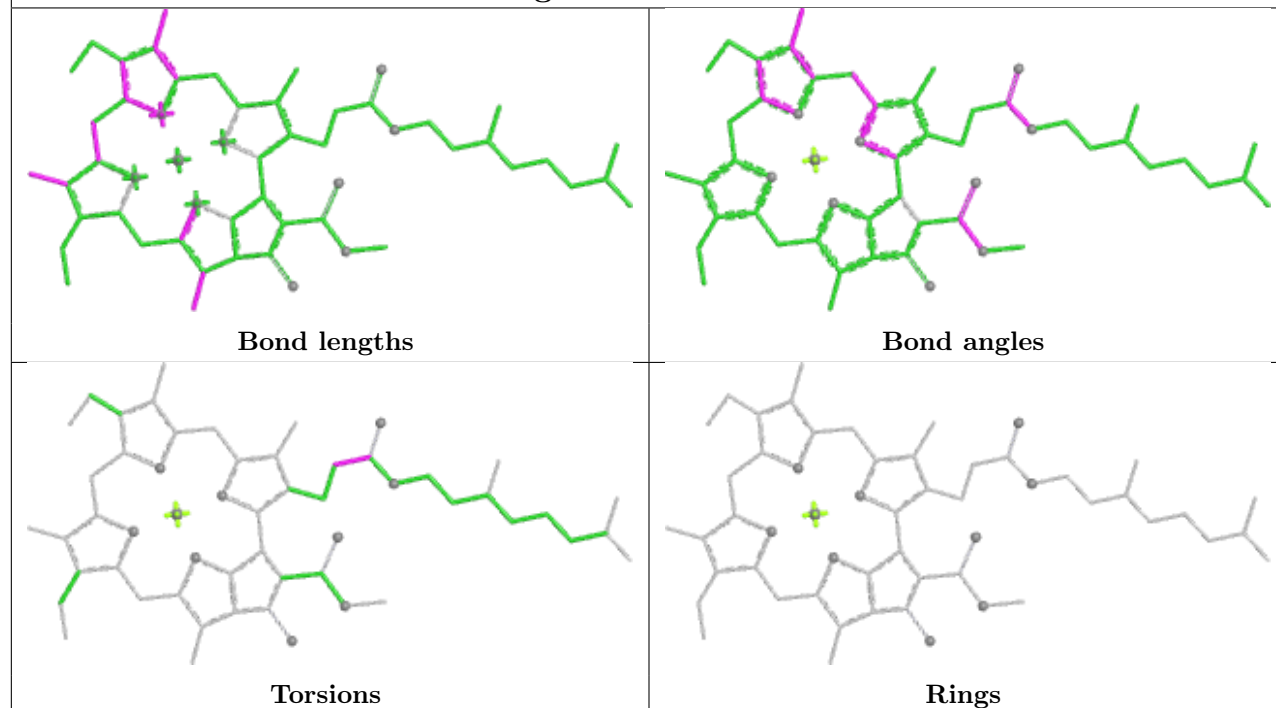
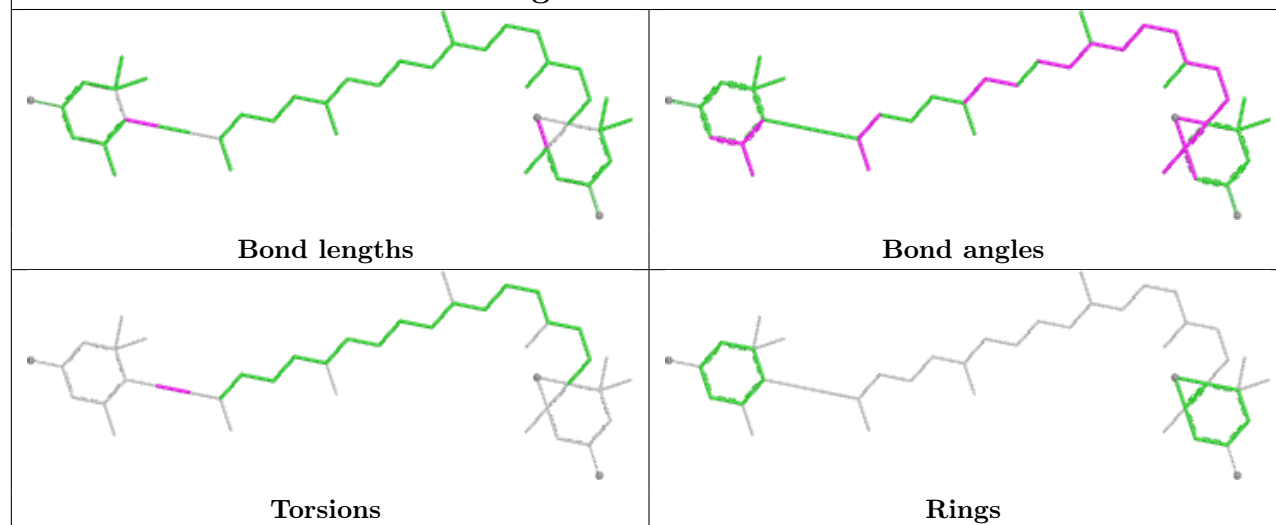
Ligand CLA a 825

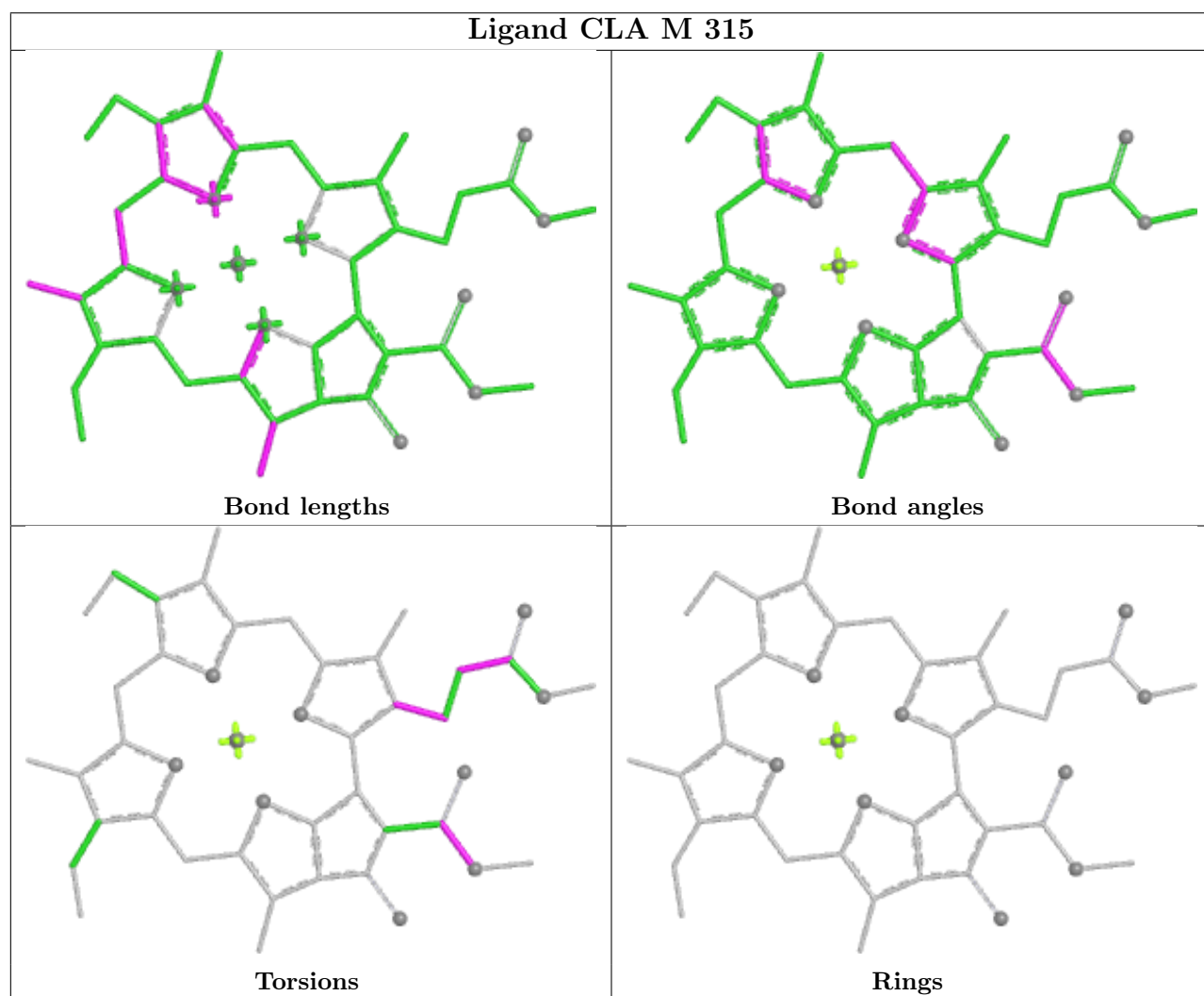
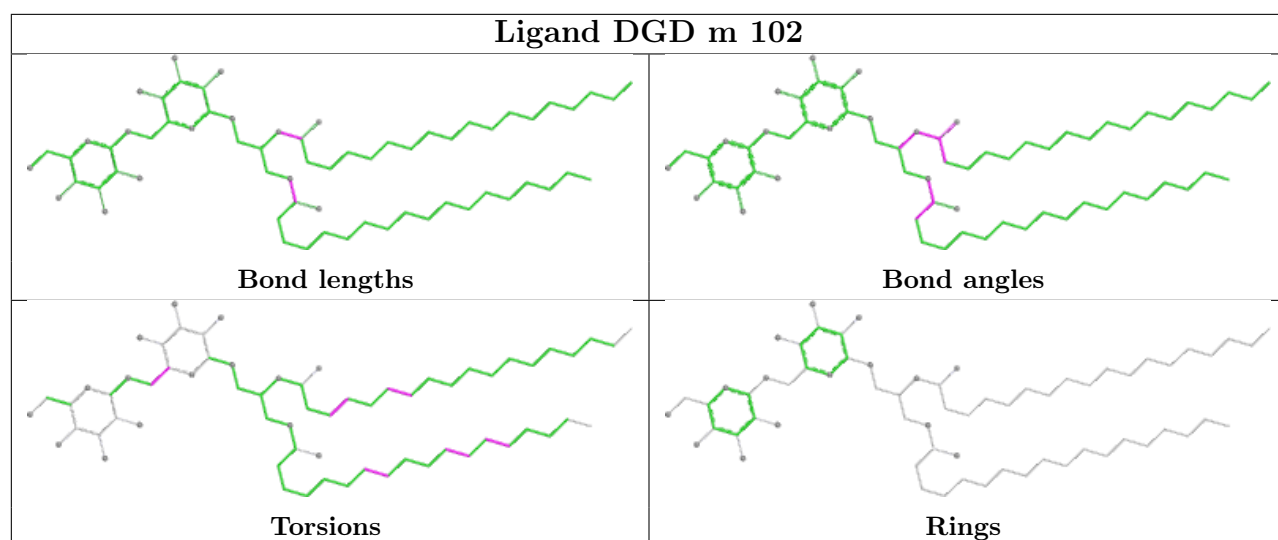


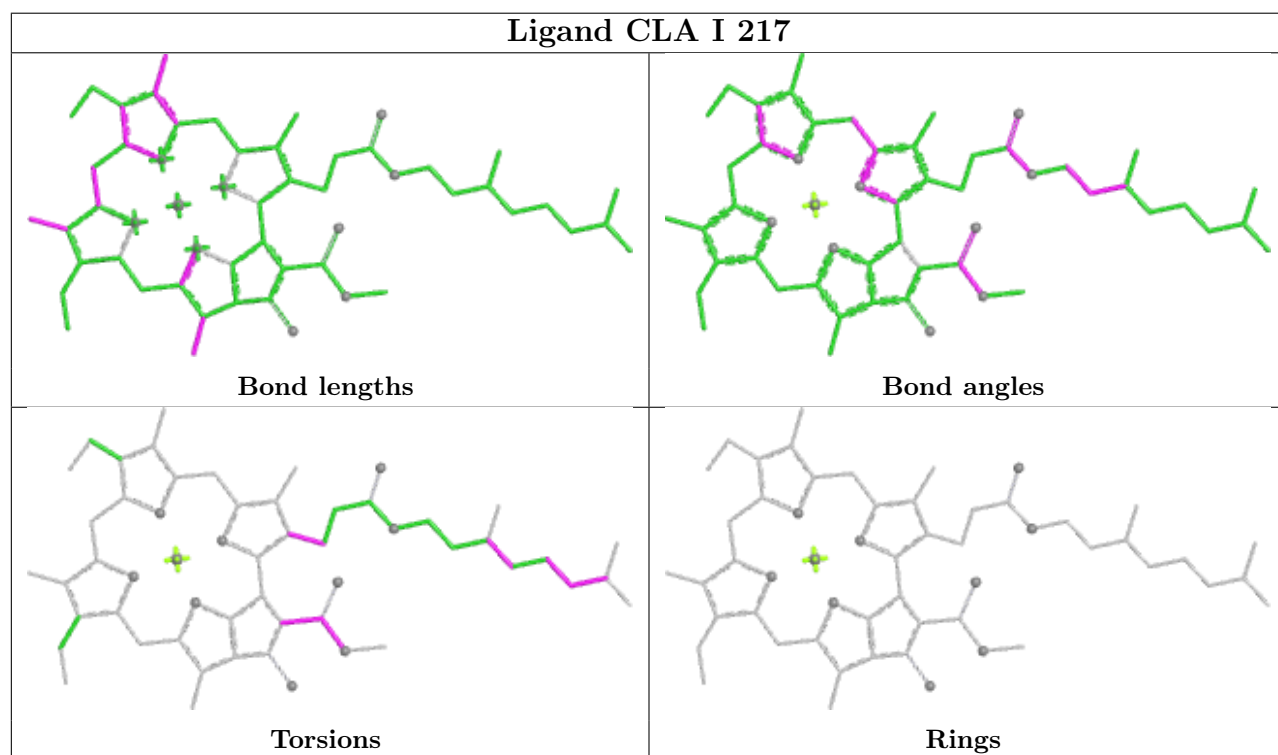
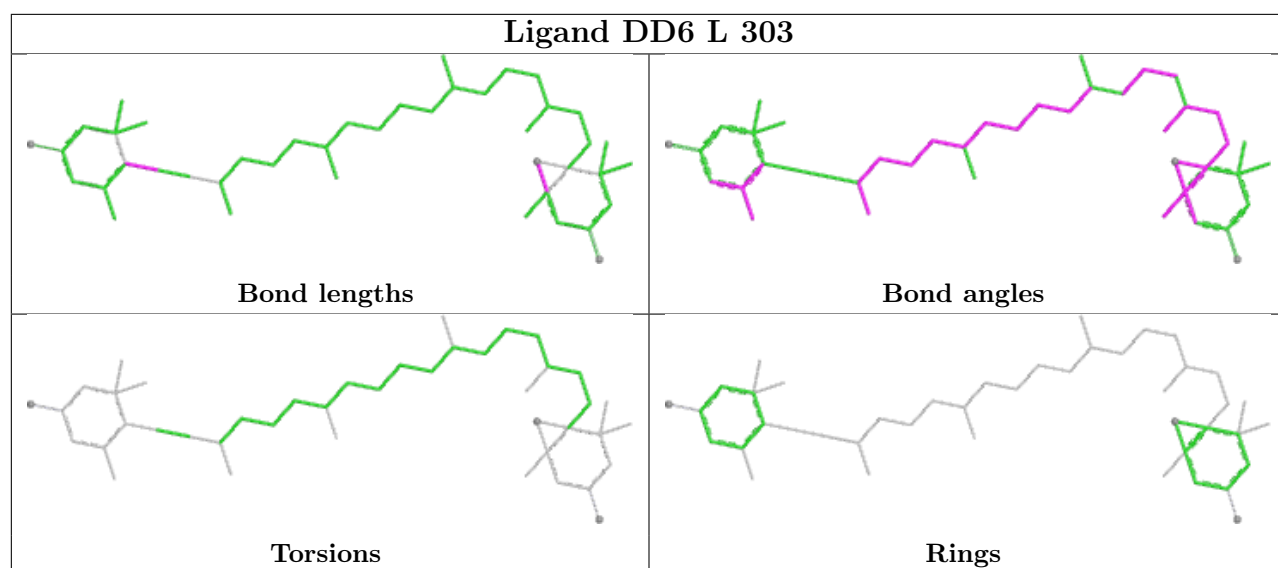
Ligand KC1 P 216



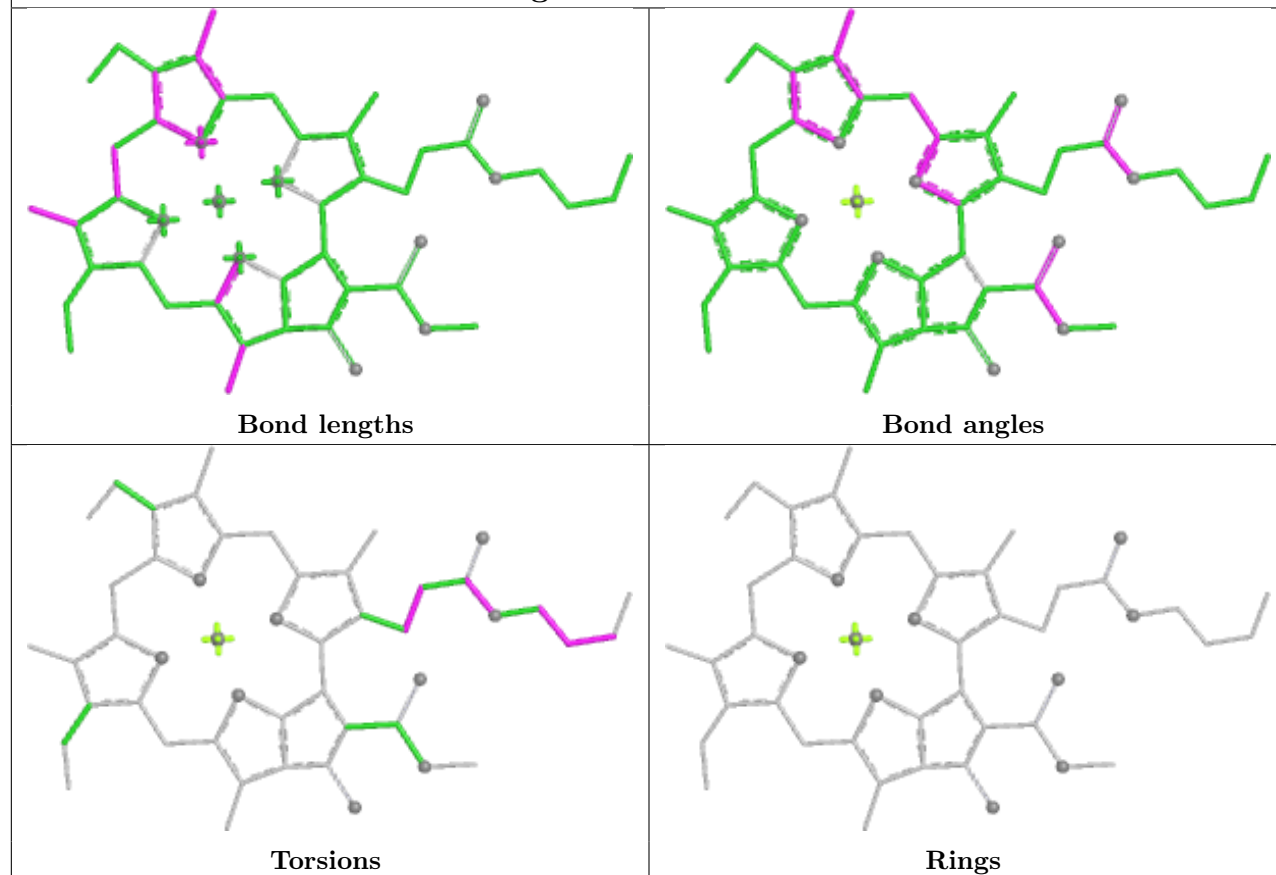


Ligand CLA L 309**Ligand DD6 N 303**

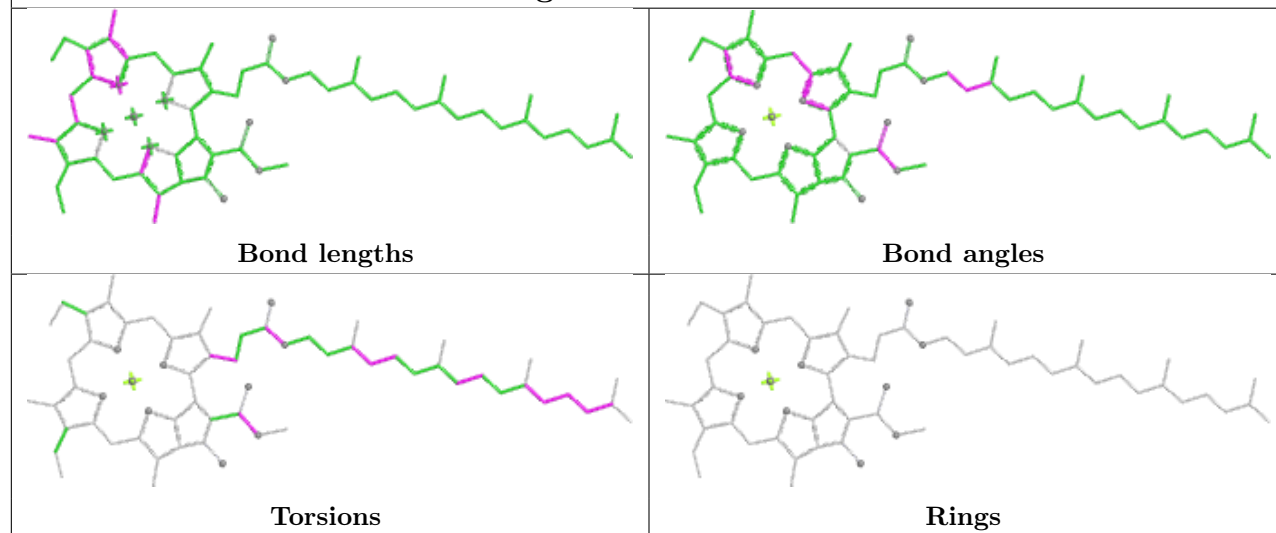




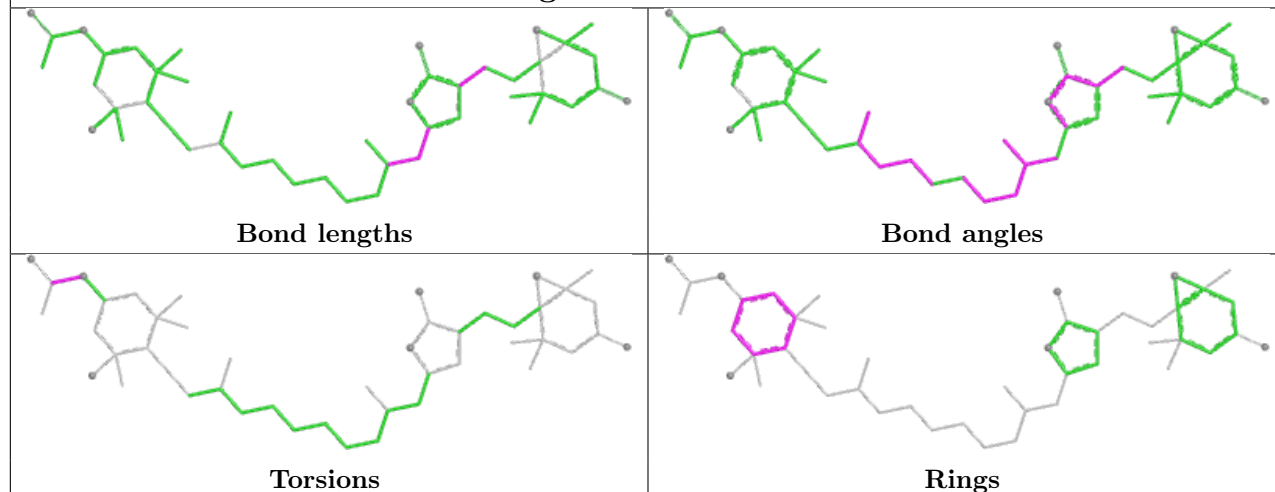
Ligand CLA G 301



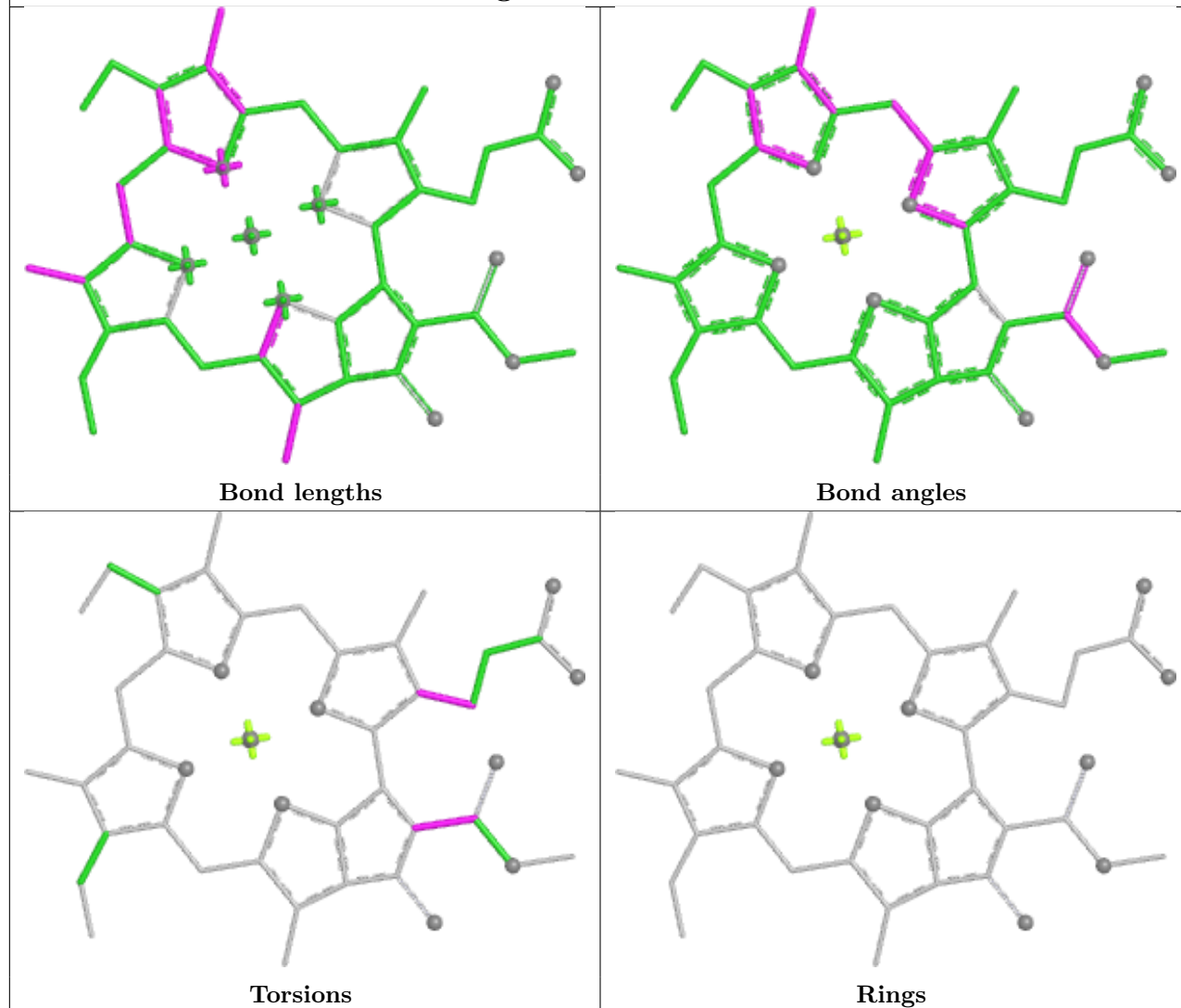
Ligand CLA J 306

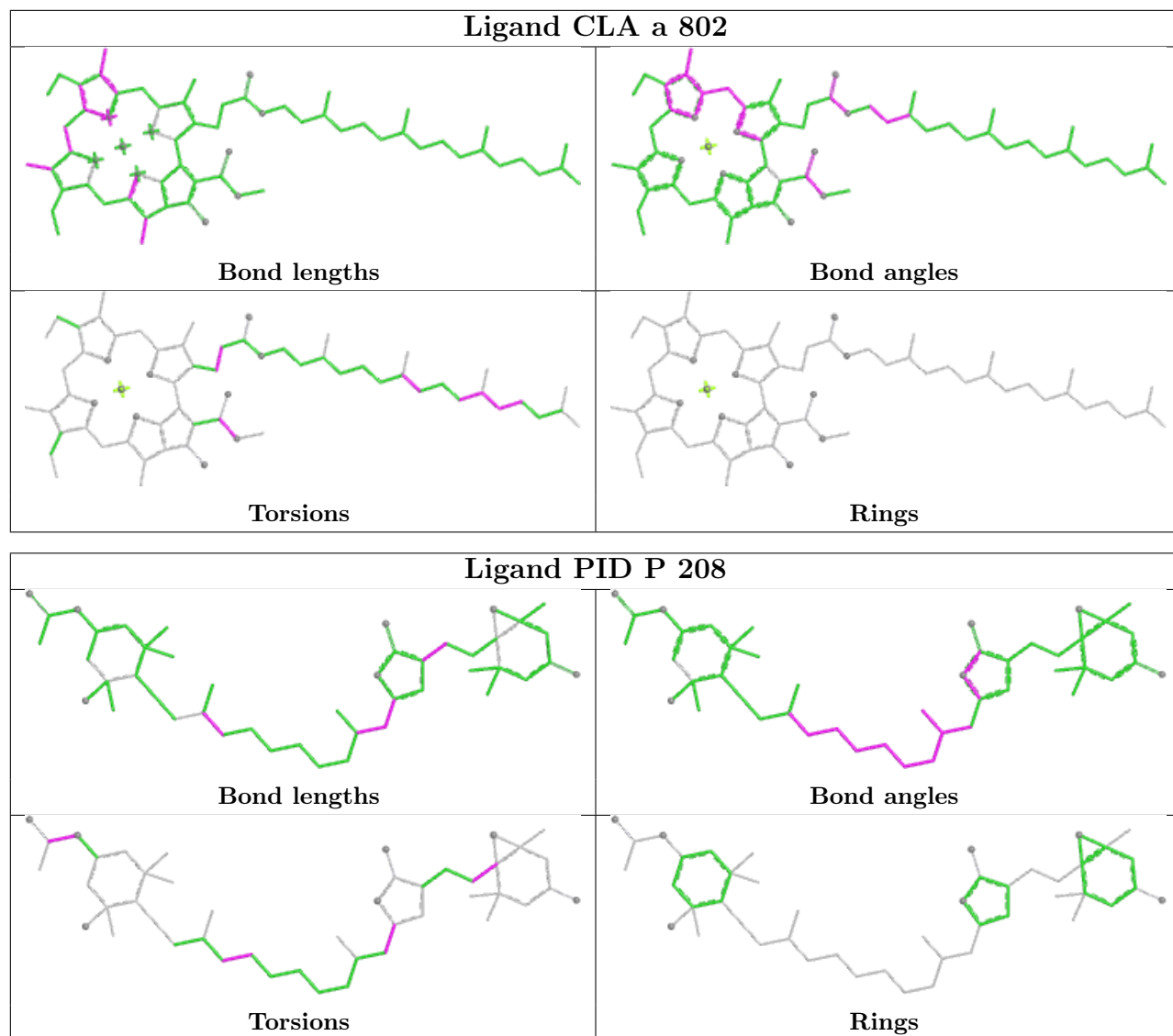


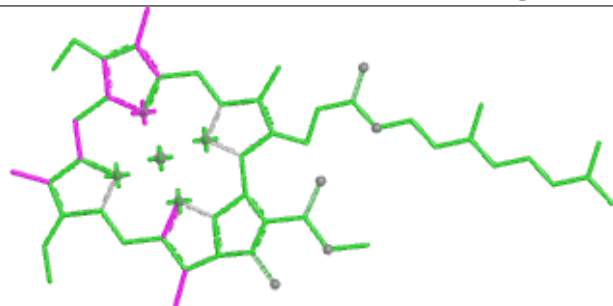
Ligand PID h 204



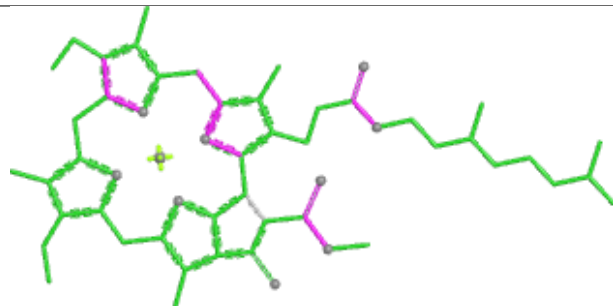
Ligand CLA a 815



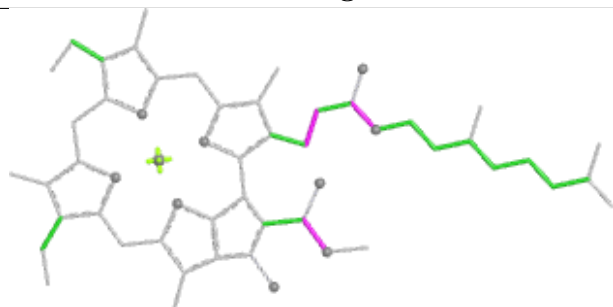


Ligand CLA A 207

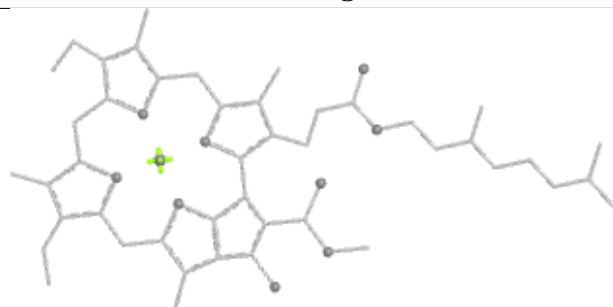
Bond lengths



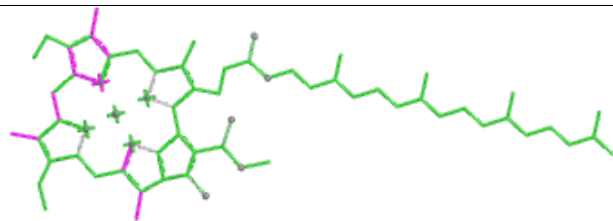
Bond angles



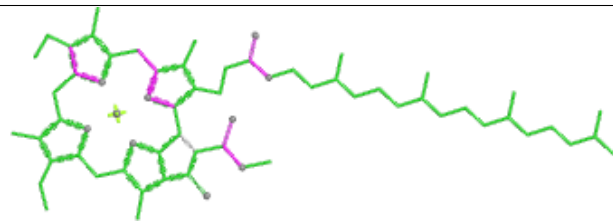
Torsions



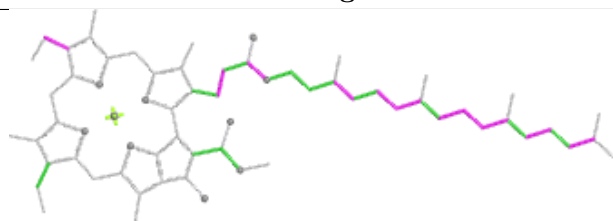
Rings

Ligand CLA G 312

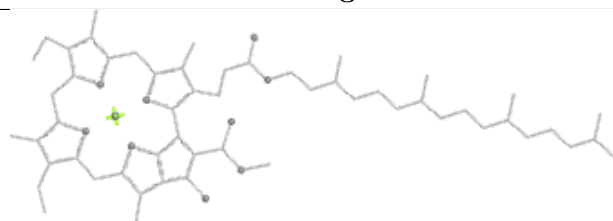
Bond lengths



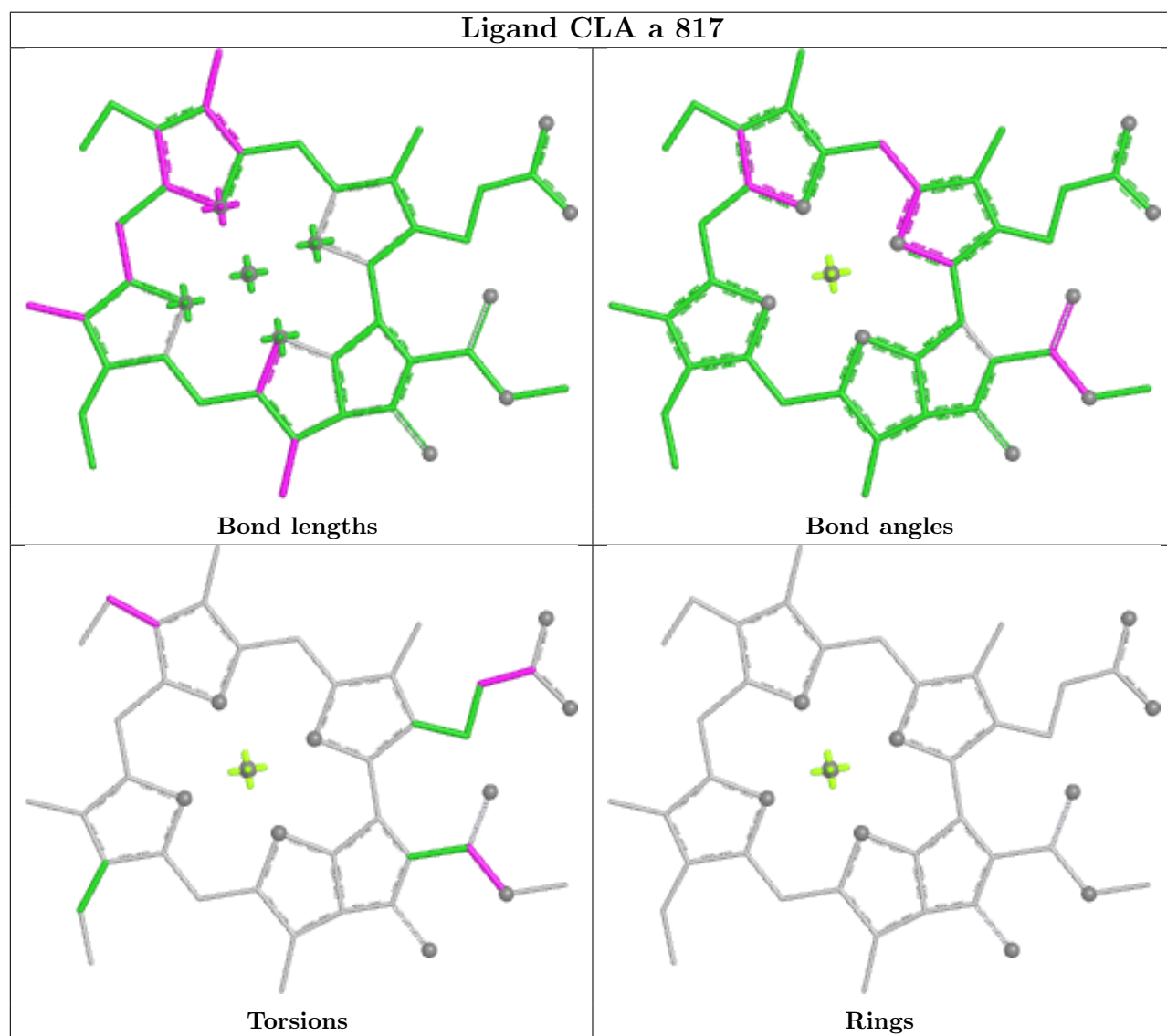
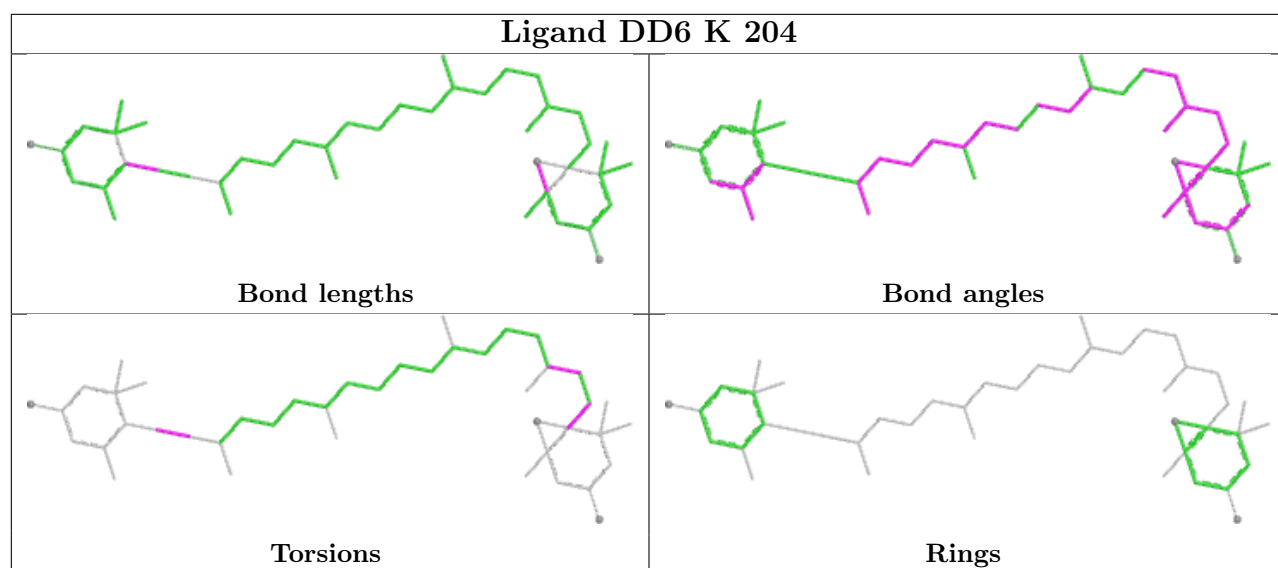
Bond angles



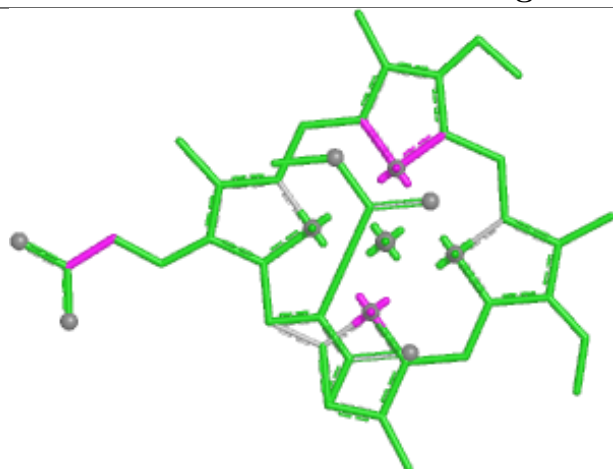
Torsions



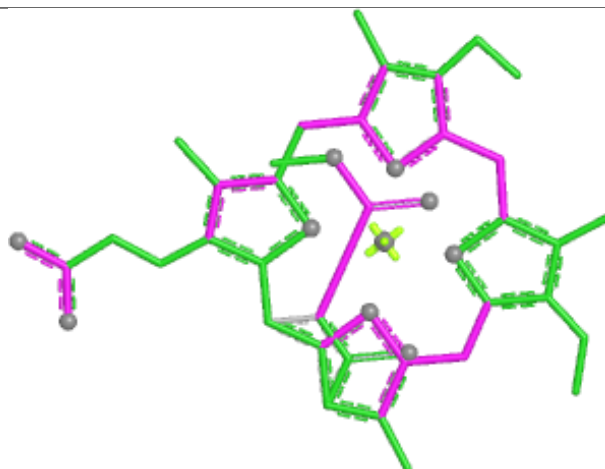
Rings



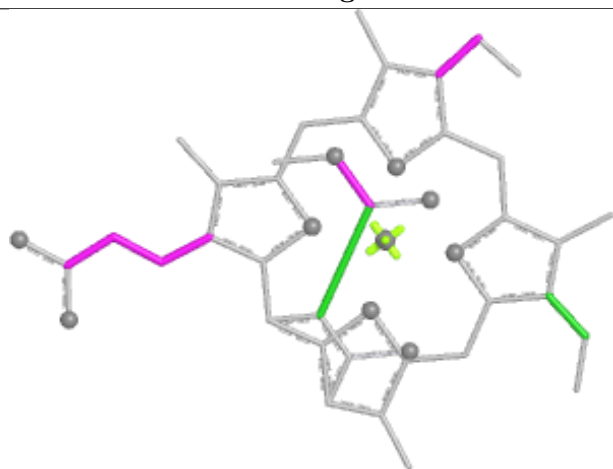
Ligand KC1 O 315



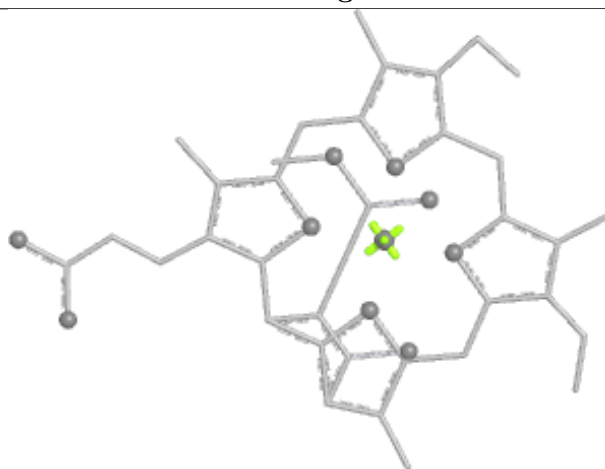
Bond lengths



Bond angles

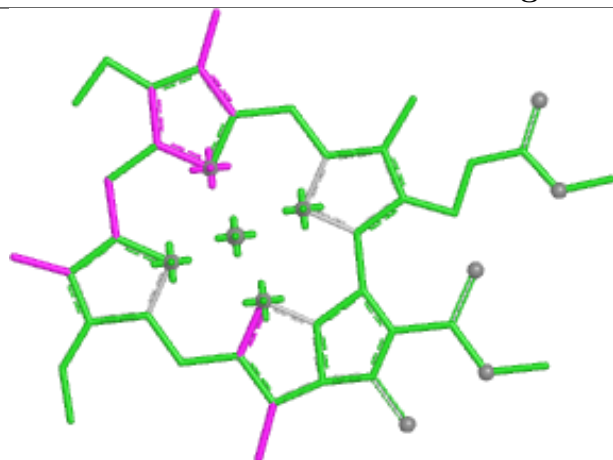


Torsions

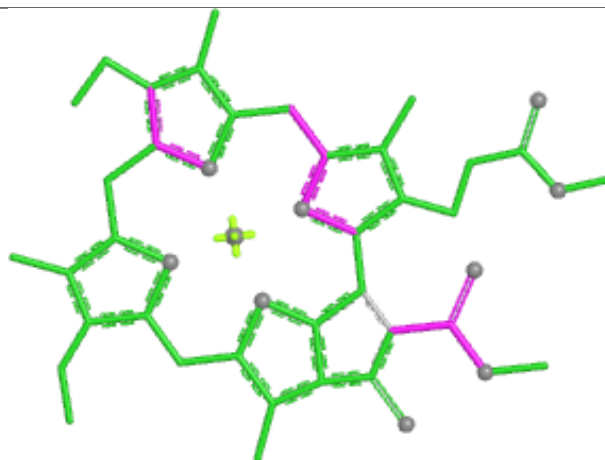


Rings

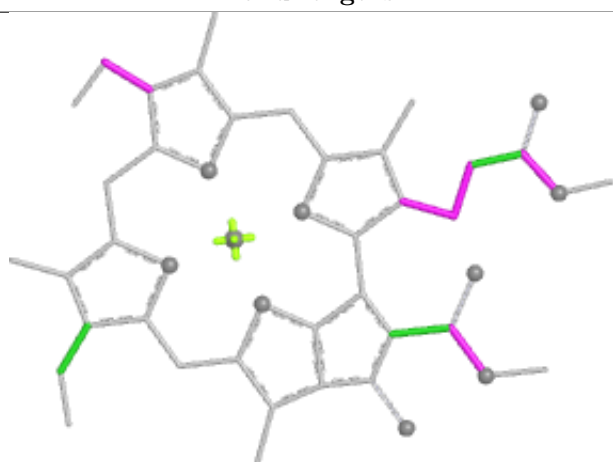
Ligand CLA I 208



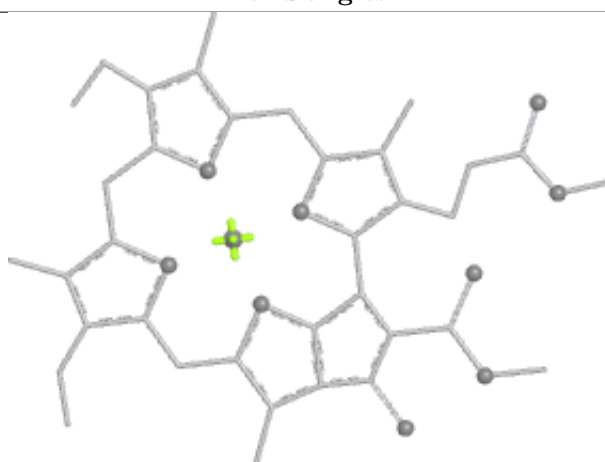
Bond lengths



Bond angles

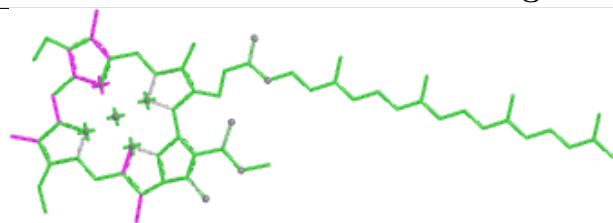


Torsions

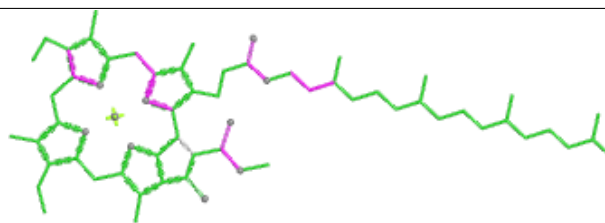


Rings

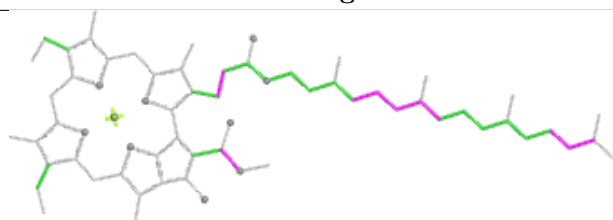
Ligand CLA i 202



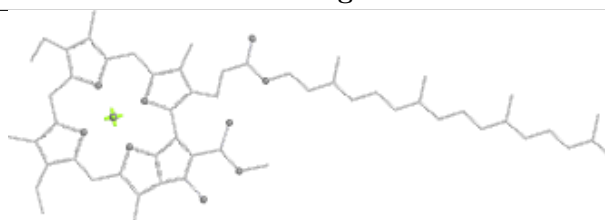
Bond lengths



Bond angles

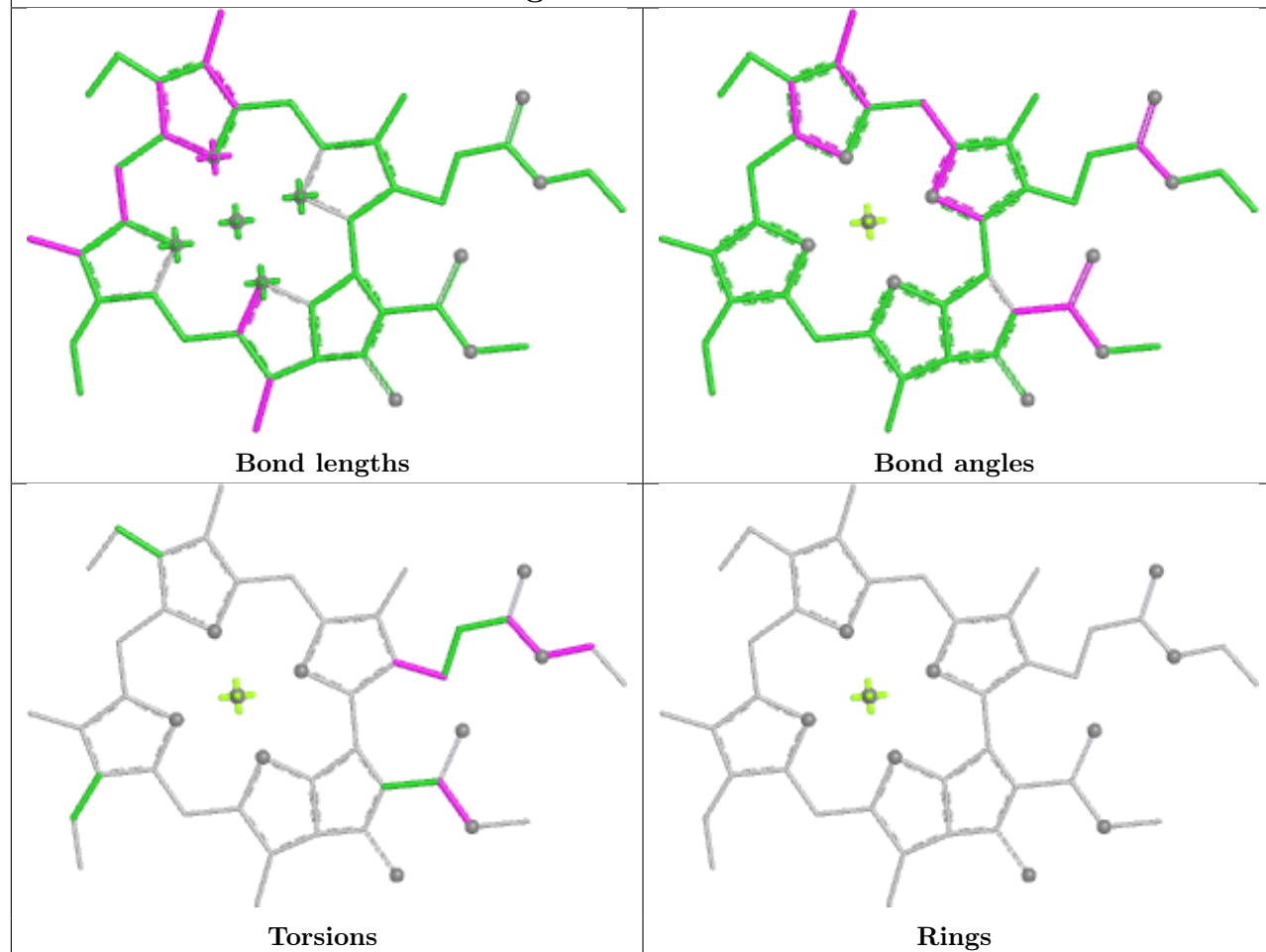


Torsions

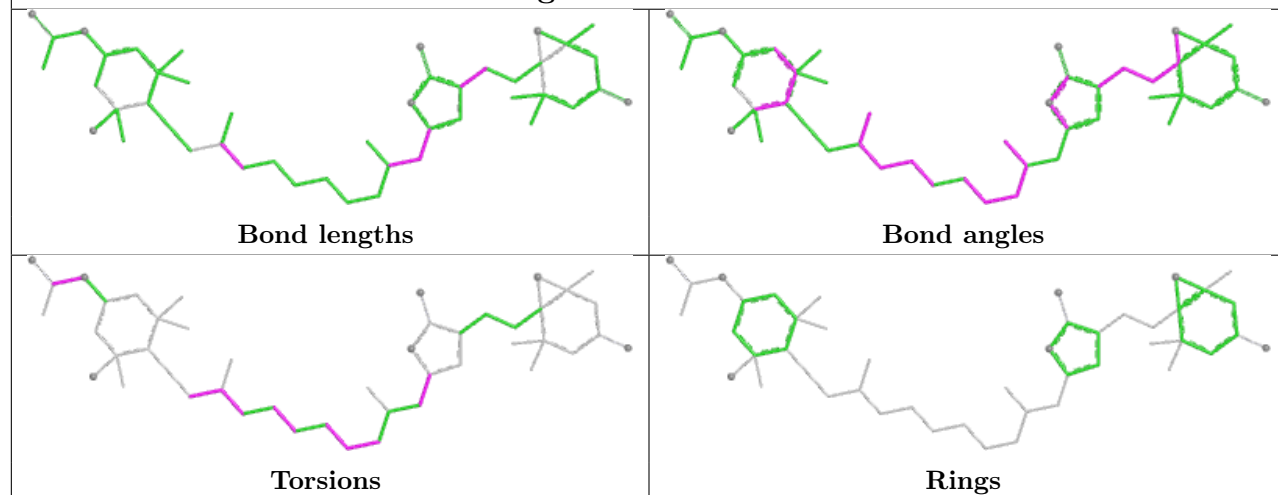


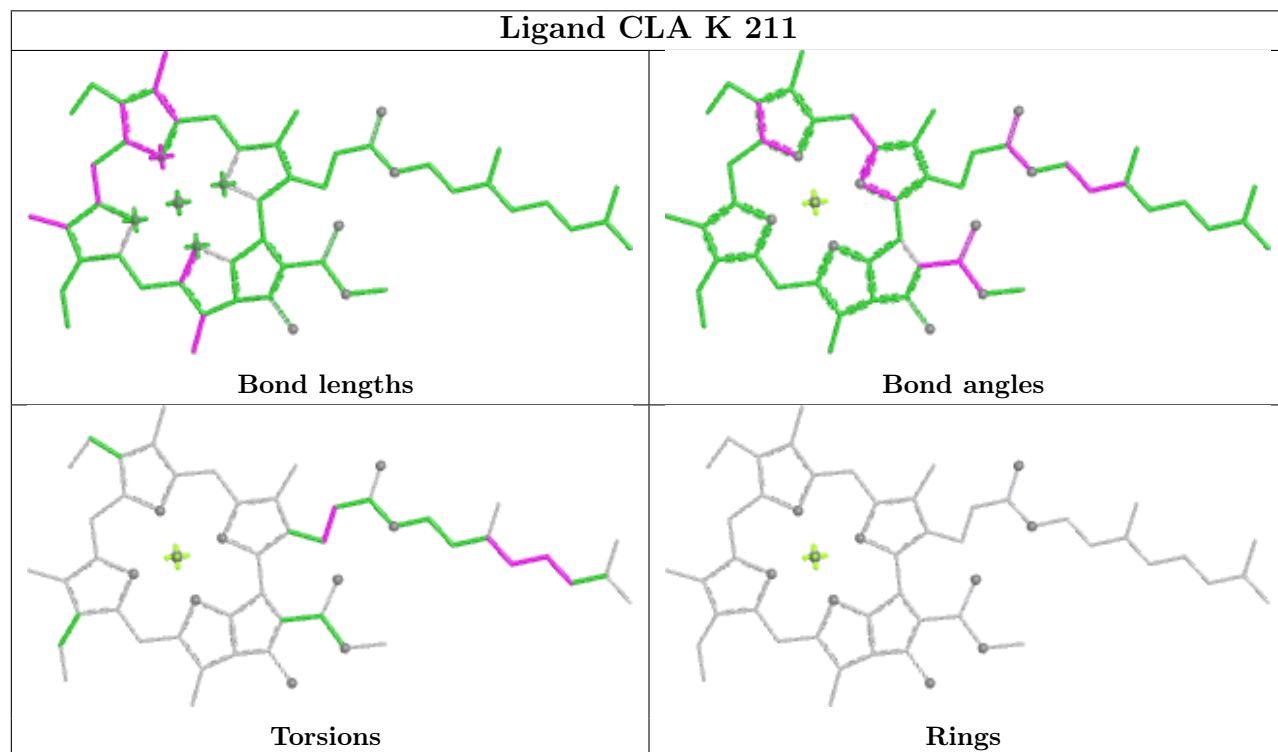
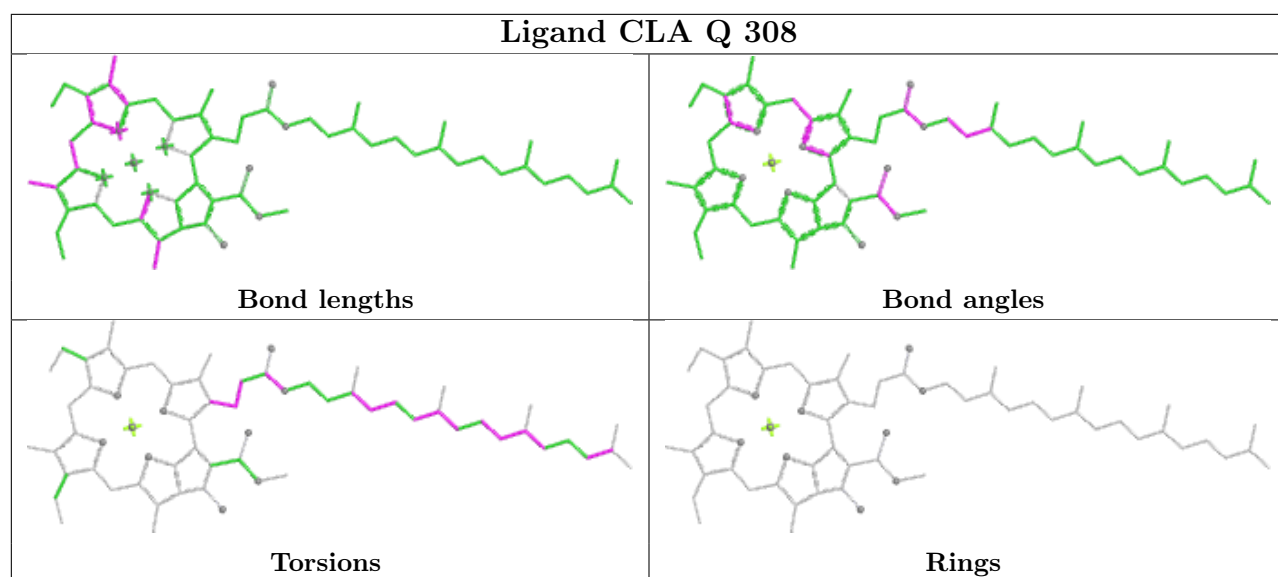
Rings

Ligand CLA N 314

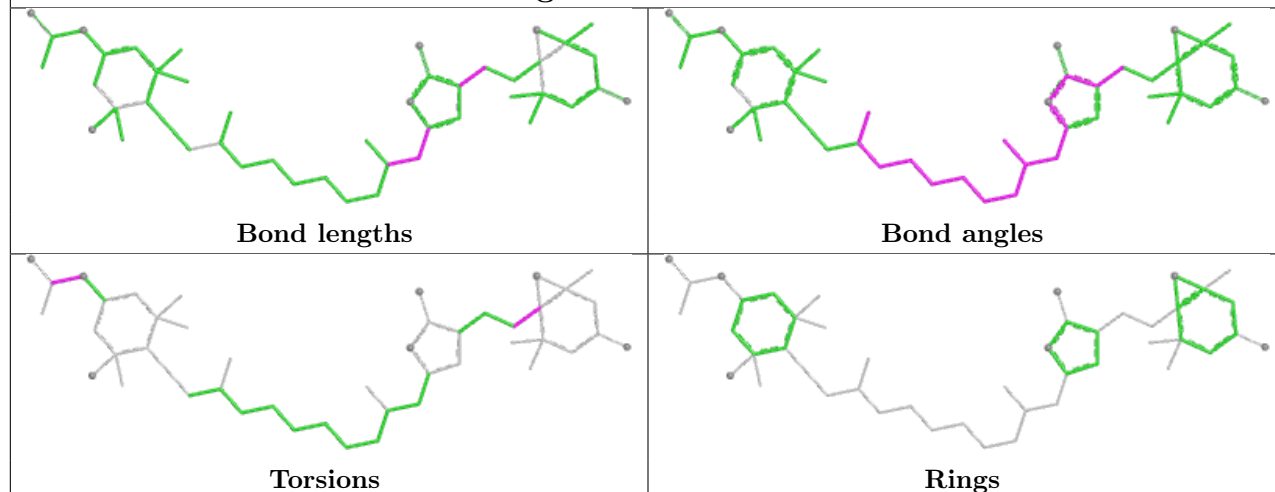


Ligand PID P 206

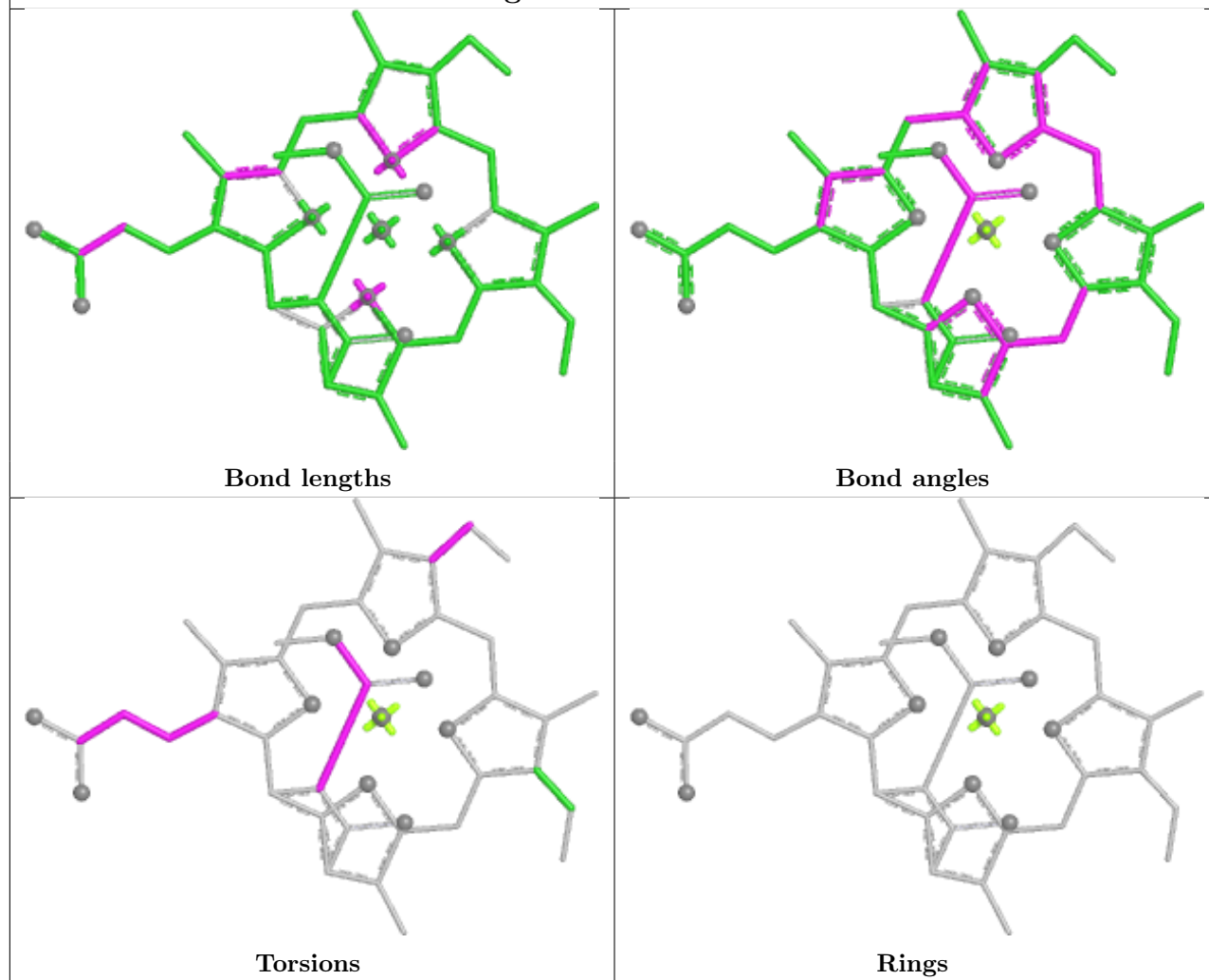




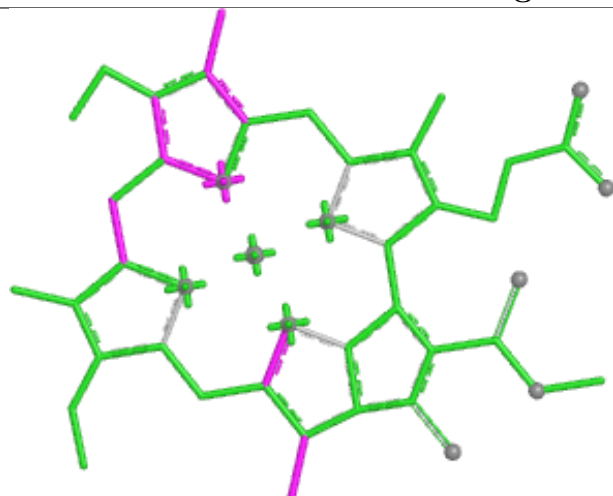
Ligand PID P 203



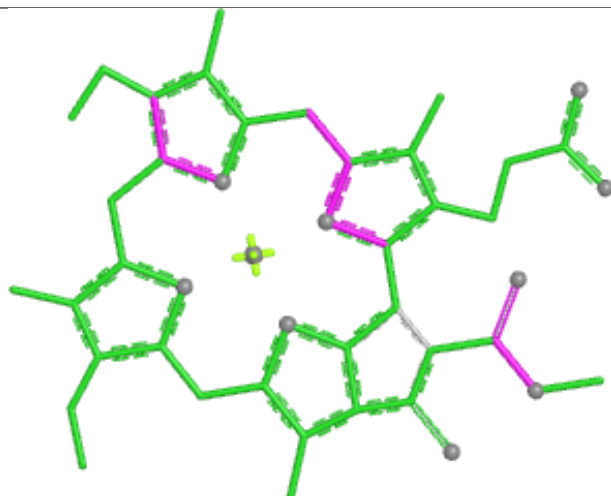
Ligand KC1 H 309



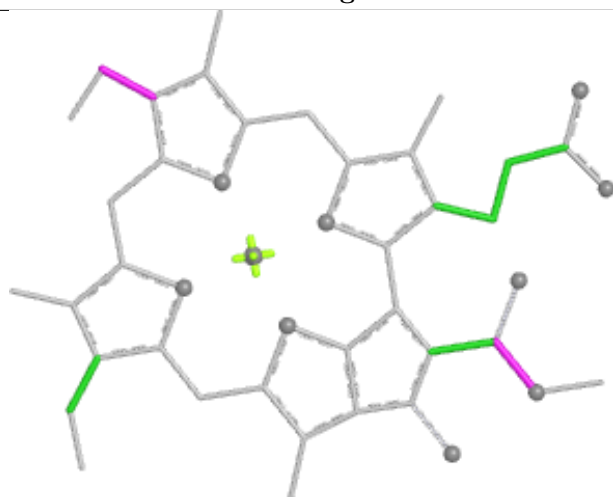
Ligand CLA B 307



Bond lengths



Bond angles

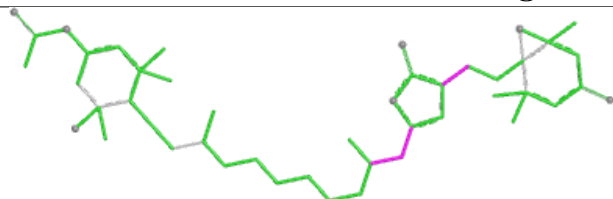


Torsions

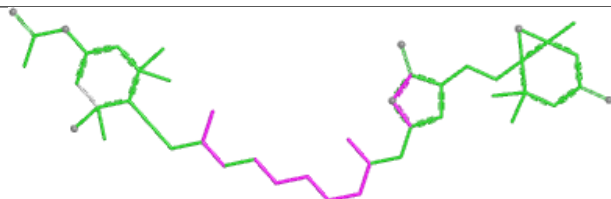


Rings

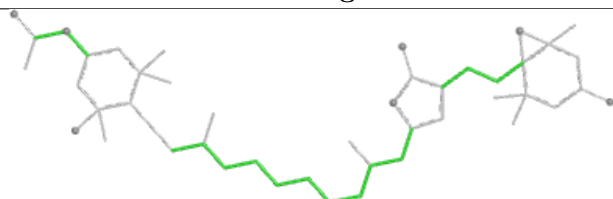
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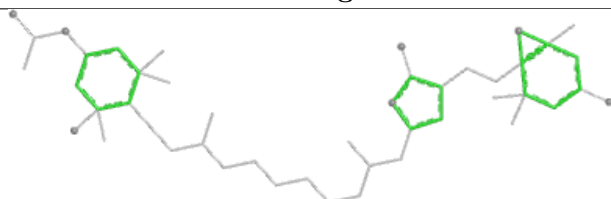
Bond lengths



Bond angles

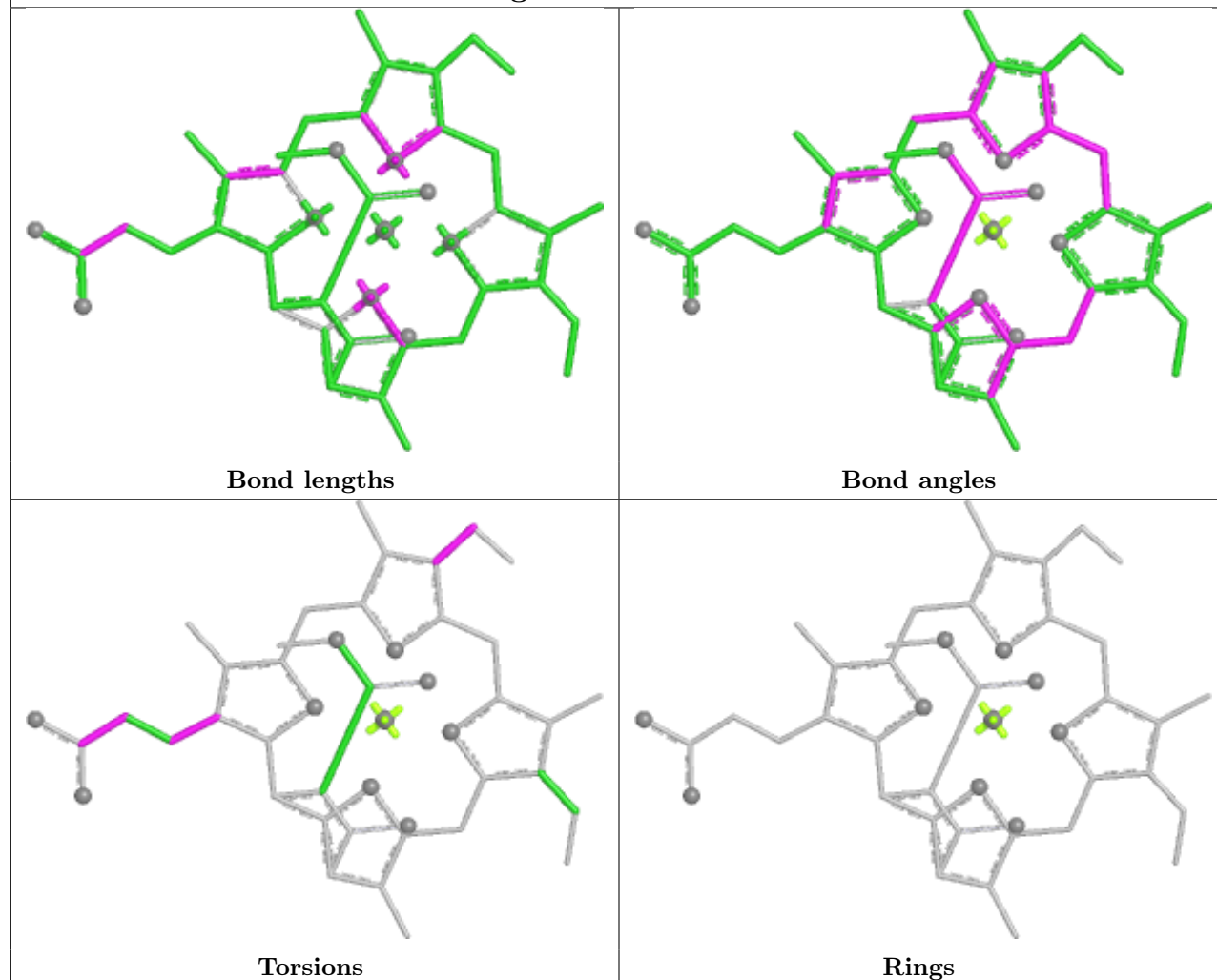


Torsions

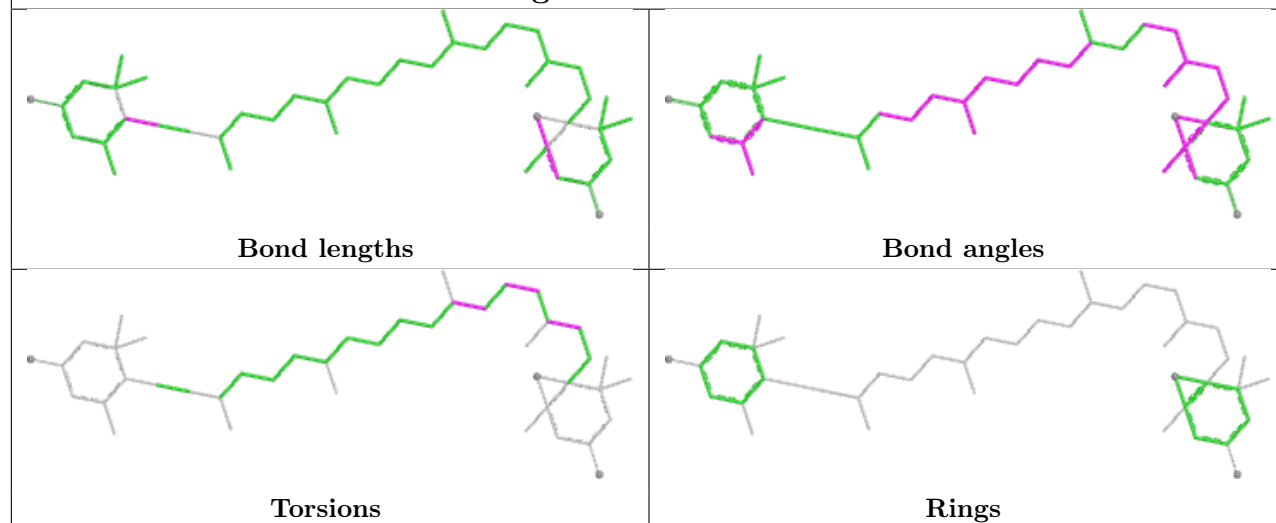


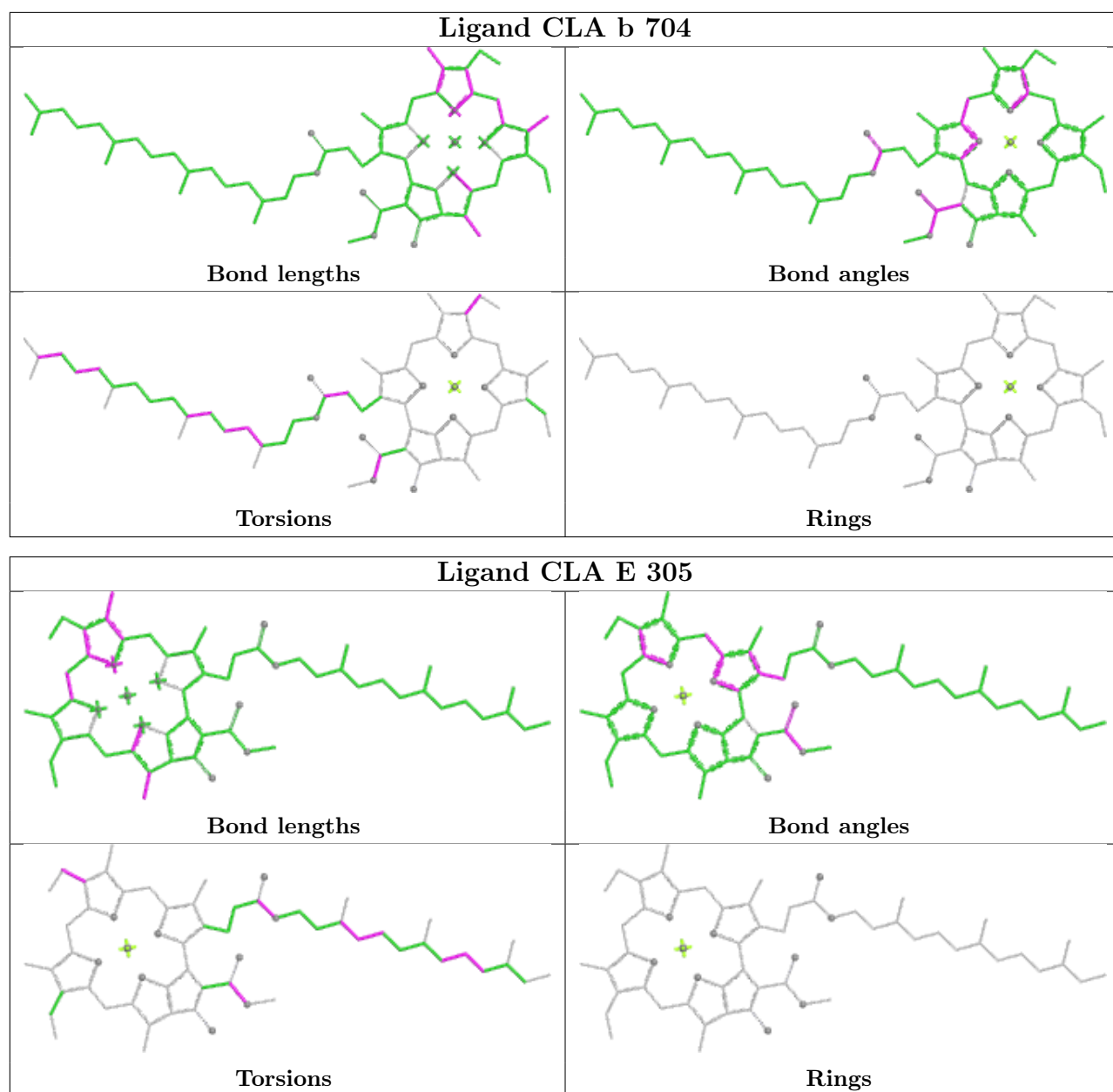
Rings

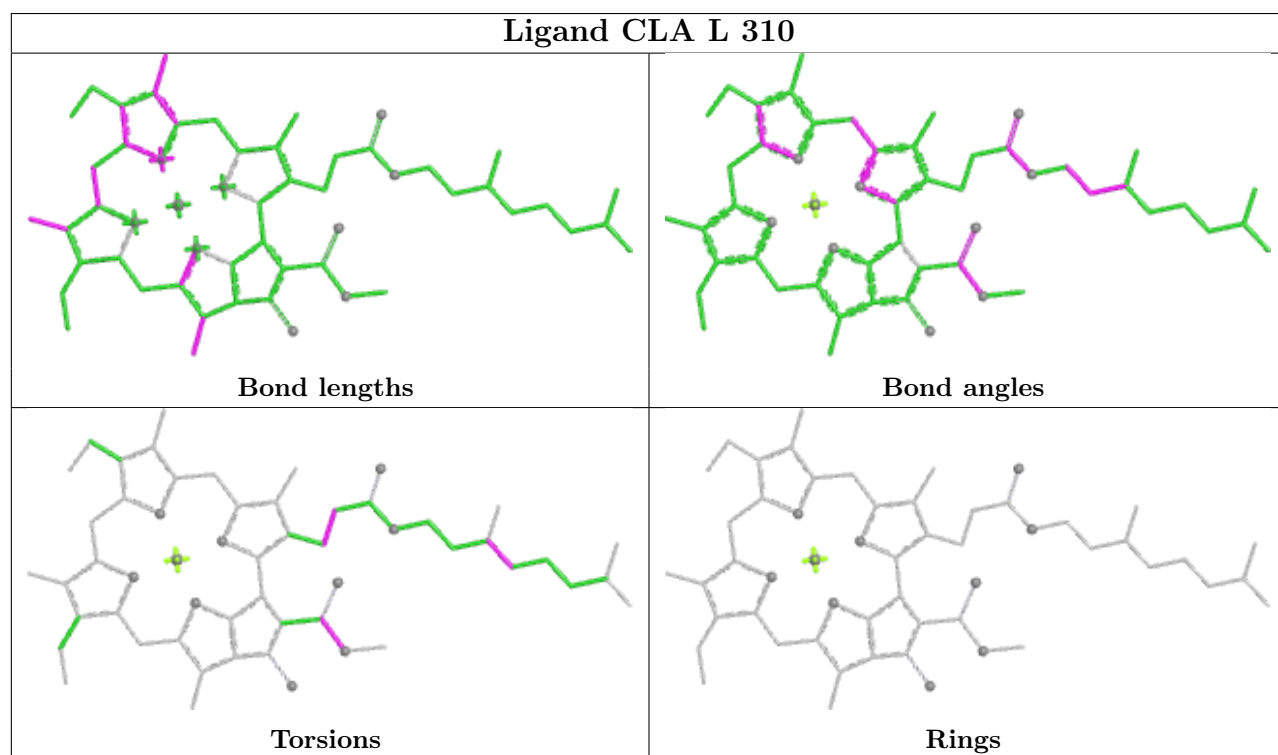
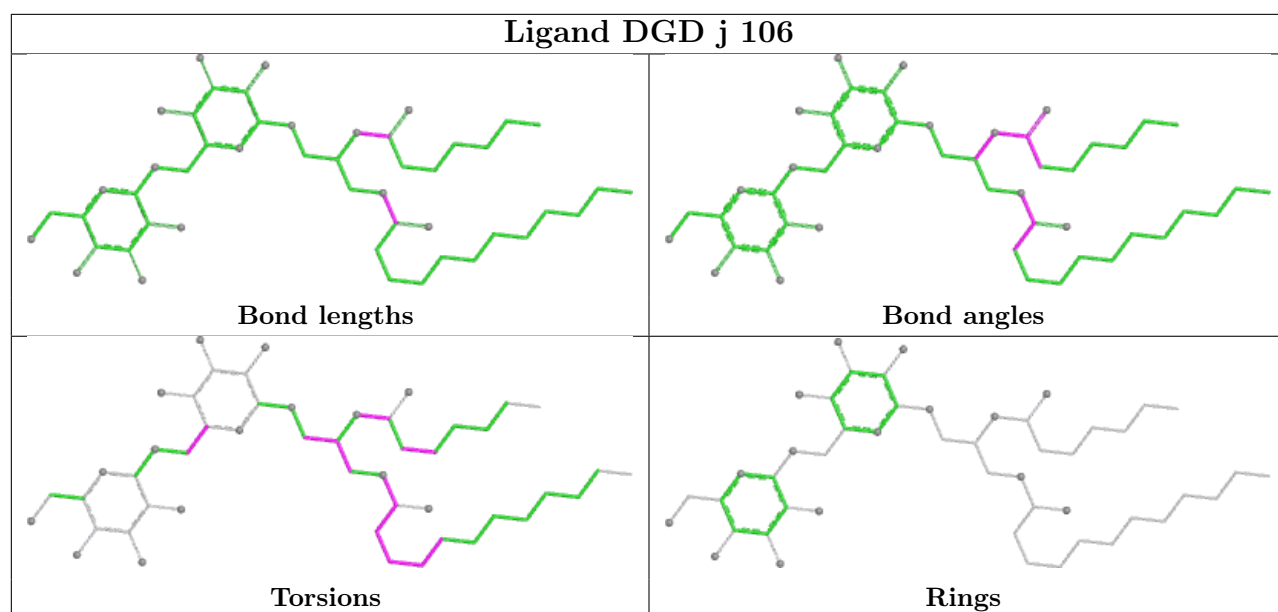
Ligand KC1 E 307

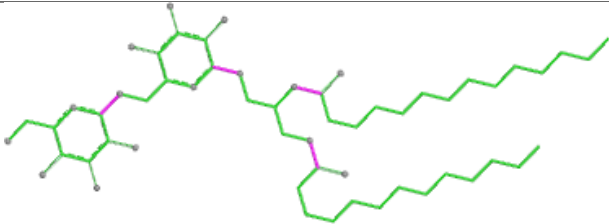
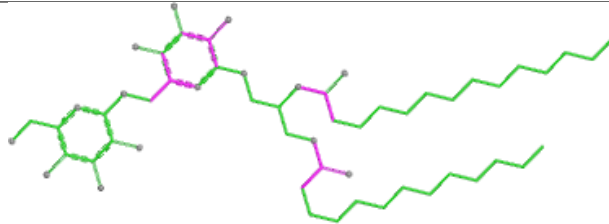
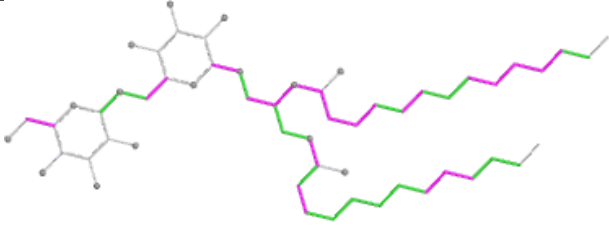
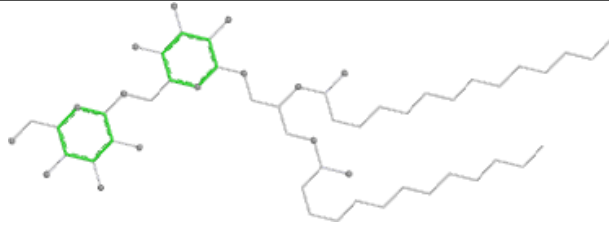


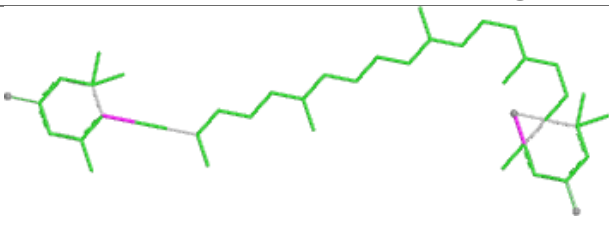
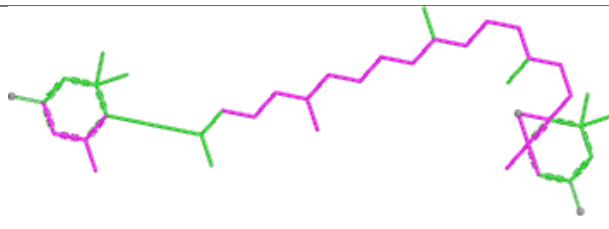
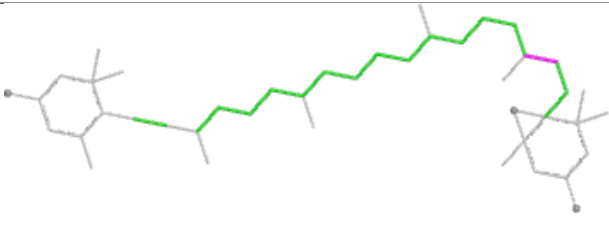
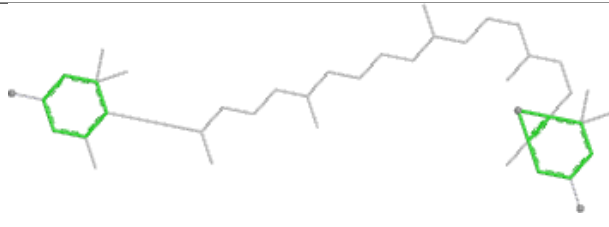
Ligand DD6 K 221

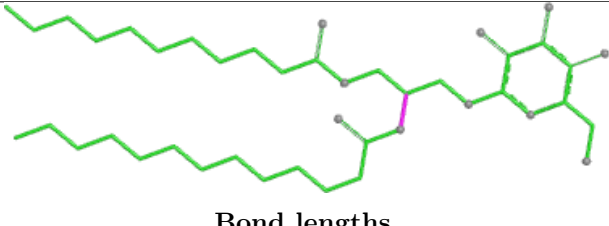
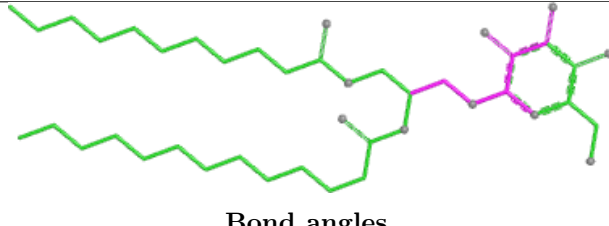
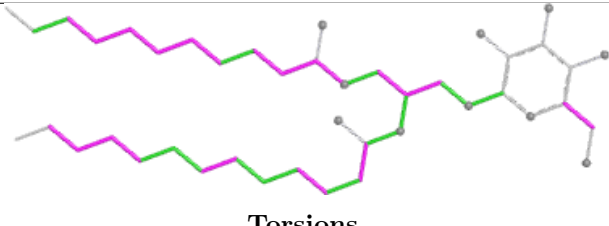
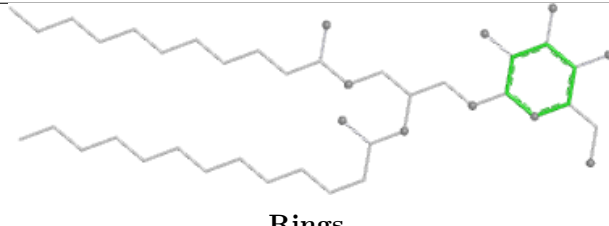




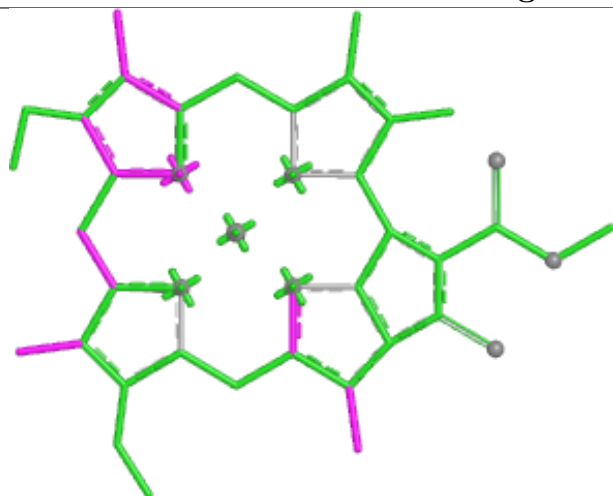


Ligand DGD b 733	
	
Bond lengths	Bond angles
	
Torsions	Rings

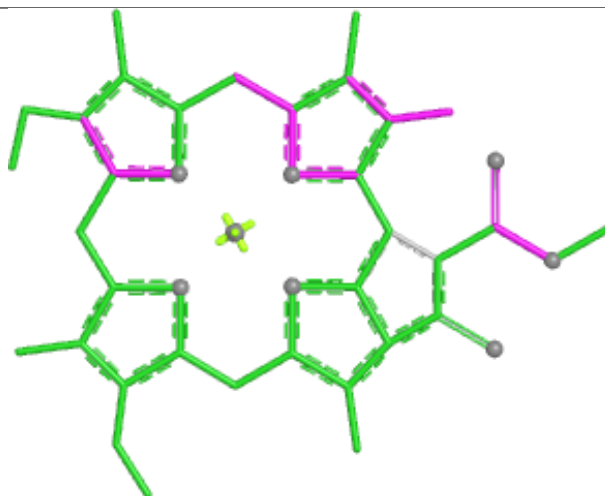
Ligand DD6 E 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

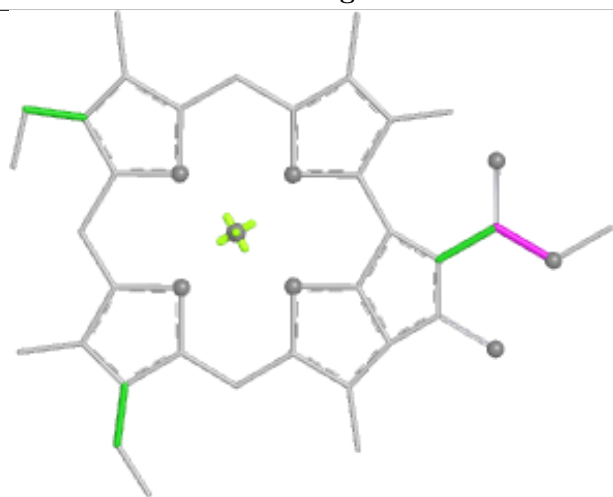
Ligand CLA J 313



Bond lengths



Bond angles

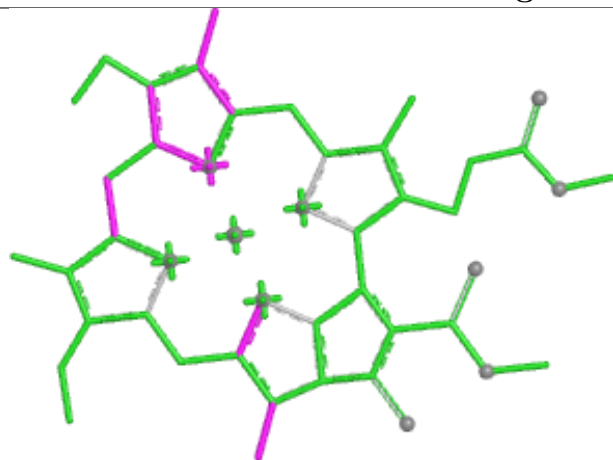


Torsions

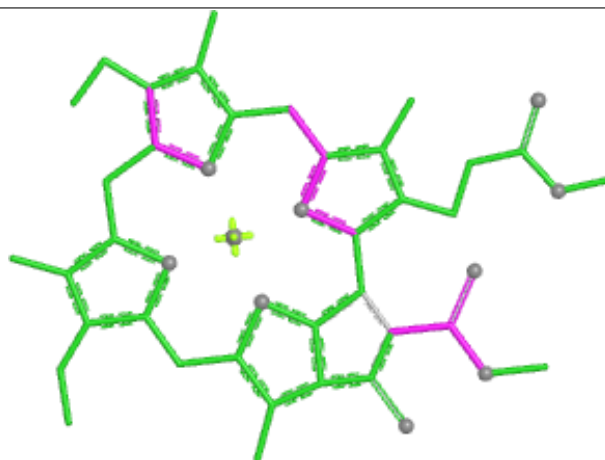


Rings

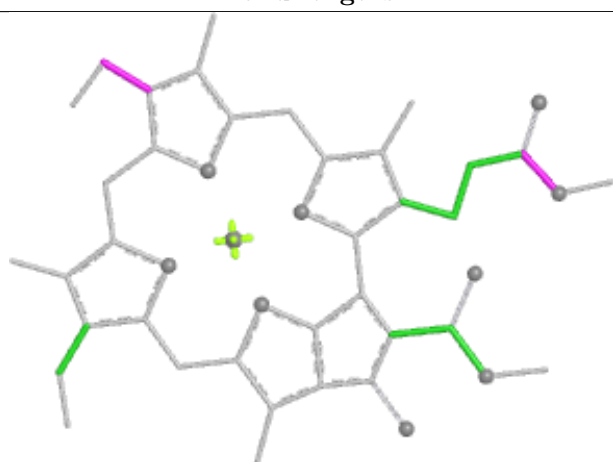
Ligand CLA F 307



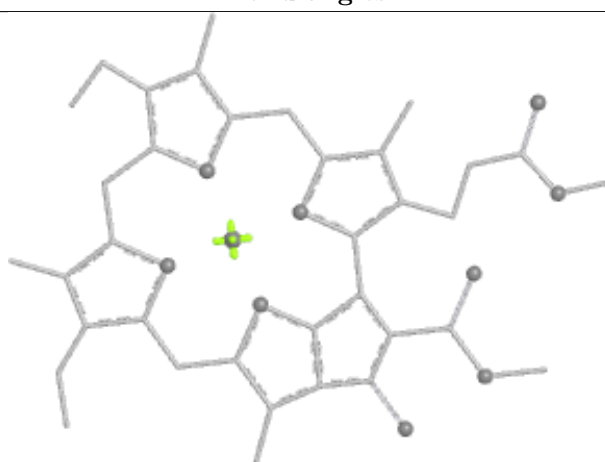
Bond lengths



Bond angles

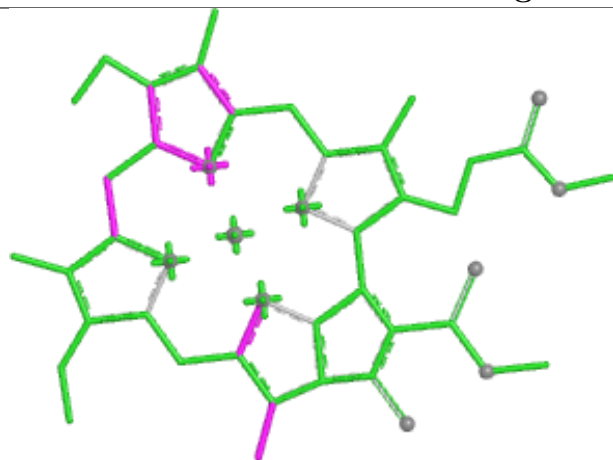


Torsions

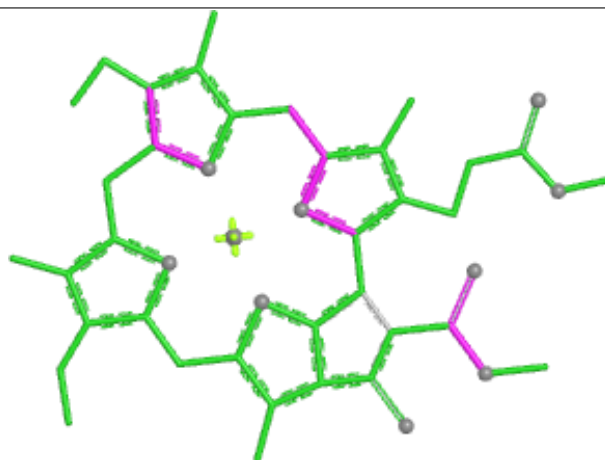


Rings

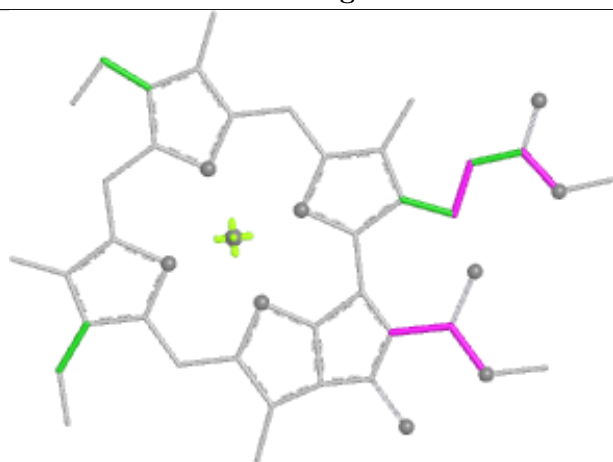
Ligand CLA T 311



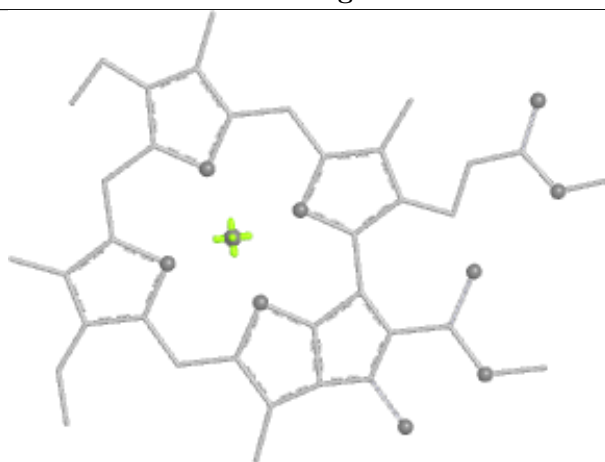
Bond lengths



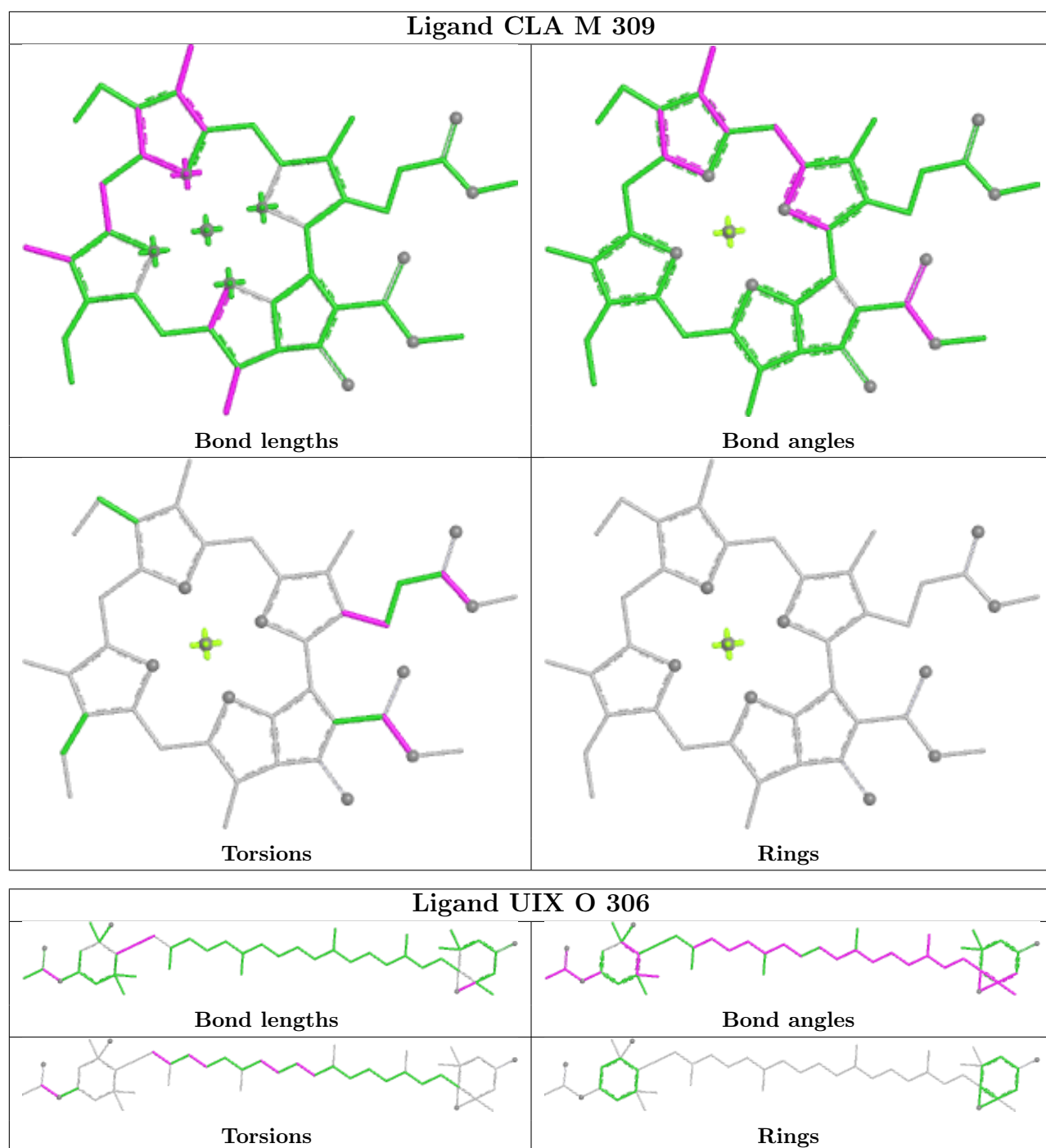
Bond angles



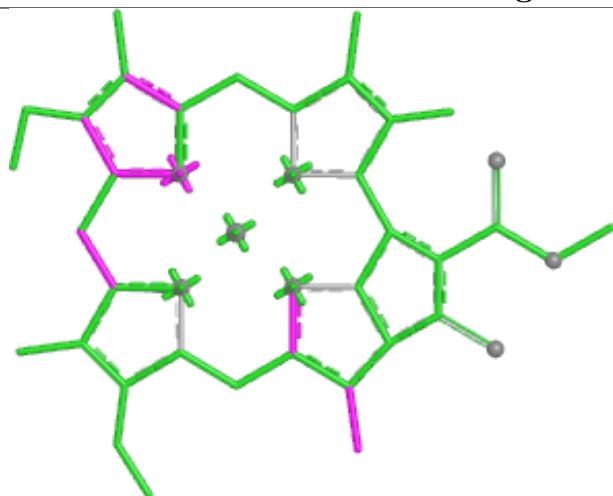
Torsions



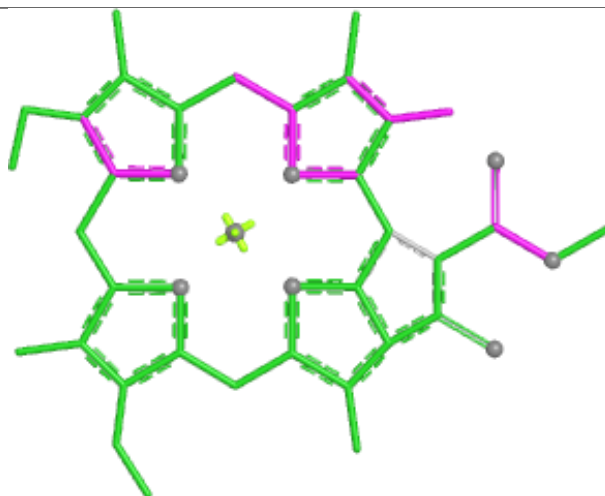
Rings



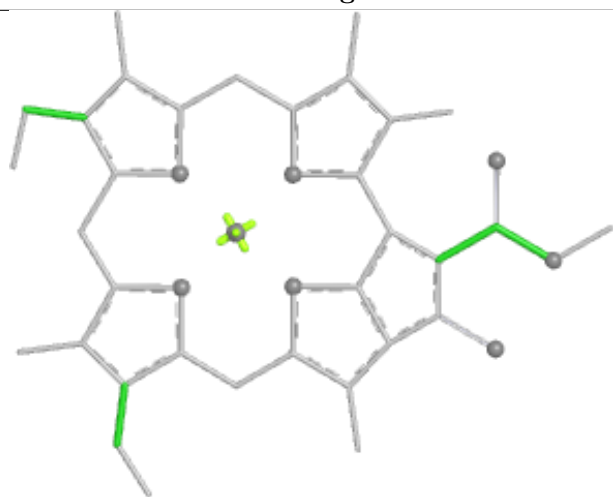
Ligand CLA E 313



Bond lengths



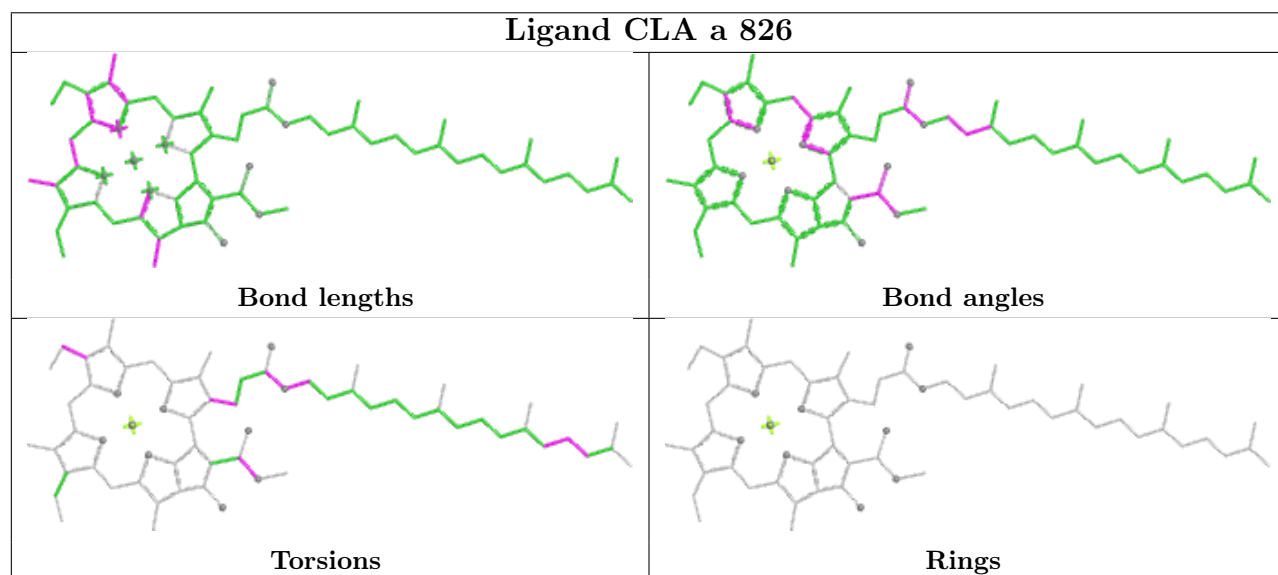
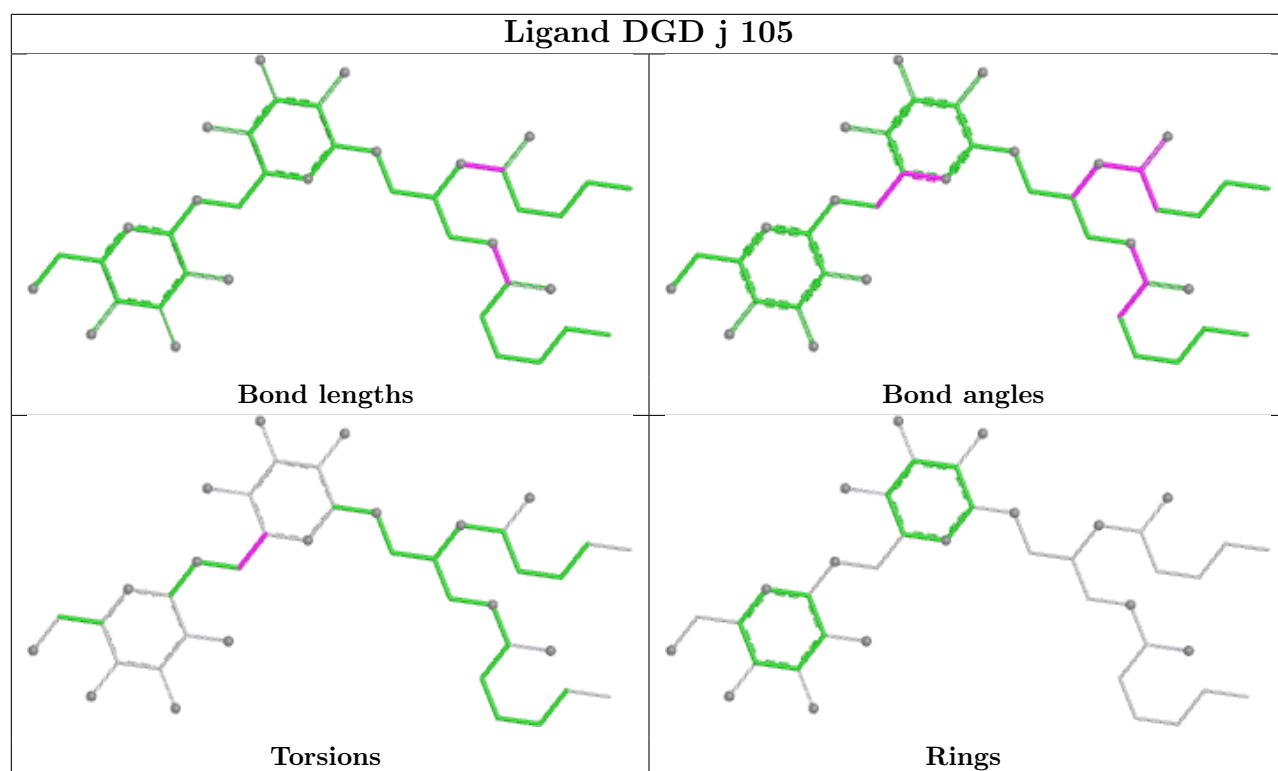
Bond angles

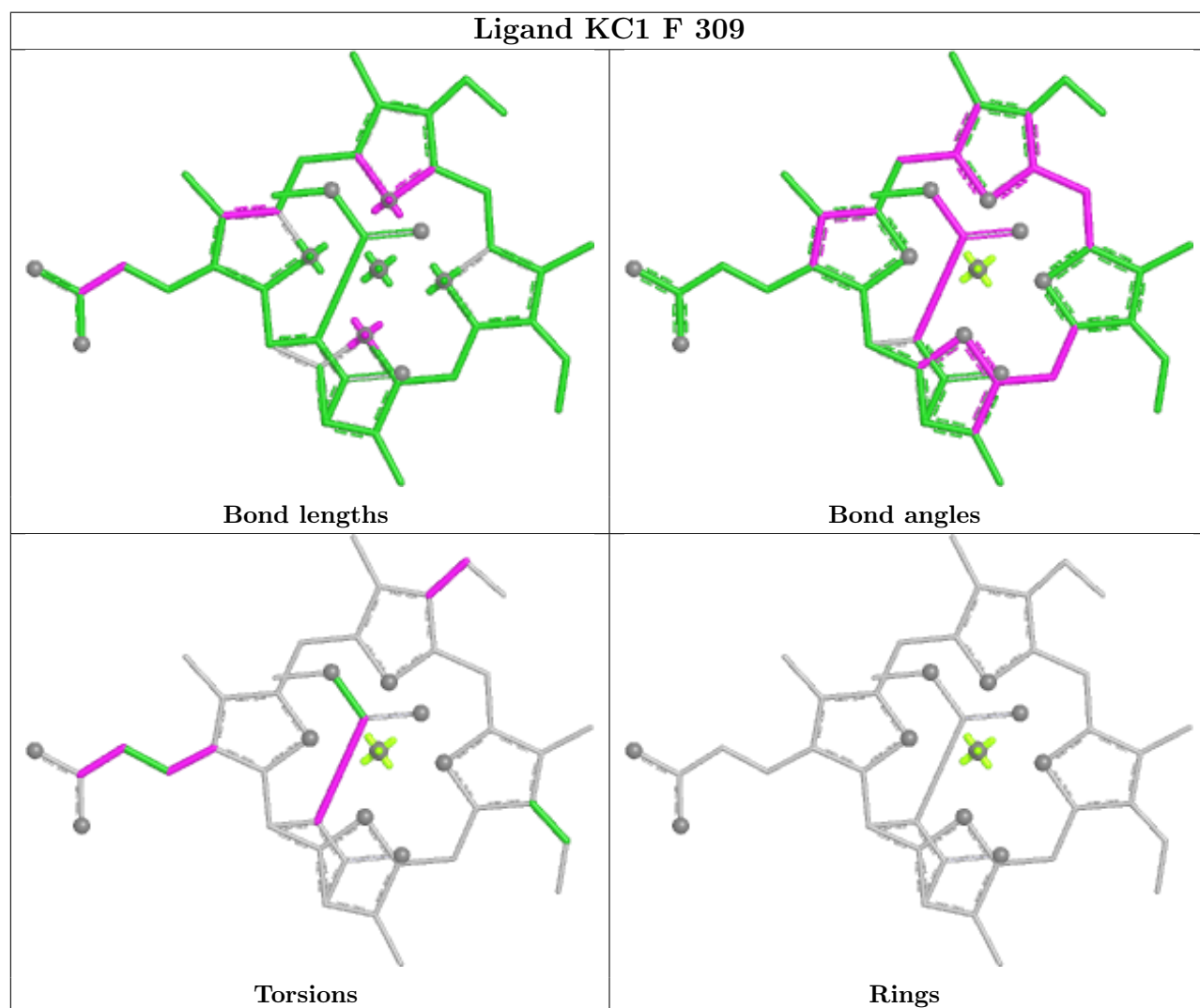
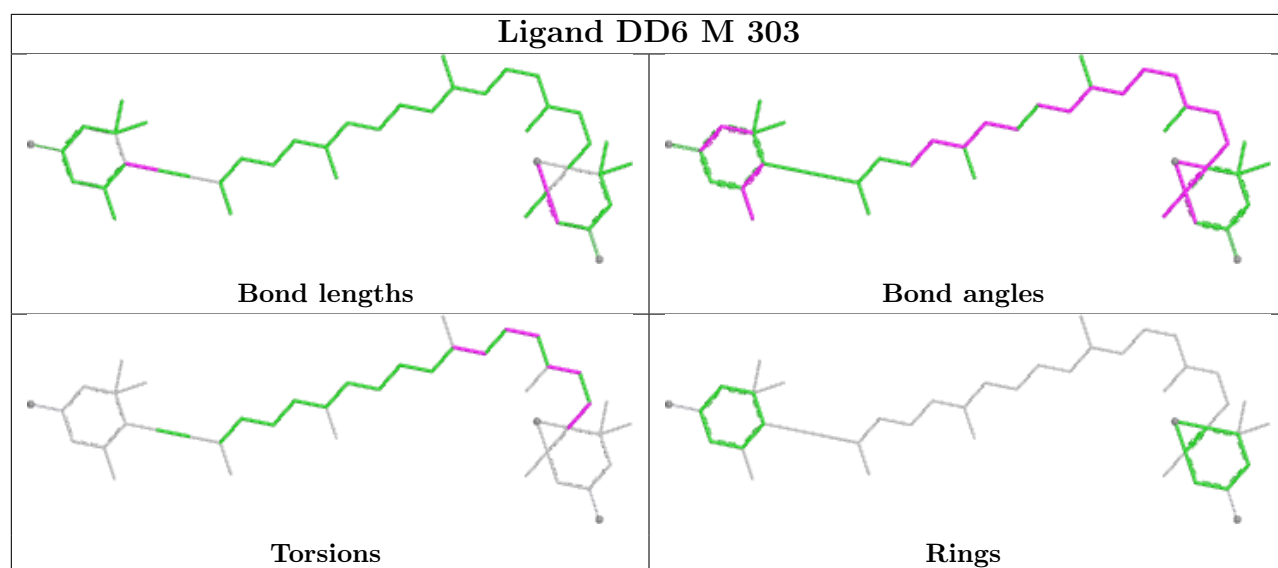


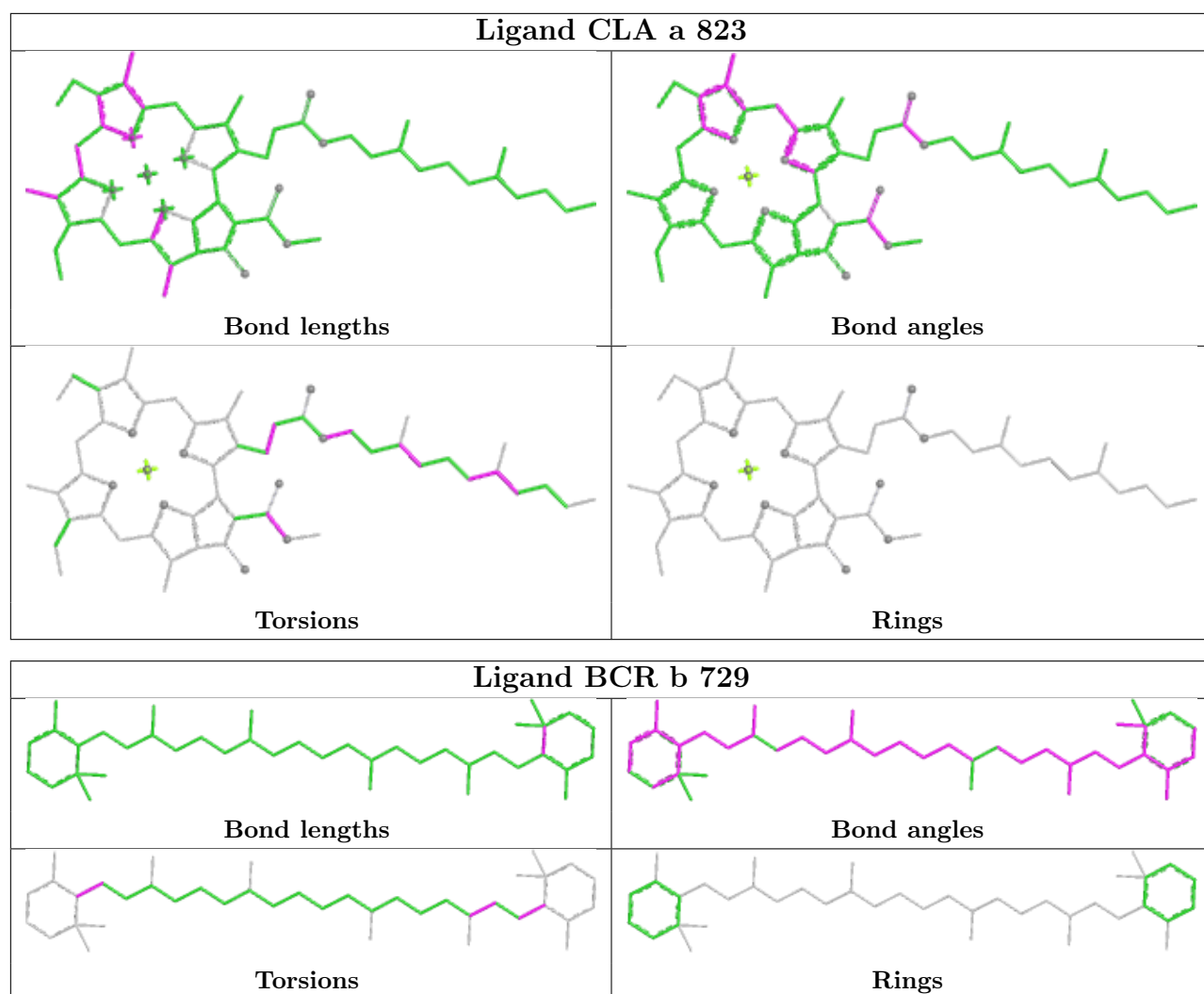
Torsions



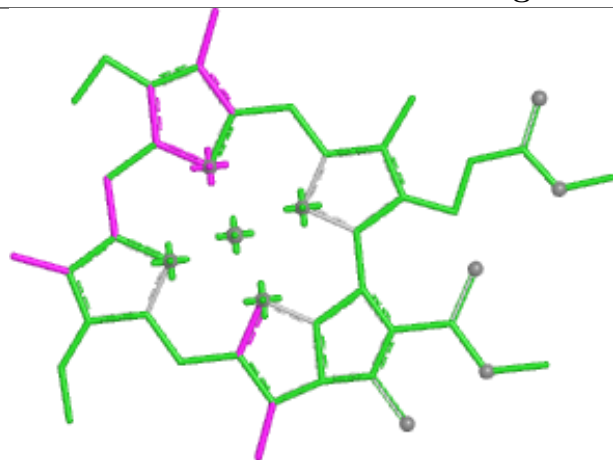
Rings



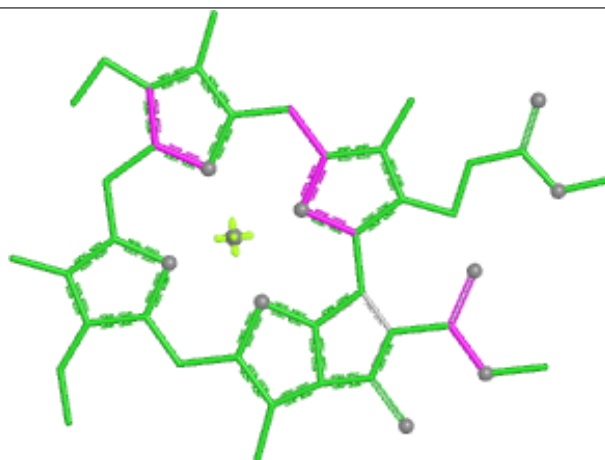




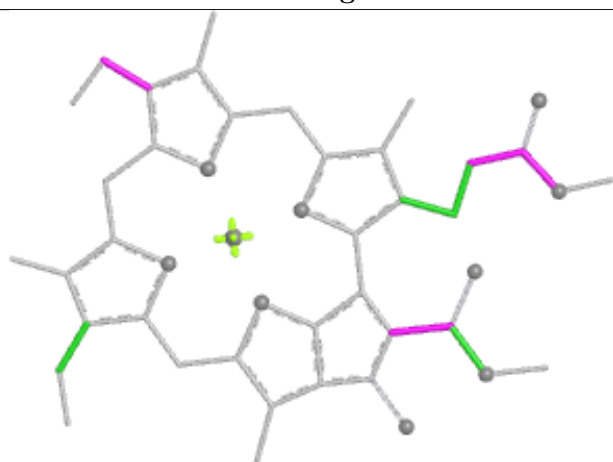
Ligand CLA K 217



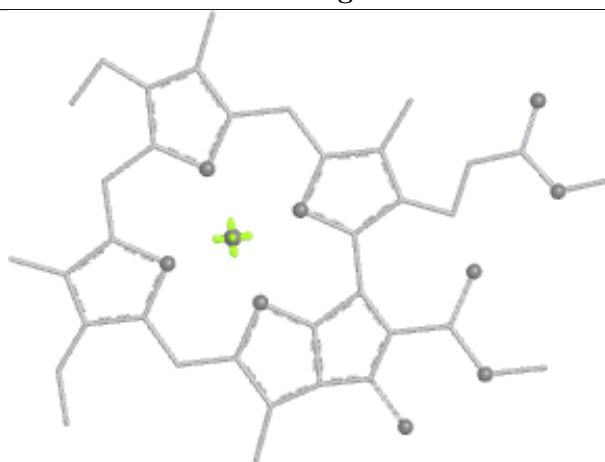
Bond lengths



Bond angles

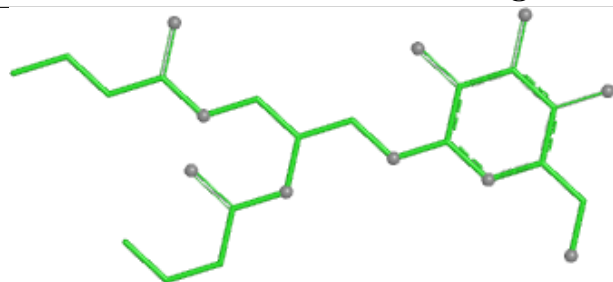


Torsions

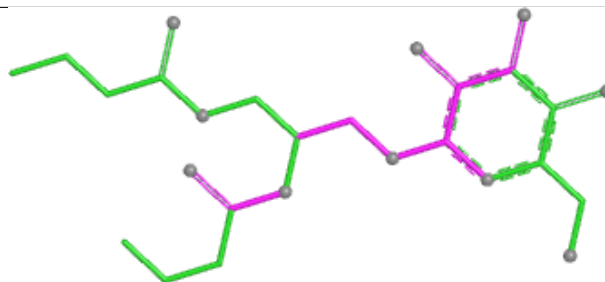


Rings

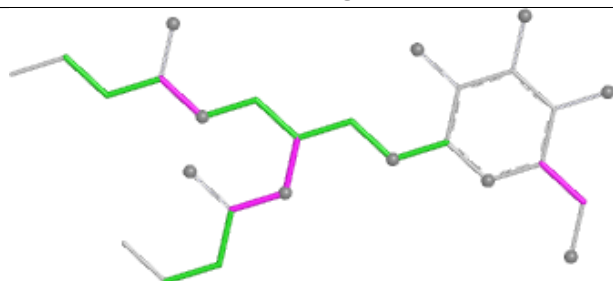
Ligand LMG P 201



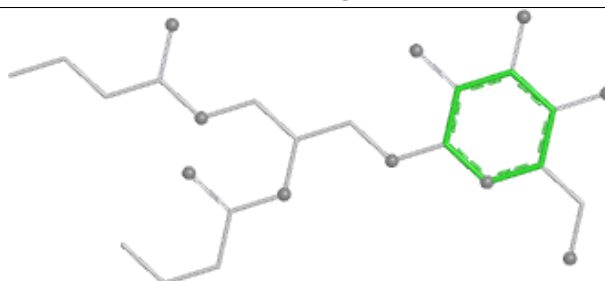
Bond lengths



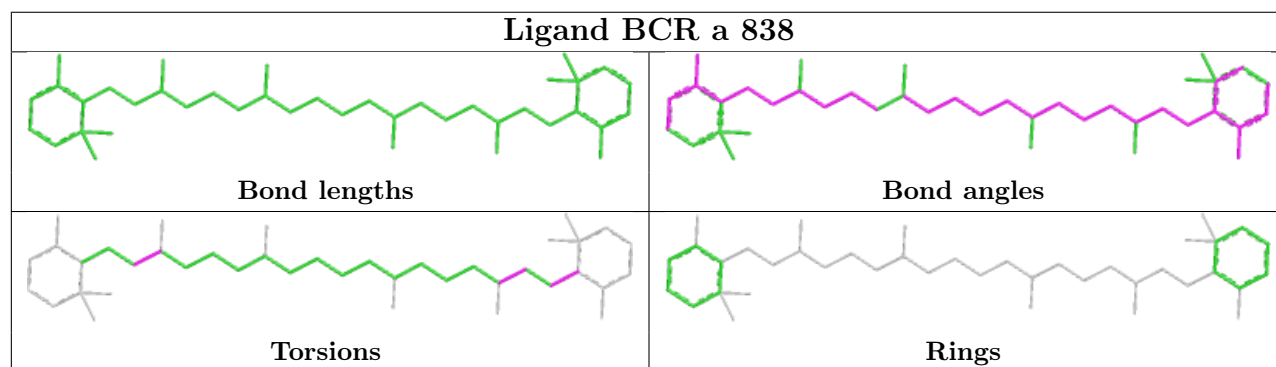
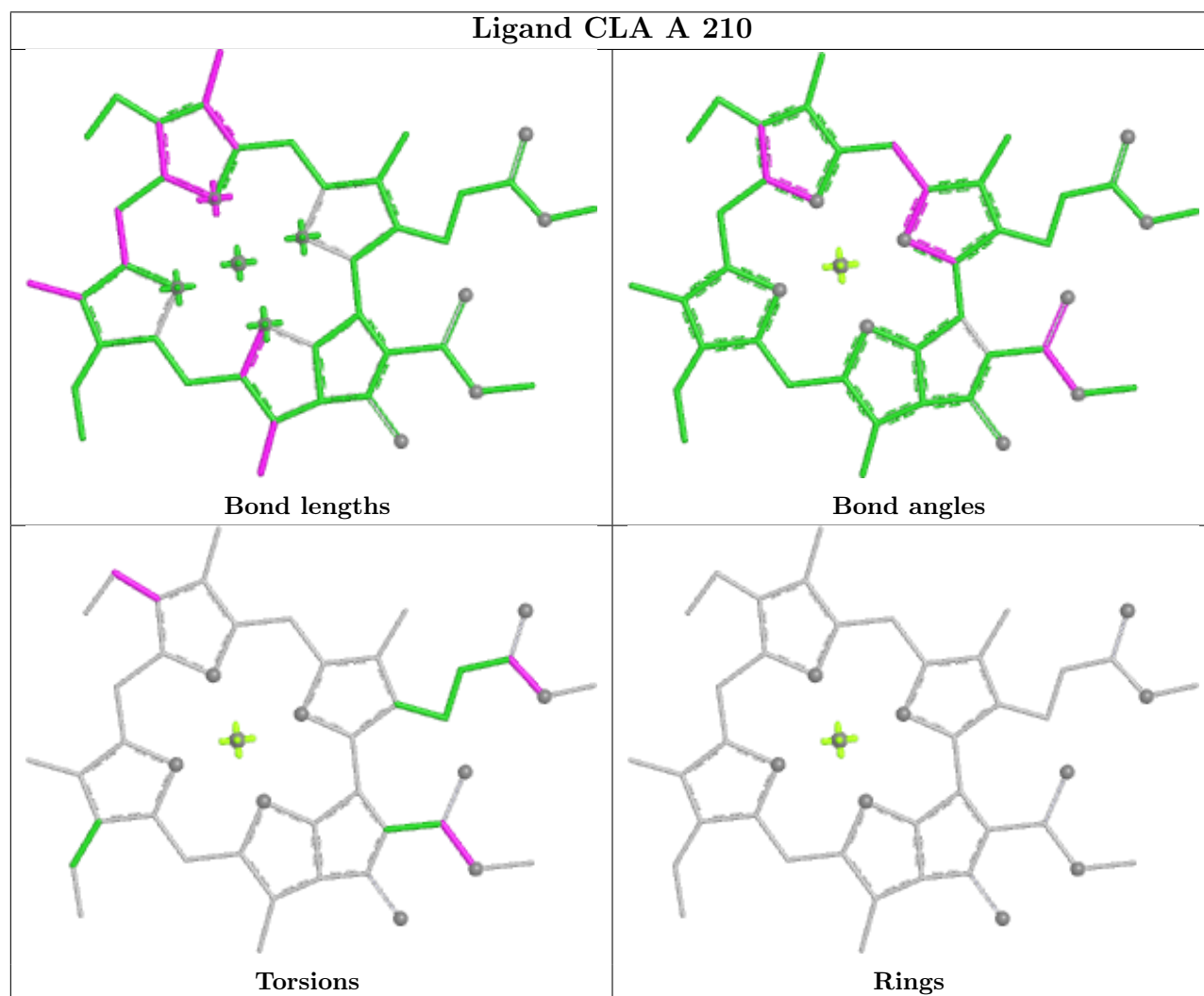
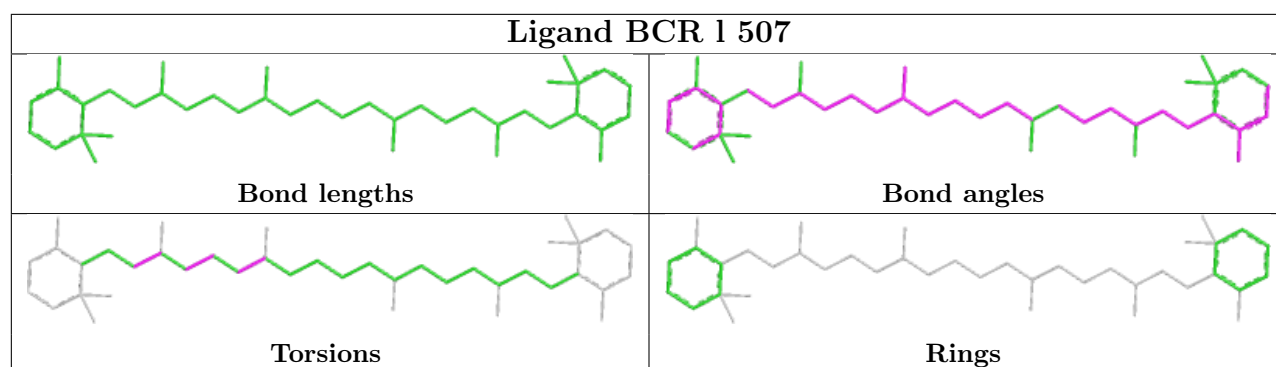
Bond angles



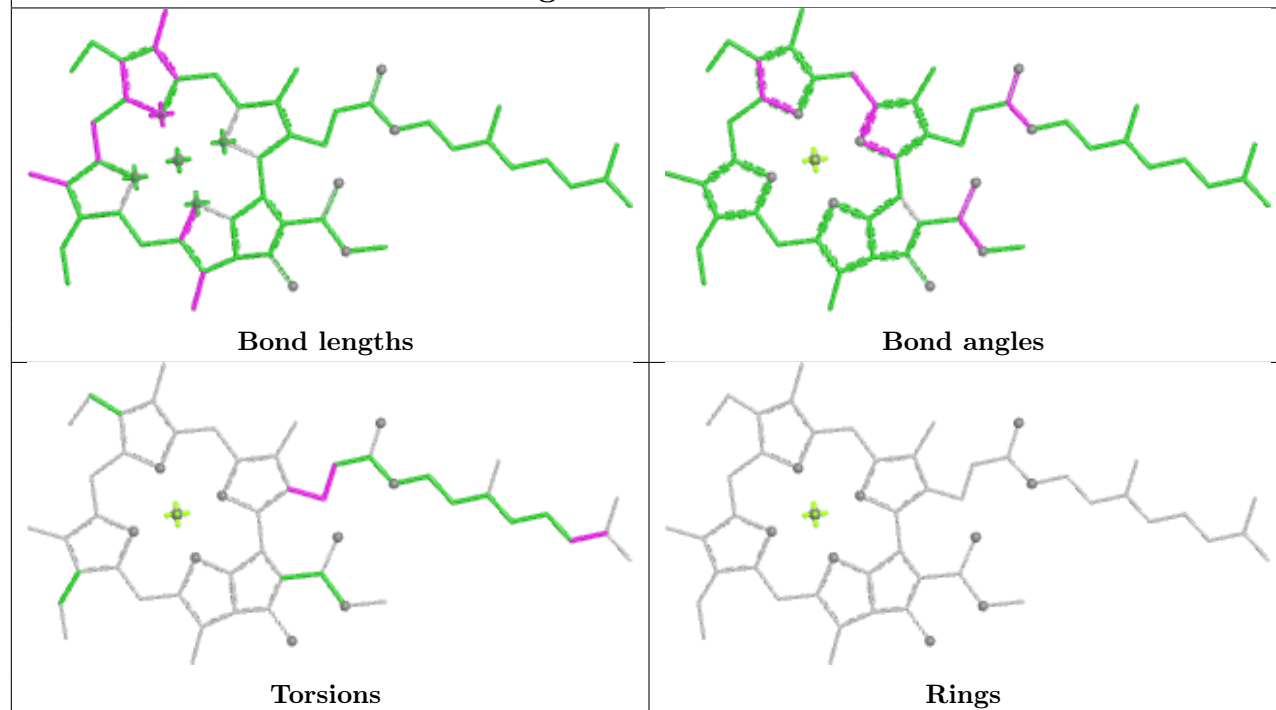
Torsions



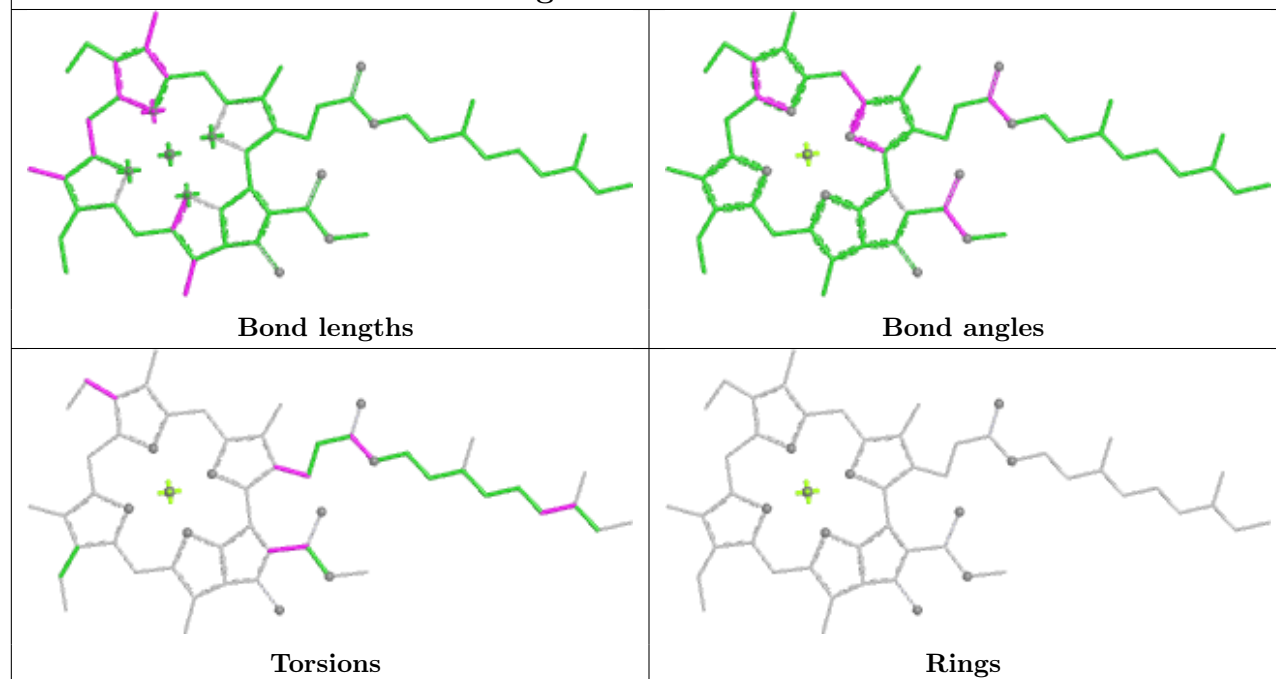
Rings



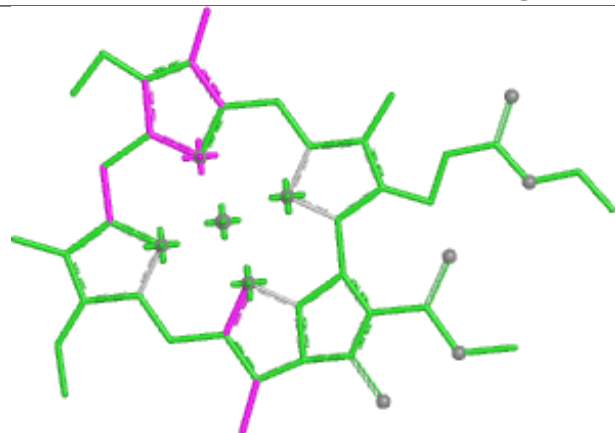
Ligand CLA I 214



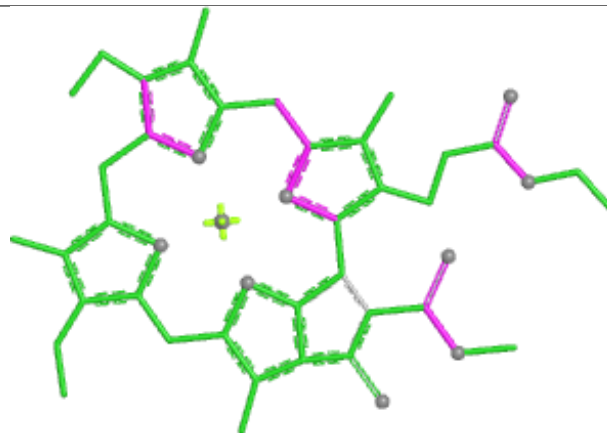
Ligand CLA a 811



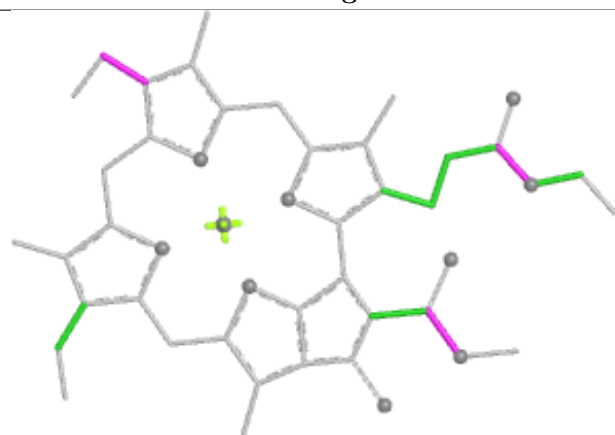
Ligand CLA N 308



Bond lengths



Bond angles

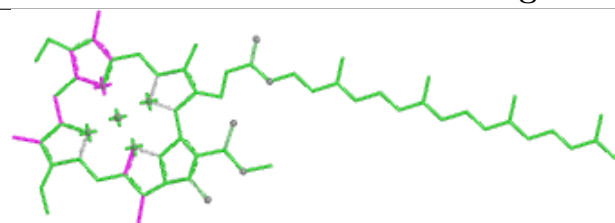


Torsions

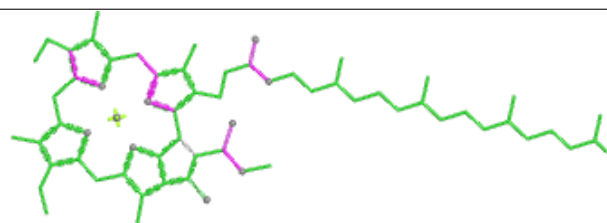


Rings

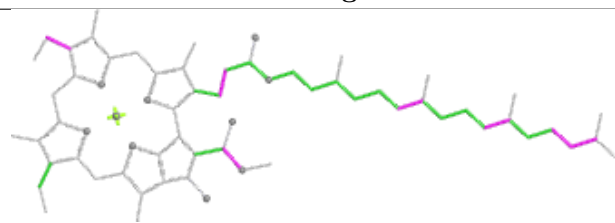
Ligand CLA b 725



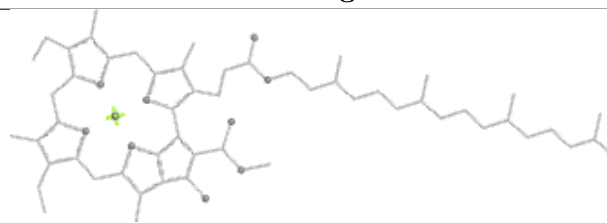
Bond lengths



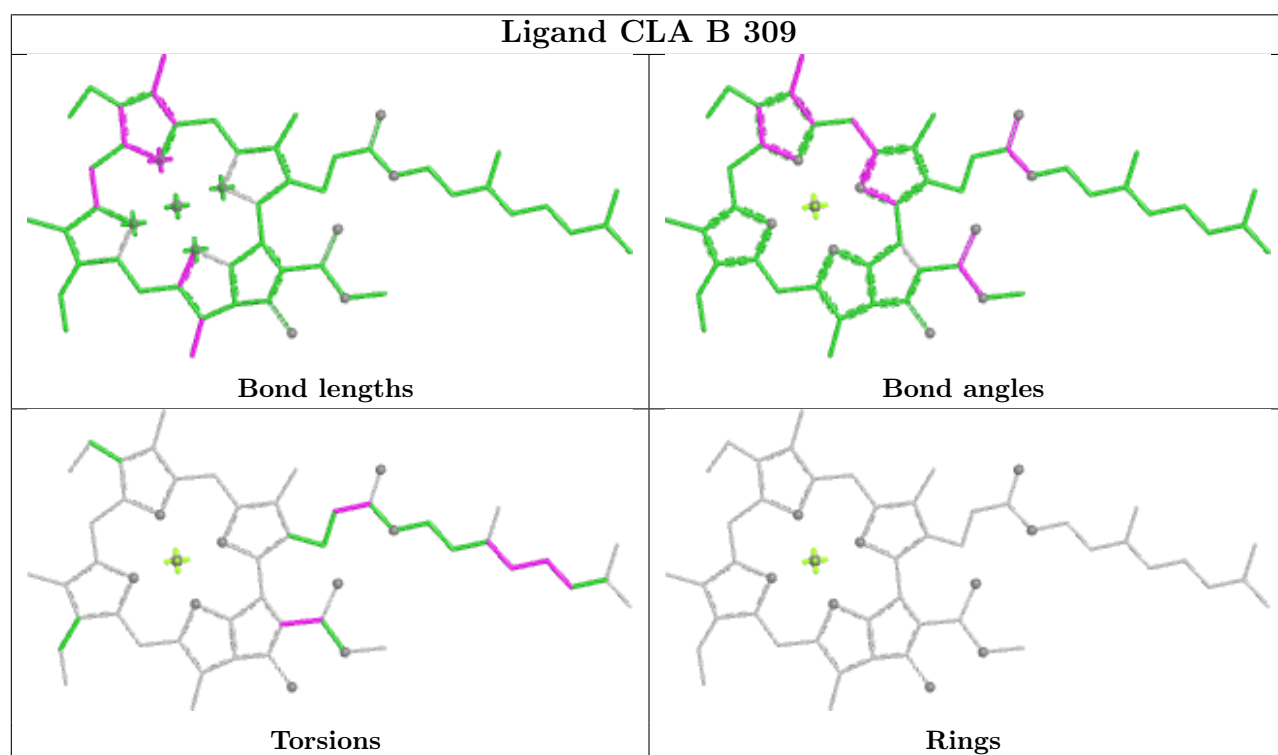
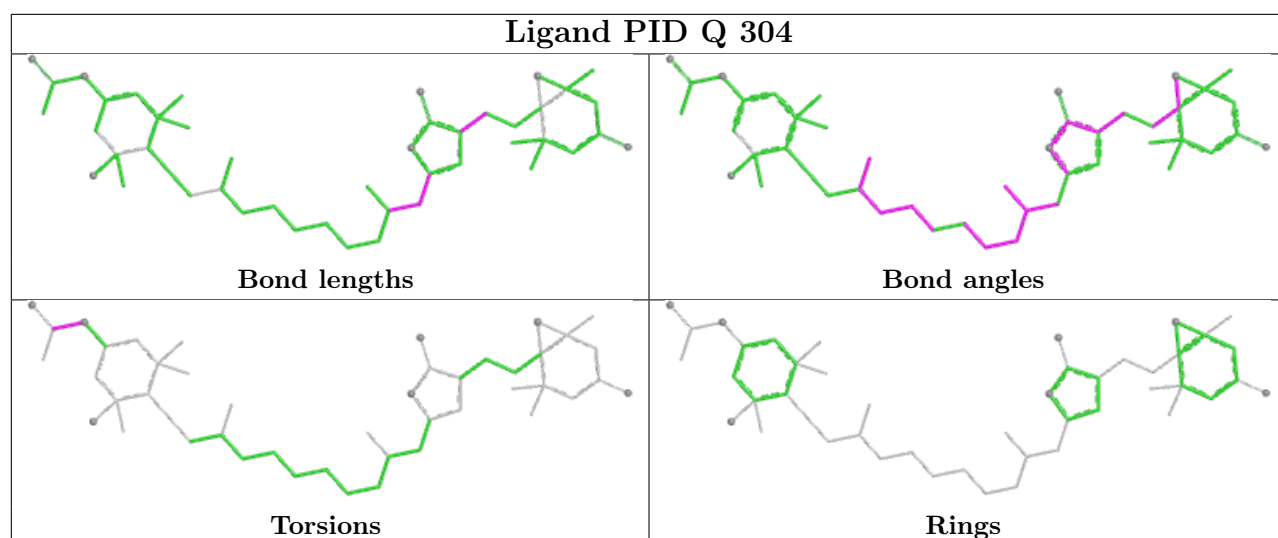
Bond angles



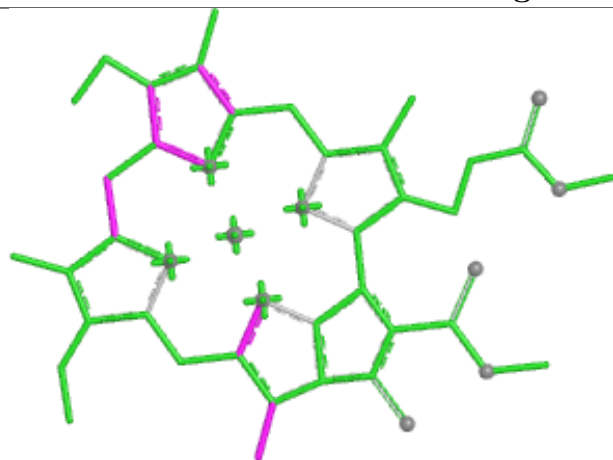
Torsions



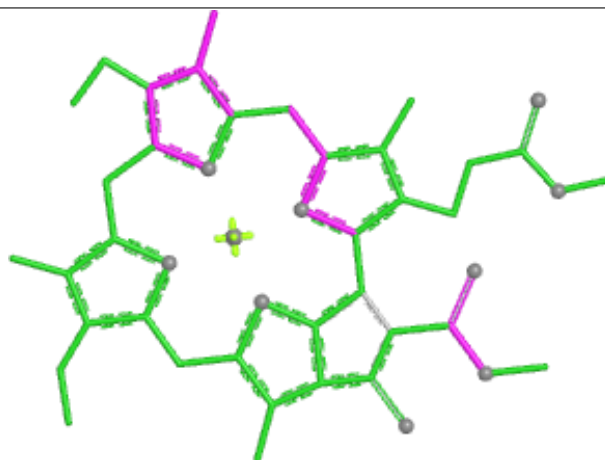
Rings



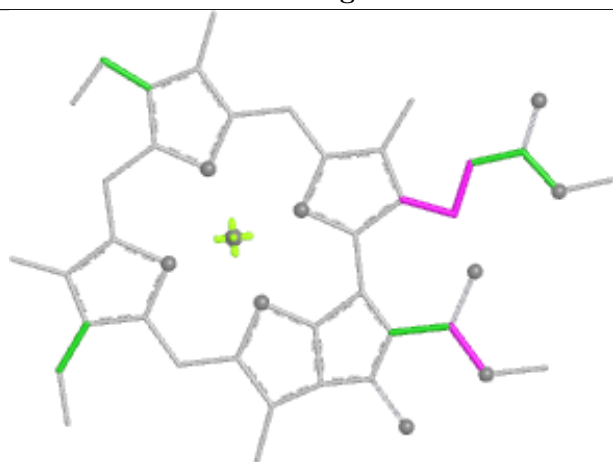
Ligand CLA H 312



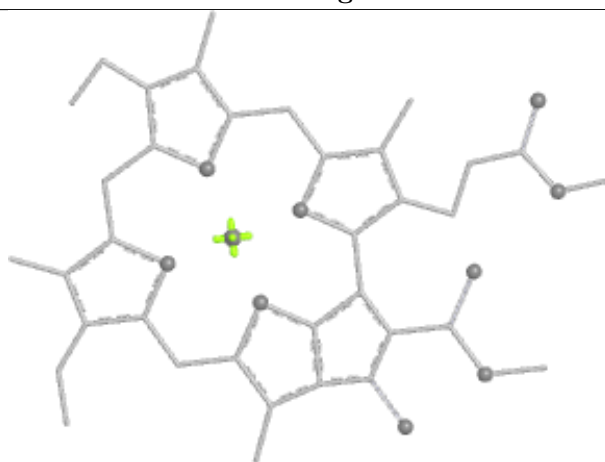
Bond lengths



Bond angles

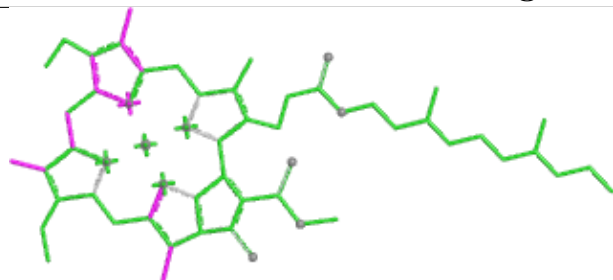


Torsions

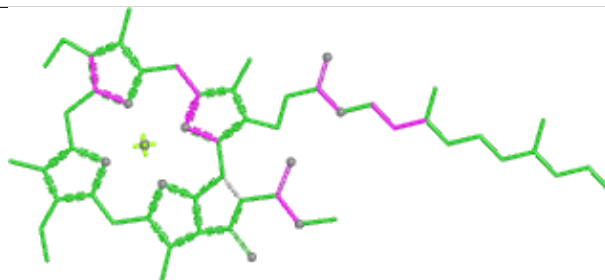


Rings

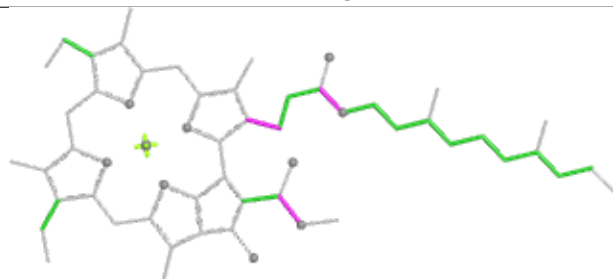
Ligand CLA a 819



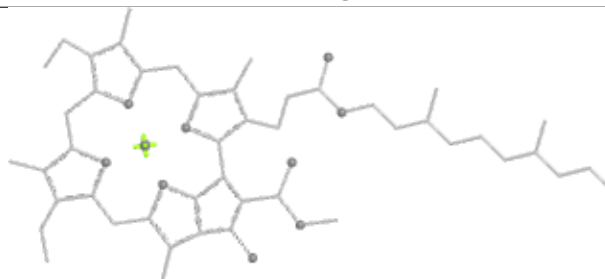
Bond lengths



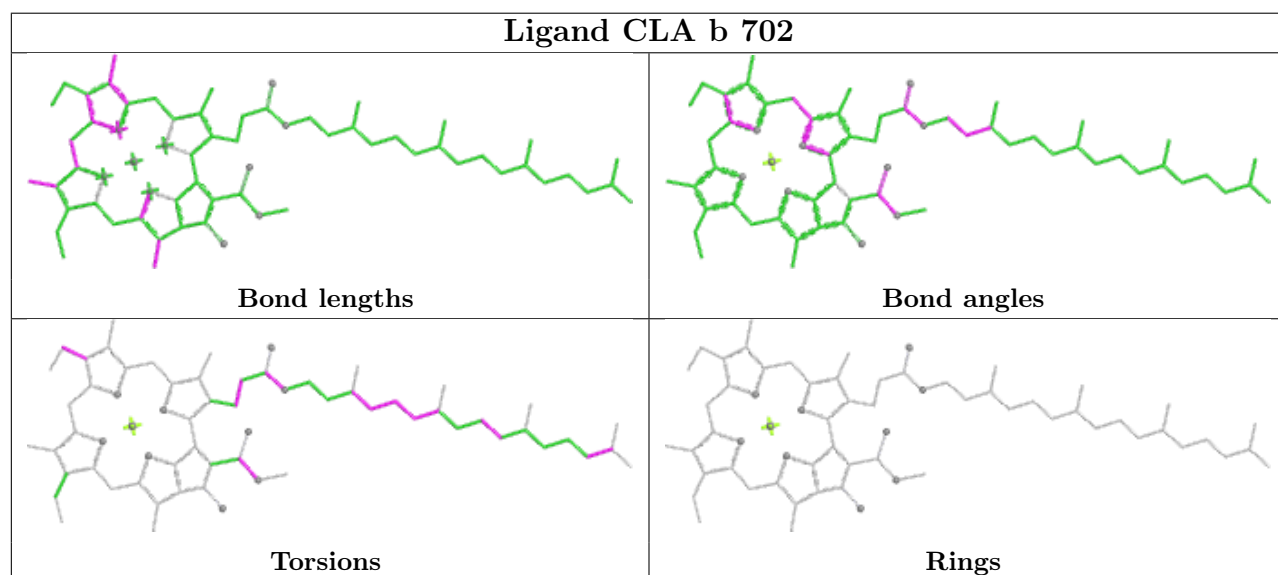
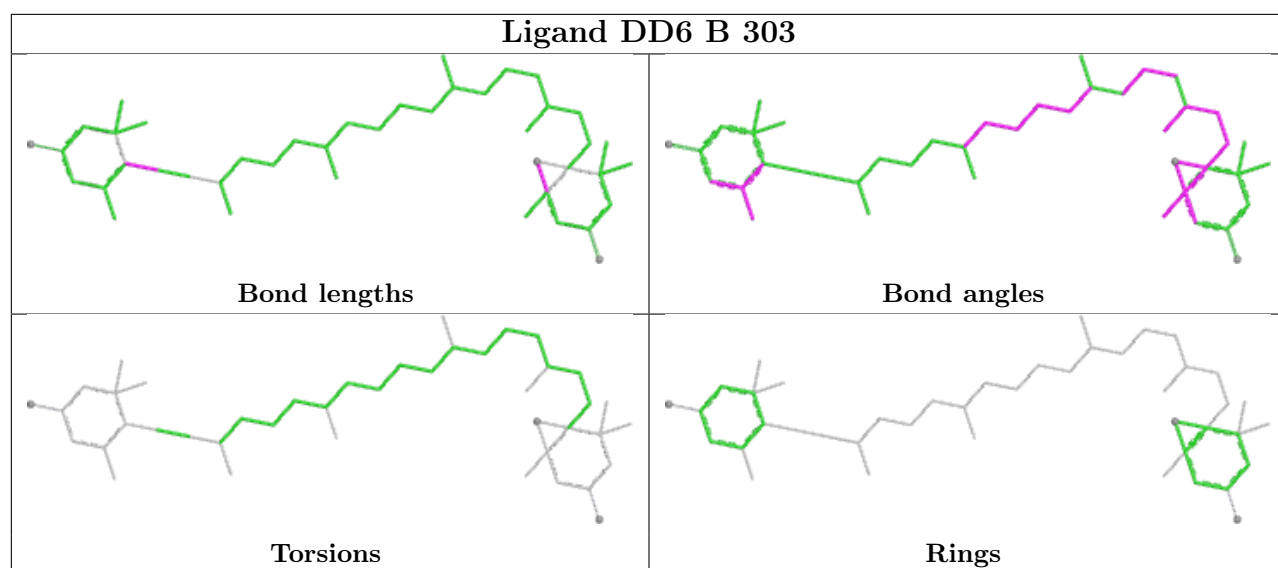
Bond angles

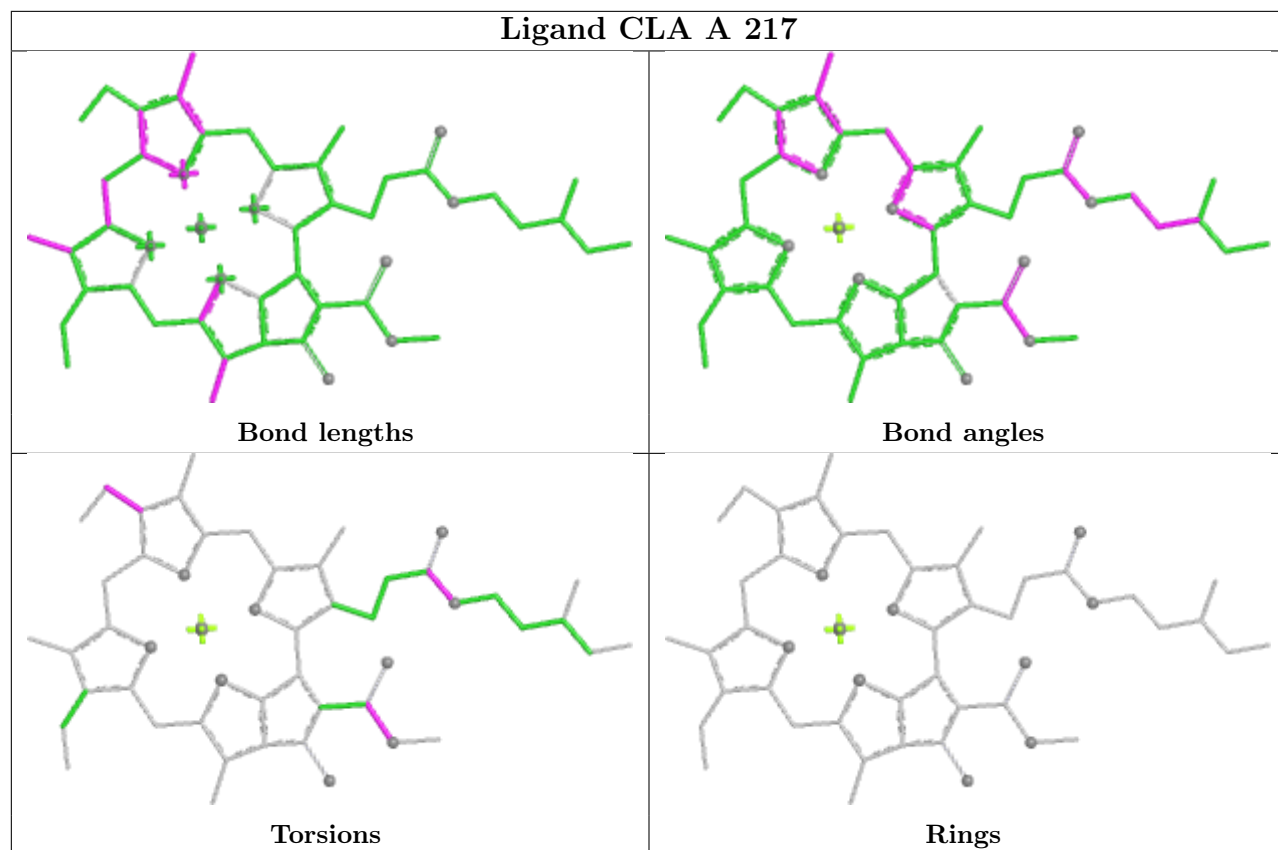


Torsions

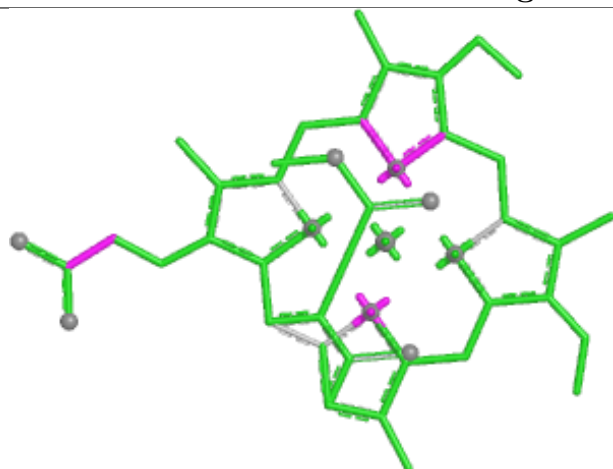


Rings

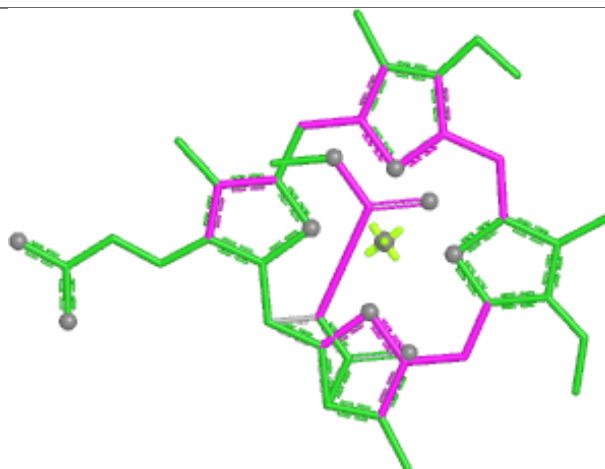




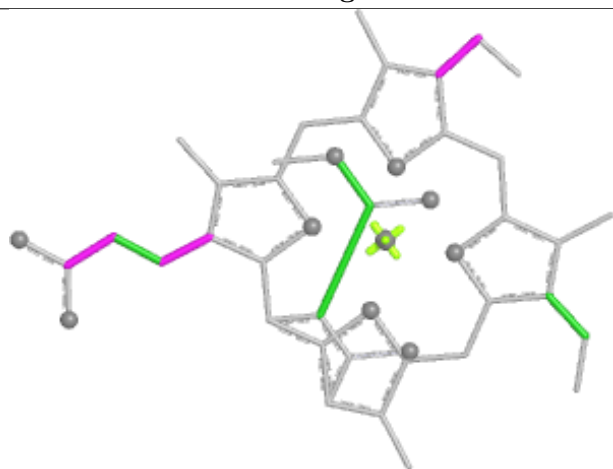
Ligand KC1 T 315



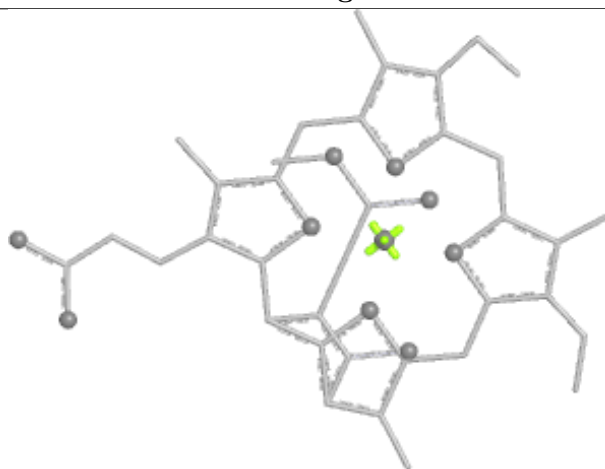
Bond lengths



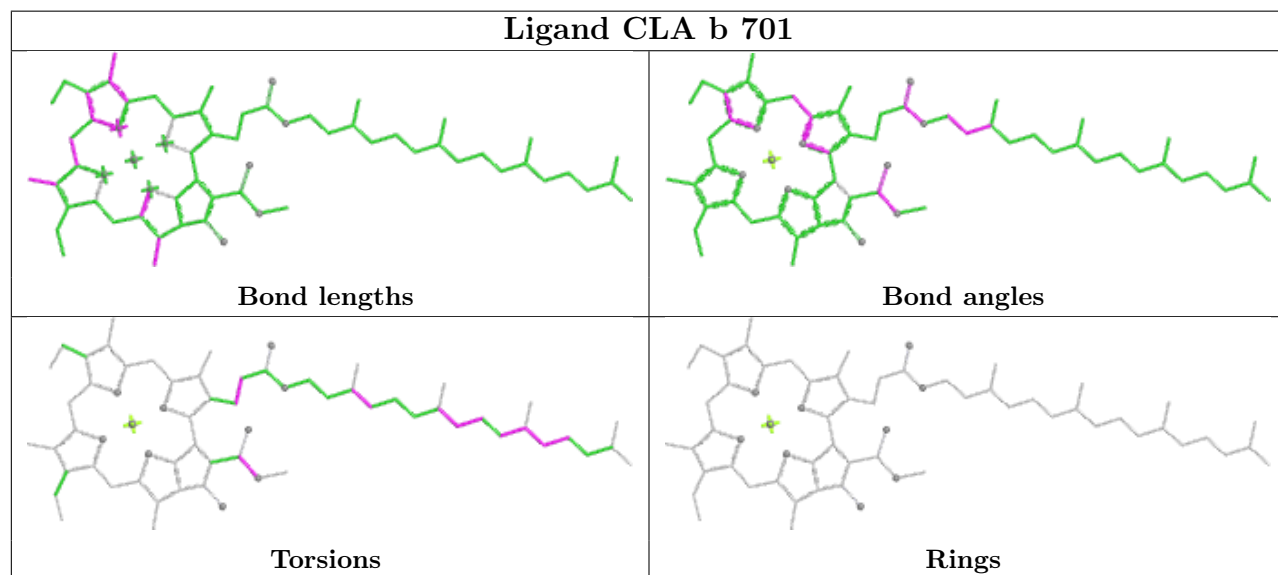
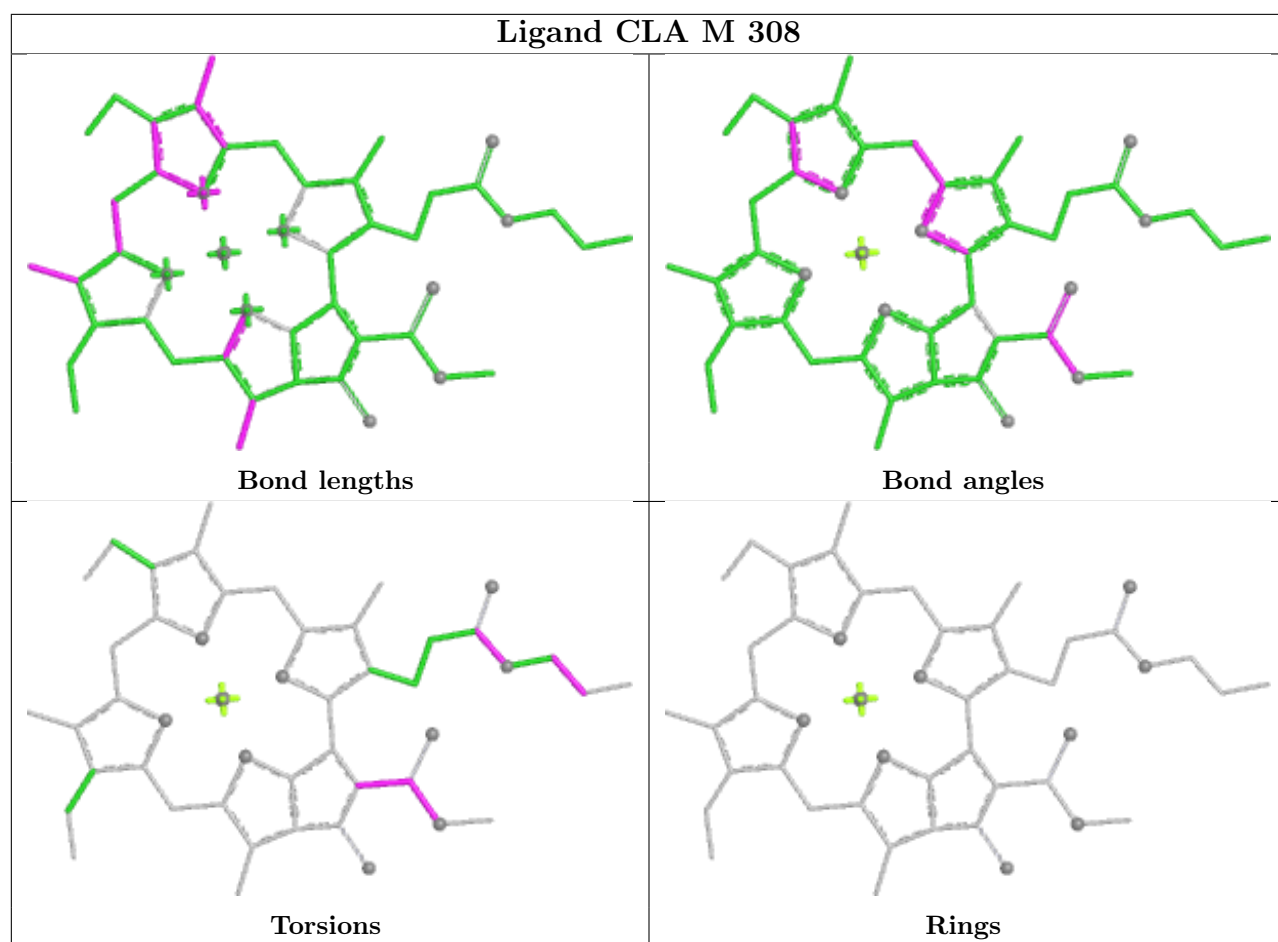
Bond angles

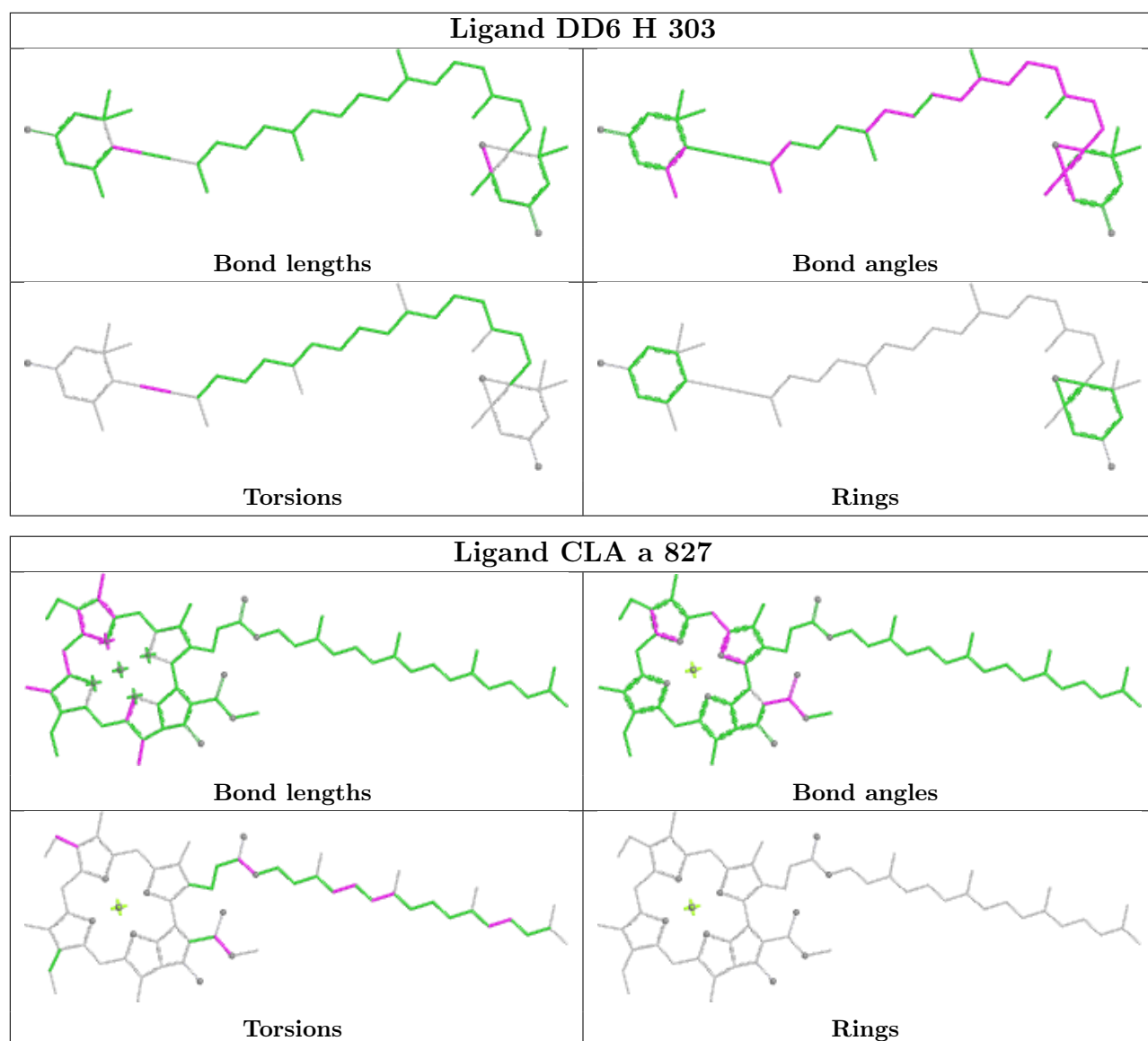


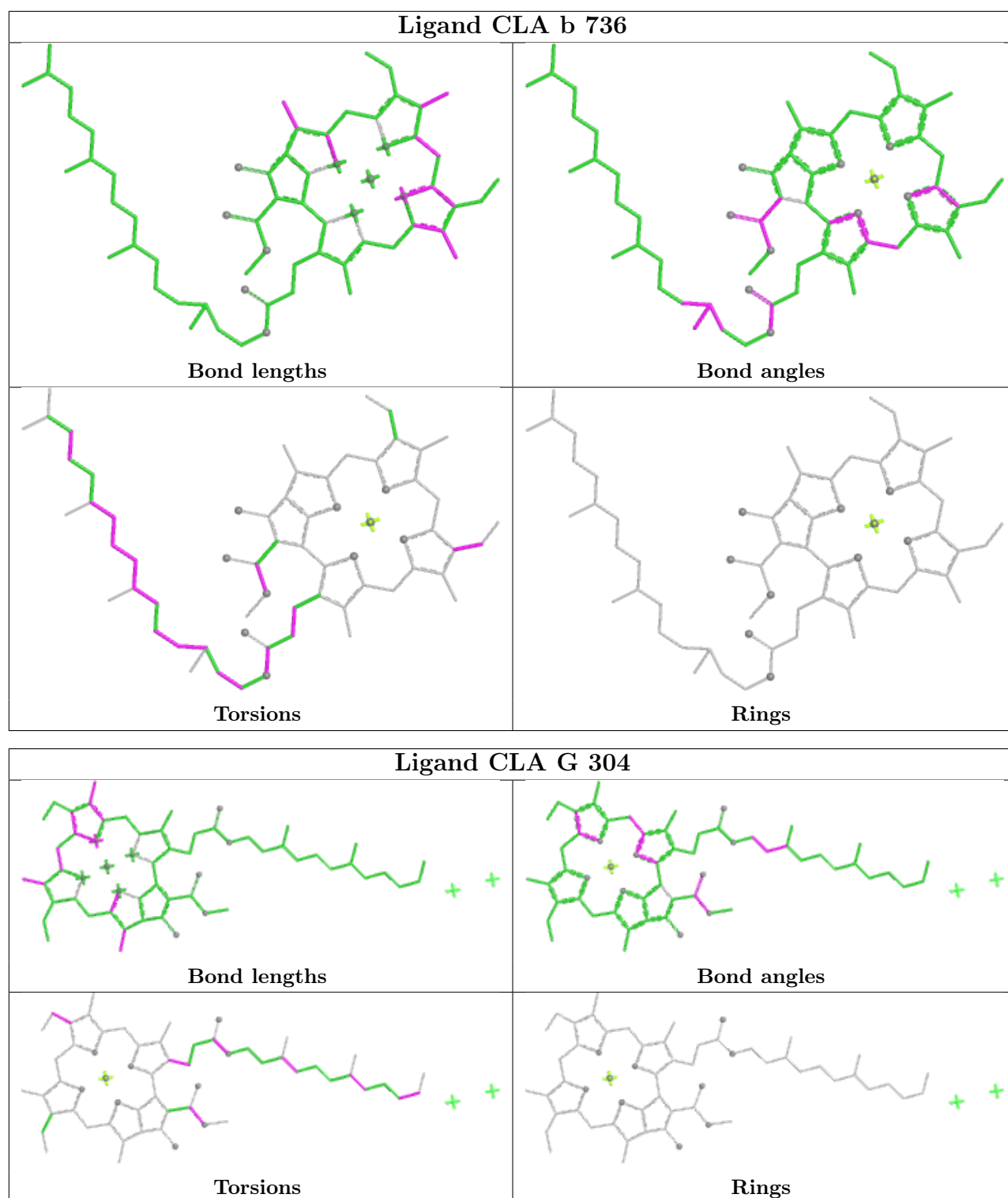
Torsions



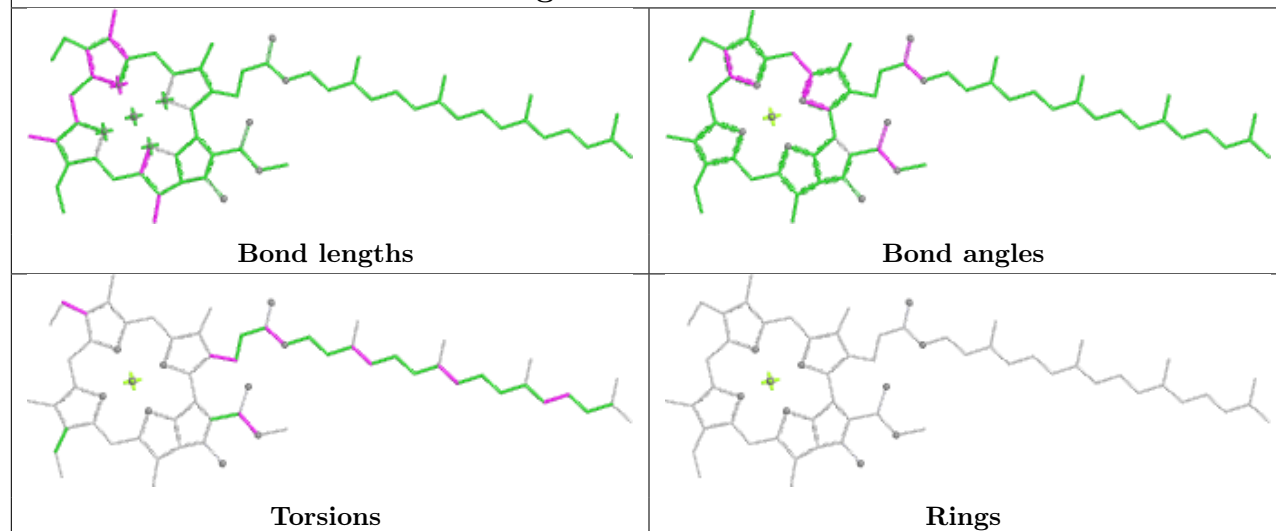
Rings



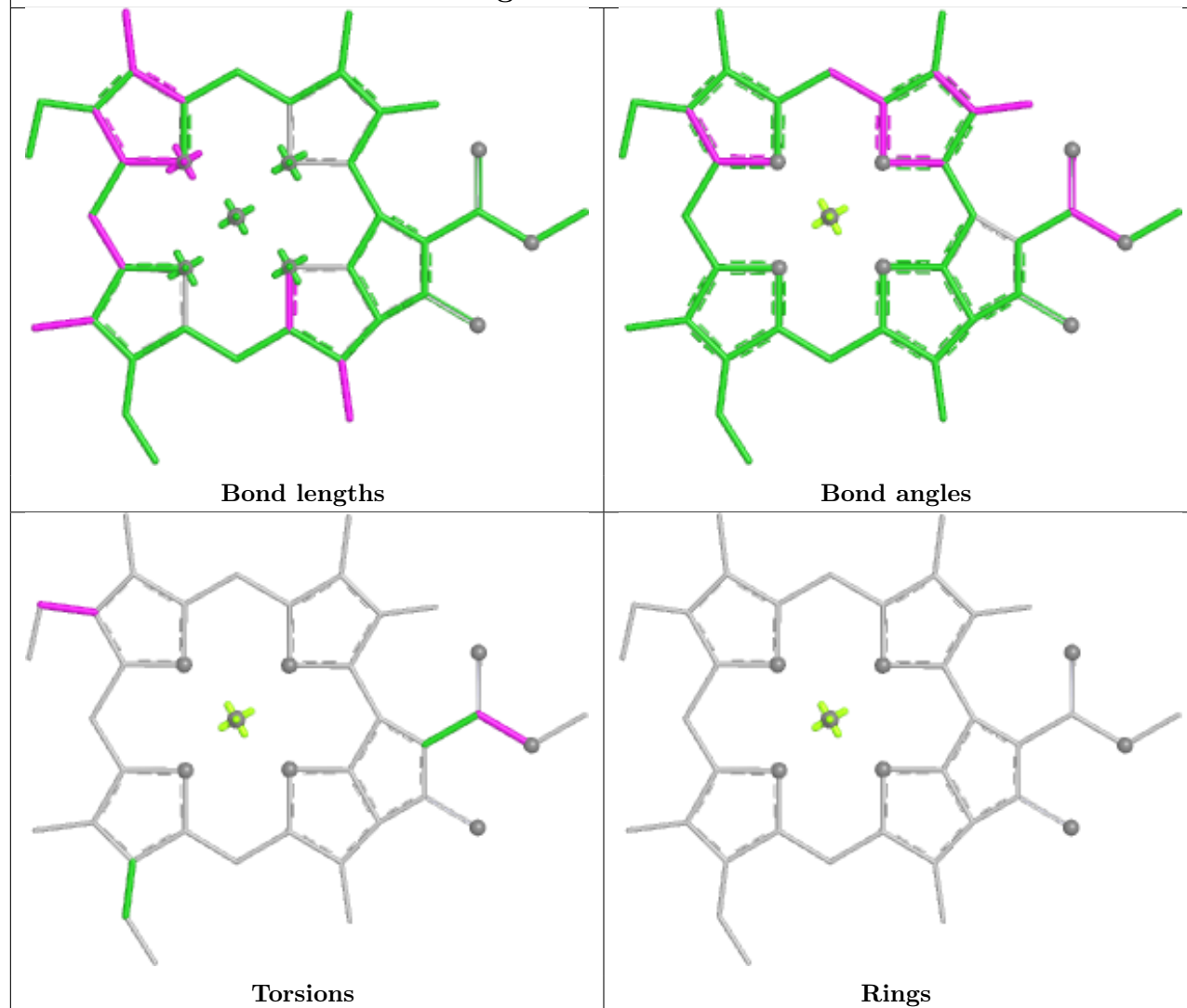




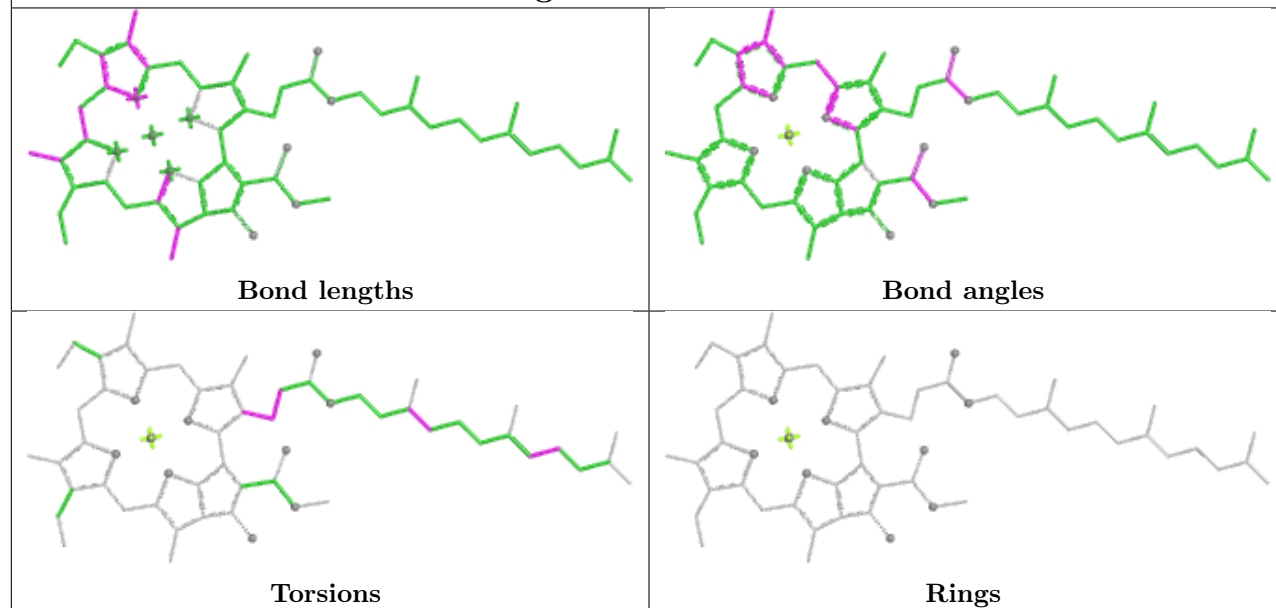
Ligand CLA a 820



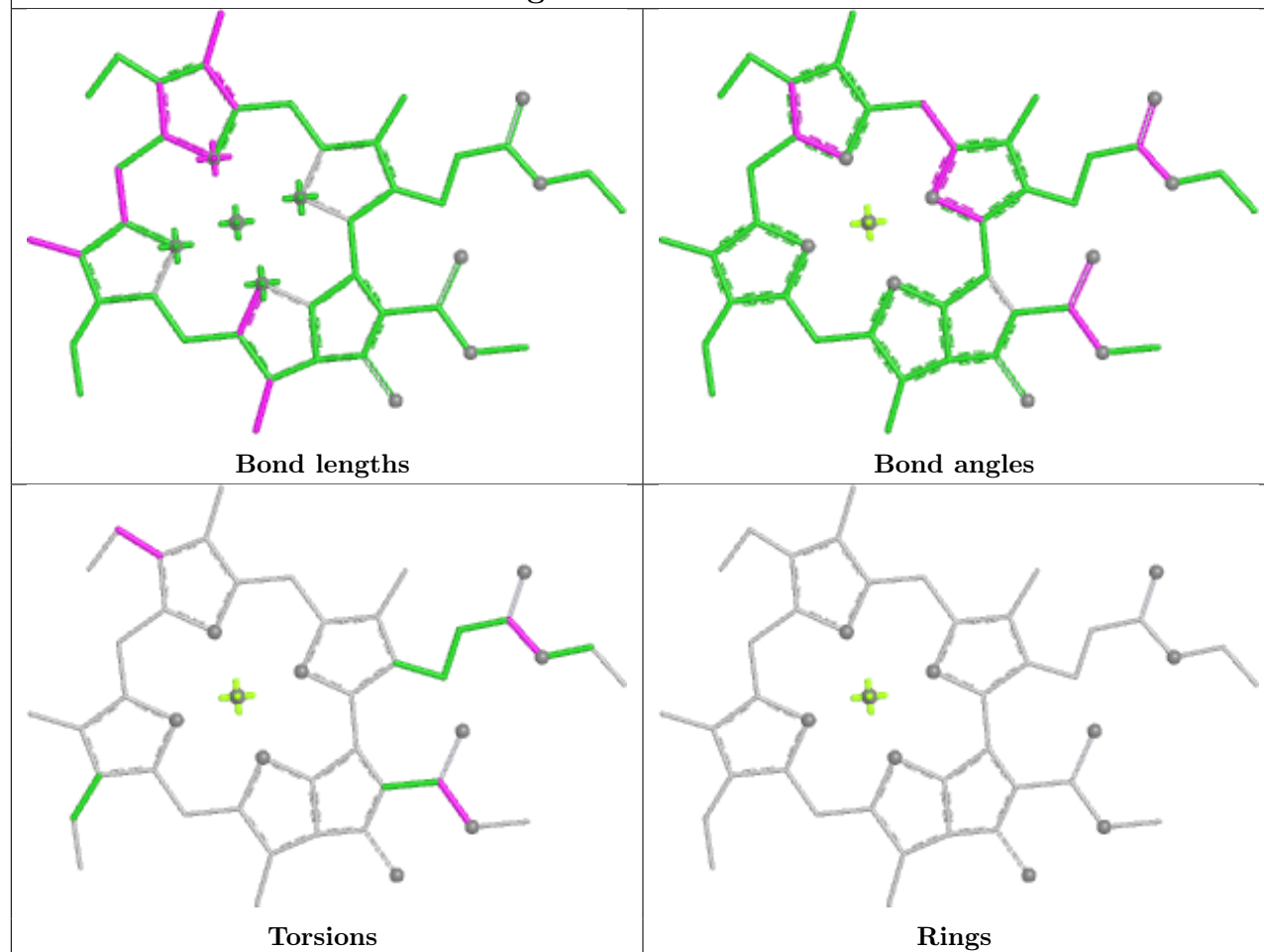
Ligand CLA L 315

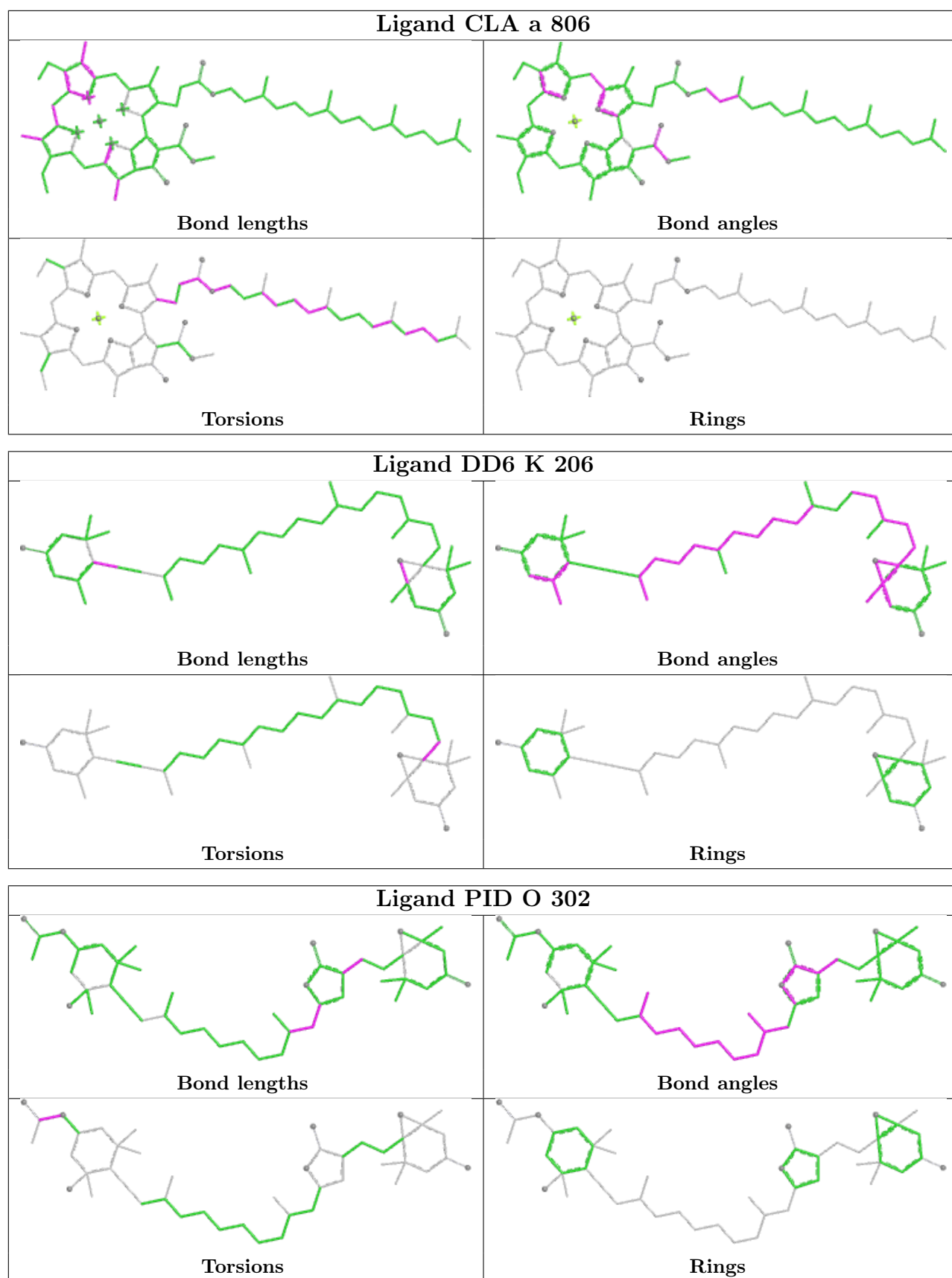


Ligand CLA h 201

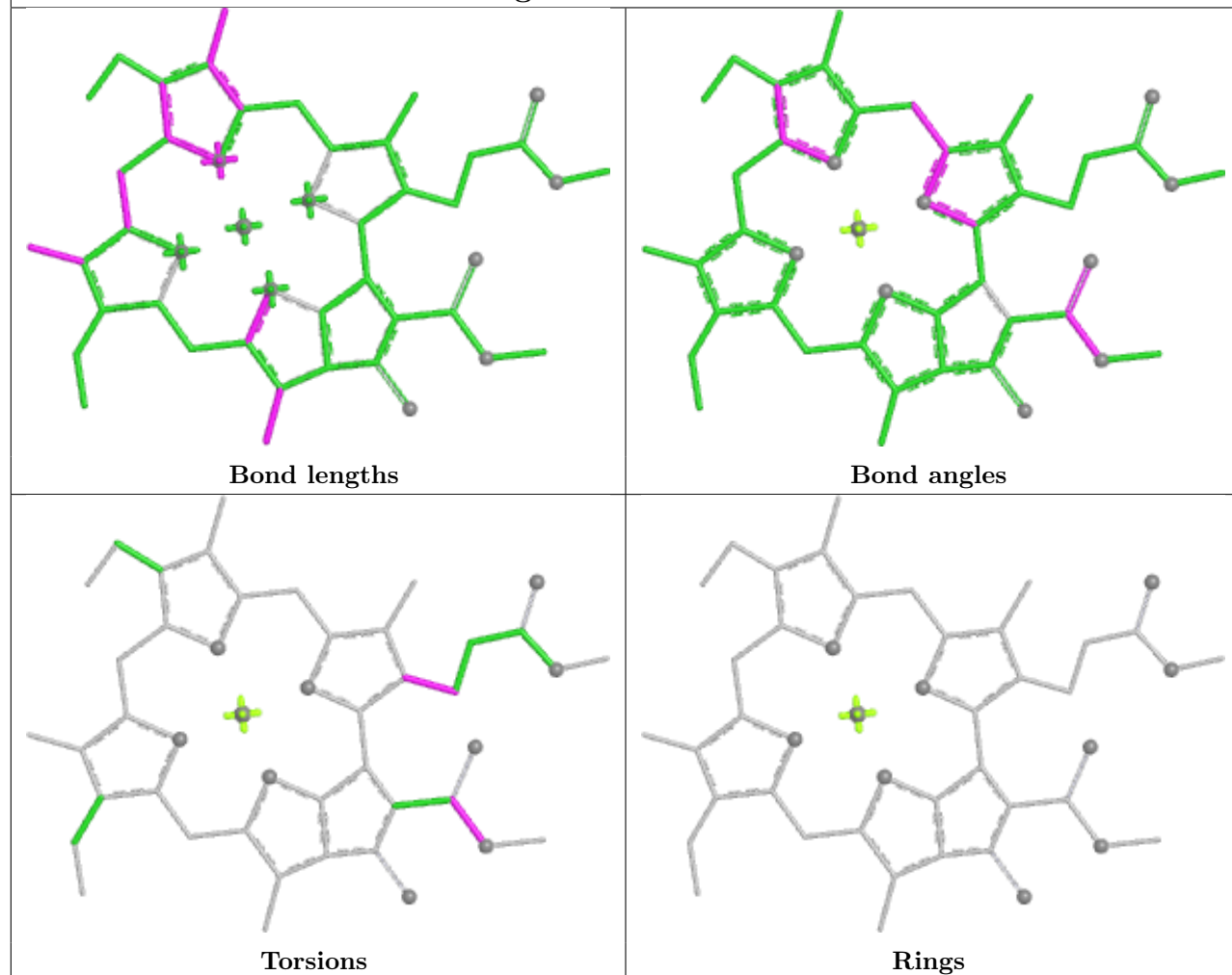


Ligand CLA C 308

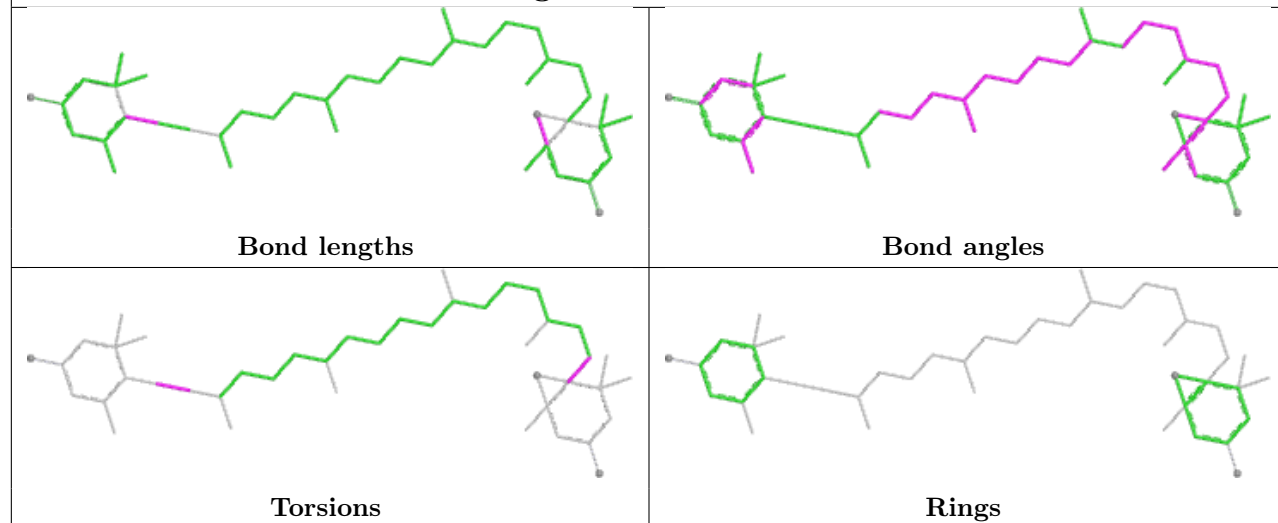




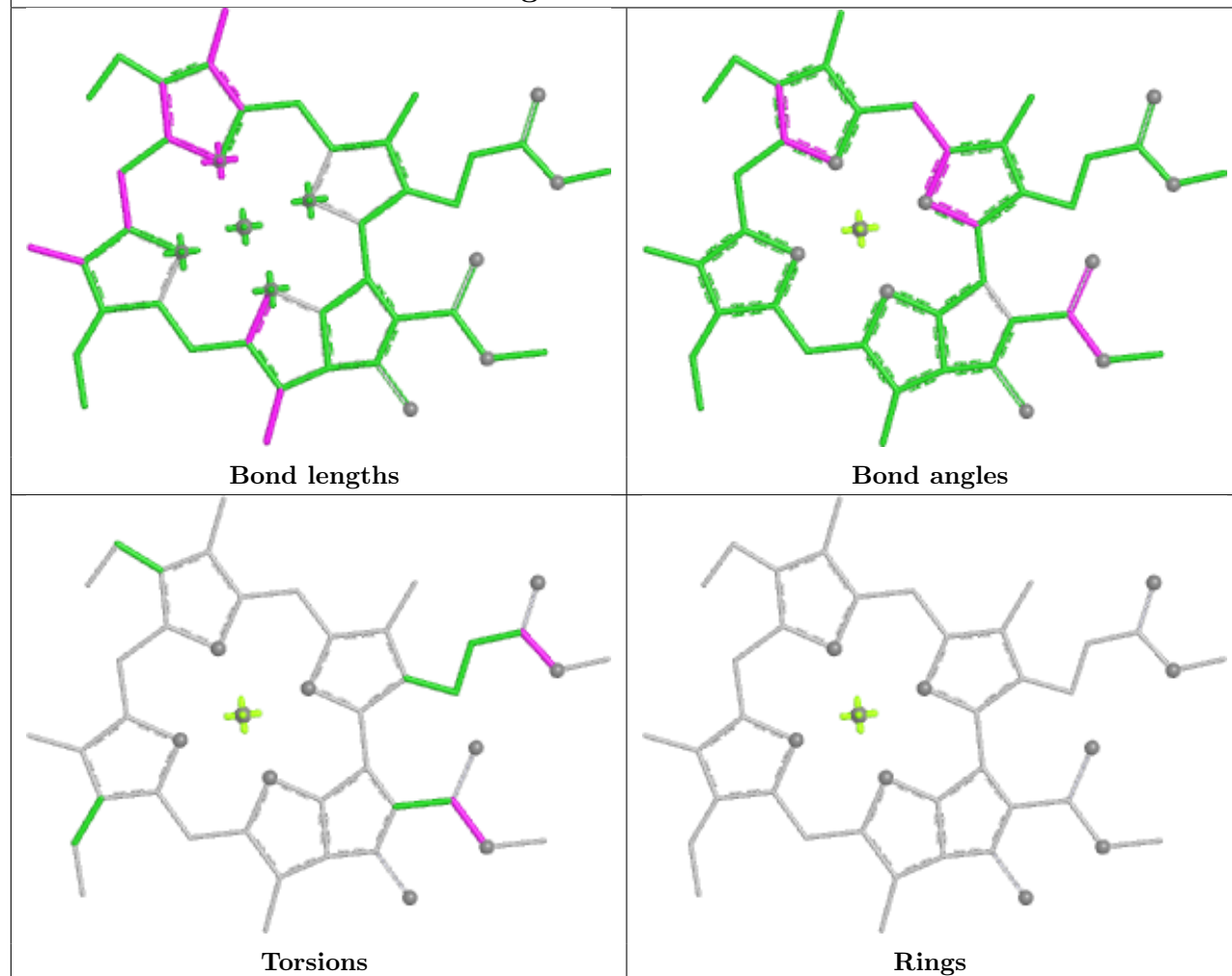
Ligand CLA F 308



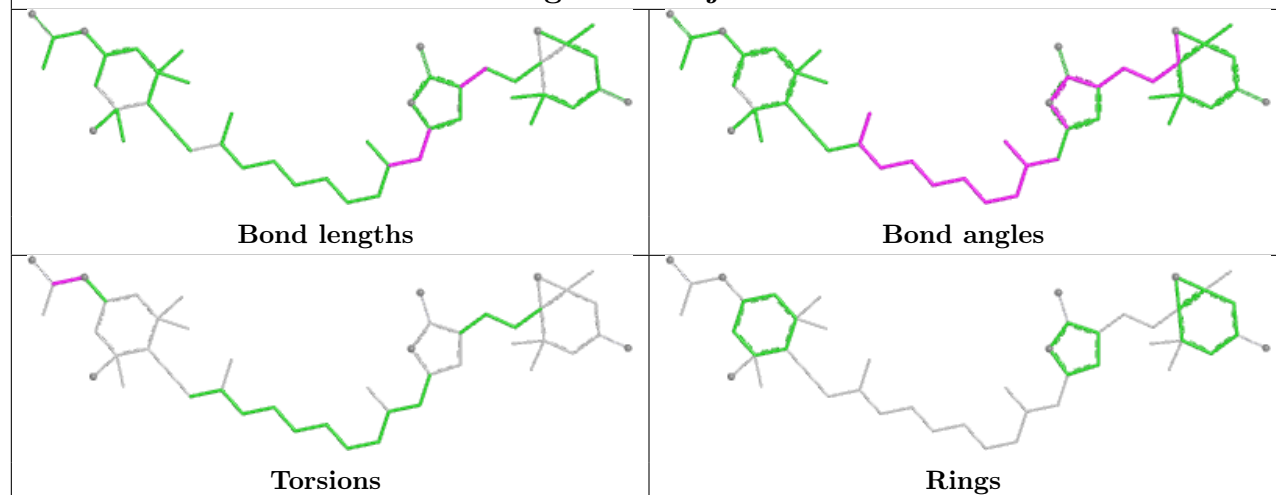
Ligand DD6 B 302

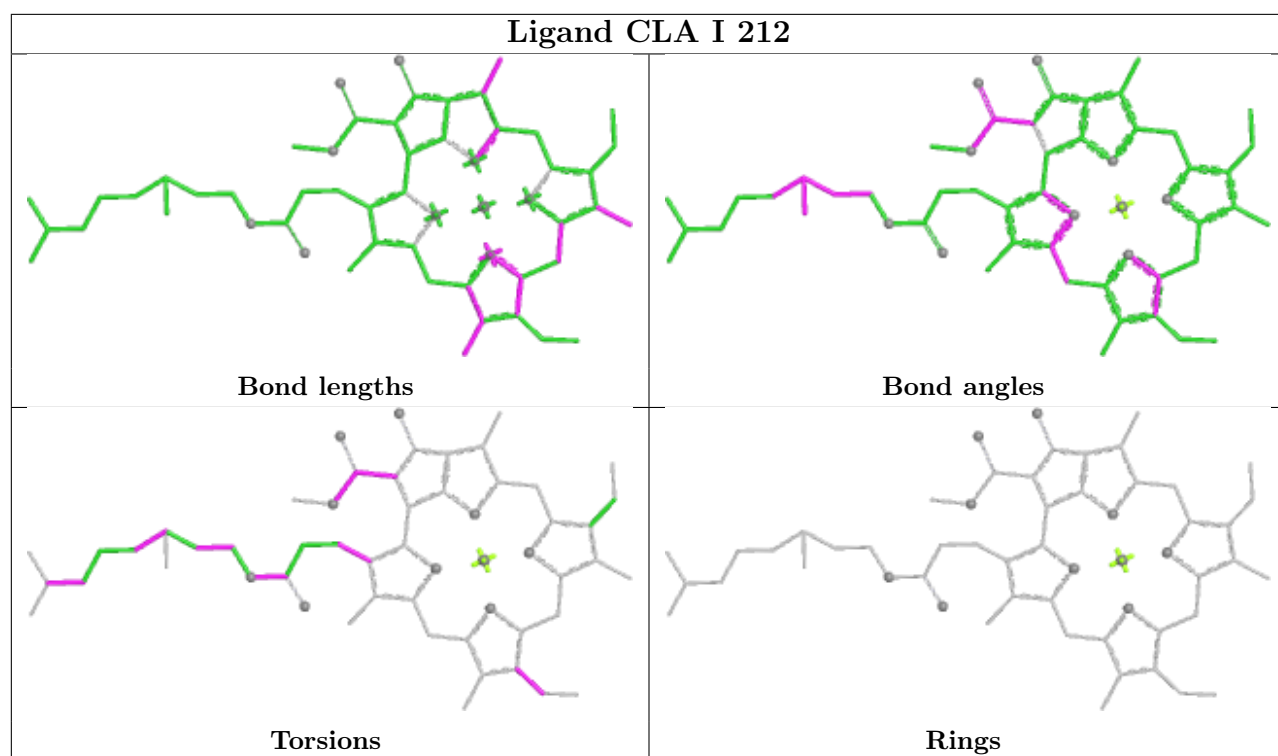


Ligand CLA f 802

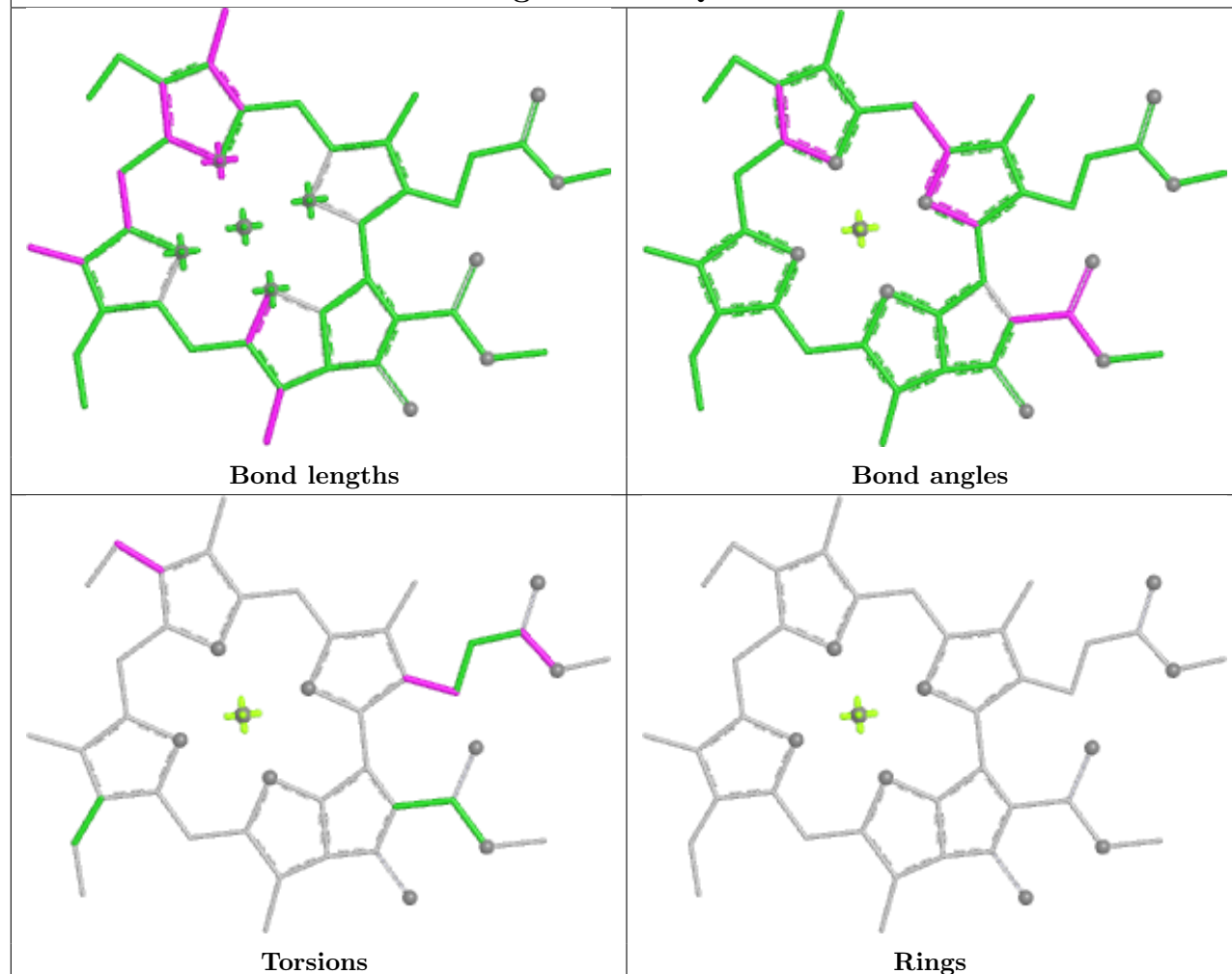


Ligand PID j 101

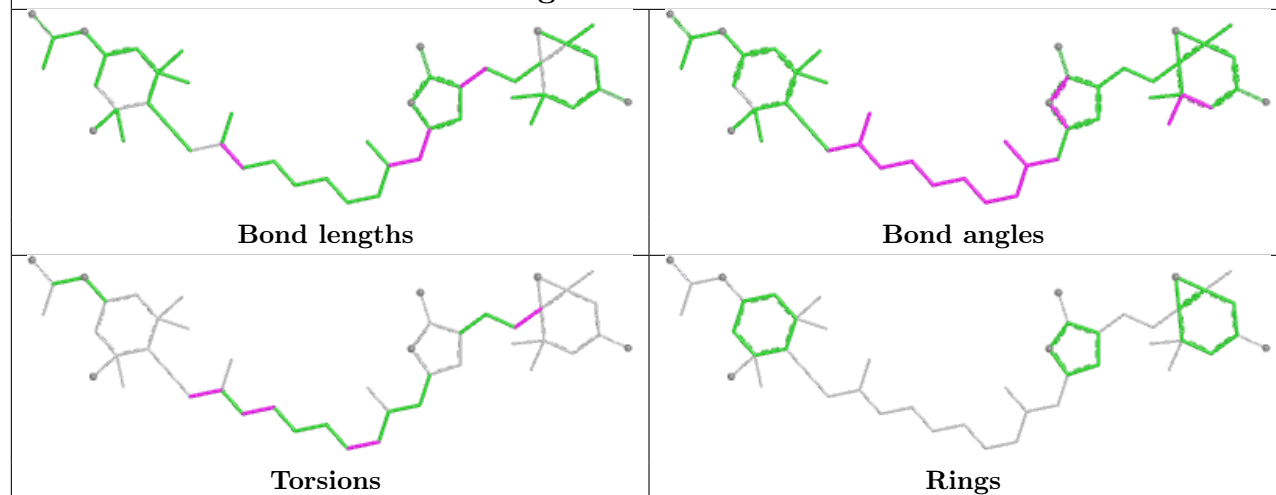


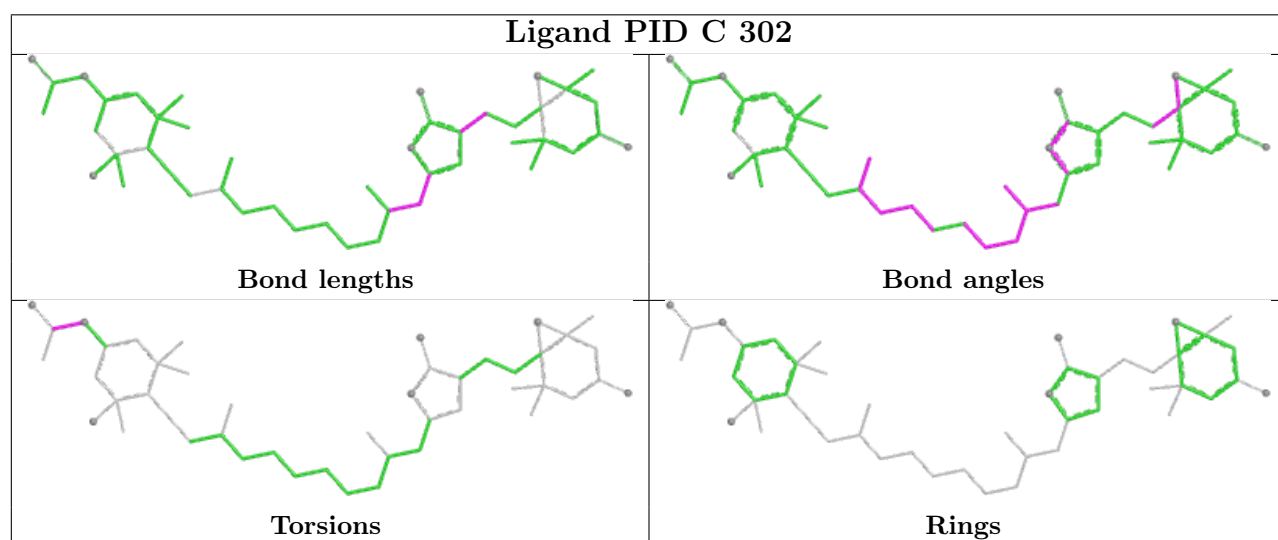
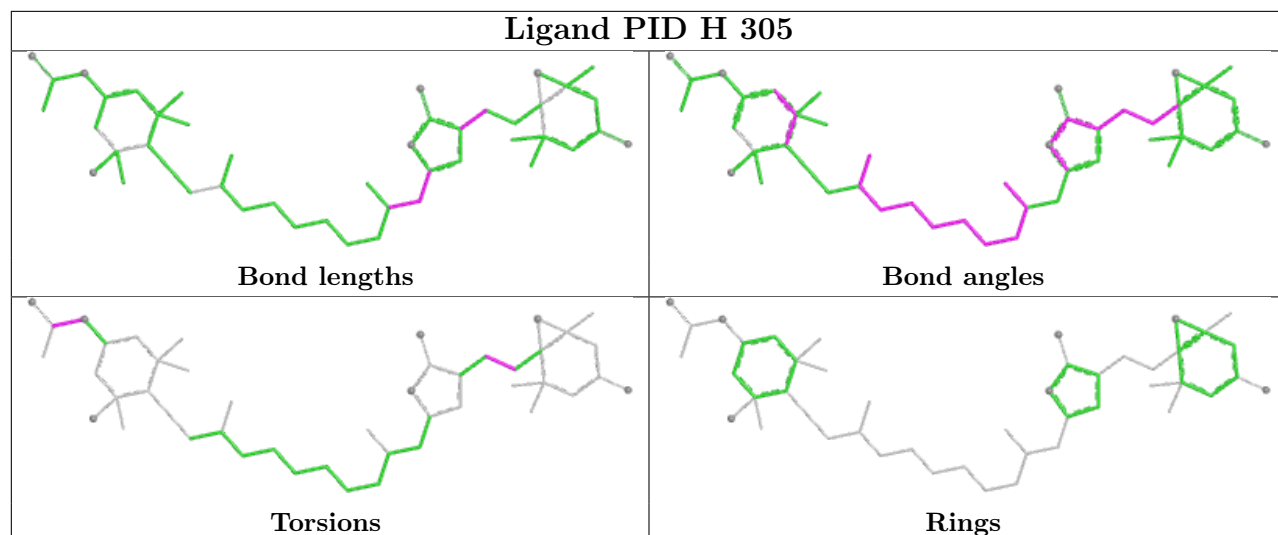


Ligand CLA Q 312

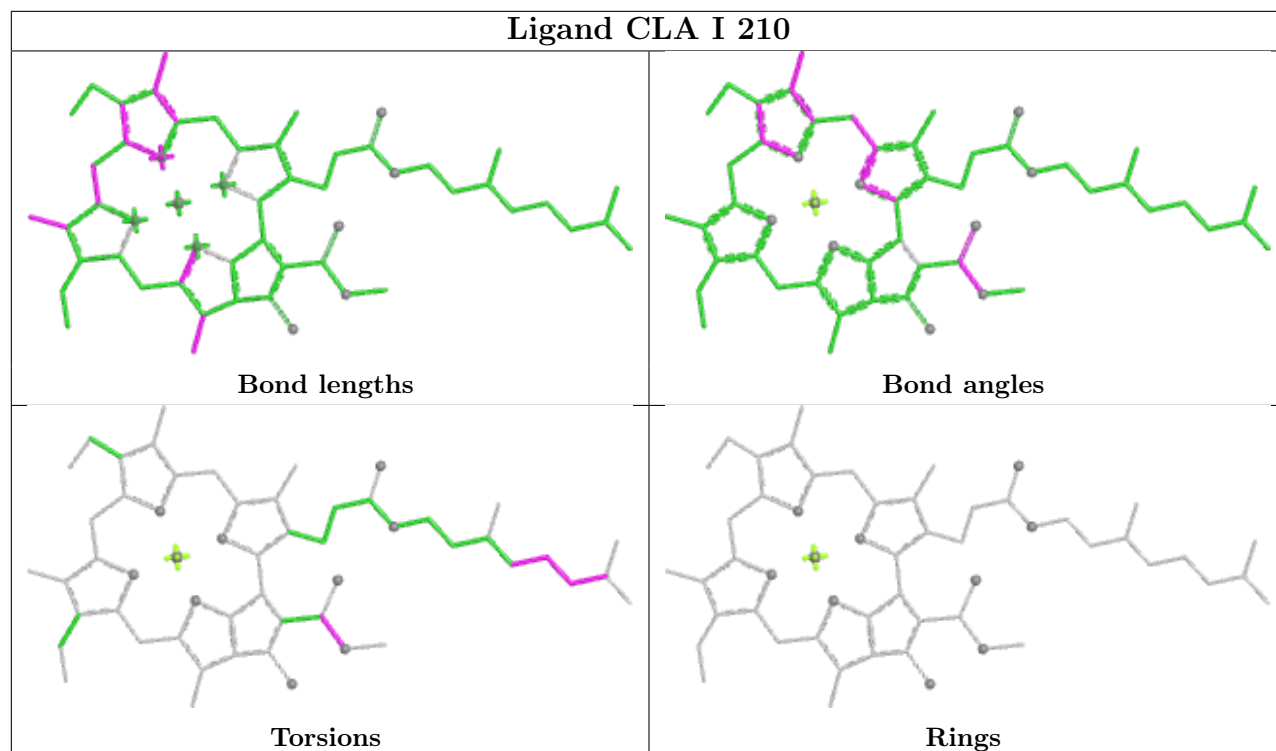


Ligand PID E 301

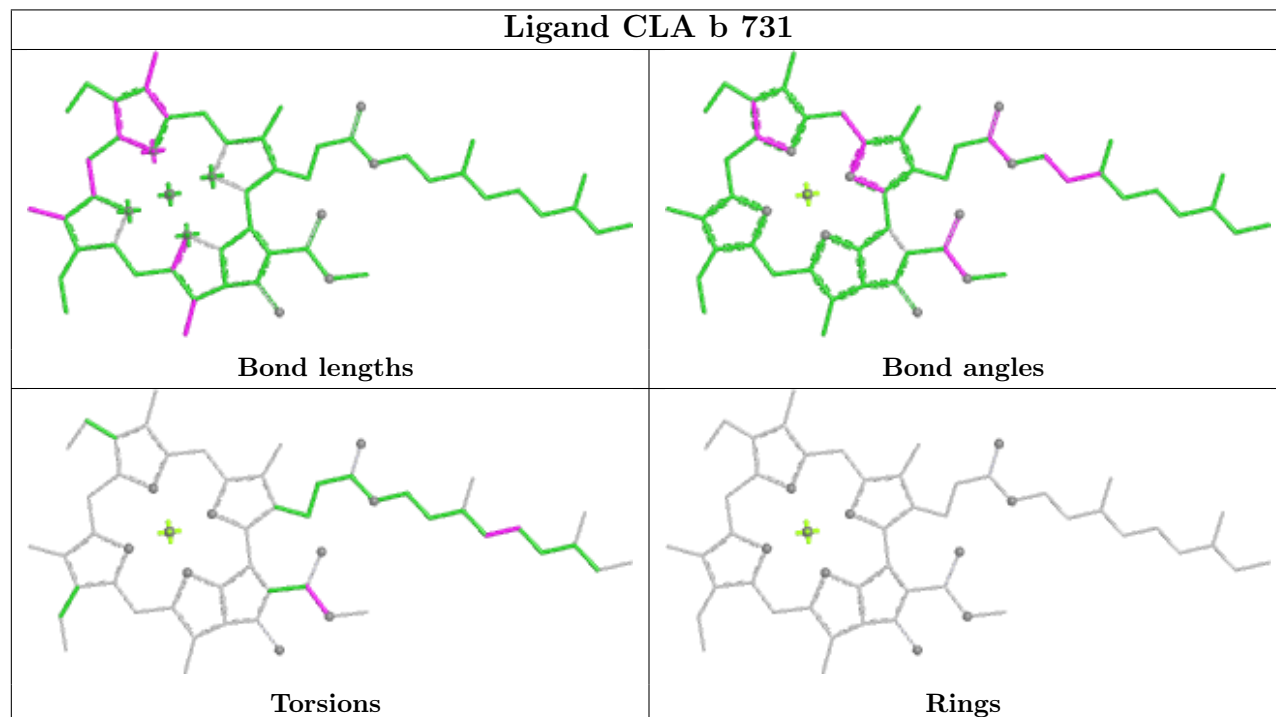




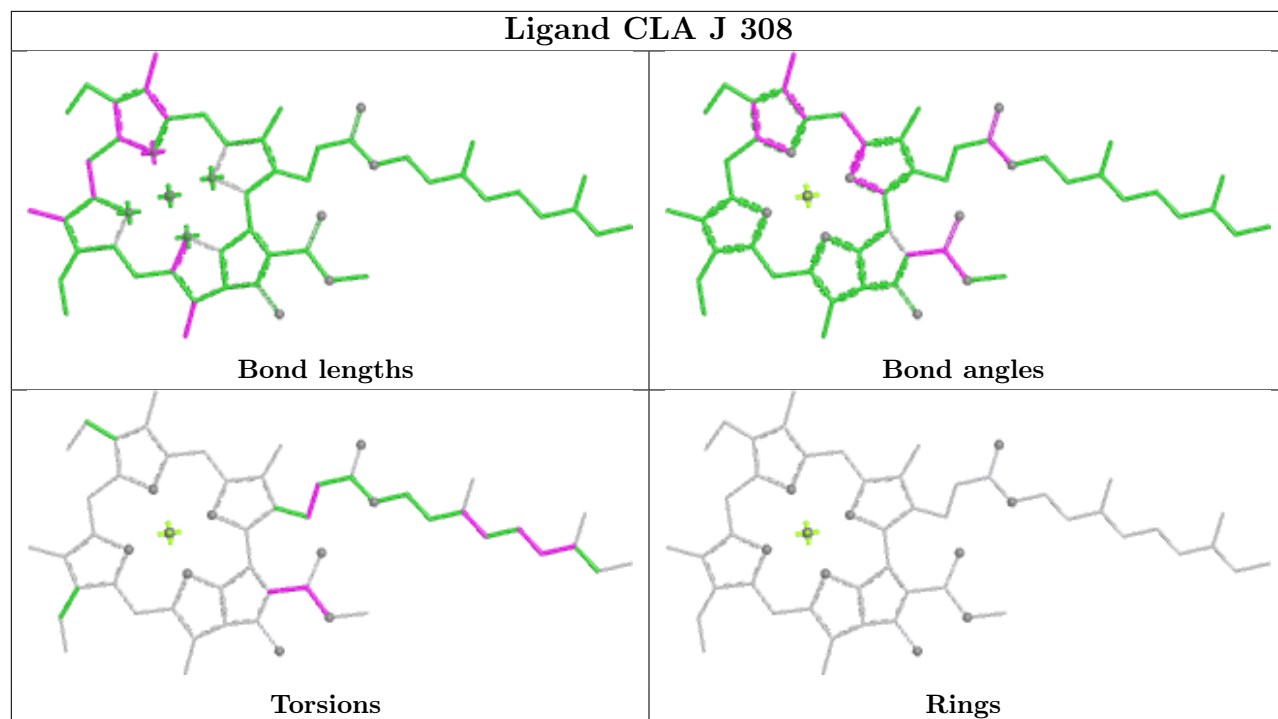
Ligand CLA I 210



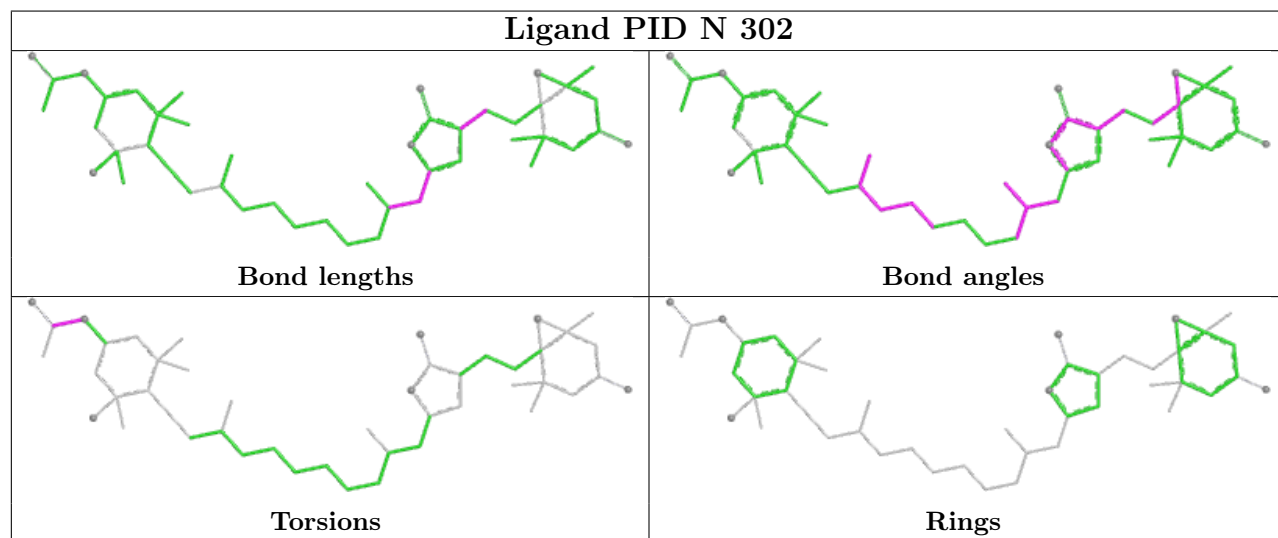
Ligand CLA b 731



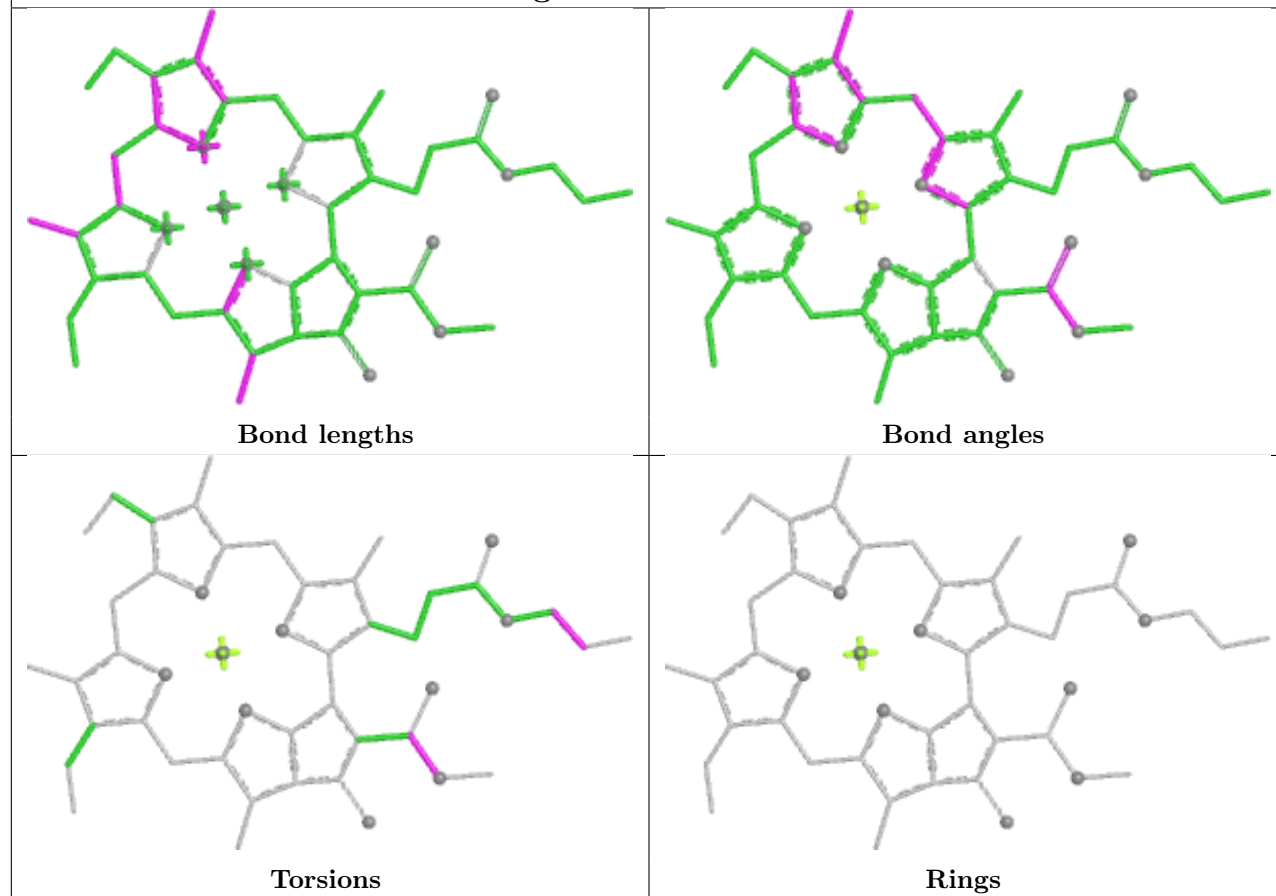
Ligand CLA J 308



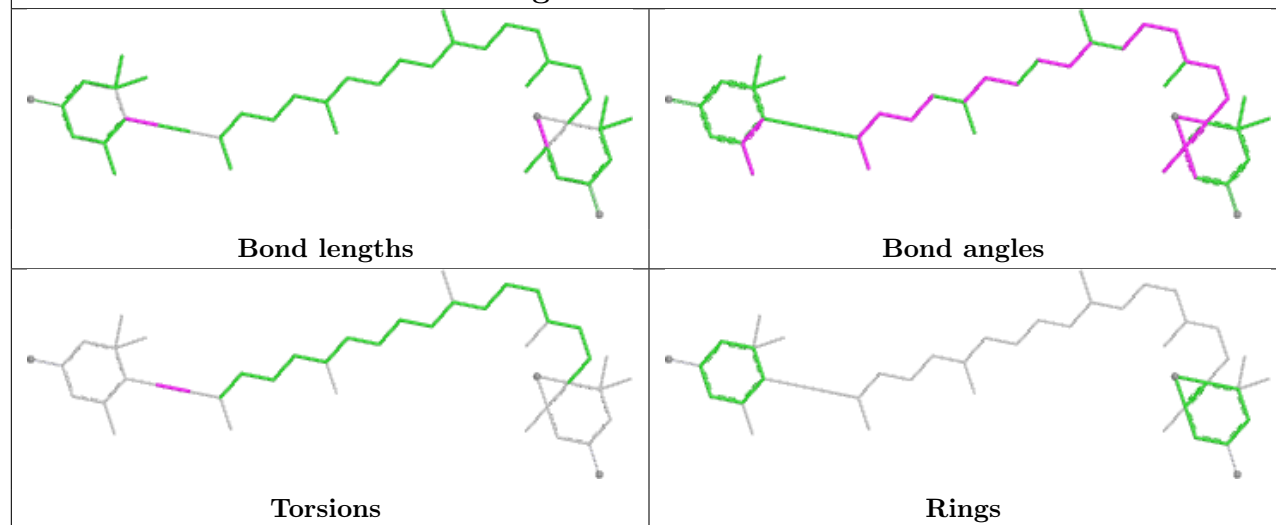
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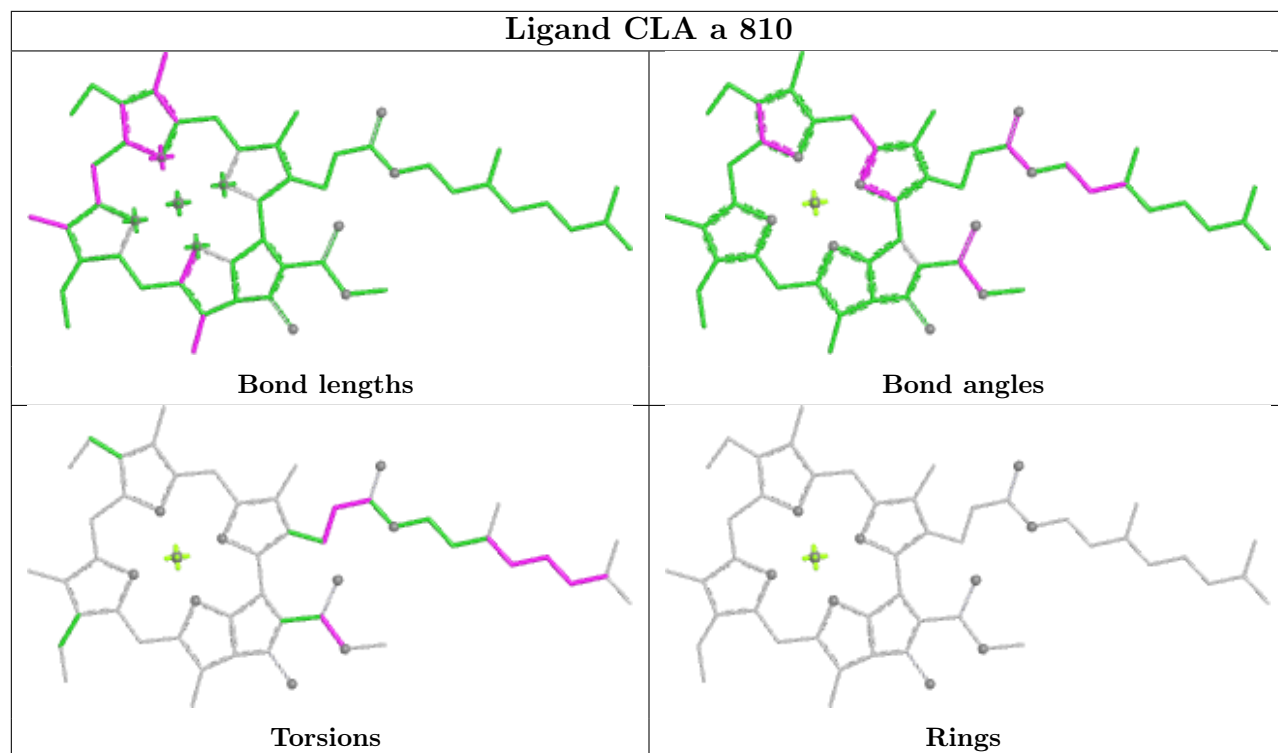
Ligand CLA E 314



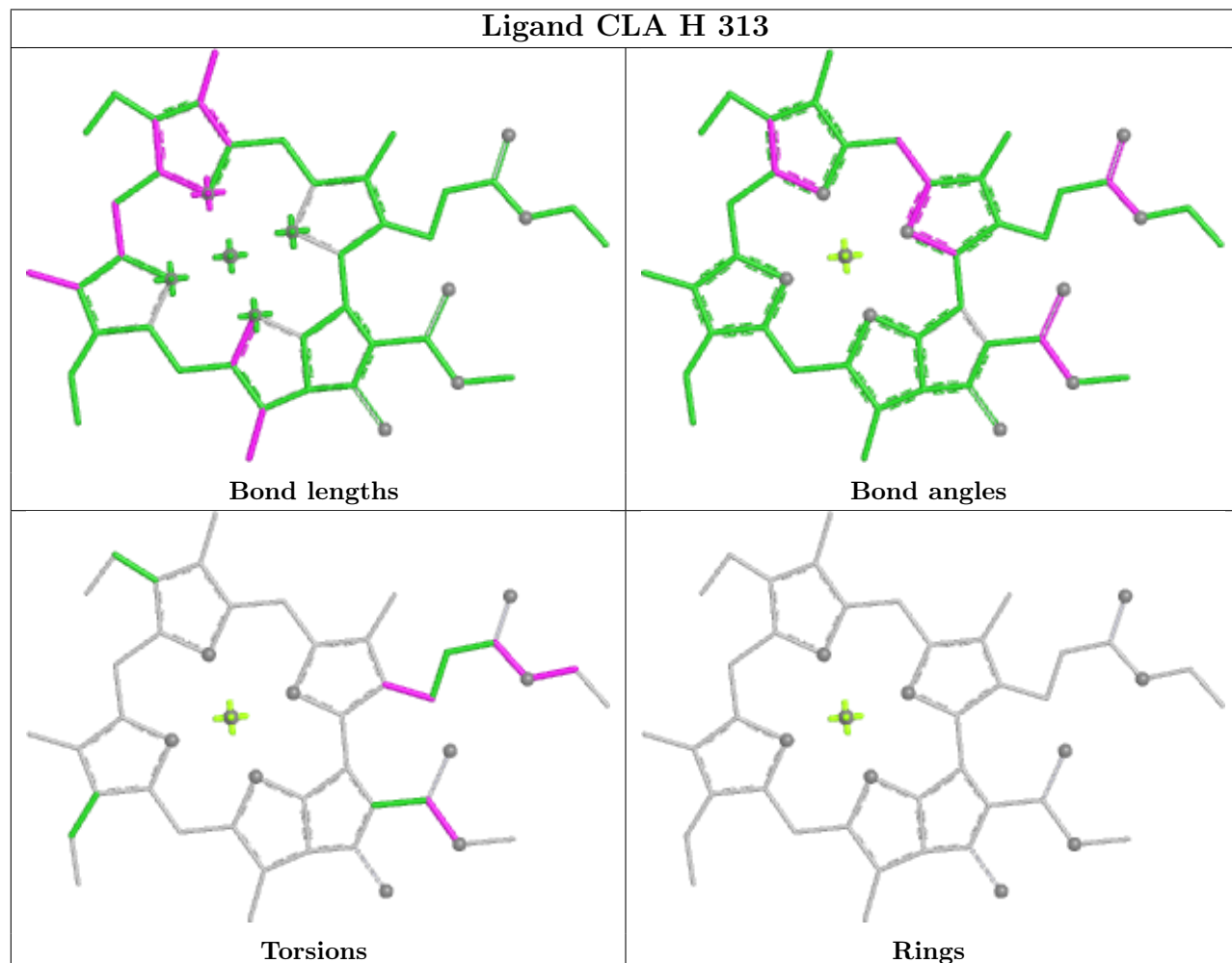
Ligand DD6 A 202



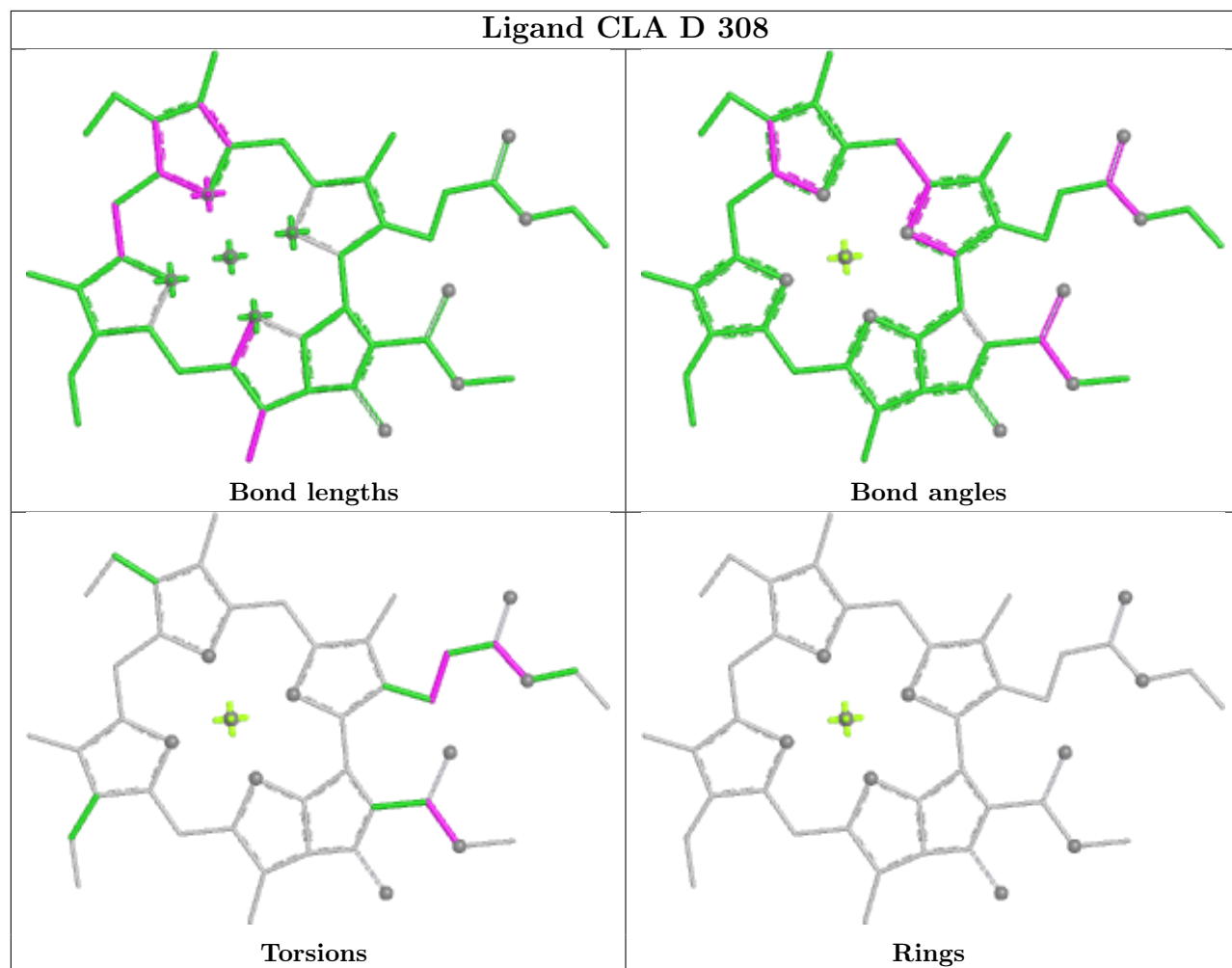
Ligand CLA a 810



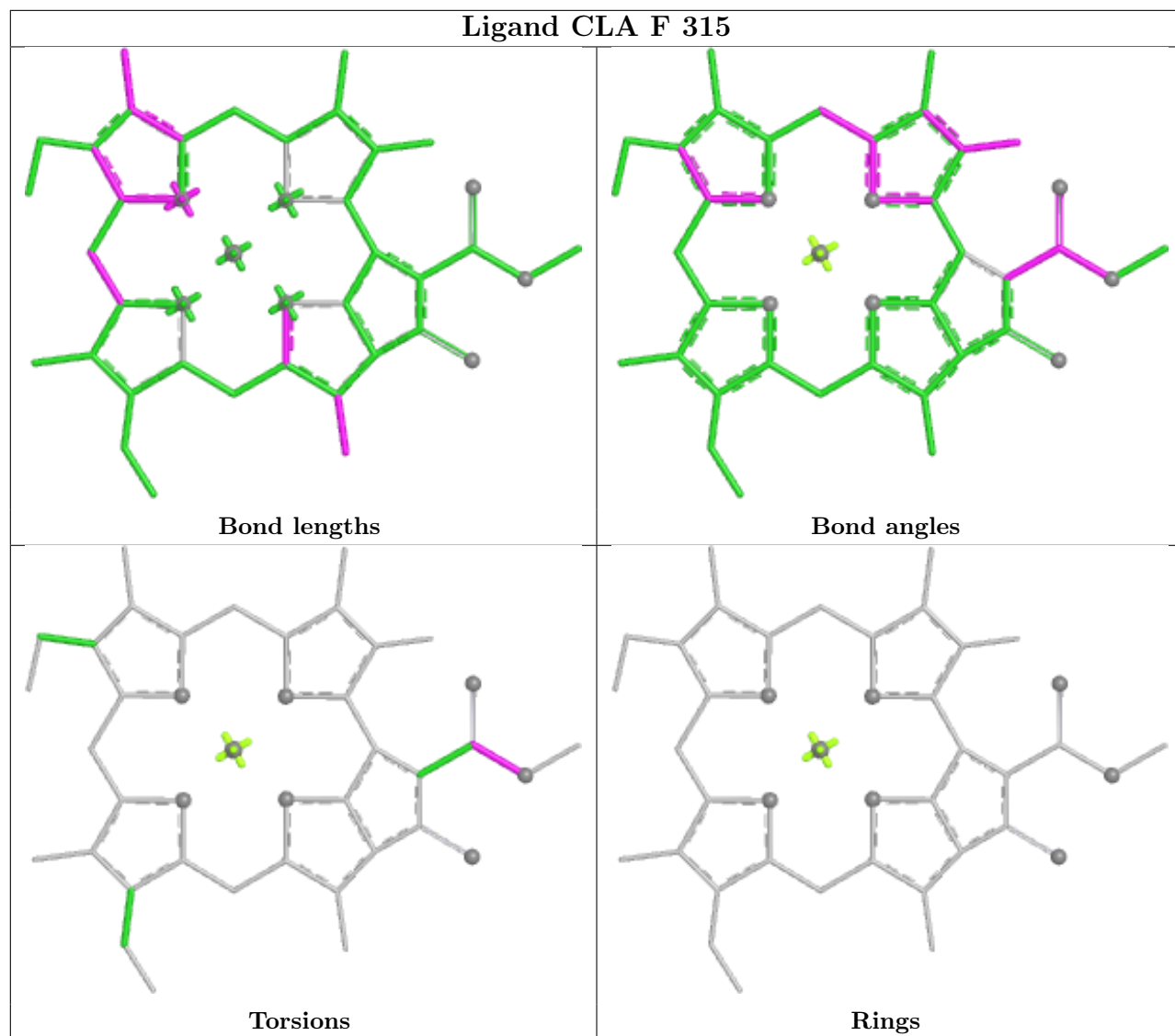
Ligand CLA H 313



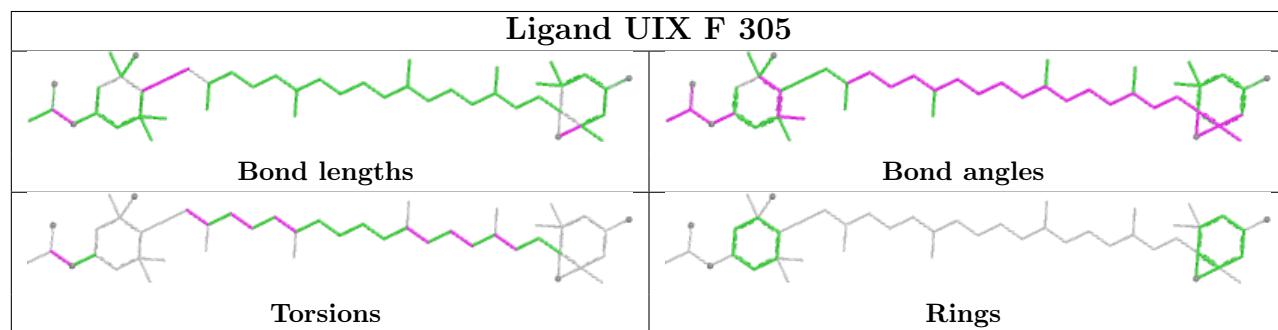
Ligand CLA D 308



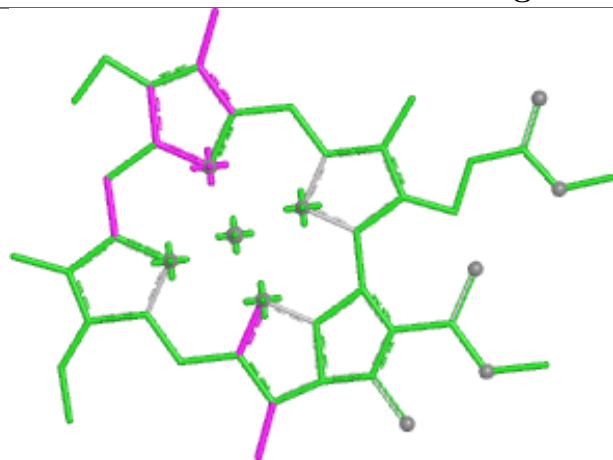
Ligand CLA F 315



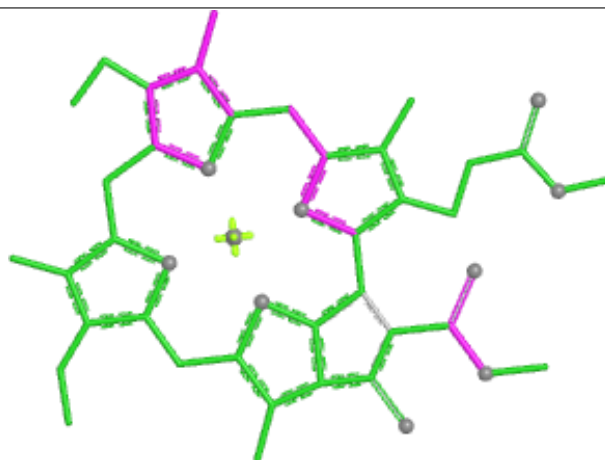
Ligand UIX F 305



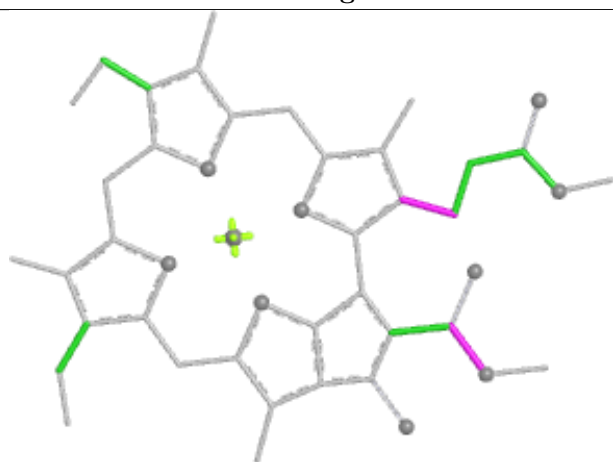
Ligand CLA O 313



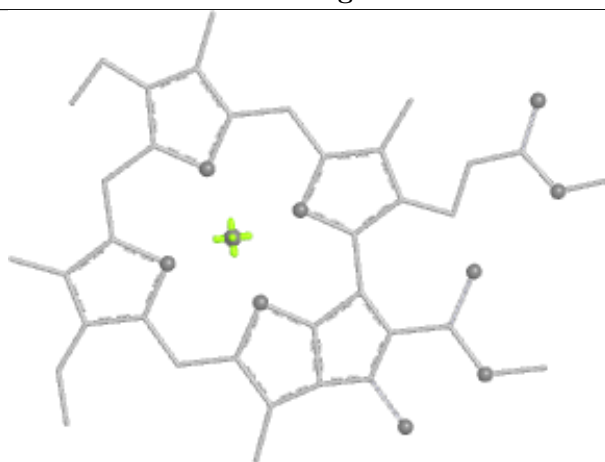
Bond lengths



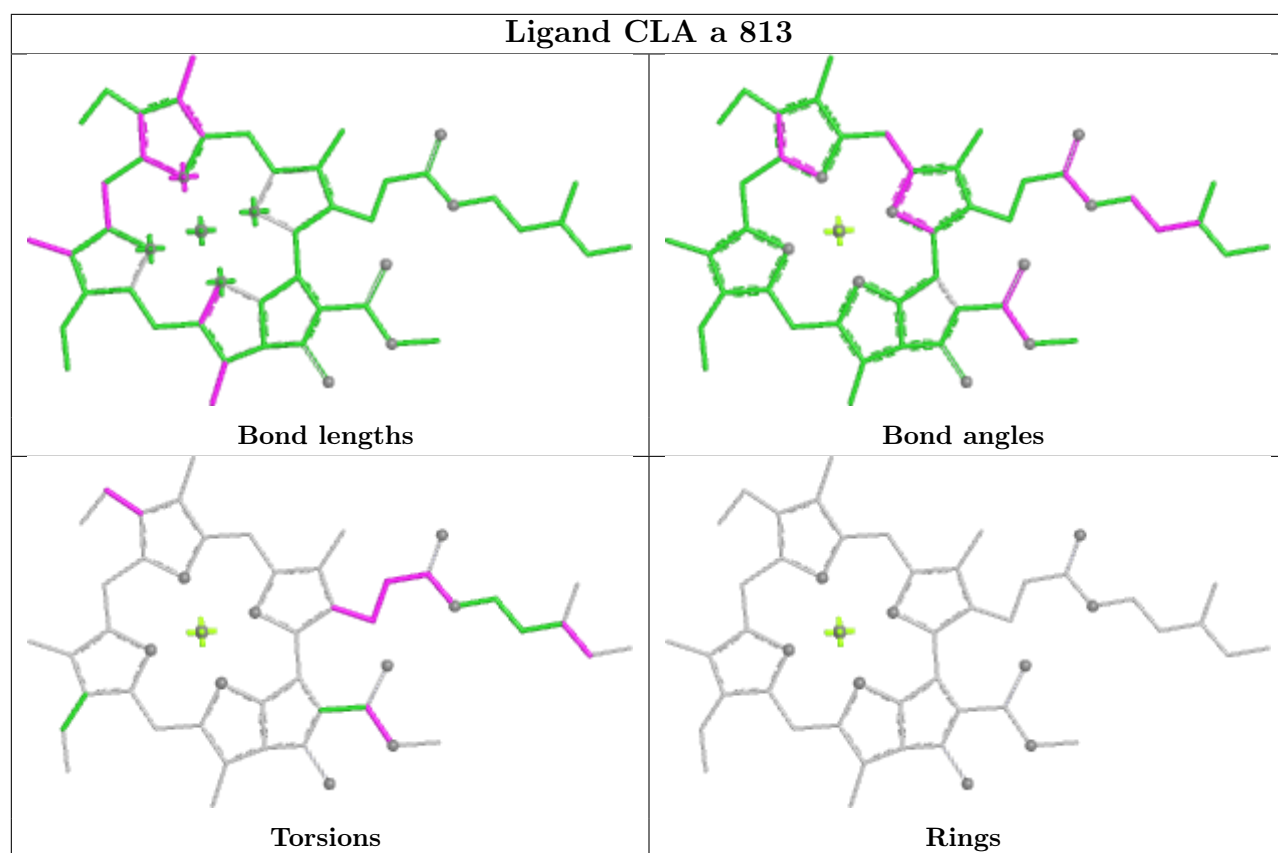
Bond angles



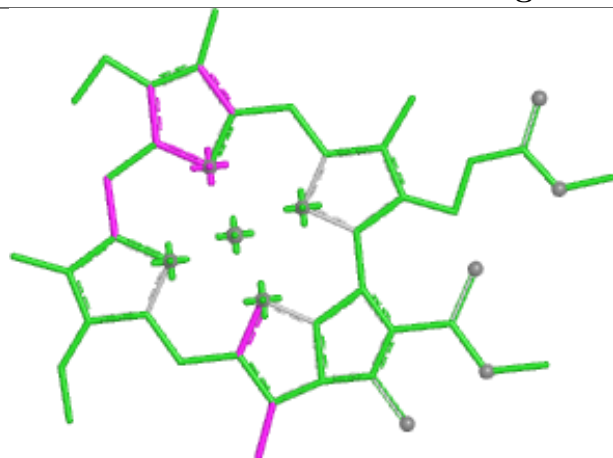
Torsions



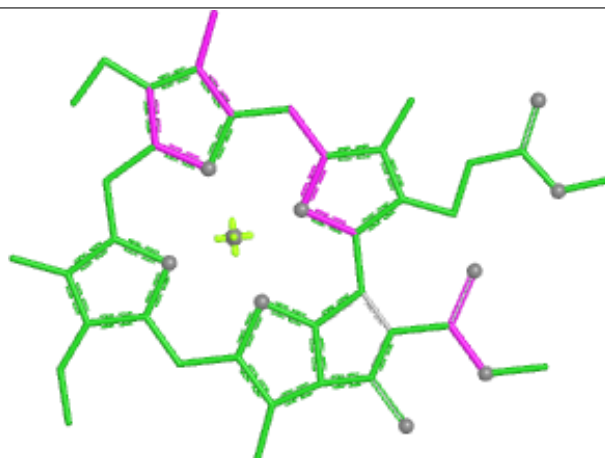
Rings



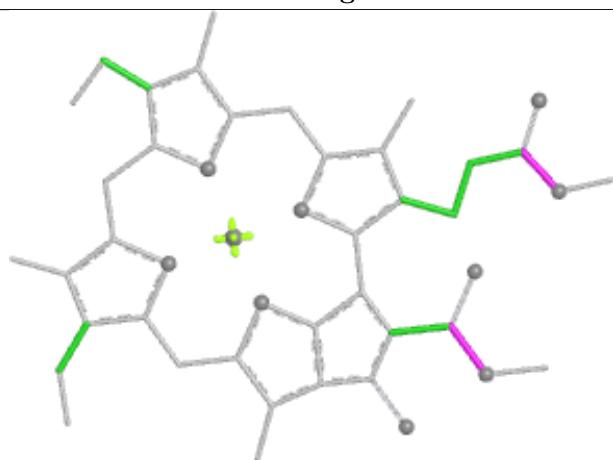
Ligand CLA E 310



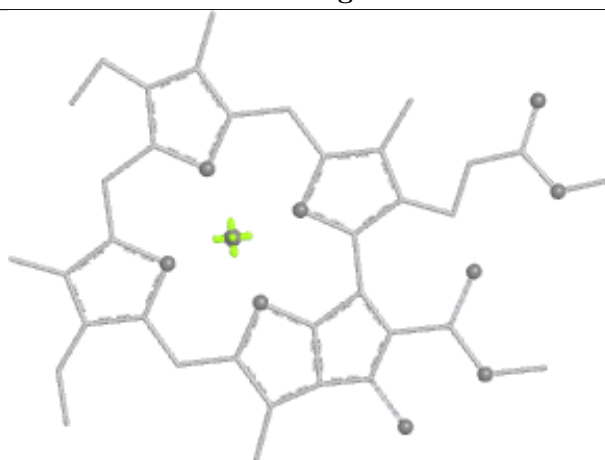
Bond lengths



Bond angles

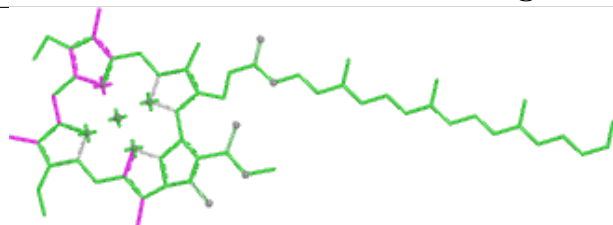


Torsions

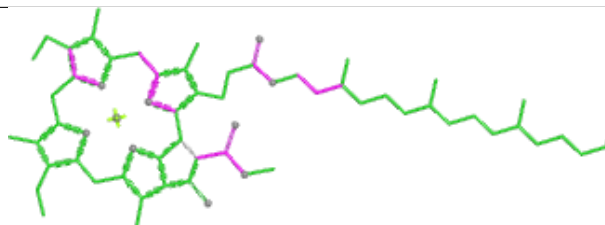


Rings

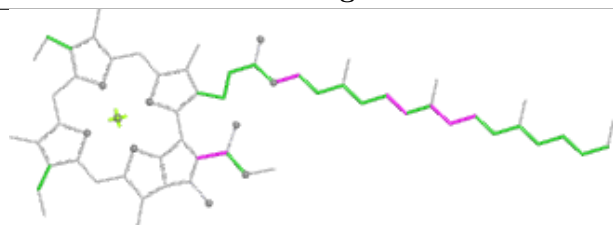
Ligand CLA b 714



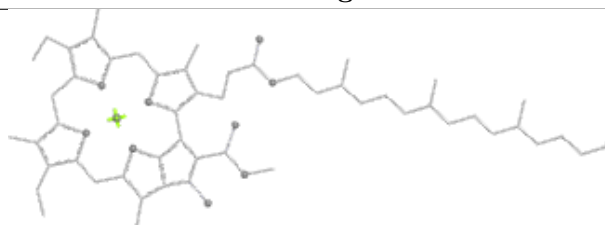
Bond lengths



Bond angles

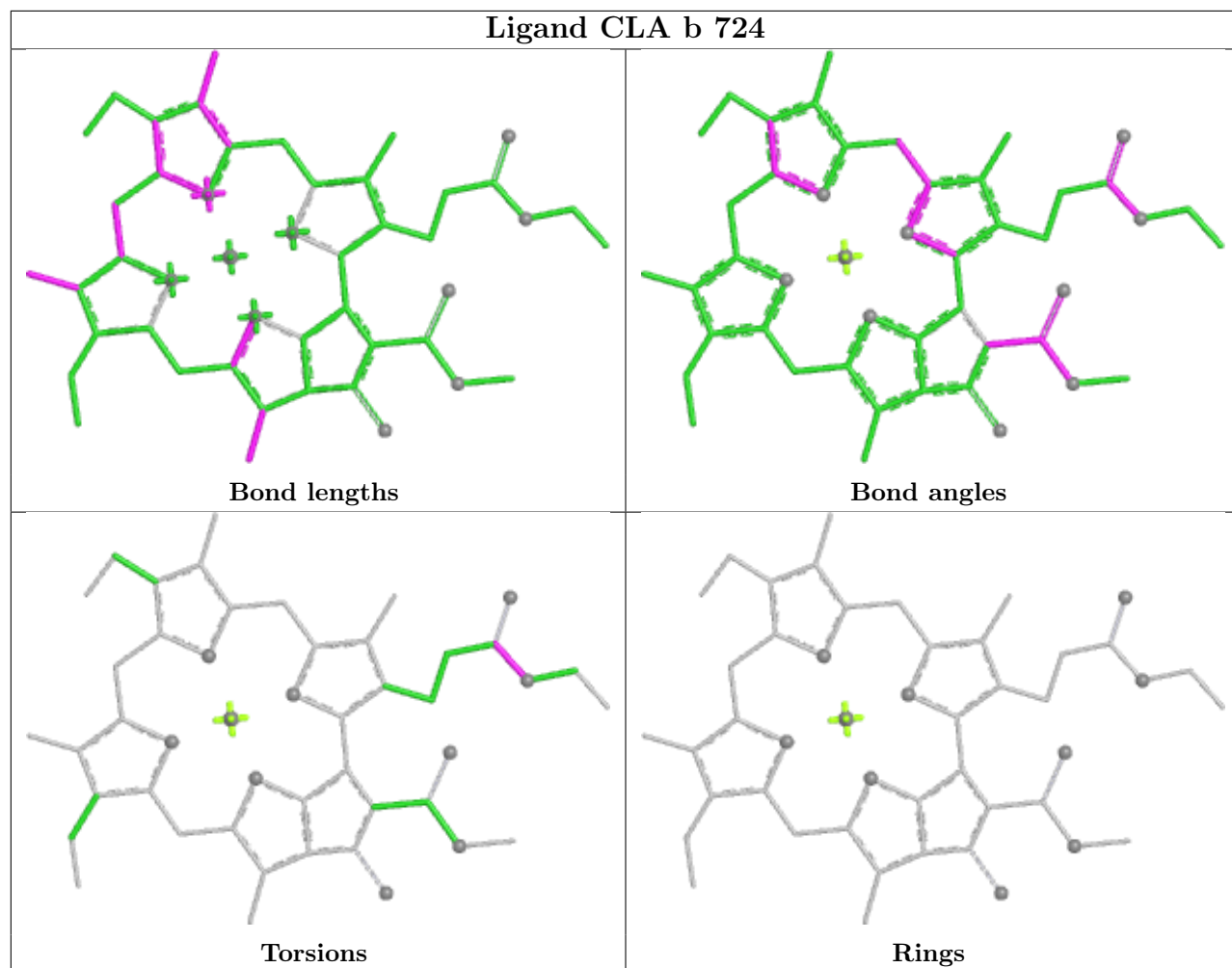


Torsions

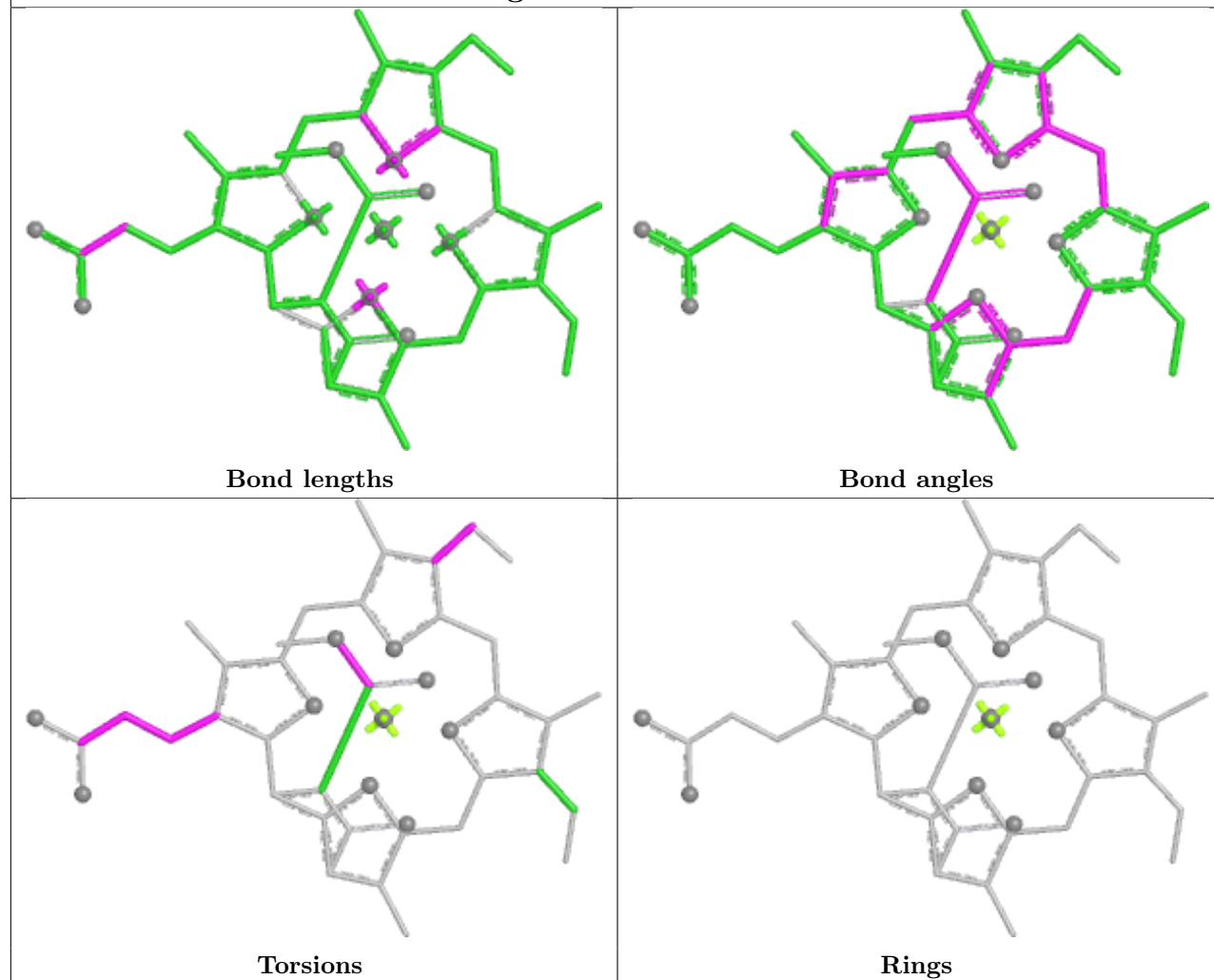


Rings

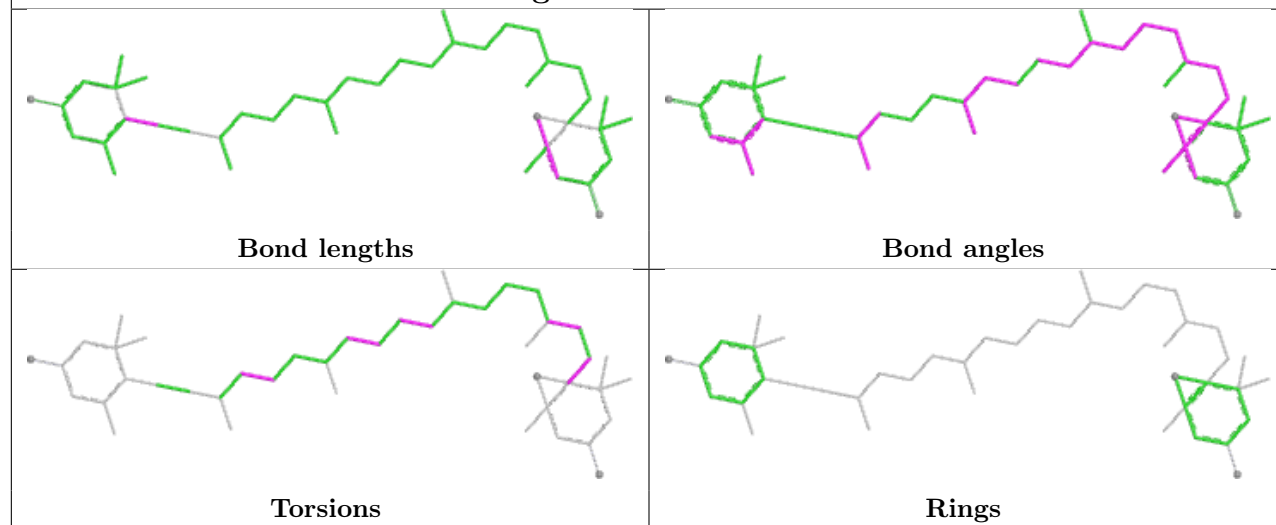
Ligand CLA b 724

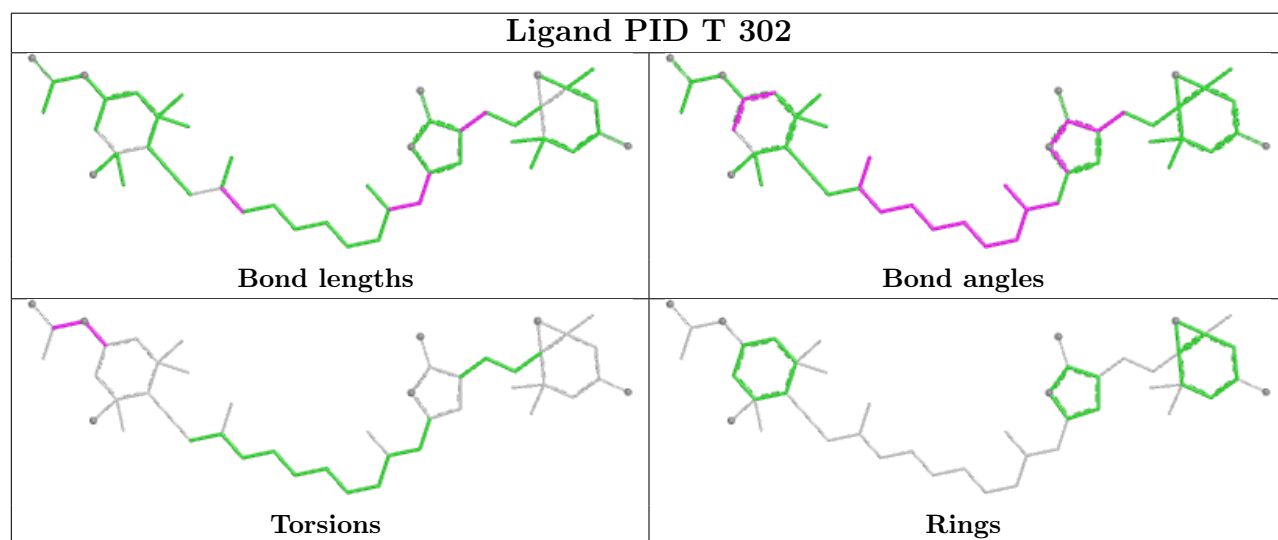
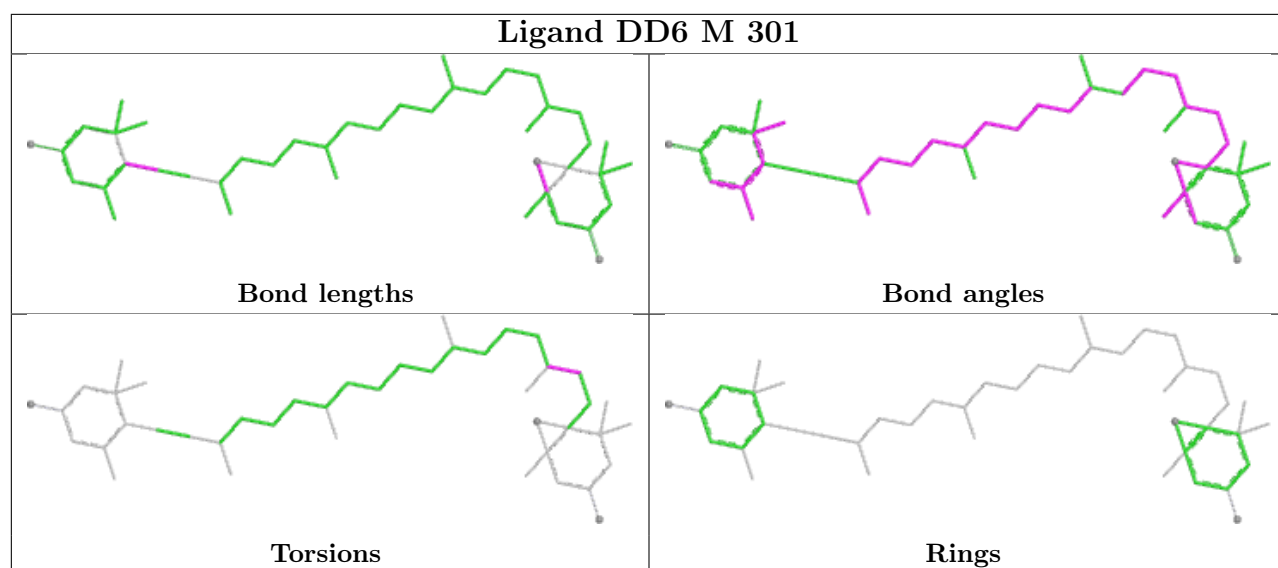


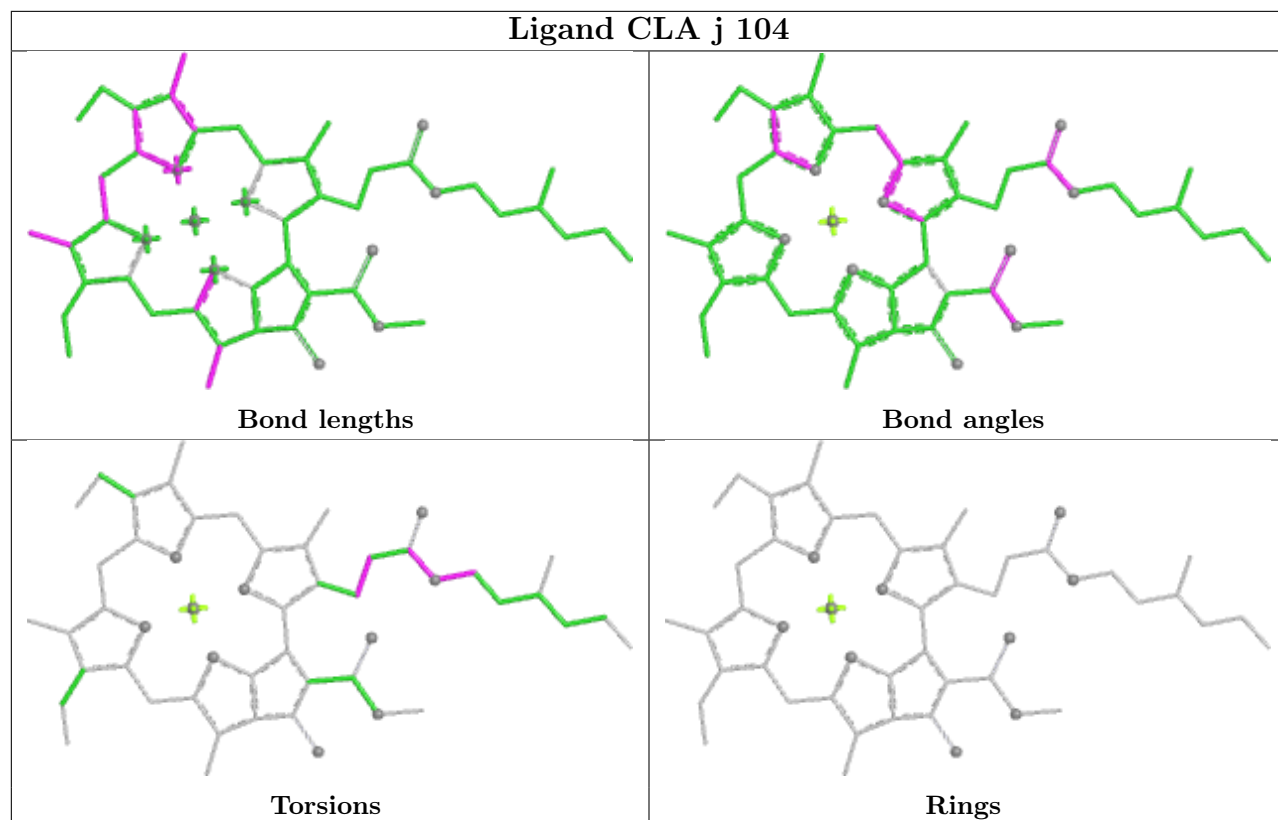
Ligand KC1 N 315



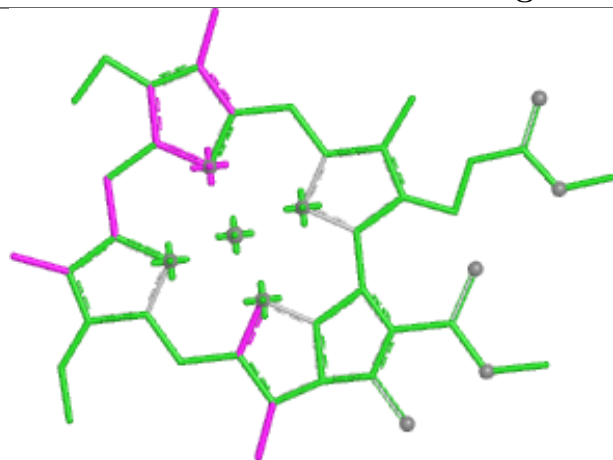
Ligand DD6 D 304



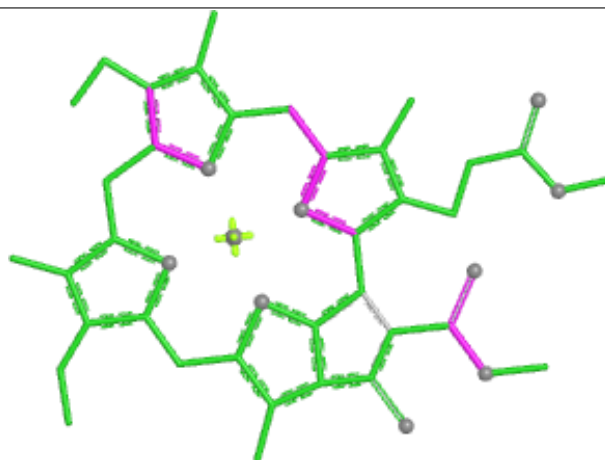




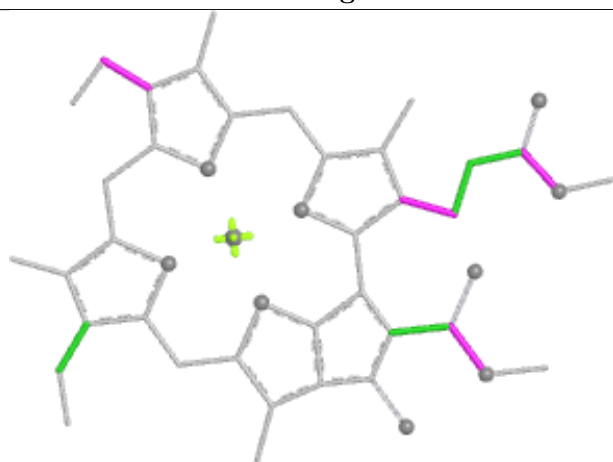
Ligand CLA F 313



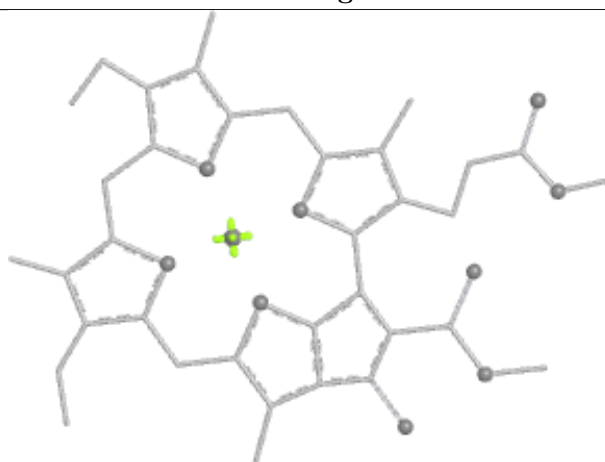
Bond lengths



Bond angles

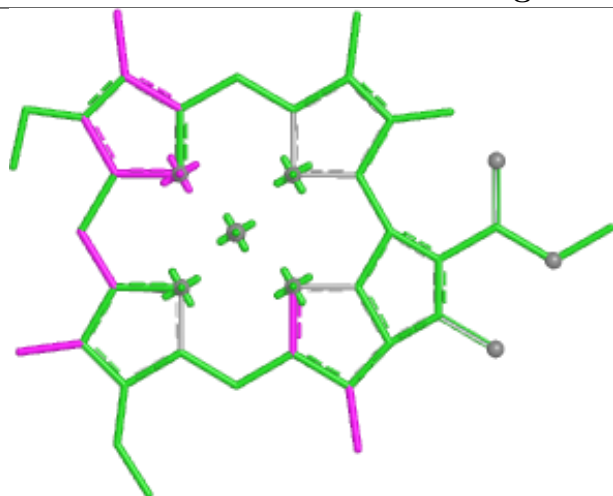


Torsions

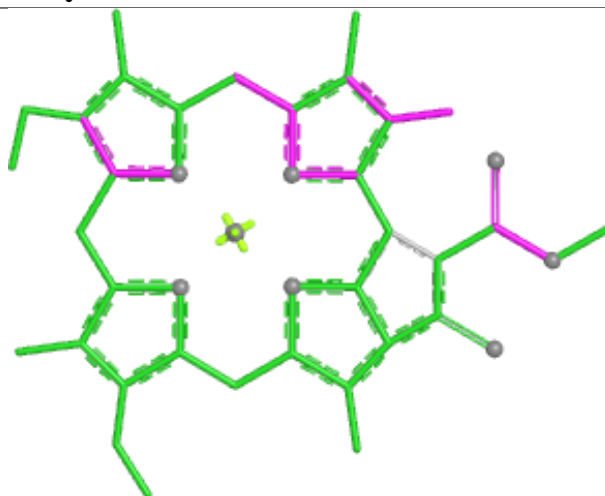


Rings

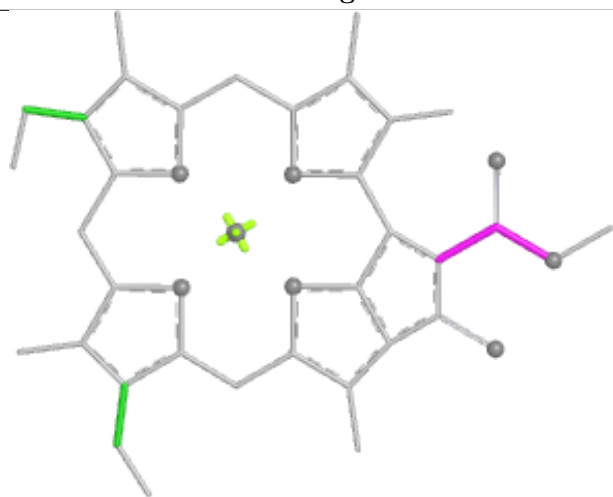
Ligand CLA Q 315



Bond lengths



Bond angles

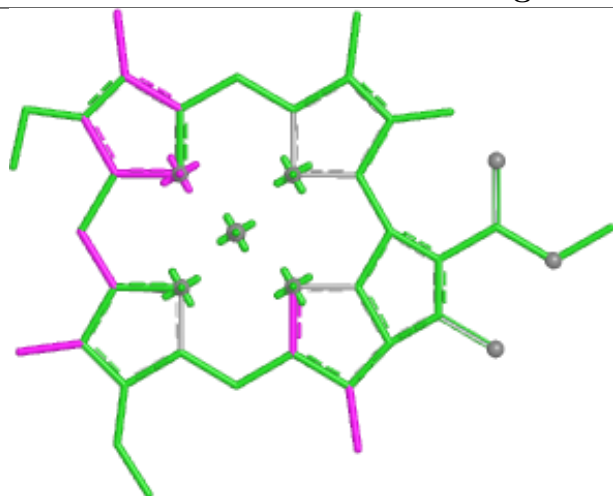


Torsions

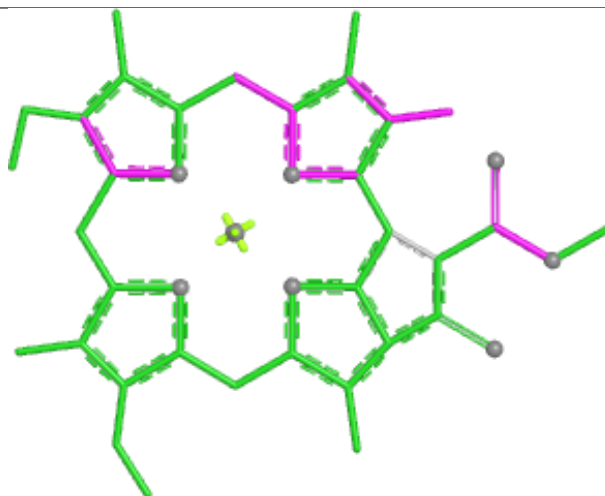


Rings

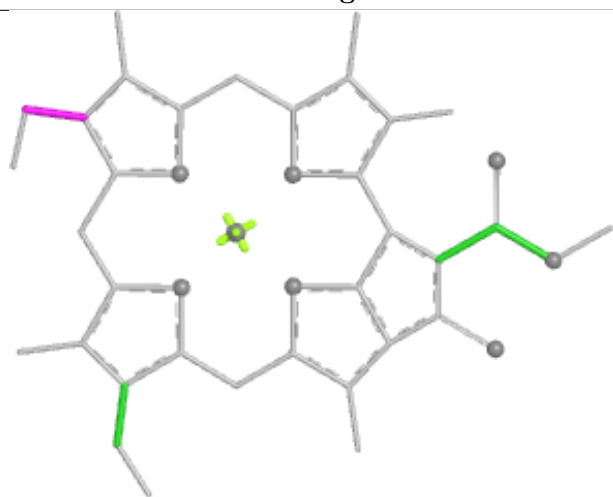
Ligand CLA A 216



Bond lengths



Bond angles

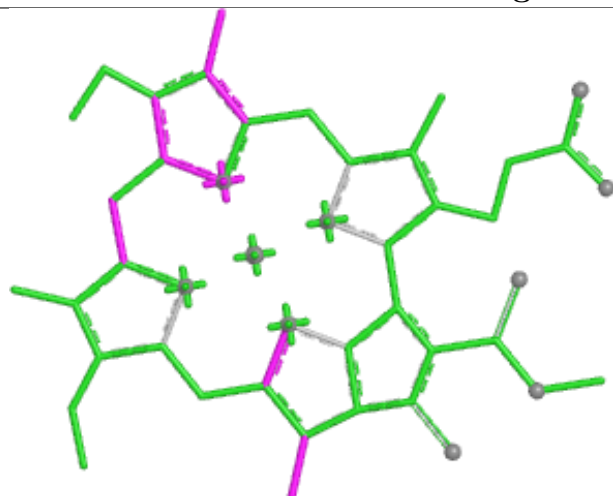


Torsions

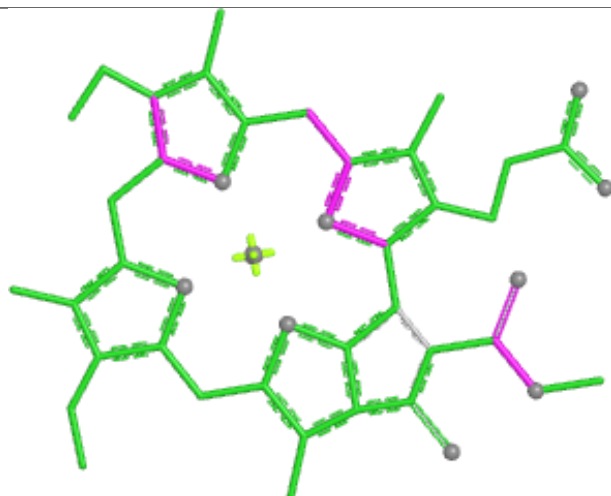


Rings

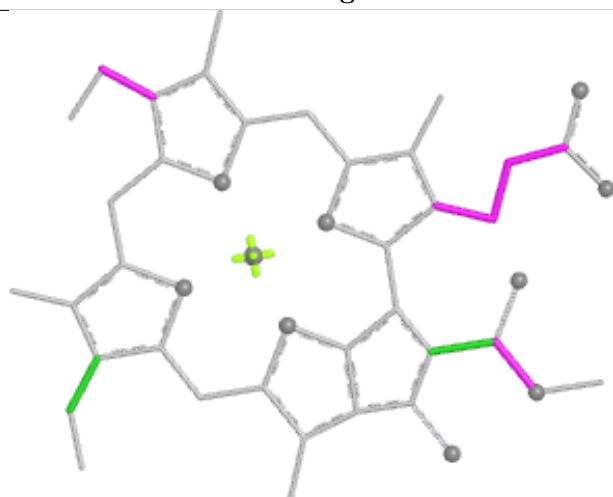
Ligand CLA K 218



Bond lengths



Bond angles

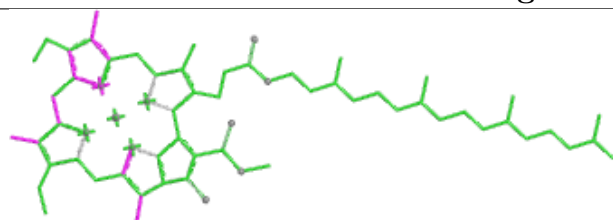


Torsions

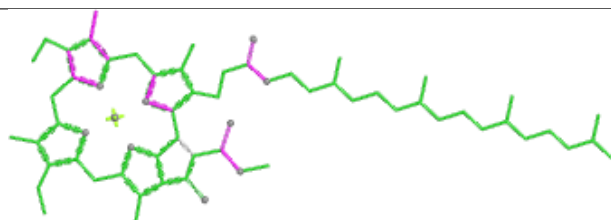


Rings

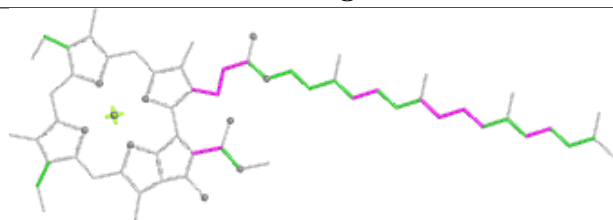
Ligand CLA b 703



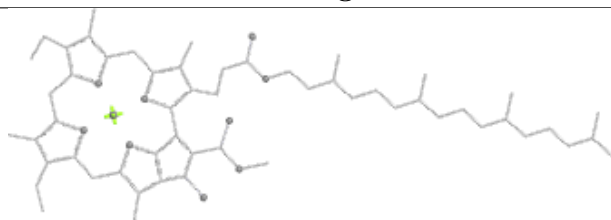
Bond lengths



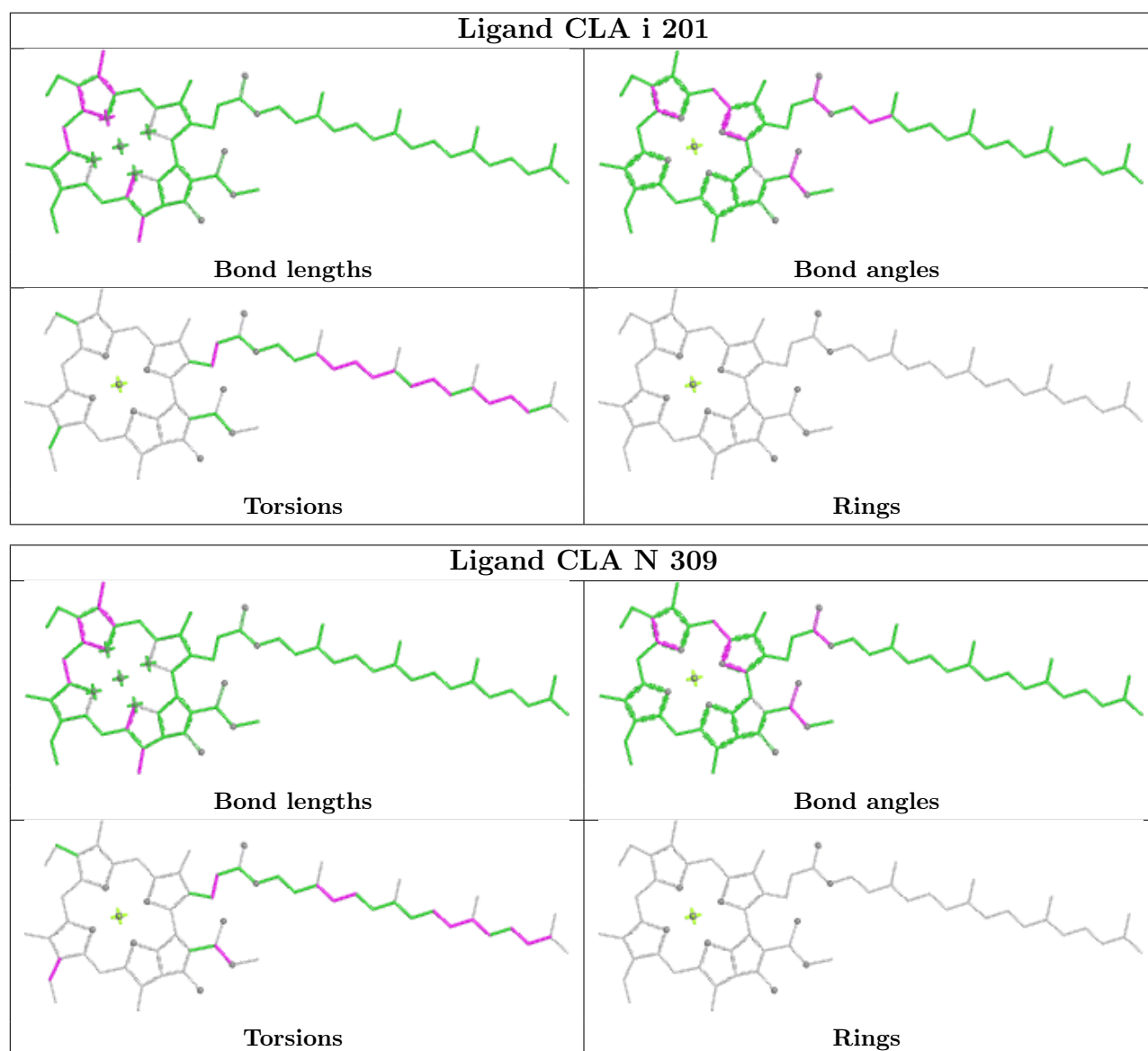
Bond angles



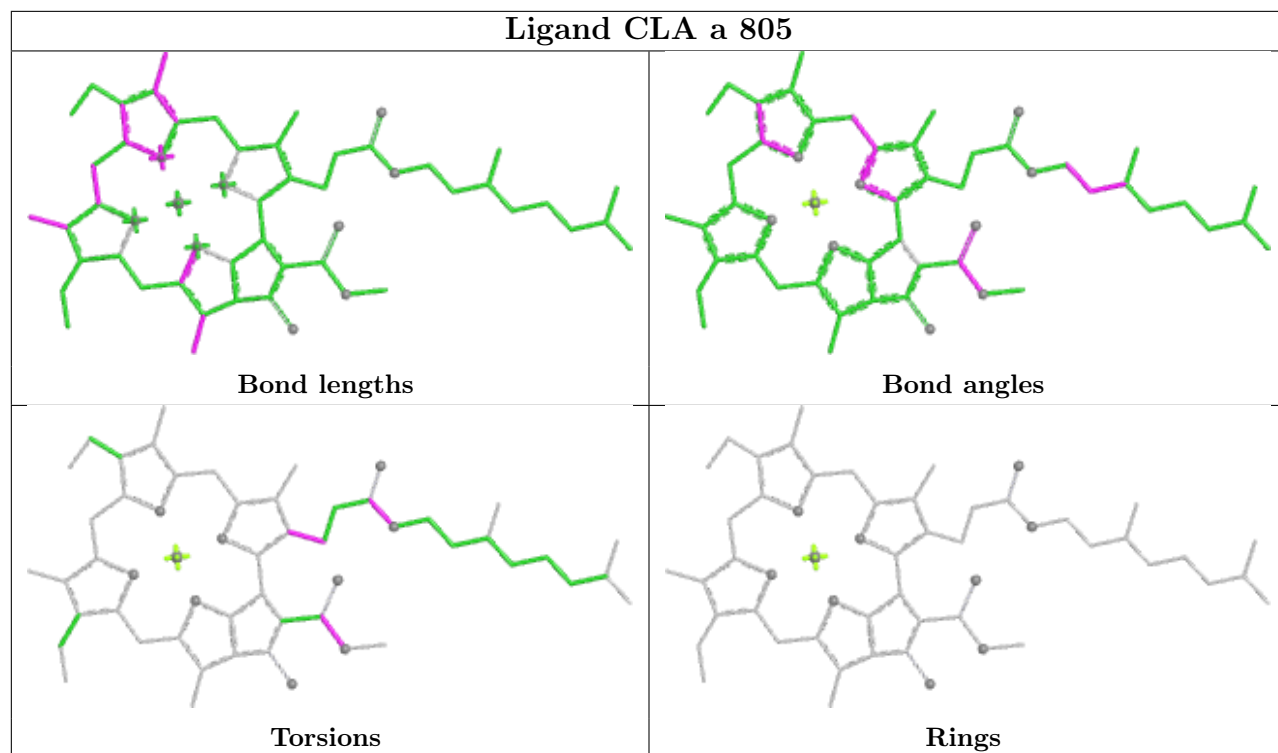
Torsions



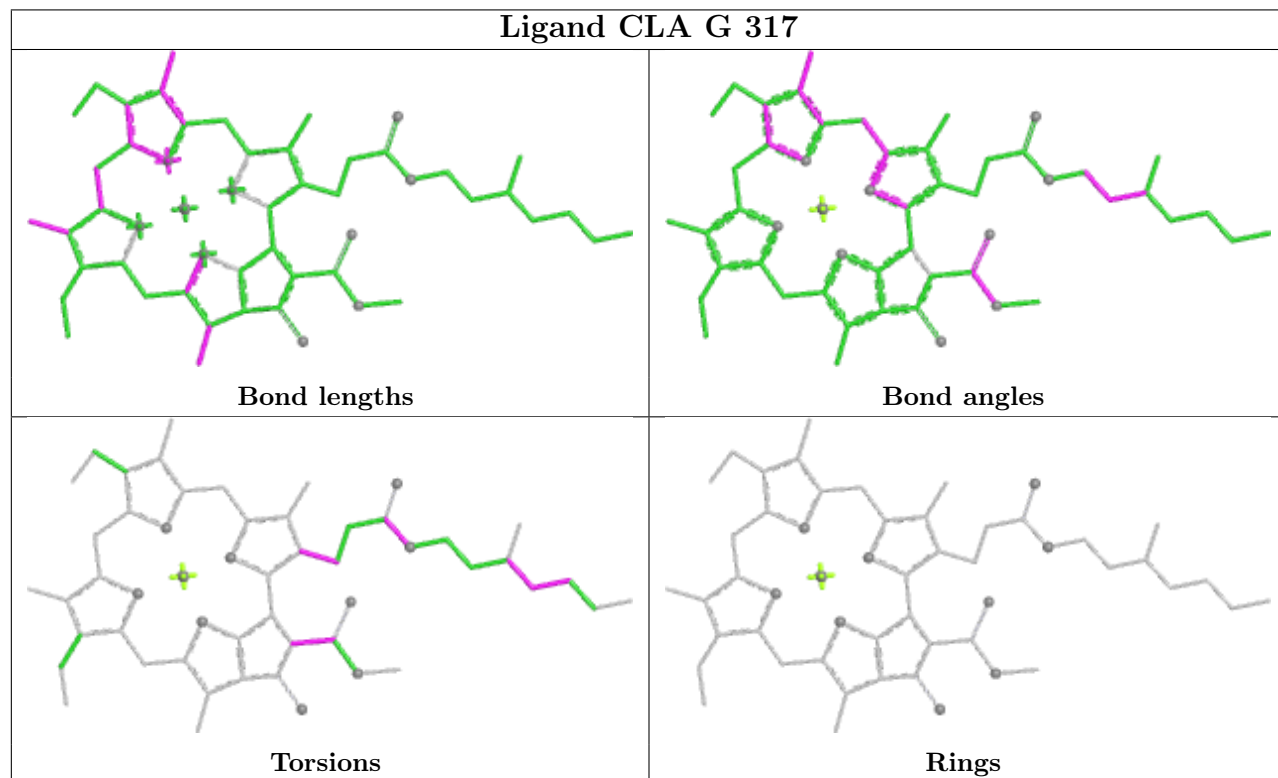
Rings

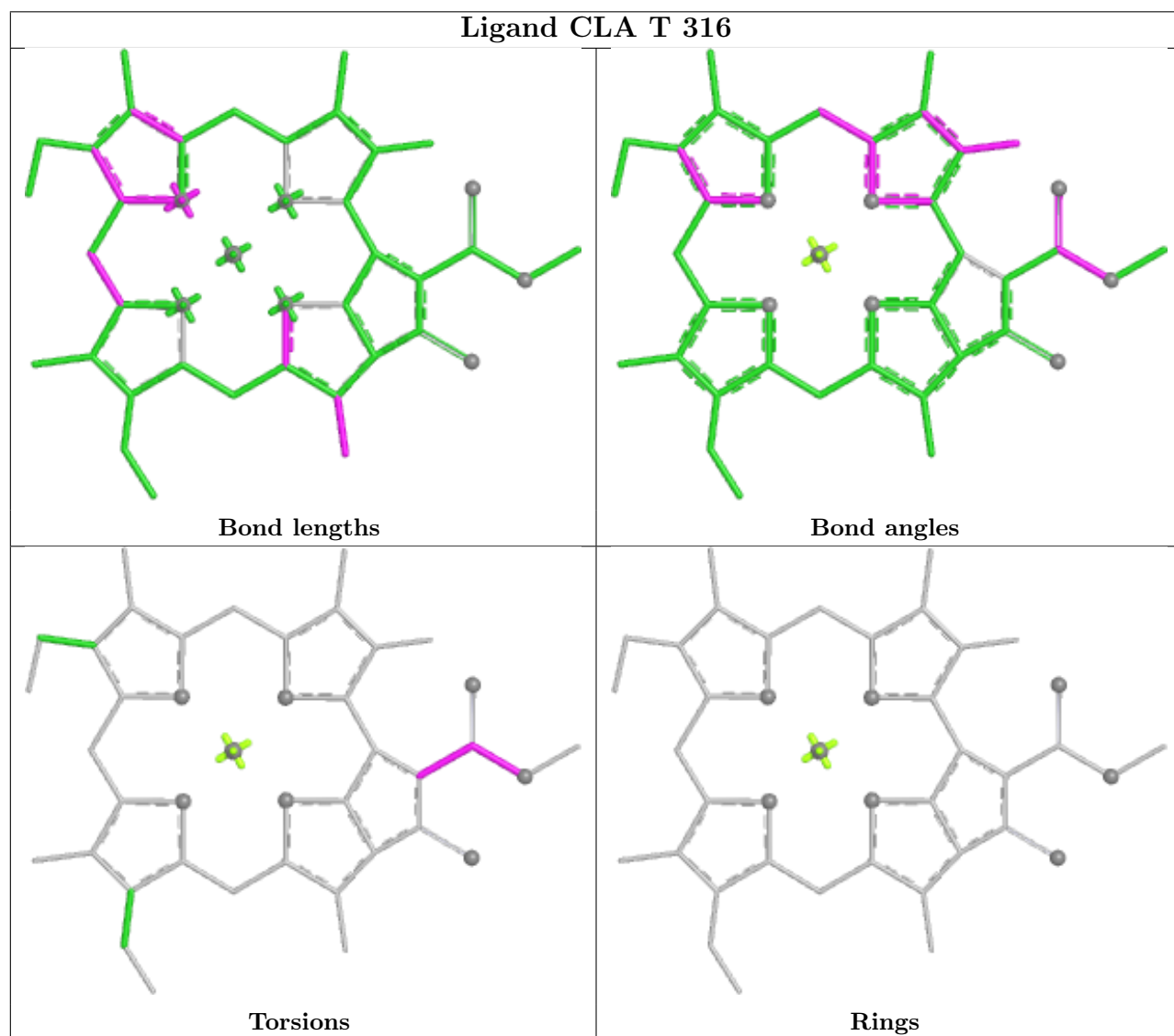
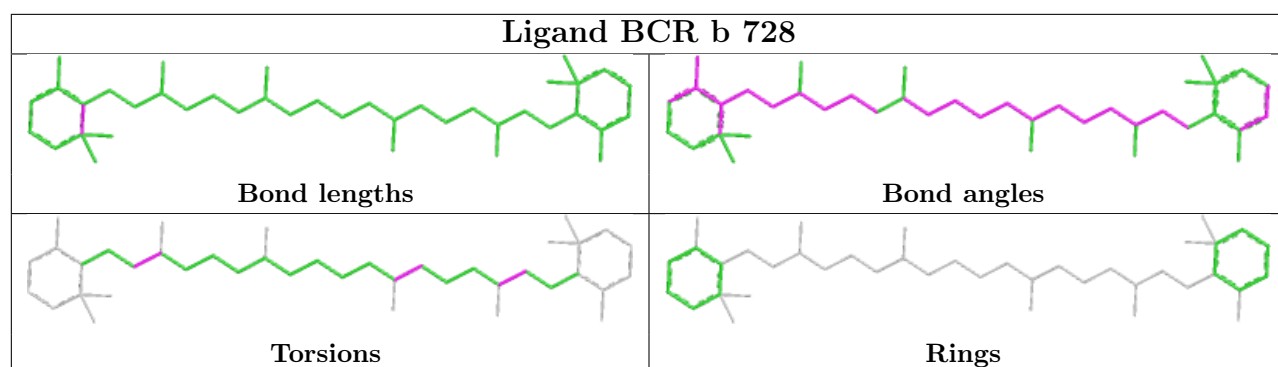


Ligand CLA a 805

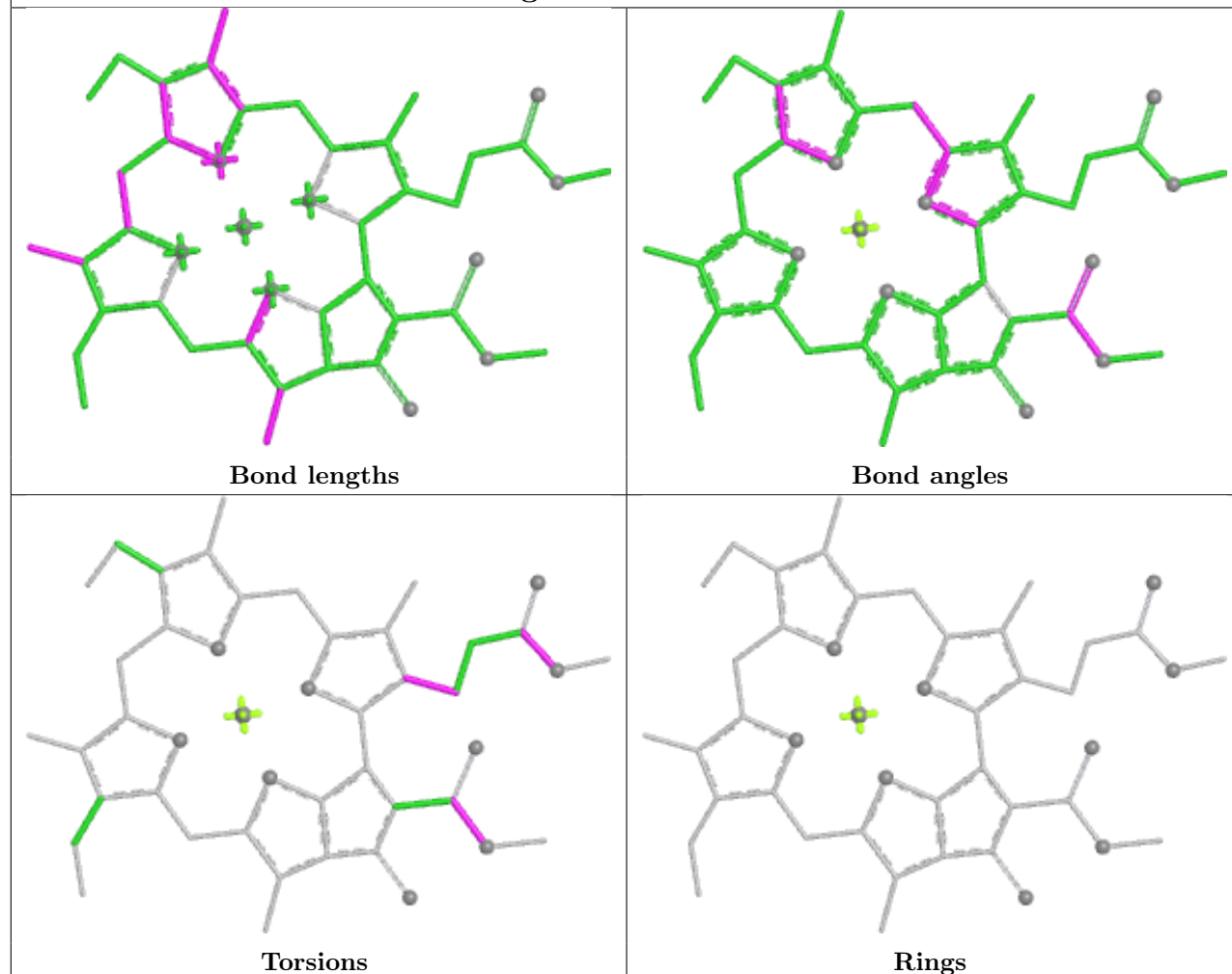


Ligand CLA G 317

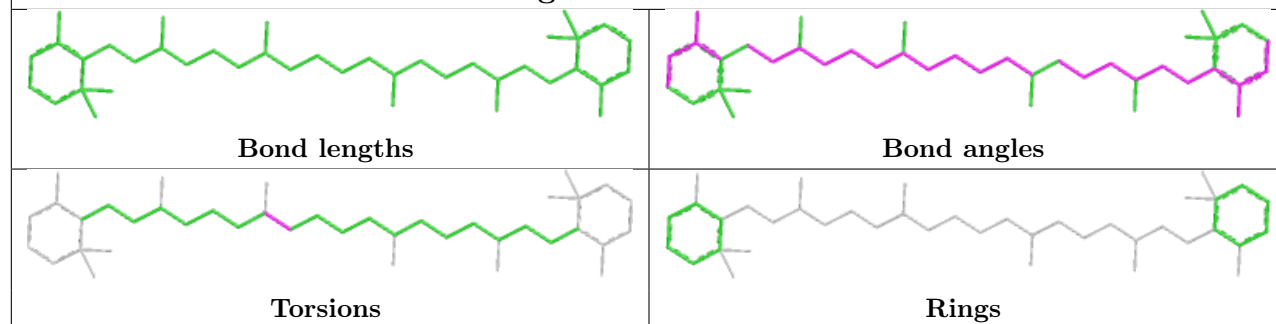




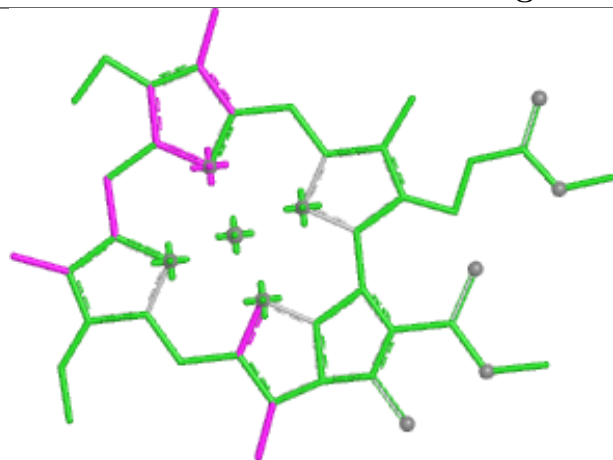
Ligand CLA f 803



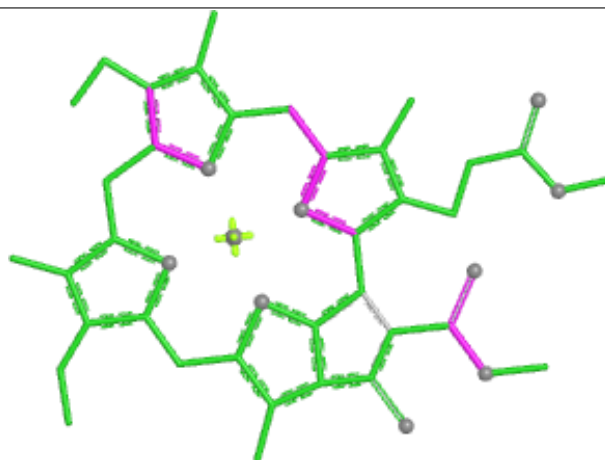
Ligand BCR f 804



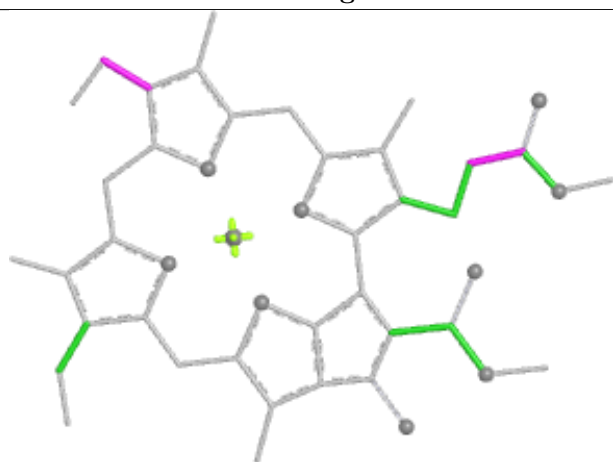
Ligand CLA F 311



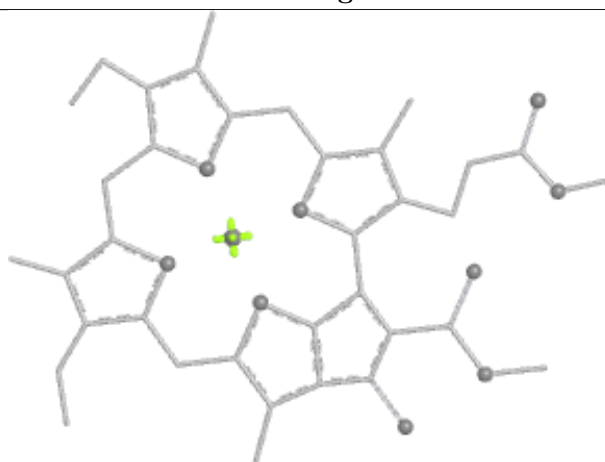
Bond lengths



Bond angles

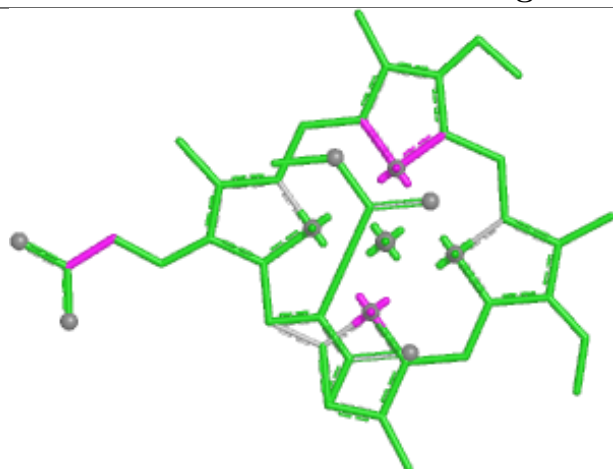


Torsions

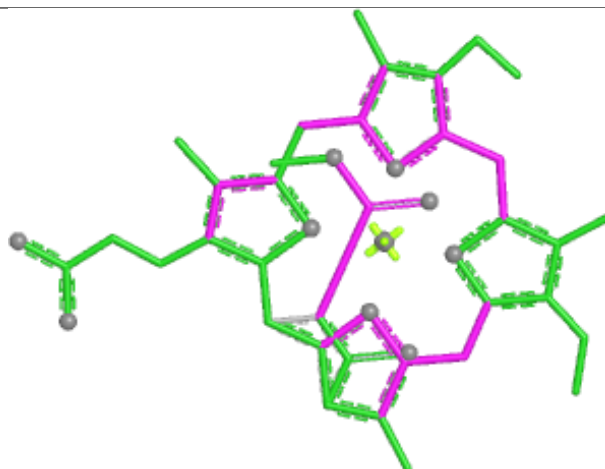


Rings

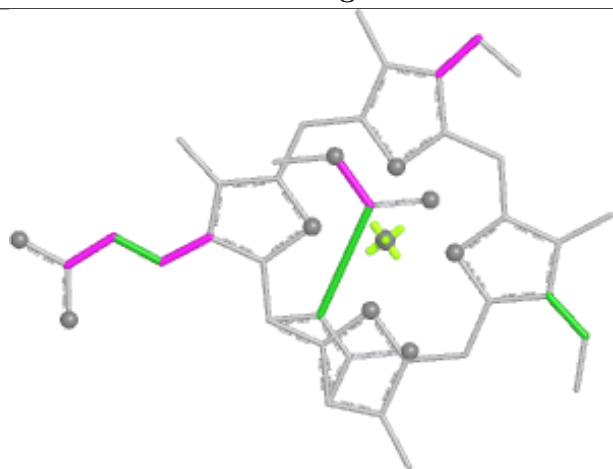
Ligand KC1 C 315



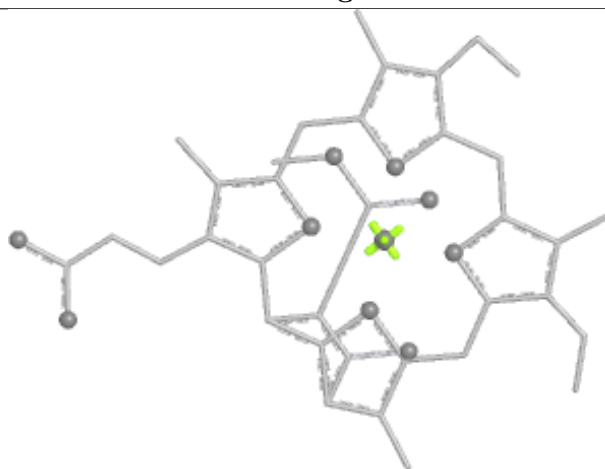
Bond lengths



Bond angles

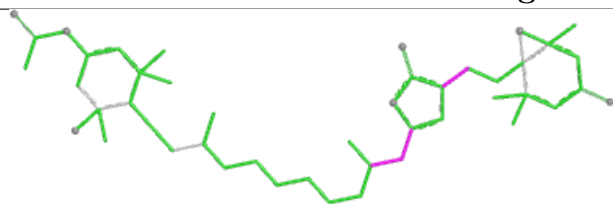


Torsions

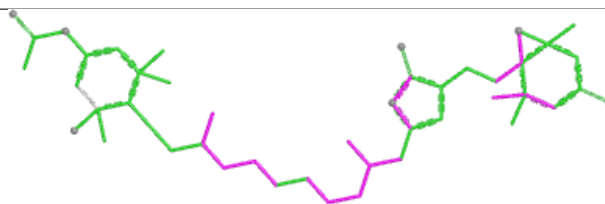


Rings

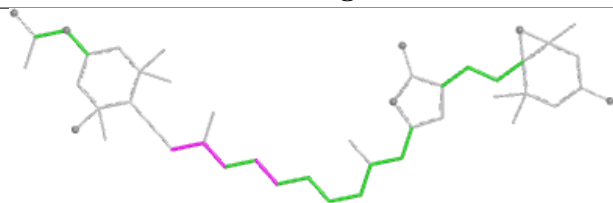
Ligand PID D 305



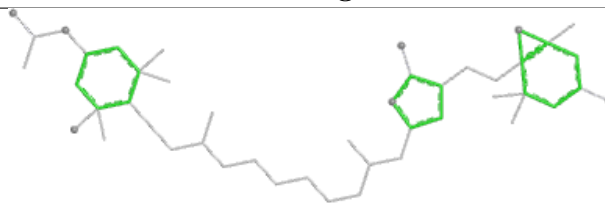
Bond lengths



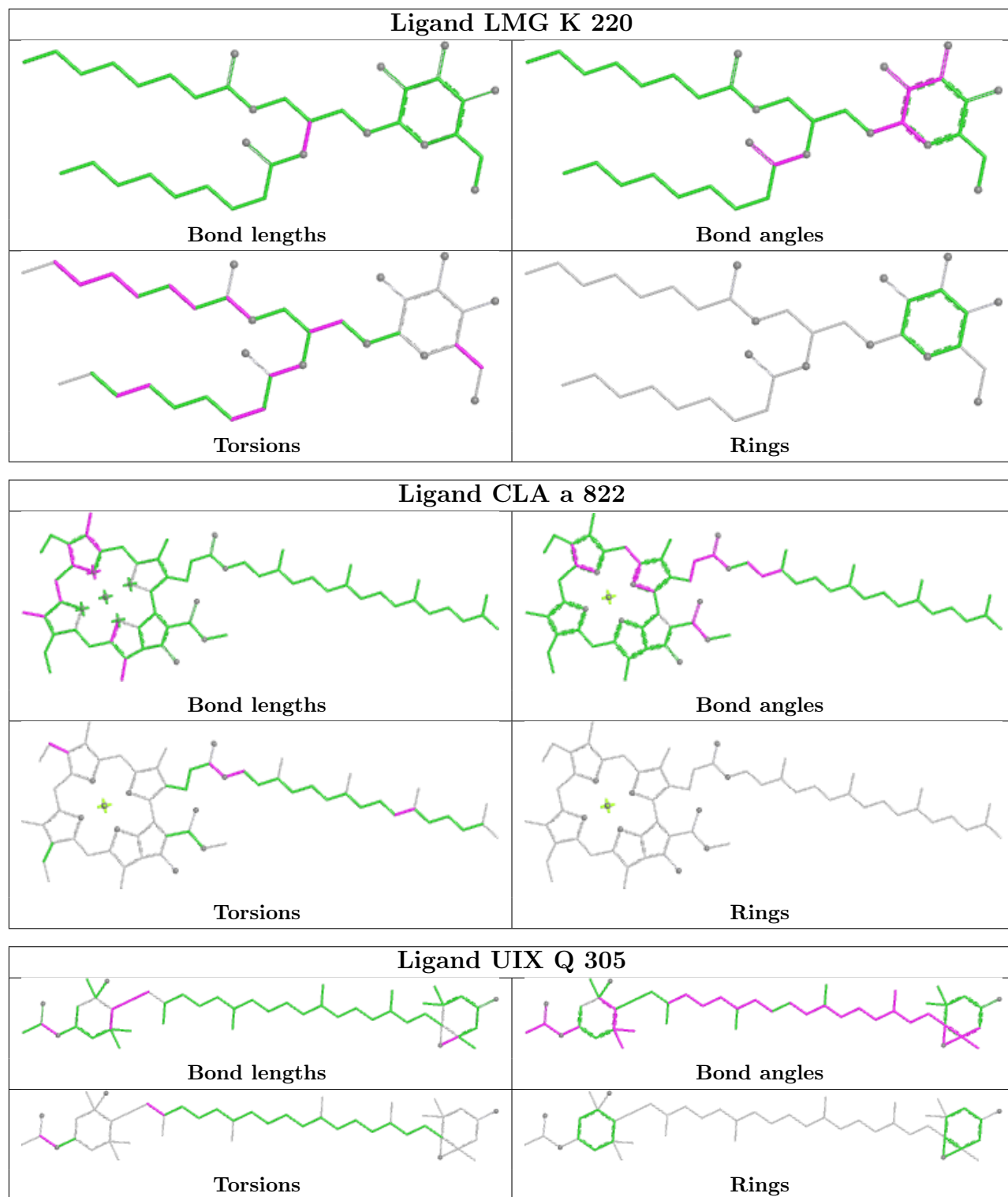
Bond angles



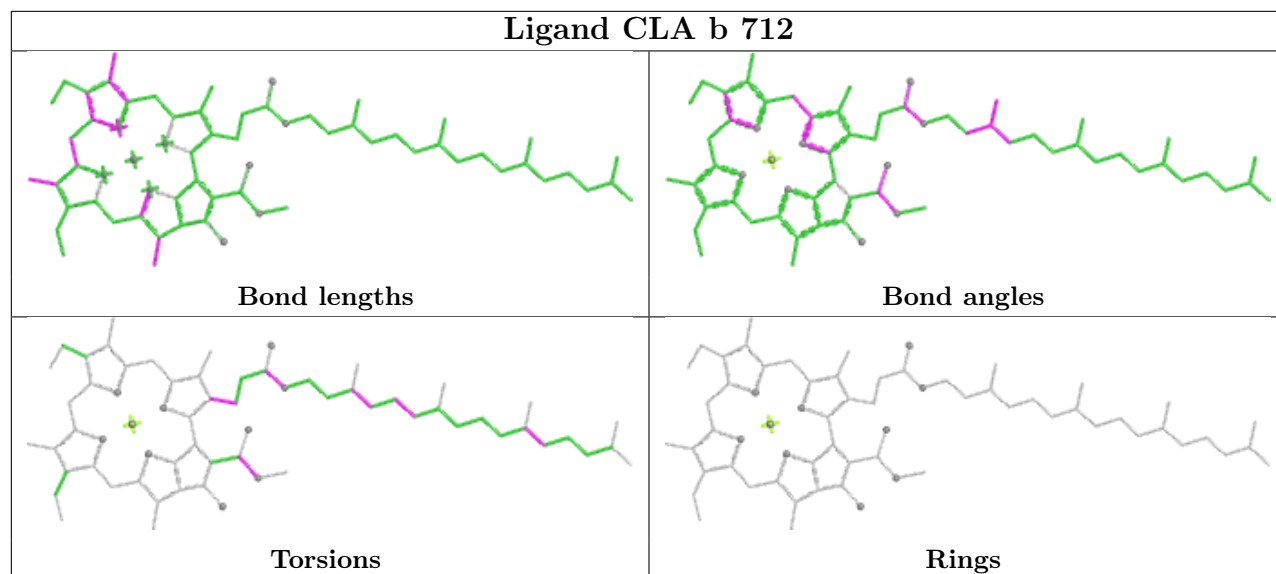
Torsions



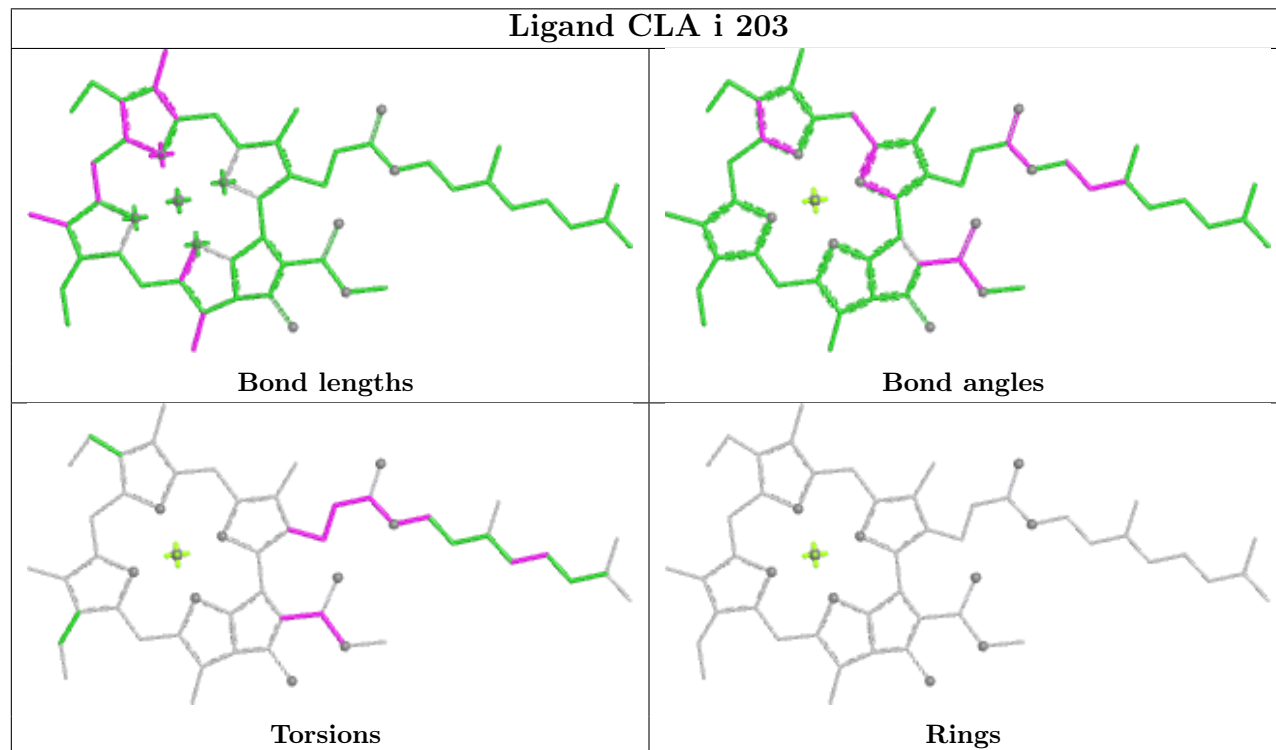
Rings



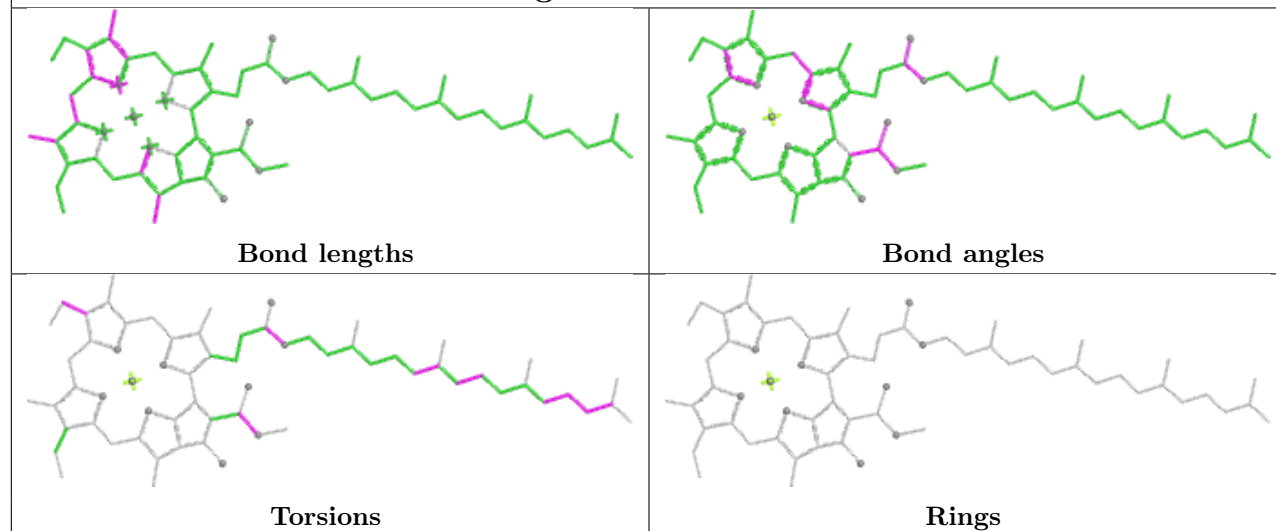
Ligand CLA b 712



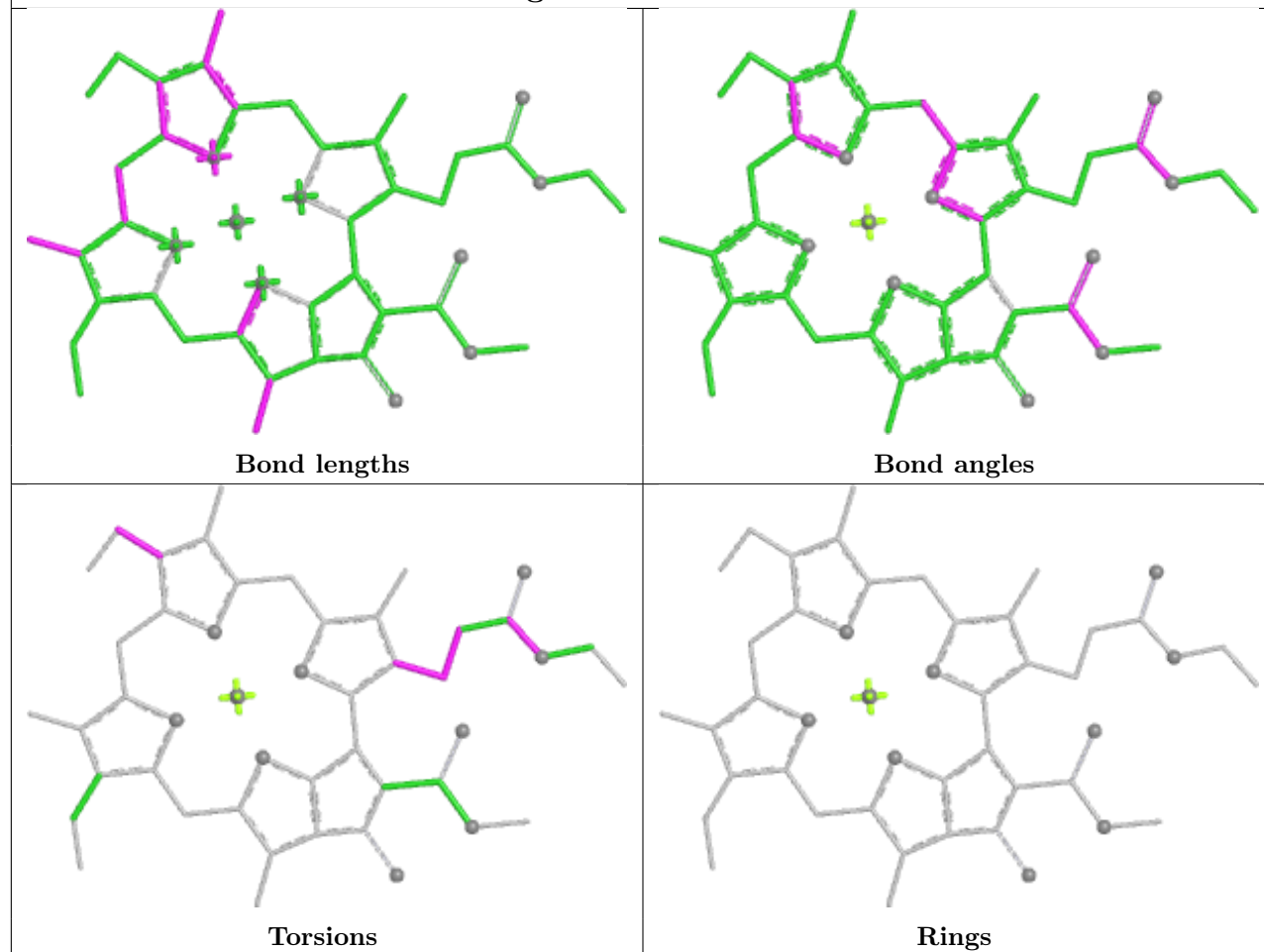
Ligand CLA i 203



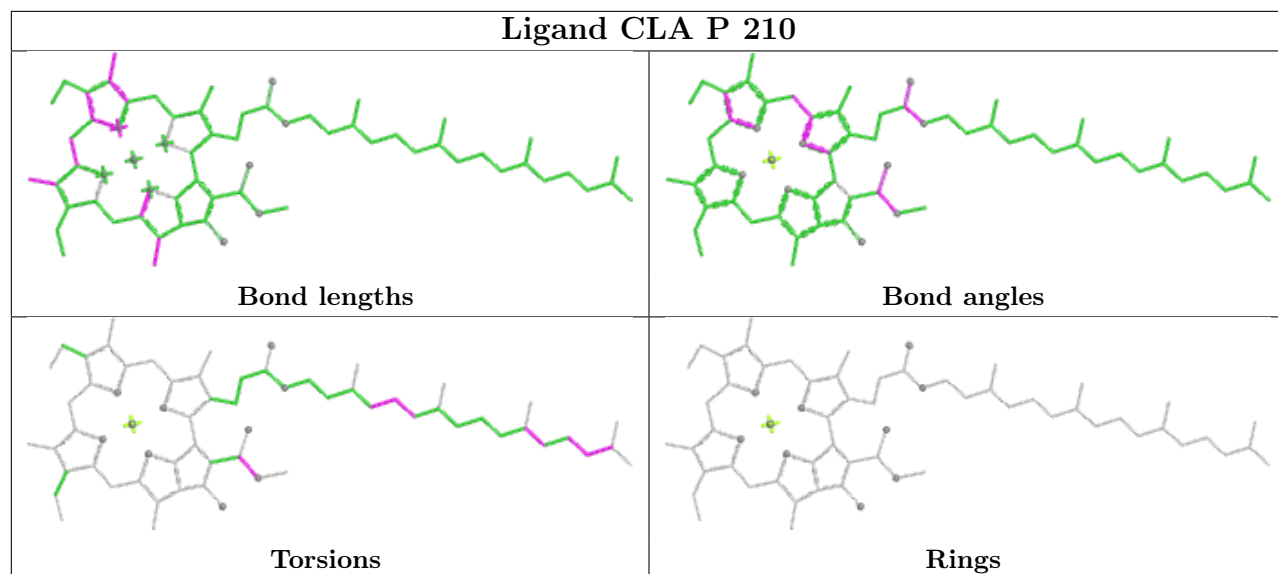
Ligand CLA b 707



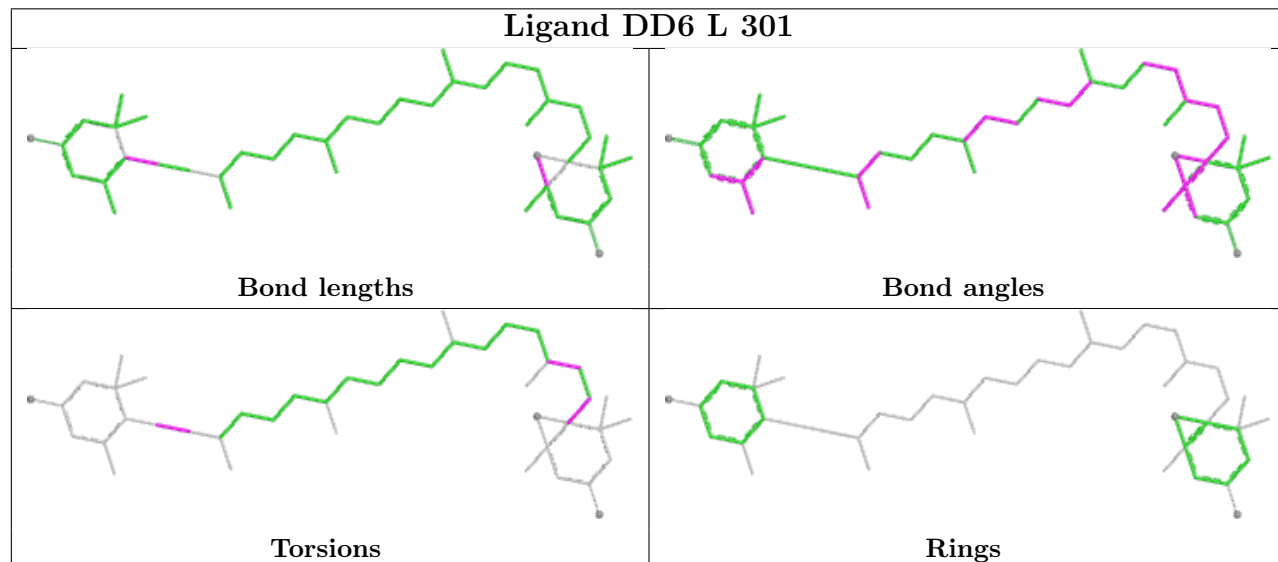
Ligand CLA A 215



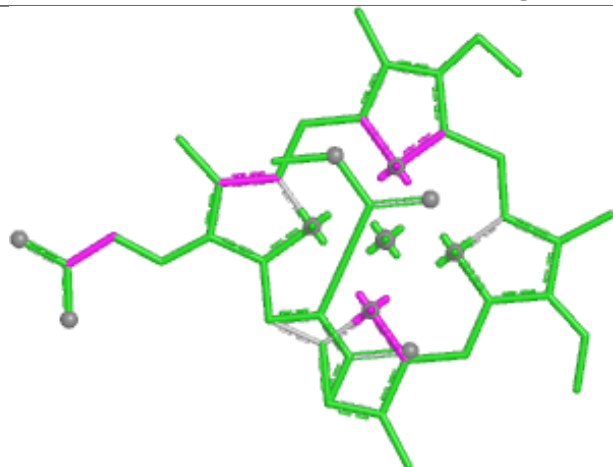
Ligand CLA P 210



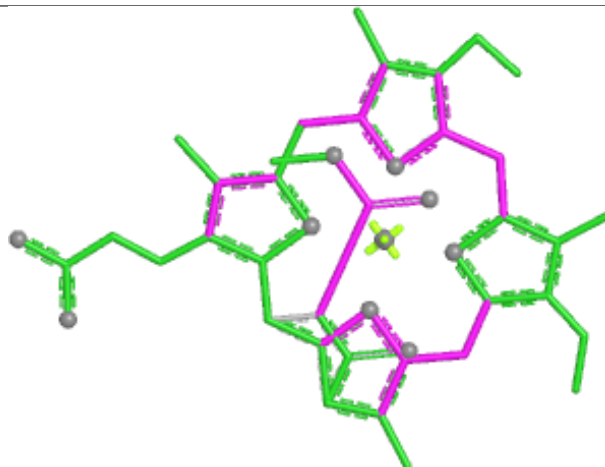
Ligand DD6 L 301



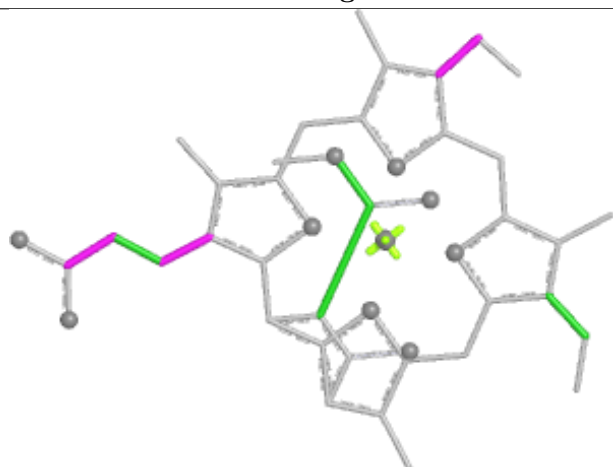
Ligand KC1 G 315



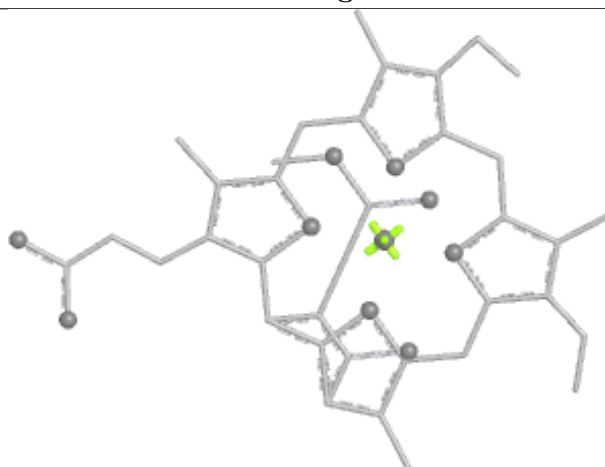
Bond lengths



Bond angles

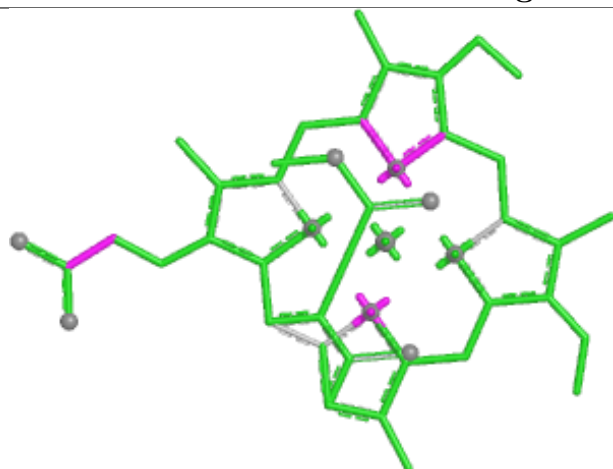


Torsions

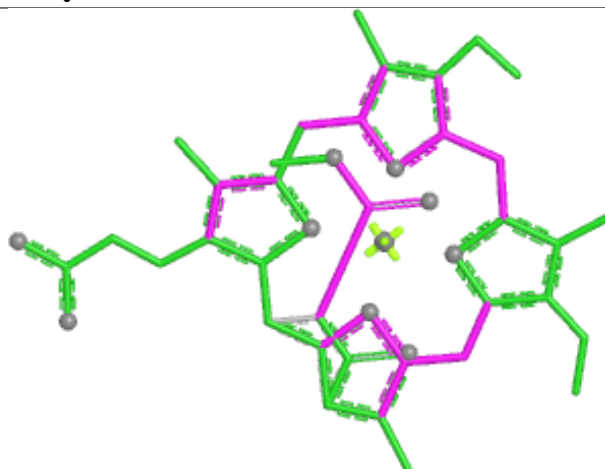


Rings

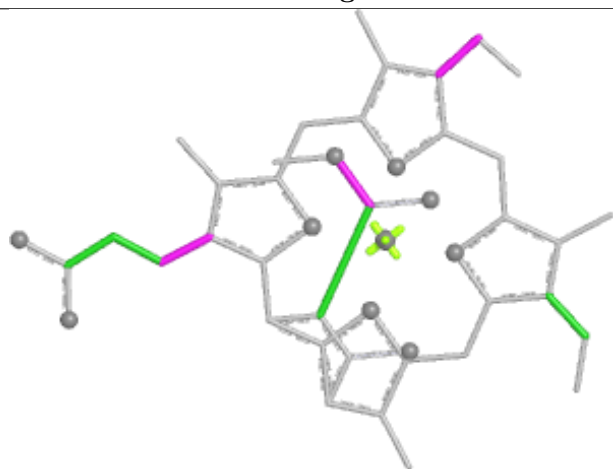
Ligand KC1 Q 309



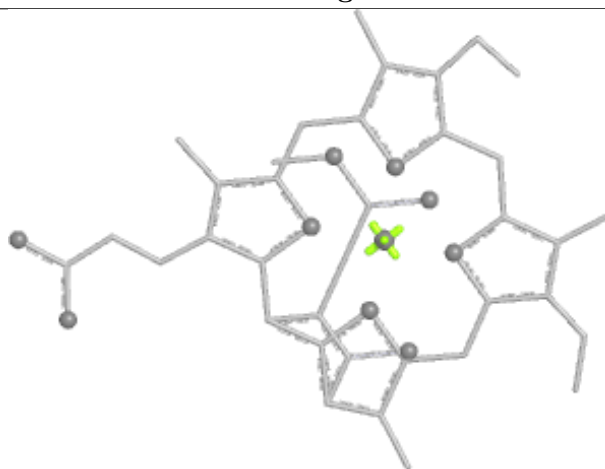
Bond lengths



Bond angles

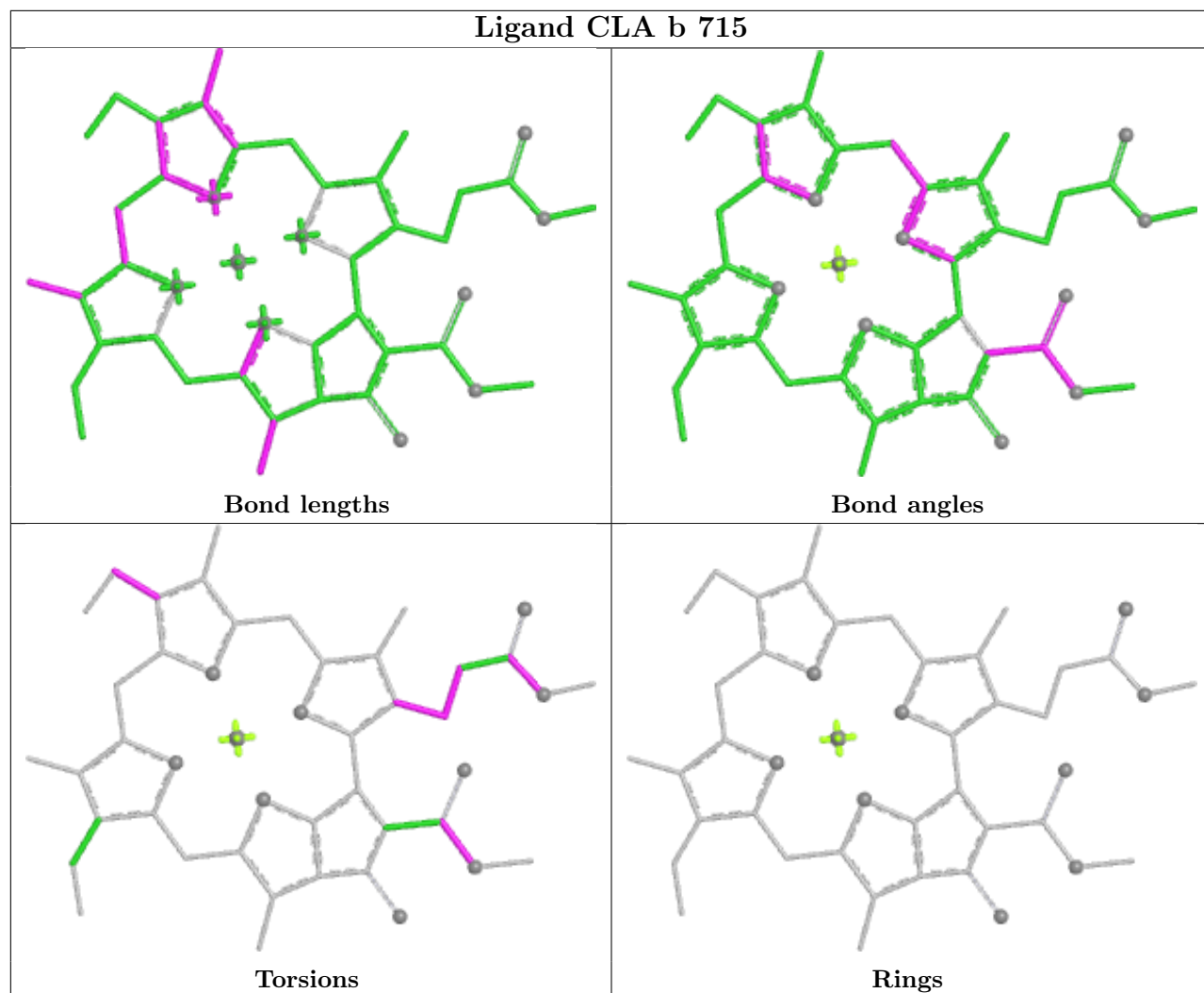


Torsions

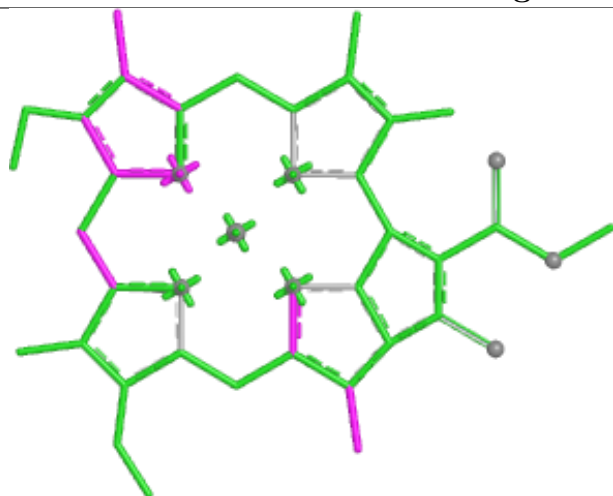


Rings

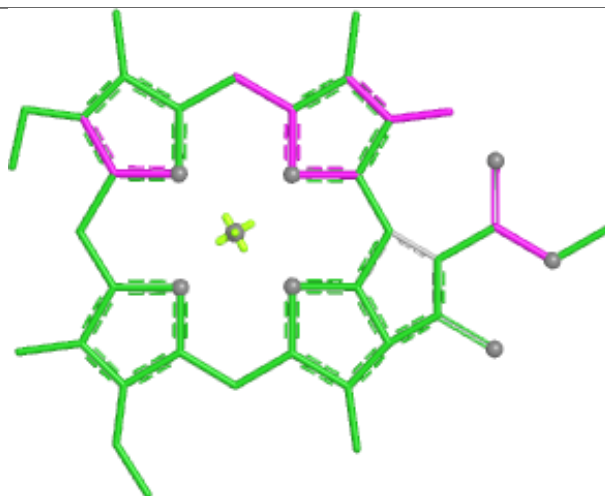
Ligand CLA b 715



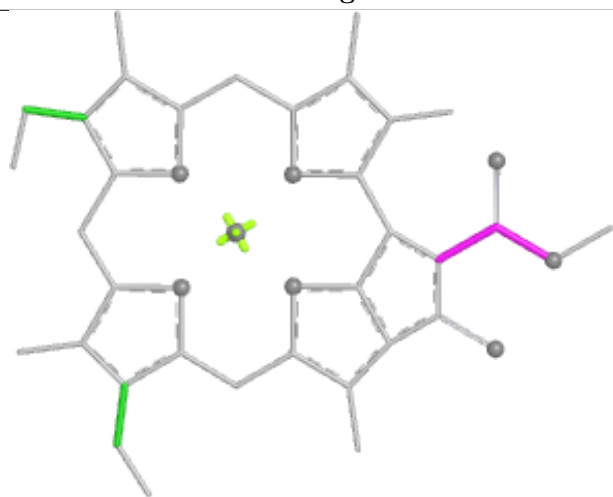
Ligand CLA N 316



Bond lengths



Bond angles

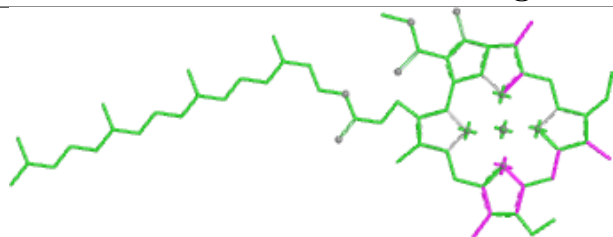


Torsions

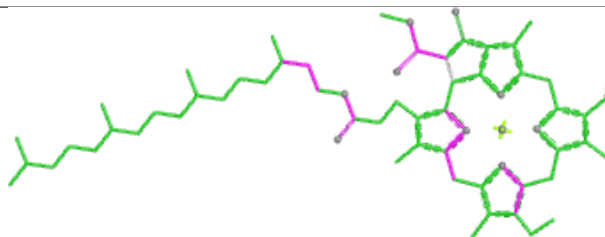


Rings

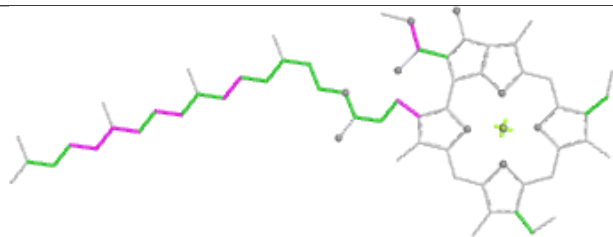
Ligand CLA G 316



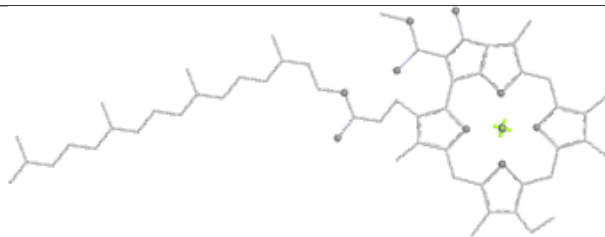
Bond lengths



Bond angles

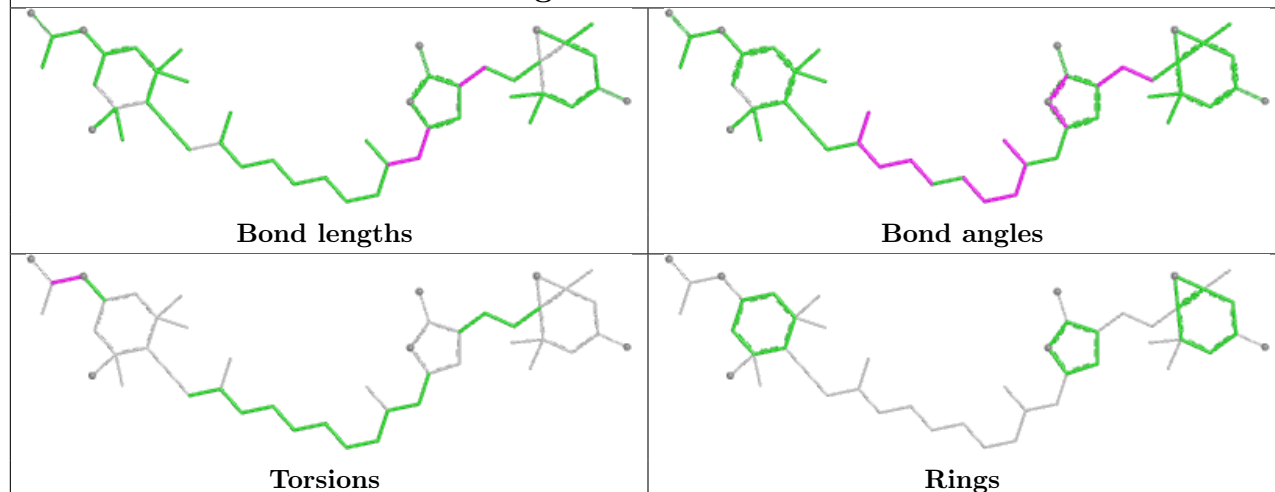


Torsions

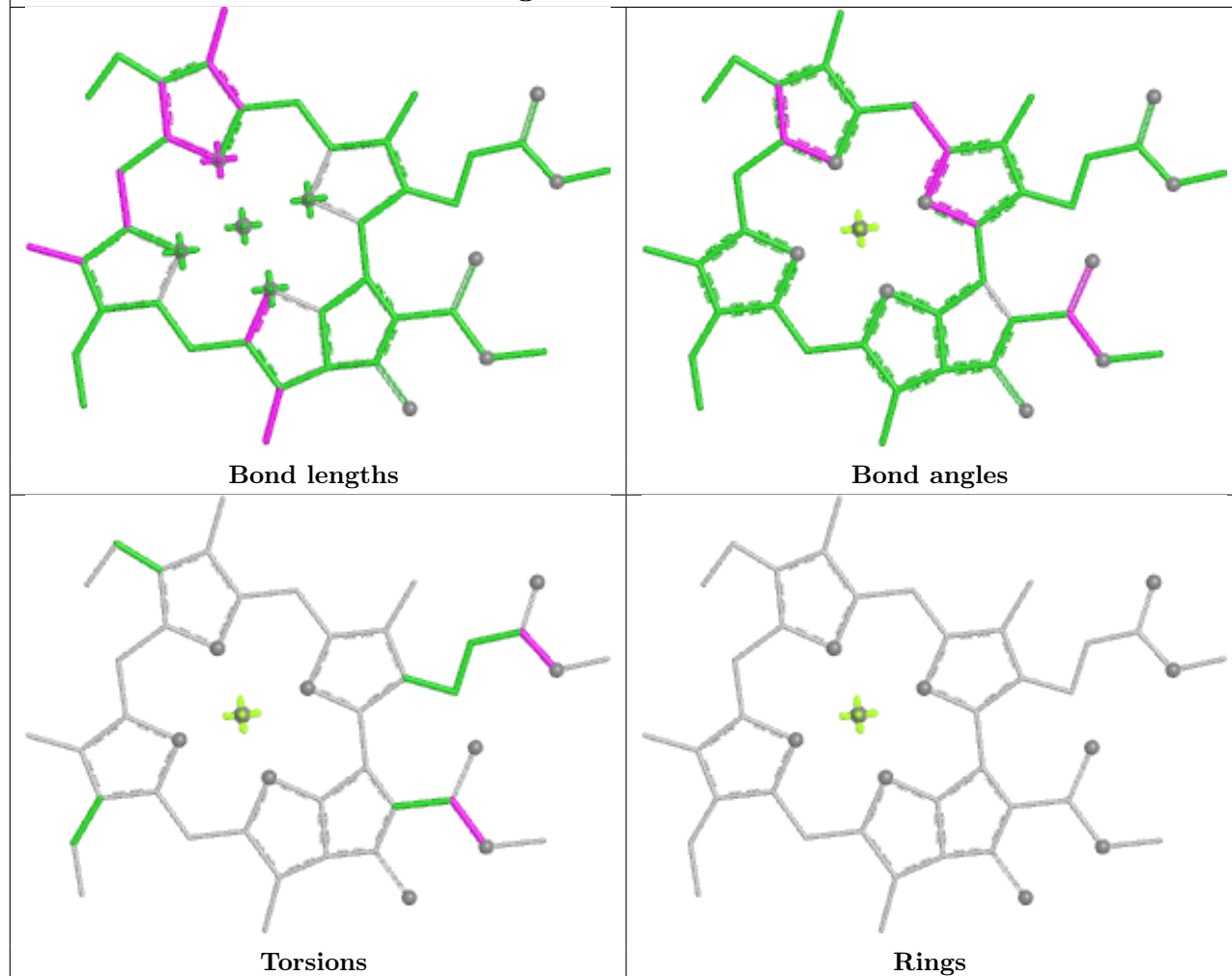


Rings

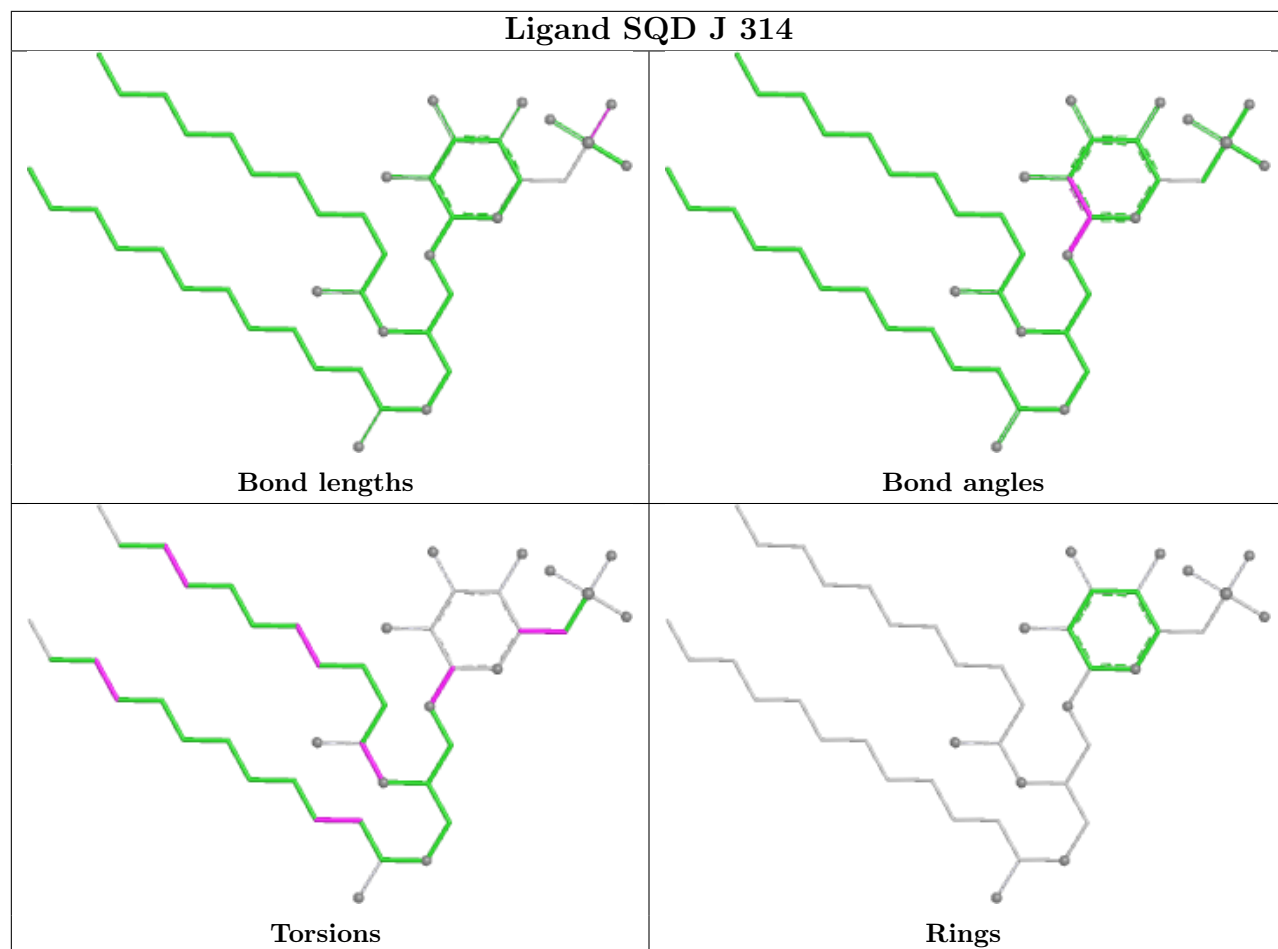
Ligand PID H 301



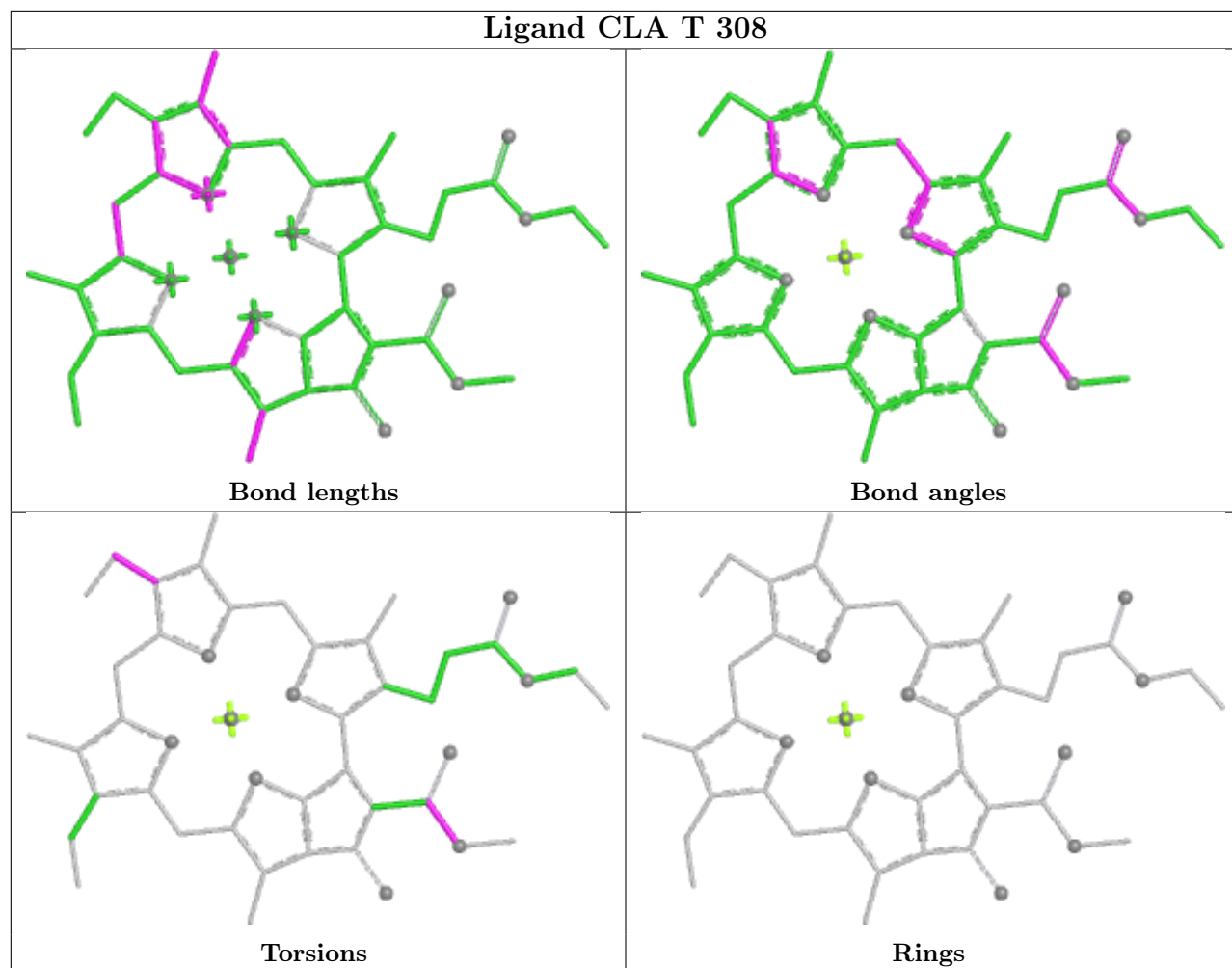
Ligand CLA a 814

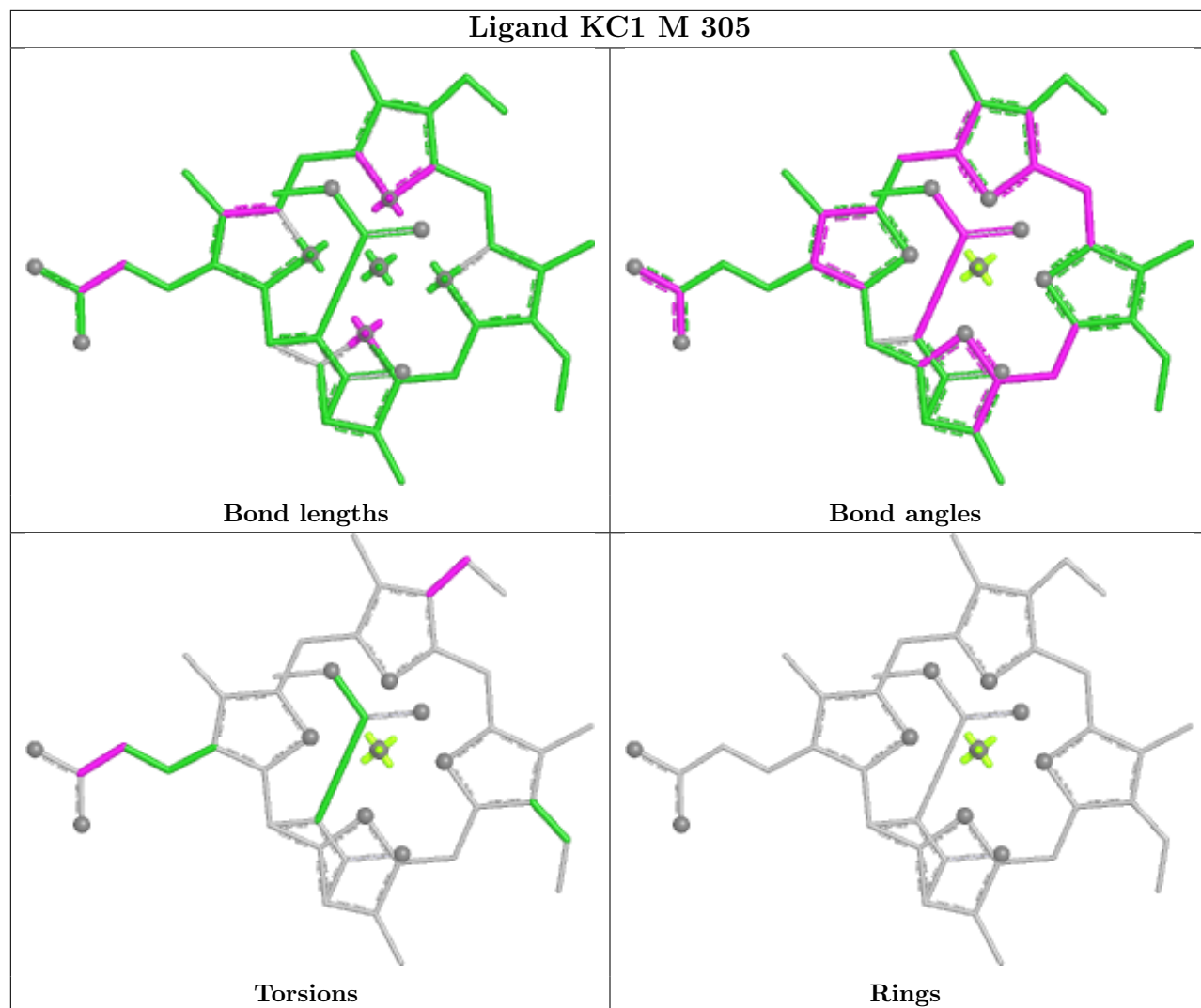


Ligand SQD J 314

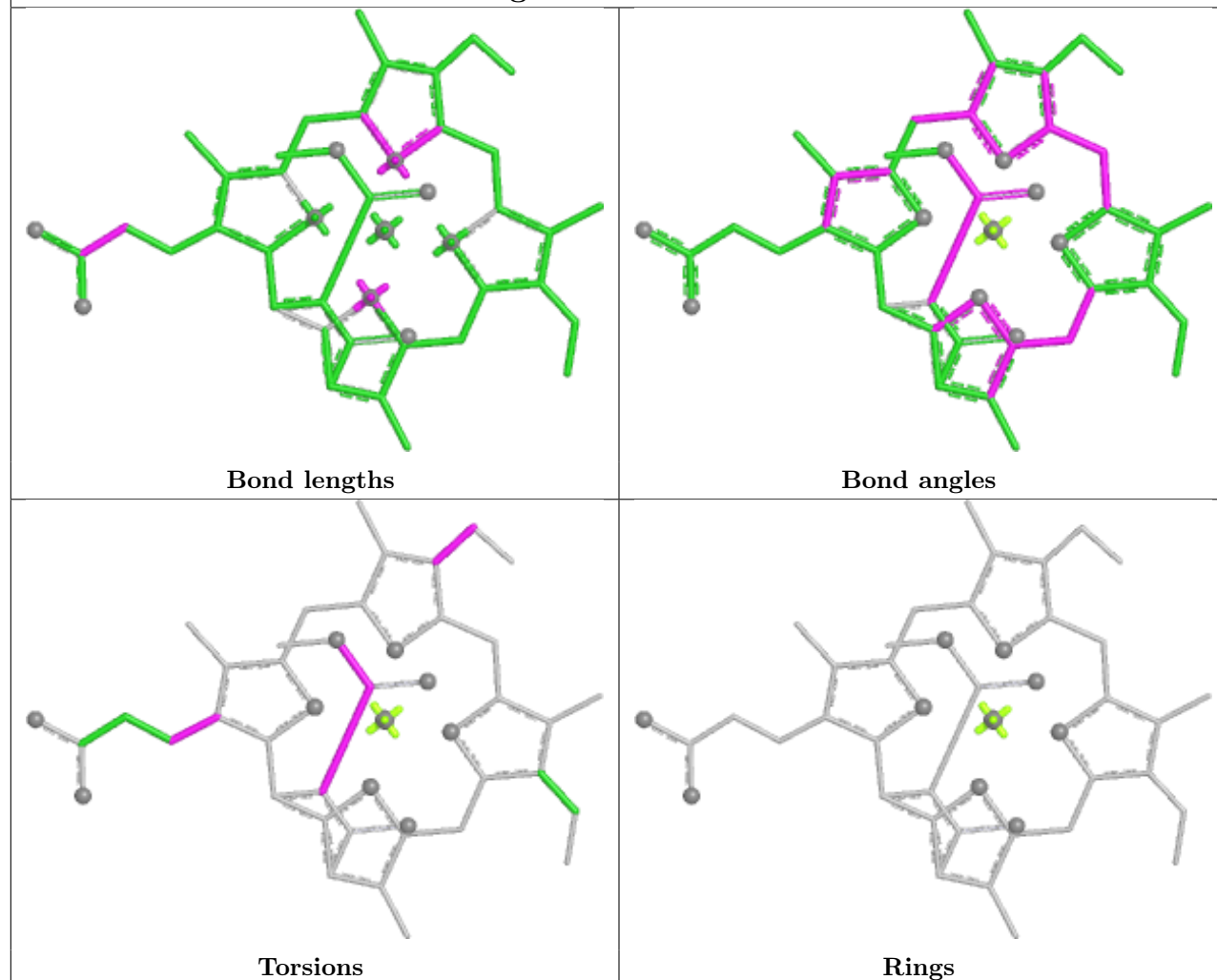


Ligand CLA T 308

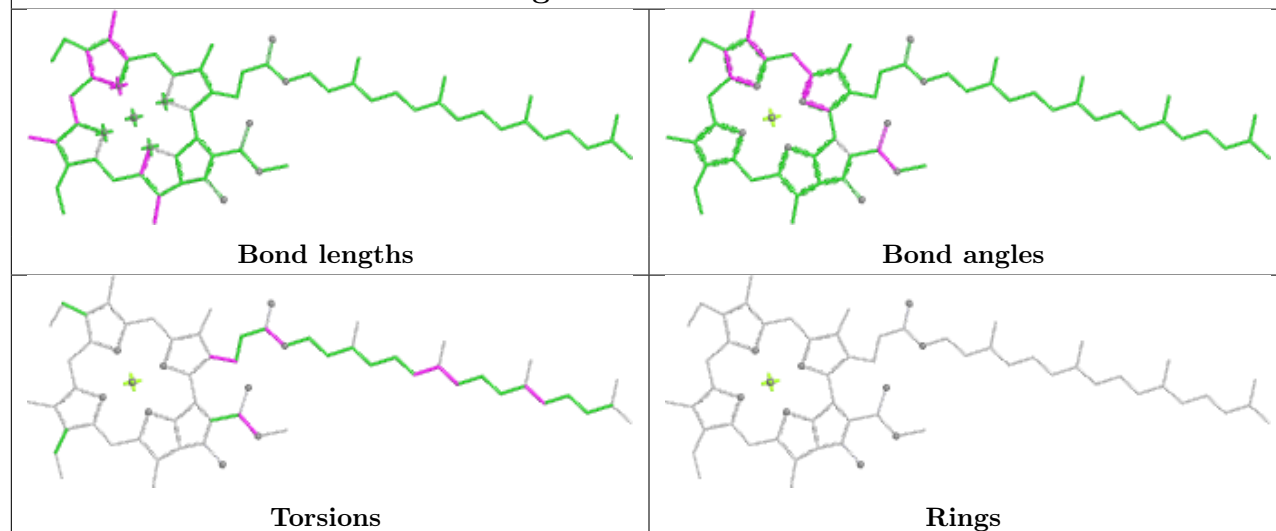




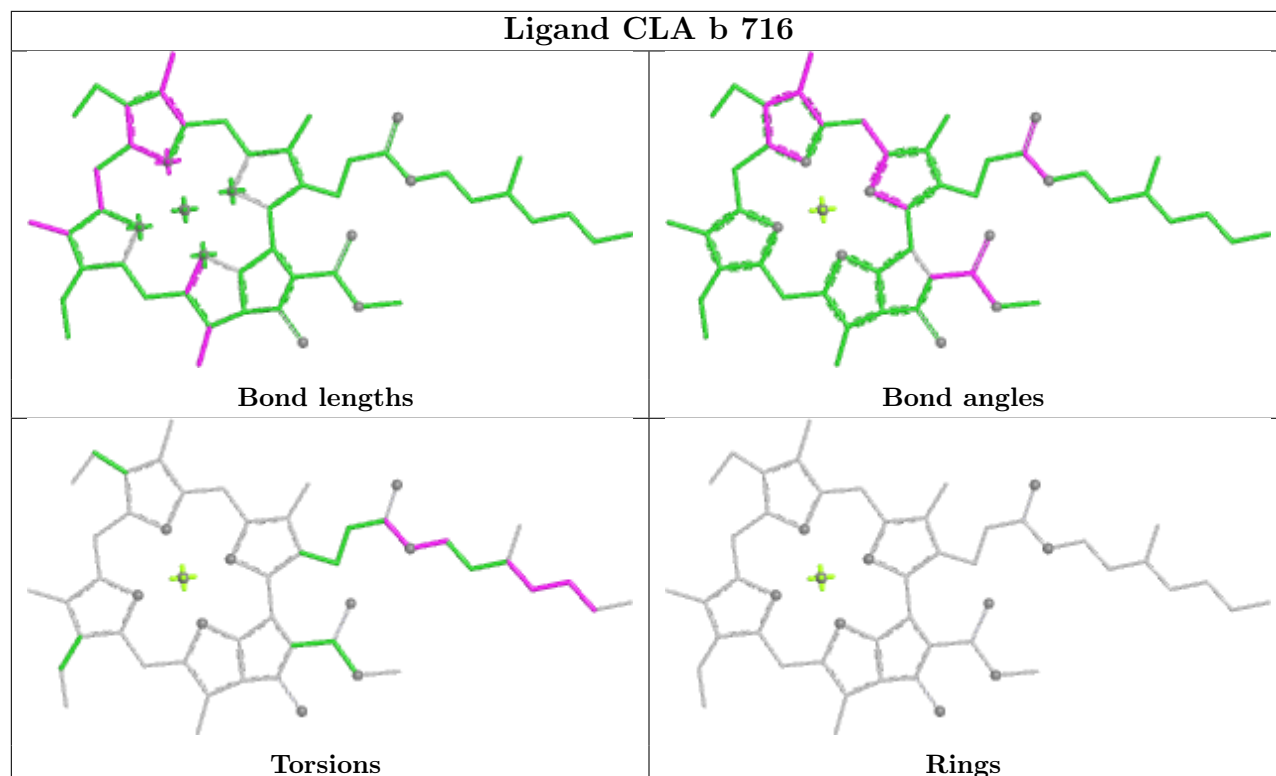
Ligand KC1 P 213



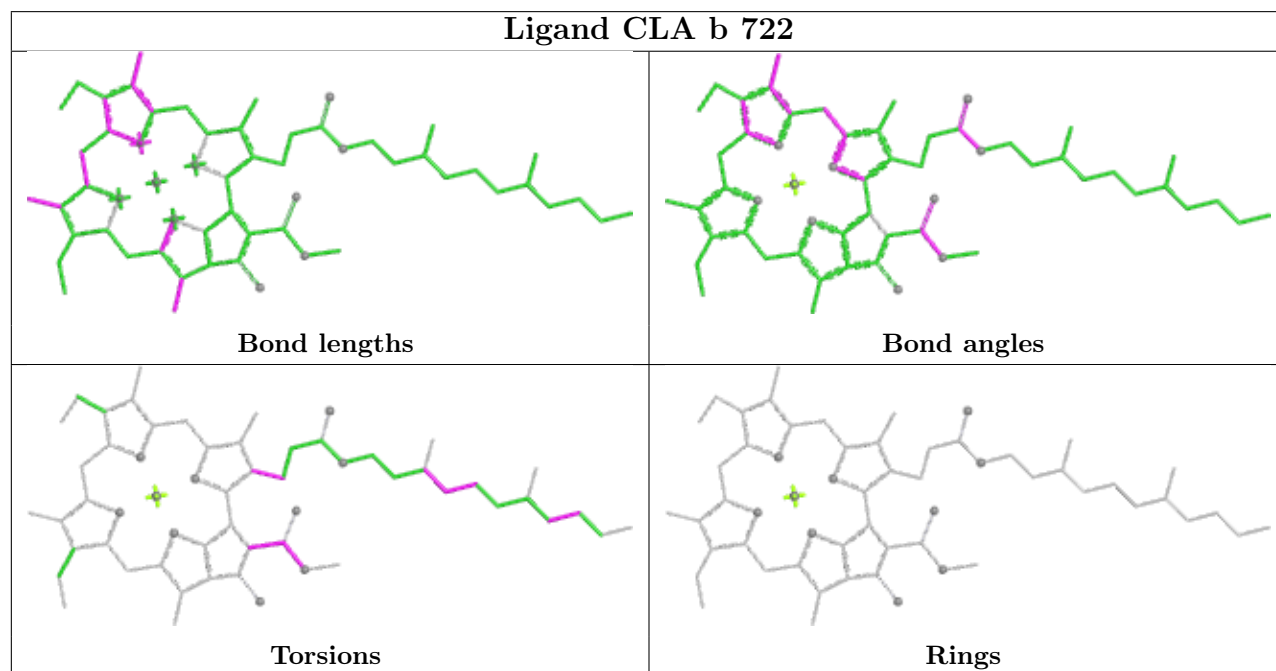
Ligand CLA B 312

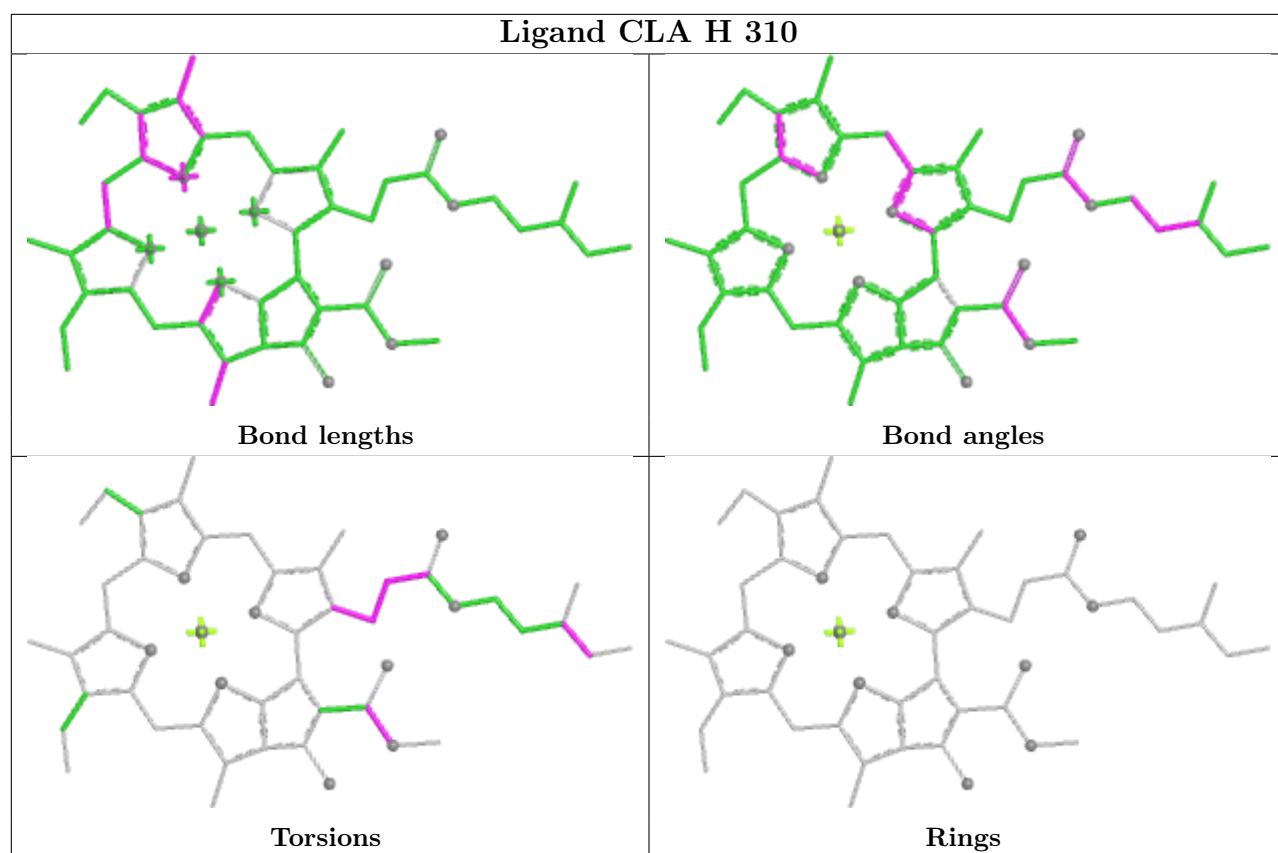


Ligand CLA b 716

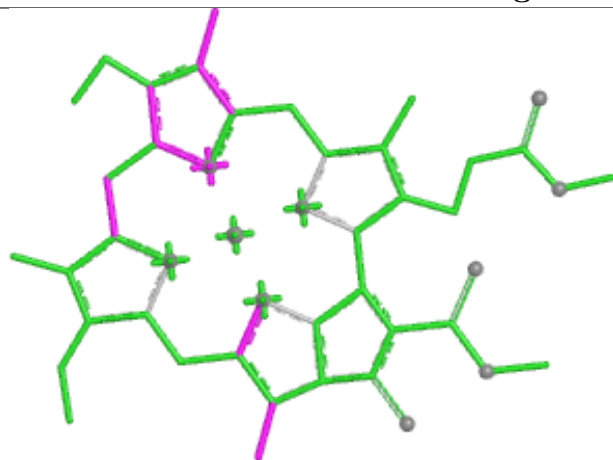


Ligand CLA b 722

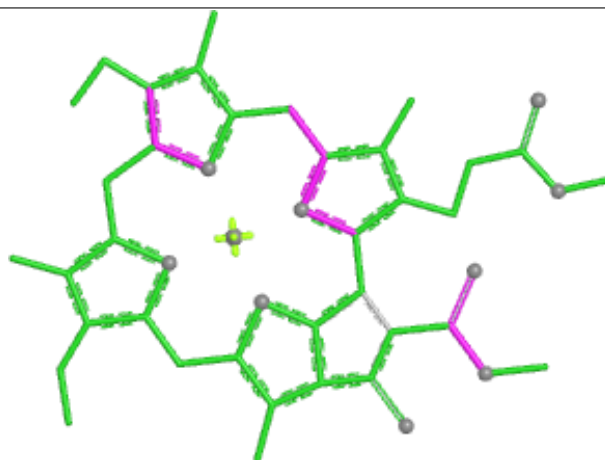




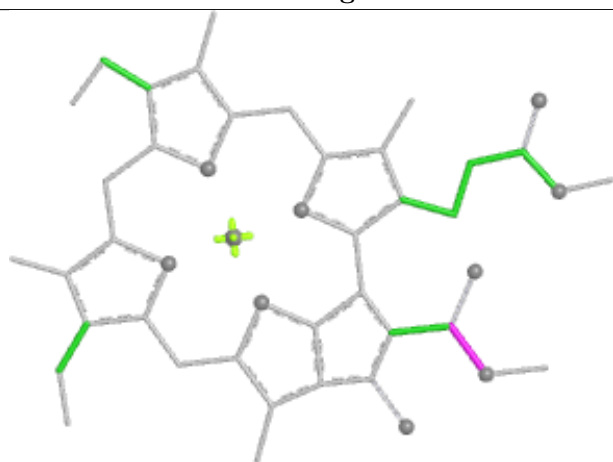
Ligand CLA D 309



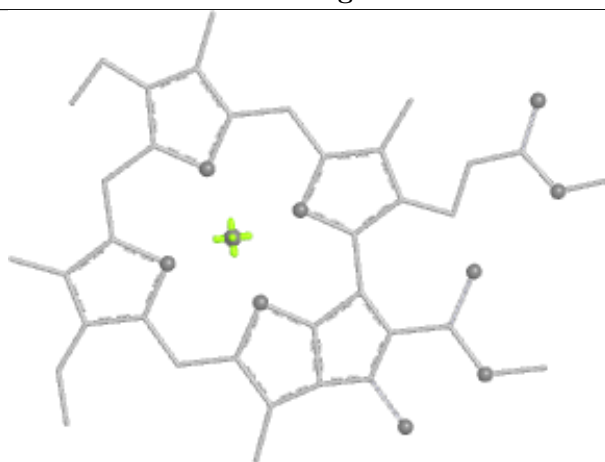
Bond lengths



Bond angles

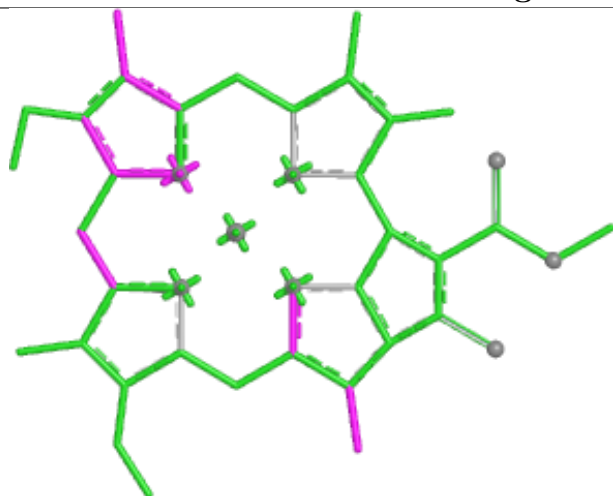


Torsions

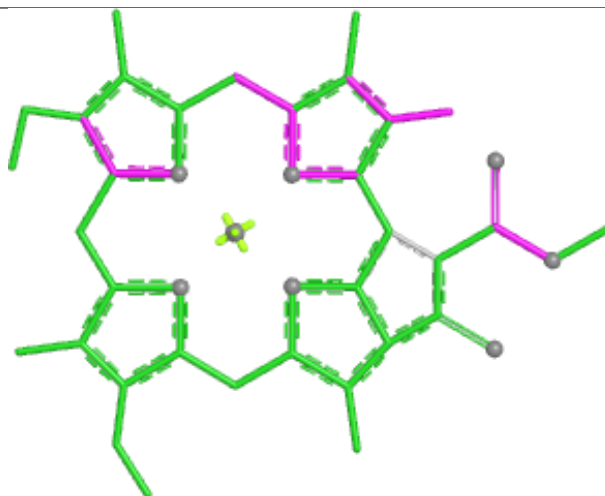


Rings

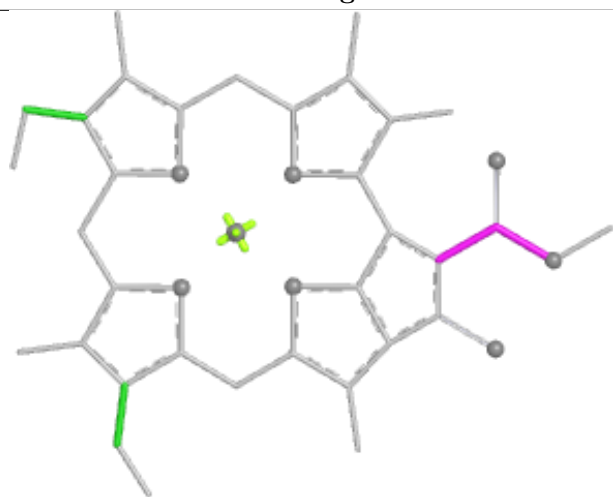
Ligand CLA C 316



Bond lengths



Bond angles

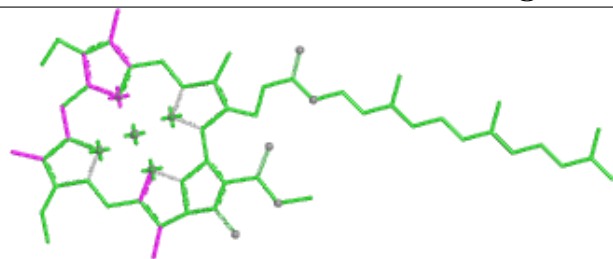


Torsions

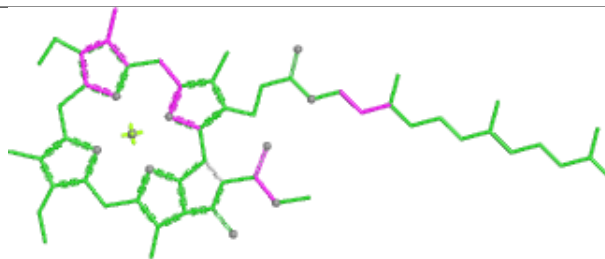


Rings

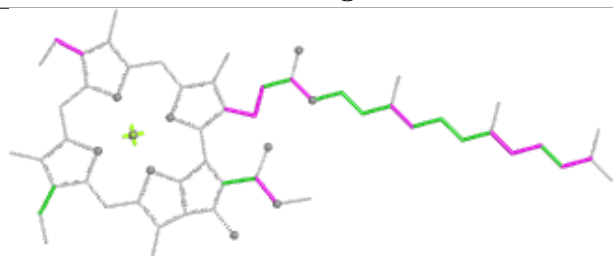
Ligand CLA a 812



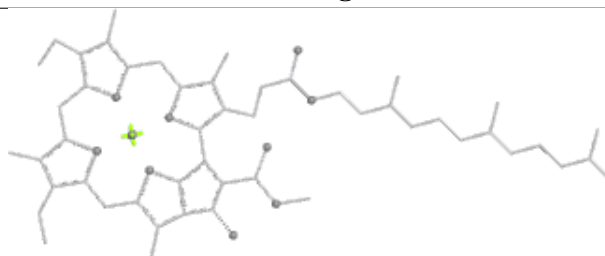
Bond lengths



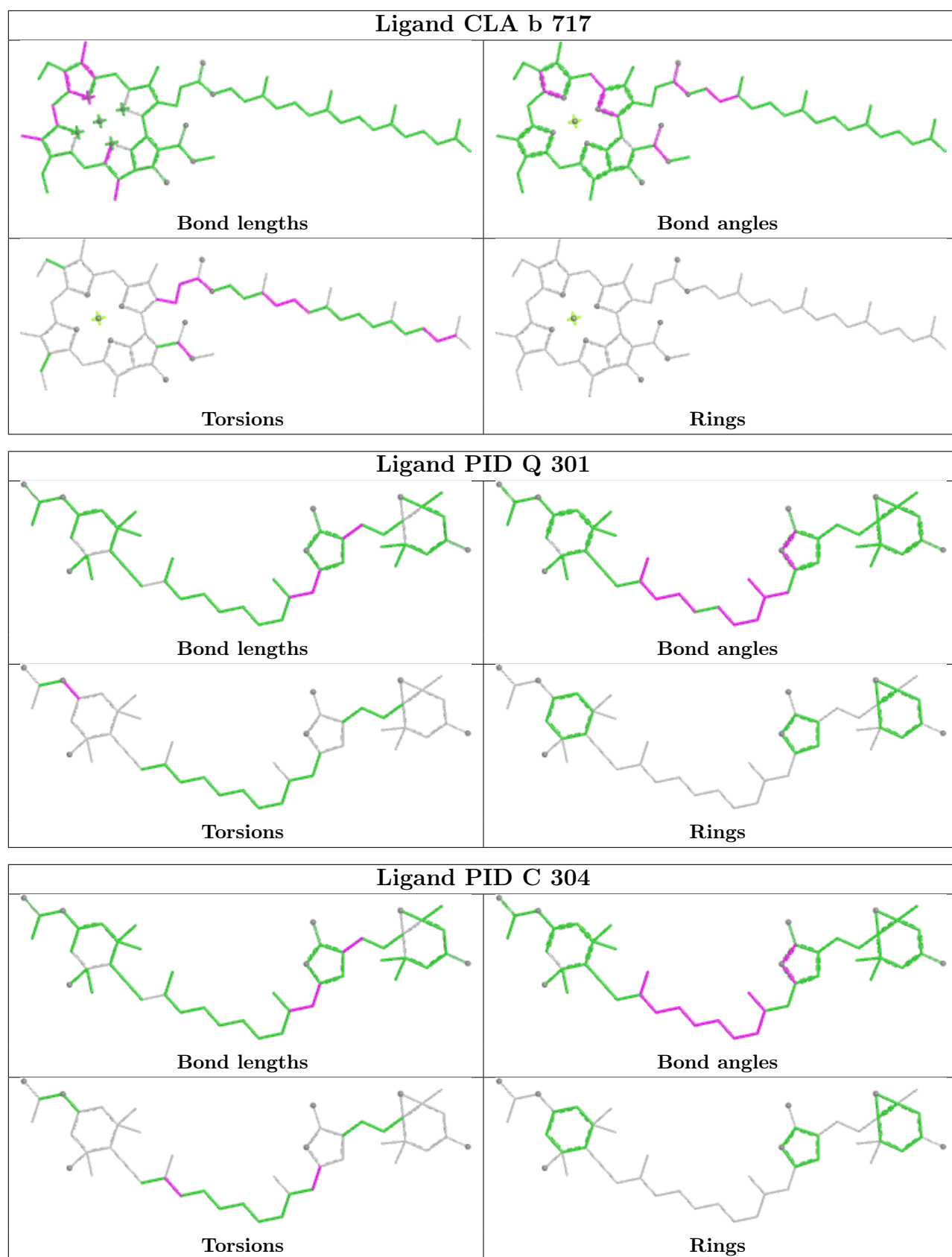
Bond angles



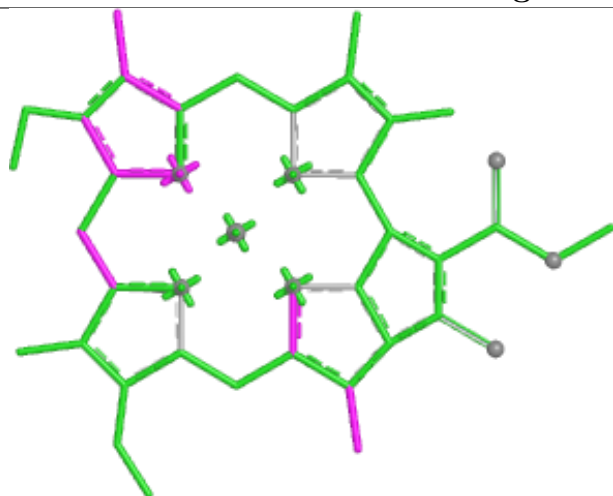
Torsions



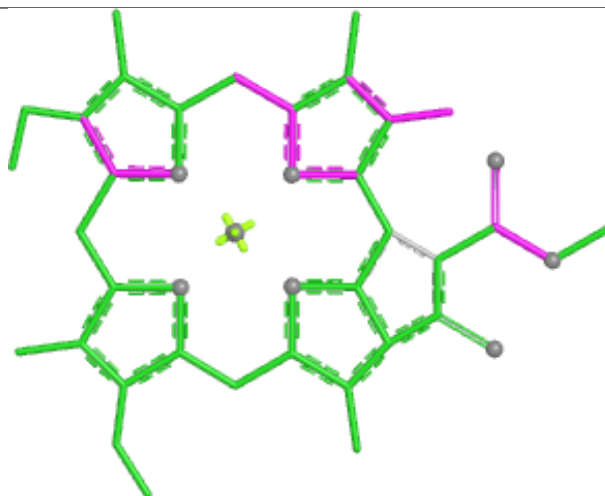
Rings



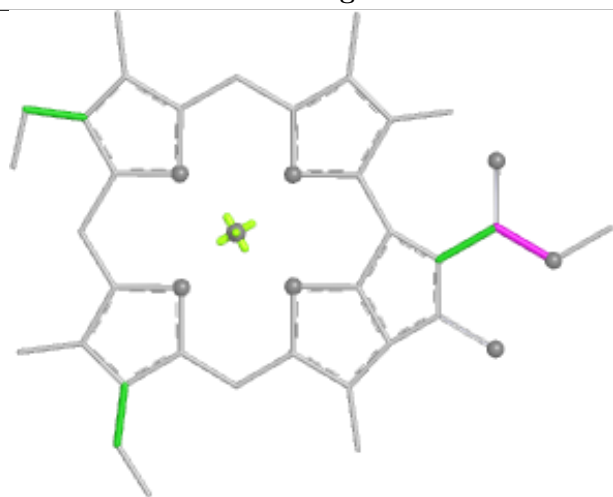
Ligand CLA G 319



Bond lengths



Bond angles

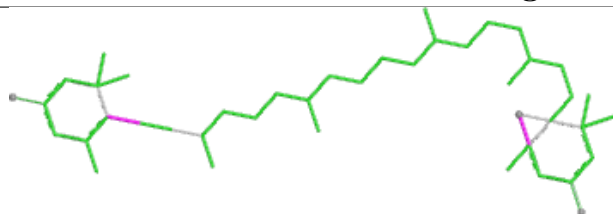


Torsions

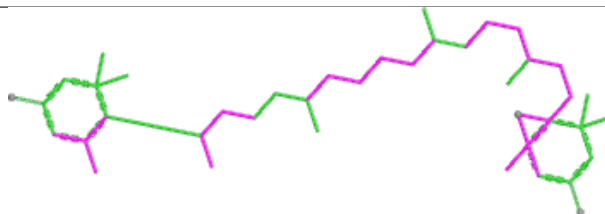


Rings

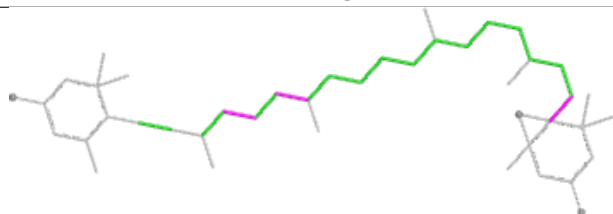
Ligand DD6 I 202



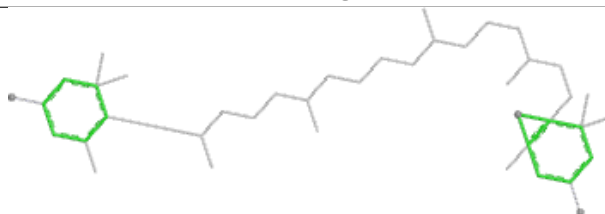
Bond lengths



Bond angles

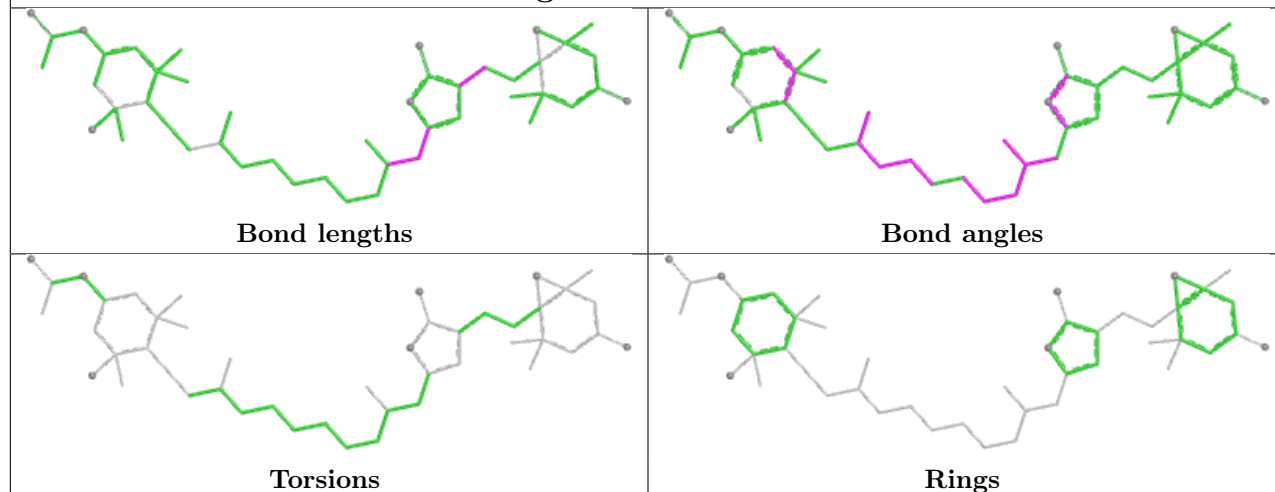


Torsions

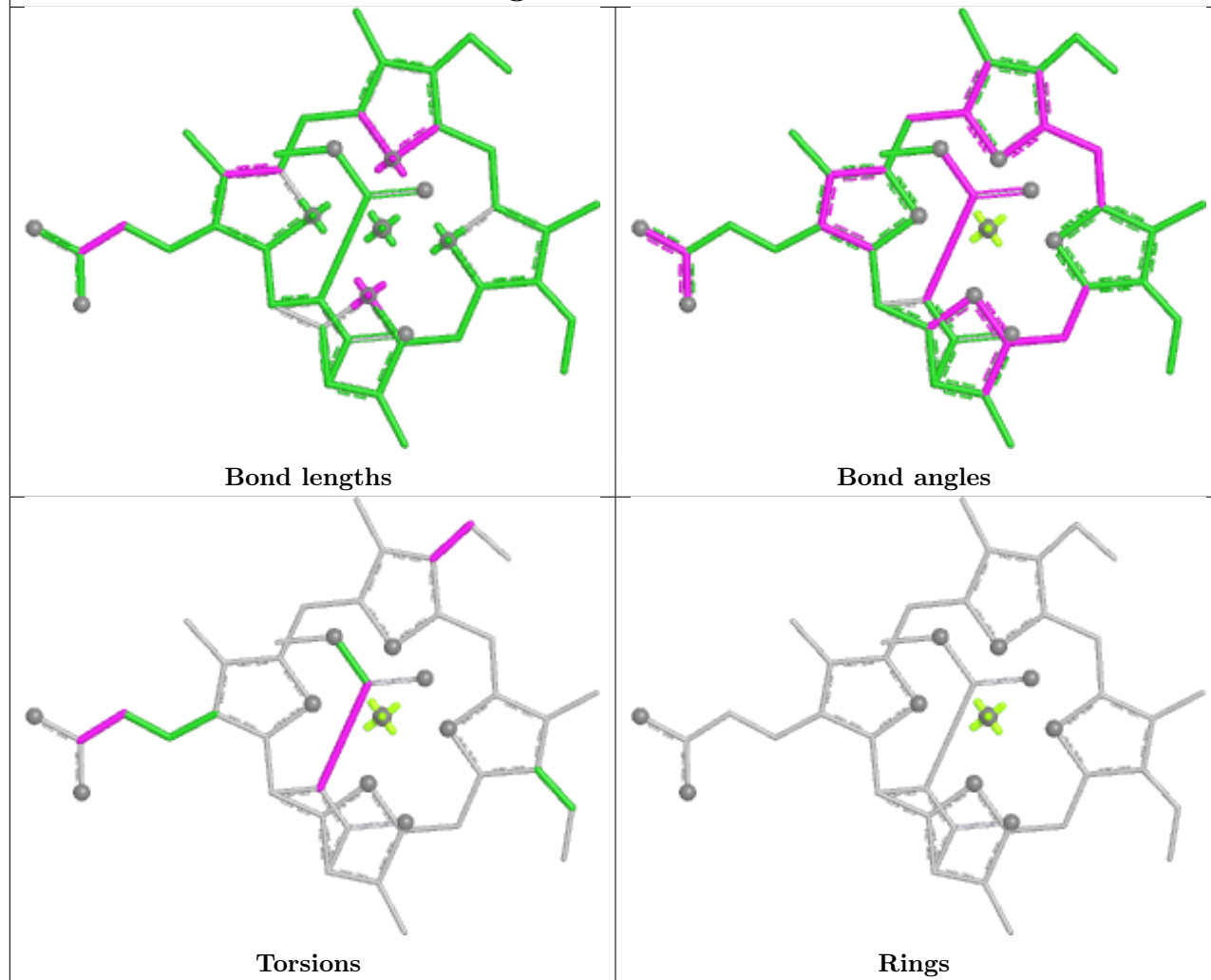


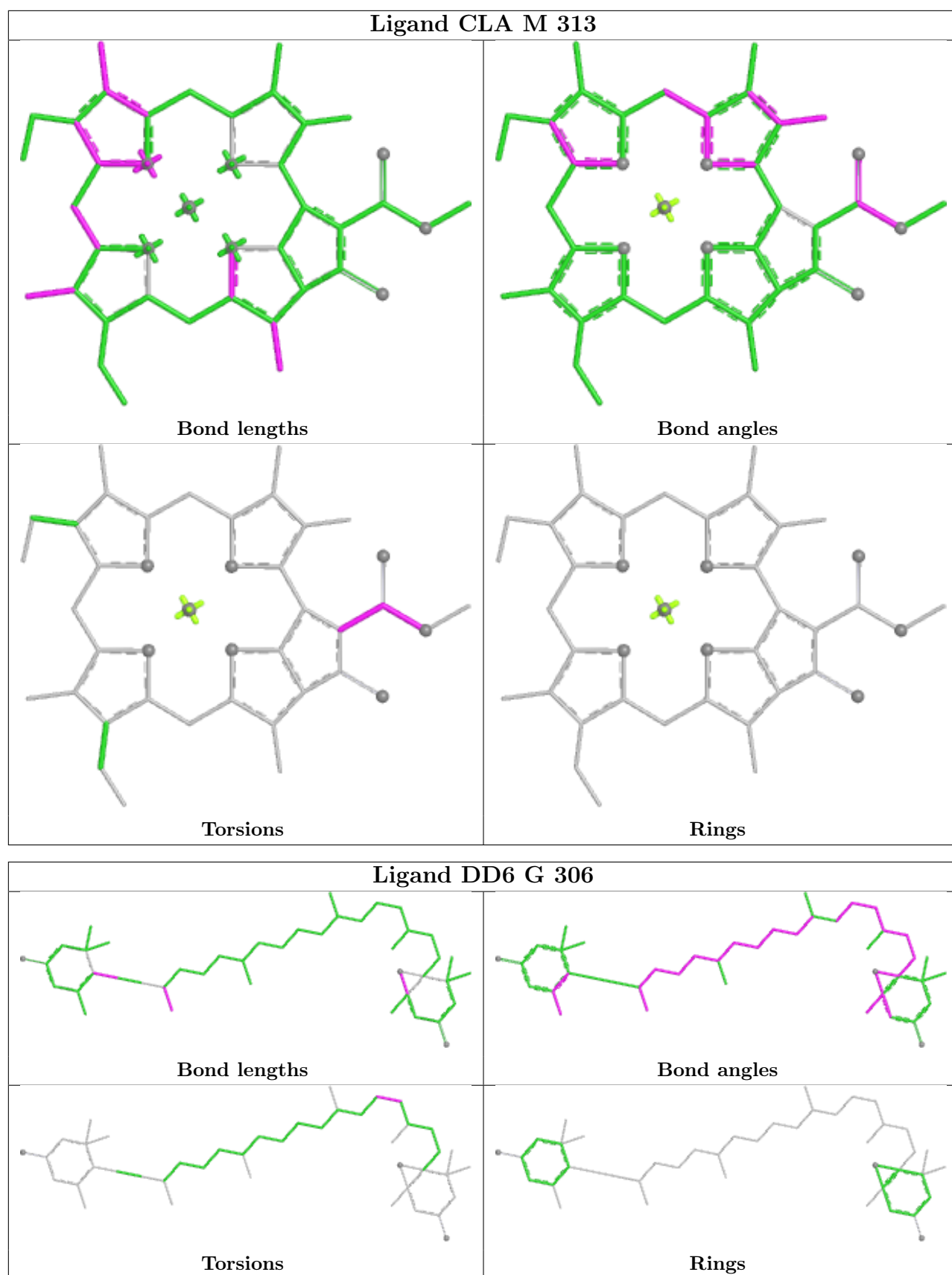
Rings

Ligand PID T 305

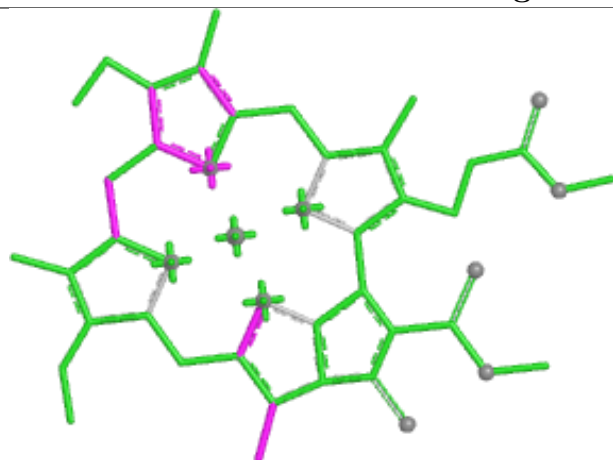


Ligand KC1 L 306

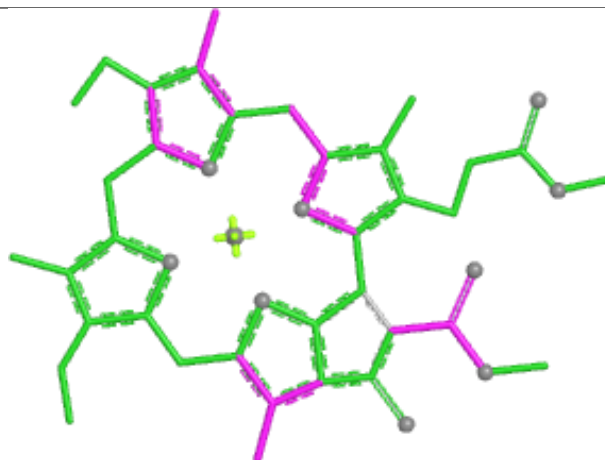




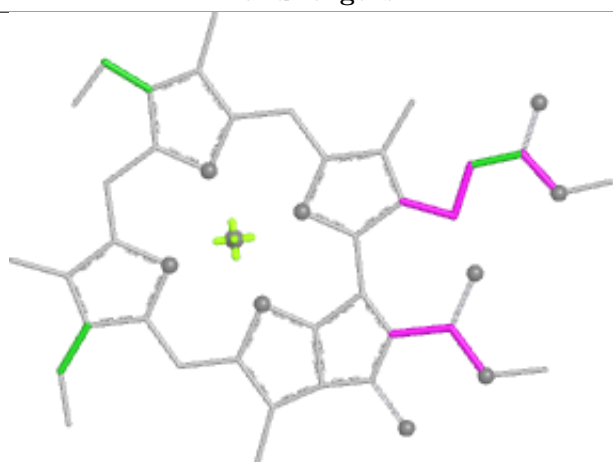
Ligand CLA N 313



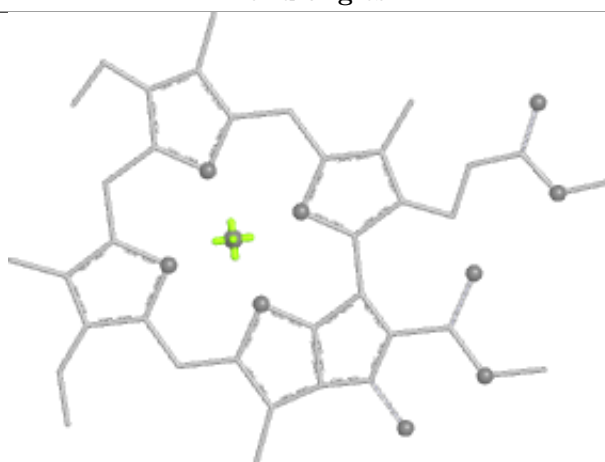
Bond lengths



Bond angles

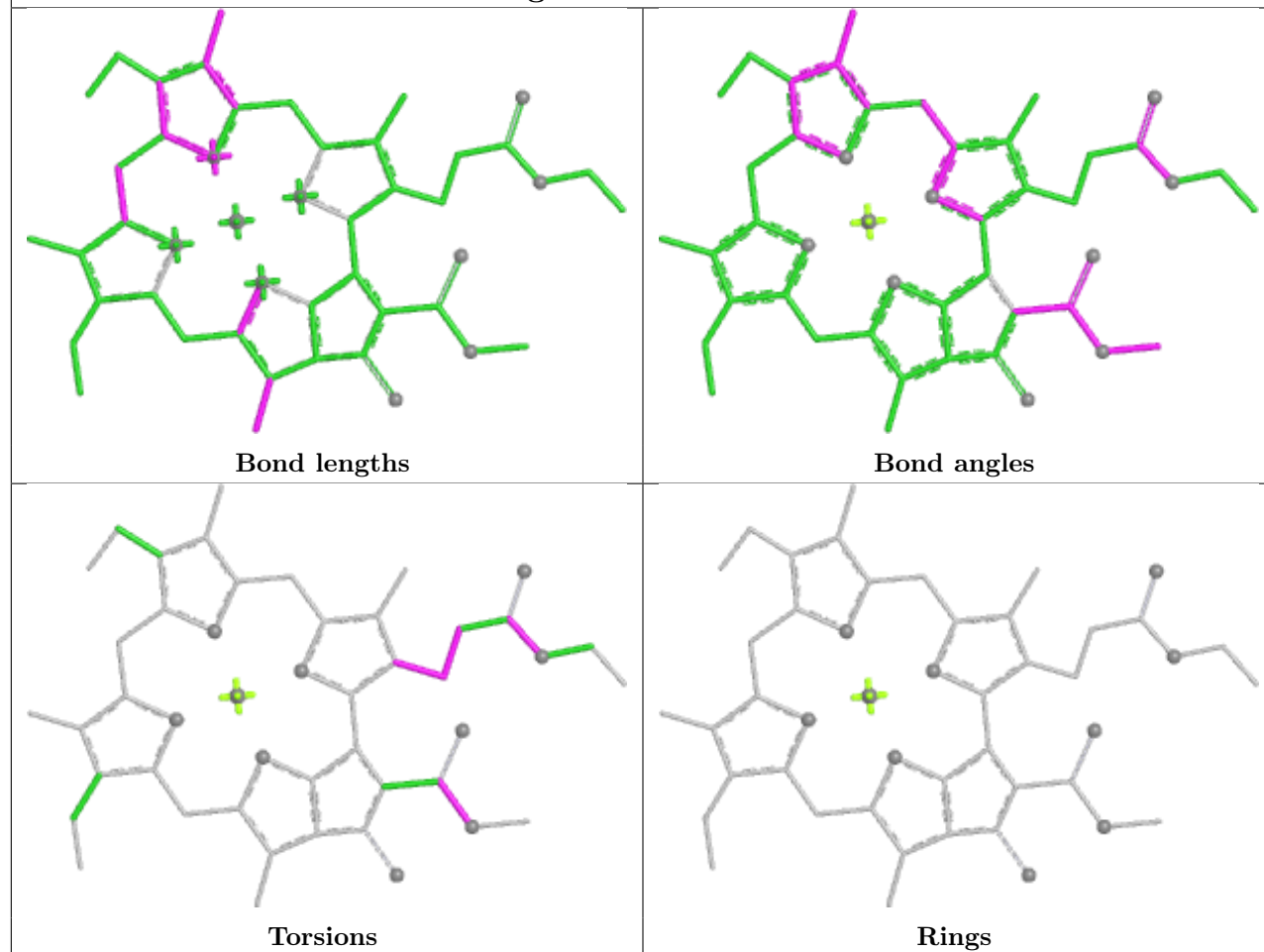


Torsions

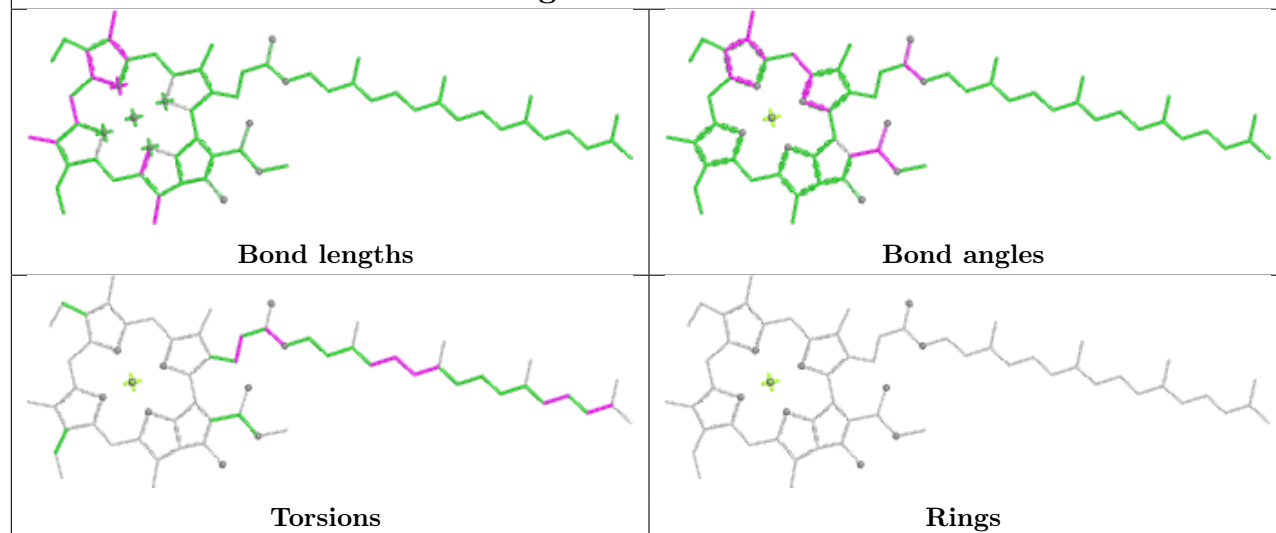


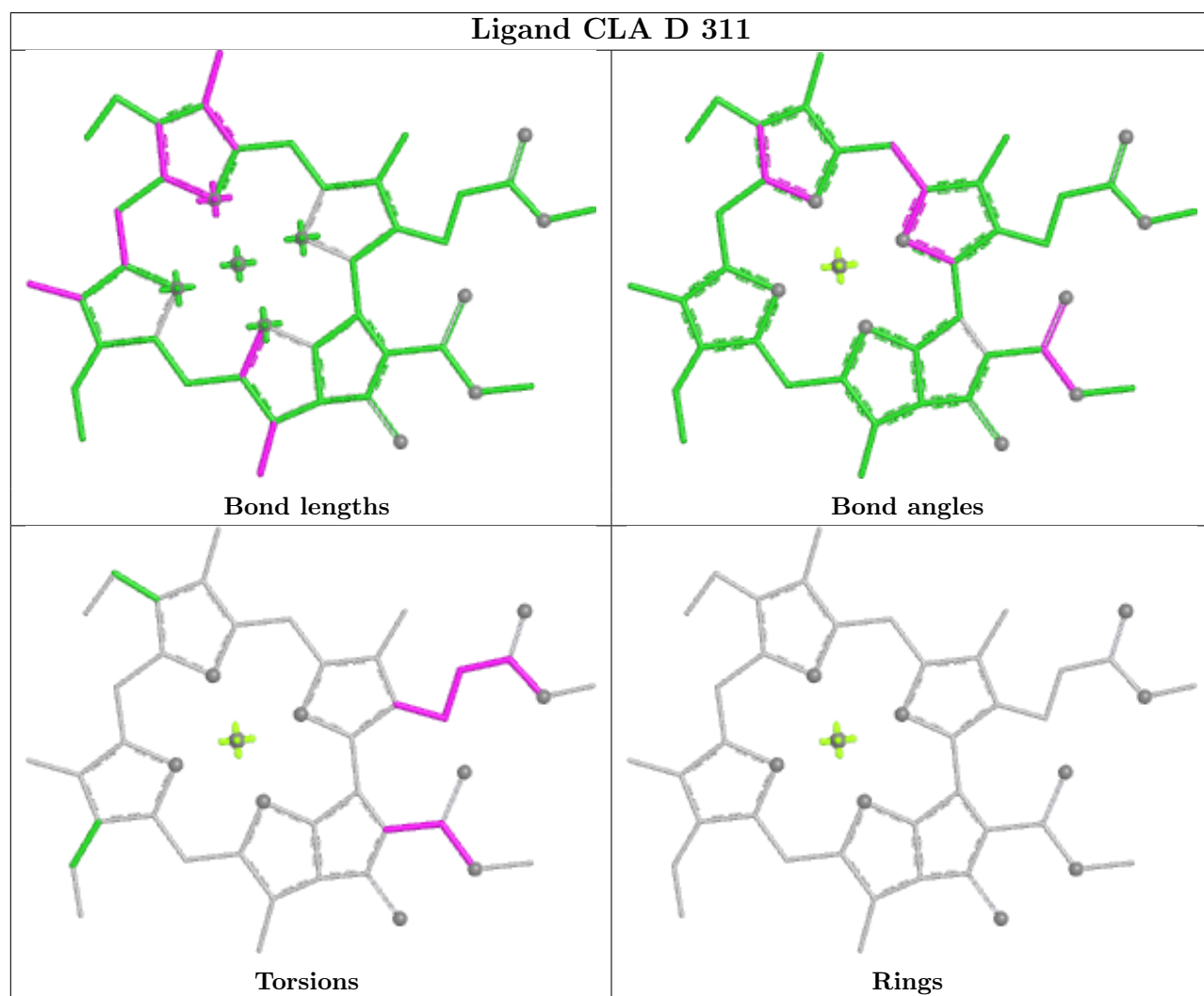
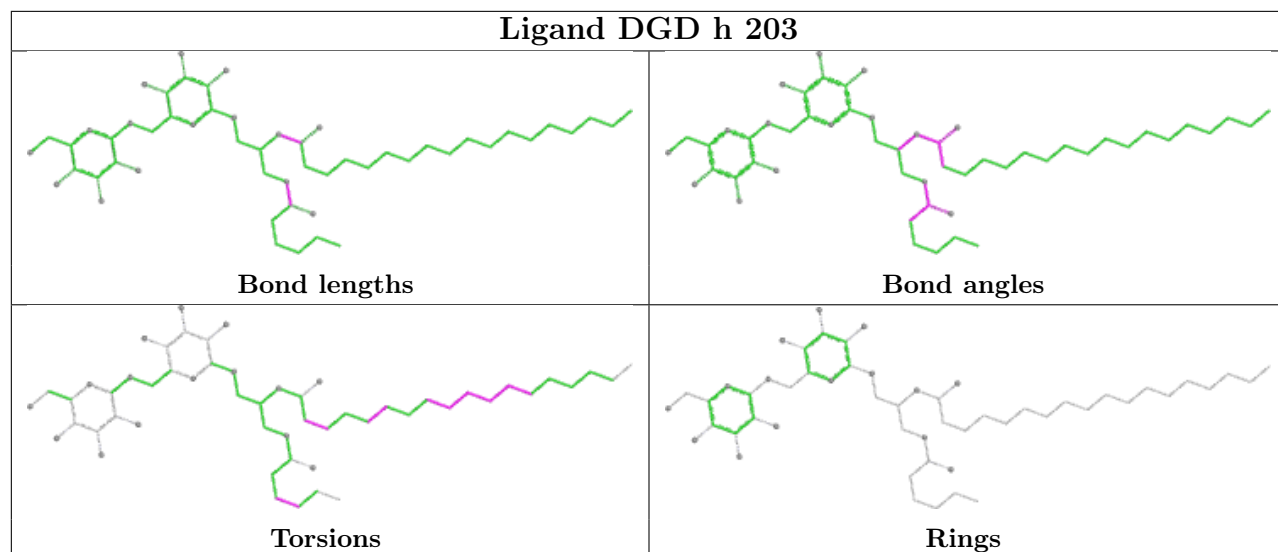
Rings

Ligand CLA T 314

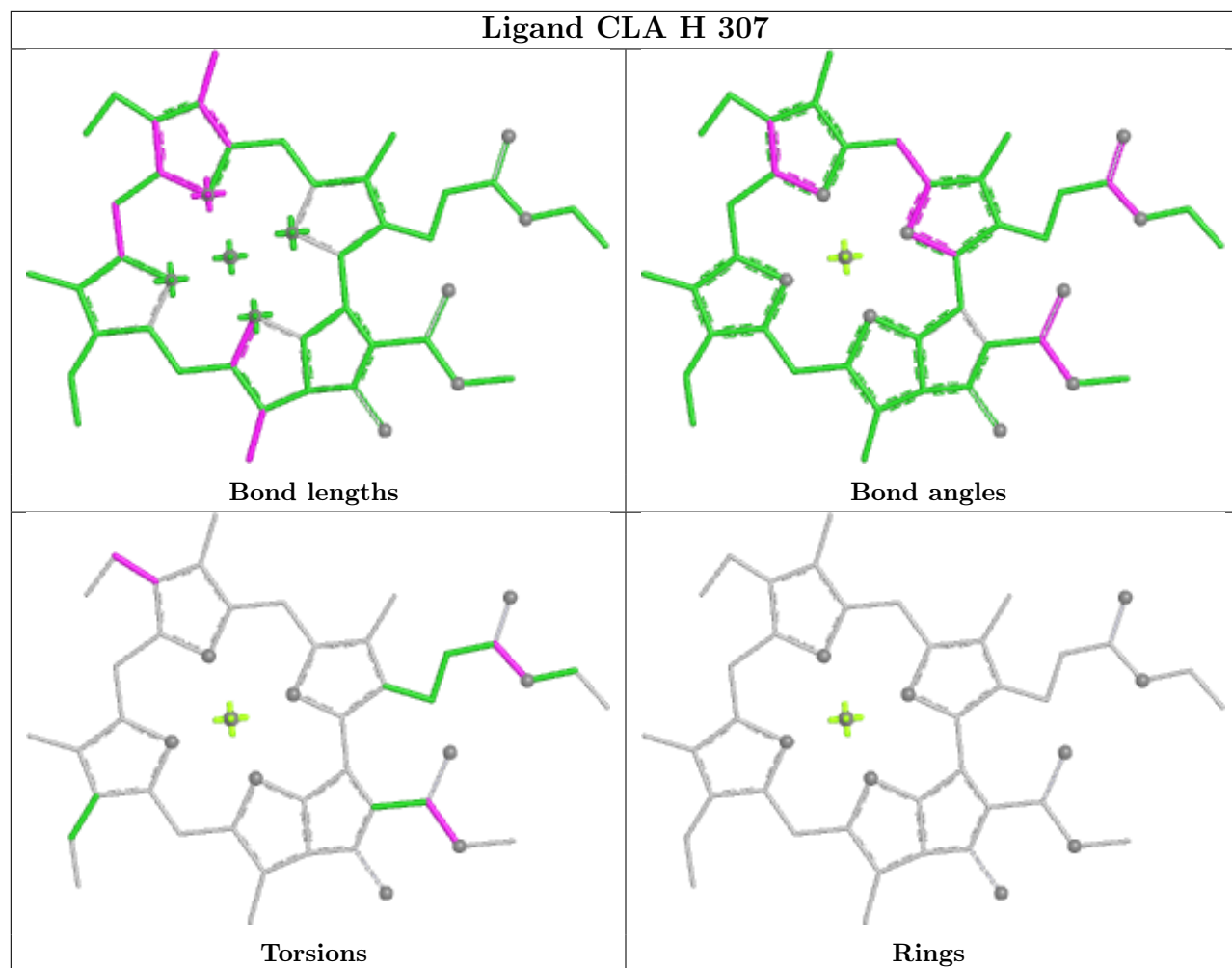


Ligand CLA I 211

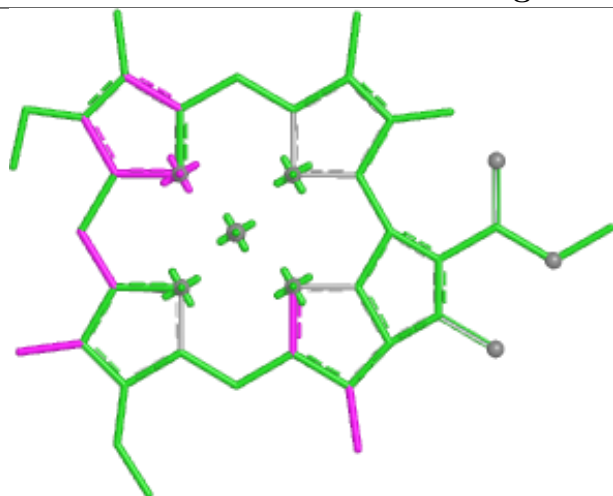




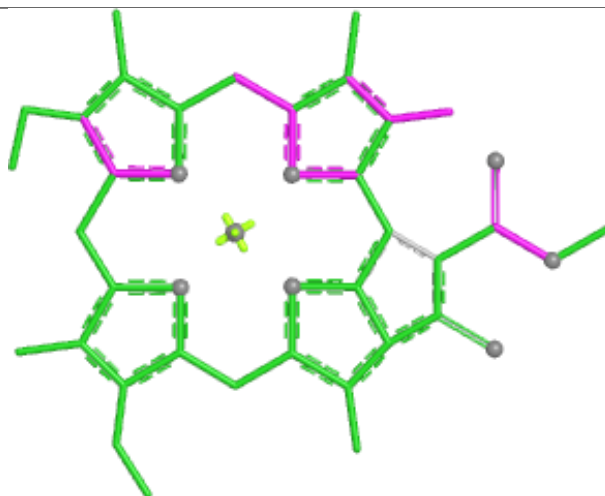
Ligand CLA H 307



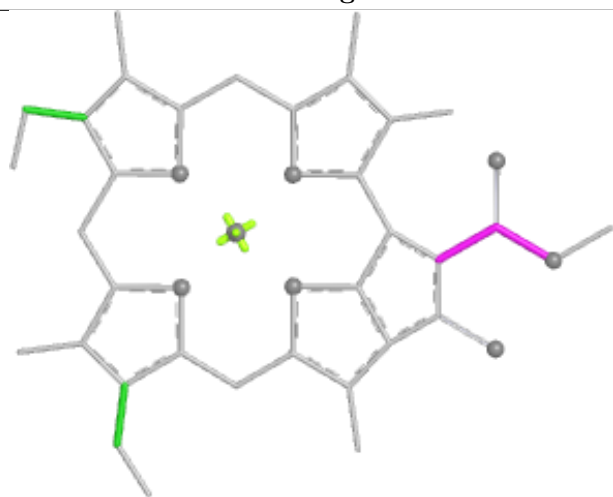
Ligand CLA D 316



Bond lengths



Bond angles

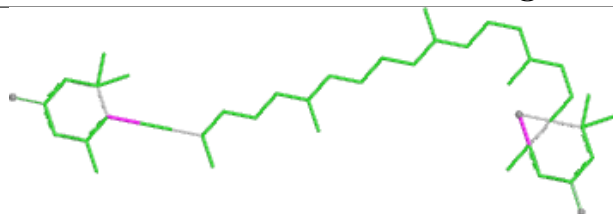


Torsions

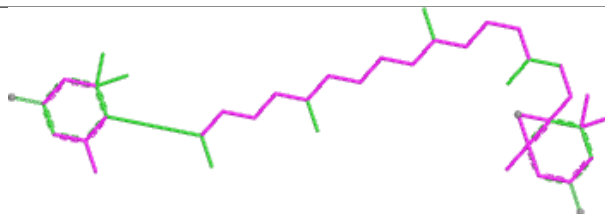


Rings

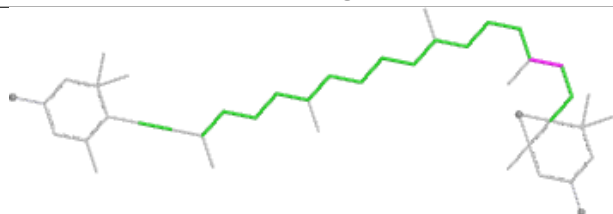
Ligand DD6 J 302



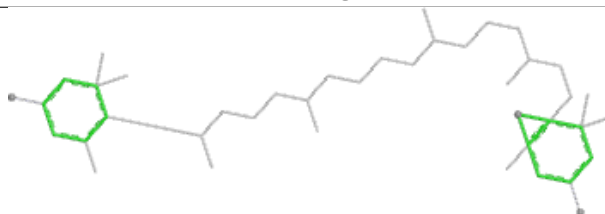
Bond lengths



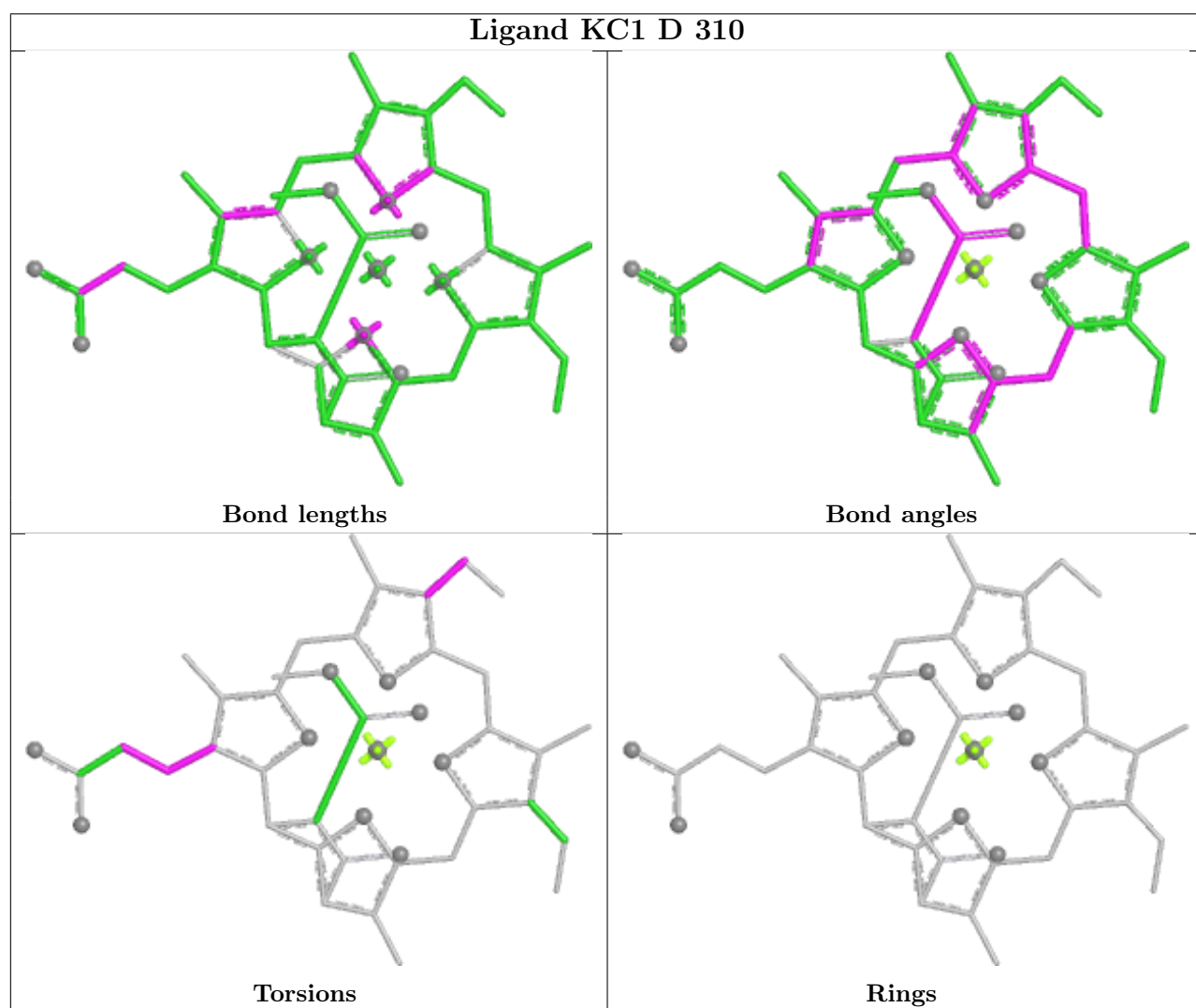
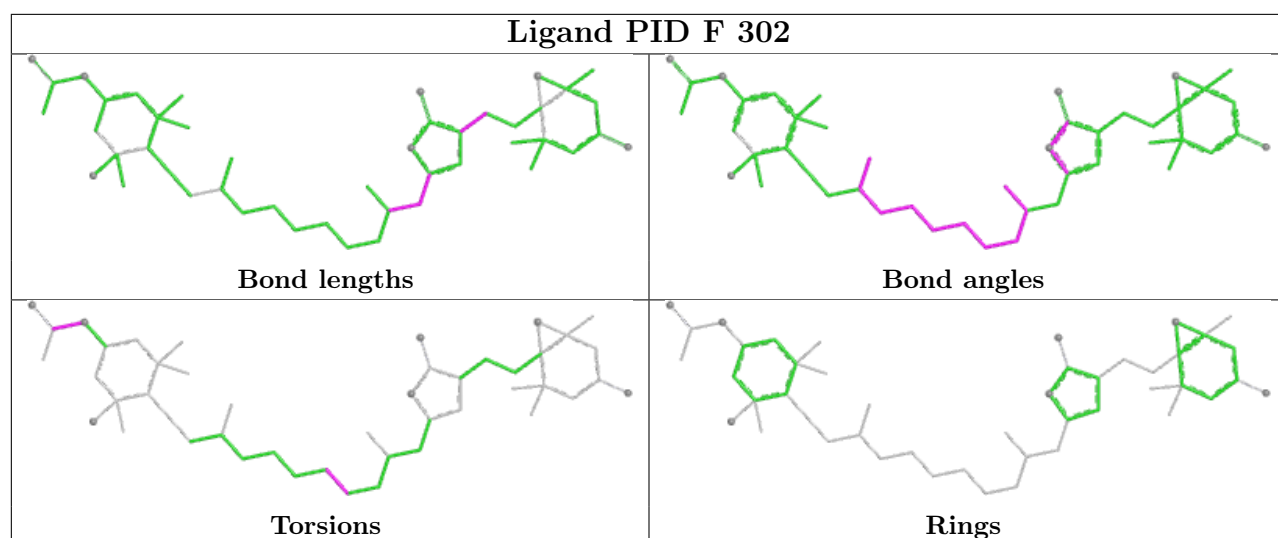
Bond angles

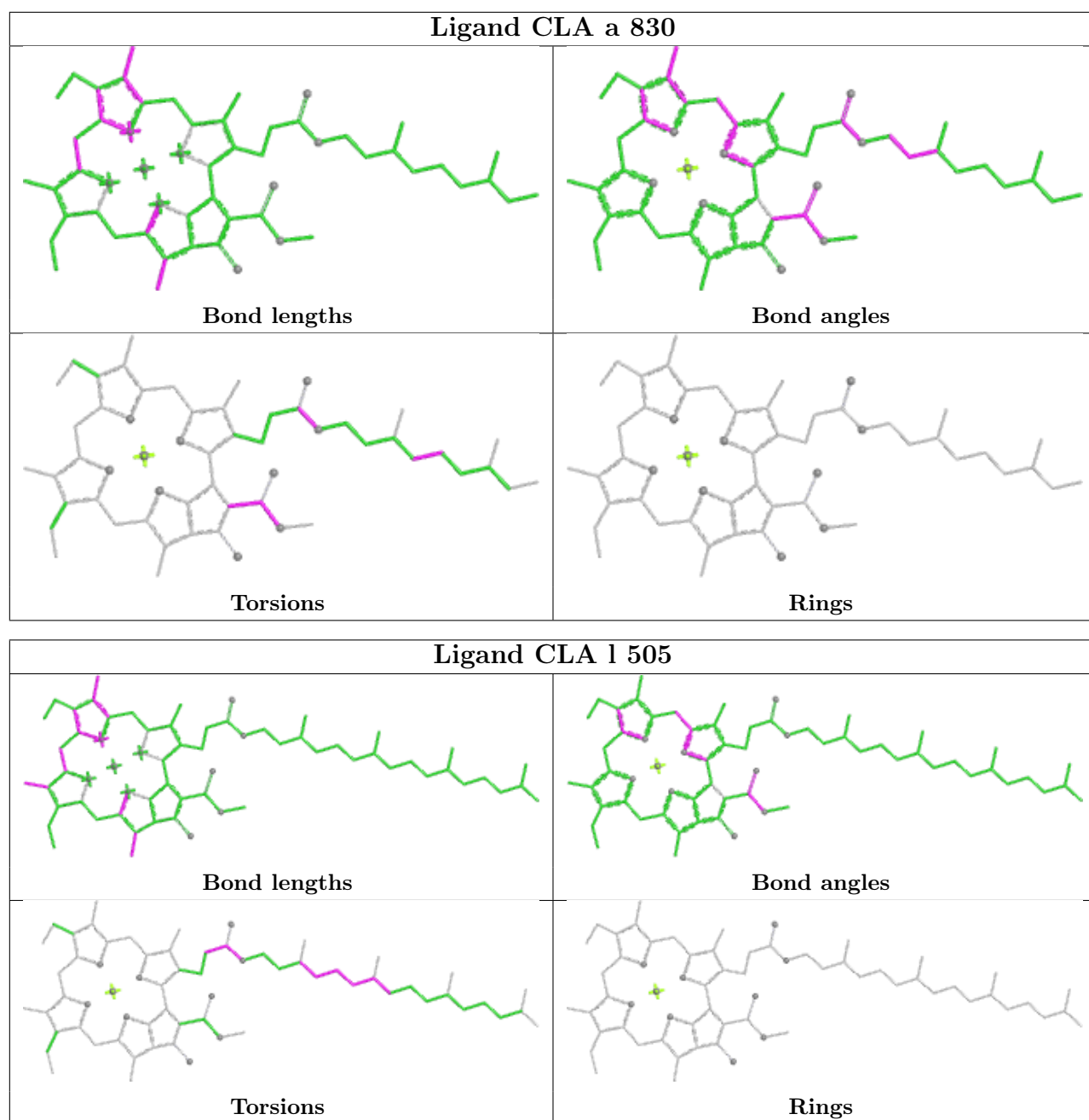


Torsions

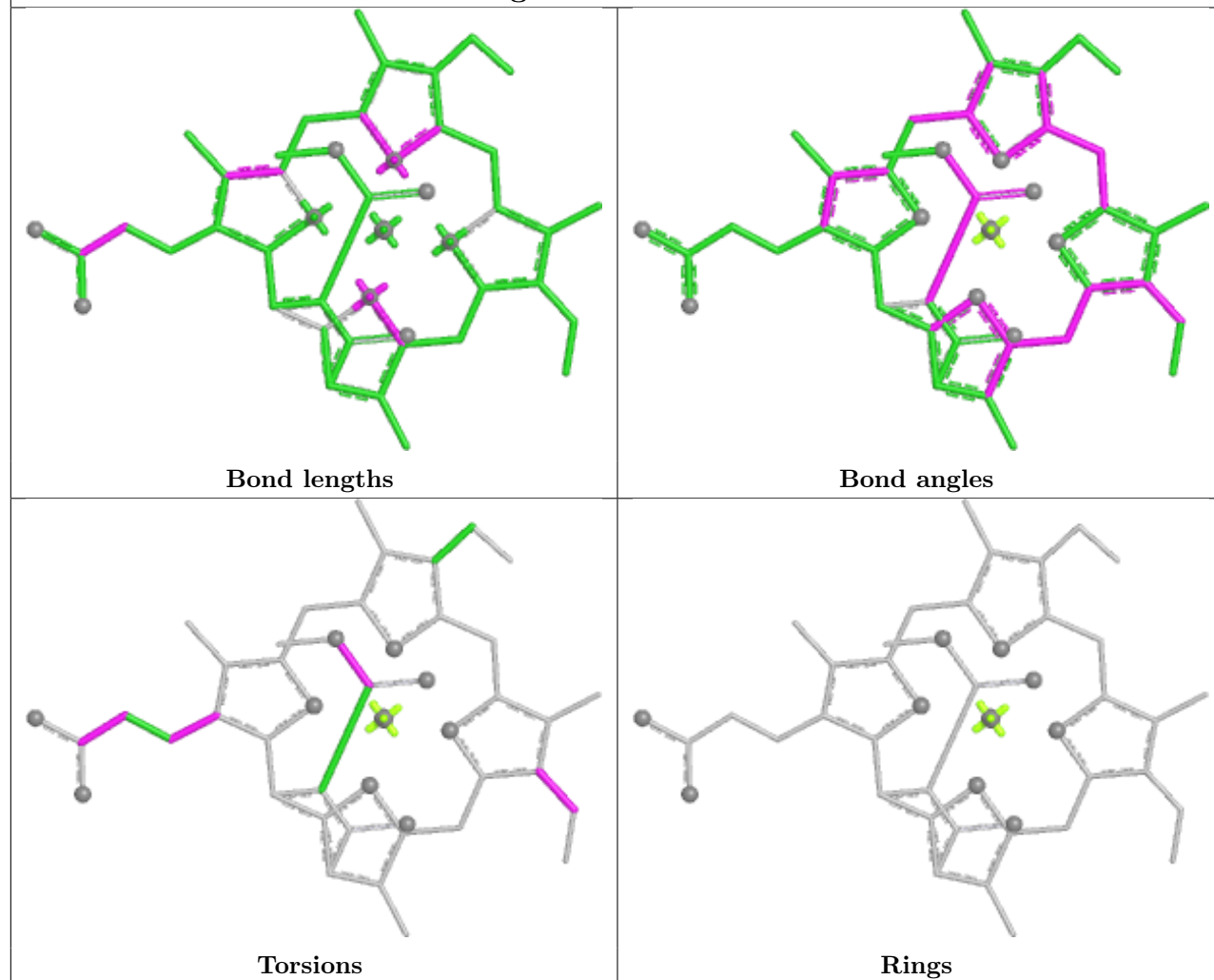


Rings

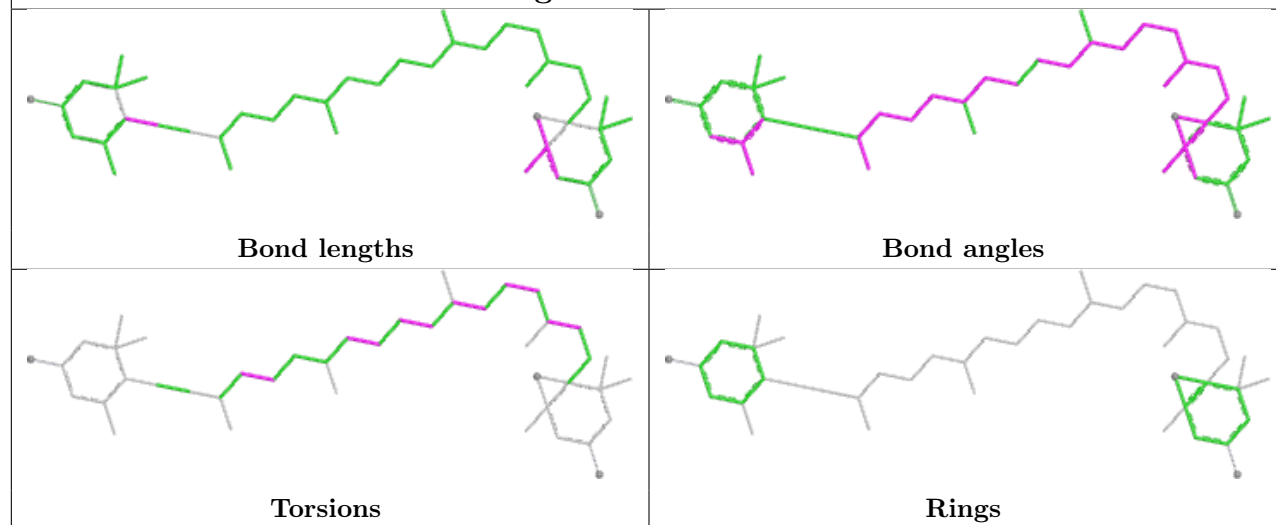


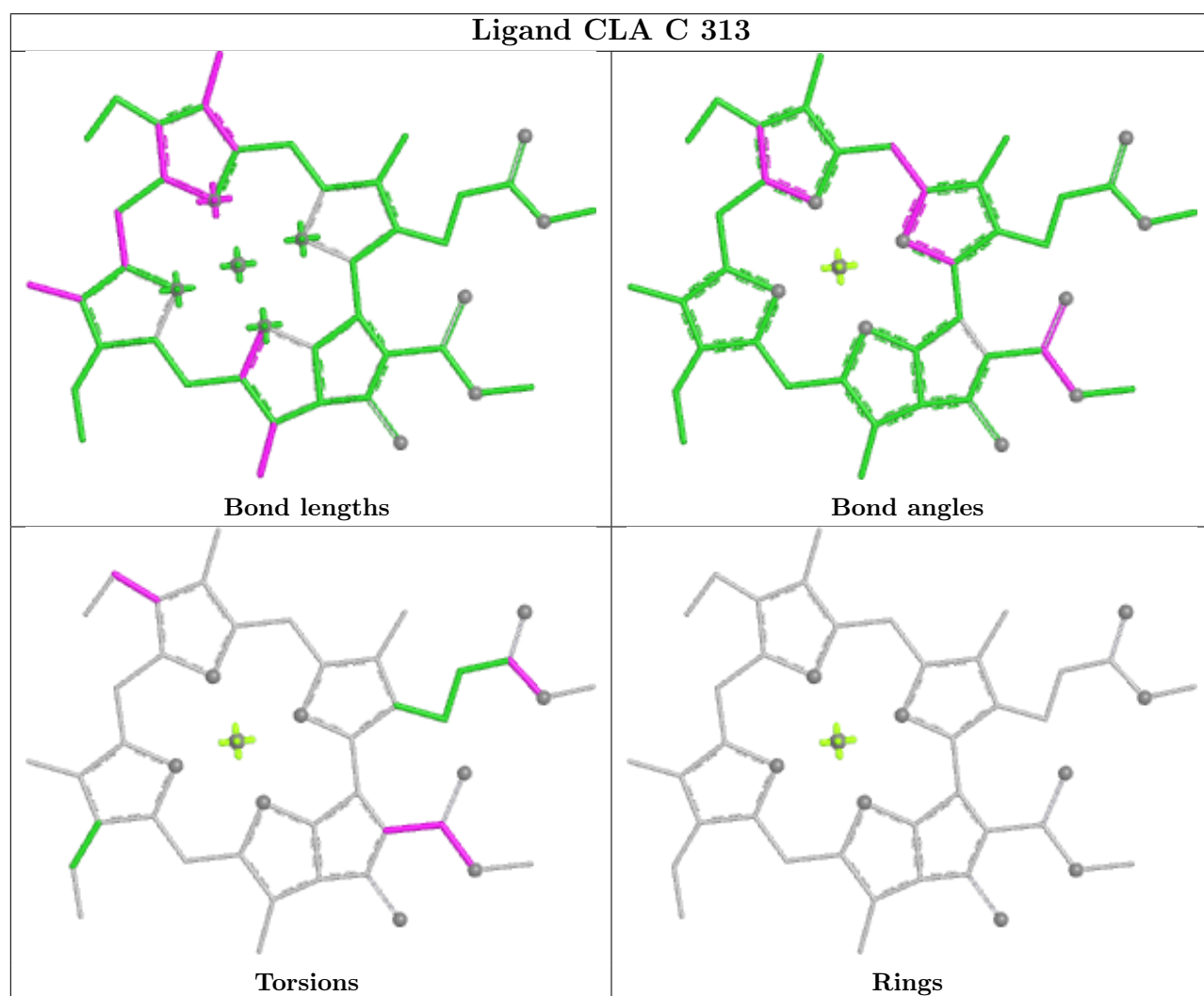
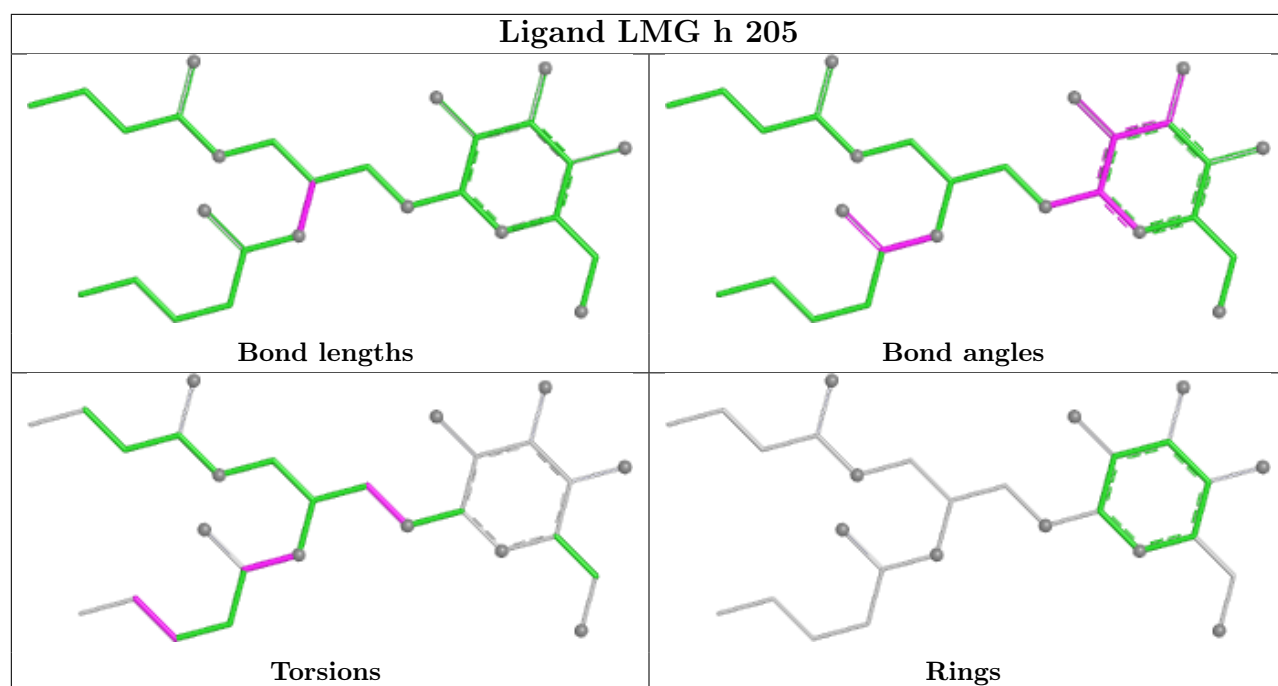


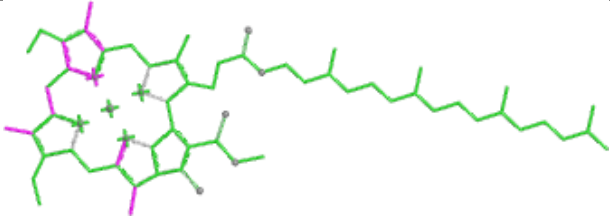
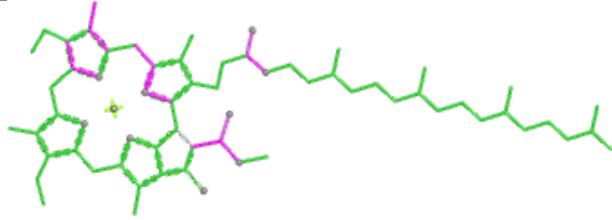
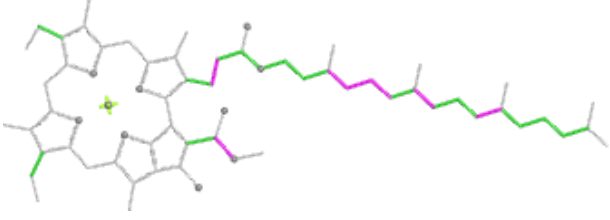
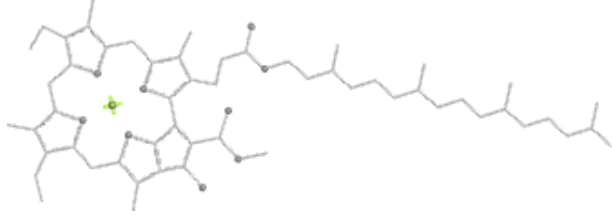
Ligand KC1 L 314

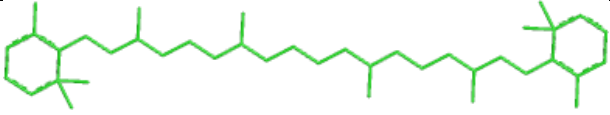
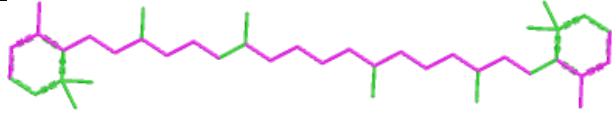
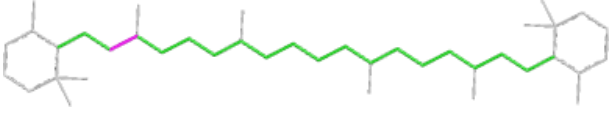
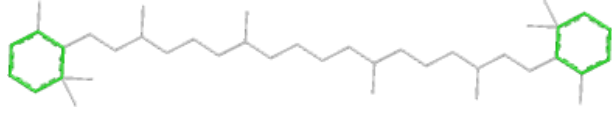


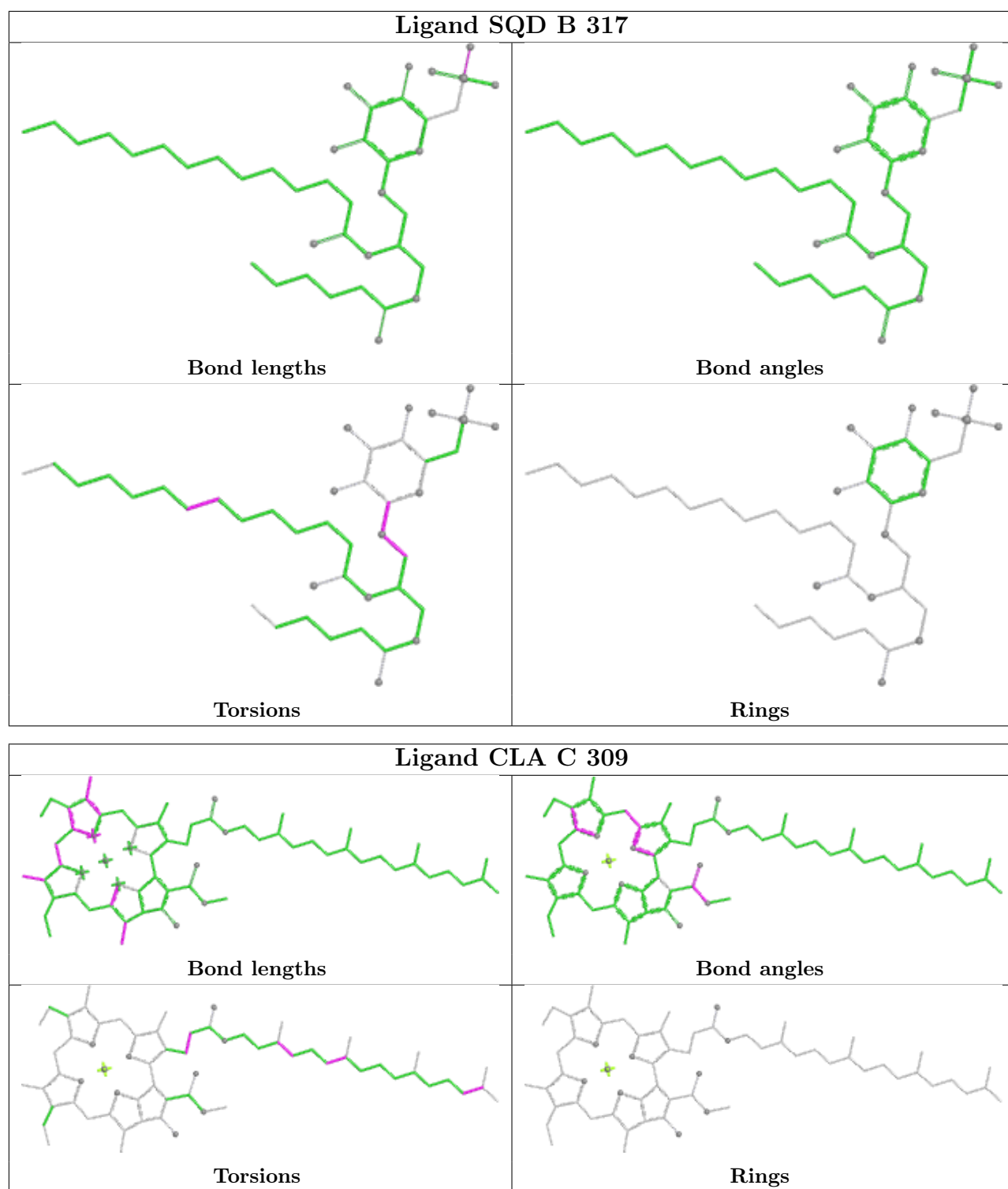
Ligand DD6 F 301



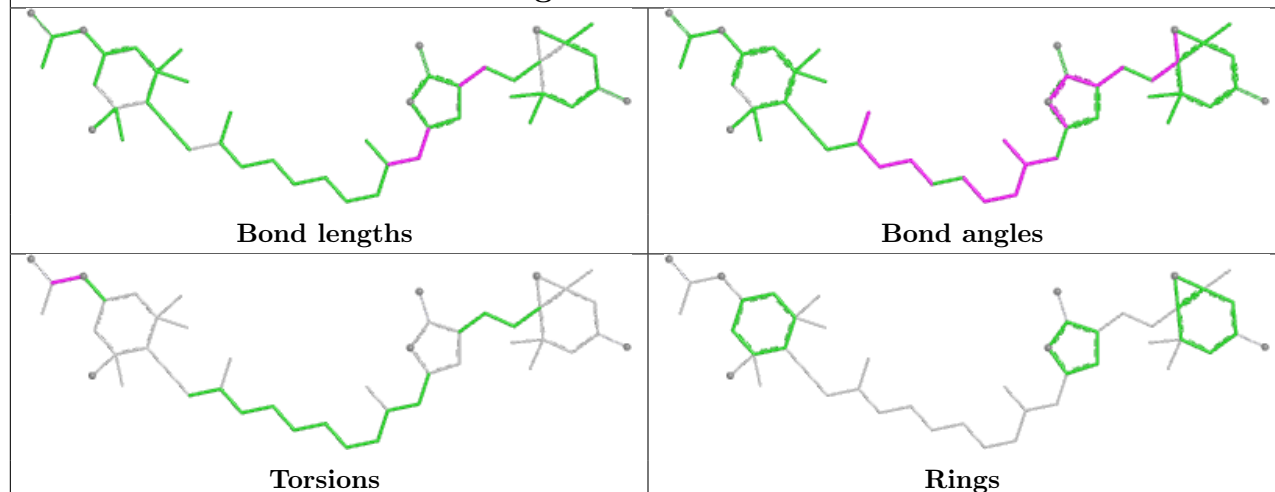


Ligand CLA E 311			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

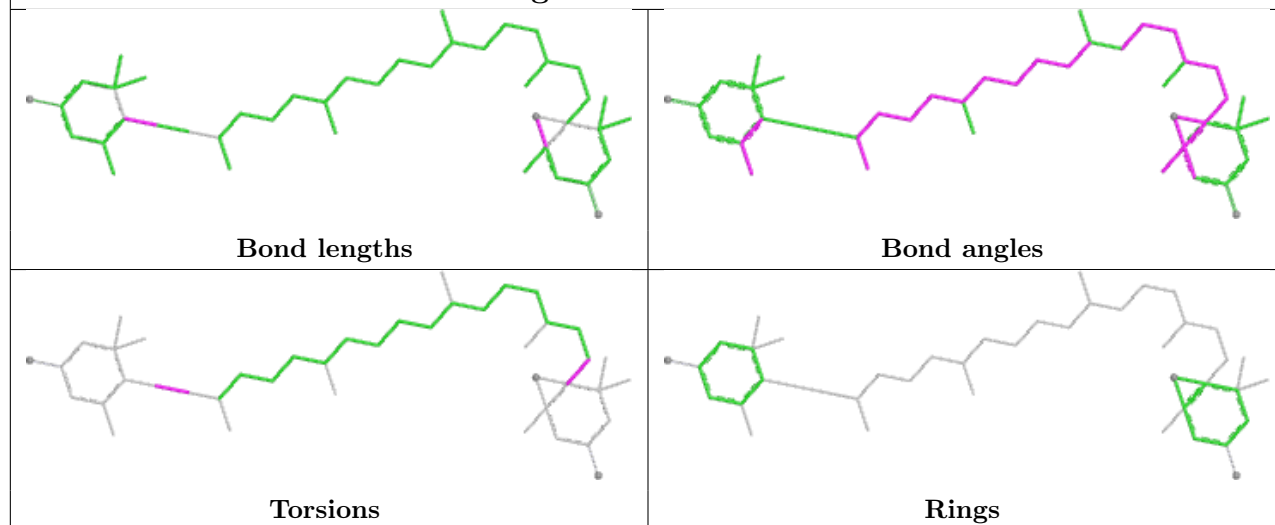
Ligand BCR a 835			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



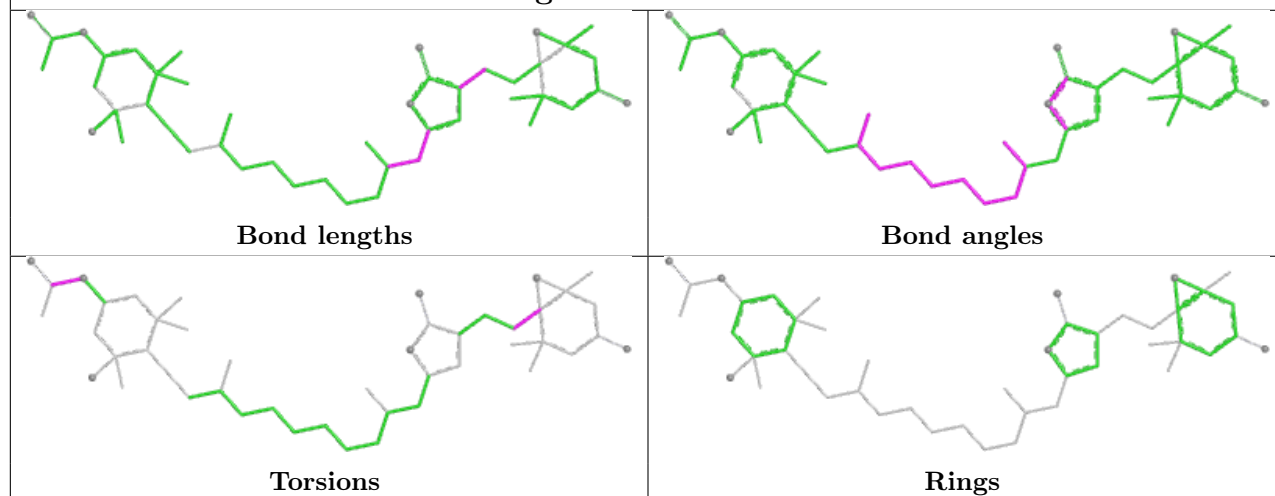
Ligand PID H 302



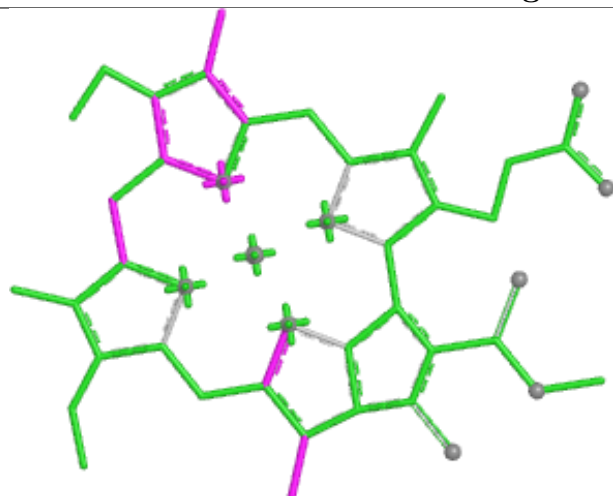
Ligand DD6 A 204



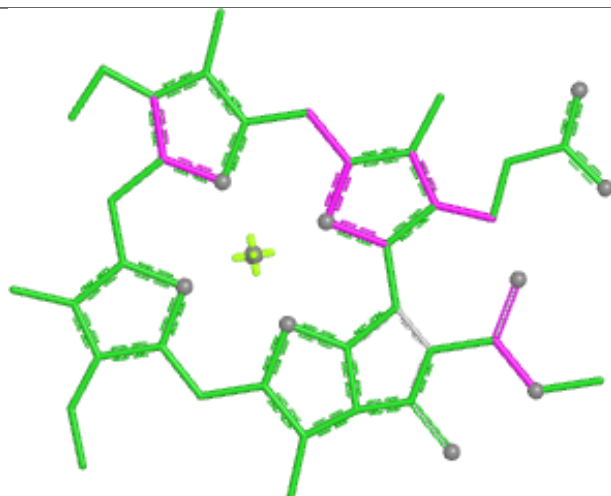
Ligand PID O 301



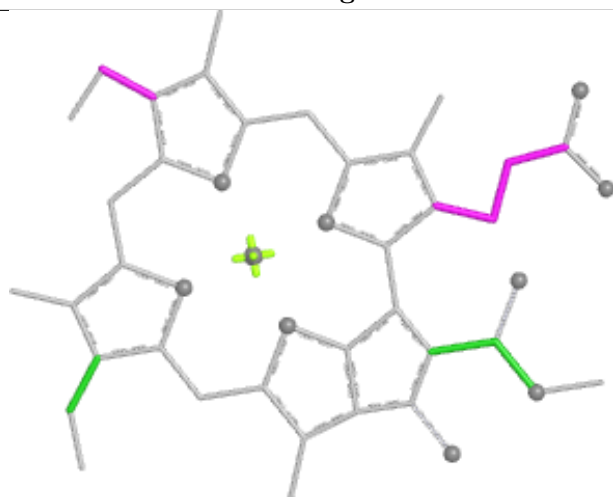
Ligand CLA 1 510



Bond lengths



Bond angles

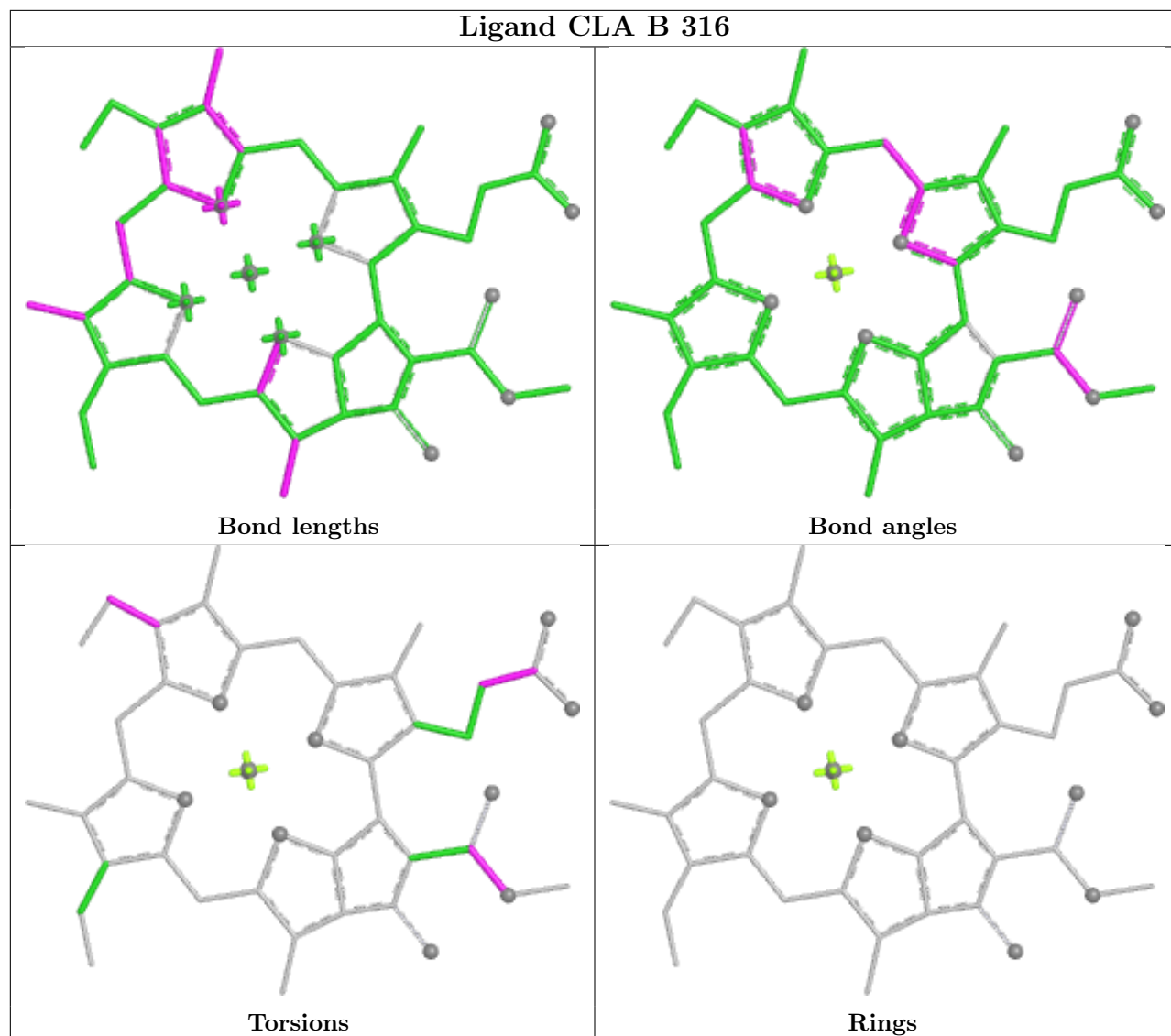


Torsions

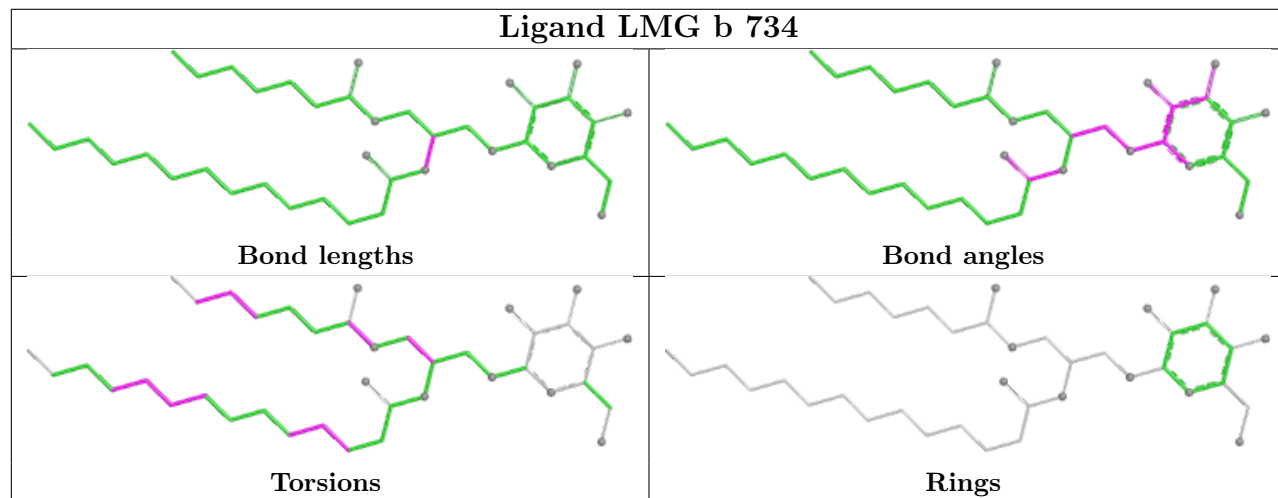


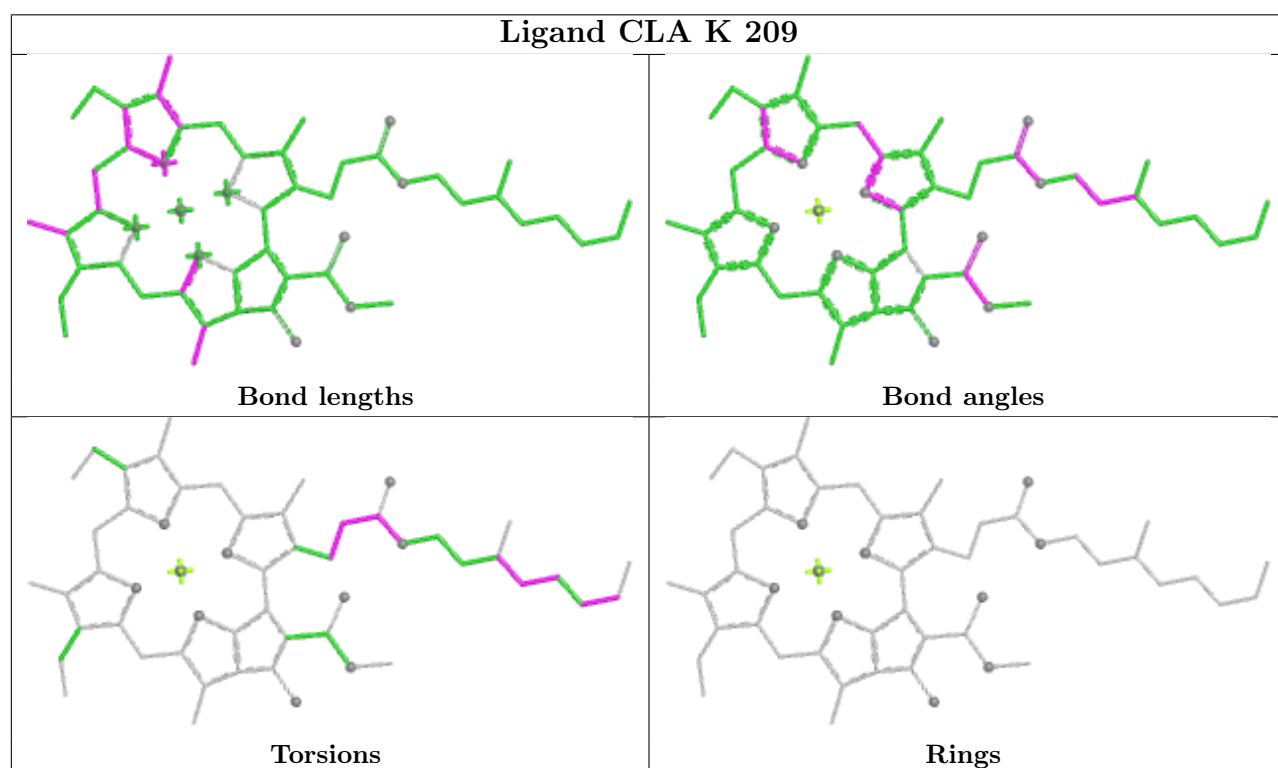
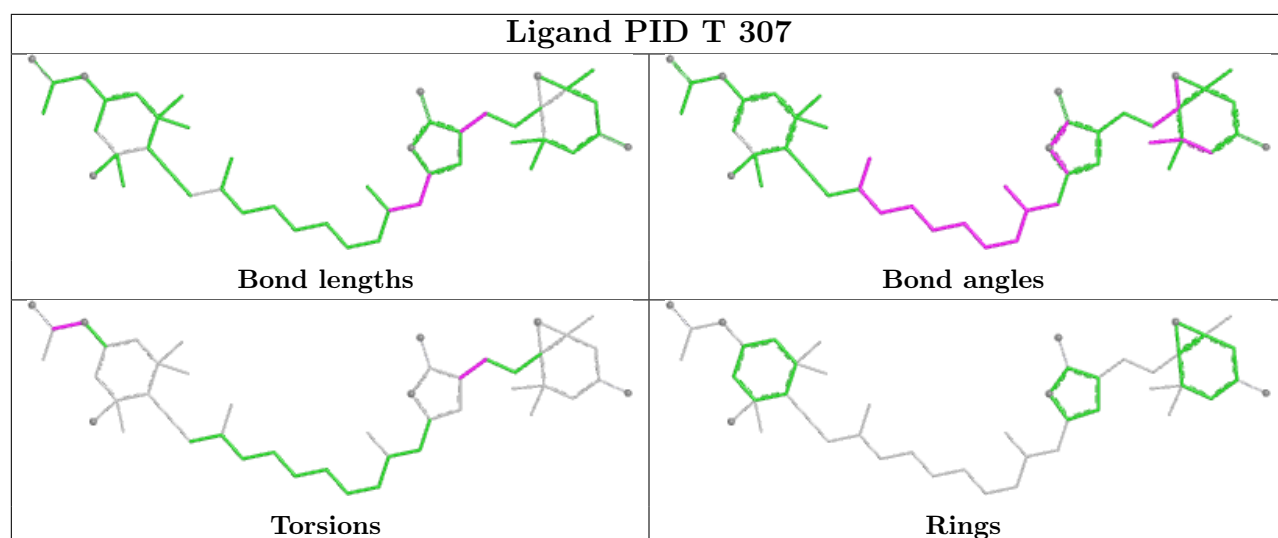
Rings

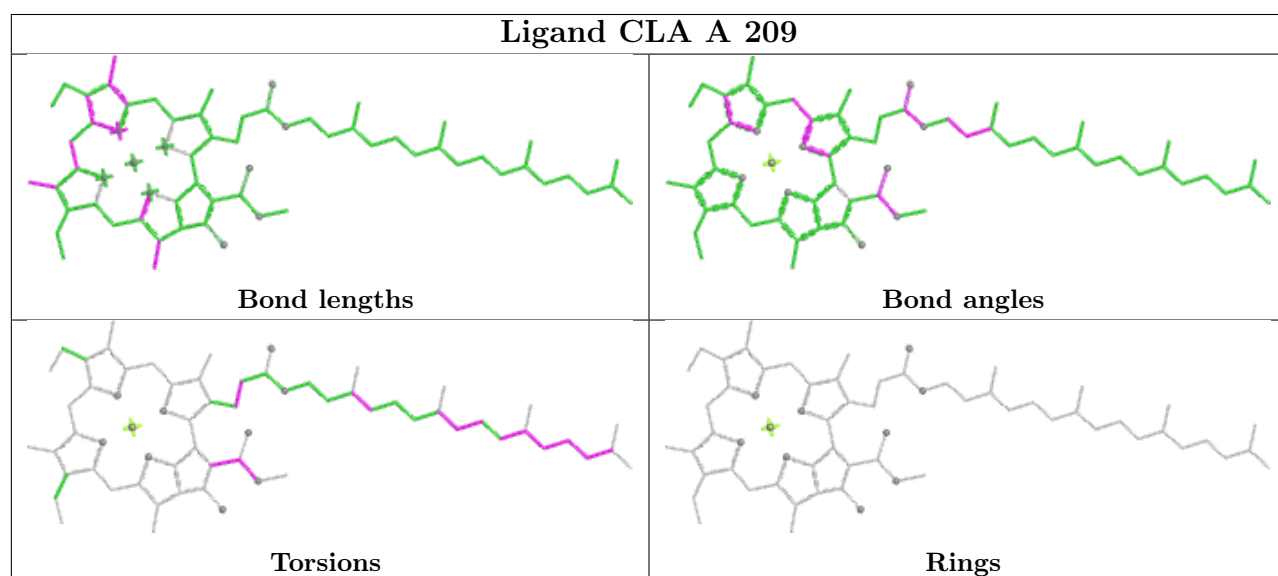
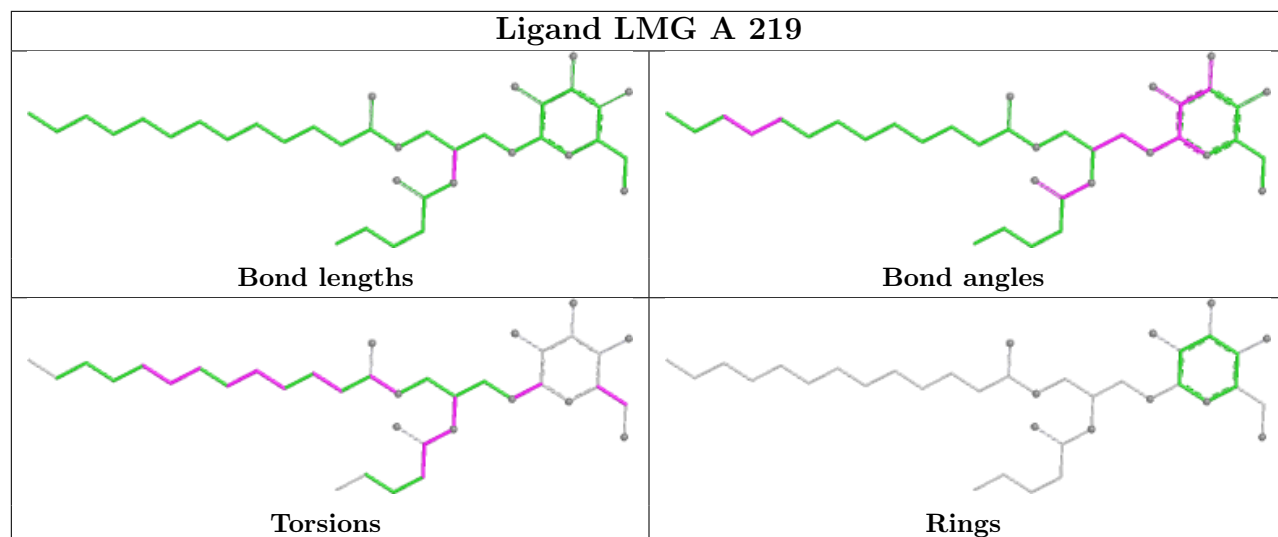
Ligand CLA B 316



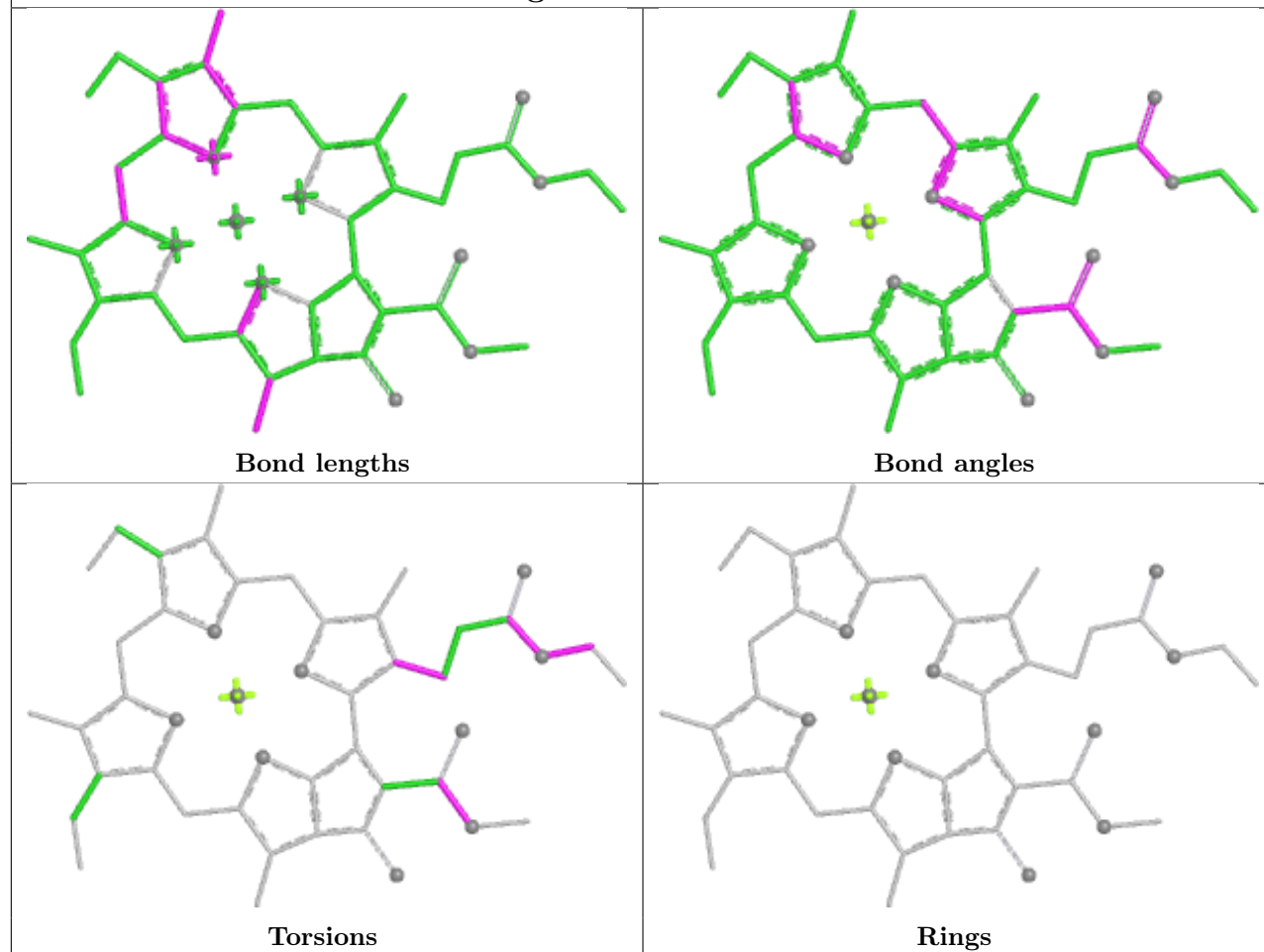
Ligand LMG b 734



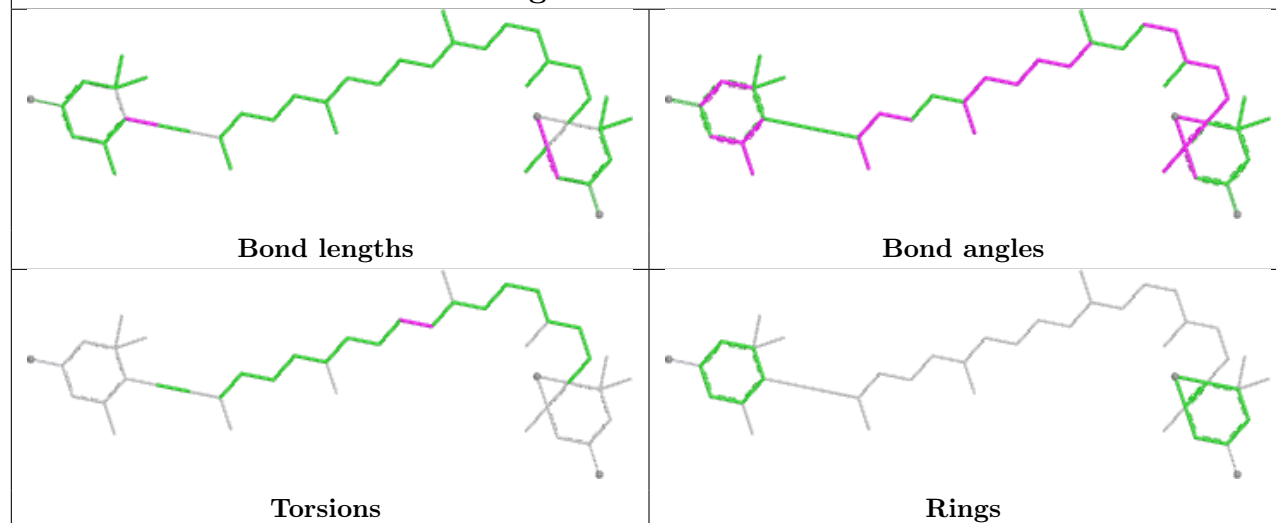




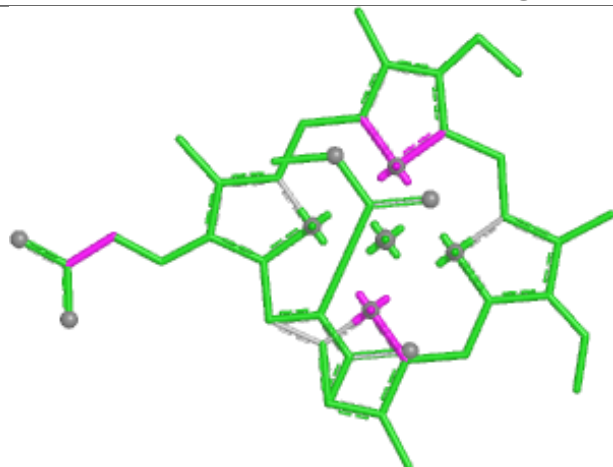
Ligand CLA C 314



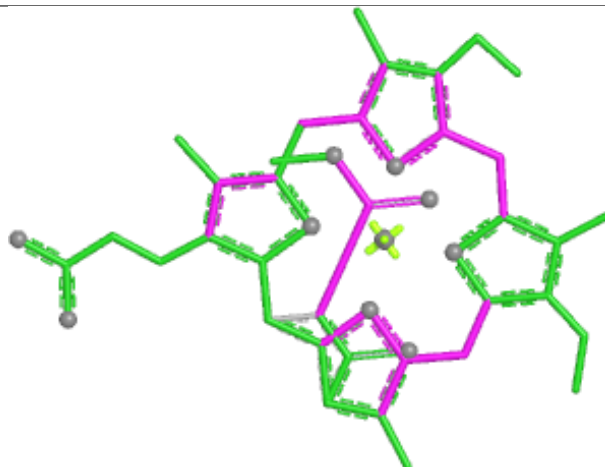
Ligand DD6 M 302



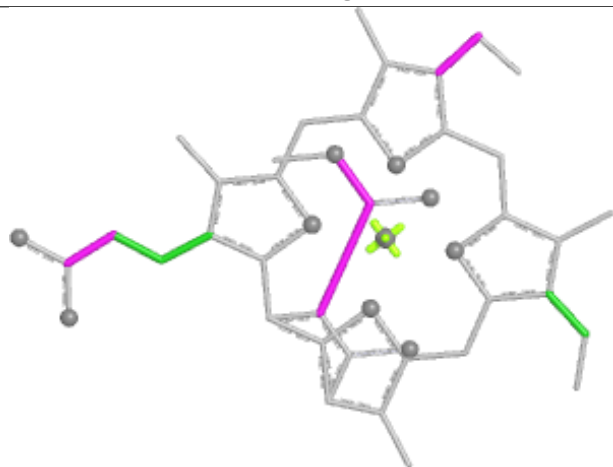
Ligand KC1 H 311



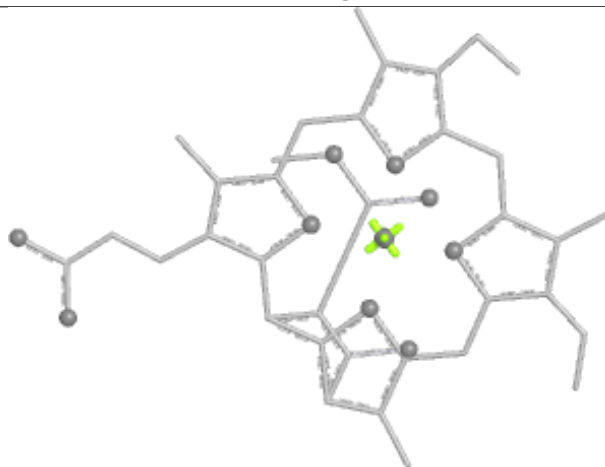
Bond lengths



Bond angles

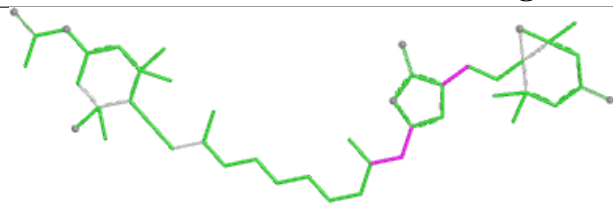


Torsions

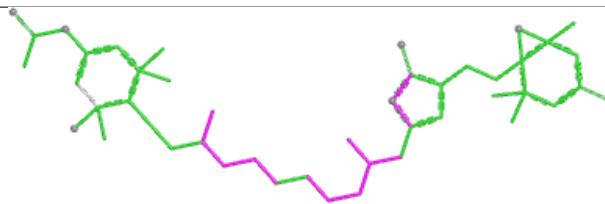


Rings

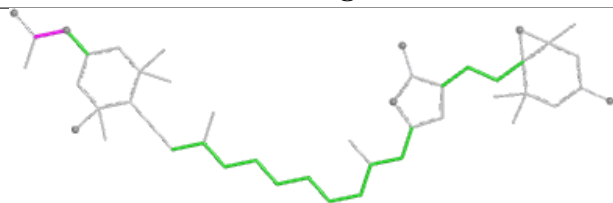
Ligand PID G 309



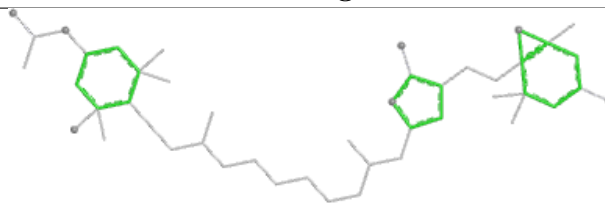
Bond lengths



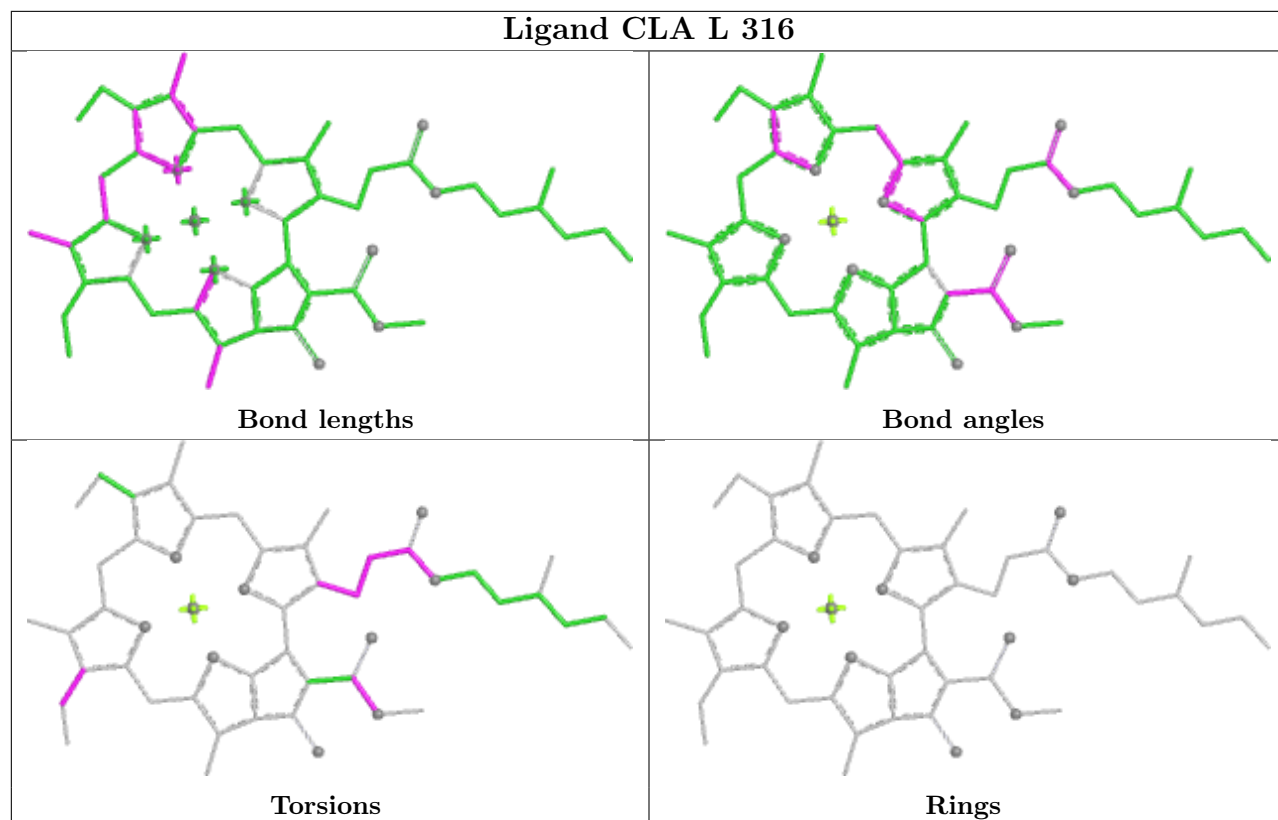
Bond angles



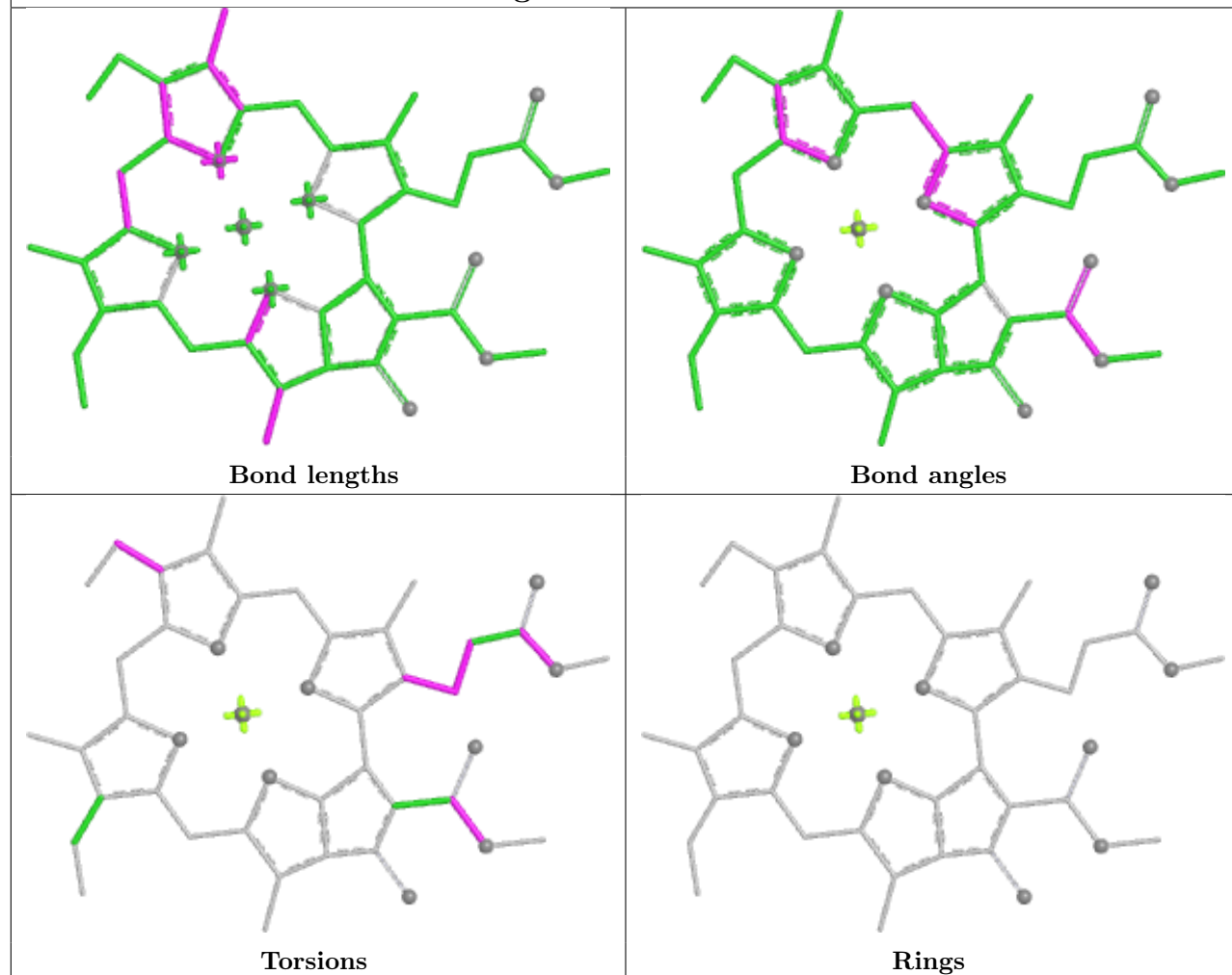
Torsions



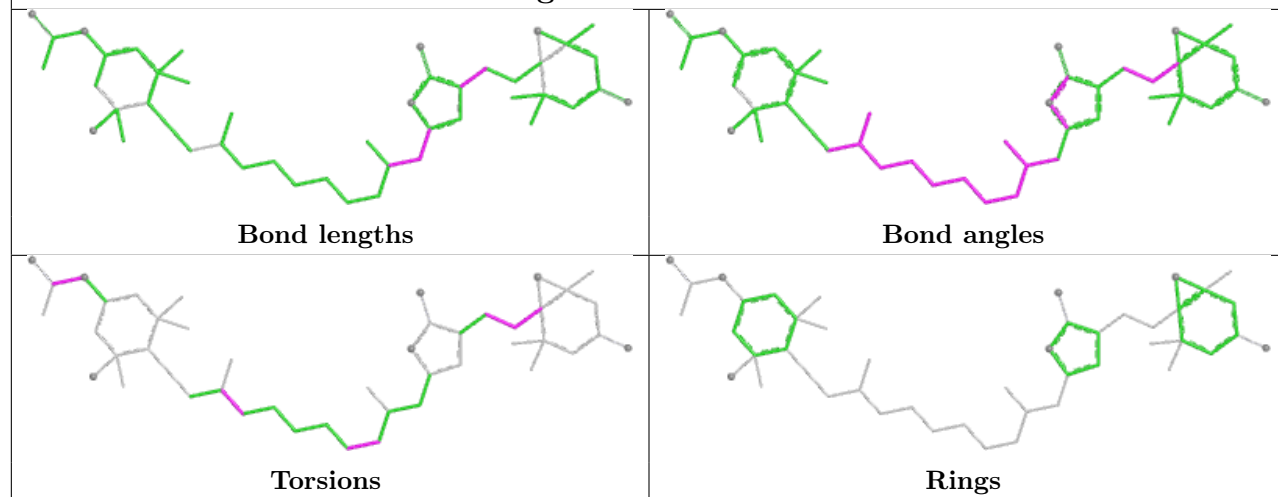
Rings



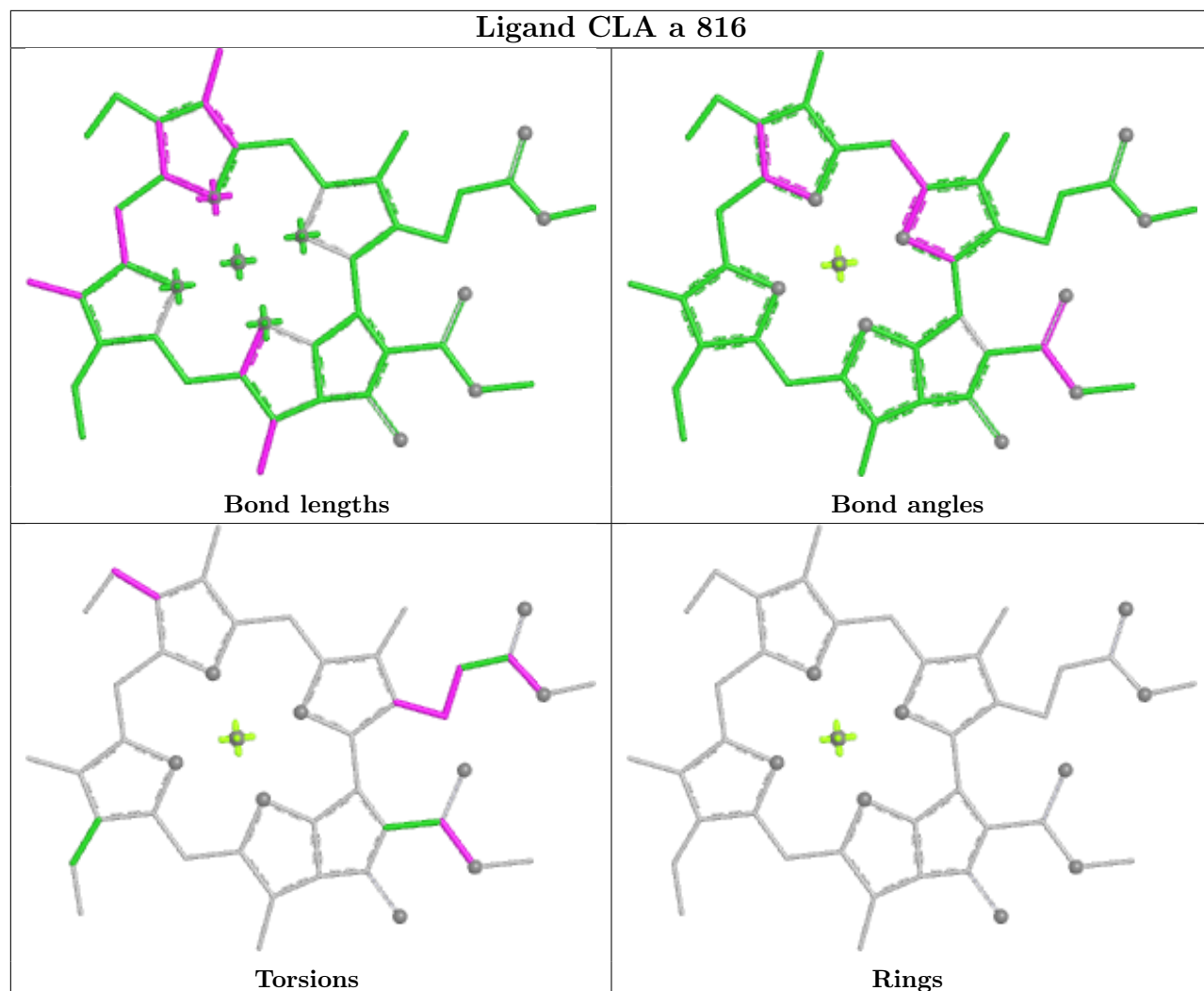
Ligand CLA P 214



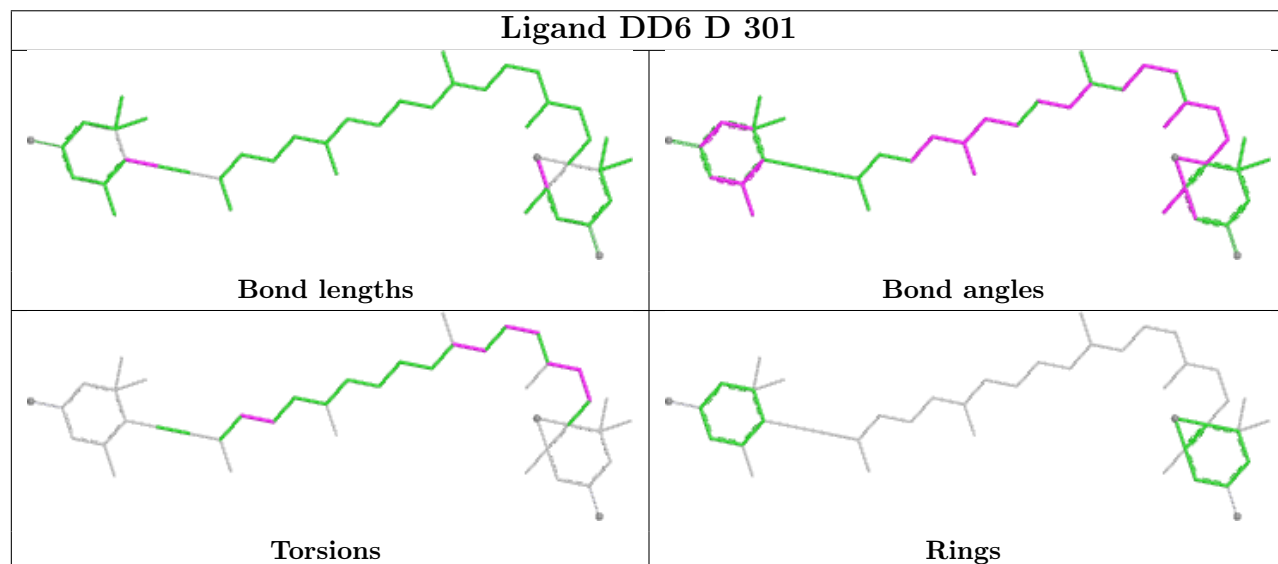
Ligand PID C 305



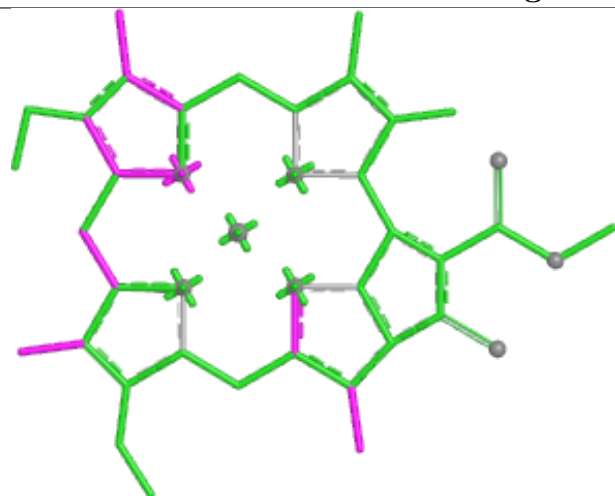
Ligand CLA a 816



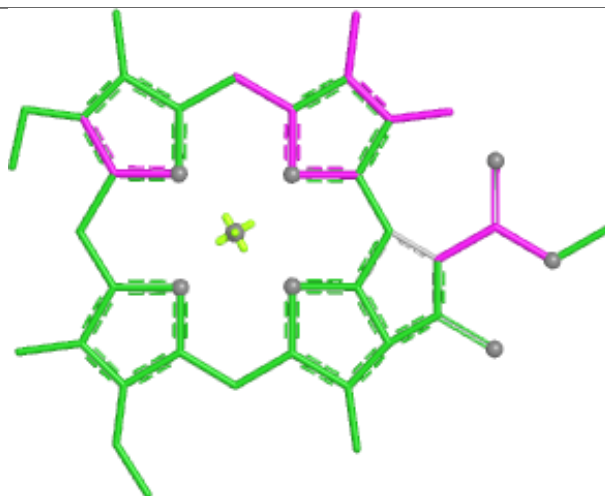
Ligand DD6 D 301



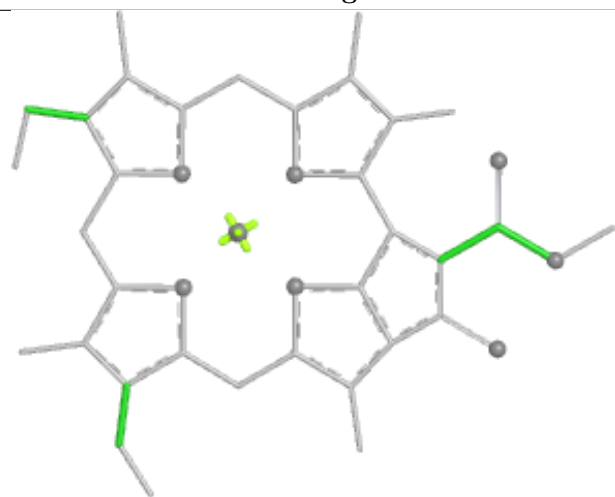
Ligand CLA I 509



Bond lengths



Bond angles

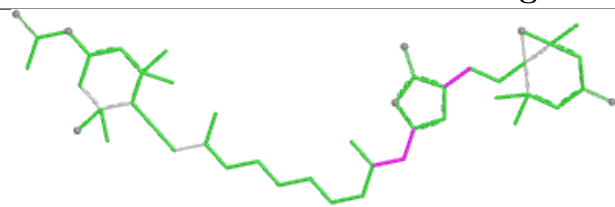


Torsions

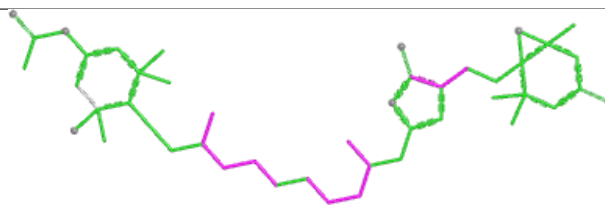


Rings

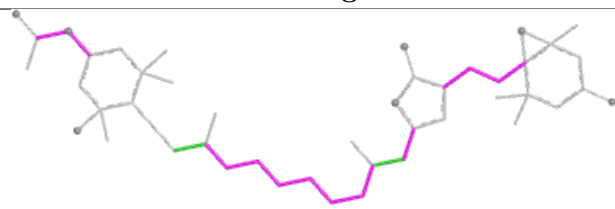
Ligand PID N 305



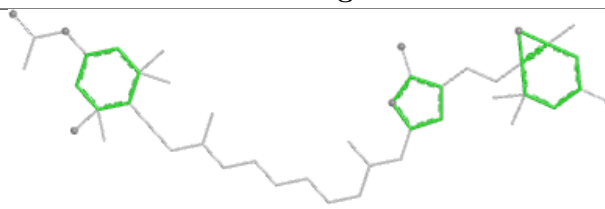
Bond lengths



Bond angles

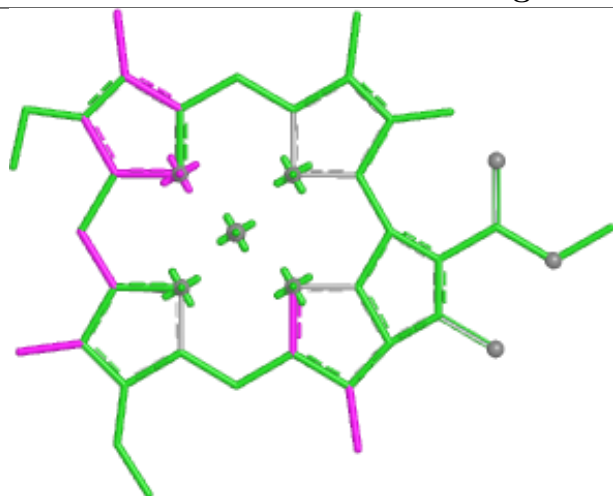


Torsions

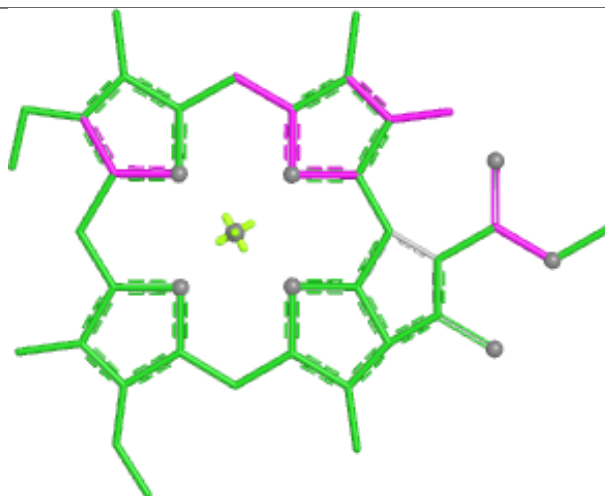


Rings

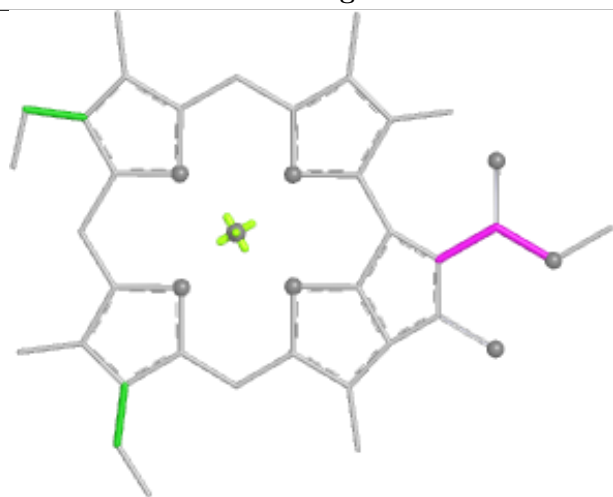
Ligand CLA K 216



Bond lengths



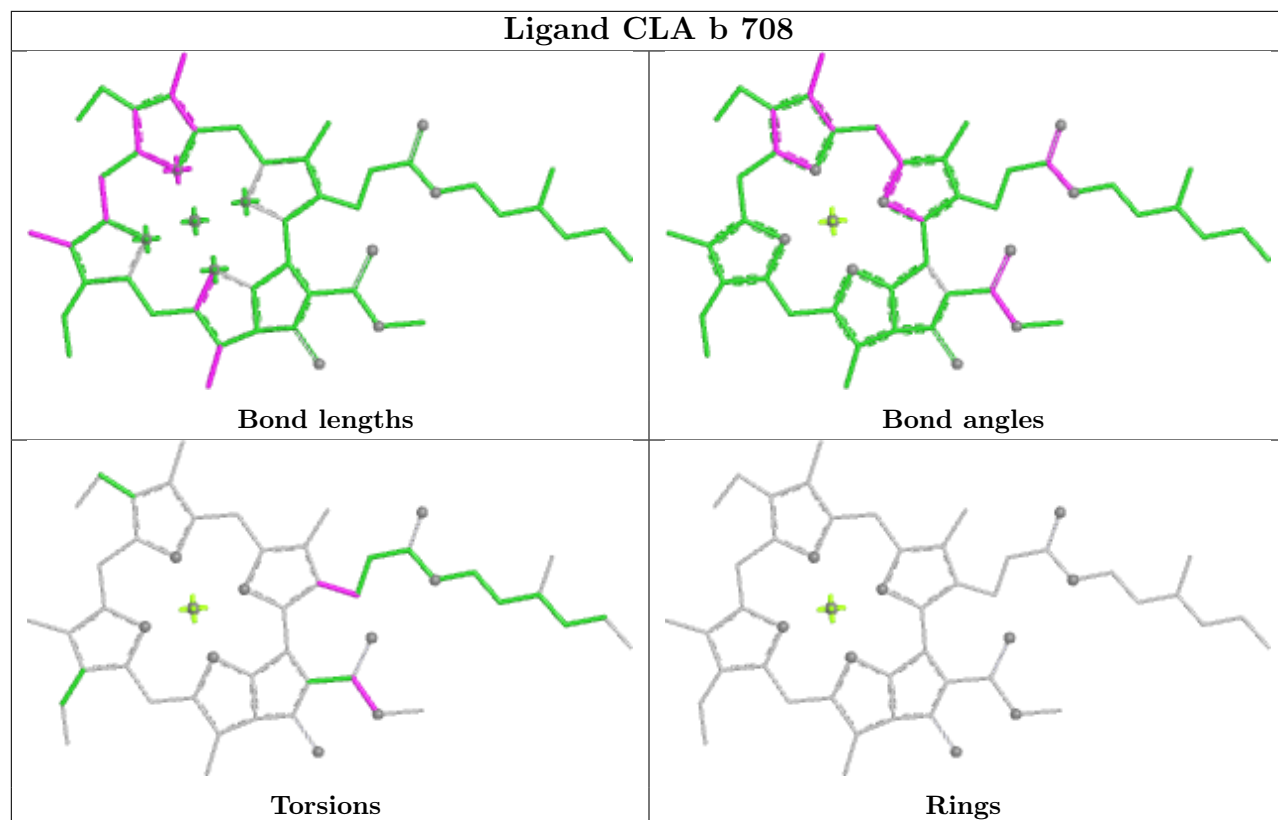
Bond angles



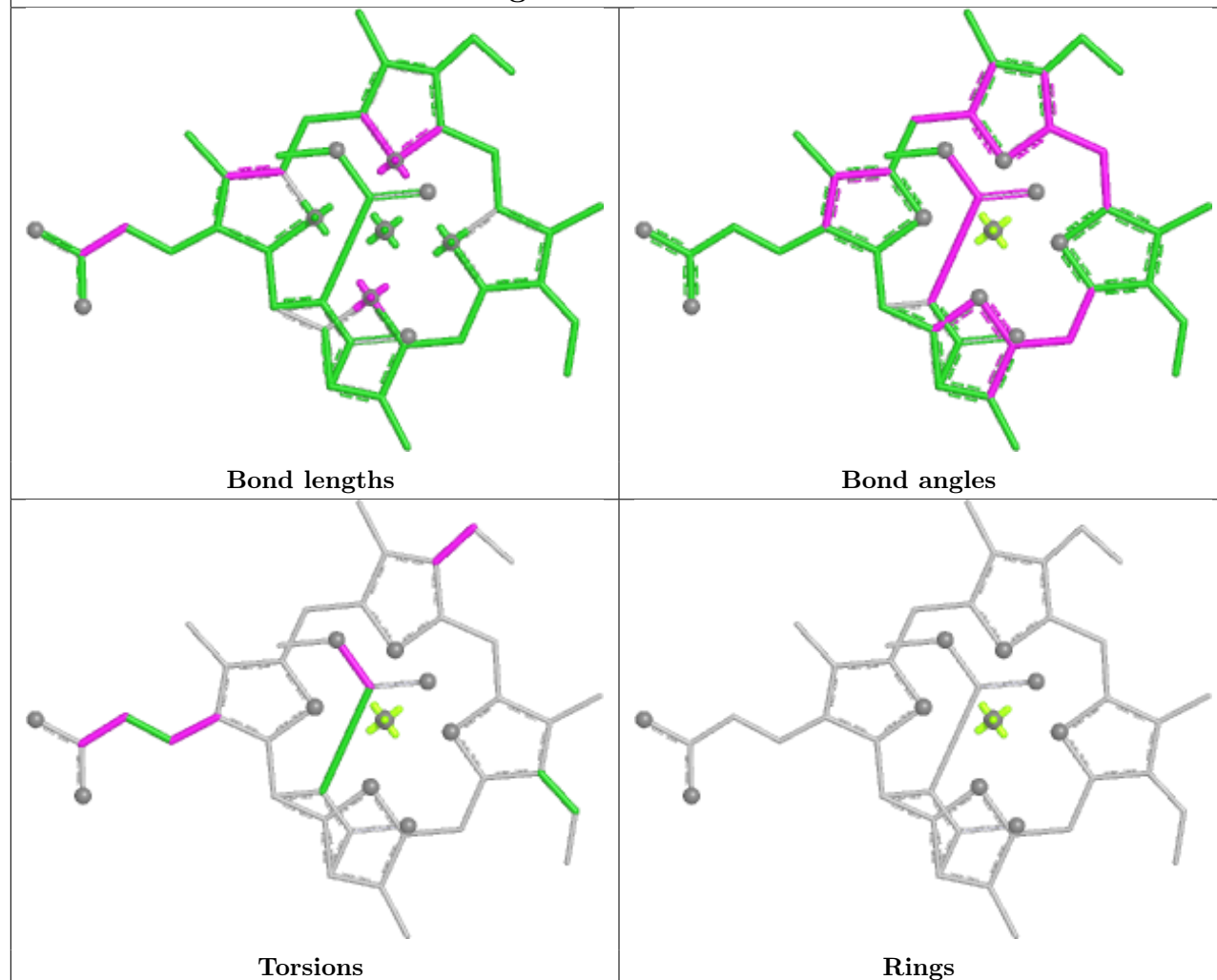
Torsions



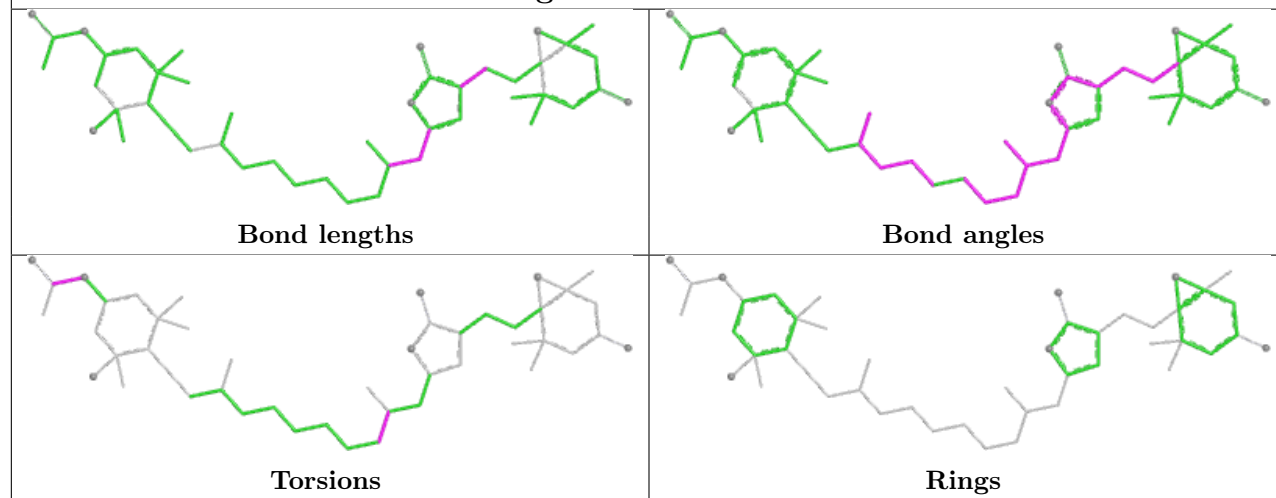
Rings



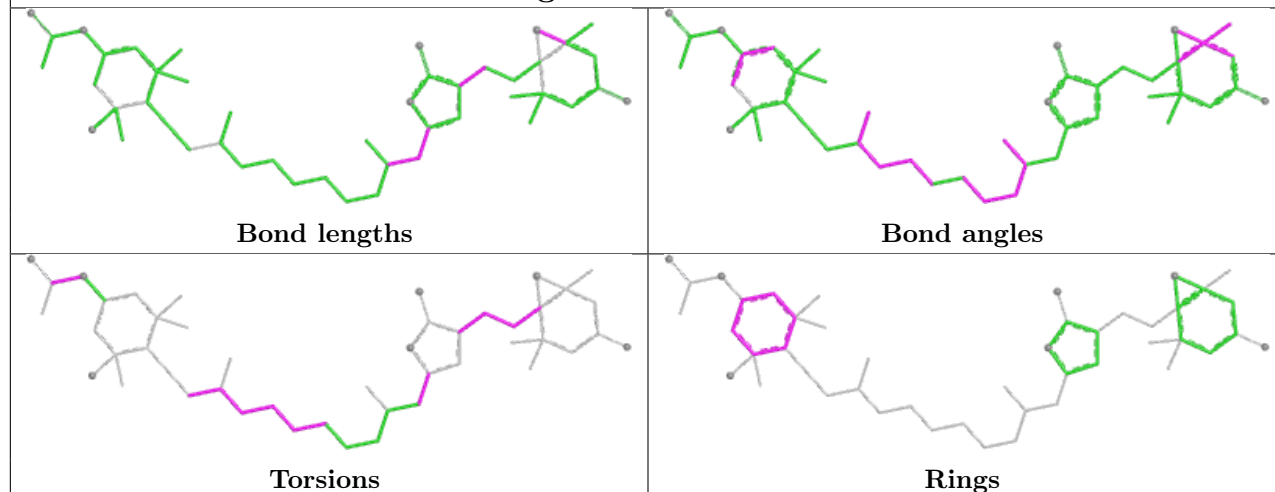
Ligand KC1 C 310



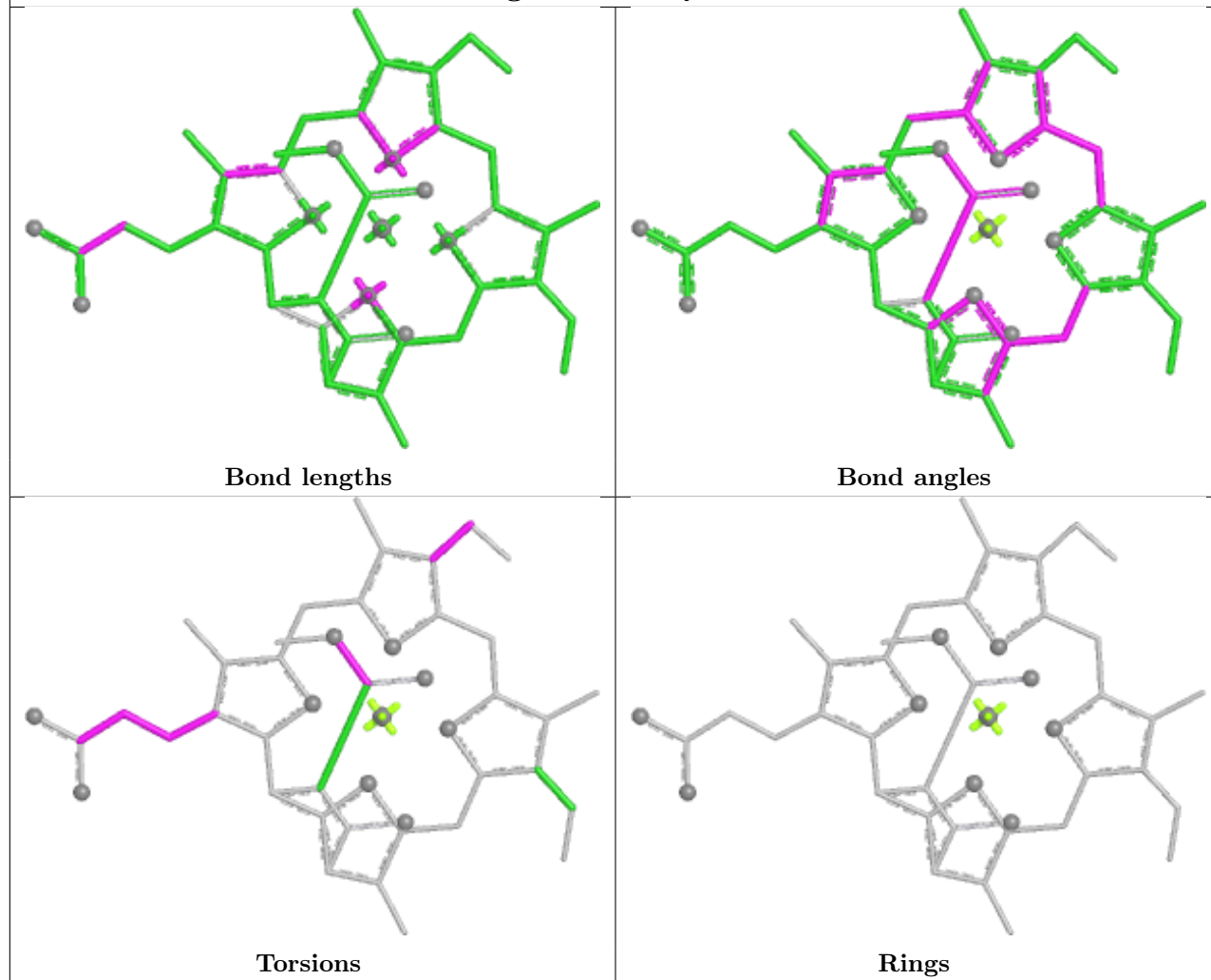
Ligand PID D 306

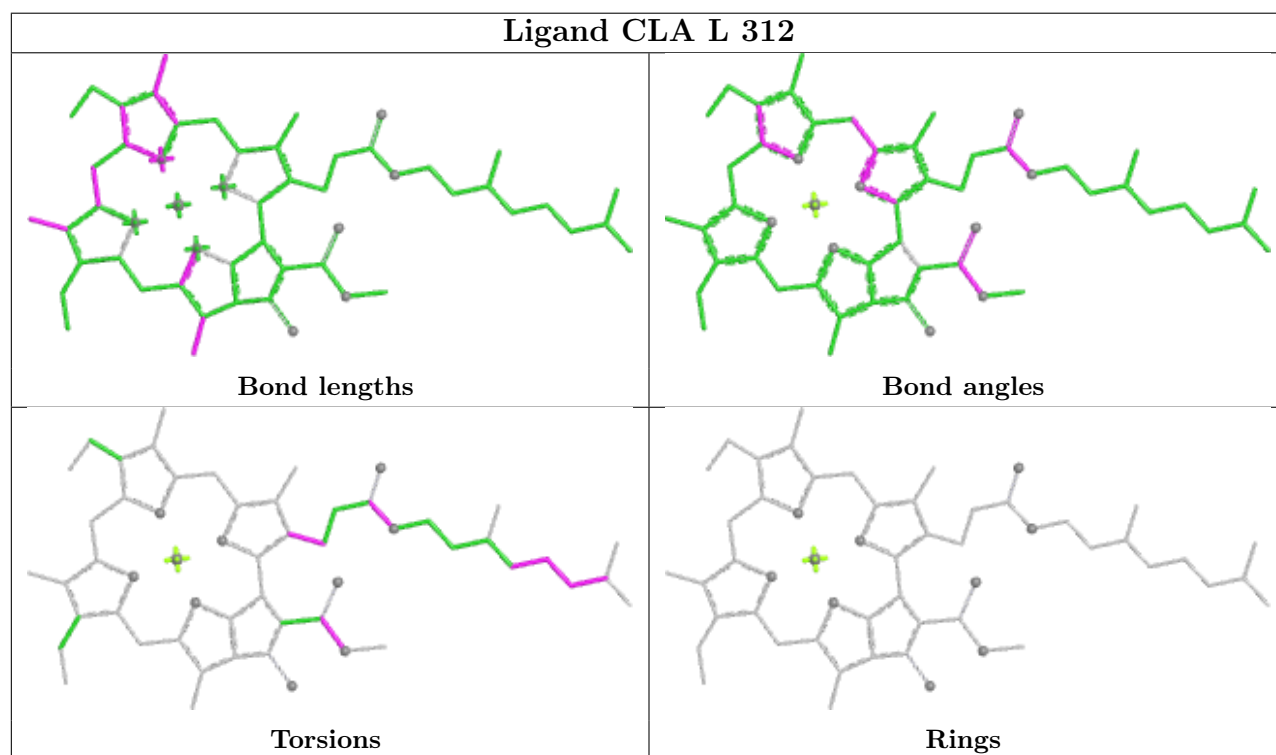
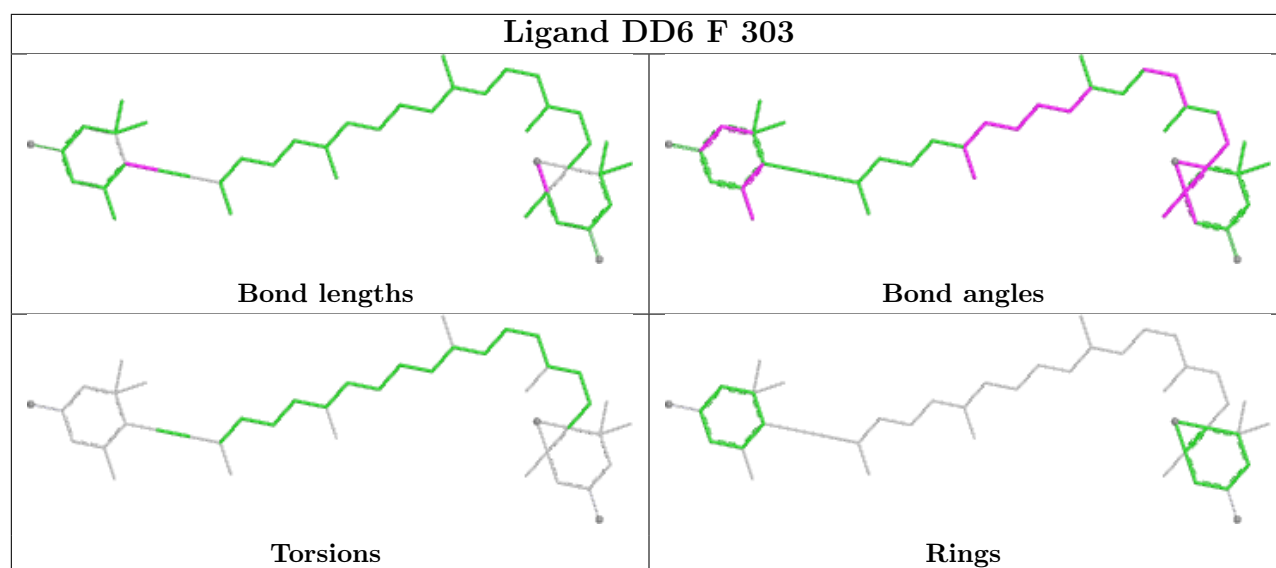


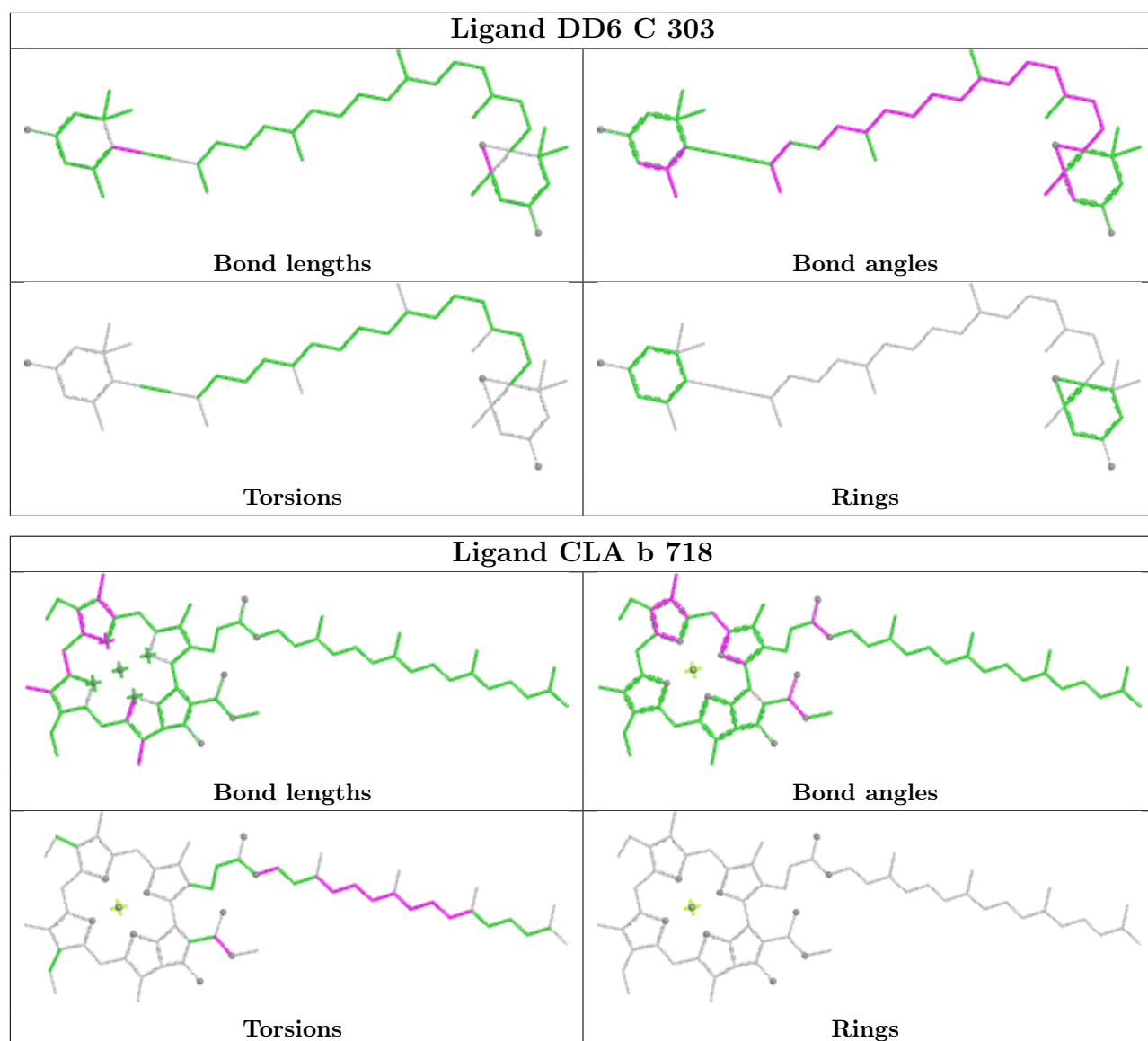
Ligand PID F 304



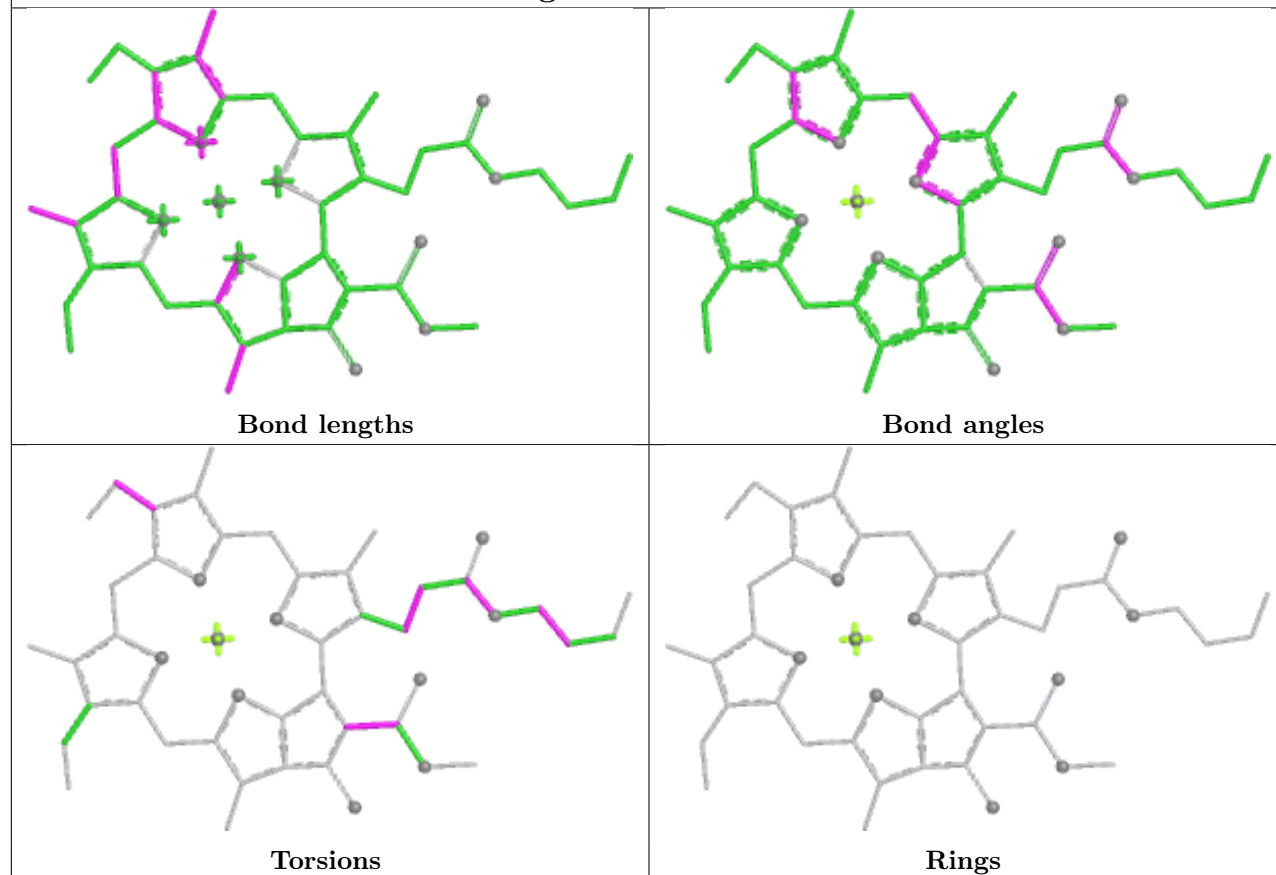
Ligand KC1 Q 314



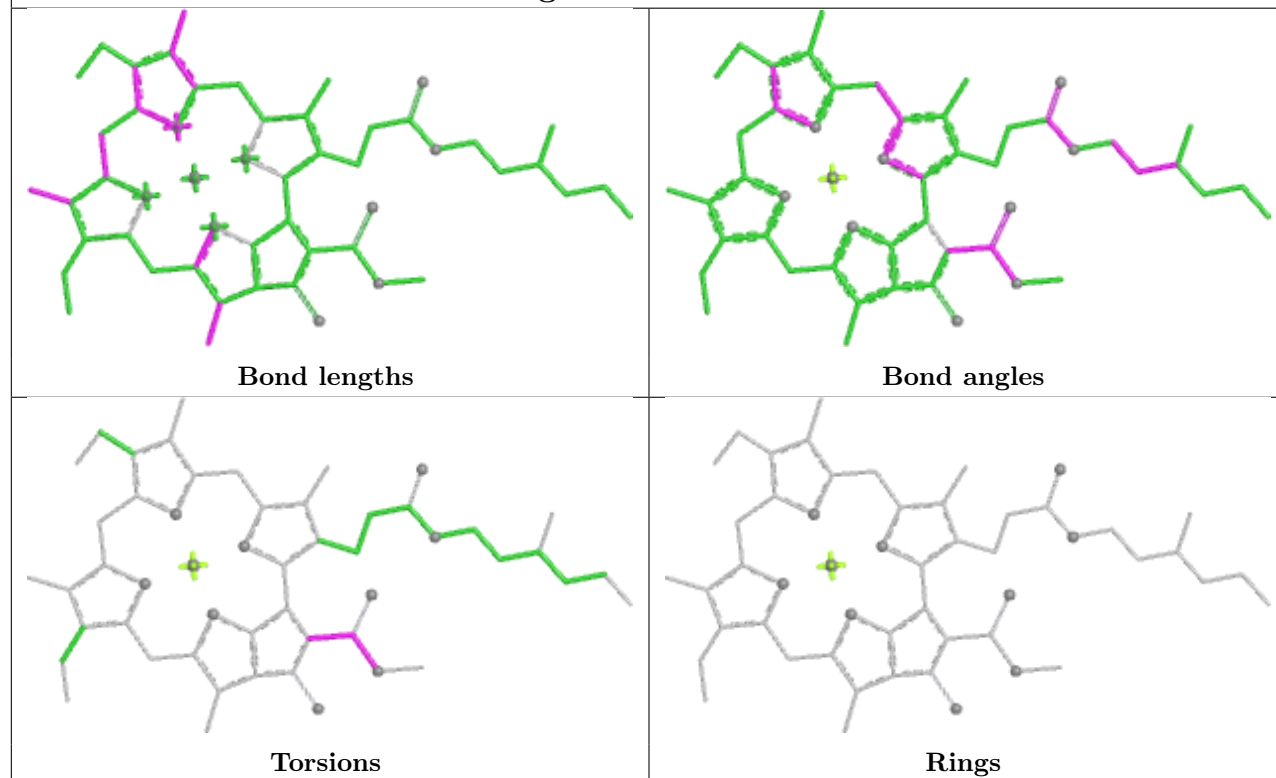


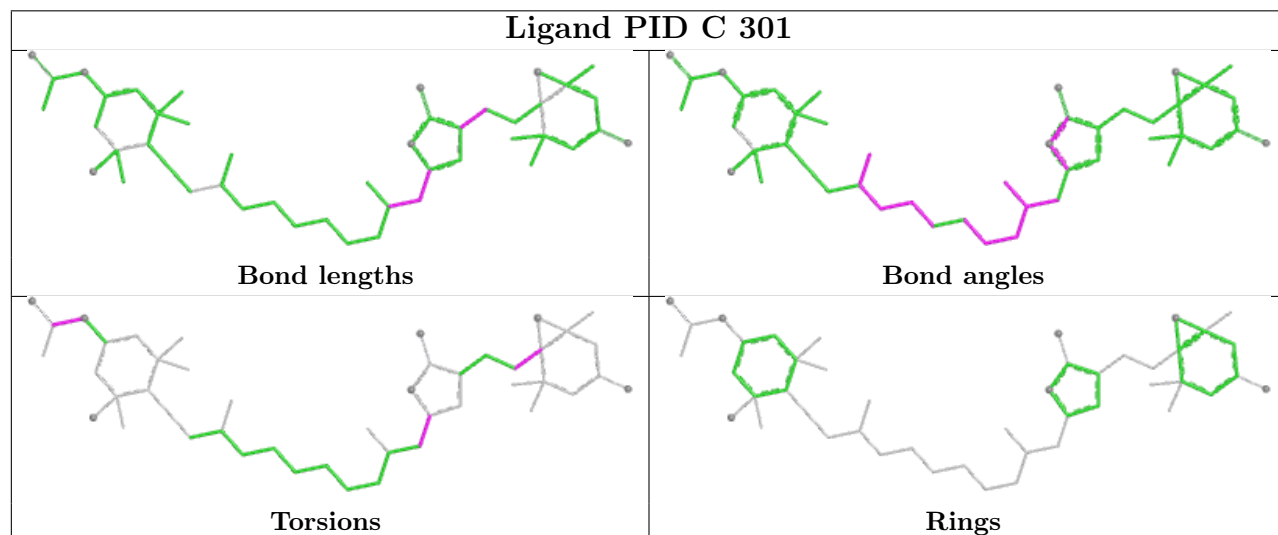
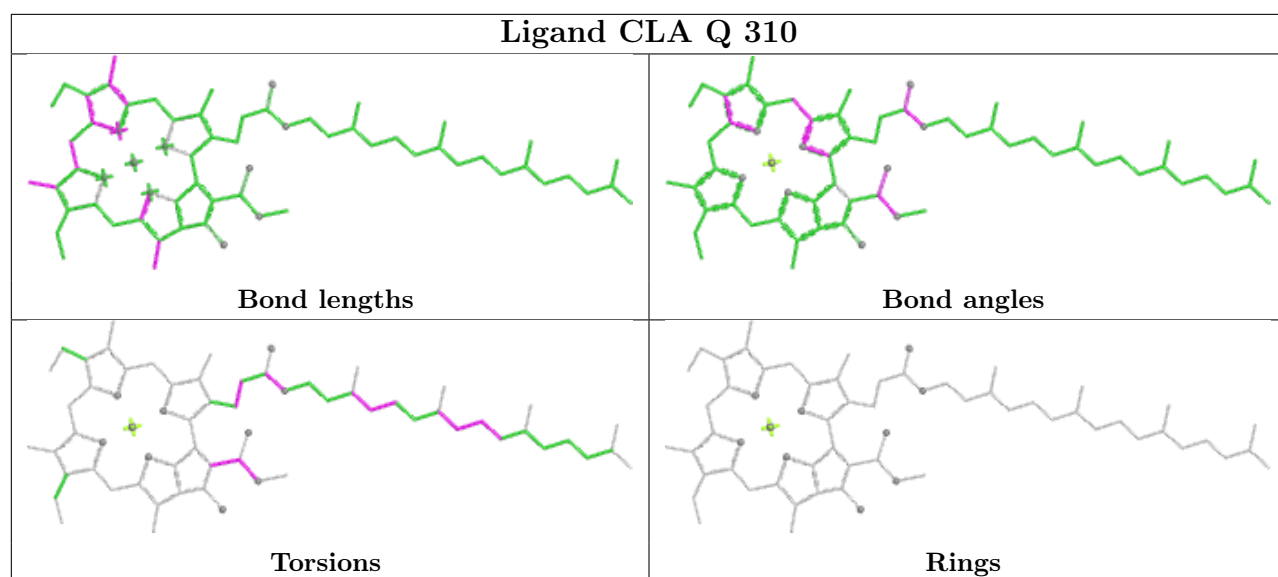


Ligand CLA I 207

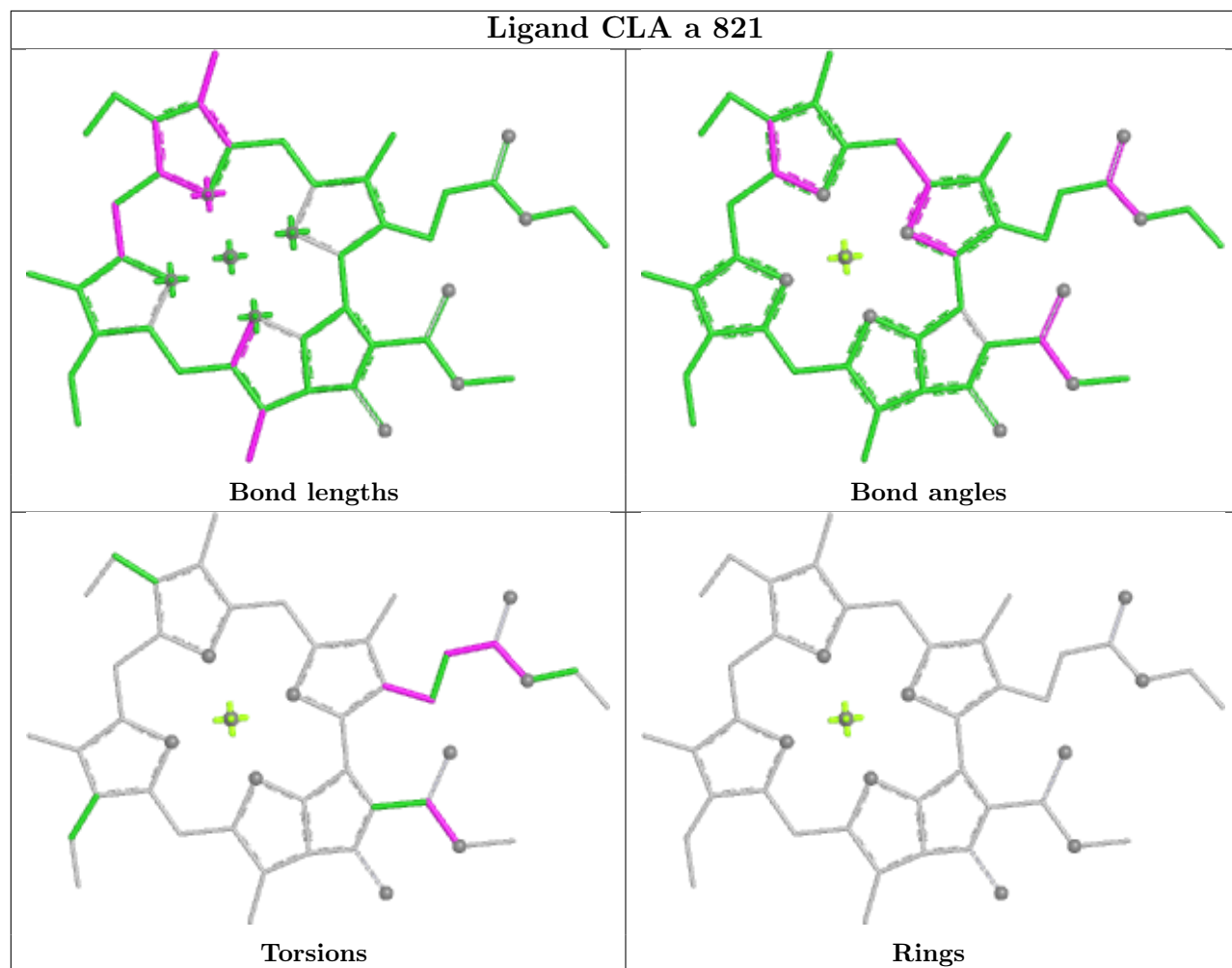


Ligand CLA I 216

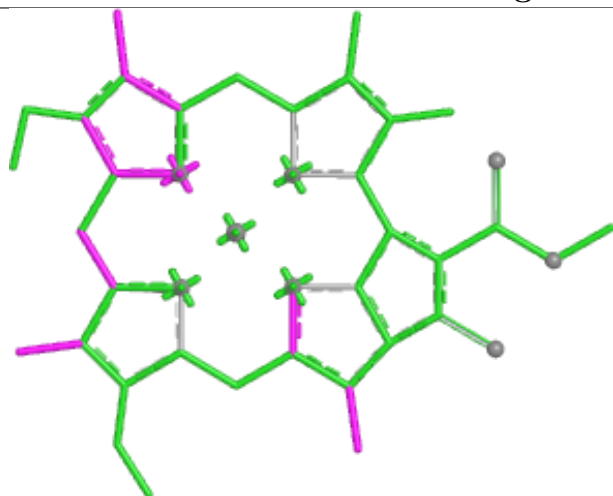




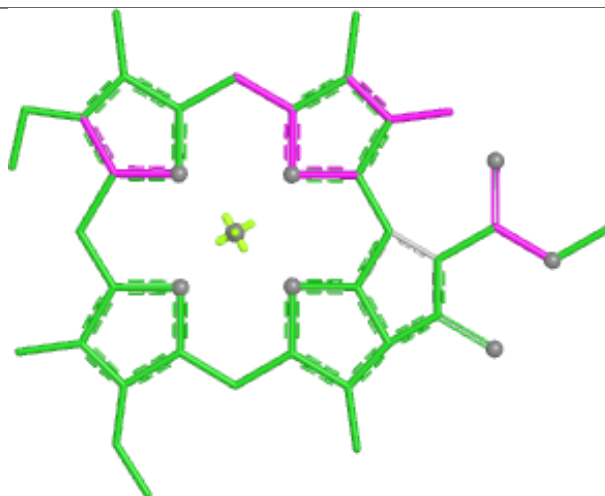
Ligand CLA a 821



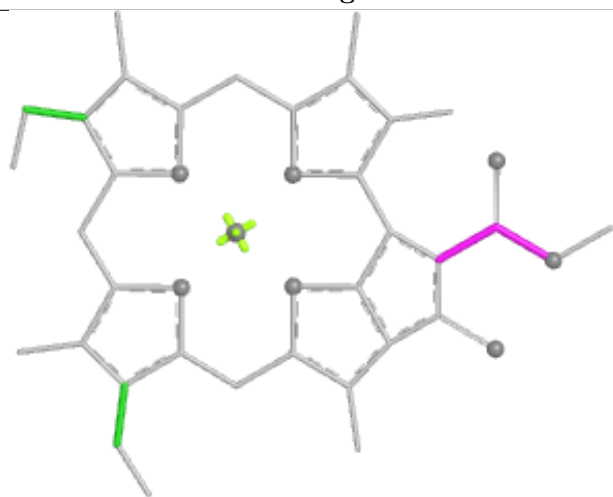
Ligand CLA B 314



Bond lengths



Bond angles

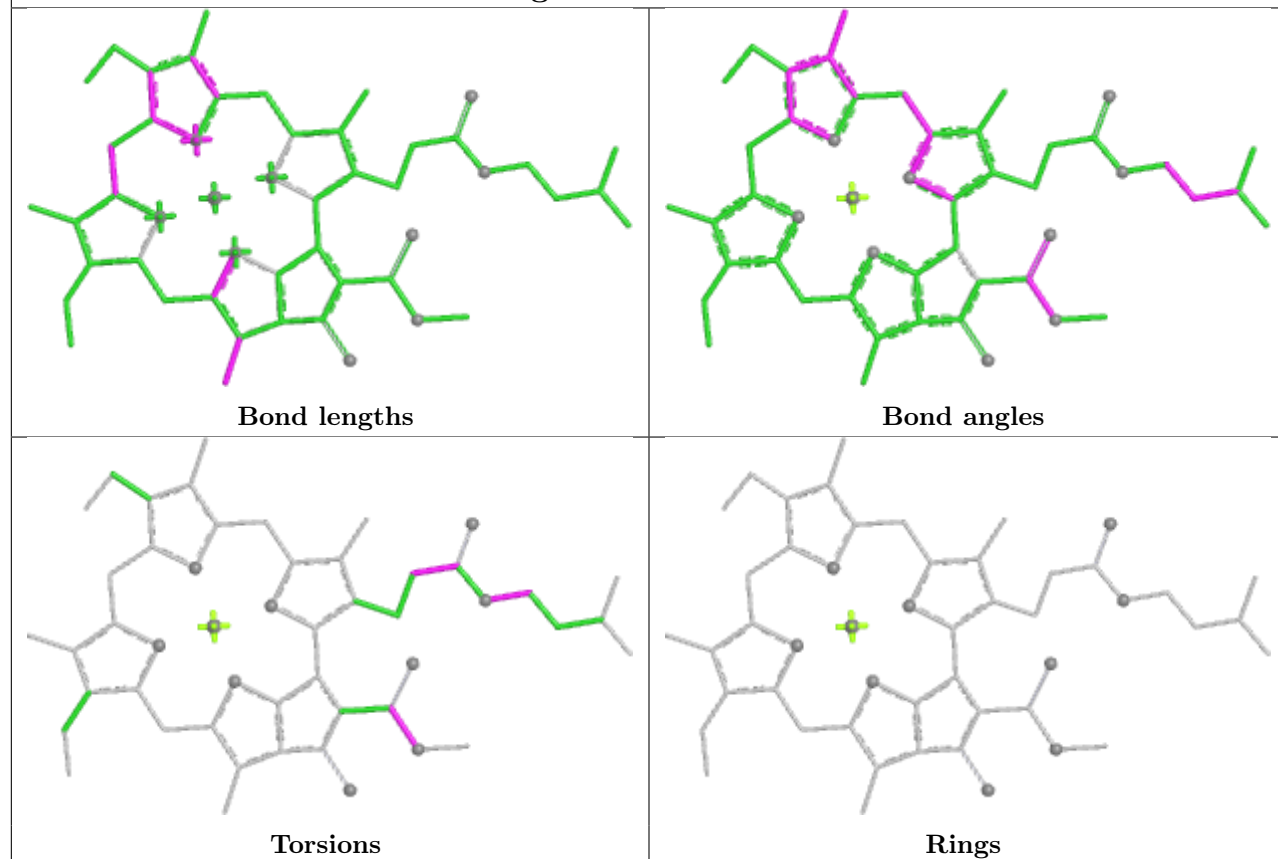


Torsions

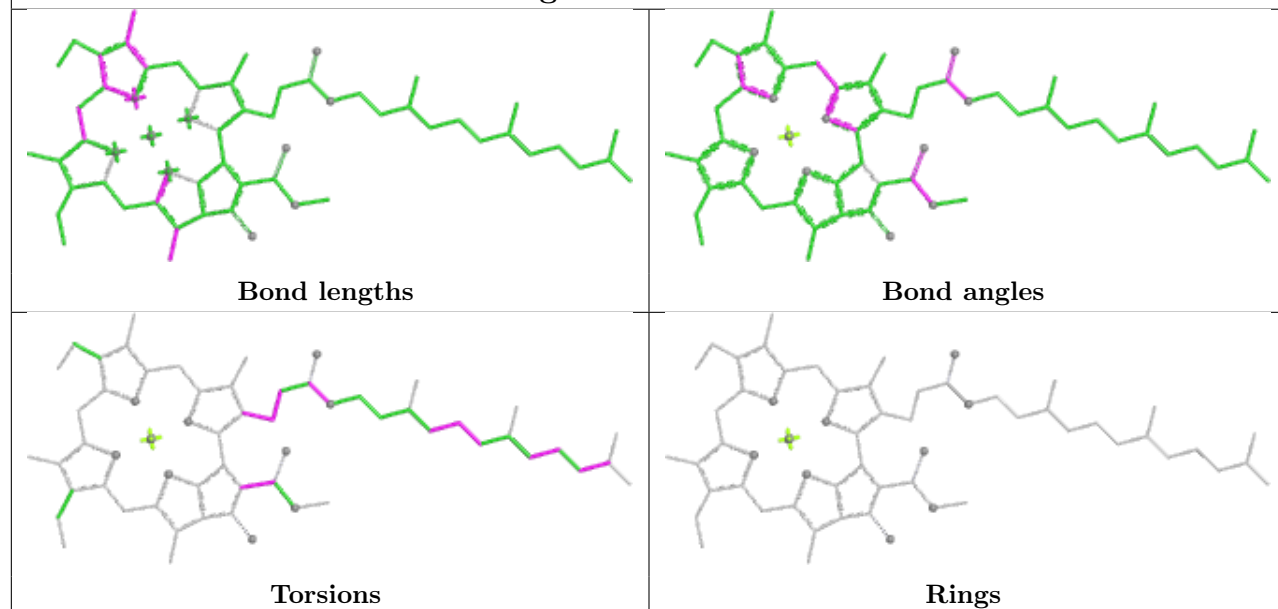


Rings

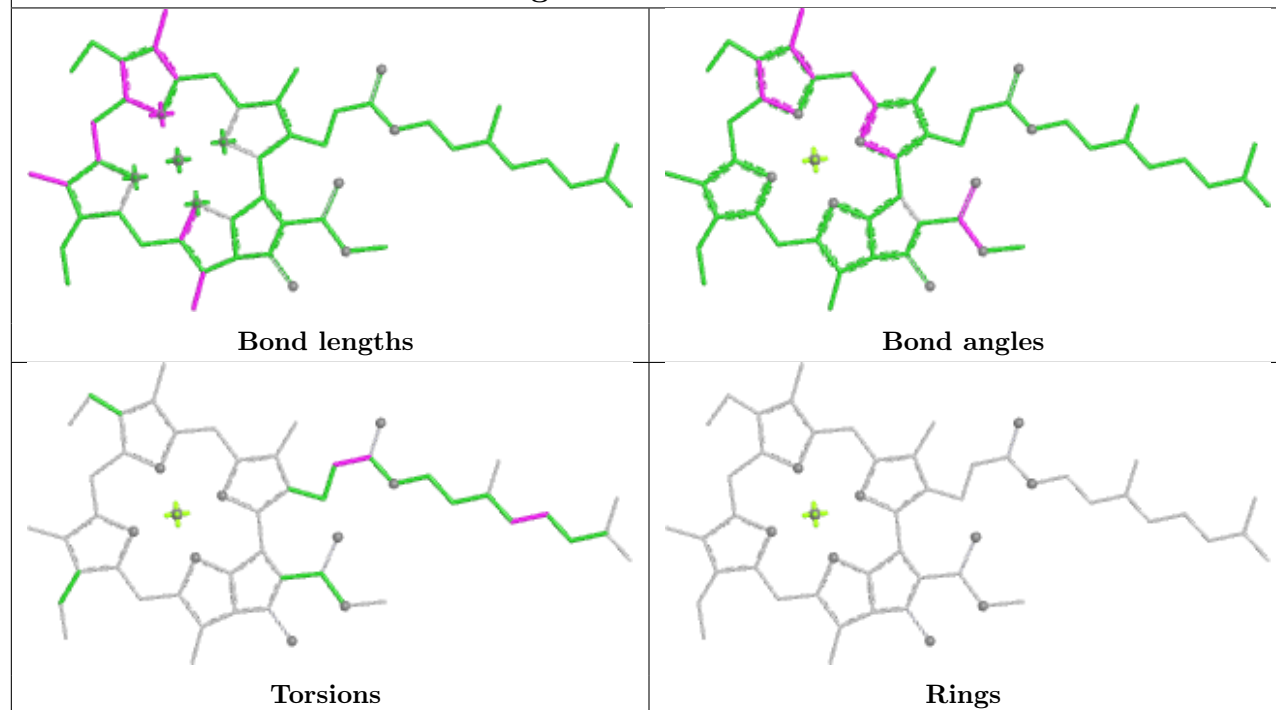
Ligand CLA K 210



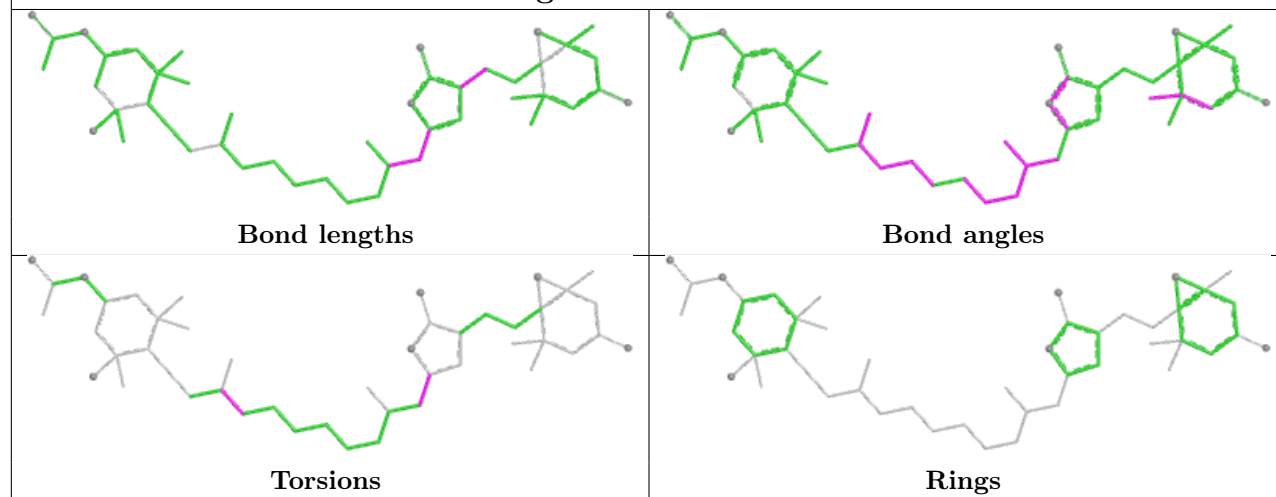
Ligand CLA f 805

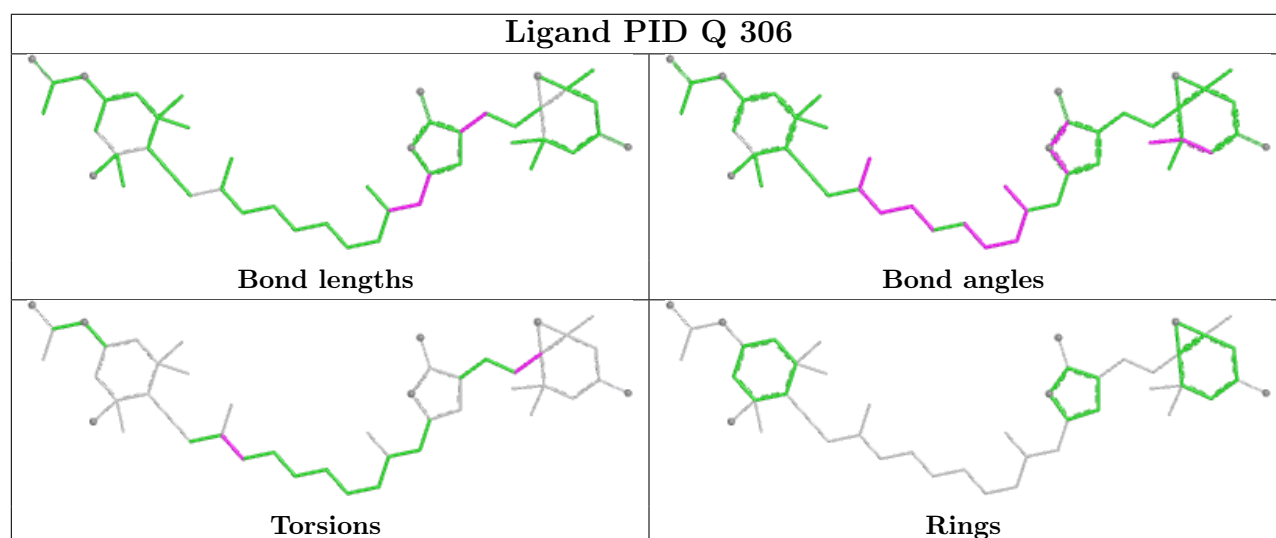
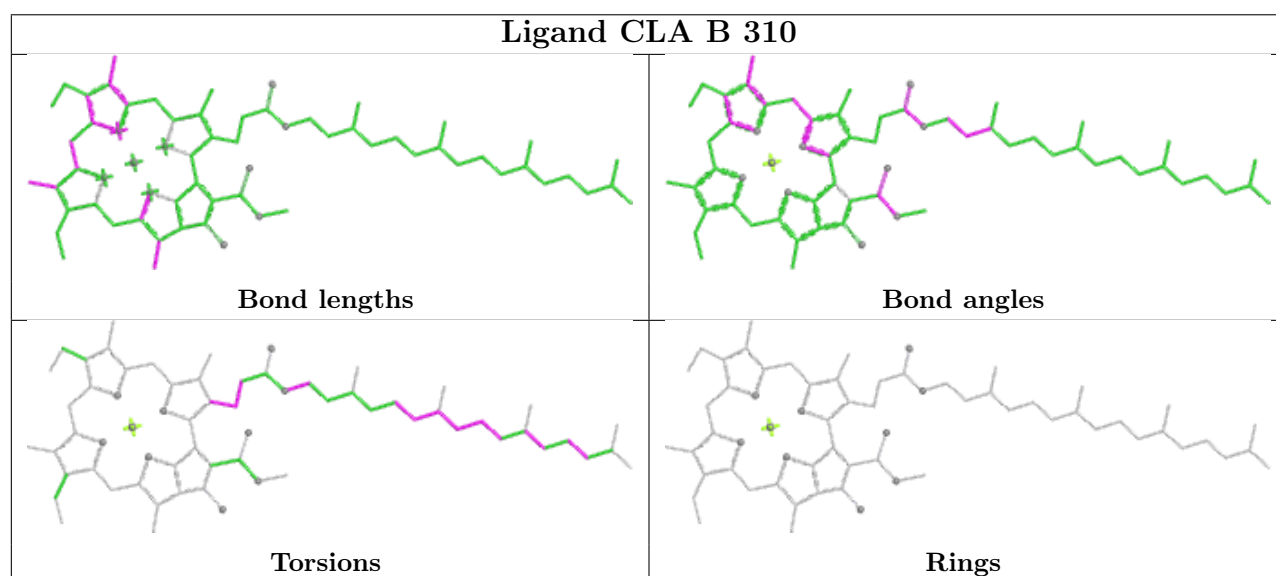
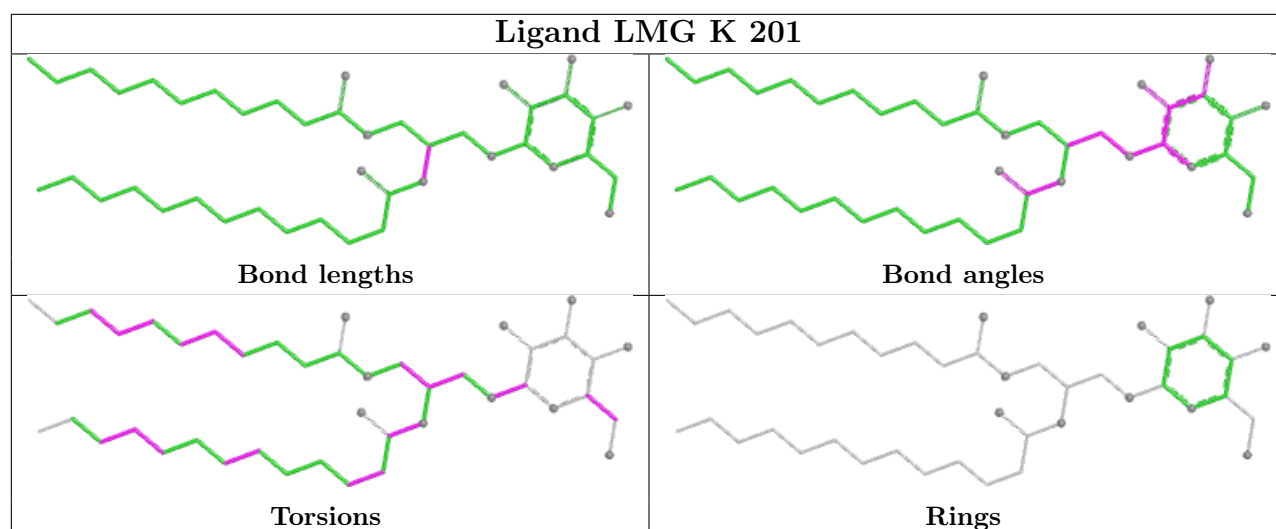


Ligand CLA G 313

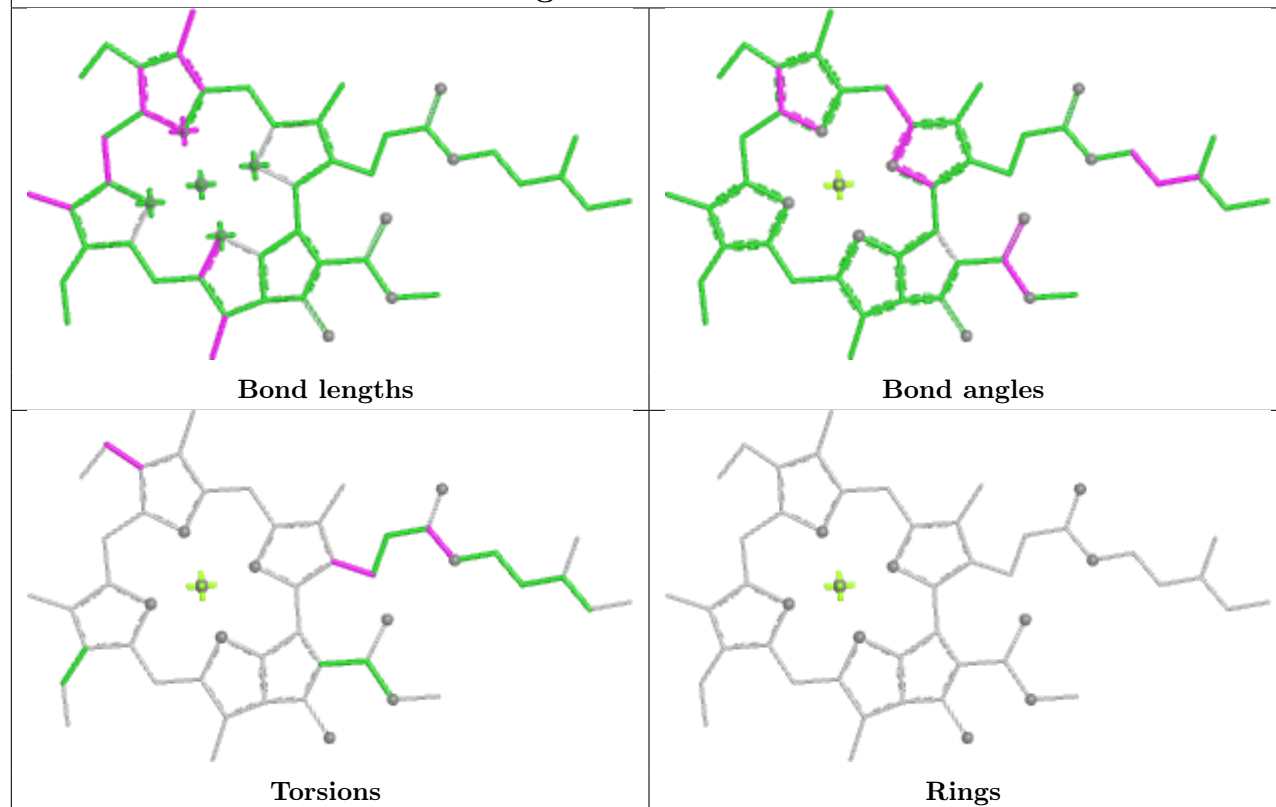


Ligand PID O 304

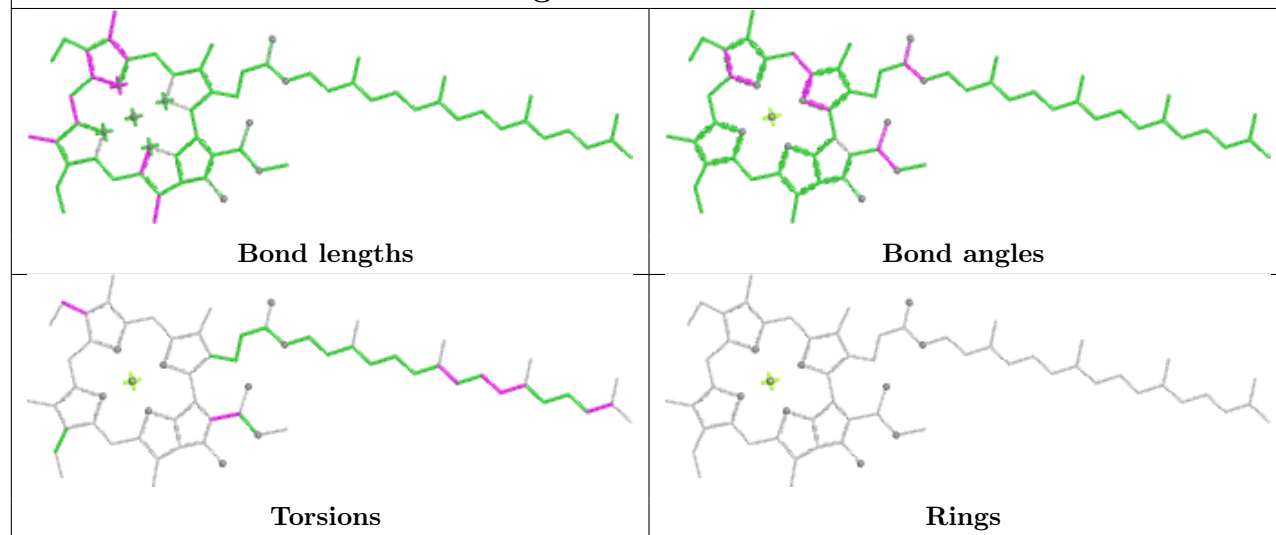


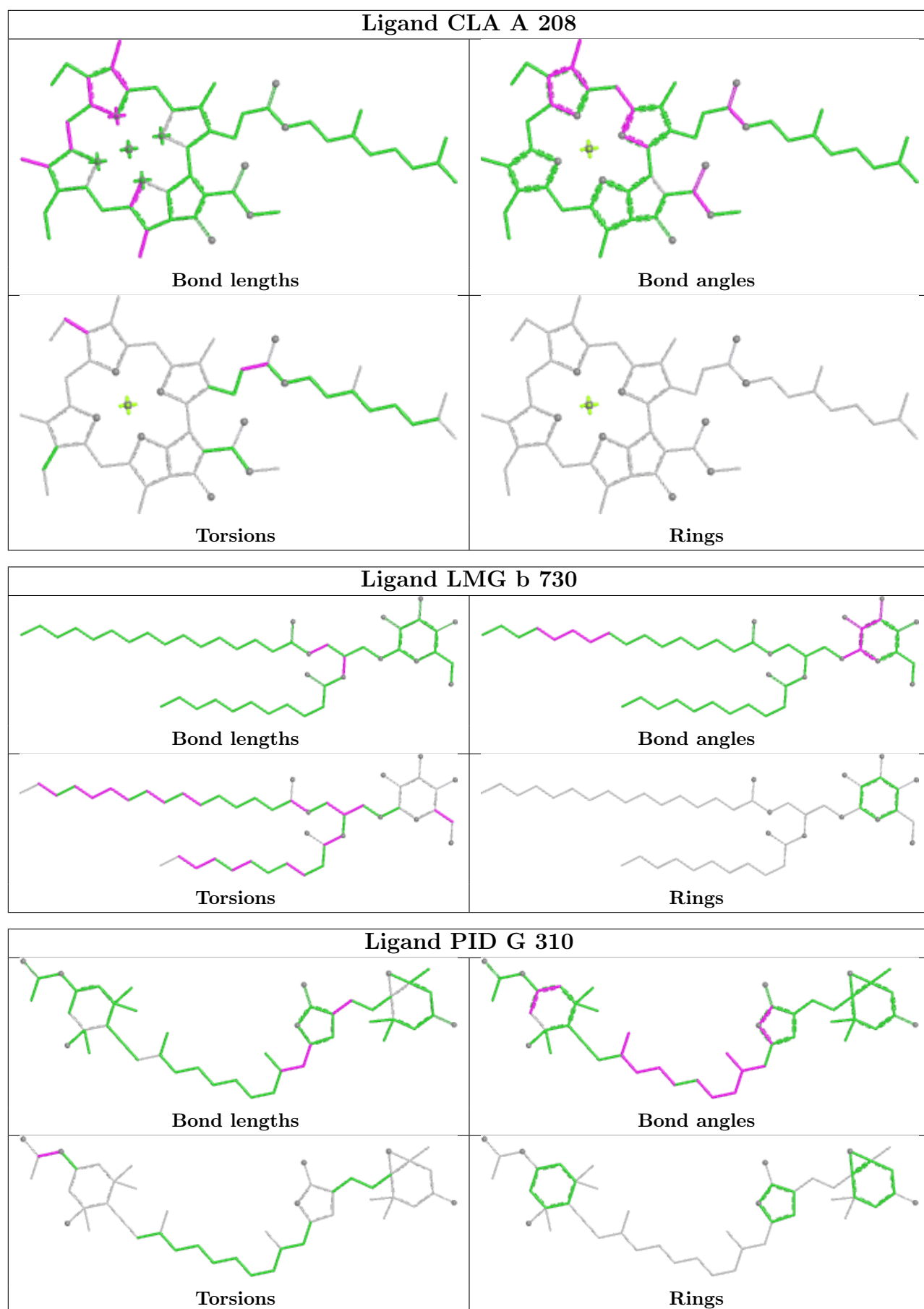


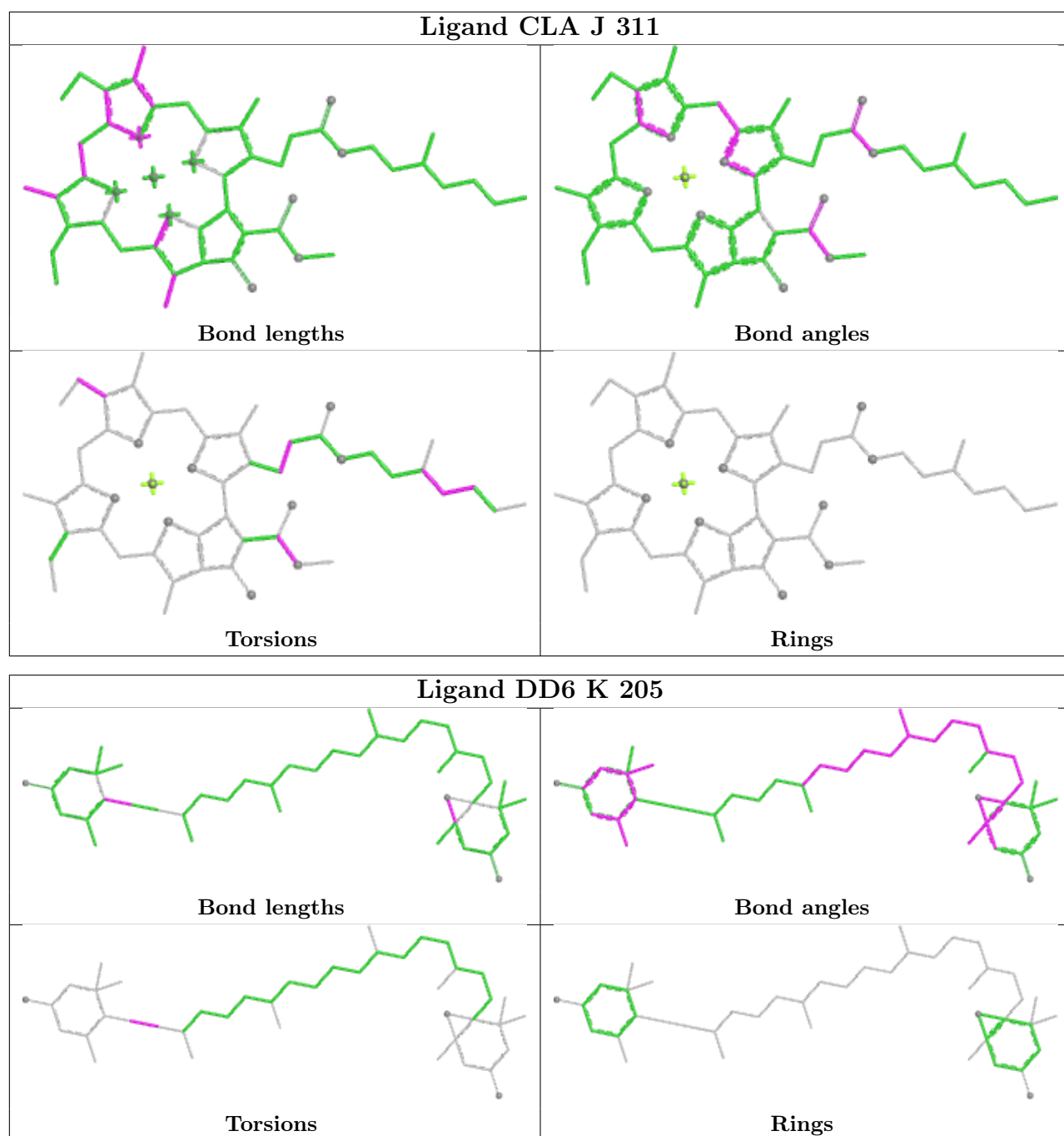
Ligand CLA a 808



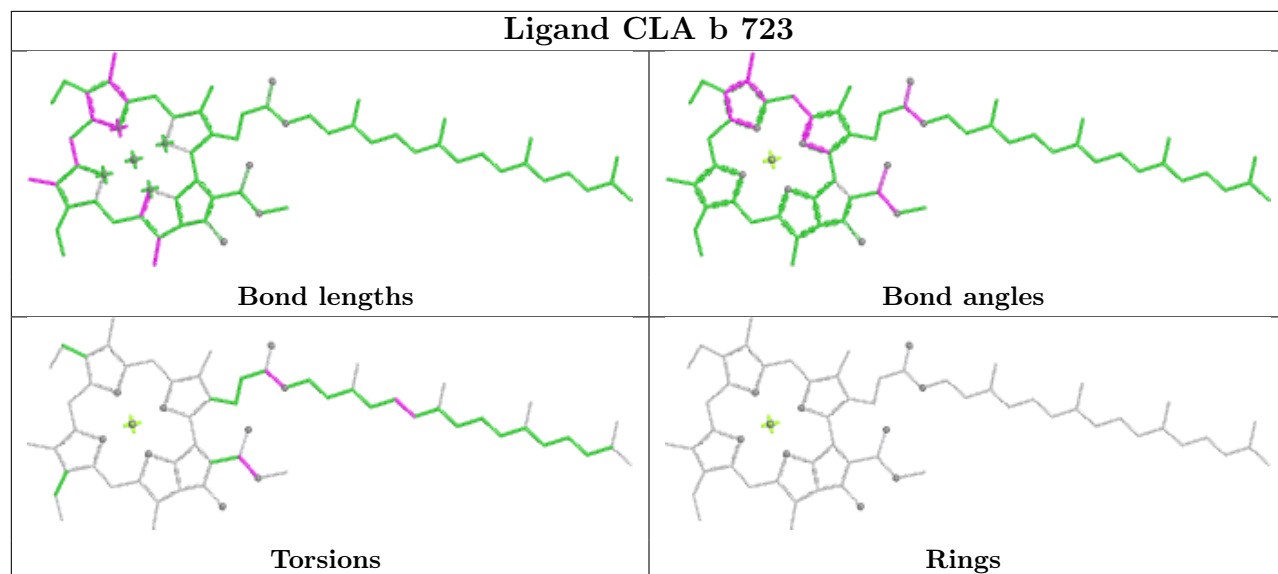
Ligand CLA E 308



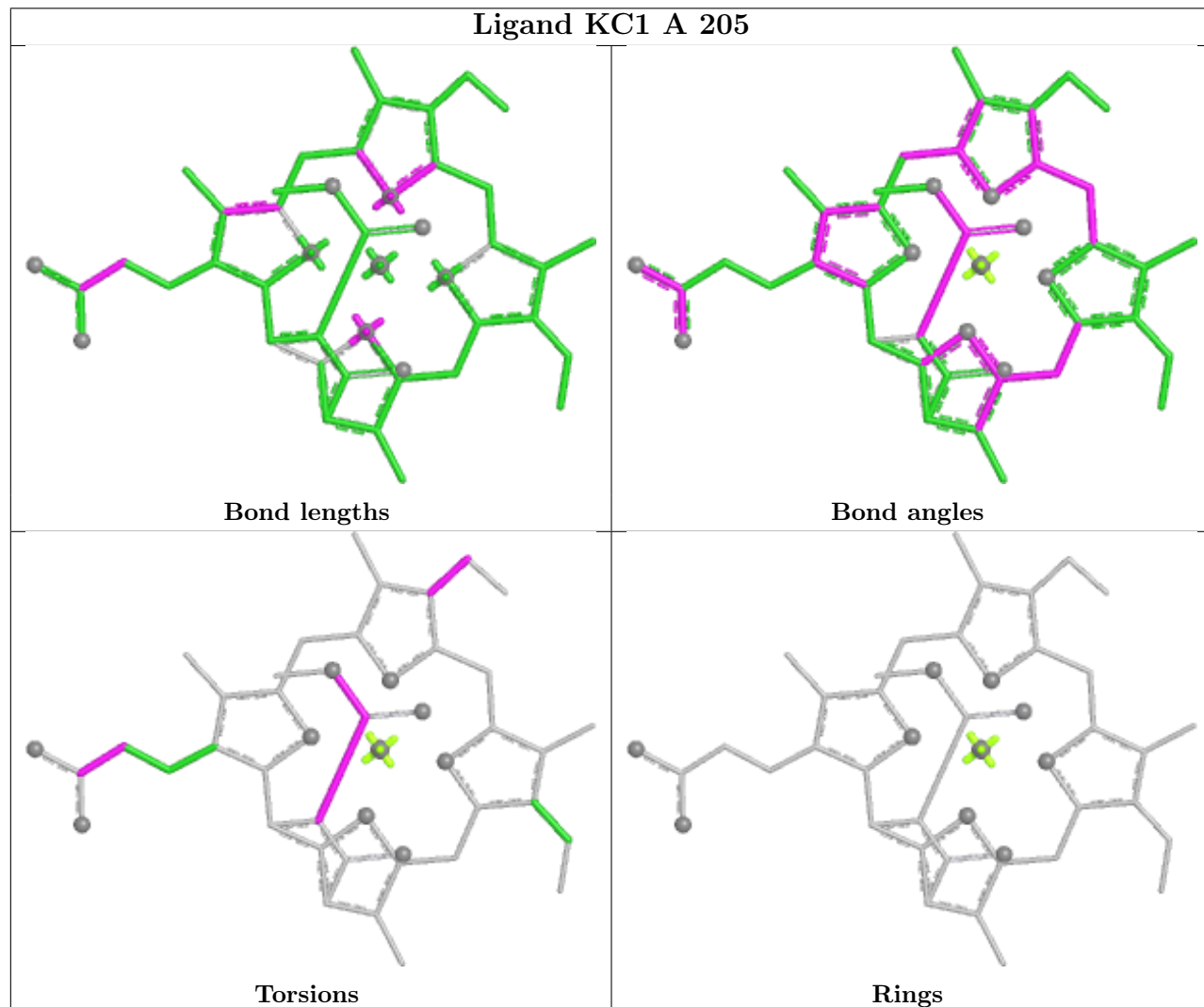




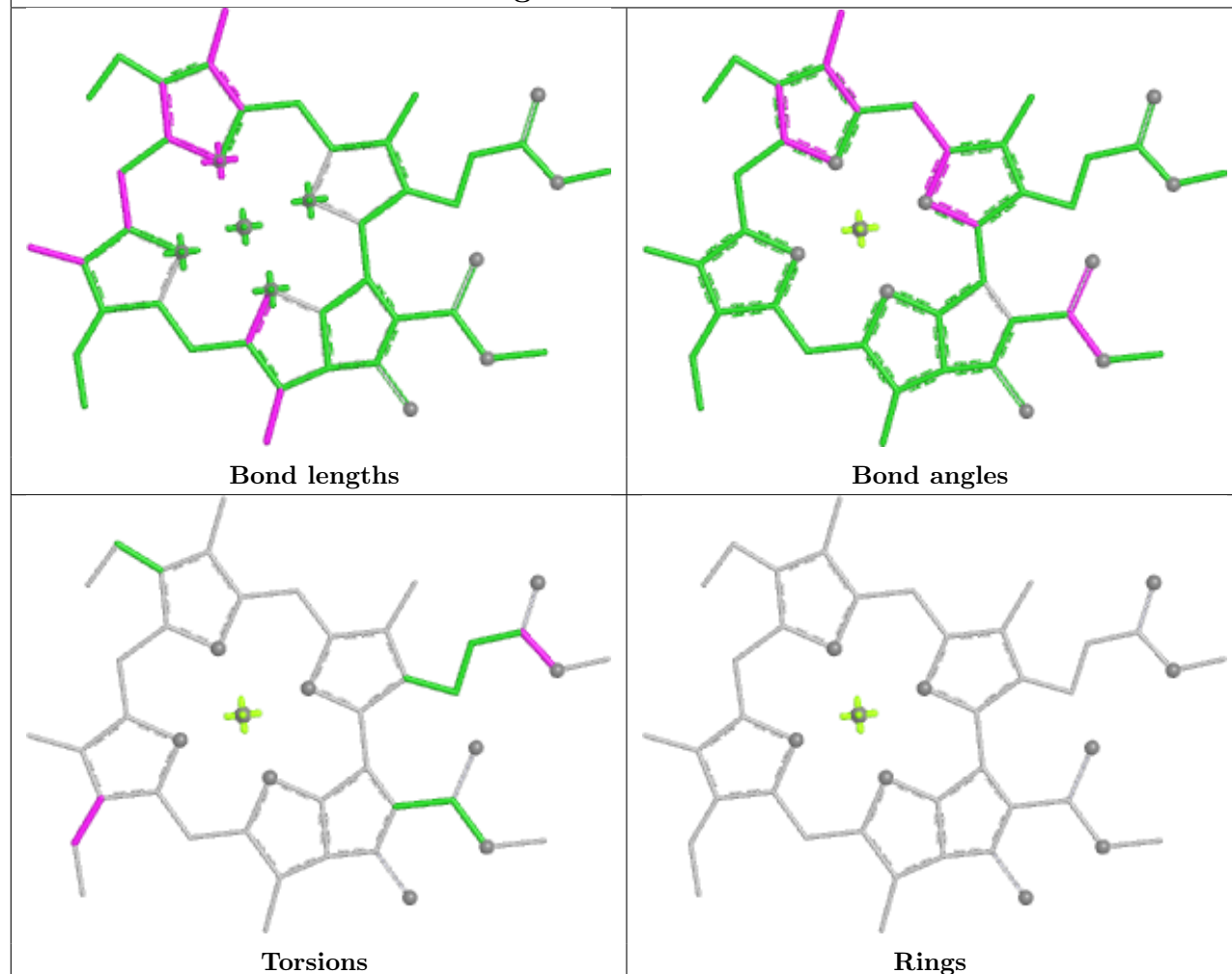
Ligand CLA b 723



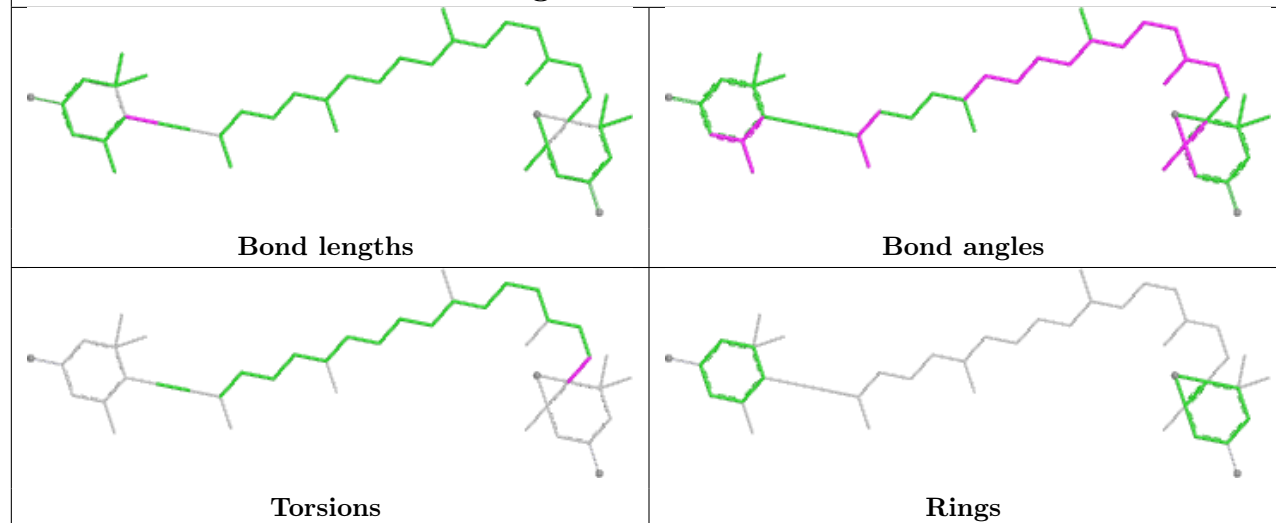
Ligand KC1 A 205



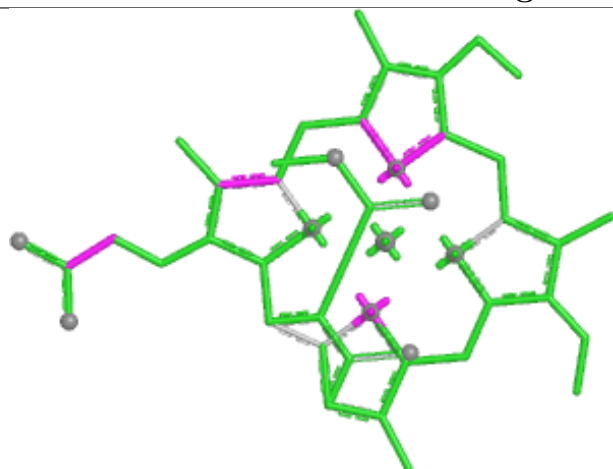
Ligand CLA B 315



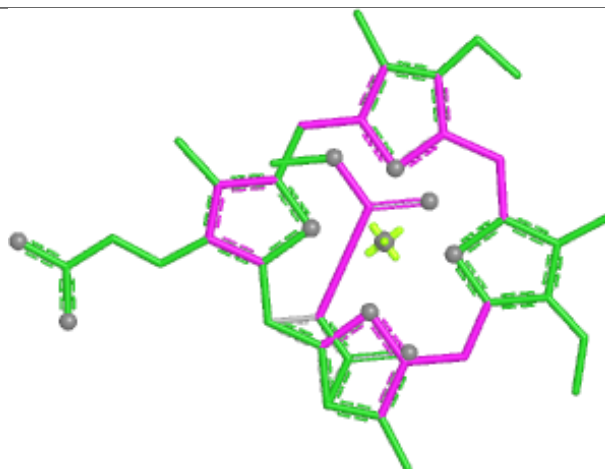
Ligand DD6 G 308



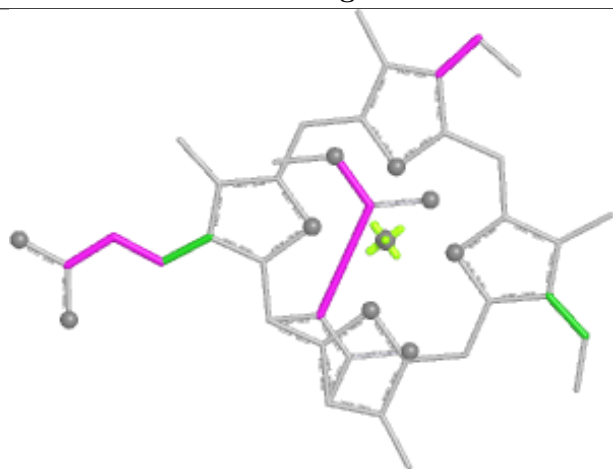
Ligand KC1 C 312



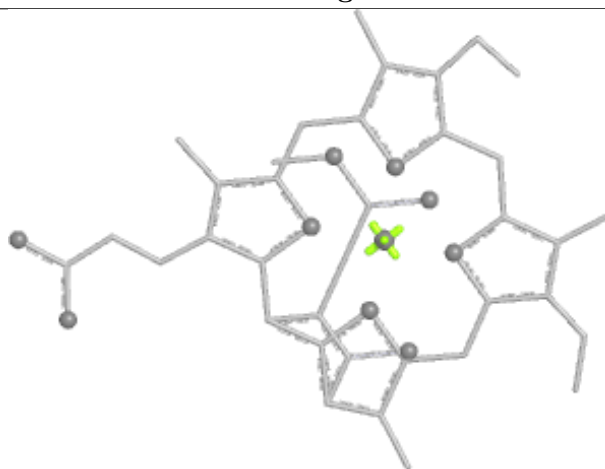
Bond lengths



Bond angles

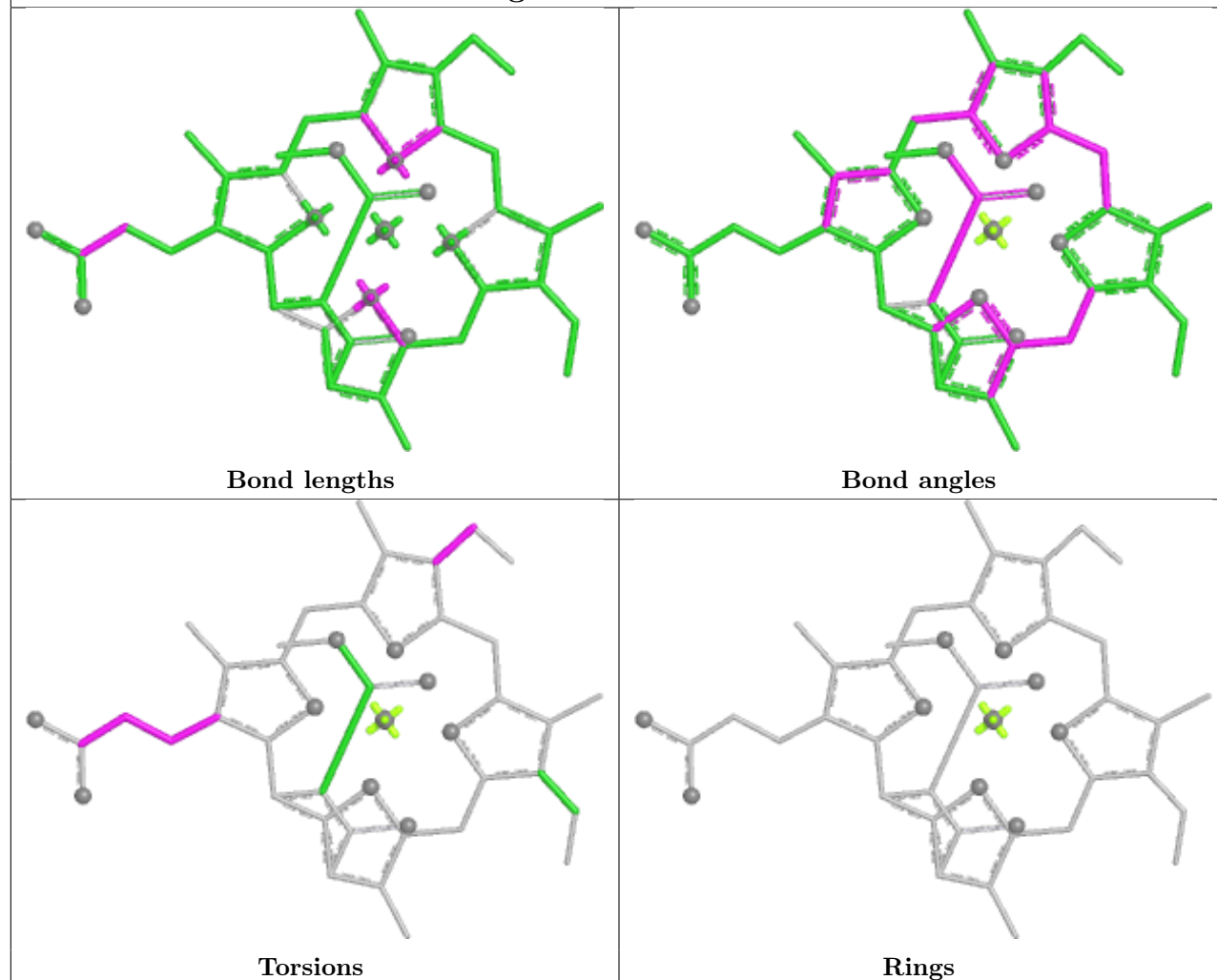


Torsions

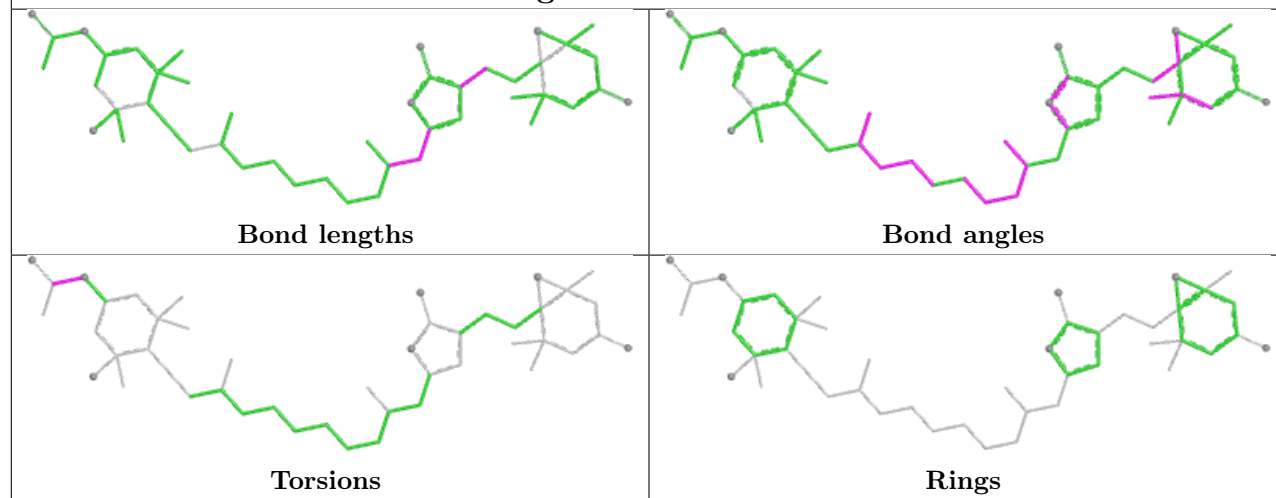


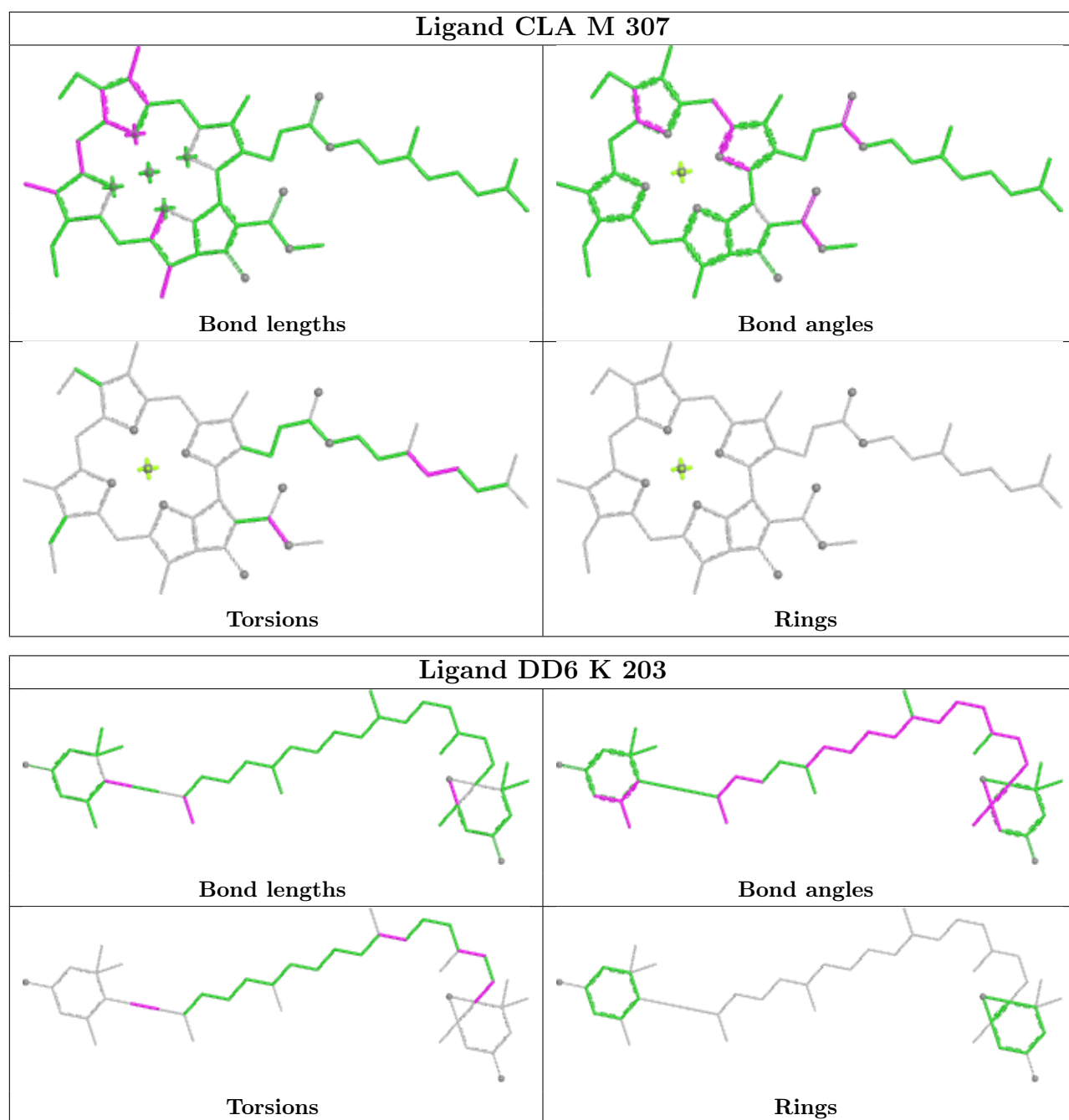
Rings

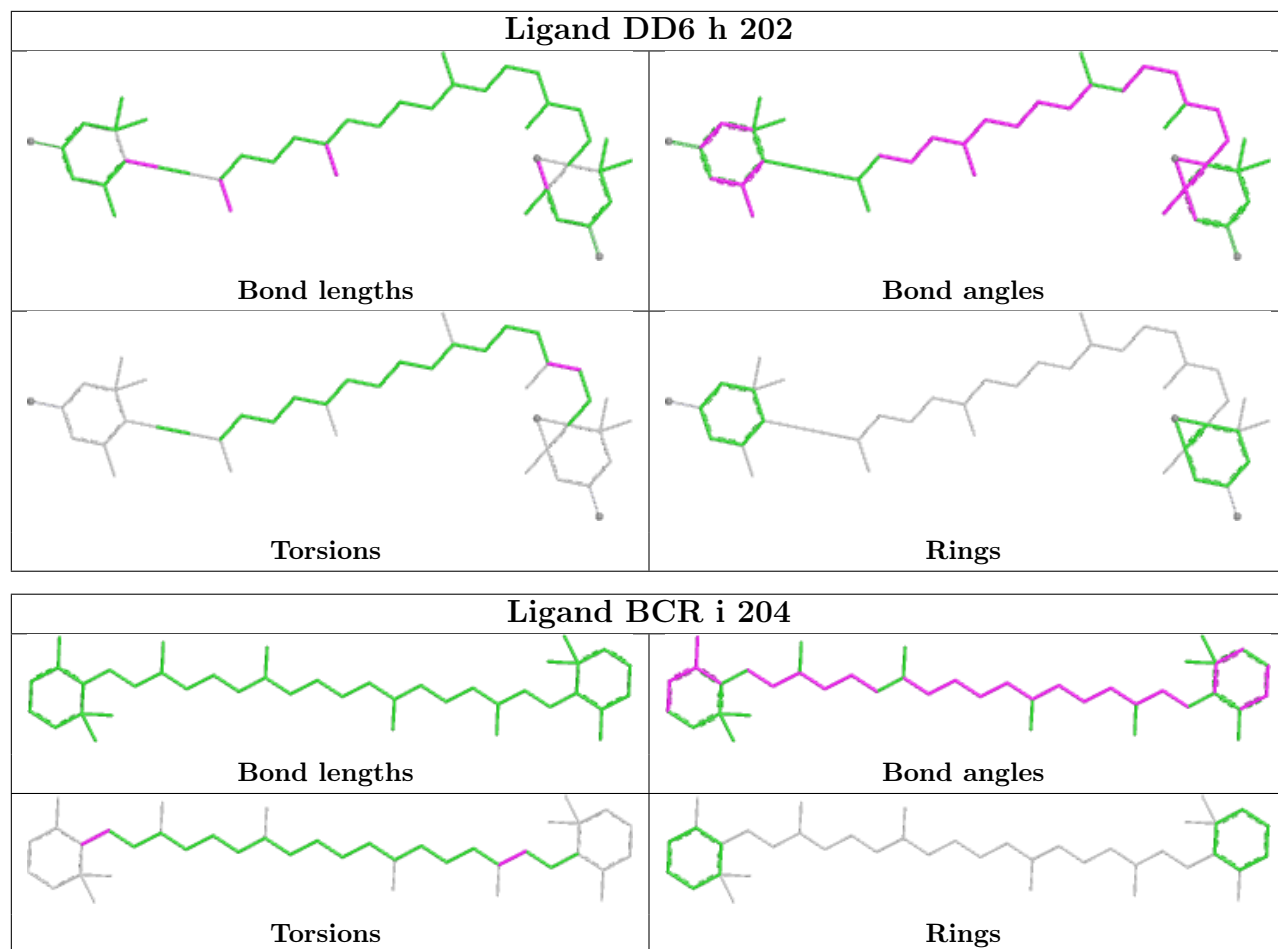
Ligand KC1 G 318



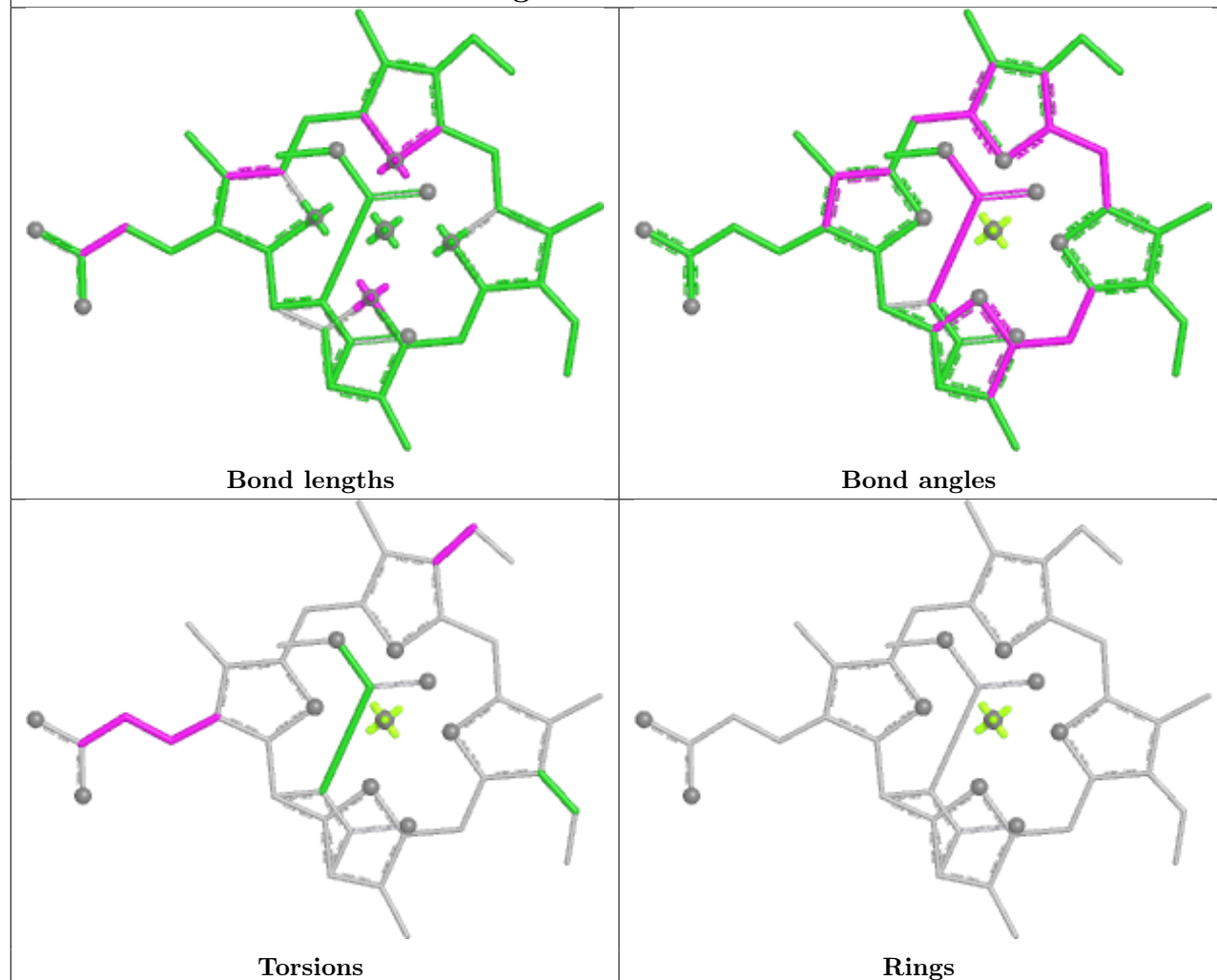
Ligand PID C 307



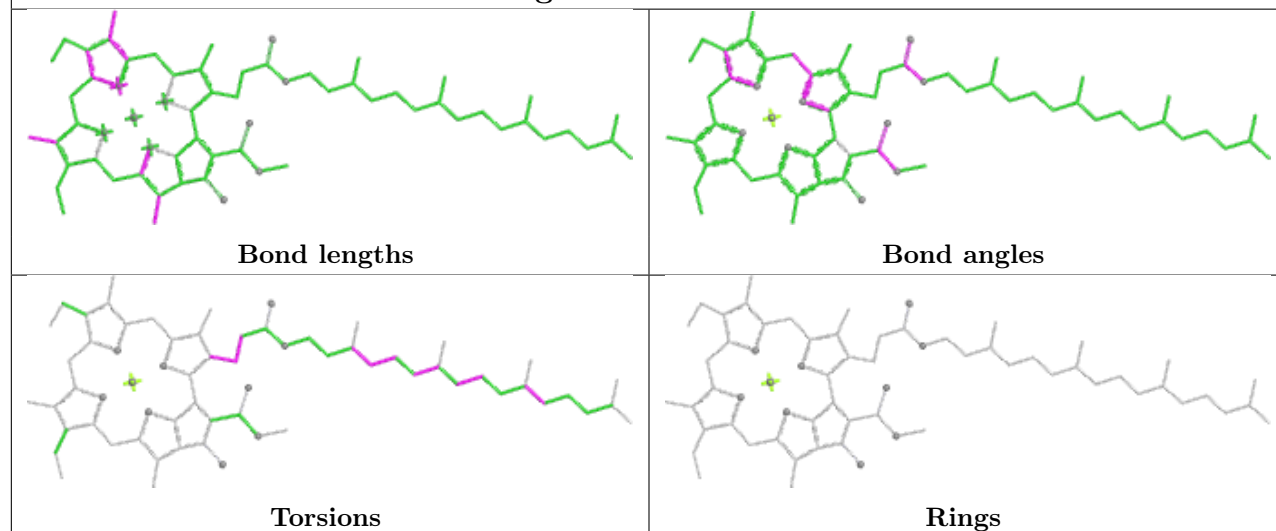




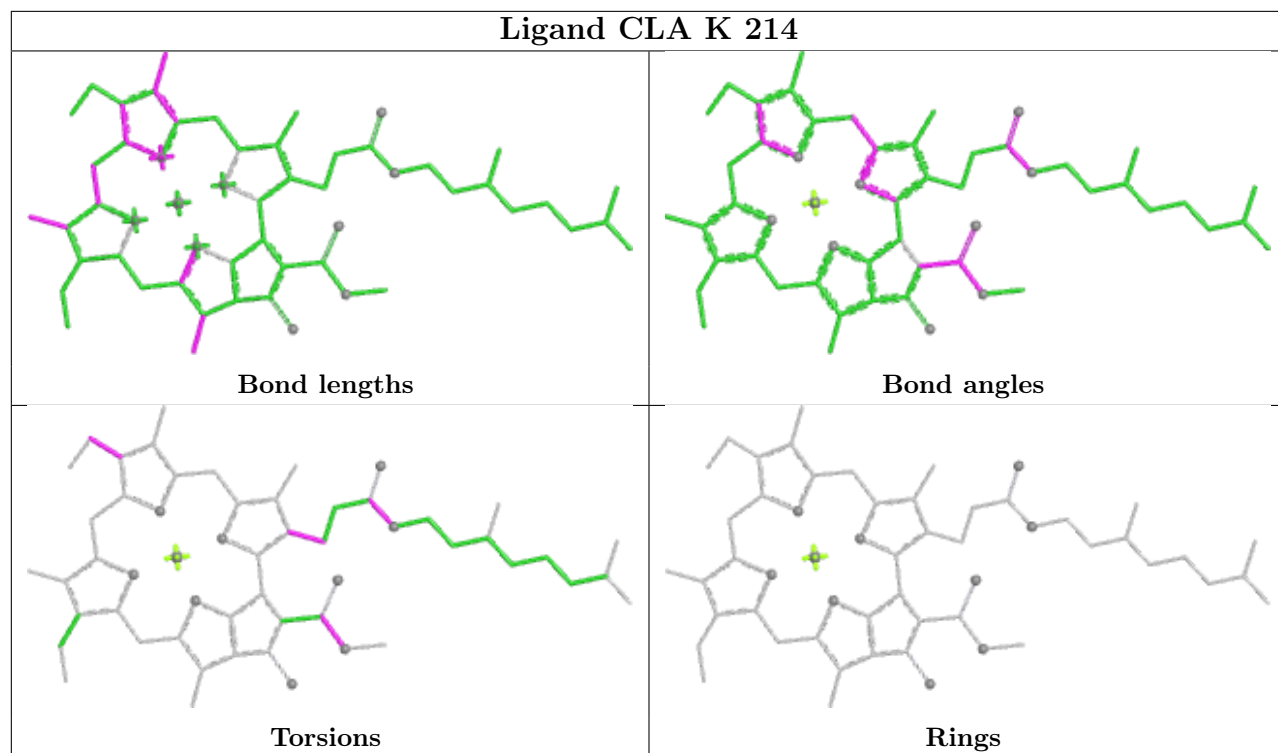
Ligand KC1 J 312



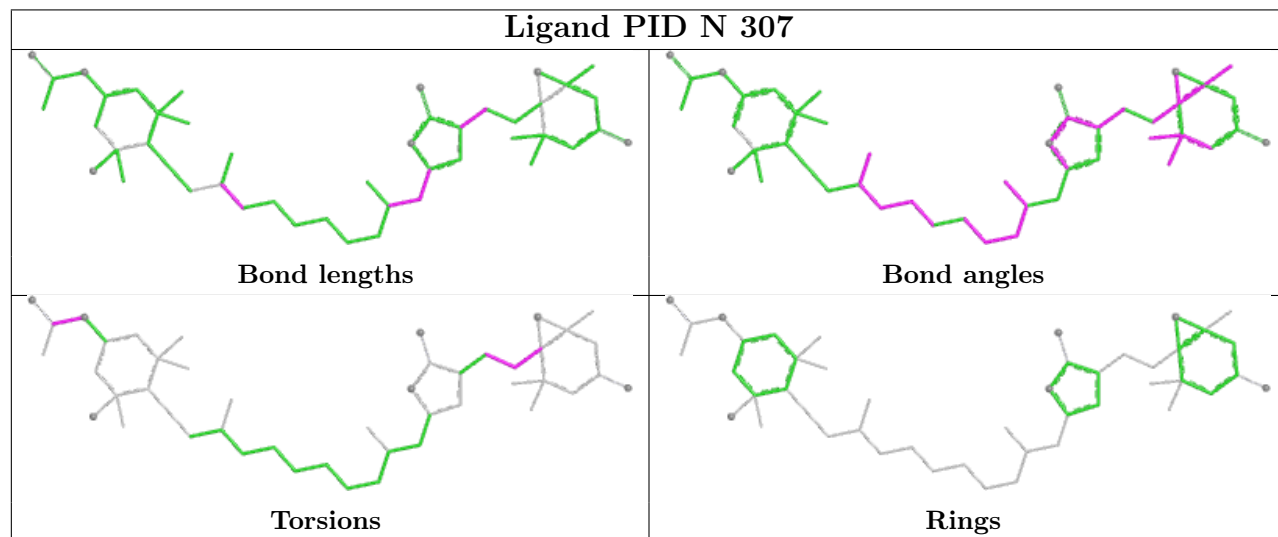
Ligand CLA b 706

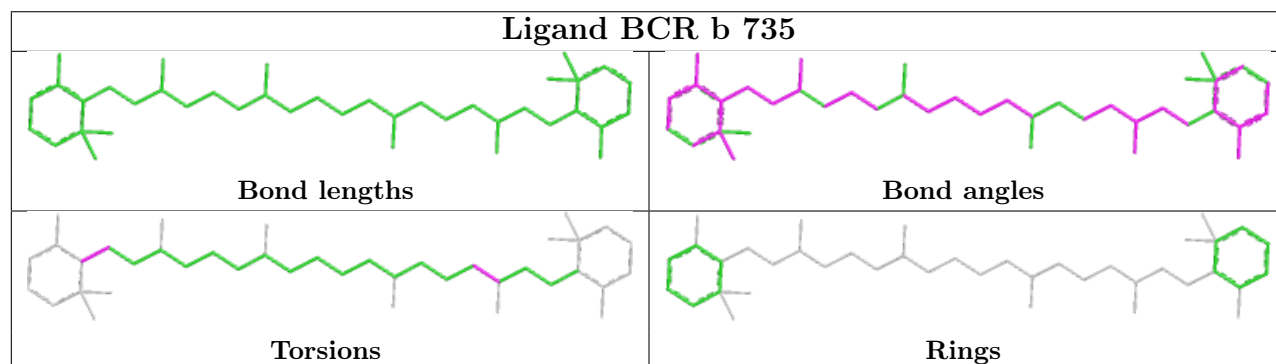
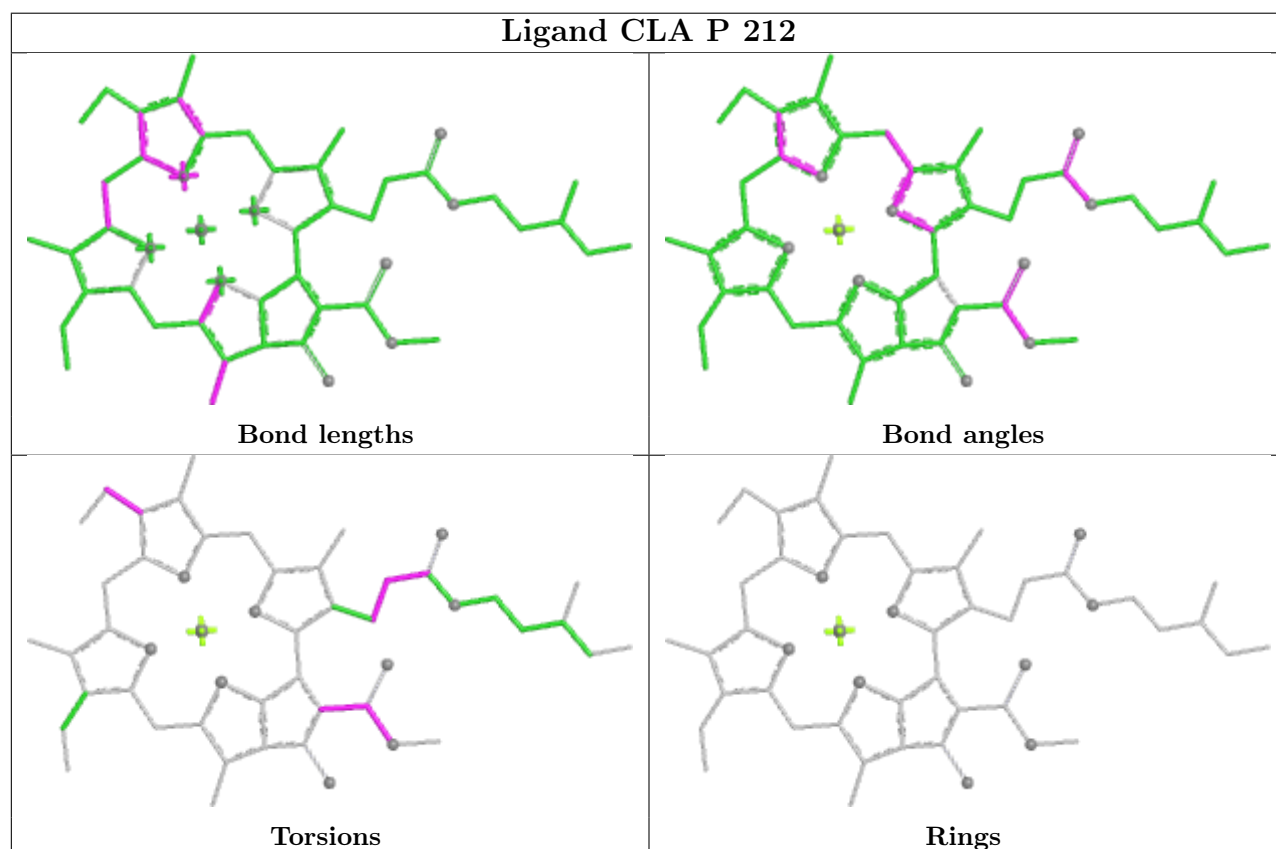
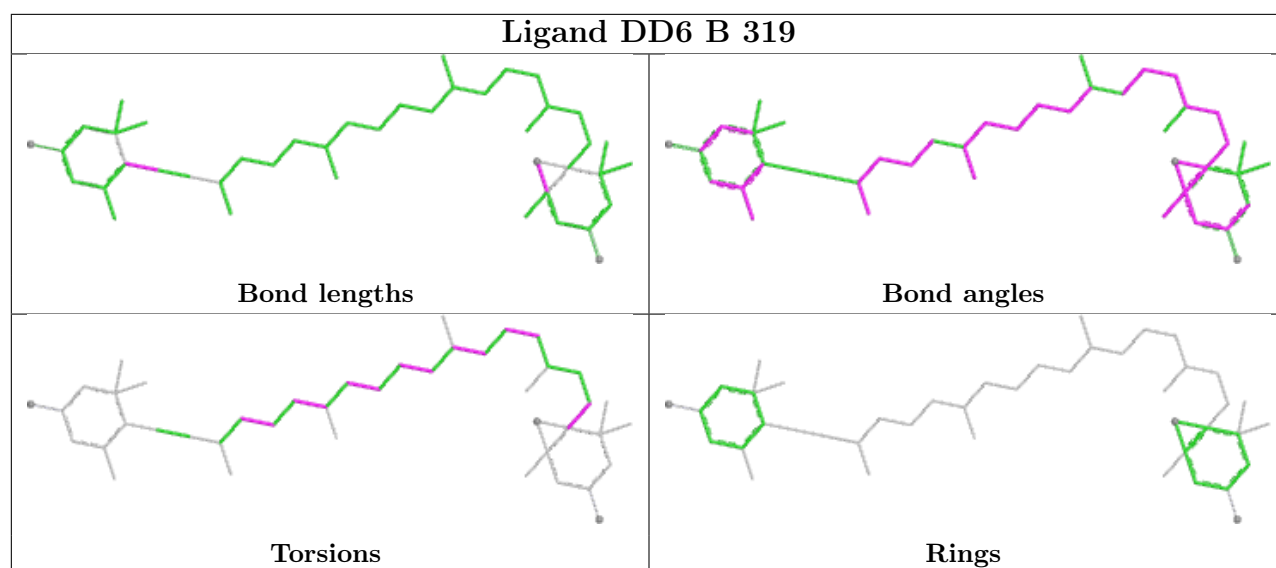


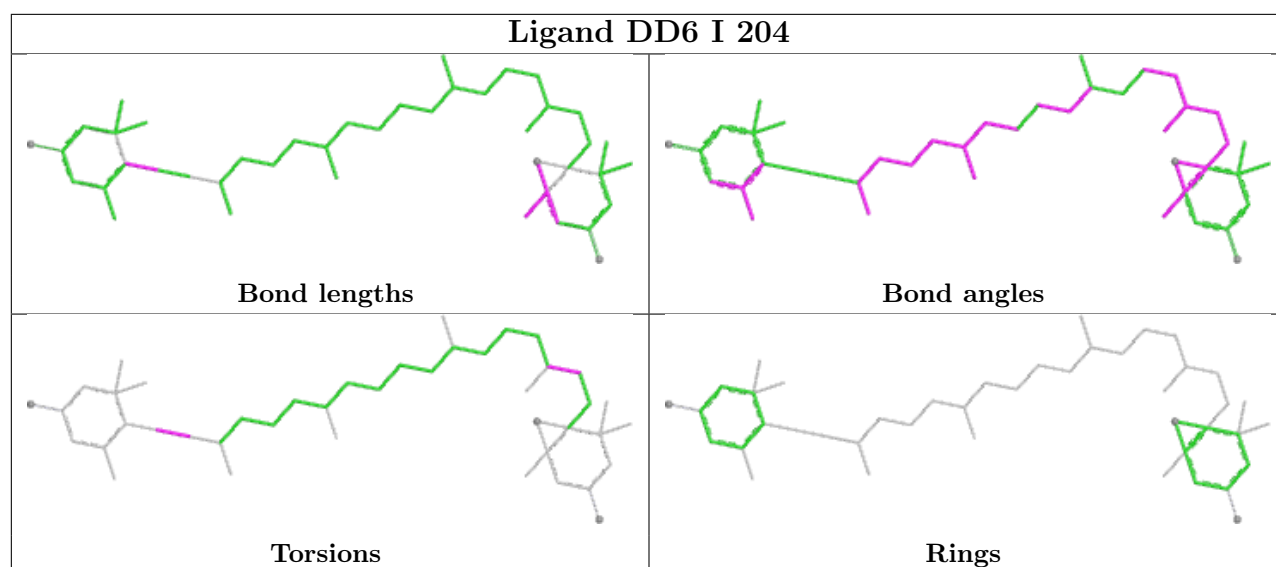
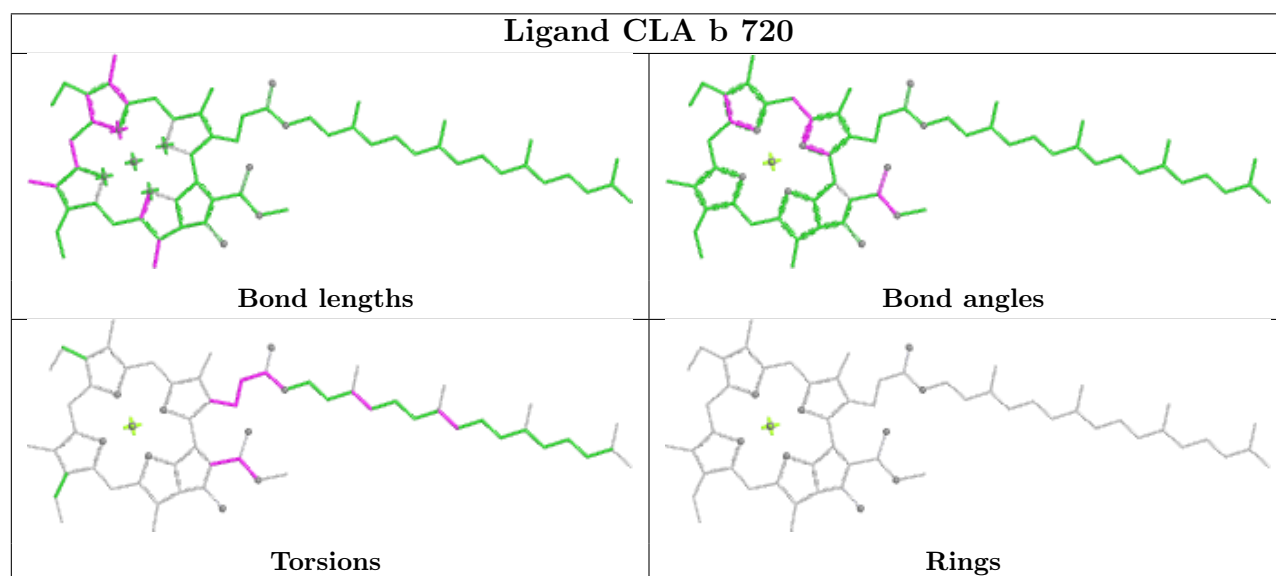
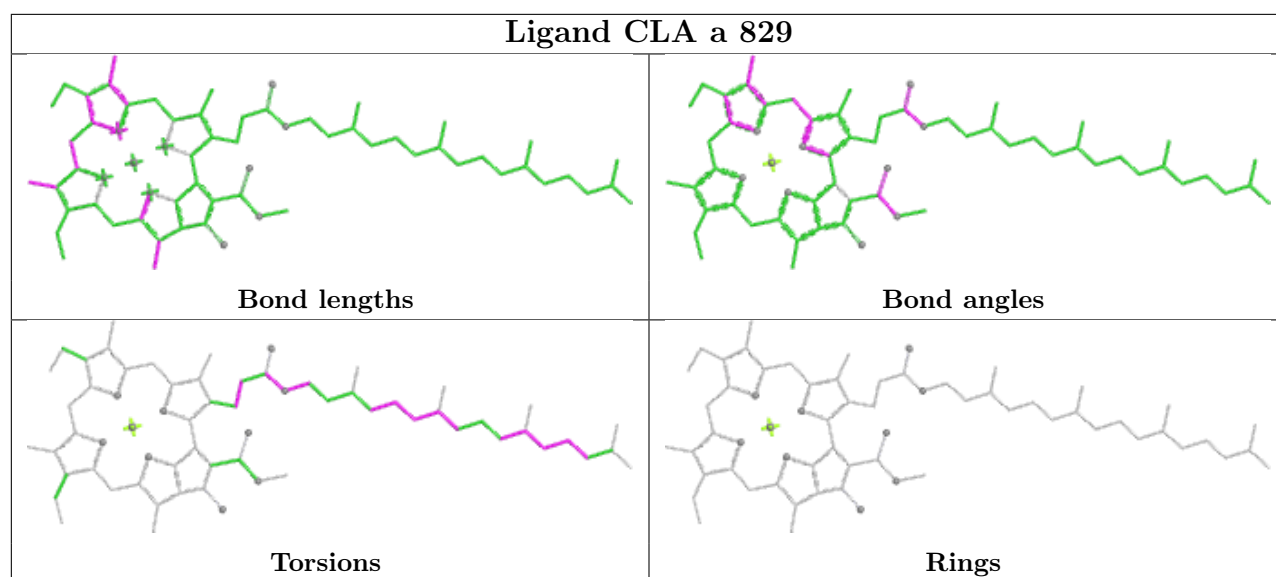
Ligand CLA K 214

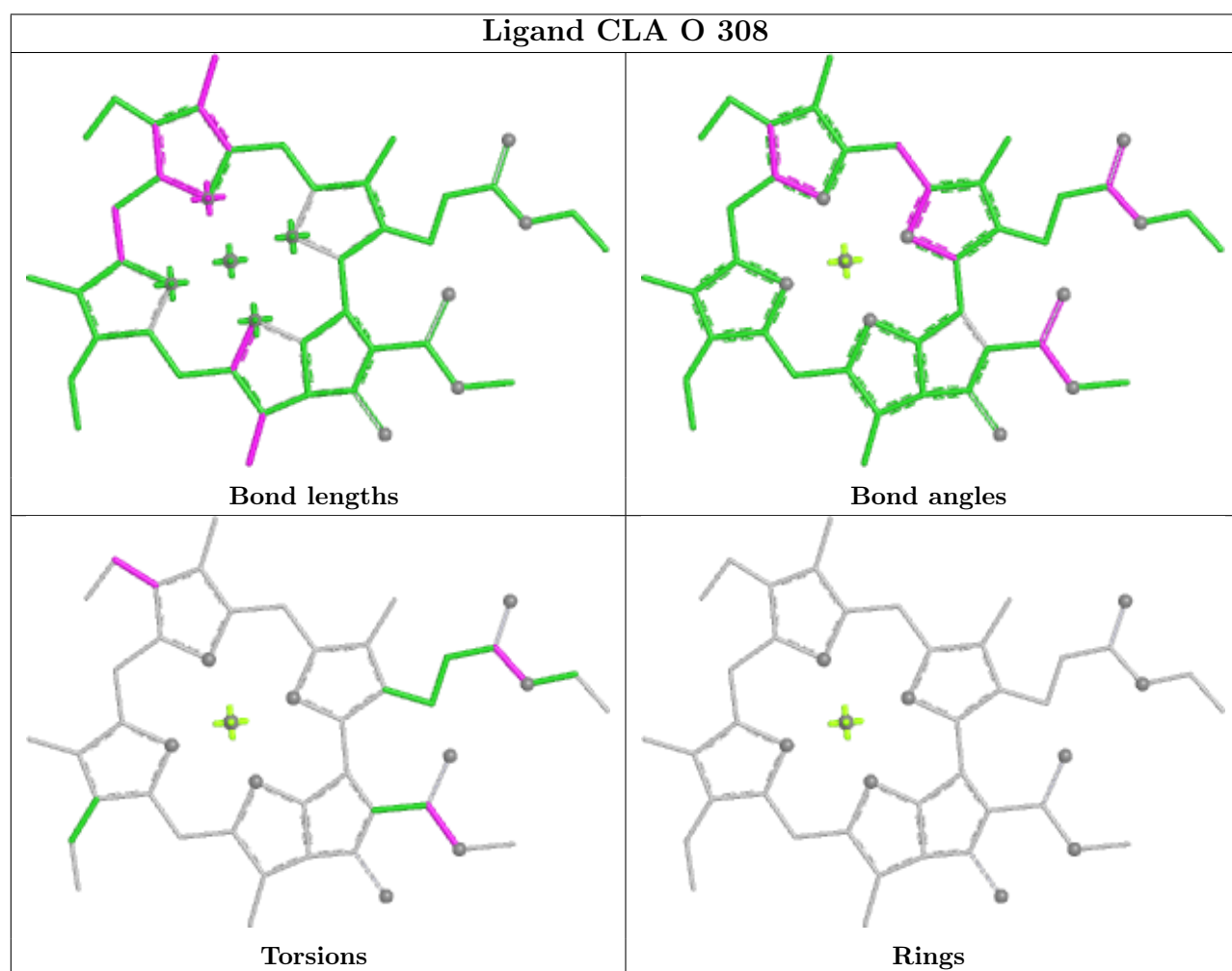
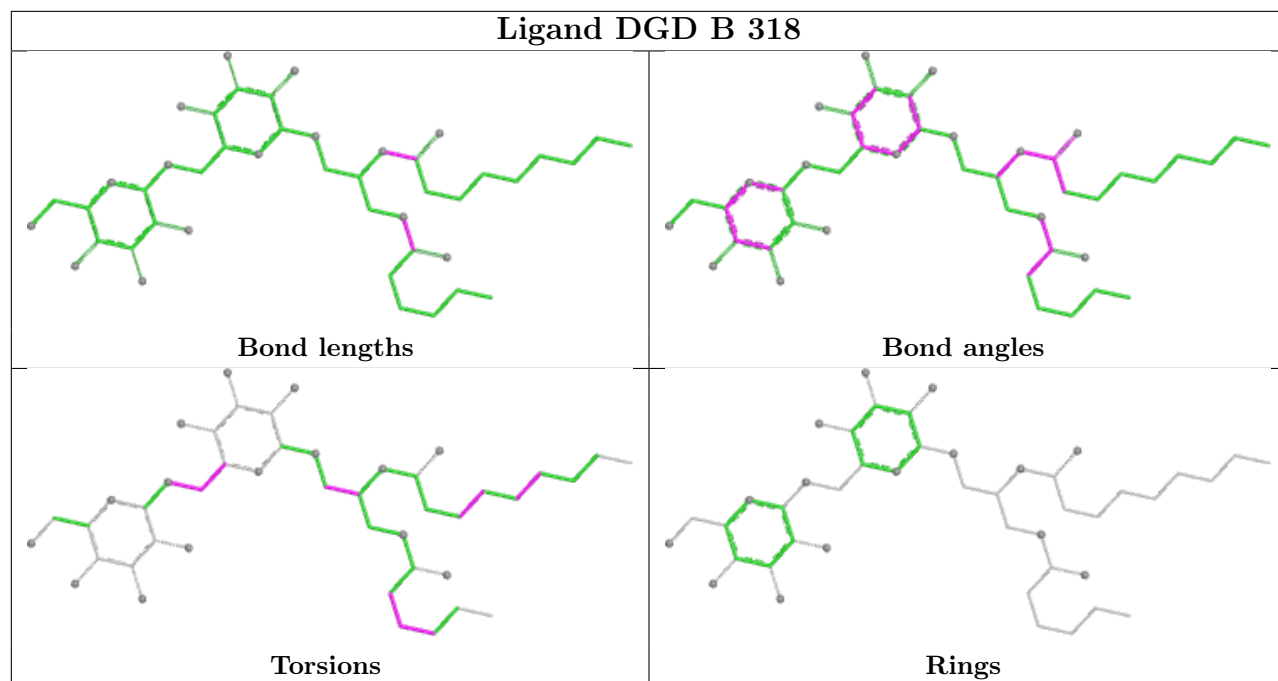


Ligand PID N 307

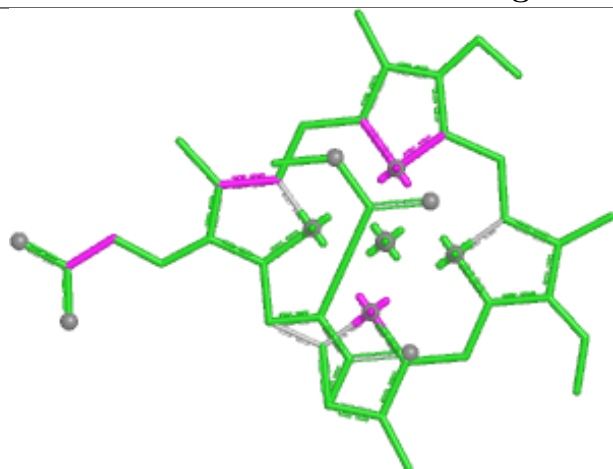




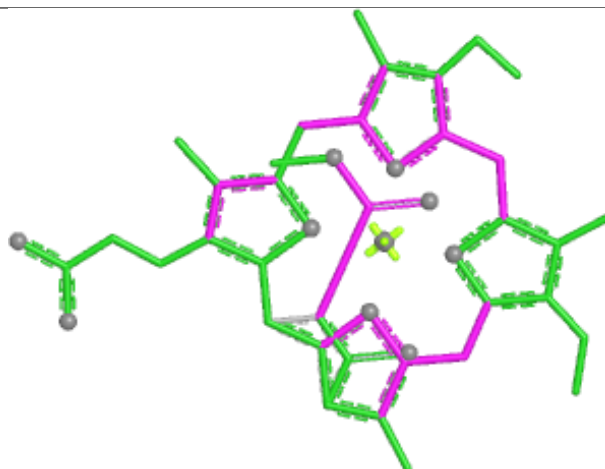




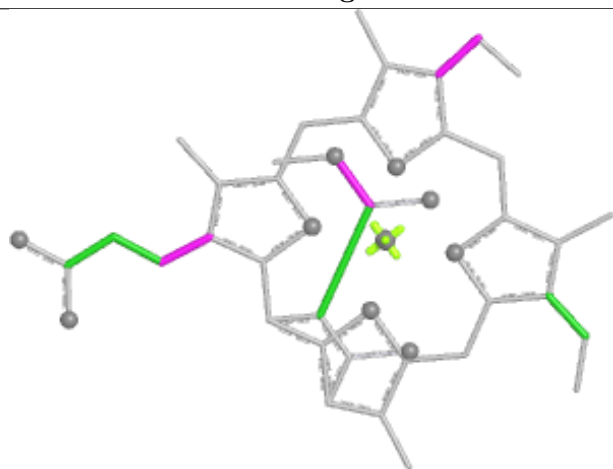
Ligand KC1 M 312



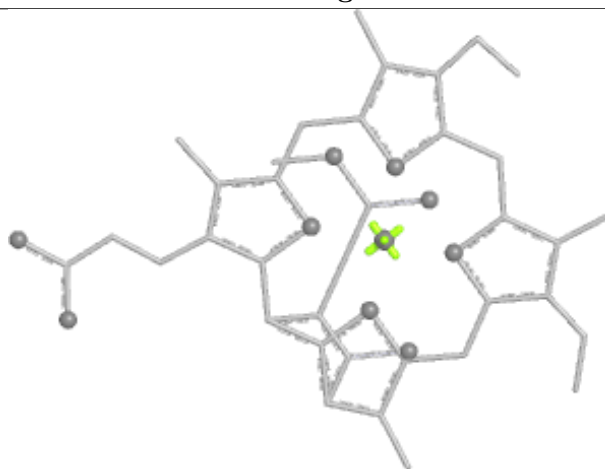
Bond lengths



Bond angles

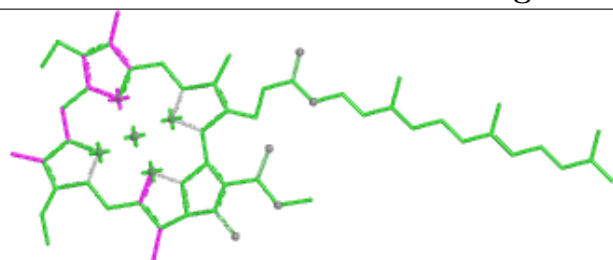


Torsions

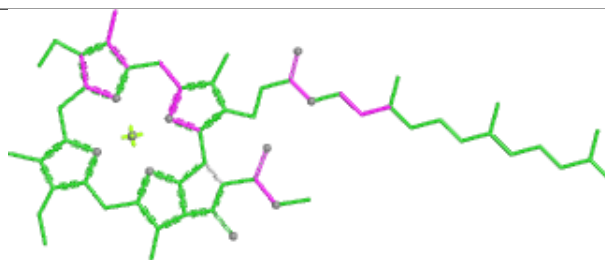


Rings

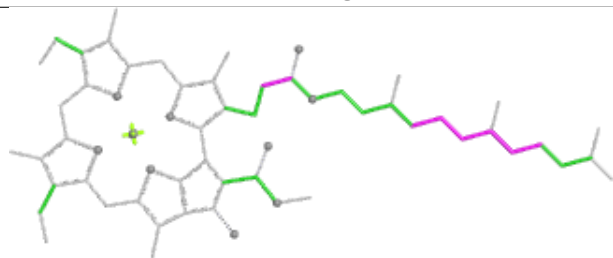
Ligand CLA A 218



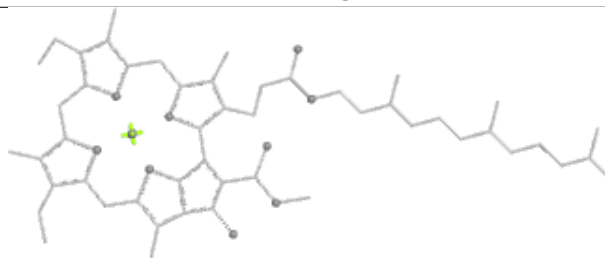
Bond lengths



Bond angles

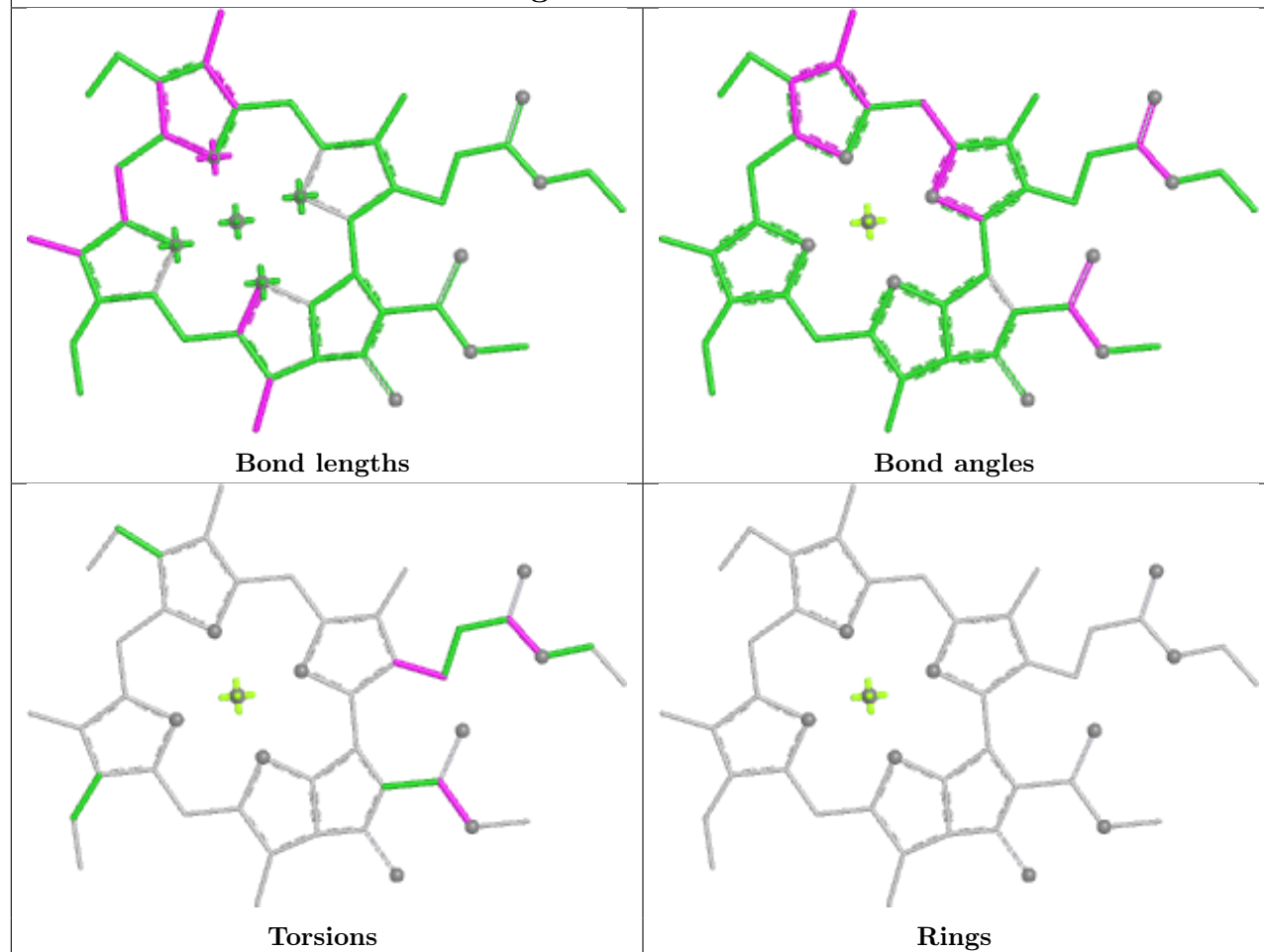


Torsions

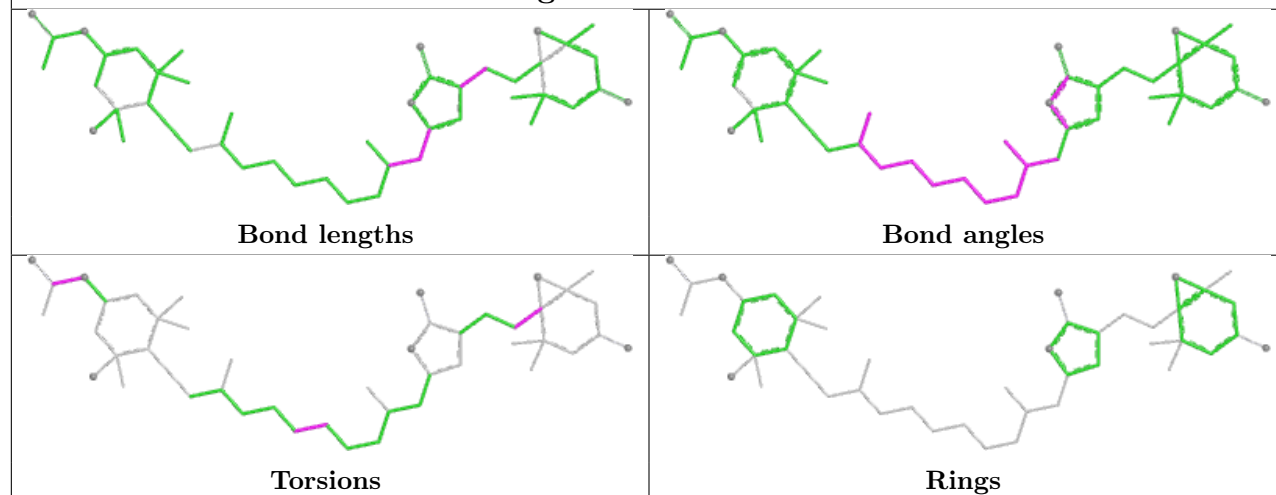


Rings

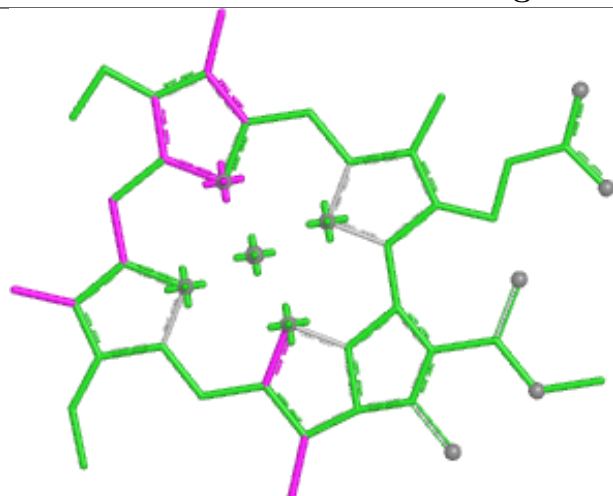
Ligand CLA J 310



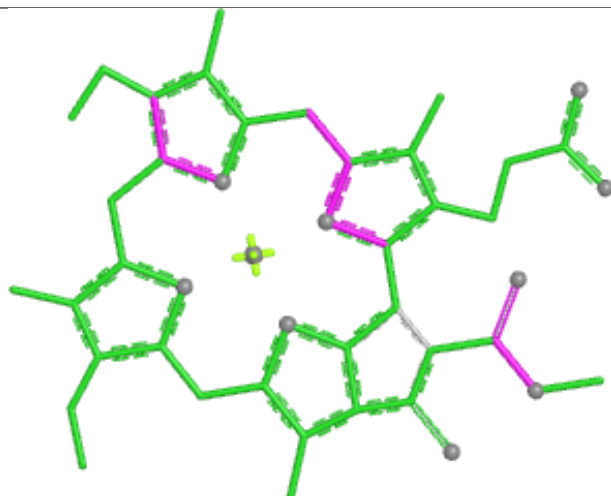
Ligand PID P 202



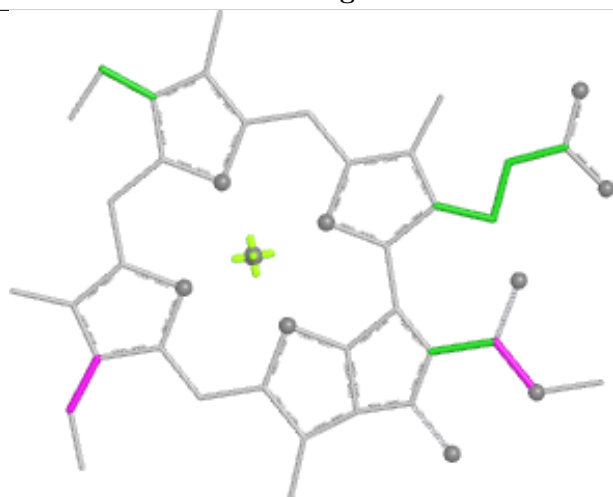
Ligand CLA D 313



Bond lengths



Bond angles

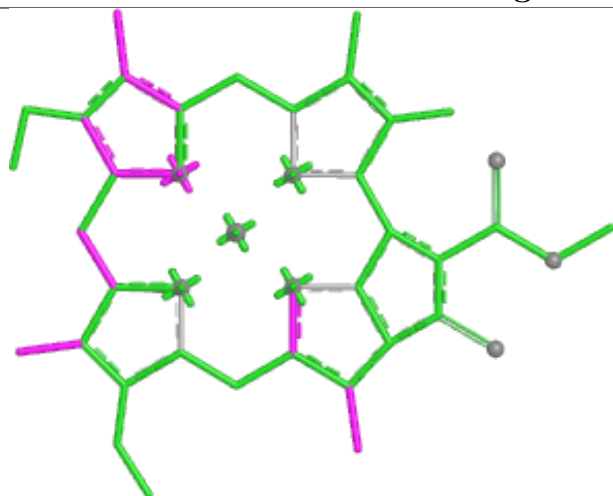


Torsions

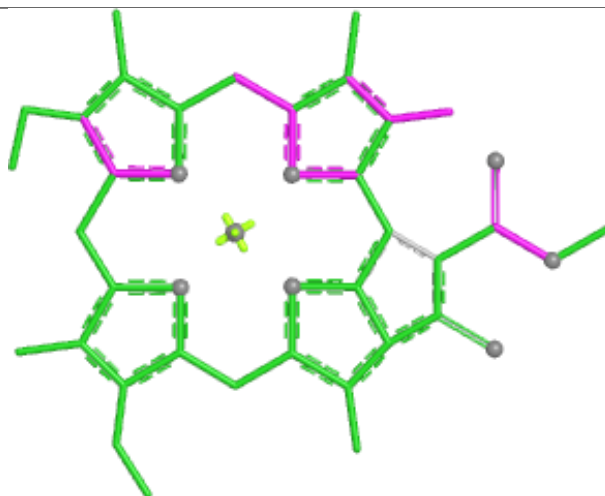


Rings

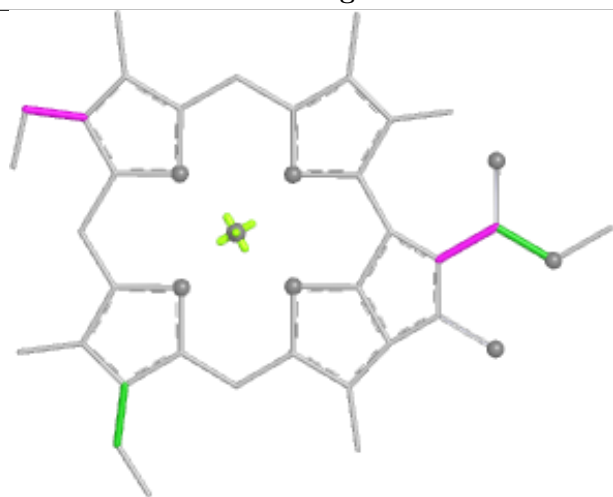
Ligand CLA A 214



Bond lengths



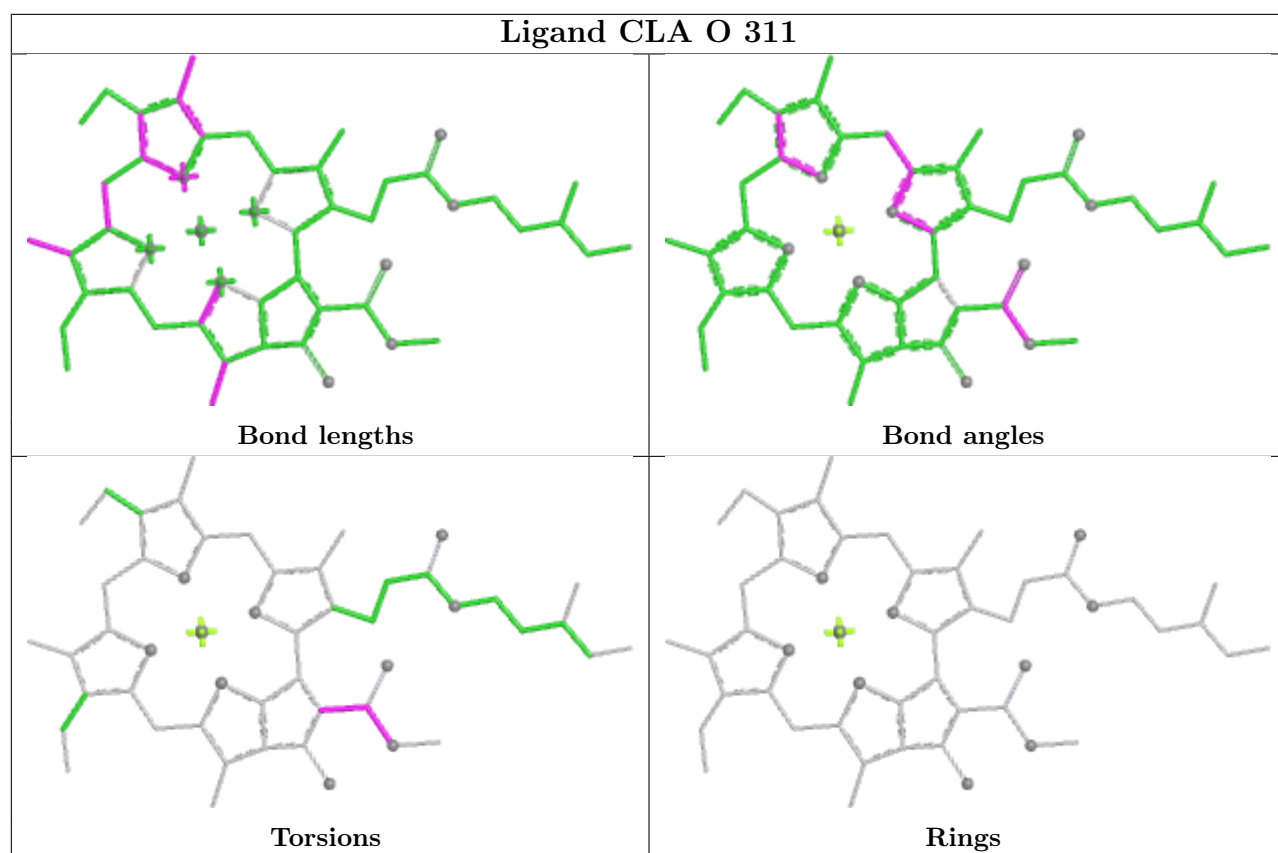
Bond angles



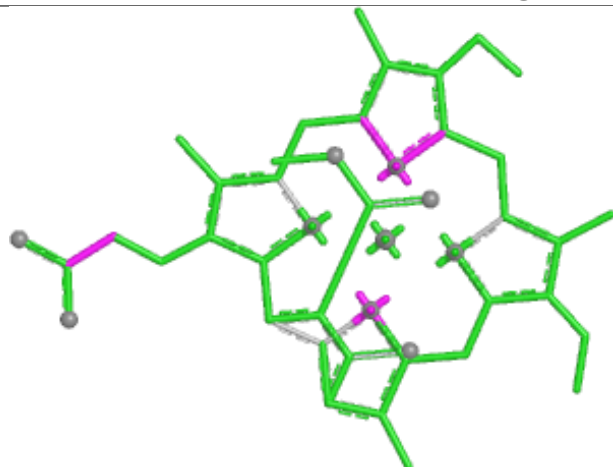
Torsions



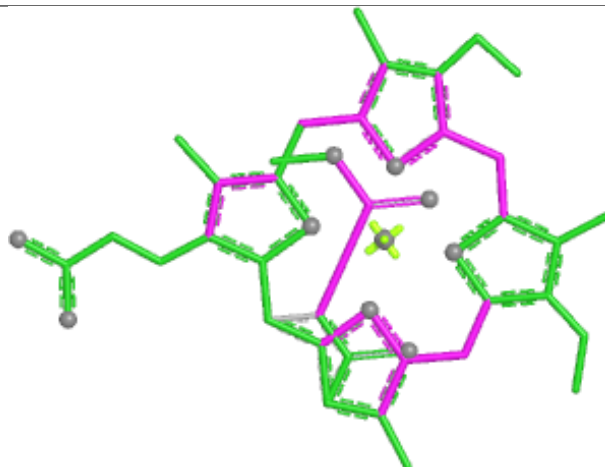
Rings



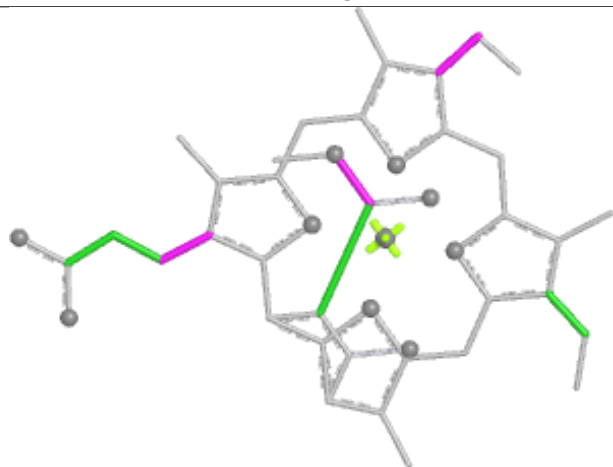
Ligand KC1 H 314



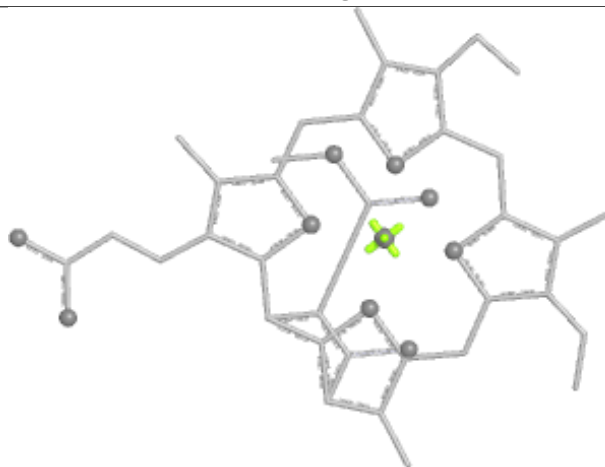
Bond lengths



Bond angles

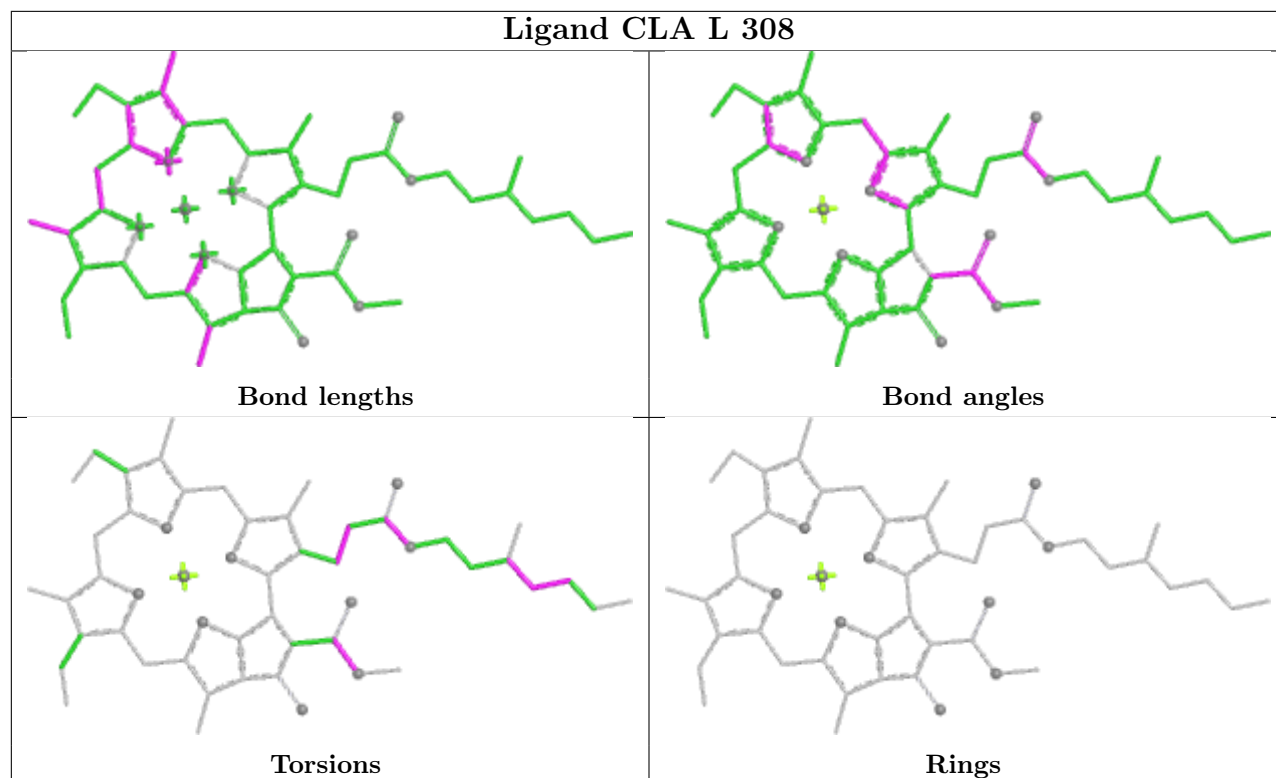


Torsions

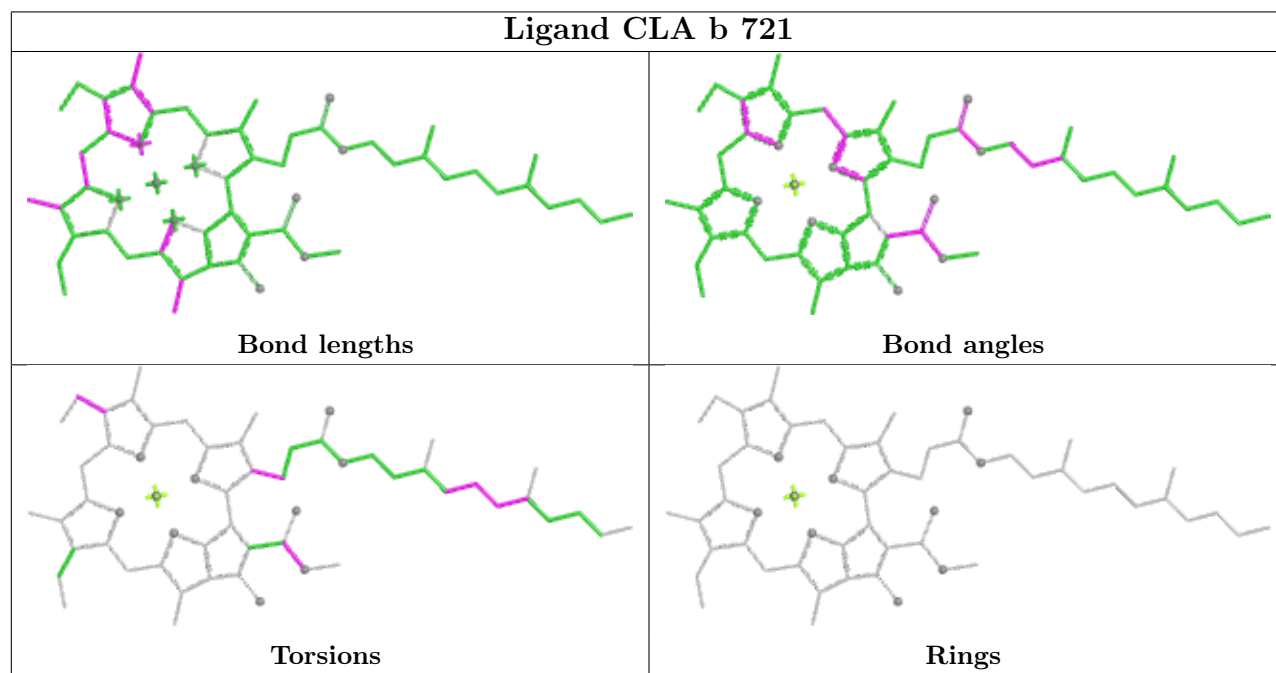


Rings

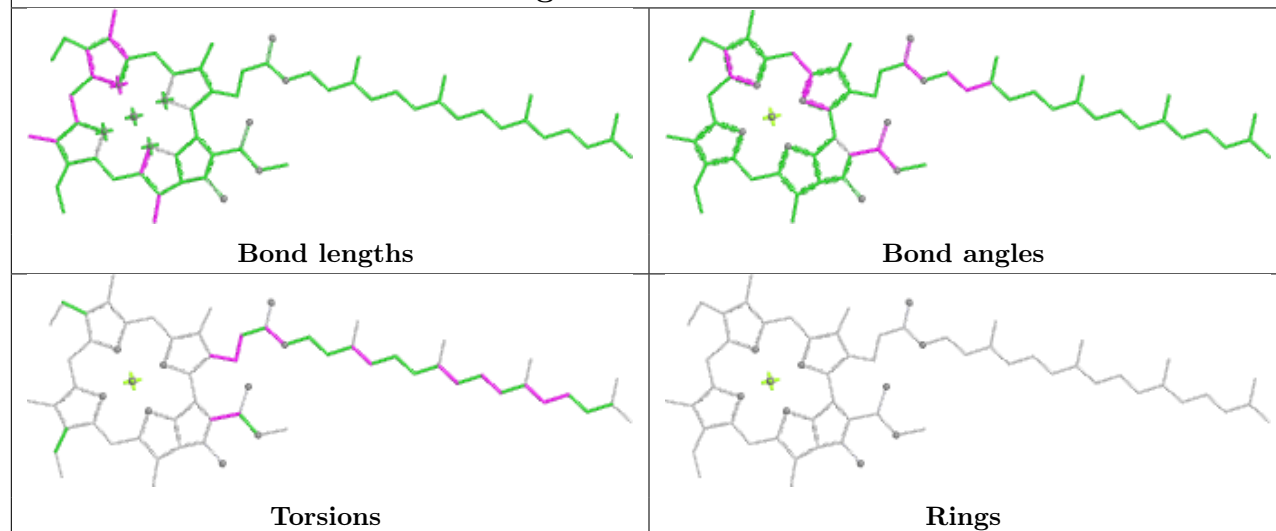
Ligand CLA L 308



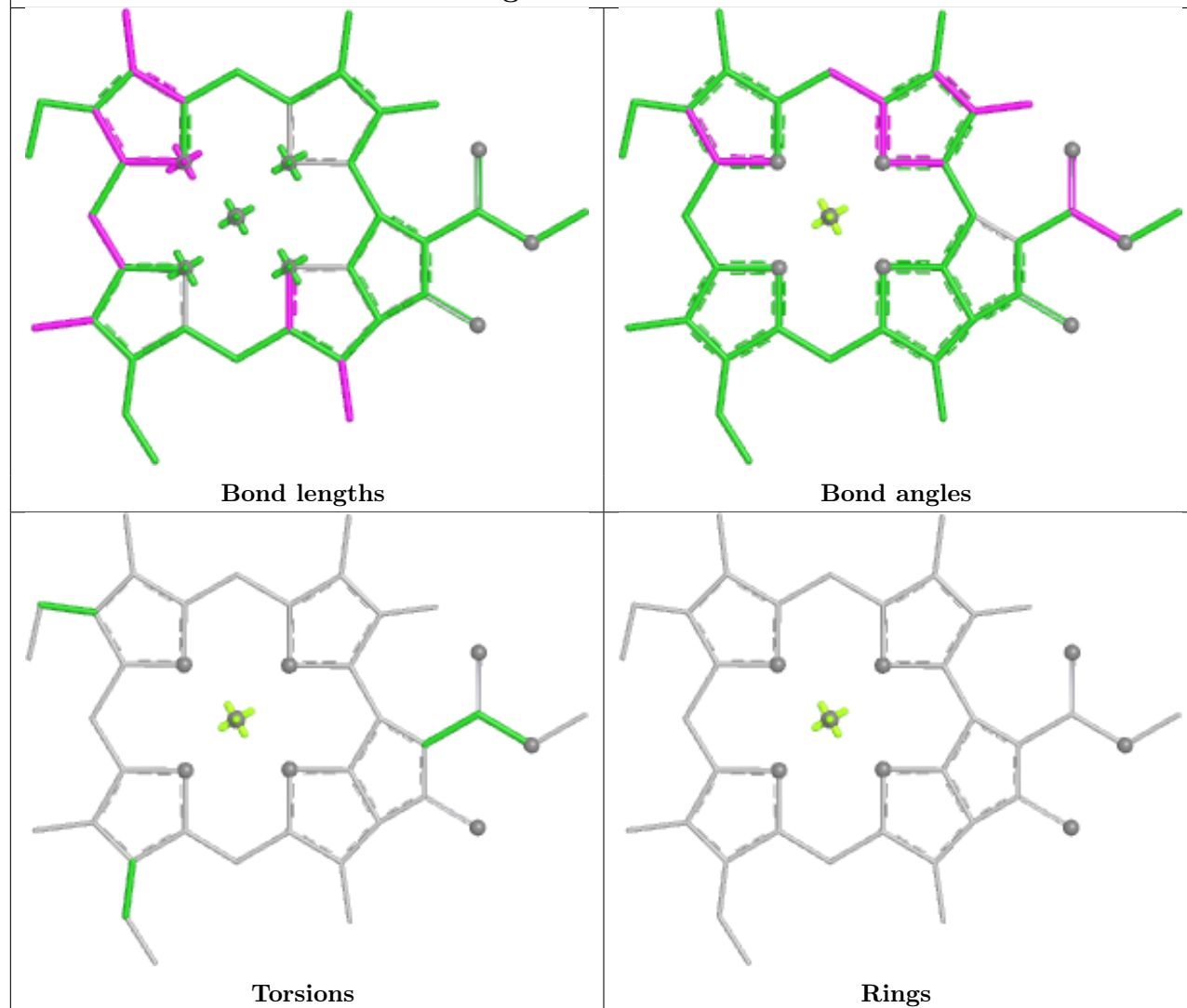
Ligand CLA b 721

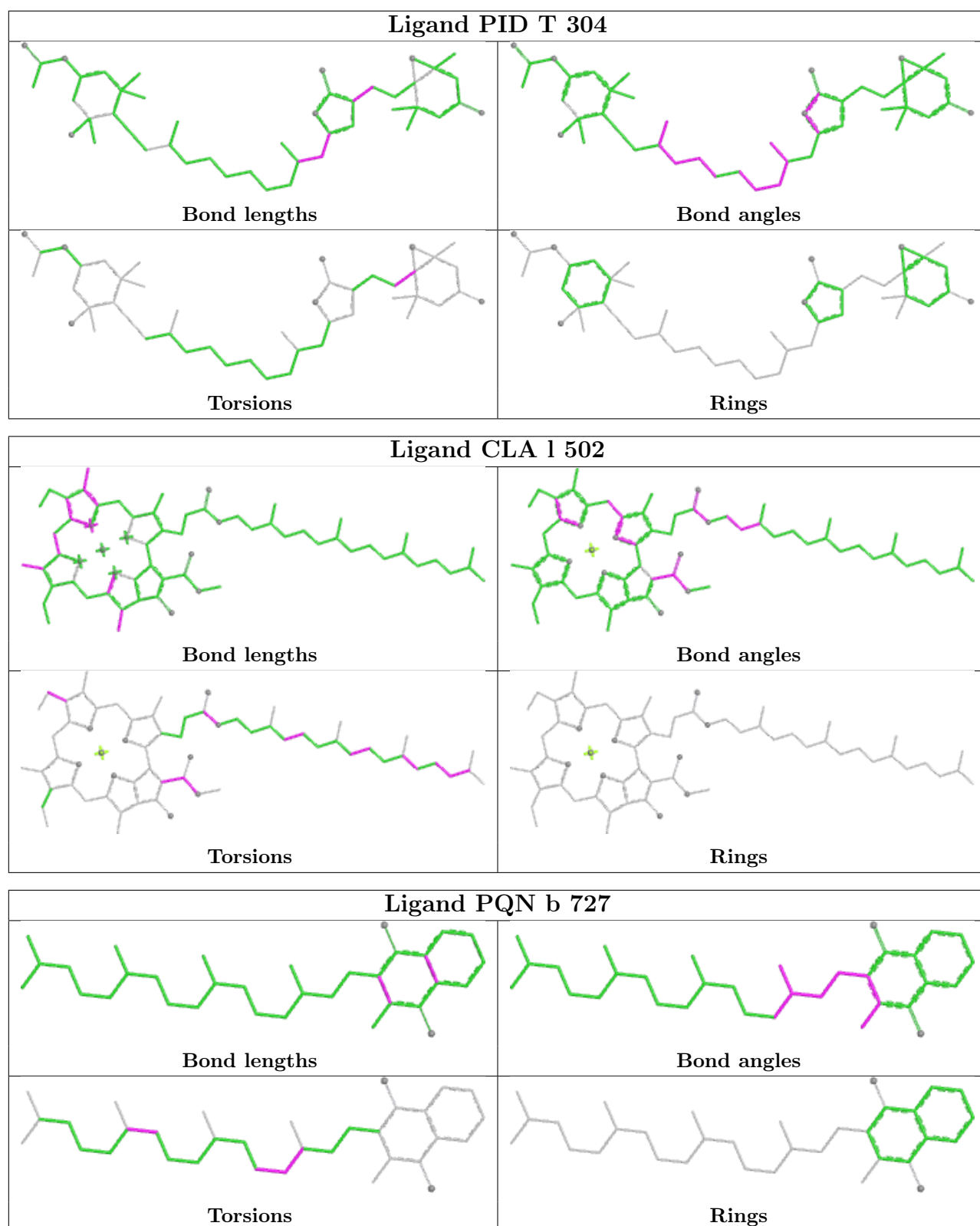


Ligand CLA a 809

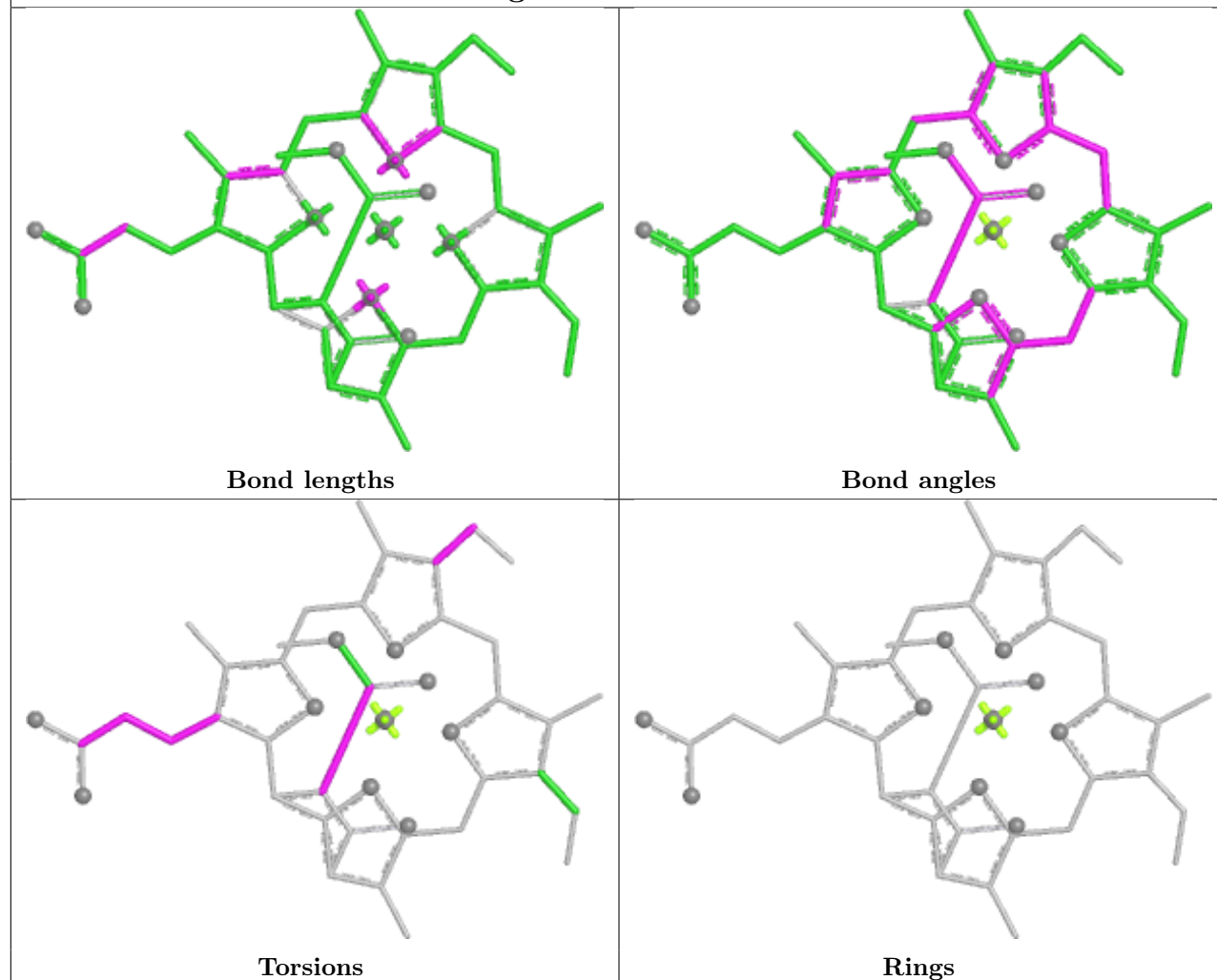


Ligand CLA l 508

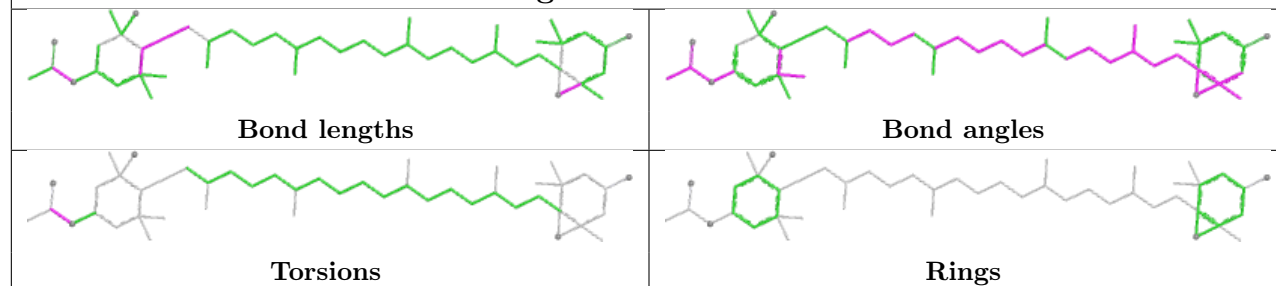




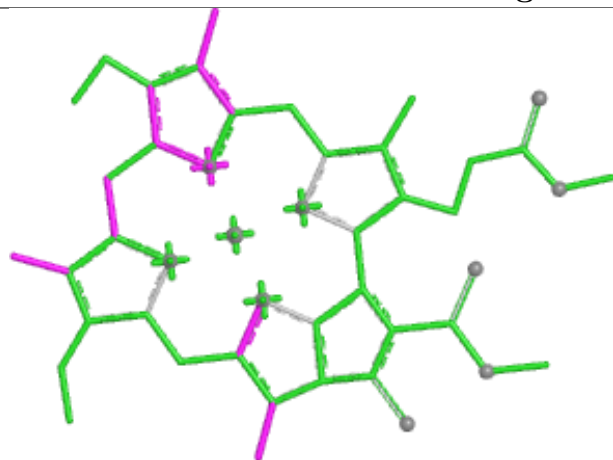
Ligand KC1 N 310



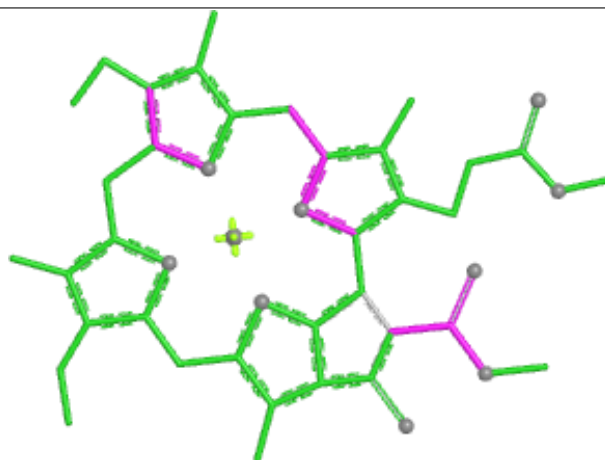
Ligand UIX E 304



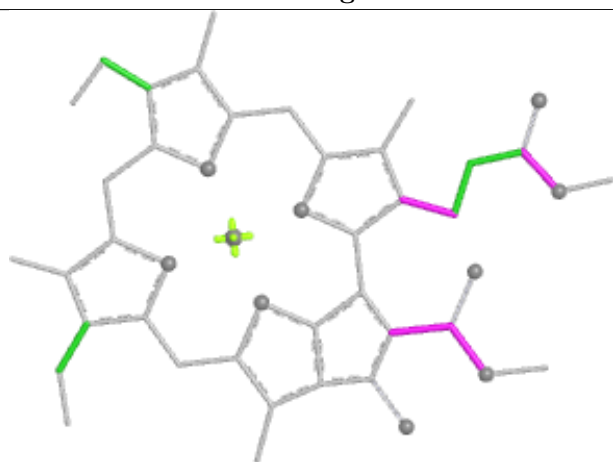
Ligand CLA F 310



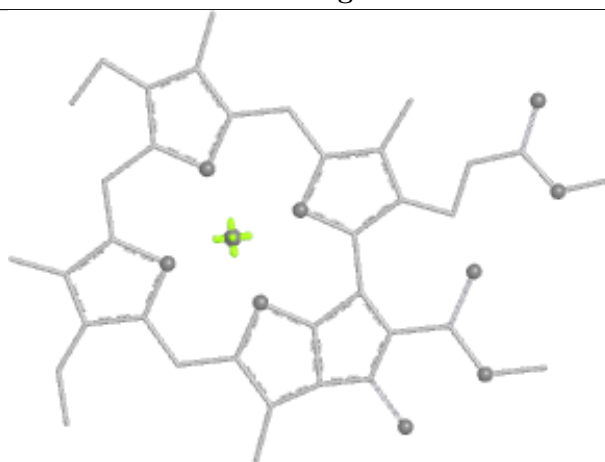
Bond lengths



Bond angles

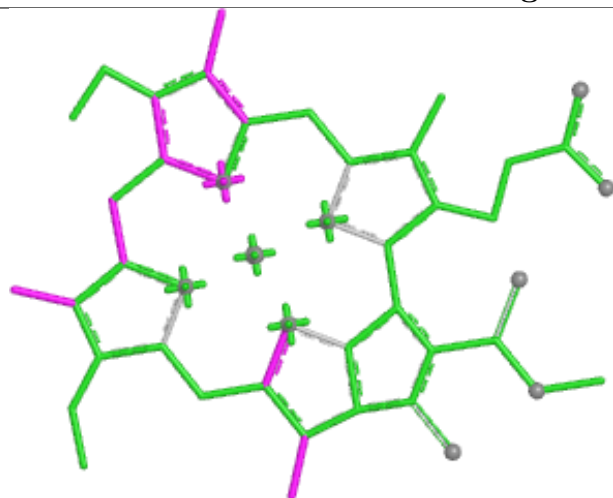


Torsions

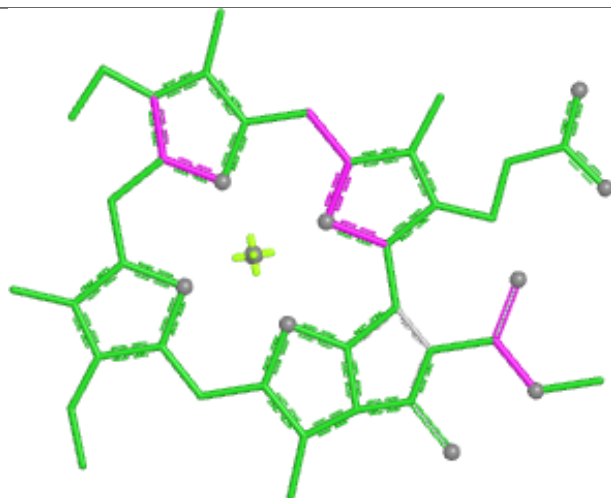


Rings

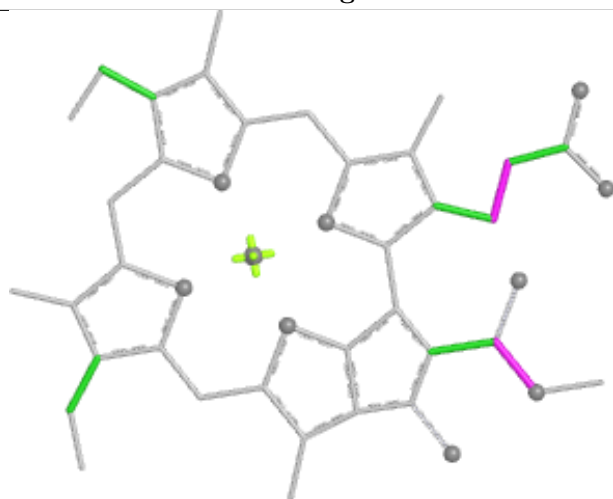
Ligand CLA I 201



Bond lengths



Bond angles

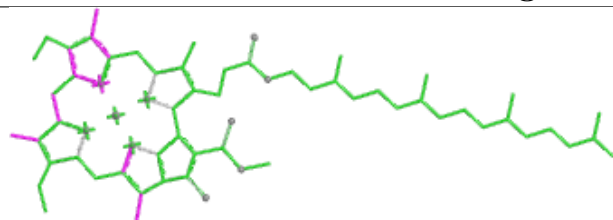


Torsions

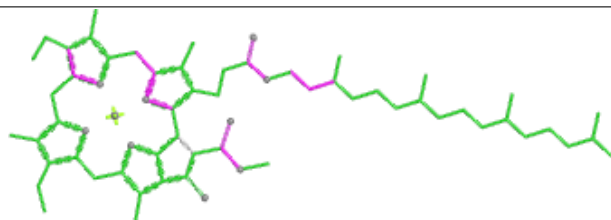


Rings

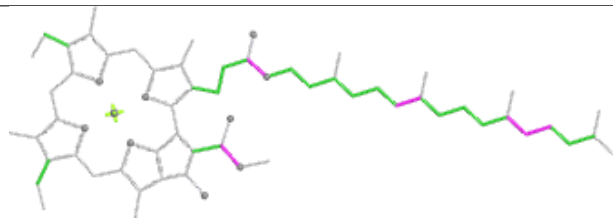
Ligand CLA a 824



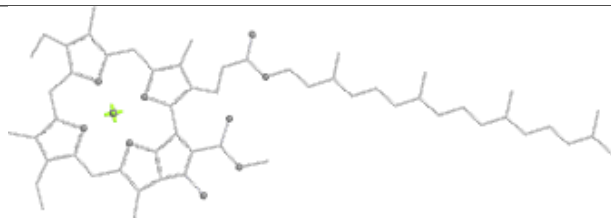
Bond lengths



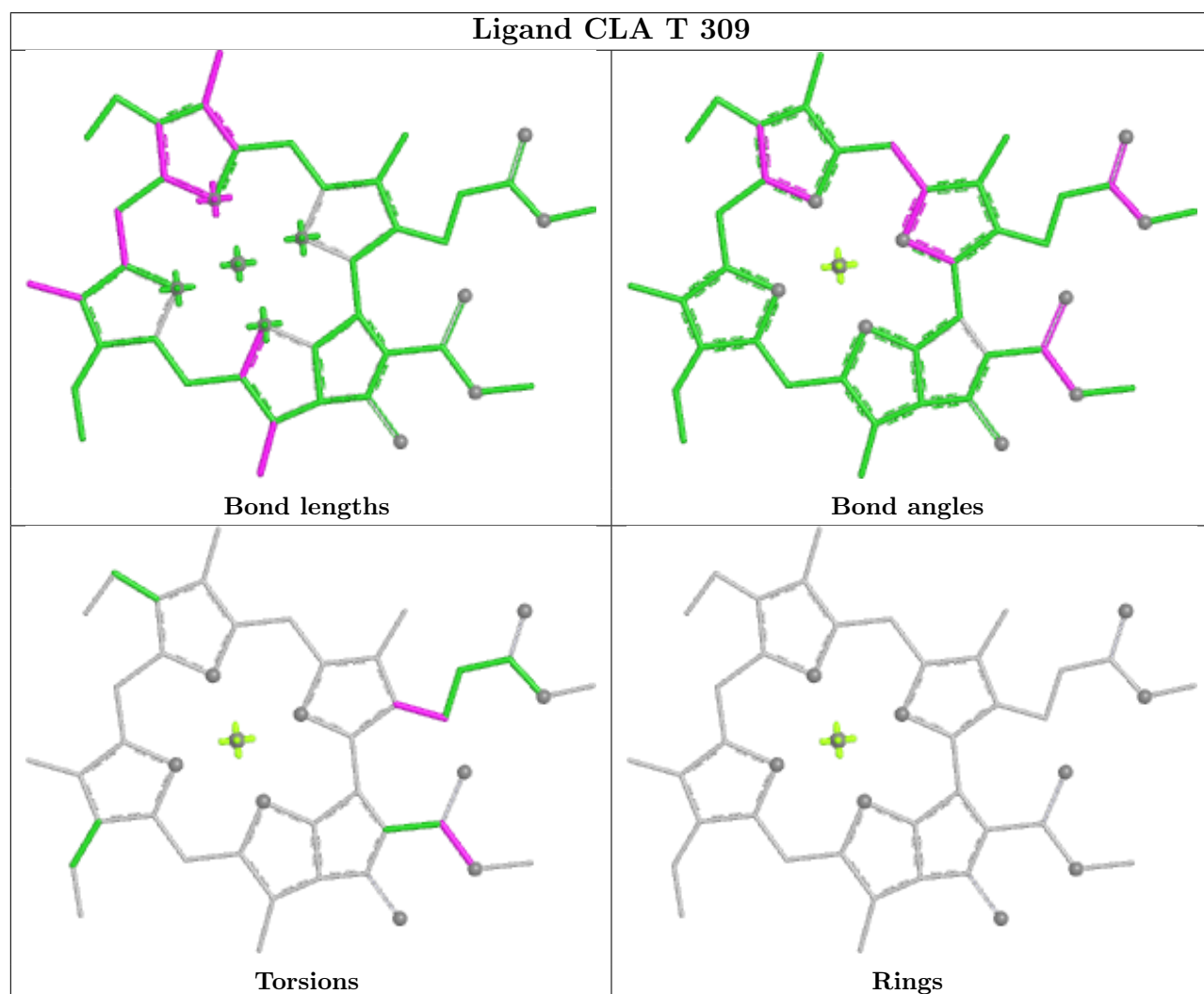
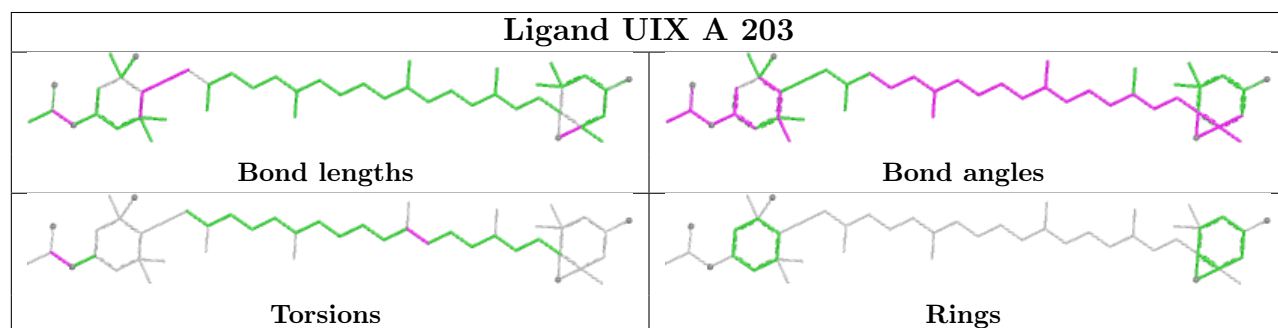
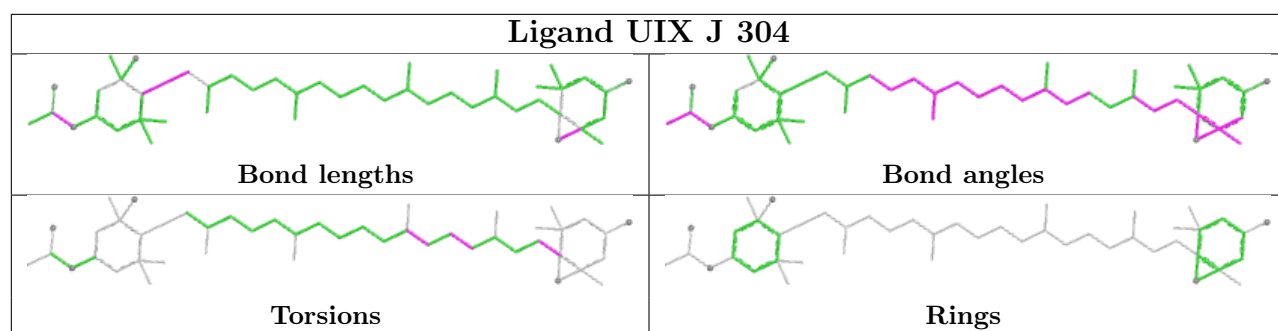
Bond angles



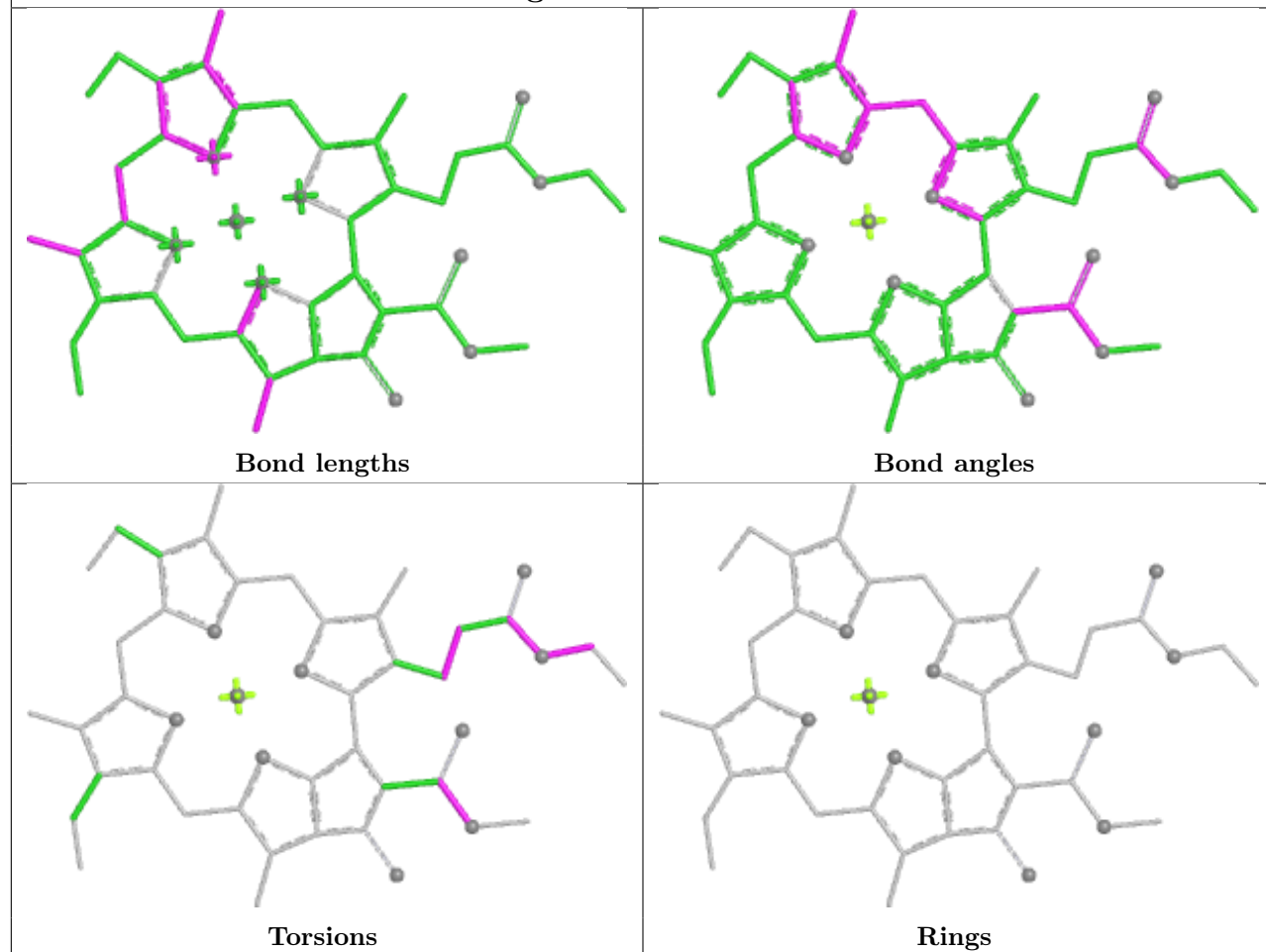
Torsions



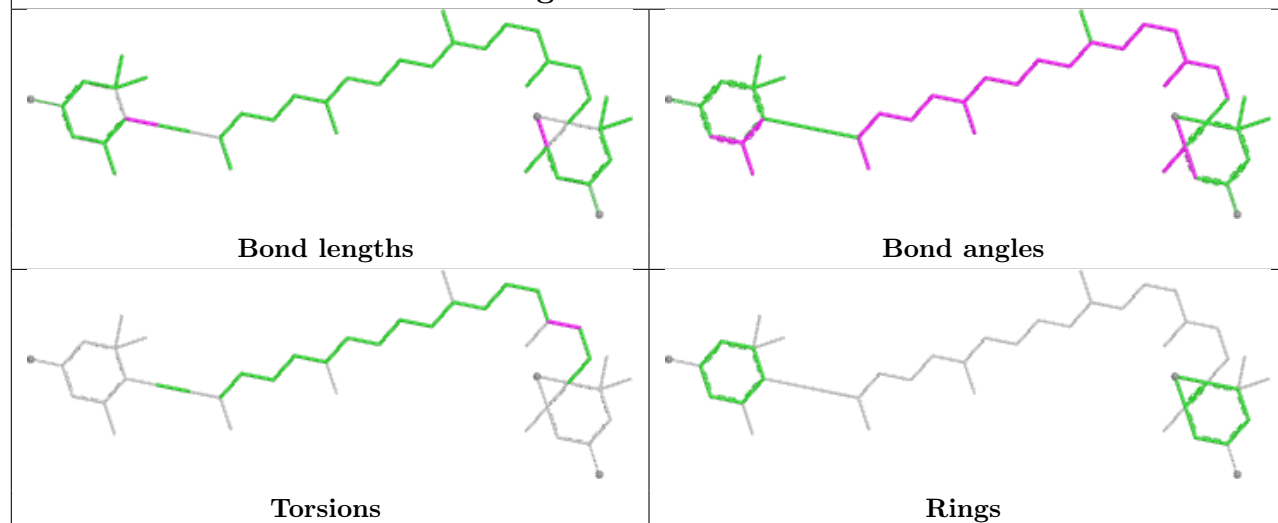
Rings

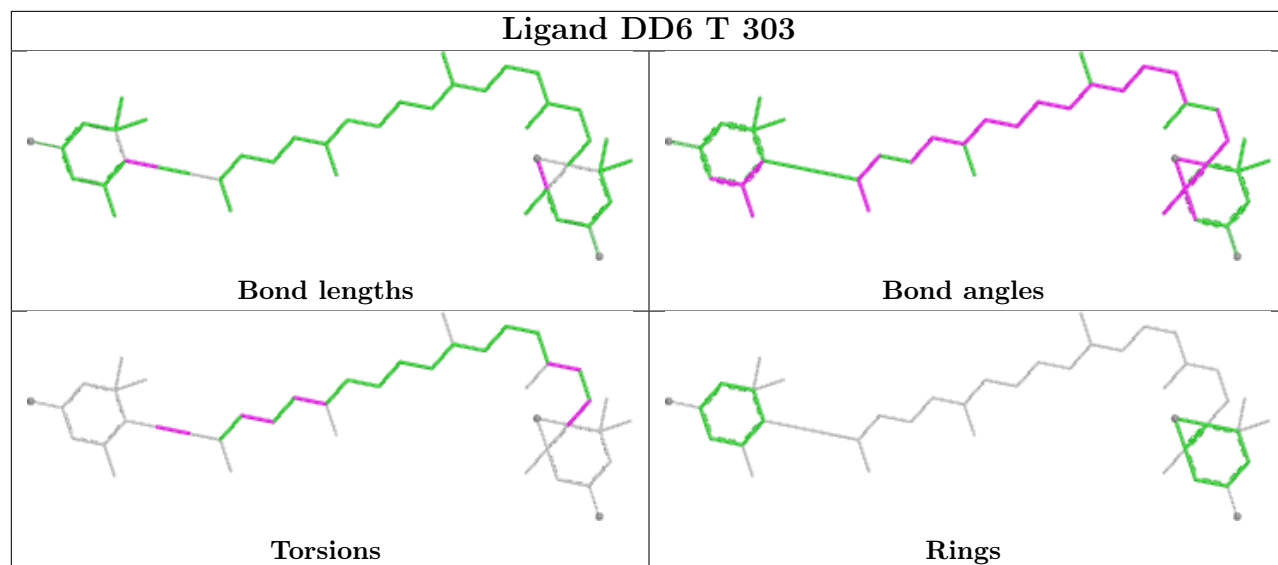
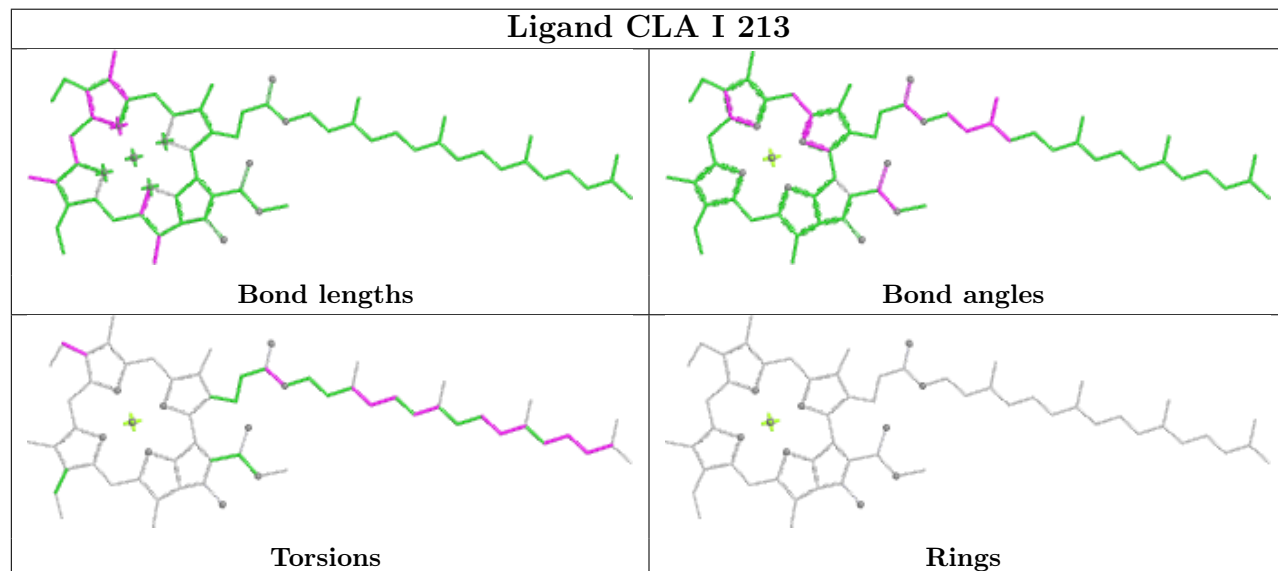


Ligand CLA O 314

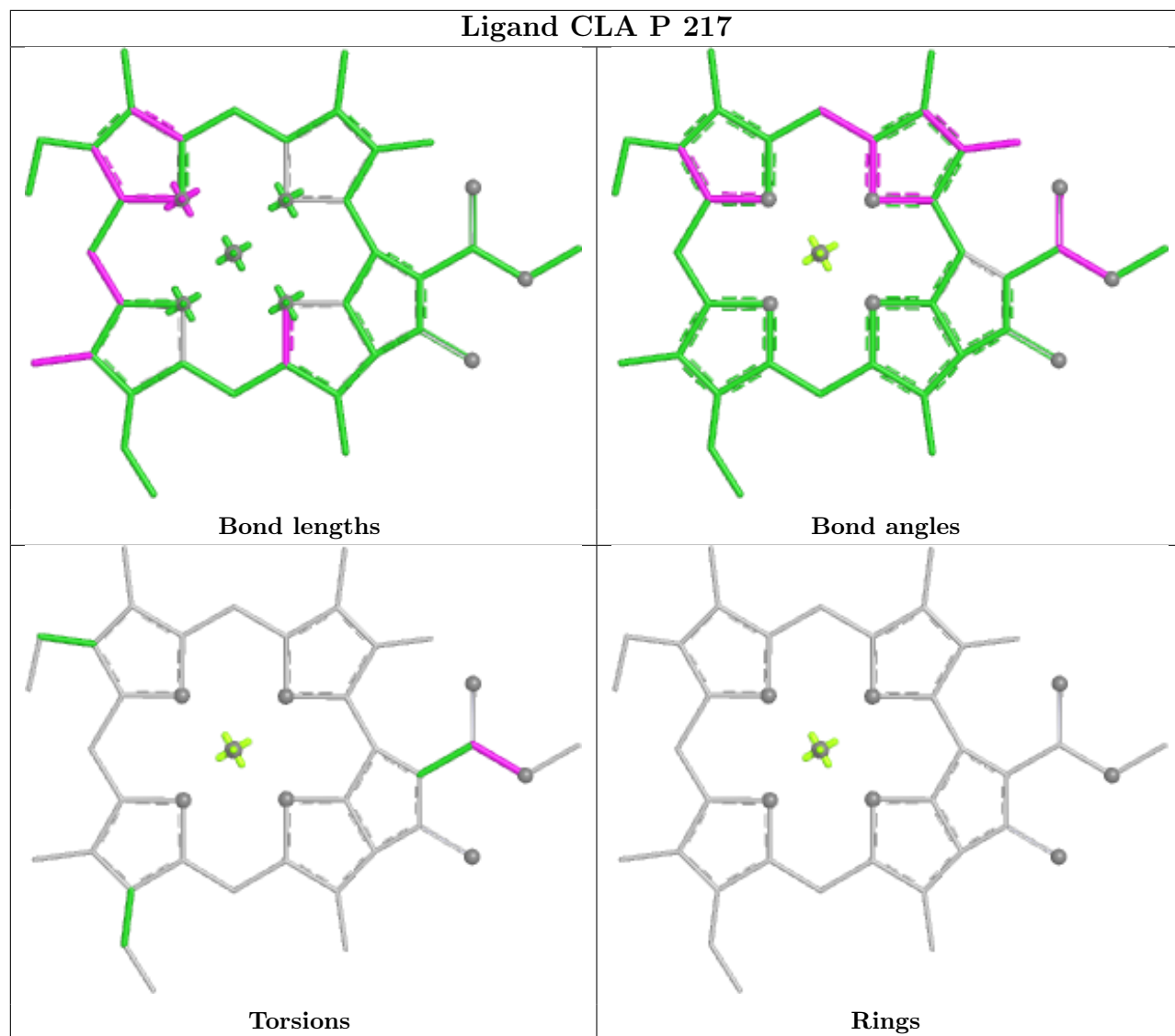


Ligand DD6 J 301

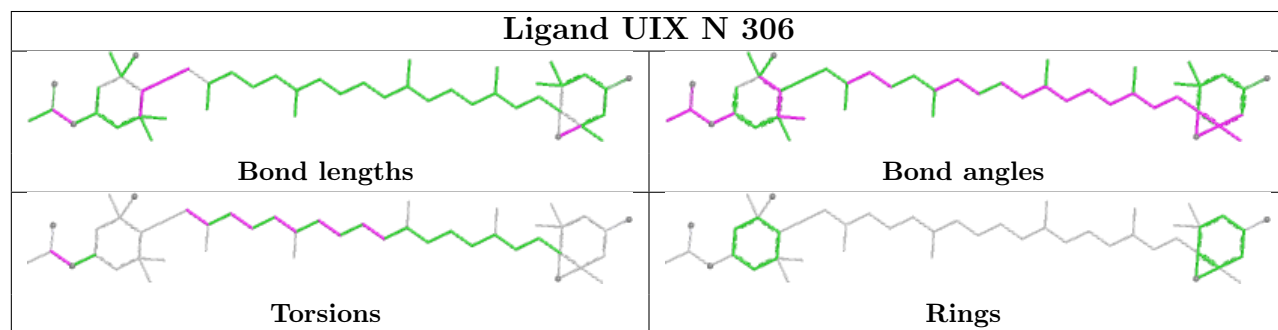


Ligand DD6 T 303**Ligand CLA I 213**

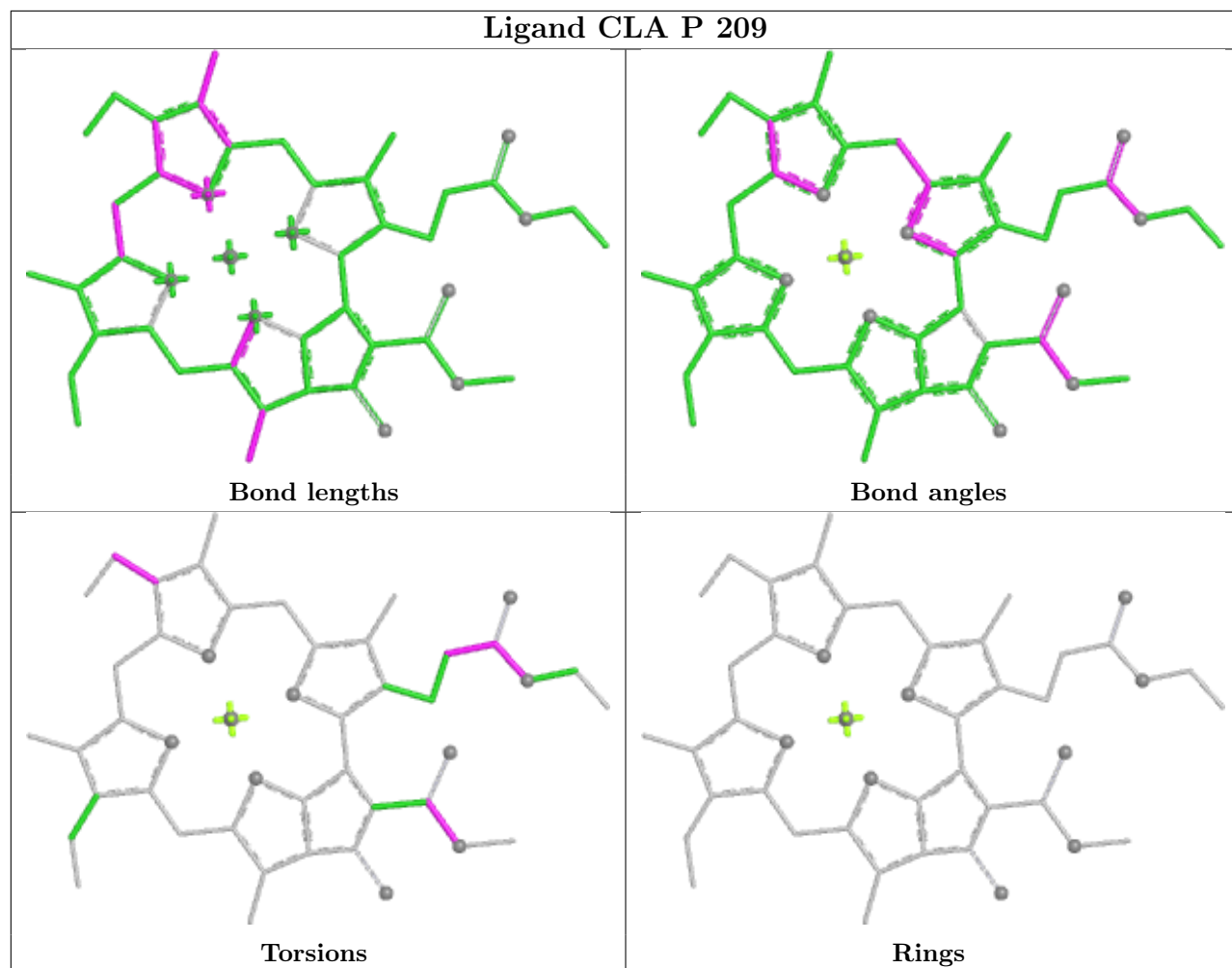
Ligand CLA P 217



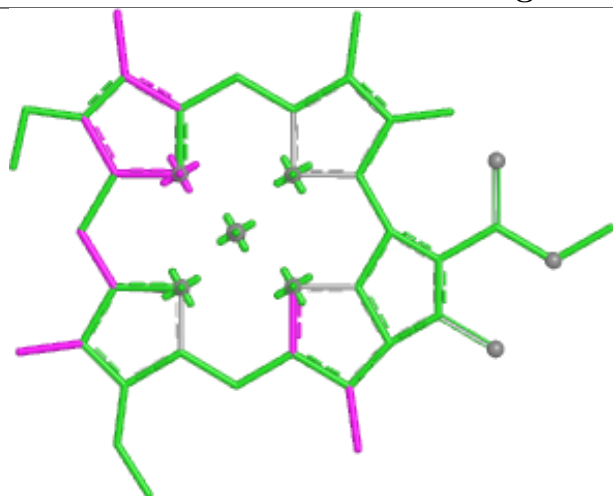
Ligand UIX N 306



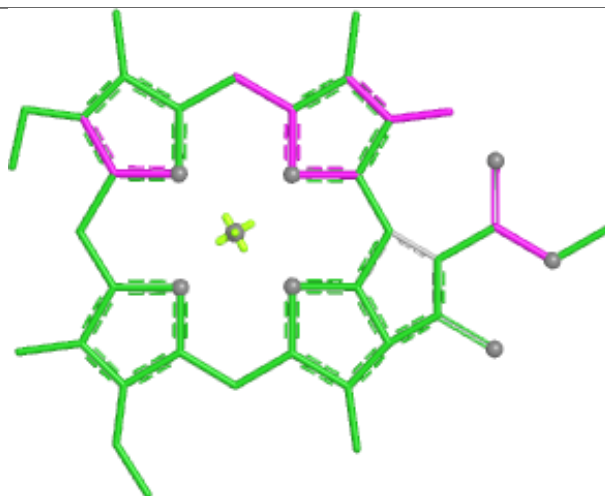
Ligand CLA P 209



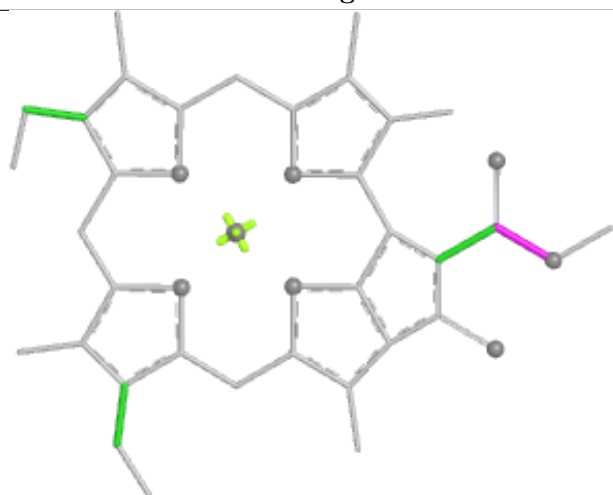
Ligand CLA F 316



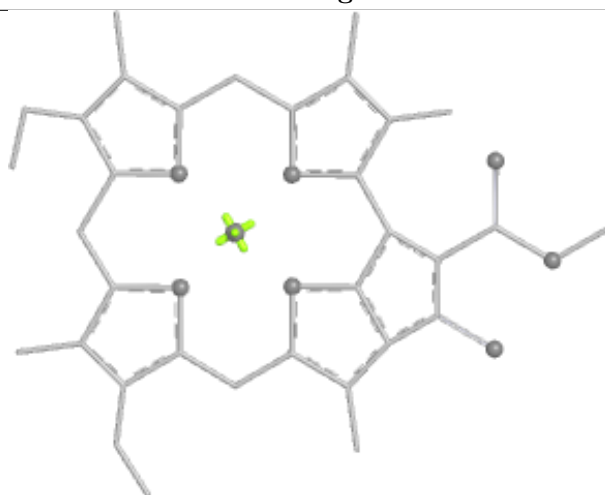
Bond lengths



Bond angles

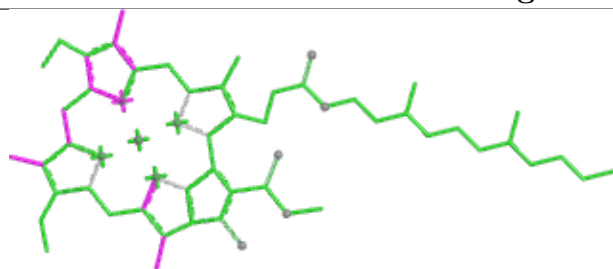


Torsions

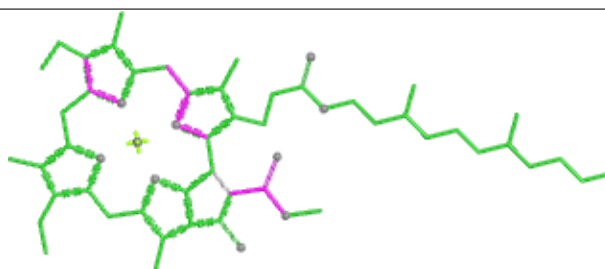


Rings

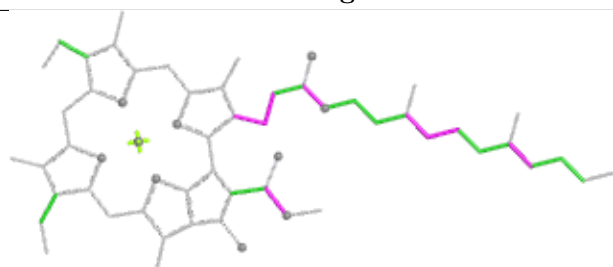
Ligand CLA b 711



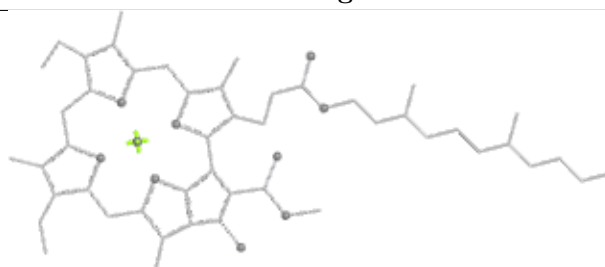
Bond lengths



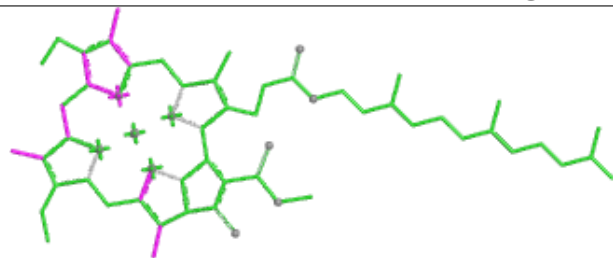
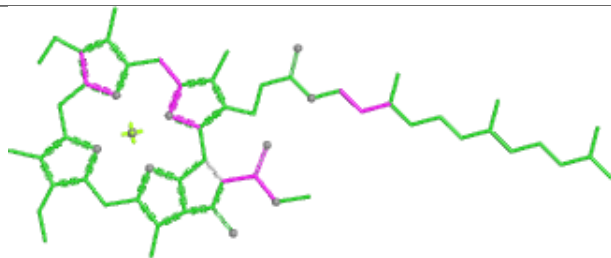
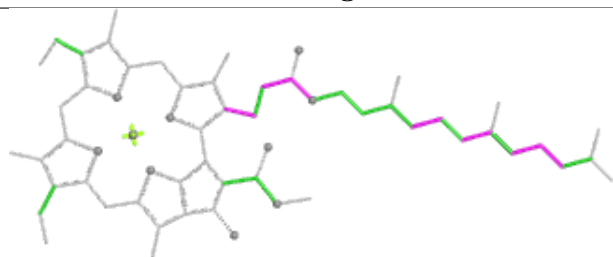
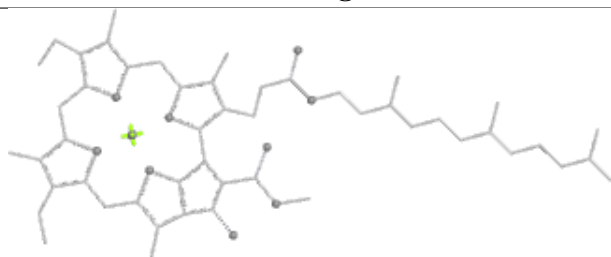
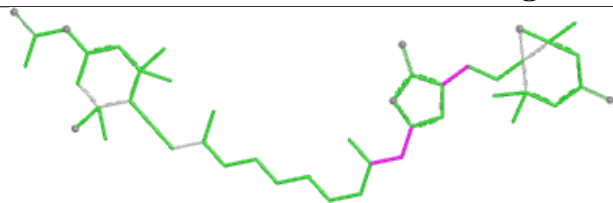
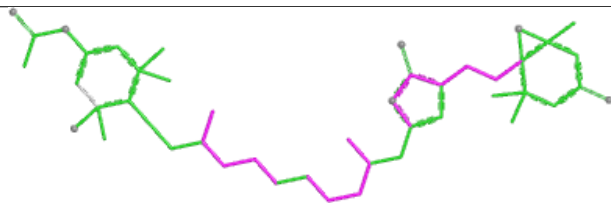
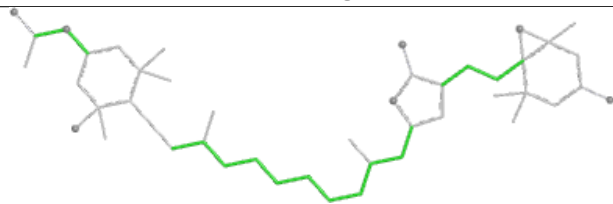
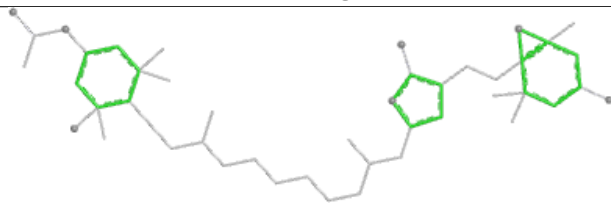
Bond angles



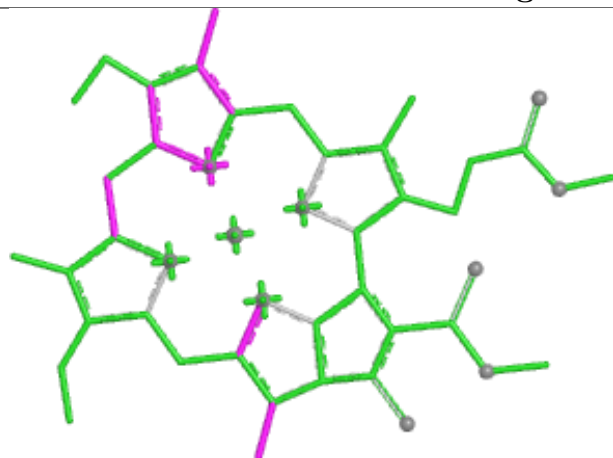
Torsions



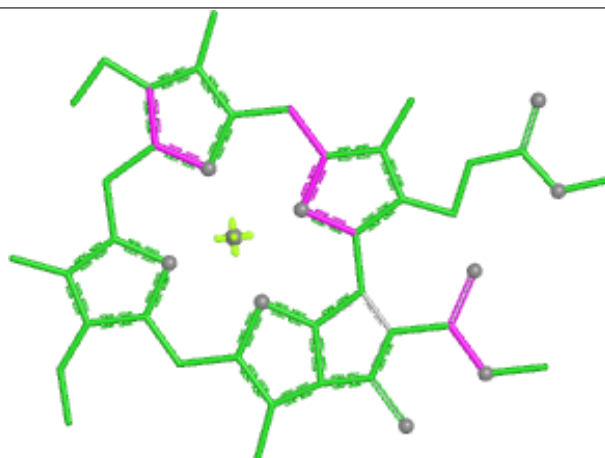
Rings

Ligand CLA 1 501**Bond lengths****Bond angles****Torsions****Rings****Ligand PID F 306****Bond lengths****Bond angles****Torsions****Rings**

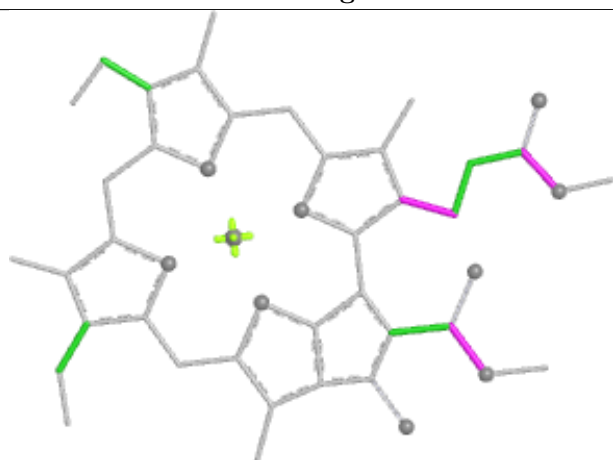
Ligand CLA L 311



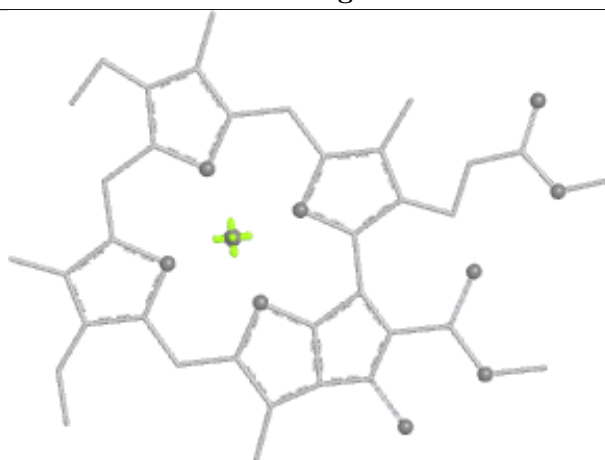
Bond lengths



Bond angles

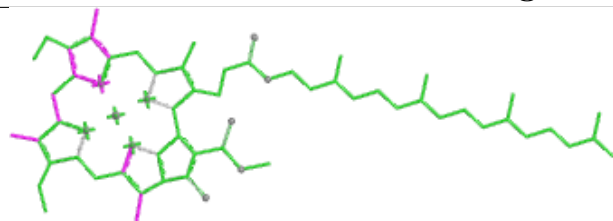


Torsions

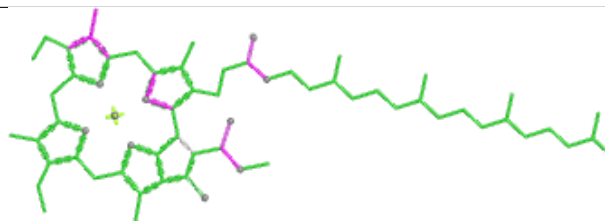


Rings

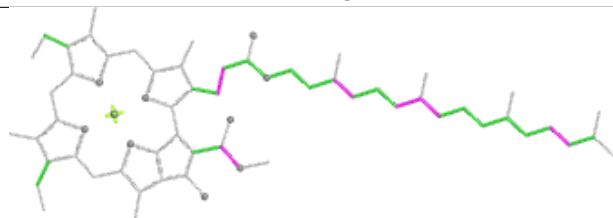
Ligand CLA a 803



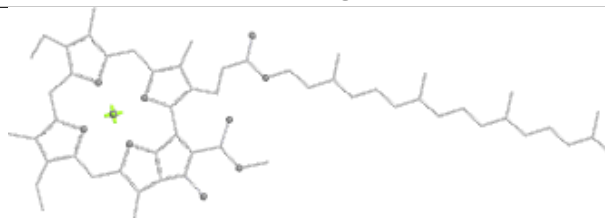
Bond lengths



Bond angles

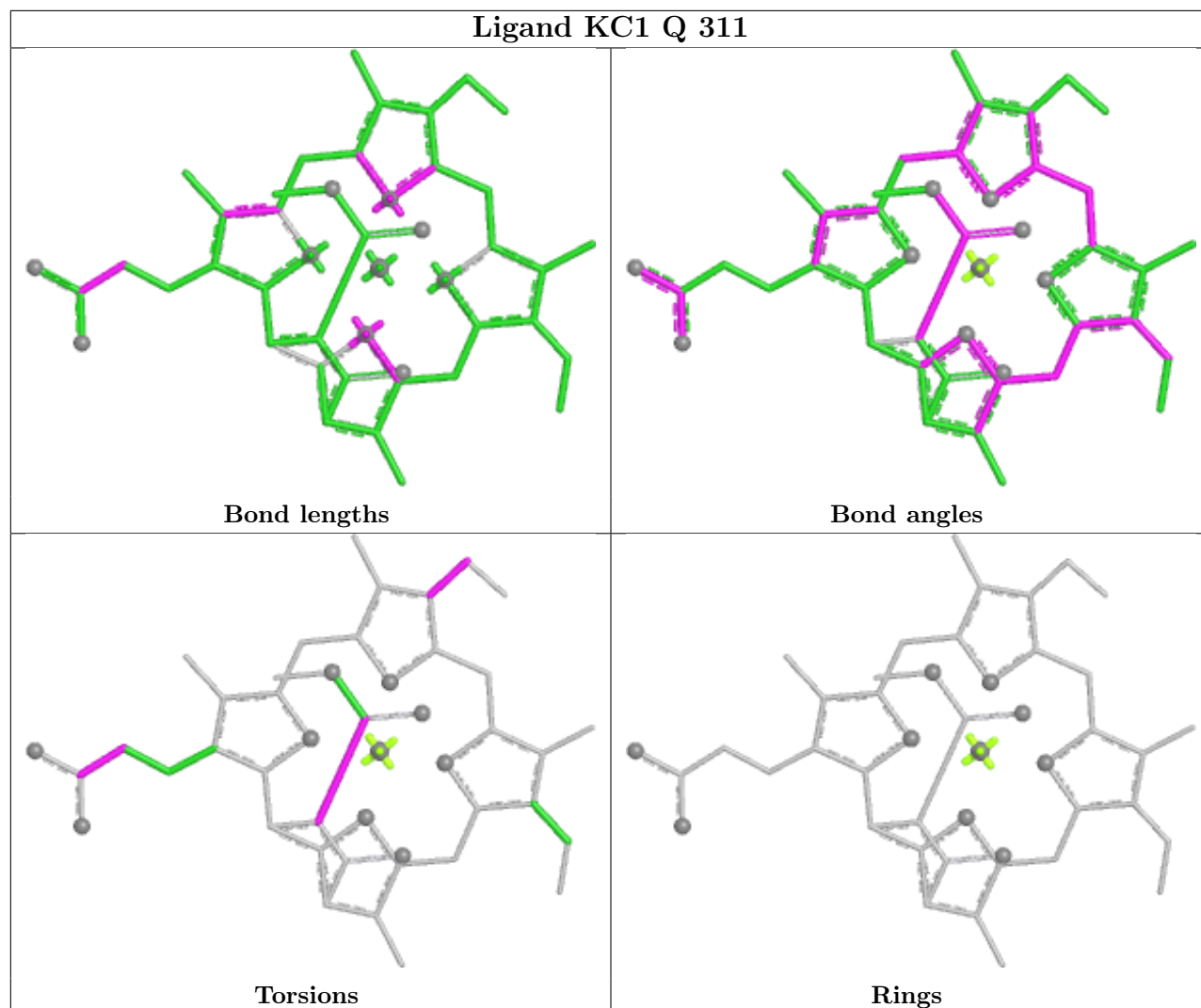


Torsions

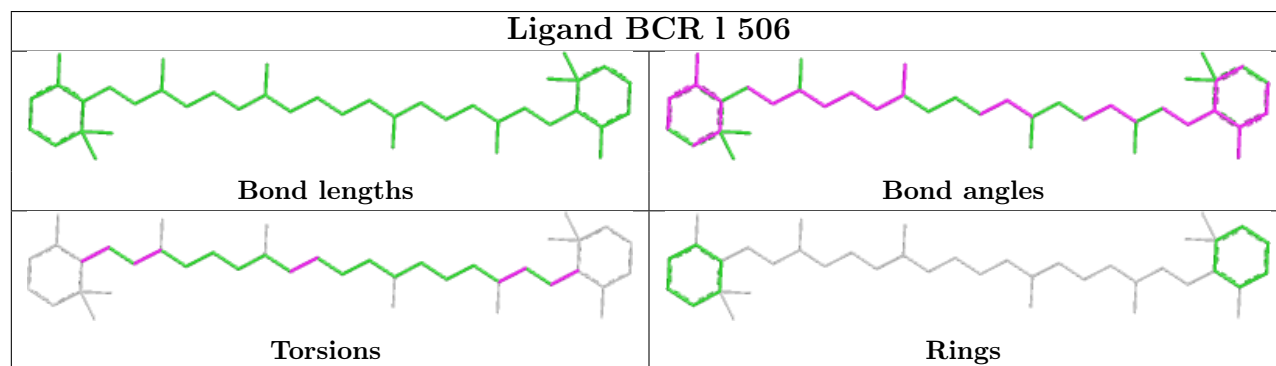


Rings

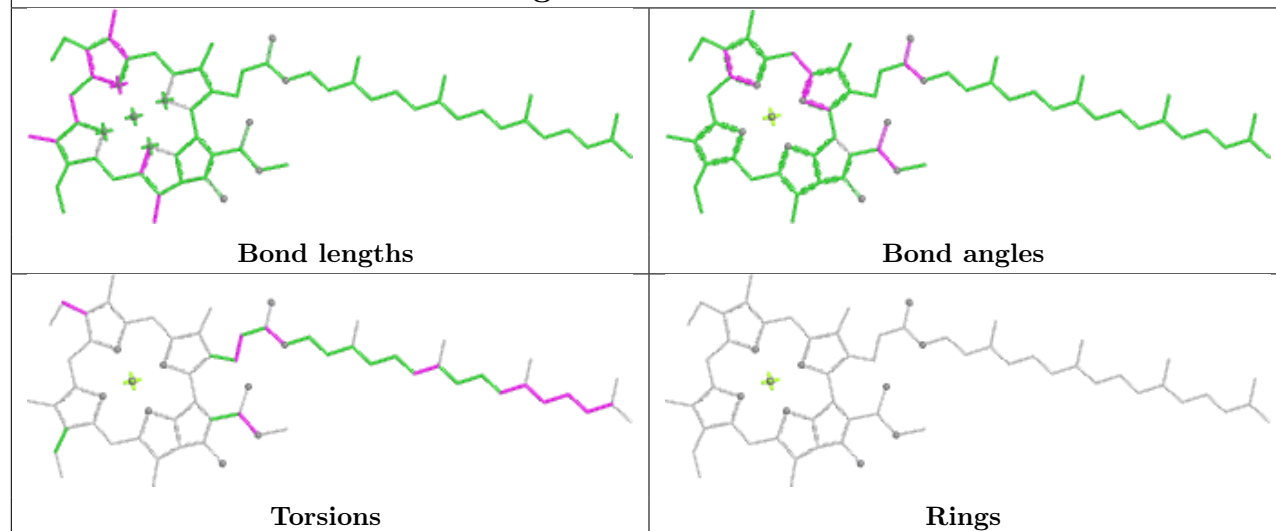
Ligand KC1 Q 311



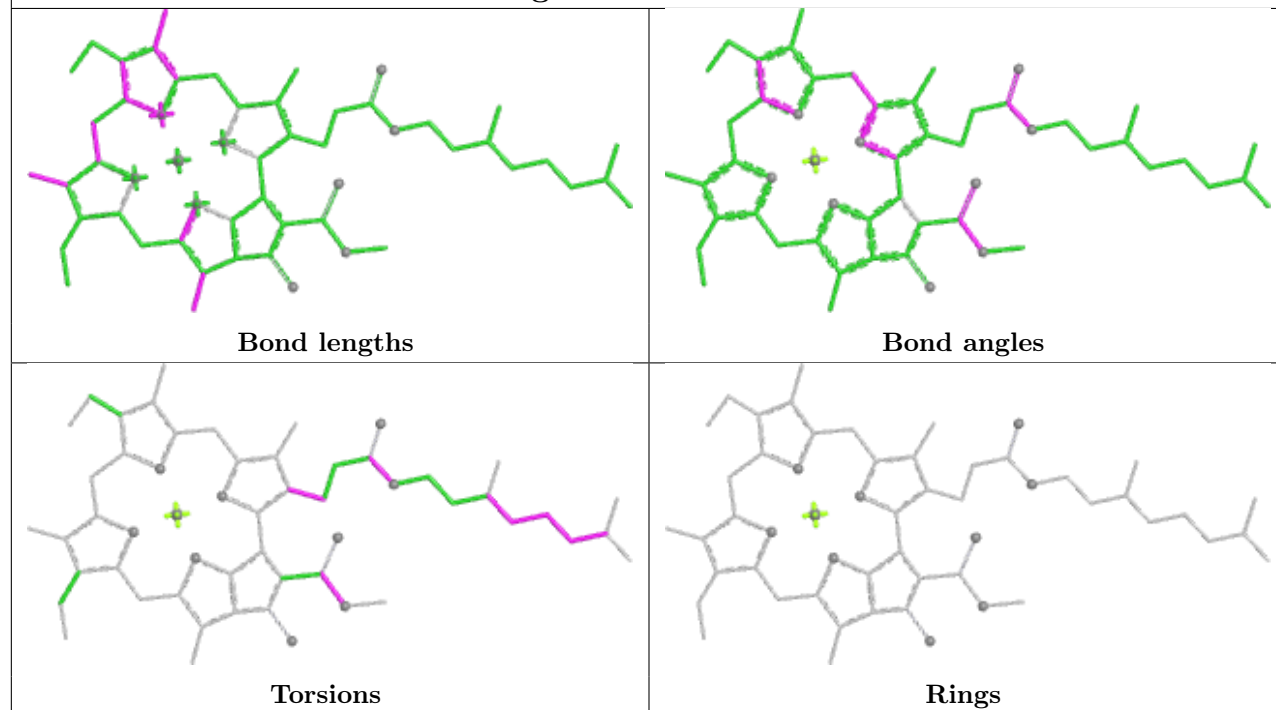
Ligand BCR 1 506



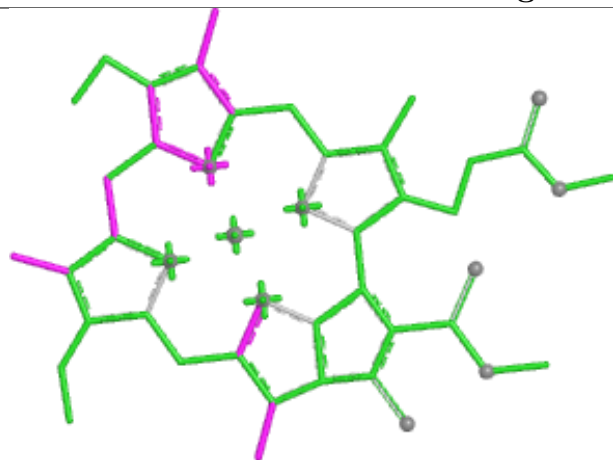
Ligand CLA E 306



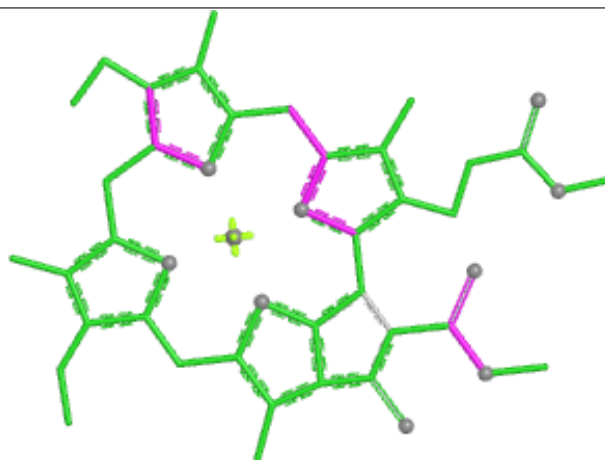
Ligand CLA A 212



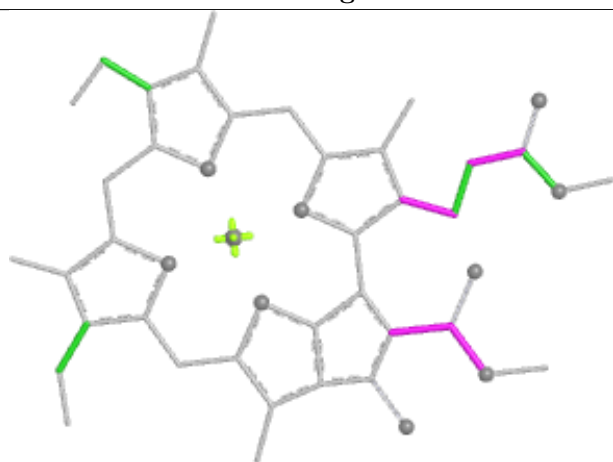
Ligand CLA b 710



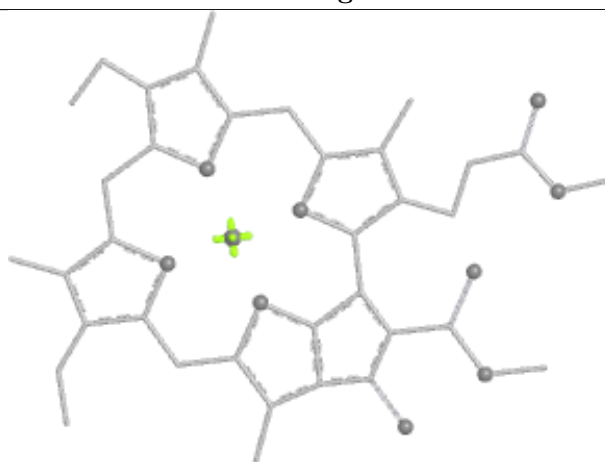
Bond lengths



Bond angles

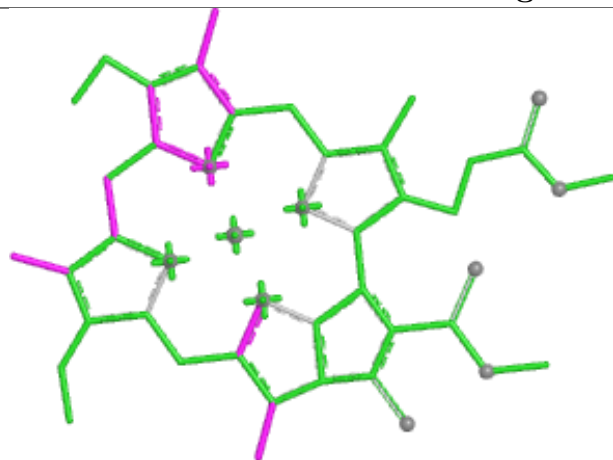


Torsions

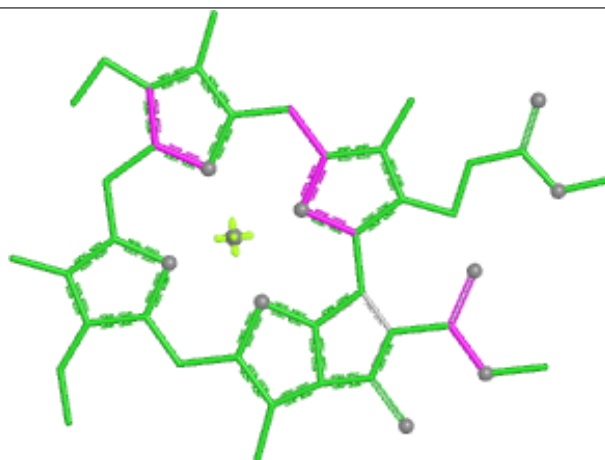


Rings

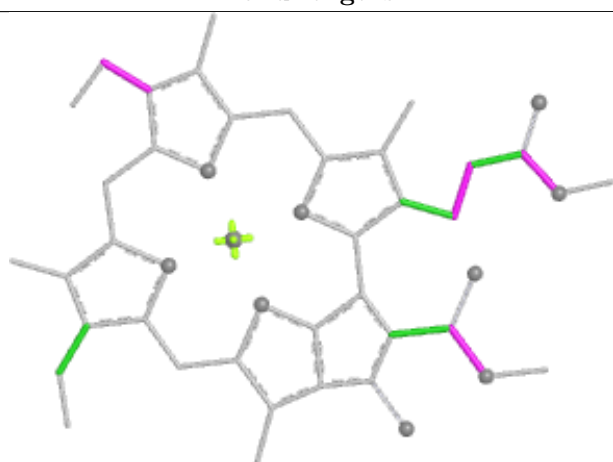
Ligand CLA L 317



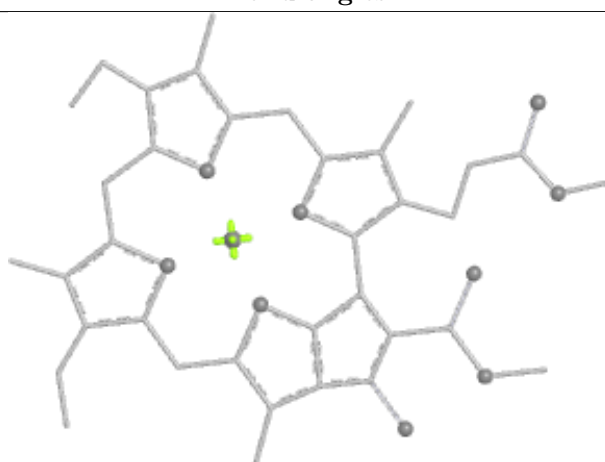
Bond lengths



Bond angles

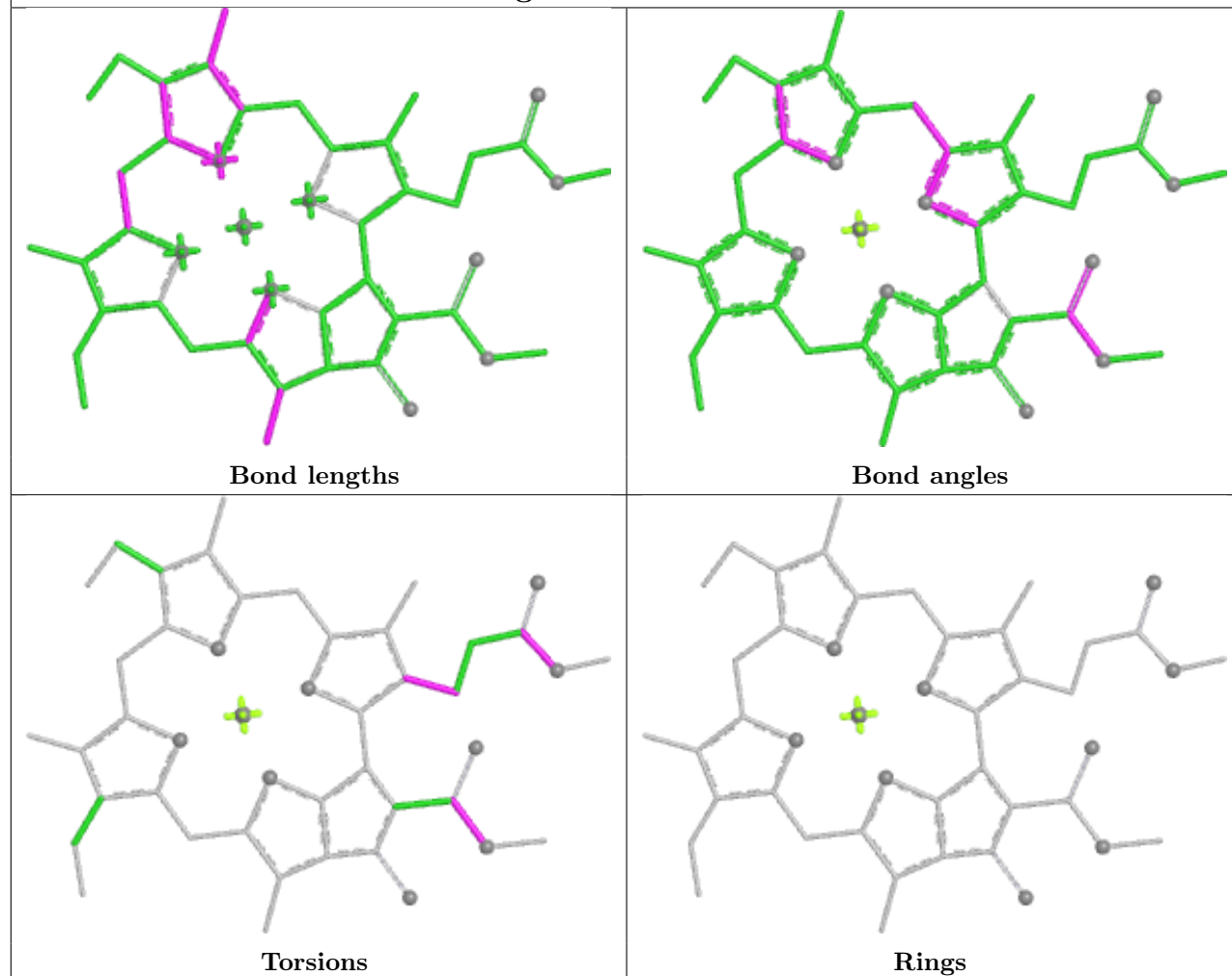


Torsions

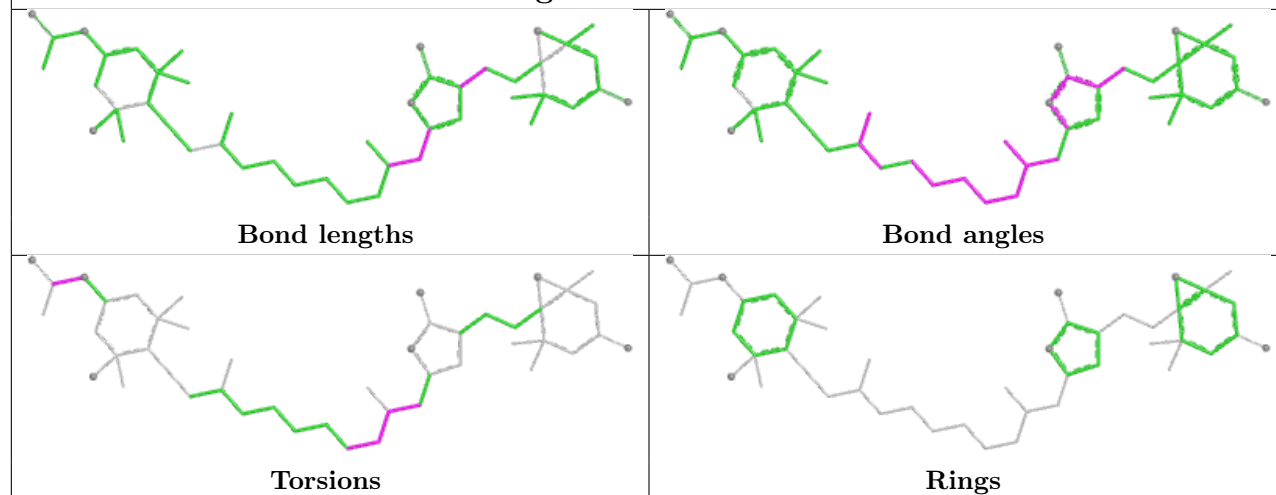


Rings

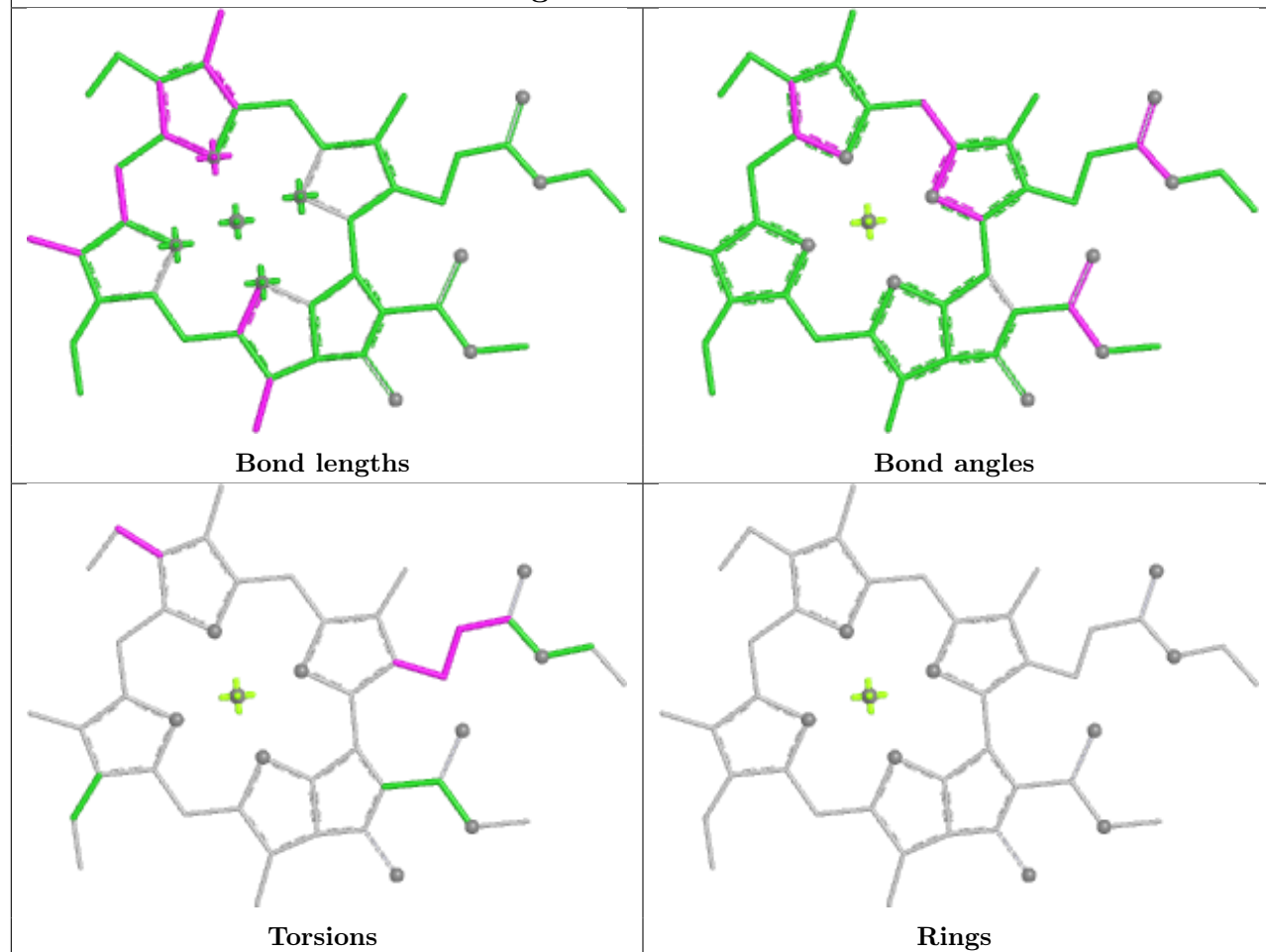
Ligand CLA F 312



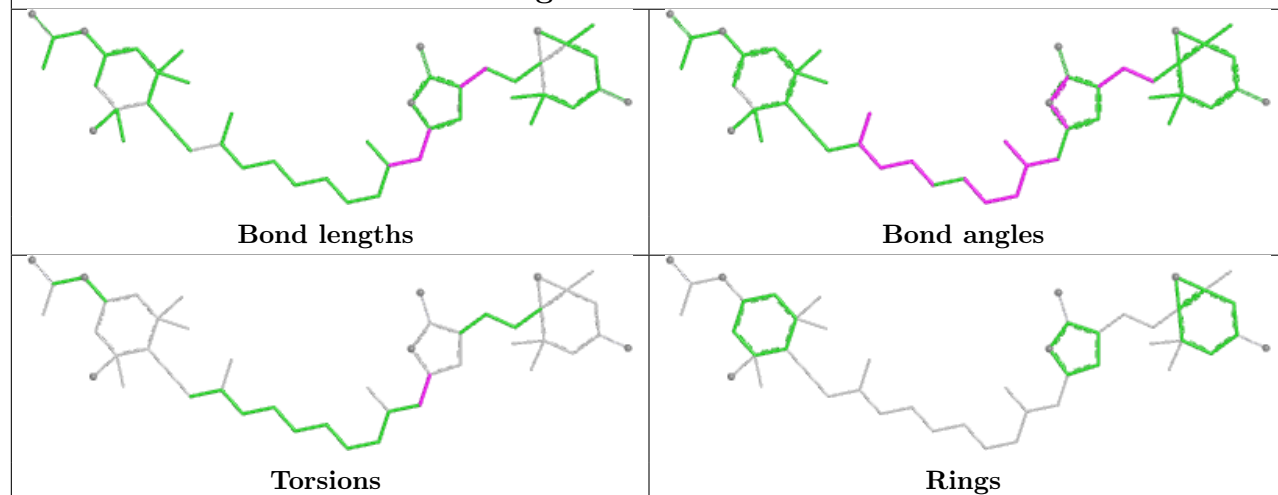
Ligand PID G 303

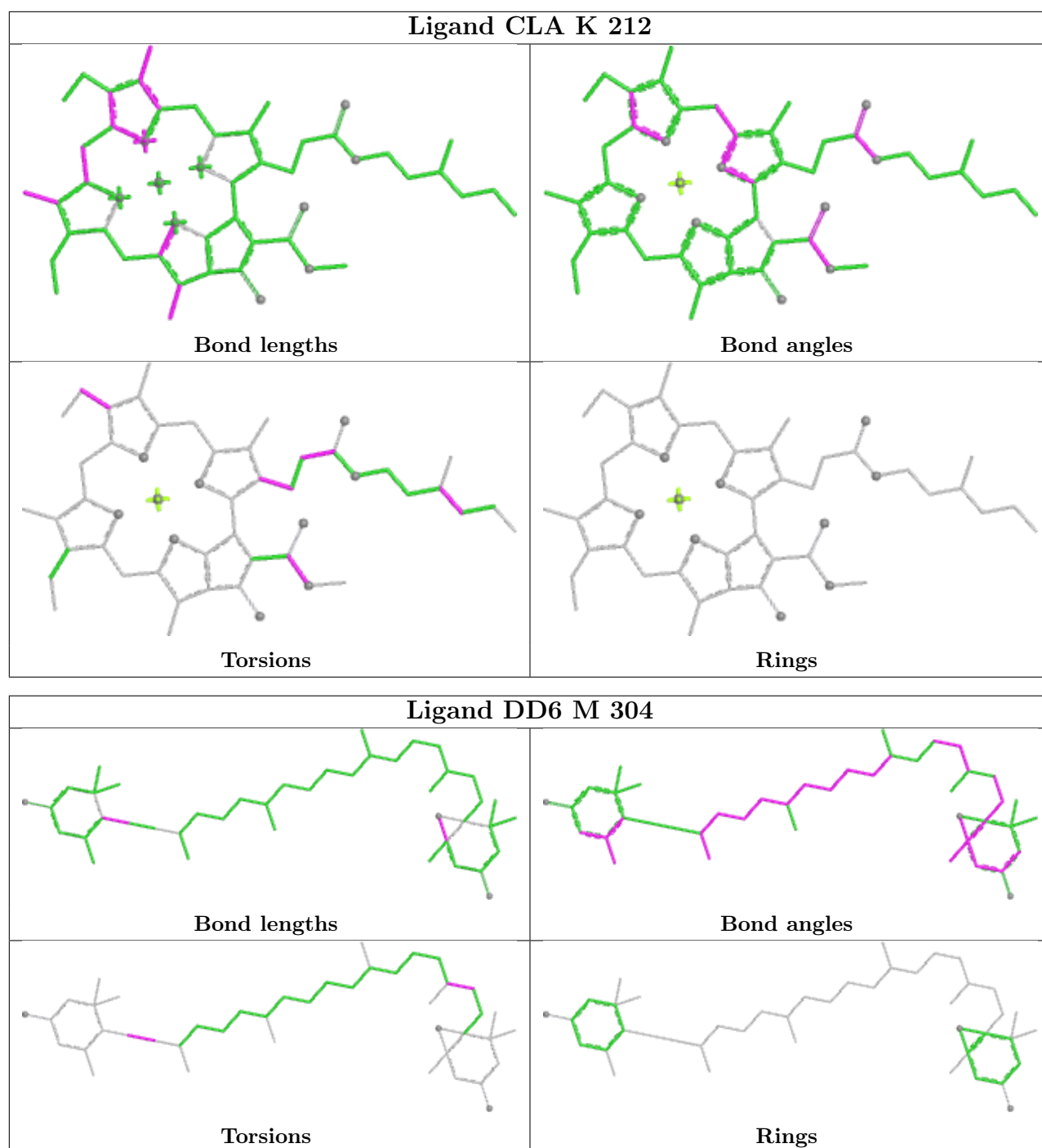


Ligand CLA a 818

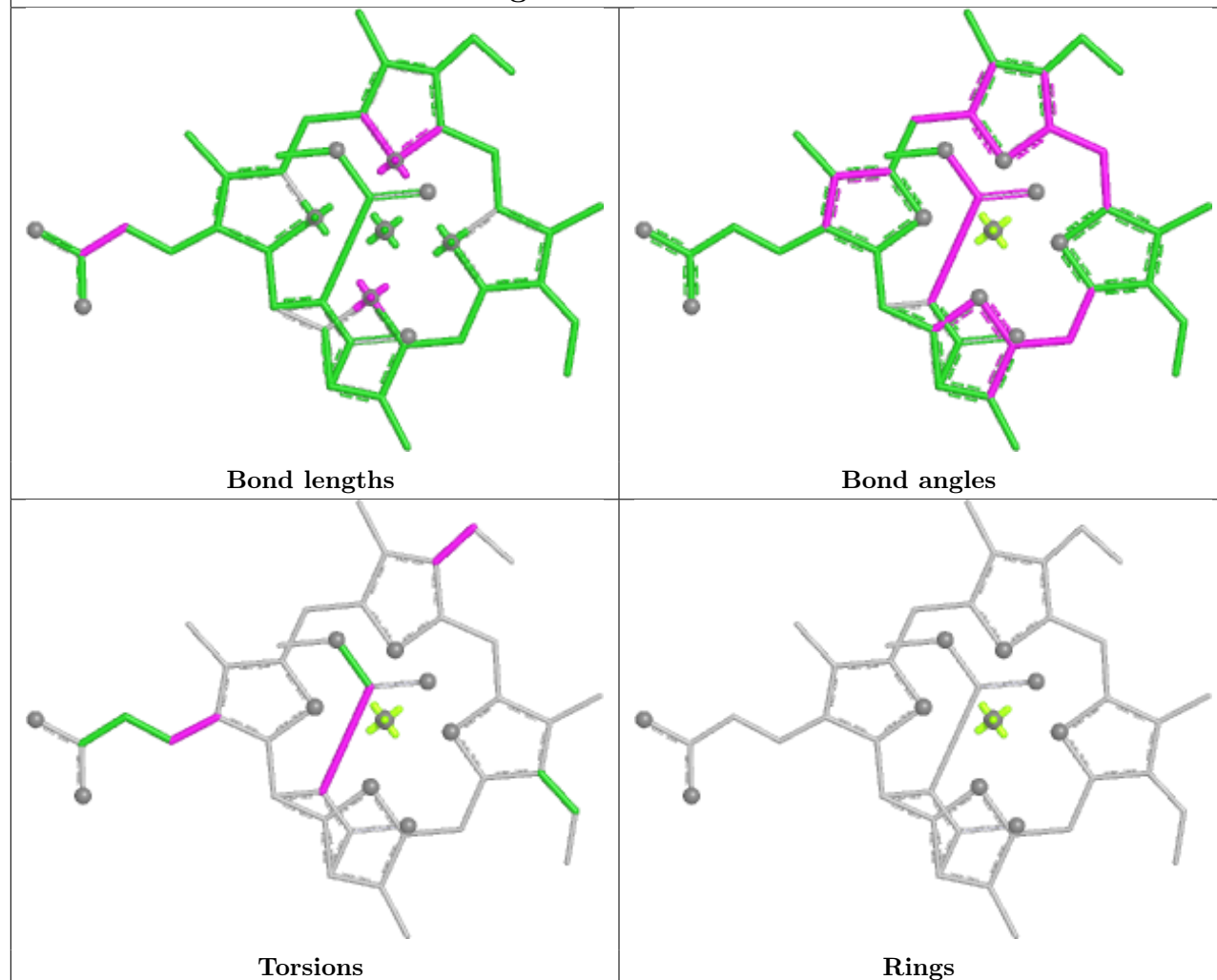


Ligand PID N 304

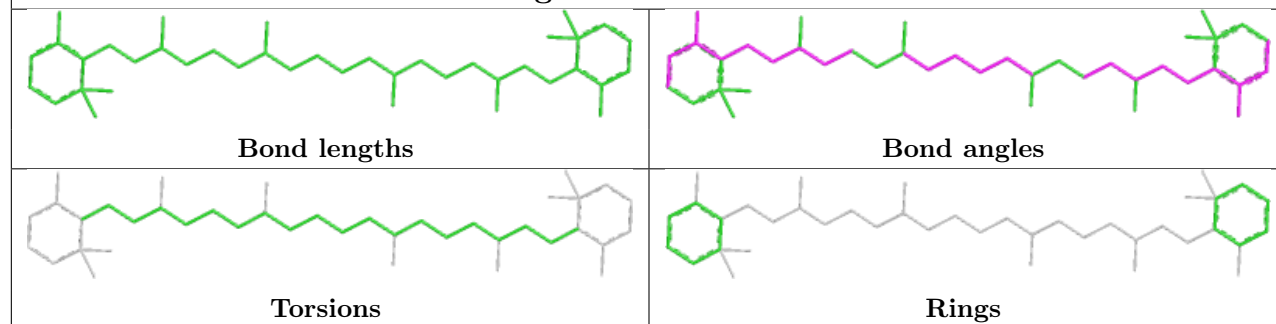




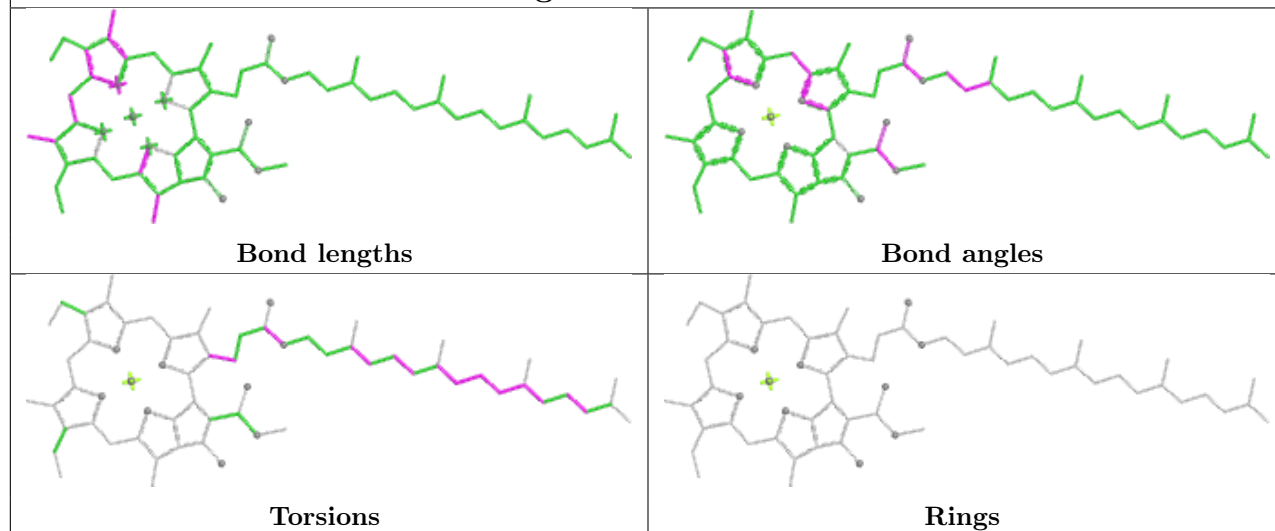
Ligand KC1 T 310



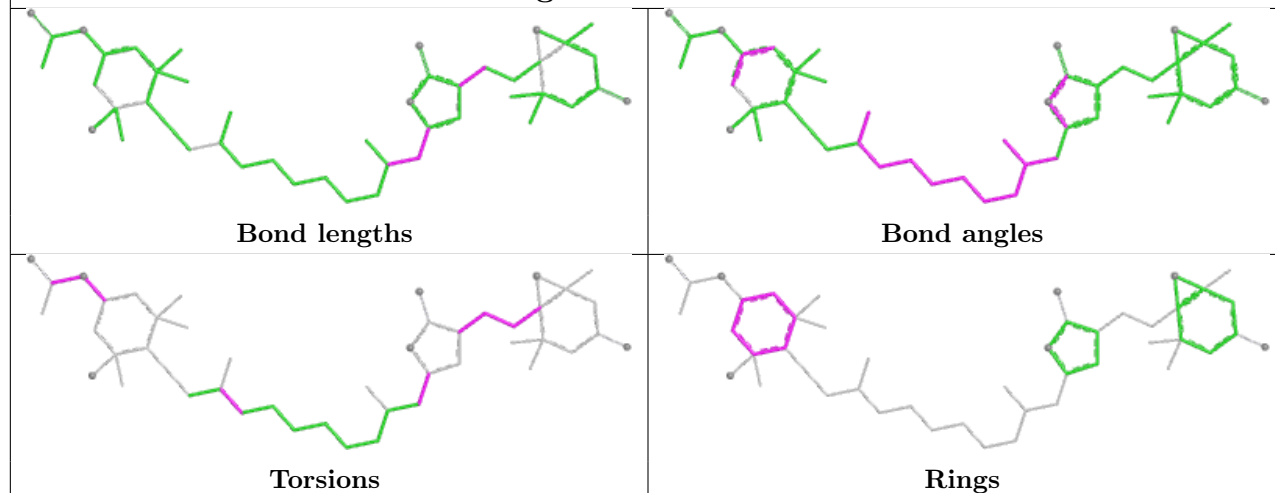
Ligand BCR a 834



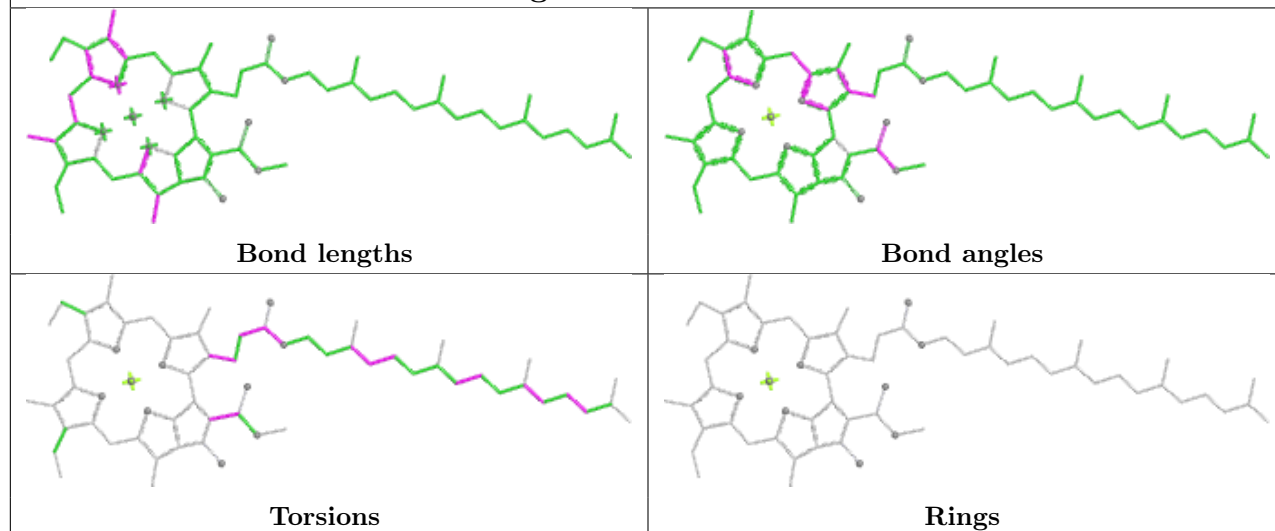
Ligand CLA a 807



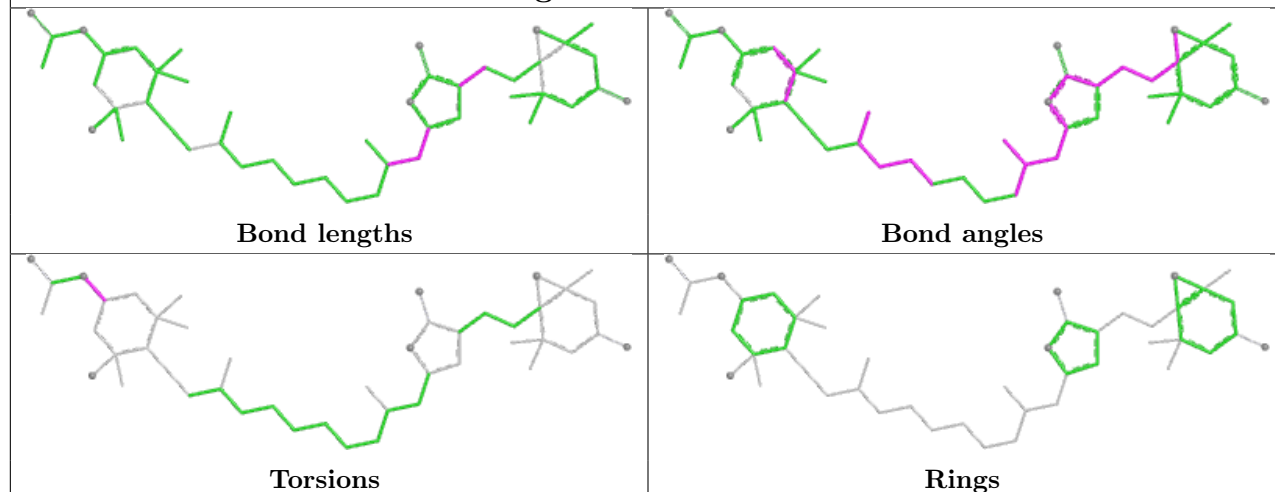
Ligand PID T 317



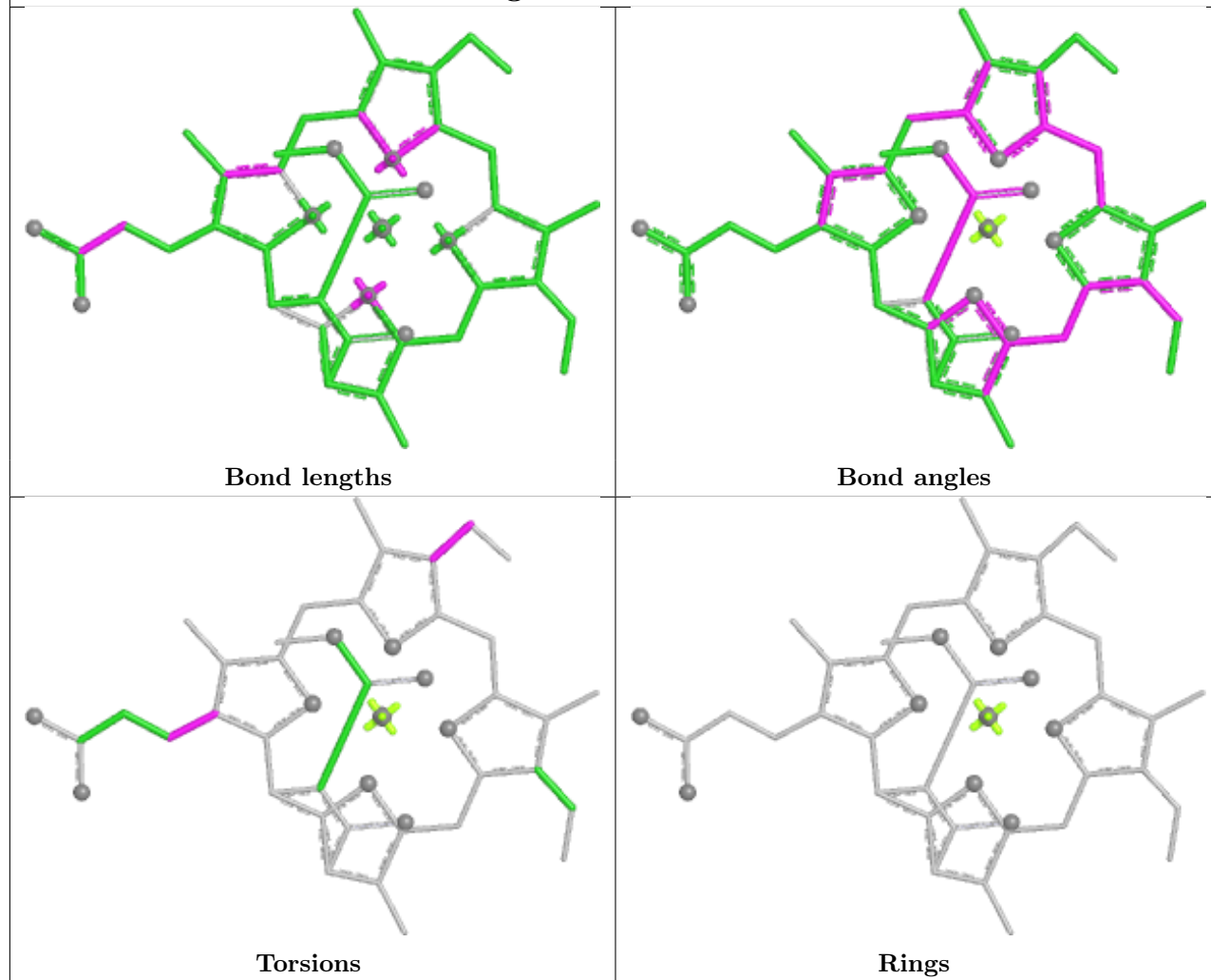
Ligand CLA G 302

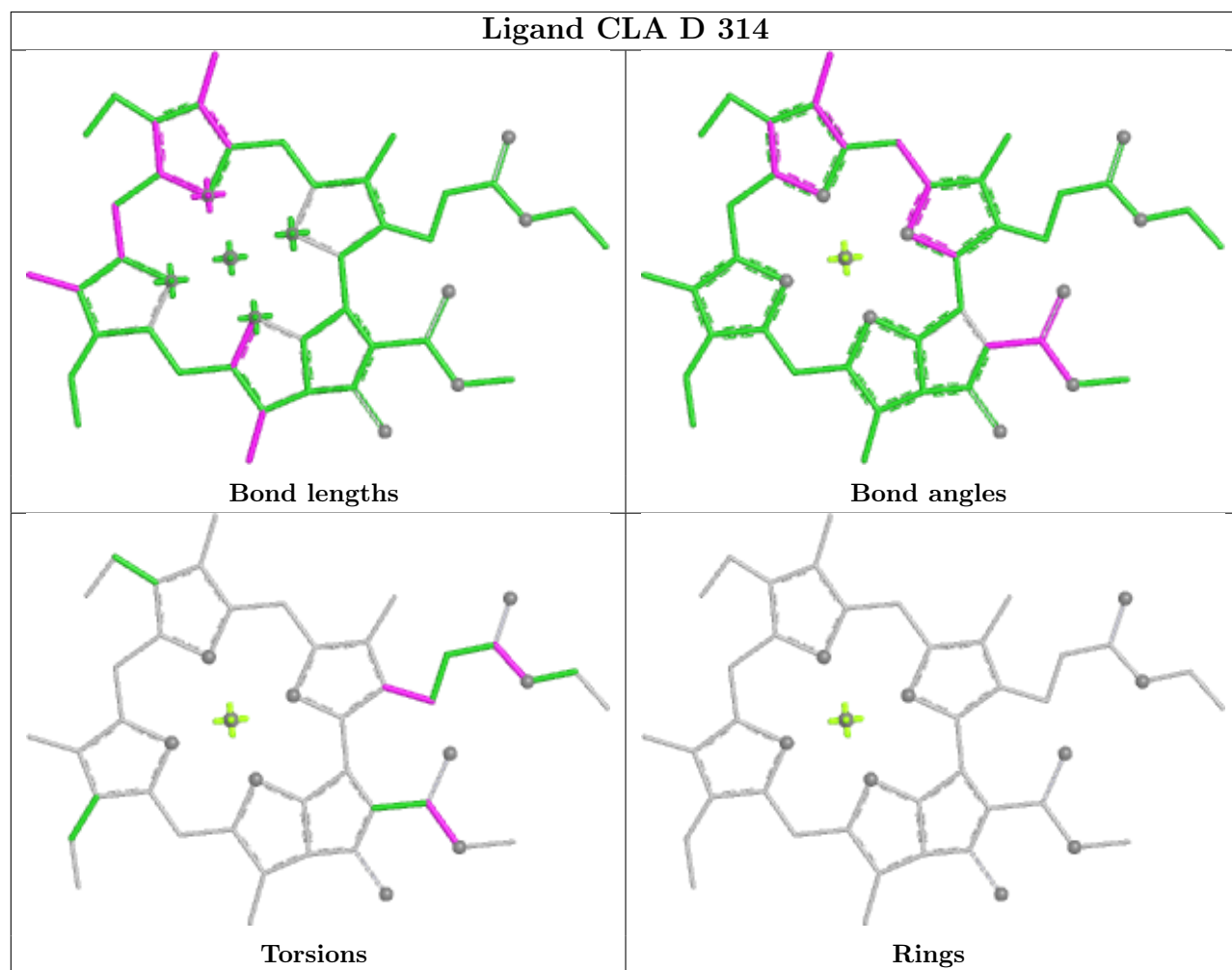
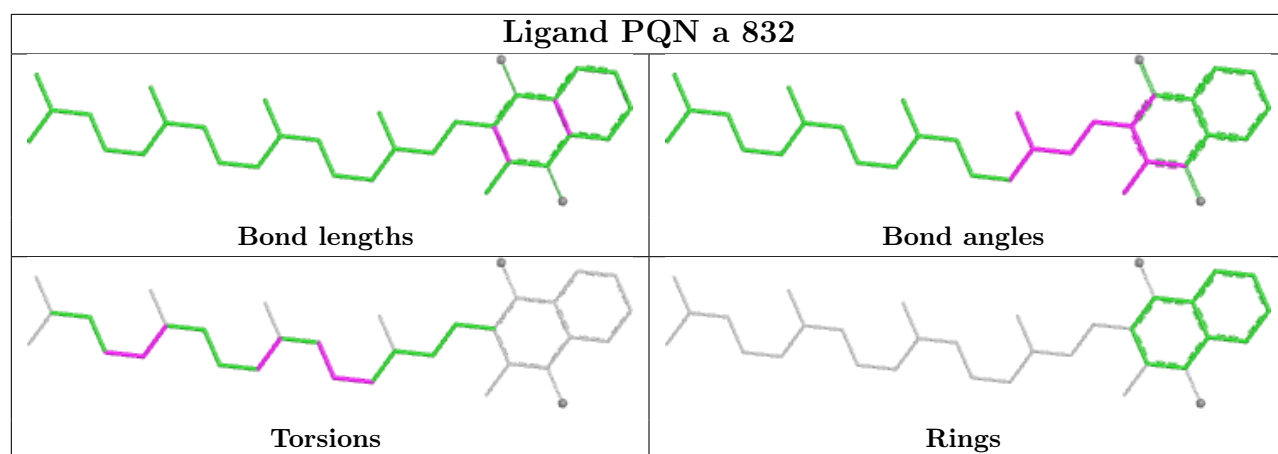


Ligand PID D 303

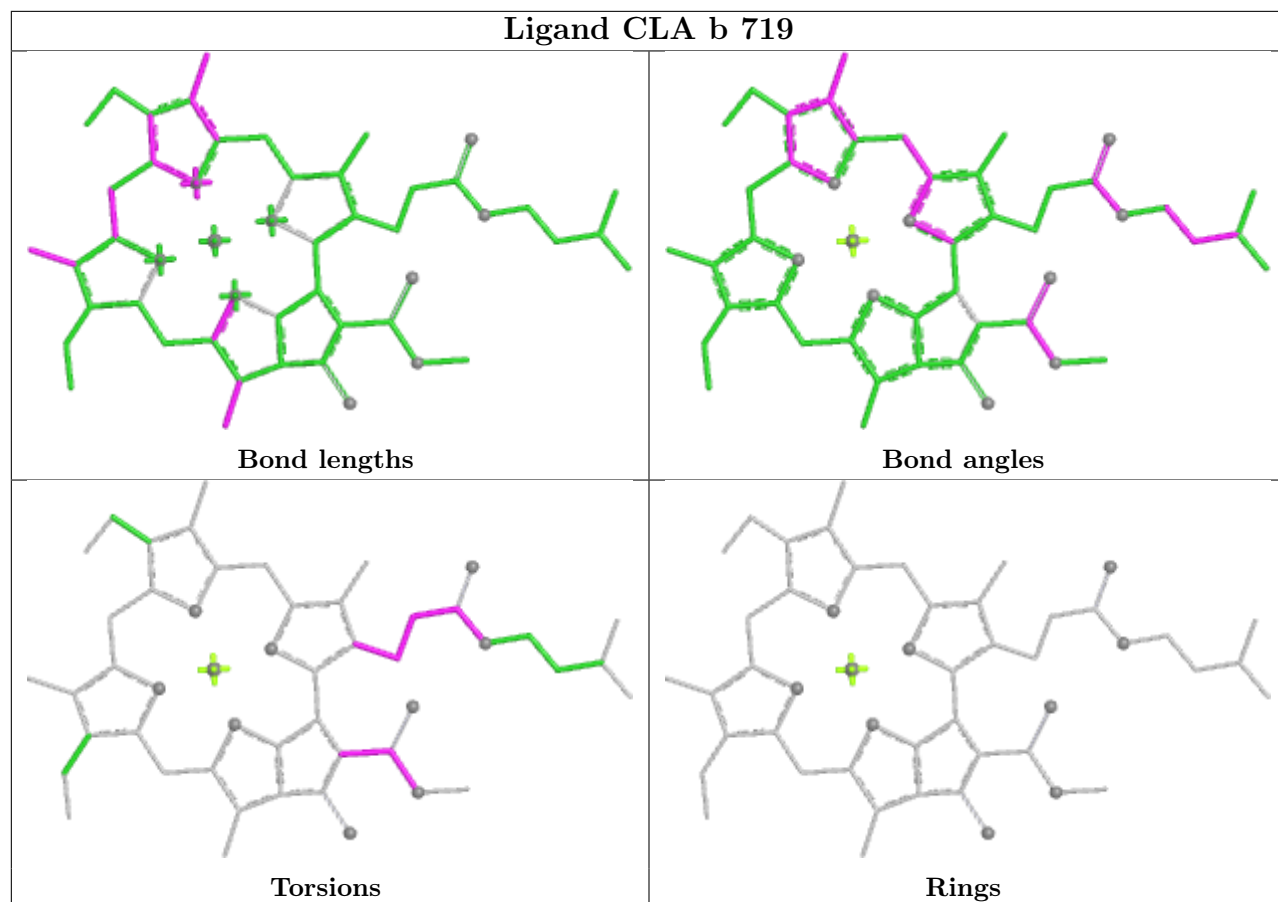


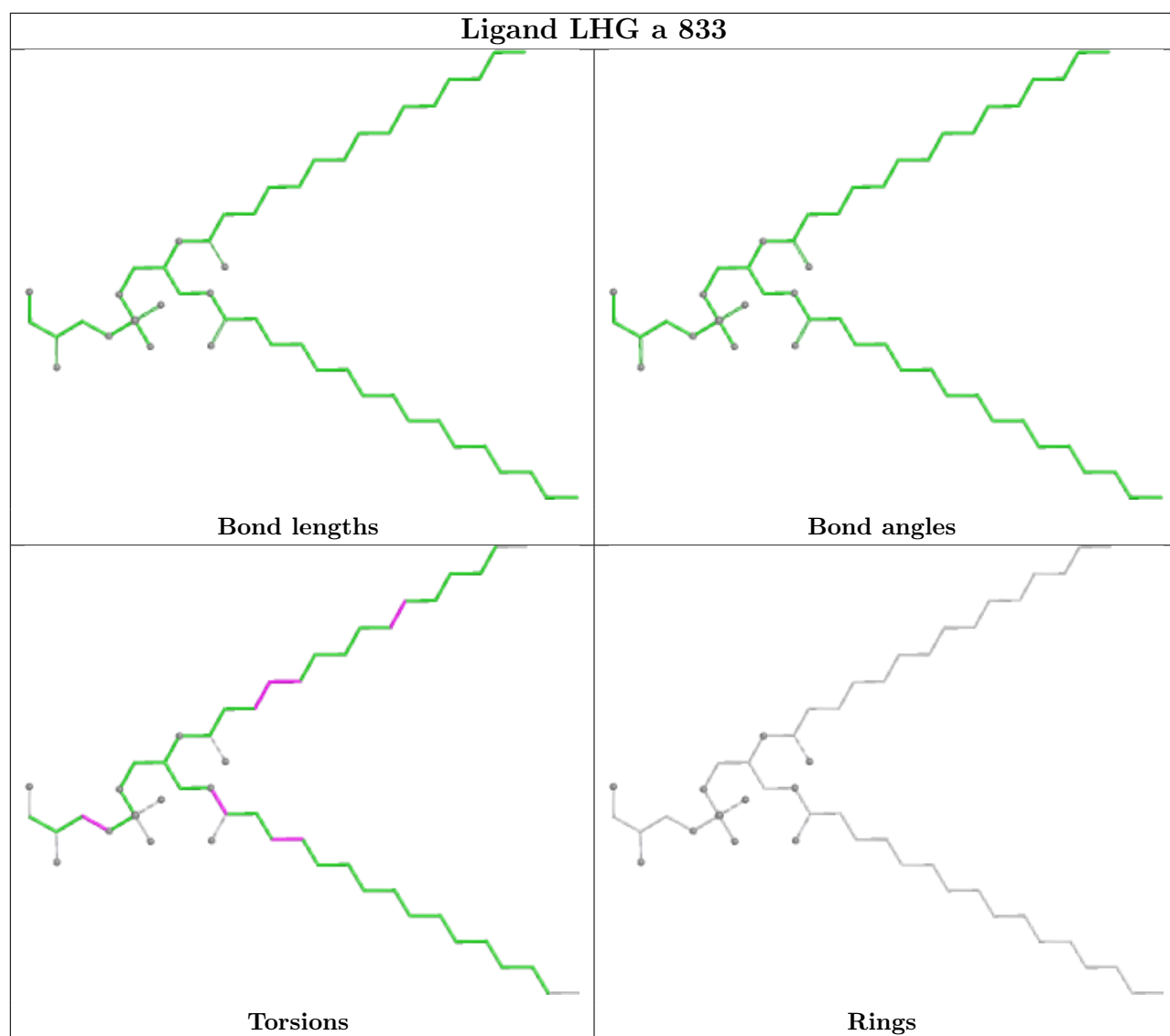
Ligand KC1 O 312



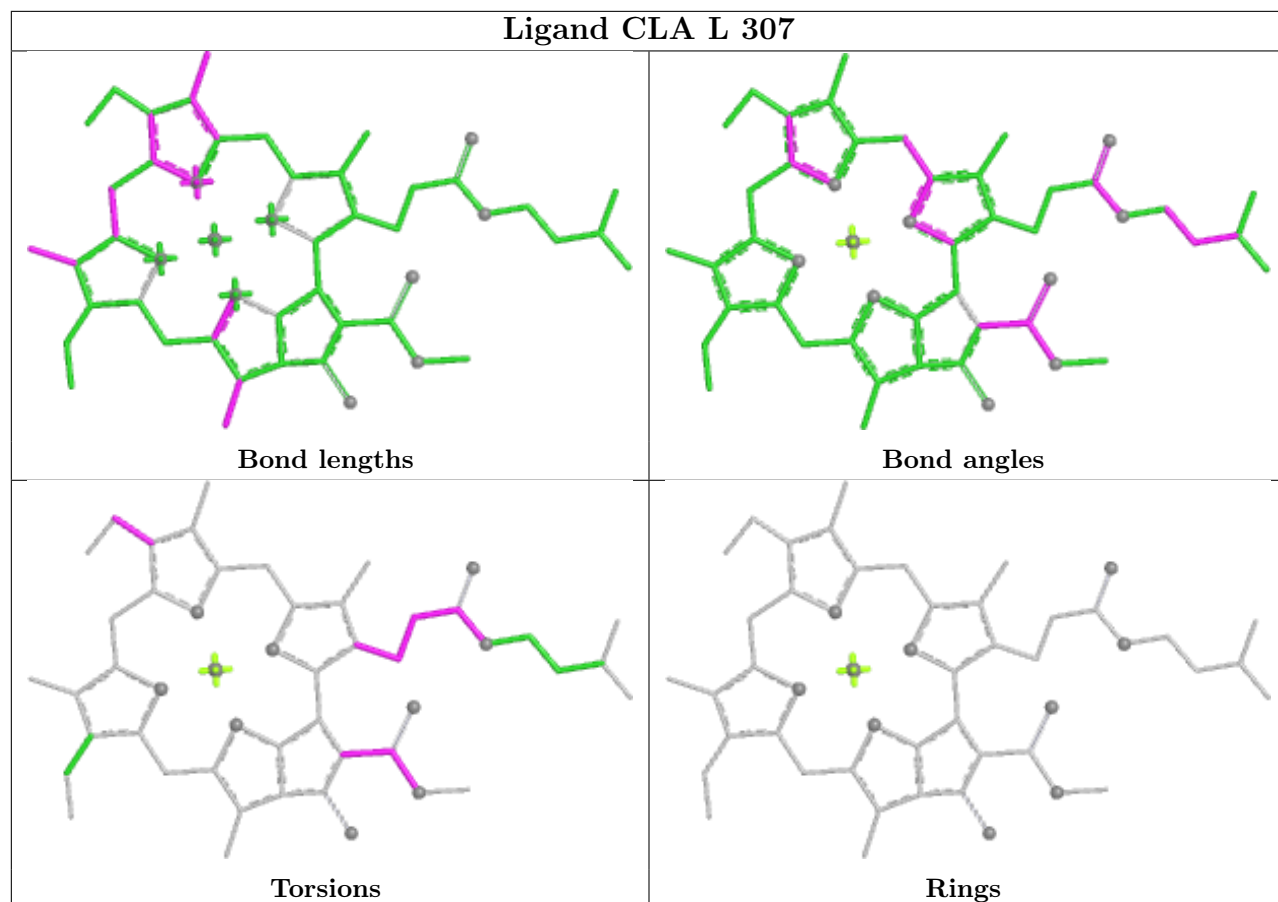


Ligand CLA b 719

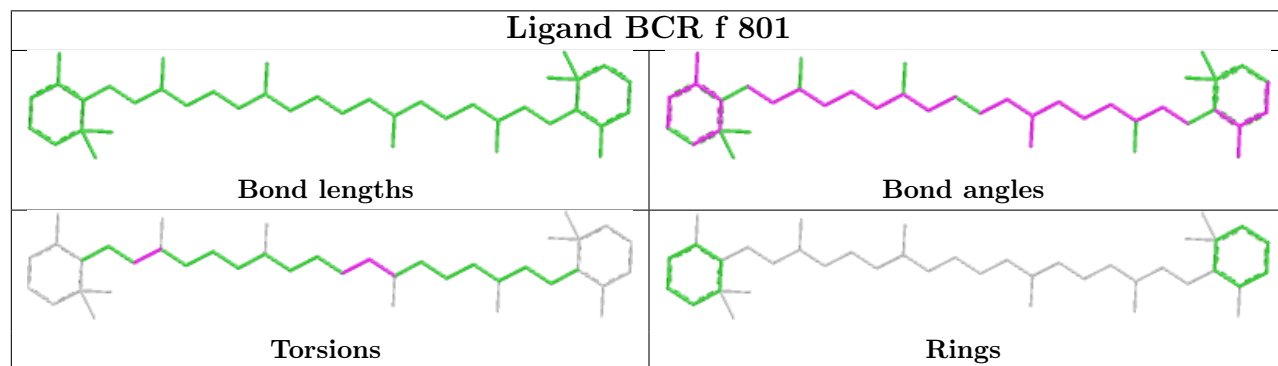




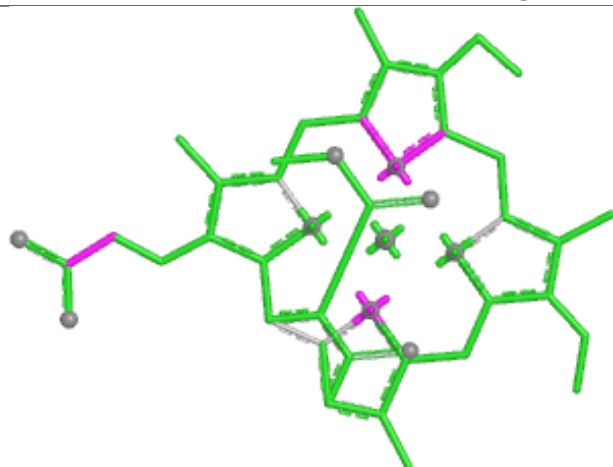
Ligand CLA L 307



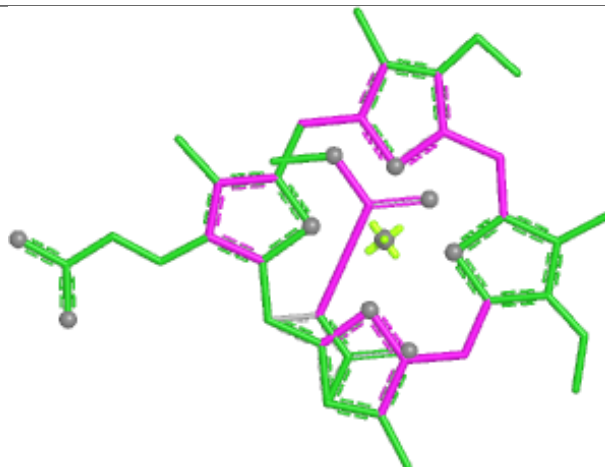
Ligand BCR f 801



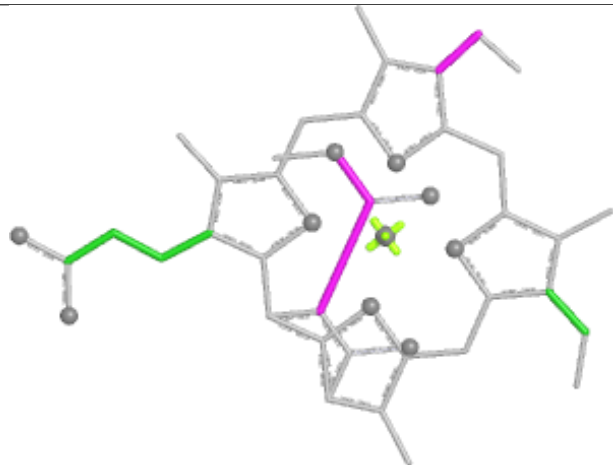
Ligand KC1 N 312



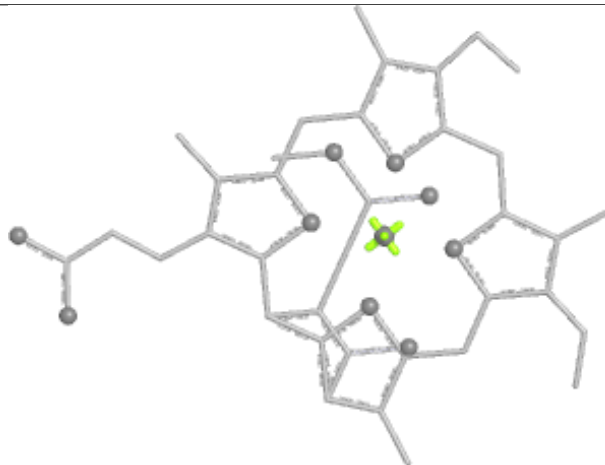
Bond lengths



Bond angles

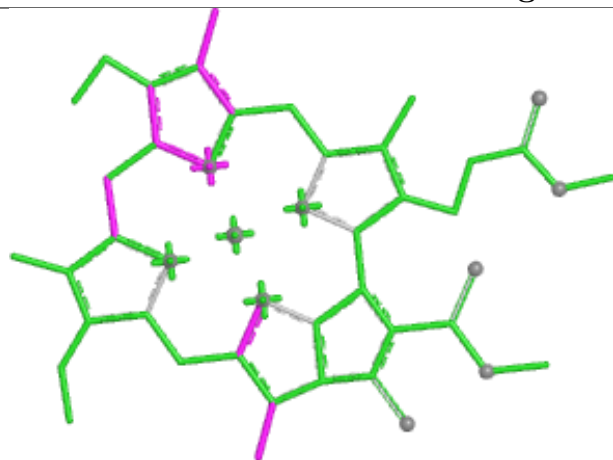


Torsions

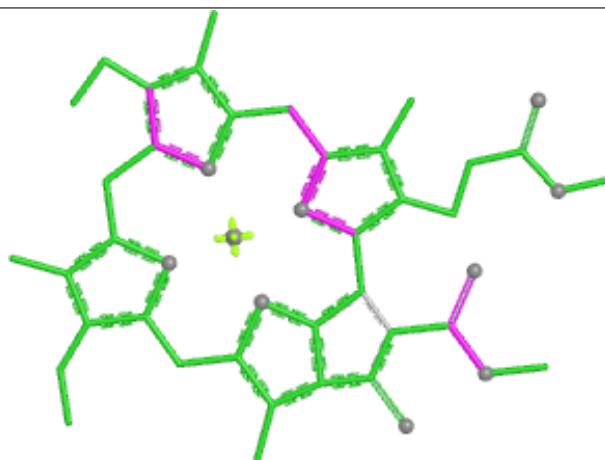


Rings

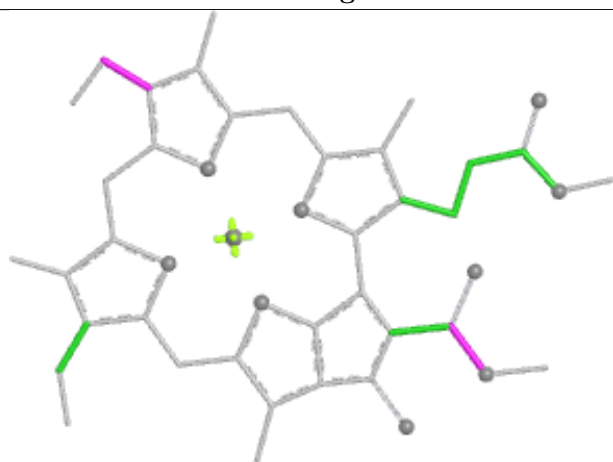
Ligand CLA J 305



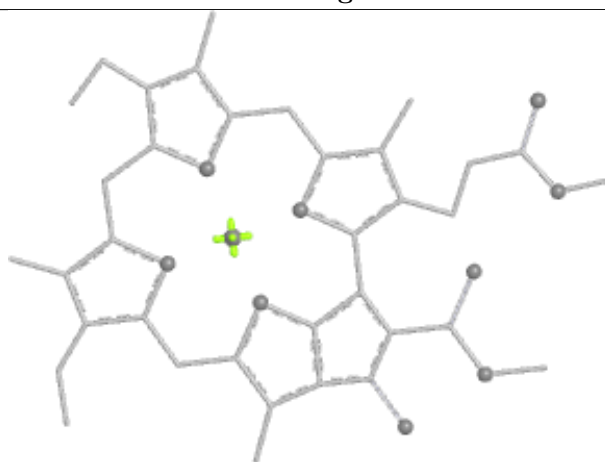
Bond lengths



Bond angles

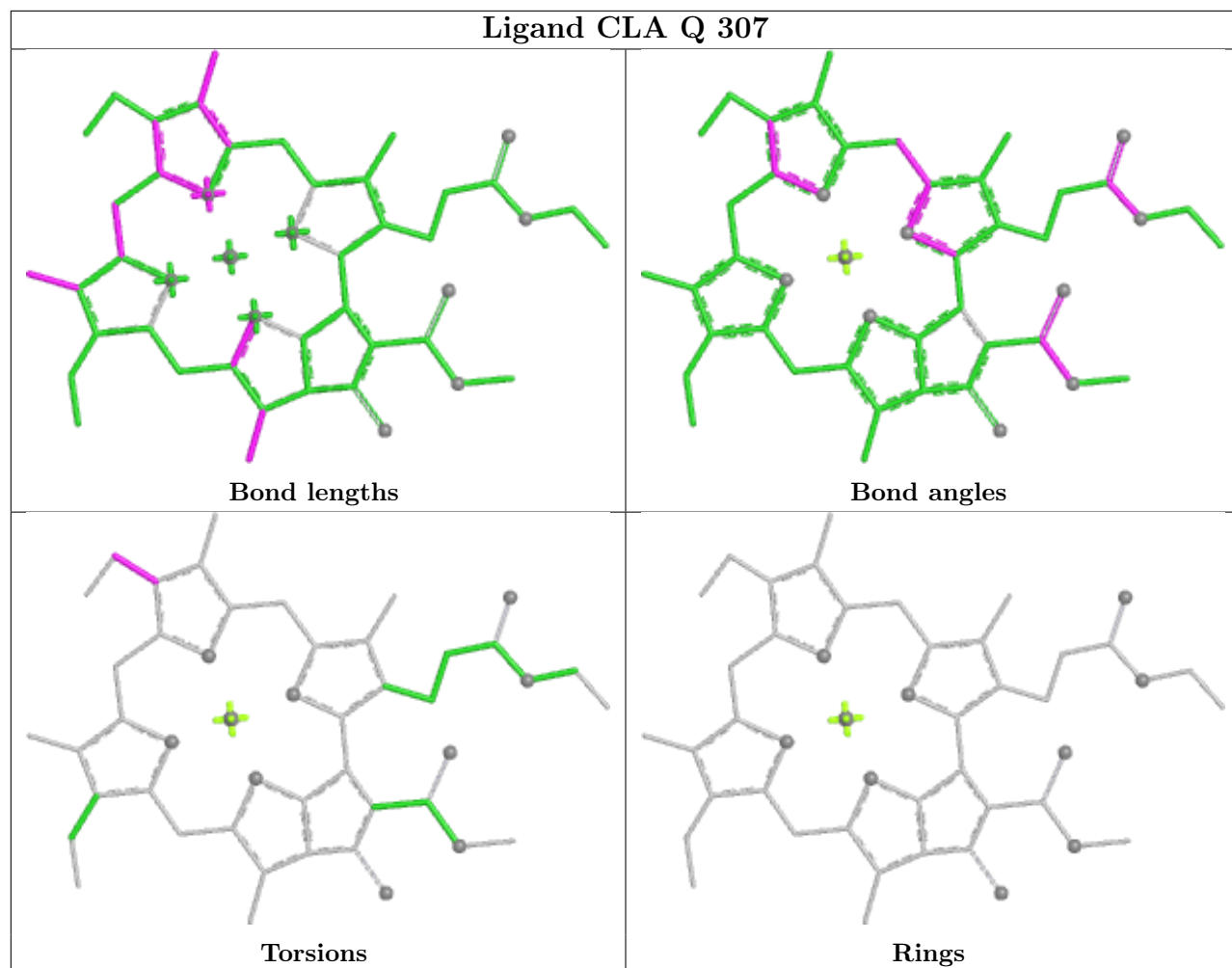


Torsions

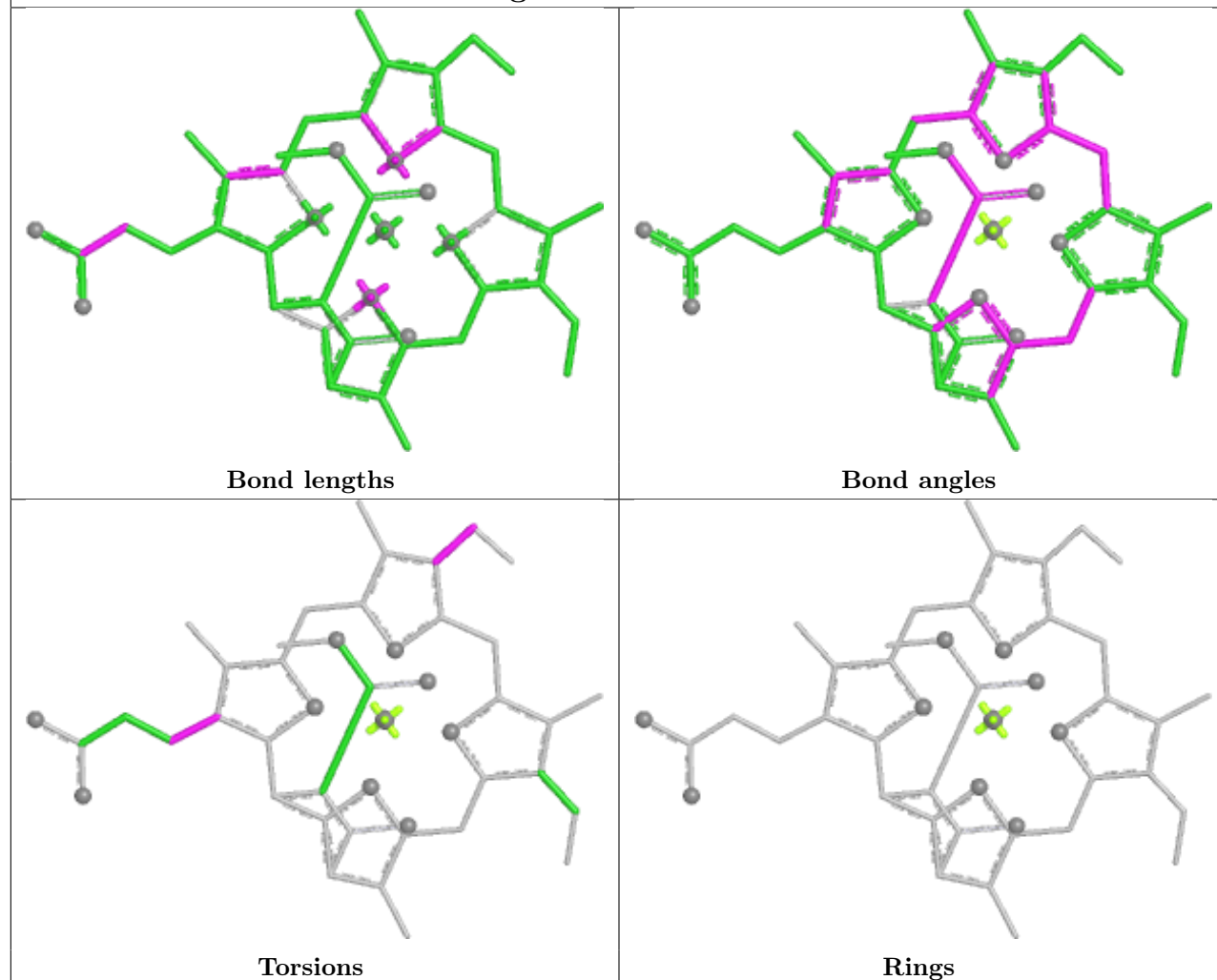


Rings

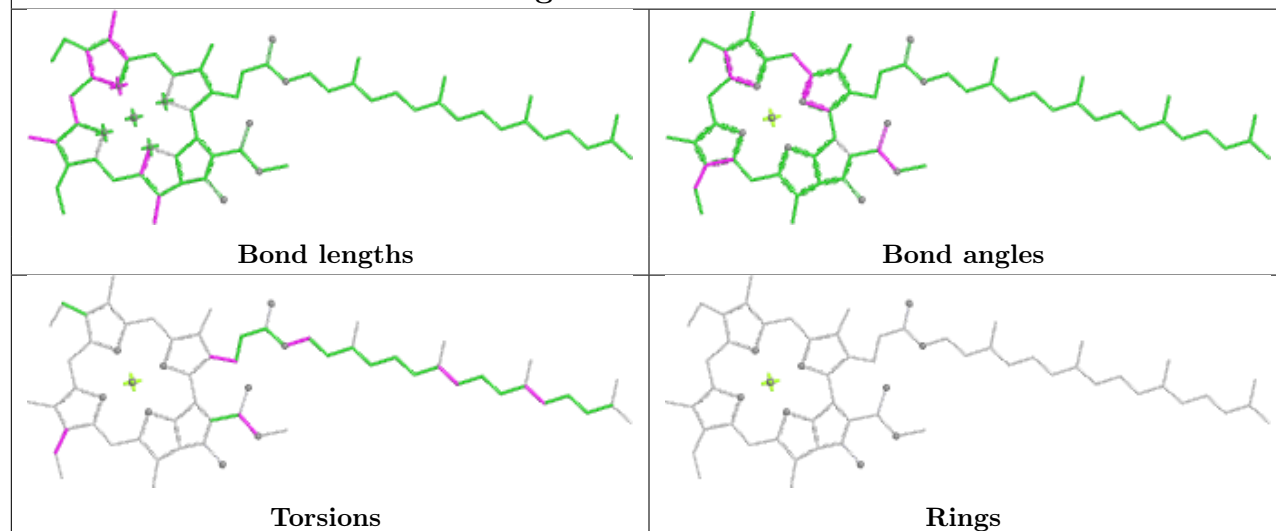
Ligand CLA Q 307



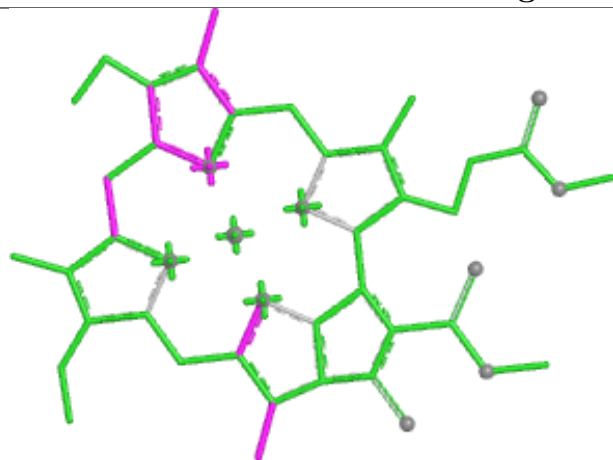
Ligand KC1 T 312



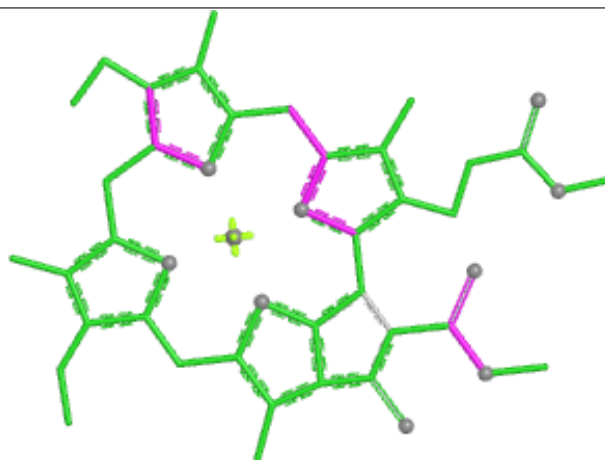
Ligand CLA b 705



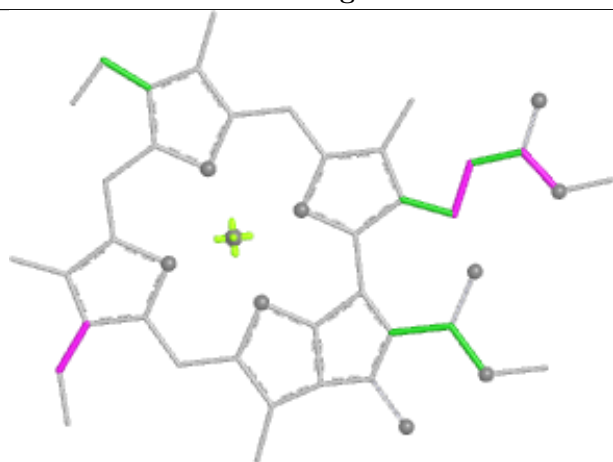
Ligand CLA J 309



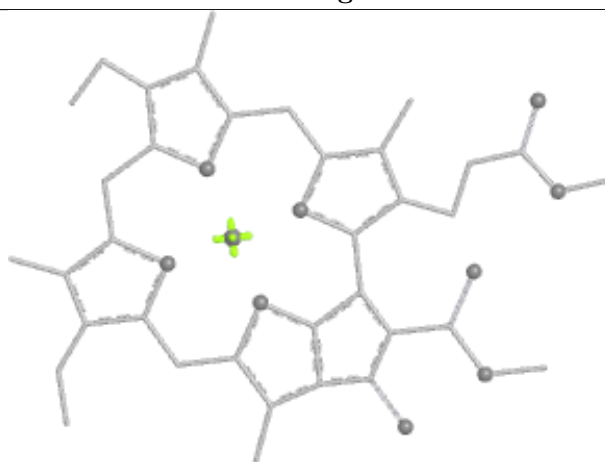
Bond lengths



Bond angles

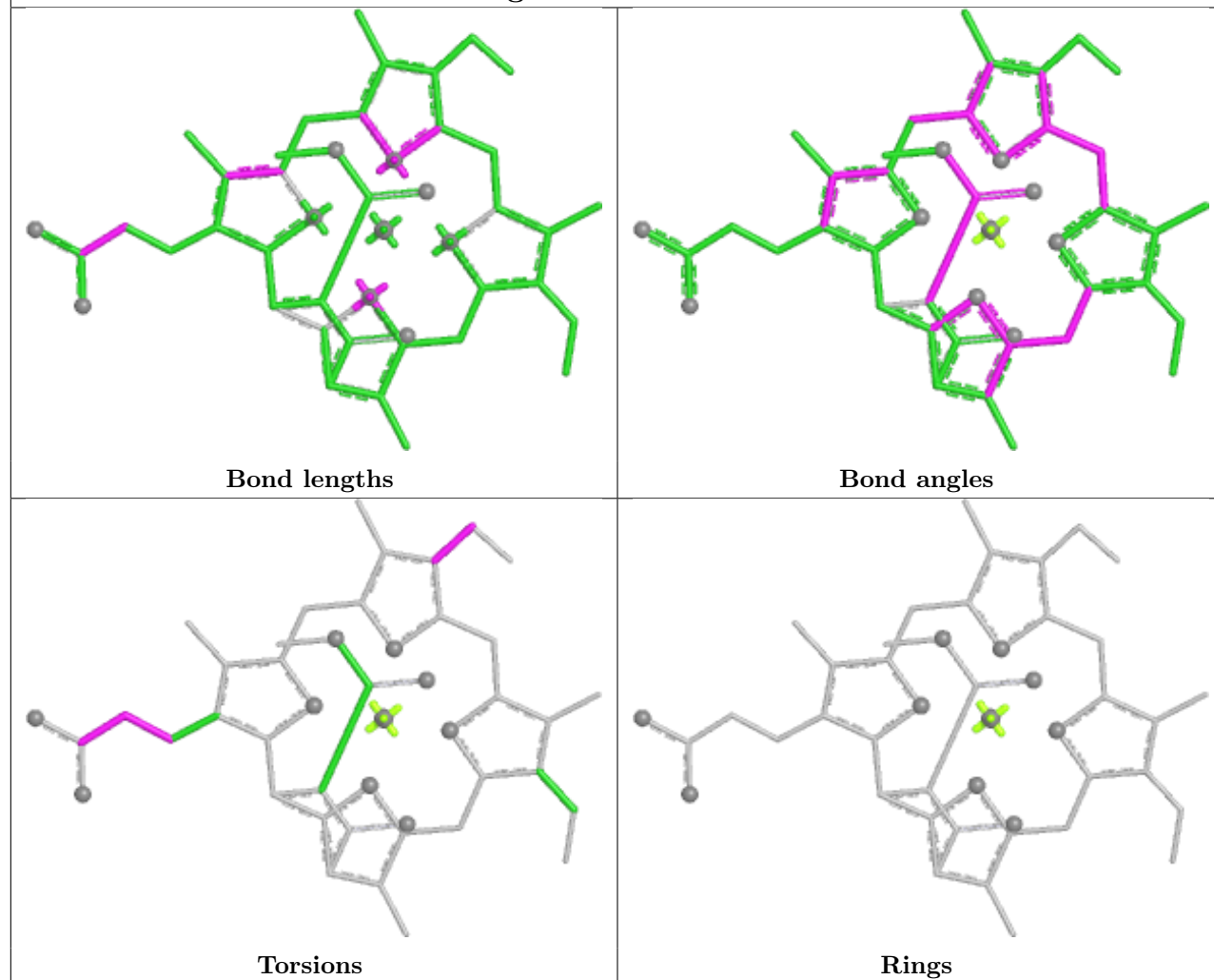


Torsions

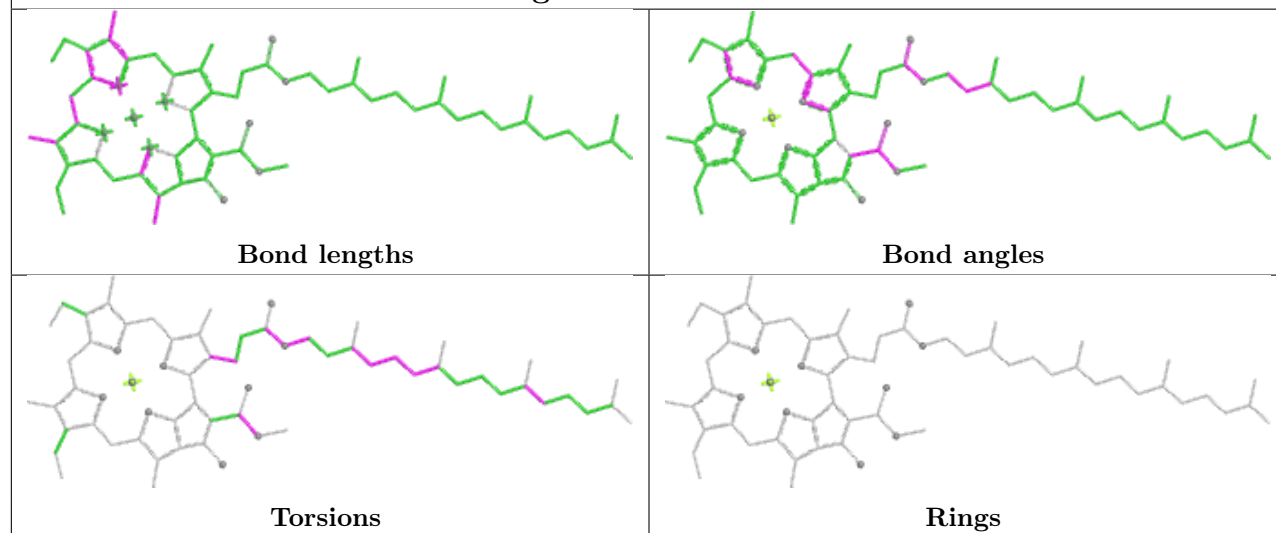


Rings

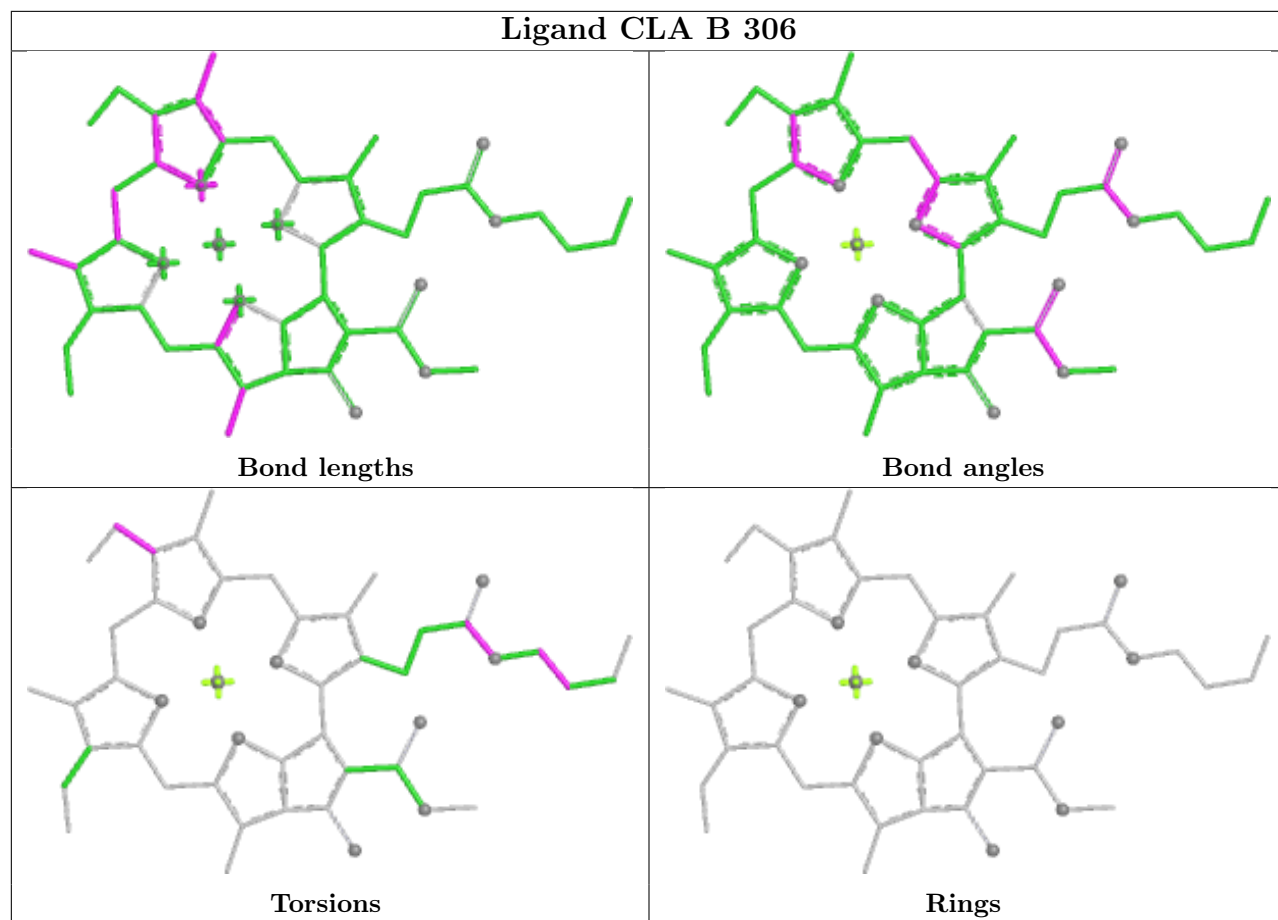
Ligand KC1 A 213



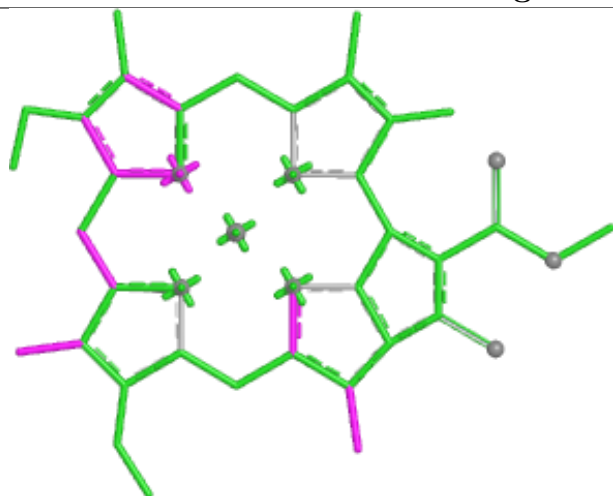
Ligand CLA B 308



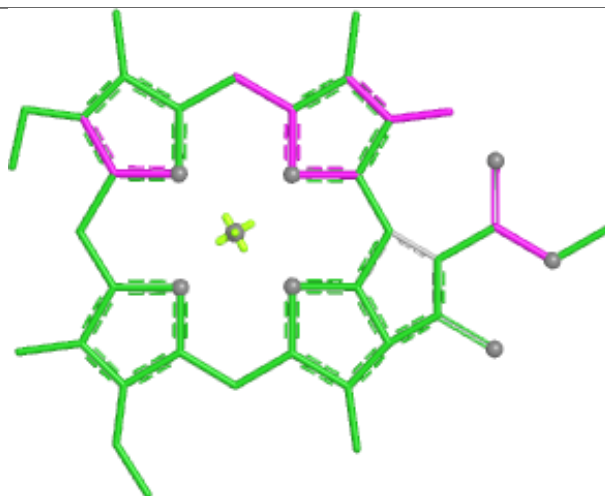
Ligand CLA B 306



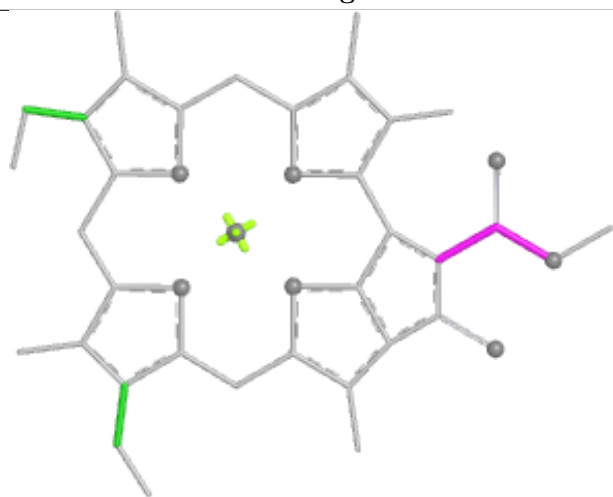
Ligand CLA O 316



Bond lengths



Bond angles

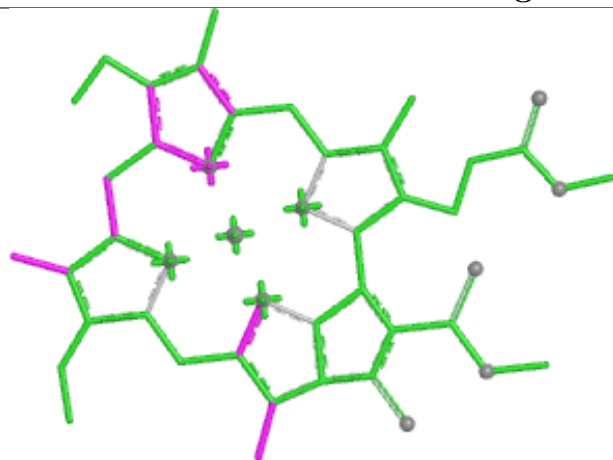


Torsions

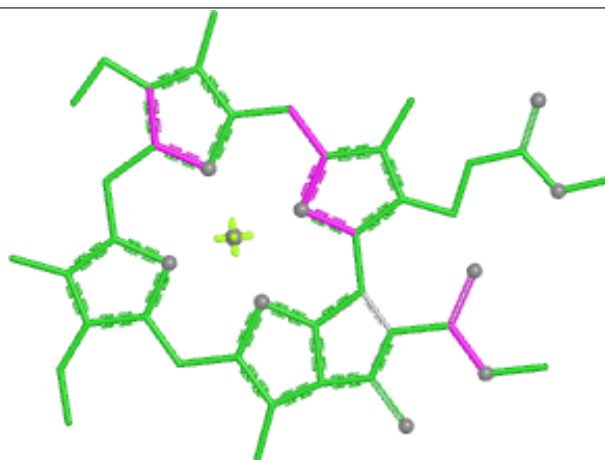


Rings

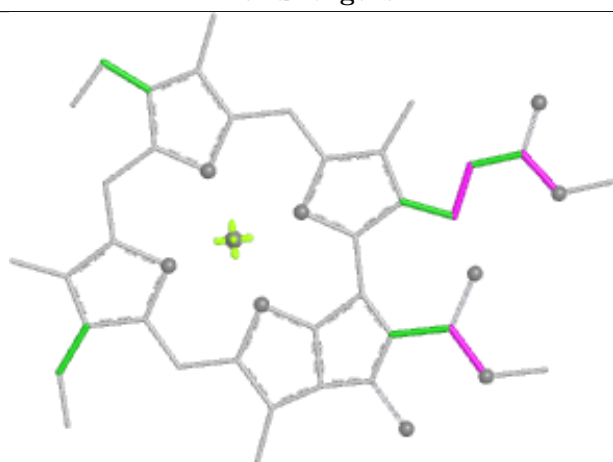
Ligand CLA T 313



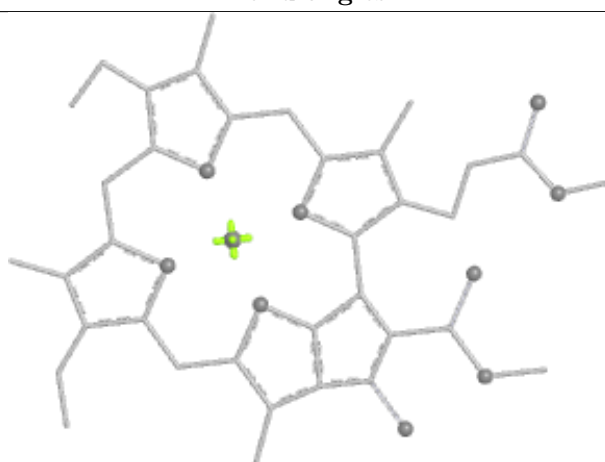
Bond lengths



Bond angles

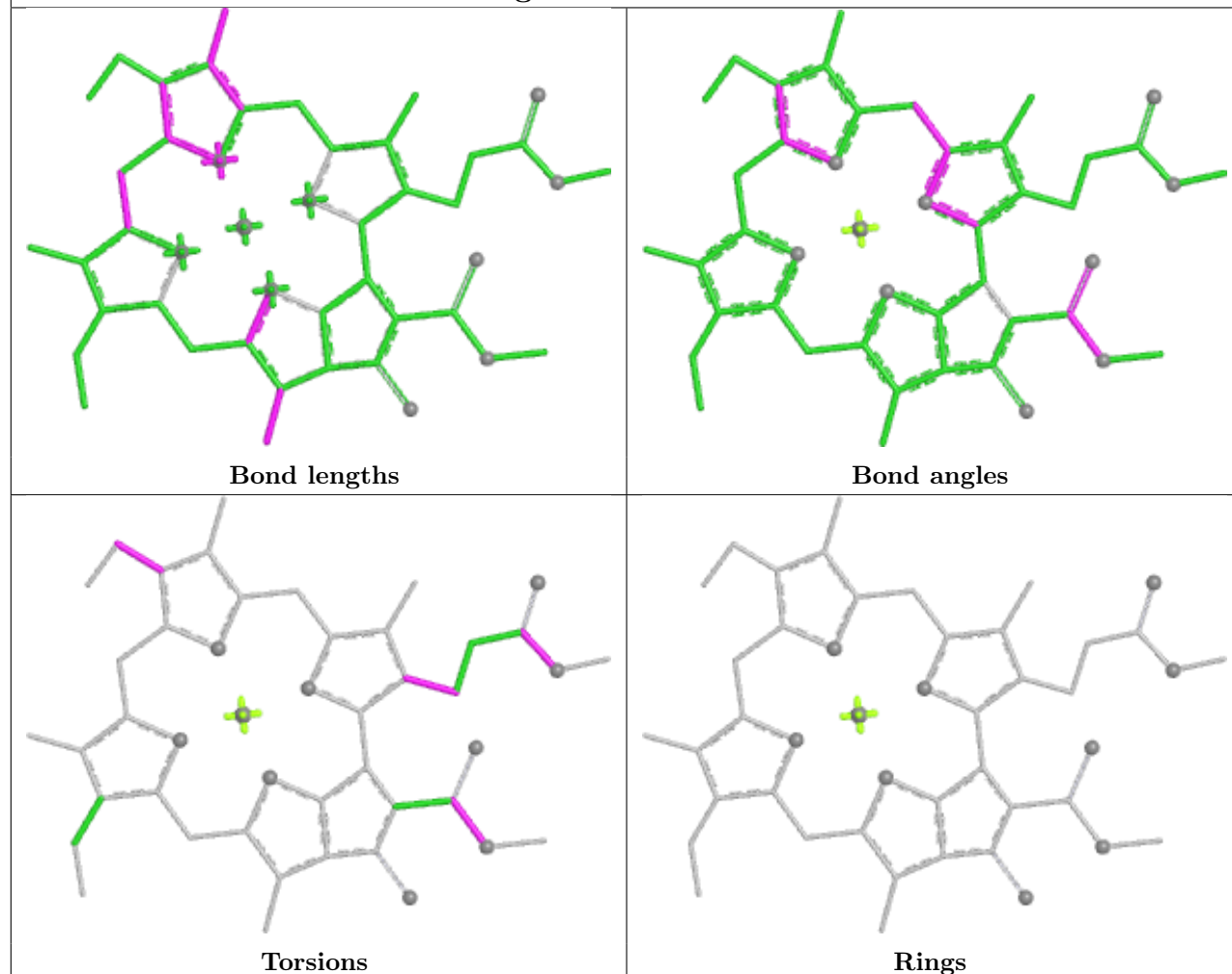


Torsions

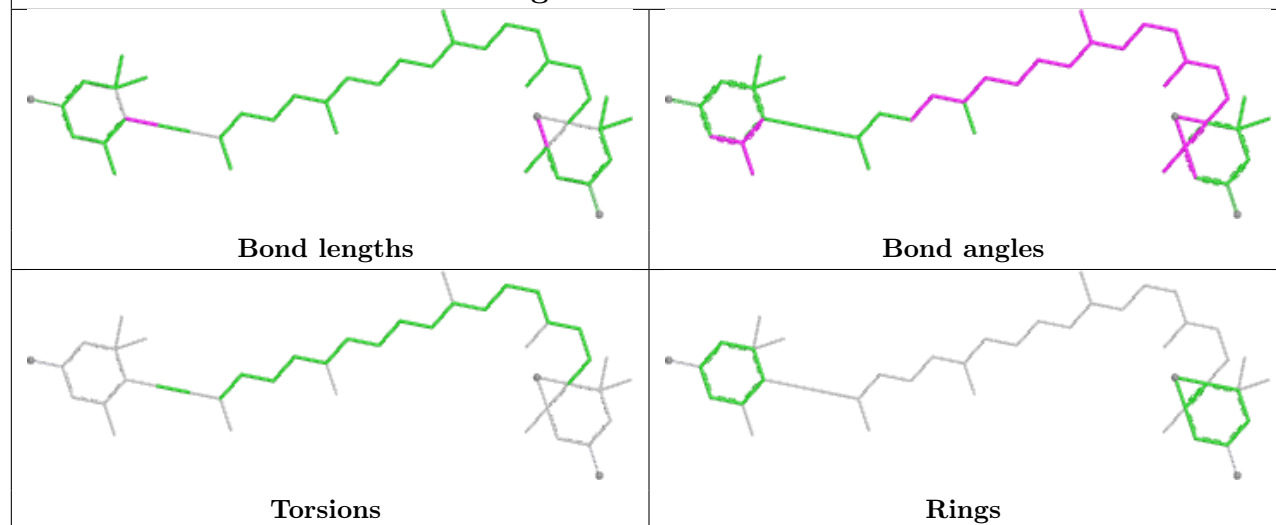


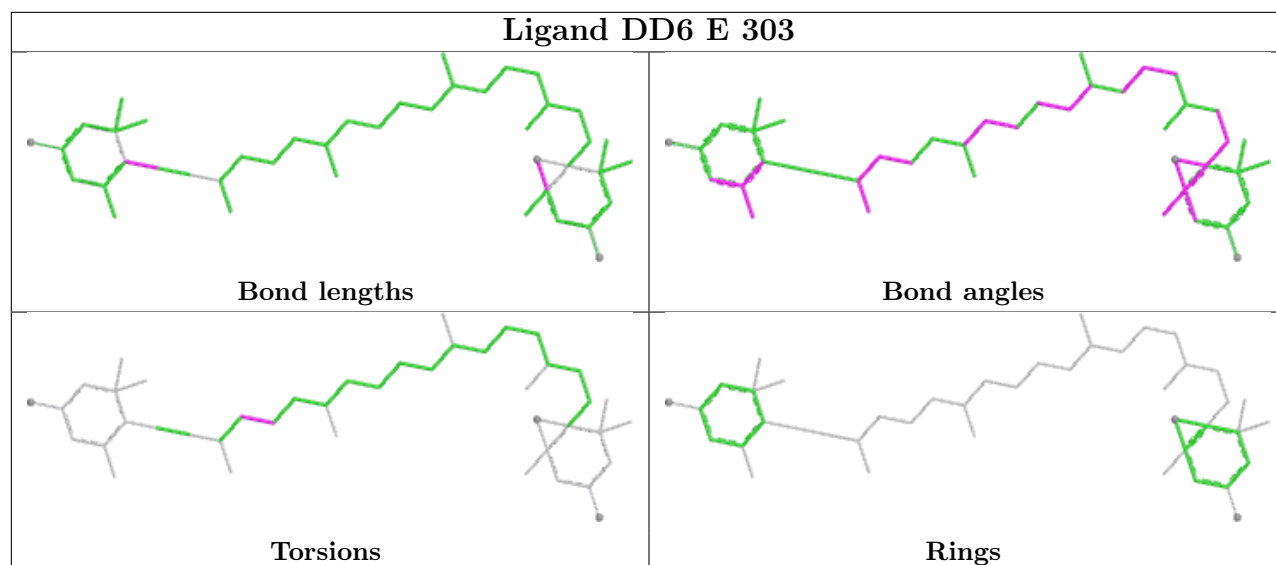
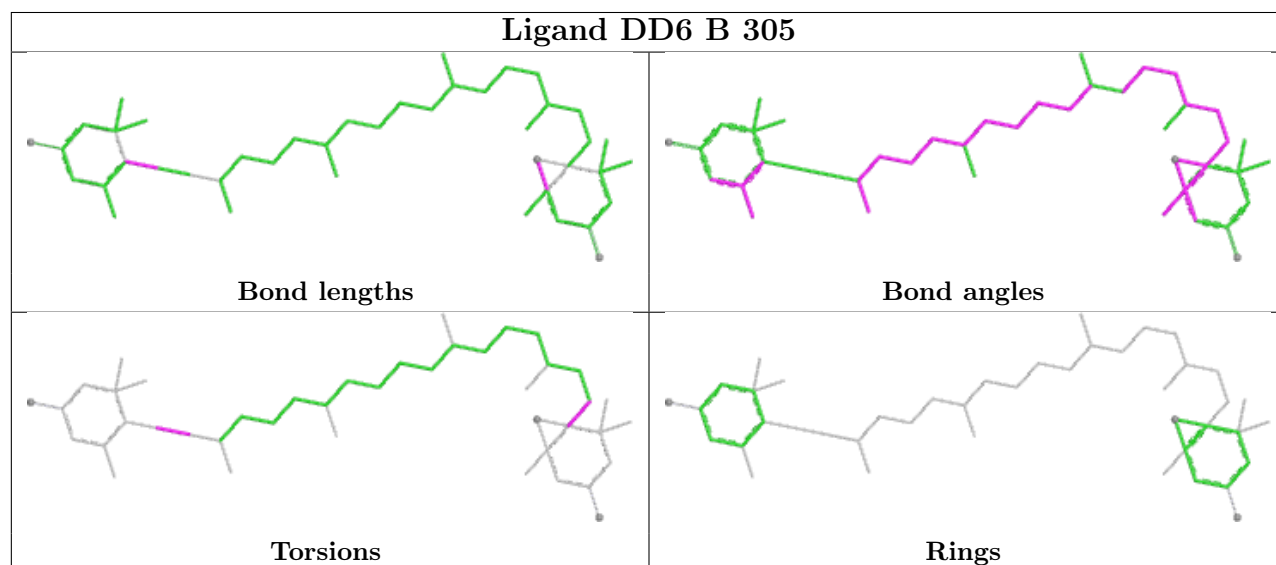
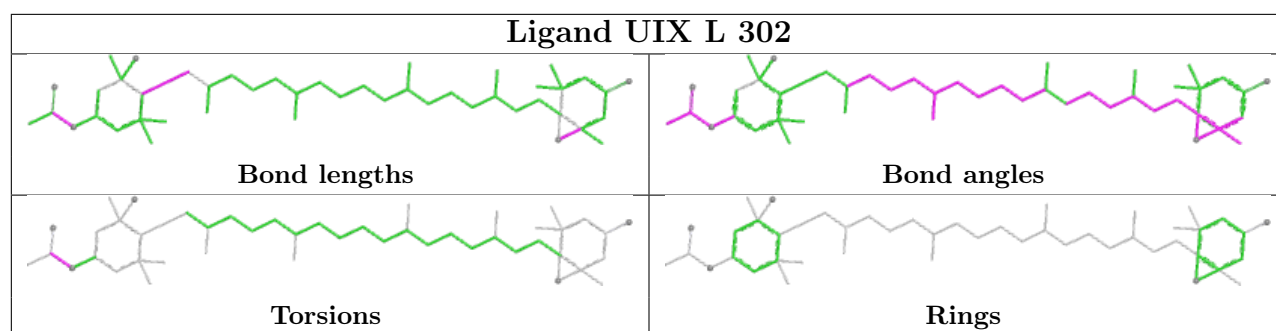
Rings

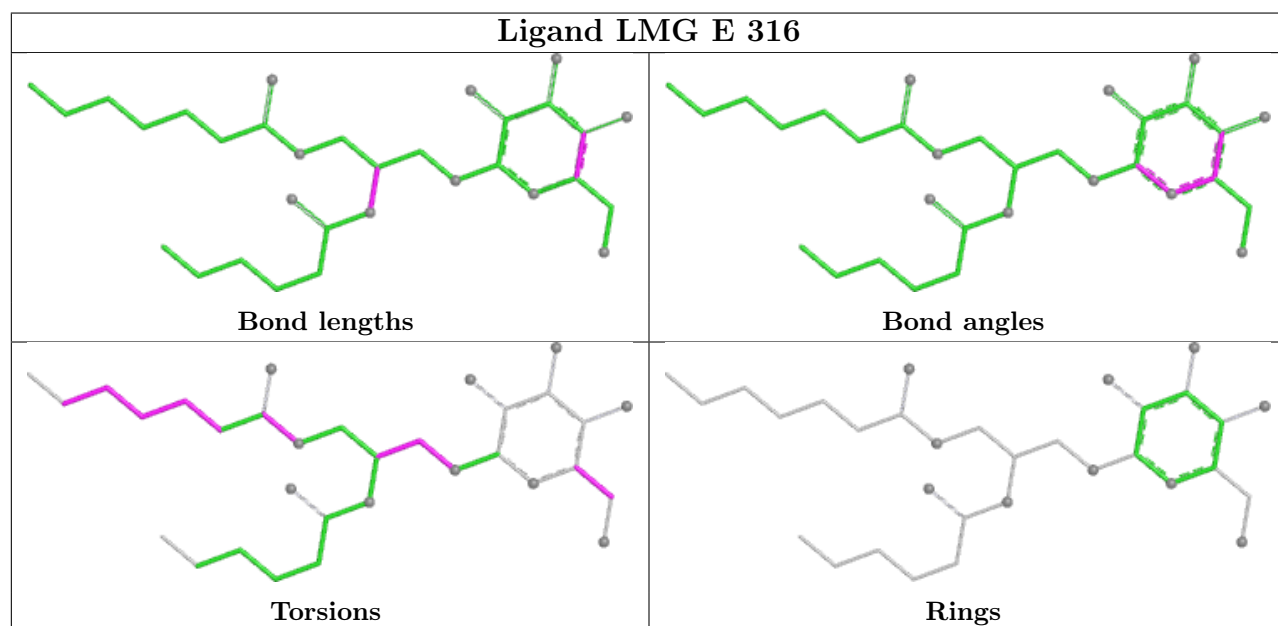
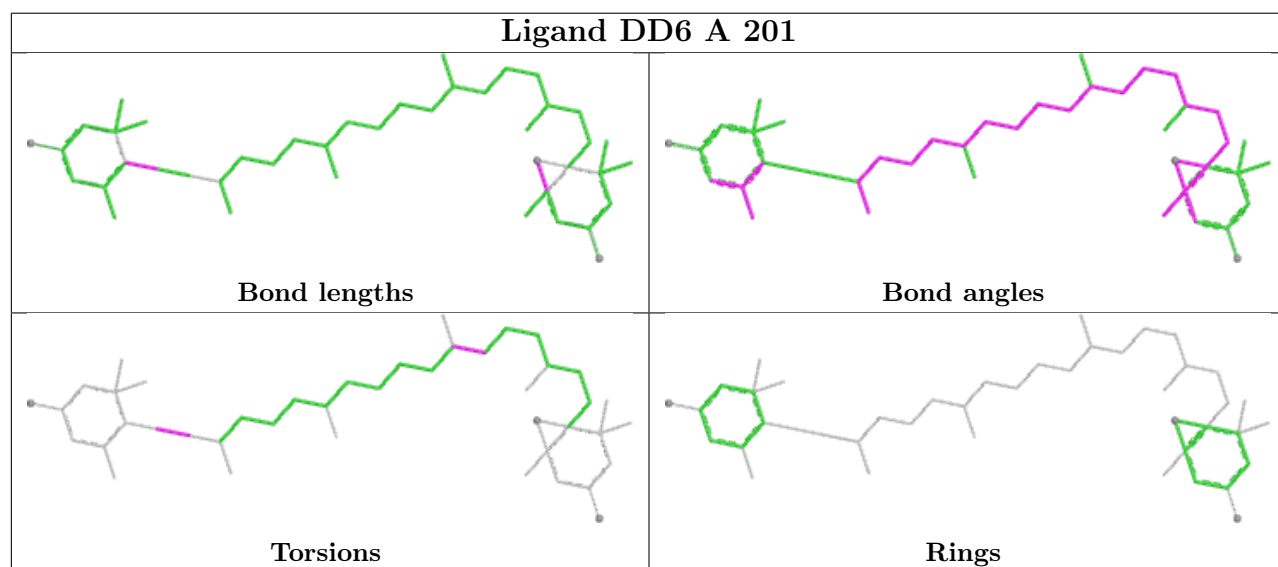
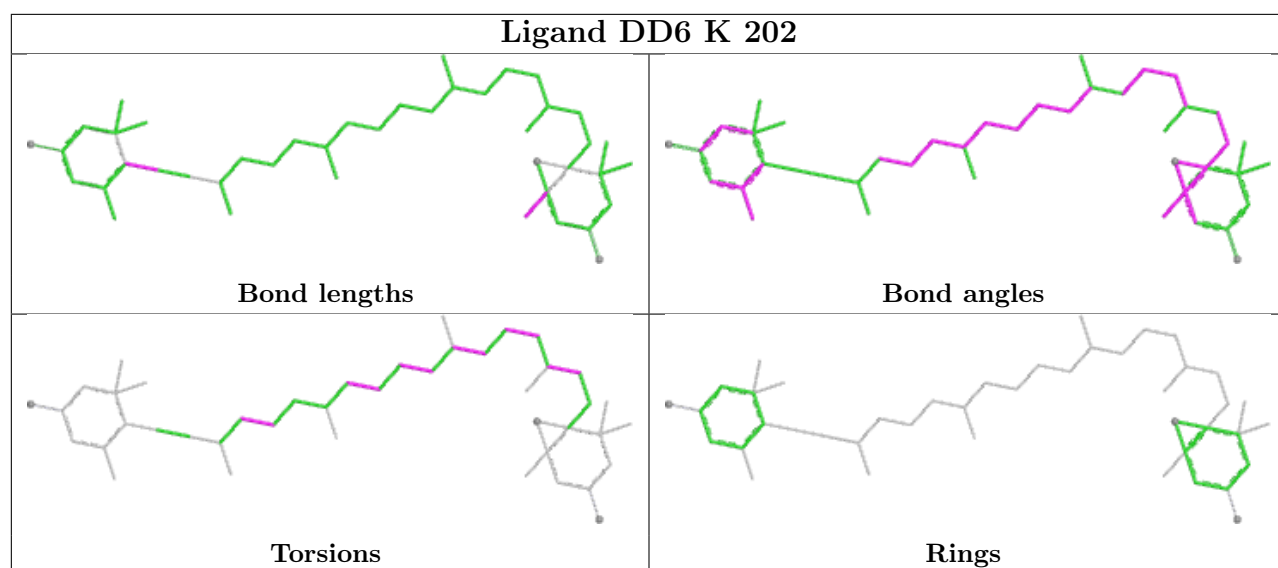
Ligand CLA E 309

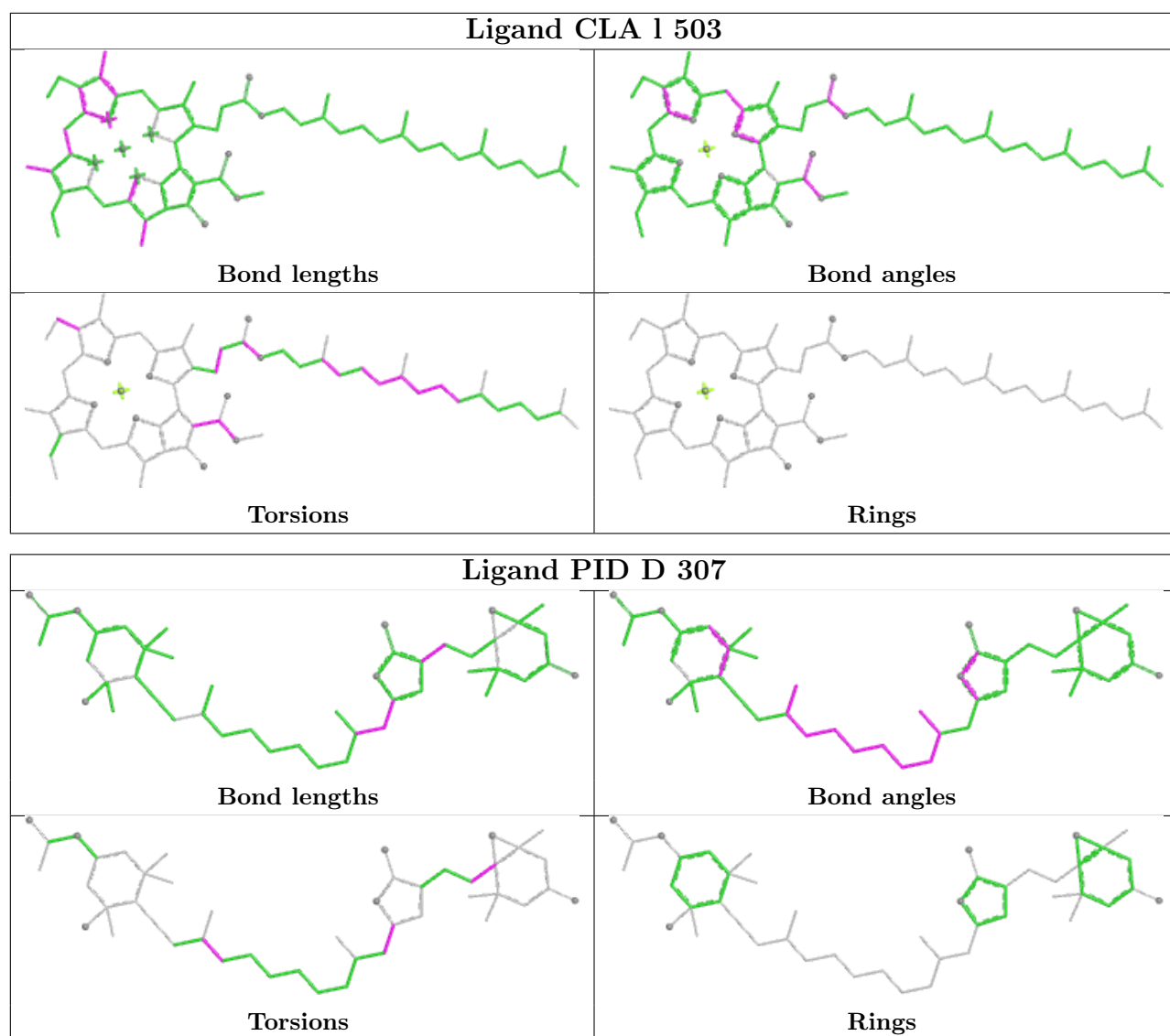


Ligand DD6 m 101

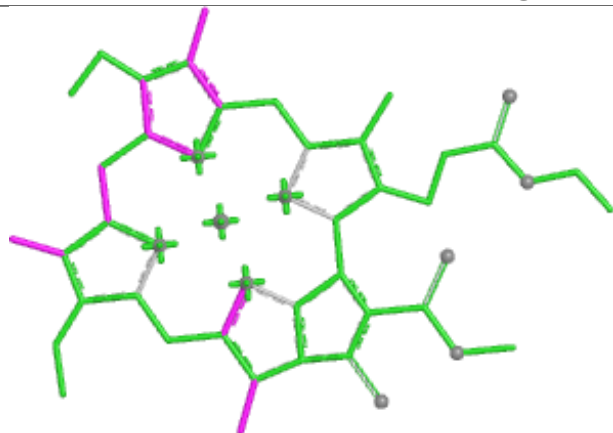




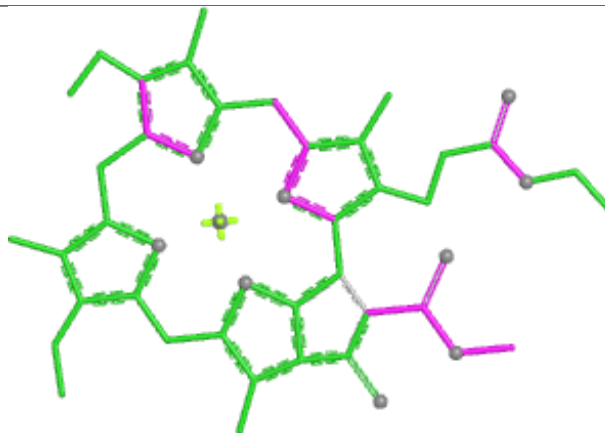




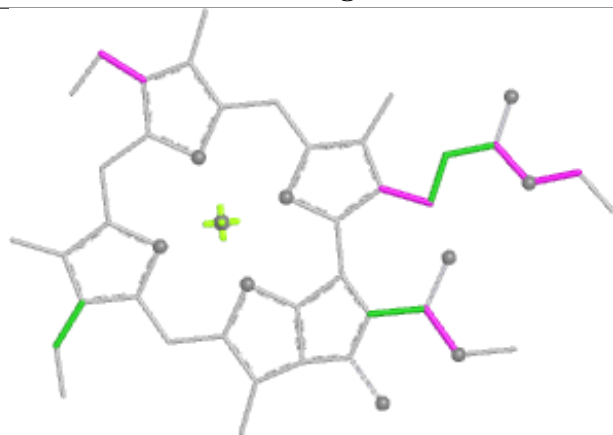
Ligand CLA P 215



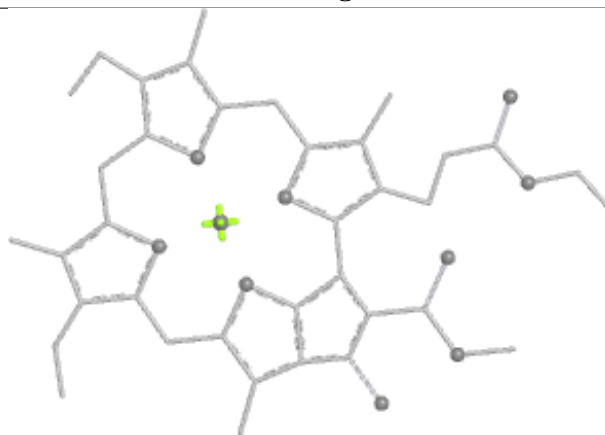
Bond lengths



Bond angles

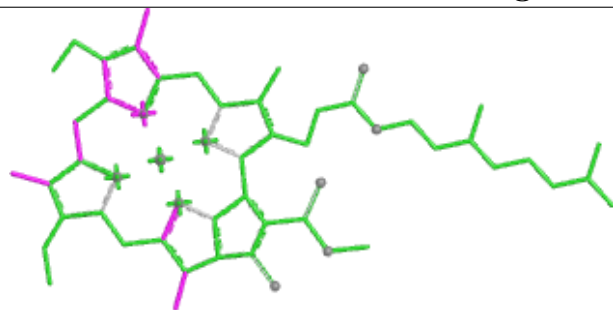


Torsions

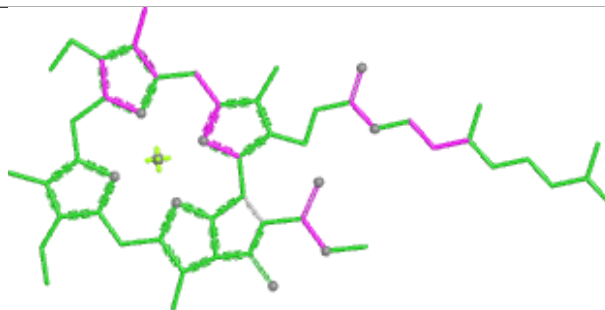


Rings

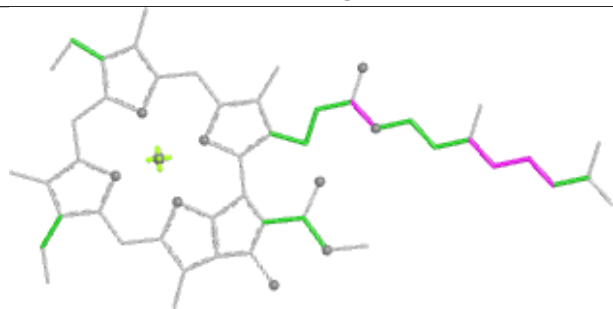
Ligand CLA A 211



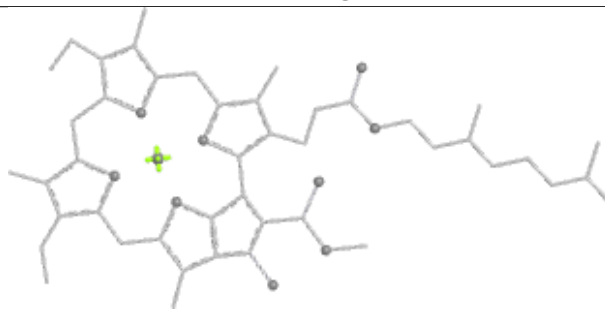
Bond lengths



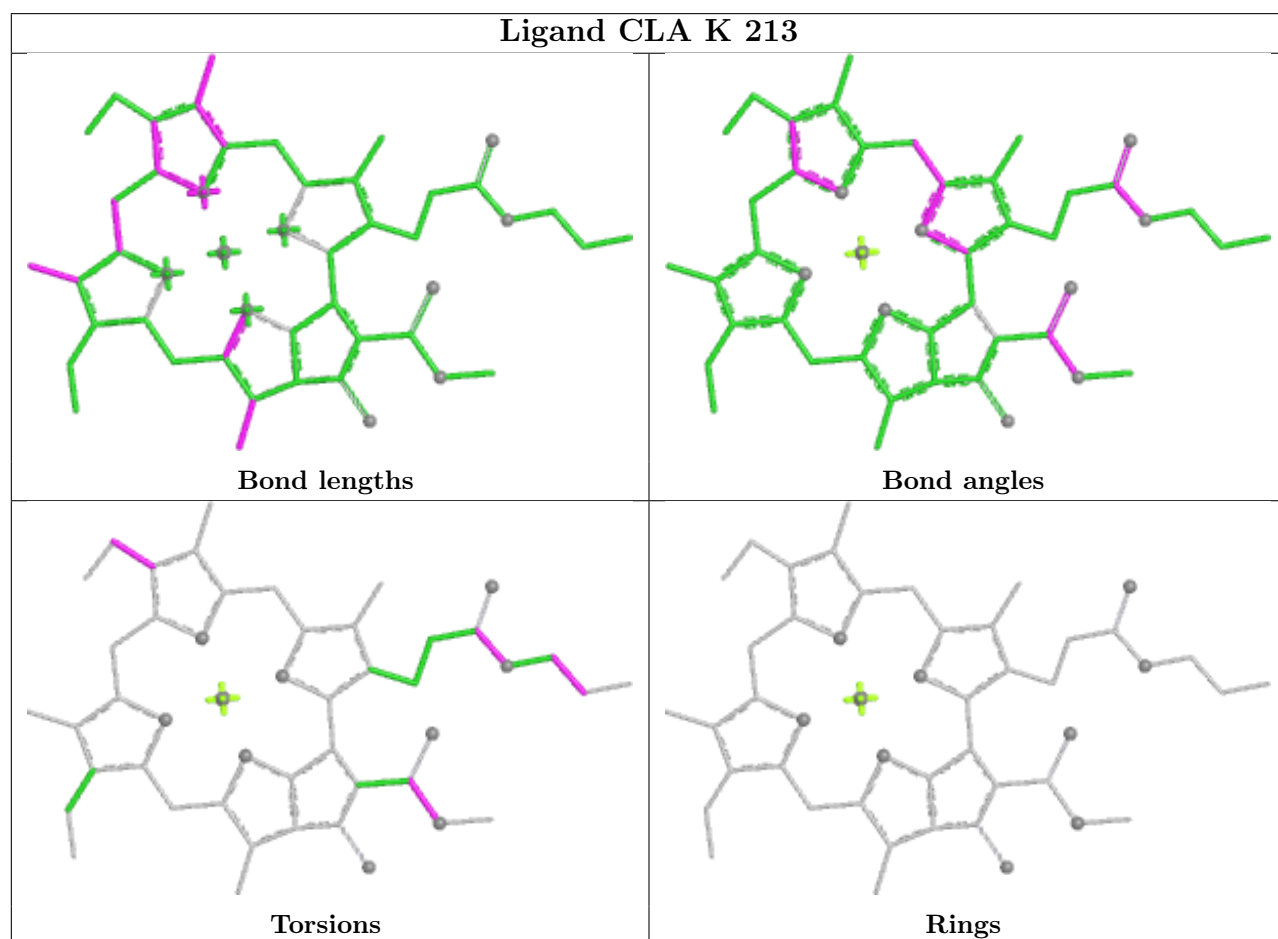
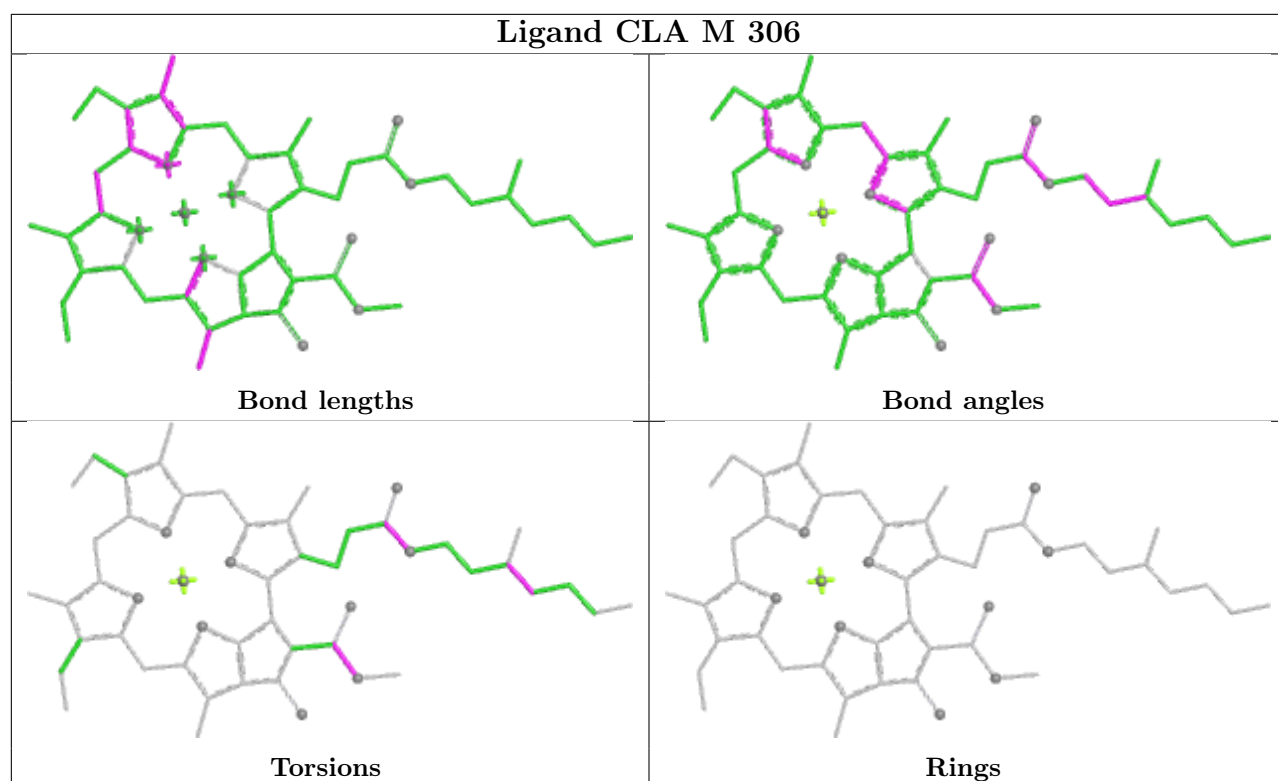
Bond angles

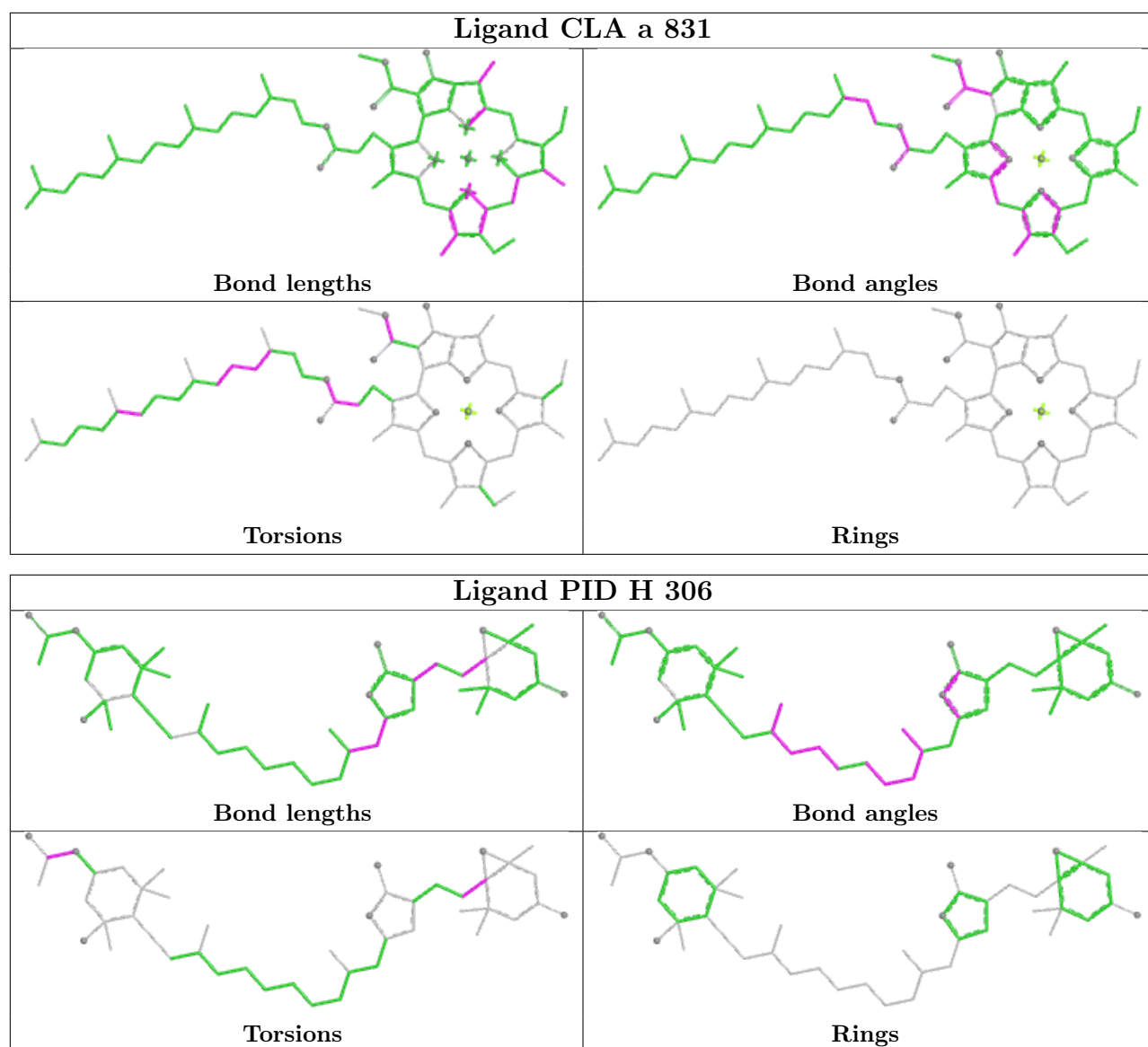


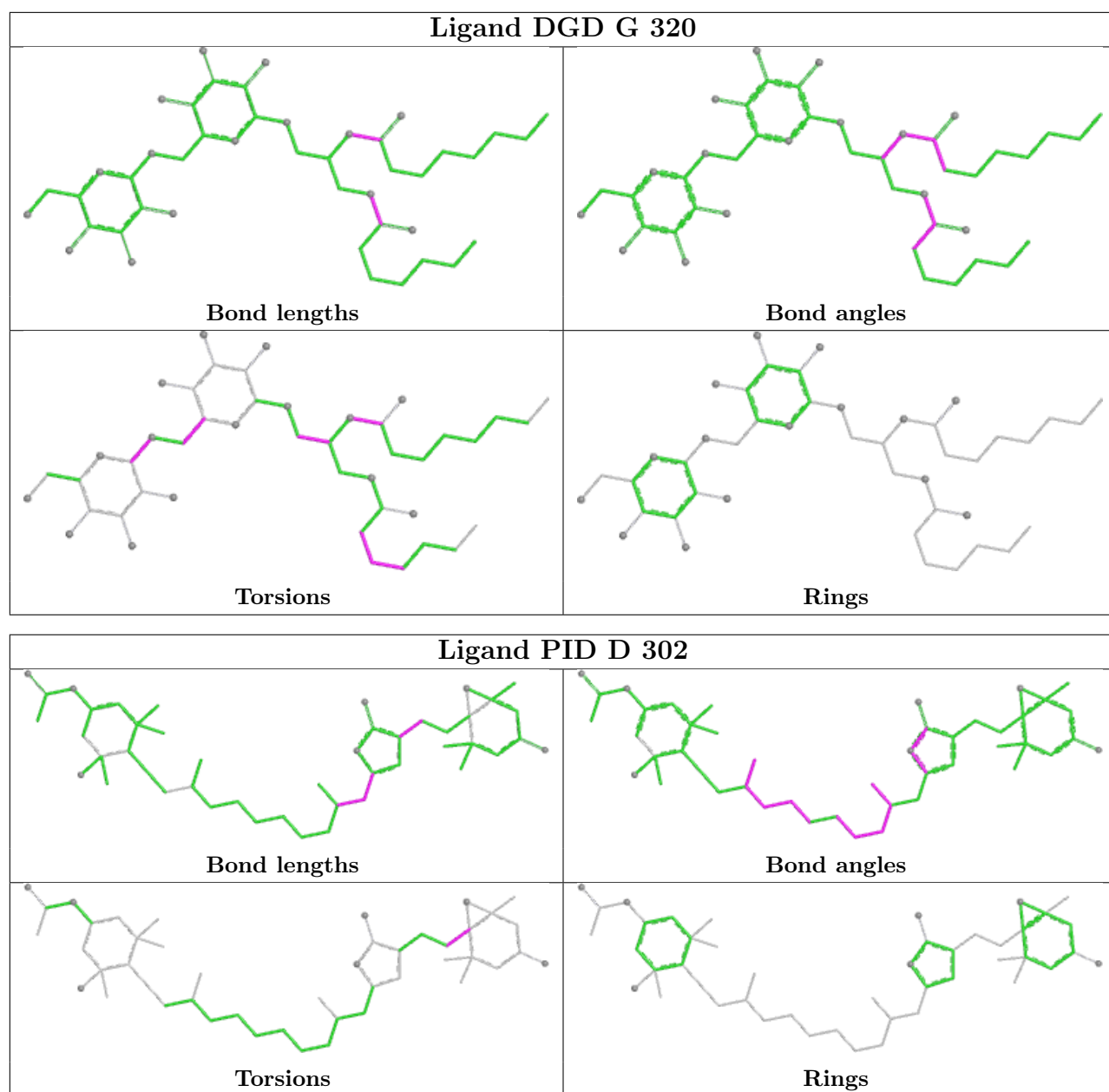
Torsions



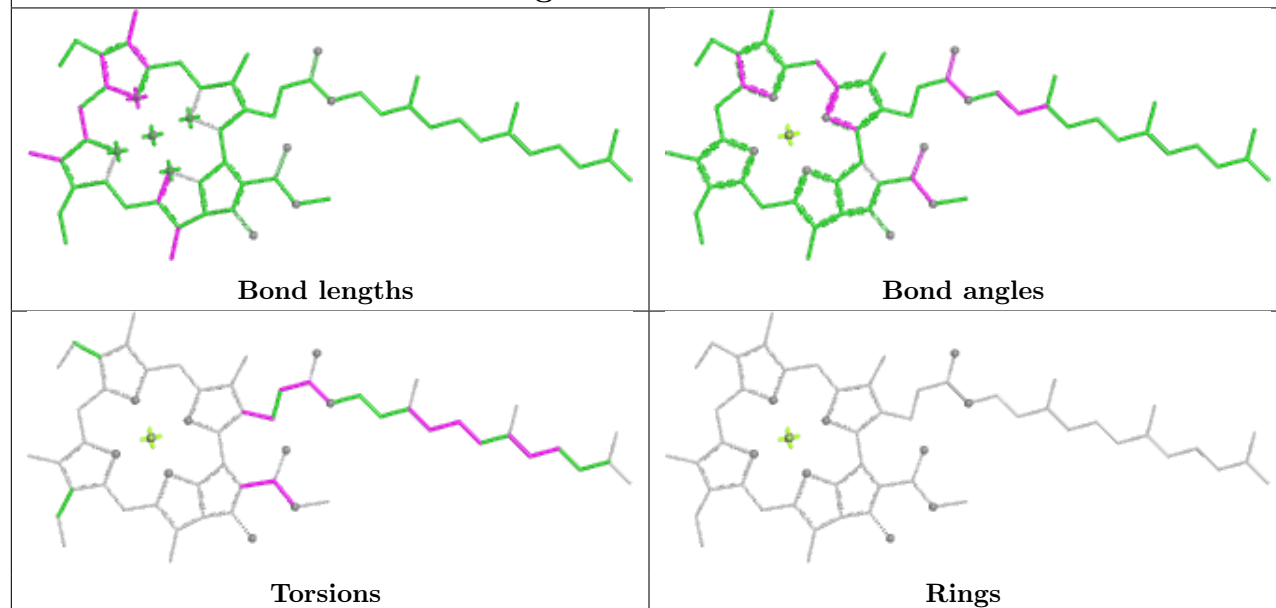
Rings



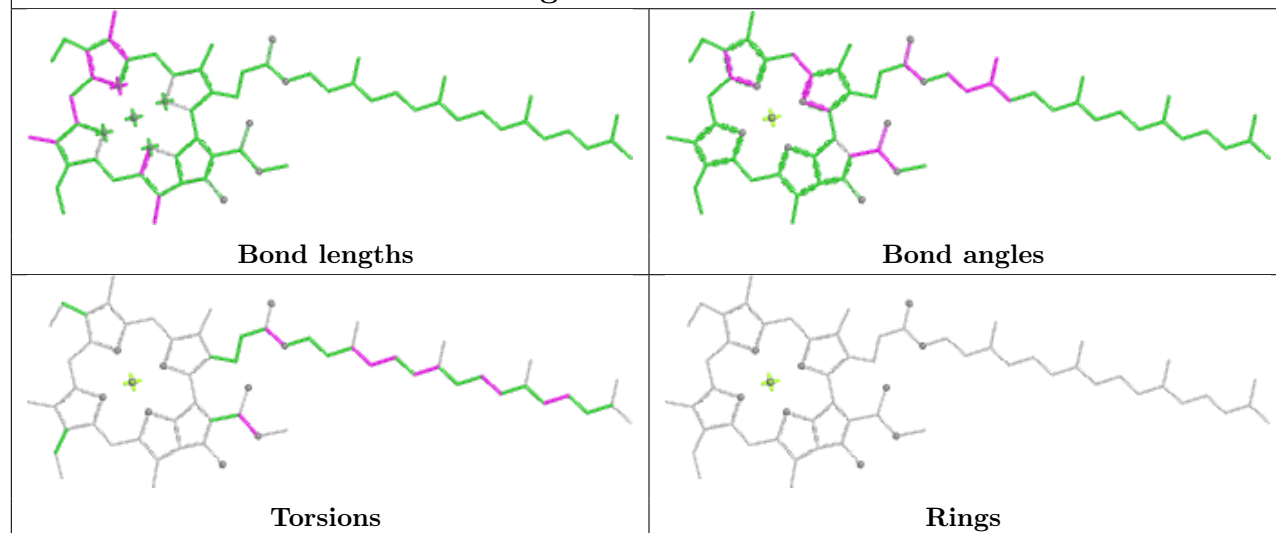


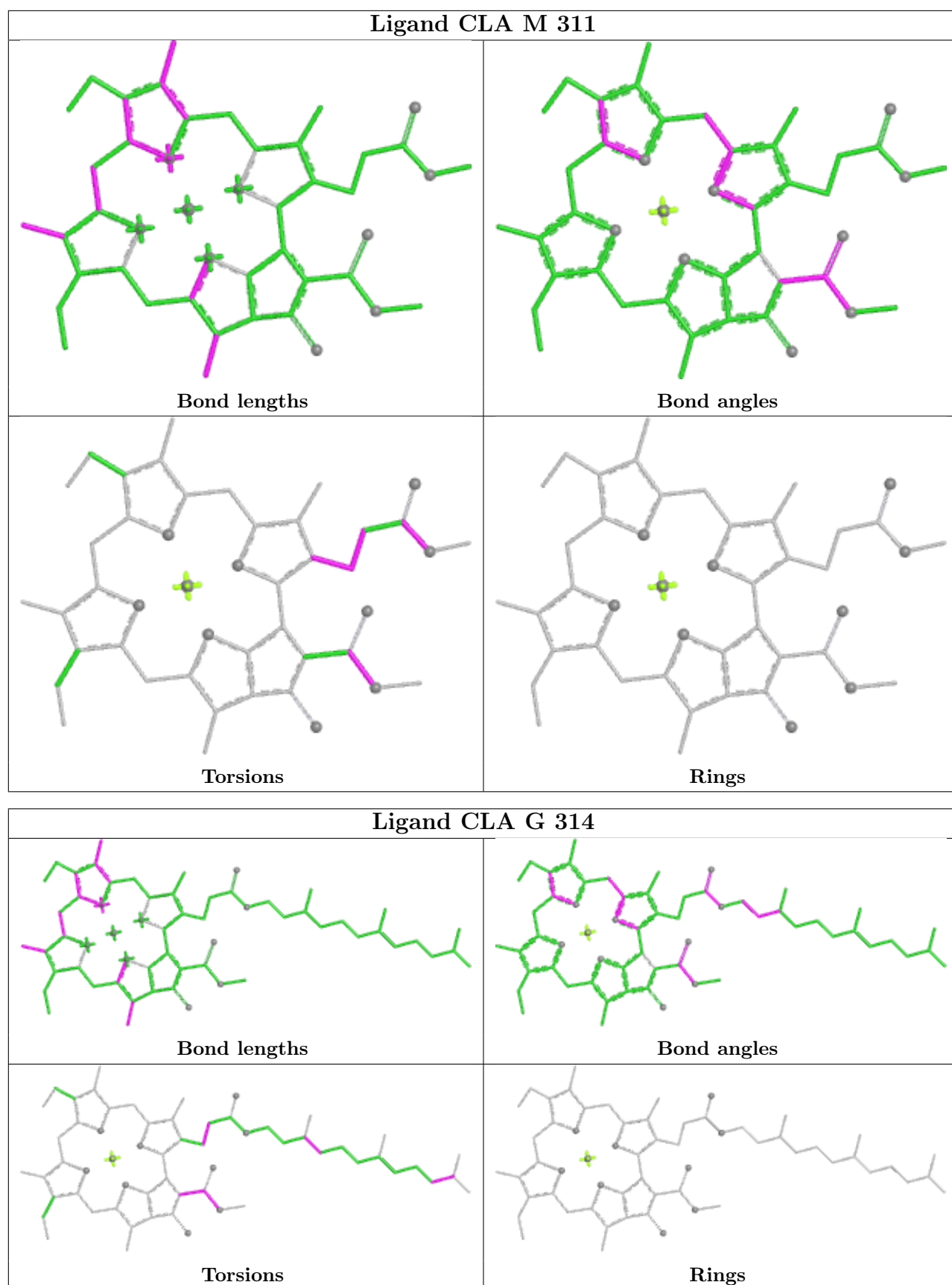


Ligand CLA b 709

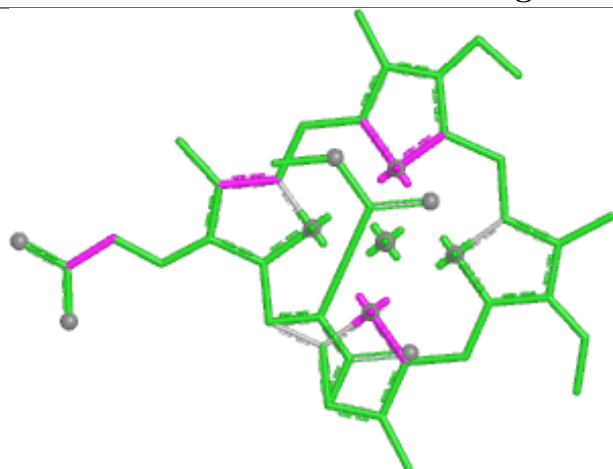


Ligand CLA l 504

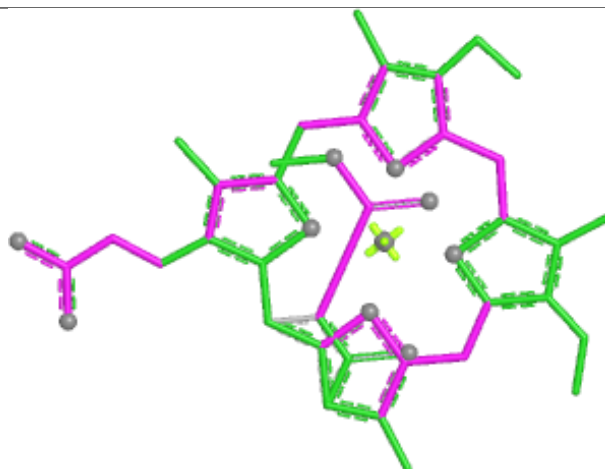




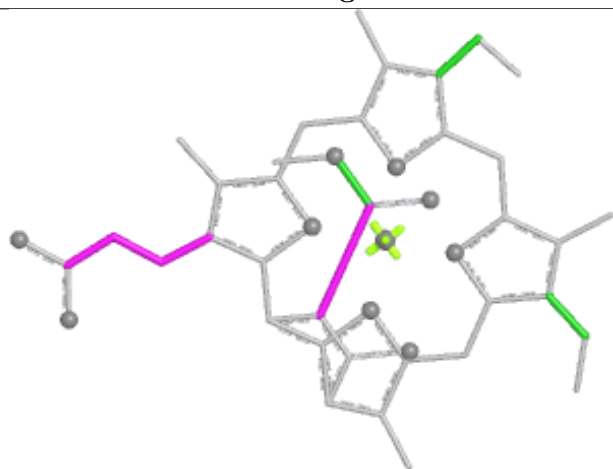
Ligand KC1 K 215



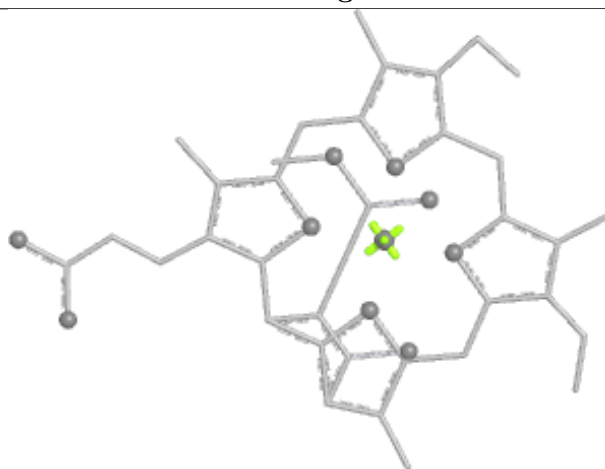
Bond lengths



Bond angles

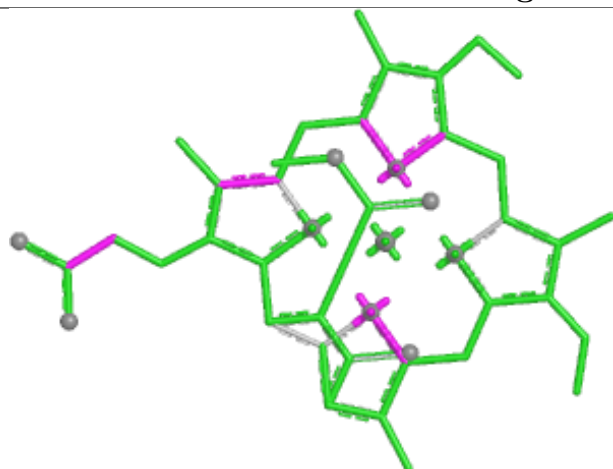


Torsions

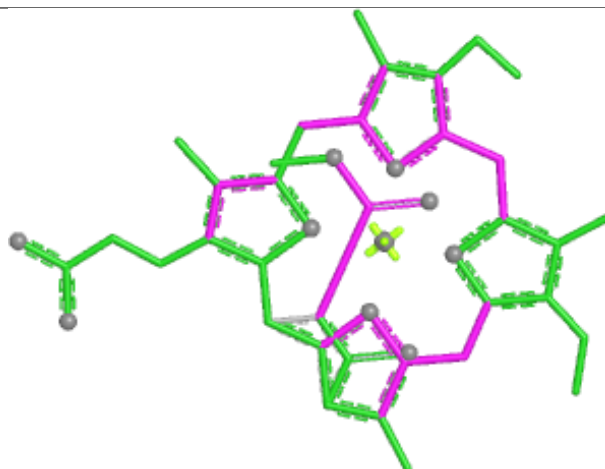


Rings

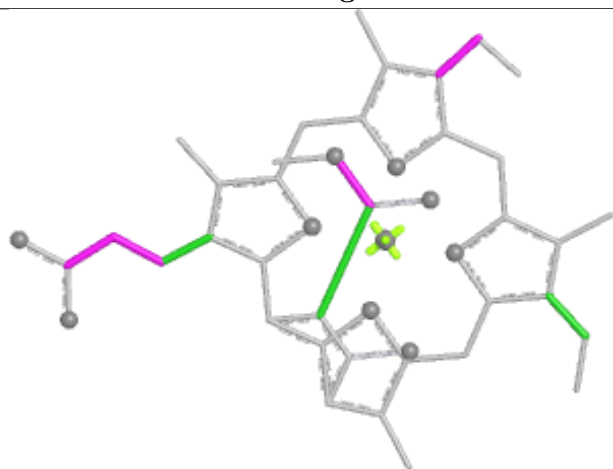
Ligand KC1 B 313



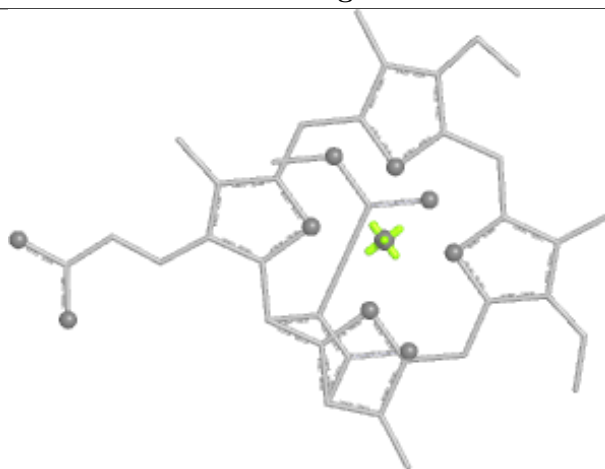
Bond lengths



Bond angles

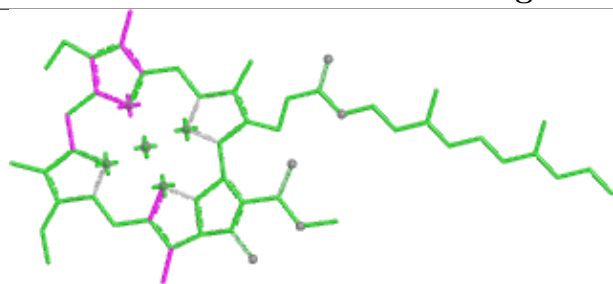


Torsions

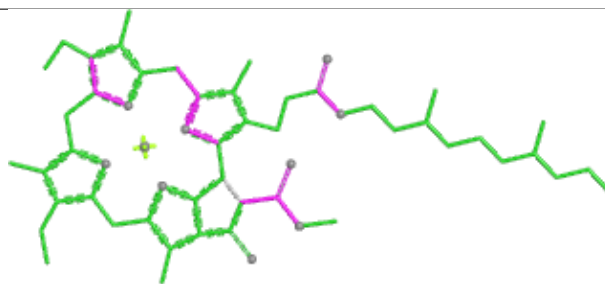


Rings

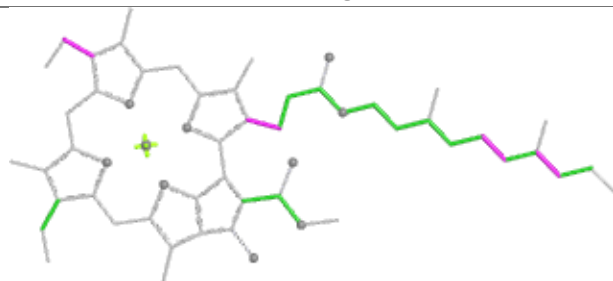
Ligand CLA E 315



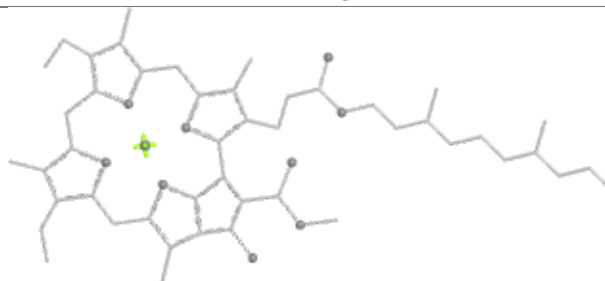
Bond lengths



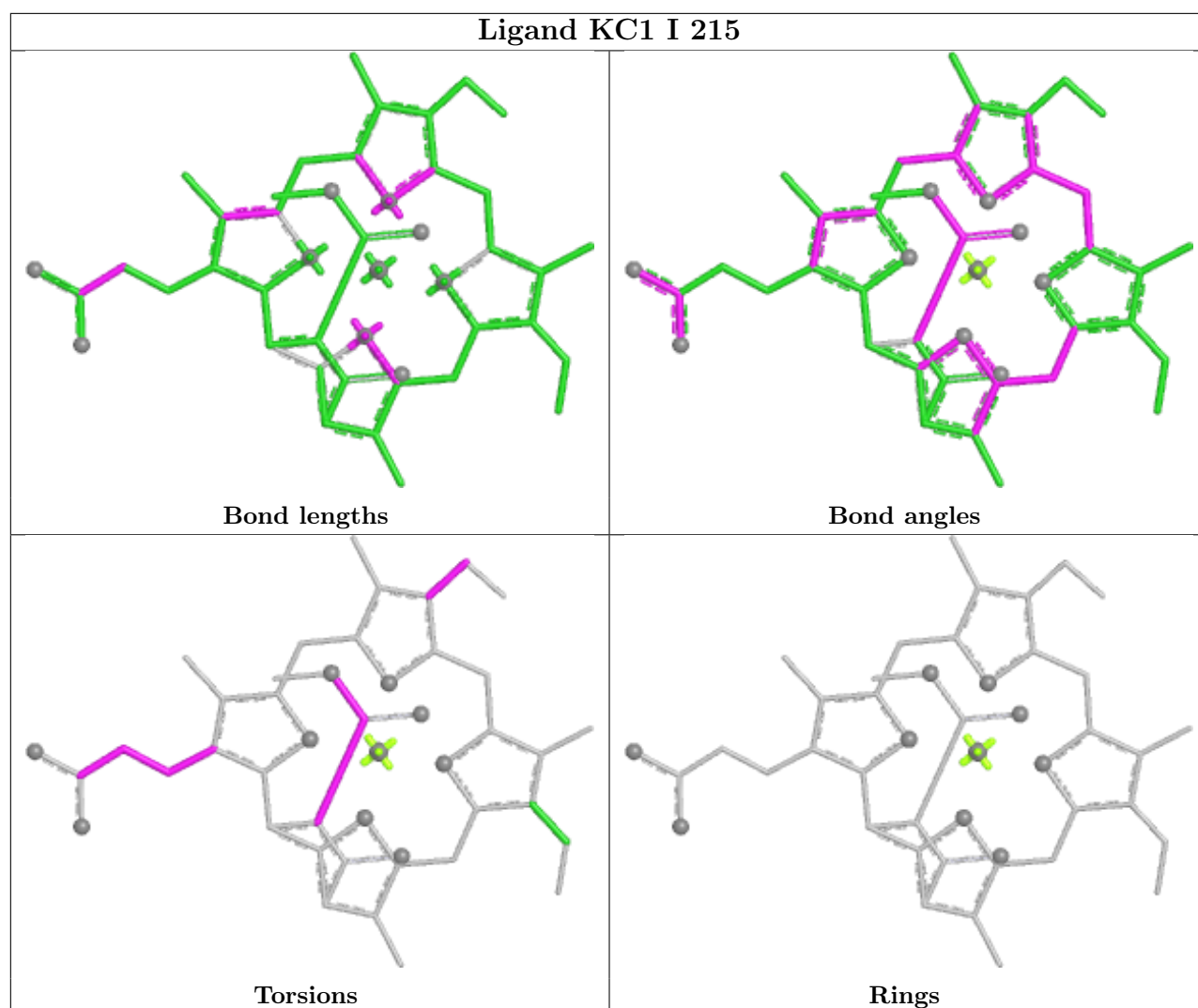
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

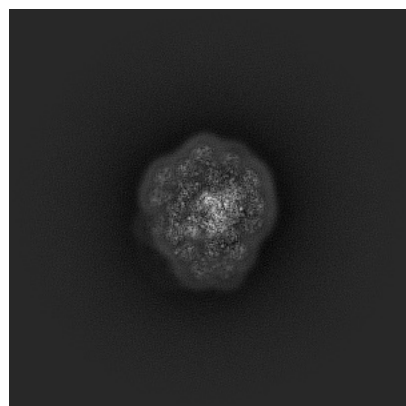
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36678. These allow visual inspection of the internal detail of the map and identification of artifacts.

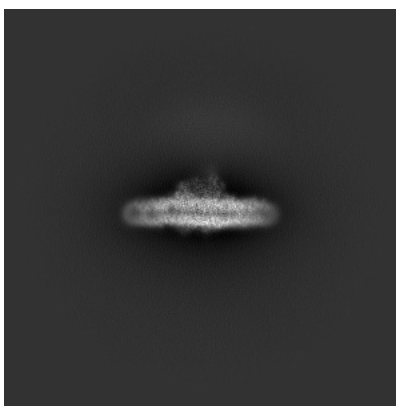
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

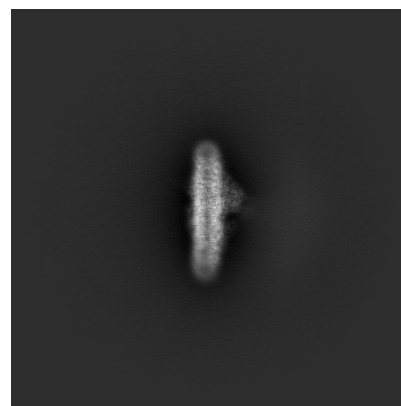
6.1.1 Primary map



X

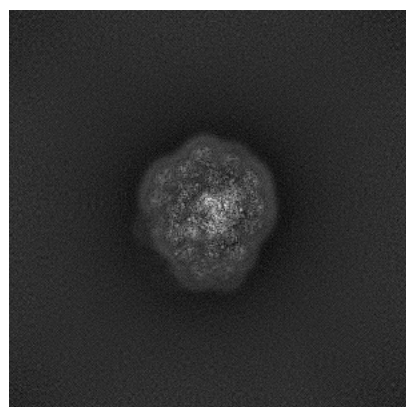


Y

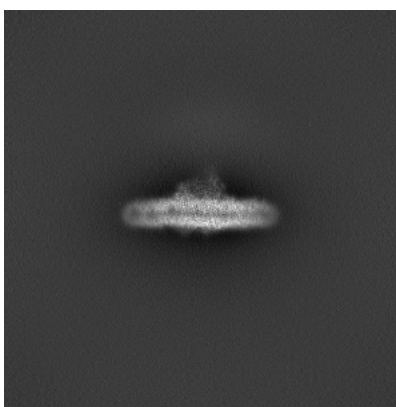


Z

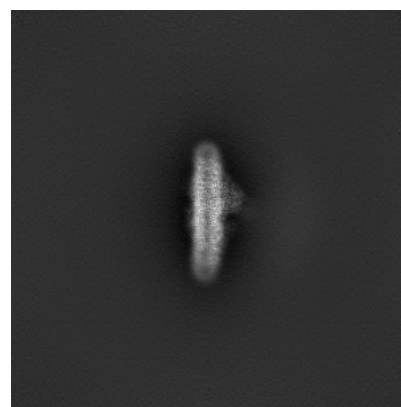
6.1.2 Raw map



X



Y

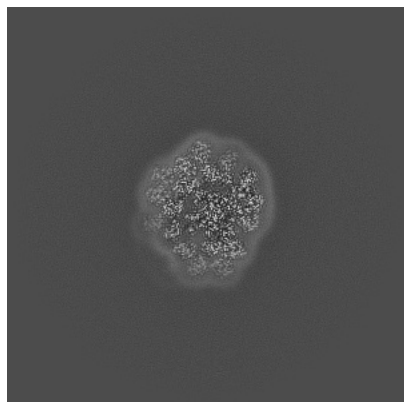


Z

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

6.2 Central slices [i](#)

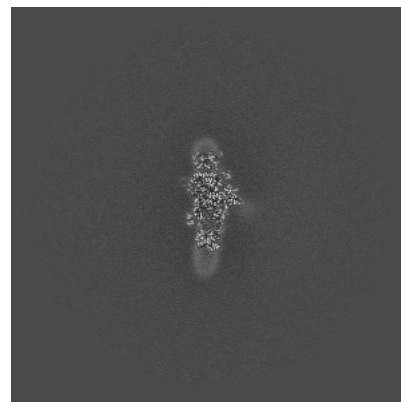
6.2.1 Primary map



X Index: 256

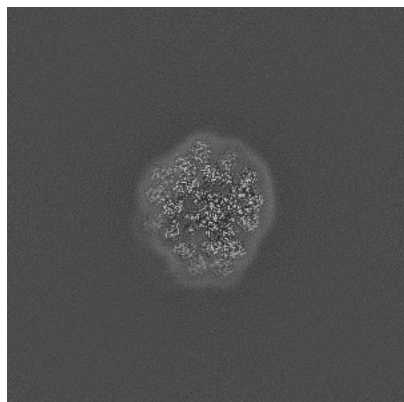


Y Index: 256

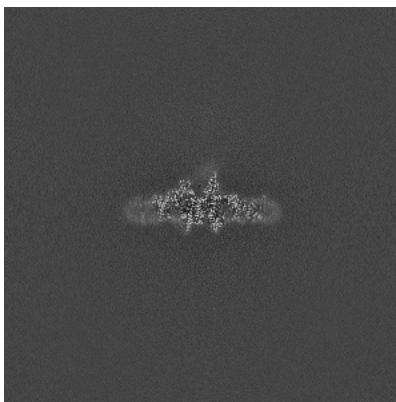


Z Index: 256

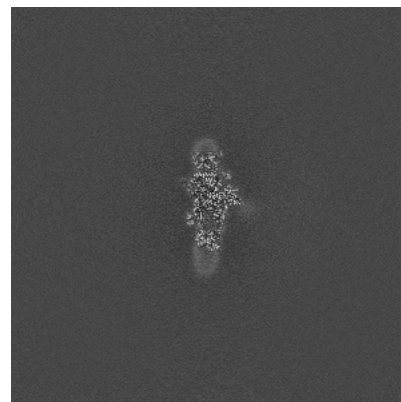
6.2.2 Raw map



X Index: 256



Y Index: 256

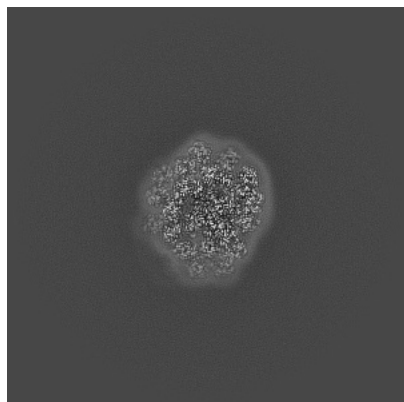


Z Index: 256

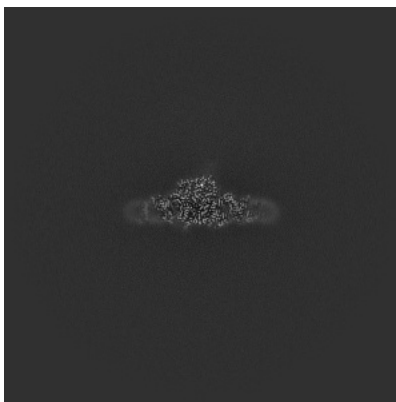
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

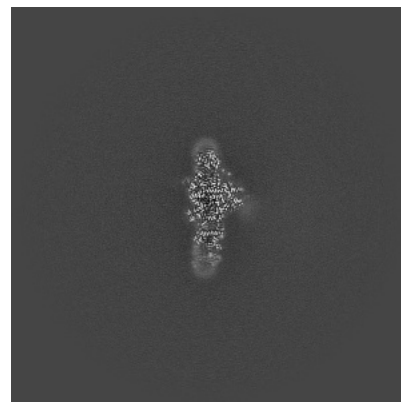
6.3.1 Primary map



X Index: 259

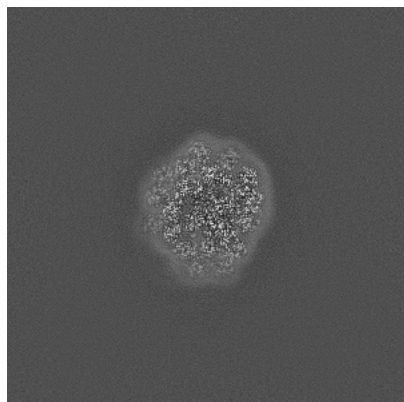


Y Index: 262

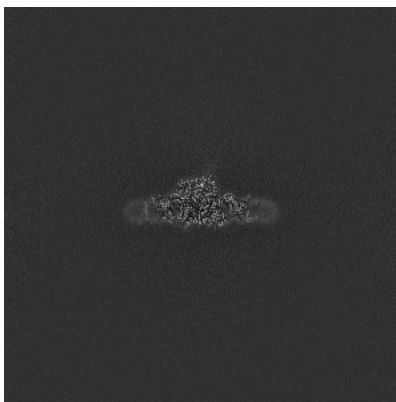


Z Index: 262

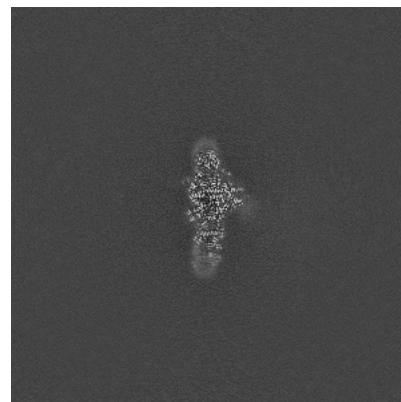
6.3.2 Raw map



X Index: 259



Y Index: 262

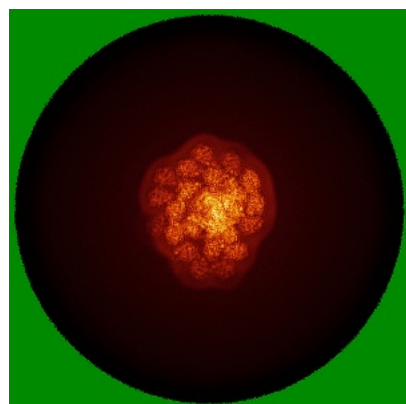


Z Index: 262

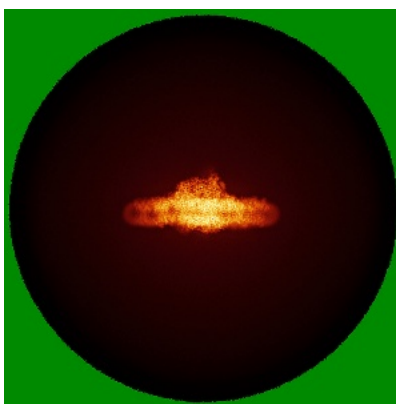
The images above show the largest variance slices of the map in three orthogonal directions.

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

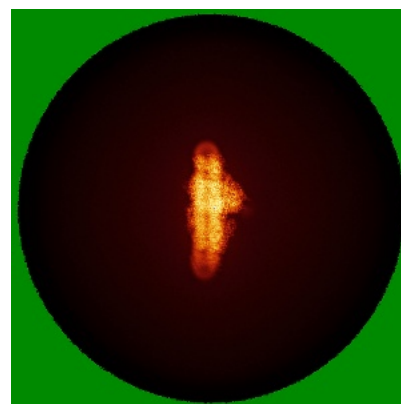
6.4.1 Primary map



X

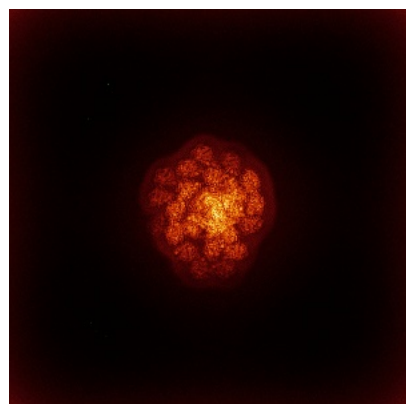


Y

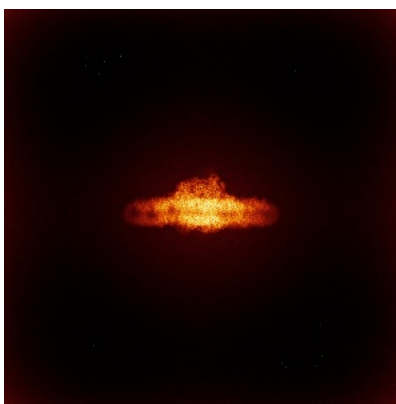


Z

6.4.2 Raw map



X



Y

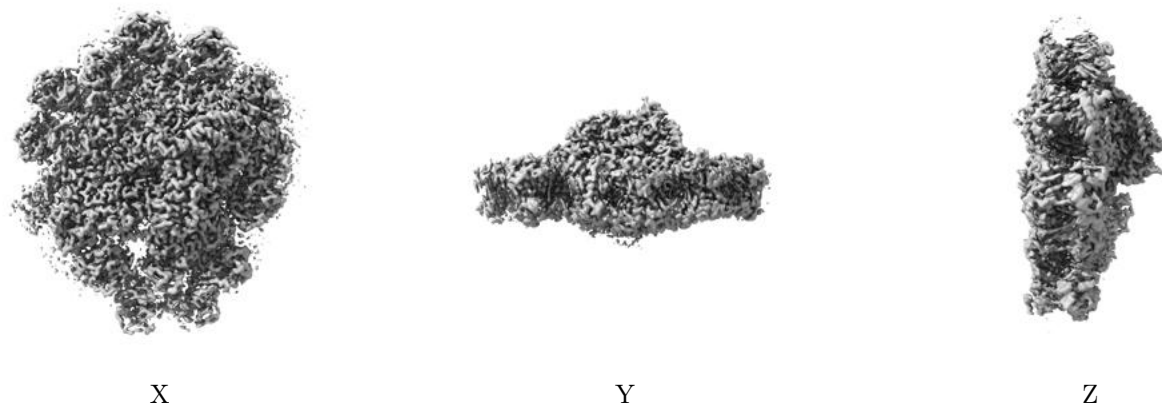


Z

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

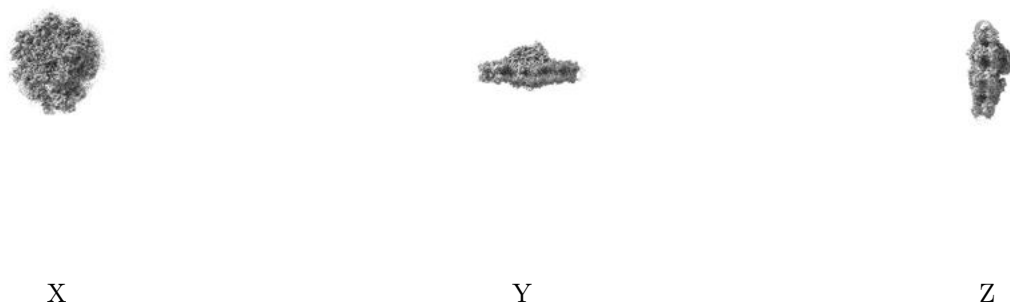
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

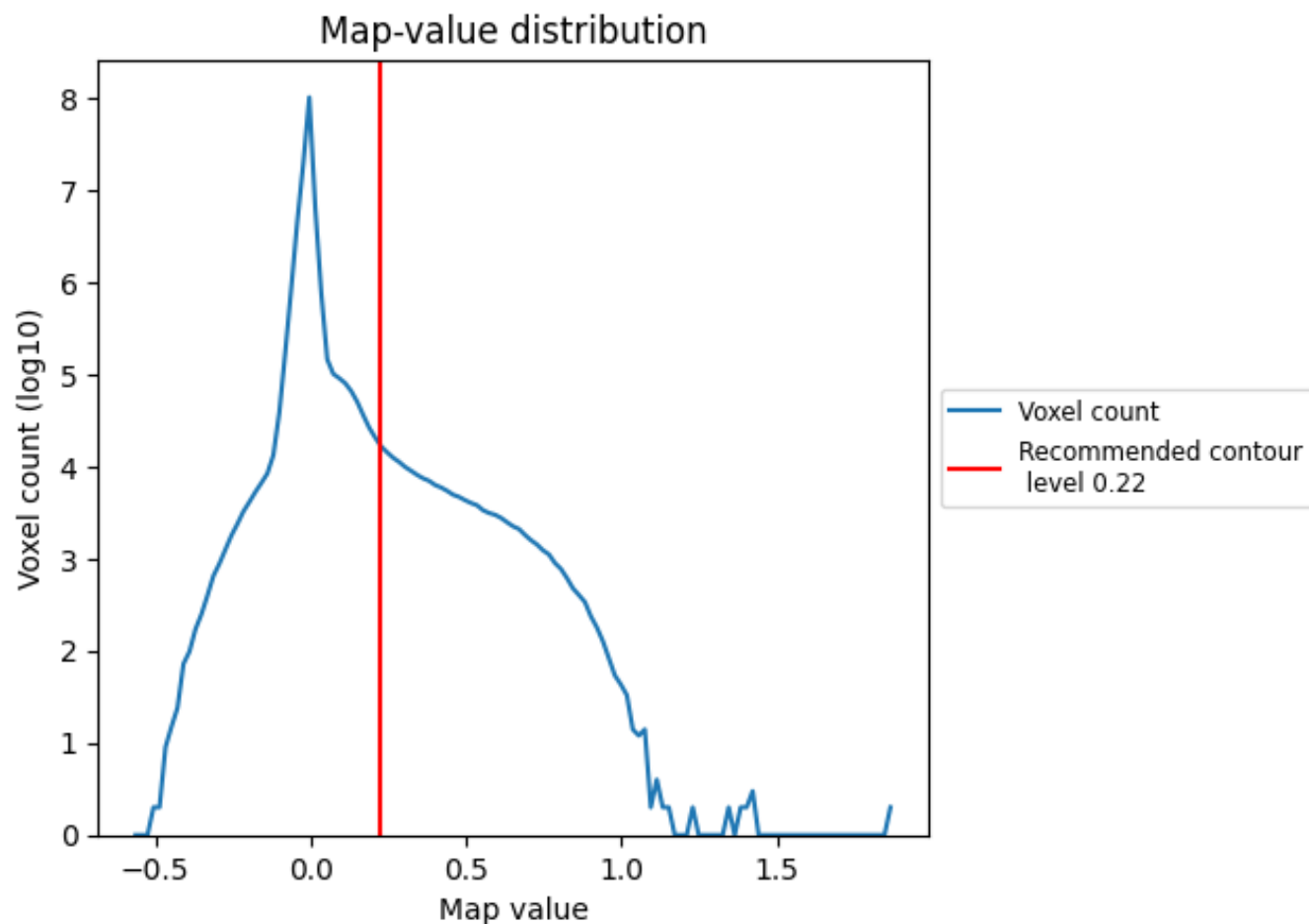
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

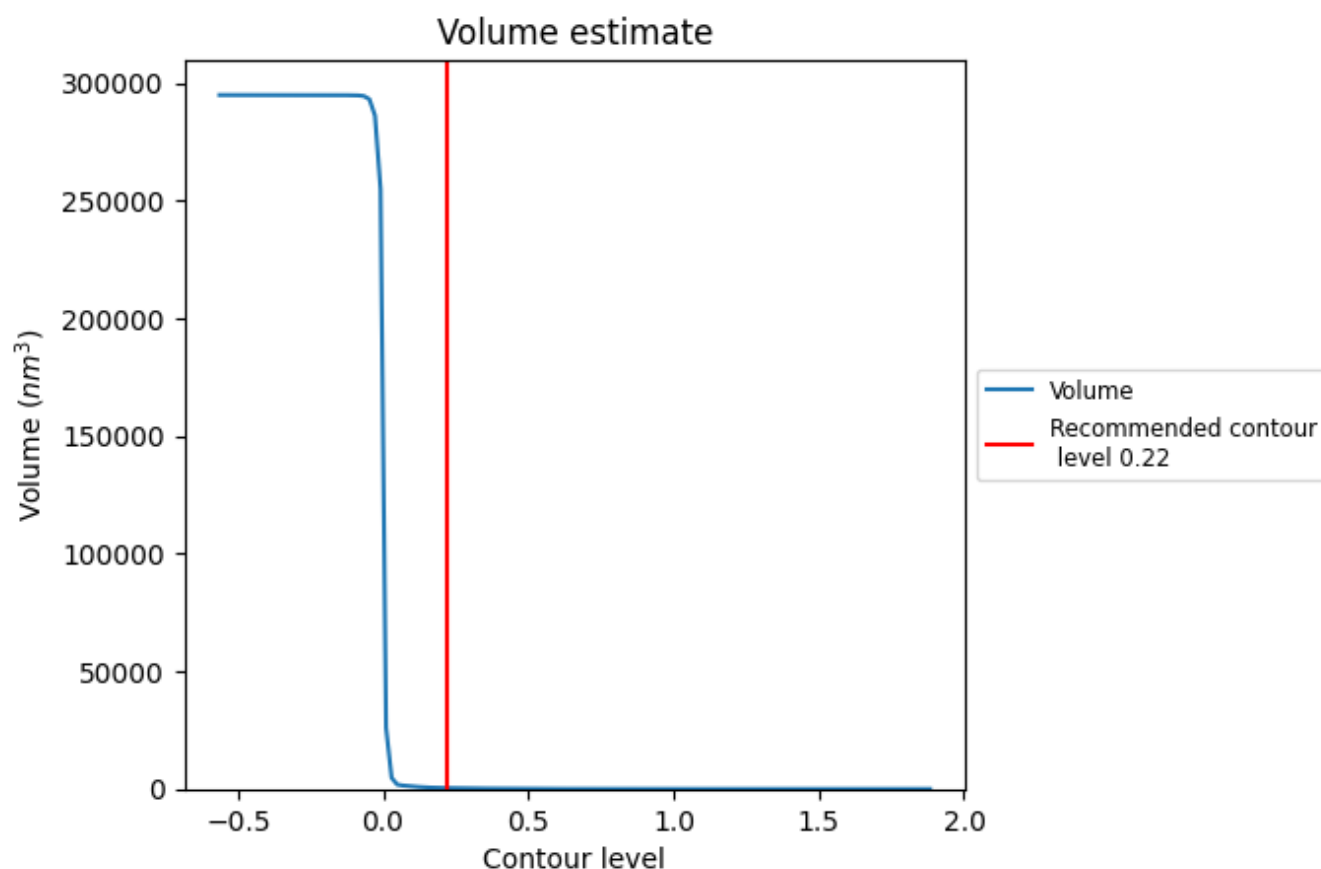
This section contains the results of statistical analysis of the map.

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.

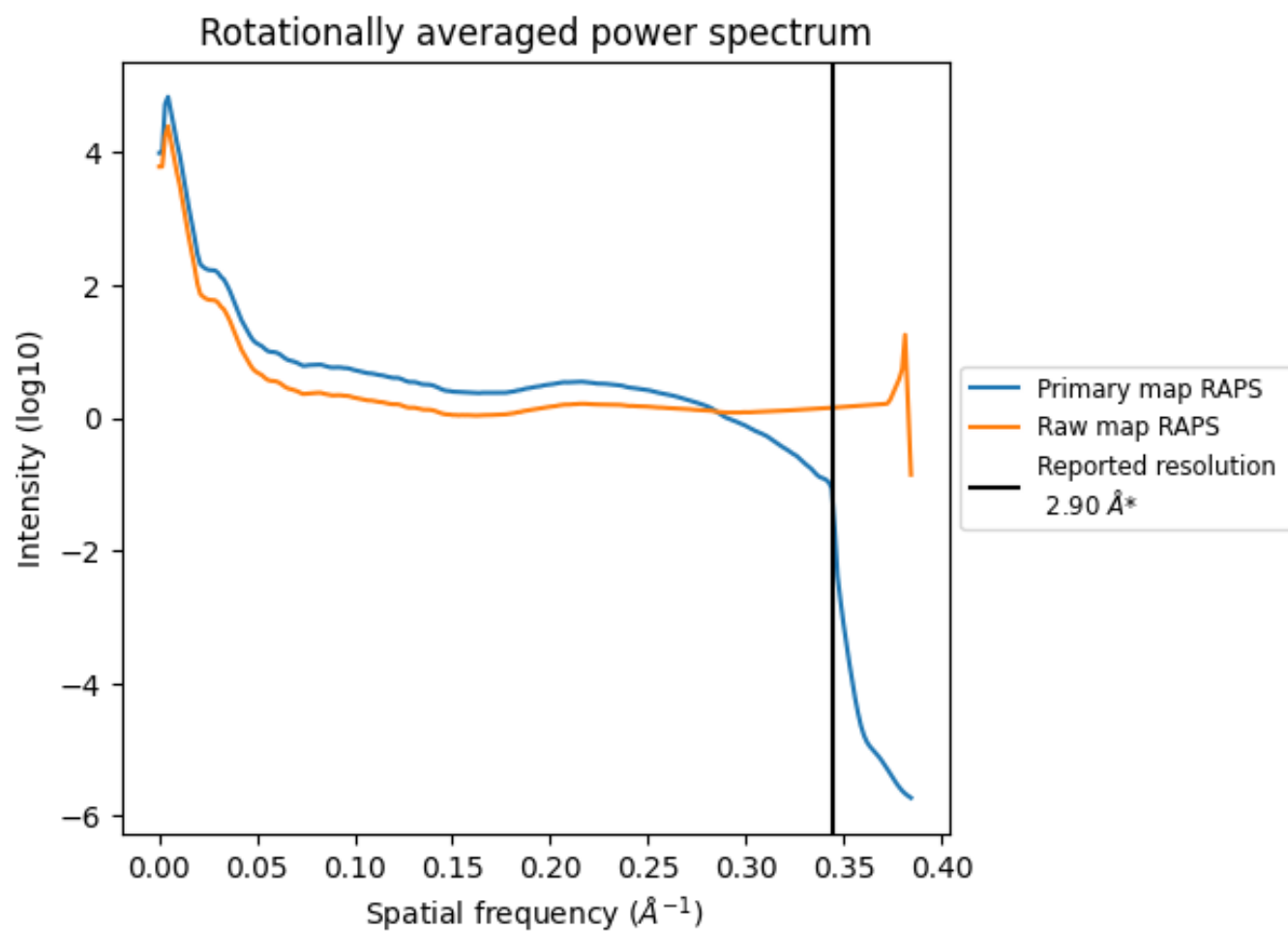
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm^3 ; this corresponds to an approximate mass of 342 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 ⓘ

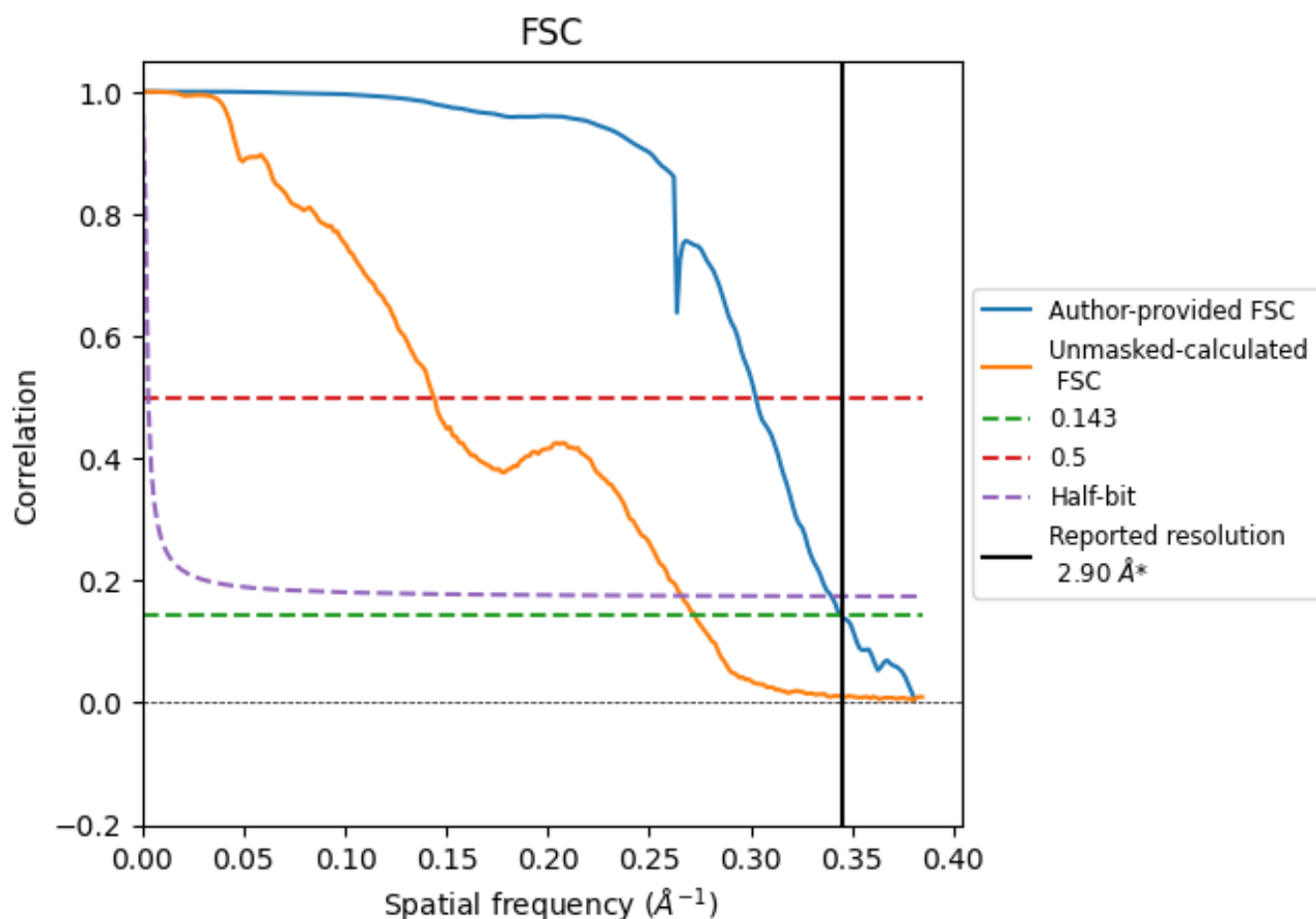


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

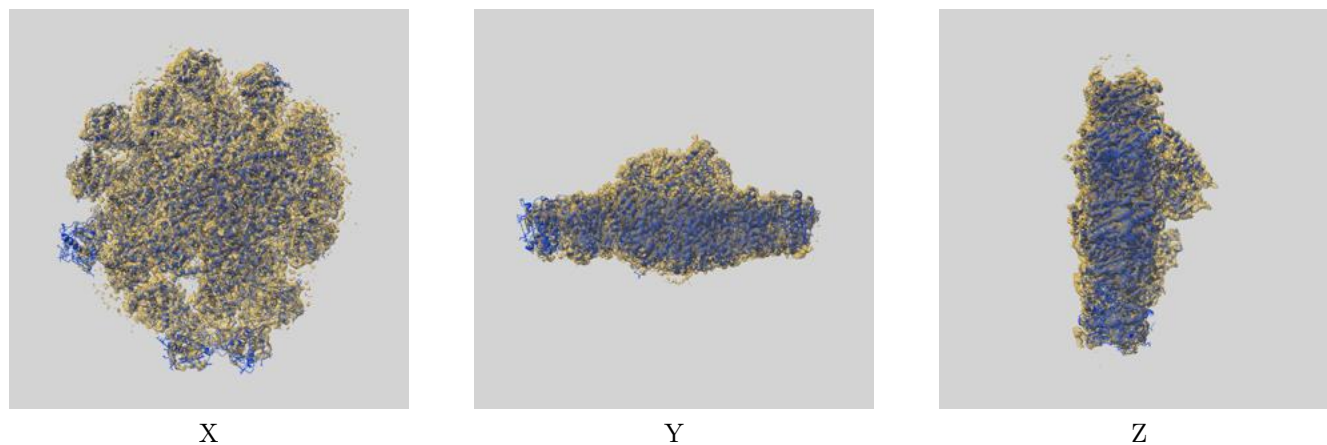
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.31	2.94
Unmasked-calculated*	3.67	6.95	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

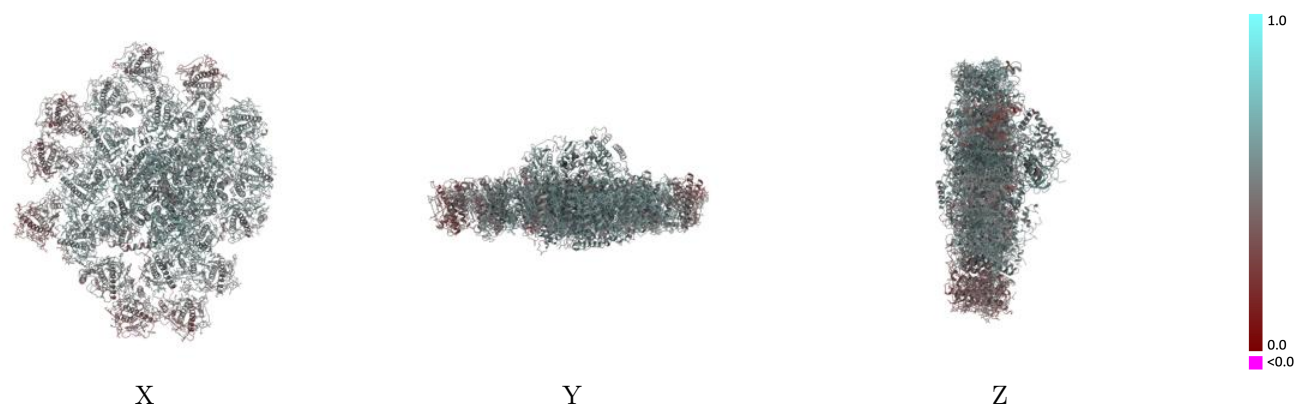
This section contains information regarding the fit between EMDB map EMD-36678 and PDB model 8JW0. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



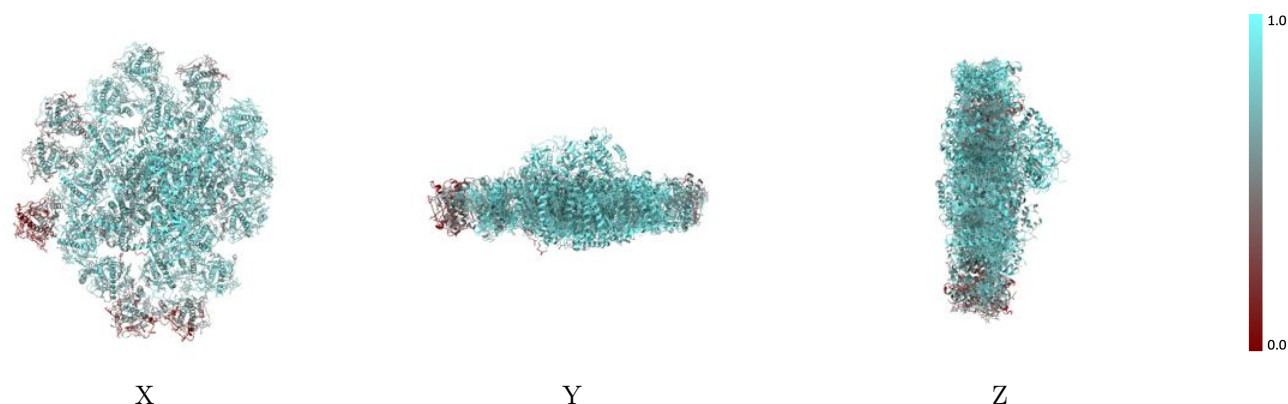
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



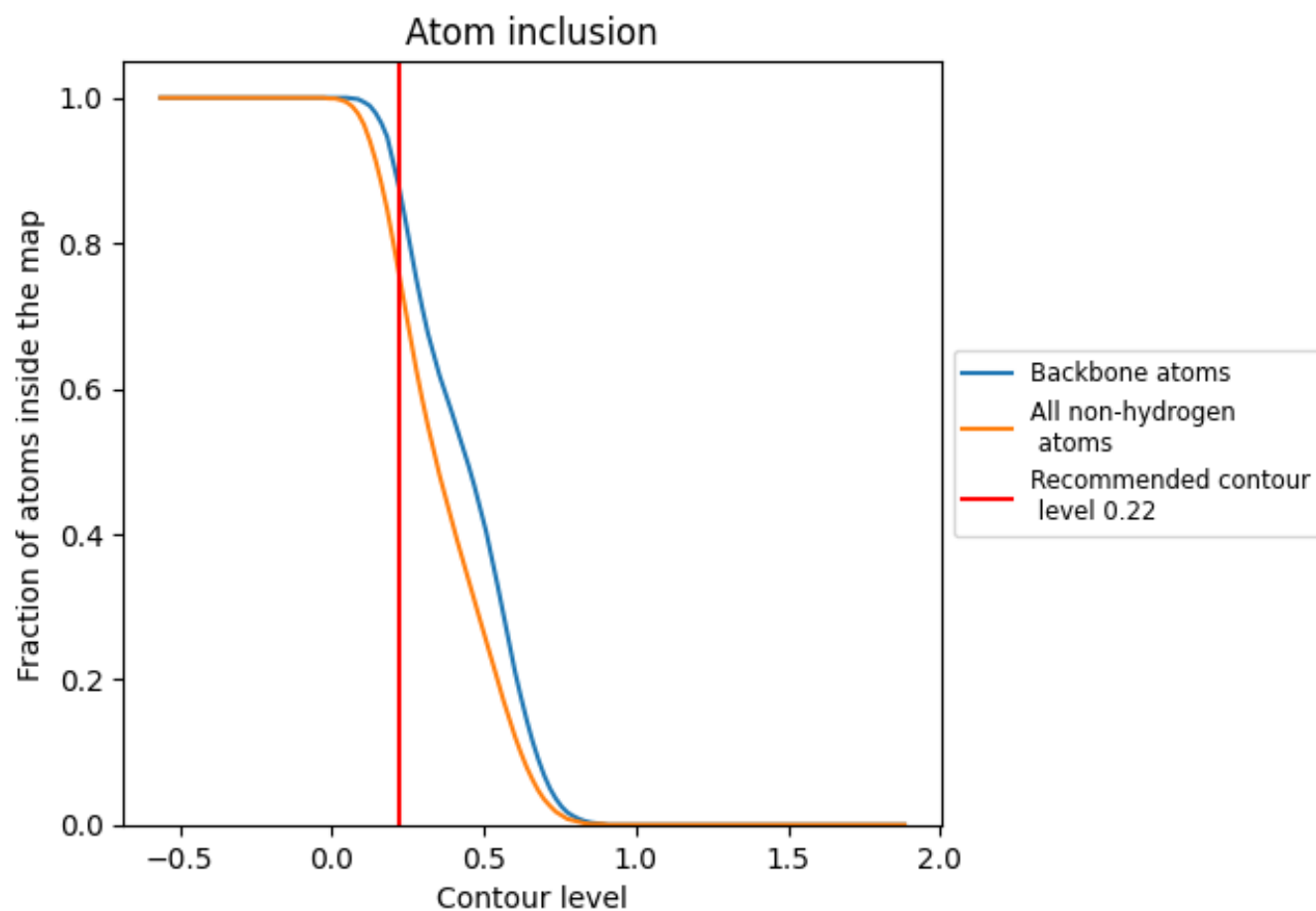
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7610	 0.5100
A	 0.8530	 0.5420
B	 0.8250	 0.5400
C	 0.7340	 0.4710
D	 0.6420	 0.4360
E	 0.7510	 0.5040
F	 0.7860	 0.5010
G	 0.8350	 0.5470
H	 0.3850	 0.3860
I	 0.8550	 0.5520
J	 0.8020	 0.5160
K	 0.8480	 0.5520
L	 0.8120	 0.5330
M	 0.7040	 0.4660
N	 0.4320	 0.3830
O	 0.5950	 0.4070
P	 0.2580	 0.3780
Q	 0.8000	 0.5110
T	 0.5580	 0.3790
a	 0.8120	 0.5450
b	 0.8740	 0.5690
c	 0.9430	 0.5590
d	 0.8890	 0.5480
e	 0.9090	 0.5690
f	 0.8360	 0.5440
h	 0.8700	 0.5530
i	 0.8300	 0.5450
j	 0.8020	 0.5450
l	 0.8340	 0.5370
m	 0.7750	 0.5380

