



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:24 PM UTC

PDB ID : 7PIN / pdb_00007pin
EMDB ID : EMD-13444
Title : Stacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-22
Resolution : 3.60 Å (reported)
Based on initial model : 6KAC

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

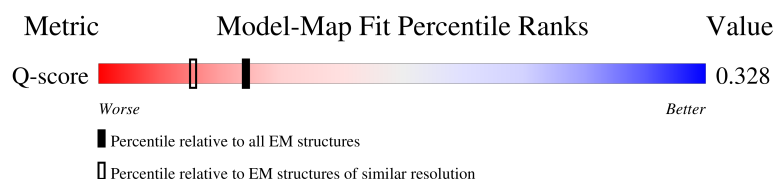
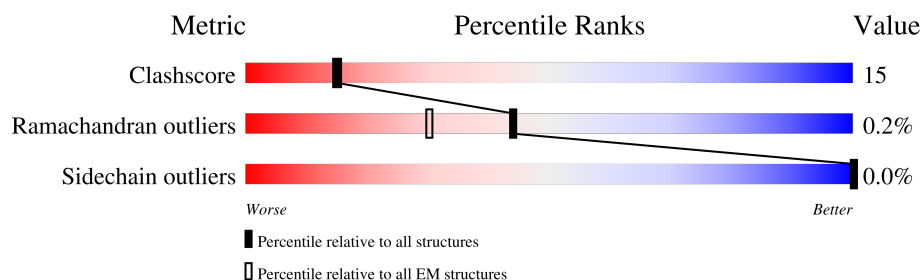
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	336	61% 70% 30%
1	A1	336	61% 63% 37%
1	a	336	54% 74% 26%
1	a1	336	70% 58% 42%

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Mol	Chain	Length	Quality of chain
2	B	484	74% 75% 25%
2	B1	484	66% 63% 37%
2	b	484	70% 69% 31%
2	b1	484	71% 68% 32%
3	V	32	94% 84% 16%
3	V1	32	69% 66% 34%
3	v	32	84% 84% 16%
3	v1	32	94% 59% 41%
4	C	449	55% 79% 21%
4	C1	449	42% 61% 38%
4	c	449	55% 81% 19%
4	c1	449	66% 63% 36%
5	D	348	63% 81% 19%
5	D1	348	63% 63% 37%
5	d	348	61% 73% 27%
5	d1	348	75% 61% 39%
6	E	76	92% 59% 41%
6	E1	76	50% 74% 26%
6	e	76	93% 75% 25%
6	e1	76	76% 67% 33%
7	F	31	74% 71% 29%
7	F1	31	58% 71% 29%
7	f	31	90% 52% 48%
7	f1	31	71% 58% 42%
8	H	67	84% 69% 31%

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Mol	Chain	Length	Quality of chain
8	H1	67	78% 63% 37%
8	h	67	88% 81% 19%
8	h1	67	84% 64% 36%
9	I	35	57% 80% 20%
9	I1	35	71% 54% 46%
9	i	35	60% 94% 6%
9	i1	35	74% 71% 29%
10	J	36	89% 83% 17%
10	J1	36	81% 75% 25%
10	j	36	86% 92% 8%
10	j1	36	81% 64% 36%
11	K	37	81% 78% 22%
11	K1	37	41% 68% 32%
11	k	37	76% 86% 14%
11	k1	37	73% 70% 30%
12	L	38	71% 84% 16%
12	L1	38	79% 74% 26%
12	l	38	74% 74% 26%
13	M	31	87% 84% 16%
13	M1	31	84% 74% 26%
13	m	31	84% 71% 29%
13	m1	31	77% 74% 26%
14	O	238	92% 77% 22%
14	O1	238	67% 65% 35%
14	o	238	94% 77% 23%

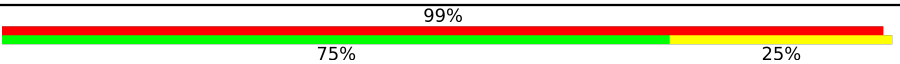
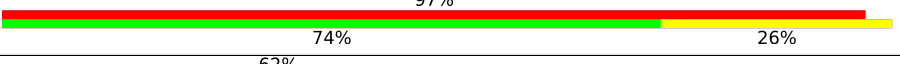
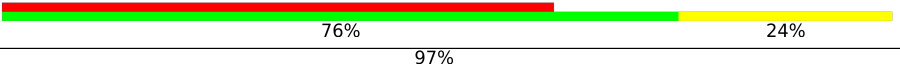
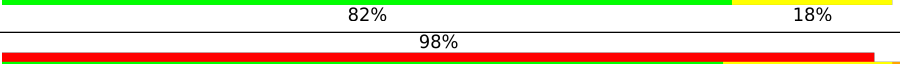
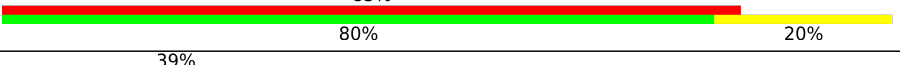
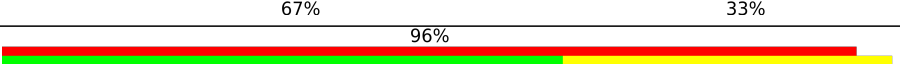
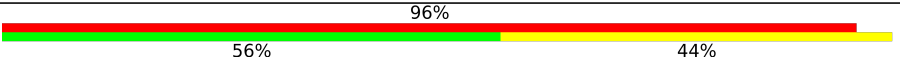
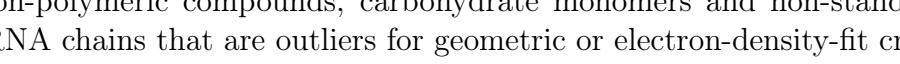
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Mol	Chain	Length	Quality of chain
14	o1	238	72% 72% 28%
15	P	187	100% 77% 23%
15	P1	187	98% 75% 25%
15	p	187	100% 72% 28%
15	p1	187	99% 73% 27%
16	T	30	83% 90% 10%
16	T1	30	83% 67% 33%
16	t	30	90% 70% 30%
16	t1	30	80% 77% 23%
17	W	44	95% 84% 16%
17	W1	44	75% 64% 36%
17	w	44	86% 73% 27%
17	w1	44	82% 57% 43%
18	X	30	97% 97% .
18	X1	30	57% 70% 30%
18	x	30	100% 67% 33%
18	x1	30	83% 77% 23%
19	Z	61	90% 90% 10%
19	Z1	61	52% 77% 23%
19	z	61	87% 87% 13%
19	z1	61	84% 80% 20%
20	N	222	94% 75% 25%
20	N1	222	37% 65% 34%
20	n	222	89% 77% 23%
20	n1	222	55% 65% 34%

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Mol	Chain	Length	Quality of chain
21	G	221	
21	G1	221	
21	g	221	
21	g1	221	
22	R	196	
22	R1	196	
22	r	196	
22	r1	196	
23	S	243	
23	S1	243	
23	s	243	
23	s1	243	
24	Y	222	
24	Y1	222	
24	y	222	
24	y1	222	
25	U	27	
25	U1	27	
25	u	27	
25	u1	27	

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	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	410	X	-	-	-
29	CLA	A1	405	X	-	-	-
29	CLA	A1	406	X	-	-	-
29	CLA	A1	407	X	-	-	-
29	CLA	A1	410	X	-	-	-
29	CLA	B	602	X	-	-	-
29	CLA	B	603	X	-	-	-
29	CLA	B	604	X	-	-	-
29	CLA	B	605	X	-	-	-
29	CLA	B	606	X	-	-	-
29	CLA	B	607	X	-	-	-
29	CLA	B	608	X	-	-	-
29	CLA	B	609	X	-	-	-
29	CLA	B	610	X	-	-	-
29	CLA	B	611	X	-	-	-
29	CLA	B	612	X	-	-	-
29	CLA	B	613	X	-	-	-
29	CLA	B	614	X	-	-	-
29	CLA	B	615	X	-	-	-
29	CLA	B	616	X	-	-	-
29	CLA	B	617	X	-	-	-
29	CLA	B1	602	X	-	-	-
29	CLA	B1	603	X	-	-	-
29	CLA	B1	604	X	-	-	-
29	CLA	B1	605	X	-	-	-
29	CLA	B1	606	X	-	-	-
29	CLA	B1	607	X	-	-	-
29	CLA	B1	608	X	-	-	-
29	CLA	B1	609	X	-	-	-
29	CLA	B1	610	X	-	-	-
29	CLA	B1	611	X	-	-	-
29	CLA	B1	612	X	-	-	-
29	CLA	B1	613	X	-	-	-
29	CLA	B1	614	X	-	-	-
29	CLA	B1	615	X	-	-	-
29	CLA	B1	616	X	-	-	-
29	CLA	B1	617	X	-	-	-
29	CLA	C	501	X	-	-	-
29	CLA	C	502	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	504	X	-	-	-
29	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	C	506	X	-	-	-
29	CLA	C	507	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	C1	501	X	-	-	-
29	CLA	C1	502	X	-	-	-
29	CLA	C1	503	X	-	-	-
29	CLA	C1	504	X	-	-	-
29	CLA	C1	505	X	-	-	-
29	CLA	C1	506	X	-	-	-
29	CLA	C1	507	X	-	-	-
29	CLA	C1	508	X	-	-	-
29	CLA	C1	509	X	-	-	-
29	CLA	C1	510	X	-	-	-
29	CLA	C1	511	X	-	-	-
29	CLA	C1	512	X	-	-	-
29	CLA	C1	513	X	-	-	-
29	CLA	D	402	X	-	-	-
29	CLA	D	403	X	-	-	-
29	CLA	D1	402	X	-	-	-
29	CLA	D1	403	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	G1	602	X	-	-	-
29	CLA	G1	603	X	-	-	-
29	CLA	G1	604	X	-	-	-
29	CLA	G1	610	X	-	-	-
29	CLA	G1	611	X	-	-	-
29	CLA	G1	612	X	-	-	-
29	CLA	G1	613	X	-	-	-
29	CLA	G1	614	X	-	-	-
29	CLA	N	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	N1	602	X	-	-	-
29	CLA	N1	603	X	-	-	-
29	CLA	N1	604	X	-	-	-
29	CLA	N1	610	X	-	-	-
29	CLA	N1	611	X	-	-	-
29	CLA	N1	612	X	-	-	-
29	CLA	N1	613	X	-	-	-
29	CLA	N1	614	X	-	-	-
29	CLA	R	602	X	-	-	-
29	CLA	R	603	X	-	-	-
29	CLA	R	604	X	-	-	-
29	CLA	R	608	X	-	-	-
29	CLA	R	609	X	-	-	-
29	CLA	R	610	X	-	-	-
29	CLA	R	612	X	-	-	-
29	CLA	R1	602	X	-	-	-
29	CLA	R1	603	X	-	-	-
29	CLA	R1	604	X	-	-	-
29	CLA	R1	608	X	-	-	-
29	CLA	R1	609	X	-	-	-
29	CLA	R1	610	X	-	-	-
29	CLA	R1	612	X	-	-	-
29	CLA	S	602	X	-	-	-
29	CLA	S	603	X	-	-	-
29	CLA	S	604	X	-	-	-
29	CLA	S	605	X	-	-	-
29	CLA	S	609	X	-	-	-
29	CLA	S	610	X	-	-	-
29	CLA	S	611	X	-	-	-
29	CLA	S	612	X	-	-	-
29	CLA	S	613	X	-	-	-
29	CLA	S	614	X	-	-	-
29	CLA	S	617	X	-	-	-
29	CLA	S1	602	X	-	-	-
29	CLA	S1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	S1	604	X	-	-	-
29	CLA	S1	605	X	-	-	-
29	CLA	S1	609	X	-	-	-
29	CLA	S1	610	X	-	-	-
29	CLA	S1	611	X	-	-	-
29	CLA	S1	612	X	-	-	-
29	CLA	S1	613	X	-	-	-
29	CLA	S1	614	X	-	-	-
29	CLA	S1	617	X	-	-	-
29	CLA	Y	602	X	-	-	-
29	CLA	Y	603	X	-	-	-
29	CLA	Y	604	X	-	-	-
29	CLA	Y	608	X	-	-	-
29	CLA	Y	610	X	-	-	-
29	CLA	Y	611	X	-	-	-
29	CLA	Y	612	X	-	-	-
29	CLA	Y	613	X	-	-	-
29	CLA	Y	614	X	-	-	-
29	CLA	Y1	602	X	-	-	-
29	CLA	Y1	603	X	-	-	-
29	CLA	Y1	604	X	-	-	-
29	CLA	Y1	608	X	-	-	-
29	CLA	Y1	610	X	-	-	-
29	CLA	Y1	611	X	-	-	-
29	CLA	Y1	612	X	-	-	-
29	CLA	Y1	613	X	-	-	-
29	CLA	Y1	614	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	a	406	X	-	-	-
29	CLA	a	407	X	-	-	-
29	CLA	a	410	X	-	-	-
29	CLA	a1	405	X	-	-	-
29	CLA	a1	406	X	-	-	-
29	CLA	a1	407	X	-	-	-
29	CLA	a1	410	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	605	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	b	609	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	b	612	X	-	-	-
29	CLA	b	613	X	-	-	-
29	CLA	b	614	X	-	-	-
29	CLA	b	615	X	-	-	-
29	CLA	b	616	X	-	-	-
29	CLA	b	617	X	-	-	-
29	CLA	b1	602	X	-	-	-
29	CLA	b1	603	X	-	-	-
29	CLA	b1	604	X	-	-	-
29	CLA	b1	605	X	-	-	-
29	CLA	b1	606	X	-	-	-
29	CLA	b1	607	X	-	-	-
29	CLA	b1	608	X	-	-	-
29	CLA	b1	609	X	-	-	-
29	CLA	b1	610	X	-	-	-
29	CLA	b1	611	X	-	-	-
29	CLA	b1	612	X	-	-	-
29	CLA	b1	613	X	-	-	-
29	CLA	b1	614	X	-	-	-
29	CLA	b1	615	X	-	-	-
29	CLA	b1	616	X	-	-	-
29	CLA	b1	617	X	-	-	-
29	CLA	c	501	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	503	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	506	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-
29	CLA	c	511	X	-	-	-
29	CLA	c	512	X	-	-	-
29	CLA	c	513	X	-	-	-
29	CLA	c1	501	X	-	-	-
29	CLA	c1	502	X	-	-	-
29	CLA	c1	503	X	-	-	-
29	CLA	c1	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	c1	505	X	-	-	-
29	CLA	c1	506	X	-	-	-
29	CLA	c1	507	X	-	-	-
29	CLA	c1	508	X	-	-	-
29	CLA	c1	509	X	-	-	-
29	CLA	c1	510	X	-	-	-
29	CLA	c1	511	X	-	-	-
29	CLA	c1	512	X	-	-	-
29	CLA	c1	513	X	-	-	-
29	CLA	d	402	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	d1	402	X	-	-	-
29	CLA	d1	403	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	612	X	-	-	-
29	CLA	g	613	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	g1	602	X	-	-	-
29	CLA	g1	603	X	-	-	-
29	CLA	g1	604	X	-	-	-
29	CLA	g1	610	X	-	-	-
29	CLA	g1	611	X	-	-	-
29	CLA	g1	612	X	-	-	-
29	CLA	g1	613	X	-	-	-
29	CLA	g1	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	612	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	n	614	X	-	-	-
29	CLA	n1	602	X	-	-	-
29	CLA	n1	603	X	-	-	-
29	CLA	n1	604	X	-	-	-
29	CLA	n1	610	X	-	-	-
29	CLA	n1	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	n1	612	X	-	-	-
29	CLA	n1	613	X	-	-	-
29	CLA	n1	614	X	-	-	-
29	CLA	r	602	X	-	-	-
29	CLA	r	603	X	-	-	-
29	CLA	r	604	X	-	-	-
29	CLA	r	608	X	-	-	-
29	CLA	r	609	X	-	-	-
29	CLA	r	610	X	-	-	-
29	CLA	r	612	X	-	-	-
29	CLA	r1	602	X	-	-	-
29	CLA	r1	603	X	-	-	-
29	CLA	r1	604	X	-	-	-
29	CLA	r1	608	X	-	-	-
29	CLA	r1	609	X	-	-	-
29	CLA	r1	610	X	-	-	-
29	CLA	r1	612	X	-	-	-
29	CLA	s	602	X	-	-	-
29	CLA	s	603	X	-	-	-
29	CLA	s	604	X	-	-	-
29	CLA	s	605	X	-	-	-
29	CLA	s	609	X	-	-	-
29	CLA	s	610	X	-	-	-
29	CLA	s	611	X	-	-	-
29	CLA	s	612	X	-	-	-
29	CLA	s	613	X	-	-	-
29	CLA	s	614	X	-	-	-
29	CLA	s	617	X	-	-	-
29	CLA	s1	602	X	-	-	-
29	CLA	s1	603	X	-	-	-
29	CLA	s1	604	X	-	-	-
29	CLA	s1	605	X	-	-	-
29	CLA	s1	609	X	-	-	-
29	CLA	s1	610	X	-	-	-
29	CLA	s1	611	X	-	-	-
29	CLA	s1	612	X	-	-	-
29	CLA	s1	613	X	-	-	-
29	CLA	s1	614	X	-	-	-
29	CLA	s1	617	X	-	-	-
29	CLA	y	602	X	-	-	-
29	CLA	y	603	X	-	-	-
29	CLA	y	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	y	608	X	-	-	-
29	CLA	y	610	X	-	-	-
29	CLA	y	611	X	-	-	-
29	CLA	y	612	X	-	-	-
29	CLA	y	613	X	-	-	-
29	CLA	y	614	X	-	-	-
29	CLA	y1	602	X	-	-	-
29	CLA	y1	603	X	-	-	-
29	CLA	y1	604	X	-	-	-
29	CLA	y1	608	X	-	-	-
29	CLA	y1	610	X	-	-	-
29	CLA	y1	611	X	-	-	-
29	CLA	y1	612	X	-	-	-
29	CLA	y1	613	X	-	-	-
29	CLA	y1	614	X	-	-	-
36	C7Z	B	620	X	-	-	-
36	C7Z	B1	620	X	-	-	-
36	C7Z	b	620	X	-	-	-
36	C7Z	b1	620	X	-	-	-
41	LMK	C	527	X	-	-	-
41	LMK	C1	527	X	-	-	-
41	LMK	c	527	X	-	-	-
41	LMK	c1	527	X	-	-	-
42	BCT	D	401	-	X	-	-
42	BCT	D1	401	-	X	-	-
42	BCT	d	401	-	X	-	-
45	RRX	H	101	X	-	-	-
45	RRX	H1	101	X	-	-	-
45	RRX	h	101	X	-	-	-
45	RRX	h1	101	X	-	-	-
48	CHL	G	601	X	-	-	-
48	CHL	G	605	X	-	-	-
48	CHL	G	606	X	-	-	-
48	CHL	G	607	X	-	-	-
48	CHL	G	608	X	-	-	-
48	CHL	G	609	X	-	-	-
48	CHL	G1	601	X	-	-	-
48	CHL	G1	605	X	-	-	-
48	CHL	G1	606	X	-	-	-
48	CHL	G1	607	X	-	-	-
48	CHL	G1	608	X	-	-	-
48	CHL	G1	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	N	601	X	-	-	-
48	CHL	N	605	X	-	-	-
48	CHL	N	606	X	-	-	-
48	CHL	N	607	X	-	-	-
48	CHL	N	608	X	-	-	-
48	CHL	N	609	X	-	-	-
48	CHL	N1	601	X	-	-	-
48	CHL	N1	605	X	-	-	-
48	CHL	N1	606	X	-	-	-
48	CHL	N1	607	X	-	-	-
48	CHL	N1	608	X	-	-	-
48	CHL	N1	609	X	-	-	-
48	CHL	R	606	X	-	-	-
48	CHL	R	607	X	-	-	-
48	CHL	R1	606	X	-	-	-
48	CHL	R1	607	X	-	-	-
48	CHL	S	601	X	-	-	-
48	CHL	S	606	X	-	-	-
48	CHL	S	607	X	-	-	-
48	CHL	S	608	X	-	-	-
48	CHL	S1	601	X	-	-	-
48	CHL	S1	606	X	-	-	-
48	CHL	S1	607	X	-	-	-
48	CHL	S1	608	X	-	-	-
48	CHL	Y	601	X	-	-	-
48	CHL	Y	605	X	-	-	-
48	CHL	Y	606	X	-	-	-
48	CHL	Y	607	X	-	-	-
48	CHL	Y	609	X	-	-	-
48	CHL	Y1	601	X	-	-	-
48	CHL	Y1	605	X	-	-	-
48	CHL	Y1	606	X	-	-	-
48	CHL	Y1	607	X	-	-	-
48	CHL	Y1	609	X	-	-	-
48	CHL	g	601	X	-	-	-
48	CHL	g	605	X	-	-	-
48	CHL	g	606	X	-	-	-
48	CHL	g	607	X	-	-	-
48	CHL	g	608	X	-	-	-
48	CHL	g	609	X	-	-	-
48	CHL	g1	601	X	-	-	-
48	CHL	g1	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	g1	606	X	-	-	-
48	CHL	g1	607	X	-	-	-
48	CHL	g1	608	X	-	-	-
48	CHL	g1	609	X	-	-	-
48	CHL	n	601	X	-	-	-
48	CHL	n	605	X	-	-	-
48	CHL	n	606	X	-	-	-
48	CHL	n	607	X	-	-	-
48	CHL	n	608	X	-	-	-
48	CHL	n	609	X	-	-	-
48	CHL	n1	601	X	-	-	-
48	CHL	n1	605	X	-	-	-
48	CHL	n1	606	X	-	-	-
48	CHL	n1	607	X	-	-	-
48	CHL	n1	608	X	-	-	-
48	CHL	n1	609	X	-	-	-
48	CHL	r	606	X	-	-	-
48	CHL	r	607	X	-	-	-
48	CHL	r1	606	X	-	-	-
48	CHL	r1	607	X	-	-	-
48	CHL	s	601	X	-	-	-
48	CHL	s	606	X	-	-	-
48	CHL	s	607	X	-	-	-
48	CHL	s	608	X	-	-	-
48	CHL	s1	601	X	-	-	-
48	CHL	s1	606	X	-	-	-
48	CHL	s1	607	X	-	-	-
48	CHL	s1	608	X	-	-	-
48	CHL	y	601	X	-	-	-
48	CHL	y	605	X	-	-	-
48	CHL	y	606	X	-	-	-
48	CHL	y	607	X	-	-	-
48	CHL	y	609	X	-	-	-
48	CHL	y1	601	X	-	-	-
48	CHL	y1	605	X	-	-	-
48	CHL	y1	606	X	-	-	-
48	CHL	y1	607	X	-	-	-
48	CHL	y1	609	X	-	-	-
49	LUT	G	621	X	-	-	-
49	LUT	R	620	X	-	-	-
49	LUT	n1	621	X	-	-	-
50	XAT	G	622	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	XAT	G1	622	X	-	-	-
50	XAT	N	622	X	-	-	-
50	XAT	N1	622	X	-	-	-
50	XAT	Y1	622	X	-	-	-
50	XAT	g	622	X	-	-	-
50	XAT	g1	622	X	-	-	-
50	XAT	n	622	X	-	-	-
50	XAT	r	621	X	-	-	-
50	XAT	r1	621	X	-	-	-
51	NEX	g	623	X	-	-	-
51	NEX	g1	623	X	-	-	-
53	ERG	R	626	X	-	-	-
53	ERG	R1	626	X	-	-	-
53	ERG	r	626	X	-	-	-
53	ERG	r1	626	X	-	-	-

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 152240 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	A1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	B1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		
3	V1	32	Total	C	N	O	0	0
			227	152	37	38		
3	v1	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	C1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	D1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		
6	E1	76	Total	C	N	O	0	0
			621	404	102	115		
6	e1	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	F1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	f1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	H1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

- Molecule 10 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		
10	j	36	Total	C	N	O	0	0
			266	183	40	43		
10	J1	36	Total	C	N	O	0	0
			266	183	40	43		
10	j1	36	Total	C	N	O	0	0
			266	183	40	43		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	L1	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		
13	M1	31	Total	C	N	O	0	0
			234	159	33	42		
13	m1	31	Total	C	N	O	0	0
			234	159	33	42		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	O1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	x1	30	Total	C	N	O	0	0
			201	132	32	37		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	Z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	N1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	G1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7
G1	180	ALA	PRO	conflict	UNP A1XKU7
g1	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	R	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

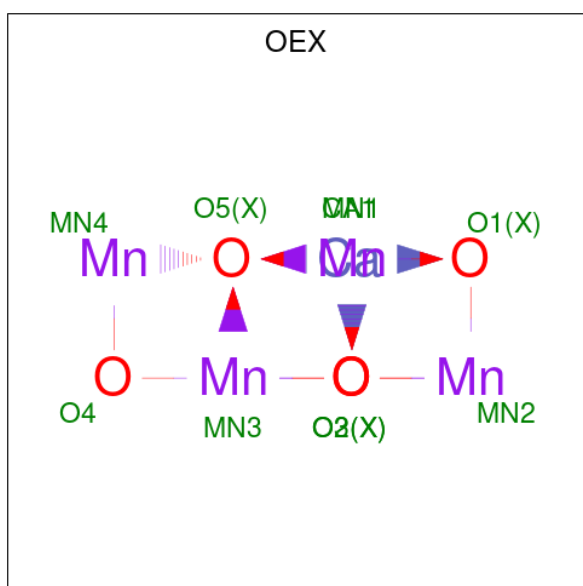
- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	U1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	A1	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	a1	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Fe	0
			1	1	
27	a	1	Total	Fe	0
			1	1	

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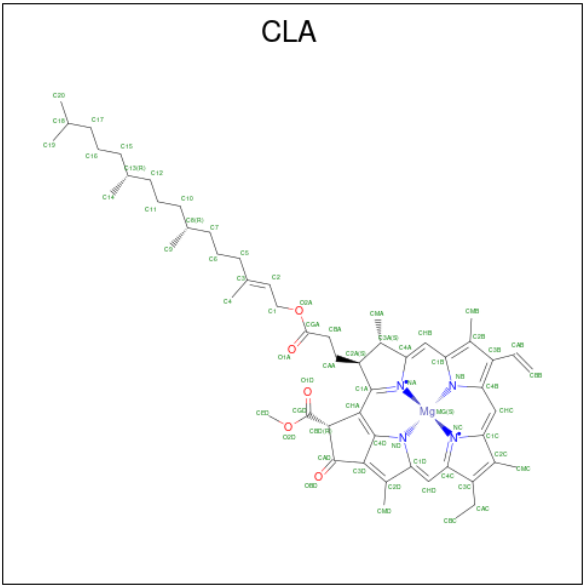
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Mol	Chain	Residues	Atoms		AltConf
27	A1	1	Total	Fe	0
			1	1	
27	a1	1	Total	Fe	0
			1	1	

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
28	A	2	Total	Cl	0
			2	2	
28	a	2	Total	Cl	0
			2	2	
28	A1	2	Total	Cl	0
			2	2	
28	a1	2	Total	Cl	0
			2	2	

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 60	C 50	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 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 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	C	1	Total 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total 65	C 55	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 65	C 55	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 65	C 55	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 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 65	C 55	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 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	N	1	Total 45	C 35	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 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 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
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 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	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 49	C 39	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	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

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

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Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	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 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	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 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 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	N1	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G1	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S1	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	n1	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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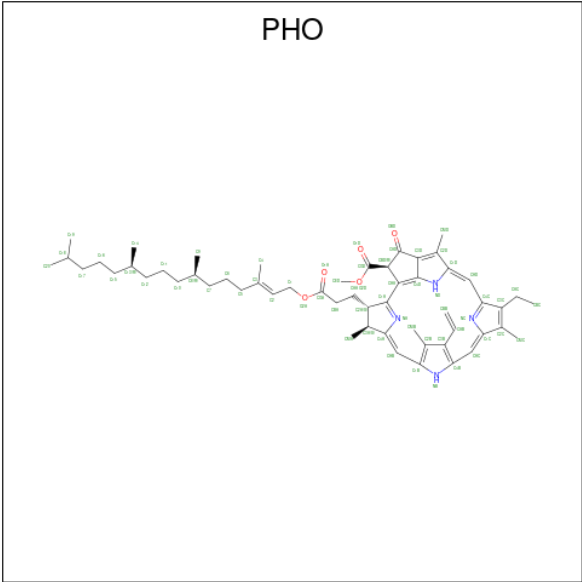
Mol	Chain	Residues	Atoms					AltConf
29	n1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g1	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r1	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	s1	1	Total 60	C 50	Mg 1	N 4	O 5	0

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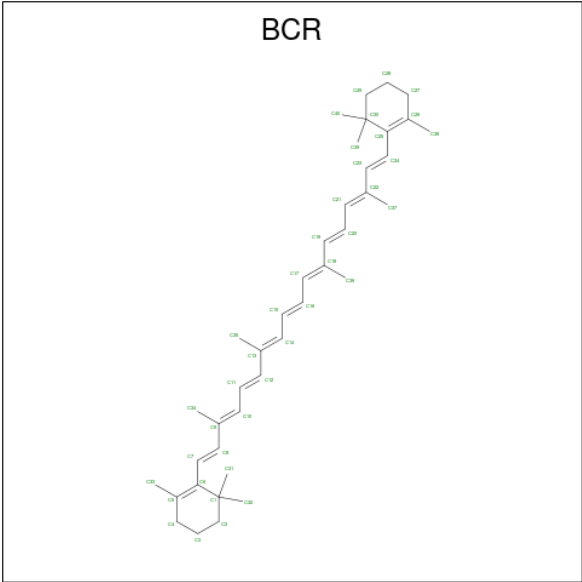
Mol	Chain	Residues	Atoms					AltConf
29	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	A1	1	Total	C	N	O	0
			64	55	4	5	
30	A1	1	Total	C	N	O	0
			64	55	4	5	
30	a1	1	Total	C	N	O	0
			64	55	4	5	
30	a1	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



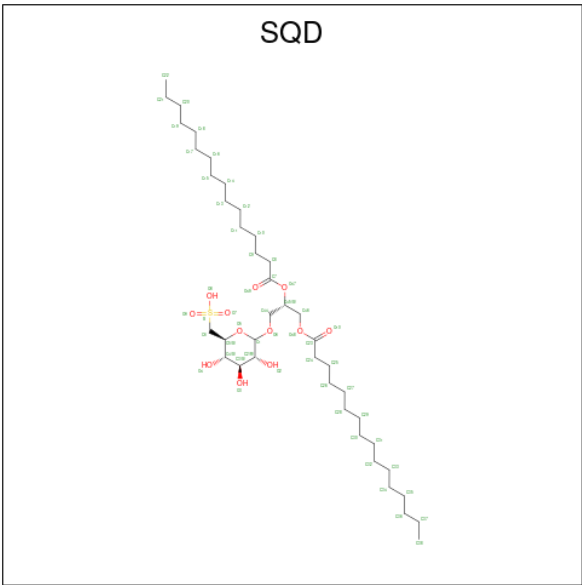
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	C	1	Total	C	0
			40	40	
31	C	1	Total	C	0
			40	40	
31	C	1	Total	C	0
			40	40	
31	C	1	Total	C	0
			40	40	
31	D	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	c	1	Total	C	0
			40	40	
31	c	1	Total	C	0
			40	40	
31	c	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	A1	1	Total C 40 40	0
31	B1	1	Total C 40 40	0
31	B1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	D1	1	Total C 40 40	0
31	a1	1	Total C 40 40	0
31	b1	1	Total C 40 40	0
31	b1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	d1	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



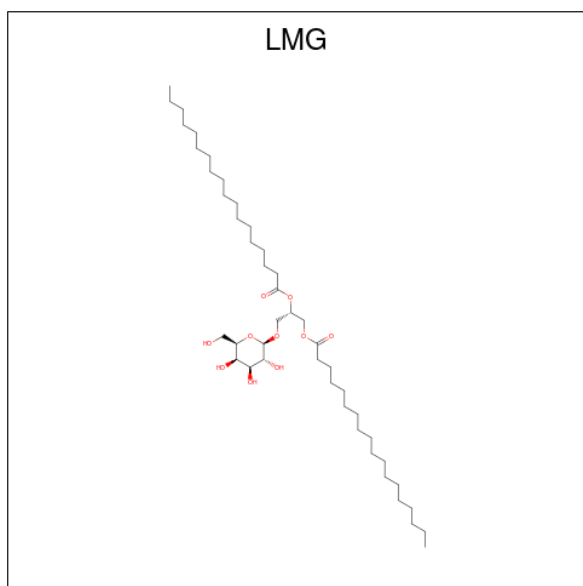
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			51	38	12	1	
32	B	1	Total	C	O	S	0
			42	29	12	1	
32	B	1	Total	C	O	S	0
			54	41	12	1	
32	C	1	Total	C	O	S	0
			54	41	12	1	
32	M	1	Total	C	O	S	0
			42	29	12	1	
32	a	1	Total	C	O	S	0
			51	38	12	1	
32	b	1	Total	C	O	S	0
			42	29	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	c	1	Total	C	O	S	0
			54	41	12	1	
32	m	1	Total	C	O	S	0
			42	29	12	1	
32	A1	1	Total	C	O	S	0
			51	38	12	1	
32	B1	1	Total	C	O	S	0
			42	29	12	1	
32	B1	1	Total	C	O	S	0
			54	41	12	1	
32	C1	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
32	M1	1	Total	C	O	S	0
			42	29	12	1	
32	a1	1	Total	C	O	S	0
			51	38	12	1	
32	b1	1	Total	C	O	S	0
			42	29	12	1	
32	b1	1	Total	C	O	S	0
			54	41	12	1	
32	c1	1	Total	C	O	S	0
			54	41	12	1	
32	m1	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O		0
			48	38	10		
33	B	1	Total	C	O		0
			44	34	10		
33	C	1	Total	C	O		0
			51	41	10		
33	C	1	Total	C	O		0
			55	45	10		
33	D	1	Total	C	O		0
			46	36	10		

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Mol	Chain	Residues	Atoms			AltConf
33	H	1	Total 48	C 38	O 10	0
33	W	1	Total 39	C 29	O 10	0
33	a	1	Total 48	C 38	O 10	0
33	b	1	Total 44	C 34	O 10	0
33	c	1	Total 51	C 41	O 10	0
33	c	1	Total 55	C 45	O 10	0
33	d	1	Total 46	C 36	O 10	0
33	h	1	Total 48	C 38	O 10	0
33	w	1	Total 39	C 29	O 10	0
33	A1	1	Total 48	C 38	O 10	0
33	B1	1	Total 44	C 34	O 10	0
33	C1	1	Total 51	C 41	O 10	0
33	C1	1	Total 55	C 45	O 10	0
33	D1	1	Total 46	C 36	O 10	0
33	H1	1	Total 48	C 38	O 10	0
33	W1	1	Total 39	C 29	O 10	0
33	a1	1	Total 48	C 38	O 10	0
33	b1	1	Total 44	C 34	O 10	0
33	c1	1	Total 51	C 41	O 10	0
33	c1	1	Total 55	C 45	O 10	0
33	d1	1	Total 46	C 36	O 10	0

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Mol	Chain	Residues	Atoms			AltConf
33	h1	1	Total	C	O	0
			48	38	10	
33	w1	1	Total	C	O	0
			39	29	10	

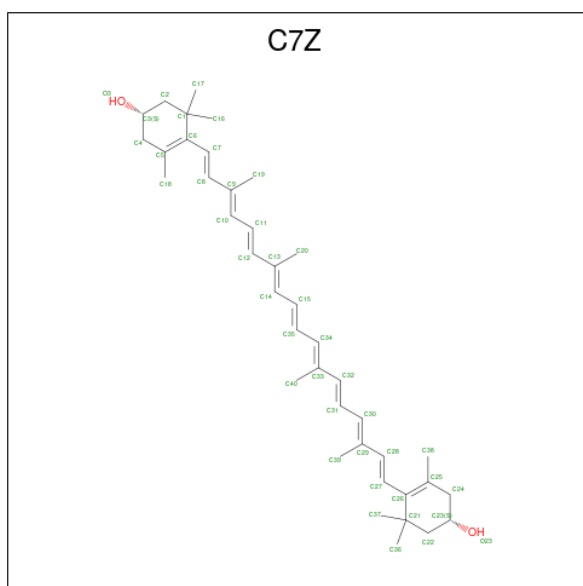
- # SPH

Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total 21	C 18	N 1	O 2	0
34	Y	1	Total 21	C 18	N 1	O 2	0
34	a	1	Total 21	C 18	N 1	O 2	0
34	y	1	Total 21	C 18	N 1	O 2	0
34	A1	1	Total 21	C 18	N 1	O 2	0
34	Y1	1	Total 21	C 18	N 1	O 2	0
34	a1	1	Total 21	C 18	N 1	O 2	0
34	y1	1	Total 21	C 18	N 1	O 2	0

- 

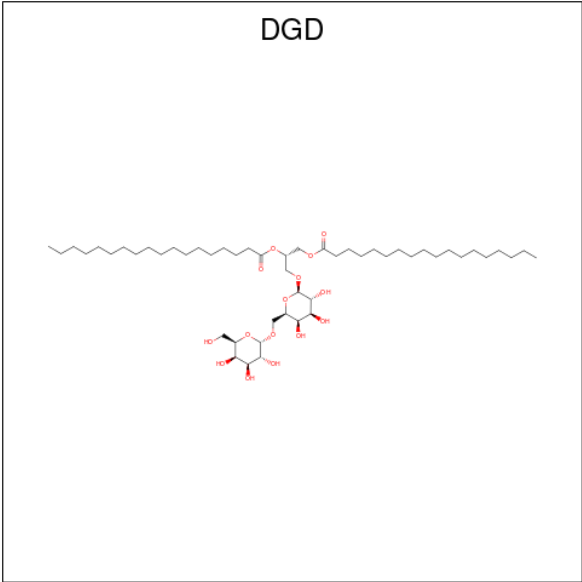
Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Na	0
			1	1	
35	a	1	Total	Na	0
			1	1	
35	A1	1	Total	Na	0
			1	1	
35	a1	1	Total	Na	0
			1	1	

- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	B1	1	Total	C	O	0
			42	40	2	
36	b1	1	Total	C	O	0
			42	40	2	

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



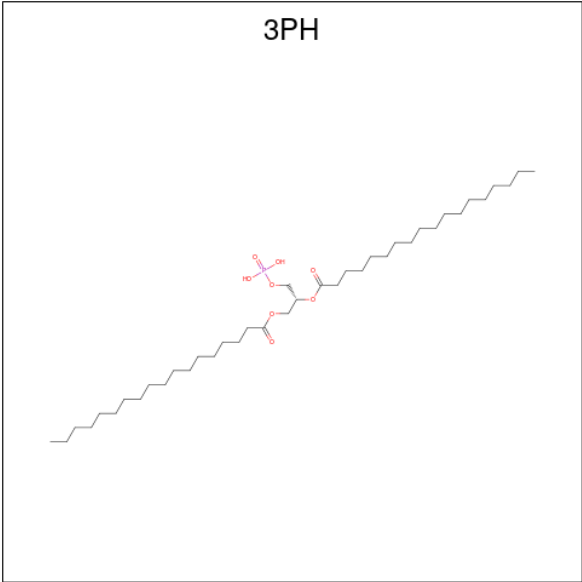
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			43	28	15	
37	C	1	Total	C	O	0
			55	40	15	
37	C	1	Total	C	O	0
			62	47	15	
37	C	1	Total	C	O	0
			59	44	15	
37	b	1	Total	C	O	0
			43	28	15	
37	c	1	Total	C	O	0
			55	40	15	
37	c	1	Total	C	O	0
			62	47	15	
37	c	1	Total	C	O	0
			59	44	15	
37	B1	1	Total	C	O	0
			43	28	15	
37	C1	1	Total	C	O	0
			55	40	15	
37	C1	1	Total	C	O	0
			62	47	15	
37	C1	1	Total	C	O	0
			59	44	15	
37	b1	1	Total	C	O	0
			43	28	15	
37	c1	1	Total	C	O	0
			55	40	15	

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Mol	Chain	Residues	Atoms			AltConf
37	c1	1	Total	C	O	0
			62	47	15	
37	c1	1	Total	C	O	0
			59	44	15	

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



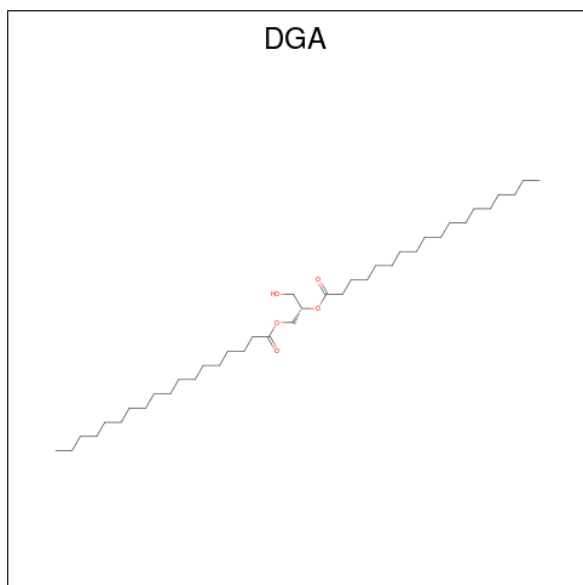
Mol	Chain	Residues	Atoms				AltConf
38	B	1	Total	C	O	P	0
			48	39	8	1	
38	T	1	Total	C	O	P	0
			48	39	8	1	
38	S	1	Total	C	O	P	0
			48	39	8	1	
38	b	1	Total	C	O	P	0
			48	39	8	1	
38	t	1	Total	C	O	P	0
			48	39	8	1	
38	s	1	Total	C	O	P	0
			48	39	8	1	
38	B1	1	Total	C	O	P	0
			48	39	8	1	
38	T1	1	Total	C	O	P	0
			48	39	8	1	
38	S1	1	Total	C	O	P	0
			48	39	8	1	

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Mol	Chain	Residues	Atoms				AltConf
38	b1	1	Total	C	O	P	0
			48	39	8	1	
38	t1	1	Total	C	O	P	0
			48	39	8	1	
38	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 39 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



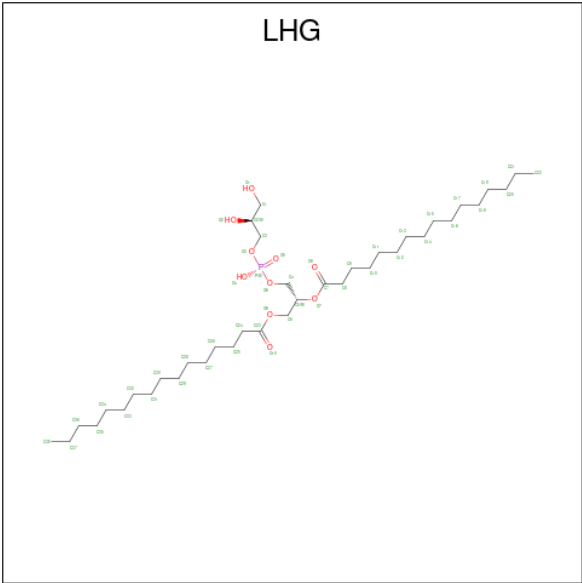
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			44	39	5	
39	C	1	Total	C	O	0
			44	39	5	
39	J	1	Total	C	O	0
			29	24	5	
39	b	1	Total	C	O	0
			44	39	5	
39	c	1	Total	C	O	0
			44	39	5	
39	j	1	Total	C	O	0
			29	24	5	
39	B1	1	Total	C	O	0
			44	39	5	
39	C1	1	Total	C	O	0
			44	39	5	

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Mol	Chain	Residues	Atoms			AltConf
39	J1	1	Total	C	O	0
			29	24	5	
39	b1	1	Total	C	O	0
			44	39	5	
39	c1	1	Total	C	O	0
			44	39	5	
39	j1	1	Total	C	O	0
			29	24	5	

- Molecule 40 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	O	P	0
			47	36	10	1	
40	D	1	Total	C	O	P	0
			44	33	10	1	
40	D	1	Total	C	O	P	0
			49	38	10	1	
40	D	1	Total	C	O	P	0
			39	28	10	1	
40	L	1	Total	C	O	P	0
			49	38	10	1	
40	N	1	Total	C	O	P	0
			49	38	10	1	
40	G	1	Total	C	O	P	0
			49	38	10	1	

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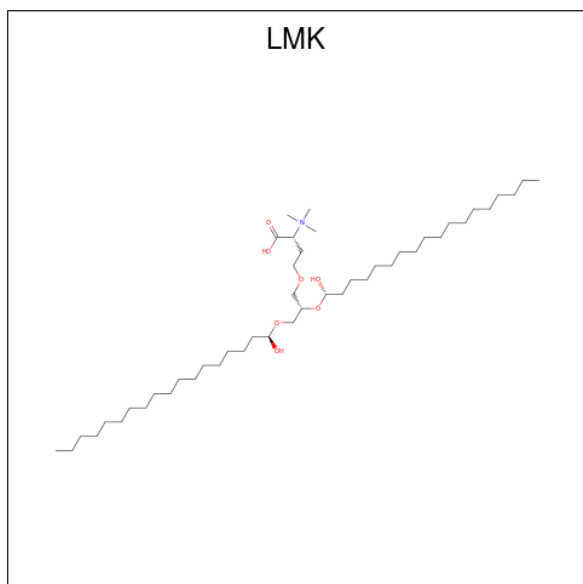
Mol	Chain	Residues	Atoms				AltConf
40	S	1	Total 45	C 34	O 10	P 1	0
40	Y	1	Total 49	C 38	O 10	P 1	0
40	c	1	Total 47	C 36	O 10	P 1	0
40	d	1	Total 44	C 33	O 10	P 1	0
40	d	1	Total 49	C 38	O 10	P 1	0
40	d	1	Total 39	C 28	O 10	P 1	0
40	l	1	Total 49	C 38	O 10	P 1	0
40	n	1	Total 49	C 38	O 10	P 1	0
40	g	1	Total 49	C 38	O 10	P 1	0
40	s	1	Total 45	C 34	O 10	P 1	0
40	y	1	Total 49	C 38	O 10	P 1	0
40	C1	1	Total 47	C 36	O 10	P 1	0
40	D1	1	Total 44	C 33	O 10	P 1	0
40	D1	1	Total 49	C 38	O 10	P 1	0
40	D1	1	Total 39	C 28	O 10	P 1	0
40	L1	1	Total 49	C 38	O 10	P 1	0
40	N1	1	Total 49	C 38	O 10	P 1	0
40	G1	1	Total 49	C 38	O 10	P 1	0
40	S1	1	Total 45	C 34	O 10	P 1	0
40	Y1	1	Total 49	C 38	O 10	P 1	0
40	c1	1	Total 47	C 36	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
40	d1	1	Total	C	O	P	0
			44	33	10	1	
40	d1	1	Total	C	O	P	0
			49	38	10	1	
40	d1	1	Total	C	O	P	0
			39	28	10	1	
40	n1	1	Total	C	O	P	0
			49	38	10	1	
40	g1	1	Total	C	O	P	0
			49	38	10	1	
40	s1	1	Total	C	O	P	0
			45	34	10	1	
40	y1	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 41 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: C₄₆H₉₄NO₇).



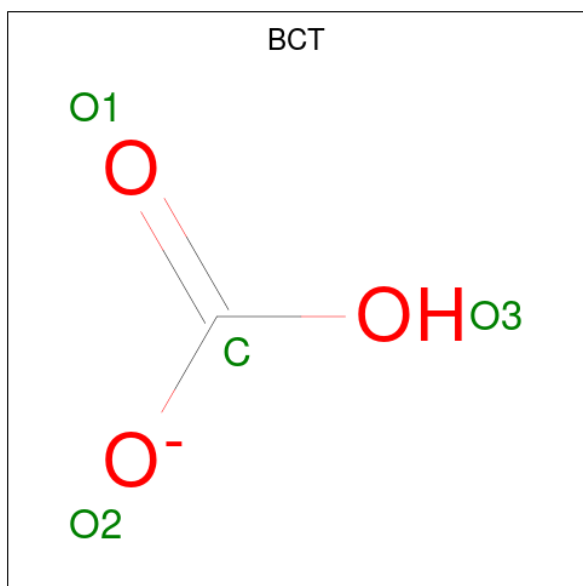
Mol	Chain	Residues	Atoms				AltConf
41	C	1	Total	C	N	O	0
			40	32	1	7	
41	c	1	Total	C	N	O	0
			40	32	1	7	
41	C1	1	Total	C	N	O	0
			40	32	1	7	

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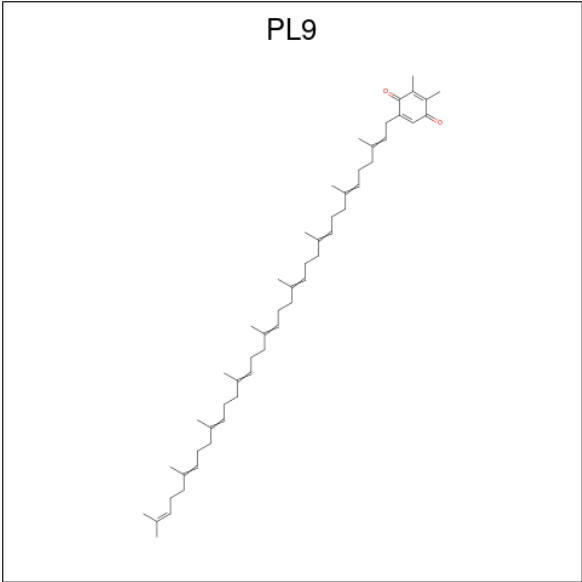
Mol	Chain	Residues	Atoms				AltConf
41	c1	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



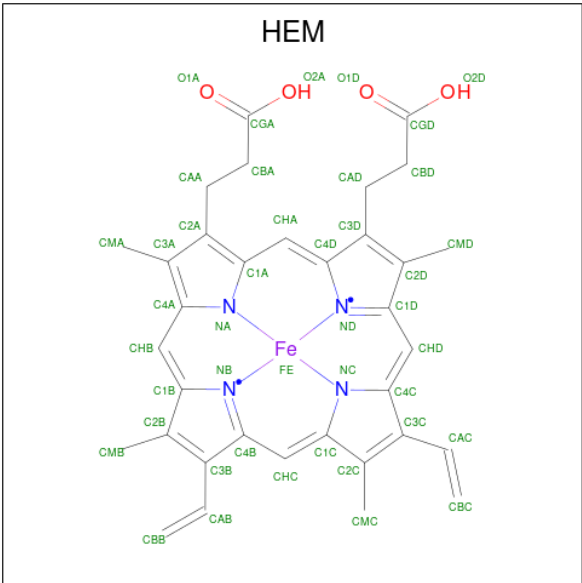
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	d	1	Total	C	O	0
			4	1	3	
42	D1	1	Total	C	O	0
			4	1	3	
42	d1	1	Total	C	O	0
			4	1	3	

- Molecule 43 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



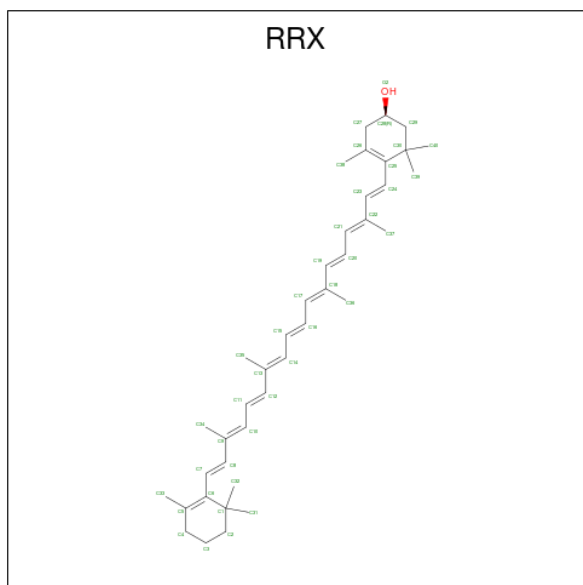
Mol	Chain	Residues	Atoms			AltConf
43	D	1	Total	C	O	0
			55	53	2	
43	d	1	Total	C	O	0
			55	53	2	
43	D1	1	Total	C	O	0
			55	53	2	
43	d1	1	Total	C	O	0
			55	53	2	

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



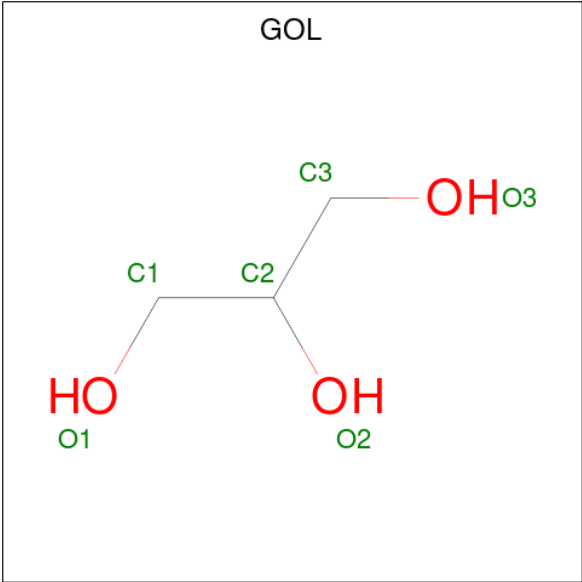
Mol	Chain	Residues	Atoms					AltConf
44	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	F1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



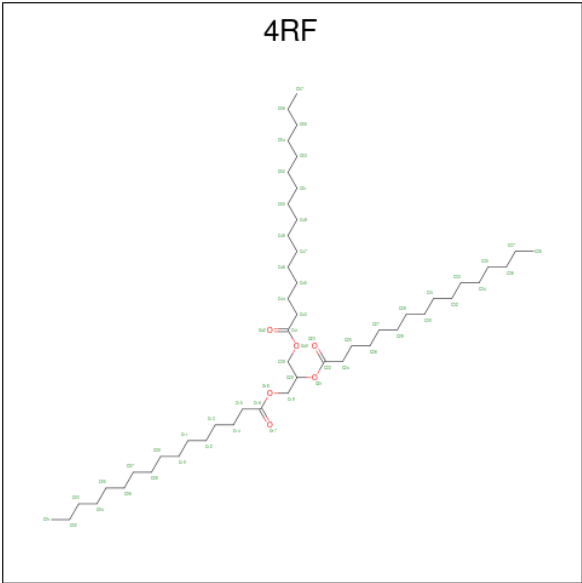
Mol	Chain	Residues	Atoms			AltConf
45	H	1	Total	C	O	0
			41	40	1	
45	h	1	Total	C	O	0
			41	40	1	
45	H1	1	Total	C	O	0
			41	40	1	
45	h1	1	Total	C	O	0
			41	40	1	

- Molecule 46 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	C	O	0
			6	3	3	
46	I1	1	Total	C	O	0
			6	3	3	

- Molecule 47 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



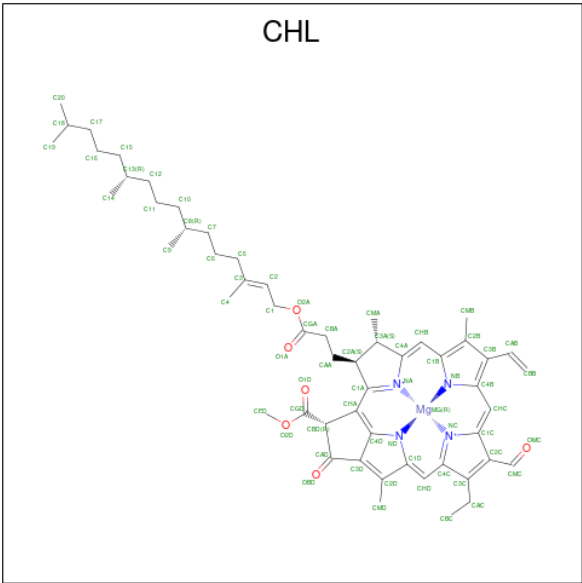
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	C	O	0
			57	51	6	
47	K	1	Total	C	O	0
			57	51	6	

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Mol	Chain	Residues	Atoms			AltConf
47	i	1	Total	C	O	0
			57	51	6	
47	k	1	Total	C	O	0
			57	51	6	
47	I1	1	Total	C	O	0
			57	51	6	
47	K1	1	Total	C	O	0
			57	51	6	
47	i1	1	Total	C	O	0
			57	51	6	
47	k1	1	Total	C	O	0
			57	51	6	

- Molecule 48 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
48	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
48	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	G	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
48	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
48	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
48	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
48	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
48	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
48	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	r	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
48	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
48	s	1	Total 61	C 50	Mg 1	N 4	O 6	0
48	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
48	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
48	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	N1	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	G1	1	Total 48	C 37	Mg 1	N 4	O 6	0
48	G1	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	G1	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	R1	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	R1	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	S1	1	Total 46	C 35	Mg 1	N 4	O 6	0
48	S1	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	S1	1	Total 43	C 34	Mg 1	N 4	O 4	0
48	S1	1	Total 61	C 50	Mg 1	N 4	O 6	0
48	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	Y1	1	Total 46	C 35	Mg 1	N 4	O 6	0
48	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0

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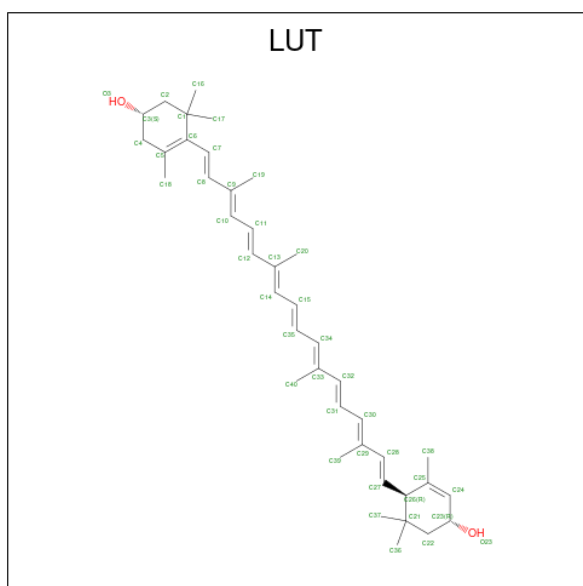
Mol	Chain	Residues	Atoms					AltConf
48	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	n1	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	g1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	g1	1	Total 48	C 37	Mg 1	N 4	O 6	0
48	g1	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	g1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	g1	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	g1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	r1	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	r1	1	Total 50	C 39	Mg 1	N 4	O 6	0
48	s1	1	Total 46	C 35	Mg 1	N 4	O 6	0
48	s1	1	Total 44	C 35	Mg 1	N 4	O 4	0
48	s1	1	Total 43	C 34	Mg 1	N 4	O 4	0
48	s1	1	Total 61	C 50	Mg 1	N 4	O 6	0
48	y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
48	y1	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 49 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms				AltConf
49	N	1	Total	C	O		0
			42	40	2		
49	N	1	Total	C	O		0
			42	40	2		
49	G	1	Total	C	O		0
			42	40	2		
49	G	1	Total	C	O		0
			42	40	2		
49	R	1	Total	C	O		0
			42	40	2		
49	S	1	Total	C	O		0
			42	40	2		
49	S	1	Total	C	O		0
			42	40	2		
49	Y	1	Total	C	O		0
			42	40	2		

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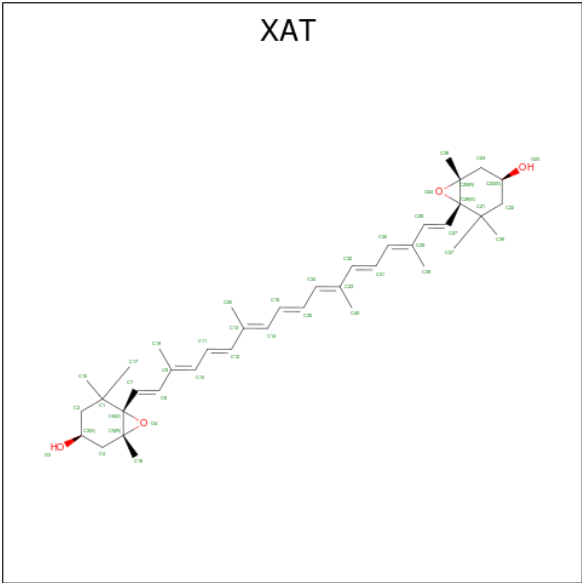
Mol	Chain	Residues	Atoms			AltConf
49	Y	1	Total	C	O	0
			42	40	2	
49	n	1	Total	C	O	0
			42	40	2	
49	n	1	Total	C	O	0
			42	40	2	
49	g	1	Total	C	O	0
			42	40	2	
49	g	1	Total	C	O	0
			42	40	2	
49	r	1	Total	C	O	0
			42	40	2	
49	s	1	Total	C	O	0
			42	40	2	
49	s	1	Total	C	O	0
			42	40	2	
49	y	1	Total	C	O	0
			42	40	2	
49	y	1	Total	C	O	0
			42	40	2	
49	N1	1	Total	C	O	0
			42	40	2	
49	N1	1	Total	C	O	0
			42	40	2	
49	G1	1	Total	C	O	0
			42	40	2	
49	G1	1	Total	C	O	0
			42	40	2	
49	R1	1	Total	C	O	0
			42	40	2	
49	S1	1	Total	C	O	0
			42	40	2	
49	S1	1	Total	C	O	0
			42	40	2	
49	Y1	1	Total	C	O	0
			42	40	2	
49	Y1	1	Total	C	O	0
			42	40	2	
49	n1	1	Total	C	O	0
			42	40	2	
49	n1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
49	g1	1	Total	C	O	0
			42	40	2	
49	g1	1	Total	C	O	0
			42	40	2	
49	r1	1	Total	C	O	0
			42	40	2	
49	s1	1	Total	C	O	0
			42	40	2	
49	s1	1	Total	C	O	0
			42	40	2	
49	y1	1	Total	C	O	0
			42	40	2	
49	y1	1	Total	C	O	0
			42	40	2	

- Molecule 50 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



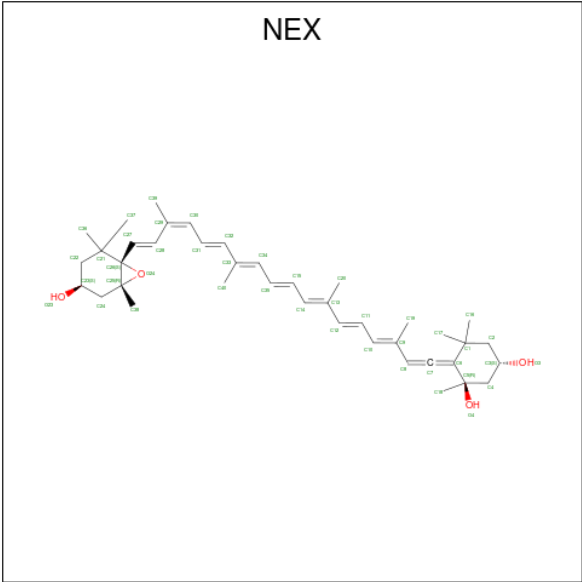
Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			44	40	4	
50	G	1	Total	C	O	0
			44	40	4	
50	R	1	Total	C	O	0
			44	40	4	
50	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
50	n	1	Total	C	O	0
			44	40	4	
50	g	1	Total	C	O	0
			44	40	4	
50	r	1	Total	C	O	0
			44	40	4	
50	y	1	Total	C	O	0
			44	40	4	
50	N1	1	Total	C	O	0
			44	40	4	
50	G1	1	Total	C	O	0
			44	40	4	
50	R1	1	Total	C	O	0
			44	40	4	
50	Y1	1	Total	C	O	0
			44	40	4	
50	n1	1	Total	C	O	0
			44	40	4	
50	g1	1	Total	C	O	0
			44	40	4	
50	r1	1	Total	C	O	0
			44	40	4	
50	y1	1	Total	C	O	0
			44	40	4	

- Molecule 51 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



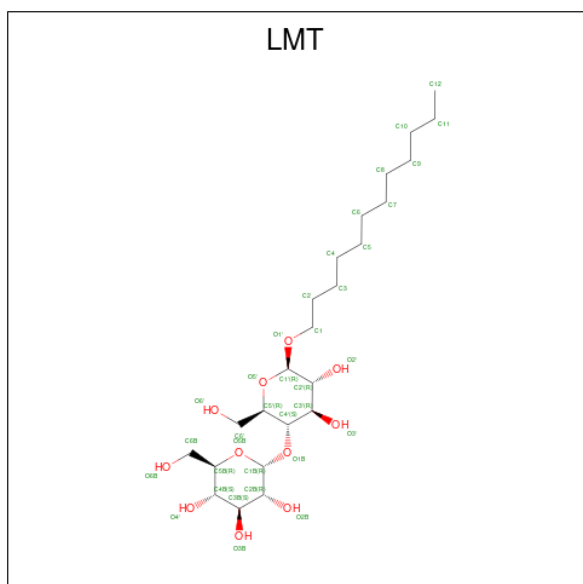
Mol	Chain	Residues	Atoms			AltConf
51	N	1	Total	C	O	0
			44	40	4	
51	G	1	Total	C	O	0
			44	40	4	
51	R	1	Total	C	O	0
			44	40	4	
51	S	1	Total	C	O	0
			44	40	4	
51	Y	1	Total	C	O	0
			44	40	4	
51	n	1	Total	C	O	0
			44	40	4	
51	g	1	Total	C	O	0
			44	40	4	
51	r	1	Total	C	O	0
			44	40	4	
51	s	1	Total	C	O	0
			44	40	4	
51	y	1	Total	C	O	0
			44	40	4	
51	N1	1	Total	C	O	0
			44	40	4	
51	G1	1	Total	C	O	0
			44	40	4	
51	R1	1	Total	C	O	0
			44	40	4	
51	S1	1	Total	C	O	0
			44	40	4	

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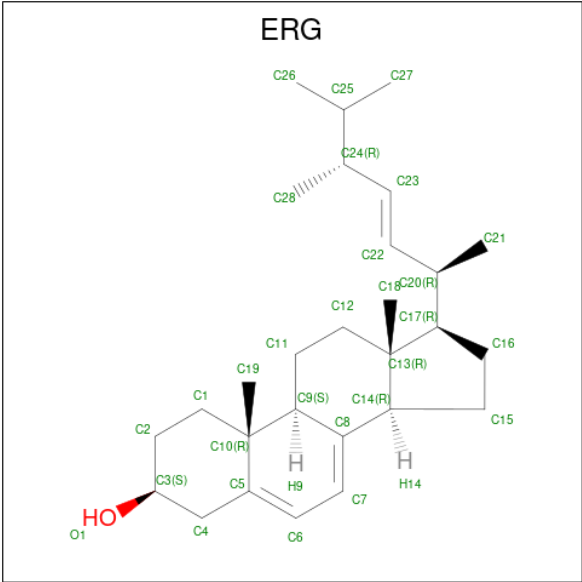
Mol	Chain	Residues	Atoms			AltConf
51	Y1	1	Total	C	O	0
			44	40	4	
51	n1	1	Total	C	O	0
			44	40	4	
51	g1	1	Total	C	O	0
			44	40	4	
51	r1	1	Total	C	O	0
			44	40	4	
51	s1	1	Total	C	O	0
			44	40	4	
51	y1	1	Total	C	O	0
			44	40	4	

- Molecule 52 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



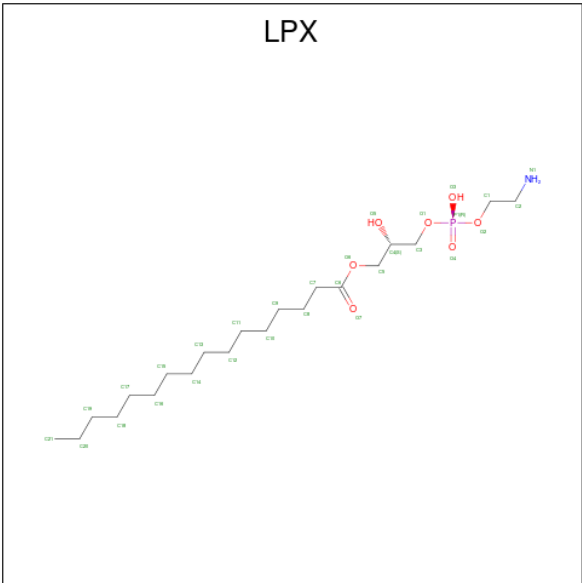
Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			35	24	11	
52	r	1	Total	C	O	0
			35	24	11	
52	R1	1	Total	C	O	0
			35	24	11	
52	r1	1	Total	C	O	0
			35	24	11	

- Molecule 53 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



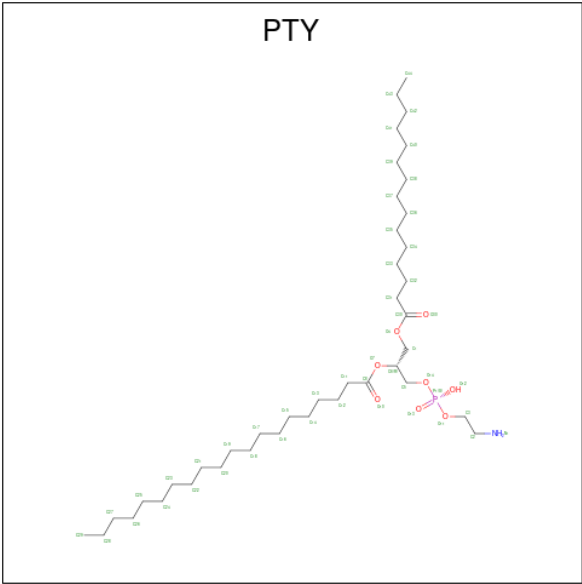
Mol	Chain	Residues	Atoms			AltConf
53	R	1	Total	C	O	0
			29	28	1	
53	r	1	Total	C	O	0
			29	28	1	
53	R1	1	Total	C	O	0
			29	28	1	
53	r1	1	Total	C	O	0
			29	28	1	

- Molecule 54 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
54	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	S1	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s1	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 55 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
55	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	y	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	y	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	Y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	Y1	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	y1	1	Total	C	N	O	P	0
			19	9	1	8	1	

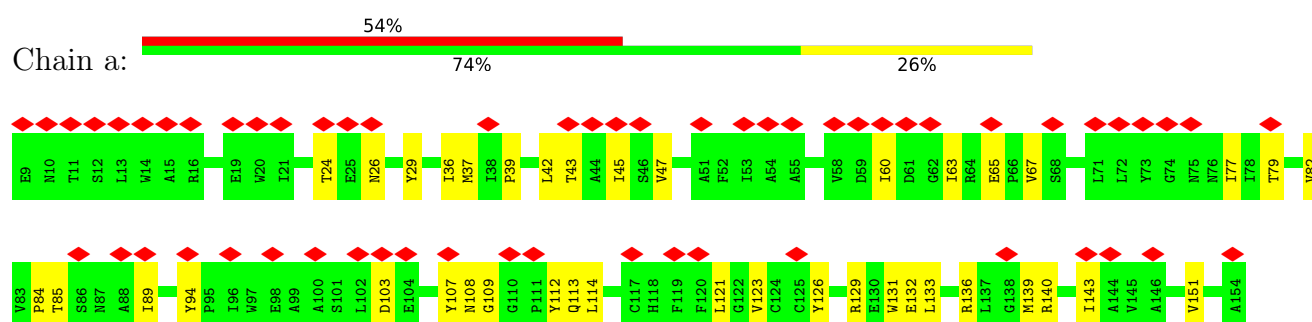
3 Residue-property plots

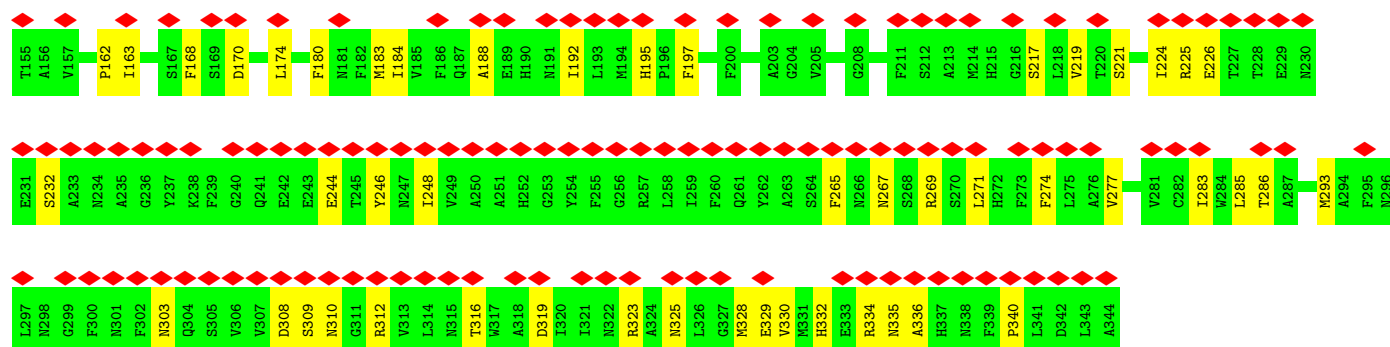
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 II protein D1

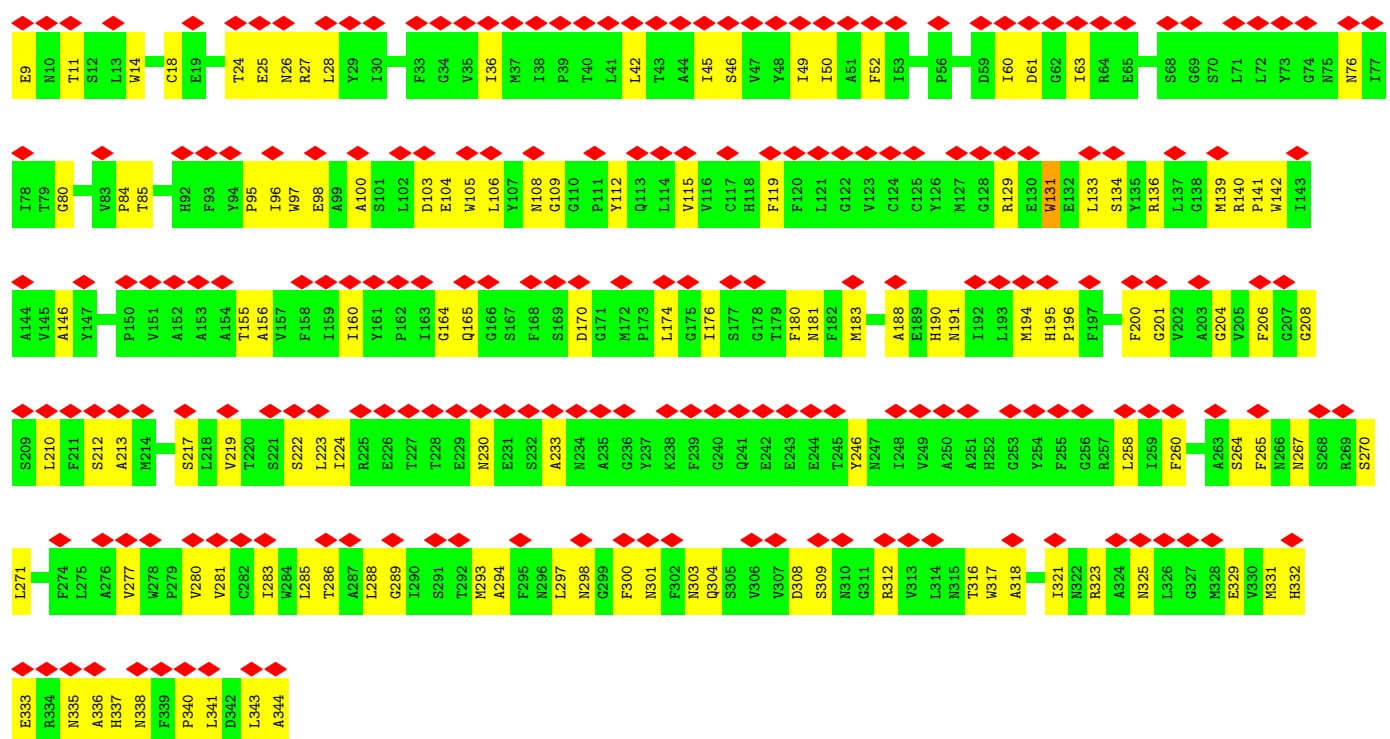


• Molecule 1: Photosystem II protein D1



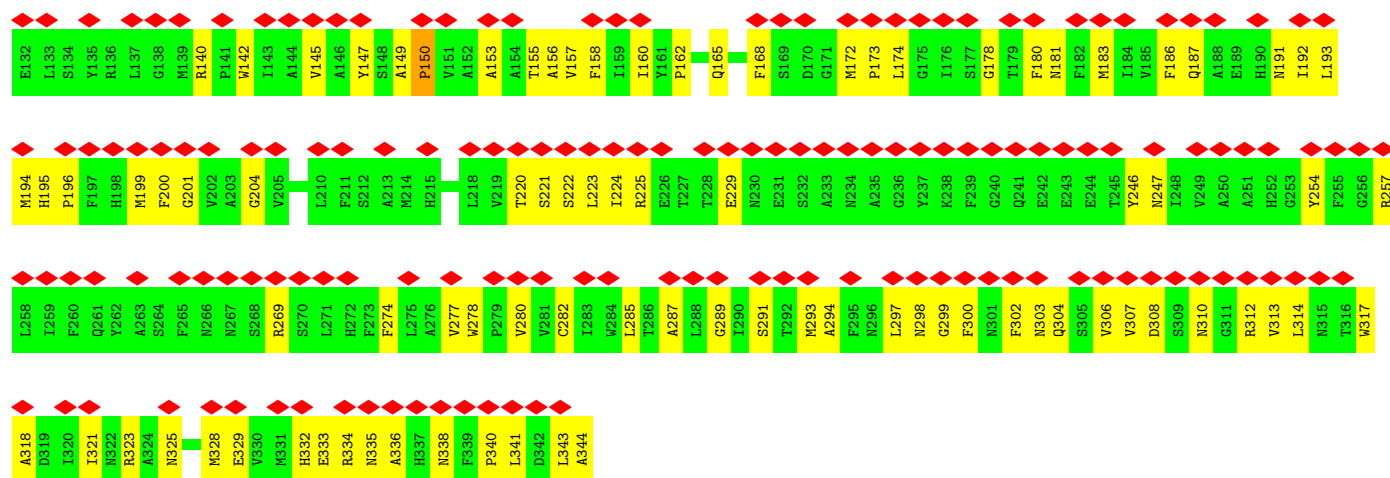


• Molecule 1: Photosystem II protein D1

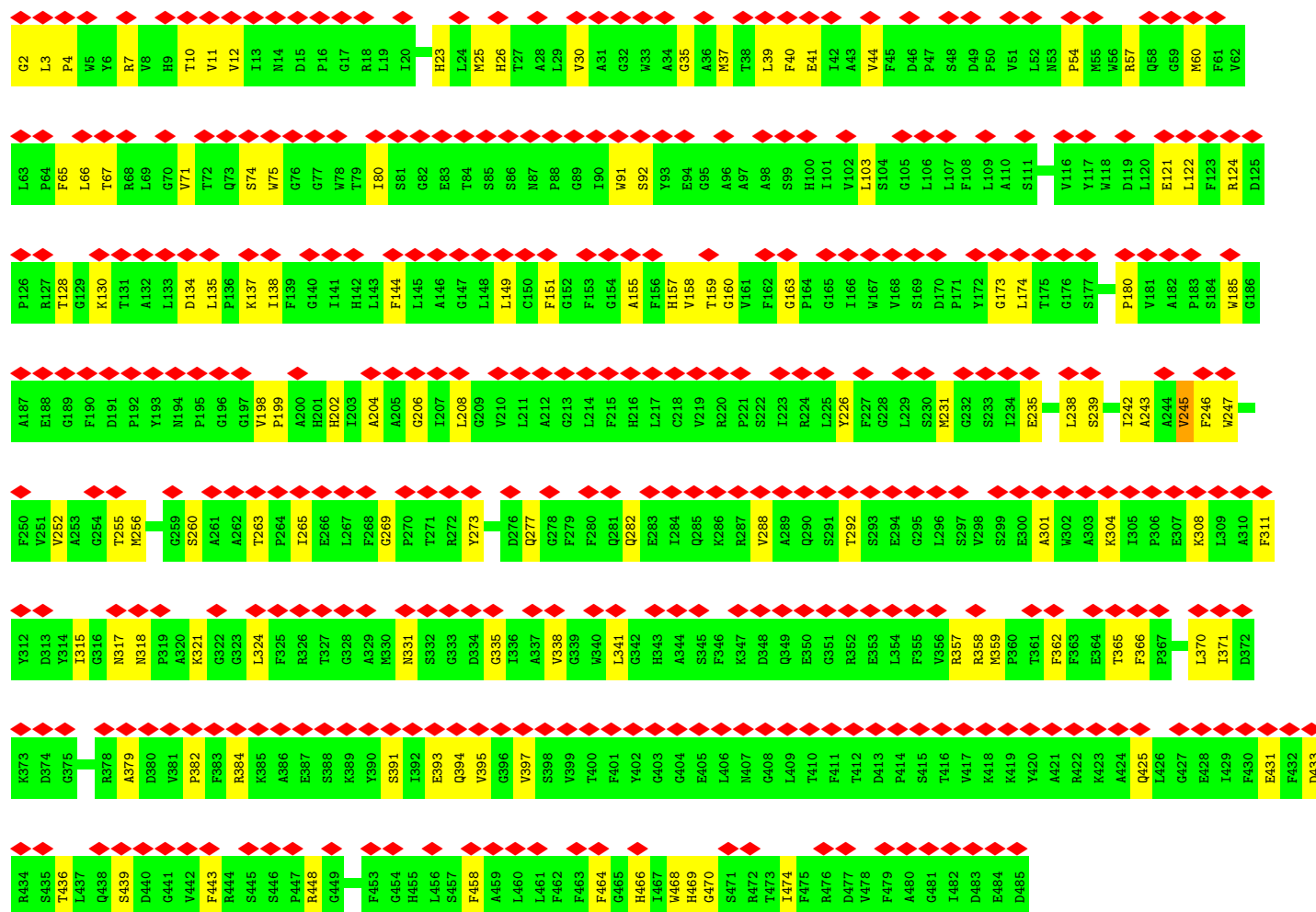
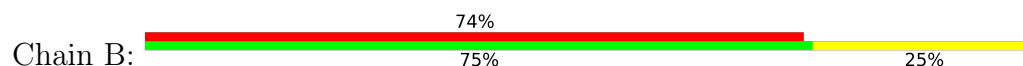


• Molecule 1: Photosystem II protein D1



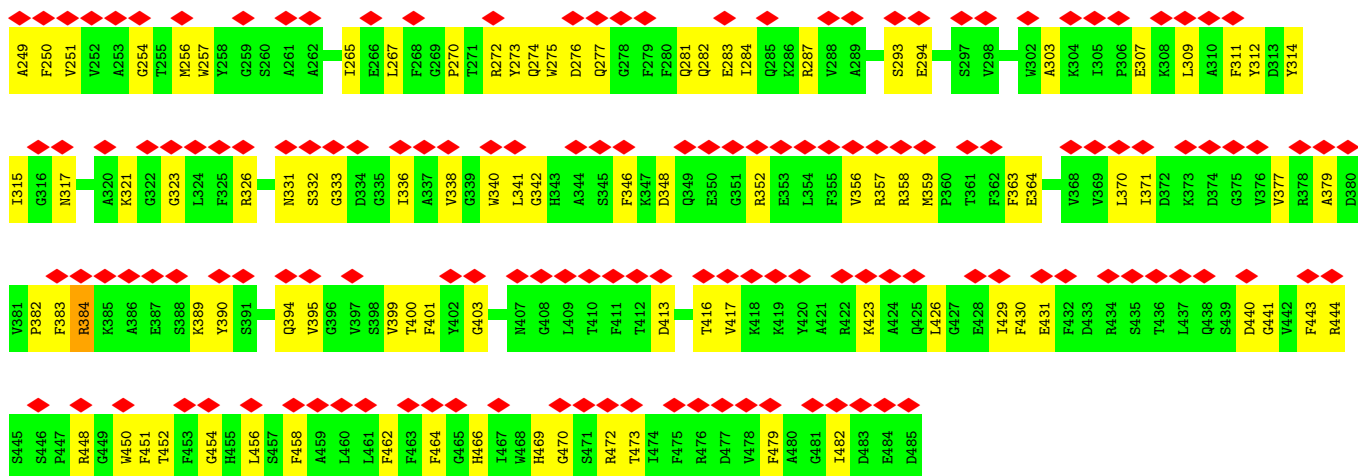


• Molecule 2: Photosystem II CP47 reaction center protein

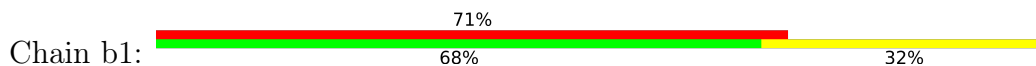


• Molecule 2: Photosystem II CP47 reaction center protein

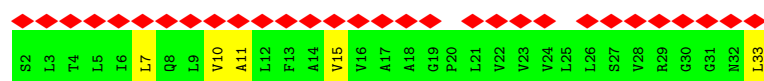
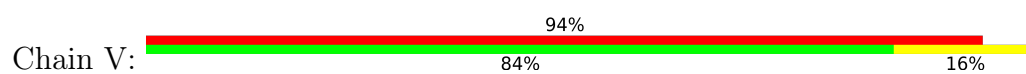




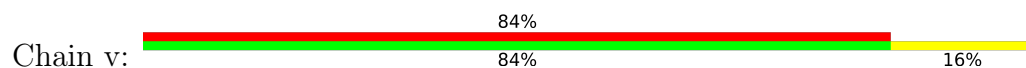
• Molecule 2: Photosystem II CP47 reaction center protein



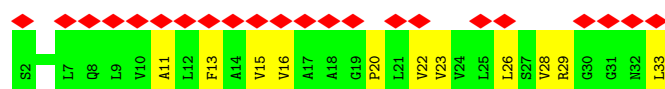
• Molecule 3: Photosystem II reaction center protein Ycf12



• Molecule 3: Photosystem II reaction center protein Ycf12



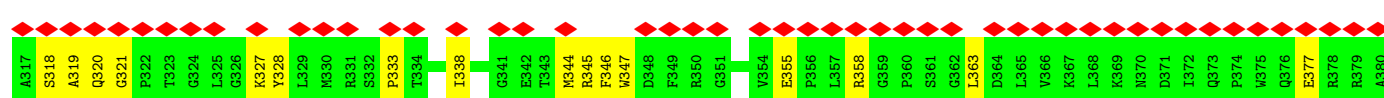
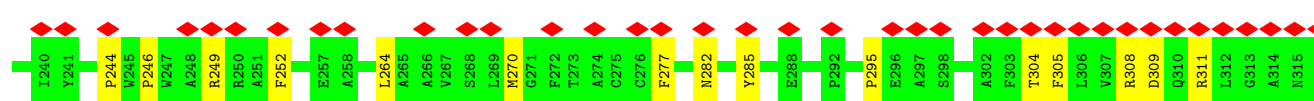
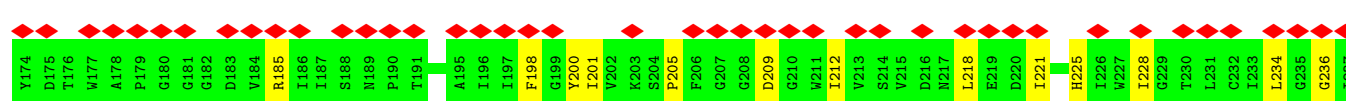
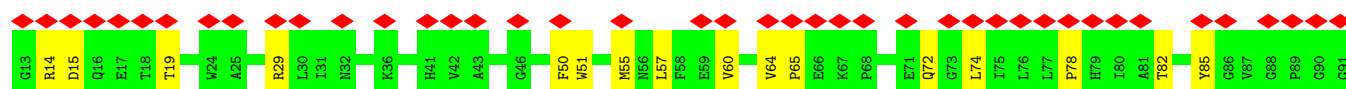
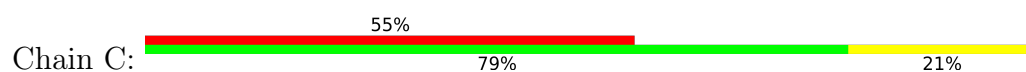
• Molecule 3: Photosystem II reaction center protein Ycf12

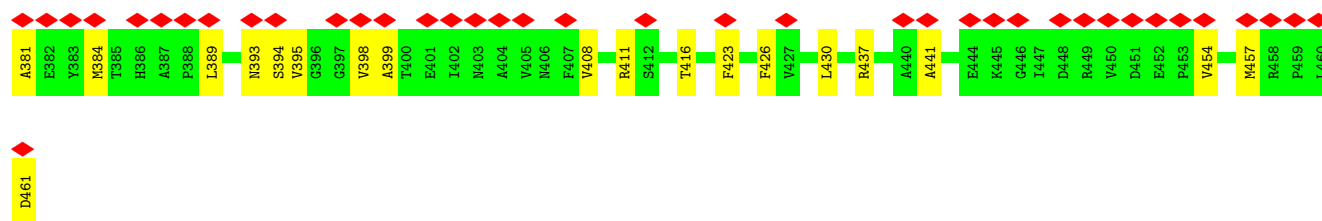


• Molecule 3: Photosystem II reaction center protein Ycf12

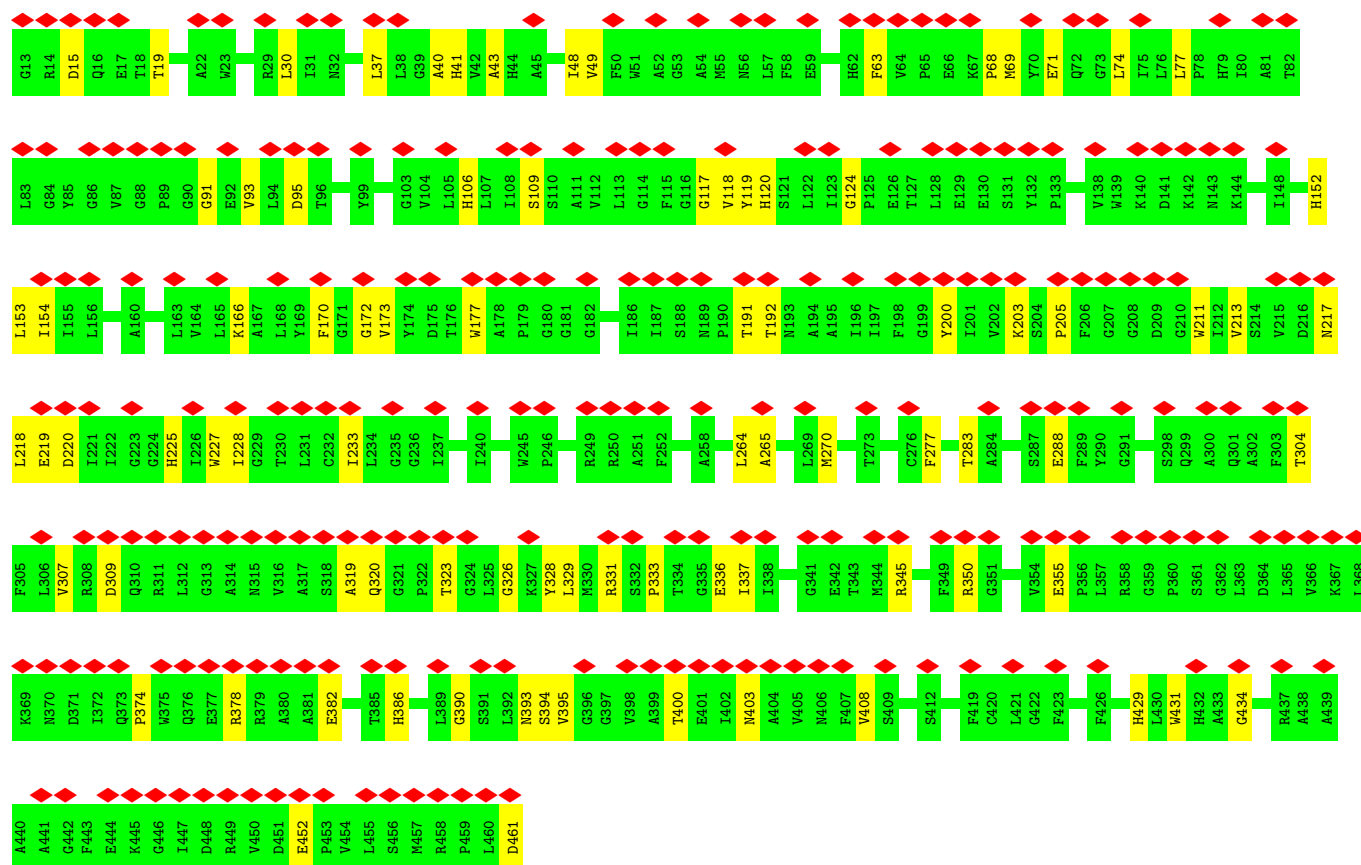
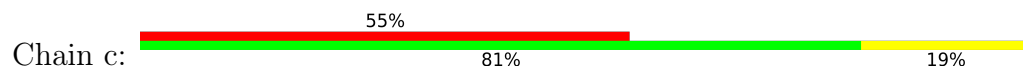


• Molecule 4: Photosystem II CP43 reaction center protein

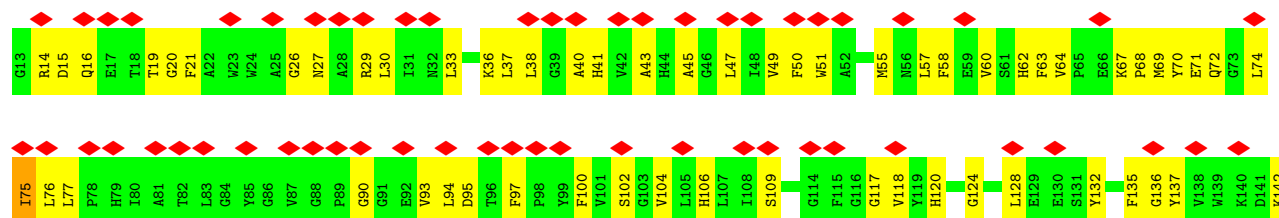
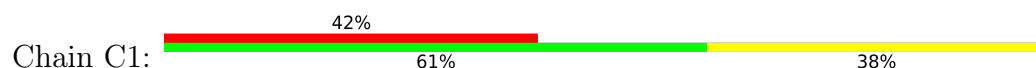


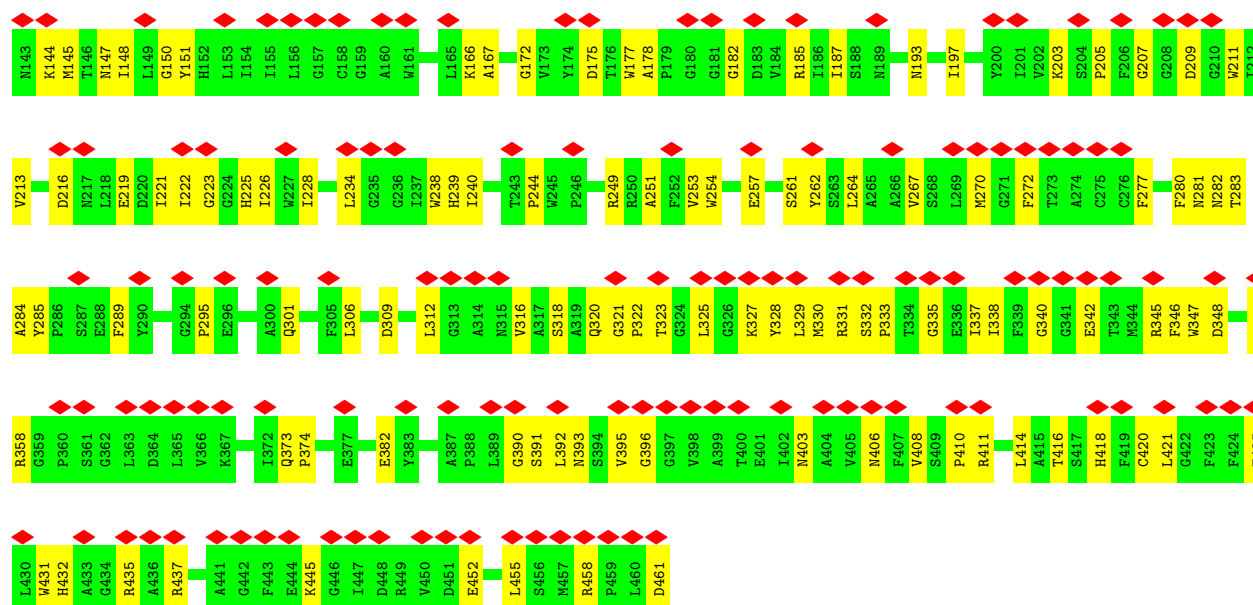


• Molecule 4: Photosystem II CP43 reaction center protein

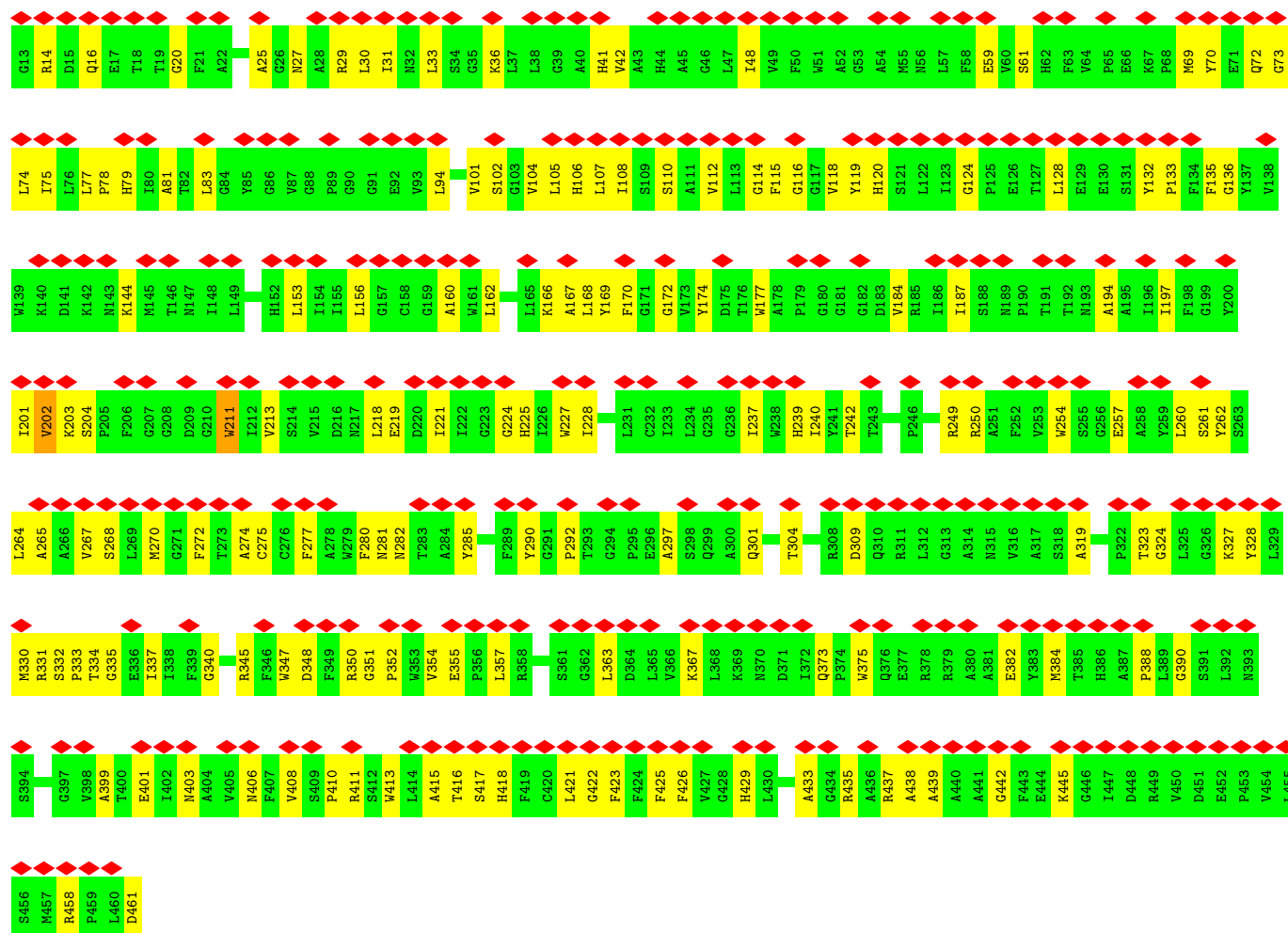


• Molecule 4: Photosystem II CP43 reaction center protein

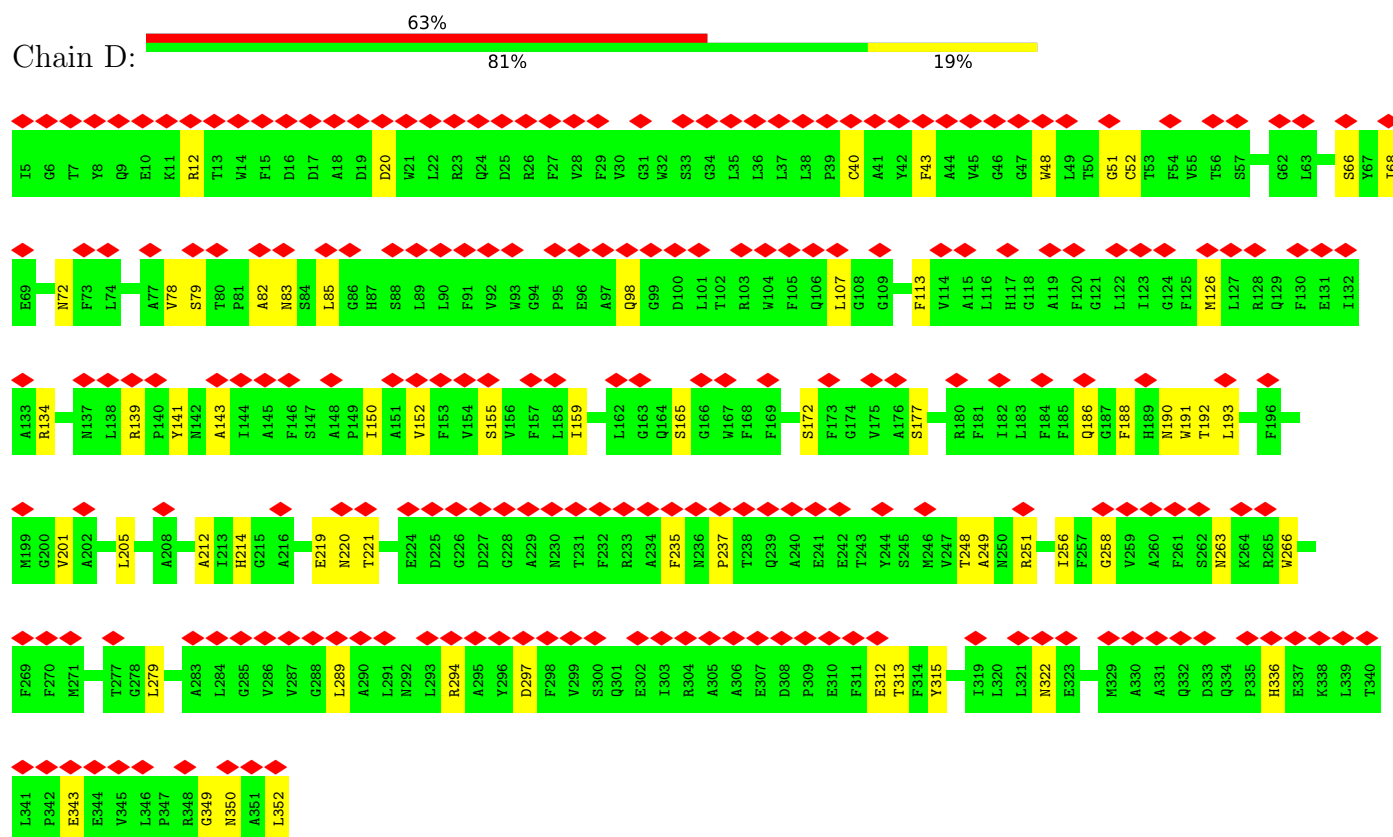




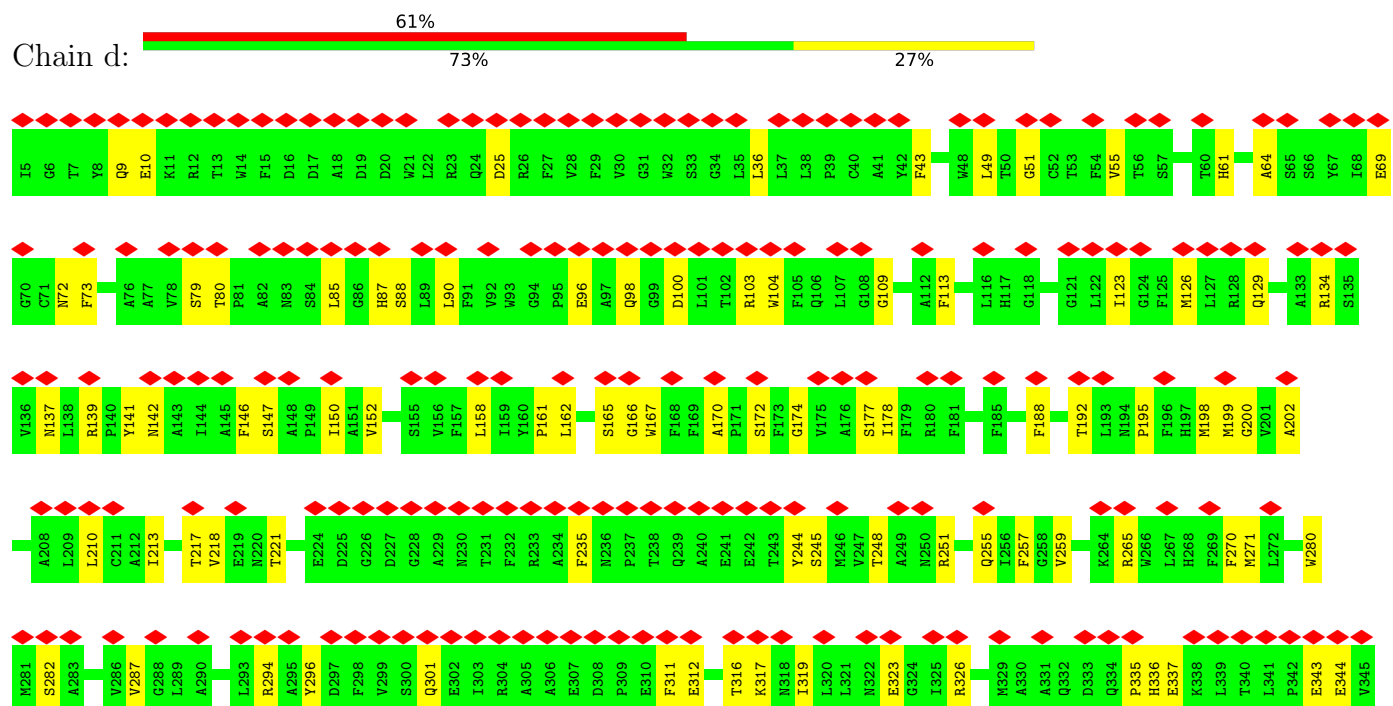
• Molecule 4: Photosystem II CP43 reaction center protein

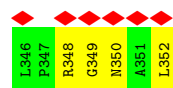


- Molecule 5: Photosystem II D2 protein

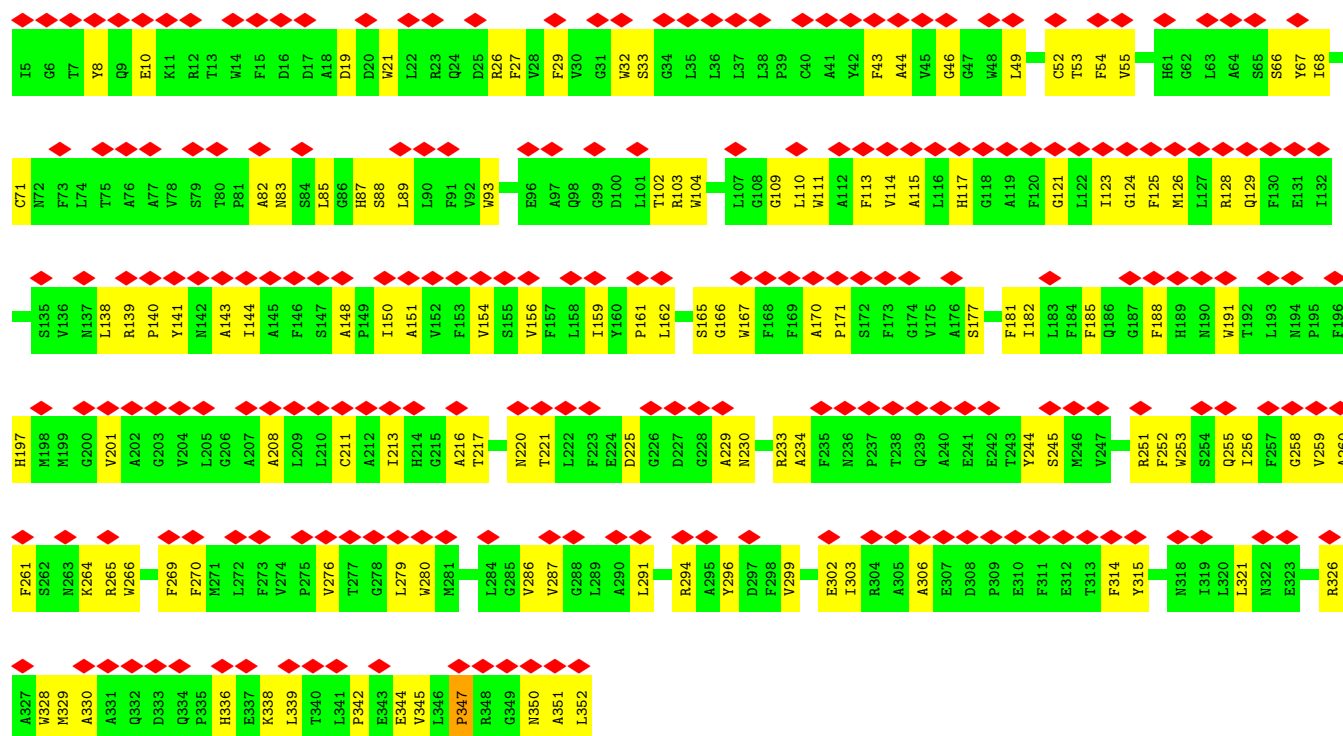


- Molecule 5: Photosystem II D2 protein

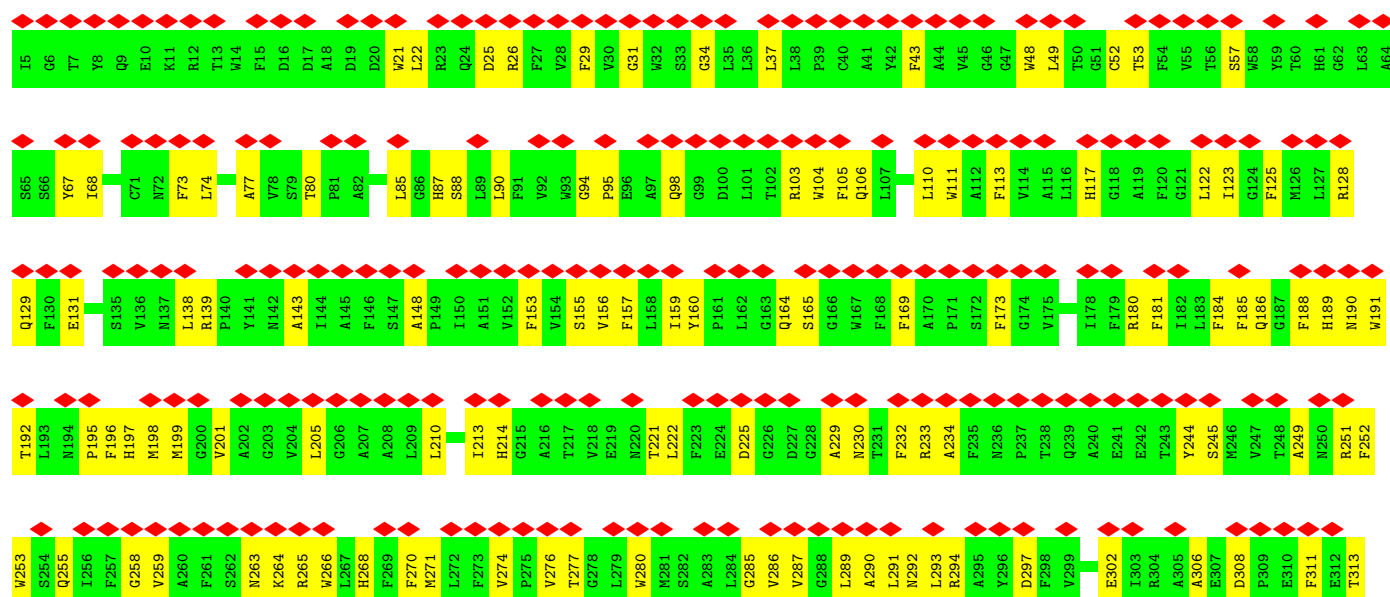
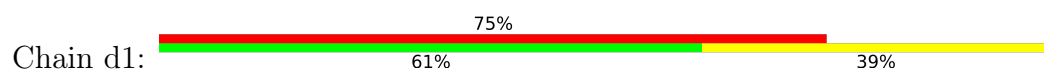


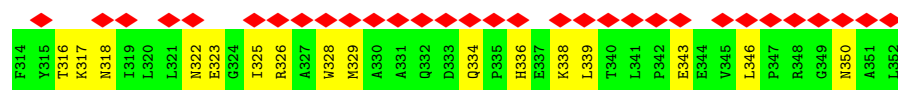


• Molecule 5: Photosystem II D2 protein

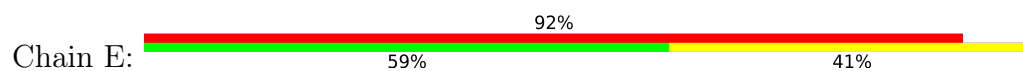


• Molecule 5: Photosystem II D2 protein

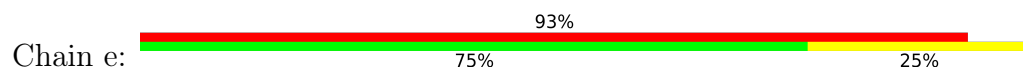




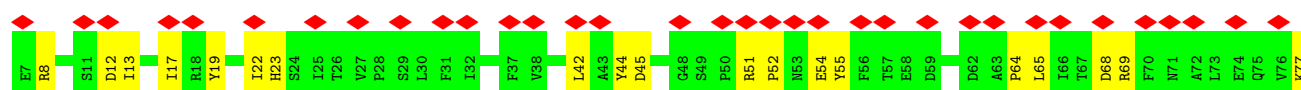
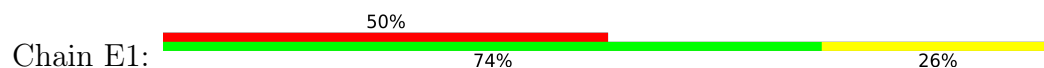
• Molecule 6: Cytochrome b559 subunit alpha



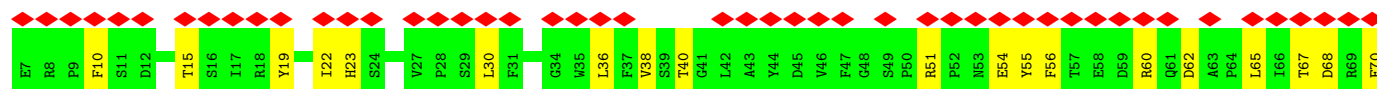
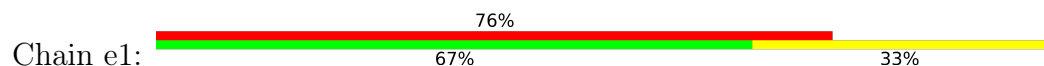
• Molecule 6: Cytochrome b559 subunit alpha



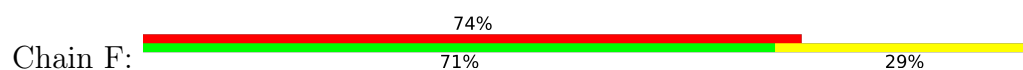
• Molecule 6: Cytochrome b559 subunit alpha

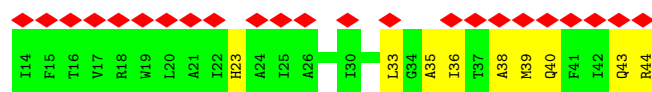


• Molecule 6: Cytochrome b559 subunit alpha

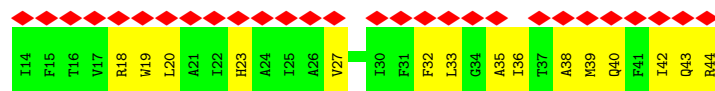


• Molecule 7: Cytochrome b559 subunit beta

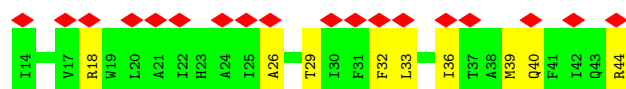




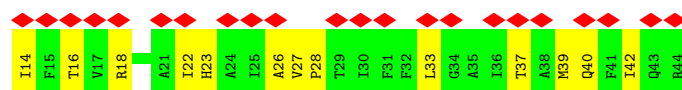
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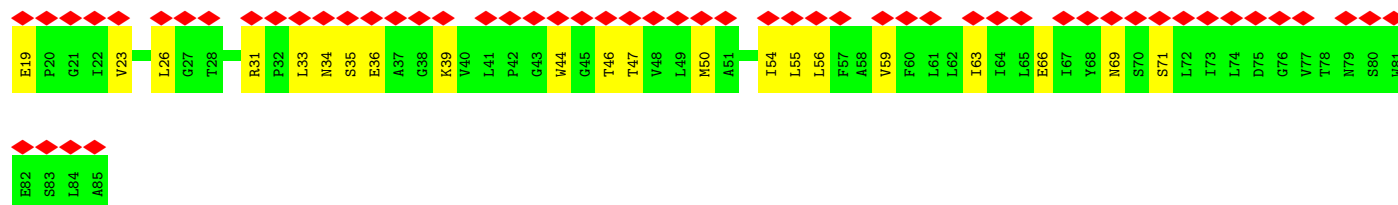
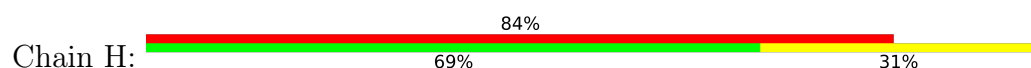
• Molecule 7: Cytochrome b559 subunit beta



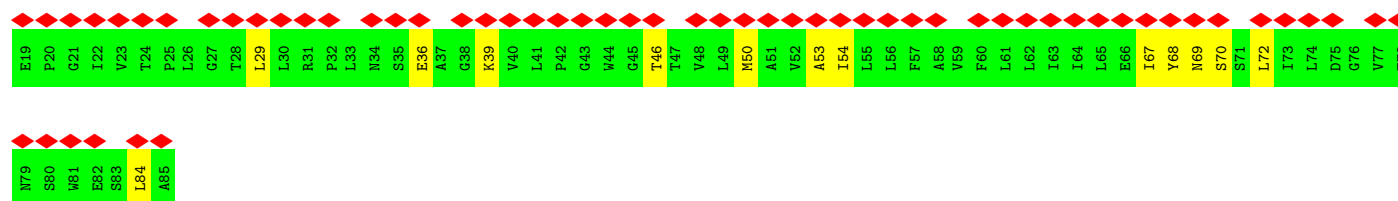
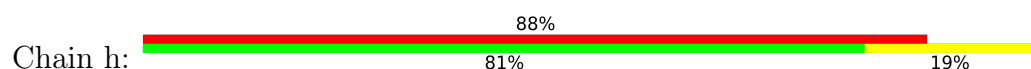
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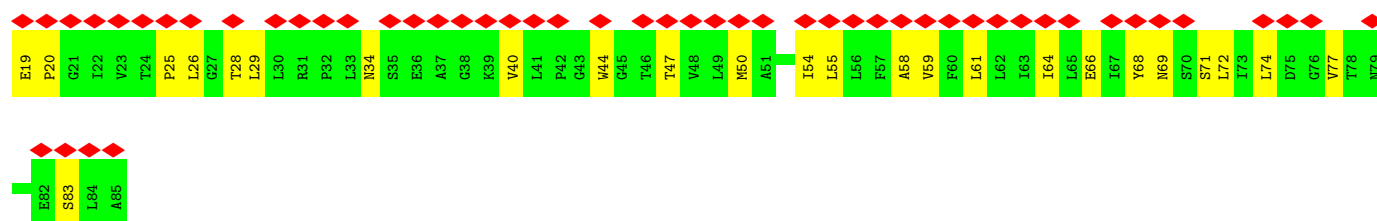
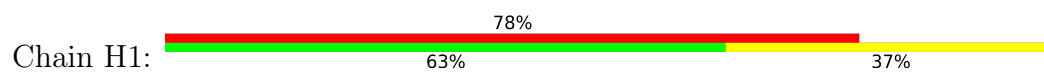
• Molecule 8: Photosystem II reaction center protein H



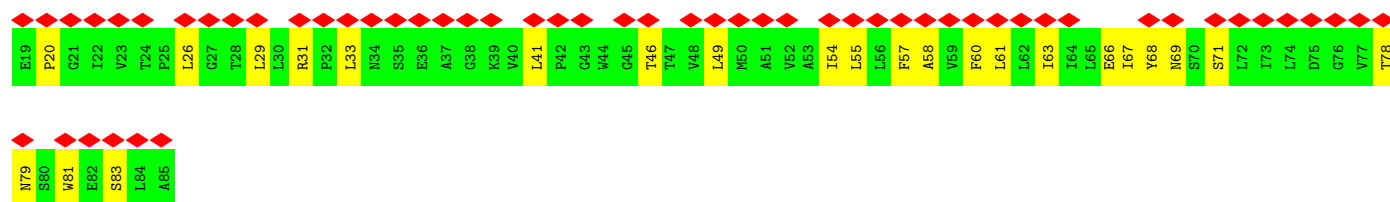
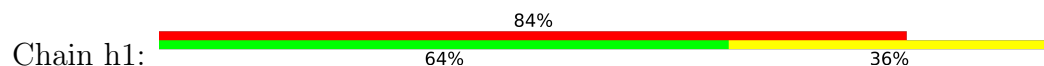
• Molecule 8: Photosystem II reaction center protein H



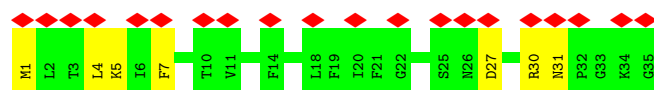
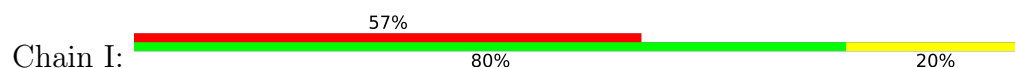
• Molecule 8: Photosystem II reaction center protein H



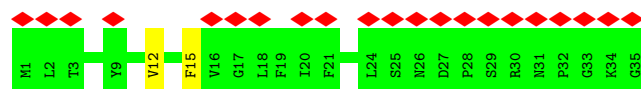
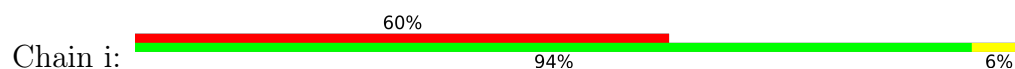
- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I



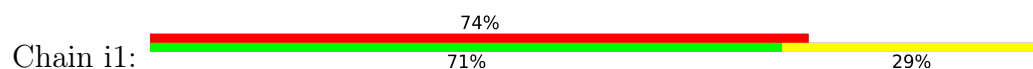
- Molecule 9: Photosystem II reaction center protein I



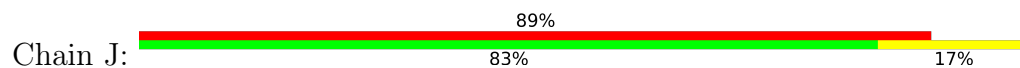
- Molecule 9: Photosystem II reaction center protein I



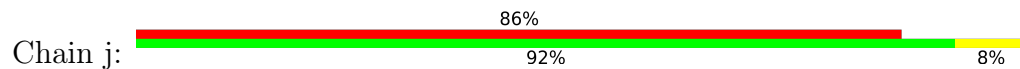
- Molecule 9: Photosystem II reaction center protein I



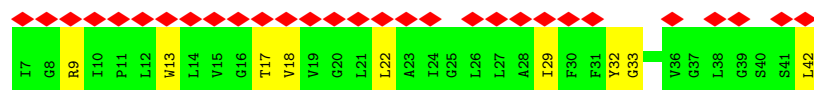
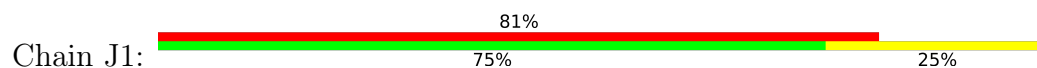
• Molecule 10: PsbJ



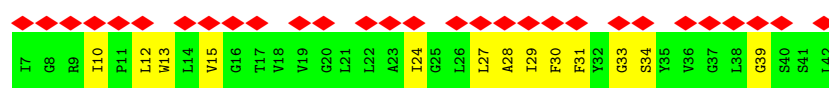
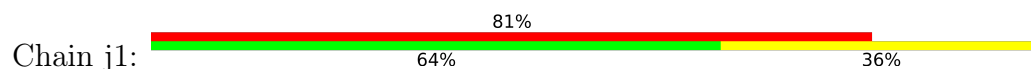
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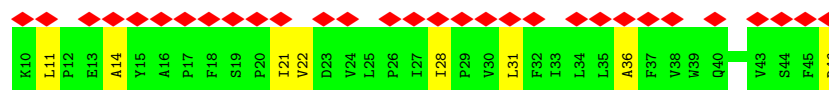
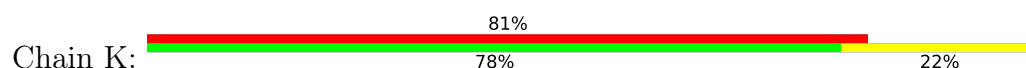
• Molecule 10: PsbJ



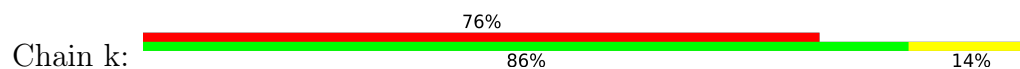
• Molecule 10: PsbJ



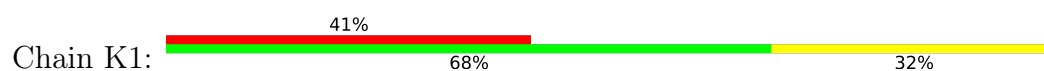
• Molecule 11: Photosystem II reaction center protein K

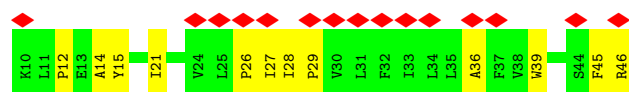


• Molecule 11: Photosystem II reaction center protein K

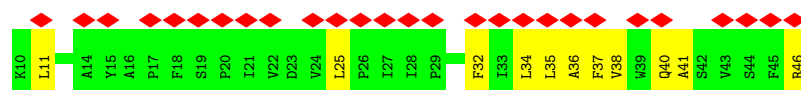
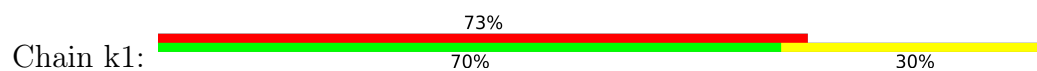


• Molecule 11: Photosystem II reaction center protein K

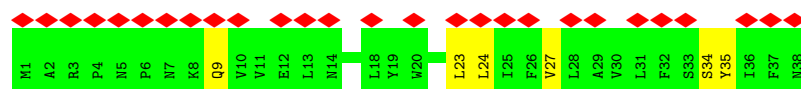
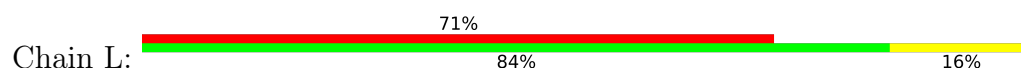




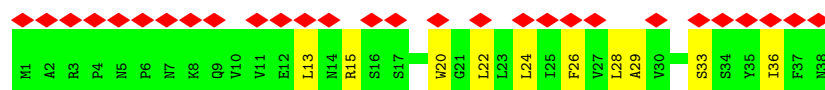
- Molecule 11: Photosystem II reaction center protein K



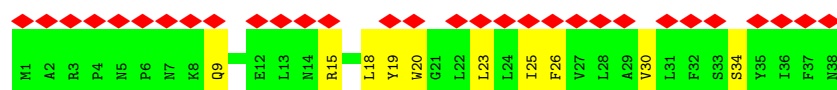
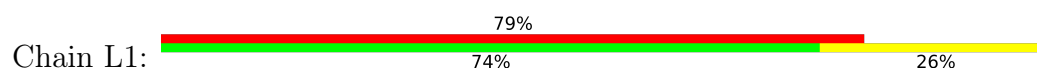
- Molecule 12: Photosystem II reaction center protein L



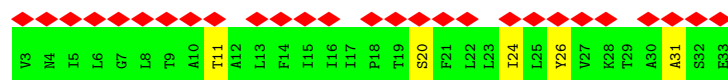
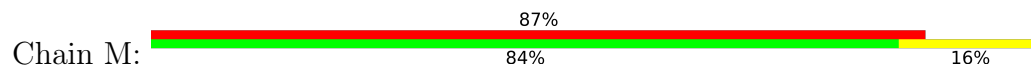
- Molecule 12: Photosystem II reaction center protein L



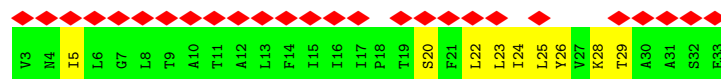
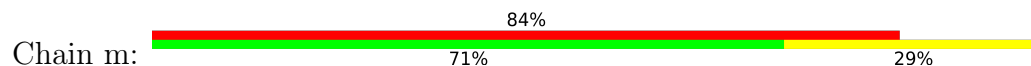
- Molecule 12: Photosystem II reaction center protein L



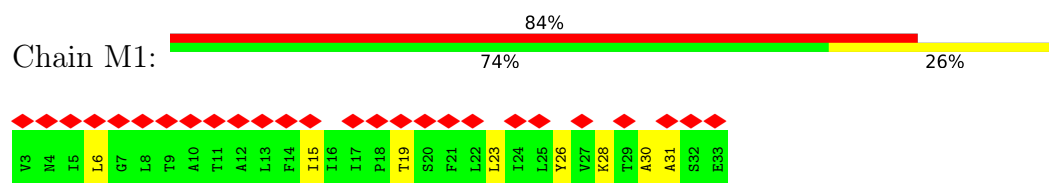
- Molecule 13: PsbM



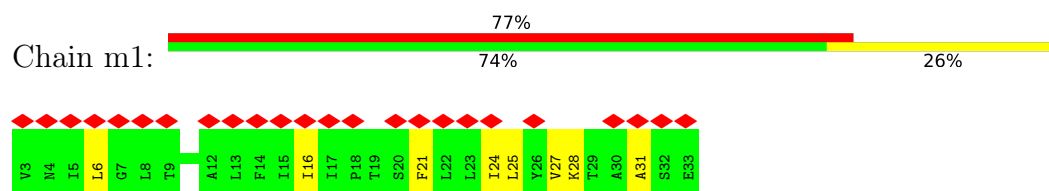
- Molecule 13: PsbM



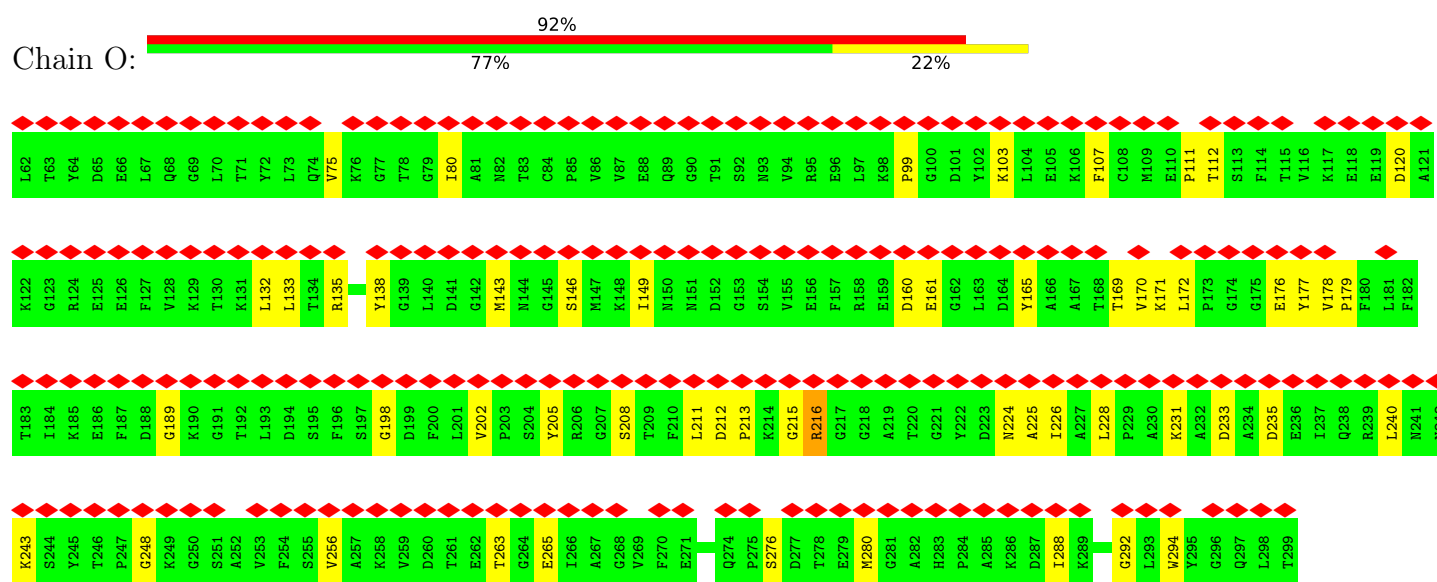
- Molecule 13: PsbM



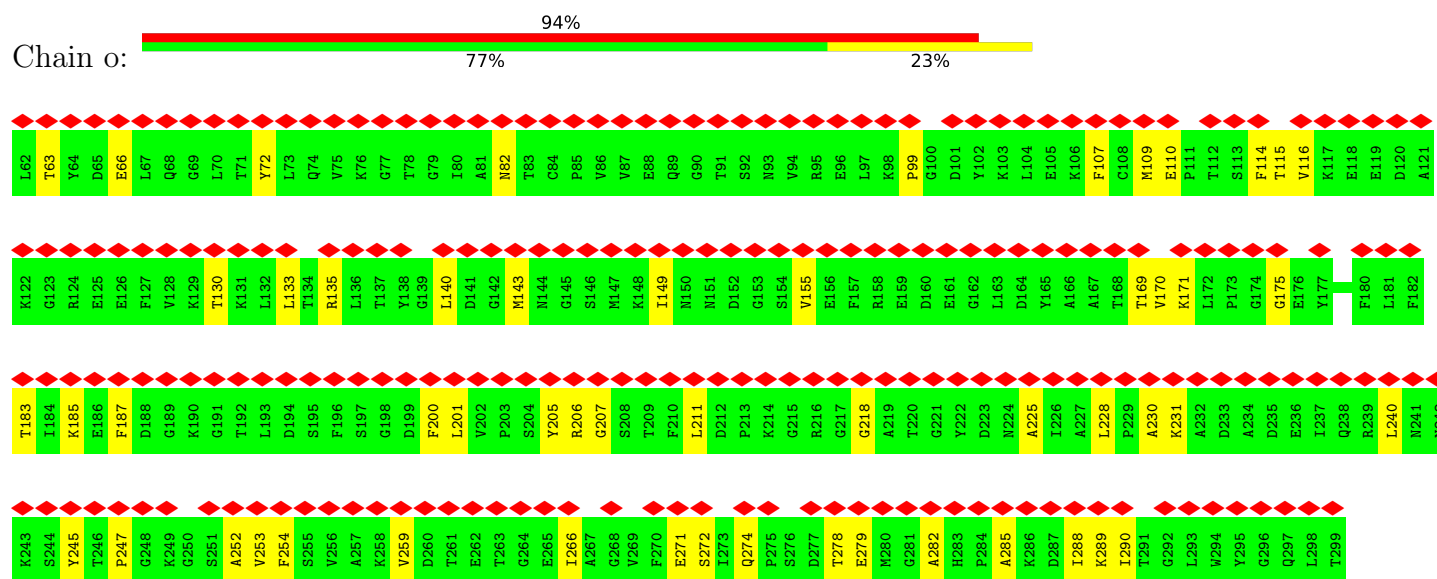
- Molecule 13: PsbM



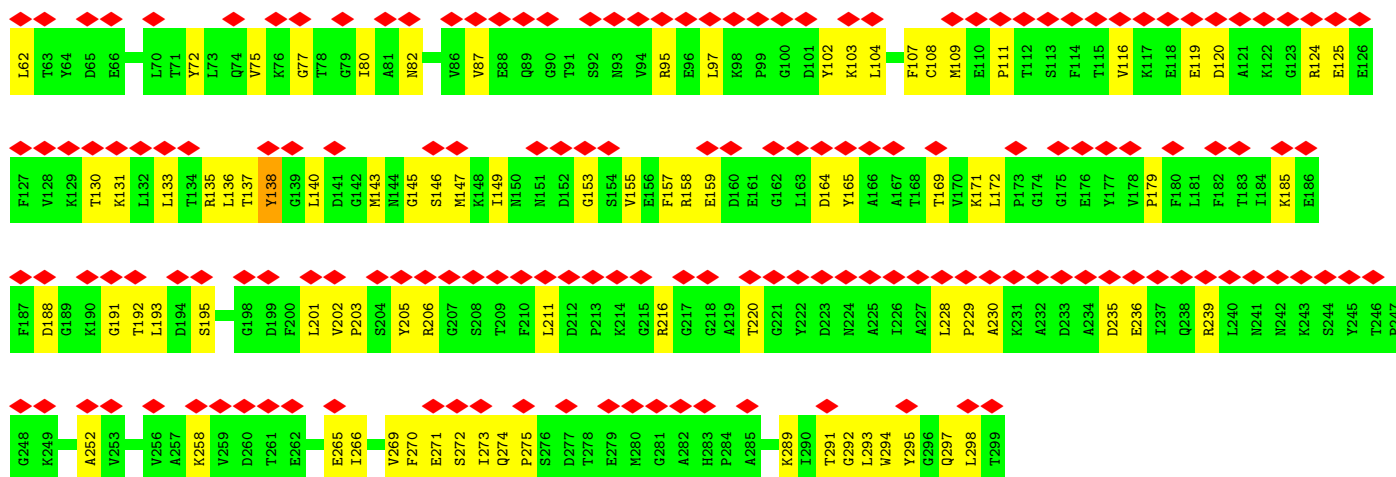
- Molecule 14: PsbO



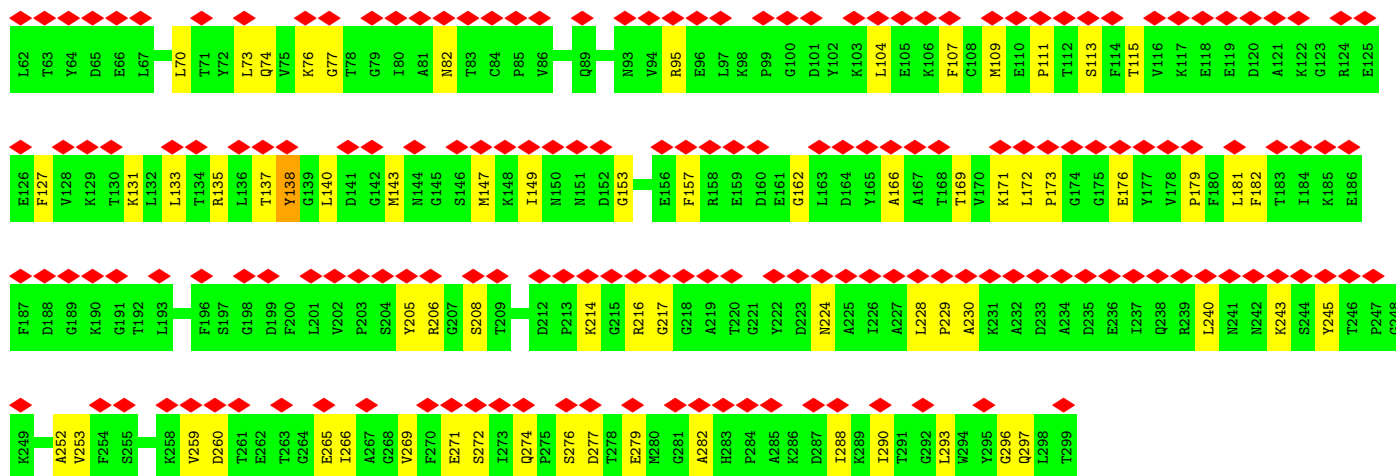
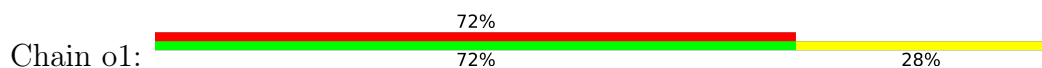
- Molecule 14: PsbO



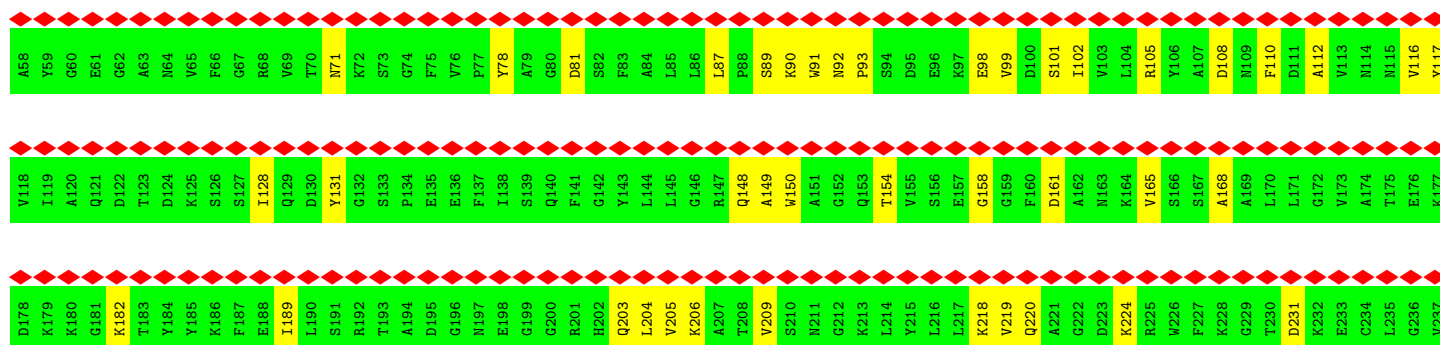
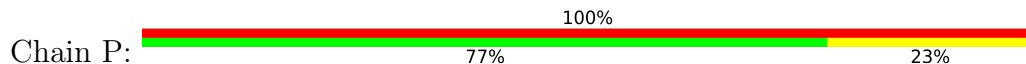
- Molecule 14: PsbO

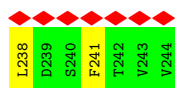


• Molecule 14: PsbO

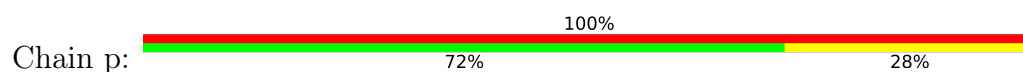


• Molecule 15: PsbP

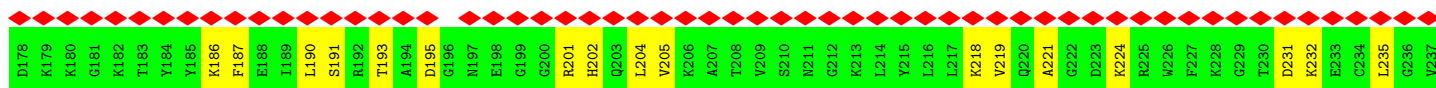
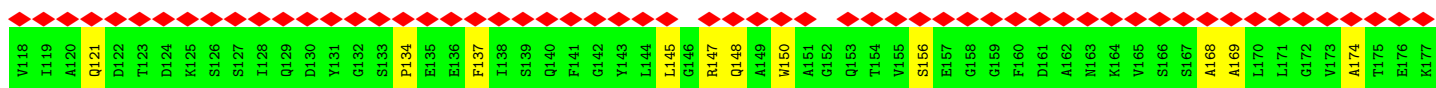
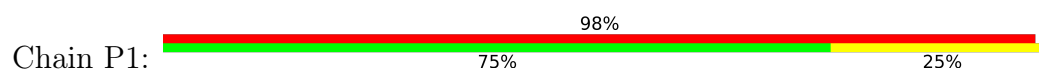




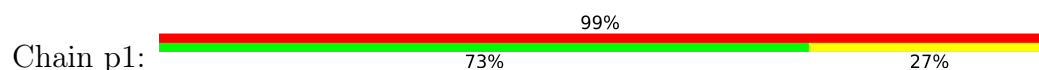
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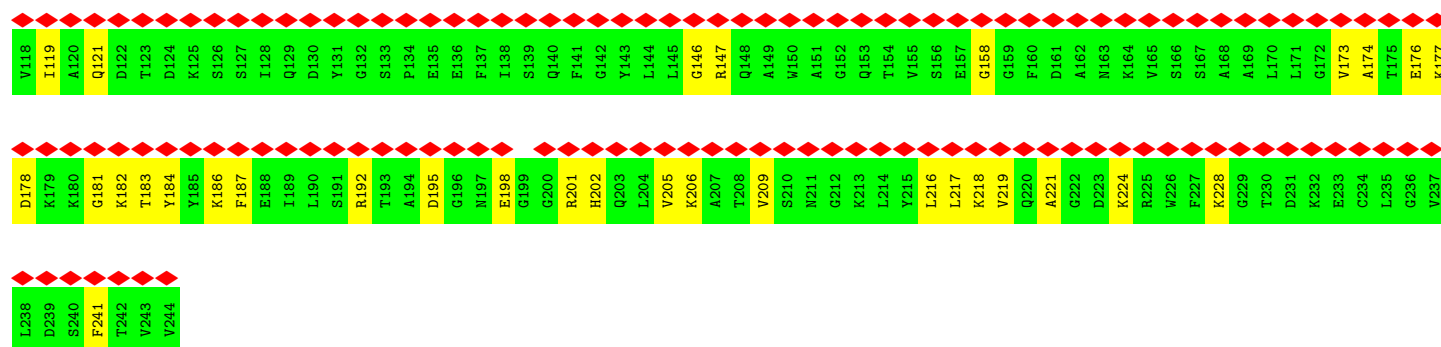


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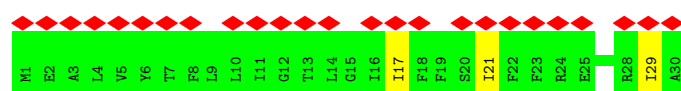
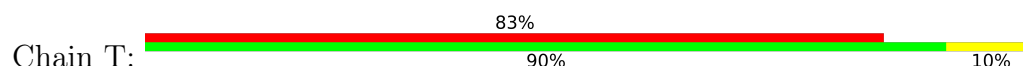


• Molecule 15: PsbP

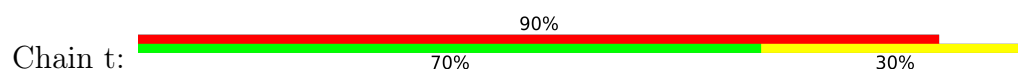




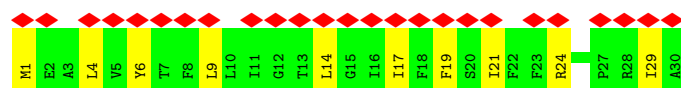
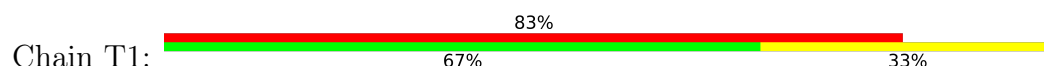
• Molecule 16: Photosystem II reaction center protein T



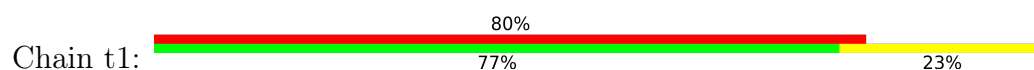
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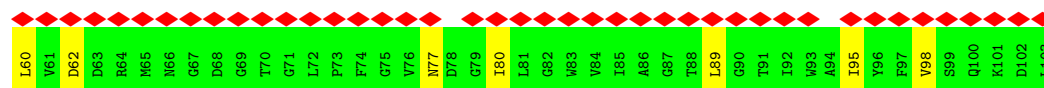
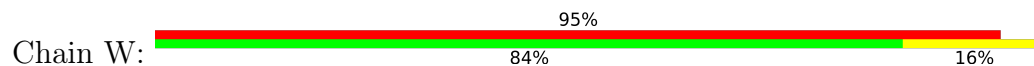
• Molecule 16: Photosystem II reaction center protein T



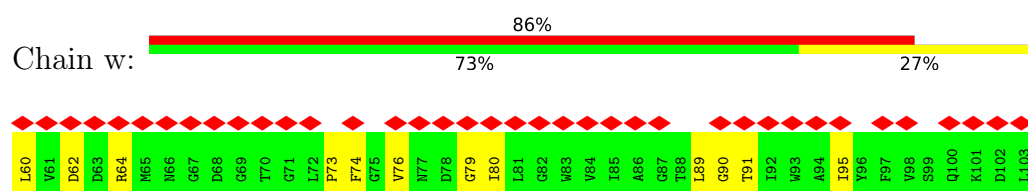
• Molecule 16: Photosystem II reaction center protein T



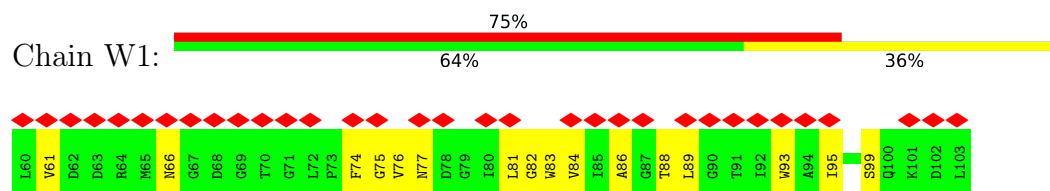
• Molecule 17: PsbW



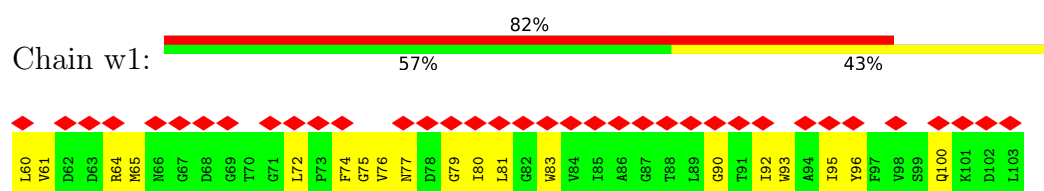
• Molecule 17: PsbW



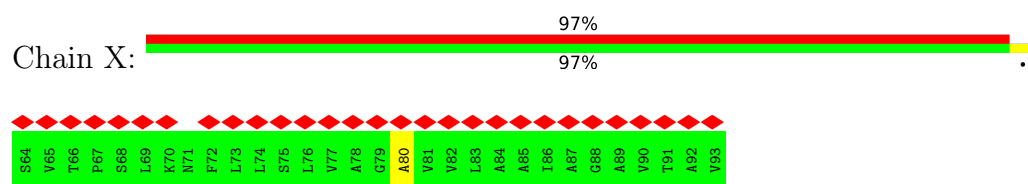
• Molecule 17: PsbW



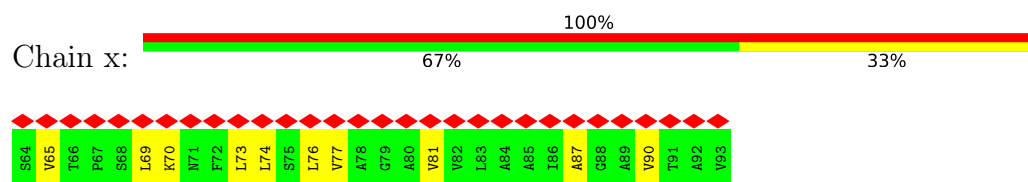
• Molecule 17: PsbW



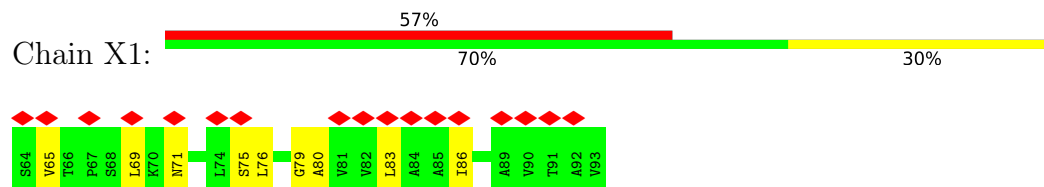
• Molecule 18: PsbX



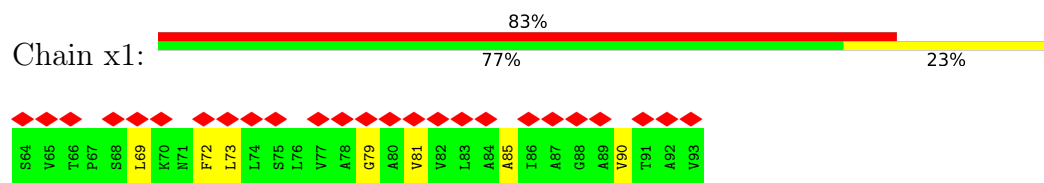
• Molecule 18: PsbX



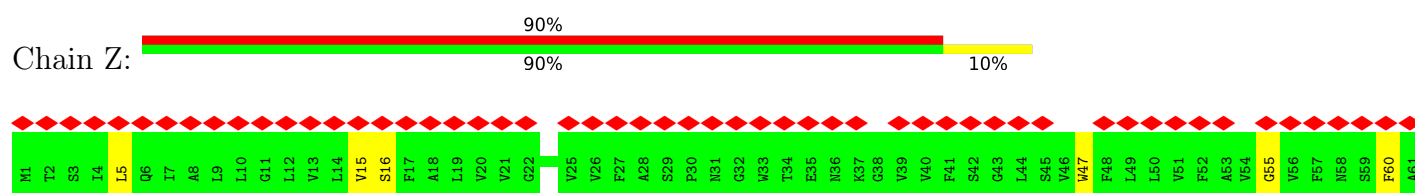
• Molecule 18: PsbX



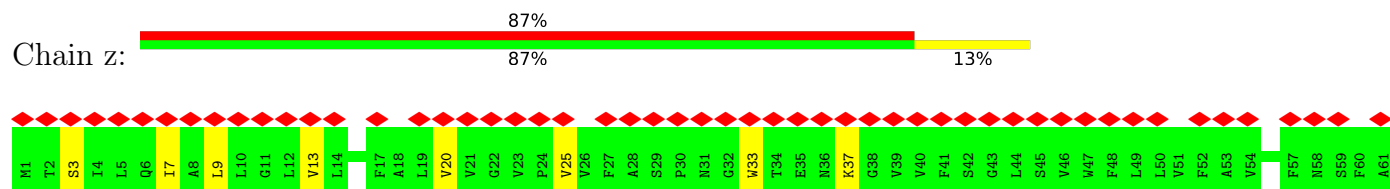
• Molecule 18: PsbX



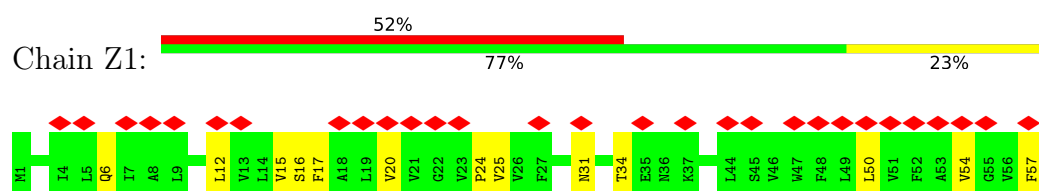
• Molecule 19: Photosystem II reaction center protein Z



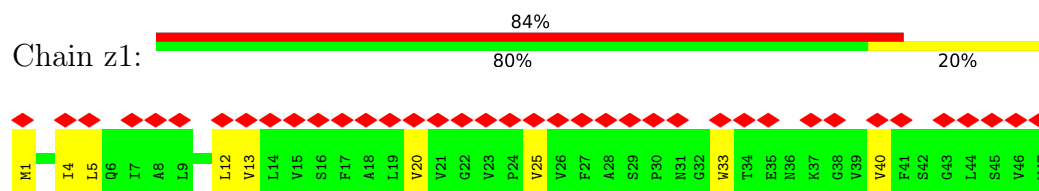
• Molecule 19: Photosystem II reaction center protein Z



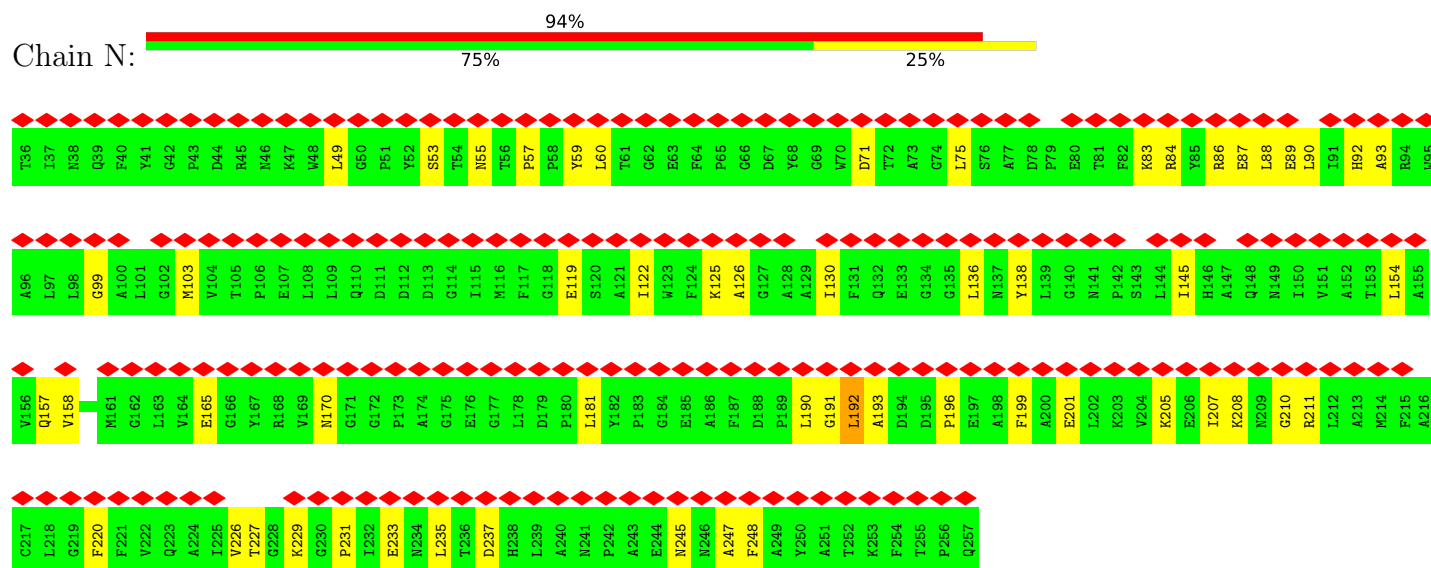
• Molecule 19: Photosystem II reaction center protein Z



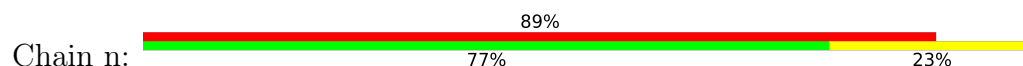
• Molecule 19: Photosystem II reaction center protein Z

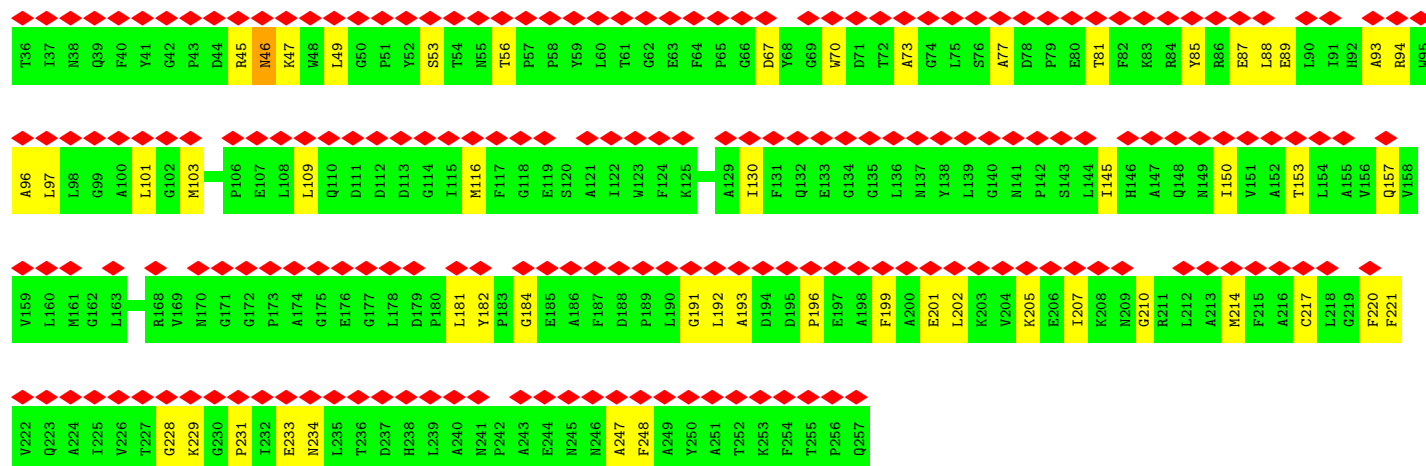


• Molecule 20: LHCII M3

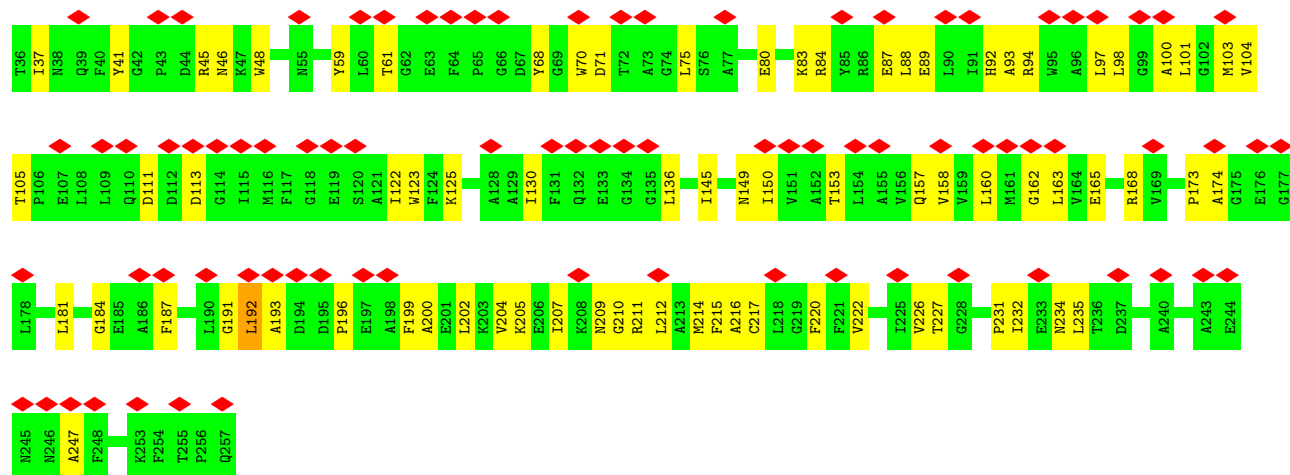


• Molecule 20: LHCII M3

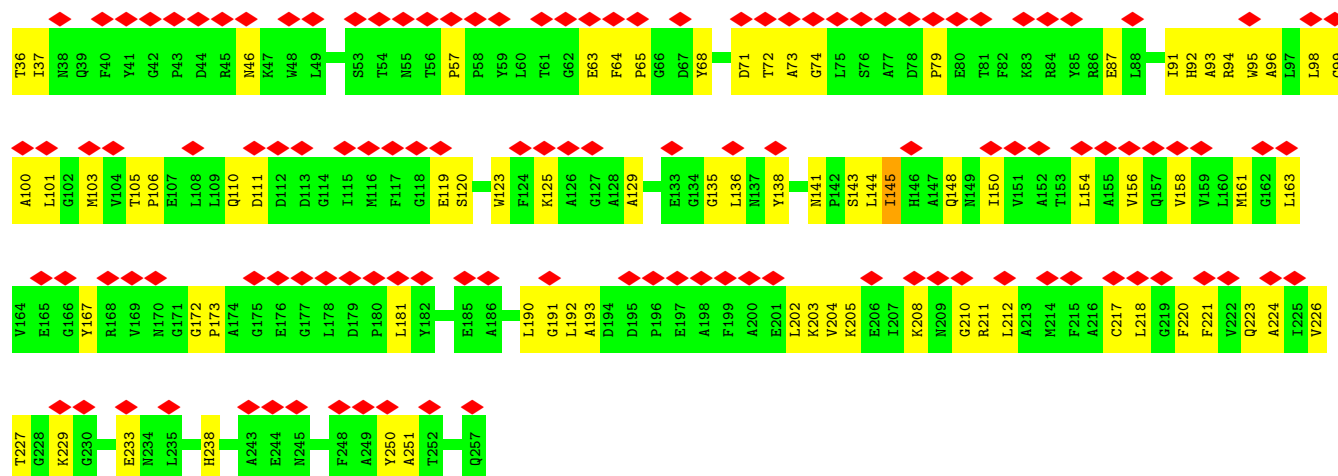




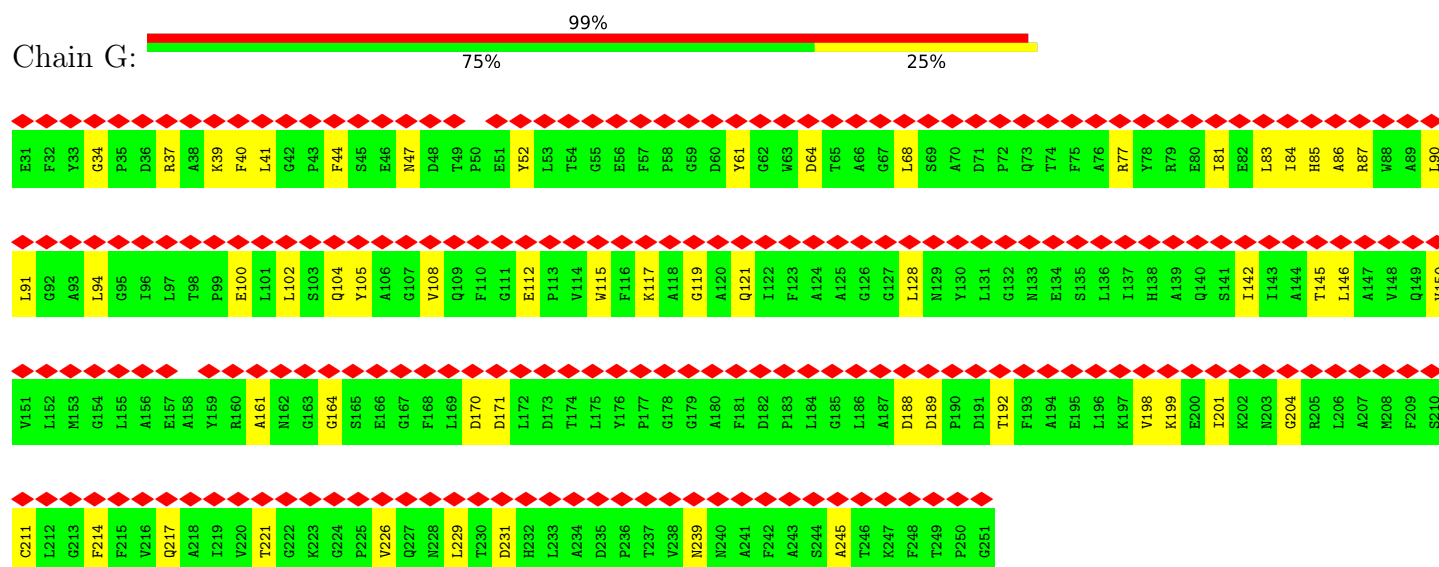
• Molecule 20: LHCII M3



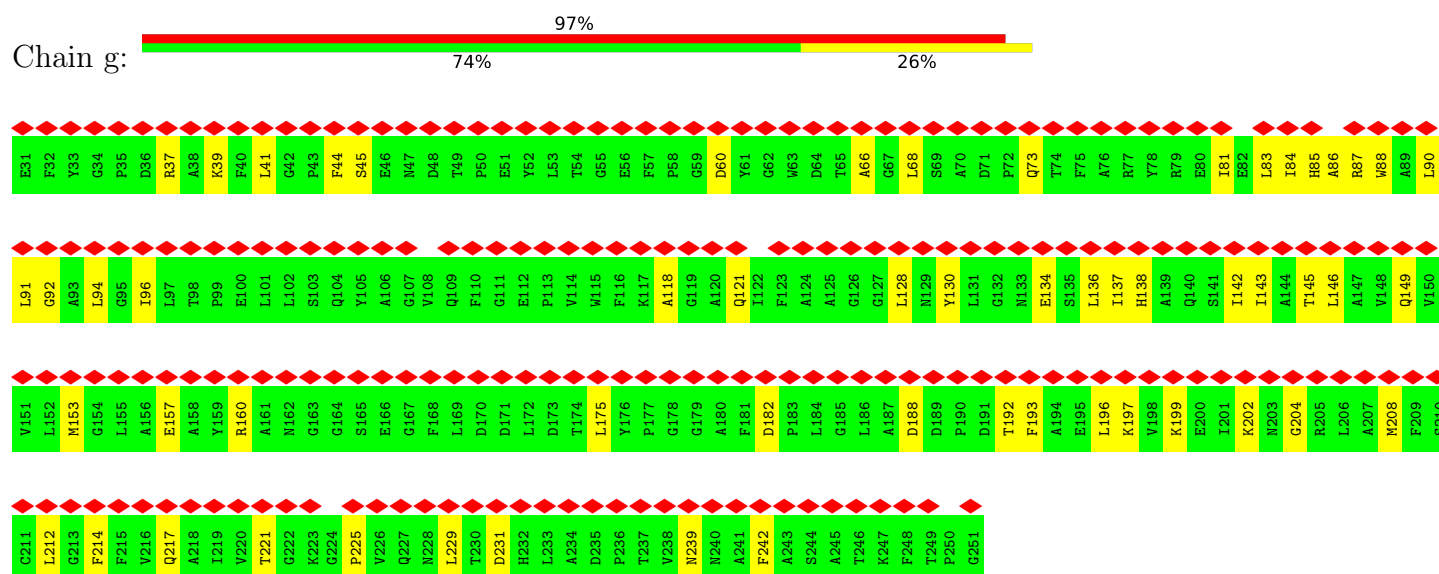
• Molecule 20: LHCII M3



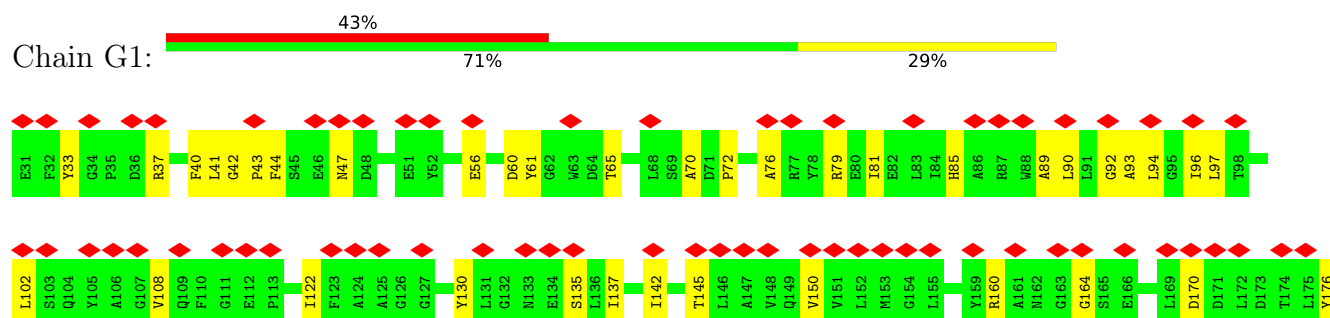
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

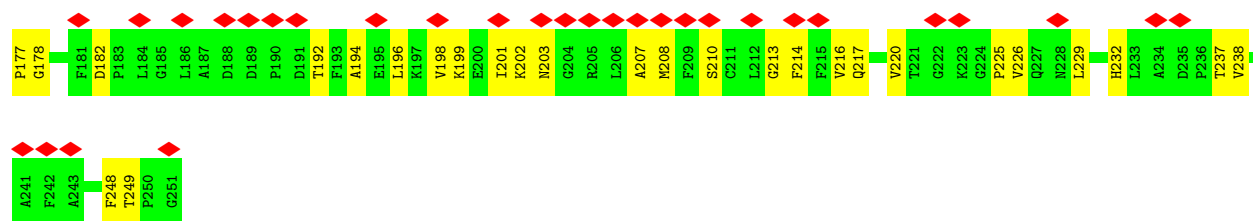


• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

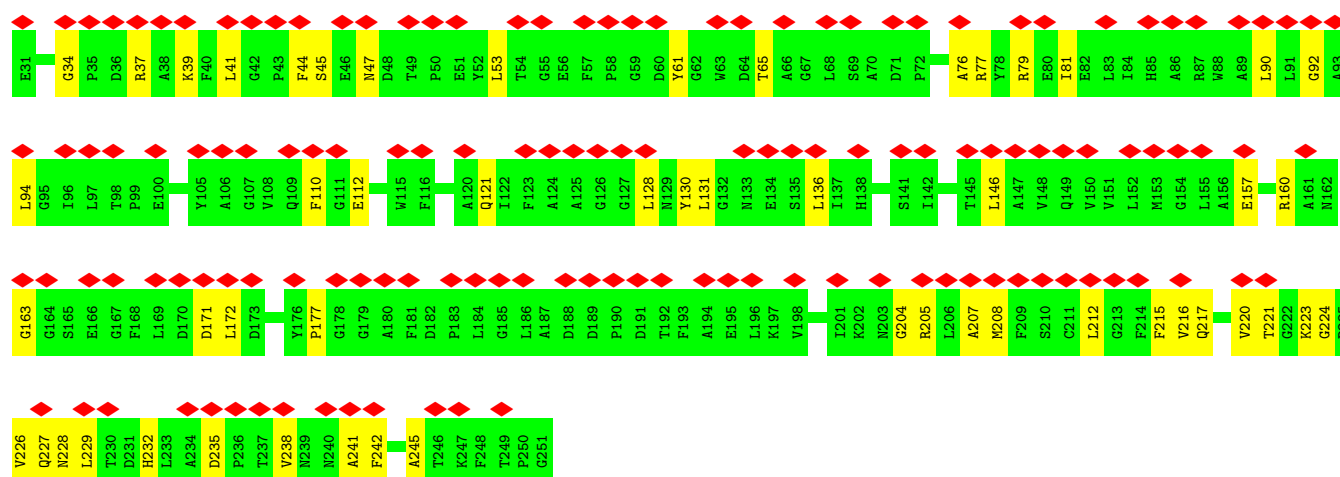
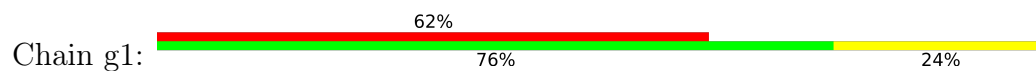


• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

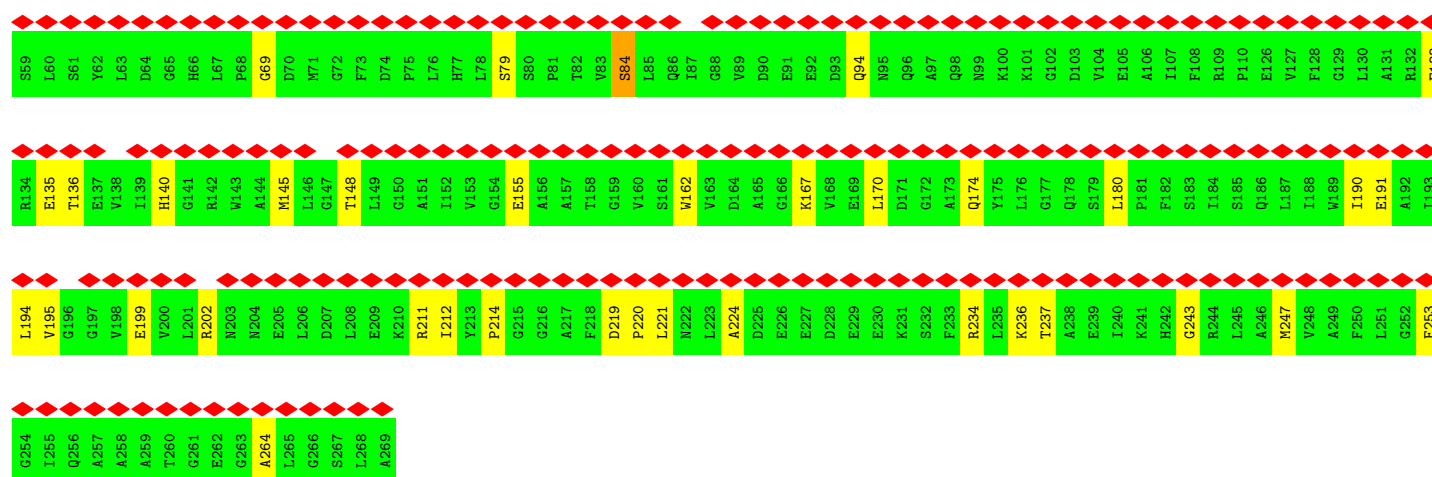
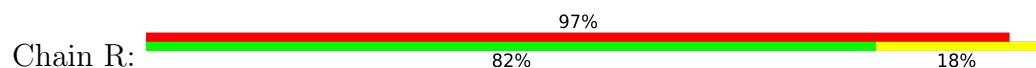




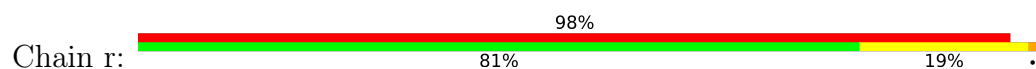
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

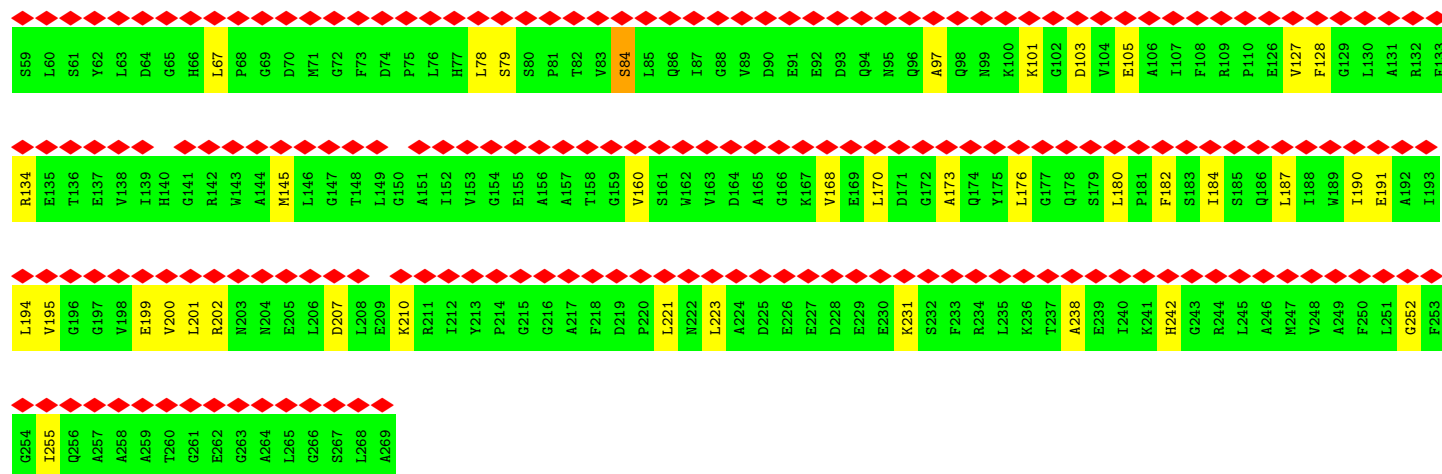


- Molecule 22: CP29

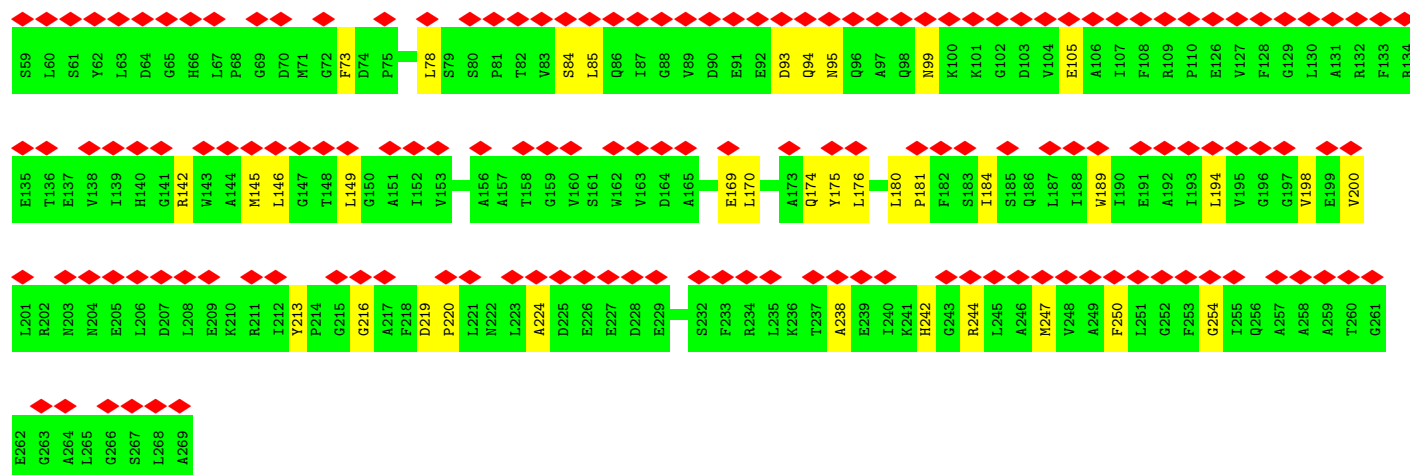
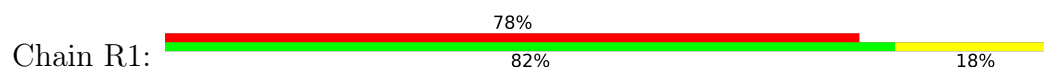


- Molecule 22: CP29

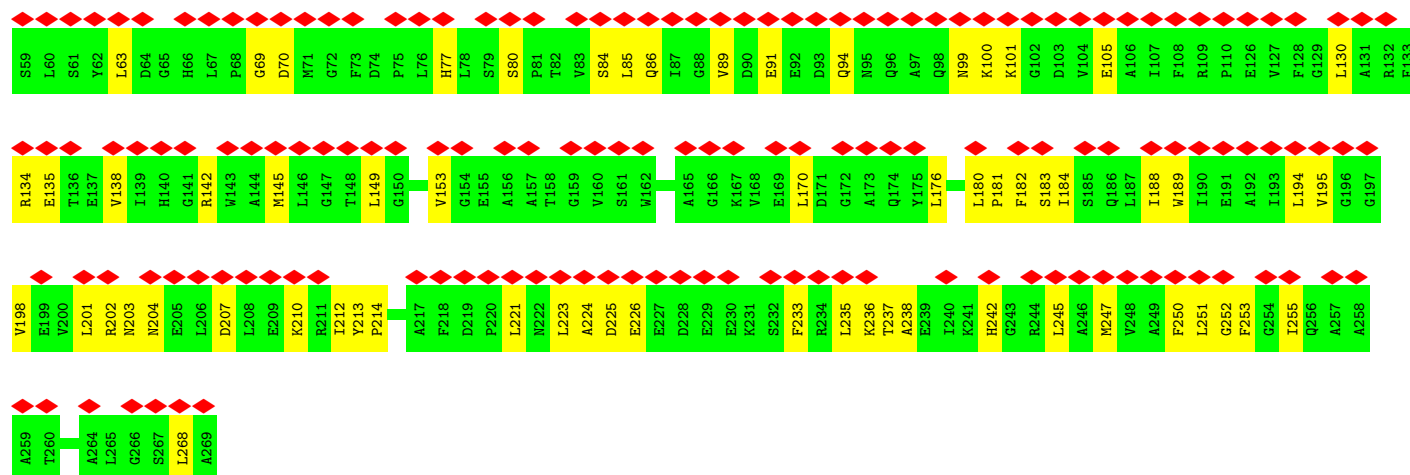
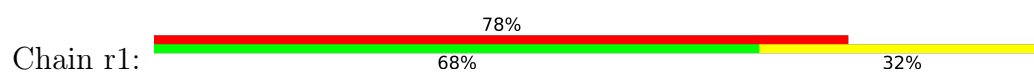




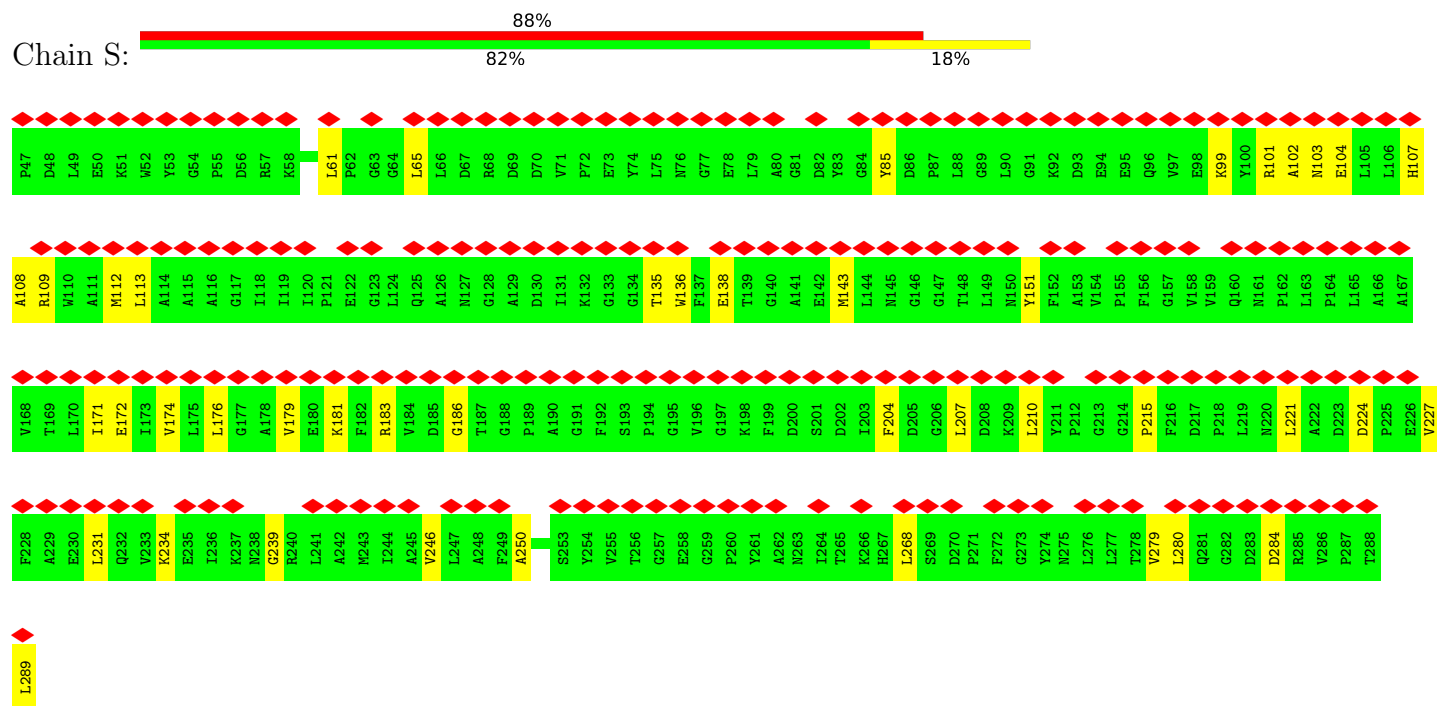
• Molecule 22: CP29



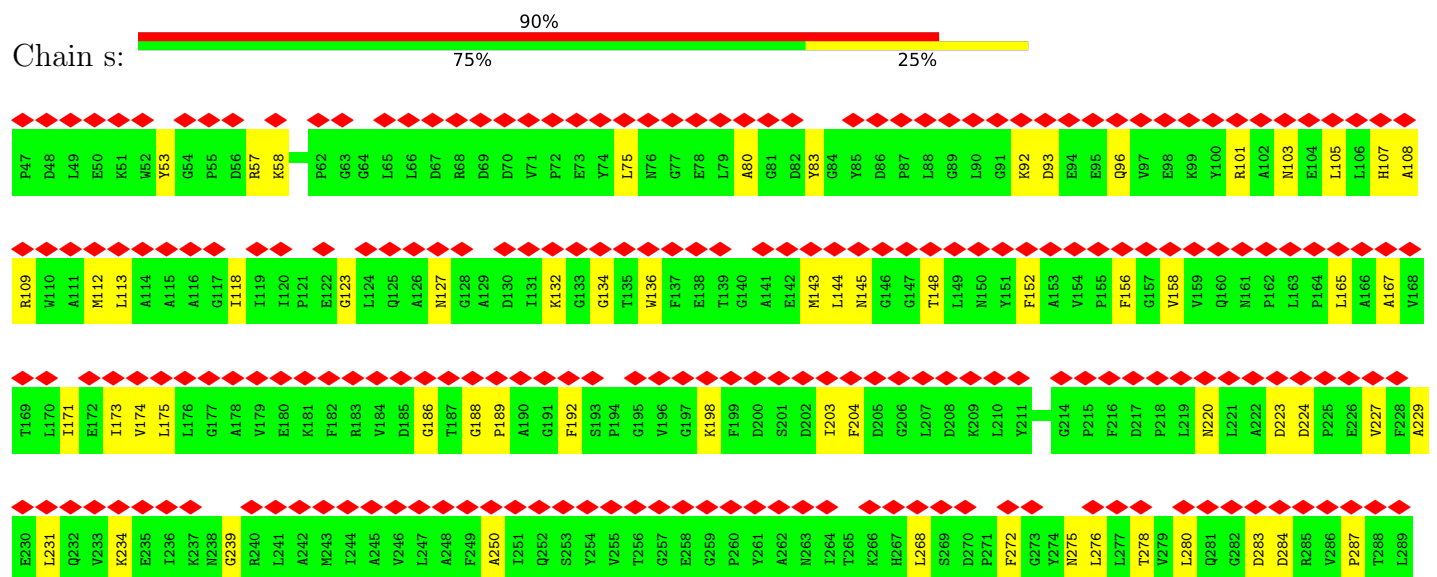
• Molecule 22: CP29



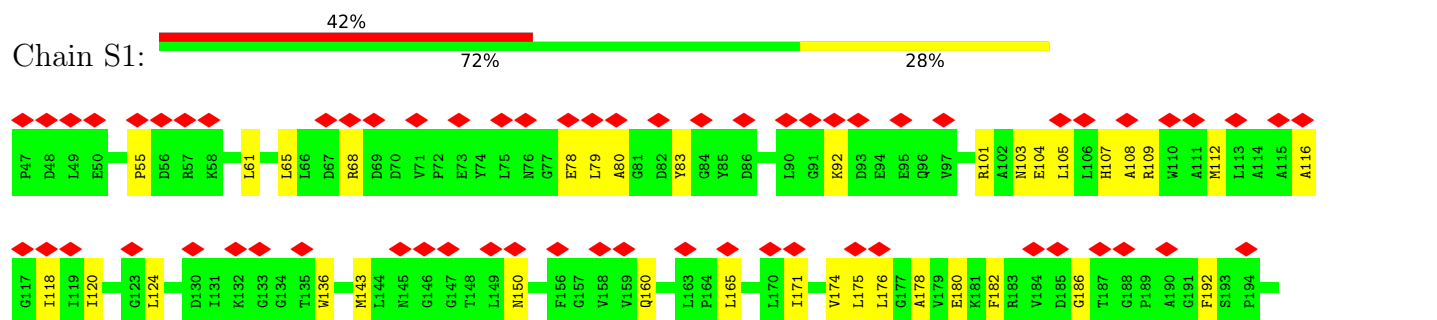
• Molecule 23: CP26

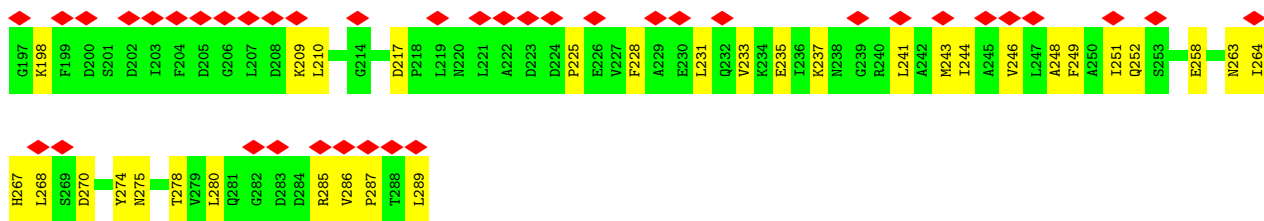


• Molecule 23: CP26

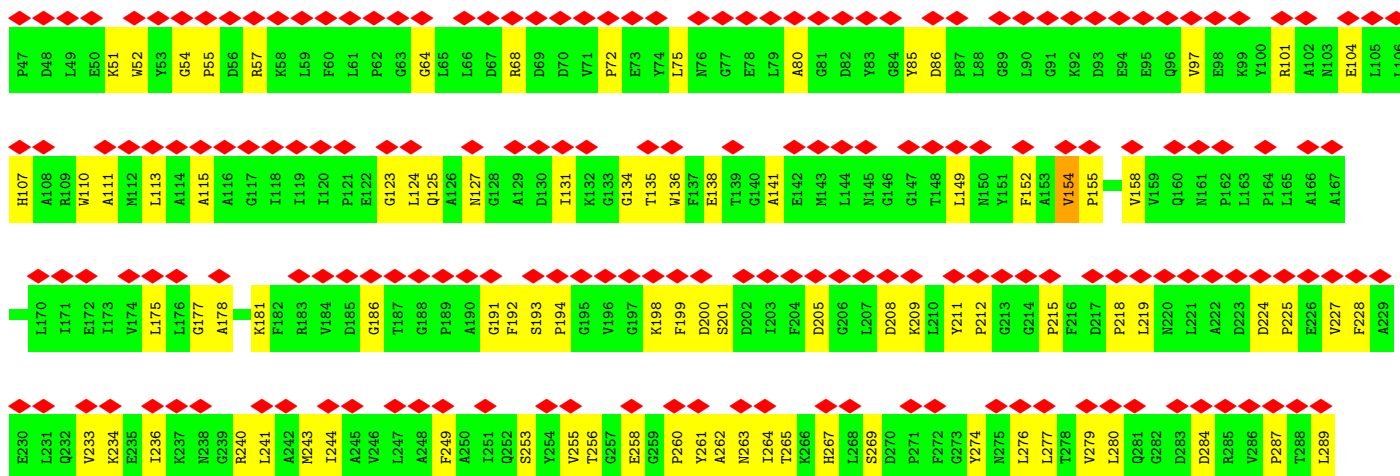
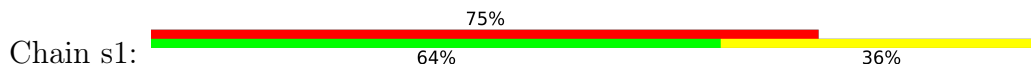


• Molecule 23: CP26

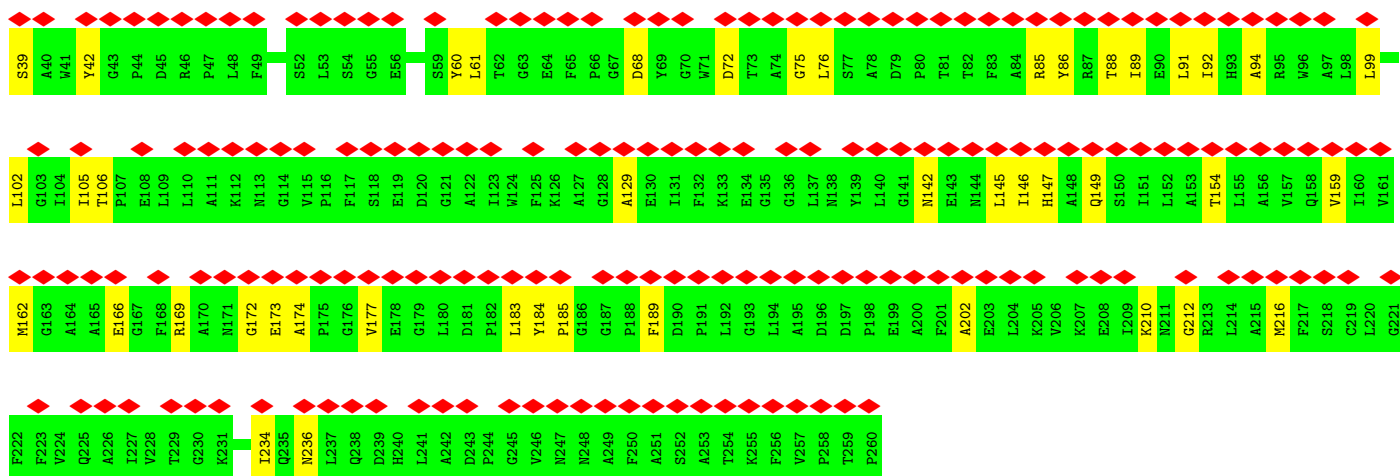
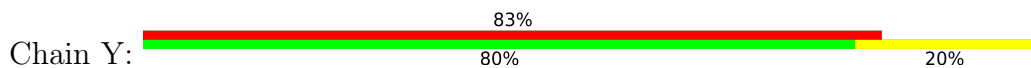




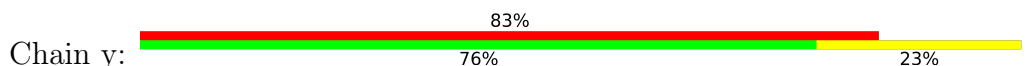
• Molecule 23: CP26

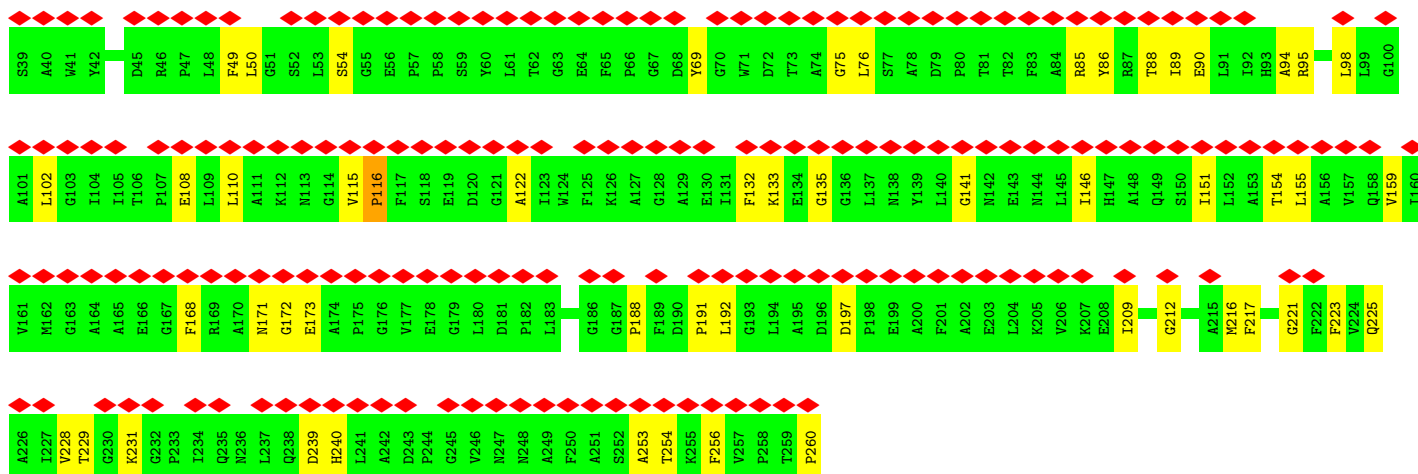


• Molecule 24: LHCII M1

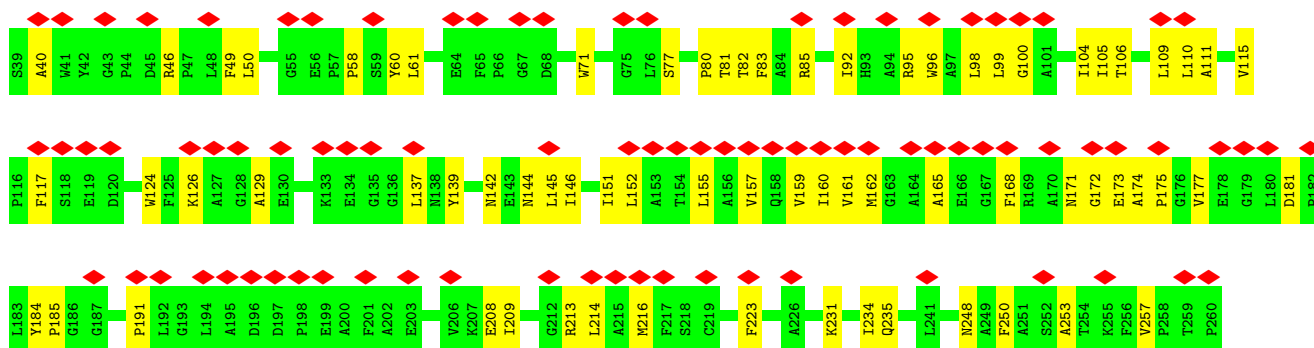
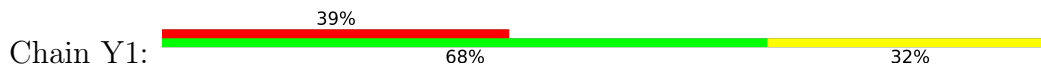


• Molecule 24: LHCII M1

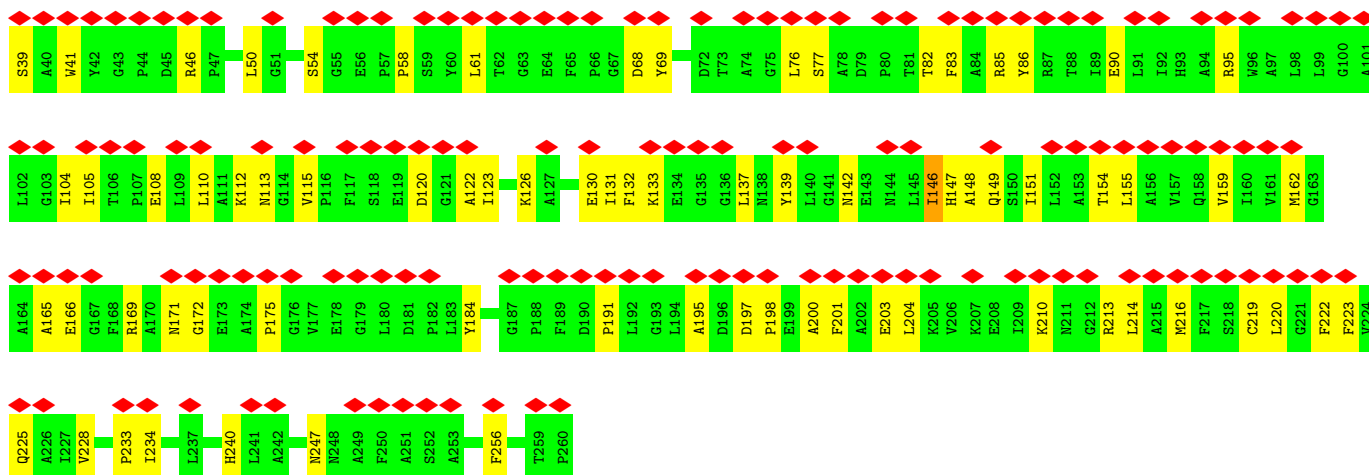




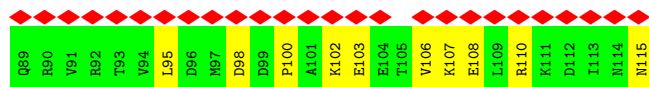
• Molecule 24: LHCII M1



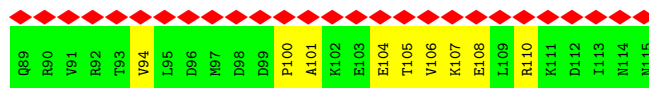
• Molecule 24: LHCII M1



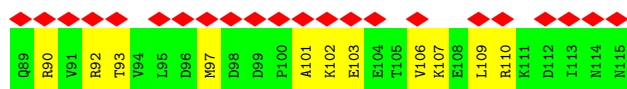
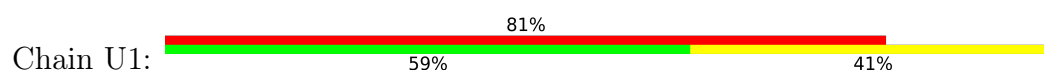
• Molecule 25: PsbU



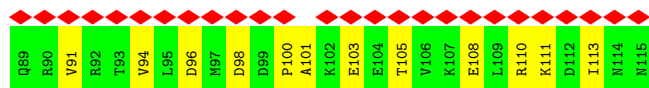
• Molecule 25: PsbU



• Molecule 25: PsbU



• Molecule 25: PsbU



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.036	Depositor
Map size ($\text{\AA}$)	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.96, 0.96, 0.96	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, LUT, CL, FE2, SEP, XAT, LPX, OEX, NEX, 3PH, LMK, NA, C7Z, SQD, BCR, PTY, LMG, DGD, PHO, ERG, BCT, 4RF, CHL, RRX, DGA, CLA, HEM, SPH, LHG, GOL, LMT

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	0.34	0/2723	0.57	0/3715
1	A1	0.27	0/2723	0.61	2/3715 (0.1%)
1	a	0.34	0/2723	0.57	0/3715
1	a1	0.28	0/2723	0.65	2/3715 (0.1%)
2	B	0.31	0/3912	0.59	2/5327 (0.0%)
2	B1	0.27	0/3912	0.60	2/5327 (0.0%)
2	b	0.31	0/3912	0.54	1/5327 (0.0%)
2	b1	0.25	0/3912	0.56	3/5327 (0.1%)
3	V	0.25	0/228	0.57	0/311
3	V1	0.19	0/228	0.47	0/311
3	v	0.24	0/228	0.55	0/311
3	v1	0.25	0/228	0.67	0/311
4	C	0.39	2/3602 (0.1%)	0.65	4/4913 (0.1%)
4	C1	0.26	0/3602	0.54	1/4913 (0.0%)
4	c	0.31	0/3602	0.51	0/4913
4	c1	0.32	2/3602 (0.1%)	0.66	4/4913 (0.1%)
5	D	0.36	0/2860	0.60	2/3899 (0.1%)
5	D1	0.28	0/2860	0.63	2/3899 (0.1%)
5	d	0.32	0/2860	0.57	0/3899
5	d1	0.29	0/2860	0.64	0/3899
6	E	0.26	0/639	0.60	0/870
6	E1	0.26	0/639	0.63	0/870
6	e	0.50	1/639 (0.2%)	0.84	3/870 (0.3%)
6	e1	0.23	0/639	0.62	0/870
7	F	0.29	0/259	0.56	0/351
7	F1	0.26	0/259	0.58	0/351
7	f	0.37	0/259	0.71	0/351
7	f1	0.26	0/259	0.71	0/351
8	H	0.34	0/513	0.68	0/703
8	H1	0.25	0/513	0.57	0/703
8	h	0.30	0/513	0.58	0/703

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	h1	0.24	0/513	0.57	0/703
9	I	0.35	0/287	0.52	0/386
9	I1	0.24	0/287	0.57	0/386
9	i	0.30	0/287	0.55	0/386
9	i1	0.26	0/287	0.63	0/386
10	J	0.24	0/272	0.46	0/369
10	J1	0.21	0/272	0.55	0/369
10	j	0.27	0/272	0.56	0/369
10	j1	0.21	0/272	0.59	0/369
11	K	0.36	0/308	0.73	0/423
11	K1	0.28	0/308	0.64	0/423
11	k	0.33	0/308	0.58	0/423
11	k1	0.32	0/308	0.70	0/423
12	L	0.27	0/321	0.46	0/435
12	L1	0.35	0/321	0.68	0/435
12	l	0.33	0/321	0.59	0/435
13	M	0.30	0/237	0.53	0/323
13	M1	0.23	0/237	0.57	0/323
13	m	0.35	0/237	0.78	1/323 (0.3%)
13	m1	0.26	0/237	0.60	0/323
14	O	0.28	0/1855	0.63	0/2505
14	O1	0.27	0/1855	0.62	0/2505
14	o	0.28	0/1855	0.58	0/2505
14	o1	0.43	1/1855 (0.1%)	0.78	4/2505 (0.2%)
15	P	0.21	0/1473	0.56	2/1988 (0.1%)
15	P1	0.21	0/1473	0.53	0/1988
15	p	0.23	0/1473	0.53	0/1988
15	p1	0.27	0/1473	0.58	0/1988
16	T	0.29	0/254	0.60	0/342
16	T1	0.32	0/254	0.65	0/342
16	t	0.26	0/254	0.42	0/342
16	t1	0.24	0/254	0.57	0/342
17	W	0.28	0/339	0.63	0/460
17	W1	0.26	0/339	0.54	0/460
17	w	0.27	0/339	0.53	0/460
17	w1	0.24	0/339	0.60	0/460
18	X	0.26	0/202	0.55	0/276
18	X1	0.24	0/202	0.52	0/276
18	x	0.28	0/202	0.62	0/276
18	x1	0.22	0/202	0.55	0/276
19	Z	0.23	0/469	0.45	0/641
19	Z1	0.22	0/469	0.59	1/641 (0.2%)
19	z	0.24	0/469	0.45	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	z1	0.19	0/469	0.49	0/641
20	N	0.28	0/1751	0.56	0/2386
20	N1	0.25	0/1751	0.54	0/2386
20	n	0.29	0/1750	0.55	0/2382
20	n1	0.39	2/1750 (0.1%)	0.71	5/2382 (0.2%)
21	G	0.26	0/1725	0.58	0/2348
21	G1	0.28	0/1725	0.61	2/2348 (0.1%)
21	g	0.27	0/1725	0.60	0/2348
21	g1	0.25	0/1725	0.58	0/2348
22	R	0.26	0/1506	0.56	0/2035
22	R1	0.21	0/1506	0.50	0/2035
22	r	0.24	0/1506	0.56	0/2035
22	r1	0.24	0/1506	0.59	0/2035
23	S	0.28	0/1903	0.60	0/2590
23	S1	0.25	0/1903	0.59	0/2590
23	s	0.28	0/1903	0.63	0/2590
23	s1	0.34	1/1903 (0.1%)	0.71	3/2590 (0.1%)
24	Y	0.30	0/1715	0.51	0/2338
24	Y1	0.26	0/1715	0.58	0/2338
24	y	0.29	0/1715	0.53	1/2338 (0.0%)
24	y1	0.23	0/1715	0.53	0/2338
25	U	0.32	0/224	0.63	0/298
25	U1	0.33	0/224	0.62	0/298
25	u	0.33	0/224	0.67	0/298
25	u1	0.30	0/224	0.67	0/298
All	All	0.29	9/117985 (0.0%)	0.59	47/160485 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	A1	0	1
2	B1	0	1
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o1	111	PRO	CG-CD	-13.88	1.03	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	65	PRO	CG-CD	-12.67	1.07	1.50
6	e	28	PRO	CG-CD	-10.34	1.15	1.50
4	c1	352	PRO	CG-CD	-8.86	1.20	1.50
20	n1	57	PRO	CG-CD	-8.42	1.22	1.50

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	65	PRO	N-CD-CG	-18.59	75.32	103.20
14	o1	111	PRO	N-CD-CG	-18.29	75.77	103.20
23	s1	155	PRO	N-CD-CG	-12.66	88.60	103.80
6	e	28	PRO	N-CD-CG	-12.50	84.44	103.20
20	n1	57	PRO	N-CD-CG	-12.30	84.74	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ARG	Sidechain
1	A1	131	TRP	Peptide
2	B1	384	ARG	Sidechain

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	2638	0	2541	95	0
1	A1	2638	0	2541	120	0
1	a	2638	0	2541	73	0
1	a1	2638	0	2541	128	0
2	B	3783	0	3663	99	0
2	B1	3783	0	3663	150	0
2	b	3783	0	3663	114	0
2	b1	3783	0	3663	137	0
3	V	227	0	261	4	0
3	V1	227	0	261	12	0
3	v	227	0	261	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	v1	227	0	261	10	0
4	C	3483	0	3376	76	0
4	C1	3483	0	3376	151	0
4	c	3483	0	3376	68	0
4	c1	3483	0	3376	154	0
5	D	2766	0	2654	61	0
5	D1	2766	0	2654	123	0
5	d	2766	0	2655	80	0
5	d1	2766	0	2655	149	0
6	E	621	0	605	25	0
6	E1	621	0	605	20	0
6	e	621	0	605	17	0
6	e1	621	0	605	23	0
7	F	252	0	265	9	0
7	F1	252	0	265	11	0
7	f	252	0	265	16	0
7	f1	252	0	265	13	0
8	H	503	0	532	18	0
8	H1	503	0	532	25	0
8	h	503	0	532	13	0
8	h1	503	0	532	23	0
9	I	279	0	288	7	0
9	I1	279	0	288	18	0
9	i	279	0	288	3	0
9	i1	279	0	288	12	0
10	J	266	0	286	6	0
10	J1	266	0	286	8	0
10	j	266	0	286	3	0
10	j1	266	0	286	15	0
11	K	297	0	312	7	0
11	K1	297	0	312	14	0
11	k	297	0	312	5	0
11	k1	297	0	312	16	0
12	L	313	0	325	8	0
12	L1	313	0	325	12	0
12	l	313	0	325	10	0
13	M	234	0	258	6	0
13	M1	234	0	258	9	0
13	m	234	0	258	8	0
13	m1	234	0	258	7	0
14	O	1820	0	1776	42	0
14	O1	1820	0	1776	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	o	1820	0	1776	34	0
14	o1	1820	0	1776	50	0
15	P	1444	0	1403	32	0
15	P1	1444	0	1403	33	0
15	p	1444	0	1403	40	0
15	p1	1444	0	1403	40	0
16	T	247	0	260	2	0
16	T1	247	0	260	15	0
16	t	247	0	260	12	0
16	t1	247	0	260	7	0
17	W	332	0	323	7	0
17	W1	332	0	323	21	0
17	w	332	0	323	11	0
17	w1	332	0	323	18	0
18	X	201	0	224	2	0
18	X1	201	0	224	7	0
18	x	201	0	224	6	0
18	x1	201	0	224	5	0
19	Z	457	0	478	5	0
19	Z1	457	0	478	10	0
19	z	457	0	478	6	0
19	z1	457	0	478	11	0
20	N	1703	0	1641	46	0
20	N1	1703	0	1641	72	0
20	n	1703	0	1641	43	0
20	n1	1703	0	1641	69	0
21	G	1680	0	1614	45	0
21	G1	1680	0	1613	52	0
21	g	1680	0	1614	53	0
21	g1	1680	0	1614	43	0
22	R	1490	0	1454	32	0
22	R1	1490	0	1454	31	0
22	r	1490	0	1454	31	0
22	r1	1490	0	1454	54	0
23	S	1856	0	1816	31	0
23	S1	1856	0	1816	61	0
23	s	1856	0	1816	45	0
23	s1	1856	0	1816	65	0
24	Y	1667	0	1624	44	0
24	Y1	1667	0	1624	62	0
24	y	1667	0	1624	45	0
24	y1	1667	0	1624	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	U	224	0	226	11	0
25	U1	224	0	226	11	0
25	u	224	0	226	7	0
25	u1	224	0	226	13	0
26	A	10	0	0	1	0
26	A1	10	0	0	0	0
26	a	10	0	0	0	0
26	a1	10	0	0	1	0
27	A	1	0	0	0	0
27	A1	1	0	0	0	0
27	a	1	0	0	0	0
27	a1	1	0	0	0	0
28	A	2	0	0	1	0
28	A1	2	0	0	1	0
28	a	2	0	0	1	0
28	a1	2	0	0	1	0
29	A	240	0	242	17	0
29	A1	240	0	240	18	0
29	B	1040	0	1149	71	0
29	B1	1040	0	1147	93	0
29	C	845	0	933	55	0
29	C1	845	0	930	67	0
29	D	130	0	144	10	0
29	D1	130	0	143	10	0
29	G	466	0	467	24	0
29	G1	466	0	467	35	0
29	N	468	0	469	27	0
29	N1	468	0	468	43	0
29	R	409	0	391	19	0
29	R1	409	0	391	26	0
29	S	625	0	588	21	0
29	S1	625	0	586	25	0
29	Y	570	0	613	51	0
29	Y1	570	0	612	48	0
29	a	239	0	242	14	0
29	a1	239	0	241	29	0
29	b	1040	0	1151	62	0
29	b1	1040	0	1146	80	0
29	c	845	0	934	43	0
29	c1	845	0	931	69	0
29	d	130	0	143	8	0
29	d1	130	0	143	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	g	466	0	468	20	0
29	g1	466	0	465	36	0
29	n	468	0	468	21	0
29	n1	468	0	469	38	0
29	r	409	0	392	18	0
29	r1	409	0	390	23	0
29	s	625	0	588	22	0
29	s1	625	0	586	34	0
29	y	570	0	614	38	0
29	y1	570	0	612	51	0
30	A	128	0	148	11	0
30	A1	128	0	148	13	0
30	a	128	0	148	7	0
30	a1	128	0	148	20	0
31	A	40	0	53	2	0
31	A1	40	0	53	4	0
31	B	80	0	106	3	0
31	B1	80	0	105	2	0
31	C	160	0	210	16	0
31	C1	160	0	209	22	0
31	D	40	0	53	3	0
31	D1	40	0	53	4	0
31	a	40	0	53	3	0
31	a1	40	0	53	4	0
31	b	80	0	106	6	0
31	b1	80	0	106	6	0
31	c	160	0	211	12	0
31	c1	160	0	211	30	0
31	d	40	0	53	3	0
31	d1	40	0	53	3	0
32	A	51	0	68	5	0
32	A1	51	0	68	6	0
32	B	96	0	124	6	0
32	B1	96	0	124	6	0
32	C	54	0	77	4	0
32	C1	54	0	77	3	0
32	M	42	0	47	4	0
32	M1	42	0	47	4	0
32	a	51	0	68	2	0
32	a1	51	0	68	3	0
32	b	96	0	124	7	0
32	b1	96	0	124	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	c	54	0	77	0	0
32	c1	54	0	77	4	0
32	m	42	0	47	6	0
32	m1	42	0	47	3	0
33	A	48	0	66	3	0
33	A1	48	0	66	10	0
33	B	44	0	58	2	0
33	B1	44	0	58	5	0
33	C	106	0	158	7	0
33	C1	106	0	158	13	0
33	D	46	0	62	2	0
33	D1	46	0	62	2	0
33	H	48	0	66	2	0
33	H1	48	0	66	15	0
33	W	39	0	48	2	0
33	W1	39	0	48	8	0
33	a	48	0	66	5	0
33	a1	48	0	66	8	0
33	b	44	0	58	5	0
33	b1	44	0	58	5	0
33	c	106	0	158	12	0
33	c1	106	0	158	7	0
33	d	46	0	62	2	0
33	d1	46	0	62	2	0
33	h	48	0	66	5	0
33	h1	48	0	66	4	0
33	w	39	0	48	6	0
33	w1	39	0	48	4	0
34	A	21	0	37	1	0
34	A1	21	0	37	4	0
34	Y	21	0	37	4	0
34	Y1	21	0	37	7	0
34	a	21	0	37	3	0
34	a1	21	0	37	1	0
34	y	21	0	37	4	0
34	y1	21	0	37	2	0
35	A	1	0	0	0	0
35	A1	1	0	0	0	0
35	a	1	0	0	0	0
35	a1	1	0	0	0	0
36	B	42	0	0	0	0
36	B1	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	b	42	0	0	0	0
36	b1	42	0	0	0	0
37	B	43	0	44	3	0
37	B1	43	0	44	2	0
37	C	176	0	226	13	0
37	C1	176	0	226	31	0
37	b	43	0	44	3	0
37	b1	43	0	44	4	0
37	c	176	0	226	10	0
37	c1	176	0	226	26	0
38	B	48	0	75	7	0
38	B1	48	0	75	6	0
38	S	48	0	75	7	0
38	S1	48	0	75	4	0
38	T	48	0	75	2	0
38	T1	48	0	75	8	0
38	b	48	0	75	6	0
38	b1	48	0	75	8	0
38	s	48	0	75	6	0
38	s1	48	0	75	5	0
38	t	48	0	75	2	0
38	t1	48	0	75	5	0
39	B	44	0	76	1	0
39	B1	44	0	76	1	0
39	C	44	0	76	3	0
39	C1	44	0	76	6	0
39	J	29	0	40	2	0
39	J1	29	0	40	4	0
39	b	44	0	76	5	0
39	b1	44	0	76	4	0
39	c	44	0	76	9	0
39	c1	44	0	76	4	0
39	j	29	0	40	3	0
39	j1	29	0	40	4	0
40	C	47	0	67	7	0
40	C1	47	0	67	8	0
40	D	132	0	183	11	0
40	D1	132	0	183	12	0
40	G	49	0	74	4	0
40	G1	49	0	74	6	0
40	L	49	0	74	5	0
40	L1	49	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	N	49	0	74	4	0
40	N1	49	0	74	5	0
40	S	45	0	63	5	0
40	S1	45	0	63	5	0
40	Y	49	0	74	6	0
40	Y1	49	0	74	6	0
40	c	47	0	67	4	0
40	c1	47	0	67	11	0
40	d	132	0	183	12	0
40	d1	132	0	183	17	0
40	g	49	0	74	7	0
40	g1	49	0	74	7	0
40	l	49	0	74	4	0
40	n	49	0	74	3	0
40	n1	49	0	74	10	0
40	s	45	0	63	4	0
40	s1	45	0	63	7	0
40	y	49	0	74	5	0
40	y1	49	0	74	6	0
41	C	40	0	0	0	0
41	C1	40	0	0	0	0
41	c	40	0	0	0	0
41	c1	40	0	0	0	0
42	D	4	0	0	0	0
42	D1	4	0	0	1	0
42	d	4	0	0	0	0
42	d1	4	0	1	0	0
43	D	55	0	80	4	0
43	D1	55	0	80	11	0
43	d	55	0	80	7	0
43	d1	55	0	80	8	0
44	F	43	0	30	3	0
44	F1	43	0	30	3	0
44	f	43	0	30	1	0
44	f1	43	0	30	3	0
45	H	41	0	56	1	0
45	H1	41	0	56	3	0
45	h	41	0	56	3	0
45	h1	41	0	56	4	0
46	I	6	0	8	0	0
46	I1	6	0	8	0	0
47	I	57	0	98	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	I1	57	0	98	9	0
47	K	57	0	98	2	0
47	K1	57	0	98	5	0
47	i	57	0	98	6	0
47	i1	57	0	98	2	0
47	k	57	0	98	2	0
47	k1	57	0	98	2	0
48	G	340	0	306	18	0
48	G1	340	0	306	19	0
48	N	380	0	383	18	0
48	N1	380	0	383	37	0
48	R	94	0	67	4	0
48	R1	94	0	67	3	0
48	S	194	0	144	9	0
48	S1	194	0	144	12	0
48	Y	310	0	307	7	0
48	Y1	310	0	308	21	0
48	g	340	0	306	15	0
48	g1	340	0	306	19	0
48	n	380	0	385	18	0
48	n1	380	0	383	29	0
48	r	94	0	66	3	0
48	r1	94	0	67	6	0
48	s	194	0	146	9	0
48	s1	194	0	146	14	0
48	y	310	0	308	7	0
48	y1	310	0	308	15	0
49	G	84	0	110	13	0
49	G1	84	0	110	16	0
49	N	84	0	110	8	0
49	N1	84	0	110	12	0
49	R	42	0	55	6	0
49	R1	42	0	55	4	0
49	S	84	0	110	7	0
49	S1	84	0	110	13	0
49	Y	84	0	110	8	0
49	Y1	84	0	110	14	0
49	g	84	0	110	13	0
49	g1	84	0	110	22	0
49	n	84	0	110	5	0
49	n1	84	0	110	14	0
49	r	42	0	55	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	r1	42	0	55	7	0
49	s	84	0	110	4	0
49	s1	84	0	110	10	0
49	y	84	0	110	5	0
49	y1	84	0	110	13	0
50	G	44	0	56	6	0
50	G1	44	0	56	10	0
50	N	44	0	56	5	0
50	N1	44	0	56	9	0
50	R	44	0	56	4	0
50	R1	44	0	56	5	0
50	Y	44	0	56	6	0
50	Y1	44	0	56	4	0
50	g	44	0	56	9	0
50	g1	44	0	56	6	0
50	n	44	0	56	6	0
50	n1	44	0	56	5	0
50	r	44	0	56	2	0
50	r1	44	0	56	5	0
50	y	44	0	56	4	0
50	y1	44	0	56	9	0
51	G	44	0	54	0	0
51	G1	44	0	54	0	0
51	N	44	0	54	3	0
51	N1	44	0	55	6	0
51	R	44	0	54	2	0
51	R1	44	0	54	4	0
51	S	44	0	54	0	0
51	S1	44	0	55	4	0
51	Y	44	0	54	2	0
51	Y1	44	0	54	3	0
51	g	44	0	54	1	0
51	g1	44	0	54	0	0
51	n	44	0	54	3	0
51	n1	44	0	54	6	0
51	r	44	0	54	3	0
51	r1	44	0	54	5	0
51	s	44	0	54	3	0
51	s1	44	0	56	6	0
51	y	44	0	54	1	0
51	y1	44	0	55	2	0
52	R	35	0	44	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	R1	35	0	45	7	0
52	r	35	0	44	4	0
52	r1	35	0	45	2	0
53	R	29	0	38	7	0
53	R1	29	0	38	9	0
53	r	29	0	38	7	0
53	r1	29	0	38	5	0
54	S	30	0	43	4	0
54	S1	30	0	43	2	0
54	s	30	0	43	3	0
54	s1	30	0	43	3	0
55	Y	69	0	90	5	0
55	Y1	69	0	90	3	0
55	y	69	0	90	9	0
55	y1	69	0	90	9	0
All	All	152240	0	154365	4580	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 4580 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)
53:r:626:ERG:O1	53:r:626:ERG:C3	1.70	1.38
53:r1:626:ERG:O1	53:r1:626:ERG:C3	1.70	1.37
53:R:626:ERG:O1	53:R:626:ERG:C3	1.70	1.36
53:R1:626:ERG:O1	53:R1:626:ERG:C3	1.70	1.35
24:y1:76:LEU:CD1	29:y1:602:CLA:H42	1.79	1.10

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	335/336 (100%)	321 (96%)	14 (4%)	0	100	100
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a	335/336 (100%)	318 (95%)	17 (5%)	0	100	100
1	a1	335/336 (100%)	314 (94%)	21 (6%)	0	100	100
2	B	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	B1	482/484 (100%)	447 (93%)	35 (7%)	0	100	100
2	b	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	b1	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	V1	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	30 (100%)	0	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	430 (96%)	17 (4%)	0	100	100
4	C1	447/449 (100%)	421 (94%)	26 (6%)	0	100	100
4	c	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
4	c1	447/449 (100%)	421 (94%)	25 (6%)	1 (0%)	43	72
5	D	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
5	D1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
5	d	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
5	d1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
6	E	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	E1	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	e	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	H1	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	29 (88%)	4 (12%)	0	100	100
9	i1	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
10	j1	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	K1	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k1	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	36 (100%)	0	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	29 (100%)	0	0	100	100
13	M1	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	215 (91%)	19 (8%)	2 (1%)	16	49
14	O1	236/238 (99%)	212 (90%)	23 (10%)	1 (0%)	30	61
14	o	236/238 (99%)	218 (92%)	17 (7%)	1 (0%)	30	61
14	o1	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	30	61
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	170 (92%)	15 (8%)	0	100	100
15	p1	185/187 (99%)	169 (91%)	16 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	2	22
16	T1	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	2	22
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	t1	28/30 (93%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	W	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
17	W1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	Z1	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
19	z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
20	N	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	14	46
20	N1	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	14	46
20	n	218/222 (98%)	199 (91%)	17 (8%)	2 (1%)	14	46
20	n1	218/222 (98%)	202 (93%)	14 (6%)	2 (1%)	14	46
21	G	219/221 (99%)	196 (90%)	23 (10%)	0	100	100
21	G1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
21	g	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
21	g1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
22	R	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	R1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
22	r	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	r1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
23	S	241/243 (99%)	219 (91%)	21 (9%)	1 (0%)	30	61
23	S1	241/243 (99%)	208 (86%)	32 (13%)	1 (0%)	30	61
23	s	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	16	49
23	s1	241/243 (99%)	214 (89%)	26 (11%)	1 (0%)	30	61
24	Y	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	57
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	57
24	y	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	y1	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	57
25	U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
25	U1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u1	25/27 (93%)	25 (100%)	0	0	100	100
All	All	14636/14846 (99%)	13696 (94%)	915 (6%)	25 (0%)	44	72

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
20	n	192	LEU
23	s	284	ASP

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	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	276 (100%)	0	100	100
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	388 (100%)	0	100	100
2	B1	388/388 (100%)	388 (100%)	0	100	100
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	387 (100%)	1 (0%)	86	83
3	V	25/25 (100%)	25 (100%)	0	100	100
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	v1	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	C1	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
5	d1	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	K1	33/33 (100%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k	33/33 (100%)	33 (100%)	0	100	100
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	M1	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
13	m1	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	194 (100%)	1 (0%)	81	80
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	194 (100%)	1 (0%)	81	80
15	P	151/151 (100%)	151 (100%)	0	100	100
15	P1	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
15	p1	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z	50/50 (100%)	50 (100%)	0	100	100
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	78	79
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	R1	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
22	r1	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
23	s1	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
25	u1	26/26 (100%)	26 (100%)	0	100	100
All	All	11841/11837 (100%)	11837 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	n	46	ASN
14	O1	138	TYR

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Mol	Chain	Res	Type
2	b1	425	GLN
14	o1	138	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
8	h1	79	ASN
18	x1	71	ASN
17	w	100	GLN
15	p	140	GLN
20	n1	245	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
22	SEP	r1	84	22	8,9,10	1.59	1 (12%)	7,12,14	1.30	1 (14%)
22	SEP	R1	84	22	8,9,10	1.58	1 (12%)	7,12,14	1.44	1 (14%)
22	SEP	R	84	22	8,9,10	1.64	1 (12%)	7,12,14	1.30	1 (14%)
22	SEP	r	84	22	8,9,10	1.57	1 (12%)	7,12,14	1.14	1 (14%)

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
22	SEP	r1	84	22	-	6/6/8/10	-
22	SEP	R1	84	22	-	5/6/8/10	-
22	SEP	R	84	22	-	3/6/8/10	-
22	SEP	r	84	22	-	2/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.52	1.61	1.50
22	r1	84	SEP	P-O1P	3.44	1.61	1.50
22	R1	84	SEP	P-O1P	3.44	1.61	1.50
22	r	84	SEP	P-O1P	3.36	1.60	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R1	84	SEP	OG-CB-CA	3.23	111.29	108.14
22	r1	84	SEP	OG-CB-CA	2.79	110.86	108.14
22	R	84	SEP	OG-CB-CA	2.49	110.57	108.14
22	r	84	SEP	OG-CB-CA	2.30	110.39	108.14

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R	84	SEP	C-CA-CB-OG
22	R1	84	SEP	N-CA-CB-OG
22	R1	84	SEP	C-CA-CB-OG
22	R1	84	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	84	SEP	1	0
22	r	84	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 721 ligands modelled in this entry, 16 are monoatomic - leaving 705 for Mogul analysis.

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
29	CLA	B1	608	-	69,73,73	1.38	6 (8%)	82,113,113	1.87	19 (23%)
48	CHL	y1	601	24	60,74,74	1.25	8 (13%)	58,114,114	1.71	12 (20%)
29	CLA	S	611	40	69,73,73	1.36	6 (8%)	82,113,113	1.88	17 (20%)
49	LUT	g	620	-	42,43,43	2.41	1 (2%)	51,60,60	2.10	15 (29%)
47	4RF	i1	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.94	3 (5%)
29	CLA	D	403	-	69,73,73	1.35	6 (8%)	82,113,113	1.96	20 (24%)
29	CLA	A1	407	-	54,58,73	1.57	7 (12%)	64,95,113	2.05	18 (28%)
33	LMG	w	201	-	39,39,55	0.97	2 (5%)	47,47,63	1.30	5 (10%)
48	CHL	g1	608	-	38,52,74	1.69	9 (23%)	31,87,114	2.29	11 (35%)
33	LMG	B	622	-	44,44,55	0.96	3 (6%)	52,52,63	1.25	2 (3%)
39	DGA	c1	524	-	43,43,43	1.17	3 (6%)	45,45,45	1.51	4 (8%)
48	CHL	G1	608	-	38,52,74	1.84	10 (26%)	31,87,114	2.40	12 (38%)
29	CLA	c1	502	-	69,73,73	1.41	6 (8%)	82,113,113	1.78	16 (19%)
29	CLA	B	608	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	17 (20%)
48	CHL	S	608	-	55,69,74	1.46	8 (14%)	52,108,114	1.82	13 (25%)
42	BCT	d	401	-	3,3,3	3.21	1 (33%)	2,3,3	2.89	2 (100%)
29	CLA	n1	613	-	69,73,73	1.36	7 (10%)	82,113,113	2.04	19 (23%)
29	CLA	s1	602	-	64,68,73	1.41	7 (10%)	76,107,113	2.15	20 (26%)
37	DGD	B1	623	-	44,44,67	0.87	1 (2%)	58,58,81	1.22	6 (10%)
29	CLA	R1	602	-	64,68,73	1.45	8 (12%)	76,107,113	1.94	18 (23%)
29	CLA	S1	613	-	59,63,73	1.43	6 (10%)	70,101,113	2.05	17 (24%)
29	CLA	b	609	-	69,73,73	1.42	8 (11%)	82,113,113	1.90	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	s1	614	-	59,63,73	1.48	8 (13%)	70,101,113	2.06	19 (27%)
48	CHL	s1	607	-	37,51,74	1.63	8 (21%)	30,86,114	2.53	10 (33%)
36	C7Z	b1	620	-	43,43,43	5.49	26 (60%)	56,60,60	2.31	18 (32%)
29	CLA	c	510	-	69,73,73	1.37	6 (8%)	82,113,113	1.96	19 (23%)
40	LHG	C1	525	-	46,46,48	0.39	0	49,52,54	1.05	3 (6%)
49	LUT	s1	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.34	14 (27%)
40	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.05	2 (4%)
38	3PH	b	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.19	3 (6%)
50	XAT	N	622	-	41,47,47	0.66	1 (2%)	54,74,74	2.14	12 (22%)
29	CLA	R	604	-	53,57,73	1.55	7 (13%)	61,93,113	2.20	15 (24%)
31	BCR	A1	411	-	41,41,41	1.65	5 (12%)	56,56,56	4.34	15 (26%)
50	XAT	G	622	-	41,47,47	0.70	1 (2%)	54,74,74	2.08	17 (31%)
49	LUT	g1	620	-	42,43,43	2.43	1 (2%)	51,60,60	1.90	13 (25%)
29	CLA	b	603	-	69,73,73	1.39	7 (10%)	82,113,113	1.92	18 (21%)
48	CHL	r	606	-	38,52,74	1.66	9 (23%)	31,87,114	2.36	10 (32%)
52	LMT	R1	625	-	36,36,36	1.24	6 (16%)	47,47,47	1.17	4 (8%)
29	CLA	n	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
29	CLA	r	612	-	64,68,73	1.43	6 (9%)	76,107,113	1.92	17 (22%)
49	LUT	R1	620	-	42,43,43	2.45	1 (2%)	51,60,60	2.00	12 (23%)
33	LMG	A	413	-	48,48,55	1.14	6 (12%)	56,56,63	1.21	5 (8%)
29	CLA	g	610	-	69,73,73	1.35	7 (10%)	82,113,113	2.00	20 (24%)
33	LMG	c1	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.12	4 (6%)
29	CLA	B	614	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	18 (21%)
31	BCR	C	517	-	41,41,41	1.61	5 (12%)	56,56,56	4.49	18 (32%)
39	DGA	J1	101	-	28,28,43	1.29	3 (10%)	30,30,45	1.35	2 (6%)
29	CLA	C1	509	-	69,73,73	1.36	7 (10%)	82,113,113	1.96	16 (19%)
29	CLA	S1	617	23	54,58,73	1.54	8 (14%)	64,95,113	2.15	19 (29%)
45	RRX	H	101	-	42,42,42	4.97	24 (57%)	56,58,58	2.94	22 (39%)
29	CLA	N	612	-	49,53,73	1.64	8 (16%)	58,89,113	2.01	12 (20%)
33	LMG	b	622	-	44,44,55	0.98	3 (6%)	52,52,63	1.16	2 (3%)
29	CLA	y1	614	-	69,73,73	1.38	8 (11%)	82,113,113	1.83	20 (24%)
40	LHG	g1	624	-	48,48,48	0.41	0	51,54,54	1.12	4 (7%)
50	XAT	g1	622	-	41,47,47	0.77	1 (2%)	54,74,74	1.91	17 (31%)
29	CLA	Y	608	-	54,58,73	1.55	7 (12%)	64,95,113	2.13	19 (29%)
31	BCR	a1	411	-	41,41,41	1.66	5 (12%)	56,56,56	4.23	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	D	404	-	41,41,41	1.61	4 (9%)	56,56,56	4.36	14 (25%)
29	CLA	g	604	-	53,57,73	1.56	7 (13%)	61,93,113	2.12	18 (29%)
51	NEX	S1	623	-	40,46,46	2.61	10 (25%)	50,70,70	1.76	10 (20%)
29	CLA	G1	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	16 (19%)
49	LUT	s	620	-	42,43,43	2.45	1 (2%)	51,60,60	1.81	15 (29%)
29	CLA	S1	602	23	64,68,73	1.40	8 (12%)	76,107,113	2.01	19 (25%)
31	BCR	C	515	-	41,41,41	1.65	6 (14%)	56,56,56	4.36	17 (30%)
29	CLA	s1	609	-	64,68,73	1.39	7 (10%)	76,107,113	2.05	18 (23%)
29	CLA	C	508	-	69,73,73	1.44	6 (8%)	82,113,113	1.89	19 (23%)
29	CLA	G	612	-	47,51,73	1.65	5 (10%)	55,86,113	2.09	16 (29%)
41	LMK	C1	527	-	39,39,53	1.52	2 (5%)	39,46,60	1.50	2 (5%)
51	NEX	Y1	623	-	40,46,46	2.56	12 (30%)	50,70,70	1.95	15 (30%)
29	CLA	a1	410	-	64,68,73	1.45	8 (12%)	76,107,113	2.04	20 (26%)
29	CLA	C1	505	-	69,73,73	1.37	7 (10%)	82,113,113	1.87	17 (20%)
29	CLA	R	602	-	64,68,73	1.45	8 (12%)	76,107,113	1.90	20 (26%)
29	CLA	c	507	-	69,73,73	1.40	7 (10%)	82,113,113	1.94	17 (20%)
54	LPX	S	625	-	29,29,29	1.04	2 (6%)	31,33,33	0.95	1 (3%)
33	LMG	C1	523	-	55,55,55	1.26	6 (10%)	63,63,63	1.16	6 (9%)
48	CHL	n1	608	-	44,58,74	1.38	7 (15%)	37,94,114	2.13	13 (35%)
29	CLA	b1	609	-	69,73,73	1.36	7 (10%)	82,113,113	1.97	16 (19%)
29	CLA	s	605	-	54,58,73	1.55	7 (12%)	64,95,113	2.16	18 (28%)
29	CLA	r1	609	-	64,68,73	1.40	7 (10%)	76,107,113	1.96	21 (27%)
29	CLA	N	614	-	53,57,73	1.56	6 (11%)	61,93,113	2.25	18 (29%)
48	CHL	N	607	-	60,74,74	1.29	8 (13%)	58,114,114	1.74	15 (25%)
48	CHL	s	608	-	55,69,74	1.54	10 (18%)	52,108,114	1.81	12 (23%)
49	LUT	g1	621	-	42,43,43	2.45	1 (2%)	51,60,60	2.23	13 (25%)
29	CLA	S	613	-	59,63,73	1.49	7 (11%)	70,101,113	2.03	14 (20%)
48	CHL	G	601	21	60,74,74	1.38	8 (13%)	58,114,114	1.69	11 (18%)
29	CLA	d1	403	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	19 (23%)
37	DGD	C	519	-	63,63,67	1.24	7 (11%)	77,77,81	1.02	2 (2%)
29	CLA	R1	610	-	64,68,73	1.44	8 (12%)	76,107,113	2.15	19 (25%)
29	CLA	A	407	-	54,58,73	1.55	8 (14%)	64,95,113	2.13	17 (26%)
47	4RF	I1	102	-	56,56,56	1.07	5 (8%)	59,59,59	1.00	4 (6%)
48	CHL	Y1	609	-	60,74,74	1.24	8 (13%)	58,114,114	1.74	13 (22%)
48	CHL	y1	605	24	40,54,74	1.73	10 (25%)	34,90,114	2.11	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	a1	405	-	69,73,73	1.35	6 (8%)	82,113,113	1.96	17 (20%)
51	NEX	G1	623	-	40,46,46	2.70	11 (27%)	50,70,70	2.04	12 (24%)
49	LUT	Y	621	-	42,43,43	2.41	1 (2%)	51,60,60	1.85	15 (29%)
29	CLA	B	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.87	18 (21%)
32	SQD	C	526	-	52,54,54	0.80	1 (1%)	62,65,65	0.87	2 (3%)
34	SPH	A	414	-	19,20,20	0.68	1 (5%)	18,21,21	1.13	2 (11%)
29	CLA	y	602	24	69,73,73	1.39	6 (8%)	82,113,113	1.82	17 (20%)
49	LUT	r	620	-	42,43,43	2.44	1 (2%)	51,60,60	2.01	13 (25%)
29	CLA	b1	608	-	69,73,73	1.40	7 (10%)	82,113,113	1.88	19 (23%)
48	CHL	y1	607	-	60,74,74	1.18	7 (11%)	58,114,114	1.62	10 (17%)
50	XAT	N1	622	-	41,47,47	0.71	1 (2%)	54,74,74	2.08	15 (27%)
29	CLA	s1	617	-	54,58,73	1.53	8 (14%)	64,95,113	2.08	19 (29%)
29	CLA	R	610	-	64,68,73	1.48	8 (12%)	76,107,113	2.10	21 (27%)
29	CLA	B1	610	-	69,73,73	1.37	6 (8%)	82,113,113	1.81	15 (18%)
37	DGD	C1	518	-	56,56,67	1.06	4 (7%)	70,70,81	1.07	5 (7%)
53	ERG	r1	626	-	32,32,32	7.94	20 (62%)	45,50,50	2.86	17 (37%)
48	CHL	g	605	21	42,56,74	1.42	8 (19%)	36,92,114	2.19	13 (36%)
32	SQD	b	626	-	52,54,54	0.81	0	62,65,65	0.85	1 (1%)
29	CLA	R	609	-	64,68,73	1.42	7 (10%)	76,107,113	4.16	19 (25%)
49	LUT	S1	621	-	42,43,43	2.49	2 (4%)	51,60,60	1.85	15 (29%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.50	5 (9%)
29	CLA	b	616	-	69,73,73	1.35	7 (10%)	82,113,113	1.80	19 (23%)
29	CLA	b1	617	-	69,73,73	1.38	5 (7%)	82,113,113	1.87	19 (23%)
29	CLA	g	614	-	53,57,73	1.57	8 (15%)	61,93,113	2.14	16 (26%)
48	CHL	g	607	-	60,74,74	1.31	10 (16%)	58,114,114	1.66	11 (18%)
37	DGD	B	623	-	44,44,67	0.90	1 (2%)	58,58,81	1.35	5 (8%)
32	SQD	b	621	-	40,42,54	0.85	0	50,53,65	0.94	2 (4%)
33	LMG	c	523	-	55,55,55	1.28	6 (10%)	63,63,63	1.13	3 (4%)
48	CHL	g	608	-	38,52,74	1.69	8 (21%)	31,87,114	2.26	11 (35%)
29	CLA	a	407	-	53,57,73	1.55	7 (13%)	61,93,113	2.39	17 (27%)
48	CHL	N	601	20	60,74,74	1.48	9 (15%)	58,114,114	1.81	11 (18%)
29	CLA	c1	501	-	69,73,73	1.39	7 (10%)	82,113,113	1.95	19 (23%)
48	CHL	N1	606	-	60,74,74	1.51	10 (16%)	58,114,114	1.80	11 (18%)
34	SPH	a	414	-	19,20,20	0.72	1 (5%)	18,21,21	1.12	1 (5%)
37	DGD	C1	519	-	63,63,67	1.22	7 (11%)	77,77,81	1.06	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	r	610	-	64,68,73	1.42	7 (10%)	76,107,113	2.07	21 (27%)
29	CLA	B1	605	-	69,73,73	1.35	7 (10%)	82,113,113	1.95	20 (24%)
48	CHL	Y	609	-	60,74,74	1.54	10 (16%)	58,114,114	1.60	11 (18%)
33	LMG	a1	413	-	48,48,55	1.11	5 (10%)	56,56,63	1.32	5 (8%)
48	CHL	Y	606	-	60,74,74	1.38	8 (13%)	58,114,114	1.68	12 (20%)
29	CLA	s1	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.97	20 (24%)
51	NEX	y1	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.95	18 (36%)
29	CLA	y	610	24	69,73,73	1.35	7 (10%)	82,113,113	1.93	19 (23%)
29	CLA	s	603	-	69,73,73	1.40	7 (10%)	82,113,113	1.95	19 (23%)
29	CLA	G	613	-	69,73,73	1.35	6 (8%)	82,113,113	1.96	22 (26%)
40	LHG	S	624	29	44,44,48	0.43	0	47,50,54	1.07	4 (8%)
29	CLA	d	403	-	69,73,73	1.38	7 (10%)	82,113,113	1.89	18 (21%)
40	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.49	4 (7%)
29	CLA	C	510	-	69,73,73	1.39	6 (8%)	82,113,113	1.86	18 (21%)
48	CHL	G	607	-	60,74,74	1.37	9 (15%)	58,114,114	1.67	11 (18%)
48	CHL	r1	607	-	44,58,74	1.52	8 (18%)	37,94,114	1.99	12 (32%)
29	CLA	G1	602	-	69,73,73	1.42	6 (8%)	82,113,113	1.99	20 (24%)
29	CLA	c	512	-	69,73,73	1.42	9 (13%)	82,113,113	1.86	20 (24%)
51	NEX	g	623	-	40,46,46	2.84	12 (30%)	50,70,70	1.89	15 (30%)
31	BCR	d1	404	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	23 (41%)
54	LPX	s	625	-	29,29,29	1.05	2 (6%)	31,33,33	0.95	1 (3%)
29	CLA	Y	611	-	69,73,73	1.34	8 (11%)	82,113,113	1.79	14 (17%)
55	PTY	Y	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.02	2 (3%)
39	DGA	B1	625	-	43,43,43	1.17	3 (6%)	45,45,45	1.46	3 (6%)
31	BCR	d	404	-	41,41,41	1.59	4 (9%)	56,56,56	4.43	16 (28%)
48	CHL	r	607	-	44,58,74	1.64	8 (18%)	37,94,114	2.06	11 (29%)
33	LMG	D1	411	-	46,46,55	1.03	4 (8%)	54,54,63	1.13	3 (5%)
51	NEX	S	623	-	40,46,46	2.79	11 (27%)	50,70,70	1.85	12 (24%)
49	LUT	N	620	-	42,43,43	2.43	1 (2%)	51,60,60	1.80	15 (29%)
52	LMT	r	625	-	36,36,36	1.19	5 (13%)	47,47,47	1.17	3 (6%)
52	LMT	r1	625	-	36,36,36	1.16	4 (11%)	47,47,47	1.09	3 (6%)
49	LUT	y1	621	-	42,43,43	2.47	1 (2%)	51,60,60	2.24	13 (25%)
29	CLA	c	508	-	69,73,73	1.39	7 (10%)	82,113,113	1.82	15 (18%)
29	CLA	S1	611	40	69,73,73	1.40	8 (11%)	82,113,113	1.90	16 (19%)
29	CLA	n1	612	-	49,53,73	1.64	8 (16%)	58,89,113	1.98	14 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	R	603	-	64,68,73	1.47	8 (12%)	76,107,113	1.91	18 (23%)
32	SQD	a1	412	-	49,51,54	0.81	1 (2%)	59,62,65	0.89	2 (3%)
39	DGA	j1	101	-	28,28,43	1.34	3 (10%)	30,30,45	1.27	2 (6%)
32	SQD	c1	526	-	52,54,54	0.79	0	62,65,65	0.86	3 (4%)
29	CLA	S	604	-	59,63,73	1.45	7 (11%)	70,101,113	2.07	21 (30%)
29	CLA	y1	612	-	69,73,73	1.35	7 (10%)	82,113,113	1.93	22 (26%)
29	CLA	C1	501	-	69,73,73	1.36	7 (10%)	82,113,113	2.03	21 (25%)
29	CLA	a1	407	-	53,57,73	1.57	6 (11%)	61,93,113	2.30	17 (27%)
29	CLA	B1	615	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	19 (23%)
48	CHL	n	609	-	60,74,74	1.20	7 (11%)	58,114,114	1.81	12 (20%)
29	CLA	b1	602	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	20 (24%)
26	OEX	A	401	1,4	0,15,15	-	-	-	-	-
29	CLA	c	501	-	69,73,73	1.35	7 (10%)	82,113,113	1.96	18 (21%)
38	3PH	T1	101	-	47,47,47	0.85	4 (8%)	50,52,52	1.11	2 (4%)
51	NEX	g1	623	-	40,46,46	2.65	11 (27%)	50,70,70	1.91	15 (30%)
29	CLA	C1	510	-	69,73,73	1.36	8 (11%)	82,113,113	1.85	17 (20%)
33	LMG	H1	102	-	48,48,55	1.15	5 (10%)	56,56,63	1.17	3 (5%)
29	CLA	A	406	-	69,73,73	1.36	7 (10%)	82,113,113	1.98	18 (21%)
29	CLA	b	605	-	69,73,73	1.39	7 (10%)	82,113,113	2.10	21 (25%)
29	CLA	b1	611	-	69,73,73	1.43	6 (8%)	82,113,113	1.93	18 (21%)
33	LMG	h	102	-	48,48,55	1.14	5 (10%)	56,56,63	1.23	4 (7%)
38	3PH	t1	101	-	47,47,47	0.88	3 (6%)	50,52,52	1.08	2 (4%)
40	LHG	s1	624	29	44,44,48	0.44	0	47,50,54	1.09	4 (8%)
29	CLA	G	614	-	53,57,73	1.57	7 (13%)	61,93,113	2.19	18 (29%)
38	3PH	s	626	-	47,47,47	0.88	3 (6%)	50,52,52	4.49	4 (8%)
29	CLA	c1	508	-	69,73,73	1.38	7 (10%)	82,113,113	1.84	18 (21%)
29	CLA	r	609	-	64,68,73	1.43	6 (9%)	76,107,113	1.92	17 (22%)
36	C7Z	b	620	-	43,43,43	5.41	26 (60%)	56,60,60	2.54	18 (32%)
45	RRX	H1	101	-	42,42,42	5.06	24 (57%)	56,58,58	2.41	19 (33%)
29	CLA	y	603	-	69,73,73	1.36	8 (11%)	82,113,113	2.04	19 (23%)
48	CHL	Y1	605	-	40,54,74	1.46	7 (17%)	34,90,114	2.24	10 (29%)
40	LHG	n1	624	-	48,48,48	0.42	0	51,54,54	1.09	3 (5%)
29	CLA	g	612	-	47,51,73	1.68	6 (12%)	55,86,113	2.09	14 (25%)
40	LHG	d1	410	-	38,38,48	0.45	0	41,44,54	1.06	2 (4%)
48	CHL	g	606	-	44,58,74	1.72	8 (18%)	37,94,114	2.02	12 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PTY	Y1	626	-	49,49,49	0.90	4 (8%)	52,54,54	1.05	2 (3%)
47	4RF	K1	101	-	56,56,56	1.08	3 (5%)	59,59,59	0.85	3 (5%)
29	CLA	n	610	-	69,73,73	1.40	8 (11%)	82,113,113	2.00	19 (23%)
29	CLA	B	607	-	69,73,73	1.38	8 (11%)	82,113,113	1.85	19 (23%)
29	CLA	N	611	-	53,57,73	1.56	6 (11%)	61,93,113	2.14	17 (27%)
29	CLA	s	609	-	64,68,73	1.43	7 (10%)	76,107,113	1.93	15 (19%)
29	CLA	c	503	-	69,73,73	1.38	7 (10%)	82,113,113	1.86	20 (24%)
37	DGD	c1	519	-	63,63,67	1.25	7 (11%)	77,77,81	1.05	3 (3%)
36	C7Z	B	620	-	43,43,43	5.36	26 (60%)	56,60,60	2.41	20 (35%)
29	CLA	r1	610	-	64,68,73	1.45	7 (10%)	76,107,113	1.88	15 (19%)
37	DGD	c	519	-	63,63,67	1.23	7 (11%)	77,77,81	1.03	2 (2%)
39	DGA	J	101	-	28,28,43	1.33	3 (10%)	30,30,45	1.29	2 (6%)
29	CLA	B1	603	-	69,73,73	1.40	8 (11%)	82,113,113	1.99	21 (25%)
29	CLA	c	509	-	69,73,73	1.37	7 (10%)	82,113,113	1.81	16 (19%)
29	CLA	y	613	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	14 (17%)
29	CLA	c1	510	-	69,73,73	1.40	6 (8%)	82,113,113	1.86	17 (20%)
48	CHL	N	608	-	44,58,74	1.71	8 (18%)	37,94,114	2.10	11 (29%)
48	CHL	G1	606	-	44,58,74	1.54	7 (15%)	37,94,114	2.06	13 (35%)
29	CLA	Y1	613	-	69,73,73	1.35	7 (10%)	82,113,113	2.01	18 (21%)
49	LUT	r1	620	-	42,43,43	2.46	2 (4%)	51,60,60	2.38	15 (29%)
29	CLA	Y	613	24	69,73,73	1.38	7 (10%)	82,113,113	2.06	22 (26%)
33	LMG	D	411	-	46,46,55	1.02	4 (8%)	54,54,63	1.01	2 (3%)
29	CLA	C	503	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	19 (23%)
29	CLA	y1	611	40	69,73,73	1.36	7 (10%)	82,113,113	1.95	17 (20%)
48	CHL	G1	605	21	42,56,74	1.42	8 (19%)	36,92,114	2.37	11 (30%)
47	4RF	I	102	-	56,56,56	1.06	4 (7%)	59,59,59	0.98	4 (6%)
51	NEX	r1	622	-	40,46,46	2.69	11 (27%)	50,70,70	2.30	12 (24%)
39	DGA	B	625	-	43,43,43	1.12	2 (4%)	45,45,45	1.52	3 (6%)
29	CLA	A	410	-	64,68,73	1.45	7 (10%)	76,107,113	2.02	20 (26%)
33	LMG	B1	622	-	44,44,55	0.98	3 (6%)	52,52,63	1.09	4 (7%)
29	CLA	B	611	-	69,73,73	1.39	7 (10%)	82,113,113	1.90	19 (23%)
31	BCR	C	516	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	14 (25%)
48	CHL	Y1	606	-	60,74,74	1.54	8 (13%)	58,114,114	1.75	12 (20%)
48	CHL	n	601	20	60,74,74	1.70	8 (13%)	58,114,114	1.80	11 (18%)
29	CLA	B1	607	-	69,73,73	1.36	7 (10%)	82,113,113	2.00	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	r1	608	-	64,68,73	1.43	6 (9%)	76,107,113	1.94	17 (22%)
29	CLA	s	613	-	59,63,73	1.44	6 (10%)	70,101,113	2.11	20 (28%)
29	CLA	N1	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.20	16 (26%)
32	SQD	B	626	-	52,54,54	0.78	0	62,65,65	0.85	2 (3%)
48	CHL	N1	607	-	60,74,74	1.32	7 (11%)	58,114,114	1.83	15 (25%)
29	CLA	A1	406	-	69,73,73	1.40	7 (10%)	82,113,113	1.94	18 (21%)
29	CLA	B	616	-	69,73,73	1.36	8 (11%)	82,113,113	1.88	21 (25%)
29	CLA	Y	614	-	69,73,73	1.36	7 (10%)	82,113,113	1.95	20 (24%)
29	CLA	S1	603	-	69,73,73	1.39	7 (10%)	82,113,113	1.92	18 (21%)
48	CHL	Y	607	-	60,74,74	1.00	6 (10%)	58,114,114	1.83	13 (22%)
48	CHL	R1	606	-	38,52,74	1.80	9 (23%)	31,87,114	2.49	10 (32%)
29	CLA	r	608	-	64,68,73	1.42	8 (12%)	76,107,113	1.86	18 (23%)
29	CLA	A	405	-	69,73,73	1.38	6 (8%)	82,113,113	1.92	16 (19%)
29	CLA	S	605	23	54,58,73	1.58	7 (12%)	64,95,113	2.27	18 (28%)
49	LUT	R	620	-	42,43,43	2.43	1 (2%)	51,60,60	2.18	17 (33%)
29	CLA	A1	405	-	69,73,73	1.35	7 (10%)	82,113,113	1.86	16 (19%)
40	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
29	CLA	Y1	608	-	54,58,73	1.58	7 (12%)	64,95,113	2.15	18 (28%)
48	CHL	s	606	-	38,52,74	1.80	7 (18%)	31,87,114	2.41	10 (32%)
49	LUT	s1	620	-	42,43,43	2.49	1 (2%)	51,60,60	1.92	17 (33%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.13	3 (6%)
48	CHL	g	601	21	60,74,74	1.51	8 (13%)	58,114,114	1.72	11 (18%)
29	CLA	g	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.98	20 (24%)
29	CLA	C	504	-	69,73,73	1.34	7 (10%)	82,113,113	1.83	16 (19%)
29	CLA	B1	617	-	69,73,73	1.39	7 (10%)	82,113,113	1.90	16 (19%)
49	LUT	s	621	-	42,43,43	2.39	2 (4%)	51,60,60	1.84	15 (29%)
29	CLA	g1	612	21	47,51,73	1.65	8 (17%)	55,86,113	2.18	15 (27%)
32	SQD	a	412	-	49,51,54	0.80	1 (2%)	59,62,65	0.85	2 (3%)
40	LHG	S1	624	29	44,44,48	0.45	0	47,50,54	1.14	4 (8%)
29	CLA	B1	604	-	69,73,73	1.39	6 (8%)	82,113,113	1.73	16 (19%)
40	LHG	y	624	29	48,48,48	0.40	0	51,54,54	1.08	5 (9%)
32	SQD	B1	626	-	52,54,54	0.78	0	62,65,65	0.85	2 (3%)
29	CLA	a1	406	-	69,73,73	1.39	7 (10%)	82,113,113	1.94	19 (23%)
40	LHG	Y1	624	-	48,48,48	0.40	0	51,54,54	1.13	4 (7%)
29	CLA	S	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.82	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B1	616	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	17 (20%)
48	CHL	R1	607	-	44,58,74	1.43	8 (18%)	37,94,114	2.41	10 (27%)
29	CLA	b1	606	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	17 (20%)
50	XAT	r	621	-	41,47,47	0.73	1 (2%)	54,74,74	2.00	13 (24%)
30	PHO	A	408	-	58,69,69	2.07	9 (15%)	55,99,99	1.54	6 (10%)
29	CLA	B	604	-	69,73,73	1.39	7 (10%)	82,113,113	1.84	16 (19%)
29	CLA	n1	602	20	69,73,73	1.33	8 (11%)	82,113,113	1.93	20 (24%)
29	CLA	r1	602	-	64,68,73	1.42	6 (9%)	76,107,113	1.99	20 (26%)
48	CHL	n	608	-	44,58,74	1.71	7 (15%)	37,94,114	1.99	13 (35%)
29	CLA	C	509	-	69,73,73	1.38	7 (10%)	82,113,113	1.95	17 (20%)
33	LMG	w1	201	-	39,39,55	0.94	2 (5%)	47,47,63	1.18	3 (6%)
29	CLA	C1	507	-	69,73,73	1.39	7 (10%)	82,113,113	1.84	18 (21%)
48	CHL	g1	601	-	60,74,74	1.34	9 (15%)	58,114,114	1.70	12 (20%)
29	CLA	c1	505	-	69,73,73	1.34	8 (11%)	82,113,113	1.99	19 (23%)
48	CHL	G1	601	21	60,74,74	1.38	9 (15%)	58,114,114	1.60	9 (15%)
48	CHL	N1	605	20	60,74,74	1.43	9 (15%)	58,114,114	1.60	9 (15%)
29	CLA	G1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	19 (23%)
29	CLA	b1	615	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	15 (18%)
29	CLA	r1	603	-	64,68,73	1.40	6 (9%)	76,107,113	1.98	19 (25%)
43	PL9	d1	405	-	55,55,55	1.10	3 (5%)	68,69,69	1.54	14 (20%)
48	CHL	G	609	21	60,74,74	1.46	10 (16%)	58,114,114	1.71	14 (24%)
29	CLA	b	606	-	69,73,73	1.37	7 (10%)	82,113,113	1.96	17 (20%)
51	NEX	R1	622	-	40,46,46	2.64	10 (25%)	50,70,70	2.31	15 (30%)
48	CHL	Y	605	24	40,54,74	1.80	9 (22%)	34,90,114	2.04	9 (26%)
37	DGD	c	518	-	56,56,67	1.05	4 (7%)	70,70,81	1.14	4 (5%)
31	BCR	B1	618	-	41,41,41	1.60	4 (9%)	56,56,56	4.57	19 (33%)
29	CLA	B	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	19 (23%)
29	CLA	n	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.25	22 (36%)
29	CLA	B1	613	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	17 (20%)
29	CLA	y1	613	-	69,73,73	1.34	6 (8%)	82,113,113	1.97	19 (23%)
48	CHL	n	607	-	60,74,74	1.31	7 (11%)	58,114,114	1.66	11 (18%)
48	CHL	g1	607	-	60,74,74	1.26	8 (13%)	58,114,114	1.78	12 (20%)
29	CLA	R1	612	-	64,68,73	1.43	6 (9%)	76,107,113	1.97	19 (25%)
31	BCR	c	514	-	41,41,41	1.63	5 (12%)	56,56,56	4.42	12 (21%)
33	LMG	W1	201	-	39,39,55	0.96	2 (5%)	47,47,63	1.38	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	BCT	D	401	27	3,3,3	3.23	1 (33%)	2,3,3	2.80	2 (100%)
29	CLA	b1	613	-	69,73,73	1.37	7 (10%)	82,113,113	1.96	16 (19%)
48	CHL	Y1	601	-	60,74,74	1.79	9 (15%)	58,114,114	1.48	11 (18%)
29	CLA	Y1	603	-	69,73,73	1.38	8 (11%)	82,113,113	1.87	18 (21%)
29	CLA	C	513	-	69,73,73	1.38	7 (10%)	82,113,113	1.90	18 (21%)
37	DGD	C	518	-	56,56,67	1.05	4 (7%)	70,70,81	0.96	2 (2%)
48	CHL	G	606	-	44,58,74	1.73	9 (20%)	37,94,114	2.15	11 (29%)
51	NEX	n	623	-	40,46,46	2.79	12 (30%)	50,70,70	1.59	10 (20%)
29	CLA	G	611	40	69,73,73	1.36	6 (8%)	82,113,113	1.91	18 (21%)
38	3PH	B	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.14	2 (4%)
53	ERG	R	626	-	32,32,32	7.96	19 (59%)	45,50,50	3.35	19 (42%)
31	BCR	c1	516	-	41,41,41	1.64	4 (9%)	56,56,56	4.59	13 (23%)
31	BCR	b	618	-	41,41,41	1.65	5 (12%)	56,56,56	4.63	19 (33%)
31	BCR	c	516	-	41,41,41	1.64	4 (9%)	56,56,56	4.40	11 (19%)
45	RRX	h1	101	-	42,42,42	4.96	24 (57%)	56,58,58	2.74	23 (41%)
31	BCR	b1	619	-	41,41,41	1.65	4 (9%)	56,56,56	4.53	15 (26%)
32	SQD	m1	101	-	40,42,54	0.87	0	50,53,65	0.91	3 (6%)
44	HEM	f	101	6,7	50,50,50	1.45	7 (14%)	67,82,82	1.05	3 (4%)
49	LUT	n1	621	-	42,43,43	2.43	1 (2%)	51,60,60	2.00	18 (35%)
29	CLA	B	605	-	69,73,73	1.40	7 (10%)	82,113,113	2.00	18 (21%)
29	CLA	y1	603	-	69,73,73	1.38	7 (10%)	82,113,113	1.86	18 (21%)
46	GOL	I	101	-	5,5,5	0.55	0	5,5,5	0.42	0
30	PHO	a	409	-	58,69,69	2.09	10 (17%)	55,99,99	1.59	11 (20%)
29	CLA	N	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.98	20 (24%)
37	DGD	C1	520	-	60,60,67	1.18	6 (10%)	74,74,81	0.96	2 (2%)
29	CLA	c	513	-	69,73,73	1.40	8 (11%)	82,113,113	1.98	18 (21%)
51	NEX	Y	623	-	40,46,46	2.70	11 (27%)	50,70,70	1.90	13 (26%)
49	LUT	y	621	-	42,43,43	2.45	2 (4%)	51,60,60	1.79	13 (25%)
48	CHL	G1	607	-	60,74,74	1.39	10 (16%)	58,114,114	1.68	11 (18%)
31	BCR	c	515	-	41,41,41	1.71	5 (12%)	56,56,56	4.33	16 (28%)
29	CLA	c1	503	-	69,73,73	1.36	7 (10%)	82,113,113	1.98	21 (25%)
33	LMG	h1	102	-	48,48,55	1.12	5 (10%)	56,56,63	1.24	5 (8%)
29	CLA	g	603	-	69,73,73	1.38	7 (10%)	82,113,113	1.94	20 (24%)
29	CLA	y	604	-	69,73,73	1.36	7 (10%)	82,113,113	1.94	19 (23%)
50	XAT	R1	621	-	41,47,47	0.70	1 (2%)	54,74,74	1.87	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	C1	513	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	19 (23%)
50	XAT	G1	622	-	41,47,47	0.79	1 (2%)	54,74,74	1.85	17 (31%)
29	CLA	Y1	602	-	69,73,73	1.39	8 (11%)	82,113,113	2.00	17 (20%)
30	PHO	A	409	-	58,69,69	2.08	9 (15%)	55,99,99	1.66	7 (12%)
40	LHG	y1	624	29	48,48,48	0.42	0	51,54,54	0.99	2 (3%)
39	DGA	C1	524	-	43,43,43	1.20	3 (6%)	45,45,45	1.55	4 (8%)
29	CLA	s	610	-	69,73,73	1.39	7 (10%)	82,113,113	1.90	20 (24%)
30	PHO	a	408	-	58,69,69	2.12	12 (20%)	55,99,99	1.59	7 (12%)
29	CLA	S1	612	-	49,53,73	1.61	6 (12%)	58,89,113	2.02	13 (22%)
33	LMG	b1	622	-	44,44,55	0.96	3 (6%)	52,52,63	1.17	4 (7%)
49	LUT	N1	621	-	42,43,43	2.43	2 (4%)	51,60,60	2.02	16 (31%)
51	NEX	s1	623	-	40,46,46	2.78	14 (35%)	50,70,70	3.06	15 (30%)
29	CLA	g1	604	-	53,57,73	1.54	7 (13%)	61,93,113	2.16	18 (29%)
31	BCR	C1	514	-	41,41,41	1.66	5 (12%)	56,56,56	4.22	12 (21%)
29	CLA	b	612	-	69,73,73	1.37	7 (10%)	82,113,113	1.95	15 (18%)
29	CLA	G1	604	-	53,57,73	1.57	6 (11%)	61,93,113	2.26	19 (31%)
31	BCR	B1	619	-	41,41,41	1.58	4 (9%)	56,56,56	4.60	16 (28%)
37	DGD	b1	623	-	44,44,67	0.92	3 (6%)	58,58,81	1.31	6 (10%)
29	CLA	b1	607	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	18 (21%)
32	SQD	B	621	-	40,42,54	0.86	0	50,53,65	0.94	3 (6%)
33	LMG	c1	523	-	55,55,55	1.28	6 (10%)	63,63,63	1.14	3 (4%)
29	CLA	S1	605	-	54,58,73	1.58	8 (14%)	64,95,113	2.08	18 (28%)
29	CLA	g1	614	-	53,57,73	1.60	9 (16%)	61,93,113	2.20	18 (29%)
29	CLA	B1	611	-	69,73,73	1.39	6 (8%)	82,113,113	1.99	16 (19%)
47	4RF	k	101	-	56,56,56	1.07	4 (7%)	59,59,59	0.85	3 (5%)
50	XAT	r1	621	-	41,47,47	0.77	1 (2%)	54,74,74	2.12	19 (35%)
47	4RF	K	101	-	56,56,56	1.09	3 (5%)	59,59,59	0.92	3 (5%)
29	CLA	R	608	-	64,68,73	1.46	9 (14%)	76,107,113	1.96	16 (21%)
29	CLA	s	604	-	59,63,73	1.48	7 (11%)	70,101,113	1.96	16 (22%)
29	CLA	N1	612	-	49,53,73	1.62	7 (14%)	58,89,113	2.07	13 (22%)
29	CLA	B1	602	-	69,73,73	1.39	7 (10%)	82,113,113	1.94	17 (20%)
29	CLA	N1	611	-	53,57,73	1.56	7 (13%)	61,93,113	2.21	18 (29%)
48	CHL	n	606	-	60,74,74	1.56	9 (15%)	58,114,114	1.70	12 (20%)
29	CLA	n1	604	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	15 (18%)
29	CLA	s	614	-	59,63,73	1.48	6 (10%)	70,101,113	2.01	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	C1	508	-	69,73,73	1.39	7 (10%)	82,113,113	1.74	18 (21%)
48	CHL	s	607	-	37,51,74	1.67	8 (21%)	30,86,114	2.60	10 (33%)
50	XAT	n1	622	-	41,47,47	0.68	1 (2%)	54,74,74	2.01	14 (25%)
55	PTY	y	627	-	18,18,49	1.33	3 (16%)	21,23,54	1.54	2 (9%)
30	PHO	a1	409	-	58,69,69	2.19	10 (17%)	55,99,99	1.73	9 (16%)
29	CLA	C	512	-	69,73,73	1.38	6 (8%)	82,113,113	1.87	16 (19%)
44	HEM	f1	101	7	50,50,50	1.61	7 (14%)	67,82,82	1.06	3 (4%)
51	NEX	r	622	-	40,46,46	2.68	10 (25%)	50,70,70	1.70	12 (24%)
29	CLA	b1	604	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	20 (24%)
29	CLA	C	511	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	17 (20%)
29	CLA	r1	604	-	53,57,73	1.57	7 (13%)	61,93,113	2.13	16 (26%)
32	SQD	b1	626	-	52,54,54	0.79	1 (1%)	62,65,65	0.86	2 (3%)
29	CLA	Y	602	-	69,73,73	1.40	7 (10%)	82,113,113	1.93	19 (23%)
31	BCR	C1	516	-	41,41,41	1.62	4 (9%)	56,56,56	4.83	16 (28%)
49	LUT	Y1	621	-	42,43,43	2.41	1 (2%)	51,60,60	2.22	13 (25%)
48	CHL	n1	607	-	60,74,74	1.28	7 (11%)	58,114,114	1.82	13 (22%)
49	LUT	Y1	620	-	42,43,43	2.49	1 (2%)	51,60,60	1.74	13 (25%)
29	CLA	b1	616	-	69,73,73	1.40	7 (10%)	82,113,113	1.86	15 (18%)
33	LMG	A1	413	-	48,48,55	1.12	5 (10%)	56,56,63	1.21	5 (8%)
29	CLA	S	603	-	69,73,73	1.38	7 (10%)	82,113,113	1.78	17 (20%)
34	SPH	A1	414	-	19,20,20	0.69	1 (5%)	18,21,21	1.20	1 (5%)
29	CLA	N	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	20 (24%)
29	CLA	Y1	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	18 (21%)
29	CLA	s1	612	-	49,53,73	1.67	9 (18%)	58,89,113	1.92	12 (20%)
29	CLA	y	608	-	54,58,73	1.58	8 (14%)	64,95,113	2.10	18 (28%)
29	CLA	s	612	-	49,53,73	1.63	7 (14%)	58,89,113	2.03	17 (29%)
37	DGD	c	520	-	60,60,67	1.15	6 (10%)	74,74,81	1.04	3 (4%)
40	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.02	2 (4%)
48	CHL	S1	608	-	55,69,74	1.25	7 (12%)	52,108,114	1.85	13 (25%)
48	CHL	s1	606	-	38,52,74	1.67	7 (18%)	31,87,114	2.21	10 (32%)
29	CLA	s1	611	40	69,73,73	1.37	6 (8%)	82,113,113	1.94	18 (21%)
50	XAT	g	622	-	41,47,47	0.76	1 (2%)	54,74,74	2.24	16 (29%)
34	SPH	a1	414	-	19,20,20	0.76	1 (5%)	18,21,21	1.00	1 (5%)
29	CLA	g1	613	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	20 (24%)
41	LMK	C	527	-	39,39,53	1.49	2 (5%)	39,46,60	1.59	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	G1	610	-	69,73,73	1.38	8 (11%)	82,113,113	1.95	20 (24%)
29	CLA	b	607	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	19 (23%)
29	CLA	d1	402	-	69,73,73	1.39	7 (10%)	82,113,113	1.87	18 (21%)
29	CLA	y1	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	21 (25%)
43	PL9	D1	405	-	55,55,55	1.18	5 (9%)	68,69,69	1.71	13 (19%)
34	SPH	y	625	-	19,20,20	0.62	0	18,21,21	1.25	2 (11%)
48	CHL	G	605	21	42,56,74	1.54	8 (19%)	36,92,114	2.24	10 (27%)
31	BCR	D1	404	-	41,41,41	1.65	5 (12%)	56,56,56	4.47	15 (26%)
49	LUT	G1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.73	12 (23%)
40	LHG	L1	101	-	48,48,48	0.37	0	51,54,54	1.13	3 (5%)
29	CLA	N	613	-	69,73,73	1.37	6 (8%)	82,113,113	1.92	13 (15%)
29	CLA	g1	610	-	69,73,73	1.32	6 (8%)	82,113,113	2.13	21 (25%)
29	CLA	g	613	-	69,73,73	1.34	6 (8%)	82,113,113	1.93	21 (25%)
29	CLA	n	612	-	49,53,73	1.62	6 (12%)	58,89,113	2.00	15 (25%)
55	PTY	Y	627	-	18,18,49	1.35	3 (16%)	21,23,54	1.44	2 (9%)
29	CLA	C1	512	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	22 (26%)
29	CLA	Y1	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	18 (21%)
31	BCR	C1	517	-	41,41,41	1.63	4 (9%)	56,56,56	4.60	15 (26%)
29	CLA	R1	608	-	64,68,73	1.42	7 (10%)	76,107,113	1.98	20 (26%)
33	LMG	d	411	-	46,46,55	1.04	4 (8%)	54,54,63	1.20	4 (7%)
29	CLA	n	611	-	53,57,73	1.56	6 (11%)	61,93,113	2.20	19 (31%)
39	DGA	j	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.30	2 (6%)
29	CLA	C1	511	-	69,73,73	1.36	7 (10%)	82,113,113	2.05	21 (25%)
52	LMT	R	625	-	36,36,36	1.19	6 (16%)	47,47,47	1.15	3 (6%)
26	OEX	a	401	1,4	0,15,15	-	-	-		
29	CLA	R	612	-	64,68,73	1.43	8 (12%)	76,107,113	2.02	20 (26%)
29	CLA	S	612	-	49,53,73	1.64	7 (14%)	58,89,113	2.08	12 (20%)
29	CLA	D1	402	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	19 (23%)
40	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.10	3 (7%)
29	CLA	S1	604	-	59,63,73	1.48	7 (11%)	70,101,113	2.07	19 (27%)
48	CHL	R	606	-	38,52,74	2.46	10 (26%)	31,87,114	1.97	9 (29%)
29	CLA	C	506	-	69,73,73	1.41	7 (10%)	82,113,113	1.96	19 (23%)
48	CHL	S	606	-	38,52,74	1.73	8 (21%)	31,87,114	2.05	11 (35%)
31	BCR	c1	514	-	41,41,41	1.61	4 (9%)	56,56,56	4.65	16 (28%)
29	CLA	b	604	-	69,73,73	1.40	7 (10%)	82,113,113	1.78	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	n1	610	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	19 (23%)
29	CLA	b1	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.82	17 (20%)
29	CLA	c	502	-	69,73,73	1.37	7 (10%)	82,113,113	1.93	18 (21%)
39	DGA	b	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.46	3 (6%)
29	CLA	R1	609	-	64,68,73	1.39	7 (10%)	76,107,113	4.19	21 (27%)
29	CLA	Y1	604	-	69,73,73	1.37	5 (7%)	82,113,113	1.87	17 (20%)
29	CLA	a	406	-	69,73,73	1.36	7 (10%)	82,113,113	2.09	19 (23%)
53	ERG	r	626	-	32,32,32	7.97	20 (62%)	45,50,50	3.21	14 (31%)
39	DGA	C	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.51	3 (6%)
29	CLA	s1	604	-	59,63,73	1.48	5 (8%)	70,101,113	2.04	16 (22%)
31	BCR	a	411	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	13 (23%)
38	3PH	t	101	-	47,47,47	0.86	4 (8%)	50,52,52	1.21	3 (6%)
40	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.17	4 (9%)
48	CHL	g1	609	-	60,74,74	1.39	10 (16%)	58,114,114	1.56	9 (15%)
51	NEX	n1	623	-	40,46,46	2.63	10 (25%)	50,70,70	1.59	10 (20%)
47	4RF	i	101	-	56,56,56	1.08	3 (5%)	59,59,59	0.95	4 (6%)
29	CLA	B1	609	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	15 (18%)
30	PHO	a1	408	-	58,69,69	2.14	11 (18%)	55,99,99	1.42	9 (16%)
29	CLA	s	611	40	69,73,73	1.35	7 (10%)	82,113,113	1.85	14 (17%)
49	LUT	y1	620	-	42,43,43	2.45	1 (2%)	51,60,60	1.95	8 (15%)
31	BCR	B	619	-	41,41,41	1.66	5 (12%)	56,56,56	3.97	20 (35%)
33	LMG	a	413	-	48,48,55	1.12	5 (10%)	56,56,63	1.20	3 (5%)
51	NEX	G	623	-	40,46,46	2.75	12 (30%)	50,70,70	1.88	12 (24%)
39	DGA	b1	625	-	43,43,43	1.16	2 (4%)	45,45,45	1.51	3 (6%)
29	CLA	s1	605	-	54,58,73	1.57	9 (16%)	64,95,113	2.15	18 (28%)
29	CLA	B1	606	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	19 (23%)
31	BCR	c1	517	-	41,41,41	1.61	5 (12%)	56,56,56	4.52	19 (33%)
38	3PH	B1	624	-	47,47,47	0.87	3 (6%)	50,52,52	1.12	2 (4%)
49	LUT	n1	620	-	42,43,43	2.46	1 (2%)	51,60,60	1.65	9 (17%)
53	ERG	R1	626	-	32,32,32	7.85	20 (62%)	45,50,50	3.05	19 (42%)
29	CLA	c1	509	-	69,73,73	1.38	9 (13%)	82,113,113	1.72	14 (17%)
29	CLA	S	614	-	59,63,73	1.49	6 (10%)	70,101,113	2.01	17 (24%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
48	CHL	S	607	-	37,51,74	1.80	9 (24%)	30,86,114	2.38	11 (36%)
38	3PH	b1	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.17	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	CHL	y1	609	-	60,74,74	1.23	9 (15%)	58,114,114	1.60	11 (18%)
29	CLA	G	603	-	69,73,73	1.34	8 (11%)	82,113,113	1.94	23 (28%)
48	CHL	s1	601	23	40,54,74	2.12	7 (17%)	34,90,114	1.92	9 (26%)
48	CHL	s	601	-	40,54,74	1.78	9 (22%)	34,90,114	2.22	10 (29%)
54	LPX	S1	625	-	29,29,29	1.05	2 (6%)	31,33,33	0.94	1 (3%)
29	CLA	B	606	-	69,73,73	1.36	7 (10%)	82,113,113	1.99	17 (20%)
40	LHG	N	624	-	48,48,48	0.41	0	51,54,54	1.09	3 (5%)
48	CHL	g1	606	-	44,58,74	2.01	8 (18%)	37,94,114	1.98	11 (29%)
29	CLA	b1	605	-	69,73,73	1.34	6 (8%)	82,113,113	2.01	20 (24%)
48	CHL	y1	606	-	60,74,74	1.19	7 (11%)	58,114,114	1.79	11 (18%)
29	CLA	g1	611	-	69,73,73	1.38	8 (11%)	82,113,113	1.80	16 (19%)
29	CLA	B	602	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
40	LHG	g	624	-	48,48,48	0.39	0	51,54,54	0.98	2 (3%)
48	CHL	g1	605	-	42,56,74	1.61	8 (19%)	36,92,114	2.14	11 (30%)
29	CLA	a	405	-	69,73,73	1.38	6 (8%)	82,113,113	1.89	20 (24%)
29	CLA	r	603	-	64,68,73	1.44	8 (12%)	76,107,113	1.84	16 (21%)
41	LMK	c	527	-	39,39,53	1.55	3 (7%)	39,46,60	1.28	2 (5%)
33	LMG	c	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.17	5 (8%)
48	CHL	g	609	-	60,74,74	1.47	10 (16%)	58,114,114	1.85	12 (20%)
49	LUT	S	620	-	42,43,43	2.37	2 (4%)	51,60,60	1.95	19 (37%)
29	CLA	y	612	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	18 (21%)
29	CLA	N1	613	-	69,73,73	1.37	6 (8%)	82,113,113	1.90	20 (24%)
41	LMK	c1	527	-	39,39,53	1.56	3 (7%)	39,46,60	1.27	2 (5%)
48	CHL	n1	601	-	60,74,74	1.29	7 (11%)	58,114,114	1.92	13 (22%)
40	LHG	d	410	-	38,38,48	0.44	0	41,44,54	1.12	3 (7%)
40	LHG	s	624	29	44,44,48	0.44	0	47,50,54	1.14	3 (6%)
48	CHL	y	605	24	40,54,74	1.64	7 (17%)	34,90,114	2.14	11 (32%)
31	BCR	B	618	-	41,41,41	1.65	5 (12%)	56,56,56	4.49	17 (30%)
51	NEX	N	623	-	40,46,46	2.73	11 (27%)	50,70,70	1.56	9 (18%)
51	NEX	R	622	-	40,46,46	2.78	13 (32%)	50,70,70	1.95	12 (24%)
48	CHL	n1	609	-	60,74,74	1.20	8 (13%)	58,114,114	1.70	11 (18%)
55	PTY	Y1	627	-	18,18,49	1.32	3 (16%)	21,23,54	1.46	2 (9%)
33	LMG	C1	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.15	2 (3%)
45	RRX	h	101	-	42,42,42	4.86	24 (57%)	56,58,58	3.21	25 (44%)
29	CLA	y1	610	24	69,73,73	1.41	8 (11%)	82,113,113	1.91	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	CHL	s1	608	-	55,69,74	2.03	9 (16%)	52,108,114	1.64	9 (17%)
40	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.07	4 (7%)
29	CLA	N	603	-	69,73,73	1.33	7 (10%)	82,113,113	1.97	20 (24%)
29	CLA	b	617	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	17 (20%)
48	CHL	S	601	23	40,54,74	2.05	8 (20%)	34,90,114	2.05	11 (32%)
29	CLA	N	604	-	69,73,73	1.38	6 (8%)	82,113,113	1.96	19 (23%)
33	LMG	C	523	-	55,55,55	1.28	6 (10%)	63,63,63	1.14	3 (4%)
29	CLA	B	612	-	69,73,73	1.39	7 (10%)	82,113,113	1.82	14 (17%)
38	3PH	S	626	-	47,47,47	0.87	3 (6%)	50,52,52	4.50	4 (8%)
29	CLA	C	501	-	69,73,73	1.35	7 (10%)	82,113,113	1.94	19 (23%)
34	SPH	Y1	625	-	19,20,20	0.66	0	18,21,21	1.05	1 (5%)
29	CLA	c1	512	-	69,73,73	1.39	6 (8%)	82,113,113	1.88	18 (21%)
29	CLA	C1	502	-	69,73,73	1.39	6 (8%)	82,113,113	1.89	18 (21%)
48	CHL	n1	606	-	60,74,74	1.43	8 (13%)	58,114,114	1.61	11 (18%)
29	CLA	c1	506	-	69,73,73	1.34	6 (8%)	82,113,113	1.93	19 (23%)
31	BCR	c	517	-	41,41,41	1.61	4 (9%)	56,56,56	4.46	15 (26%)
49	LUT	y	620	-	42,43,43	2.41	2 (4%)	51,60,60	1.76	16 (31%)
48	CHL	R	607	-	44,58,74	1.45	8 (18%)	37,94,114	2.24	12 (32%)
48	CHL	n	605	20	60,74,74	1.69	10 (16%)	58,114,114	1.75	10 (17%)
29	CLA	y1	604	-	69,73,73	1.34	6 (8%)	82,113,113	1.98	17 (20%)
29	CLA	r1	612	-	64,68,73	1.42	7 (10%)	76,107,113	1.90	20 (26%)
32	SQD	c	526	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
29	CLA	b	608	-	69,73,73	1.34	7 (10%)	82,113,113	1.87	16 (19%)
29	CLA	r	602	22	64,68,73	1.45	7 (10%)	76,107,113	1.89	20 (26%)
48	CHL	G	608	-	38,52,74	1.68	9 (23%)	31,87,114	2.30	11 (35%)
48	CHL	y	606	-	60,74,74	1.54	9 (15%)	58,114,114	1.68	12 (20%)
55	PTY	y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.08	2 (3%)
29	CLA	y	611	40	69,73,73	1.36	7 (10%)	82,113,113	1.75	14 (17%)
29	CLA	S1	610	-	69,73,73	1.37	6 (8%)	82,113,113	1.91	18 (21%)
33	LMG	d1	411	-	46,46,55	1.04	4 (8%)	54,54,63	1.13	2 (3%)
26	OEX	A1	401	1,4	0,15,15	-	-	-	-	-
48	CHL	Y	601	24	60,74,74	1.52	9 (15%)	58,114,114	1.77	11 (18%)
29	CLA	b	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	15 (18%)
29	CLA	Y	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.96	22 (26%)
40	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	SQD	A	412	-	49,51,54	0.80	1 (2%)	59,62,65	0.87	2 (3%)
49	LUT	N	621	-	42,43,43	2.49	1 (2%)	51,60,60	1.83	11 (21%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.11	2 (4%)
29	CLA	g	602	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	22 (26%)
32	SQD	M1	101	-	40,42,54	0.89	0	50,53,65	0.90	2 (4%)
26	OEX	a1	401	1	0,15,15	-	-	-	-	-
29	CLA	B1	612	-	69,73,73	1.37	6 (8%)	82,113,113	1.95	20 (24%)
49	LUT	g	621	-	42,43,43	2.47	2 (4%)	51,60,60	1.75	12 (23%)
32	SQD	m	101	-	40,42,54	0.90	0	50,53,65	0.92	2 (4%)
29	CLA	b	610	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	18 (21%)
29	CLA	c1	507	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	18 (21%)
37	DGD	b	623	-	44,44,67	0.89	2 (4%)	58,58,81	1.26	5 (8%)
50	XAT	R	621	-	41,47,47	0.69	1 (2%)	54,74,74	1.99	16 (29%)
30	PHO	A1	409	-	58,69,69	2.15	10 (17%)	55,99,99	1.68	7 (12%)
32	SQD	b1	621	-	40,42,54	0.87	0	50,53,65	0.91	2 (4%)
40	LHG	d1	409	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
34	SPH	Y	625	-	19,20,20	0.65	0	18,21,21	1.00	0
50	XAT	Y1	622	-	41,47,47	0.71	1 (2%)	54,74,74	3.84	22 (40%)
51	NEX	N1	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.46	8 (16%)
48	CHL	N1	601	-	60,74,74	1.26	9 (15%)	58,114,114	1.62	11 (18%)
49	LUT	G1	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.04	9 (17%)
48	CHL	r1	606	-	38,52,74	2.08	8 (21%)	31,87,114	2.38	8 (25%)
29	CLA	N1	603	-	69,73,73	1.36	6 (8%)	82,113,113	2.00	24 (29%)
29	CLA	n1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	19 (23%)
37	DGD	C	520	-	60,60,67	1.16	6 (10%)	74,74,81	1.07	3 (4%)
29	CLA	n	603	-	69,73,73	1.36	6 (8%)	82,113,113	1.98	23 (28%)
55	PTY	y1	627	-	18,18,49	1.30	2 (11%)	21,23,54	1.49	2 (9%)
46	GOL	I1	101	-	5,5,5	0.57	0	5,5,5	0.33	0
29	CLA	b	615	-	69,73,73	1.36	7 (10%)	82,113,113	1.94	17 (20%)
29	CLA	Y1	612	-	69,73,73	1.39	7 (10%)	82,113,113	1.89	19 (23%)
29	CLA	g1	602	-	69,73,73	1.38	8 (11%)	82,113,113	1.87	21 (25%)
29	CLA	y1	608	-	54,58,73	1.54	7 (12%)	64,95,113	2.08	18 (28%)
48	CHL	N	609	-	60,74,74	1.38	8 (13%)	58,114,114	1.69	13 (22%)
29	CLA	Y	612	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	18 (21%)
55	PTY	y	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LHG	G	624	29	48,48,48	0.37	0	51,54,54	1.07	3 (5%)
29	CLA	r	604	-	53,57,73	1.54	7 (13%)	61,93,113	2.26	14 (22%)
48	CHL	S1	606	-	38,52,74	1.70	8 (21%)	31,87,114	2.21	10 (32%)
38	3PH	T	101	-	47,47,47	0.85	4 (8%)	50,52,52	1.20	2 (4%)
29	CLA	S1	609	-	64,68,73	1.40	7 (10%)	76,107,113	2.00	18 (23%)
29	CLA	D1	403	-	69,73,73	1.37	9 (13%)	82,113,113	1.92	21 (25%)
29	CLA	B	613	-	69,73,73	1.41	7 (10%)	82,113,113	1.91	15 (18%)
29	CLA	b1	603	-	69,73,73	1.37	6 (8%)	82,113,113	1.93	21 (25%)
39	DGA	c	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.55	3 (6%)
47	4RF	k1	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.89	3 (5%)
29	CLA	s	617	-	54,58,73	1.55	7 (12%)	64,95,113	2.20	19 (29%)
31	BCR	c1	515	-	41,41,41	1.66	4 (9%)	56,56,56	4.53	12 (21%)
29	CLA	G	610	21	69,73,73	1.38	7 (10%)	82,113,113	1.91	17 (20%)
29	CLA	n	613	-	69,73,73	1.37	6 (8%)	82,113,113	2.01	16 (19%)
48	CHL	y	601	24	60,74,74	1.45	9 (15%)	58,114,114	1.68	11 (18%)
29	CLA	C1	506	-	69,73,73	1.37	6 (8%)	82,113,113	1.92	18 (21%)
50	XAT	y	622	-	41,47,47	0.72	1 (2%)	54,74,74	3.69	18 (33%)
49	LUT	G	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.93	16 (31%)
50	XAT	Y	622	-	41,47,47	0.69	1 (2%)	54,74,74	3.79	16 (29%)
29	CLA	d	402	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	18 (21%)
32	SQD	B1	621	-	40,42,54	0.87	0	50,53,65	0.89	2 (4%)
33	LMG	H	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.12	2 (3%)
29	CLA	b	611	-	69,73,73	1.38	7 (10%)	82,113,113	1.90	20 (24%)
29	CLA	G	602	-	69,73,73	1.37	7 (10%)	82,113,113	1.97	18 (21%)
29	CLA	y	614	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	20 (24%)
48	CHL	y	607	-	60,74,74	1.26	7 (11%)	58,114,114	1.74	13 (22%)
48	CHL	Y1	607	-	60,74,74	1.59	7 (11%)	58,114,114	1.69	12 (20%)
48	CHL	G1	609	-	60,74,74	1.46	9 (15%)	58,114,114	1.67	11 (18%)
29	CLA	C1	503	-	69,73,73	1.40	8 (11%)	82,113,113	1.90	19 (23%)
31	BCR	A	411	-	41,41,41	1.65	4 (9%)	56,56,56	4.40	14 (25%)
40	LHG	d	409	-	48,48,48	0.42	0	51,54,54	1.08	3 (5%)
44	HEM	F1	101	7	50,50,50	1.42	6 (12%)	67,82,82	1.23	6 (8%)
29	CLA	G1	612	-	47,51,73	1.69	7 (14%)	55,86,113	2.08	14 (25%)
29	CLA	B	615	-	69,73,73	1.37	8 (11%)	82,113,113	1.92	17 (20%)
29	CLA	C	502	-	69,73,73	1.38	7 (10%)	82,113,113	1.89	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	DGD	c1	518	-	56,56,67	1.09	5 (8%)	70,70,81	1.12	4 (5%)
29	CLA	N1	602	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	17 (20%)
44	HEM	F	101	6,7	50,50,50	1.36	7 (14%)	67,82,82	1.06	1 (1%)
48	CHL	N1	609	-	60,74,74	1.15	7 (11%)	58,114,114	1.67	12 (20%)
54	LPX	s1	625	-	29,29,29	1.03	2 (6%)	31,33,33	1.06	2 (6%)
29	CLA	c1	504	-	69,73,73	1.37	7 (10%)	82,113,113	1.98	15 (18%)
50	XAT	n	622	-	41,47,47	0.73	1 (2%)	54,74,74	2.10	13 (24%)
29	CLA	S	617	23	54,58,73	1.51	7 (12%)	64,95,113	2.15	18 (28%)
29	CLA	A1	410	-	64,68,73	1.40	7 (10%)	76,107,113	2.02	21 (27%)
30	PHO	A1	408	-	58,69,69	2.17	10 (17%)	55,99,99	1.59	9 (16%)
29	CLA	c	504	-	69,73,73	1.33	7 (10%)	82,113,113	1.92	18 (21%)
40	LHG	d1	408	-	43,43,48	0.40	0	46,49,54	1.06	2 (4%)
29	CLA	c	511	4	69,73,73	1.38	7 (10%)	82,113,113	1.89	18 (21%)
29	CLA	b	614	-	69,73,73	1.36	7 (10%)	82,113,113	2.00	16 (19%)
34	SPH	y1	625	-	19,20,20	0.64	0	18,21,21	1.30	2 (11%)
29	CLA	s1	613	-	59,63,73	1.51	8 (13%)	70,101,113	2.00	19 (27%)
36	C7Z	B1	620	-	43,43,43	5.48	26 (60%)	56,60,60	2.28	19 (33%)
29	CLA	S	609	-	64,68,73	1.43	7 (10%)	76,107,113	1.89	17 (22%)
29	CLA	n1	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.30	17 (27%)
32	SQD	A1	412	-	49,51,54	0.81	1 (2%)	59,62,65	0.92	3 (5%)
29	CLA	R1	603	-	64,68,73	1.45	7 (10%)	76,107,113	1.80	14 (18%)
49	LUT	S1	620	-	42,43,43	2.43	1 (2%)	51,60,60	1.75	9 (17%)
48	CHL	S1	601	23	40,54,74	1.82	8 (20%)	34,90,114	2.01	11 (32%)
31	BCR	b1	618	-	41,41,41	1.73	5 (12%)	56,56,56	4.39	18 (32%)
29	CLA	D	402	-	69,73,73	1.39	6 (8%)	82,113,113	1.82	16 (19%)
31	BCR	C1	515	-	41,41,41	1.59	4 (9%)	56,56,56	3.89	17 (30%)
49	LUT	G	621	-	42,43,43	2.45	1 (2%)	51,60,60	1.85	12 (23%)
43	PL9	d	405	-	55,55,55	1.68	10 (18%)	68,69,69	1.51	10 (14%)
29	CLA	C1	504	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	18 (21%)
37	DGD	c1	520	-	60,60,67	1.18	6 (10%)	74,74,81	1.01	3 (4%)
33	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.20	4 (6%)
29	CLA	N1	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.86	19 (23%)
29	CLA	c1	513	-	69,73,73	1.39	8 (11%)	82,113,113	1.96	19 (23%)
29	CLA	G1	614	-	53,57,73	1.54	6 (11%)	61,93,113	2.23	17 (27%)
29	CLA	B	609	-	69,73,73	1.38	7 (10%)	82,113,113	2.09	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	Y	610	-	69,73,73	1.38	7 (10%)	82,113,113	2.02	18 (21%)
29	CLA	b1	612	-	69,73,73	1.38	7 (10%)	82,113,113	2.03	18 (21%)
38	3PH	S1	626	-	47,47,47	0.88	4 (8%)	50,52,52	4.49	4 (8%)
42	BCT	D1	401	27	3,3,3	3.23	1 (33%)	2,3,3	3.11	2 (100%)
49	LUT	N1	620	-	42,43,43	2.47	1 (2%)	51,60,60	1.80	10 (19%)
29	CLA	G	604	-	53,57,73	1.58	7 (13%)	61,93,113	2.15	20 (32%)
49	LUT	n	620	-	42,43,43	2.43	1 (2%)	51,60,60	1.98	16 (31%)
49	LUT	S	621	-	42,43,43	2.33	1 (2%)	51,60,60	2.03	19 (37%)
49	LUT	Y	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.72	12 (23%)
29	CLA	b	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	21 (25%)
51	NEX	y	623	-	40,46,46	2.73	11 (27%)	50,70,70	1.90	14 (28%)
29	CLA	B1	614	-	69,73,73	1.38	8 (11%)	82,113,113	1.88	16 (19%)
50	XAT	y1	622	-	41,47,47	0.77	1 (2%)	54,74,74	3.88	17 (31%)
29	CLA	g1	603	-	69,73,73	1.39	7 (10%)	82,113,113	1.79	16 (19%)
48	CHL	N1	608	-	44,58,74	1.58	8 (18%)	37,94,114	2.29	13 (35%)
29	CLA	Y	604	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	18 (21%)
42	BCT	d1	401	-	3,3,3	1.19	0	2,3,3	4.40	2 (100%)
40	LHG	D1	409	-	48,48,48	0.41	0	51,54,54	1.08	3 (5%)
40	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.06	4 (8%)
48	CHL	n1	605	-	60,74,74	1.75	8 (13%)	58,114,114	1.64	11 (18%)
29	CLA	S	602	-	64,68,73	1.47	7 (10%)	76,107,113	2.03	16 (21%)
29	CLA	s1	610	-	69,73,73	1.38	6 (8%)	82,113,113	1.89	18 (21%)
40	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.09	2 (3%)
29	CLA	B	617	-	69,73,73	1.37	7 (10%)	82,113,113	1.94	16 (19%)
32	SQD	M	101	-	40,42,54	0.88	0	50,53,65	0.90	2 (4%)
29	CLA	b1	614	-	69,73,73	1.38	9 (13%)	82,113,113	1.84	18 (21%)
48	CHL	N	606	-	60,74,74	1.54	8 (13%)	58,114,114	1.60	12 (20%)
51	NEX	s	623	-	40,46,46	2.80	12 (30%)	50,70,70	2.10	15 (30%)
29	CLA	a	410	-	64,68,73	1.41	7 (10%)	76,107,113	2.02	20 (26%)
29	CLA	c	505	-	69,73,73	1.40	7 (10%)	82,113,113	1.92	16 (19%)
48	CHL	N	605	20	60,74,74	1.58	9 (15%)	58,114,114	1.71	12 (20%)
29	CLA	s	602	-	64,68,73	1.41	6 (9%)	76,107,113	1.99	21 (27%)
31	BCR	C	514	-	41,41,41	1.66	5 (12%)	56,56,56	4.45	14 (25%)
29	CLA	S1	614	-	59,63,73	1.48	6 (10%)	70,101,113	2.04	19 (27%)
29	CLA	C	507	-	69,73,73	1.39	7 (10%)	82,113,113	1.94	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	PL9	D	405	-	55,55,55	1.52	6 (10%)	68,69,69	1.44	10 (14%)
48	CHL	S1	607	-	37,51,74	1.75	8 (21%)	30,86,114	2.19	11 (36%)
29	CLA	G1	613	-	69,73,73	1.35	7 (10%)	82,113,113	2.04	20 (24%)
33	LMG	W	201	-	39,39,55	0.94	2 (5%)	47,47,63	1.23	4 (8%)
29	CLA	Y1	614	-	69,73,73	1.36	6 (8%)	82,113,113	1.94	20 (24%)
29	CLA	C	505	-	69,73,73	1.39	7 (10%)	82,113,113	1.92	17 (20%)
29	CLA	R1	604	-	53,57,73	1.57	7 (13%)	61,93,113	2.20	15 (24%)
29	CLA	c	506	-	69,73,73	1.40	7 (10%)	82,113,113	1.90	19 (23%)
29	CLA	n	602	-	69,73,73	1.42	8 (11%)	82,113,113	1.85	20 (24%)
38	3PH	s1	626	-	47,47,47	0.87	4 (8%)	50,52,52	4.46	4 (8%)
40	LHG	C	525	-	46,46,48	0.42	0	49,52,54	1.05	3 (6%)
29	CLA	N1	604	-	69,73,73	1.36	7 (10%)	82,113,113	2.05	17 (20%)
48	CHL	y	609	-	60,74,74	1.54	8 (13%)	58,114,114	1.69	12 (20%)
49	LUT	n	621	-	42,43,43	2.49	1 (2%)	51,60,60	1.58	12 (23%)
31	BCR	b	619	-	41,41,41	1.65	5 (12%)	56,56,56	4.31	15 (26%)
29	CLA	n1	611	-	53,57,73	1.56	6 (11%)	61,93,113	2.18	20 (32%)
29	CLA	c1	511	-	69,73,73	1.35	6 (8%)	82,113,113	1.97	20 (24%)
32	SQD	C1	526	-	52,54,54	0.80	0	62,65,65	0.82	2 (3%)

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
29	CLA	B1	608	-	1/1/15/20	26/39/115/115	-
48	CHL	y1	601	24	4/4/20/26	4/39/137/137	-
29	CLA	S	611	40	1/1/15/20	16/39/115/115	-
49	LUT	g	620	-	-	4/29/67/67	0/2/2/2
47	4RF	i1	101	-	-	30/59/59/59	-
29	CLA	D	403	-	1/1/15/20	17/39/115/115	-
29	CLA	A1	407	-	1/1/12/20	7/21/97/115	-
33	LMG	w	201	-	-	17/34/54/70	0/1/1/1
48	CHL	g1	608	-	3/3/15/26	2/13/111/137	-
33	LMG	B	622	-	-	20/39/59/70	0/1/1/1
39	DGA	c1	524	-	-	28/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	G1	608	-	2/2/15/26	3/13/111/137	-
29	CLA	c1	502	-	1/1/15/20	14/39/115/115	-
29	CLA	B	608	-	1/1/15/20	26/39/115/115	-
48	CHL	S	608	-	4/4/19/26	9/33/131/137	-
29	CLA	n1	613	-	1/1/15/20	18/39/115/115	-
29	CLA	s1	602	-	1/1/14/20	12/33/109/115	-
37	DGD	B1	623	-	-	12/32/72/95	0/2/2/2
29	CLA	R1	602	-	1/1/14/20	15/33/109/115	-
29	CLA	S1	613	-	1/1/13/20	11/27/103/115	-
29	CLA	b	609	-	1/1/15/20	13/39/115/115	-
29	CLA	s1	614	-	1/1/13/20	17/27/103/115	-
48	CHL	s1	607	-	3/3/15/26	2/12/110/137	-
36	C7Z	b1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
29	CLA	c	510	-	1/1/15/20	15/39/115/115	-
40	LHG	C1	525	-	-	28/51/51/53	-
49	LUT	s1	621	-	-	5/29/67/67	0/2/2/2
40	LHG	D1	408	-	-	26/48/48/53	-
38	3PH	b	624	-	-	23/49/49/49	-
50	XAT	N	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	R	604	-	1/1/11/20	8/20/96/115	-
31	BCR	A1	411	-	-	7/29/63/63	0/2/2/2
50	XAT	G	622	-	1/1/12/26	2/31/93/93	0/4/4/4
49	LUT	g1	620	-	-	6/29/67/67	0/2/2/2
29	CLA	b	603	-	1/1/15/20	20/39/115/115	-
48	CHL	r	606	-	3/3/15/26	2/13/111/137	-
52	LMT	R1	625	-	-	10/21/61/61	0/2/2/2
29	CLA	n	604	-	1/1/15/20	15/39/115/115	-
29	CLA	r	612	-	1/1/14/20	16/33/109/115	-
49	LUT	R1	620	-	-	9/29/67/67	0/2/2/2
33	LMG	A	413	-	-	15/43/63/70	0/1/1/1
29	CLA	g	610	-	1/1/15/20	17/39/115/115	-
33	LMG	c1	521	-	-	14/46/66/70	0/1/1/1
29	CLA	B	614	-	1/1/15/20	10/39/115/115	-
31	BCR	C	517	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGA	J1	101	-	-	15/30/30/45	-
29	CLA	C1	509	-	1/1/15/20	12/39/115/115	-
29	CLA	S1	617	23	1/1/12/20	7/21/97/115	-
45	RRX	H	101	-	1/1/11/25	6/29/65/65	0/2/2/2
29	CLA	N	612	-	1/1/11/20	6/15/91/115	-
33	LMG	b	622	-	-	17/39/59/70	0/1/1/1
29	CLA	y1	614	-	1/1/15/20	17/39/115/115	-
40	LHG	g1	624	-	-	34/53/53/53	-
50	XAT	g1	622	-	1/1/12/26	7/31/93/93	0/4/4/4
29	CLA	Y	608	-	1/1/12/20	9/21/97/115	-
31	BCR	a1	411	-	-	6/29/63/63	0/2/2/2
31	BCR	D	404	-	-	13/29/63/63	0/2/2/2
29	CLA	g	604	-	1/1/11/20	8/20/96/115	-
51	NEX	S1	623	-	-	4/27/83/83	0/3/3/3
29	CLA	G1	611	-	1/1/15/20	18/39/115/115	-
49	LUT	s	620	-	-	0/29/67/67	0/2/2/2
29	CLA	S1	602	23	1/1/14/20	19/33/109/115	-
31	BCR	C	515	-	-	9/29/63/63	0/2/2/2
29	CLA	s1	609	-	1/1/14/20	15/33/109/115	-
29	CLA	C	508	-	1/1/15/20	9/39/115/115	-
29	CLA	G	612	-	1/1/10/20	6/13/89/115	-
41	LMK	C1	527	-	2/2/6/6	19/46/46/60	-
51	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
29	CLA	a1	410	-	1/1/14/20	11/33/109/115	-
29	CLA	C1	505	-	1/1/15/20	17/39/115/115	-
29	CLA	R	602	-	1/1/14/20	11/33/109/115	-
29	CLA	c	507	-	1/1/15/20	16/39/115/115	-
54	LPX	S	625	-	-	14/31/31/31	-
33	LMG	C1	523	-	-	19/50/70/70	0/1/1/1
48	CHL	n1	608	-	3/3/16/26	5/20/118/137	-
29	CLA	b1	609	-	1/1/15/20	18/39/115/115	-
29	CLA	s	605	-	1/1/12/20	11/21/97/115	-
29	CLA	r1	609	-	1/1/14/20	19/33/109/115	-
29	CLA	N	614	-	1/1/11/20	7/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	N	607	-	4/4/20/26	6/39/137/137	-
48	CHL	s	608	-	4/4/19/26	7/33/131/137	-
49	LUT	g1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	S	613	-	1/1/13/20	10/27/103/115	-
48	CHL	G	601	21	4/4/20/26	7/39/137/137	-
29	CLA	d1	403	-	1/1/15/20	11/39/115/115	-
37	DGD	C	519	-	-	25/51/91/95	0/2/2/2
29	CLA	R1	610	-	1/1/14/20	17/33/109/115	-
29	CLA	A	407	-	1/1/12/20	7/21/97/115	-
48	CHL	y1	605	24	3/3/16/26	2/15/113/137	-
48	CHL	Y1	609	-	4/4/20/26	6/39/137/137	-
47	4RF	I1	102	-	-	24/59/59/59	-
29	CLA	a1	405	-	1/1/15/20	16/39/115/115	-
51	NEX	G1	623	-	-	12/27/83/83	0/3/3/3
49	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	B	603	-	1/1/15/20	21/39/115/115	-
32	SQD	C	526	-	-	23/49/69/69	0/1/1/1
34	SPH	A	414	-	-	12/21/21/21	-
29	CLA	y	602	24	1/1/15/20	14/39/115/115	-
49	LUT	r	620	-	-	7/29/67/67	0/2/2/2
29	CLA	b1	608	-	1/1/15/20	24/39/115/115	-
48	CHL	y1	607	-	4/4/20/26	6/39/137/137	-
50	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	s1	617	-	1/1/12/20	9/21/97/115	-
29	CLA	R	610	-	1/1/14/20	14/33/109/115	-
29	CLA	B1	610	-	1/1/15/20	21/39/115/115	-
37	DGD	C1	518	-	-	12/44/84/95	0/2/2/2
53	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
48	CHL	g	605	21	4/4/16/26	3/18/116/137	-
32	SQD	b	626	-	-	19/49/69/69	0/1/1/1
29	CLA	R	609	-	1/1/14/20	13/33/109/115	-
49	LUT	S1	621	-	-	7/29/67/67	0/2/2/2
40	LHG	L	101	-	-	37/53/53/53	-
29	CLA	b	616	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b1	617	-	1/1/15/20	16/39/115/115	-
29	CLA	g	614	-	1/1/11/20	12/20/96/115	-
48	CHL	g	607	-	4/4/20/26	9/39/137/137	-
37	DGD	B	623	-	-	14/32/72/95	0/2/2/2
32	SQD	b	621	-	-	18/37/57/69	0/1/1/1
33	LMG	c	523	-	-	20/50/70/70	0/1/1/1
48	CHL	g	608	-	3/3/15/26	4/13/111/137	-
29	CLA	a	407	-	1/1/11/20	9/20/96/115	-
48	CHL	N	601	20	4/4/20/26	5/39/137/137	-
29	CLA	c1	501	-	1/1/15/20	18/39/115/115	-
48	CHL	N1	606	-	4/4/20/26	12/39/137/137	-
34	SPH	a	414	-	-	11/21/21/21	-
37	DGD	C1	519	-	-	21/51/91/95	0/2/2/2
29	CLA	r	610	-	1/1/14/20	13/33/109/115	-
29	CLA	B1	605	-	1/1/15/20	15/39/115/115	-
48	CHL	Y	609	-	4/4/20/26	8/39/137/137	-
33	LMG	a1	413	-	-	20/43/63/70	0/1/1/1
48	CHL	Y	606	-	4/4/20/26	9/39/137/137	-
29	CLA	s1	603	-	1/1/15/20	18/39/115/115	-
51	NEX	y1	623	-	-	10/27/83/83	0/3/3/3
29	CLA	y	610	24	1/1/15/20	12/39/115/115	-
29	CLA	s	603	-	1/1/15/20	17/39/115/115	-
29	CLA	G	613	-	1/1/15/20	18/39/115/115	-
40	LHG	S	624	29	-	26/49/49/53	-
29	CLA	d	403	-	1/1/15/20	16/39/115/115	-
40	LHG	l	101	-	-	37/53/53/53	-
29	CLA	C	510	-	1/1/15/20	12/39/115/115	-
48	CHL	G	607	-	4/4/20/26	10/39/137/137	-
48	CHL	r1	607	-	3/3/16/26	2/20/118/137	-
29	CLA	G1	602	-	1/1/15/20	24/39/115/115	-
29	CLA	c	512	-	1/1/15/20	17/39/115/115	-
51	NEX	g	623	-	1/1/12/25	8/27/83/83	0/3/3/3
31	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
54	LPX	s	625	-	-	13/31/31/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y	611	-	1/1/15/20	12/39/115/115	-
55	PTY	Y	626	-	-	29/53/53/53	-
39	DGA	B1	625	-	-	25/45/45/45	-
31	BCR	d	404	-	-	13/29/63/63	0/2/2/2
48	CHL	r	607	-	3/3/16/26	6/20/118/137	-
33	LMG	D1	411	-	-	10/41/61/70	0/1/1/1
51	NEX	S	623	-	-	8/27/83/83	0/3/3/3
49	LUT	N	620	-	-	2/29/67/67	0/2/2/2
52	LMT	r	625	-	-	13/21/61/61	0/2/2/2
52	LMT	r1	625	-	-	11/21/61/61	0/2/2/2
49	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
29	CLA	c	508	-	1/1/15/20	8/39/115/115	-
29	CLA	S1	611	40	1/1/15/20	16/39/115/115	-
29	CLA	n1	612	-	1/1/11/20	6/15/91/115	-
29	CLA	R	603	-	1/1/14/20	16/33/109/115	-
32	SQD	a1	412	-	-	19/46/66/69	0/1/1/1
39	DGA	j1	101	-	-	20/30/30/45	-
32	SQD	c1	526	-	-	20/49/69/69	0/1/1/1
29	CLA	S	604	-	1/1/13/20	12/27/103/115	-
29	CLA	y1	612	-	1/1/15/20	17/39/115/115	-
29	CLA	C1	501	-	1/1/15/20	14/39/115/115	-
29	CLA	a1	407	-	1/1/11/20	7/20/96/115	-
29	CLA	B1	615	-	1/1/15/20	13/39/115/115	-
48	CHL	n	609	-	4/4/20/26	5/39/137/137	-
29	CLA	b1	602	-	1/1/15/20	22/39/115/115	-
29	CLA	c	501	-	1/1/15/20	20/39/115/115	-
51	NEX	g1	623	-	1/1/12/25	7/27/83/83	0/3/3/3
38	3PH	T1	101	-	-	29/49/49/49	-
29	CLA	C1	510	-	1/1/15/20	17/39/115/115	-
33	LMG	H1	102	-	-	17/43/63/70	0/1/1/1
29	CLA	A	406	-	1/1/15/20	12/39/115/115	-
29	CLA	b	605	-	1/1/15/20	19/39/115/115	-
29	CLA	b1	611	-	1/1/15/20	10/39/115/115	-
33	LMG	h	102	-	-	11/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	3PH	t1	101	-	-	30/49/49/49	-
40	LHG	s1	624	29	-	26/49/49/53	-
29	CLA	G	614	-	1/1/11/20	10/20/96/115	-
38	3PH	s	626	-	-	22/49/49/49	-
29	CLA	c1	508	-	1/1/15/20	9/39/115/115	-
29	CLA	r	609	-	1/1/14/20	10/33/109/115	-
36	C7Z	b	620	-	1/1/12/26	13/29/67/67	0/2/2/2
45	RRX	H1	101	-	1/1/11/25	8/29/65/65	0/2/2/2
29	CLA	y	603	-	1/1/15/20	20/39/115/115	-
48	CHL	Y1	605	-	3/3/16/26	3/15/113/137	-
40	LHG	n1	624	-	-	28/53/53/53	-
29	CLA	g	612	-	1/1/10/20	8/13/89/115	-
48	CHL	g	606	-	3/3/16/26	4/20/118/137	-
40	LHG	d1	410	-	-	32/43/43/53	-
55	PTY	Y1	626	-	-	25/53/53/53	-
47	4RF	K1	101	-	-	32/59/59/59	-
29	CLA	n	610	-	1/1/15/20	17/39/115/115	-
29	CLA	B	607	-	1/1/15/20	16/39/115/115	-
29	CLA	N	611	-	1/1/11/20	9/20/96/115	-
29	CLA	s	609	-	1/1/14/20	16/33/109/115	-
29	CLA	c	503	-	1/1/15/20	20/39/115/115	-
37	DGD	c1	519	-	-	26/51/91/95	0/2/2/2
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	r1	610	-	1/1/14/20	13/33/109/115	-
37	DGD	c	519	-	-	23/51/91/95	0/2/2/2
39	DGA	J	101	-	-	11/30/30/45	-
29	CLA	B1	603	-	1/1/15/20	17/39/115/115	-
29	CLA	c	509	-	1/1/15/20	16/39/115/115	-
29	CLA	y	613	-	1/1/15/20	22/39/115/115	-
29	CLA	c1	510	-	1/1/15/20	13/39/115/115	-
48	CHL	N	608	-	3/3/16/26	3/20/118/137	-
48	CHL	G1	606	-	3/3/16/26	3/20/118/137	-
29	CLA	Y1	613	-	1/1/15/20	21/39/115/115	-
49	LUT	r1	620	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y	613	24	1/1/15/20	21/39/115/115	-
33	LMG	D	411	-	-	11/41/61/70	0/1/1/1
29	CLA	C	503	-	1/1/15/20	18/39/115/115	-
29	CLA	y1	611	40	1/1/15/20	18/39/115/115	-
48	CHL	G1	605	21	4/4/16/26	2/18/116/137	-
47	4RF	I	102	-	-	30/59/59/59	-
51	NEX	r1	622	-	-	8/27/83/83	0/3/3/3
39	DGA	B	625	-	-	23/45/45/45	-
29	CLA	A	410	-	1/1/14/20	13/33/109/115	-
33	LMG	B1	622	-	-	16/39/59/70	0/1/1/1
29	CLA	B	611	-	1/1/15/20	13/39/115/115	-
48	CHL	Y1	606	-	4/4/20/26	7/39/137/137	-
31	BCR	C	516	-	-	13/29/63/63	0/2/2/2
48	CHL	n	601	20	4/4/20/26	3/39/137/137	-
29	CLA	B1	607	-	1/1/15/20	16/39/115/115	-
29	CLA	r1	608	-	1/1/14/20	14/33/109/115	-
29	CLA	s	613	-	1/1/13/20	9/27/103/115	-
29	CLA	N1	614	-	1/1/11/20	6/20/96/115	-
48	CHL	N1	607	-	4/4/20/26	10/39/137/137	-
32	SQD	B	626	-	-	24/49/69/69	0/1/1/1
29	CLA	A1	406	-	1/1/15/20	17/39/115/115	-
29	CLA	B	616	-	1/1/15/20	7/39/115/115	-
29	CLA	Y	614	-	1/1/15/20	18/39/115/115	-
29	CLA	S1	603	-	1/1/15/20	14/39/115/115	-
48	CHL	Y	607	-	4/4/20/26	8/39/137/137	-
48	CHL	R1	606	-	3/3/15/26	3/13/111/137	-
29	CLA	r	608	-	1/1/14/20	15/33/109/115	-
29	CLA	A	405	-	1/1/15/20	11/39/115/115	-
29	CLA	S	605	23	1/1/12/20	9/21/97/115	-
49	LUT	R	620	-	1/1/12/27	1/29/67/67	0/2/2/2
29	CLA	A1	405	-	1/1/15/20	12/39/115/115	-
40	LHG	G1	624	-	-	28/53/53/53	-
29	CLA	Y1	608	-	1/1/12/20	9/21/97/115	-
48	CHL	s	606	-	3/3/15/26	0/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	LUT	s1	620	-	-	6/29/67/67	0/2/2/2
40	LHG	c	525	-	-	29/51/51/53	-
48	CHL	g	601	21	4/4/20/26	13/39/137/137	-
29	CLA	g	611	-	1/1/15/20	15/39/115/115	-
29	CLA	C	504	-	1/1/15/20	14/39/115/115	-
29	CLA	B1	617	-	1/1/15/20	17/39/115/115	-
49	LUT	s	621	-	-	3/29/67/67	0/2/2/2
29	CLA	g1	612	21	1/1/10/20	5/13/89/115	-
32	SQD	a	412	-	-	14/46/66/69	0/1/1/1
40	LHG	S1	624	29	-	31/49/49/53	-
29	CLA	B1	604	-	1/1/15/20	12/39/115/115	-
40	LHG	y	624	29	-	29/53/53/53	-
32	SQD	B1	626	-	-	17/49/69/69	0/1/1/1
29	CLA	a1	406	-	1/1/15/20	14/39/115/115	-
40	LHG	Y1	624	-	-	18/53/53/53	-
29	CLA	S	610	-	1/1/15/20	22/39/115/115	-
29	CLA	B1	616	-	1/1/15/20	13/39/115/115	-
48	CHL	R1	607	-	3/3/16/26	2/20/118/137	-
29	CLA	b1	606	-	1/1/15/20	13/39/115/115	-
50	XAT	r	621	-	2/2/12/26	2/31/93/93	0/4/4/4
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
29	CLA	B	604	-	1/1/15/20	18/39/115/115	-
29	CLA	n1	602	20	1/1/15/20	18/39/115/115	-
29	CLA	r1	602	-	1/1/14/20	13/33/109/115	-
48	CHL	n	608	-	3/3/16/26	4/20/118/137	-
29	CLA	C	509	-	1/1/15/20	20/39/115/115	-
33	LMG	w1	201	-	-	17/34/54/70	0/1/1/1
29	CLA	C1	507	-	1/1/15/20	15/39/115/115	-
48	CHL	g1	601	-	4/4/20/26	8/39/137/137	-
29	CLA	c1	505	-	1/1/15/20	17/39/115/115	-
48	CHL	G1	601	21	4/4/20/26	9/39/137/137	-
48	CHL	N1	605	20	4/4/20/26	9/39/137/137	-
29	CLA	G1	603	-	1/1/15/20	22/39/115/115	-
29	CLA	b1	615	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	r1	603	-	1/1/14/20	18/33/109/115	-
48	CHL	G	609	21	4/4/20/26	9/39/137/137	-
43	PL9	d1	405	-	-	19/53/73/73	0/1/1/1
29	CLA	b	606	-	1/1/15/20	13/39/115/115	-
51	NEX	R1	622	-	-	14/27/83/83	0/3/3/3
48	CHL	Y	605	24	3/3/16/26	1/15/113/137	-
37	DGD	c	518	-	-	9/44/84/95	0/2/2/2
31	BCR	B1	618	-	-	15/29/63/63	0/2/2/2
29	CLA	B	610	-	1/1/15/20	21/39/115/115	-
29	CLA	n	614	-	1/1/11/20	6/20/96/115	-
29	CLA	B1	613	-	1/1/15/20	16/39/115/115	-
29	CLA	y1	613	-	1/1/15/20	18/39/115/115	-
48	CHL	n	607	-	4/4/20/26	7/39/137/137	-
48	CHL	g1	607	-	4/4/20/26	9/39/137/137	-
29	CLA	R1	612	-	1/1/14/20	19/33/109/115	-
31	BCR	c	514	-	-	14/29/63/63	0/2/2/2
33	LMG	W1	201	-	-	17/34/54/70	0/1/1/1
29	CLA	b1	613	-	1/1/15/20	15/39/115/115	-
48	CHL	Y1	601	-	4/4/20/26	3/39/137/137	-
29	CLA	Y1	603	-	1/1/15/20	15/39/115/115	-
29	CLA	C	513	-	1/1/15/20	22/39/115/115	-
37	DGD	C	518	-	-	17/44/84/95	0/2/2/2
48	CHL	G	606	-	3/3/16/26	4/20/118/137	-
51	NEX	n	623	-	-	4/27/83/83	1/3/3/3
29	CLA	G	611	40	1/1/15/20	17/39/115/115	-
38	3PH	B	624	-	-	34/49/49/49	-
53	ERG	R	626	-	5/5/11/15	6/13/71/71	0/4/4/4
31	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
31	BCR	b	618	-	-	9/29/63/63	0/2/2/2
31	BCR	c	516	-	-	15/29/63/63	0/2/2/2
45	RRX	h1	101	-	1/1/11/25	10/29/65/65	0/2/2/2
31	BCR	b1	619	-	-	9/29/63/63	0/2/2/2
32	SQD	m1	101	-	-	22/37/57/69	0/1/1/1
44	HEM	f	101	6,7	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	LUT	n1	621	-	1/1/12/27	5/29/67/67	0/2/2/2
29	CLA	B	605	-	1/1/15/20	20/39/115/115	-
29	CLA	y1	603	-	1/1/15/20	20/39/115/115	-
46	GOL	I	101	-	-	2/4/4/4	-
30	PHO	a	409	-	-	11/37/103/103	0/5/6/6
29	CLA	N	610	-	1/1/15/20	19/39/115/115	-
37	DGD	C1	520	-	-	16/48/88/95	0/2/2/2
29	CLA	c	513	-	1/1/15/20	22/39/115/115	-
51	NEX	Y	623	-	-	7/27/83/83	0/3/3/3
49	LUT	y	621	-	-	2/29/67/67	0/2/2/2
48	CHL	G1	607	-	4/4/20/26	13/39/137/137	-
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2
29	CLA	c1	503	-	1/1/15/20	19/39/115/115	-
33	LMG	h1	102	-	-	22/43/63/70	0/1/1/1
29	CLA	g	603	-	1/1/15/20	22/39/115/115	-
29	CLA	y	604	-	1/1/15/20	15/39/115/115	-
50	XAT	R1	621	-	-	4/31/93/93	0/4/4/4
29	CLA	C1	513	-	1/1/15/20	15/39/115/115	-
50	XAT	G1	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	Y1	602	-	1/1/15/20	20/39/115/115	-
30	PHO	A	409	-	-	14/37/103/103	0/5/6/6
40	LHG	y1	624	29	-	25/53/53/53	-
39	DGA	C1	524	-	-	23/45/45/45	-
29	CLA	s	610	-	1/1/15/20	19/39/115/115	-
30	PHO	a	408	-	-	10/37/103/103	0/5/6/6
29	CLA	S1	612	-	1/1/11/20	6/15/91/115	-
33	LMG	b1	622	-	-	19/39/59/70	0/1/1/1
49	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
51	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
29	CLA	g1	604	-	1/1/11/20	8/20/96/115	-
31	BCR	C1	514	-	-	12/29/63/63	0/2/2/2
29	CLA	b	612	-	1/1/15/20	12/39/115/115	-
29	CLA	G1	604	-	1/1/11/20	9/20/96/115	-
31	BCR	B1	619	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	b1	623	-	-	13/32/72/95	0/2/2/2
29	CLA	b1	607	-	1/1/15/20	12/39/115/115	-
32	SQD	B	621	-	-	20/37/57/69	0/1/1/1
33	LMG	c1	523	-	-	17/50/70/70	0/1/1/1
29	CLA	S1	605	-	1/1/12/20	8/21/97/115	-
29	CLA	g1	614	-	1/1/11/20	12/20/96/115	-
29	CLA	B1	611	-	1/1/15/20	14/39/115/115	-
50	XAT	r1	621	-	1/1/12/26	1/31/93/93	0/4/4/4
47	4RF	k	101	-	-	31/59/59/59	-
47	4RF	K	101	-	-	32/59/59/59	-
29	CLA	R	608	-	1/1/14/20	19/33/109/115	-
29	CLA	s	604	-	1/1/13/20	10/27/103/115	-
29	CLA	N1	612	-	1/1/11/20	7/15/91/115	-
29	CLA	B1	602	-	1/1/15/20	24/39/115/115	-
29	CLA	N1	611	-	1/1/11/20	10/20/96/115	-
48	CHL	n	606	-	4/4/20/26	7/39/137/137	-
29	CLA	n1	604	-	1/1/15/20	14/39/115/115	-
29	CLA	s	614	-	1/1/13/20	4/27/103/115	-
29	CLA	C1	508	-	1/1/15/20	11/39/115/115	-
48	CHL	s	607	-	3/3/15/26	2/12/110/137	-
50	XAT	n1	622	-	-	4/31/93/93	0/4/4/4
55	PTY	y	627	-	-	14/20/20/53	-
30	PHO	a1	409	-	-	11/37/103/103	0/5/6/6
29	CLA	C	512	-	1/1/15/20	13/39/115/115	-
44	HEM	f1	101	7	-	3/14/54/54	-
51	NEX	r	622	-	-	9/27/83/83	0/3/3/3
29	CLA	b1	604	-	1/1/15/20	20/39/115/115	-
29	CLA	C	511	-	1/1/15/20	12/39/115/115	-
29	CLA	r1	604	-	1/1/11/20	8/20/96/115	-
32	SQD	b1	626	-	-	25/49/69/69	0/1/1/1
29	CLA	Y	602	-	1/1/15/20	18/39/115/115	-
31	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
49	LUT	Y1	621	-	-	6/29/67/67	0/2/2/2
48	CHL	n1	607	-	4/4/20/26	6/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	LUT	Y1	620	-	-	6/29/67/67	0/2/2/2
29	CLA	b1	616	-	1/1/15/20	9/39/115/115	-
33	LMG	A1	413	-	-	18/43/63/70	0/1/1/1
29	CLA	S	603	-	1/1/15/20	17/39/115/115	-
34	SPH	A1	414	-	-	15/21/21/21	-
29	CLA	N	602	-	1/1/15/20	14/39/115/115	-
29	CLA	Y1	611	-	1/1/15/20	17/39/115/115	-
29	CLA	s1	612	-	1/1/11/20	7/15/91/115	-
29	CLA	y	608	-	1/1/12/20	8/21/97/115	-
29	CLA	s	612	-	1/1/11/20	7/15/91/115	-
48	CHL	s1	606	-	3/3/15/26	2/13/111/137	-
48	CHL	S1	608	-	4/4/19/26	6/33/131/137	-
37	DGD	c	520	-	-	9/48/88/95	0/2/2/2
40	LHG	c1	525	-	-	32/51/51/53	-
29	CLA	s1	611	40	1/1/15/20	20/39/115/115	-
50	XAT	g	622	-	2/2/12/26	3/31/93/93	0/4/4/4
34	SPH	a1	414	-	-	10/21/21/21	-
29	CLA	g1	613	-	1/1/15/20	21/39/115/115	-
41	LMK	C	527	-	2/2/6/6	20/46/46/60	-
29	CLA	G1	610	-	1/1/15/20	14/39/115/115	-
29	CLA	b	607	-	1/1/15/20	15/39/115/115	-
29	CLA	d1	402	-	1/1/15/20	11/39/115/115	-
29	CLA	y1	602	-	1/1/15/20	17/39/115/115	-
43	PL9	D1	405	-	-	18/53/73/73	0/1/1/1
34	SPH	y	625	-	-	8/21/21/21	-
48	CHL	G	605	21	4/4/16/26	3/18/116/137	-
31	BCR	D1	404	-	-	14/29/63/63	0/2/2/2
49	LUT	G1	620	-	-	5/29/67/67	0/2/2/2
40	LHG	L1	101	-	-	36/53/53/53	-
29	CLA	N	613	-	1/1/15/20	17/39/115/115	-
29	CLA	g1	610	-	1/1/15/20	16/39/115/115	-
29	CLA	g	613	-	1/1/15/20	20/39/115/115	-
29	CLA	n	612	-	1/1/11/20	6/15/91/115	-
55	PTY	Y	627	-	-	13/20/20/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C1	512	-	1/1/15/20	15/39/115/115	-
29	CLA	Y1	610	-	1/1/15/20	11/39/115/115	-
31	BCR	C1	517	-	-	10/29/63/63	0/2/2/2
29	CLA	R1	608	-	1/1/14/20	11/33/109/115	-
33	LMG	d	411	-	-	19/41/61/70	0/1/1/1
29	CLA	n	611	-	1/1/11/20	10/20/96/115	-
39	DGA	j	101	-	-	19/30/30/45	-
29	CLA	C1	511	-	1/1/15/20	12/39/115/115	-
52	LMT	R	625	-	-	9/21/61/61	0/2/2/2
29	CLA	R	612	-	1/1/14/20	13/33/109/115	-
29	CLA	S	612	-	1/1/11/20	6/15/91/115	-
29	CLA	D1	402	-	1/1/15/20	11/39/115/115	-
40	LHG	D1	410	-	-	25/43/43/53	-
29	CLA	S1	604	-	1/1/13/20	12/27/103/115	-
48	CHL	R	606	-	3/3/15/26	1/13/111/137	-
29	CLA	C	506	-	1/1/15/20	14/39/115/115	-
48	CHL	S	606	-	3/3/15/26	1/13/111/137	-
31	BCR	c1	514	-	-	12/29/63/63	0/2/2/2
29	CLA	b	604	-	1/1/15/20	13/39/115/115	-
29	CLA	n1	610	-	1/1/15/20	20/39/115/115	-
29	CLA	b1	610	-	1/1/15/20	18/39/115/115	-
29	CLA	c	502	-	1/1/15/20	12/39/115/115	-
39	DGA	b	625	-	-	24/45/45/45	-
29	CLA	R1	609	-	1/1/14/20	14/33/109/115	-
29	CLA	Y1	604	-	1/1/15/20	15/39/115/115	-
29	CLA	a	406	-	1/1/15/20	14/39/115/115	-
53	ERG	r	626	-	5/5/11/15	8/13/71/71	0/4/4/4
39	DGA	C	524	-	-	19/45/45/45	-
29	CLA	s1	604	-	1/1/13/20	8/27/103/115	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
38	3PH	t	101	-	-	27/49/49/49	-
48	CHL	g1	609	-	4/4/20/26	6/39/137/137	-
40	LHG	D	410	-	-	25/43/43/53	-
51	NEX	n1	623	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	4RF	i	101	-	-	31/59/59/59	-
29	CLA	B1	609	-	1/1/15/20	17/39/115/115	-
30	PHO	a1	408	-	-	18/37/103/103	0/5/6/6
29	CLA	s	611	40	1/1/15/20	15/39/115/115	-
49	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
31	BCR	B	619	-	-	7/29/63/63	0/2/2/2
33	LMG	a	413	-	-	20/43/63/70	0/1/1/1
51	NEX	G	623	-	-	5/27/83/83	0/3/3/3
39	DGA	b1	625	-	-	22/45/45/45	-
29	CLA	s1	605	-	1/1/12/20	9/21/97/115	-
29	CLA	B1	606	-	1/1/15/20	19/39/115/115	-
31	BCR	c1	517	-	-	9/29/63/63	0/2/2/2
38	3PH	B1	624	-	-	25/49/49/49	-
49	LUT	n1	620	-	-	4/29/67/67	0/2/2/2
53	ERG	R1	626	-	5/5/11/15	10/13/71/71	0/4/4/4
29	CLA	c1	509	-	1/1/15/20	23/39/115/115	-
29	CLA	S	614	-	1/1/13/20	8/27/103/115	-
48	CHL	y1	609	-	4/4/20/26	7/39/137/137	-
48	CHL	S	607	-	3/3/15/26	2/12/110/137	-
38	3PH	b1	624	-	-	24/49/49/49	-
40	LHG	D	409	-	-	24/53/53/53	-
29	CLA	G	603	-	1/1/15/20	15/39/115/115	-
48	CHL	s1	601	23	3/3/16/26	2/15/113/137	-
48	CHL	s	601	-	3/3/16/26	2/15/113/137	-
54	LPX	S1	625	-	-	15/31/31/31	-
29	CLA	B	606	-	1/1/15/20	16/39/115/115	-
48	CHL	g1	606	-	3/3/16/26	2/20/118/137	-
40	LHG	N	624	-	-	29/53/53/53	-
29	CLA	b1	605	-	1/1/15/20	18/39/115/115	-
48	CHL	y1	606	-	4/4/20/26	8/39/137/137	-
29	CLA	g1	611	-	1/1/15/20	18/39/115/115	-
29	CLA	B	602	-	1/1/15/20	18/39/115/115	-
40	LHG	g	624	-	-	26/53/53/53	-
48	CHL	g1	605	-	4/4/16/26	4/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	a	405	-	1/1/15/20	12/39/115/115	-
29	CLA	r	603	-	1/1/14/20	16/33/109/115	-
41	LMK	c	527	-	2/2/6/6	13/46/46/60	-
33	LMG	c	521	-	-	13/46/66/70	0/1/1/1
48	CHL	g	609	-	4/4/20/26	9/39/137/137	-
49	LUT	S	620	-	-	3/29/67/67	0/2/2/2
29	CLA	y	612	-	1/1/15/20	19/39/115/115	-
29	CLA	N1	613	-	1/1/15/20	12/39/115/115	-
41	LMK	c1	527	-	2/2/6/6	13/46/46/60	-
48	CHL	n1	601	-	4/4/20/26	10/39/137/137	-
40	LHG	d	410	-	-	20/43/43/53	-
48	CHL	y	605	24	3/3/16/26	5/15/113/137	-
40	LHG	s	624	29	-	25/49/49/53	-
31	BCR	B	618	-	-	11/29/63/63	0/2/2/2
51	NEX	N	623	-	-	4/27/83/83	1/3/3/3
51	NEX	R	622	-	-	8/27/83/83	0/3/3/3
48	CHL	n1	609	-	4/4/20/26	5/39/137/137	-
55	PTY	Y1	627	-	-	10/20/20/53	-
48	CHL	s1	608	-	4/4/19/26	3/33/131/137	-
45	RRX	h	101	-	1/1/11/25	4/29/65/65	0/2/2/2
29	CLA	y1	610	24	1/1/15/20	11/39/115/115	-
33	LMG	C1	521	-	-	13/46/66/70	0/1/1/1
40	LHG	Y	624	-	-	28/53/53/53	-
29	CLA	N	603	-	1/1/15/20	18/39/115/115	-
29	CLA	b	617	-	1/1/15/20	15/39/115/115	-
48	CHL	S	601	23	3/3/16/26	3/15/113/137	-
29	CLA	N	604	-	1/1/15/20	21/39/115/115	-
33	LMG	C	523	-	-	20/50/70/70	0/1/1/1
29	CLA	B	612	-	1/1/15/20	14/39/115/115	-
38	3PH	S	626	-	-	24/49/49/49	-
29	CLA	C	501	-	1/1/15/20	19/39/115/115	-
34	SPH	Y1	625	-	-	9/21/21/21	-
29	CLA	c1	512	-	1/1/15/20	17/39/115/115	-
29	CLA	C1	502	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	n1	606	-	4/4/20/26	8/39/137/137	-
29	CLA	c1	506	-	1/1/15/20	16/39/115/115	-
31	BCR	c	517	-	-	8/29/63/63	0/2/2/2
49	LUT	y	620	-	-	3/29/67/67	0/2/2/2
48	CHL	R	607	-	3/3/16/26	6/20/118/137	-
48	CHL	n	605	20	4/4/20/26	7/39/137/137	-
29	CLA	y1	604	-	1/1/15/20	15/39/115/115	-
29	CLA	r1	612	-	1/1/14/20	15/33/109/115	-
32	SQD	c	526	-	-	19/49/69/69	0/1/1/1
29	CLA	b	608	-	1/1/15/20	25/39/115/115	-
29	CLA	r	602	22	1/1/14/20	13/33/109/115	-
48	CHL	G	608	-	3/3/15/26	3/13/111/137	-
48	CHL	y	606	-	4/4/20/26	14/39/137/137	-
55	PTY	y1	626	-	-	31/53/53/53	-
29	CLA	y	611	40	1/1/15/20	14/39/115/115	-
29	CLA	S1	610	-	1/1/15/20	20/39/115/115	-
33	LMG	d1	411	-	-	19/41/61/70	0/1/1/1
48	CHL	Y	601	24	4/4/20/26	3/39/137/137	-
29	CLA	b	613	-	1/1/15/20	17/39/115/115	-
29	CLA	Y	603	-	1/1/15/20	18/39/115/115	-
40	LHG	N1	624	-	-	33/53/53/53	-
32	SQD	A	412	-	-	24/46/66/69	0/1/1/1
49	LUT	N	621	-	-	3/29/67/67	0/2/2/2
40	LHG	D	408	-	-	23/48/48/53	-
29	CLA	g	602	-	1/1/15/20	22/39/115/115	-
32	SQD	M1	101	-	-	16/37/57/69	0/1/1/1
29	CLA	B1	612	-	1/1/15/20	12/39/115/115	-
49	LUT	g	621	-	-	3/29/67/67	0/2/2/2
32	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	b	610	-	1/1/15/20	14/39/115/115	-
29	CLA	c1	507	-	1/1/15/20	17/39/115/115	-
37	DGD	b	623	-	-	13/32/72/95	0/2/2/2
50	XAT	R	621	-	-	2/31/93/93	0/4/4/4
30	PHO	A1	409	-	-	11/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	b1	621	-	-	16/37/57/69	0/1/1/1
40	LHG	d1	409	-	-	30/53/53/53	-
34	SPH	Y	625	-	-	10/21/21/21	-
50	XAT	Y1	622	-	1/1/12/26	4/31/93/93	0/4/4/4
51	NEX	N1	623	-	-	6/27/83/83	0/3/3/3
48	CHL	N1	601	-	4/4/20/26	8/39/137/137	-
49	LUT	G1	621	-	-	3/29/67/67	0/2/2/2
48	CHL	r1	606	-	3/3/15/26	3/13/111/137	-
29	CLA	N1	603	-	1/1/15/20	16/39/115/115	-
29	CLA	n1	603	-	1/1/15/20	13/39/115/115	-
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
29	CLA	n	603	-	1/1/15/20	24/39/115/115	-
55	PTY	y1	627	-	-	11/20/20/53	-
46	GOL	l1	101	-	-	2/4/4/4	-
29	CLA	b	615	-	1/1/15/20	18/39/115/115	-
29	CLA	Y1	612	-	1/1/15/20	20/39/115/115	-
29	CLA	g1	602	-	1/1/15/20	17/39/115/115	-
29	CLA	y1	608	-	1/1/12/20	9/21/97/115	-
48	CHL	N	609	-	4/4/20/26	11/39/137/137	-
29	CLA	Y	612	-	1/1/15/20	15/39/115/115	-
55	PTY	y	626	-	-	26/53/53/53	-
40	LHG	G	624	29	-	32/53/53/53	-
29	CLA	r	604	-	1/1/11/20	9/20/96/115	-
48	CHL	S1	606	-	3/3/15/26	1/13/111/137	-
38	3PH	T	101	-	-	26/49/49/49	-
29	CLA	S1	609	-	1/1/14/20	12/33/109/115	-
29	CLA	D1	403	-	1/1/15/20	17/39/115/115	-
29	CLA	B	613	-	1/1/15/20	18/39/115/115	-
29	CLA	b1	603	-	1/1/15/20	19/39/115/115	-
39	DGA	c	524	-	-	31/45/45/45	-
47	4RF	k1	101	-	-	37/59/59/59	-
29	CLA	s	617	-	1/1/12/20	8/21/97/115	-
31	BCR	c1	515	-	-	11/29/63/63	0/2/2/2
29	CLA	G	610	21	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	n	613	-	1/1/15/20	15/39/115/115	-
48	CHL	y	601	24	4/4/20/26	7/39/137/137	-
29	CLA	C1	506	-	1/1/15/20	18/39/115/115	-
50	XAT	y	622	-	-	8/31/93/93	0/4/4/4
49	LUT	G	620	-	-	3/29/67/67	0/2/2/2
50	XAT	Y	622	-	-	6/31/93/93	0/4/4/4
29	CLA	d	402	-	1/1/15/20	11/39/115/115	-
32	SQD	B1	621	-	-	11/37/57/69	0/1/1/1
33	LMG	H	102	-	-	14/43/63/70	0/1/1/1
29	CLA	b	611	-	1/1/15/20	7/39/115/115	-
29	CLA	G	602	-	1/1/15/20	17/39/115/115	-
29	CLA	y	614	-	1/1/15/20	16/39/115/115	-
48	CHL	y	607	-	4/4/20/26	9/39/137/137	-
48	CHL	Y1	607	-	4/4/20/26	7/39/137/137	-
48	CHL	G1	609	-	4/4/20/26	7/39/137/137	-
29	CLA	C1	503	-	1/1/15/20	18/39/115/115	-
31	BCR	A	411	-	-	9/29/63/63	0/2/2/2
40	LHG	d	409	-	-	26/53/53/53	-
44	HEM	F1	101	7	-	1/14/54/54	-
29	CLA	G1	612	-	1/1/10/20	8/13/89/115	-
29	CLA	B	615	-	1/1/15/20	14/39/115/115	-
29	CLA	C	502	-	1/1/15/20	13/39/115/115	-
37	DGD	c1	518	-	-	13/44/84/95	0/2/2/2
29	CLA	N1	602	-	1/1/15/20	16/39/115/115	-
44	HEM	F	101	6,7	-	1/14/54/54	-
48	CHL	N1	609	-	4/4/20/26	7/39/137/137	-
54	LPX	s1	625	-	-	17/31/31/31	-
29	CLA	c1	504	-	1/1/15/20	19/39/115/115	-
50	XAT	n	622	-	1/1/12/26	4/31/93/93	0/4/4/4
29	CLA	S	617	23	1/1/12/20	7/21/97/115	-
29	CLA	A1	410	-	1/1/14/20	12/33/109/115	-
30	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
29	CLA	c	504	-	1/1/15/20	18/39/115/115	-
40	LHG	d1	408	-	-	30/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	511	4	1/1/15/20	9/39/115/115	-
29	CLA	b	614	-	1/1/15/20	13/39/115/115	-
34	SPH	y1	625	-	-	12/21/21/21	-
29	CLA	s1	613	-	1/1/13/20	12/27/103/115	-
36	C7Z	B1	620	-	1/1/12/26	7/29/67/67	0/2/2/2
29	CLA	S	609	-	1/1/14/20	12/33/109/115	-
29	CLA	n1	614	-	1/1/11/20	10/20/96/115	-
32	SQD	A1	412	-	-	16/46/66/69	0/1/1/1
29	CLA	R1	603	-	1/1/14/20	17/33/109/115	-
49	LUT	S1	620	-	-	3/29/67/67	0/2/2/2
48	CHL	S1	601	23	3/3/16/26	1/15/113/137	-
31	BCR	b1	618	-	-	11/29/63/63	0/2/2/2
29	CLA	D	402	-	1/1/15/20	17/39/115/115	-
31	BCR	C1	515	-	-	12/29/63/63	0/2/2/2
49	LUT	G	621	-	1/1/12/27	3/29/67/67	0/2/2/2
43	PL9	d	405	-	-	9/53/73/73	0/1/1/1
29	CLA	C1	504	-	1/1/15/20	18/39/115/115	-
37	DGD	c1	520	-	-	11/48/88/95	0/2/2/2
33	LMG	C	521	-	-	16/46/66/70	0/1/1/1
29	CLA	N1	610	-	1/1/15/20	19/39/115/115	-
29	CLA	c1	513	-	1/1/15/20	22/39/115/115	-
29	CLA	G1	614	-	1/1/11/20	7/20/96/115	-
29	CLA	B	609	-	1/1/15/20	12/39/115/115	-
29	CLA	Y	610	-	1/1/15/20	13/39/115/115	-
29	CLA	b1	612	-	1/1/15/20	17/39/115/115	-
38	3PH	S1	626	-	-	30/49/49/49	-
49	LUT	N1	620	-	-	6/29/67/67	0/2/2/2
29	CLA	G	604	-	1/1/11/20	8/20/96/115	-
49	LUT	n	620	-	-	3/29/67/67	0/2/2/2
49	LUT	S	621	-	-	2/29/67/67	0/2/2/2
49	LUT	Y	620	-	-	5/29/67/67	0/2/2/2
29	CLA	b	602	-	1/1/15/20	21/39/115/115	-
51	NEX	y	623	-	-	6/27/83/83	0/3/3/3
29	CLA	B1	614	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	XAT	y1	622	-	-	6/31/93/93	0/4/4/4
29	CLA	g1	603	-	1/1/15/20	17/39/115/115	-
48	CHL	N1	608	-	3/3/16/26	3/20/118/137	-
29	CLA	Y	604	-	1/1/15/20	17/39/115/115	-
40	LHG	D1	409	-	-	31/53/53/53	-
48	CHL	n1	605	-	4/4/20/26	6/39/137/137	-
40	LHG	d	408	-	-	26/48/48/53	-
29	CLA	S	602	-	1/1/14/20	16/33/109/115	-
29	CLA	s1	610	-	1/1/15/20	21/39/115/115	-
40	LHG	n	624	-	-	35/53/53/53	-
29	CLA	B	617	-	1/1/15/20	19/39/115/115	-
32	SQD	M	101	-	-	24/37/57/69	0/1/1/1
29	CLA	b1	614	-	1/1/15/20	12/39/115/115	-
48	CHL	N	606	-	4/4/20/26	10/39/137/137	-
51	NEX	s	623	-	-	4/27/83/83	0/3/3/3
29	CLA	a	410	-	1/1/14/20	15/33/109/115	-
29	CLA	c	505	-	1/1/15/20	19/39/115/115	-
48	CHL	N	605	20	4/4/20/26	9/39/137/137	-
29	CLA	s	602	-	1/1/14/20	18/33/109/115	-
31	BCR	C	514	-	-	17/29/63/63	0/2/2/2
29	CLA	S1	614	-	1/1/13/20	10/27/103/115	-
29	CLA	C	507	-	1/1/15/20	14/39/115/115	-
48	CHL	S1	607	-	3/3/15/26	2/12/110/137	-
43	PL9	D	405	-	-	9/53/73/73	0/1/1/1
29	CLA	G1	613	-	1/1/15/20	13/39/115/115	-
33	LMG	W	201	-	-	13/34/54/70	0/1/1/1
29	CLA	Y1	614	-	1/1/15/20	14/39/115/115	-
29	CLA	C	505	-	1/1/15/20	16/39/115/115	-
29	CLA	R1	604	-	1/1/11/20	10/20/96/115	-
29	CLA	c	506	-	1/1/15/20	16/39/115/115	-
29	CLA	n	602	-	1/1/15/20	18/39/115/115	-
38	3PH	s1	626	-	-	27/49/49/49	-
40	LHG	C	525	-	-	32/51/51/53	-
29	CLA	N1	604	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	y	609	-	4/4/20/26	8/39/137/137	-
49	LUT	n	621	-	-	2/29/67/67	0/2/2/2
31	BCR	b	619	-	-	6/29/63/63	0/2/2/2
29	CLA	n1	611	-	1/1/11/20	10/20/96/115	-
29	CLA	c1	511	-	1/1/15/20	18/39/115/115	-
32	SQD	C1	526	-	-	25/49/69/69	0/1/1/1

The worst 5 of 4153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	R	626	ERG	C1-C10	-24.08	1.10	1.54
53	r	626	ERG	C1-C10	-23.87	1.10	1.54
53	R1	626	ERG	C1-C10	-23.80	1.10	1.54
53	r1	626	ERG	C1-C10	-23.64	1.11	1.54
53	r	626	ERG	C10-C9	-21.45	1.28	1.55

The worst 5 of 8995 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L	101	LHG	O7-C7-C8	22.89	161.00	111.48
40	l	101	LHG	O7-C7-C8	22.88	160.99	111.48
38	S	626	3PH	O21-C21-C22	22.11	159.31	111.48
38	S1	626	3PH	O21-C21-C22	22.06	159.19	111.48
38	s	626	3PH	O21-C21-C22	22.01	159.10	111.48

5 of 696 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	A	410	CLA	ND
29	B	602	CLA	ND

5 of 9356 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	A	407	CLA	C2-C1-O2A-CGA
29	B	602	CLA	C3A-C2A-CAA-CBA

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	N	623	NEX	C1-C2-C3-C4-C5-C6
51	n	623	NEX	C1-C2-C3-C4-C5-C6

662 monomers are involved in 2295 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B1	608	CLA	7	0
29	S	611	CLA	3	0
49	g	620	LUT	4	0
47	i1	101	4RF	2	0
29	D	403	CLA	4	0
29	A1	407	CLA	2	0
33	w	201	LMG	6	0
48	g1	608	CHL	2	0
33	B	622	LMG	2	0
39	c1	524	DGA	4	0
48	G1	608	CHL	2	0
29	c1	502	CLA	7	0
29	B	608	CLA	4	0
48	S	608	CHL	3	0
29	n1	613	CLA	10	0
29	s1	602	CLA	4	0
37	B1	623	DGD	2	0
29	R1	602	CLA	4	0
29	S1	613	CLA	2	0
29	b	609	CLA	4	0
29	s1	614	CLA	2	0
48	s1	607	CHL	3	0
29	c	510	CLA	2	0
40	C1	525	LHG	8	0
49	s1	621	LUT	6	0
40	D1	408	LHG	3	0
38	b	624	3PH	6	0
50	N	622	XAT	5	0
31	A1	411	BCR	4	0
50	G	622	XAT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	g1	620	LUT	9	0
29	b	603	CLA	5	0
48	r	606	CHL	2	0
52	R1	625	LMT	7	0
29	n	604	CLA	1	0
29	r	612	CLA	1	0
49	R1	620	LUT	4	0
33	A	413	LMG	3	0
29	g	610	CLA	3	0
33	c1	521	LMG	3	0
29	B	614	CLA	6	0
31	C	517	BCR	1	0
39	J1	101	DGA	4	0
29	C1	509	CLA	3	0
45	H	101	RRX	1	0
29	N	612	CLA	3	0
33	b	622	LMG	5	0
29	y1	614	CLA	6	0
40	g1	624	LHG	7	0
50	g1	622	XAT	6	0
29	Y	608	CLA	2	0
31	a1	411	BCR	4	0
31	D	404	BCR	3	0
29	g	604	CLA	1	0
51	S1	623	NEX	4	0
29	G1	611	CLA	6	0
49	s	620	LUT	3	0
29	S1	602	CLA	6	0
31	C	515	BCR	3	0
29	s1	609	CLA	6	0
29	C	508	CLA	3	0
29	G	612	CLA	1	0
51	Y1	623	NEX	3	0
29	a1	410	CLA	11	0
29	C1	505	CLA	4	0
29	R	602	CLA	4	0
29	c	507	CLA	6	0
54	S	625	LPX	4	0
33	C1	523	LMG	4	0
48	n1	608	CHL	5	0
29	b1	609	CLA	8	0
29	r1	609	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	N	614	CLA	1	0
48	N	607	CHL	3	0
48	s	608	CHL	5	0
49	g1	621	LUT	13	0
29	S	613	CLA	1	0
48	G	601	CHL	4	0
29	d1	403	CLA	4	0
37	C	519	DGD	9	0
29	R1	610	CLA	7	0
29	A	407	CLA	1	0
47	I1	102	4RF	9	0
48	Y1	609	CHL	7	0
48	y1	605	CHL	1	0
29	a1	405	CLA	9	0
49	Y	621	LUT	6	0
29	B	603	CLA	8	0
32	C	526	SQD	4	0
34	A	414	SPH	1	0
29	y	602	CLA	9	0
49	r	620	LUT	4	0
29	b1	608	CLA	4	0
48	y1	607	CHL	8	0
50	N1	622	XAT	9	0
29	s1	617	CLA	1	0
29	R	610	CLA	5	0
29	B1	610	CLA	5	0
37	C1	518	DGD	11	0
53	r1	626	ERG	5	0
48	g	605	CHL	1	0
32	b	626	SQD	2	0
29	R	609	CLA	3	0
49	S1	621	LUT	6	0
40	L	101	LHG	5	0
29	b	616	CLA	8	0
29	b1	617	CLA	7	0
29	g	614	CLA	2	0
48	g	607	CHL	2	0
37	B	623	DGD	3	0
32	b	621	SQD	5	0
33	c	523	LMG	8	0
48	g	608	CHL	1	0
29	a	407	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	N	601	CHL	4	0
29	c1	501	CLA	8	0
48	N1	606	CHL	7	0
34	a	414	SPH	3	0
37	C1	519	DGD	8	0
29	r	610	CLA	5	0
29	B1	605	CLA	4	0
48	Y	609	CHL	3	0
33	a1	413	LMG	8	0
29	s1	603	CLA	3	0
51	y1	623	NEX	2	0
29	y	610	CLA	1	0
29	s	603	CLA	2	0
29	G	613	CLA	2	0
40	S	624	LHG	5	0
29	d	403	CLA	3	0
40	l	101	LHG	4	0
29	C	510	CLA	2	0
48	G	607	CHL	6	0
48	r1	607	CHL	2	0
29	G1	602	CLA	8	0
29	c	512	CLA	1	0
51	g	623	NEX	1	0
31	d1	404	BCR	3	0
54	s	625	LPX	3	0
29	Y	611	CLA	3	0
55	Y	626	PTY	5	0
39	B1	625	DGA	1	0
31	d	404	BCR	3	0
48	r	607	CHL	1	0
33	D1	411	LMG	2	0
49	N	620	LUT	6	0
52	r	625	LMT	4	0
52	r1	625	LMT	2	0
49	y1	621	LUT	7	0
29	c	508	CLA	4	0
29	S1	611	CLA	4	0
29	n1	612	CLA	1	0
29	R	603	CLA	2	0
32	a1	412	SQD	3	0
39	j1	101	DGA	4	0
32	c1	526	SQD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	S	604	CLA	3	0
29	y1	612	CLA	6	0
29	C1	501	CLA	8	0
29	a1	407	CLA	3	0
29	B1	615	CLA	5	0
48	n	609	CHL	2	0
29	b1	602	CLA	2	0
26	A	401	OEX	1	0
29	c	501	CLA	5	0
38	T1	101	3PH	8	0
29	C1	510	CLA	2	0
33	H1	102	LMG	15	0
29	A	406	CLA	6	0
29	b	605	CLA	4	0
29	b1	611	CLA	7	0
33	h	102	LMG	5	0
38	t1	101	3PH	5	0
40	s1	624	LHG	7	0
29	G	614	CLA	1	0
38	s	626	3PH	6	0
29	c1	508	CLA	8	0
29	r	609	CLA	2	0
45	H1	101	RRX	3	0
29	y	603	CLA	3	0
48	Y1	605	CHL	2	0
40	n1	624	LHG	10	0
29	g	612	CLA	1	0
40	d1	410	LHG	7	0
48	g	606	CHL	3	0
55	Y1	626	PTY	3	0
47	K1	101	4RF	5	0
29	n	610	CLA	3	0
29	B	607	CLA	5	0
29	N	611	CLA	4	0
29	s	609	CLA	2	0
29	c	503	CLA	4	0
37	c1	519	DGD	9	0
29	r1	610	CLA	6	0
37	c	519	DGD	1	0
39	J	101	DGA	2	0
29	B1	603	CLA	13	0
29	c	509	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	613	CLA	6	0
29	c1	510	CLA	5	0
48	N	608	CHL	1	0
48	G1	606	CHL	1	0
29	Y1	613	CLA	4	0
49	r1	620	LUT	7	0
29	Y	613	CLA	9	0
33	D	411	LMG	2	0
29	C	503	CLA	2	0
29	y1	611	CLA	4	0
48	G1	605	CHL	1	0
47	I	102	4RF	2	0
51	r1	622	NEX	5	0
39	B	625	DGA	1	0
29	A	410	CLA	6	0
33	B1	622	LMG	5	0
29	B	611	CLA	2	0
31	C	516	BCR	2	0
48	Y1	606	CHL	4	0
48	n	601	CHL	2	0
29	B1	607	CLA	4	0
29	r1	608	CLA	3	0
29	s	613	CLA	2	0
32	B	626	SQD	4	0
48	N1	607	CHL	8	0
29	A1	406	CLA	4	0
29	B	616	CLA	7	0
29	Y	614	CLA	9	0
29	S1	603	CLA	1	0
48	Y	607	CHL	1	0
48	R1	606	CHL	2	0
29	r	608	CLA	4	0
29	A	405	CLA	4	0
49	R	620	LUT	6	0
29	A1	405	CLA	6	0
40	G1	624	LHG	6	0
29	Y1	608	CLA	5	0
48	s	606	CHL	3	0
49	s1	620	LUT	4	0
40	c	525	LHG	4	0
48	g	601	CHL	4	0
29	g	611	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	C	504	CLA	7	0
29	B1	617	CLA	7	0
49	s	621	LUT	1	0
29	g1	612	CLA	1	0
32	a	412	SQD	2	0
40	S1	624	LHG	5	0
29	B1	604	CLA	5	0
40	y	624	LHG	5	0
32	B1	626	SQD	3	0
29	a1	406	CLA	9	0
40	Y1	624	LHG	6	0
29	S	610	CLA	6	0
29	B1	616	CLA	11	0
48	R1	607	CHL	2	0
29	b1	606	CLA	8	0
50	r	621	XAT	2	0
30	A	408	PHO	5	0
29	B	604	CLA	4	0
29	n1	602	CLA	7	0
29	r1	602	CLA	4	0
29	C	509	CLA	3	0
33	w1	201	LMG	4	0
29	C1	507	CLA	8	0
48	g1	601	CHL	7	0
29	c1	505	CLA	9	0
48	G1	601	CHL	3	0
48	N1	605	CHL	4	0
29	G1	603	CLA	9	0
29	b1	615	CLA	3	0
29	r1	603	CLA	2	0
43	d1	405	PL9	8	0
48	G	609	CHL	4	0
29	b	606	CLA	5	0
51	R1	622	NEX	4	0
48	Y	605	CHL	2	0
37	c	518	DGD	7	0
31	B1	618	BCR	2	0
29	B	610	CLA	7	0
29	B1	613	CLA	3	0
29	y1	613	CLA	5	0
48	n	607	CHL	7	0
48	g1	607	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	R1	612	CLA	2	0
31	c	514	BCR	3	0
33	W1	201	LMG	8	0
29	b1	613	CLA	6	0
48	Y1	601	CHL	4	0
29	Y1	603	CLA	5	0
29	C	513	CLA	10	0
37	C	518	DGD	4	0
48	G	606	CHL	2	0
51	n	623	NEX	3	0
29	G	611	CLA	3	0
38	B	624	3PH	7	0
53	R	626	ERG	7	0
31	c1	516	BCR	7	0
31	b	618	BCR	5	0
31	c	516	BCR	5	0
45	h1	101	RRX	4	0
31	b1	619	BCR	4	0
32	m1	101	SQD	3	0
44	f	101	HEM	1	0
49	n1	621	LUT	10	0
29	B	605	CLA	5	0
29	y1	603	CLA	6	0
30	a	409	PHO	2	0
29	N	610	CLA	4	0
37	C1	520	DGD	12	0
29	c	513	CLA	3	0
51	Y	623	NEX	2	0
49	y	621	LUT	3	0
48	G1	607	CHL	6	0
31	c	515	BCR	3	0
29	c1	503	CLA	5	0
33	h1	102	LMG	4	0
29	g	603	CLA	4	0
29	y	604	CLA	1	0
50	R1	621	XAT	5	0
29	C1	513	CLA	14	0
50	G1	622	XAT	10	0
29	Y1	602	CLA	10	0
30	A	409	PHO	6	0
40	y1	624	LHG	6	0
39	C1	524	DGA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	s	610	CLA	5	0
30	a	408	PHO	5	0
33	b1	622	LMG	5	0
49	N1	621	LUT	7	0
51	s1	623	NEX	6	0
29	g1	604	CLA	3	0
31	C1	514	BCR	9	0
29	b	612	CLA	2	0
29	G1	604	CLA	3	0
31	B1	619	BCR	1	0
37	b1	623	DGD	4	0
29	b1	607	CLA	5	0
32	B	621	SQD	2	0
33	c1	523	LMG	4	0
29	g1	614	CLA	1	0
29	B1	611	CLA	6	0
47	k	101	4RF	2	0
50	r1	621	XAT	5	0
47	K	101	4RF	2	0
29	R	608	CLA	4	0
29	s	604	CLA	2	0
29	N1	612	CLA	3	0
29	B1	602	CLA	5	0
29	N1	611	CLA	3	0
48	n	606	CHL	6	0
29	n1	604	CLA	6	0
29	s	614	CLA	1	0
29	C1	508	CLA	7	0
48	s	607	CHL	2	0
50	n1	622	XAT	5	0
30	a1	409	PHO	11	0
29	C	512	CLA	3	0
44	f1	101	HEM	3	0
51	r	622	NEX	3	0
29	b1	604	CLA	9	0
29	C	511	CLA	1	0
29	r1	604	CLA	1	0
32	b1	626	SQD	4	0
29	Y	602	CLA	15	0
31	C1	516	BCR	3	0
49	Y1	621	LUT	8	0
48	n1	607	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	Y1	620	LUT	6	0
29	b1	616	CLA	3	0
33	A1	413	LMG	10	0
29	S	603	CLA	3	0
34	A1	414	SPH	4	0
29	N	602	CLA	6	0
29	Y1	611	CLA	8	0
29	s1	612	CLA	1	0
29	y	608	CLA	3	0
29	s	612	CLA	2	0
37	c	520	DGD	2	0
40	c1	525	LHG	11	0
48	S1	608	CHL	5	0
48	s1	606	CHL	2	0
29	s1	611	CLA	7	0
50	g	622	XAT	9	0
34	a1	414	SPH	1	0
29	g1	613	CLA	7	0
29	G1	610	CLA	2	0
29	b	607	CLA	4	0
29	d1	402	CLA	9	0
29	y1	602	CLA	17	0
43	D1	405	PL9	11	0
34	y	625	SPH	4	0
48	G	605	CHL	1	0
31	D1	404	BCR	4	0
49	G1	620	LUT	6	0
40	L1	101	LHG	6	0
29	N	613	CLA	4	0
29	g1	610	CLA	4	0
29	g	613	CLA	2	0
29	n	612	CLA	1	0
29	C1	512	CLA	8	0
29	Y1	610	CLA	4	0
31	C1	517	BCR	5	0
29	R1	608	CLA	2	0
33	d	411	LMG	2	0
39	j	101	DGA	3	0
29	C1	511	CLA	7	0
52	R	625	LMT	4	0
29	R	612	CLA	1	0
29	D1	402	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	D1	410	LHG	4	0
29	S1	604	CLA	3	0
48	R	606	CHL	2	0
29	C	506	CLA	7	0
48	S	606	CHL	3	0
31	c1	514	BCR	9	0
29	b	604	CLA	3	0
29	n1	610	CLA	4	0
29	b1	610	CLA	9	0
29	c	502	CLA	3	0
39	b	625	DGA	5	0
29	R1	609	CLA	4	0
29	Y1	604	CLA	7	0
29	a	406	CLA	5	0
53	r	626	ERG	7	0
39	C	524	DGA	3	0
29	s1	604	CLA	3	0
31	a	411	BCR	3	0
38	t	101	3PH	2	0
40	D	410	LHG	2	0
48	g1	609	CHL	4	0
51	n1	623	NEX	6	0
47	i	101	4RF	6	0
29	B1	609	CLA	9	0
30	a1	408	PHO	9	0
29	s	611	CLA	6	0
49	y1	620	LUT	6	0
33	a	413	LMG	5	0
39	b1	625	DGA	4	0
29	B1	606	CLA	5	0
31	c1	517	BCR	8	0
38	B1	624	3PH	6	0
49	n1	620	LUT	4	0
53	R1	626	ERG	9	0
29	c1	509	CLA	4	0
40	D	409	LHG	6	0
48	S	607	CHL	1	0
38	b1	624	3PH	8	0
48	y1	609	CHL	6	0
29	G	603	CLA	3	0
48	s1	601	CHL	4	0
54	S1	625	LPX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	606	CLA	8	0
40	N	624	LHG	4	0
48	g1	606	CHL	2	0
29	b1	605	CLA	9	0
48	y1	606	CHL	1	0
29	g1	611	CLA	3	0
29	B	602	CLA	2	0
40	g	624	LHG	7	0
48	g1	605	CHL	2	0
29	a	405	CLA	3	0
29	r	603	CLA	3	0
33	c	521	LMG	4	0
48	g	609	CHL	4	0
49	S	620	LUT	2	0
29	y	612	CLA	5	0
29	N1	613	CLA	10	0
48	n1	601	CHL	6	0
40	d	410	LHG	3	0
40	s	624	LHG	4	0
48	y	605	CHL	1	0
31	B	618	BCR	3	0
51	N	623	NEX	3	0
51	R	622	NEX	2	0
48	n1	609	CHL	4	0
33	C1	521	LMG	9	0
45	h	101	RRX	3	0
29	y1	610	CLA	7	0
48	s1	608	CHL	5	0
40	Y	624	LHG	6	0
29	N	603	CLA	4	0
29	b	617	CLA	5	0
48	S	601	CHL	2	0
29	N	604	CLA	2	0
33	C	523	LMG	4	0
29	B	612	CLA	8	0
38	S	626	3PH	7	0
29	C	501	CLA	8	0
34	Y1	625	SPH	7	0
29	c1	512	CLA	5	0
29	C1	502	CLA	2	0
48	n1	606	CHL	7	0
29	c1	506	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	517	BCR	1	0
49	y	620	LUT	2	0
48	R	607	CHL	2	0
48	n	605	CHL	4	0
29	y1	604	CLA	2	0
29	r1	612	CLA	3	0
29	b	608	CLA	7	0
29	r	602	CLA	2	0
48	G	608	CHL	2	0
48	y	606	CHL	2	0
55	y1	626	PTY	9	0
29	y	611	CLA	6	0
29	S1	610	CLA	6	0
33	d1	411	LMG	2	0
48	Y	601	CHL	1	0
29	b	613	CLA	4	0
29	Y	603	CLA	4	0
40	N1	624	LHG	5	0
32	A	412	SQD	5	0
49	N	621	LUT	2	0
40	D	408	LHG	3	0
29	g	602	CLA	6	0
32	M1	101	SQD	4	0
26	a1	401	OEX	1	0
29	B1	612	CLA	9	0
49	g	621	LUT	9	0
32	m	101	SQD	6	0
29	b	610	CLA	6	0
29	c1	507	CLA	8	0
37	b	623	DGD	3	0
50	R	621	XAT	4	0
30	A1	409	PHO	8	0
32	b1	621	SQD	4	0
40	d1	409	LHG	6	0
34	Y	625	SPH	4	0
50	Y1	622	XAT	4	0
51	N1	623	NEX	6	0
48	N1	601	CHL	8	0
49	G1	621	LUT	10	0
48	r1	606	CHL	4	0
29	N1	603	CLA	7	0
29	n1	603	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	C	520	DGD	2	0
29	n	603	CLA	5	0
29	b	615	CLA	6	0
29	Y1	612	CLA	6	0
29	g1	602	CLA	12	0
29	y1	608	CLA	2	0
48	N	609	CHL	5	0
29	Y	612	CLA	2	0
55	y	626	PTY	9	0
40	G	624	LHG	4	0
29	r	604	CLA	1	0
48	S1	606	CHL	4	0
38	T	101	3PH	2	0
29	S1	609	CLA	2	0
29	D1	403	CLA	2	0
29	B	613	CLA	5	0
29	b1	603	CLA	3	0
39	c	524	DGA	9	0
47	k1	101	4RF	2	0
31	c1	515	BCR	7	0
29	G	610	CLA	6	0
29	n	613	CLA	8	0
48	y	601	CHL	1	0
29	C1	506	CLA	5	0
50	y	622	XAT	4	0
49	G	620	LUT	6	0
50	Y	622	XAT	6	0
29	d	402	CLA	5	0
32	B1	621	SQD	3	0
33	H	102	LMG	2	0
29	b	611	CLA	5	0
29	G	602	CLA	8	0
29	y	614	CLA	7	0
48	y	607	CHL	3	0
48	Y1	607	CHL	4	0
48	G1	609	CHL	6	0
29	C1	503	CLA	2	0
31	A	411	BCR	2	0
40	d	409	LHG	7	0
44	F1	101	HEM	3	0
29	B	615	CLA	2	0
29	C	502	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	c1	518	DGD	11	0
29	N1	602	CLA	8	0
44	F	101	HEM	3	0
48	N1	609	CHL	9	0
54	s1	625	LPX	3	0
29	c1	504	CLA	4	0
50	n	622	XAT	6	0
29	S	617	CLA	1	0
29	A1	410	CLA	7	0
30	A1	408	PHO	5	0
29	c	504	CLA	4	0
40	d1	408	LHG	4	0
29	c	511	CLA	4	0
29	b	614	CLA	4	0
34	y1	625	SPH	2	0
29	s1	613	CLA	4	0
29	S	609	CLA	3	0
29	n1	614	CLA	1	0
32	A1	412	SQD	6	0
29	R1	603	CLA	6	0
49	S1	620	LUT	7	0
48	S1	601	CHL	2	0
31	b1	618	BCR	2	0
29	D	402	CLA	6	0
31	C1	515	BCR	5	0
49	G	621	LUT	7	0
43	d	405	PL9	7	0
29	C1	504	CLA	6	0
37	c1	520	DGD	6	0
33	C	521	LMG	3	0
29	N1	610	CLA	8	0
29	c1	513	CLA	8	0
29	G1	614	CLA	3	0
29	B	609	CLA	8	0
29	Y	610	CLA	4	0
29	b1	612	CLA	6	0
38	S1	626	3PH	4	0
42	D1	401	BCT	1	0
49	N1	620	LUT	5	0
29	G	604	CLA	2	0
49	n	620	LUT	3	0
49	S	621	LUT	5	0

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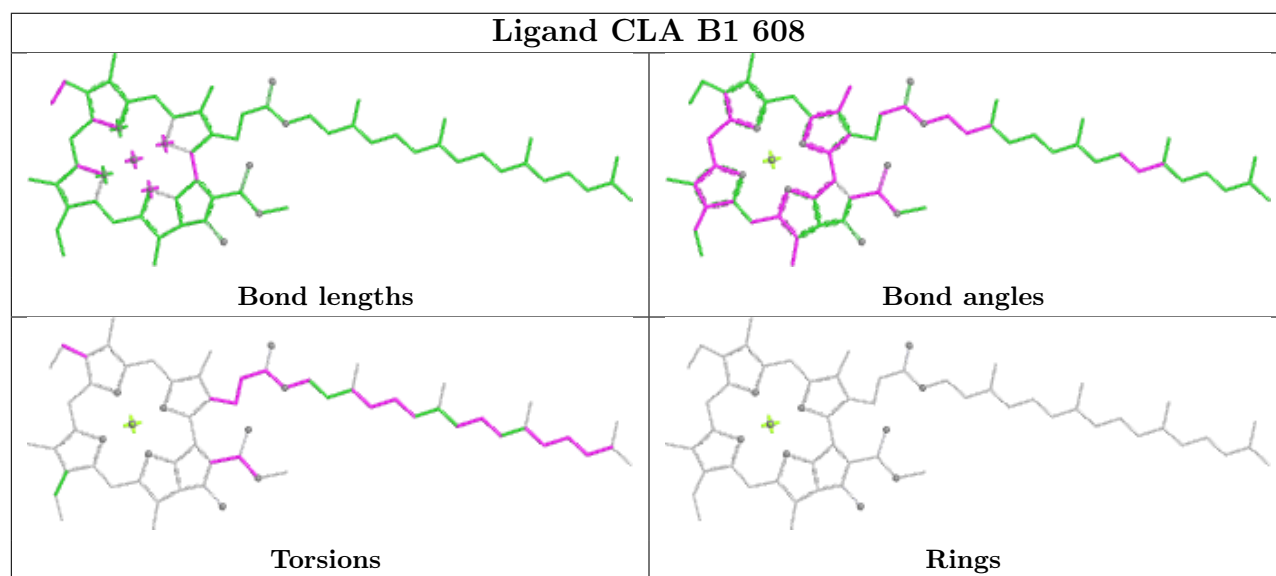
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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29	b	602	CLA	1	0
51	y	623	NEX	1	0
29	B1	614	CLA	8	0
50	y1	622	XAT	9	0
29	g1	603	CLA	8	0
48	N1	608	CHL	4	0
29	Y	604	CLA	4	0
40	D1	409	LHG	5	0
40	d	408	LHG	2	0
48	n1	605	CHL	3	0
29	S	602	CLA	3	0
29	s1	610	CLA	6	0
40	n	624	LHG	3	0
29	B	617	CLA	5	0
32	M	101	SQD	4	0
29	b1	614	CLA	7	0
48	N	606	CHL	3	0
51	s	623	NEX	3	0
29	a	410	CLA	6	0
29	c	505	CLA	5	0
48	N	605	CHL	3	0
29	s	602	CLA	1	0
31	C	514	BCR	10	0
29	S1	614	CLA	1	0
29	C	507	CLA	4	0
43	D	405	PL9	4	0
48	S1	607	CHL	1	0
29	G1	613	CLA	6	0
33	W	201	LMG	2	0
29	Y1	614	CLA	3	0
29	C	505	CLA	6	0
29	R1	604	CLA	2	0
29	c	506	CLA	6	0
29	n	602	CLA	4	0
38	s1	626	3PH	5	0
40	C	525	LHG	7	0
29	N1	604	CLA	5	0
48	y	609	CHL	2	0
49	n	621	LUT	2	0
31	b	619	BCR	1	0
29	n1	611	CLA	2	0

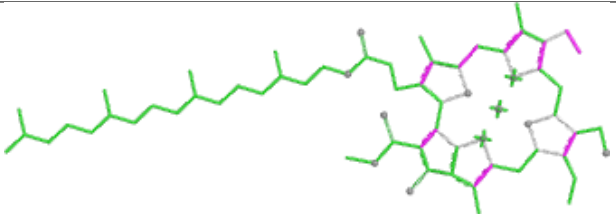
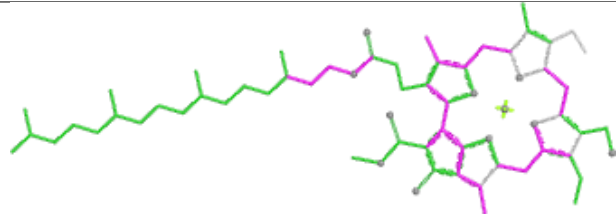
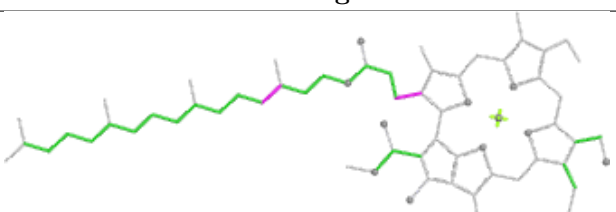
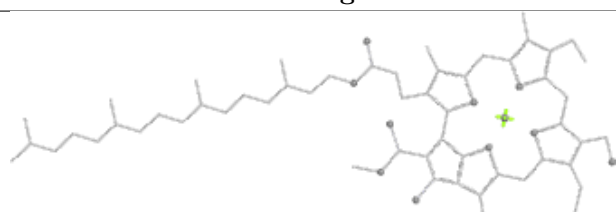
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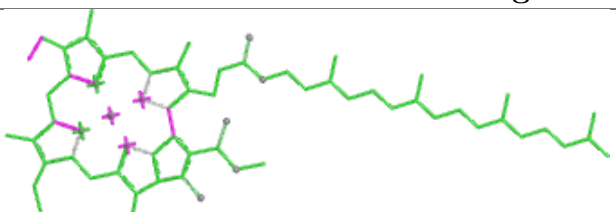
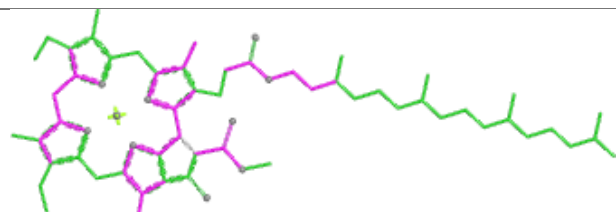
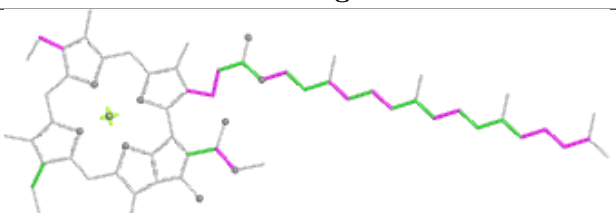
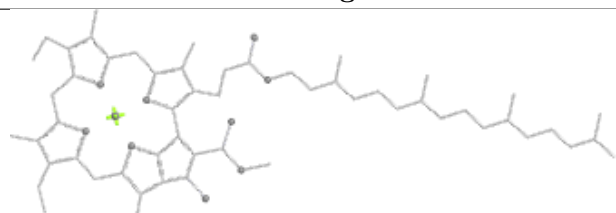
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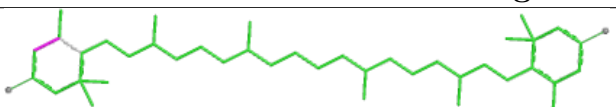
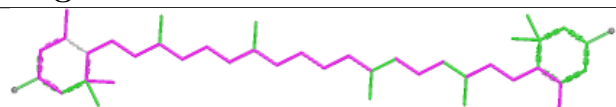
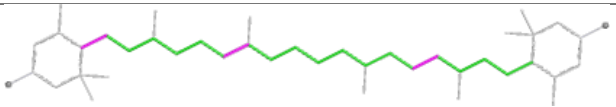
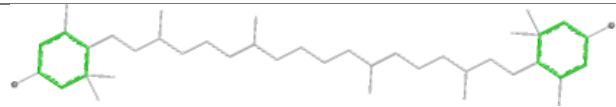
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c1	511	CLA	9	0
32	C1	526	SQD	3	0

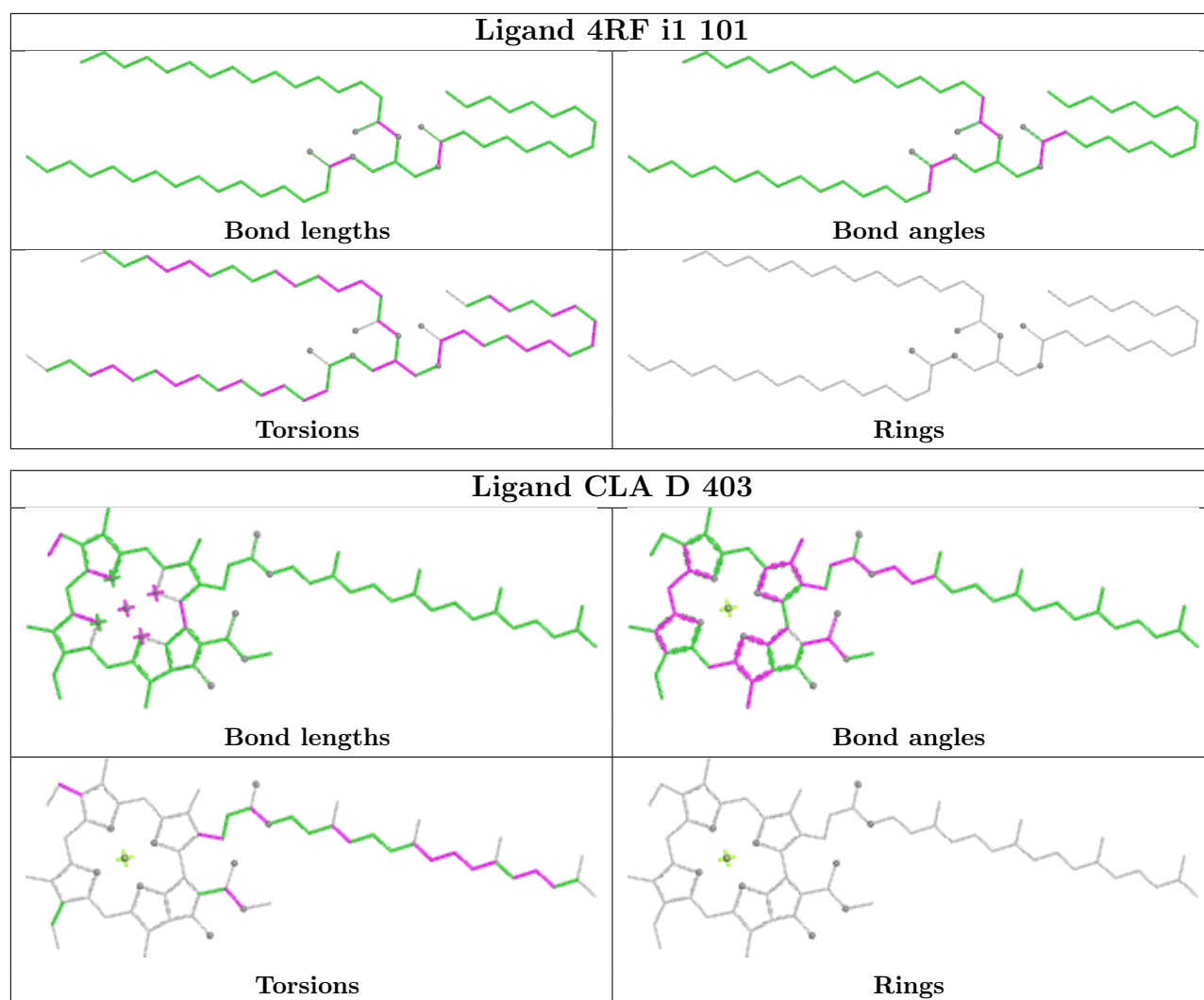
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

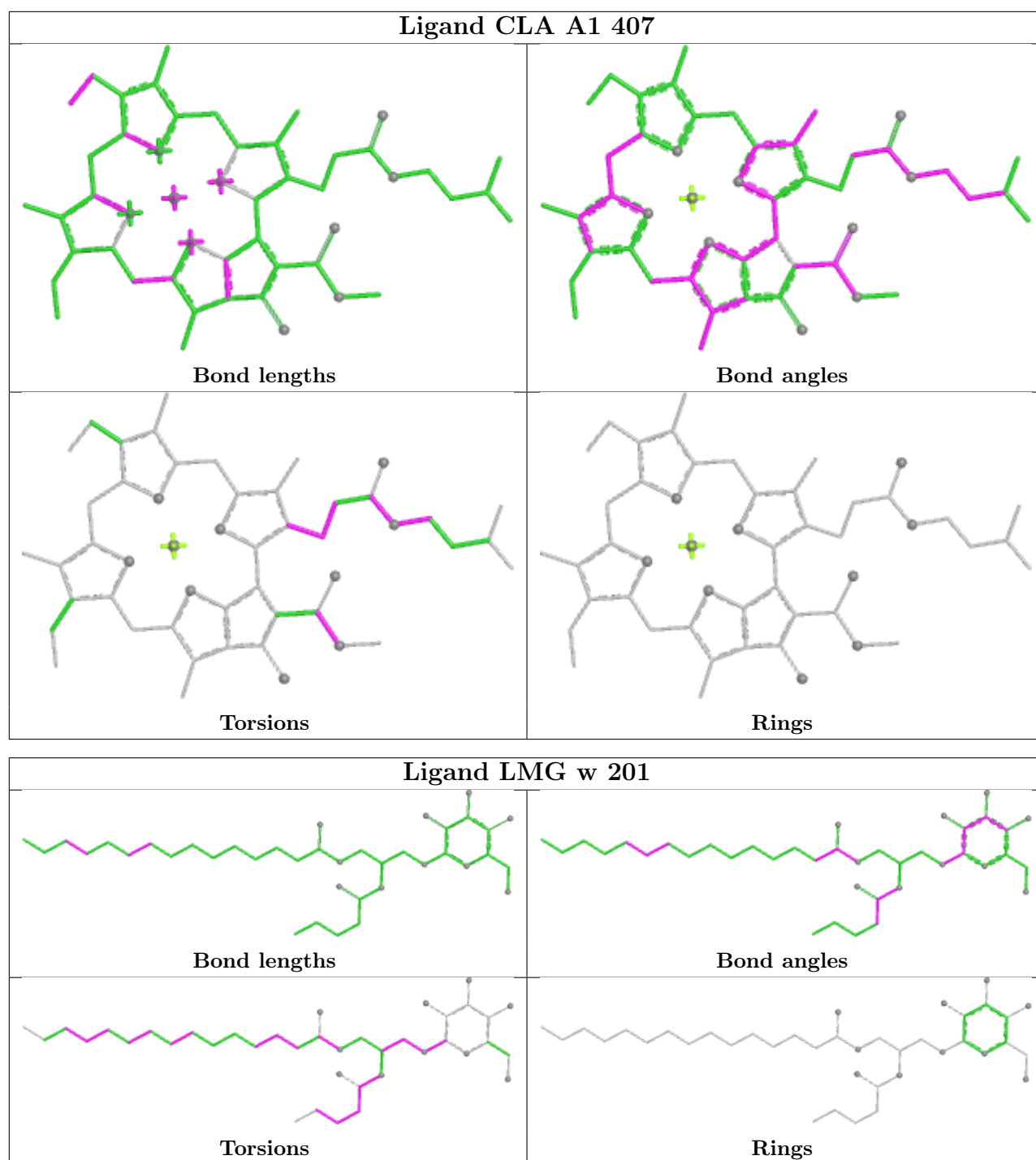


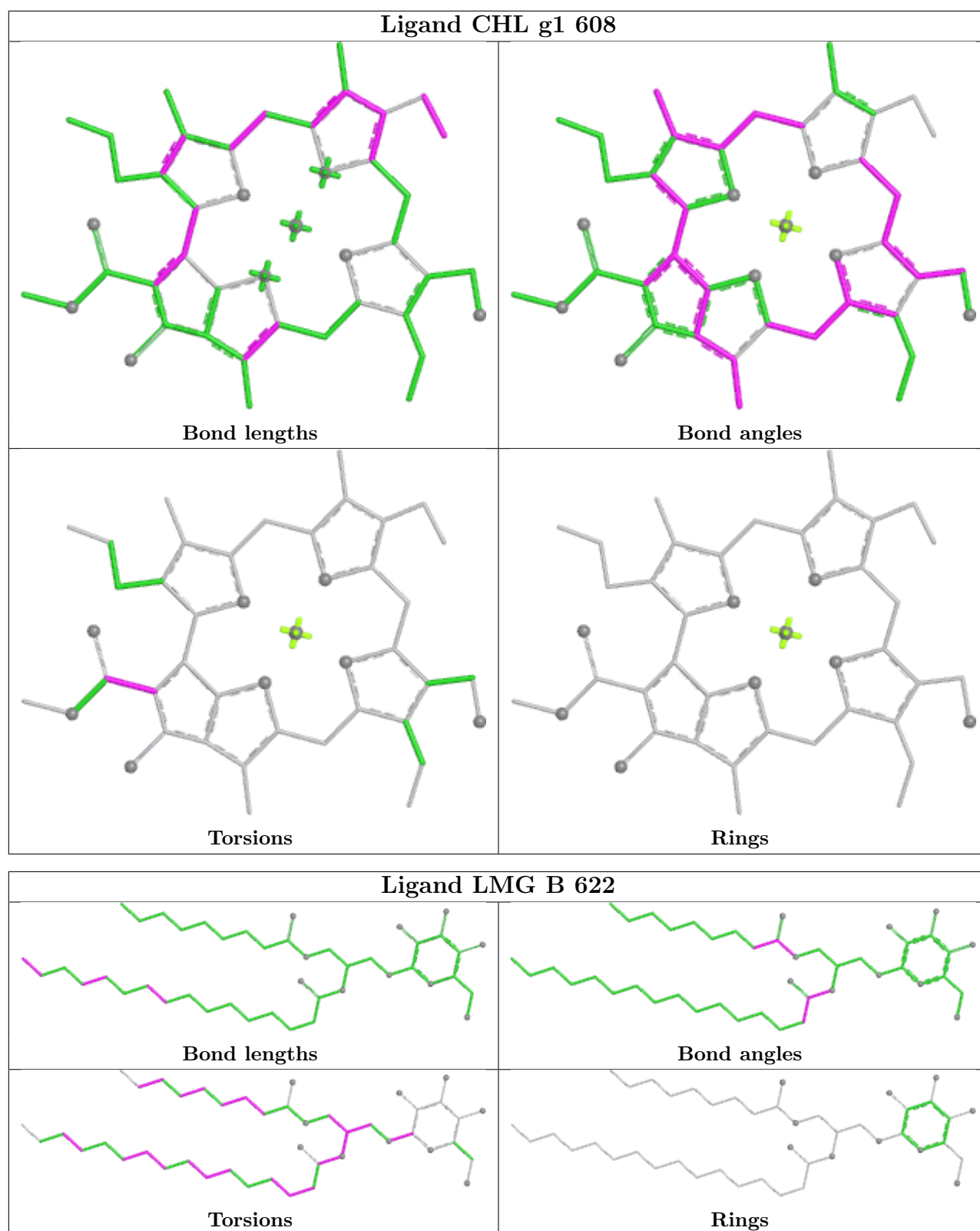
Ligand CHL y1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

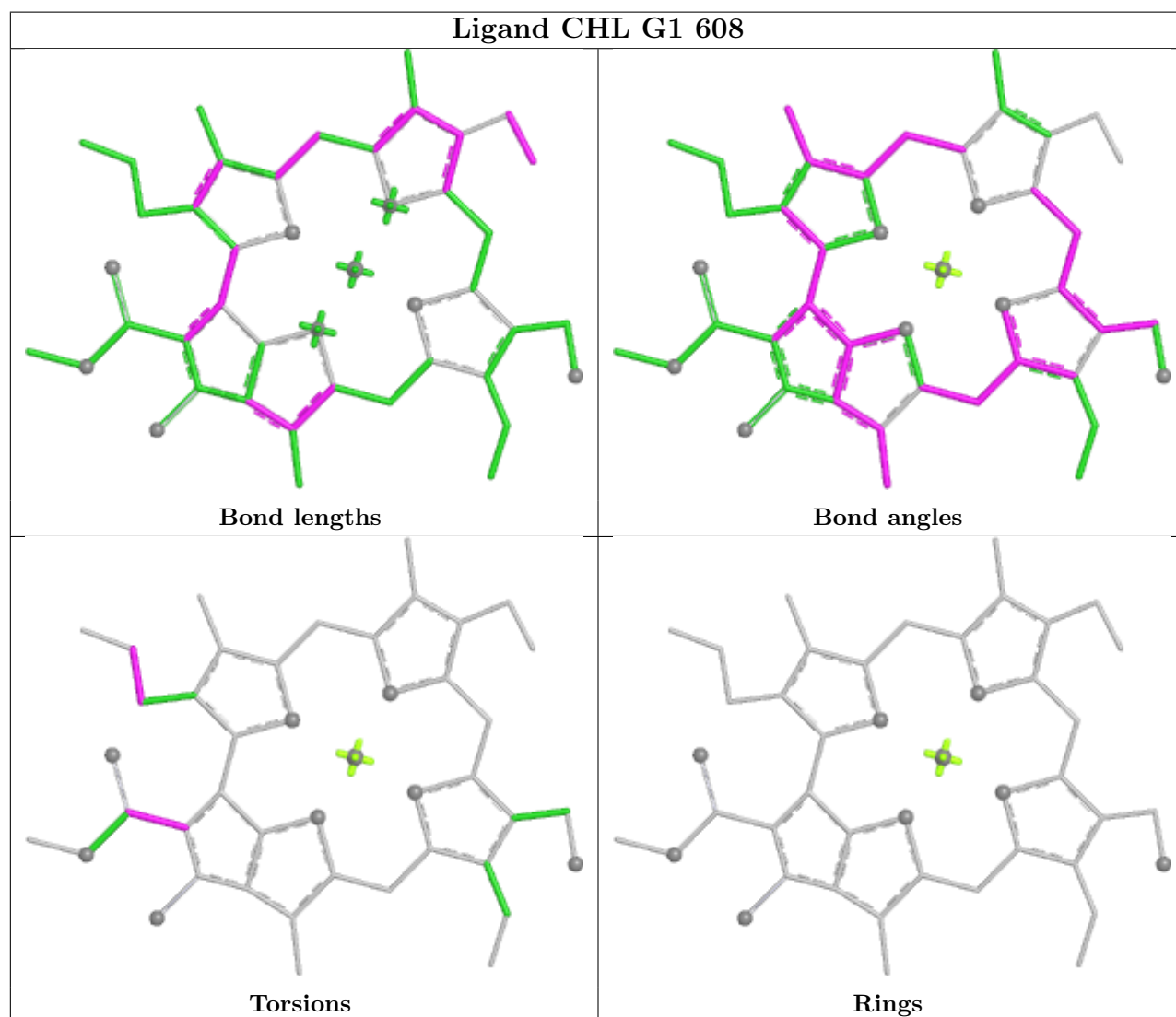
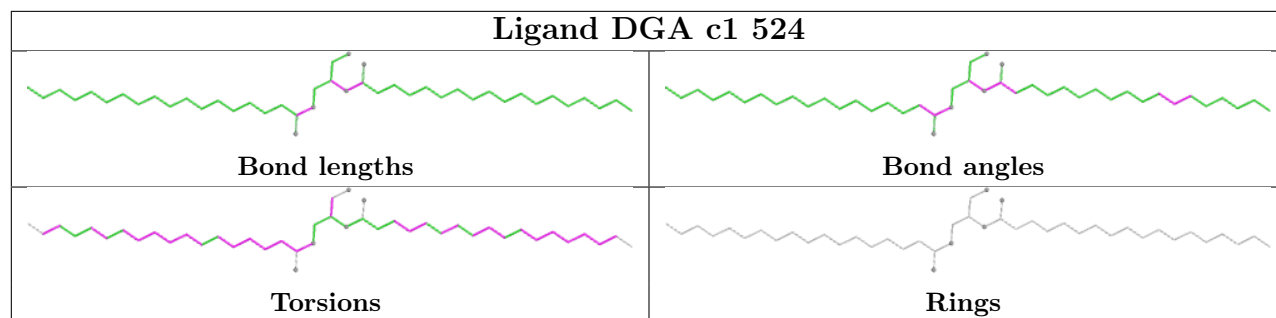
Ligand CLA S 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

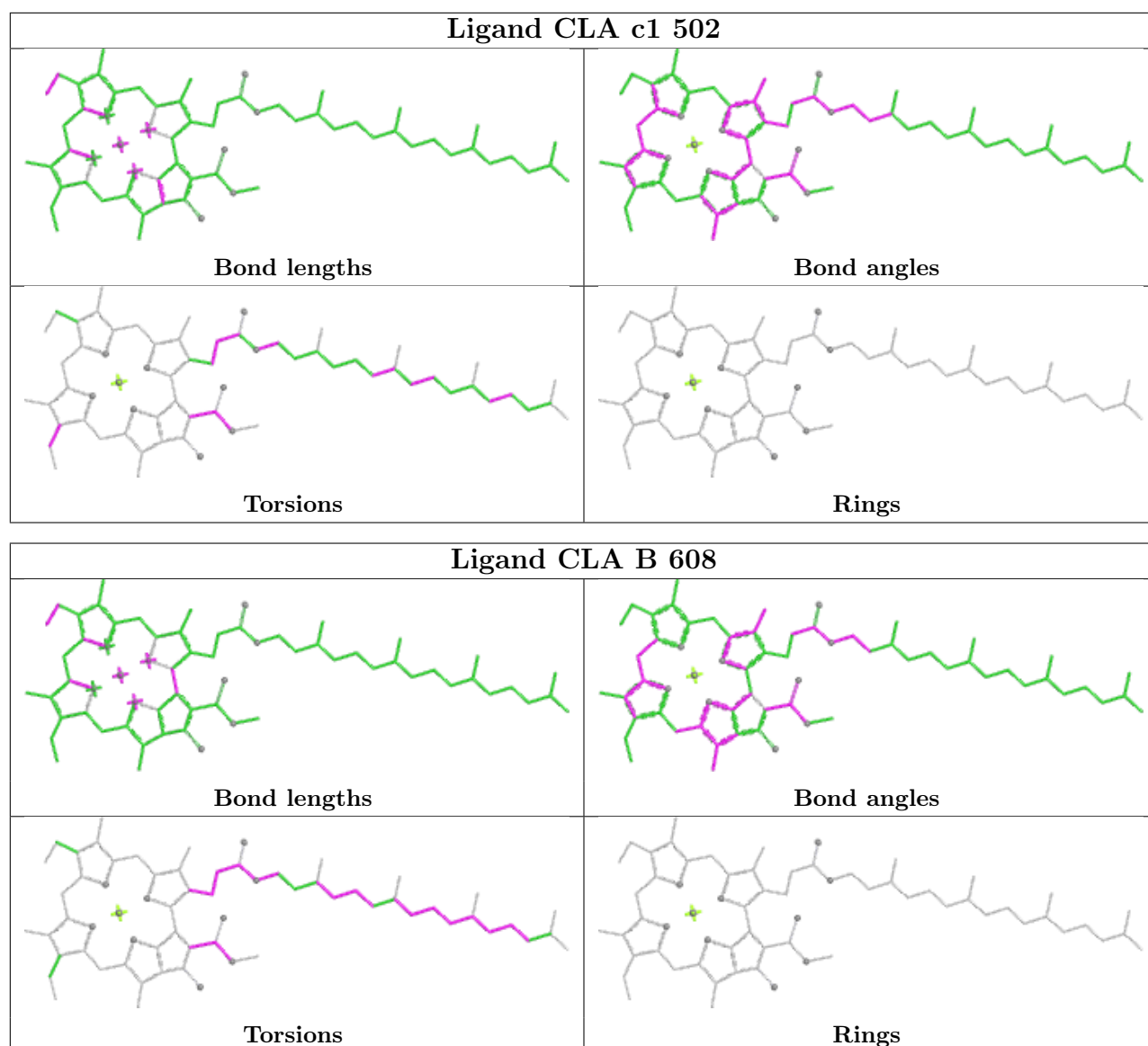
Ligand LUT g 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

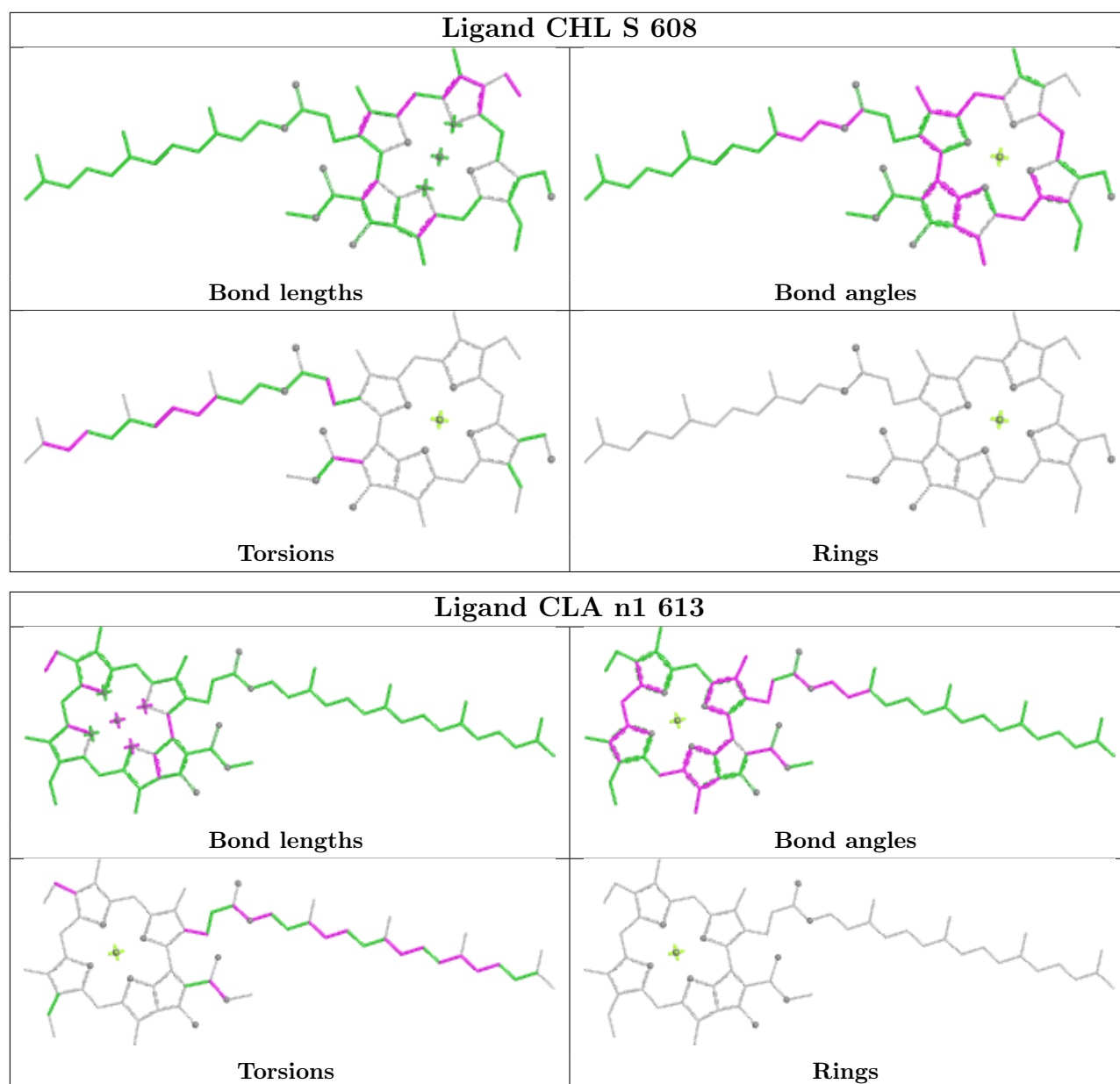


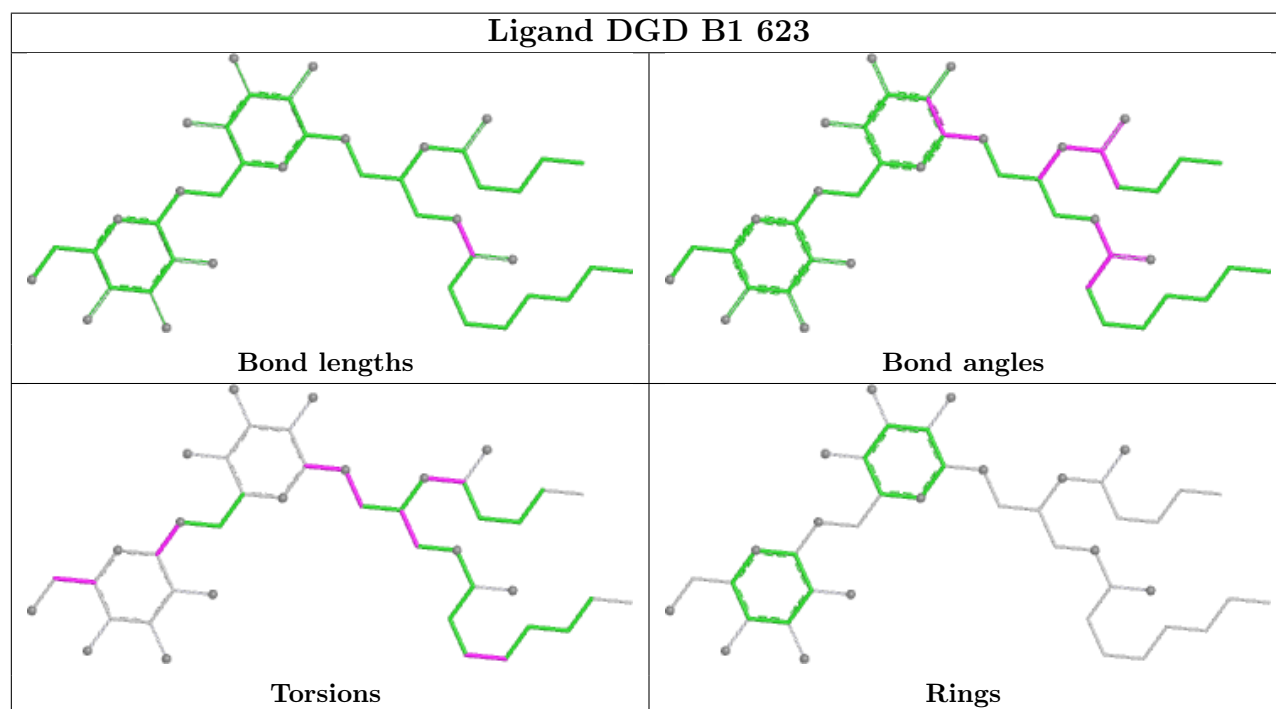
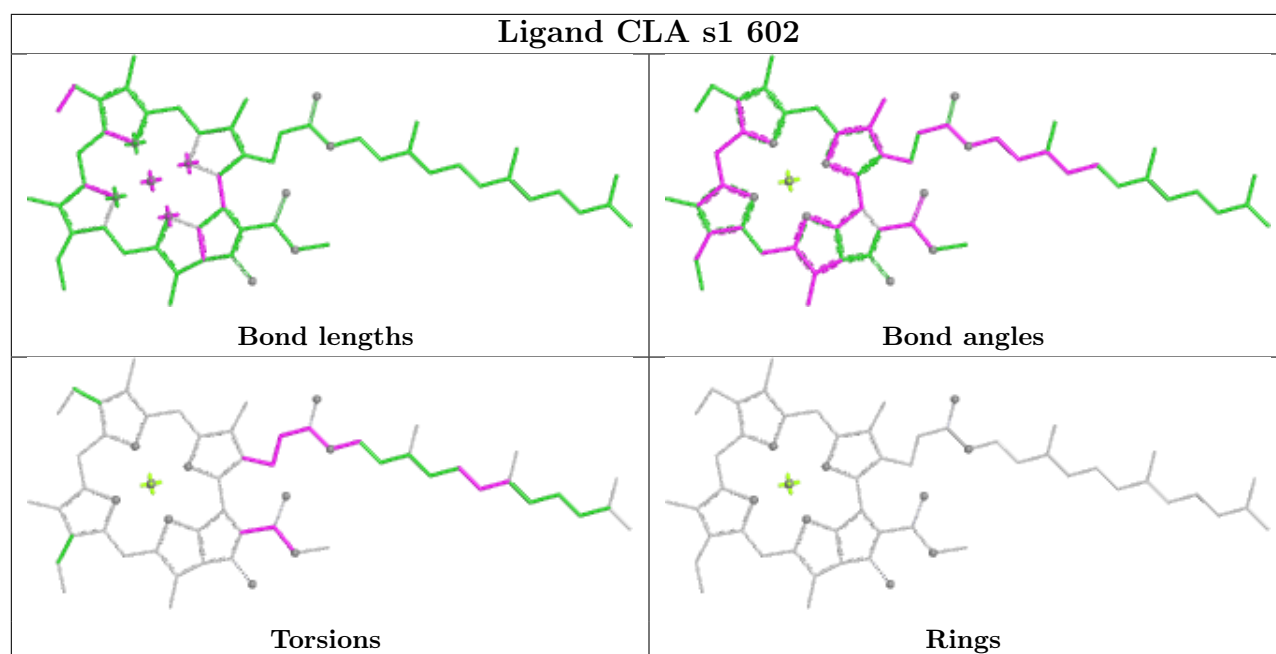


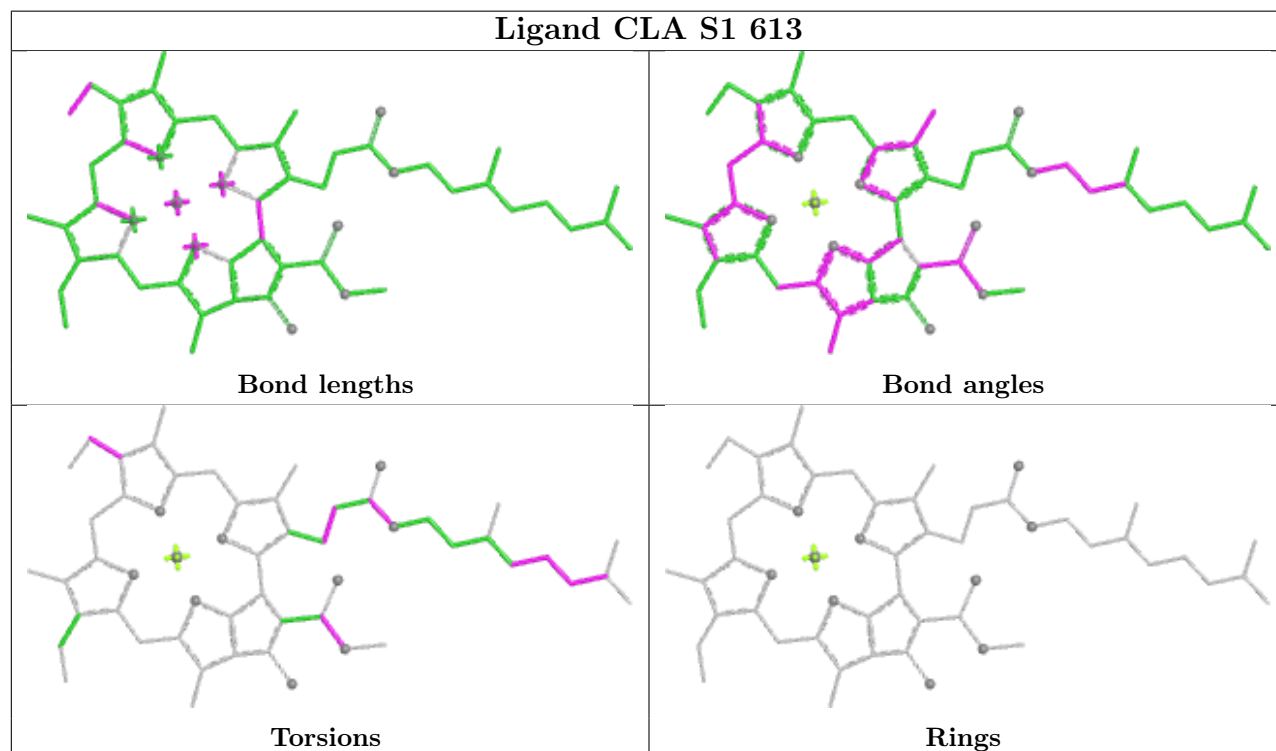
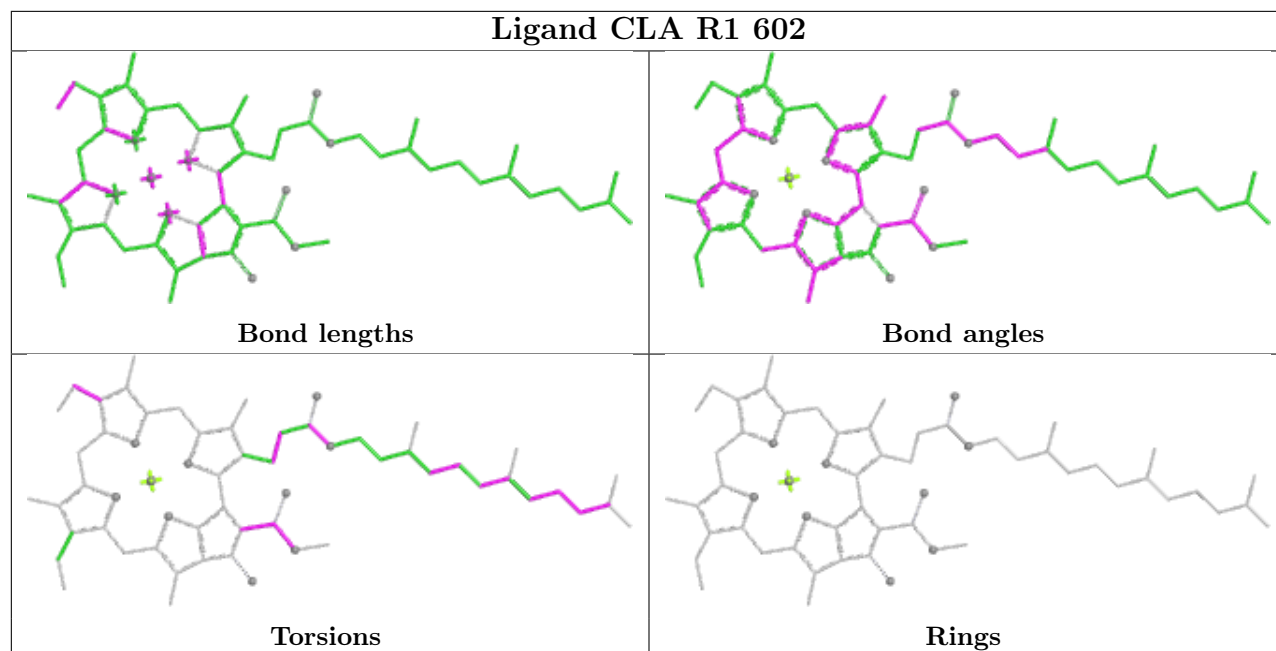


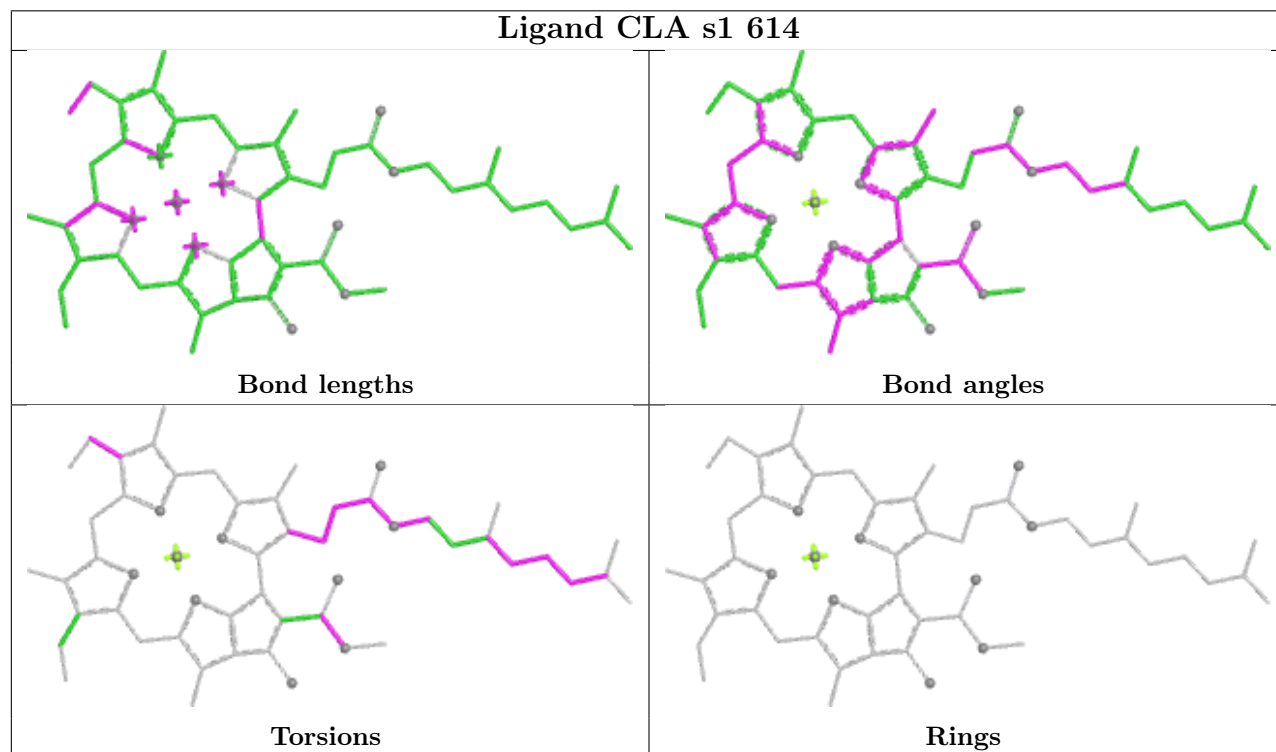
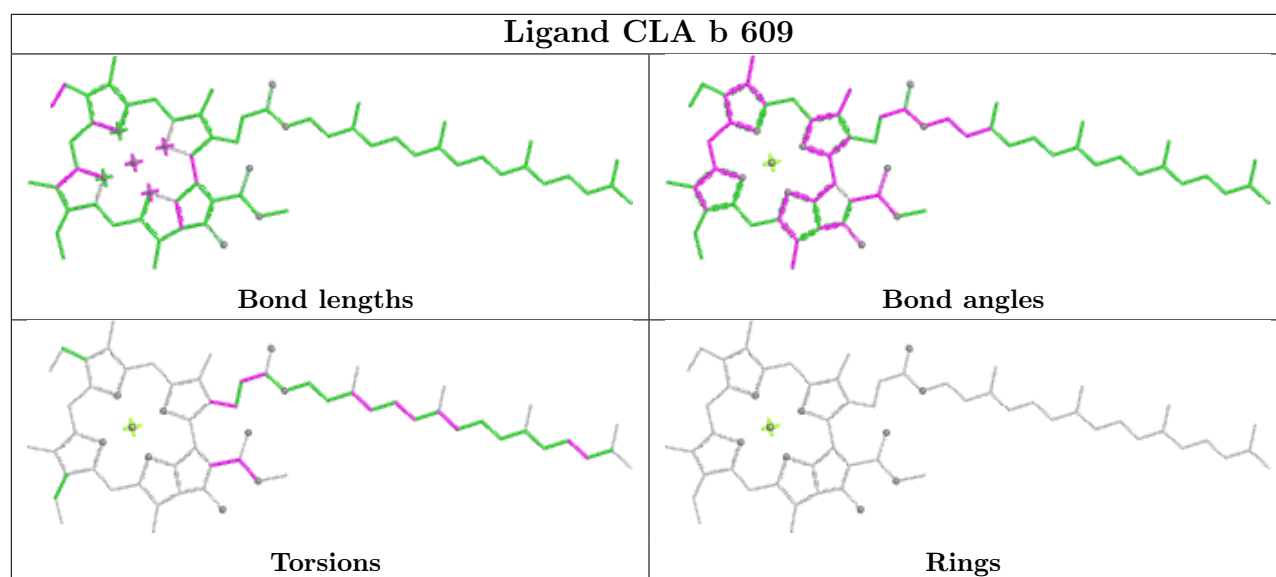


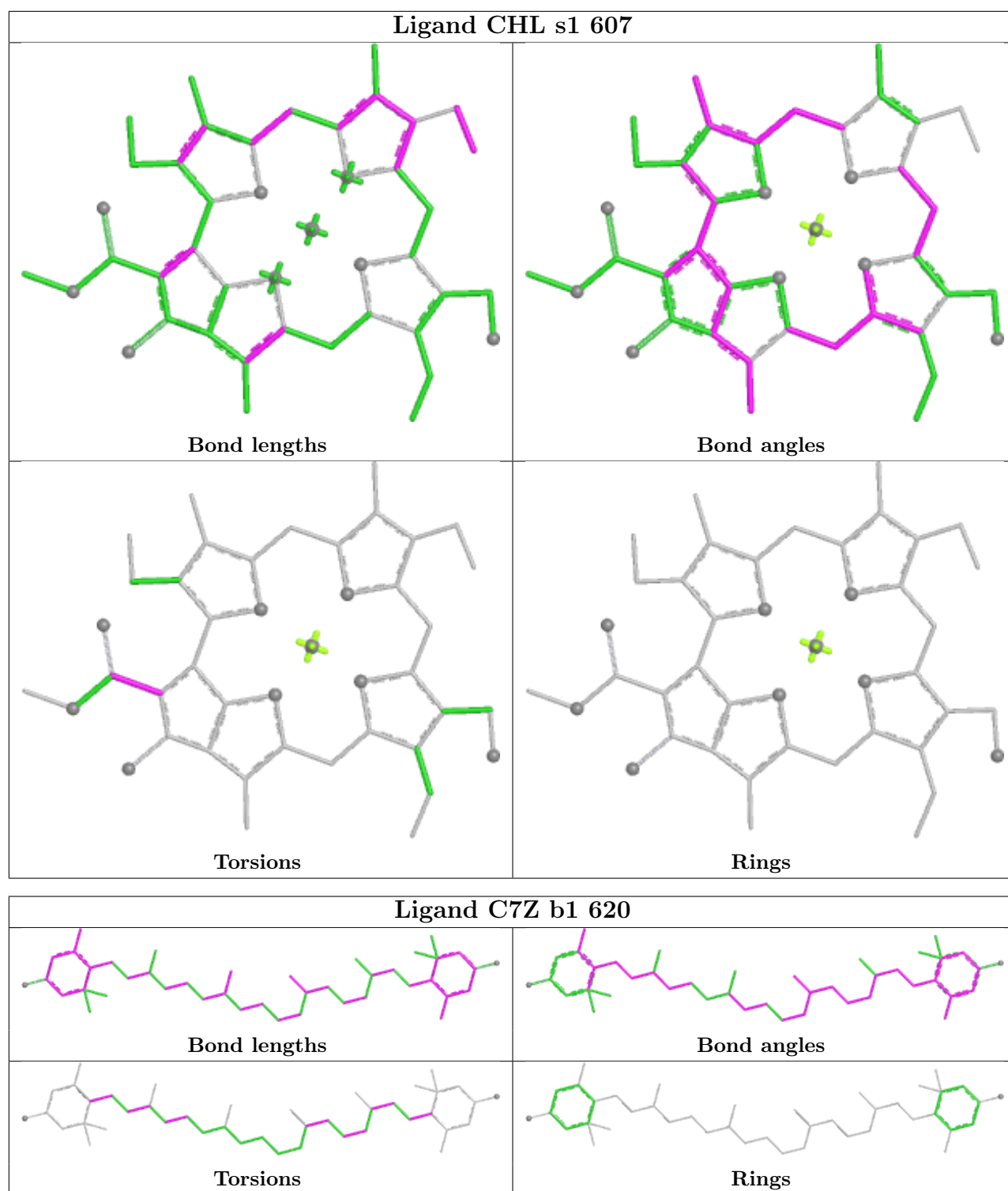


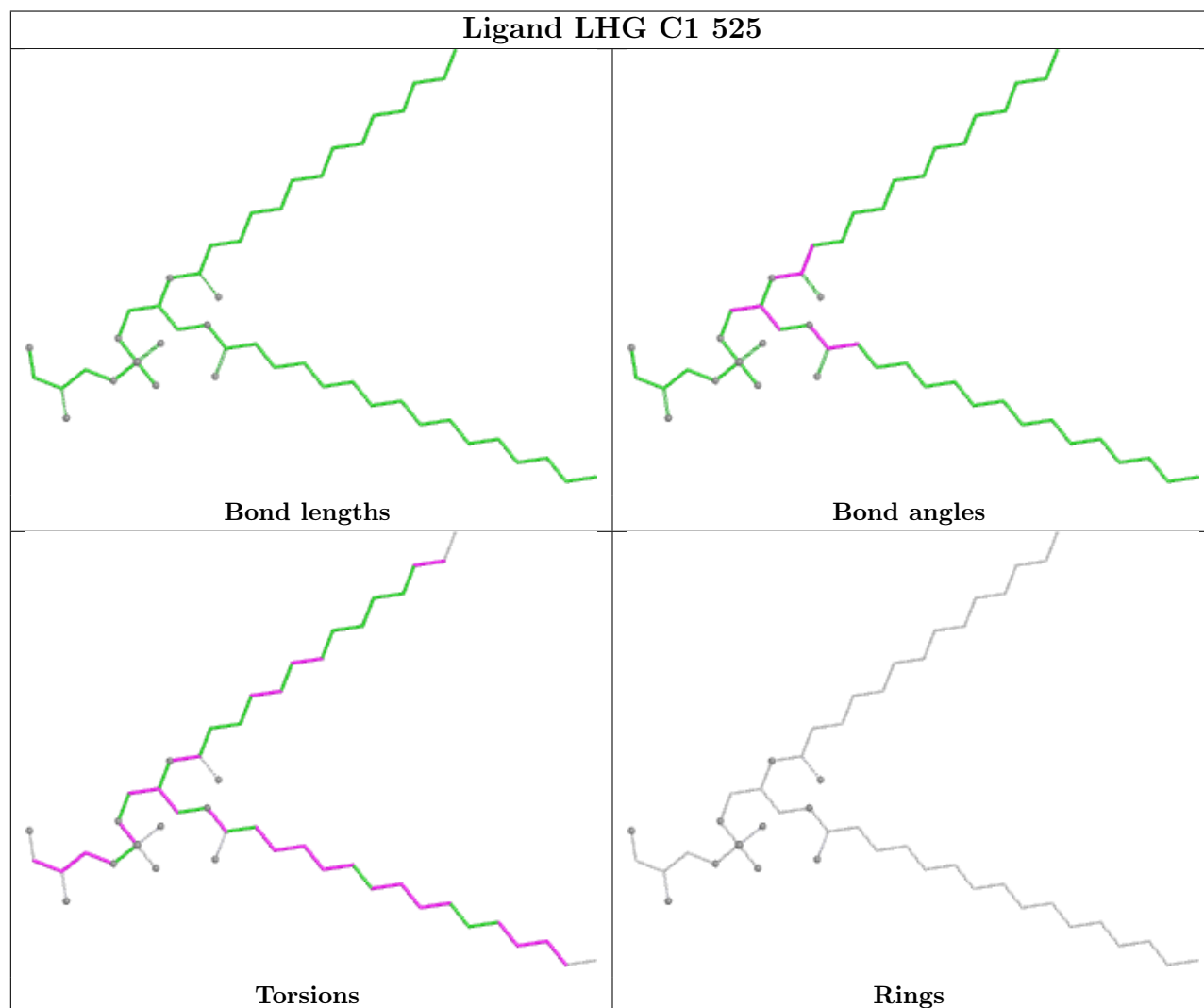
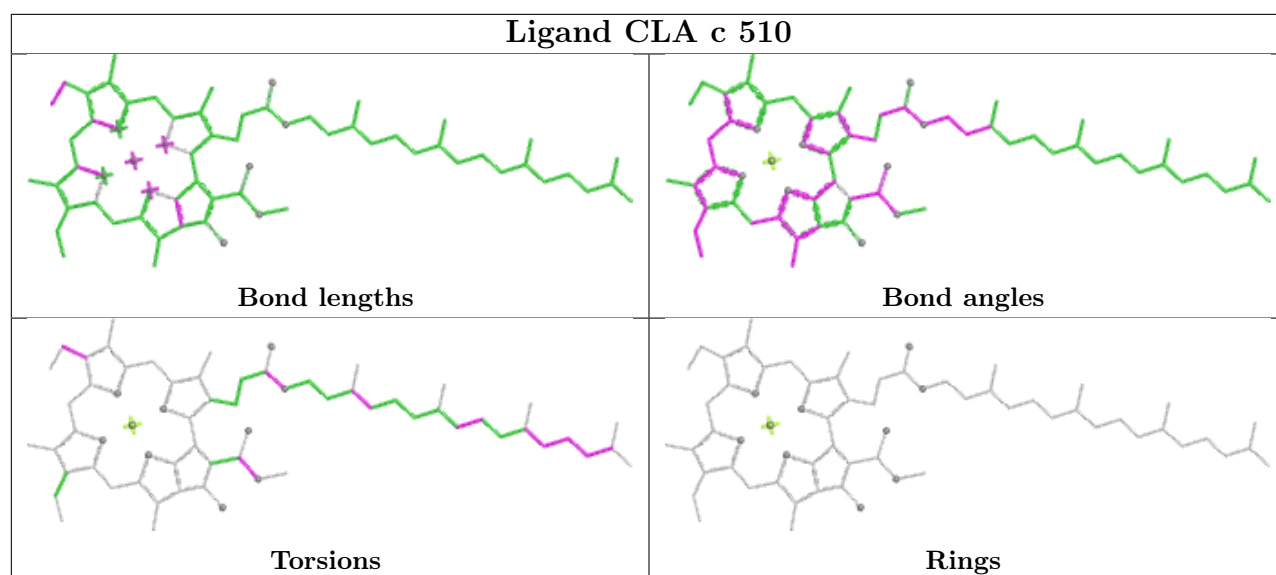


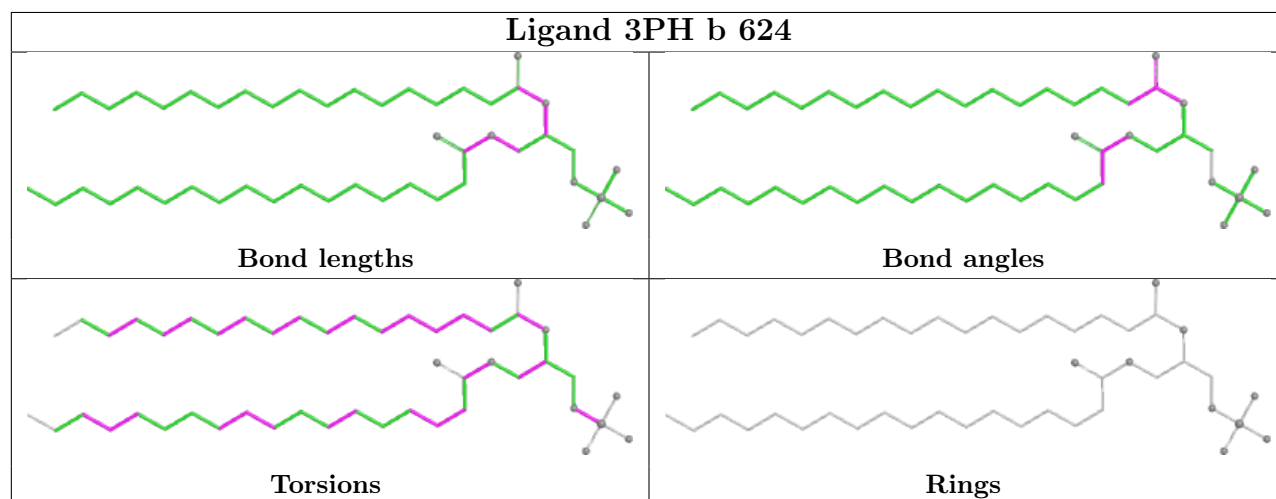
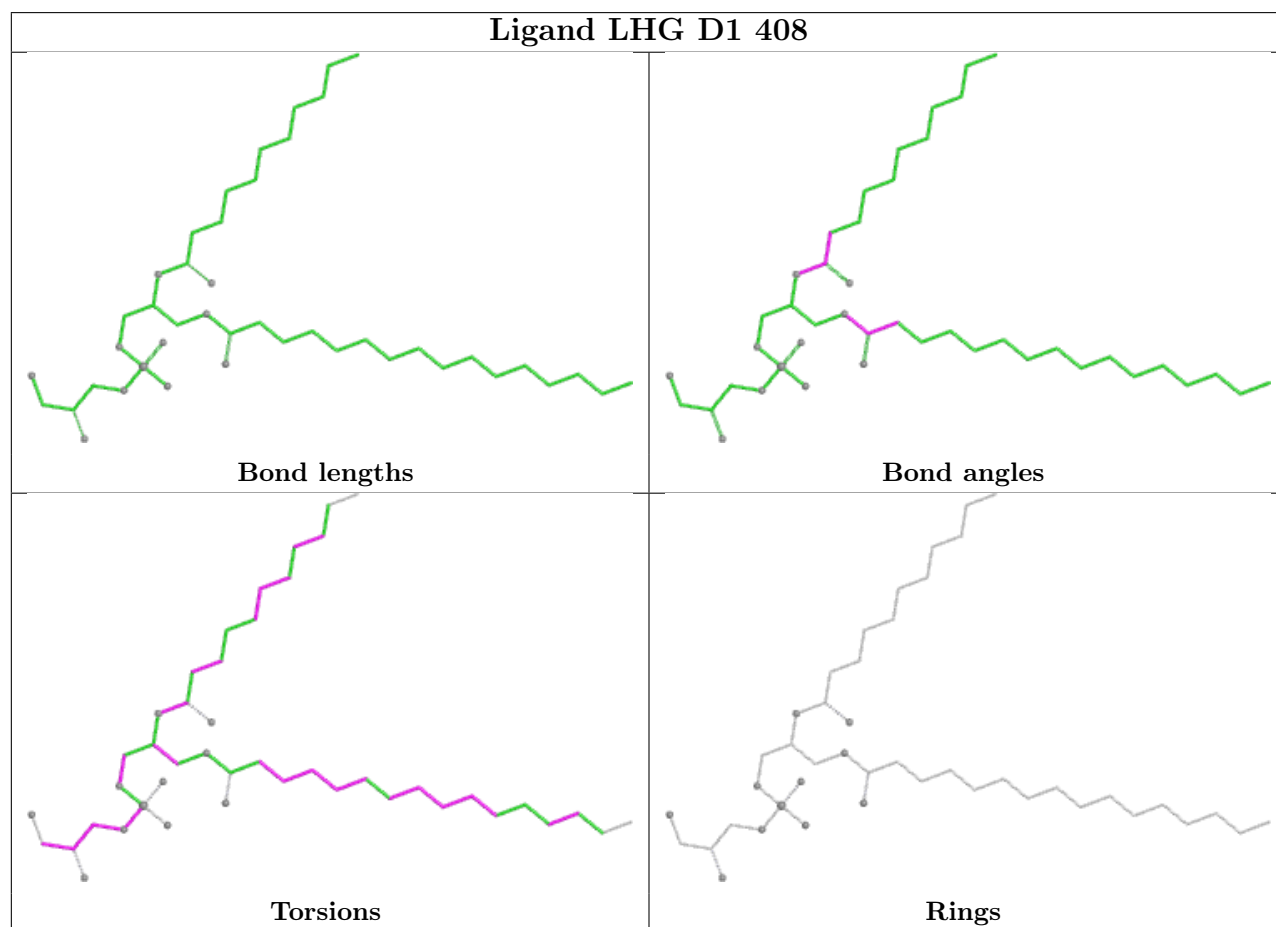
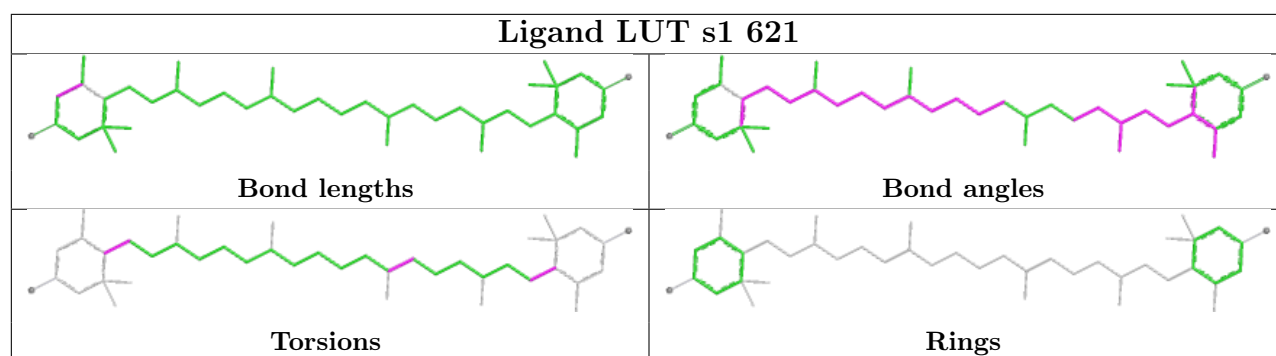


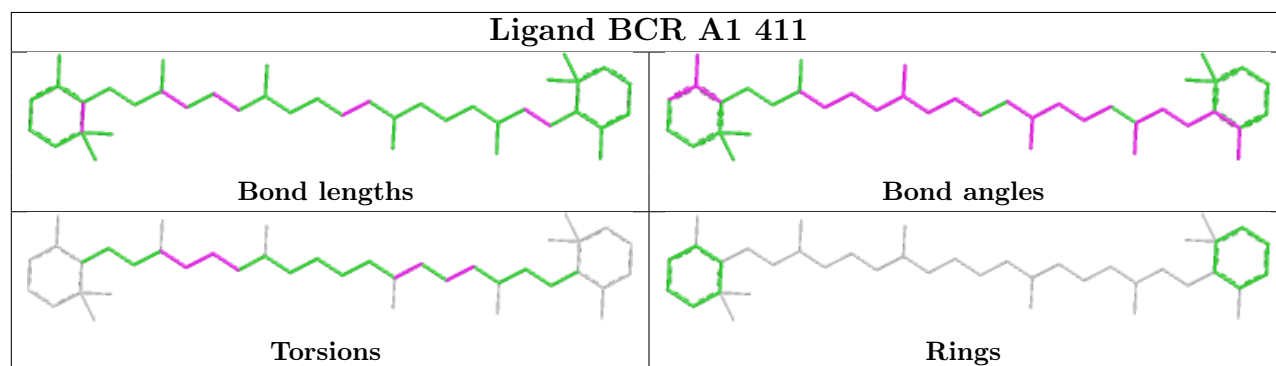
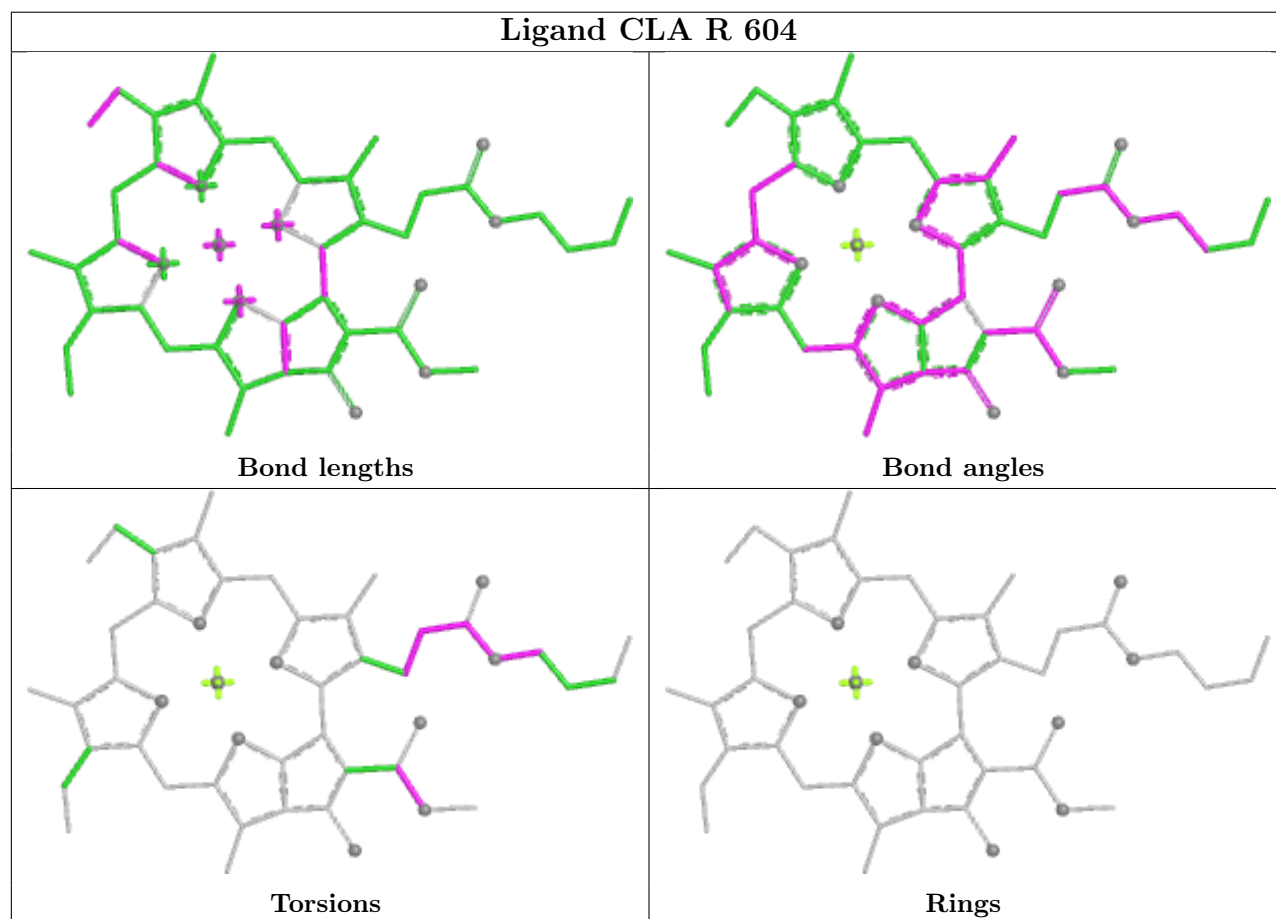
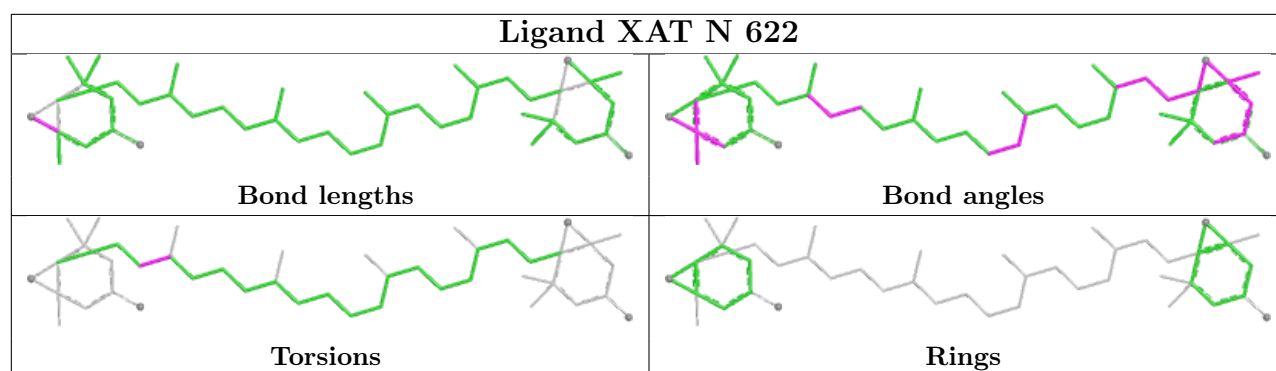


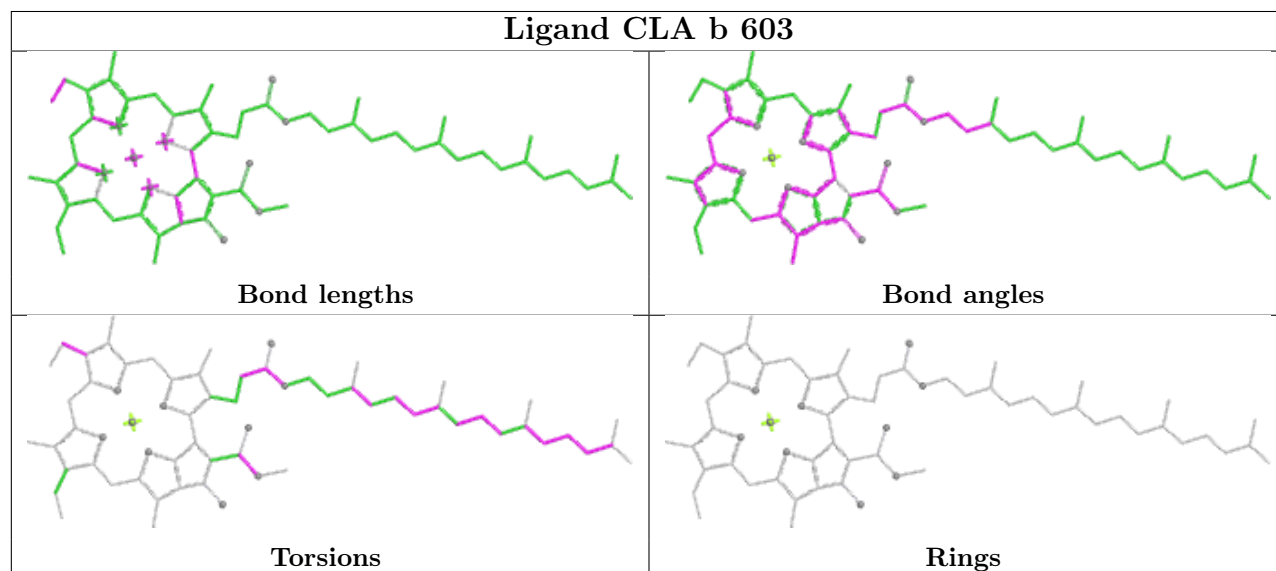
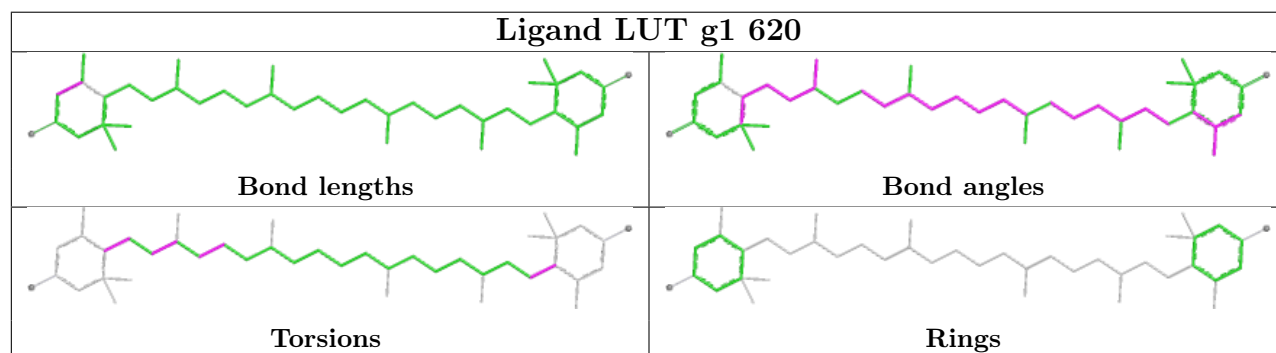
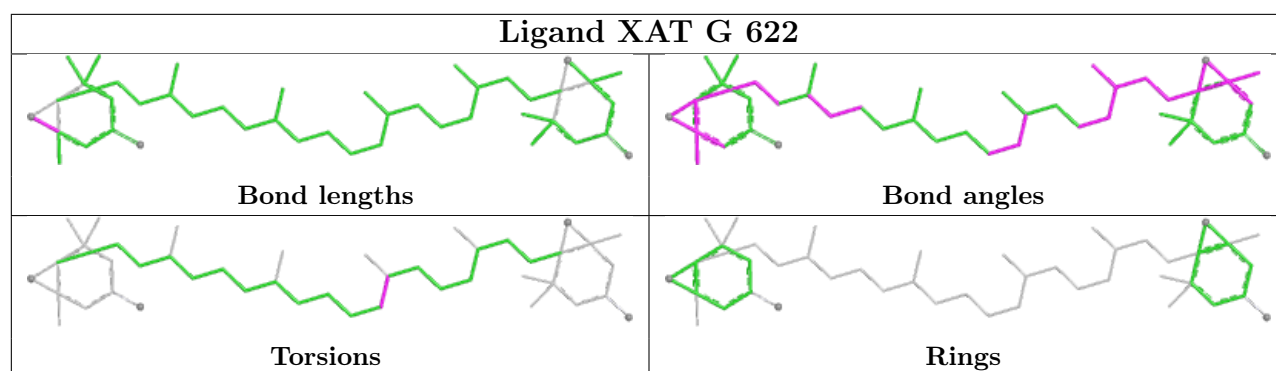


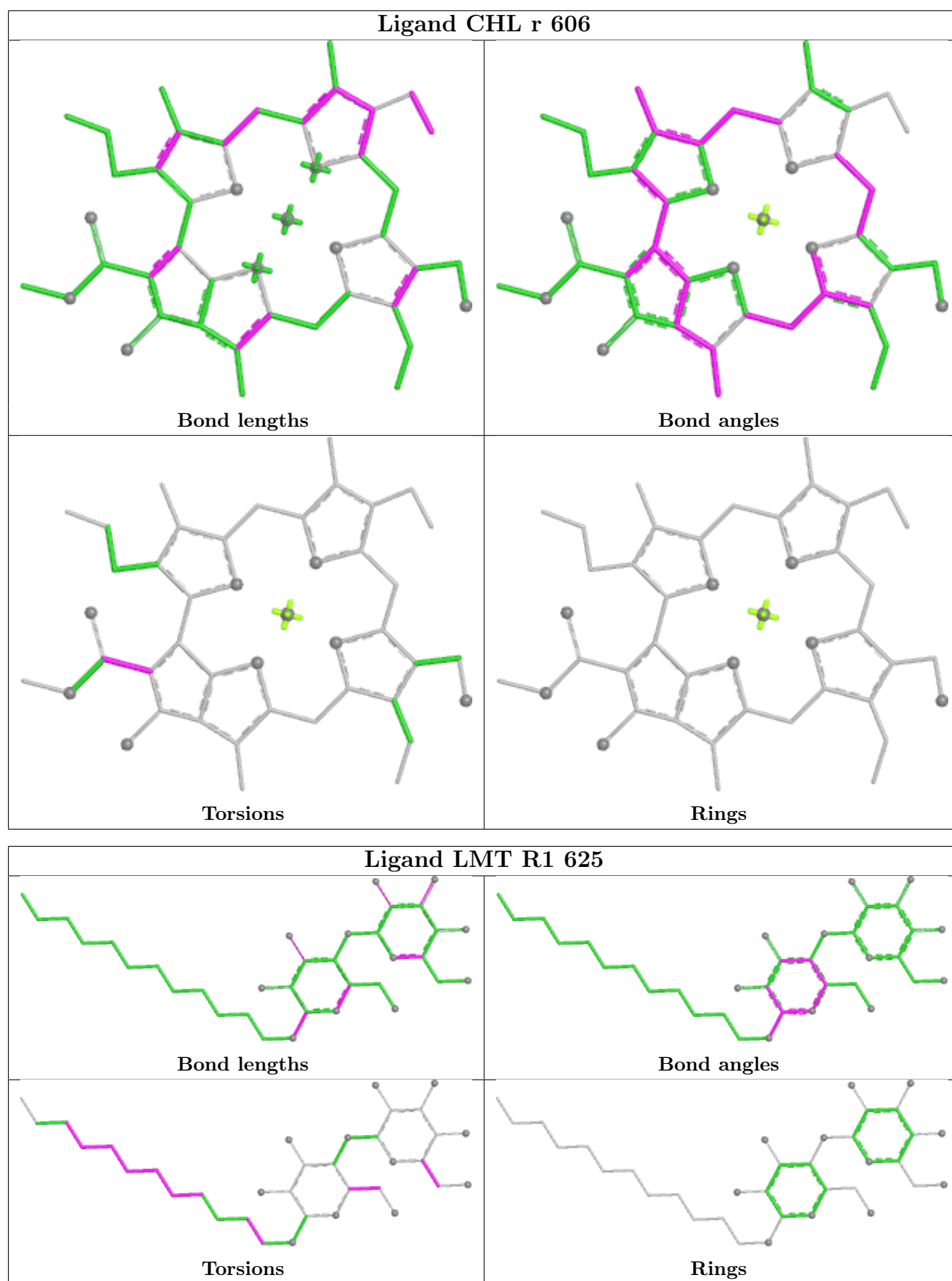


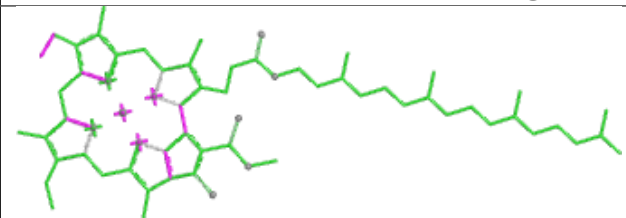
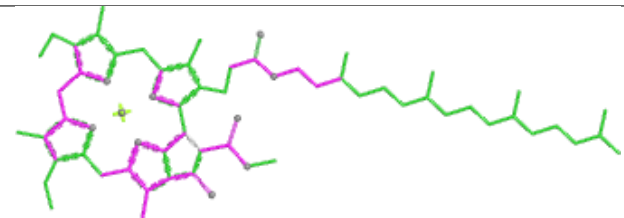
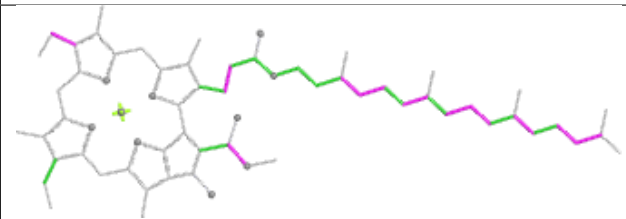
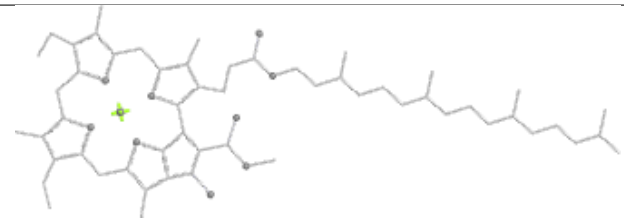


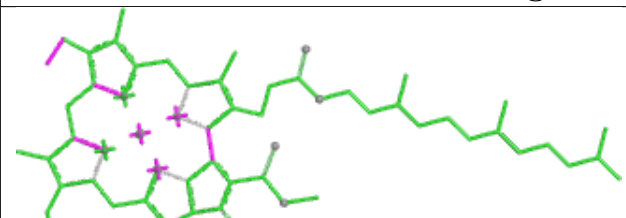
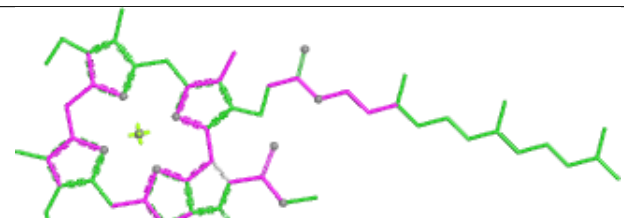
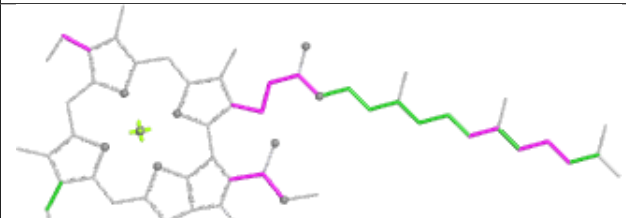
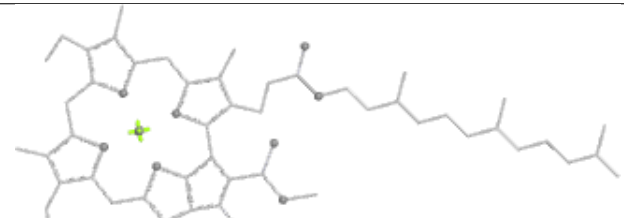


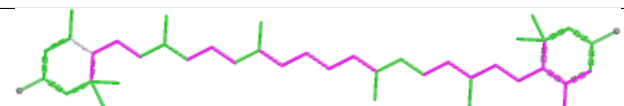
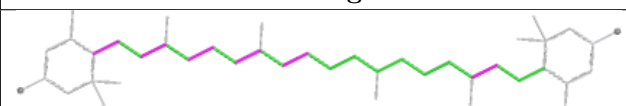
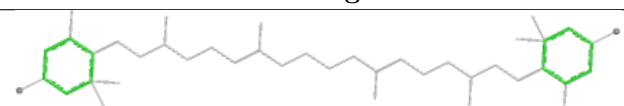


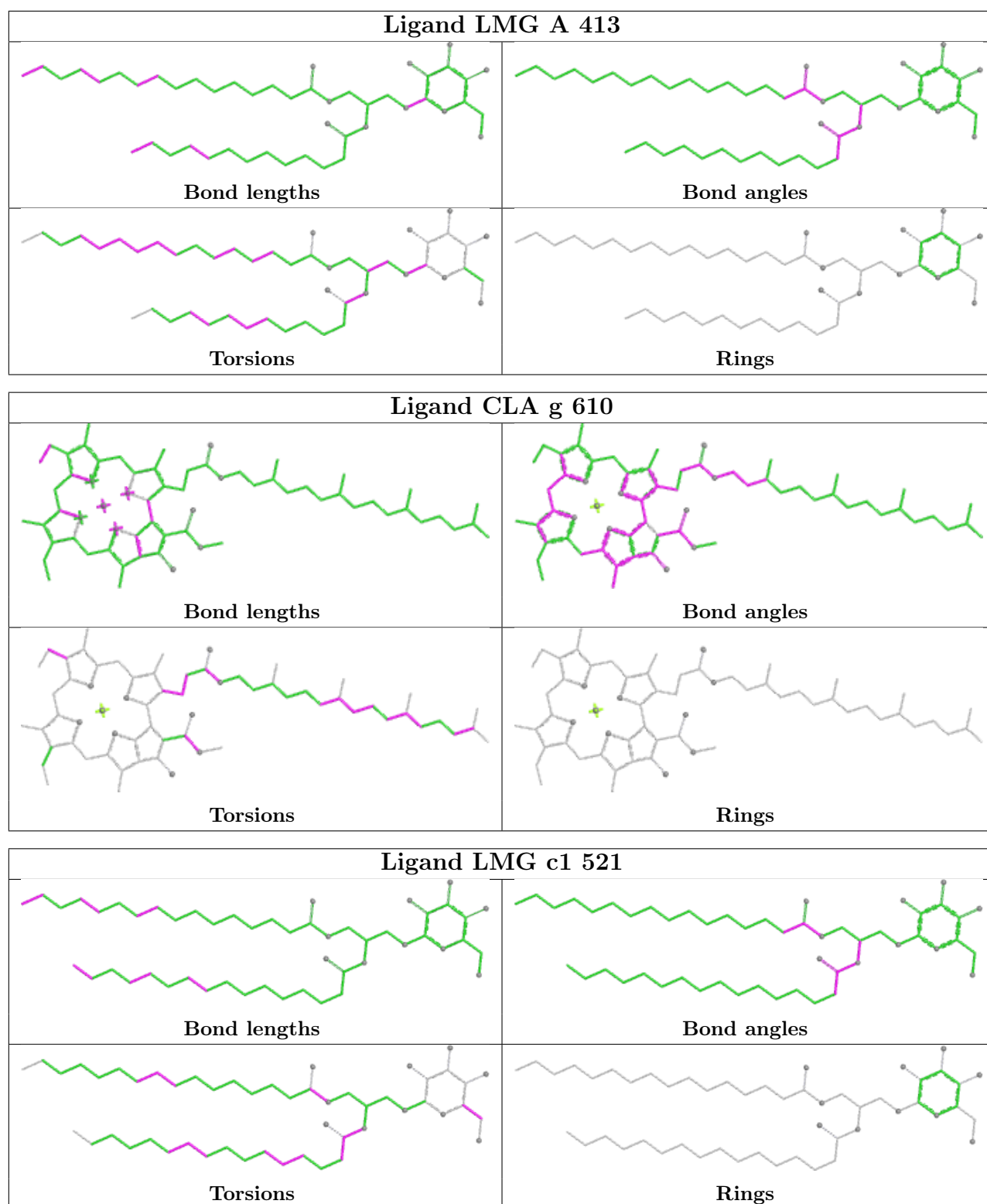


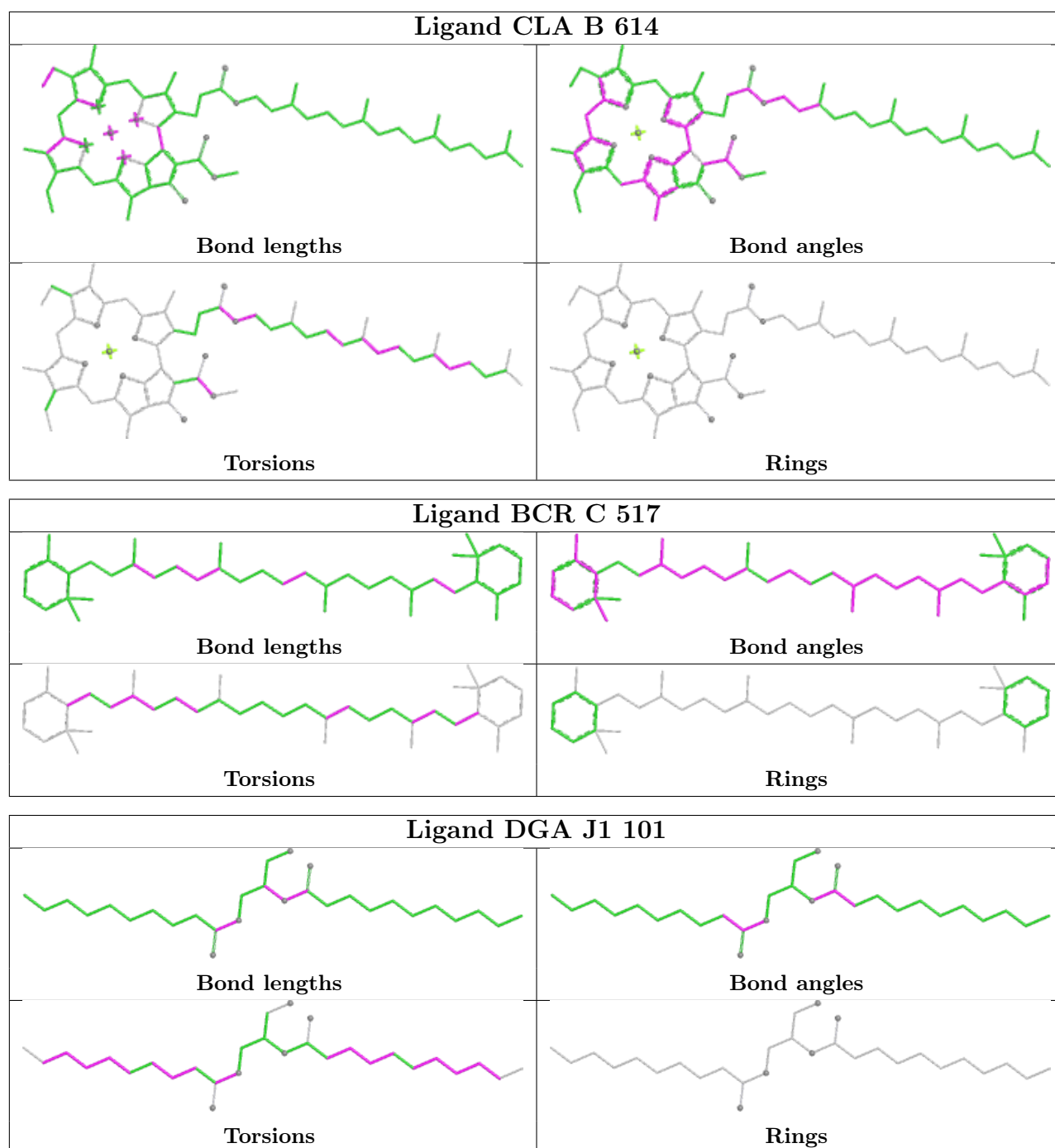


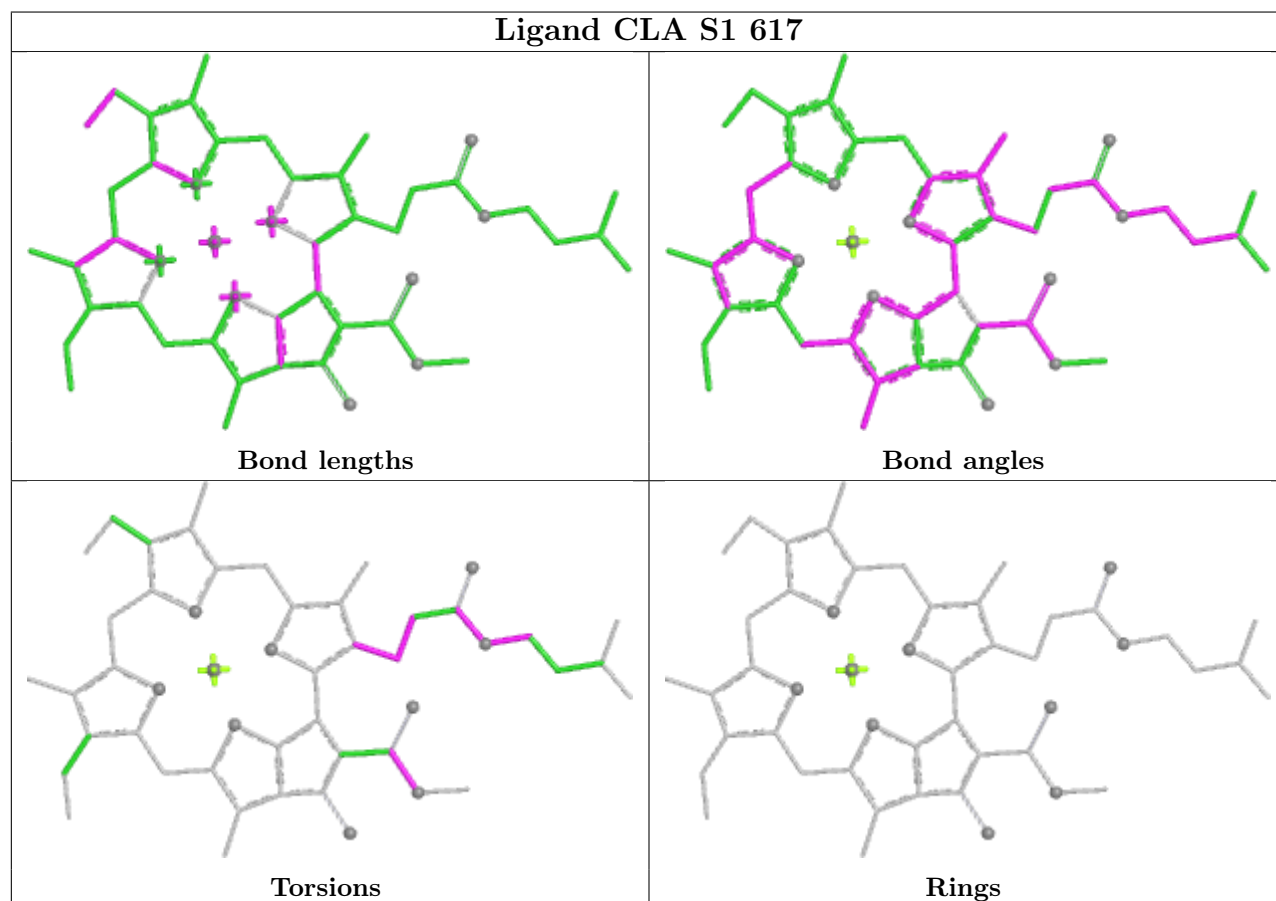
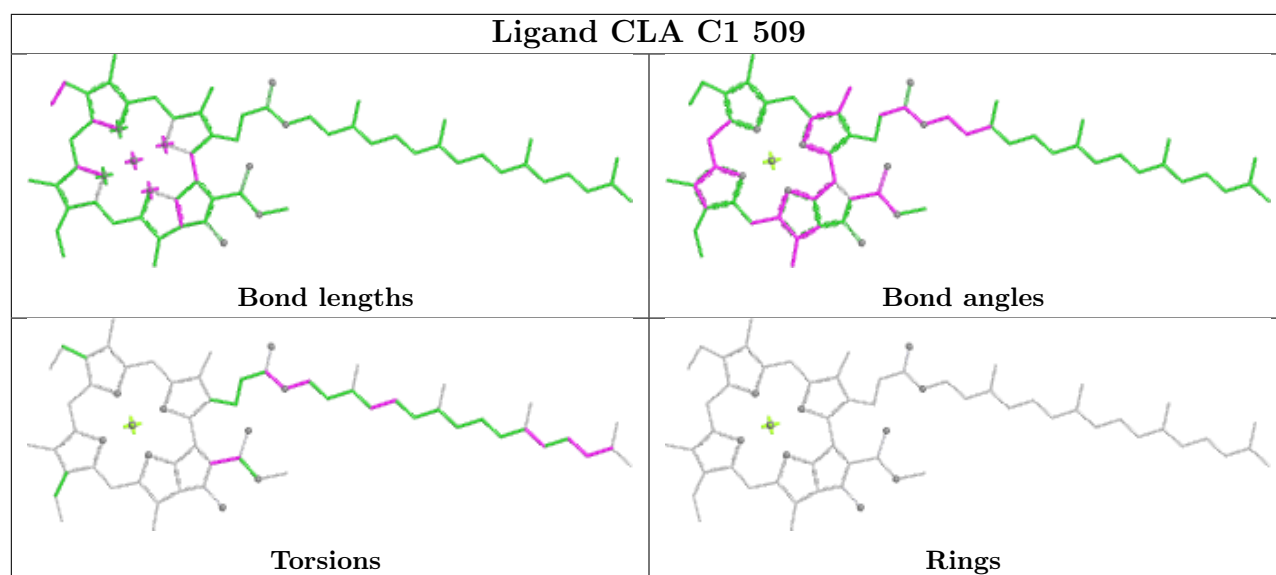
Ligand CLA n 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

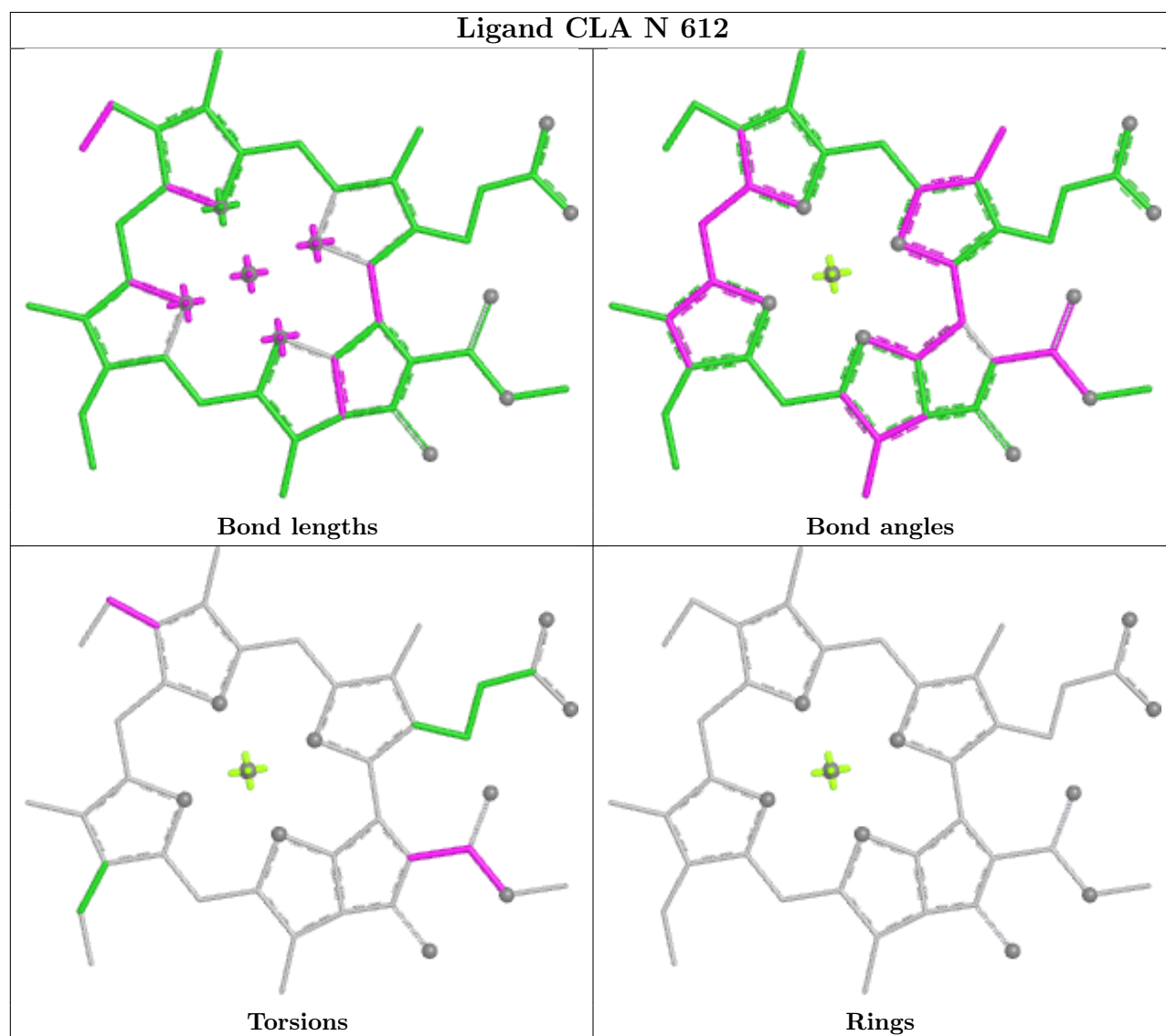
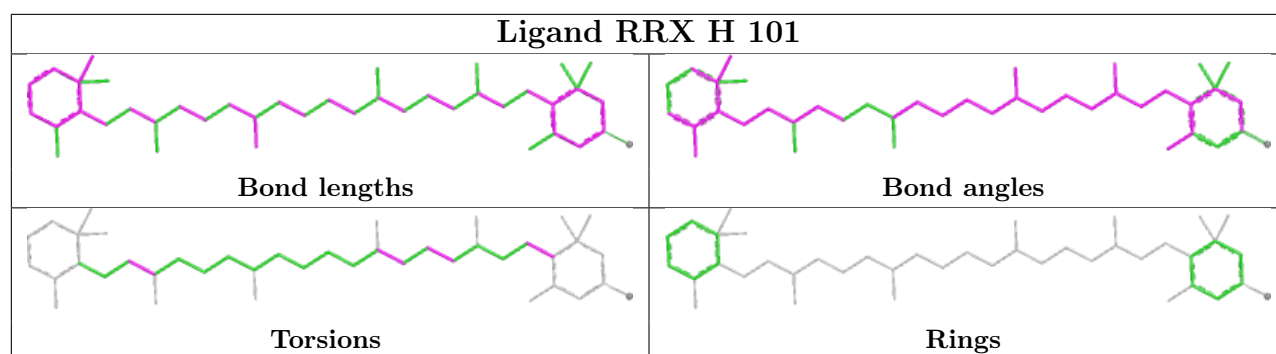
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Bond lengths	Bond angles
	
Torsions	Rings

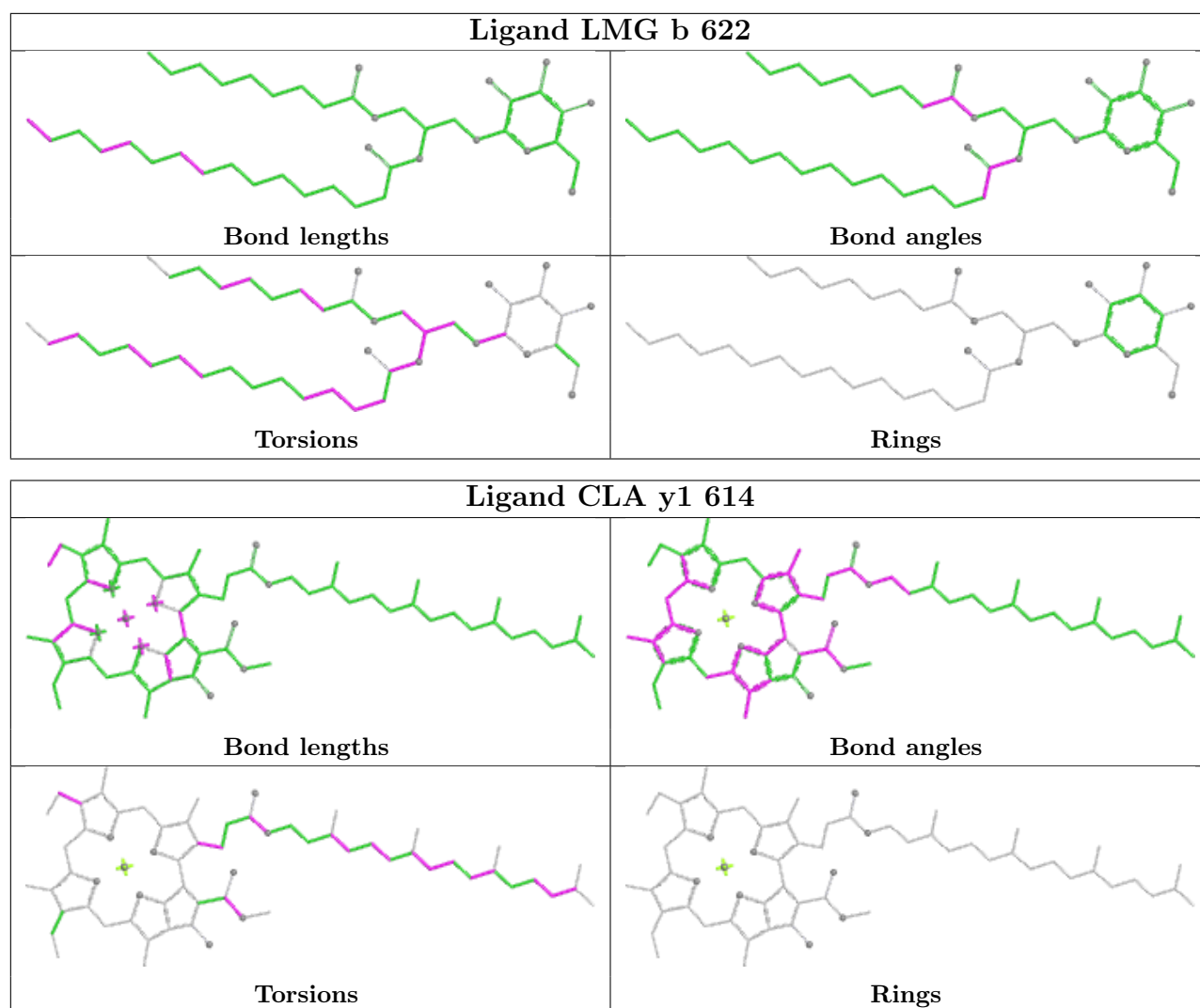
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Bond lengths	Bond angles
	
Torsions	Rings

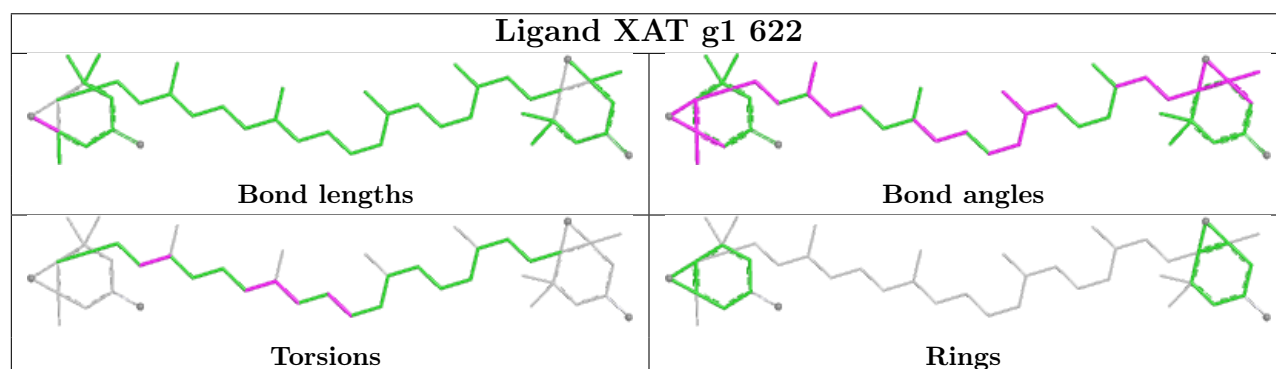
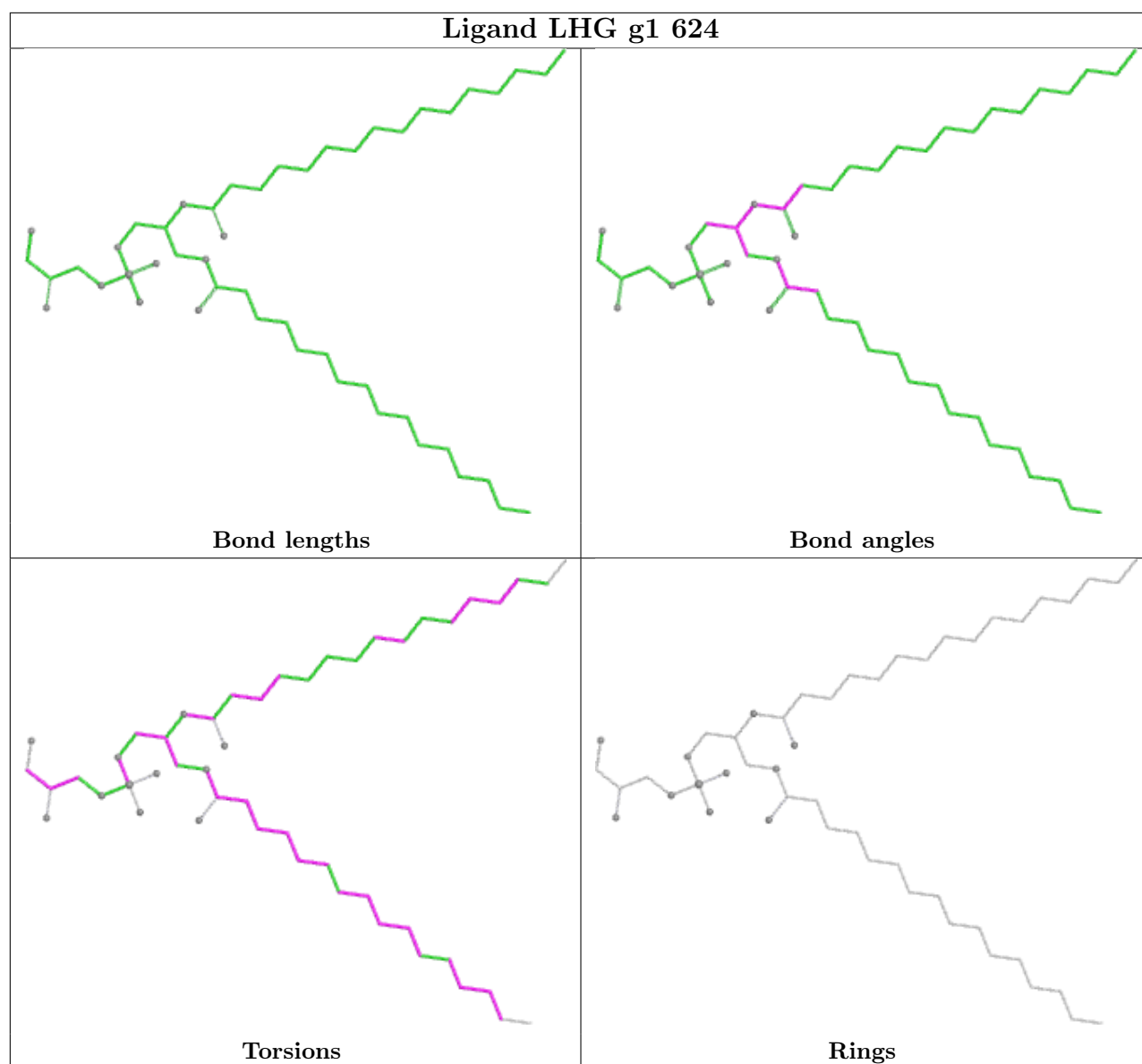


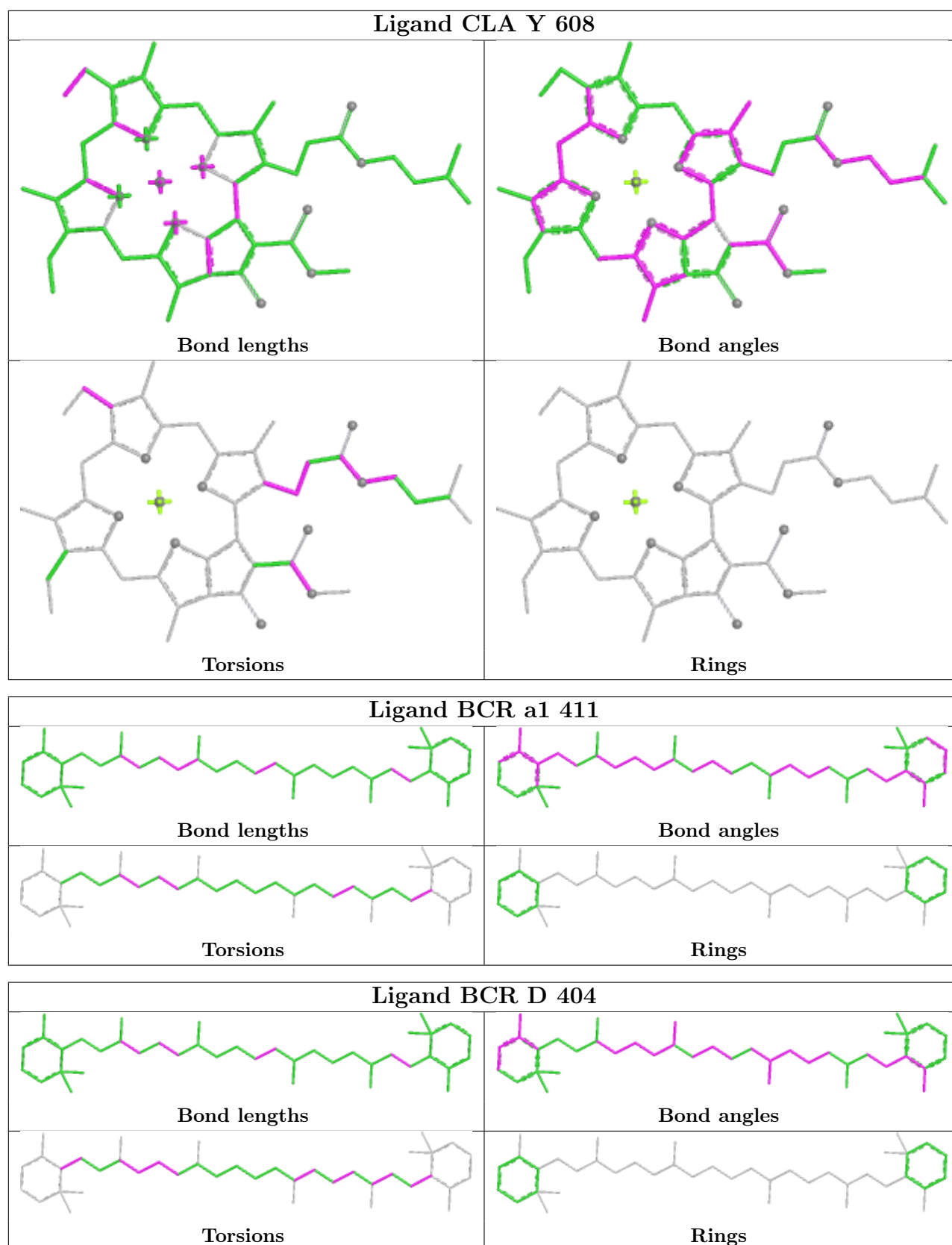


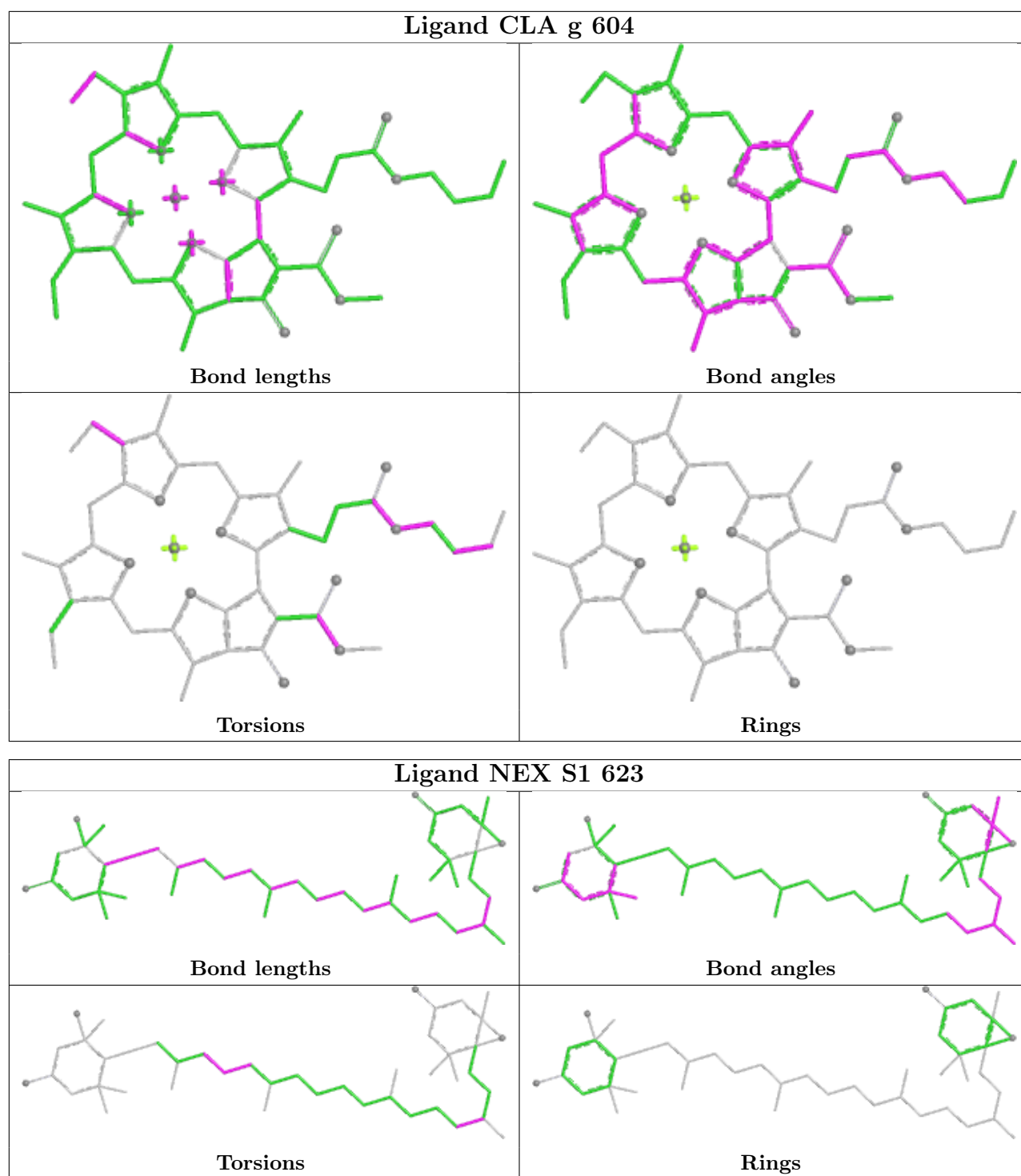


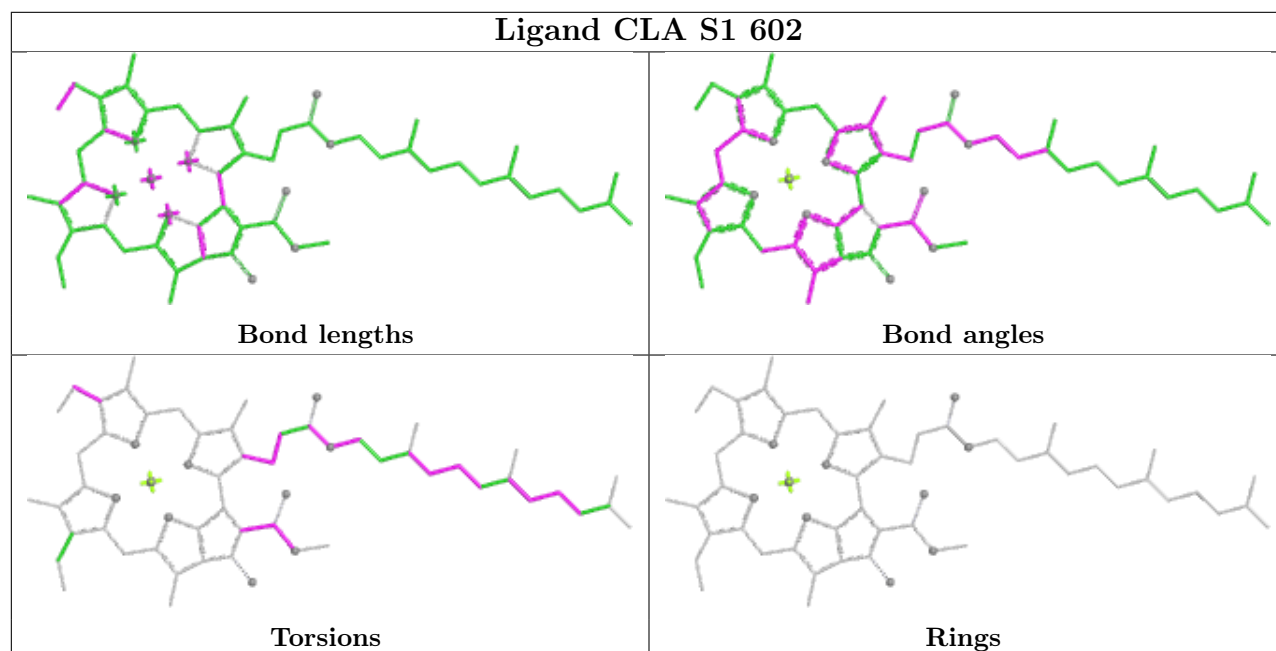
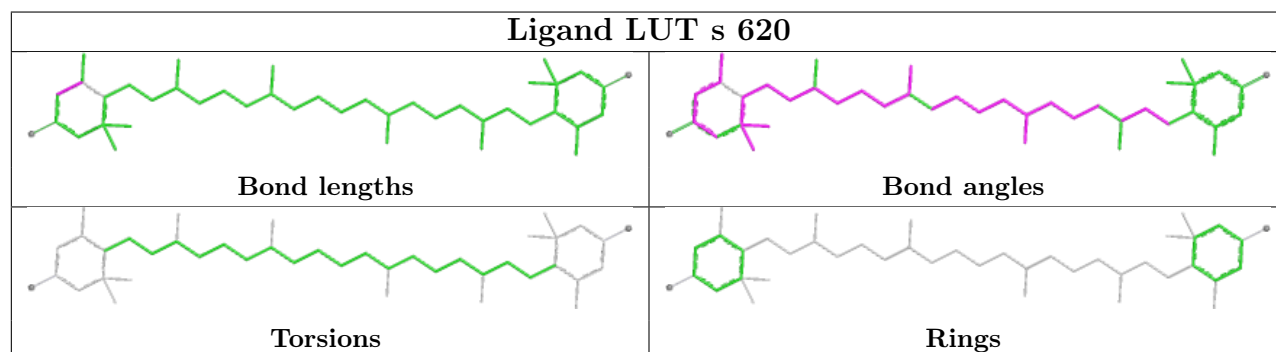
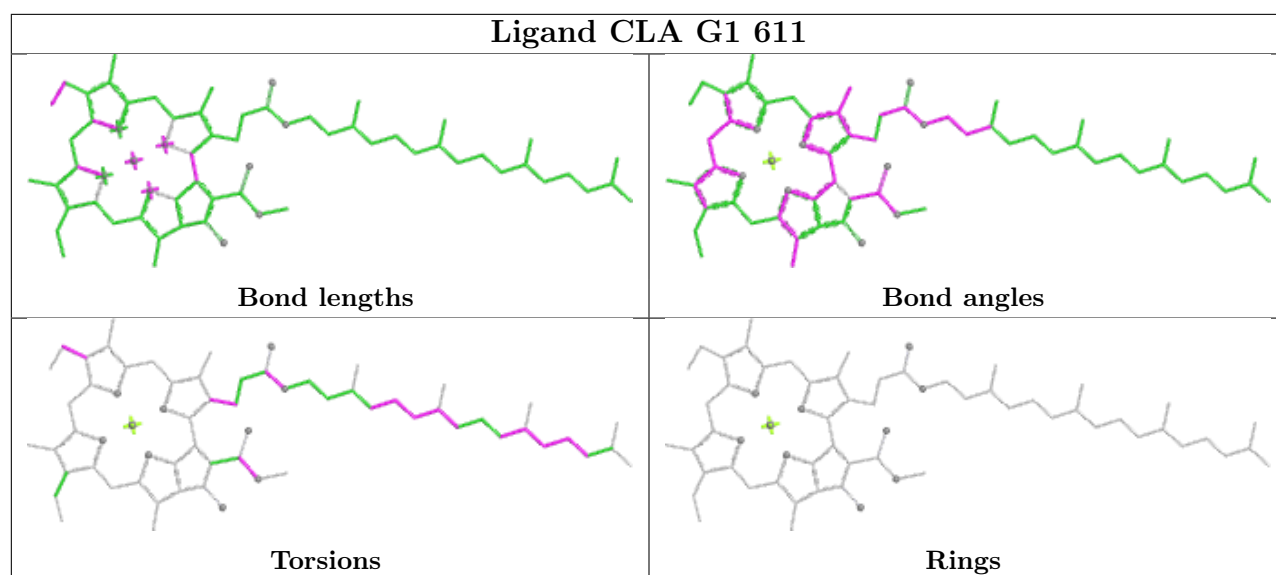


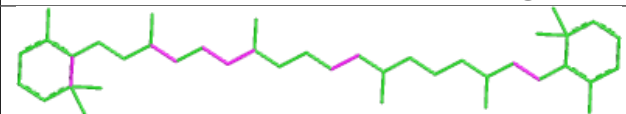
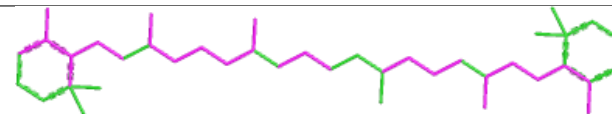
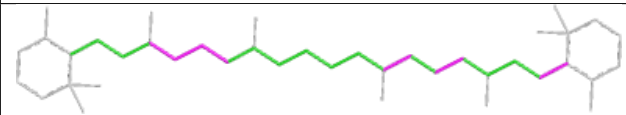
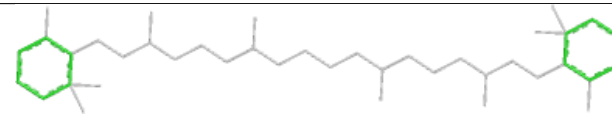


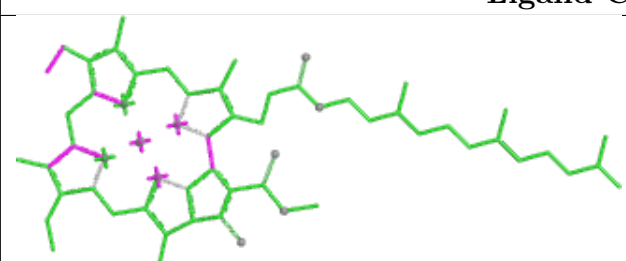
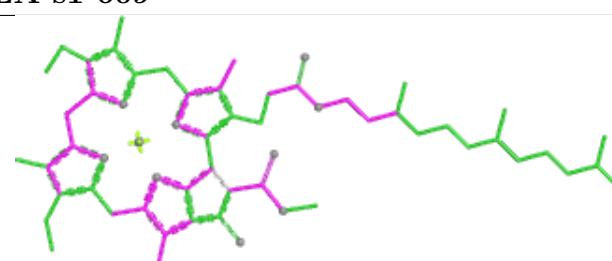
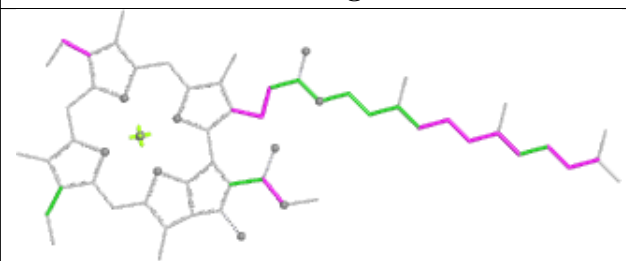
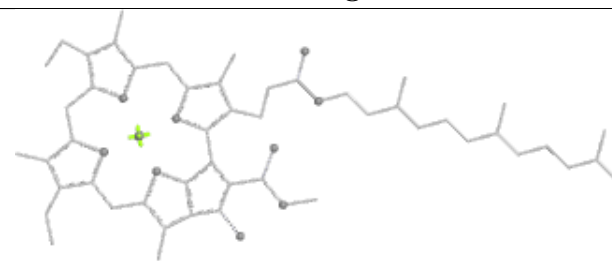


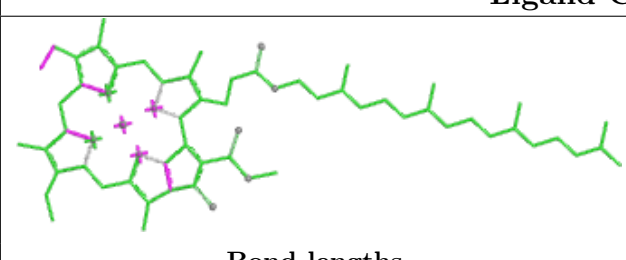
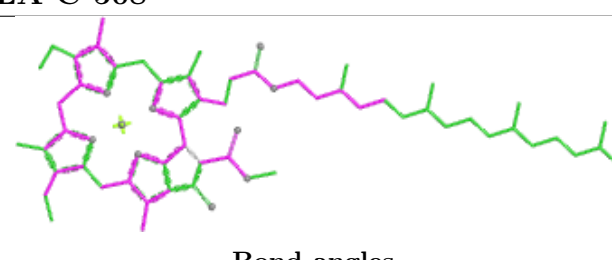
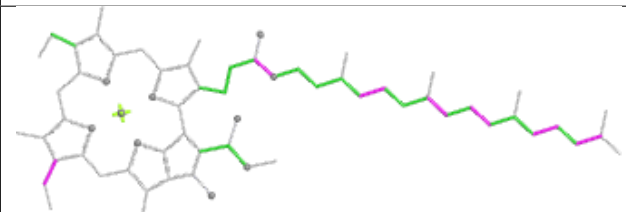
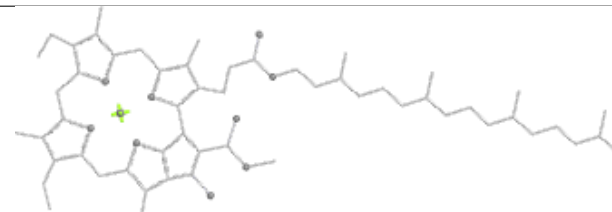


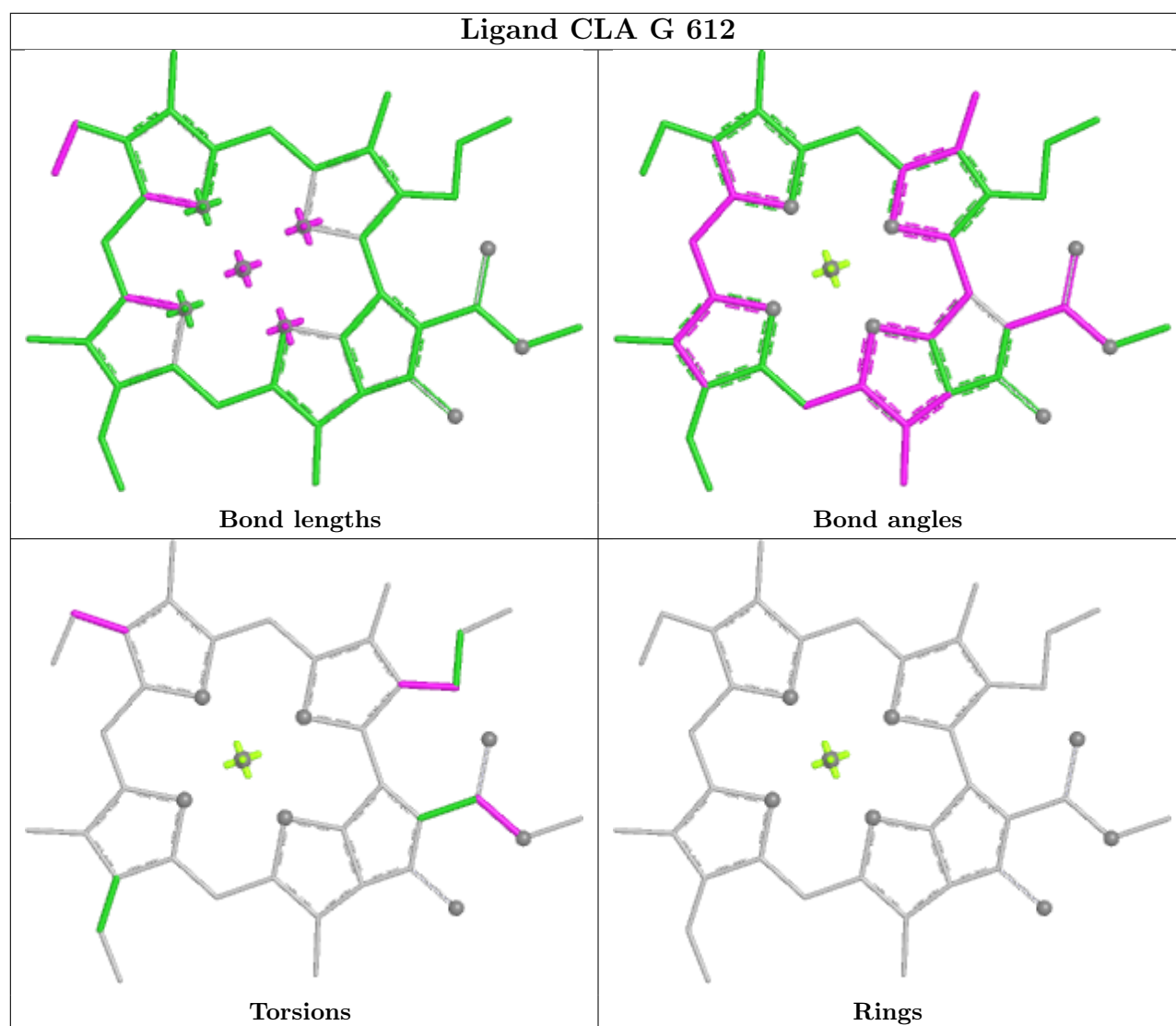


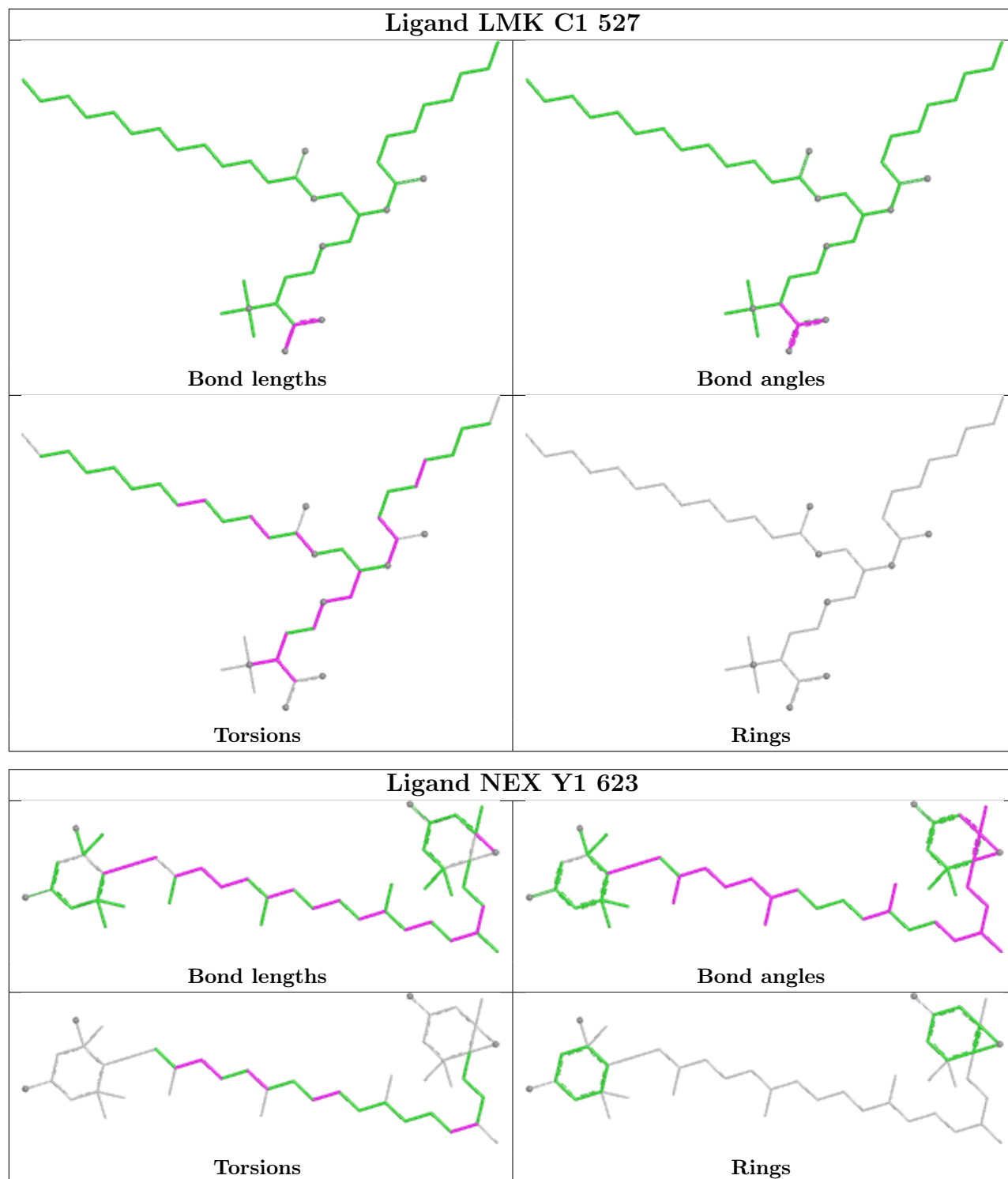


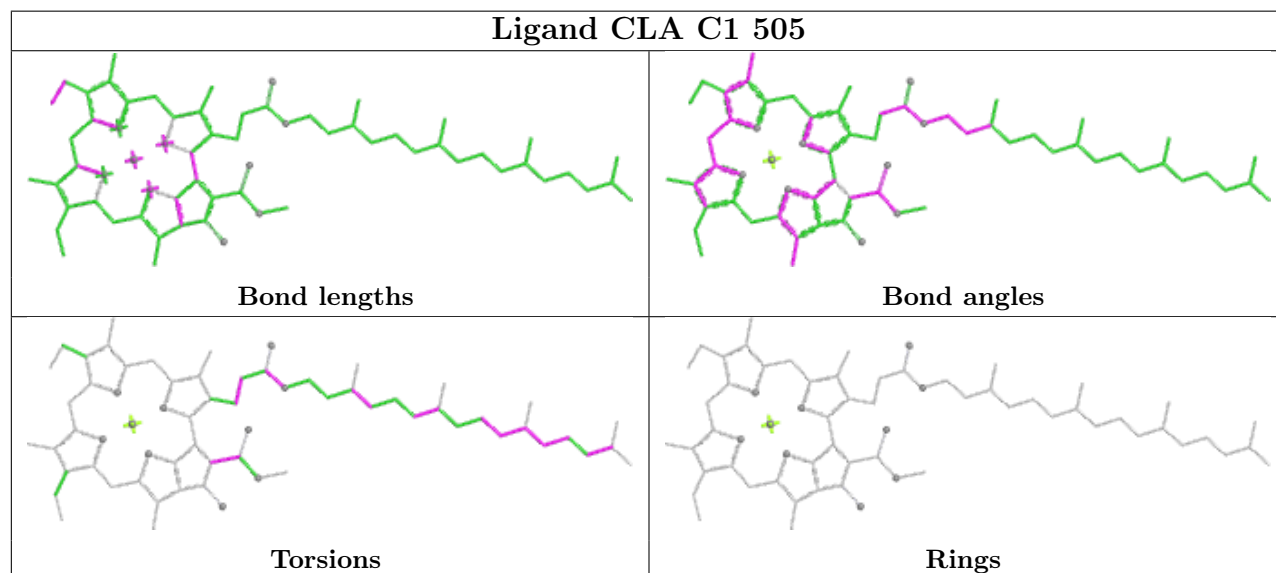
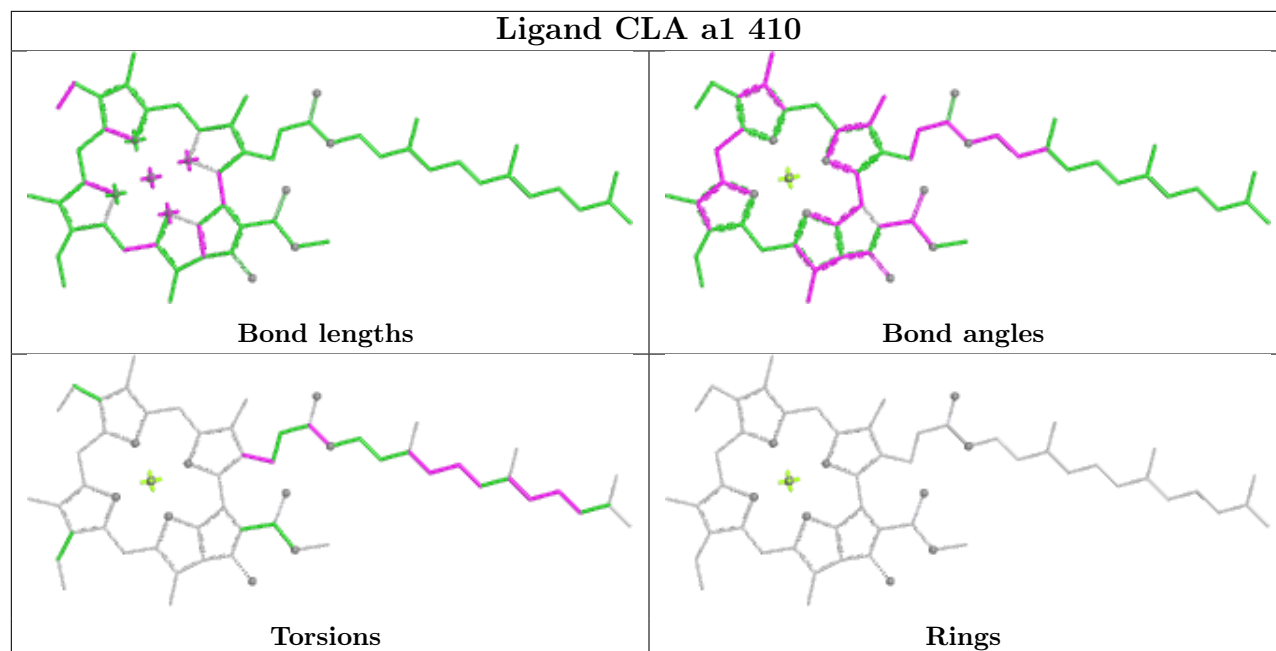
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

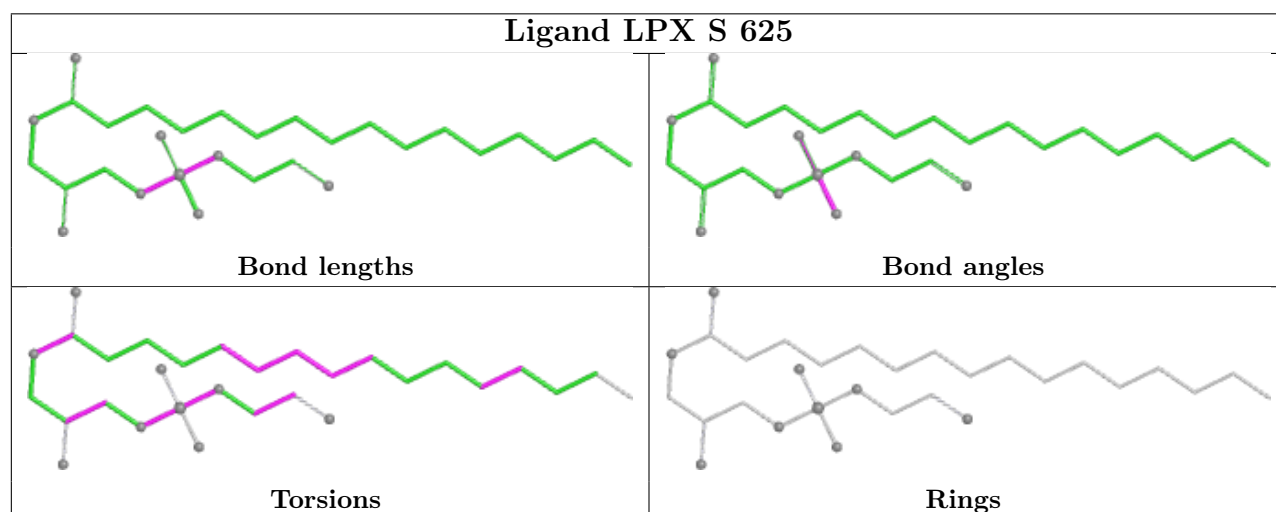
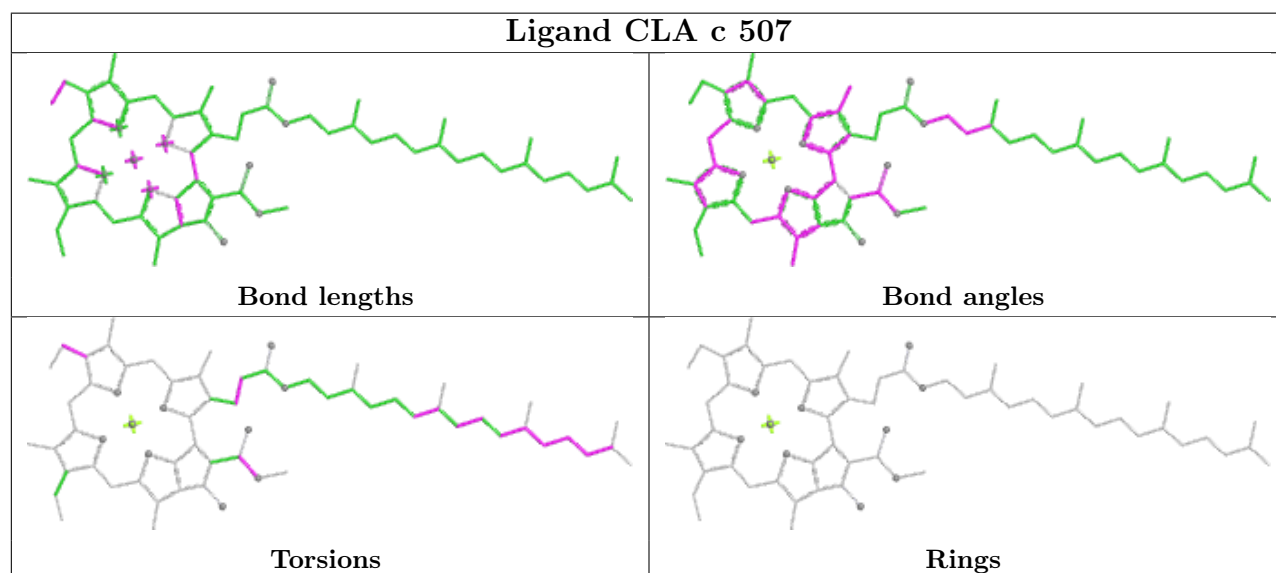
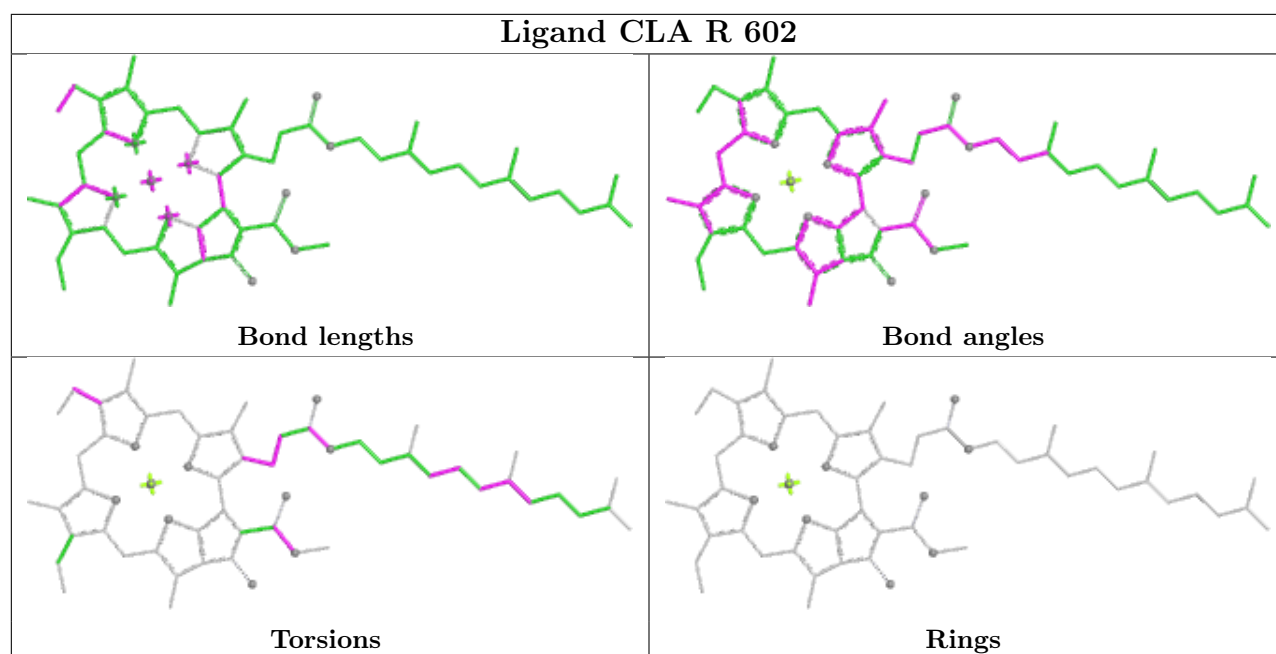
Ligand CLA s1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

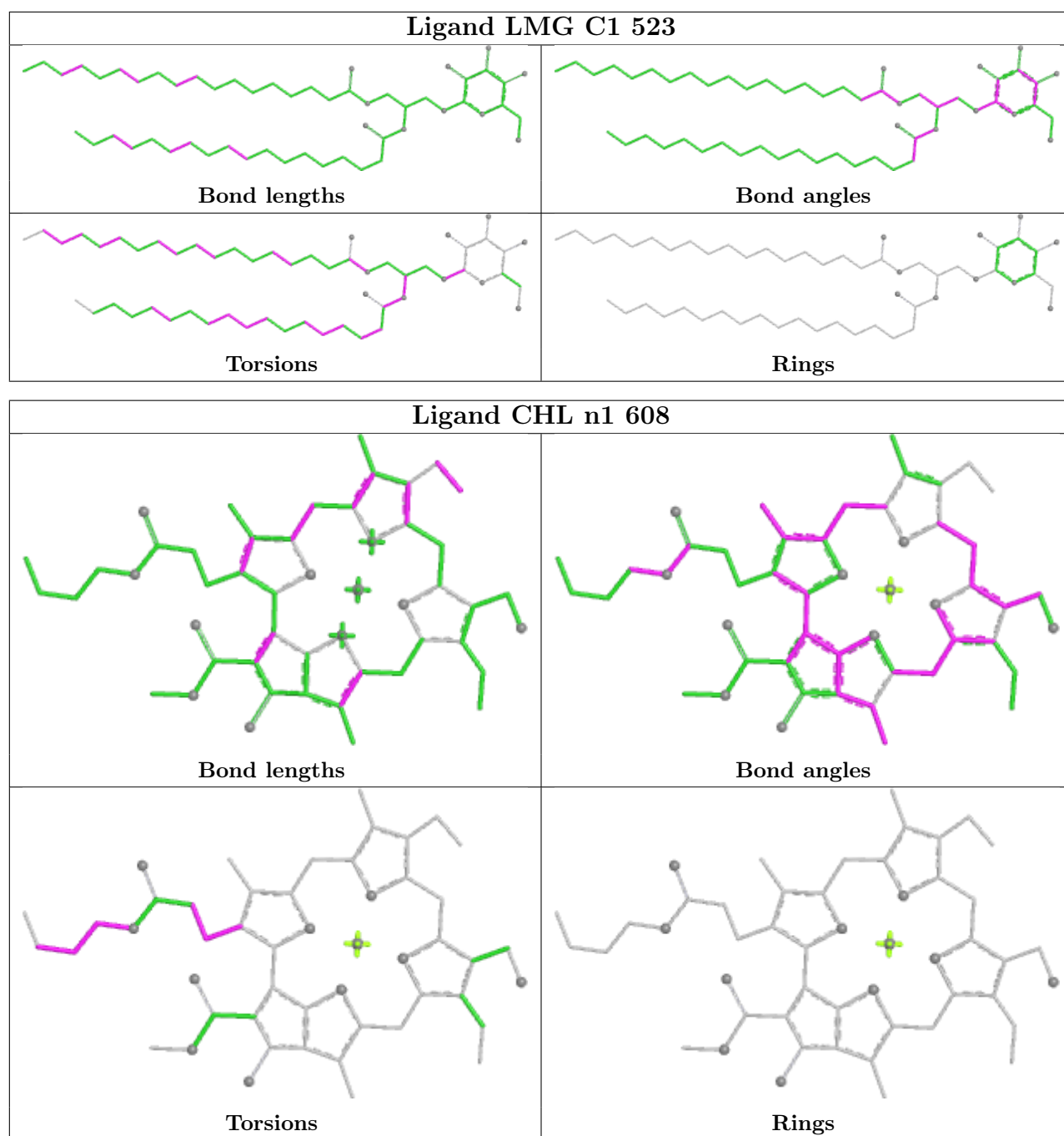
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Bond lengths	Bond angles
	
Torsions	Rings

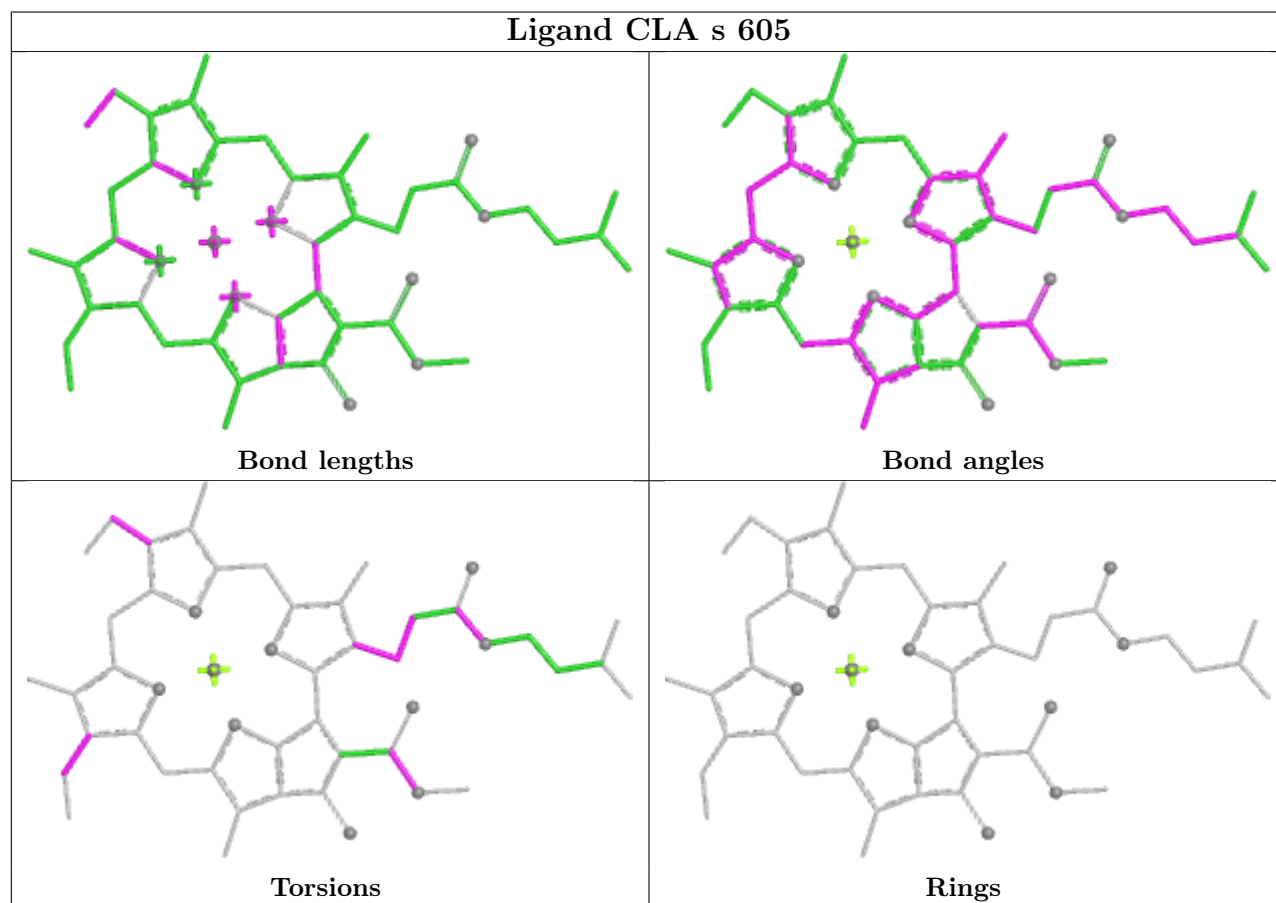
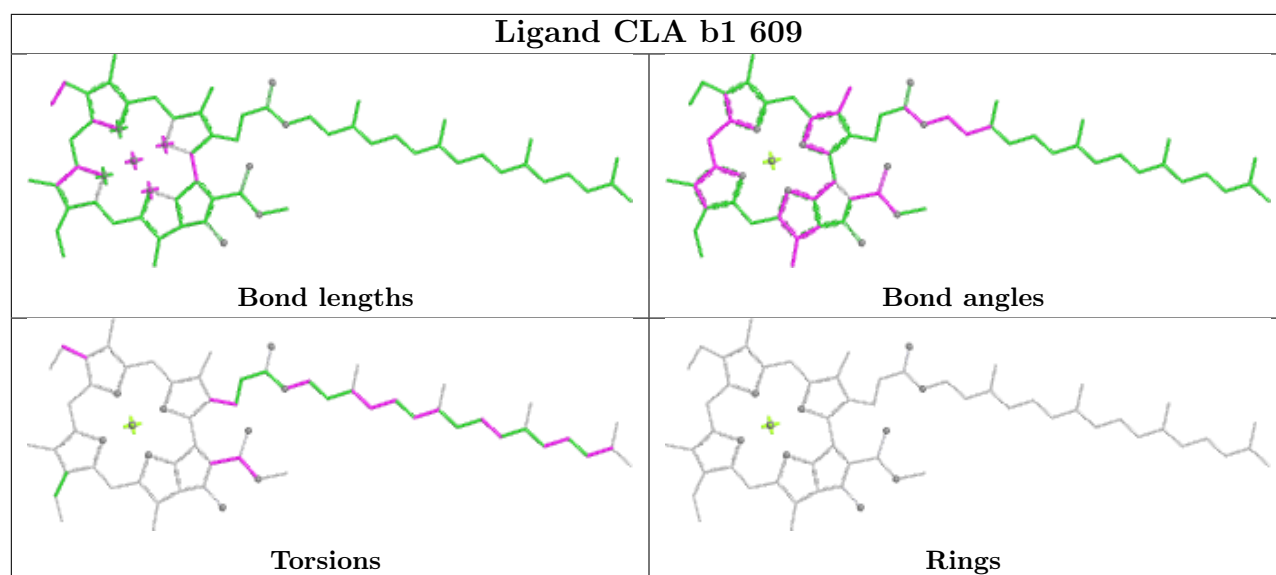


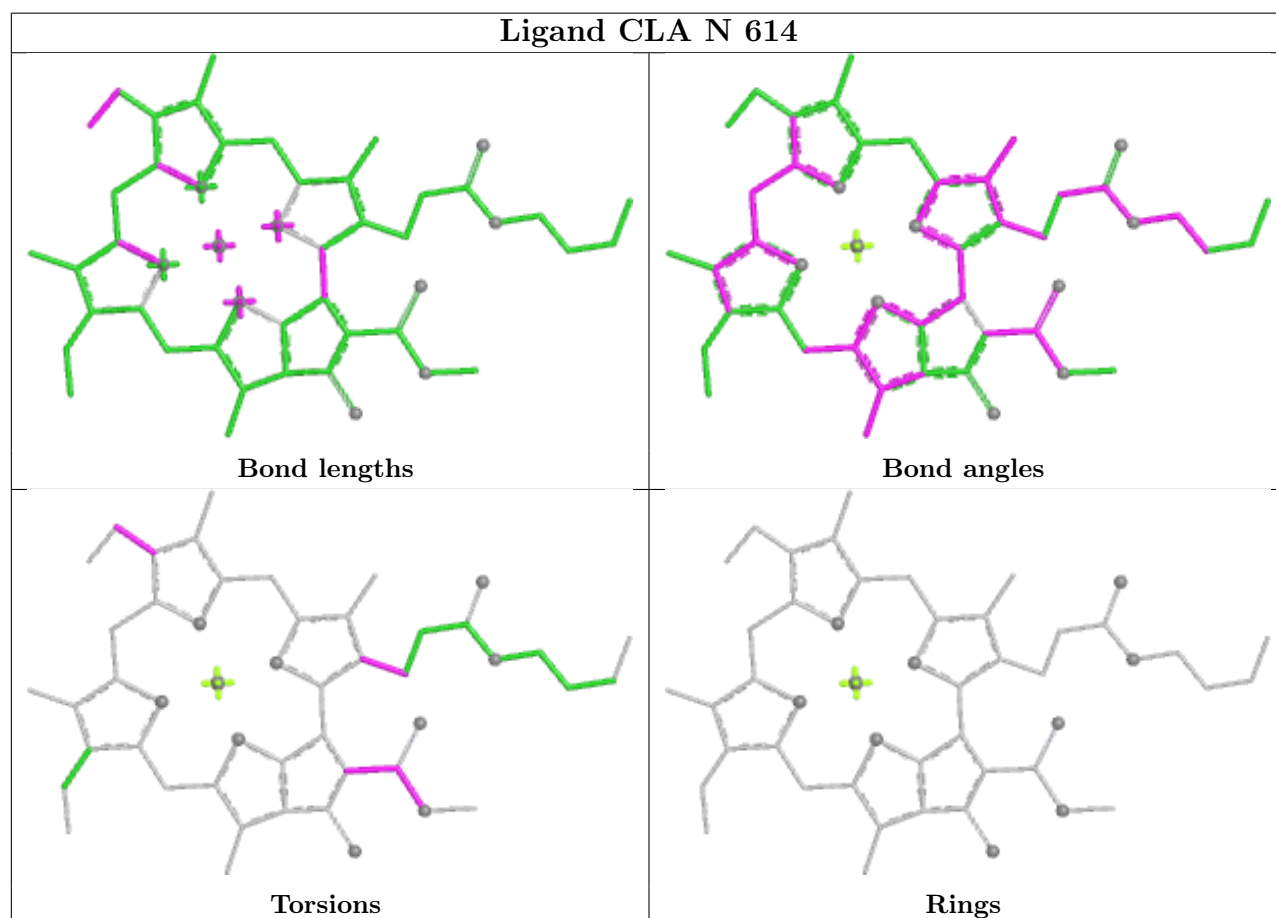
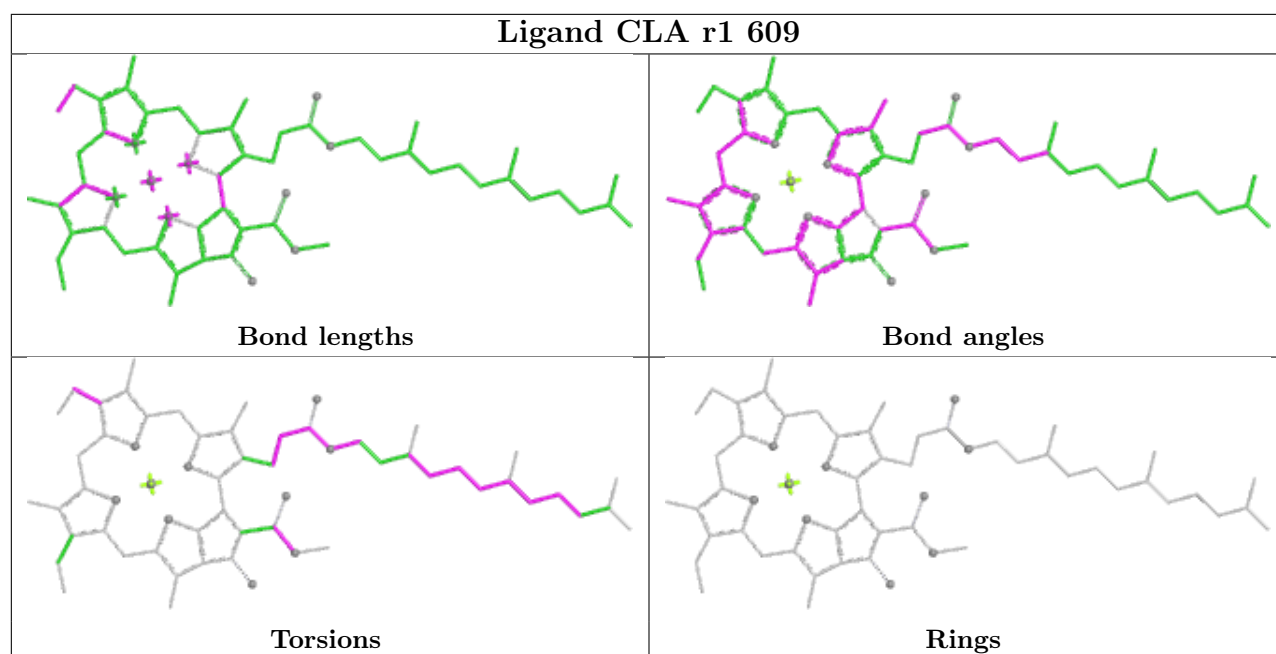


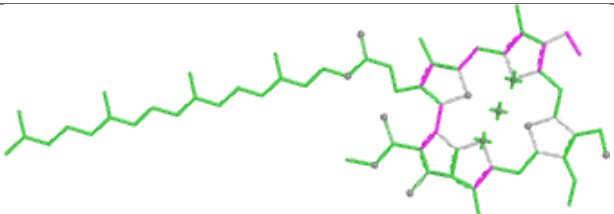
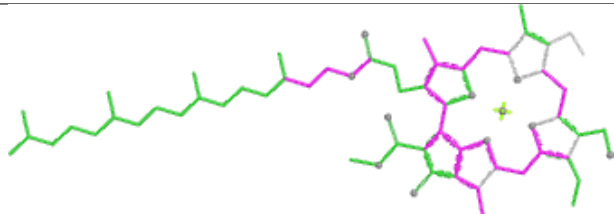
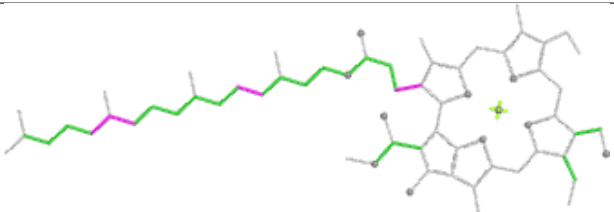
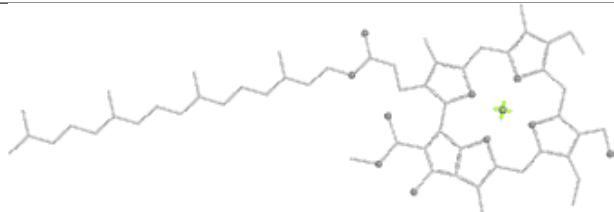


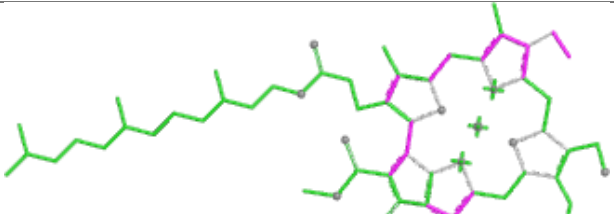
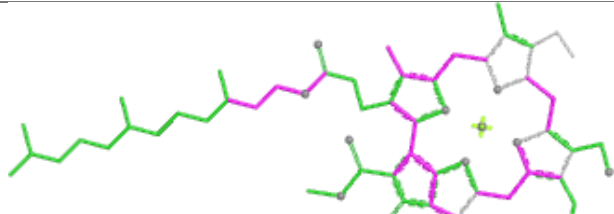
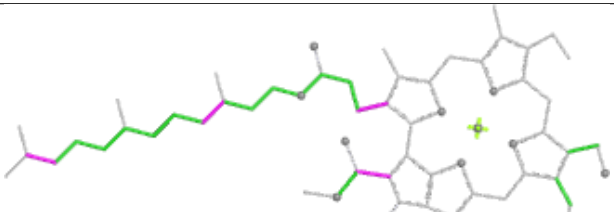
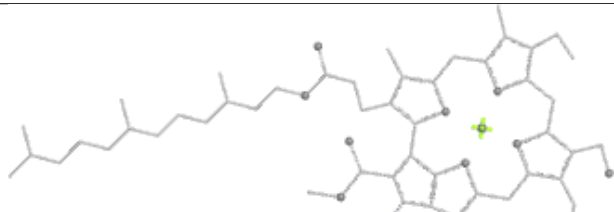


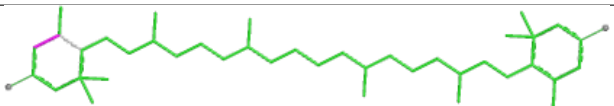
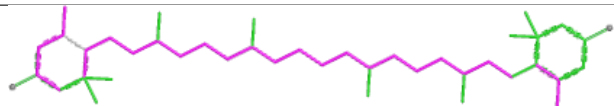
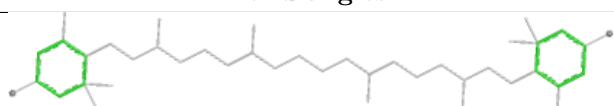


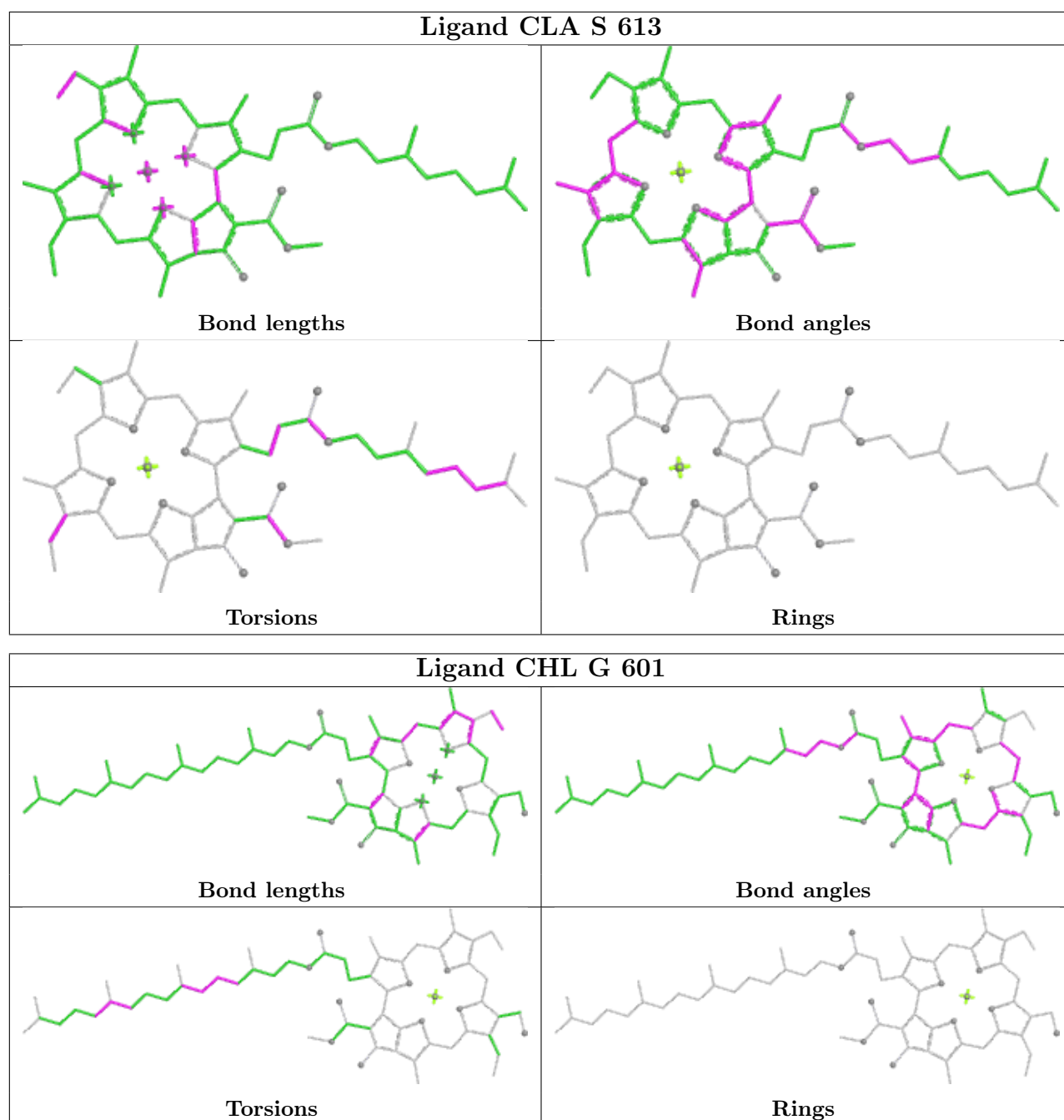


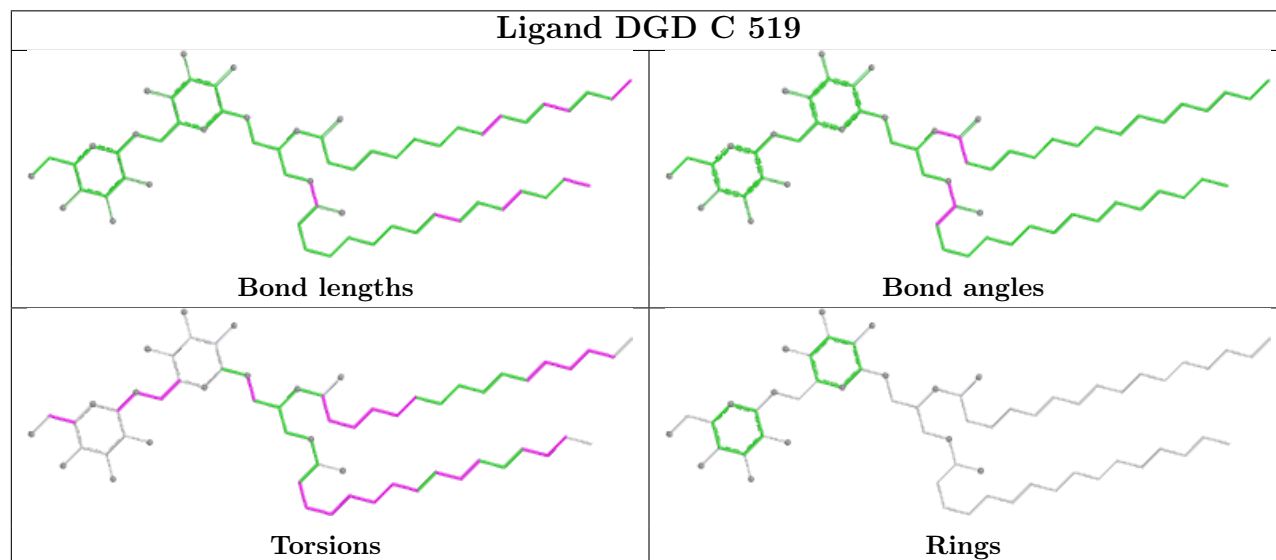
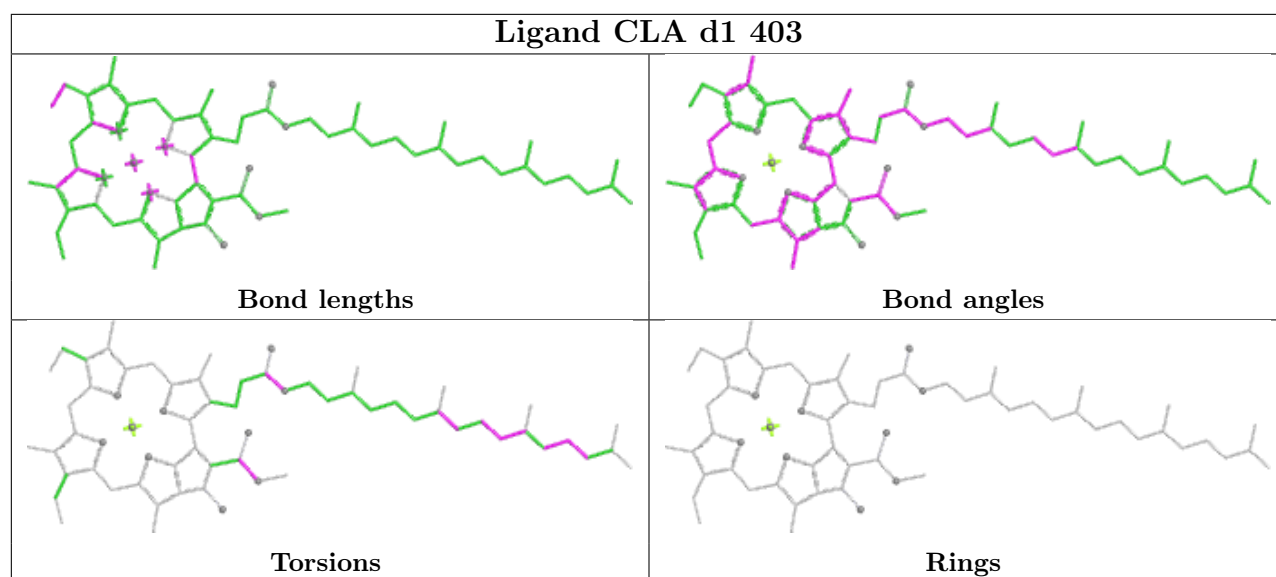


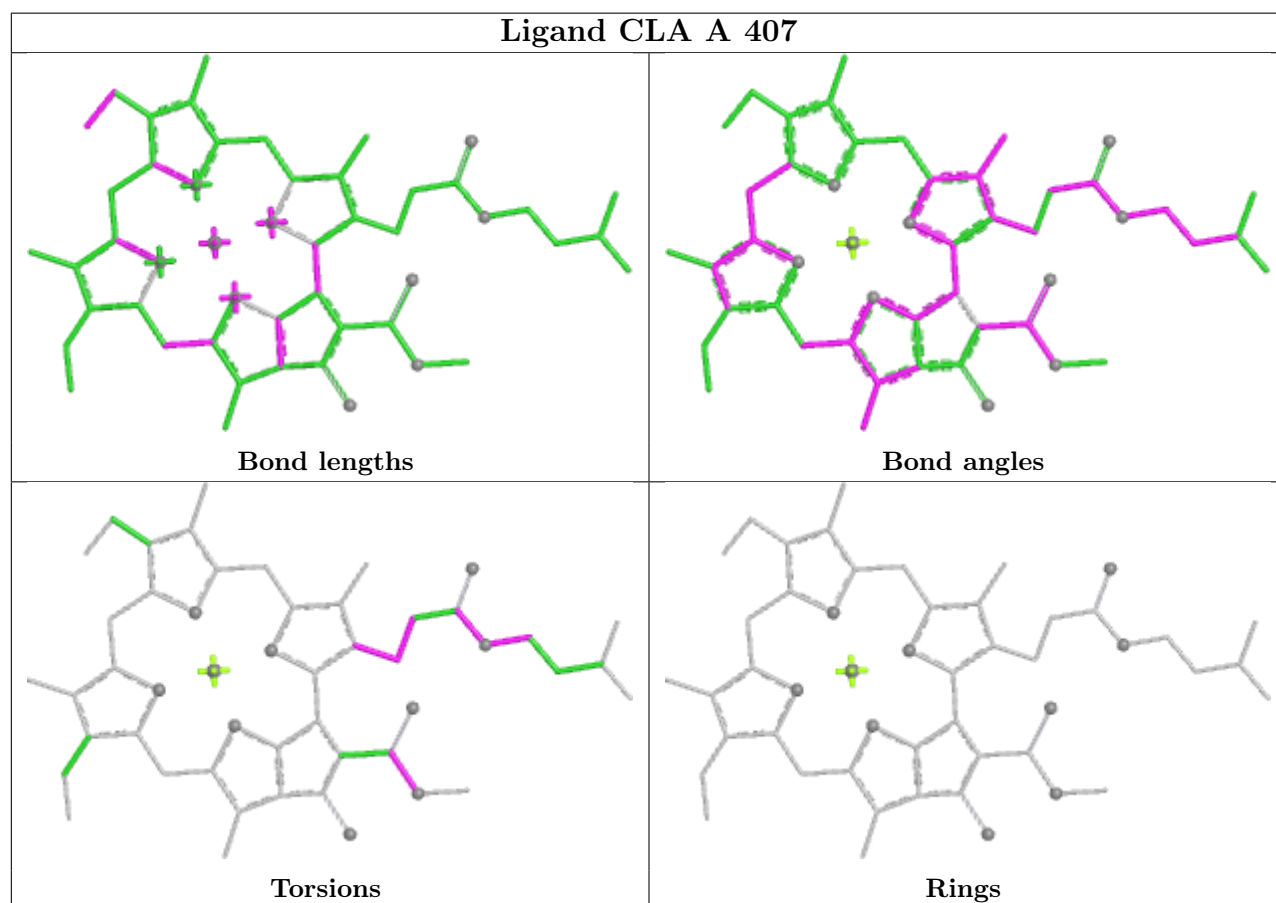
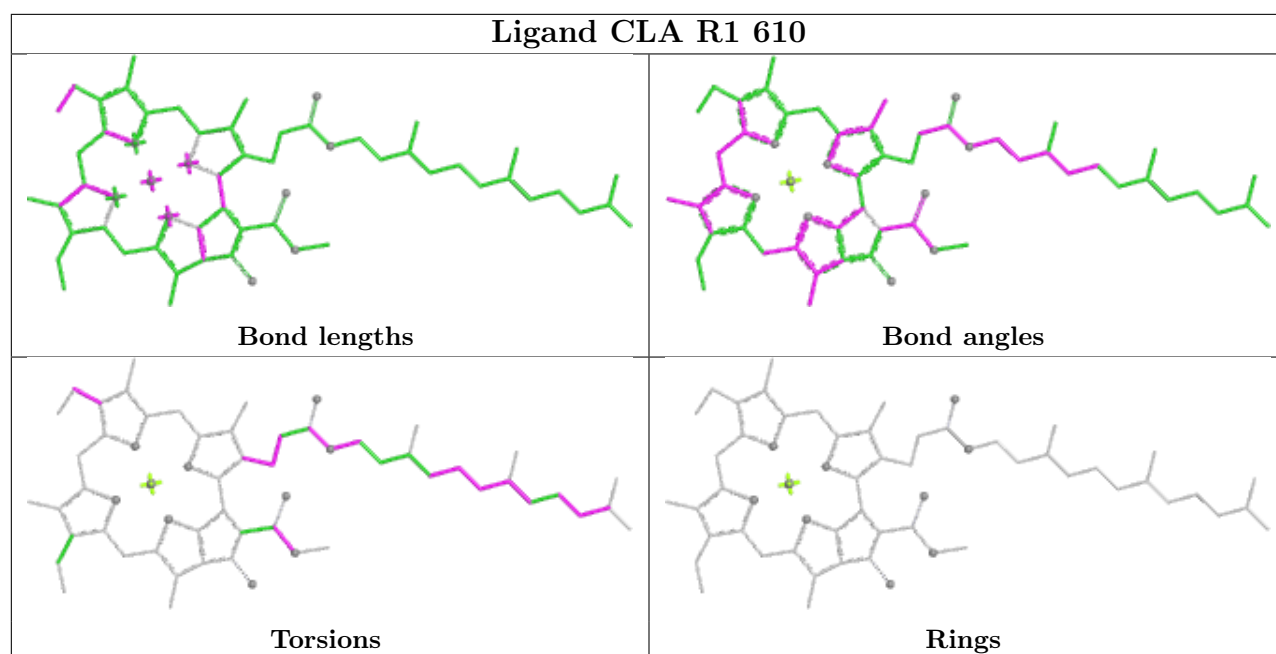
Ligand CHL N 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

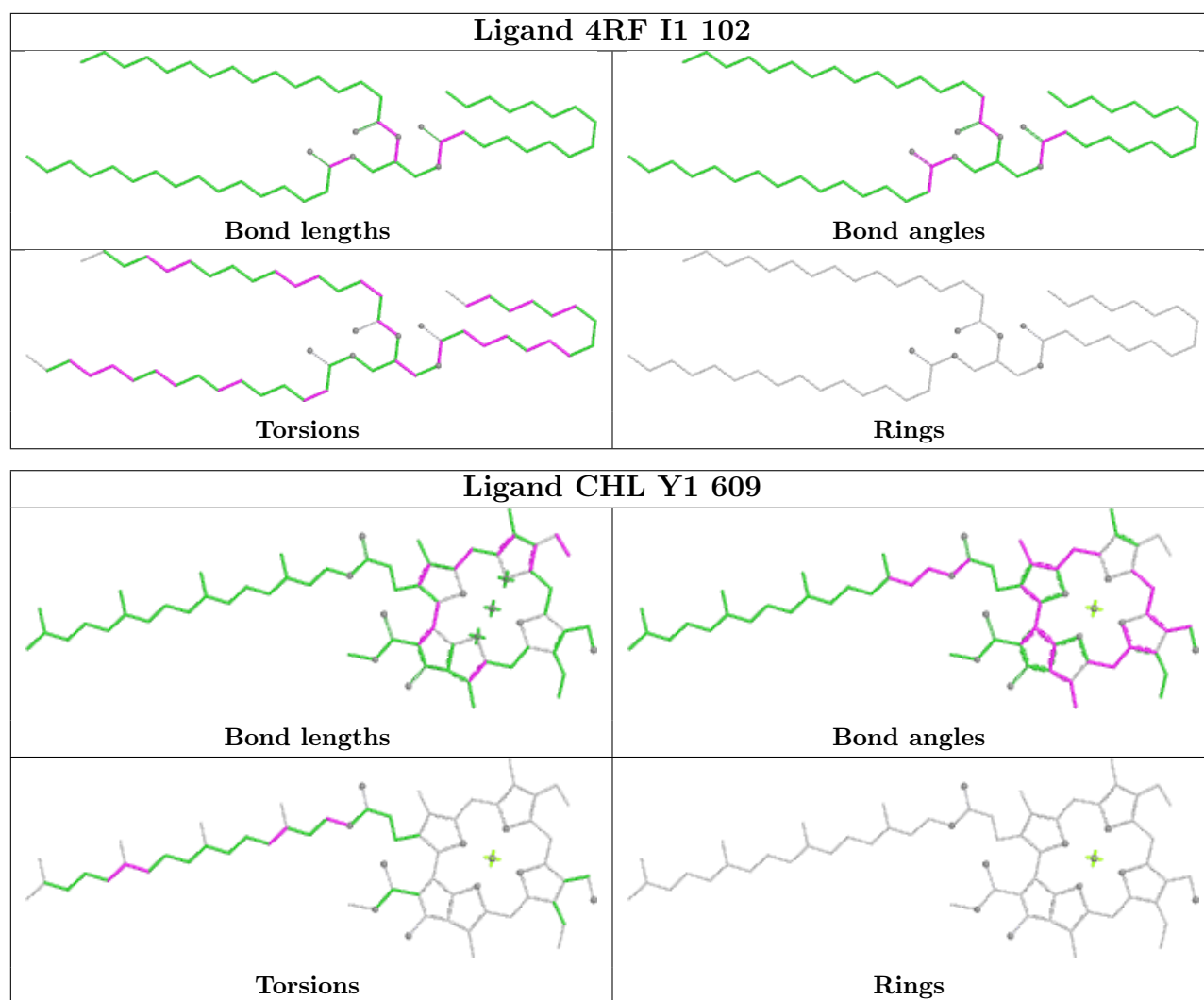
Ligand CHL s 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

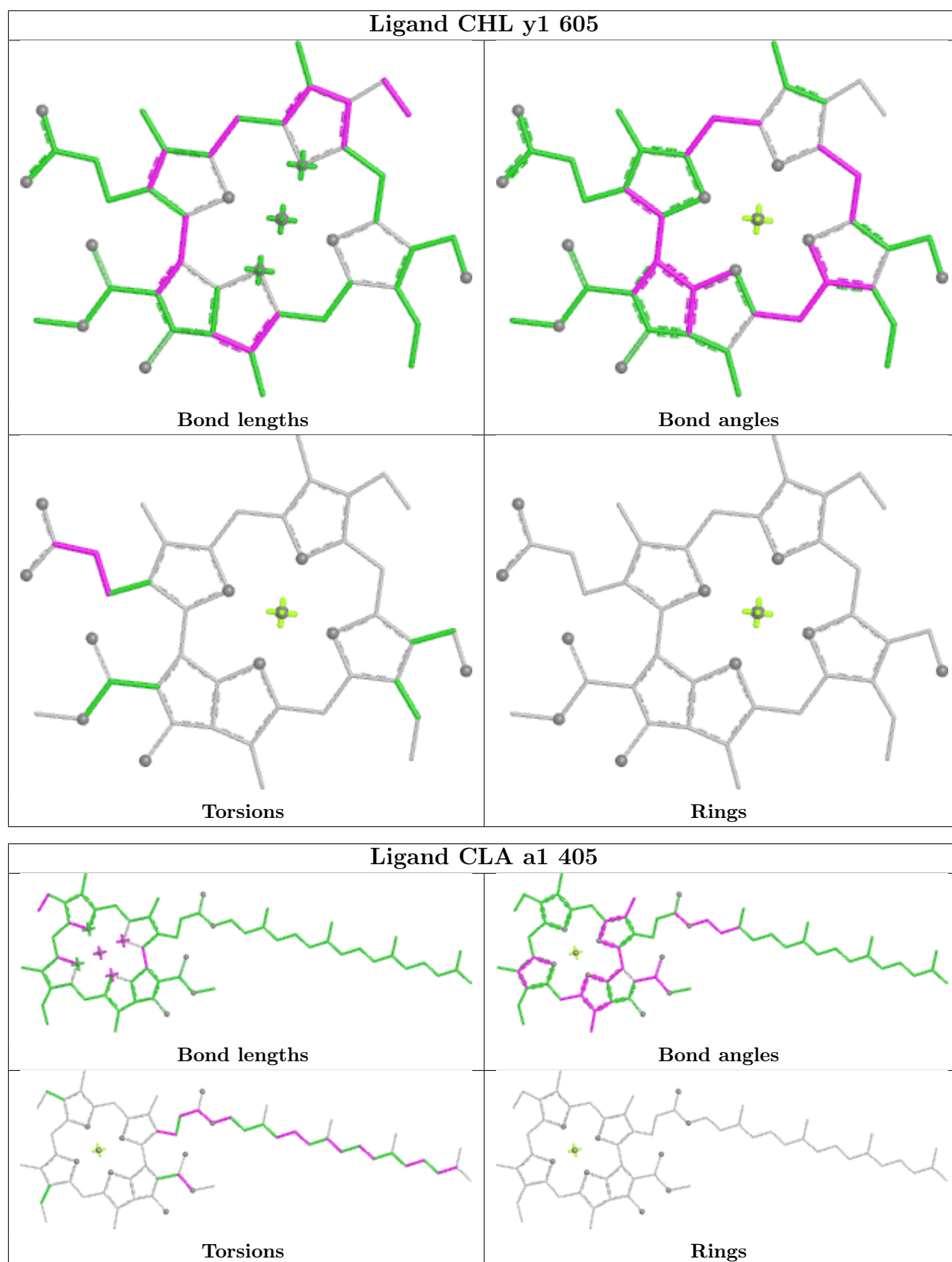
Ligand LUT g1 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

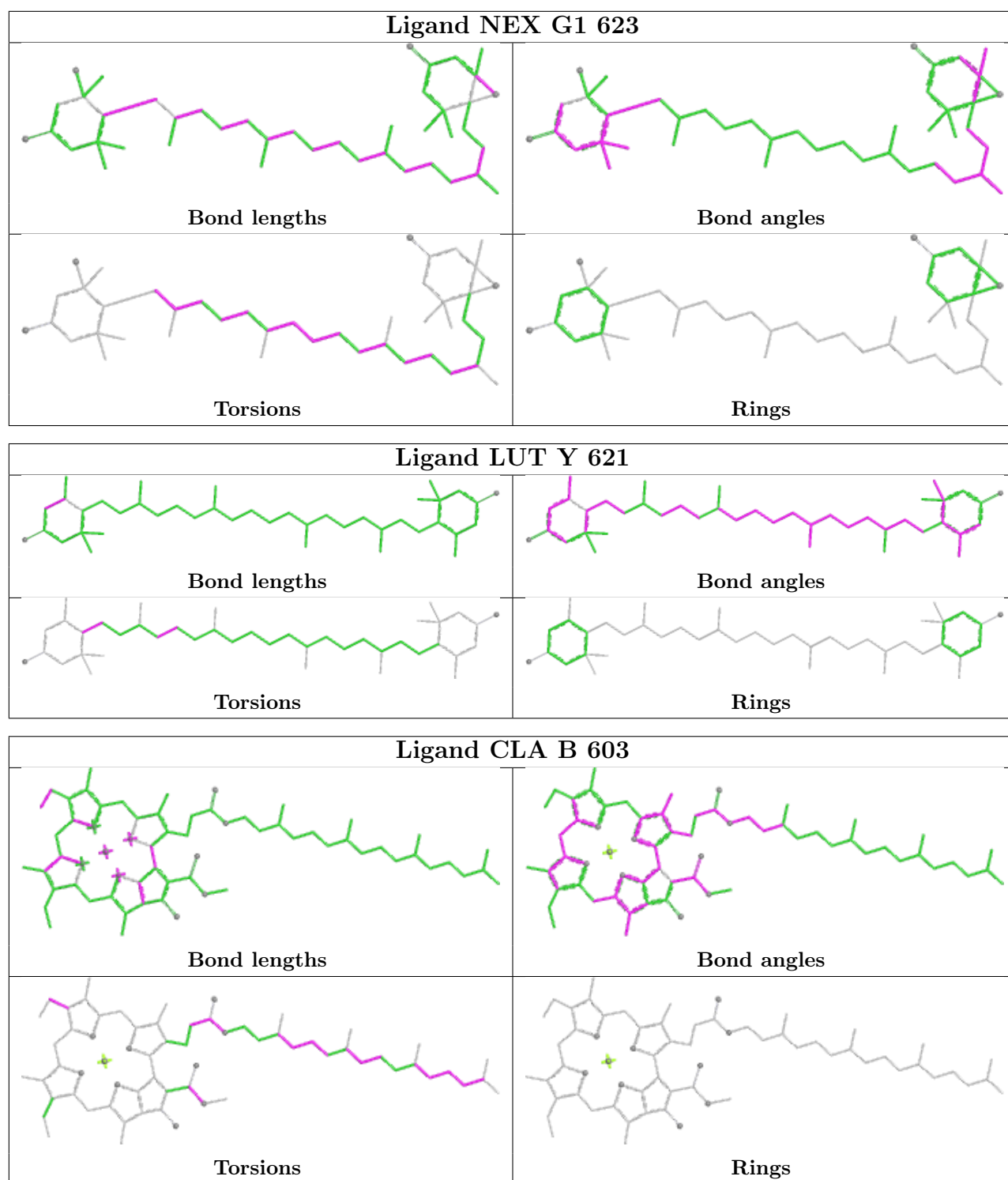


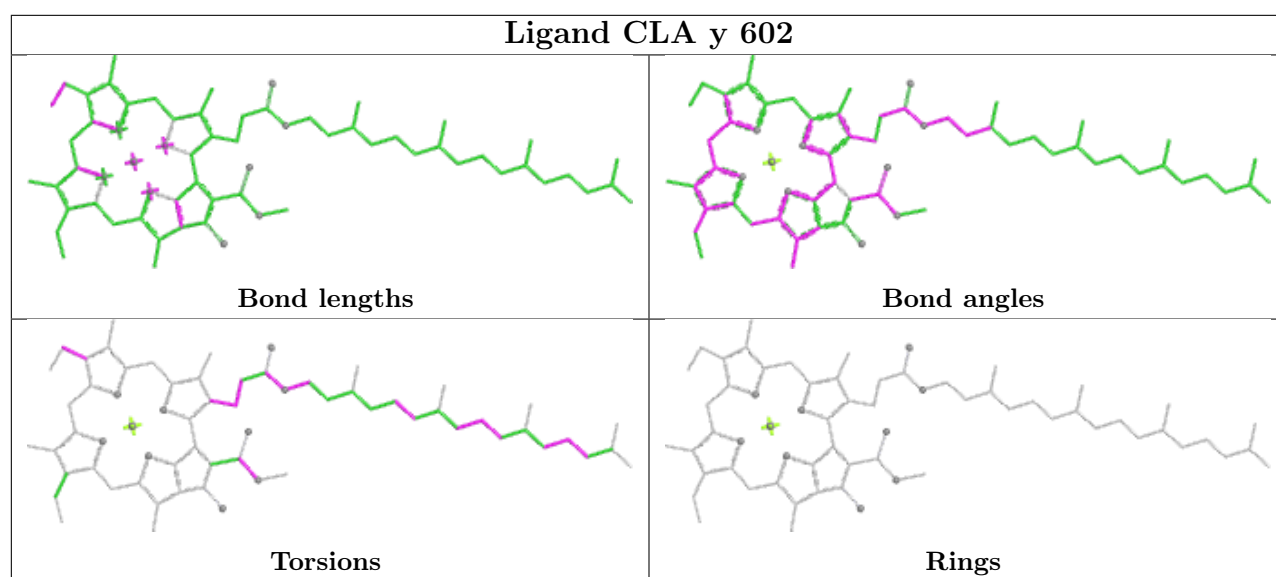
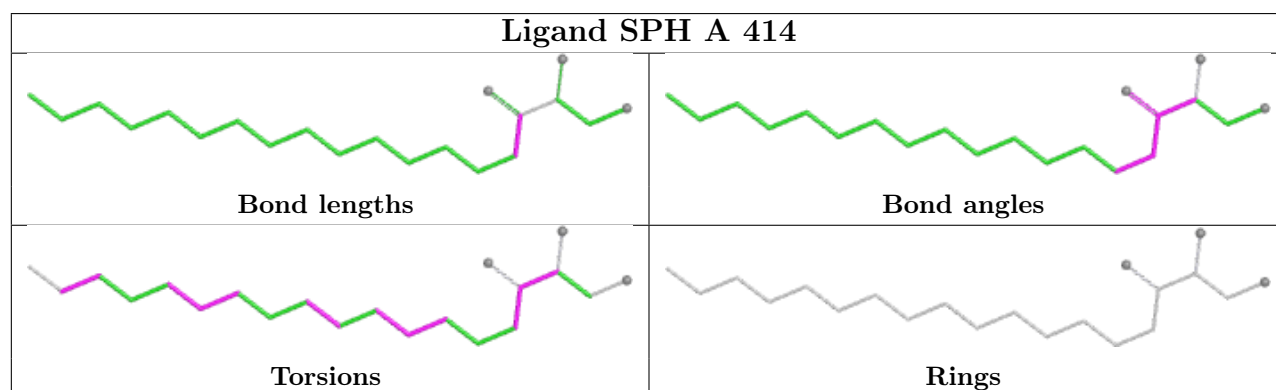
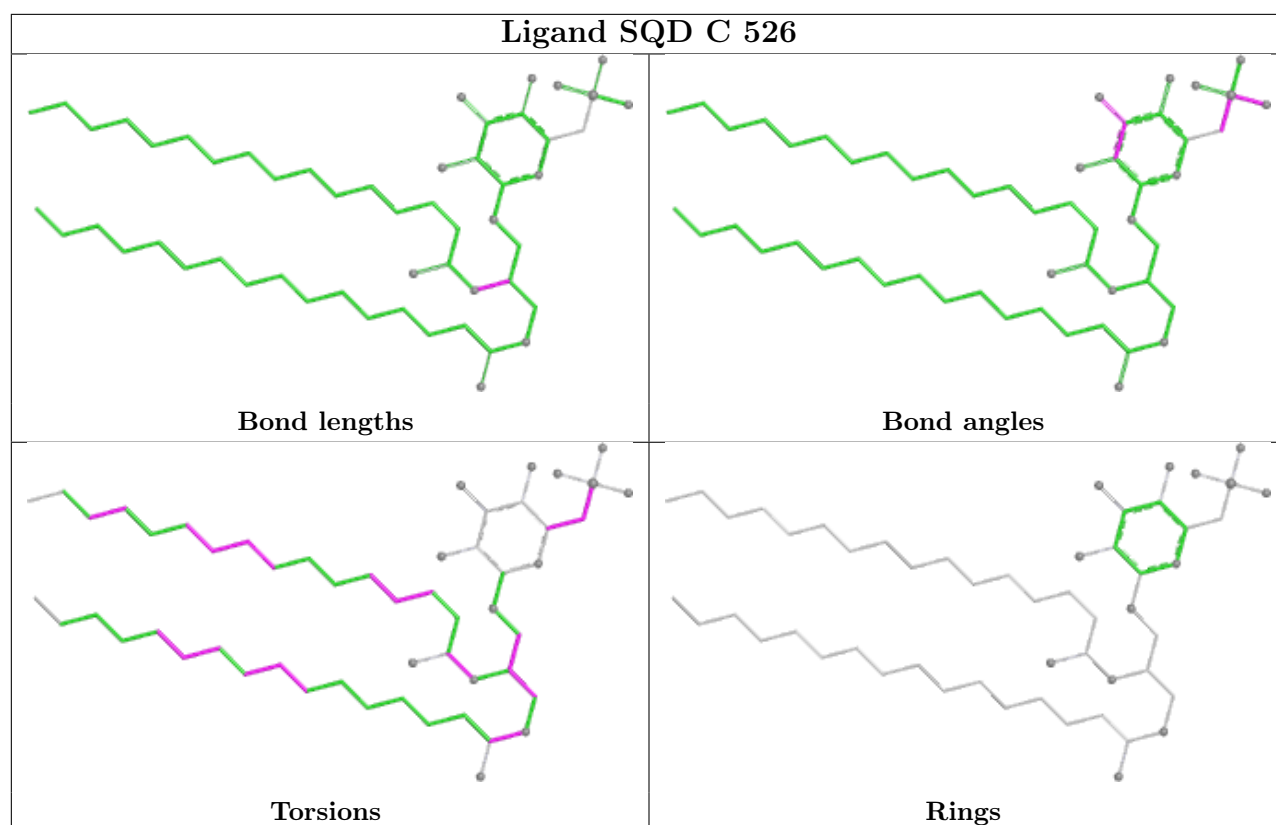


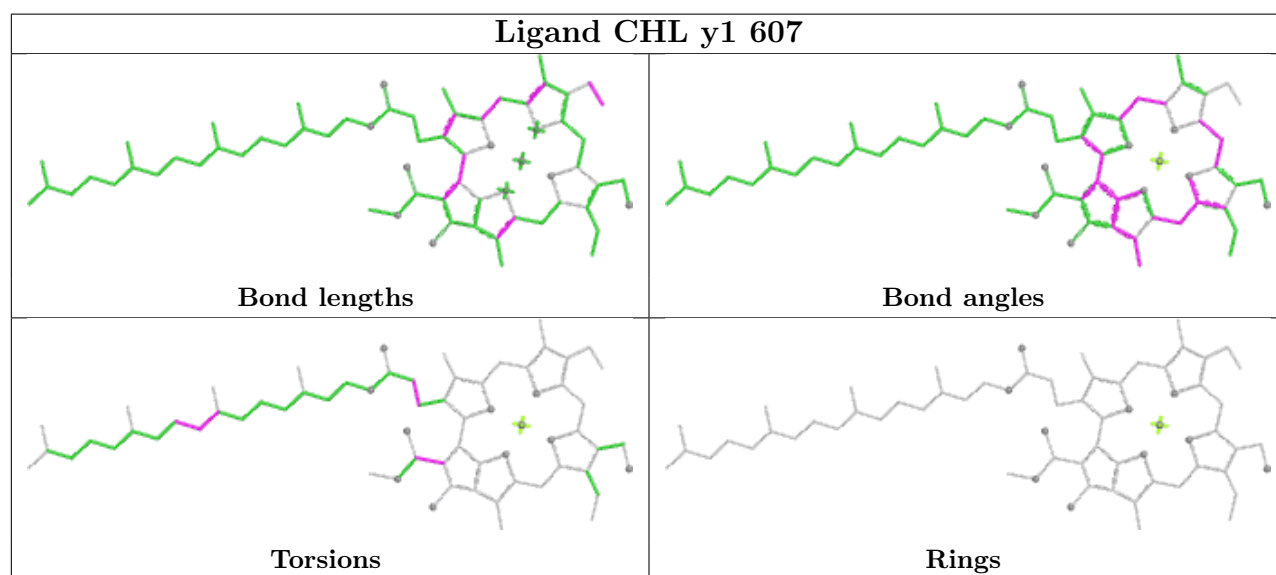
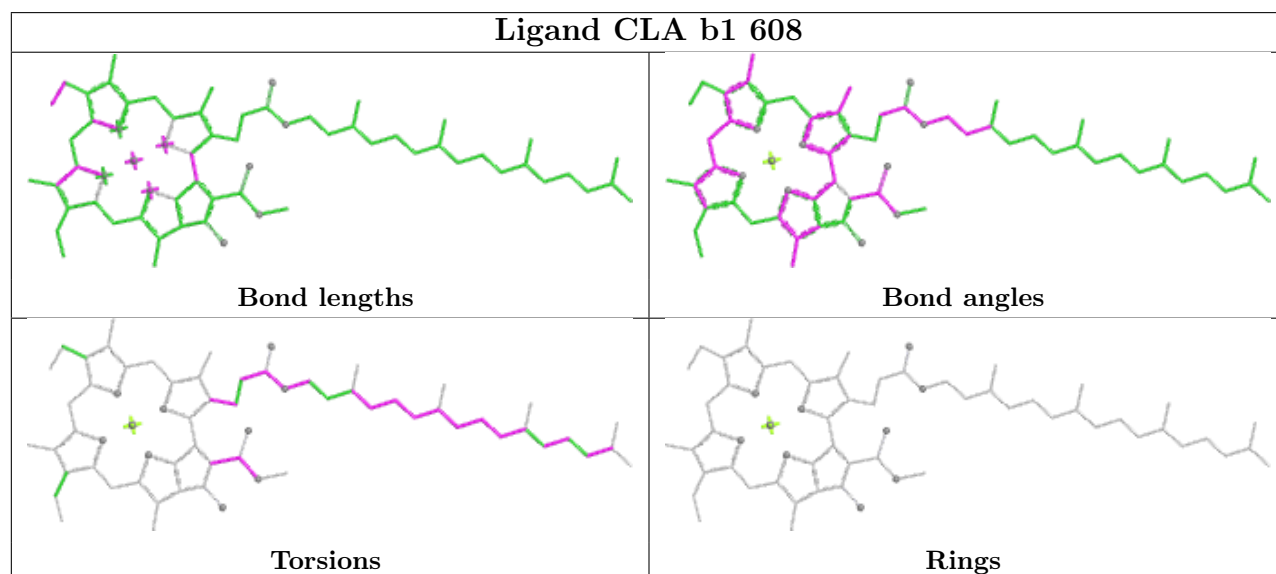
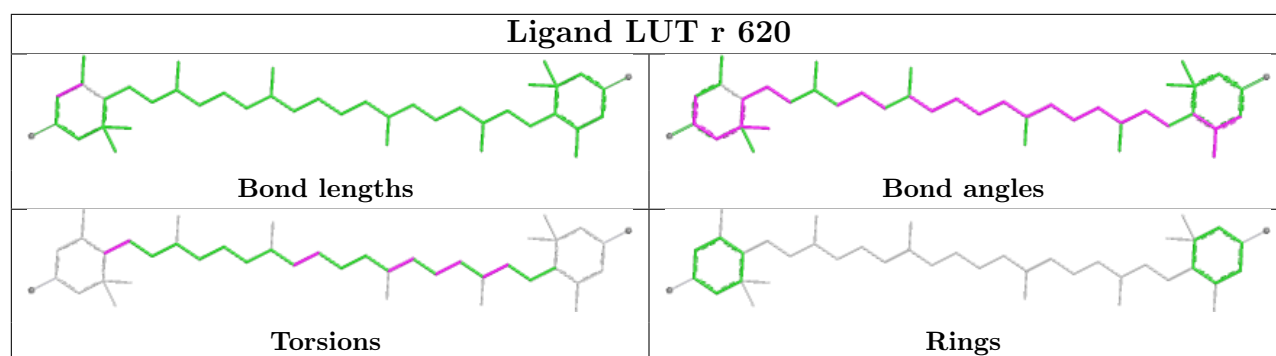


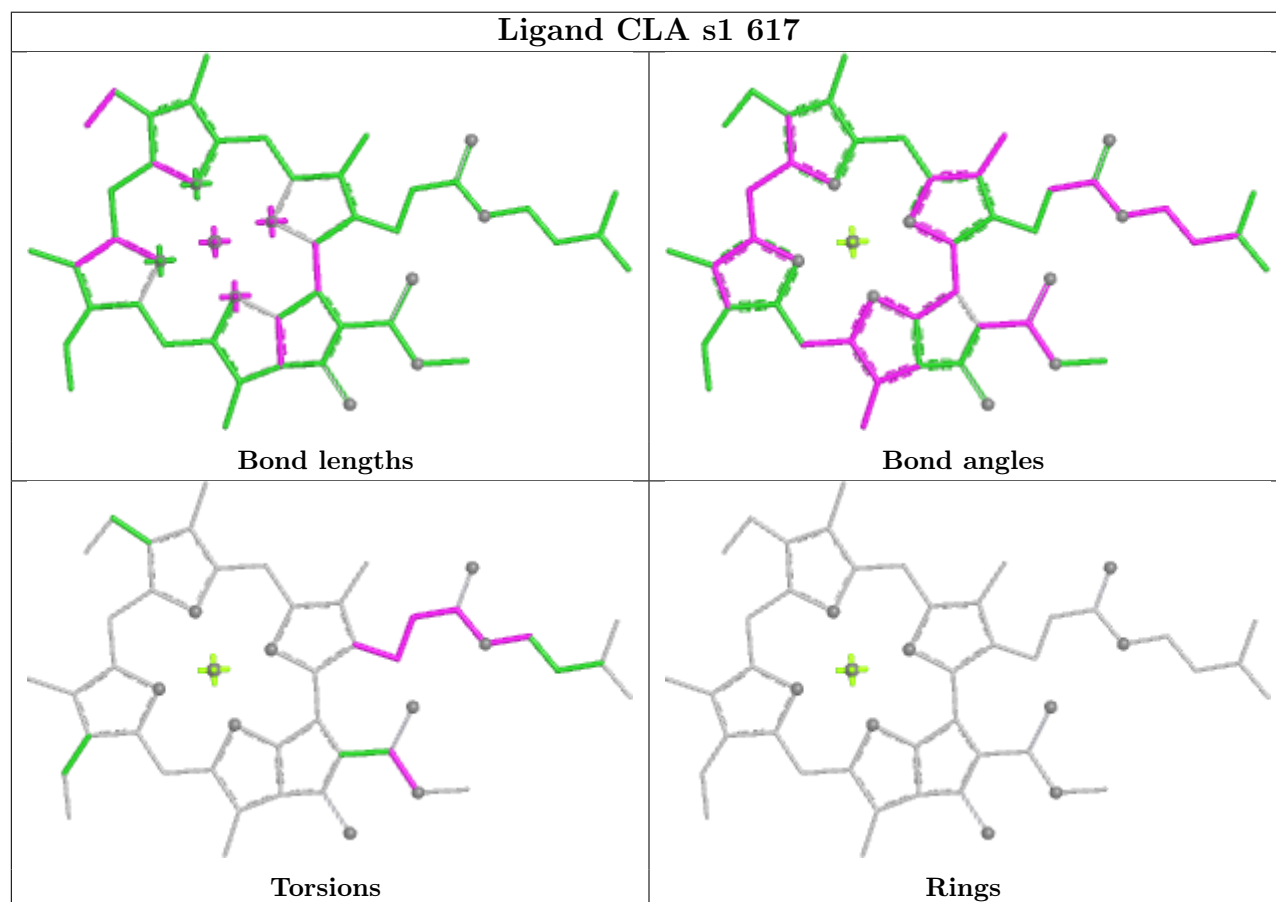
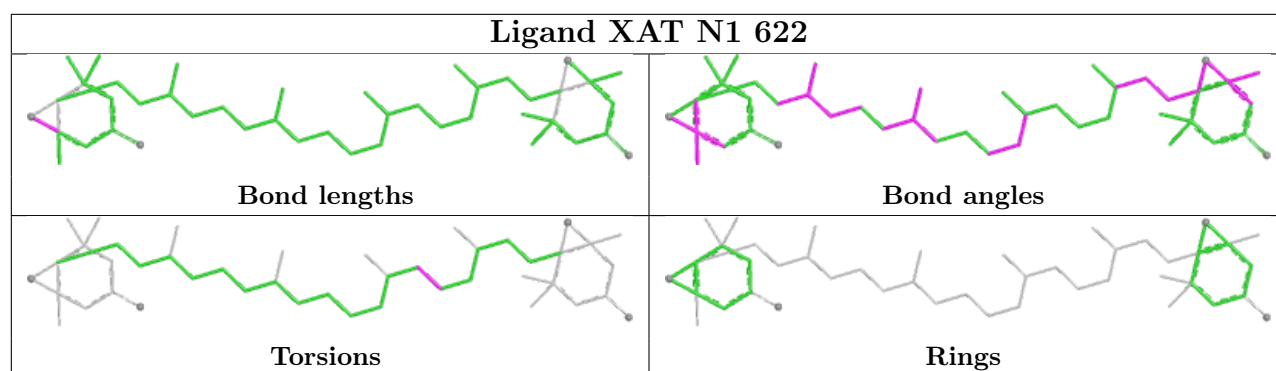


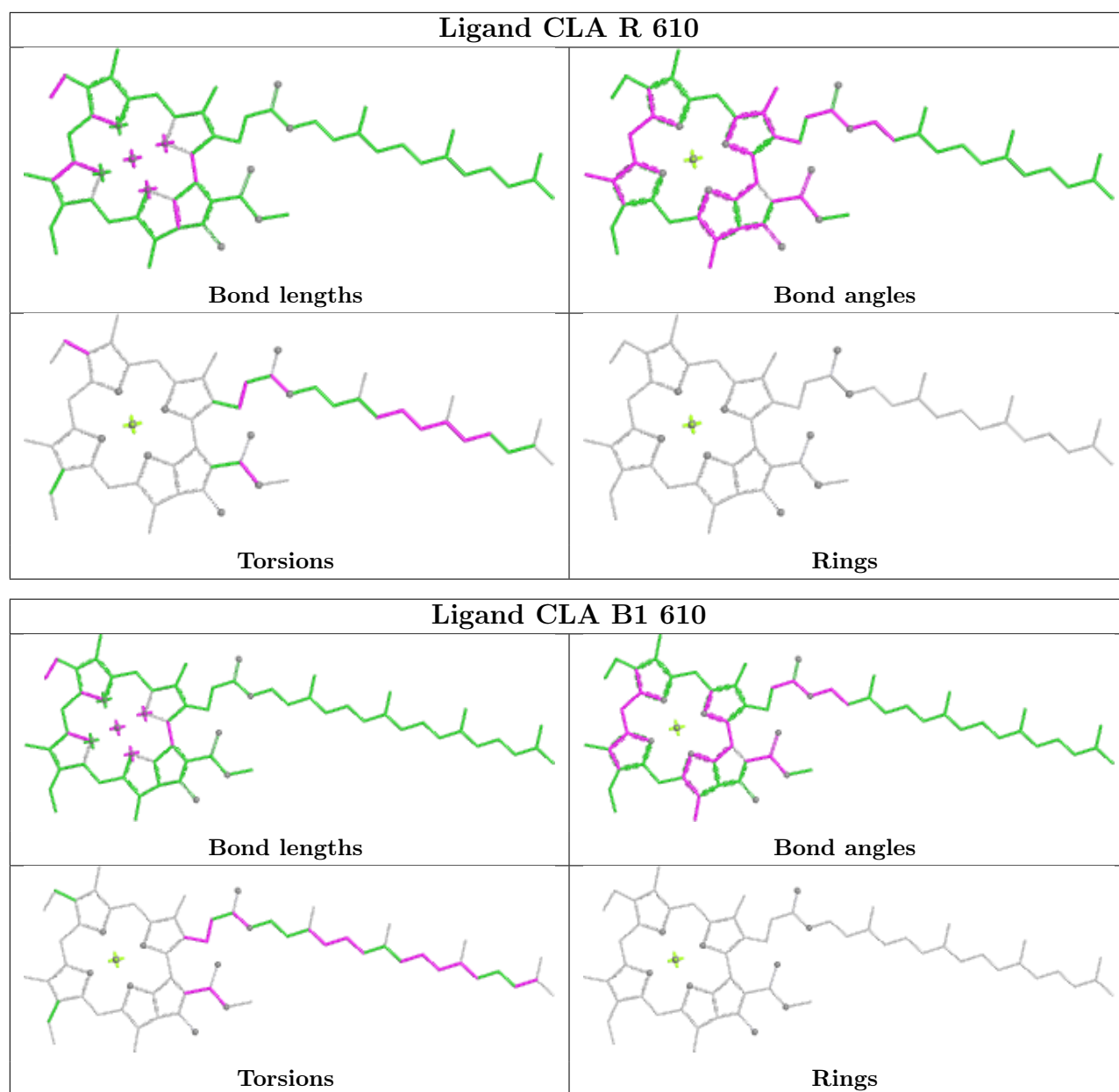


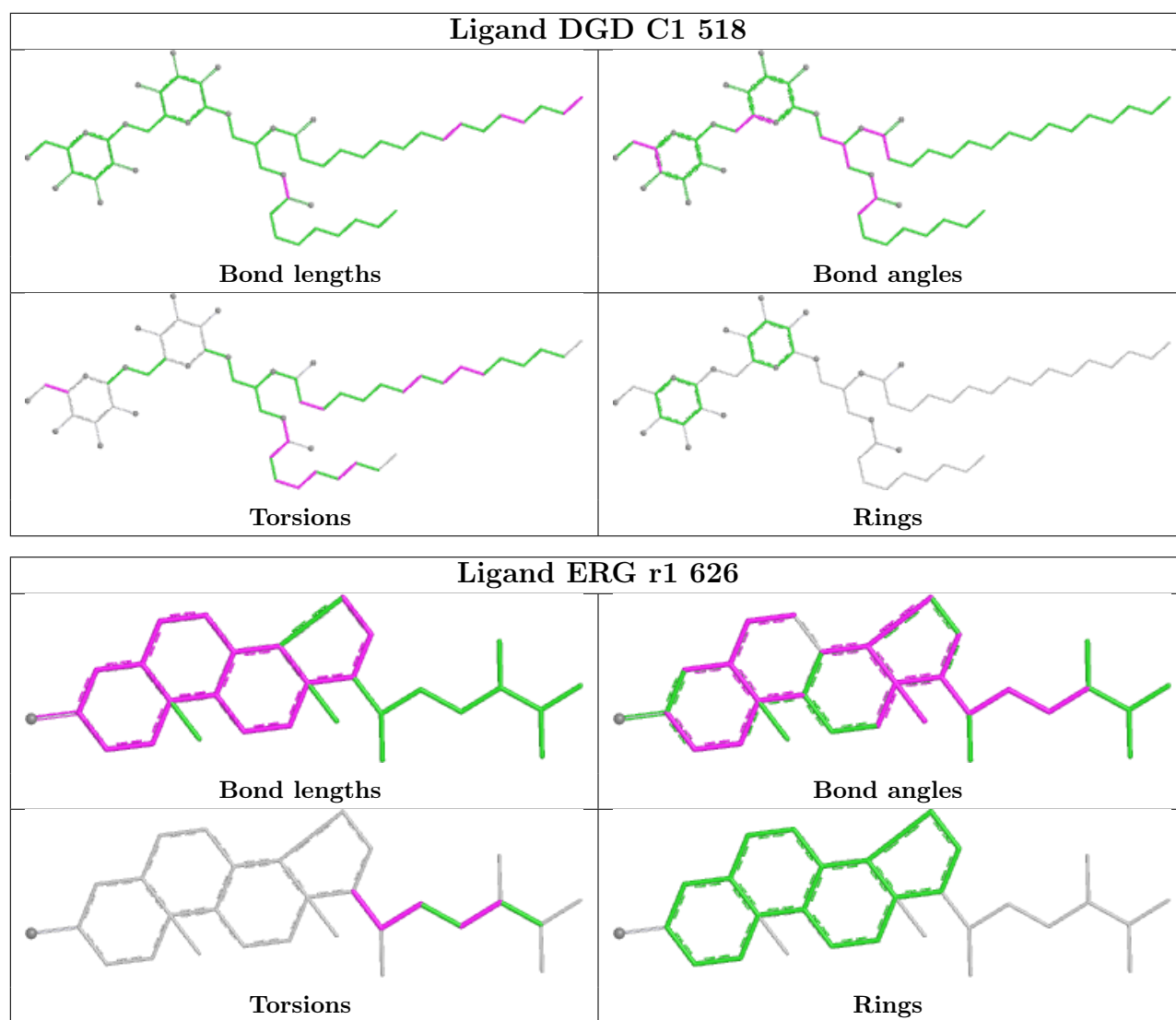


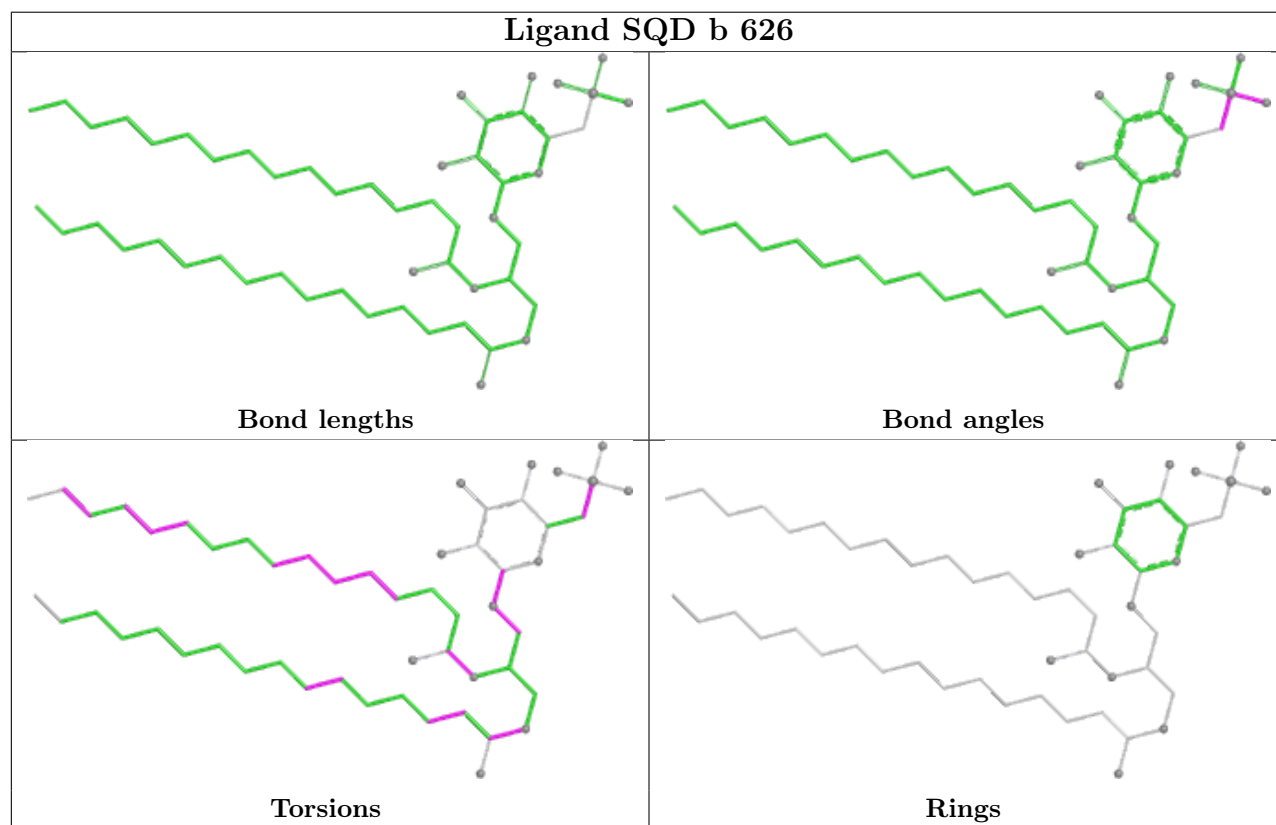
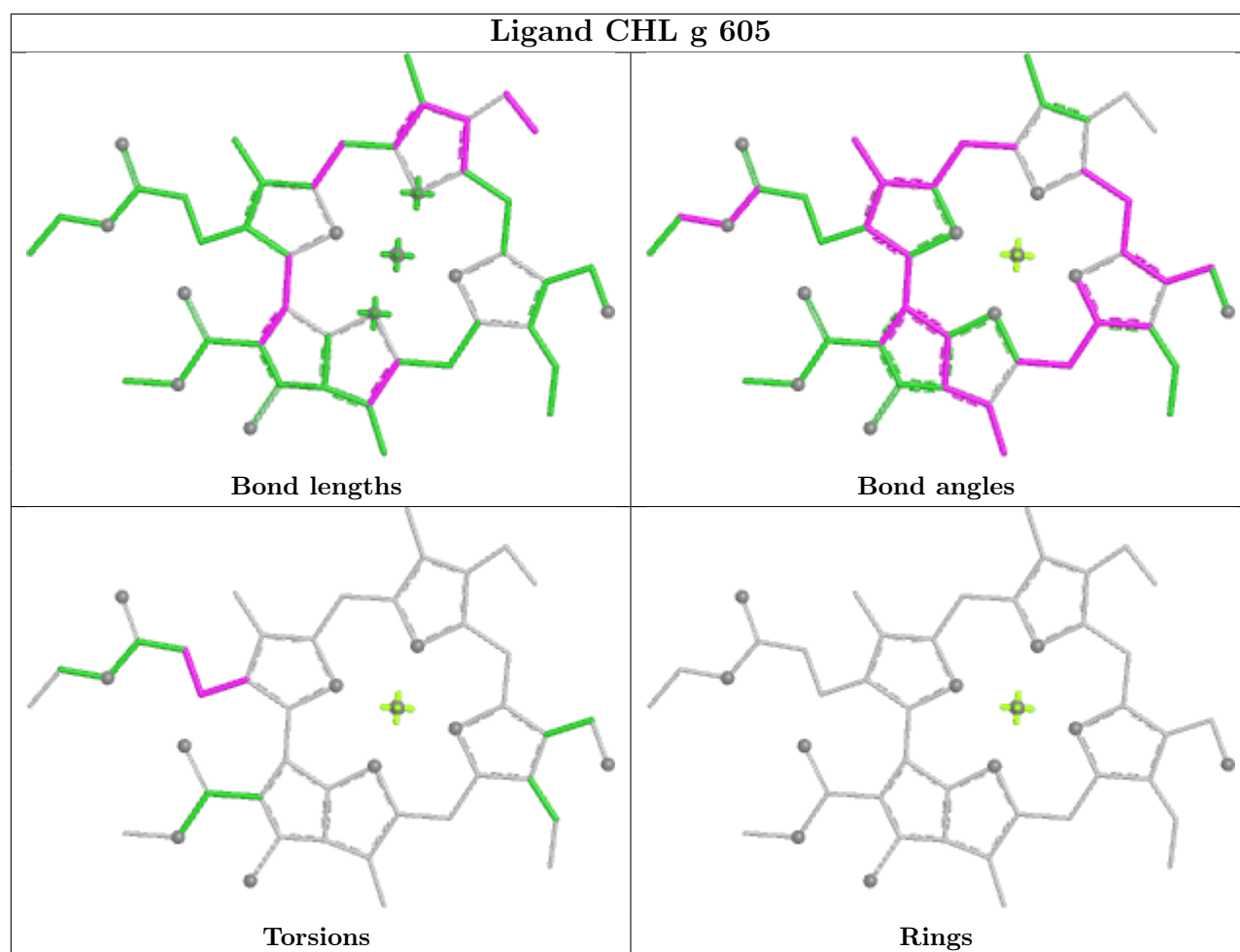


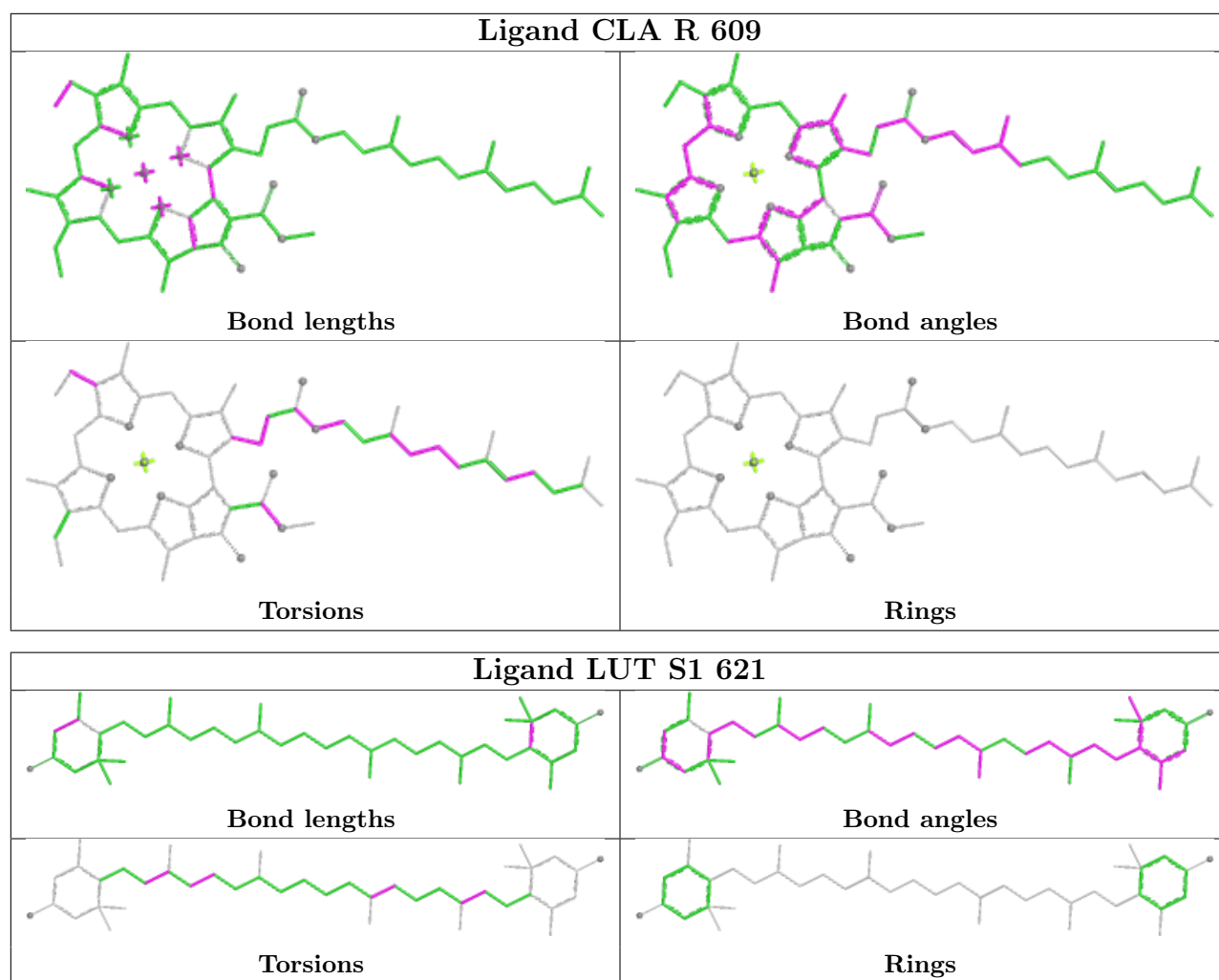


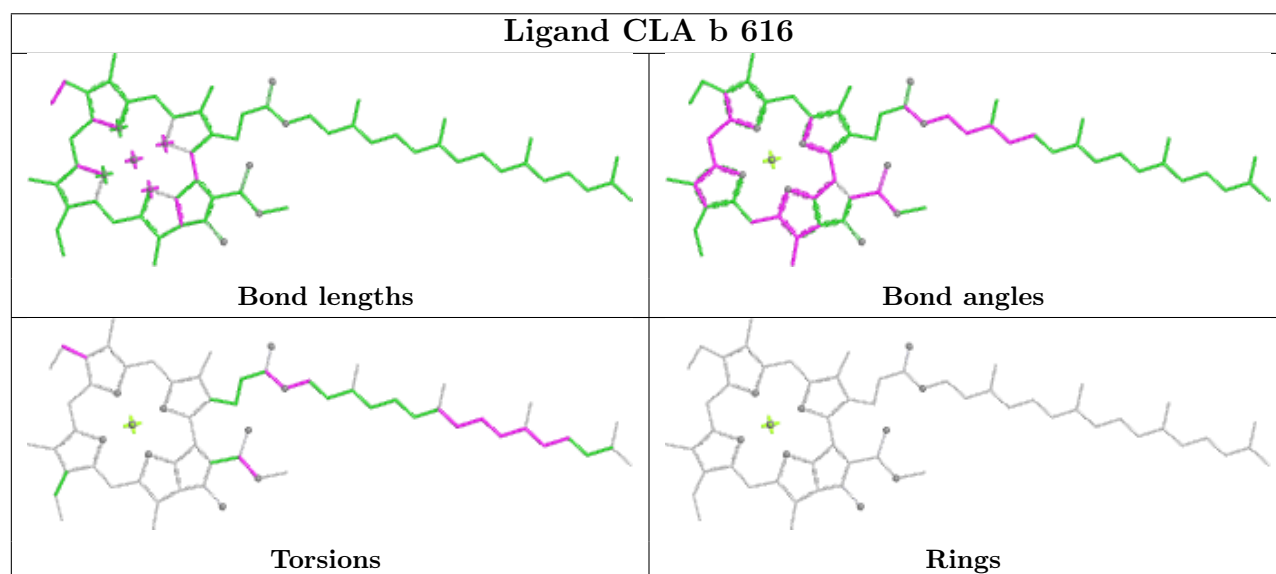
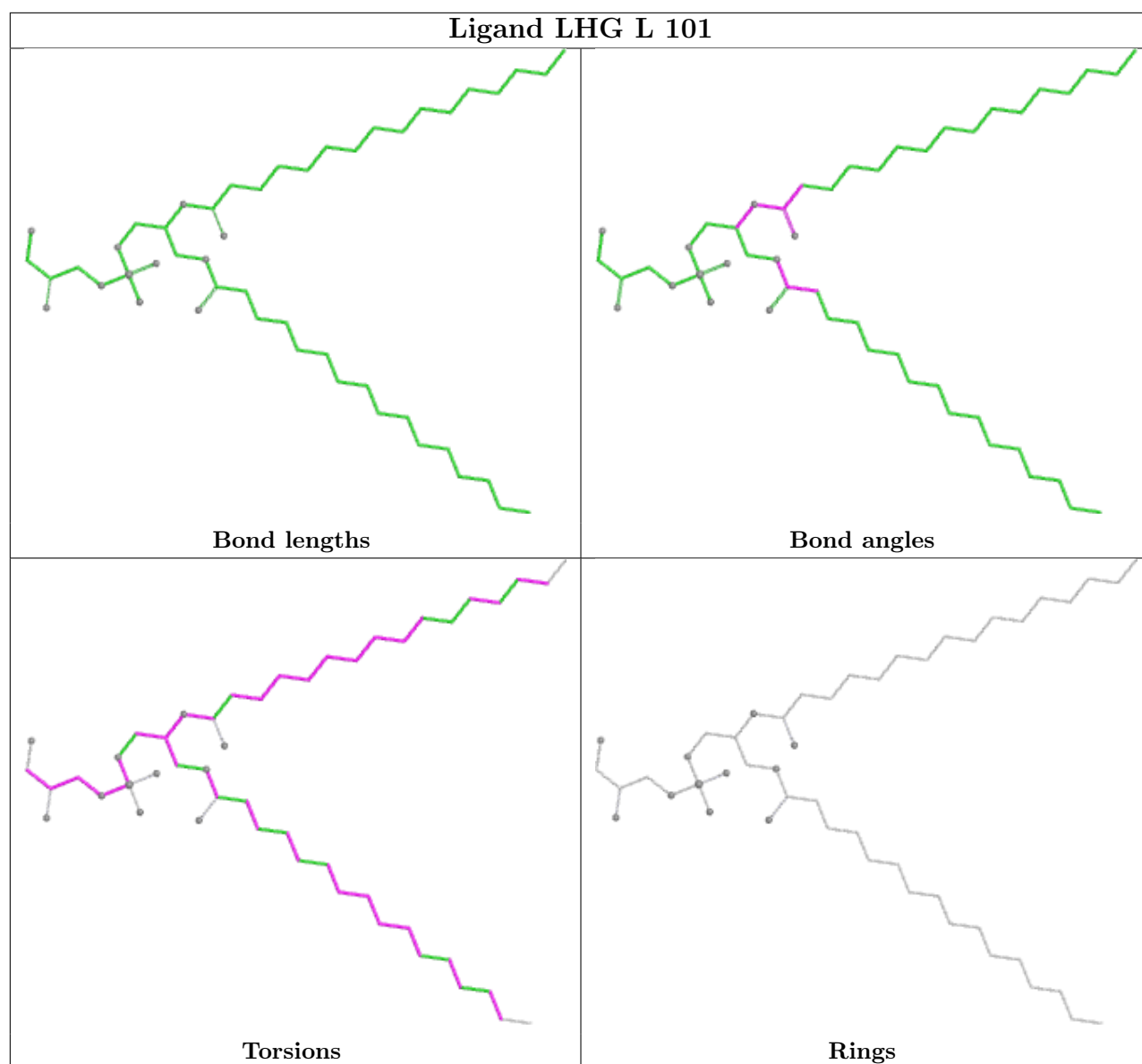


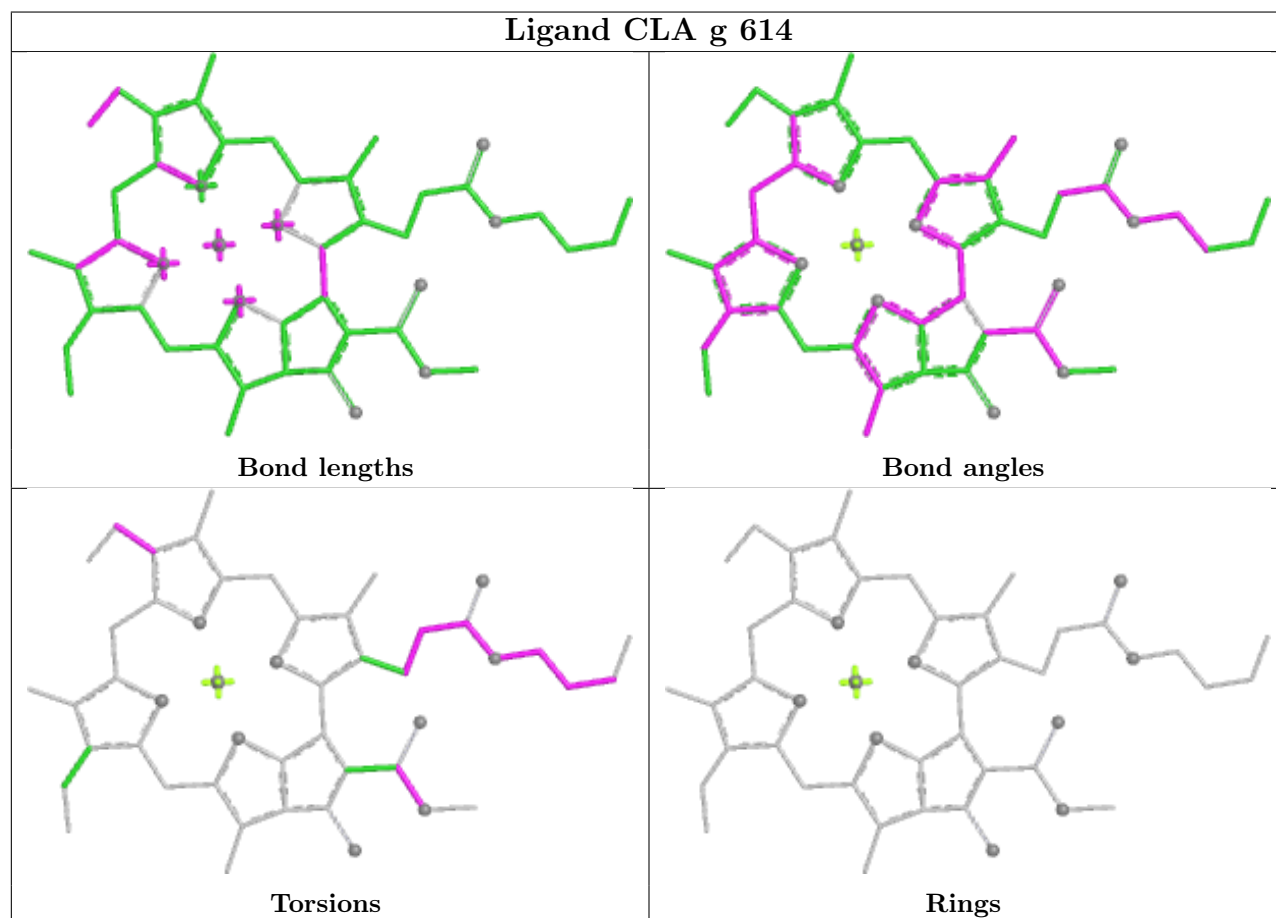
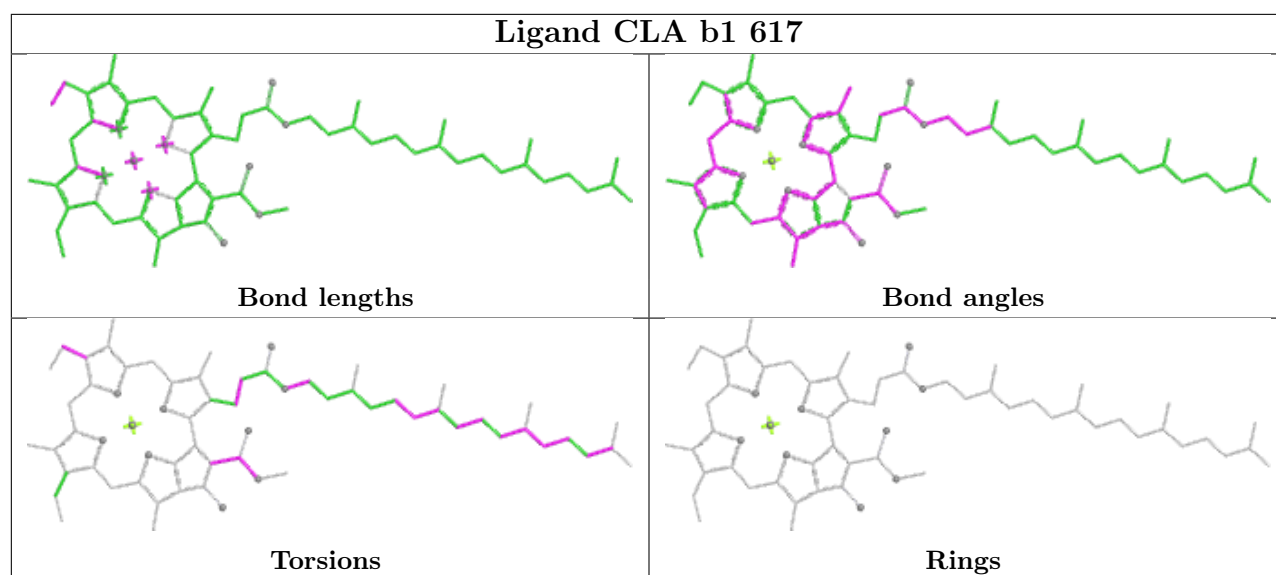


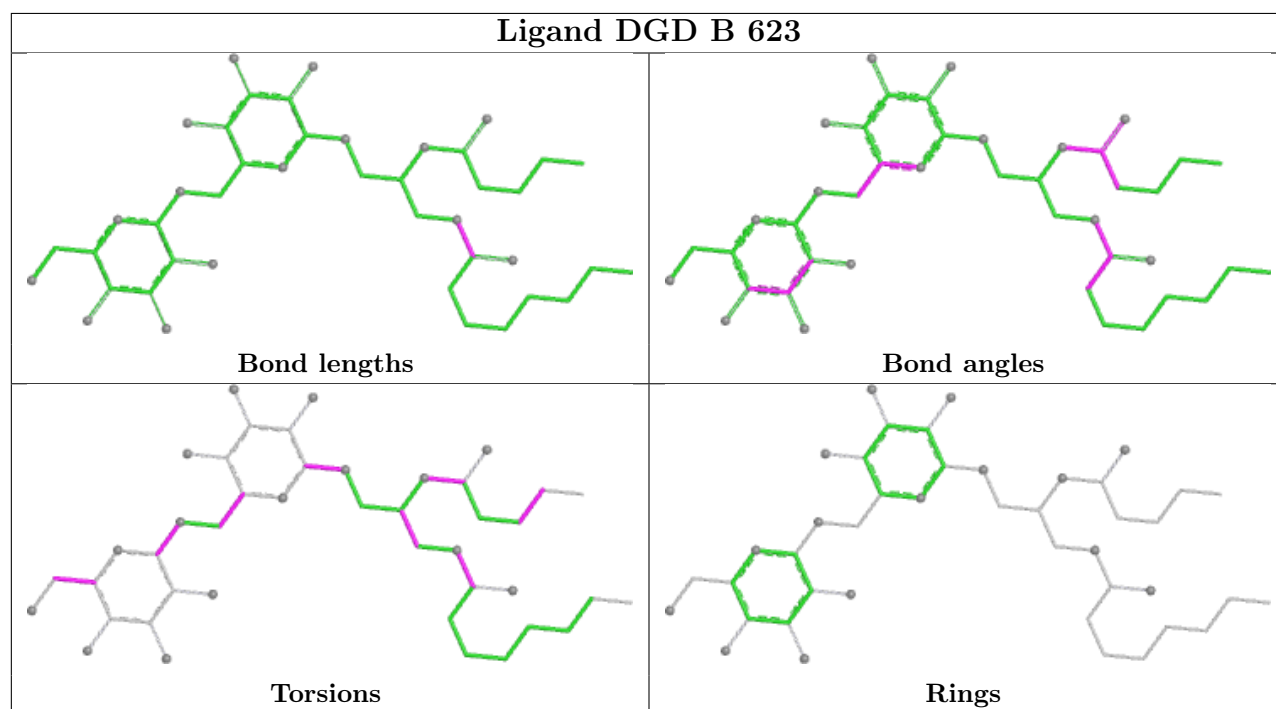
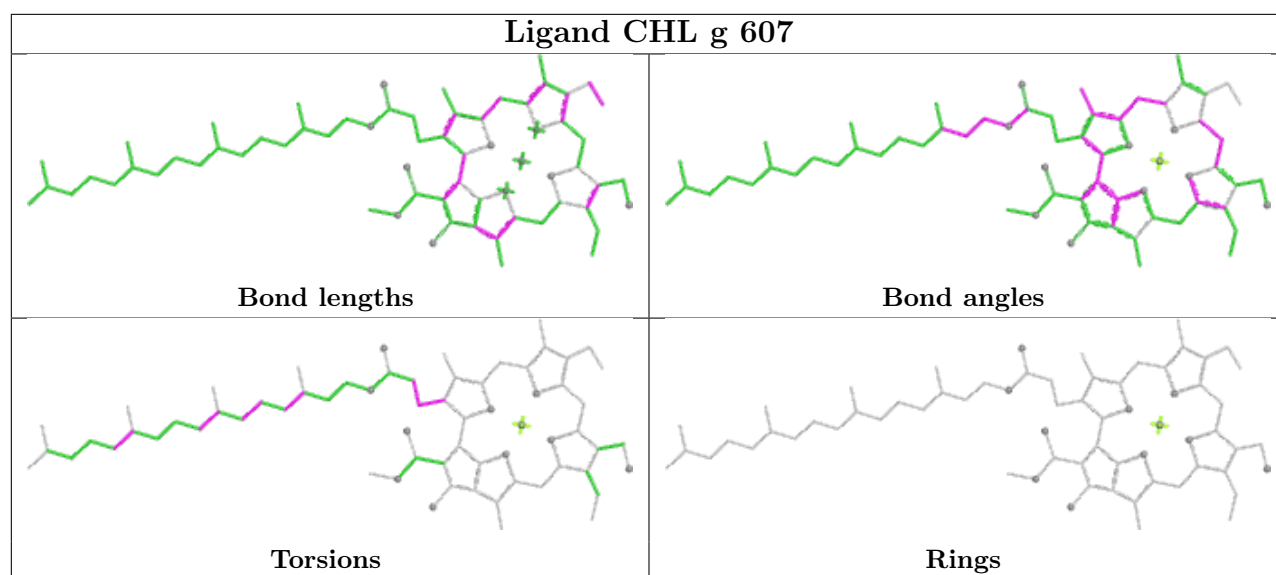


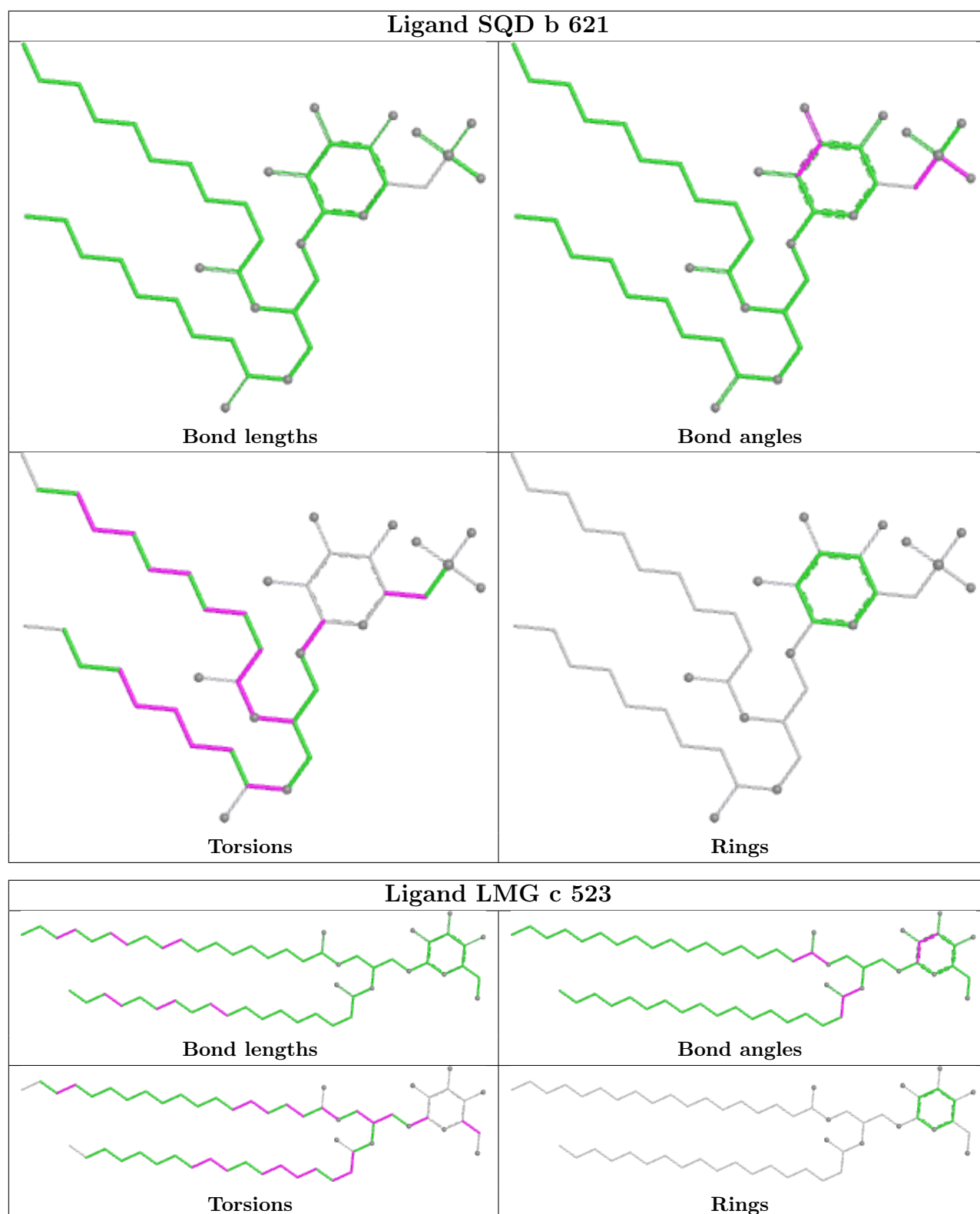




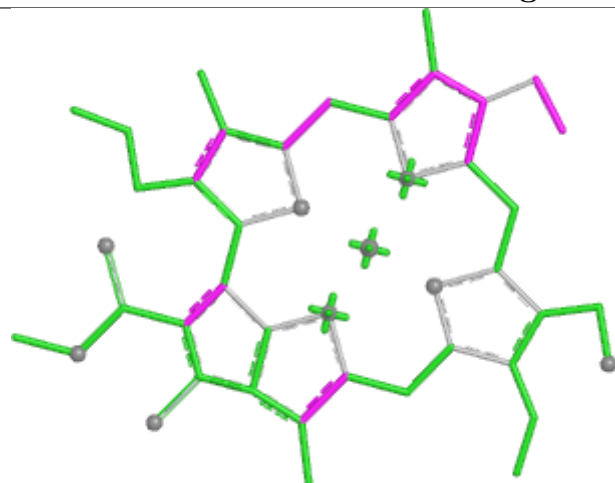




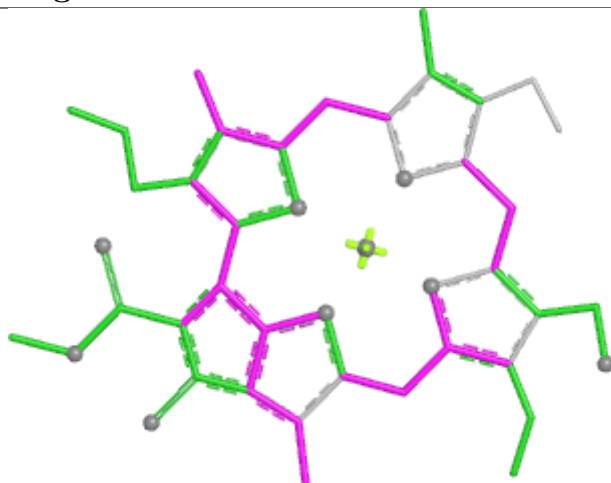




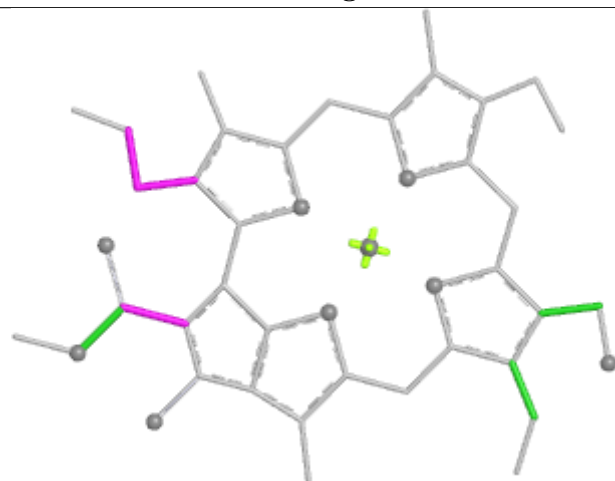
Ligand CHL g 608



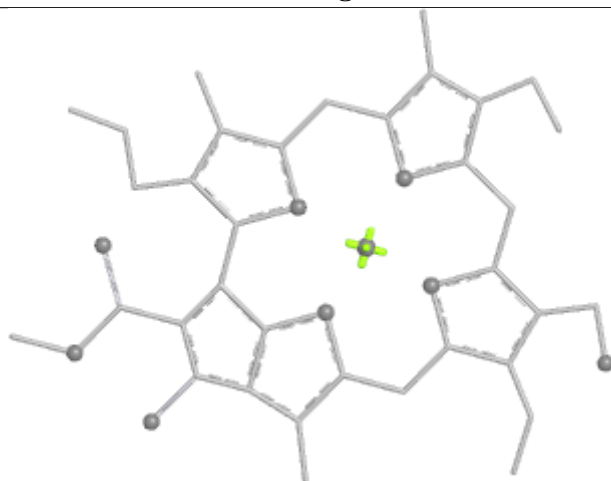
Bond lengths



Bond angles

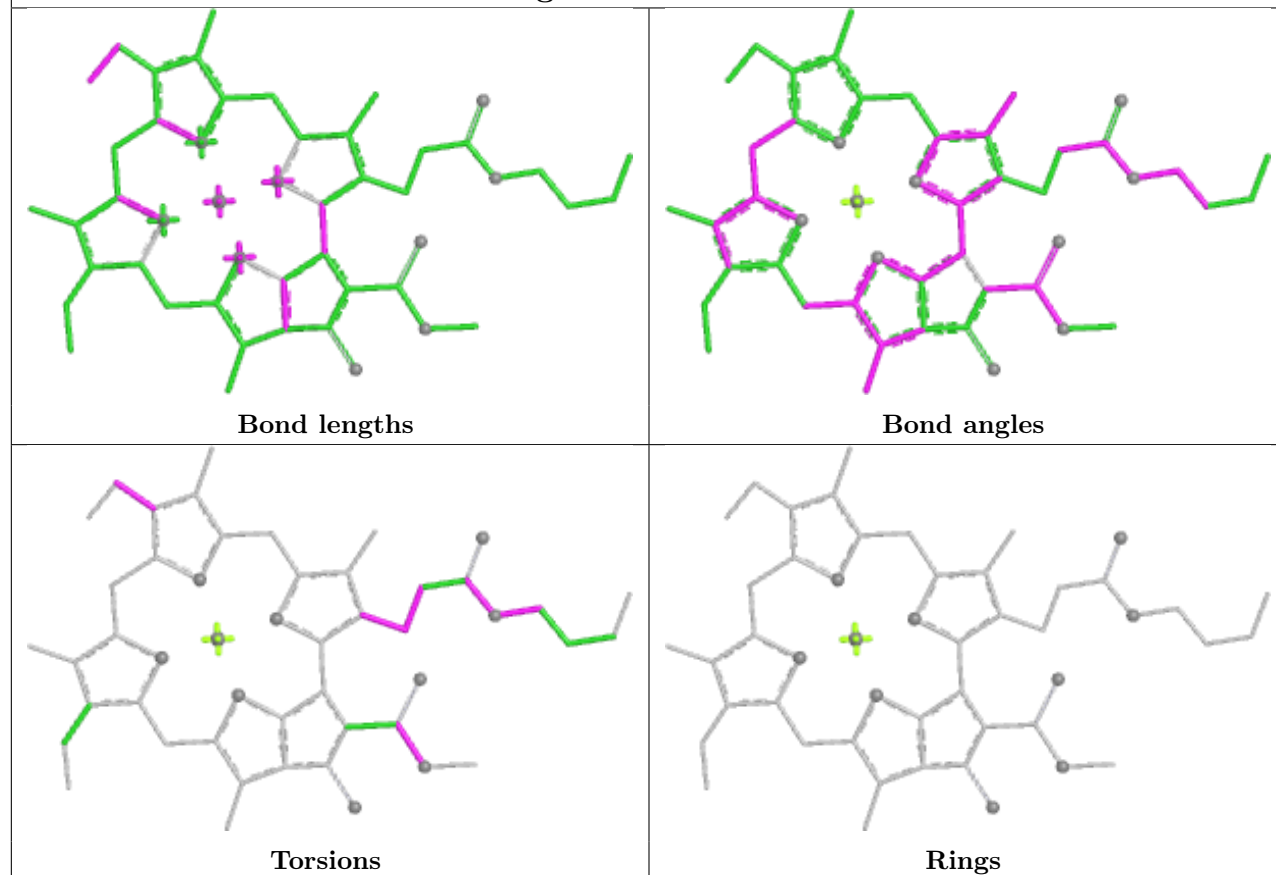


Torsions

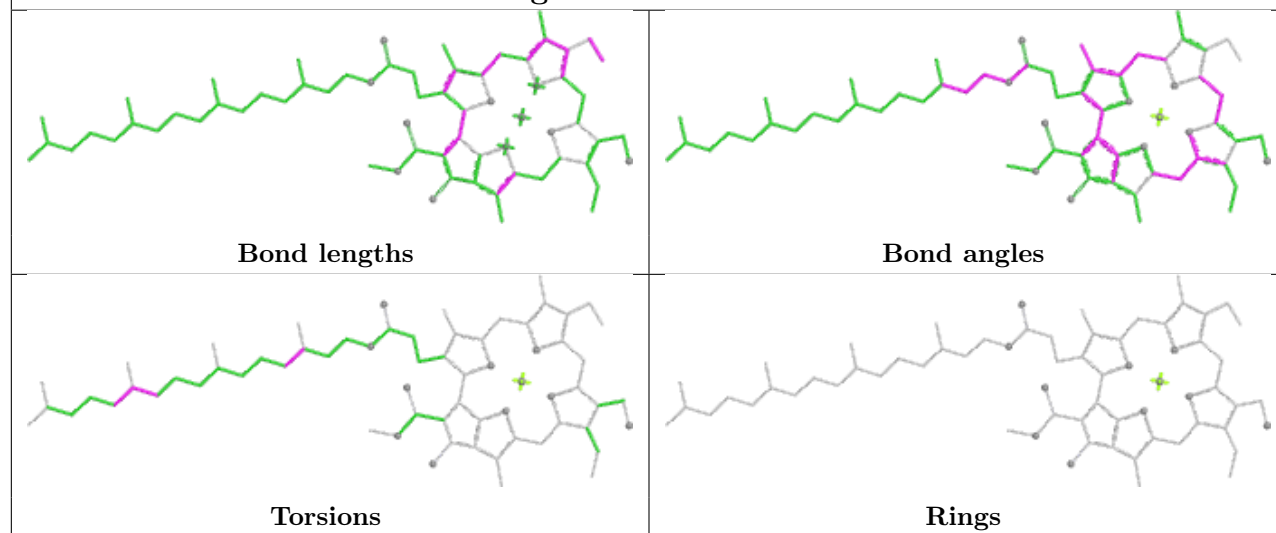


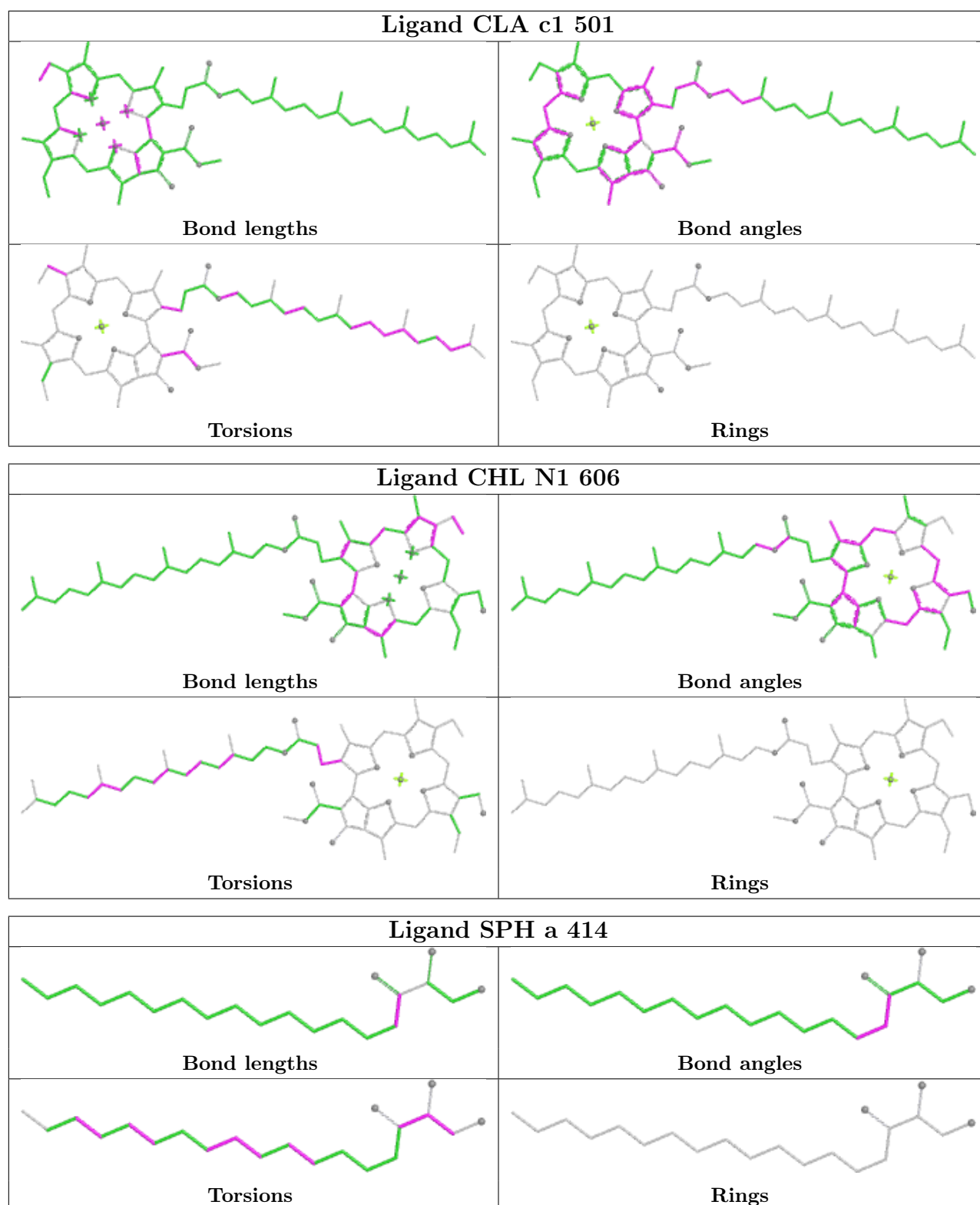
Rings

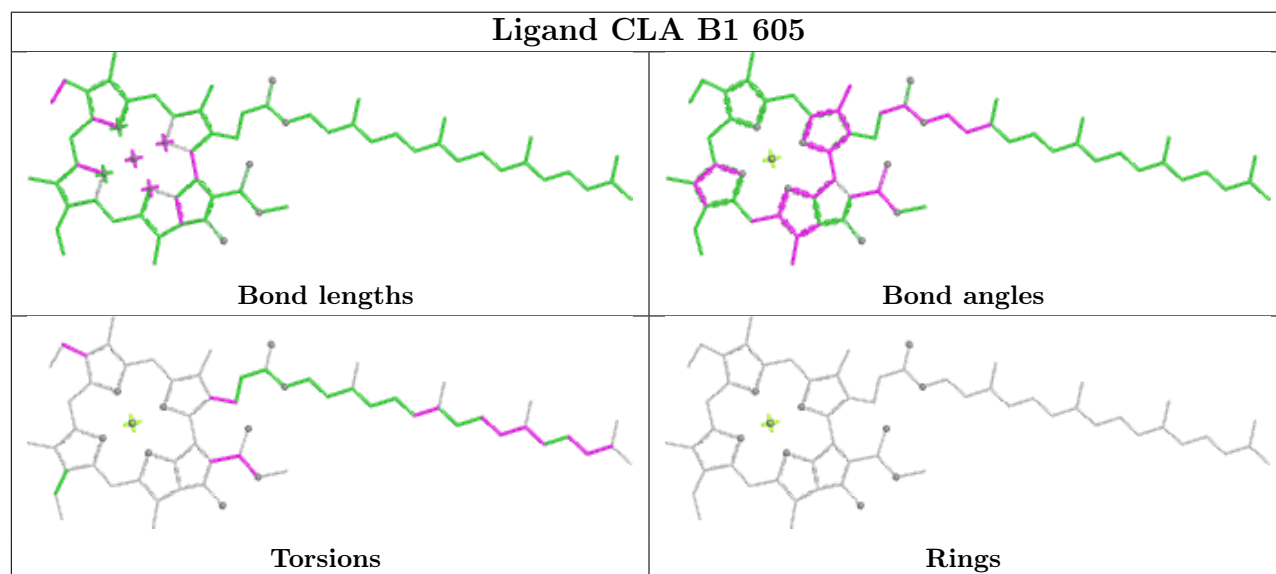
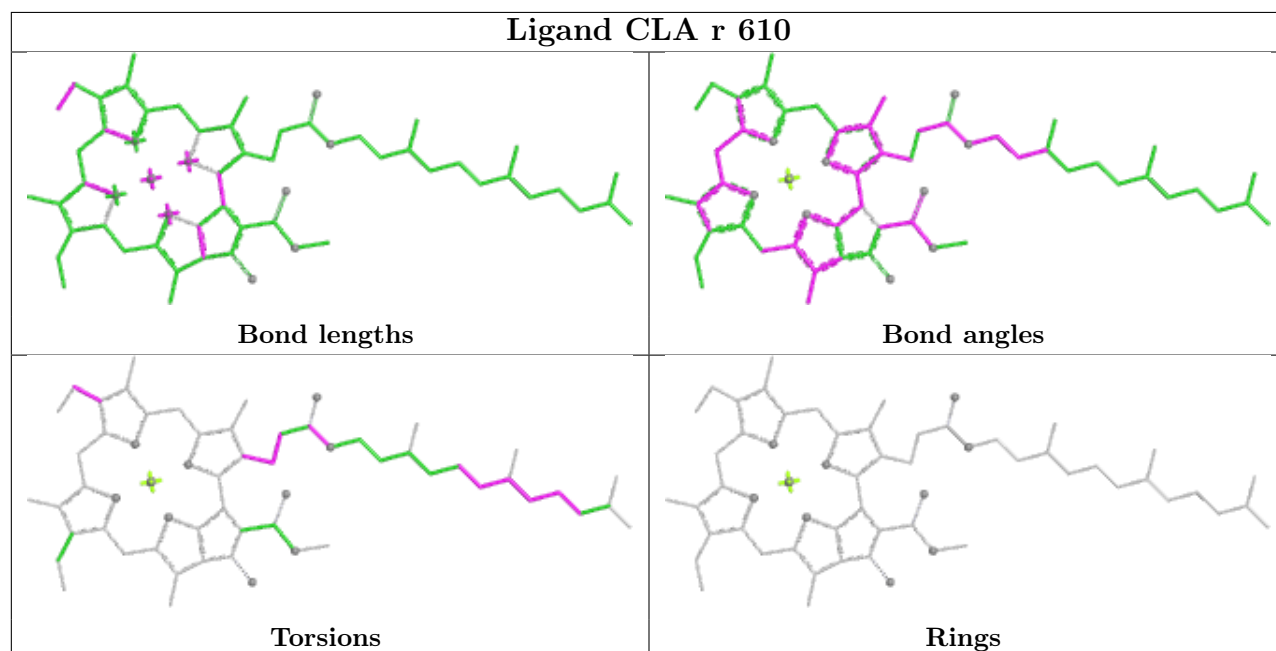
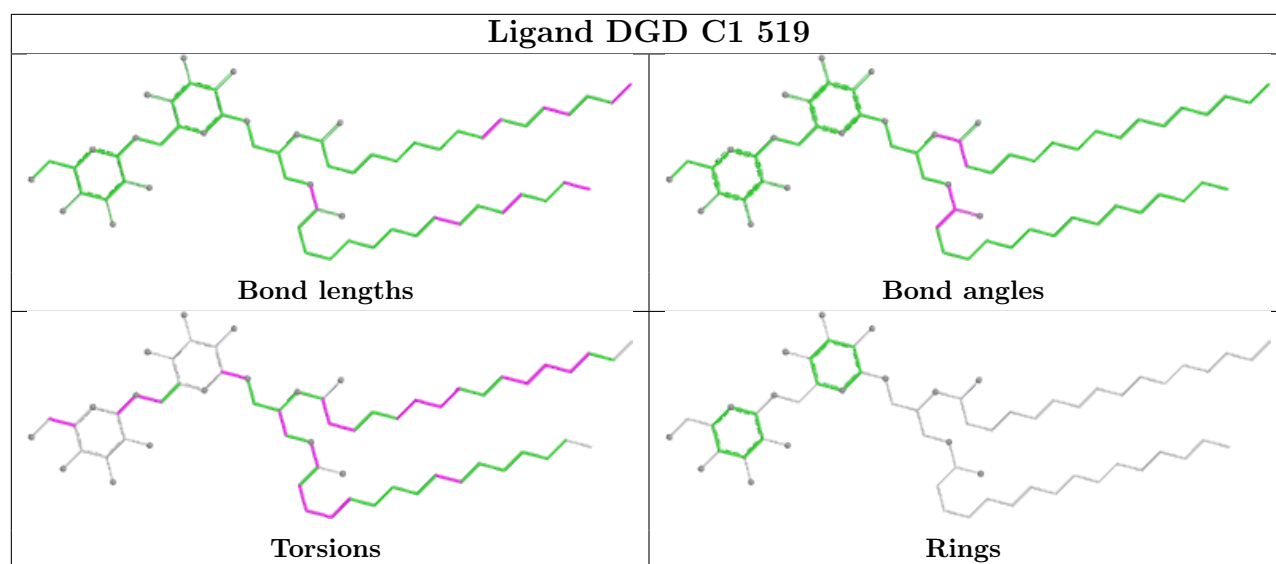
Ligand CLA a 407

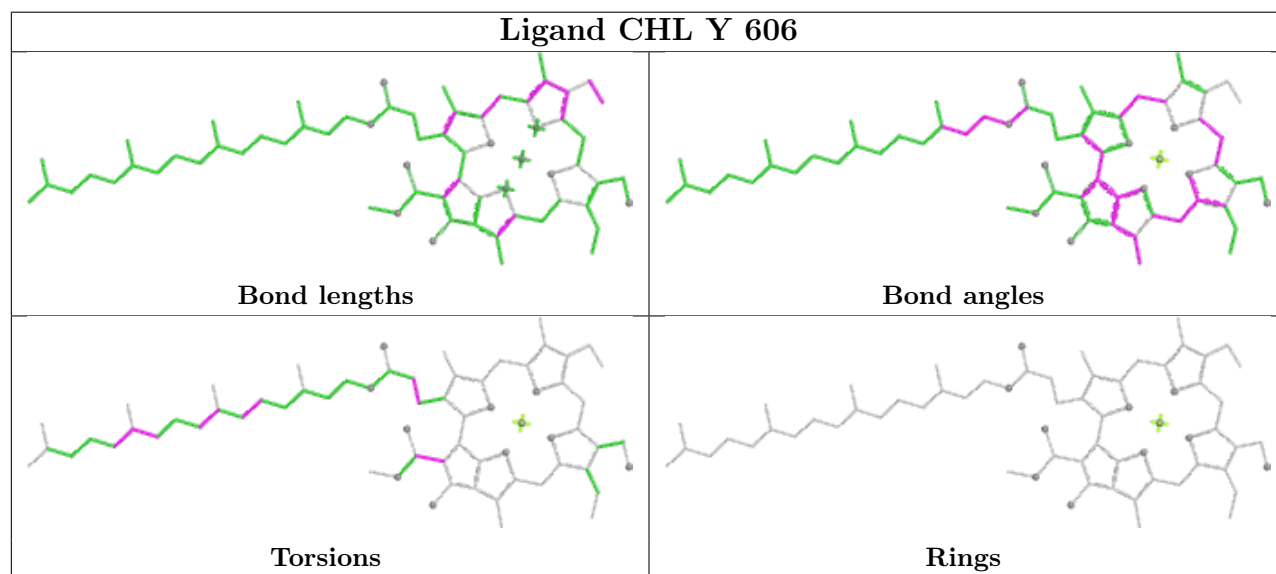
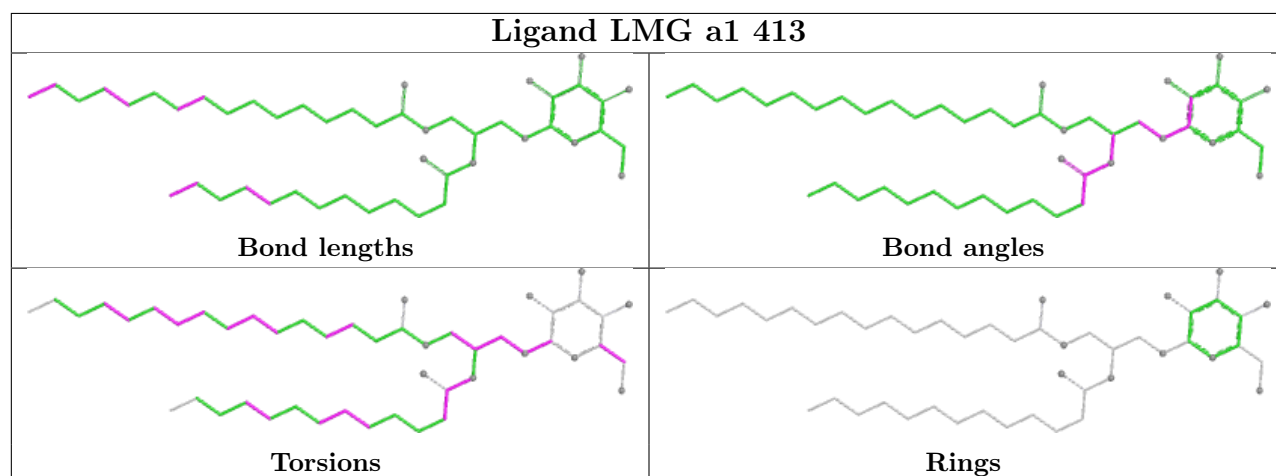
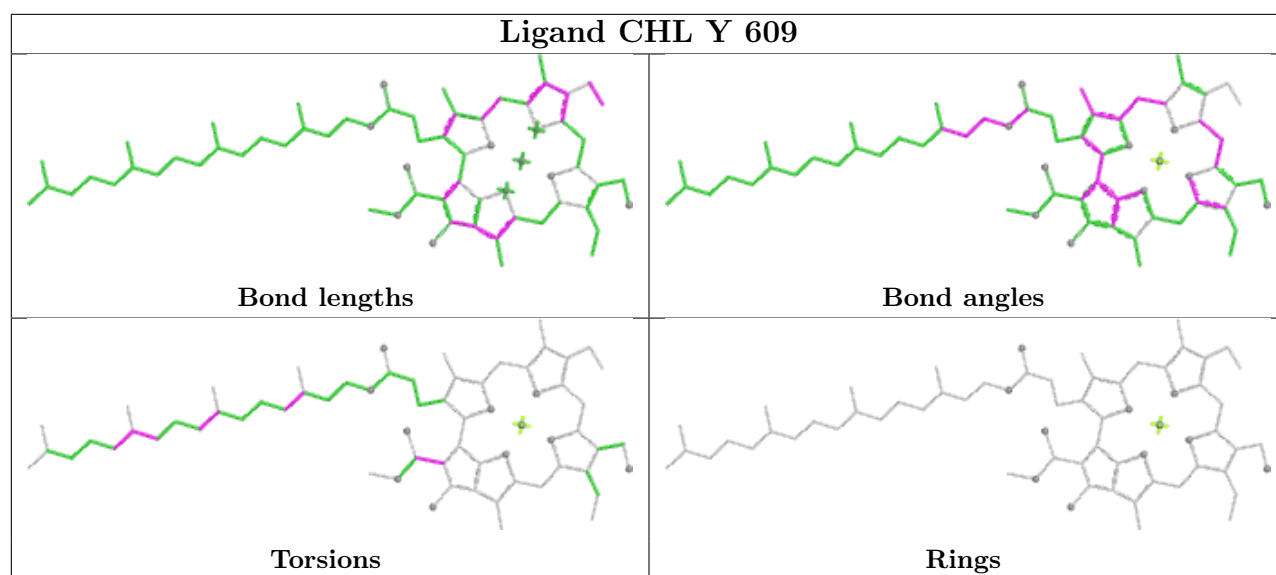


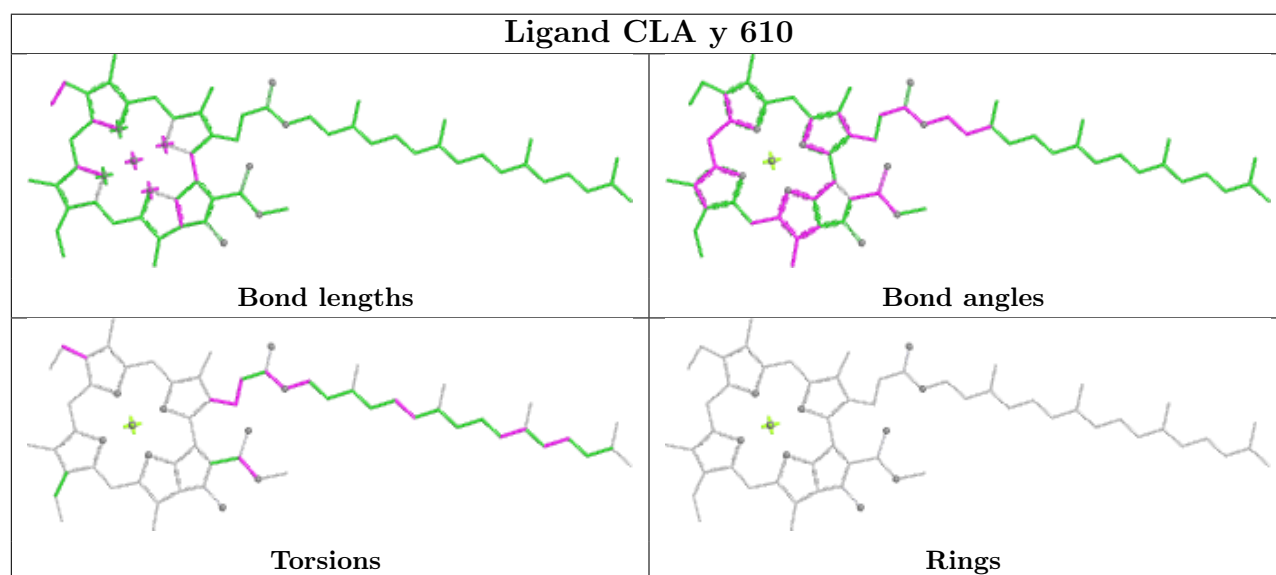
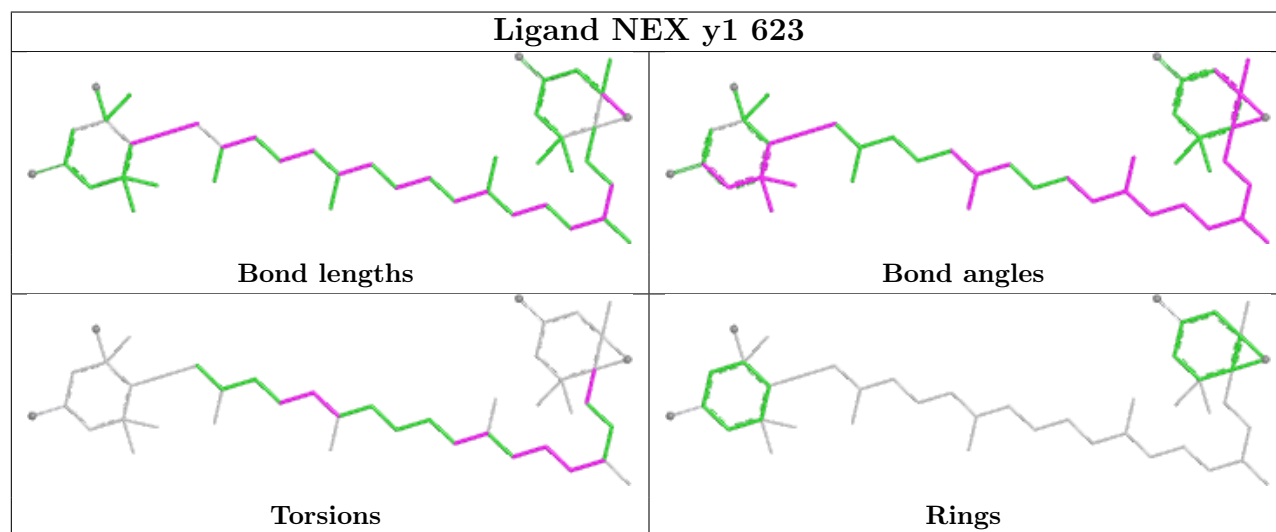
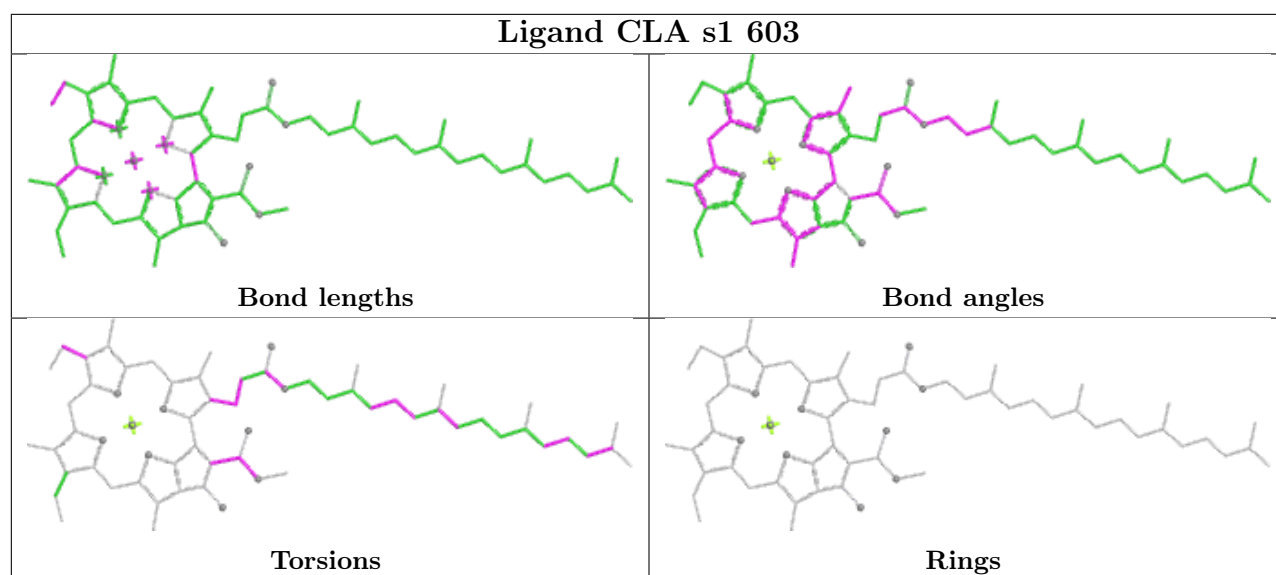
Ligand CHL N 601

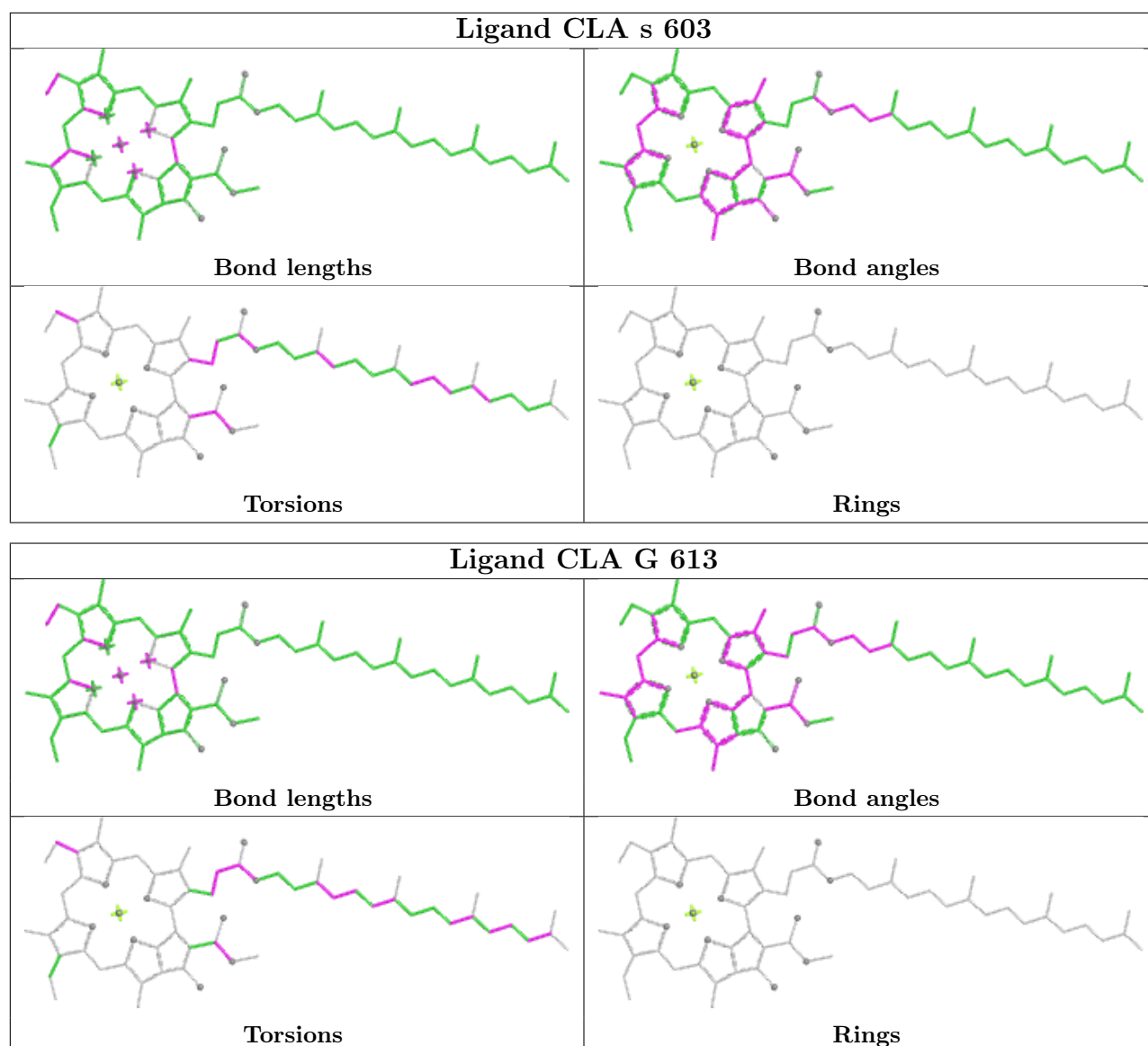


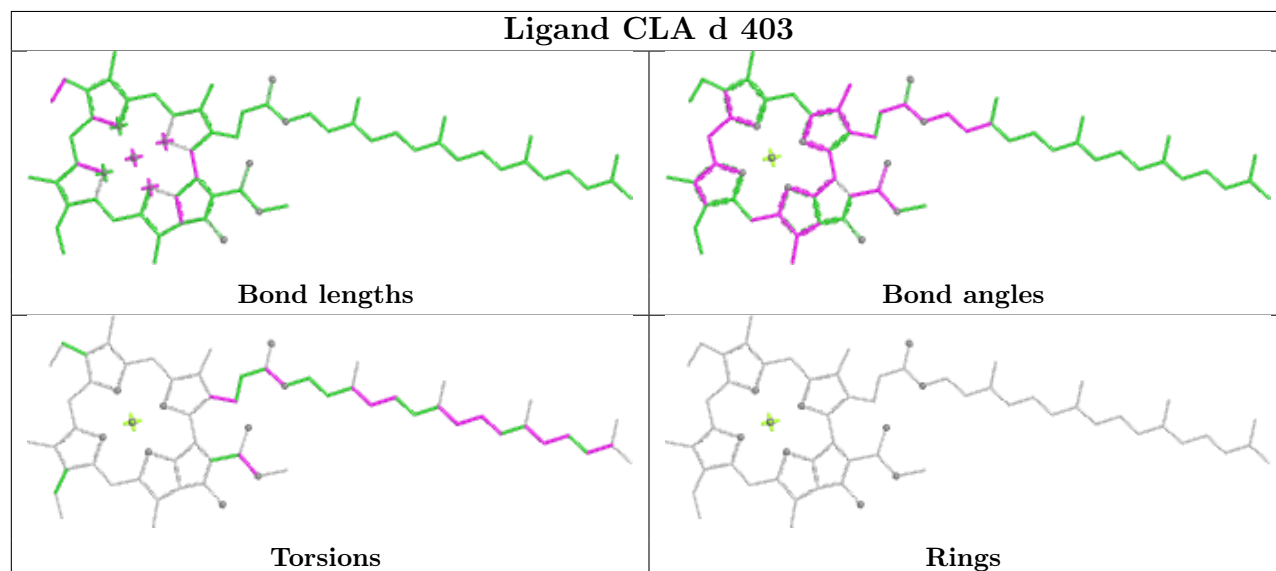
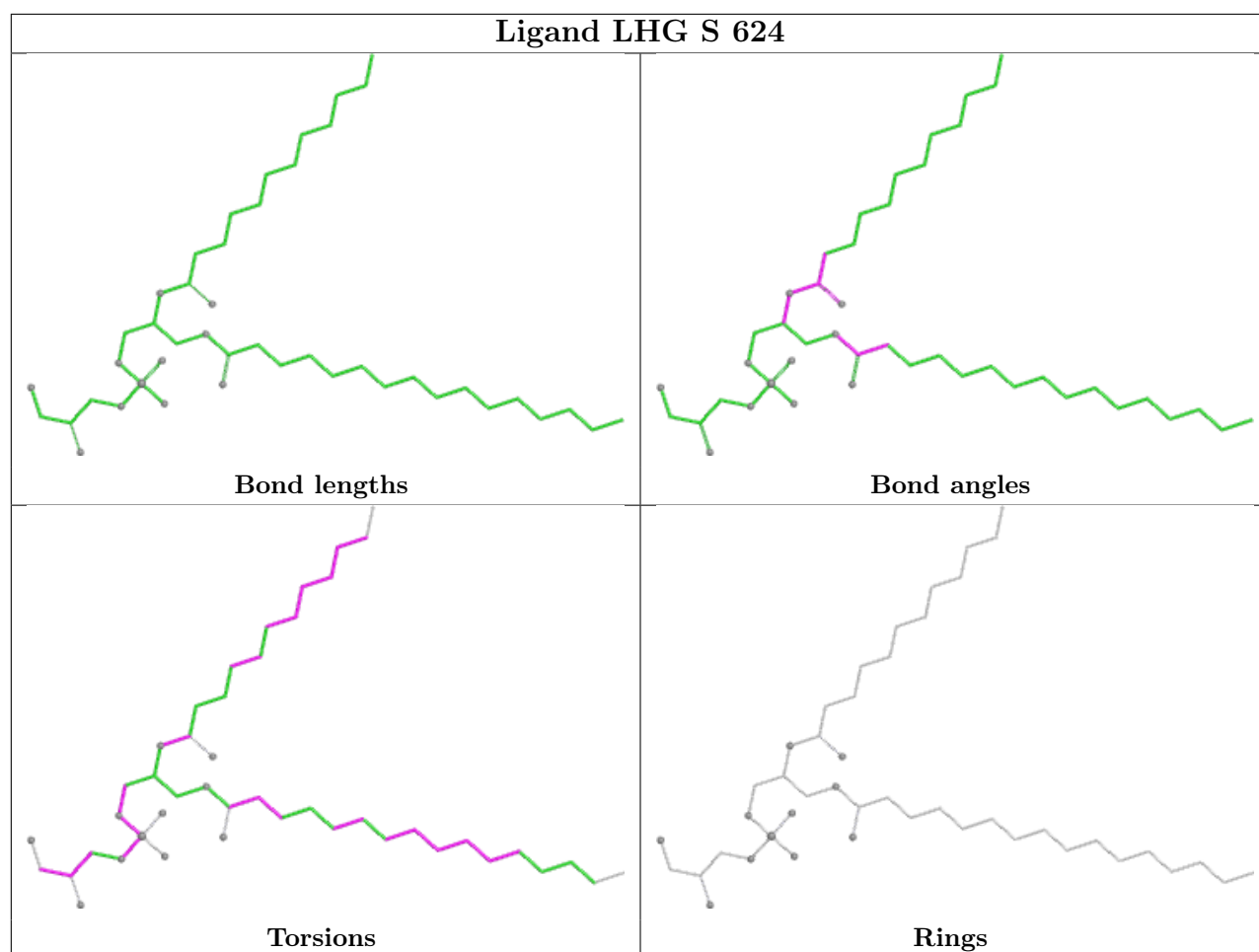


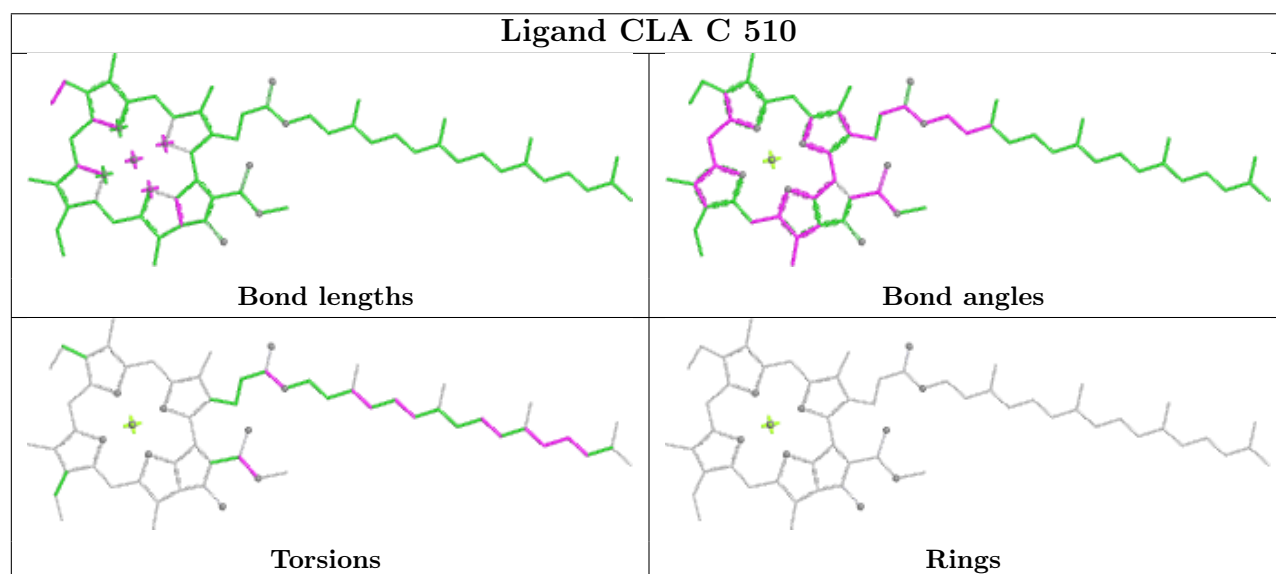
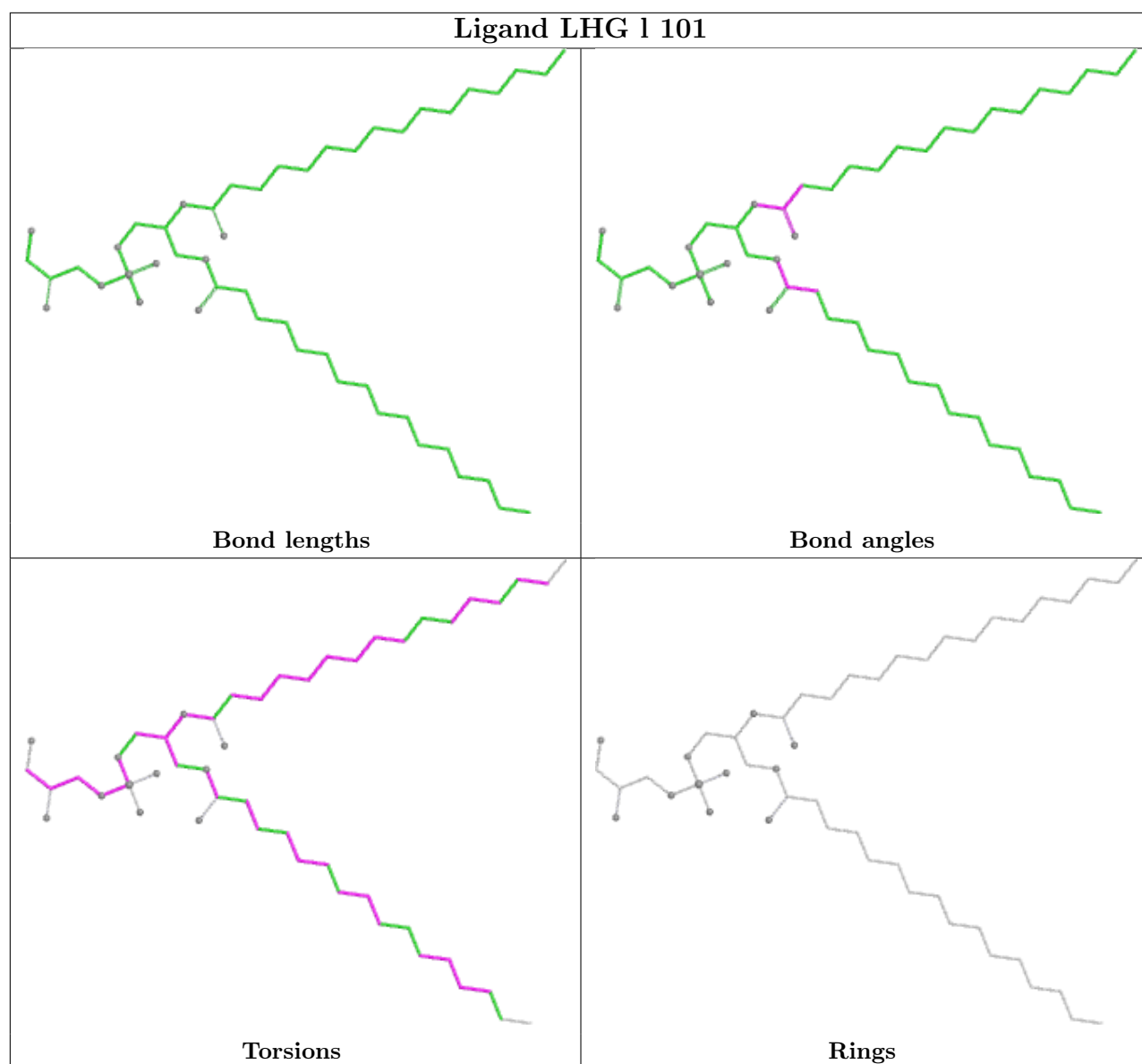


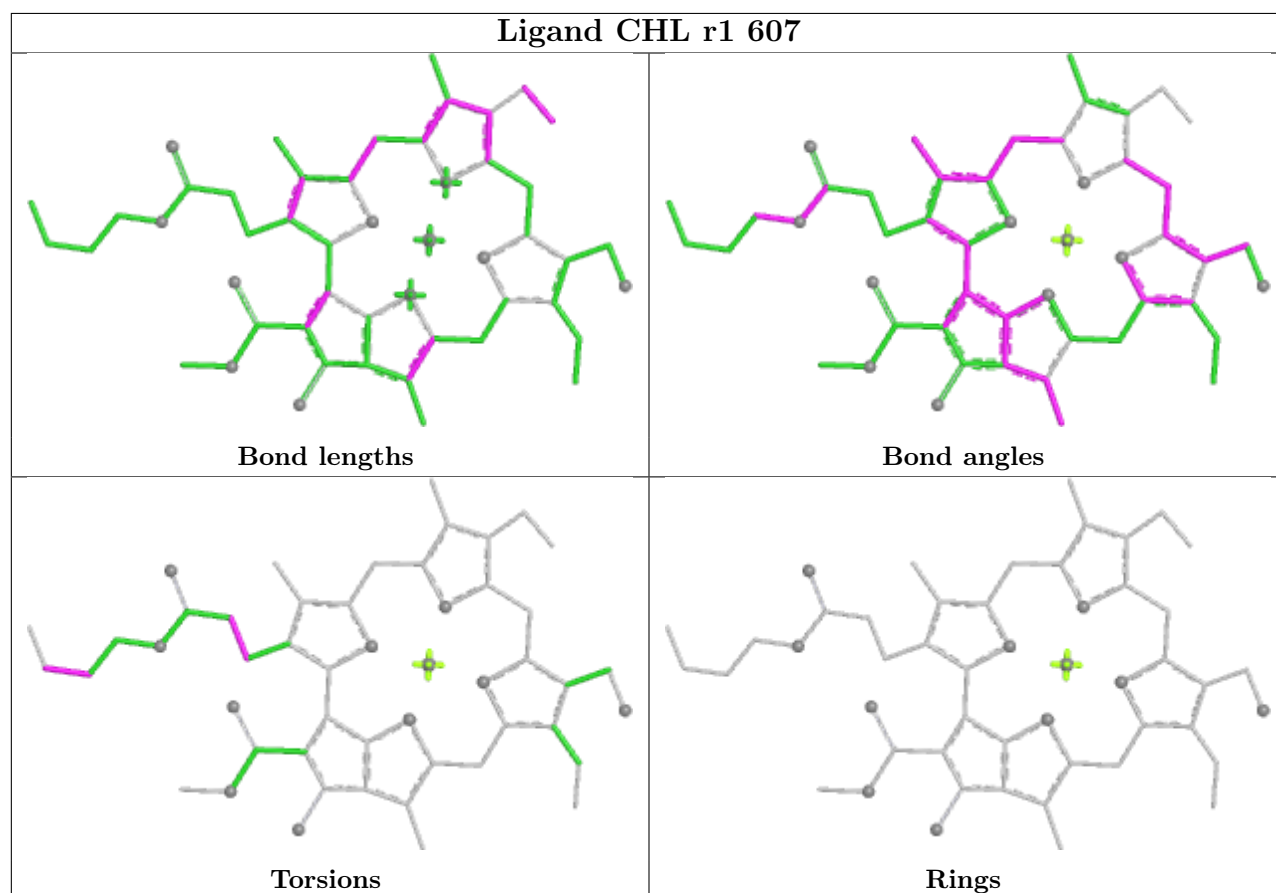
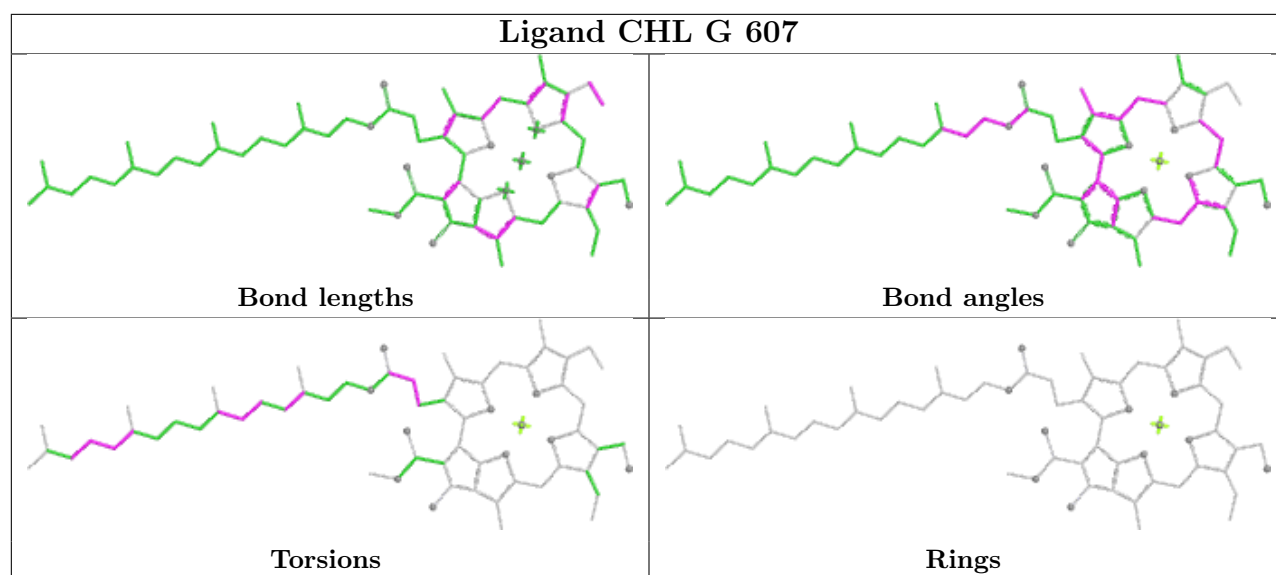


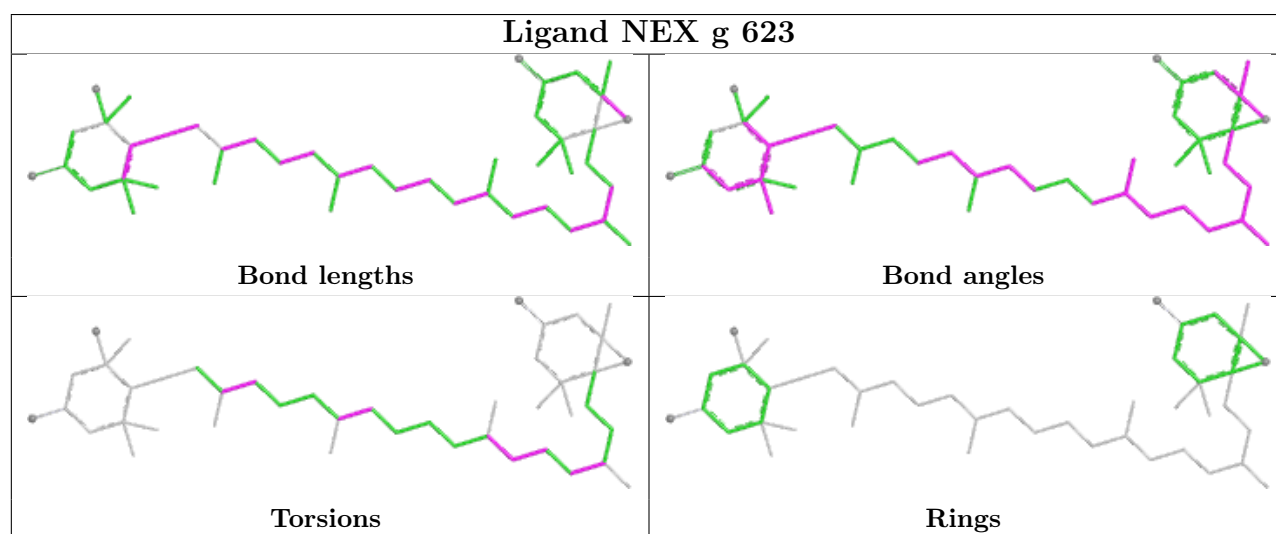
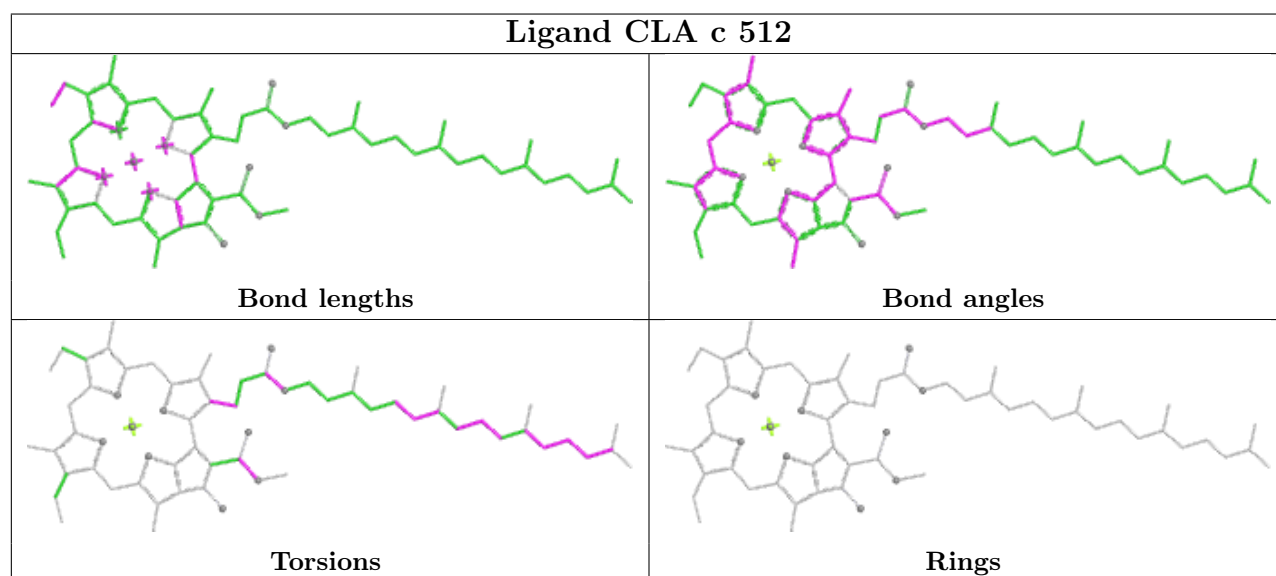
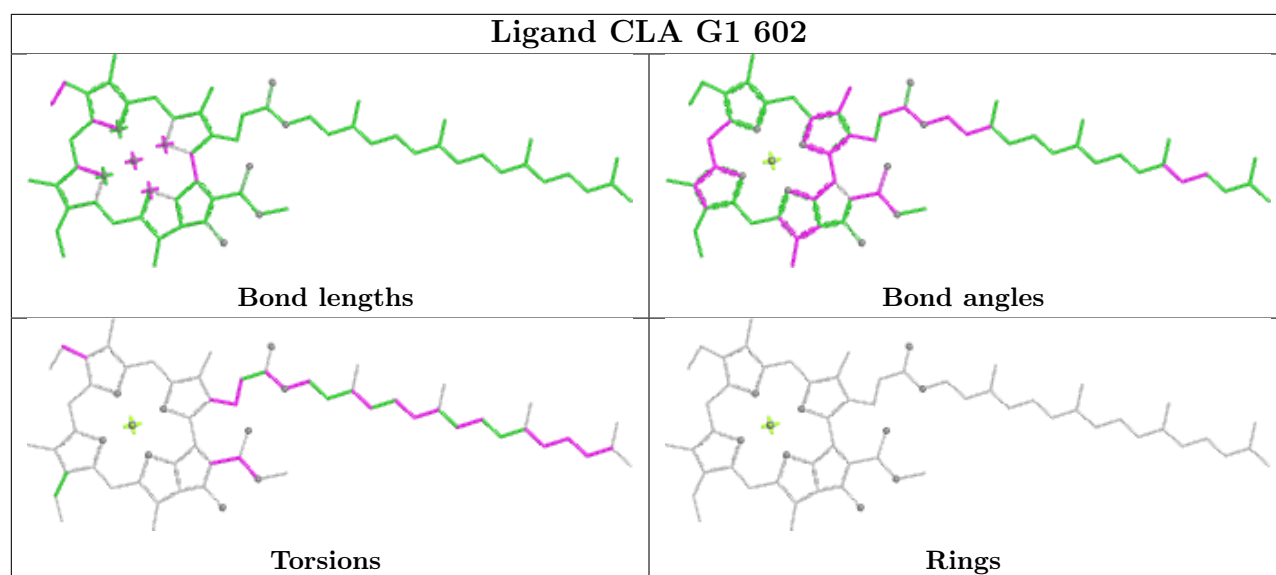


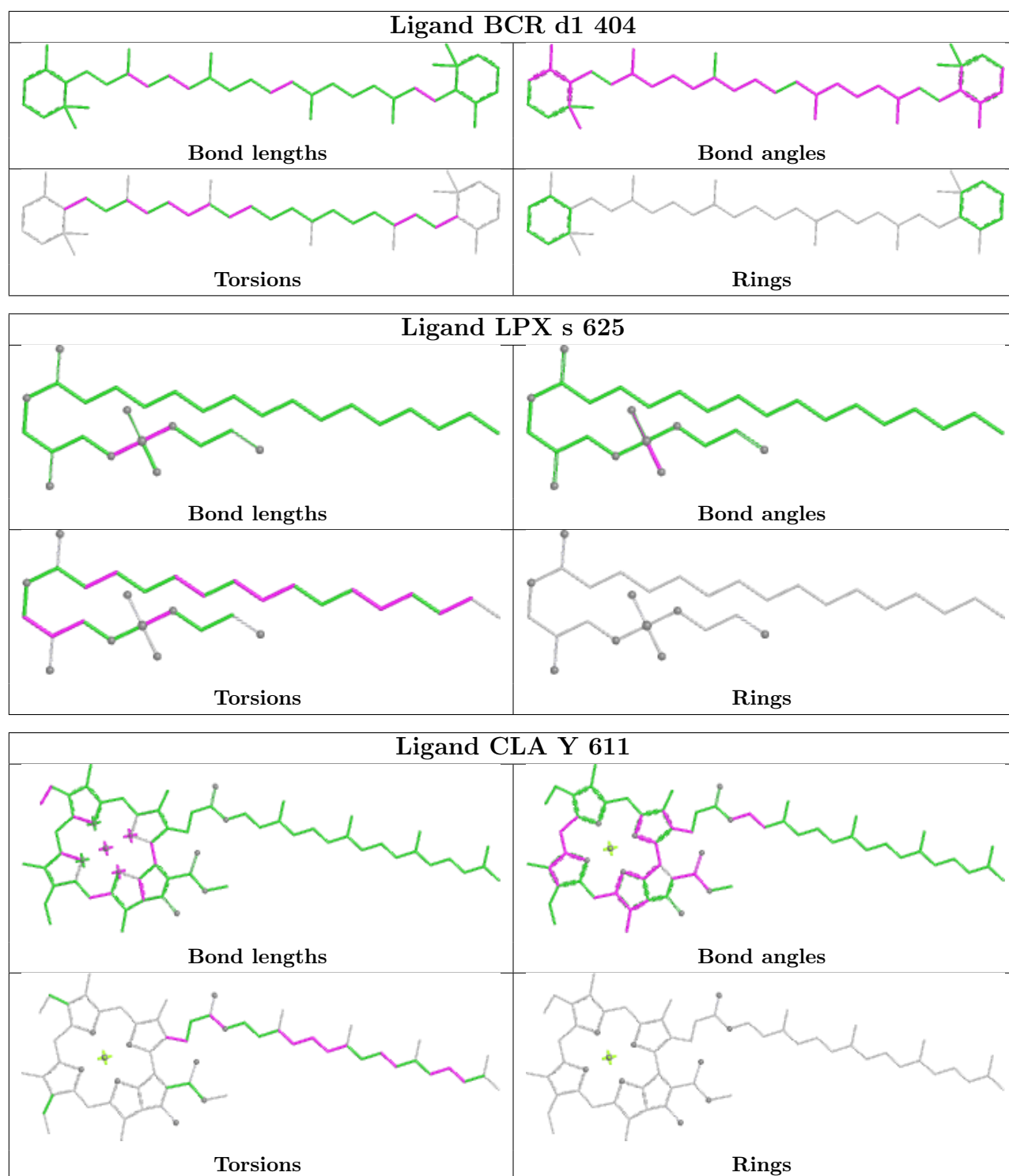


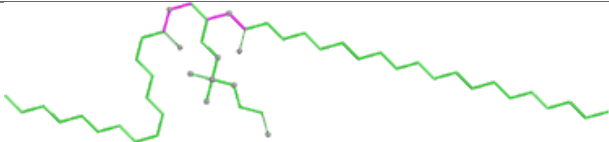
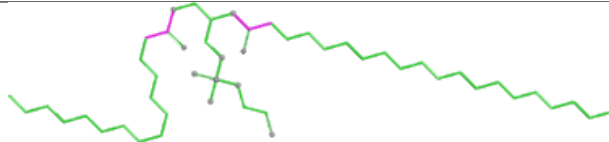
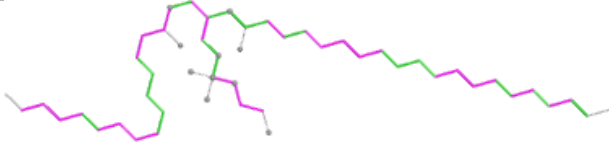
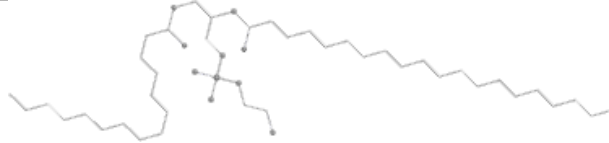


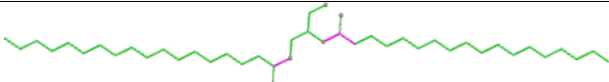
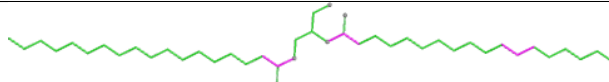
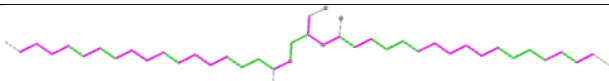
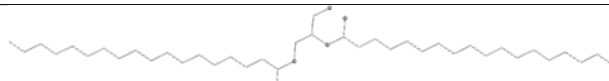


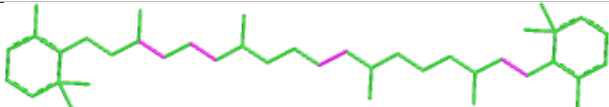
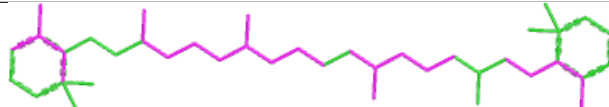
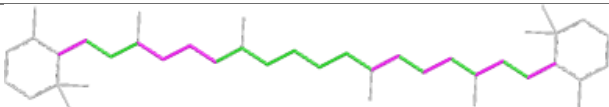
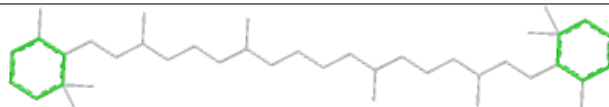


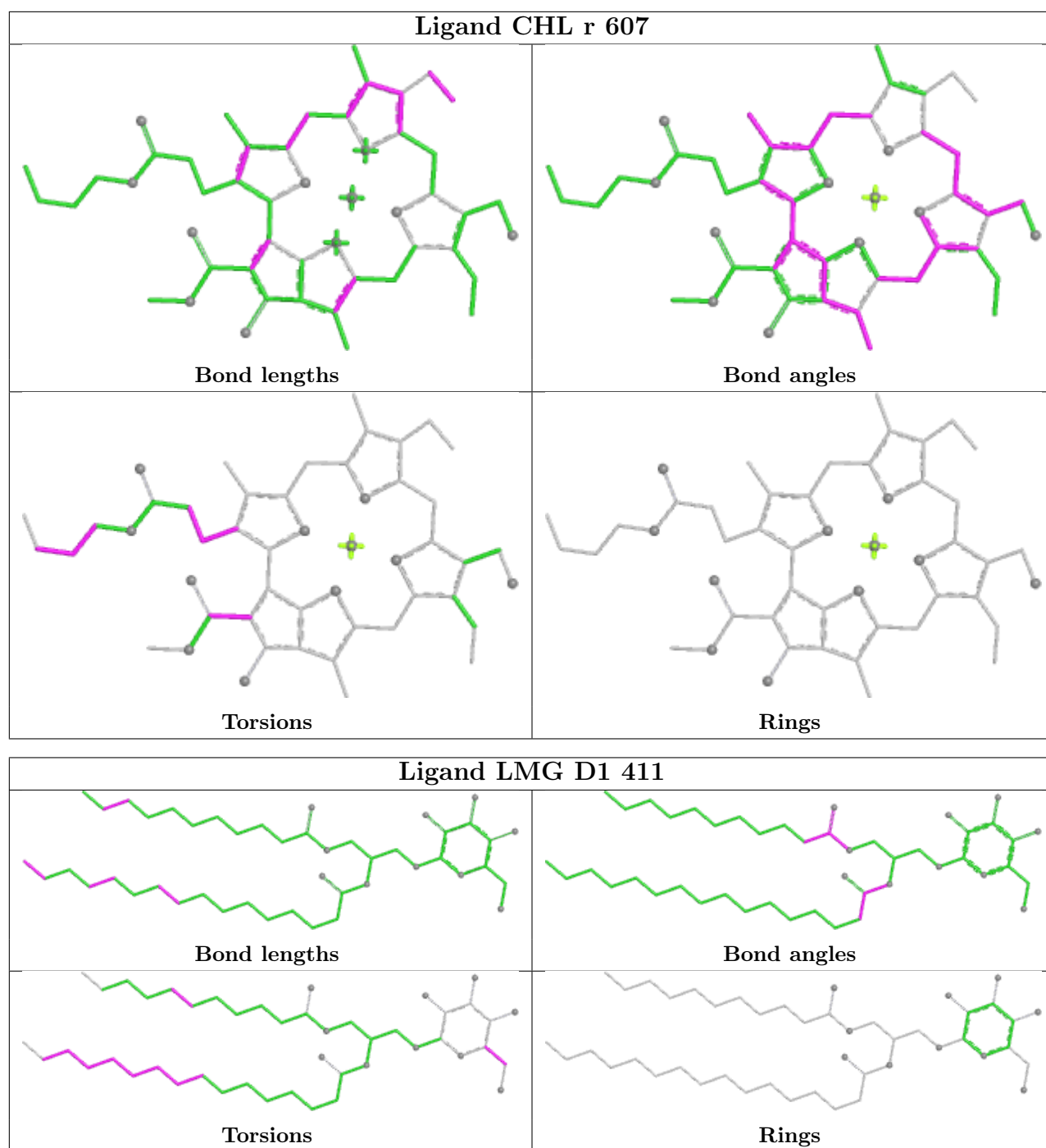


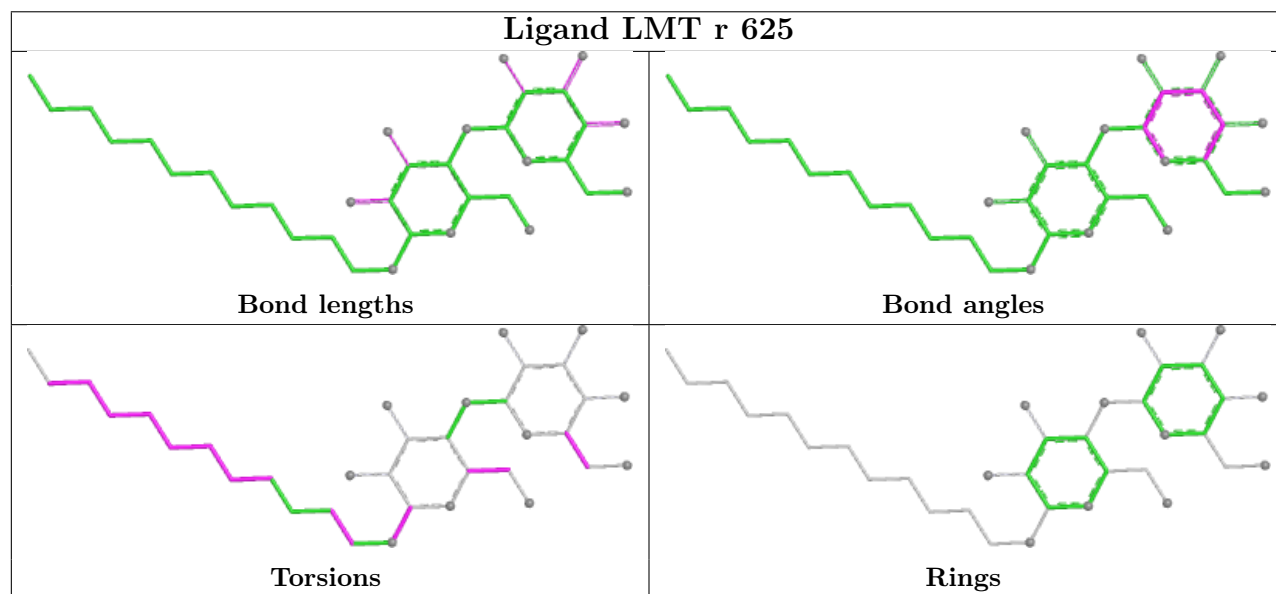
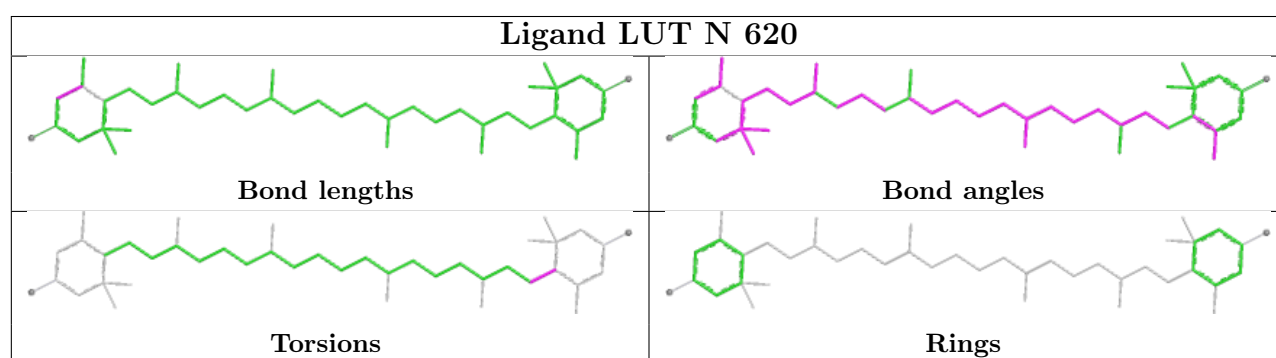
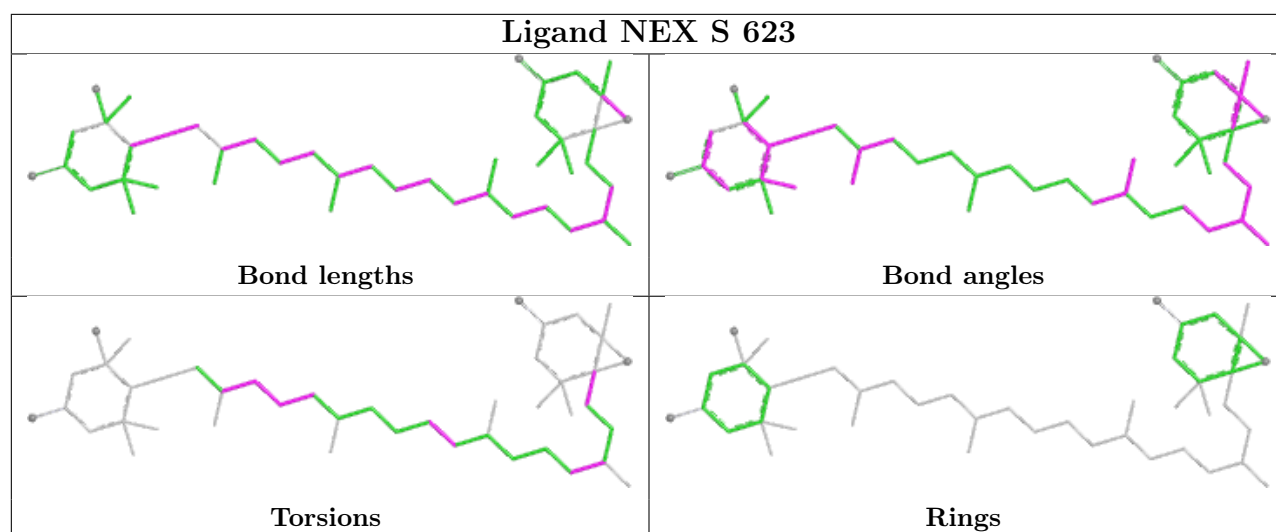


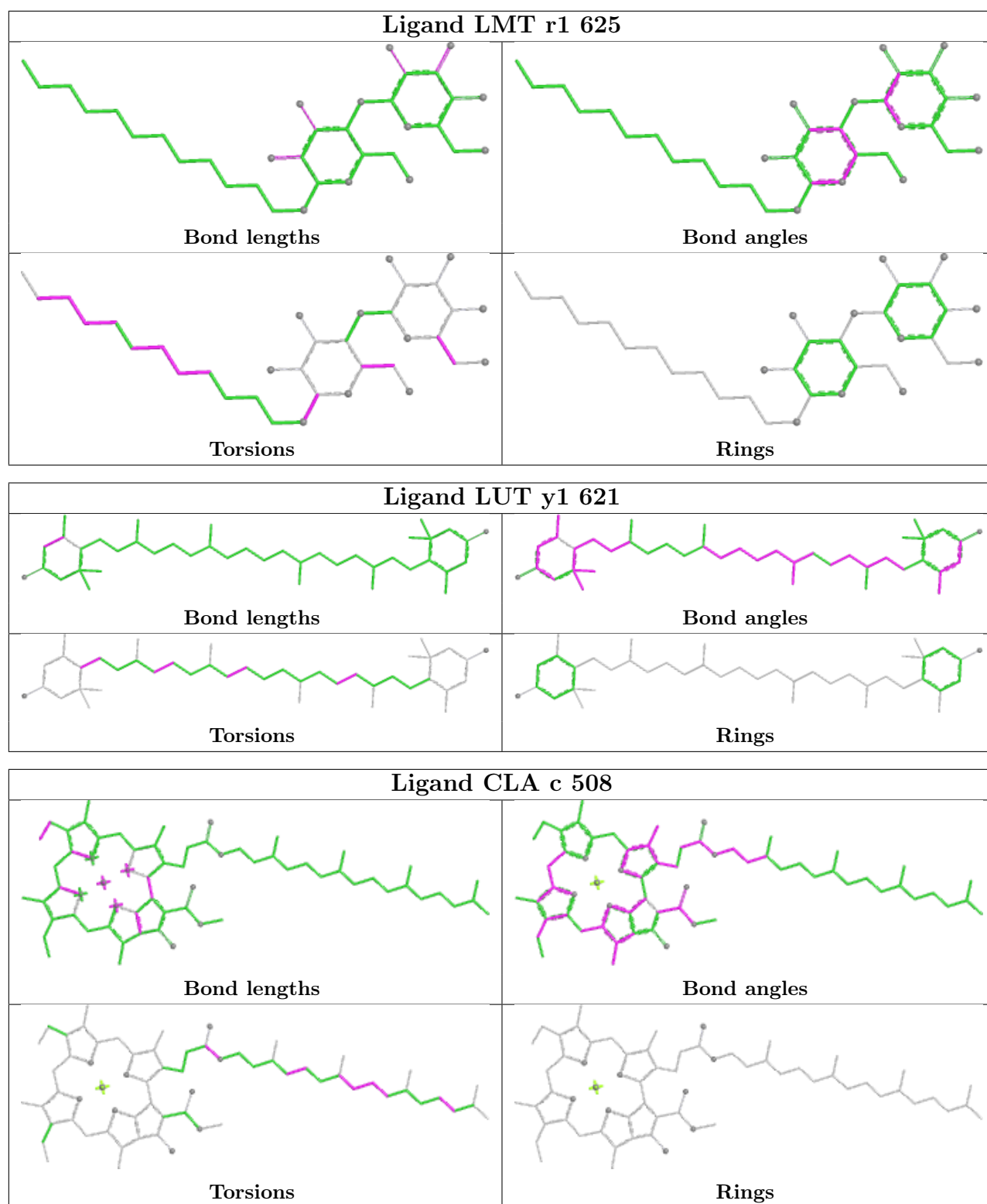
Ligand PTY Y 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

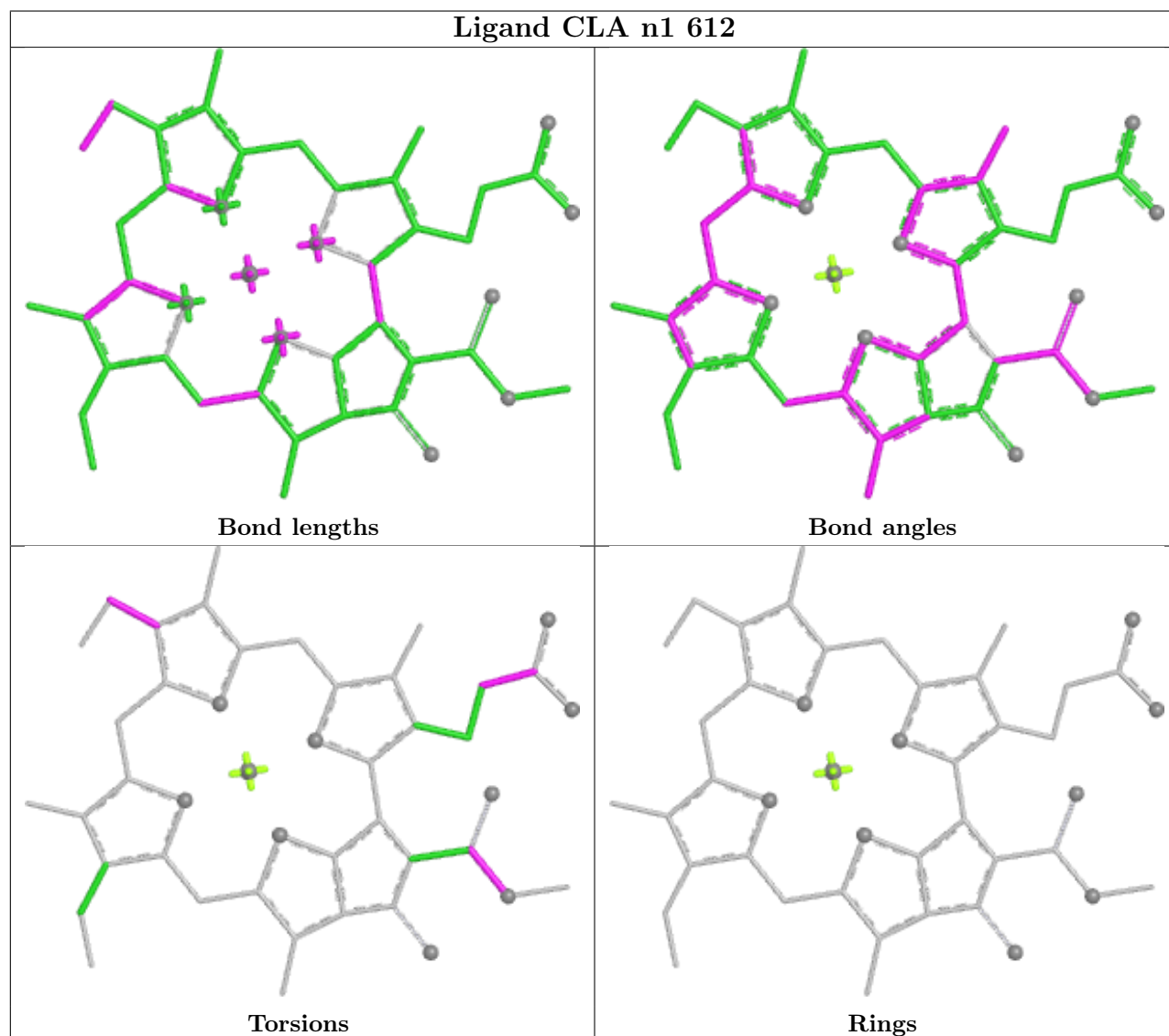
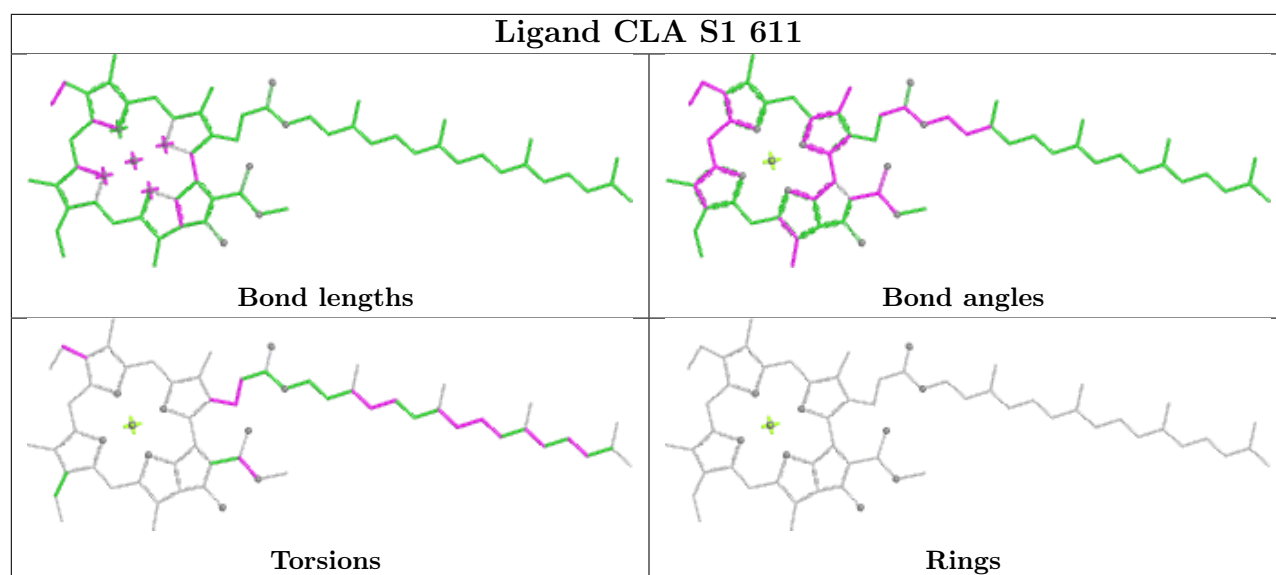
Ligand DGA B1 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

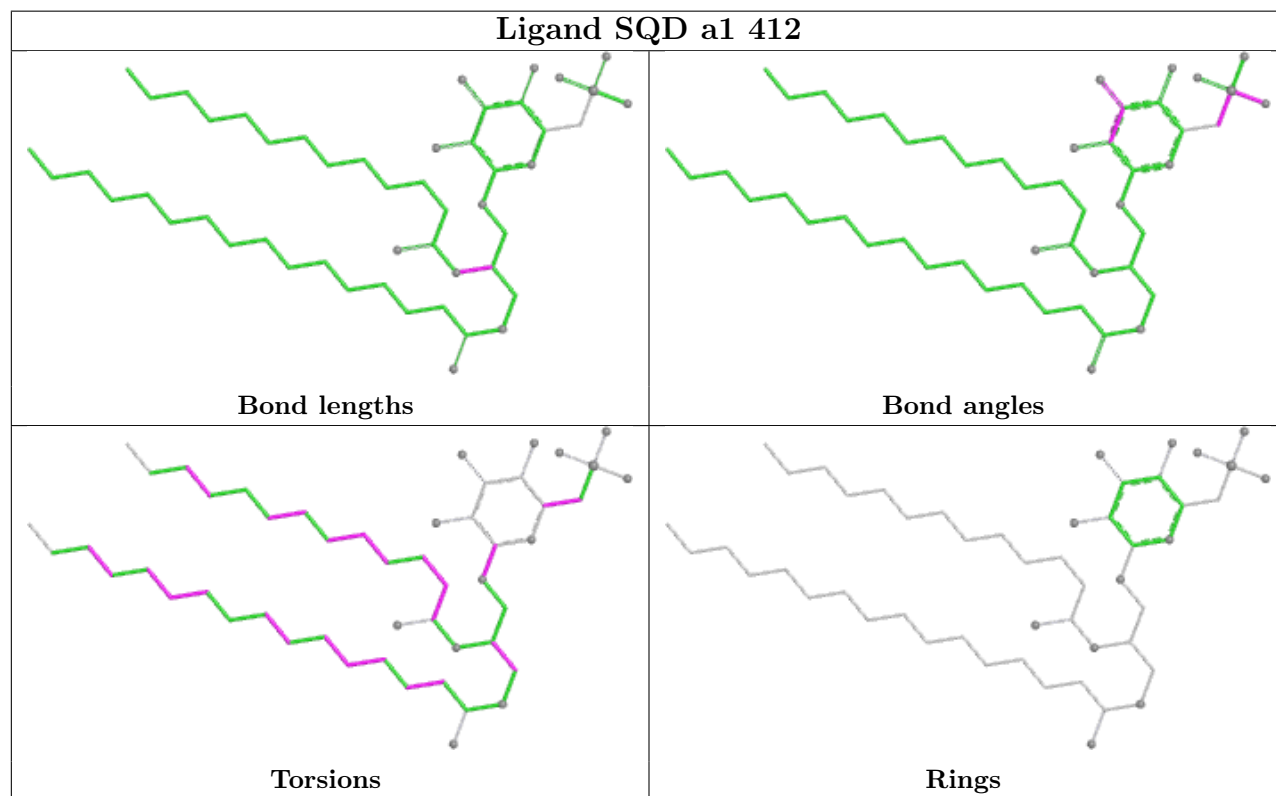
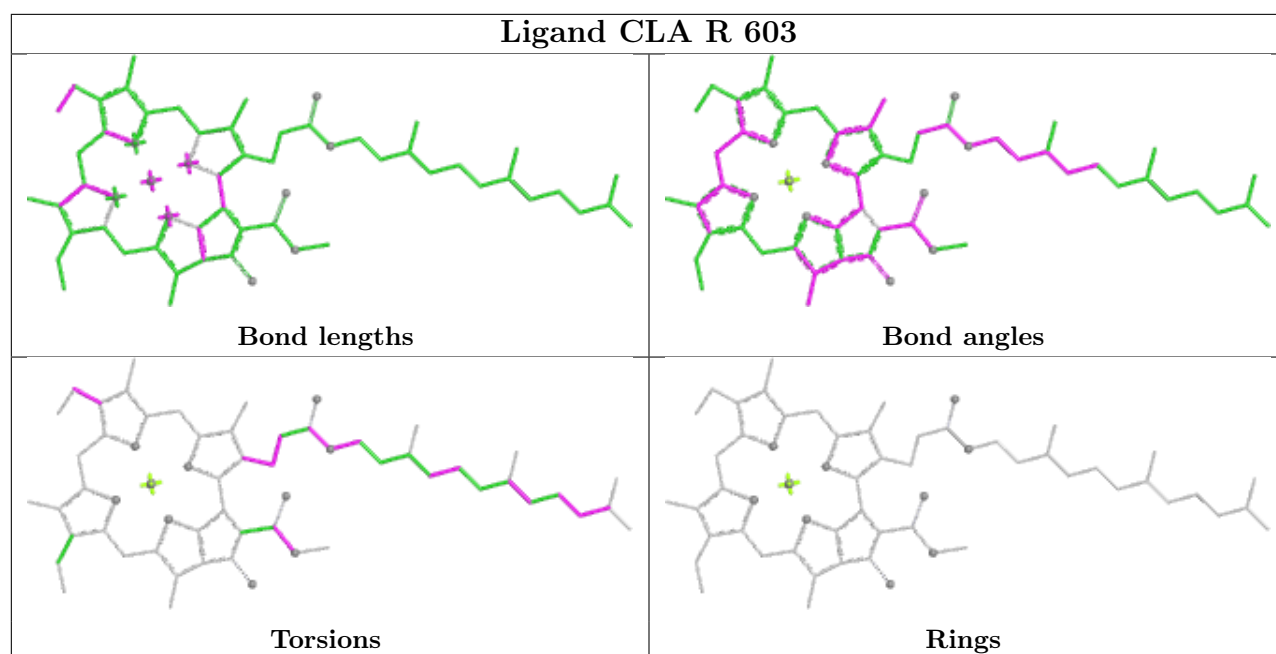
Ligand BCR d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

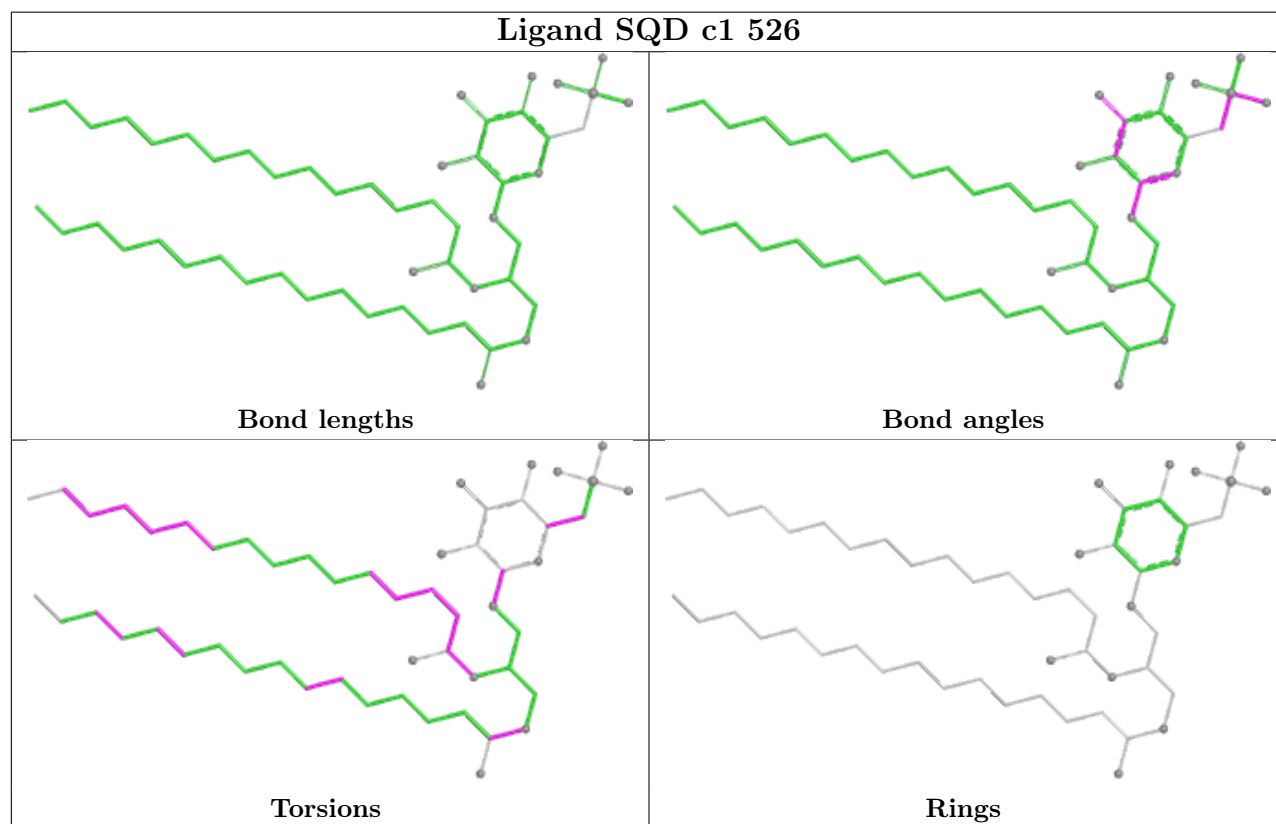
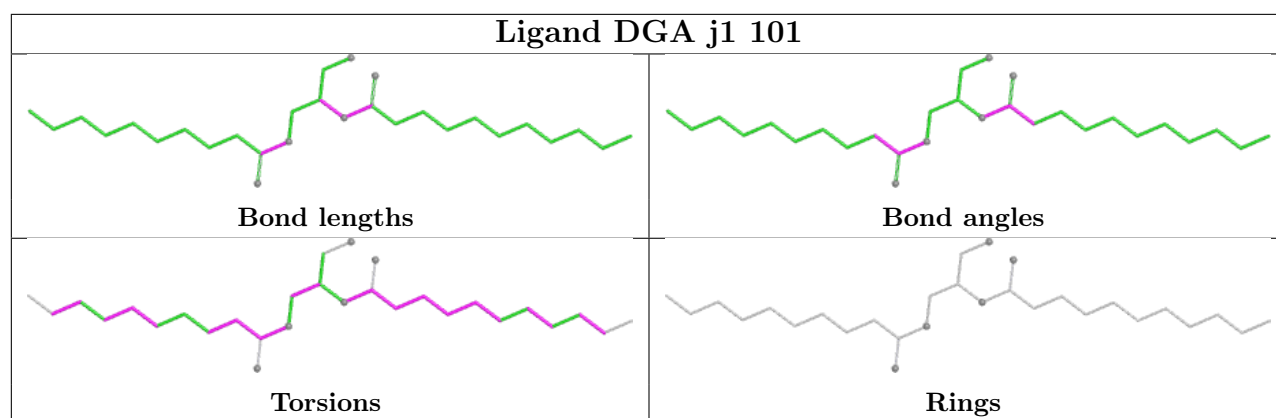




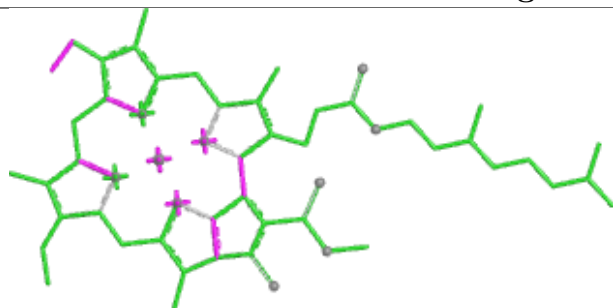




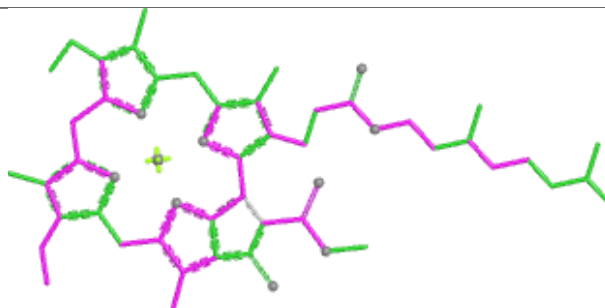




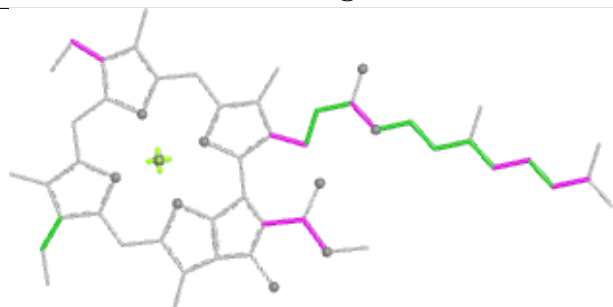
Ligand CLA S 604



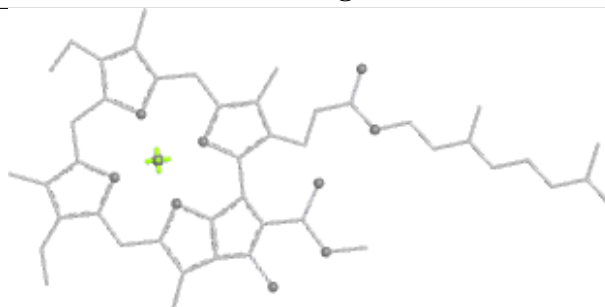
Bond lengths



Bond angles

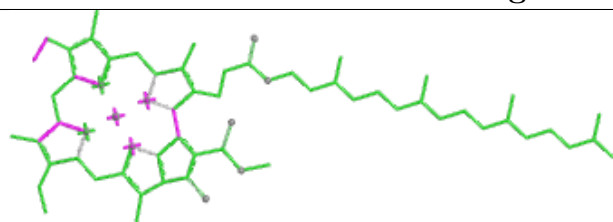


Torsions

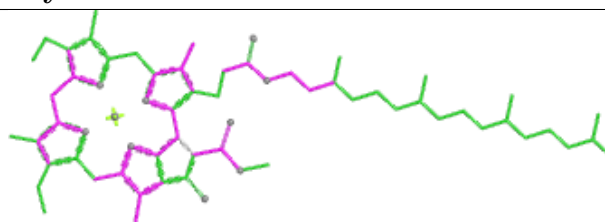


Rings

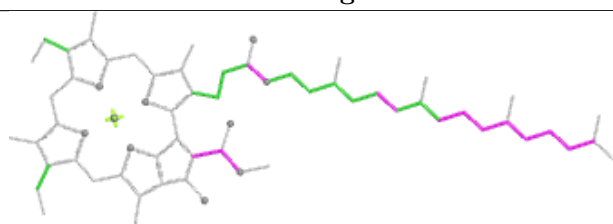
Ligand CLA y1 612



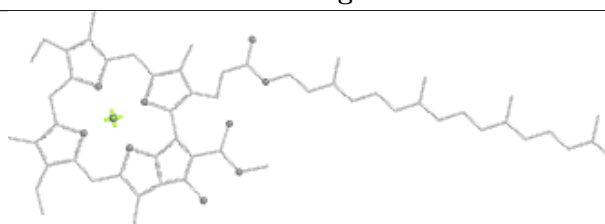
Bond lengths



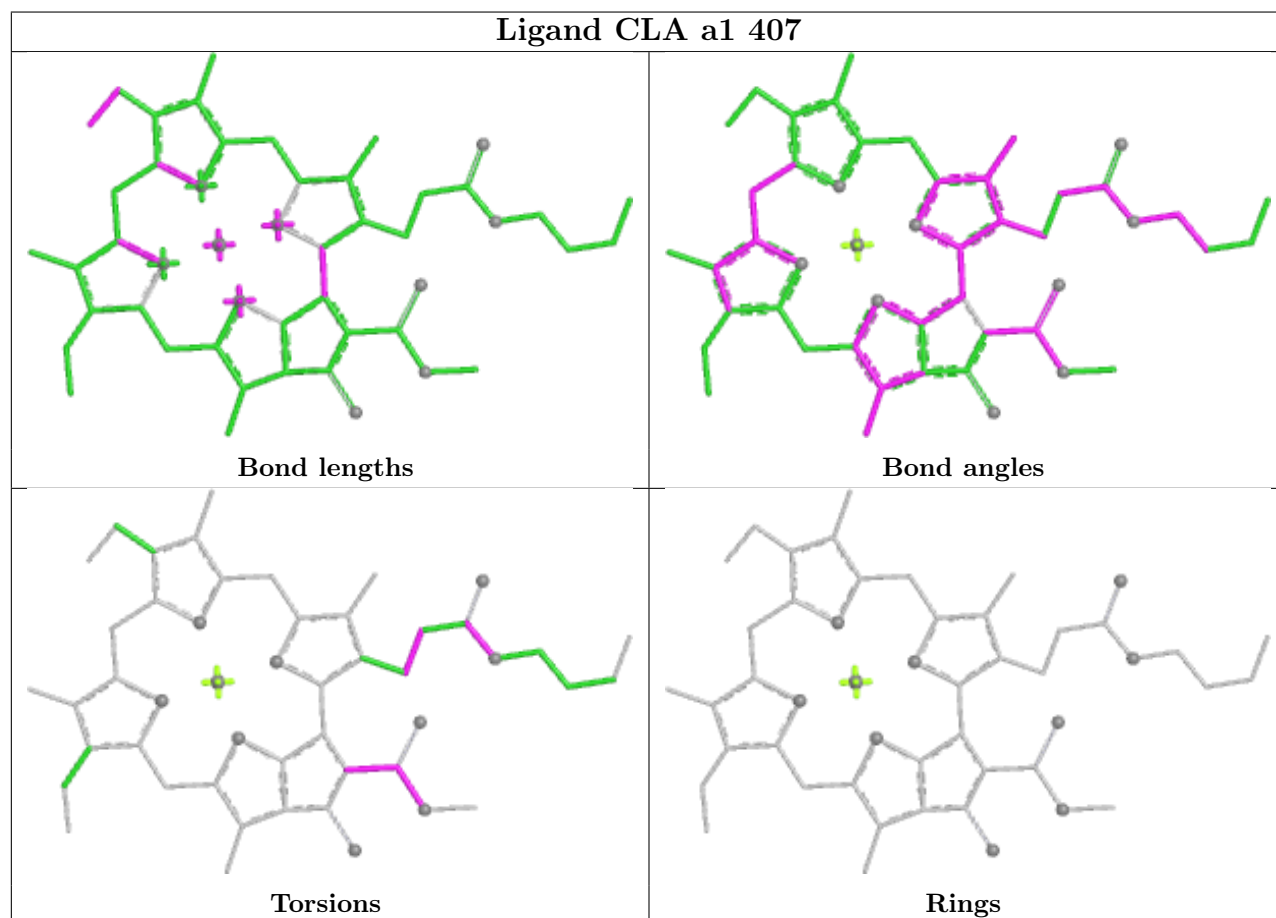
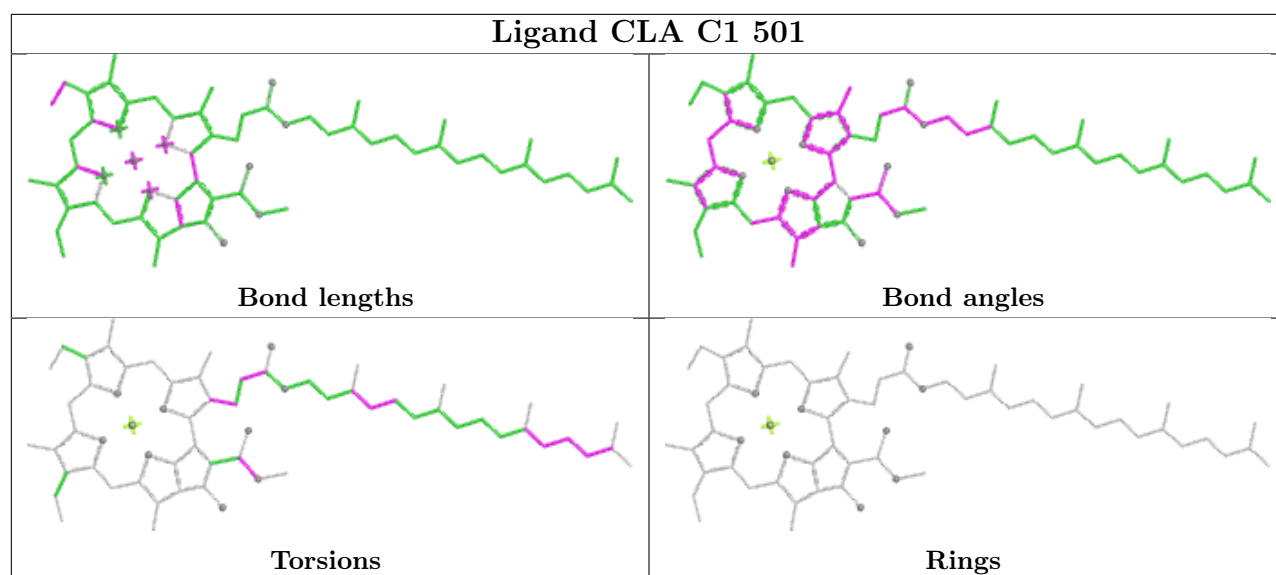
Bond angles

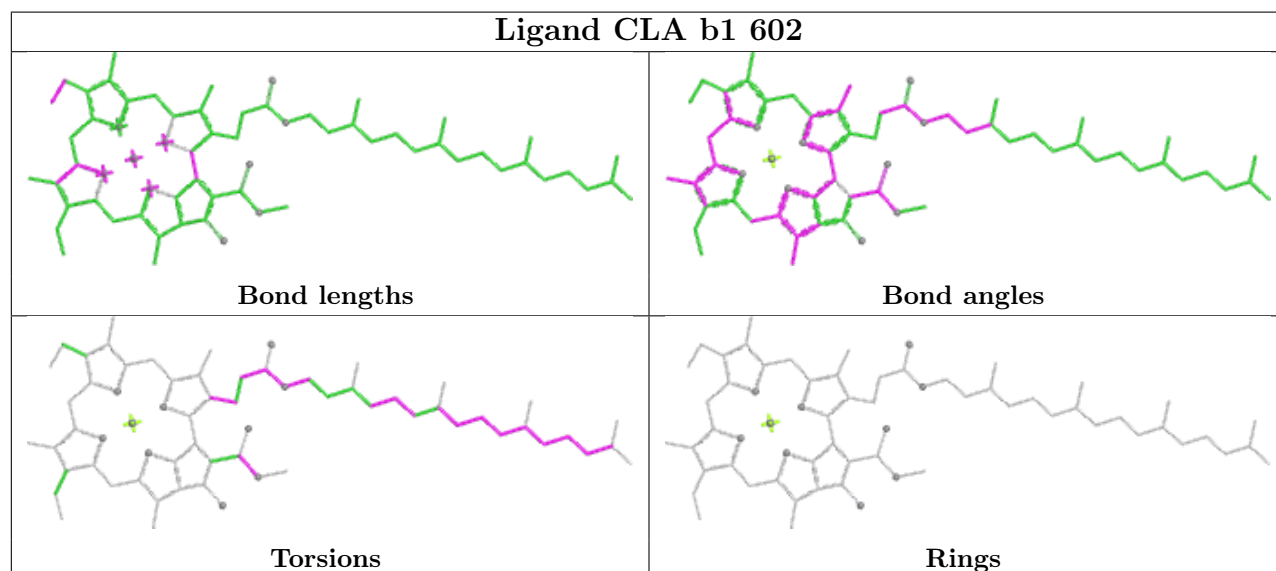
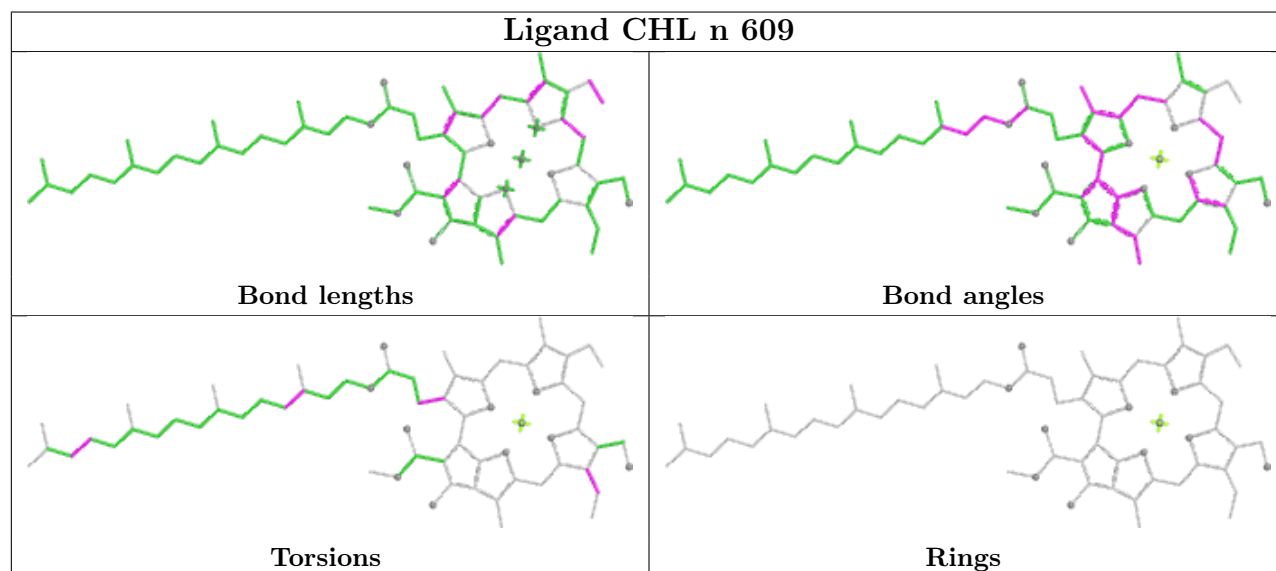
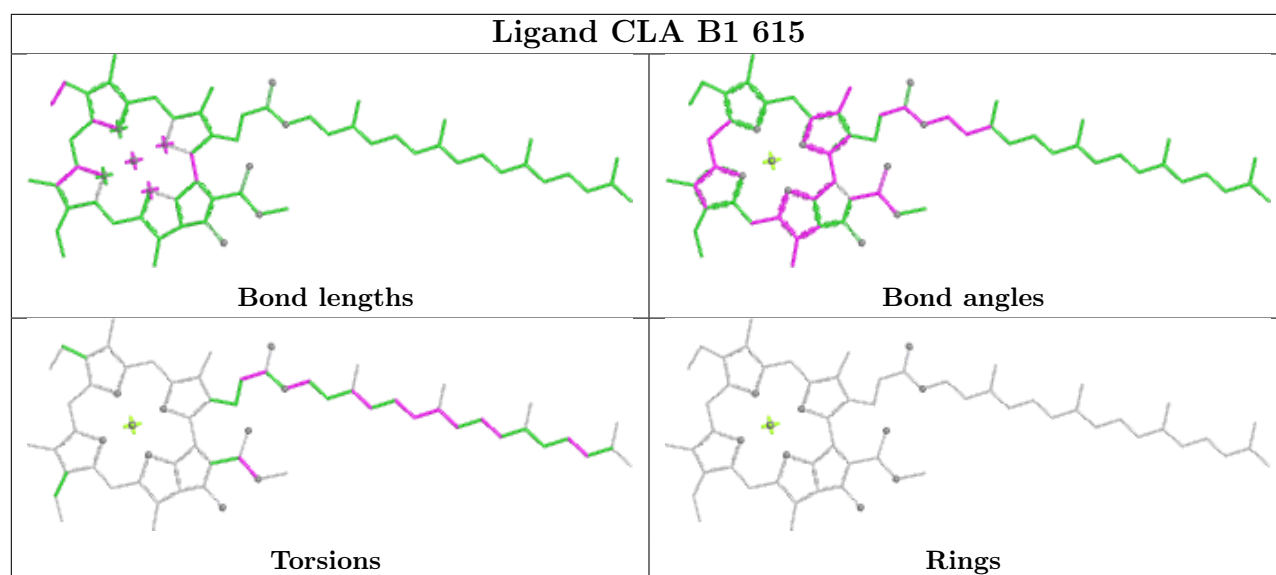


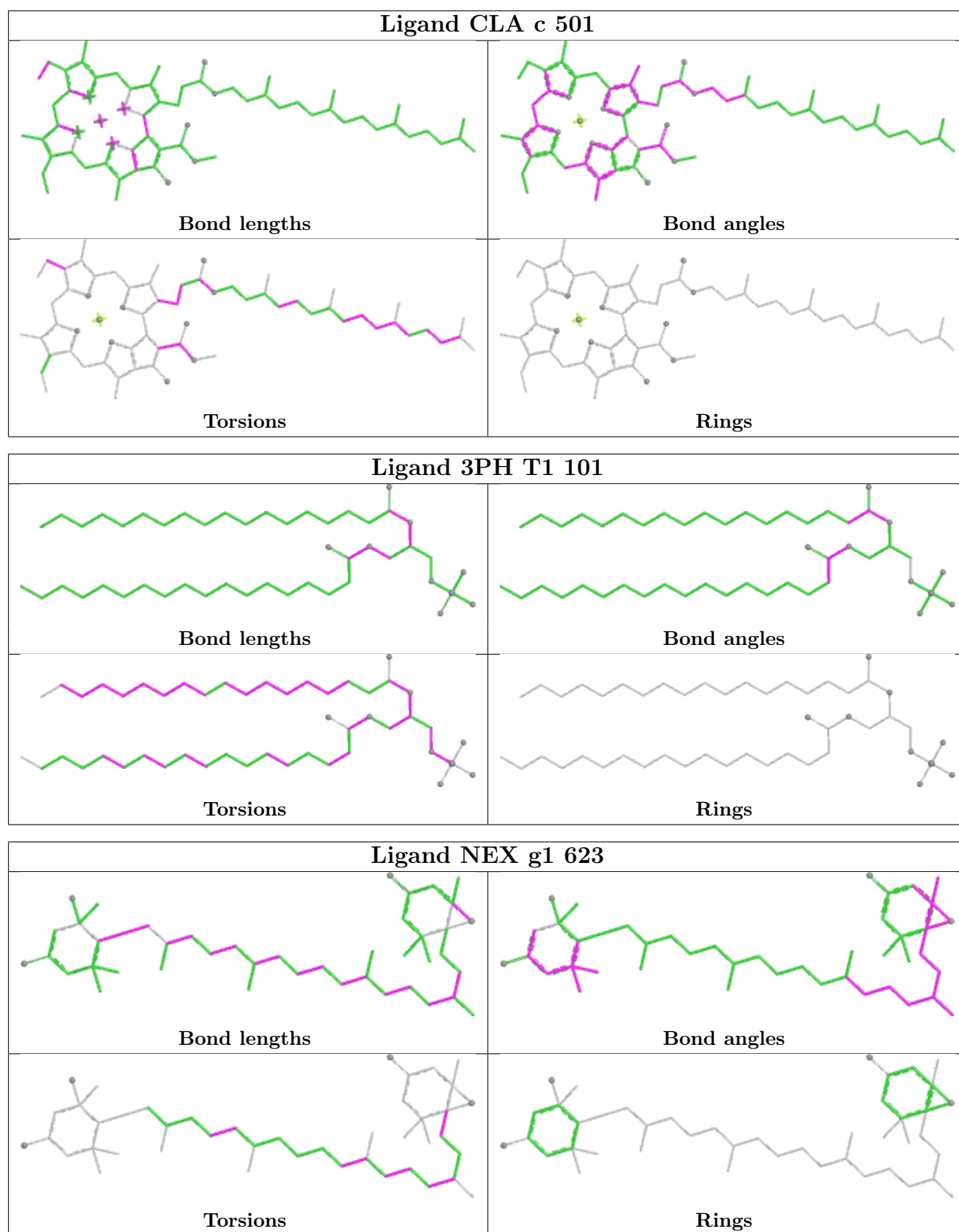
Torsions

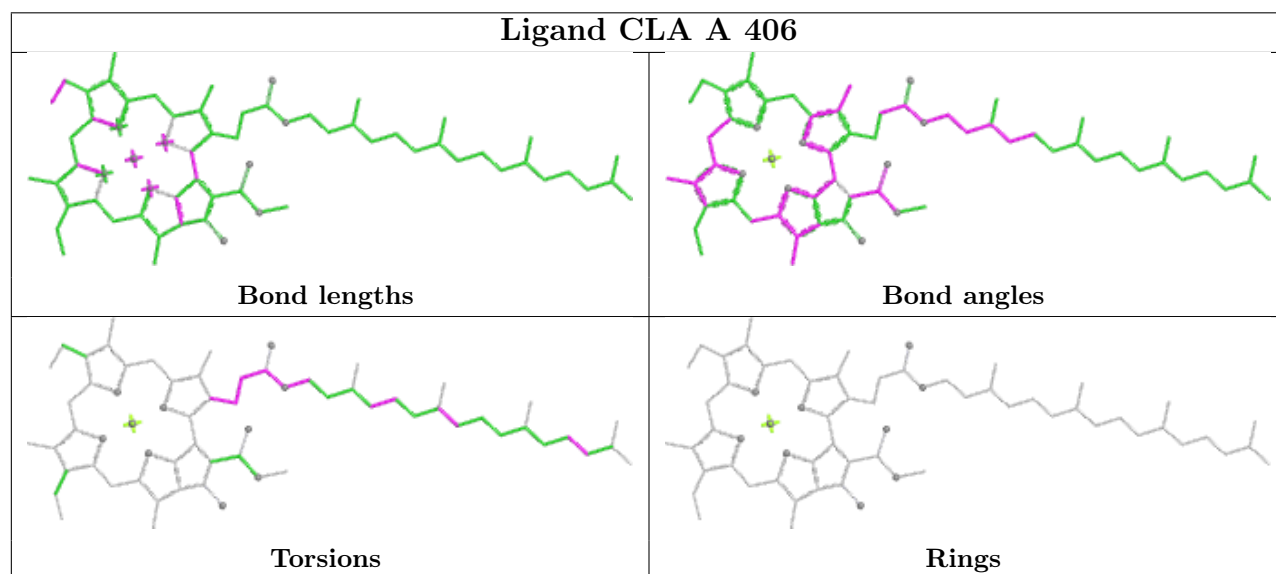
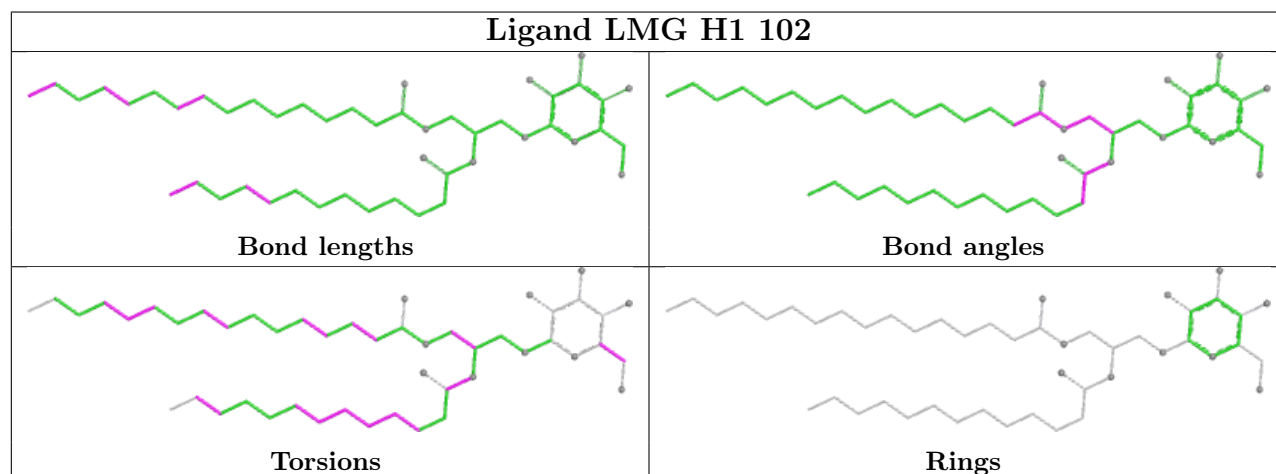
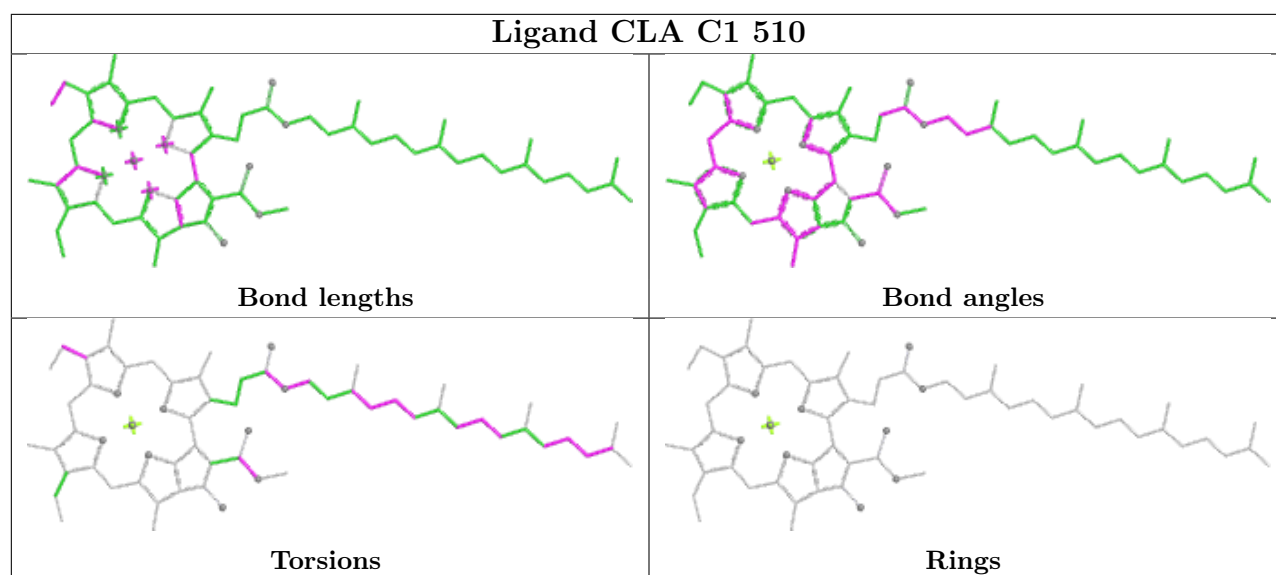


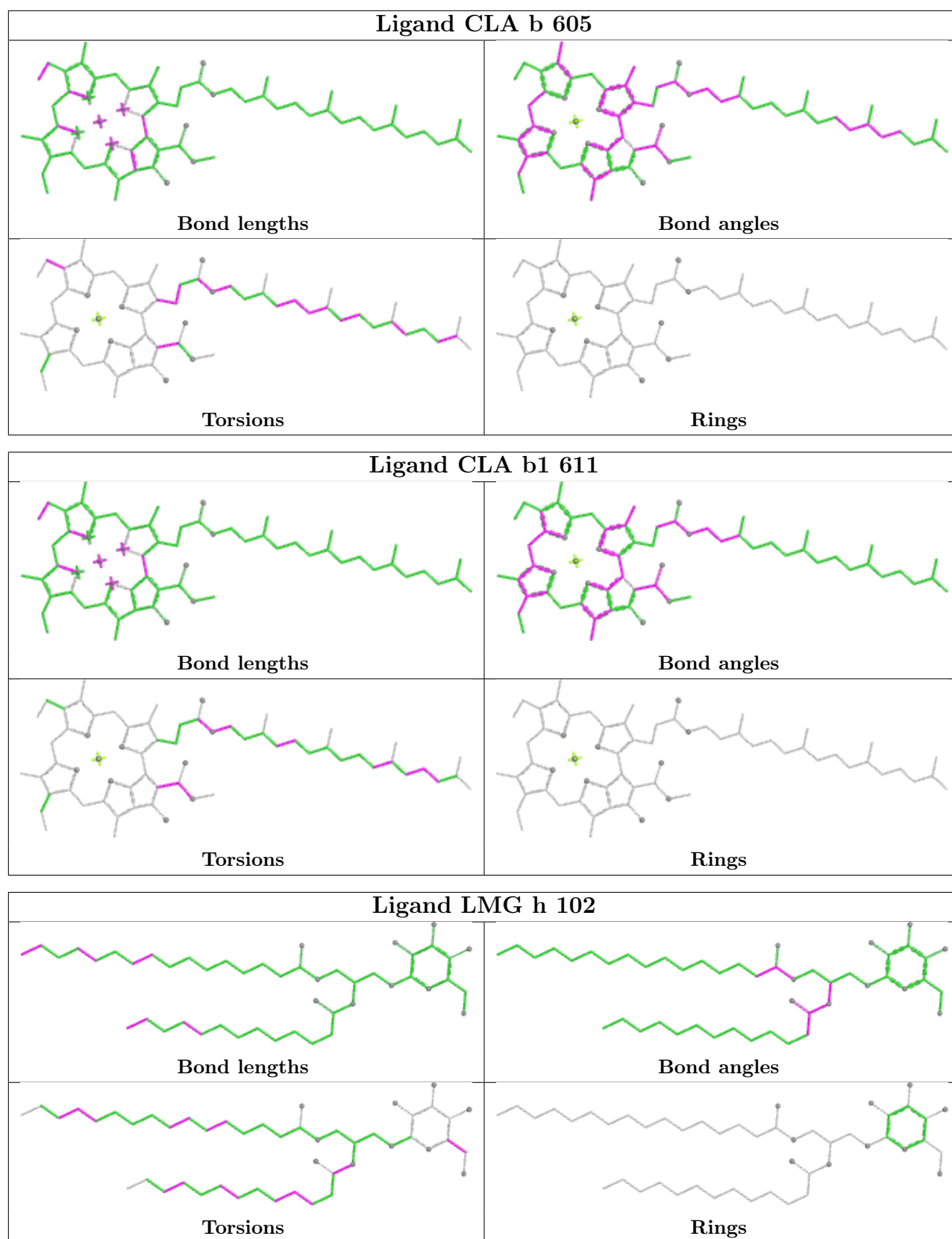
Rings

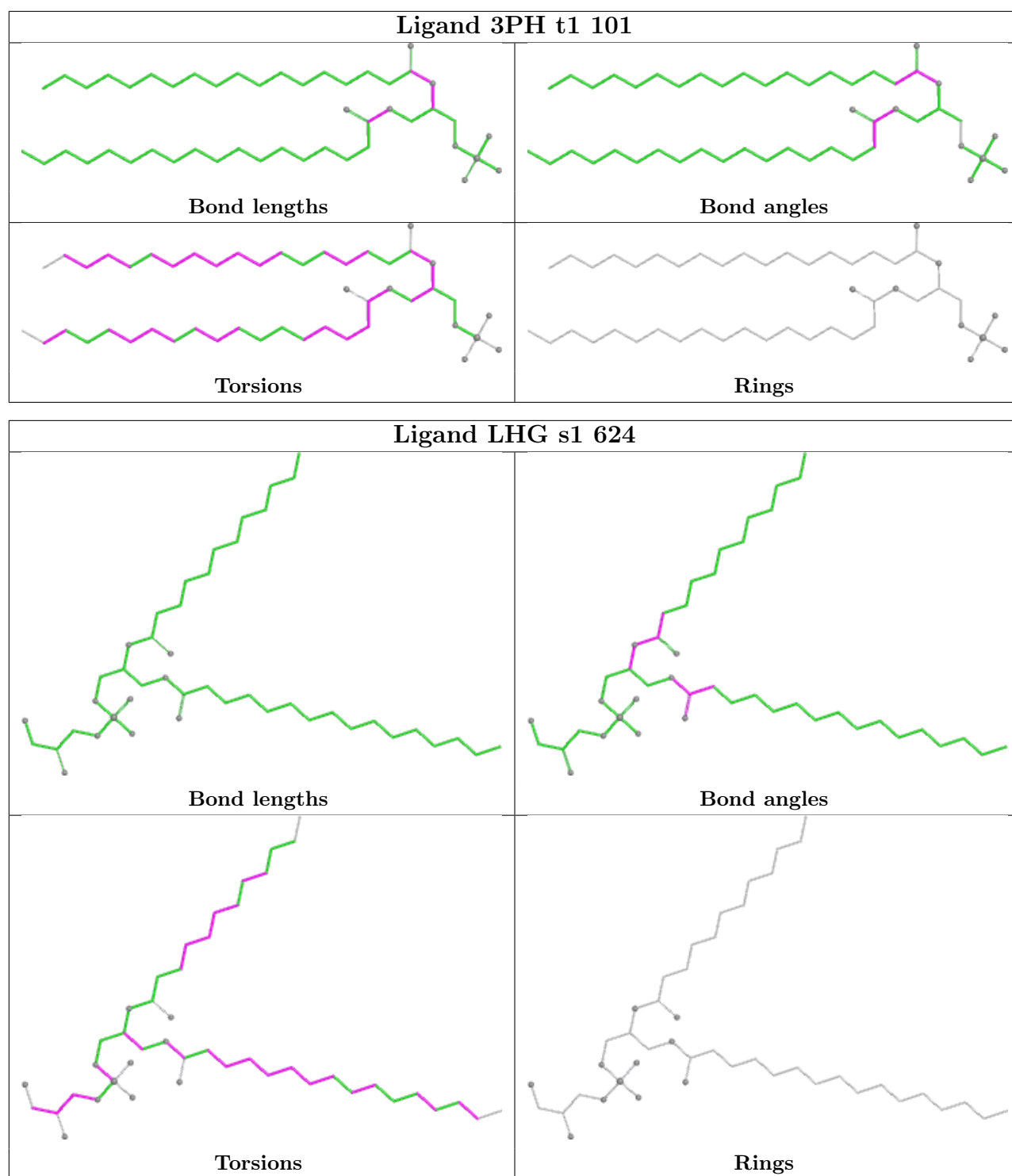


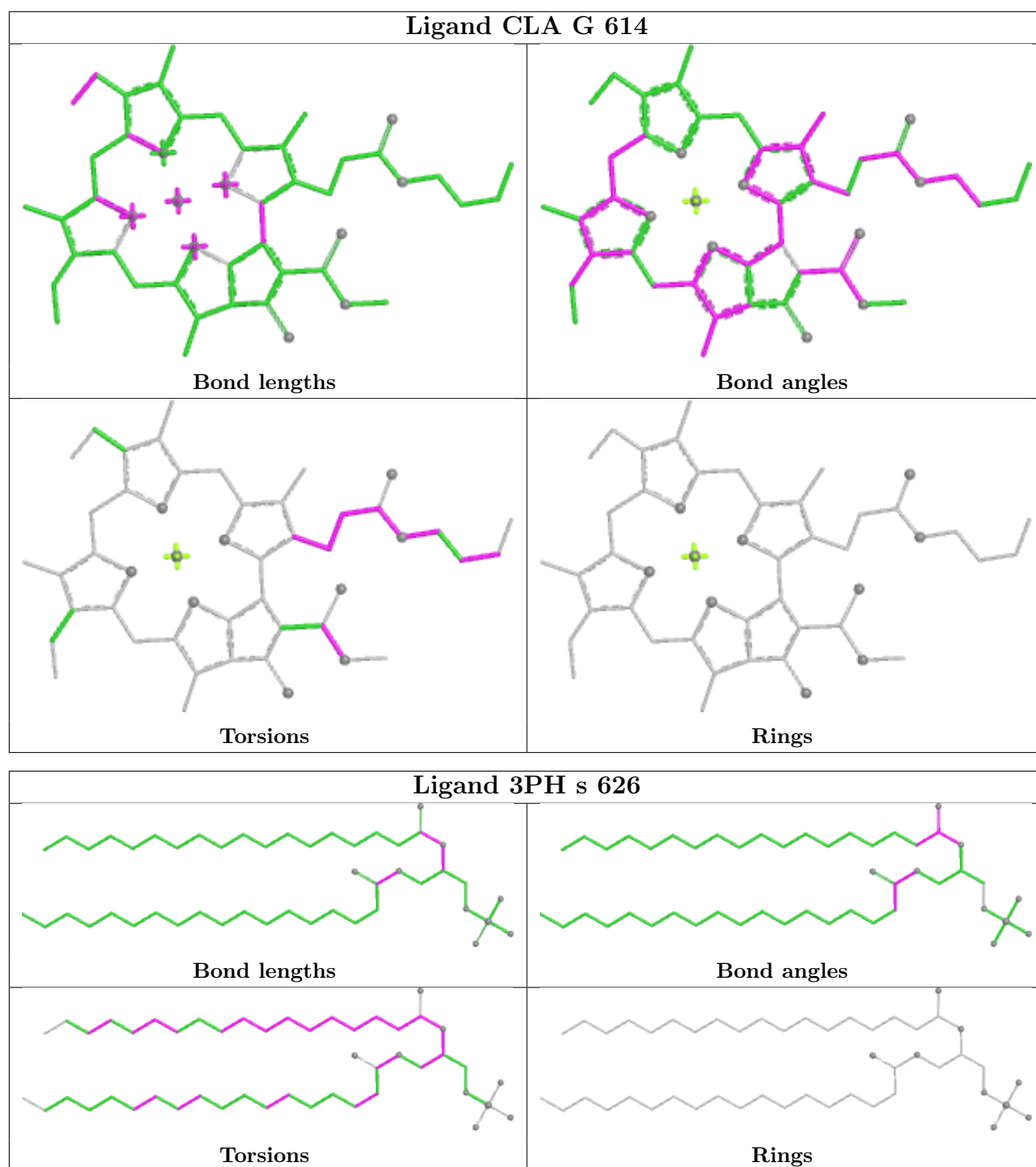


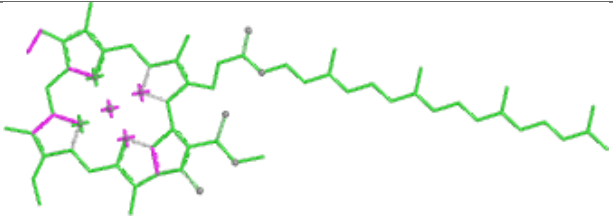
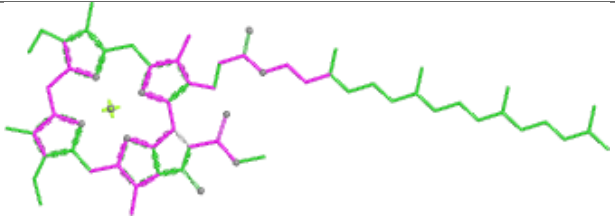
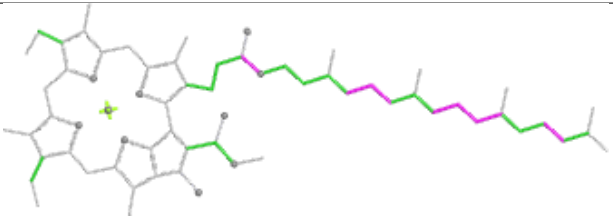
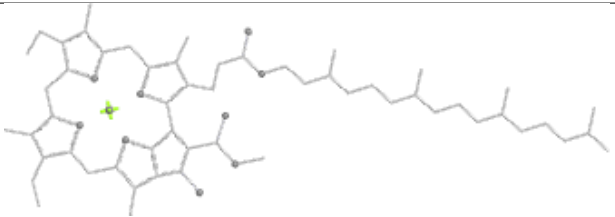
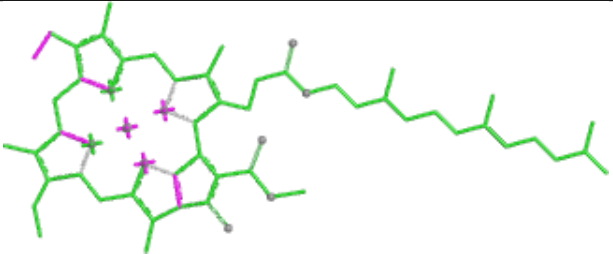
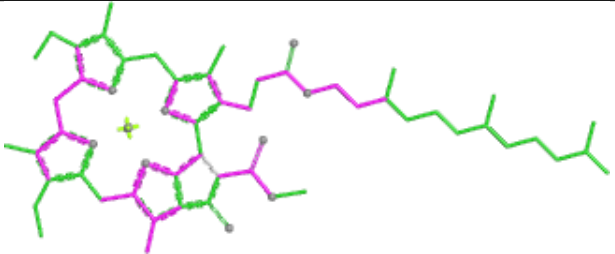
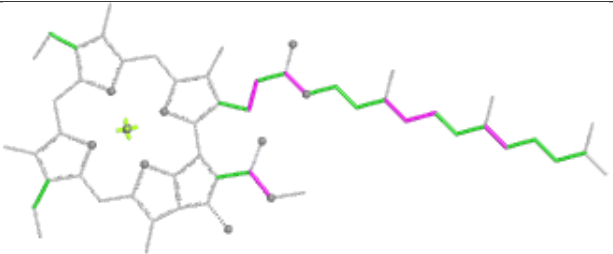
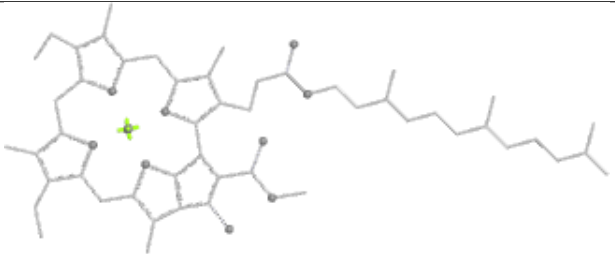
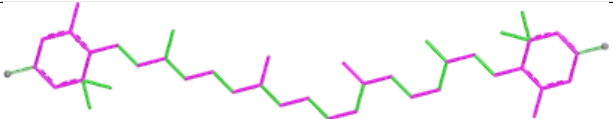
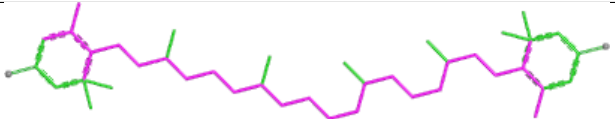
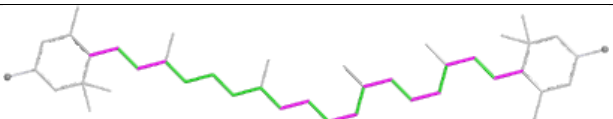
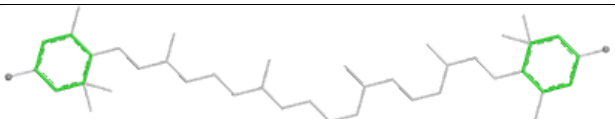


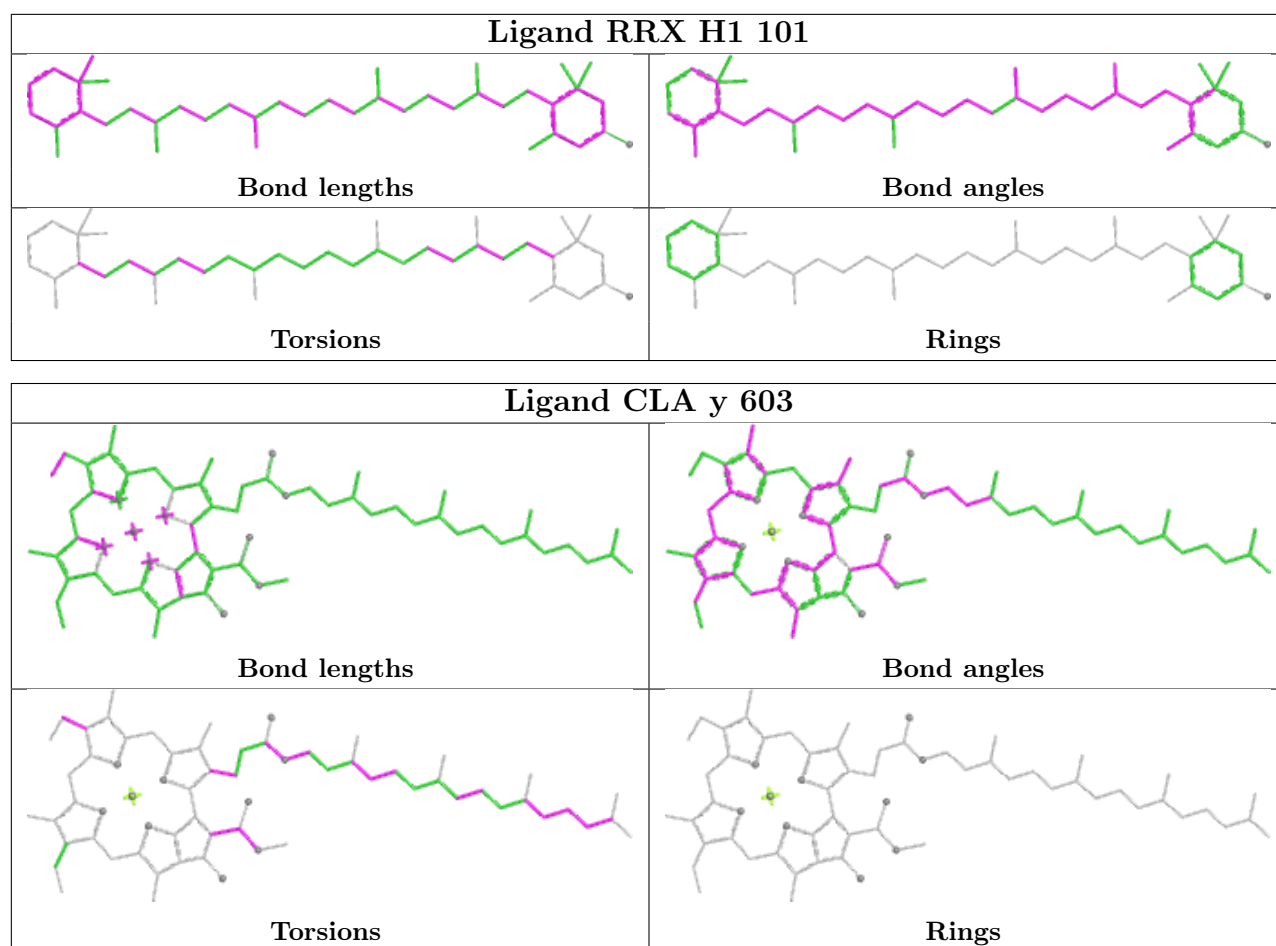




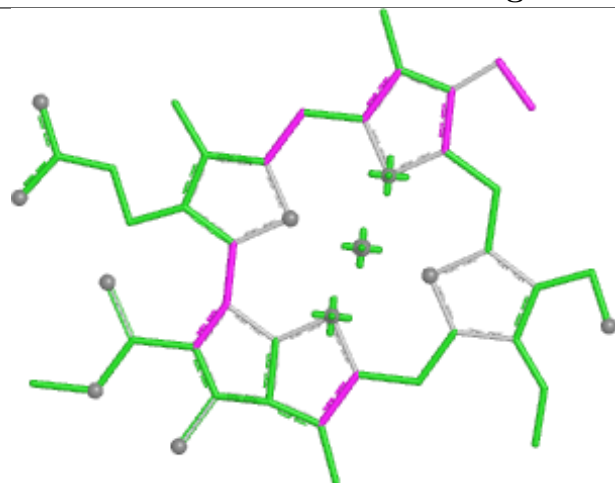




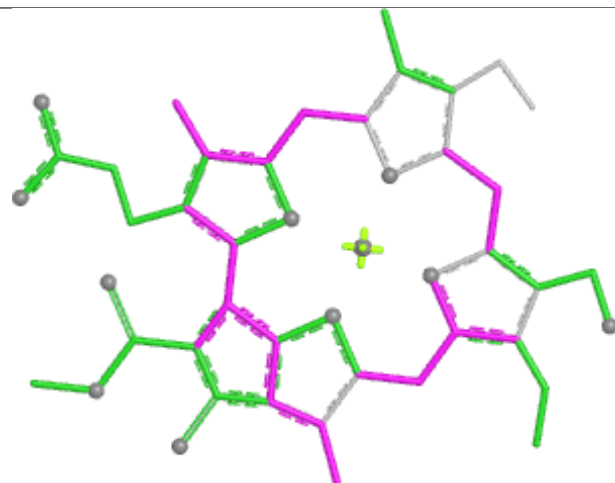
Ligand CLA c1 508	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA r 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand C7Z b 620	
 Bond lengths	 Bond angles
 Torsions	 Rings



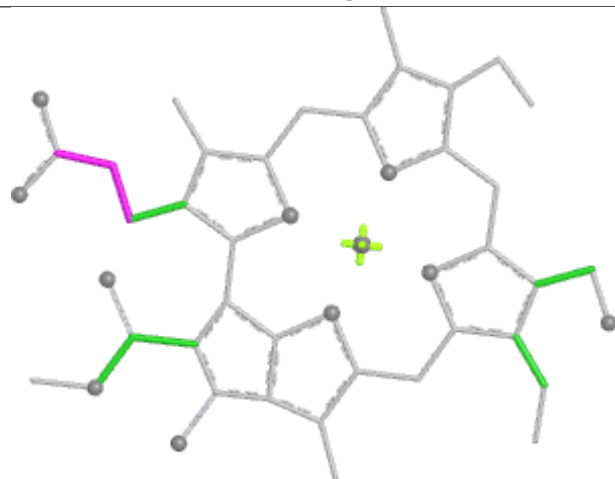
Ligand CHL Y1 605



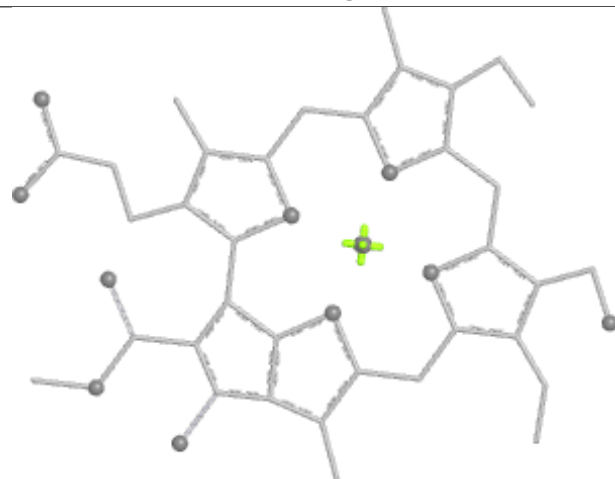
Bond lengths



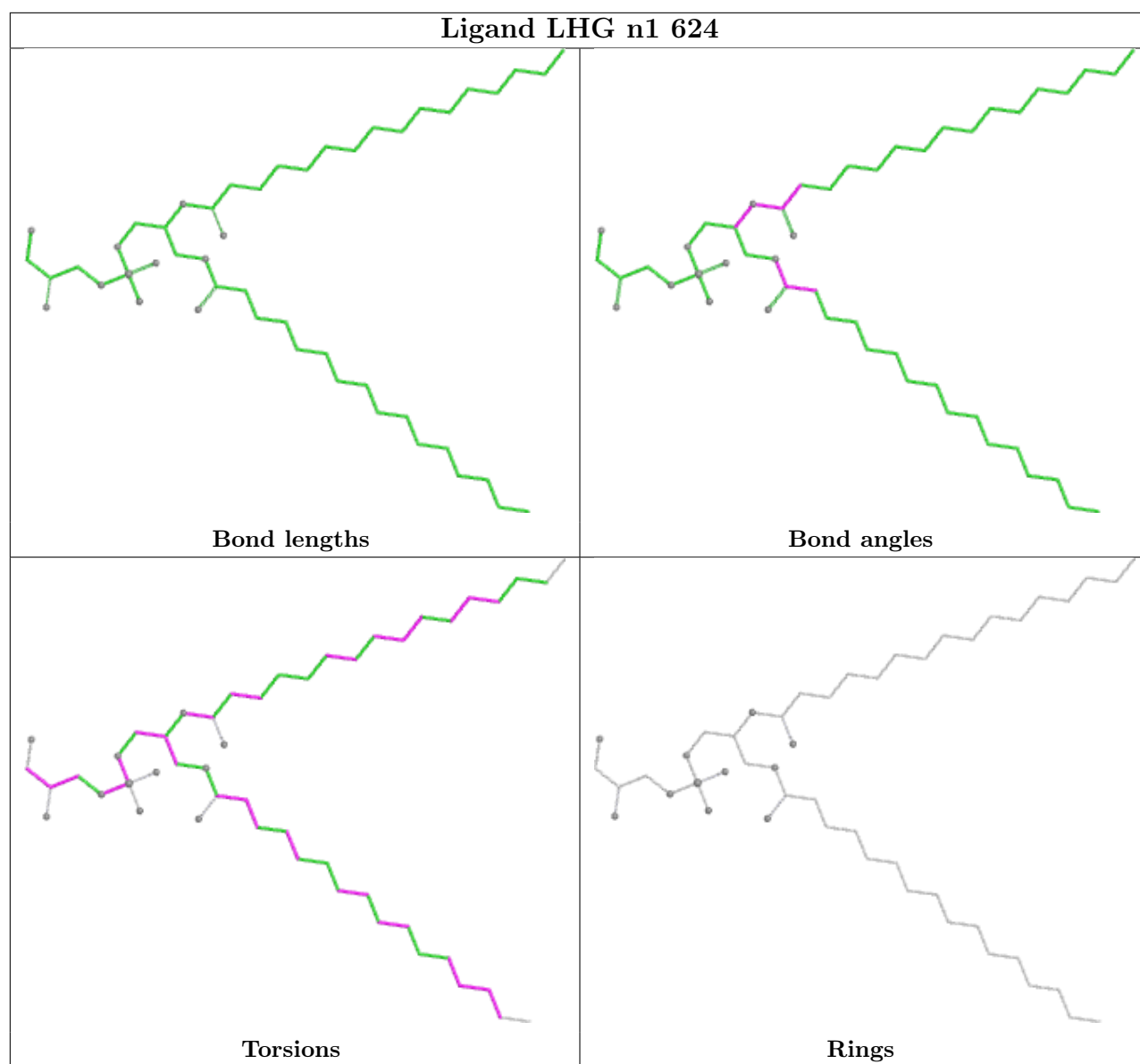
Bond angles



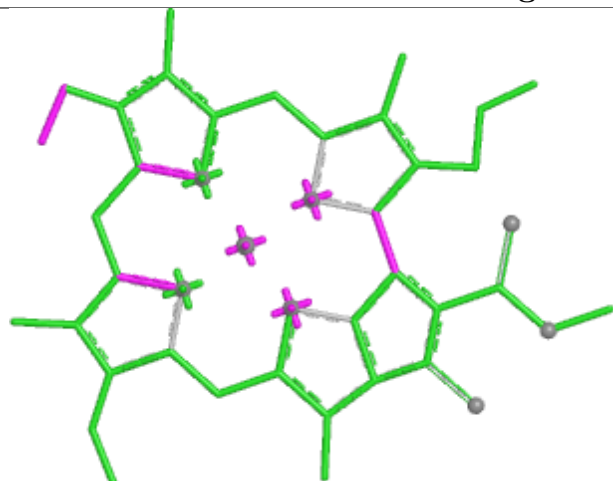
Torsions



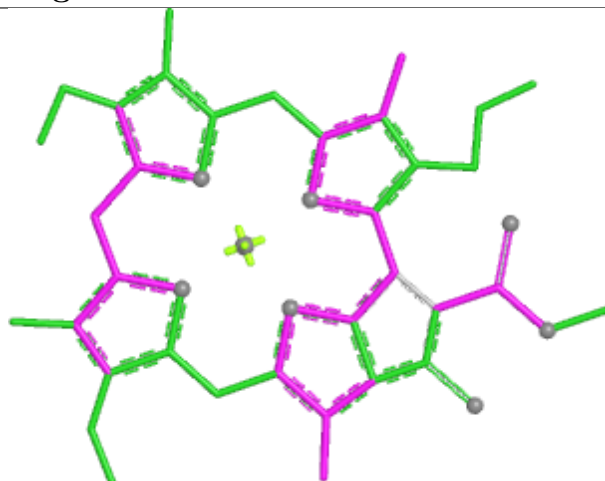
Rings



Ligand CLA g 612



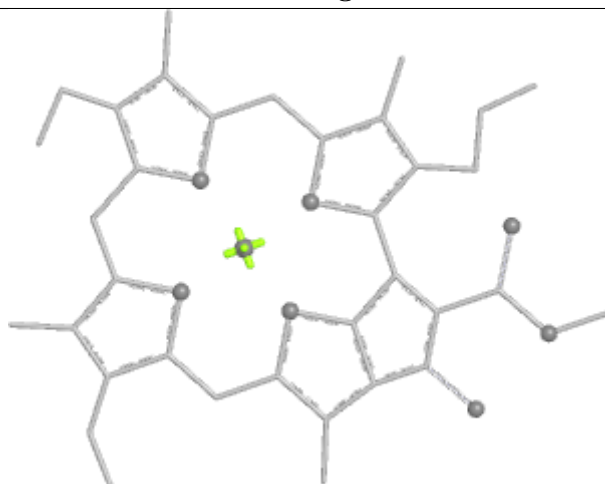
Bond lengths



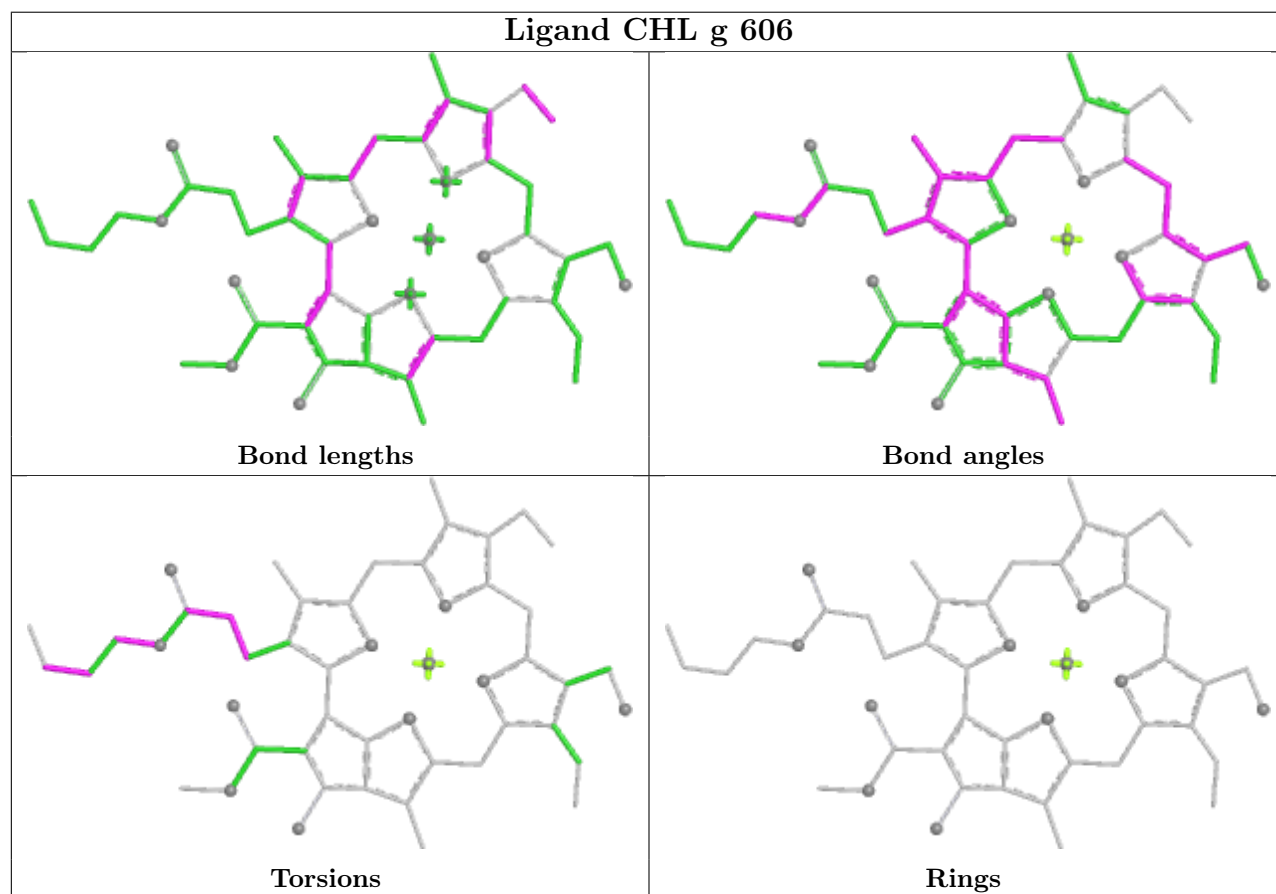
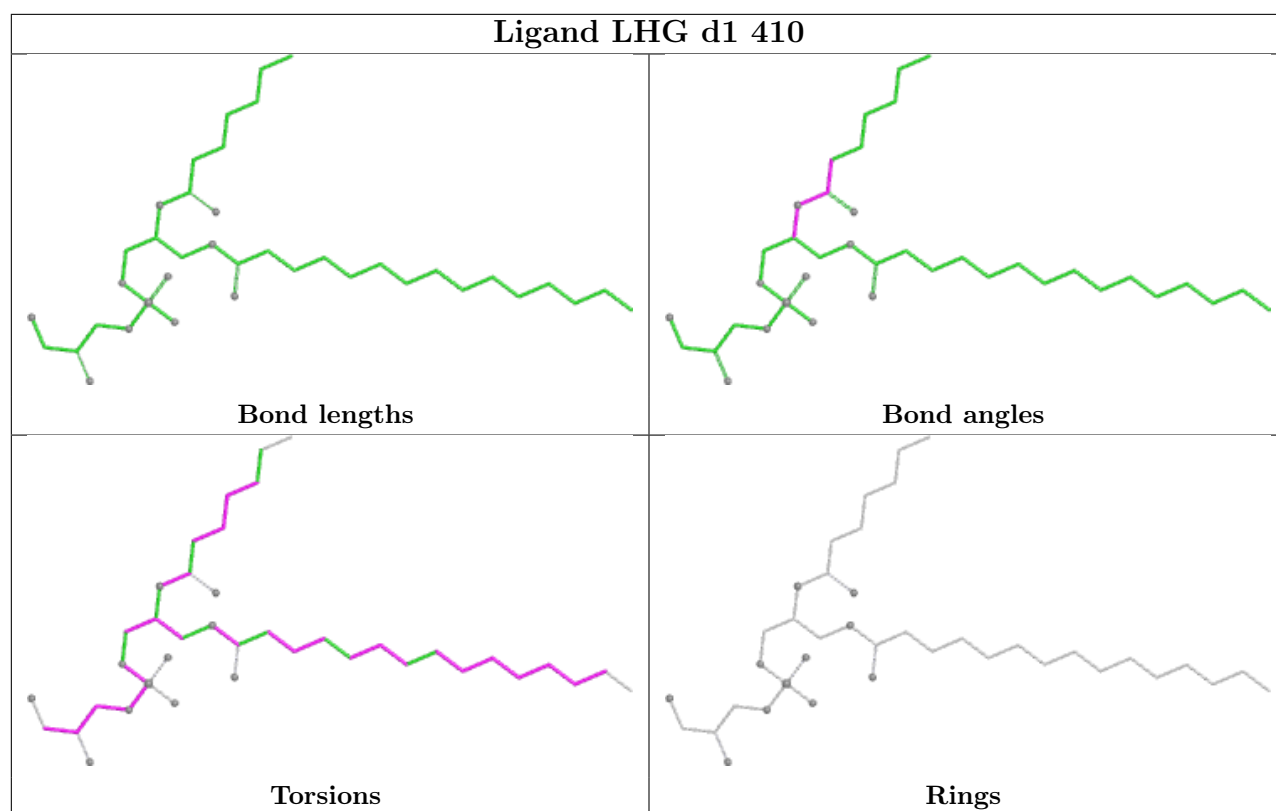
Bond angles

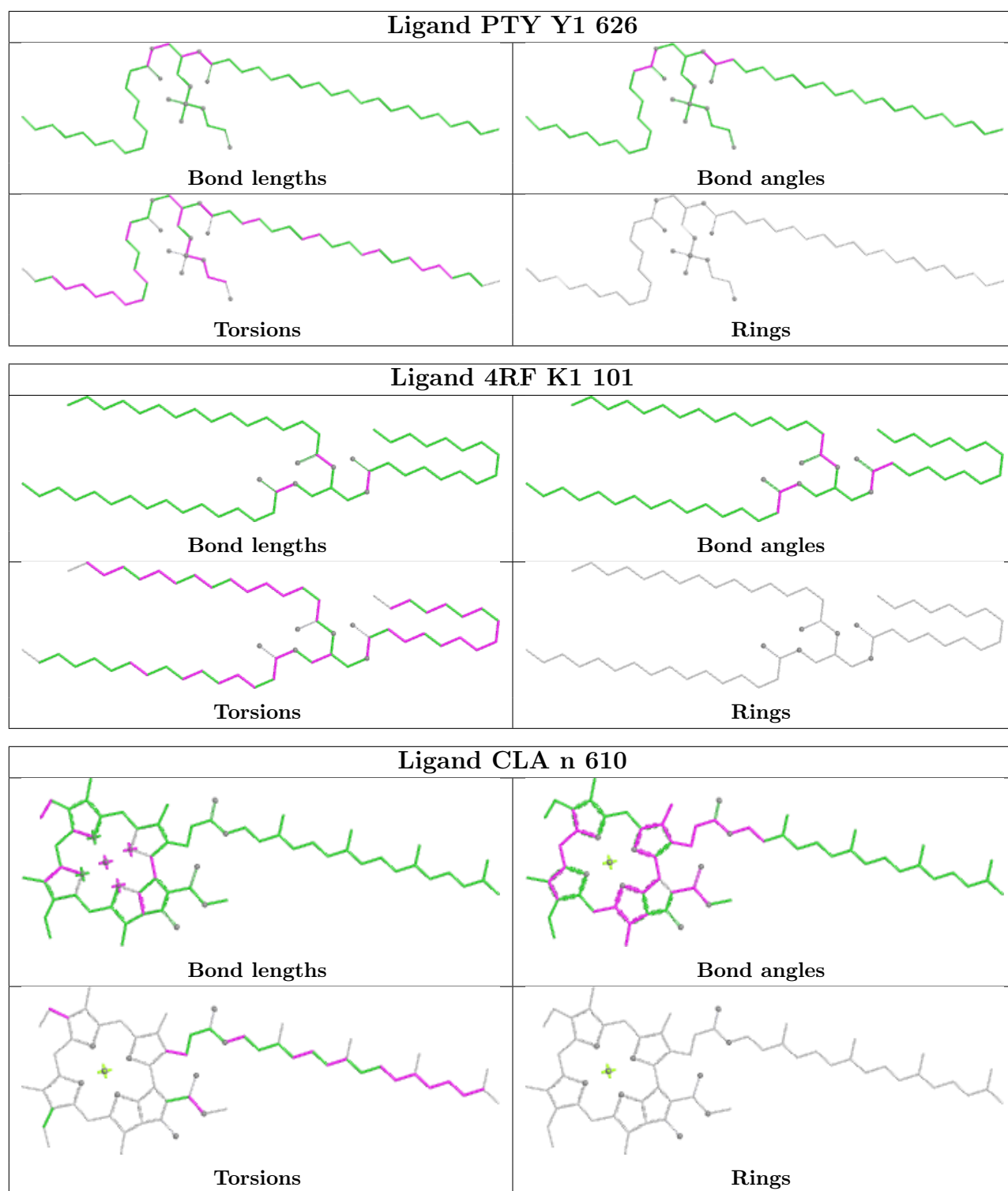


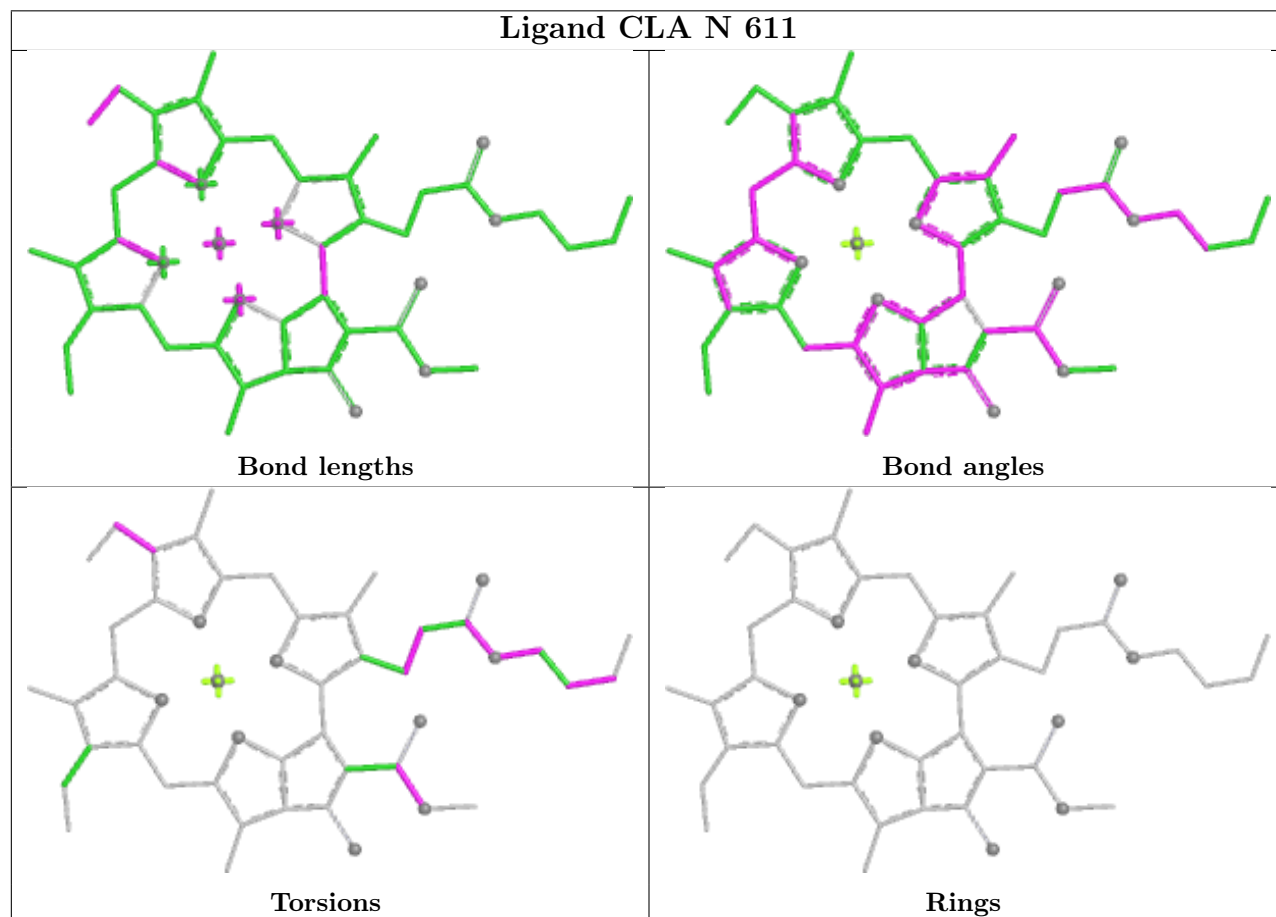
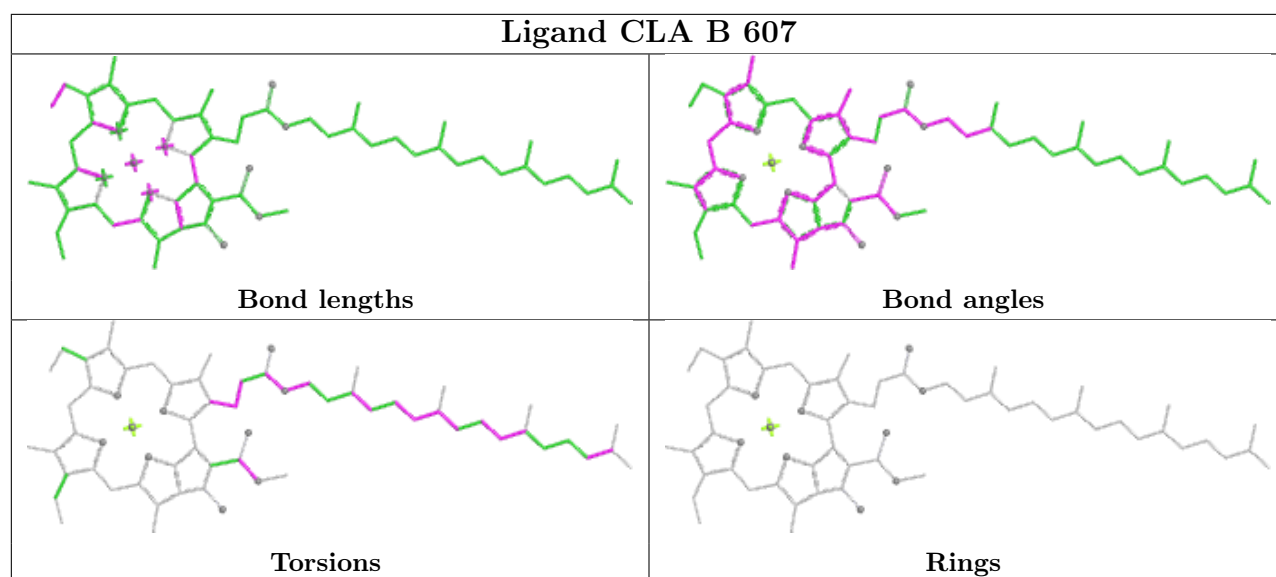
Torsions

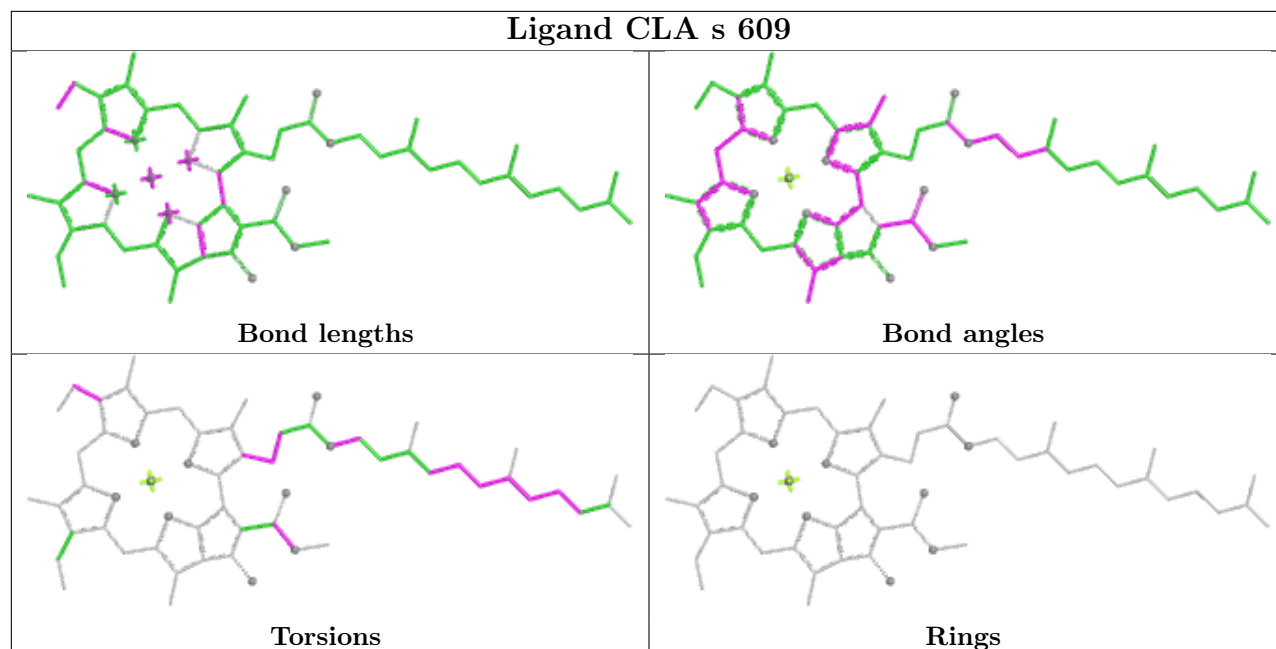
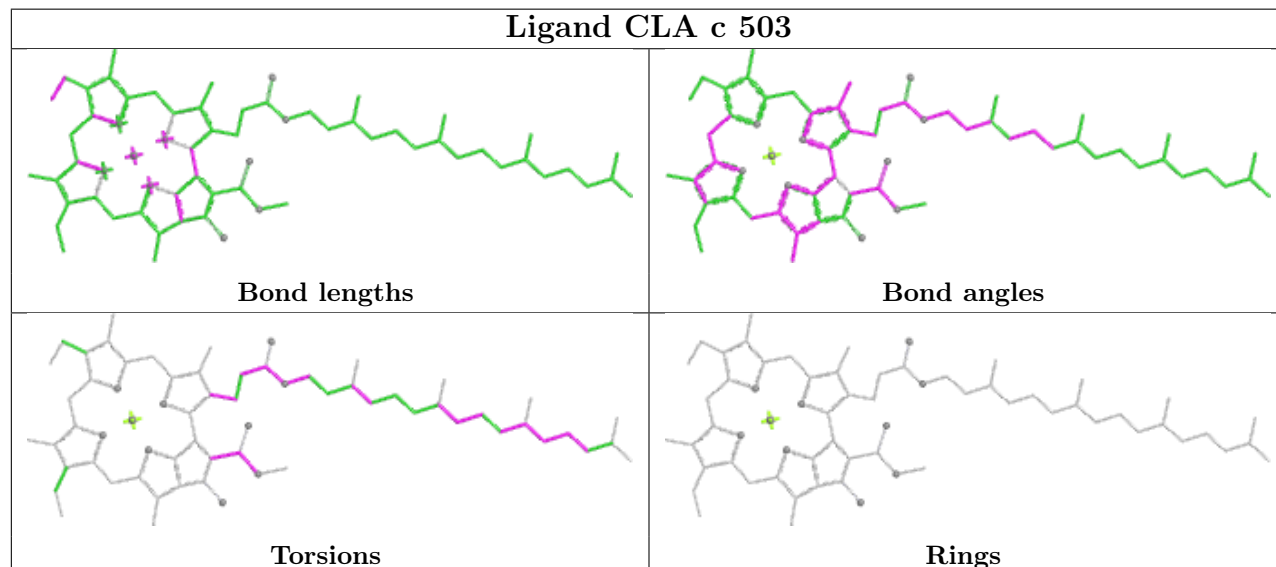
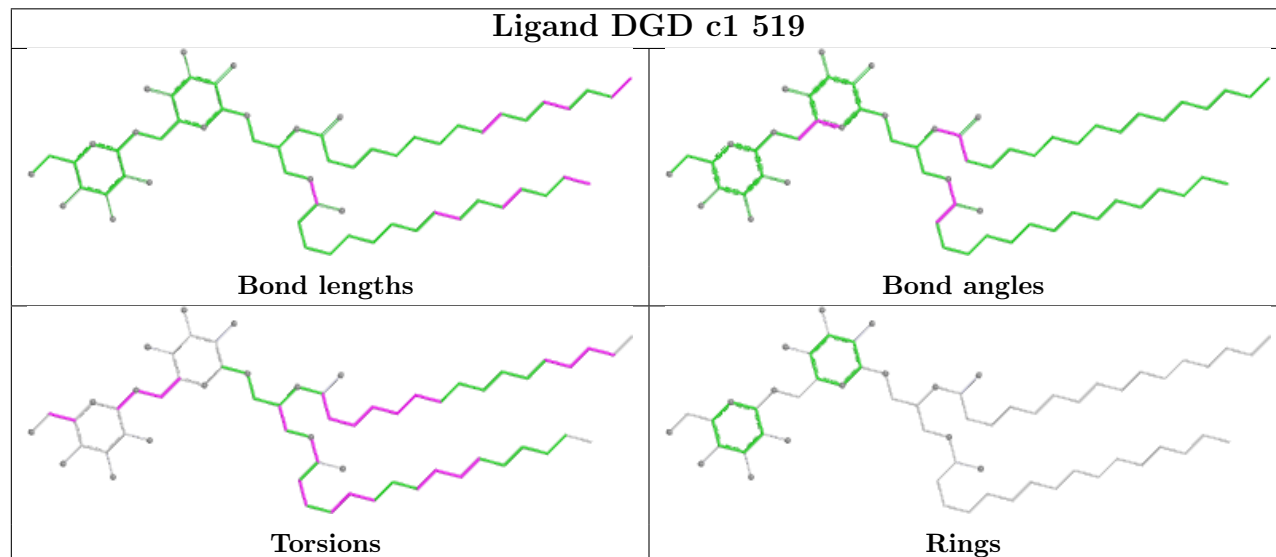


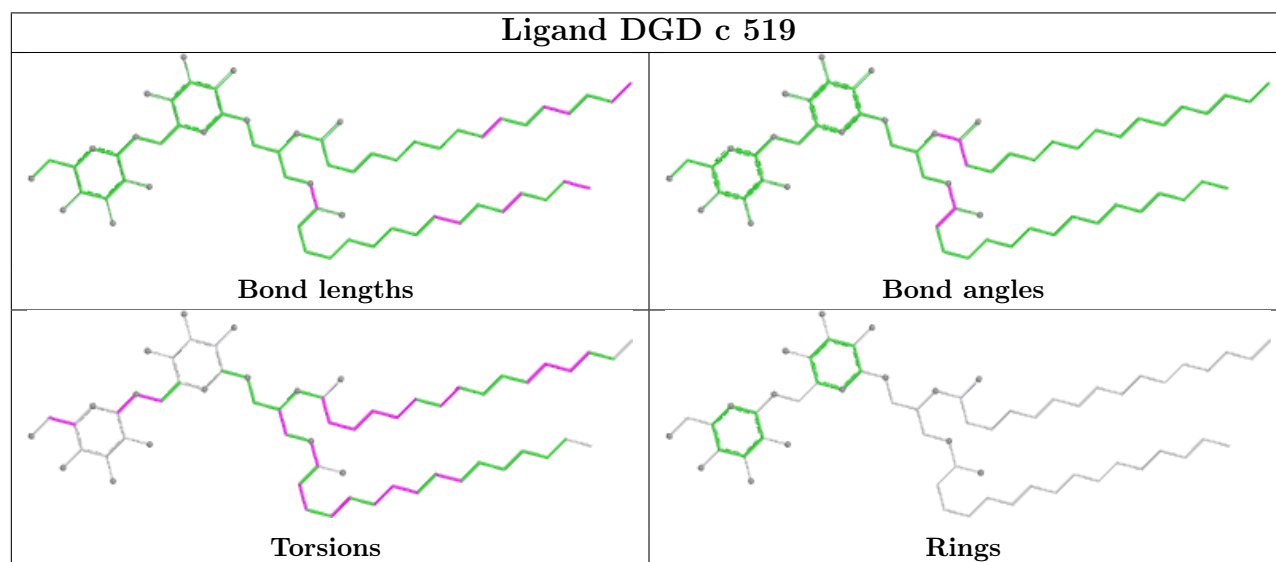
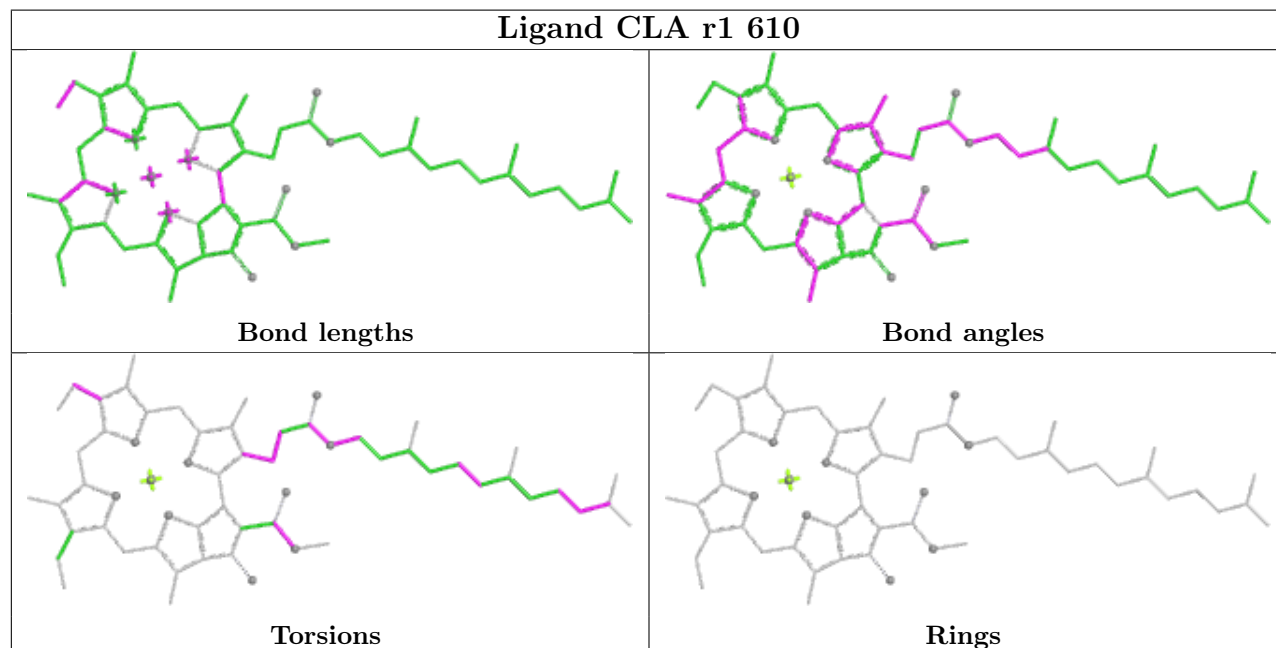
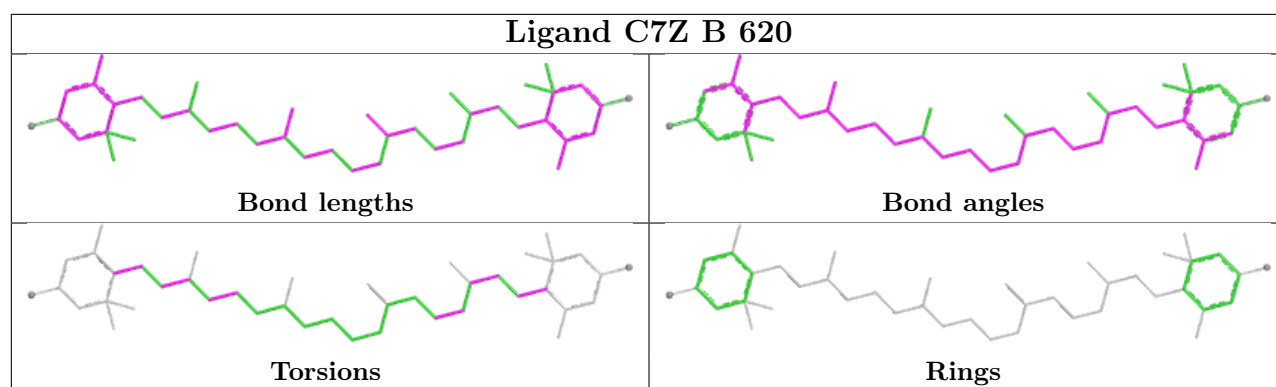
Rings

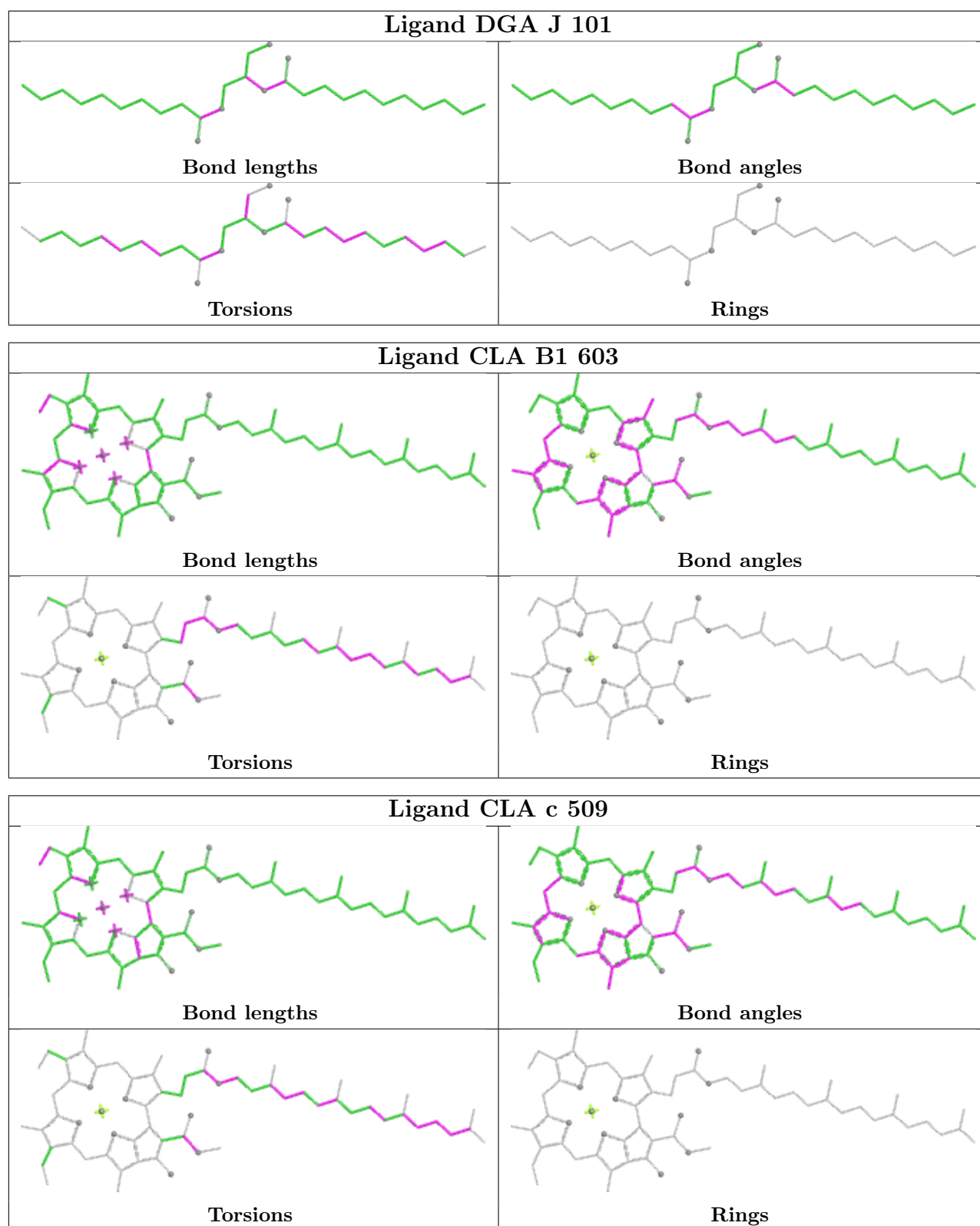


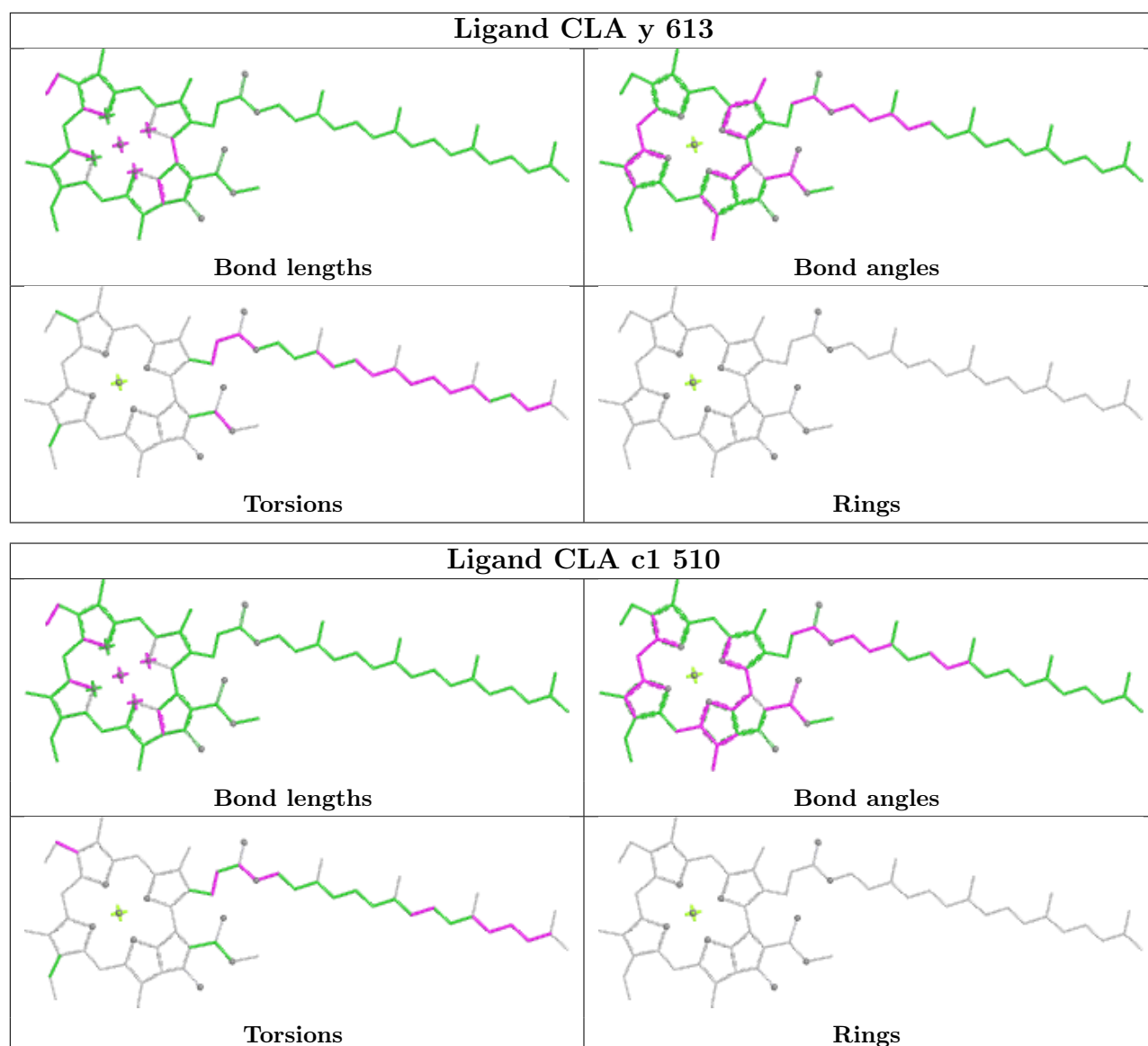


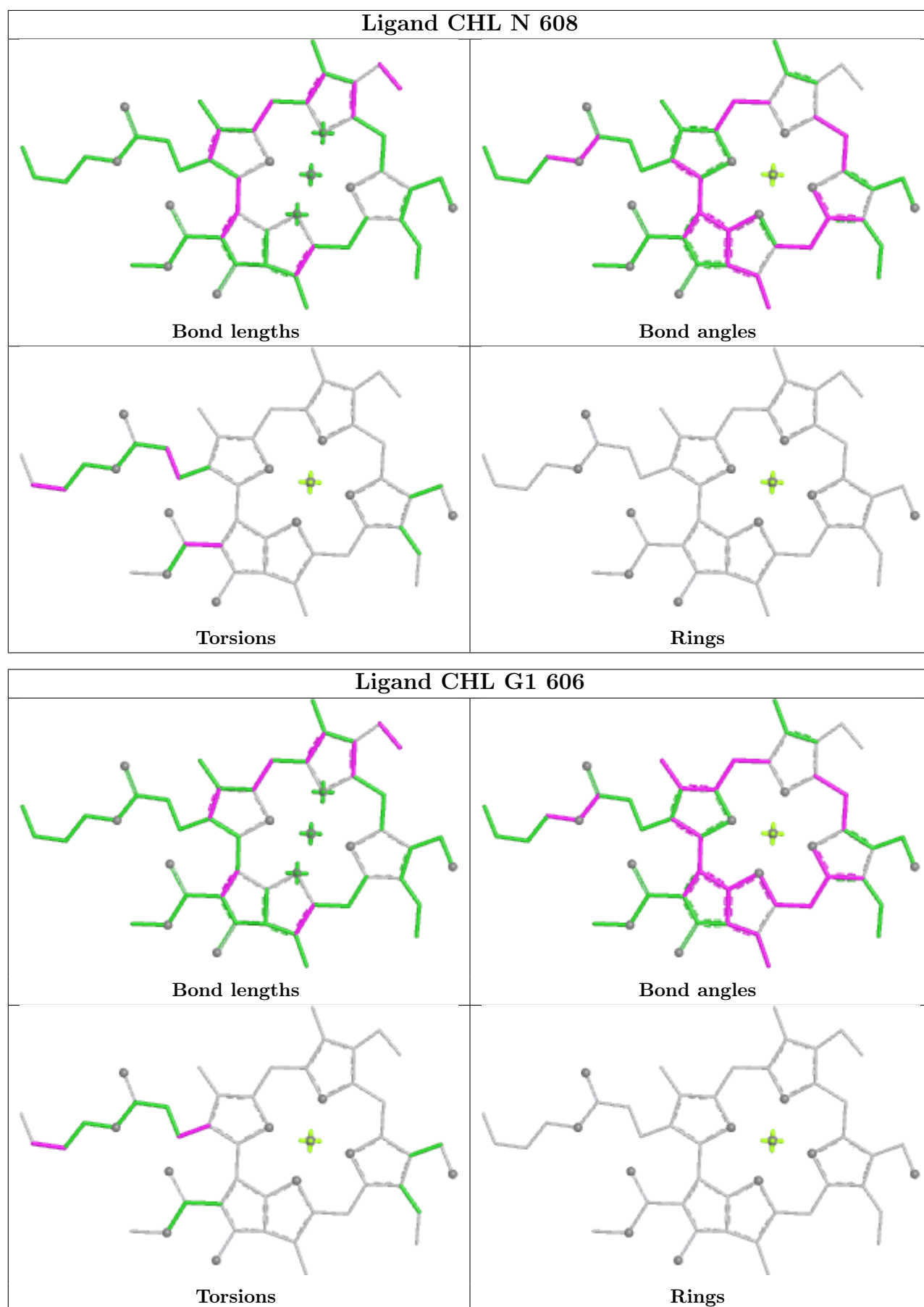


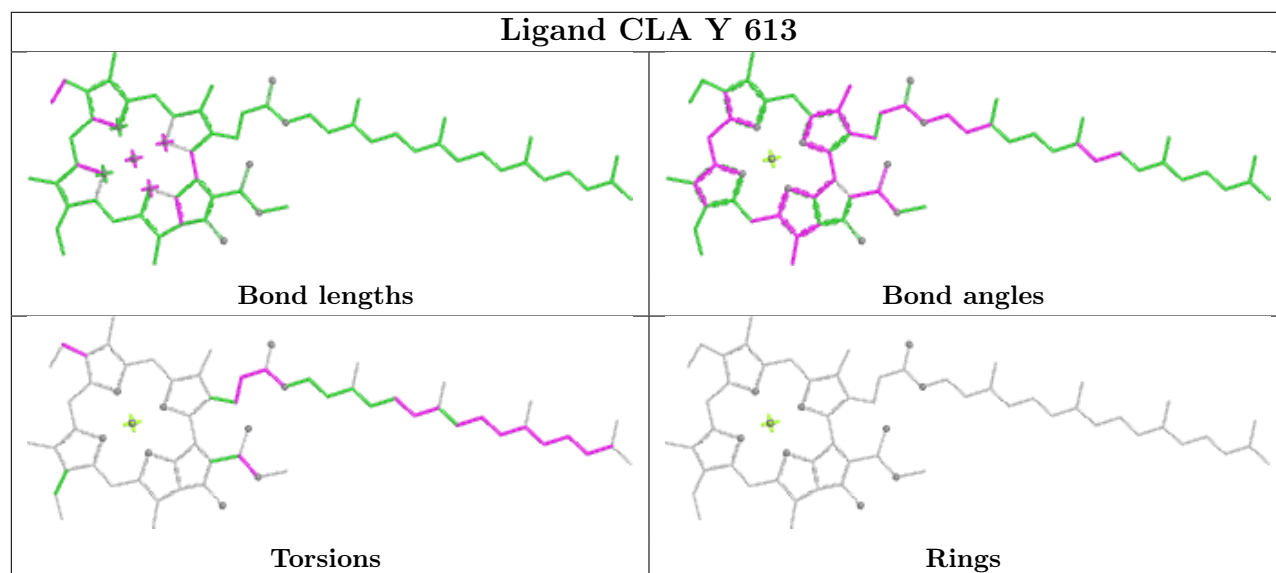
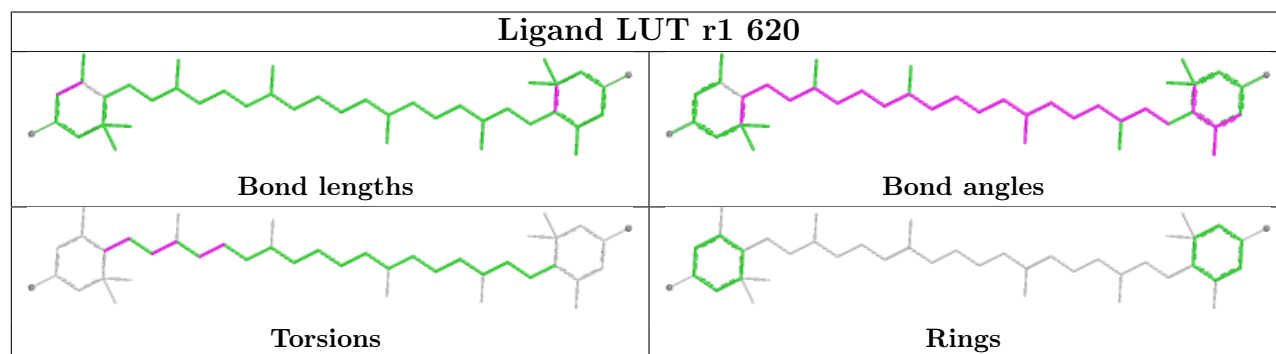
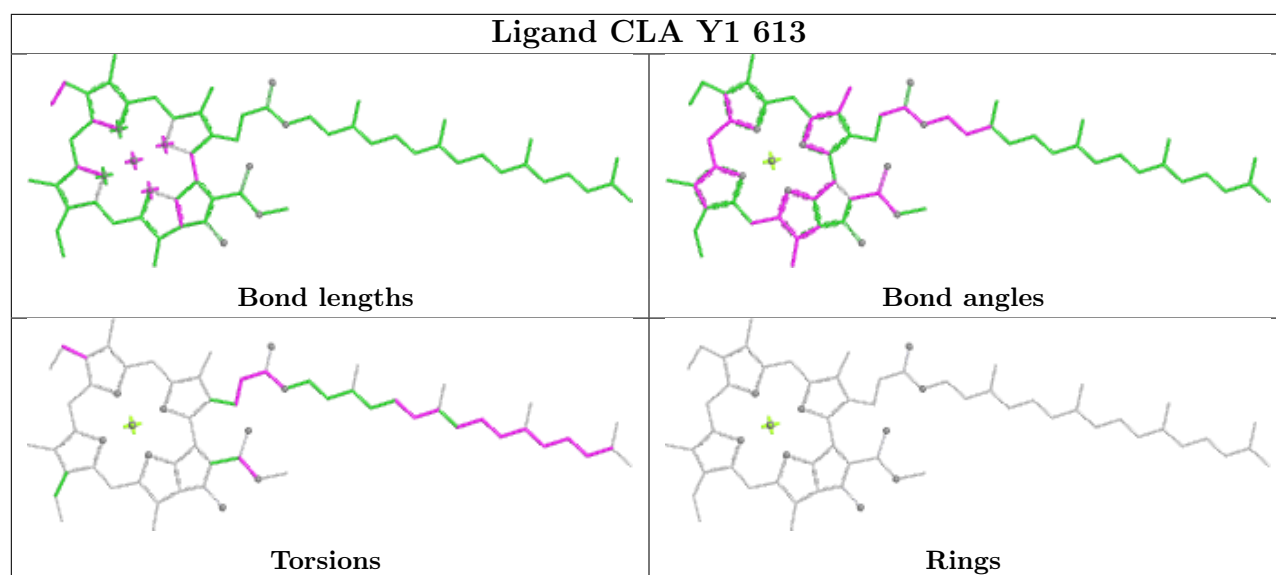
Ligand CLA s 609**Ligand CLA c 503****Ligand DGD c1 519**

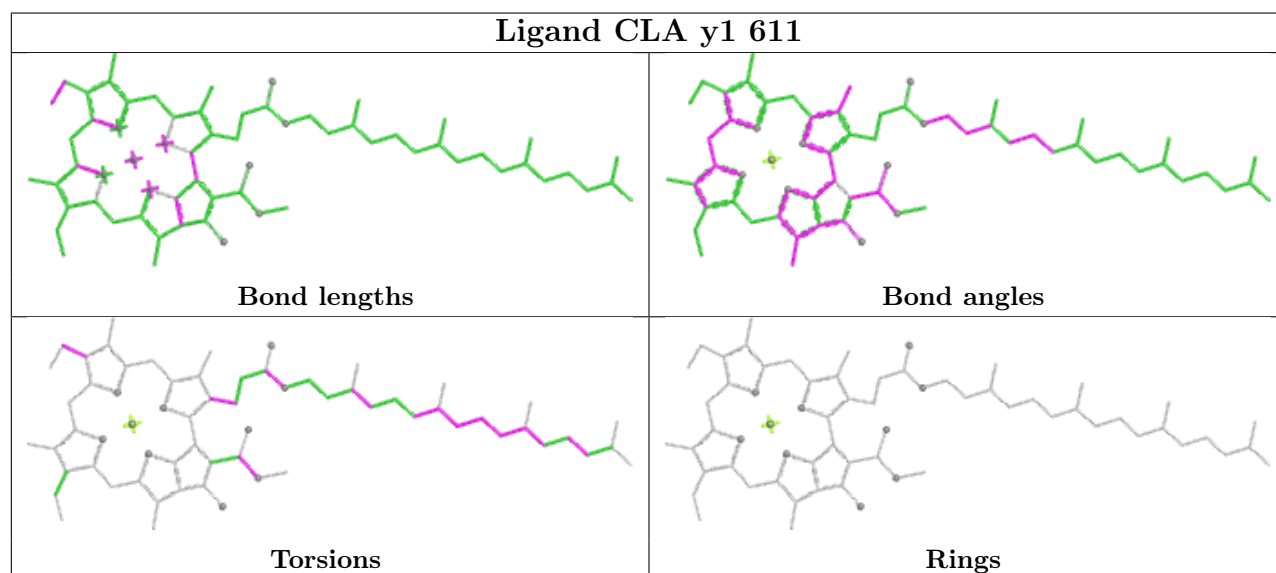
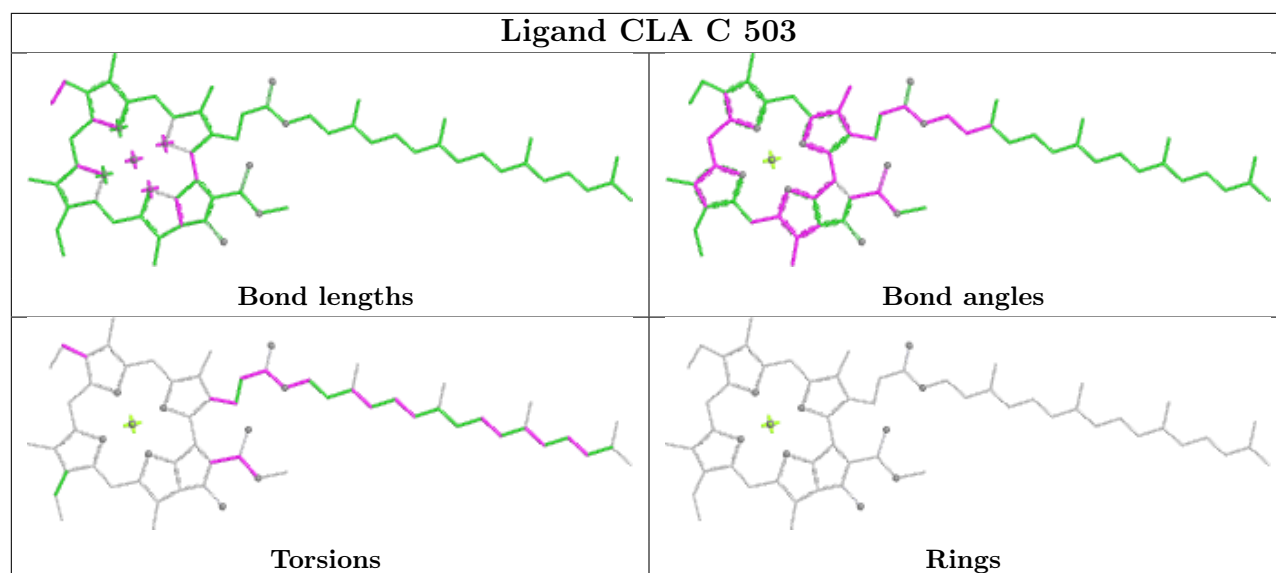
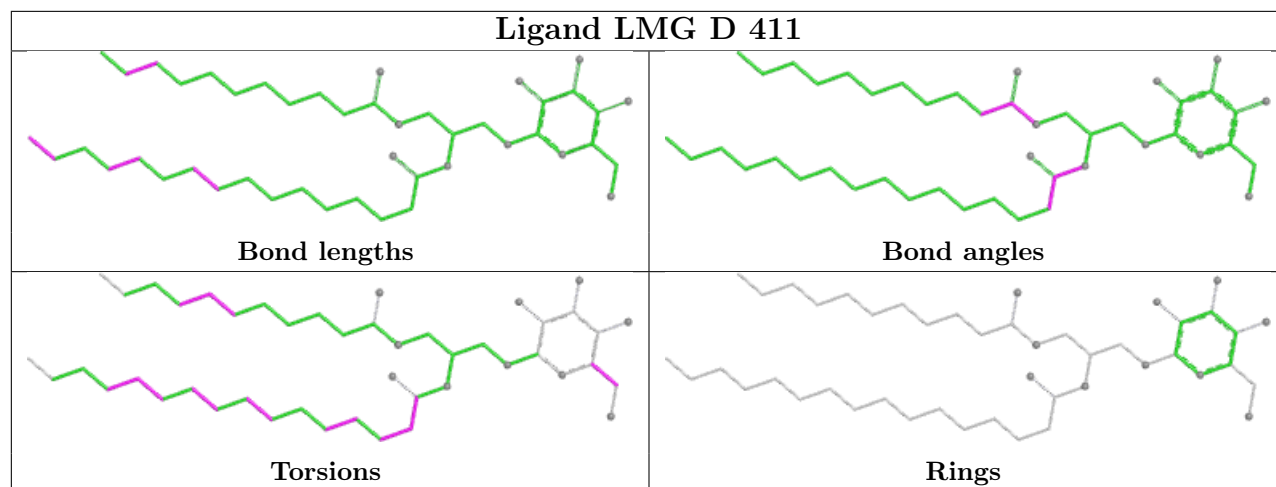


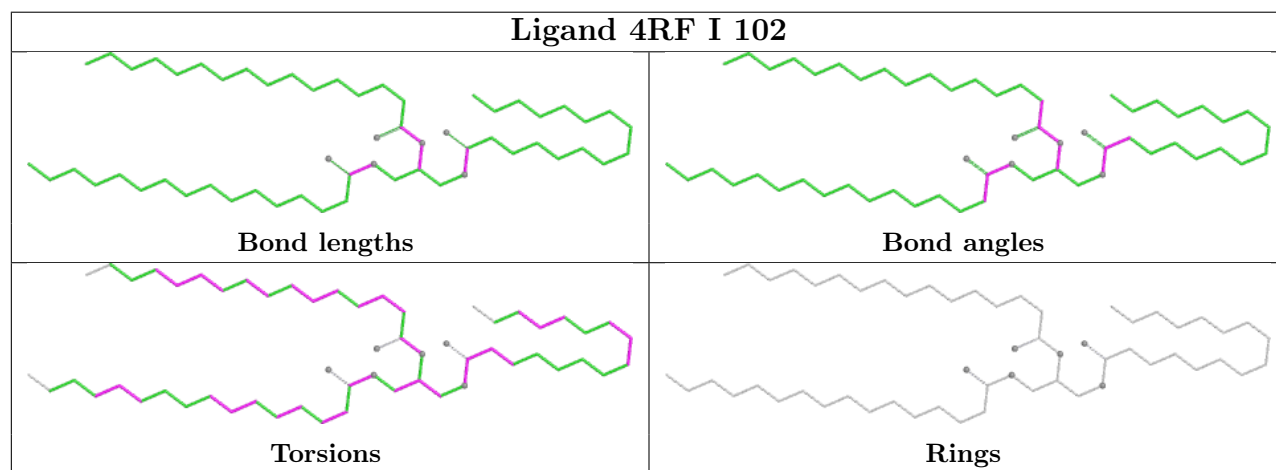
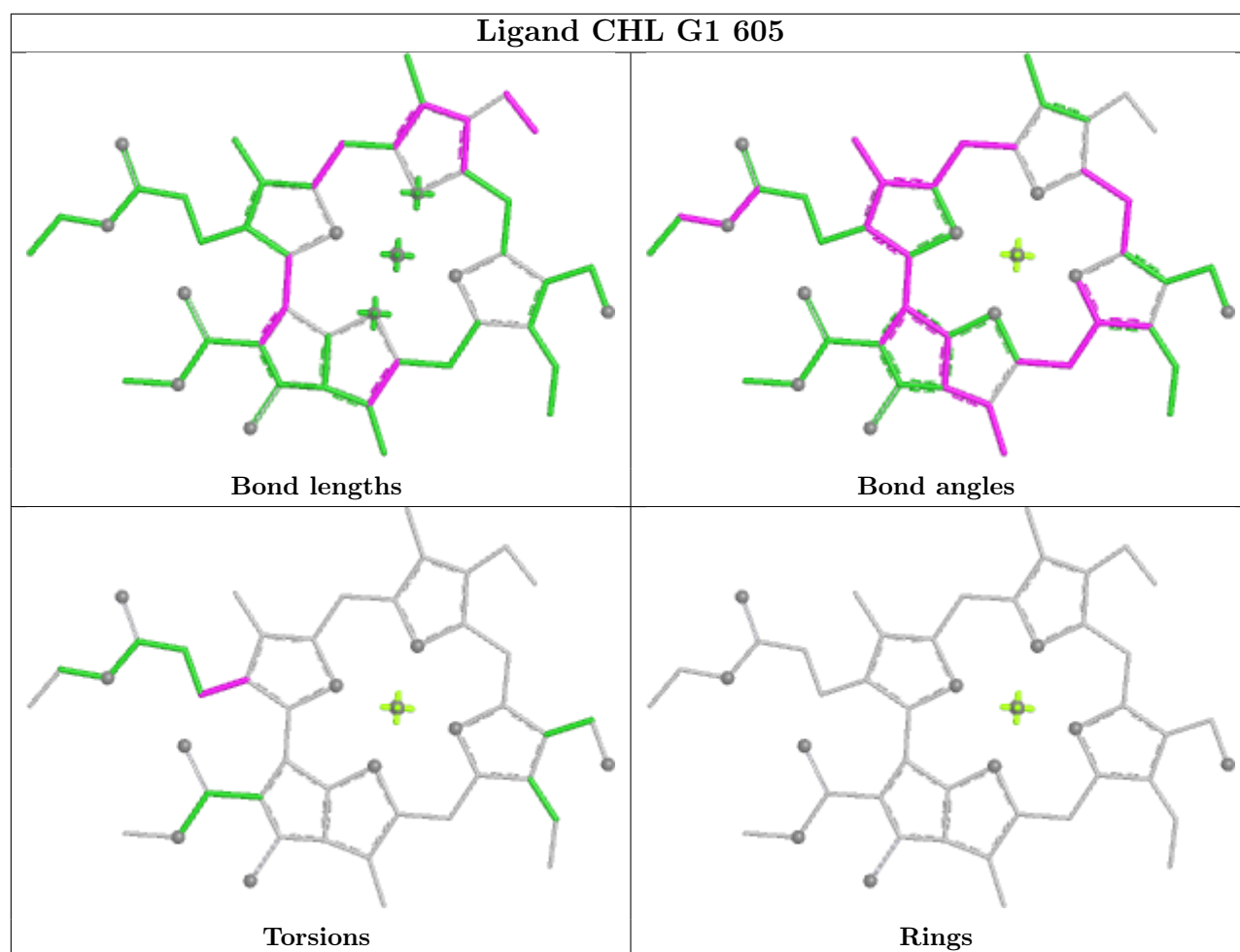


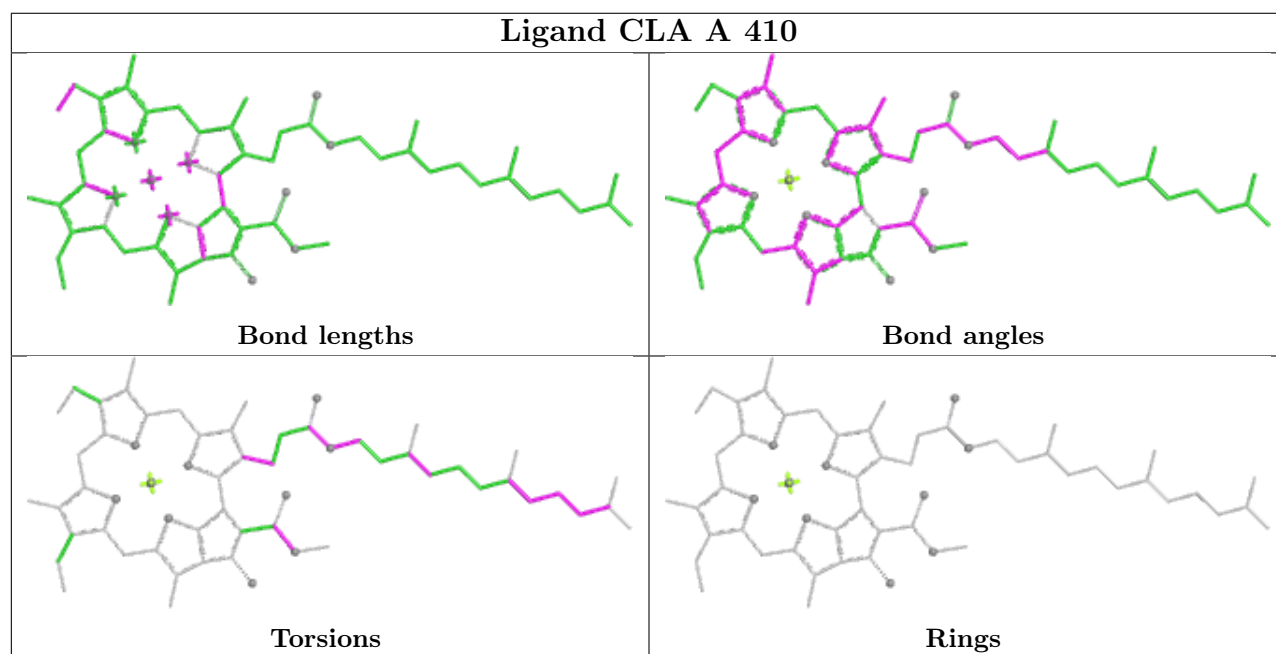
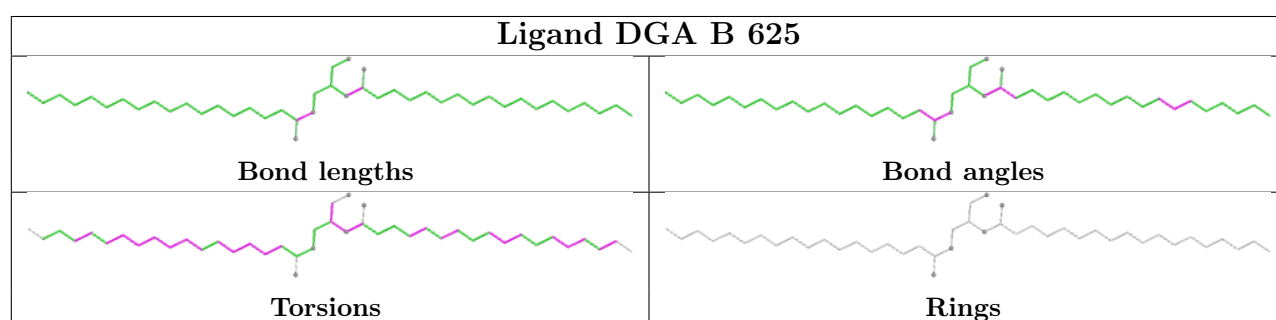
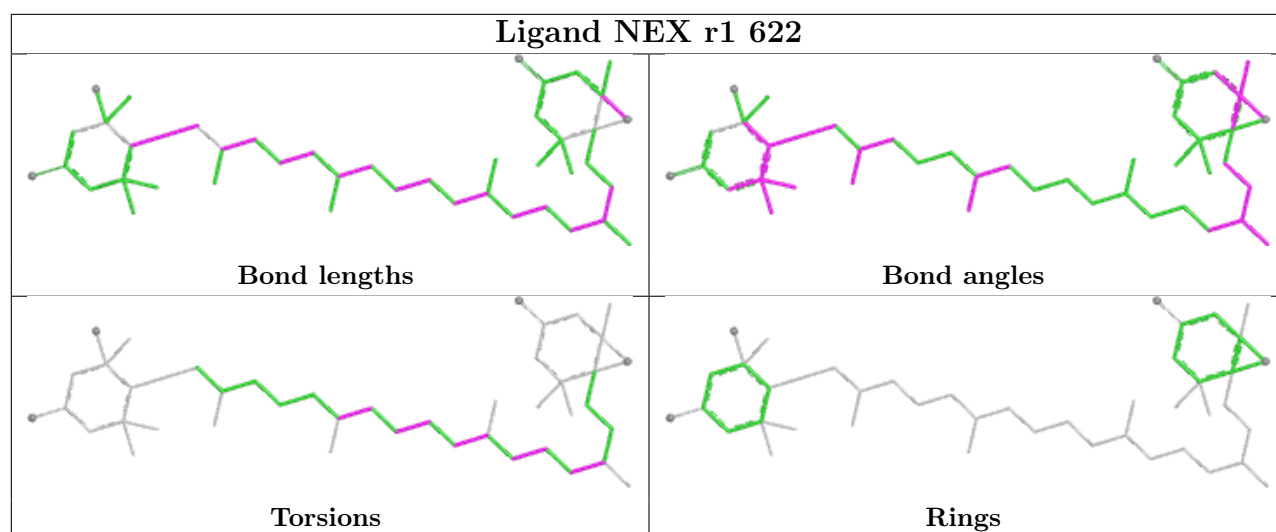


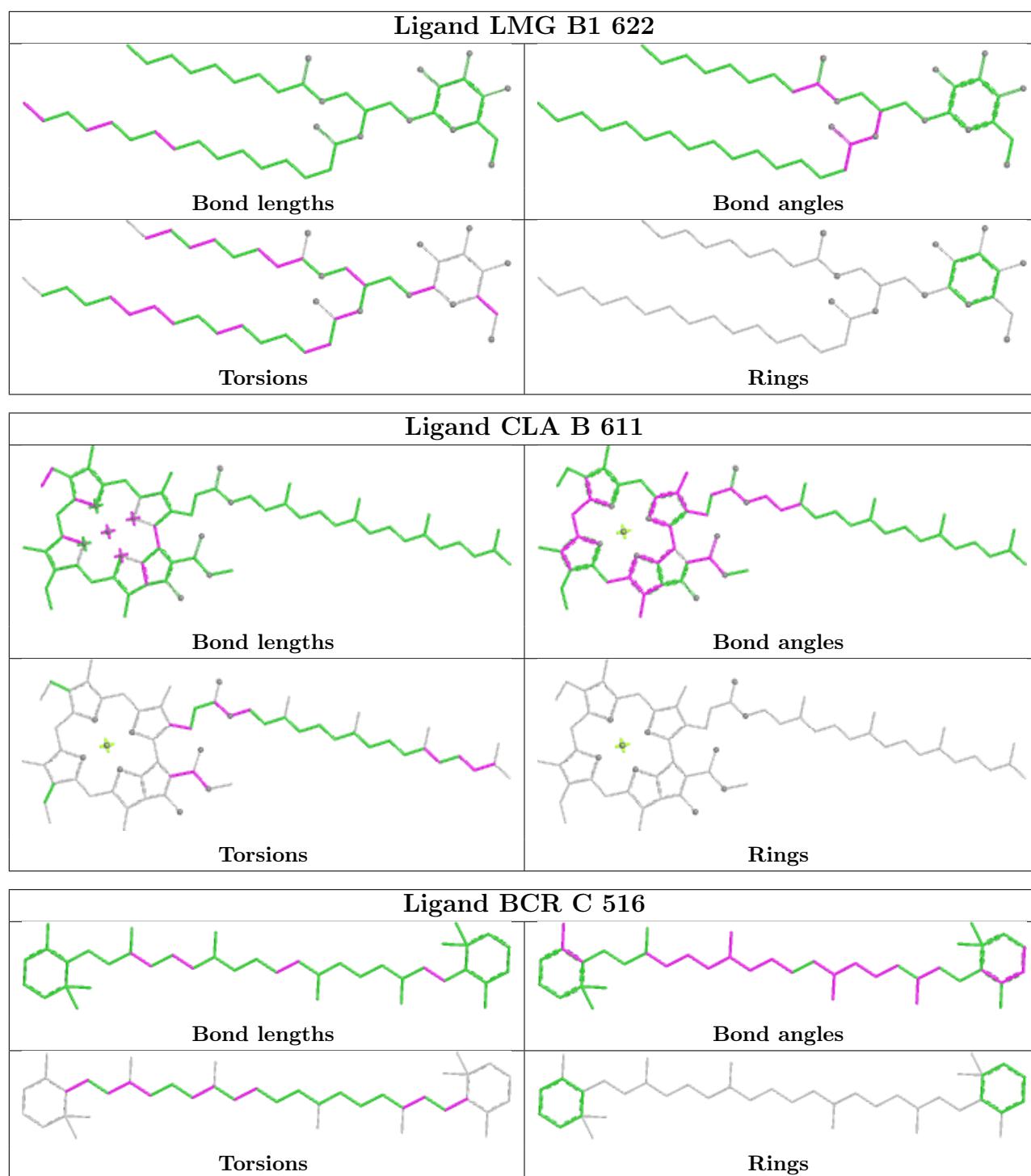


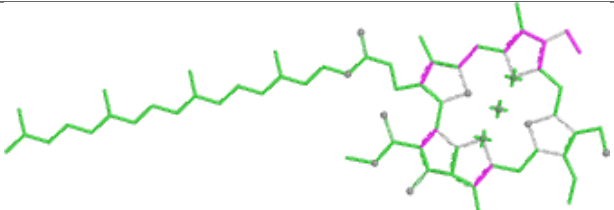
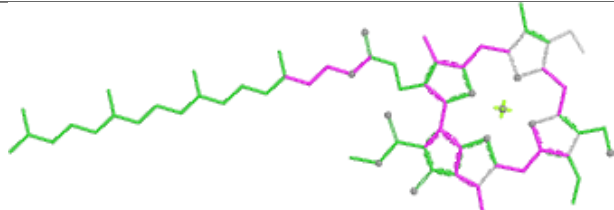
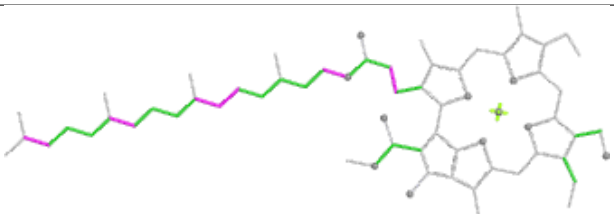
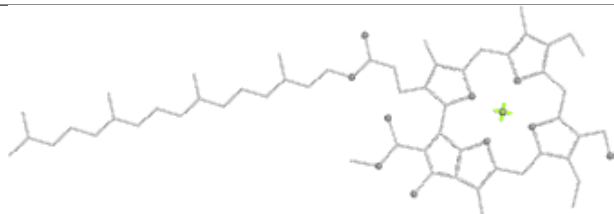


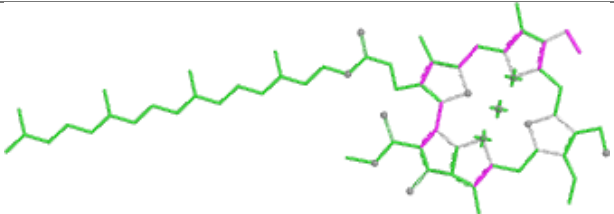
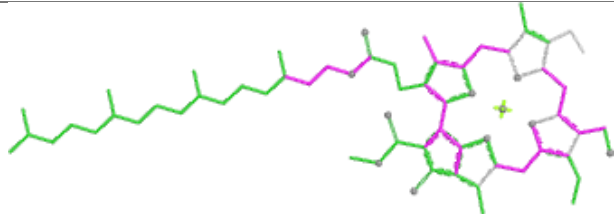
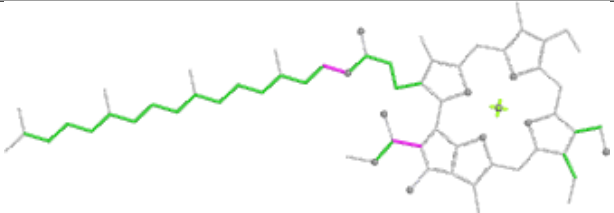
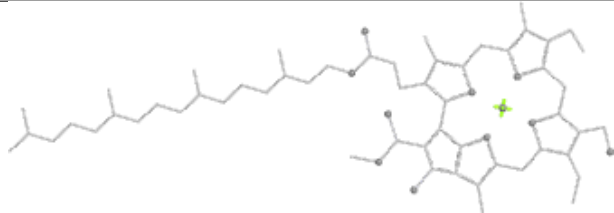


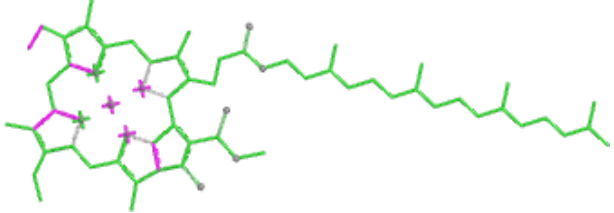
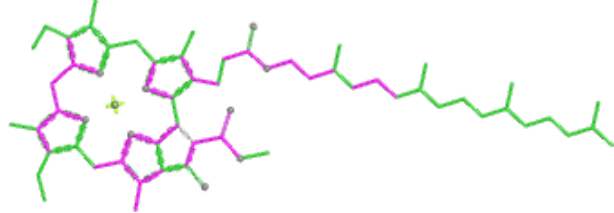
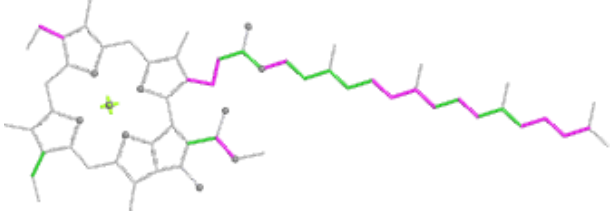
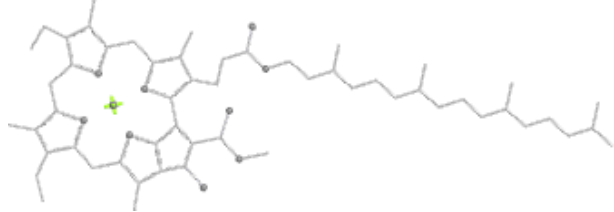


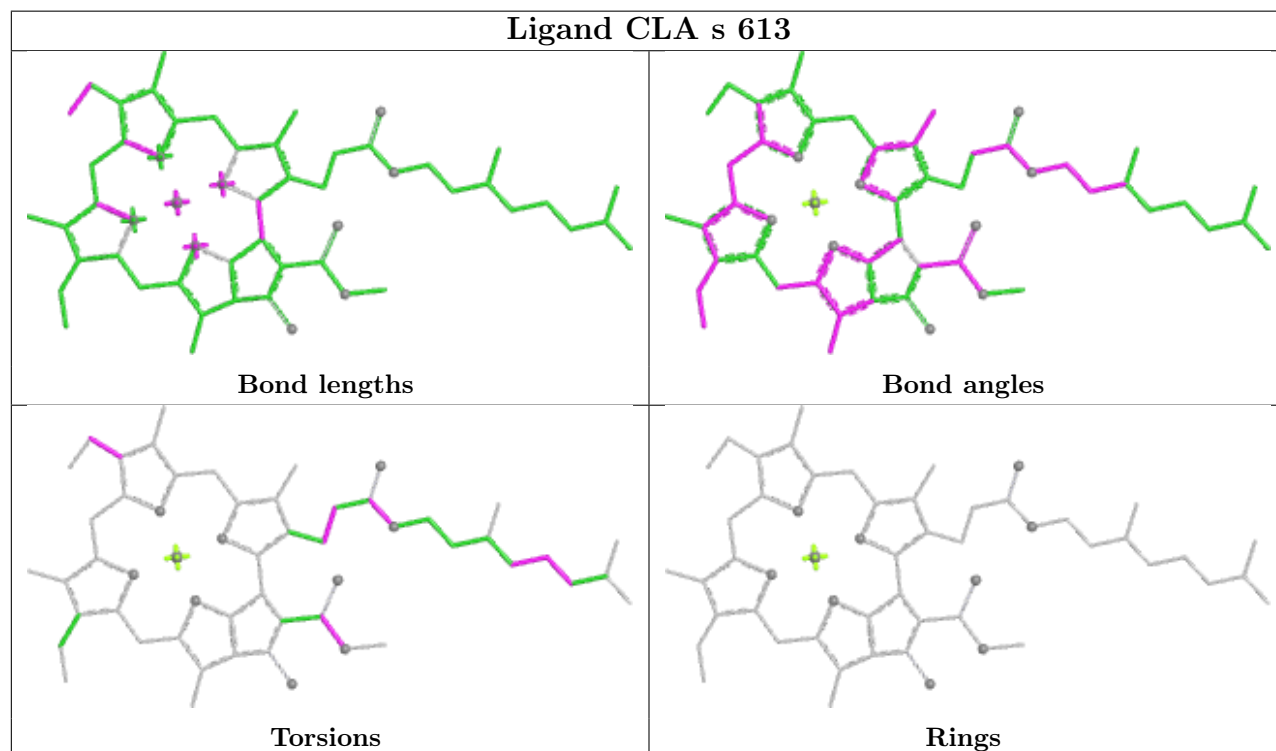
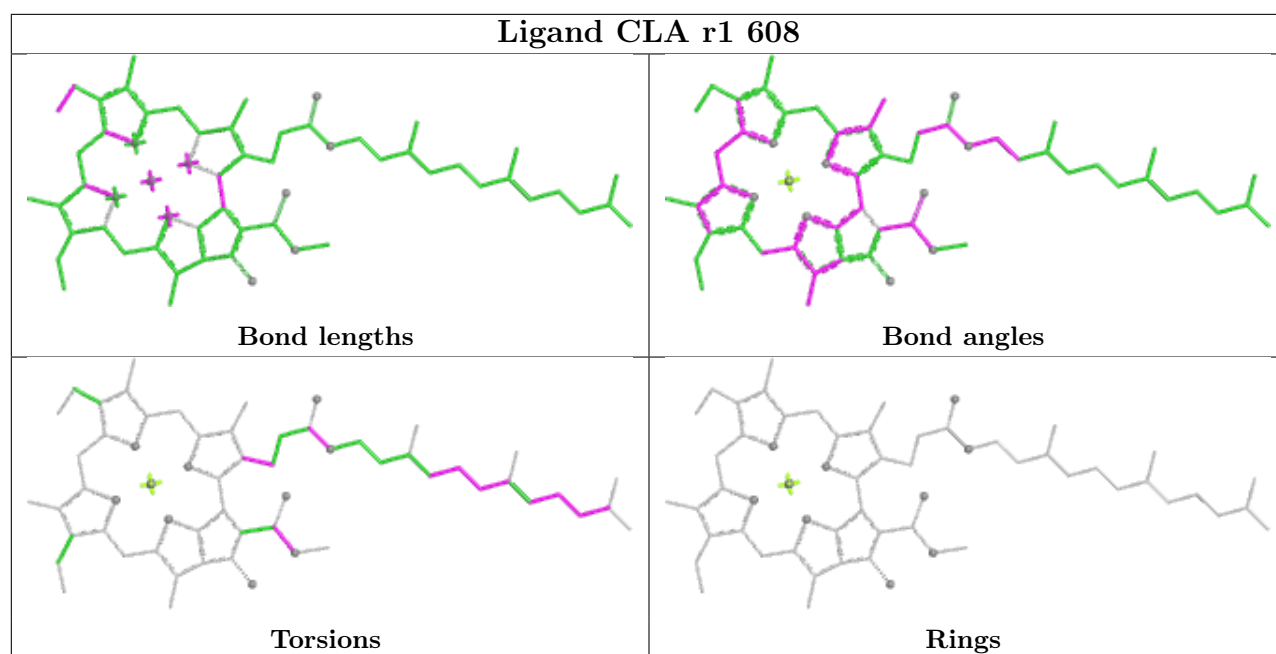




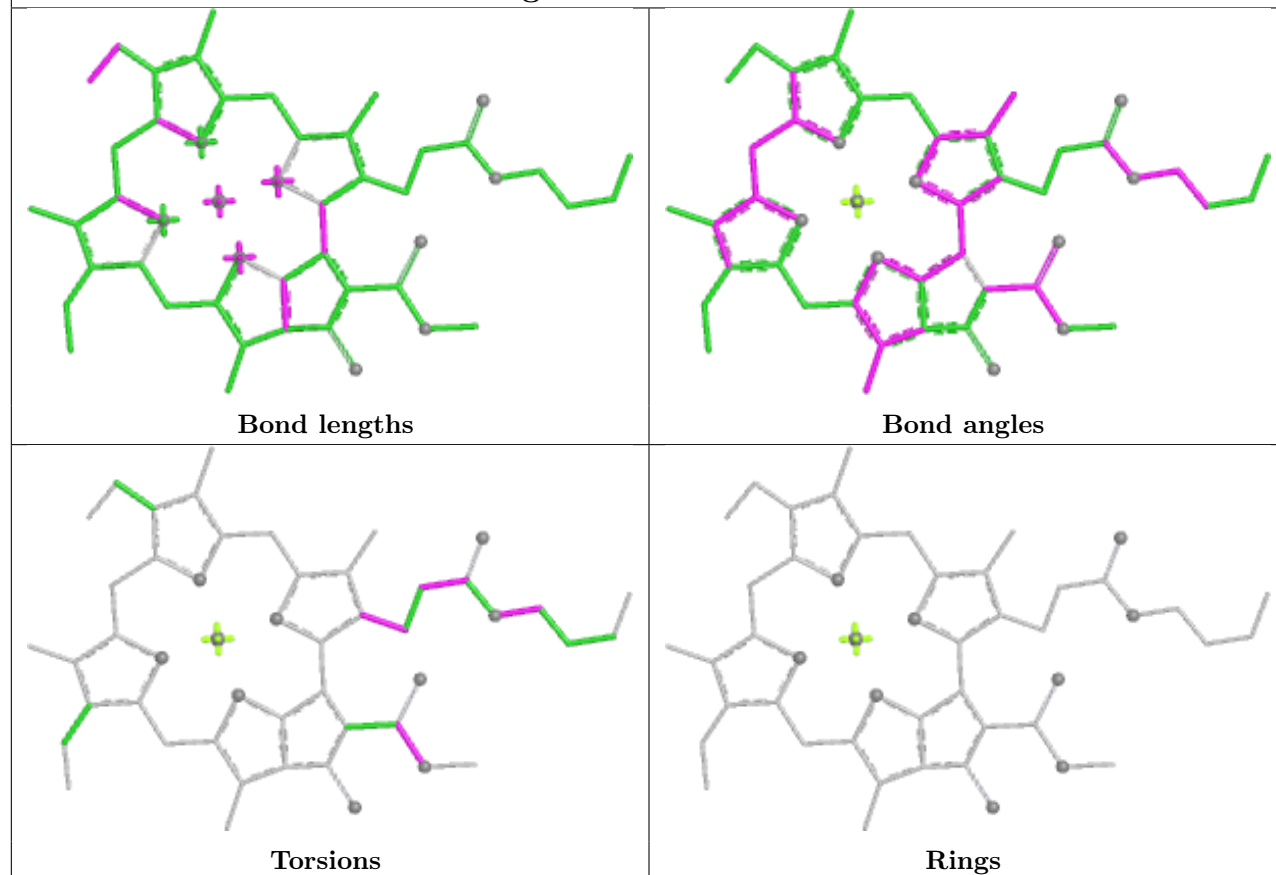
Ligand CHL Y1 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL n 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

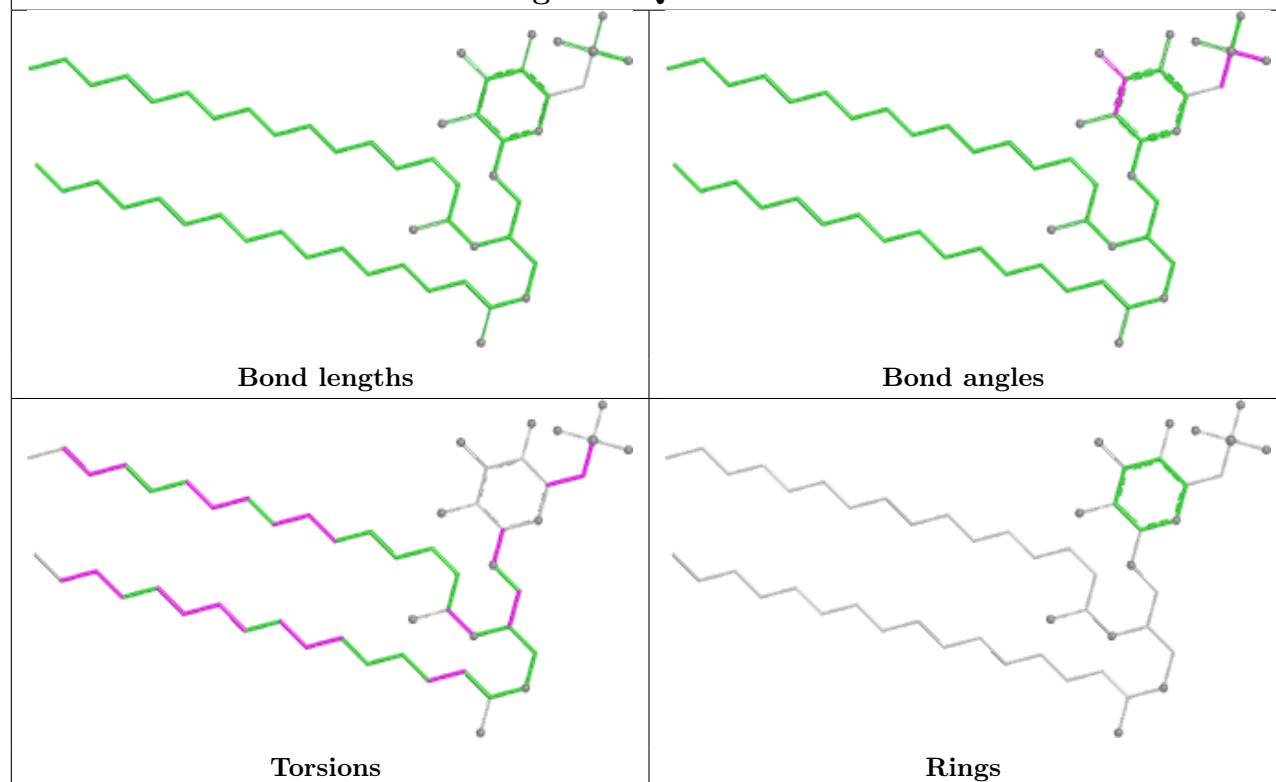
Ligand CLA B1 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

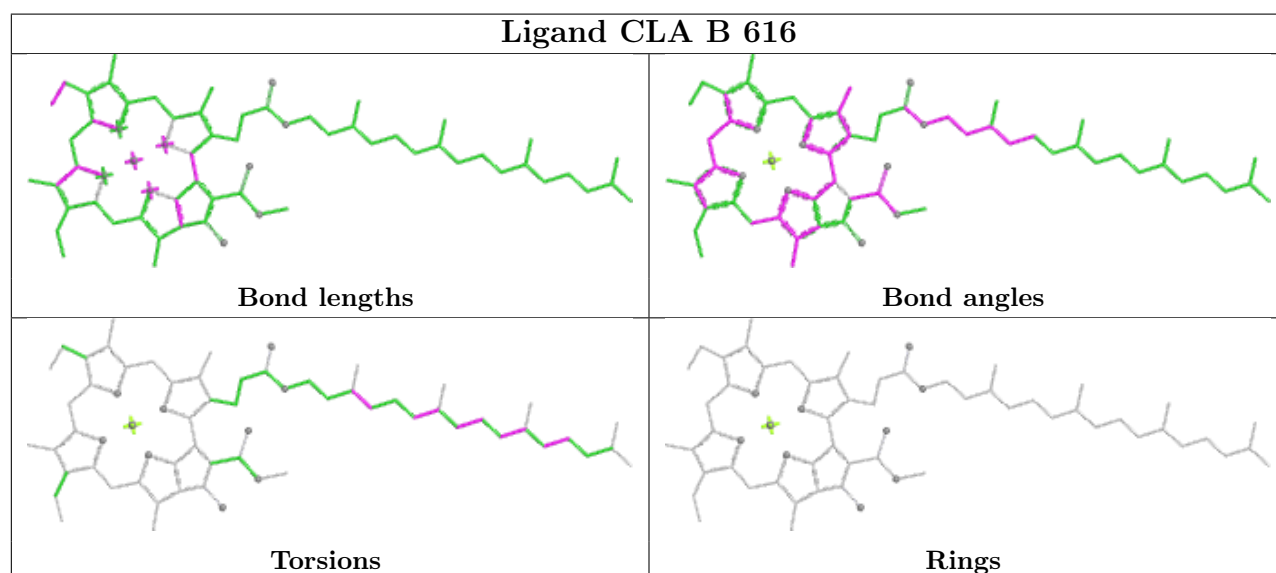
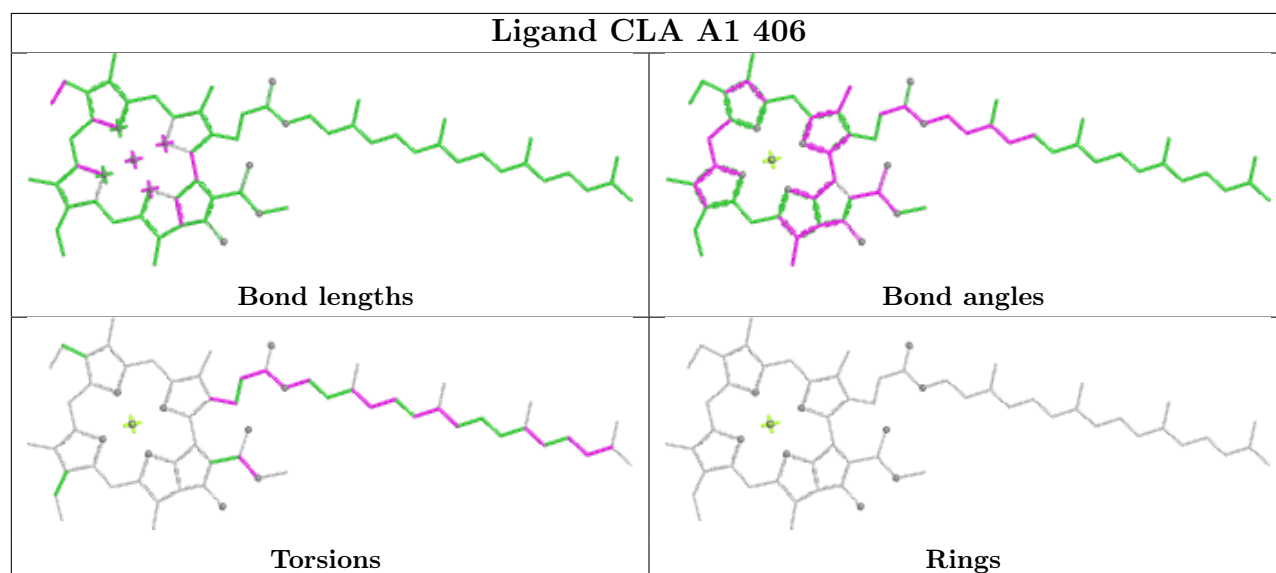
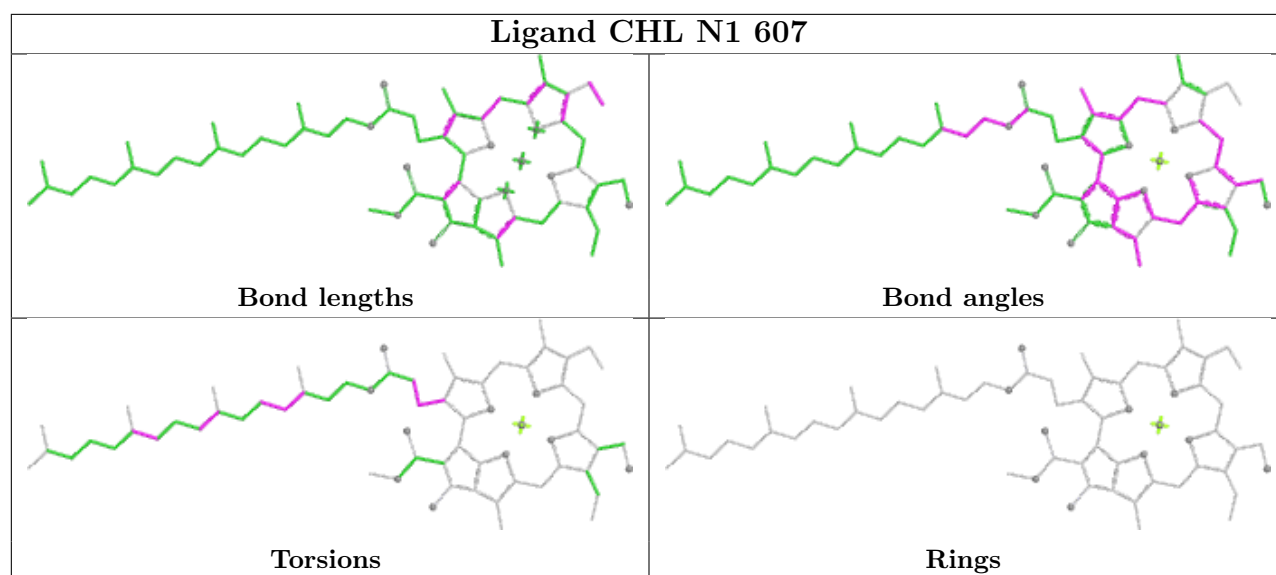


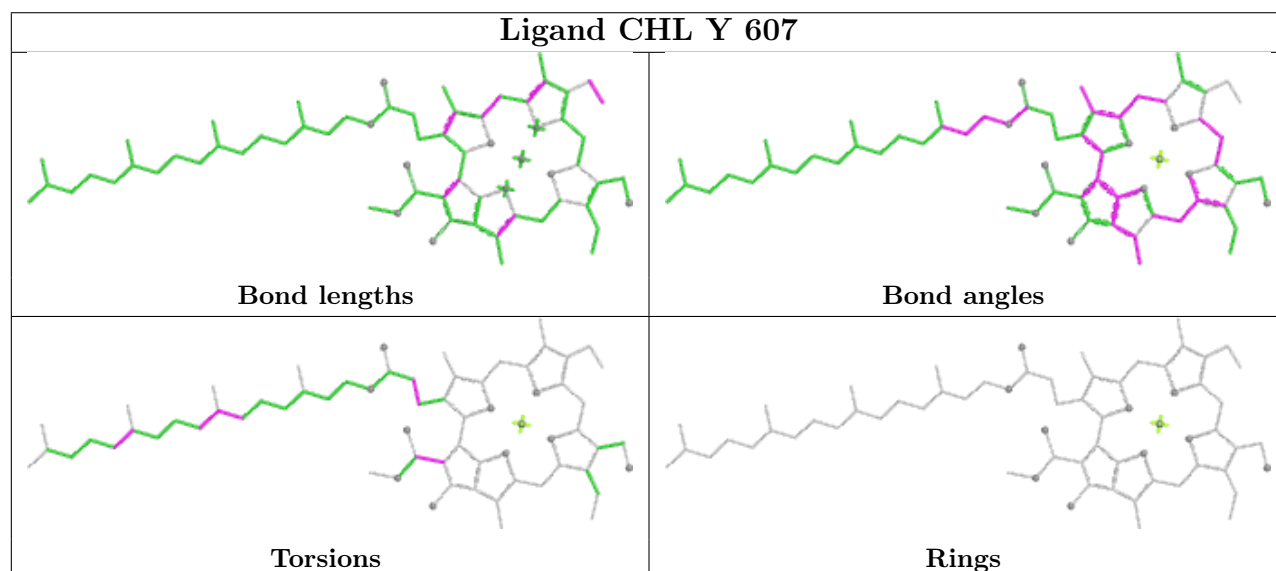
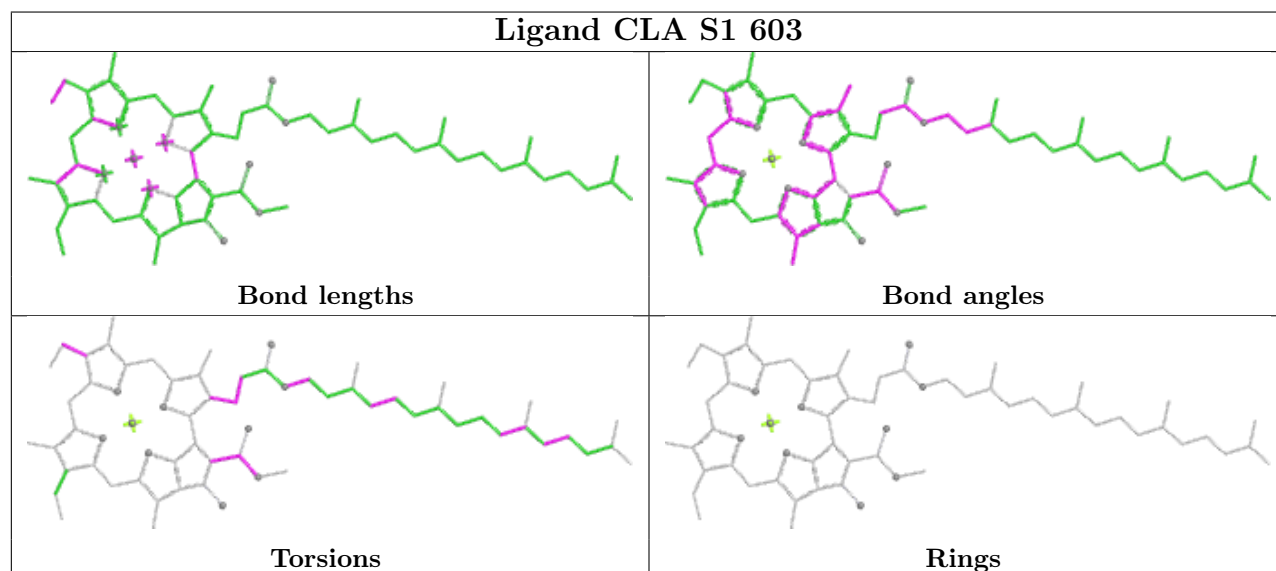
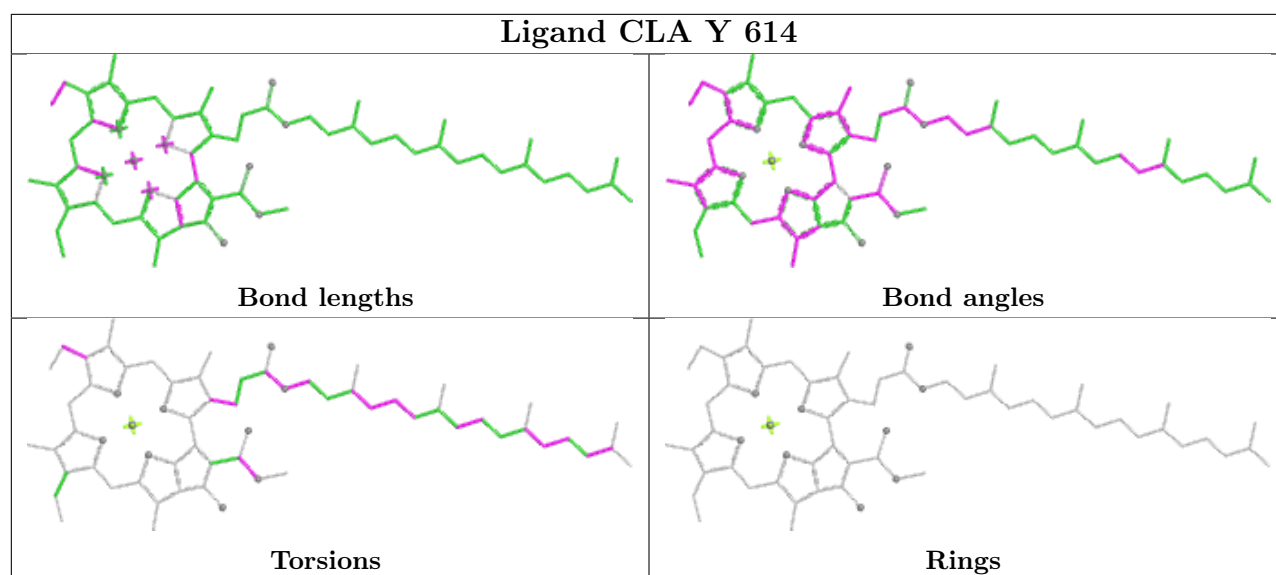
Ligand CLA N1 614



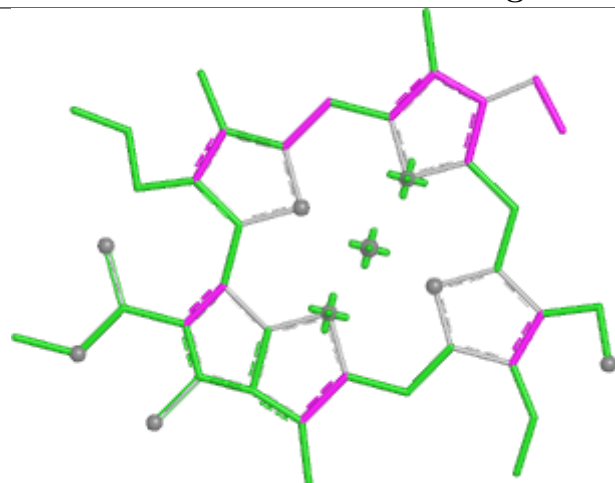
Ligand SQD B 626



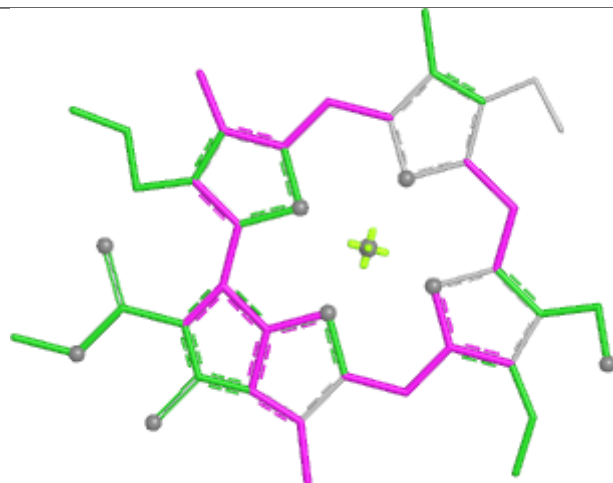




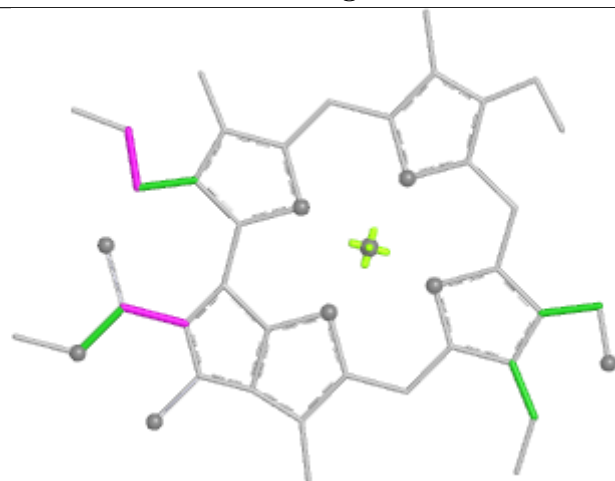
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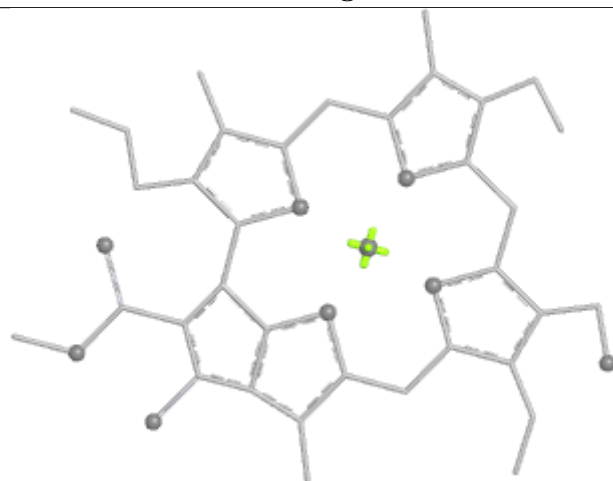
Bond lengths



Bond angles

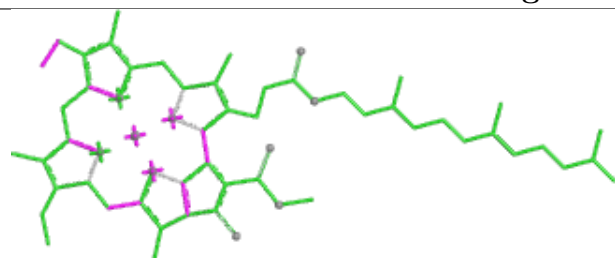


Torsions

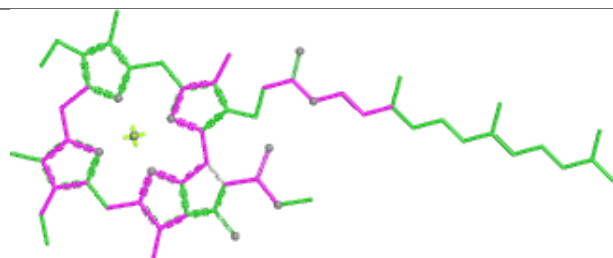


Rings

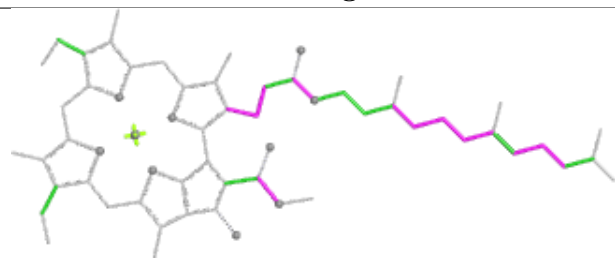
Ligand CLA r 608



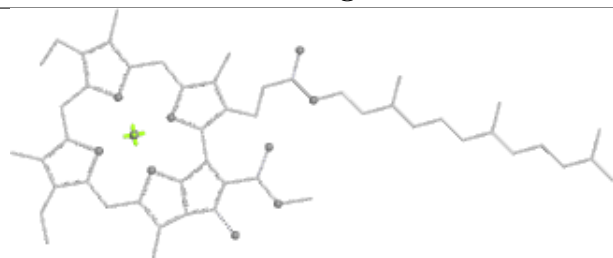
Bond lengths



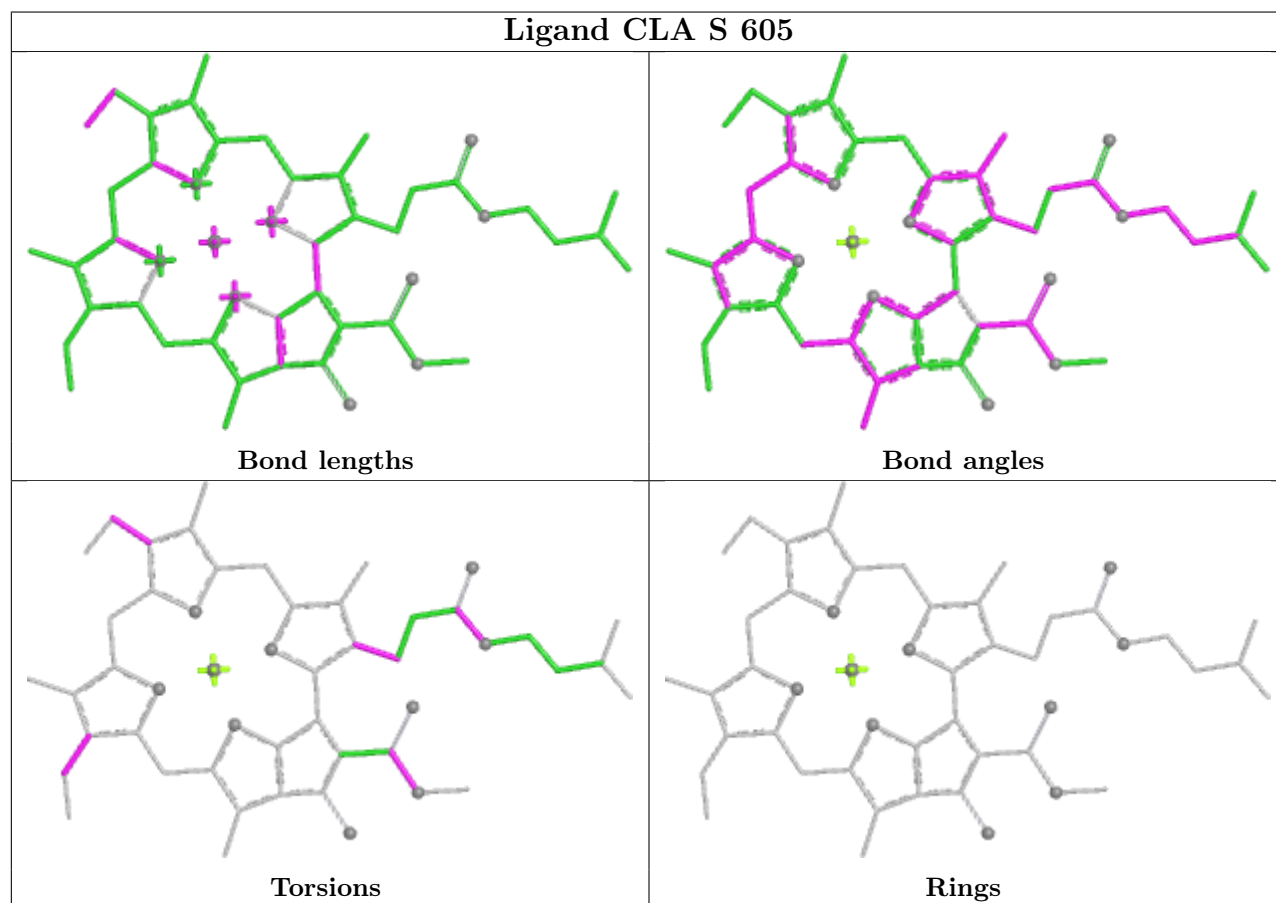
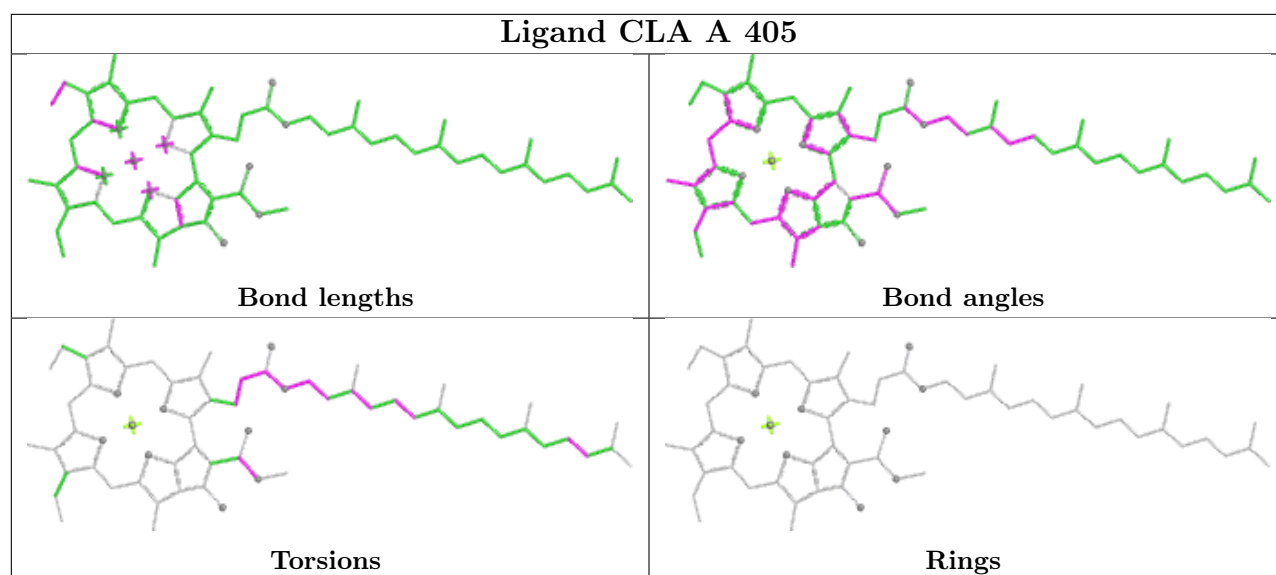
Bond angles

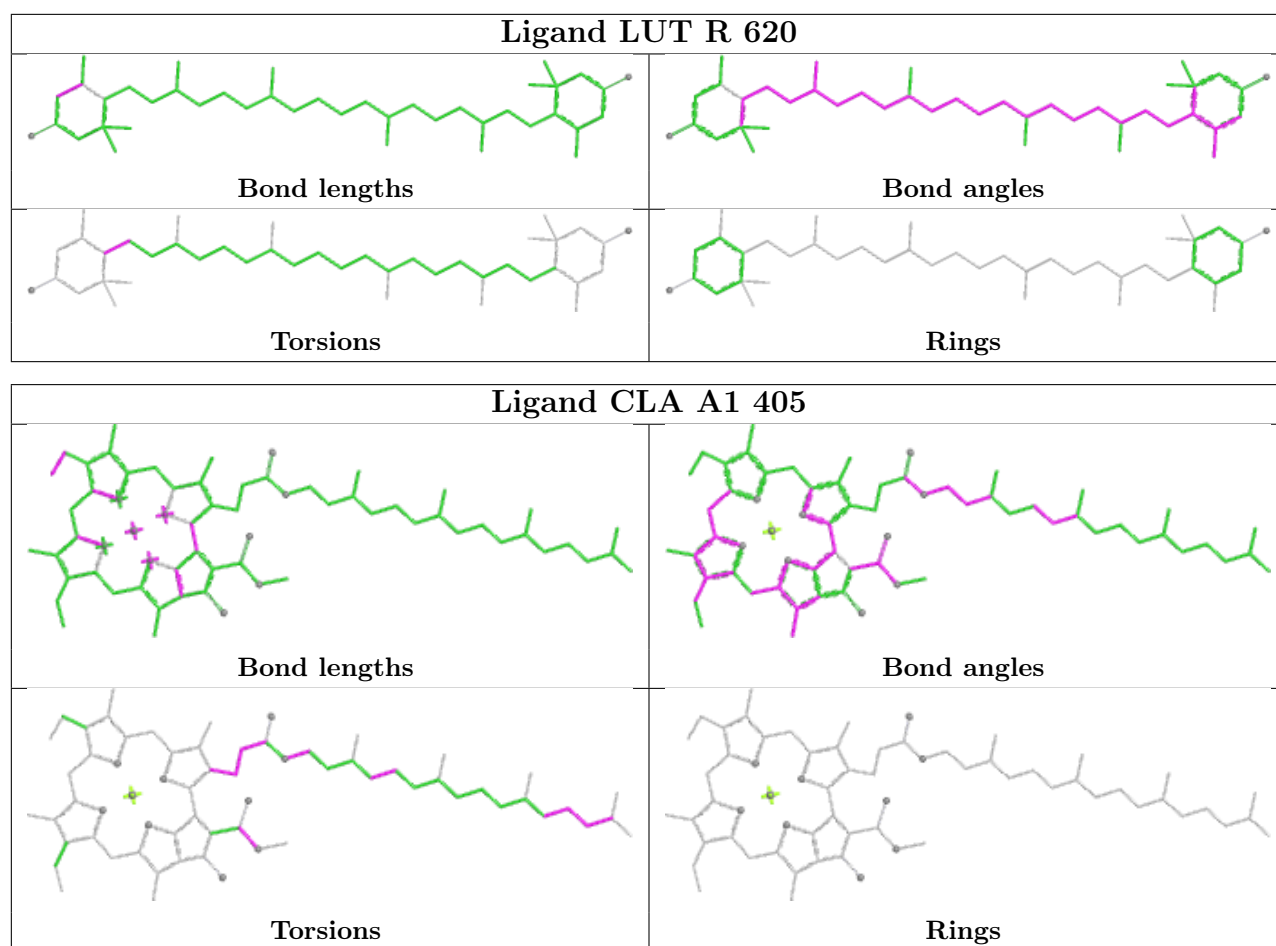


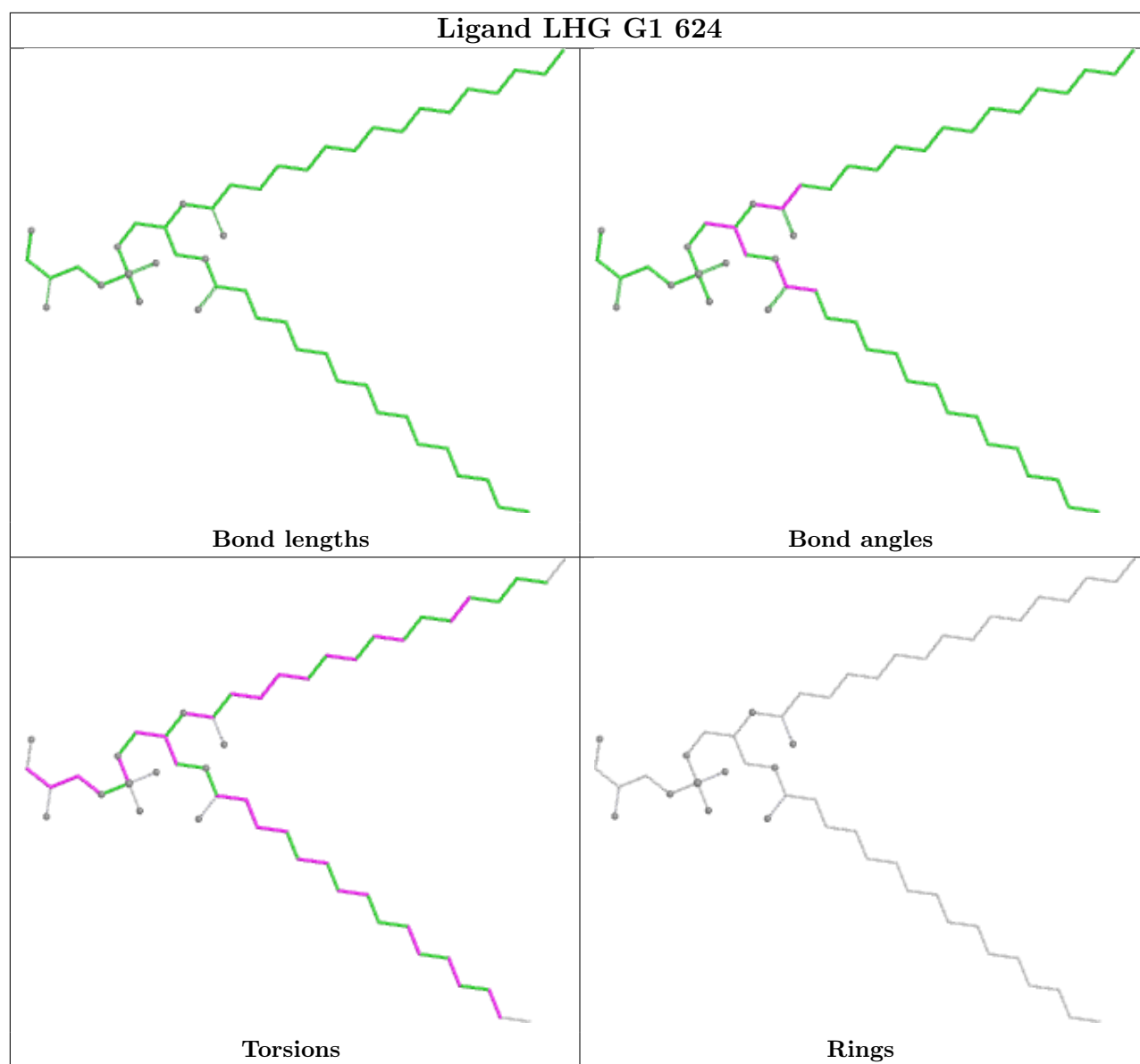
Torsions



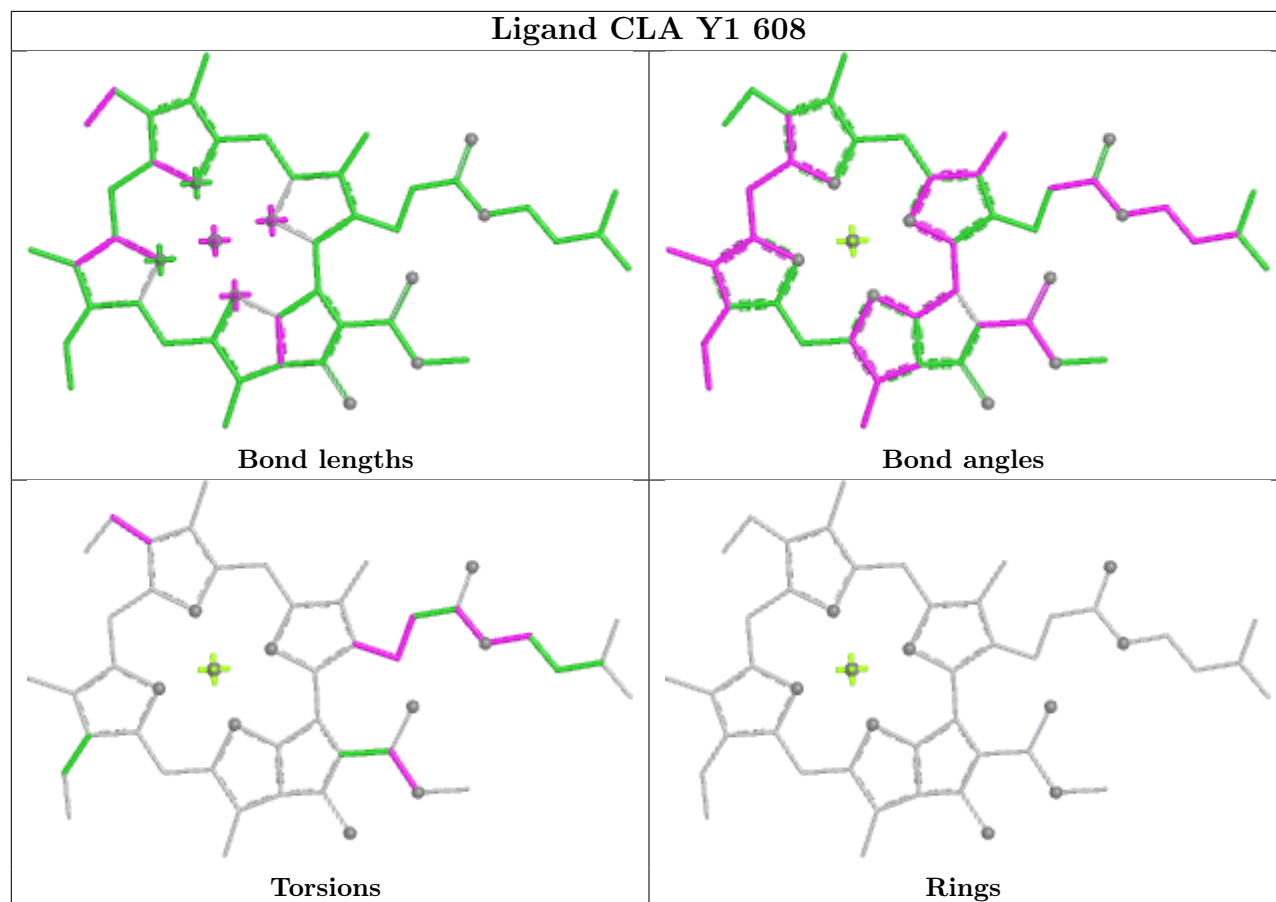
Rings



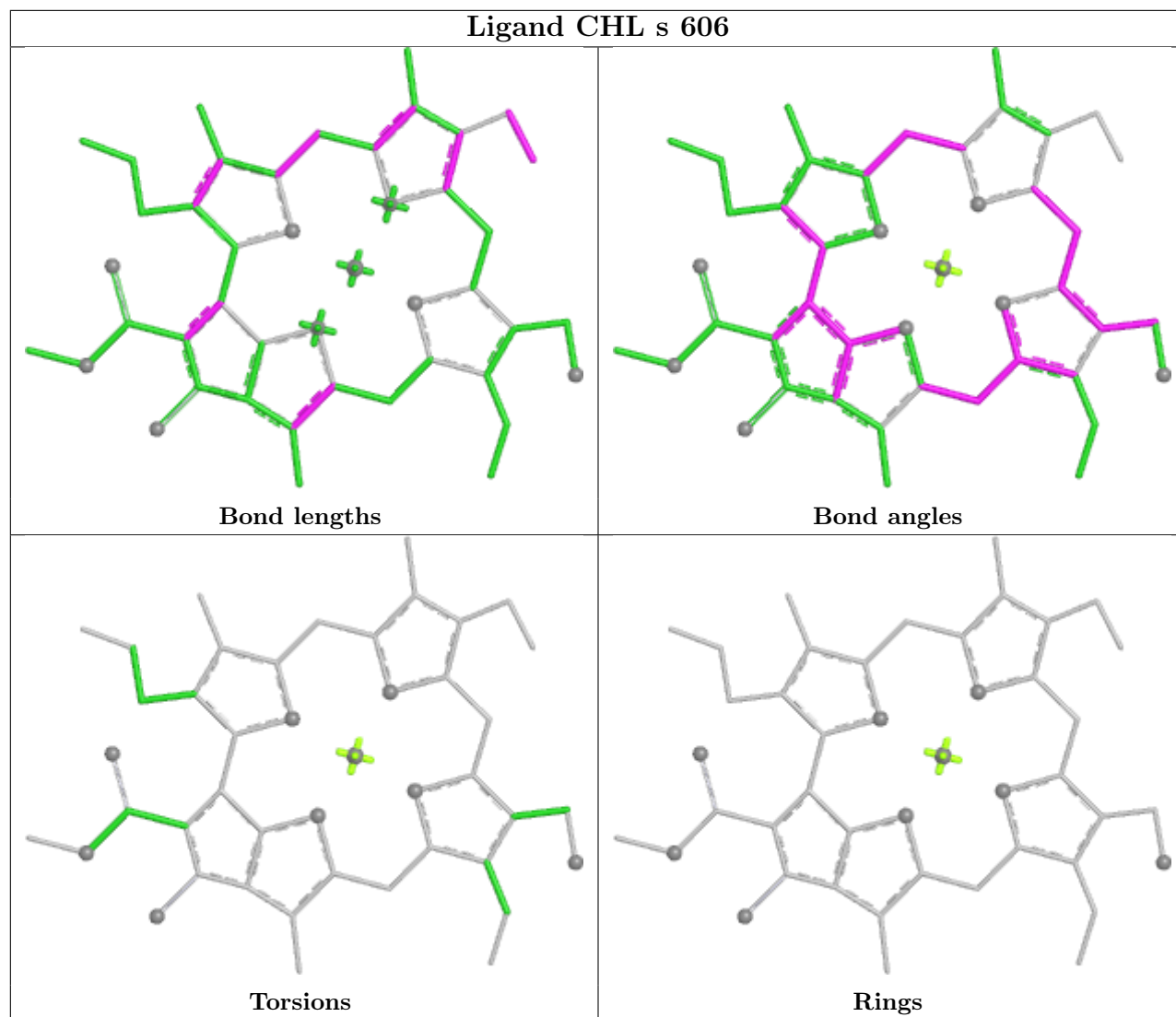




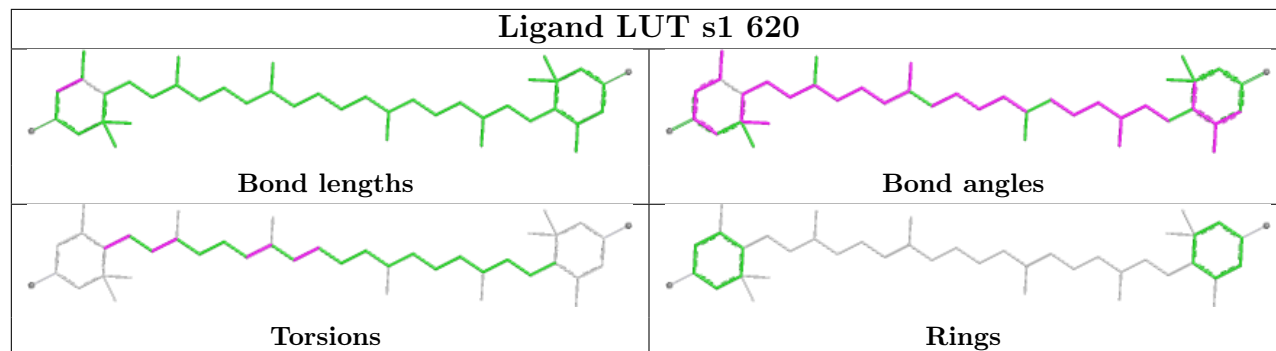
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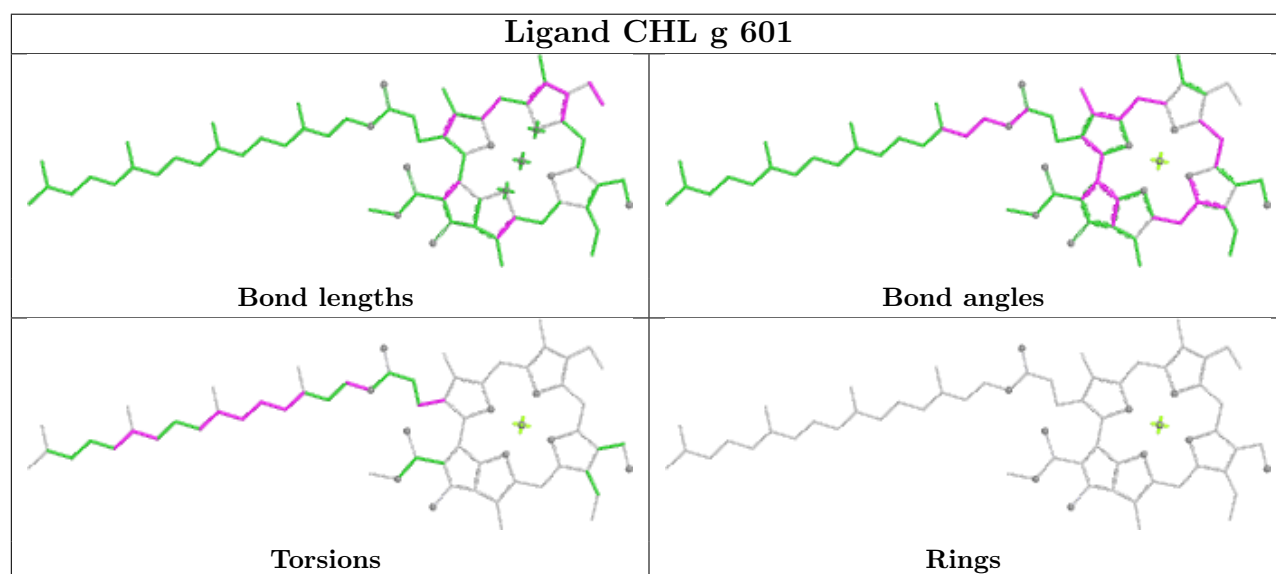
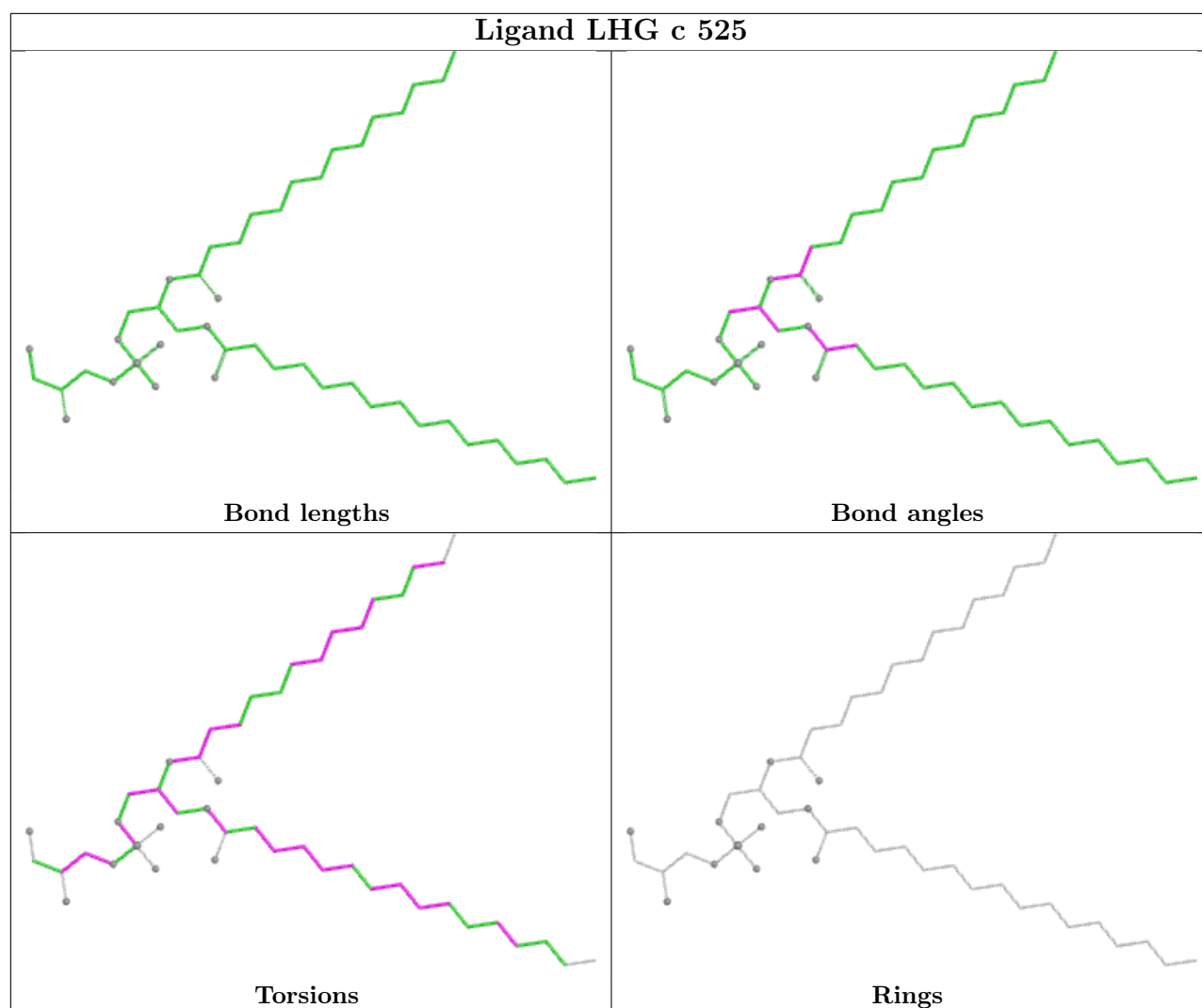


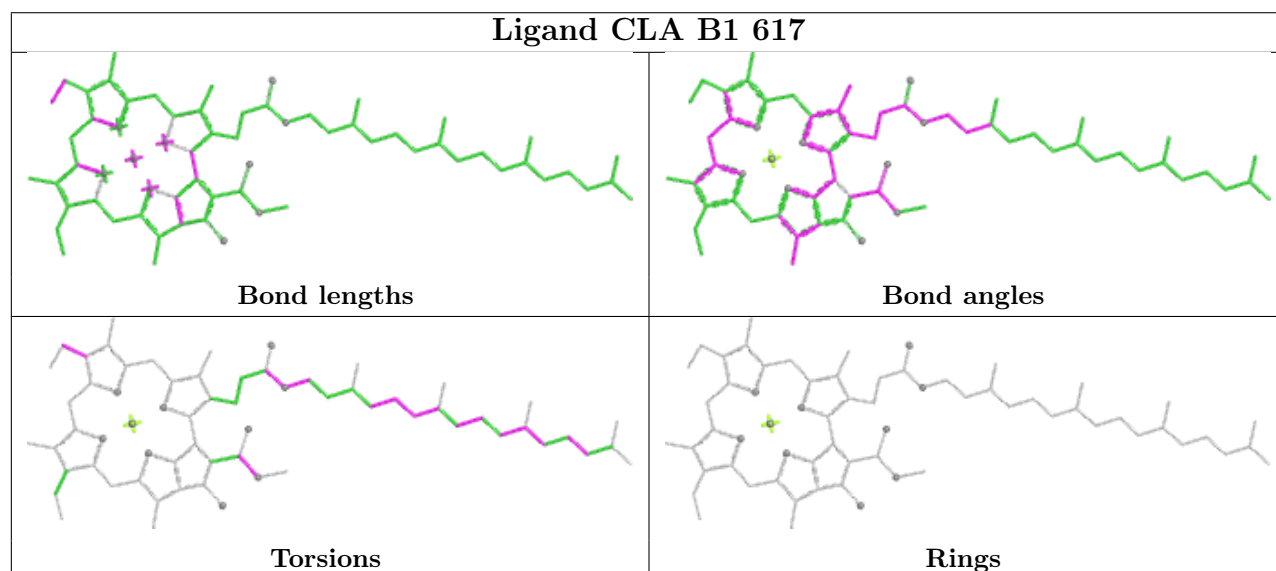
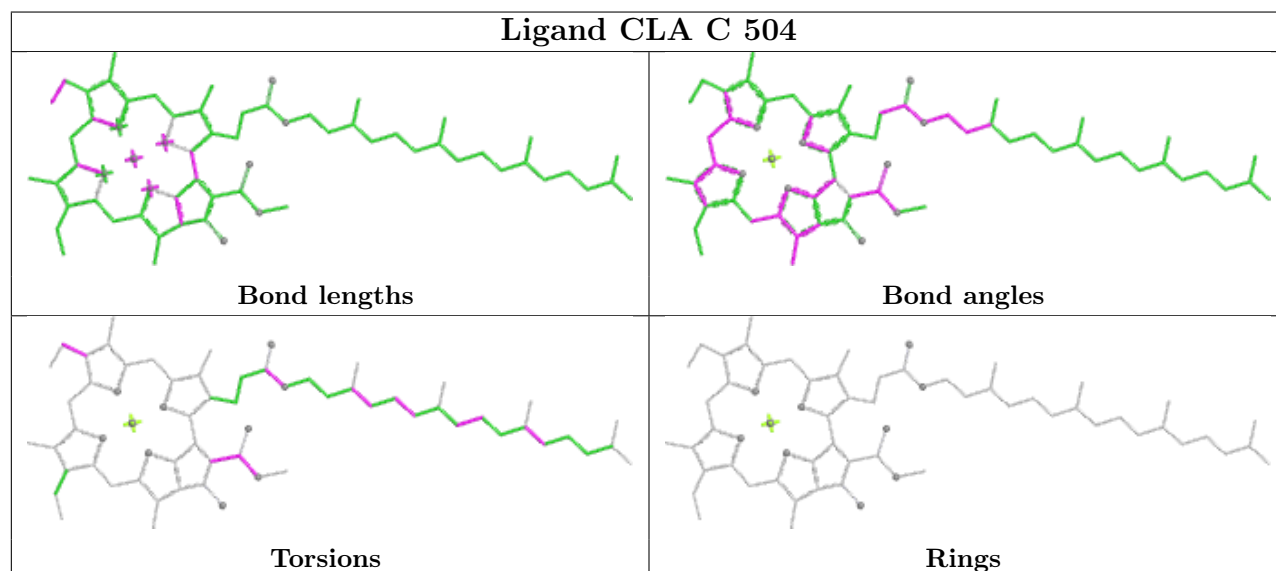
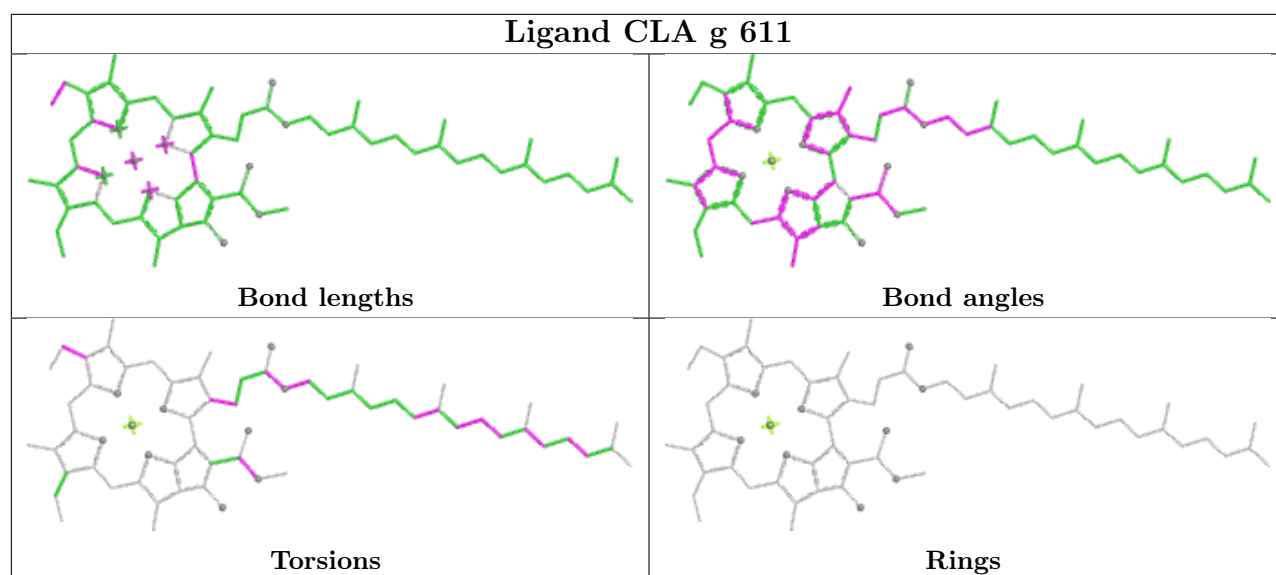
Ligand CHL s 606



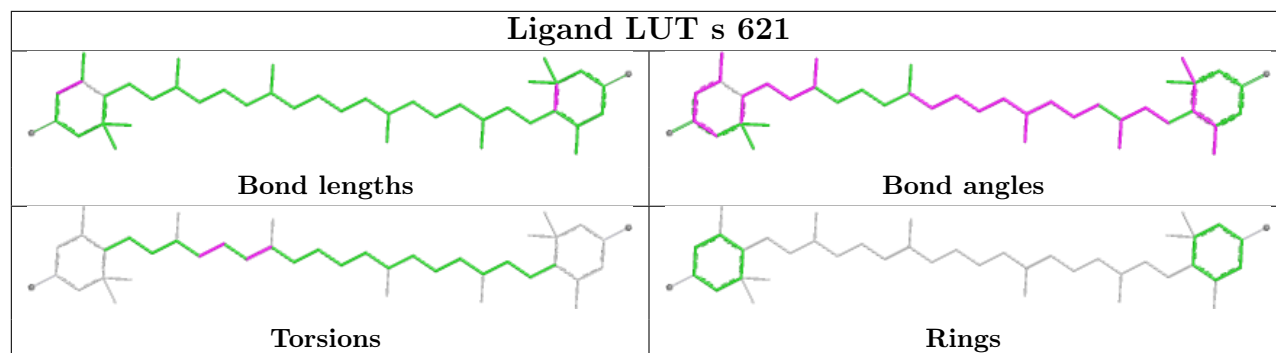
Ligand LUT s1 620



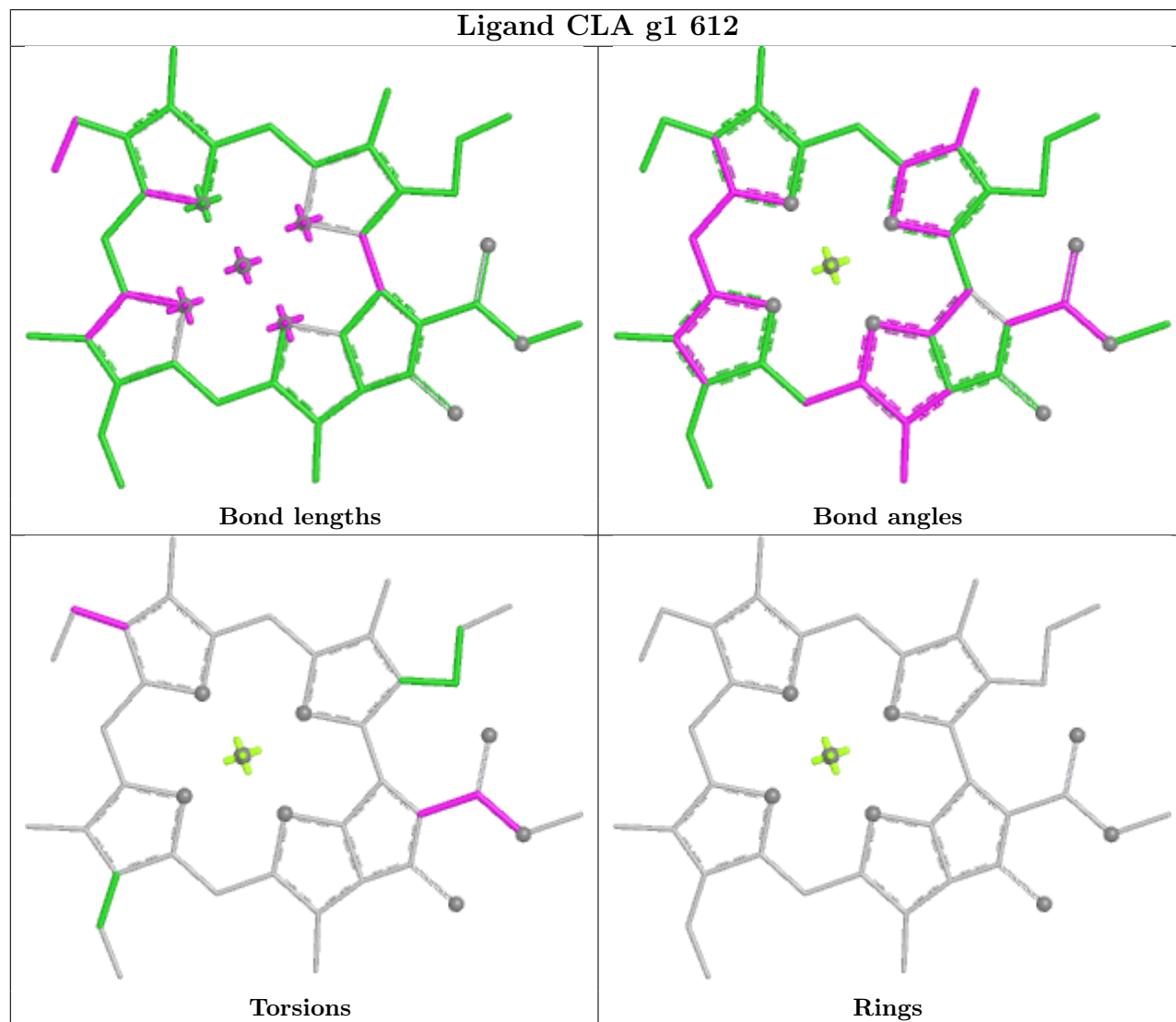


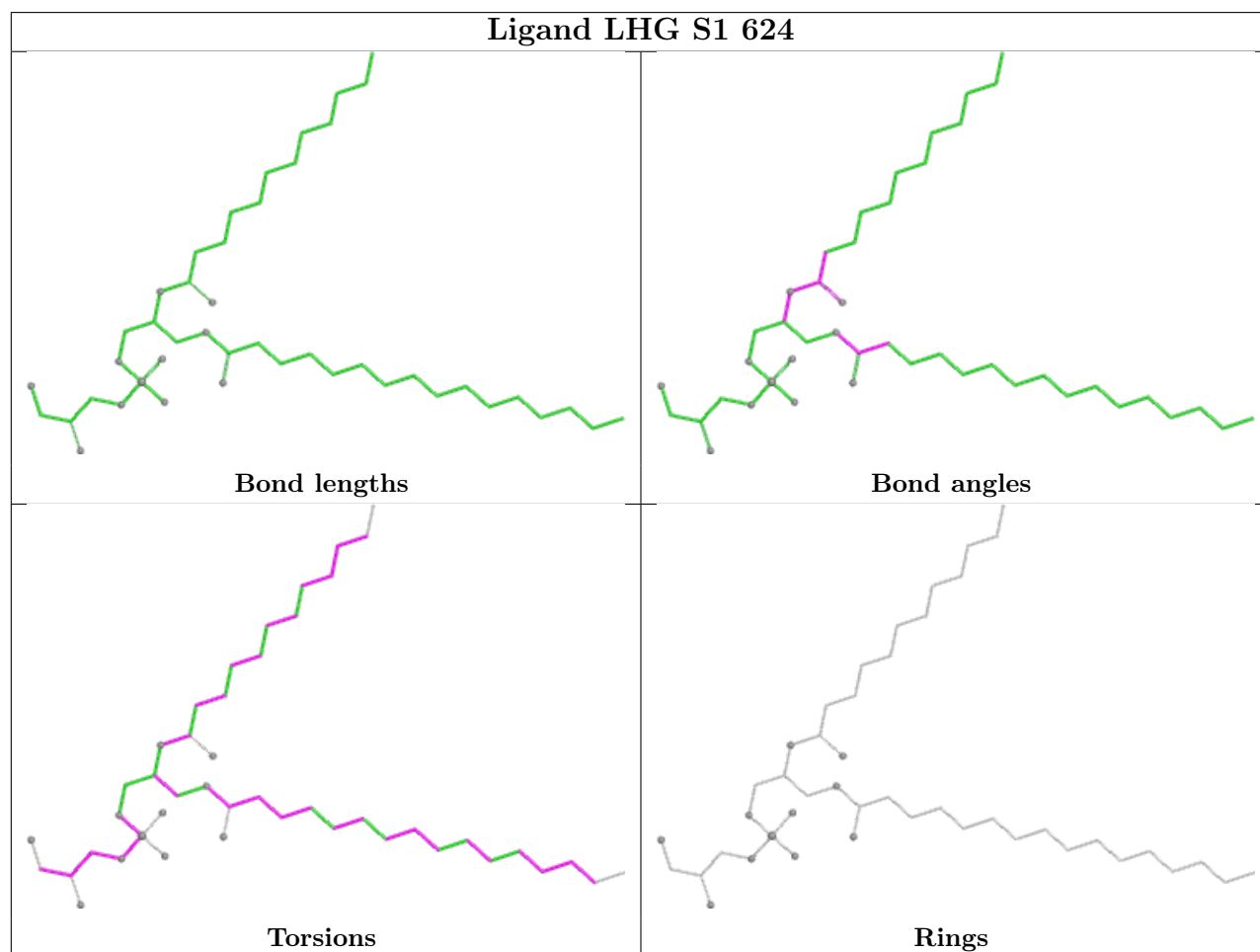
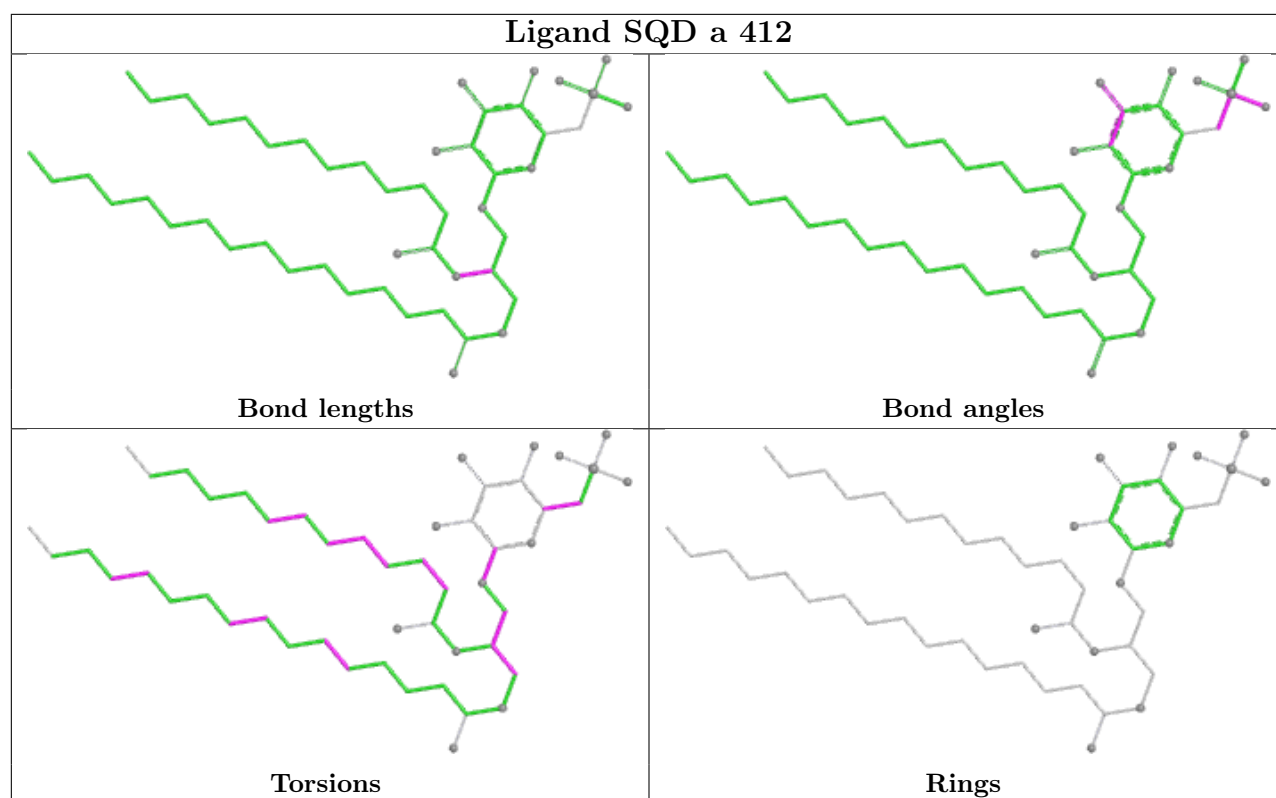


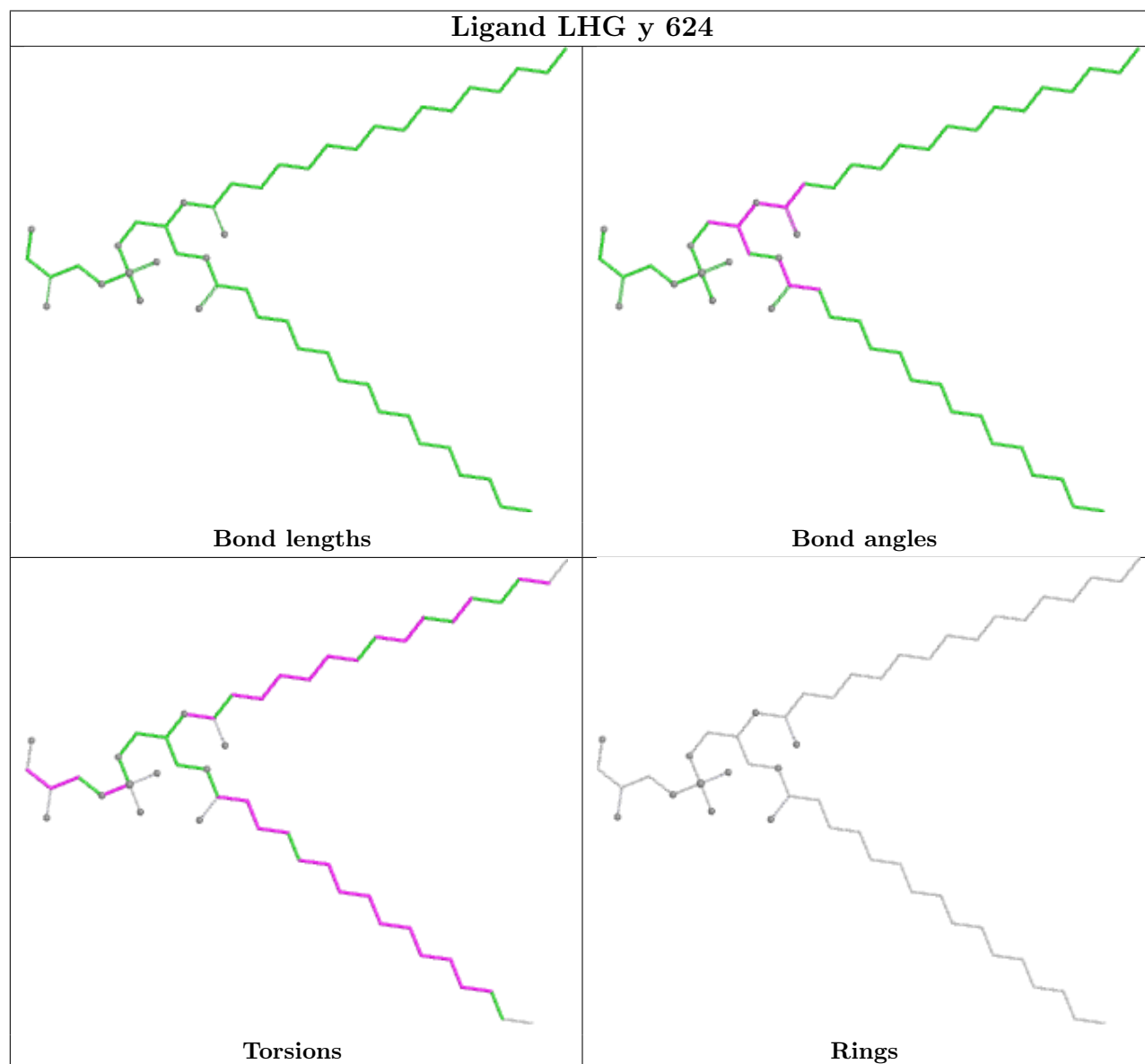
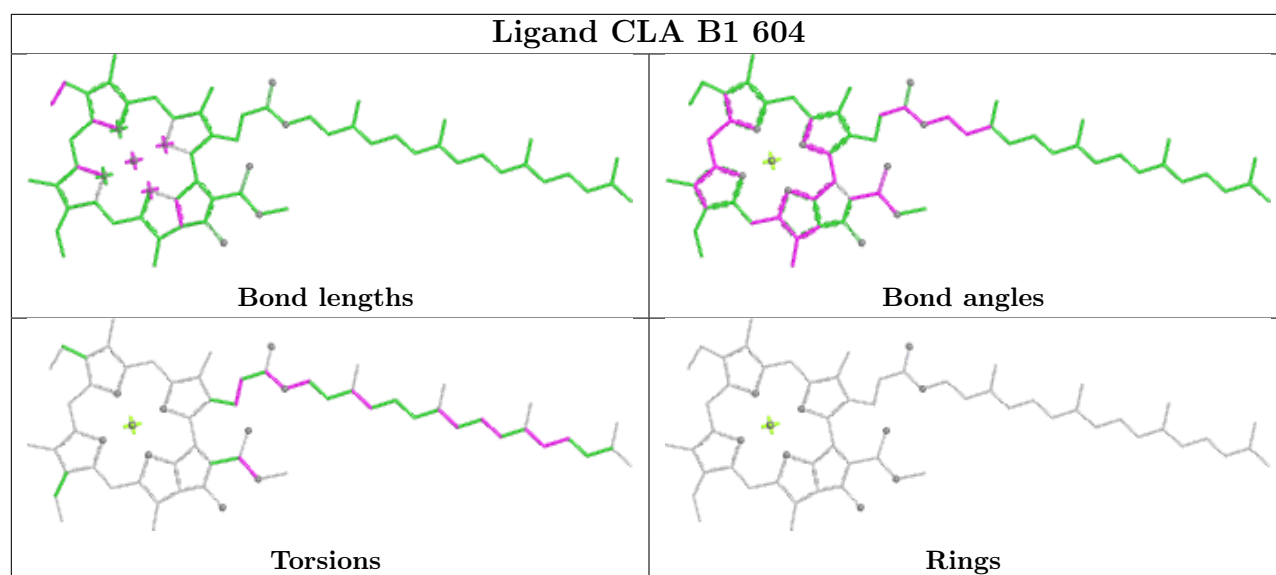
Ligand LUT s 621

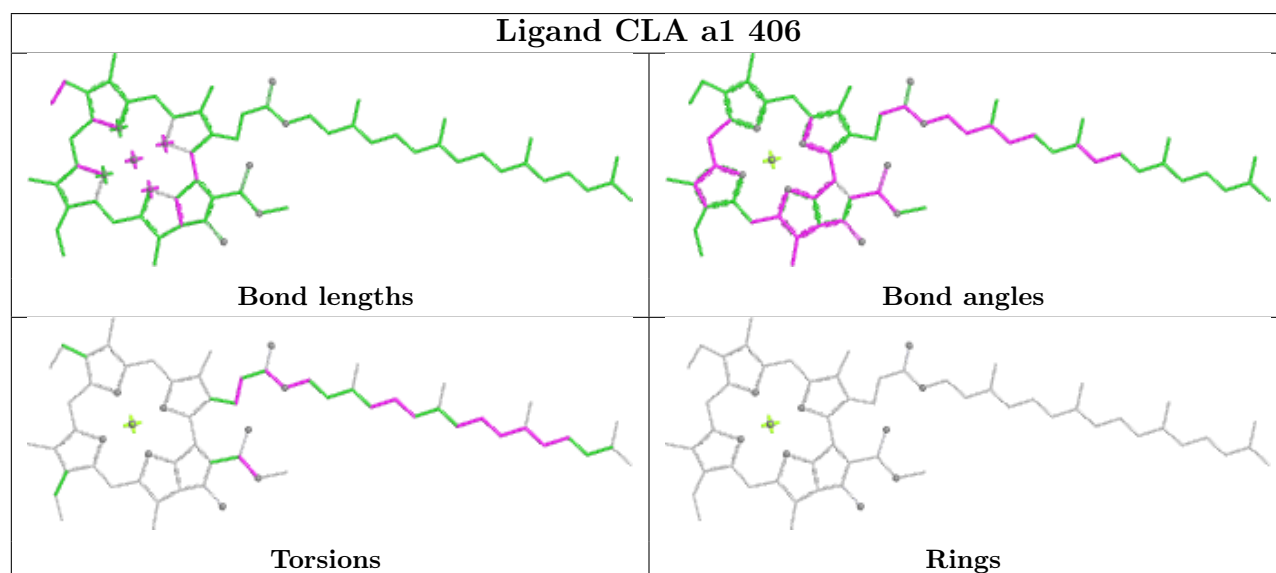
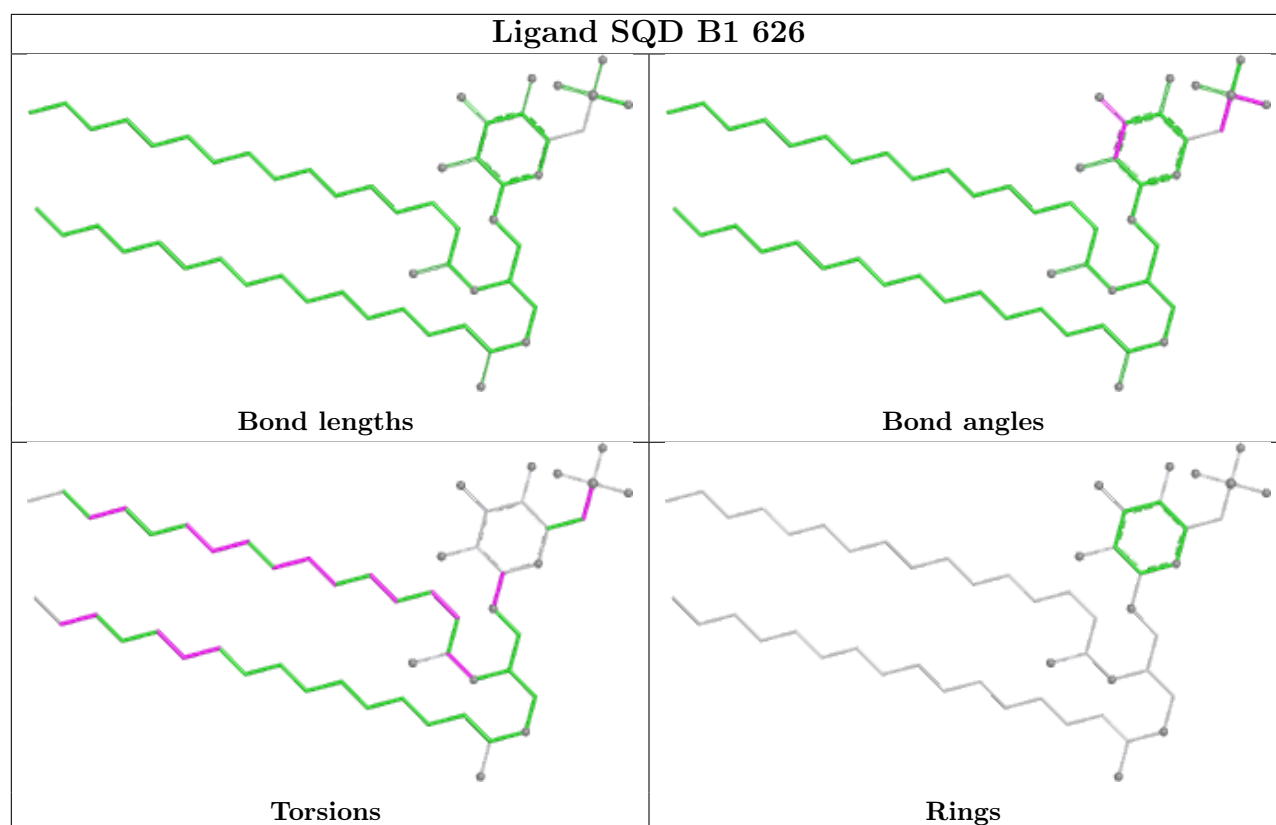


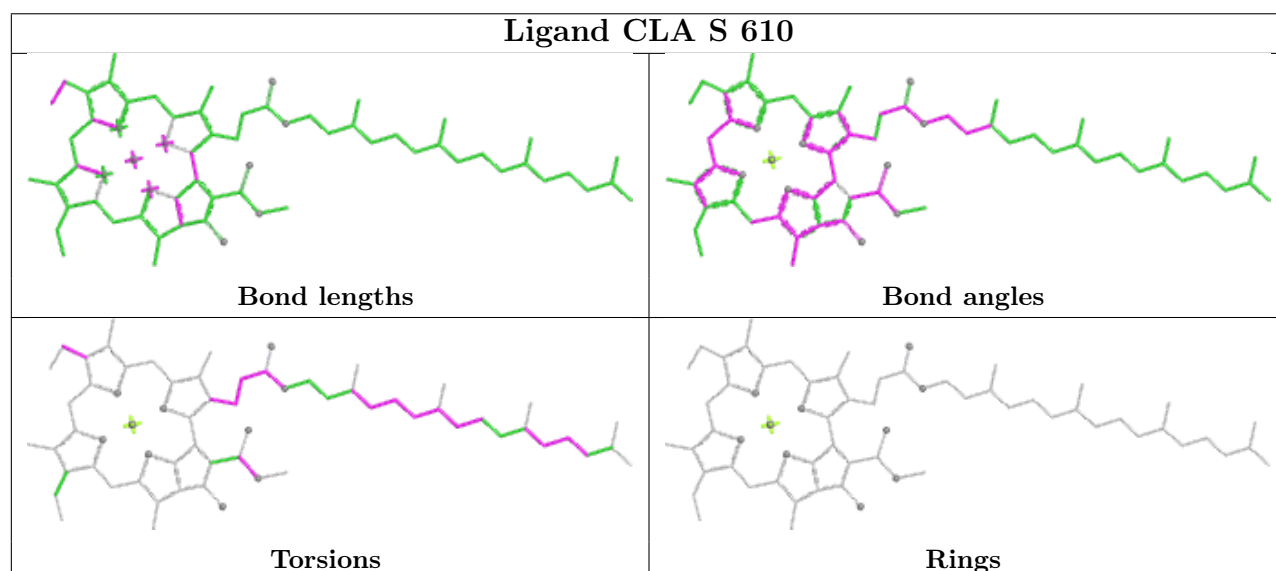
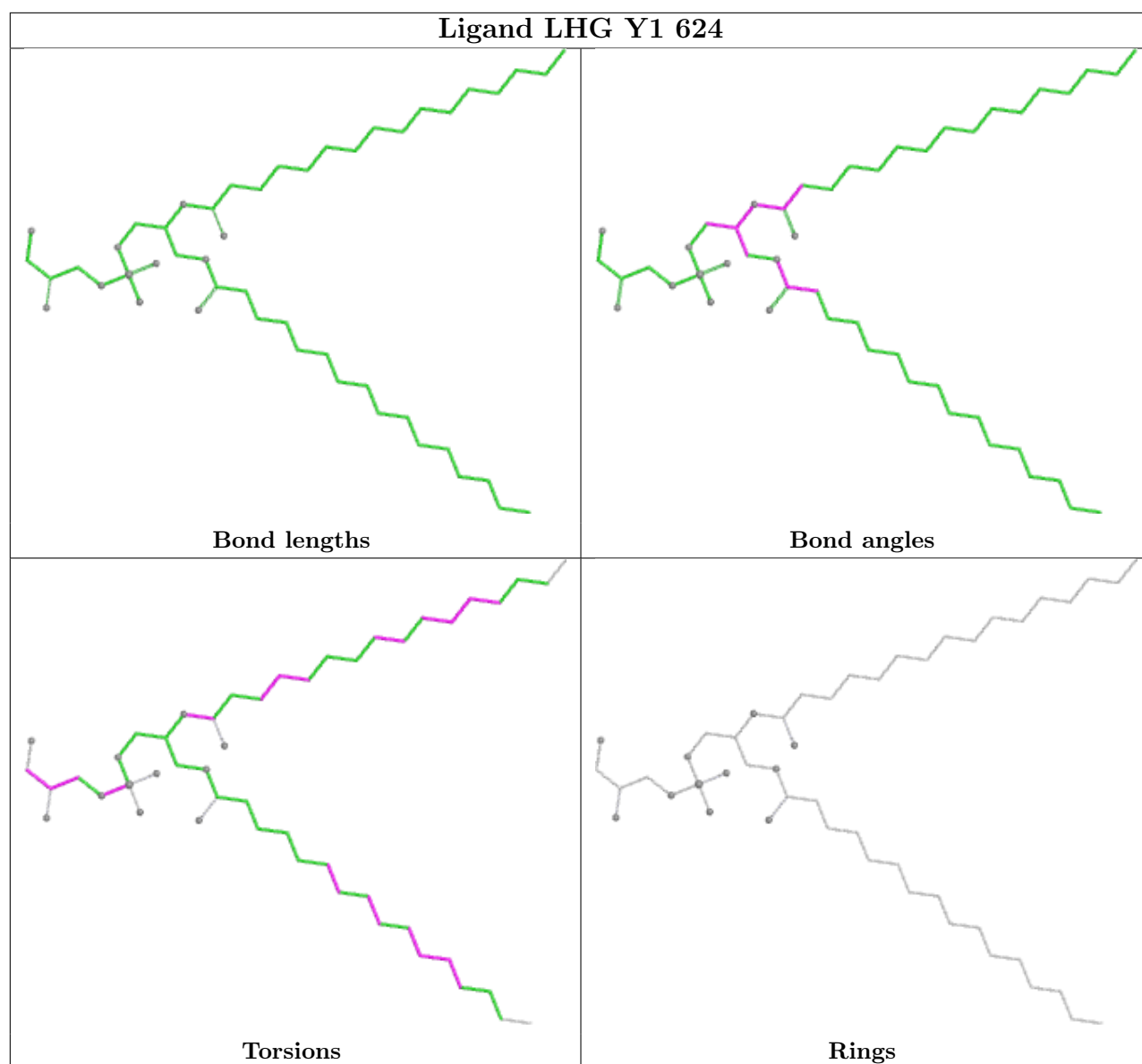
Ligand CLA g1 612

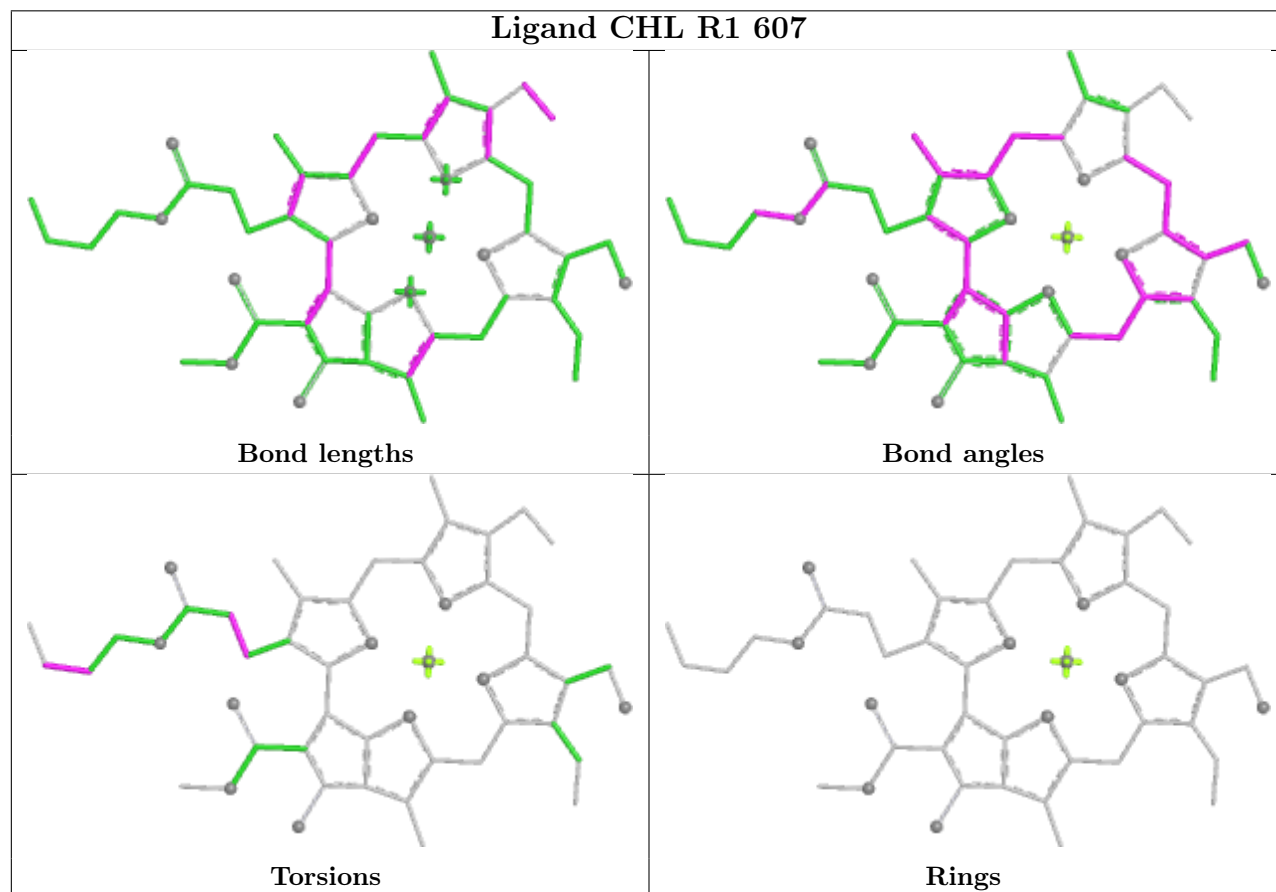
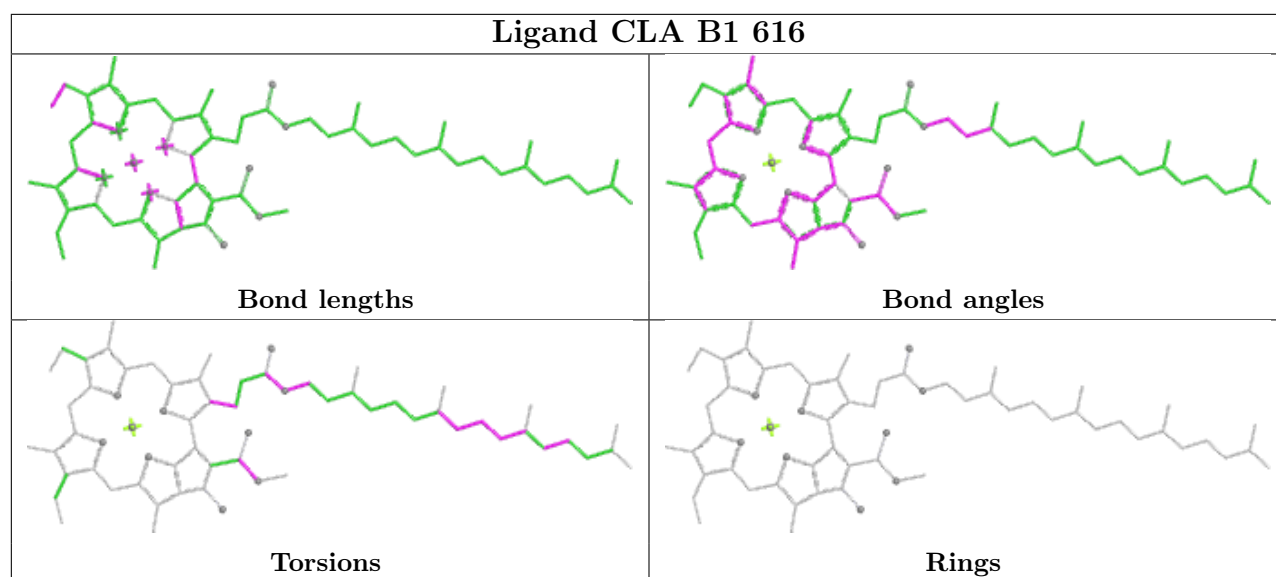


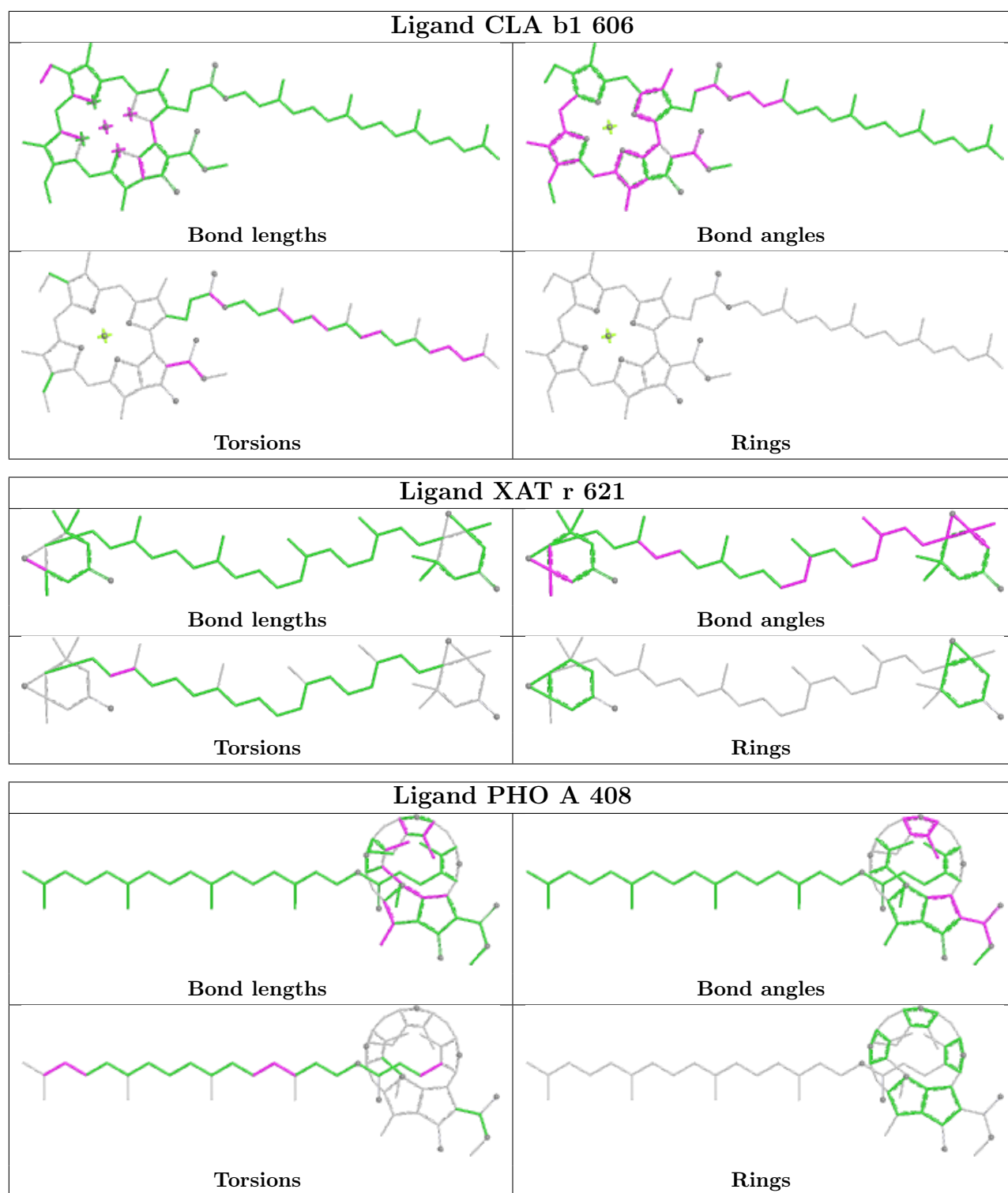


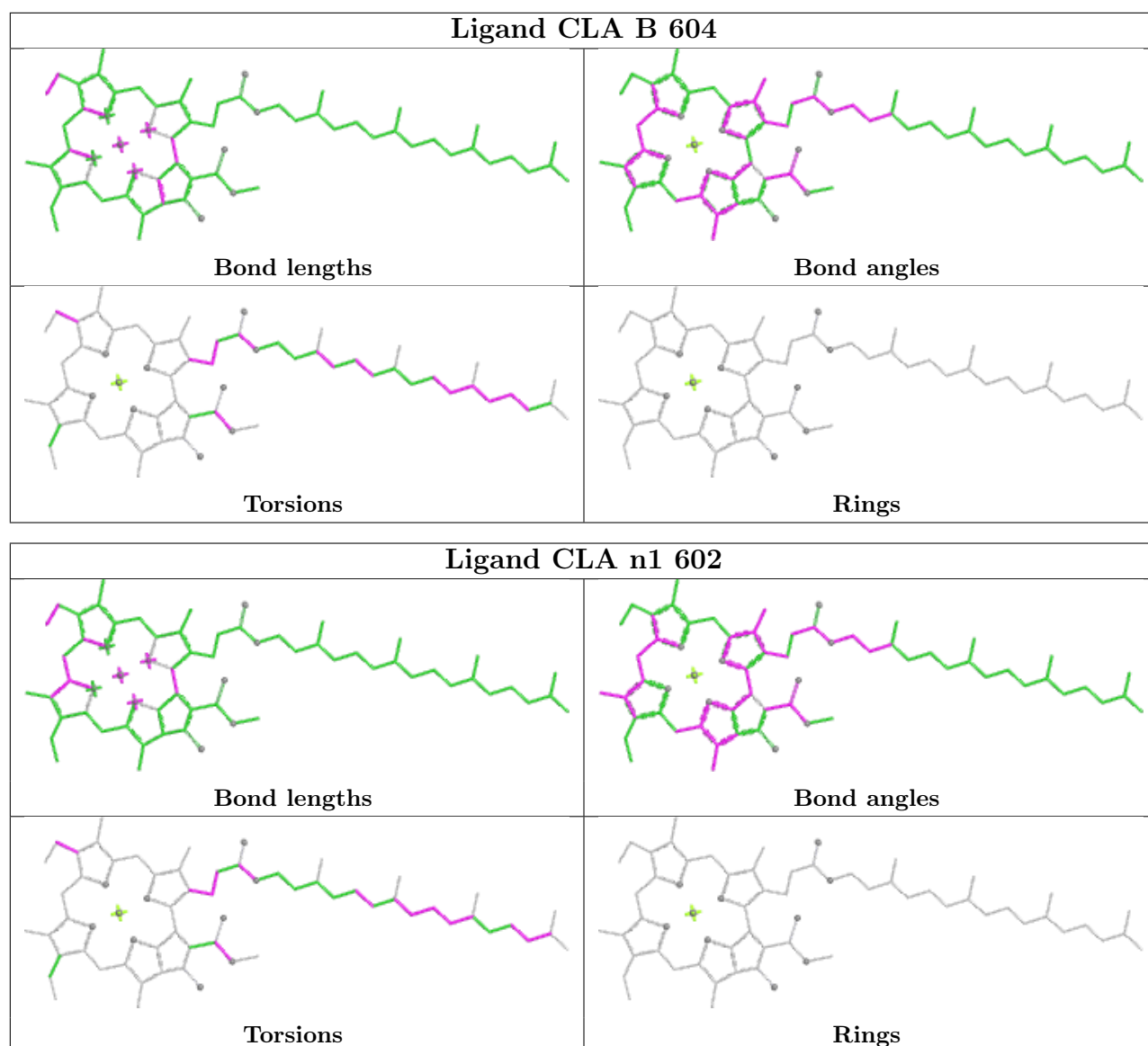


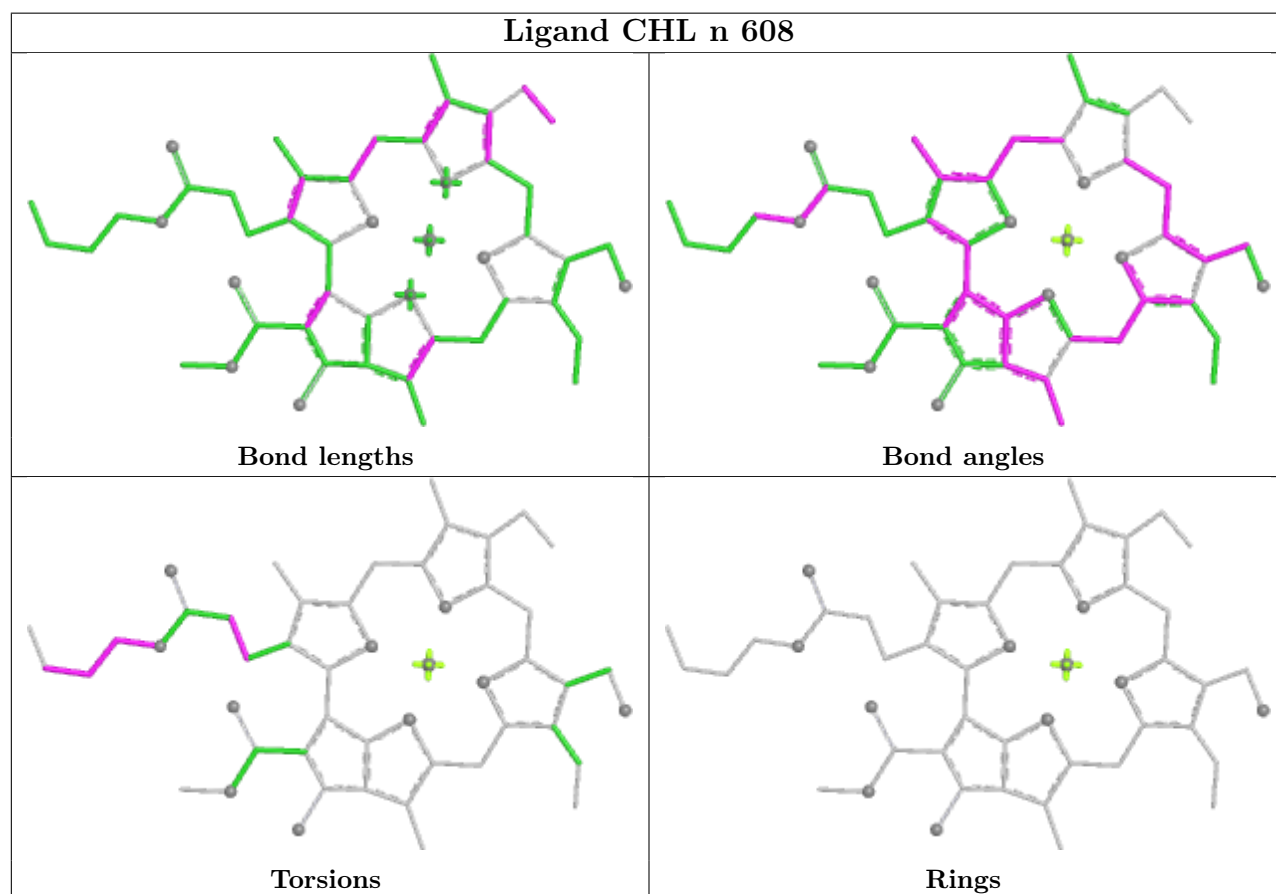
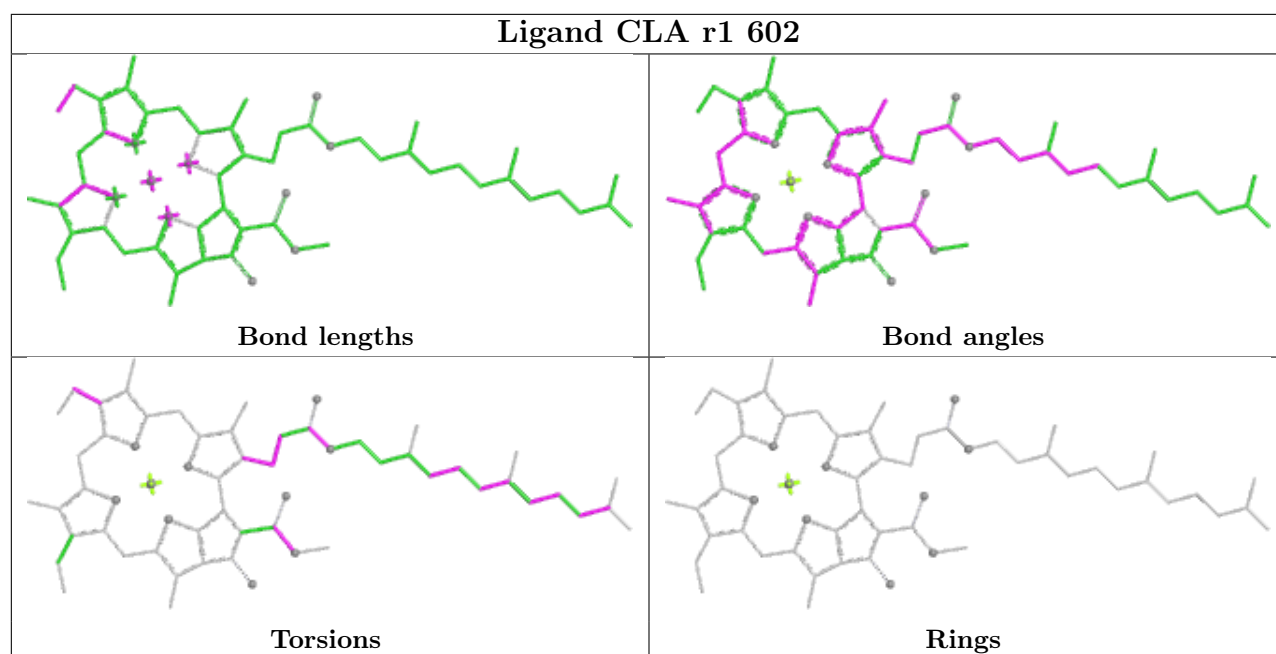


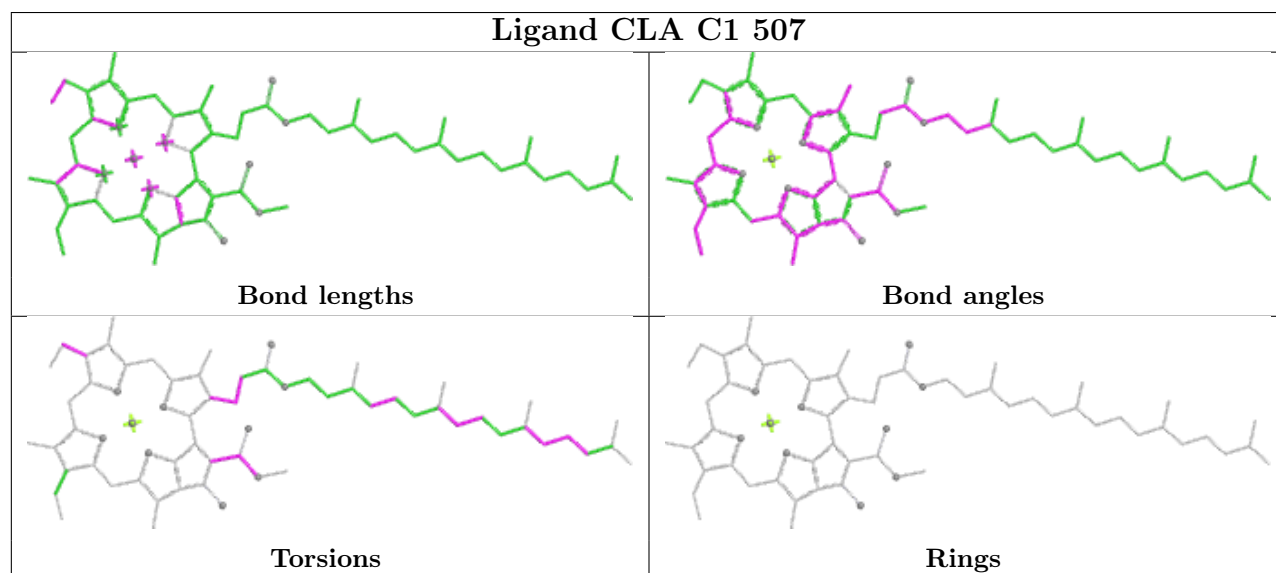
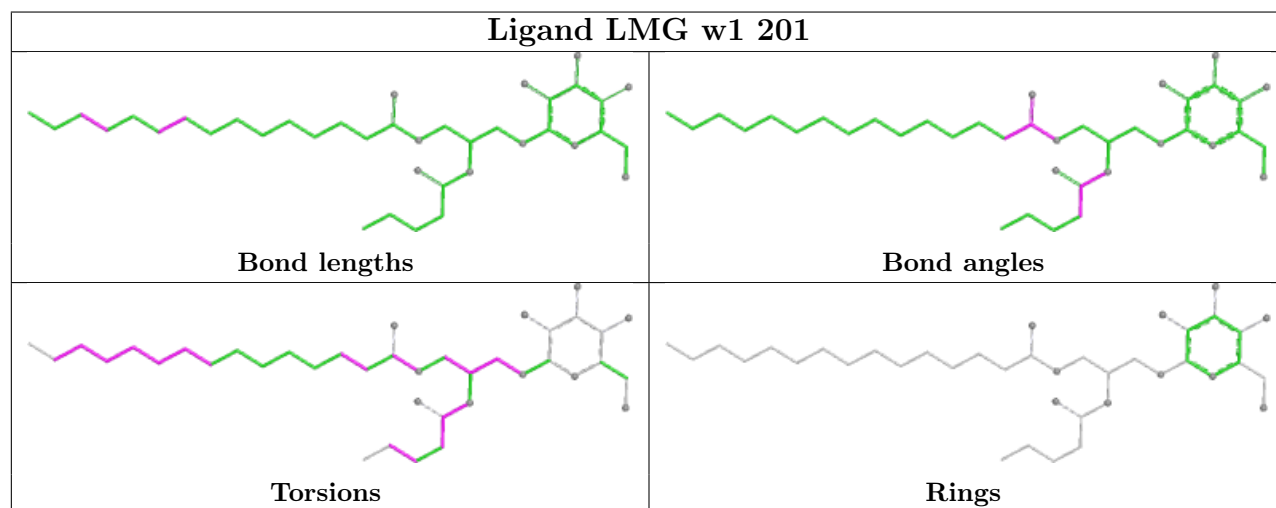
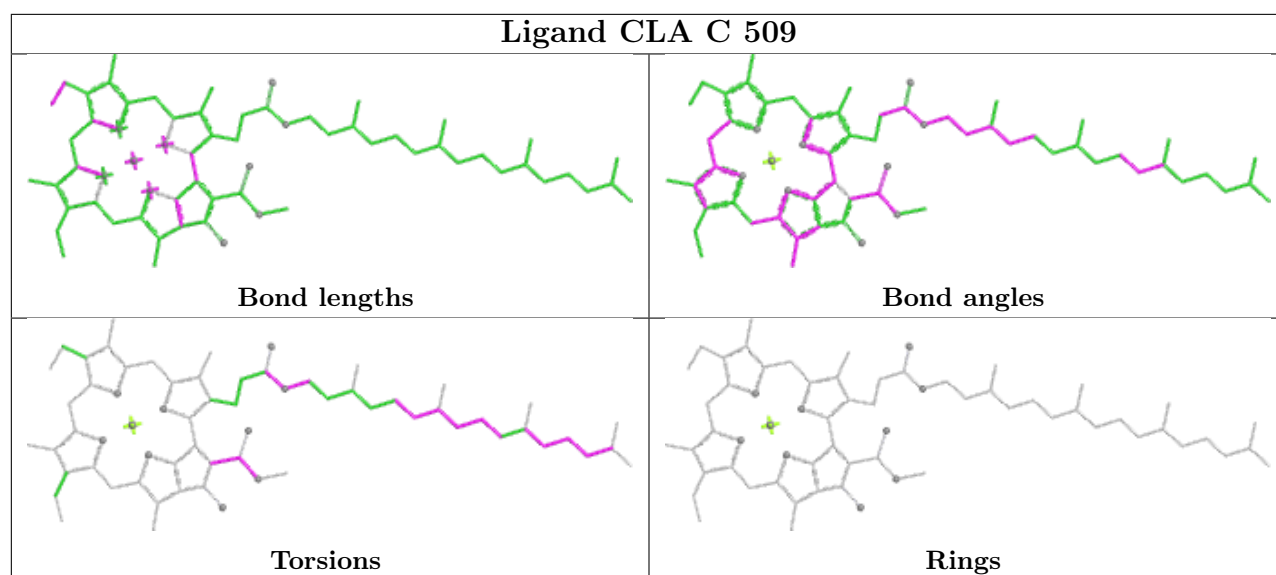


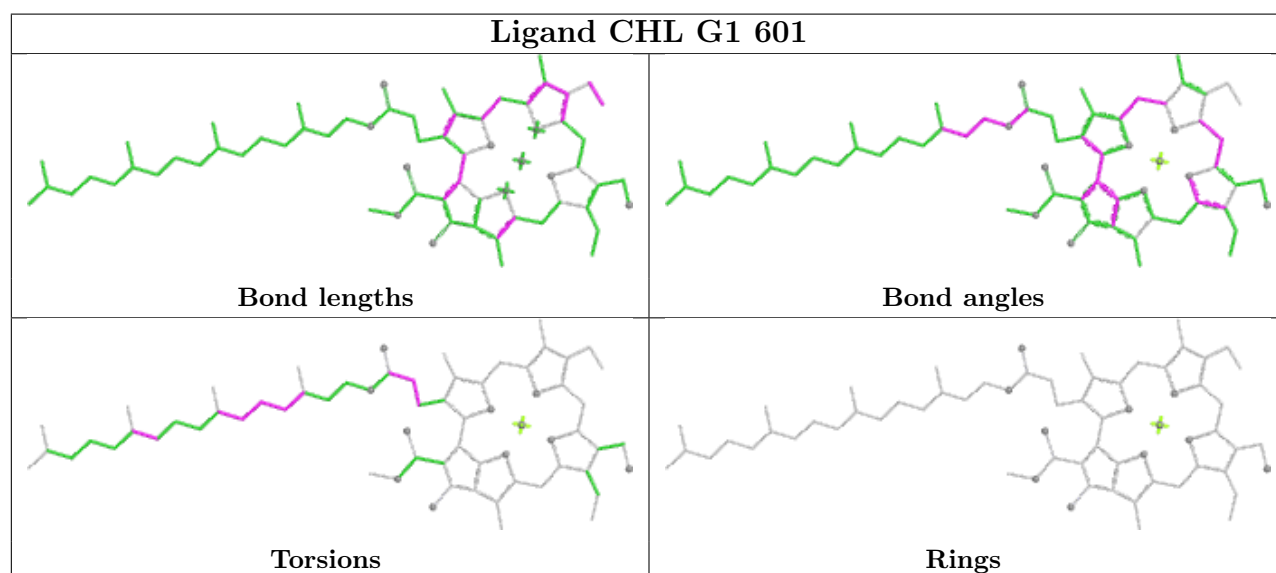
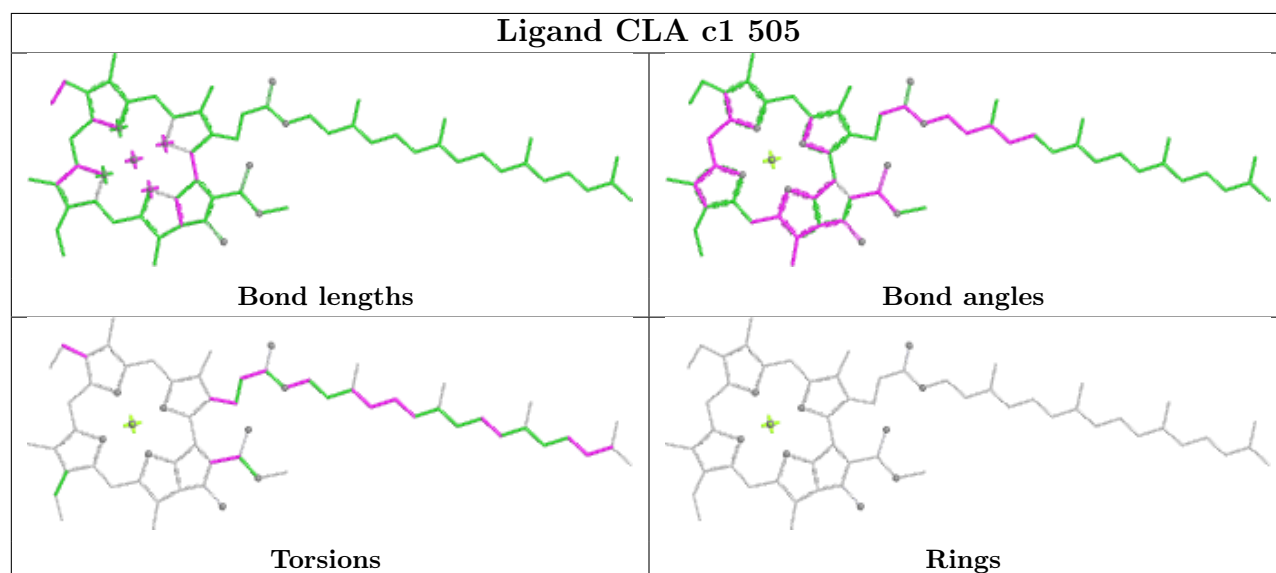
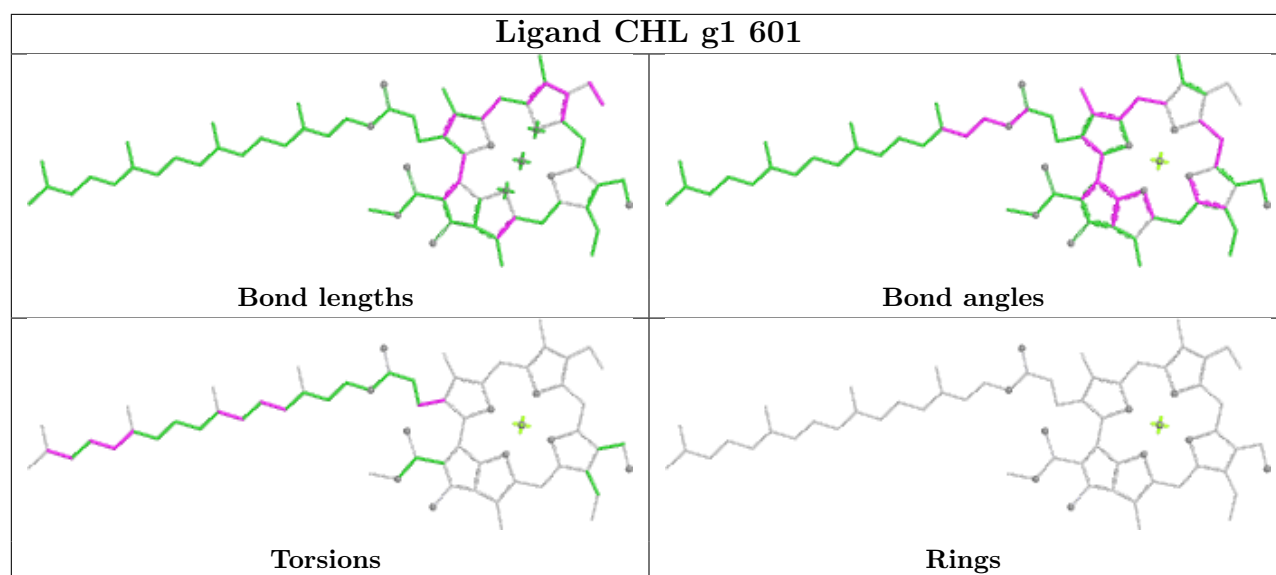


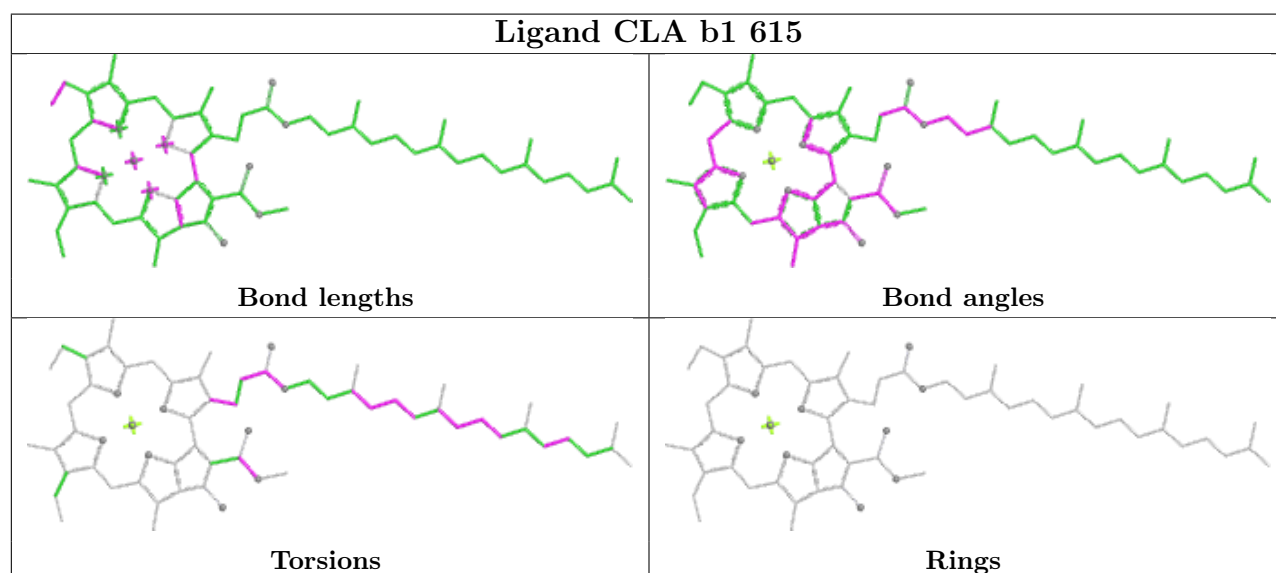
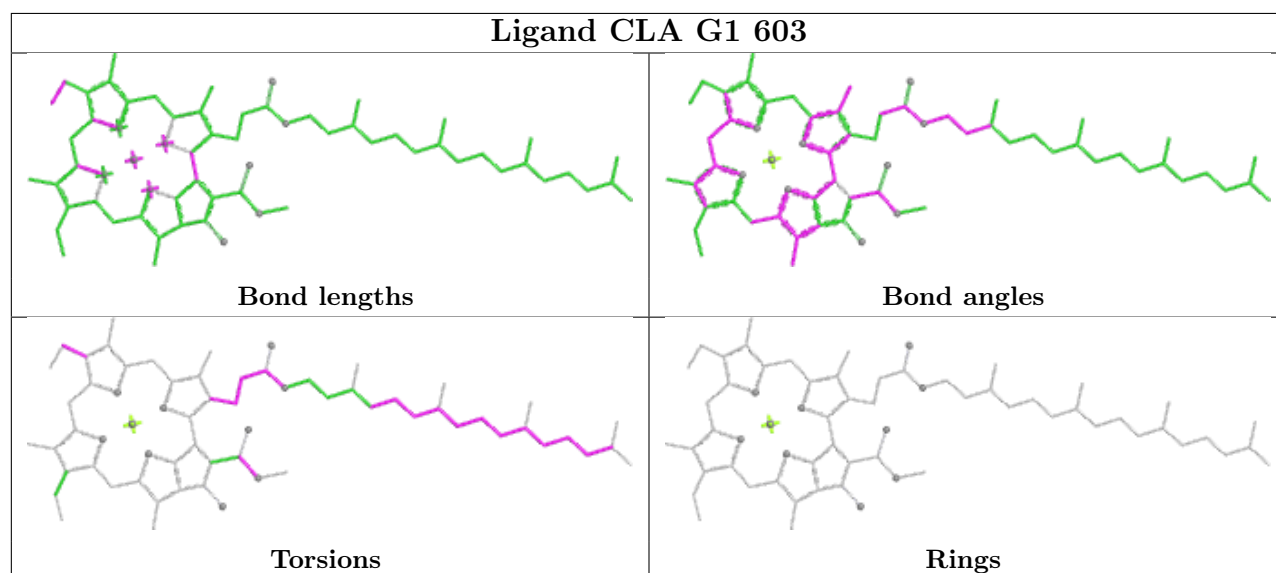
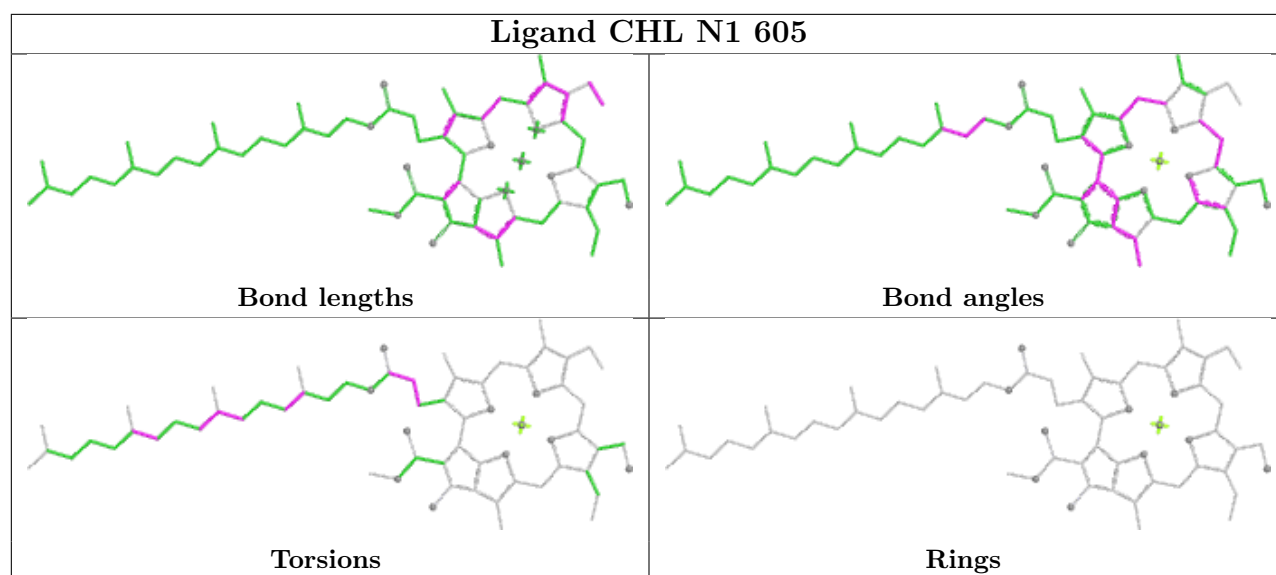


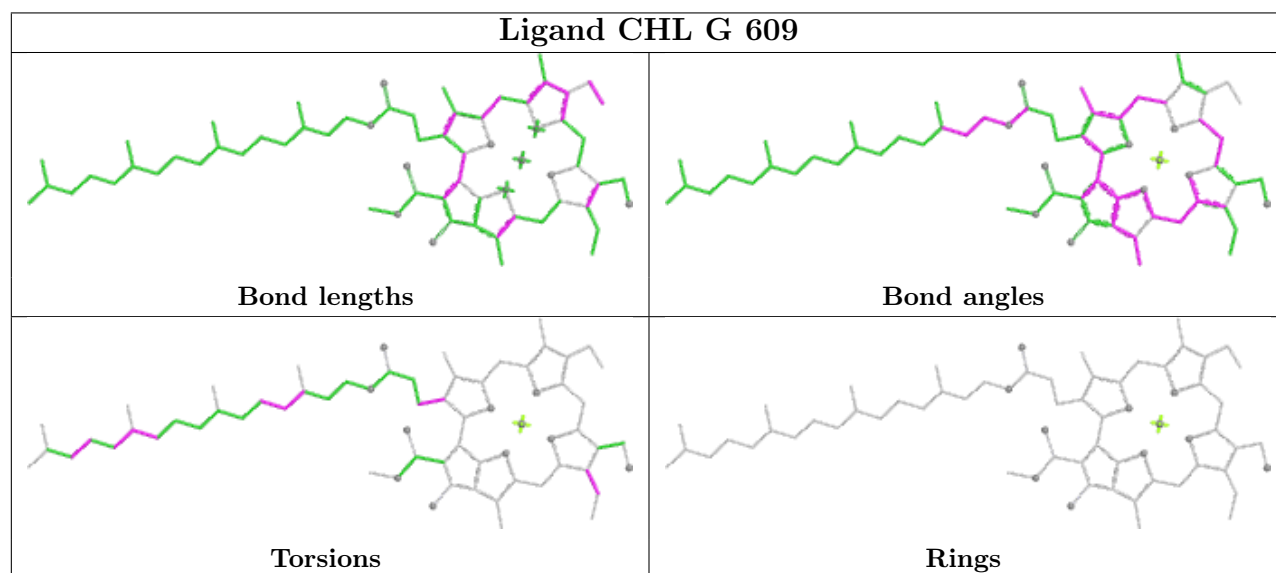
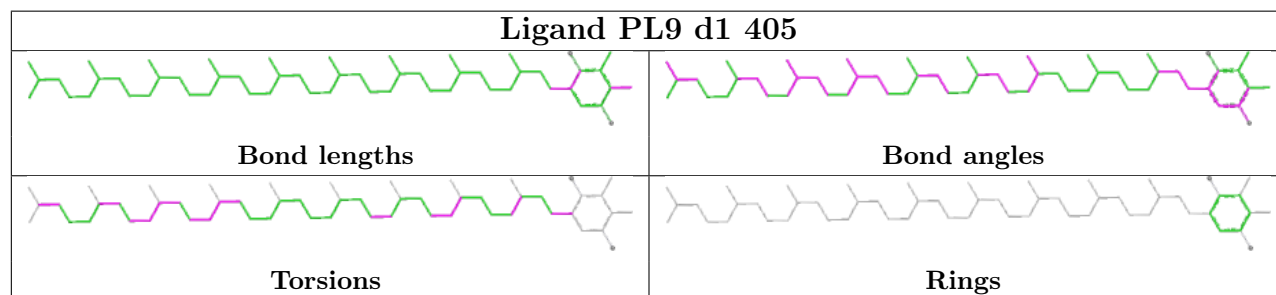
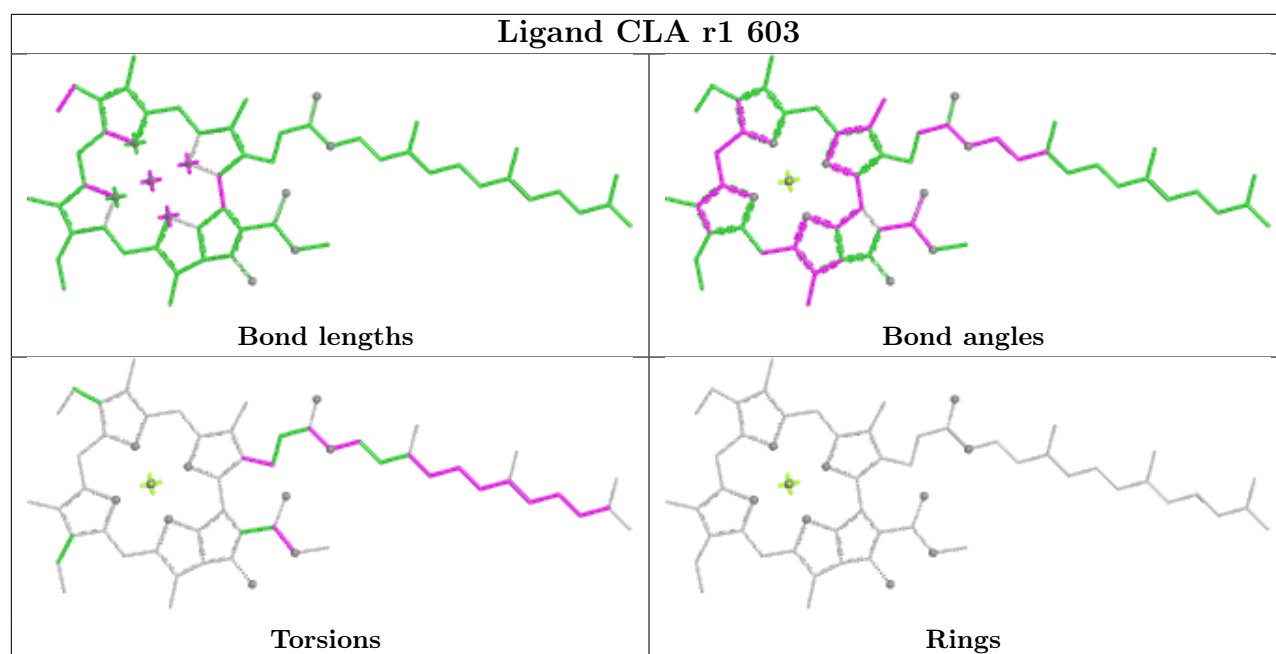


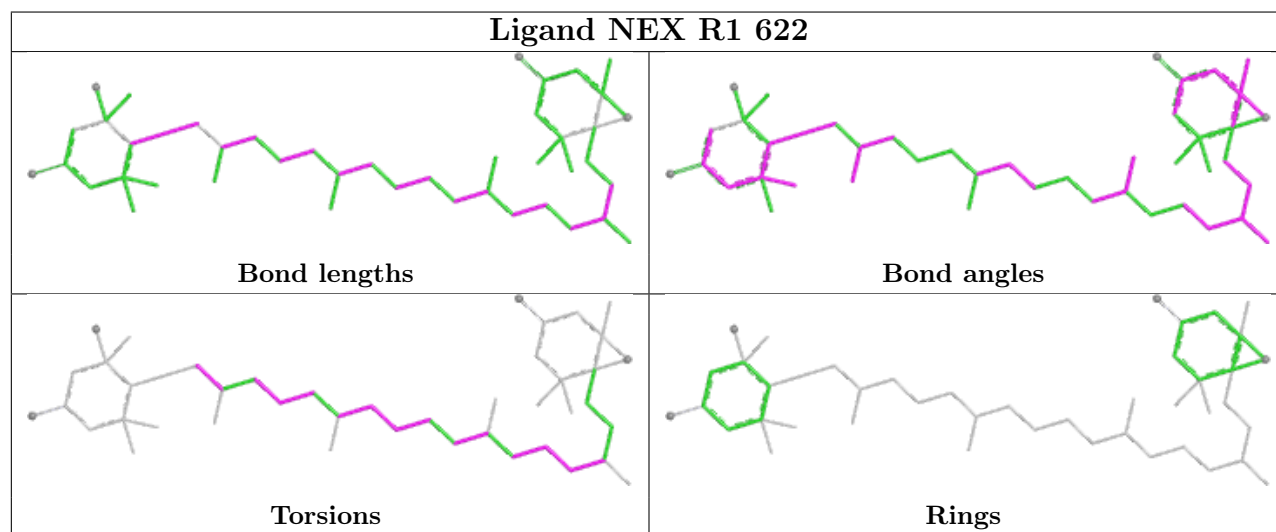
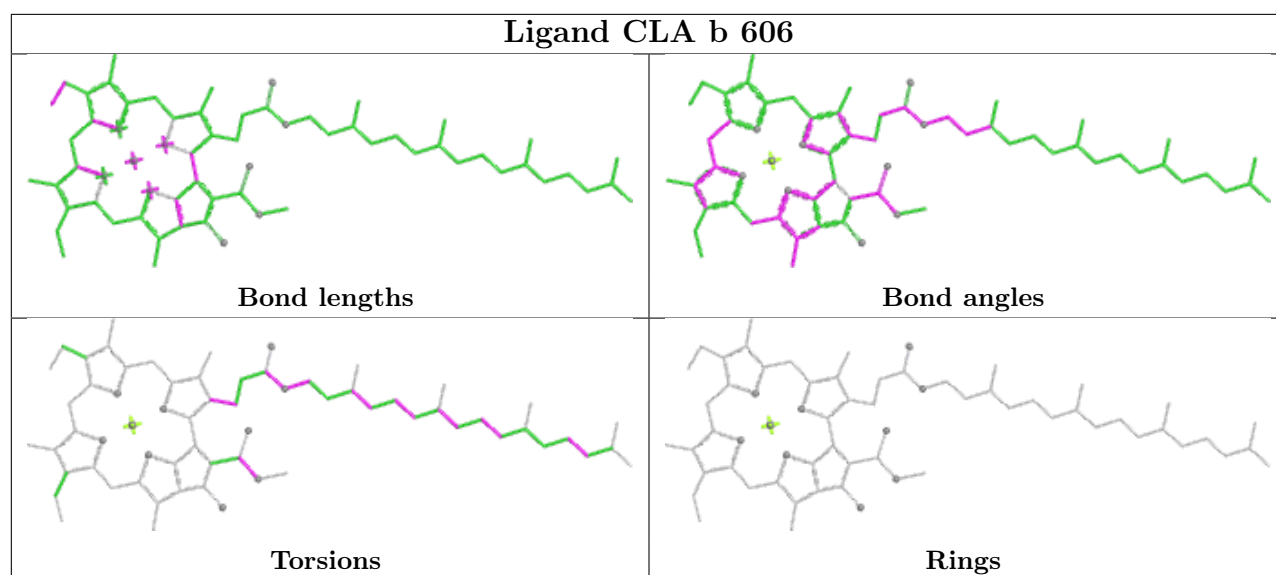




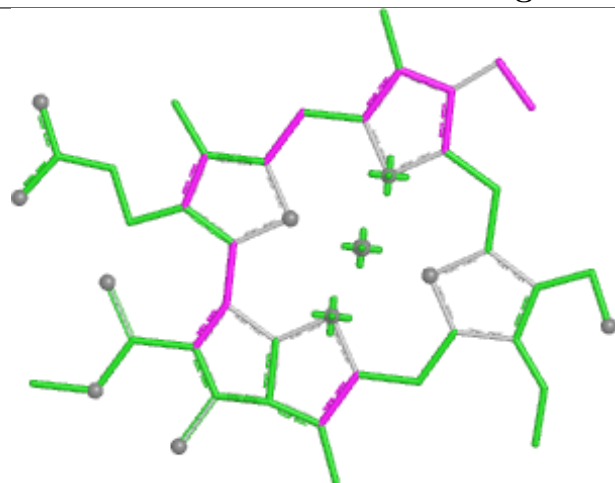




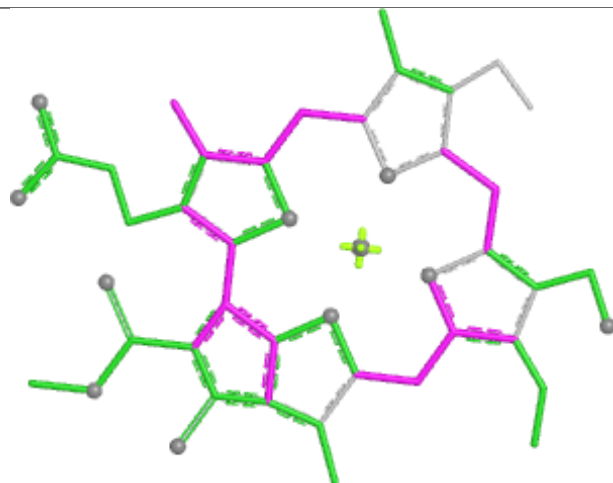




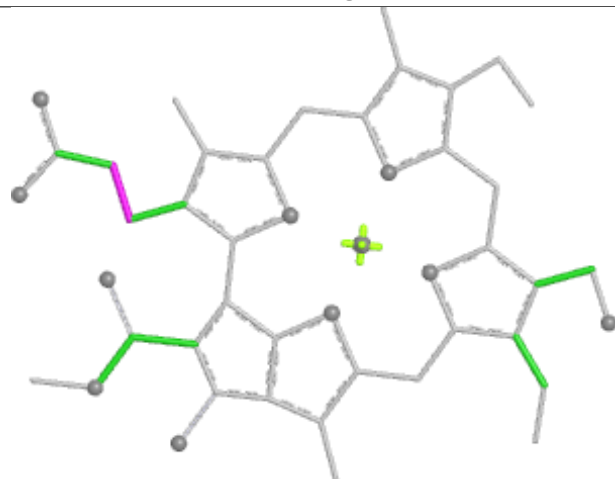
Ligand CHL Y 605



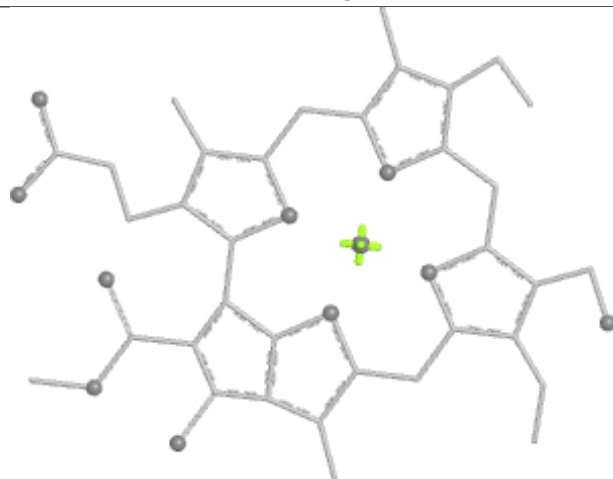
Bond lengths



Bond angles

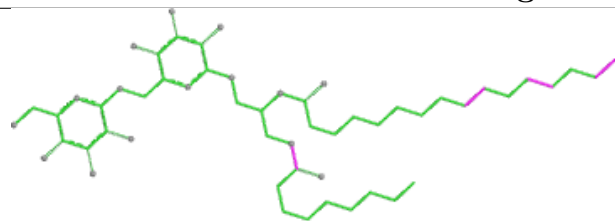


Torsions

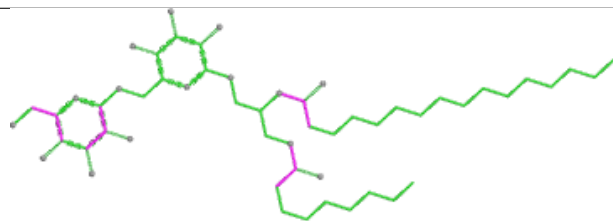


Rings

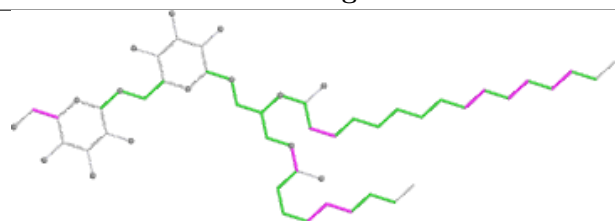
Ligand DGD c 518



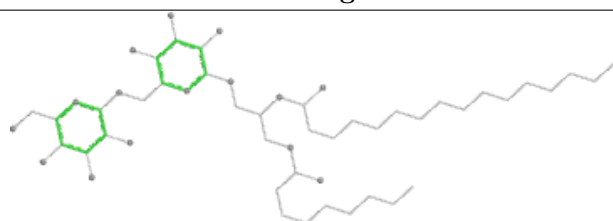
Bond lengths



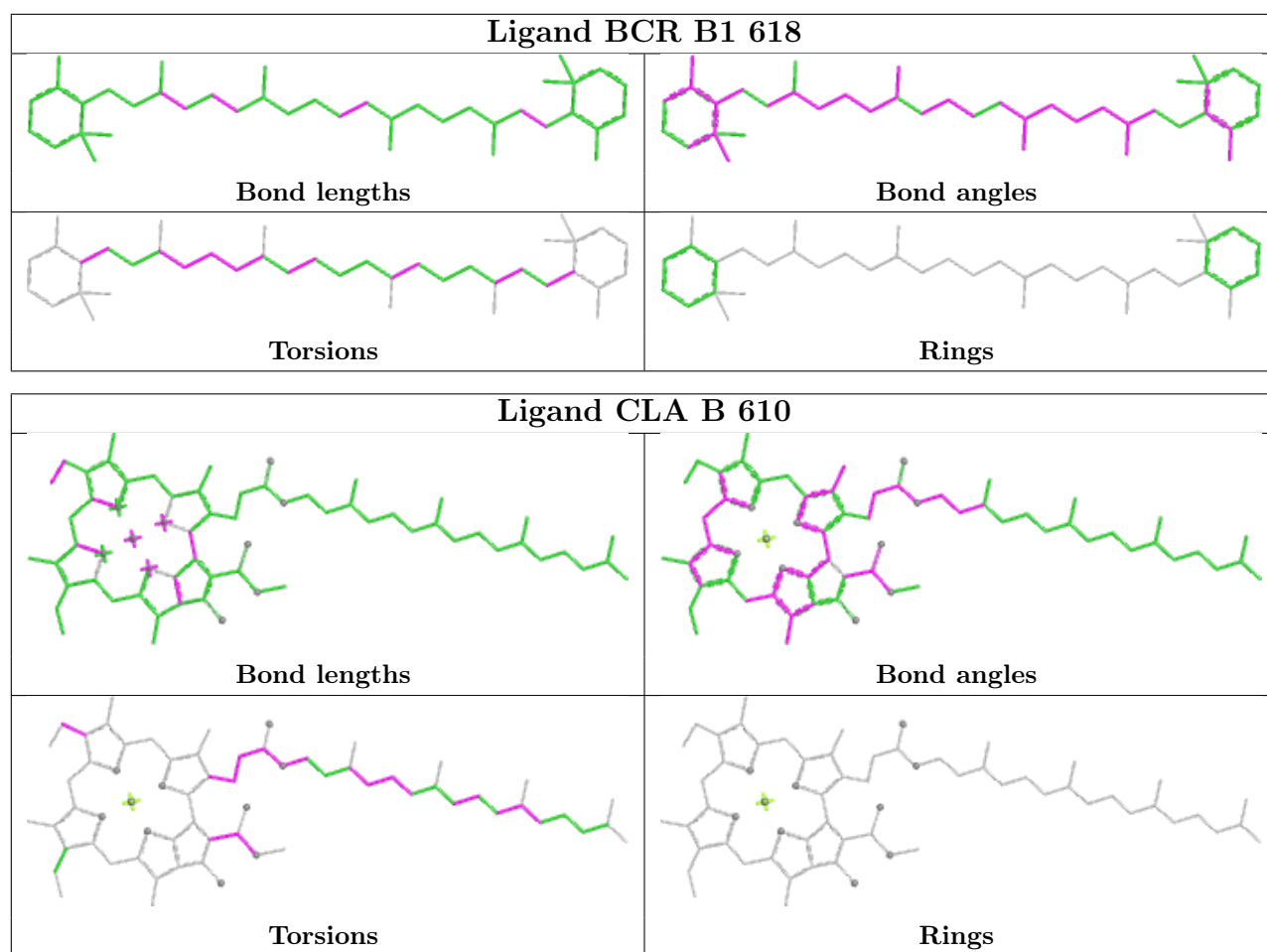
Bond angles



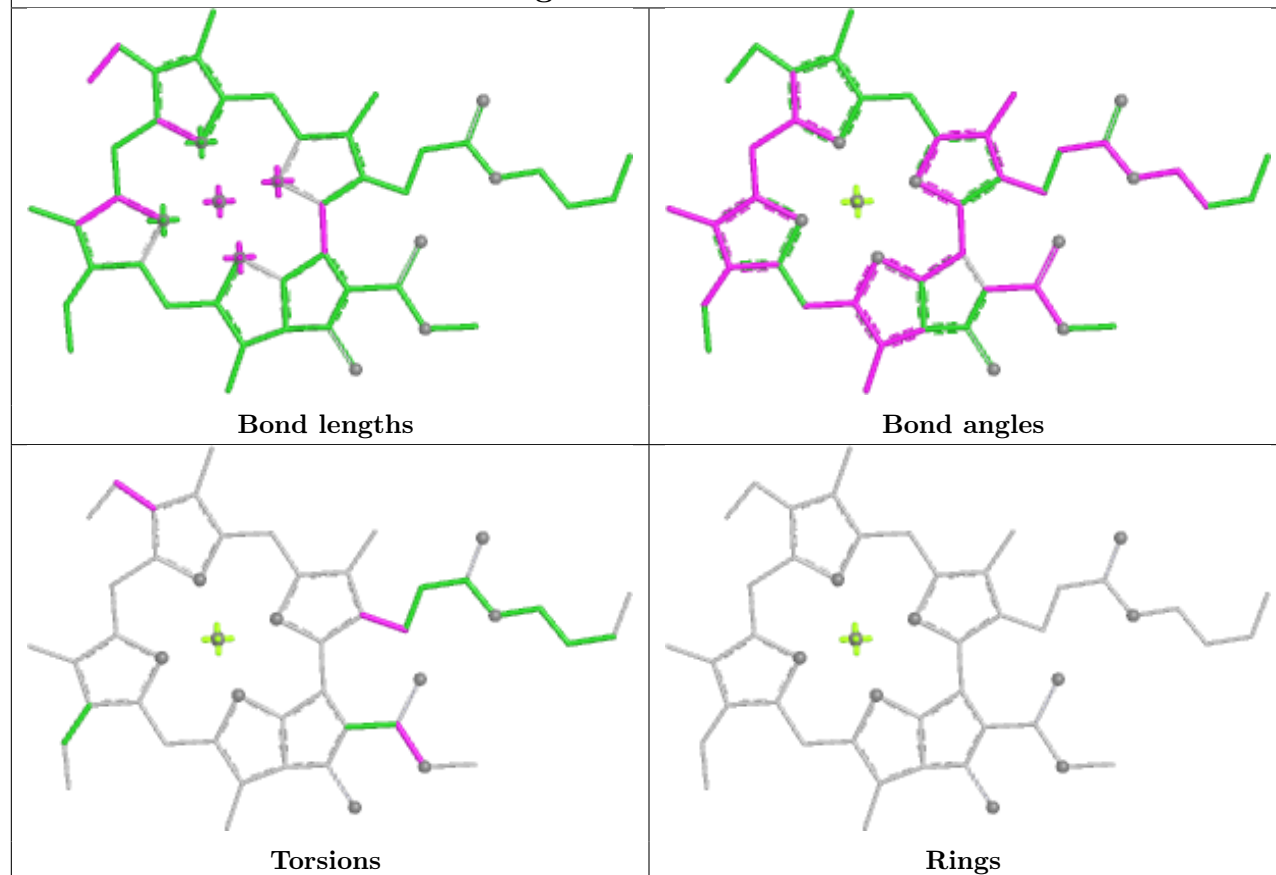
Torsions



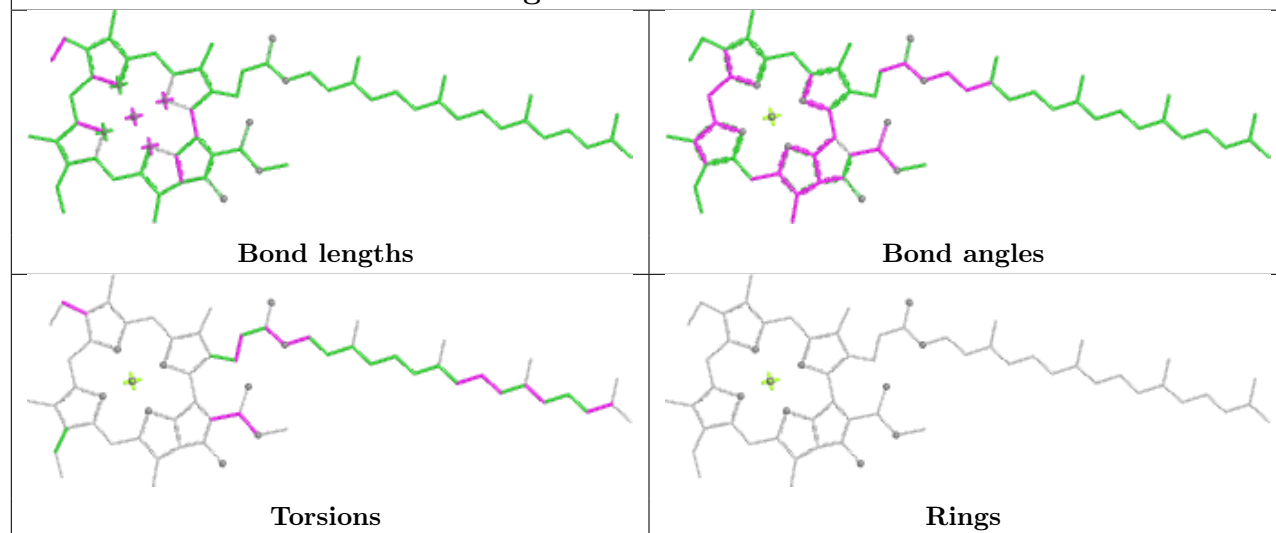
Rings

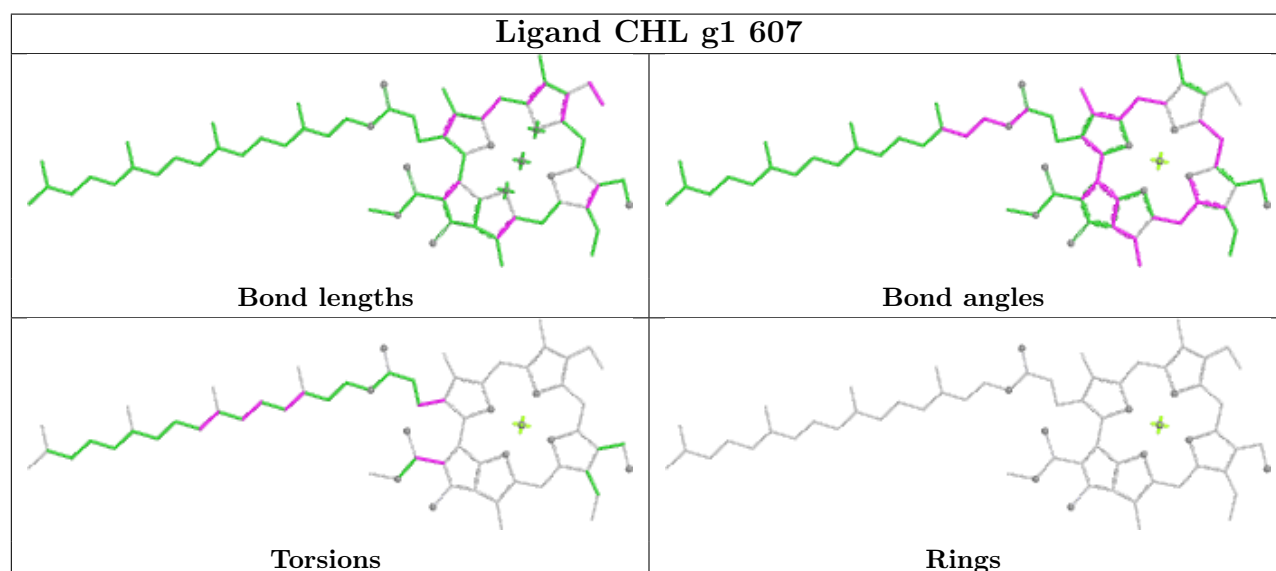
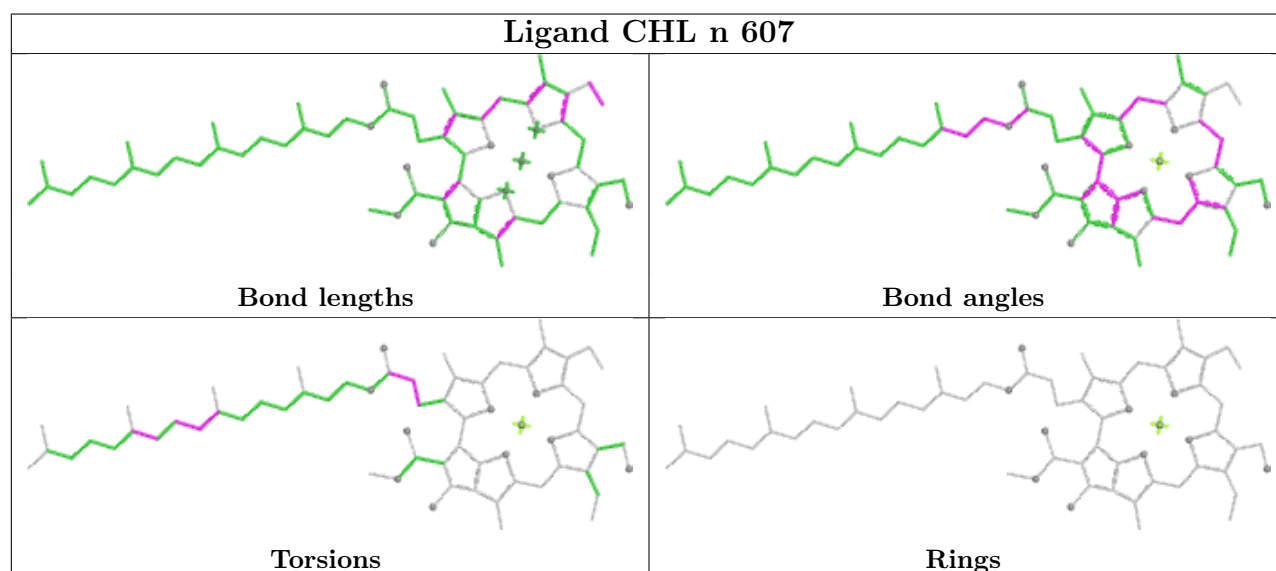
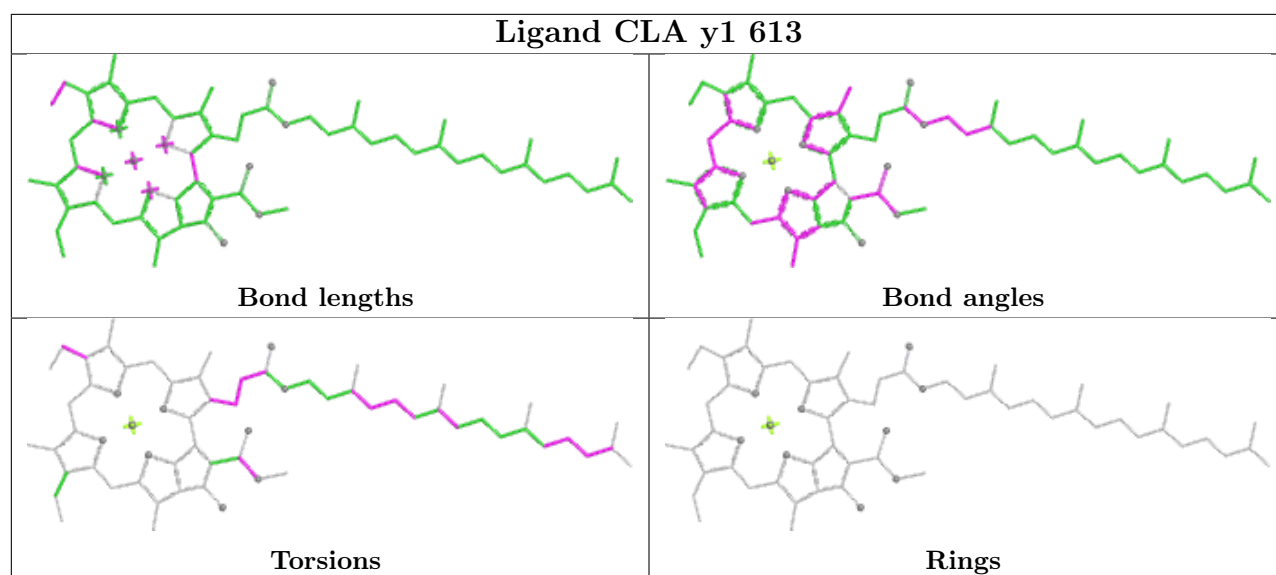


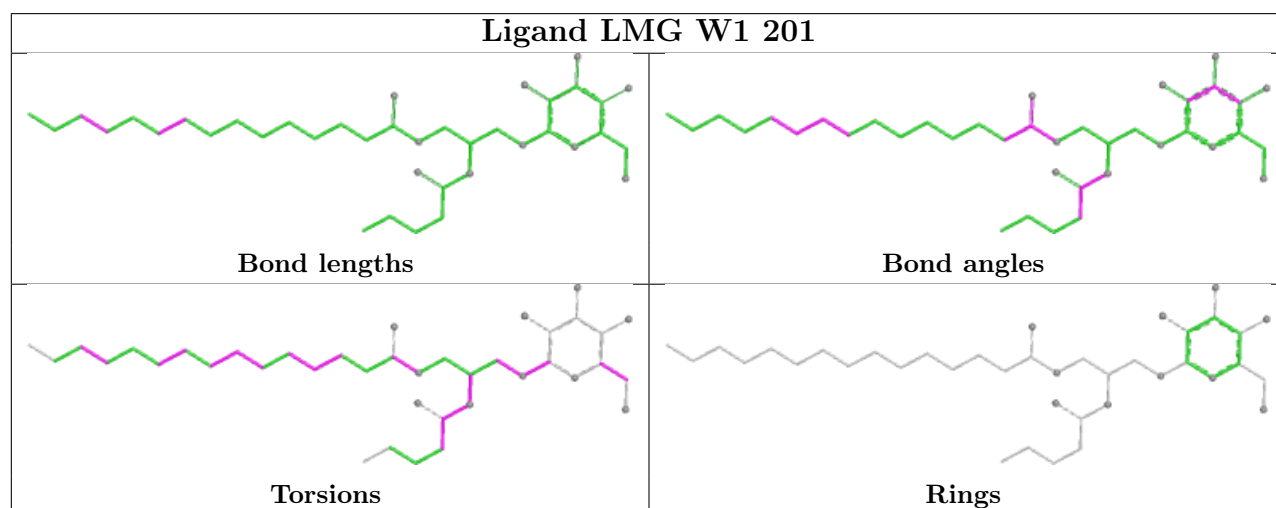
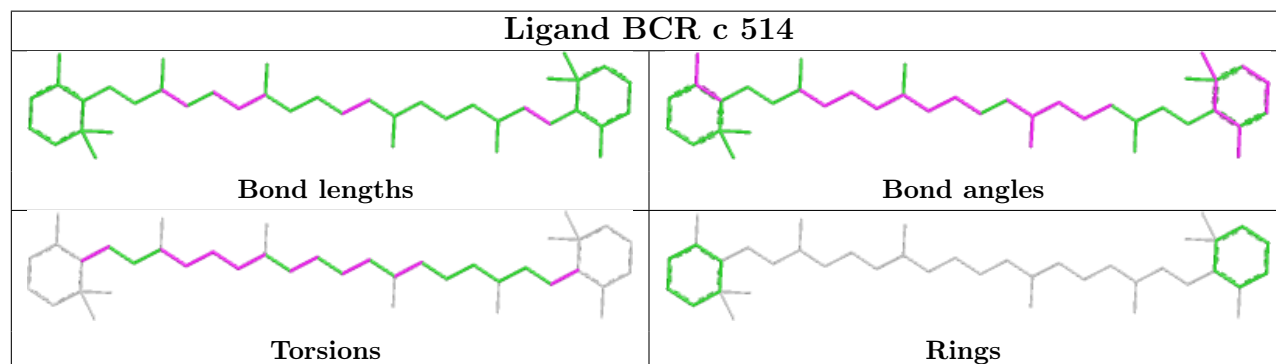
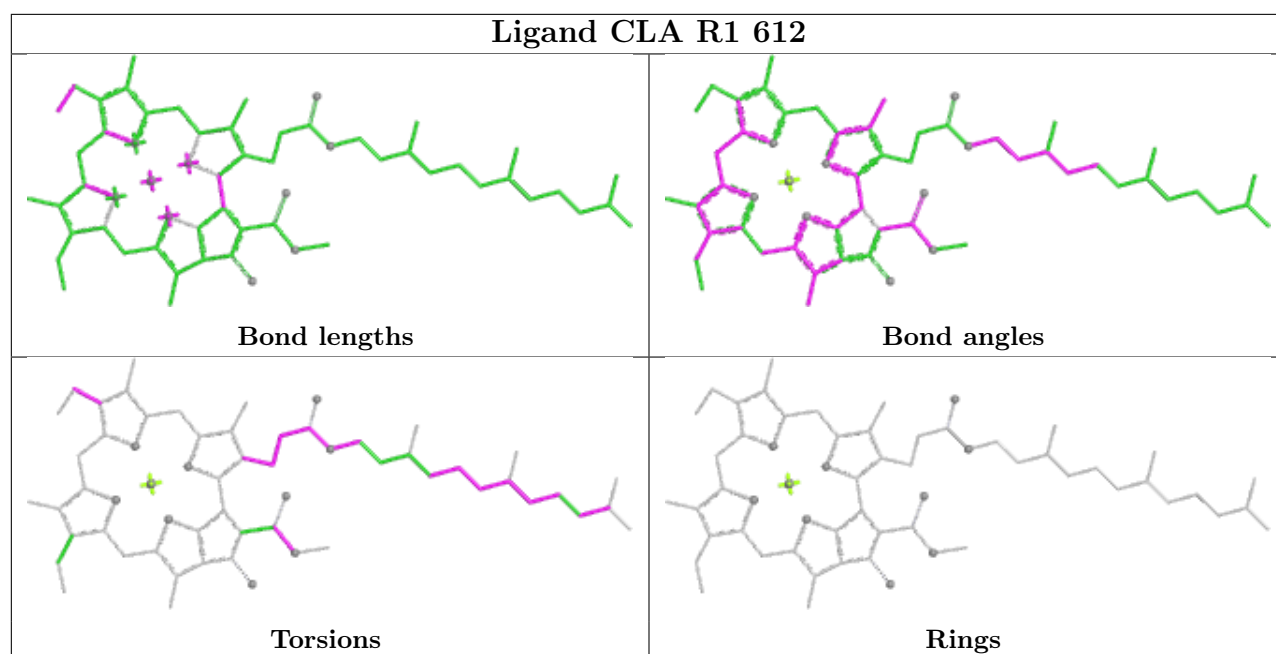
Ligand CLA n 614

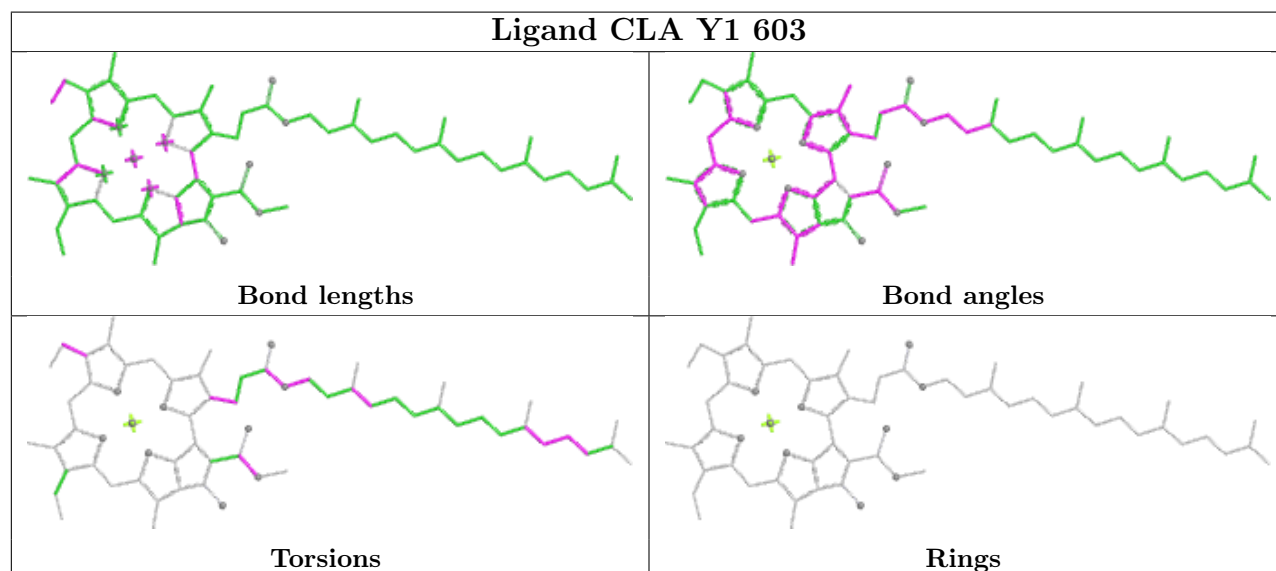
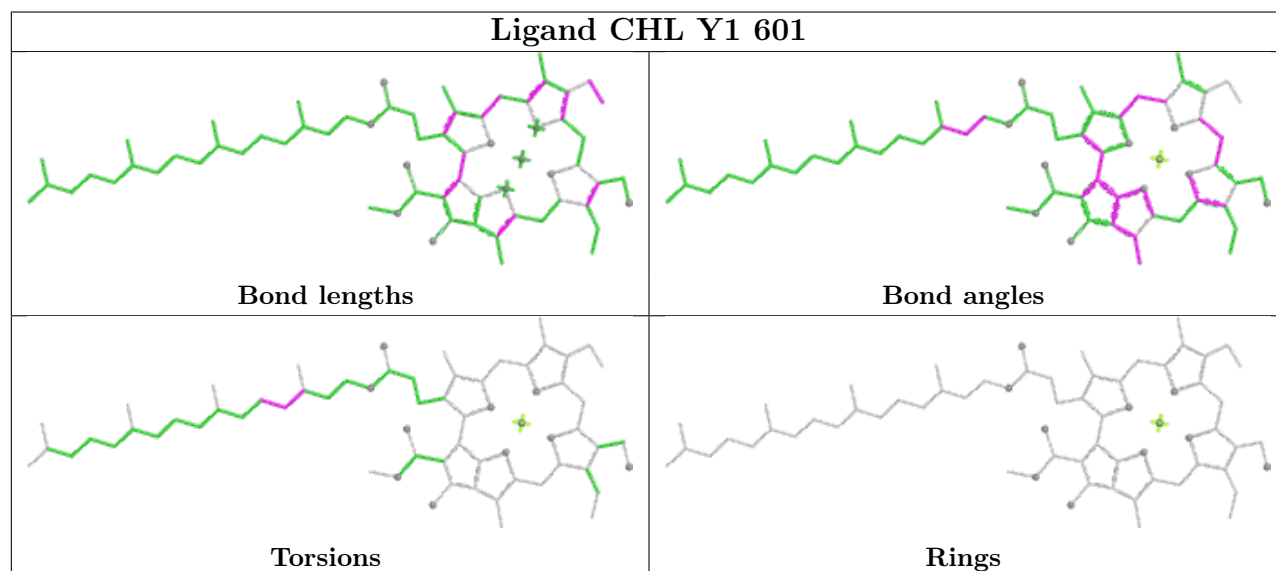
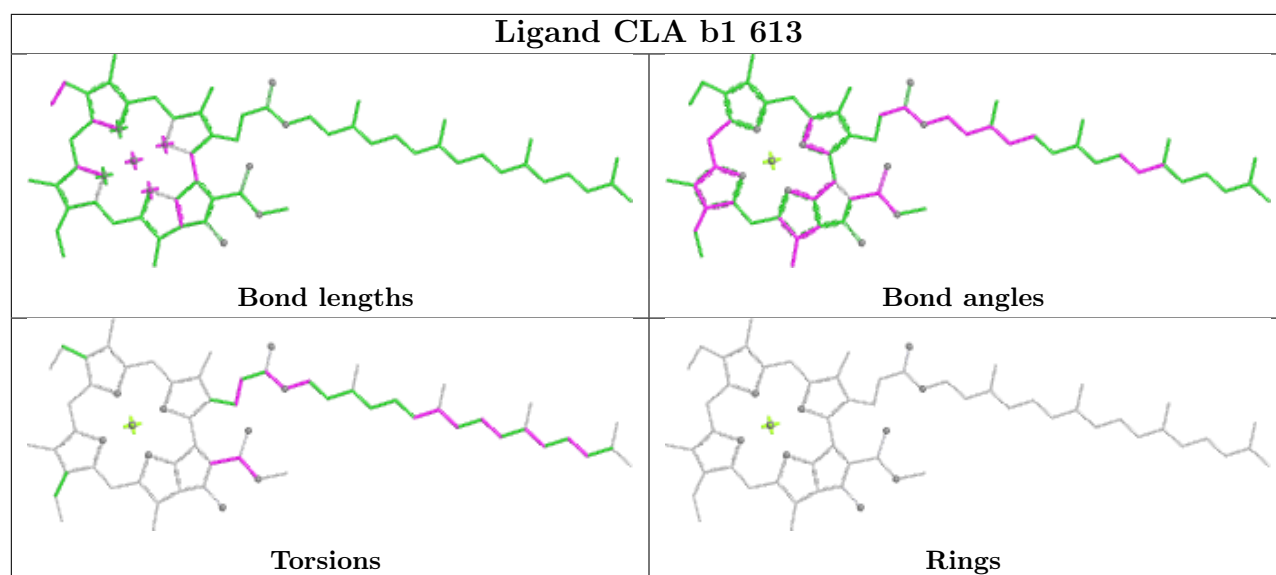


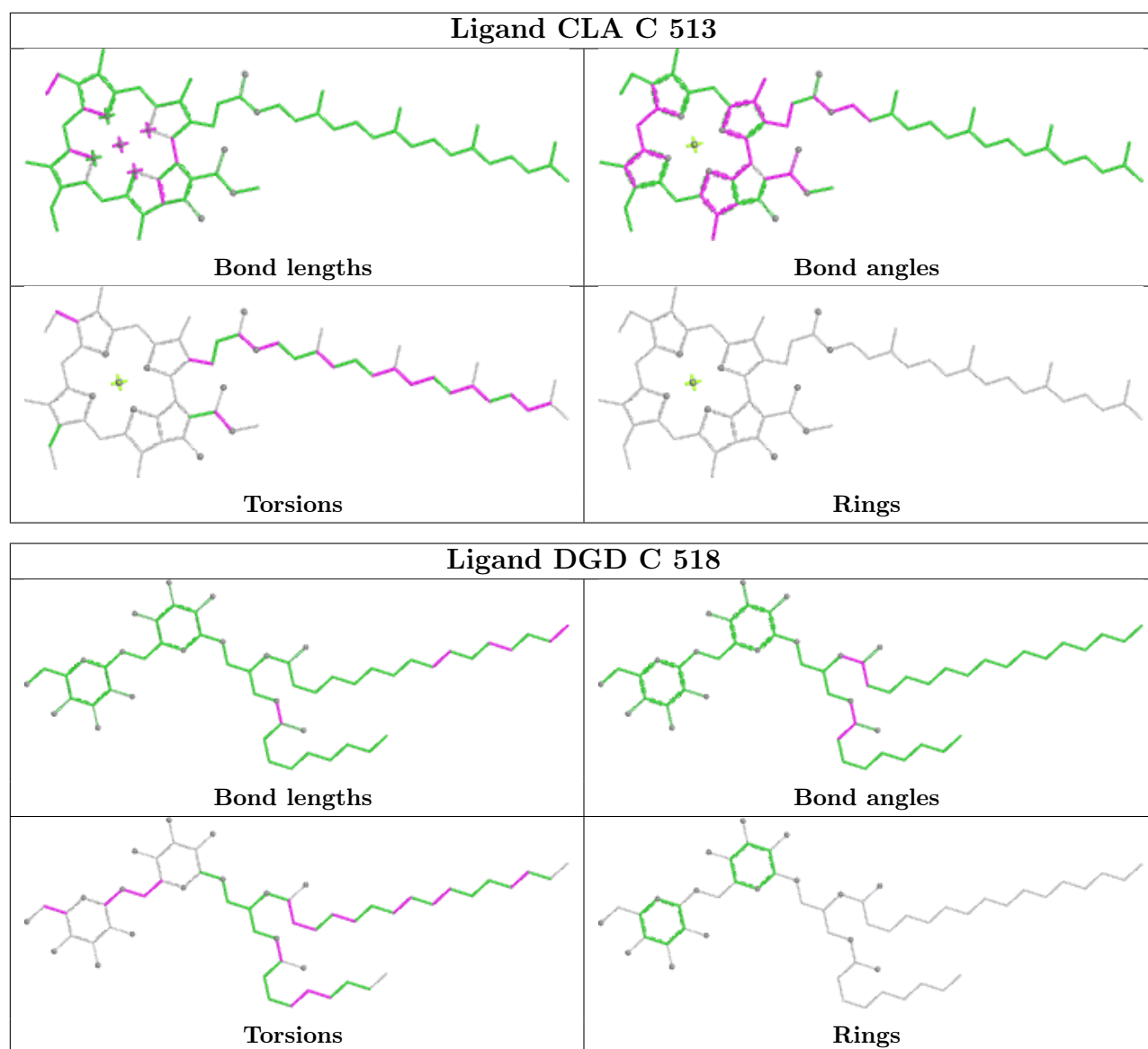
Ligand CLA B1 613

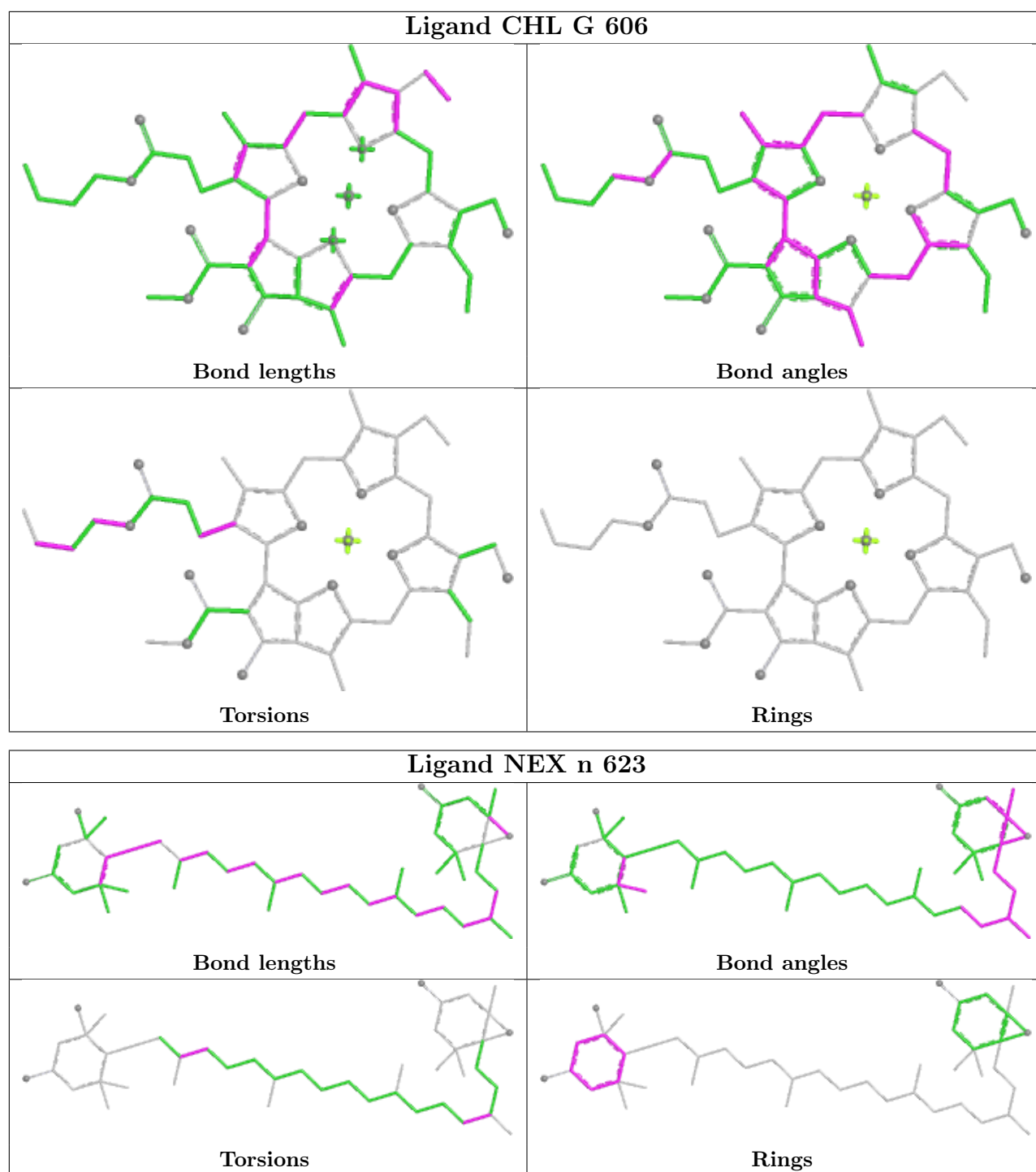


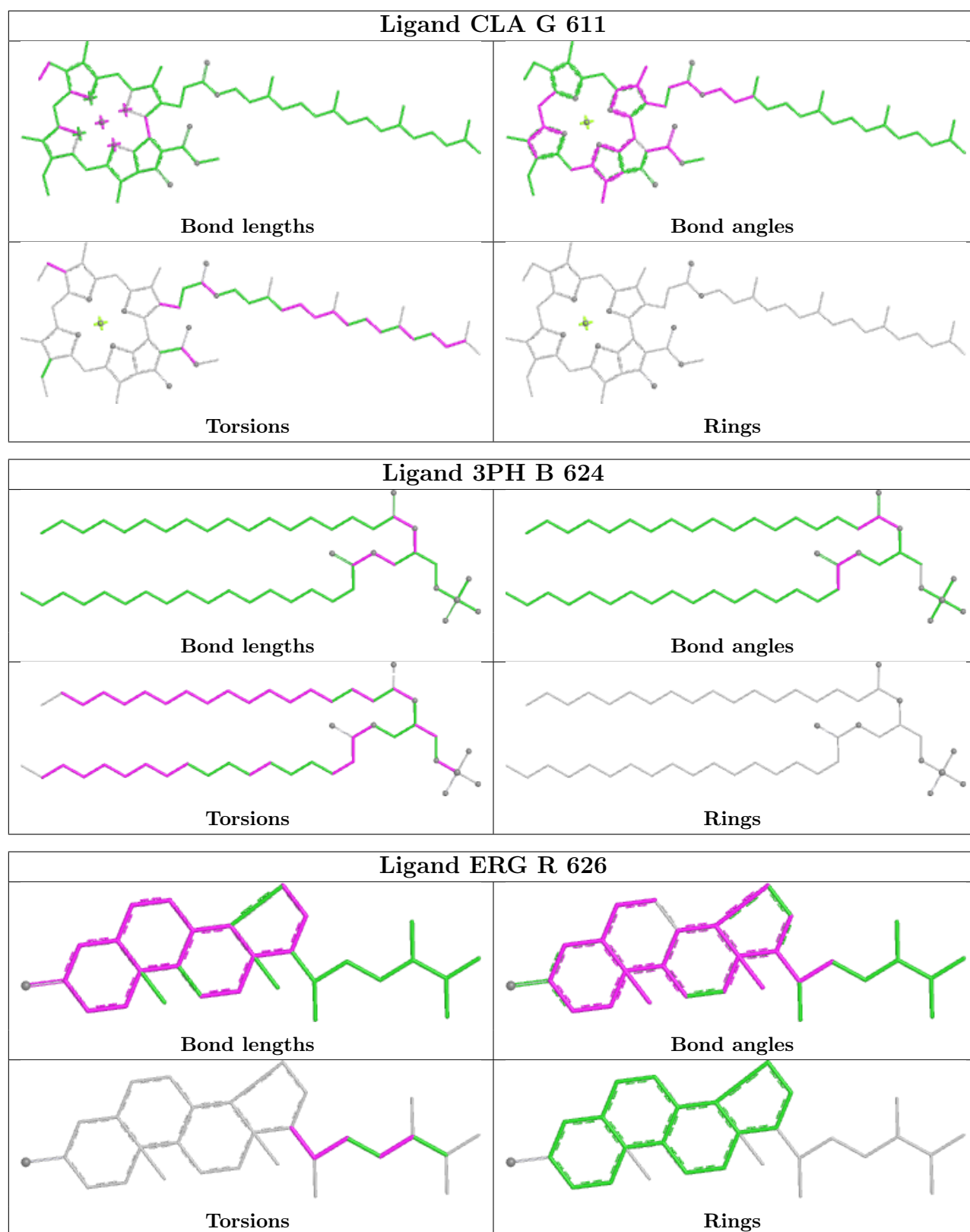


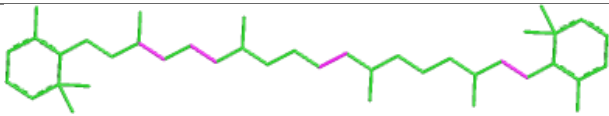
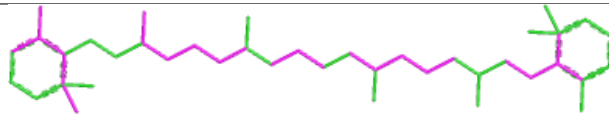
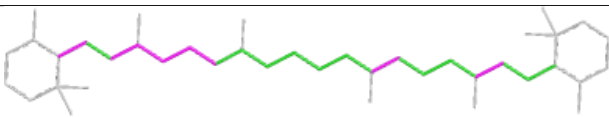
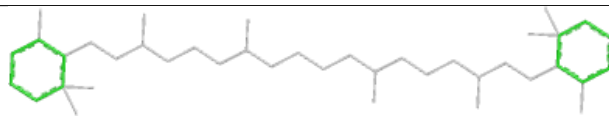


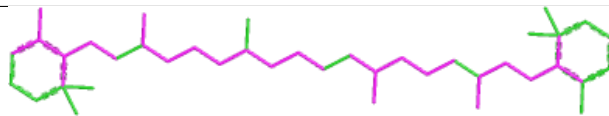
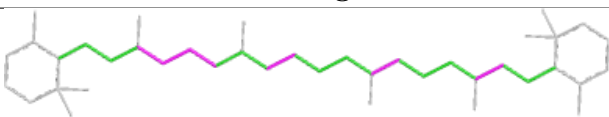
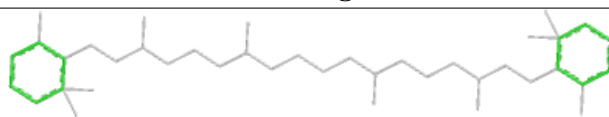


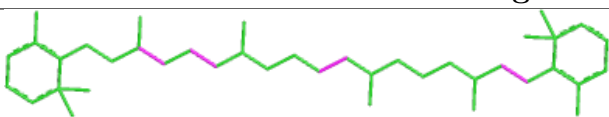
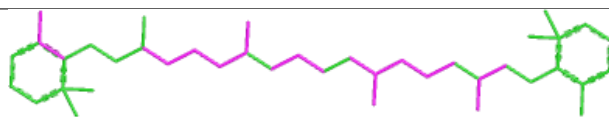
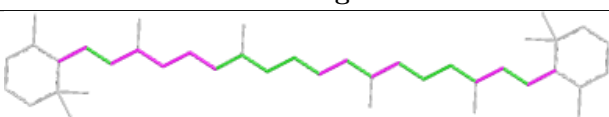
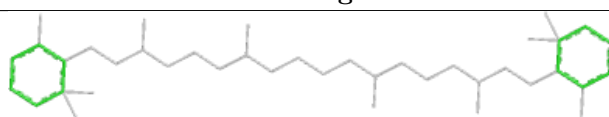


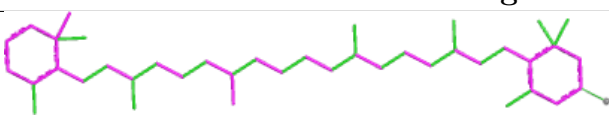
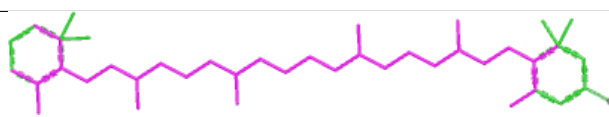
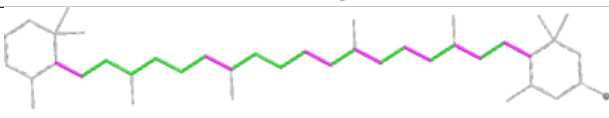
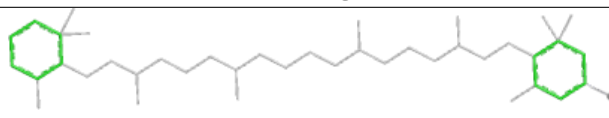


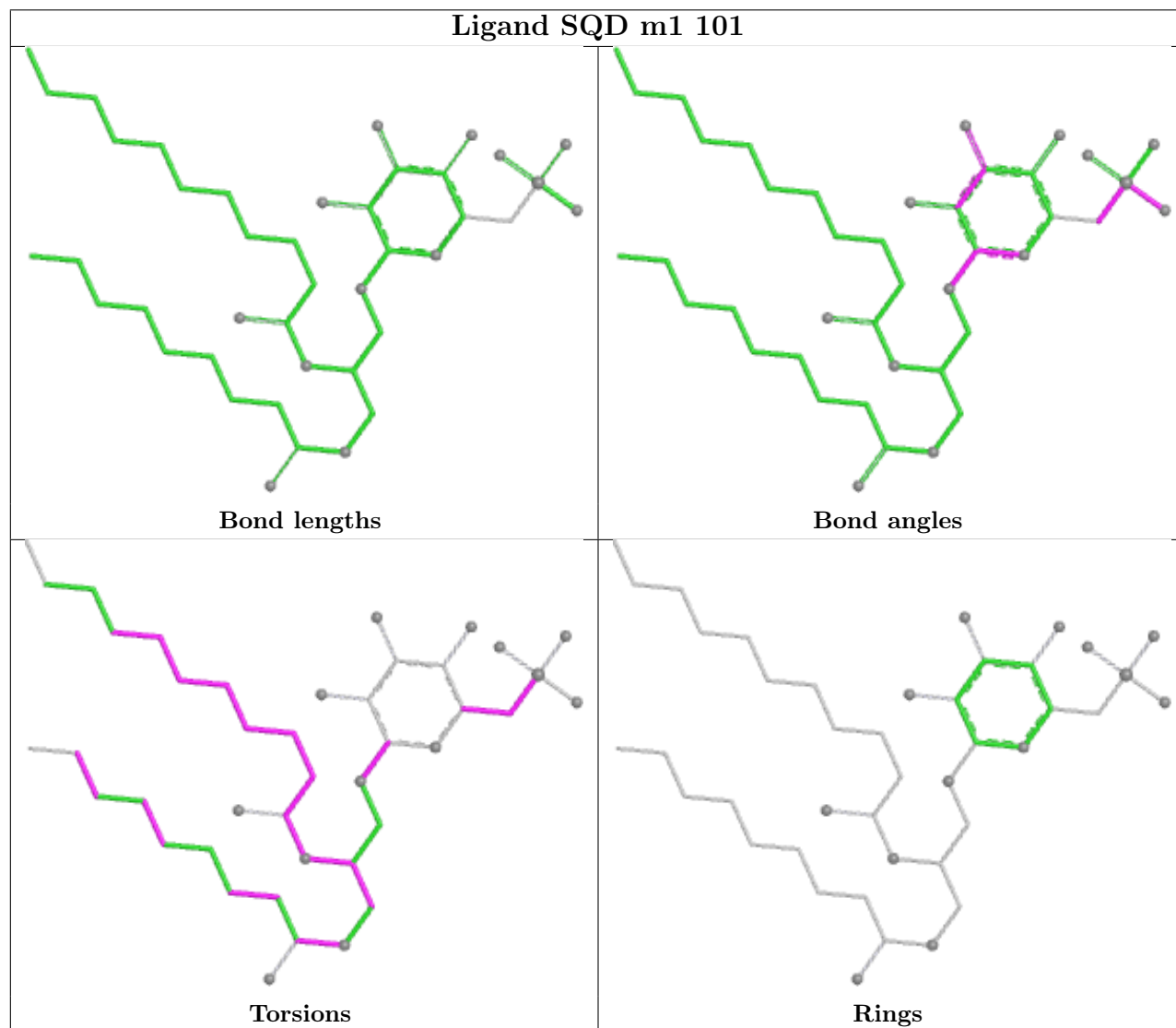
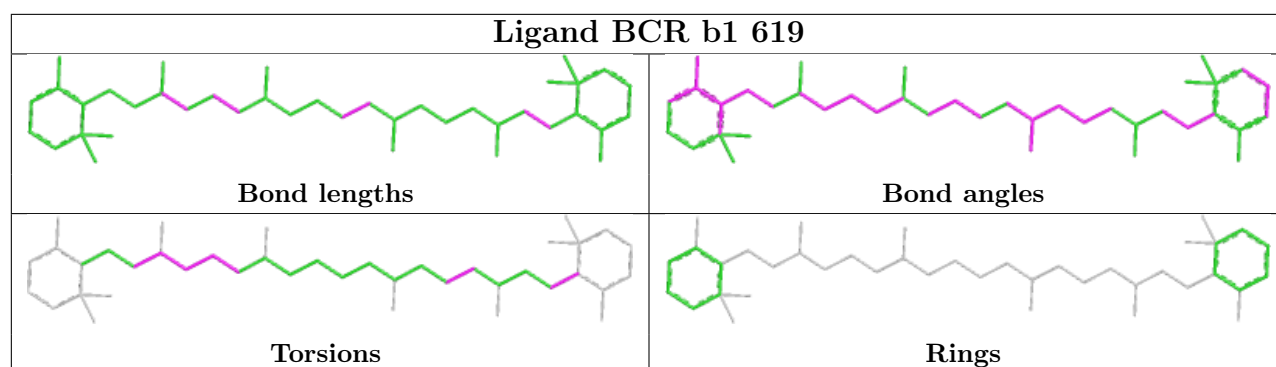


Ligand BCR c1 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

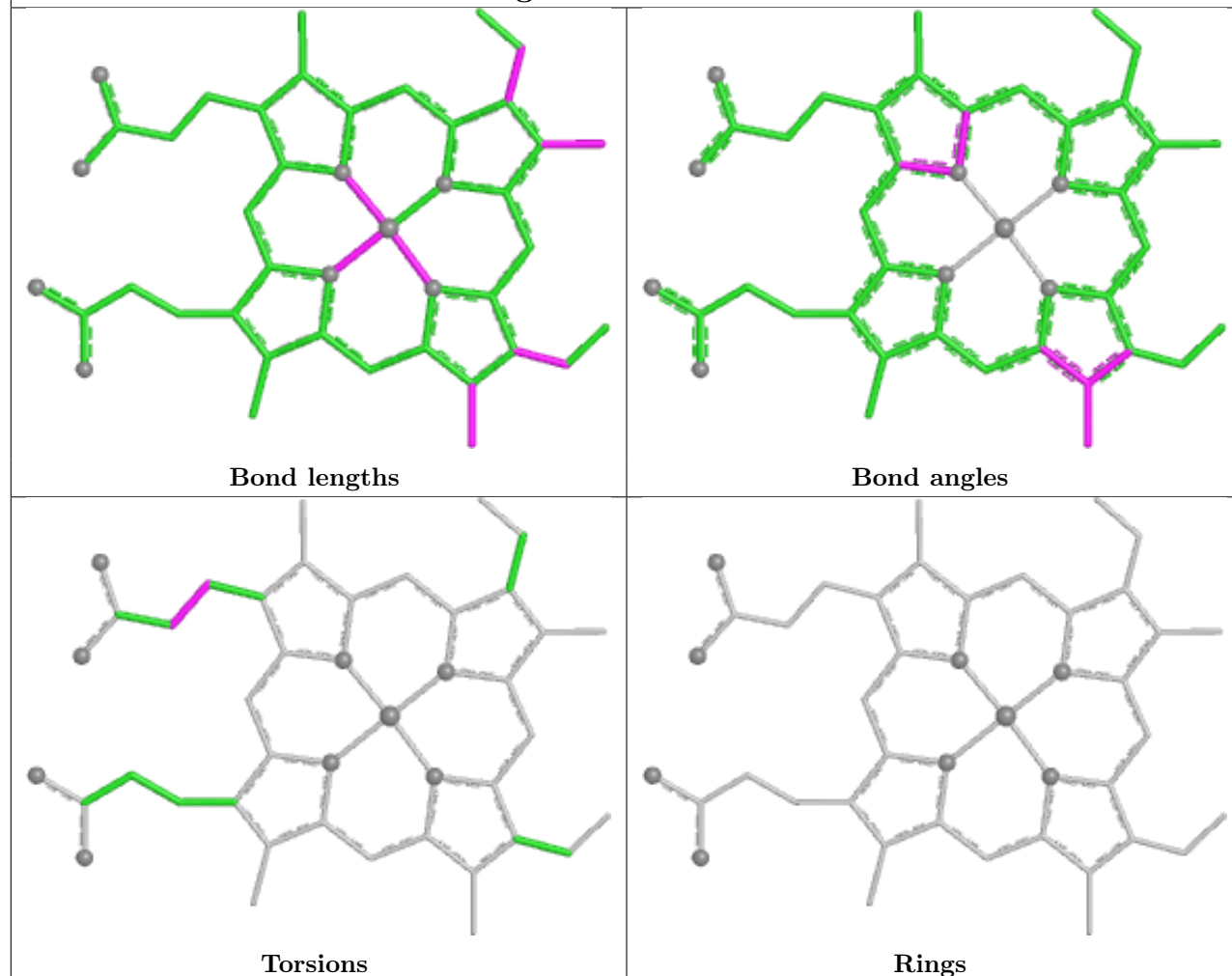
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

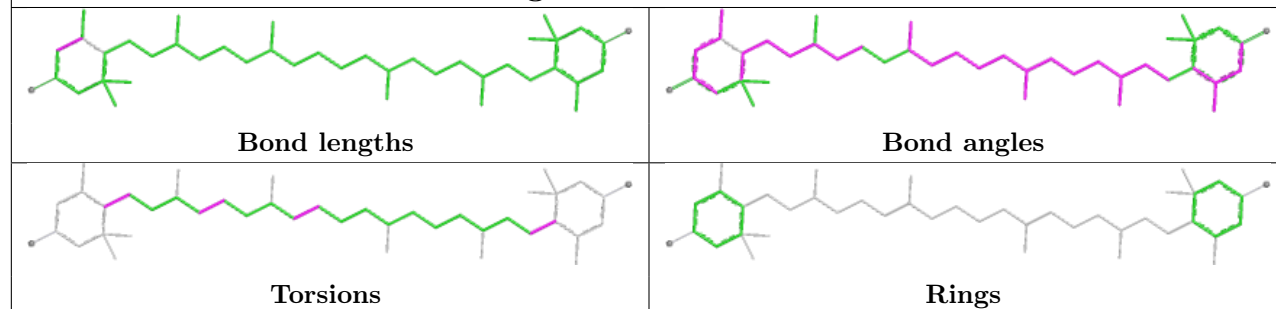
Ligand RRX h1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

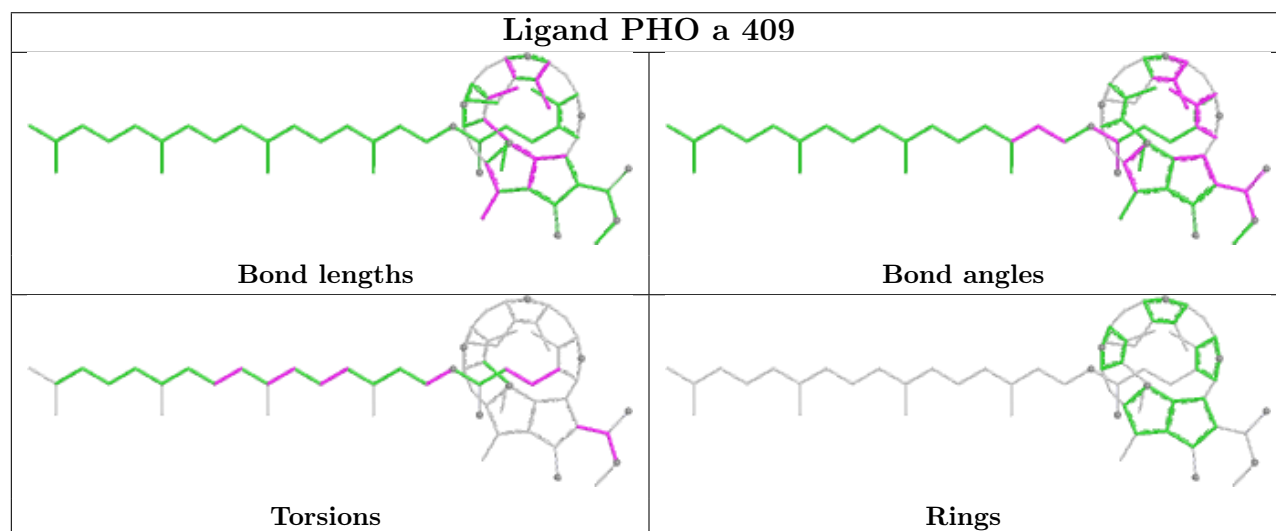
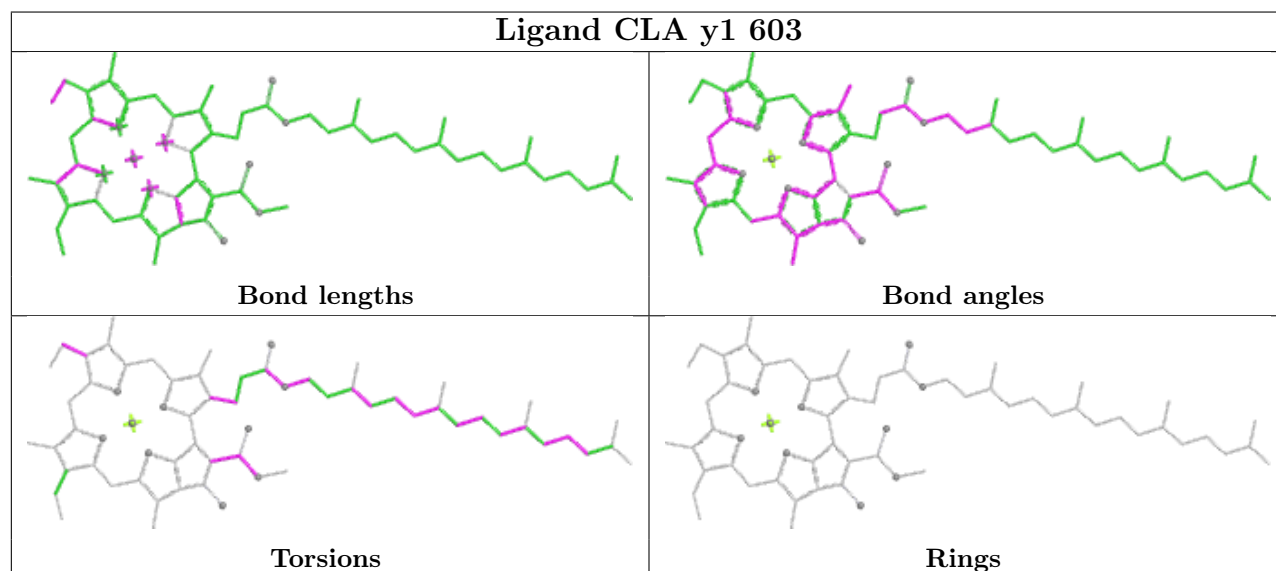
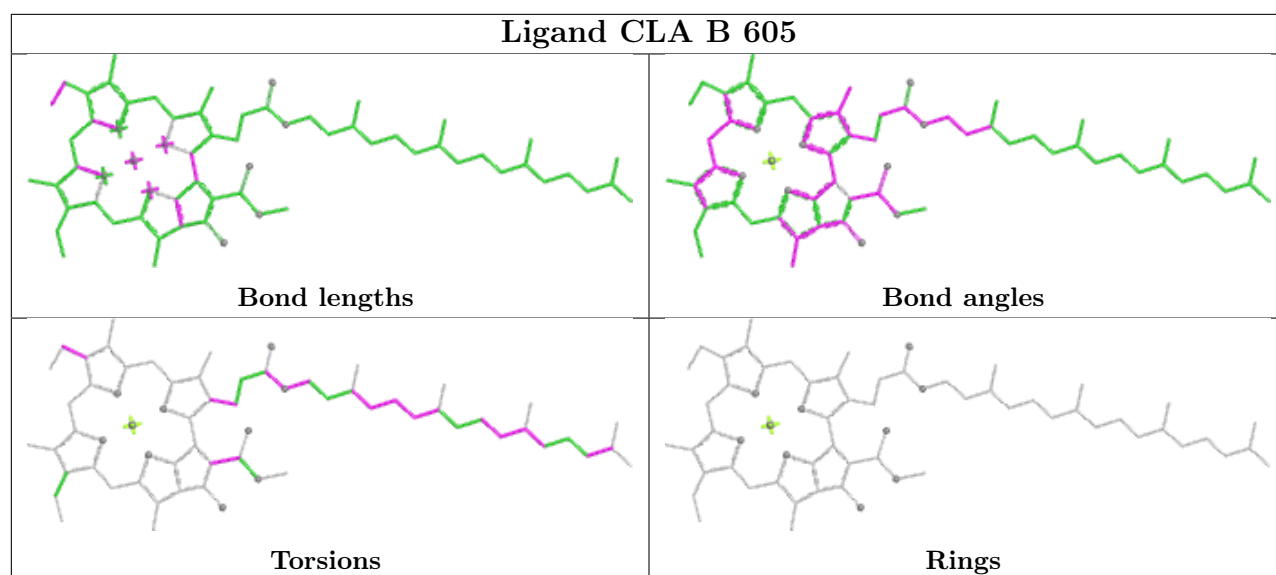


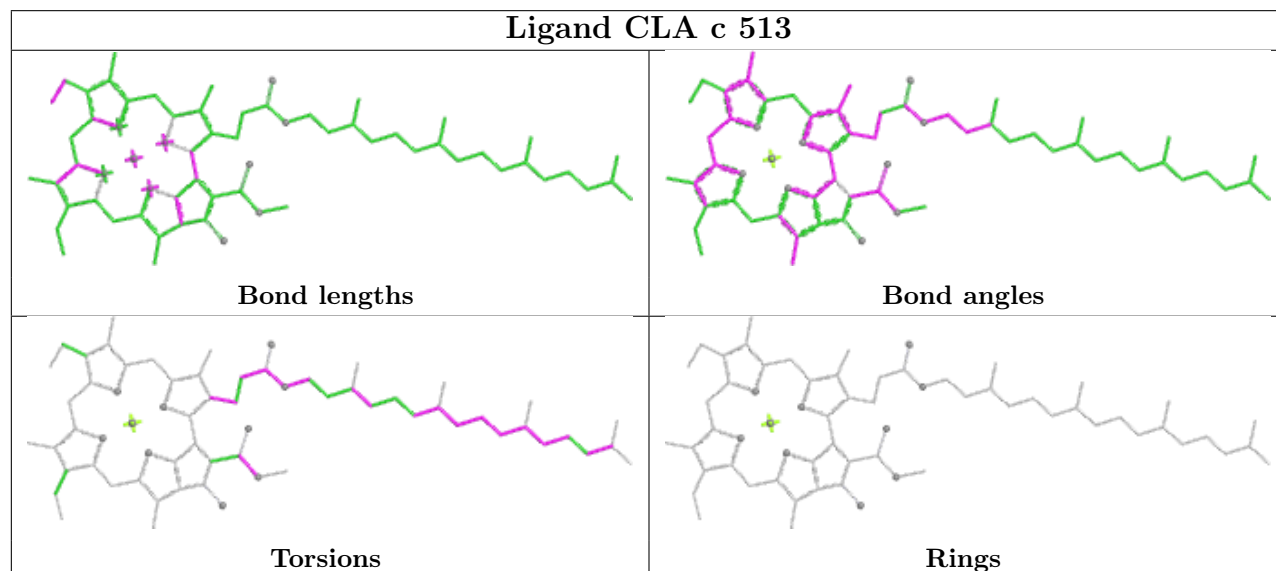
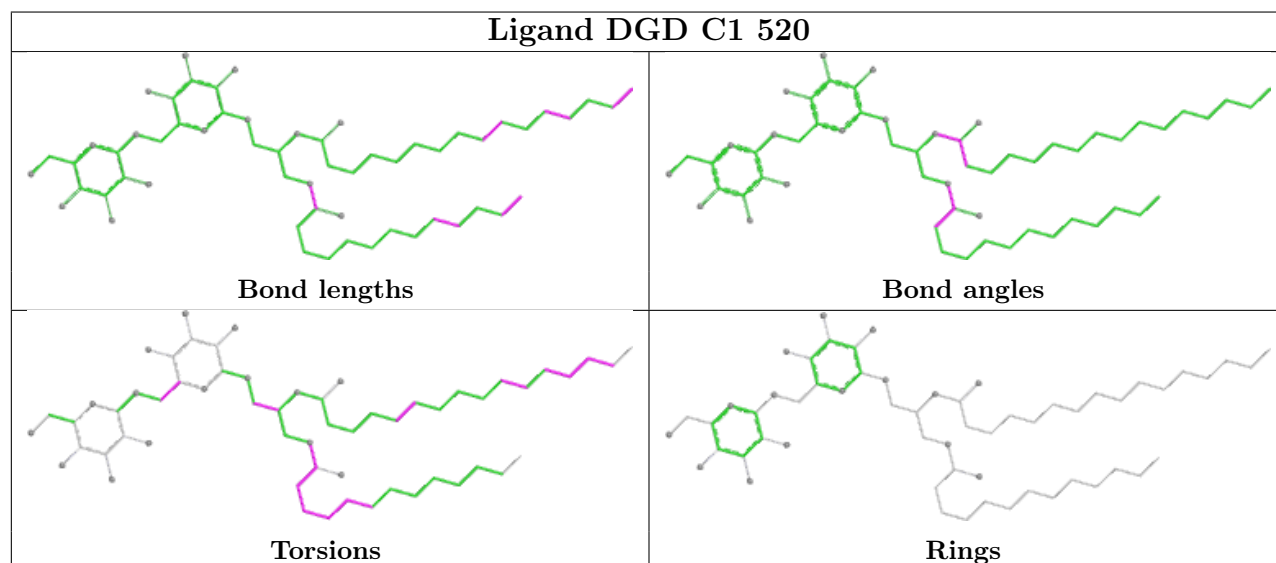
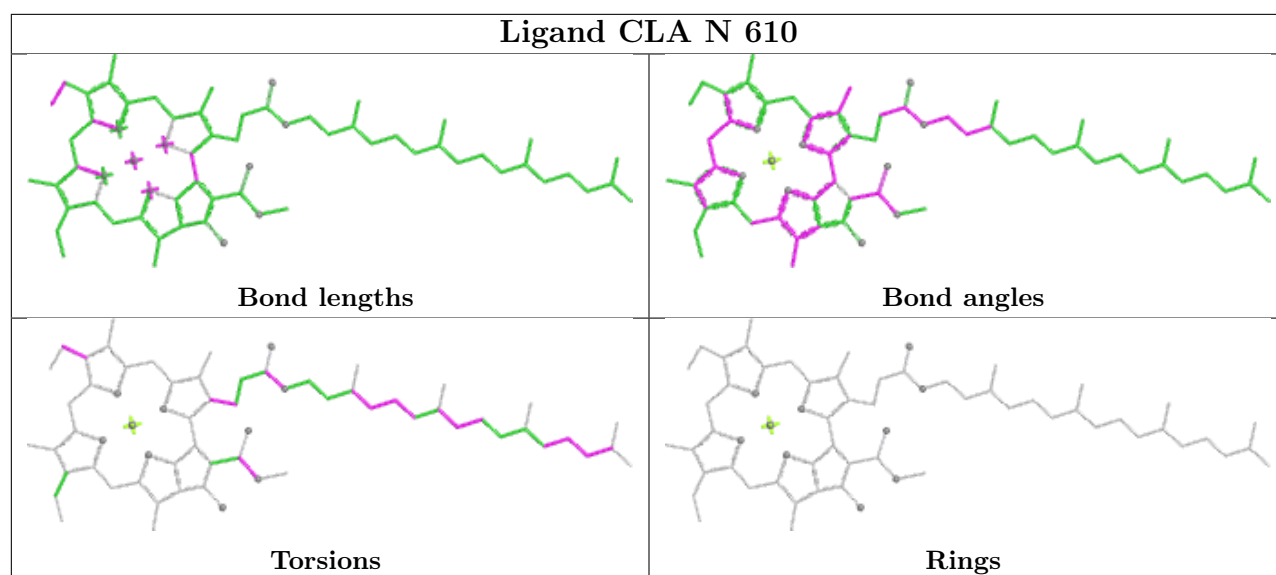
Ligand HEM f 101

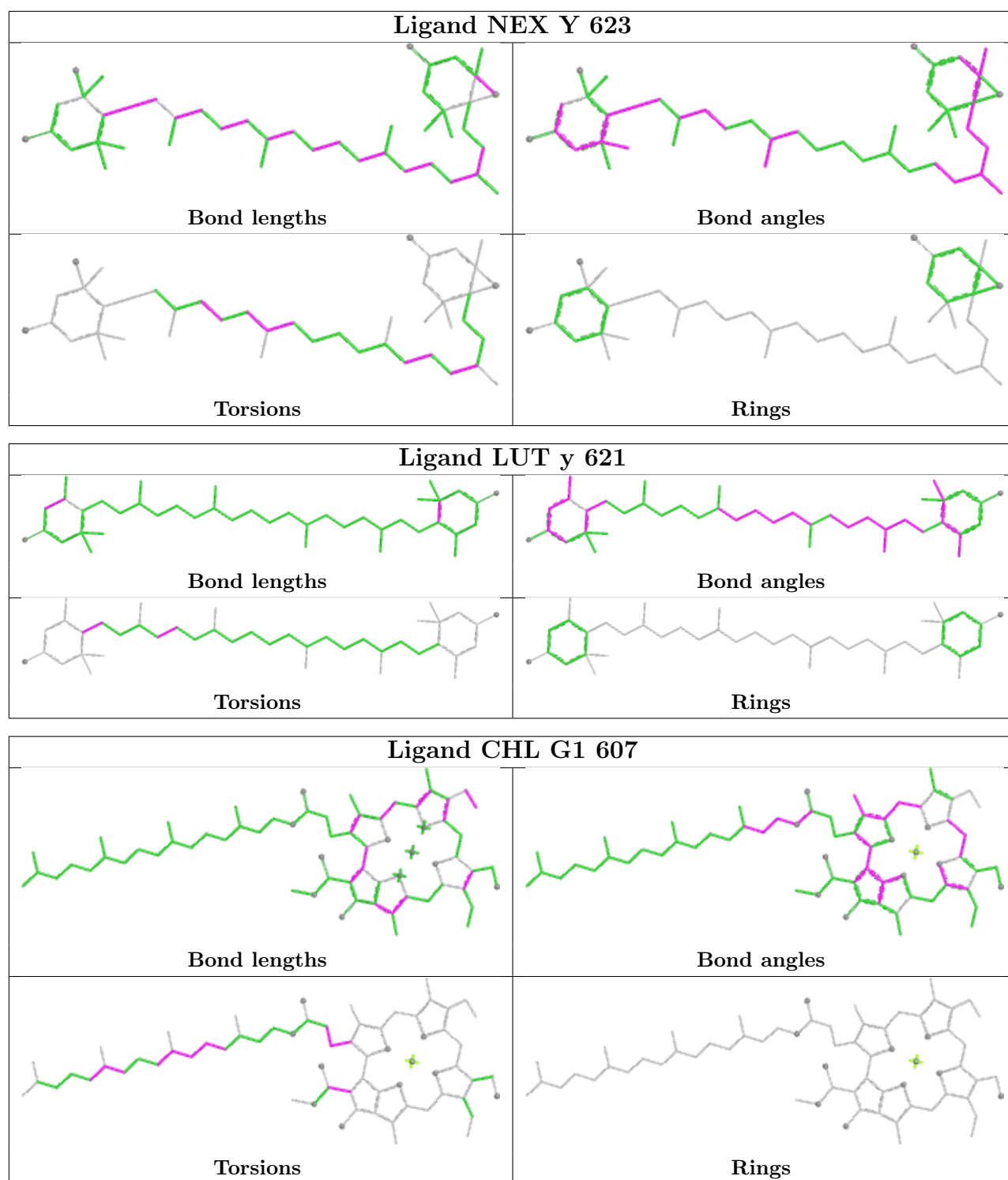


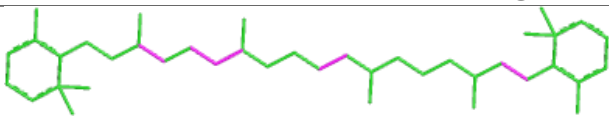
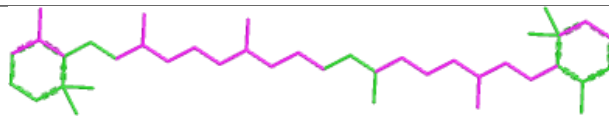
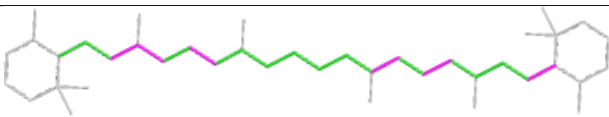
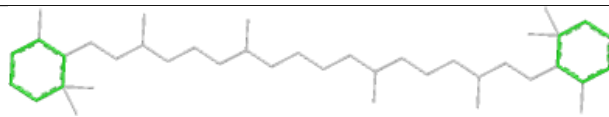
Ligand LUT n1 621

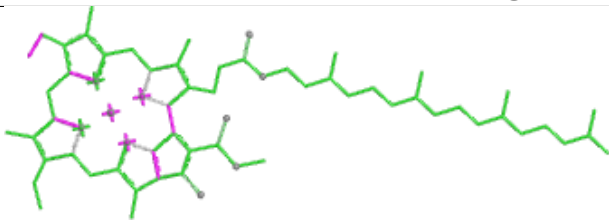
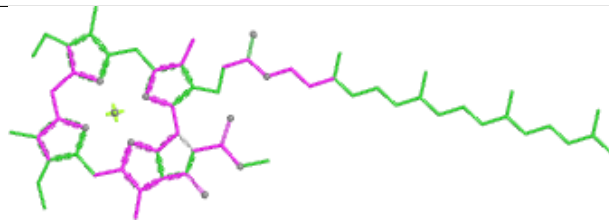
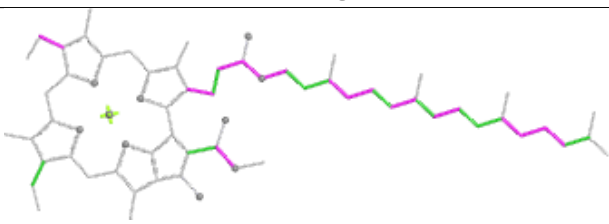
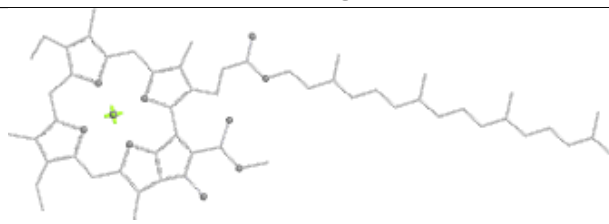


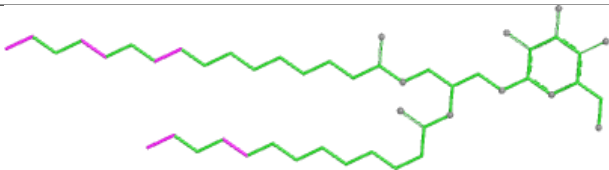
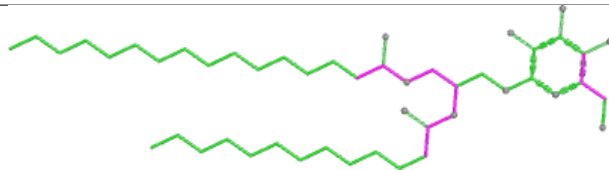
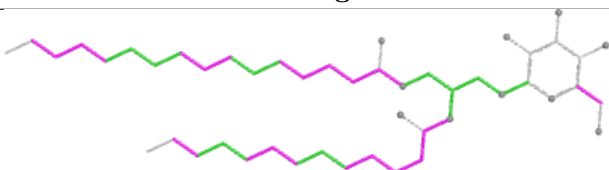
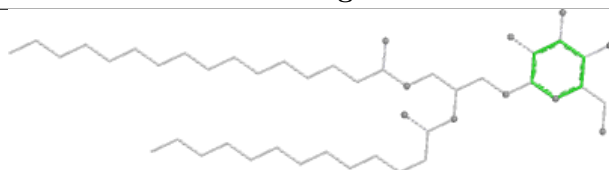


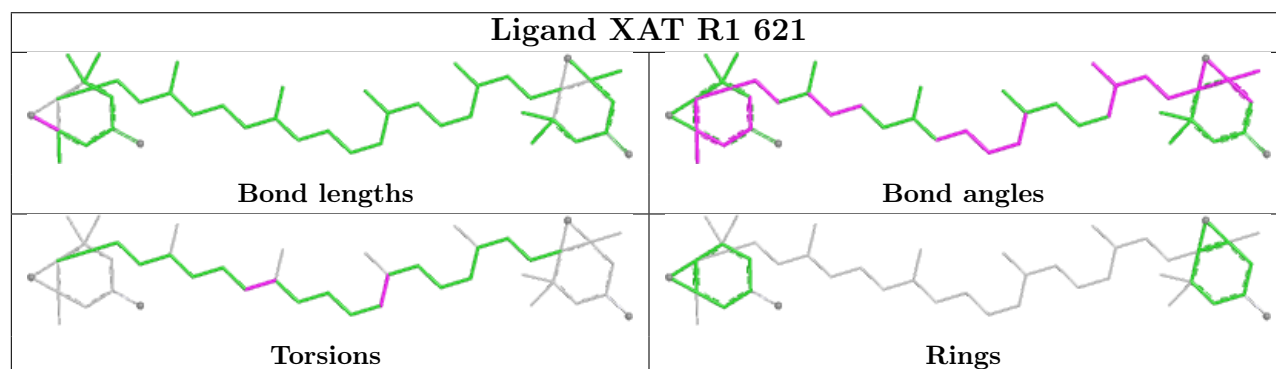
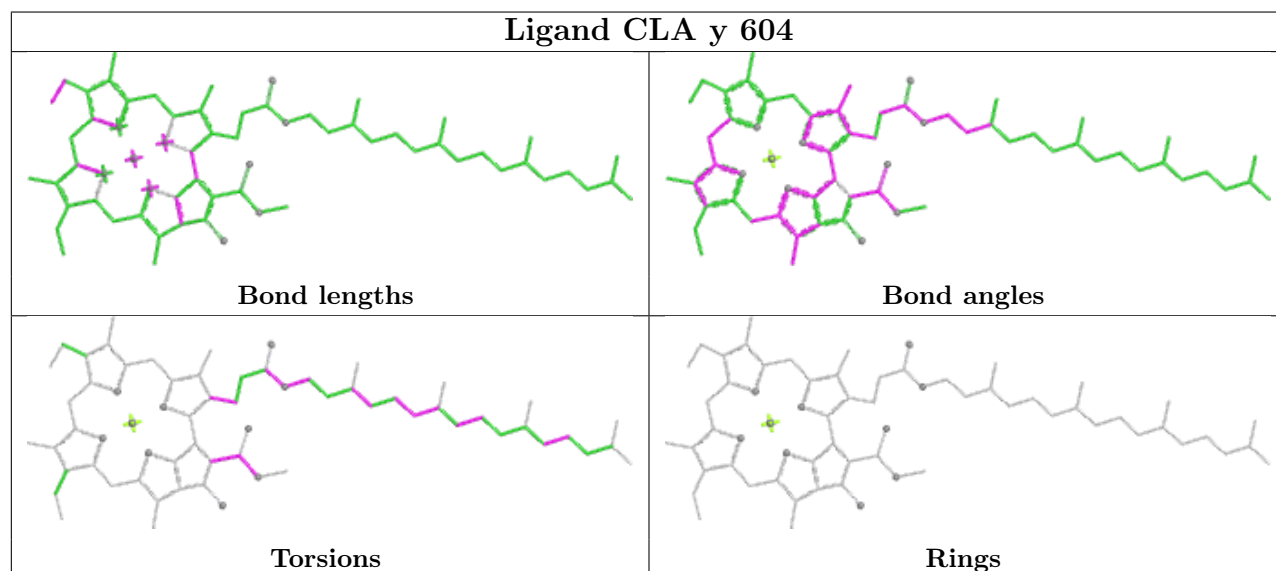
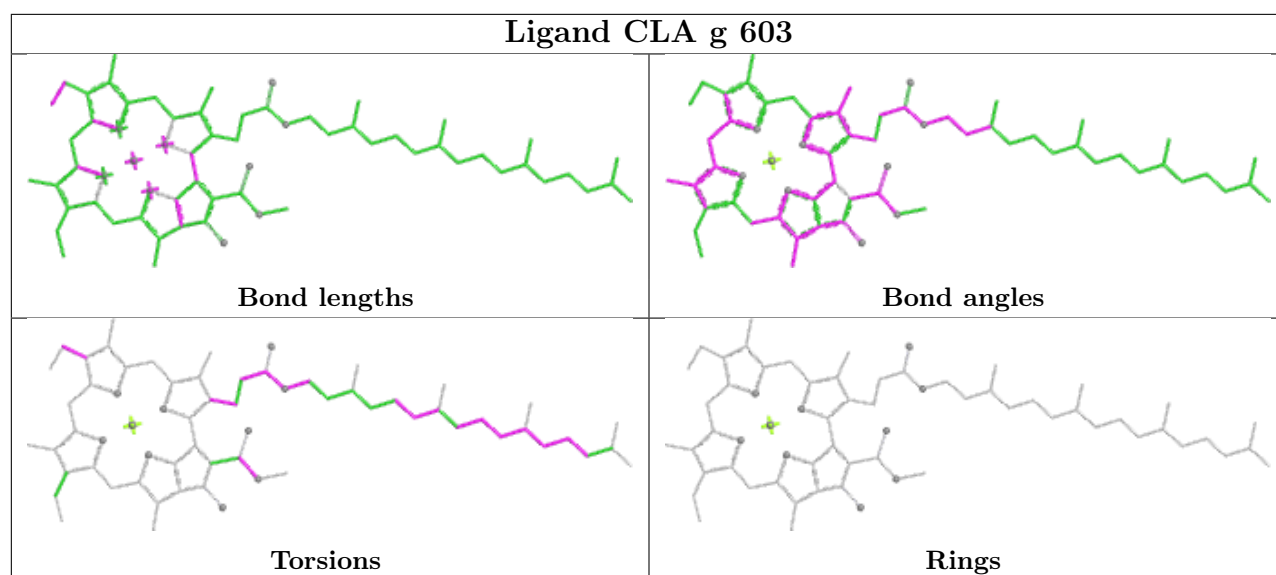


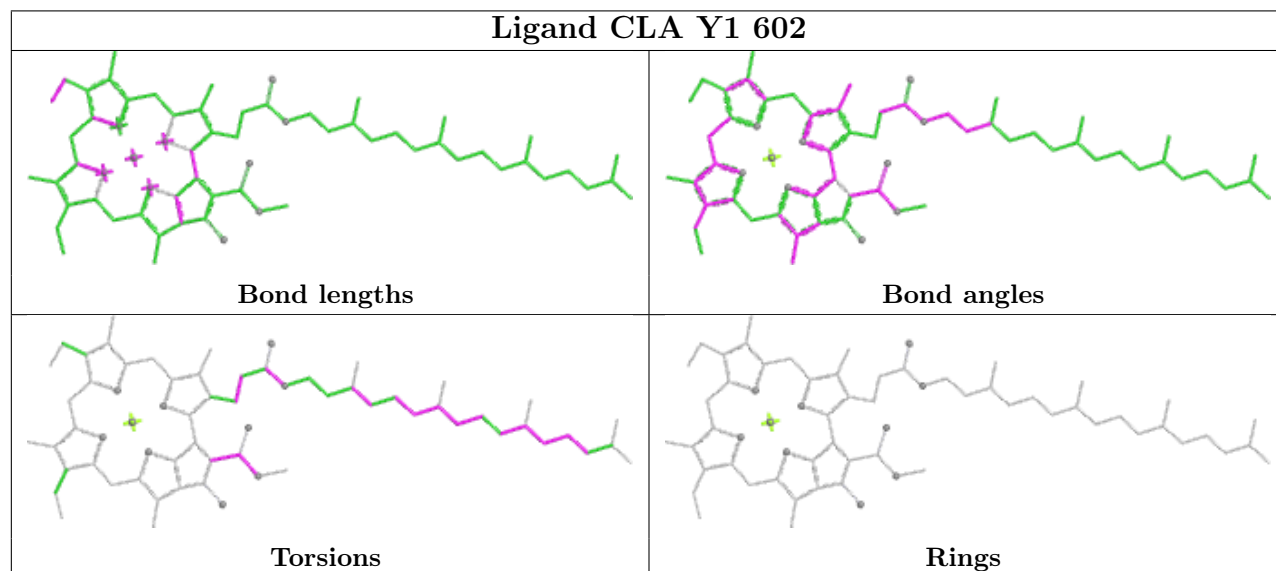
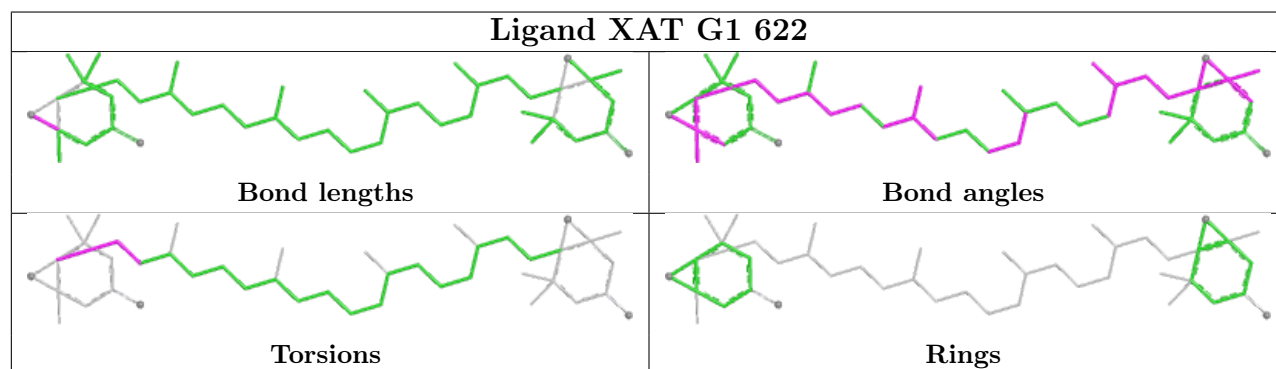
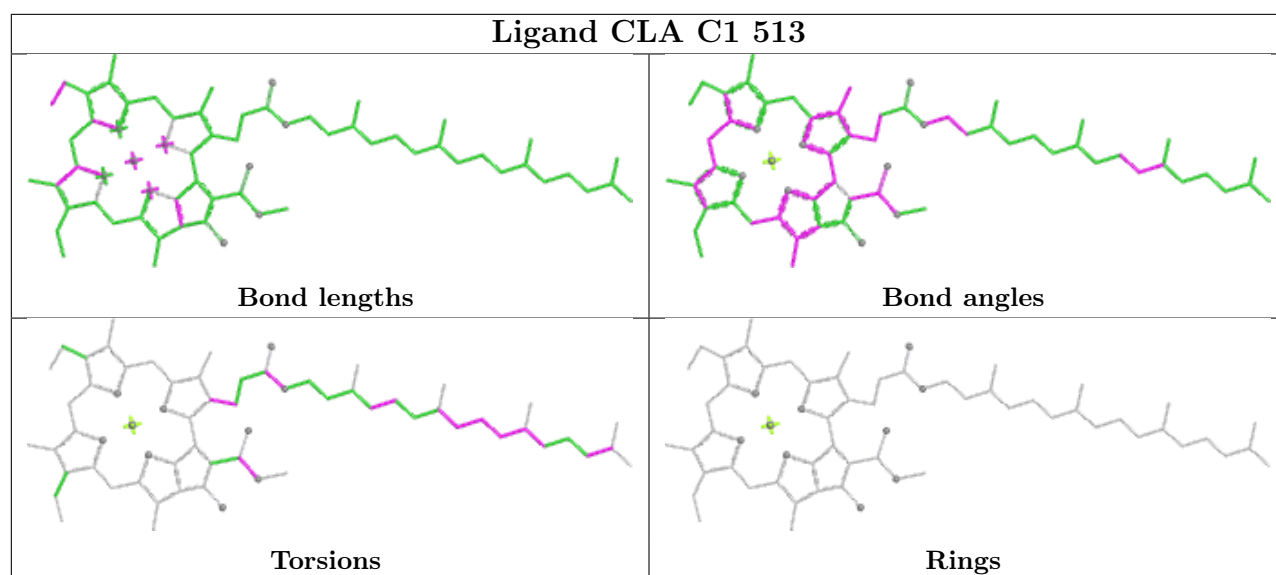


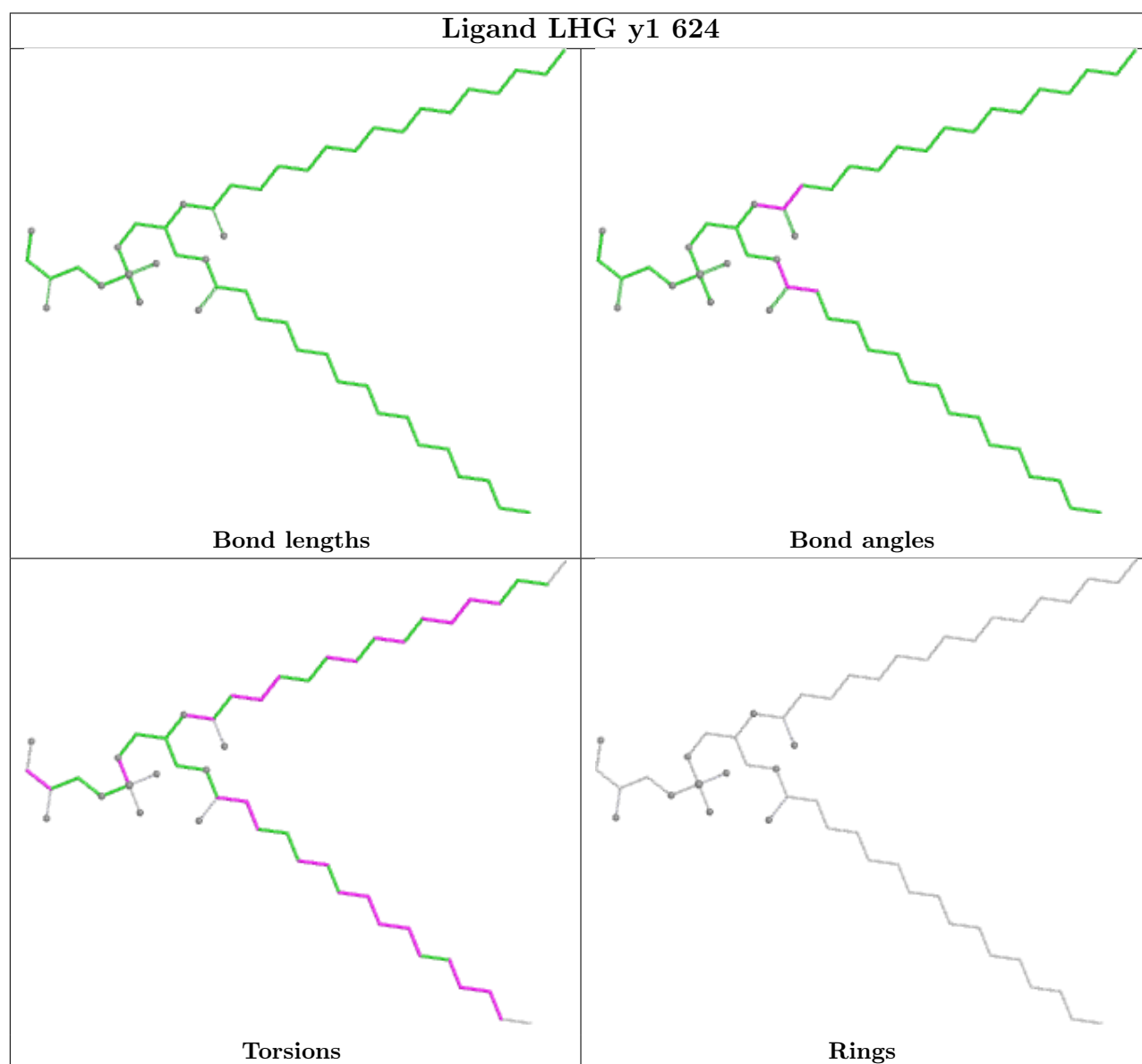
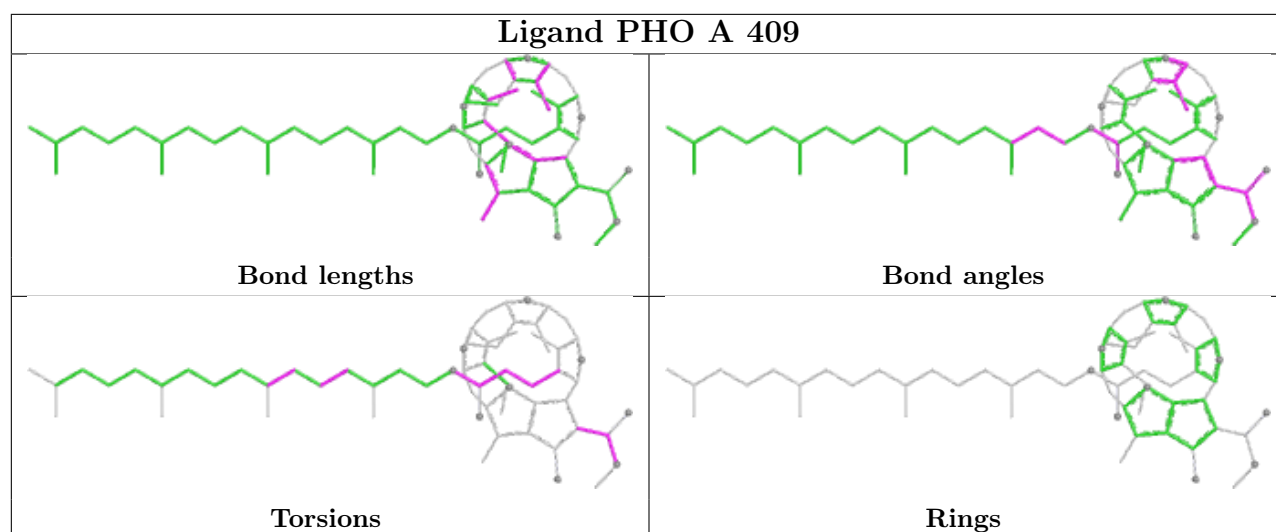
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

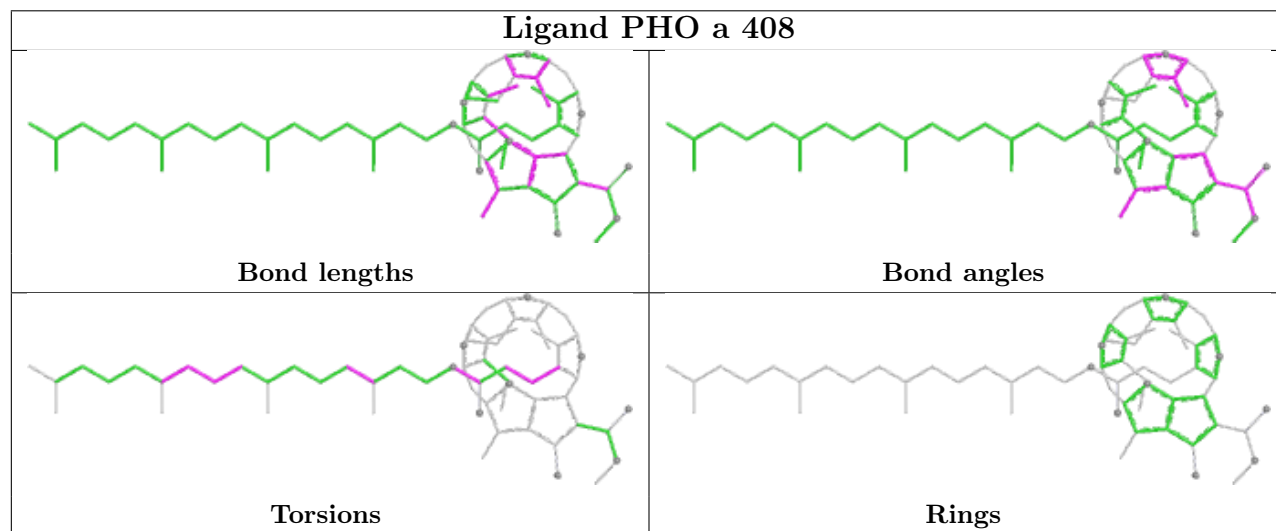
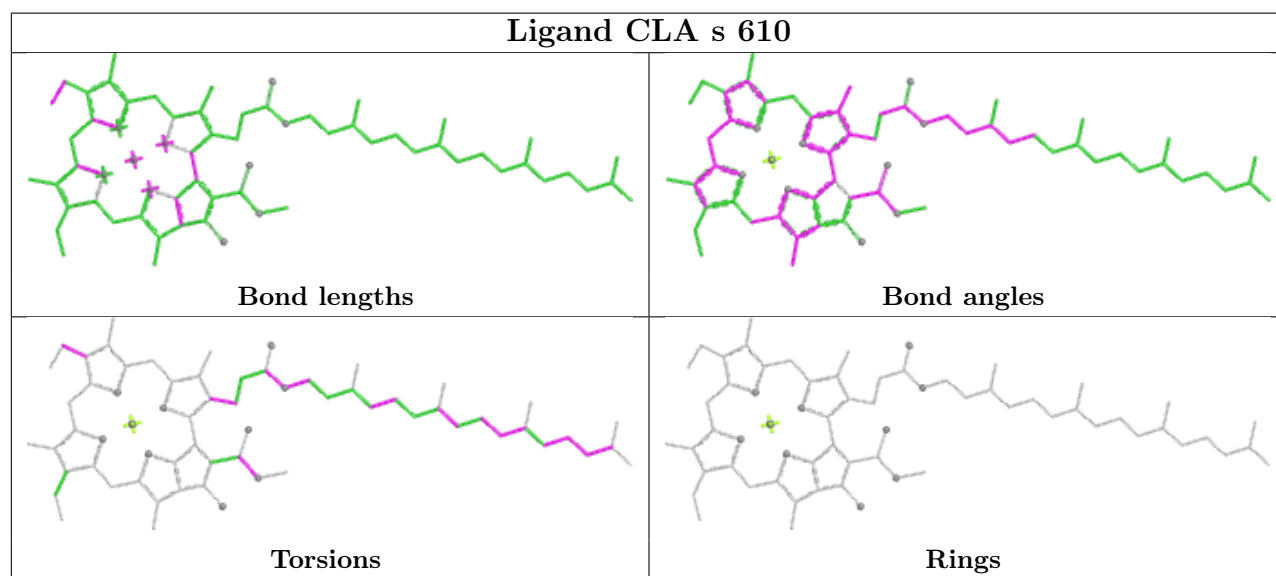
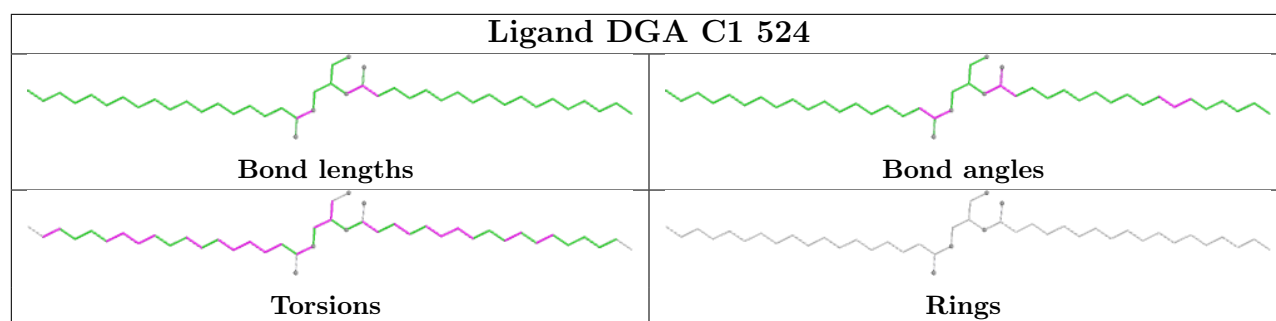
Ligand CLA c1 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

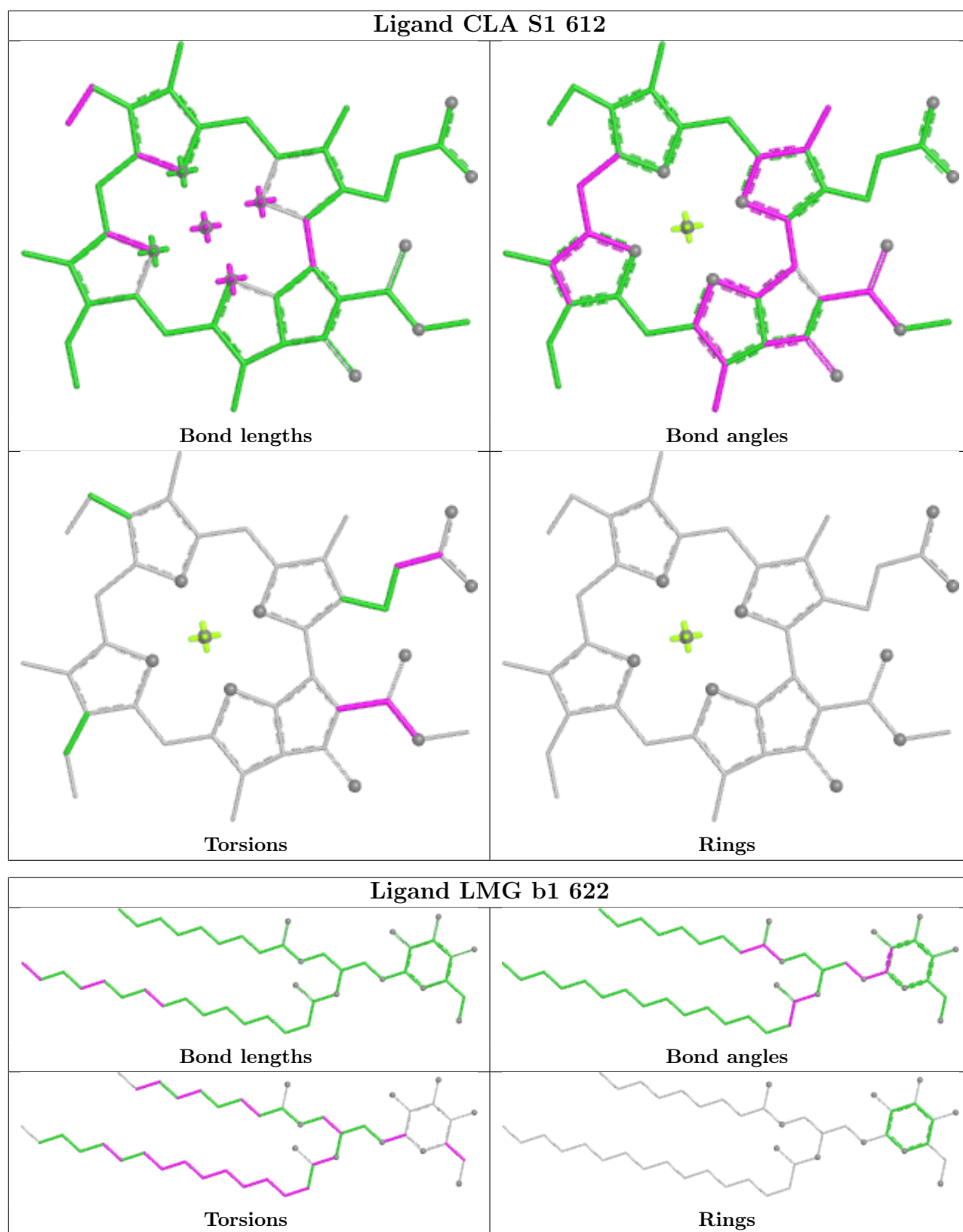
Ligand LMG h1 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

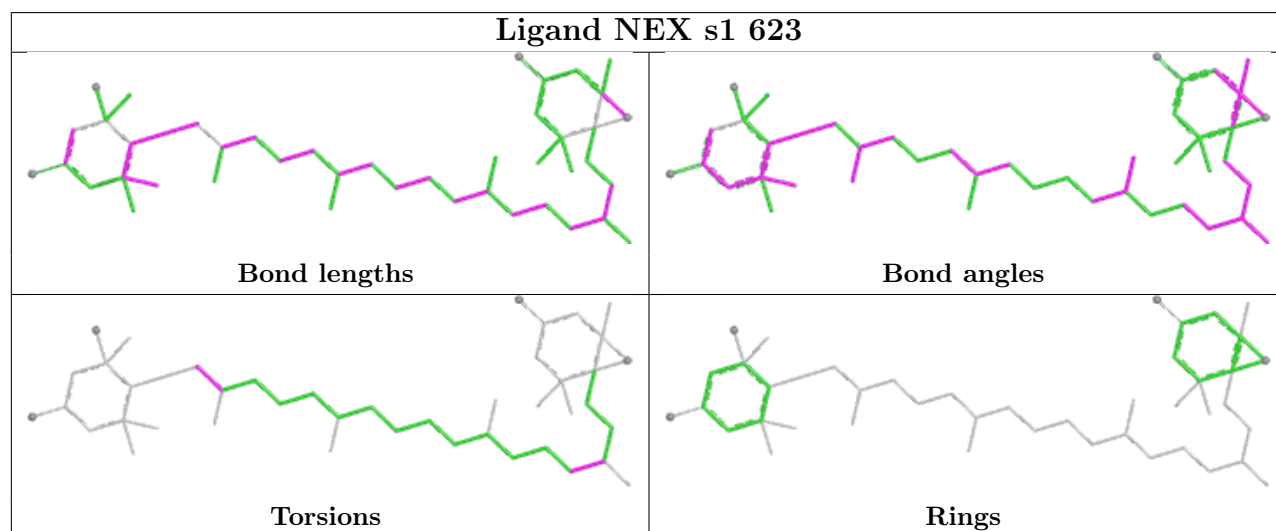
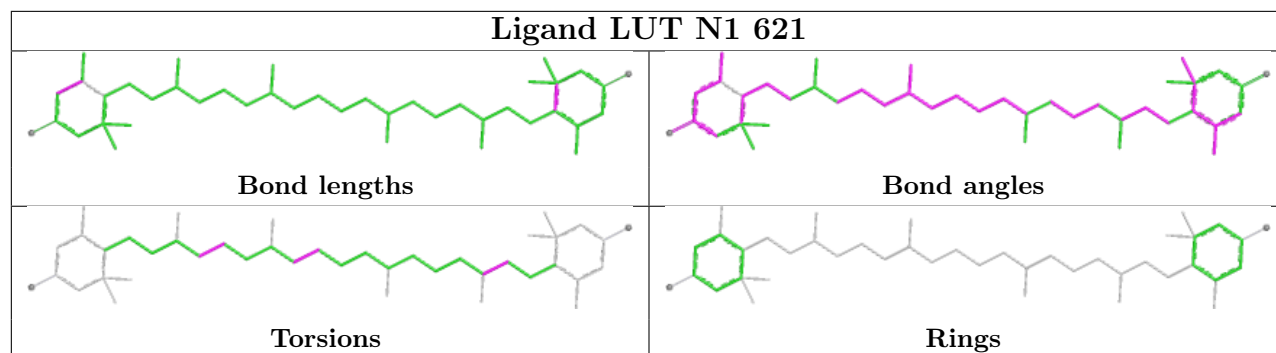


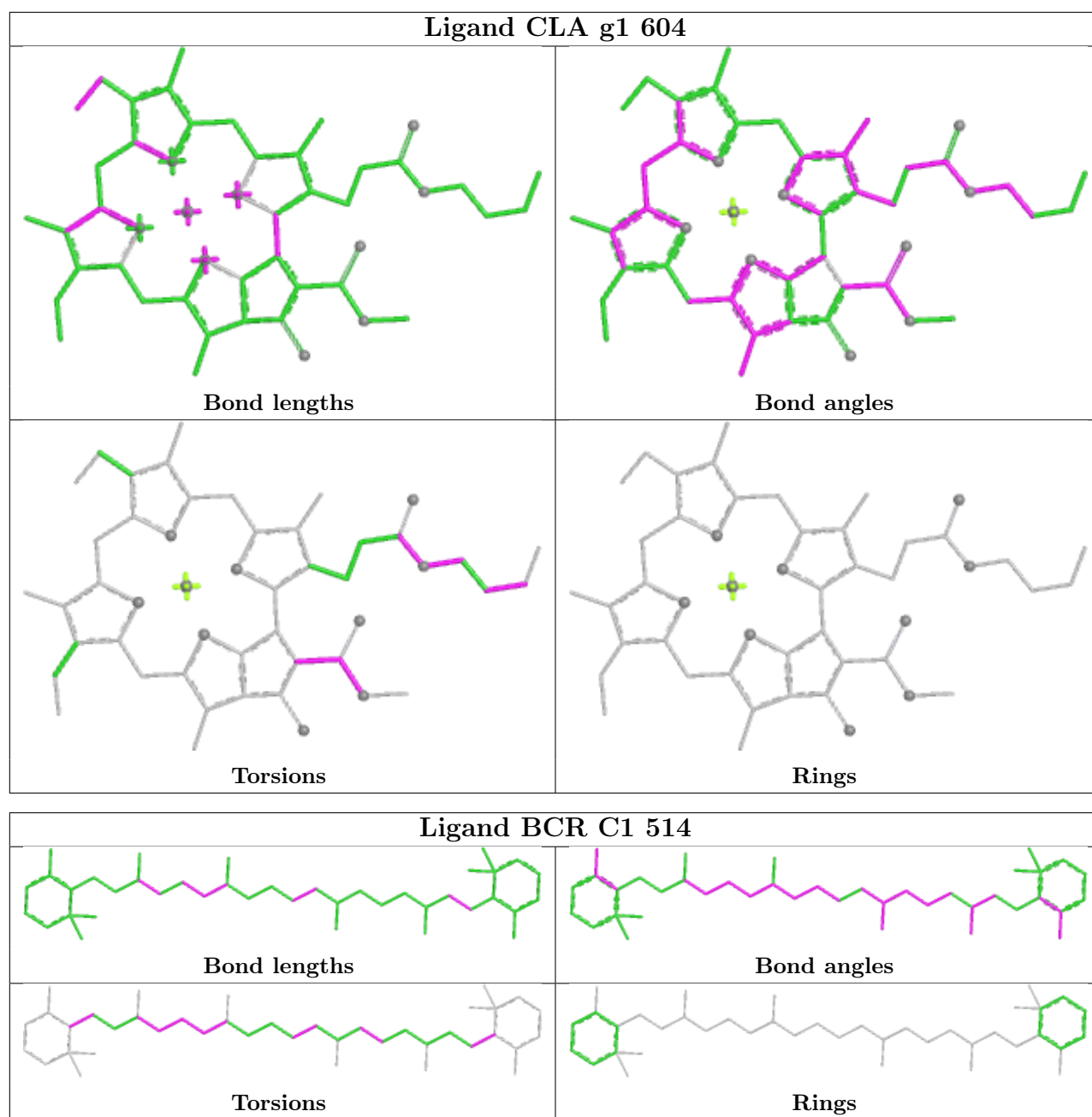




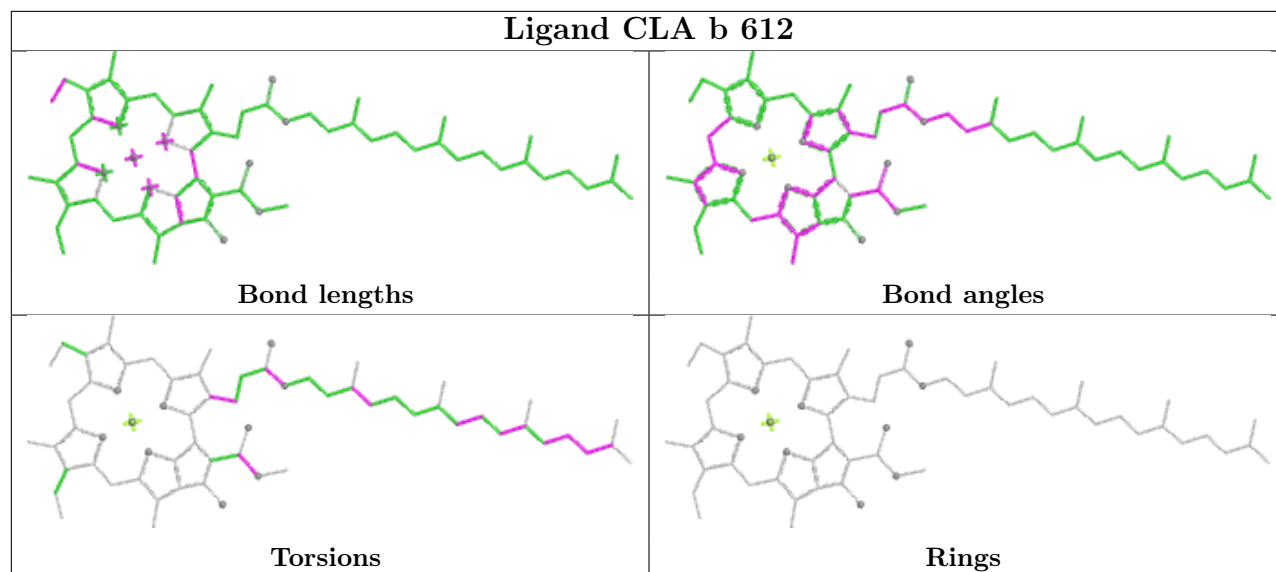




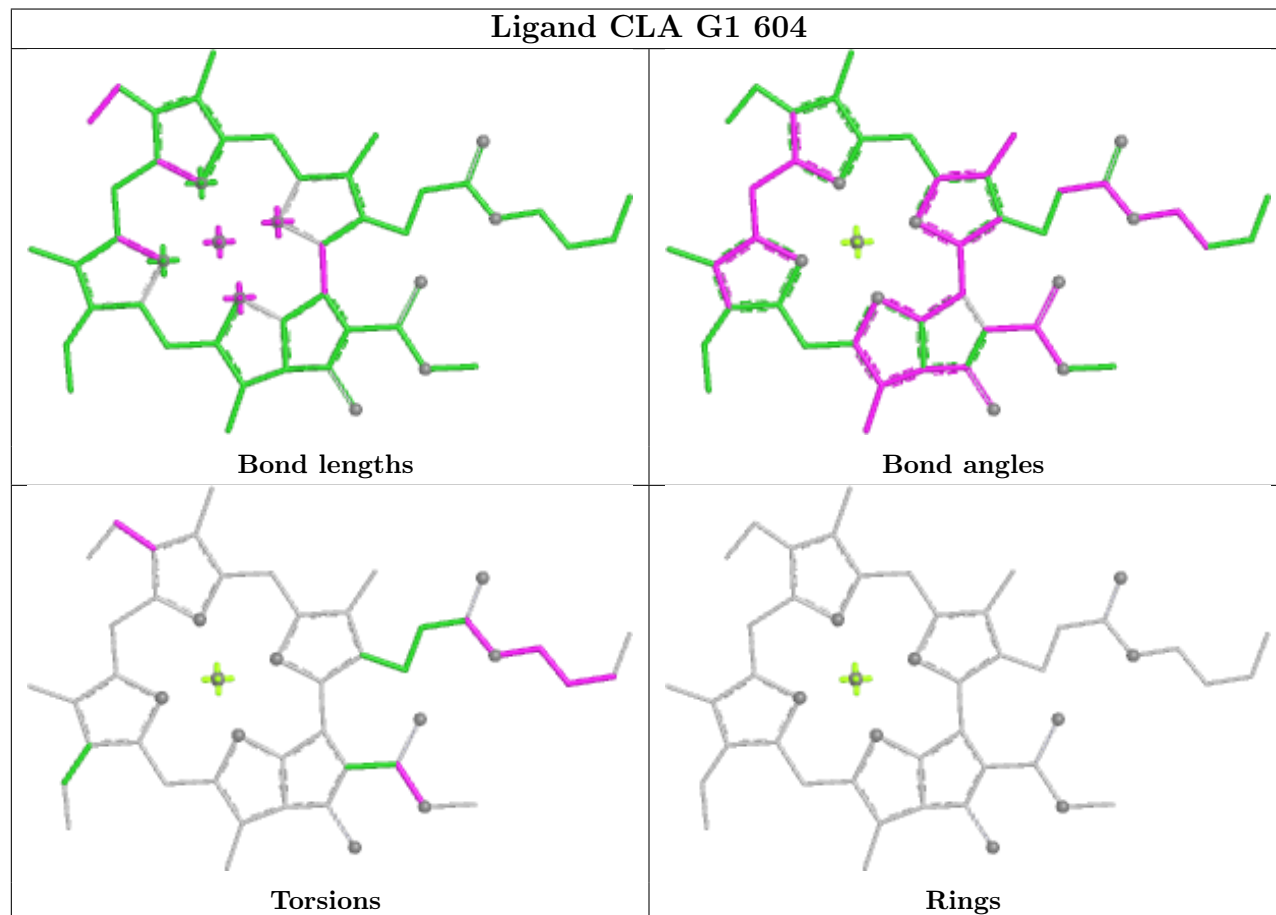


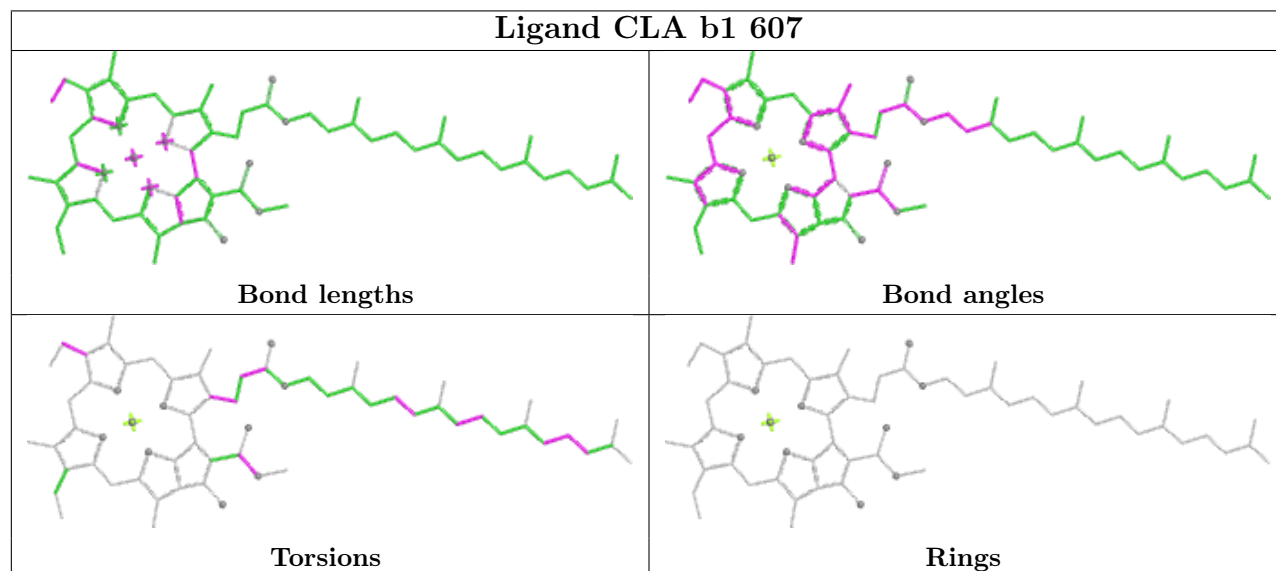
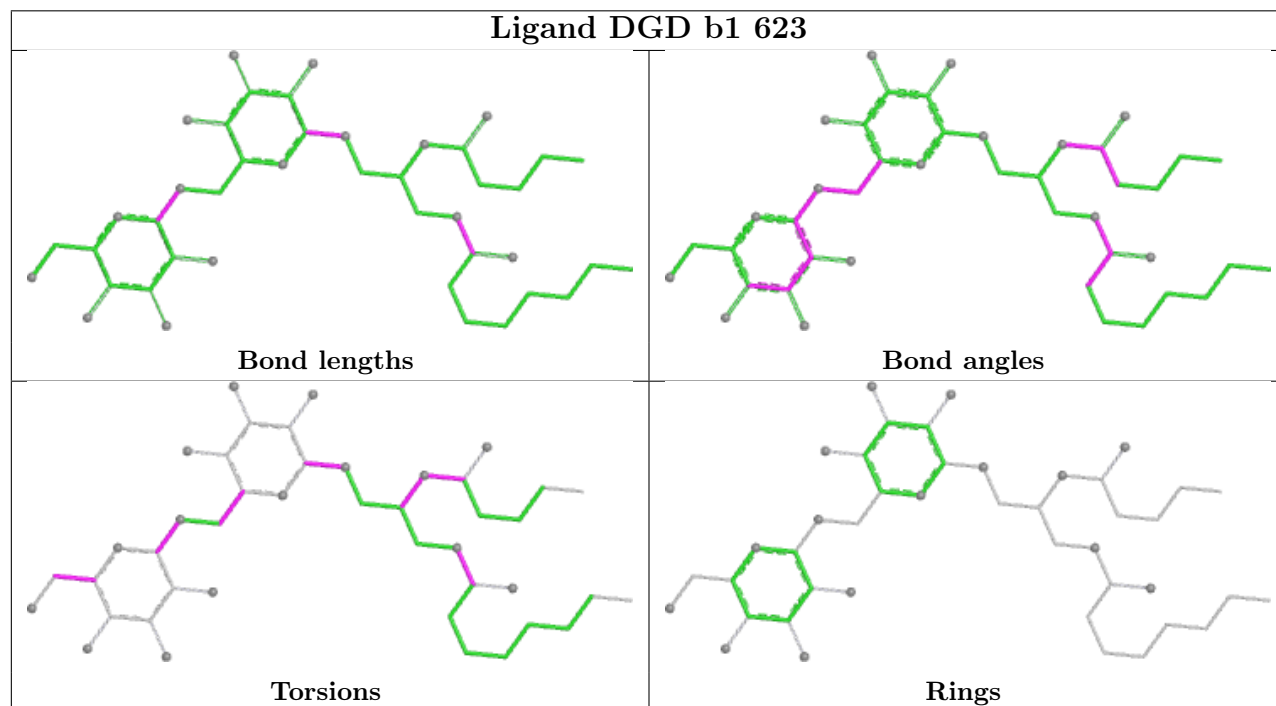
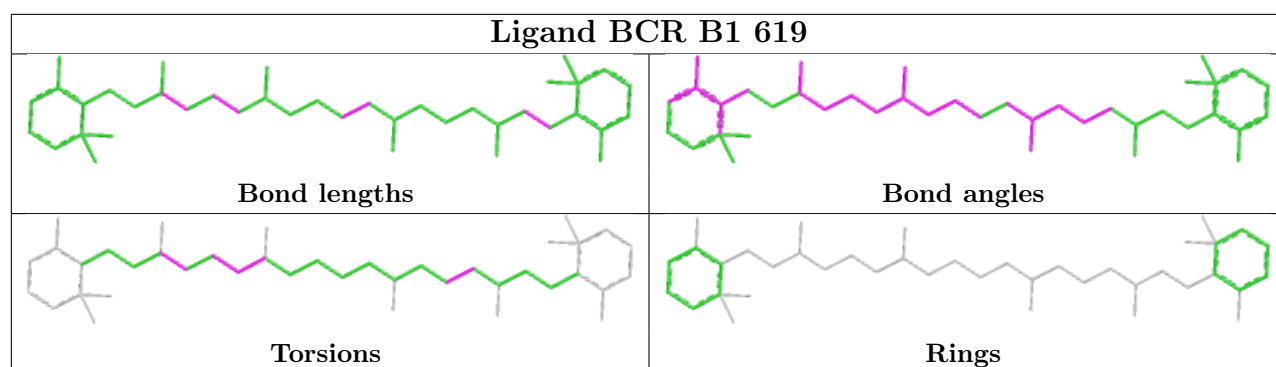


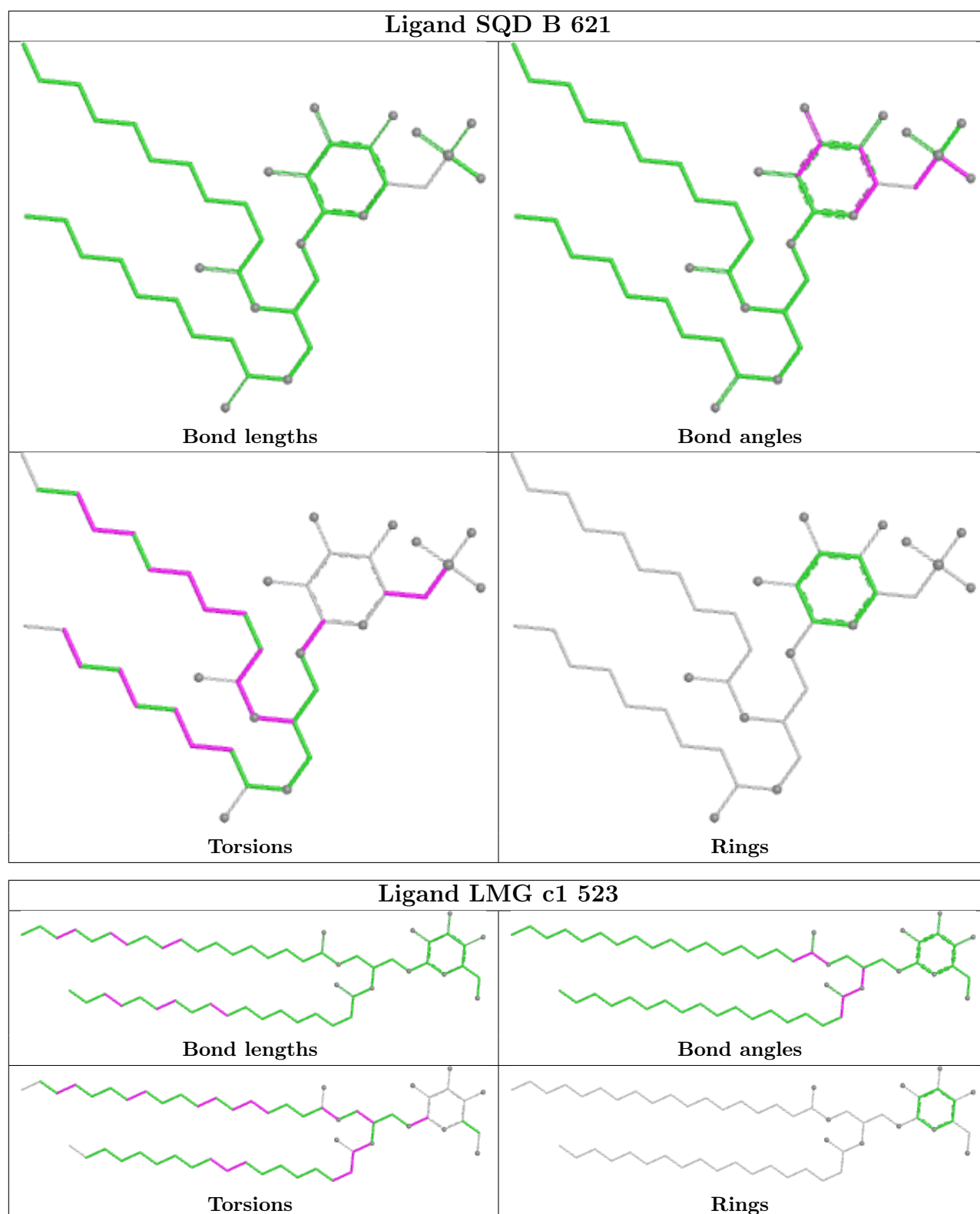
Ligand CLA b 612

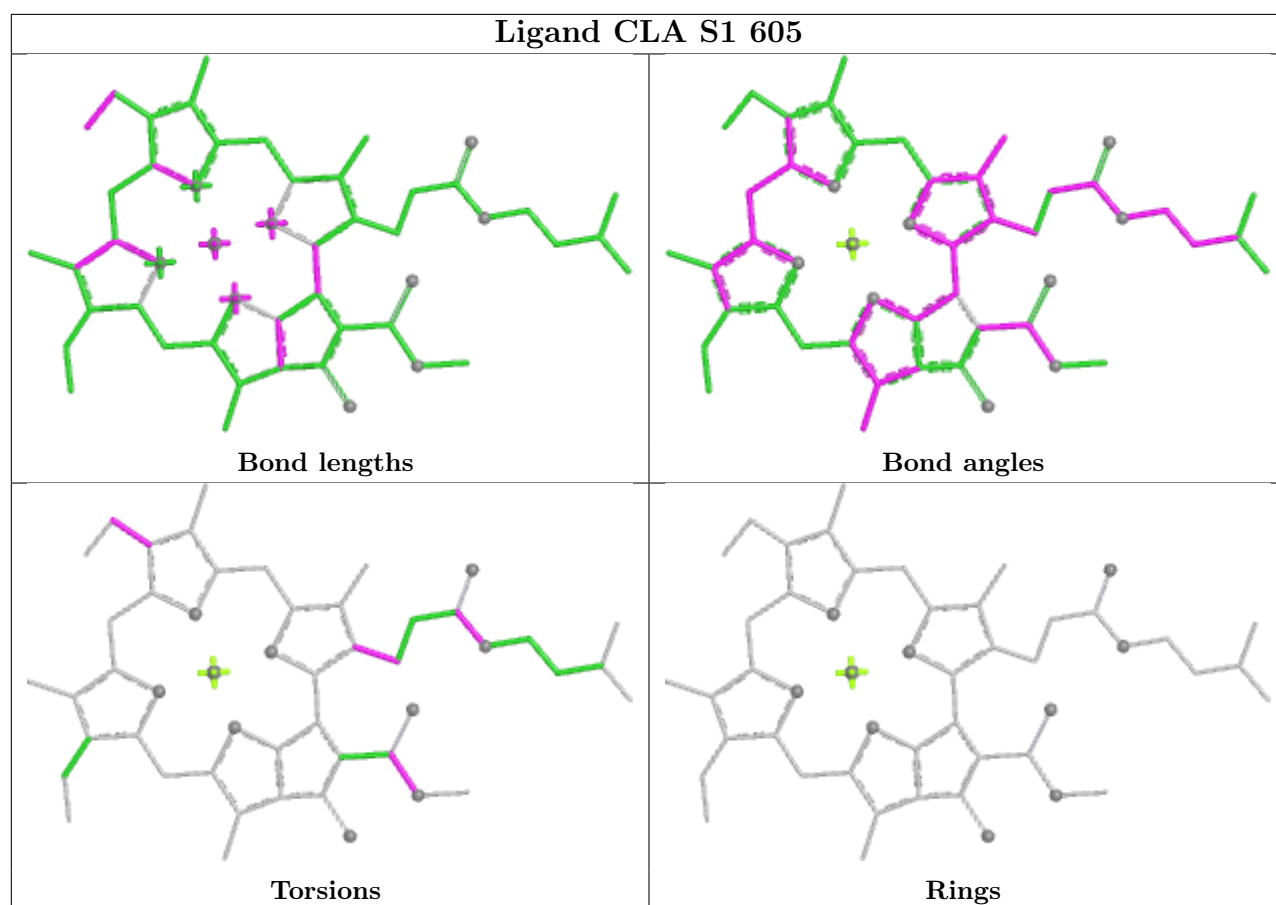


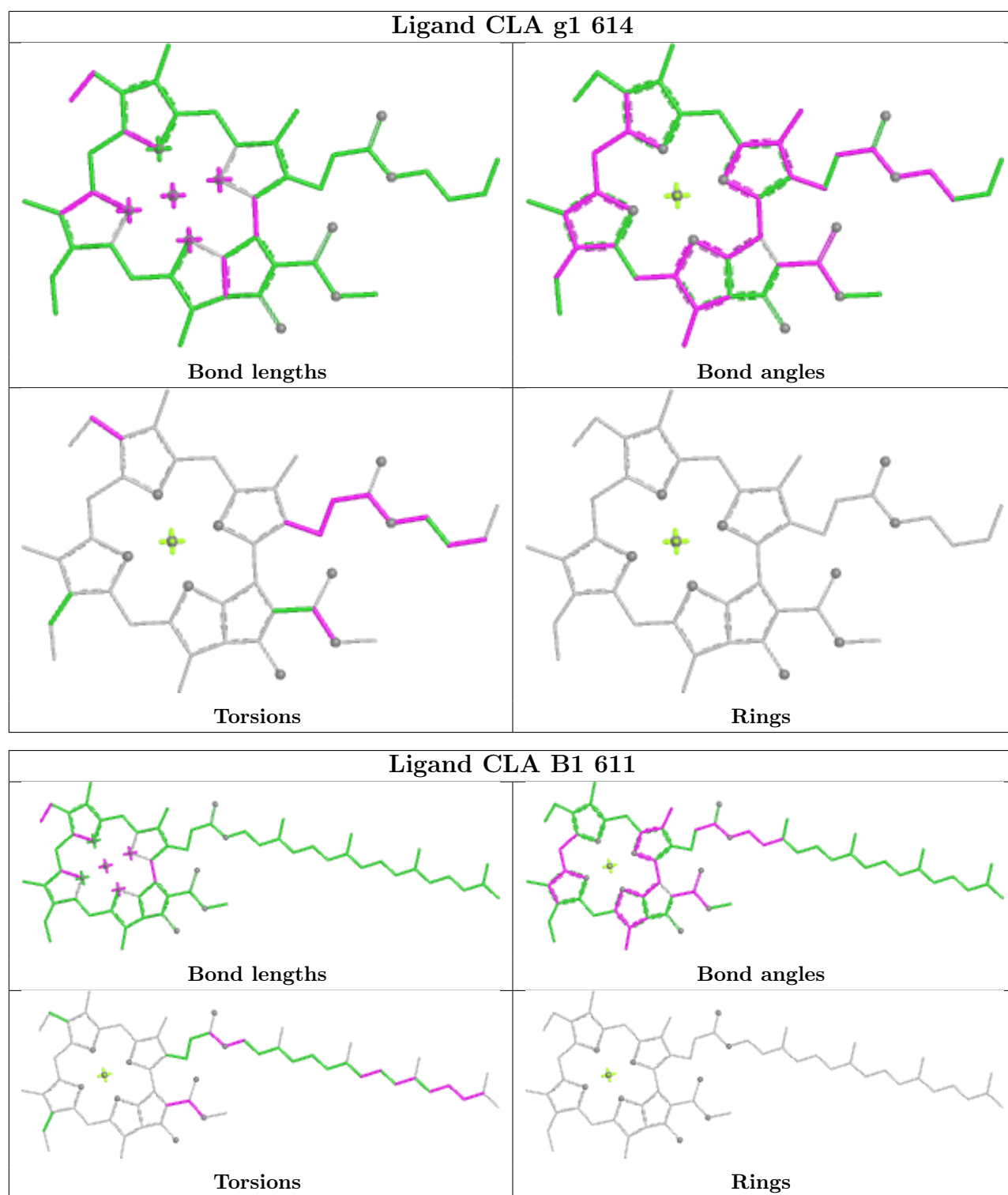
Ligand CLA G1 604

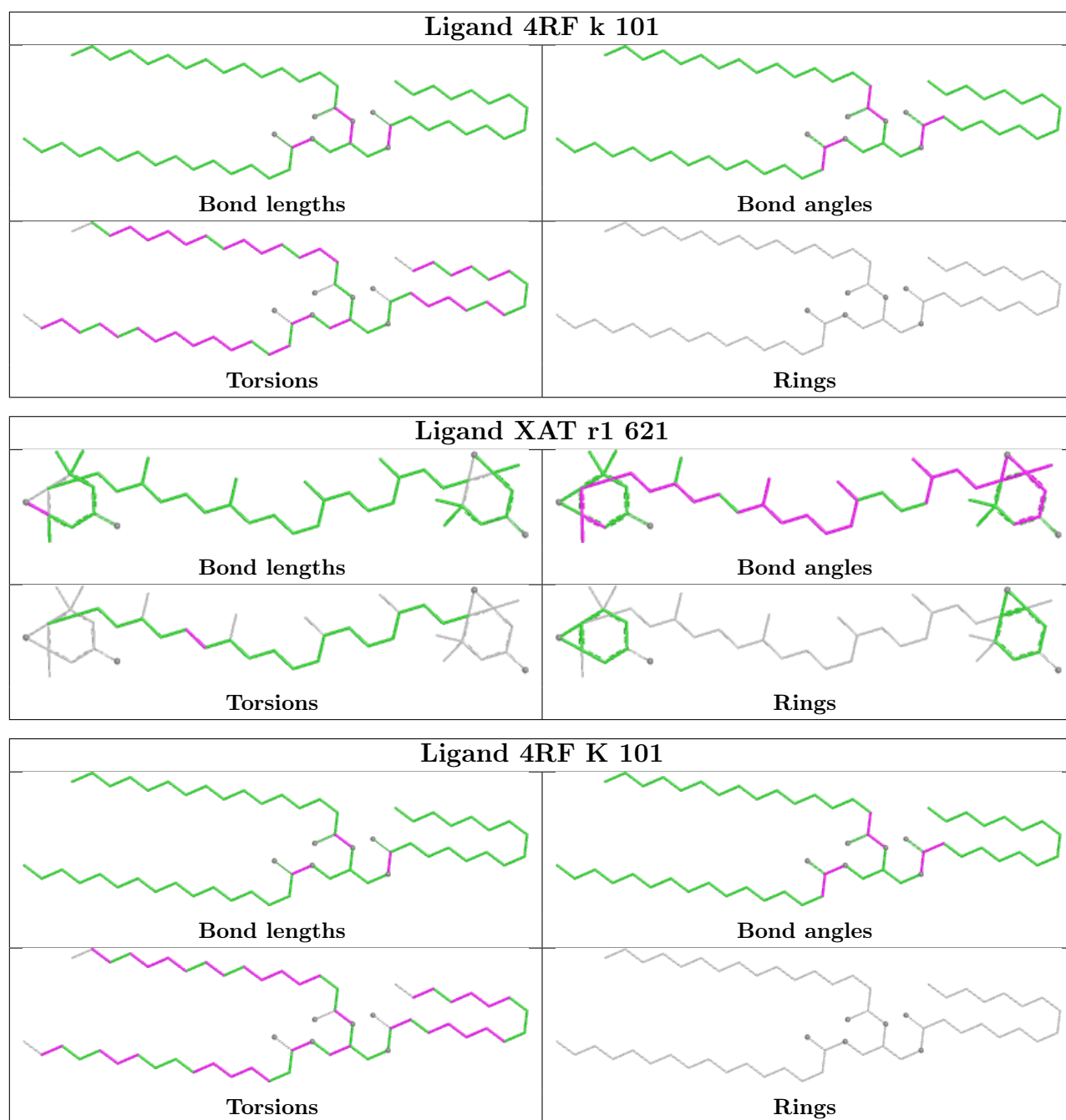




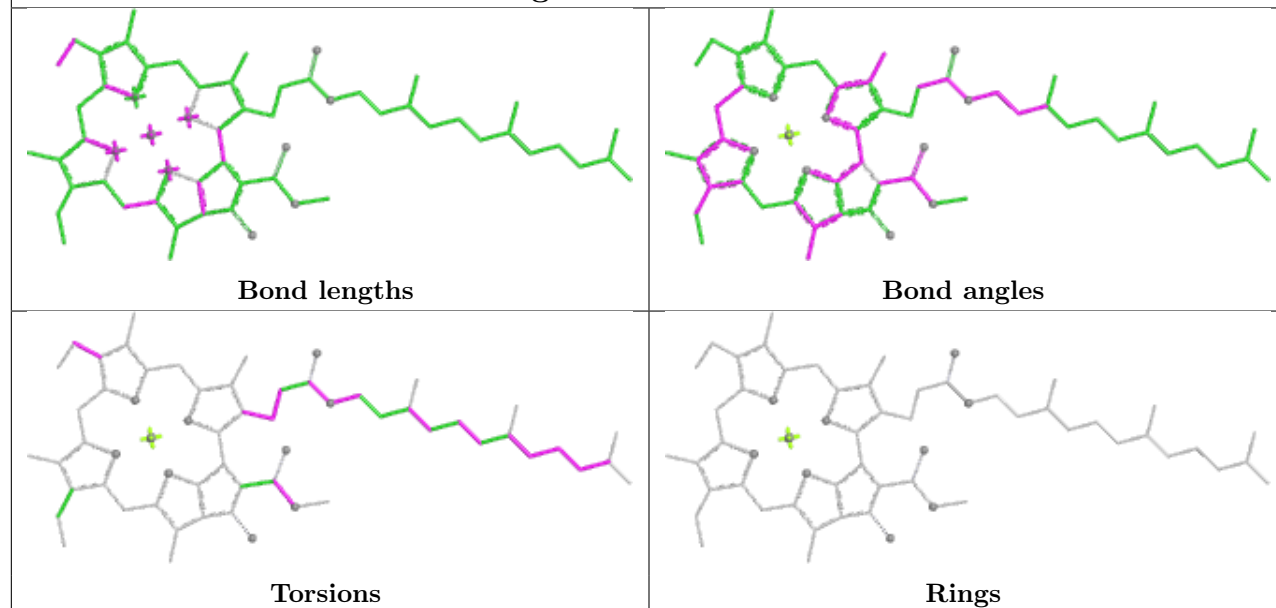




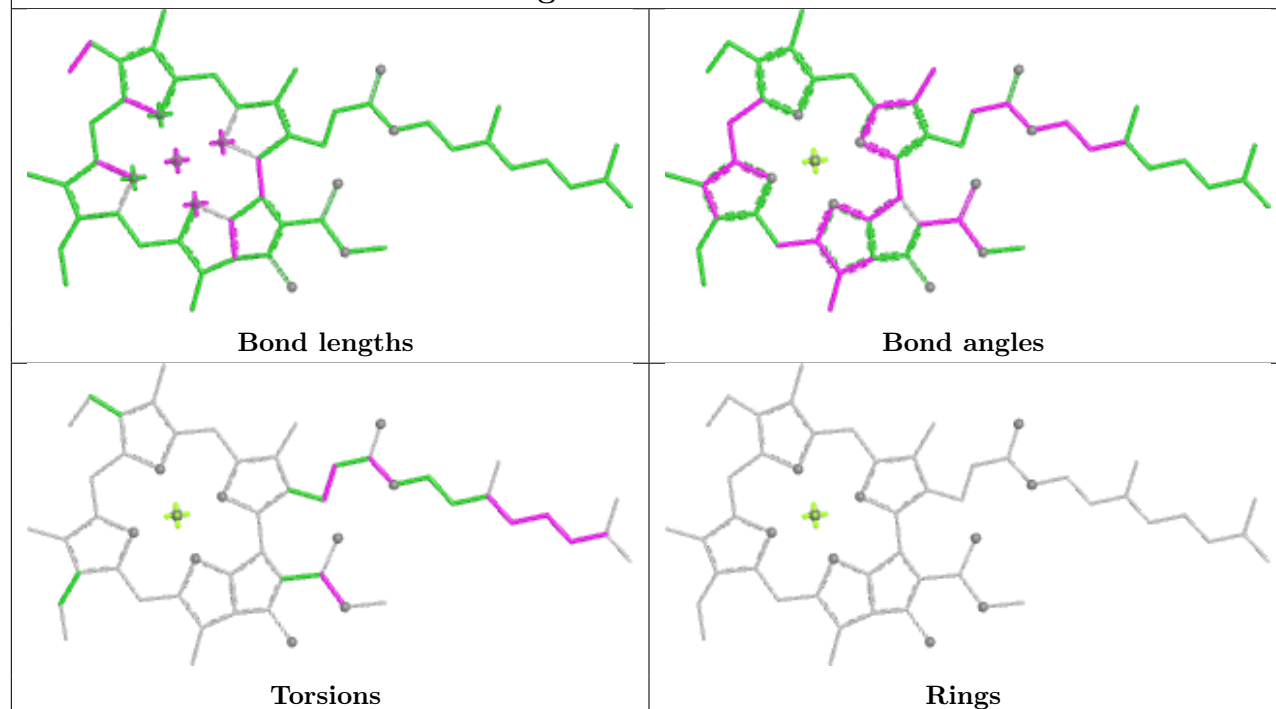




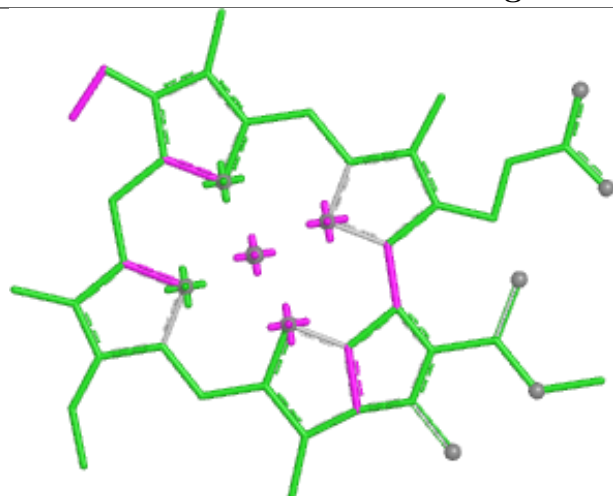
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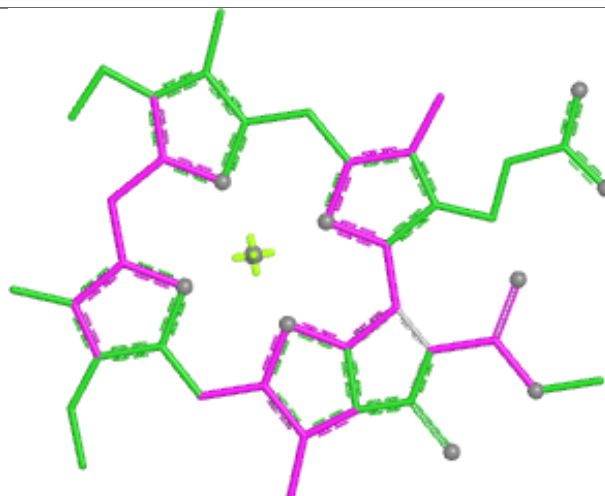
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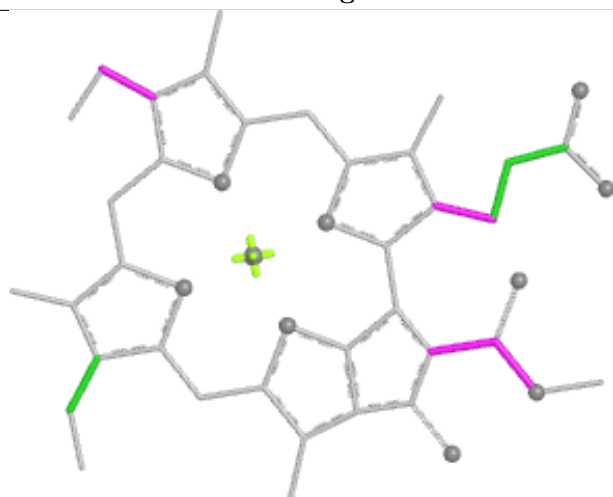
Ligand CLA N1 612



Bond lengths



Bond angles

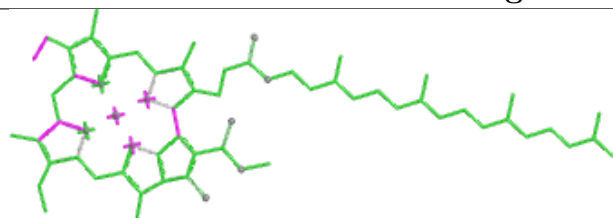


Torsions

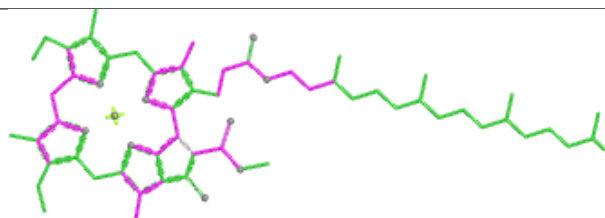


Rings

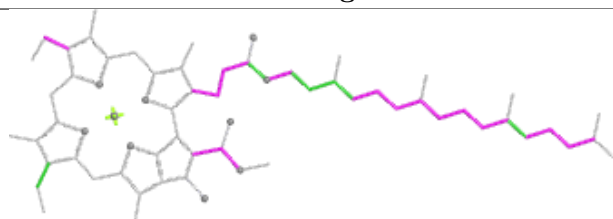
Ligand CLA B1 602



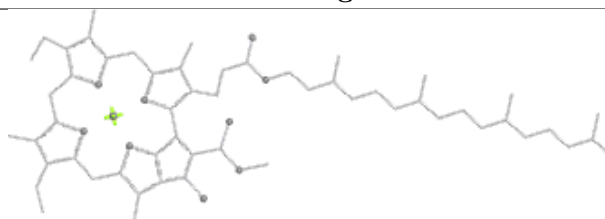
Bond lengths



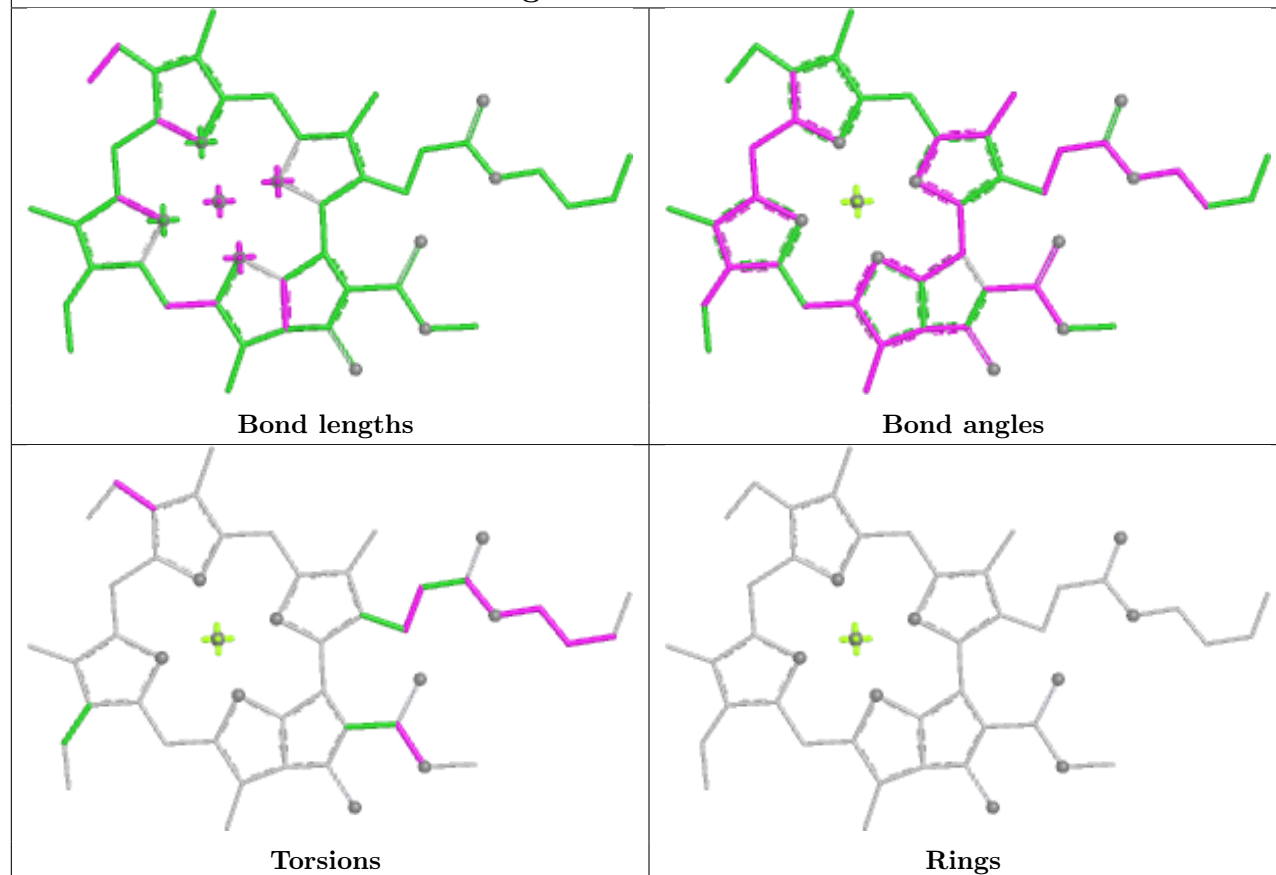
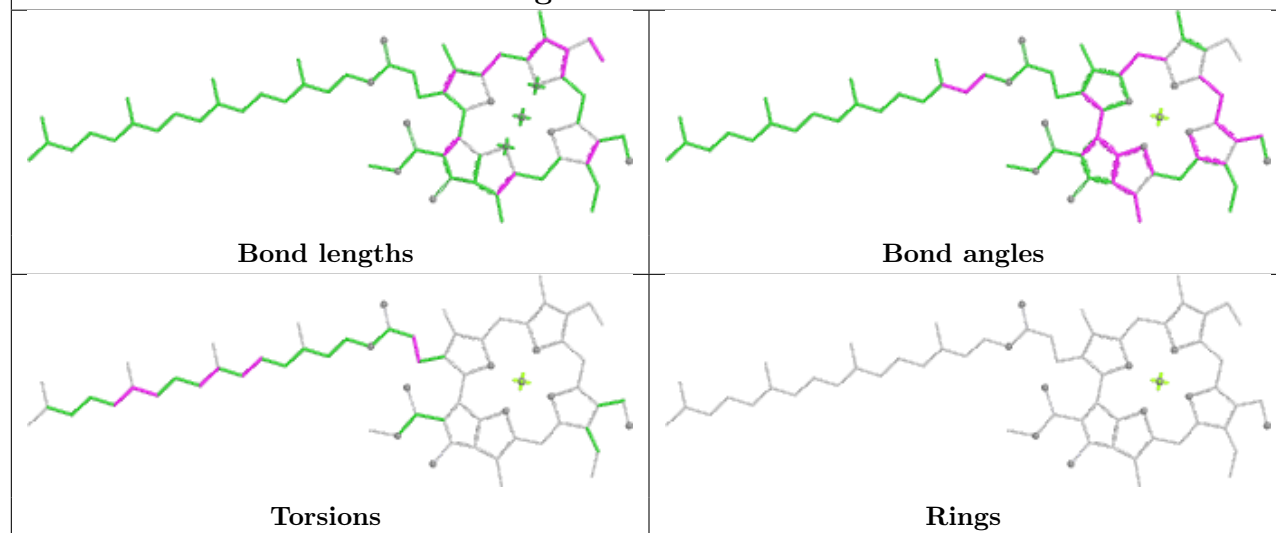
Bond angles

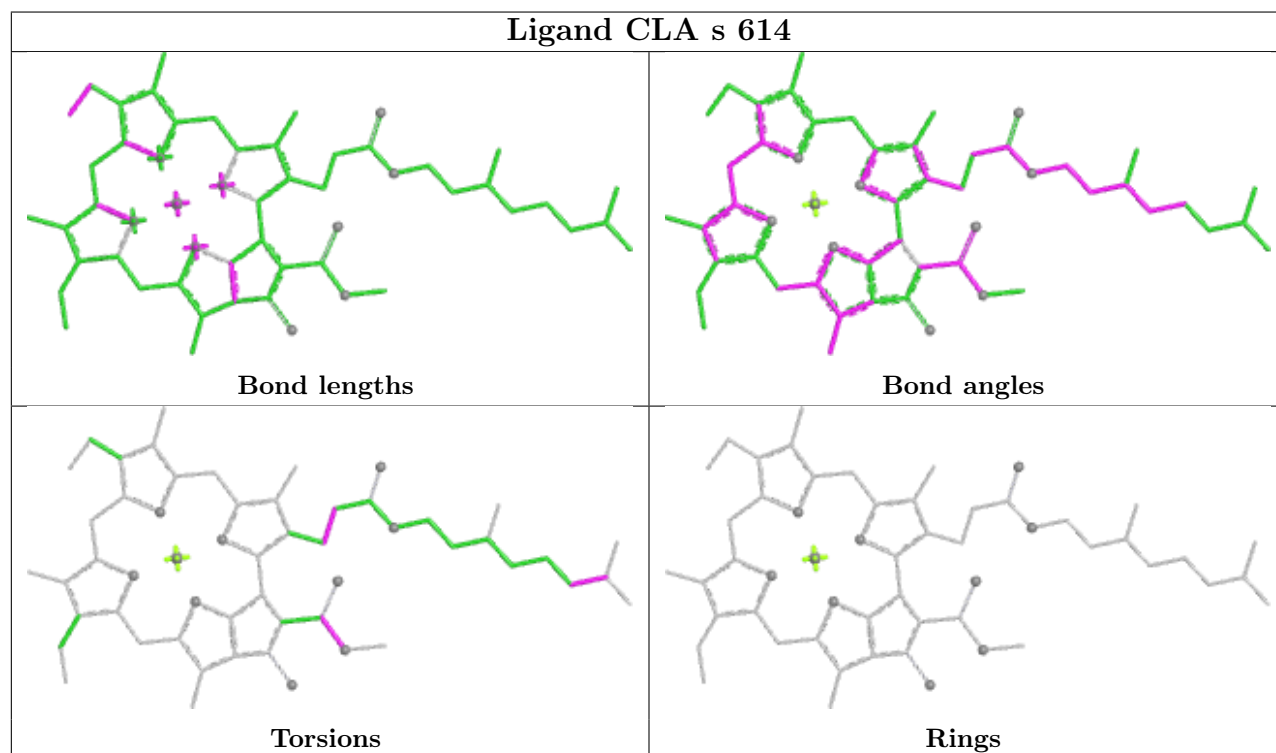
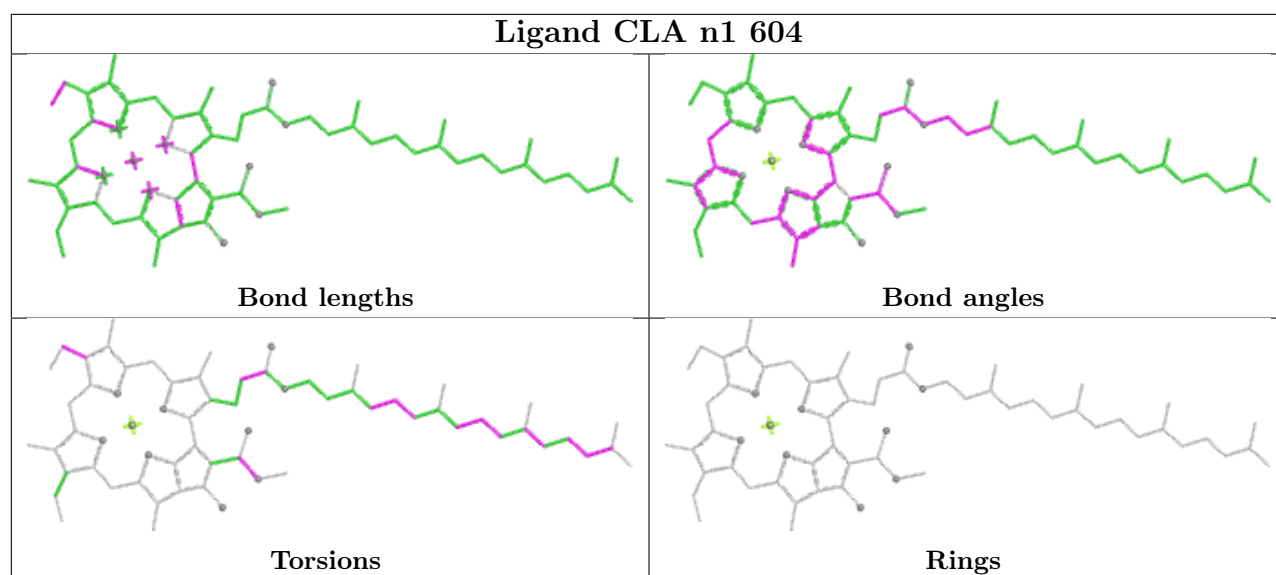


Torsions

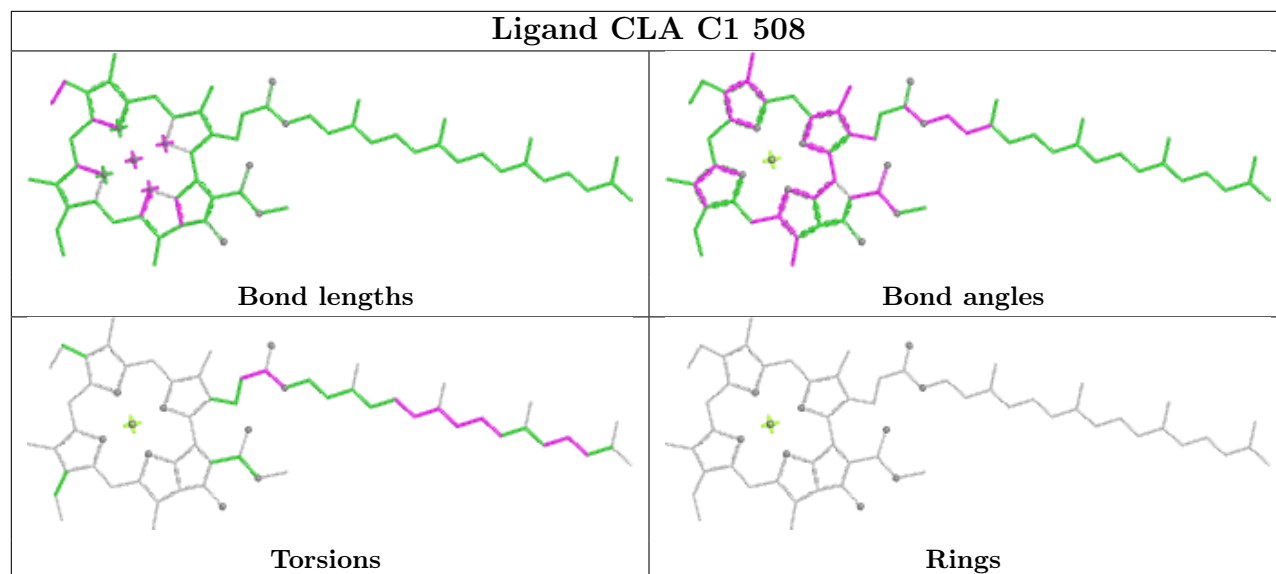


Rings

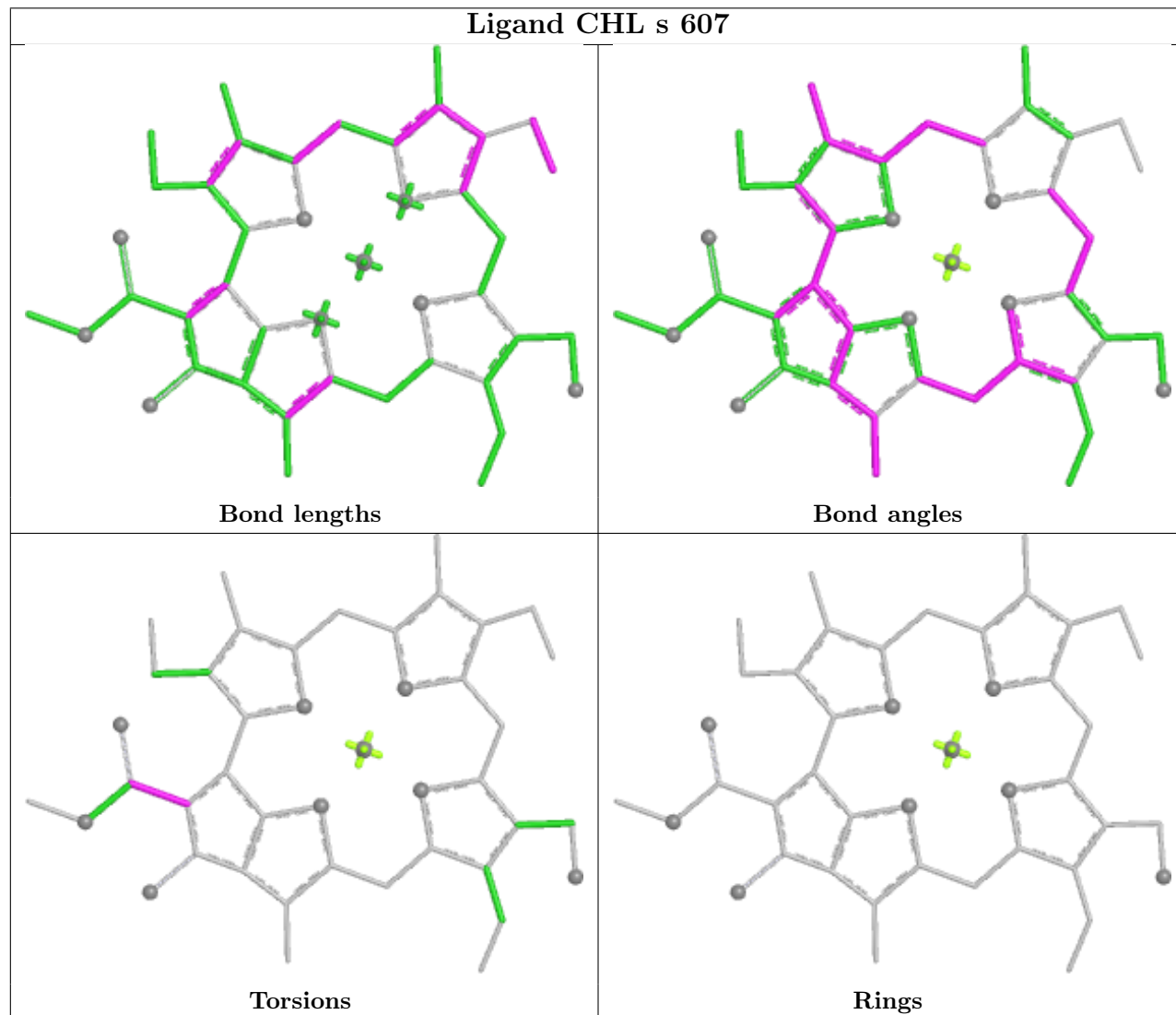
Ligand CLA N1 611**Ligand CHL n 606**

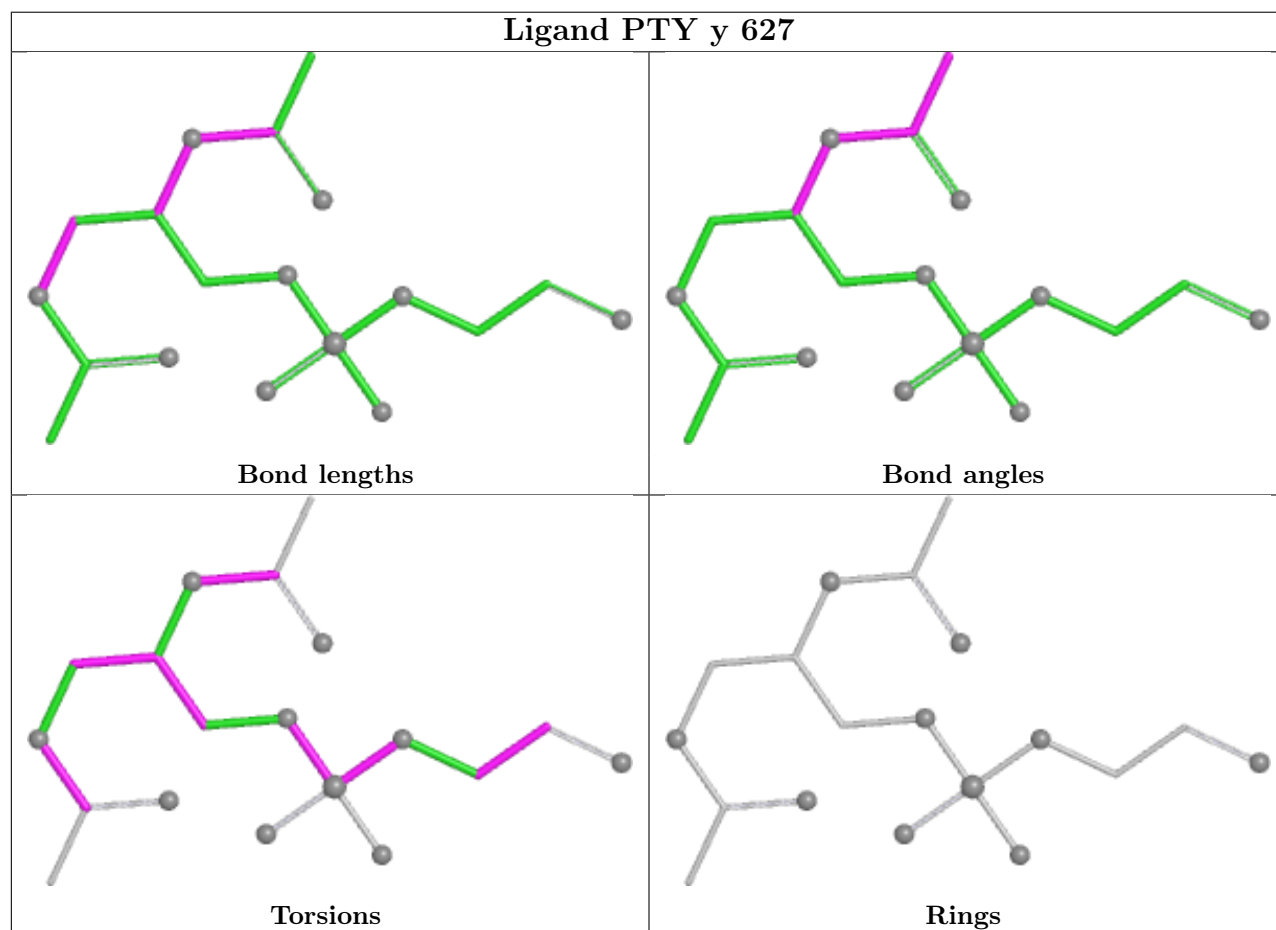
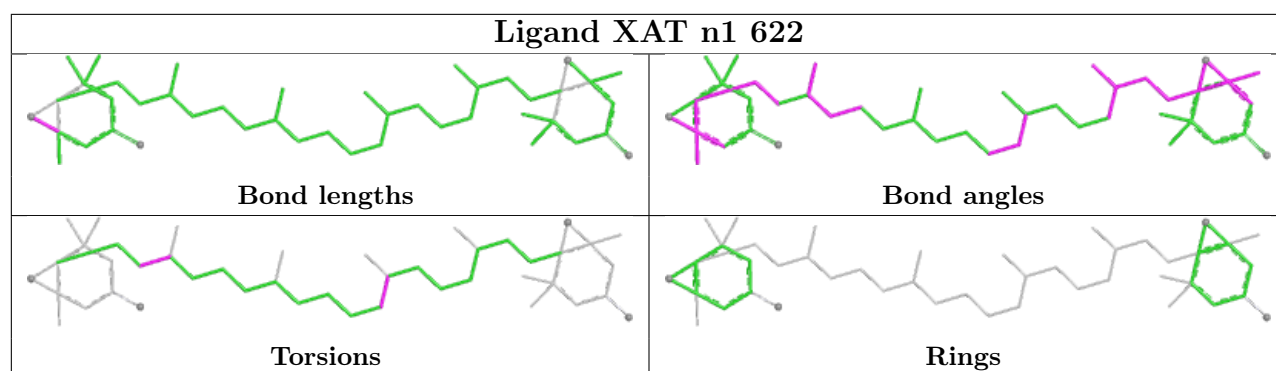


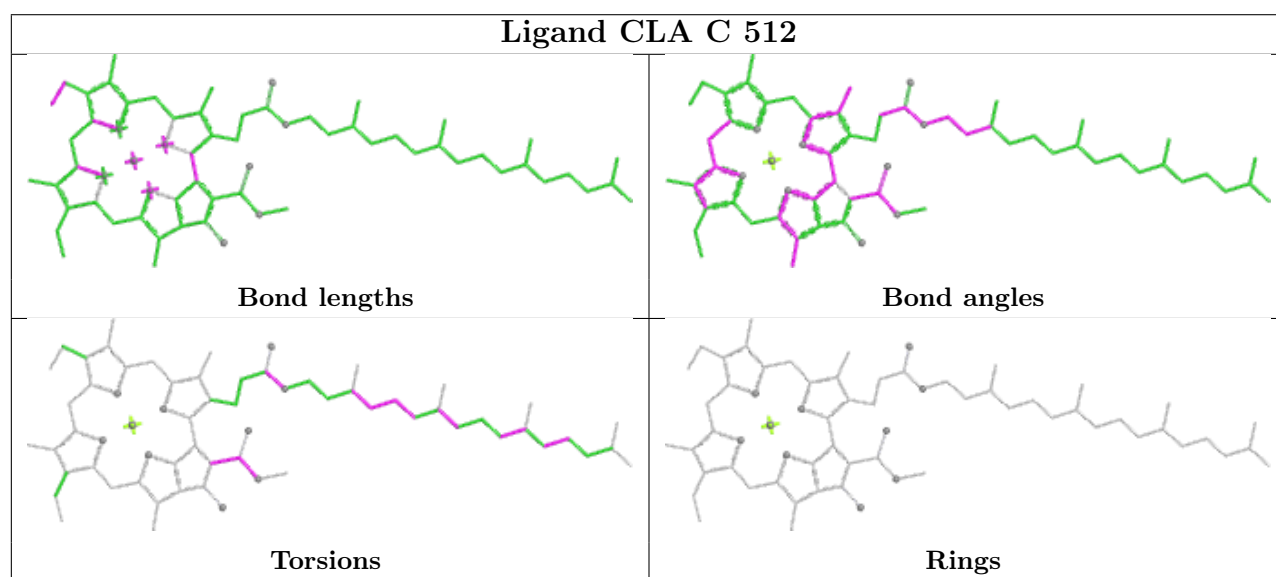
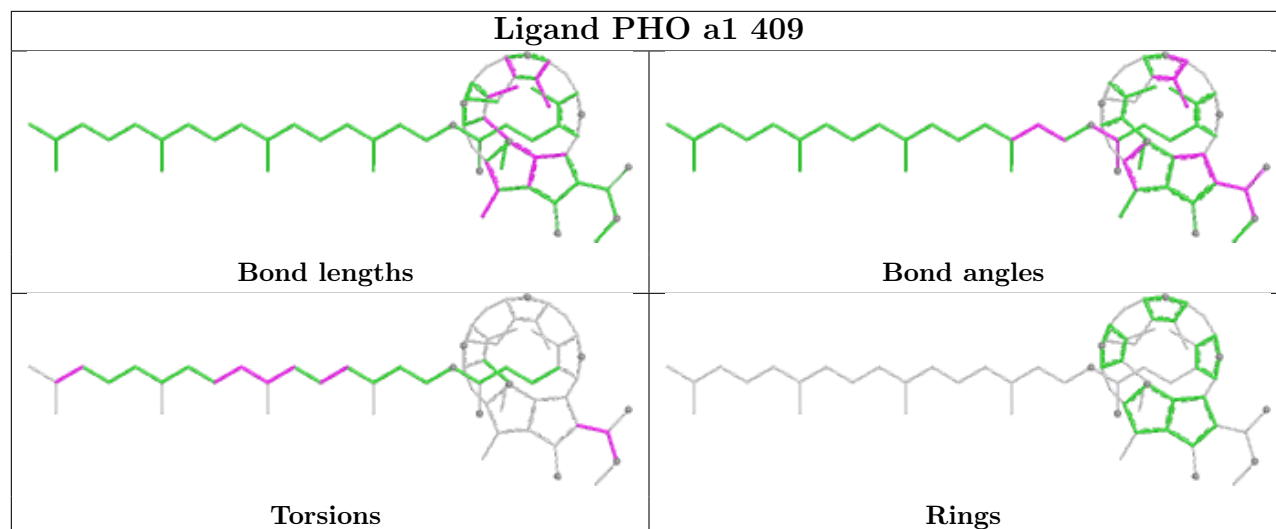
Ligand CLA C1 508

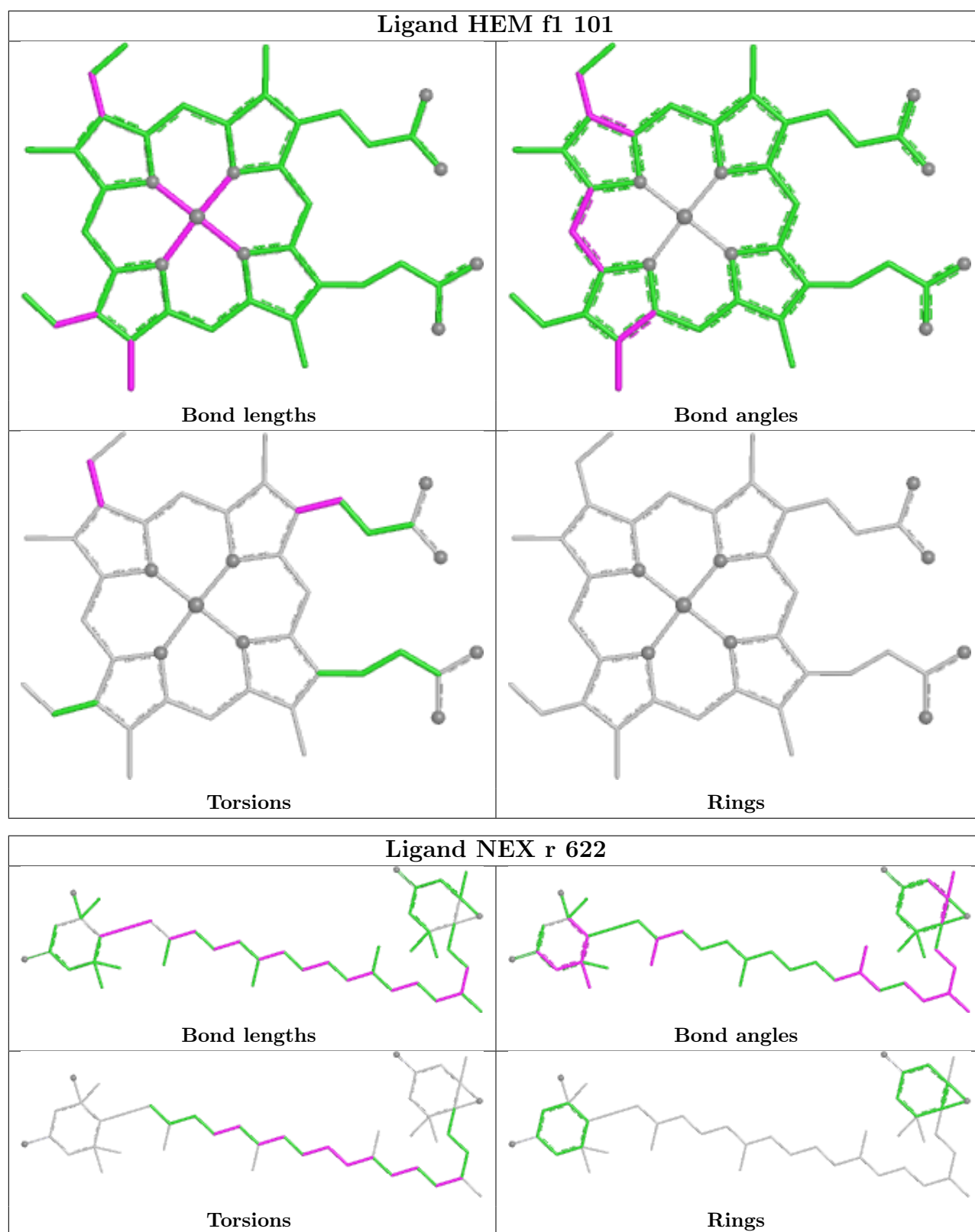


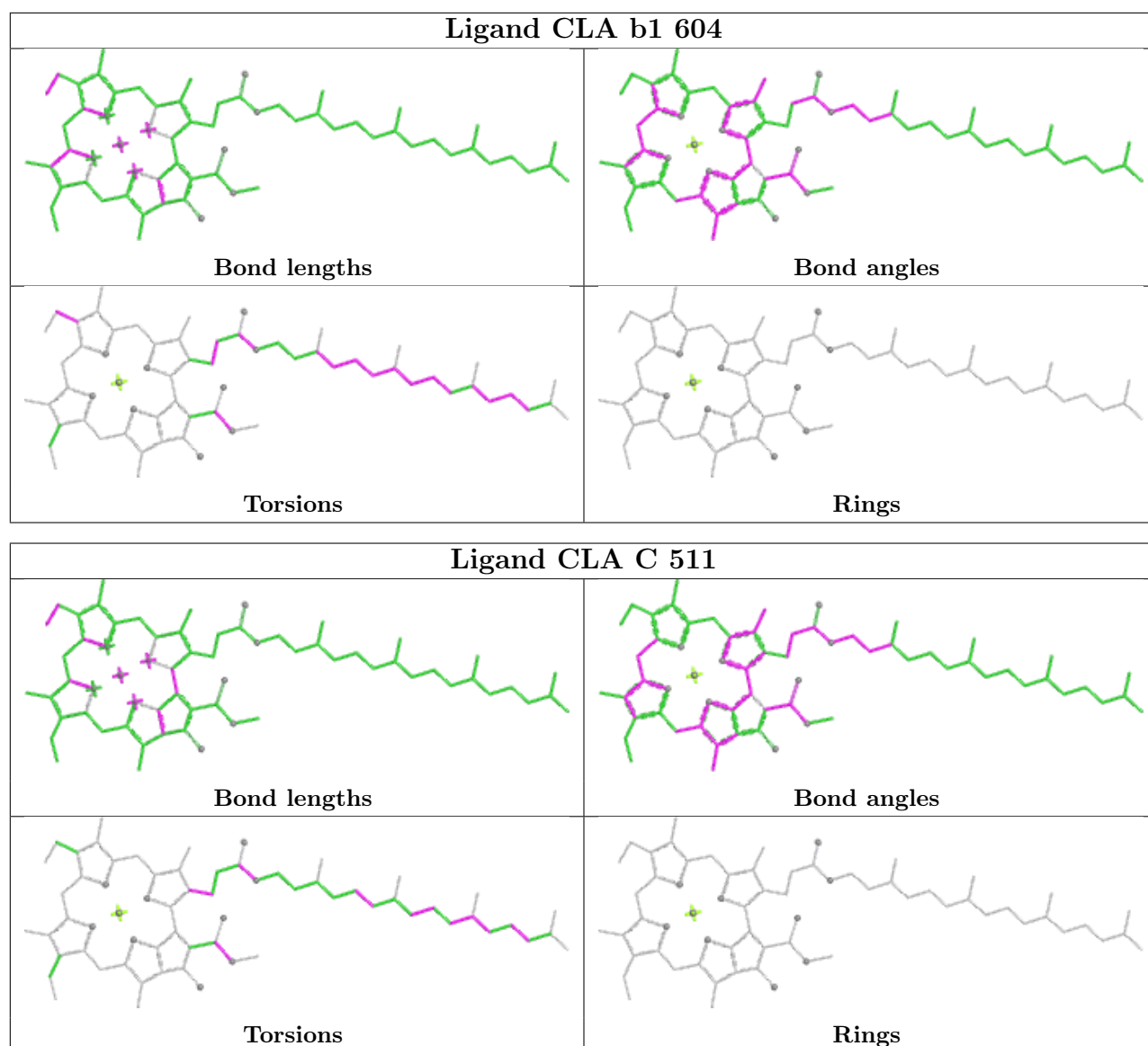
Ligand CHL s 607

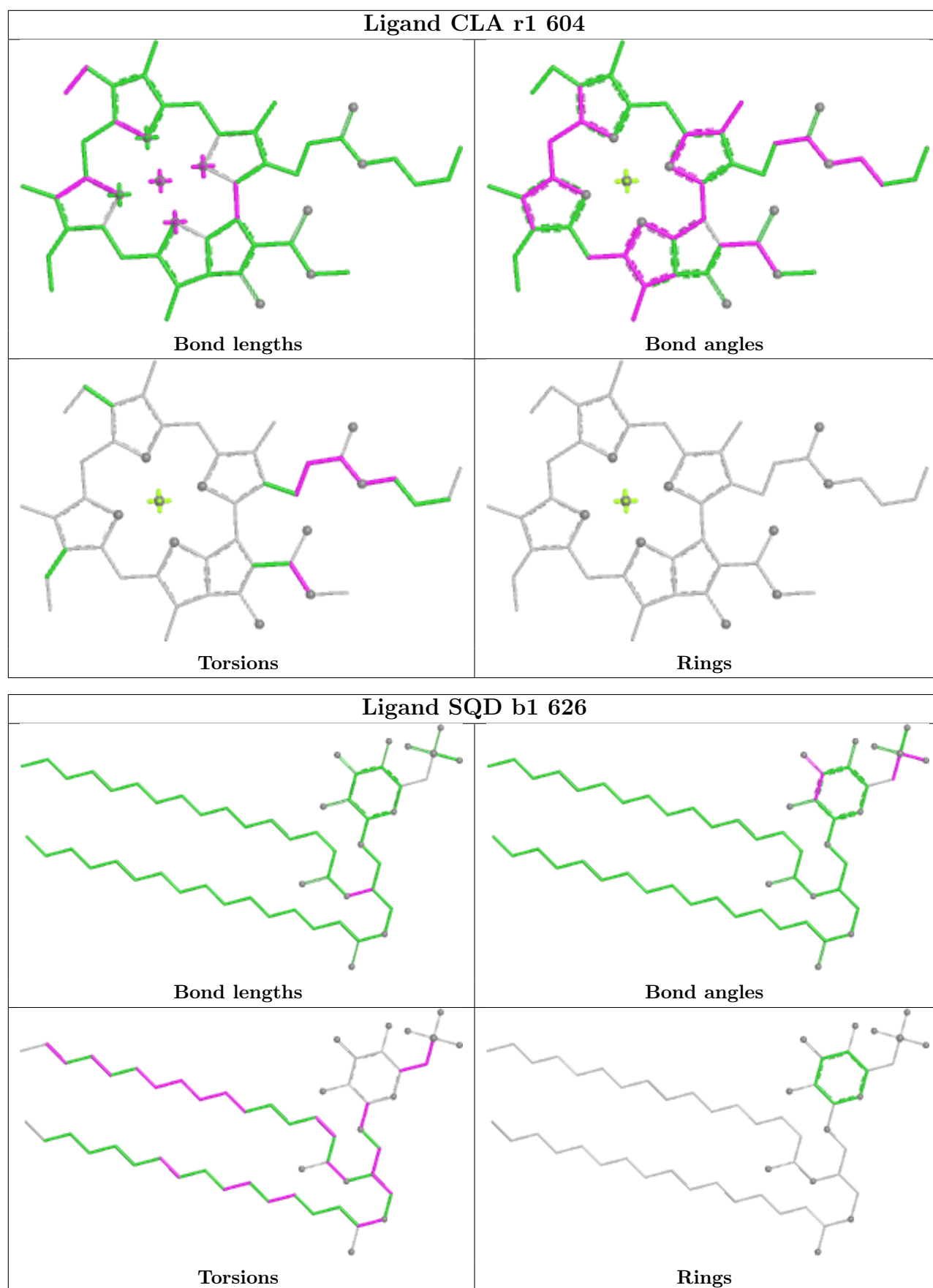


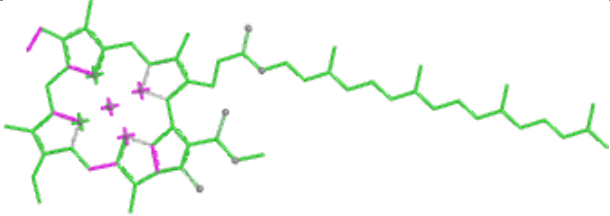
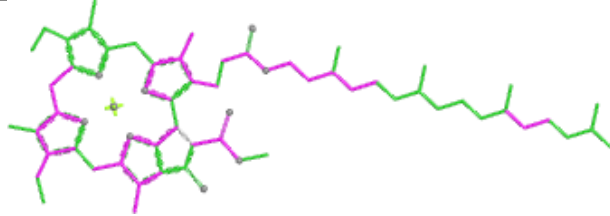
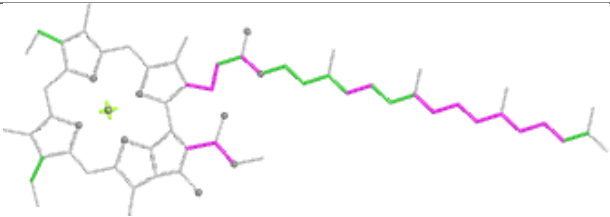
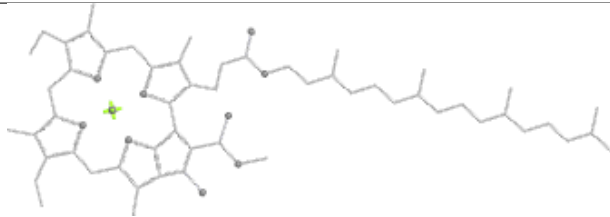
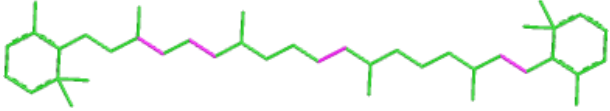
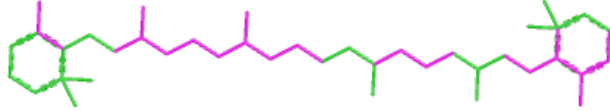
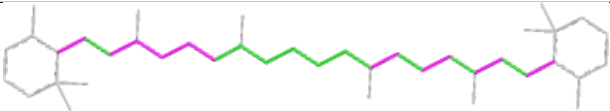
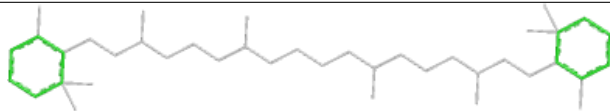
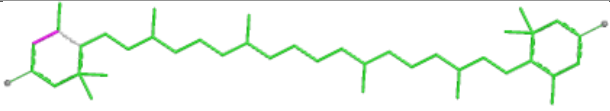
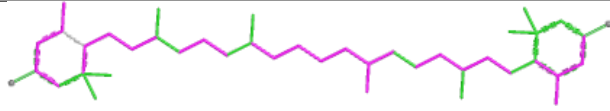
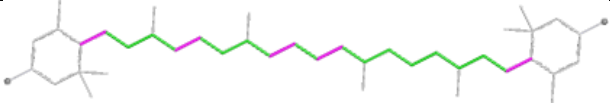
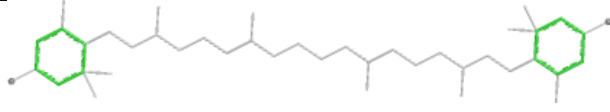


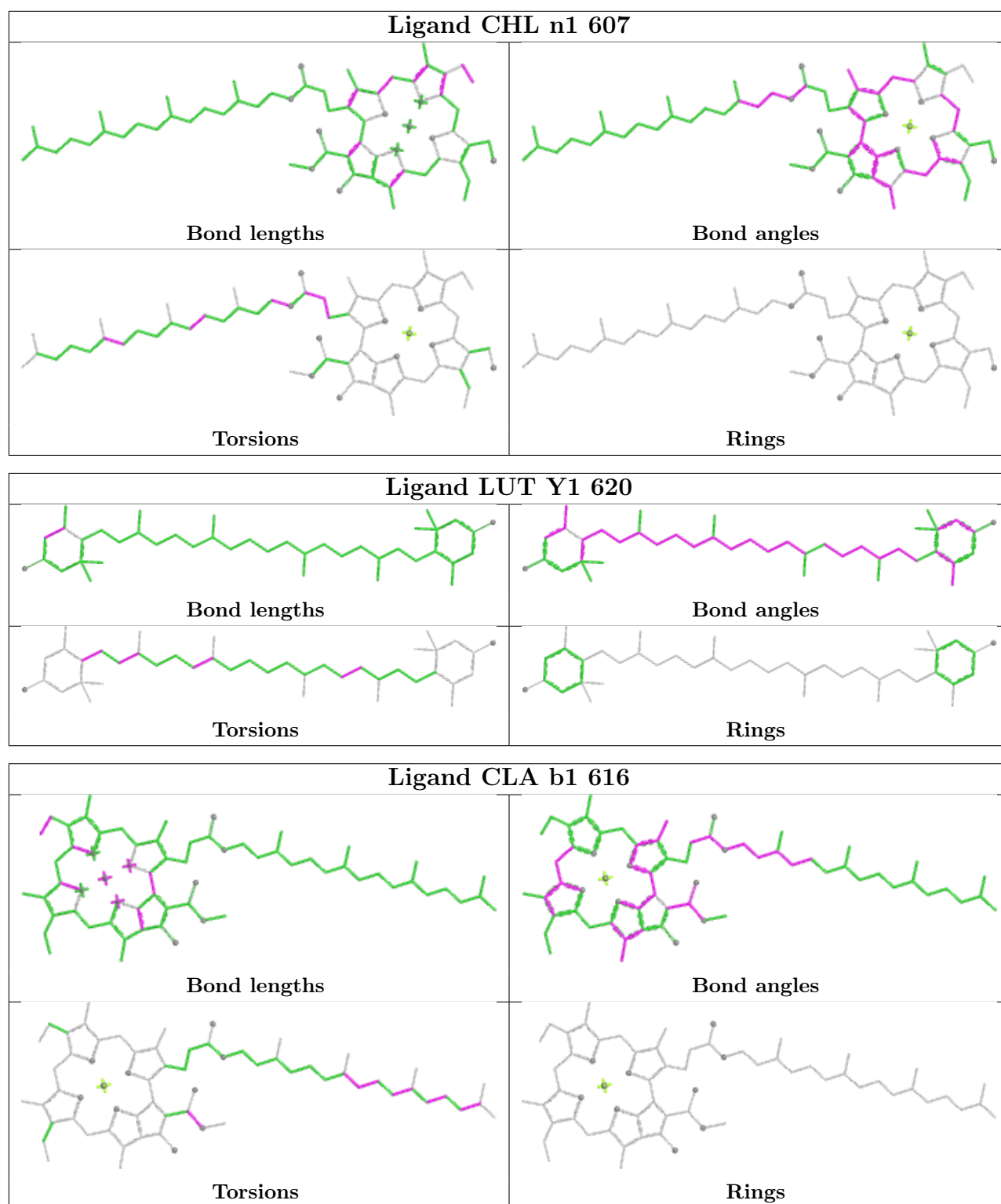


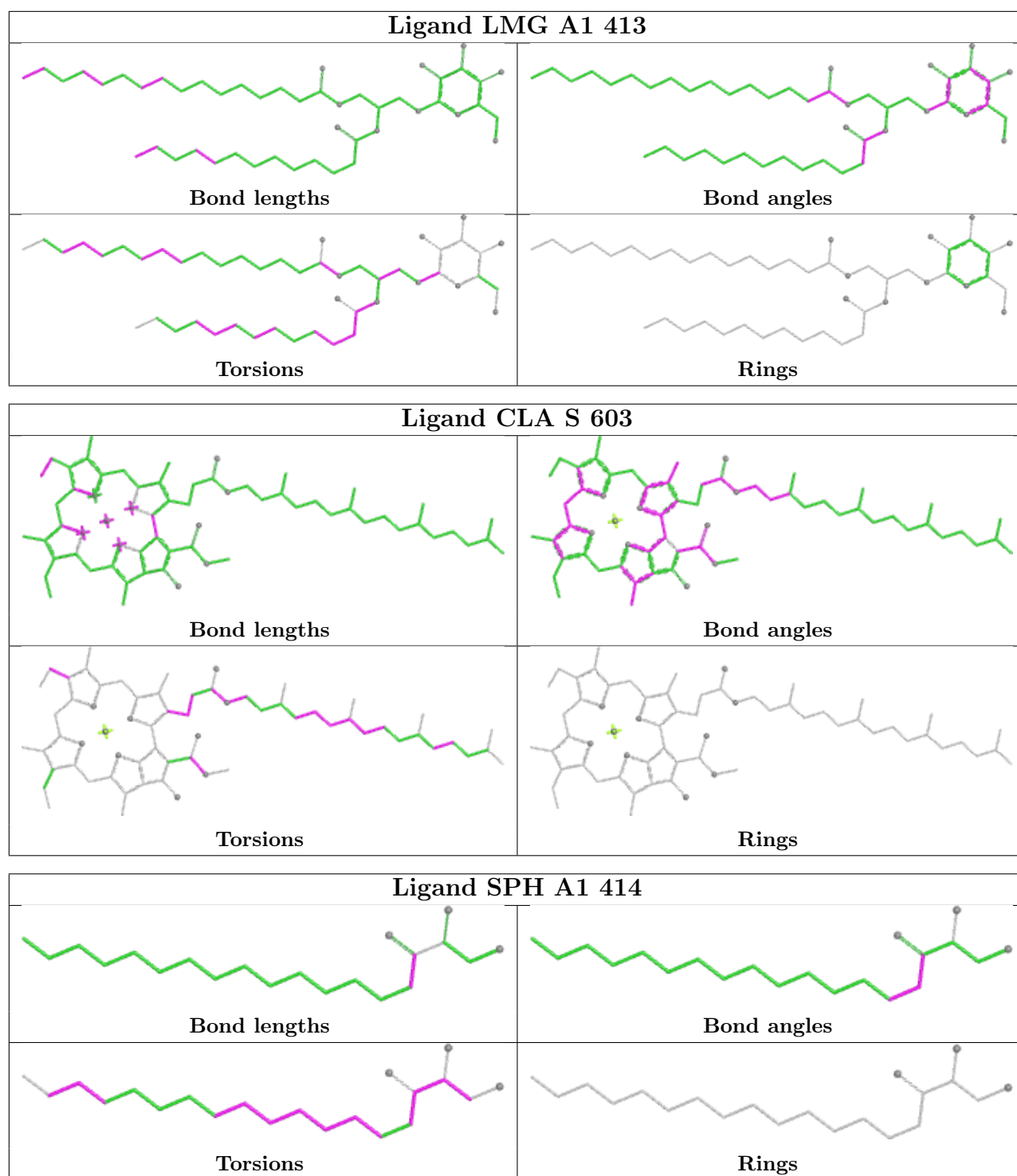


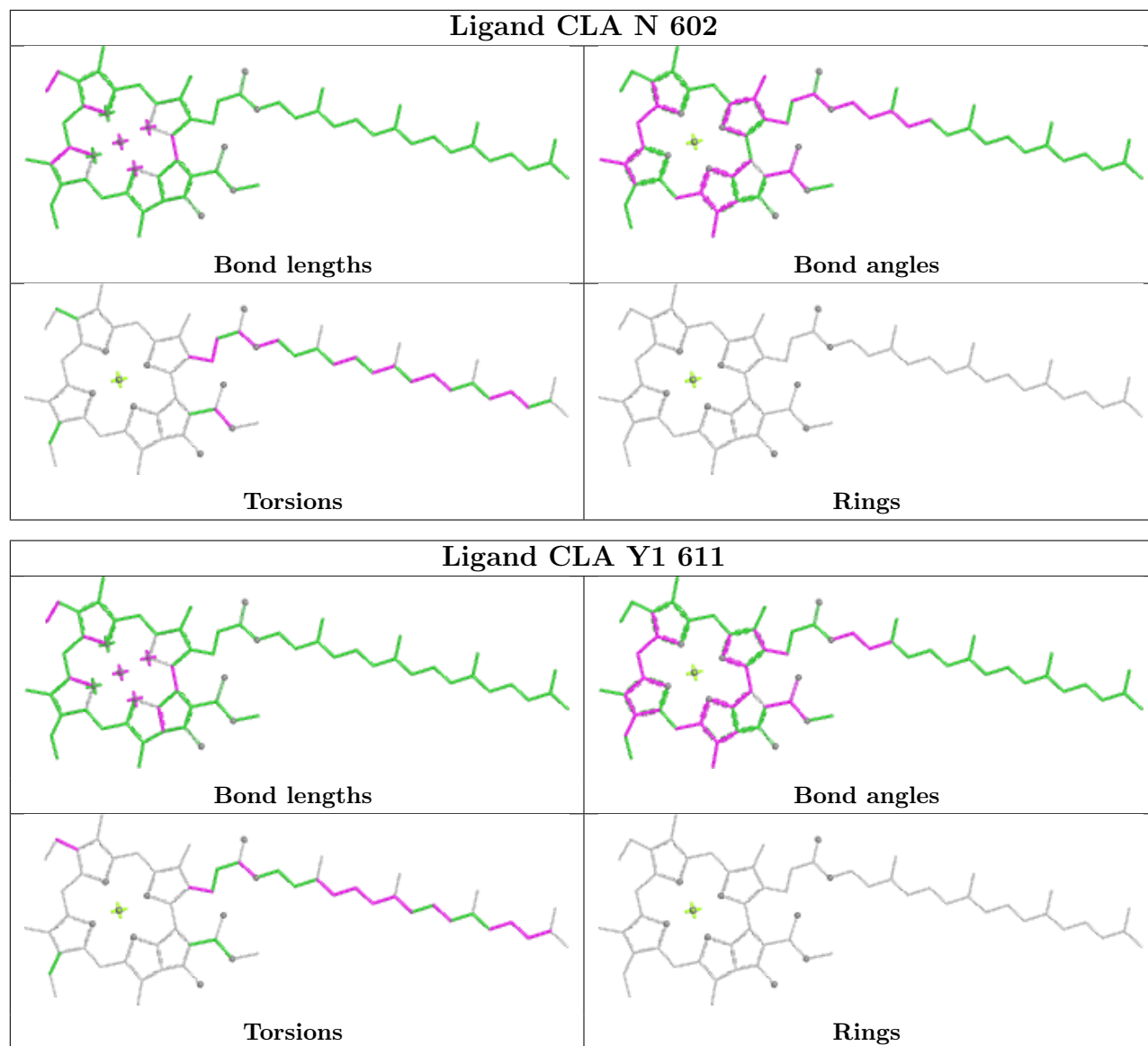


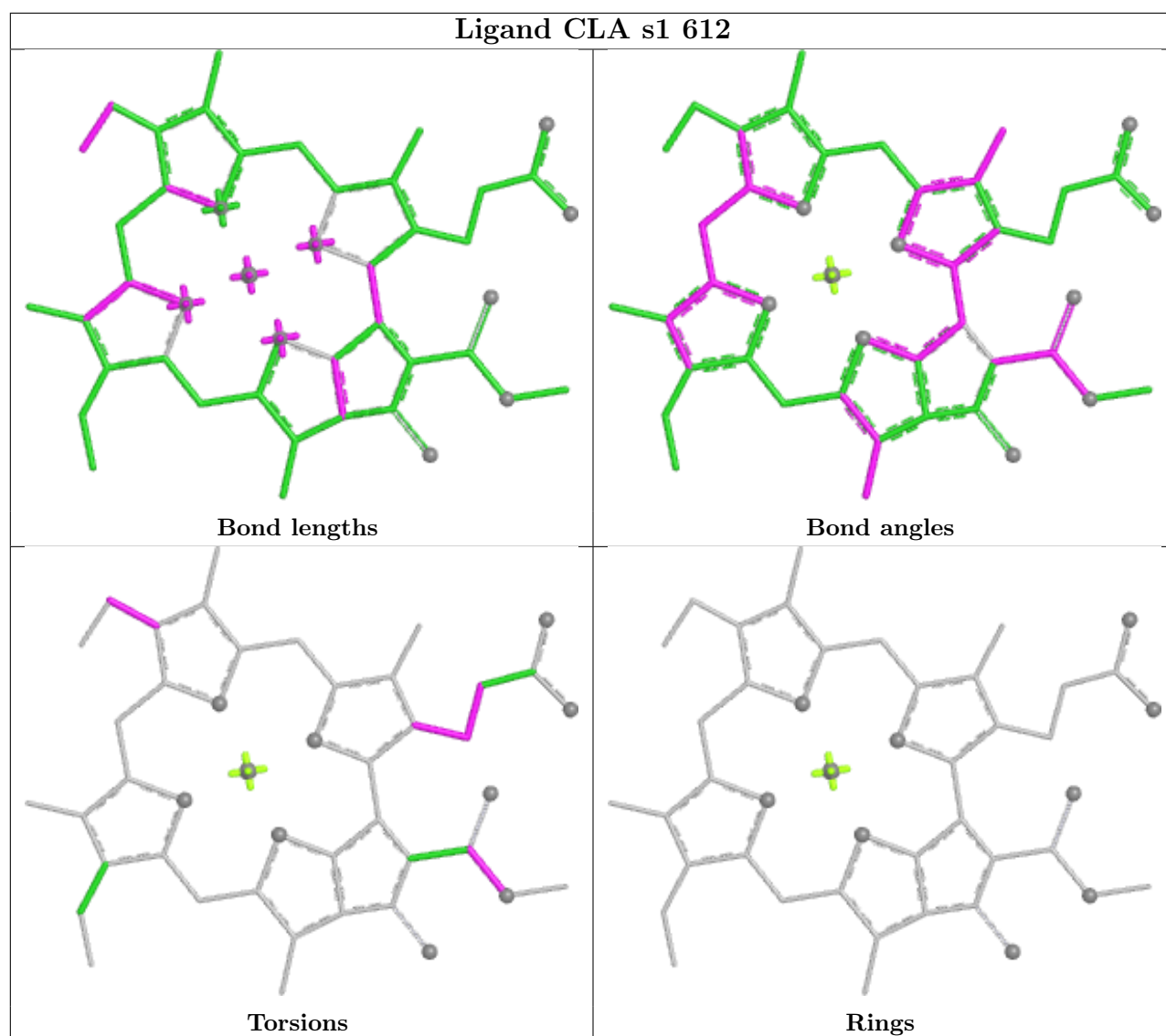


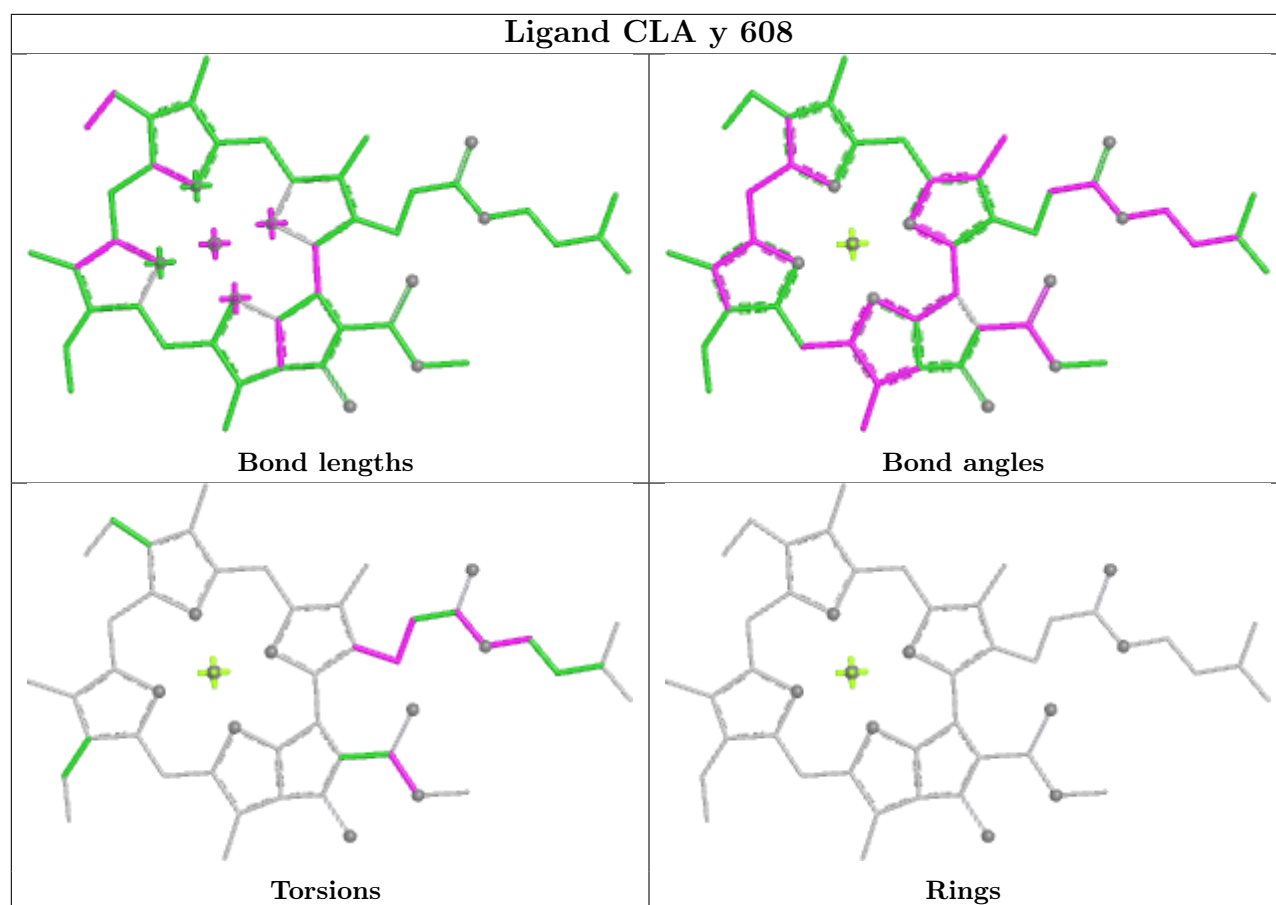
Ligand CLA Y 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C1 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT Y1 621	
 Bond lengths	 Bond angles
 Torsions	 Rings



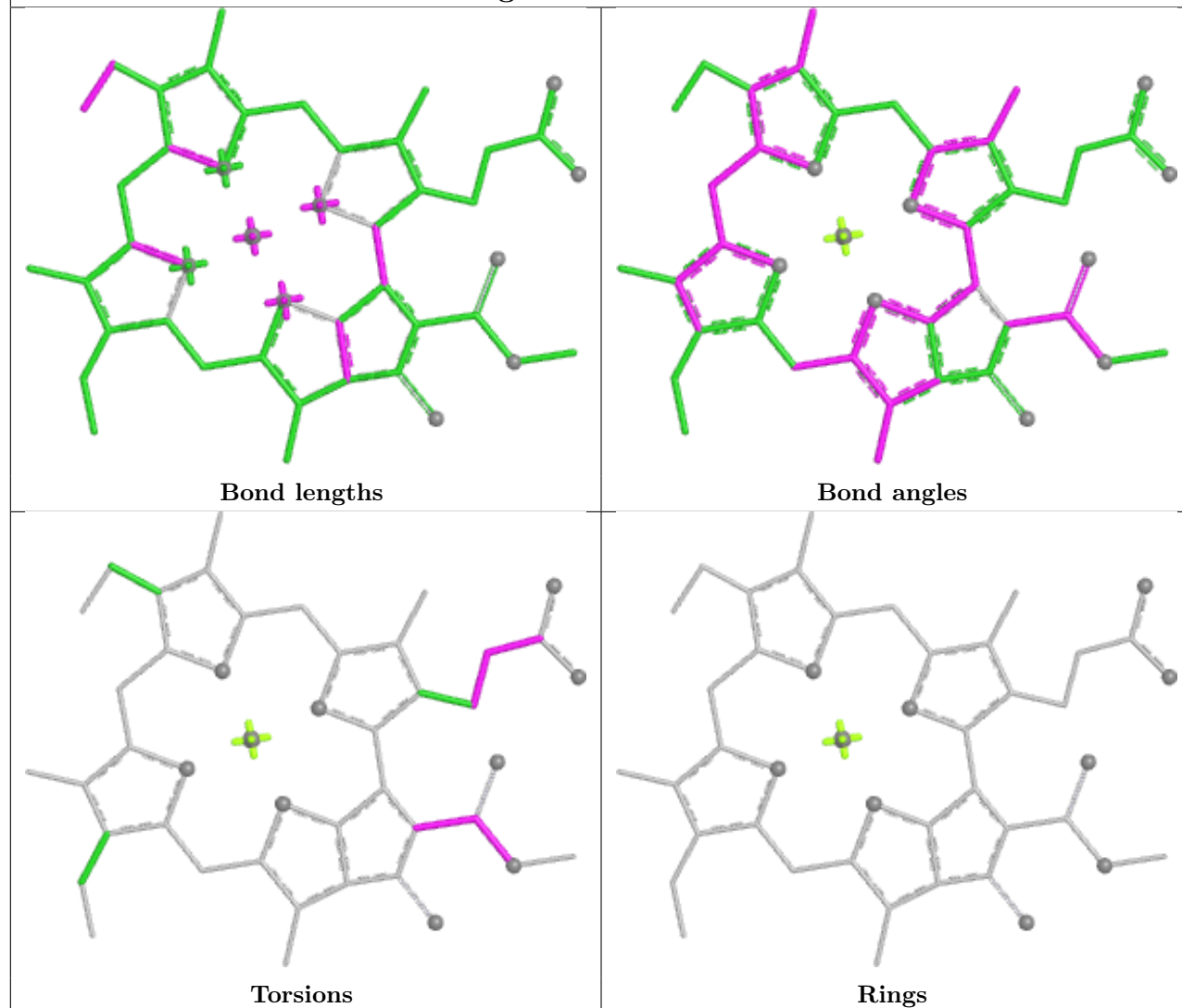




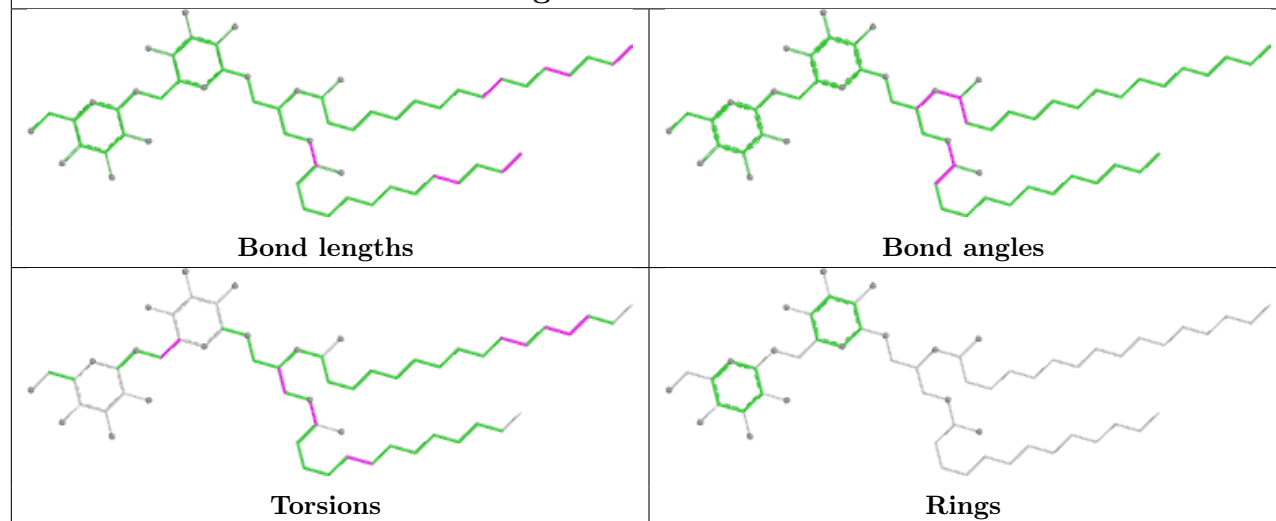


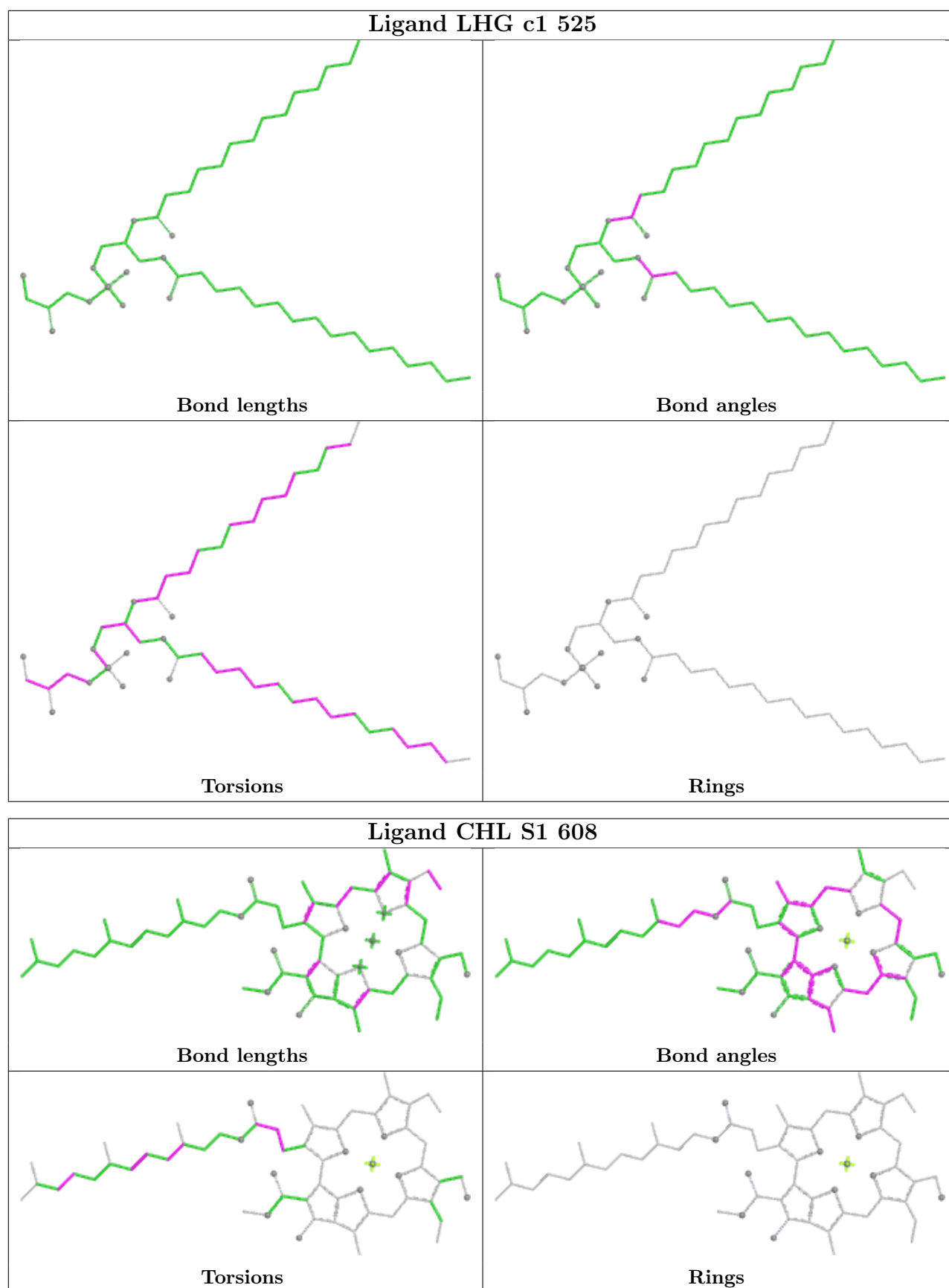


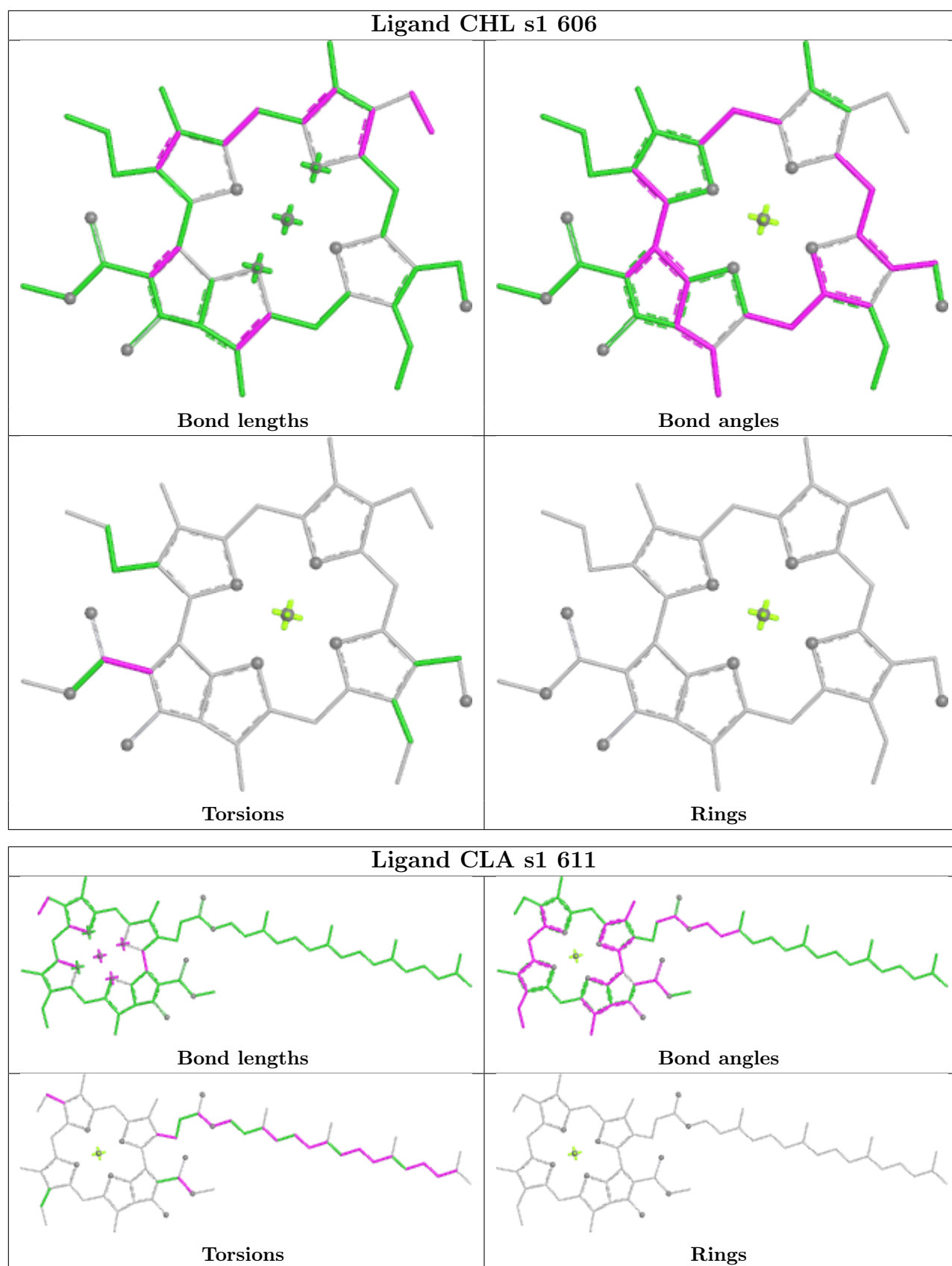
Ligand CLA s 612

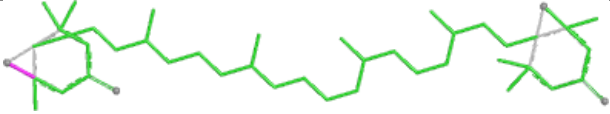
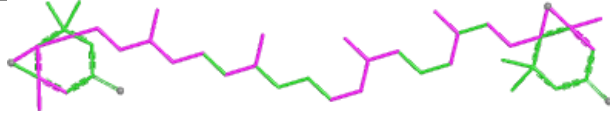
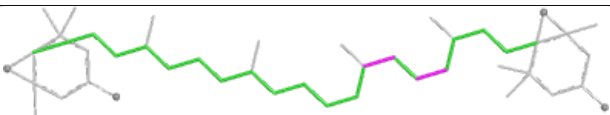
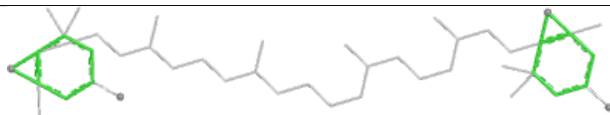
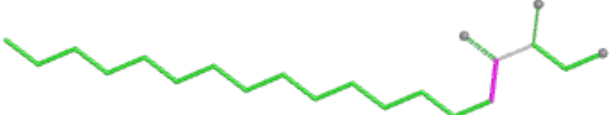
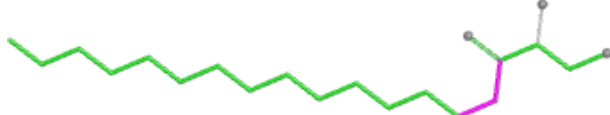
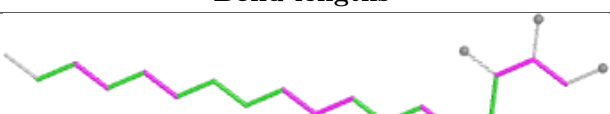
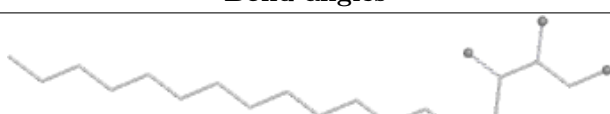
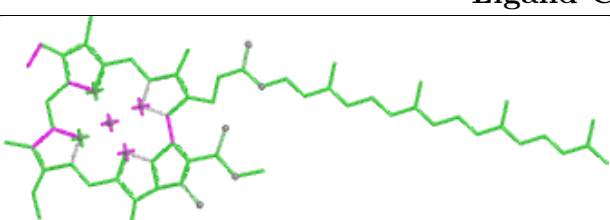
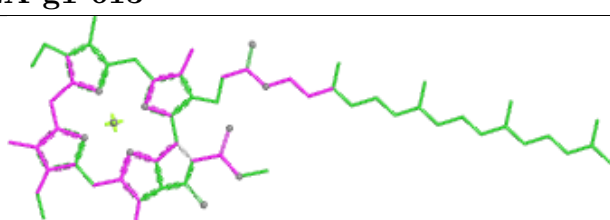
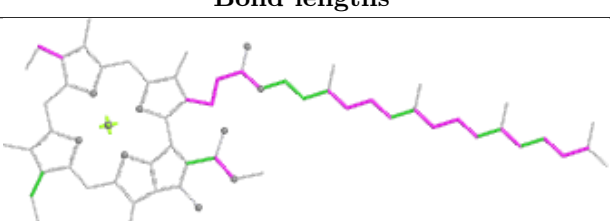
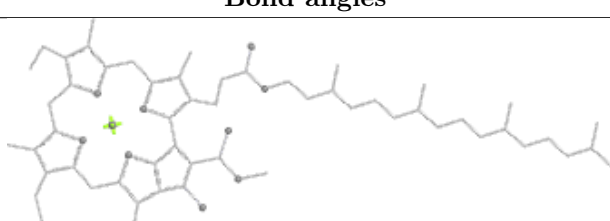


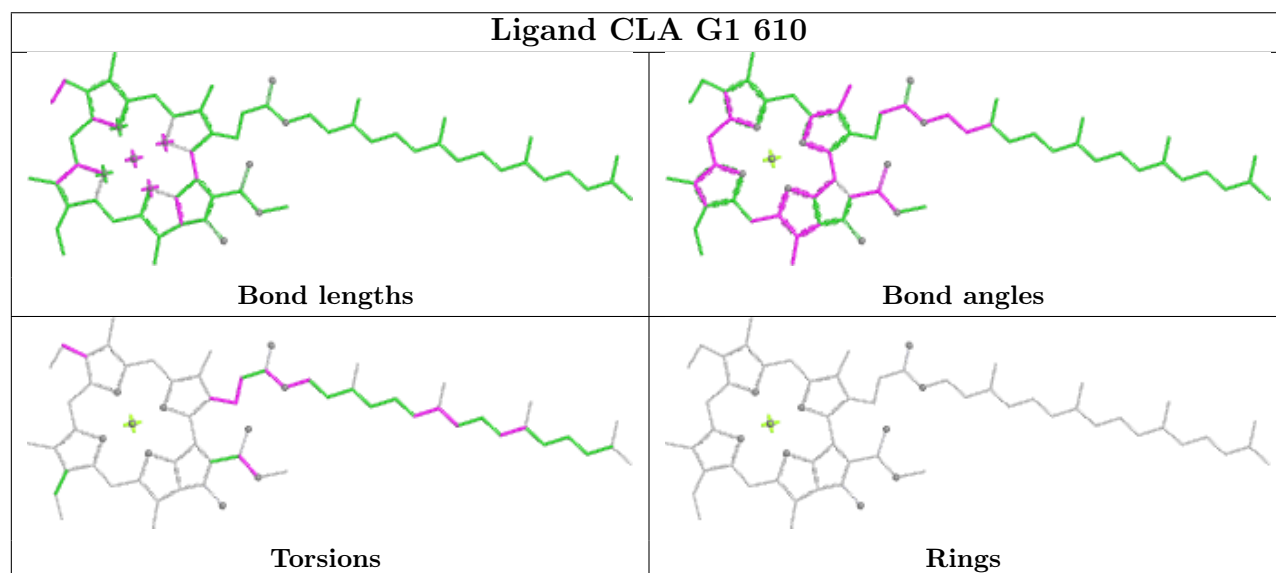
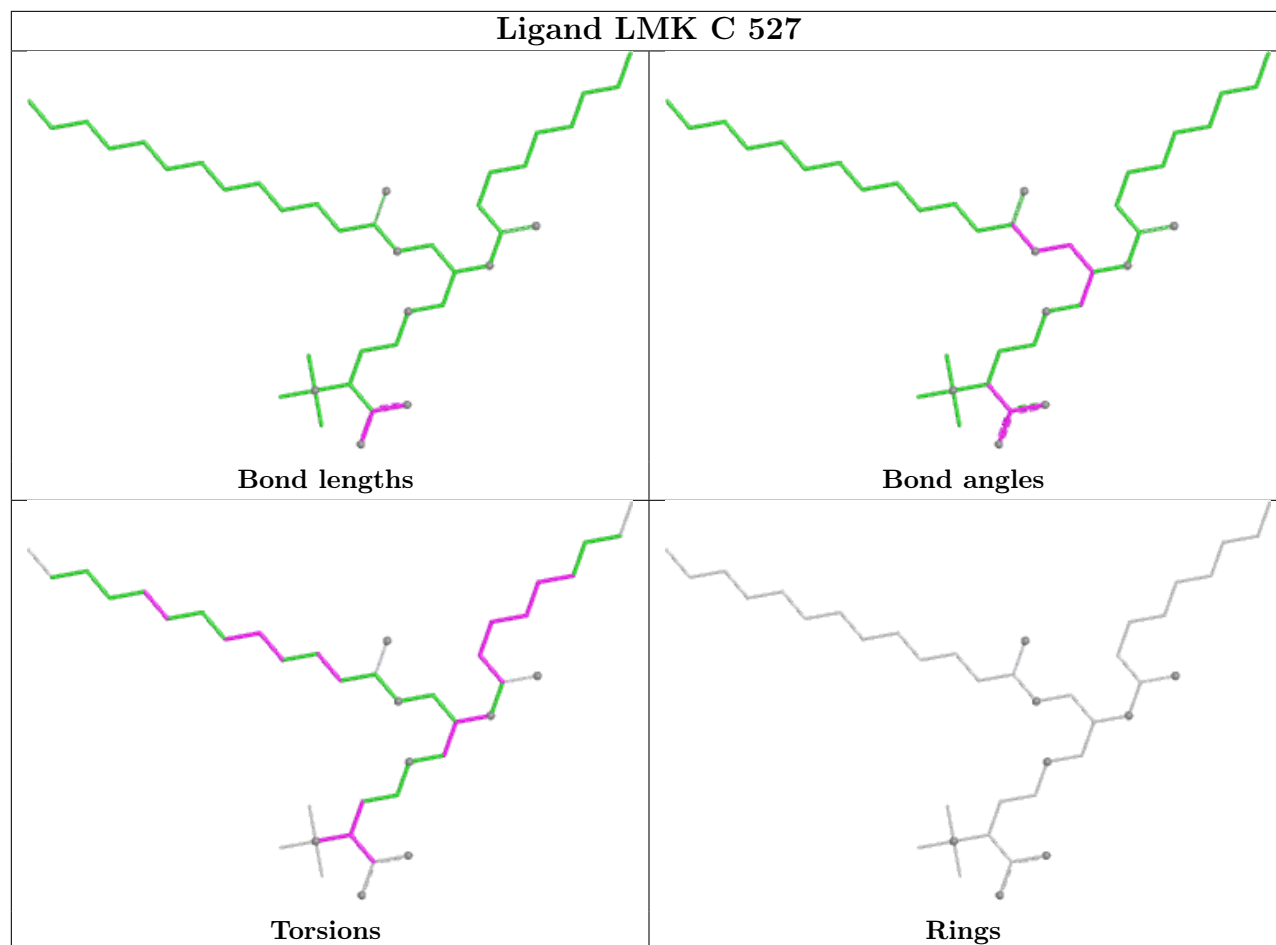
Ligand DGD c 520

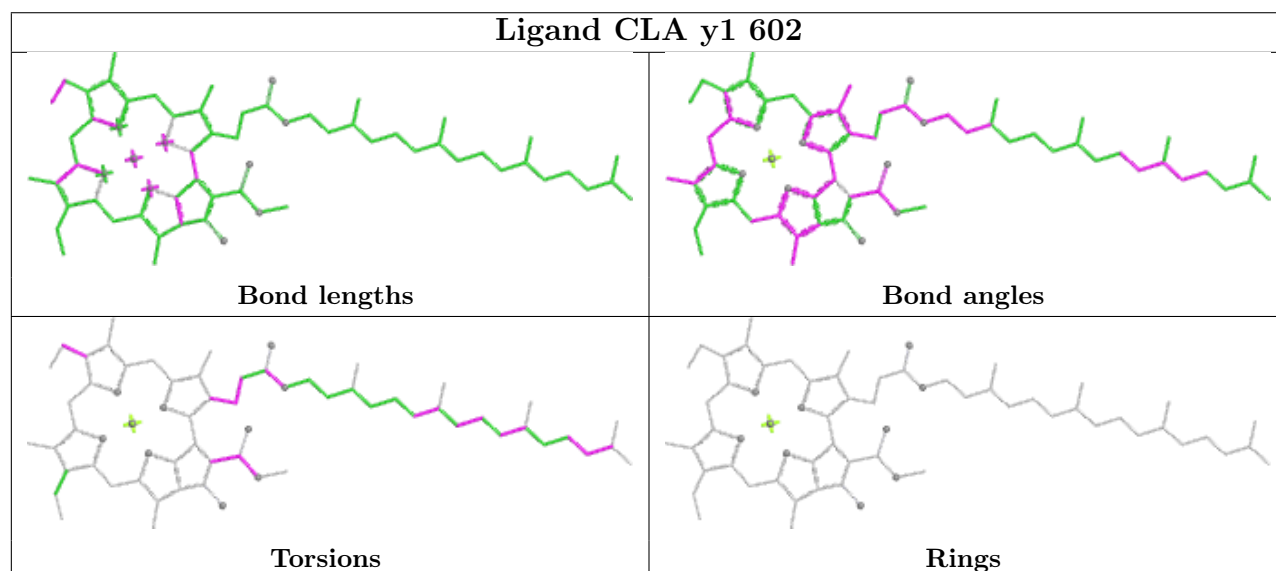
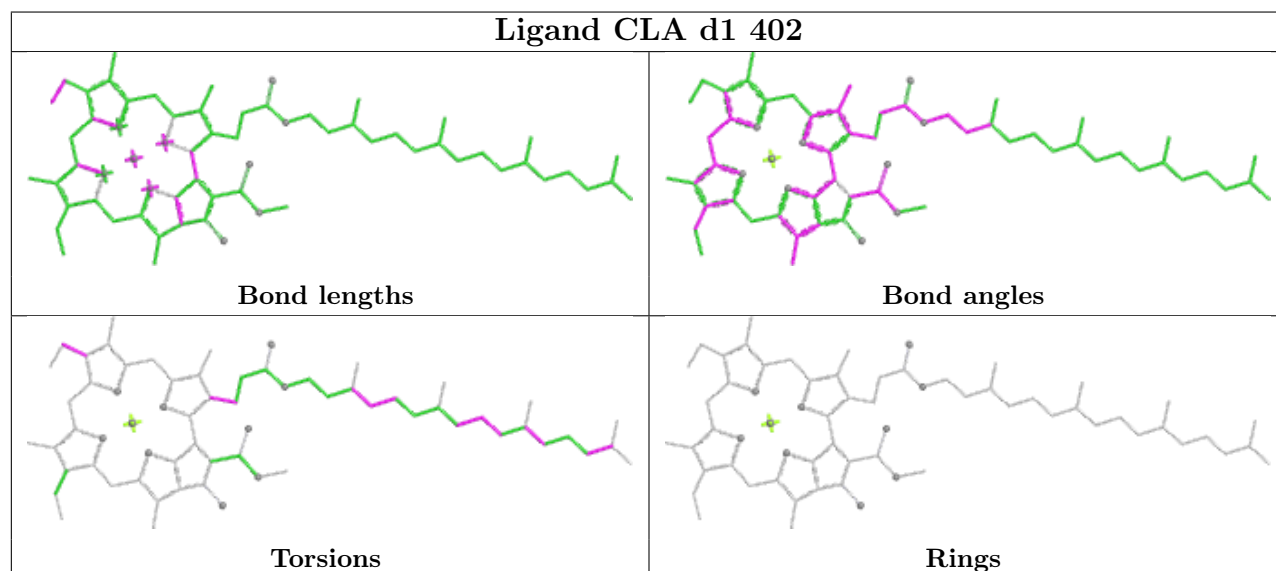
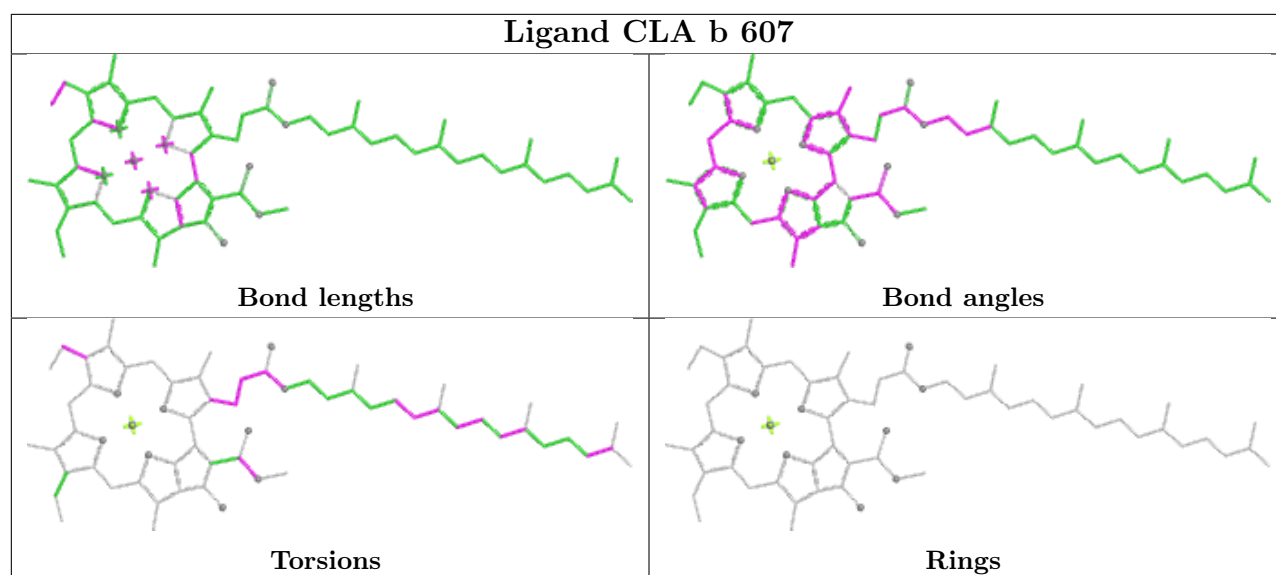


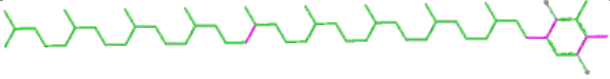
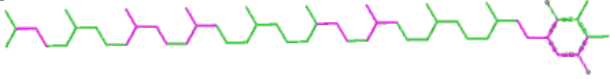
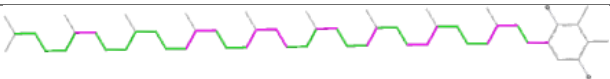
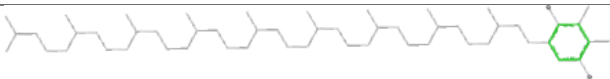
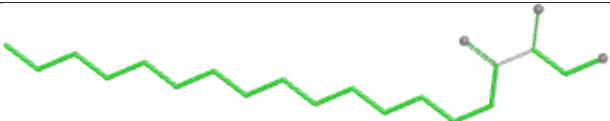
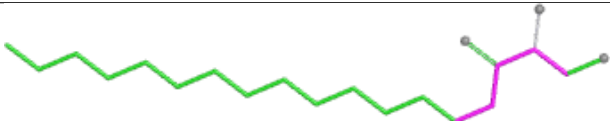
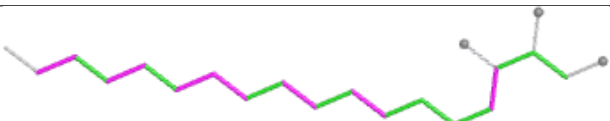
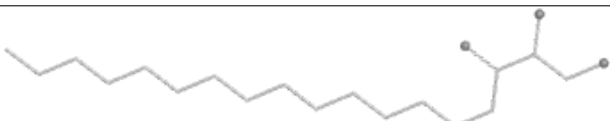
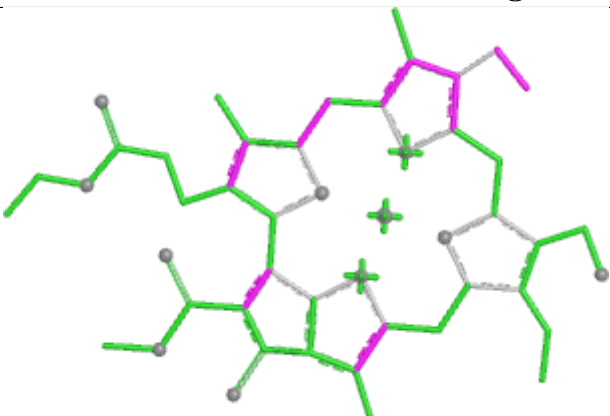
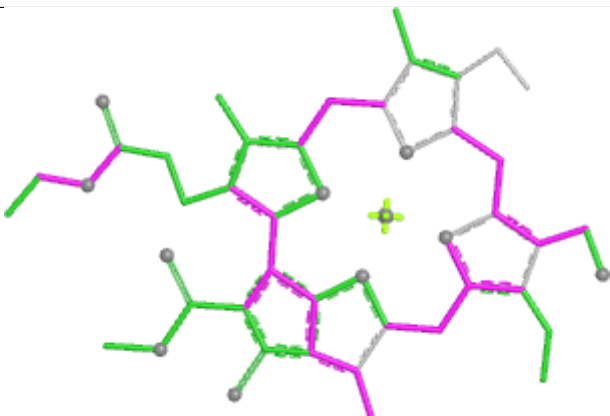
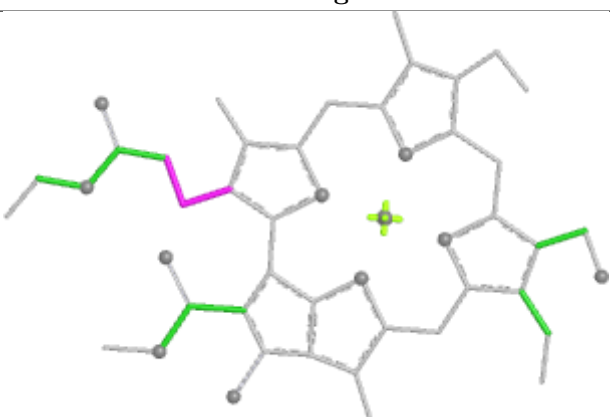
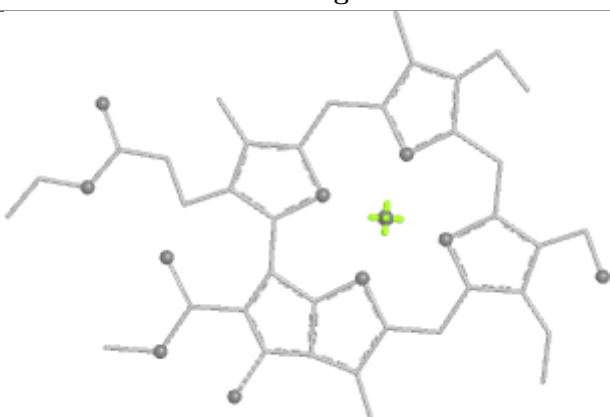


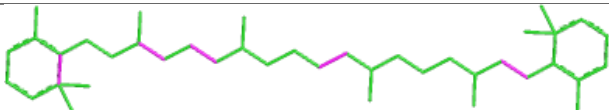
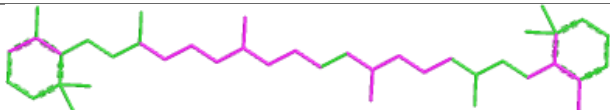
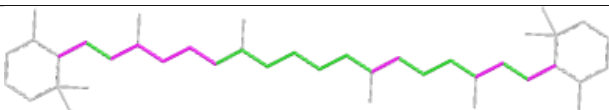
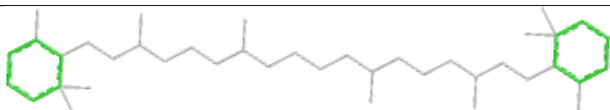


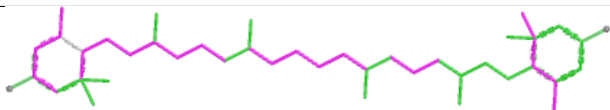
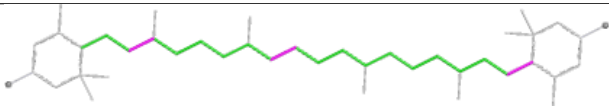
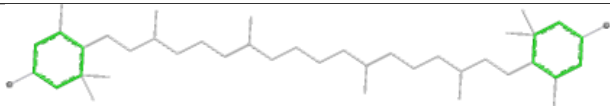
Ligand XAT g 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPH a1 414	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA g1 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

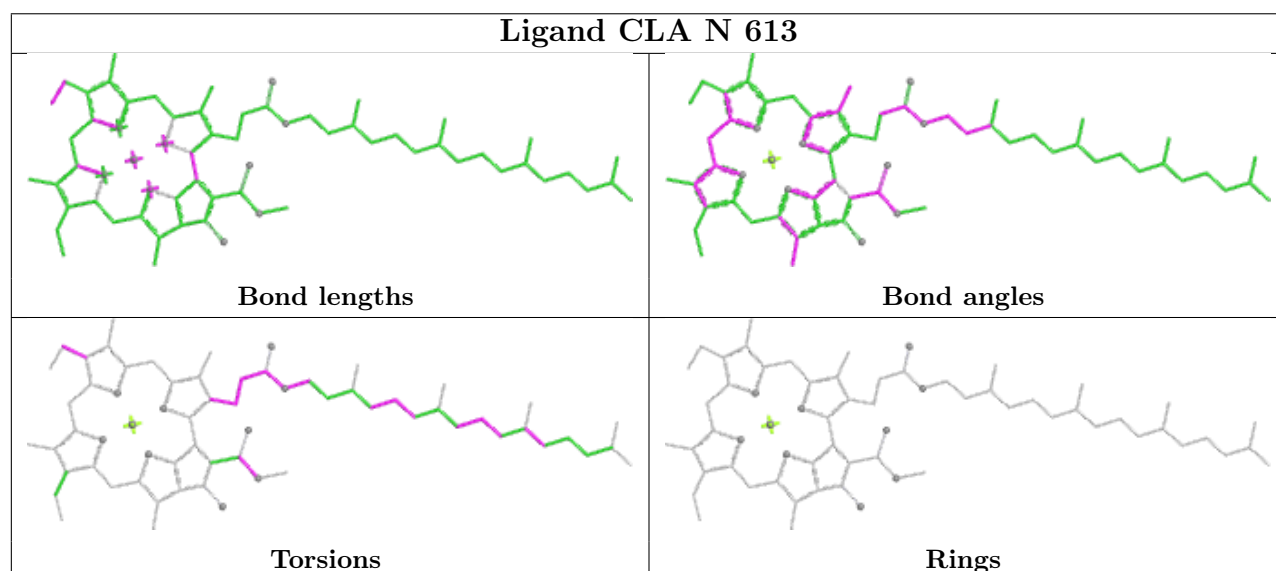
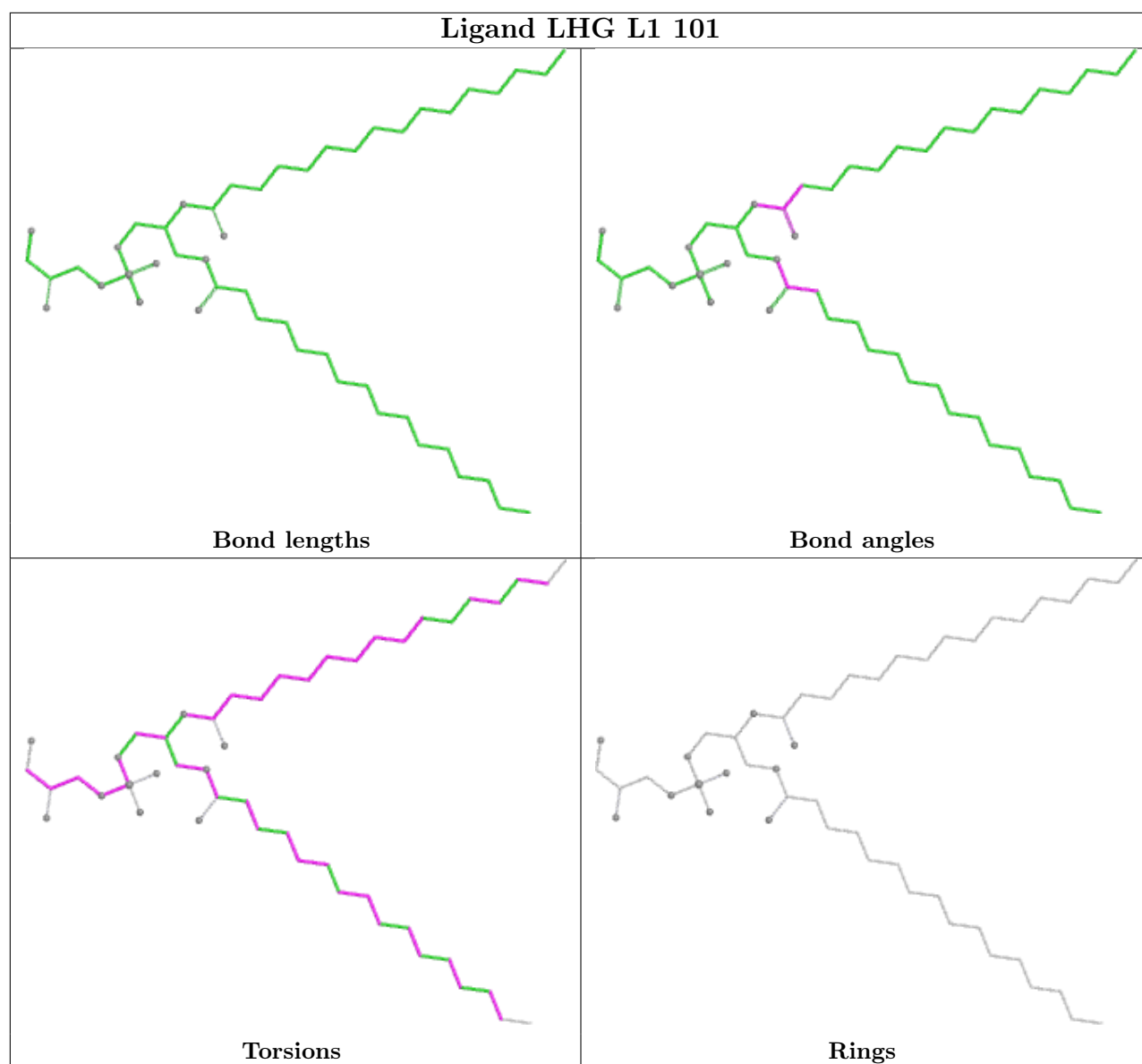


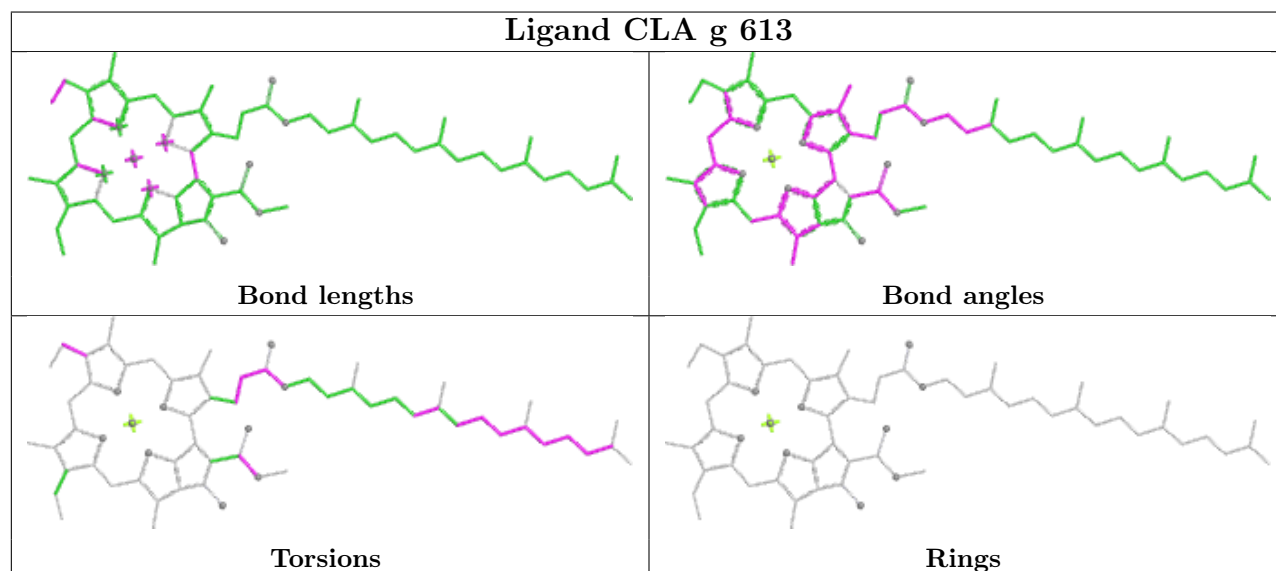
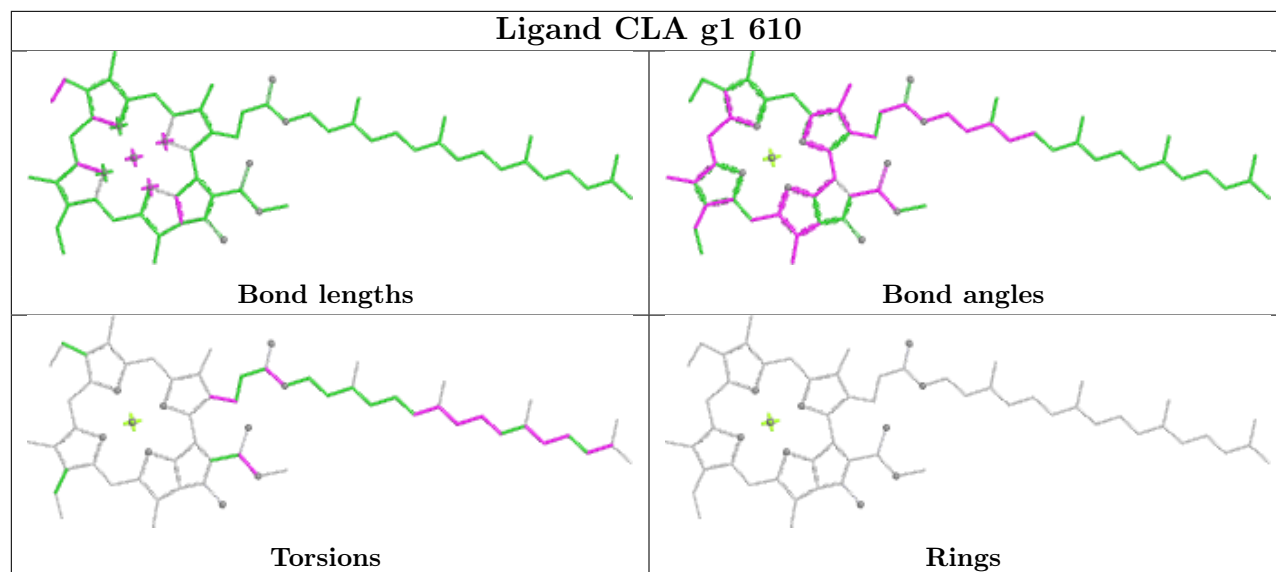


Ligand PL9 D1 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPH y 625	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL G 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

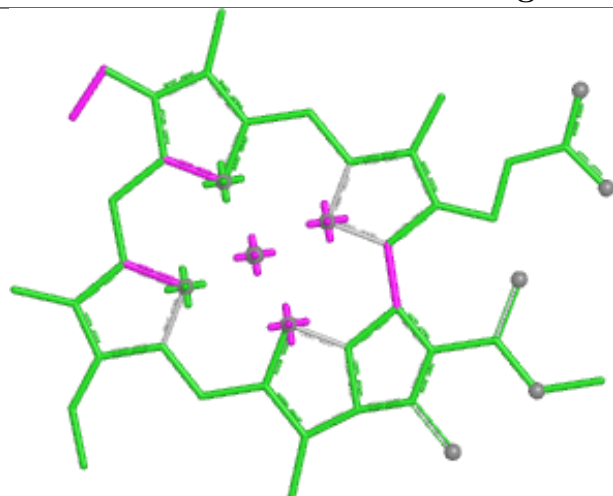
Ligand BCR D1 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT G1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

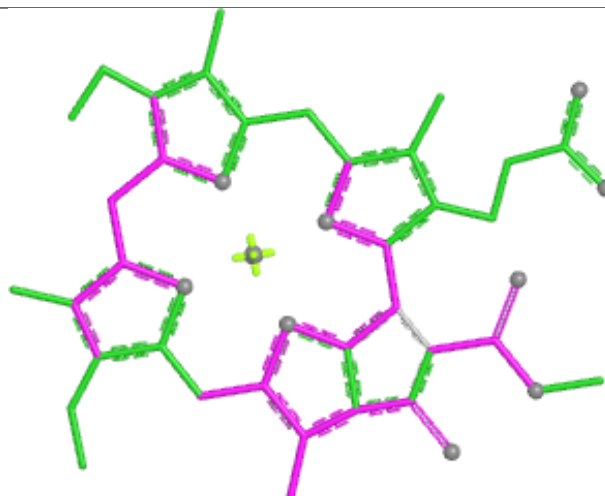




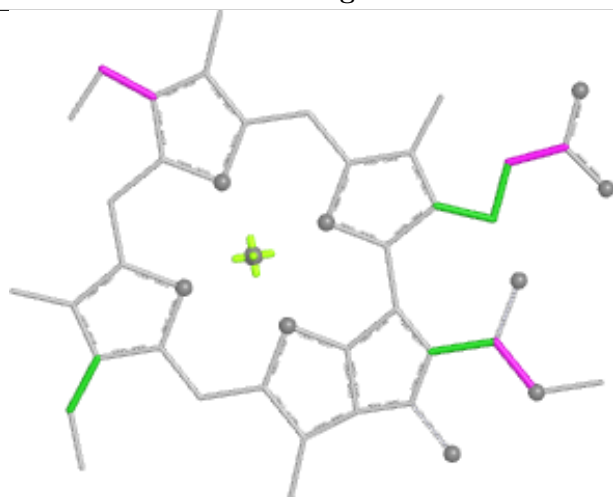
Ligand CLA n 612



Bond lengths



Bond angles

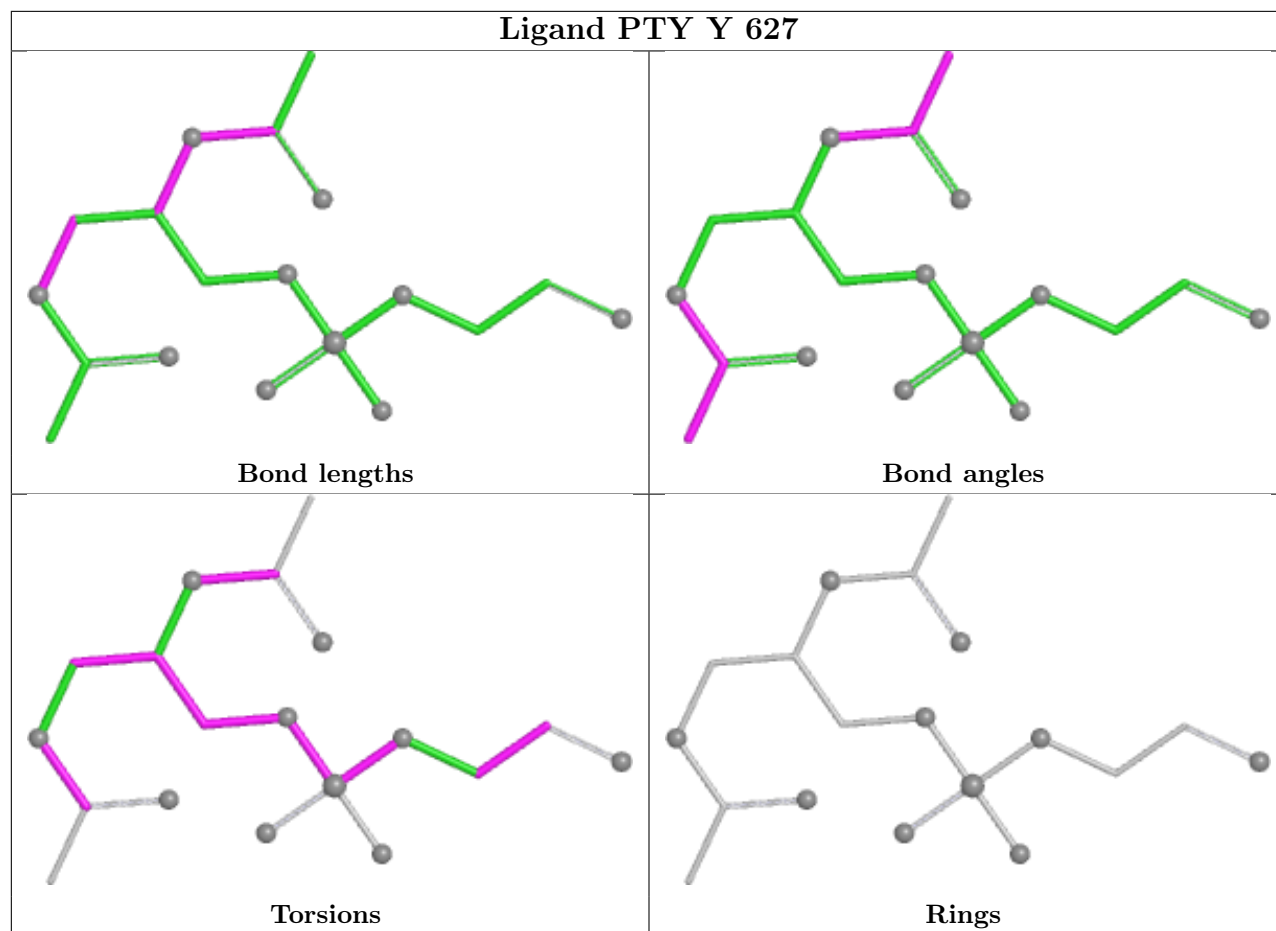


Torsions

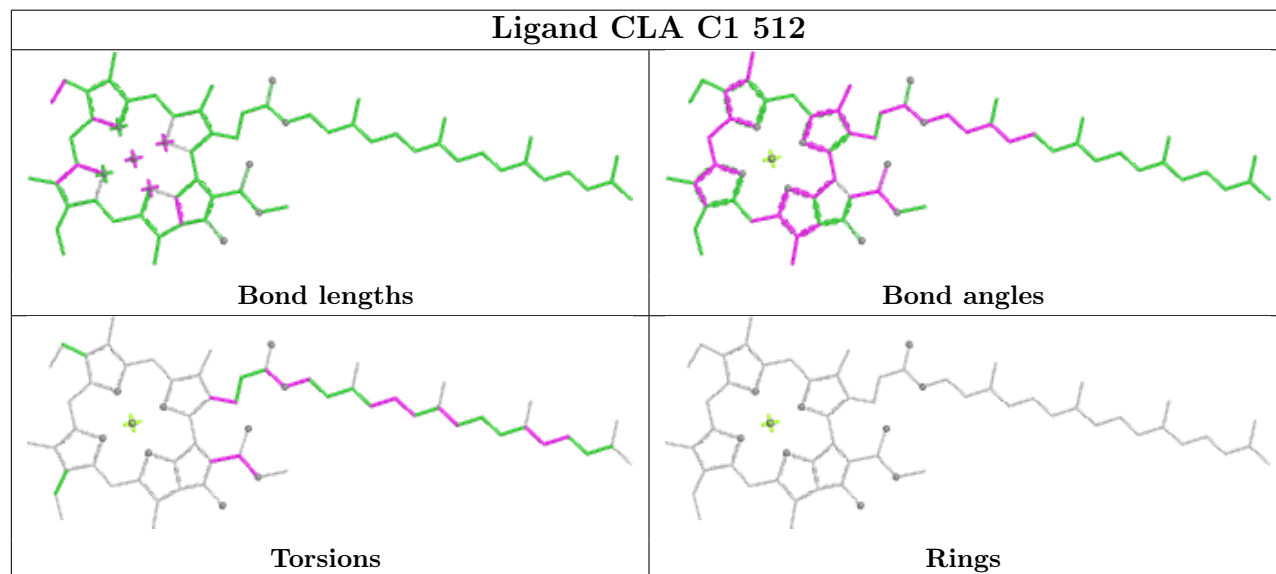


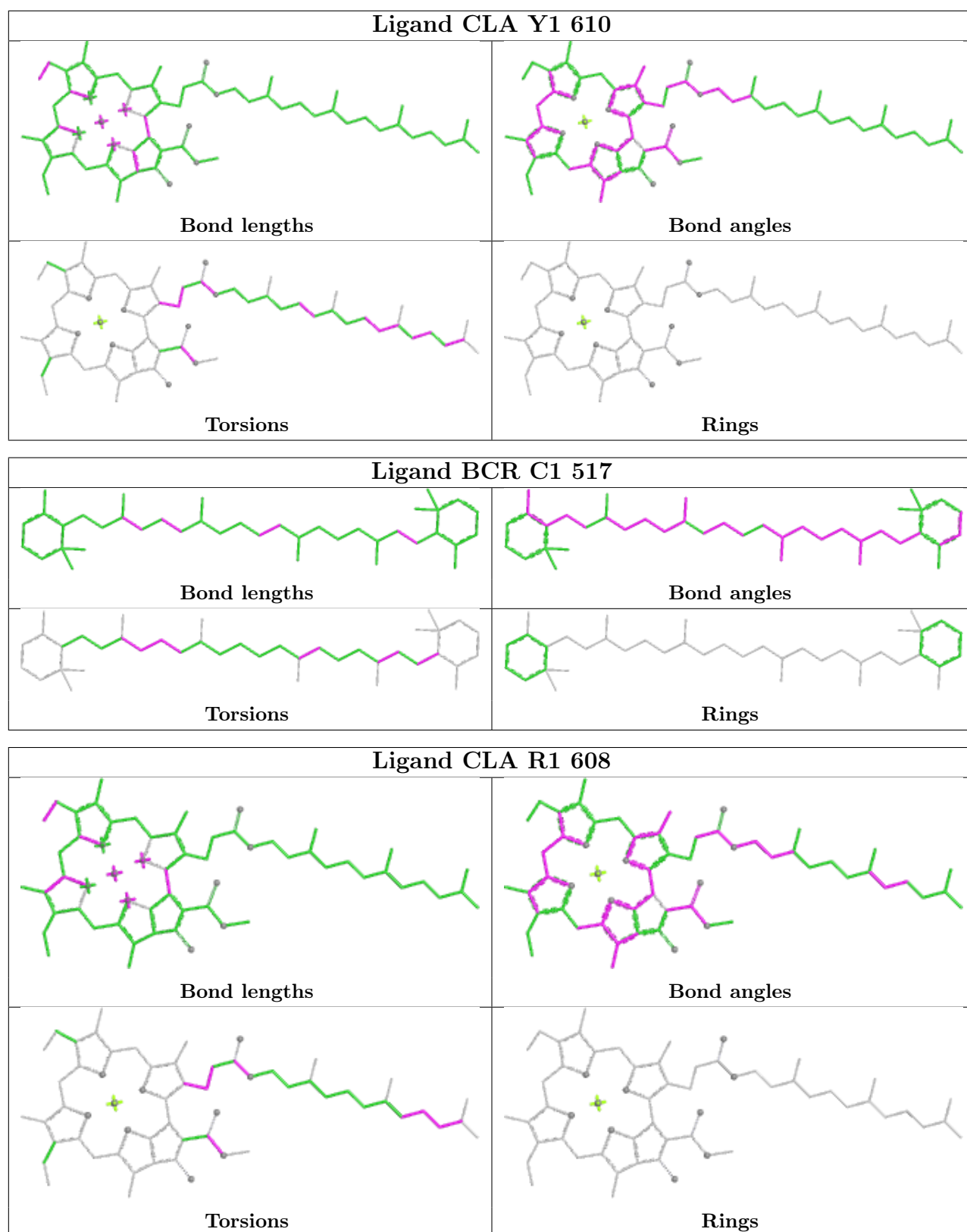
Rings

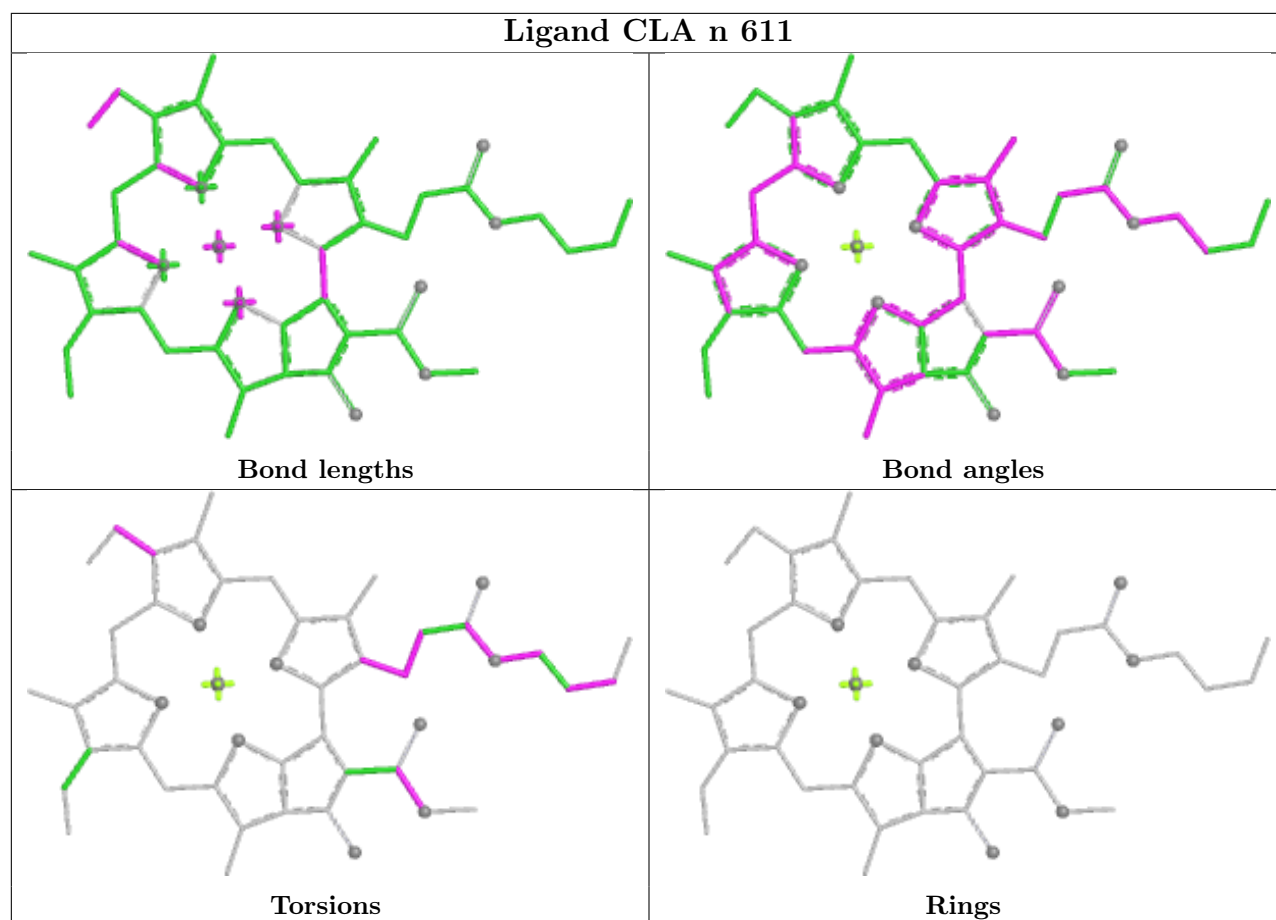
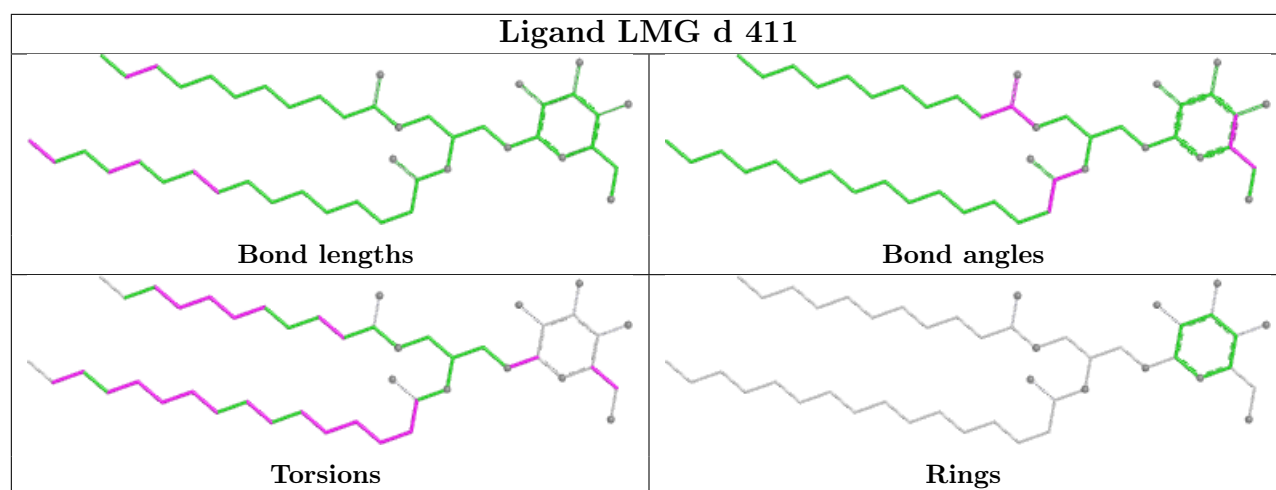
Ligand PTY Y 627

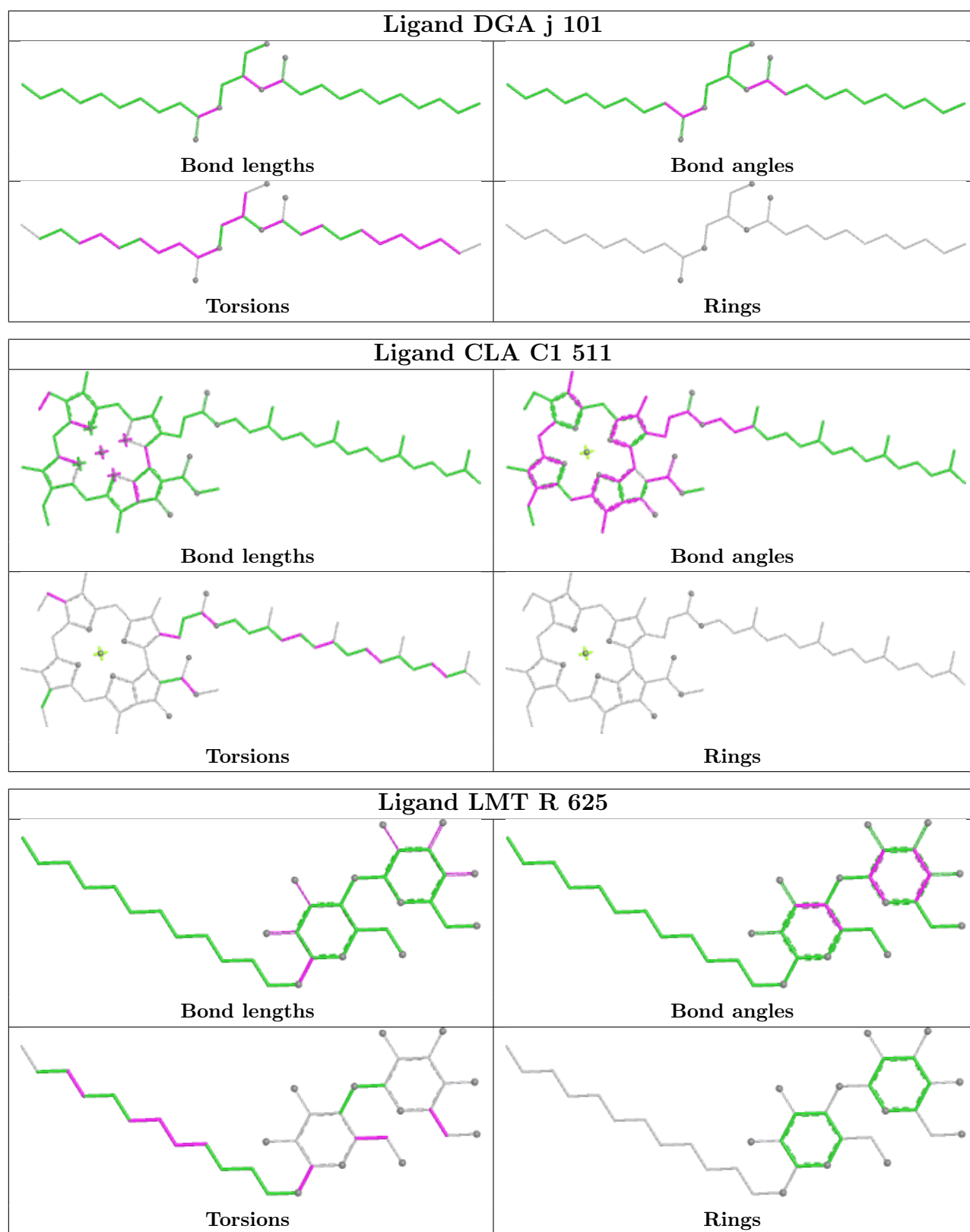


Ligand CLA C1 512

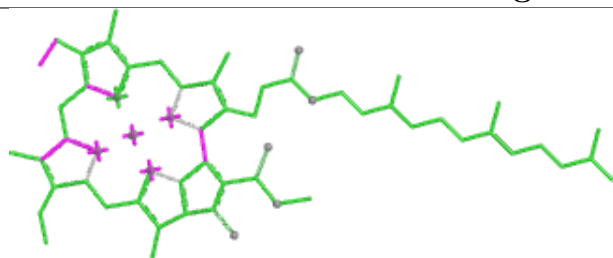




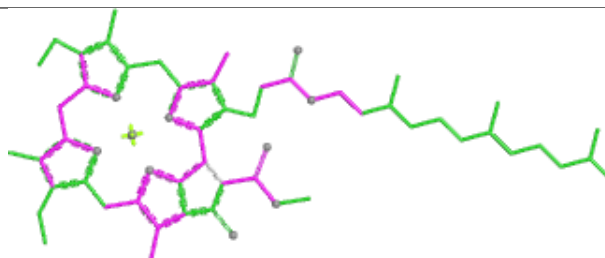




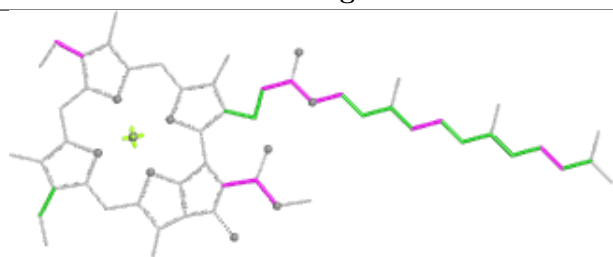
Ligand CLA R 612



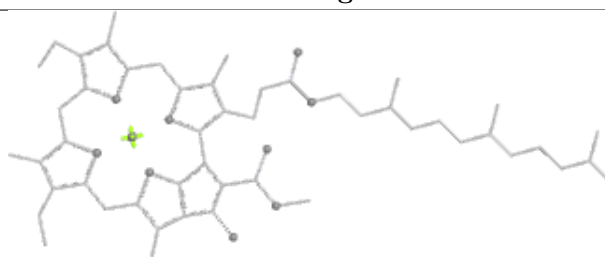
Bond lengths



Bond angles

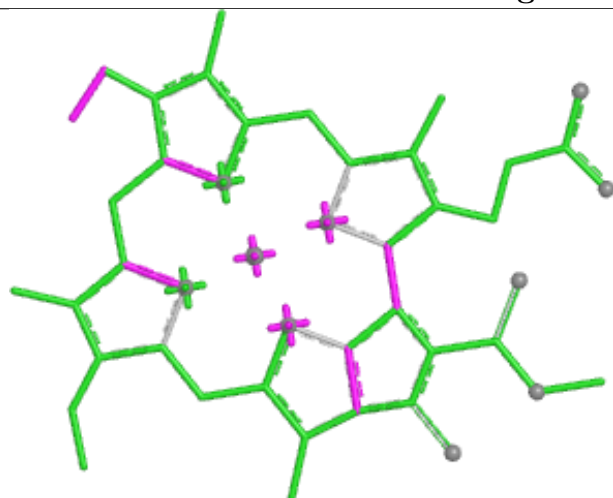


Torsions

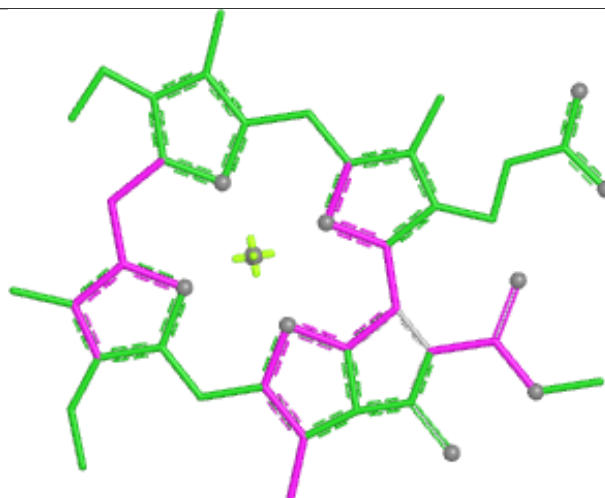


Rings

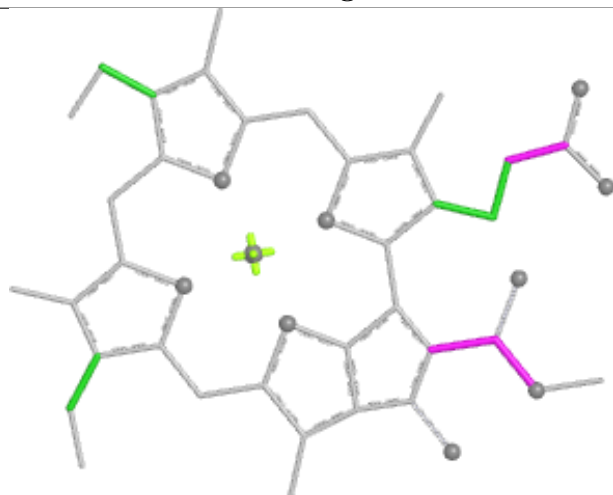
Ligand CLA S 612



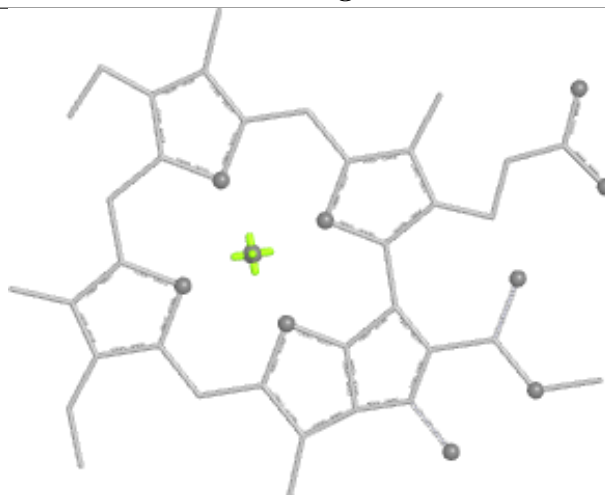
Bond lengths



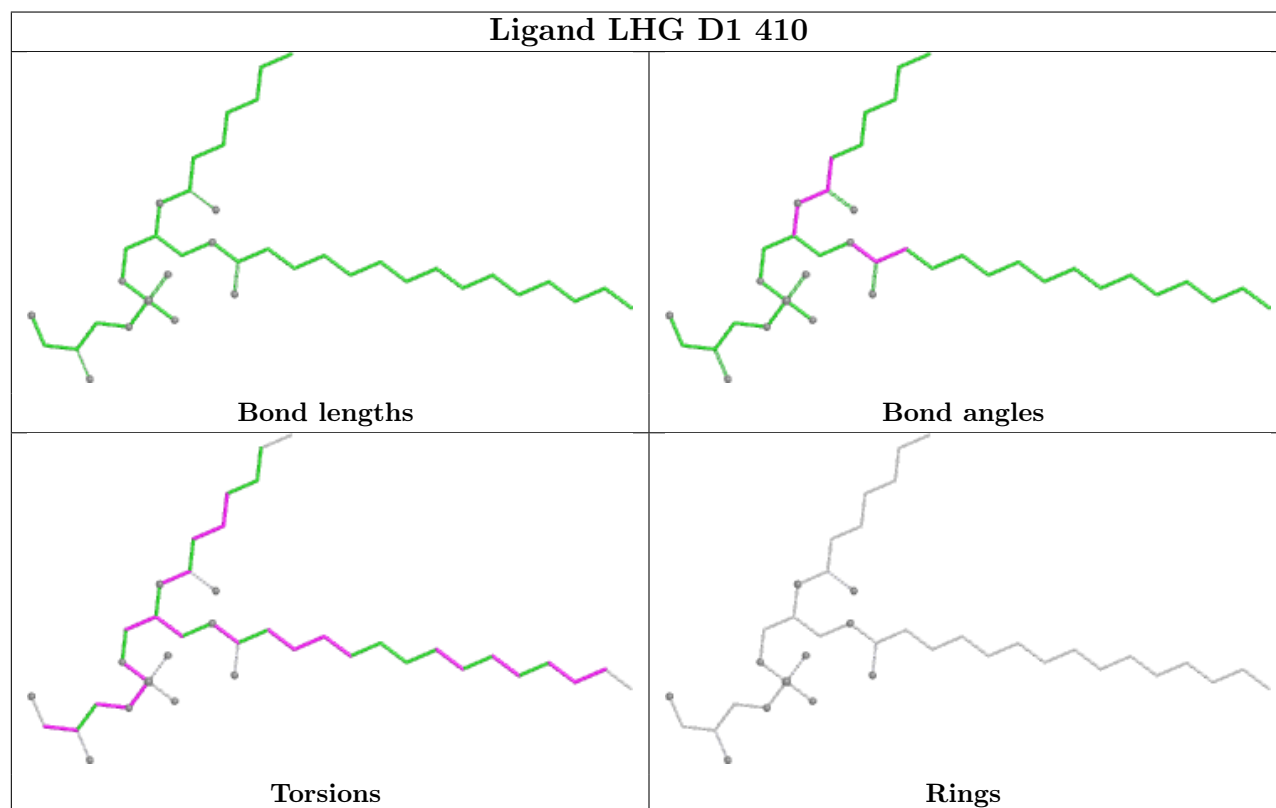
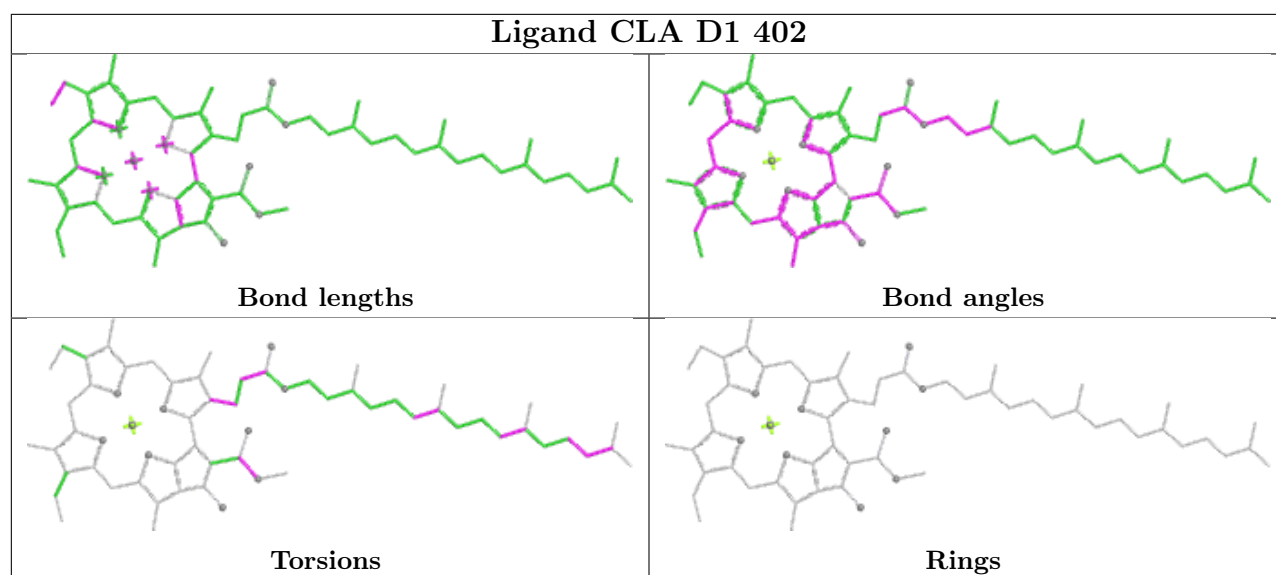
Bond angles

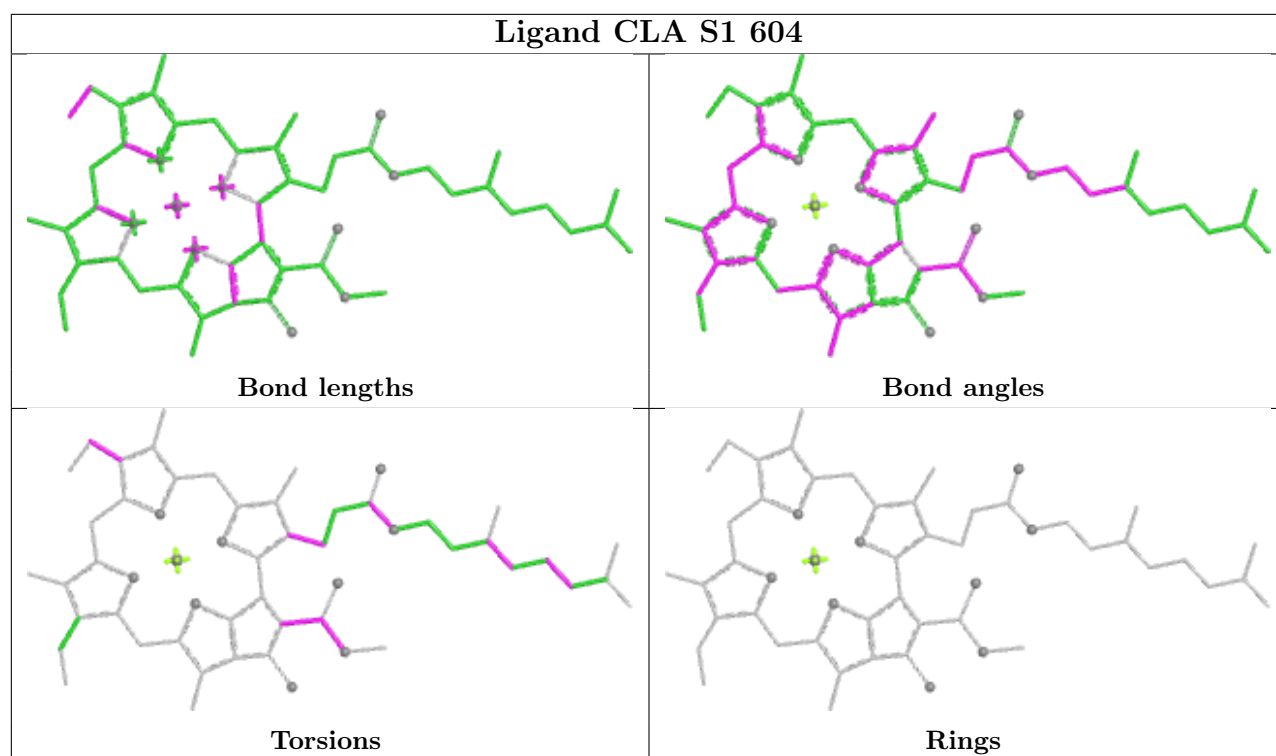


Torsions

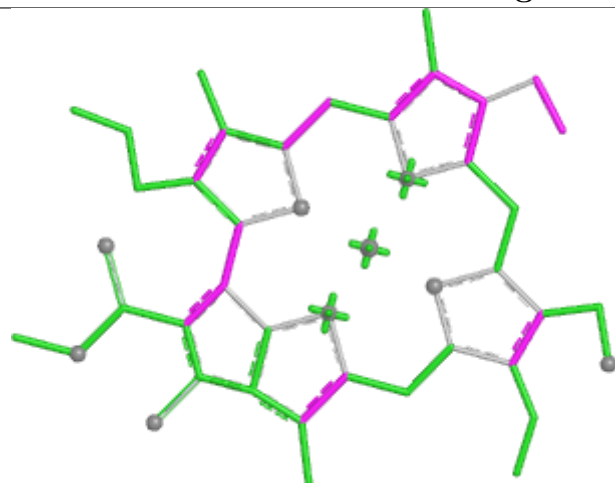


Rings

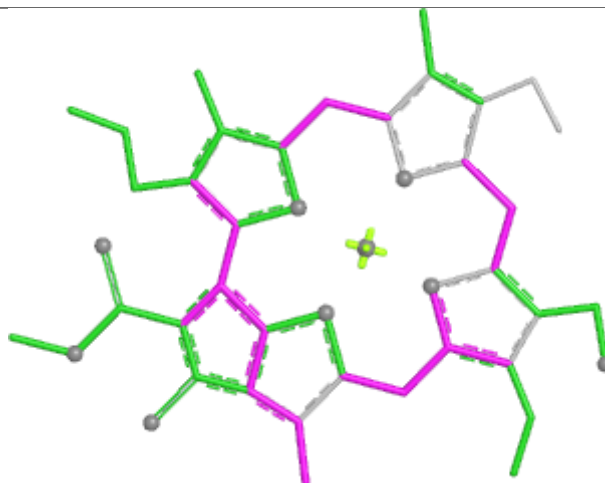




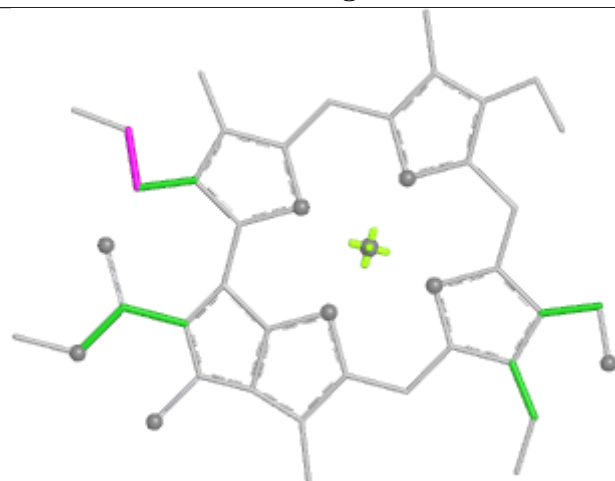
Ligand CHL R 606



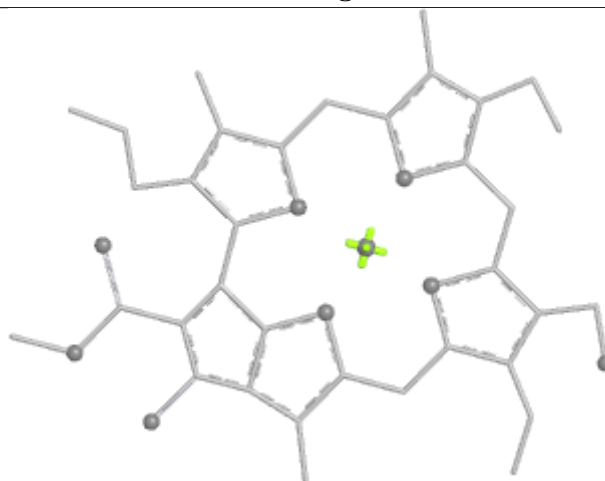
Bond lengths



Bond angles

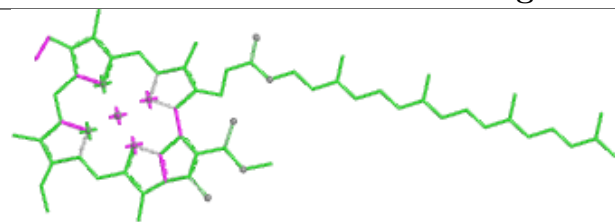


Torsions

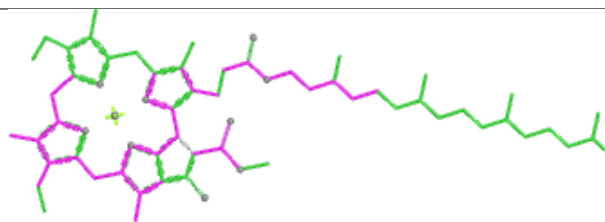


Rings

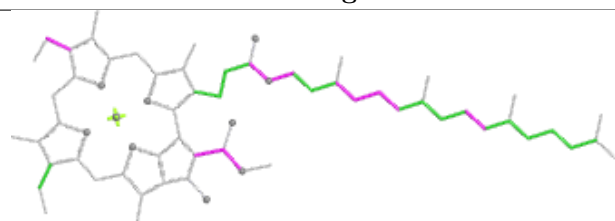
Ligand CLA C 506



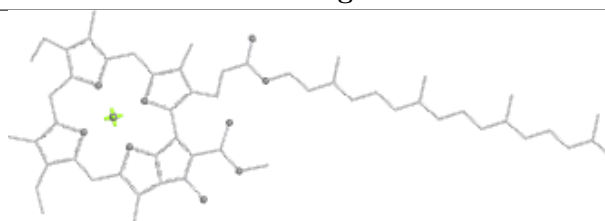
Bond lengths



Bond angles

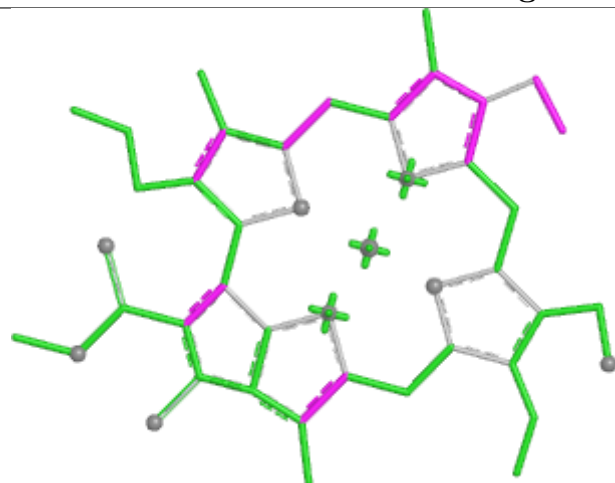


Torsions

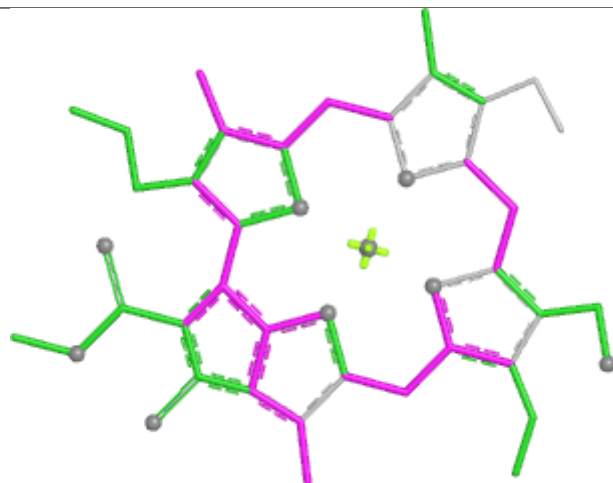


Rings

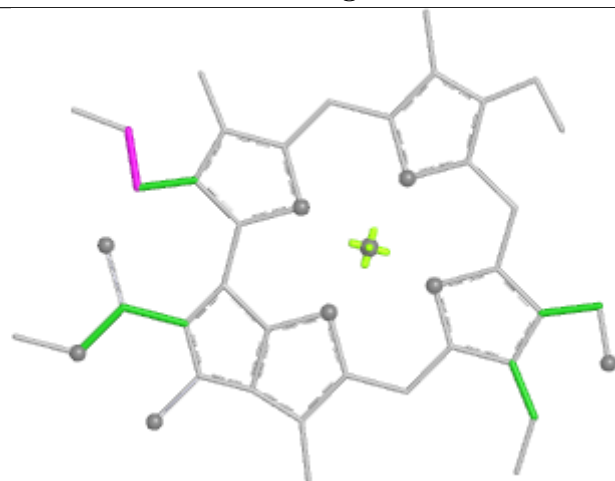
Ligand CHL S 606



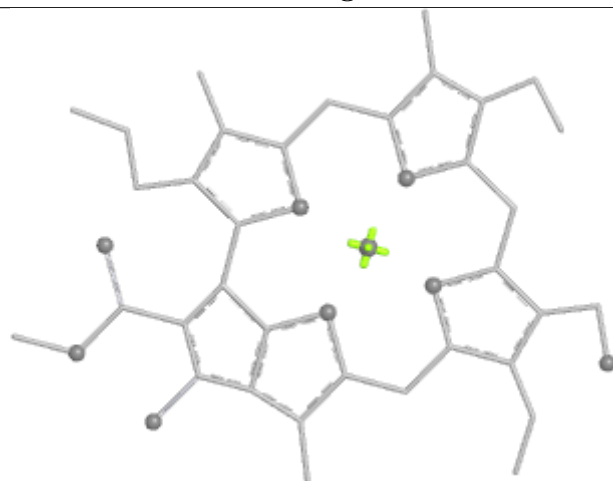
Bond lengths



Bond angles

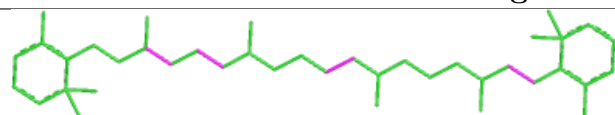


Torsions

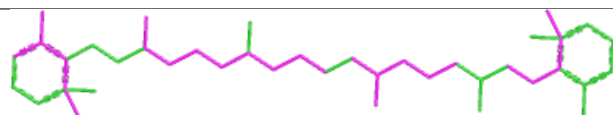


Rings

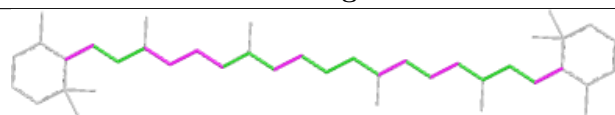
Ligand BCR c1 514



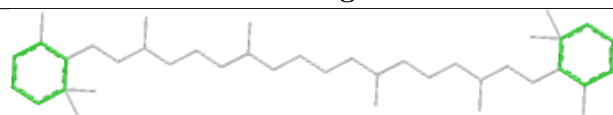
Bond lengths



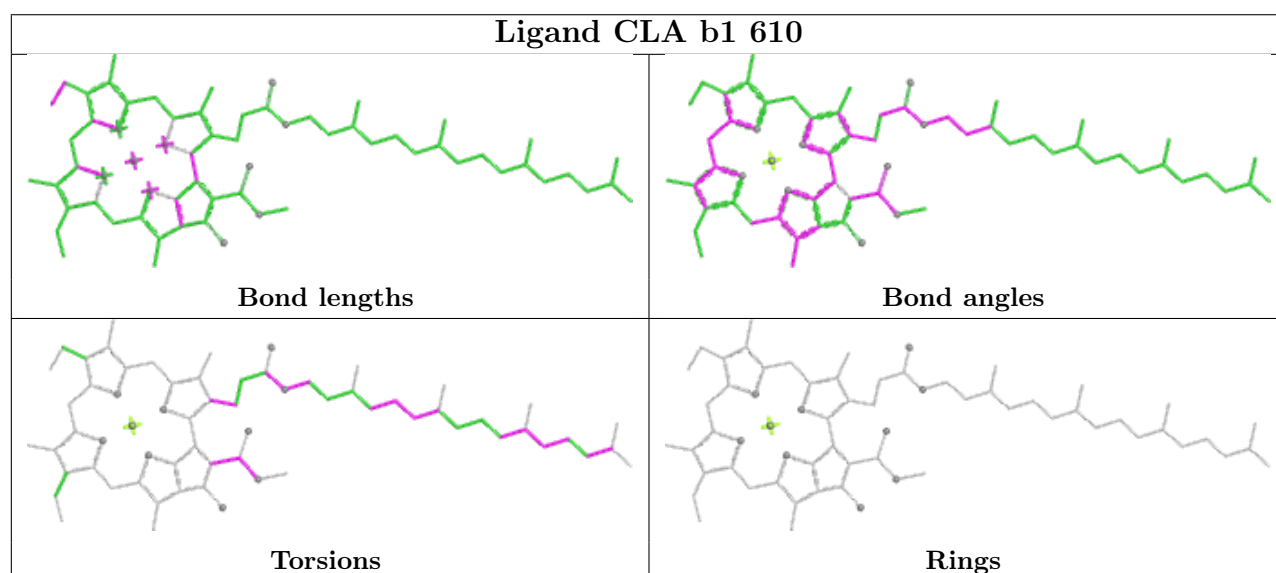
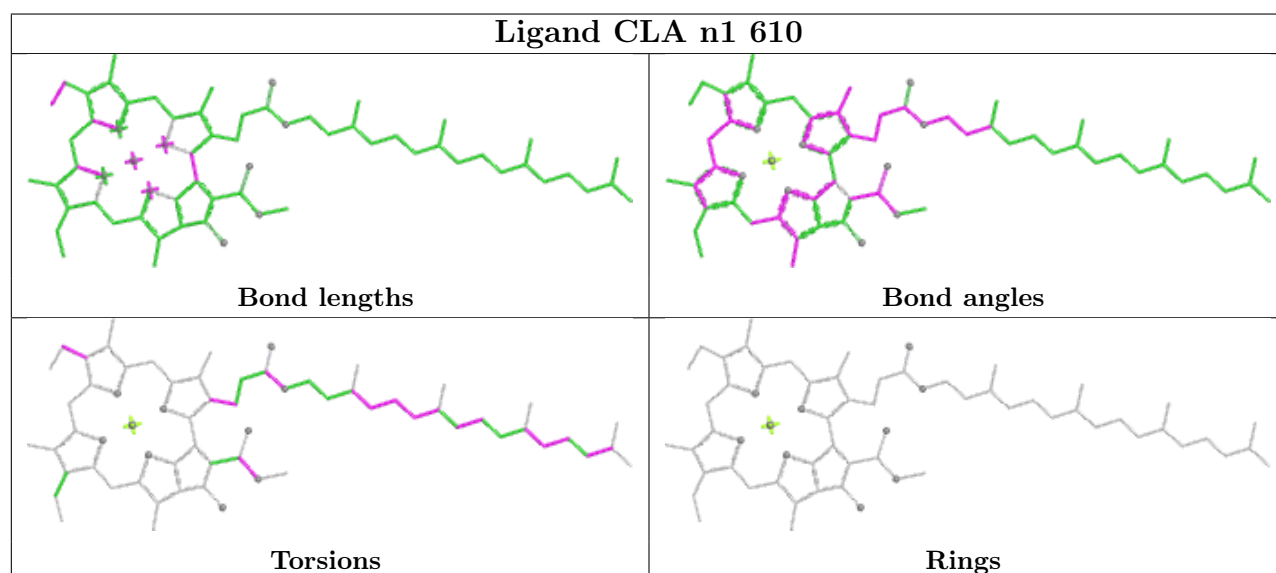
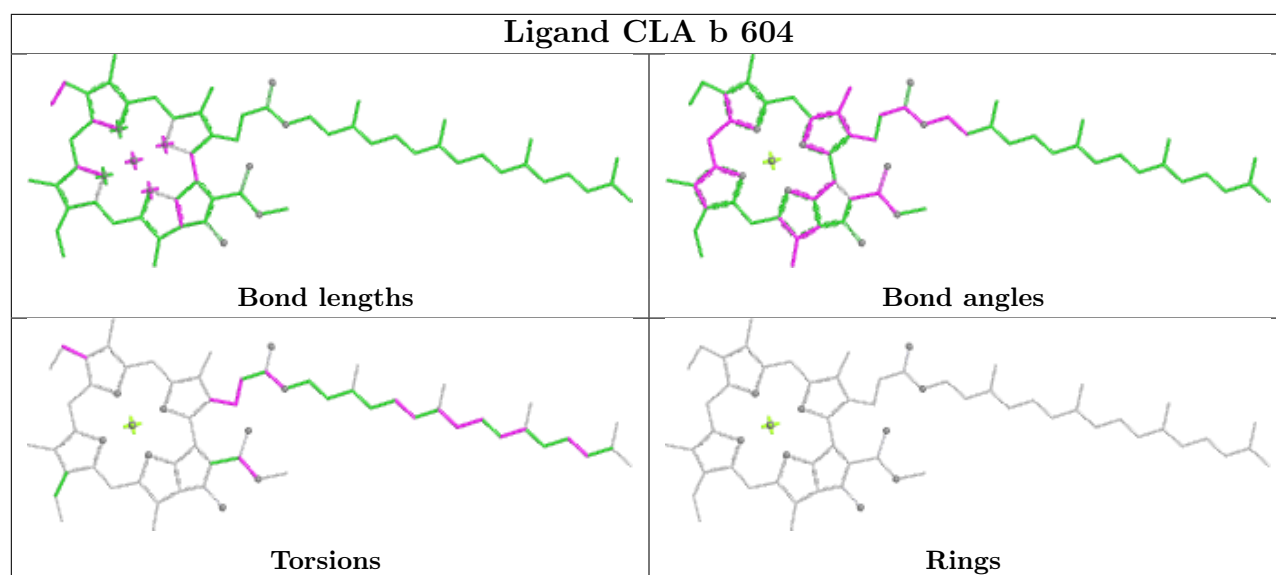
Bond angles

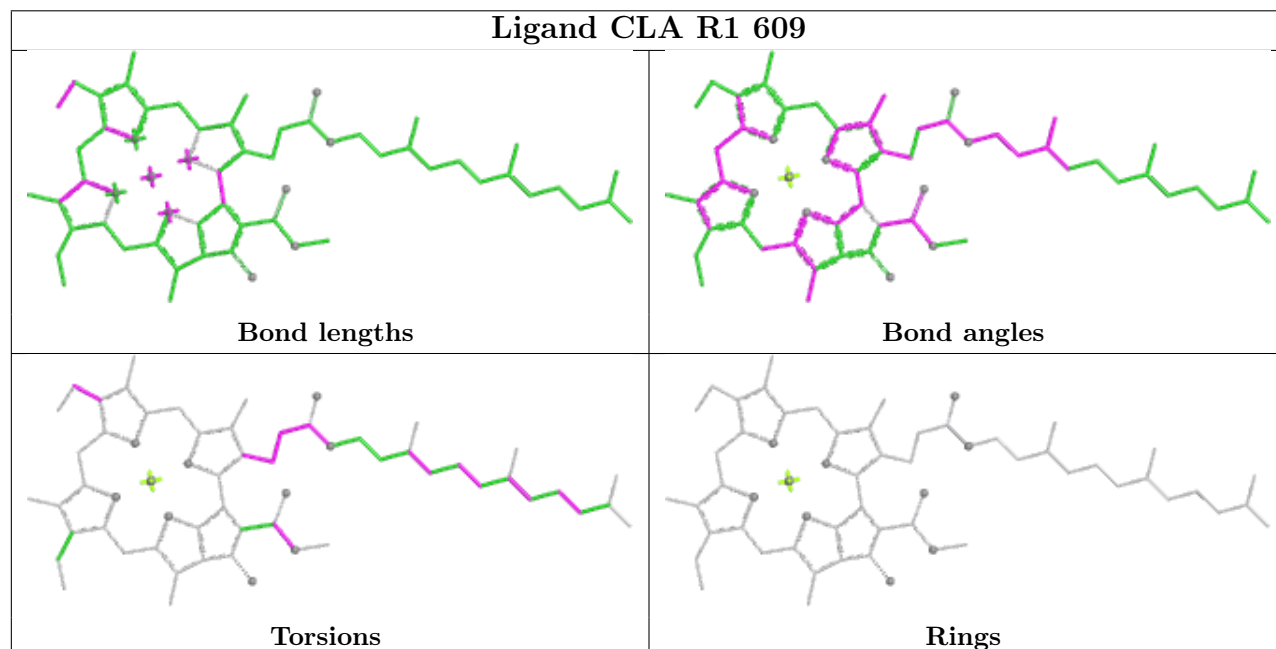
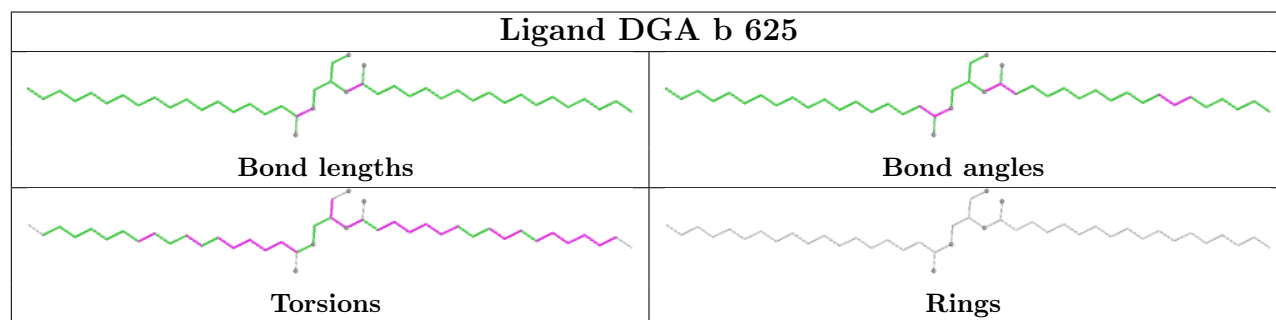
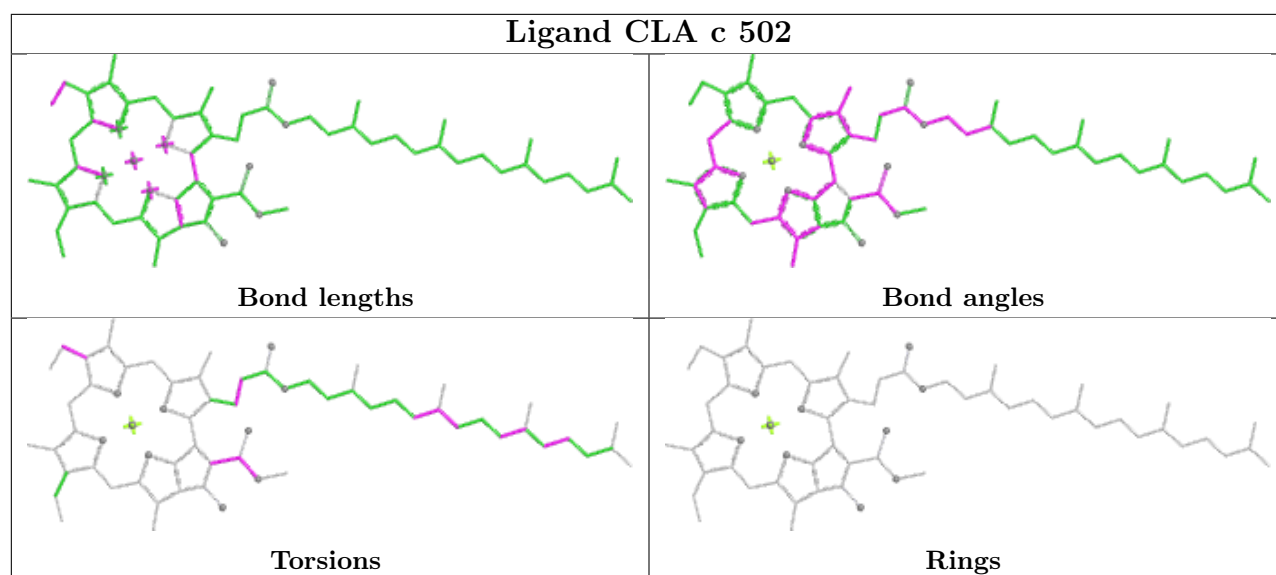


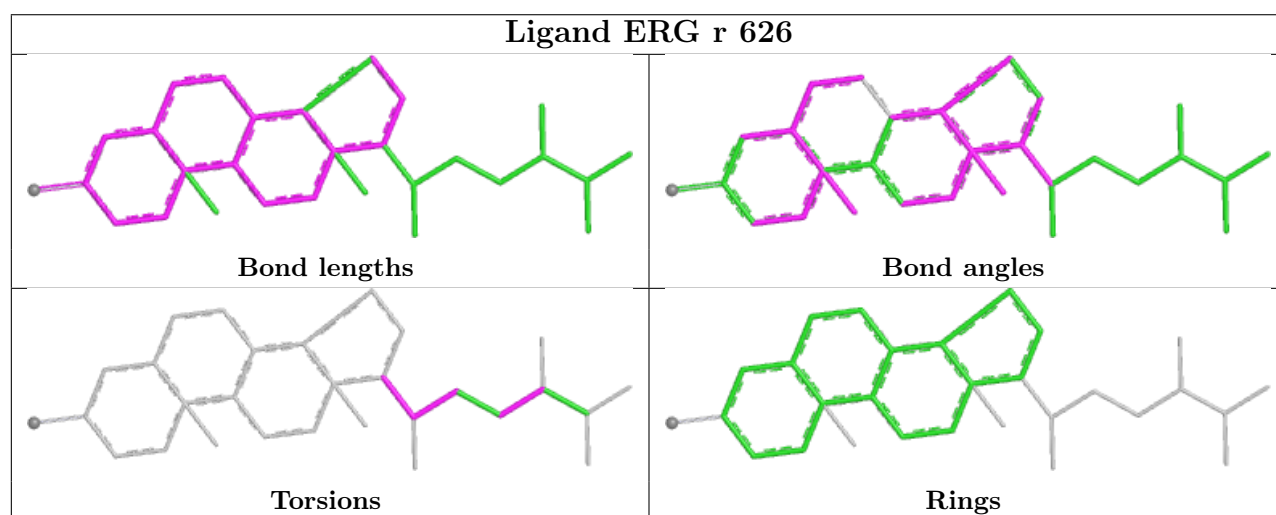
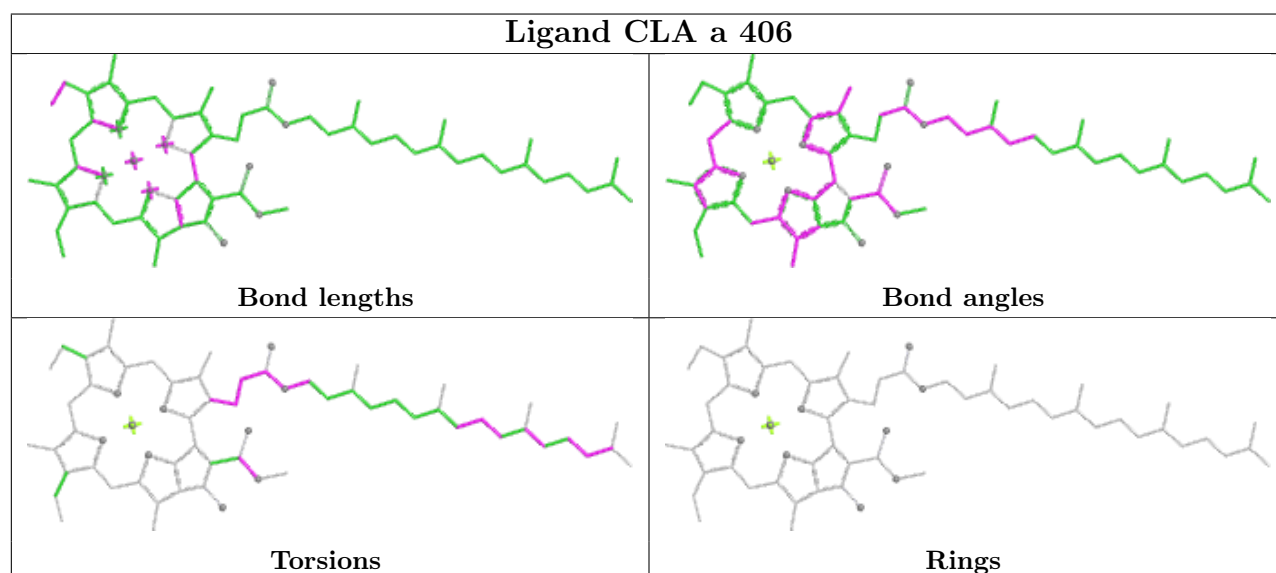
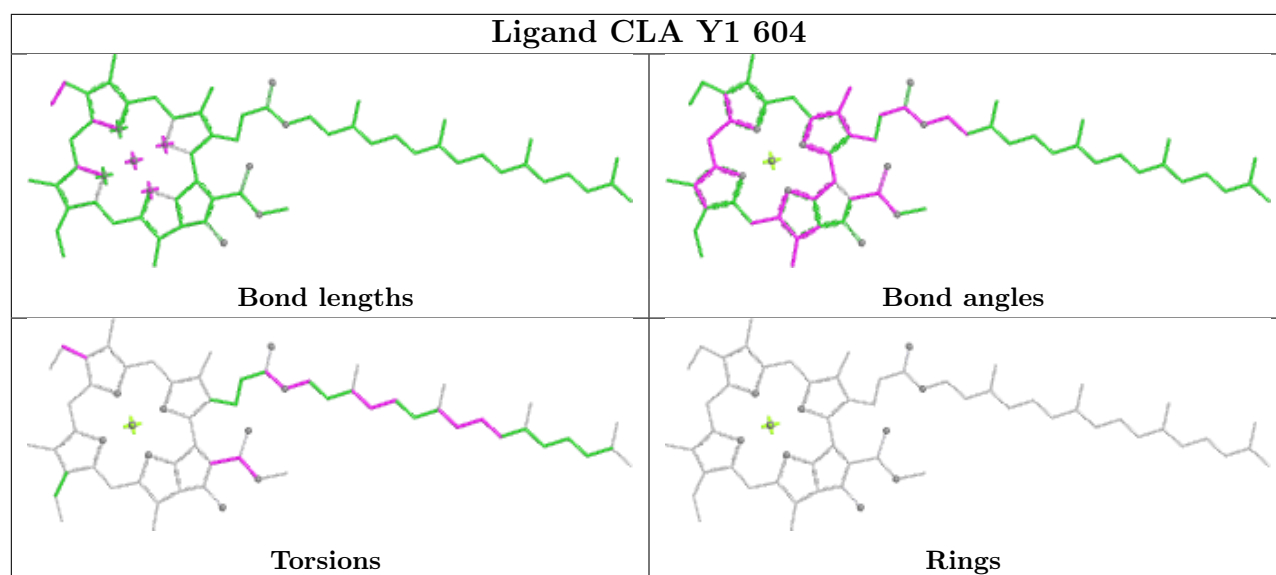
Torsions

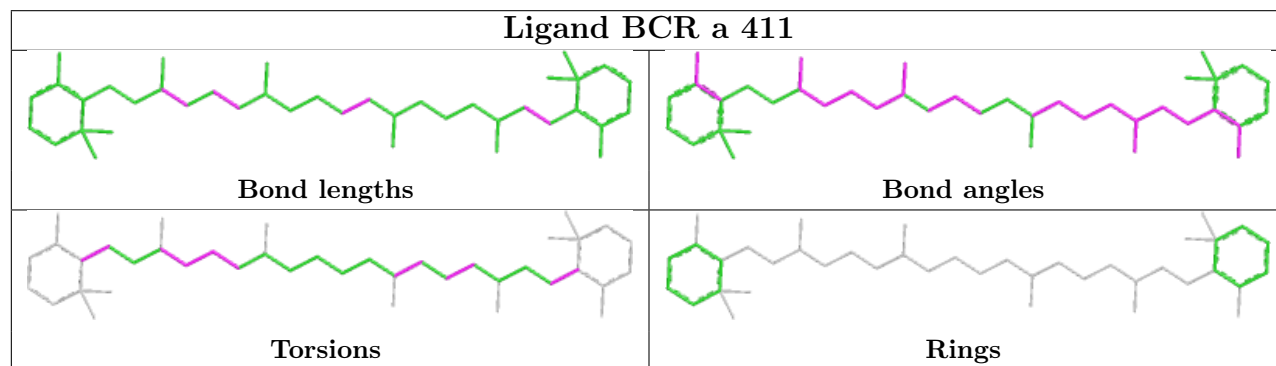
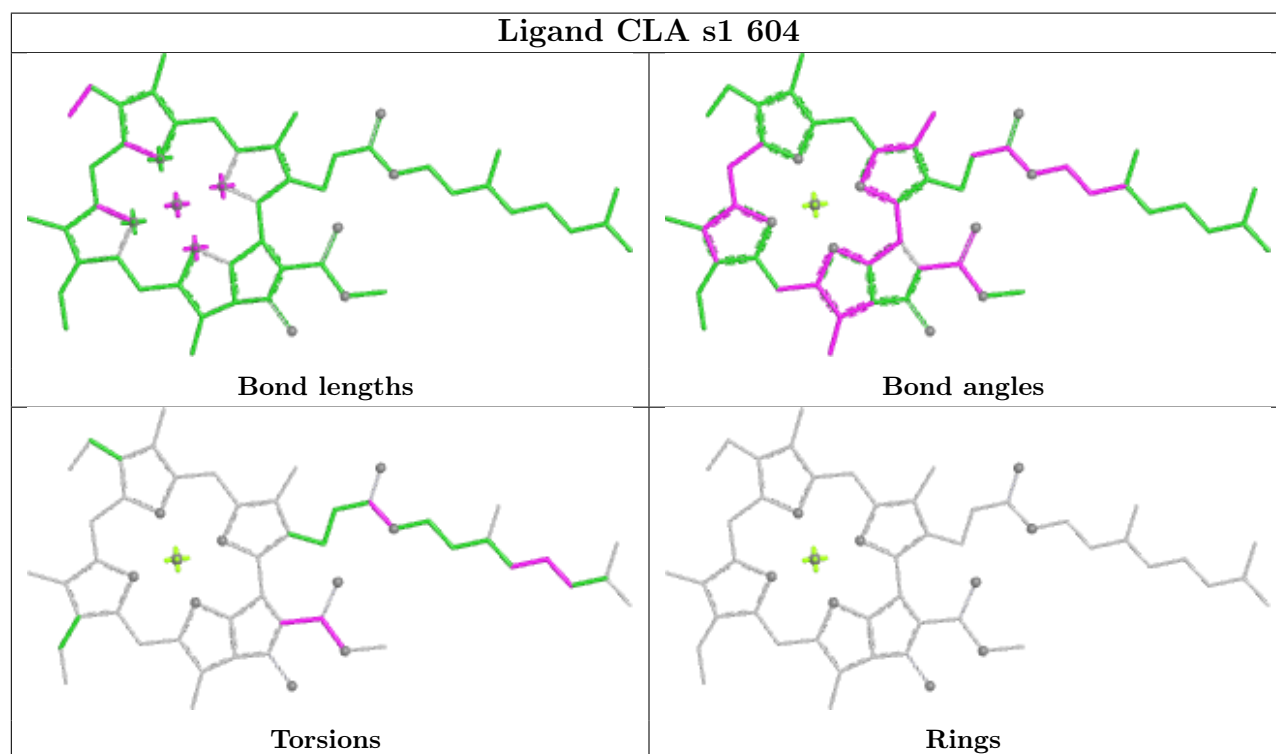
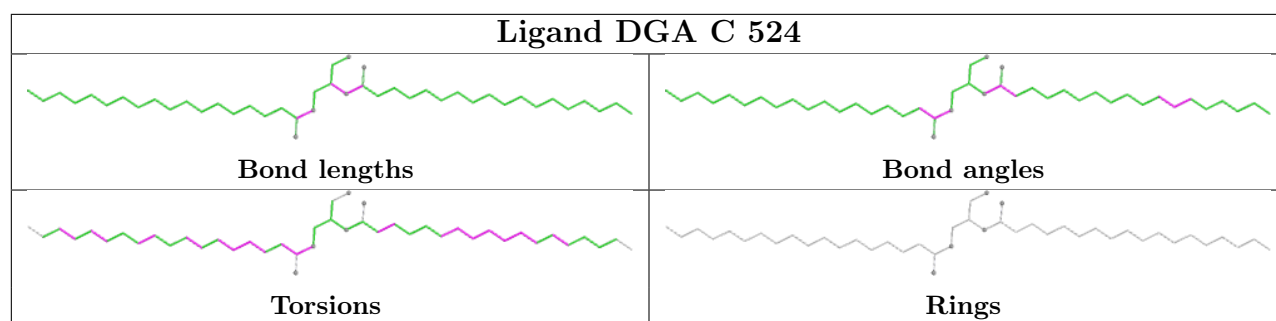


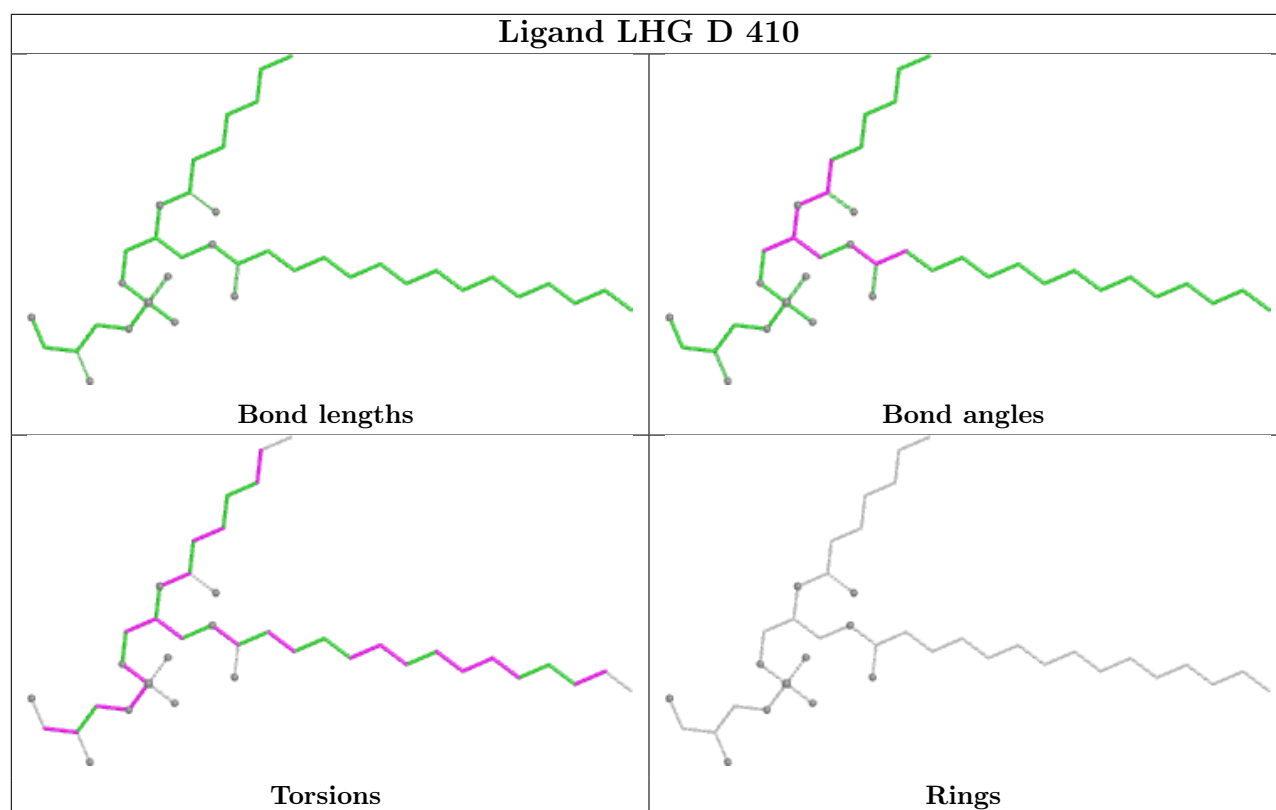
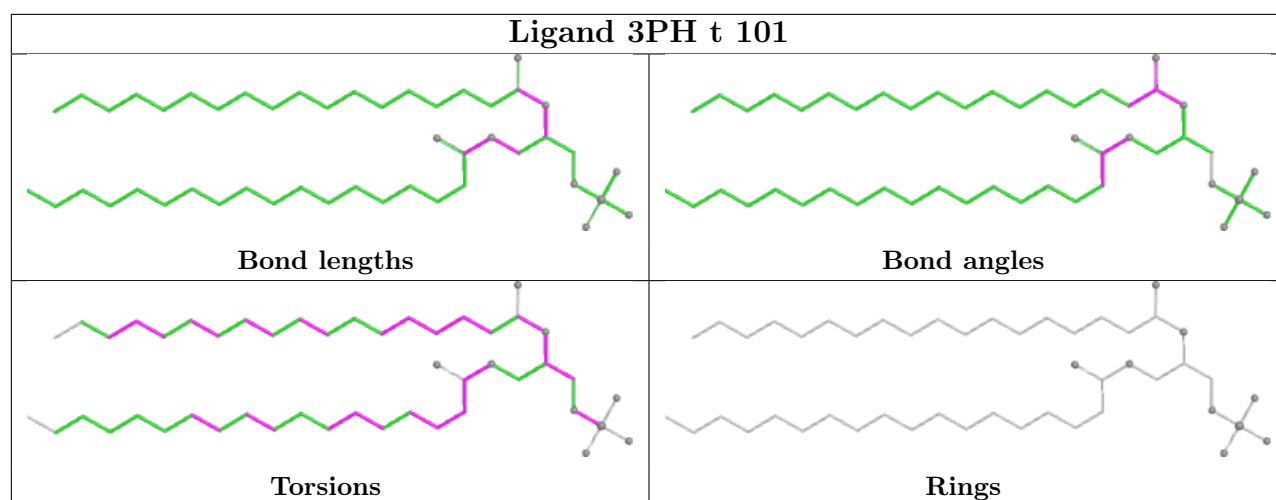
Rings

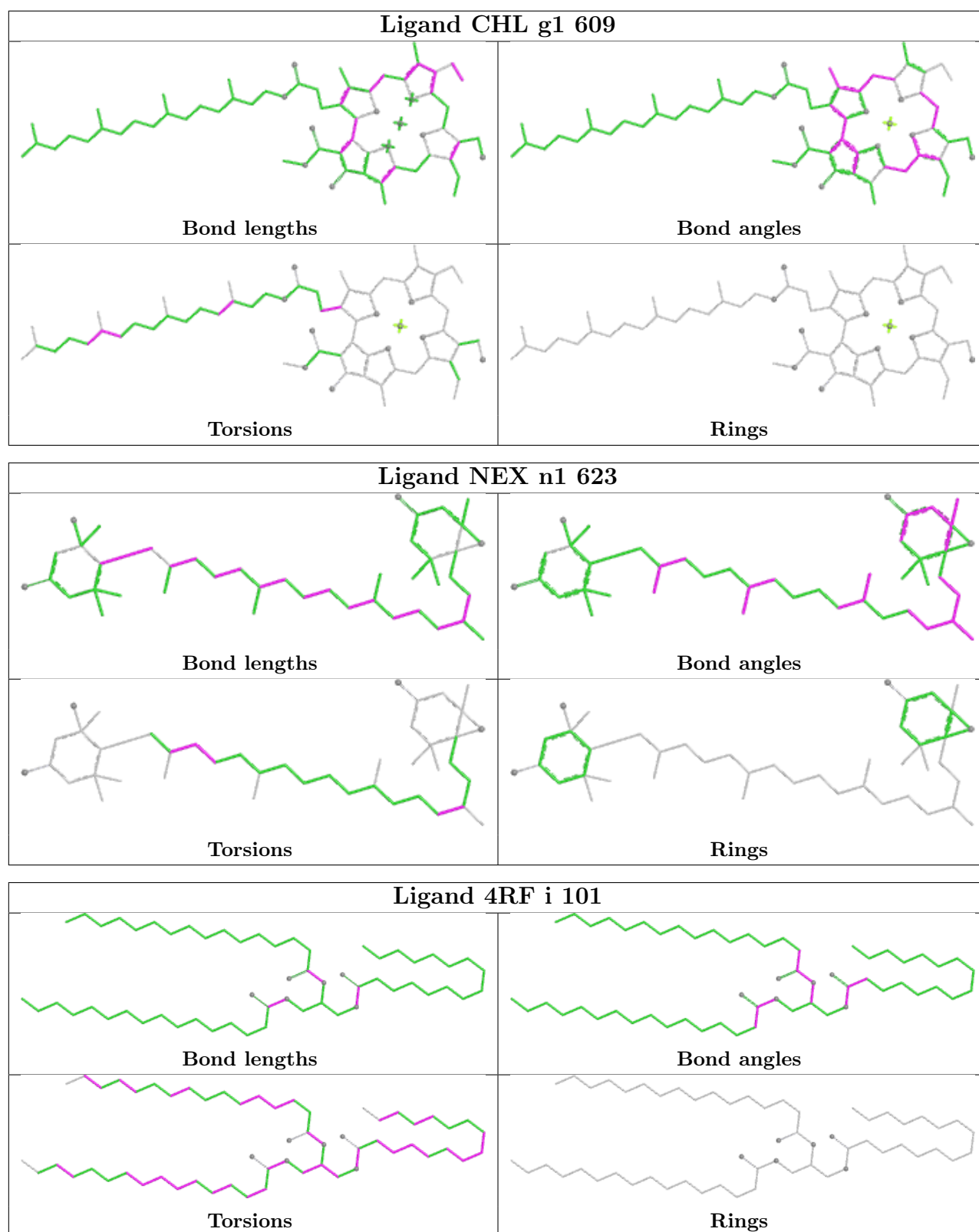


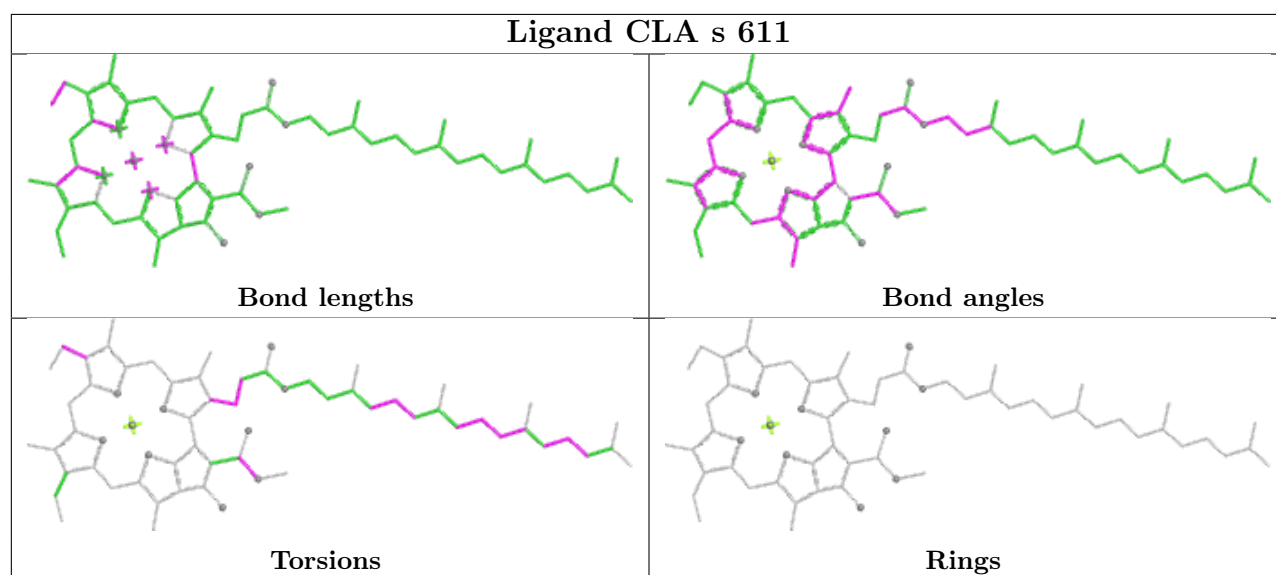
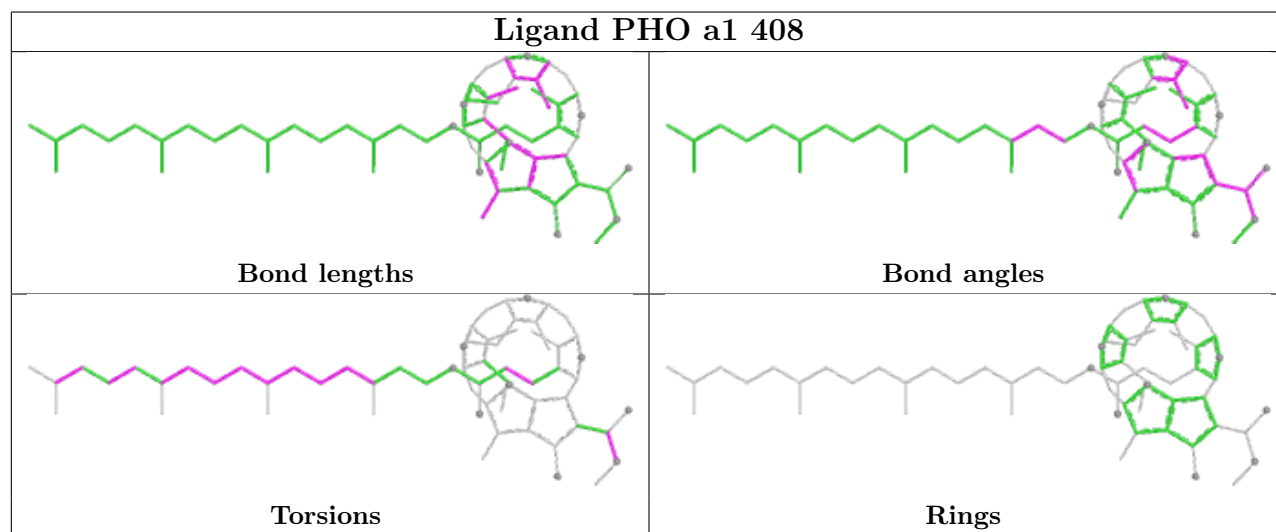
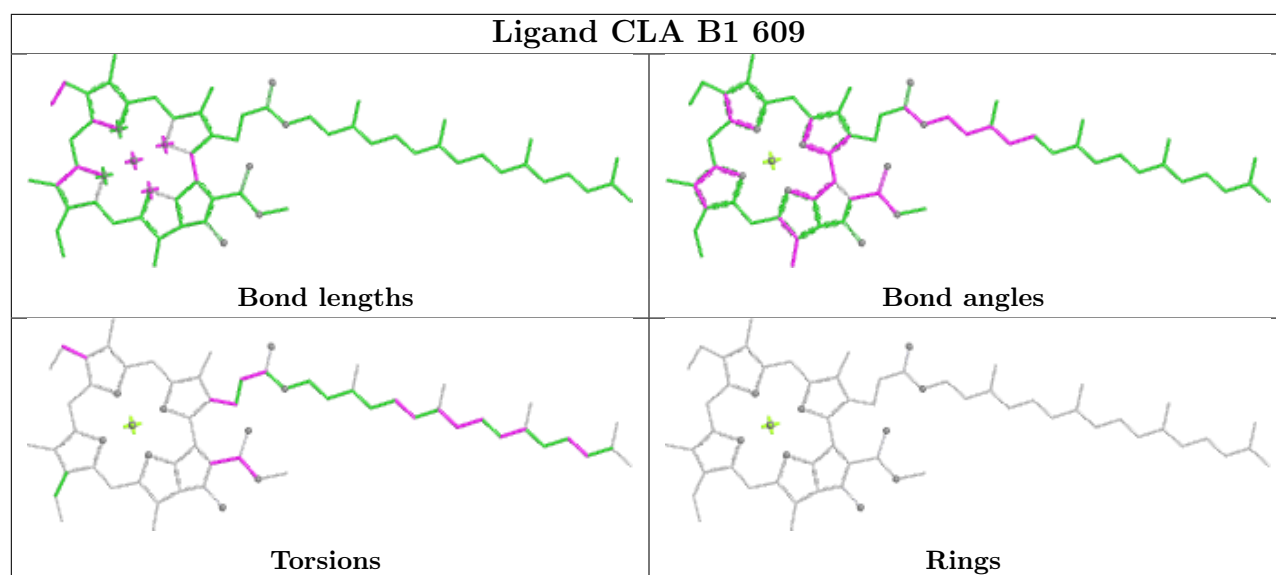


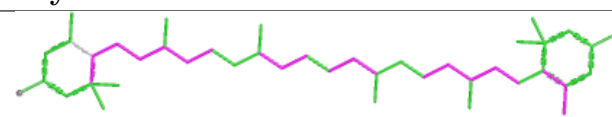
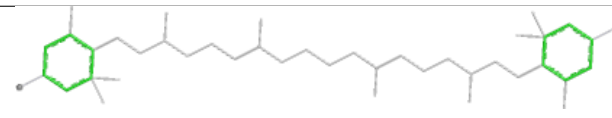


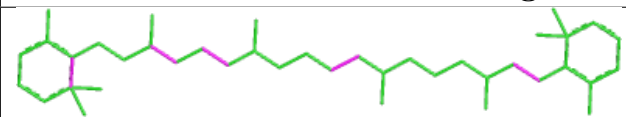
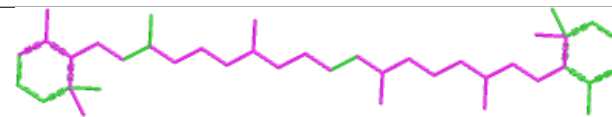
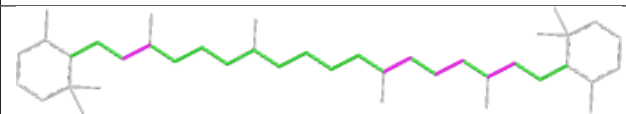
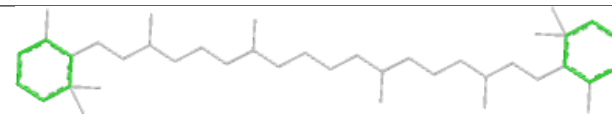


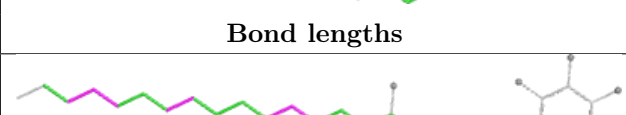
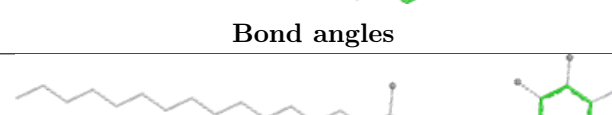


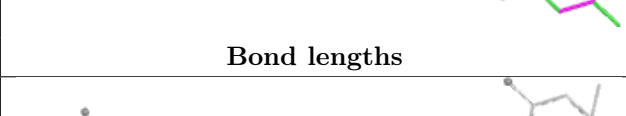
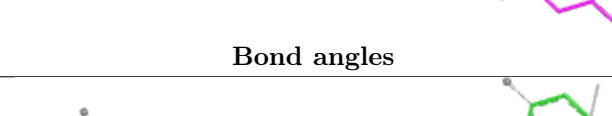


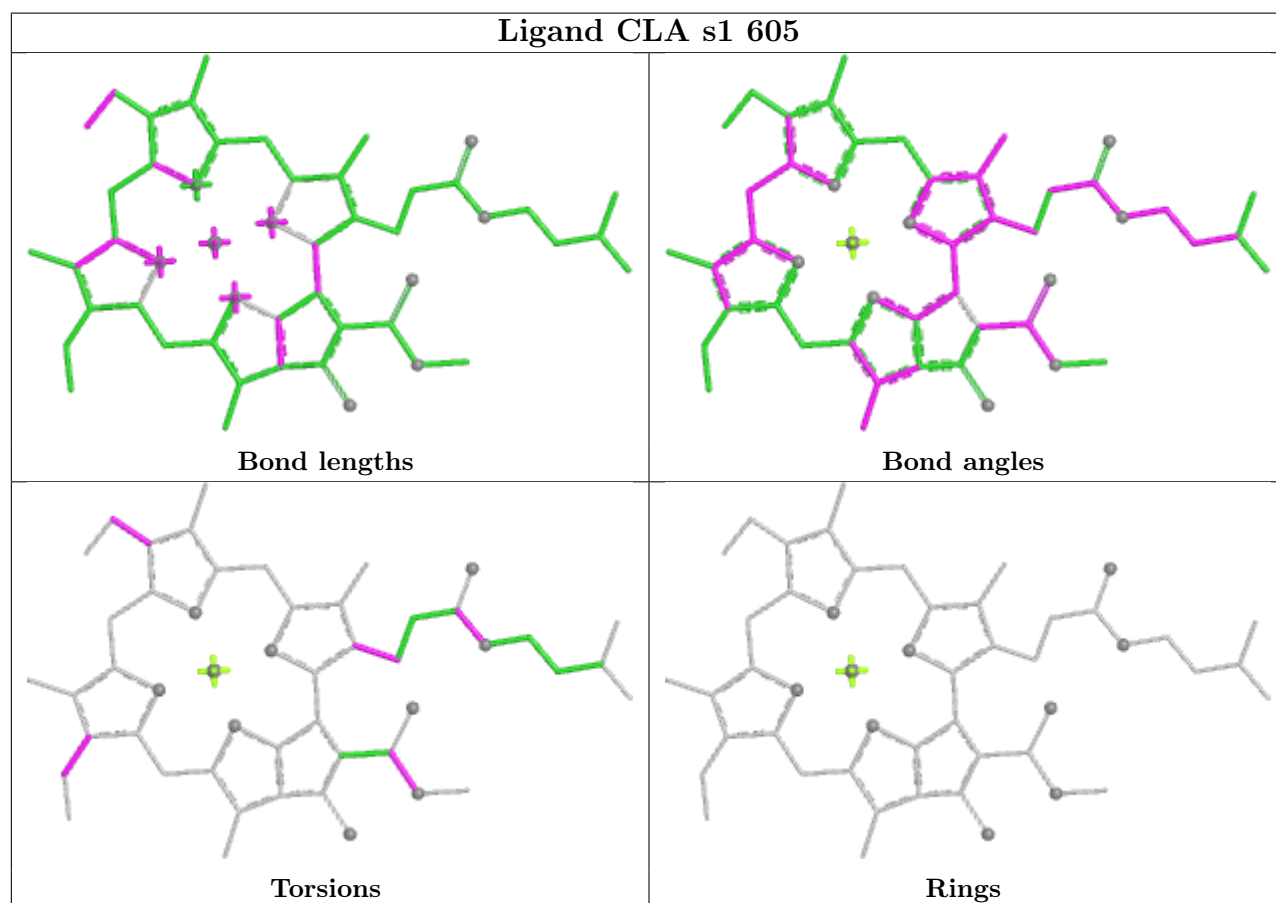
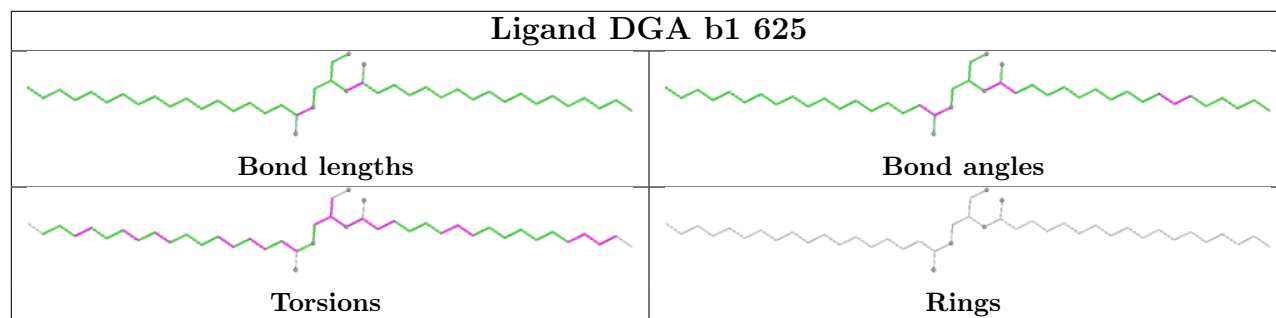


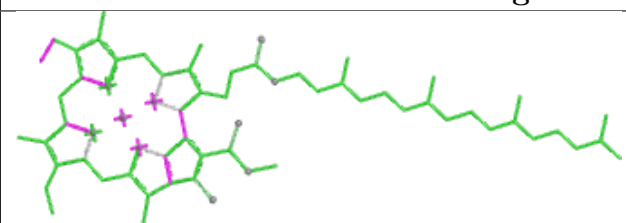
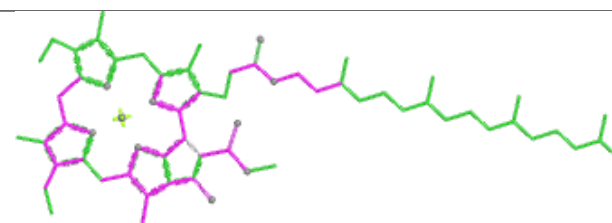
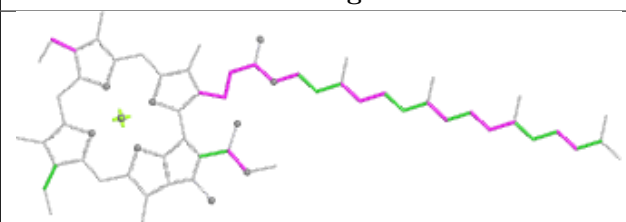
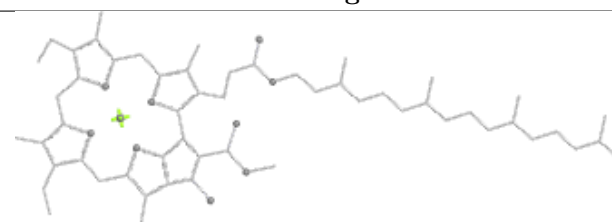
Ligand LUT y1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

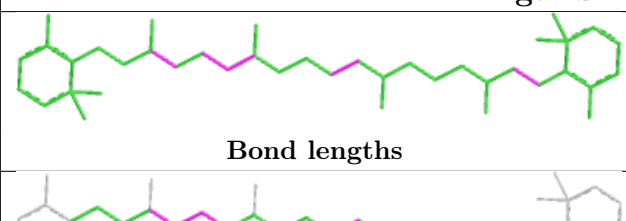
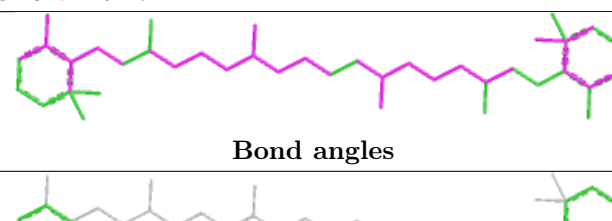
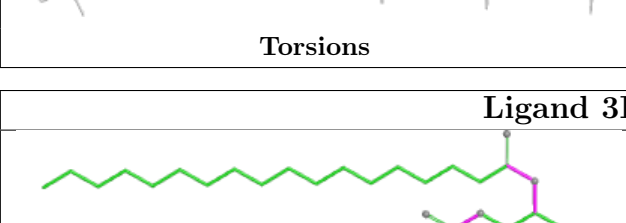
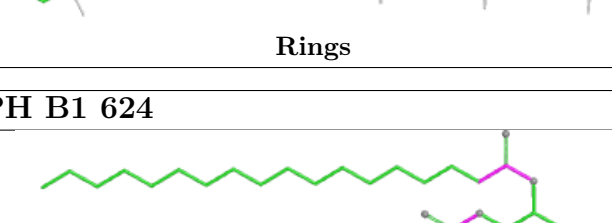
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

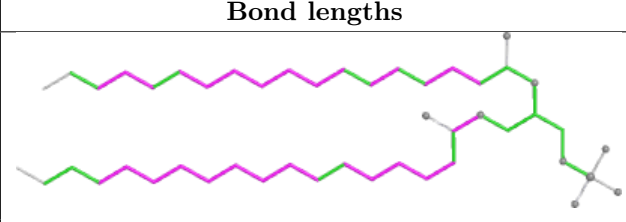
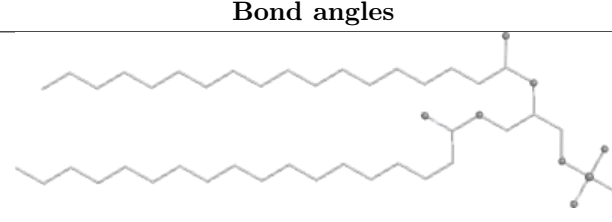
Ligand LMG a 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

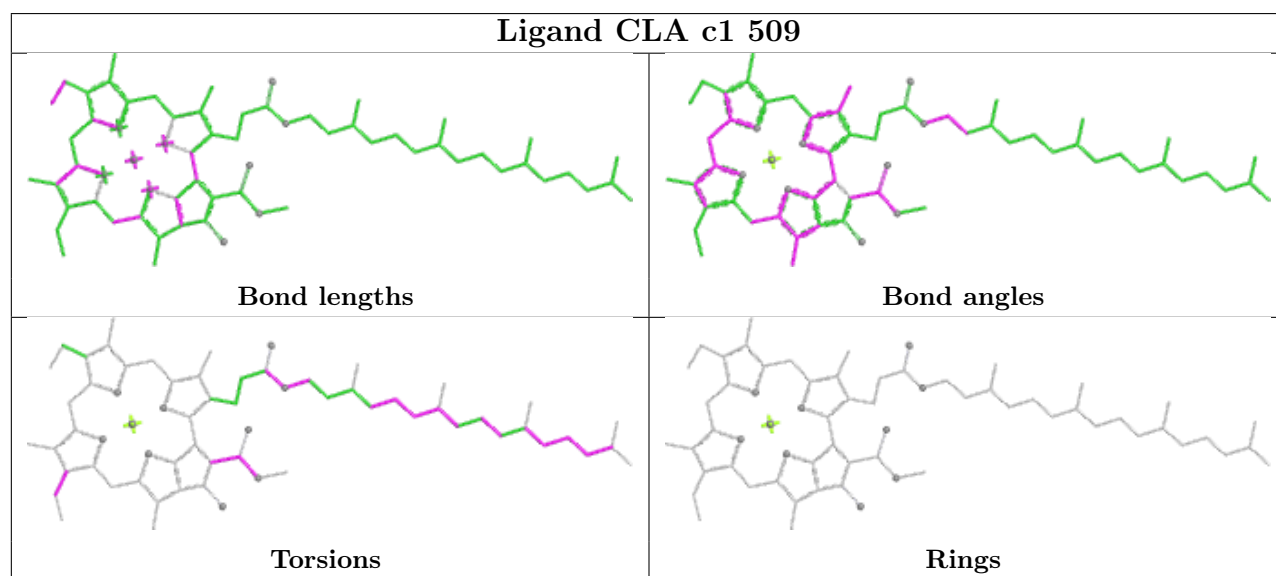
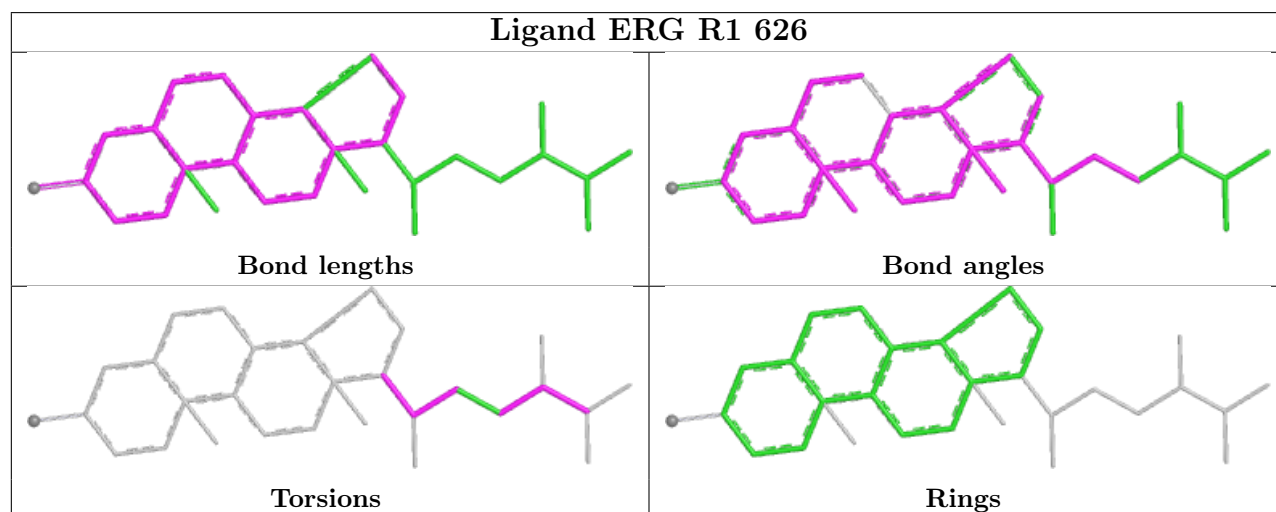
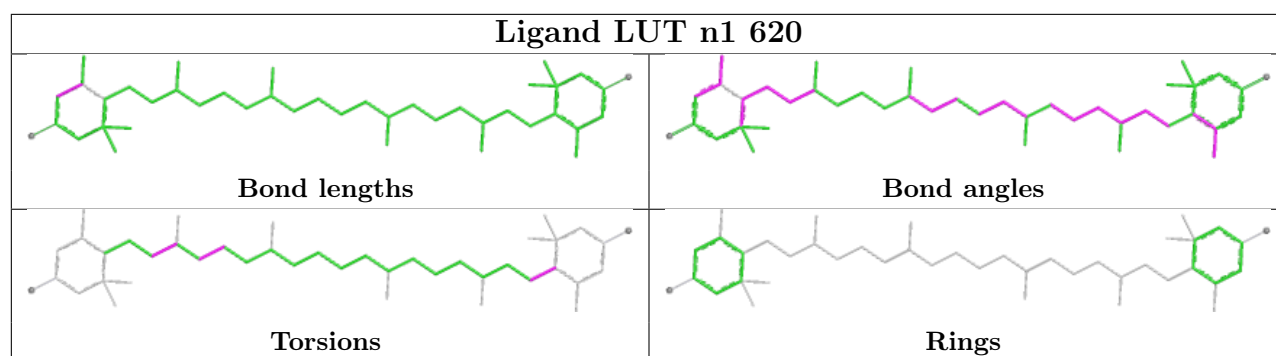
Ligand NEX G 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

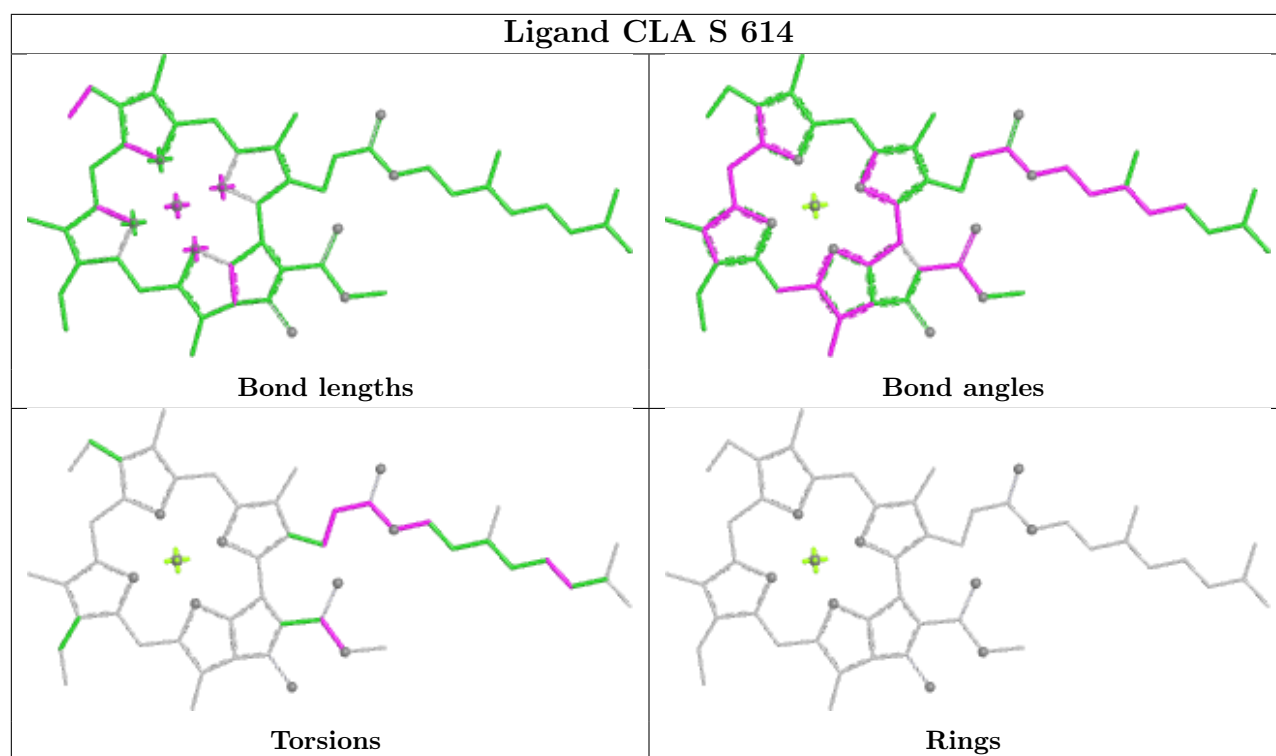


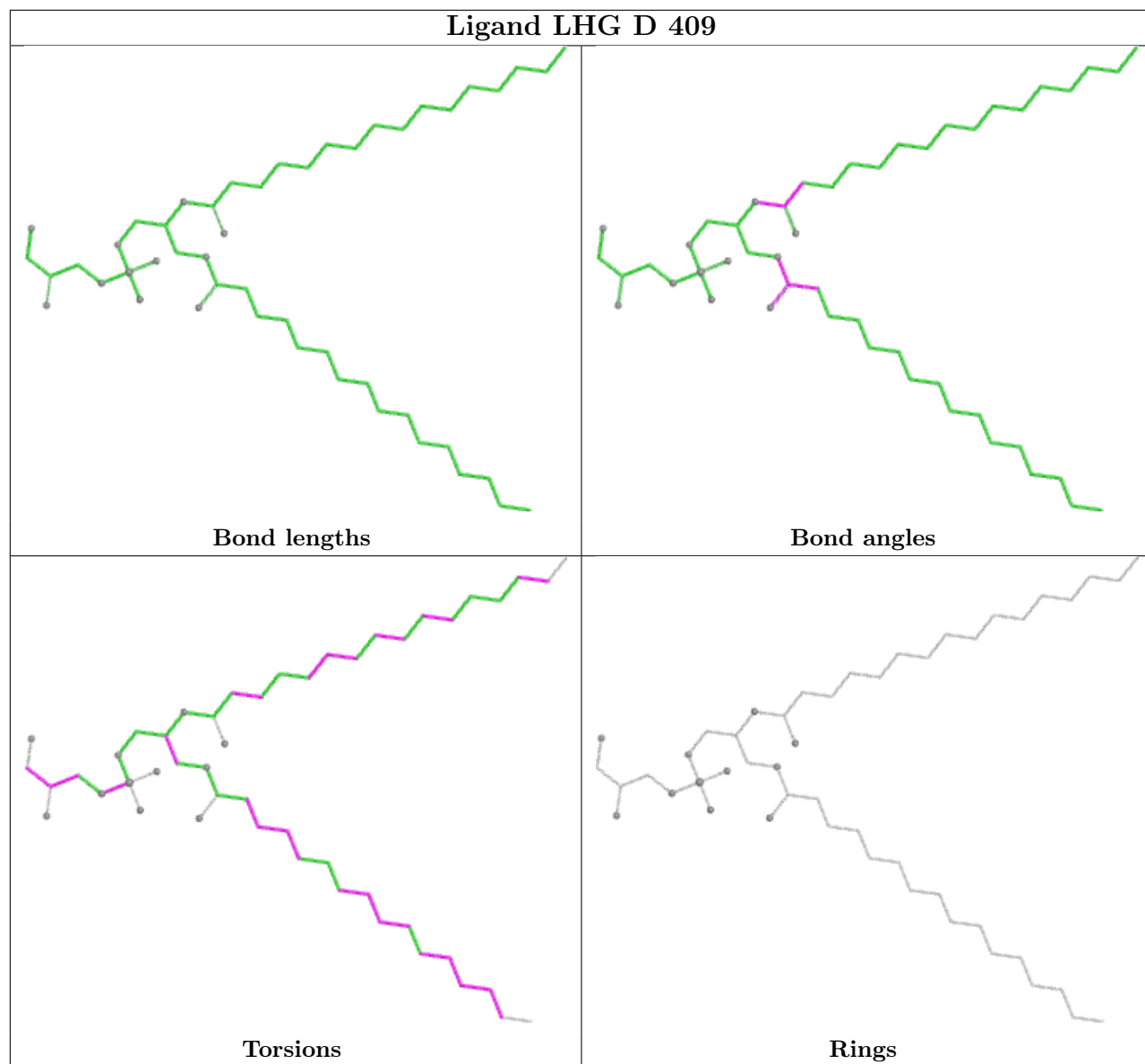
Ligand CLA B1 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c1 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

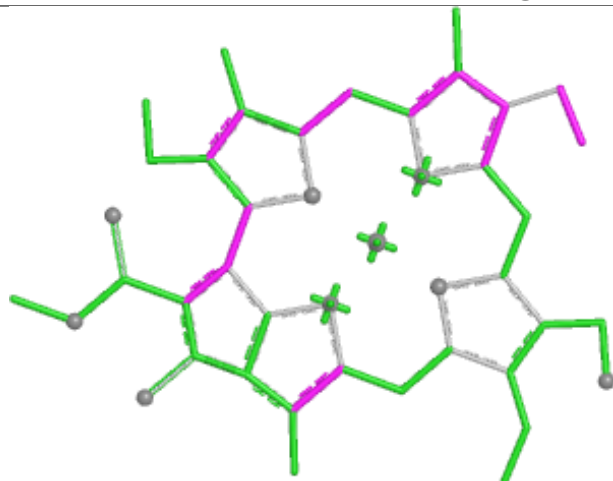
Ligand 3PH B1 624	
	
Bond lengths	Bond angles
	
Torsions	Rings



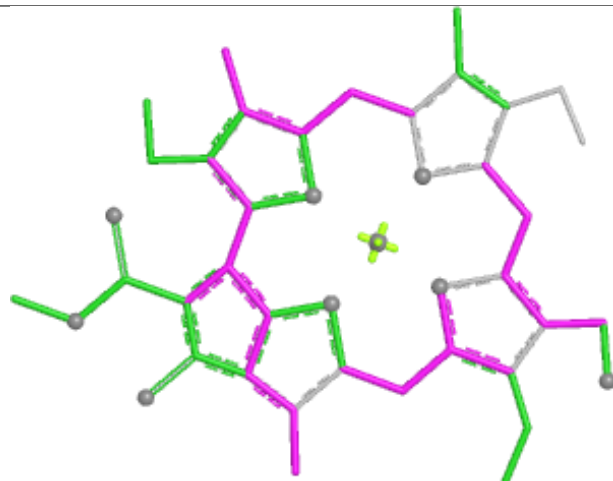




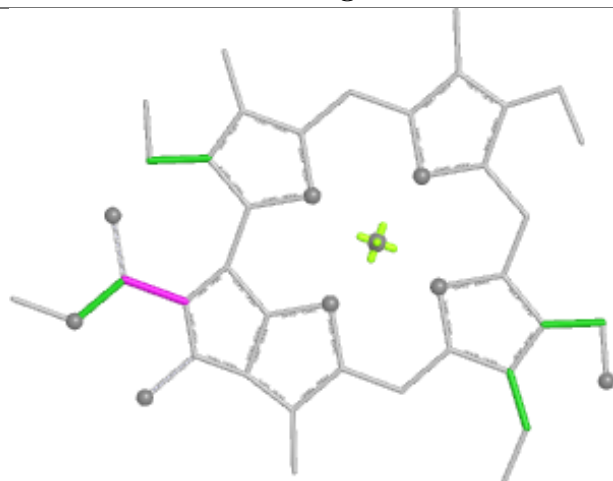
Ligand CHL S 607



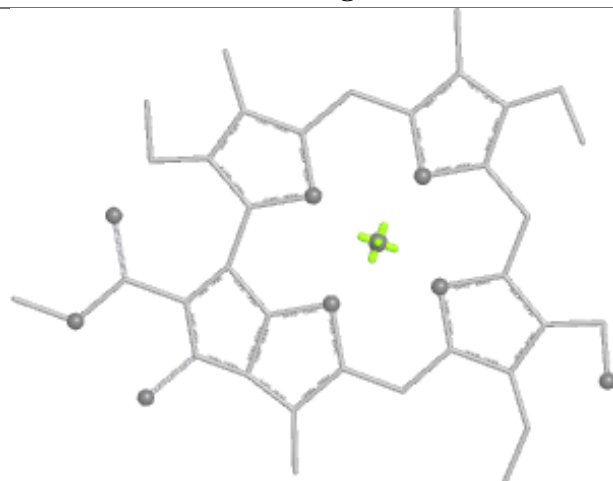
Bond lengths



Bond angles

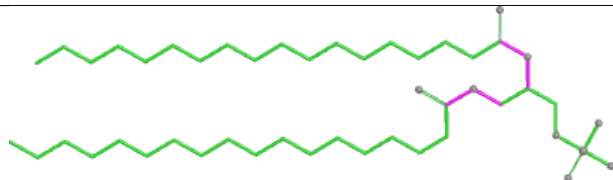


Torsions

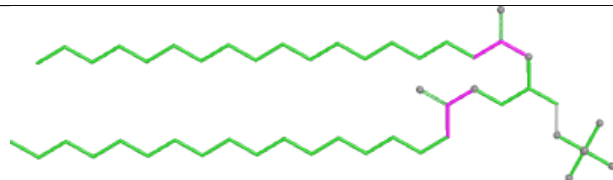


Rings

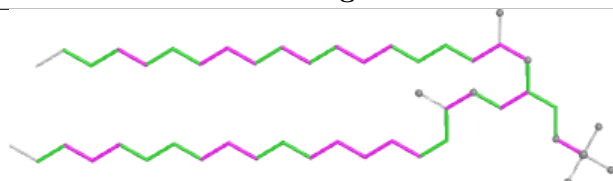
Ligand 3PH b1 624



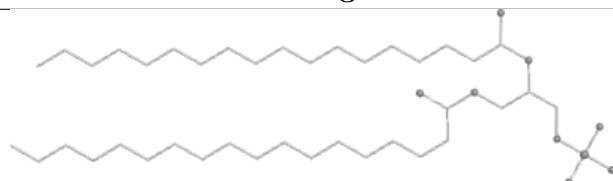
Bond lengths



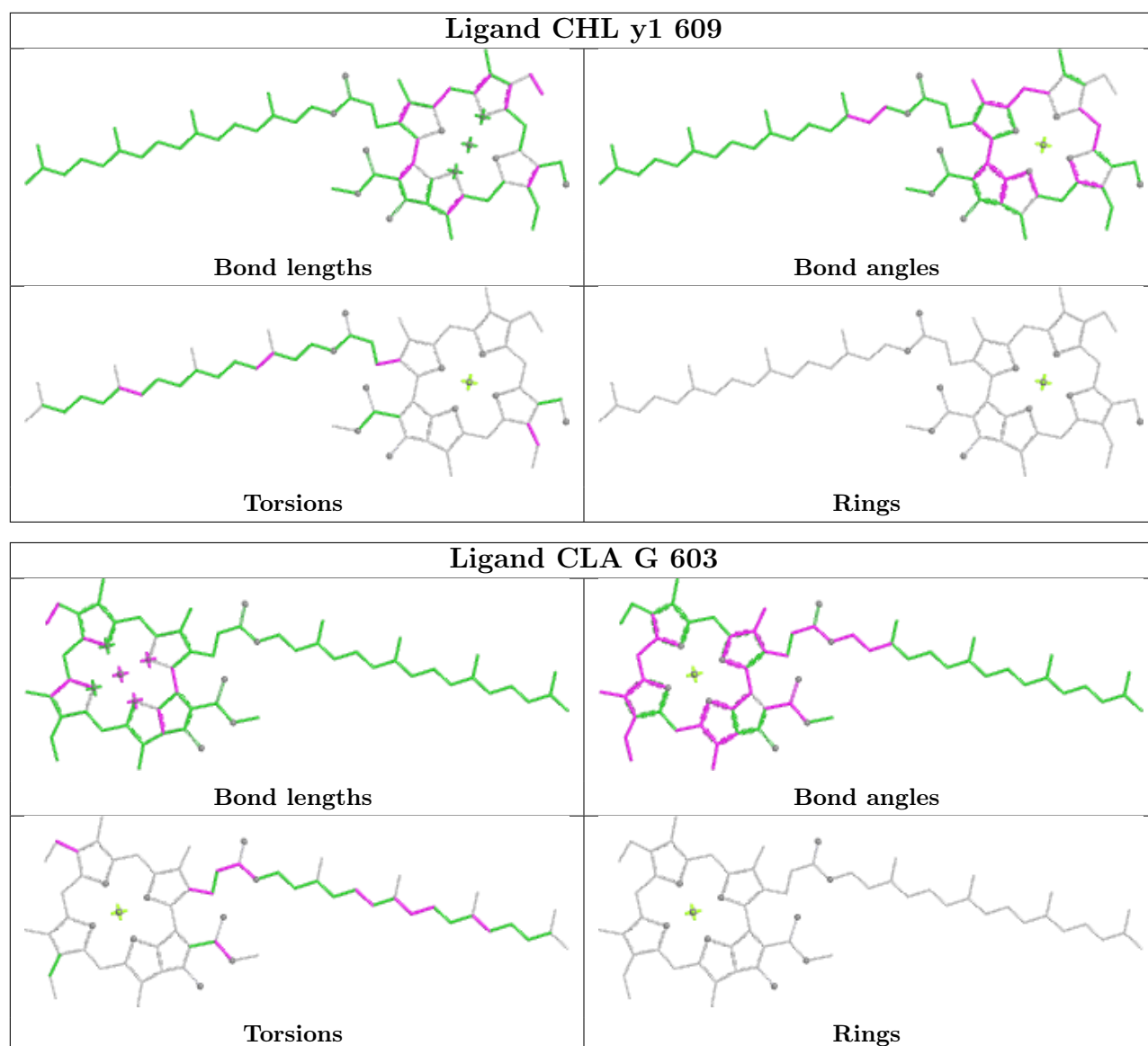
Bond angles

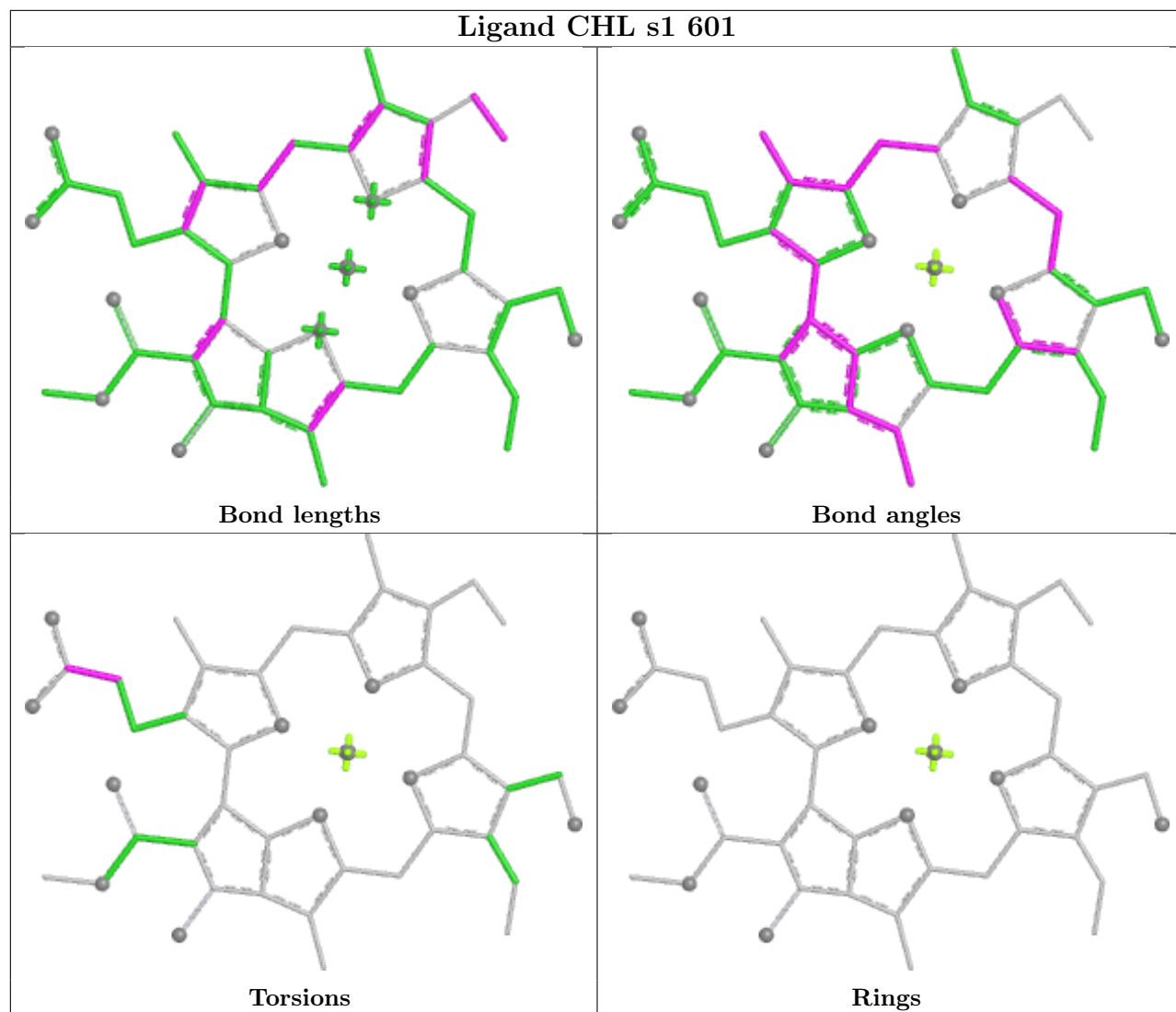


Torsions

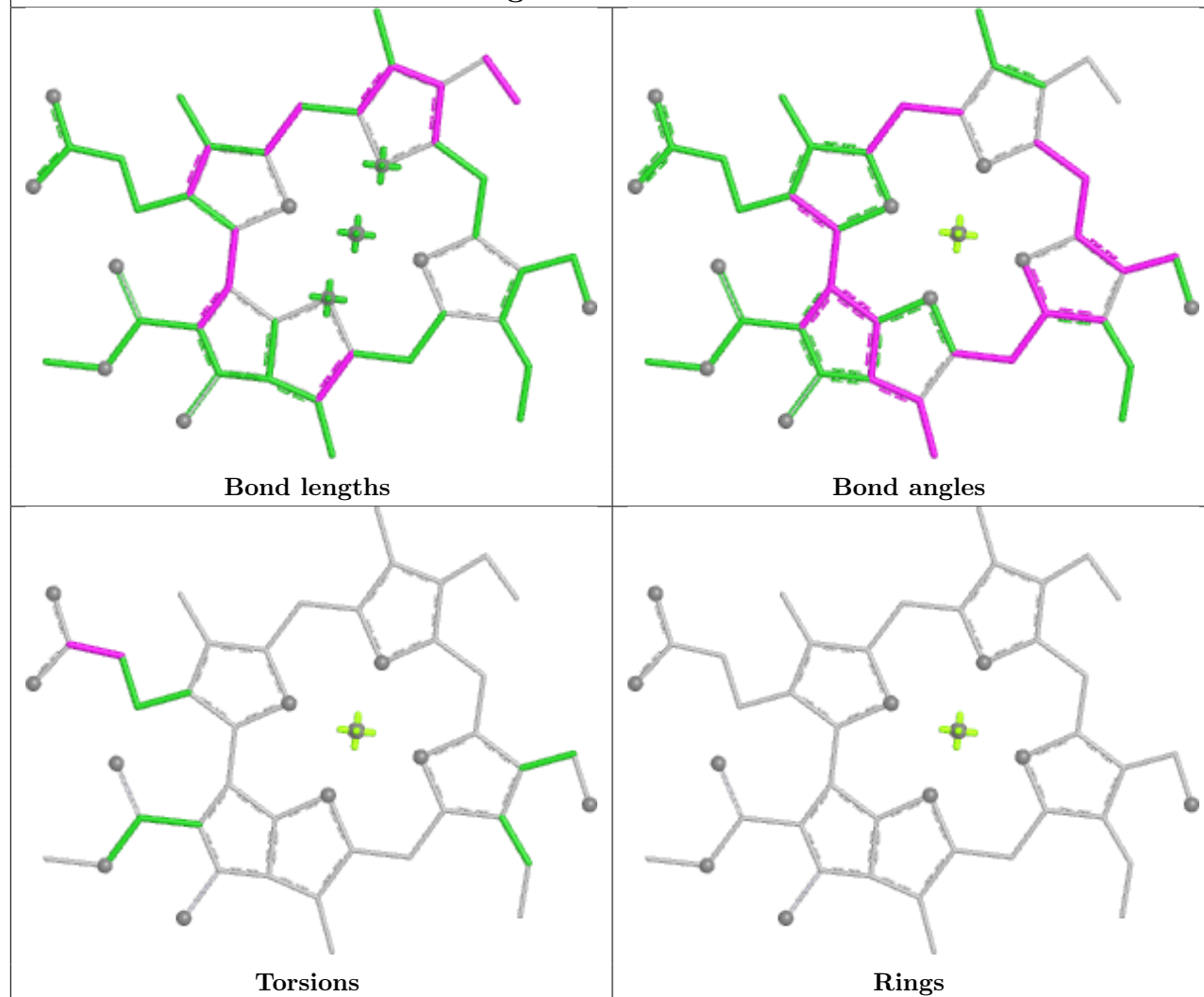


Rings

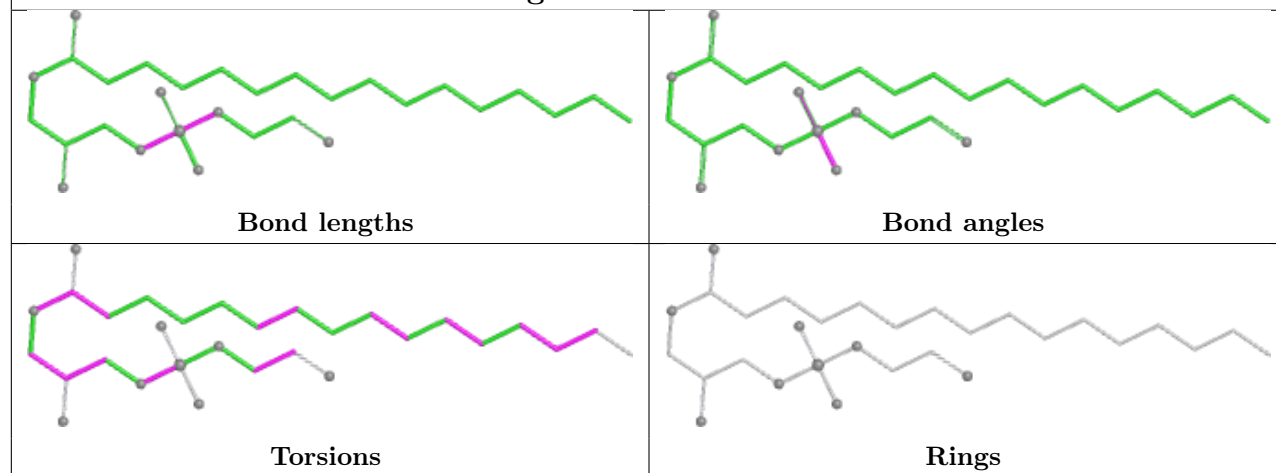


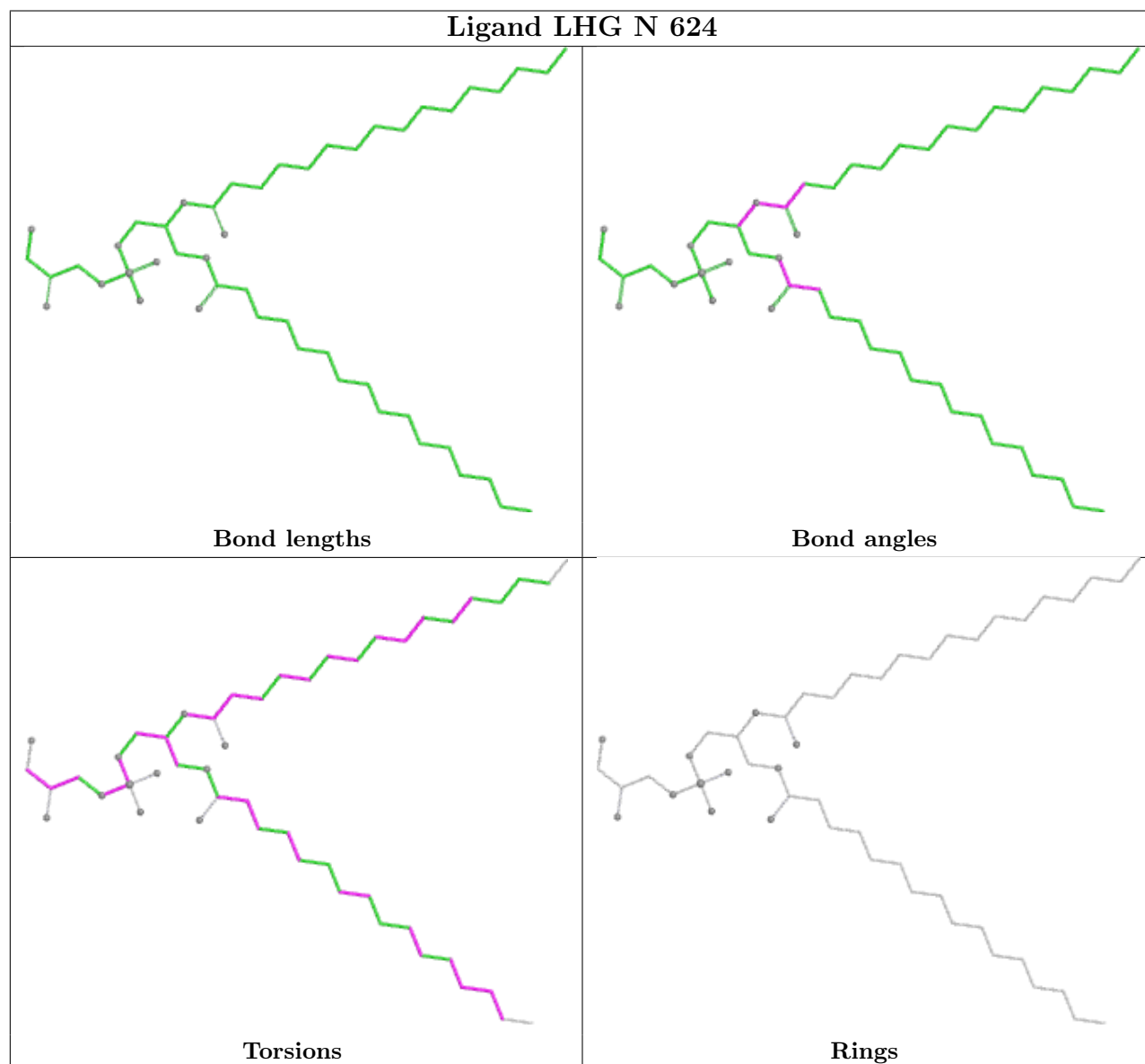
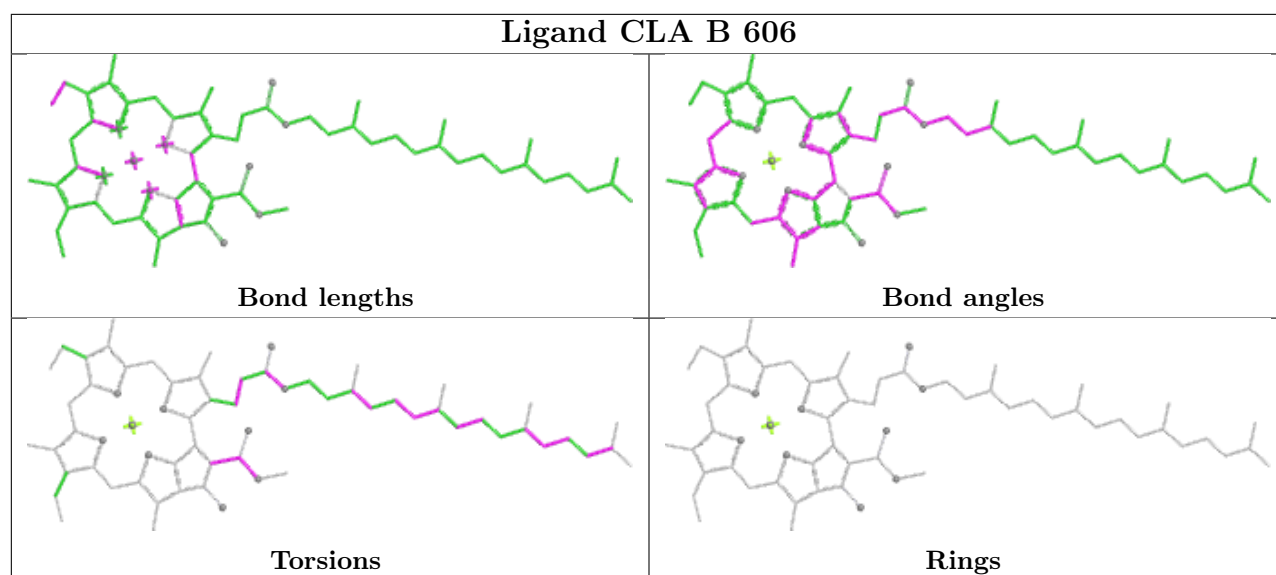


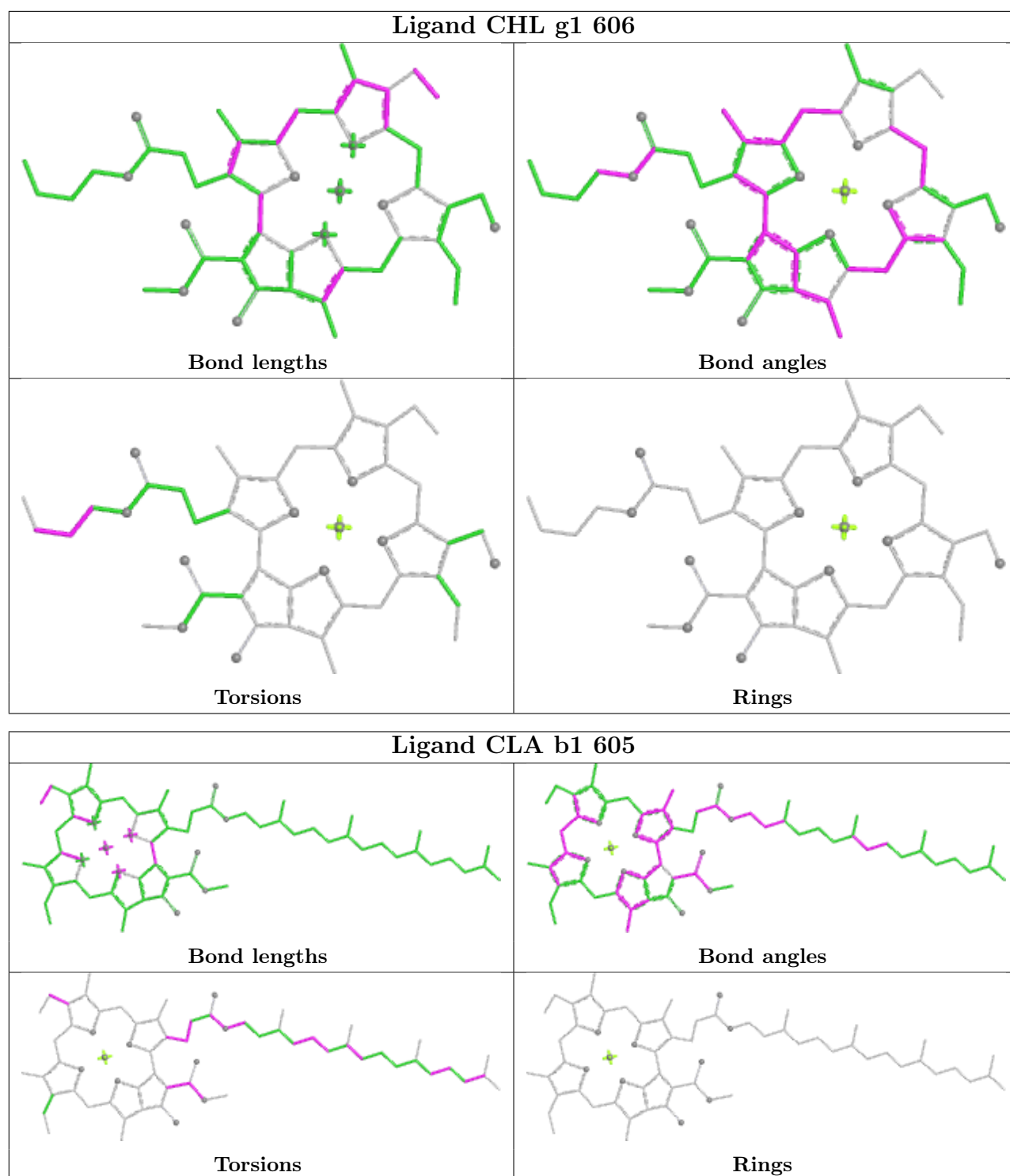
Ligand CHL s 601

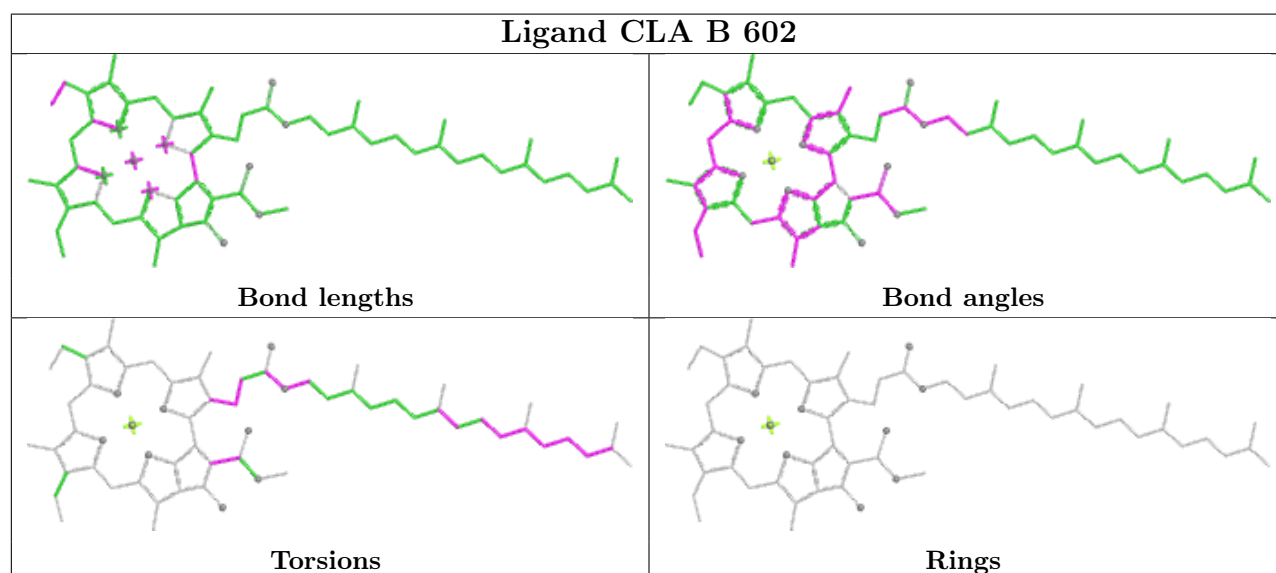
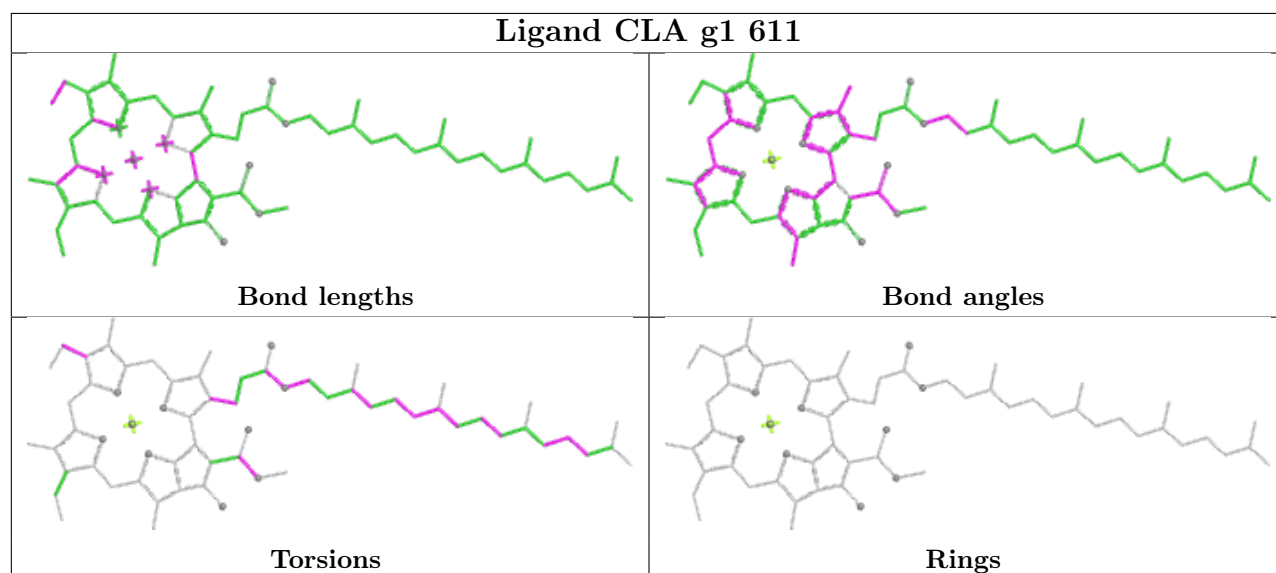
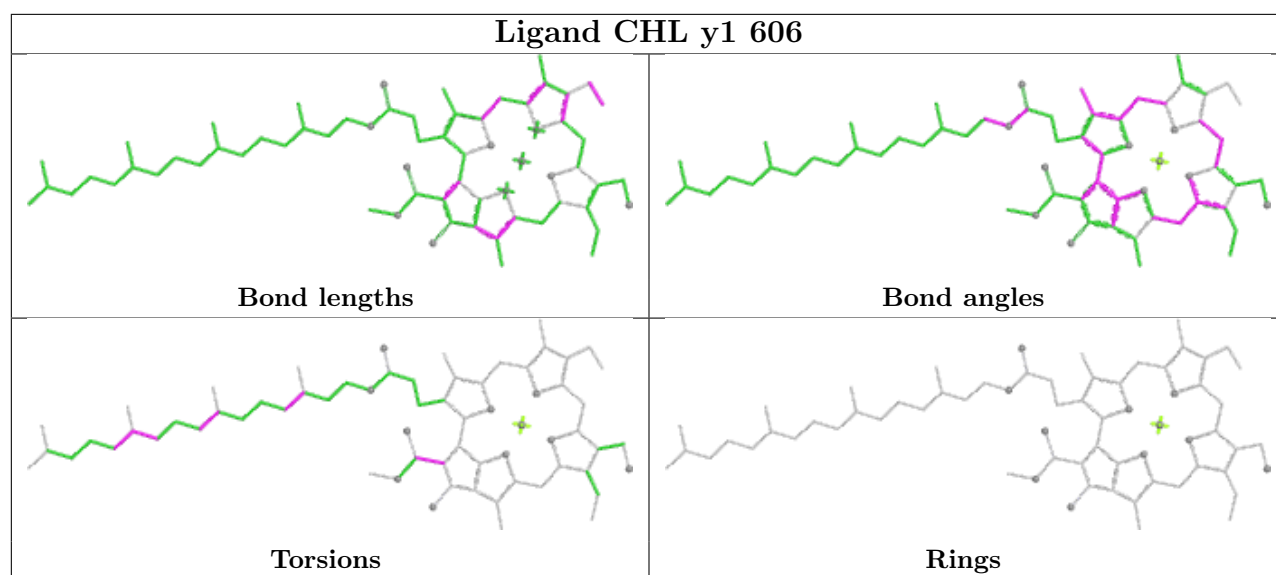


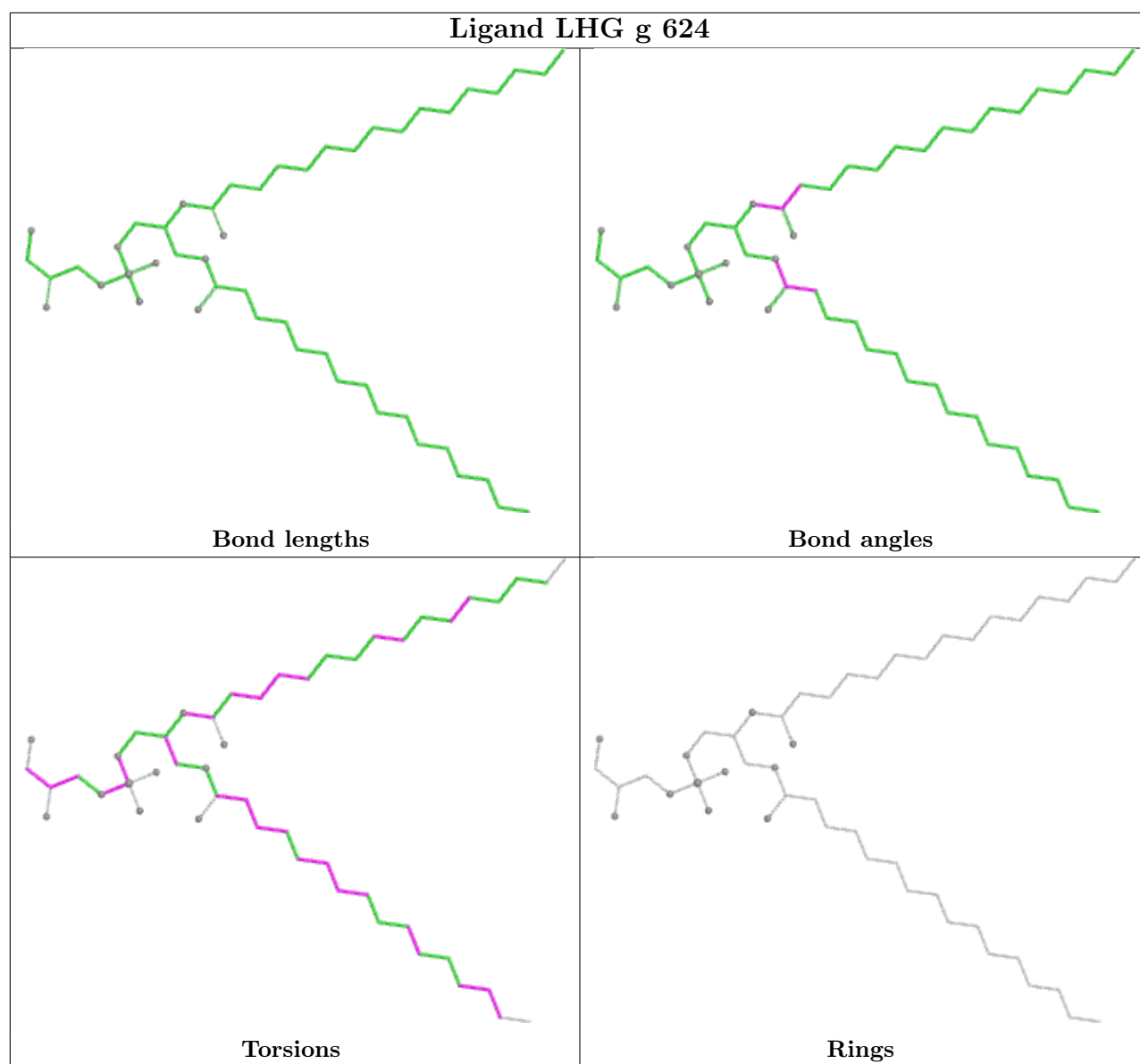
Ligand LPX S1 625

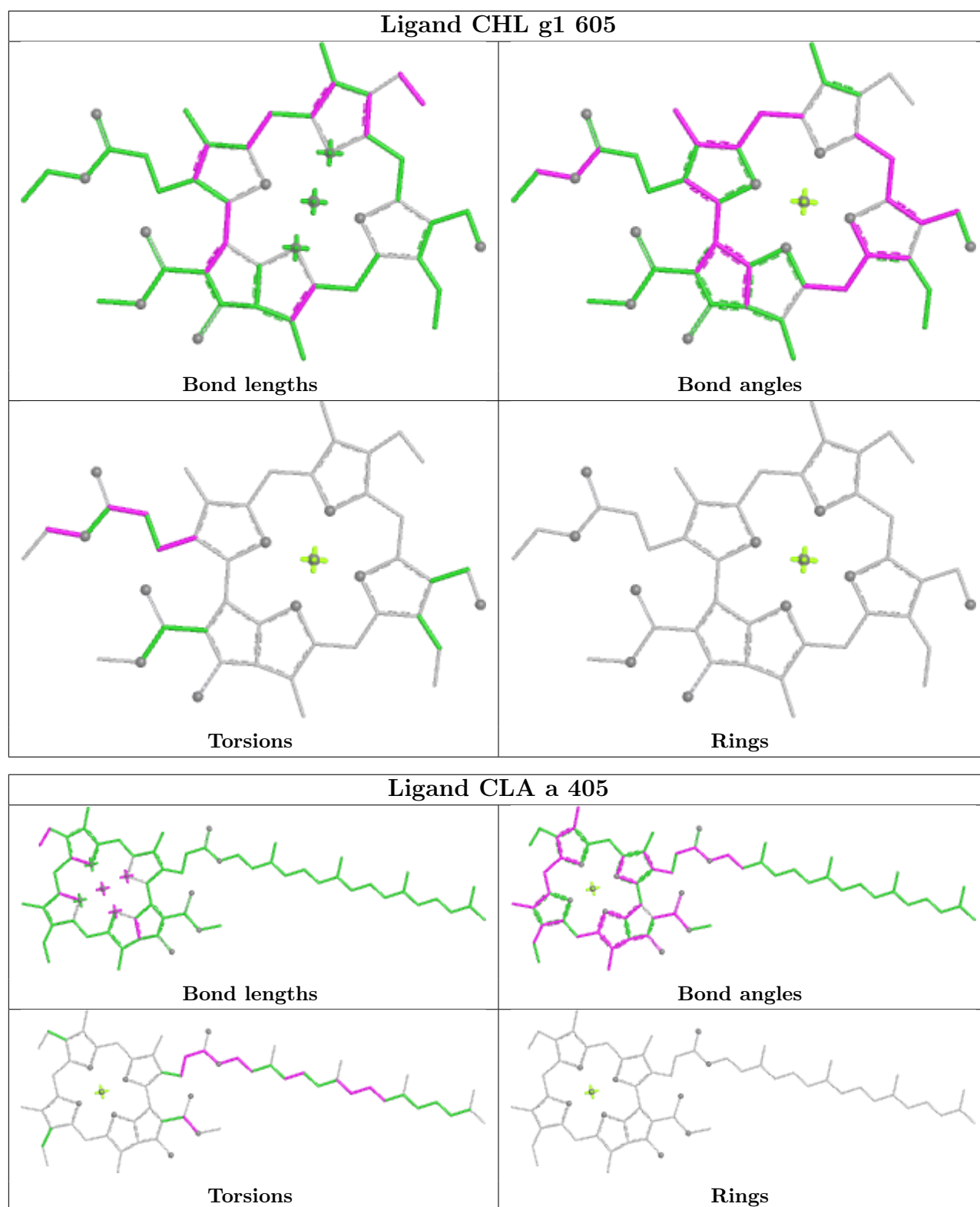


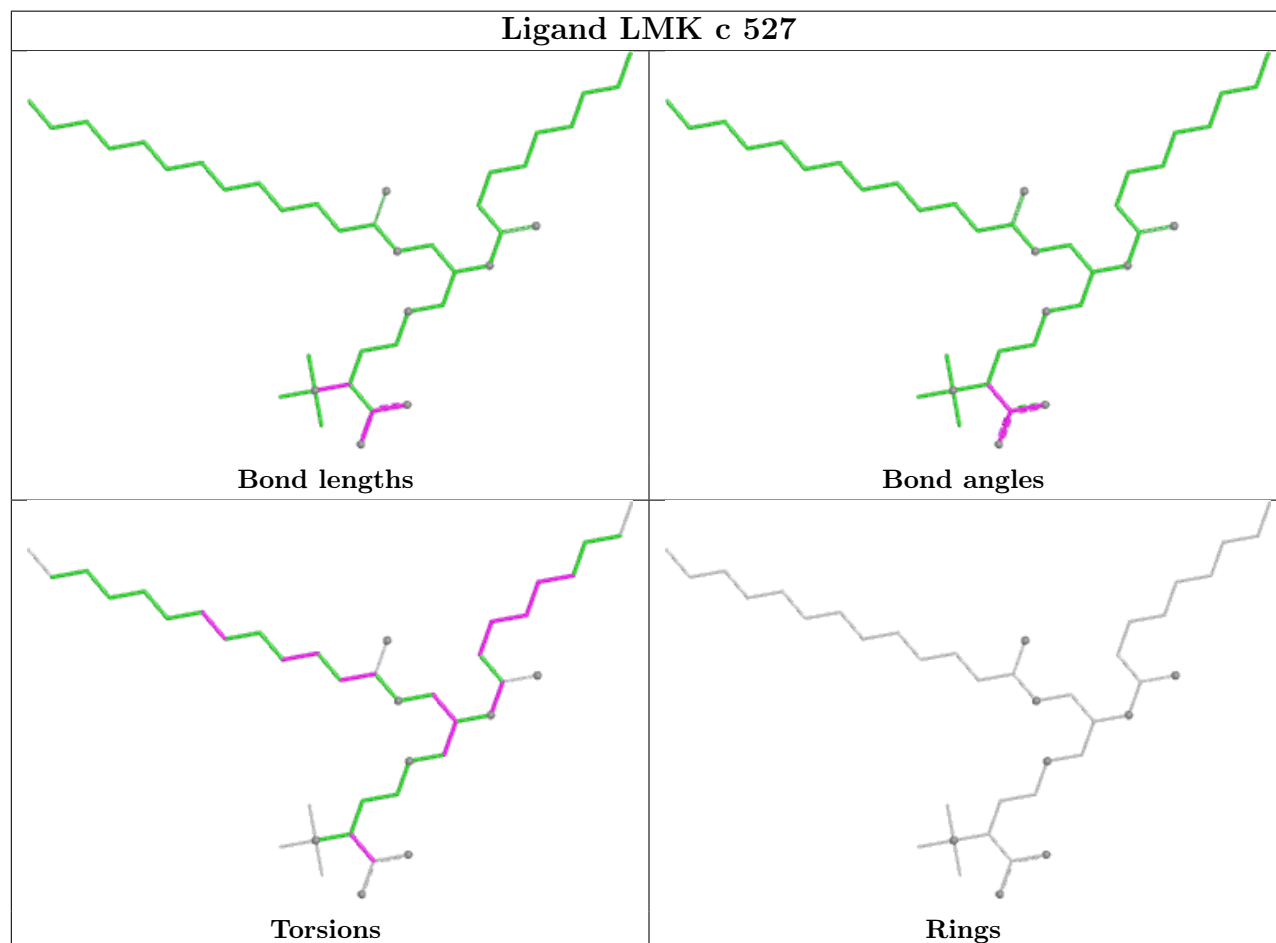
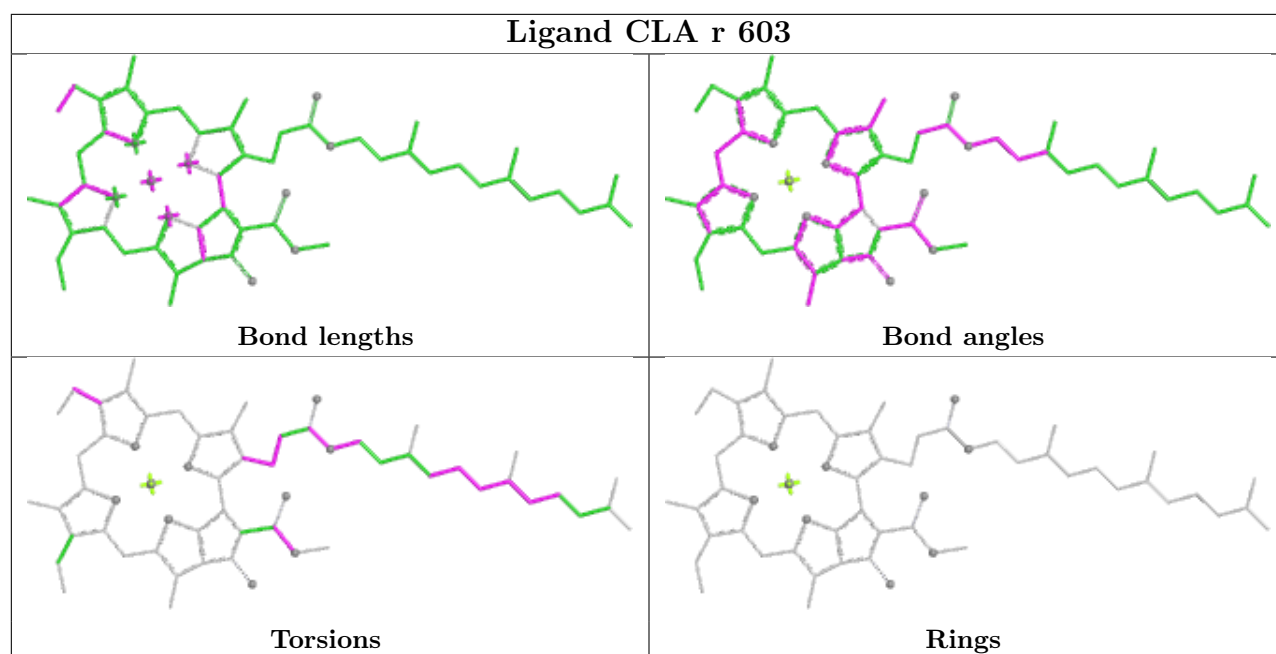


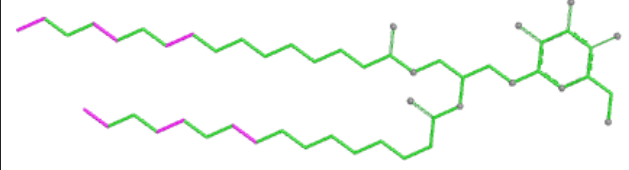
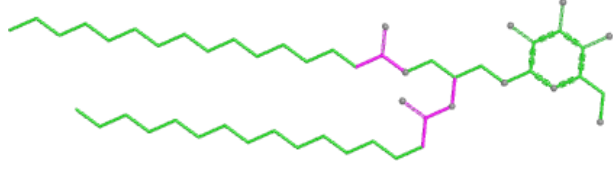
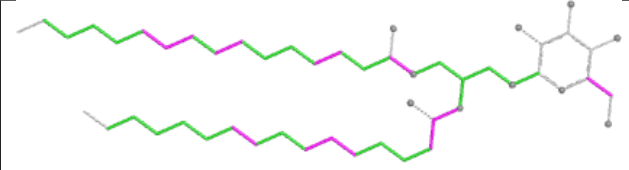
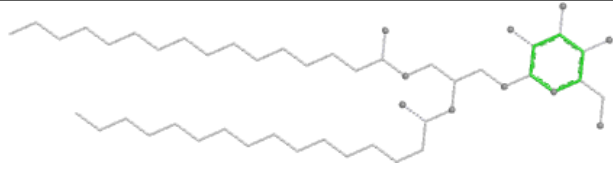
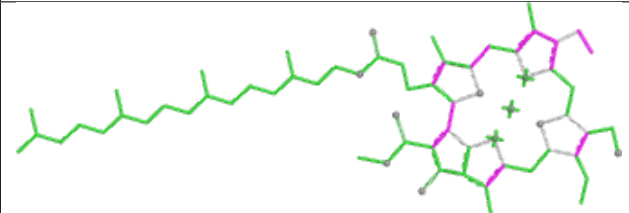
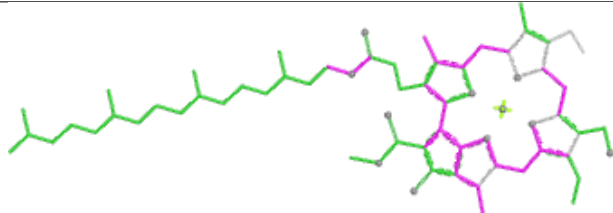
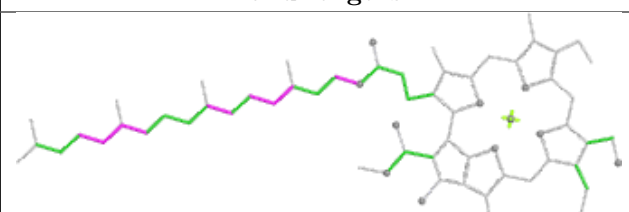
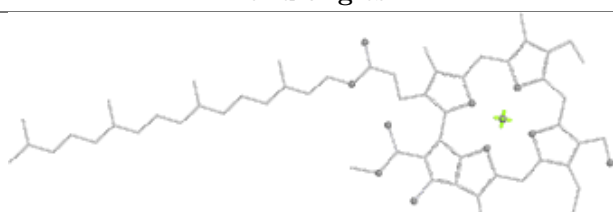
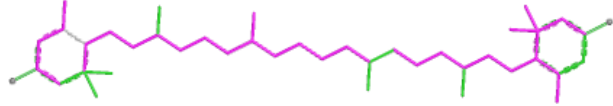
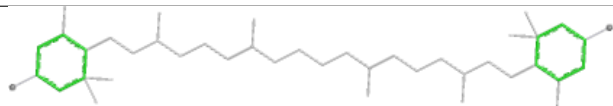


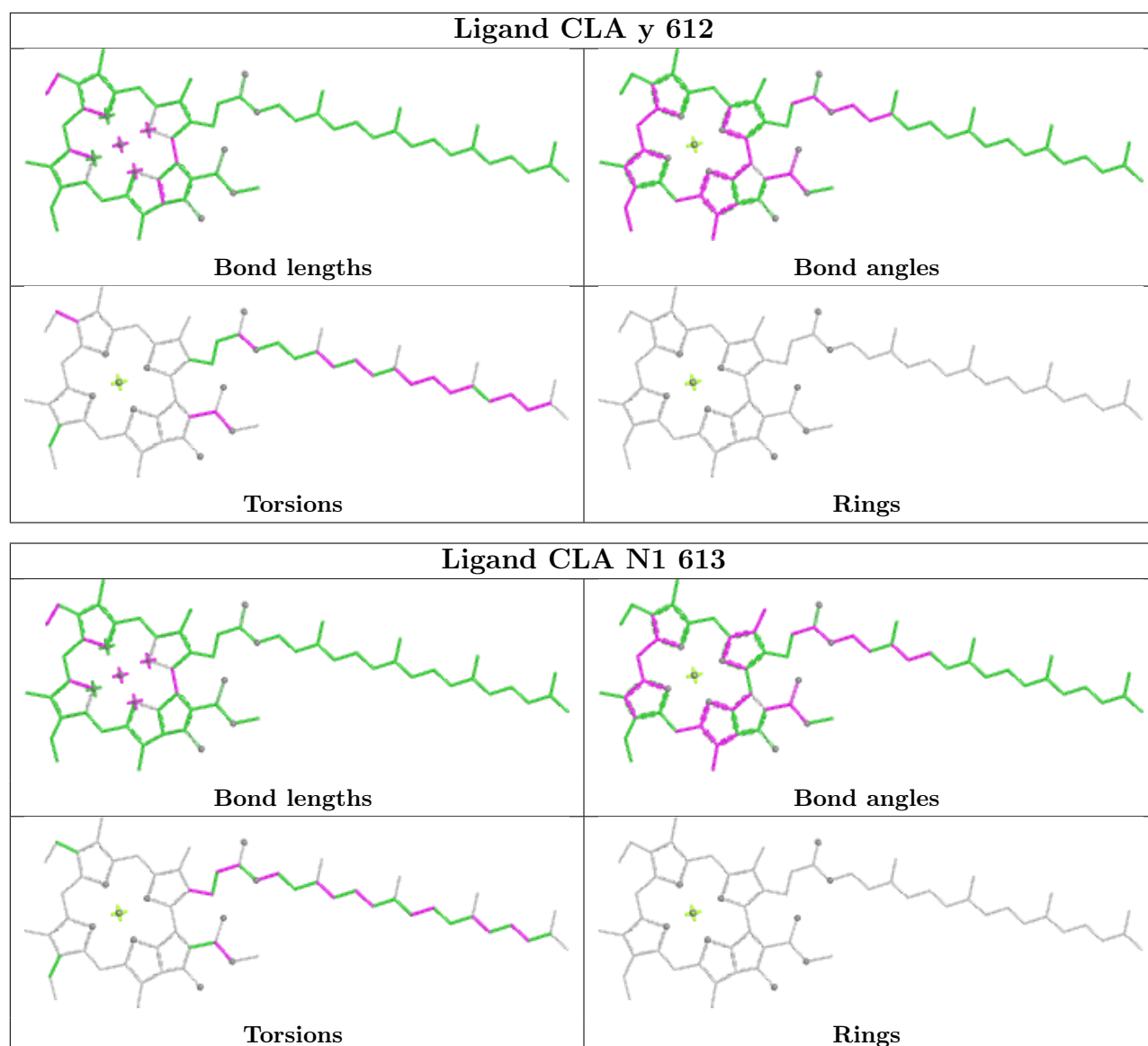


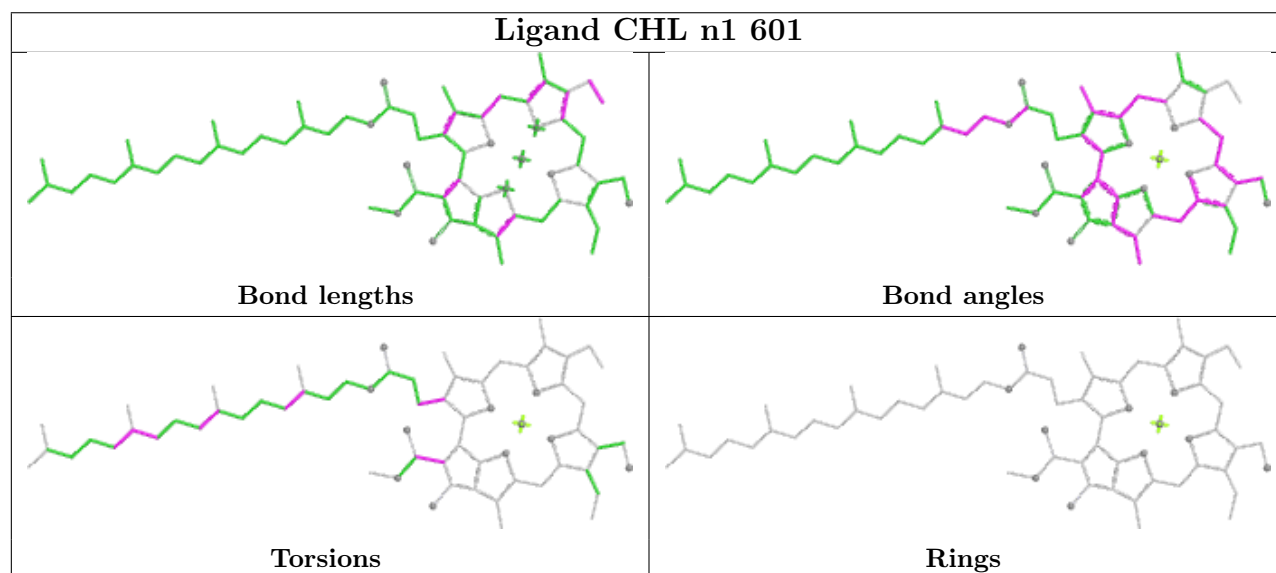
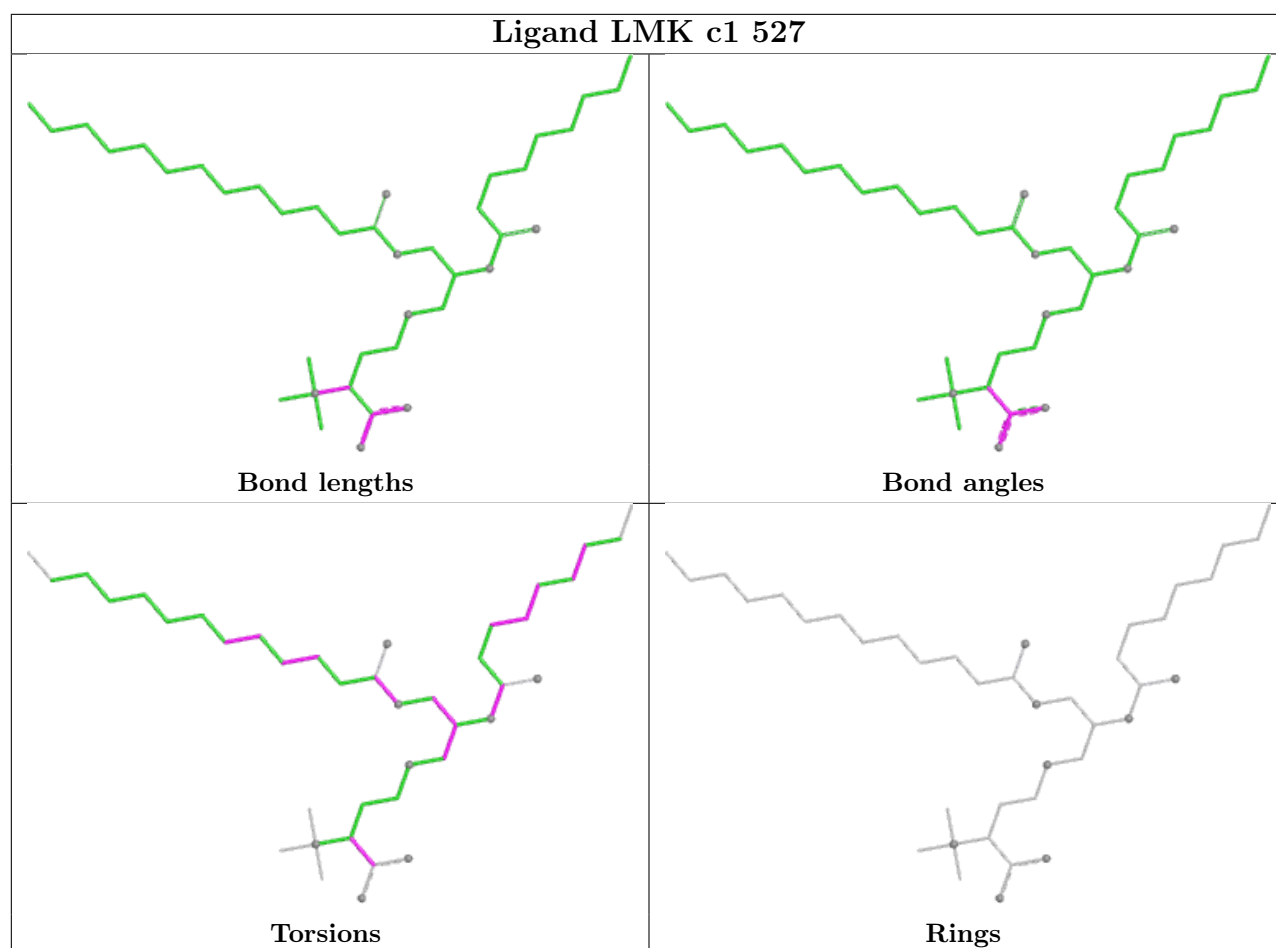


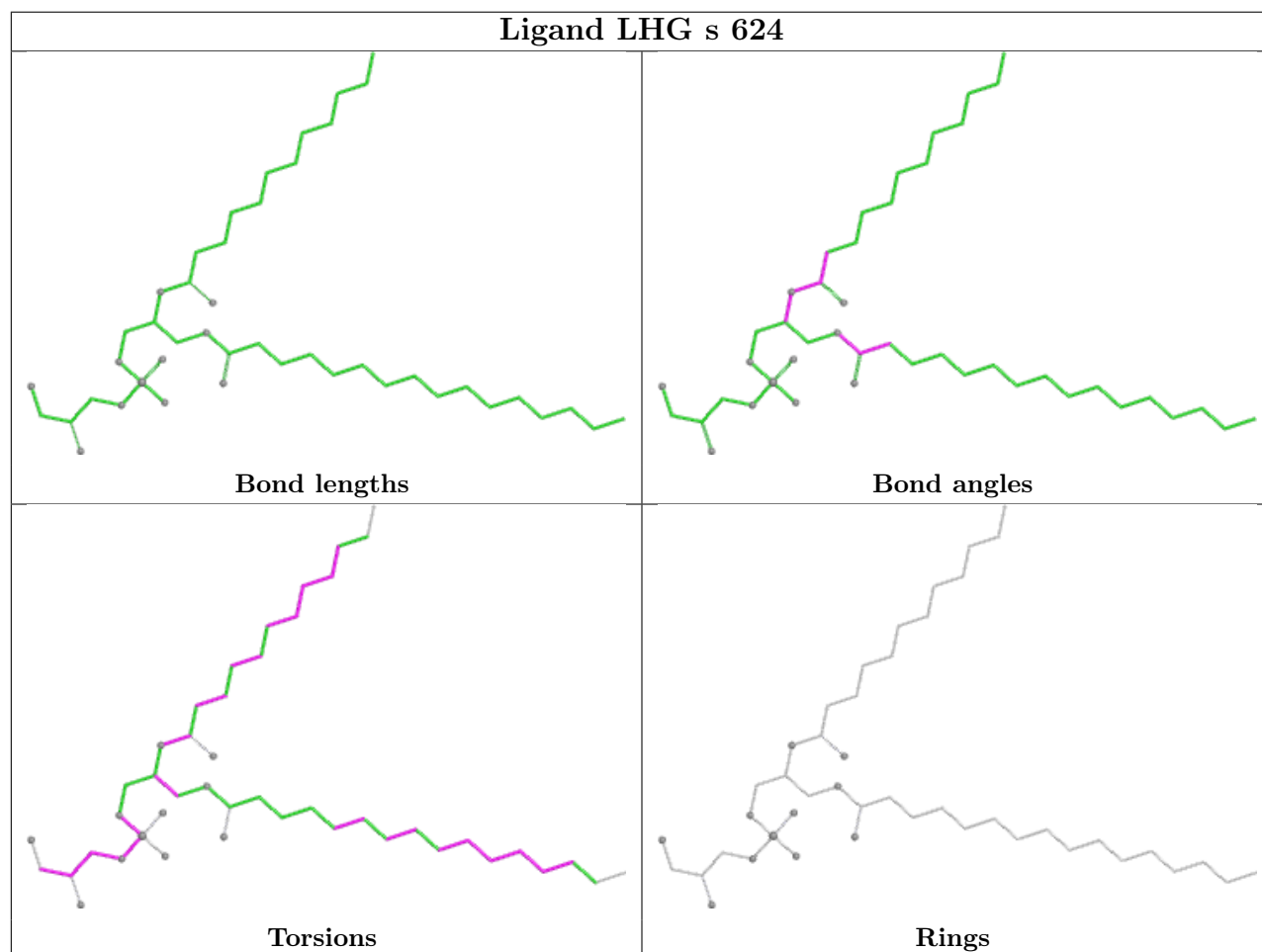
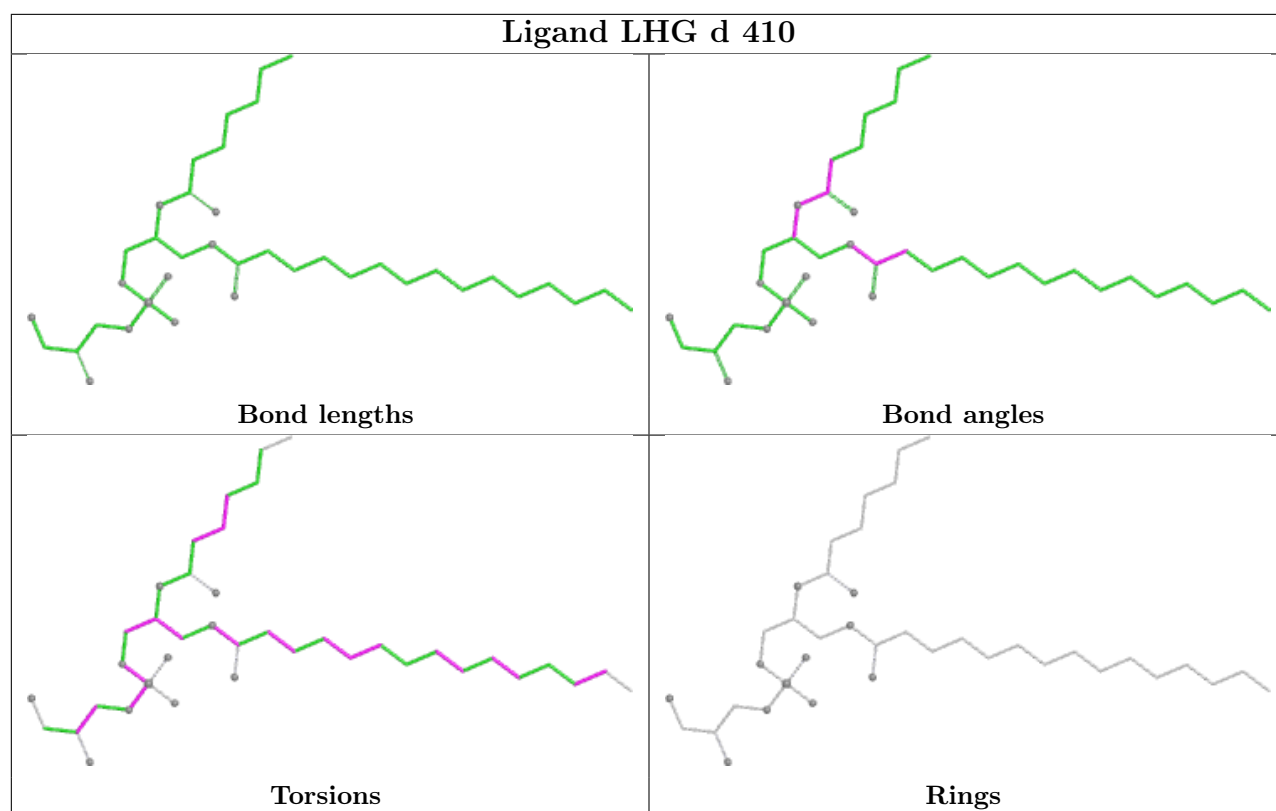


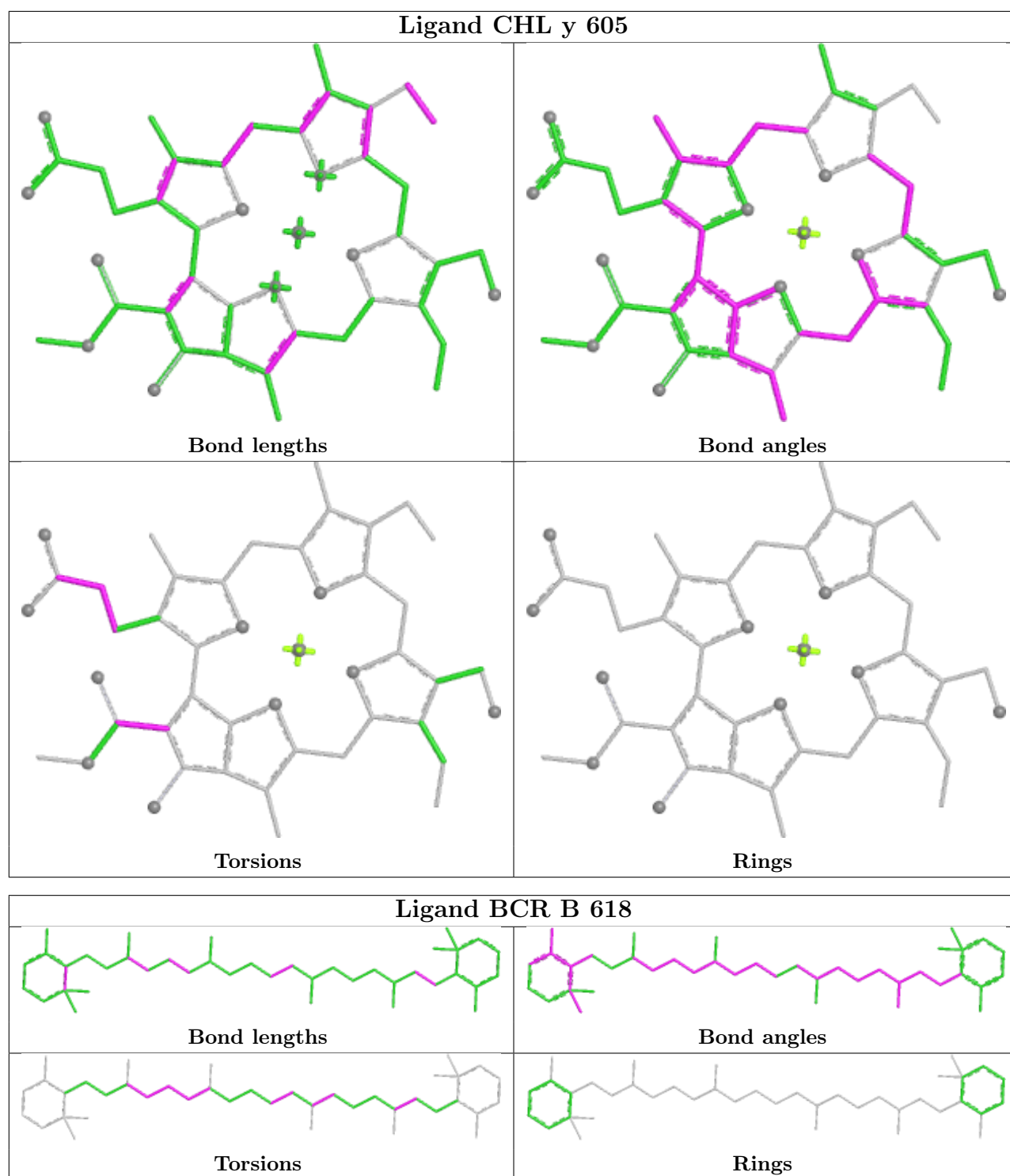


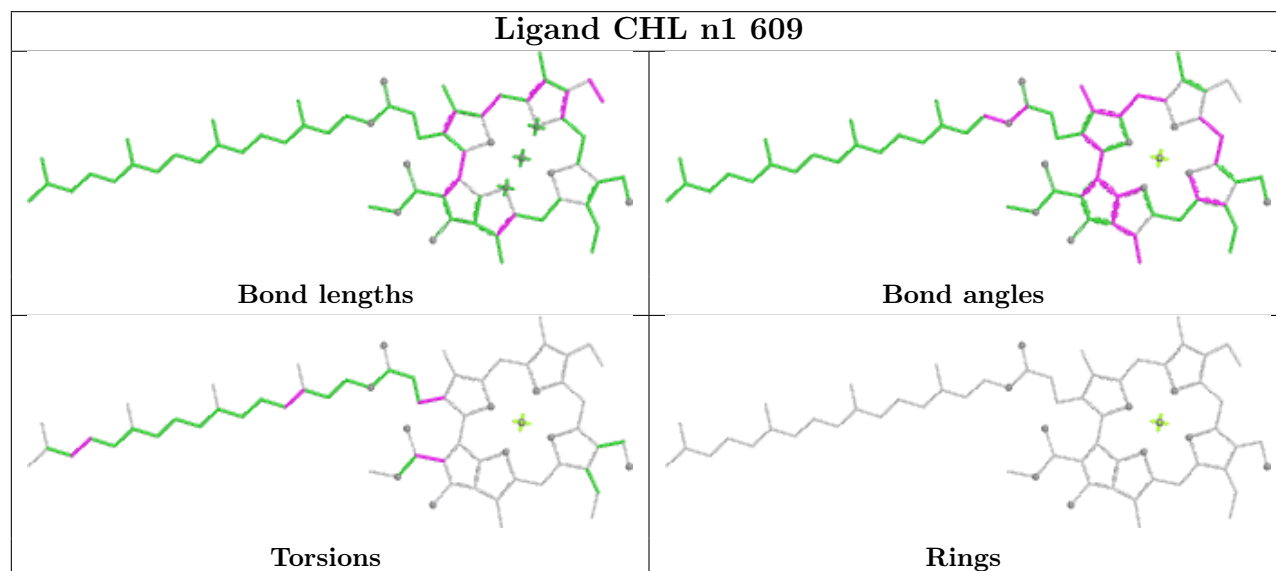
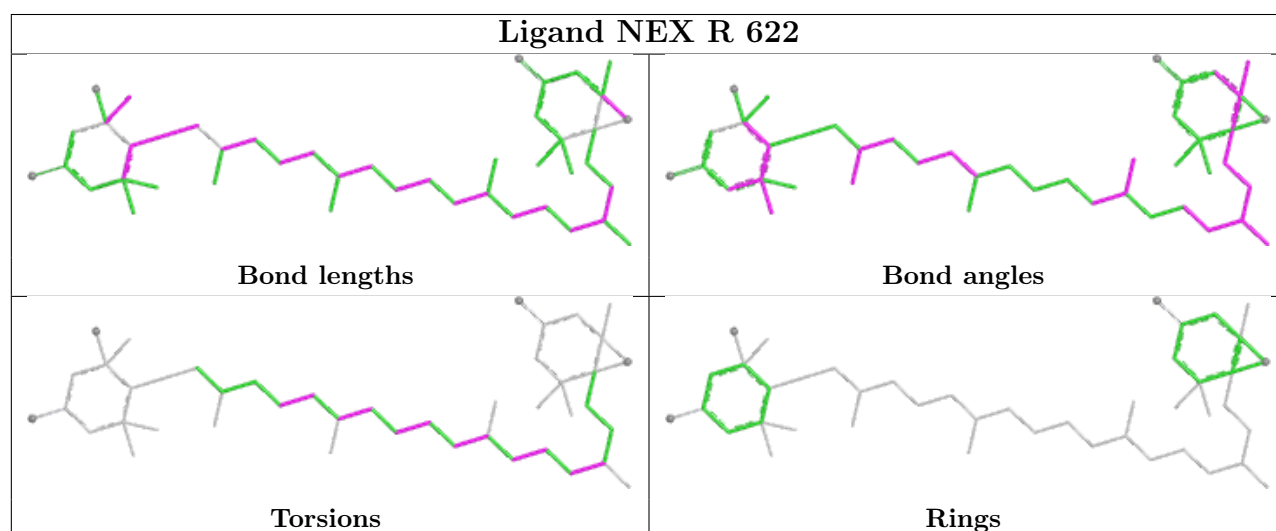
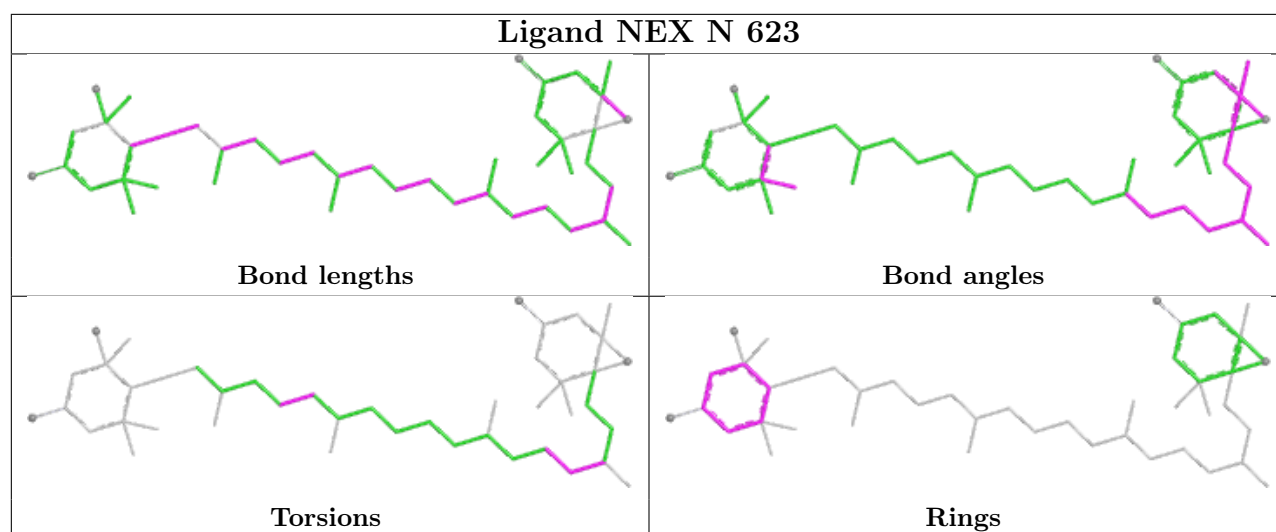
Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL g 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT S 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

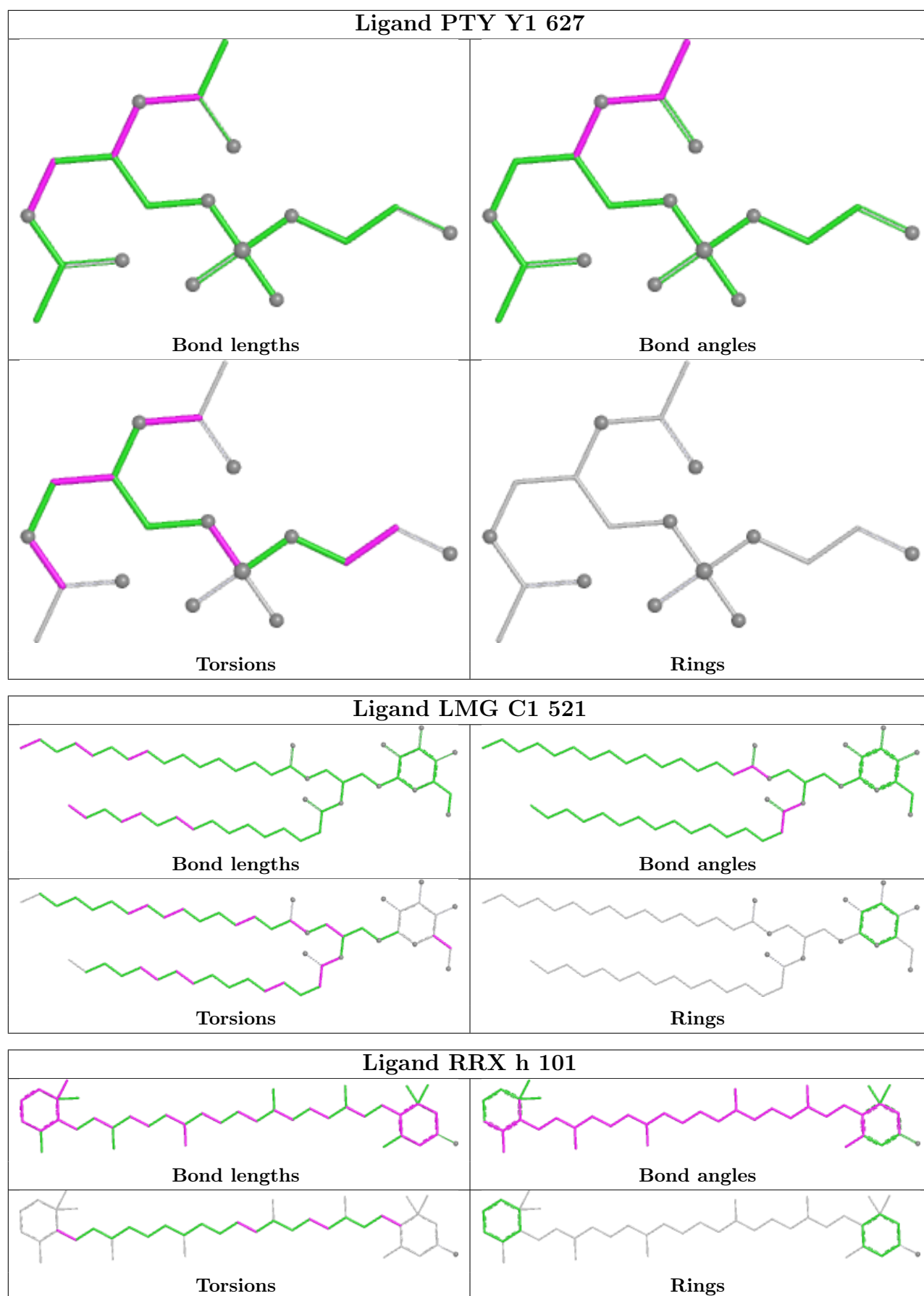


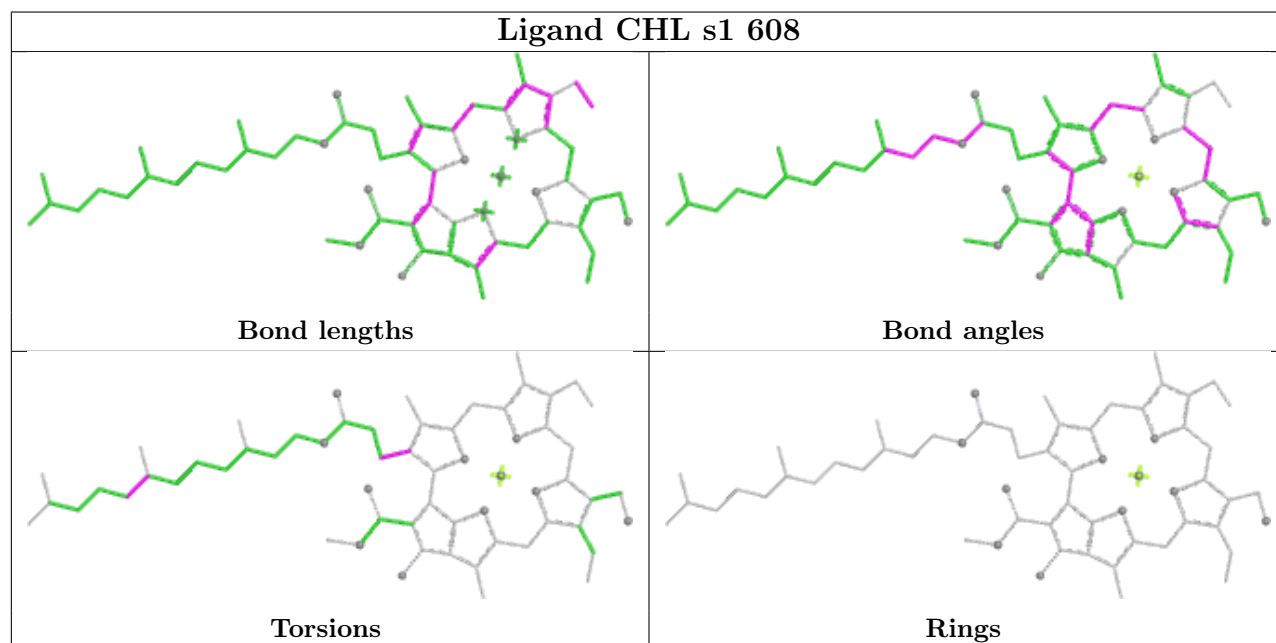
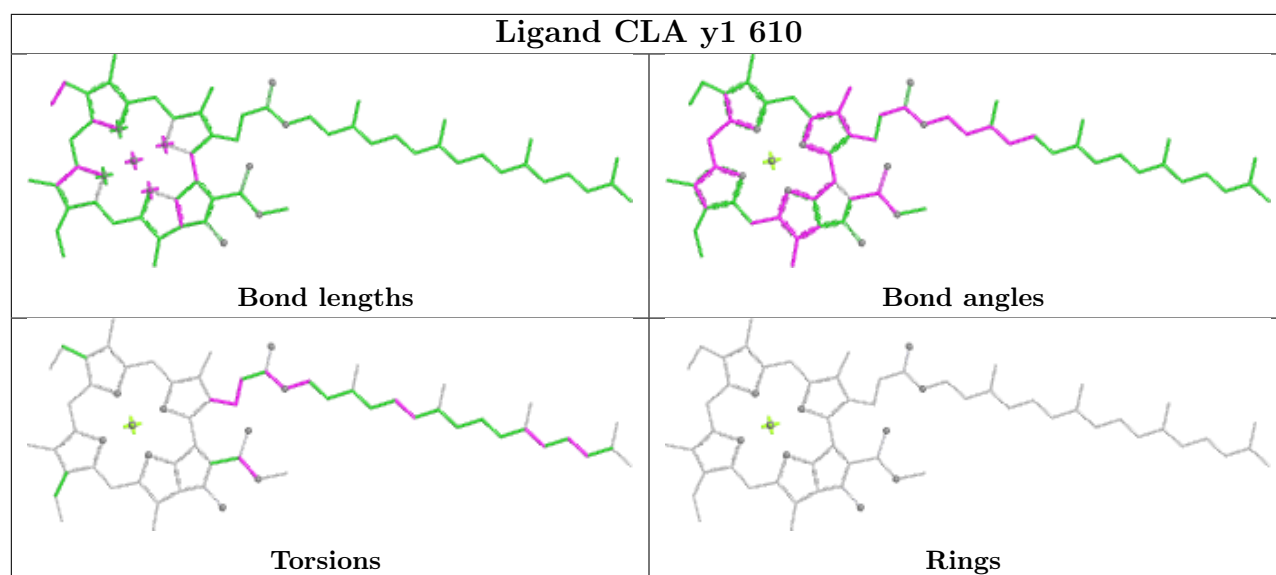


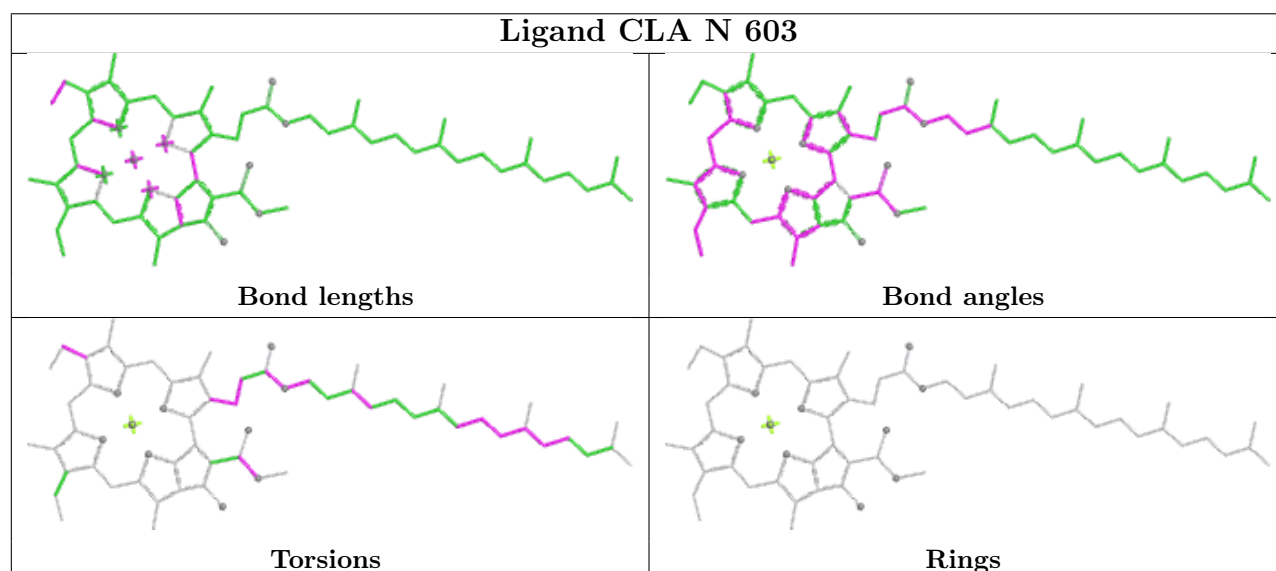
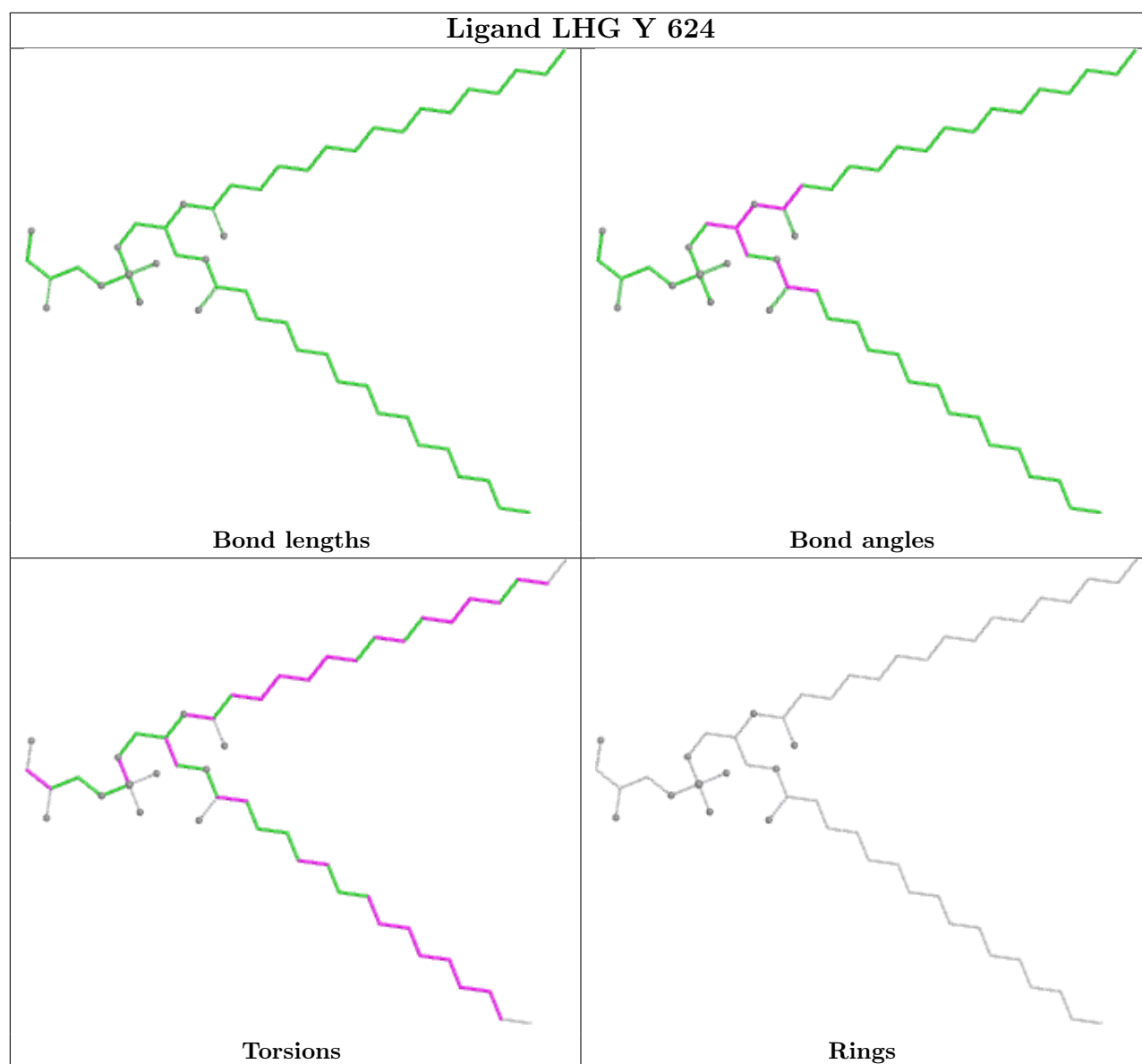


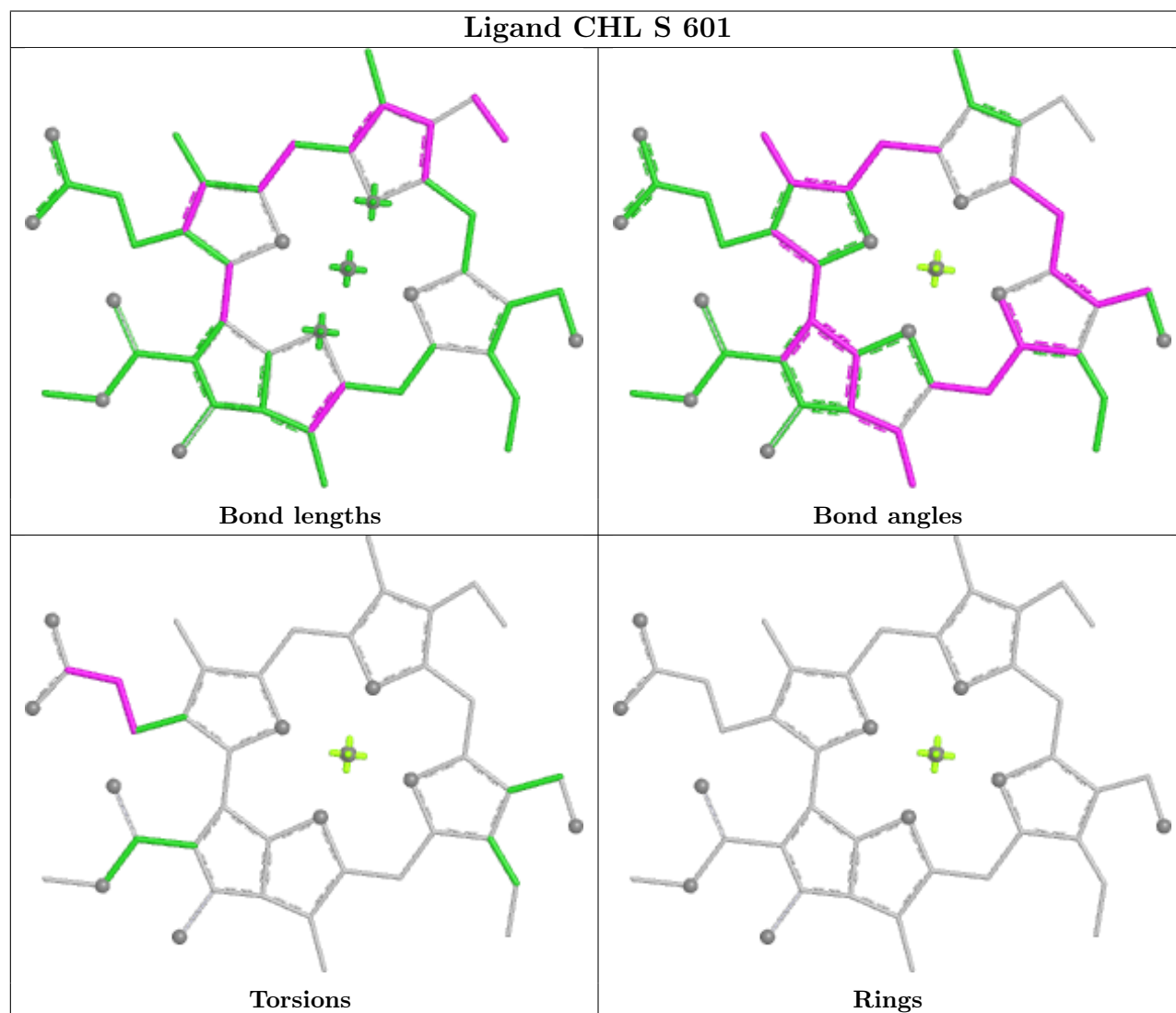
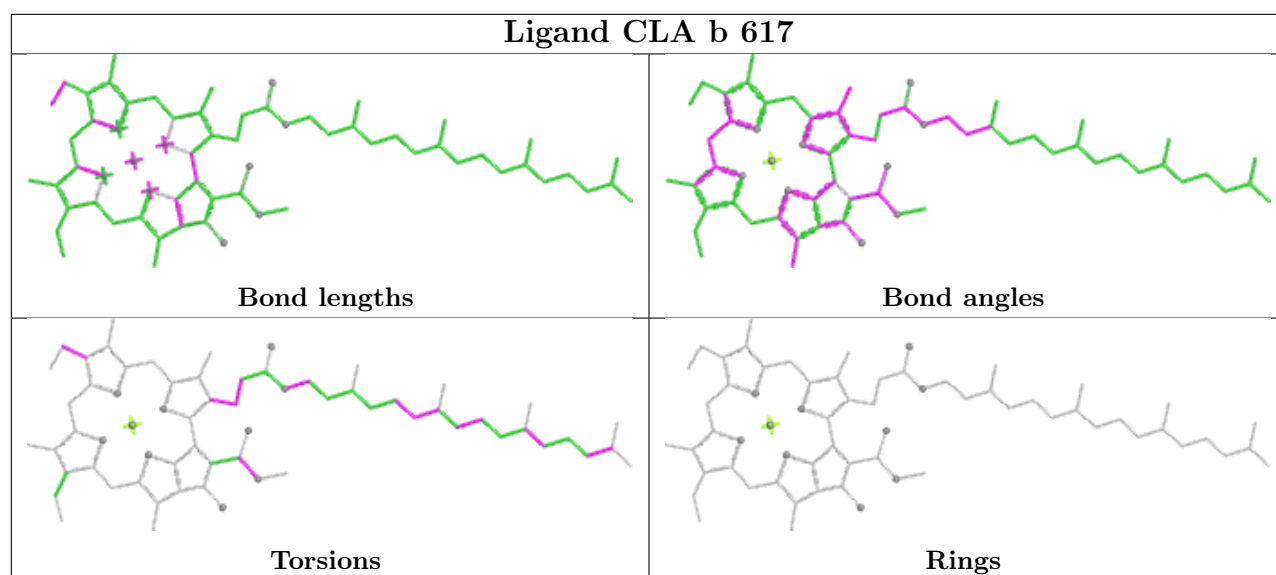


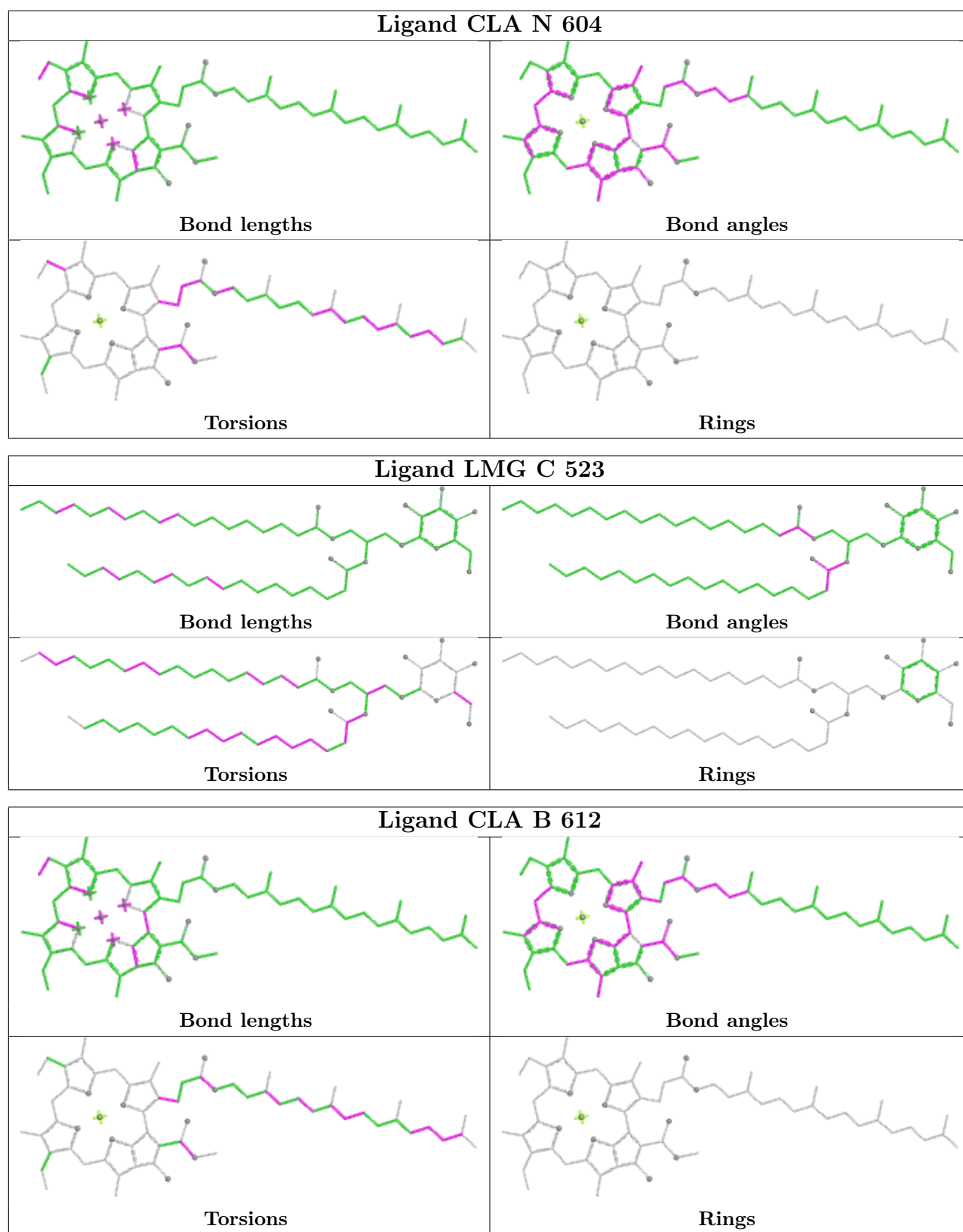


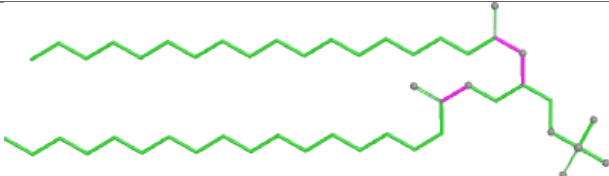
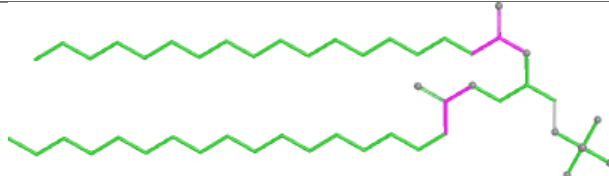
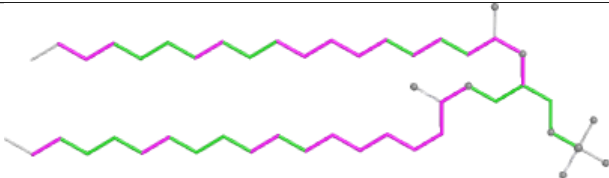
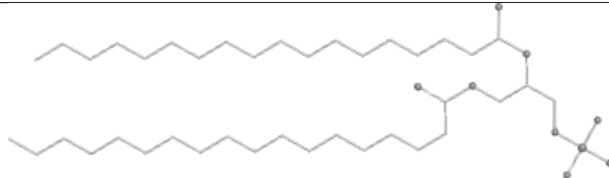


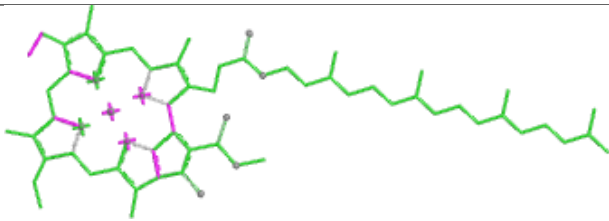
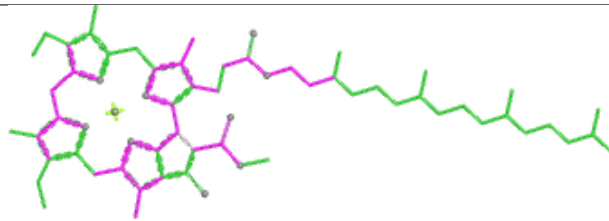
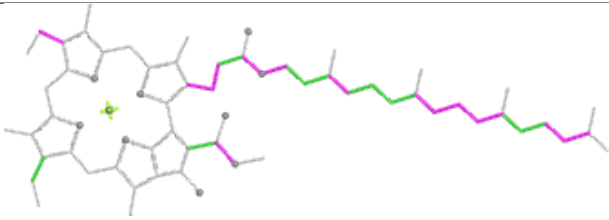
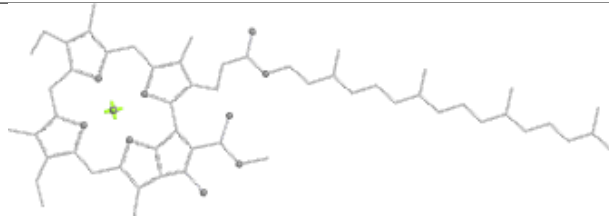


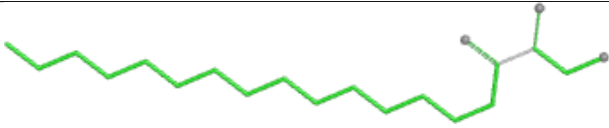
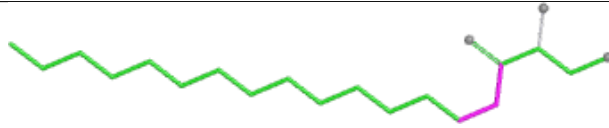
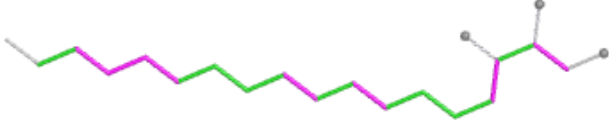
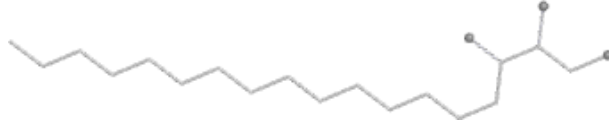


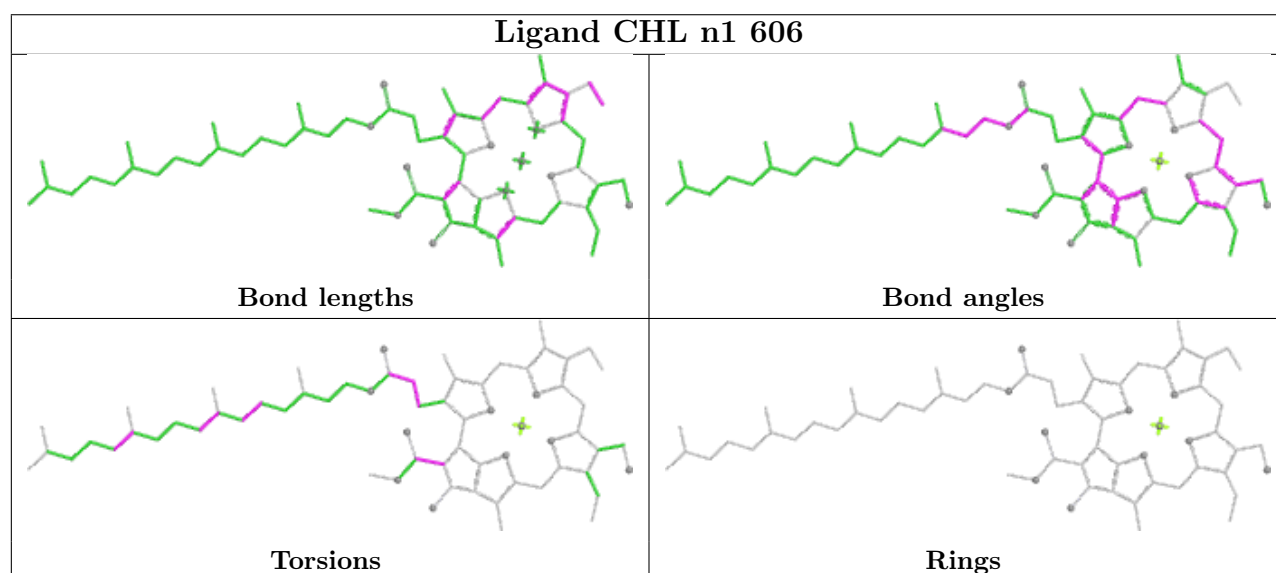
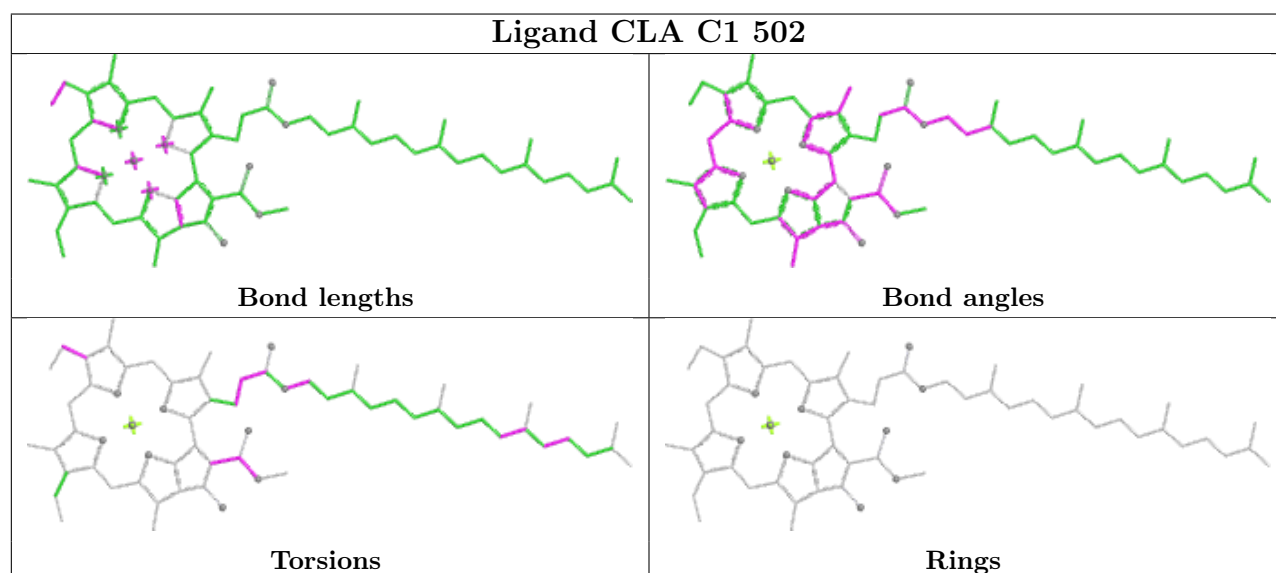
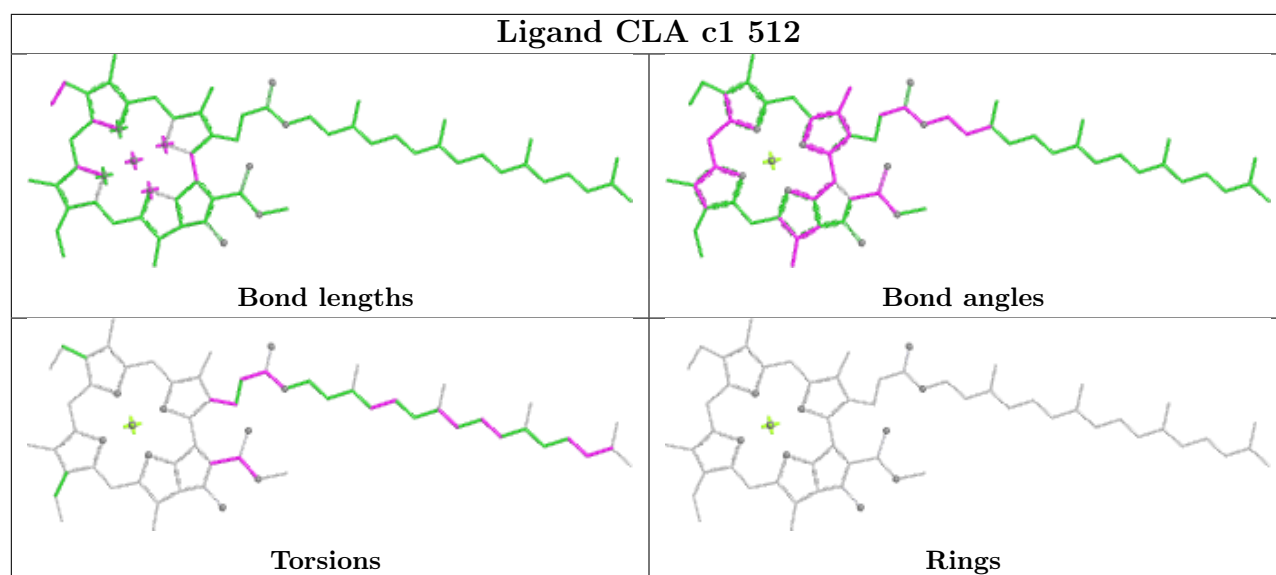


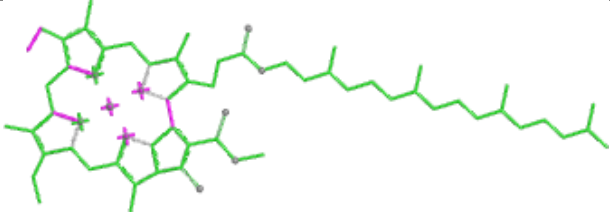
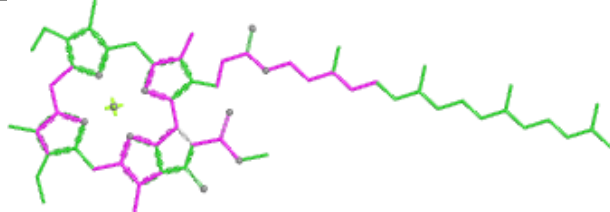
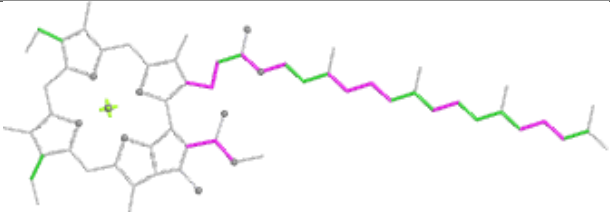
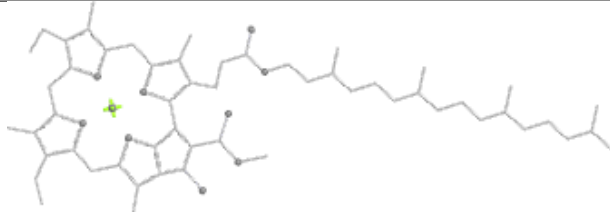
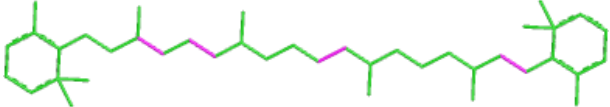
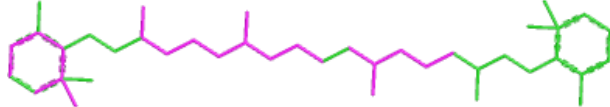
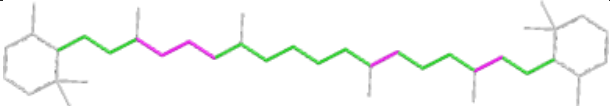
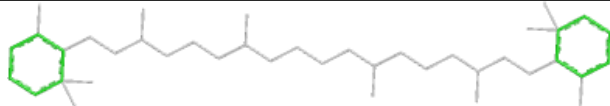
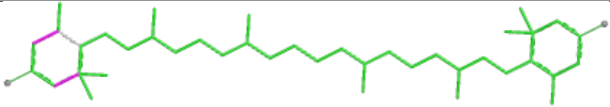
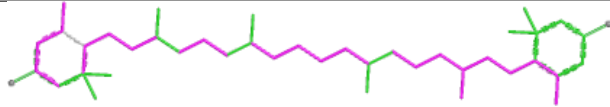
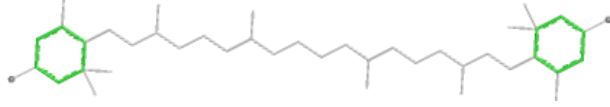


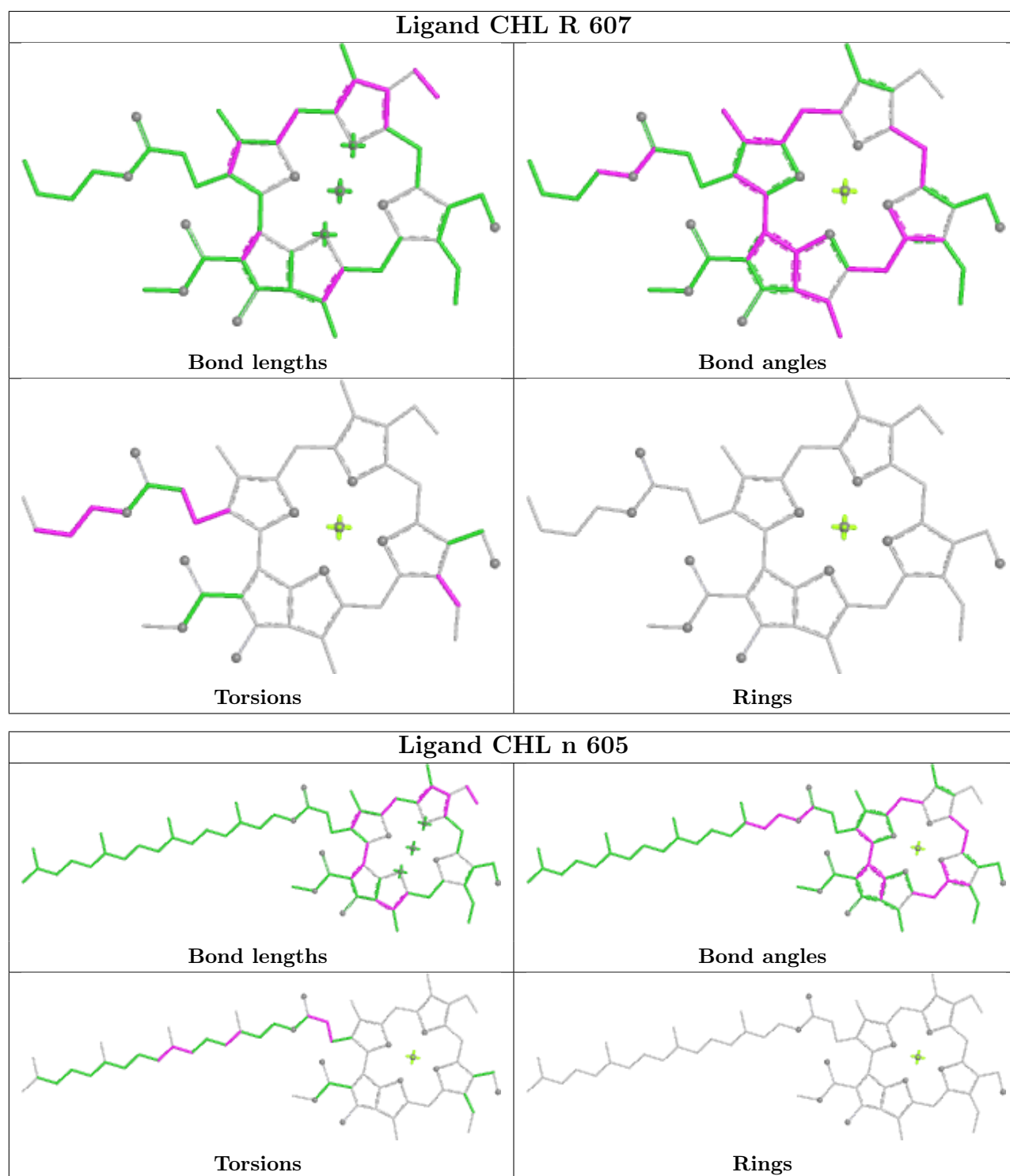
Ligand 3PH S 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

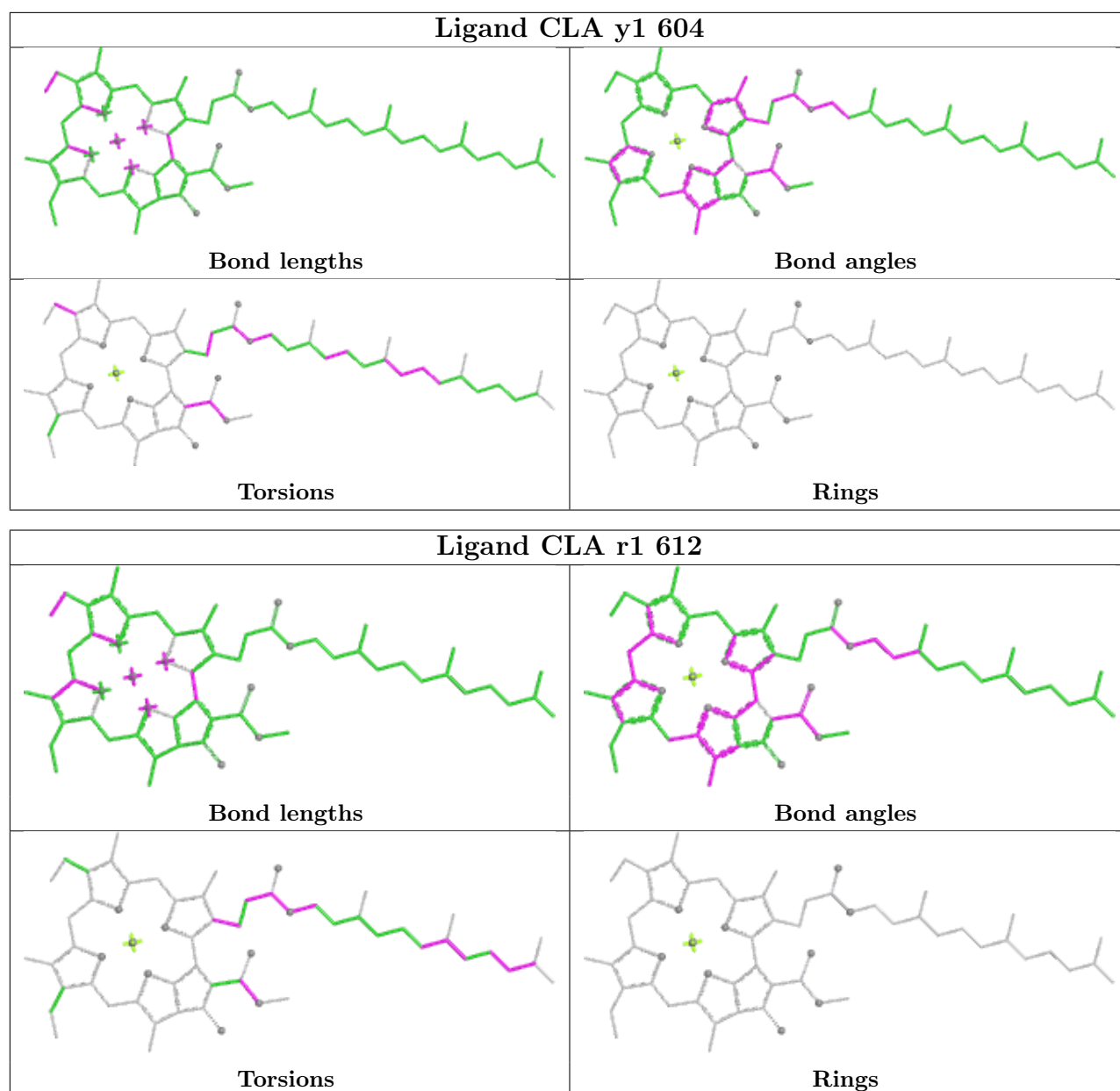
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Bond lengths	Bond angles
	
Torsions	Rings

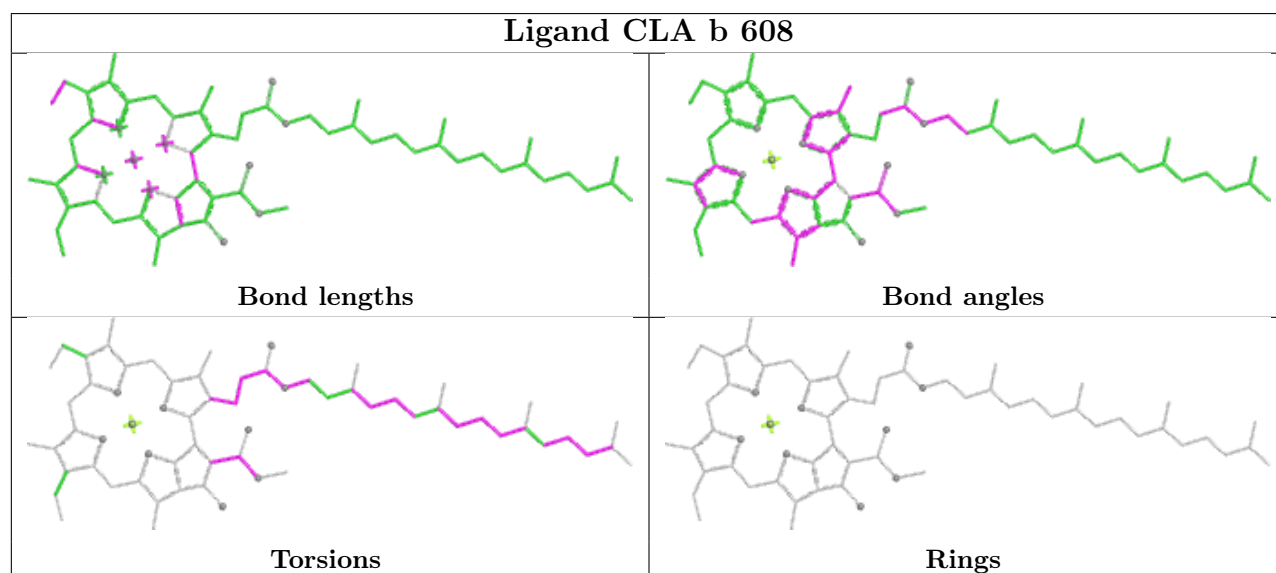
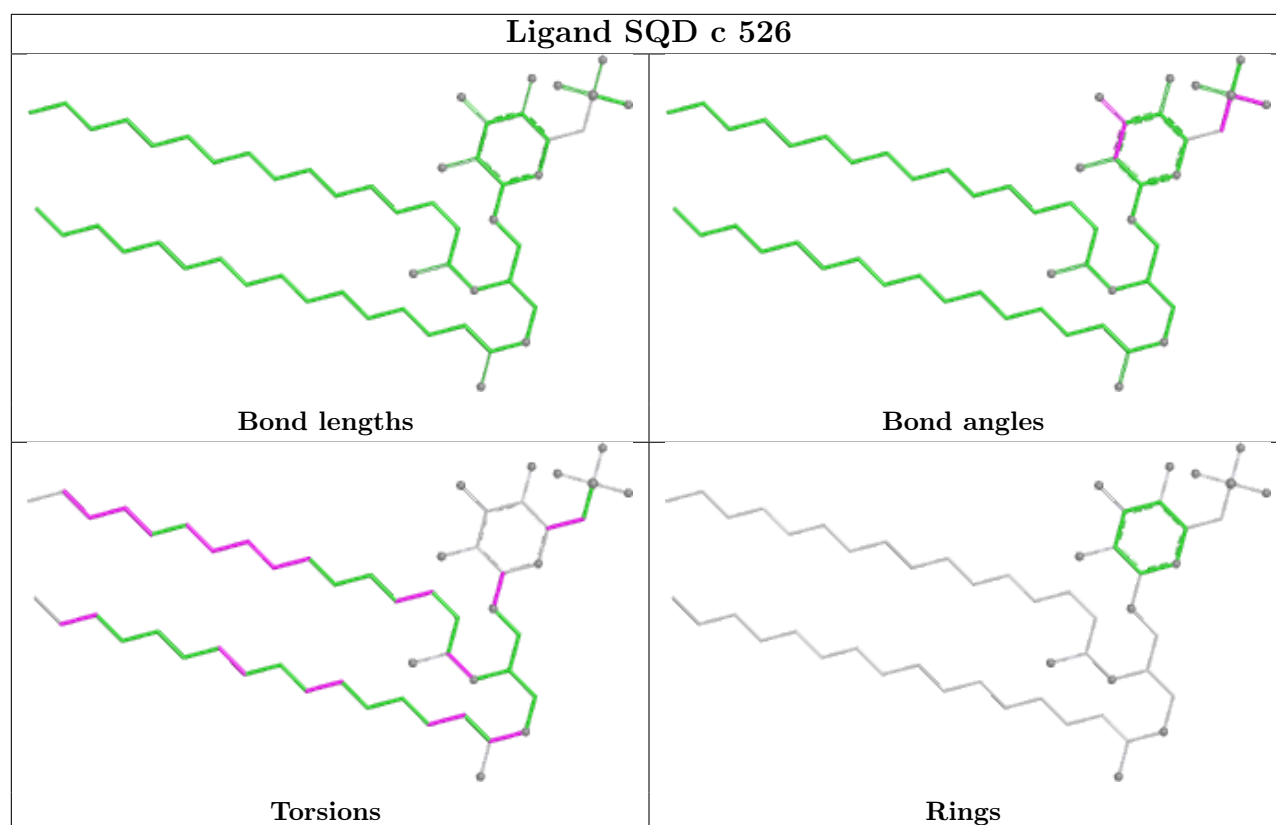
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Bond lengths	Bond angles
	
Torsions	Rings



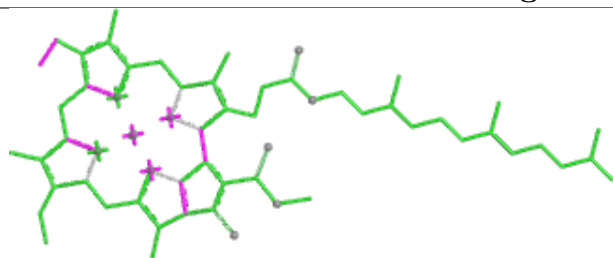
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 517	
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 Torsions	 Rings
Ligand LUT y 620	
 Bond lengths	 Bond angles
 Torsions	 Rings



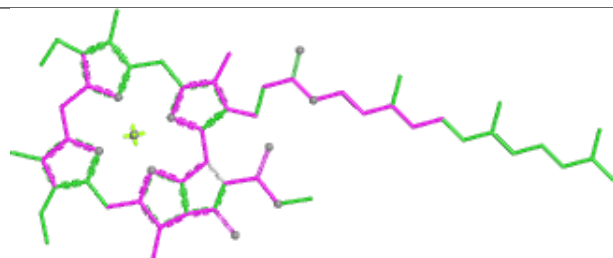




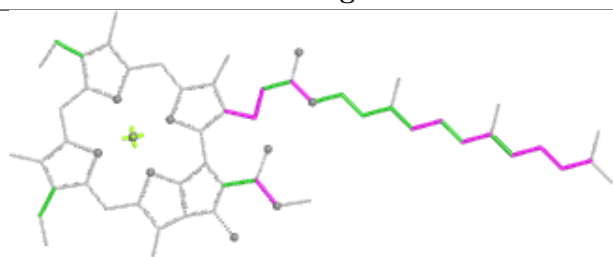
Ligand CLA r 602



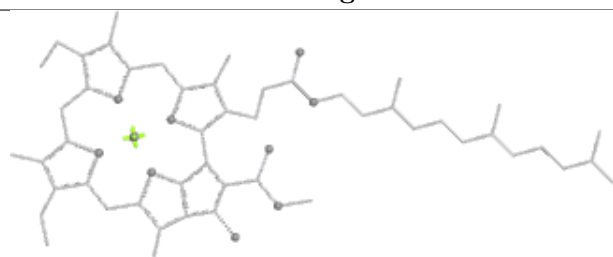
Bond lengths



Bond angles

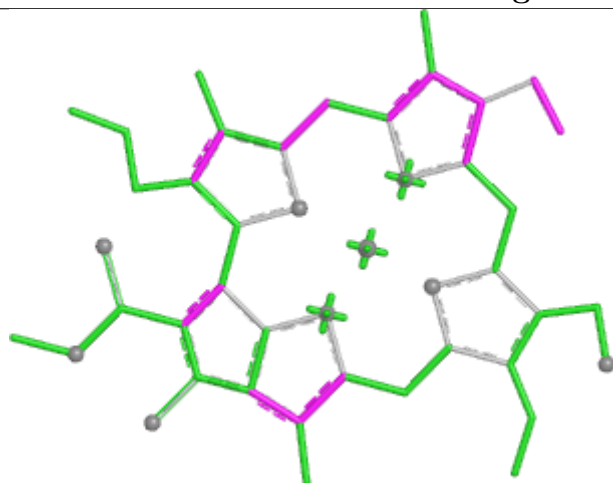


Torsions

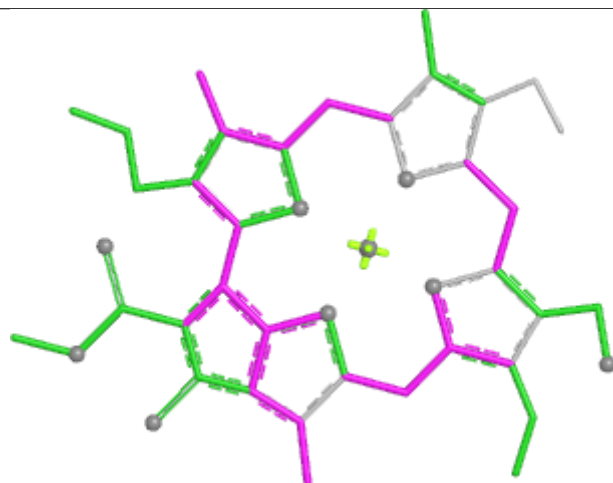


Rings

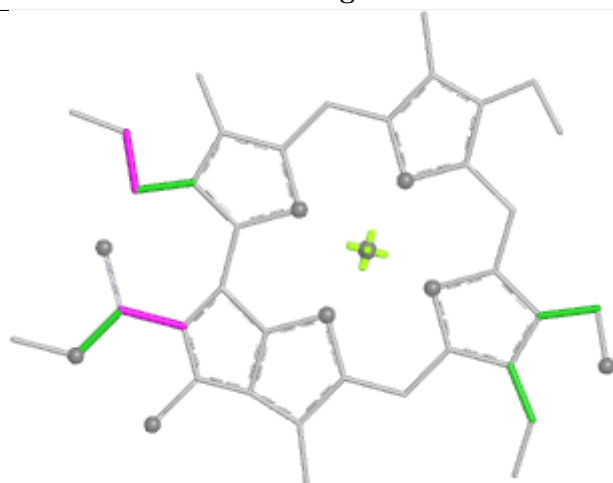
Ligand CHL G 608



Bond lengths



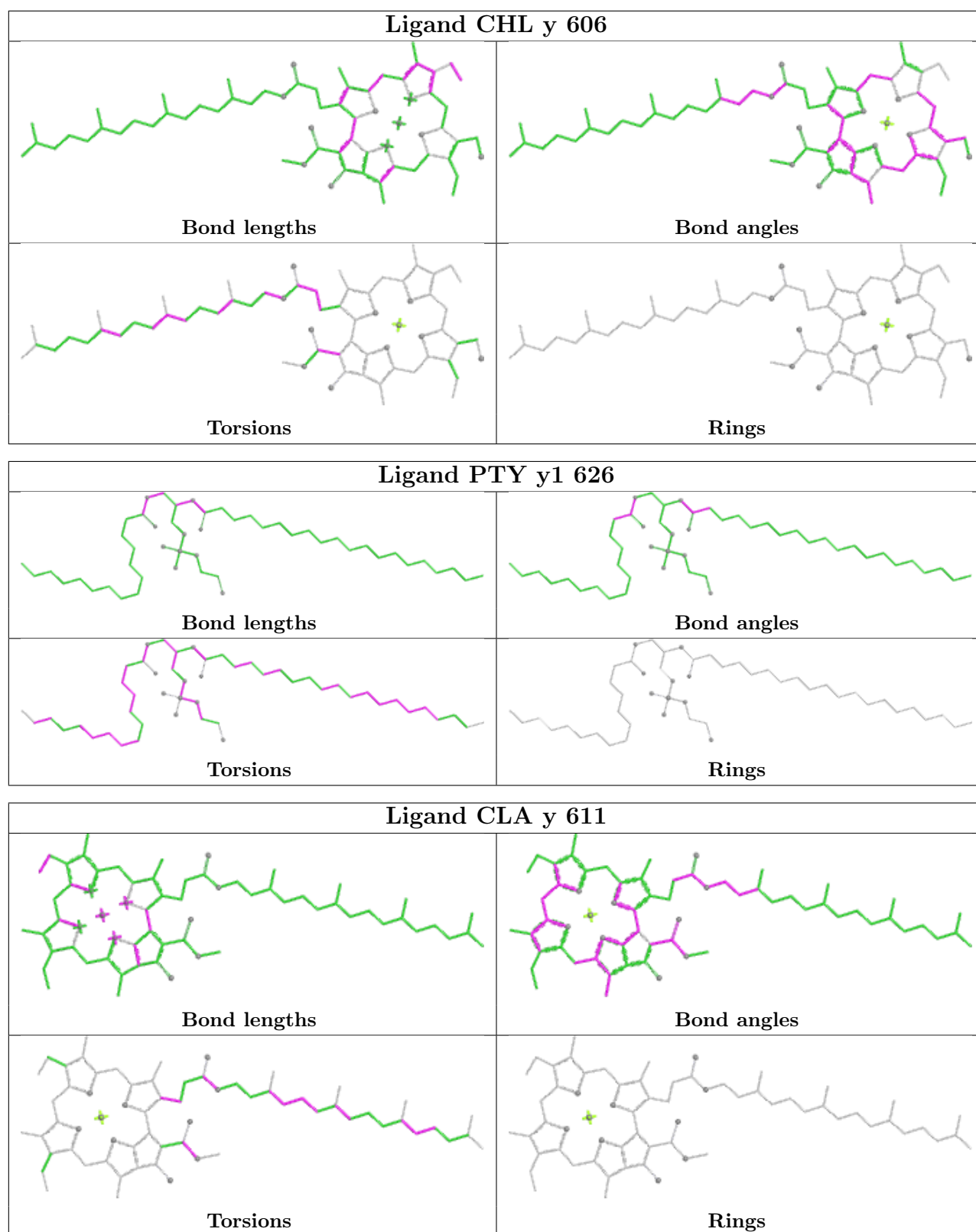
Bond angles

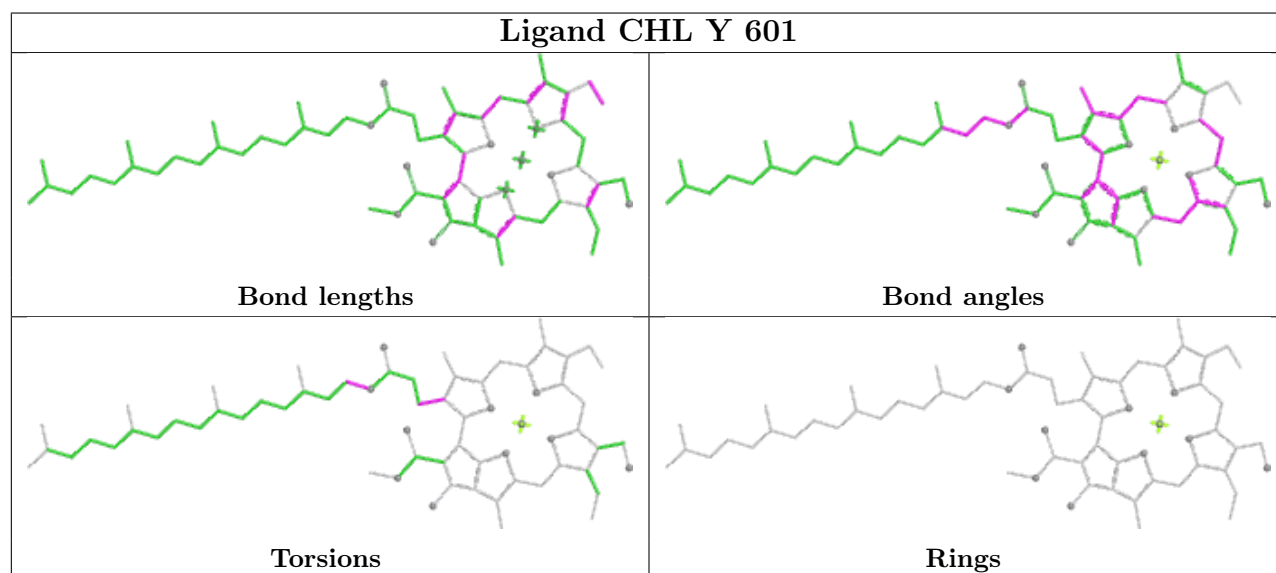
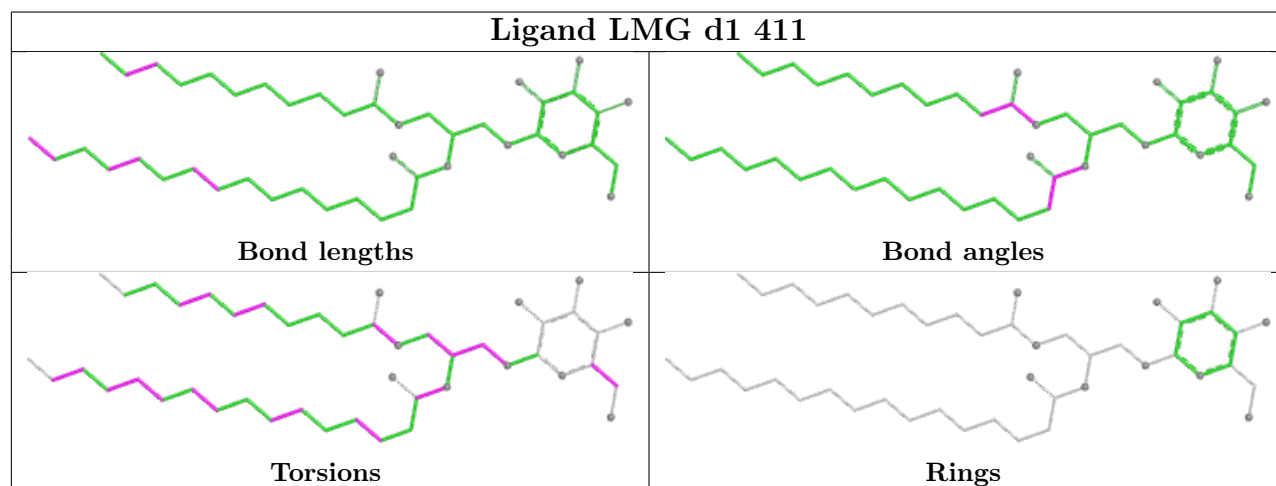
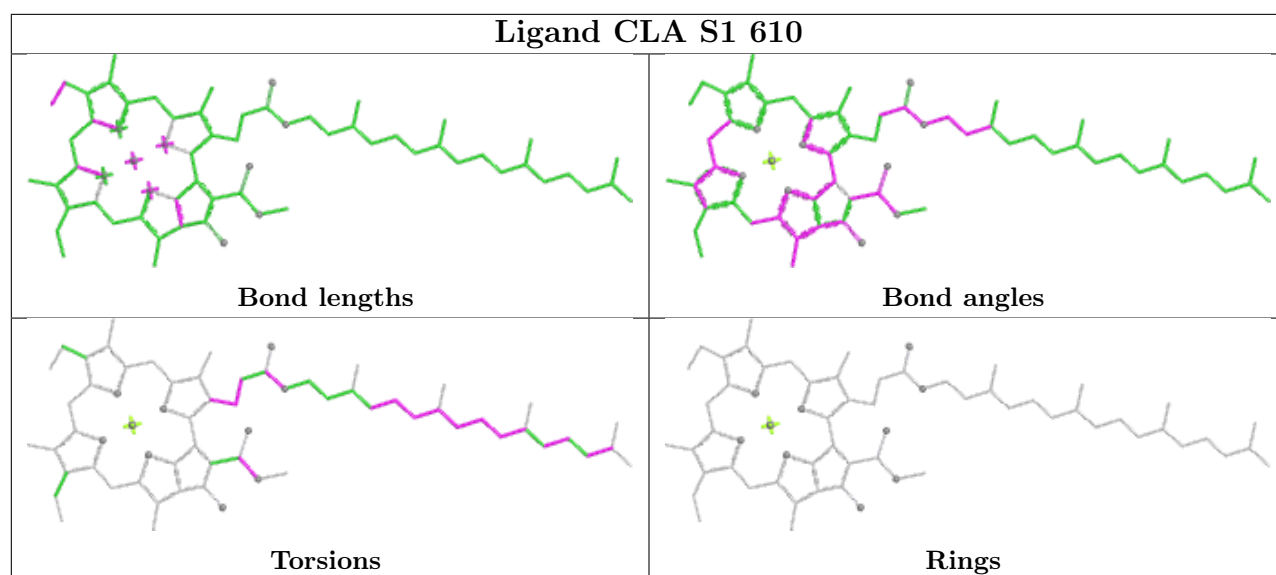


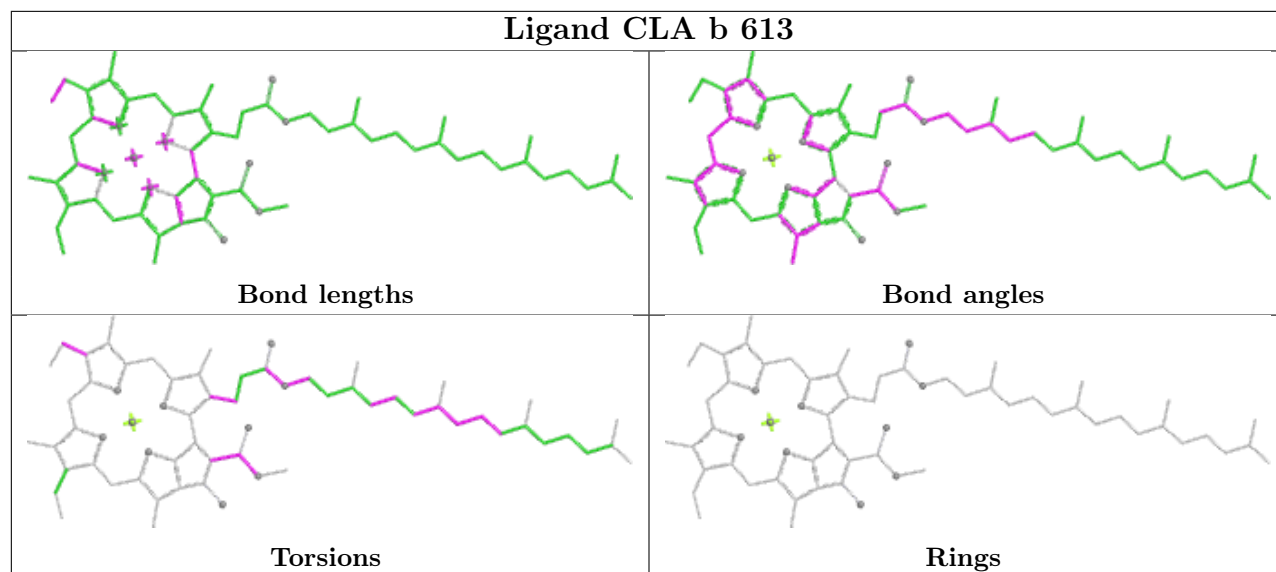
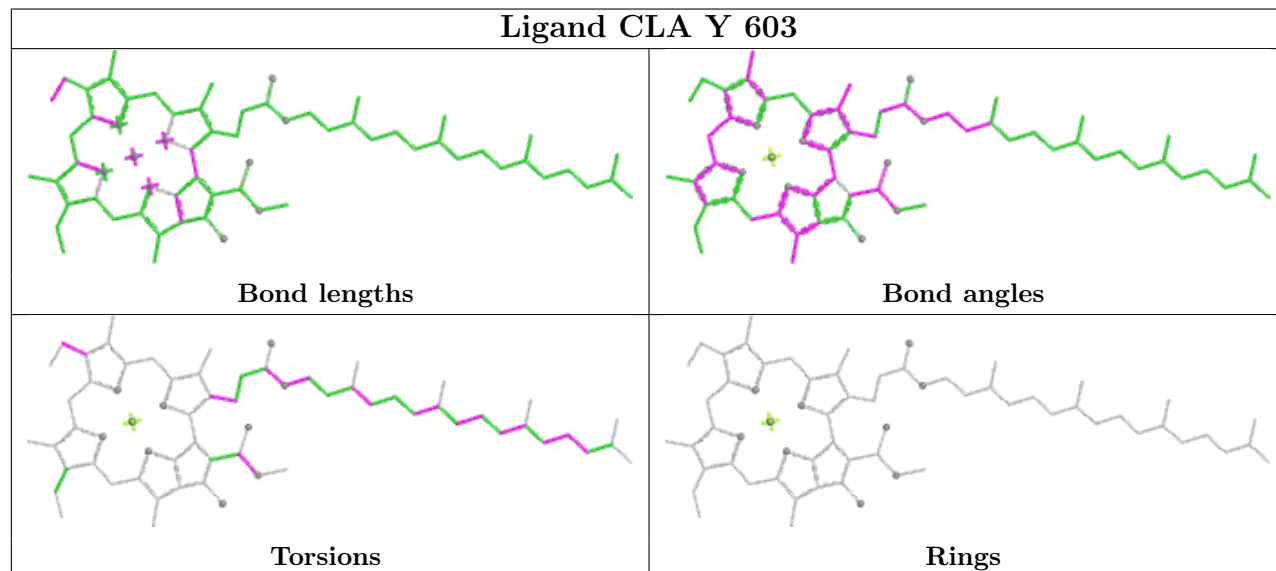
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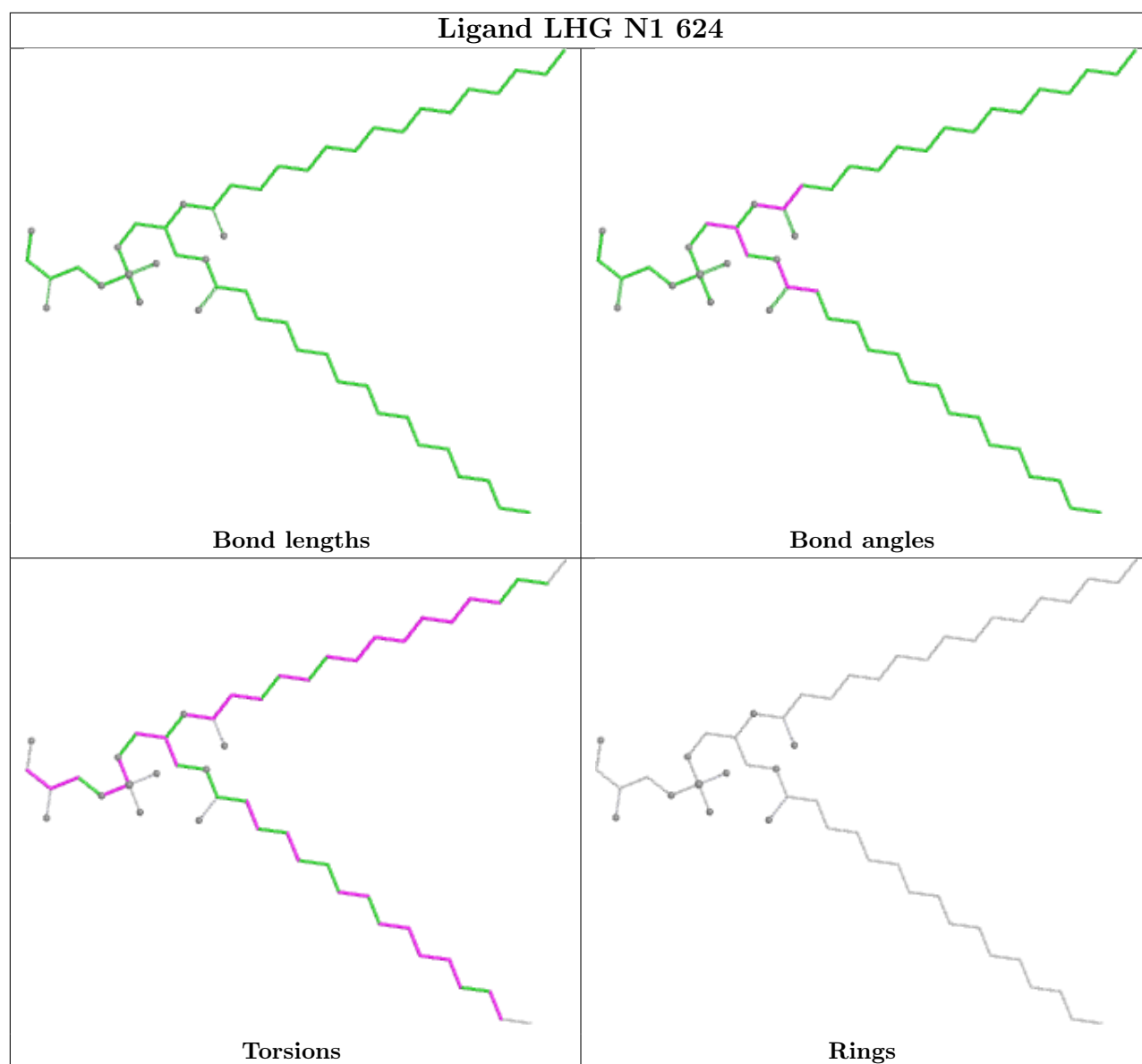


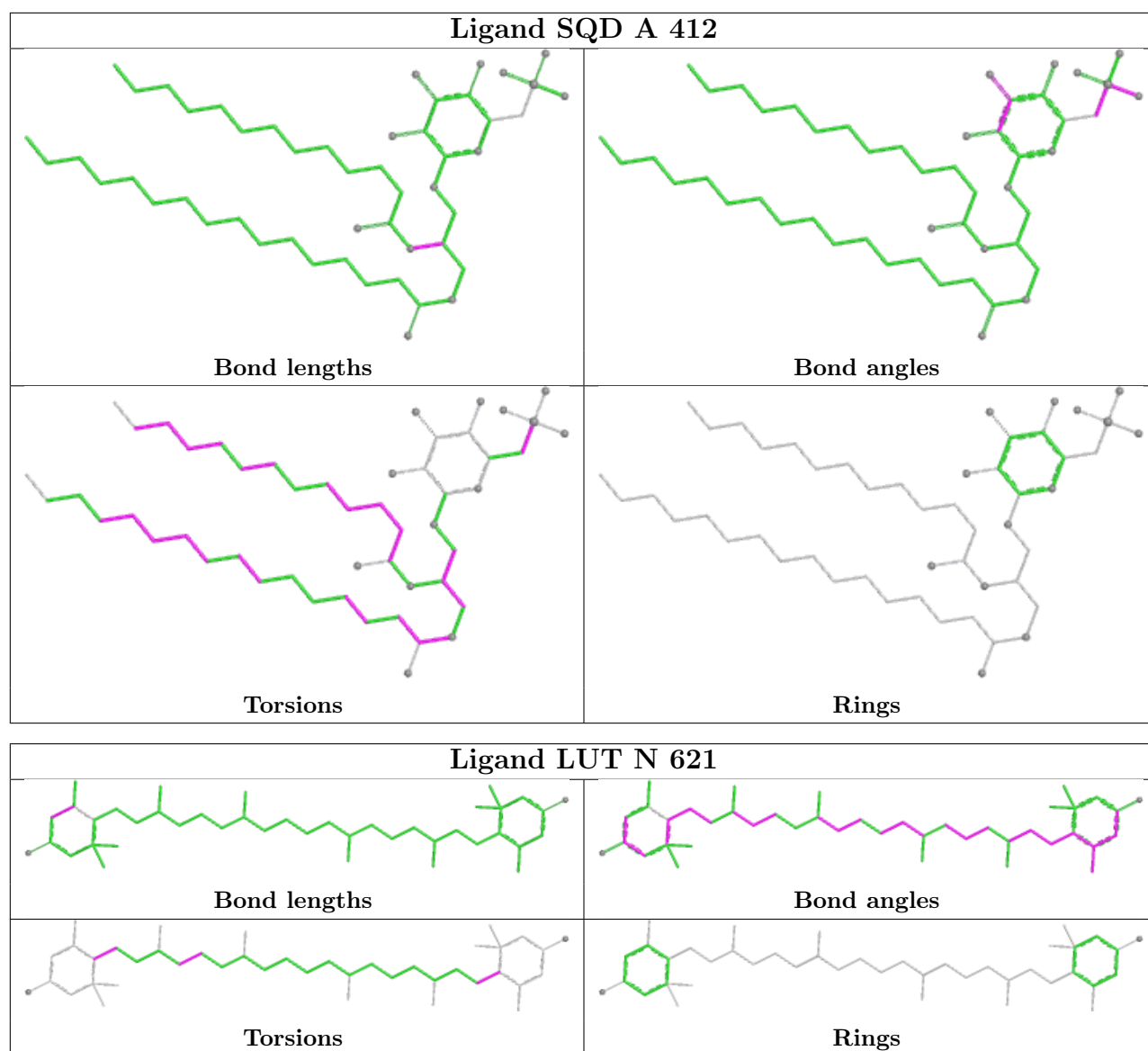
Rings

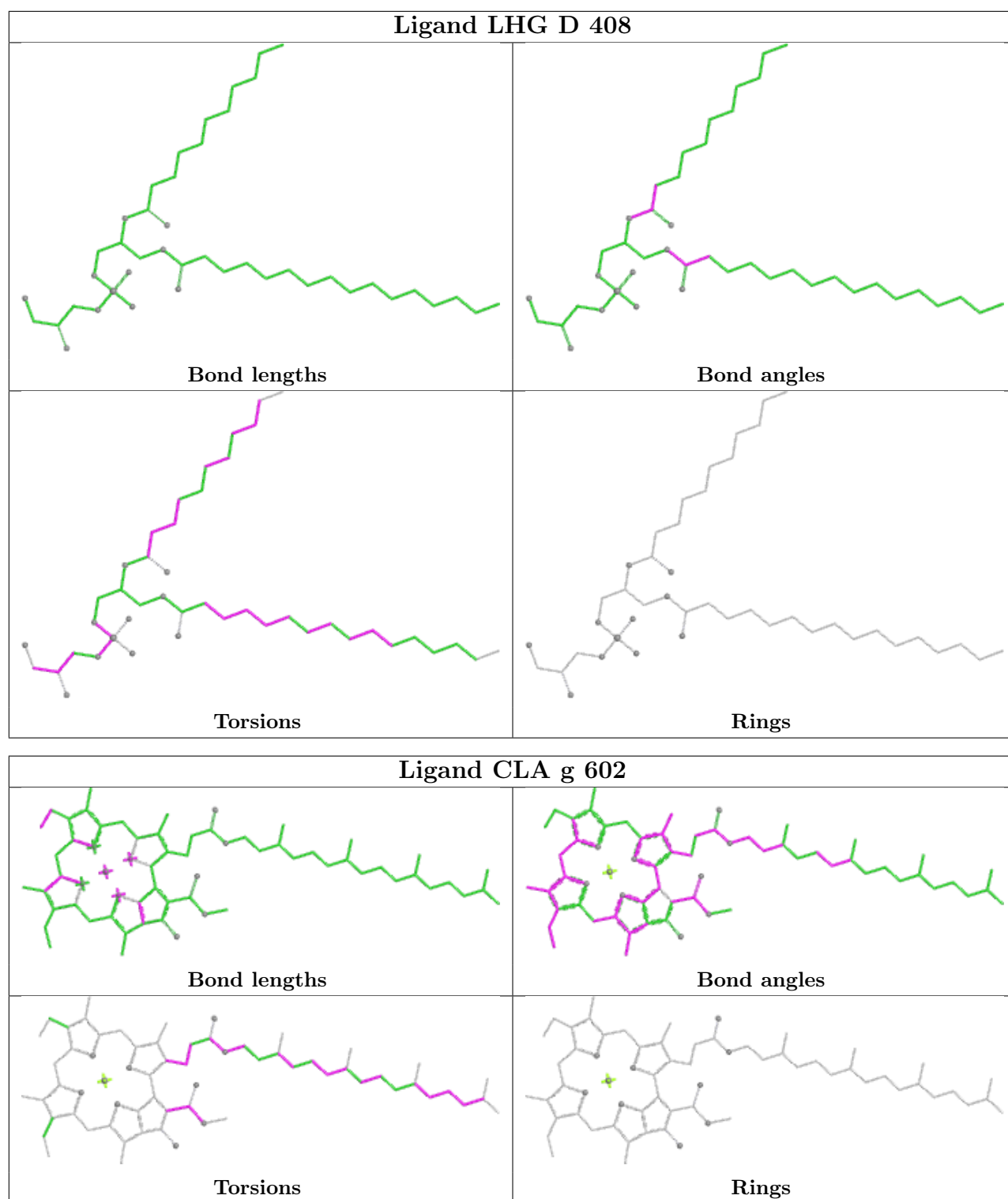


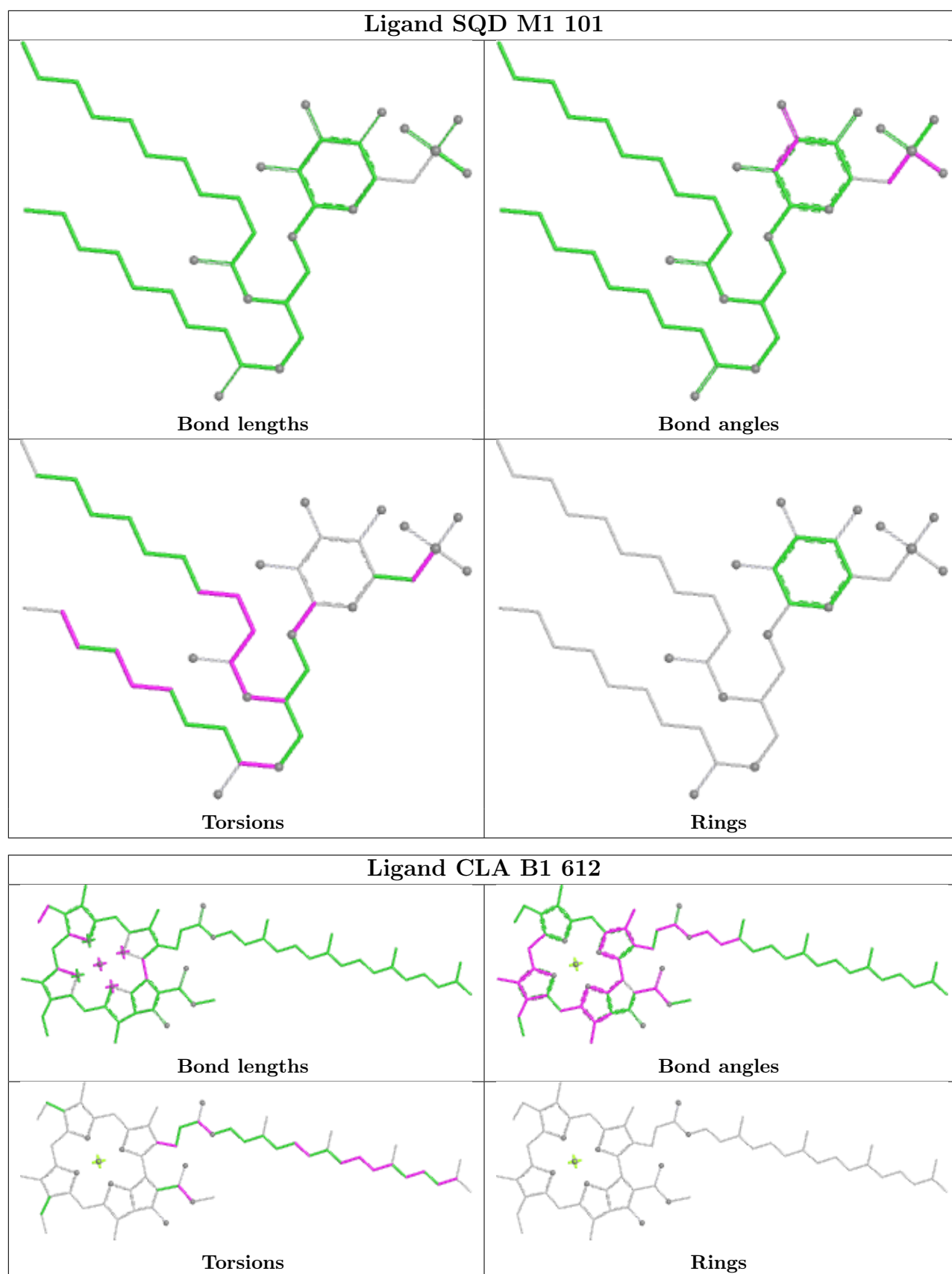


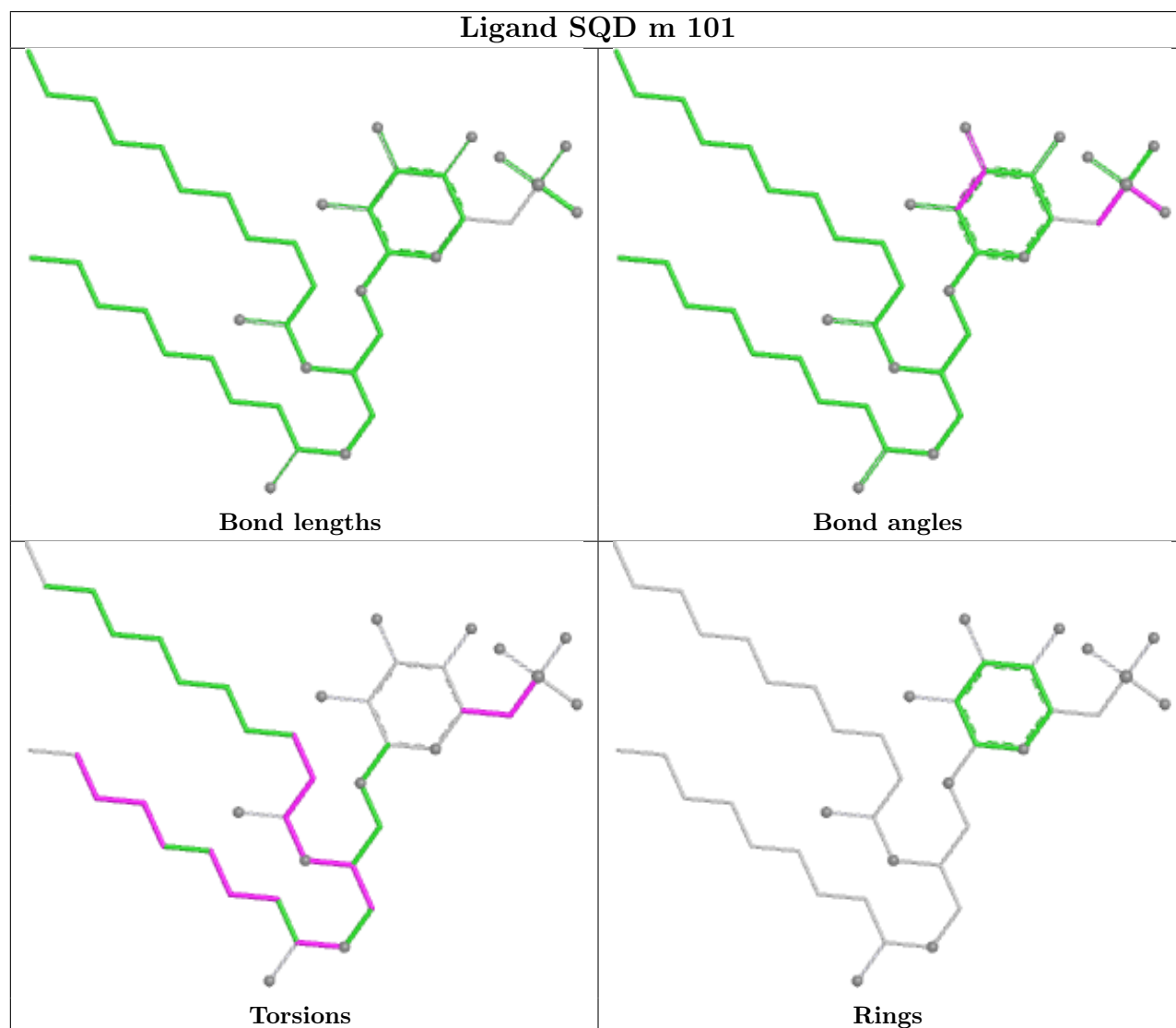
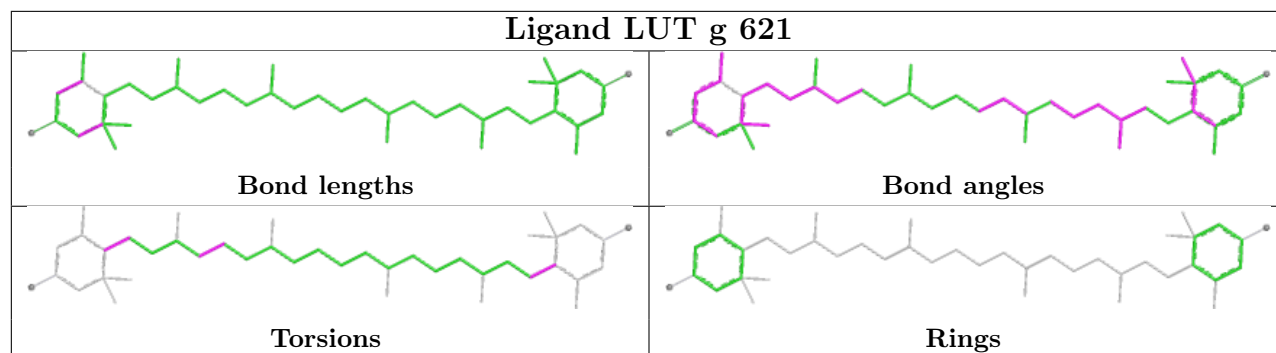
Ligand CLA b 613**Ligand CLA Y 603**

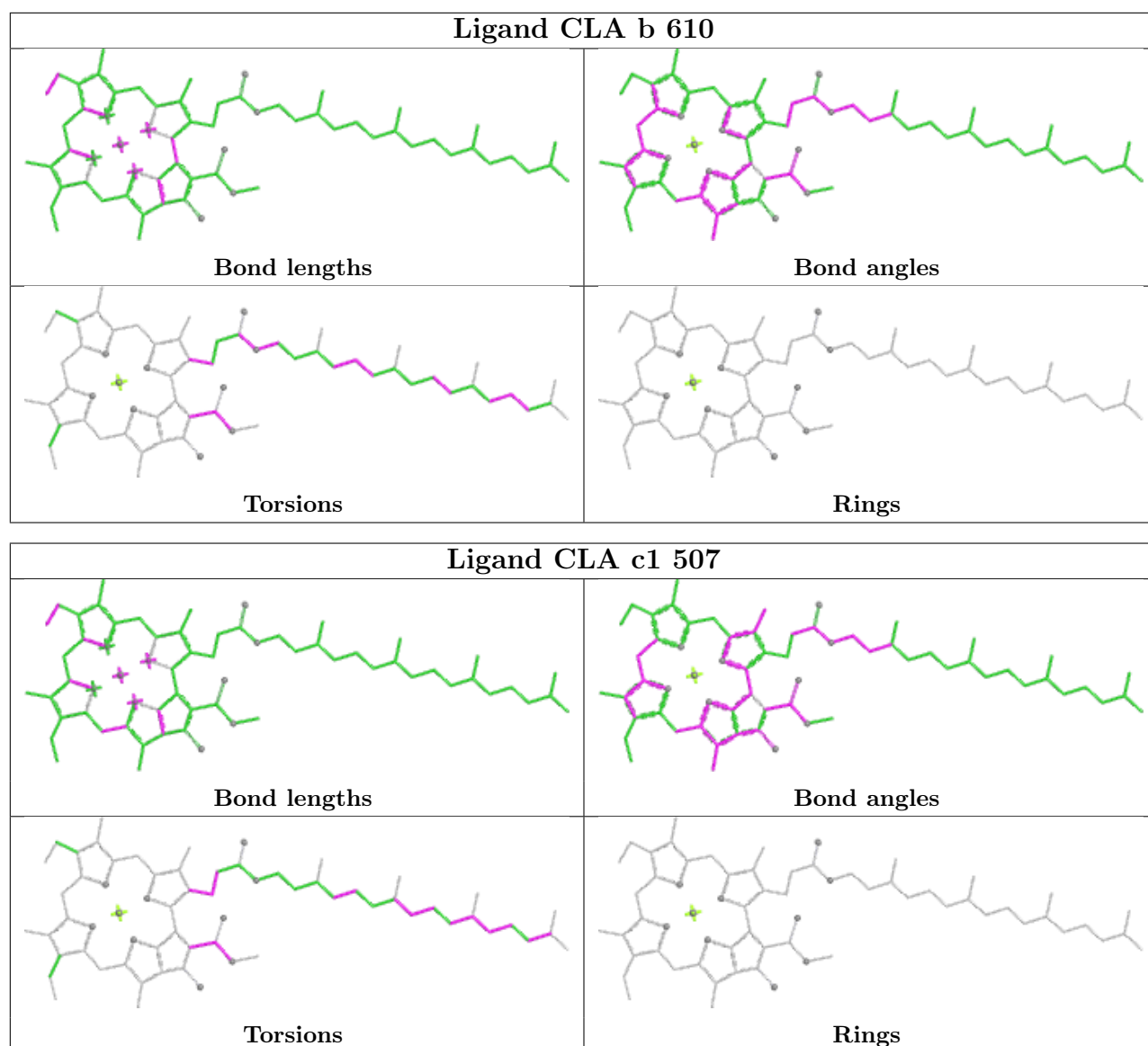


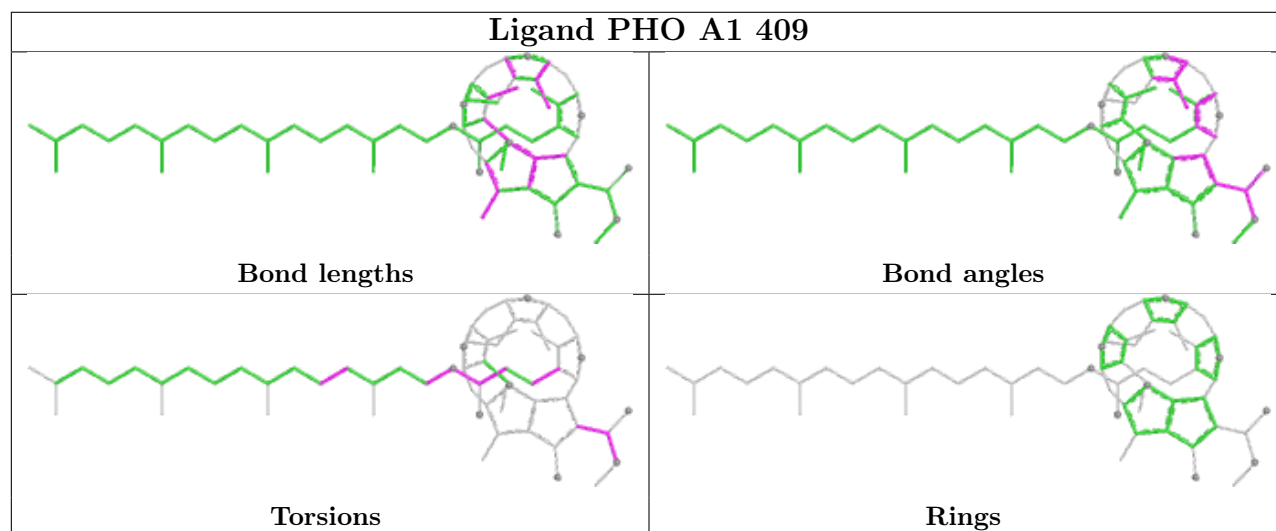
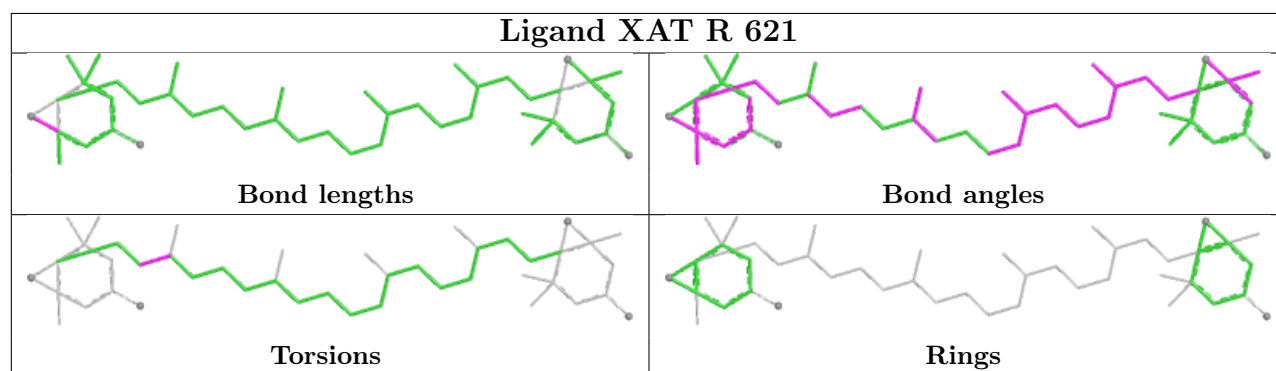
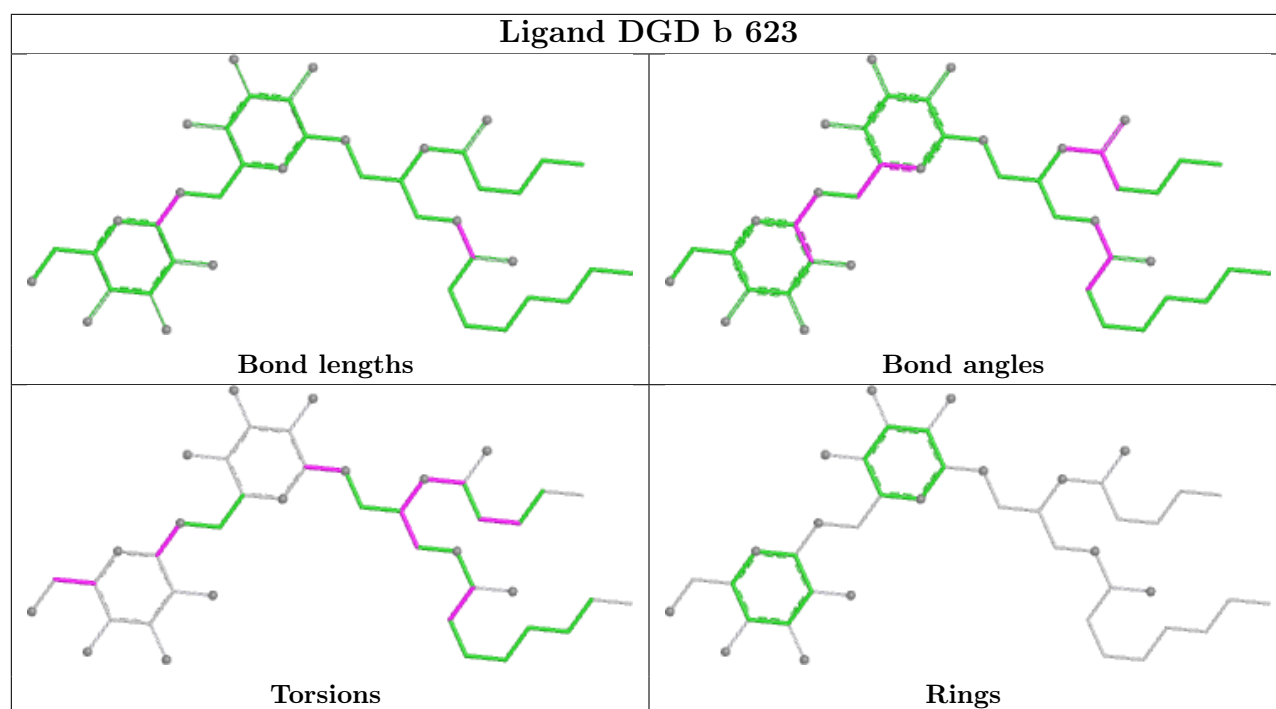


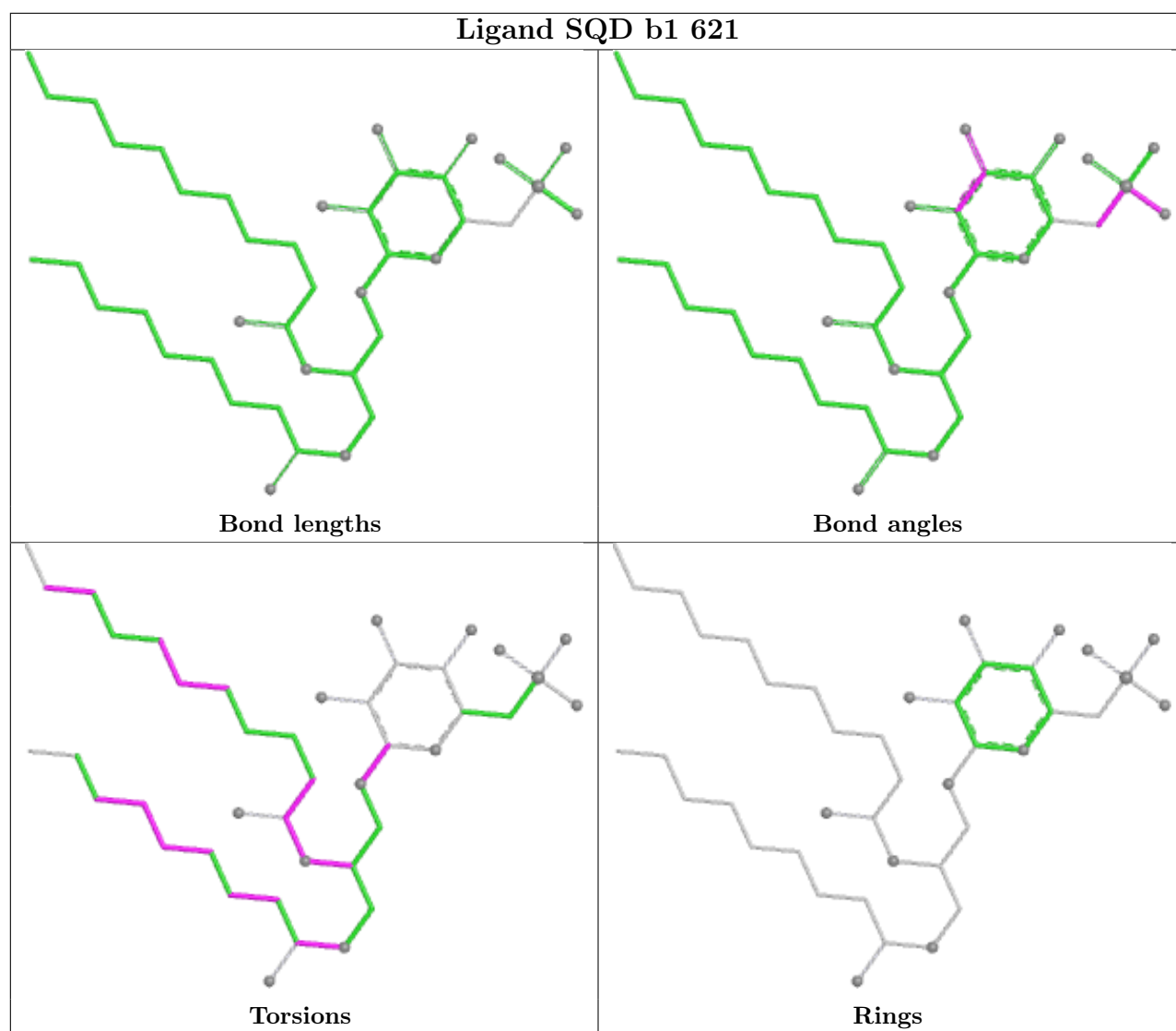


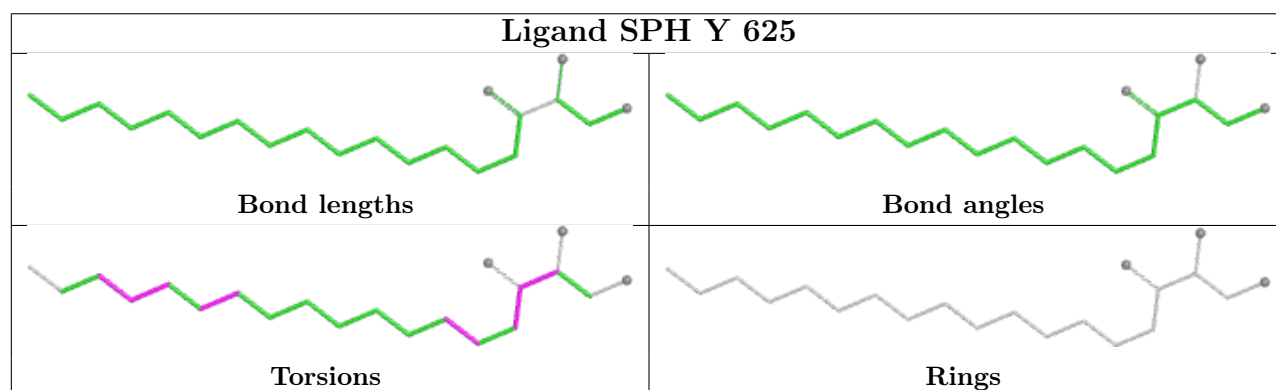
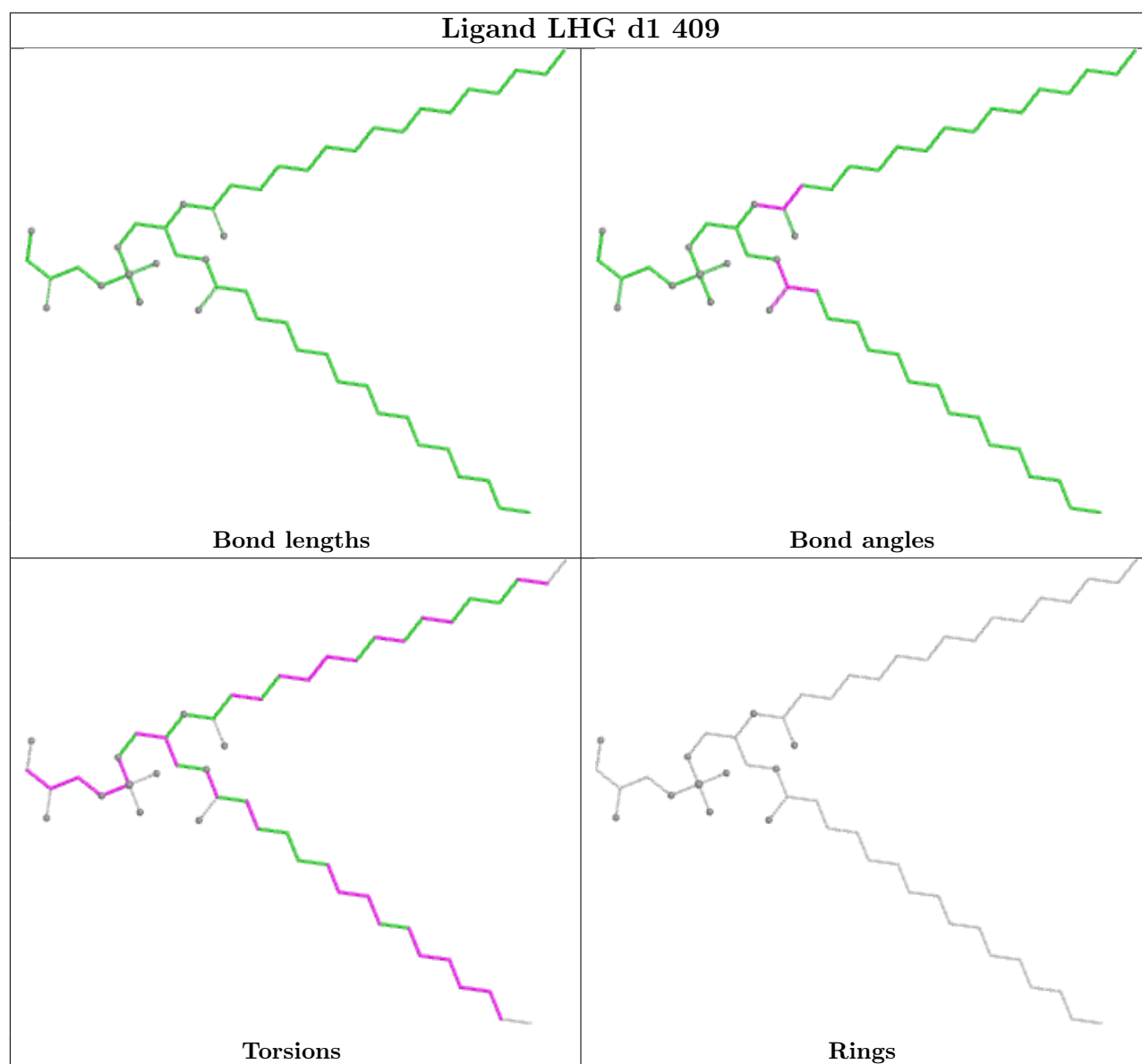


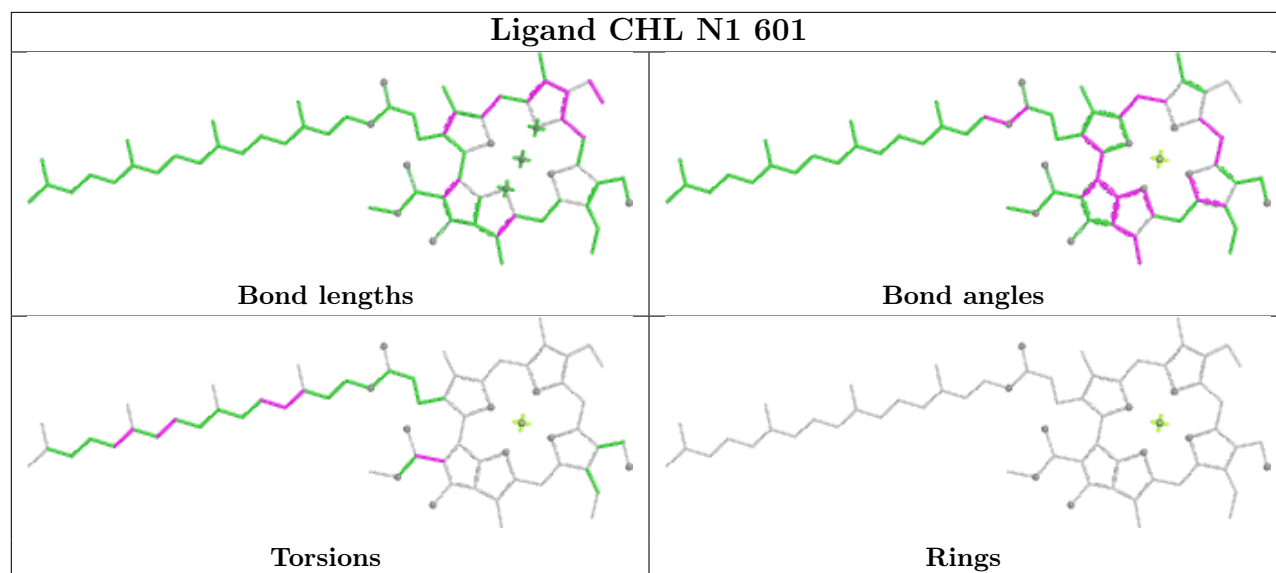
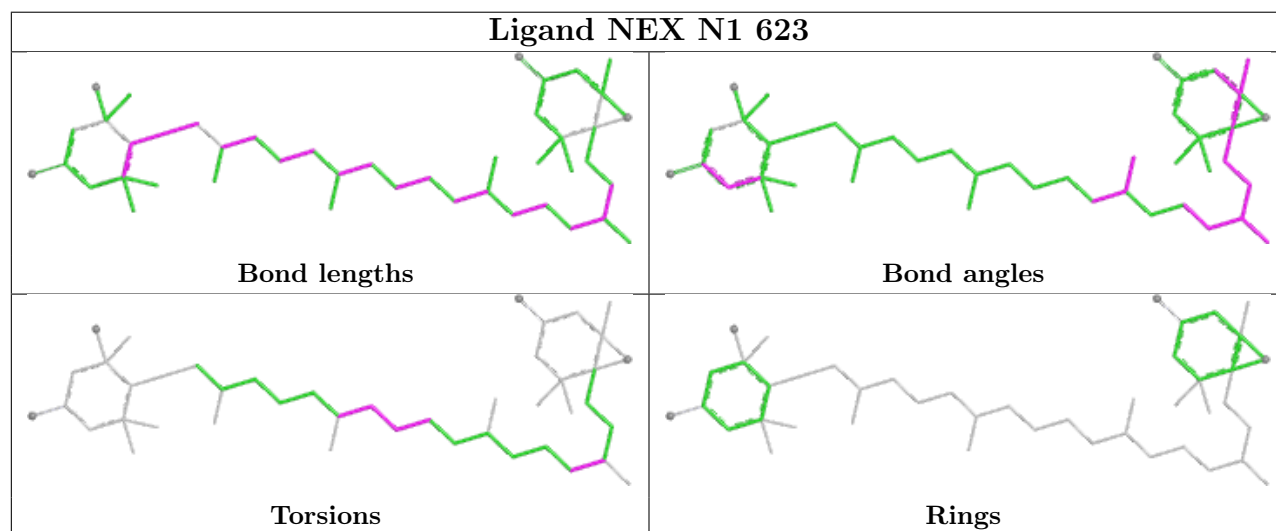
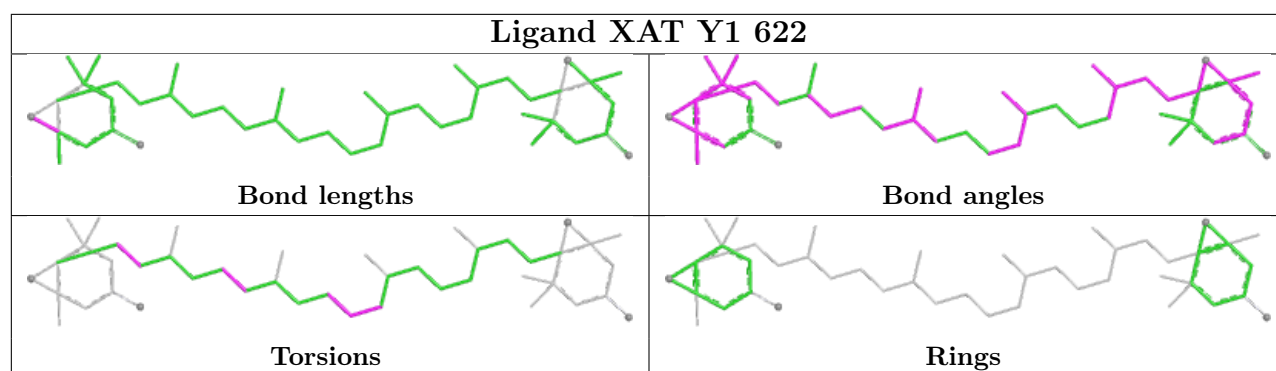


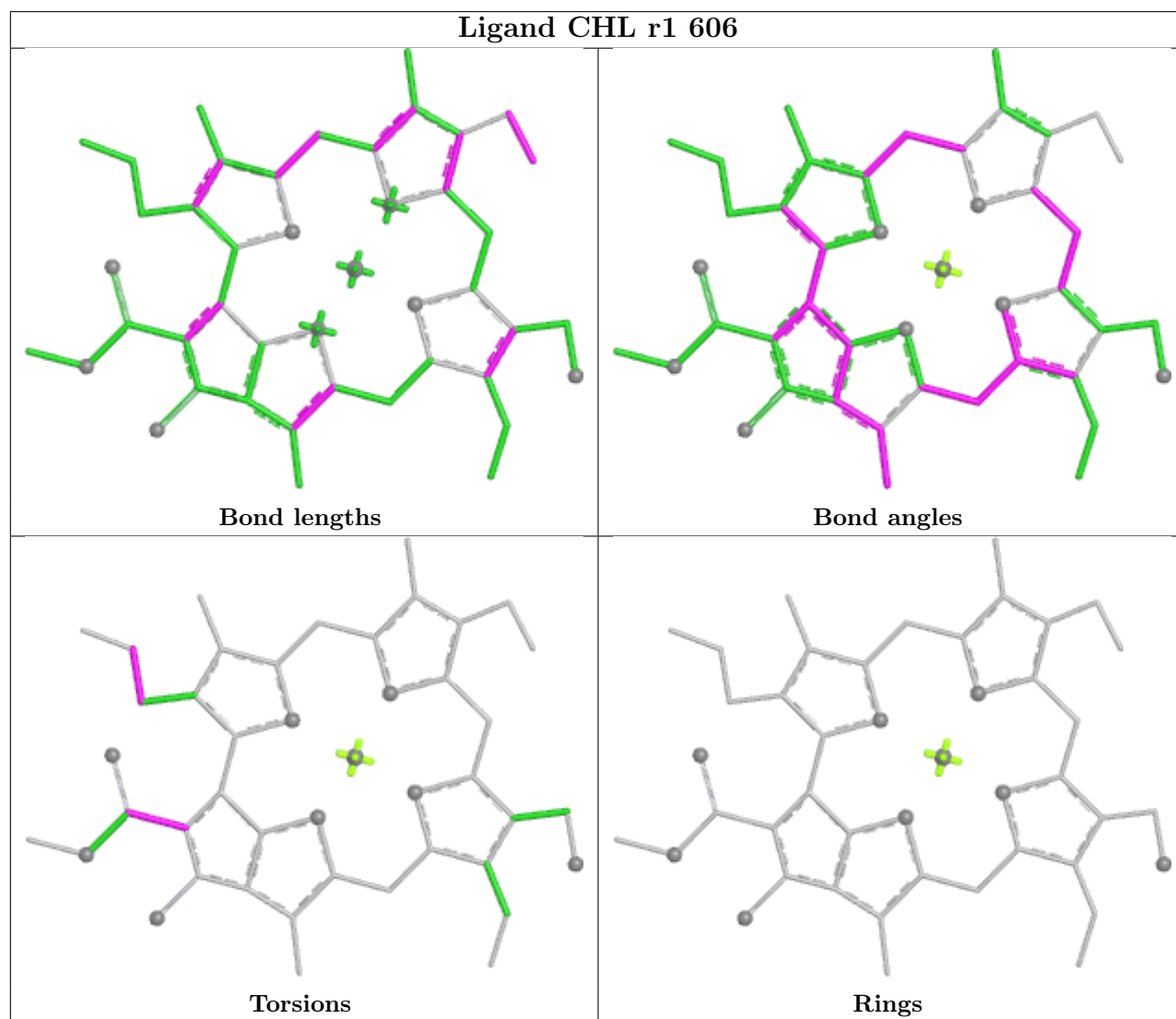
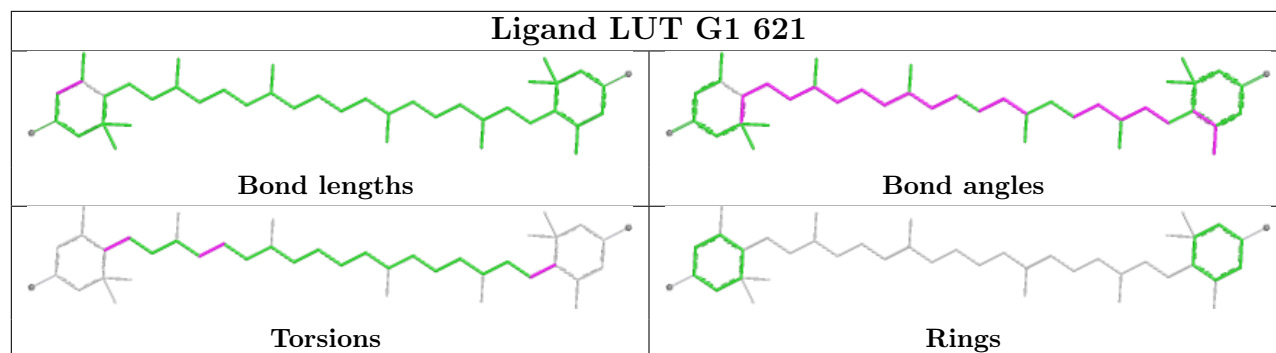


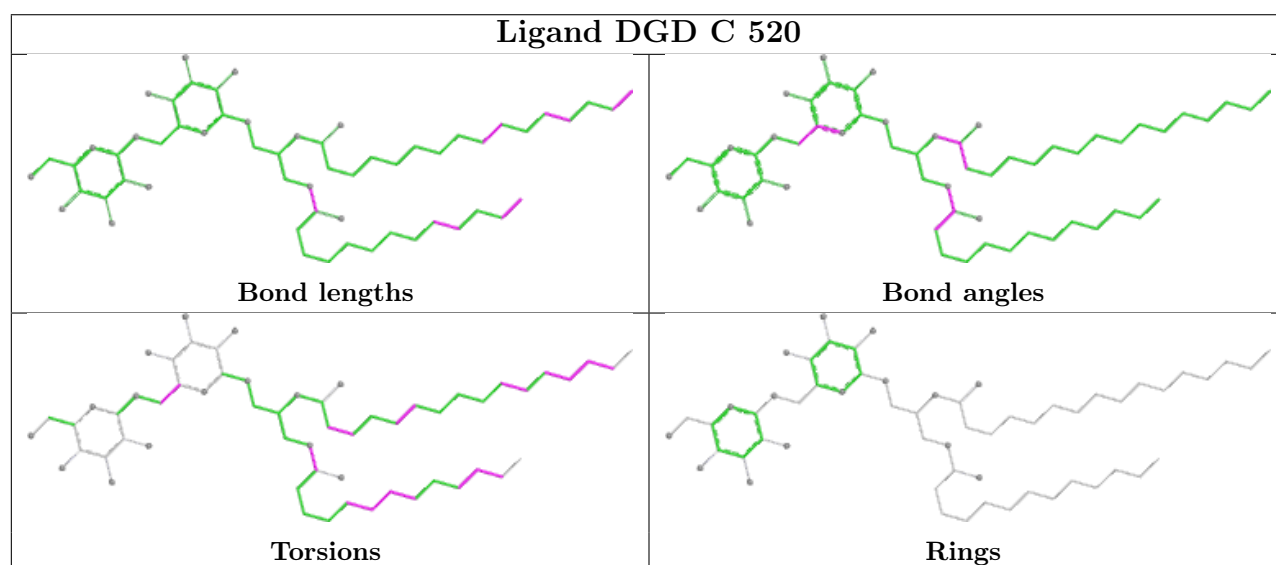
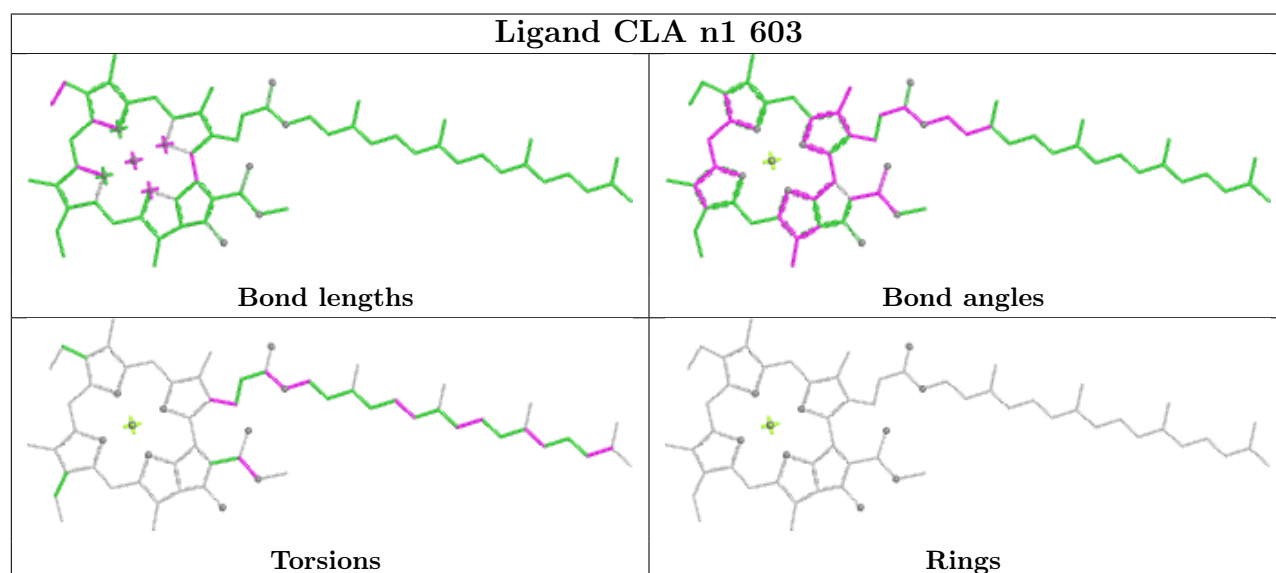
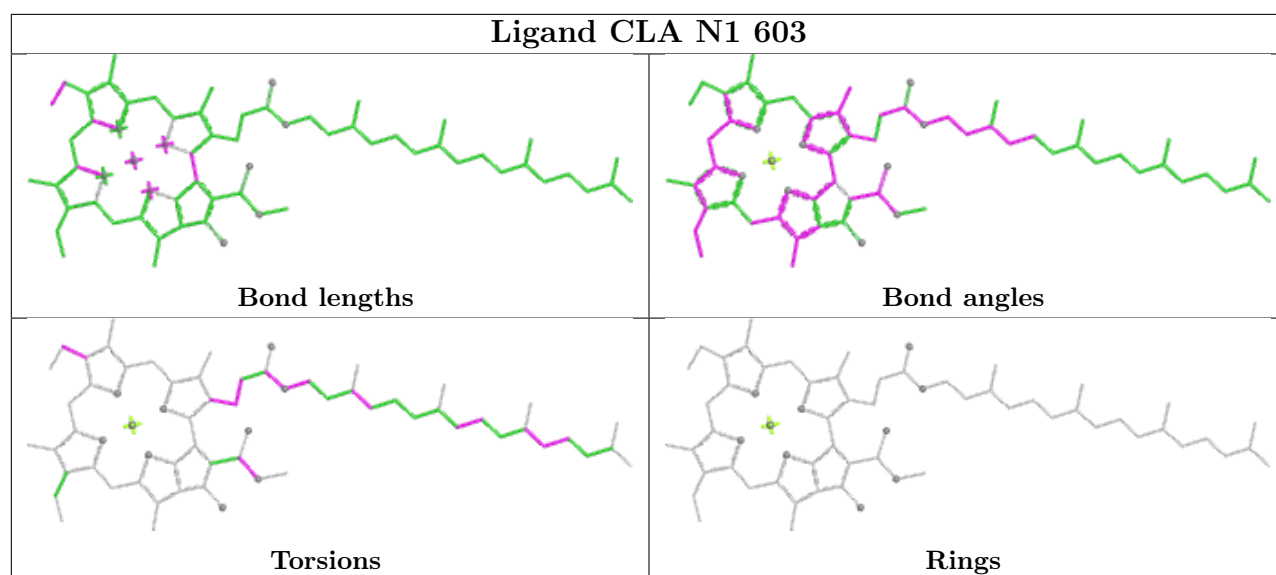


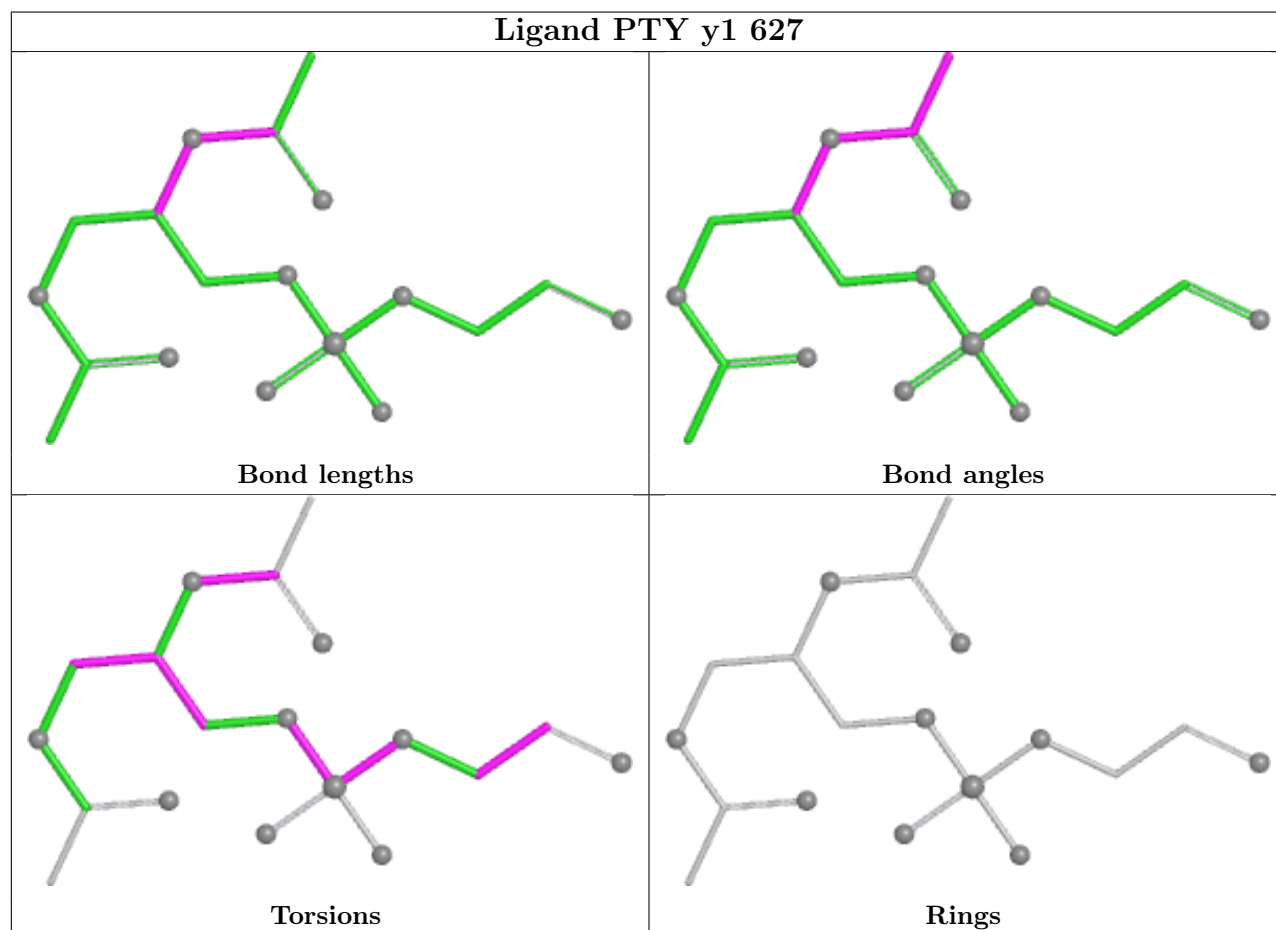
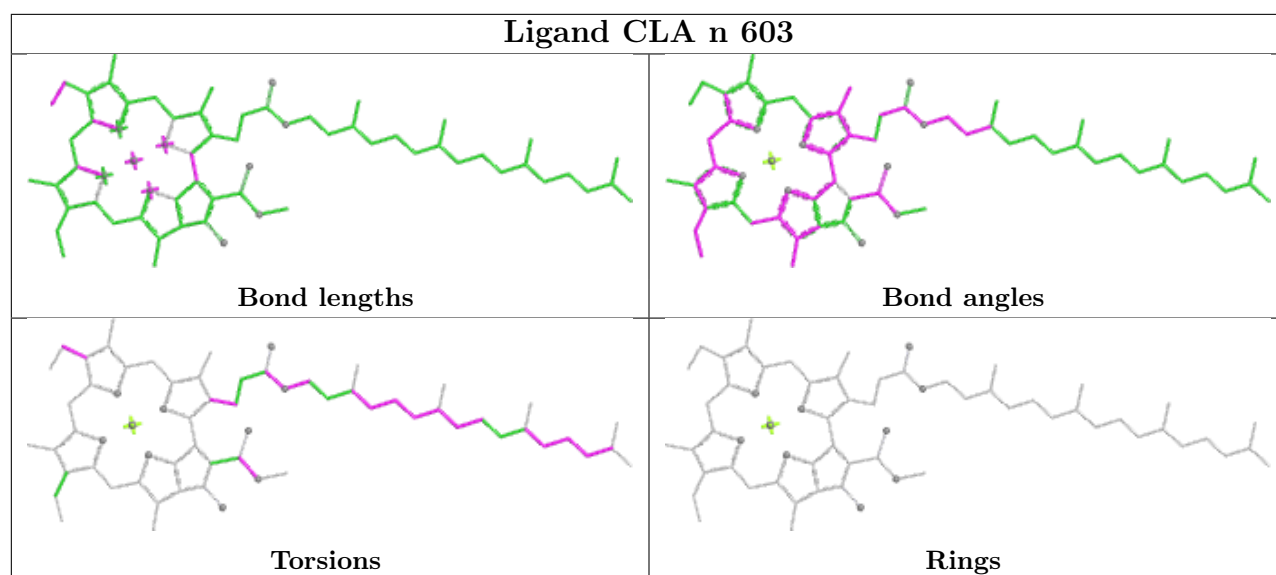


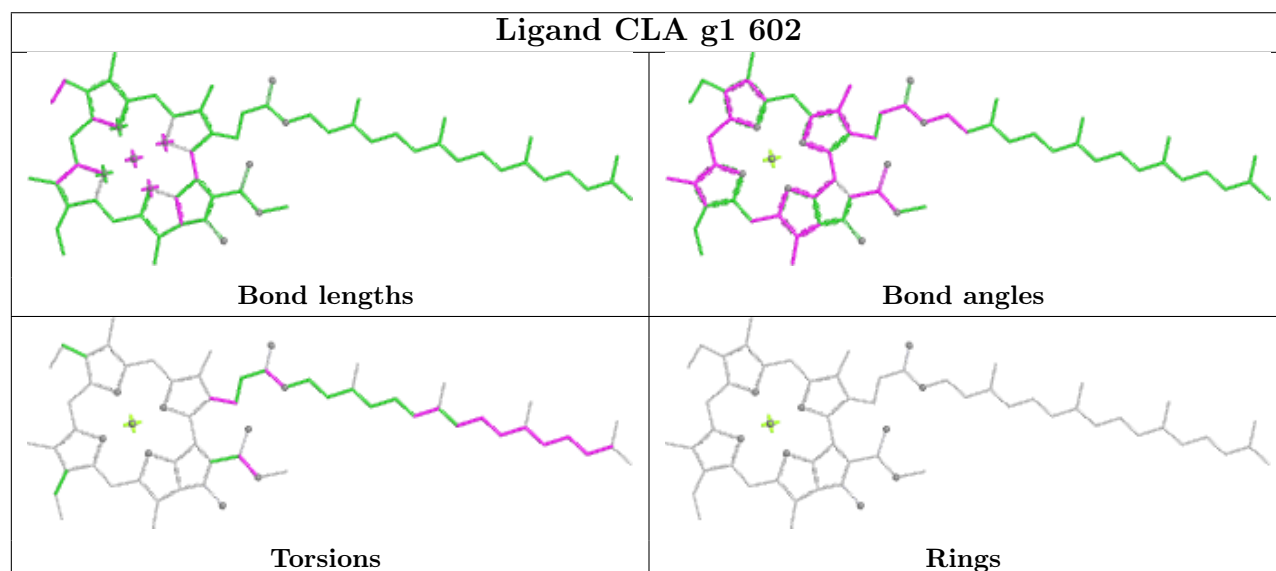
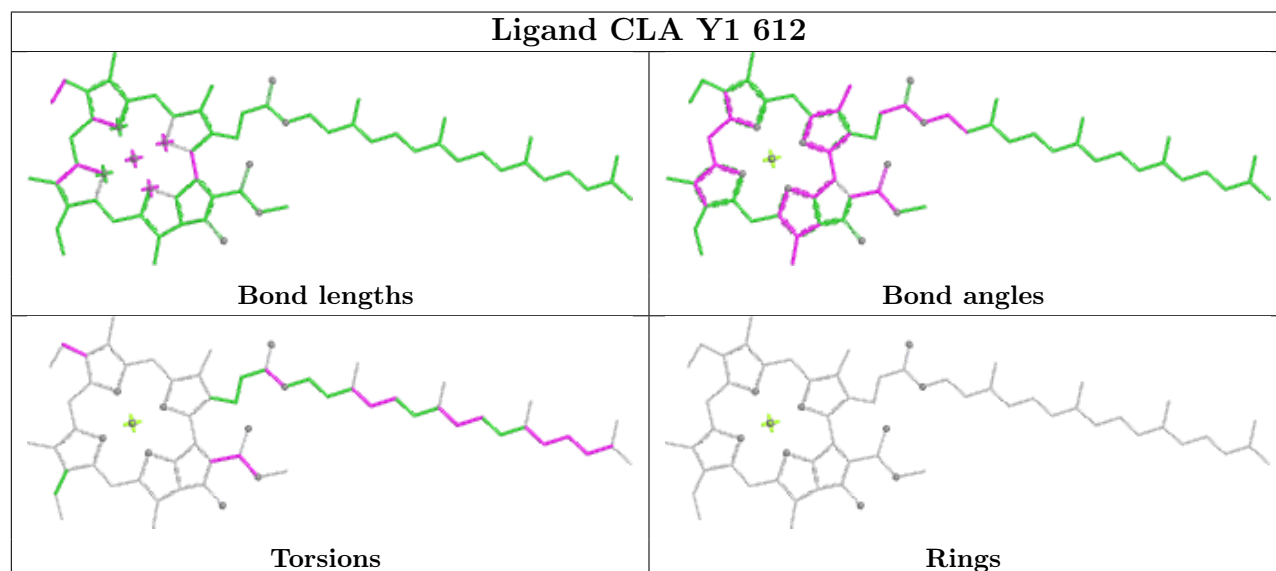
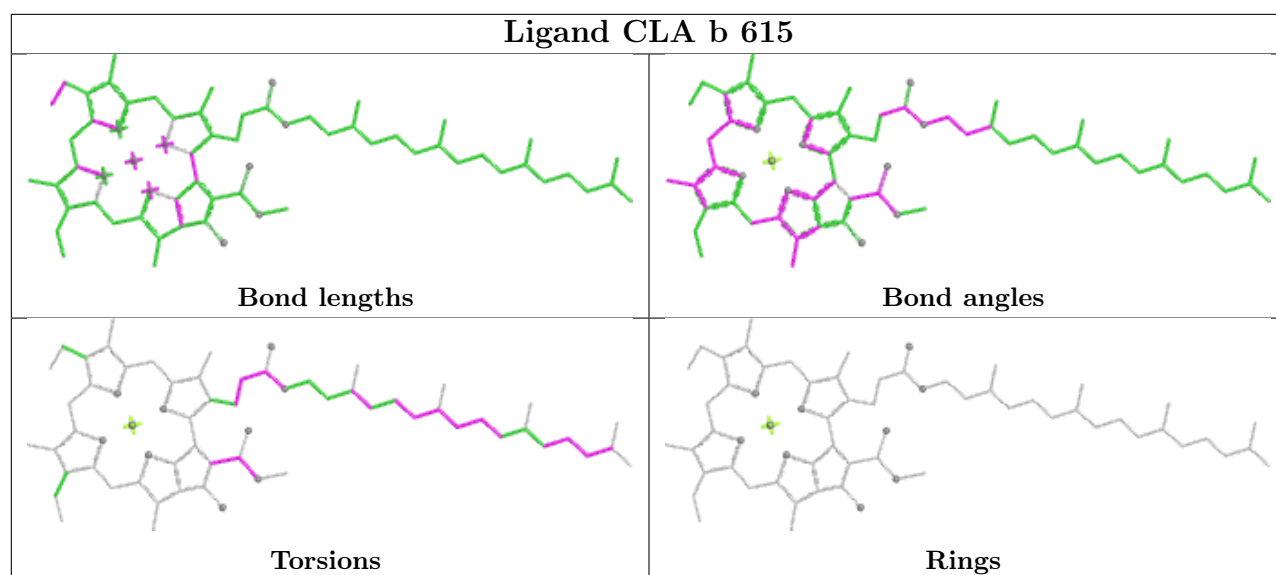


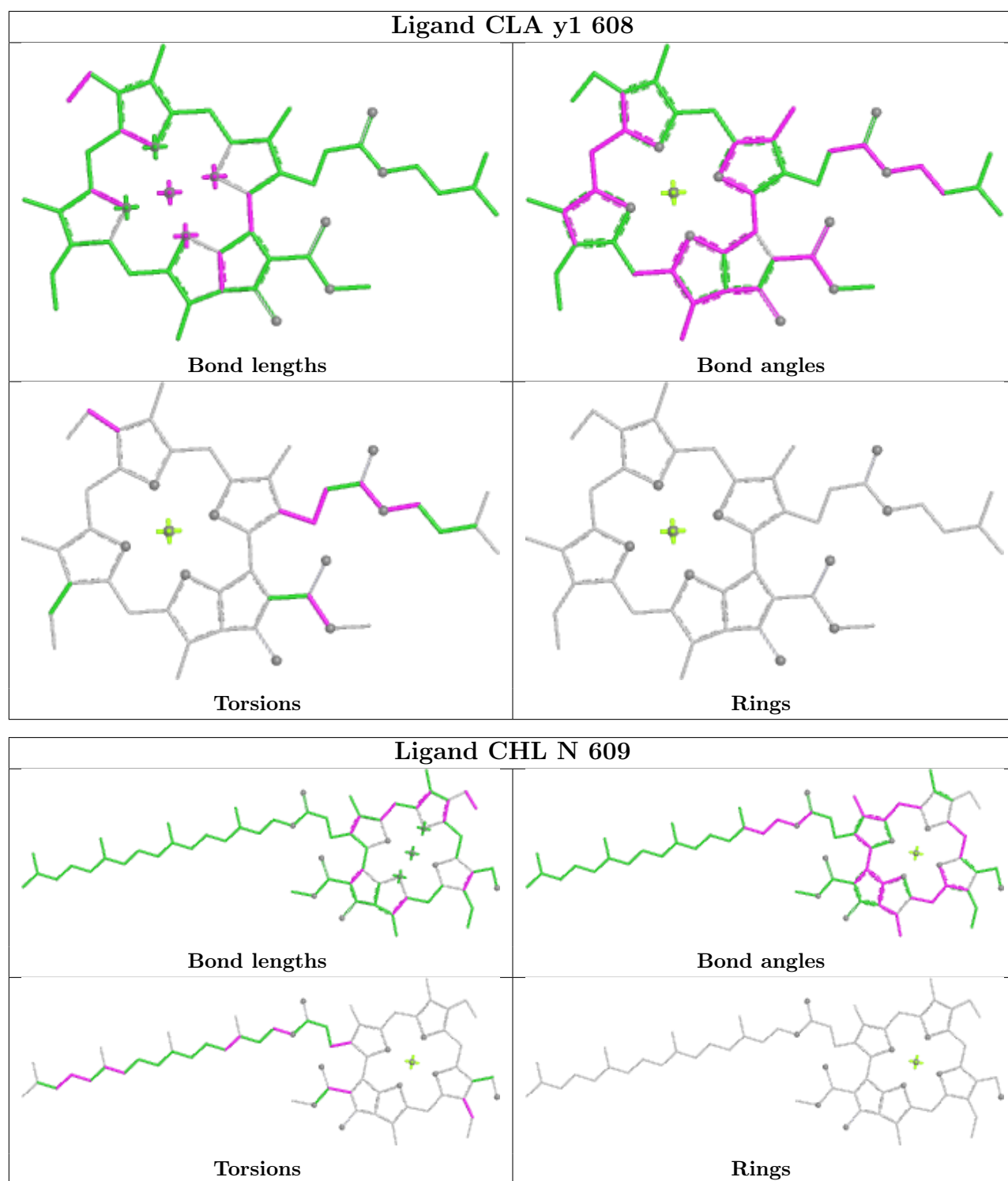


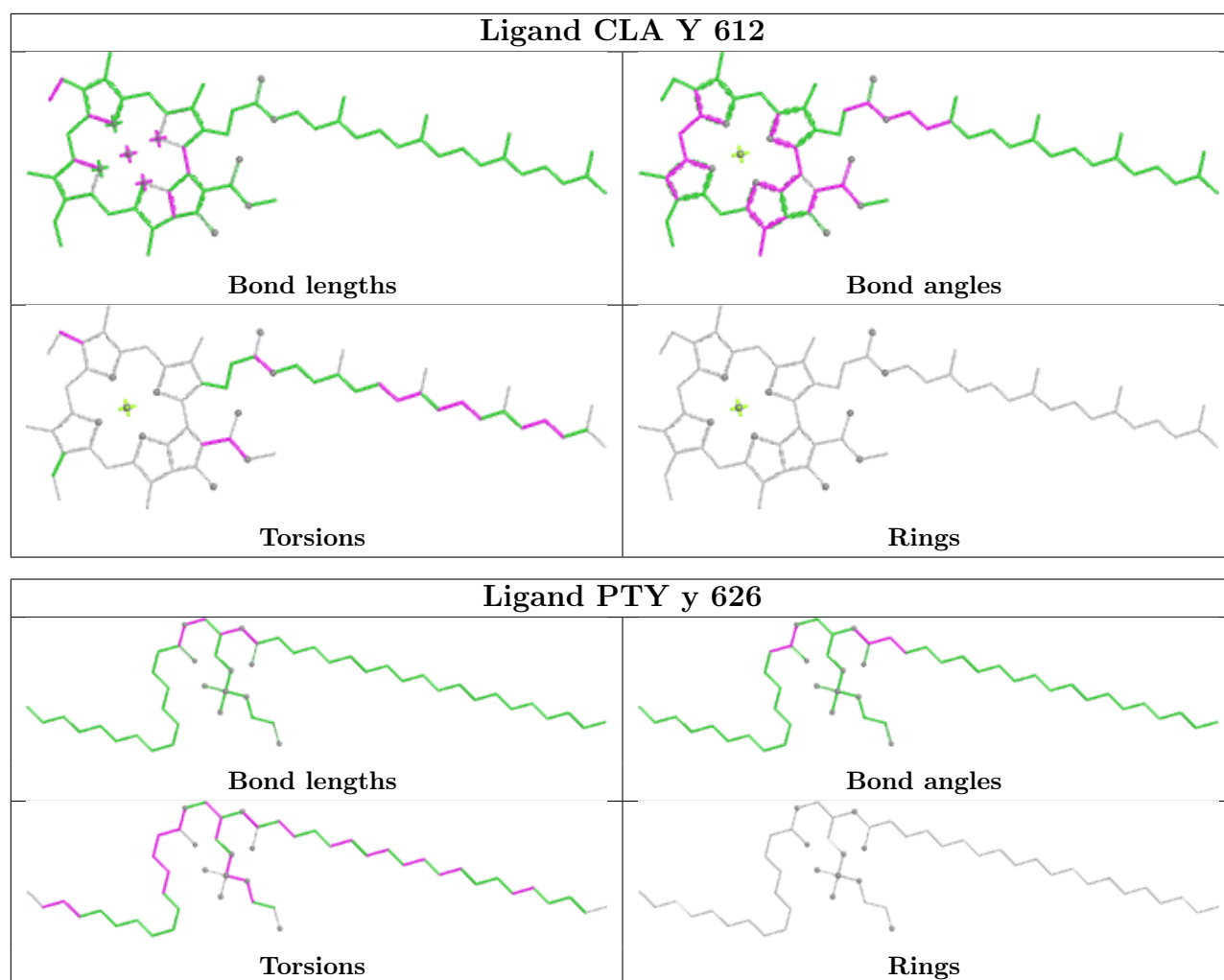


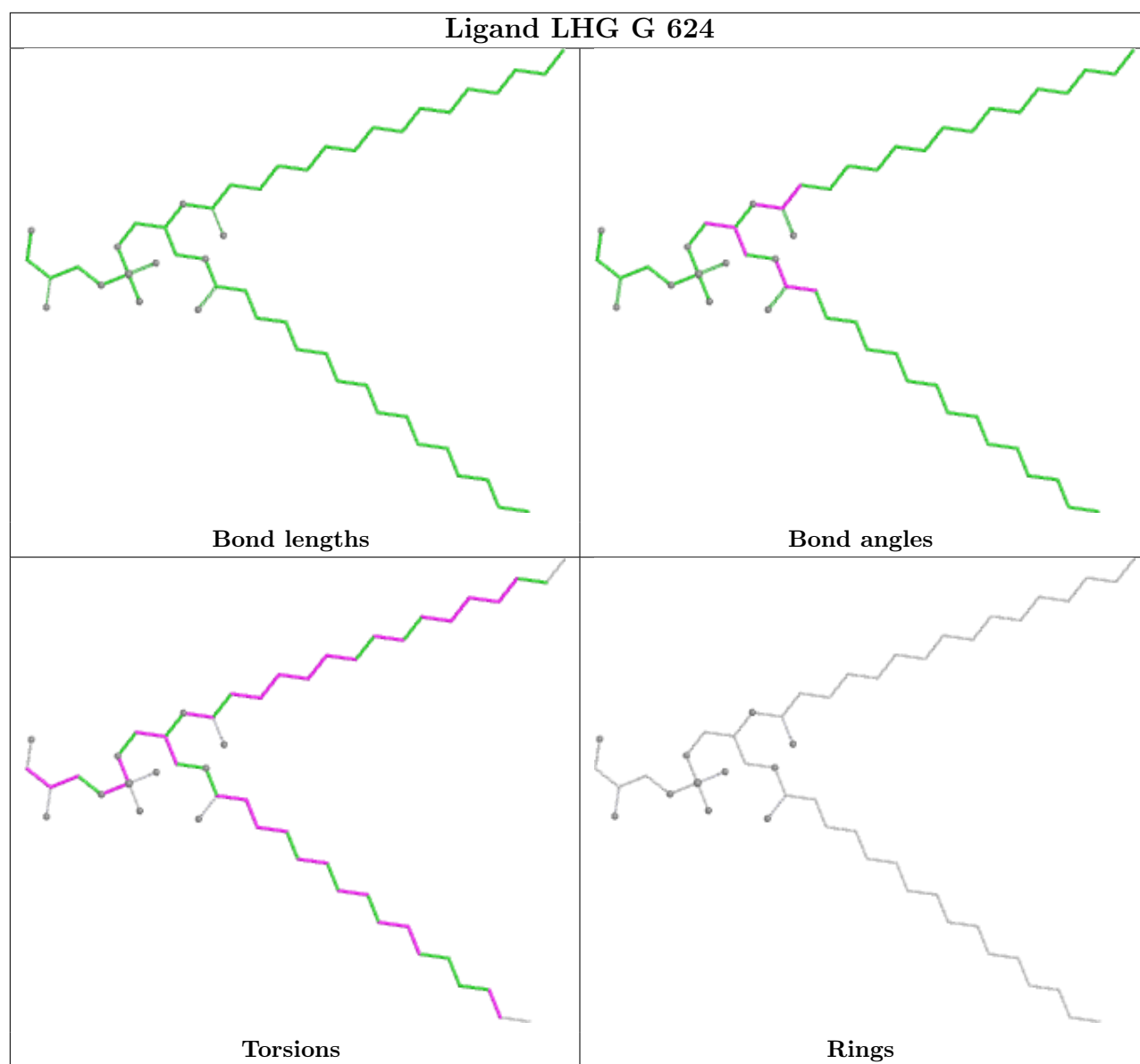




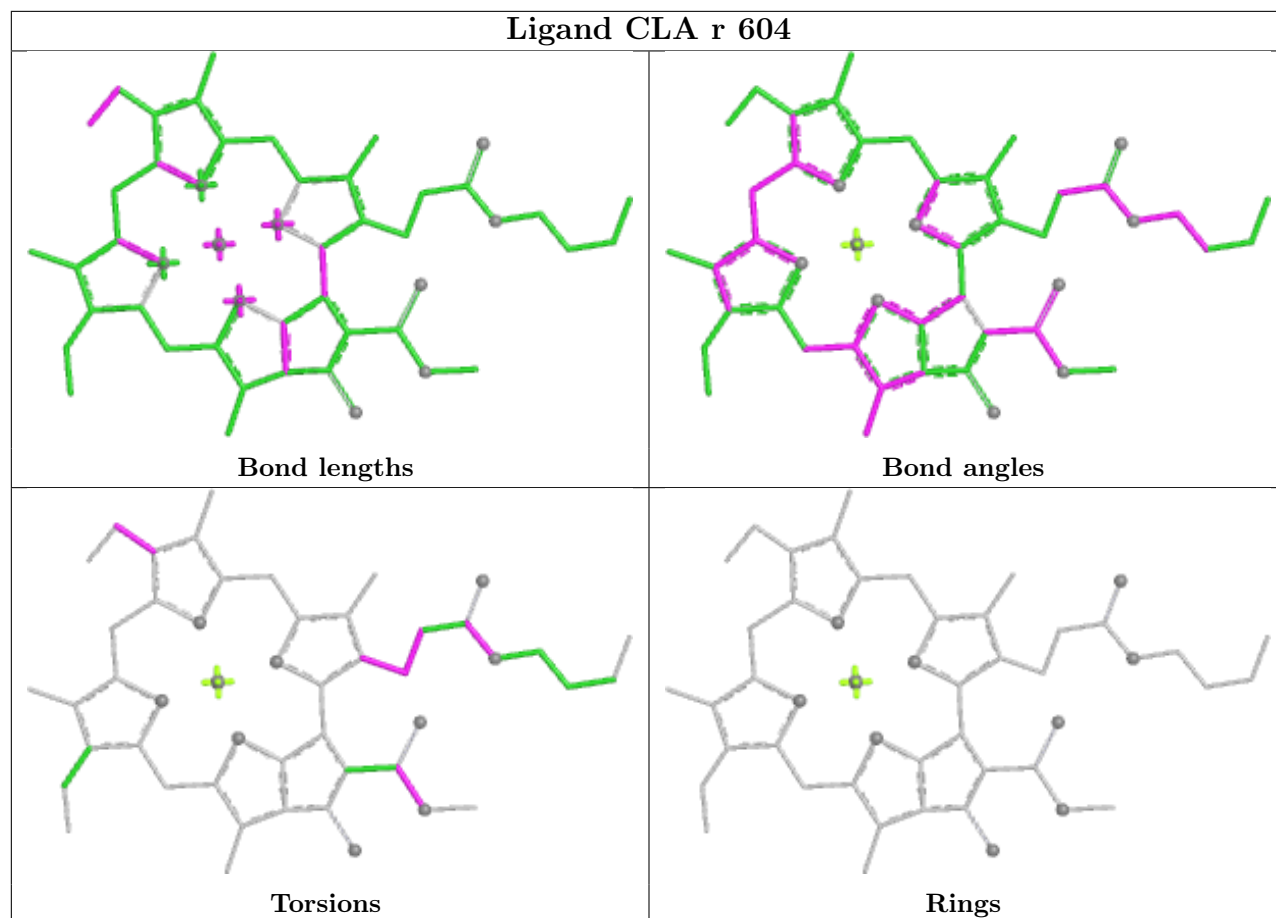


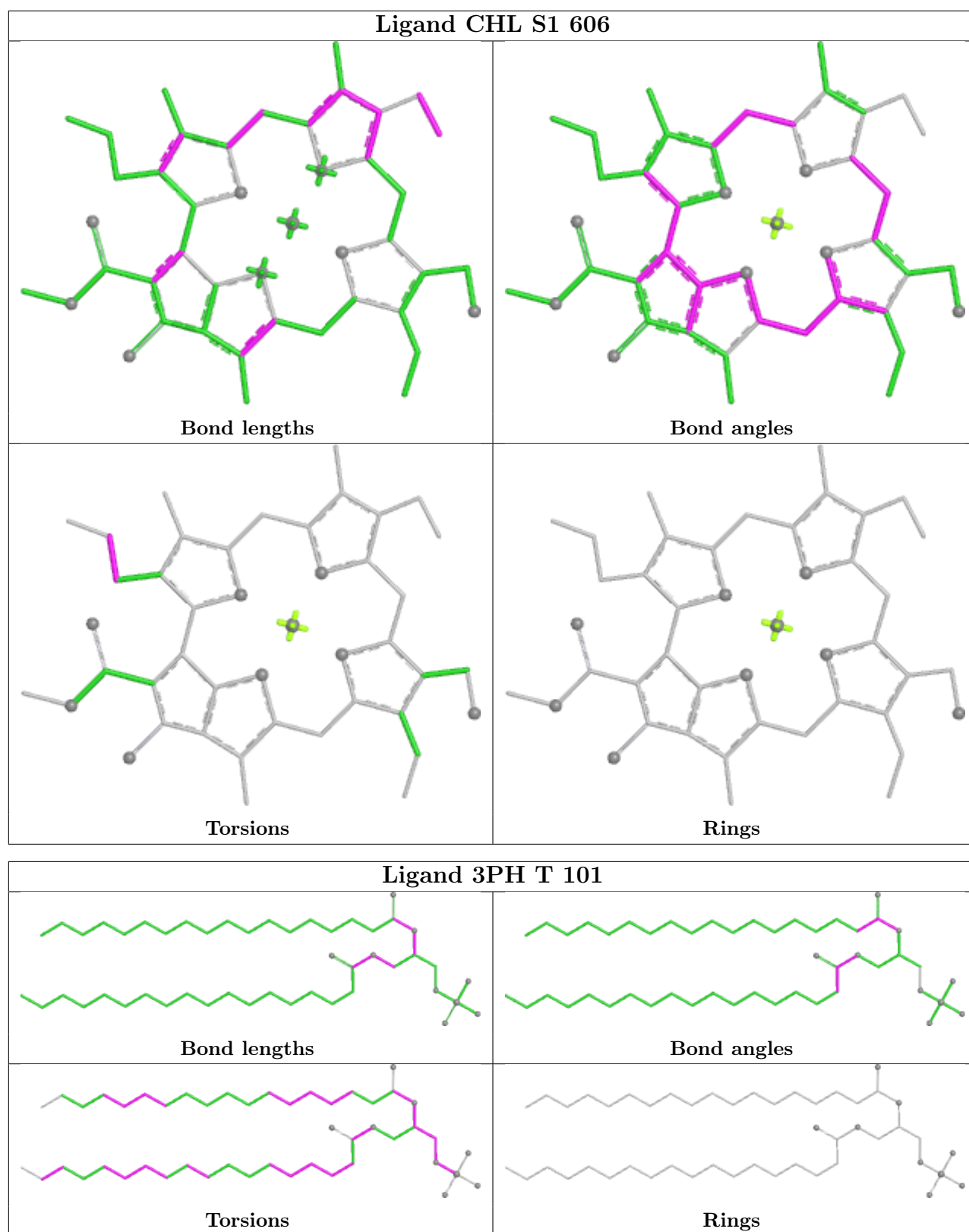


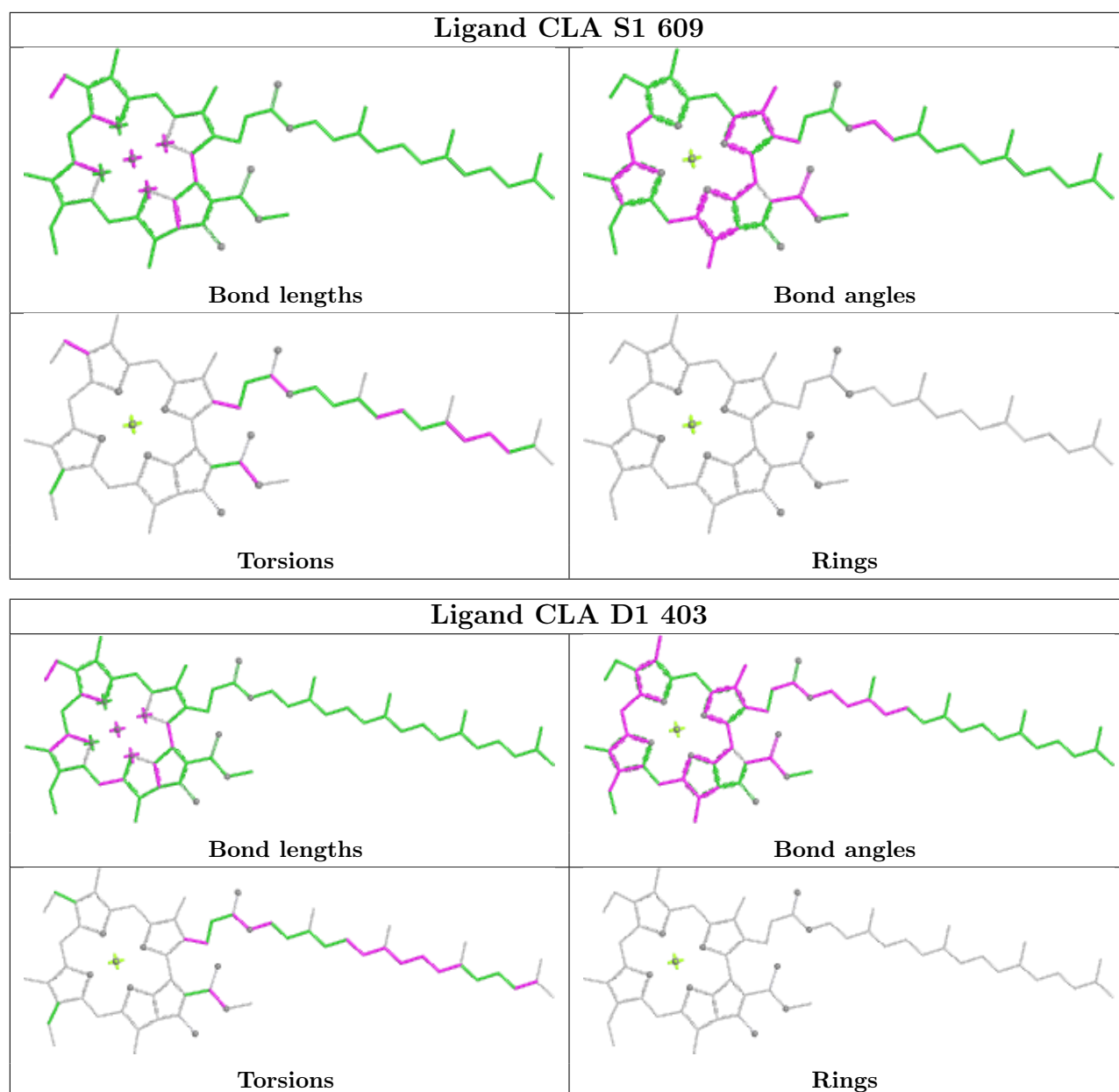


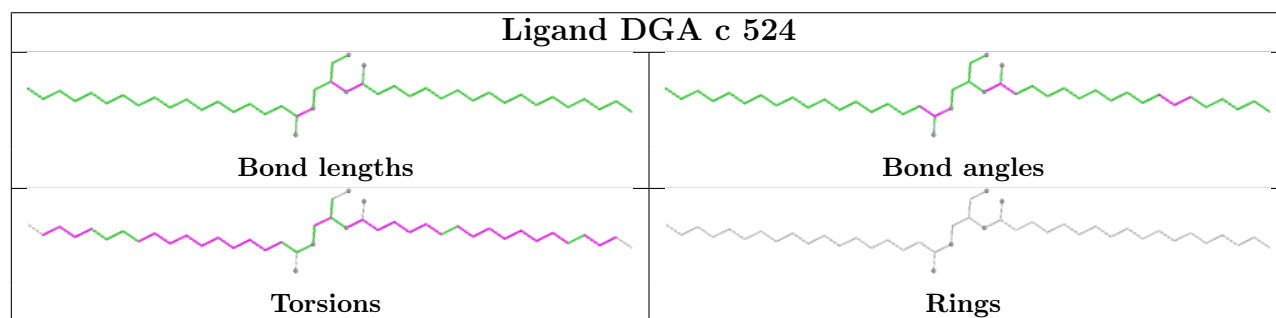
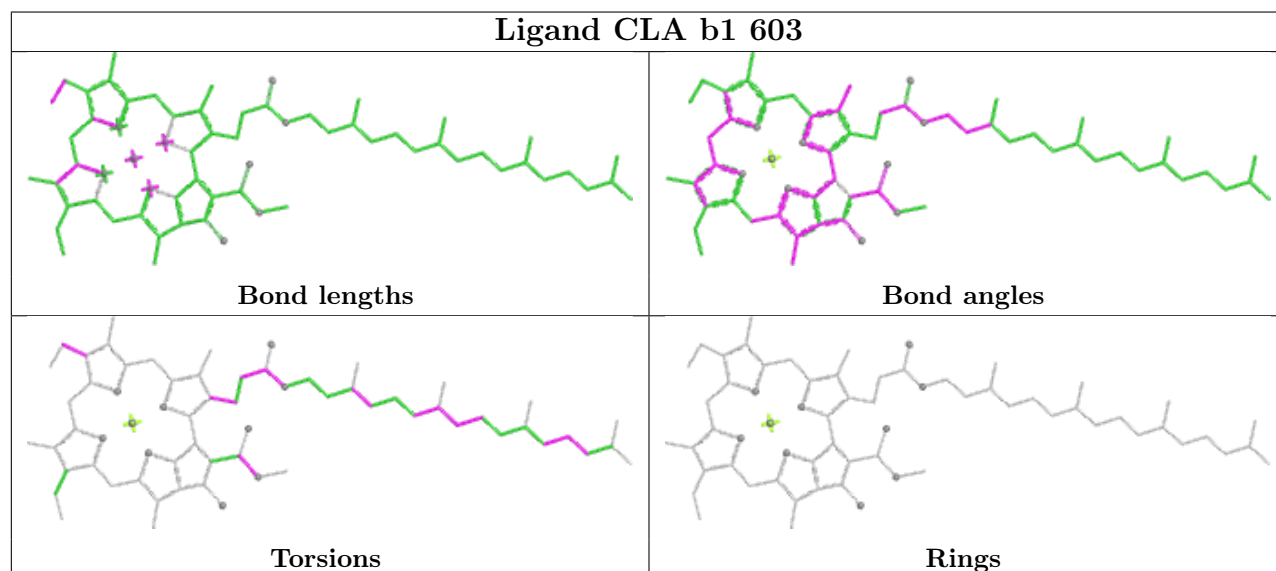
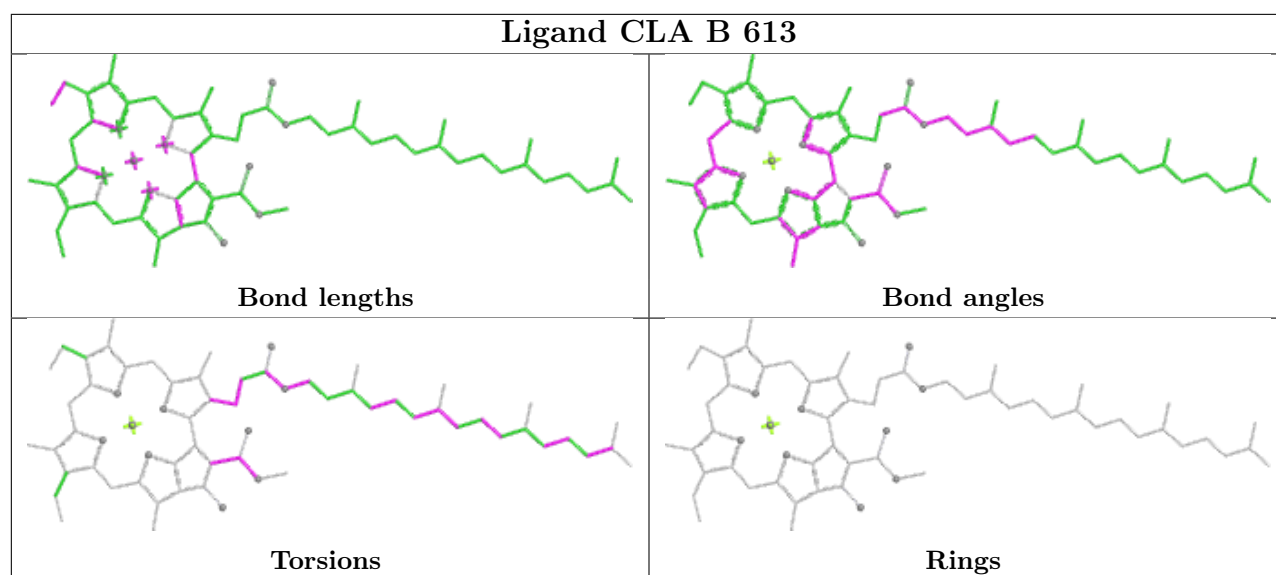


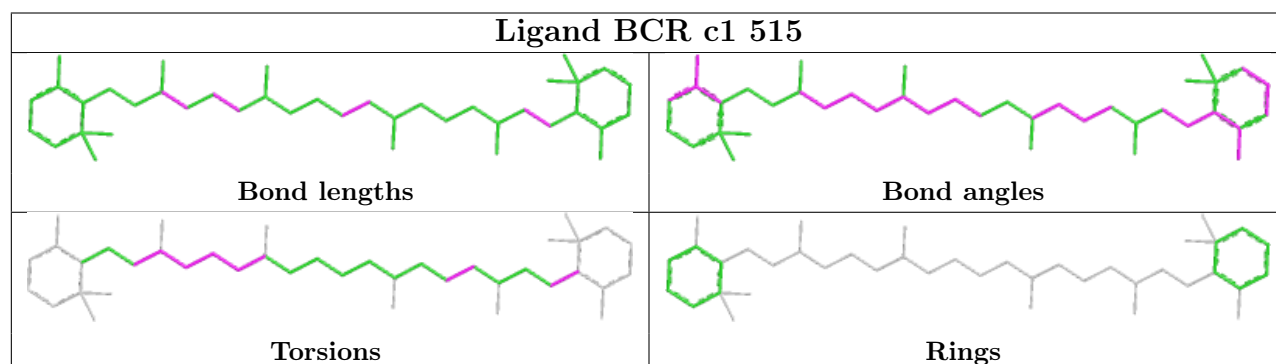
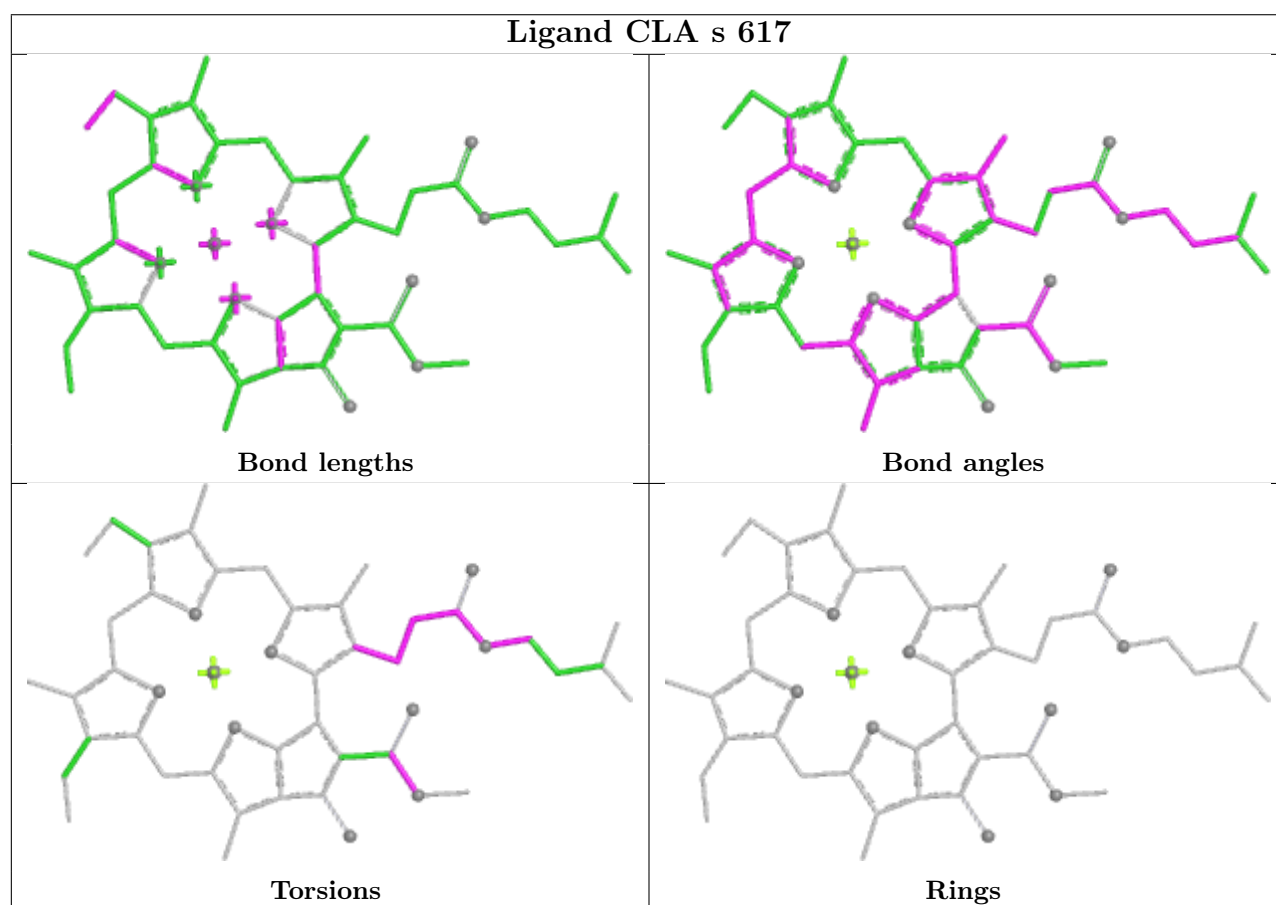
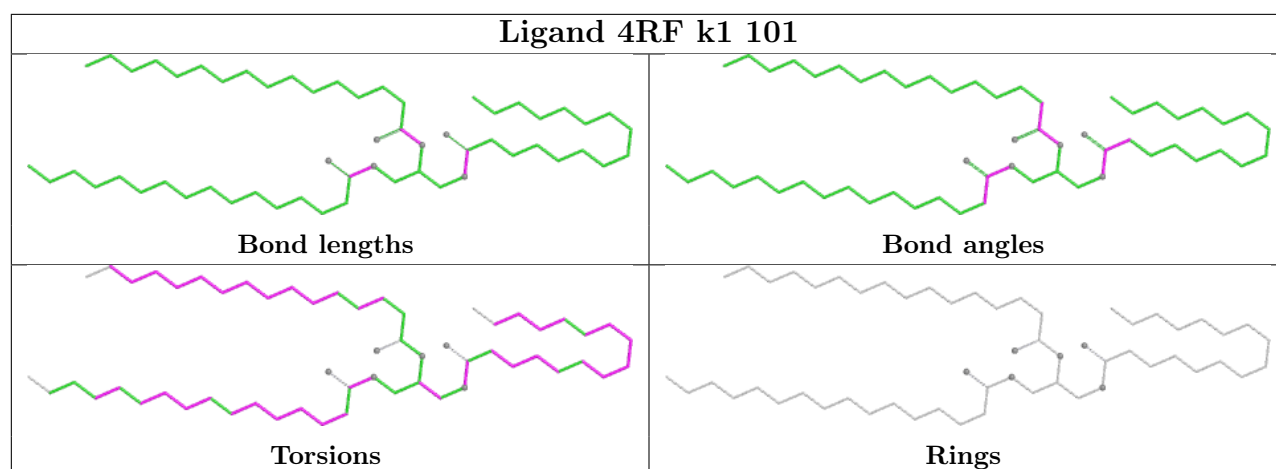
Ligand CLA r 604

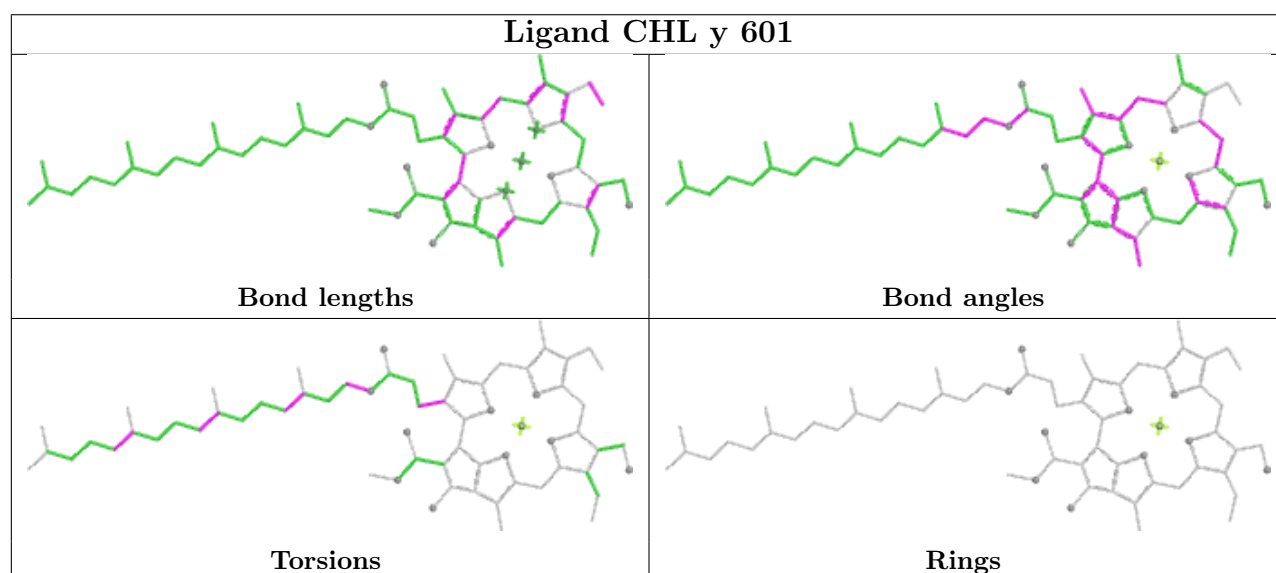
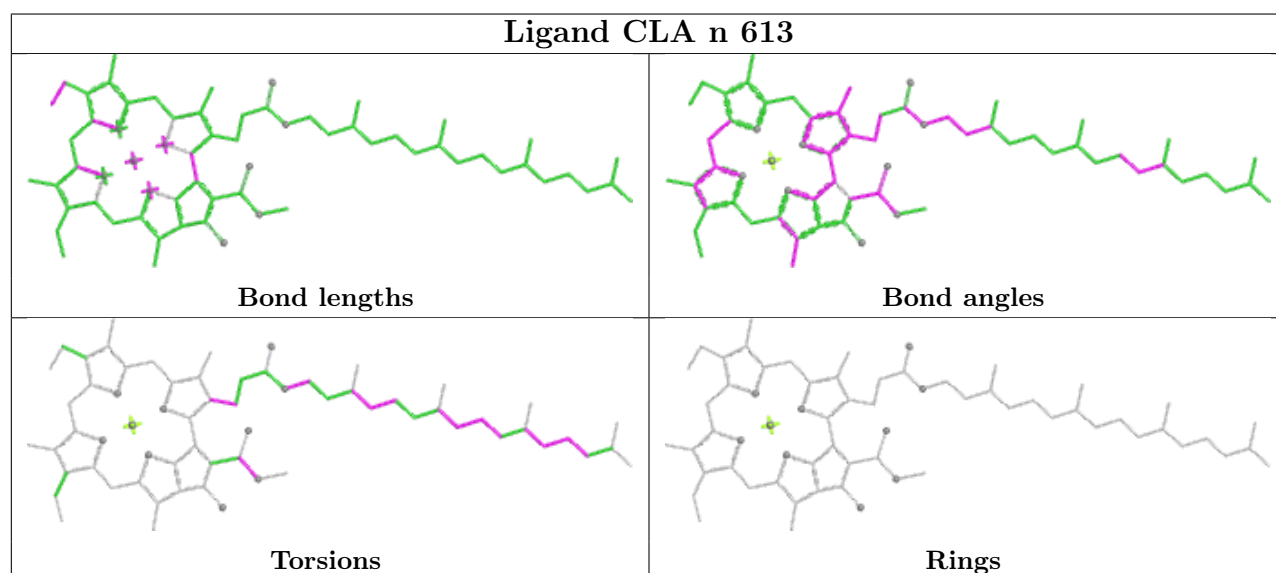
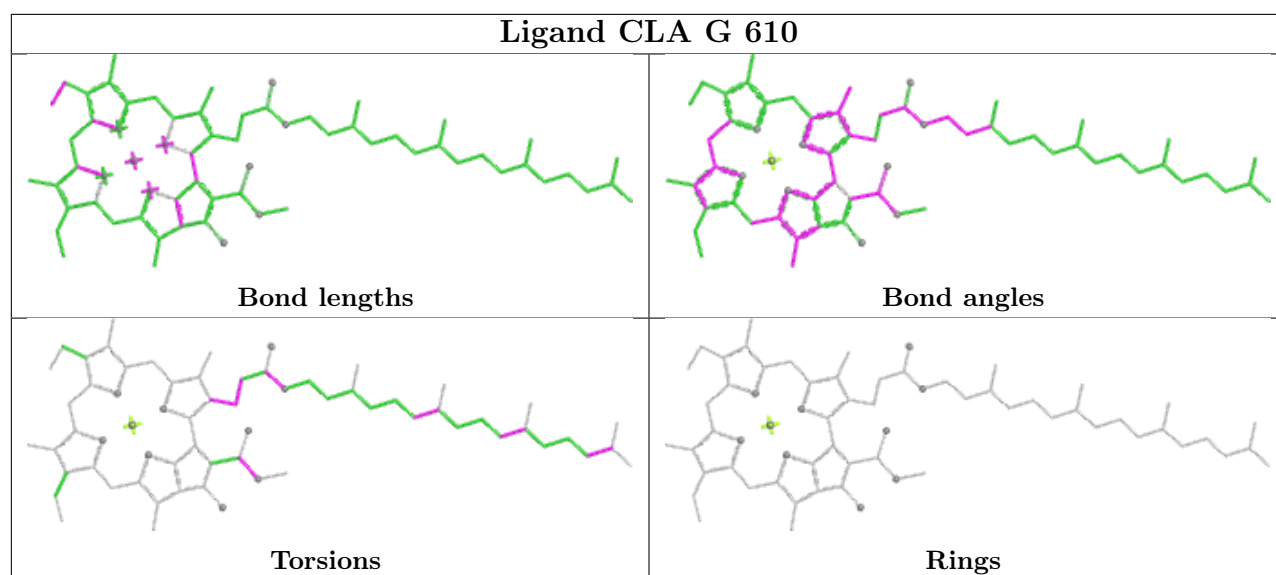


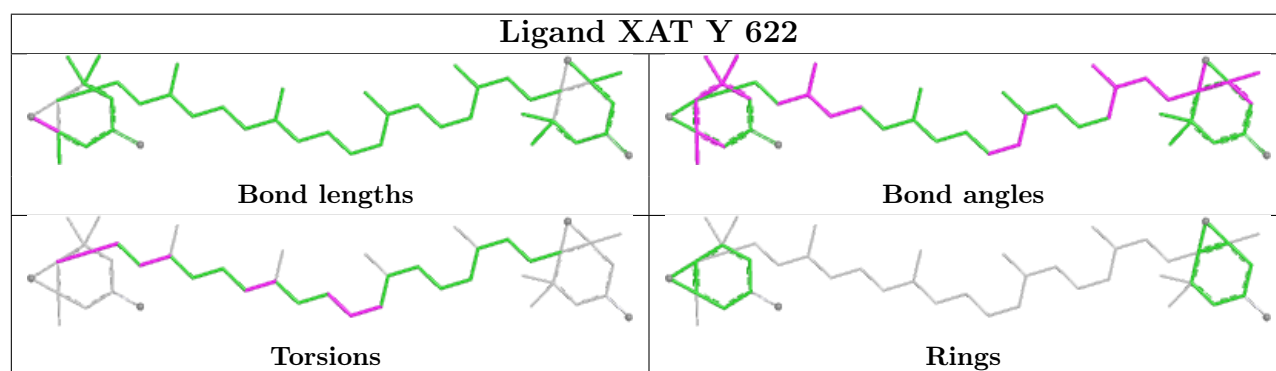
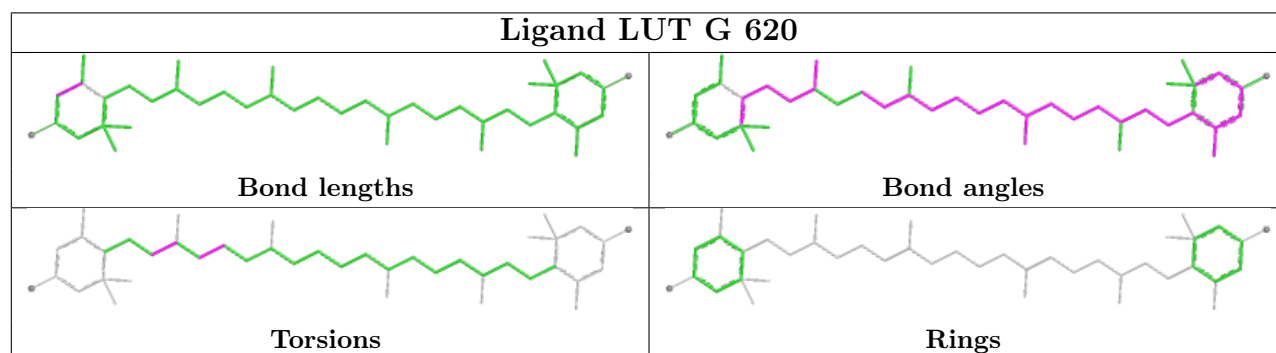
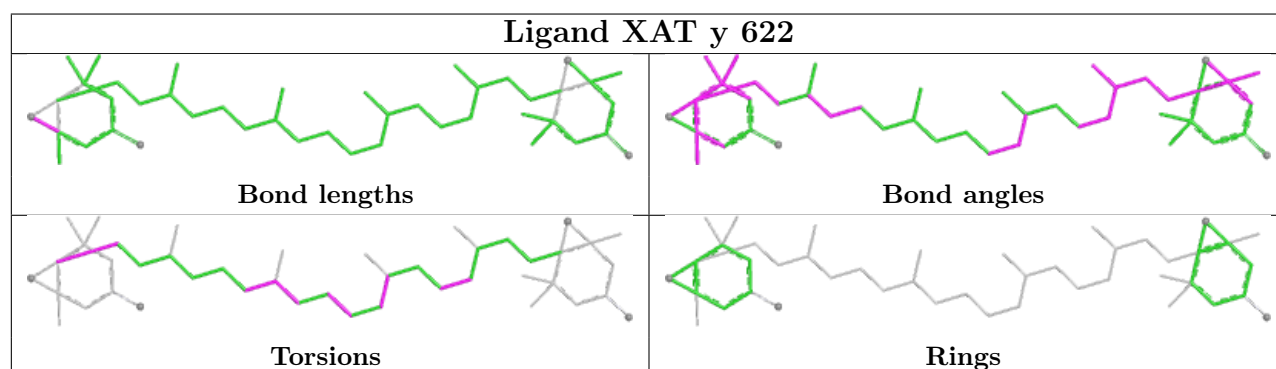
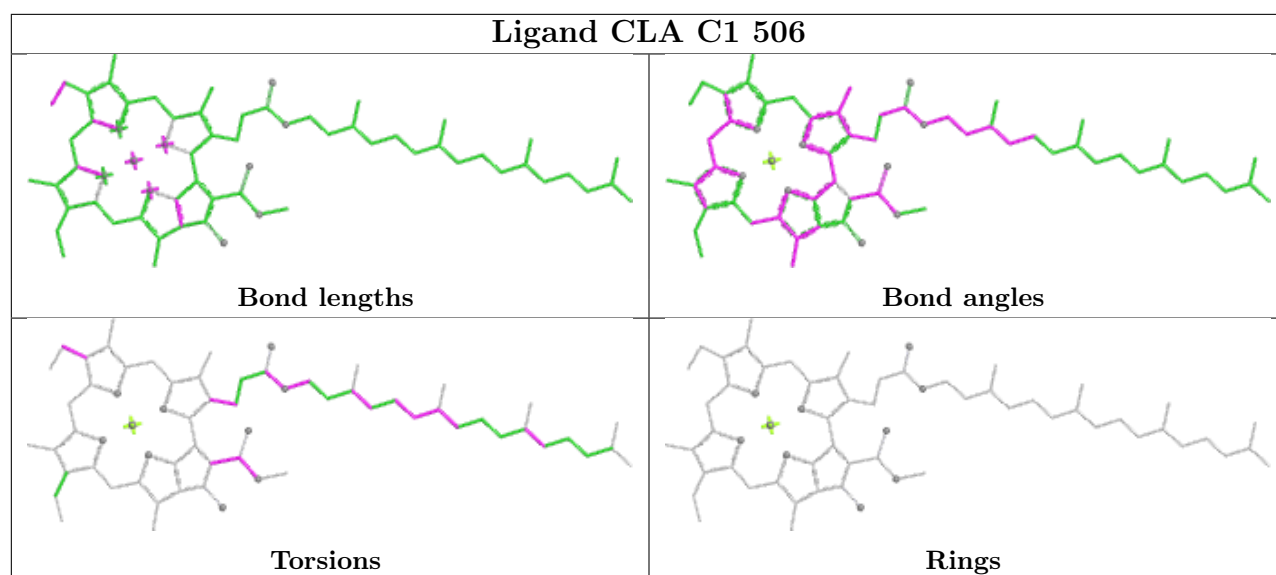


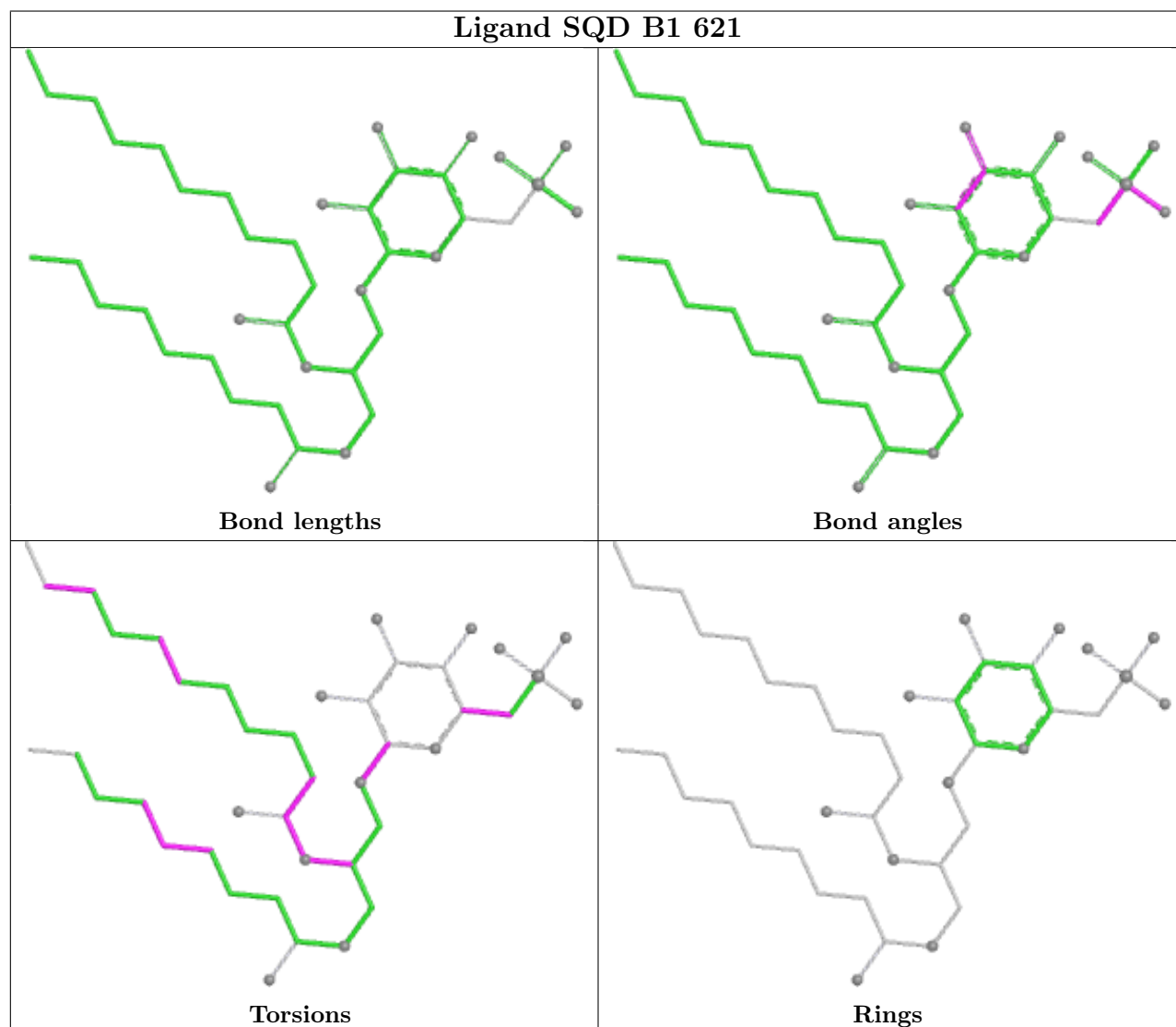
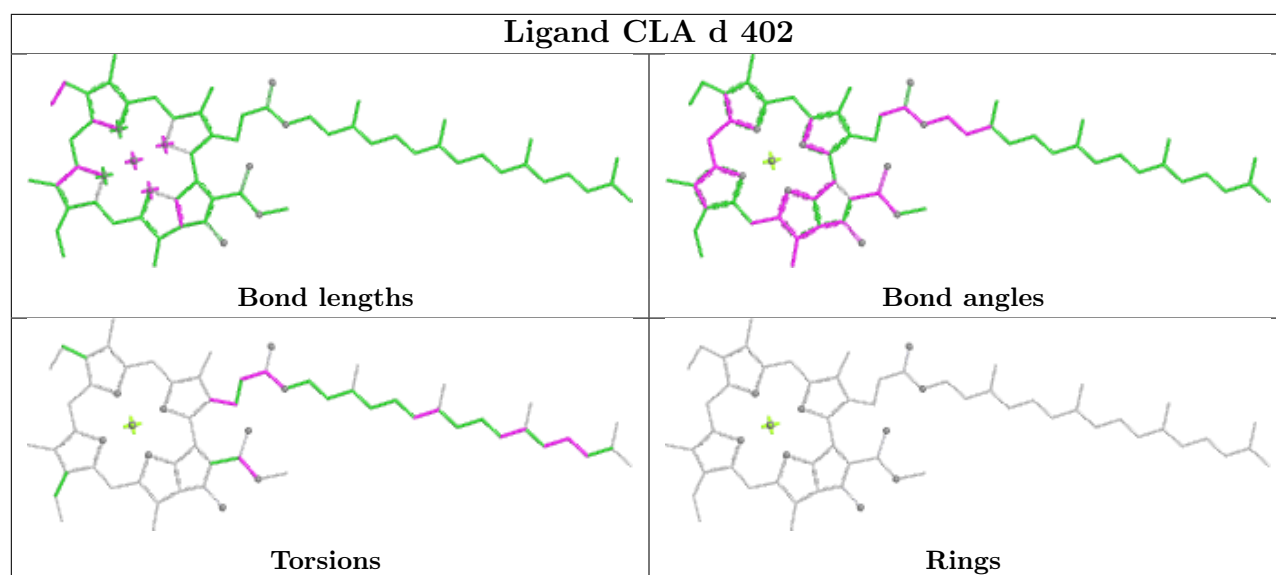


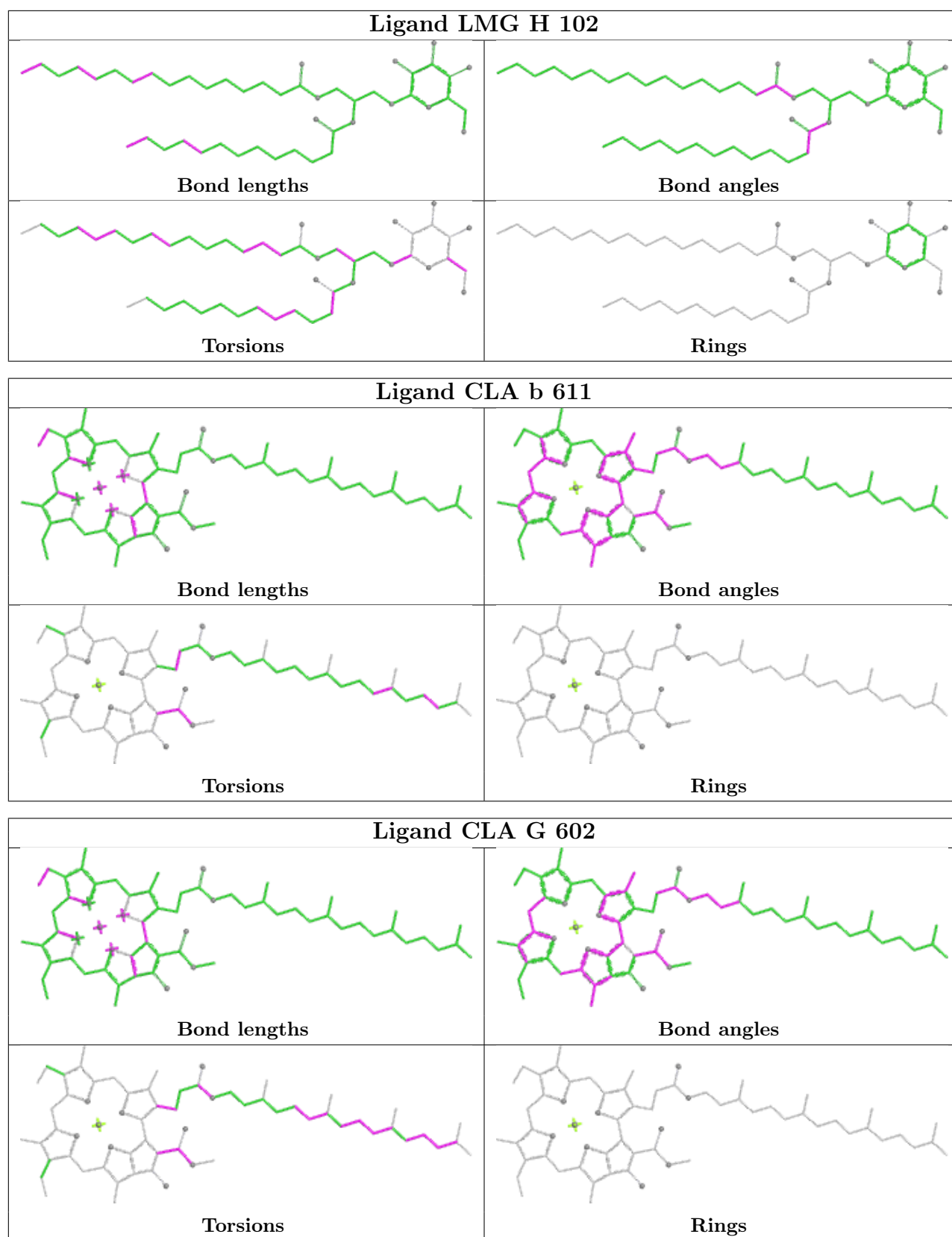


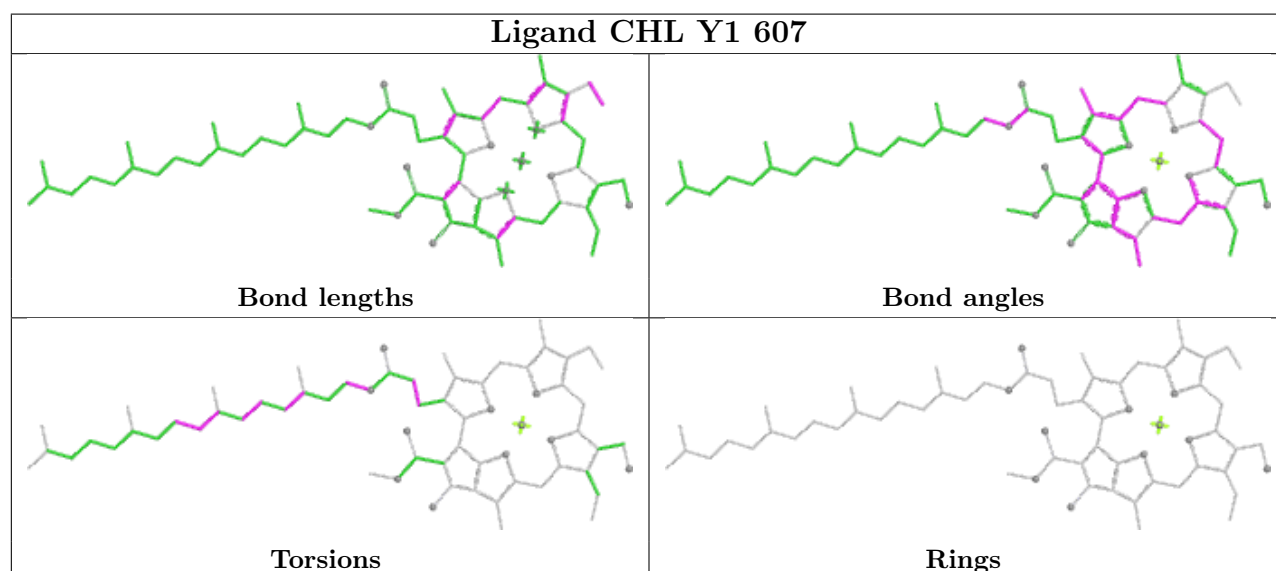
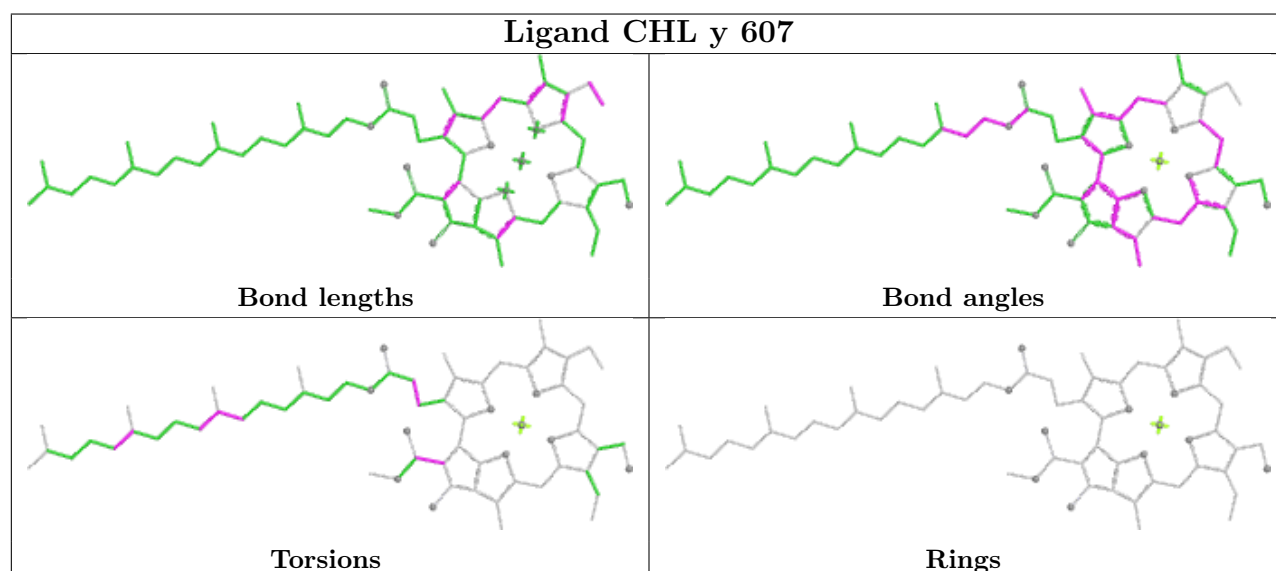
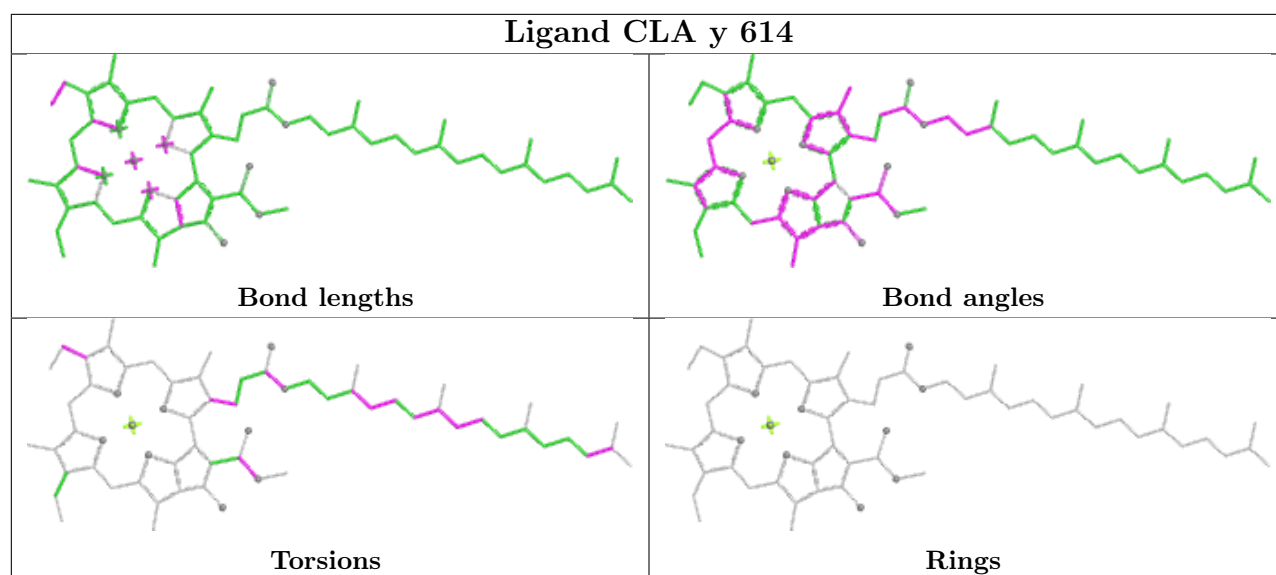


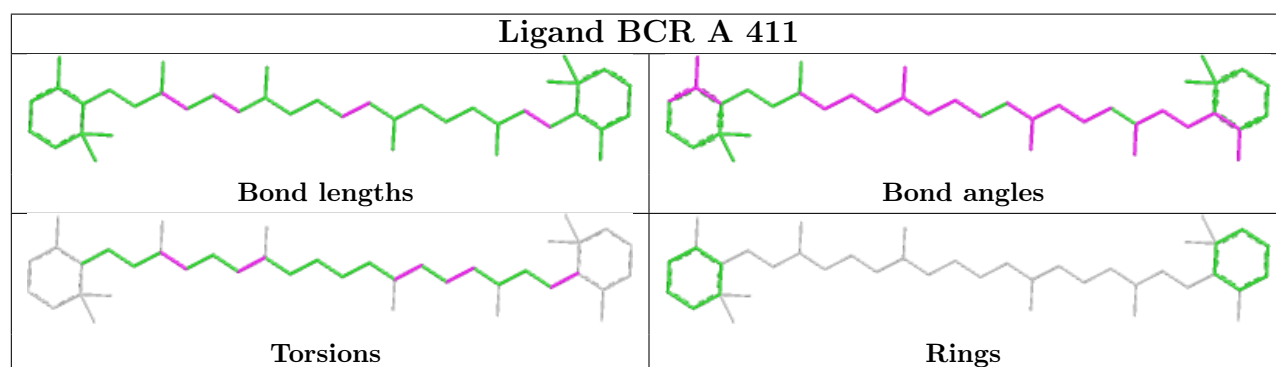
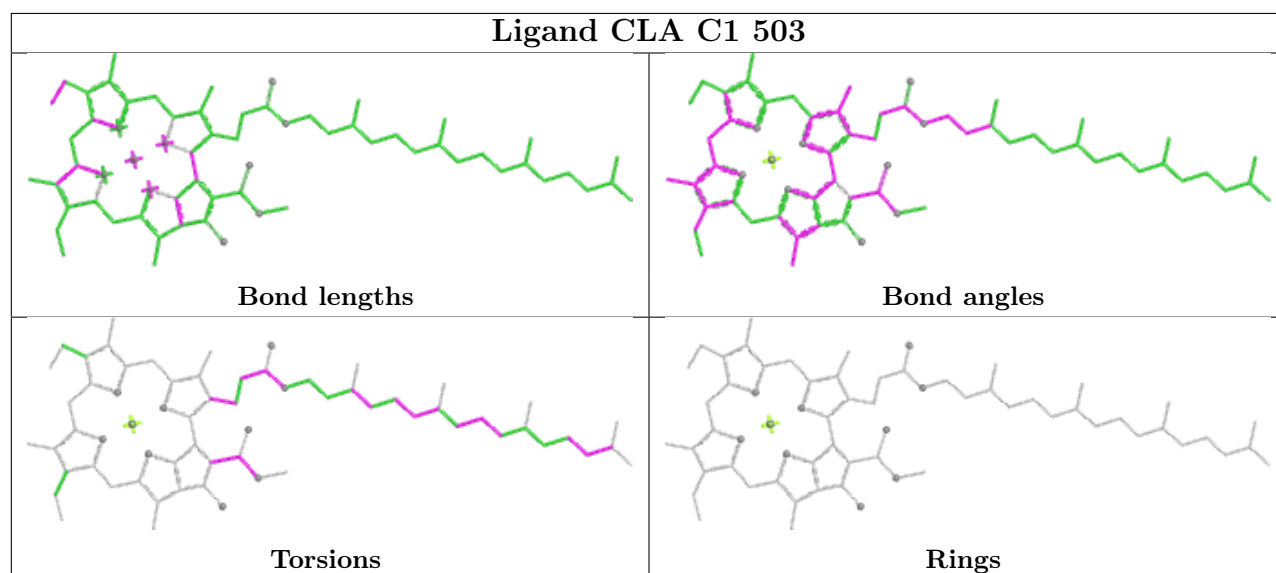
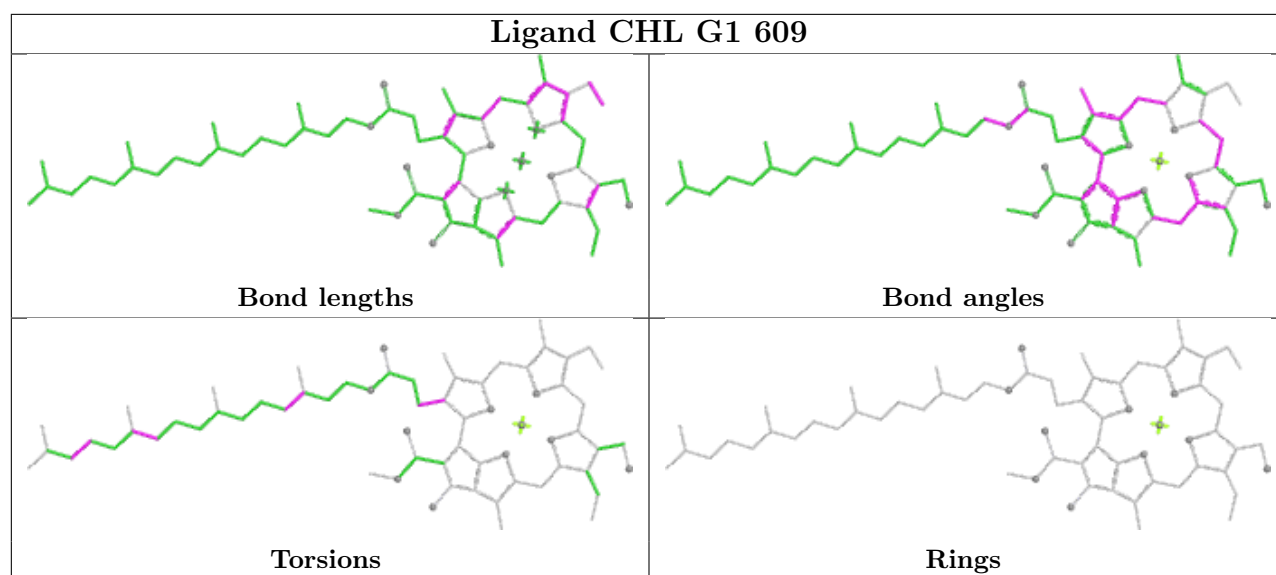


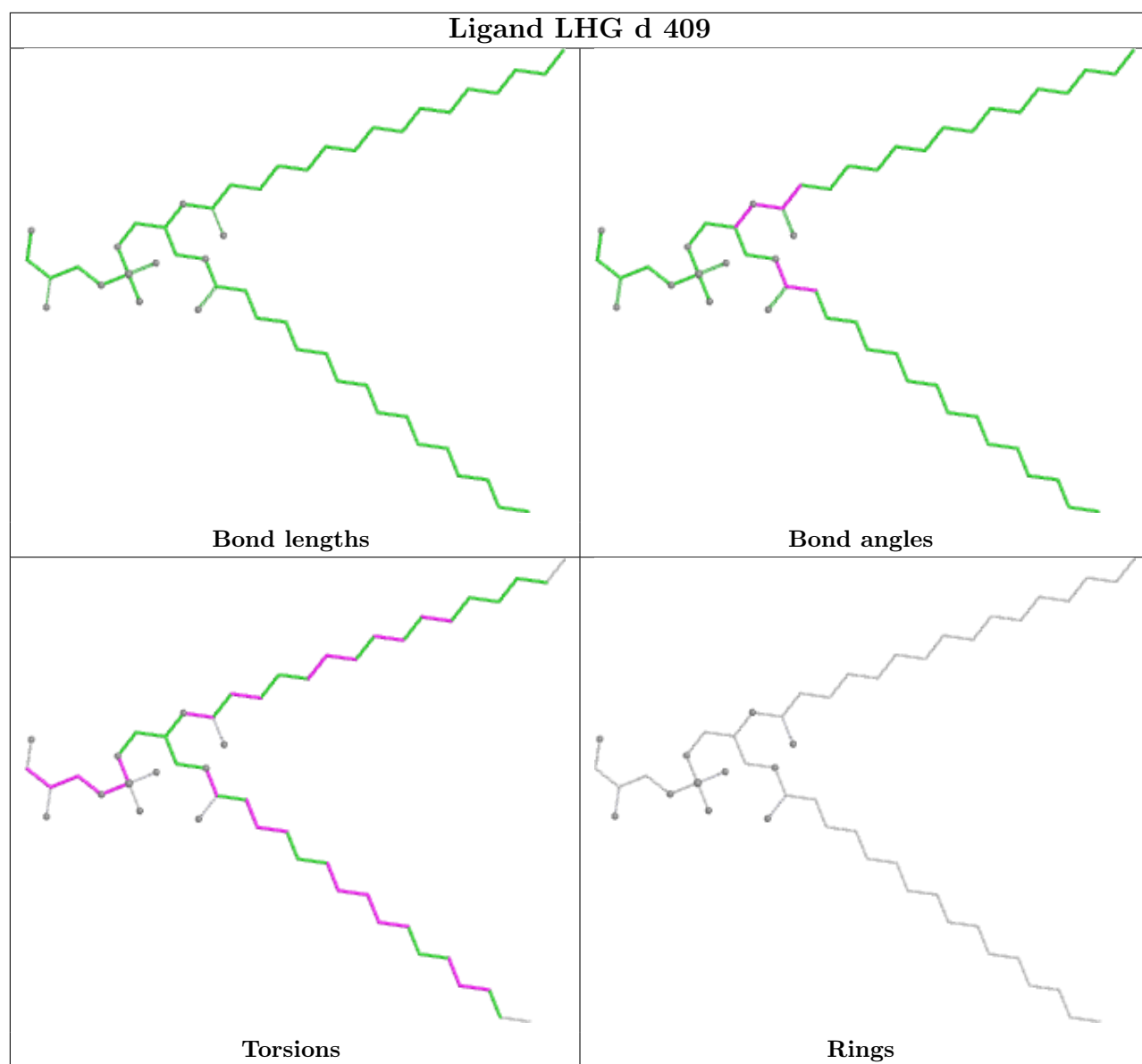




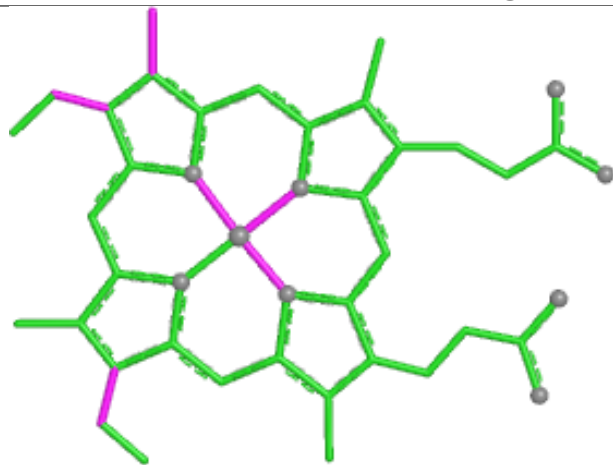




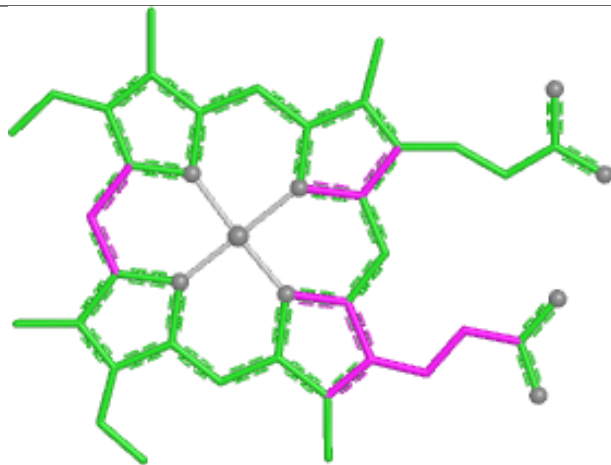




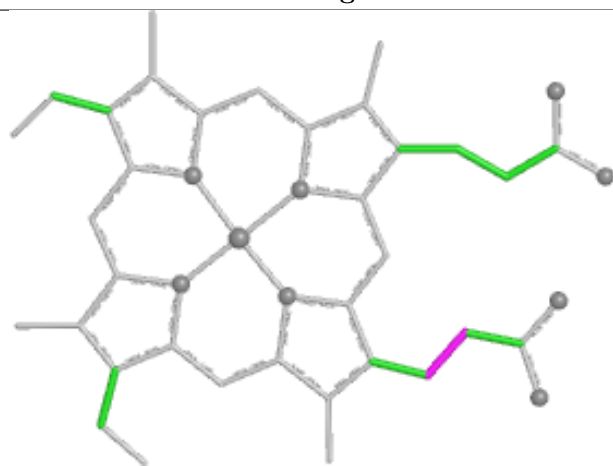
Ligand HEM F1 101



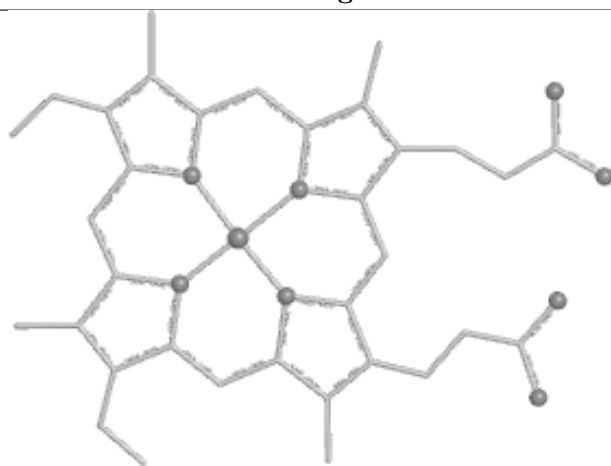
Bond lengths



Bond angles

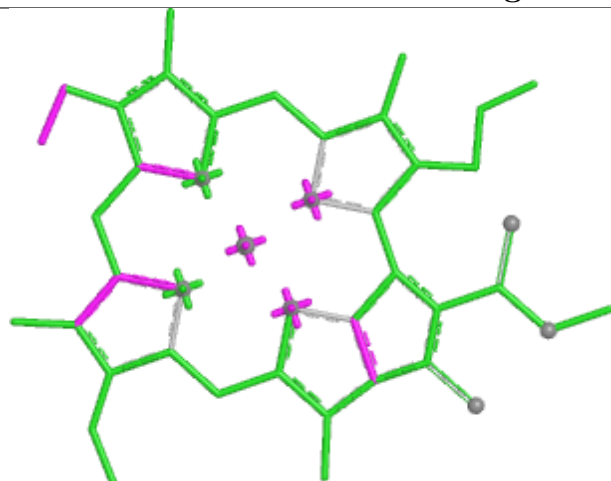


Torsions

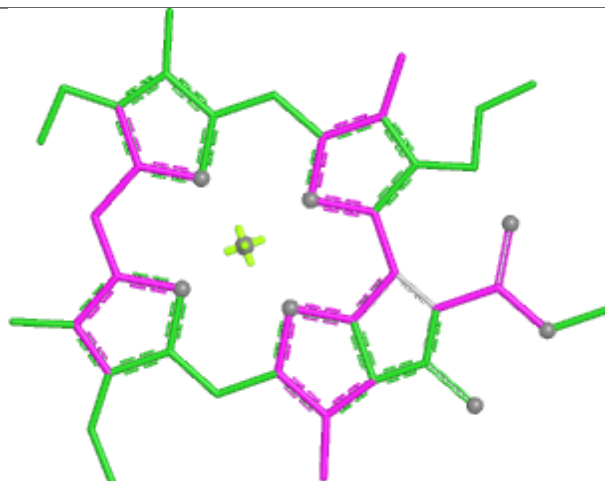


Rings

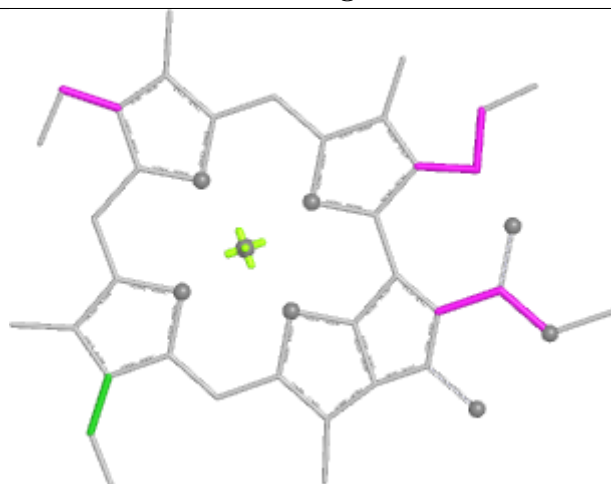
Ligand CLA G1 612



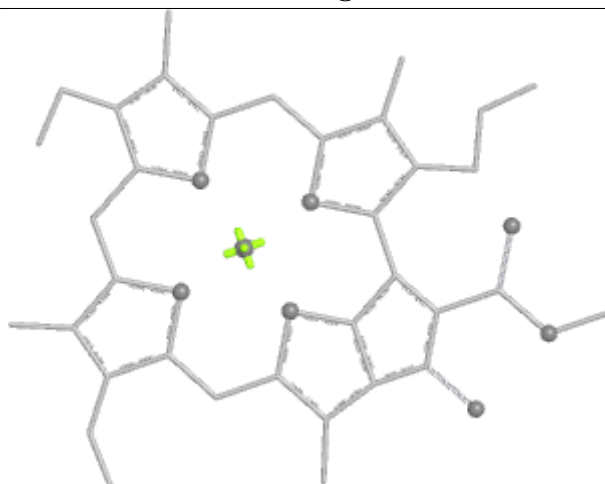
Bond lengths



Bond angles

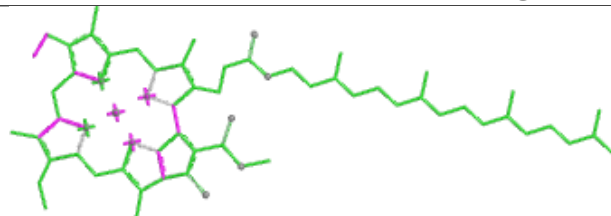


Torsions

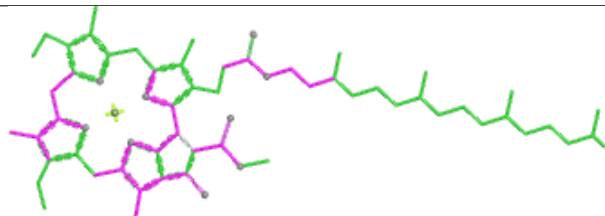


Rings

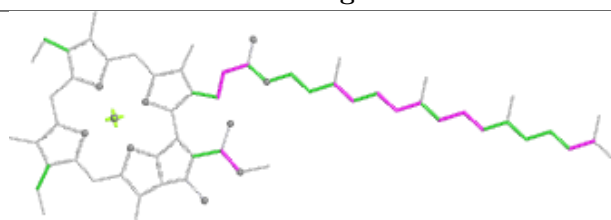
Ligand CLA B 615



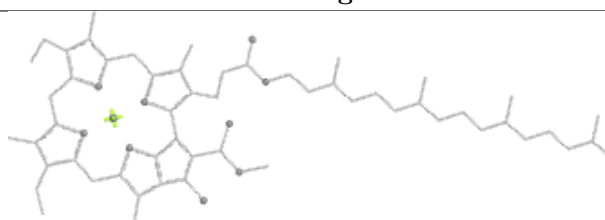
Bond lengths



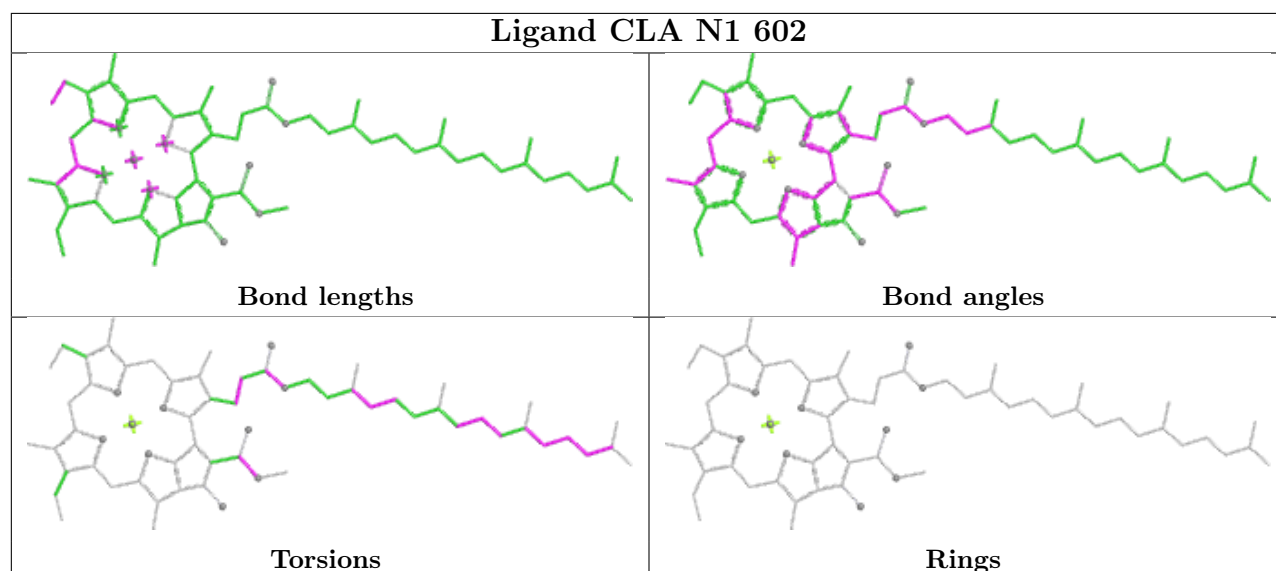
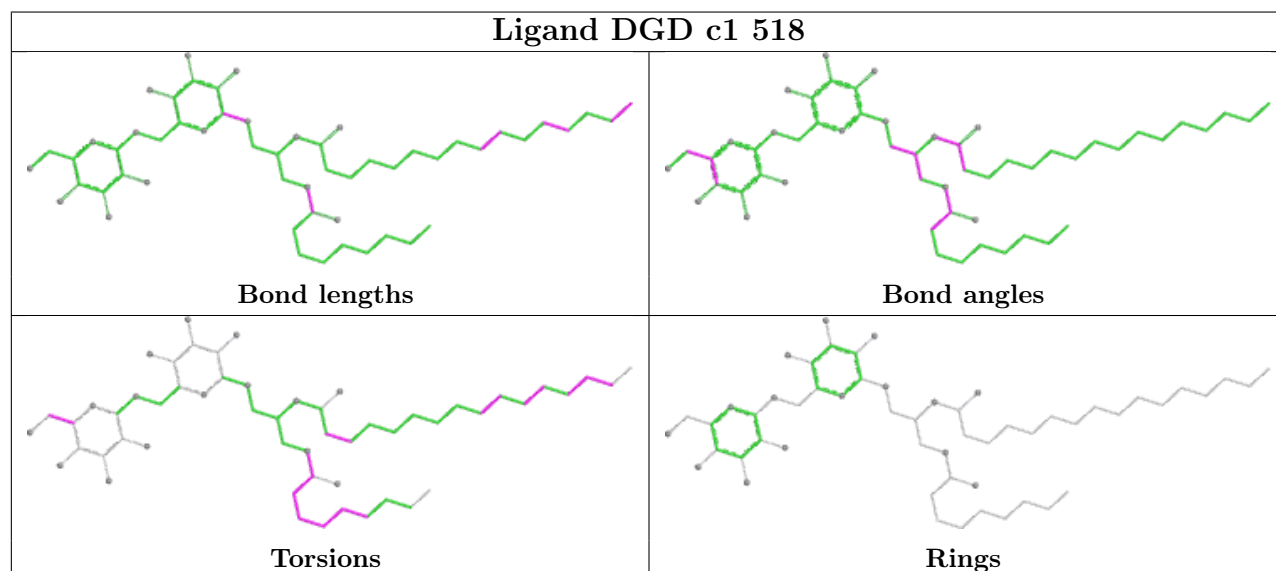
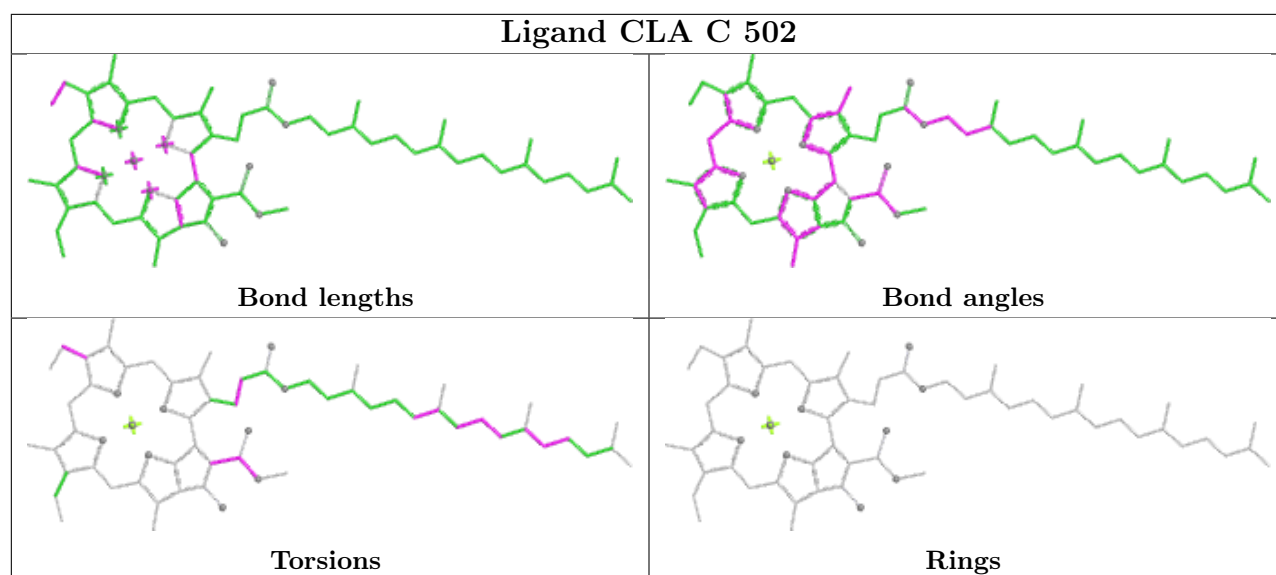
Bond angles

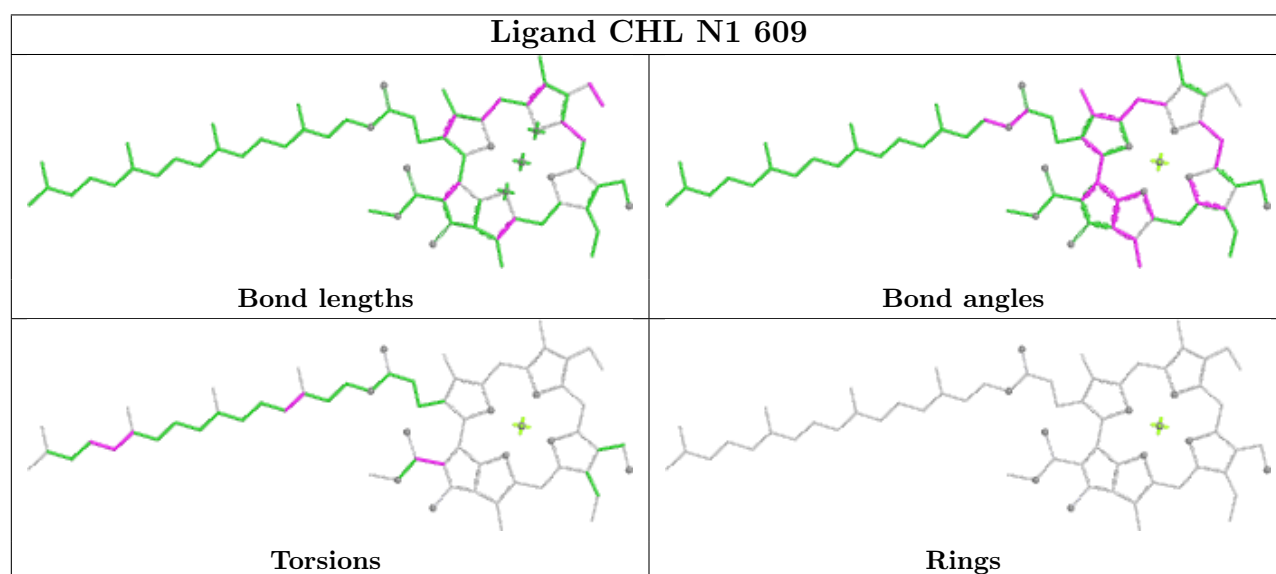
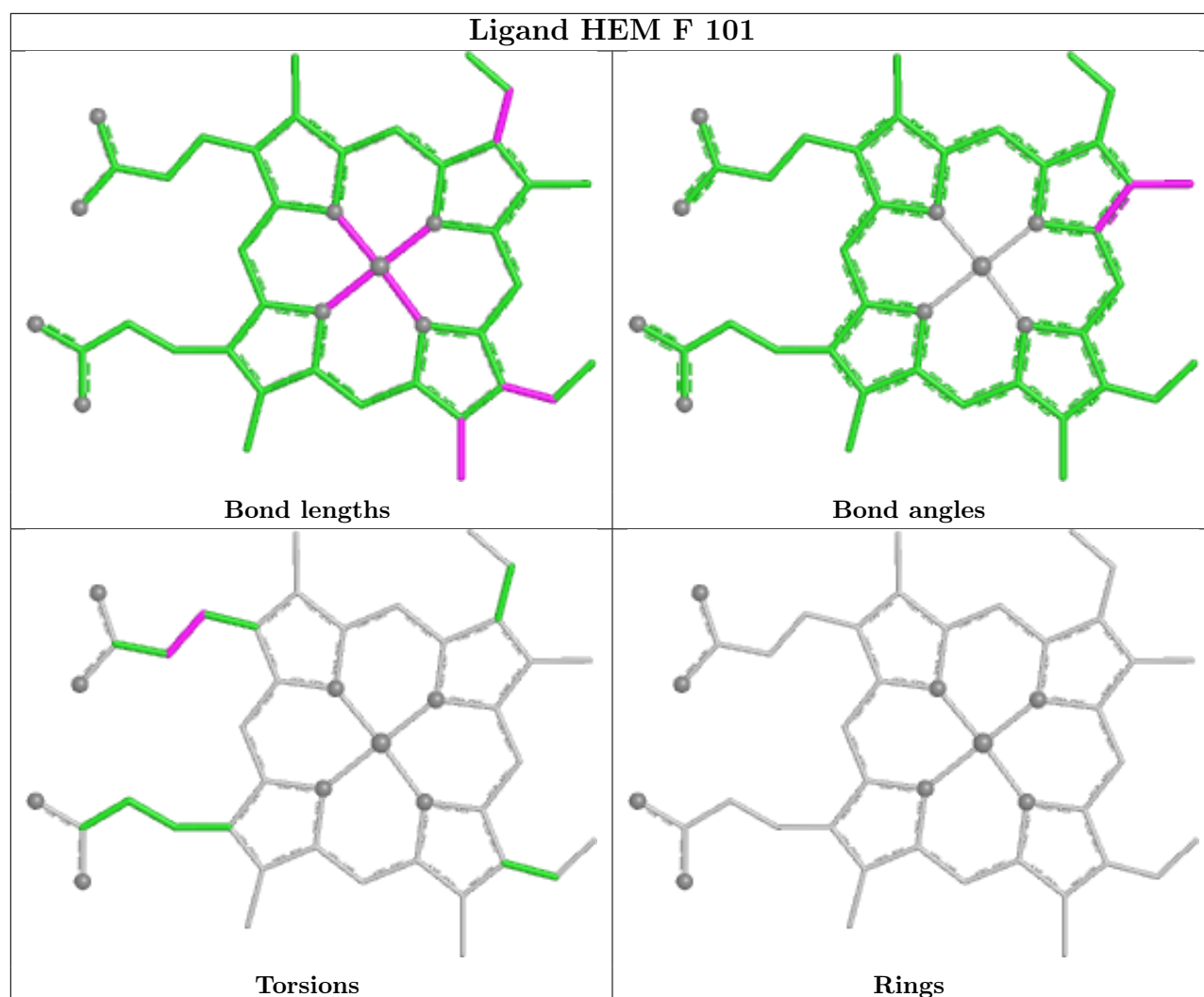


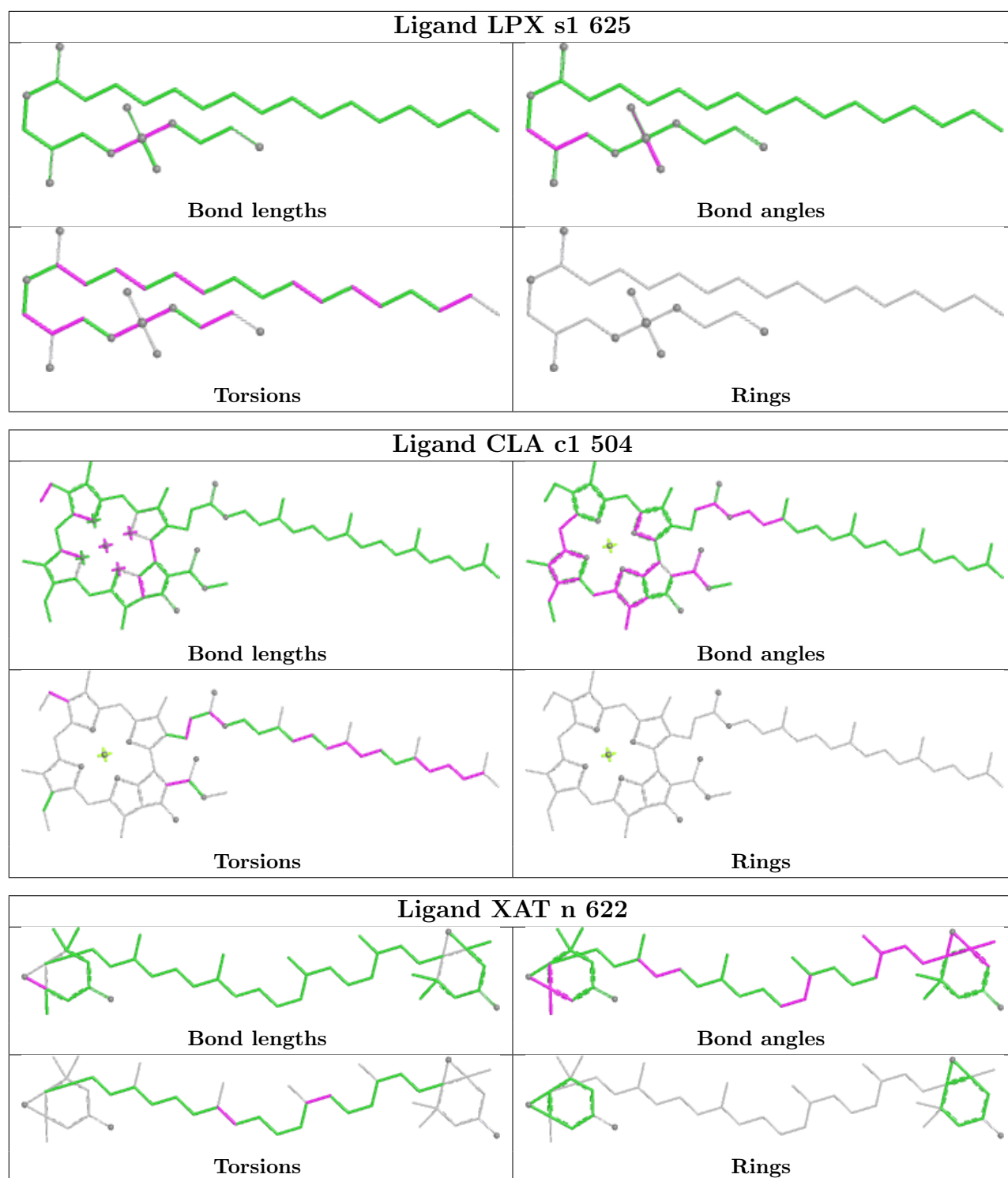
Torsions



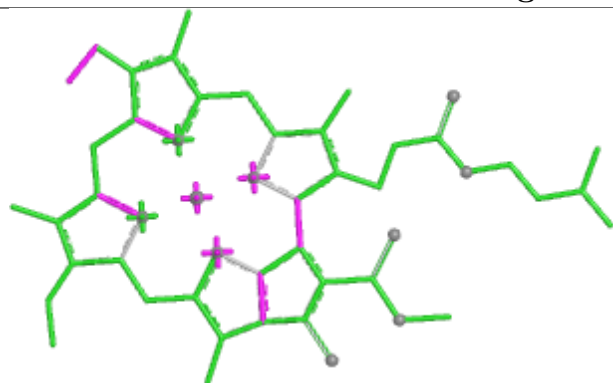
Rings



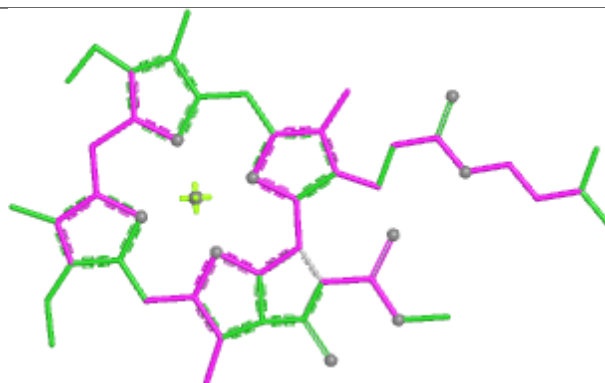




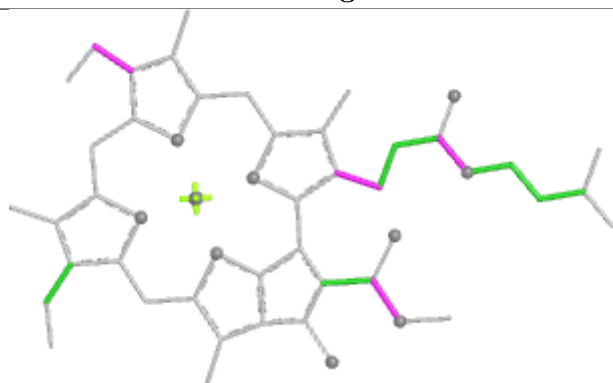
Ligand CLA S 617



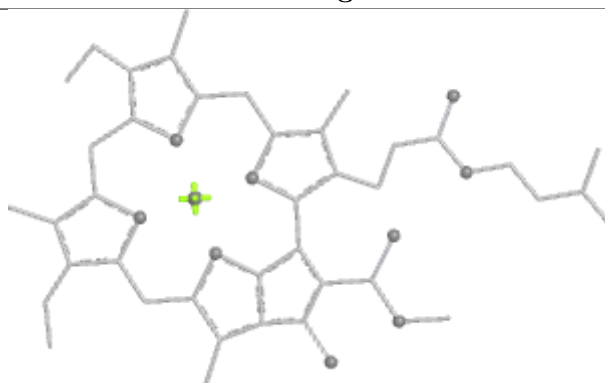
Bond lengths



Bond angles

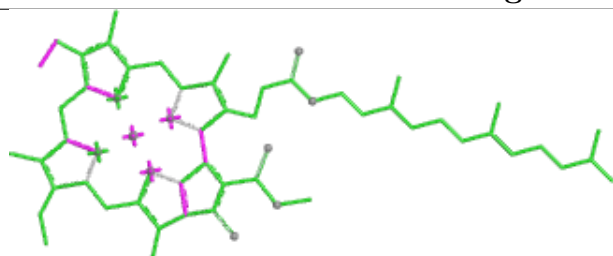


Torsions

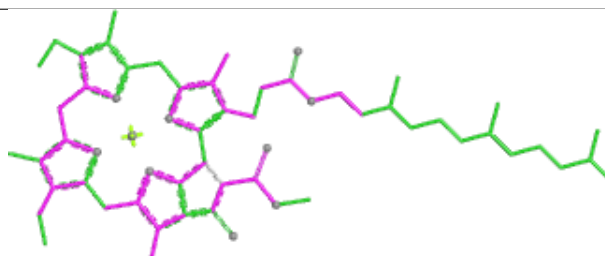


Rings

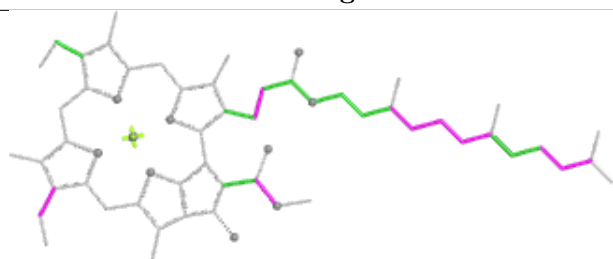
Ligand CLA A1 410



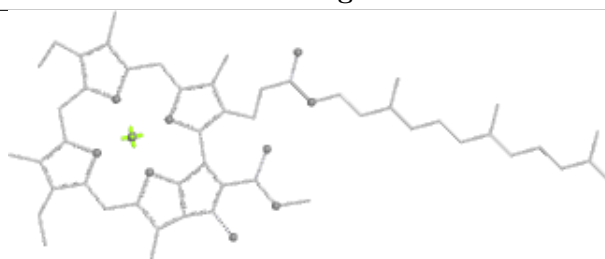
Bond lengths



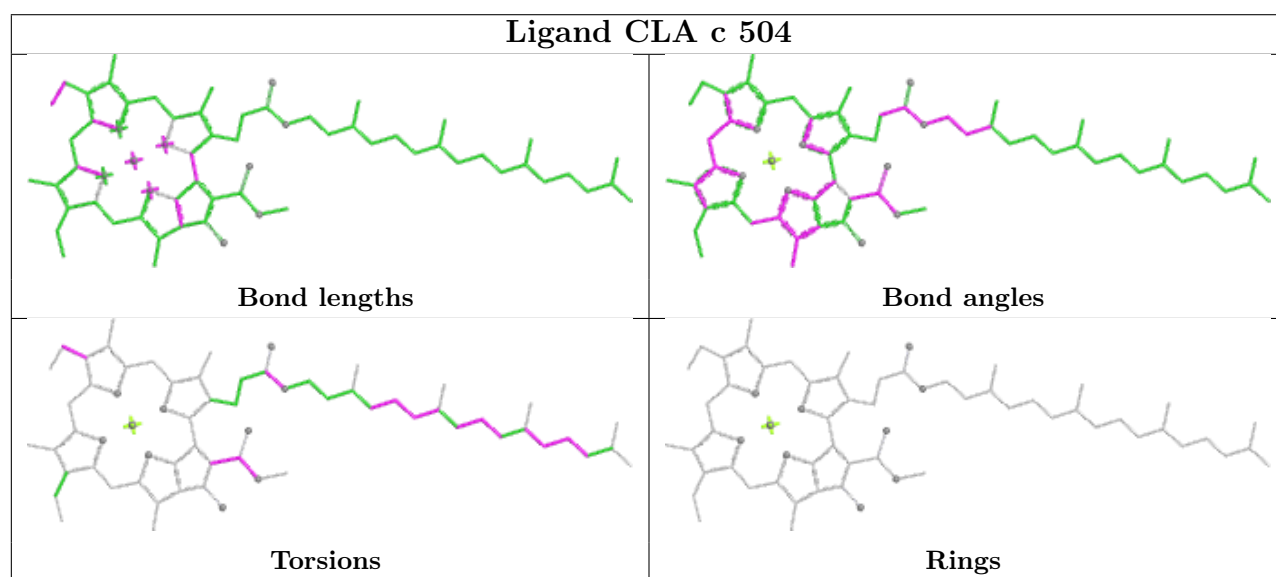
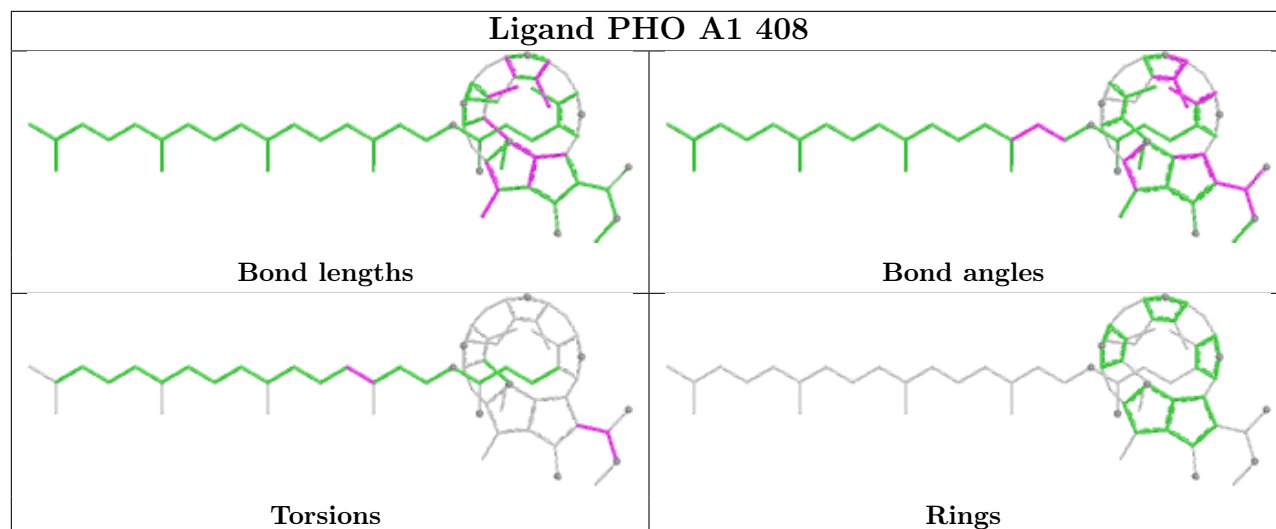
Bond angles

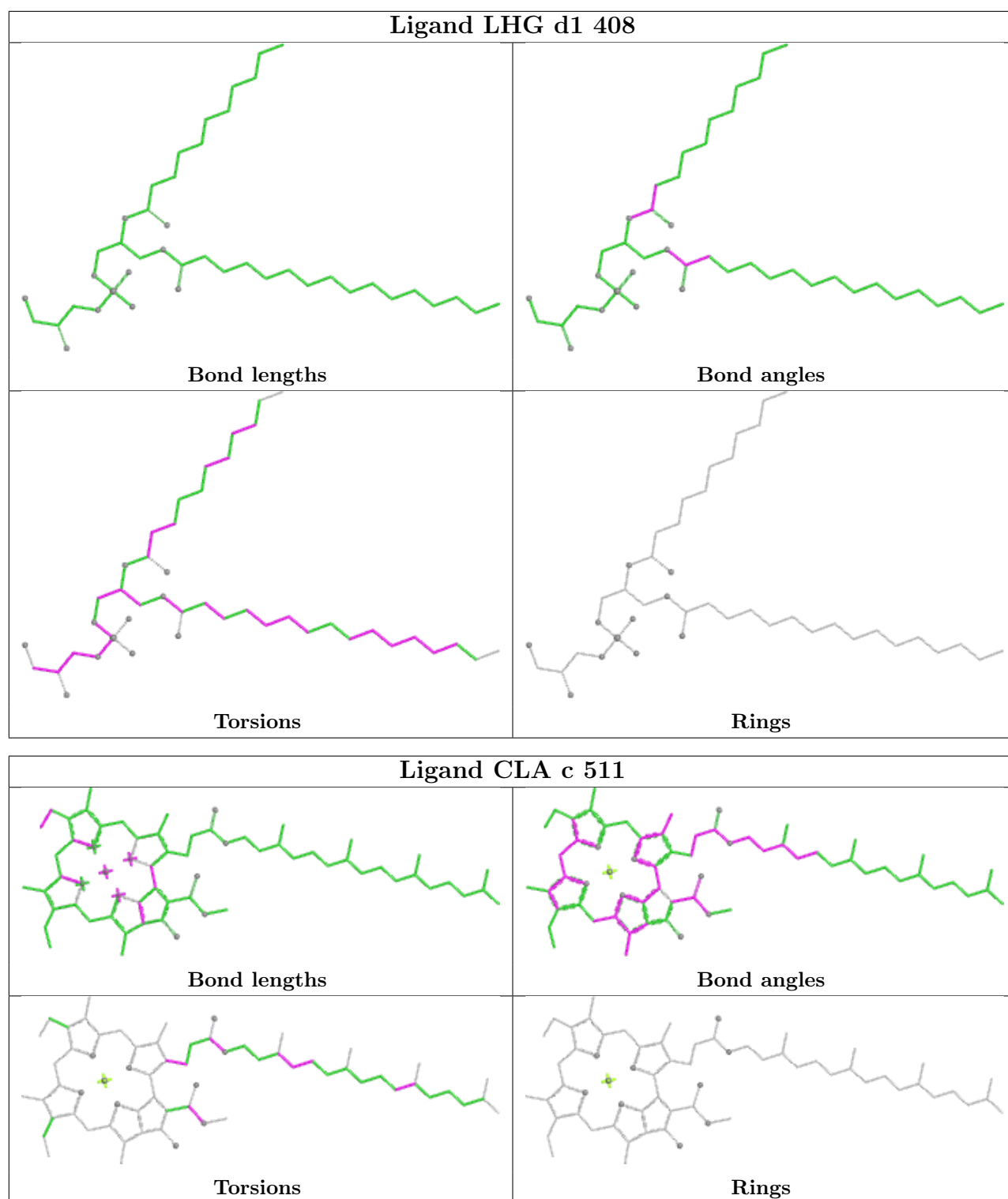


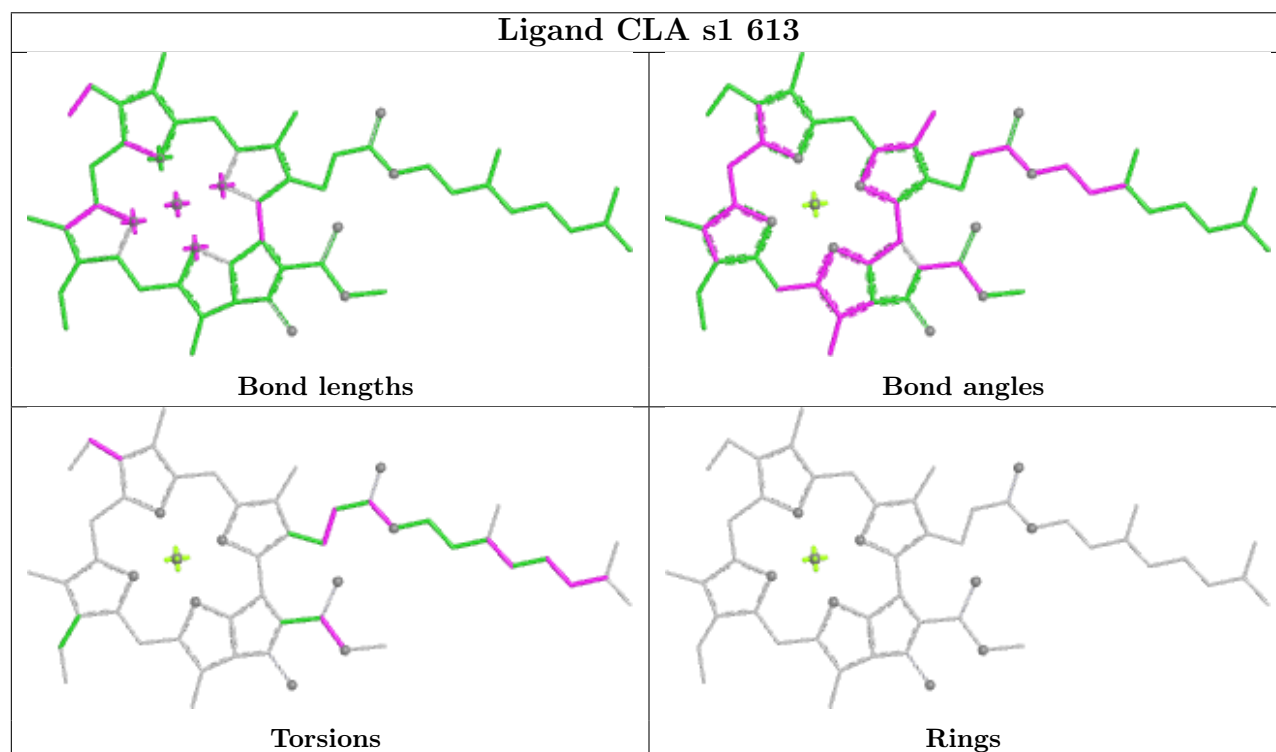
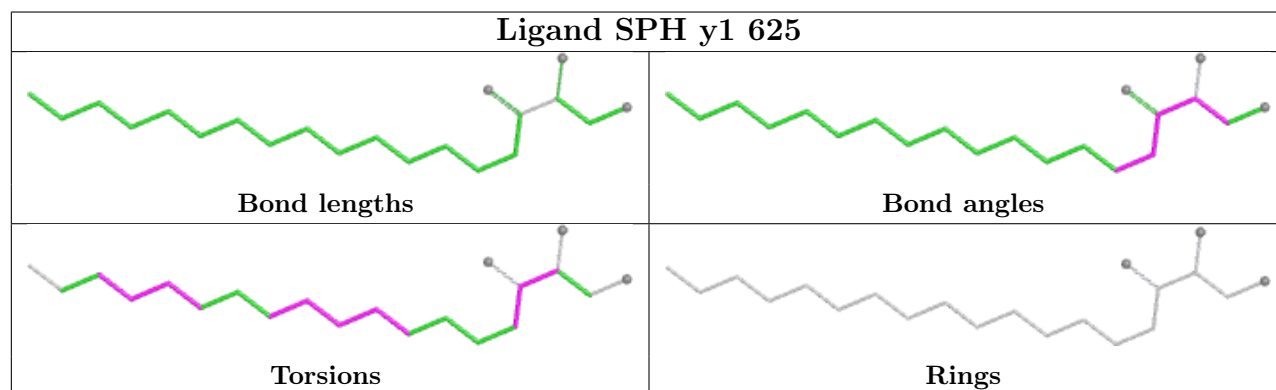
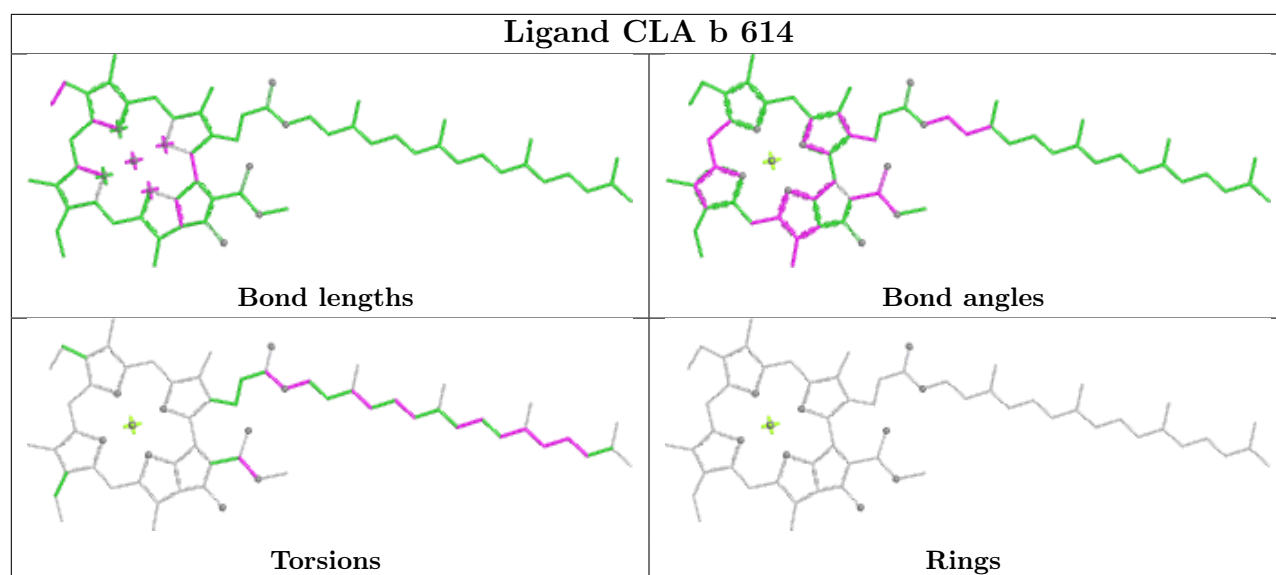
Torsions

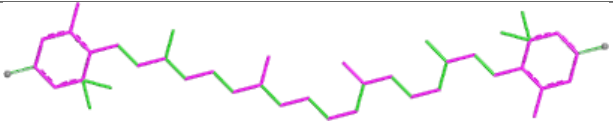
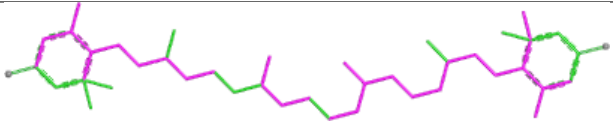
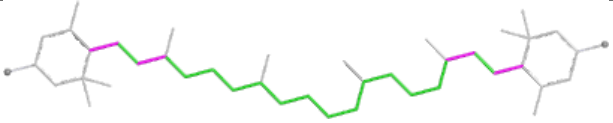
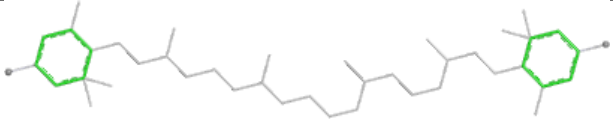
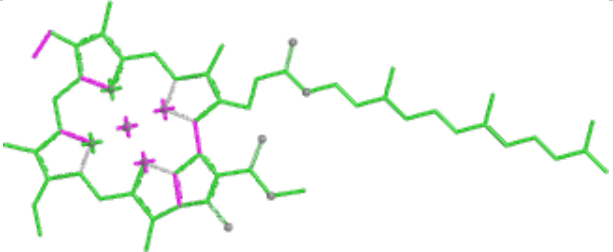
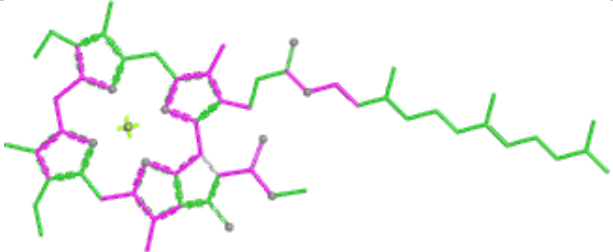
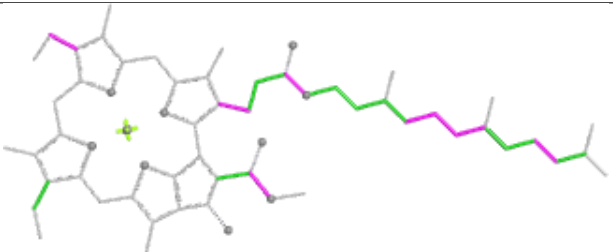
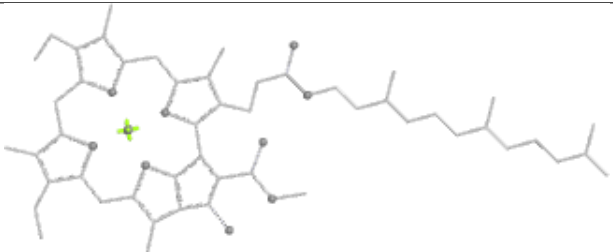


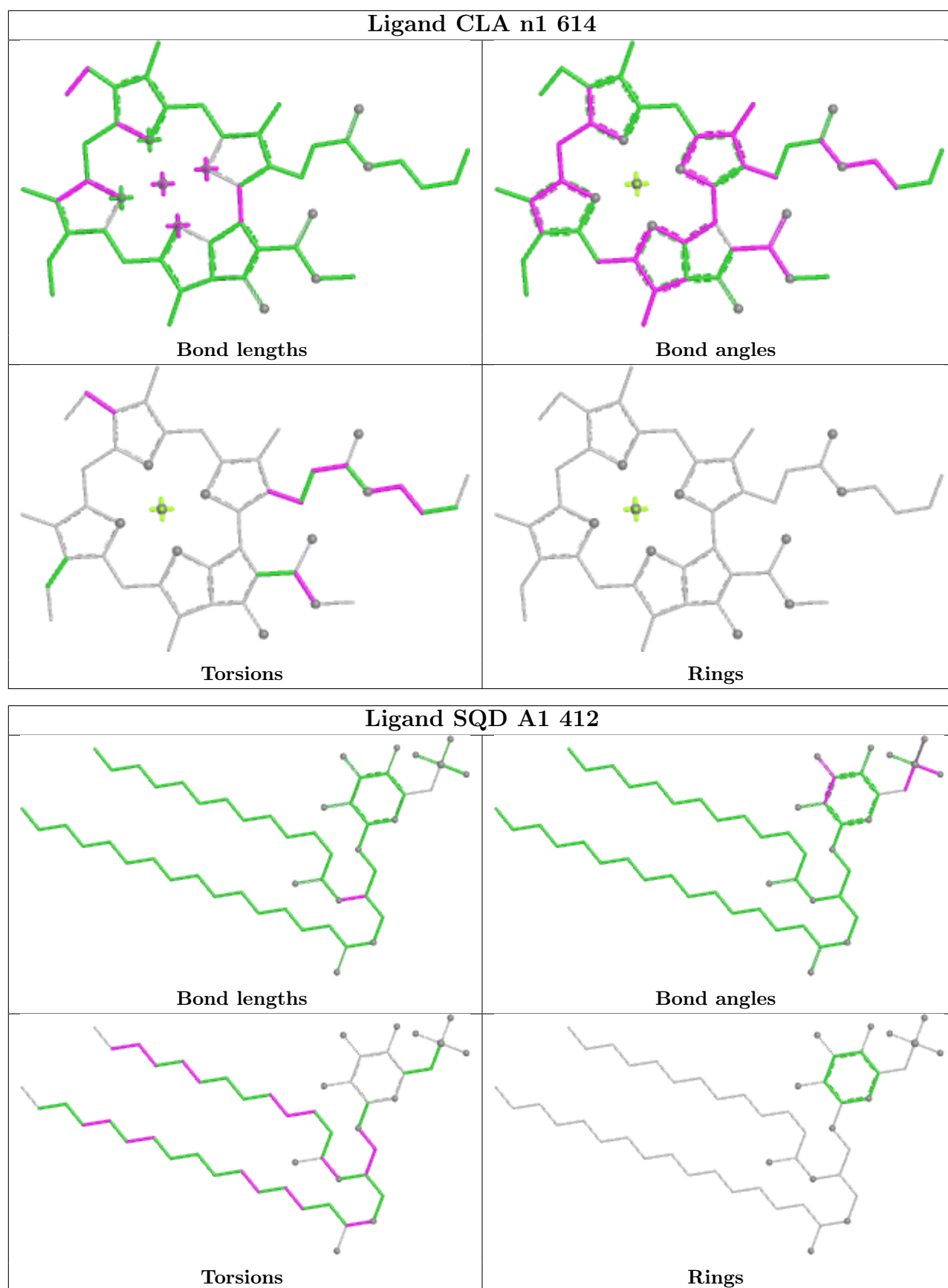
Rings

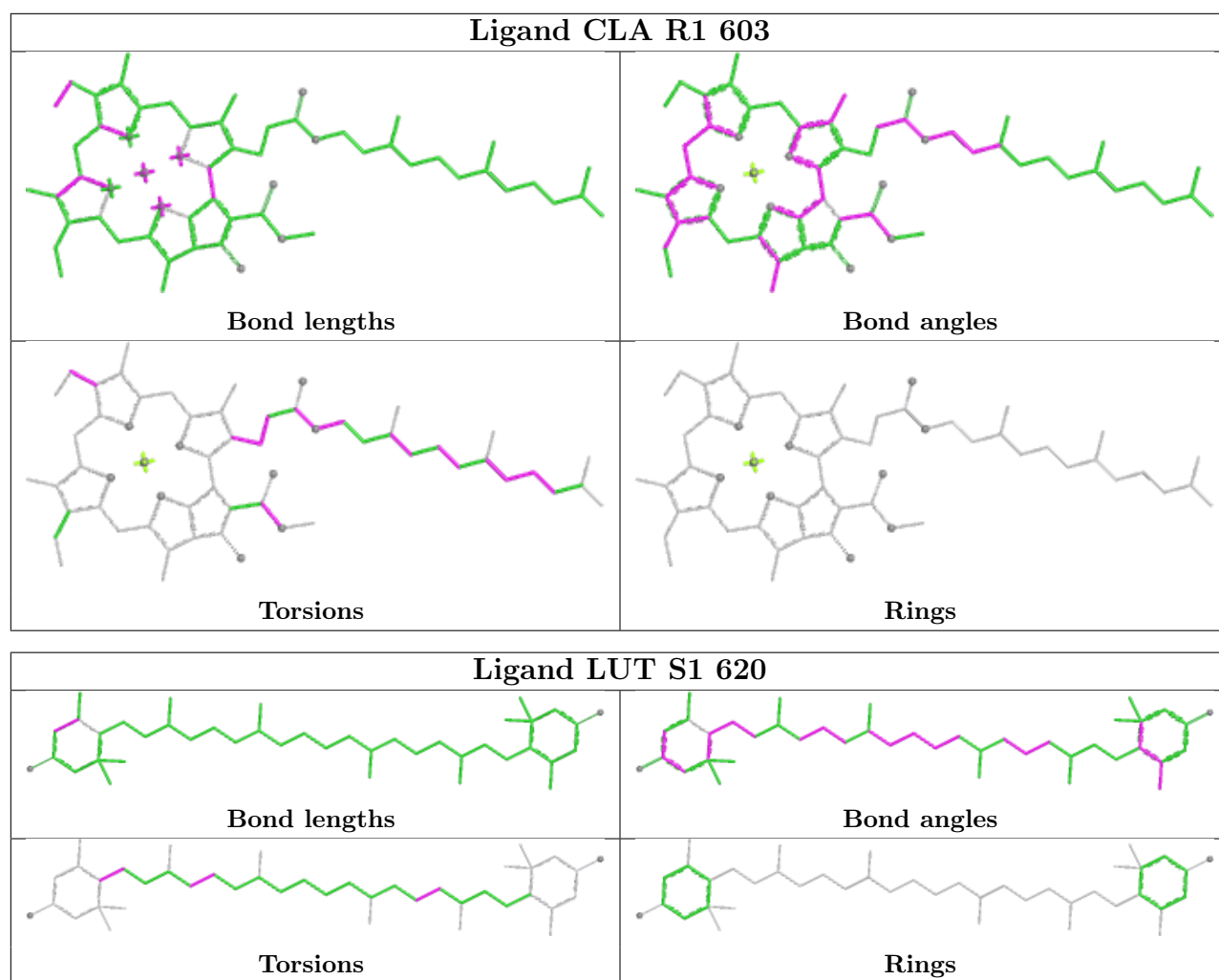


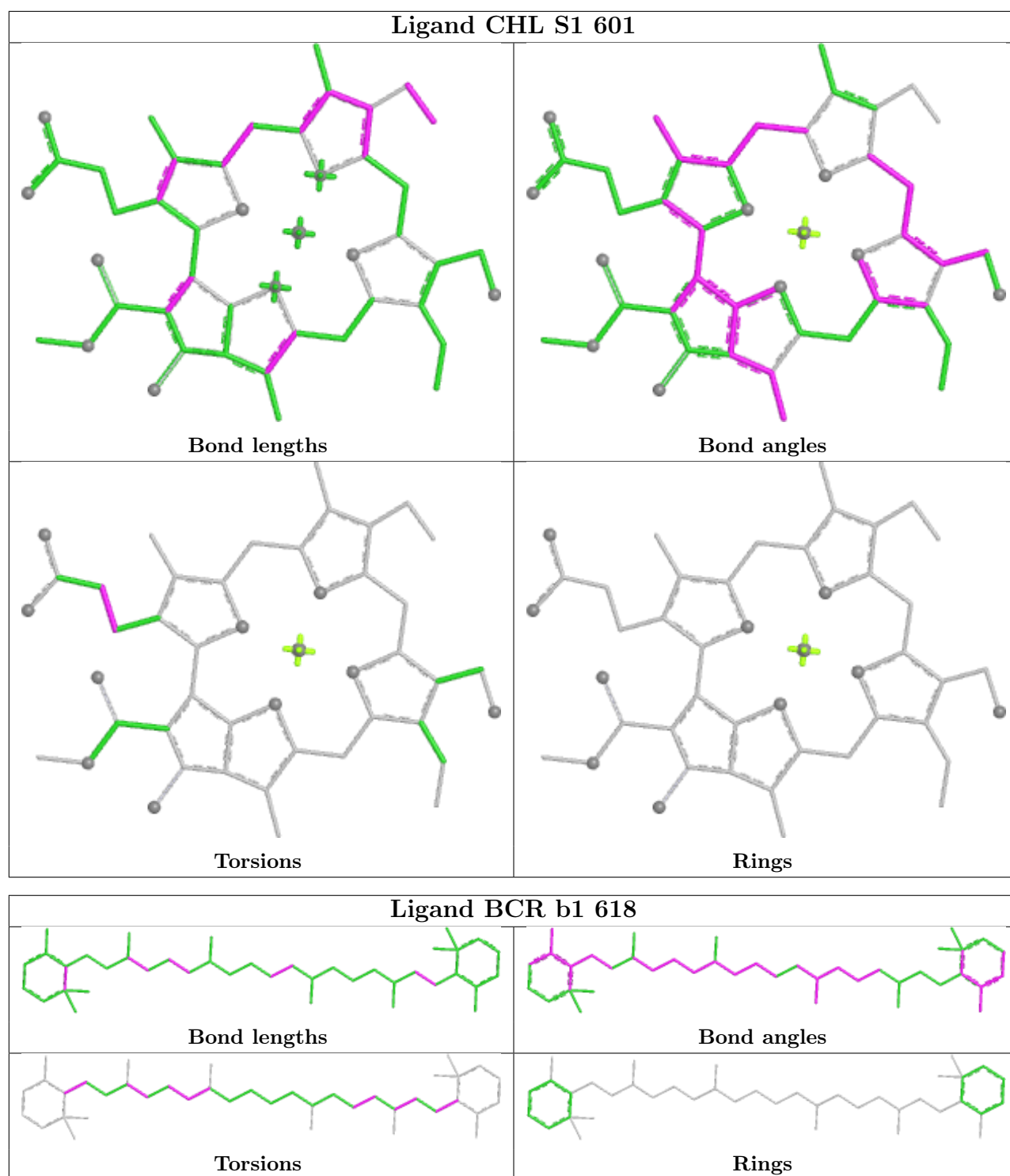


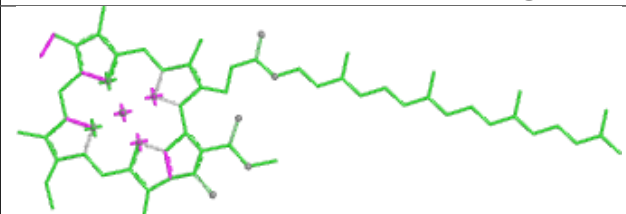
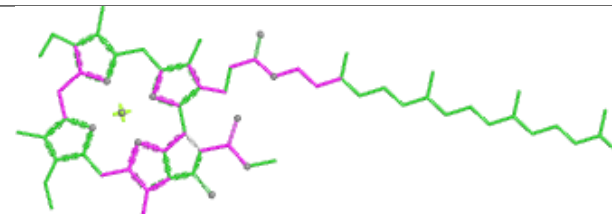
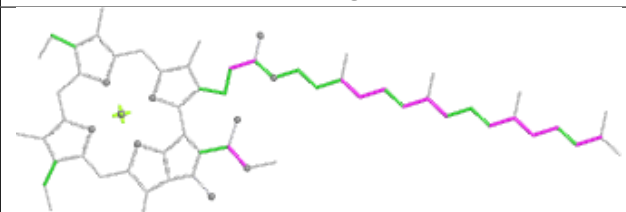
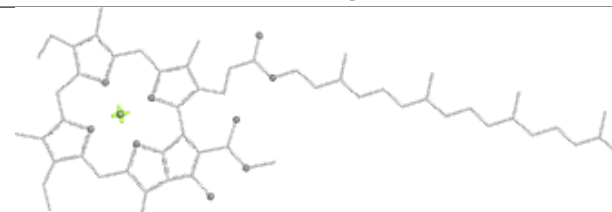


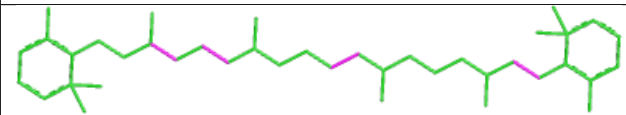
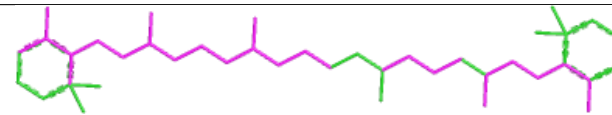
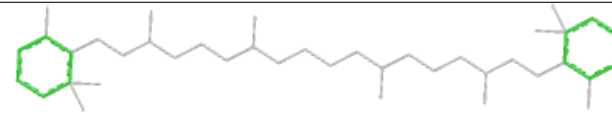
Ligand C7Z B1 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA S 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

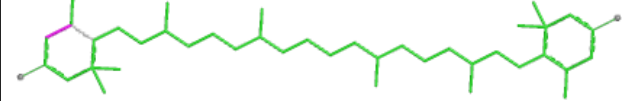
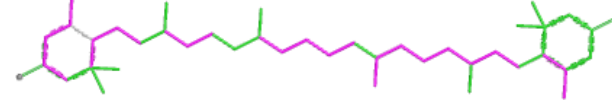
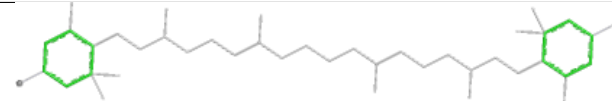




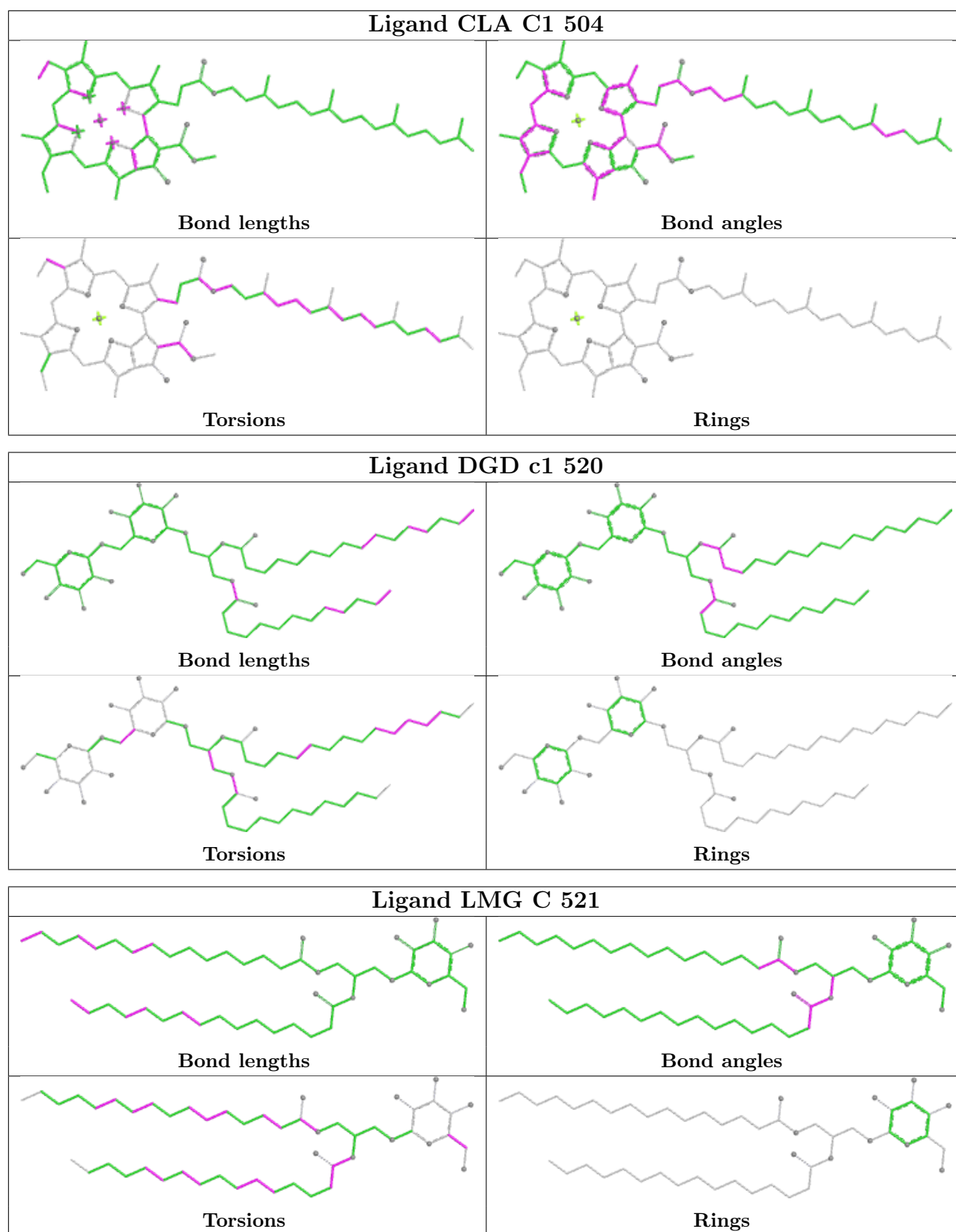


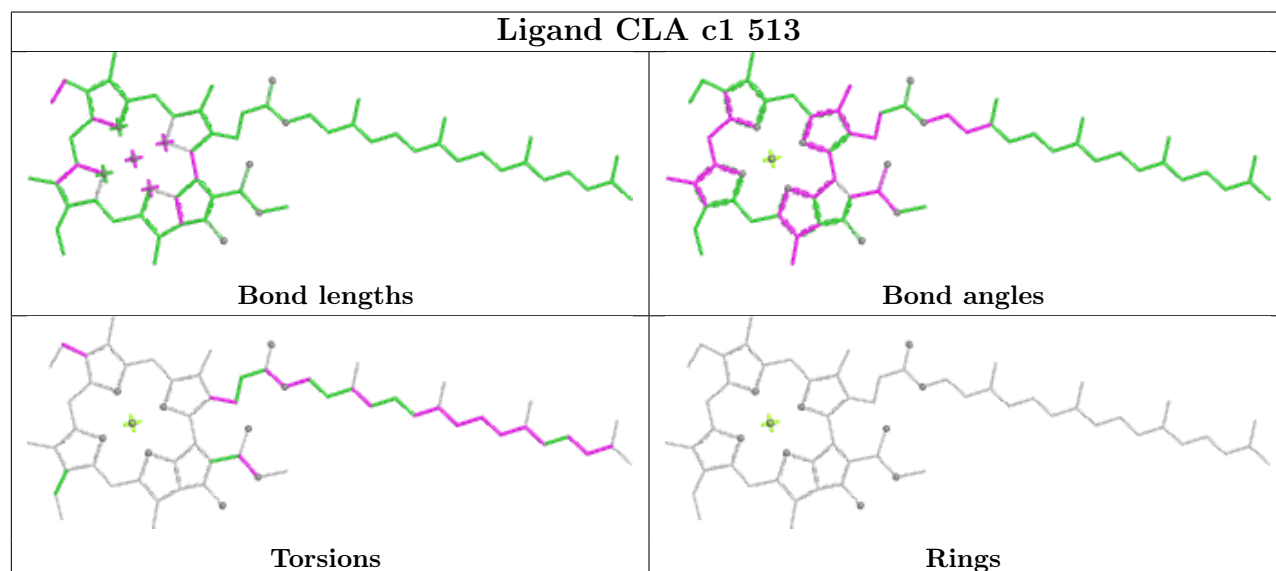
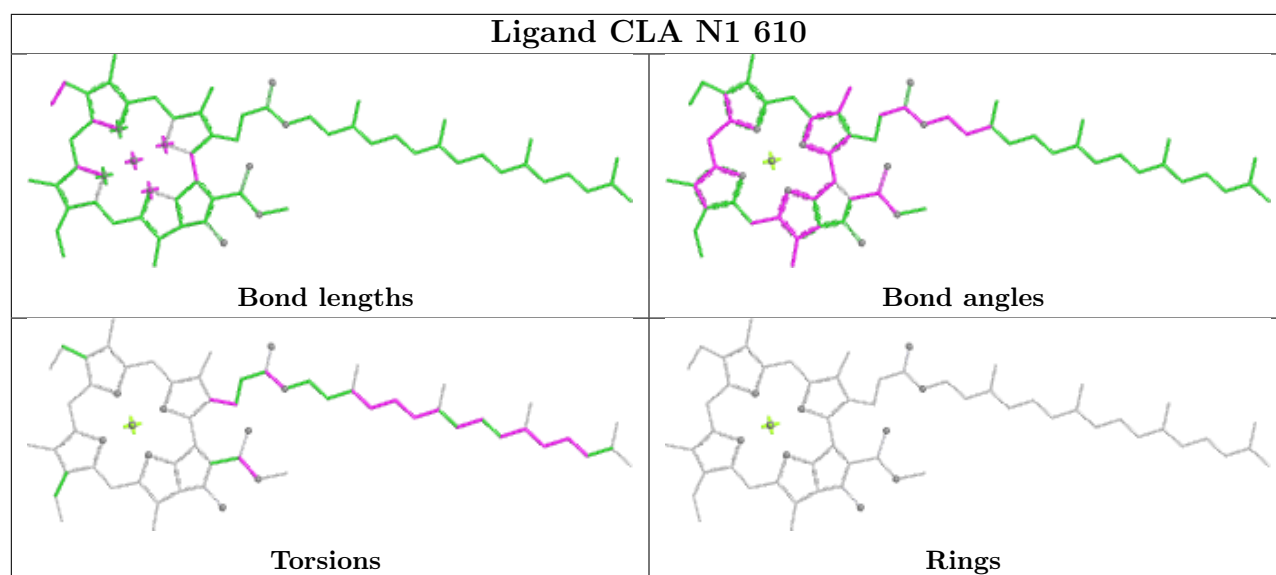
Ligand CLA D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C1 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

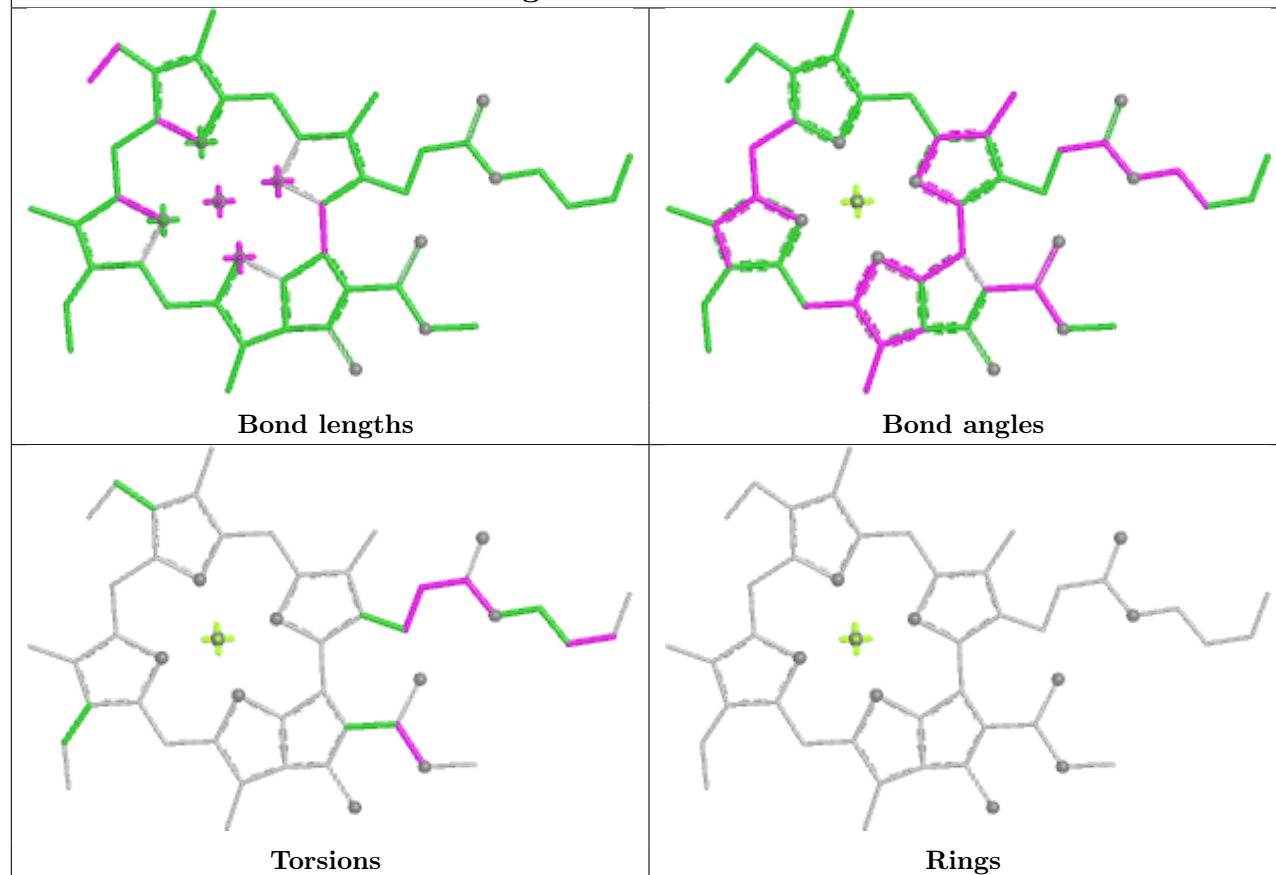
Ligand LUT G 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

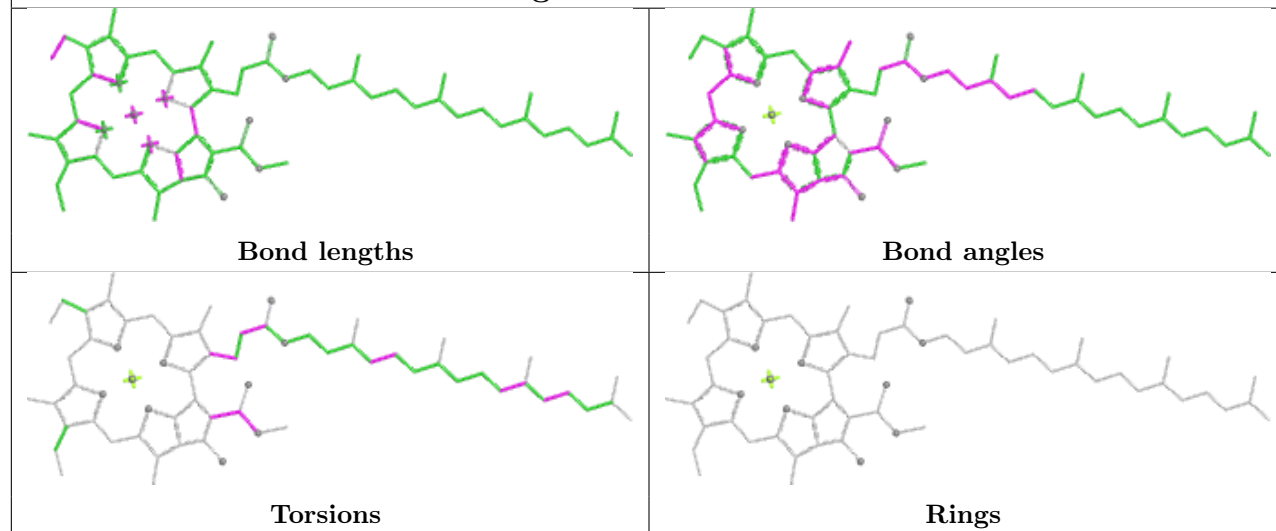


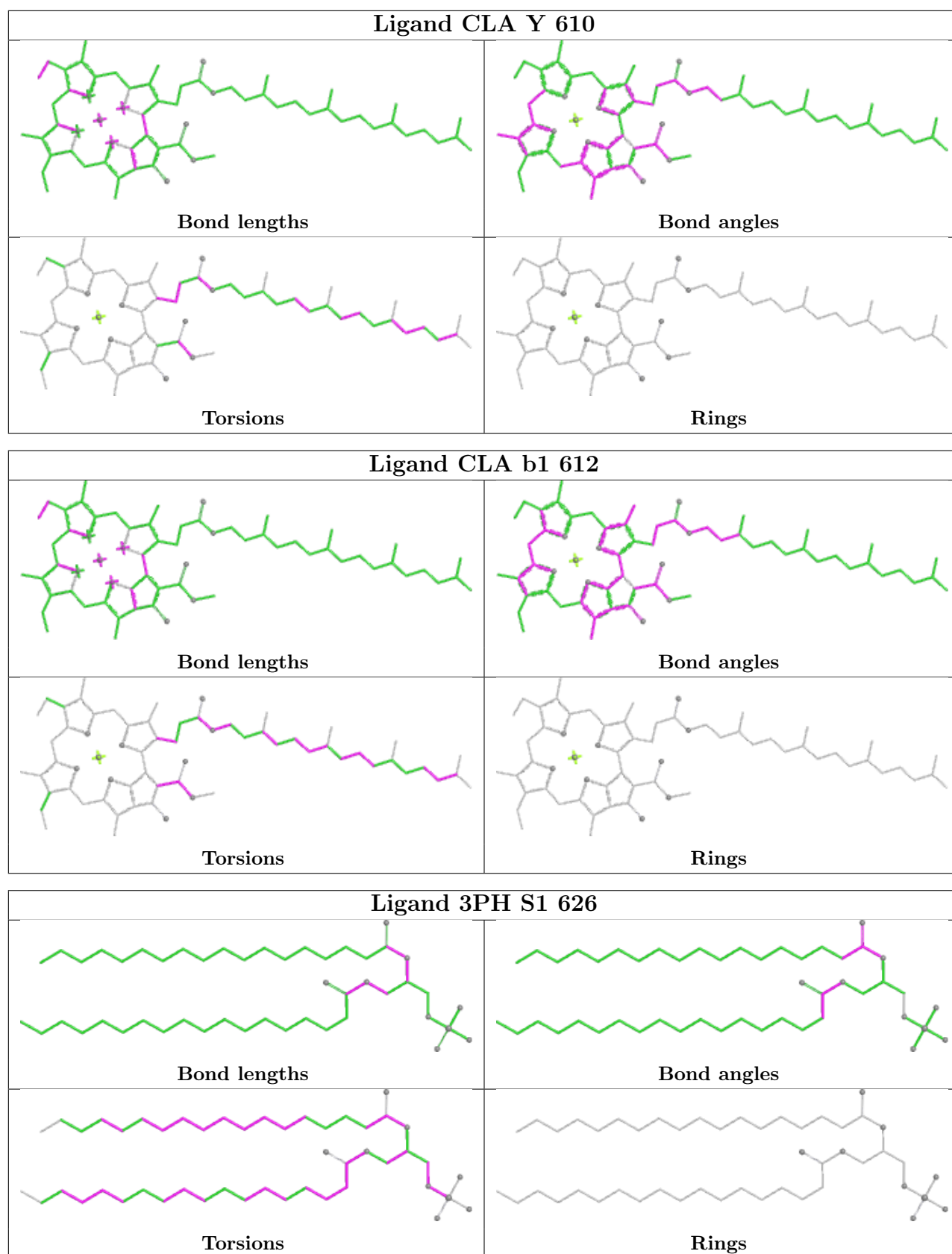


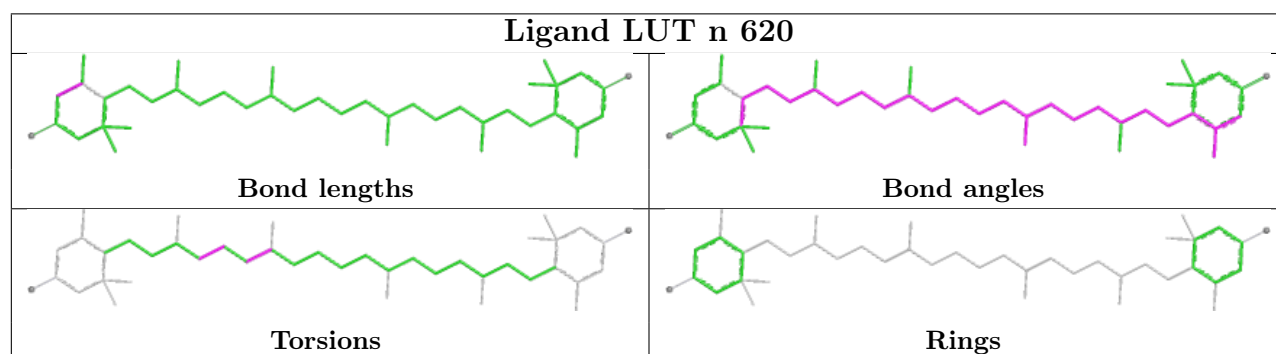
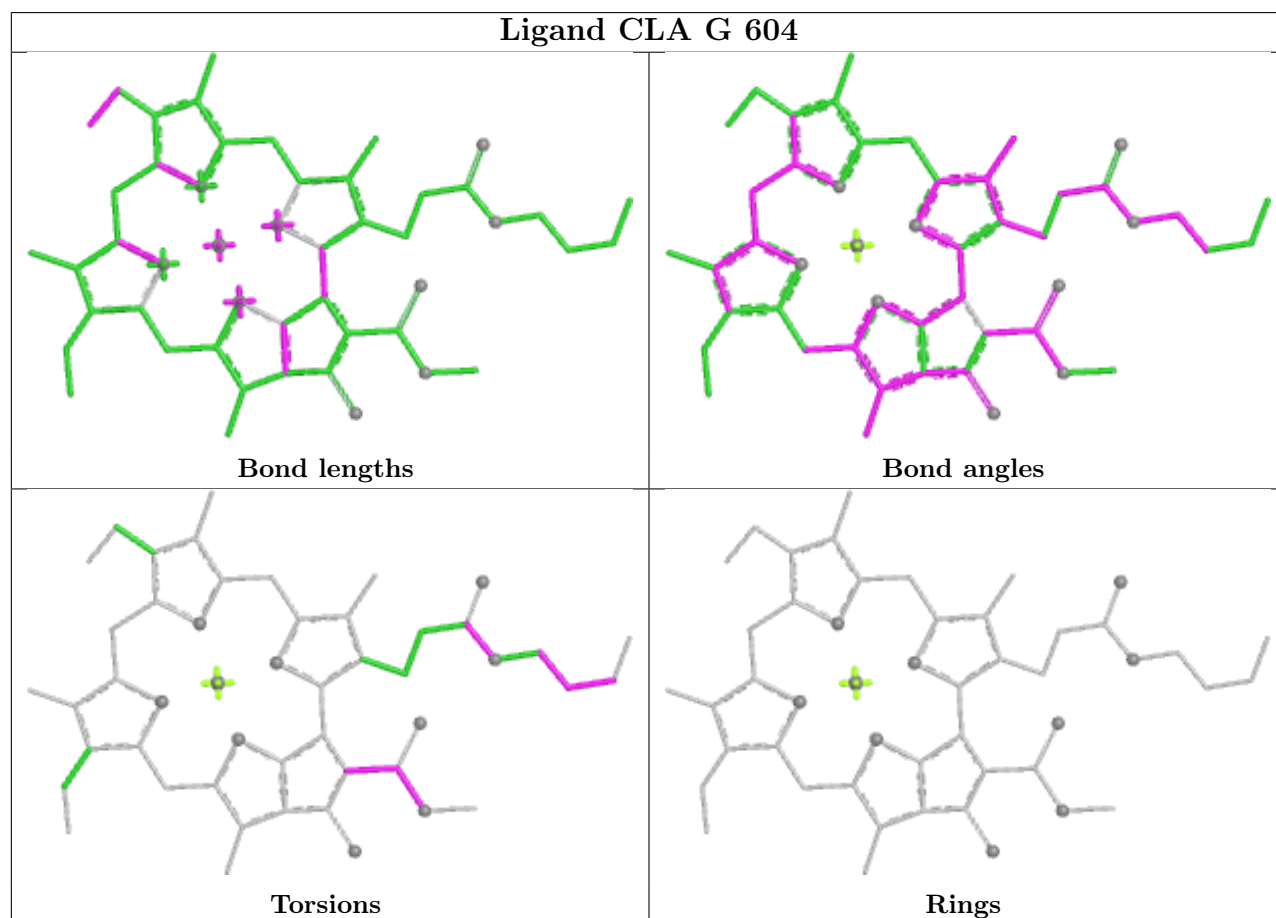
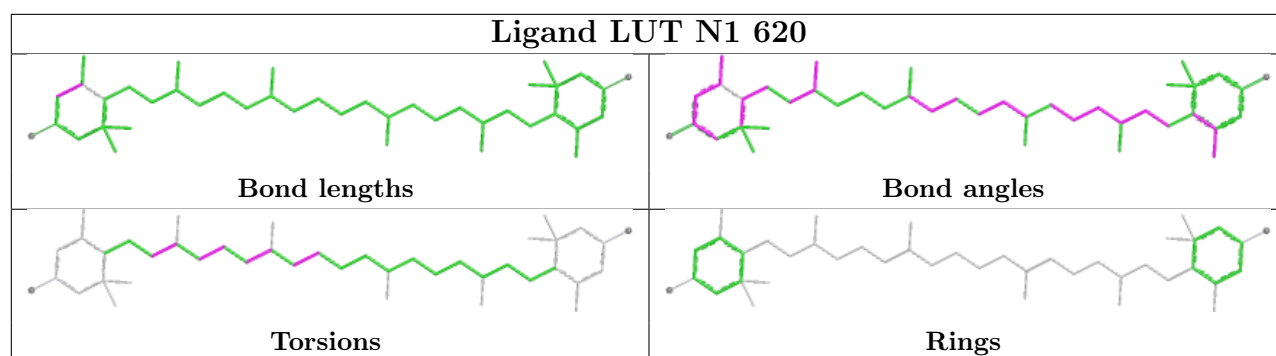
Ligand CLA G1 614

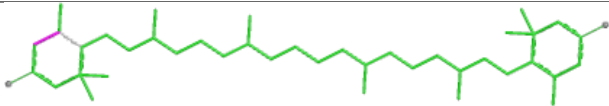
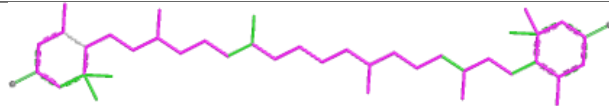
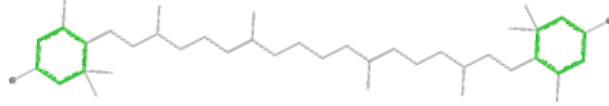


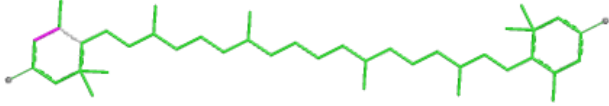
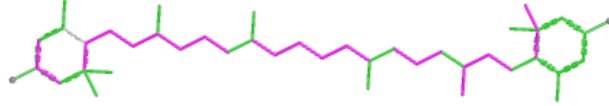
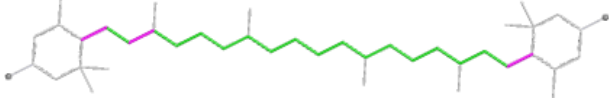
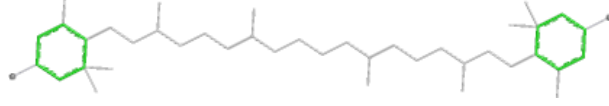
Ligand CLA B 609

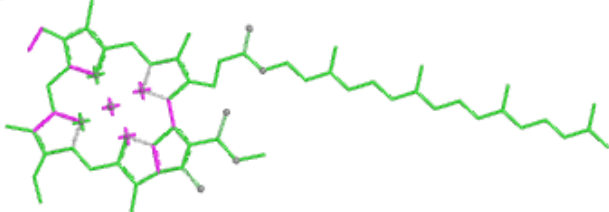
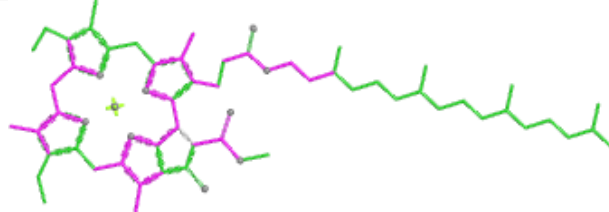
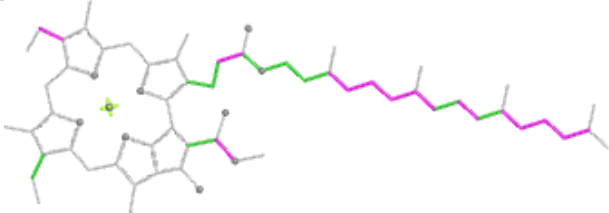
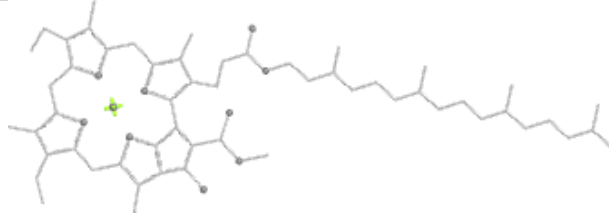


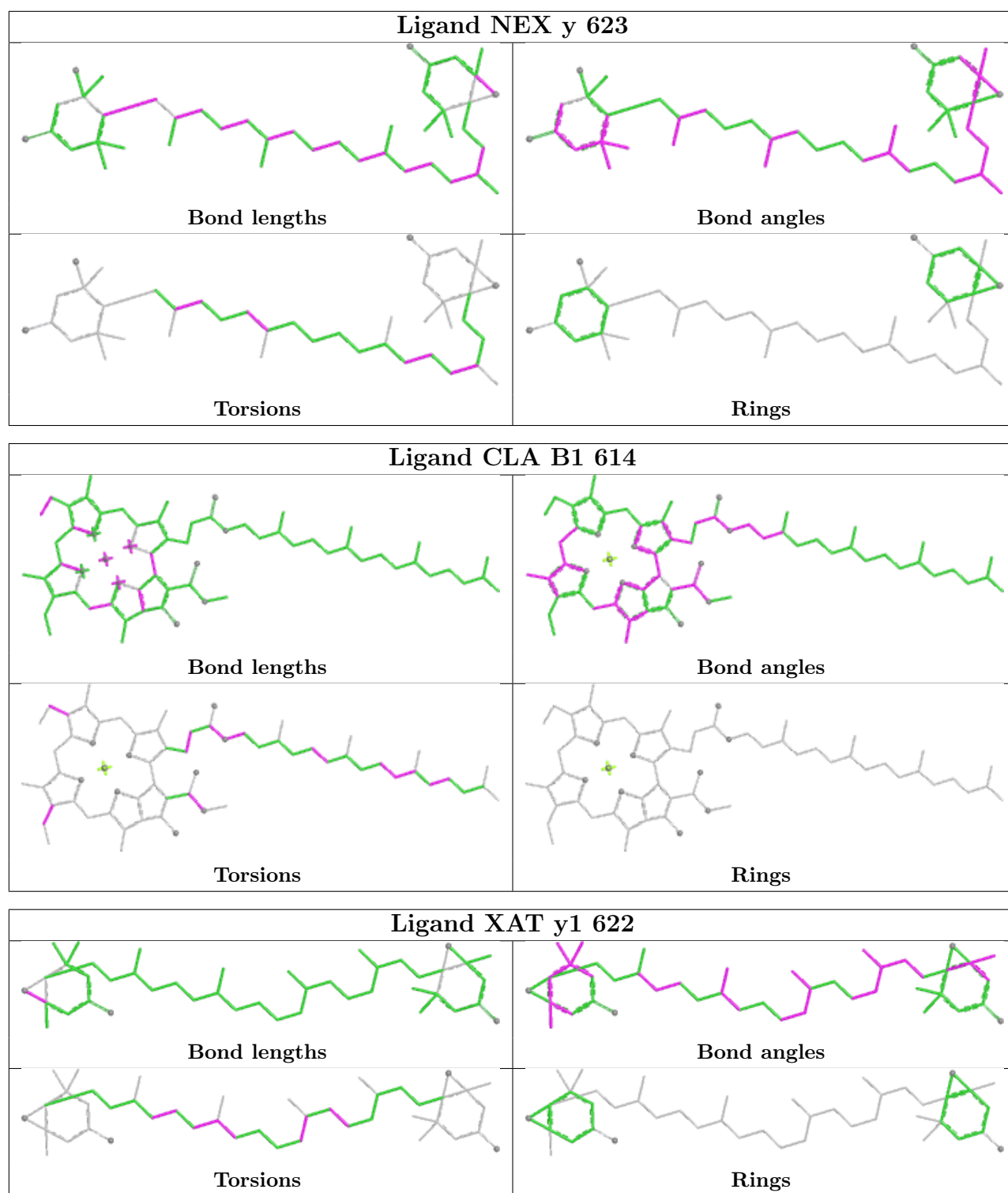


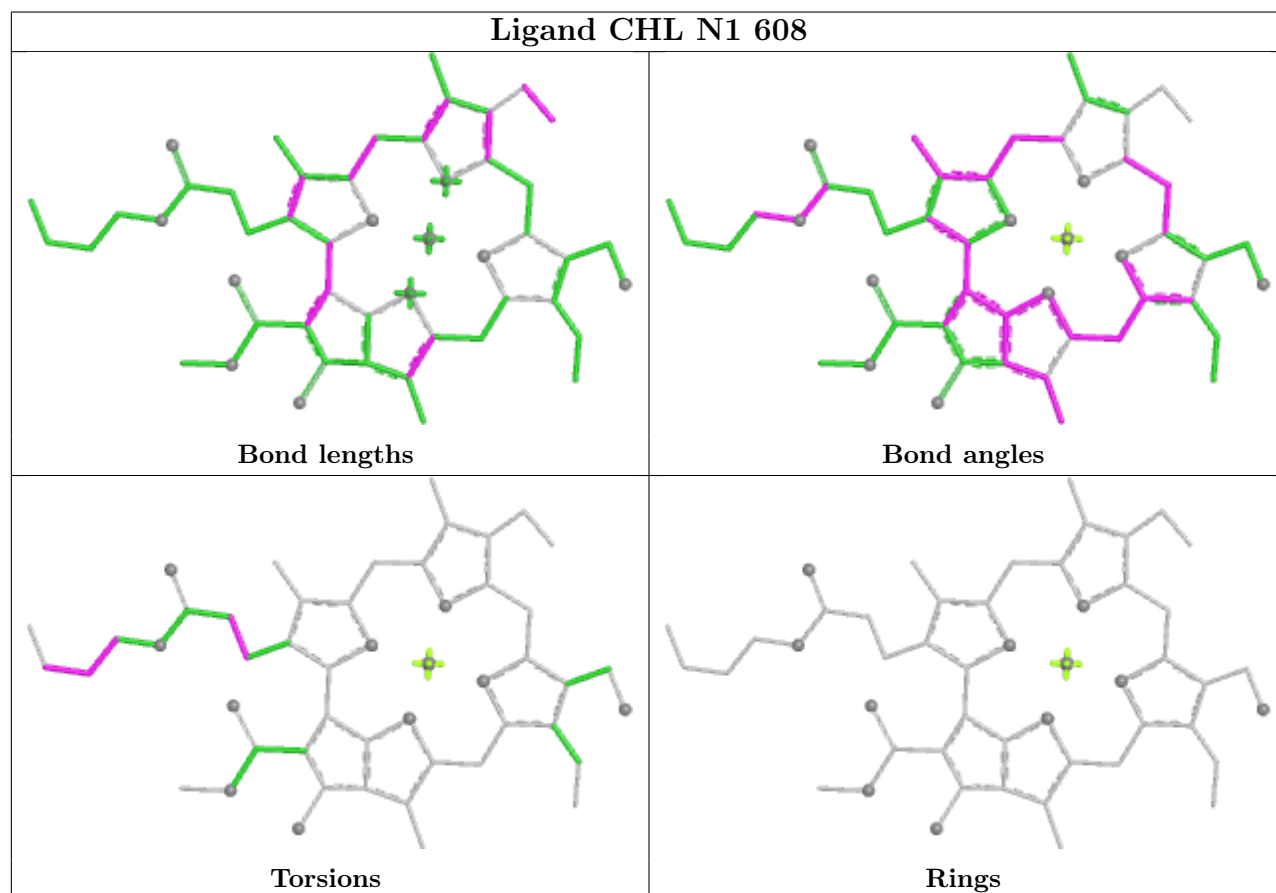
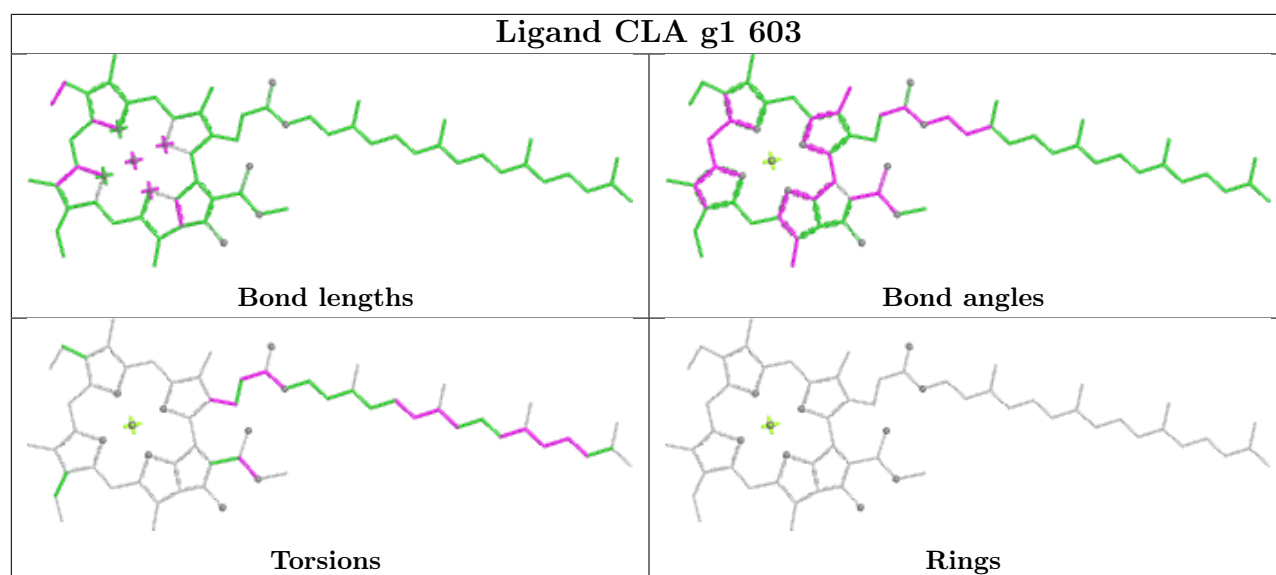


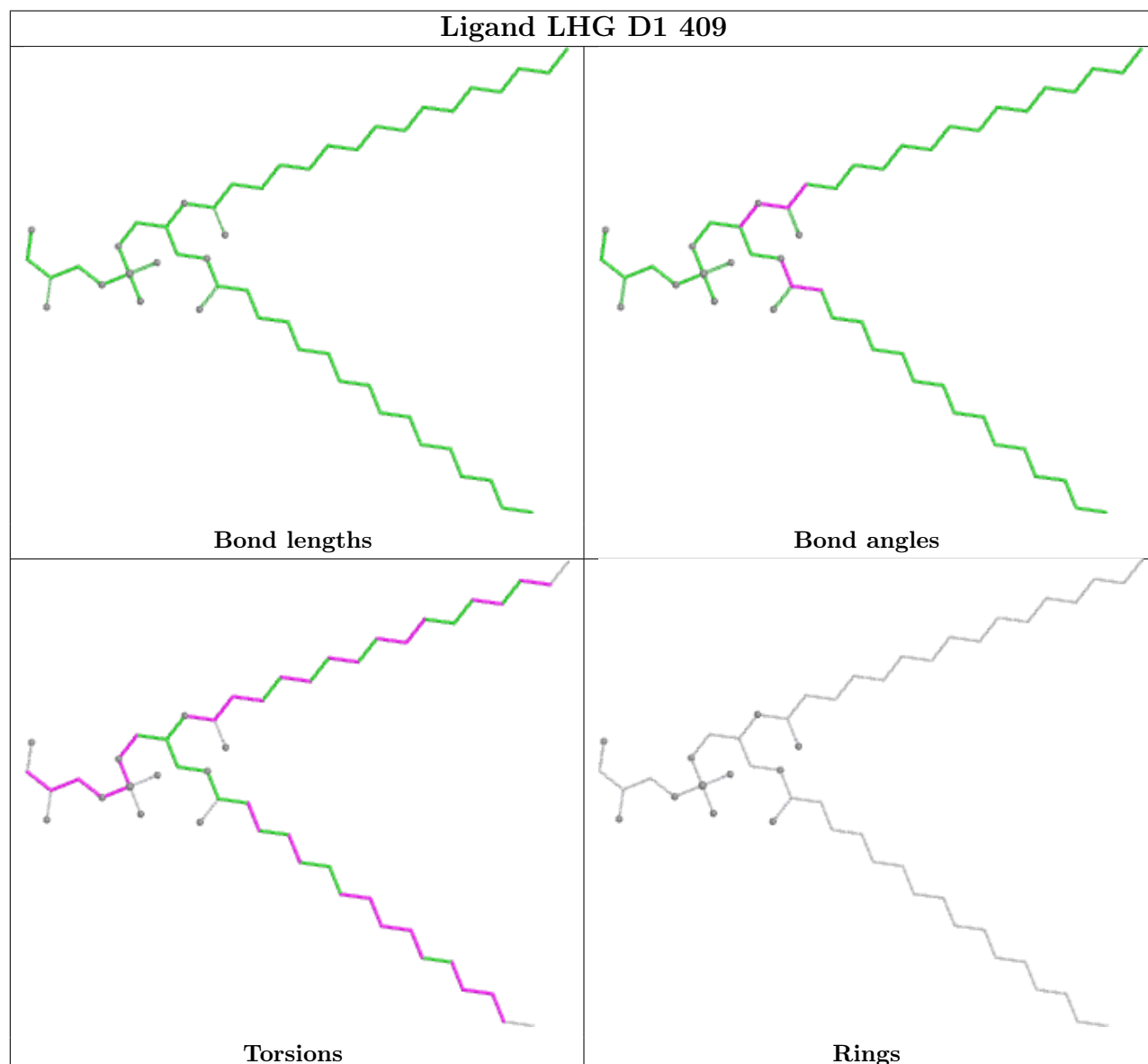
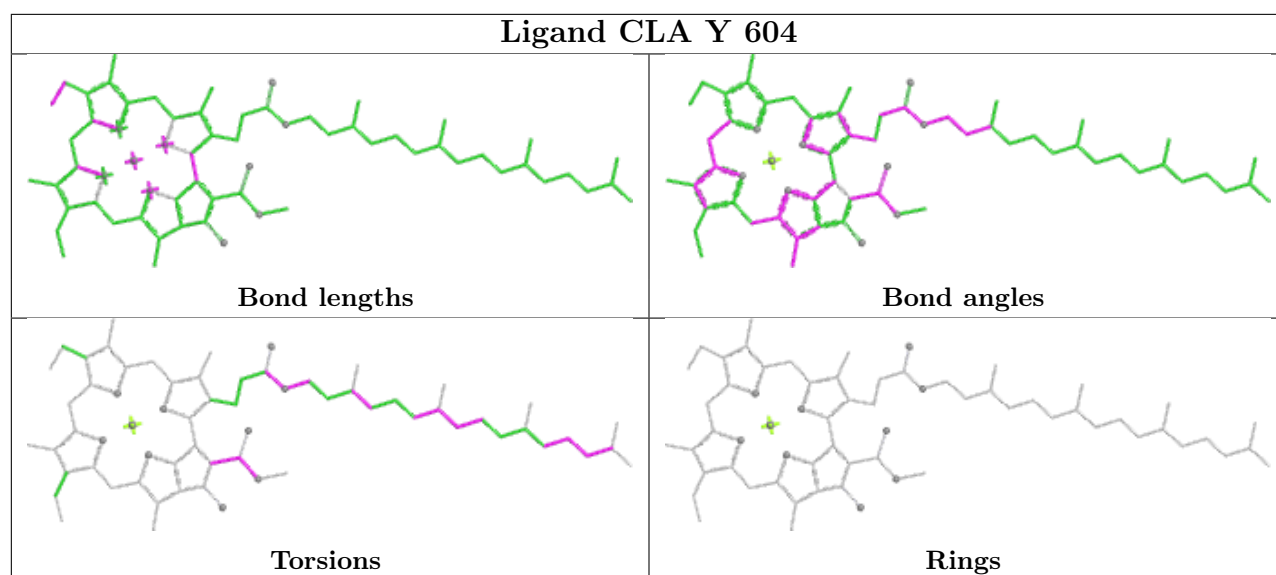
Ligand LUT S 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

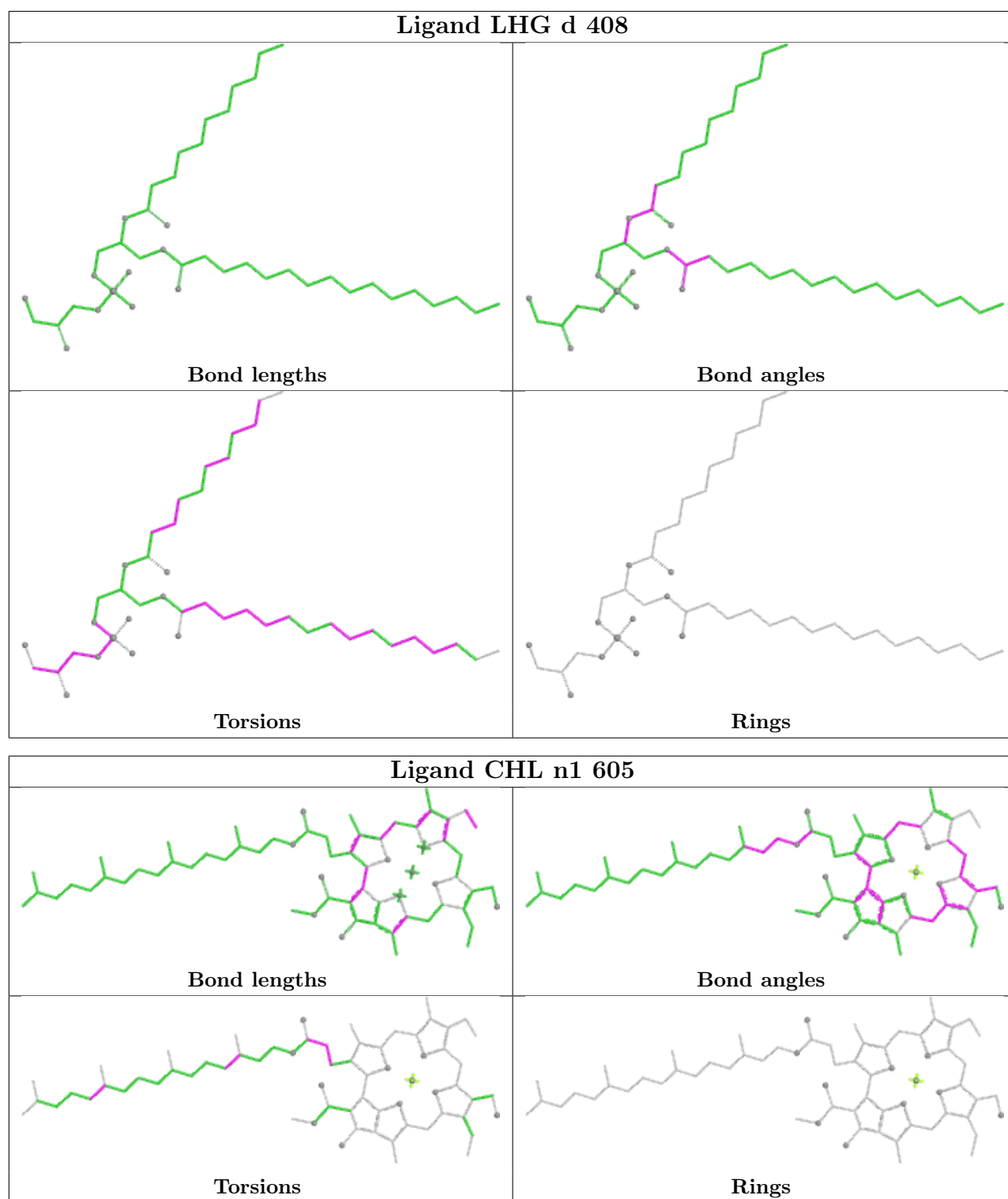
Ligand LUT Y 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

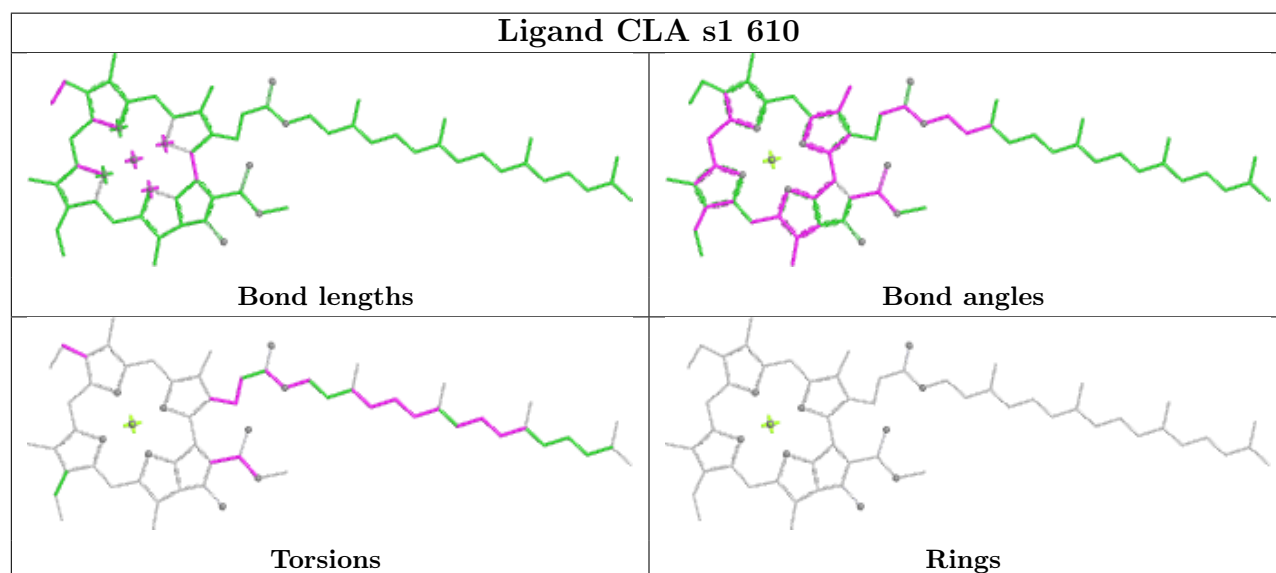
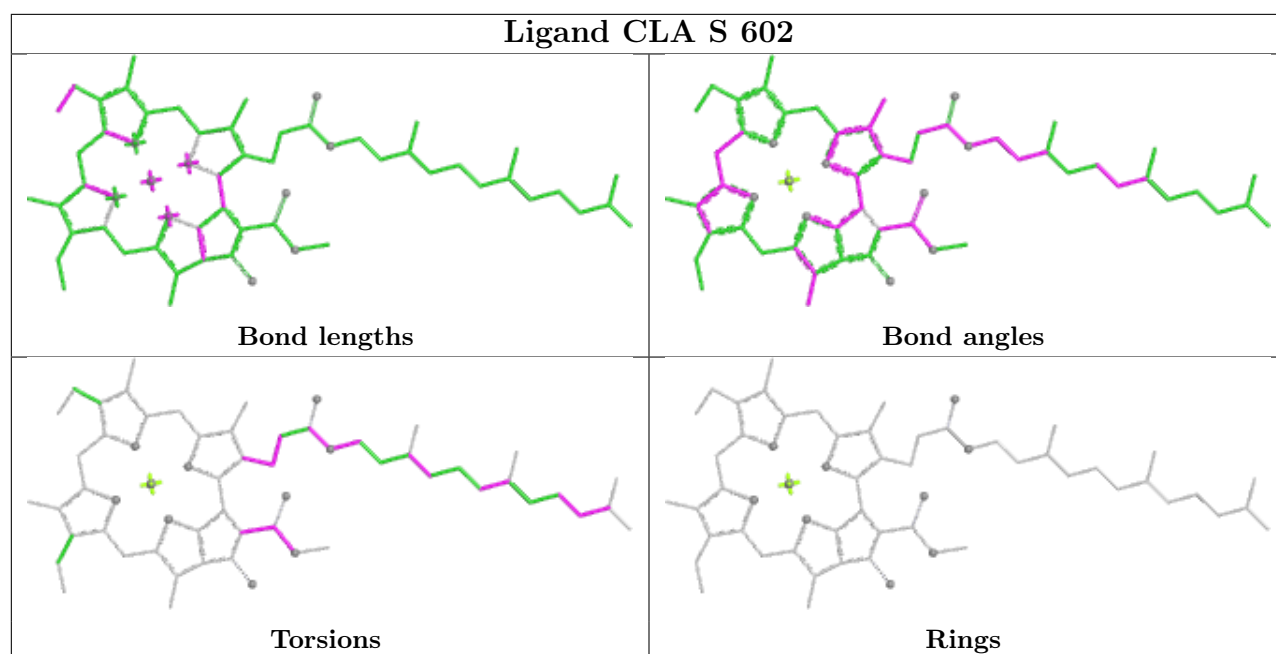
Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

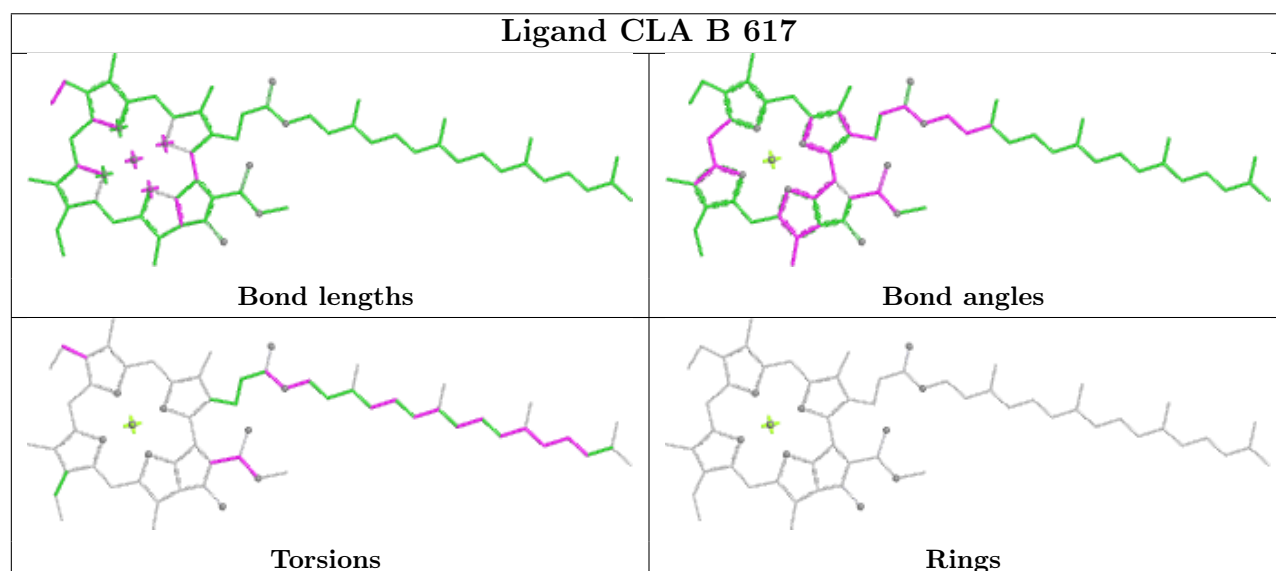
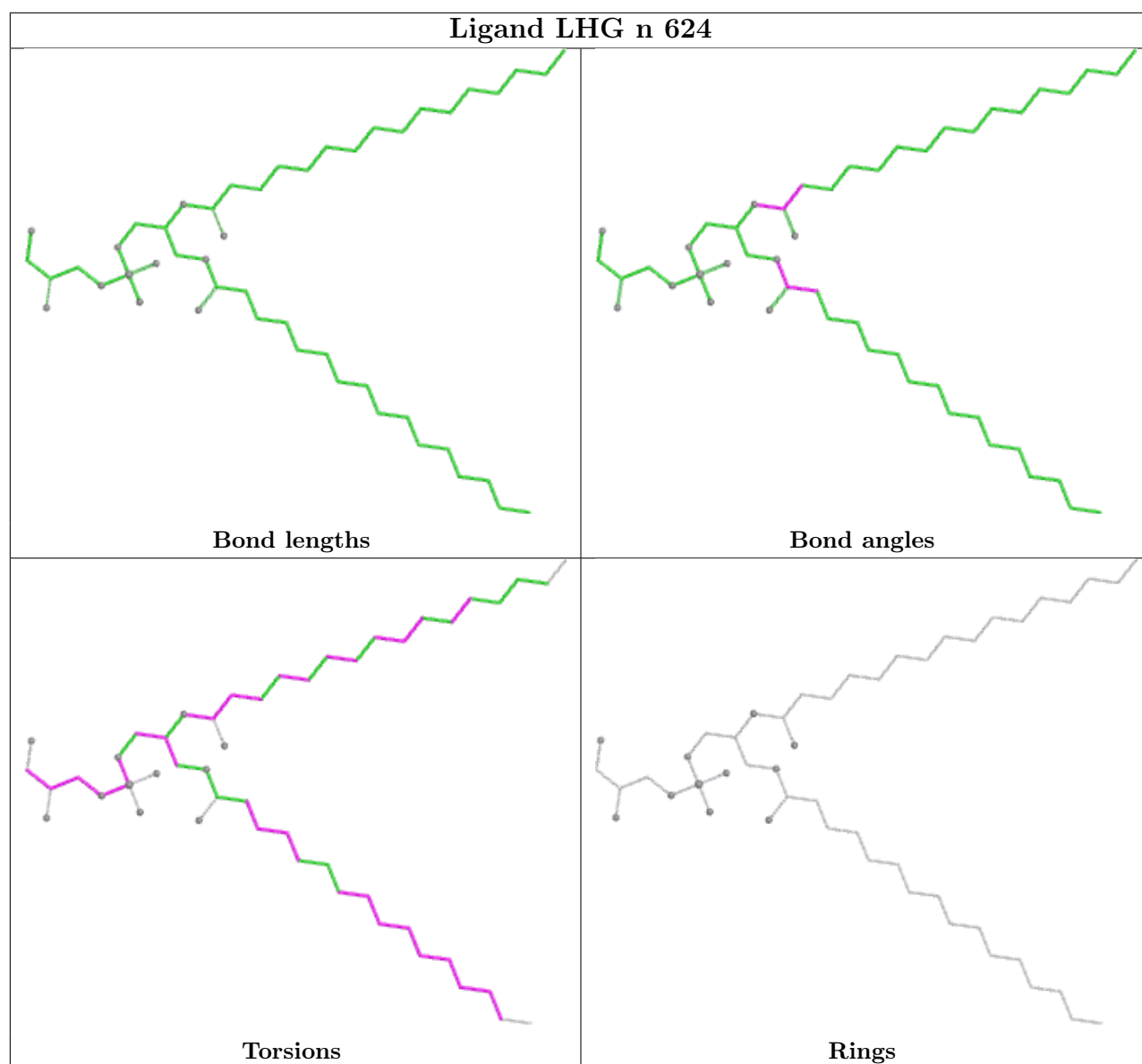


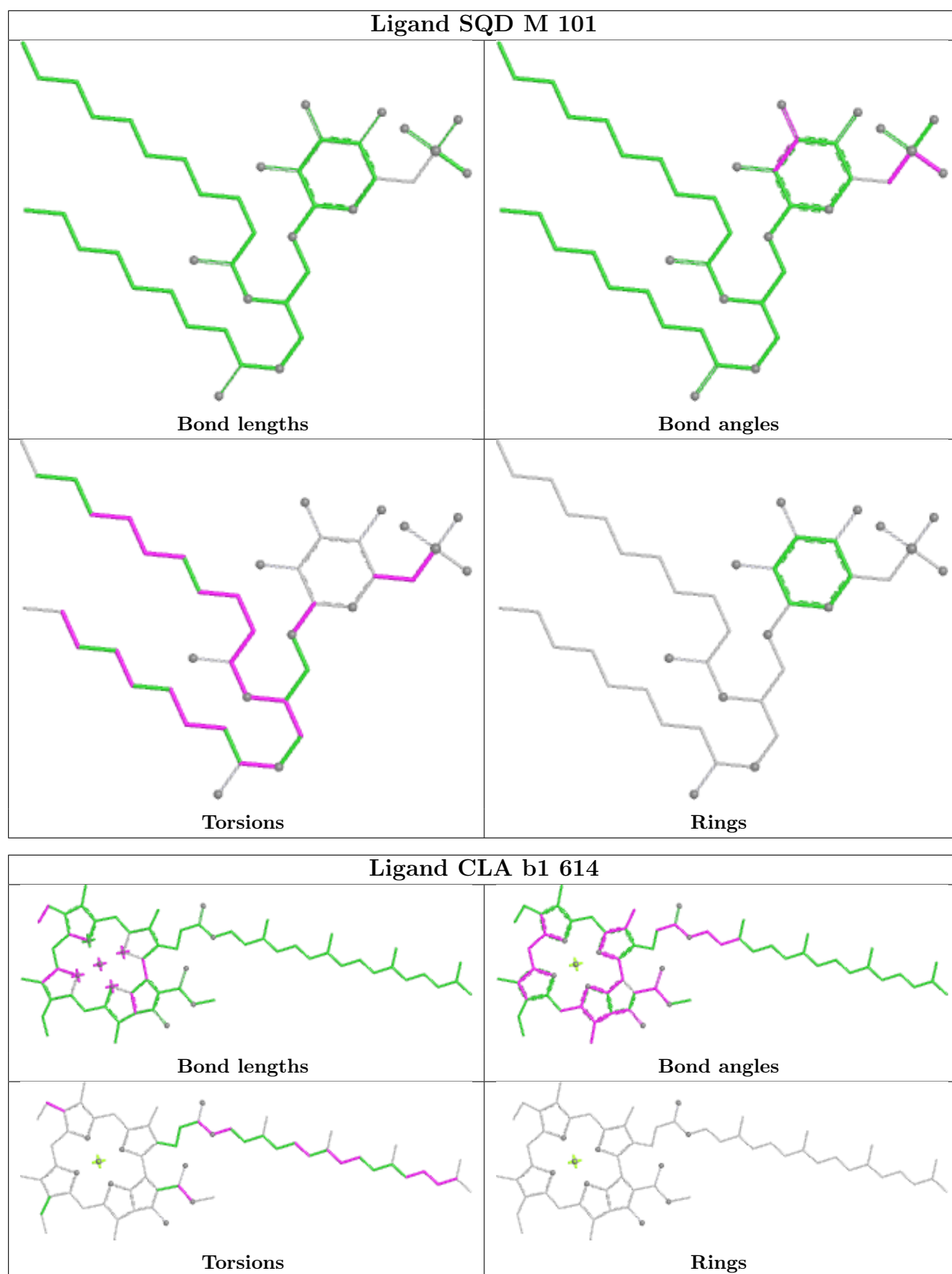


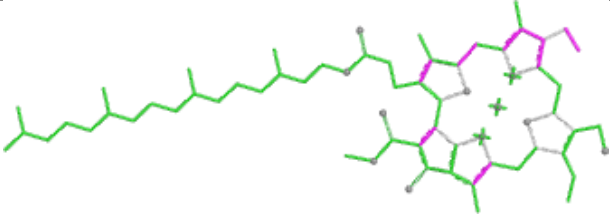
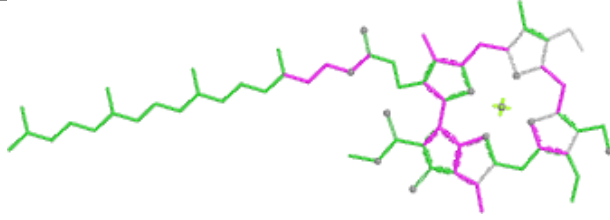
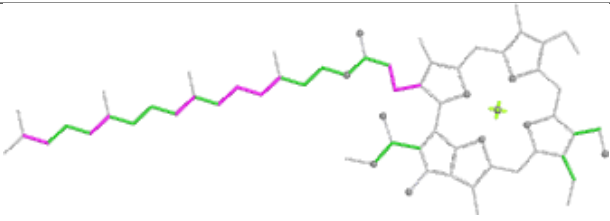
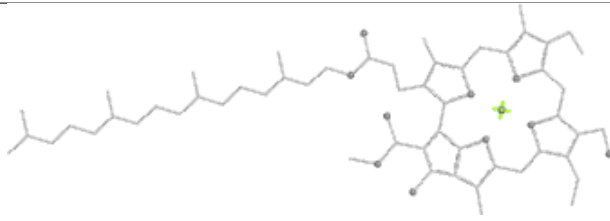
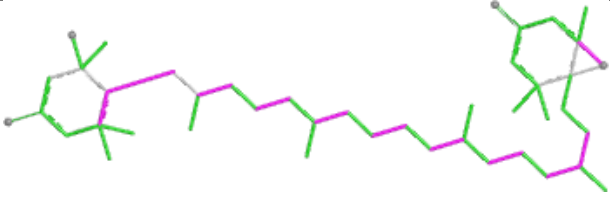
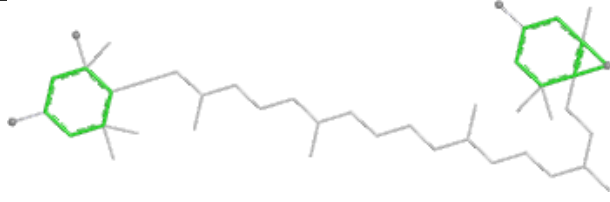
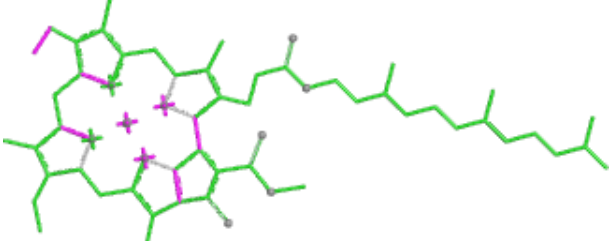
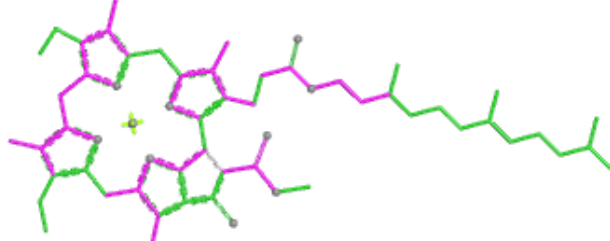
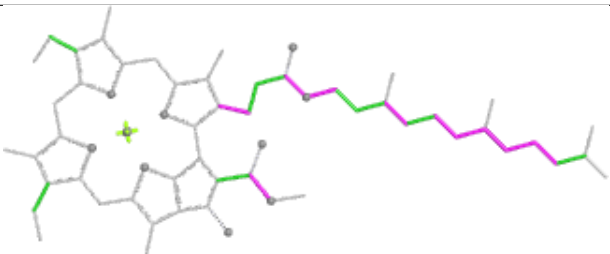
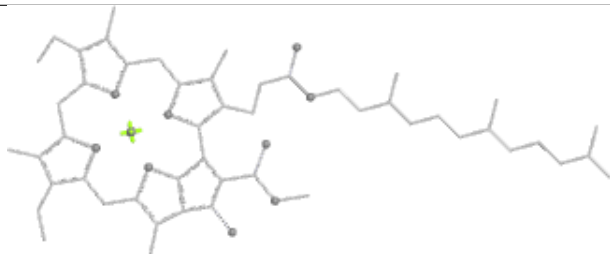


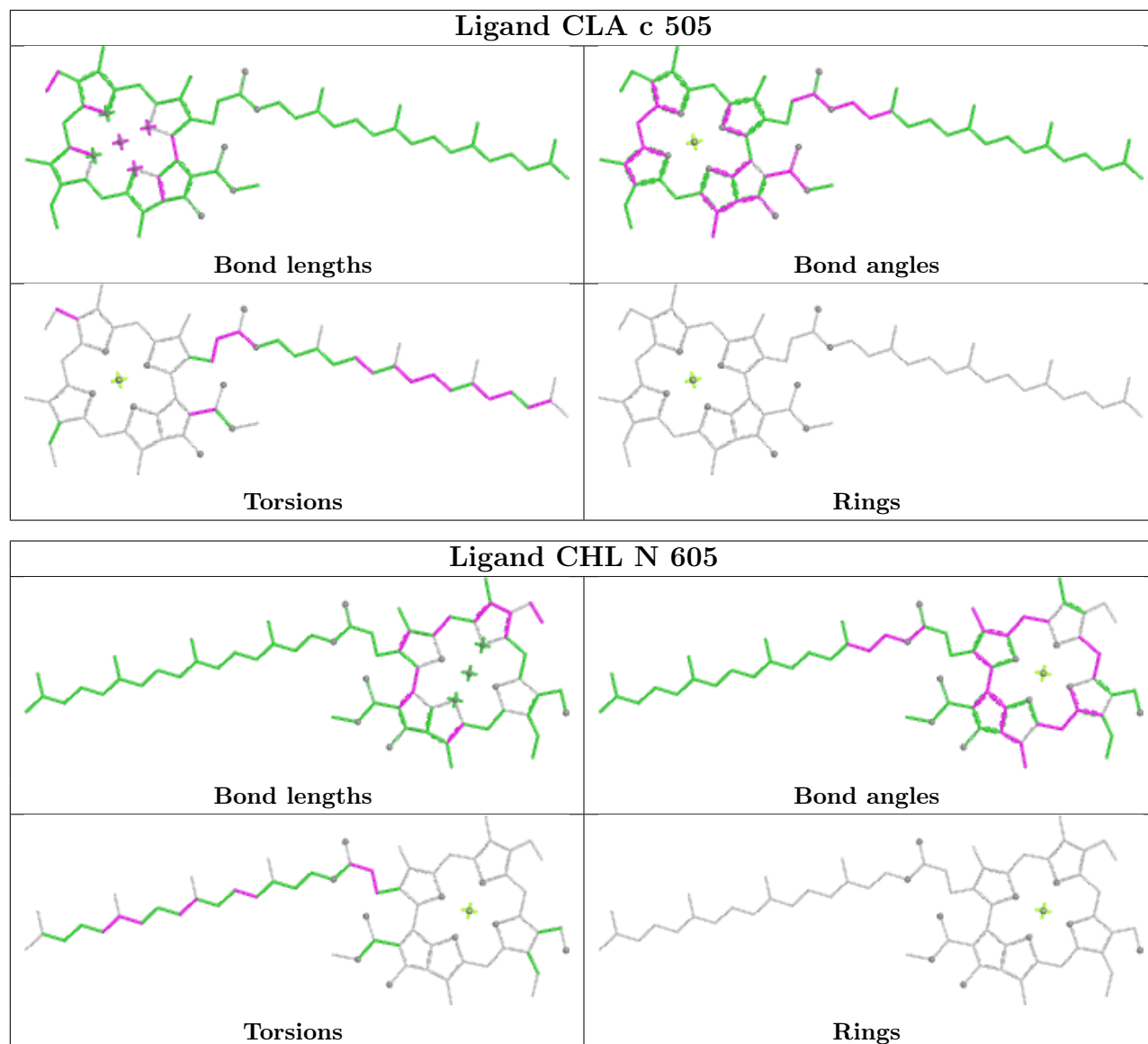


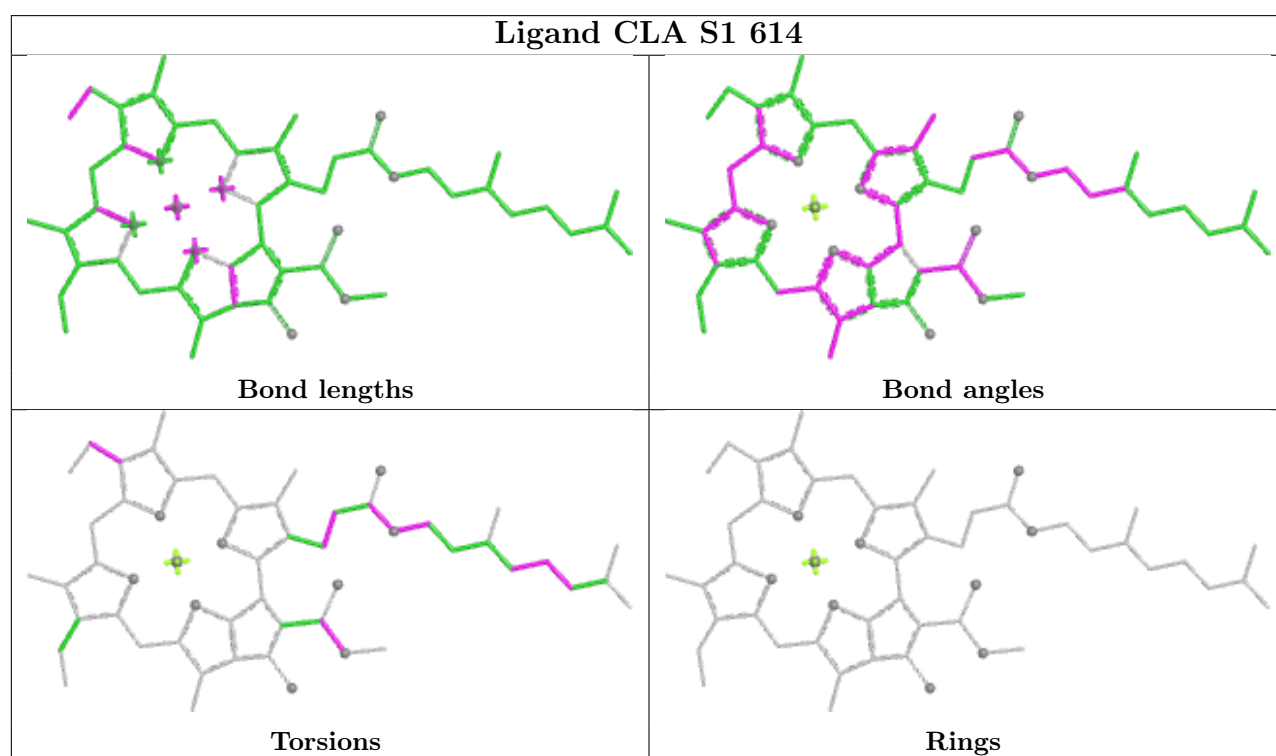
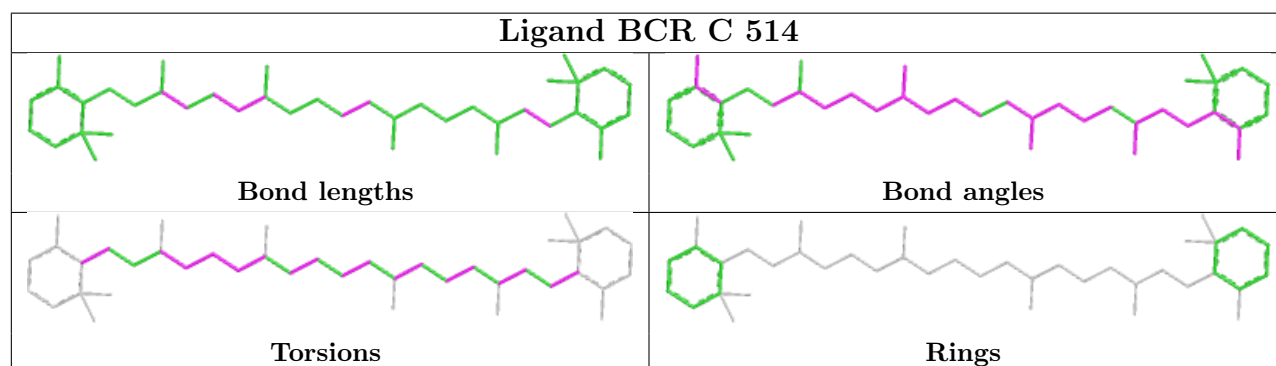
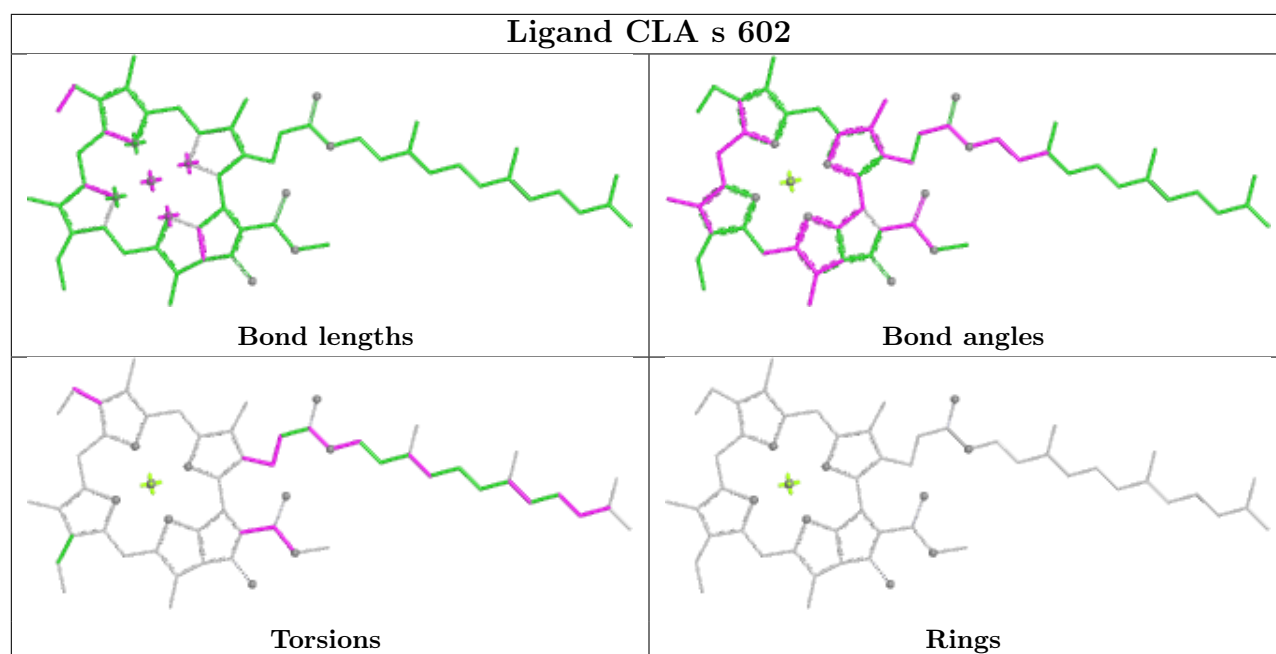


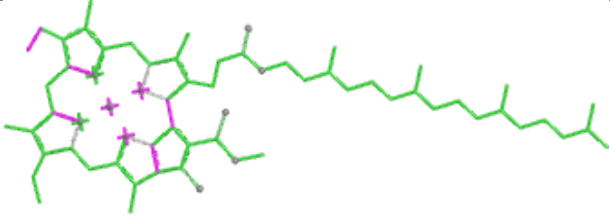
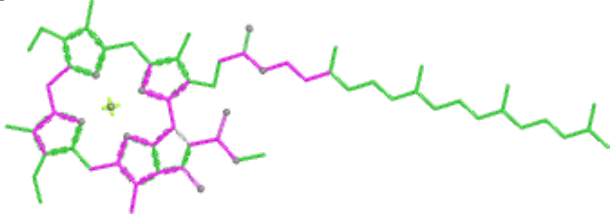
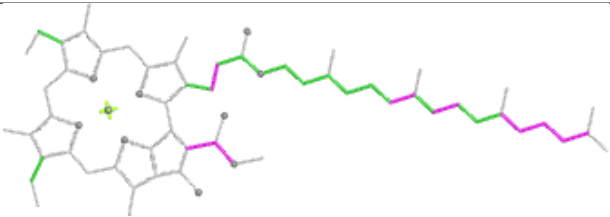
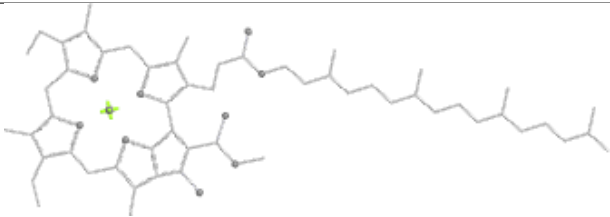
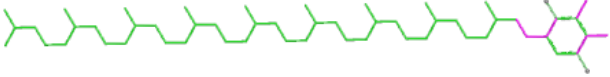
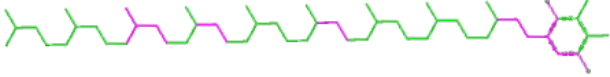
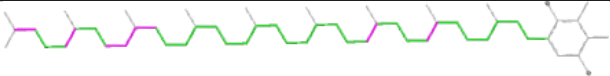
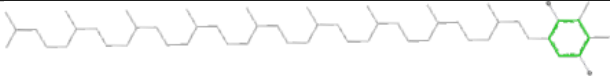


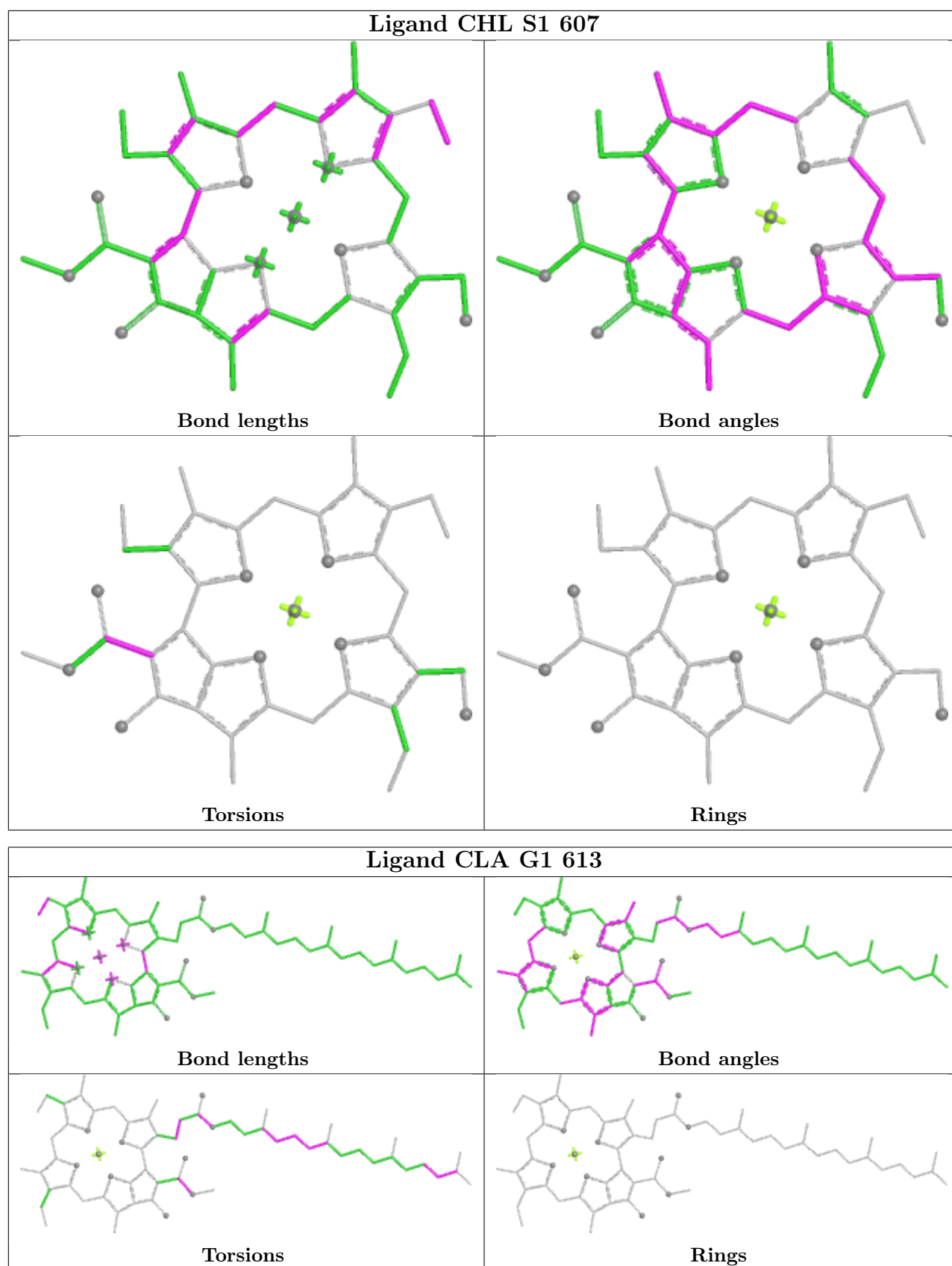


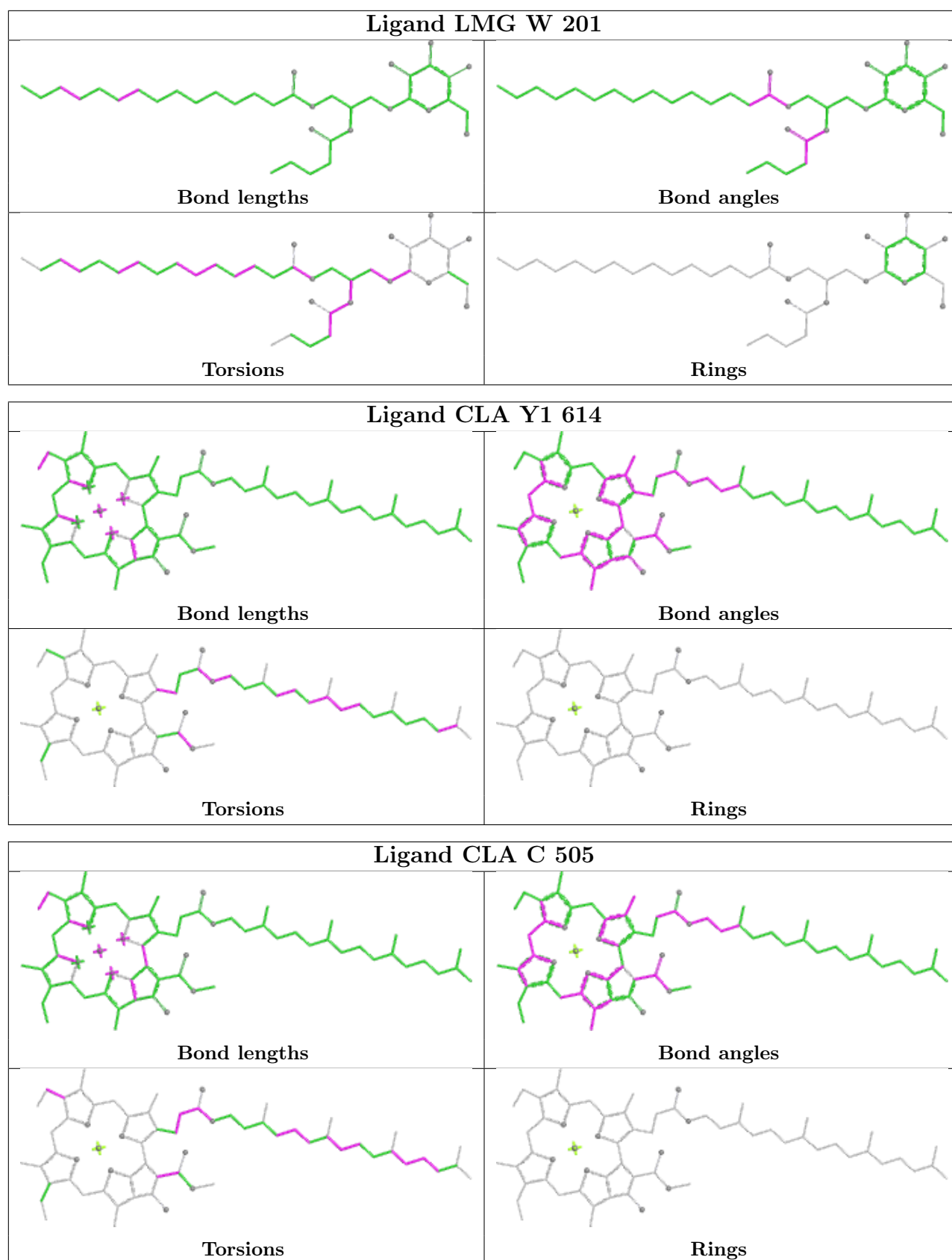
Ligand CHL N 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NEX s 623	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings



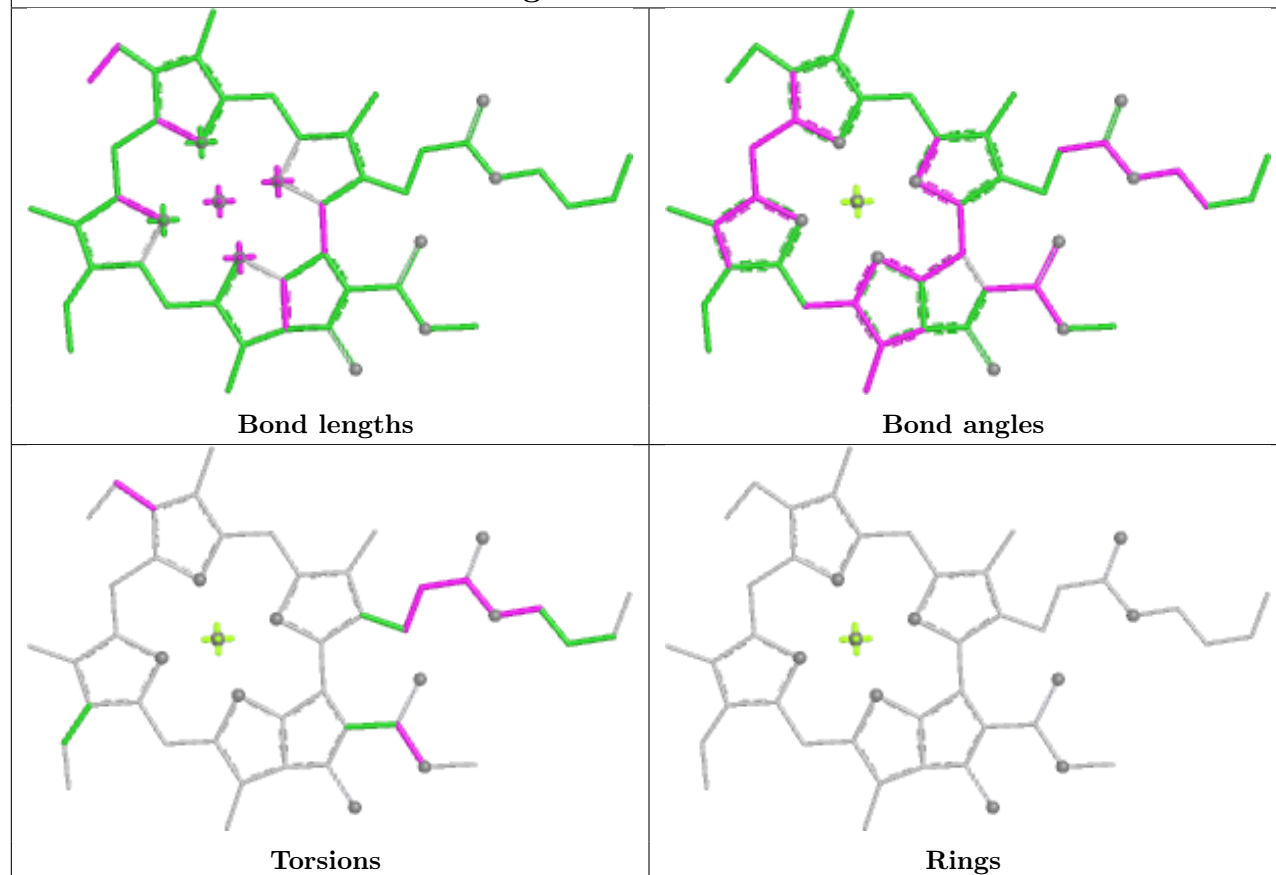


Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

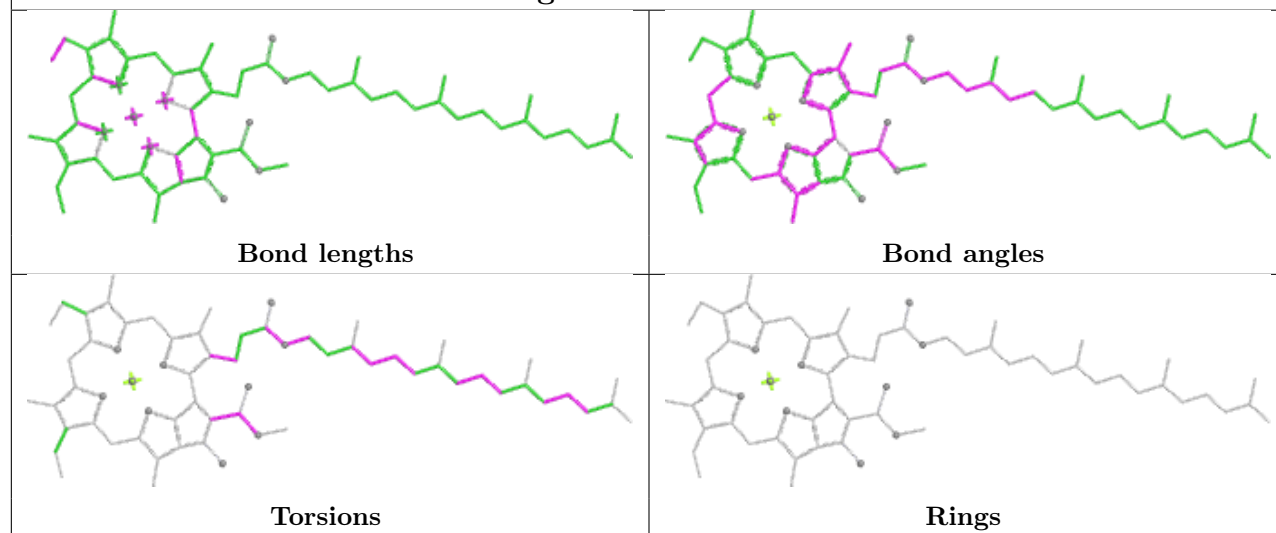


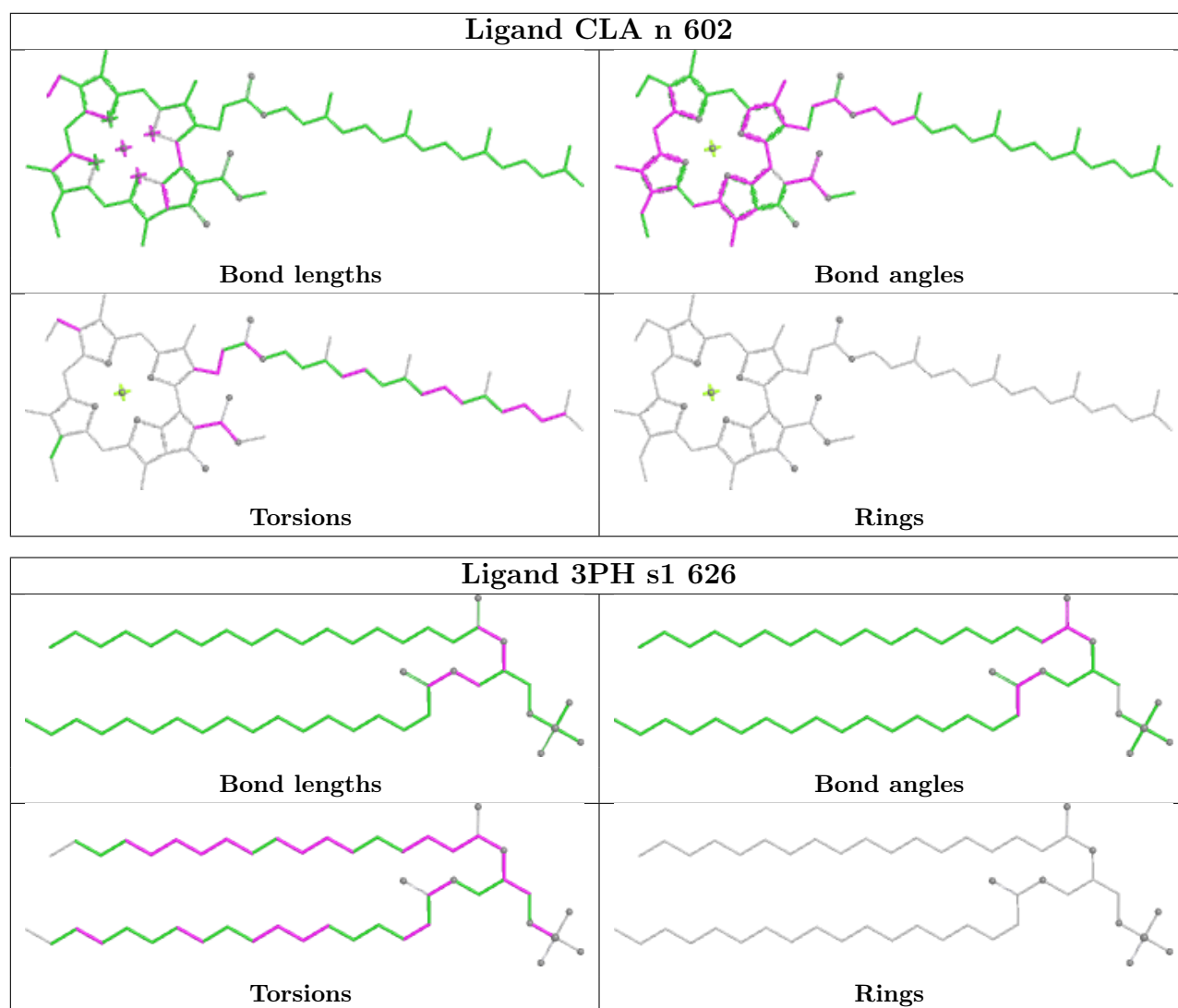


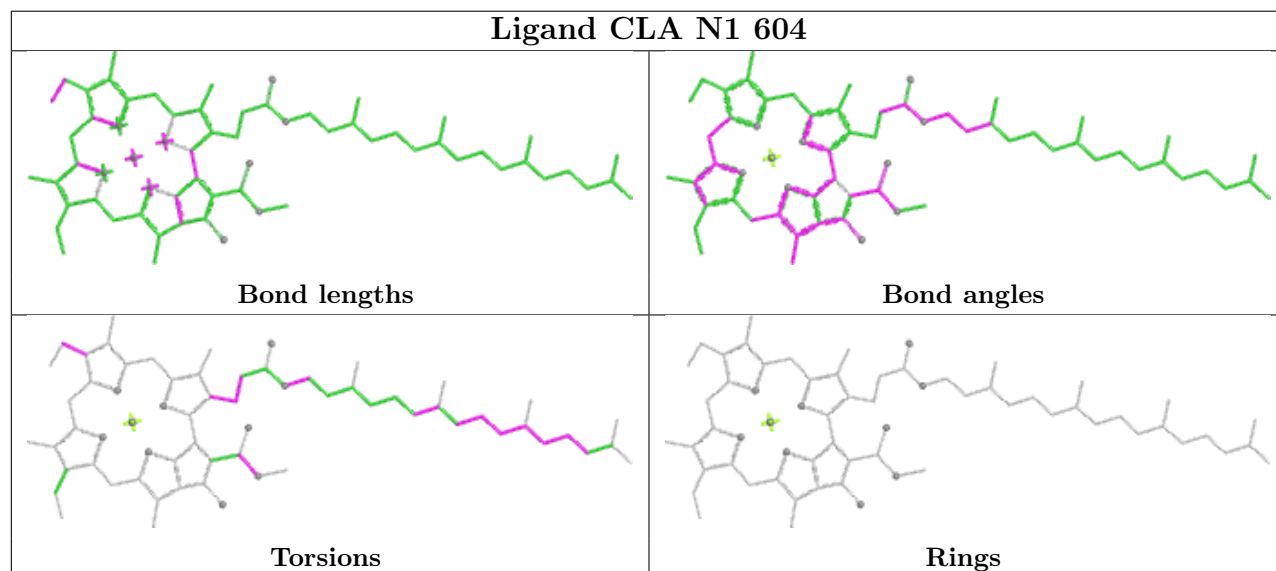
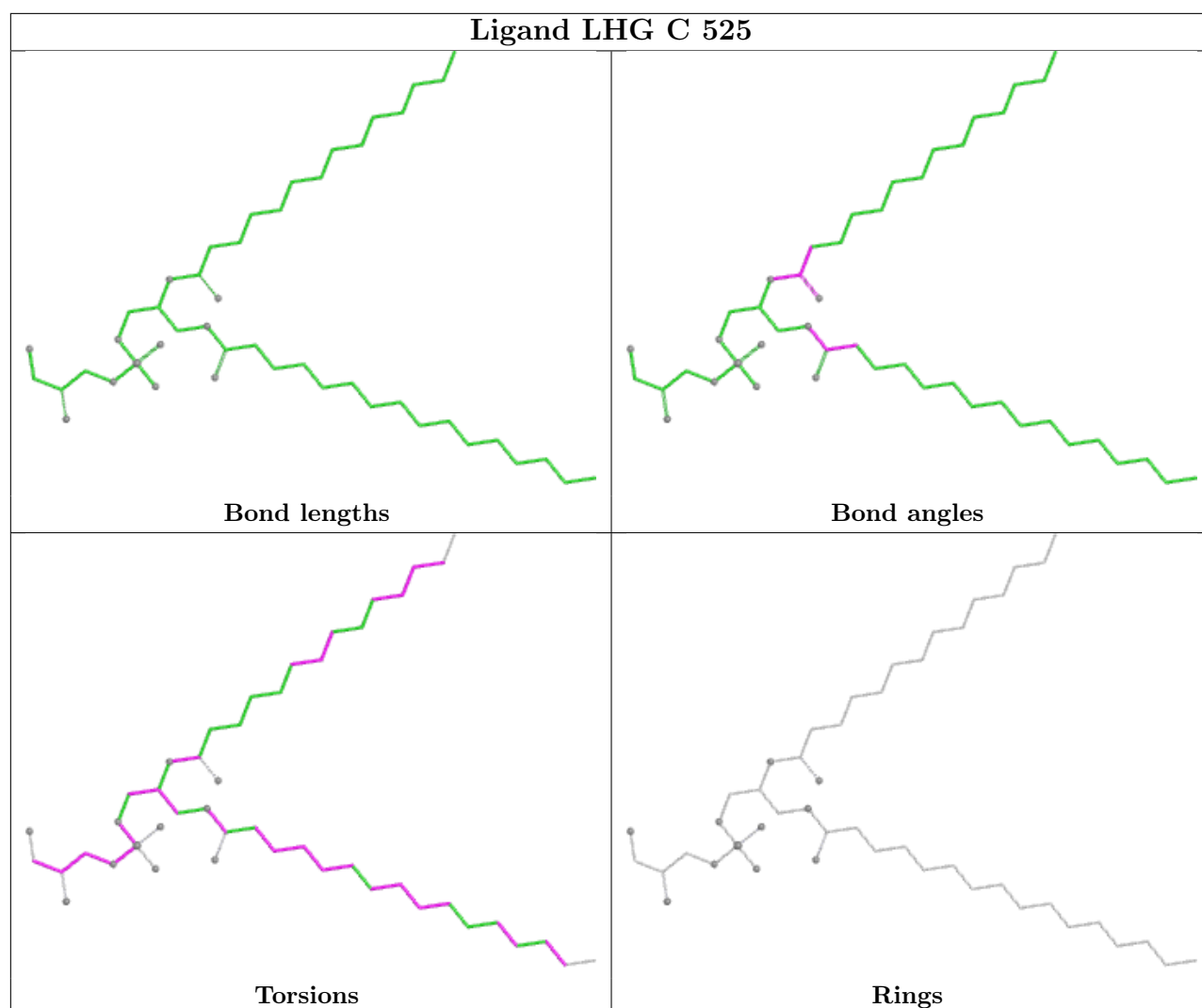
Ligand CLA R1 604

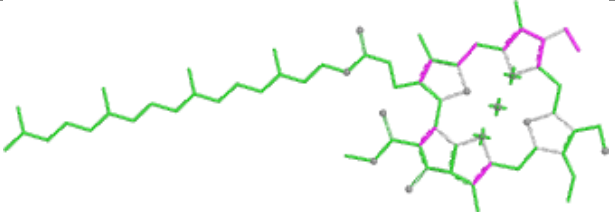
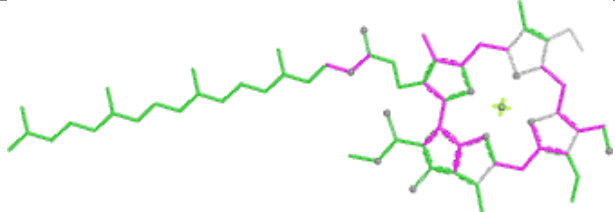
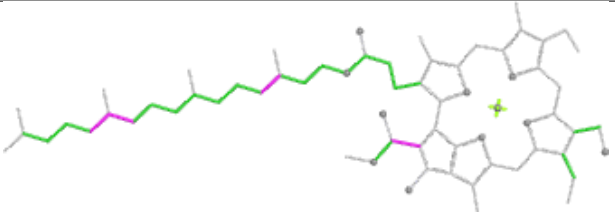
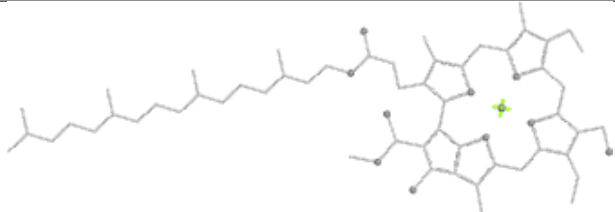
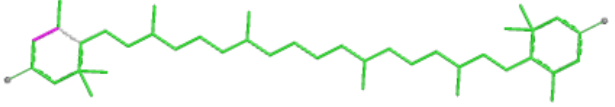
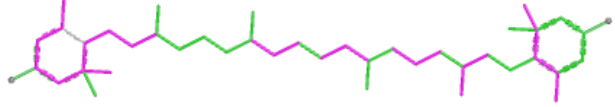
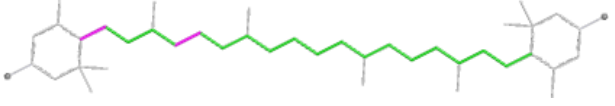
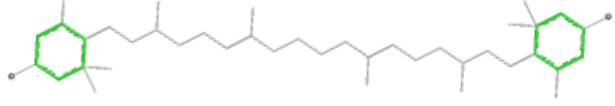
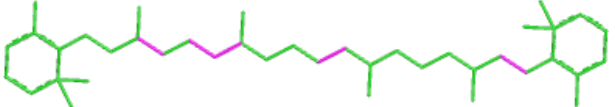
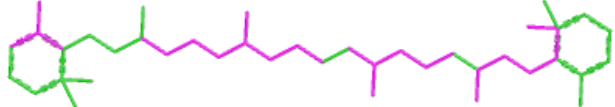
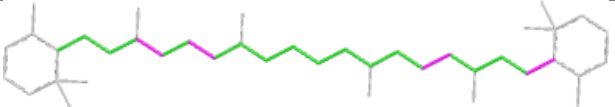
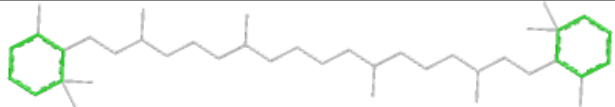


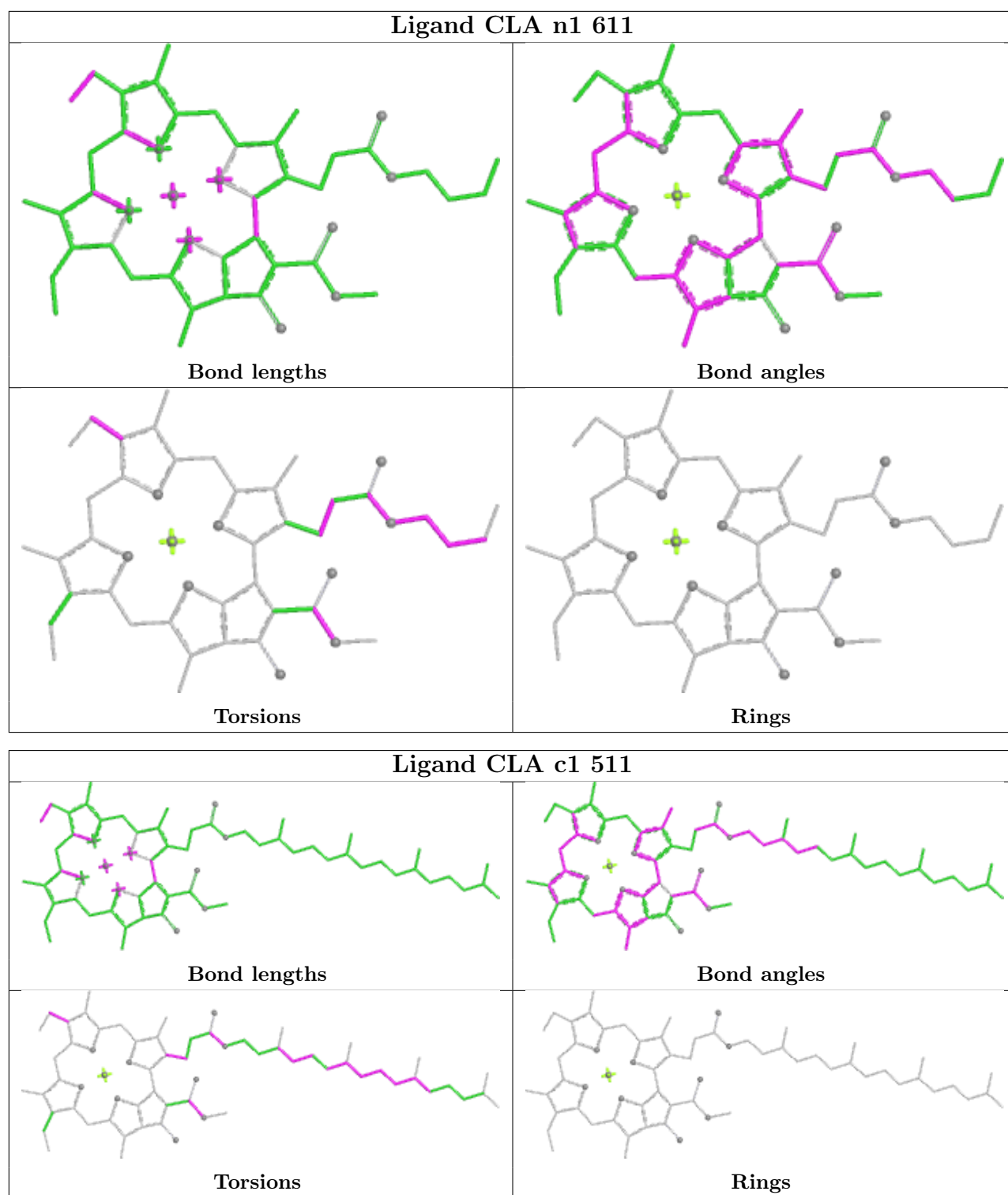
Ligand CLA c 506

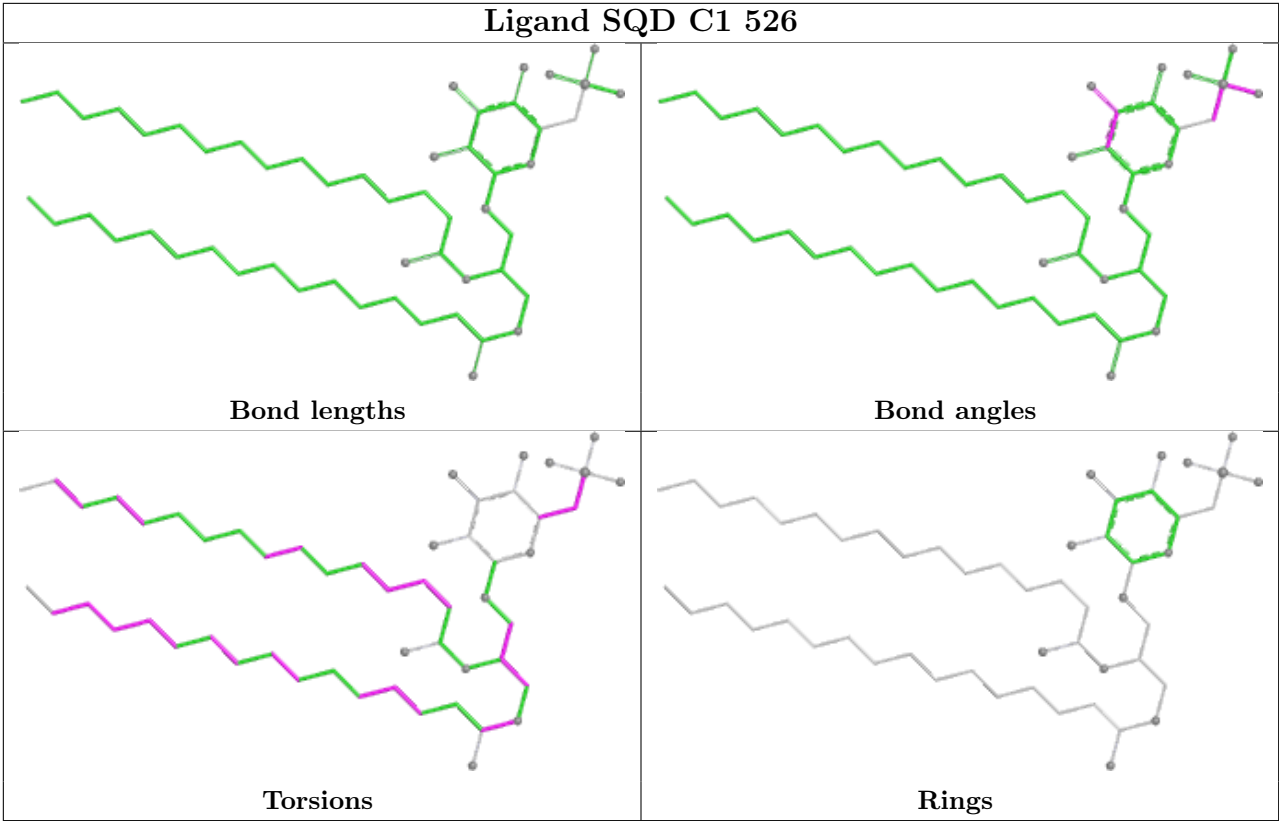






Ligand CHL y 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT n 621	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	r1	1
22	R1	1
22	R	1
20	n1	1
20	n	1
21	G1	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.15
1	r1	110:PRO	C	126:GLU	N	13.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R1	110:PRO	C	126:GLU	N	12.94
1	R	110:PRO	C	126:GLU	N	12.16
1	n1	57:PRO	C	58:PRO	N	3.54

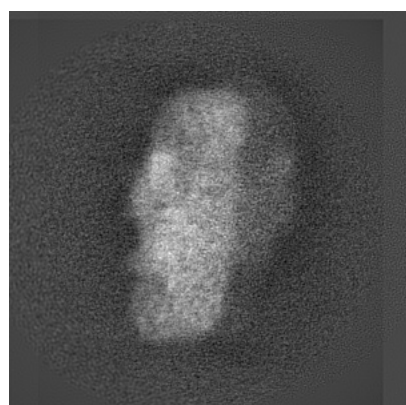
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13444. These allow visual inspection of the internal detail of the map and identification of artifacts.

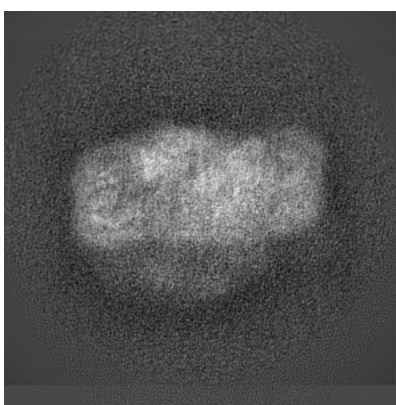
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

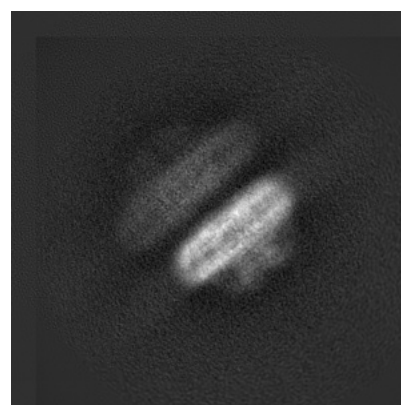
6.1.1 Primary map



X



Y

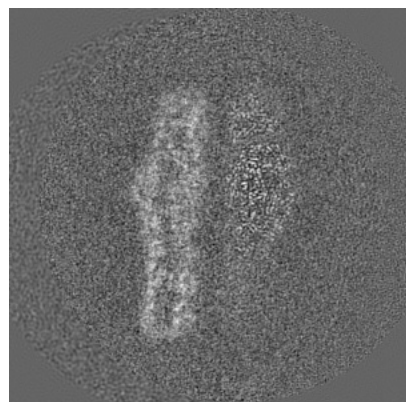


Z

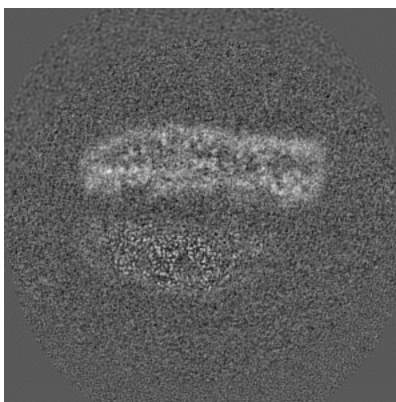
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

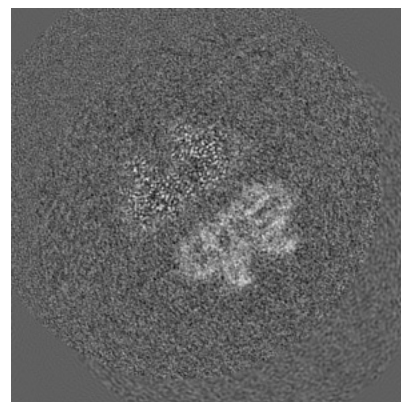
6.2.1 Primary map



X Index: 240



Y Index: 240

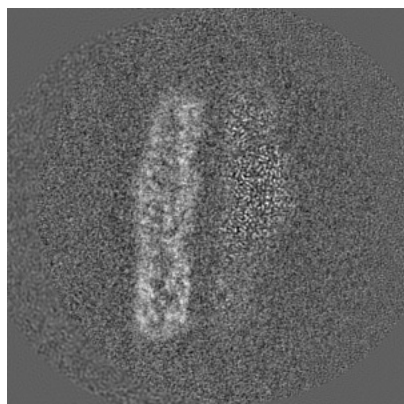


Z Index: 240

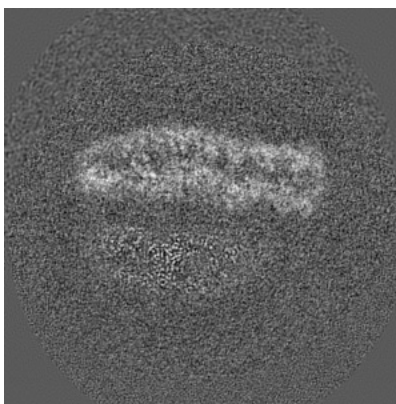
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

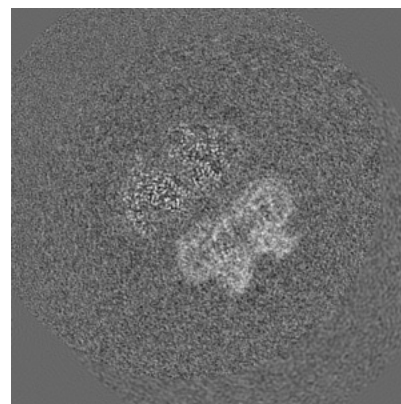
6.3.1 Primary map



X Index: 232



Y Index: 233

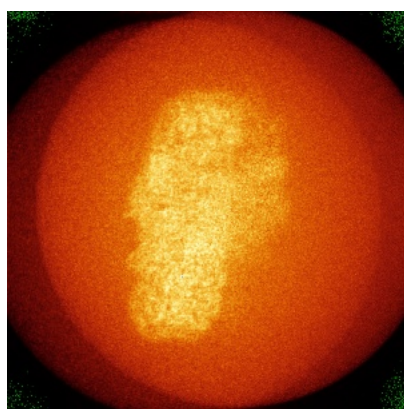


Z Index: 236

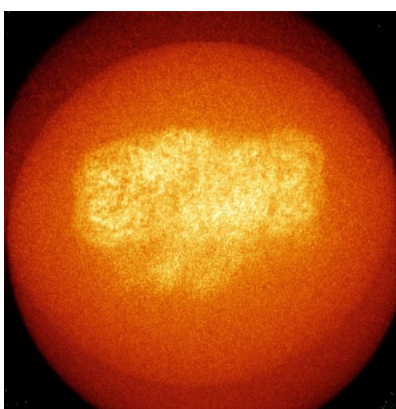
The images above show the largest variance slices of the map in three orthogonal directions.

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

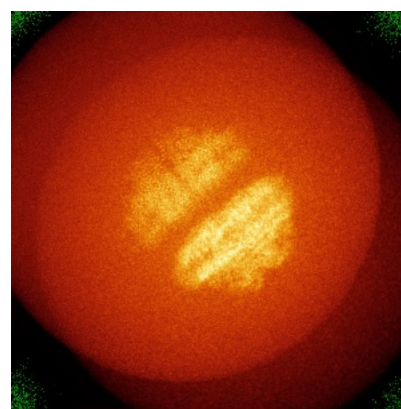
6.4.1 Primary map



X



Y

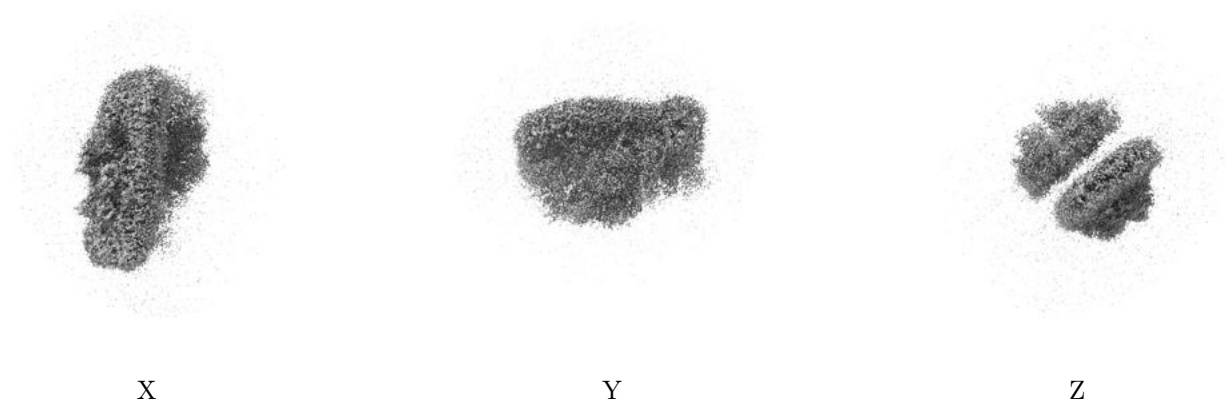


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

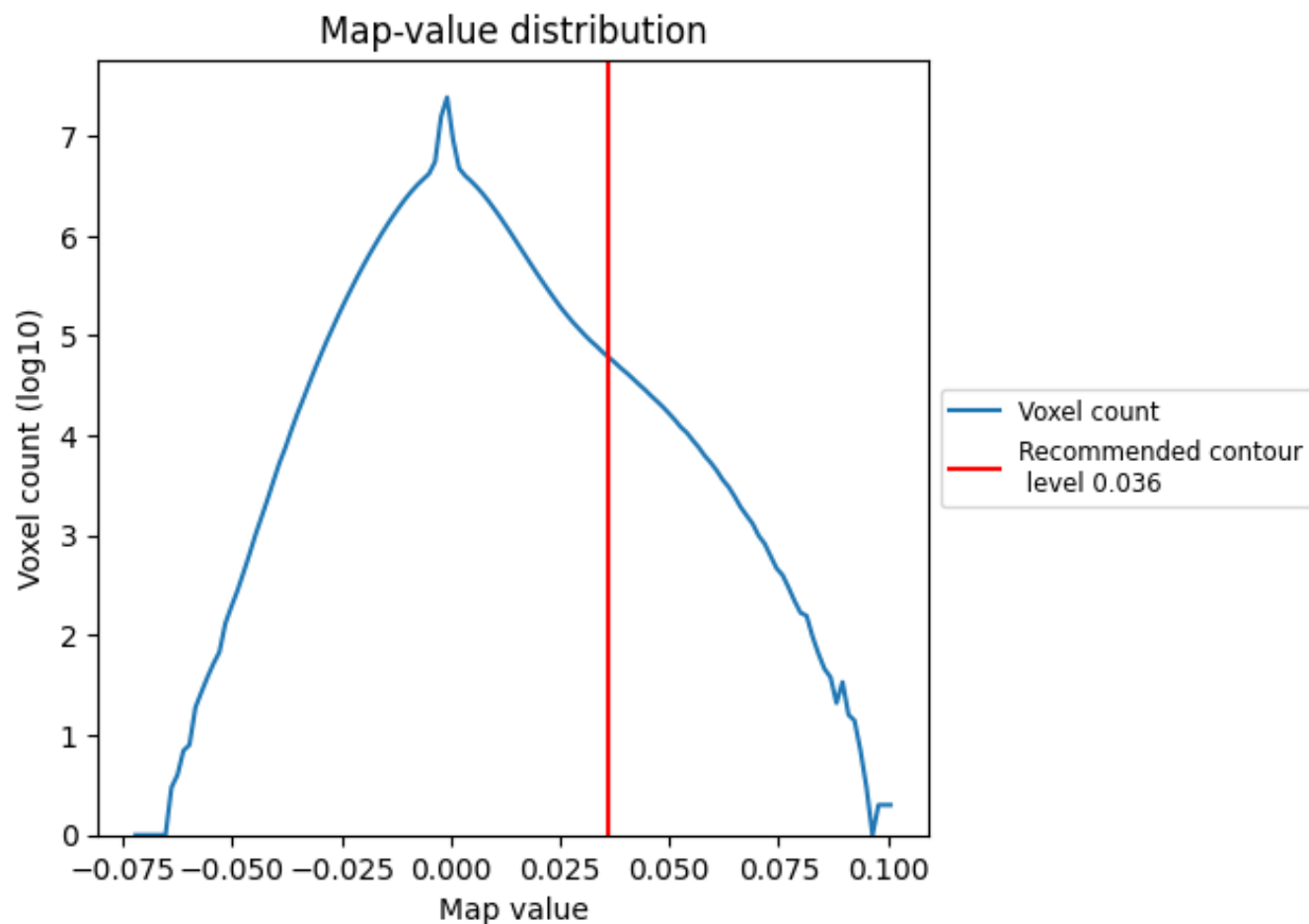
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

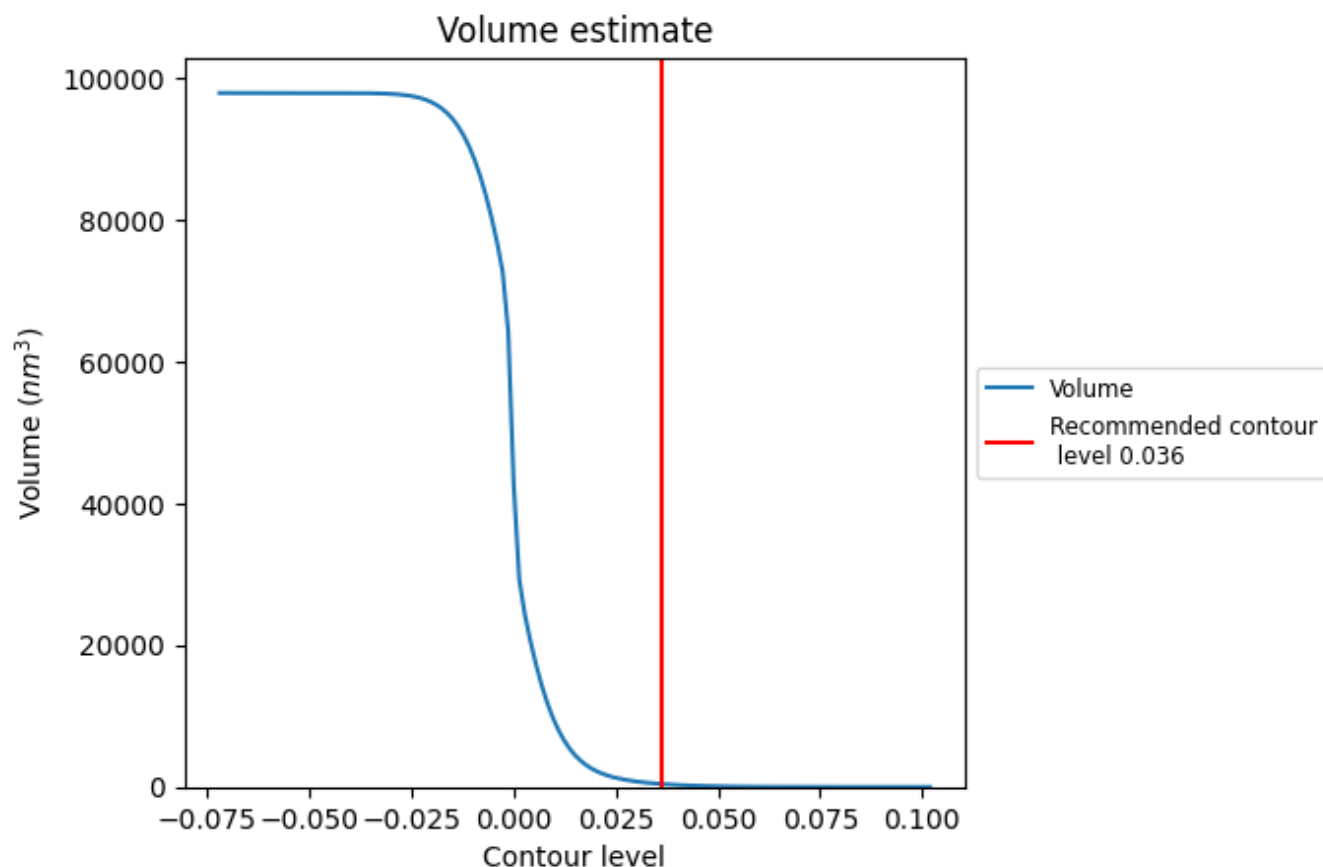
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

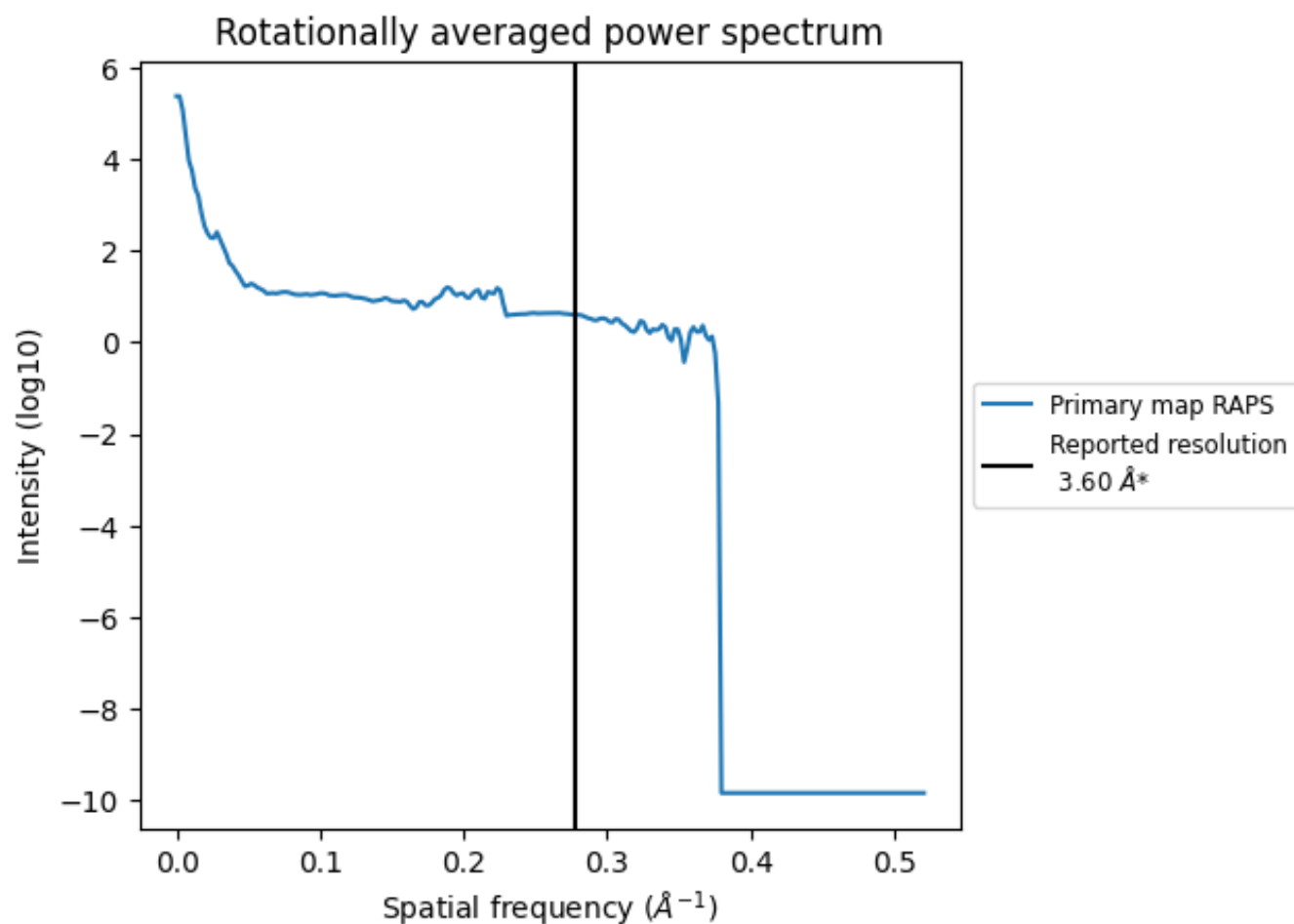
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm³; this corresponds to an approximate mass of 387 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 ⓘ

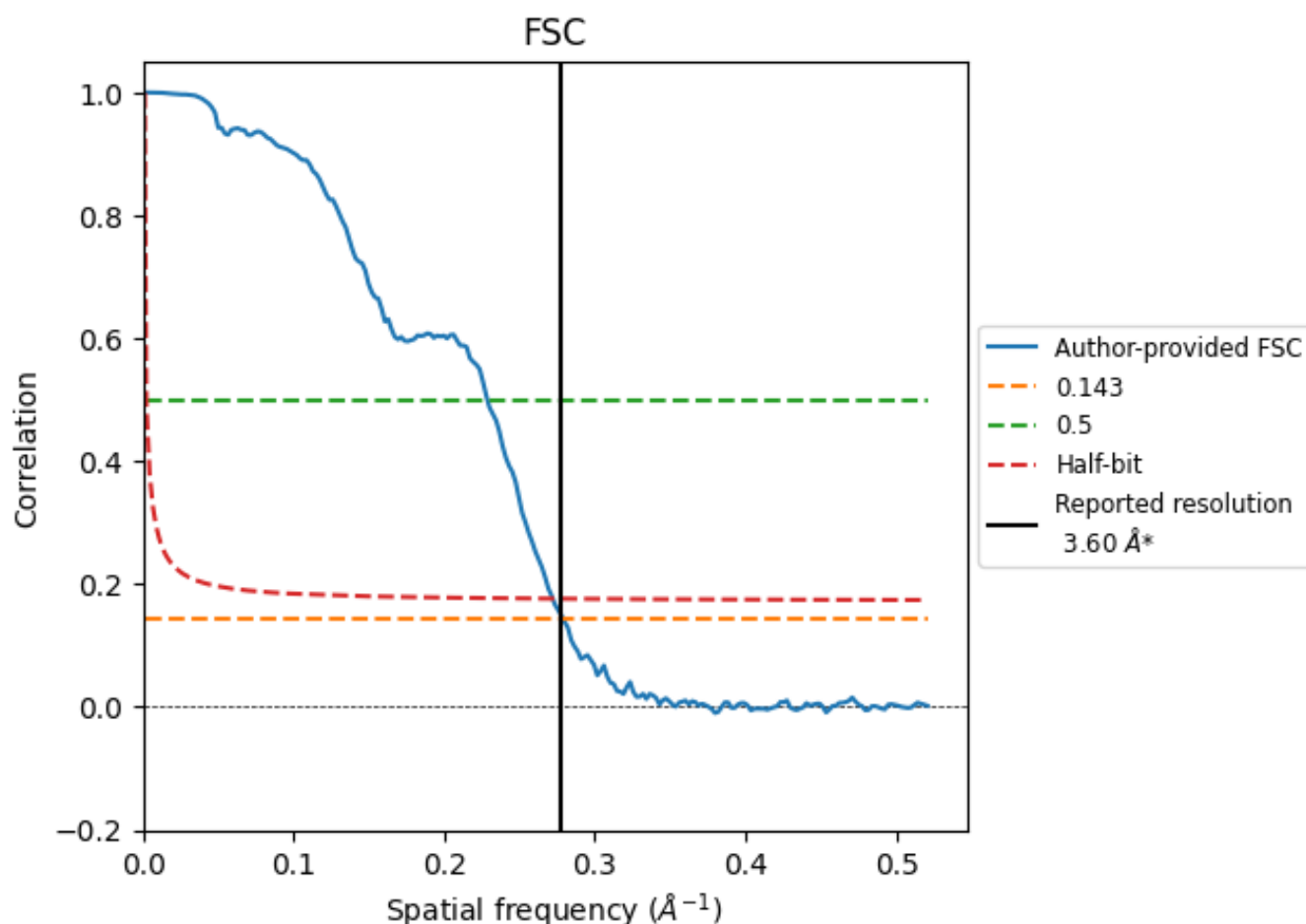


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

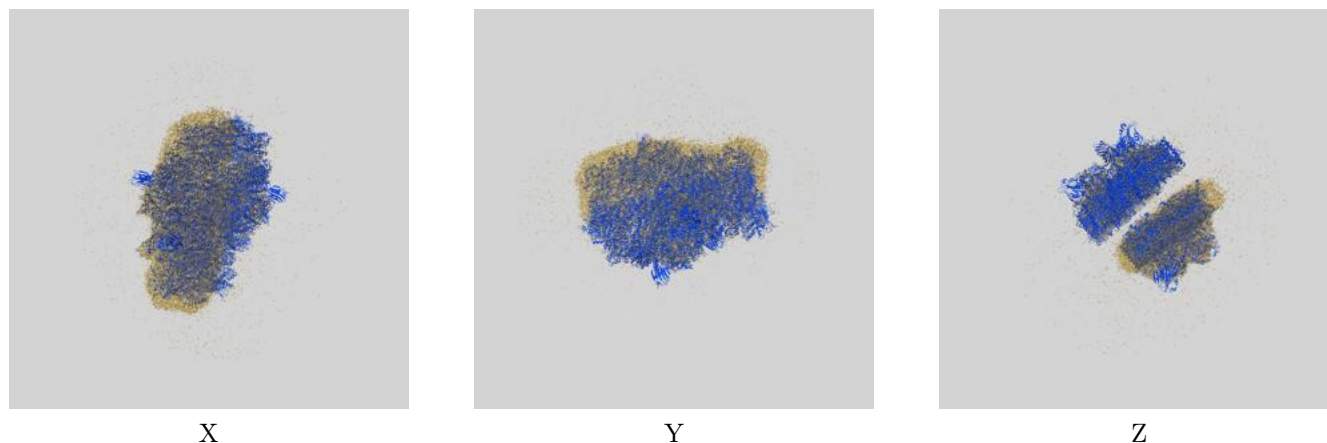
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.37	3.68
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

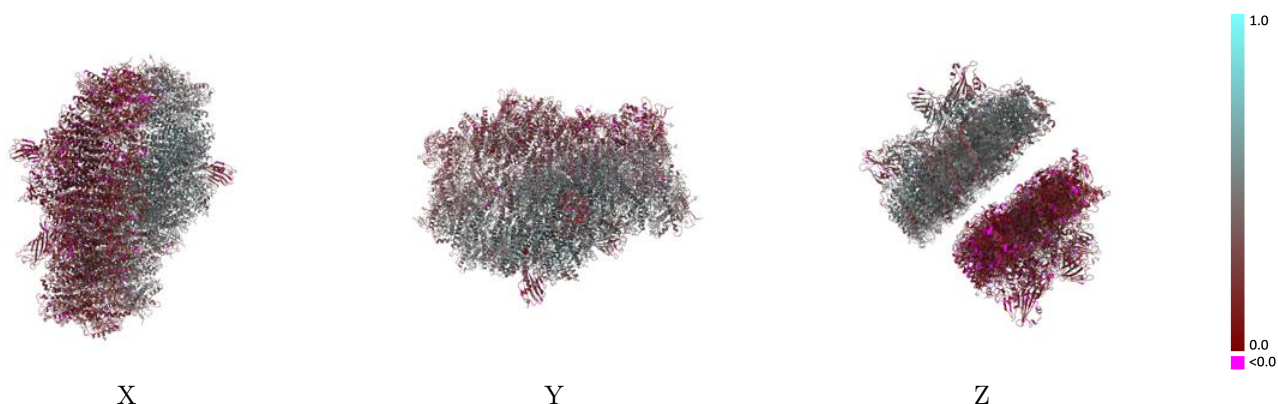
This section contains information regarding the fit between EMDB map EMD-13444 and PDB model 7PIN. Per-residue inclusion information can be found in section [3](#) on page [73](#).

9.1 Map-model overlay [i](#)



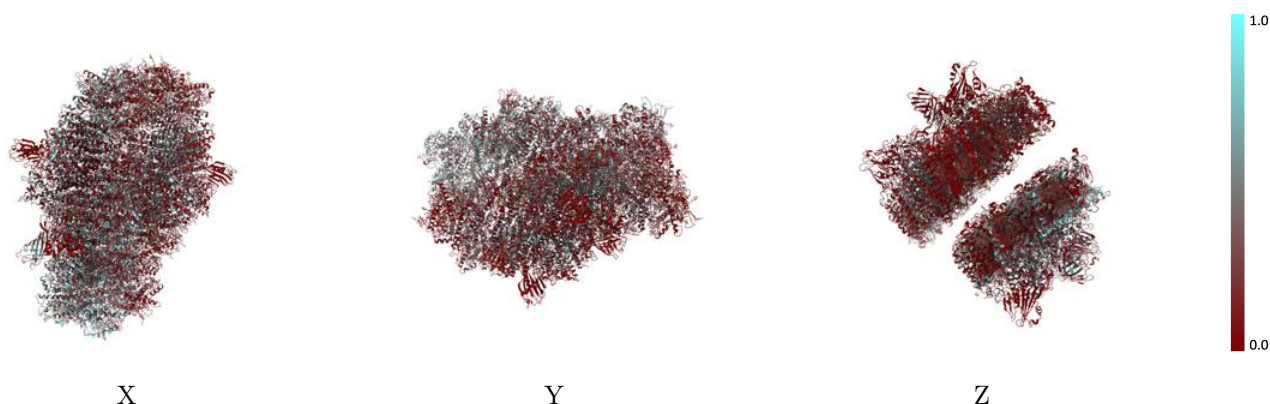
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



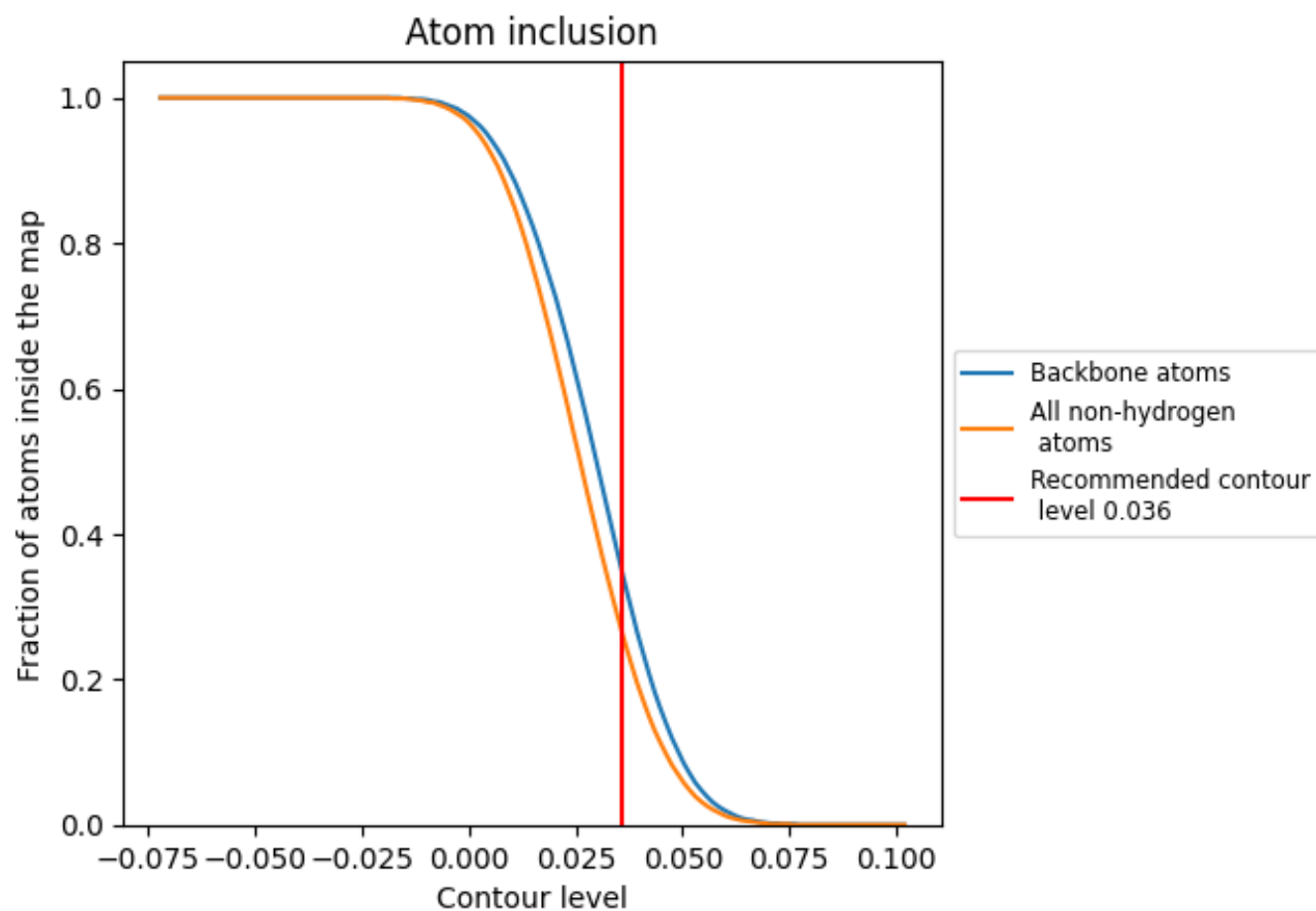
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 26% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2620	 0.3280
A	 0.3530	 0.5260
A1	 0.3490	 0.2350
B	 0.2800	 0.5100
B1	 0.2940	 0.2060
C	 0.3490	 0.5370
C1	 0.4040	 0.2440
D	 0.3190	 0.5320
D1	 0.3360	 0.2300
E	 0.1680	 0.4510
E1	 0.3960	 0.2140
F	 0.2270	 0.4540
F1	 0.3850	 0.1930
G	 0.1010	 0.4070
G1	 0.4160	 0.1980
H	 0.2160	 0.4790
H1	 0.2710	 0.1950
I	 0.2710	 0.4970
I1	 0.2800	 0.2390
J	 0.1660	 0.4880
J1	 0.2520	 0.1960
K	 0.2340	 0.4820
K1	 0.3910	 0.2320
L	 0.2820	 0.5100
L1	 0.2230	 0.2170
M	 0.1850	 0.4500
M1	 0.1740	 0.2160
N	 0.1410	 0.4480
N1	 0.4420	 0.2080
O	 0.1150	 0.4130
O1	 0.3020	 0.2040
P	 0.0010	 0.2320
P1	 0.0250	 0.1680
R	 0.0980	 0.3800
R1	 0.2380	 0.1720



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Chain	Atom inclusion	Q-score
S	 0.1780	 0.4500
S1	 0.4390	 0.2170
T	 0.1700	 0.4490
T1	 0.1940	 0.2630
U	 0.0830	 0.3800
U1	 0.2200	 0.2430
V	 0.1470	 0.4630
V1	 0.2800	 0.2330
W	 0.1420	 0.4380
W1	 0.2650	 0.2450
X	 0.1290	 0.3870
X1	 0.3880	 0.2580
Y	 0.2290	 0.4840
Y1	 0.4010	 0.2140
Z	 0.1710	 0.4810
Z1	 0.3890	 0.2370
a	 0.3670	 0.5310
a1	 0.2620	 0.1770
b	 0.2920	 0.5100
b1	 0.2540	 0.1730
c	 0.3480	 0.5280
c1	 0.2840	 0.1760
d	 0.3360	 0.5210
d1	 0.2310	 0.1470
e	 0.1580	 0.4380
e1	 0.2260	 0.1560
f	 0.1640	 0.4470
f1	 0.2730	 0.1240
g	 0.0990	 0.3840
g1	 0.3060	 0.1490
h	 0.2150	 0.4800
h1	 0.1890	 0.1490
i	 0.2940	 0.4960
i1	 0.2430	 0.2320
j	 0.2100	 0.4710
j1	 0.2070	 0.1650
k	 0.2460	 0.4880
k1	 0.2370	 0.1790
l	 0.2790	 0.5200
m	 0.1820	 0.4480
m1	 0.2000	 0.2000
n	 0.1580	 0.4320

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Chain	Atom inclusion	Q-score
n1	 0.3230	 0.1490
o	 0.1070	 0.4000
o1	 0.2650	 0.2040
p	 0.0010	 0.2150
p1	 0.0250	 0.1470
r	 0.0910	 0.3850
r1	 0.2370	 0.1650
s	 0.1790	 0.4480
s1	 0.2430	 0.1250
t	 0.2150	 0.4900
t1	 0.1700	 0.2200
u	 0.0370	 0.3030
u1	 0.1280	 0.1660
v	 0.1690	 0.4370
v1	 0.1470	 0.1550
w	 0.1640	 0.4320
w1	 0.2460	 0.2170
x	 0.0850	 0.3690
x1	 0.2090	 0.1910
y	 0.2250	 0.4760
y1	 0.2950	 0.1590
z	 0.1690	 0.4790
z1	 0.1960	 0.1480