



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:52 AM UTC

PDB ID : 7QCO / pdb\_00007qco  
EMDB ID : EMD-13898  
Title : The structure of Photosystem I tetramer from *Chroococcidiopsis* TS-821, a thermophilic, unicellular, non-heterocyst-forming cyanobacterium  
Authors : Semchonok, D.A.; Mondal, J.; Cooper, J.C.; Schlum, K.; Li, M.; Amin, M.; Sorzano, C.O.S.; Ramirez-Aportela, E.; Kastiris, P.L.; Boekema, E.J.; Guskov, A.; Bruce, B.D.  
Deposited on : 2021-11-24  
Resolution : 3.70 Å(reported)  
Based on initial model : 1JB0

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

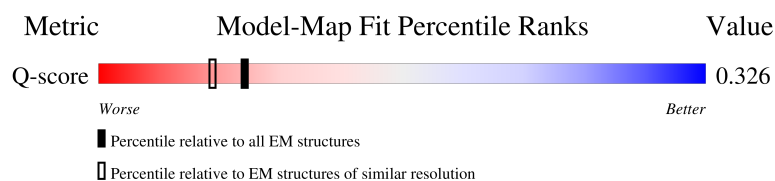
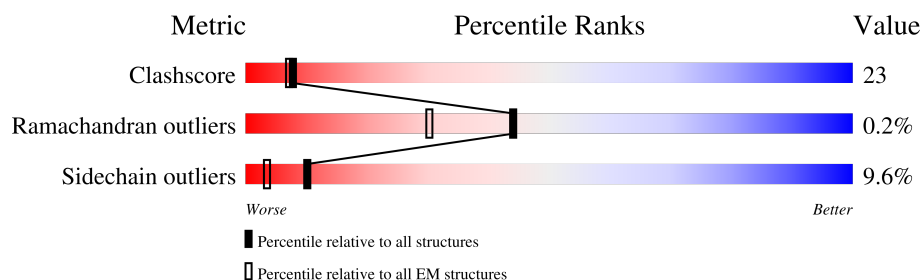
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11569 ( 3.20 - 4.20 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 752    |                  |
| 1   | E     | 752    |                  |
| 1   | a     | 752    |                  |

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Validation Pipeline (wwPDB-VP) : 2.49

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | e     | 752    |                  |
| 2   | B     | 737    |                  |
| 2   | G     | 737    |                  |
| 2   | b     | 737    |                  |
| 2   | g     | 737    |                  |
| 3   | C     | 82     |                  |
| 3   | H     | 82     |                  |
| 3   | c     | 82     |                  |
| 3   | h     | 82     |                  |
| 4   | D     | 168    |                  |
| 4   | N     | 168    |                  |
| 4   | d     | 168    |                  |
| 4   | n     | 168    |                  |
| 5   | V     | 126    |                  |
| 5   | W     | 126    |                  |
| 5   | v     | 126    |                  |
| 5   | w     | 126    |                  |
| 6   | F     | 164    |                  |
| 6   | O     | 164    |                  |
| 6   | f     | 164    |                  |
| 6   | o     | 164    |                  |
| 7   | I     | 39     |                  |
| 7   | P     | 39     |                  |
| 7   | i     | 39     |                  |
| 7   | p     | 39     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8   | J     | 49     |                  |
| 8   | Q     | 49     |                  |
| 8   | j     | 49     |                  |
| 8   | q     | 49     |                  |
| 9   | K     | 93     |                  |
| 9   | R     | 93     |                  |
| 9   | k     | 93     |                  |
| 9   | r     | 93     |                  |
| 10  | L     | 172    |                  |
| 10  | S     | 172    |                  |
| 10  | l     | 172    |                  |
| 10  | s     | 172    |                  |
| 11  | M     | 31     |                  |
| 11  | T     | 31     |                  |
| 11  | m     | 31     |                  |
| 11  | t     | 31     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | A     | 803 | X         | -        | -       | -                |
| 13  | CLA  | A     | 804 | X         | -        | -       | -                |
| 13  | CLA  | A     | 805 | X         | -        | -       | -                |
| 13  | CLA  | A     | 806 | X         | -        | -       | -                |
| 13  | CLA  | A     | 807 | X         | -        | -       | -                |
| 13  | CLA  | A     | 808 | X         | -        | -       | -                |
| 13  | CLA  | A     | 809 | X         | -        | -       | -                |
| 13  | CLA  | A     | 810 | X         | -        | -       | -                |
| 13  | CLA  | A     | 811 | X         | -        | -       | -                |
| 13  | CLA  | A     | 812 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | A     | 813 | X         | -        | -       | -                |
| 13  | CLA  | A     | 814 | X         | -        | -       | -                |
| 13  | CLA  | A     | 815 | X         | -        | -       | -                |
| 13  | CLA  | A     | 816 | X         | -        | -       | -                |
| 13  | CLA  | A     | 817 | X         | -        | -       | -                |
| 13  | CLA  | A     | 818 | X         | -        | -       | -                |
| 13  | CLA  | A     | 819 | X         | -        | -       | -                |
| 13  | CLA  | A     | 820 | X         | -        | -       | -                |
| 13  | CLA  | A     | 821 | X         | -        | -       | -                |
| 13  | CLA  | A     | 822 | X         | -        | -       | -                |
| 13  | CLA  | A     | 823 | X         | -        | -       | -                |
| 13  | CLA  | A     | 824 | X         | -        | -       | -                |
| 13  | CLA  | A     | 825 | X         | -        | -       | -                |
| 13  | CLA  | A     | 826 | X         | -        | -       | -                |
| 13  | CLA  | A     | 827 | X         | -        | -       | -                |
| 13  | CLA  | A     | 828 | X         | -        | -       | -                |
| 13  | CLA  | A     | 829 | X         | -        | -       | -                |
| 13  | CLA  | A     | 830 | X         | -        | -       | -                |
| 13  | CLA  | A     | 831 | X         | -        | -       | -                |
| 13  | CLA  | A     | 832 | X         | -        | -       | -                |
| 13  | CLA  | A     | 833 | X         | -        | -       | -                |
| 13  | CLA  | A     | 834 | X         | -        | -       | -                |
| 13  | CLA  | A     | 835 | X         | -        | -       | -                |
| 13  | CLA  | A     | 836 | X         | -        | -       | -                |
| 13  | CLA  | A     | 838 | X         | -        | -       | -                |
| 13  | CLA  | A     | 839 | X         | -        | -       | -                |
| 13  | CLA  | A     | 840 | X         | -        | -       | -                |
| 13  | CLA  | A     | 841 | X         | -        | -       | -                |
| 13  | CLA  | A     | 842 | X         | -        | -       | -                |
| 13  | CLA  | A     | 843 | X         | -        | -       | -                |
| 13  | CLA  | A     | 844 | X         | -        | -       | -                |
| 13  | CLA  | A     | 845 | X         | -        | -       | -                |
| 13  | CLA  | A     | 853 | X         | -        | -       | -                |
| 13  | CLA  | B     | 801 | X         | -        | -       | -                |
| 13  | CLA  | B     | 802 | X         | -        | -       | -                |
| 13  | CLA  | B     | 804 | X         | -        | -       | -                |
| 13  | CLA  | B     | 805 | X         | -        | -       | -                |
| 13  | CLA  | B     | 806 | X         | -        | -       | -                |
| 13  | CLA  | B     | 807 | X         | -        | -       | -                |
| 13  | CLA  | B     | 808 | X         | -        | -       | -                |
| 13  | CLA  | B     | 809 | X         | -        | -       | -                |
| 13  | CLA  | B     | 810 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | B     | 811 | X         | -        | -       | -                |
| 13  | CLA  | B     | 812 | X         | -        | -       | -                |
| 13  | CLA  | B     | 813 | X         | -        | -       | -                |
| 13  | CLA  | B     | 814 | X         | -        | -       | -                |
| 13  | CLA  | B     | 815 | X         | -        | -       | -                |
| 13  | CLA  | B     | 816 | X         | -        | -       | -                |
| 13  | CLA  | B     | 817 | X         | -        | -       | -                |
| 13  | CLA  | B     | 818 | X         | -        | -       | -                |
| 13  | CLA  | B     | 819 | X         | -        | -       | -                |
| 13  | CLA  | B     | 820 | X         | -        | -       | -                |
| 13  | CLA  | B     | 821 | X         | -        | -       | -                |
| 13  | CLA  | B     | 822 | X         | -        | -       | -                |
| 13  | CLA  | B     | 823 | X         | -        | -       | -                |
| 13  | CLA  | B     | 824 | X         | -        | -       | -                |
| 13  | CLA  | B     | 825 | X         | -        | -       | -                |
| 13  | CLA  | B     | 826 | X         | -        | -       | -                |
| 13  | CLA  | B     | 827 | X         | -        | -       | -                |
| 13  | CLA  | B     | 828 | X         | -        | -       | -                |
| 13  | CLA  | B     | 829 | X         | -        | -       | -                |
| 13  | CLA  | B     | 830 | X         | -        | -       | -                |
| 13  | CLA  | B     | 831 | X         | -        | -       | -                |
| 13  | CLA  | B     | 832 | X         | -        | -       | -                |
| 13  | CLA  | B     | 833 | X         | -        | -       | -                |
| 13  | CLA  | B     | 834 | X         | -        | -       | -                |
| 13  | CLA  | B     | 835 | X         | -        | -       | -                |
| 13  | CLA  | B     | 836 | X         | -        | -       | -                |
| 13  | CLA  | B     | 837 | X         | -        | -       | -                |
| 13  | CLA  | B     | 838 | X         | -        | -       | -                |
| 13  | CLA  | B     | 839 | X         | -        | -       | -                |
| 13  | CLA  | B     | 840 | X         | -        | -       | -                |
| 13  | CLA  | B     | 841 | X         | -        | -       | -                |
| 13  | CLA  | E     | 803 | X         | -        | -       | -                |
| 13  | CLA  | E     | 804 | X         | -        | -       | -                |
| 13  | CLA  | E     | 805 | X         | -        | -       | -                |
| 13  | CLA  | E     | 806 | X         | -        | -       | -                |
| 13  | CLA  | E     | 807 | X         | -        | -       | -                |
| 13  | CLA  | E     | 808 | X         | -        | -       | -                |
| 13  | CLA  | E     | 809 | X         | -        | -       | -                |
| 13  | CLA  | E     | 810 | X         | -        | -       | -                |
| 13  | CLA  | E     | 811 | X         | -        | -       | -                |
| 13  | CLA  | E     | 812 | X         | -        | -       | -                |
| 13  | CLA  | E     | 813 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | E     | 814 | X         | -        | -       | -                |
| 13  | CLA  | E     | 815 | X         | -        | -       | -                |
| 13  | CLA  | E     | 816 | X         | -        | -       | -                |
| 13  | CLA  | E     | 817 | X         | -        | -       | -                |
| 13  | CLA  | E     | 818 | X         | -        | -       | -                |
| 13  | CLA  | E     | 819 | X         | -        | -       | -                |
| 13  | CLA  | E     | 820 | X         | -        | -       | -                |
| 13  | CLA  | E     | 821 | X         | -        | -       | -                |
| 13  | CLA  | E     | 822 | X         | -        | -       | -                |
| 13  | CLA  | E     | 823 | X         | -        | -       | -                |
| 13  | CLA  | E     | 824 | X         | -        | -       | -                |
| 13  | CLA  | E     | 825 | X         | -        | -       | -                |
| 13  | CLA  | E     | 826 | X         | -        | -       | -                |
| 13  | CLA  | E     | 827 | X         | -        | -       | -                |
| 13  | CLA  | E     | 828 | X         | -        | -       | -                |
| 13  | CLA  | E     | 829 | X         | -        | -       | -                |
| 13  | CLA  | E     | 830 | X         | -        | -       | -                |
| 13  | CLA  | E     | 831 | X         | -        | -       | -                |
| 13  | CLA  | E     | 832 | X         | -        | -       | -                |
| 13  | CLA  | E     | 833 | X         | -        | -       | -                |
| 13  | CLA  | E     | 834 | X         | -        | -       | -                |
| 13  | CLA  | E     | 835 | X         | -        | -       | -                |
| 13  | CLA  | E     | 836 | X         | -        | -       | -                |
| 13  | CLA  | E     | 837 | X         | -        | -       | -                |
| 13  | CLA  | E     | 839 | X         | -        | -       | -                |
| 13  | CLA  | E     | 840 | X         | -        | -       | -                |
| 13  | CLA  | E     | 841 | X         | -        | -       | -                |
| 13  | CLA  | E     | 842 | X         | -        | -       | -                |
| 13  | CLA  | E     | 843 | X         | -        | -       | -                |
| 13  | CLA  | E     | 844 | X         | -        | -       | -                |
| 13  | CLA  | E     | 845 | X         | -        | -       | -                |
| 13  | CLA  | E     | 846 | X         | -        | -       | -                |
| 13  | CLA  | F     | 202 | X         | -        | -       | -                |
| 13  | CLA  | G     | 801 | X         | -        | -       | -                |
| 13  | CLA  | G     | 802 | X         | -        | -       | -                |
| 13  | CLA  | G     | 803 | X         | -        | -       | -                |
| 13  | CLA  | G     | 804 | X         | -        | -       | -                |
| 13  | CLA  | G     | 805 | X         | -        | -       | -                |
| 13  | CLA  | G     | 806 | X         | -        | -       | -                |
| 13  | CLA  | G     | 807 | X         | -        | -       | -                |
| 13  | CLA  | G     | 808 | X         | -        | -       | -                |
| 13  | CLA  | G     | 809 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | G     | 810 | X         | -        | -       | -                |
| 13  | CLA  | G     | 811 | X         | -        | -       | -                |
| 13  | CLA  | G     | 812 | X         | -        | -       | -                |
| 13  | CLA  | G     | 813 | X         | -        | -       | -                |
| 13  | CLA  | G     | 814 | X         | -        | -       | -                |
| 13  | CLA  | G     | 815 | X         | -        | -       | -                |
| 13  | CLA  | G     | 816 | X         | -        | -       | -                |
| 13  | CLA  | G     | 817 | X         | -        | -       | -                |
| 13  | CLA  | G     | 818 | X         | -        | -       | -                |
| 13  | CLA  | G     | 819 | X         | -        | -       | -                |
| 13  | CLA  | G     | 820 | X         | -        | -       | -                |
| 13  | CLA  | G     | 821 | X         | -        | -       | -                |
| 13  | CLA  | G     | 822 | X         | -        | -       | -                |
| 13  | CLA  | G     | 823 | X         | -        | -       | -                |
| 13  | CLA  | G     | 824 | X         | -        | -       | -                |
| 13  | CLA  | G     | 825 | X         | -        | -       | -                |
| 13  | CLA  | G     | 826 | X         | -        | -       | -                |
| 13  | CLA  | G     | 827 | X         | -        | -       | -                |
| 13  | CLA  | G     | 828 | X         | -        | -       | -                |
| 13  | CLA  | G     | 829 | X         | -        | -       | -                |
| 13  | CLA  | G     | 830 | X         | -        | -       | -                |
| 13  | CLA  | G     | 831 | X         | -        | -       | -                |
| 13  | CLA  | G     | 832 | X         | -        | -       | -                |
| 13  | CLA  | G     | 833 | X         | -        | -       | -                |
| 13  | CLA  | G     | 834 | X         | -        | -       | -                |
| 13  | CLA  | G     | 835 | X         | -        | -       | -                |
| 13  | CLA  | G     | 836 | X         | -        | -       | -                |
| 13  | CLA  | G     | 837 | X         | -        | -       | -                |
| 13  | CLA  | G     | 838 | X         | -        | -       | -                |
| 13  | CLA  | G     | 839 | X         | -        | -       | -                |
| 13  | CLA  | G     | 840 | X         | -        | -       | -                |
| 13  | CLA  | G     | 841 | X         | -        | -       | -                |
| 13  | CLA  | K     | 101 | X         | -        | -       | -                |
| 13  | CLA  | K     | 102 | X         | -        | -       | -                |
| 13  | CLA  | L     | 202 | X         | -        | -       | -                |
| 13  | CLA  | L     | 203 | X         | -        | -       | -                |
| 13  | CLA  | L     | 204 | X         | -        | -       | -                |
| 13  | CLA  | O     | 203 | X         | -        | -       | -                |
| 13  | CLA  | R     | 102 | X         | -        | -       | -                |
| 13  | CLA  | S     | 203 | X         | -        | -       | -                |
| 13  | CLA  | S     | 204 | X         | -        | -       | -                |
| 13  | CLA  | S     | 206 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | a     | 804 | X         | -        | -       | -                |
| 13  | CLA  | a     | 805 | X         | -        | -       | -                |
| 13  | CLA  | a     | 806 | X         | -        | -       | -                |
| 13  | CLA  | a     | 807 | X         | -        | -       | -                |
| 13  | CLA  | a     | 808 | X         | -        | -       | -                |
| 13  | CLA  | a     | 809 | X         | -        | -       | -                |
| 13  | CLA  | a     | 810 | X         | -        | -       | -                |
| 13  | CLA  | a     | 811 | X         | -        | -       | -                |
| 13  | CLA  | a     | 812 | X         | -        | -       | -                |
| 13  | CLA  | a     | 813 | X         | -        | -       | -                |
| 13  | CLA  | a     | 814 | X         | -        | -       | -                |
| 13  | CLA  | a     | 815 | X         | -        | -       | -                |
| 13  | CLA  | a     | 816 | X         | -        | -       | -                |
| 13  | CLA  | a     | 817 | X         | -        | -       | -                |
| 13  | CLA  | a     | 818 | X         | -        | -       | -                |
| 13  | CLA  | a     | 819 | X         | -        | -       | -                |
| 13  | CLA  | a     | 820 | X         | -        | -       | -                |
| 13  | CLA  | a     | 821 | X         | -        | -       | -                |
| 13  | CLA  | a     | 822 | X         | -        | -       | -                |
| 13  | CLA  | a     | 823 | X         | -        | -       | -                |
| 13  | CLA  | a     | 824 | X         | -        | -       | -                |
| 13  | CLA  | a     | 825 | X         | -        | -       | -                |
| 13  | CLA  | a     | 826 | X         | -        | -       | -                |
| 13  | CLA  | a     | 827 | X         | -        | -       | -                |
| 13  | CLA  | a     | 828 | X         | -        | -       | -                |
| 13  | CLA  | a     | 829 | X         | -        | -       | -                |
| 13  | CLA  | a     | 830 | X         | -        | -       | -                |
| 13  | CLA  | a     | 831 | X         | -        | -       | -                |
| 13  | CLA  | a     | 832 | X         | -        | -       | -                |
| 13  | CLA  | a     | 833 | X         | -        | -       | -                |
| 13  | CLA  | a     | 834 | X         | -        | -       | -                |
| 13  | CLA  | a     | 835 | X         | -        | -       | -                |
| 13  | CLA  | a     | 836 | X         | -        | -       | -                |
| 13  | CLA  | a     | 837 | X         | -        | -       | -                |
| 13  | CLA  | a     | 839 | X         | -        | -       | -                |
| 13  | CLA  | a     | 840 | X         | -        | -       | -                |
| 13  | CLA  | a     | 841 | X         | -        | -       | -                |
| 13  | CLA  | a     | 842 | X         | -        | -       | -                |
| 13  | CLA  | a     | 843 | X         | -        | -       | -                |
| 13  | CLA  | a     | 844 | X         | -        | -       | -                |
| 13  | CLA  | a     | 845 | X         | -        | -       | -                |
| 13  | CLA  | a     | 852 | X         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | b     | 801 | X         | -        | -       | -                |
| 13  | CLA  | b     | 802 | X         | -        | -       | -                |
| 13  | CLA  | b     | 803 | X         | -        | -       | -                |
| 13  | CLA  | b     | 804 | X         | -        | -       | -                |
| 13  | CLA  | b     | 805 | X         | -        | -       | -                |
| 13  | CLA  | b     | 806 | X         | -        | -       | -                |
| 13  | CLA  | b     | 807 | X         | -        | -       | -                |
| 13  | CLA  | b     | 808 | X         | -        | -       | -                |
| 13  | CLA  | b     | 809 | X         | -        | -       | -                |
| 13  | CLA  | b     | 810 | X         | -        | -       | -                |
| 13  | CLA  | b     | 811 | X         | -        | -       | -                |
| 13  | CLA  | b     | 812 | X         | -        | -       | -                |
| 13  | CLA  | b     | 813 | X         | -        | -       | -                |
| 13  | CLA  | b     | 814 | X         | -        | -       | -                |
| 13  | CLA  | b     | 815 | X         | -        | -       | -                |
| 13  | CLA  | b     | 816 | X         | -        | -       | -                |
| 13  | CLA  | b     | 817 | X         | -        | -       | -                |
| 13  | CLA  | b     | 818 | X         | -        | -       | -                |
| 13  | CLA  | b     | 819 | X         | -        | -       | -                |
| 13  | CLA  | b     | 820 | X         | -        | -       | -                |
| 13  | CLA  | b     | 821 | X         | -        | -       | -                |
| 13  | CLA  | b     | 822 | X         | -        | -       | -                |
| 13  | CLA  | b     | 823 | X         | -        | -       | -                |
| 13  | CLA  | b     | 824 | X         | -        | -       | -                |
| 13  | CLA  | b     | 825 | X         | -        | -       | -                |
| 13  | CLA  | b     | 826 | X         | -        | -       | -                |
| 13  | CLA  | b     | 827 | X         | -        | -       | -                |
| 13  | CLA  | b     | 828 | X         | -        | -       | -                |
| 13  | CLA  | b     | 829 | X         | -        | -       | -                |
| 13  | CLA  | b     | 830 | X         | -        | -       | -                |
| 13  | CLA  | b     | 831 | X         | -        | -       | -                |
| 13  | CLA  | b     | 832 | X         | -        | -       | -                |
| 13  | CLA  | b     | 833 | X         | -        | -       | -                |
| 13  | CLA  | b     | 834 | X         | -        | -       | -                |
| 13  | CLA  | b     | 835 | X         | -        | -       | -                |
| 13  | CLA  | b     | 836 | X         | -        | -       | -                |
| 13  | CLA  | b     | 837 | X         | -        | -       | -                |
| 13  | CLA  | b     | 838 | X         | -        | -       | -                |
| 13  | CLA  | b     | 839 | X         | -        | -       | -                |
| 13  | CLA  | b     | 840 | X         | -        | -       | -                |
| 13  | CLA  | e     | 803 | X         | -        | -       | -                |
| 13  | CLA  | e     | 804 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CLA  | e     | 805 | X         | -        | -       | -                |
| 13  | CLA  | e     | 806 | X         | -        | -       | -                |
| 13  | CLA  | e     | 807 | X         | -        | -       | -                |
| 13  | CLA  | e     | 808 | X         | -        | -       | -                |
| 13  | CLA  | e     | 809 | X         | -        | -       | -                |
| 13  | CLA  | e     | 810 | X         | -        | -       | -                |
| 13  | CLA  | e     | 811 | X         | -        | -       | -                |
| 13  | CLA  | e     | 812 | X         | -        | -       | -                |
| 13  | CLA  | e     | 813 | X         | -        | -       | -                |
| 13  | CLA  | e     | 814 | X         | -        | -       | -                |
| 13  | CLA  | e     | 815 | X         | -        | -       | -                |
| 13  | CLA  | e     | 816 | X         | -        | -       | -                |
| 13  | CLA  | e     | 817 | X         | -        | -       | -                |
| 13  | CLA  | e     | 818 | X         | -        | -       | -                |
| 13  | CLA  | e     | 819 | X         | -        | -       | -                |
| 13  | CLA  | e     | 820 | X         | -        | -       | -                |
| 13  | CLA  | e     | 821 | X         | -        | -       | -                |
| 13  | CLA  | e     | 822 | X         | -        | -       | -                |
| 13  | CLA  | e     | 823 | X         | -        | -       | -                |
| 13  | CLA  | e     | 824 | X         | -        | -       | -                |
| 13  | CLA  | e     | 825 | X         | -        | -       | -                |
| 13  | CLA  | e     | 826 | X         | -        | -       | -                |
| 13  | CLA  | e     | 827 | X         | -        | -       | -                |
| 13  | CLA  | e     | 828 | X         | -        | -       | -                |
| 13  | CLA  | e     | 829 | X         | -        | -       | -                |
| 13  | CLA  | e     | 830 | X         | -        | -       | -                |
| 13  | CLA  | e     | 831 | X         | -        | -       | -                |
| 13  | CLA  | e     | 832 | X         | -        | -       | -                |
| 13  | CLA  | e     | 833 | X         | -        | -       | -                |
| 13  | CLA  | e     | 834 | X         | -        | -       | -                |
| 13  | CLA  | e     | 835 | X         | -        | -       | -                |
| 13  | CLA  | e     | 837 | X         | -        | -       | -                |
| 13  | CLA  | e     | 838 | X         | -        | -       | -                |
| 13  | CLA  | e     | 839 | X         | -        | -       | -                |
| 13  | CLA  | e     | 840 | X         | -        | -       | -                |
| 13  | CLA  | e     | 841 | X         | -        | -       | -                |
| 13  | CLA  | e     | 842 | X         | -        | -       | -                |
| 13  | CLA  | e     | 843 | X         | -        | -       | -                |
| 13  | CLA  | e     | 844 | X         | -        | -       | -                |
| 13  | CLA  | e     | 852 | X         | -        | -       | -                |
| 13  | CLA  | f     | 203 | X         | -        | -       | -                |
| 13  | CLA  | g     | 801 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 13  | CLA  | g     | 802  | X         | -        | -       | -                |
| 13  | CLA  | g     | 803  | X         | -        | -       | -                |
| 13  | CLA  | g     | 805  | X         | -        | -       | -                |
| 13  | CLA  | g     | 806  | X         | -        | -       | -                |
| 13  | CLA  | g     | 807  | X         | -        | -       | -                |
| 13  | CLA  | g     | 808  | X         | -        | -       | -                |
| 13  | CLA  | g     | 809  | X         | -        | -       | -                |
| 13  | CLA  | g     | 810  | X         | -        | -       | -                |
| 13  | CLA  | g     | 811  | X         | -        | -       | -                |
| 13  | CLA  | g     | 812  | X         | -        | -       | -                |
| 13  | CLA  | g     | 813  | X         | -        | -       | -                |
| 13  | CLA  | g     | 814  | X         | -        | -       | -                |
| 13  | CLA  | g     | 815  | X         | -        | -       | -                |
| 13  | CLA  | g     | 816  | X         | -        | -       | -                |
| 13  | CLA  | g     | 817  | X         | -        | -       | -                |
| 13  | CLA  | g     | 818  | X         | -        | -       | -                |
| 13  | CLA  | g     | 819  | X         | -        | -       | -                |
| 13  | CLA  | g     | 820  | X         | -        | -       | -                |
| 13  | CLA  | g     | 821  | X         | -        | -       | -                |
| 13  | CLA  | g     | 822  | X         | -        | -       | -                |
| 13  | CLA  | g     | 823  | X         | -        | -       | -                |
| 13  | CLA  | g     | 824  | X         | -        | -       | -                |
| 13  | CLA  | g     | 825  | X         | -        | -       | -                |
| 13  | CLA  | g     | 826  | X         | -        | -       | -                |
| 13  | CLA  | g     | 827  | X         | -        | -       | -                |
| 13  | CLA  | g     | 828  | X         | -        | -       | -                |
| 13  | CLA  | g     | 829  | X         | -        | -       | -                |
| 13  | CLA  | g     | 830  | X         | -        | -       | -                |
| 13  | CLA  | g     | 831  | X         | -        | -       | -                |
| 13  | CLA  | g     | 832  | X         | -        | -       | -                |
| 13  | CLA  | g     | 833  | X         | -        | -       | -                |
| 13  | CLA  | g     | 834  | X         | -        | -       | -                |
| 13  | CLA  | g     | 835  | X         | -        | -       | -                |
| 13  | CLA  | g     | 836  | X         | -        | -       | -                |
| 13  | CLA  | g     | 837  | X         | -        | -       | -                |
| 13  | CLA  | g     | 838  | X         | -        | -       | -                |
| 13  | CLA  | g     | 839  | X         | -        | -       | -                |
| 13  | CLA  | g     | 840  | X         | -        | -       | -                |
| 13  | CLA  | g     | 841  | X         | -        | -       | -                |
| 13  | CLA  | g     | 842  | X         | -        | -       | -                |
| 13  | CLA  | k     | 4002 | X         | -        | -       | -                |
| 13  | CLA  | l     | 201  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 13  | CLA  | l     | 203  | X         | -        | -       | -                |
| 13  | CLA  | l     | 204  | X         | -        | -       | -                |
| 13  | CLA  | l     | 205  | X         | -        | -       | -                |
| 13  | CLA  | o     | 202  | X         | -        | -       | -                |
| 13  | CLA  | r     | 101  | X         | -        | -       | -                |
| 13  | CLA  | r     | 102  | X         | -        | -       | -                |
| 13  | CLA  | s     | 202  | X         | -        | -       | -                |
| 13  | CLA  | s     | 203  | X         | -        | -       | -                |
| 13  | CLA  | s     | 205  | X         | -        | -       | -                |
| 15  | BCR  | E     | 849  | -         | -        | X       | -                |
| 15  | BCR  | R     | 101  | -         | -        | X       | -                |
| 15  | BCR  | a     | 848  | -         | -        | X       | -                |
| 15  | BCR  | a     | 849  | -         | -        | X       | -                |
| 15  | BCR  | k     | 4001 | -         | -        | X       | -                |
| 16  | SF4  | C     | 101  | -         | -        | X       | -                |
| 16  | SF4  | C     | 102  | -         | -        | X       | -                |
| 16  | SF4  | H     | 101  | -         | -        | X       | -                |
| 16  | SF4  | H     | 102  | -         | -        | X       | -                |
| 16  | SF4  | c     | 101  | -         | -        | X       | -                |
| 16  | SF4  | c     | 102  | -         | -        | X       | -                |
| 16  | SF4  | h     | 101  | -         | -        | X       | -                |
| 16  | SF4  | h     | 102  | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 90396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 728      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5713  | 3744 | 976 | 968 | 25 |         |       |
| 1   | E     | 728      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5713  | 3744 | 976 | 968 | 25 |         |       |
| 1   | e     | 728      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5713  | 3744 | 976 | 968 | 25 |         |       |
| 1   | a     | 728      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5713  | 3744 | 976 | 968 | 25 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 734      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5857  | 3861 | 984 | 996 | 16 |         |       |
| 2   | G     | 734      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5857  | 3861 | 984 | 996 | 16 |         |       |
| 2   | g     | 734      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5857  | 3861 | 984 | 996 | 16 |         |       |
| 2   | b     | 734      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5857  | 3861 | 984 | 996 | 16 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 81       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 605   | 370 | 105 | 119 | 11 |         |       |
| 3   | H     | 81       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 605   | 370 | 105 | 119 | 11 |         |       |
| 3   | h     | 81       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 605   | 370 | 105 | 119 | 11 |         |       |
| 3   | c     | 81       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 605   | 370 | 105 | 119 | 11 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 689 | 189 | 198 | 4 |         |       |
| 4   | N     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 680 | 187 | 195 | 4 |         |       |
| 4   | n     | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 689 | 189 | 198 | 4 |         |       |
| 4   | d     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 680 | 187 | 195 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | V     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 494   | 315 | 86 | 93 |         |       |
| 5   | W     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 494   | 315 | 86 | 93 |         |       |
| 5   | v     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 494   | 315 | 86 | 93 |         |       |
| 5   | w     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 494   | 315 | 86 | 93 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1093  | 700 | 188 | 202 | 3 |         |       |
| 6   | O     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1093  | 700 | 188 | 202 | 3 |         |       |
| 6   | o     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1093  | 700 | 188 | 202 | 3 |         |       |
| 6   | f     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1093  | 700 | 188 | 202 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | I     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 295   | 199 | 42 | 52 | 2 |         |       |
| 7   | P     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 295   | 199 | 42 | 52 | 2 |         |       |
| 7   | p     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 295   | 199 | 42 | 52 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | i     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 295   | 199 | 42 | 52 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 8   | J     | 37       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 311   | 218 | 44 | 49 |  |         |       |
| 8   | Q     | 37       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 311   | 218 | 44 | 49 |  |         |       |
| 8   | q     | 37       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 311   | 218 | 44 | 49 |  |         |       |
| 8   | j     | 37       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 311   | 218 | 44 | 49 |  |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | K     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 474   | 316 | 80 | 77 | 1 |         |       |
| 9   | R     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 474   | 316 | 80 | 77 | 1 |         |       |
| 9   | r     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 474   | 316 | 80 | 77 | 1 |         |       |
| 9   | k     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 474   | 316 | 80 | 77 | 1 |         |       |

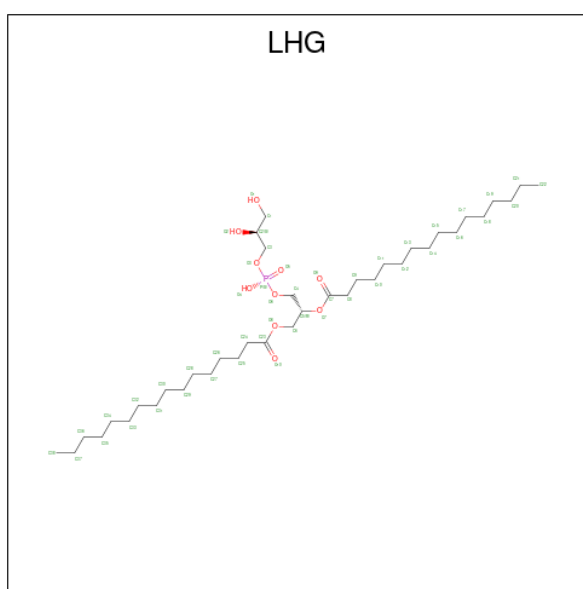
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | L     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 738 | 189 | 205 | 2 |         |       |
| 10  | S     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 738 | 189 | 205 | 2 |         |       |
| 10  | s     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 738 | 189 | 205 | 2 |         |       |
| 10  | l     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 738 | 189 | 205 | 2 |         |       |

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

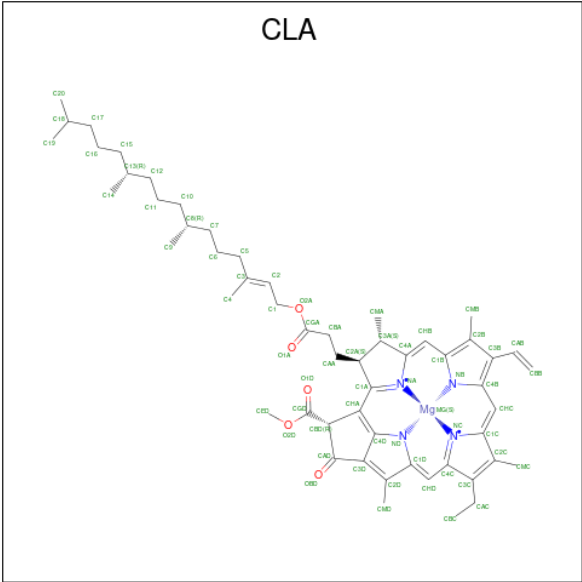
| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | M     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 238   | 159 | 36 | 42 | 1 |         |       |
| 11  | T     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 238   | 159 | 36 | 42 | 1 |         |       |
| 11  | t     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 238   | 159 | 36 | 42 | 1 |         |       |
| 11  | m     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 238   | 159 | 36 | 42 | 1 |         |       |

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 12  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 12  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 12  | e     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 12  | e     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 12  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | K     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 13  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | L     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | L     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | E     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | E     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | E     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | E     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | E     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | E     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | E     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | E     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 13  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | O     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | R     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | e     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | e     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | e     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | o     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | r     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | r     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | s     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | s     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | a     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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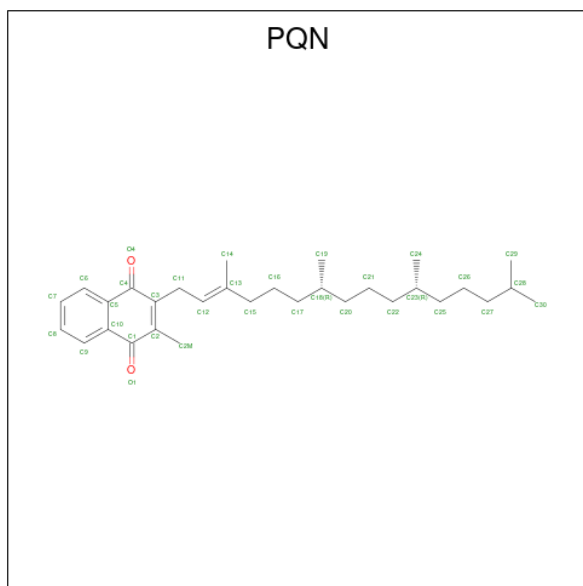
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 13  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 13  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 13  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 13  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



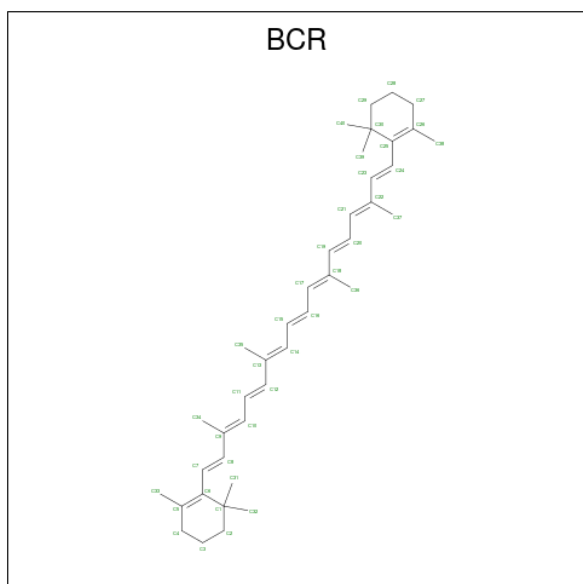
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 14  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 14  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 14  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 14  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 14  | e     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 14  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 14  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 14  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 15  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 15  | A     | 1        | Total C<br>40 40 | 0       |
| 15  | B     | 1        | Total C<br>40 40 | 0       |
| 15  | B     | 1        | Total C<br>40 40 | 0       |
| 15  | B     | 1        | Total C<br>40 40 | 0       |
| 15  | B     | 1        | Total C<br>40 40 | 0       |
| 15  | B     | 1        | Total C<br>40 40 | 0       |
| 15  | B     | 1        | Total C<br>40 40 | 0       |
| 15  | F     | 1        | Total C<br>40 40 | 0       |
| 15  | I     | 1        | Total C<br>40 40 | 0       |
| 15  | J     | 1        | Total C<br>40 40 | 0       |
| 15  | J     | 1        | Total C<br>40 40 | 0       |
| 15  | L     | 1        | Total C<br>40 40 | 0       |
| 15  | L     | 1        | Total C<br>40 40 | 0       |
| 15  | E     | 1        | Total C<br>40 40 | 0       |
| 15  | E     | 1        | Total C<br>40 40 | 0       |
| 15  | E     | 1        | Total C<br>40 40 | 0       |
| 15  | E     | 1        | Total C<br>40 40 | 0       |
| 15  | E     | 1        | Total C<br>40 40 | 0       |
| 15  | E     | 1        | Total C<br>40 40 | 0       |
| 15  | G     | 1        | Total C<br>40 40 | 0       |
| 15  | G     | 1        | Total C<br>40 40 | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 15  | G     | 1        | Total C<br>40 40 | 0       |
| 15  | G     | 1        | Total C<br>40 40 | 0       |
| 15  | G     | 1        | Total C<br>40 40 | 0       |
| 15  | G     | 1        | Total C<br>40 40 | 0       |
| 15  | O     | 1        | Total C<br>40 40 | 0       |
| 15  | O     | 1        | Total C<br>40 40 | 0       |
| 15  | P     | 1        | Total C<br>40 40 | 0       |
| 15  | Q     | 1        | Total C<br>40 40 | 0       |
| 15  | R     | 1        | Total C<br>40 40 | 0       |
| 15  | S     | 1        | Total C<br>40 40 | 0       |
| 15  | S     | 1        | Total C<br>40 40 | 0       |
| 15  | S     | 1        | Total C<br>40 40 | 0       |
| 15  | T     | 1        | Total C<br>40 40 | 0       |
| 15  | e     | 1        | Total C<br>40 40 | 0       |
| 15  | e     | 1        | Total C<br>40 40 | 0       |
| 15  | e     | 1        | Total C<br>40 40 | 0       |
| 15  | e     | 1        | Total C<br>40 40 | 0       |
| 15  | e     | 1        | Total C<br>40 40 | 0       |
| 15  | e     | 1        | Total C<br>40 40 | 0       |
| 15  | g     | 1        | Total C<br>40 40 | 0       |
| 15  | g     | 1        | Total C<br>40 40 | 0       |

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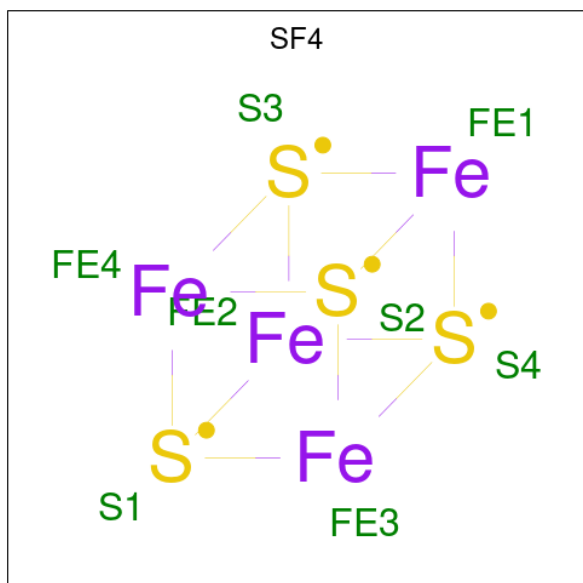
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 15  | g     | 1        | Total C<br>40 40 | 0       |
| 15  | g     | 1        | Total C<br>40 40 | 0       |
| 15  | g     | 1        | Total C<br>40 40 | 0       |
| 15  | g     | 1        | Total C<br>40 40 | 0       |
| 15  | o     | 1        | Total C<br>40 40 | 0       |
| 15  | p     | 1        | Total C<br>40 40 | 0       |
| 15  | q     | 1        | Total C<br>40 40 | 0       |
| 15  | q     | 1        | Total C<br>40 40 | 0       |
| 15  | s     | 1        | Total C<br>40 40 | 0       |
| 15  | s     | 1        | Total C<br>40 40 | 0       |
| 15  | a     | 1        | Total C<br>40 40 | 0       |
| 15  | a     | 1        | Total C<br>40 40 | 0       |
| 15  | a     | 1        | Total C<br>40 40 | 0       |
| 15  | a     | 1        | Total C<br>40 40 | 0       |
| 15  | a     | 1        | Total C<br>40 40 | 0       |
| 15  | a     | 1        | Total C<br>40 40 | 0       |
| 15  | a     | 1        | Total C<br>40 40 | 0       |
| 15  | b     | 1        | Total C<br>40 40 | 0       |
| 15  | b     | 1        | Total C<br>40 40 | 0       |
| 15  | b     | 1        | Total C<br>40 40 | 0       |
| 15  | b     | 1        | Total C<br>40 40 | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 15  | b     | 1        | Total C<br>40 40 | 0       |
| 15  | b     | 1        | Total C<br>40 40 | 0       |
| 15  | f     | 1        | Total C<br>40 40 | 0       |
| 15  | f     | 1        | Total C<br>40 40 | 0       |
| 15  | i     | 1        | Total C<br>40 40 | 0       |
| 15  | j     | 1        | Total C<br>40 40 | 0       |
| 15  | k     | 1        | Total C<br>40 40 | 0       |
| 15  | l     | 1        | Total C<br>40 40 | 0       |
| 15  | l     | 1        | Total C<br>40 40 | 0       |
| 15  | m     | 1        | Total C<br>40 40 | 0       |

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms               | AltConf |
|-----|-------|----------|---------------------|---------|
| 16  | B     | 1        | Total Fe S<br>8 4 4 | 0       |

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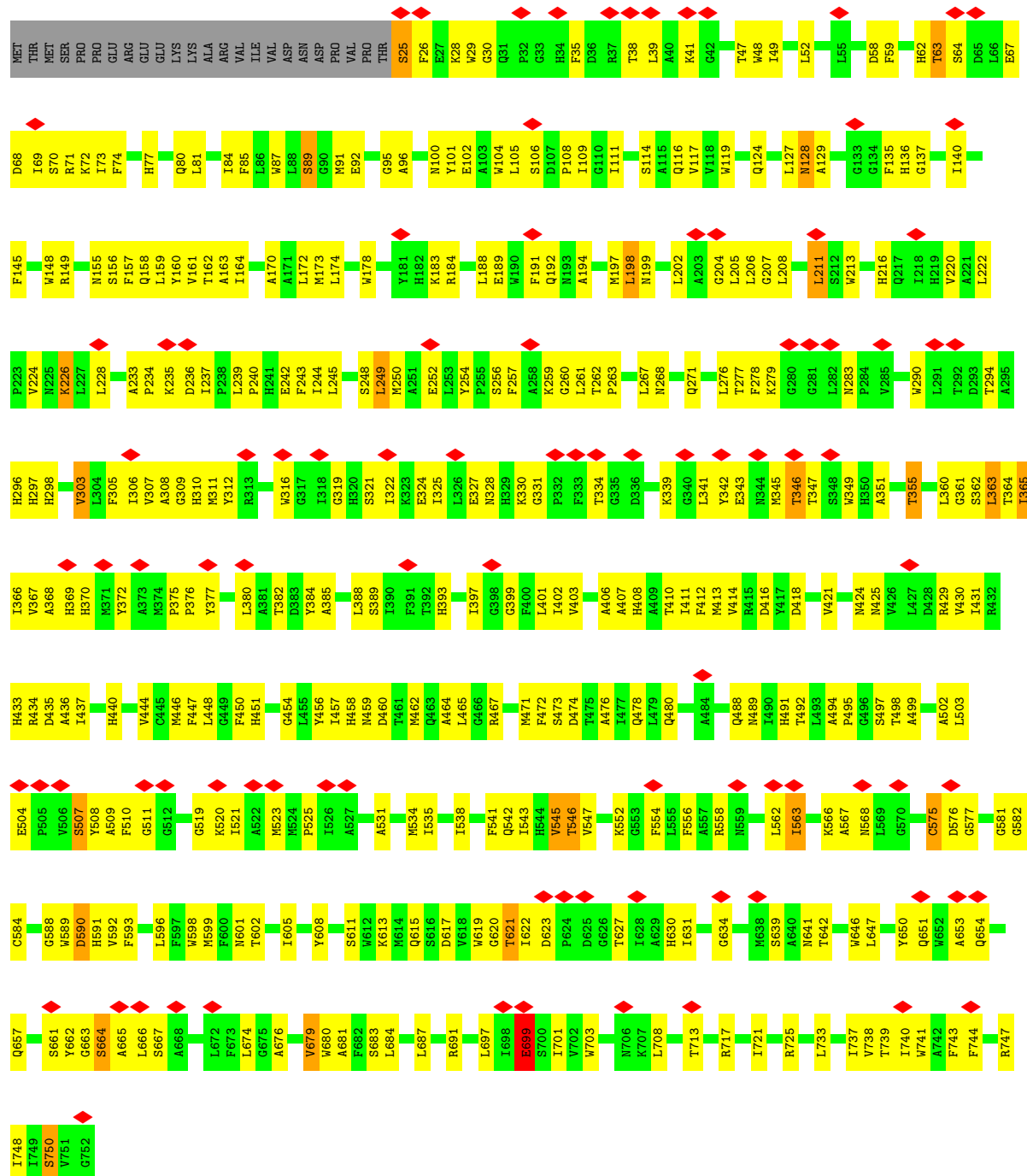
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| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 16  | C     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | C     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | E     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | H     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | H     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | g     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | h     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | h     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | a     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | c     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 16  | c     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |





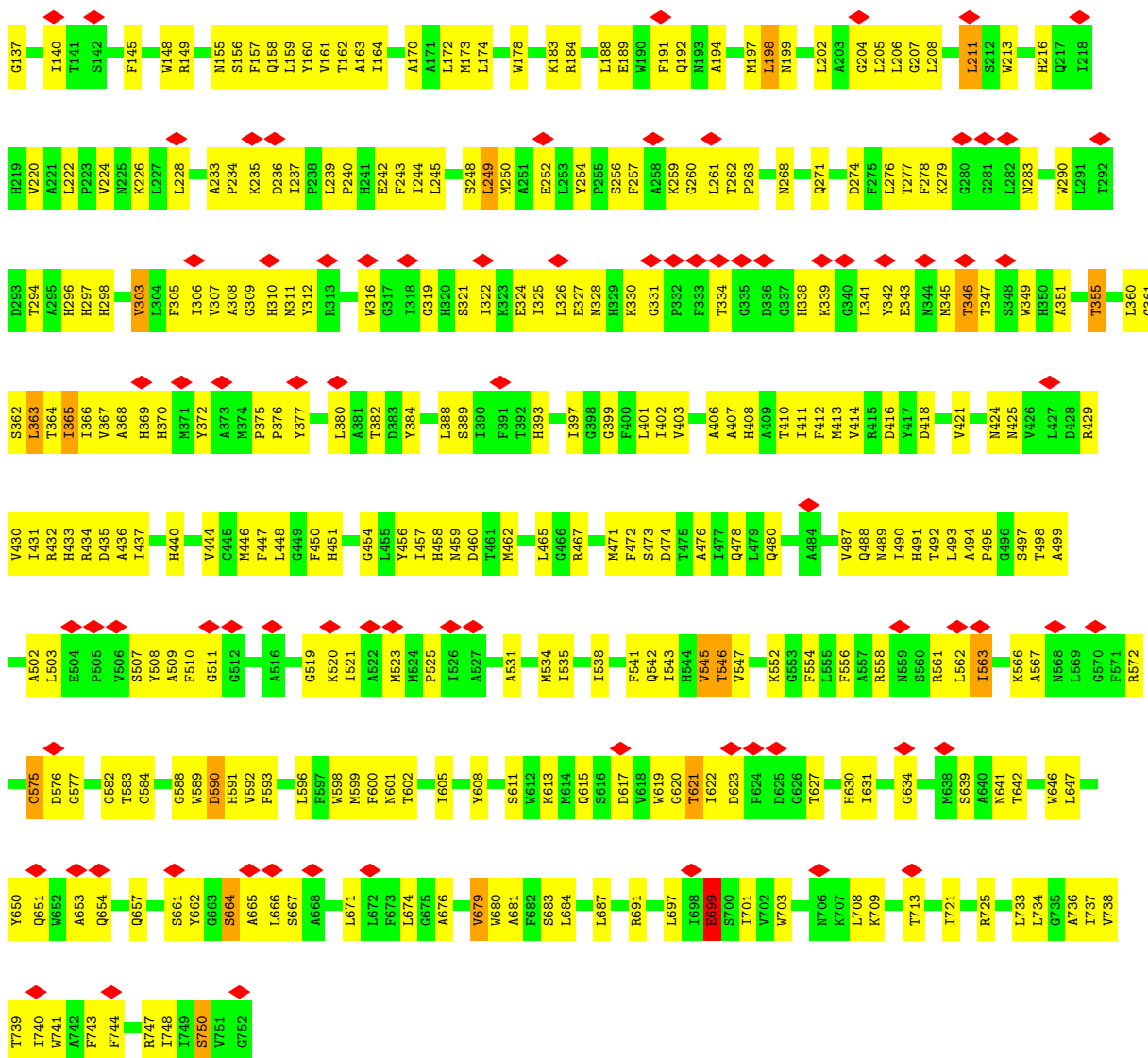
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



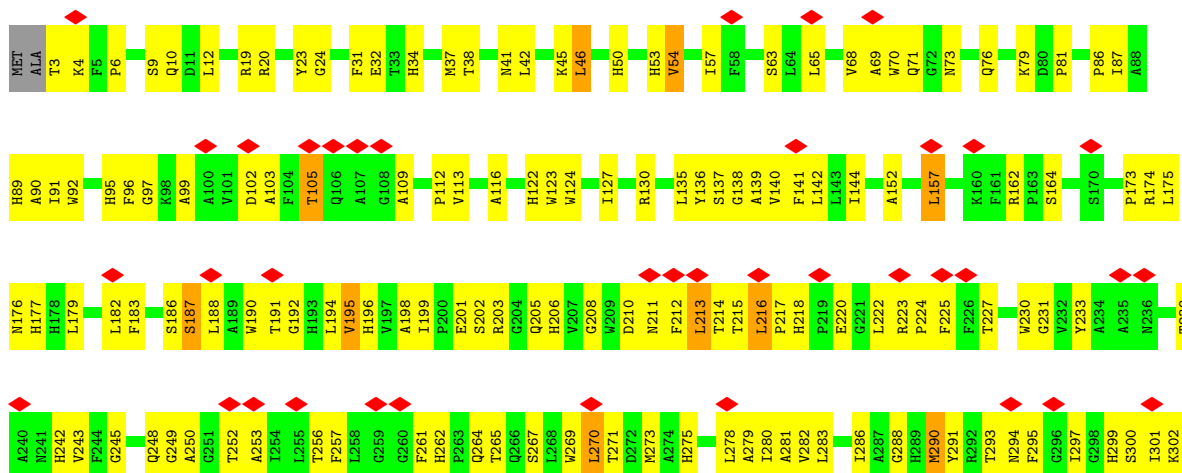
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

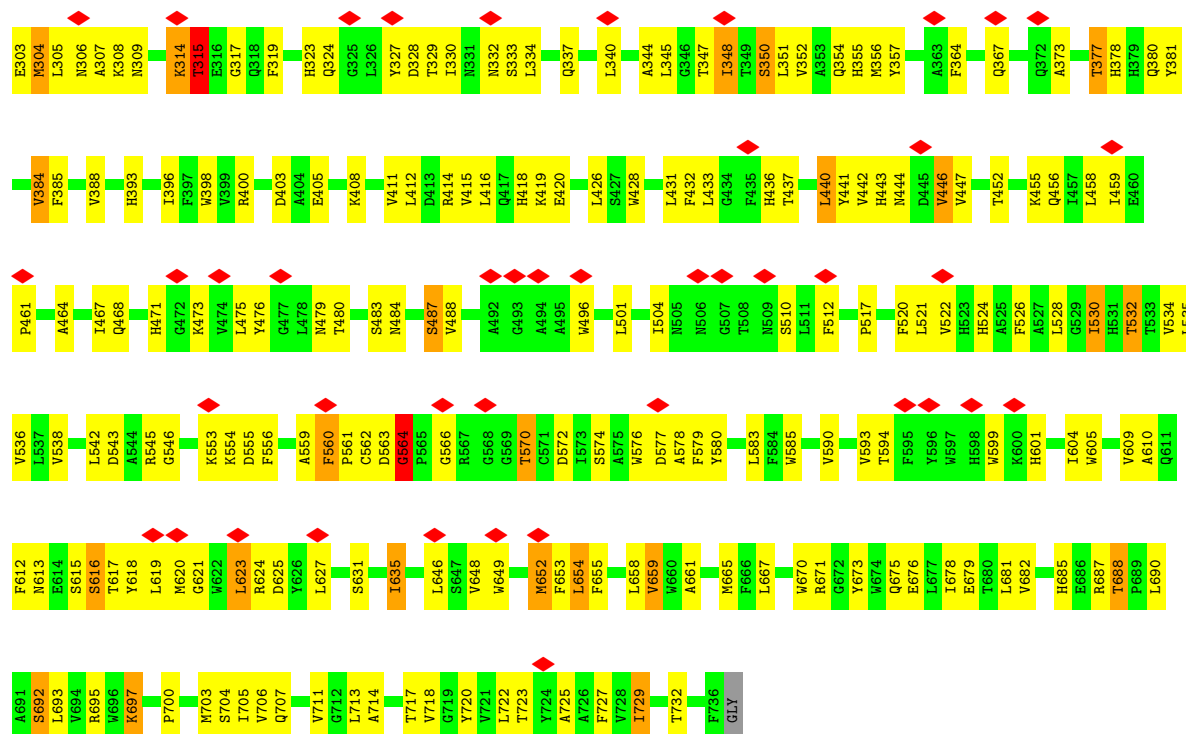




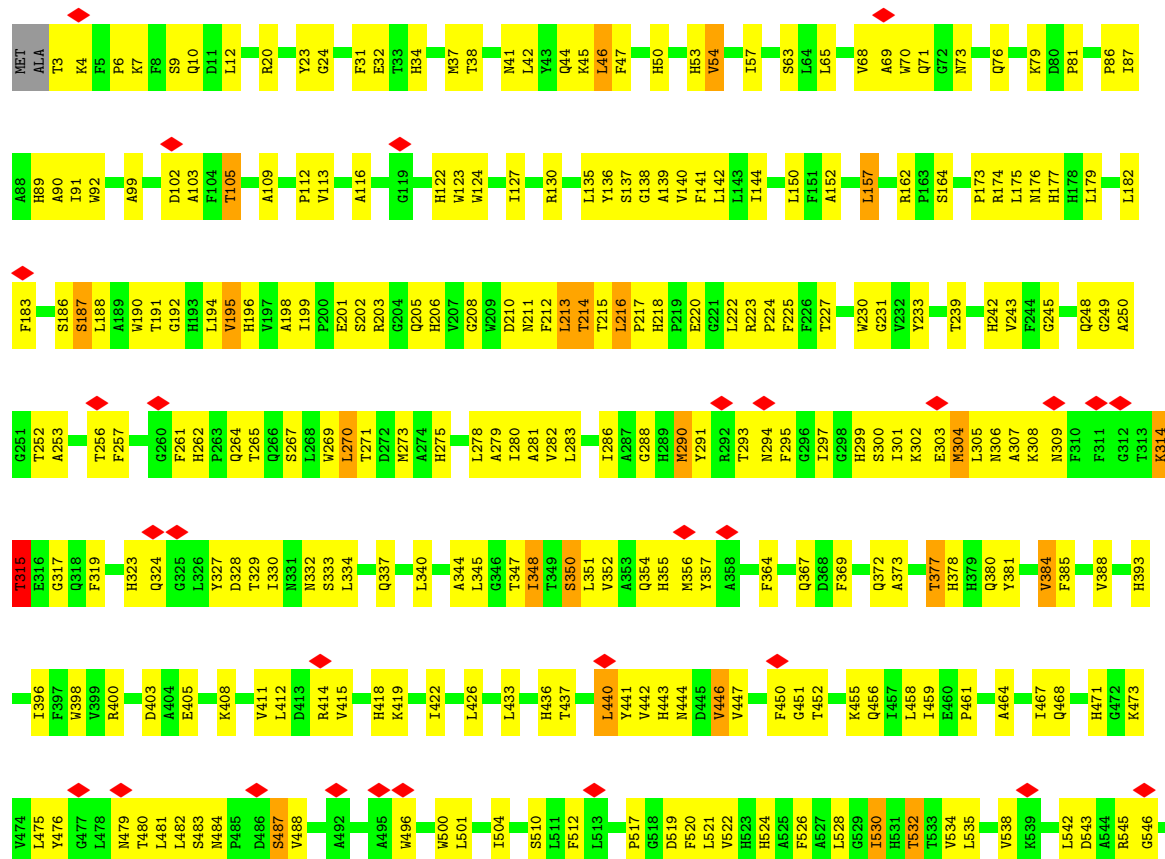


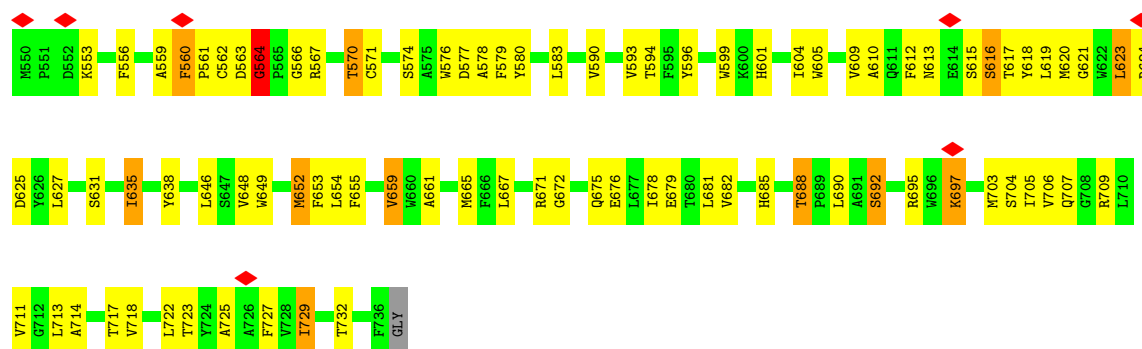
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



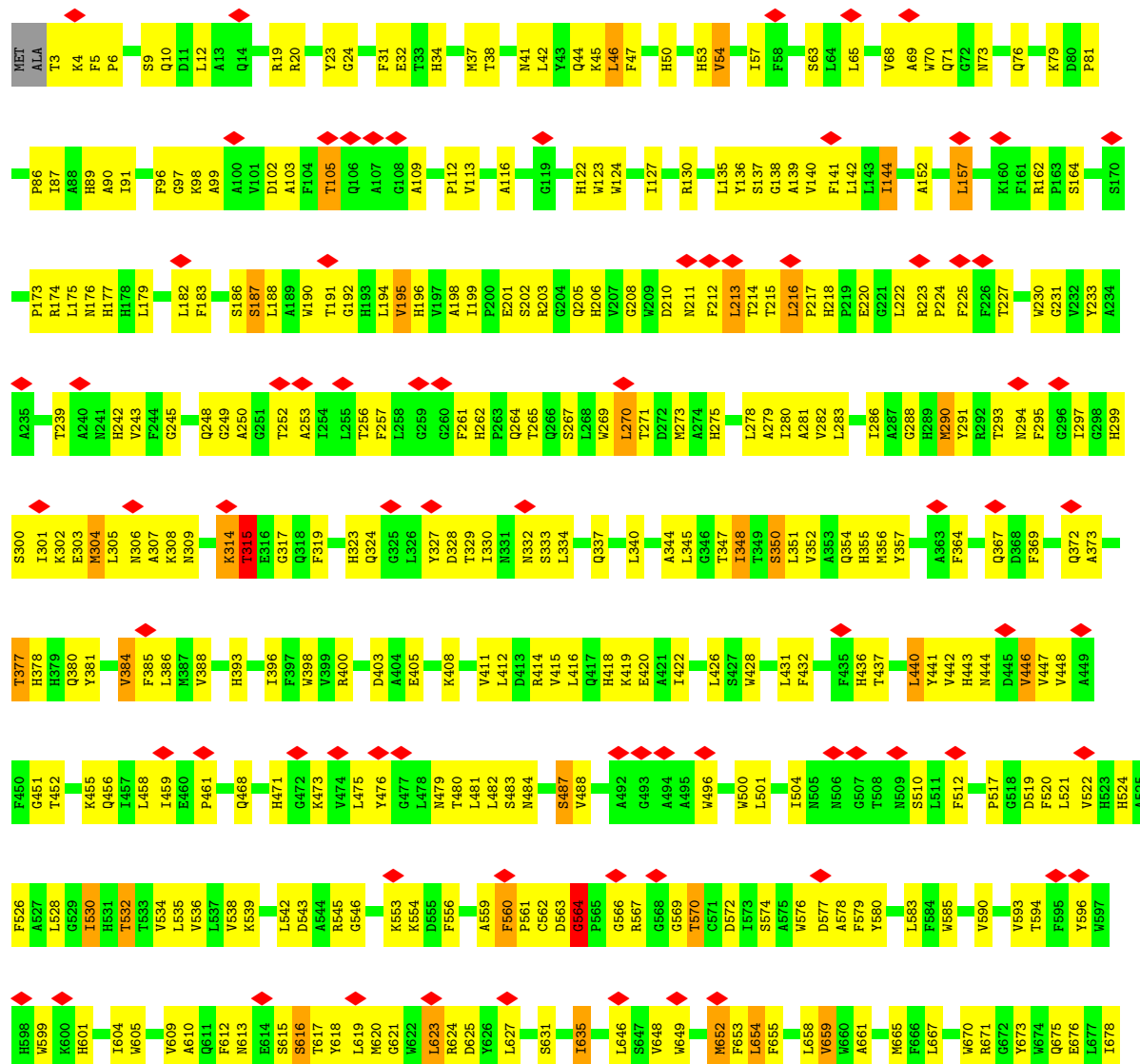


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

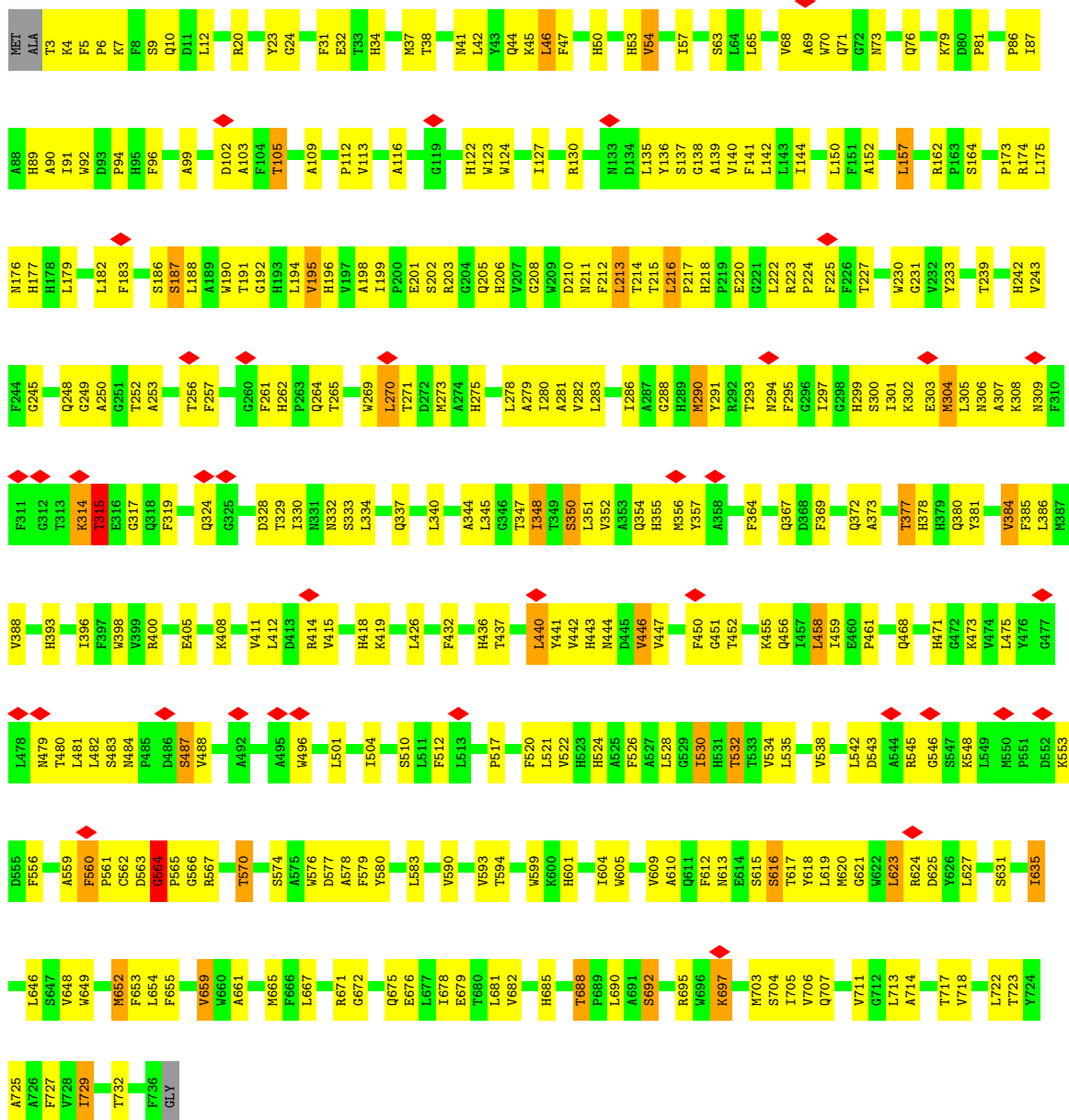




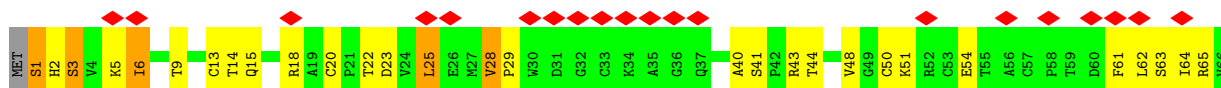
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

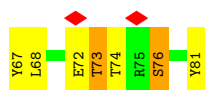


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

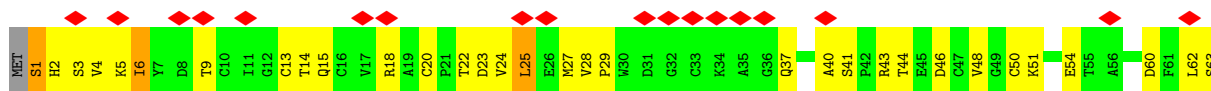


- Molecule 3: Photosystem I iron-sulfur center

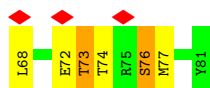
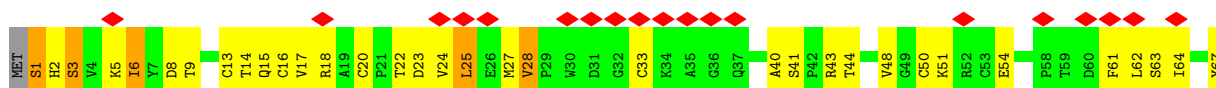




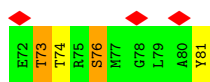
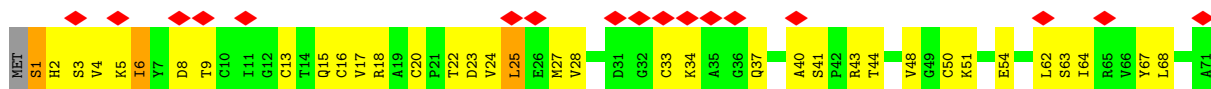
• Molecule 3: Photosystem I iron-sulfur center



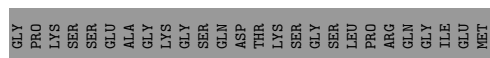
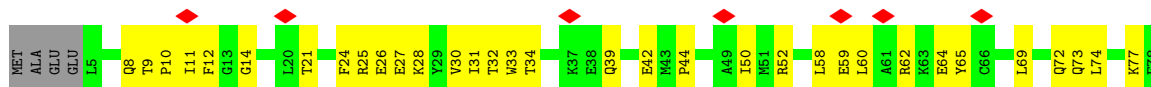
• Molecule 3: Photosystem I iron-sulfur center



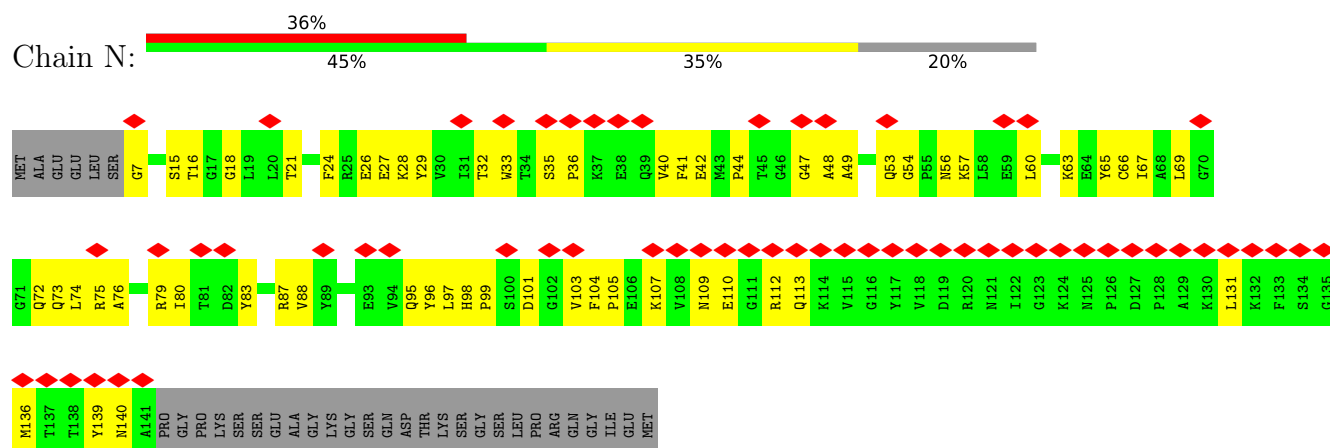
• Molecule 3: Photosystem I iron-sulfur center



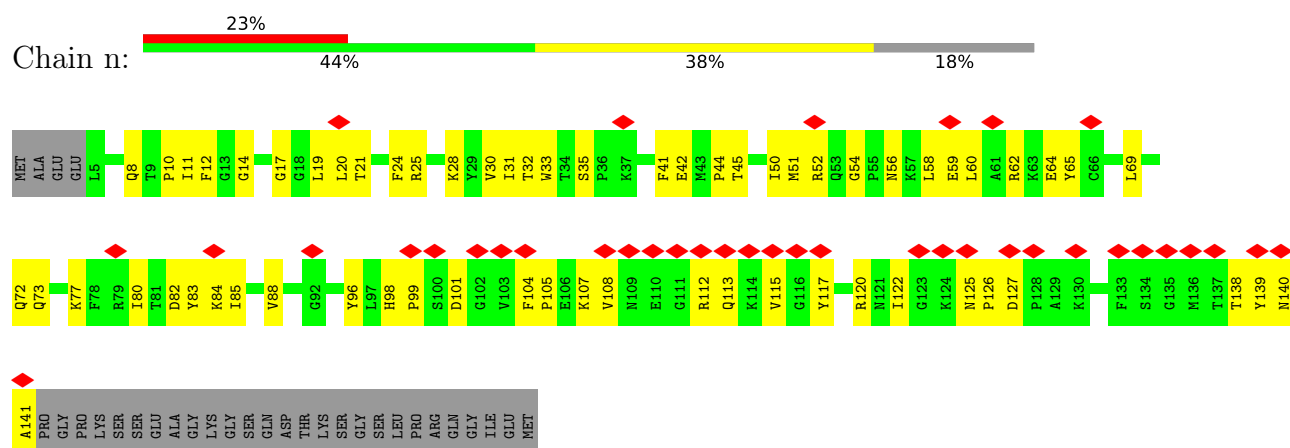
• Molecule 4: Photosystem I reaction center subunit II



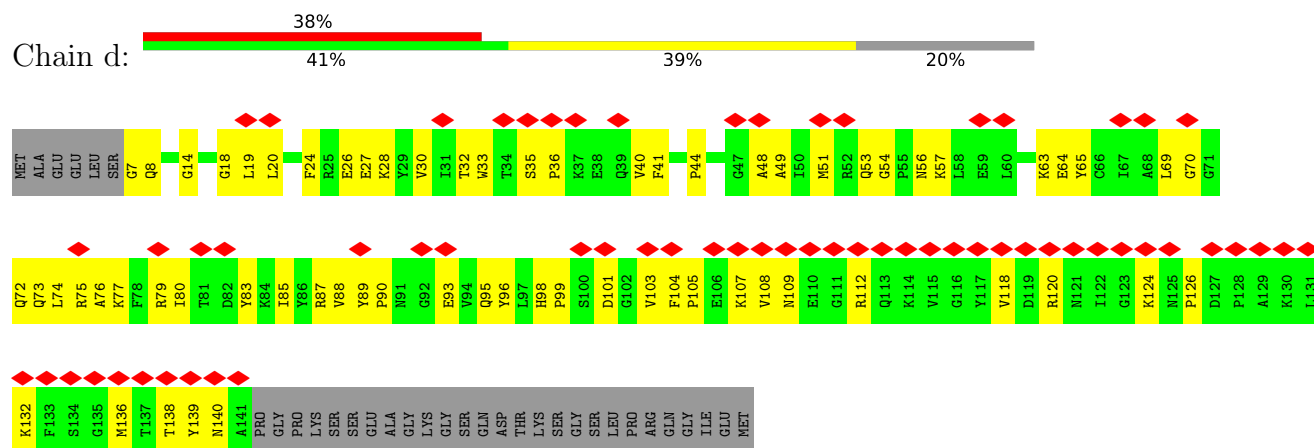
- Molecule 4: Photosystem I reaction center subunit II



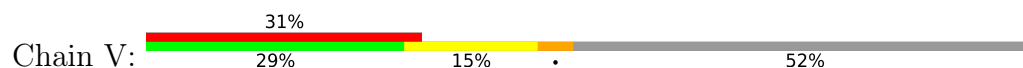
- Molecule 4: Photosystem I reaction center subunit II

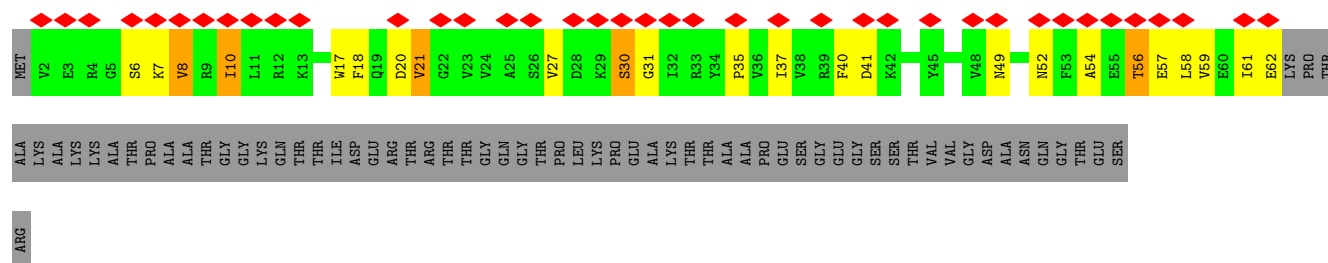


- Molecule 4: Photosystem I reaction center subunit II

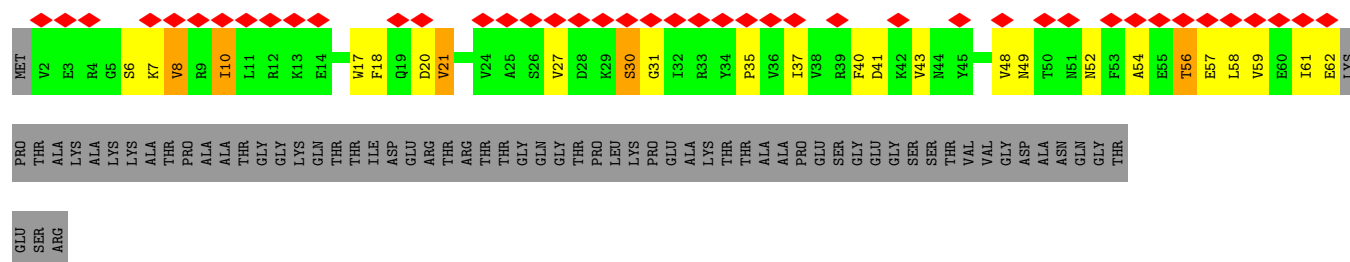
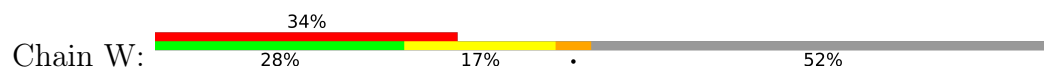


- Molecule 5: Photosystem I reaction center subunit IV

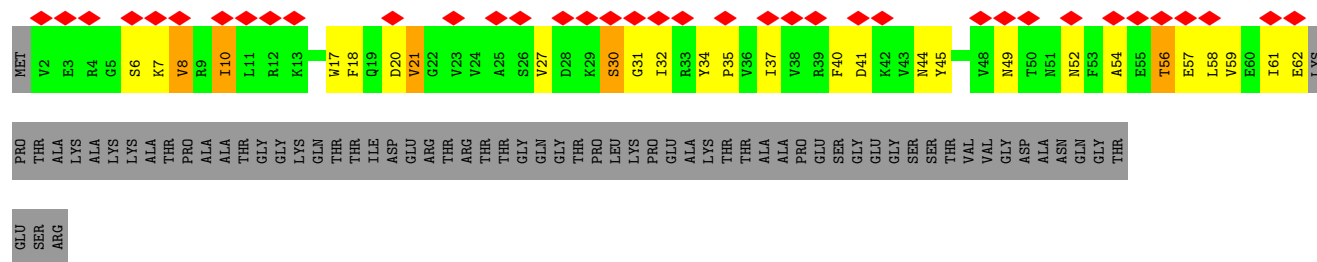




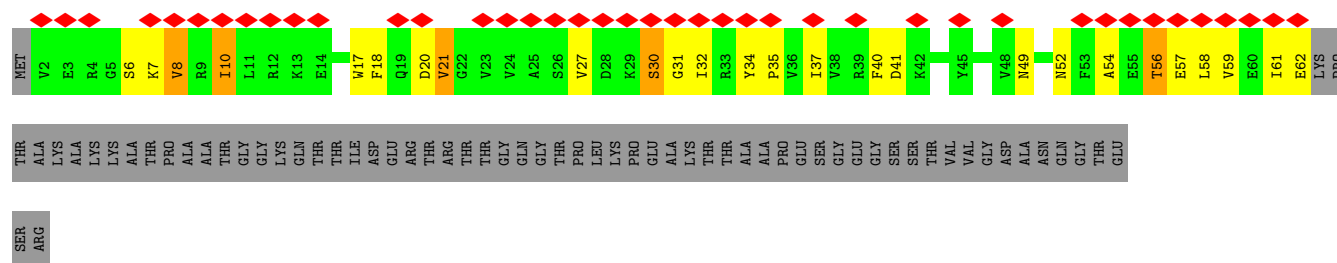
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV

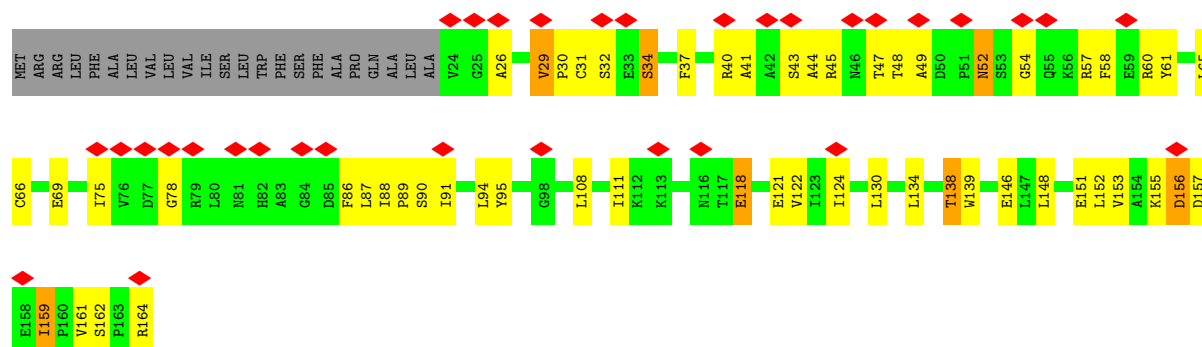


- Molecule 5: Photosystem I reaction center subunit IV

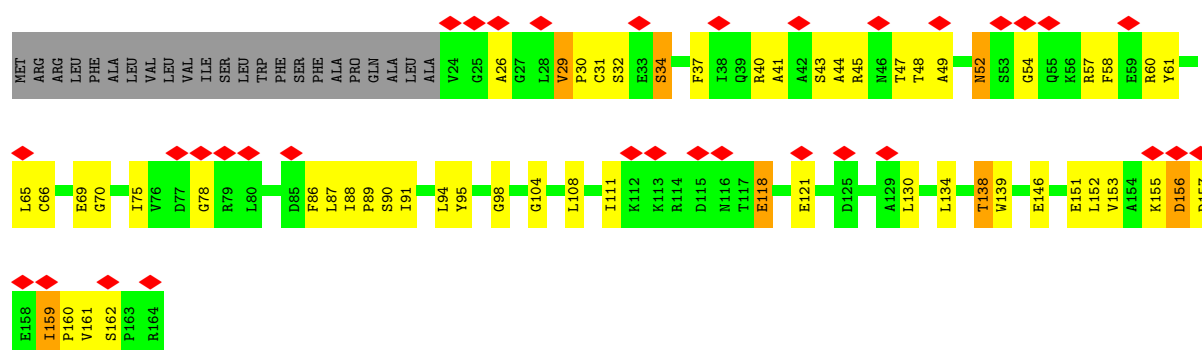


- Molecule 6: Photosystem I reaction center subunit III

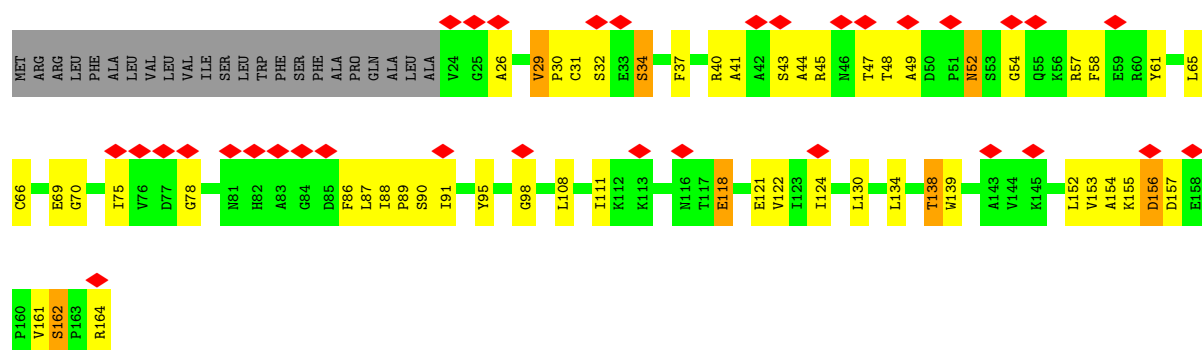




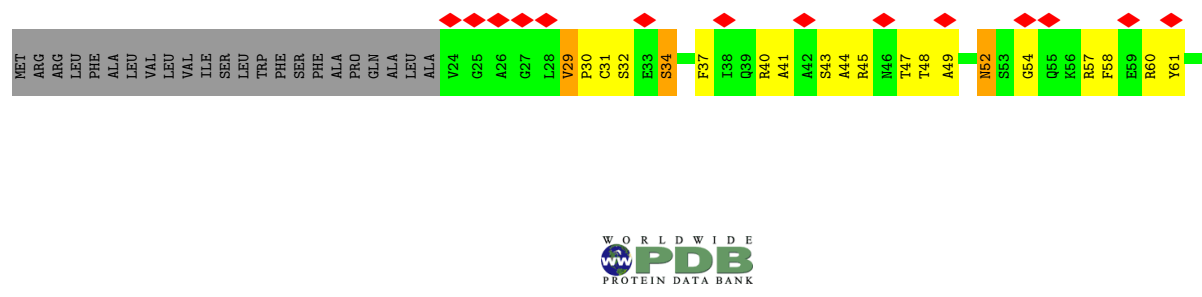
• Molecule 6: Photosystem I reaction center subunit III



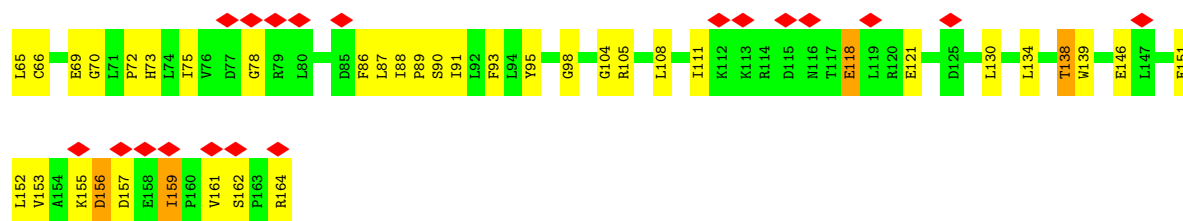
• Molecule 6: Photosystem I reaction center subunit III



• Molecule 6: Photosystem I reaction center subunit III







• Molecule 7: Photosystem I reaction center subunit VIII



• Molecule 7: Photosystem I reaction center subunit VIII



• Molecule 7: Photosystem I reaction center subunit VIII



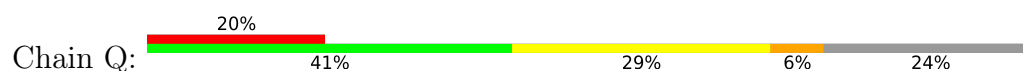
• Molecule 7: Photosystem I reaction center subunit VIII

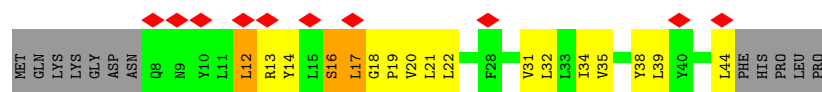


• Molecule 8: Photosystem I reaction center subunit IX

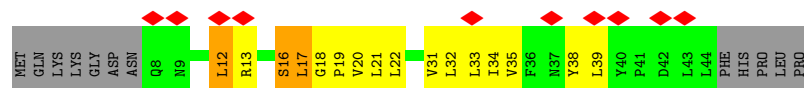
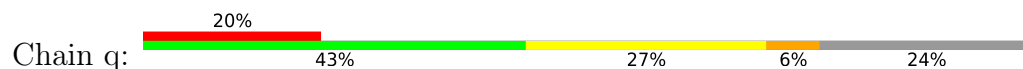


• Molecule 8: Photosystem I reaction center subunit IX

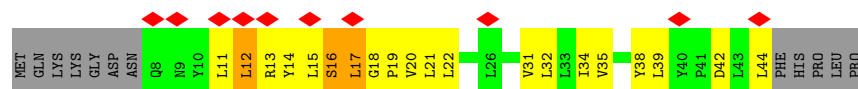




• Molecule 8: Photosystem I reaction center subunit IX



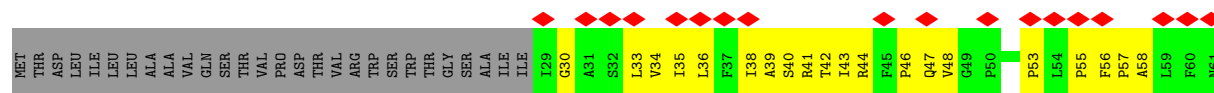
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: Photosystem I reaction center subunit Psak

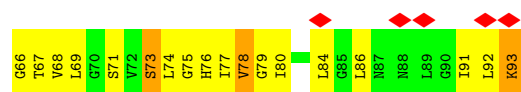


• Molecule 9: Photosystem I reaction center subunit Psak

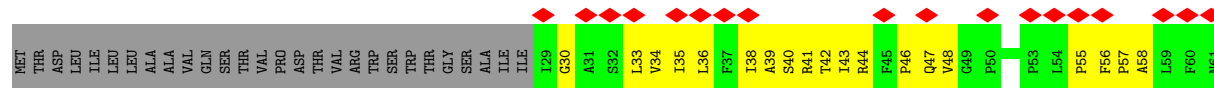


• Molecule 9: Photosystem I reaction center subunit Psak

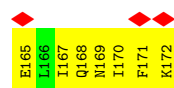
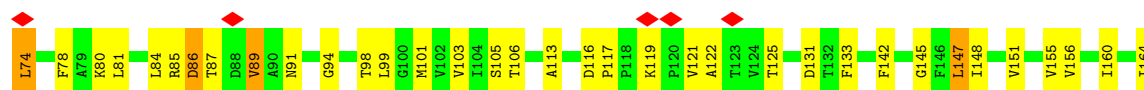
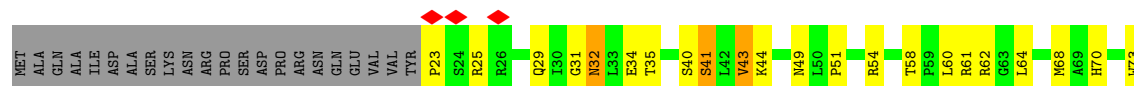




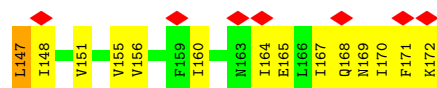
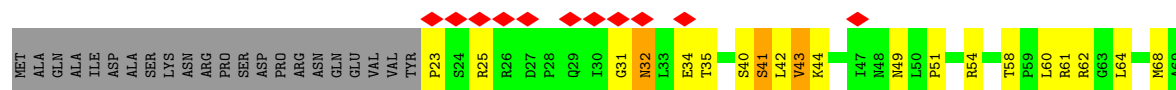
• Molecule 9: Photosystem I reaction center subunit PsaK



• Molecule 10: Photosystem I reaction center subunit XI

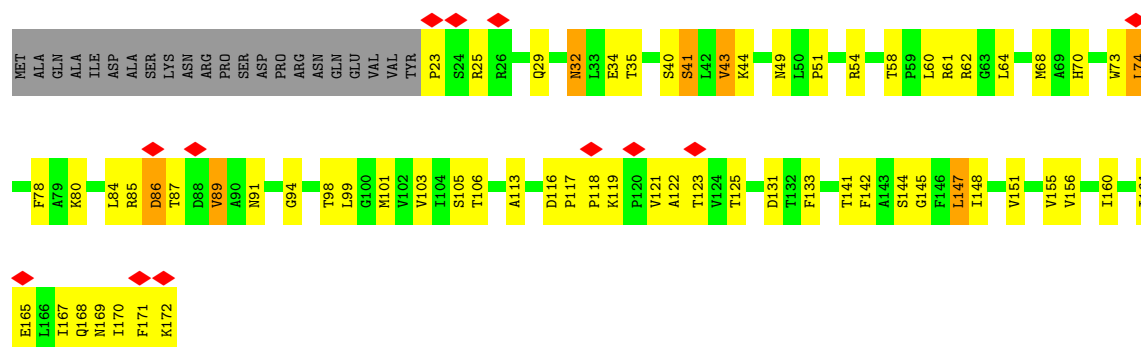


• Molecule 10: Photosystem I reaction center subunit XI

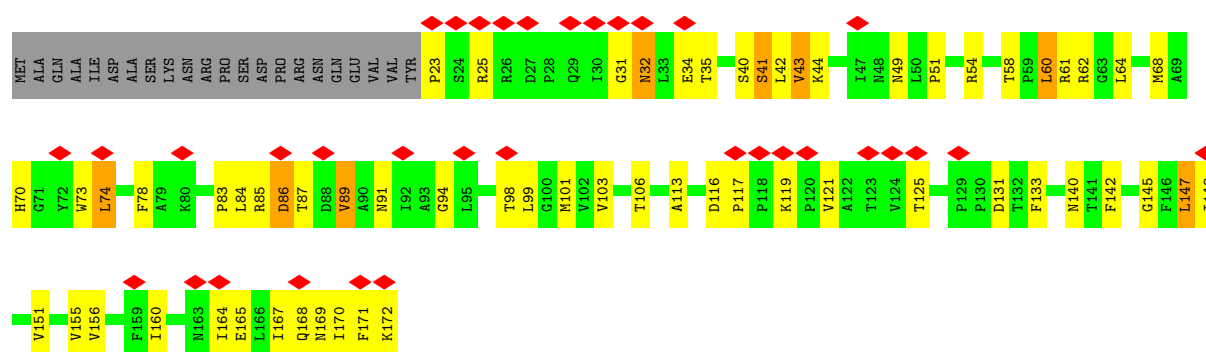


• Molecule 10: Photosystem I reaction center subunit XI





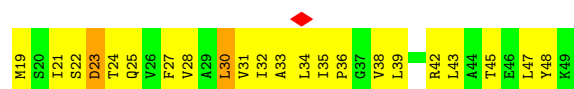
• Molecule 10: Photosystem I reaction center subunit XI



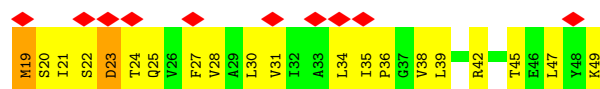
• Molecule 11: Photosystem I reaction center subunit XII



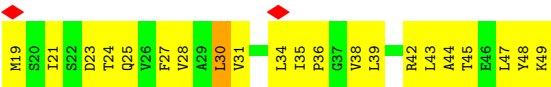
• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C2                               | Depositor |
| Number of particles used             | 66130                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 4.3                                     | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.053                                   | Depositor |
| Minimum map value                    | -0.029                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.0125                                  | Depositor |
| Map size (Å)                         | 425.47202, 425.47202, 425.47202         | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.108, 1.108, 1.108                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, BCR, PQN, LHG, SF4

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     | 0.21         | 0/5908  | 0.46        | 1/8056 (0.0%) |
| 1   | E     | 0.21         | 0/5908  | 0.46        | 1/8056 (0.0%) |
| 1   | a     | 0.21         | 0/5908  | 0.46        | 1/8056 (0.0%) |
| 1   | e     | 0.21         | 0/5908  | 0.46        | 1/8056 (0.0%) |
| 2   | B     | 0.20         | 0/6072  | 0.45        | 0/8301        |
| 2   | G     | 0.20         | 0/6072  | 0.45        | 0/8301        |
| 2   | b     | 0.20         | 0/6072  | 0.45        | 0/8301        |
| 2   | g     | 0.20         | 0/6072  | 0.45        | 0/8301        |
| 3   | C     | 0.18         | 0/615   | 0.42        | 0/833         |
| 3   | H     | 0.18         | 0/615   | 0.42        | 0/833         |
| 3   | c     | 0.18         | 0/615   | 0.42        | 0/833         |
| 3   | h     | 0.18         | 0/615   | 0.42        | 0/833         |
| 4   | D     | 0.17         | 0/1105  | 0.42        | 0/1489        |
| 4   | N     | 0.18         | 0/1091  | 0.45        | 0/1470        |
| 4   | d     | 0.18         | 0/1091  | 0.46        | 0/1470        |
| 4   | n     | 0.18         | 0/1105  | 0.40        | 0/1489        |
| 5   | V     | 0.19         | 0/502   | 0.51        | 0/678         |
| 5   | W     | 0.19         | 0/502   | 0.51        | 0/678         |
| 5   | v     | 0.19         | 0/502   | 0.52        | 0/678         |
| 5   | w     | 0.19         | 0/502   | 0.51        | 0/678         |
| 6   | F     | 0.20         | 0/1119  | 0.45        | 0/1522        |
| 6   | O     | 0.20         | 0/1119  | 0.45        | 0/1522        |
| 6   | f     | 0.20         | 0/1119  | 0.45        | 0/1522        |
| 6   | o     | 0.20         | 0/1119  | 0.45        | 0/1522        |
| 7   | I     | 0.21         | 0/302   | 0.54        | 0/411         |
| 7   | P     | 0.21         | 0/302   | 0.54        | 0/411         |
| 7   | i     | 0.21         | 0/302   | 0.54        | 0/411         |
| 7   | p     | 0.21         | 0/302   | 0.54        | 0/411         |
| 8   | J     | 0.18         | 0/321   | 0.44        | 0/441         |
| 8   | Q     | 0.18         | 0/321   | 0.43        | 0/441         |
| 8   | j     | 0.18         | 0/321   | 0.44        | 0/441         |
| 8   | q     | 0.18         | 0/321   | 0.43        | 0/441         |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 9   | K     | 0.21         | 0/484   | 0.63        | 0/659          |
| 9   | R     | 0.21         | 0/484   | 0.63        | 0/659          |
| 9   | k     | 0.21         | 0/484   | 0.63        | 0/659          |
| 9   | r     | 0.21         | 0/484   | 0.63        | 0/659          |
| 10  | L     | 0.21         | 0/1165  | 0.49        | 0/1597         |
| 10  | S     | 0.21         | 0/1165  | 0.49        | 0/1597         |
| 10  | l     | 0.21         | 0/1165  | 0.49        | 0/1597         |
| 10  | s     | 0.21         | 0/1165  | 0.49        | 0/1597         |
| 11  | M     | 0.24         | 0/241   | 0.58        | 0/326          |
| 11  | T     | 0.24         | 0/241   | 0.58        | 0/326          |
| 11  | m     | 0.24         | 0/241   | 0.58        | 0/326          |
| 11  | t     | 0.24         | 0/241   | 0.58        | 0/326          |
| All | All   | 0.20         | 0/71308 | 0.46        | 4/97214 (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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 3                   |
| 2   | G     | 0                   | 3                   |
| 2   | b     | 0                   | 3                   |
| 2   | g     | 0                   | 3                   |
| 10  | L     | 0                   | 1                   |
| 10  | S     | 0                   | 1                   |
| 10  | l     | 0                   | 1                   |
| 10  | s     | 0                   | 1                   |
| All | All   | 0                   | 16                  |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | e     | 699 | GLU  | CA-CB-CG | 6.37 | 126.85      | 114.10   |
| 1   | a     | 699 | GLU  | CA-CB-CG | 6.37 | 126.83      | 114.10   |
| 1   | A     | 699 | GLU  | CA-CB-CG | 6.36 | 126.83      | 114.10   |
| 1   | E     | 699 | GLU  | CA-CB-CG | 6.36 | 126.83      | 114.10   |

There are no chirality outliers.

5 of 16 planarity outliers are listed below:



| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 315 | THR  | Peptide |
| 2   | B     | 560 | PHE  | Peptide |
| 2   | B     | 564 | GLY  | Peptide |
| 2   | G     | 315 | THR  | Peptide |
| 10  | L     | 117 | PRO  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5713  | 0        | 5565     | 290     | 0            |
| 1   | E     | 5713  | 0        | 5565     | 285     | 0            |
| 1   | a     | 5713  | 0        | 5565     | 346     | 0            |
| 1   | e     | 5713  | 0        | 5565     | 304     | 0            |
| 2   | B     | 5857  | 0        | 5642     | 293     | 0            |
| 2   | G     | 5857  | 0        | 5642     | 280     | 0            |
| 2   | b     | 5857  | 0        | 5642     | 275     | 0            |
| 2   | g     | 5857  | 0        | 5642     | 309     | 0            |
| 3   | C     | 605   | 0        | 590      | 33      | 0            |
| 3   | H     | 605   | 0        | 590      | 30      | 0            |
| 3   | c     | 605   | 0        | 590      | 38      | 0            |
| 3   | h     | 605   | 0        | 590      | 36      | 0            |
| 4   | D     | 1080  | 0        | 1083     | 58      | 0            |
| 4   | N     | 1066  | 0        | 1067     | 51      | 0            |
| 4   | d     | 1066  | 0        | 1067     | 65      | 0            |
| 4   | n     | 1080  | 0        | 1083     | 58      | 0            |
| 5   | V     | 494   | 0        | 493      | 16      | 0            |
| 5   | W     | 494   | 0        | 493      | 18      | 0            |
| 5   | v     | 494   | 0        | 493      | 22      | 0            |
| 5   | w     | 494   | 0        | 493      | 18      | 0            |
| 6   | F     | 1093  | 0        | 1095     | 38      | 0            |
| 6   | O     | 1093  | 0        | 1095     | 39      | 0            |
| 6   | f     | 1093  | 0        | 1095     | 43      | 0            |
| 6   | o     | 1093  | 0        | 1095     | 39      | 0            |
| 7   | I     | 295   | 0        | 314      | 13      | 0            |
| 7   | P     | 295   | 0        | 314      | 17      | 0            |
| 7   | i     | 295   | 0        | 314      | 21      | 0            |
| 7   | p     | 295   | 0        | 314      | 15      | 0            |
| 8   | J     | 311   | 0        | 323      | 18      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | Q     | 311   | 0        | 323      | 12      | 0            |
| 8   | j     | 311   | 0        | 323      | 17      | 0            |
| 8   | q     | 311   | 0        | 323      | 15      | 0            |
| 9   | K     | 474   | 0        | 521      | 29      | 0            |
| 9   | R     | 474   | 0        | 521      | 40      | 0            |
| 9   | k     | 474   | 0        | 521      | 34      | 0            |
| 9   | r     | 474   | 0        | 521      | 29      | 0            |
| 10  | L     | 1134  | 0        | 1151     | 54      | 0            |
| 10  | S     | 1134  | 0        | 1151     | 46      | 0            |
| 10  | l     | 1134  | 0        | 1151     | 44      | 0            |
| 10  | s     | 1134  | 0        | 1151     | 63      | 0            |
| 11  | M     | 238   | 0        | 257      | 10      | 0            |
| 11  | T     | 238   | 0        | 257      | 15      | 0            |
| 11  | m     | 238   | 0        | 257      | 17      | 0            |
| 11  | t     | 238   | 0        | 257      | 11      | 0            |
| 12  | A     | 87    | 0        | 123      | 5       | 0            |
| 12  | a     | 49    | 0        | 74       | 3       | 0            |
| 12  | e     | 87    | 0        | 123      | 5       | 0            |
| 13  | A     | 2175  | 0        | 1688     | 122     | 0            |
| 13  | B     | 1954  | 0        | 1504     | 99      | 0            |
| 13  | E     | 2166  | 0        | 1678     | 121     | 0            |
| 13  | F     | 45    | 0        | 33       | 2       | 0            |
| 13  | G     | 1999  | 0        | 1537     | 105     | 0            |
| 13  | K     | 86    | 0        | 62       | 4       | 0            |
| 13  | L     | 145   | 0        | 111      | 12      | 0            |
| 13  | O     | 45    | 0        | 33       | 1       | 0            |
| 13  | R     | 45    | 0        | 33       | 2       | 0            |
| 13  | S     | 135   | 0        | 99       | 10      | 0            |
| 13  | a     | 2125  | 0        | 1649     | 183     | 0            |
| 13  | b     | 1940  | 0        | 1488     | 106     | 0            |
| 13  | e     | 2125  | 0        | 1649     | 117     | 0            |
| 13  | f     | 45    | 0        | 33       | 0       | 0            |
| 13  | g     | 2004  | 0        | 1543     | 98      | 0            |
| 13  | k     | 45    | 0        | 33       | 2       | 0            |
| 13  | l     | 190   | 0        | 144      | 12      | 0            |
| 13  | o     | 45    | 0        | 33       | 2       | 0            |
| 13  | r     | 86    | 0        | 62       | 3       | 0            |
| 13  | s     | 145   | 0        | 111      | 24      | 0            |
| 14  | A     | 33    | 0        | 46       | 10      | 0            |
| 14  | B     | 33    | 0        | 46       | 2       | 0            |
| 14  | E     | 33    | 0        | 46       | 4       | 0            |
| 14  | G     | 33    | 0        | 46       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | a     | 33    | 0        | 46       | 2       | 0            |
| 14  | b     | 33    | 0        | 46       | 1       | 0            |
| 14  | e     | 33    | 0        | 46       | 1       | 0            |
| 14  | g     | 33    | 0        | 46       | 2       | 0            |
| 15  | A     | 240   | 0        | 336      | 31      | 0            |
| 15  | B     | 240   | 0        | 336      | 10      | 0            |
| 15  | E     | 240   | 0        | 336      | 47      | 0            |
| 15  | F     | 40    | 0        | 56       | 6       | 0            |
| 15  | G     | 240   | 0        | 336      | 16      | 0            |
| 15  | I     | 40    | 0        | 56       | 0       | 0            |
| 15  | J     | 80    | 0        | 112      | 2       | 0            |
| 15  | L     | 80    | 0        | 112      | 6       | 0            |
| 15  | O     | 80    | 0        | 112      | 9       | 0            |
| 15  | P     | 40    | 0        | 56       | 0       | 0            |
| 15  | Q     | 40    | 0        | 56       | 0       | 0            |
| 15  | R     | 40    | 0        | 56       | 37      | 0            |
| 15  | S     | 120   | 0        | 168      | 10      | 0            |
| 15  | T     | 40    | 0        | 56       | 3       | 0            |
| 15  | a     | 280   | 0        | 392      | 86      | 0            |
| 15  | b     | 240   | 0        | 336      | 15      | 0            |
| 15  | e     | 240   | 0        | 336      | 32      | 0            |
| 15  | f     | 80    | 0        | 112      | 8       | 0            |
| 15  | g     | 240   | 0        | 336      | 13      | 0            |
| 15  | i     | 40    | 0        | 56       | 3       | 0            |
| 15  | j     | 40    | 0        | 56       | 4       | 0            |
| 15  | k     | 40    | 0        | 56       | 33      | 0            |
| 15  | l     | 80    | 0        | 112      | 6       | 0            |
| 15  | m     | 40    | 0        | 56       | 6       | 0            |
| 15  | o     | 40    | 0        | 56       | 3       | 0            |
| 15  | p     | 40    | 0        | 56       | 1       | 0            |
| 15  | q     | 80    | 0        | 112      | 1       | 0            |
| 15  | s     | 80    | 0        | 112      | 6       | 0            |
| 16  | B     | 8     | 0        | 0        | 1       | 0            |
| 16  | C     | 16    | 0        | 0        | 4       | 0            |
| 16  | E     | 8     | 0        | 0        | 1       | 0            |
| 16  | H     | 16    | 0        | 0        | 4       | 0            |
| 16  | a     | 8     | 0        | 0        | 1       | 0            |
| 16  | c     | 16    | 0        | 0        | 4       | 0            |
| 16  | g     | 8     | 0        | 0        | 1       | 0            |
| 16  | h     | 16    | 0        | 0        | 4       | 0            |
| All | All   | 90396 | 0        | 86683    | 4001    | 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 23.

The worst 5 of 4001 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) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:a:680:TRP:CE3 | 13:a:852:CLA:HHB  | 1.40                     | 1.54              |
| 1:a:680:TRP:CZ3 | 13:a:852:CLA:HHB  | 1.50                     | 1.41              |
| 1:a:680:TRP:CZ3 | 13:a:852:CLA:HMB1 | 1.55                     | 1.41              |
| 1:a:680:TRP:CE2 | 13:a:852:CLA:H3A  | 1.65                     | 1.31              |
| 10:L:80:LYS:HD3 | 13:L:204:CLA:C5   | 1.61                     | 1.28              |

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     | 726/752 (96%) | 625 (86%) | 101 (14%) | 0        | 100         | 100 |
| 1   | E     | 726/752 (96%) | 625 (86%) | 101 (14%) | 0        | 100         | 100 |
| 1   | a     | 726/752 (96%) | 625 (86%) | 101 (14%) | 0        | 100         | 100 |
| 1   | e     | 726/752 (96%) | 626 (86%) | 100 (14%) | 0        | 100         | 100 |
| 2   | B     | 732/737 (99%) | 642 (88%) | 87 (12%)  | 3 (0%)   | 30          | 60  |
| 2   | G     | 732/737 (99%) | 642 (88%) | 87 (12%)  | 3 (0%)   | 30          | 60  |
| 2   | b     | 732/737 (99%) | 644 (88%) | 85 (12%)  | 3 (0%)   | 30          | 60  |
| 2   | g     | 732/737 (99%) | 642 (88%) | 87 (12%)  | 3 (0%)   | 30          | 60  |
| 3   | C     | 79/82 (96%)   | 65 (82%)  | 14 (18%)  | 0        | 100         | 100 |
| 3   | H     | 79/82 (96%)   | 65 (82%)  | 14 (18%)  | 0        | 100         | 100 |
| 3   | c     | 79/82 (96%)   | 65 (82%)  | 14 (18%)  | 0        | 100         | 100 |
| 3   | h     | 79/82 (96%)   | 66 (84%)  | 13 (16%)  | 0        | 100         | 100 |
| 4   | D     | 135/168 (80%) | 115 (85%) | 20 (15%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | N     | 133/168 (79%) | 113 (85%) | 20 (15%) | 0        | 100         | 100 |
| 4   | d     | 133/168 (79%) | 114 (86%) | 19 (14%) | 0        | 100         | 100 |
| 4   | n     | 135/168 (80%) | 117 (87%) | 18 (13%) | 0        | 100         | 100 |
| 5   | V     | 59/126 (47%)  | 47 (80%)  | 12 (20%) | 0        | 100         | 100 |
| 5   | W     | 59/126 (47%)  | 47 (80%)  | 12 (20%) | 0        | 100         | 100 |
| 5   | v     | 59/126 (47%)  | 47 (80%)  | 12 (20%) | 0        | 100         | 100 |
| 5   | w     | 59/126 (47%)  | 47 (80%)  | 12 (20%) | 0        | 100         | 100 |
| 6   | F     | 139/164 (85%) | 120 (86%) | 19 (14%) | 0        | 100         | 100 |
| 6   | O     | 139/164 (85%) | 120 (86%) | 19 (14%) | 0        | 100         | 100 |
| 6   | f     | 139/164 (85%) | 120 (86%) | 19 (14%) | 0        | 100         | 100 |
| 6   | o     | 139/164 (85%) | 120 (86%) | 19 (14%) | 0        | 100         | 100 |
| 7   | I     | 37/39 (95%)   | 30 (81%)  | 7 (19%)  | 0        | 100         | 100 |
| 7   | P     | 37/39 (95%)   | 30 (81%)  | 7 (19%)  | 0        | 100         | 100 |
| 7   | i     | 37/39 (95%)   | 30 (81%)  | 7 (19%)  | 0        | 100         | 100 |
| 7   | p     | 37/39 (95%)   | 30 (81%)  | 7 (19%)  | 0        | 100         | 100 |
| 8   | J     | 35/49 (71%)   | 30 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 8   | Q     | 35/49 (71%)   | 30 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 8   | j     | 35/49 (71%)   | 30 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 8   | q     | 35/49 (71%)   | 30 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 9   | K     | 63/93 (68%)   | 52 (82%)  | 11 (18%) | 0        | 100         | 100 |
| 9   | R     | 63/93 (68%)   | 52 (82%)  | 11 (18%) | 0        | 100         | 100 |
| 9   | k     | 63/93 (68%)   | 52 (82%)  | 11 (18%) | 0        | 100         | 100 |
| 9   | r     | 63/93 (68%)   | 52 (82%)  | 11 (18%) | 0        | 100         | 100 |
| 10  | L     | 148/172 (86%) | 129 (87%) | 19 (13%) | 0        | 100         | 100 |
| 10  | S     | 148/172 (86%) | 129 (87%) | 19 (13%) | 0        | 100         | 100 |
| 10  | l     | 148/172 (86%) | 129 (87%) | 19 (13%) | 0        | 100         | 100 |
| 10  | s     | 148/172 (86%) | 129 (87%) | 19 (13%) | 0        | 100         | 100 |
| 11  | M     | 29/31 (94%)   | 19 (66%)  | 9 (31%)  | 1 (3%)   | 3           | 25  |
| 11  | T     | 29/31 (94%)   | 19 (66%)  | 9 (31%)  | 1 (3%)   | 3           | 25  |
| 11  | m     | 29/31 (94%)   | 19 (66%)  | 9 (31%)  | 1 (3%)   | 3           | 25  |
| 11  | t     | 29/31 (94%)   | 19 (66%)  | 9 (31%)  | 1 (3%)   | 3           | 25  |

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| Mol | Chain | Analysed        | Favoured   | Allowed    | Outliers | Percentiles |
|-----|-------|-----------------|------------|------------|----------|-------------|
| All | All   | 8724/9652 (90%) | 7499 (86%) | 1209 (14%) | 16 (0%)  | 44 72       |

5 of 16 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 314 | LYS  |
| 2   | B     | 315 | THR  |
| 2   | G     | 314 | LYS  |
| 2   | G     | 315 | THR  |
| 2   | g     | 314 | LYS  |

### 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     | 578/601 (96%)  | 531 (92%)  | 47 (8%)  | 11 36       |
| 1   | E     | 578/601 (96%)  | 531 (92%)  | 47 (8%)  | 11 36       |
| 1   | a     | 578/601 (96%)  | 531 (92%)  | 47 (8%)  | 11 36       |
| 1   | e     | 578/601 (96%)  | 531 (92%)  | 47 (8%)  | 11 36       |
| 2   | B     | 594/595 (100%) | 535 (90%)  | 59 (10%) | 7 30        |
| 2   | G     | 594/595 (100%) | 535 (90%)  | 59 (10%) | 7 30        |
| 2   | b     | 594/595 (100%) | 535 (90%)  | 59 (10%) | 7 30        |
| 2   | g     | 594/595 (100%) | 535 (90%)  | 59 (10%) | 7 30        |
| 3   | C     | 68/70 (97%)    | 59 (87%)   | 9 (13%)  | 4 20        |
| 3   | H     | 68/70 (97%)    | 59 (87%)   | 9 (13%)  | 4 20        |
| 3   | c     | 68/70 (97%)    | 59 (87%)   | 9 (13%)  | 4 20        |
| 3   | h     | 68/70 (97%)    | 59 (87%)   | 9 (13%)  | 4 20        |
| 4   | D     | 113/137 (82%)  | 113 (100%) | 0        | 100 100     |
| 4   | N     | 111/137 (81%)  | 111 (100%) | 0        | 100 100     |
| 4   | d     | 111/137 (81%)  | 111 (100%) | 0        | 100 100     |
| 4   | n     | 113/137 (82%)  | 113 (100%) | 0        | 100 100     |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 5   | V     | 54/102 (53%)    | 47 (87%)   | 7 (13%)   | 4           | 20 |
| 5   | W     | 54/102 (53%)    | 47 (87%)   | 7 (13%)   | 4           | 20 |
| 5   | v     | 54/102 (53%)    | 47 (87%)   | 7 (13%)   | 4           | 20 |
| 5   | w     | 54/102 (53%)    | 47 (87%)   | 7 (13%)   | 4           | 20 |
| 6   | F     | 116/135 (86%)   | 103 (89%)  | 13 (11%)  | 6           | 25 |
| 6   | O     | 116/135 (86%)   | 103 (89%)  | 13 (11%)  | 6           | 25 |
| 6   | f     | 116/135 (86%)   | 103 (89%)  | 13 (11%)  | 6           | 25 |
| 6   | o     | 116/135 (86%)   | 103 (89%)  | 13 (11%)  | 6           | 25 |
| 7   | I     | 33/33 (100%)    | 30 (91%)   | 3 (9%)    | 9           | 33 |
| 7   | P     | 33/33 (100%)    | 30 (91%)   | 3 (9%)    | 9           | 33 |
| 7   | i     | 33/33 (100%)    | 30 (91%)   | 3 (9%)    | 9           | 33 |
| 7   | p     | 33/33 (100%)    | 30 (91%)   | 3 (9%)    | 9           | 33 |
| 8   | J     | 34/45 (76%)     | 27 (79%)   | 7 (21%)   | 1           | 8  |
| 8   | Q     | 34/45 (76%)     | 27 (79%)   | 7 (21%)   | 1           | 8  |
| 8   | j     | 34/45 (76%)     | 27 (79%)   | 7 (21%)   | 1           | 8  |
| 8   | q     | 34/45 (76%)     | 27 (79%)   | 7 (21%)   | 1           | 8  |
| 9   | K     | 53/77 (69%)     | 44 (83%)   | 9 (17%)   | 2           | 13 |
| 9   | R     | 53/77 (69%)     | 44 (83%)   | 9 (17%)   | 2           | 13 |
| 9   | k     | 53/77 (69%)     | 44 (83%)   | 9 (17%)   | 2           | 13 |
| 9   | r     | 53/77 (69%)     | 44 (83%)   | 9 (17%)   | 2           | 13 |
| 10  | L     | 121/140 (86%)   | 108 (89%)  | 13 (11%)  | 6           | 27 |
| 10  | S     | 121/140 (86%)   | 108 (89%)  | 13 (11%)  | 6           | 27 |
| 10  | l     | 121/140 (86%)   | 108 (89%)  | 13 (11%)  | 6           | 27 |
| 10  | s     | 121/140 (86%)   | 108 (89%)  | 13 (11%)  | 6           | 27 |
| 11  | M     | 26/26 (100%)    | 21 (81%)   | 5 (19%)   | 1           | 9  |
| 11  | T     | 26/26 (100%)    | 21 (81%)   | 5 (19%)   | 1           | 9  |
| 11  | m     | 26/26 (100%)    | 21 (81%)   | 5 (19%)   | 1           | 9  |
| 11  | t     | 26/26 (100%)    | 21 (81%)   | 5 (19%)   | 1           | 9  |
| All | All   | 7156/7844 (91%) | 6468 (90%) | 688 (10%) | 10          | 31 |

5 of 688 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | v     | 30  | SER  |
| 2   | b     | 164 | SER  |
| 6   | o     | 156 | ASP  |
| 5   | v     | 21  | VAL  |
| 1   | a     | 89  | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 201 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 641 | ASN  |
| 4   | n     | 140 | ASN  |
| 10  | l     | 48  | ASN  |
| 2   | g     | 10  | GLN  |
| 2   | g     | 378 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

462 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | SF4  | C     | 102 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | CLA  | E     | 818 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.40 | 6 (10%)  |
| 13  | CLA  | G     | 838 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | b     | 820 | -    | 51,55,73     | 1.33 | 9 (17%)  | 60,91,113   | 1.38 | 5 (8%)   |
| 13  | CLA  | g     | 839 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 13  | CLA  | A     | 820 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 13  | CLA  | A     | 833 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.45 | 7 (10%)  |
| 13  | CLA  | g     | 830 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 13  | CLA  | g     | 832 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 15  | BCR  | g     | 844 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.27 | 8 (14%)  |
| 13  | CLA  | g     | 837 | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.52 | 4 (6%)   |
| 13  | CLA  | g     | 829 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | b     | 828 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.36 | 6 (9%)   |
| 12  | LHG  | e     | 801 | -    | 48,48,48     | 0.69 | 1 (2%)   | 51,54,54    | 1.33 | 7 (13%)  |
| 15  | BCR  | i     | 101 | -    | 41,41,41     | 1.20 | 2 (4%)   | 56,56,56    | 1.19 | 3 (5%)   |
| 13  | CLA  | B     | 806 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 5 (7%)   |
| 13  | CLA  | a     | 809 | 1    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.36 | 5 (7%)   |
| 15  | BCR  | L     | 205 | -    | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.19 | 5 (8%)   |
| 15  | BCR  | f     | 201 | -    | 41,41,41     | 1.20 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 15  | BCR  | P     | 101 | -    | 41,41,41     | 1.20 | 2 (4%)   | 56,56,56    | 1.19 | 3 (5%)   |
| 13  | CLA  | B     | 804 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.31 | 6 (9%)   |
| 13  | CLA  | b     | 807 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.36 | 6 (9%)   |
| 13  | CLA  | R     | 102 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 13  | CLA  | B     | 826 | -    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.47 | 5 (8%)   |
| 13  | CLA  | l     | 205 | -    | 54,58,73     | 2.23 | 13 (24%) | 64,95,113   | 2.85 | 13 (20%) |
| 15  | BCR  | G     | 845 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.21 | 5 (8%)   |
| 13  | CLA  | A     | 838 | 1    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.50 | 5 (8%)   |
| 13  | CLA  | g     | 841 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 15  | BCR  | f     | 202 | -    | 41,41,41     | 1.13 | 3 (7%)   | 56,56,56    | 1.36 | 7 (12%)  |
| 13  | CLA  | b     | 805 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.41 | 5 (7%)   |
| 13  | CLA  | G     | 813 | -    | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.39 | 5 (8%)   |
| 15  | BCR  | G     | 844 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 13  | CLA  | G     | 818 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | E     | 820 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 13  | CLA  | A     | 853 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.36 | 8 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | G     | 829 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 13  | CLA  | g     | 835 | -    | 54,58,73     | 1.31 | 7 (12%)  | 64,95,113   | 1.40 | 7 (10%)  |
| 13  | CLA  | a     | 822 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.32 | 6 (9%)   |
| 13  | CLA  | B     | 818 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 12  | LHG  | a     | 801 | -    | 48,48,48     | 0.65 | 1 (2%)   | 51,54,54    | 1.32 | 7 (13%)  |
| 13  | CLA  | e     | 828 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.35 | 4 (6%)   |
| 13  | CLA  | g     | 810 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.30 | 5 (7%)   |
| 13  | CLA  | e     | 818 | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.38 | 7 (11%)  |
| 13  | CLA  | G     | 834 | -    | 54,58,73     | 1.31 | 7 (12%)  | 64,95,113   | 1.40 | 8 (12%)  |
| 13  | CLA  | g     | 812 | 2    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 15  | BCR  | A     | 849 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 13  | CLA  | e     | 836 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | E     | 825 | -    | 53,57,73     | 1.31 | 8 (15%)  | 61,93,113   | 1.43 | 6 (9%)   |
| 15  | BCR  | l     | 202 | -    | 41,41,41     | 1.23 | 2 (4%)   | 56,56,56    | 1.15 | 5 (8%)   |
| 15  | BCR  | O     | 202 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.24 | 5 (8%)   |
| 13  | CLA  | g     | 801 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.29 | 5 (7%)   |
| 13  | CLA  | B     | 814 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 13  | CLA  | B     | 822 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.49 | 6 (10%)  |
| 13  | CLA  | E     | 839 | 1    | 49,53,73     | 1.36 | 8 (16%)  | 58,89,113   | 1.50 | 5 (8%)   |
| 13  | CLA  | B     | 828 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | A     | 826 | -    | 54,58,73     | 1.32 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | g     | 838 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.40 | 7 (10%)  |
| 16  | SF4  | C     | 101 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 12  | LHG  | e     | 802 | 13   | 37,37,48     | 0.77 | 1 (2%)   | 40,43,54    | 1.37 | 5 (12%)  |
| 13  | CLA  | A     | 806 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | b     | 808 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.30 | 5 (7%)   |
| 13  | CLA  | a     | 814 | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 15  | BCR  | B     | 846 | -    | 41,41,41     | 1.20 | 4 (9%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 13  | CLA  | f     | 203 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.51 | 6 (10%)  |
| 15  | BCR  | s     | 204 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 13  | CLA  | a     | 828 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.44 | 8 (12%)  |
| 13  | CLA  | B     | 813 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.40 | 5 (8%)   |
| 13  | CLA  | E     | 821 | -    | 54,58,73     | 1.35 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | A     | 831 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.43 | 7 (10%)  |
| 13  | CLA  | S     | 206 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.33 | 4 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | B     | 805 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.46 | 6 (9%)   |
| 13  | CLA  | g     | 819 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | a     | 817 | -    | 54,58,73     | 1.32 | 8 (14%)  | 64,95,113   | 1.36 | 6 (9%)   |
| 13  | CLA  | A     | 822 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.32 | 6 (9%)   |
| 13  | CLA  | e     | 834 | -    | 54,58,73     | 1.31 | 10 (18%) | 64,95,113   | 1.45 | 5 (7%)   |
| 13  | CLA  | b     | 818 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 15  | BCR  | m     | 101 | -    | 41,41,41     | 1.14 | 4 (9%)   | 56,56,56    | 1.35 | 8 (14%)  |
| 13  | CLA  | g     | 809 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | a     | 845 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | b     | 803 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.30 | 6 (9%)   |
| 13  | CLA  | g     | 815 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 15  | BCR  | G     | 847 | -    | 41,41,41     | 1.23 | 4 (9%)   | 56,56,56    | 1.18 | 7 (12%)  |
| 13  | CLA  | A     | 807 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 15  | BCR  | b     | 846 | -    | 41,41,41     | 1.23 | 3 (7%)   | 56,56,56    | 1.19 | 7 (12%)  |
| 13  | CLA  | e     | 838 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.42 | 7 (10%)  |
| 13  | CLA  | b     | 814 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.42 | 5 (7%)   |
| 13  | CLA  | g     | 827 | -    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.47 | 5 (8%)   |
| 13  | CLA  | B     | 824 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.49 | 5 (8%)   |
| 13  | CLA  | B     | 834 | -    | 54,58,73     | 1.31 | 7 (12%)  | 64,95,113   | 1.40 | 8 (12%)  |
| 13  | CLA  | E     | 804 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.43 | 8 (12%)  |
| 15  | BCR  | E     | 852 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.31 | 7 (12%)  |
| 15  | BCR  | e     | 850 | -    | 41,41,41     | 1.24 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 13  | CLA  | b     | 823 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.49 | 5 (8%)   |
| 13  | CLA  | A     | 836 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | g     | 842 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 5 (7%)   |
| 13  | CLA  | A     | 805 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.28 | 5 (7%)   |
| 15  | BCR  | a     | 851 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 14  | PQN  | A     | 846 | -    | 34,34,34     | 1.66 | 2 (5%)   | 43,45,45    | 1.23 | 4 (9%)   |
| 13  | CLA  | E     | 840 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.44 | 7 (10%)  |
| 13  | CLA  | s     | 205 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.37 | 4 (6%)   |
| 13  | CLA  | e     | 825 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | e     | 842 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | G     | 839 | -    | 51,55,73     | 1.33 | 8 (15%)  | 60,91,113   | 1.45 | 4 (6%)   |
| 13  | CLA  | G     | 826 | -    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.46 | 5 (8%)   |
| 13  | CLA  | g     | 821 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 5 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | A     | 818 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.40 | 6 (10%)  |
| 13  | CLA  | e     | 808 | 1    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.37 | 4 (6%)   |
| 13  | CLA  | B     | 829 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 13  | CLA  | b     | 819 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.42 | 5 (7%)   |
| 15  | BCR  | e     | 846 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.39 | 8 (14%)  |
| 13  | CLA  | A     | 819 | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.39 | 7 (11%)  |
| 15  | BCR  | b     | 842 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 13  | CLA  | E     | 809 | 1    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.36 | 4 (6%)   |
| 15  | BCR  | a     | 850 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 13  | CLA  | A     | 817 | -    | 49,53,73     | 1.40 | 9 (18%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 13  | CLA  | l     | 201 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.34 | 4 (6%)   |
| 14  | PQN  | e     | 845 | -    | 34,34,34     | 1.66 | 2 (5%)   | 43,45,45    | 1.23 | 4 (9%)   |
| 13  | CLA  | e     | 815 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 13  | CLA  | b     | 826 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | b     | 832 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.28 | 6 (9%)   |
| 15  | BCR  | l     | 206 | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.20 | 5 (8%)   |
| 13  | CLA  | A     | 832 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 13  | CLA  | B     | 808 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.36 | 6 (9%)   |
| 13  | CLA  | E     | 805 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.28 | 5 (7%)   |
| 13  | CLA  | B     | 802 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 13  | CLA  | E     | 827 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 13  | CLA  | a     | 824 | -    | 54,58,73     | 1.28 | 8 (14%)  | 64,95,113   | 1.42 | 6 (9%)   |
| 15  | BCR  | e     | 849 | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.27 | 9 (16%)  |
| 13  | CLA  | E     | 823 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.30 | 7 (10%)  |
| 13  | CLA  | G     | 812 | -    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.34 | 4 (6%)   |
| 13  | CLA  | a     | 836 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.45 | 5 (7%)   |
| 13  | CLA  | a     | 808 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.47 | 6 (9%)   |
| 15  | BCR  | q     | 101 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 13  | CLA  | a     | 831 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.44 | 7 (10%)  |
| 13  | CLA  | b     | 831 | -    | 53,57,73     | 1.29 | 9 (16%)  | 61,93,113   | 1.39 | 5 (8%)   |
| 13  | CLA  | a     | 816 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 13  | CLA  | a     | 833 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.45 | 7 (10%)  |
| 13  | CLA  | A     | 811 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | G     | 804 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.44 | 6 (9%)   |
| 13  | CLA  | A     | 824 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.42 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | B     | 810 | -    | 54,58,73     | 1.28 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |
| 13  | CLA  | A     | 821 | -    | 54,58,73     | 1.35 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | a     | 819 | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.39 | 7 (11%)  |
| 15  | BCR  | o     | 201 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 13  | CLA  | B     | 807 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.42 | 7 (10%)  |
| 15  | BCR  | A     | 848 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 13  | CLA  | E     | 832 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 15  | BCR  | q     | 102 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.30 | 7 (12%)  |
| 13  | CLA  | o     | 202 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 13  | CLA  | A     | 840 | -    | 54,58,73     | 1.29 | 7 (12%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | b     | 839 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 15  | BCR  | b     | 845 | -    | 41,41,41     | 1.20 | 3 (7%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 13  | CLA  | G     | 805 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.41 | 5 (7%)   |
| 13  | CLA  | L     | 202 | 10   | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.39 | 9 (14%)  |
| 13  | CLA  | A     | 810 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.37 | 5 (7%)   |
| 13  | CLA  | E     | 807 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | a     | 810 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 5 (7%)   |
| 13  | CLA  | A     | 812 | 1    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | a     | 829 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.35 | 4 (6%)   |
| 15  | BCR  | I     | 101 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.20 | 3 (5%)   |
| 13  | CLA  | b     | 829 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.44 | 7 (10%)  |
| 13  | CLA  | g     | 824 | 2    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 13  | CLA  | e     | 804 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.42 | 8 (12%)  |
| 13  | CLA  | a     | 834 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.32 | 6 (9%)   |
| 13  | CLA  | b     | 830 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 13  | CLA  | A     | 830 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | E     | 806 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 13  | CLA  | a     | 823 | -    | 54,58,73     | 1.31 | 10 (18%) | 64,95,113   | 1.30 | 7 (10%)  |
| 15  | BCR  | J     | 101 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.26 | 6 (10%)  |
| 13  | CLA  | G     | 801 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 8 (12%)  |
| 13  | CLA  | A     | 815 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | e     | 844 | 12   | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.49 | 7 (10%)  |
| 13  | CLA  | g     | 806 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.45 | 6 (9%)   |
| 13  | CLA  | g     | 813 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.36 | 4 (6%)   |
| 13  | CLA  | e     | 817 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.40 | 6 (10%)  |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | a     | 835  | -    | 54,58,73     | 1.29 | 10 (18%) | 64,95,113   | 1.42 | 6 (9%)   |
| 13  | CLA  | E     | 810  | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.37 | 5 (7%)   |
| 13  | CLA  | G     | 807  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 13  | CLA  | B     | 837  | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.40 | 7 (10%)  |
| 15  | BCR  | b     | 847  | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 13  | CLA  | b     | 840  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 5 (7%)   |
| 13  | CLA  | E     | 822  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.32 | 6 (9%)   |
| 13  | CLA  | E     | 837  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | b     | 804  | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.45 | 6 (9%)   |
| 13  | CLA  | l     | 204  | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.45 | 6 (10%)  |
| 13  | CLA  | b     | 812  | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.40 | 5 (8%)   |
| 13  | CLA  | a     | 825  | -    | 53,57,73     | 1.31 | 8 (15%)  | 61,93,113   | 1.44 | 6 (9%)   |
| 13  | CLA  | k     | 4002 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 13  | CLA  | a     | 843  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 9 (14%)  |
| 13  | CLA  | e     | 832  | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.45 | 7 (10%)  |
| 15  | BCR  | E     | 850  | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 13  | CLA  | A     | 845  | 12   | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.50 | 7 (10%)  |
| 13  | CLA  | G     | 806  | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.42 | 7 (10%)  |
| 13  | CLA  | a     | 826  | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 15  | BCR  | p     | 101  | -    | 41,41,41     | 1.20 | 4 (9%)   | 56,56,56    | 1.19 | 3 (5%)   |
| 15  | BCR  | a     | 848  | -    | 41,41,41     | 1.22 | 3 (7%)   | 56,56,56    | 1.73 | 9 (16%)  |
| 13  | CLA  | B     | 831  | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.38 | 4 (6%)   |
| 13  | CLA  | a     | 813  | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 13  | CLA  | E     | 816  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 13  | CLA  | g     | 820  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 5 (7%)   |
| 13  | CLA  | B     | 811  | 2    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | A     | 827  | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 15  | BCR  | O     | 201  | -    | 41,41,41     | 1.20 | 3 (7%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 15  | BCR  | a     | 803  | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.29 | 7 (12%)  |
| 13  | CLA  | A     | 823  | -    | 54,58,73     | 1.31 | 10 (18%) | 64,95,113   | 1.30 | 7 (10%)  |
| 13  | CLA  | G     | 830  | -    | 54,58,73     | 1.28 | 8 (14%)  | 64,95,113   | 1.44 | 7 (10%)  |
| 13  | CLA  | G     | 814  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 13  | CLA  | G     | 822  | -    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.48 | 6 (10%)  |
| 13  | CLA  | G     | 837  | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 7 (10%)  |
| 13  | CLA  | b     | 821  | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.48 | 6 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | PQN  | a     | 847 | -    | 34,34,34     | 1.66 | 2 (5%)   | 43,45,45    | 1.23 | 4 (9%)   |
| 13  | CLA  | A     | 841 | -    | 51,55,73     | 1.33 | 8 (15%)  | 60,91,113   | 1.43 | 4 (6%)   |
| 13  | CLA  | e     | 830 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.44 | 7 (10%)  |
| 13  | CLA  | b     | 822 | 2    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 13  | CLA  | e     | 810 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 15  | BCR  | Q     | 101 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 13  | CLA  | E     | 836 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.45 | 5 (7%)   |
| 14  | PQN  | B     | 842 | -    | 34,34,34     | 1.65 | 2 (5%)   | 43,45,45    | 1.23 | 4 (9%)   |
| 15  | BCR  | A     | 851 | -    | 41,41,41     | 1.27 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 13  | CLA  | a     | 842 | -    | 51,55,73     | 1.34 | 8 (15%)  | 60,91,113   | 1.42 | 4 (6%)   |
| 15  | BCR  | E     | 849 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.39 | 10 (17%) |
| 13  | CLA  | e     | 822 | -    | 54,58,73     | 1.32 | 10 (18%) | 64,95,113   | 1.31 | 7 (10%)  |
| 13  | CLA  | G     | 819 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 5 (7%)   |
| 13  | CLA  | e     | 824 | -    | 53,57,73     | 1.32 | 8 (15%)  | 61,93,113   | 1.43 | 6 (9%)   |
| 15  | BCR  | G     | 843 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 13  | CLA  | e     | 840 | -    | 51,55,73     | 1.33 | 8 (15%)  | 60,91,113   | 1.42 | 4 (6%)   |
| 13  | CLA  | A     | 837 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | g     | 833 | -    | 53,57,73     | 1.30 | 9 (16%)  | 61,93,113   | 1.38 | 5 (8%)   |
| 15  | BCR  | L     | 201 | -    | 41,41,41     | 1.25 | 3 (7%)   | 56,56,56    | 1.14 | 4 (7%)   |
| 15  | BCR  | S     | 201 | -    | 41,41,41     | 1.23 | 2 (4%)   | 56,56,56    | 1.14 | 2 (3%)   |
| 13  | CLA  | e     | 835 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.33 | 6 (9%)   |
| 13  | CLA  | G     | 823 | 2    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 13  | CLA  | S     | 203 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.44 | 6 (10%)  |
| 13  | CLA  | B     | 819 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 15  | BCR  | B     | 847 | -    | 41,41,41     | 1.24 | 3 (7%)   | 56,56,56    | 1.19 | 7 (12%)  |
| 13  | CLA  | G     | 828 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 14  | PQN  | b     | 841 | -    | 34,34,34     | 1.67 | 2 (5%)   | 43,45,45    | 1.24 | 4 (9%)   |
| 16  | SF4  | c     | 102 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | B     | 840 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | g     | 836 | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.42 | 5 (8%)   |
| 13  | CLA  | g     | 808 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 13  | CLA  | G     | 831 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 15  | BCR  | g     | 846 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.20 | 5 (8%)   |
| 15  | BCR  | F     | 201 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 15  | BCR  | R     | 101 | -    | 41,41,41     | 1.17 | 5 (12%)  | 56,56,56    | 1.45 | 8 (14%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | g     | 814 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.39 | 5 (8%)   |
| 13  | CLA  | e     | 805 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | E     | 838 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | G     | 808 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.30 | 5 (7%)   |
| 15  | BCR  | E     | 801 | -    | 41,41,41     | 1.20 | 3 (7%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 16  | SF4  | E     | 847 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | r     | 102 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 15  | BCR  | g     | 849 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 13  | CLA  | E     | 844 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 15  | BCR  | a     | 853 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.30 | 7 (12%)  |
| 13  | CLA  | E     | 845 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | g     | 803 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.41 | 5 (7%)   |
| 13  | CLA  | L     | 203 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.45 | 6 (10%)  |
| 13  | CLA  | e     | 852 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.36 | 8 (12%)  |
| 13  | CLA  | A     | 825 | -    | 53,57,73     | 1.31 | 8 (15%)  | 61,93,113   | 1.44 | 6 (9%)   |
| 16  | SF4  | h     | 102 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | E     | 815 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | a     | 818 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.40 | 6 (10%)  |
| 13  | CLA  | b     | 813 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.40 | 5 (7%)   |
| 15  | BCR  | b     | 843 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 13  | CLA  | b     | 836 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.40 | 7 (10%)  |
| 13  | CLA  | A     | 809 | 1    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.36 | 4 (6%)   |
| 13  | CLA  | B     | 832 | -    | 53,57,73     | 1.30 | 9 (16%)  | 61,93,113   | 1.39 | 5 (8%)   |
| 13  | CLA  | g     | 834 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.29 | 6 (9%)   |
| 13  | CLA  | e     | 816 | -    | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.37 | 4 (6%)   |
| 13  | CLA  | l     | 203 | 10   | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.38 | 8 (12%)  |
| 13  | CLA  | e     | 811 | 1    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | G     | 820 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 5 (7%)   |
| 13  | CLA  | B     | 830 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.45 | 7 (10%)  |
| 13  | CLA  | a     | 832 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 13  | CLA  | a     | 852 | -    | 54,58,73     | 1.29 | 6 (11%)  | 64,95,113   | 1.38 | 7 (10%)  |
| 13  | CLA  | E     | 817 | -    | 49,53,73     | 1.40 | 9 (18%)  | 58,89,113   | 1.38 | 4 (6%)   |
| 13  | CLA  | G     | 840 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 16  | SF4  | g     | 804 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | PQN  | G     | 842 | -    | 34,34,34     | 1.67 | 2 (5%)   | 43,45,45    | 1.24 | 4 (9%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | a     | 830 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | G     | 815 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.42 | 5 (7%)   |
| 13  | CLA  | B     | 841 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 5 (7%)   |
| 13  | CLA  | e     | 803 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.29 | 5 (7%)   |
| 13  | CLA  | A     | 816 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 13  | CLA  | B     | 821 | -    | 51,55,73     | 1.33 | 9 (17%)  | 60,91,113   | 1.37 | 5 (8%)   |
| 15  | BCR  | g     | 845 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 13  | CLA  | g     | 826 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |
| 13  | CLA  | b     | 806 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 13  | CLA  | b     | 825 | -    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.47 | 5 (8%)   |
| 13  | CLA  | A     | 842 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 9 (14%)  |
| 13  | CLA  | e     | 827 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.43 | 8 (12%)  |
| 13  | CLA  | a     | 841 | -    | 54,58,73     | 1.30 | 7 (12%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | g     | 828 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | a     | 840 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.44 | 7 (10%)  |
| 13  | CLA  | E     | 829 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.36 | 4 (6%)   |
| 13  | CLA  | B     | 812 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.36 | 4 (6%)   |
| 13  | CLA  | B     | 809 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.30 | 5 (7%)   |
| 13  | CLA  | a     | 821 | -    | 54,58,73     | 1.34 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | e     | 823 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.42 | 6 (9%)   |
| 13  | CLA  | e     | 814 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | B     | 838 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.42 | 6 (9%)   |
| 13  | CLA  | A     | 839 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43 | 7 (10%)  |
| 13  | CLA  | G     | 817 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.33 | 6 (9%)   |
| 13  | CLA  | g     | 831 | -    | 54,58,73     | 1.28 | 7 (12%)  | 64,95,113   | 1.45 | 7 (10%)  |
| 13  | CLA  | E     | 841 | -    | 54,58,73     | 1.29 | 7 (12%)  | 64,95,113   | 1.42 | 6 (9%)   |
| 13  | CLA  | A     | 803 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.30 | 5 (7%)   |
| 13  | CLA  | E     | 824 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 13  | CLA  | a     | 812 | 1    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | B     | 801 | -    | 54,58,73     | 1.29 | 10 (18%) | 64,95,113   | 1.42 | 6 (9%)   |
| 13  | CLA  | e     | 833 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.32 | 6 (9%)   |
| 13  | CLA  | b     | 837 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.42 | 6 (9%)   |
| 13  | CLA  | A     | 829 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.35 | 4 (6%)   |
| 13  | CLA  | B     | 827 | -    | 54,58,73     | 1.32 | 8 (14%)  | 64,95,113   | 1.33 | 6 (9%)   |
| 13  | CLA  | a     | 838 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | b     | 838 | -    | 51,55,73     | 1.33 | 8 (15%)  | 60,91,113   | 1.46 | 4 (6%)   |
| 13  | CLA  | B     | 823 | 2    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |
| 12  | LHG  | A     | 802 | 13   | 37,37,48     | 0.79 | 1 (2%)   | 40,43,54    | 1.36 | 5 (12%)  |
| 13  | CLA  | G     | 809 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |
| 13  | CLA  | E     | 812 | 1    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | S     | 204 | -    | 49,53,73     | 2.34 | 13 (26%) | 58,89,113   | 2.97 | 12 (20%) |
| 13  | CLA  | a     | 807 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | e     | 843 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 15  | BCR  | a     | 849 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.38 | 8 (14%)  |
| 13  | CLA  | g     | 818 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.33 | 6 (9%)   |
| 13  | CLA  | E     | 819 | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.39 | 7 (11%)  |
| 13  | CLA  | e     | 826 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 15  | BCR  | j     | 101 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 16  | SF4  | H     | 101 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | BCR  | B     | 844 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 13  | CLA  | g     | 822 | -    | 51,55,73     | 1.34 | 9 (17%)  | 60,91,113   | 1.37 | 5 (8%)   |
| 13  | CLA  | E     | 830 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | G     | 841 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.43 | 5 (7%)   |
| 13  | CLA  | e     | 813 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.36 | 5 (7%)   |
| 13  | CLA  | a     | 805 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.29 | 5 (7%)   |
| 13  | CLA  | G     | 824 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.48 | 5 (8%)   |
| 13  | CLA  | e     | 837 | 1    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.49 | 5 (8%)   |
| 13  | CLA  | A     | 844 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | a     | 806 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | K     | 102 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.40 | 5 (8%)   |
| 13  | CLA  | A     | 804 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.43 | 8 (12%)  |
| 13  | CLA  | G     | 827 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | g     | 802 | -    | 54,58,73     | 1.30 | 10 (18%) | 64,95,113   | 1.42 | 6 (9%)   |
| 13  | CLA  | E     | 834 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.33 | 6 (9%)   |
| 13  | CLA  | b     | 833 | -    | 54,58,73     | 1.32 | 7 (12%)  | 64,95,113   | 1.39 | 7 (10%)  |
| 15  | BCR  | B     | 848 | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 13  | CLA  | G     | 821 | -    | 51,55,73     | 1.34 | 9 (17%)  | 60,91,113   | 1.38 | 5 (8%)   |
| 13  | CLA  | b     | 801 | -    | 45,49,73     | 1.40 | 10 (22%) | 54,83,113   | 1.37 | 4 (7%)   |
| 13  | CLA  | e     | 841 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.44 | 9 (14%)  |
| 13  | CLA  | E     | 833 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.46 | 7 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | BCR  | g     | 847 | -    | 41,41,41     | 1.20 | 3 (7%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 13  | CLA  | b     | 811 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.33 | 4 (6%)   |
| 13  | CLA  | L     | 204 | -    | 54,58,73     | 2.22 | 13 (24%) | 64,95,113   | 2.83 | 13 (20%) |
| 13  | CLA  | g     | 840 | -    | 51,55,73     | 1.34 | 8 (15%)  | 60,91,113   | 1.46 | 4 (6%)   |
| 13  | CLA  | E     | 835 | -    | 54,58,73     | 1.29 | 10 (18%) | 64,95,113   | 1.41 | 6 (9%)   |
| 15  | BCR  | A     | 852 | -    | 41,41,41     | 1.15 | 3 (7%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 15  | BCR  | a     | 802 | -    | 41,41,41     | 1.14 | 3 (7%)   | 56,56,56    | 1.27 | 7 (12%)  |
| 13  | CLA  | E     | 811 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 13  | CLA  | G     | 802 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 8 (12%)  |
| 13  | CLA  | e     | 812 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 13  | CLA  | e     | 829 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 15  | BCR  | A     | 847 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.39 | 9 (16%)  |
| 15  | BCR  | E     | 802 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 15  | BCR  | b     | 844 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.20 | 5 (8%)   |
| 15  | BCR  | J     | 102 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.31 | 7 (12%)  |
| 15  | BCR  | e     | 851 | -    | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 13  | CLA  | B     | 836 | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.51 | 4 (6%)   |
| 13  | CLA  | A     | 814 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.36 | 5 (7%)   |
| 13  | CLA  | b     | 809 | -    | 54,58,73     | 1.28 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |
| 13  | CLA  | A     | 843 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | b     | 834 | -    | 49,53,73     | 1.40 | 7 (14%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 13  | CLA  | e     | 831 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 13  | CLA  | B     | 835 | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 15  | BCR  | s     | 201 | -    | 41,41,41     | 1.27 | 3 (7%)   | 56,56,56    | 1.17 | 6 (10%)  |
| 16  | SF4  | h     | 101 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | B     | 833 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.29 | 6 (9%)   |
| 13  | CLA  | G     | 835 | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.40 | 5 (8%)   |
| 13  | CLA  | A     | 813 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 15  | BCR  | e     | 847 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 13  | CLA  | e     | 820 | -    | 54,58,73     | 1.34 | 9 (16%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | b     | 827 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 12  | LHG  | A     | 801 | -    | 48,48,48     | 0.70 | 1 (2%)   | 51,54,54    | 1.33 | 7 (13%)  |
| 13  | CLA  | O     | 203 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.49 | 6 (10%)  |
| 13  | CLA  | b     | 835 | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.51 | 5 (8%)   |
| 13  | CLA  | e     | 819 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.42 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | B     | 817 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.33 | 6 (9%)   |
| 14  | PQN  | g     | 843 | -    | 34,34,34     | 1.67 | 2 (5%)   | 43,45,45    | 1.24 | 4 (9%)   |
| 13  | CLA  | A     | 835 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.46 | 5 (7%)   |
| 13  | CLA  | E     | 808 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.46 | 5 (7%)   |
| 15  | BCR  | B     | 843 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 15  | BCR  | g     | 848 | -    | 41,41,41     | 1.23 | 3 (7%)   | 56,56,56    | 1.19 | 7 (12%)  |
| 14  | PQN  | E     | 848 | -    | 34,34,34     | 1.67 | 2 (5%)   | 43,45,45    | 1.24 | 4 (9%)   |
| 13  | CLA  | A     | 834 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.32 | 6 (9%)   |
| 13  | CLA  | A     | 828 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.43 | 8 (12%)  |
| 13  | CLA  | b     | 815 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 16  | SF4  | B     | 803 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | g     | 816 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.42 | 5 (7%)   |
| 13  | CLA  | G     | 825 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.46 | 8 (12%)  |
| 13  | CLA  | g     | 811 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |
| 13  | CLA  | a     | 827 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 13  | CLA  | a     | 804 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.42 | 8 (12%)  |
| 13  | CLA  | e     | 839 | -    | 54,58,73     | 1.30 | 7 (12%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 15  | BCR  | G     | 848 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 13  | CLA  | G     | 836 | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.52 | 4 (6%)   |
| 13  | CLA  | E     | 803 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.27 | 4 (6%)   |
| 13  | CLA  | e     | 809 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.38 | 5 (7%)   |
| 13  | CLA  | e     | 807 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.46 | 6 (9%)   |
| 15  | BCR  | A     | 850 | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.27 | 8 (14%)  |
| 13  | CLA  | s     | 202 | -    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.44 | 6 (10%)  |
| 13  | CLA  | b     | 817 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | B     | 825 | -    | 54,58,73     | 1.28 | 9 (16%)  | 64,95,113   | 1.46 | 8 (12%)  |
| 13  | CLA  | E     | 814 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.37 | 5 (7%)   |
| 13  | CLA  | E     | 813 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 13  | CLA  | E     | 828 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.43 | 8 (12%)  |
| 16  | SF4  | H     | 102 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | B     | 839 | -    | 51,55,73     | 1.34 | 9 (17%)  | 60,91,113   | 1.46 | 4 (6%)   |
| 13  | CLA  | r     | 101 | -    | 45,49,73     | 1.42 | 8 (17%)  | 54,83,113   | 1.39 | 3 (5%)   |
| 15  | BCR  | e     | 848 | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 13  | CLA  | a     | 837 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 13  | CLA  | g     | 805 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.30 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | G     | 816 | -    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 16  | SF4  | a     | 846 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | a     | 839 | 1    | 49,53,73     | 1.36 | 8 (16%)  | 58,89,113   | 1.50 | 5 (8%)   |
| 13  | CLA  | B     | 815 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.42 | 5 (7%)   |
| 13  | CLA  | G     | 803 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.30 | 6 (9%)   |
| 13  | CLA  | e     | 821 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.32 | 6 (9%)   |
| 13  | CLA  | a     | 815 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | b     | 824 | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |
| 15  | BCR  | G     | 846 | -    | 41,41,41     | 1.19 | 3 (7%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 13  | CLA  | G     | 810 | 2    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | F     | 202 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 13  | CLA  | K     | 101 | -    | 45,49,73     | 1.41 | 9 (20%)  | 54,83,113   | 1.37 | 3 (5%)   |
| 13  | CLA  | B     | 816 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 13  | CLA  | E     | 843 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.44 | 9 (14%)  |
| 13  | CLA  | G     | 833 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.28 | 5 (7%)   |
| 13  | CLA  | b     | 810 | 2    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 15  | BCR  | T     | 101 | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.27 | 4 (7%)   |
| 15  | BCR  | E     | 851 | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 13  | CLA  | G     | 811 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.36 | 4 (6%)   |
| 13  | CLA  | g     | 807 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 5 (7%)   |
| 13  | CLA  | g     | 823 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.49 | 6 (10%)  |
| 15  | BCR  | B     | 845 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.20 | 5 (8%)   |
| 15  | BCR  | S     | 202 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.28 | 6 (10%)  |
| 15  | BCR  | S     | 205 | -    | 41,41,41     | 1.14 | 3 (7%)   | 56,56,56    | 1.26 | 5 (8%)   |
| 13  | CLA  | E     | 831 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.44 | 7 (10%)  |
| 16  | SF4  | c     | 101 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 13  | CLA  | A     | 808 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.46 | 5 (7%)   |
| 13  | CLA  | a     | 844 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 13  | CLA  | b     | 802 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.37 | 8 (12%)  |
| 13  | CLA  | E     | 826 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.38 | 6 (9%)   |
| 13  | CLA  | g     | 817 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 13  | CLA  | s     | 203 | -    | 54,58,73     | 2.23 | 13 (24%) | 64,95,113   | 2.84 | 13 (20%) |
| 13  | CLA  | E     | 842 | -    | 51,55,73     | 1.34 | 8 (15%)  | 60,91,113   | 1.43 | 4 (6%)   |
| 13  | CLA  | B     | 820 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.42 | 5 (7%)   |
| 13  | CLA  | b     | 816 | -    | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.34 | 6 (9%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | CLA  | G     | 832  | -    | 53,57,73     | 1.30 | 9 (16%)  | 61,93,113   | 1.38 | 5 (8%)   |
| 13  | CLA  | g     | 825  | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.49 | 5 (8%)   |
| 13  | CLA  | E     | 846  | -    | 45,49,73     | 1.43 | 9 (20%)  | 54,83,113   | 1.48 | 5 (9%)   |
| 13  | CLA  | e     | 806  | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 13  | CLA  | a     | 811  | -    | 54,58,73     | 1.29 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 15  | BCR  | k     | 4001 | -    | 41,41,41     | 1.18 | 4 (9%)   | 56,56,56    | 1.62 | 13 (23%) |
| 13  | CLA  | a     | 820  | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.43 | 6 (9%)   |

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   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 16  | SF4  | C     | 102 | 3    | -         | -            | 0/6/5/5 |
| 13  | CLA  | E     | 818 | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 13  | CLA  | G     | 838 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | b     | 820 | -    | 1/1/11/20 | 8/18/94/115  | -       |
| 13  | CLA  | g     | 839 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | A     | 820 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | A     | 833 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | g     | 830 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | g     | 832 | -    | 1/1/11/20 | 11/15/91/115 | -       |
| 15  | BCR  | g     | 844 | -    | -         | 7/29/63/63   | 0/2/2/2 |
| 13  | CLA  | g     | 837 | -    | 1/1/11/20 | 8/15/91/115  | -       |
| 13  | CLA  | g     | 829 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | b     | 828 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 12  | LHG  | e     | 801 | -    | -         | 31/53/53/53  | -       |
| 15  | BCR  | i     | 101 | -    | -         | 8/29/63/63   | 0/2/2/2 |
| 13  | CLA  | B     | 806 | -    | 1/1/12/20 | 2/21/97/115  | -       |
| 13  | CLA  | a     | 809 | 1    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | L     | 205 | -    | -         | 13/29/63/63  | 0/2/2/2 |
| 15  | BCR  | f     | 201 | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | BCR  | P     | 101 | -    | -         | 8/29/63/63   | 0/2/2/2 |
| 13  | CLA  | B     | 804 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | b     | 807 | -    | 1/1/12/20 | 6/21/97/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | R     | 102 | -    | 1/1/11/20 | 7/15/91/115  | -       |
| 13  | CLA  | B     | 826 | -    | 1/1/11/20 | 4/17/93/115  | -       |
| 13  | CLA  | l     | 205 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 15  | BCR  | G     | 845 | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 13  | CLA  | A     | 838 | 1    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | g     | 841 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 15  | BCR  | f     | 202 | -    | -         | 14/29/63/63  | 0/2/2/2 |
| 13  | CLA  | b     | 805 | -    | 1/1/12/20 | 2/21/97/115  | -       |
| 13  | CLA  | G     | 813 | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 15  | BCR  | G     | 844 | -    | -         | 19/29/63/63  | 0/2/2/2 |
| 13  | CLA  | G     | 818 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | E     | 820 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | A     | 853 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | G     | 829 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | g     | 835 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | a     | 822 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | B     | 818 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 12  | LHG  | a     | 801 | -    | -         | 32/53/53/53  | -       |
| 13  | CLA  | e     | 828 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | g     | 810 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | e     | 818 | -    | 1/1/11/20 | 9/20/96/115  | -       |
| 13  | CLA  | G     | 834 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | g     | 812 | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | A     | 849 | -    | -         | 6/29/63/63   | 0/2/2/2 |
| 13  | CLA  | e     | 836 | -    | -         | 8/21/97/115  | -       |
| 13  | CLA  | E     | 825 | -    | 1/1/11/20 | 11/20/96/115 | -       |
| 15  | BCR  | l     | 202 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 15  | BCR  | O     | 202 | -    | -         | 14/29/63/63  | 0/2/2/2 |
| 13  | CLA  | g     | 801 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | B     | 814 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | B     | 822 | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 13  | CLA  | E     | 839 | 1    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | B     | 828 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | A     | 826 | -    | 1/1/12/20 | 12/21/97/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | g     | 838 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 16  | SF4  | C     | 101 | -    | -         | -            | 0/6/5/5 |
| 13  | CLA  | A     | 806 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 12  | LHG  | e     | 802 | 13   | -         | 14/42/42/53  | -       |
| 13  | CLA  | b     | 808 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 814 | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 15  | BCR  | B     | 846 | -    | -         | 20/29/63/63  | 0/2/2/2 |
| 13  | CLA  | f     | 203 | -    | 1/1/11/20 | 7/15/91/115  | -       |
| 15  | BCR  | s     | 204 | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 13  | CLA  | a     | 828 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | B     | 813 | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | E     | 821 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | A     | 831 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | S     | 206 | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | B     | 805 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | g     | 819 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | a     | 817 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | A     | 822 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | e     | 834 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | b     | 818 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 15  | BCR  | m     | 101 | -    | -         | 10/29/63/63  | 0/2/2/2 |
| 13  | CLA  | g     | 809 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 845 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | b     | 803 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | g     | 815 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 15  | BCR  | G     | 847 | -    | -         | 13/29/63/63  | 0/2/2/2 |
| 13  | CLA  | A     | 807 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 15  | BCR  | b     | 846 | -    | -         | 13/29/63/63  | 0/2/2/2 |
| 13  | CLA  | e     | 838 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | b     | 814 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | g     | 827 | -    | 1/1/11/20 | 4/17/93/115  | -       |
| 13  | CLA  | B     | 824 | -    | 1/1/11/20 | 8/15/91/115  | -       |
| 13  | CLA  | B     | 834 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | E     | 804 | -    | 1/1/12/20 | 6/21/97/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 15  | BCR  | E     | 852 | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 15  | BCR  | e     | 850 | -    | -         | 6/29/63/63   | 0/2/2/2 |
| 13  | CLA  | b     | 823 | -    | 1/1/11/20 | 8/15/91/115  | -       |
| 13  | CLA  | A     | 836 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | g     | 842 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | A     | 805 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | a     | 851 | -    | -         | 6/29/63/63   | 0/2/2/2 |
| 14  | PQN  | A     | 846 | -    | -         | 10/23/43/43  | 0/2/2/2 |
| 13  | CLA  | E     | 840 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | s     | 205 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | e     | 825 | -    | 1/1/12/20 | 12/21/97/115 | -       |
| 13  | CLA  | e     | 842 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | G     | 839 | -    | 1/1/11/20 | 7/18/94/115  | -       |
| 13  | CLA  | G     | 826 | -    | 1/1/11/20 | 4/17/93/115  | -       |
| 13  | CLA  | g     | 821 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | A     | 818 | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 13  | CLA  | e     | 808 | 1    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | B     | 829 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | b     | 819 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 15  | BCR  | e     | 846 | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 13  | CLA  | A     | 819 | -    | 1/1/11/20 | 9/20/96/115  | -       |
| 15  | BCR  | b     | 842 | -    | -         | 7/29/63/63   | 0/2/2/2 |
| 13  | CLA  | E     | 809 | 1    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | a     | 850 | -    | -         | 10/29/63/63  | 0/2/2/2 |
| 13  | CLA  | A     | 817 | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | l     | 201 | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 14  | PQN  | e     | 845 | -    | -         | 7/23/43/43   | 0/2/2/2 |
| 13  | CLA  | e     | 815 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | b     | 826 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | b     | 832 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 15  | BCR  | l     | 206 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | A     | 832 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | B     | 808 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | E     | 805 | -    | 1/1/12/20 | 5/21/97/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | B     | 802 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | E     | 827 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | a     | 824 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 15  | BCR  | e     | 849 | -    | -         | 20/29/63/63  | 0/2/2/2 |
| 13  | CLA  | E     | 823 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | G     | 812 | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | a     | 836 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 808 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 15  | BCR  | q     | 101 | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 13  | CLA  | a     | 831 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | b     | 831 | -    | 1/1/11/20 | 6/20/96/115  | -       |
| 13  | CLA  | a     | 816 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | a     | 833 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | A     | 811 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | G     | 804 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | A     | 824 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | B     | 810 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | A     | 821 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 819 | -    | 1/1/11/20 | 9/20/96/115  | -       |
| 15  | BCR  | o     | 201 | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 13  | CLA  | B     | 807 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 15  | BCR  | A     | 848 | -    | -         | 11/29/63/63  | 0/2/2/2 |
| 13  | CLA  | E     | 832 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 15  | BCR  | q     | 102 | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 13  | CLA  | o     | 202 | -    | 1/1/11/20 | 8/15/91/115  | -       |
| 13  | CLA  | A     | 840 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | b     | 839 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 15  | BCR  | b     | 845 | -    | -         | 20/29/63/63  | 0/2/2/2 |
| 13  | CLA  | G     | 805 | -    | 1/1/12/20 | 2/21/97/115  | -       |
| 13  | CLA  | L     | 202 | 10   | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | A     | 810 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | E     | 807 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | a     | 810 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | A     | 812 | 1    | 1/1/12/20 | 8/21/97/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 13  | CLA  | a     | 829  | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 15  | BCR  | I     | 101  | -    | -         | 8/29/63/63   | 0/2/2/2 |
| 13  | CLA  | b     | 829  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | g     | 824  | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | e     | 804  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 834  | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | b     | 830  | -    | 1/1/11/20 | 11/15/91/115 | -       |
| 13  | CLA  | A     | 830  | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | E     | 806  | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | a     | 823  | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 15  | BCR  | J     | 101  | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 13  | CLA  | G     | 801  | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | A     | 815  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | e     | 844  | 12   | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | g     | 806  | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | g     | 813  | -    | 1/1/12/20 | 12/21/97/115 | -       |
| 13  | CLA  | e     | 817  | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 13  | CLA  | a     | 835  | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | E     | 810  | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | G     | 807  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | B     | 837  | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 15  | BCR  | b     | 847  | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | b     | 840  | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | E     | 822  | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | E     | 837  | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | b     | 804  | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | l     | 204  | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | b     | 812  | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | a     | 825  | -    | 1/1/11/20 | 11/20/96/115 | -       |
| 13  | CLA  | k     | 4002 | -    | 1/1/11/20 | 7/15/91/115  | -       |
| 13  | CLA  | a     | 843  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | e     | 832  | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 15  | BCR  | E     | 850  | -    | -         | 11/29/63/63  | 0/2/2/2 |
| 13  | CLA  | A     | 845  | 12   | 1/1/12/20 | 7/21/97/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | G     | 806 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | a     | 826 | -    | 1/1/12/20 | 12/21/97/115 | -       |
| 15  | BCR  | p     | 101 | -    | -         | 8/29/63/63   | 0/2/2/2 |
| 15  | BCR  | a     | 848 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | B     | 831 | -    | 1/1/11/20 | 11/15/91/115 | -       |
| 13  | CLA  | a     | 813 | -    | 1/1/11/20 | 3/15/91/115  | -       |
| 13  | CLA  | E     | 816 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | g     | 820 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | B     | 811 | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | A     | 827 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 15  | BCR  | O     | 201 | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | BCR  | a     | 803 | -    | -         | 23/29/63/63  | 0/2/2/2 |
| 13  | CLA  | A     | 823 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | G     | 830 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | G     | 814 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | G     | 822 | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 13  | CLA  | G     | 837 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | b     | 821 | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 14  | PQN  | a     | 847 | -    | -         | 10/23/43/43  | 0/2/2/2 |
| 13  | CLA  | A     | 841 | -    | 1/1/11/20 | 4/18/94/115  | -       |
| 13  | CLA  | e     | 830 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | b     | 822 | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | e     | 810 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | Q     | 101 | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 13  | CLA  | E     | 836 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 14  | PQN  | B     | 842 | -    | -         | 10/23/43/43  | 0/2/2/2 |
| 15  | BCR  | A     | 851 | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 13  | CLA  | a     | 842 | -    | 1/1/11/20 | 5/18/94/115  | -       |
| 15  | BCR  | E     | 849 | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 13  | CLA  | e     | 822 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | G     | 819 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | e     | 824 | -    | 1/1/11/20 | 11/20/96/115 | -       |
| 15  | BCR  | G     | 843 | -    | -         | 7/29/63/63   | 0/2/2/2 |
| 13  | CLA  | e     | 840 | -    | 1/1/11/20 | 5/18/94/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | A     | 837 | -    | -         | 8/21/97/115  | -       |
| 13  | CLA  | g     | 833 | -    | 1/1/11/20 | 6/20/96/115  | -       |
| 15  | BCR  | L     | 201 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 15  | BCR  | S     | 201 | -    | -         | 14/29/63/63  | 0/2/2/2 |
| 13  | CLA  | e     | 835 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | G     | 823 | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | S     | 203 | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | B     | 819 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 15  | BCR  | B     | 847 | -    | -         | 13/29/63/63  | 0/2/2/2 |
| 13  | CLA  | G     | 828 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 14  | PQN  | b     | 841 | -    | -         | 10/23/43/43  | 0/2/2/2 |
| 16  | SF4  | c     | 102 | 3    | -         | -            | 0/6/5/5 |
| 13  | CLA  | B     | 840 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | g     | 836 | -    | 1/1/11/20 | 7/15/91/115  | -       |
| 13  | CLA  | g     | 808 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | G     | 831 | -    | 1/1/11/20 | 11/15/91/115 | -       |
| 15  | BCR  | g     | 846 | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 15  | BCR  | F     | 201 | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | BCR  | R     | 101 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | g     | 814 | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | e     | 805 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | E     | 838 | -    | -         | 8/21/97/115  | -       |
| 13  | CLA  | G     | 808 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 15  | BCR  | E     | 801 | -    | -         | 10/29/63/63  | 0/2/2/2 |
| 16  | SF4  | E     | 847 | -    | -         | -            | 0/6/5/5 |
| 13  | CLA  | r     | 102 | -    | 1/1/11/20 | 7/15/91/115  | -       |
| 15  | BCR  | g     | 849 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | E     | 844 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | a     | 853 | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 13  | CLA  | E     | 845 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | g     | 803 | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | L     | 203 | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | e     | 852 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | A     | 825 | -    | 1/1/11/20 | 10/20/96/115 | -       |
| 16  | SF4  | h     | 102 | 3    | -         | -            | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | E     | 815 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 818 | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 13  | CLA  | b     | 813 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 15  | BCR  | b     | 843 | -    | -         | 19/29/63/63  | 0/2/2/2 |
| 13  | CLA  | b     | 836 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | B     | 832 | -    | 1/1/11/20 | 6/20/96/115  | -       |
| 13  | CLA  | A     | 809 | 1    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | g     | 834 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | e     | 816 | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | l     | 203 | 10   | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | e     | 811 | 1    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | G     | 820 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | B     | 830 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 832 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 852 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | E     | 817 | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | G     | 840 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 16  | SF4  | g     | 804 | -    | -         | -            | 0/6/5/5 |
| 14  | PQN  | G     | 842 | -    | -         | 10/23/43/43  | 0/2/2/2 |
| 13  | CLA  | a     | 830 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | G     | 815 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | B     | 841 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | e     | 803 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | A     | 816 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | B     | 821 | -    | 1/1/11/20 | 8/18/94/115  | -       |
| 15  | BCR  | g     | 845 | -    | -         | 19/29/63/63  | 0/2/2/2 |
| 13  | CLA  | g     | 826 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | b     | 806 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | b     | 825 | -    | 1/1/11/20 | 4/17/93/115  | -       |
| 13  | CLA  | a     | 841 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | A     | 842 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | e     | 827 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | g     | 828 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | a     | 840 | -    | 1/1/12/20 | 6/21/97/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | E     | 829 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | B     | 812 | -    | 1/1/12/20 | 12/21/97/115 | -       |
| 13  | CLA  | B     | 809 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 821 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | e     | 823 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | e     | 814 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | B     | 838 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | A     | 839 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | G     | 817 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | g     | 831 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | E     | 841 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | A     | 803 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | E     | 824 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | a     | 812 | 1    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | B     | 801 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | e     | 833 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | b     | 837 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | A     | 829 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | B     | 827 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | a     | 838 | -    | -         | 8/21/97/115  | -       |
| 13  | CLA  | b     | 838 | -    | 1/1/11/20 | 7/18/94/115  | -       |
| 13  | CLA  | B     | 823 | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 12  | LHG  | A     | 802 | 13   | -         | 17/42/42/53  | -       |
| 13  | CLA  | G     | 809 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | E     | 812 | 1    | 1/1/12/20 | 8/21/97/115  | -       |
| 13  | CLA  | S     | 204 | -    | 1/1/11/20 | 9/15/91/115  | -       |
| 13  | CLA  | a     | 807 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | e     | 843 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 15  | BCR  | a     | 849 | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 13  | CLA  | g     | 818 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | E     | 819 | -    | 1/1/11/20 | 10/20/96/115 | -       |
| 13  | CLA  | e     | 826 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 15  | BCR  | j     | 101 | -    | -         | 12/29/63/63  | 0/2/2/2 |
| 16  | SF4  | H     | 101 | -    | -         | -            | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 15  | BCR  | B     | 844 | -    | -         | 19/29/63/63  | 0/2/2/2 |
| 13  | CLA  | g     | 822 | -    | 1/1/11/20 | 8/18/94/115  | -       |
| 13  | CLA  | E     | 830 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | G     | 841 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | e     | 813 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | a     | 805 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | G     | 824 | -    | 1/1/11/20 | 8/15/91/115  | -       |
| 13  | CLA  | e     | 837 | 1    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | A     | 844 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | a     | 806 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | K     | 102 | -    | 1/1/11/20 | 7/15/91/115  | -       |
| 13  | CLA  | A     | 804 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | G     | 827 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | g     | 802 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | E     | 834 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | b     | 833 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 15  | BCR  | B     | 848 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | G     | 821 | -    | 1/1/11/20 | 8/18/94/115  | -       |
| 13  | CLA  | b     | 801 | -    | 1/1/9/20  | 4/9/81/115   | -       |
| 13  | CLA  | e     | 841 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | E     | 833 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 15  | BCR  | g     | 847 | -    | -         | 20/29/63/63  | 0/2/2/2 |
| 13  | CLA  | b     | 811 | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | L     | 204 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | g     | 840 | -    | 1/1/11/20 | 6/18/94/115  | -       |
| 13  | CLA  | E     | 835 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 15  | BCR  | A     | 852 | -    | -         | 15/29/63/63  | 0/2/2/2 |
| 15  | BCR  | a     | 802 | -    | -         | 9/29/63/63   | 0/2/2/2 |
| 13  | CLA  | E     | 811 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | G     | 802 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | e     | 812 | -    | 1/1/11/20 | 3/15/91/115  | -       |
| 13  | CLA  | e     | 829 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 15  | BCR  | A     | 847 | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 15  | BCR  | E     | 802 | -    | -         | 20/29/63/63  | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions    | Rings   |
|-----|------|-------|-----|------|-----------|-------------|---------|
| 15  | BCR  | b     | 844 | -    | -         | 17/29/63/63 | 0/2/2/2 |
| 15  | BCR  | J     | 102 | -    | -         | 12/29/63/63 | 0/2/2/2 |
| 15  | BCR  | e     | 851 | -    | -         | 16/29/63/63 | 0/2/2/2 |
| 13  | CLA  | B     | 836 | -    | 1/1/11/20 | 8/15/91/115 | -       |
| 13  | CLA  | A     | 814 | -    | 1/1/12/20 | 4/21/97/115 | -       |
| 13  | CLA  | b     | 809 | -    | 1/1/12/20 | 4/21/97/115 | -       |
| 13  | CLA  | A     | 843 | -    | 1/1/12/20 | 5/21/97/115 | -       |
| 13  | CLA  | b     | 834 | -    | 1/1/11/20 | 7/15/91/115 | -       |
| 13  | CLA  | e     | 831 | -    | 1/1/12/20 | 6/21/97/115 | -       |
| 13  | CLA  | B     | 835 | -    | 1/1/11/20 | 7/15/91/115 | -       |
| 15  | BCR  | s     | 201 | -    | -         | 18/29/63/63 | 0/2/2/2 |
| 16  | SF4  | h     | 101 | -    | -         | -           | 0/6/5/5 |
| 13  | CLA  | B     | 833 | -    | 1/1/12/20 | 4/21/97/115 | -       |
| 13  | CLA  | G     | 835 | -    | 1/1/11/20 | 7/15/91/115 | -       |
| 13  | CLA  | A     | 813 | -    | 1/1/11/20 | 3/15/91/115 | -       |
| 15  | BCR  | e     | 847 | -    | -         | 10/29/63/63 | 0/2/2/2 |
| 13  | CLA  | e     | 820 | -    | 1/1/12/20 | 6/21/97/115 | -       |
| 13  | CLA  | b     | 827 | -    | 1/1/12/20 | 8/21/97/115 | -       |
| 13  | CLA  | O     | 203 | -    | 1/1/11/20 | 7/15/91/115 | -       |
| 12  | LHG  | A     | 801 | -    | -         | 32/53/53/53 | -       |
| 13  | CLA  | b     | 835 | -    | 1/1/11/20 | 8/15/91/115 | -       |
| 13  | CLA  | e     | 819 | -    | 1/1/12/20 | 4/21/97/115 | -       |
| 13  | CLA  | B     | 817 | -    | 1/1/12/20 | 6/21/97/115 | -       |
| 14  | PQN  | g     | 843 | -    | -         | 10/23/43/43 | 0/2/2/2 |
| 13  | CLA  | A     | 835 | -    | 1/1/12/20 | 6/21/97/115 | -       |
| 13  | CLA  | E     | 808 | -    | 1/1/12/20 | 6/21/97/115 | -       |
| 15  | BCR  | B     | 843 | -    | -         | 7/29/63/63  | 0/2/2/2 |
| 15  | BCR  | g     | 848 | -    | -         | 13/29/63/63 | 0/2/2/2 |
| 14  | PQN  | E     | 848 | -    | -         | 6/23/43/43  | 0/2/2/2 |
| 13  | CLA  | A     | 834 | -    | 1/1/12/20 | 7/21/97/115 | -       |
| 13  | CLA  | A     | 828 | -    | 1/1/12/20 | 4/21/97/115 | -       |
| 13  | CLA  | b     | 815 | -    | 1/1/11/20 | 6/15/91/115 | -       |
| 16  | SF4  | B     | 803 | -    | -         | -           | 0/6/5/5 |
| 13  | CLA  | g     | 816 | -    | 1/1/12/20 | 3/21/97/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | CLA  | G     | 825 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | g     | 811 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | a     | 827 | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | a     | 804 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | e     | 839 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 15  | BCR  | G     | 848 | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | G     | 836 | -    | 1/1/11/20 | 8/15/91/115  | -       |
| 13  | CLA  | E     | 803 | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | e     | 809 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | e     | 807 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 15  | BCR  | A     | 850 | -    | -         | 20/29/63/63  | 0/2/2/2 |
| 13  | CLA  | s     | 202 | -    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | b     | 817 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | B     | 825 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | E     | 814 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | E     | 813 | -    | 1/1/11/20 | 3/15/91/115  | -       |
| 13  | CLA  | E     | 828 | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 16  | SF4  | H     | 102 | 3    | -         | -            | 0/6/5/5 |
| 13  | CLA  | B     | 839 | -    | 1/1/11/20 | 5/18/94/115  | -       |
| 13  | CLA  | r     | 101 | -    | 1/1/9/20  | 4/9/81/115   | -       |
| 15  | BCR  | e     | 848 | -    | -         | 6/29/63/63   | 0/2/2/2 |
| 13  | CLA  | a     | 837 | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | g     | 805 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | G     | 816 | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 16  | SF4  | a     | 846 | -    | -         | -            | 0/6/5/5 |
| 13  | CLA  | a     | 839 | 1    | 1/1/11/20 | 5/15/91/115  | -       |
| 13  | CLA  | B     | 815 | -    | 1/1/12/20 | 3/21/97/115  | -       |
| 13  | CLA  | G     | 803 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | e     | 821 | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | a     | 815 | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | b     | 824 | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | G     | 846 | -    | -         | 20/29/63/63  | 0/2/2/2 |
| 13  | CLA  | G     | 810 | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | F     | 202 | -    | 1/1/11/20 | 7/15/91/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 13  | CLA  | K     | 101  | -    | 1/1/9/20  | 3/9/81/115   | -       |
| 13  | CLA  | B     | 816  | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | E     | 843  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | G     | 833  | -    | 1/1/12/20 | 4/21/97/115  | -       |
| 13  | CLA  | b     | 810  | 2    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | T     | 101  | -    | -         | 9/29/63/63   | 0/2/2/2 |
| 15  | BCR  | E     | 851  | -    | -         | 6/29/63/63   | 0/2/2/2 |
| 13  | CLA  | G     | 811  | -    | 1/1/12/20 | 11/21/97/115 | -       |
| 13  | CLA  | g     | 807  | -    | 1/1/12/20 | 2/21/97/115  | -       |
| 13  | CLA  | g     | 823  | -    | 1/1/11/20 | 4/15/91/115  | -       |
| 15  | BCR  | B     | 845  | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 15  | BCR  | S     | 202  | -    | -         | 17/29/63/63  | 0/2/2/2 |
| 15  | BCR  | S     | 205  | -    | -         | 16/29/63/63  | 0/2/2/2 |
| 13  | CLA  | E     | 831  | -    | 1/1/12/20 | 8/21/97/115  | -       |
| 16  | SF4  | c     | 101  | -    | -         | -            | 0/6/5/5 |
| 13  | CLA  | A     | 808  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | a     | 844  | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 13  | CLA  | b     | 802  | -    | 1/1/12/20 | 9/21/97/115  | -       |
| 13  | CLA  | E     | 826  | -    | 1/1/12/20 | 12/21/97/115 | -       |
| 13  | CLA  | g     | 817  | -    | 1/1/11/20 | 6/15/91/115  | -       |
| 13  | CLA  | s     | 203  | -    | 1/1/12/20 | 10/21/97/115 | -       |
| 13  | CLA  | E     | 842  | -    | 1/1/11/20 | 5/18/94/115  | -       |
| 13  | CLA  | B     | 820  | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | b     | 816  | -    | 1/1/12/20 | 6/21/97/115  | -       |
| 13  | CLA  | G     | 832  | -    | 1/1/11/20 | 6/20/96/115  | -       |
| 13  | CLA  | g     | 825  | -    | 1/1/11/20 | 8/15/91/115  | -       |
| 13  | CLA  | E     | 846  | -    | 1/1/9/20  | 3/9/81/115   | -       |
| 13  | CLA  | e     | 806  | -    | 1/1/12/20 | 7/21/97/115  | -       |
| 13  | CLA  | a     | 811  | -    | 1/1/12/20 | 5/21/97/115  | -       |
| 15  | BCR  | k     | 4001 | -    | -         | 21/29/63/63  | 0/2/2/2 |
| 13  | CLA  | a     | 820  | -    | 1/1/12/20 | 4/21/97/115  | -       |

The worst 5 of 3355 bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
|-----|-------|-----|------|-------|---|-------------|----------|

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 13  | S     | 204 | CLA  | MG-ND | 9.46 | 2.24        | 2.05     |
| 13  | l     | 205 | CLA  | MG-ND | 9.45 | 2.24        | 2.05     |
| 13  | L     | 204 | CLA  | MG-ND | 9.43 | 2.24        | 2.05     |
| 13  | s     | 203 | CLA  | MG-ND | 9.40 | 2.24        | 2.05     |
| 14  | G     | 842 | PQN  | C3-C2 | 7.87 | 1.49        | 1.35     |

The worst 5 of 2678 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | l     | 205 | CLA  | C4A-NA-C1A  | 17.20 | 114.53      | 106.68   |
| 13  | s     | 203 | CLA  | C4A-NA-C1A  | 17.16 | 114.51      | 106.68   |
| 13  | S     | 204 | CLA  | C4A-NA-C1A  | 17.11 | 114.49      | 106.68   |
| 13  | L     | 204 | CLA  | C4A-NA-C1A  | 17.07 | 114.47      | 106.68   |
| 13  | l     | 205 | CLA  | C2A-C1A-CHA | 7.38  | 136.67      | 123.87   |

5 of 355 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 13  | A     | 803 | CLA  | ND   |
| 13  | A     | 804 | CLA  | ND   |
| 13  | A     | 805 | CLA  | ND   |
| 13  | A     | 806 | CLA  | ND   |
| 13  | A     | 807 | CLA  | ND   |

5 of 3595 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 12  | A     | 801 | LHG  | O1-C1-C2-C3 |
| 12  | A     | 801 | LHG  | C3-O3-P-O4  |
| 12  | A     | 801 | LHG  | C3-O3-P-O6  |
| 12  | A     | 801 | LHG  | C4-O6-P-O3  |
| 12  | A     | 801 | LHG  | C4-O6-P-O5  |

There are no ring outliers.

410 monomers are involved in 1257 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 16  | C     | 102 | SF4  | 2       | 0            |
| 13  | E     | 818 | CLA  | 1       | 0            |
| 13  | A     | 820 | CLA  | 5       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | A     | 833 | CLA  | 2       | 0            |
| 13  | g     | 830 | CLA  | 4       | 0            |
| 13  | g     | 832 | CLA  | 1       | 0            |
| 15  | g     | 844 | BCR  | 1       | 0            |
| 13  | g     | 837 | CLA  | 2       | 0            |
| 13  | g     | 829 | CLA  | 4       | 0            |
| 13  | b     | 828 | CLA  | 3       | 0            |
| 12  | e     | 801 | LHG  | 2       | 0            |
| 15  | i     | 101 | BCR  | 3       | 0            |
| 13  | a     | 809 | CLA  | 2       | 0            |
| 15  | L     | 205 | BCR  | 2       | 0            |
| 15  | f     | 201 | BCR  | 4       | 0            |
| 13  | B     | 804 | CLA  | 5       | 0            |
| 13  | b     | 807 | CLA  | 1       | 0            |
| 13  | R     | 102 | CLA  | 2       | 0            |
| 13  | B     | 826 | CLA  | 6       | 0            |
| 13  | l     | 205 | CLA  | 3       | 0            |
| 15  | G     | 845 | BCR  | 1       | 0            |
| 13  | A     | 838 | CLA  | 3       | 0            |
| 13  | g     | 841 | CLA  | 5       | 0            |
| 15  | f     | 202 | BCR  | 4       | 0            |
| 13  | b     | 805 | CLA  | 1       | 0            |
| 13  | G     | 813 | CLA  | 2       | 0            |
| 15  | G     | 844 | BCR  | 5       | 0            |
| 13  | G     | 818 | CLA  | 4       | 0            |
| 13  | E     | 820 | CLA  | 6       | 0            |
| 13  | A     | 853 | CLA  | 1       | 0            |
| 13  | G     | 829 | CLA  | 4       | 0            |
| 13  | g     | 835 | CLA  | 7       | 0            |
| 13  | a     | 822 | CLA  | 4       | 0            |
| 13  | B     | 818 | CLA  | 4       | 0            |
| 12  | a     | 801 | LHG  | 3       | 0            |
| 13  | e     | 828 | CLA  | 1       | 0            |
| 13  | G     | 834 | CLA  | 7       | 0            |
| 13  | g     | 812 | CLA  | 2       | 0            |
| 15  | A     | 849 | BCR  | 7       | 0            |
| 13  | e     | 836 | CLA  | 3       | 0            |
| 13  | E     | 825 | CLA  | 10      | 0            |
| 15  | l     | 202 | BCR  | 5       | 0            |
| 15  | O     | 202 | BCR  | 7       | 0            |
| 13  | g     | 801 | CLA  | 5       | 0            |
| 13  | B     | 814 | CLA  | 6       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | B     | 822 | CLA  | 1       | 0            |
| 13  | E     | 839 | CLA  | 2       | 0            |
| 13  | B     | 828 | CLA  | 4       | 0            |
| 13  | A     | 826 | CLA  | 5       | 0            |
| 16  | C     | 101 | SF4  | 2       | 0            |
| 12  | e     | 802 | LHG  | 3       | 0            |
| 13  | A     | 806 | CLA  | 3       | 0            |
| 13  | b     | 808 | CLA  | 3       | 0            |
| 13  | a     | 814 | CLA  | 1       | 0            |
| 15  | B     | 846 | BCR  | 1       | 0            |
| 15  | s     | 204 | BCR  | 4       | 0            |
| 13  | a     | 828 | CLA  | 1       | 0            |
| 13  | B     | 813 | CLA  | 3       | 0            |
| 13  | E     | 821 | CLA  | 7       | 0            |
| 13  | A     | 831 | CLA  | 1       | 0            |
| 13  | S     | 206 | CLA  | 2       | 0            |
| 13  | B     | 805 | CLA  | 5       | 0            |
| 13  | g     | 819 | CLA  | 3       | 0            |
| 13  | a     | 817 | CLA  | 14      | 0            |
| 13  | A     | 822 | CLA  | 4       | 0            |
| 13  | e     | 834 | CLA  | 5       | 0            |
| 13  | b     | 818 | CLA  | 4       | 0            |
| 15  | m     | 101 | BCR  | 6       | 0            |
| 13  | g     | 809 | CLA  | 1       | 0            |
| 13  | a     | 845 | CLA  | 2       | 0            |
| 13  | b     | 803 | CLA  | 2       | 0            |
| 13  | g     | 815 | CLA  | 5       | 0            |
| 15  | G     | 847 | BCR  | 1       | 0            |
| 13  | A     | 807 | CLA  | 4       | 0            |
| 15  | b     | 846 | BCR  | 2       | 0            |
| 13  | e     | 838 | CLA  | 5       | 0            |
| 13  | b     | 814 | CLA  | 1       | 0            |
| 13  | g     | 827 | CLA  | 7       | 0            |
| 13  | B     | 824 | CLA  | 8       | 0            |
| 13  | B     | 834 | CLA  | 7       | 0            |
| 13  | E     | 804 | CLA  | 4       | 0            |
| 15  | E     | 852 | BCR  | 2       | 0            |
| 15  | e     | 850 | BCR  | 3       | 0            |
| 13  | b     | 823 | CLA  | 8       | 0            |
| 13  | A     | 836 | CLA  | 6       | 0            |
| 13  | A     | 805 | CLA  | 4       | 0            |
| 15  | a     | 851 | BCR  | 8       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | A     | 846 | PQN  | 10      | 0            |
| 13  | E     | 840 | CLA  | 5       | 0            |
| 13  | s     | 205 | CLA  | 7       | 0            |
| 13  | e     | 825 | CLA  | 5       | 0            |
| 13  | G     | 839 | CLA  | 4       | 0            |
| 13  | G     | 826 | CLA  | 6       | 0            |
| 13  | A     | 818 | CLA  | 1       | 0            |
| 13  | e     | 808 | CLA  | 3       | 0            |
| 13  | B     | 829 | CLA  | 4       | 0            |
| 15  | e     | 846 | BCR  | 14      | 0            |
| 15  | b     | 842 | BCR  | 2       | 0            |
| 13  | E     | 809 | CLA  | 3       | 0            |
| 15  | a     | 850 | BCR  | 19      | 0            |
| 13  | A     | 817 | CLA  | 3       | 0            |
| 13  | l     | 201 | CLA  | 2       | 0            |
| 14  | e     | 845 | PQN  | 1       | 0            |
| 13  | e     | 815 | CLA  | 5       | 0            |
| 13  | b     | 826 | CLA  | 2       | 0            |
| 13  | b     | 832 | CLA  | 3       | 0            |
| 15  | l     | 206 | BCR  | 1       | 0            |
| 13  | A     | 832 | CLA  | 6       | 0            |
| 13  | B     | 808 | CLA  | 1       | 0            |
| 13  | E     | 805 | CLA  | 3       | 0            |
| 13  | B     | 802 | CLA  | 5       | 0            |
| 13  | a     | 824 | CLA  | 1       | 0            |
| 15  | e     | 849 | BCR  | 3       | 0            |
| 13  | E     | 823 | CLA  | 7       | 0            |
| 13  | G     | 812 | CLA  | 1       | 0            |
| 13  | a     | 836 | CLA  | 9       | 0            |
| 13  | a     | 808 | CLA  | 3       | 0            |
| 13  | a     | 831 | CLA  | 1       | 0            |
| 13  | b     | 831 | CLA  | 2       | 0            |
| 13  | a     | 816 | CLA  | 5       | 0            |
| 13  | a     | 833 | CLA  | 2       | 0            |
| 13  | A     | 811 | CLA  | 1       | 0            |
| 13  | G     | 804 | CLA  | 6       | 0            |
| 13  | B     | 810 | CLA  | 3       | 0            |
| 13  | A     | 821 | CLA  | 6       | 0            |
| 13  | a     | 819 | CLA  | 3       | 0            |
| 15  | o     | 201 | BCR  | 3       | 0            |
| 13  | B     | 807 | CLA  | 2       | 0            |
| 15  | A     | 848 | BCR  | 5       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 13  | E     | 832  | CLA  | 5       | 0            |
| 15  | q     | 102  | BCR  | 1       | 0            |
| 13  | o     | 202  | CLA  | 2       | 0            |
| 13  | A     | 840  | CLA  | 3       | 0            |
| 13  | b     | 839  | CLA  | 5       | 0            |
| 15  | b     | 845  | BCR  | 2       | 0            |
| 13  | G     | 805  | CLA  | 2       | 0            |
| 13  | L     | 202  | CLA  | 2       | 0            |
| 13  | A     | 810  | CLA  | 2       | 0            |
| 13  | E     | 807  | CLA  | 3       | 0            |
| 13  | a     | 810  | CLA  | 2       | 0            |
| 13  | A     | 812  | CLA  | 3       | 0            |
| 13  | a     | 829  | CLA  | 1       | 0            |
| 13  | b     | 829  | CLA  | 1       | 0            |
| 13  | g     | 824  | CLA  | 3       | 0            |
| 13  | e     | 804  | CLA  | 6       | 0            |
| 13  | a     | 834  | CLA  | 2       | 0            |
| 13  | b     | 830  | CLA  | 2       | 0            |
| 13  | E     | 806  | CLA  | 2       | 0            |
| 13  | a     | 823  | CLA  | 8       | 0            |
| 15  | J     | 101  | BCR  | 1       | 0            |
| 13  | G     | 801  | CLA  | 5       | 0            |
| 13  | A     | 815  | CLA  | 1       | 0            |
| 13  | e     | 844  | CLA  | 4       | 0            |
| 13  | g     | 806  | CLA  | 5       | 0            |
| 13  | g     | 813  | CLA  | 1       | 0            |
| 13  | e     | 817  | CLA  | 1       | 0            |
| 13  | E     | 810  | CLA  | 2       | 0            |
| 13  | G     | 807  | CLA  | 1       | 0            |
| 15  | b     | 847  | BCR  | 4       | 0            |
| 13  | E     | 822  | CLA  | 4       | 0            |
| 13  | E     | 837  | CLA  | 5       | 0            |
| 13  | b     | 804  | CLA  | 6       | 0            |
| 13  | l     | 204  | CLA  | 7       | 0            |
| 13  | b     | 812  | CLA  | 2       | 0            |
| 13  | a     | 825  | CLA  | 11      | 0            |
| 13  | k     | 4002 | CLA  | 2       | 0            |
| 13  | a     | 843  | CLA  | 2       | 0            |
| 13  | e     | 832  | CLA  | 2       | 0            |
| 15  | E     | 850  | BCR  | 5       | 0            |
| 13  | A     | 845  | CLA  | 5       | 0            |
| 13  | G     | 806  | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | a     | 826 | CLA  | 2       | 0            |
| 15  | p     | 101 | BCR  | 1       | 0            |
| 15  | a     | 848 | BCR  | 41      | 0            |
| 13  | B     | 831 | CLA  | 2       | 0            |
| 13  | a     | 813 | CLA  | 1       | 0            |
| 13  | E     | 816 | CLA  | 5       | 0            |
| 13  | g     | 820 | CLA  | 4       | 0            |
| 13  | B     | 811 | CLA  | 2       | 0            |
| 13  | A     | 827 | CLA  | 2       | 0            |
| 15  | O     | 201 | BCR  | 2       | 0            |
| 15  | a     | 803 | BCR  | 1       | 0            |
| 13  | A     | 823 | CLA  | 2       | 0            |
| 13  | G     | 830 | CLA  | 1       | 0            |
| 13  | G     | 814 | CLA  | 5       | 0            |
| 13  | G     | 822 | CLA  | 1       | 0            |
| 13  | b     | 821 | CLA  | 1       | 0            |
| 14  | a     | 847 | PQN  | 2       | 0            |
| 13  | A     | 841 | CLA  | 3       | 0            |
| 13  | e     | 830 | CLA  | 1       | 0            |
| 13  | b     | 822 | CLA  | 3       | 0            |
| 13  | e     | 810 | CLA  | 2       | 0            |
| 13  | E     | 836 | CLA  | 9       | 0            |
| 14  | B     | 842 | PQN  | 2       | 0            |
| 15  | A     | 851 | BCR  | 3       | 0            |
| 13  | a     | 842 | CLA  | 3       | 0            |
| 15  | E     | 849 | BCR  | 30      | 0            |
| 13  | e     | 822 | CLA  | 3       | 0            |
| 13  | G     | 819 | CLA  | 3       | 0            |
| 13  | e     | 824 | CLA  | 10      | 0            |
| 15  | G     | 843 | BCR  | 1       | 0            |
| 13  | e     | 840 | CLA  | 4       | 0            |
| 13  | A     | 837 | CLA  | 3       | 0            |
| 15  | L     | 201 | BCR  | 4       | 0            |
| 15  | S     | 201 | BCR  | 7       | 0            |
| 13  | e     | 835 | CLA  | 4       | 0            |
| 13  | G     | 823 | CLA  | 3       | 0            |
| 13  | S     | 203 | CLA  | 7       | 0            |
| 13  | B     | 819 | CLA  | 4       | 0            |
| 15  | B     | 847 | BCR  | 1       | 0            |
| 13  | G     | 828 | CLA  | 4       | 0            |
| 14  | b     | 841 | PQN  | 1       | 0            |
| 16  | c     | 102 | SF4  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | B     | 840 | CLA  | 6       | 0            |
| 13  | g     | 836 | CLA  | 2       | 0            |
| 13  | g     | 808 | CLA  | 2       | 0            |
| 13  | G     | 831 | CLA  | 2       | 0            |
| 15  | F     | 201 | BCR  | 6       | 0            |
| 15  | R     | 101 | BCR  | 37      | 0            |
| 13  | g     | 814 | CLA  | 2       | 0            |
| 13  | e     | 805 | CLA  | 3       | 0            |
| 13  | E     | 838 | CLA  | 2       | 0            |
| 13  | G     | 808 | CLA  | 1       | 0            |
| 15  | E     | 801 | BCR  | 2       | 0            |
| 16  | E     | 847 | SF4  | 1       | 0            |
| 13  | r     | 102 | CLA  | 1       | 0            |
| 15  | g     | 849 | BCR  | 4       | 0            |
| 15  | a     | 853 | BCR  | 6       | 0            |
| 13  | E     | 845 | CLA  | 3       | 0            |
| 13  | g     | 803 | CLA  | 3       | 0            |
| 13  | L     | 203 | CLA  | 3       | 0            |
| 13  | e     | 852 | CLA  | 2       | 0            |
| 13  | A     | 825 | CLA  | 10      | 0            |
| 16  | h     | 102 | SF4  | 2       | 0            |
| 13  | E     | 815 | CLA  | 1       | 0            |
| 13  | a     | 818 | CLA  | 6       | 0            |
| 13  | b     | 813 | CLA  | 5       | 0            |
| 15  | b     | 843 | BCR  | 5       | 0            |
| 13  | A     | 809 | CLA  | 3       | 0            |
| 13  | g     | 834 | CLA  | 2       | 0            |
| 13  | e     | 816 | CLA  | 4       | 0            |
| 13  | l     | 203 | CLA  | 2       | 0            |
| 13  | e     | 811 | CLA  | 2       | 0            |
| 13  | B     | 830 | CLA  | 1       | 0            |
| 13  | a     | 832 | CLA  | 6       | 0            |
| 13  | a     | 852 | CLA  | 53      | 0            |
| 13  | E     | 817 | CLA  | 3       | 0            |
| 13  | G     | 840 | CLA  | 6       | 0            |
| 16  | g     | 804 | SF4  | 1       | 0            |
| 14  | G     | 842 | PQN  | 1       | 0            |
| 13  | G     | 815 | CLA  | 1       | 0            |
| 13  | e     | 803 | CLA  | 7       | 0            |
| 13  | A     | 816 | CLA  | 5       | 0            |
| 15  | g     | 845 | BCR  | 5       | 0            |
| 13  | g     | 826 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | b     | 806 | CLA  | 2       | 0            |
| 13  | b     | 825 | CLA  | 7       | 0            |
| 13  | A     | 842 | CLA  | 4       | 0            |
| 13  | e     | 827 | CLA  | 1       | 0            |
| 13  | a     | 841 | CLA  | 3       | 0            |
| 13  | g     | 828 | CLA  | 2       | 0            |
| 13  | a     | 840 | CLA  | 5       | 0            |
| 13  | B     | 812 | CLA  | 2       | 0            |
| 13  | B     | 809 | CLA  | 1       | 0            |
| 13  | a     | 821 | CLA  | 7       | 0            |
| 13  | e     | 823 | CLA  | 1       | 0            |
| 13  | e     | 814 | CLA  | 1       | 0            |
| 13  | A     | 839 | CLA  | 5       | 0            |
| 13  | G     | 817 | CLA  | 5       | 0            |
| 13  | g     | 831 | CLA  | 1       | 0            |
| 13  | E     | 841 | CLA  | 3       | 0            |
| 13  | A     | 803 | CLA  | 7       | 0            |
| 13  | E     | 824 | CLA  | 1       | 0            |
| 13  | a     | 812 | CLA  | 4       | 0            |
| 13  | B     | 801 | CLA  | 1       | 0            |
| 13  | e     | 833 | CLA  | 4       | 0            |
| 13  | B     | 827 | CLA  | 2       | 0            |
| 13  | a     | 838 | CLA  | 2       | 0            |
| 13  | b     | 838 | CLA  | 3       | 0            |
| 13  | B     | 823 | CLA  | 3       | 0            |
| 12  | A     | 802 | LHG  | 3       | 0            |
| 13  | G     | 809 | CLA  | 3       | 0            |
| 13  | E     | 812 | CLA  | 2       | 0            |
| 13  | S     | 204 | CLA  | 2       | 0            |
| 13  | a     | 807 | CLA  | 2       | 0            |
| 15  | a     | 849 | BCR  | 26      | 0            |
| 13  | g     | 818 | CLA  | 5       | 0            |
| 13  | E     | 819 | CLA  | 1       | 0            |
| 13  | e     | 826 | CLA  | 1       | 0            |
| 15  | j     | 101 | BCR  | 4       | 0            |
| 16  | H     | 101 | SF4  | 2       | 0            |
| 15  | B     | 844 | BCR  | 4       | 0            |
| 13  | e     | 813 | CLA  | 3       | 0            |
| 13  | a     | 805 | CLA  | 3       | 0            |
| 13  | G     | 824 | CLA  | 8       | 0            |
| 13  | e     | 837 | CLA  | 2       | 0            |
| 13  | A     | 844 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | a     | 806 | CLA  | 2       | 0            |
| 13  | K     | 102 | CLA  | 2       | 0            |
| 13  | A     | 804 | CLA  | 5       | 0            |
| 13  | G     | 827 | CLA  | 2       | 0            |
| 13  | g     | 802 | CLA  | 1       | 0            |
| 13  | E     | 834 | CLA  | 2       | 0            |
| 13  | b     | 833 | CLA  | 8       | 0            |
| 15  | B     | 848 | BCR  | 4       | 0            |
| 13  | b     | 801 | CLA  | 3       | 0            |
| 13  | e     | 841 | CLA  | 2       | 0            |
| 13  | E     | 833 | CLA  | 4       | 0            |
| 15  | g     | 847 | BCR  | 1       | 0            |
| 13  | b     | 811 | CLA  | 1       | 0            |
| 13  | L     | 204 | CLA  | 8       | 0            |
| 13  | g     | 840 | CLA  | 4       | 0            |
| 13  | E     | 835 | CLA  | 1       | 0            |
| 15  | A     | 852 | BCR  | 4       | 0            |
| 15  | a     | 802 | BCR  | 2       | 0            |
| 13  | E     | 811 | CLA  | 2       | 0            |
| 13  | G     | 802 | CLA  | 1       | 0            |
| 13  | e     | 812 | CLA  | 1       | 0            |
| 15  | A     | 847 | BCR  | 12      | 0            |
| 15  | E     | 802 | BCR  | 2       | 0            |
| 15  | J     | 102 | BCR  | 1       | 0            |
| 15  | e     | 851 | BCR  | 2       | 0            |
| 13  | B     | 836 | CLA  | 2       | 0            |
| 13  | A     | 814 | CLA  | 3       | 0            |
| 13  | b     | 809 | CLA  | 3       | 0            |
| 13  | b     | 834 | CLA  | 4       | 0            |
| 13  | e     | 831 | CLA  | 5       | 0            |
| 13  | B     | 835 | CLA  | 2       | 0            |
| 15  | s     | 201 | BCR  | 2       | 0            |
| 16  | h     | 101 | SF4  | 2       | 0            |
| 13  | B     | 833 | CLA  | 2       | 0            |
| 13  | G     | 835 | CLA  | 2       | 0            |
| 13  | A     | 813 | CLA  | 1       | 0            |
| 15  | e     | 847 | BCR  | 6       | 0            |
| 13  | e     | 820 | CLA  | 7       | 0            |
| 13  | b     | 827 | CLA  | 4       | 0            |
| 12  | A     | 801 | LHG  | 2       | 0            |
| 13  | O     | 203 | CLA  | 1       | 0            |
| 13  | b     | 835 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | e     | 819 | CLA  | 4       | 0            |
| 13  | B     | 817 | CLA  | 4       | 0            |
| 14  | g     | 843 | PQN  | 2       | 0            |
| 13  | A     | 835 | CLA  | 5       | 0            |
| 13  | E     | 808 | CLA  | 3       | 0            |
| 15  | g     | 848 | BCR  | 2       | 0            |
| 14  | E     | 848 | PQN  | 4       | 0            |
| 13  | A     | 834 | CLA  | 2       | 0            |
| 13  | A     | 828 | CLA  | 1       | 0            |
| 13  | b     | 815 | CLA  | 1       | 0            |
| 16  | B     | 803 | SF4  | 1       | 0            |
| 13  | G     | 825 | CLA  | 2       | 0            |
| 13  | g     | 811 | CLA  | 2       | 0            |
| 13  | a     | 804 | CLA  | 4       | 0            |
| 13  | e     | 839 | CLA  | 3       | 0            |
| 15  | G     | 848 | BCR  | 5       | 0            |
| 13  | G     | 836 | CLA  | 2       | 0            |
| 13  | E     | 803 | CLA  | 3       | 0            |
| 13  | e     | 809 | CLA  | 2       | 0            |
| 13  | e     | 807 | CLA  | 3       | 0            |
| 15  | A     | 850 | BCR  | 3       | 0            |
| 13  | s     | 202 | CLA  | 8       | 0            |
| 13  | b     | 817 | CLA  | 3       | 0            |
| 13  | B     | 825 | CLA  | 2       | 0            |
| 13  | E     | 814 | CLA  | 3       | 0            |
| 13  | E     | 813 | CLA  | 1       | 0            |
| 13  | E     | 828 | CLA  | 1       | 0            |
| 16  | H     | 102 | SF4  | 2       | 0            |
| 13  | B     | 839 | CLA  | 3       | 0            |
| 13  | r     | 101 | CLA  | 2       | 0            |
| 15  | e     | 848 | BCR  | 7       | 0            |
| 13  | a     | 837 | CLA  | 5       | 0            |
| 13  | g     | 805 | CLA  | 5       | 0            |
| 13  | G     | 816 | CLA  | 2       | 0            |
| 16  | a     | 846 | SF4  | 1       | 0            |
| 13  | a     | 839 | CLA  | 2       | 0            |
| 13  | B     | 815 | CLA  | 1       | 0            |
| 13  | G     | 803 | CLA  | 2       | 0            |
| 13  | e     | 821 | CLA  | 4       | 0            |
| 13  | a     | 815 | CLA  | 1       | 0            |
| 13  | b     | 824 | CLA  | 2       | 0            |
| 15  | G     | 846 | BCR  | 3       | 0            |

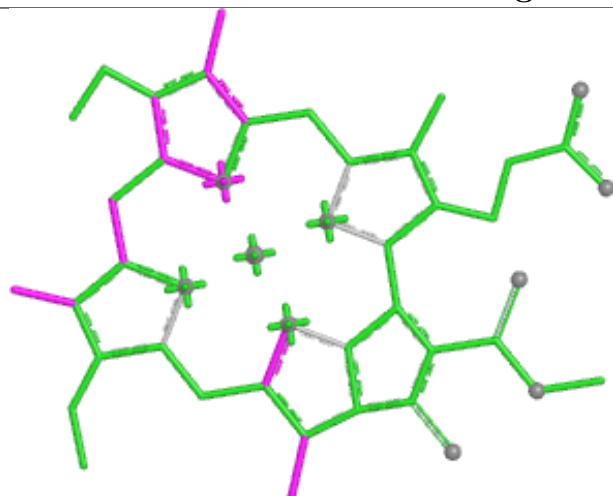
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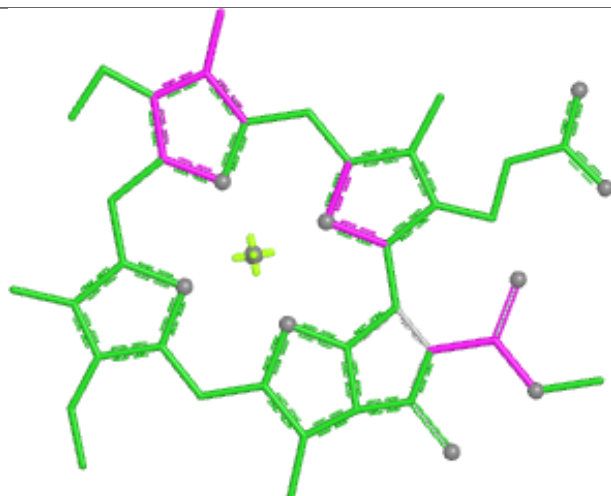
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 13  | G     | 810  | CLA  | 2       | 0            |
| 13  | F     | 202  | CLA  | 2       | 0            |
| 13  | K     | 101  | CLA  | 2       | 0            |
| 13  | B     | 816  | CLA  | 1       | 0            |
| 13  | E     | 843  | CLA  | 3       | 0            |
| 13  | G     | 833  | CLA  | 2       | 0            |
| 13  | b     | 810  | CLA  | 2       | 0            |
| 15  | T     | 101  | BCR  | 3       | 0            |
| 15  | E     | 851  | BCR  | 8       | 0            |
| 13  | G     | 811  | CLA  | 3       | 0            |
| 13  | g     | 823  | CLA  | 1       | 0            |
| 15  | S     | 202  | BCR  | 1       | 0            |
| 15  | S     | 205  | BCR  | 2       | 0            |
| 13  | E     | 831  | CLA  | 1       | 0            |
| 16  | c     | 101  | SF4  | 2       | 0            |
| 13  | A     | 808  | CLA  | 3       | 0            |
| 13  | b     | 802  | CLA  | 6       | 0            |
| 13  | E     | 826  | CLA  | 2       | 0            |
| 13  | g     | 817  | CLA  | 2       | 0            |
| 13  | s     | 203  | CLA  | 16      | 0            |
| 13  | E     | 842  | CLA  | 3       | 0            |
| 13  | b     | 816  | CLA  | 5       | 0            |
| 13  | G     | 832  | CLA  | 4       | 0            |
| 13  | g     | 825  | CLA  | 8       | 0            |
| 13  | E     | 846  | CLA  | 2       | 0            |
| 13  | e     | 806  | CLA  | 4       | 0            |
| 13  | a     | 811  | CLA  | 1       | 0            |
| 15  | k     | 4001 | BCR  | 33      | 0            |
| 13  | a     | 820  | CLA  | 5       | 0            |

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

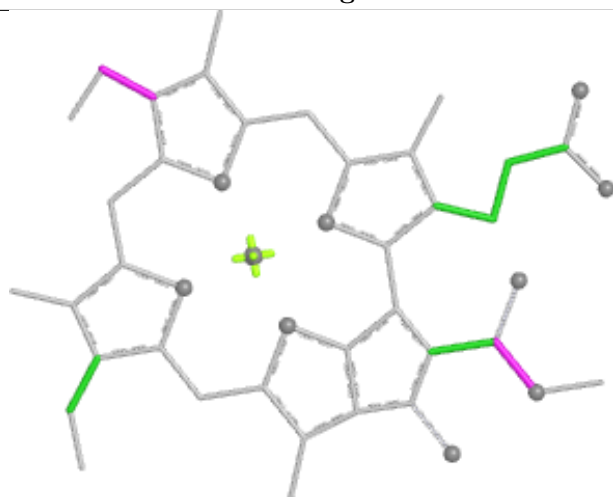
## Ligand CLA E 818



Bond lengths



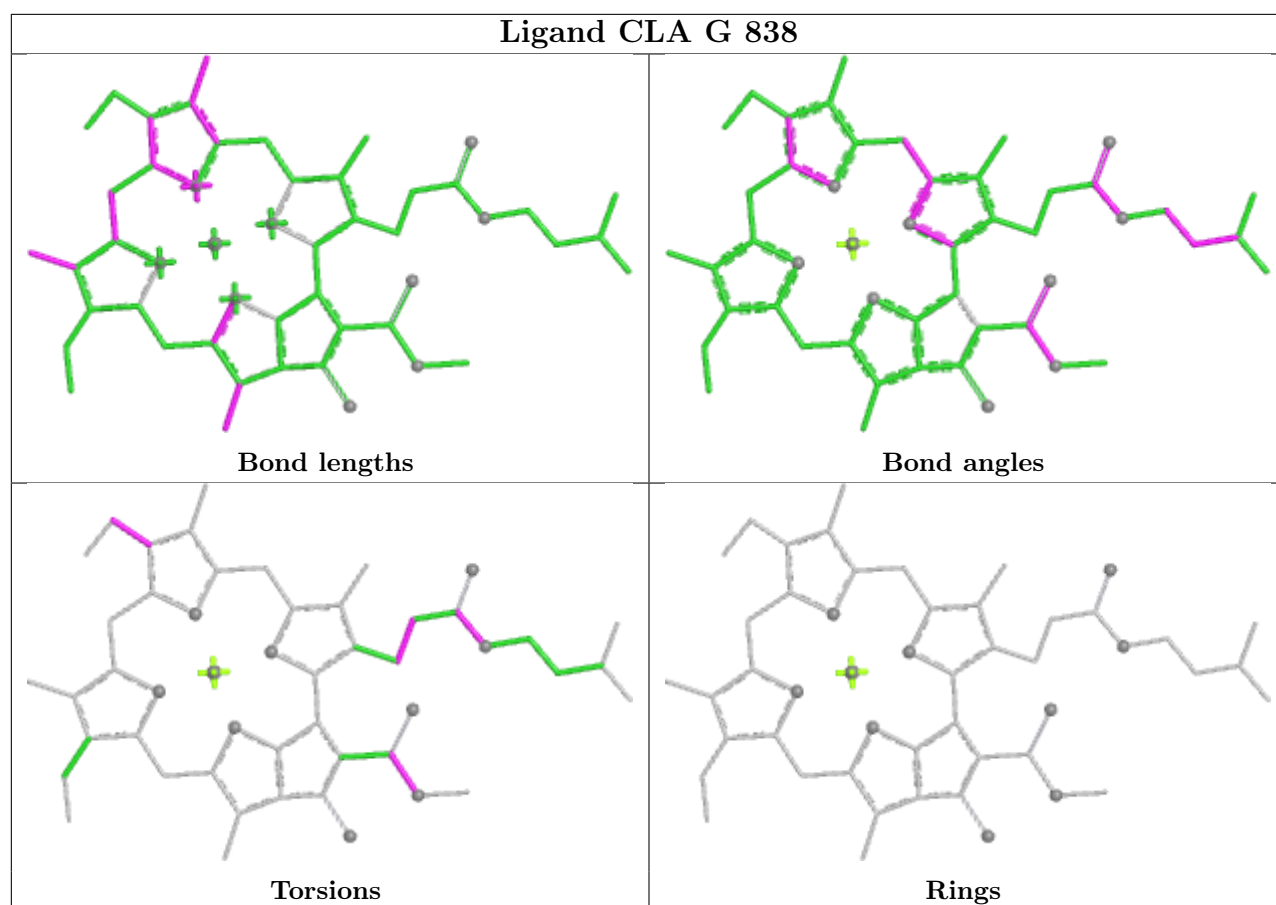
Bond angles



Torsions

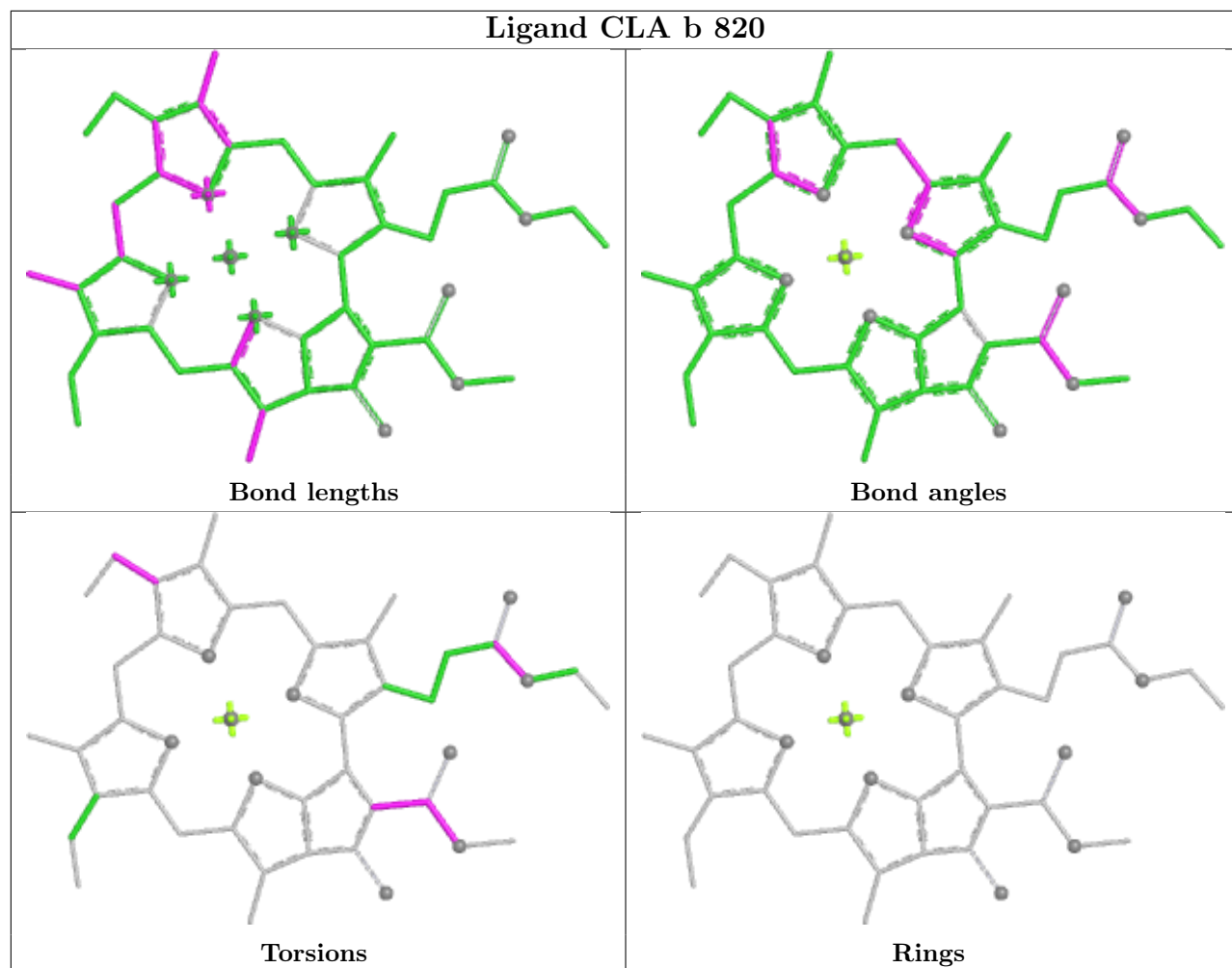


Rings

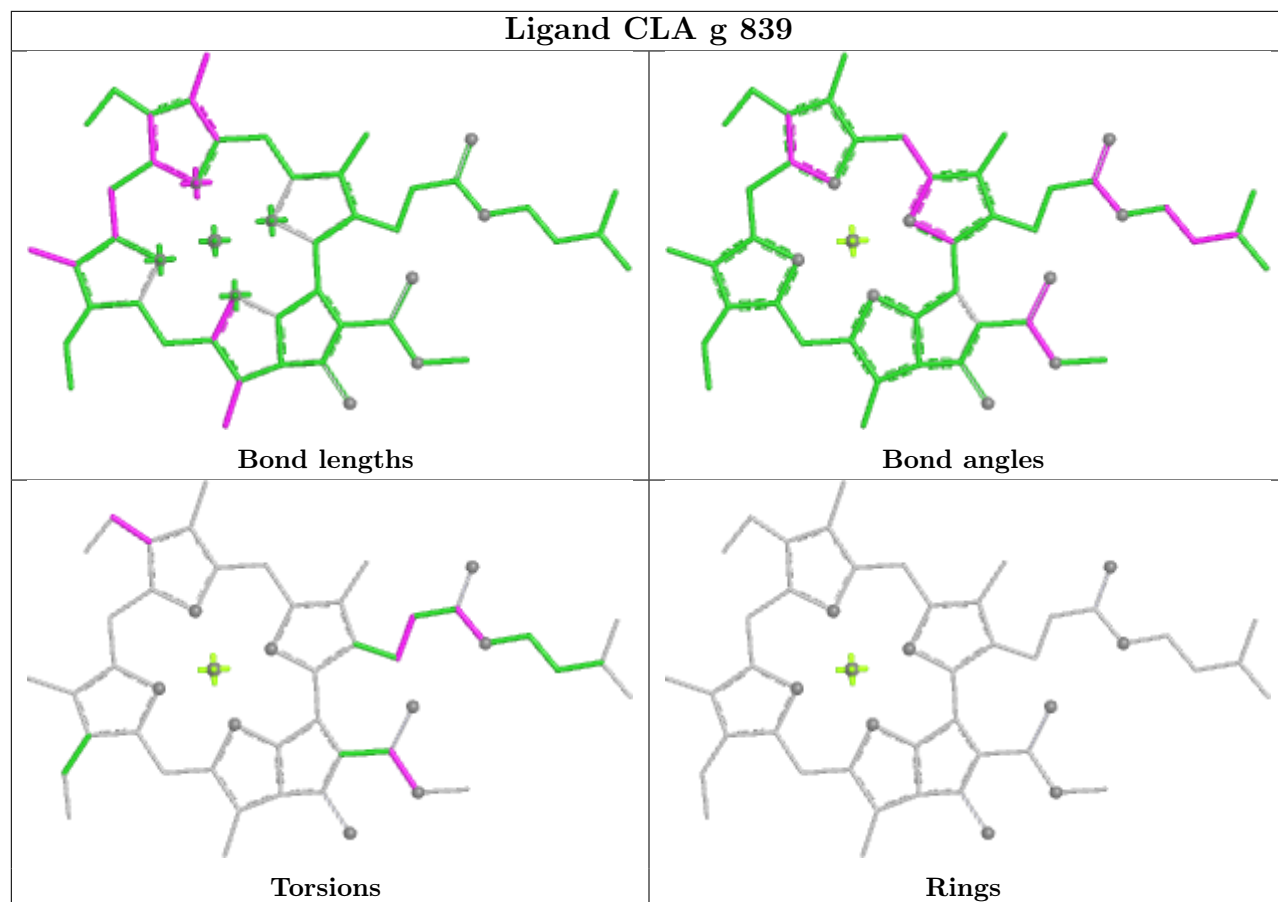




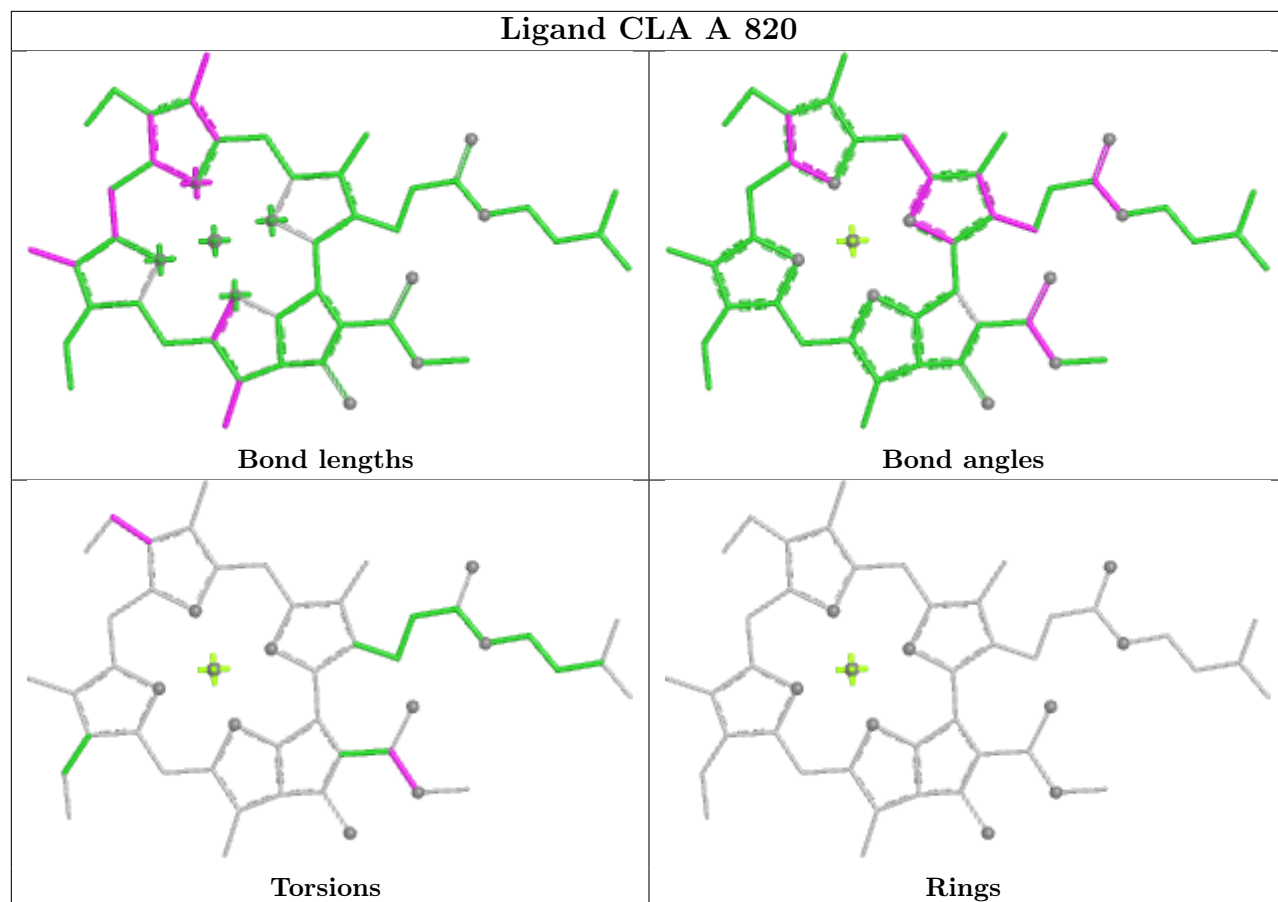
## Ligand CLA b 820



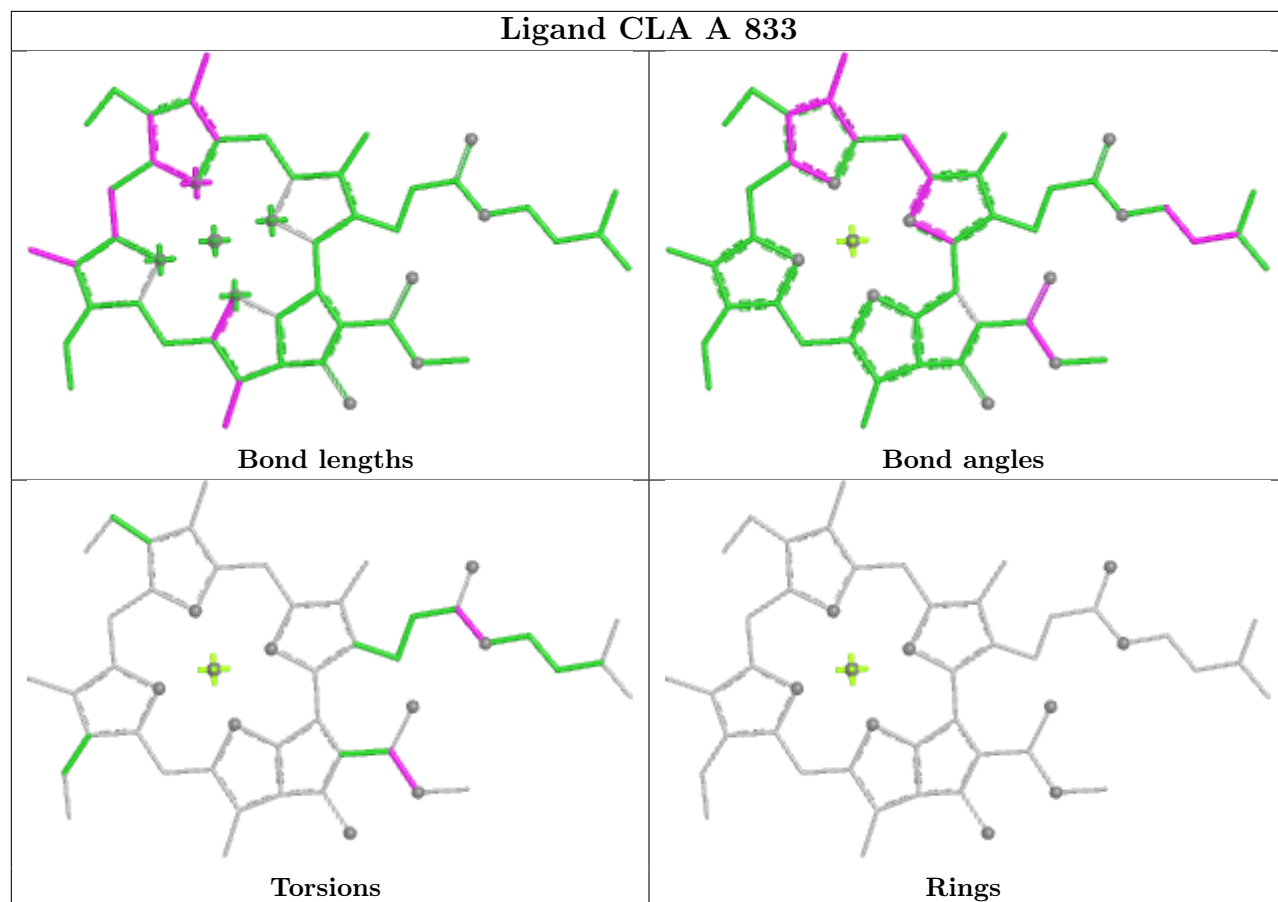
## Ligand CLA g 839



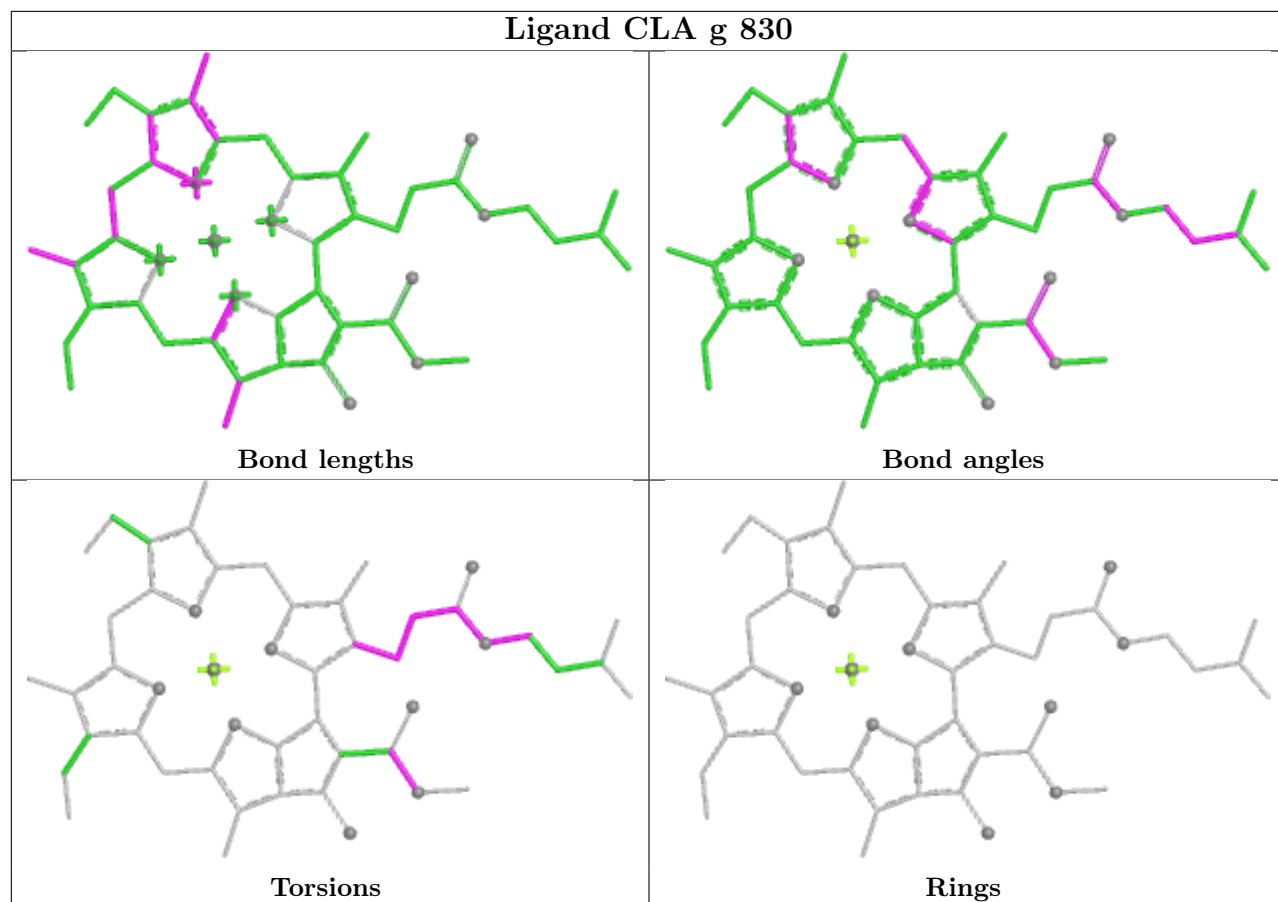
## Ligand CLA A 820



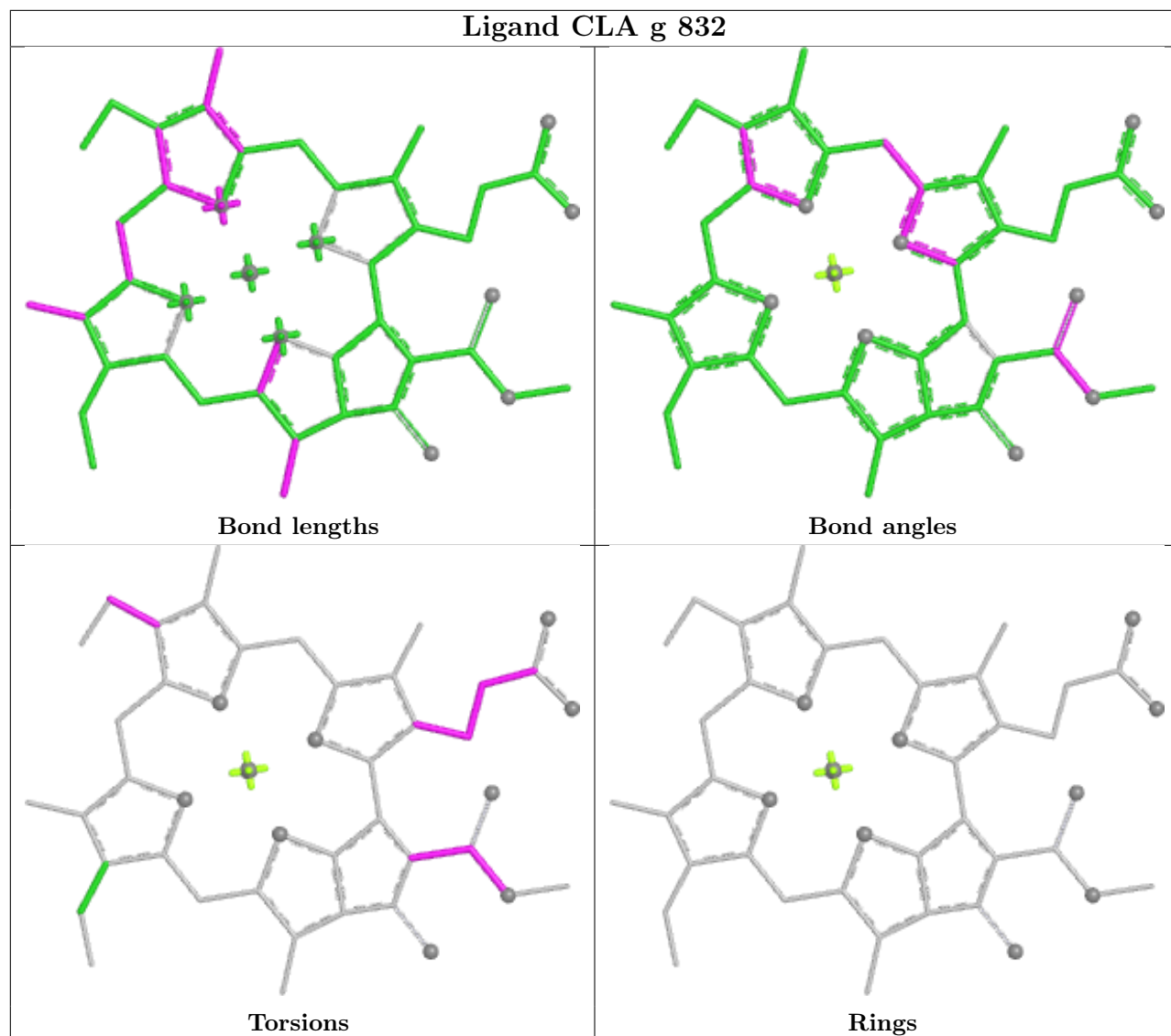
## Ligand CLA A 833



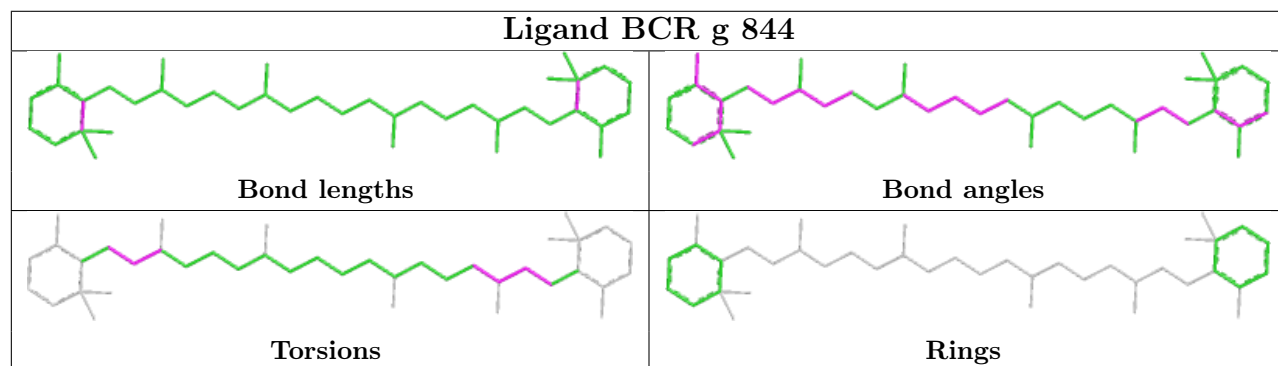
## Ligand CLA g 830



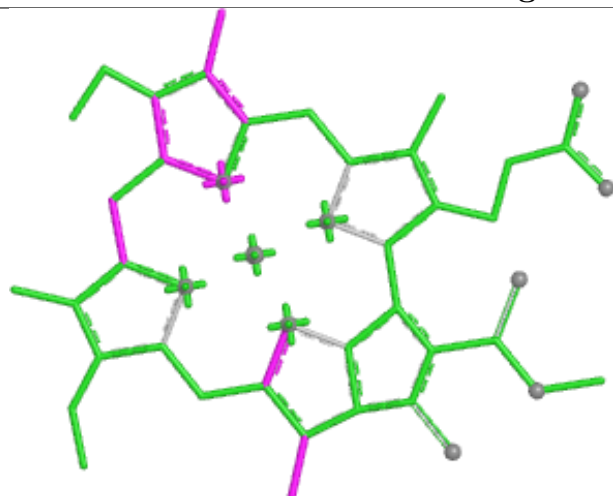
## Ligand CLA g 832



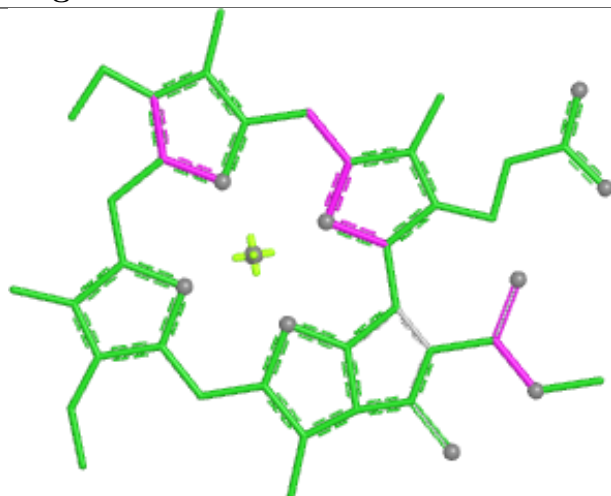
## Ligand BCR g 844



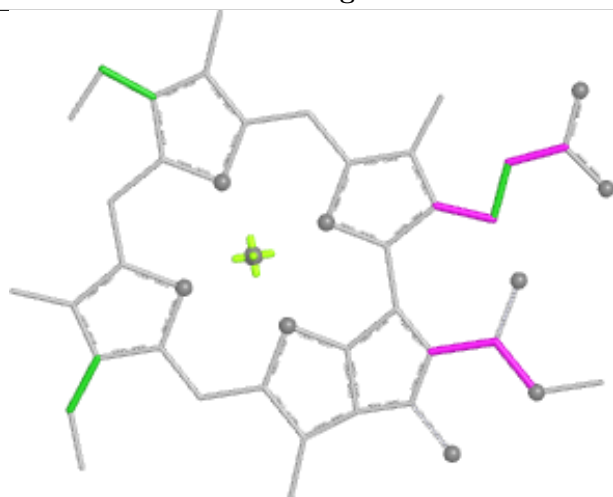
## Ligand CLA g 837



Bond lengths



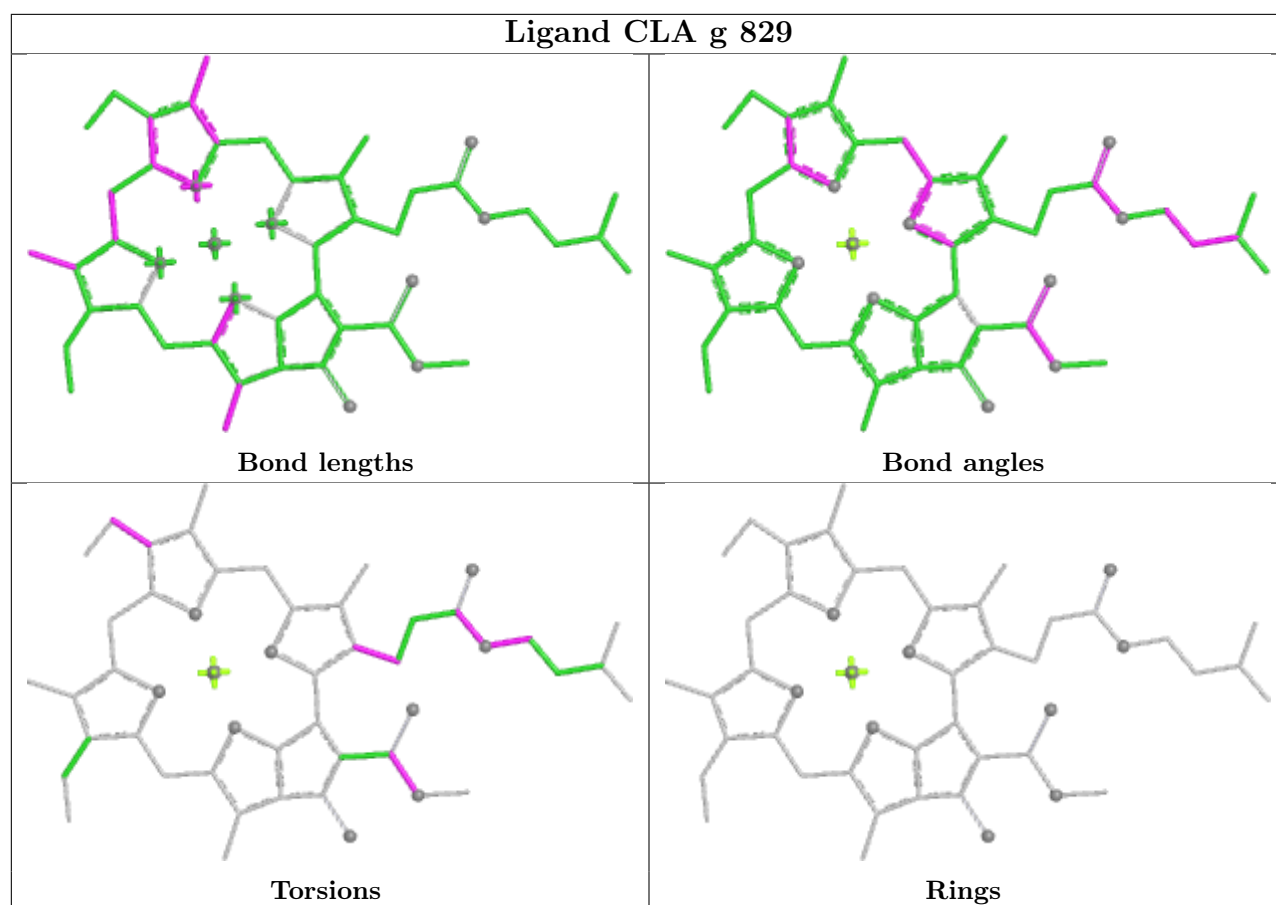
Bond angles



Torsions

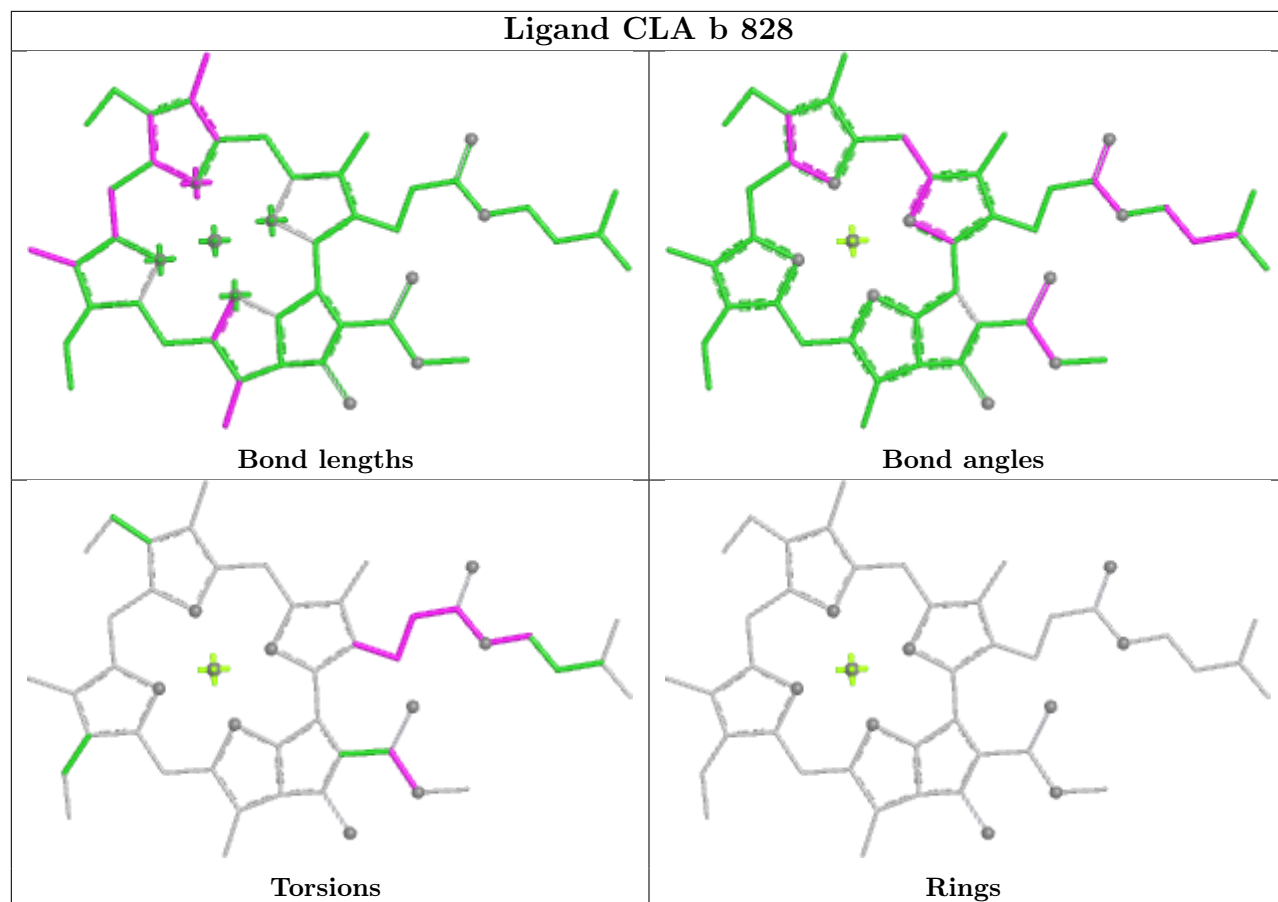


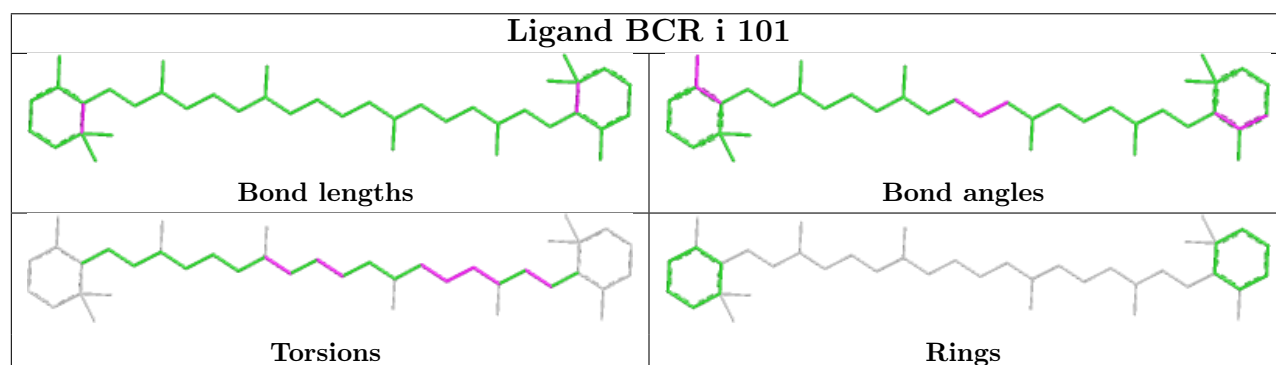
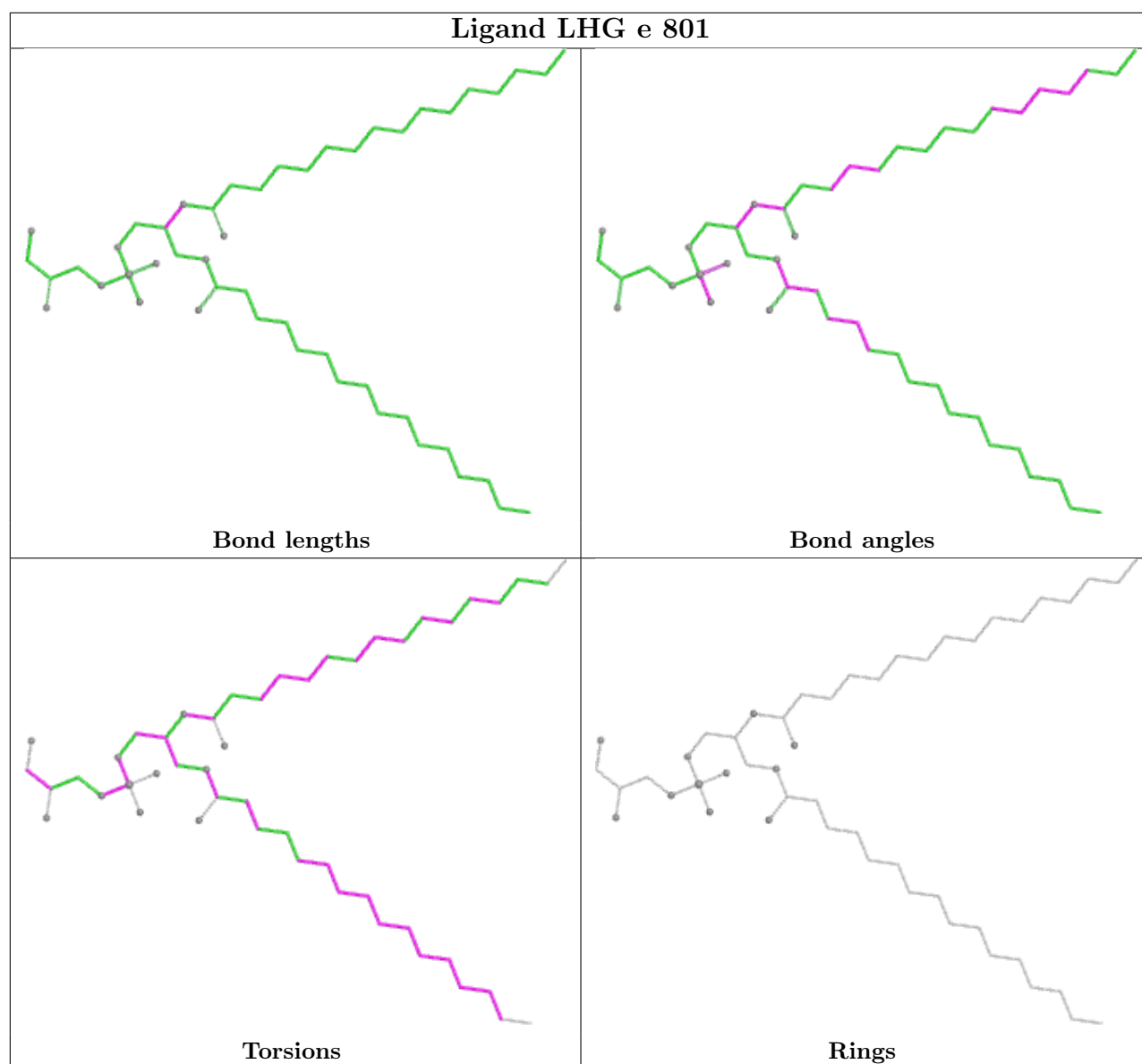
Rings

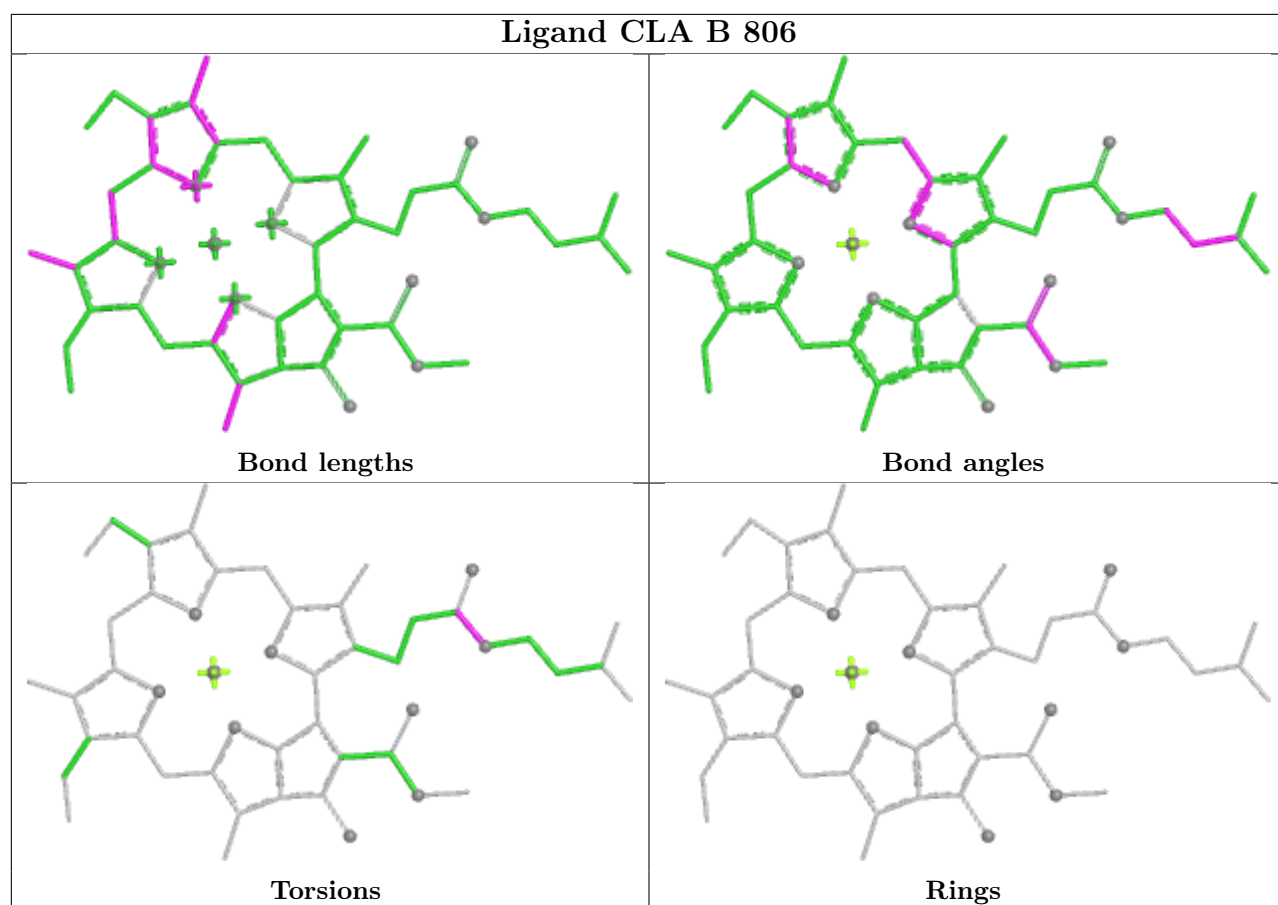


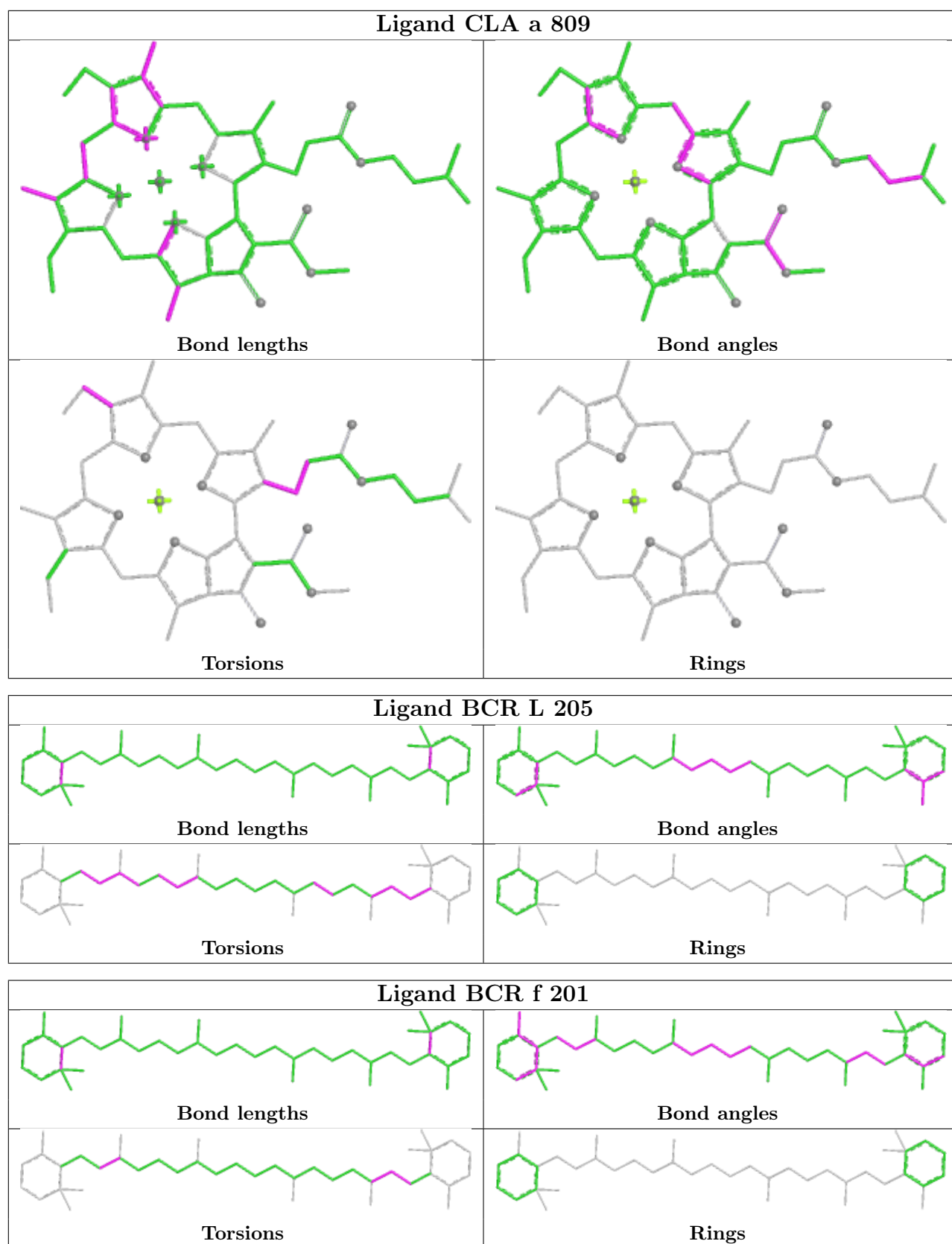


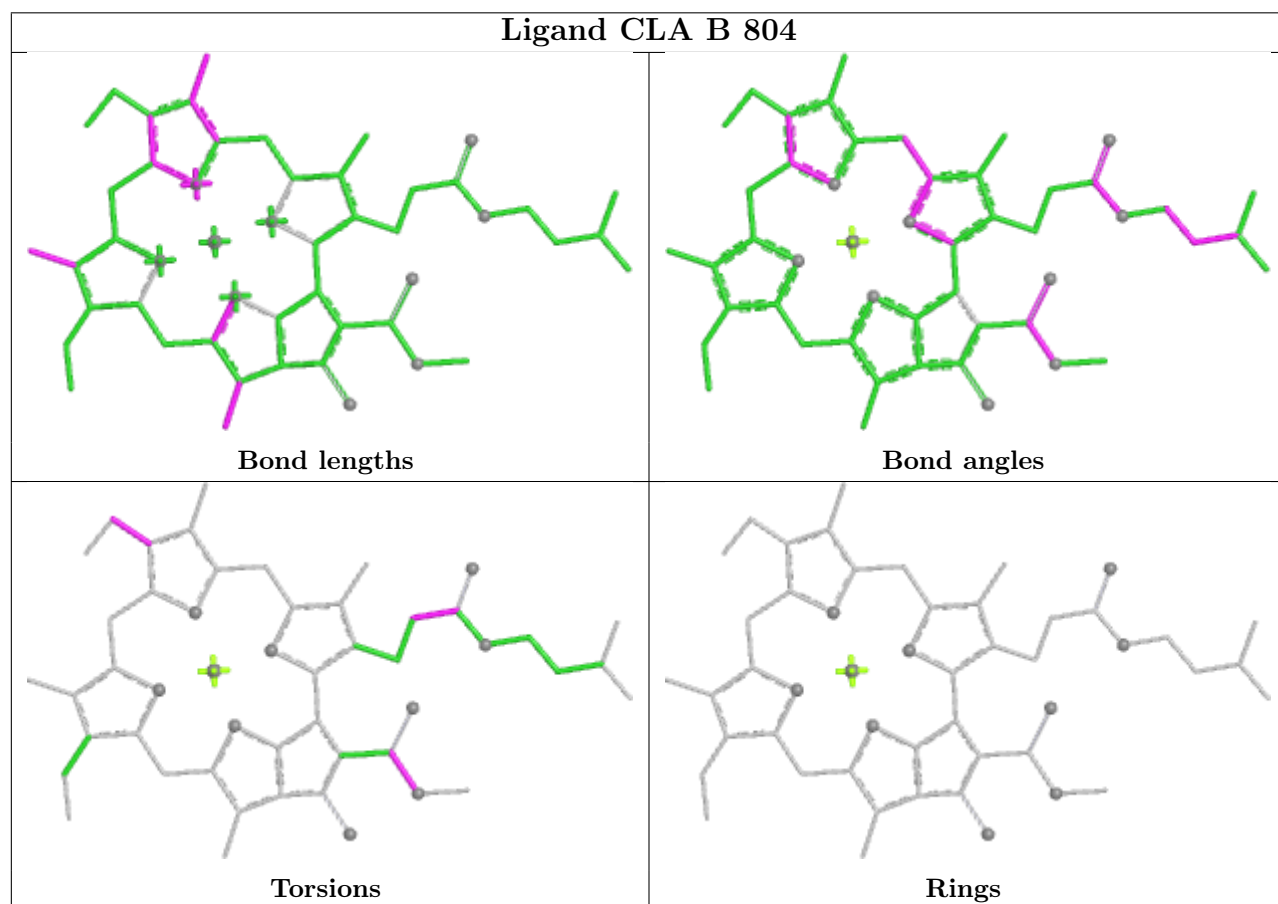
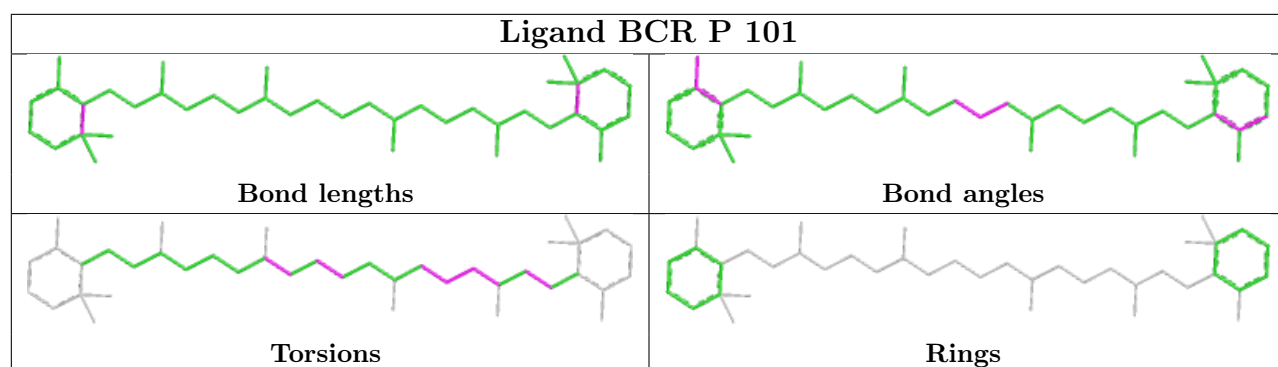
## Ligand CLA b 828



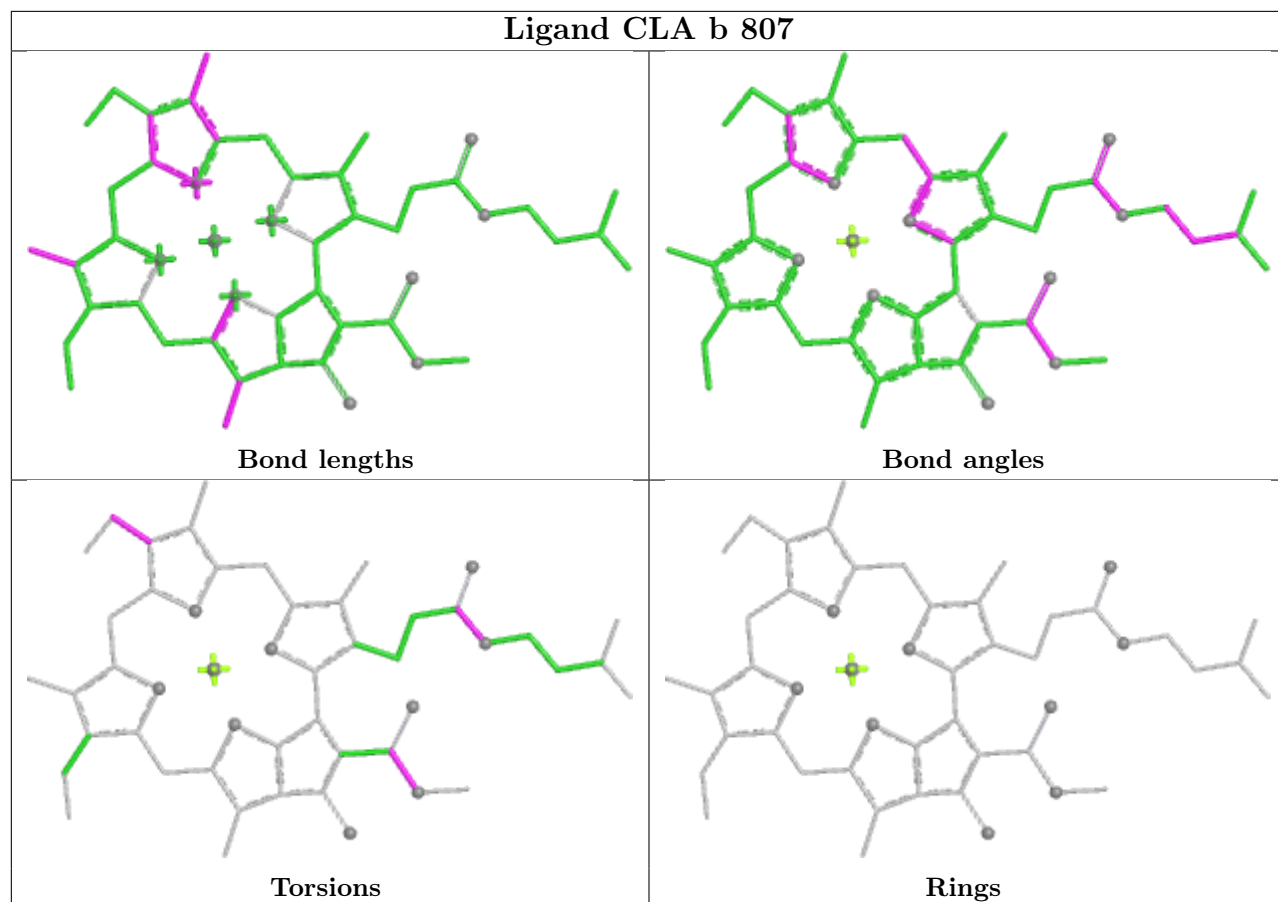




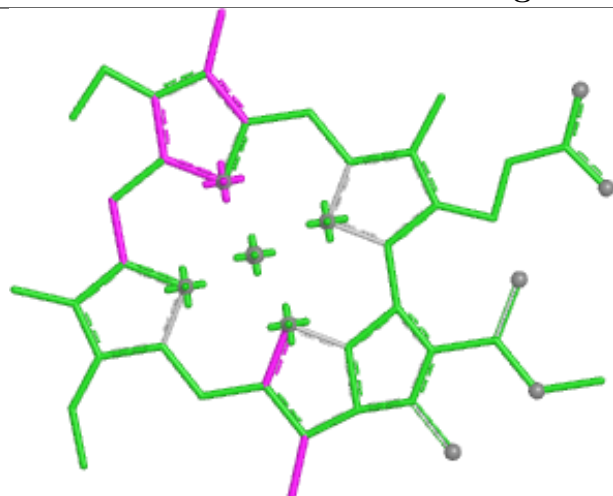




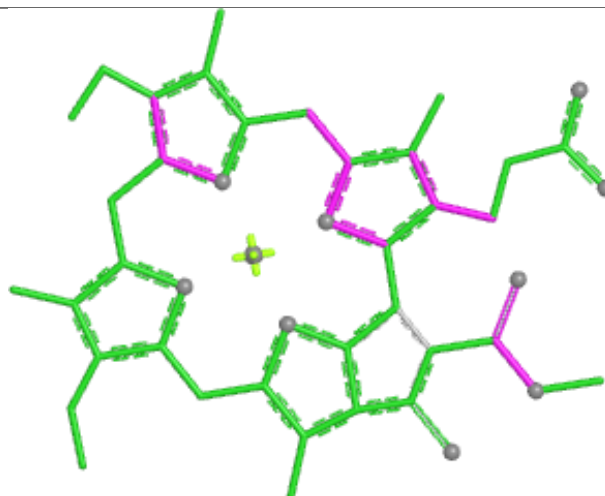
## Ligand CLA b 807



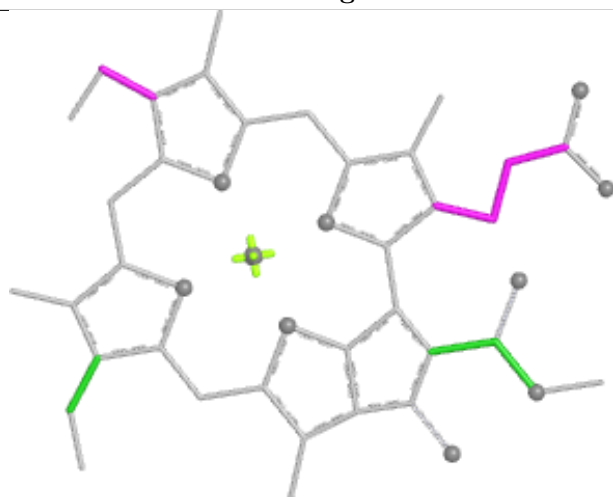
## Ligand CLA R 102



Bond lengths



Bond angles

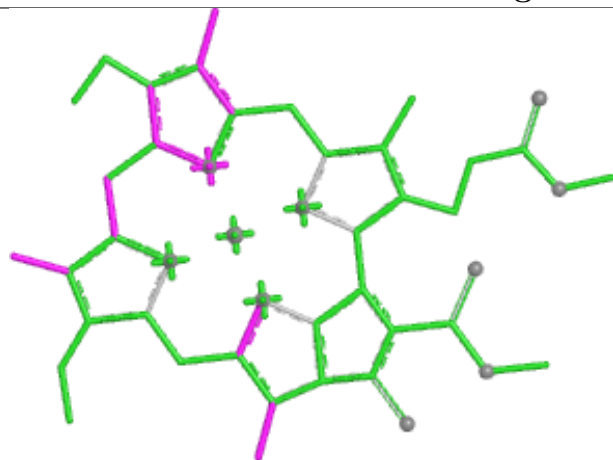


Torsions

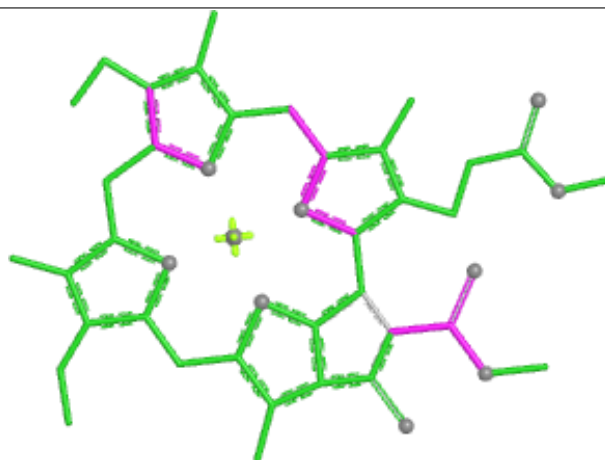


Rings

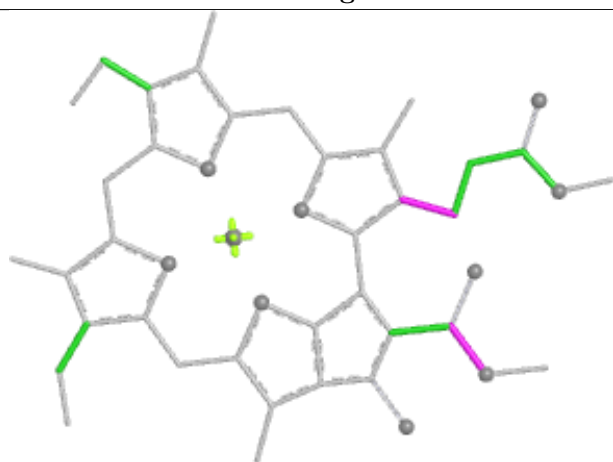
## Ligand CLA B 826



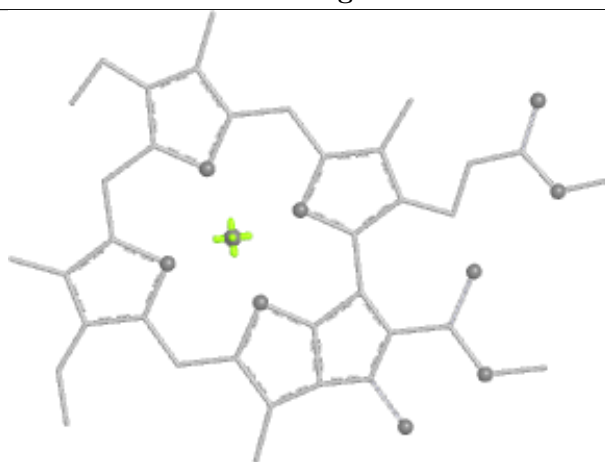
Bond lengths



Bond angles



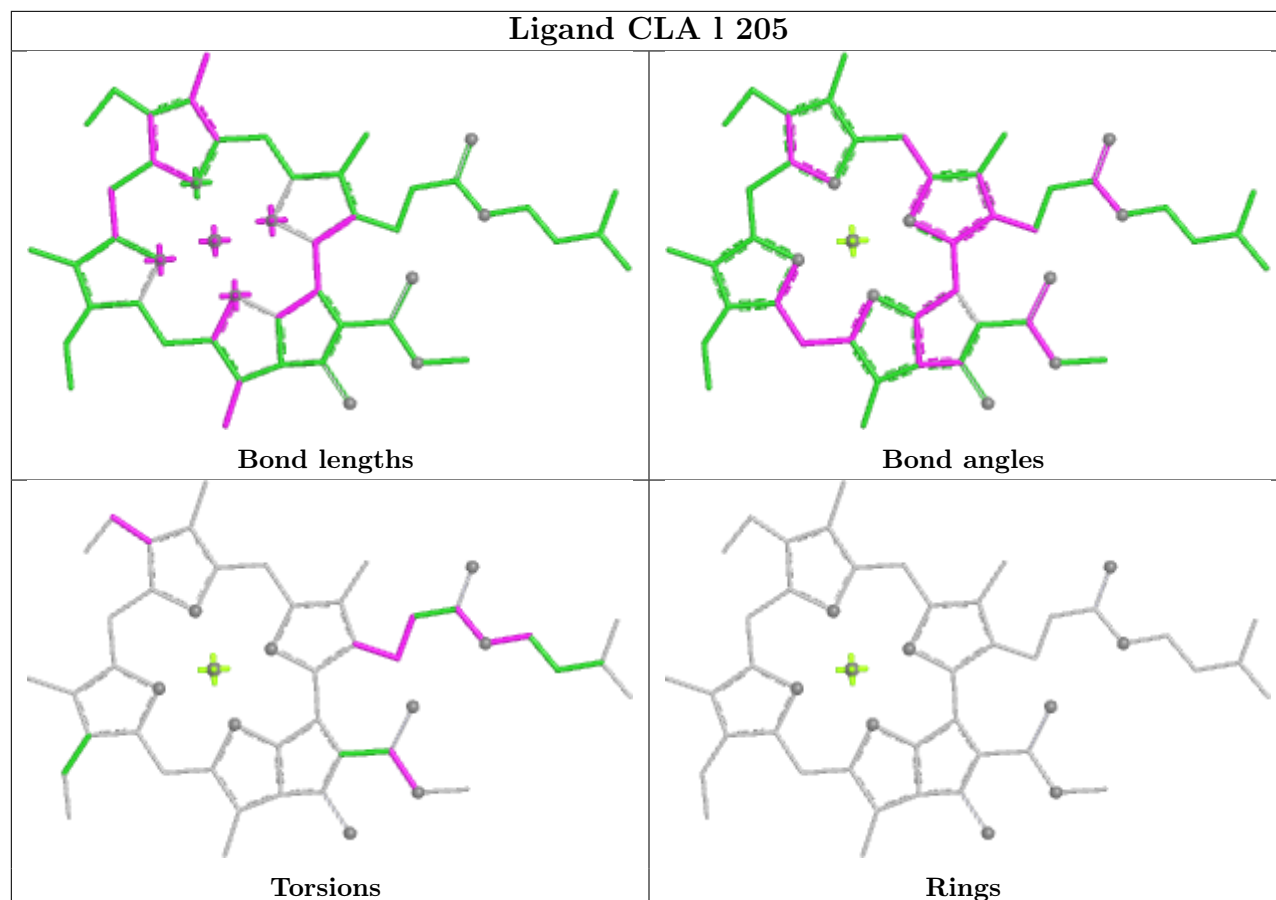
Torsions



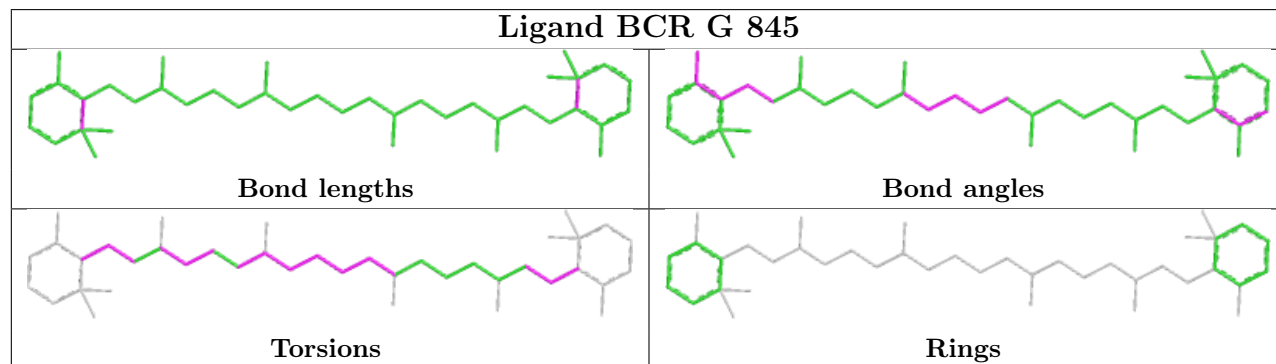
Rings



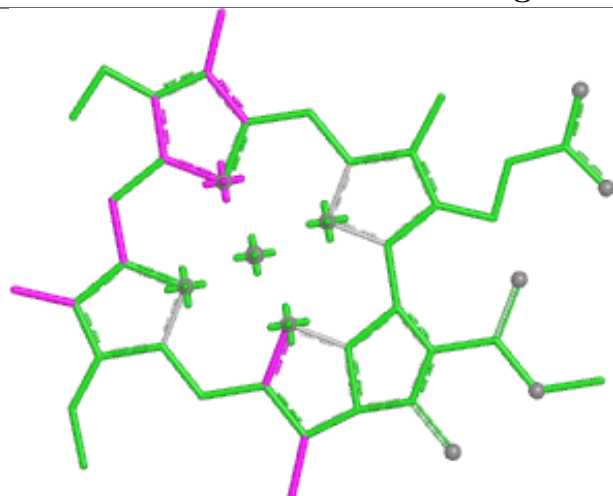
## Ligand CLA 1 205



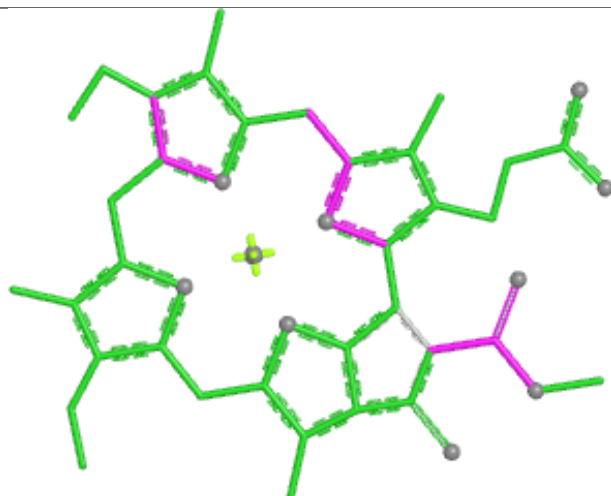
## Ligand BCR G 845



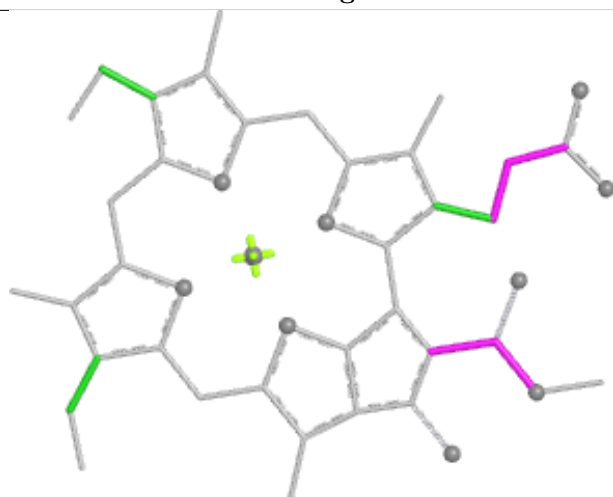
## Ligand CLA A 838



Bond lengths



Bond angles

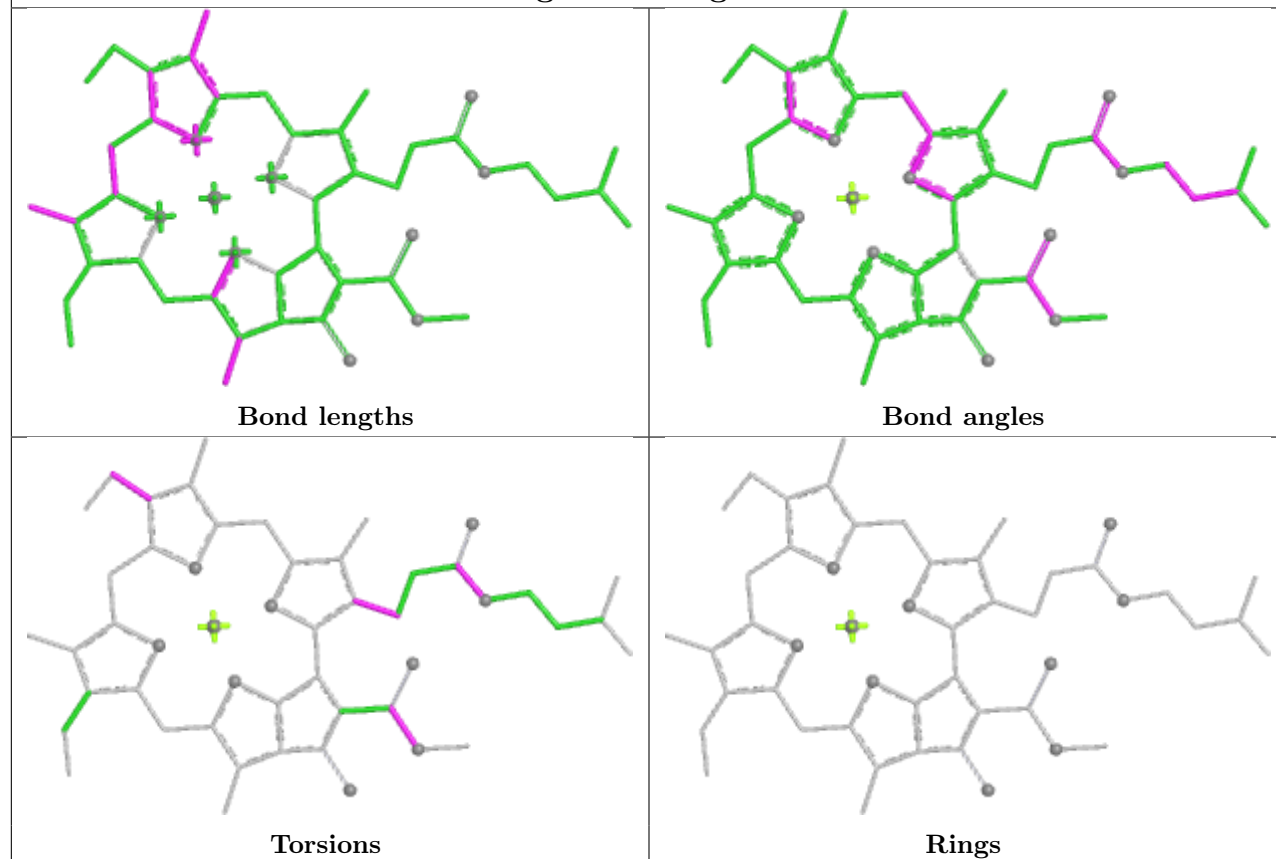


Torsions

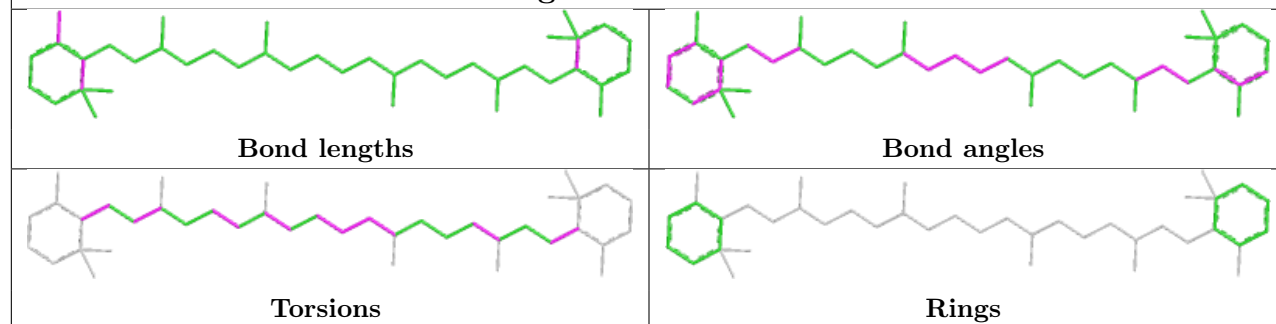


Rings

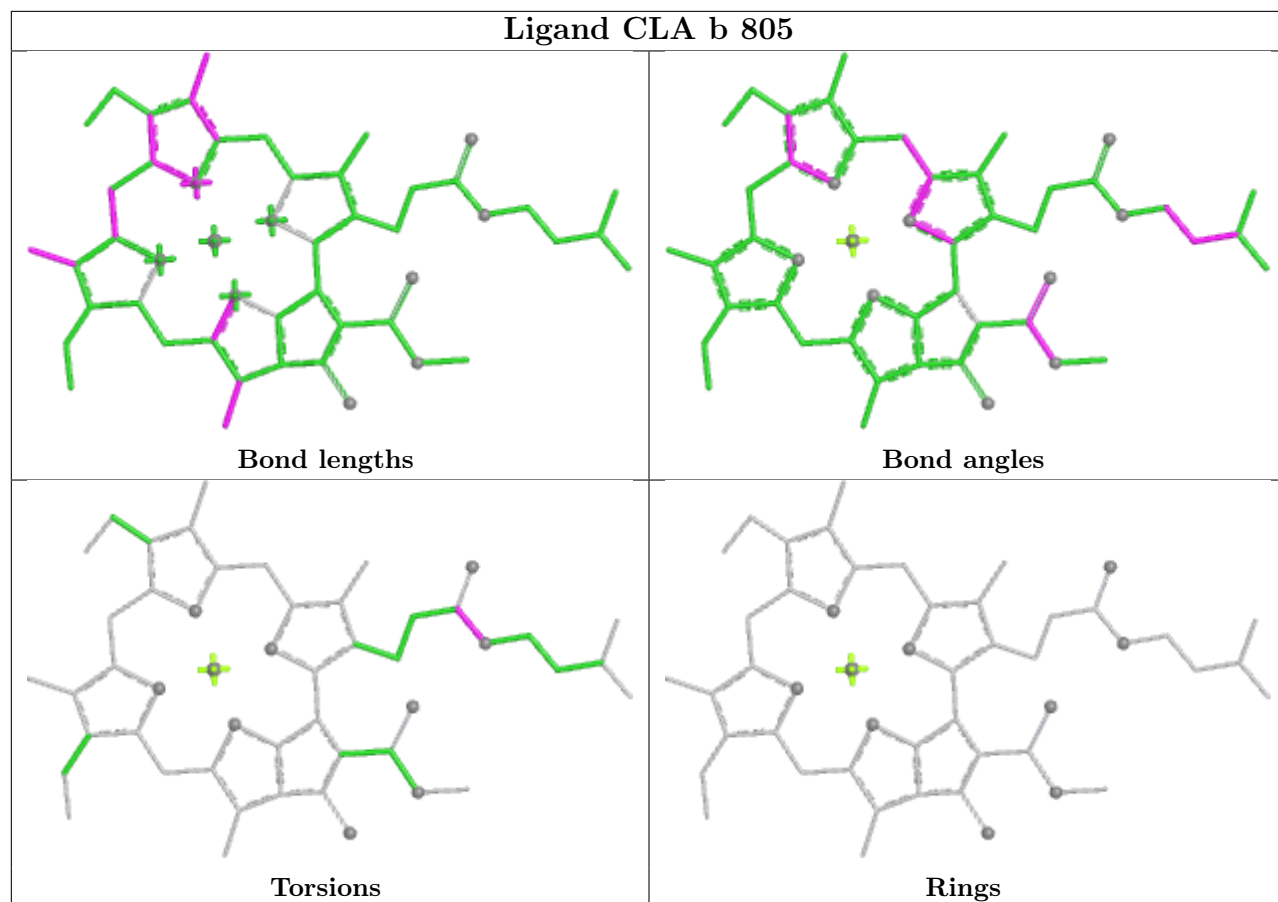
## Ligand CLA g 841

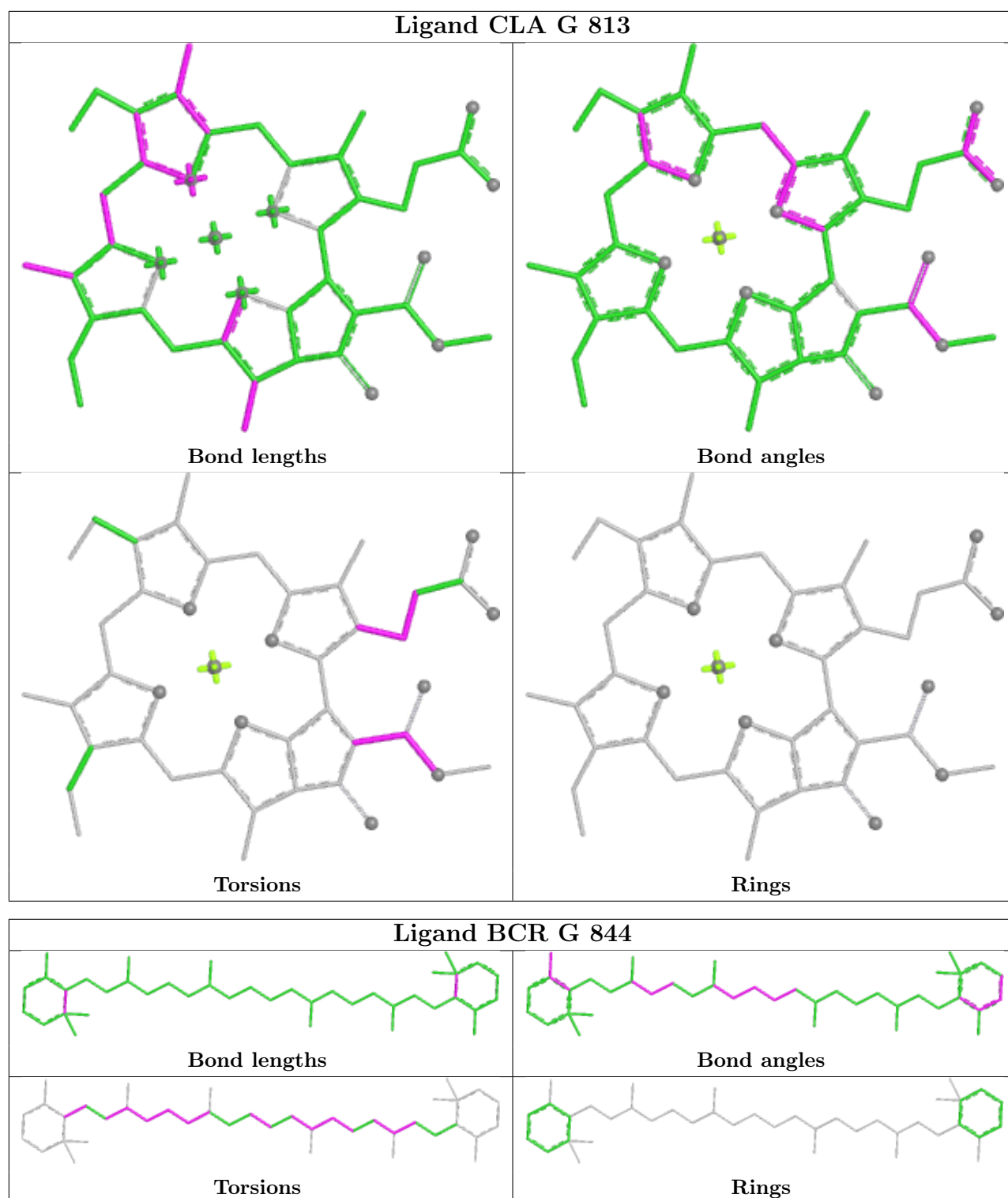


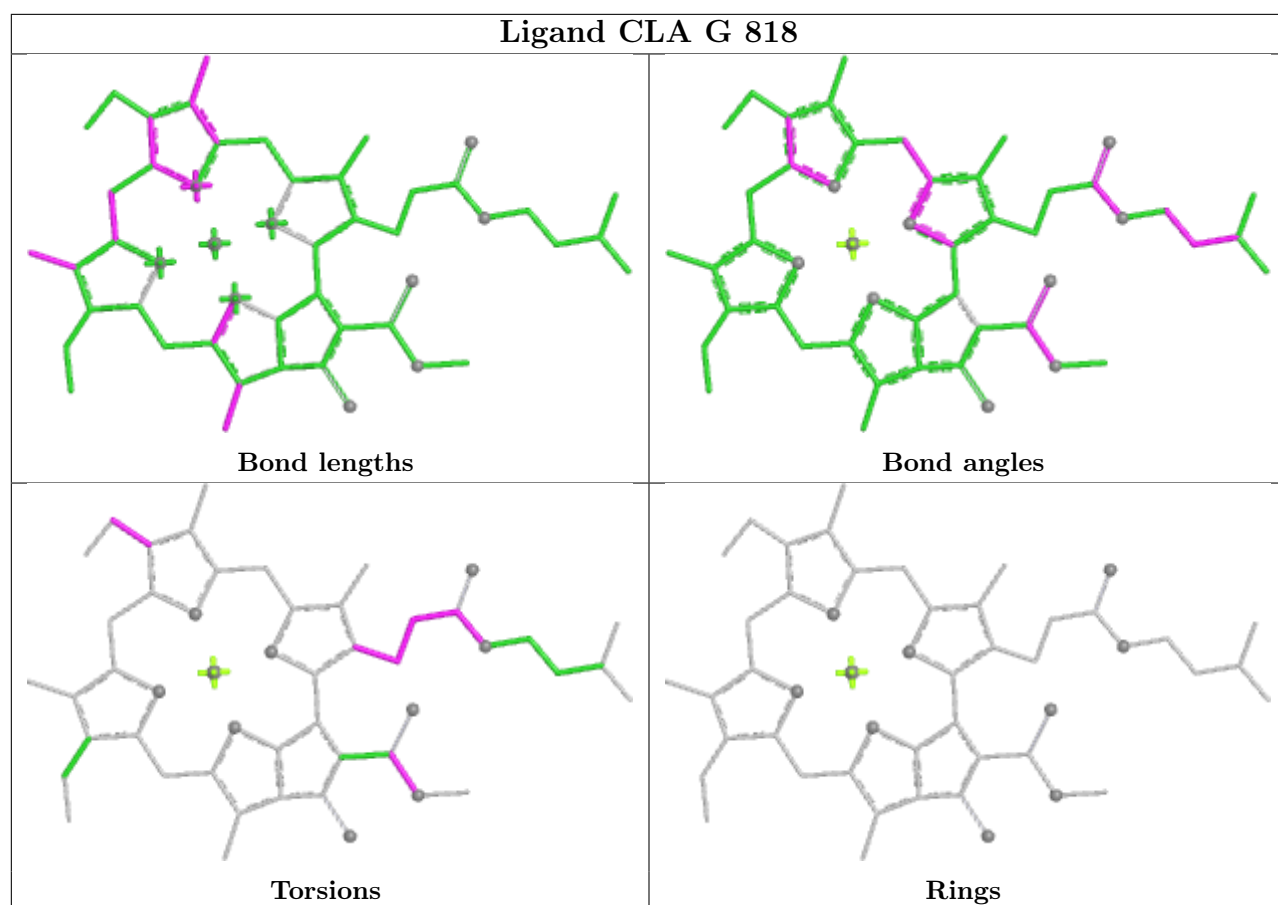
## Ligand BCR f 202



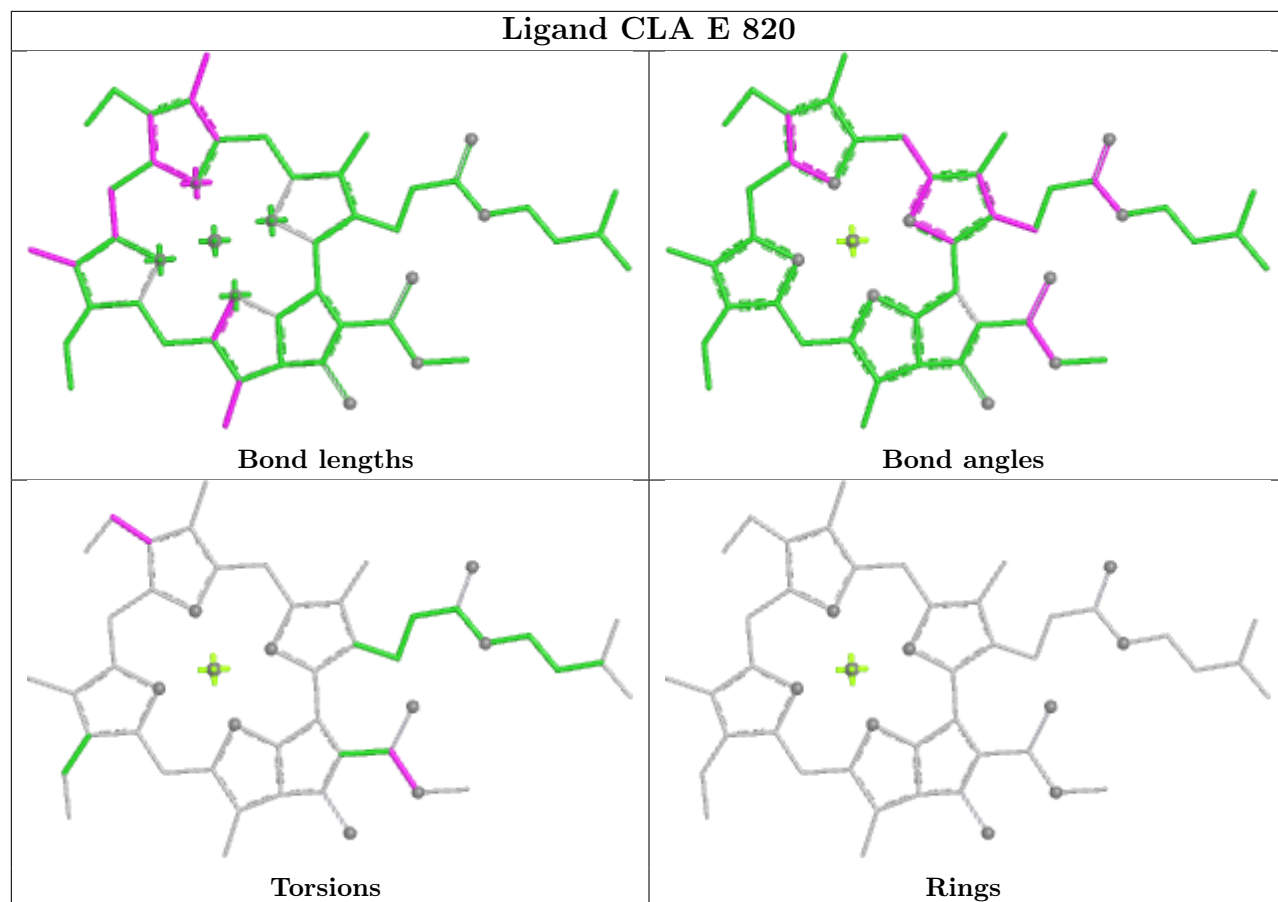
## Ligand CLA b 805



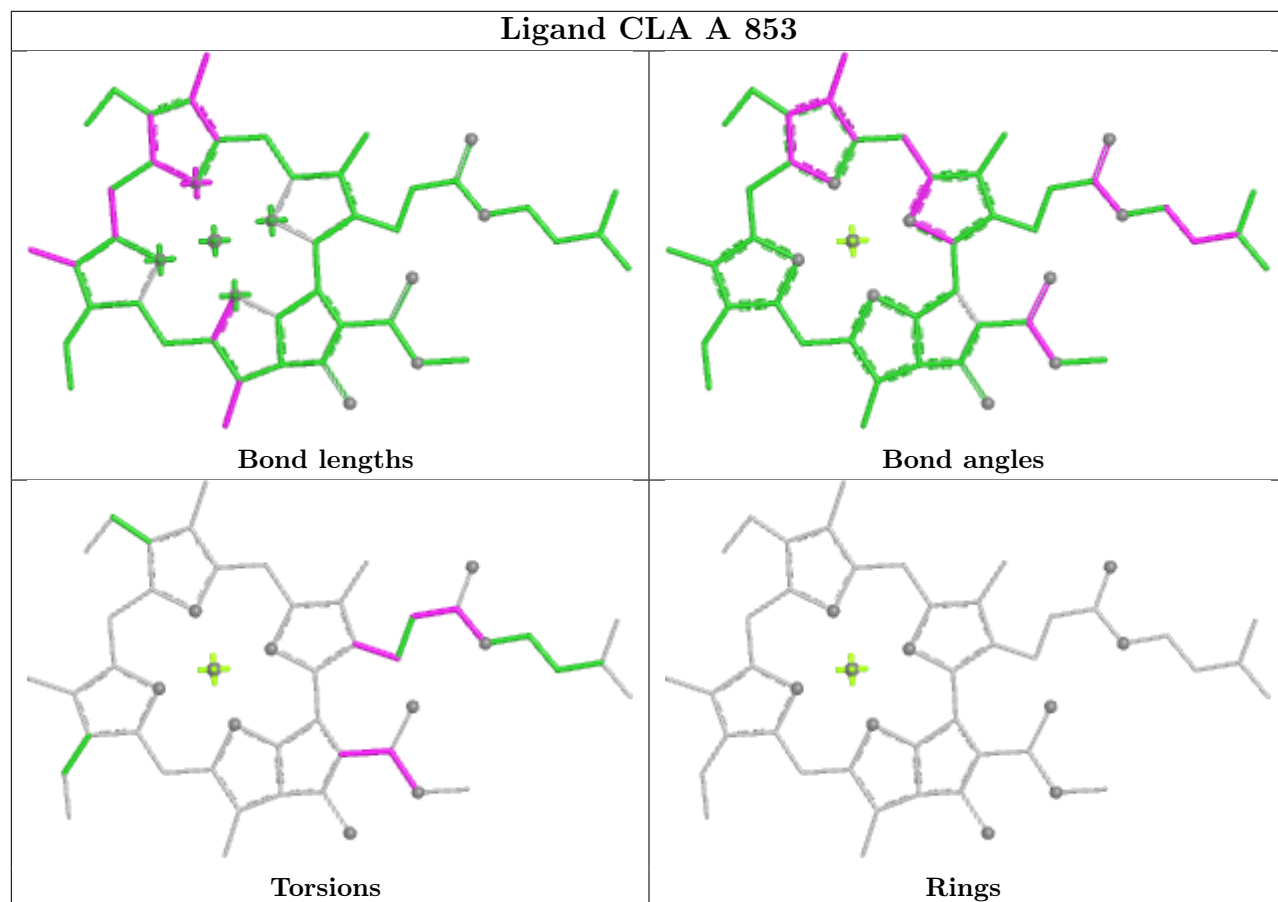




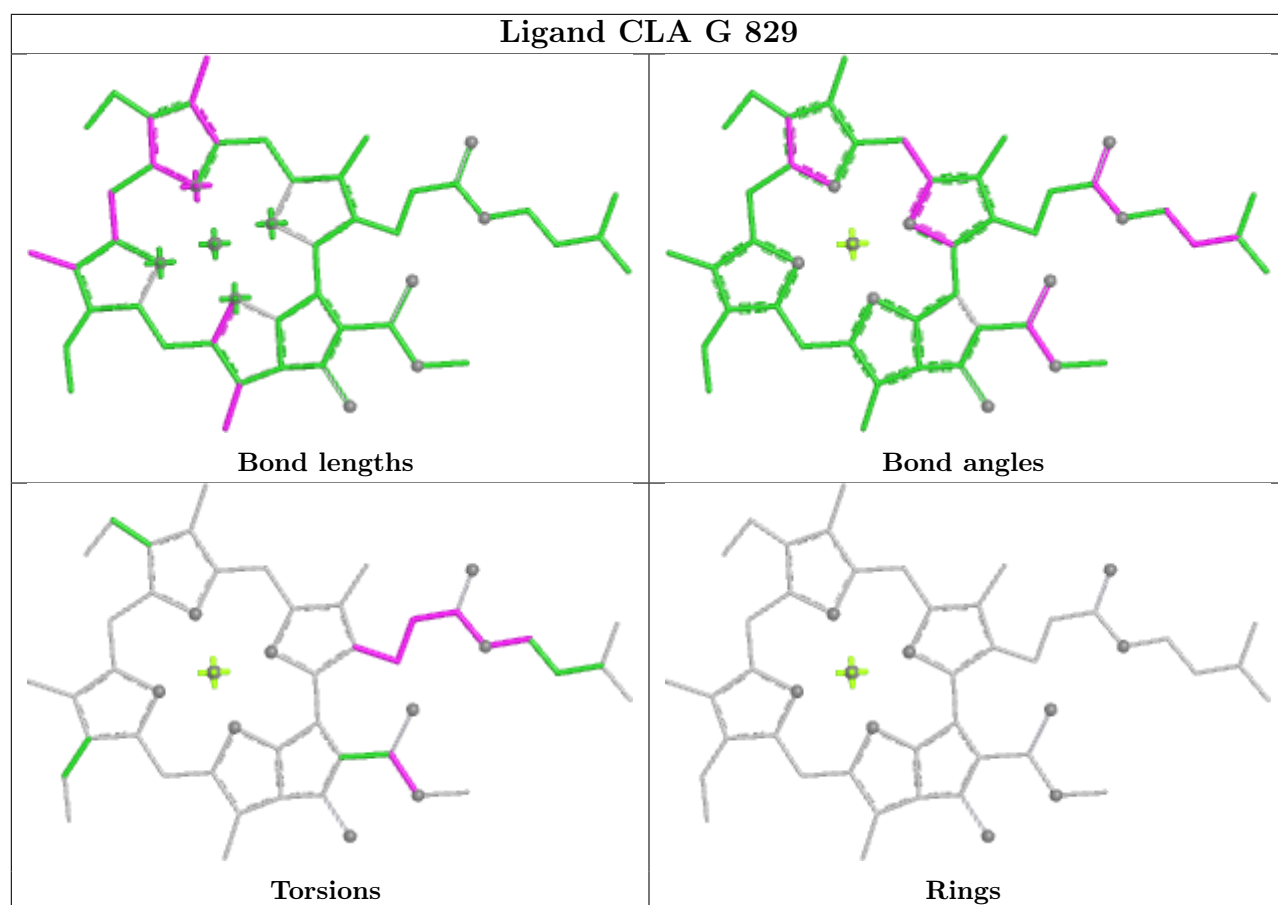
## Ligand CLA E 820



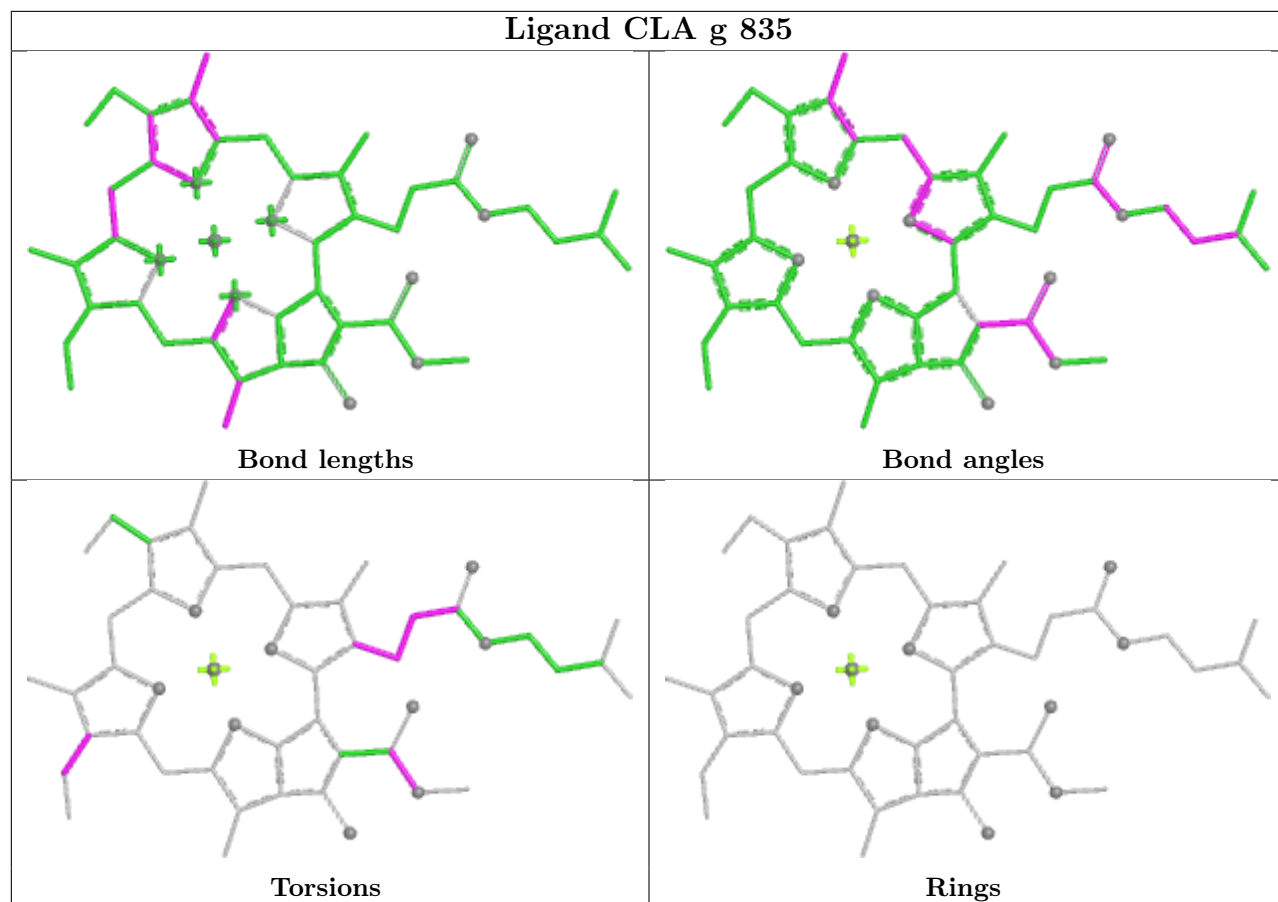
## Ligand CLA A 853



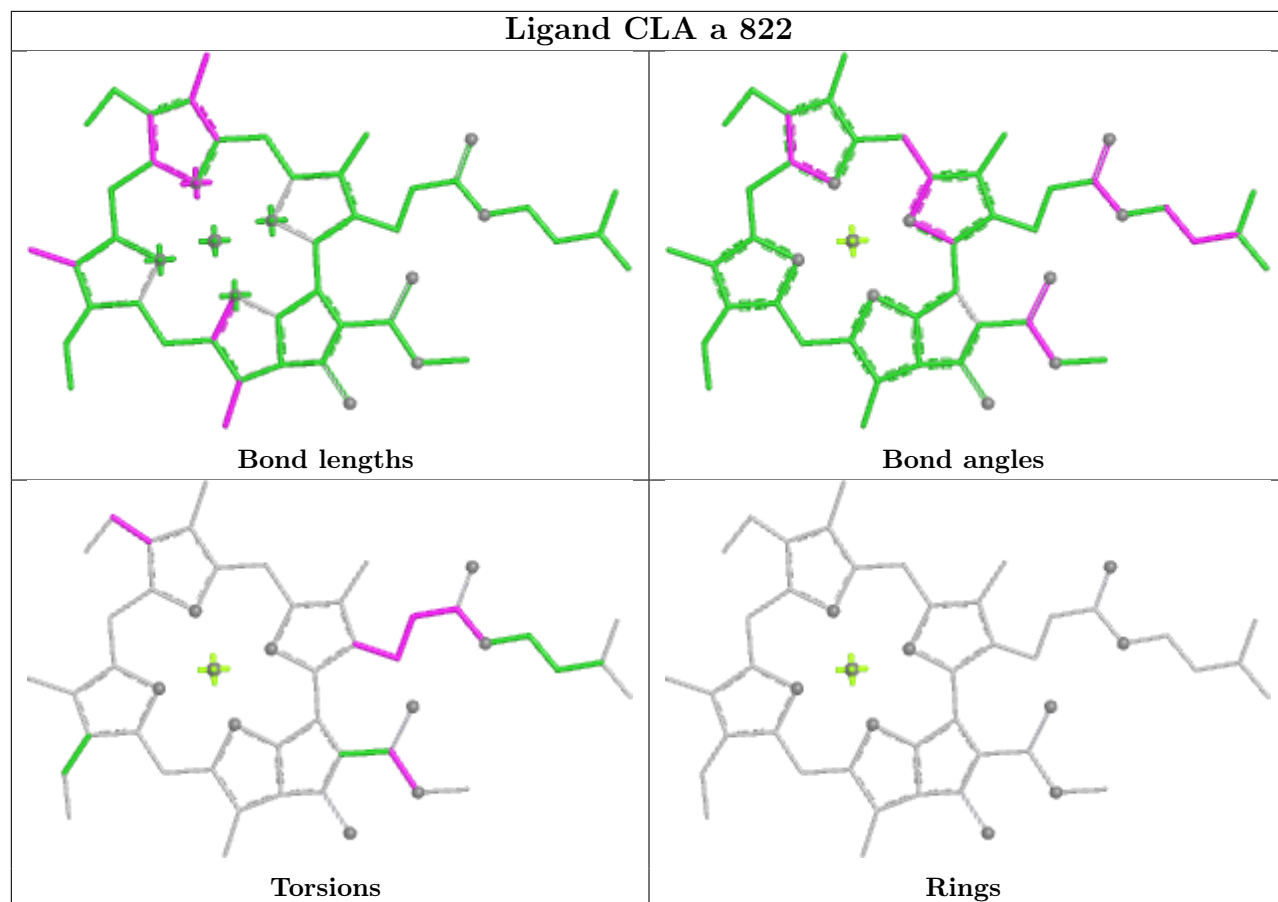


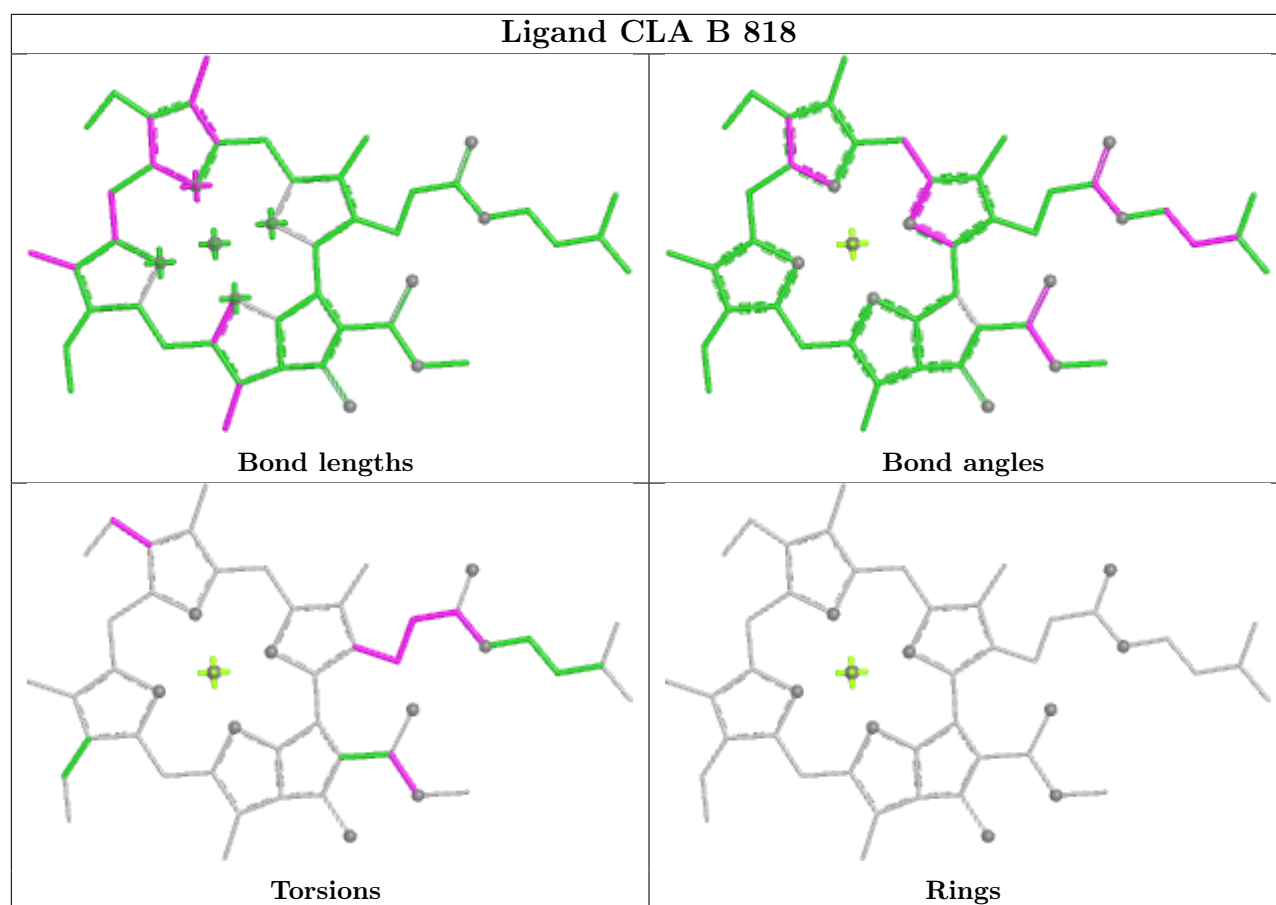


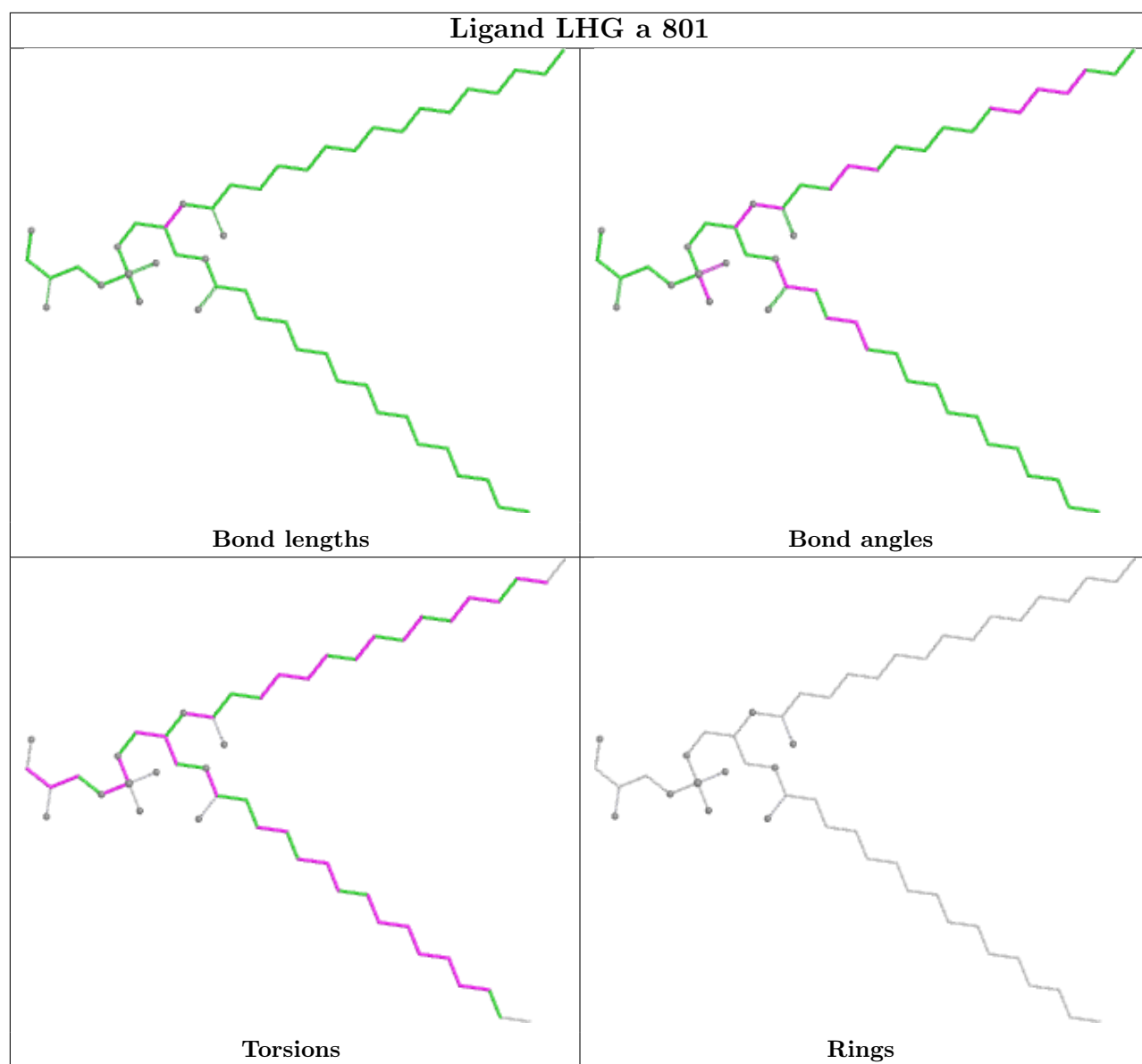
## Ligand CLA g 835



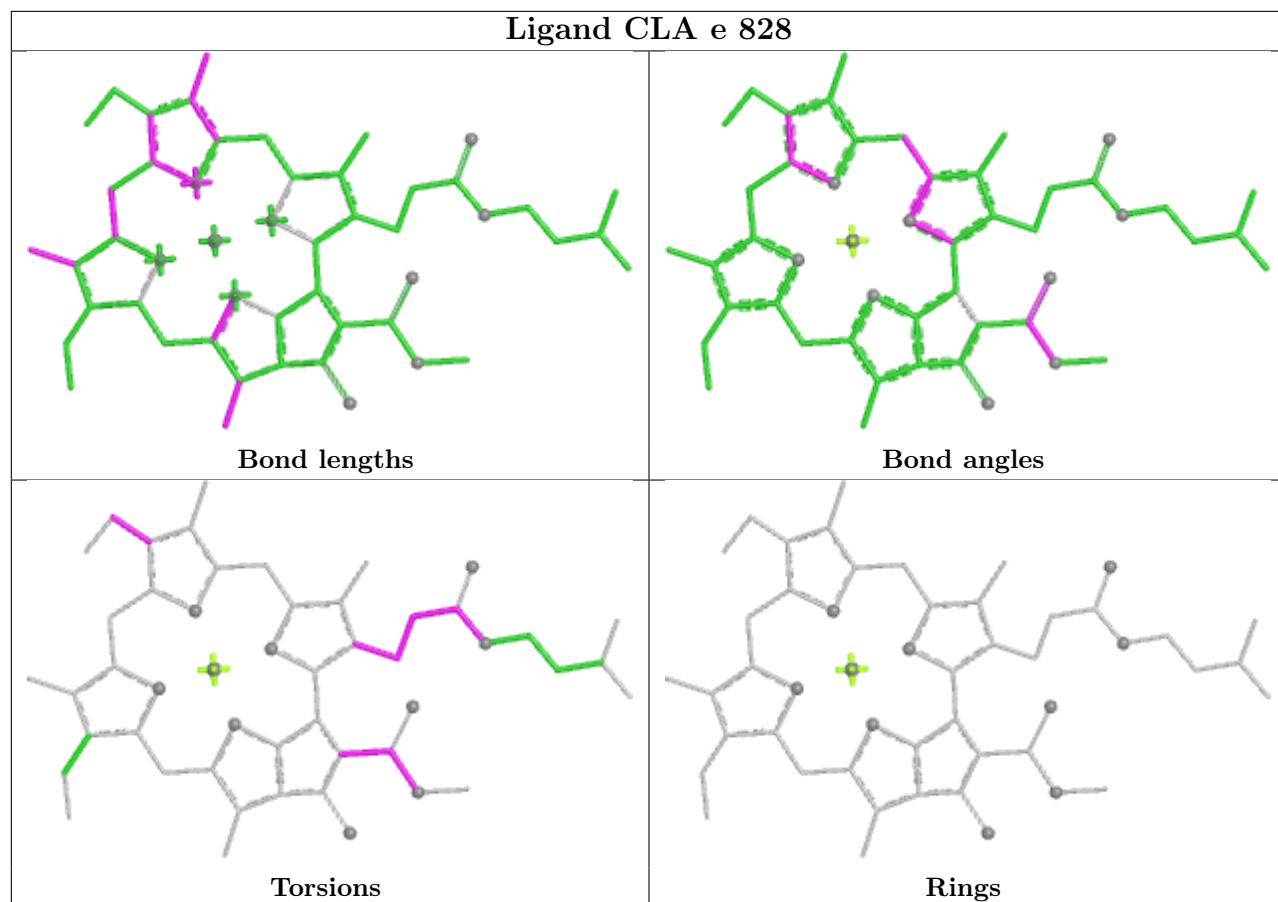
## Ligand CLA a 822



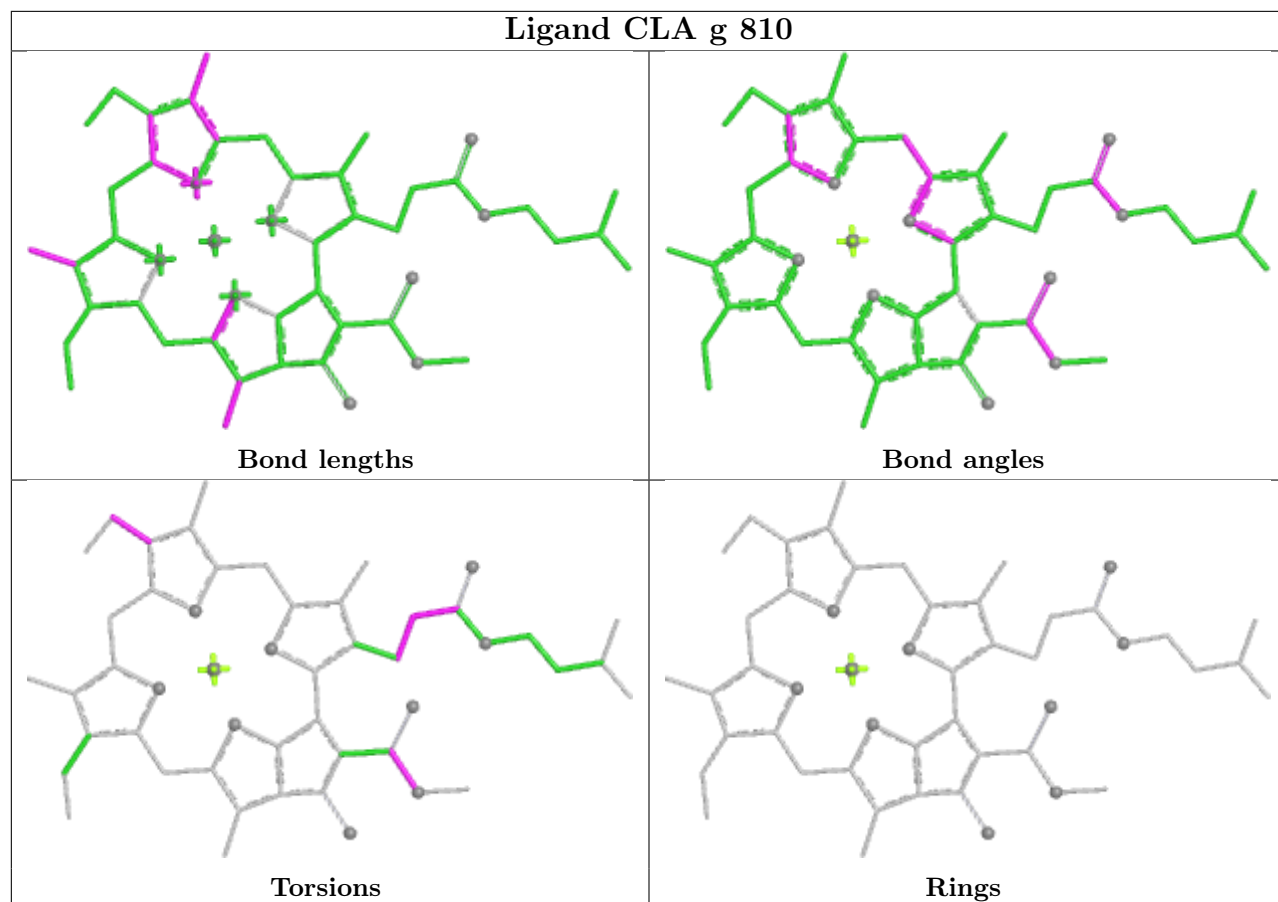




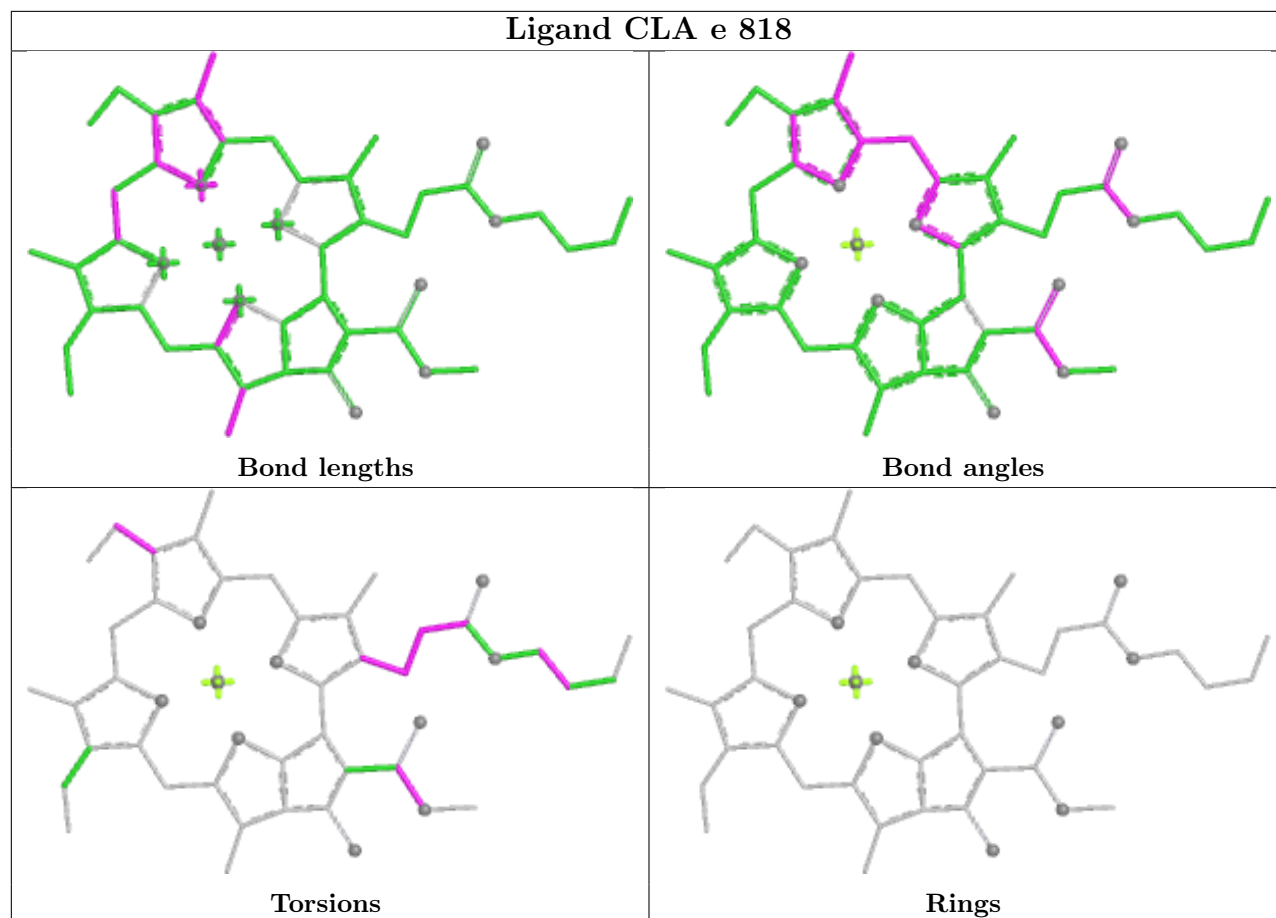
## Ligand CLA e 828



## Ligand CLA g 810

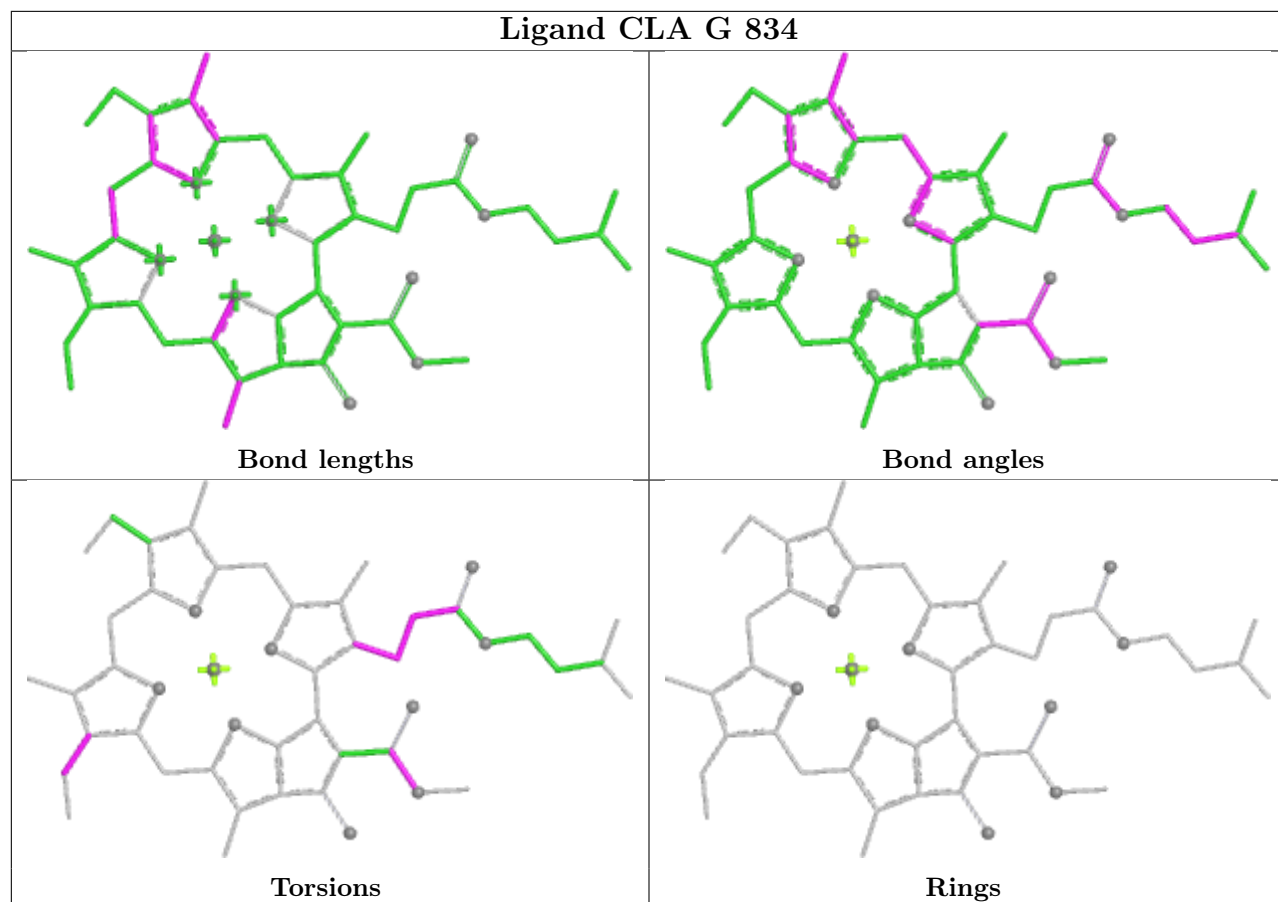


## Ligand CLA e 818

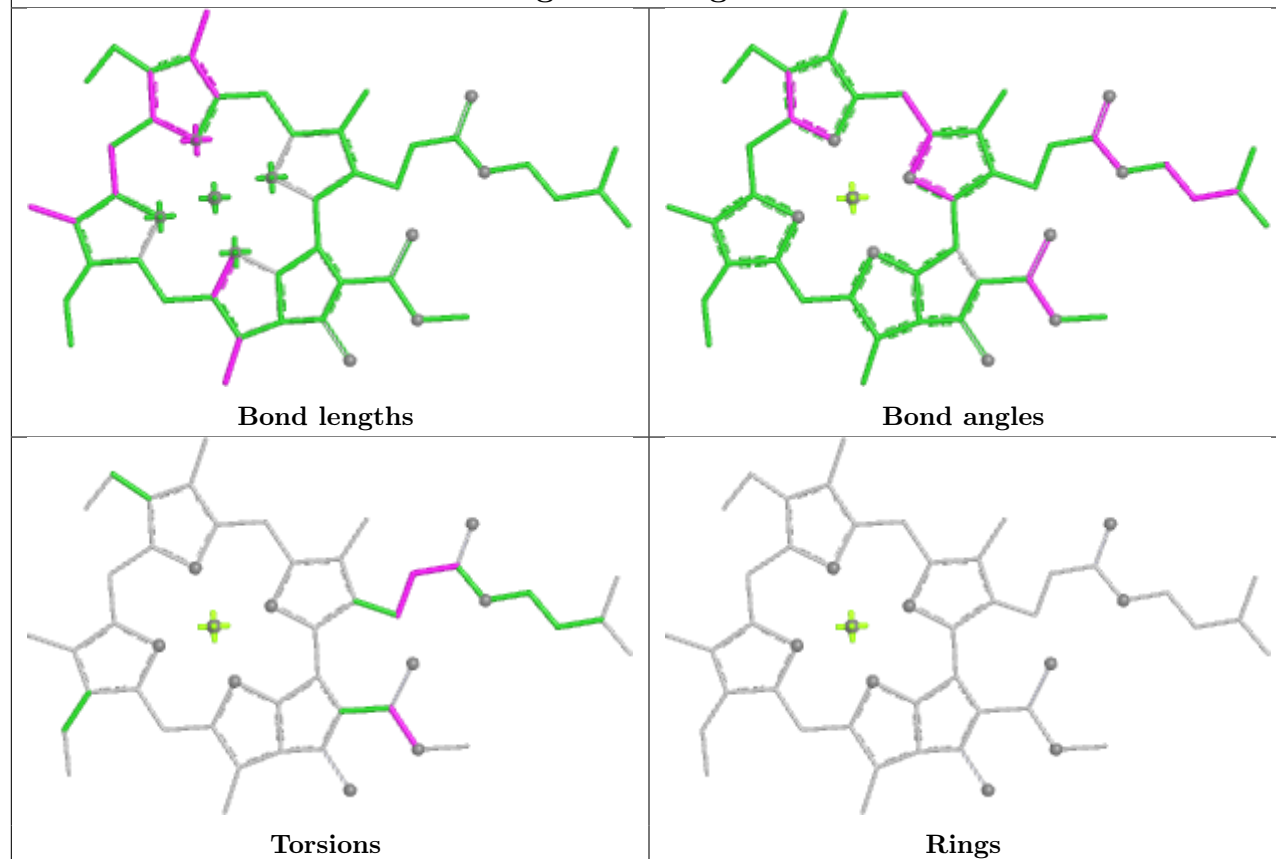




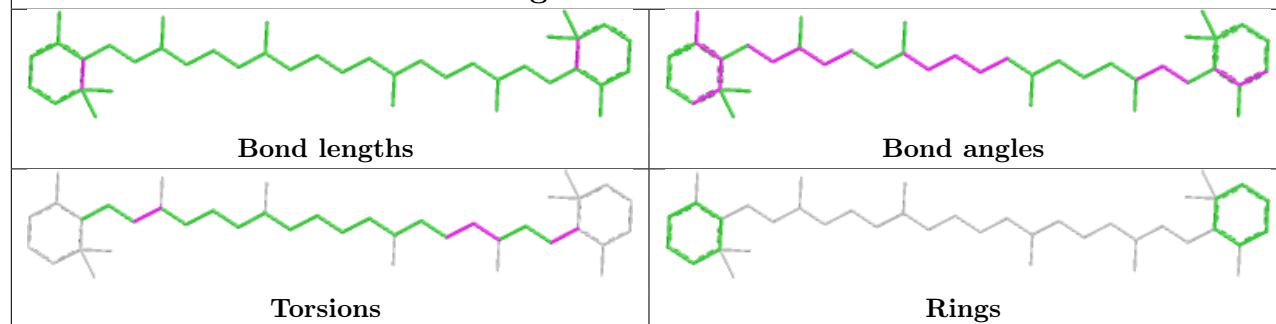
## Ligand CLA G 834



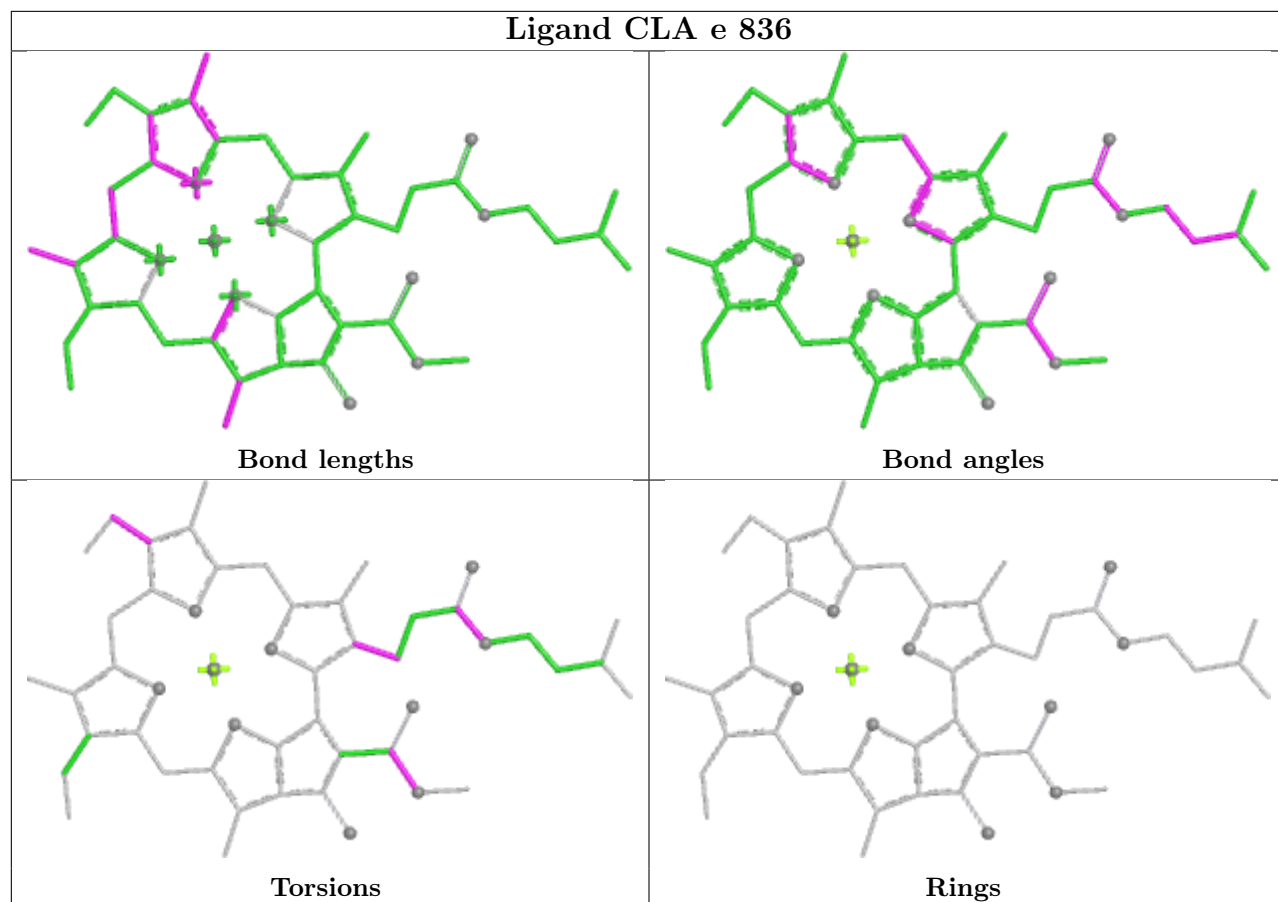
## Ligand CLA g 812

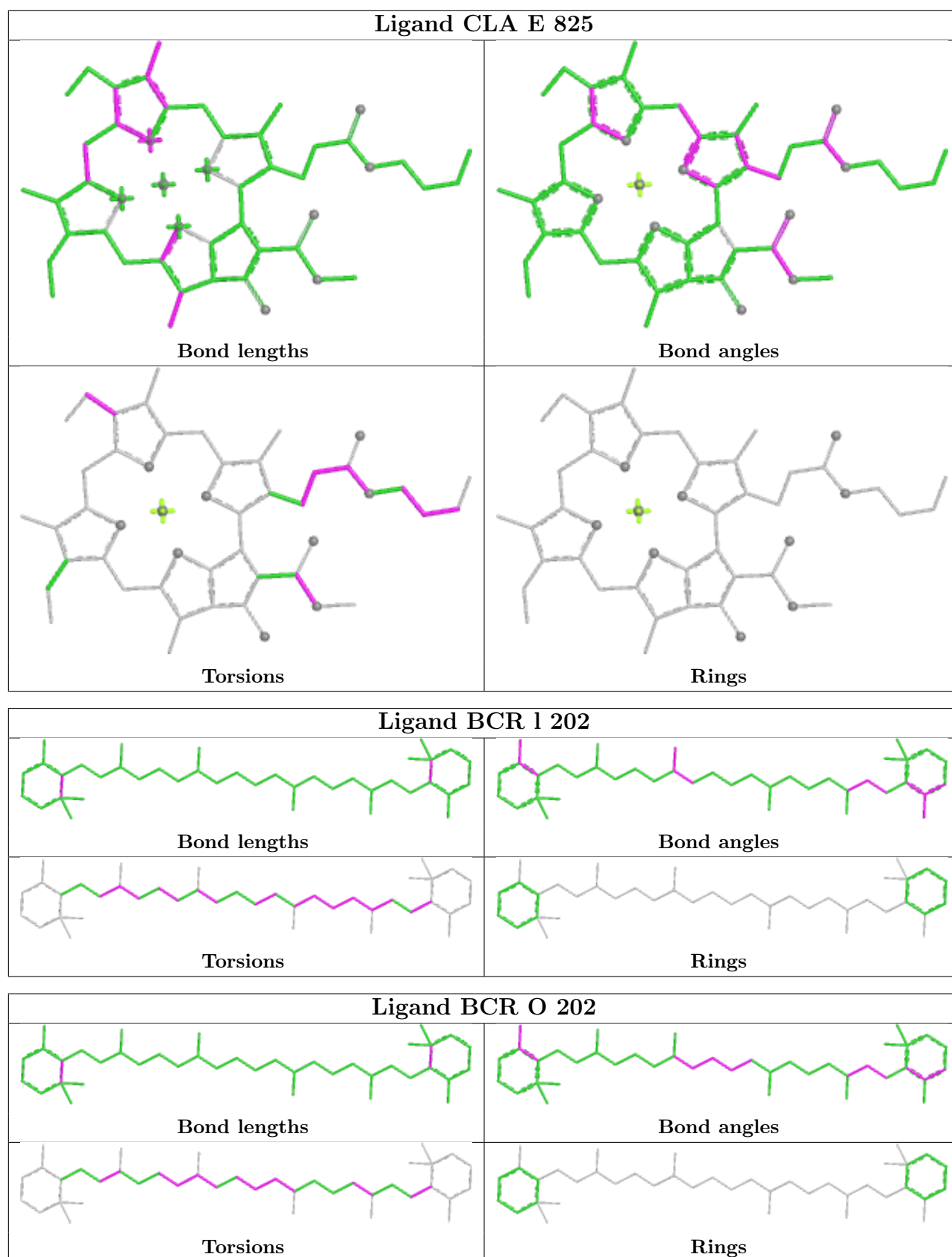


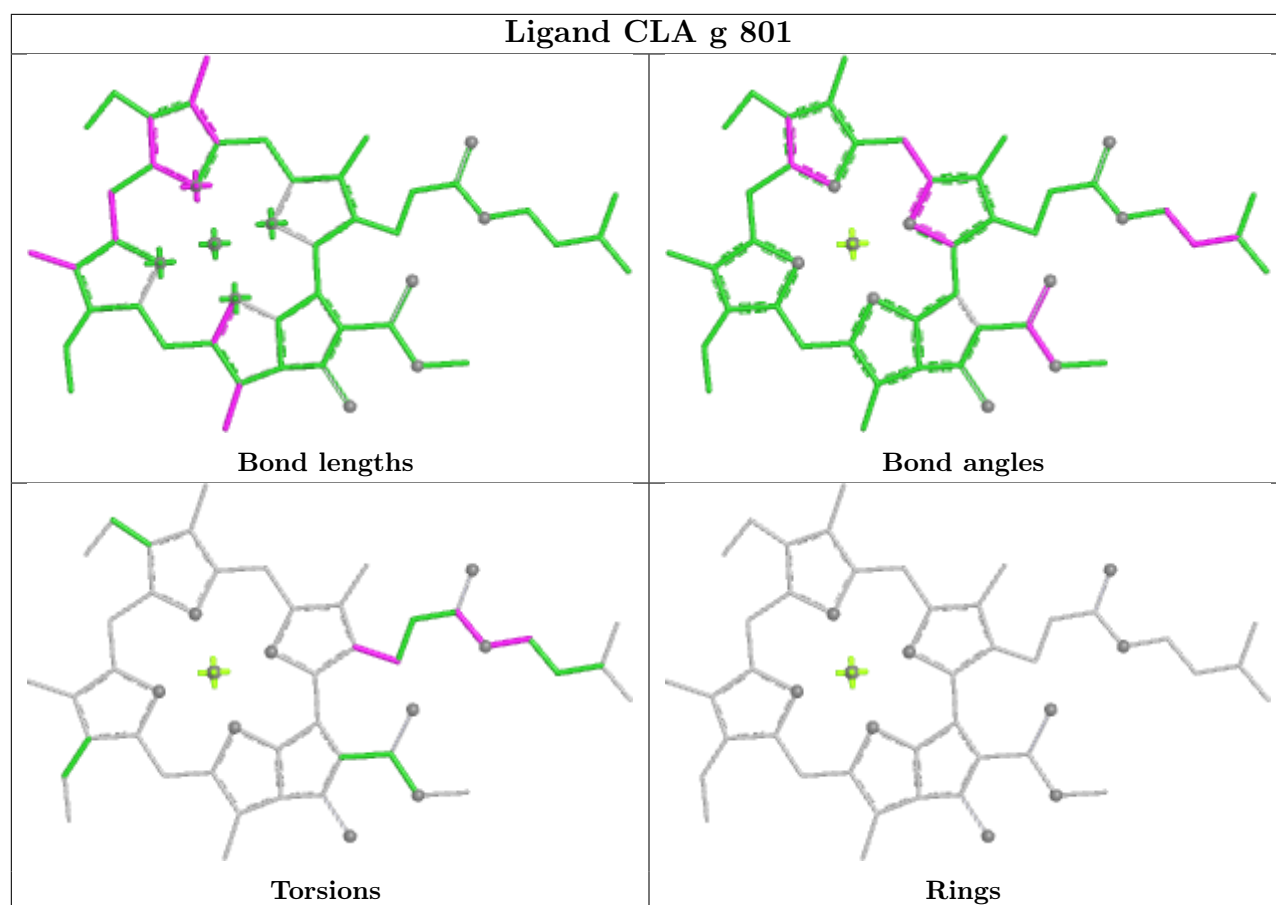
## Ligand BCR A 849



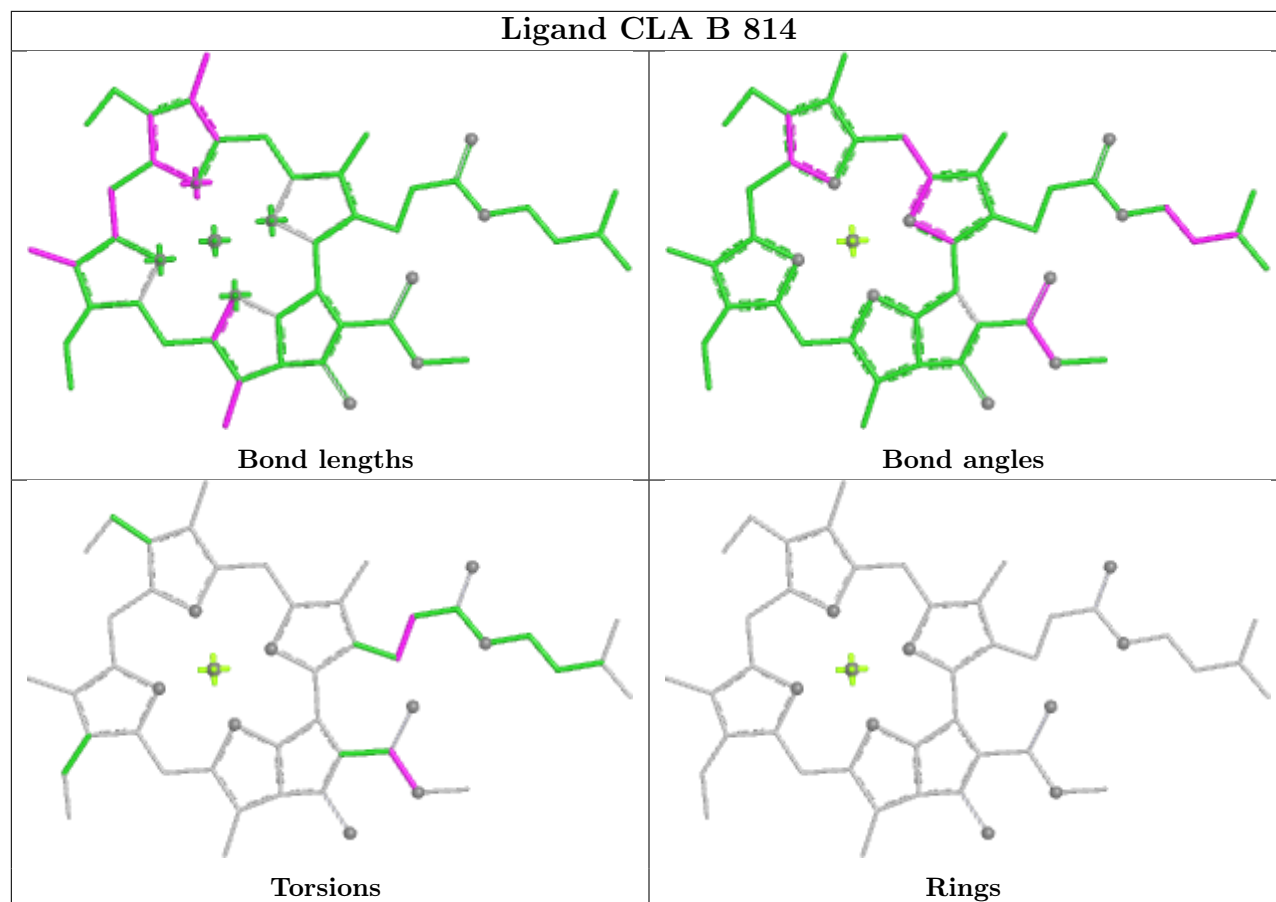
## Ligand CLA e 836



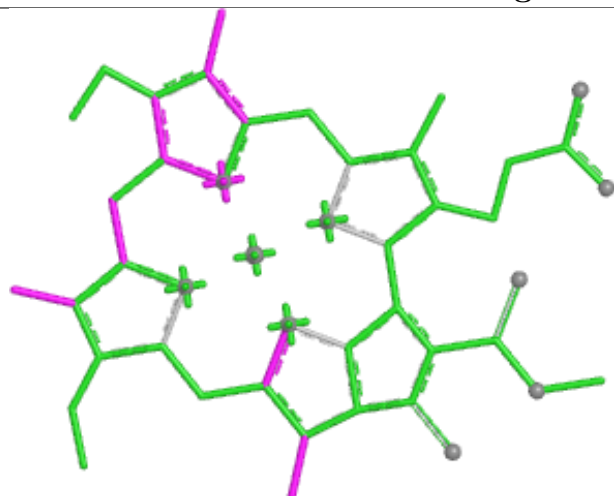




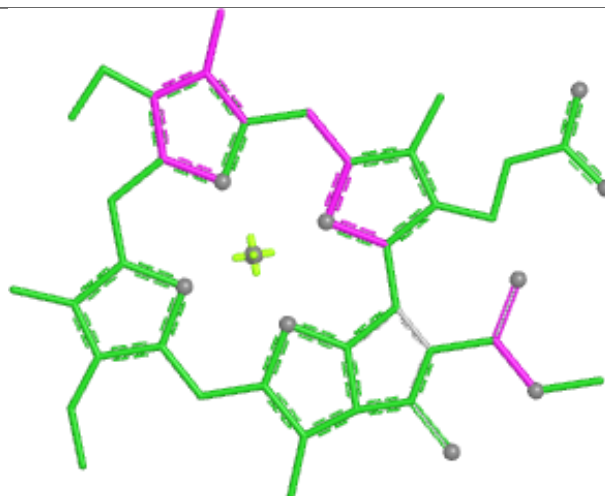
## Ligand CLA B 814



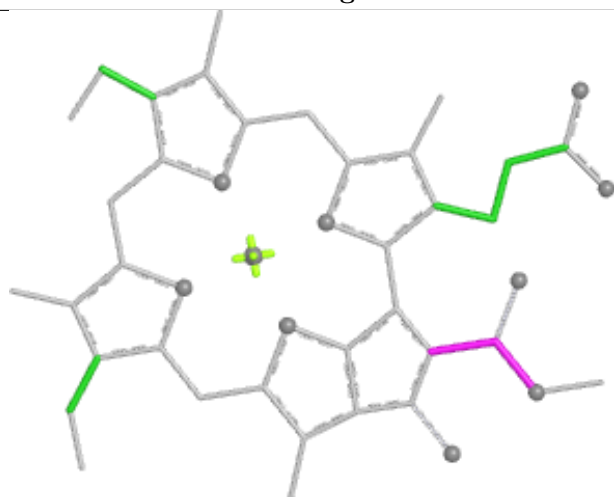
## Ligand CLA B 822



Bond lengths



Bond angles

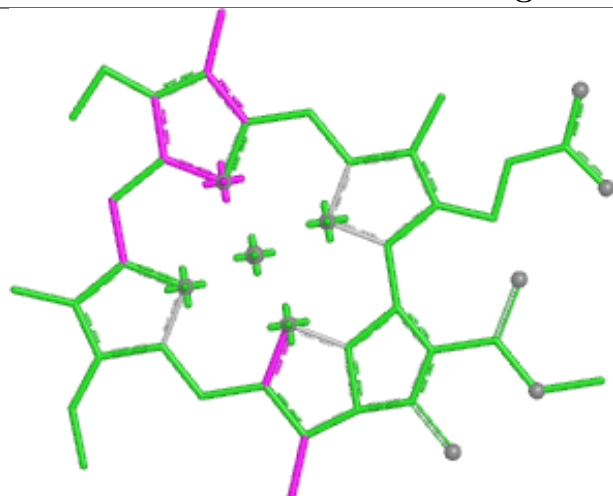


Torsions

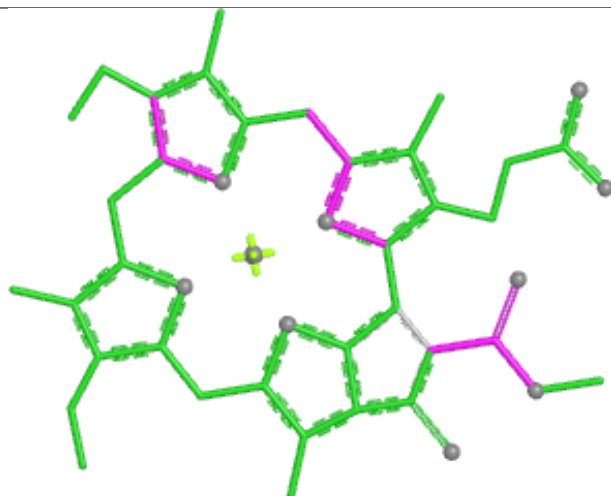


Rings

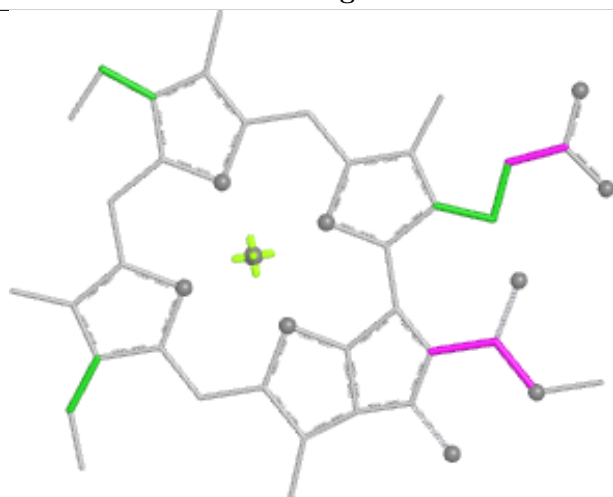
## Ligand CLA E 839



Bond lengths



Bond angles

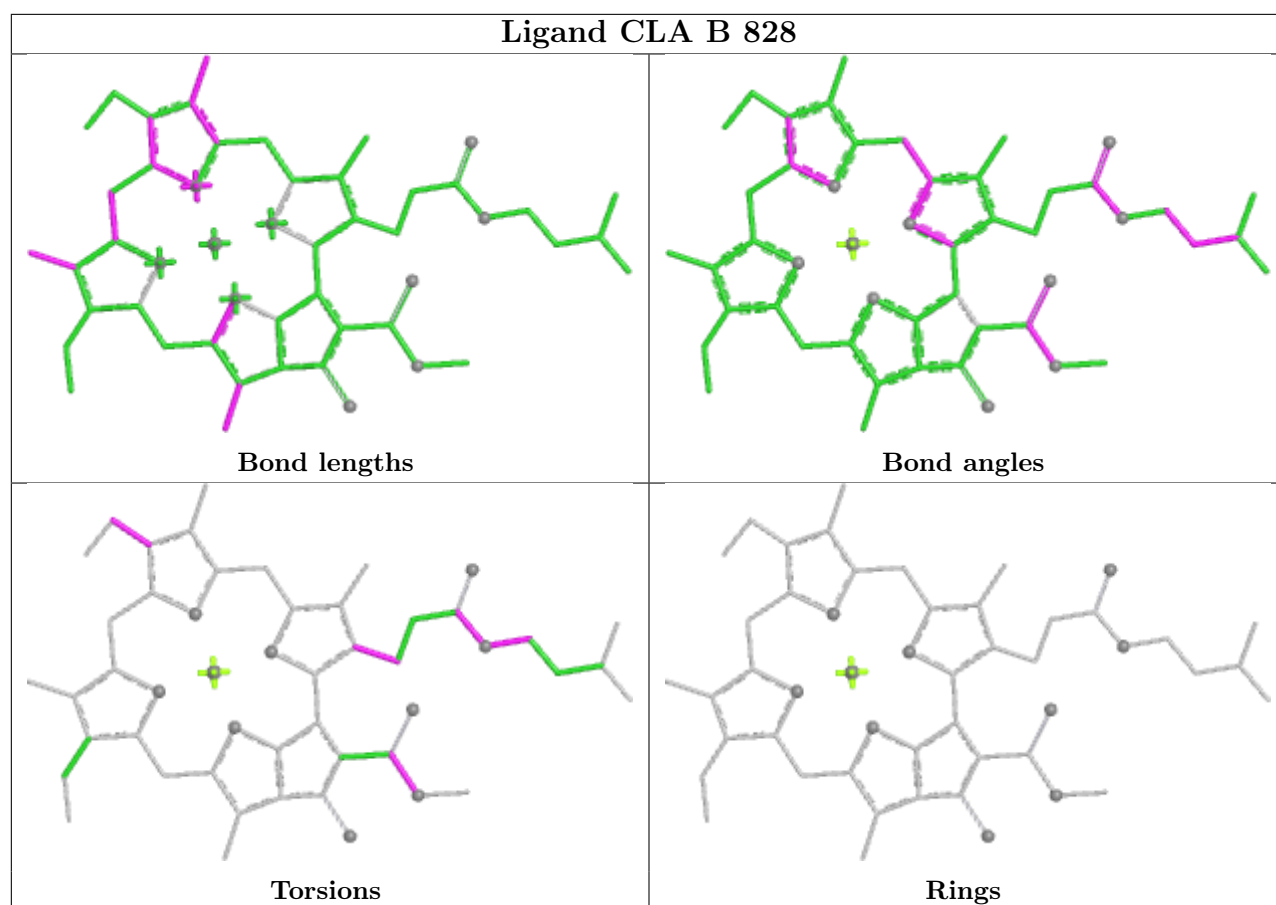


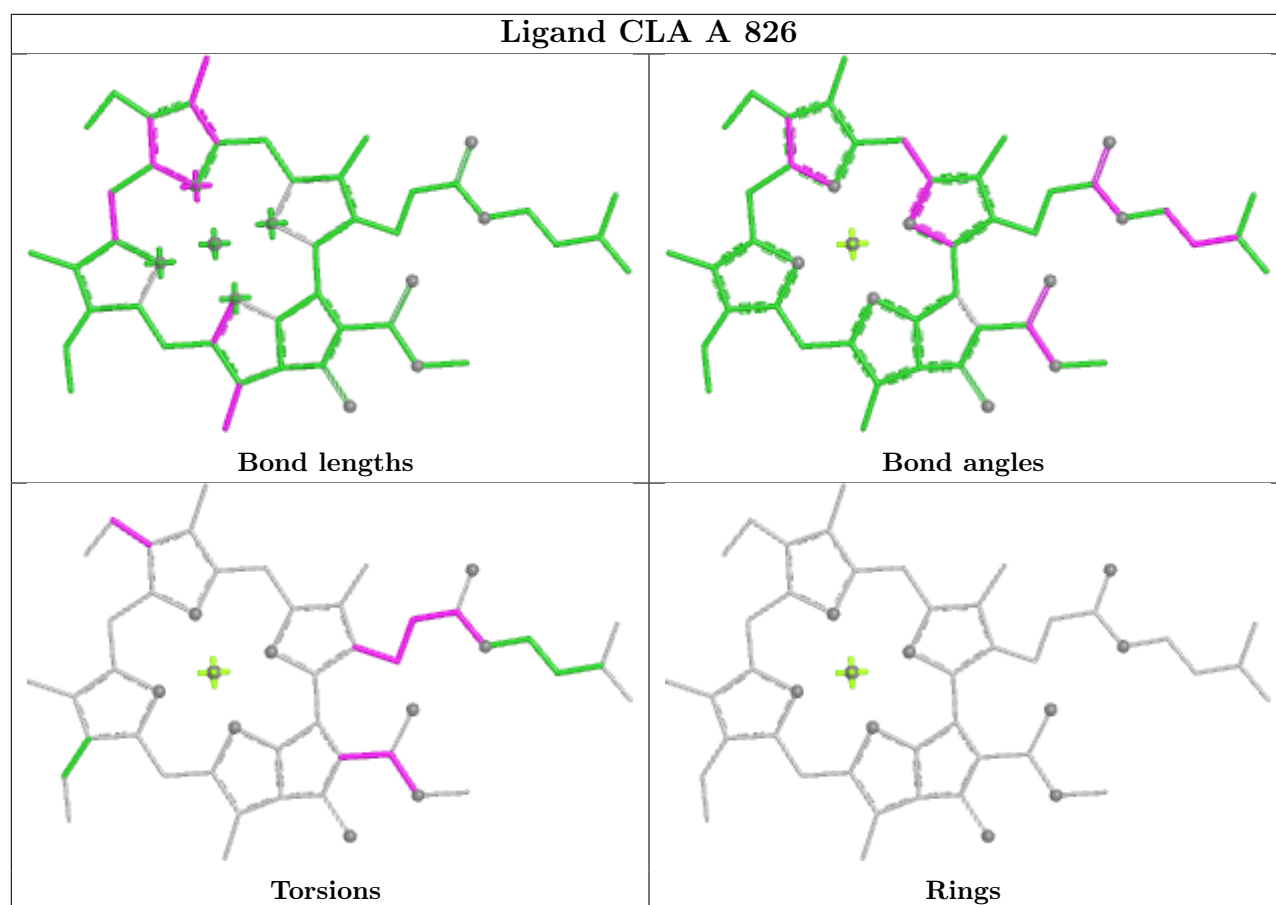
Torsions



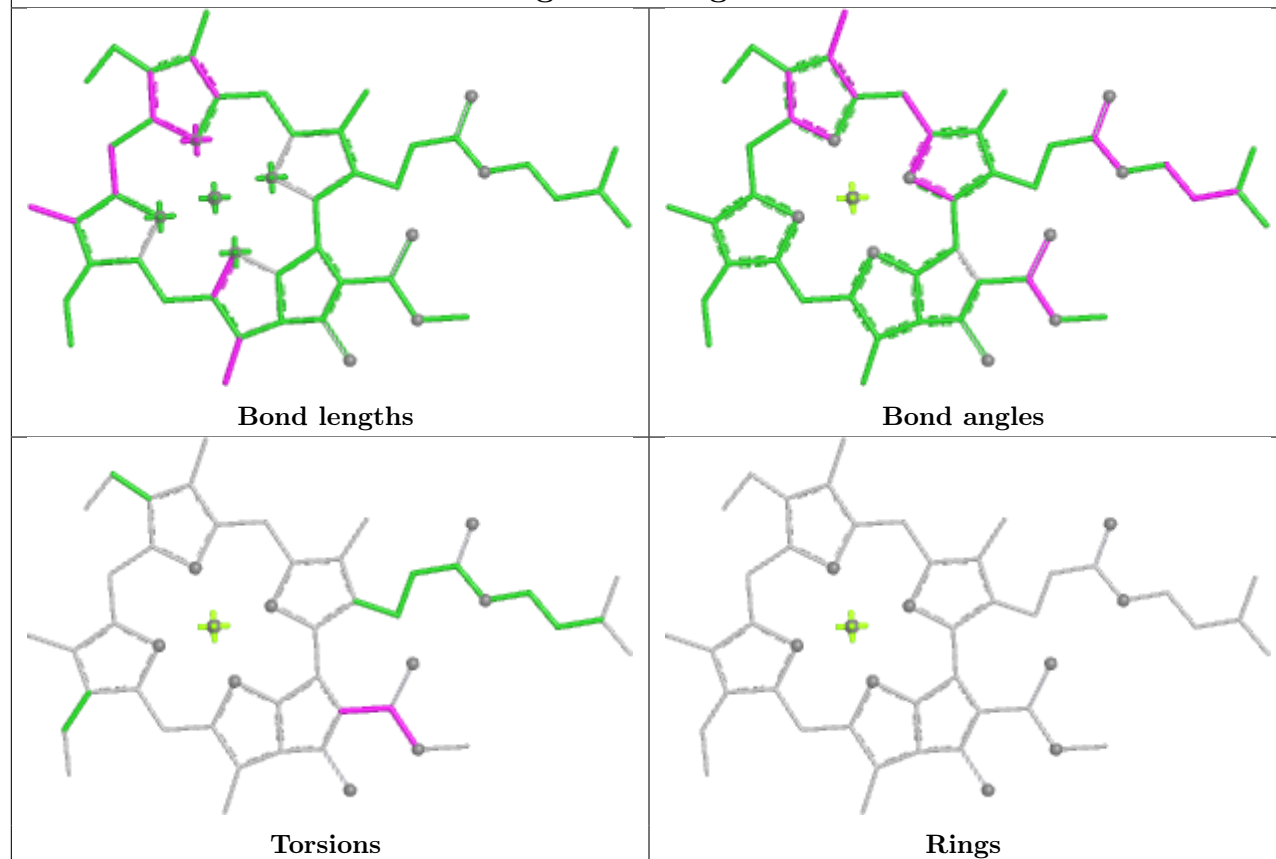
Rings



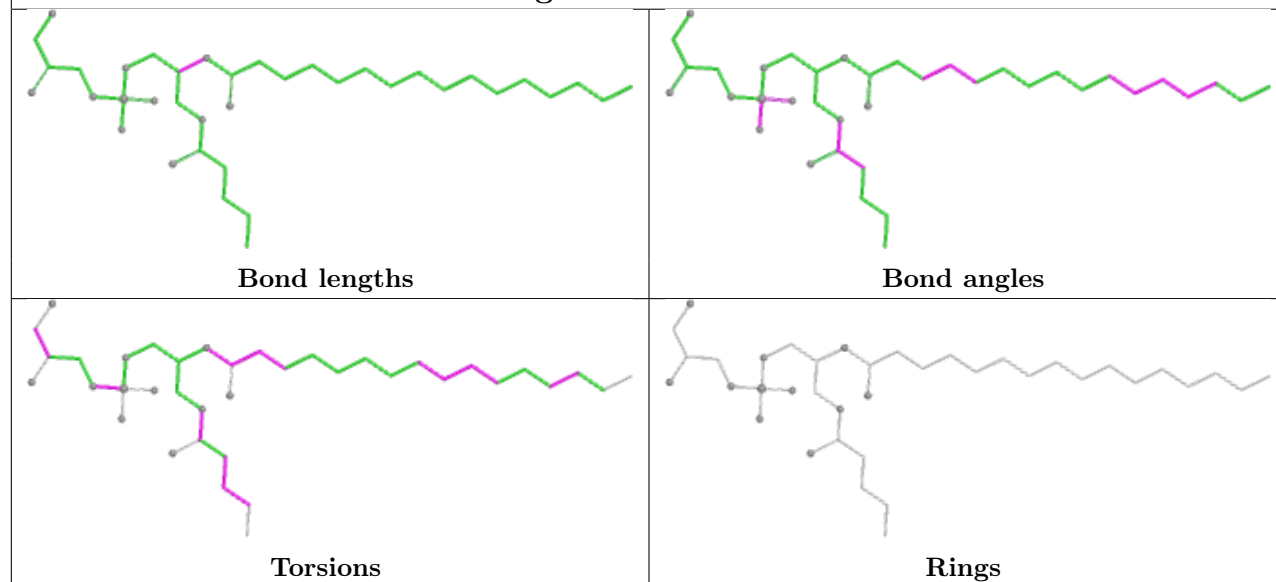




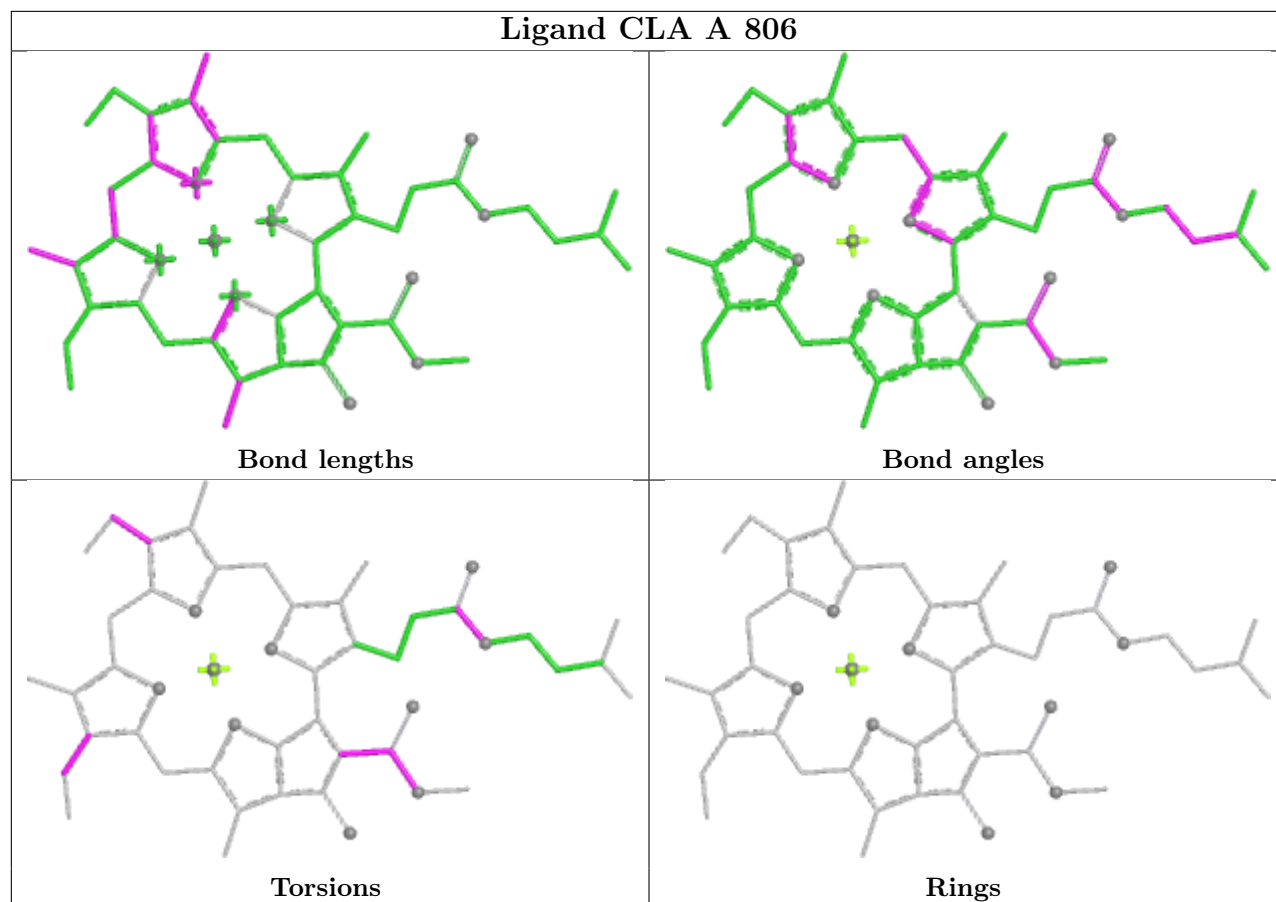
## Ligand CLA g 838



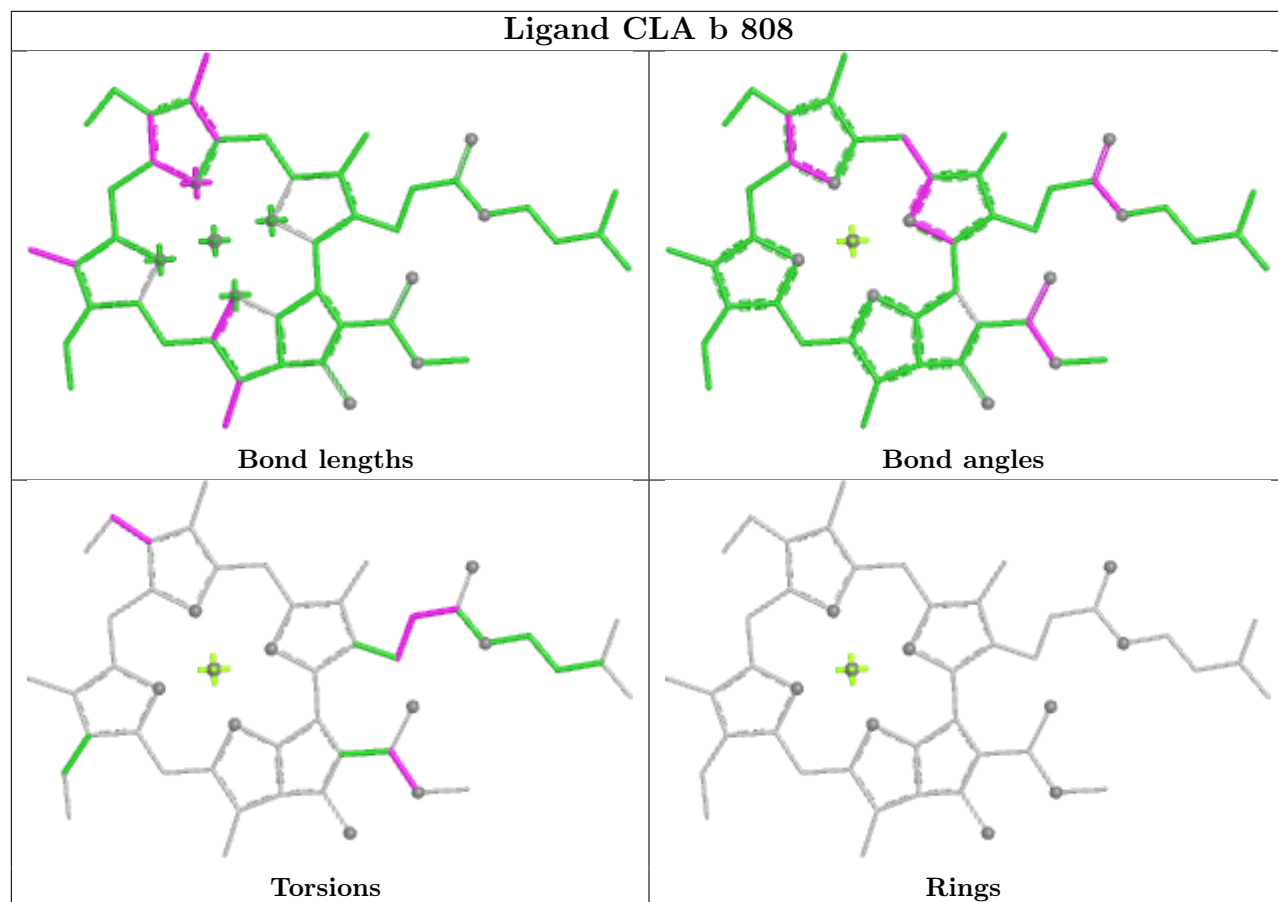
## Ligand LHG e 802



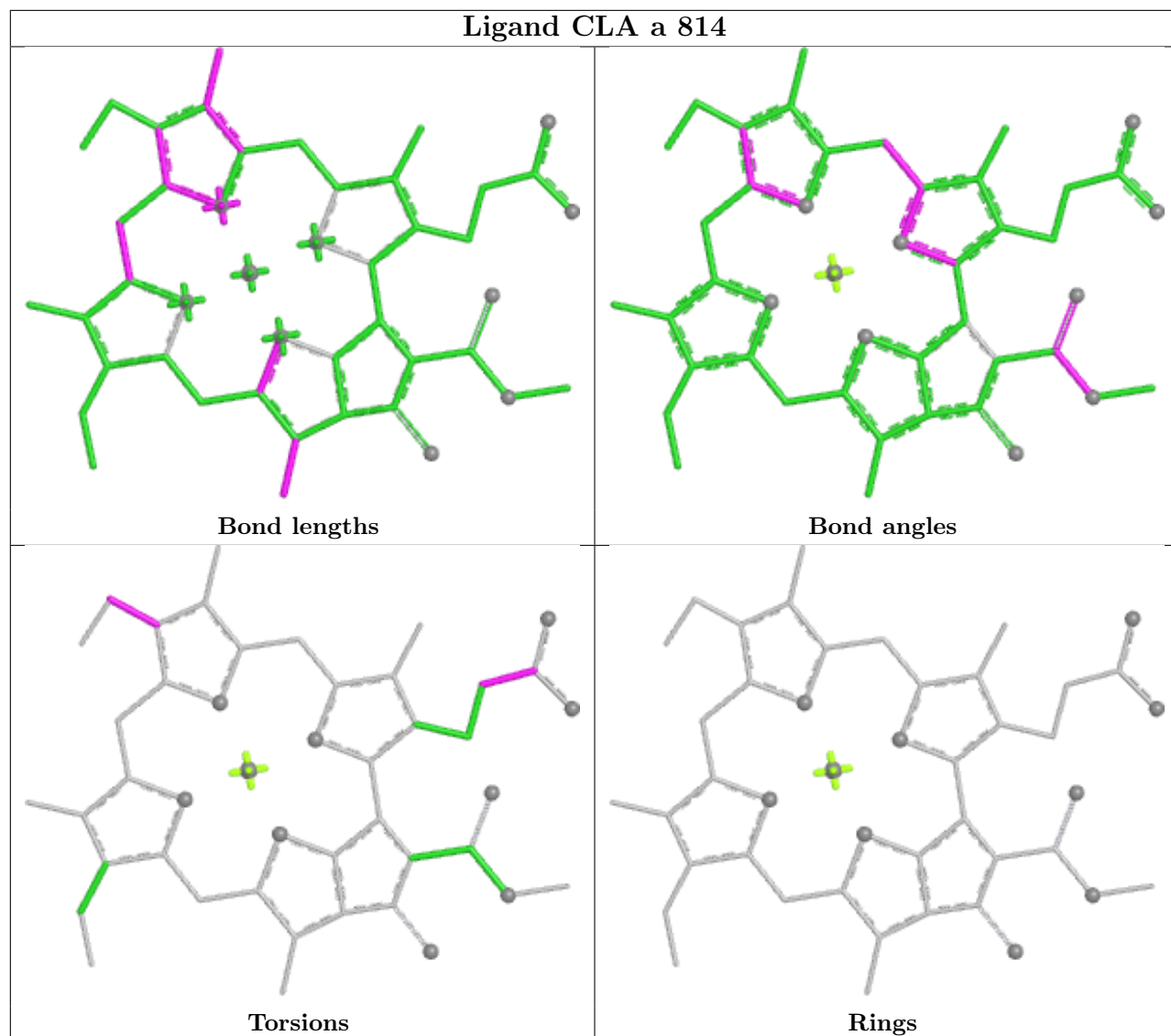
## Ligand CLA A 806



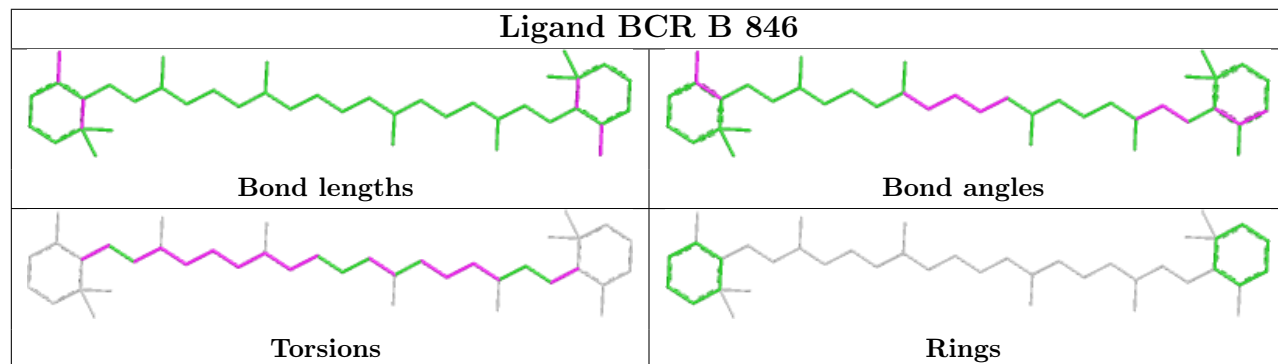
## Ligand CLA b 808



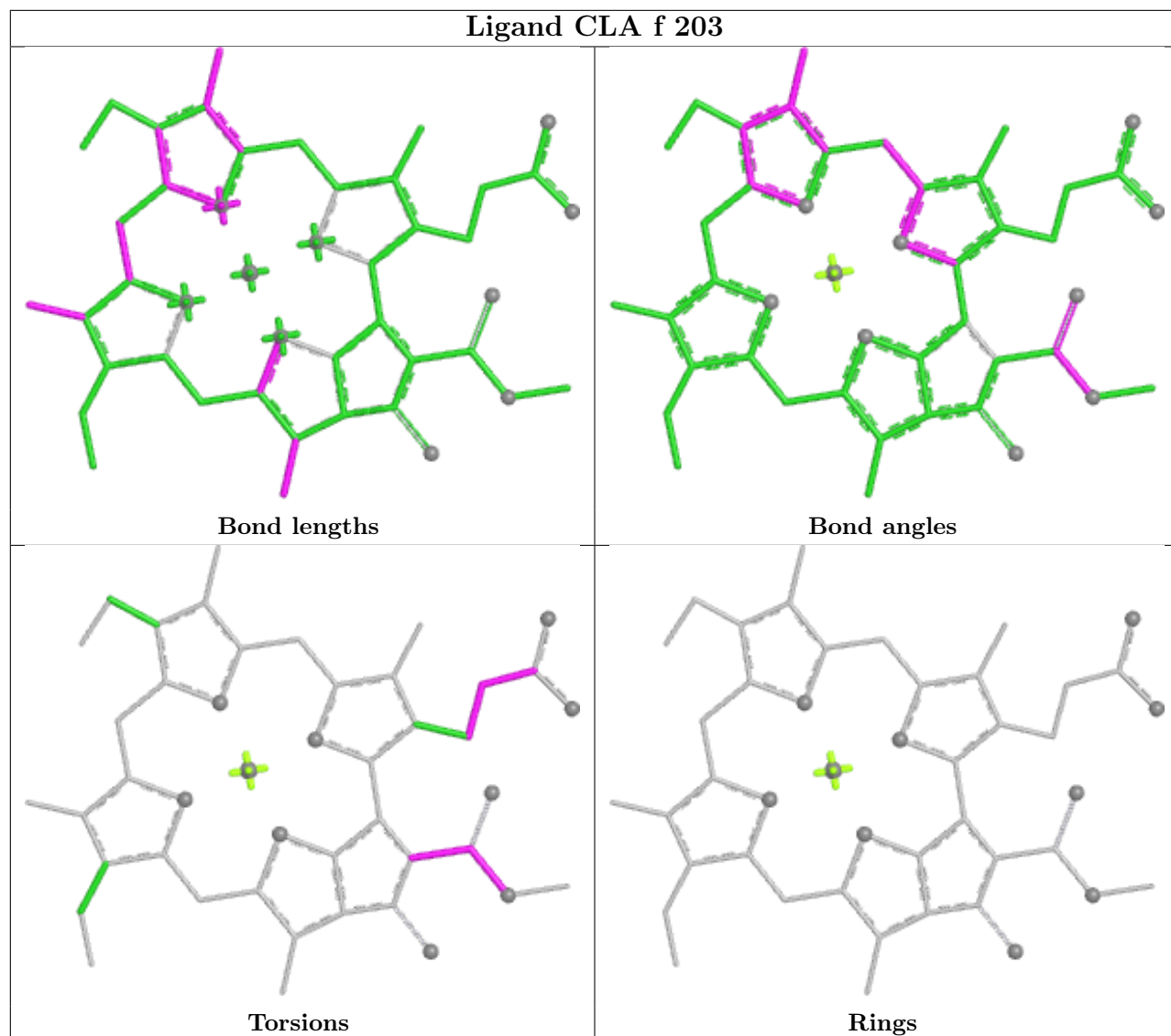
## Ligand CLA a 814



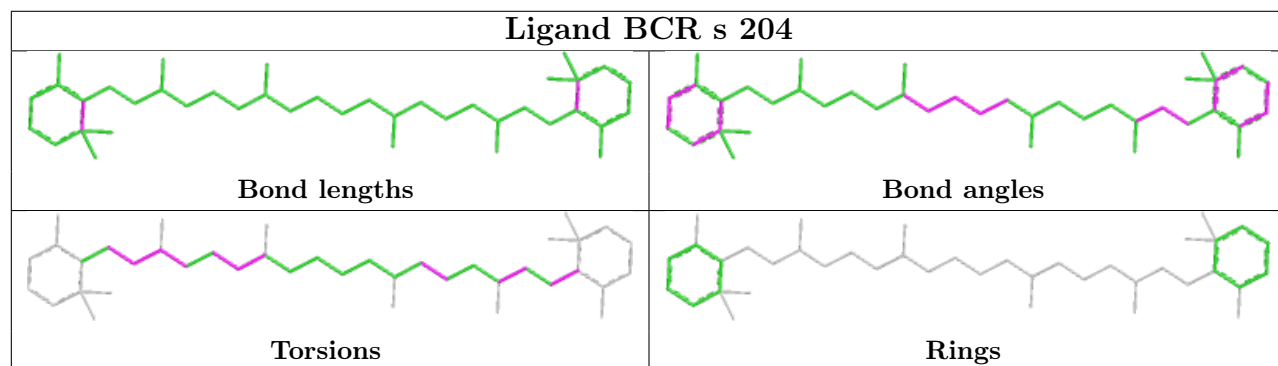
## Ligand BCR B 846



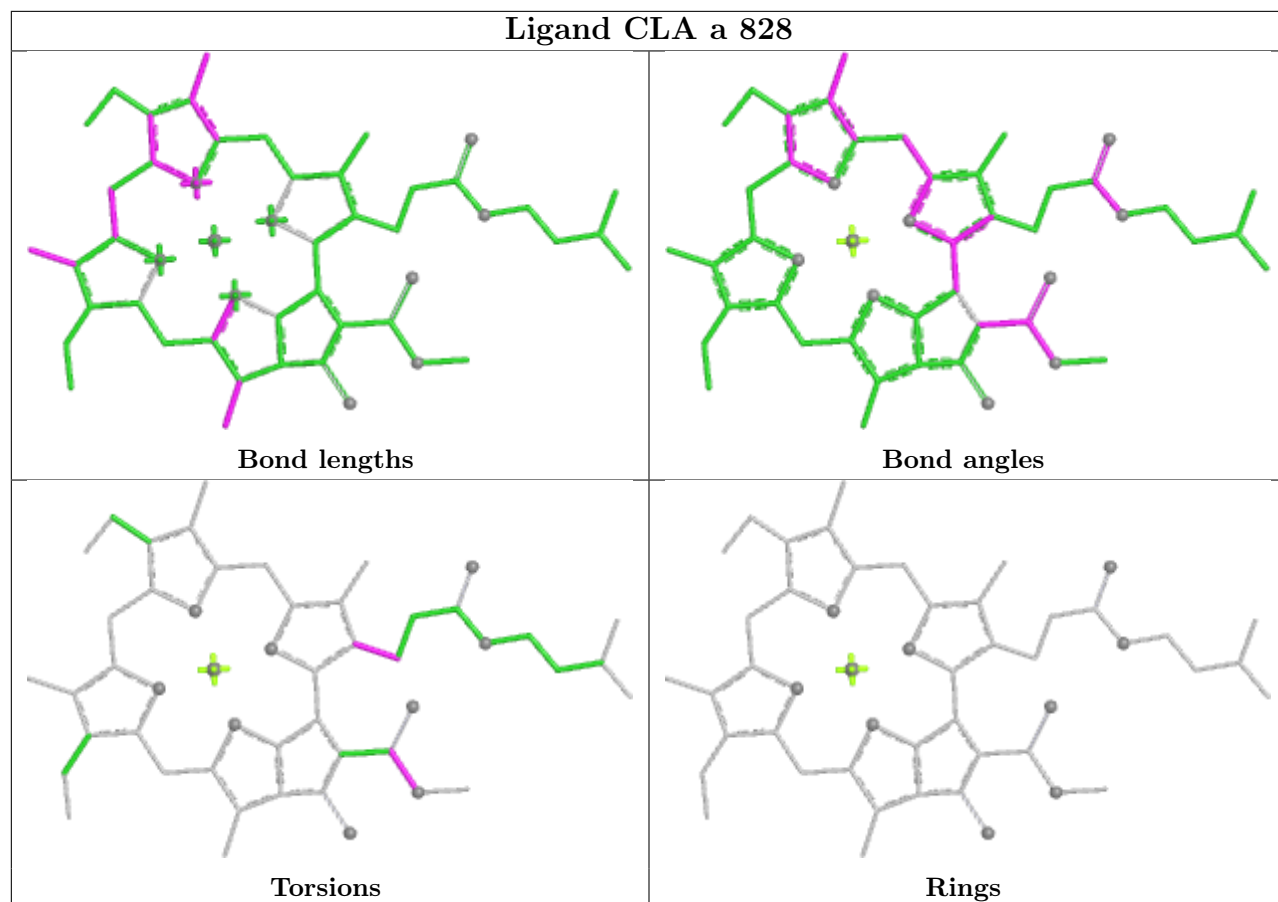
## Ligand CLA f 203



## Ligand BCR s 204

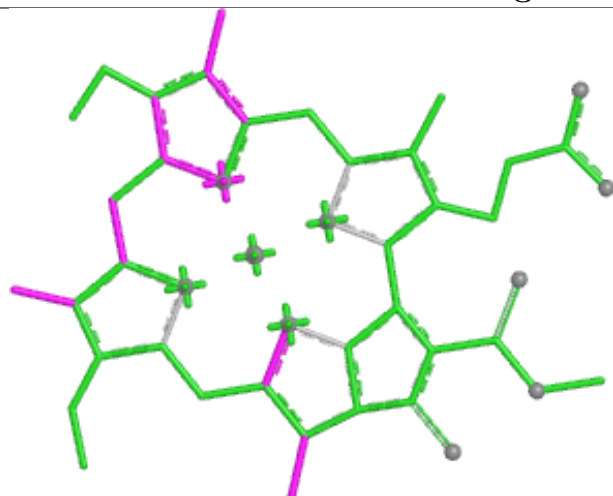


## Ligand CLA a 828

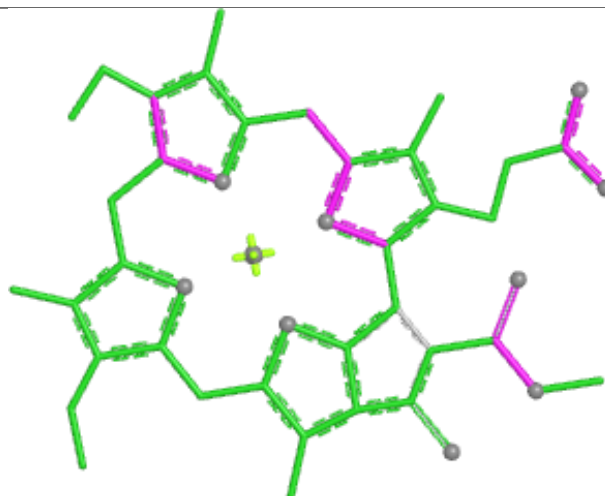




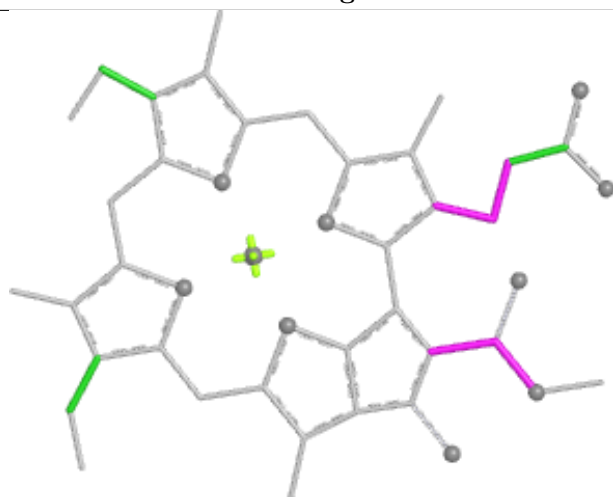
## Ligand CLA B 813



Bond lengths



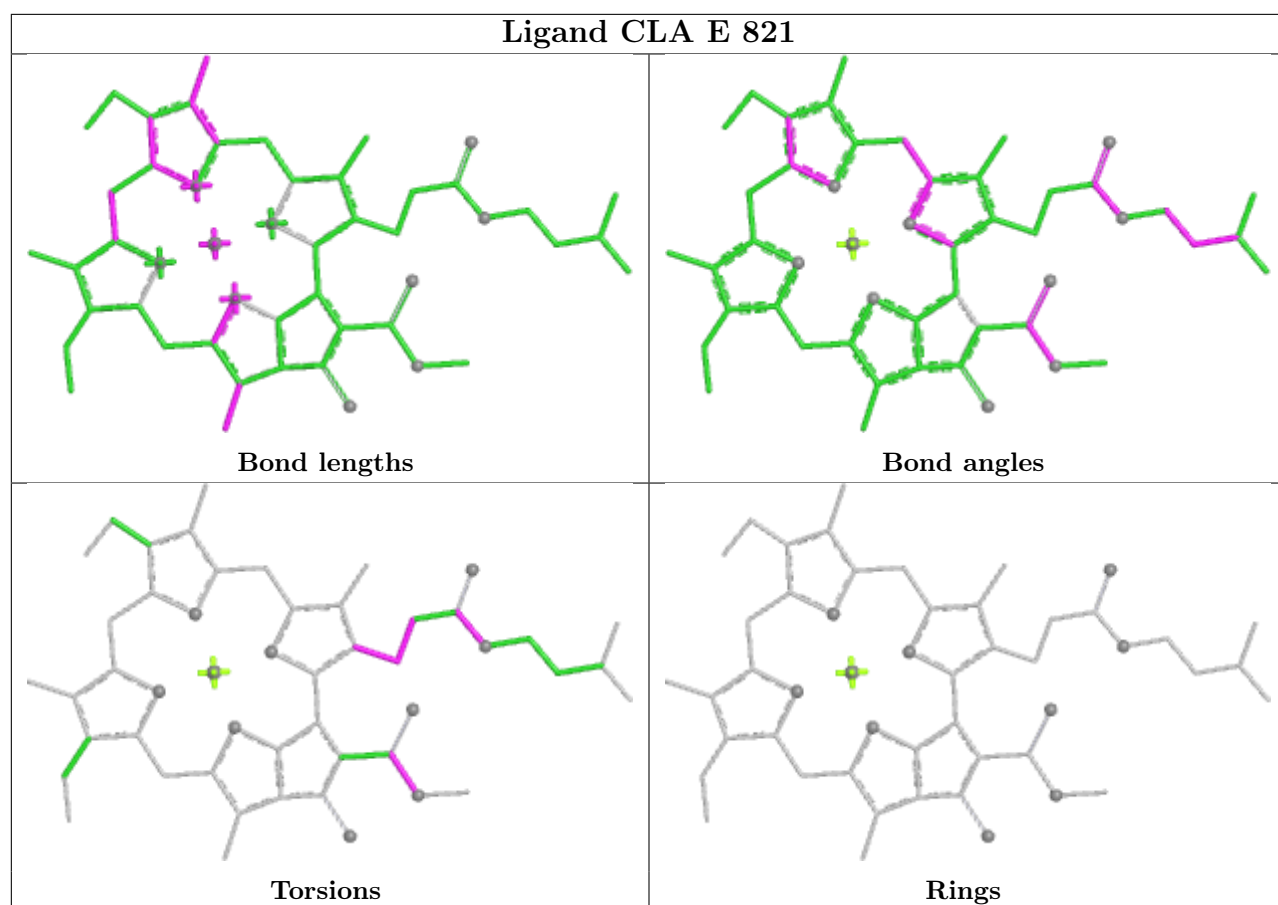
Bond angles



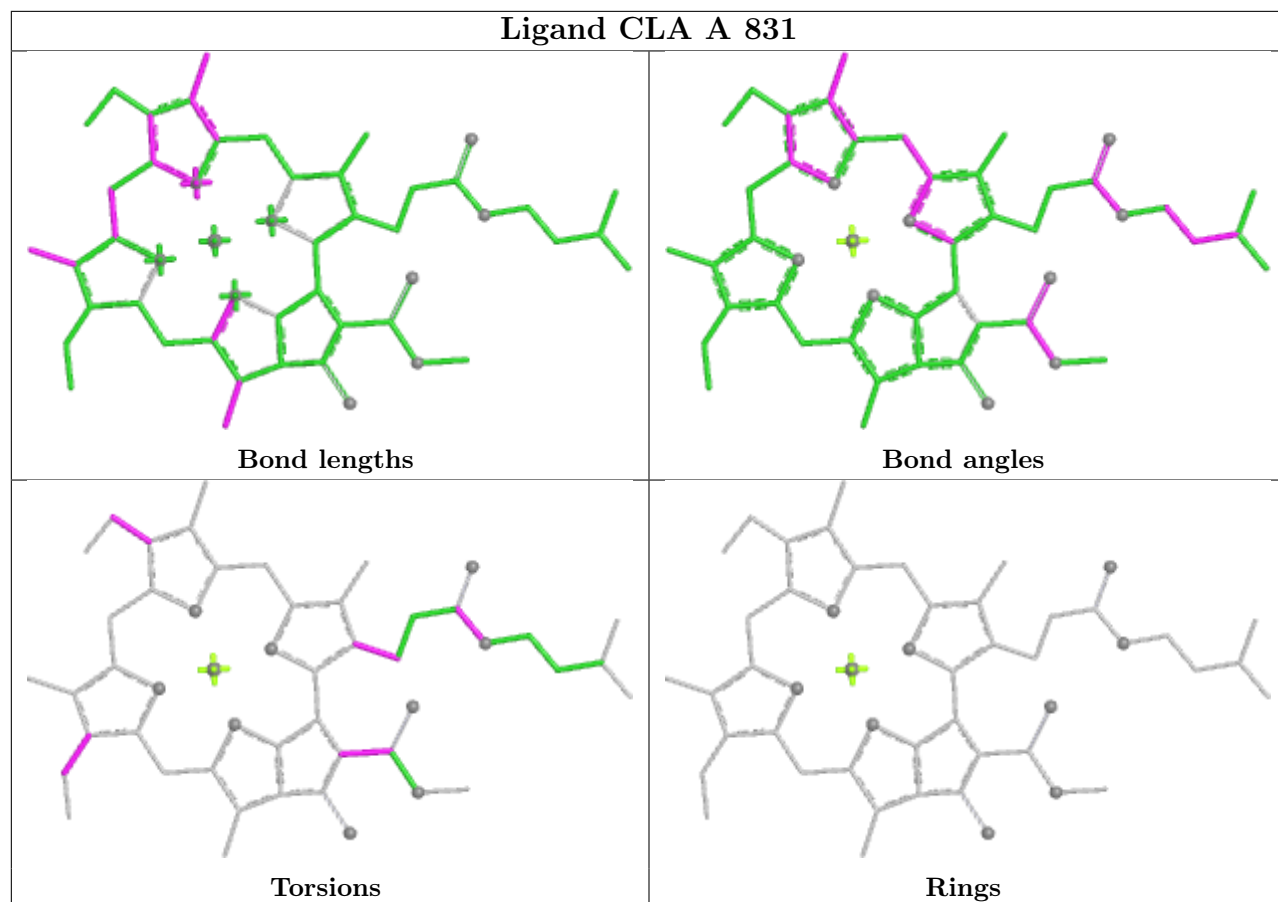
Torsions



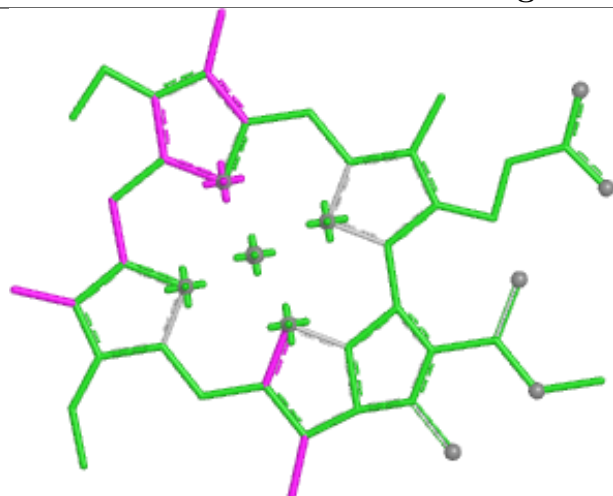
Rings



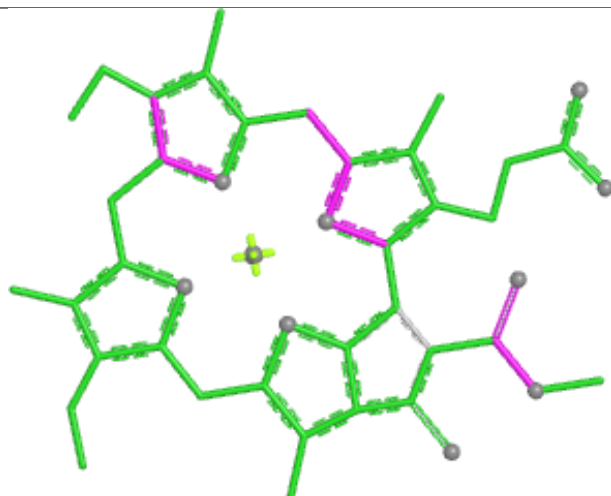
## Ligand CLA A 831



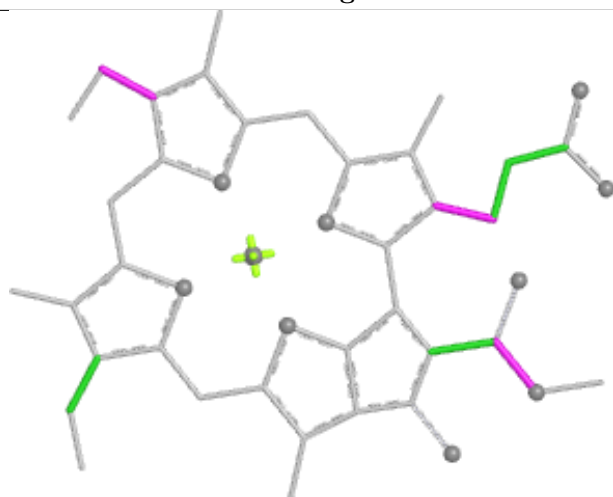
## Ligand CLA S 206



Bond lengths



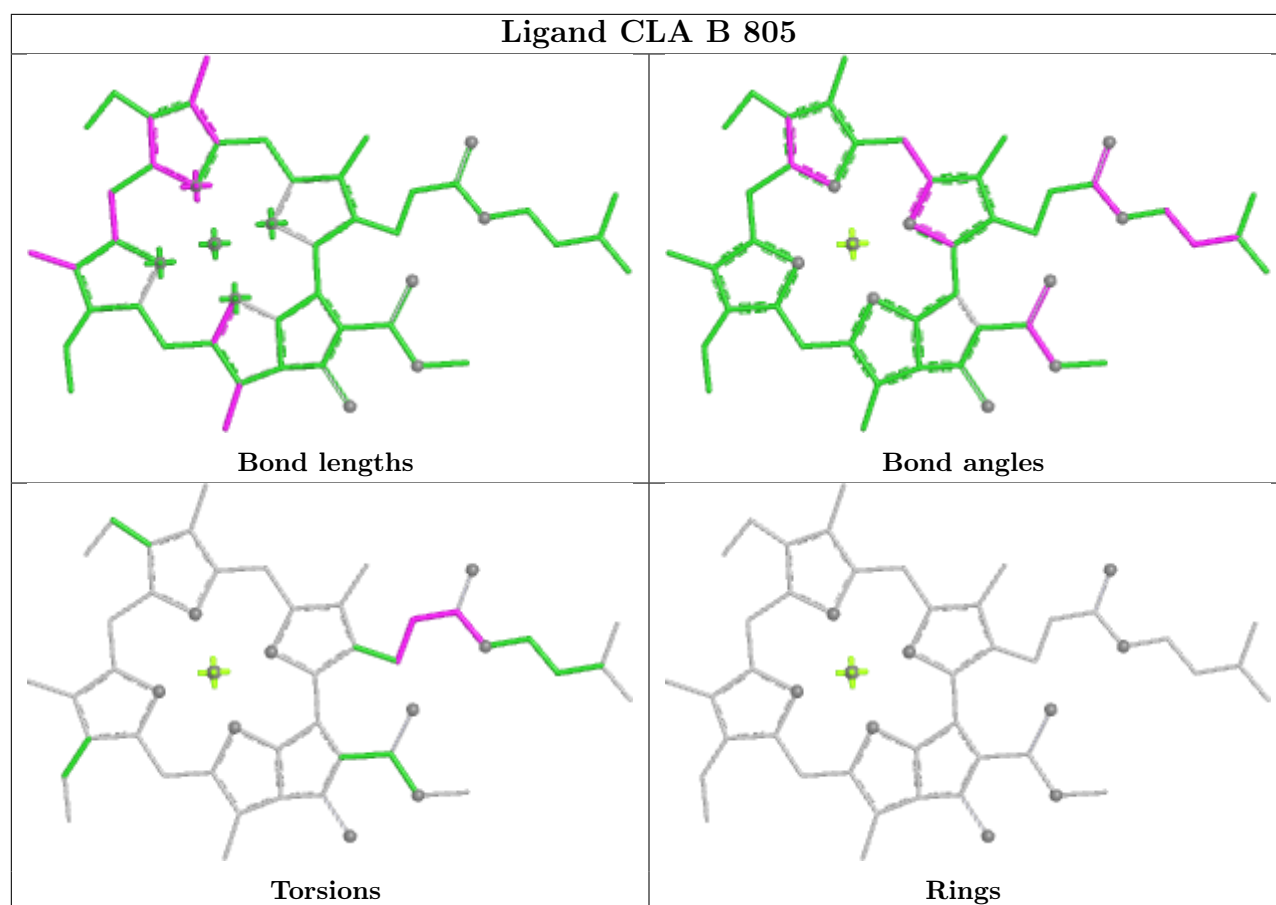
Bond angles



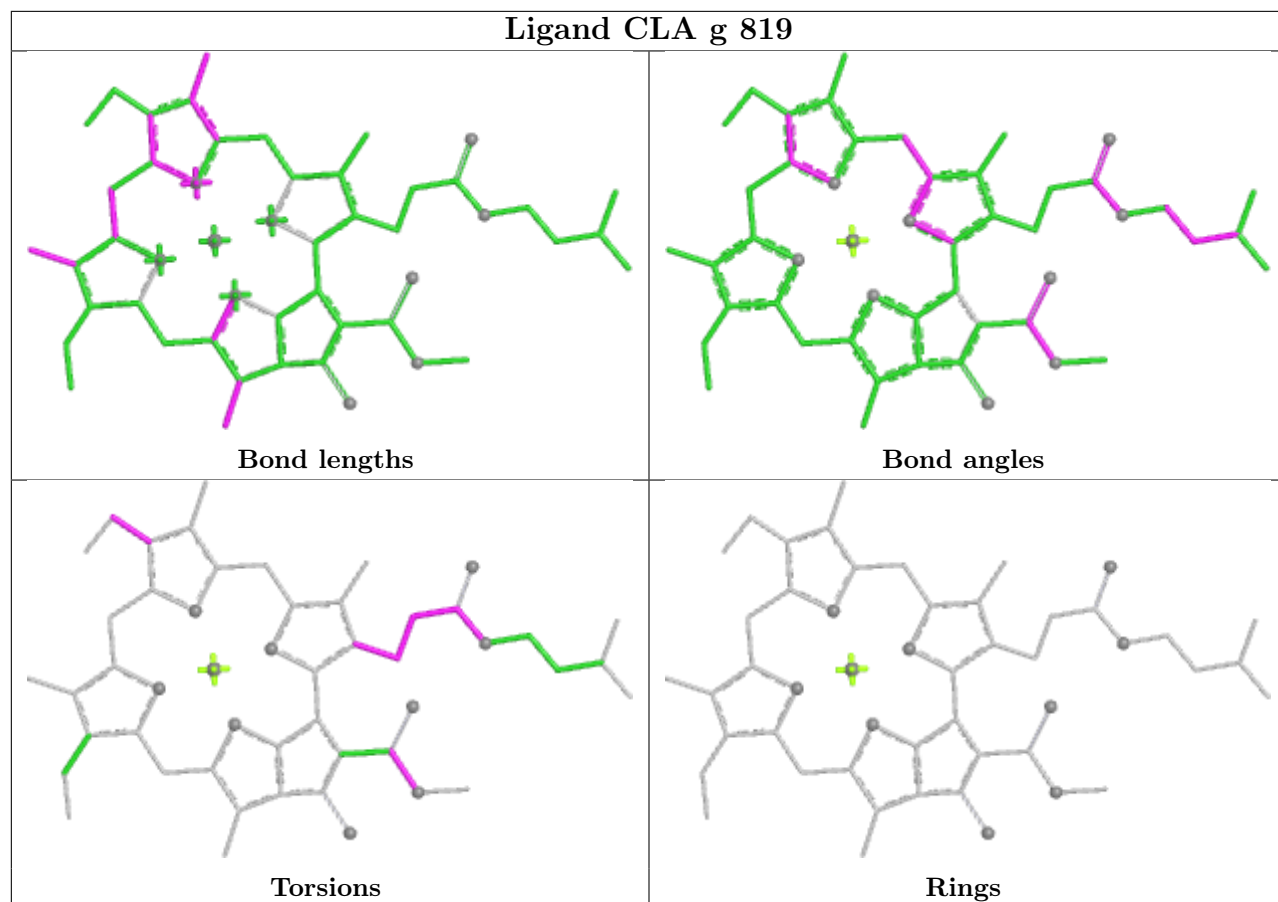
Torsions



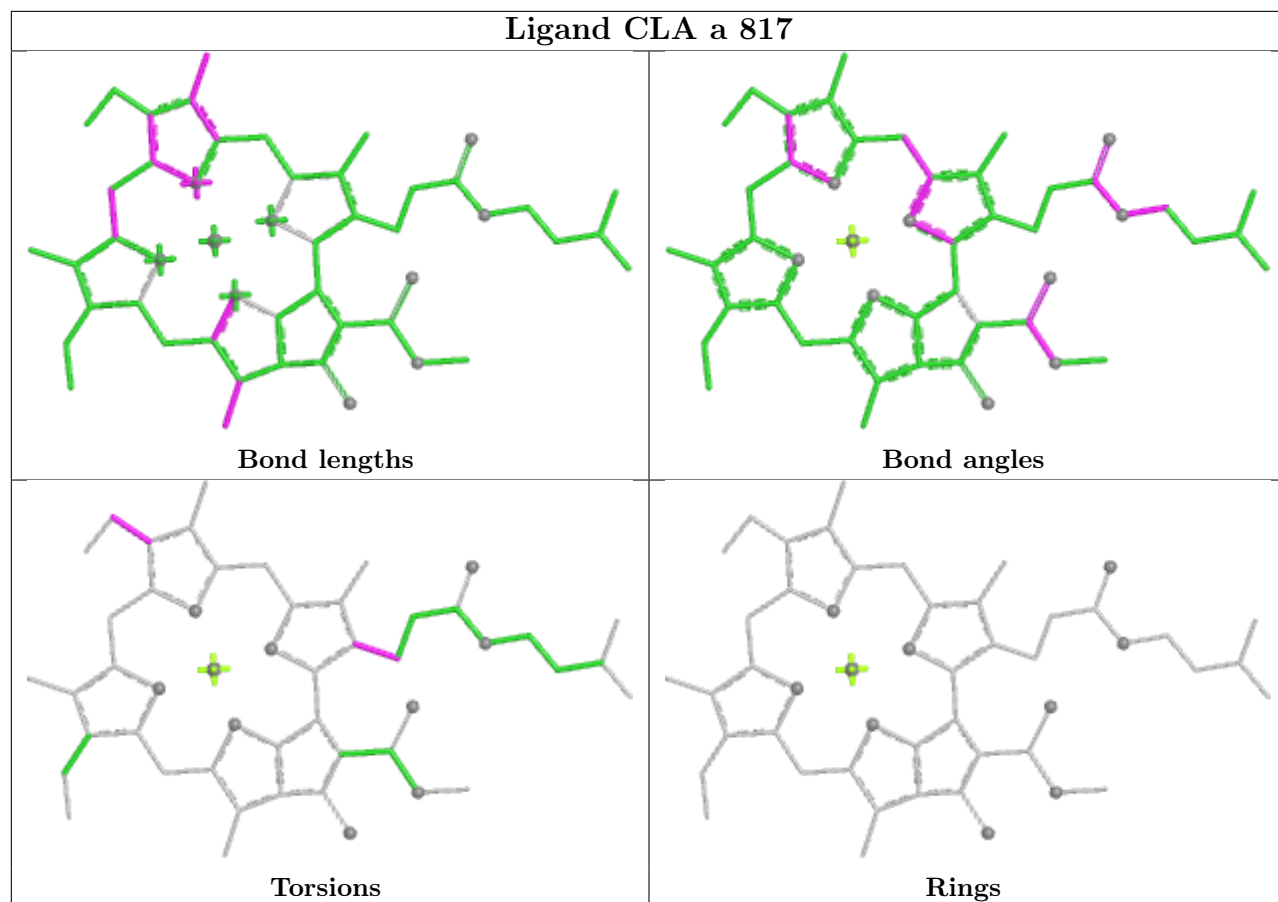
Rings

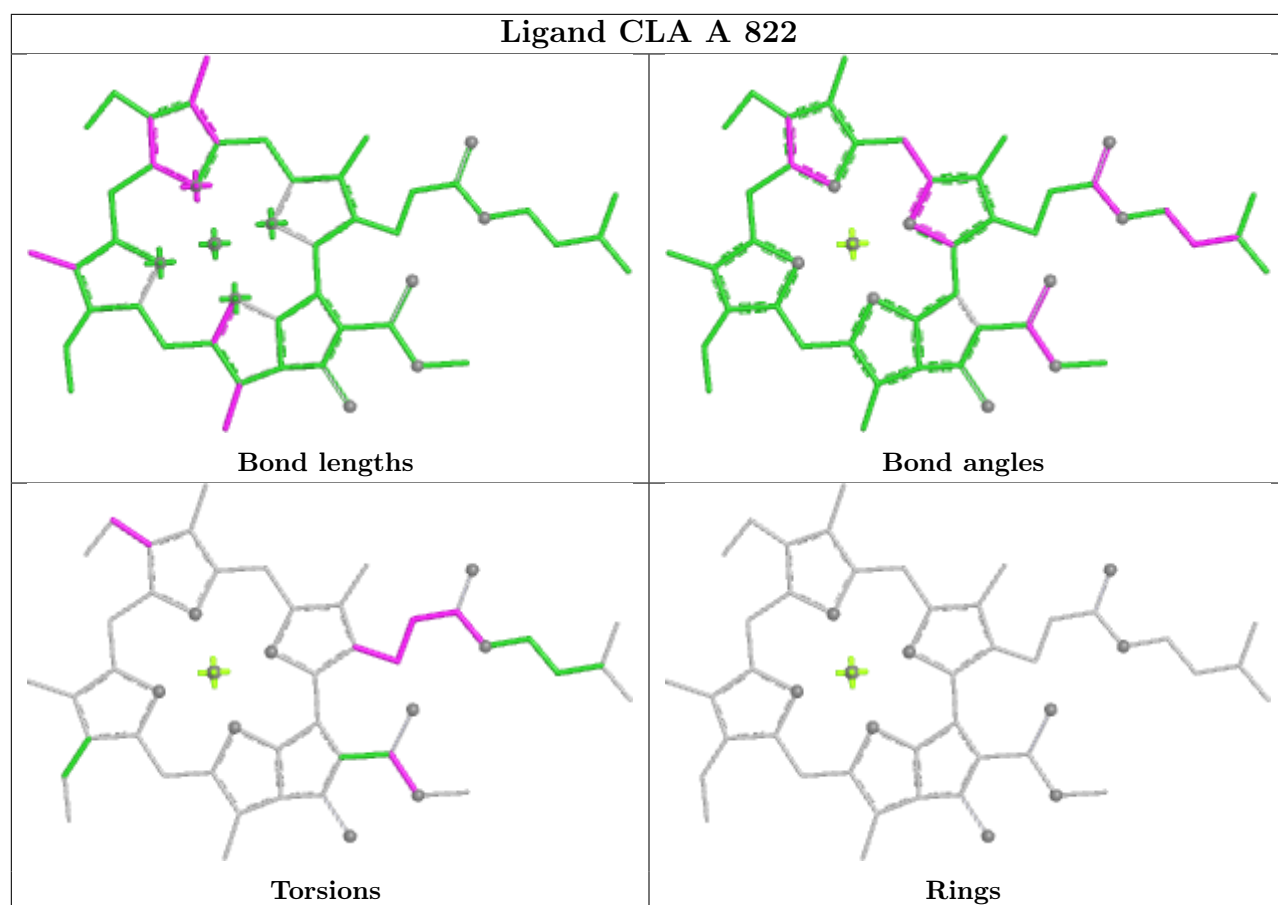


## Ligand CLA g 819



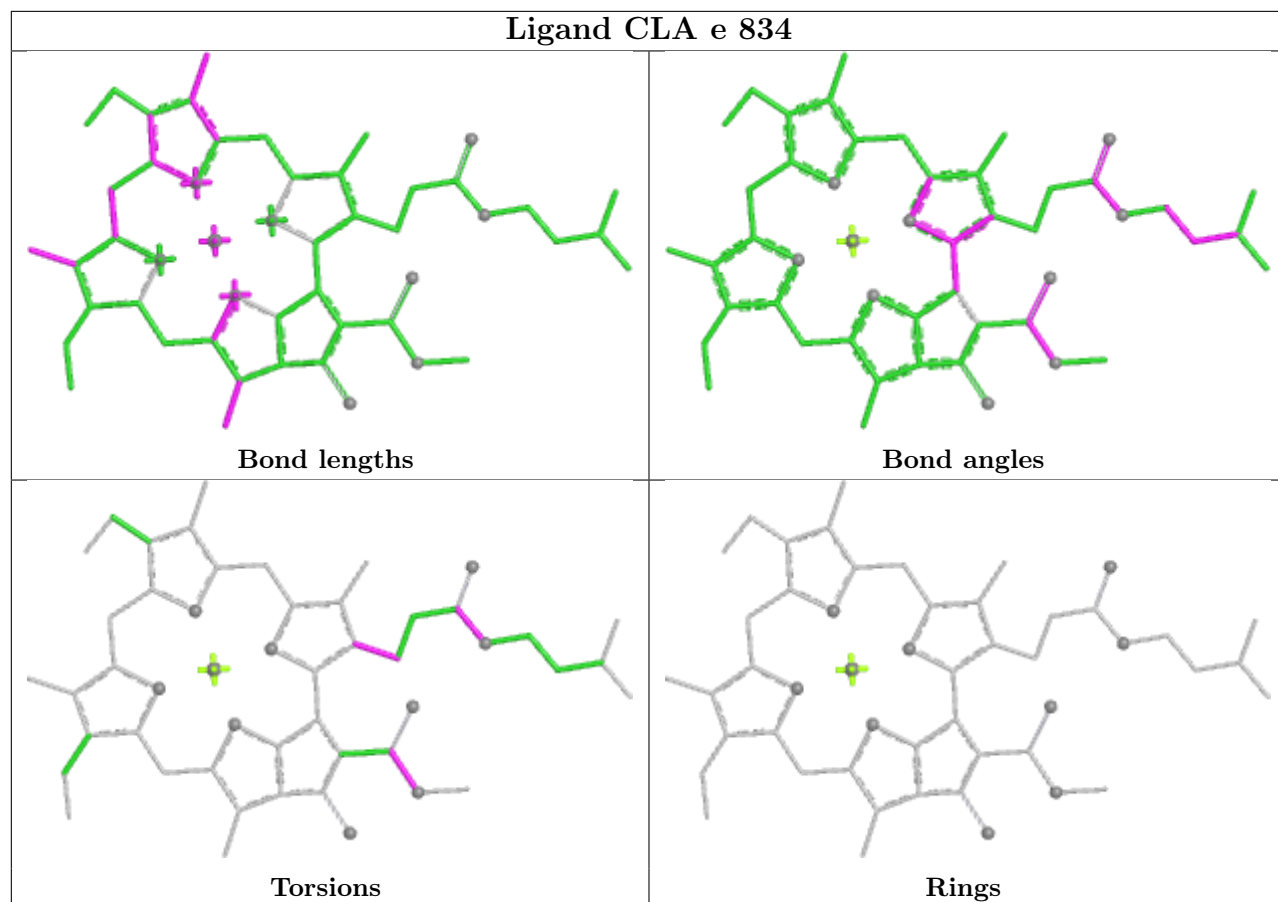
## Ligand CLA a 817



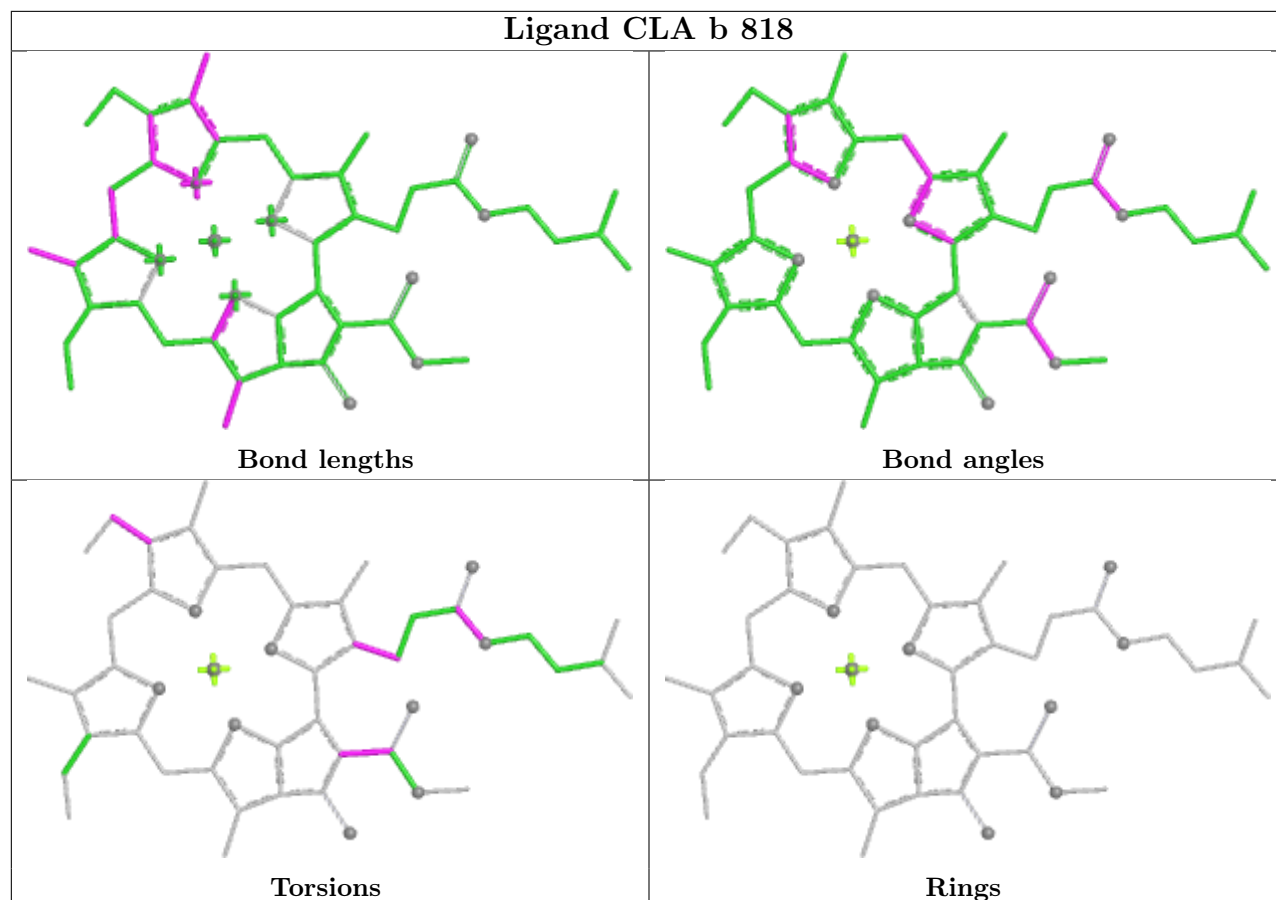




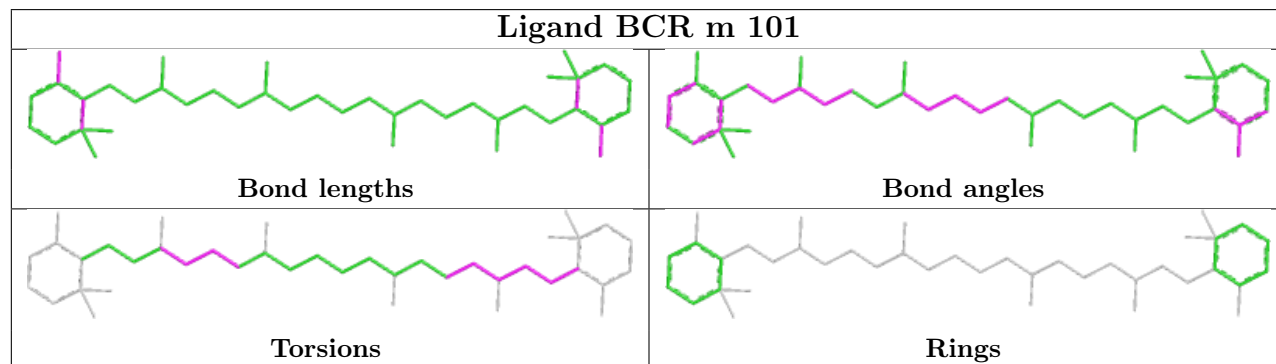
## Ligand CLA e 834



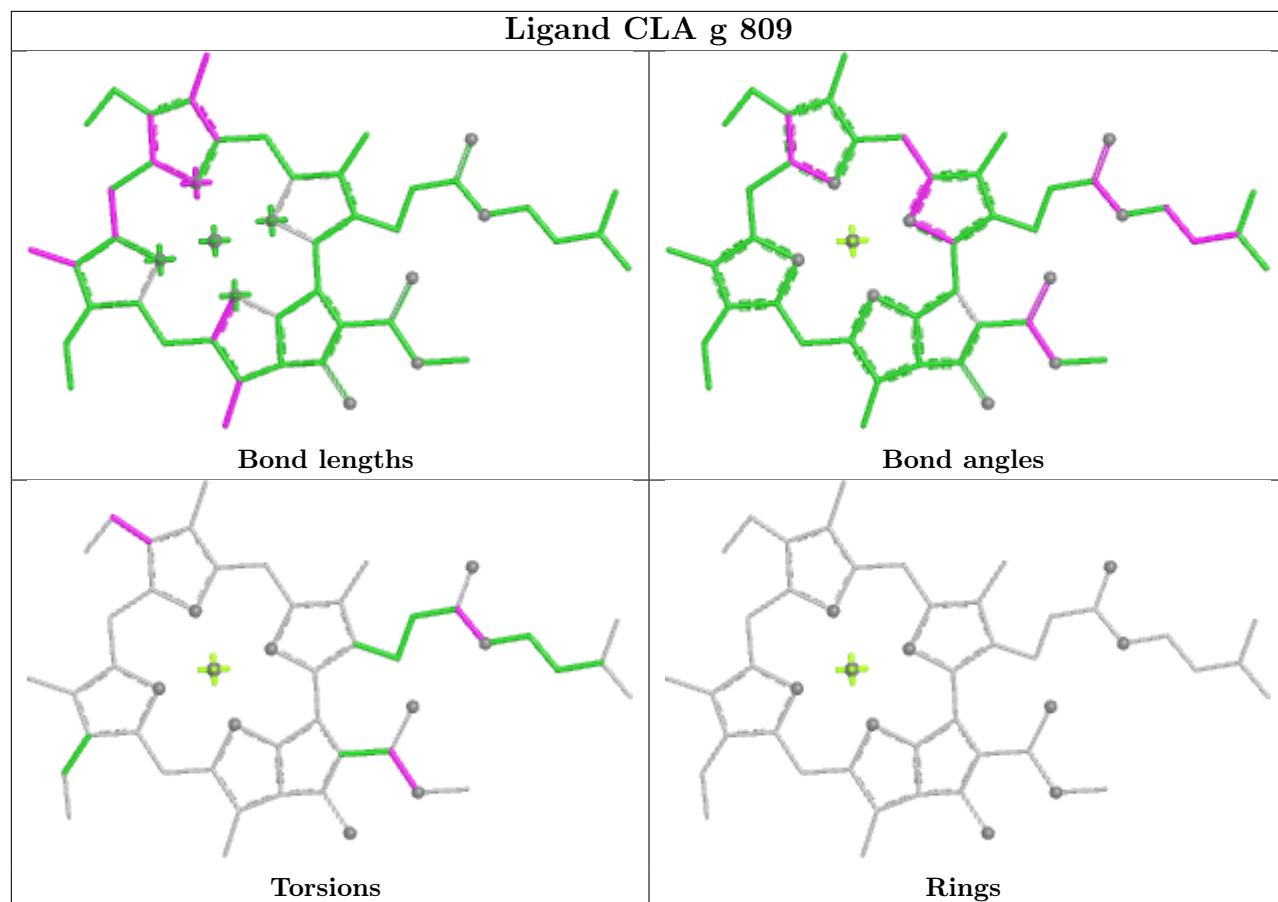
## Ligand CLA b 818



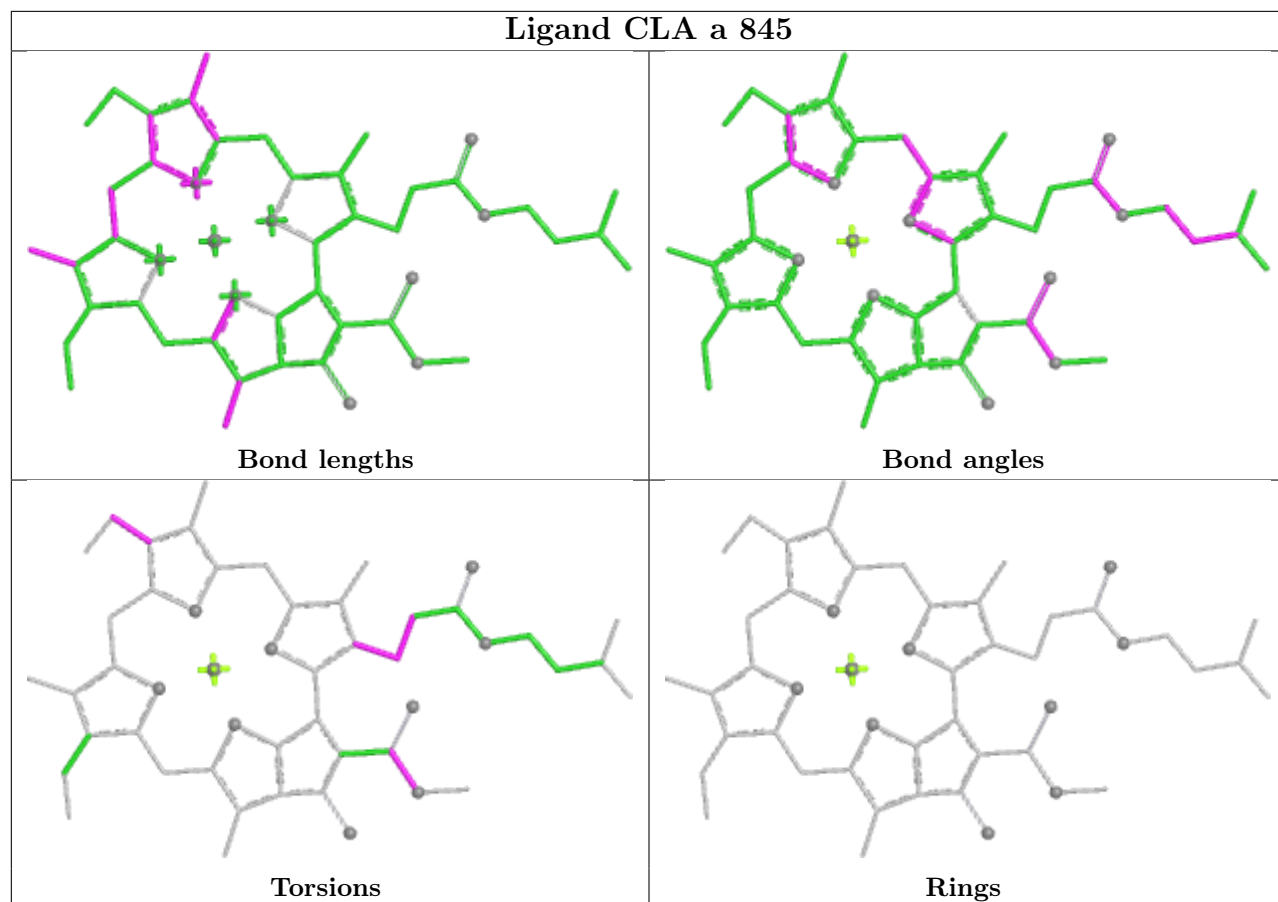
## Ligand BCR m 101



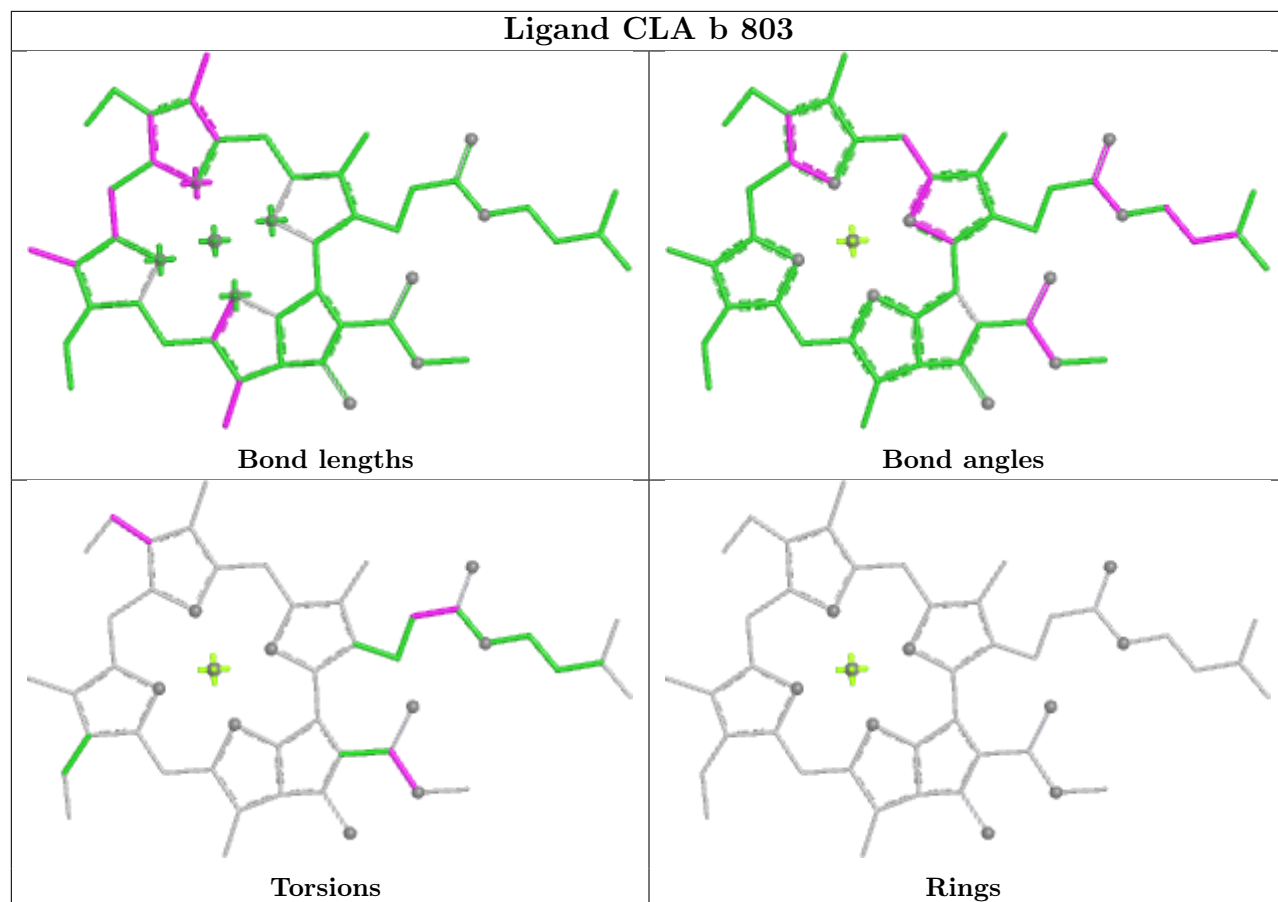
## Ligand CLA g 809



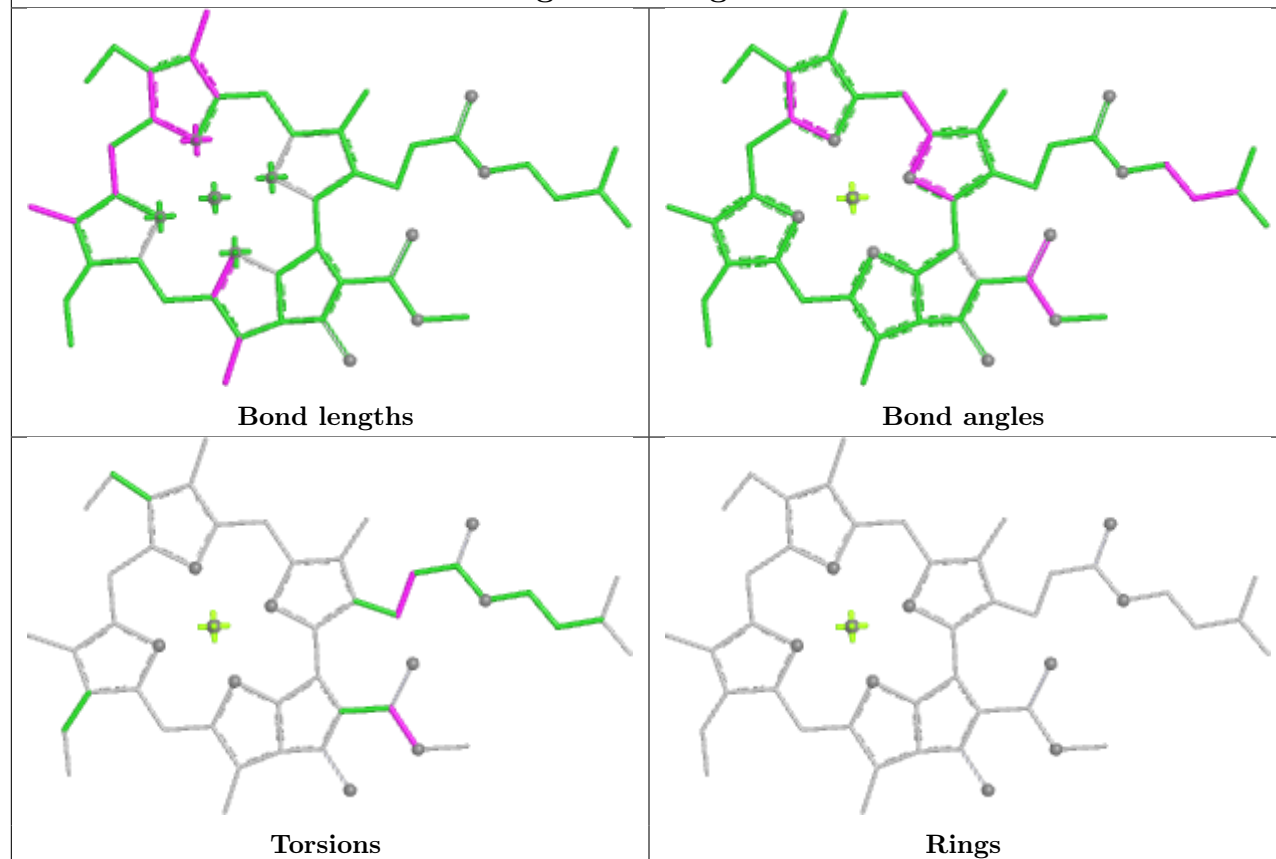
## Ligand CLA a 845



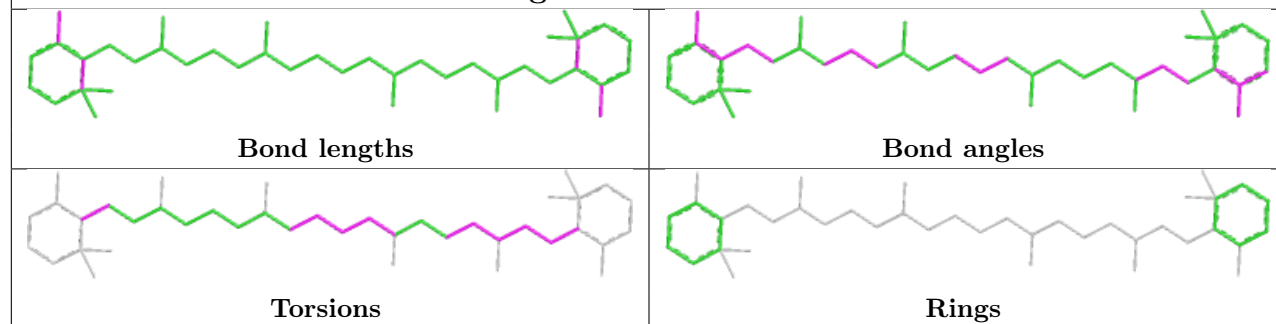
## Ligand CLA b 803



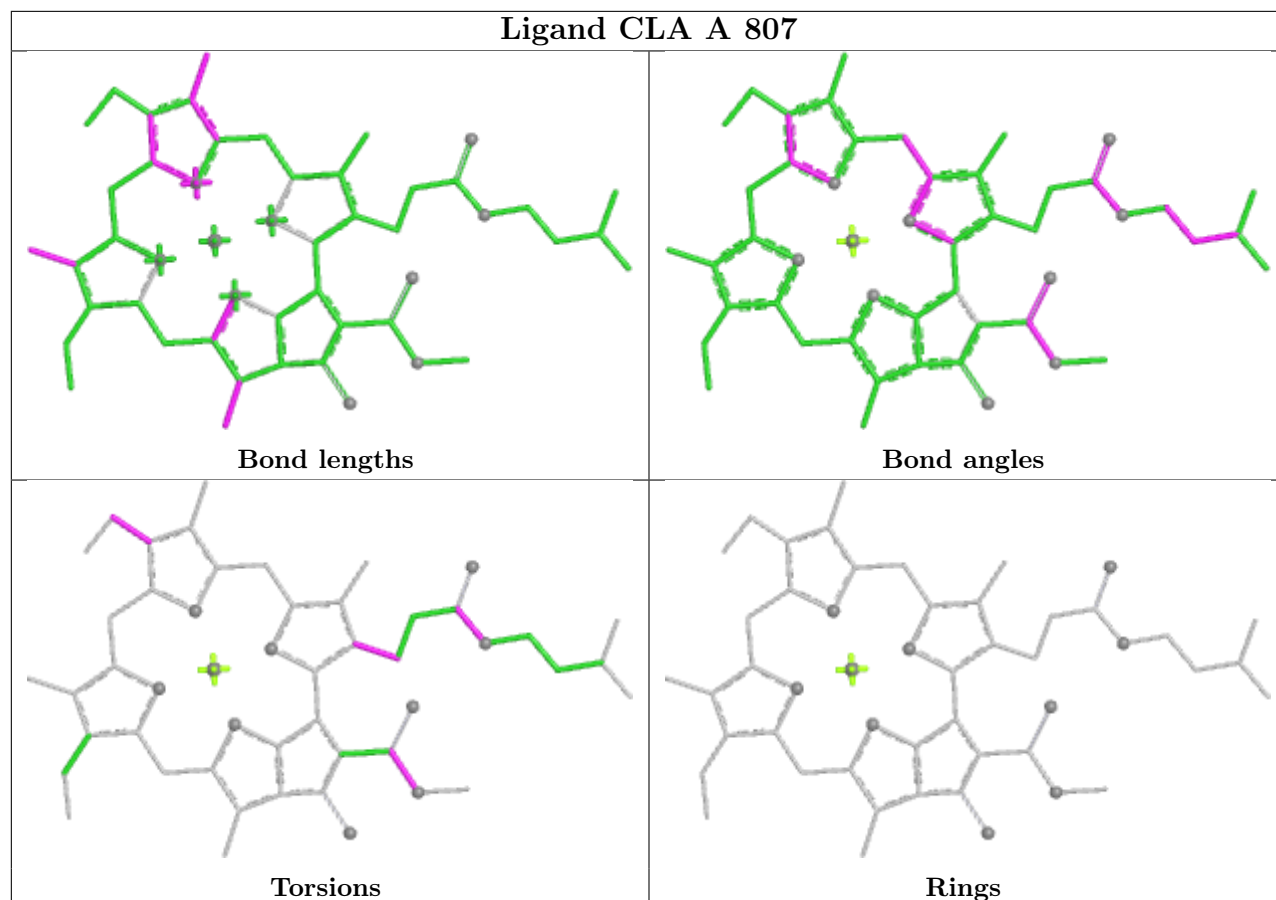
## Ligand CLA g 815



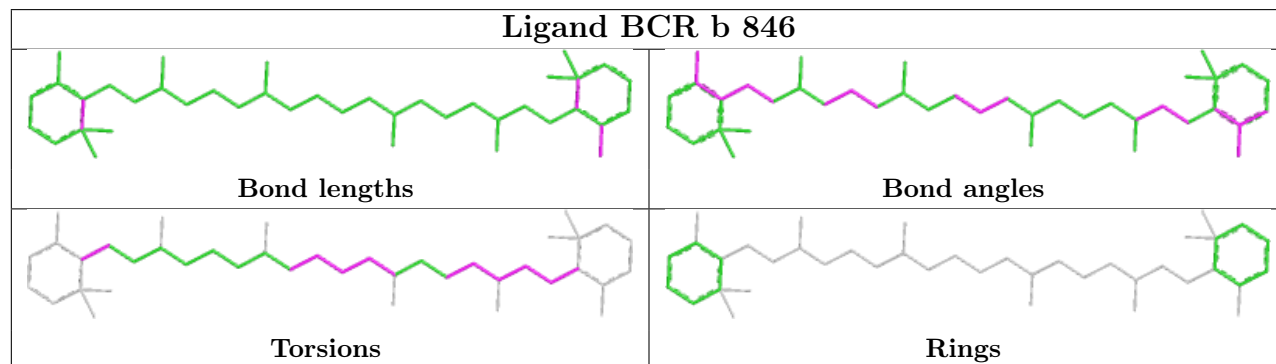
## Ligand BCR G 847



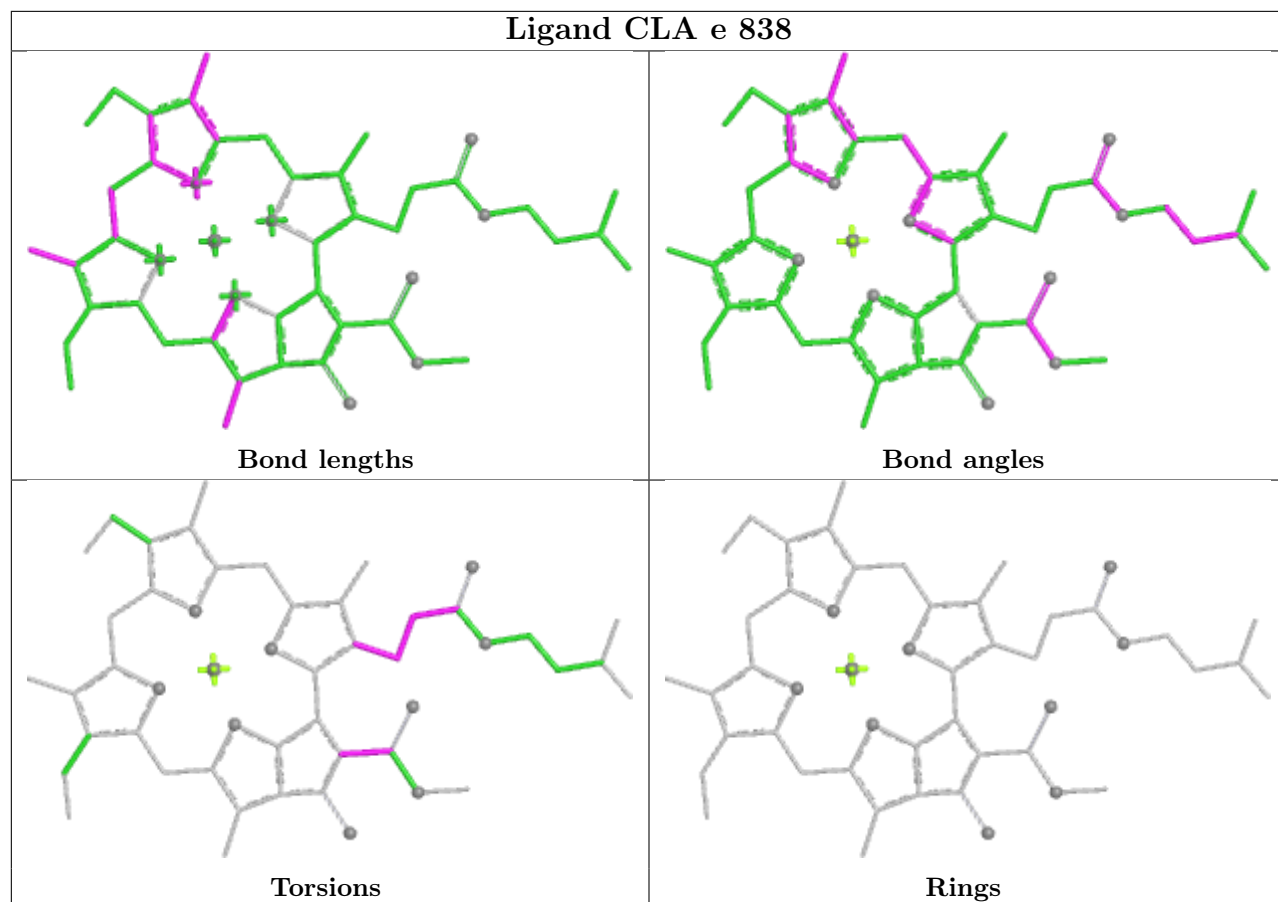
## Ligand CLA A 807



## Ligand BCR b 846

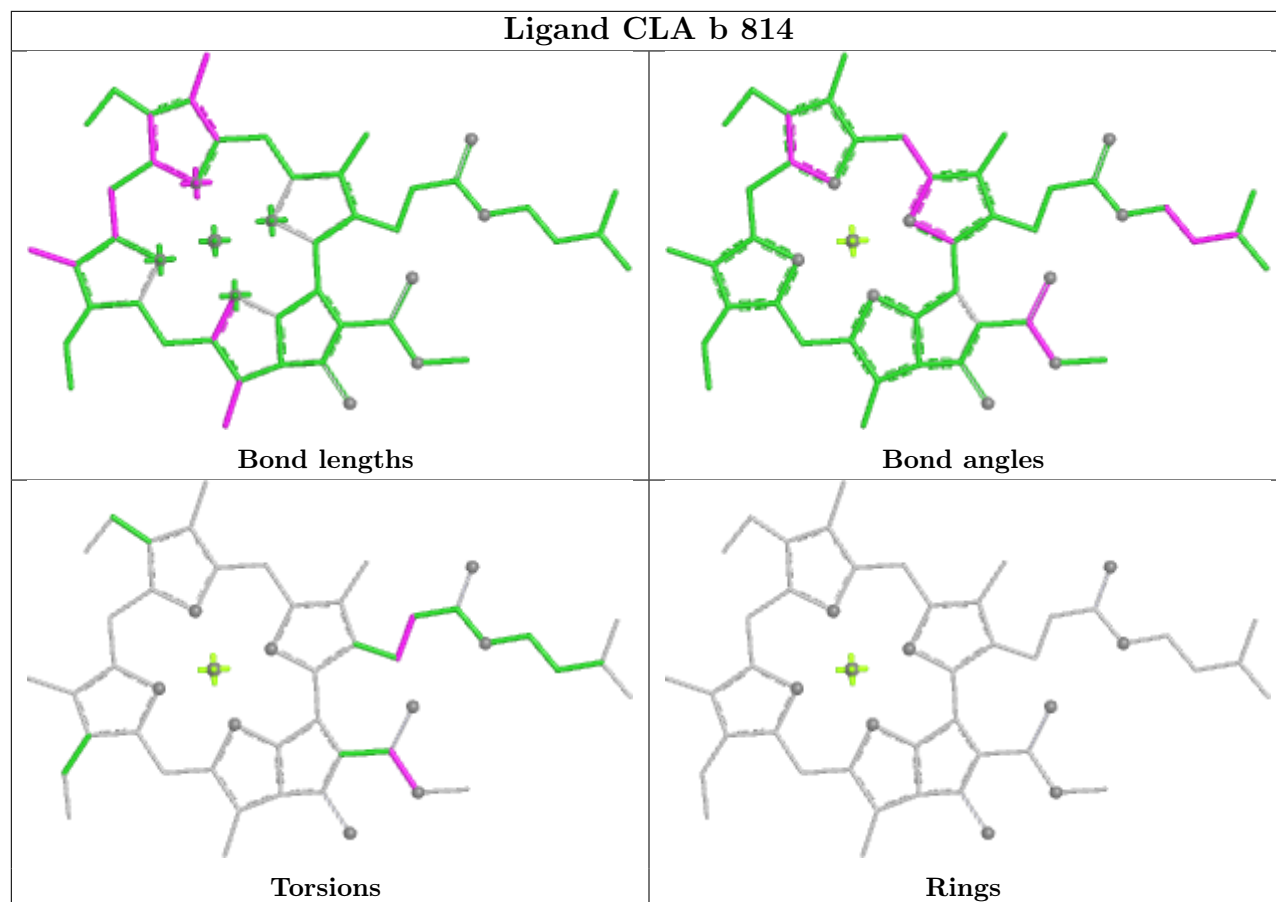


## Ligand CLA e 838

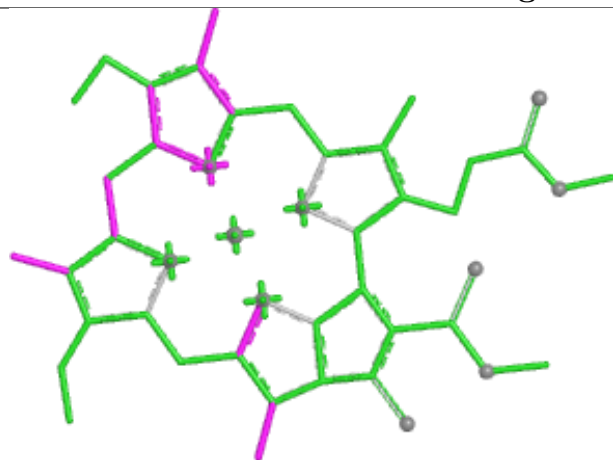




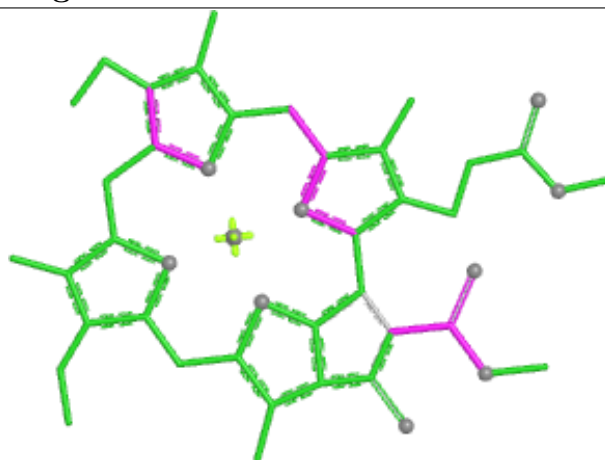
## Ligand CLA b 814



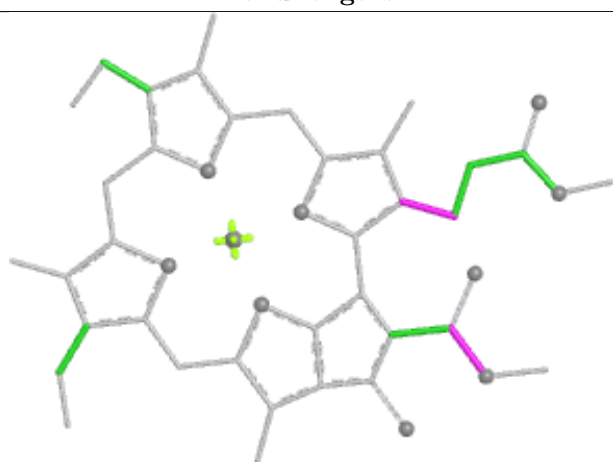
## Ligand CLA g 827



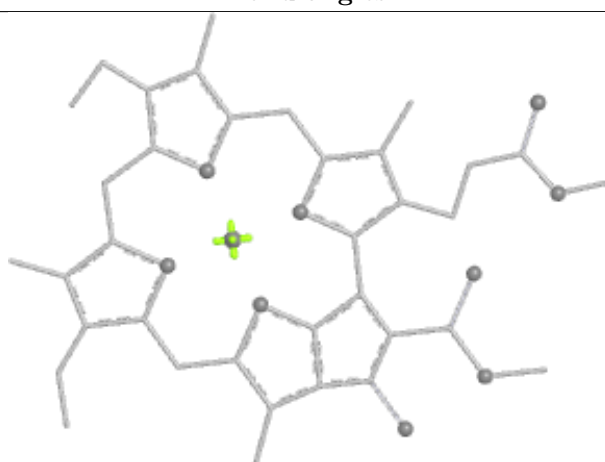
Bond lengths



Bond angles

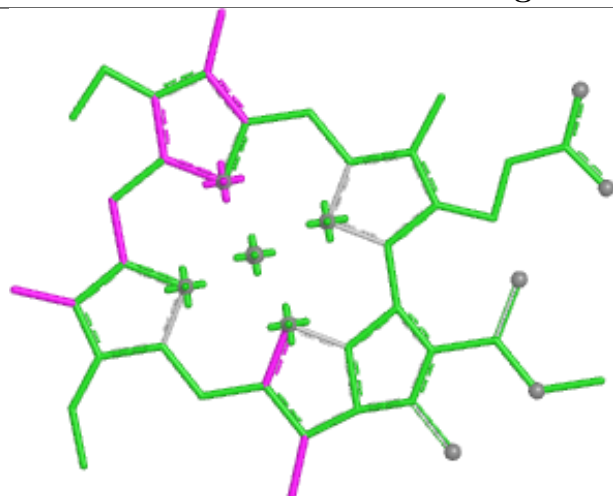


Torsions

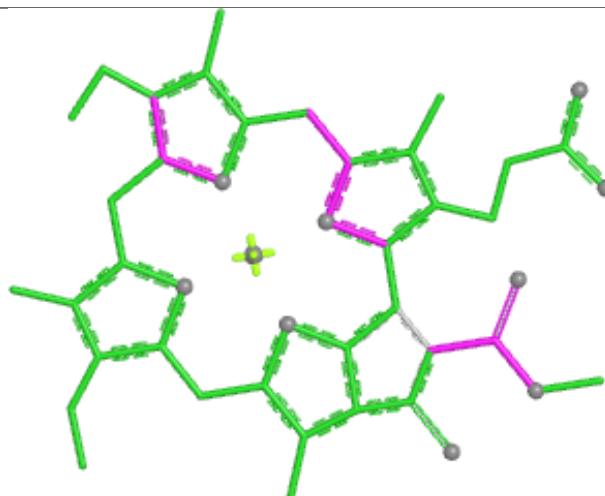


Rings

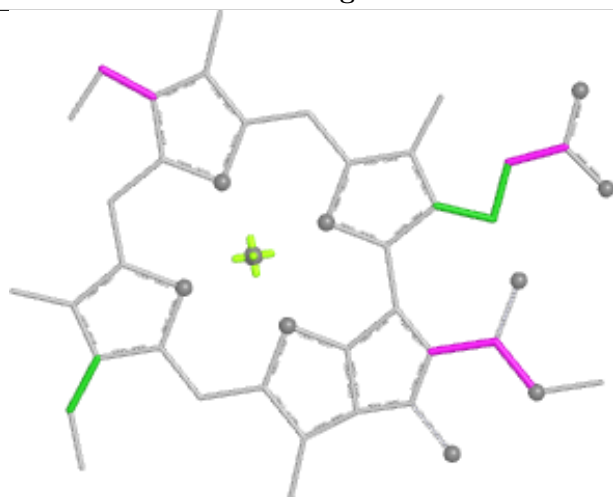
## Ligand CLA B 824



Bond lengths



Bond angles

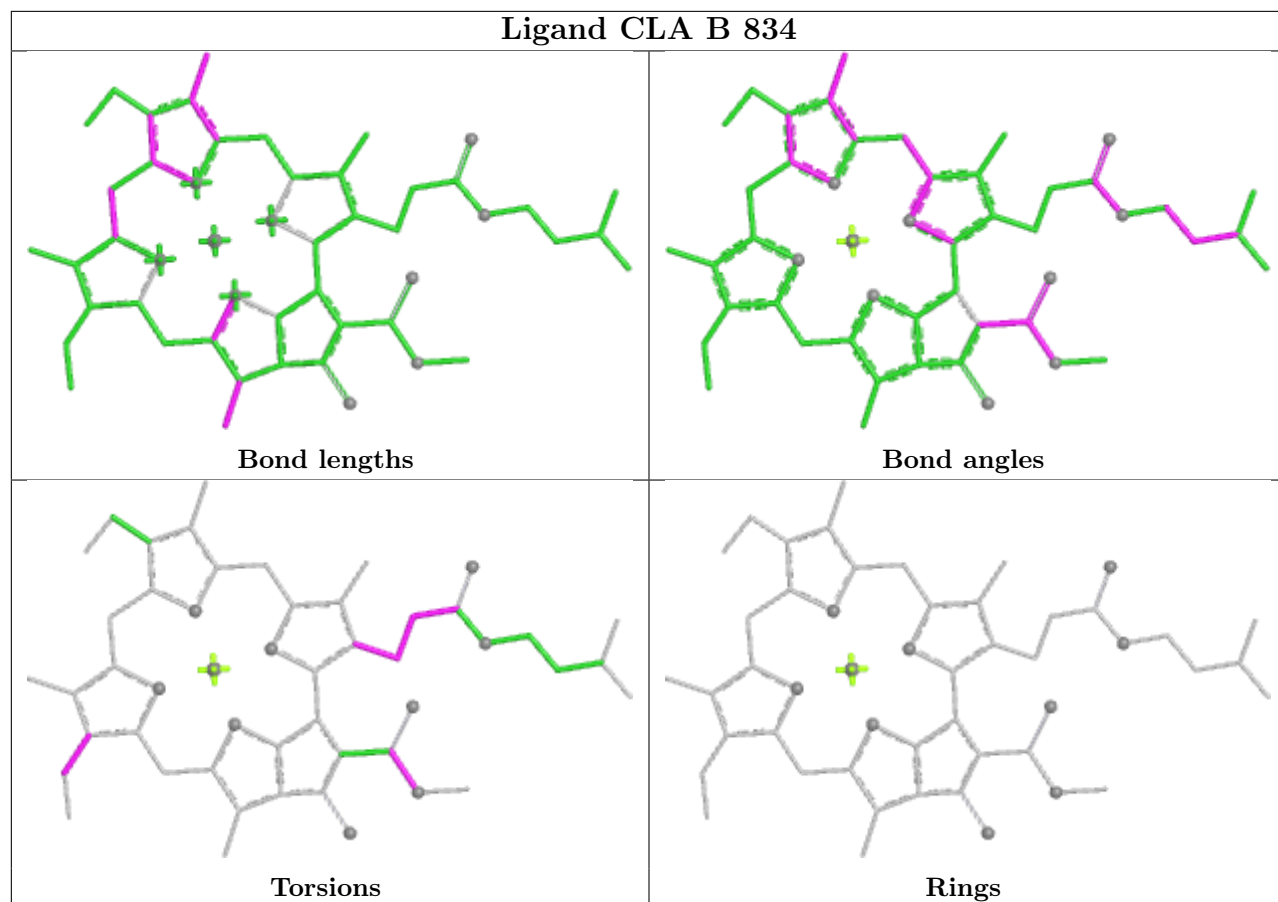


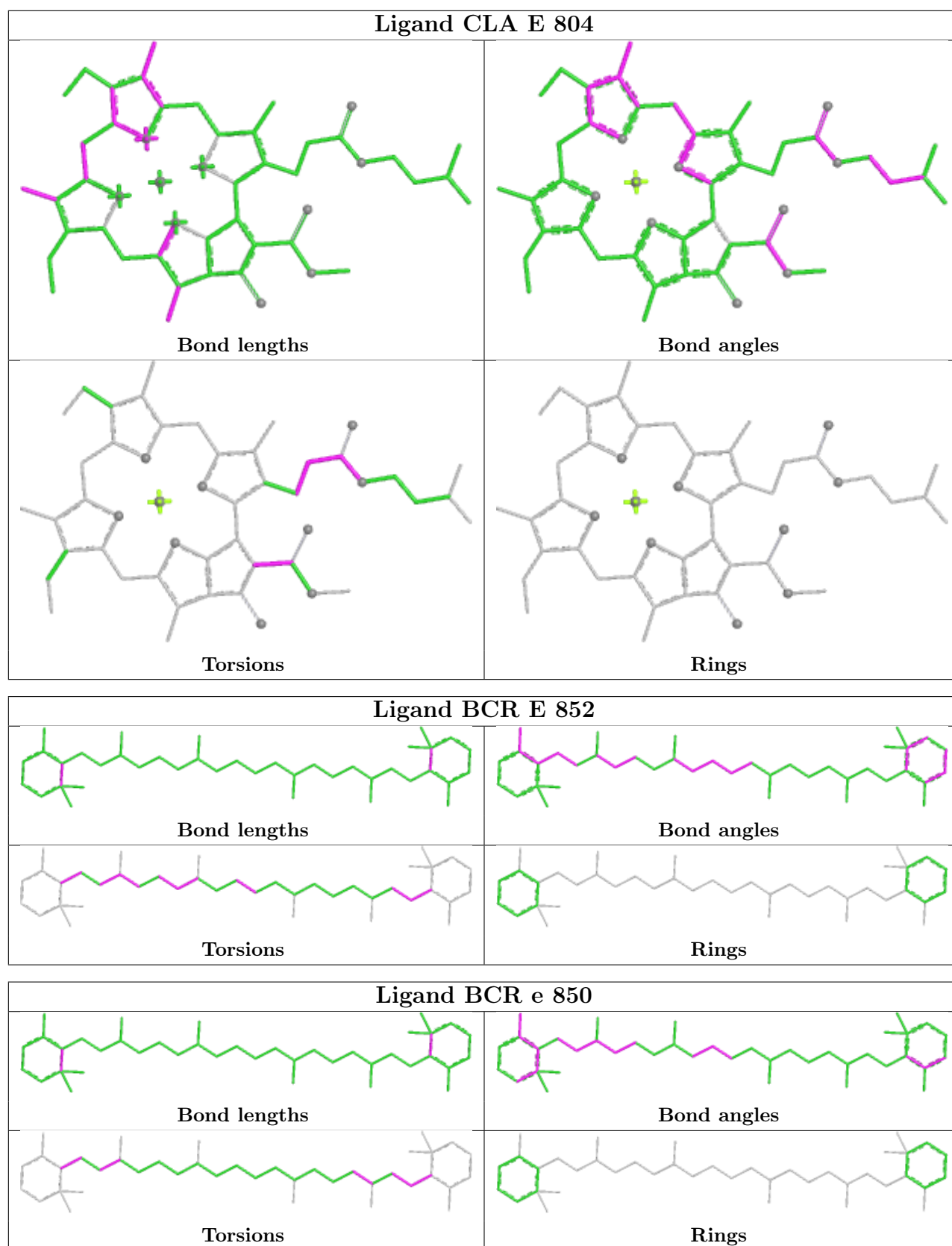
Torsions



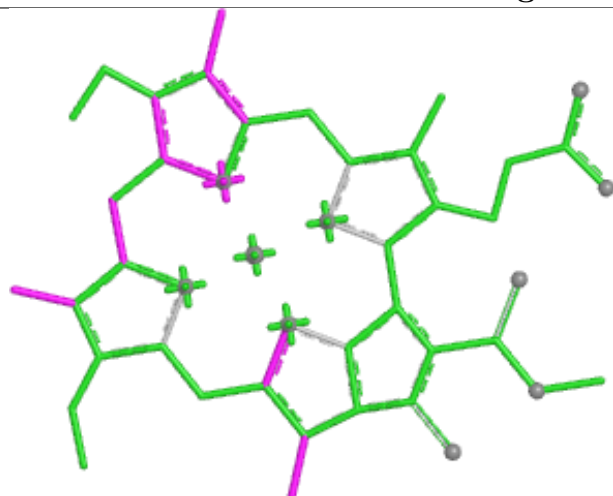
Rings

## Ligand CLA B 834

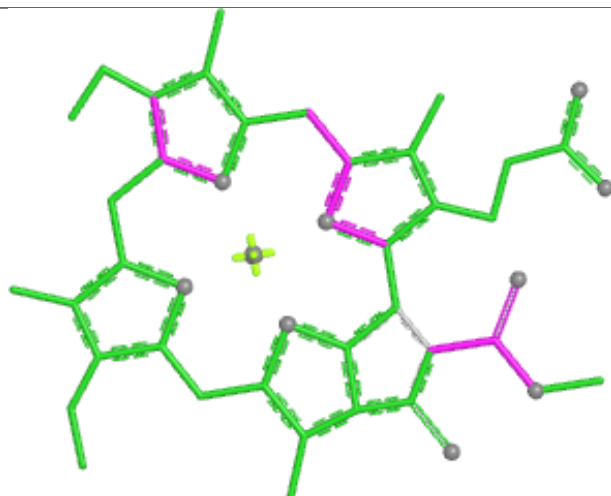




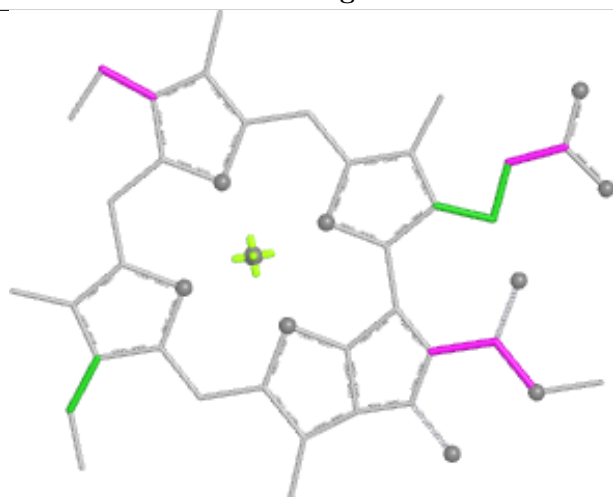
## Ligand CLA b 823



Bond lengths



Bond angles

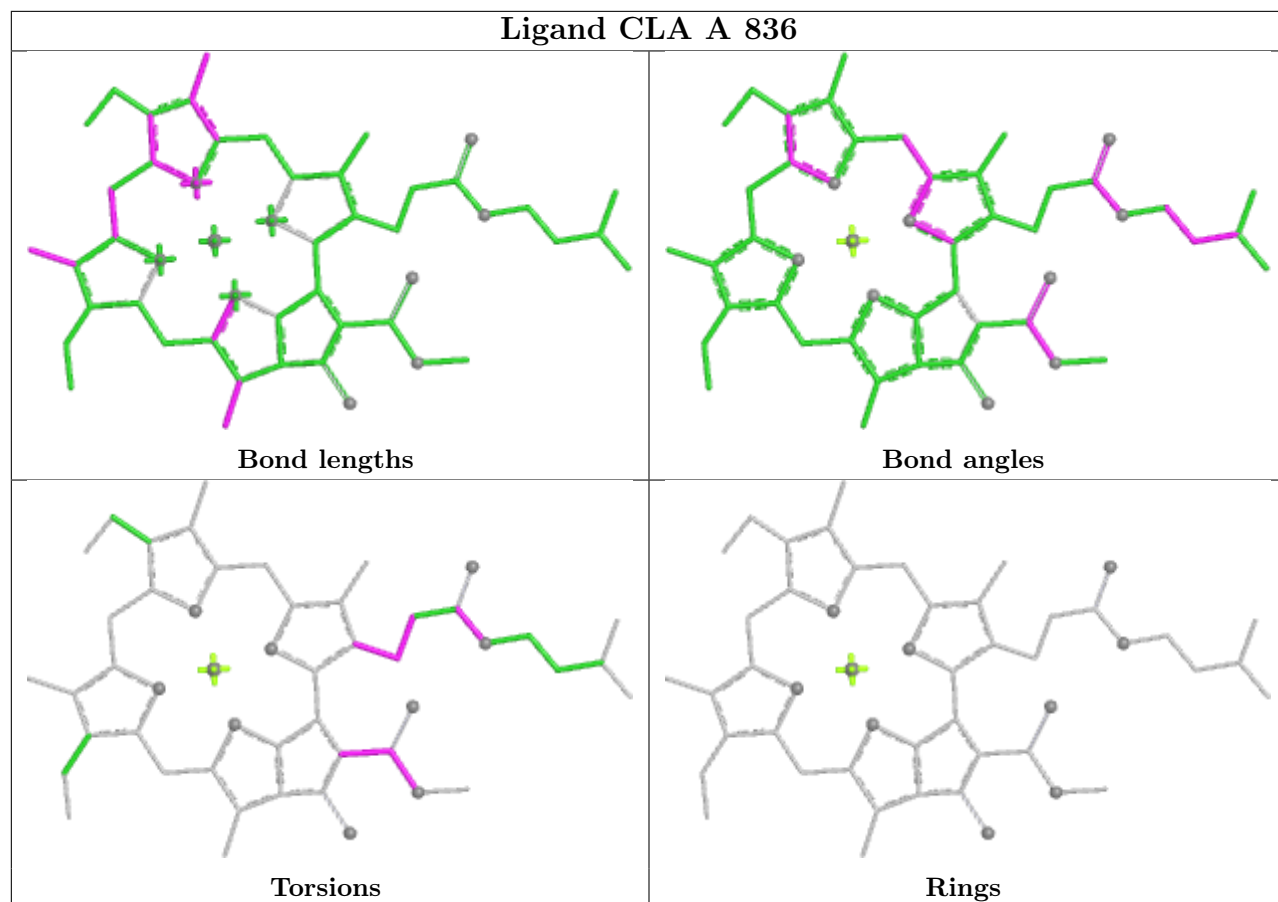


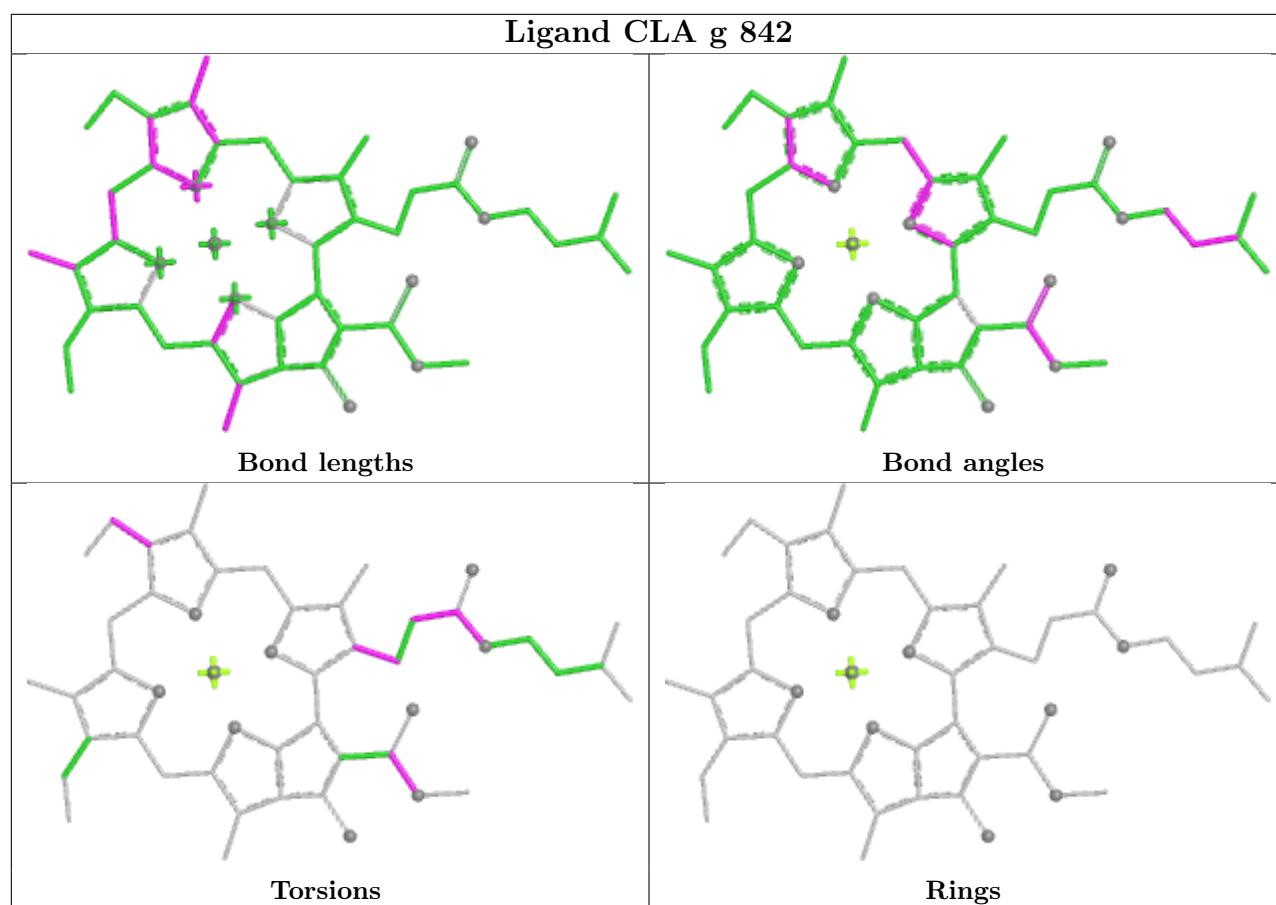
Torsions



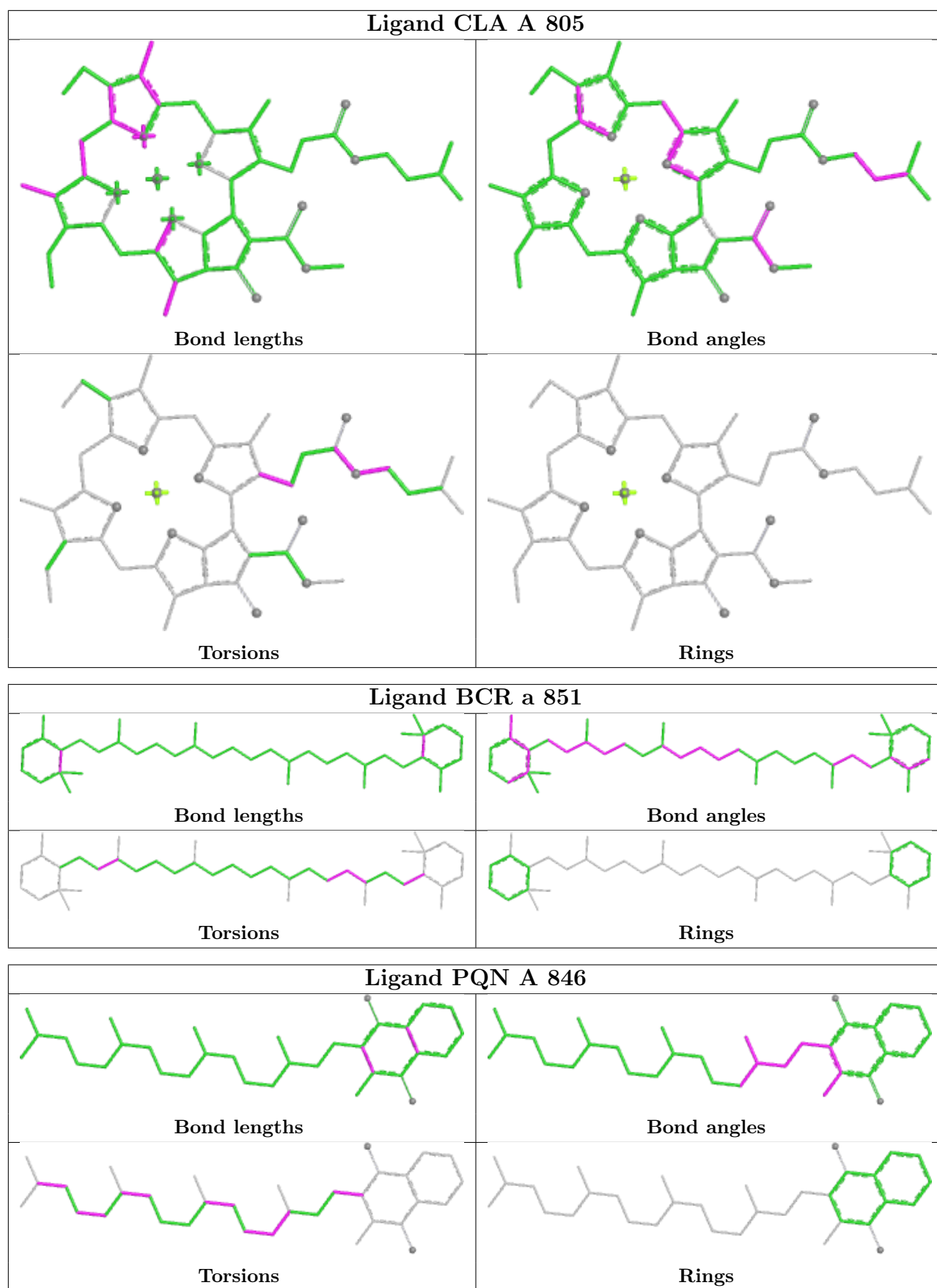
Rings

## Ligand CLA A 836

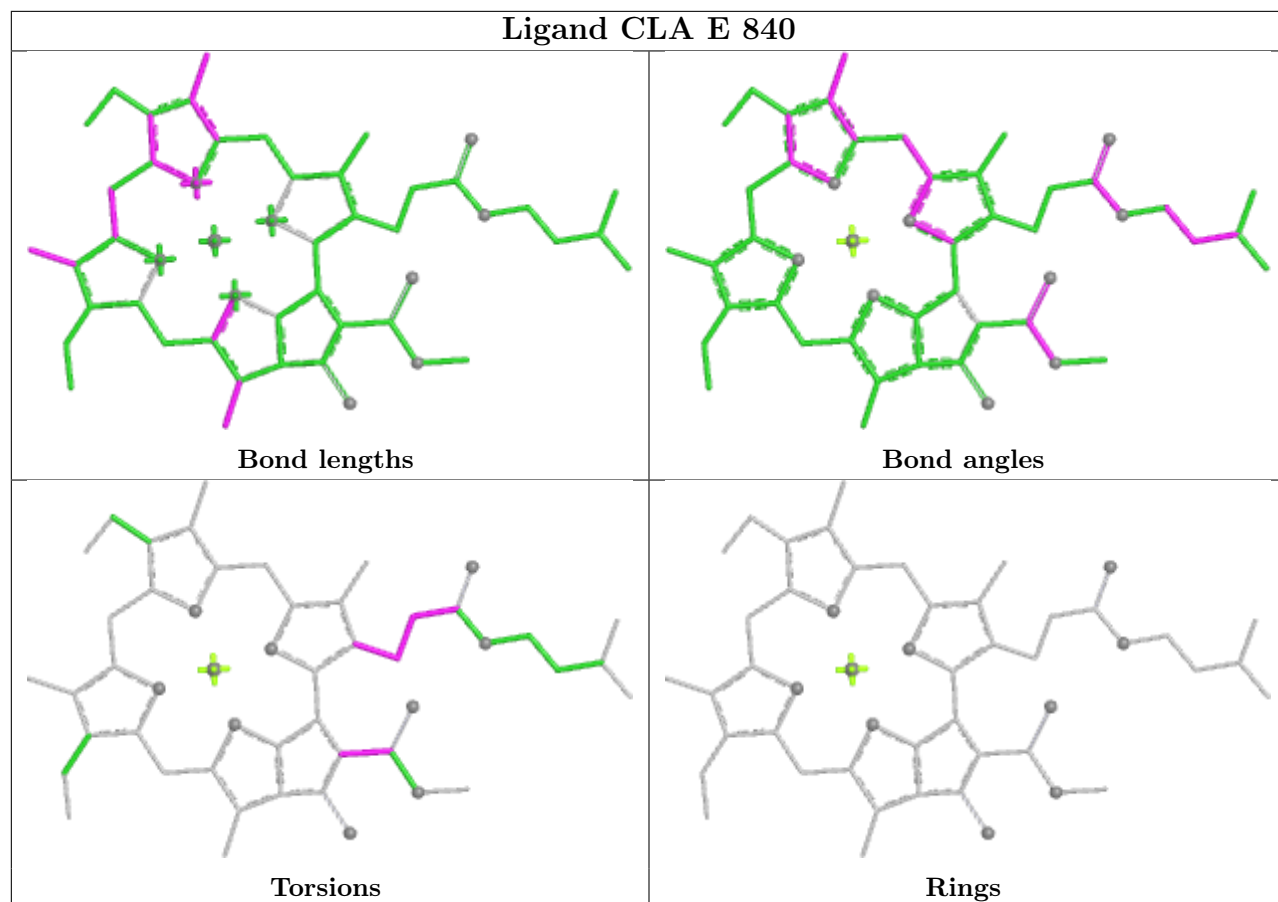




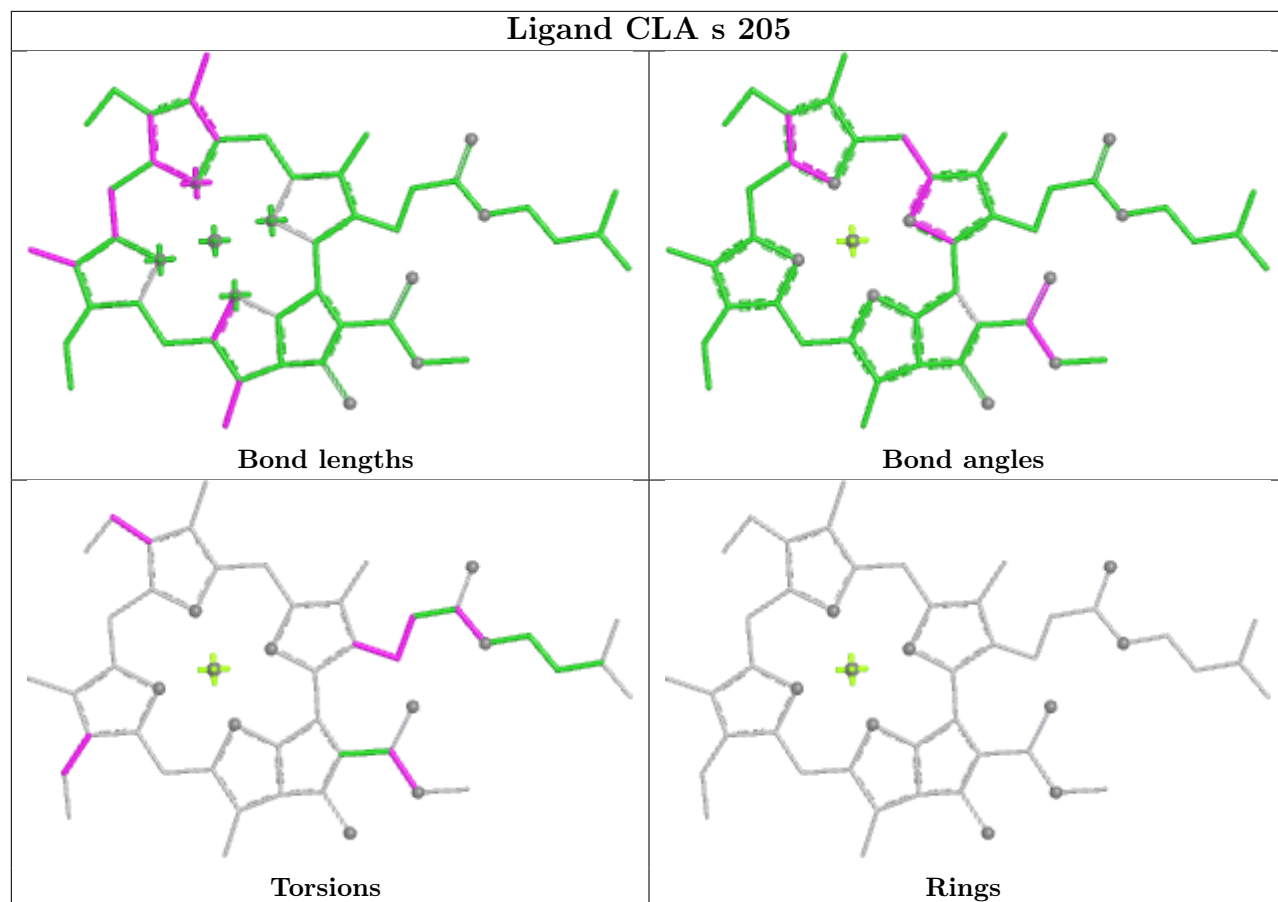




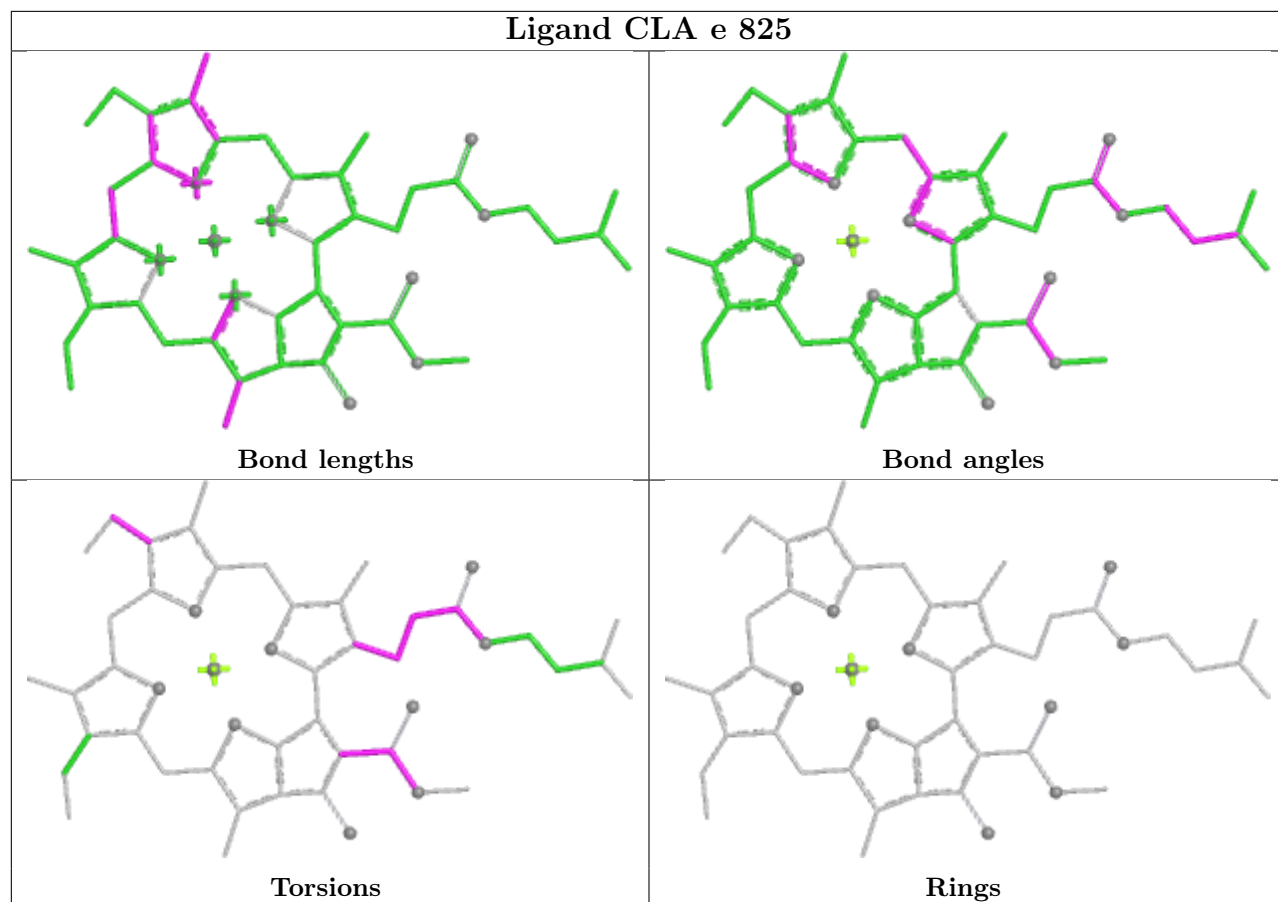
## Ligand CLA E 840



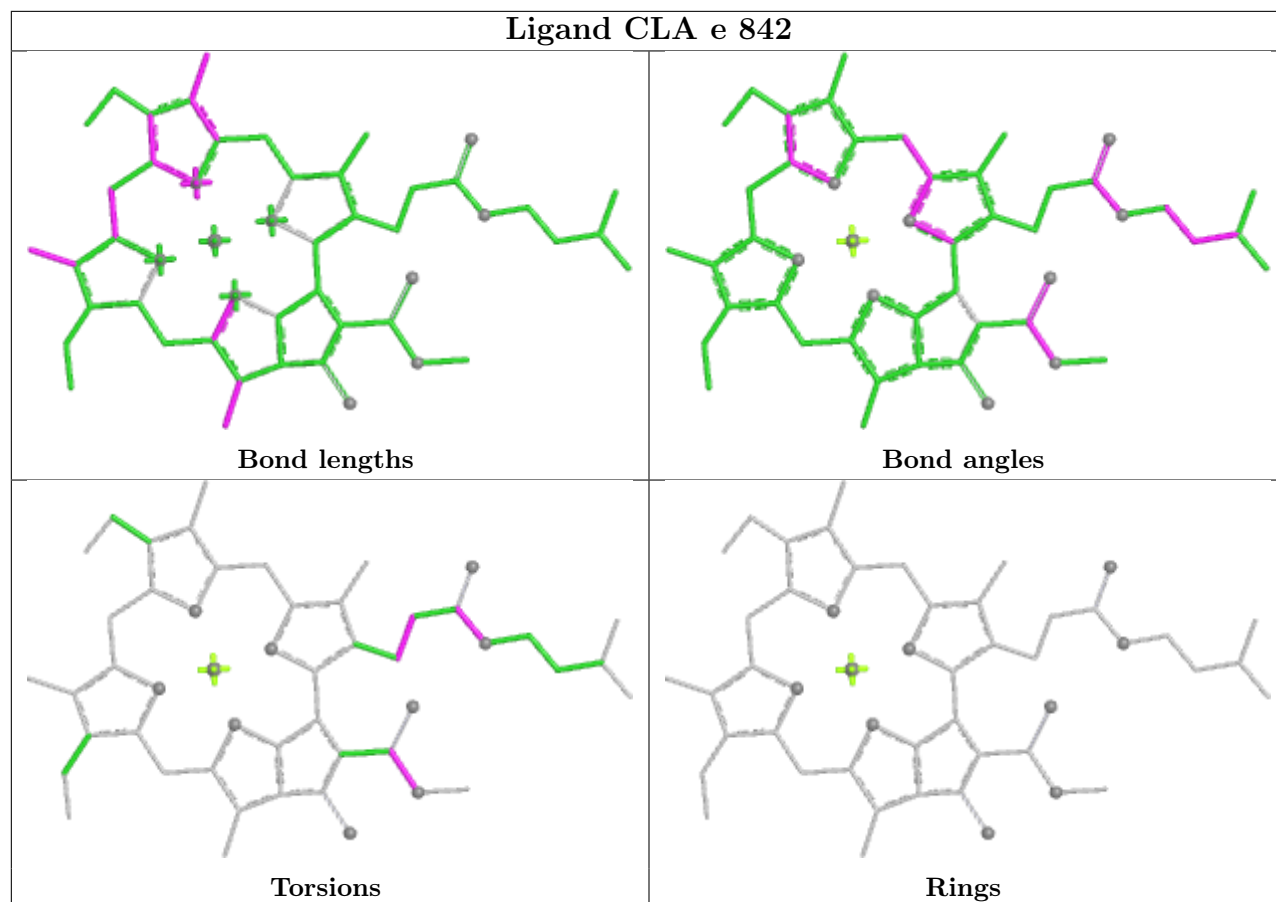
## Ligand CLA s 205



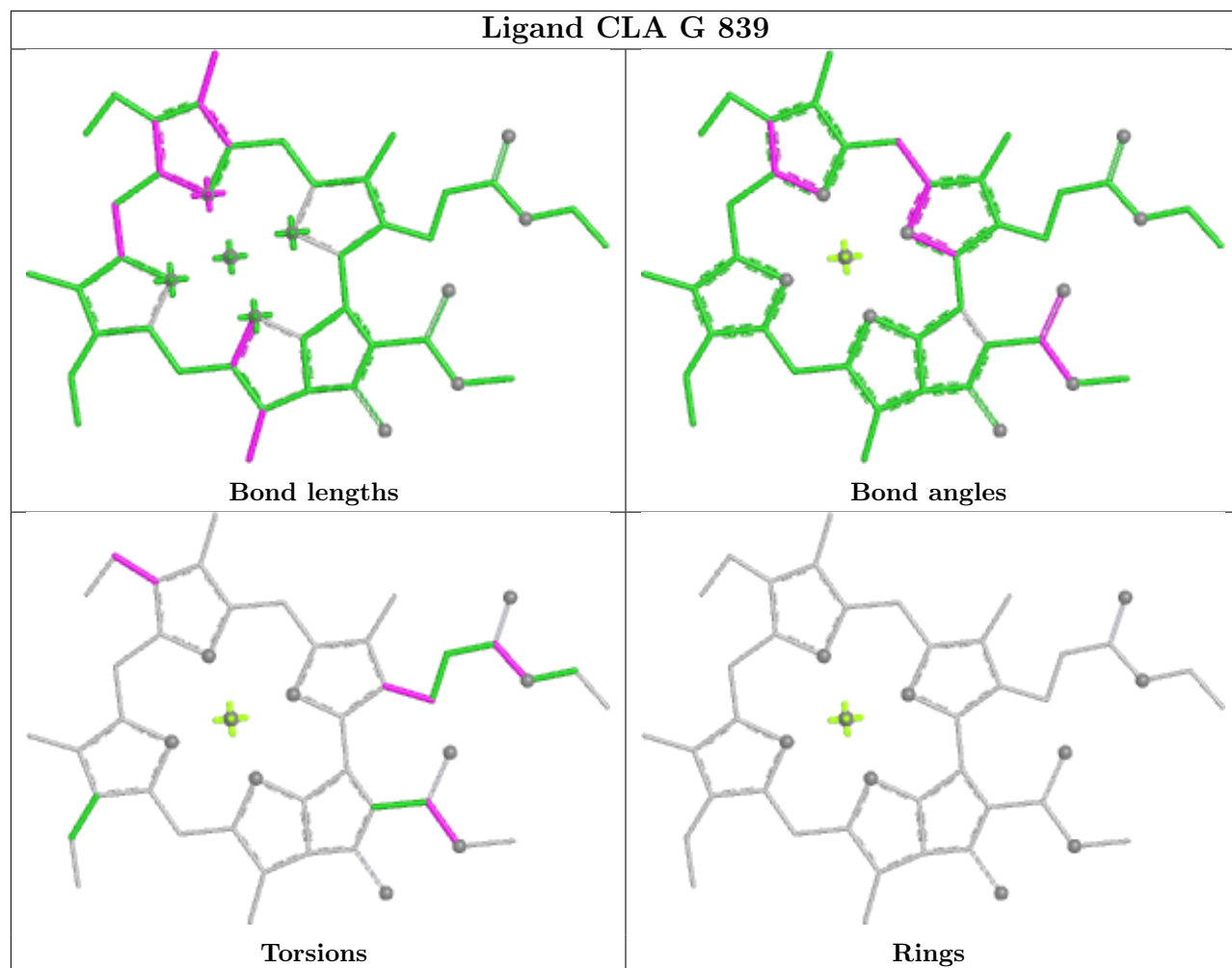
## Ligand CLA e 825



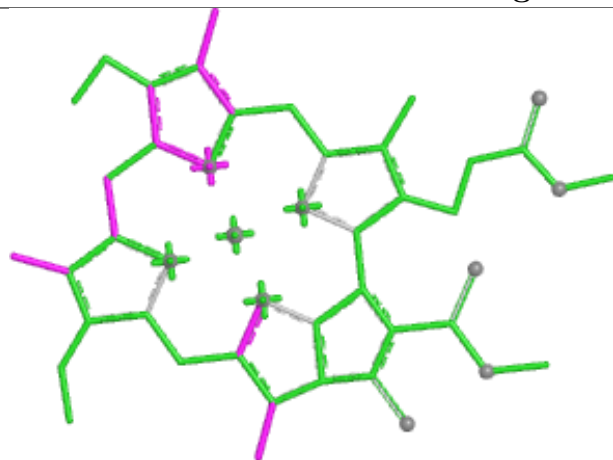
## Ligand CLA e 842



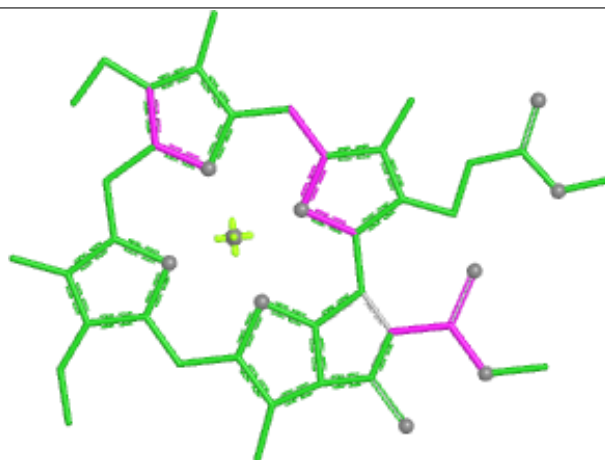
## Ligand CLA G 839



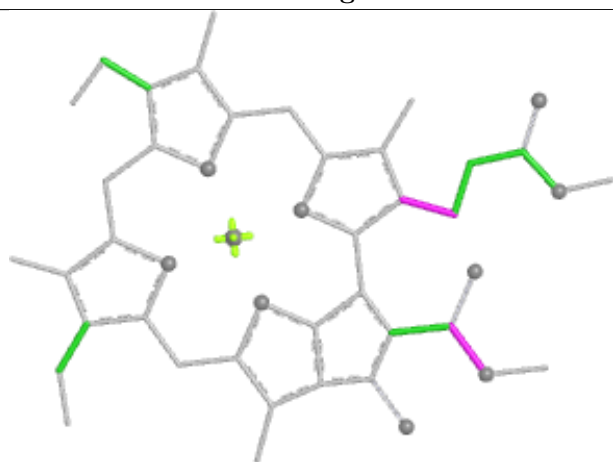
## Ligand CLA G 826



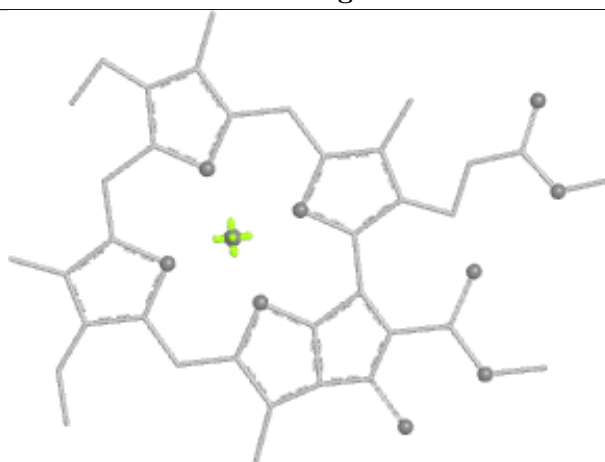
Bond lengths



Bond angles

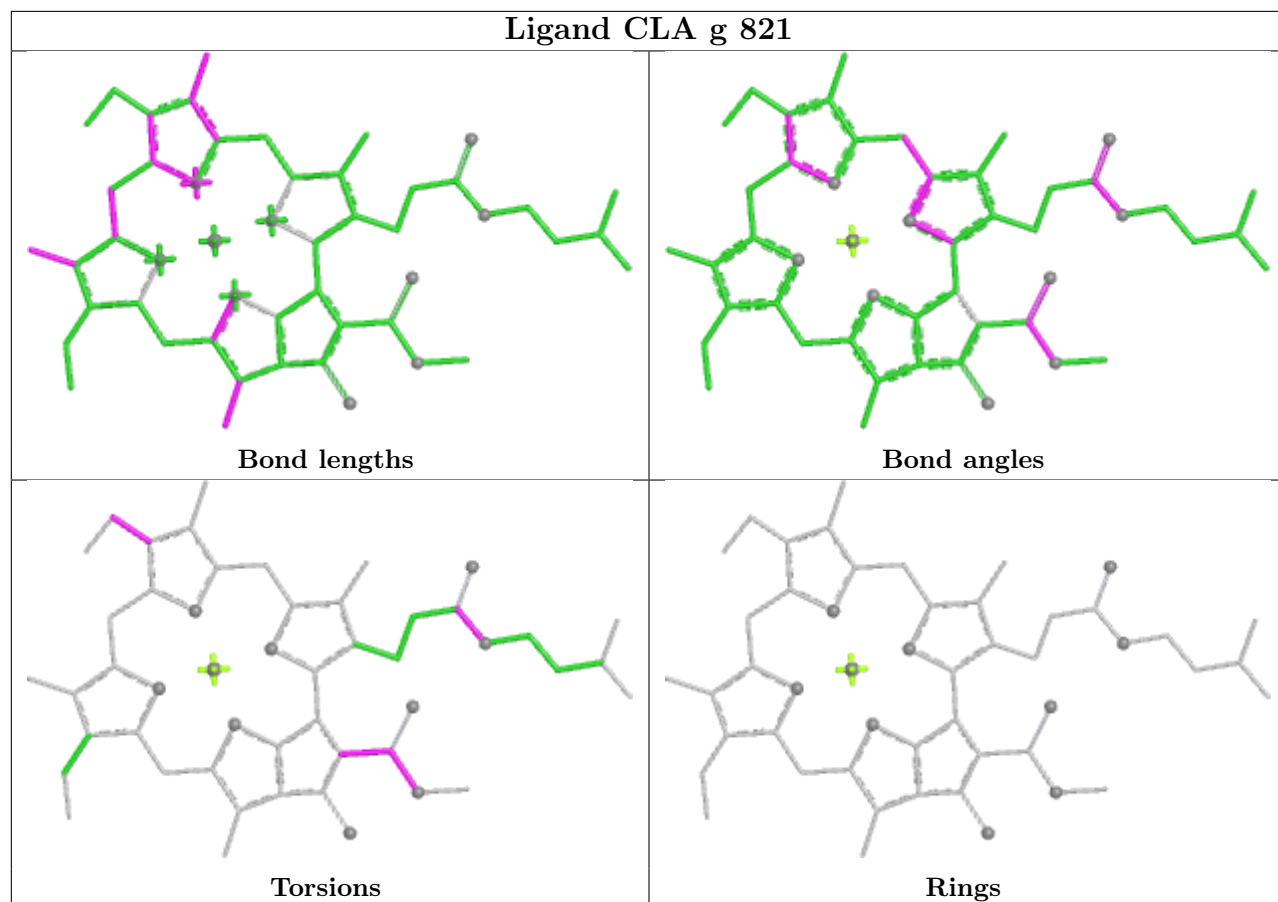


Torsions



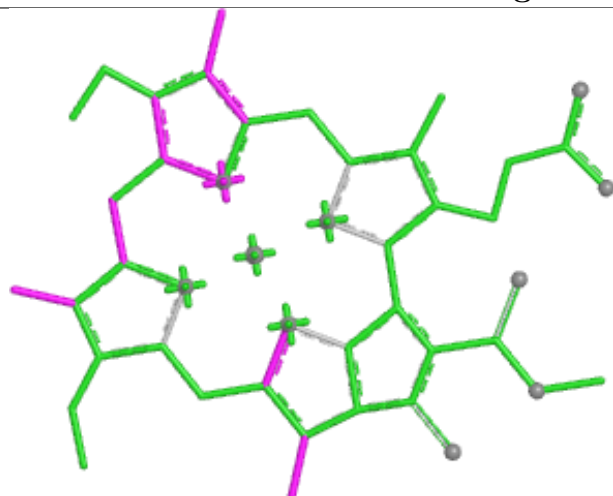
Rings

## Ligand CLA g 821

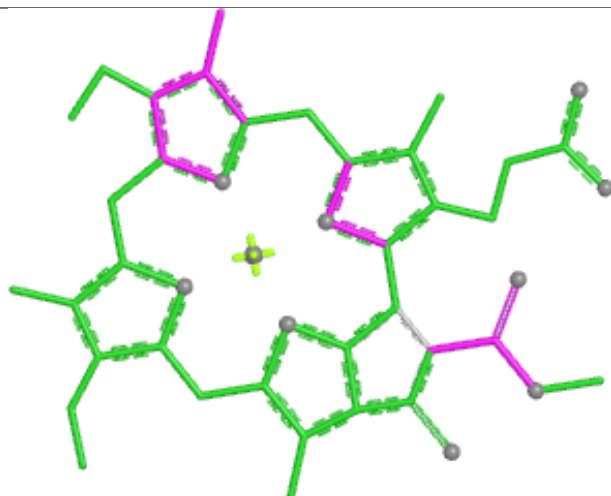




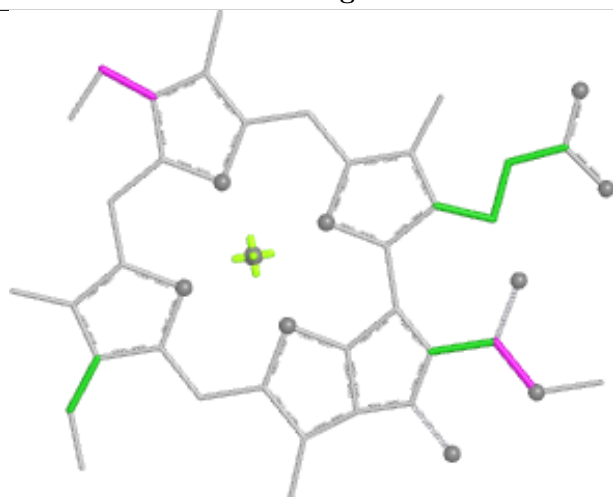
## Ligand CLA A 818



Bond lengths



Bond angles

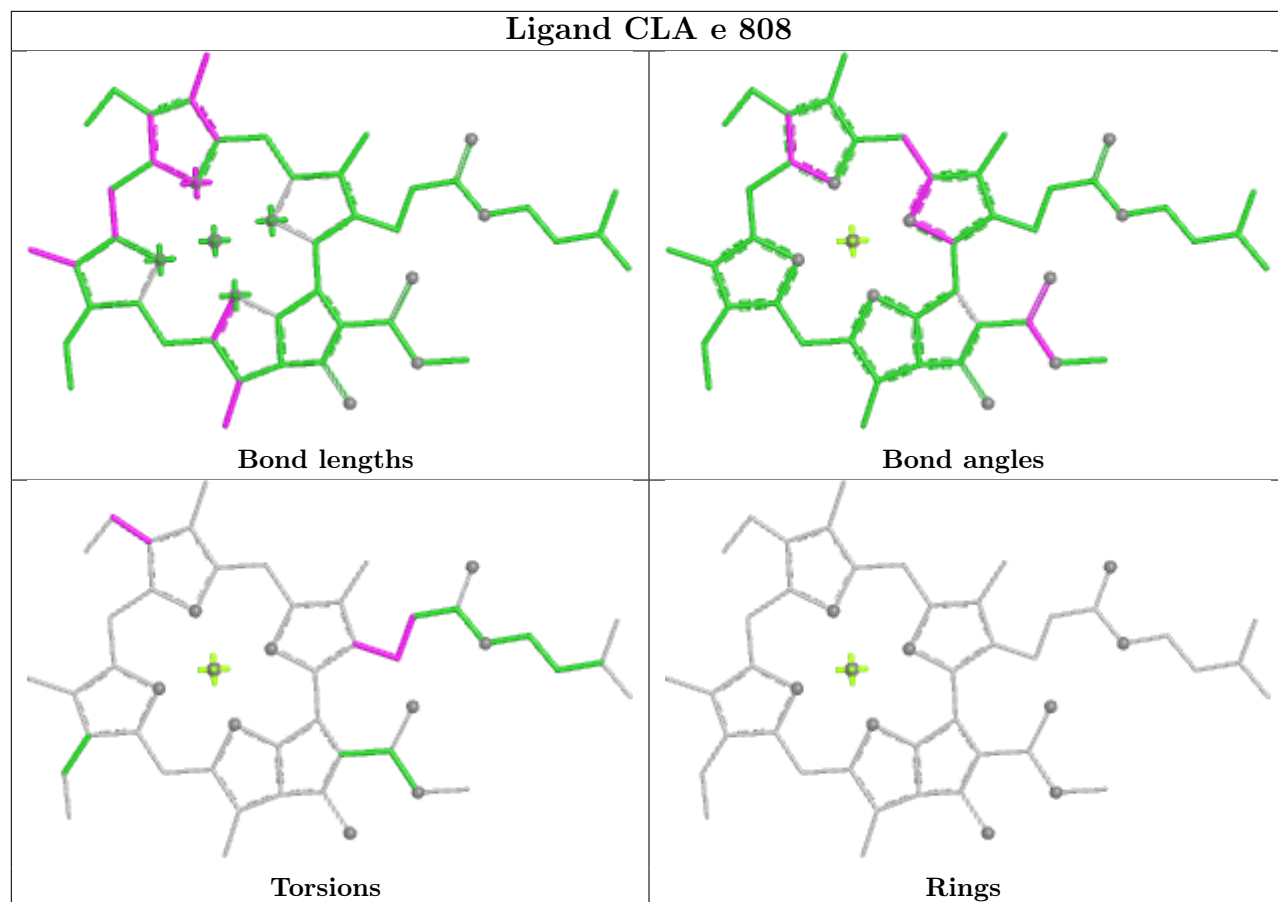


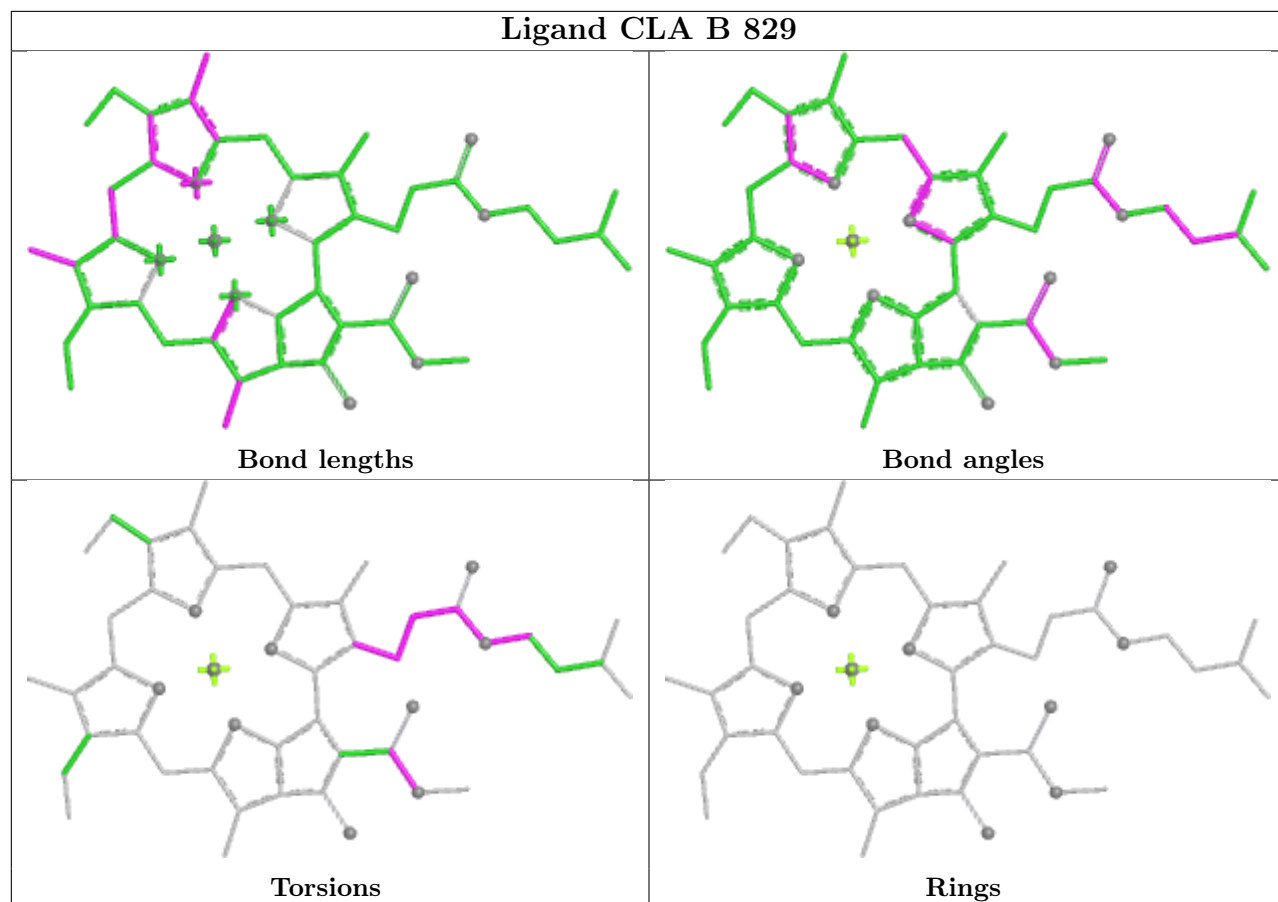
Torsions



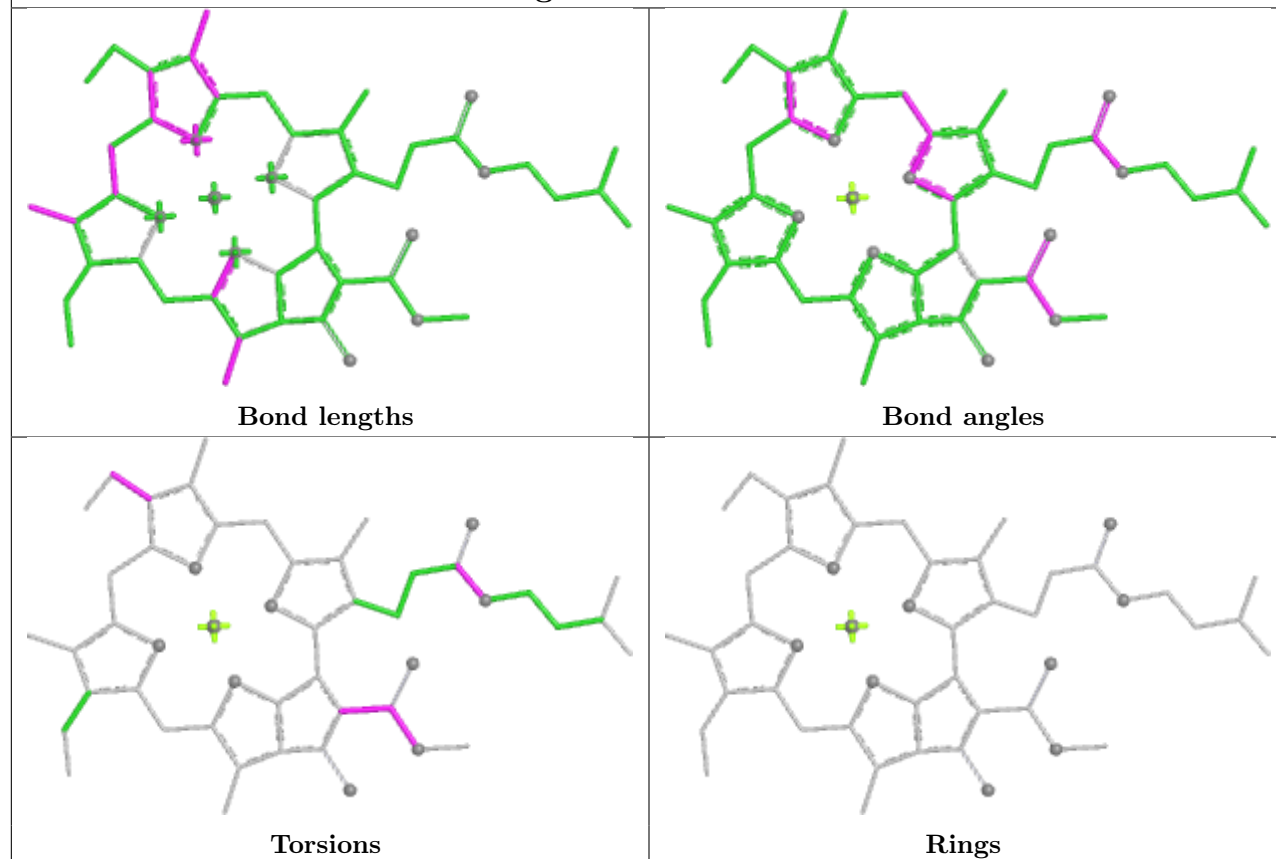
Rings

## Ligand CLA e 808

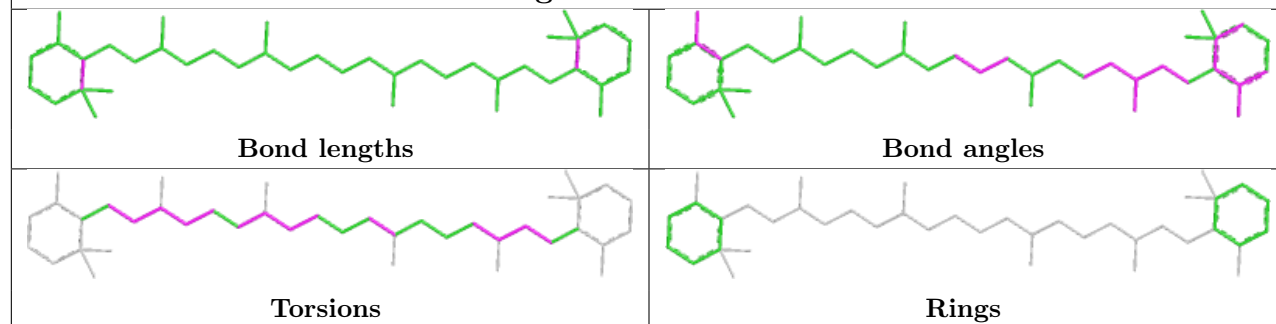


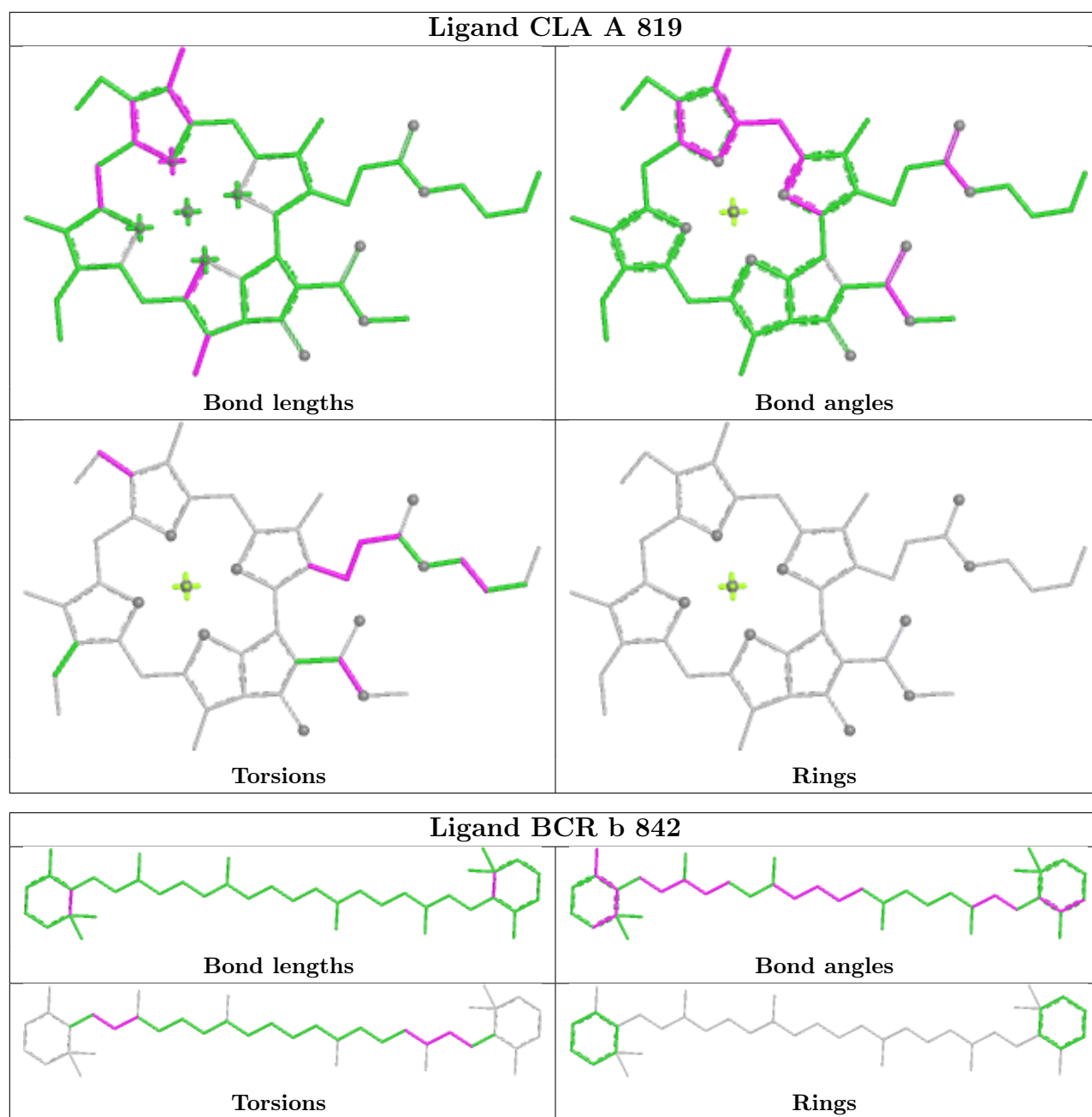


## Ligand CLA b 819

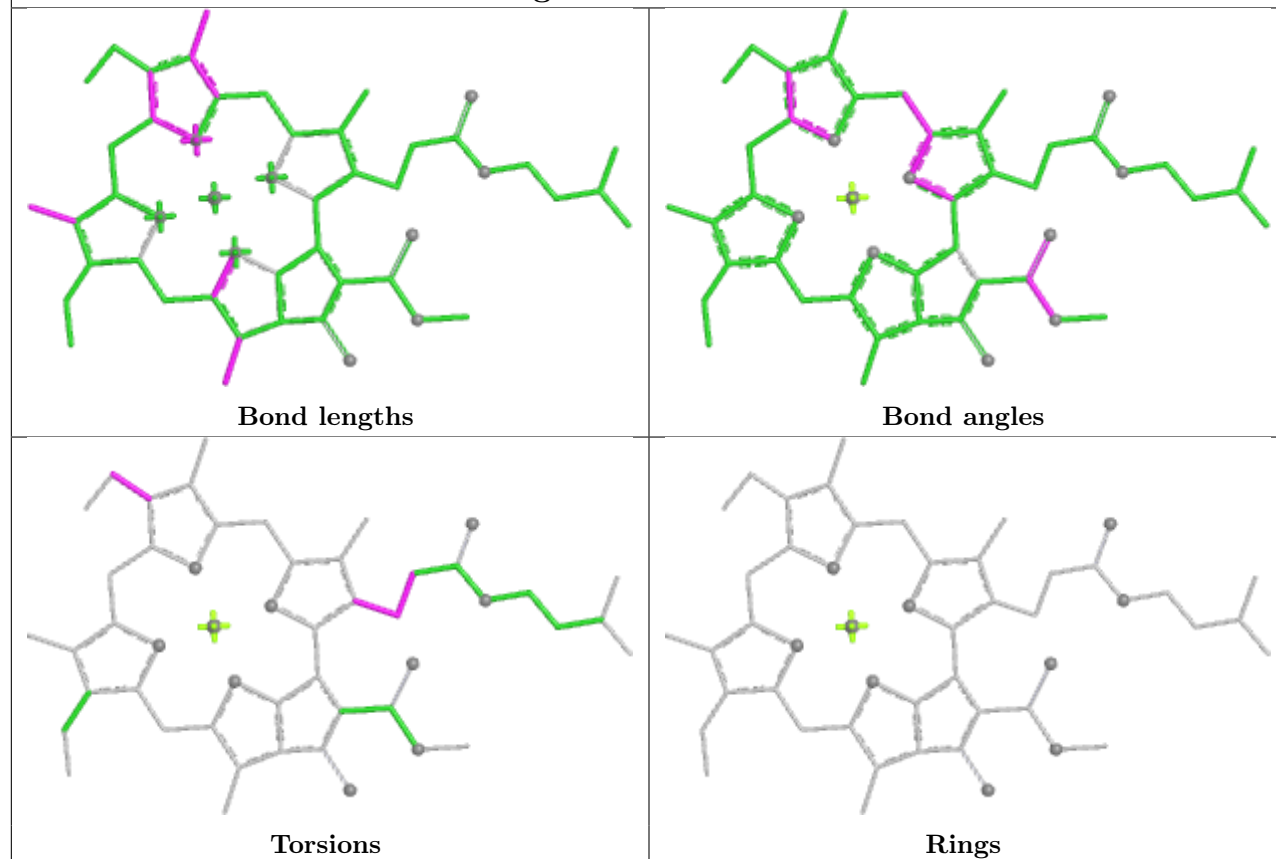


## Ligand BCR e 846

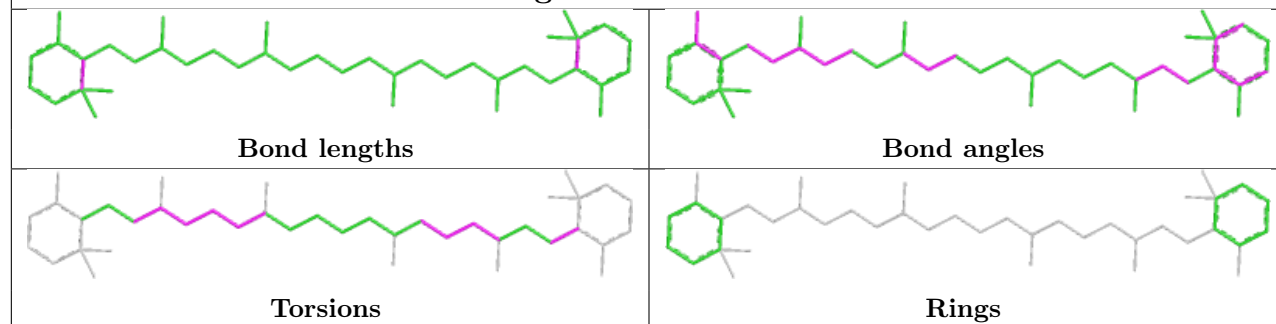




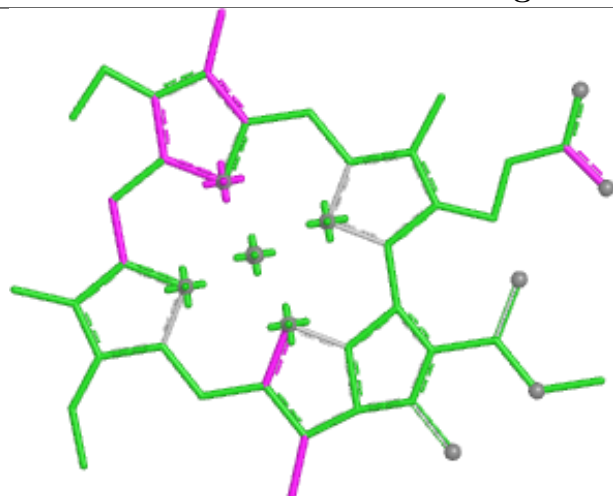
## Ligand CLA E 809



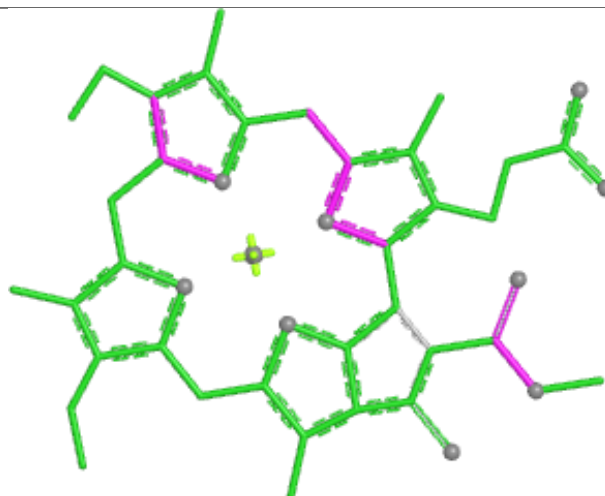
## Ligand BCR a 850



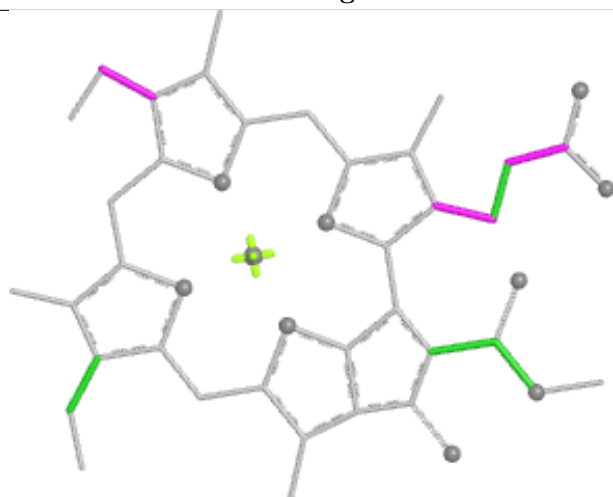
## Ligand CLA A 817



Bond lengths



Bond angles

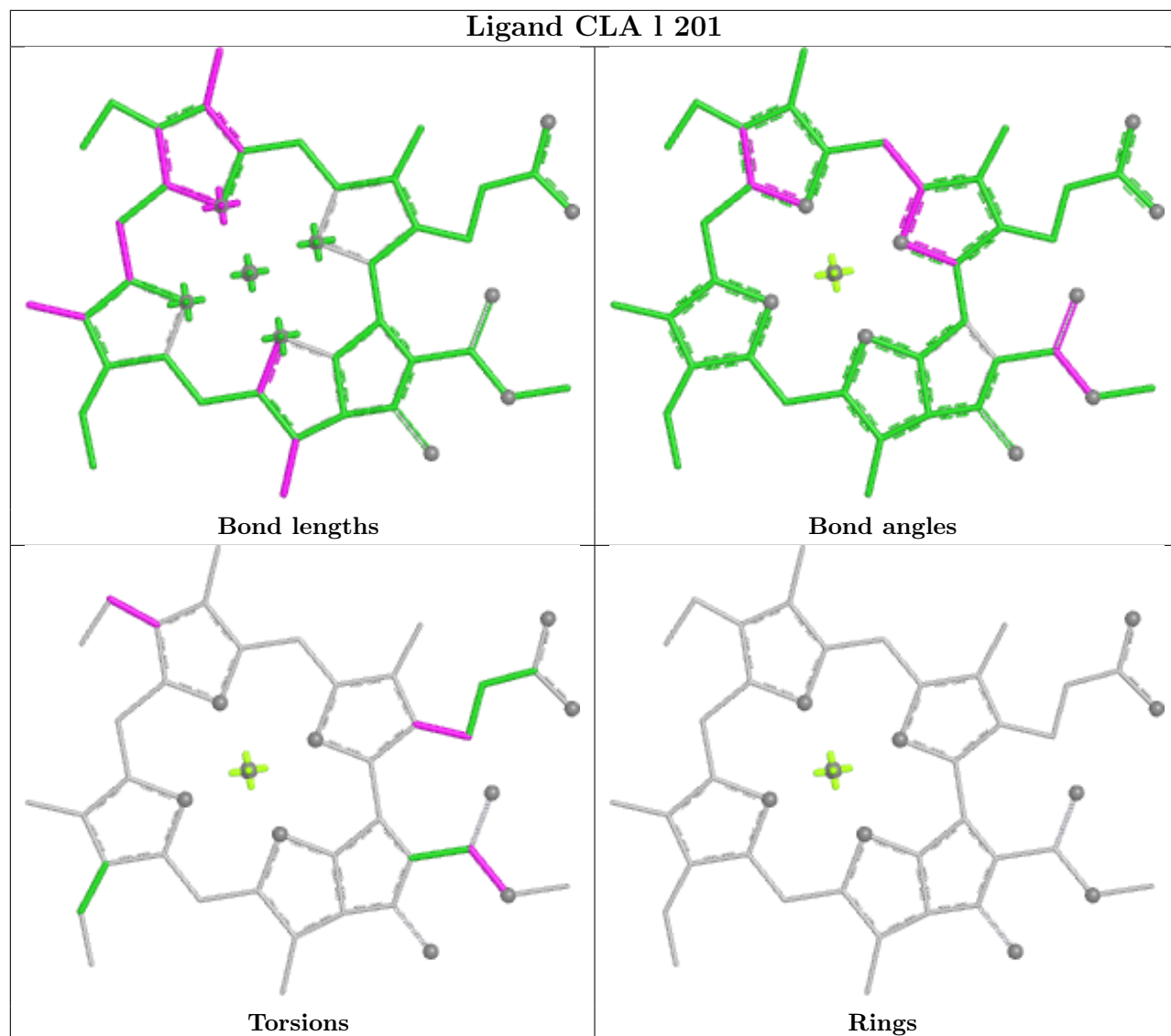


Torsions

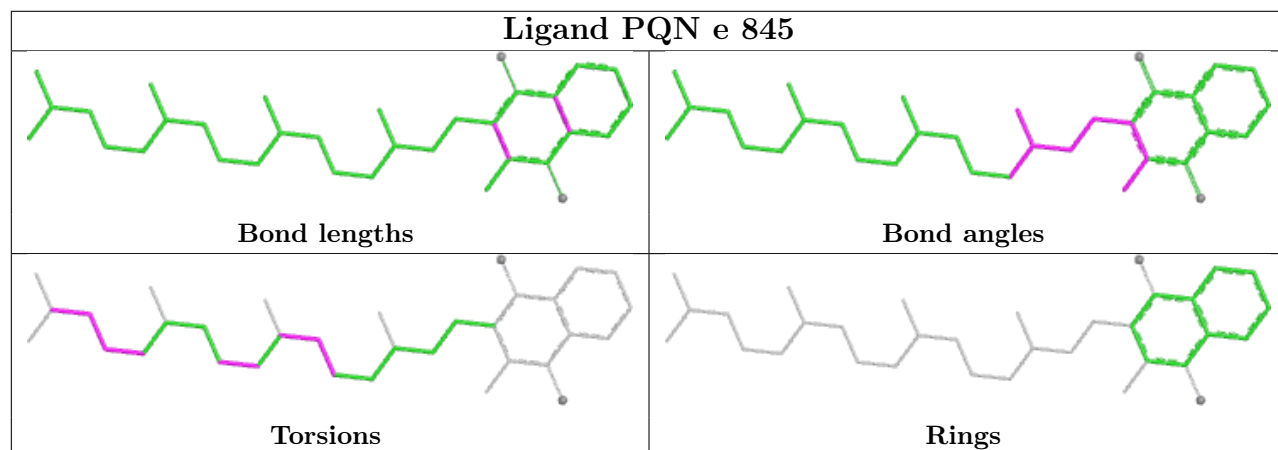


Rings

## Ligand CLA 1 201

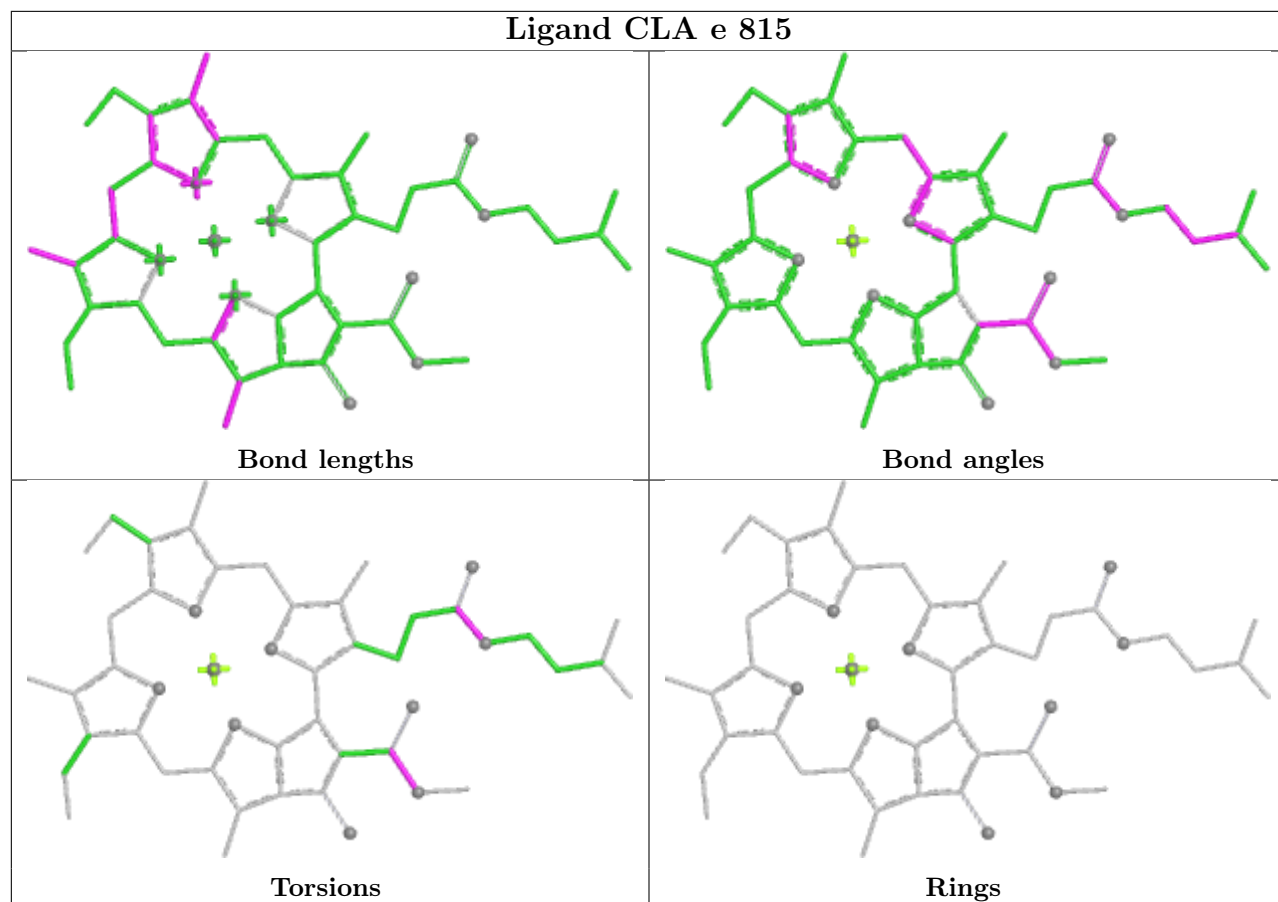


## Ligand PQN e 845

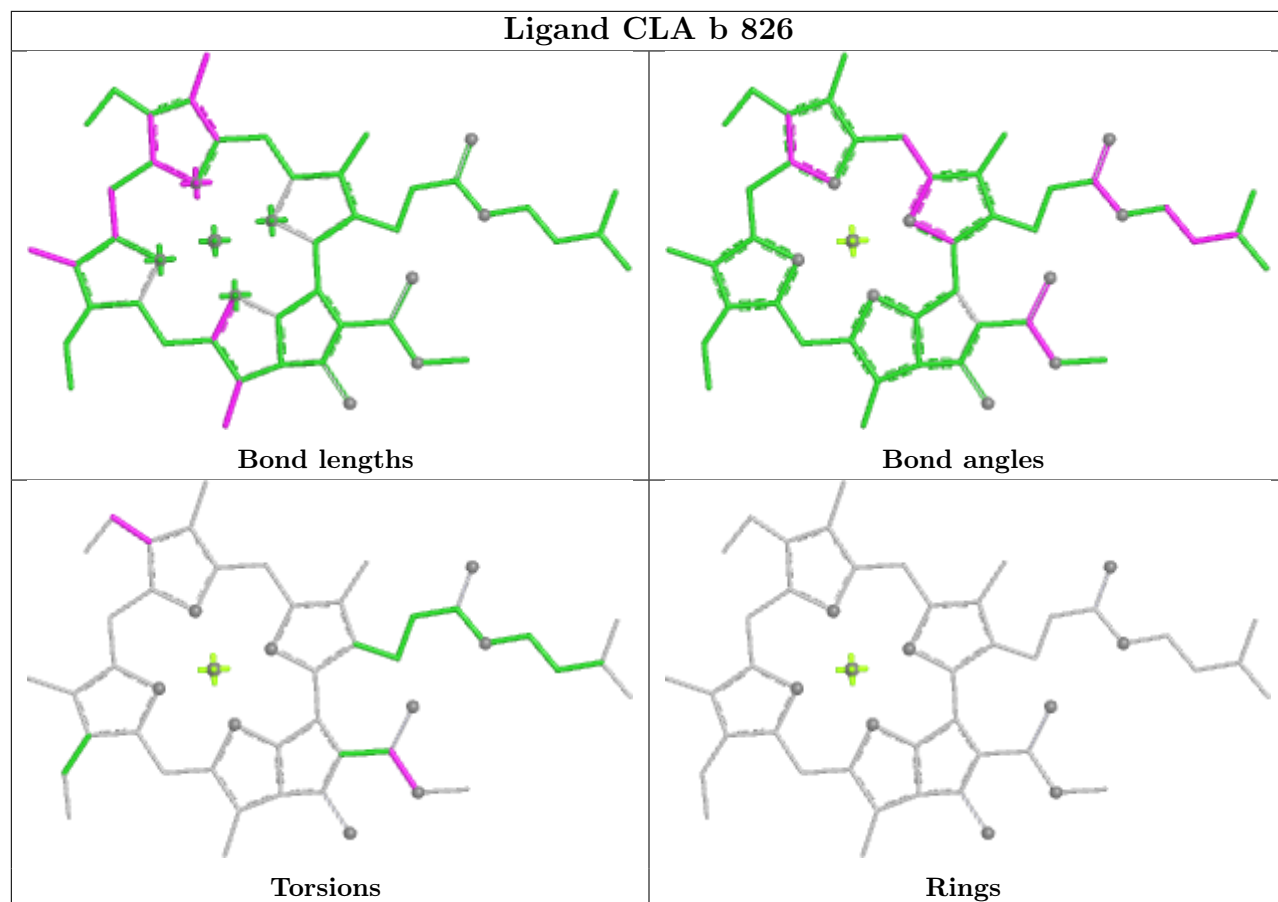




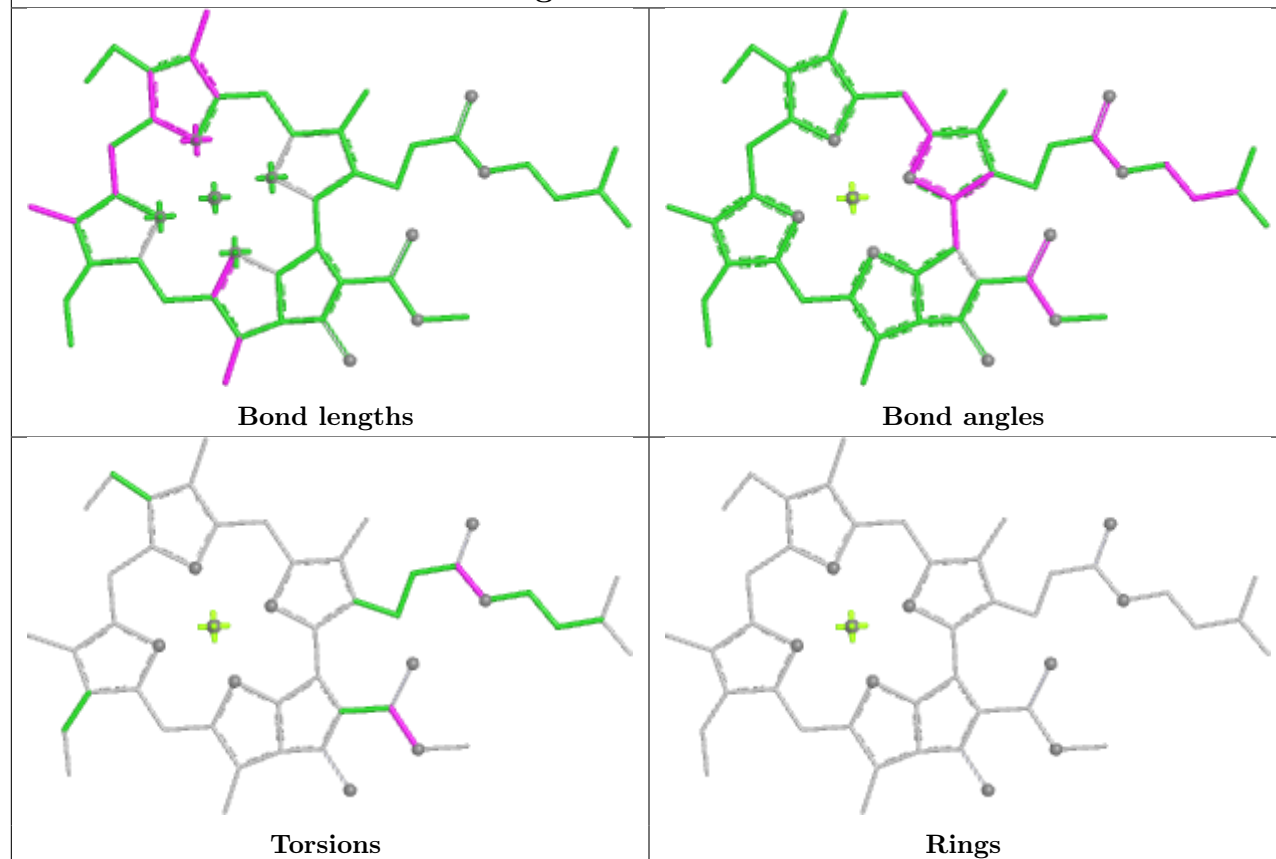
## Ligand CLA e 815



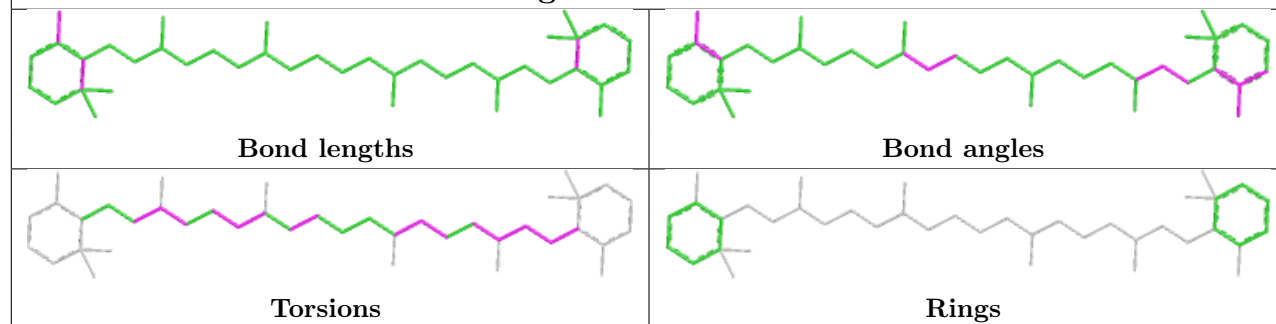
## Ligand CLA b 826

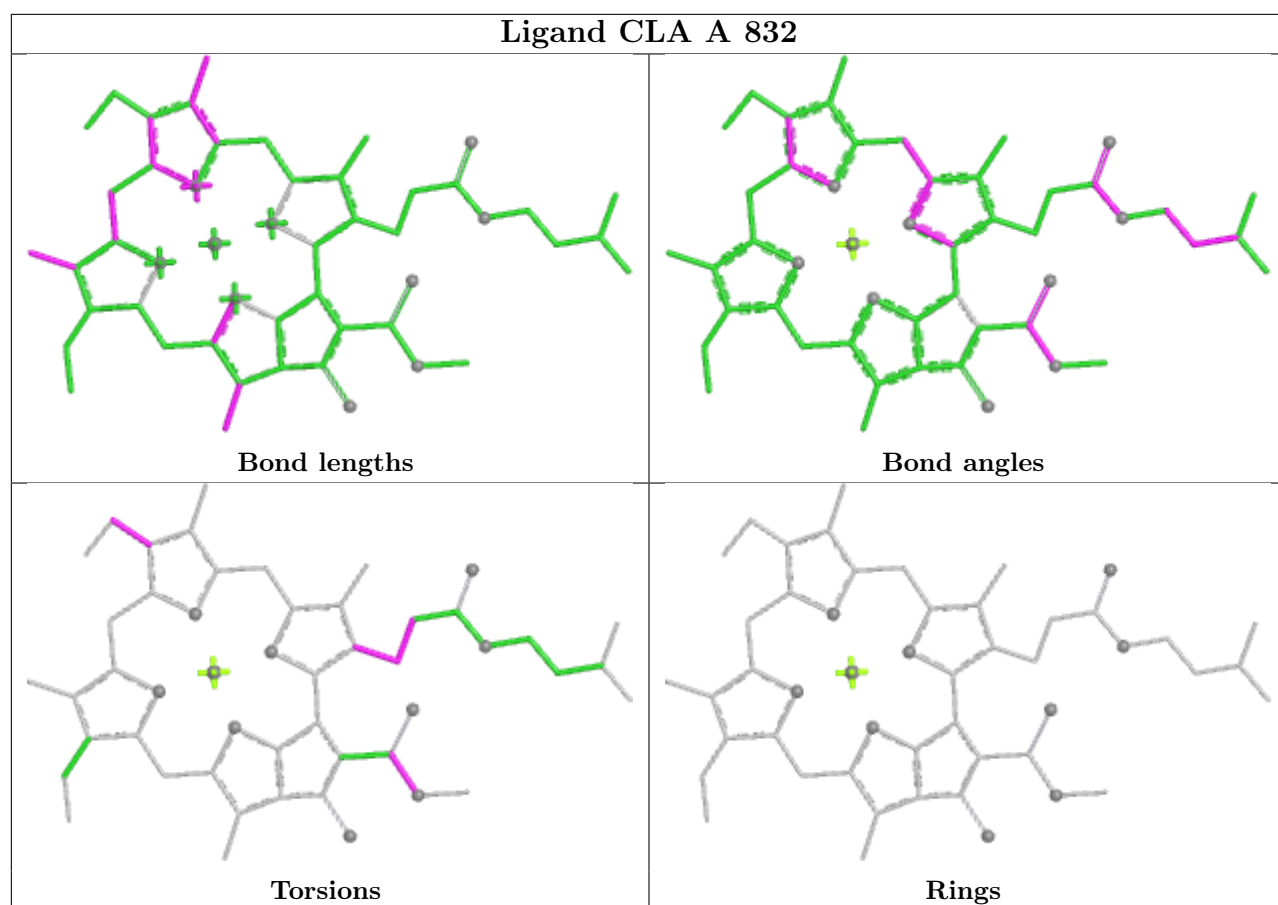


## Ligand CLA b 832

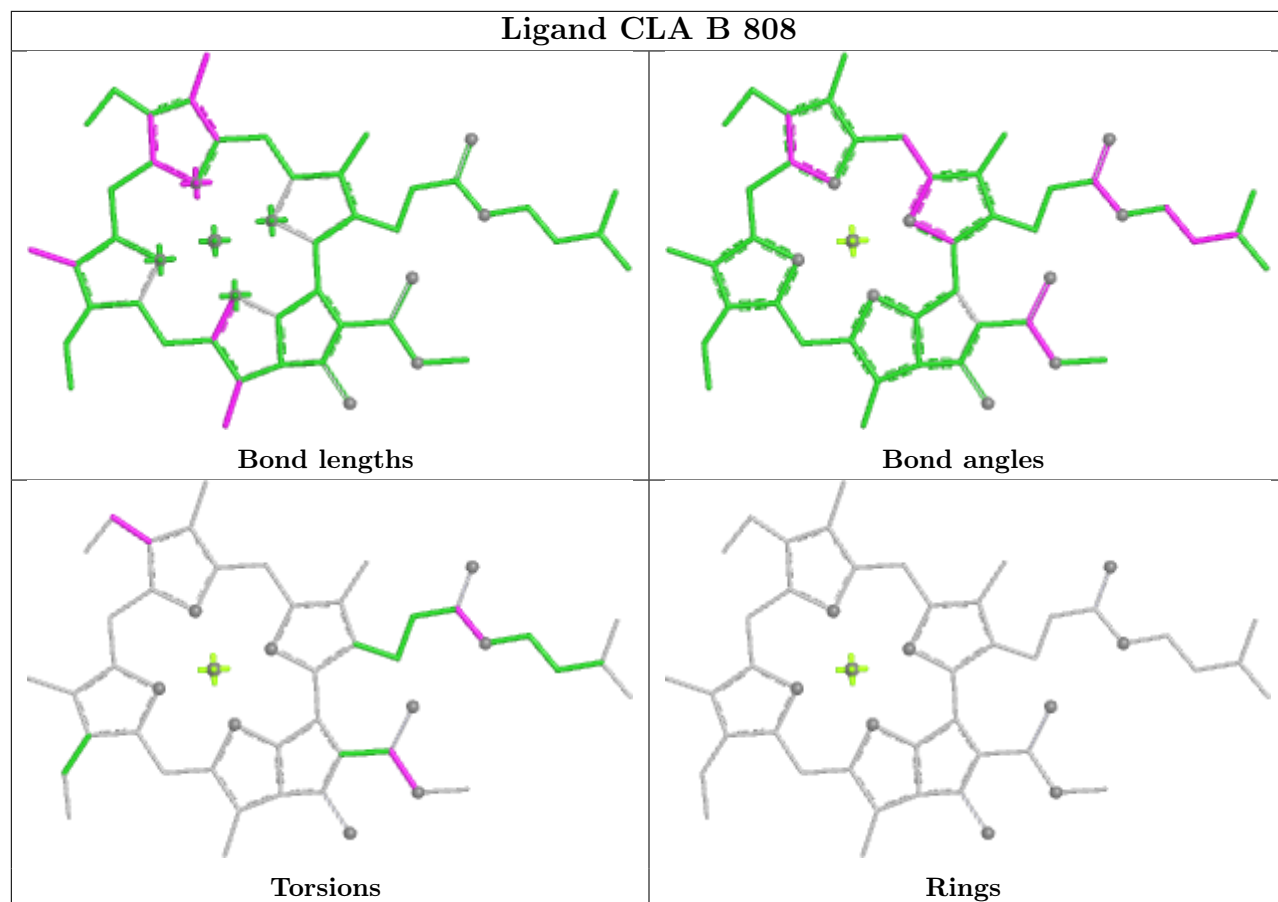


## Ligand BCR 1 206

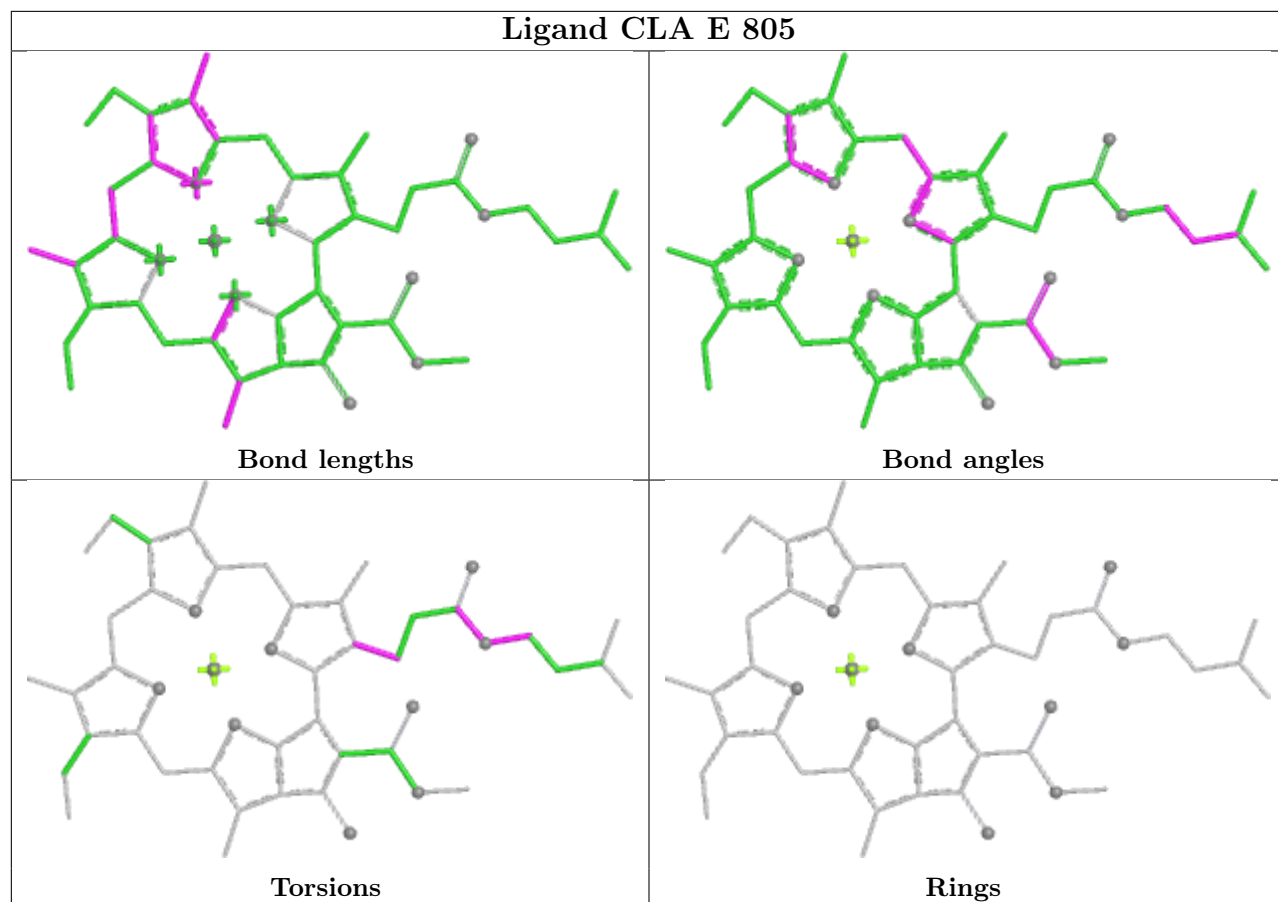


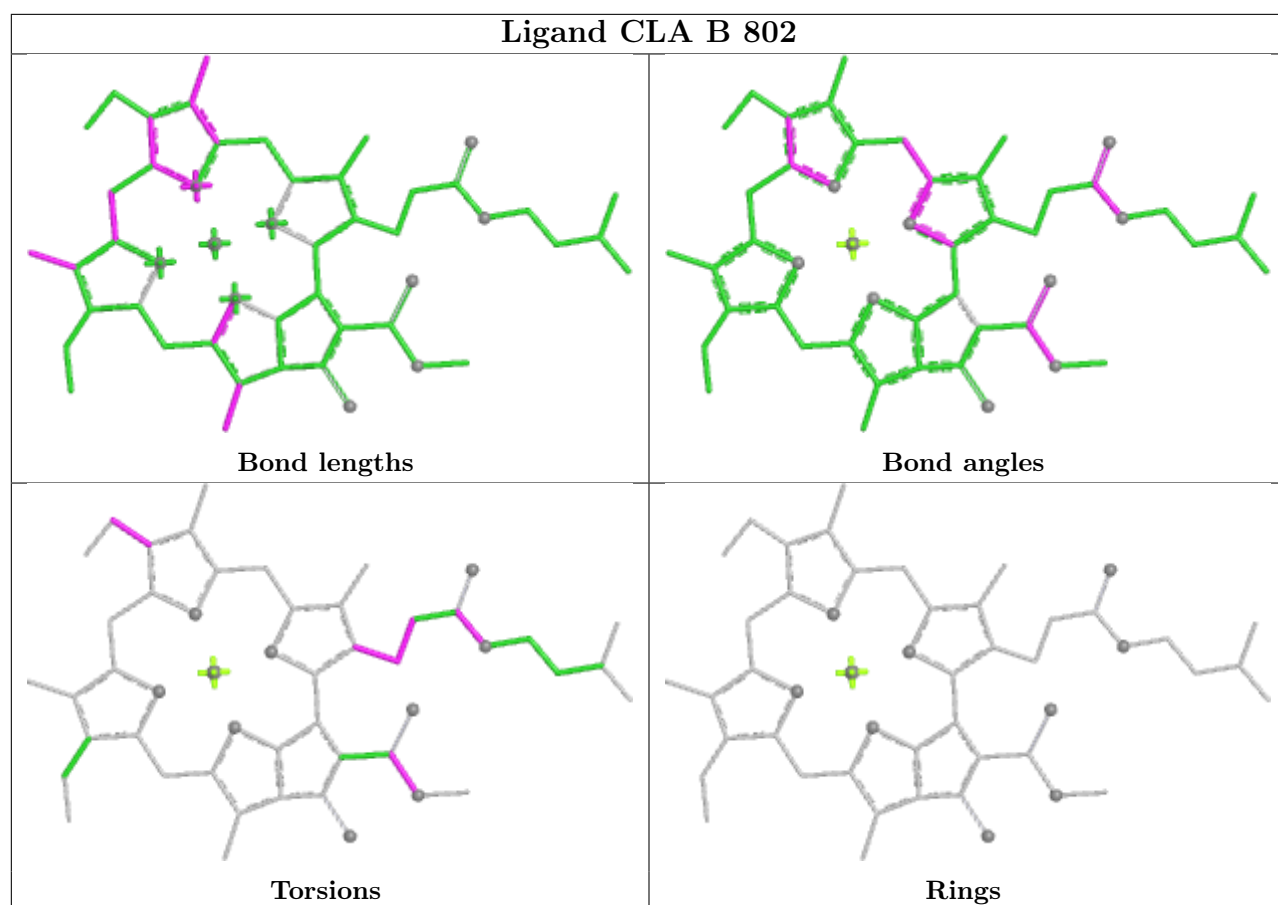


## Ligand CLA B 808

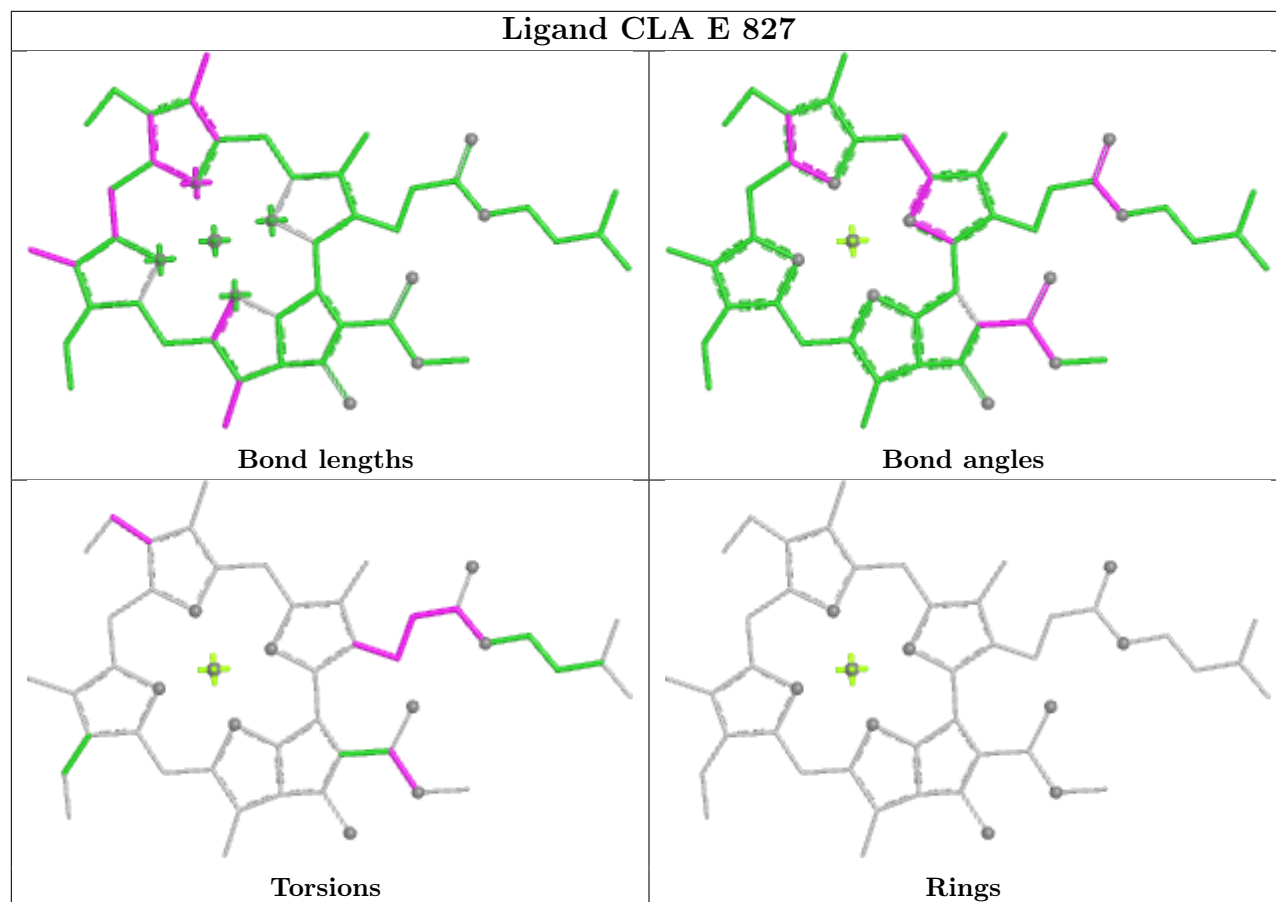


## Ligand CLA E 805



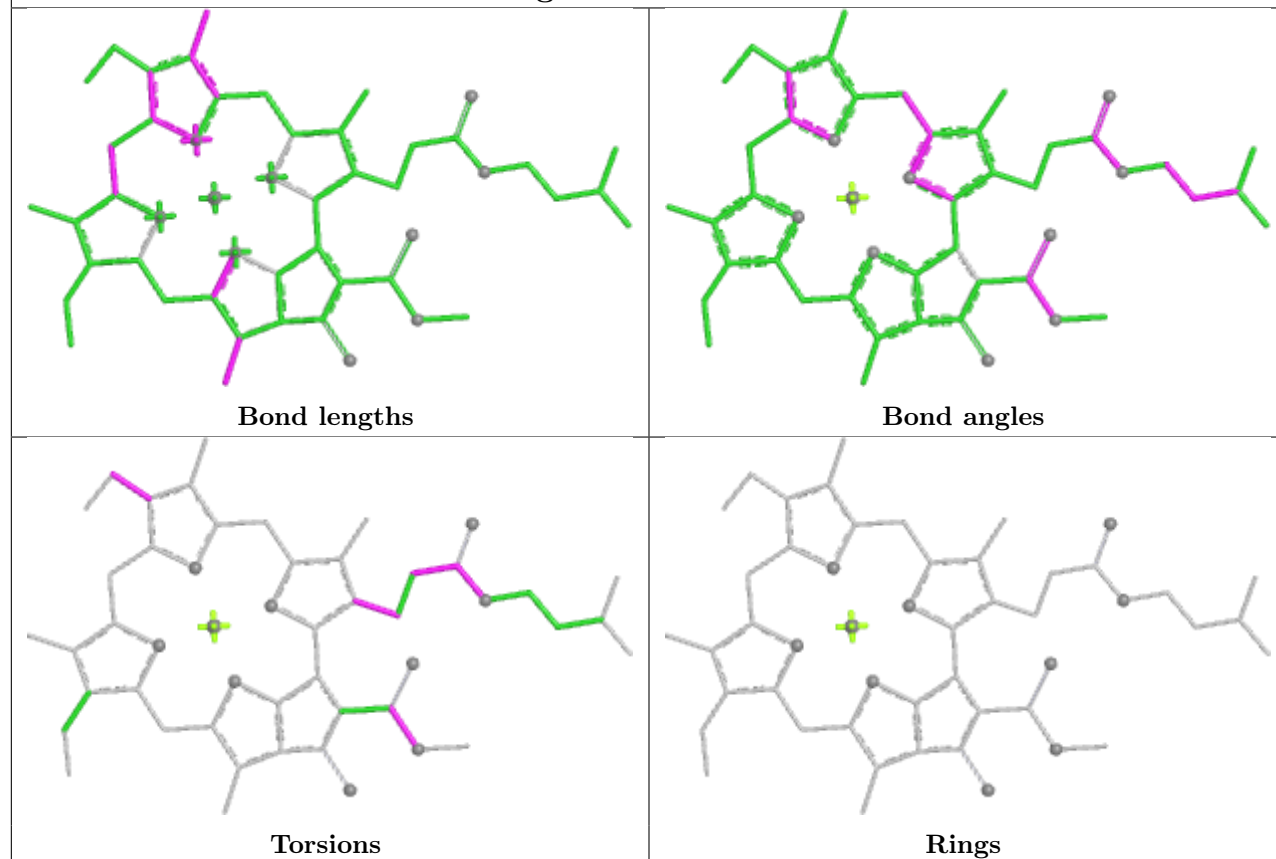


## Ligand CLA E 827

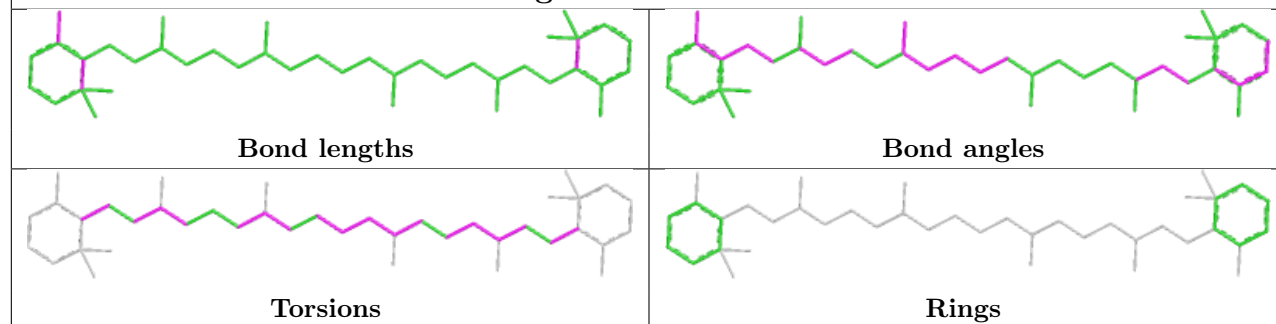




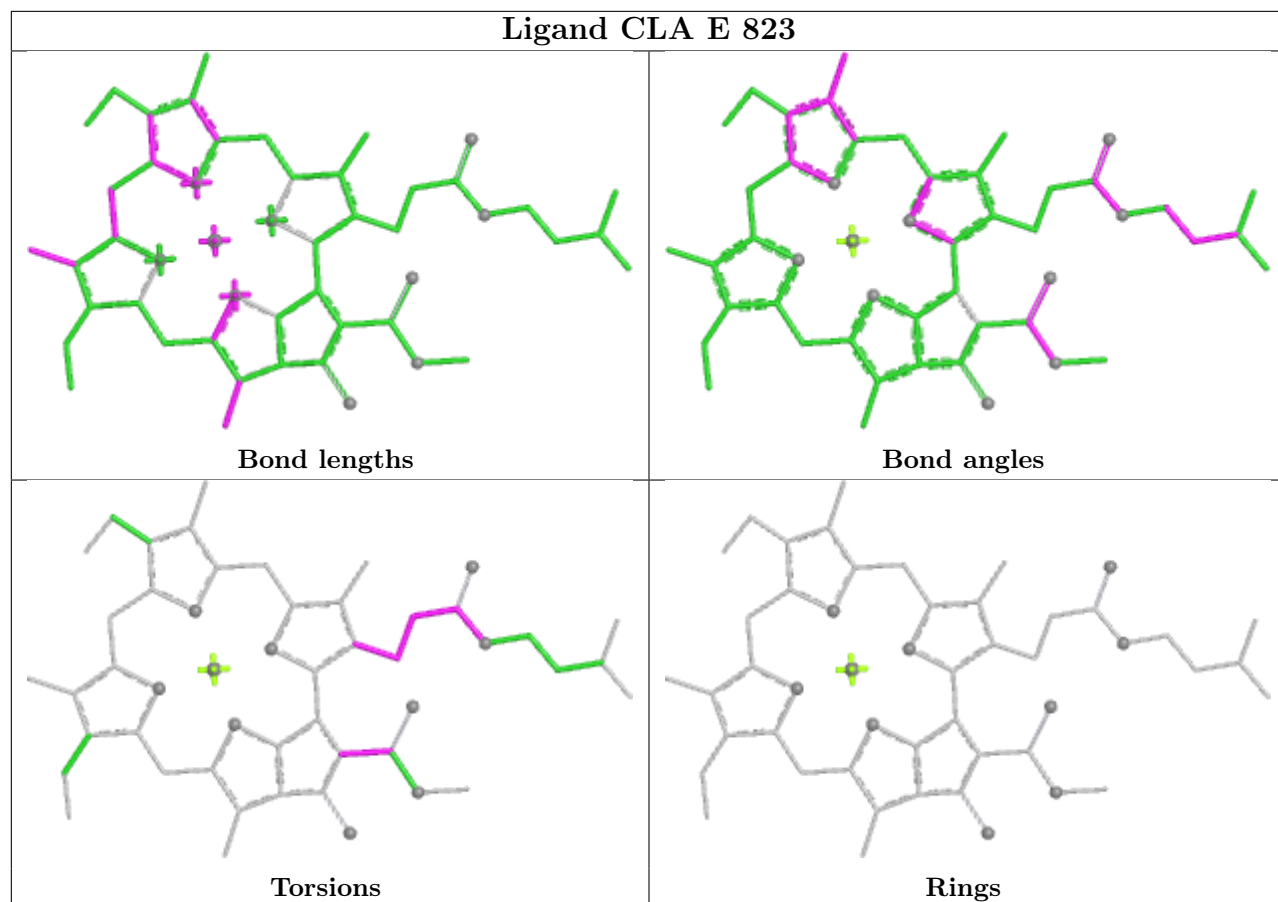
## Ligand CLA a 824

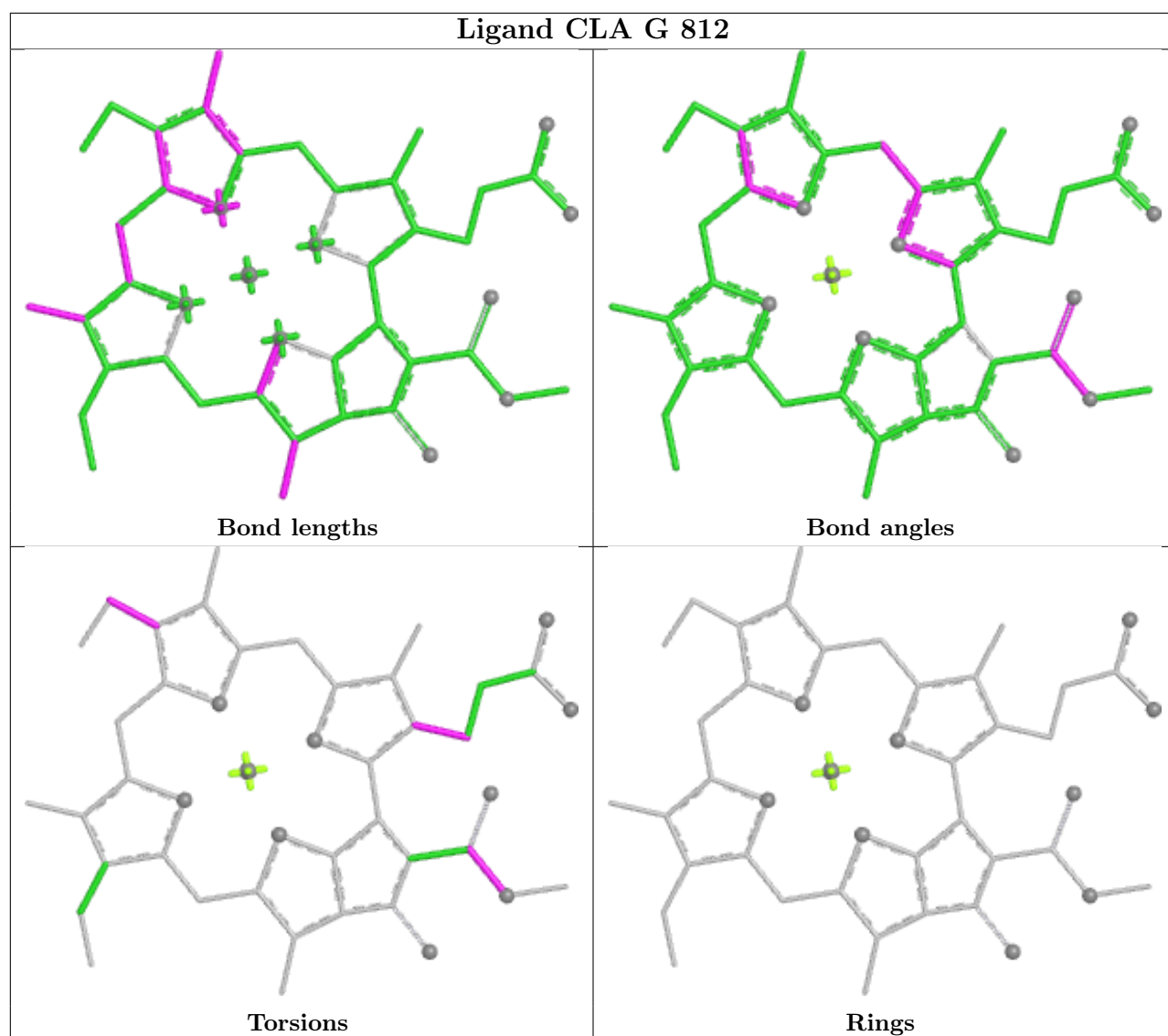


## Ligand BCR e 849

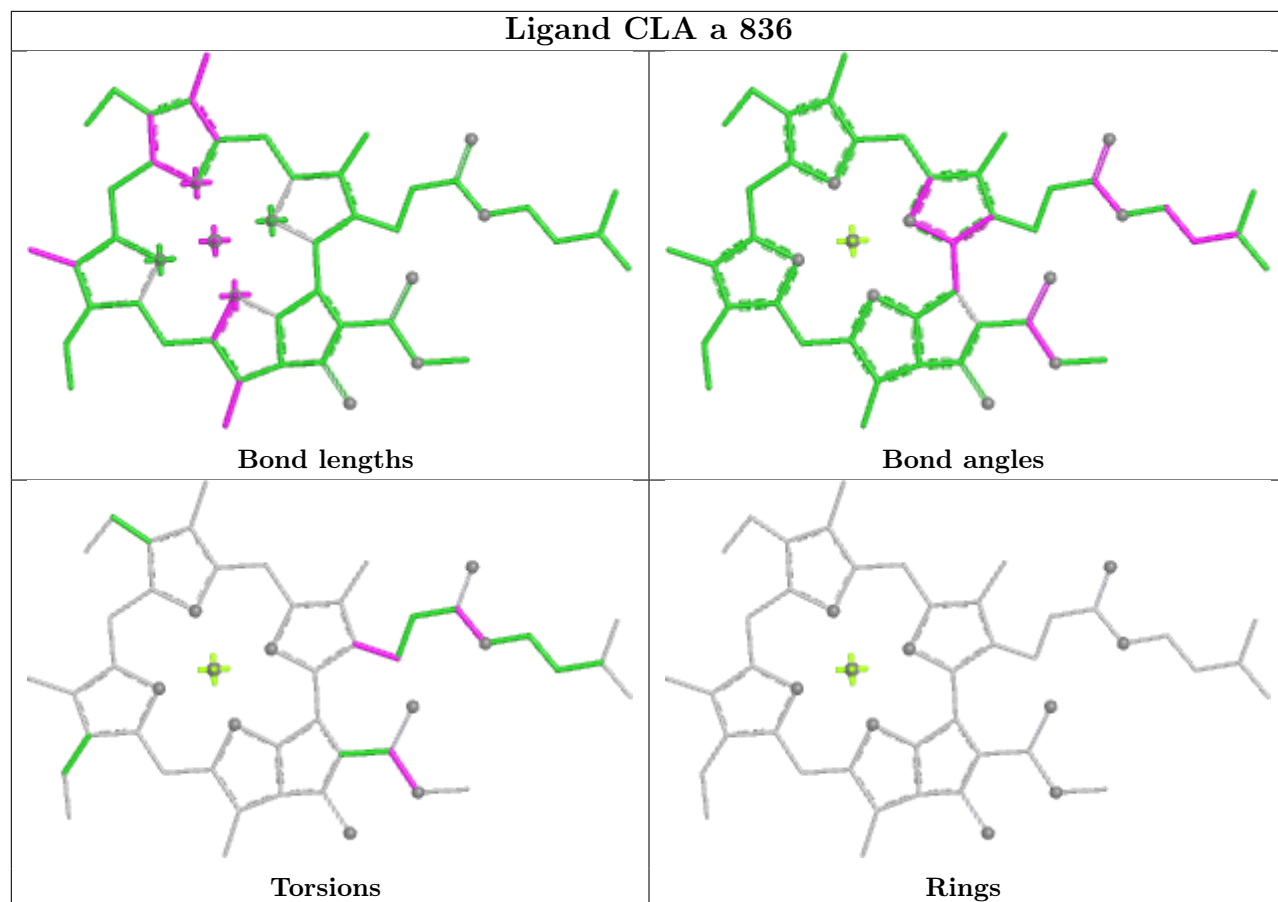


## Ligand CLA E 823

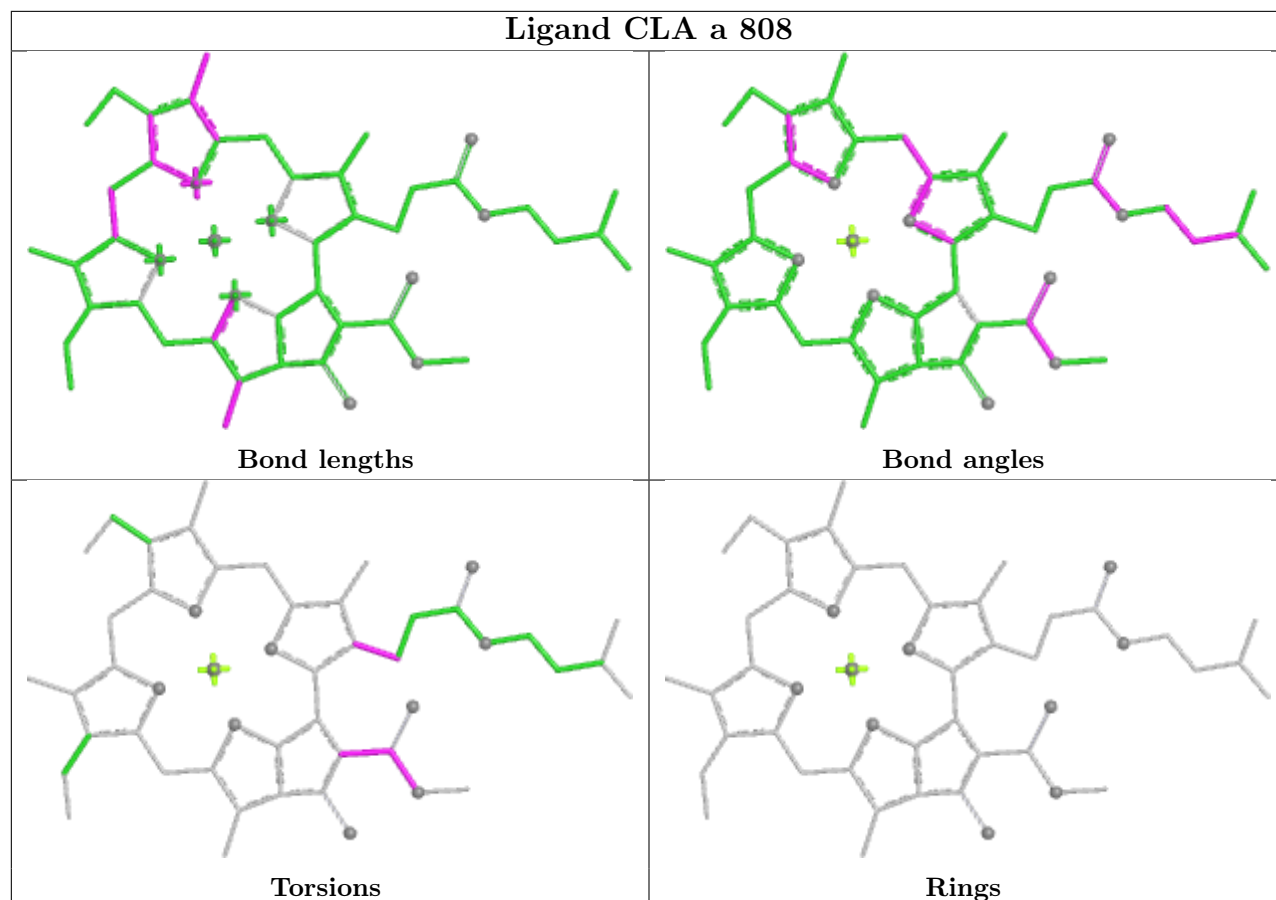




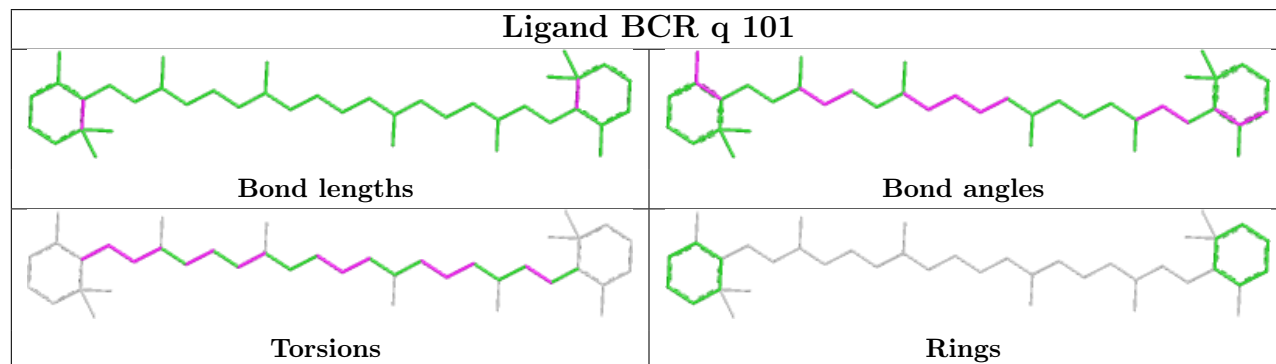
## Ligand CLA a 836



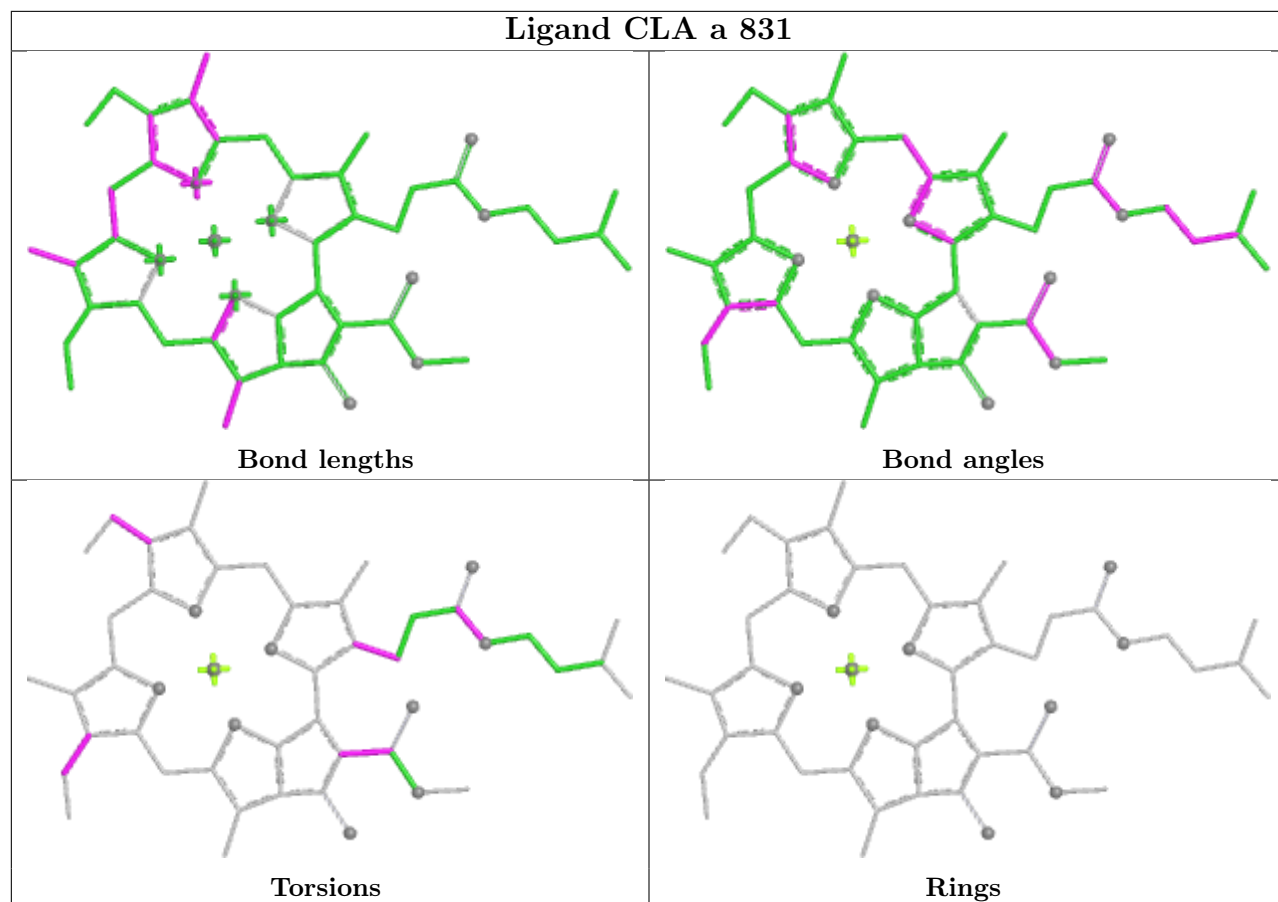
## Ligand CLA a 808



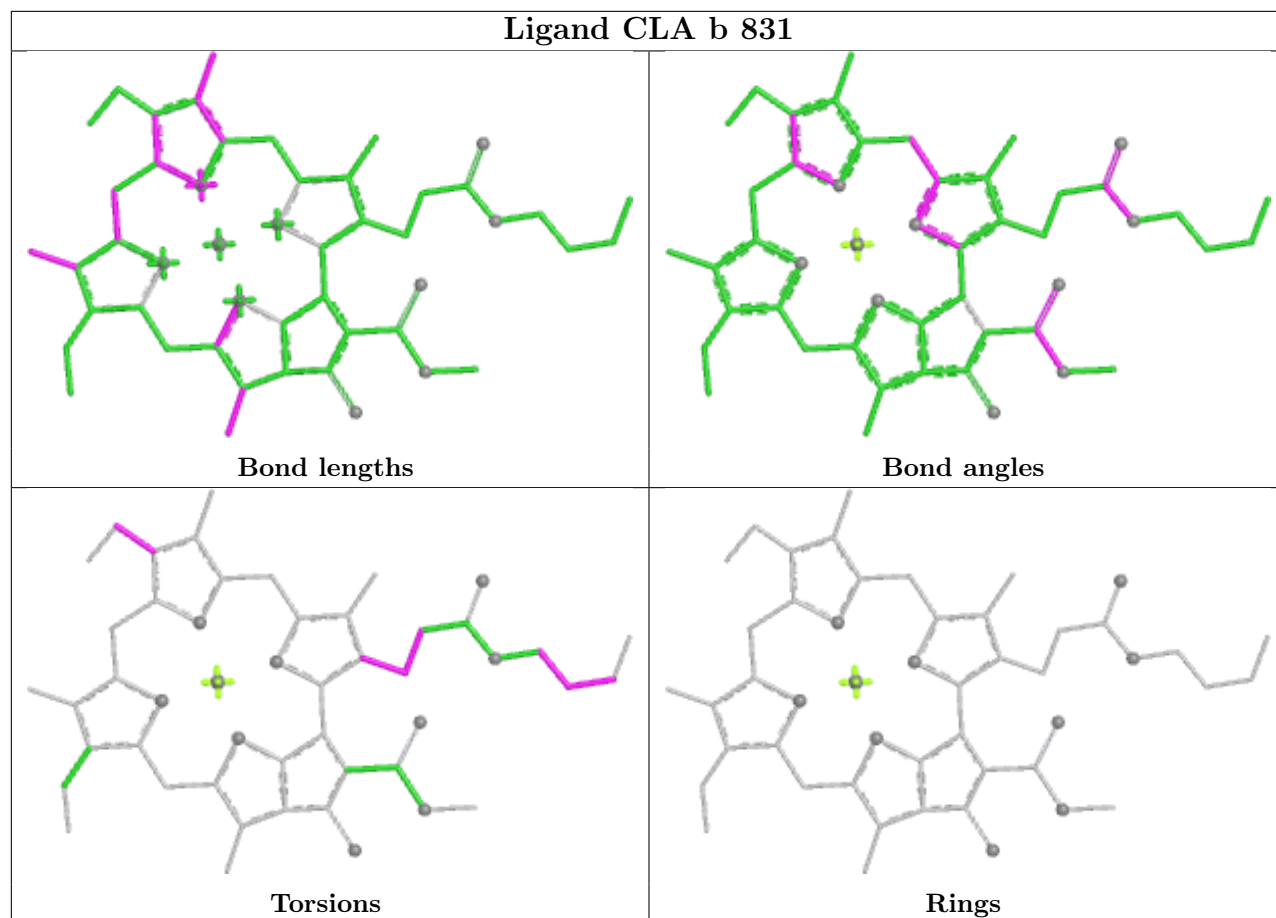
## Ligand BCR q 101



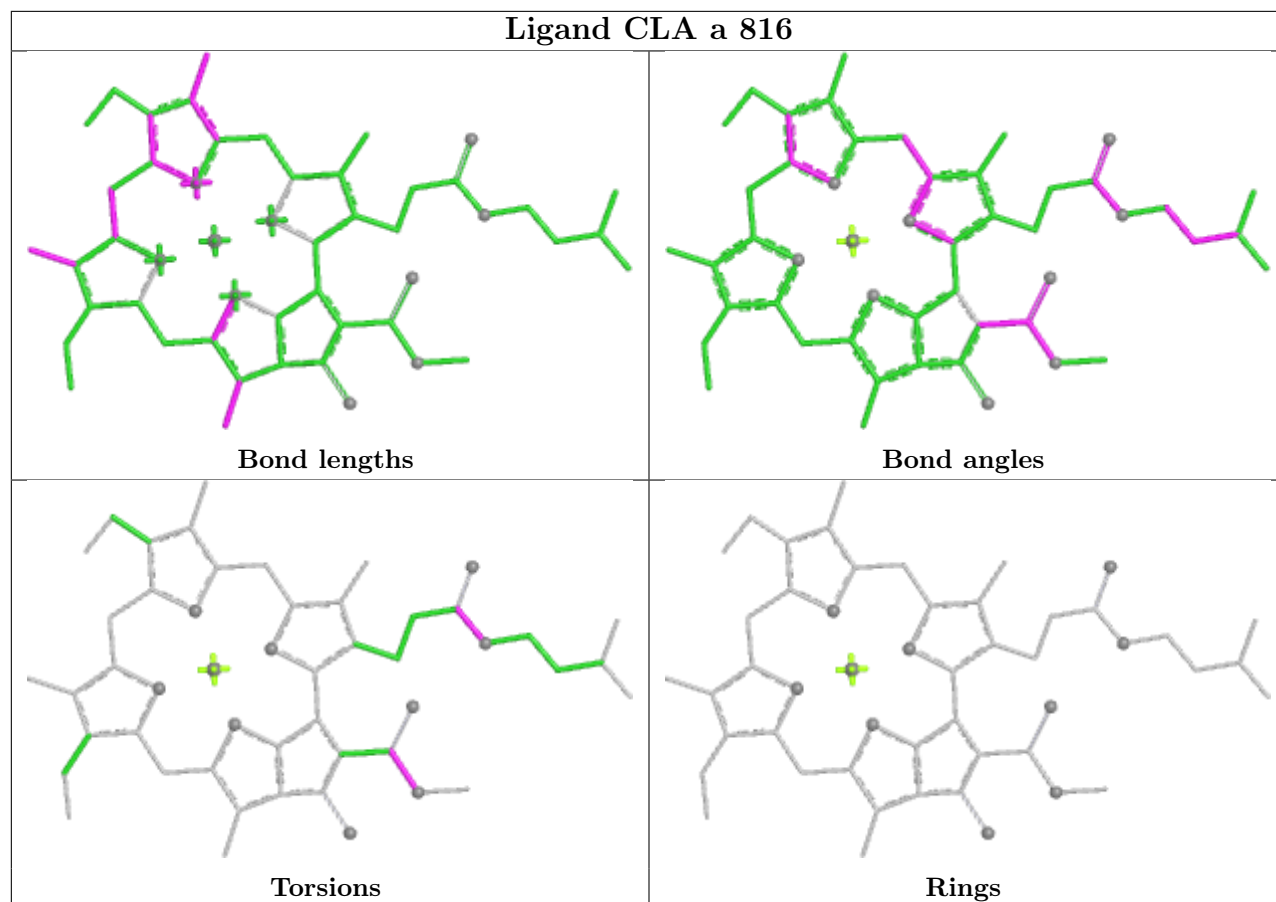
## Ligand CLA a 831



## Ligand CLA b 831

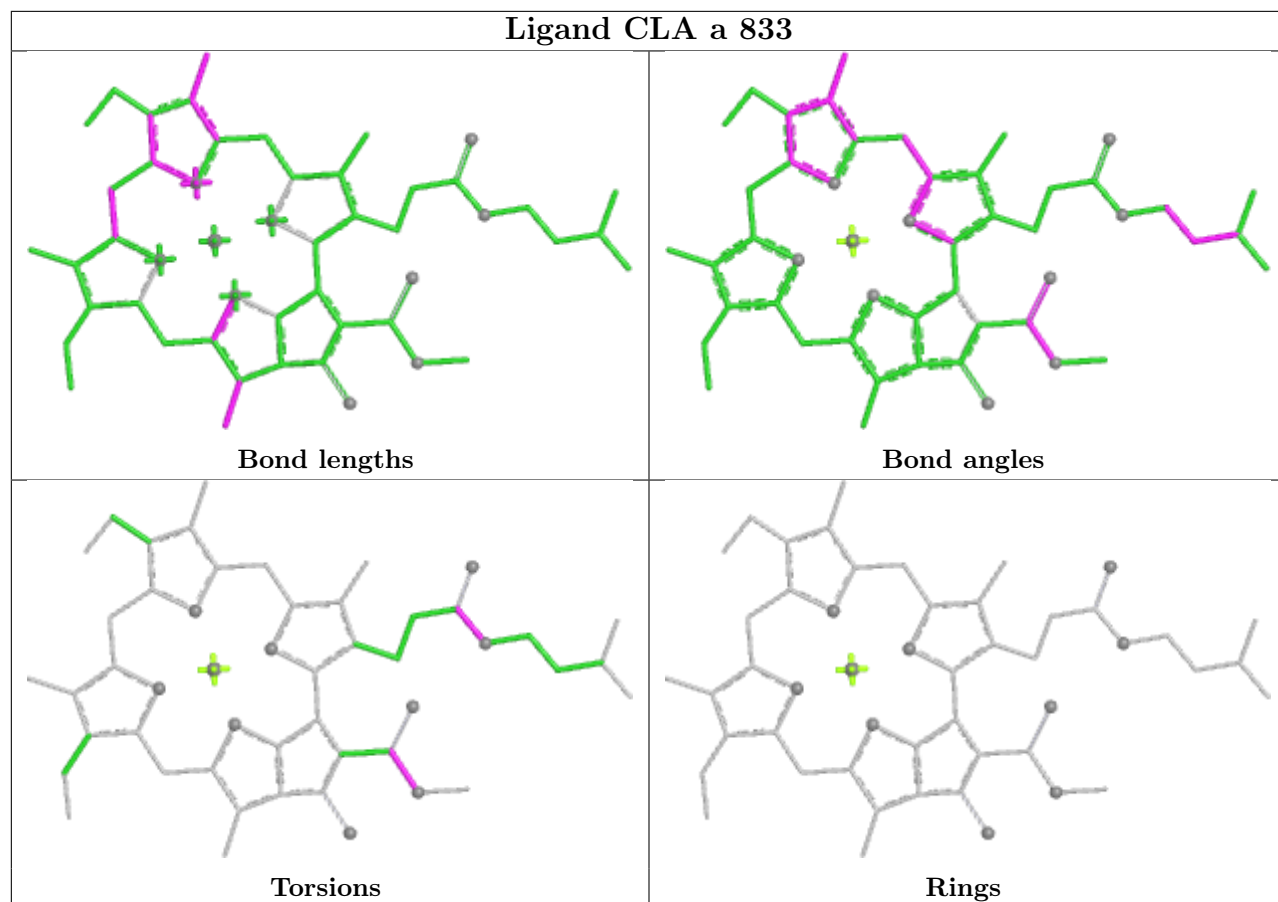


## Ligand CLA a 816

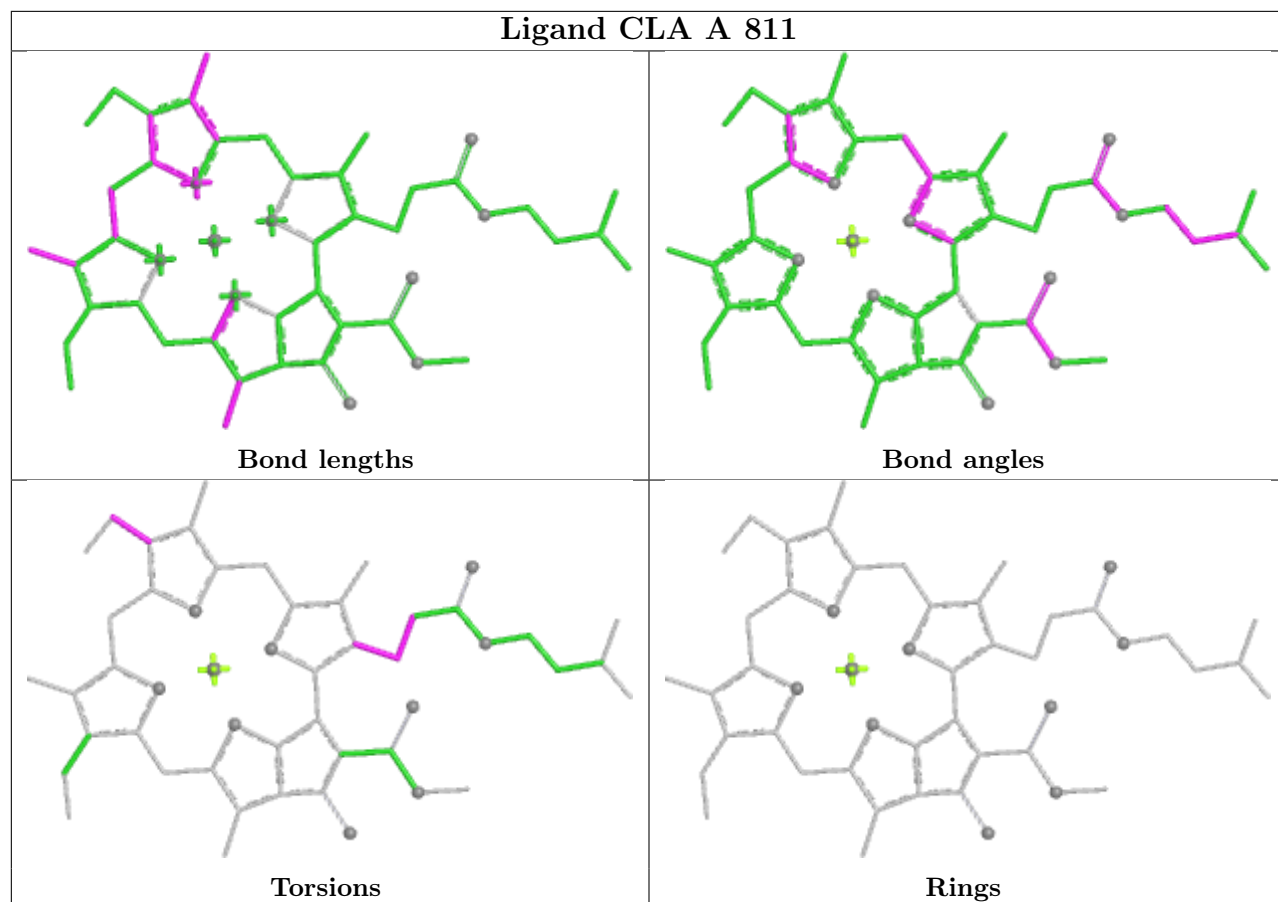


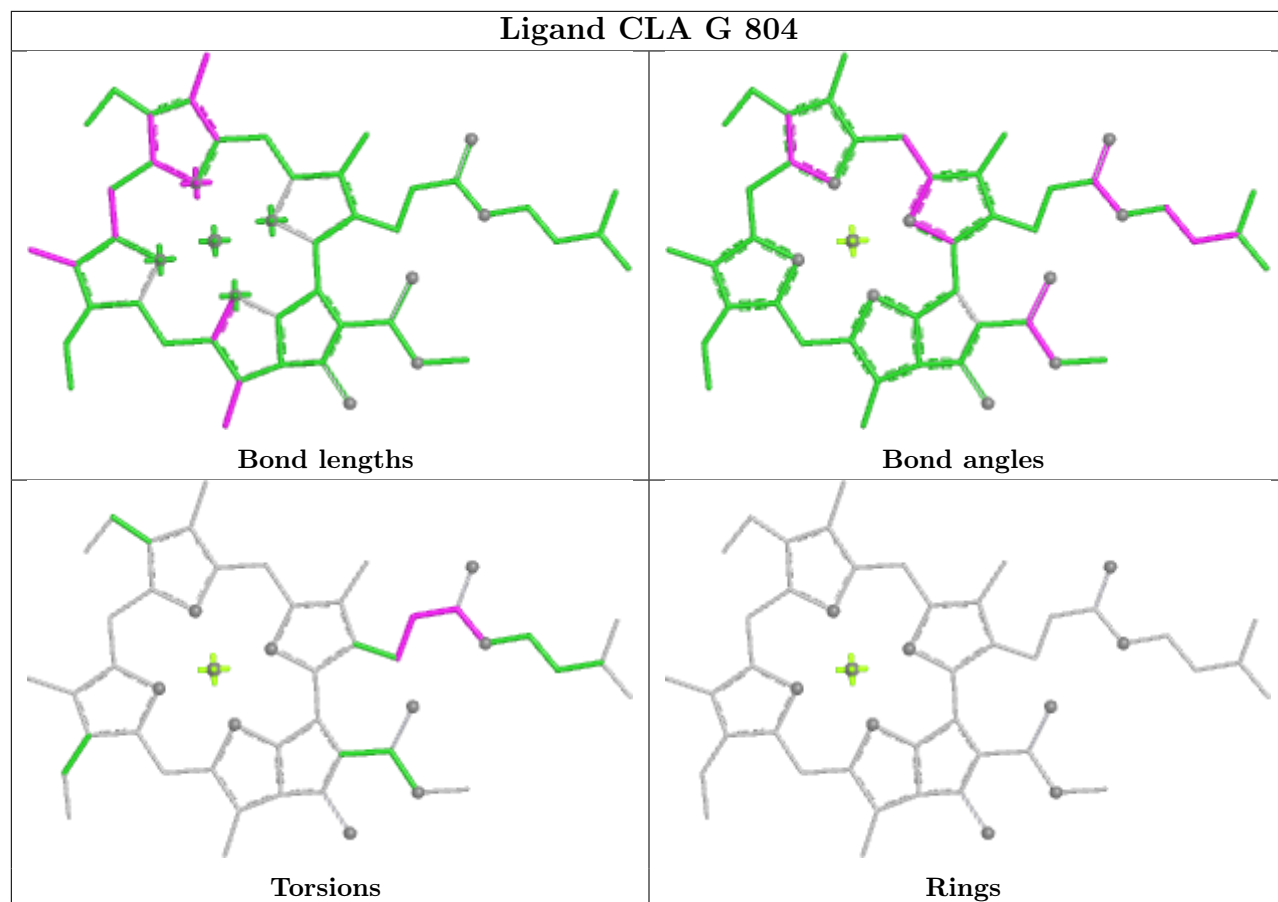


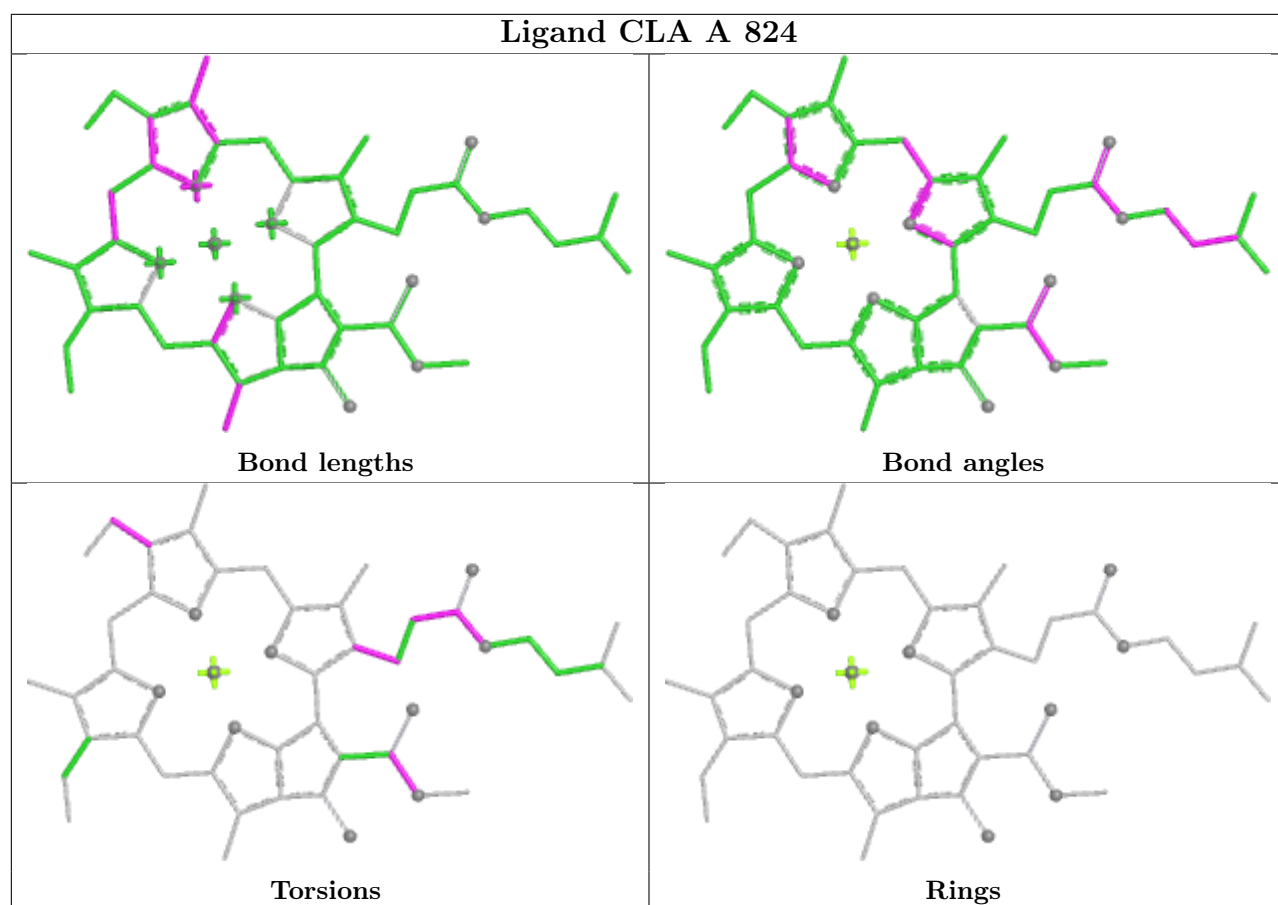
## Ligand CLA a 833

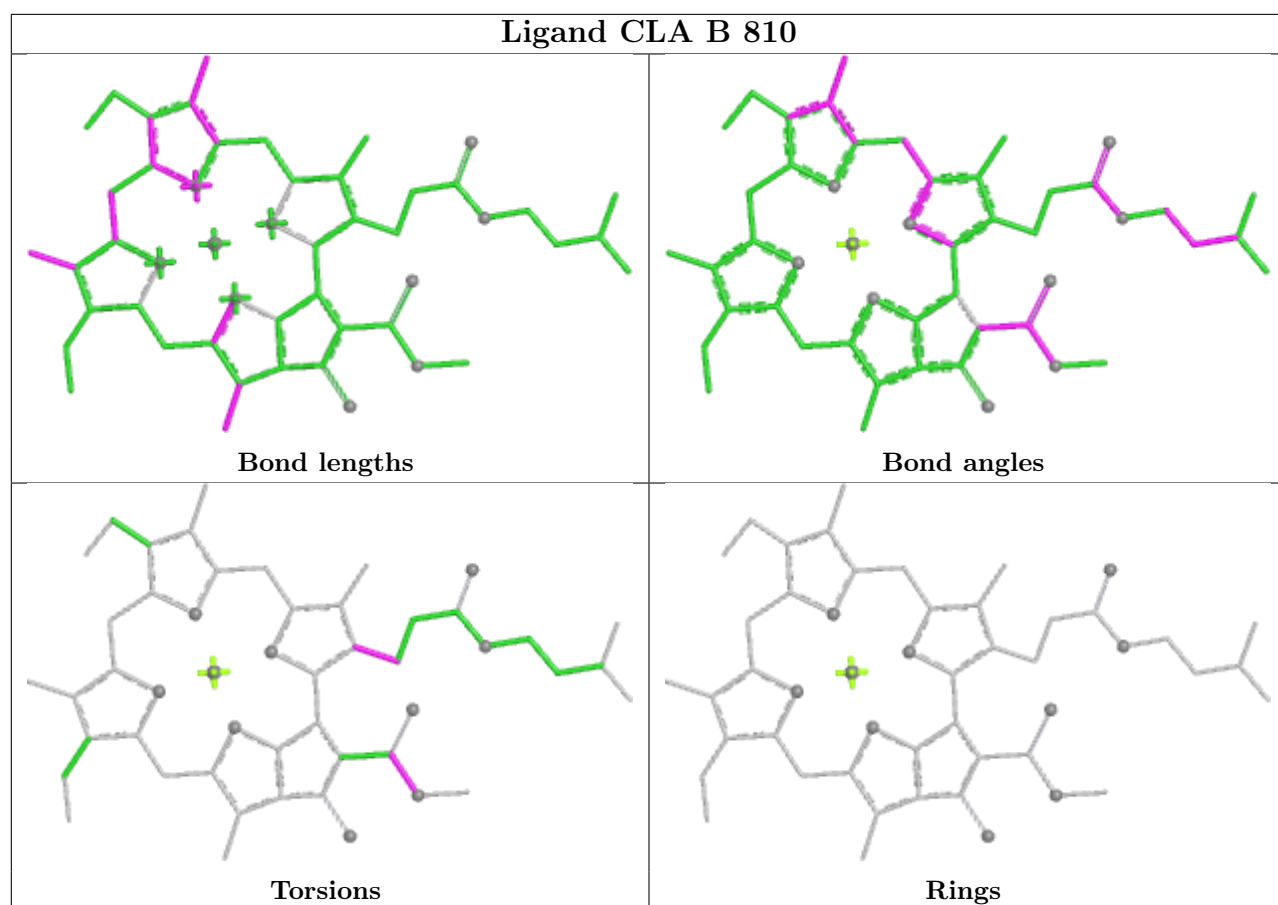


## Ligand CLA A 811

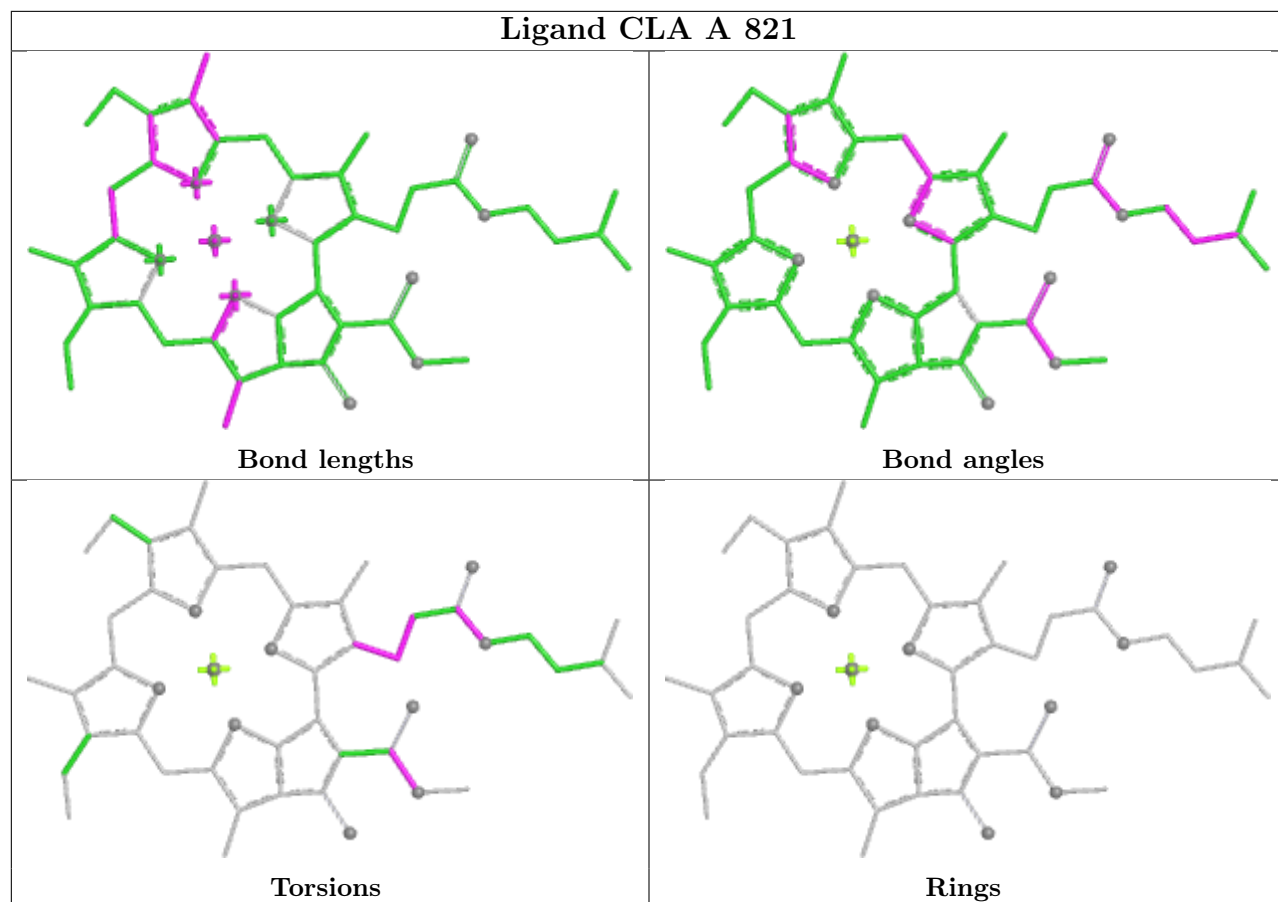




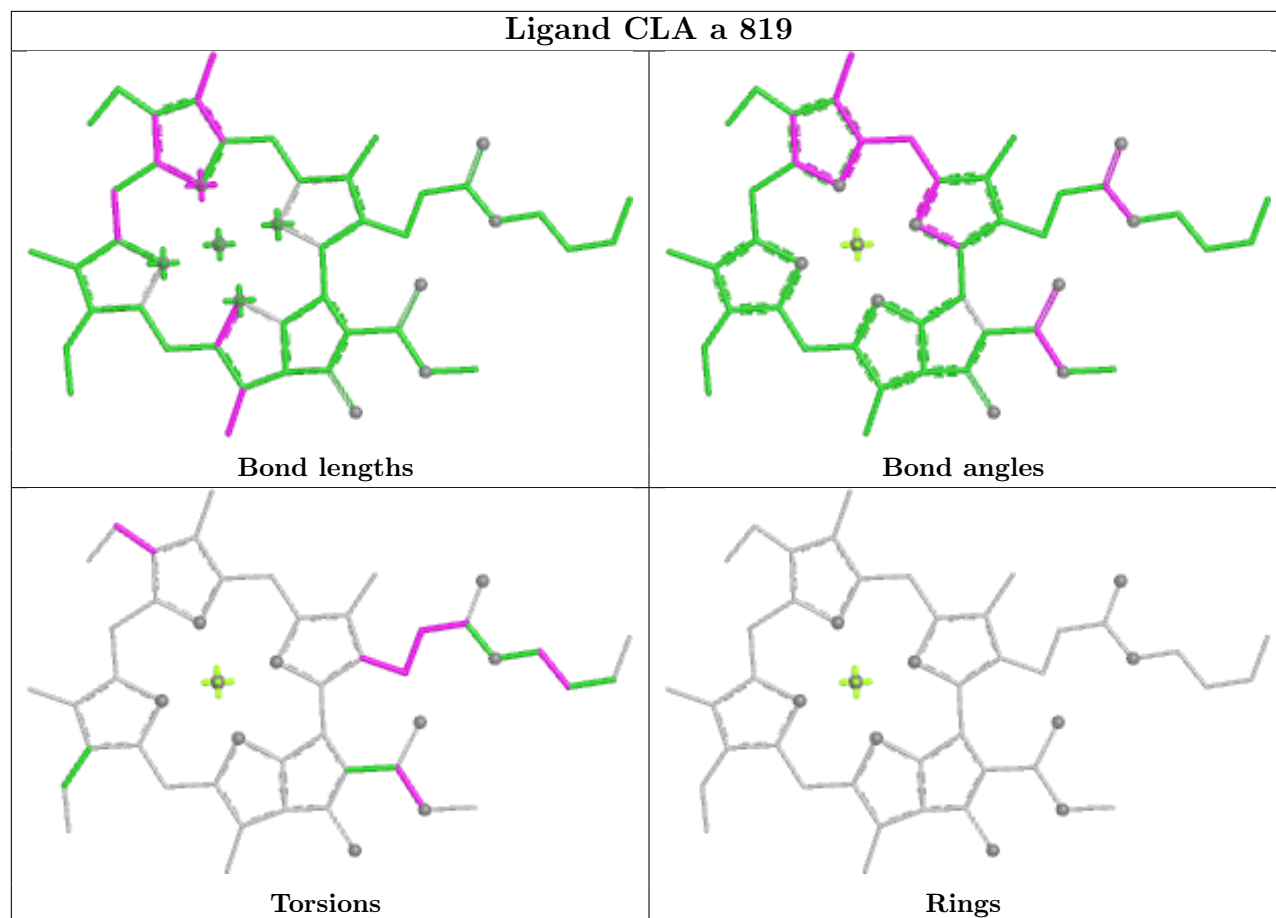




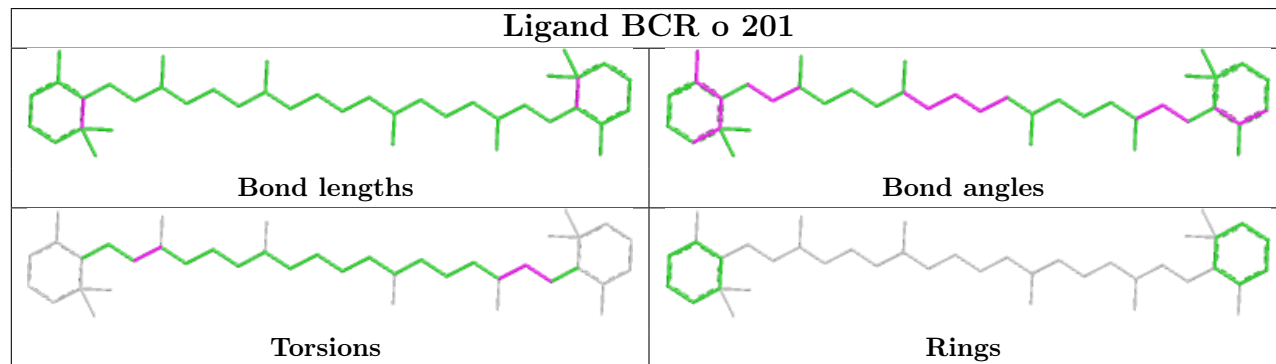
## Ligand CLA A 821



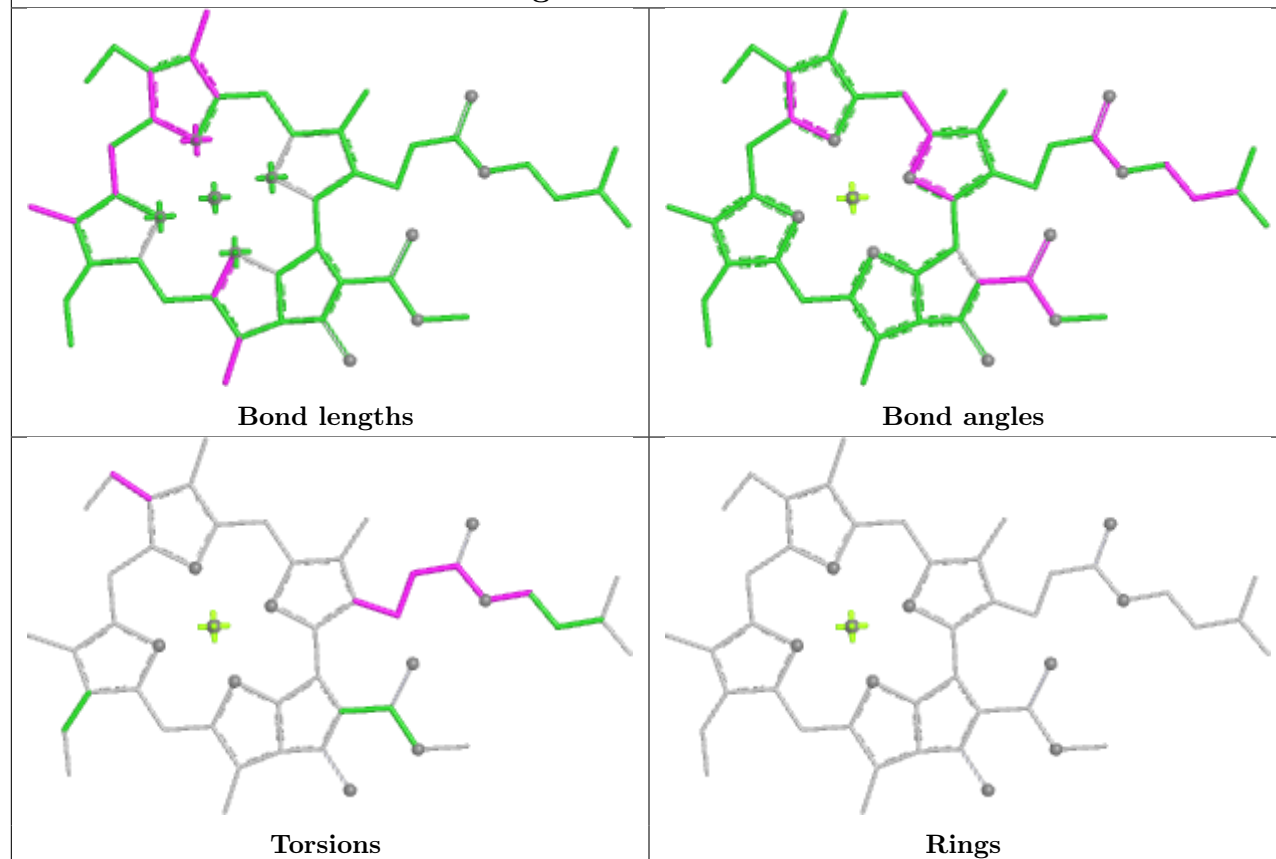
## Ligand CLA a 819



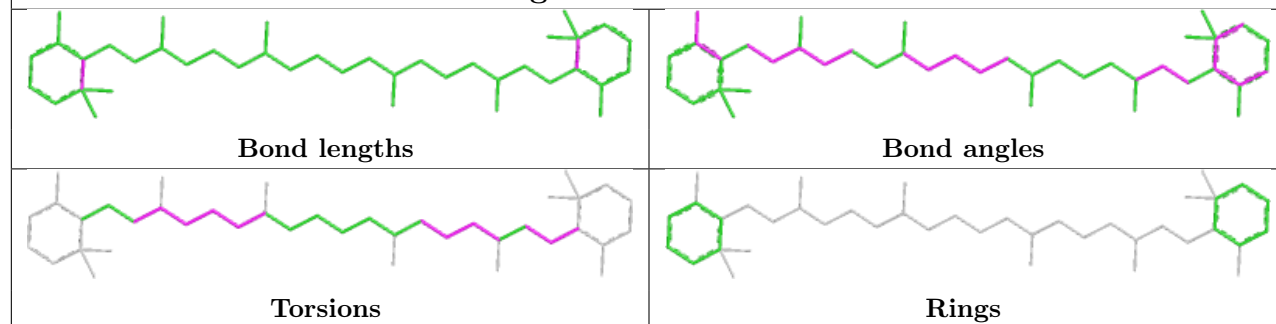
## Ligand BCR o 201



## Ligand CLA B 807

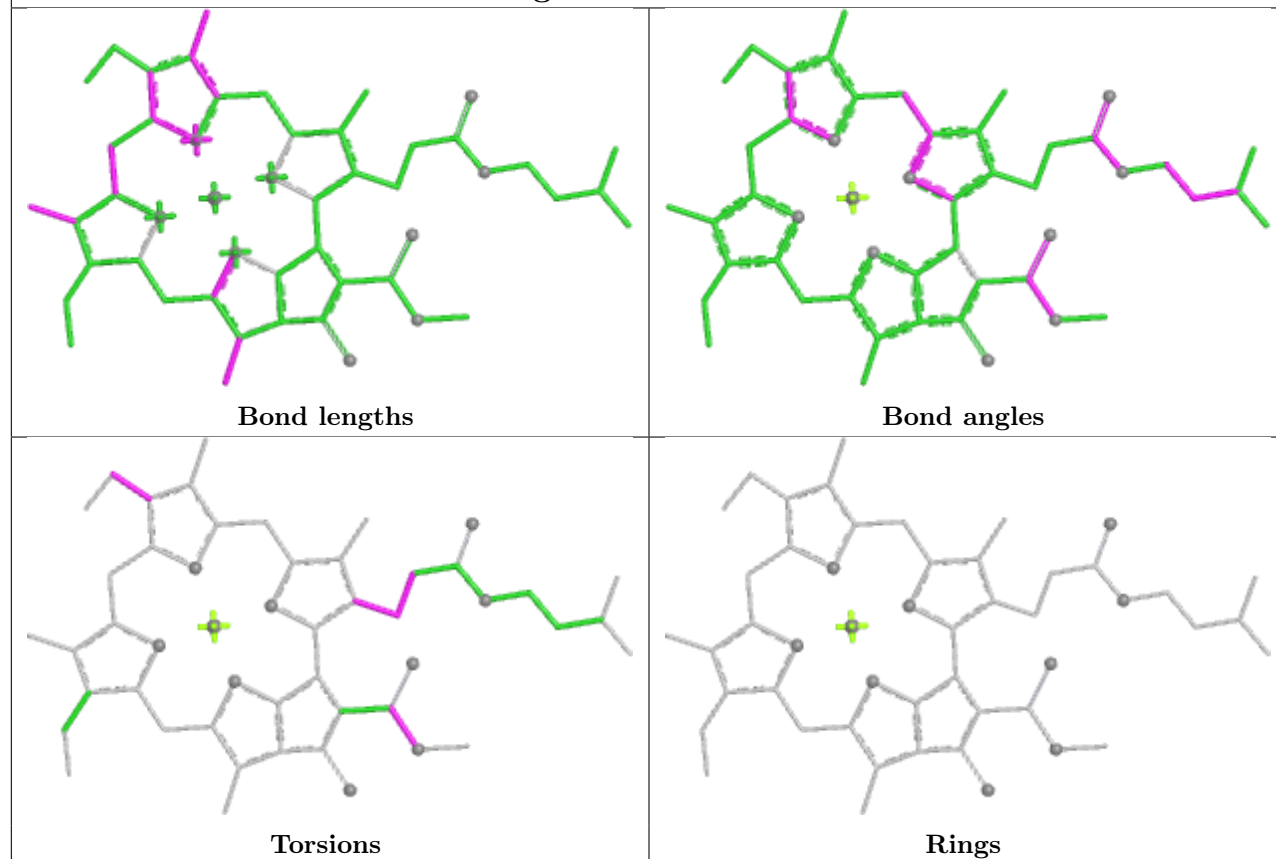


## Ligand BCR A 848

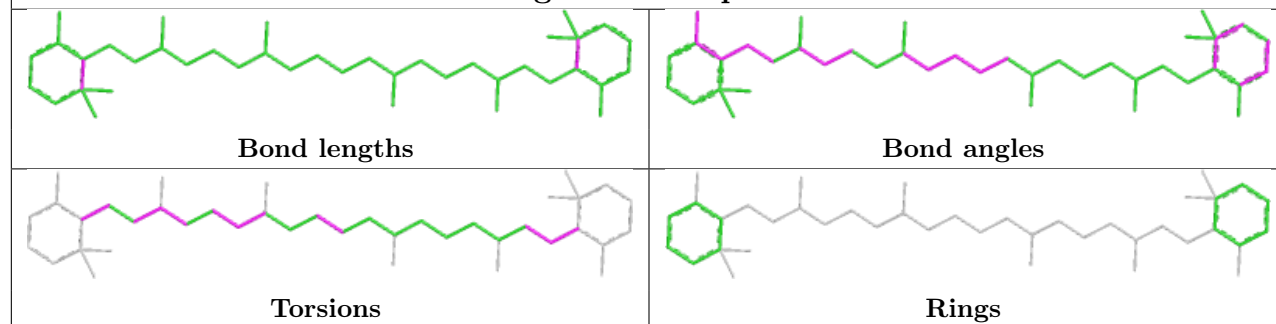




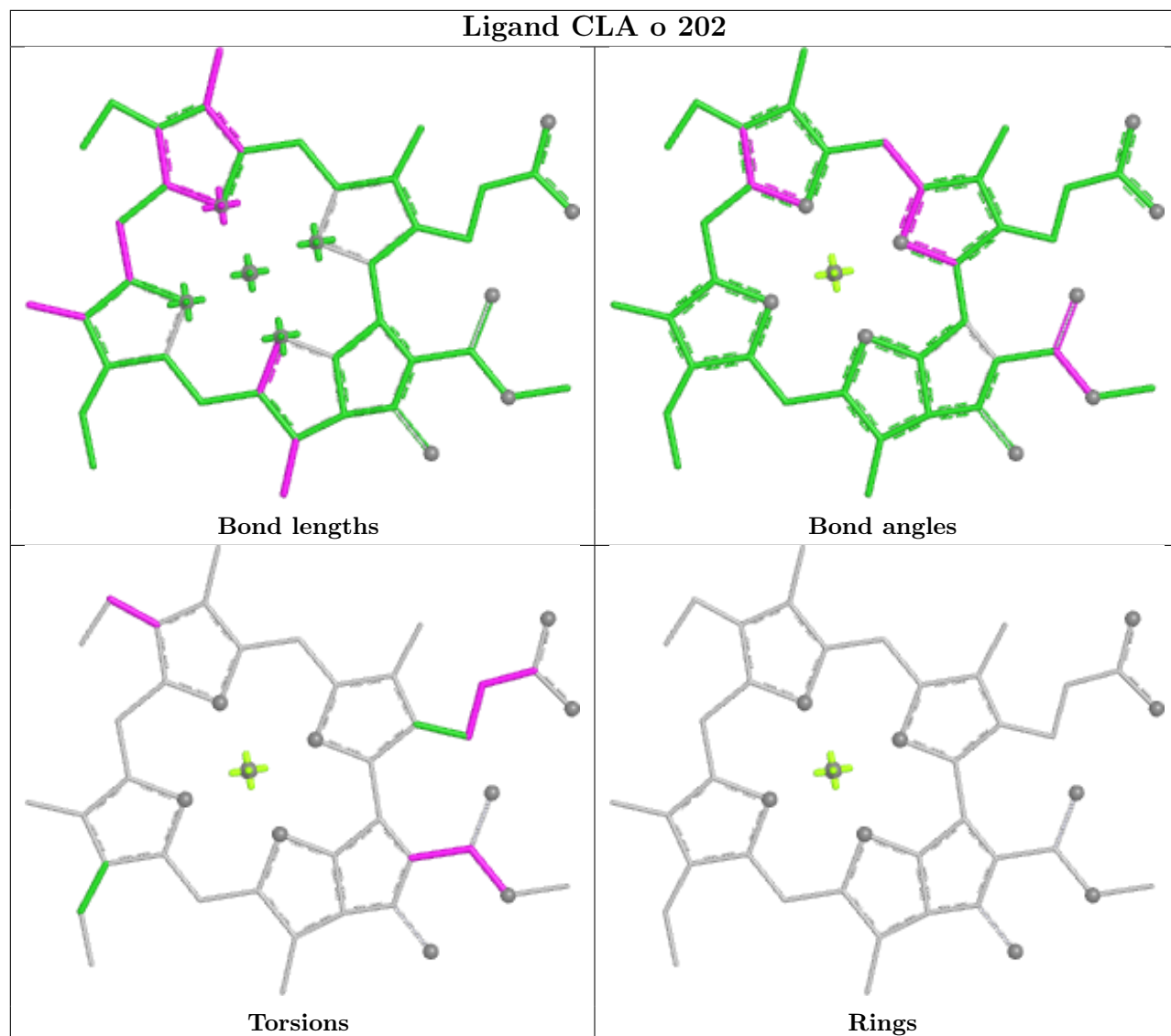
## Ligand CLA E 832

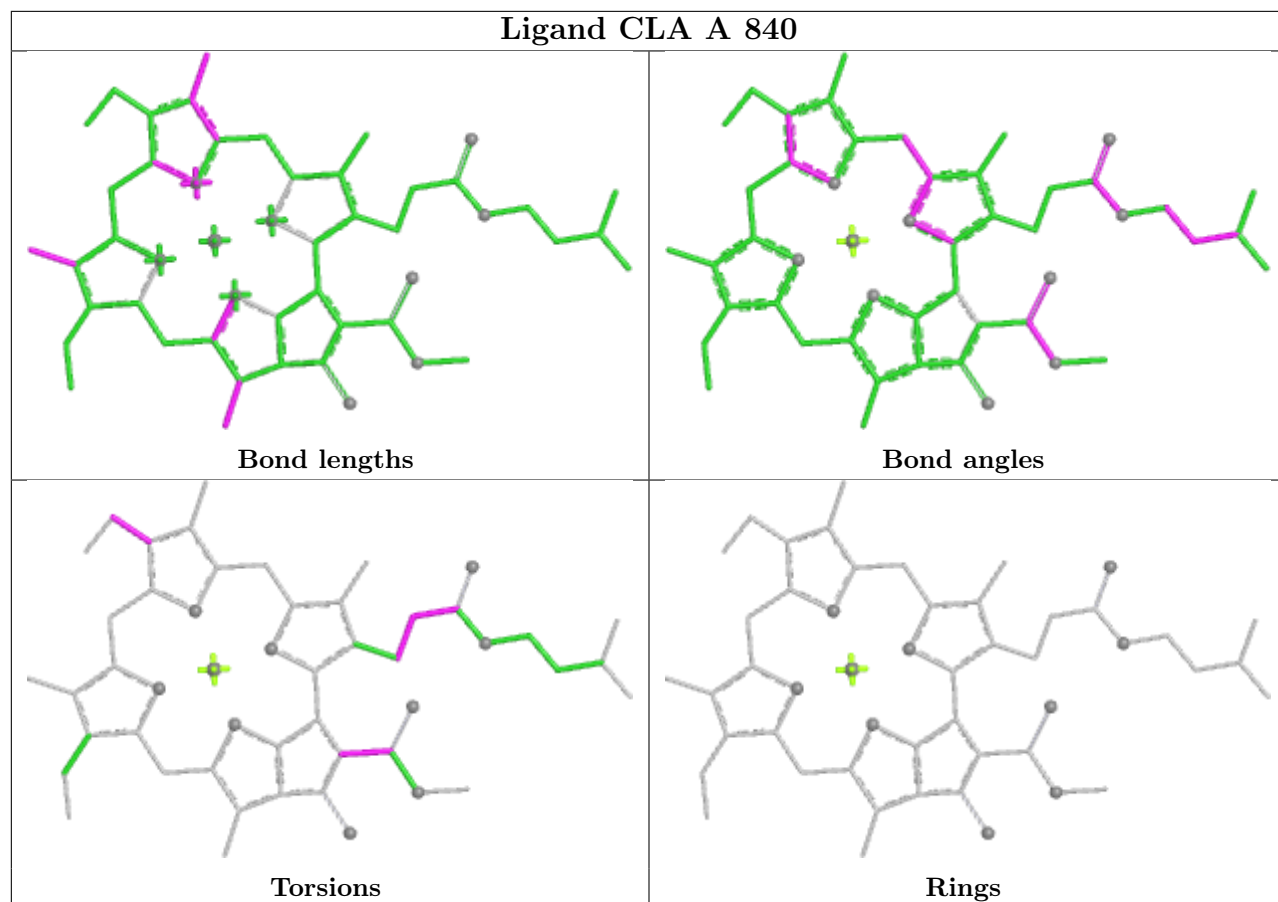


## Ligand BCR q 102

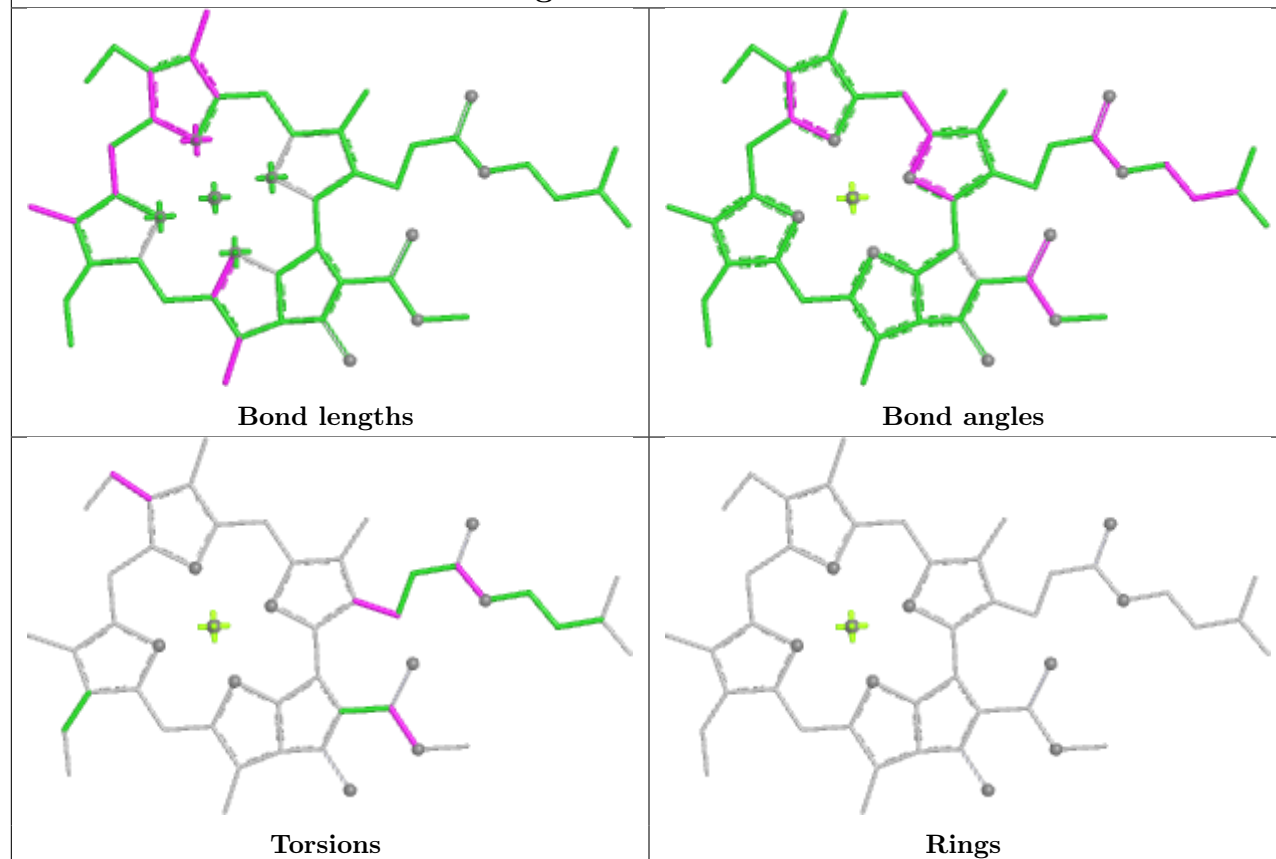


## Ligand CLA o 202

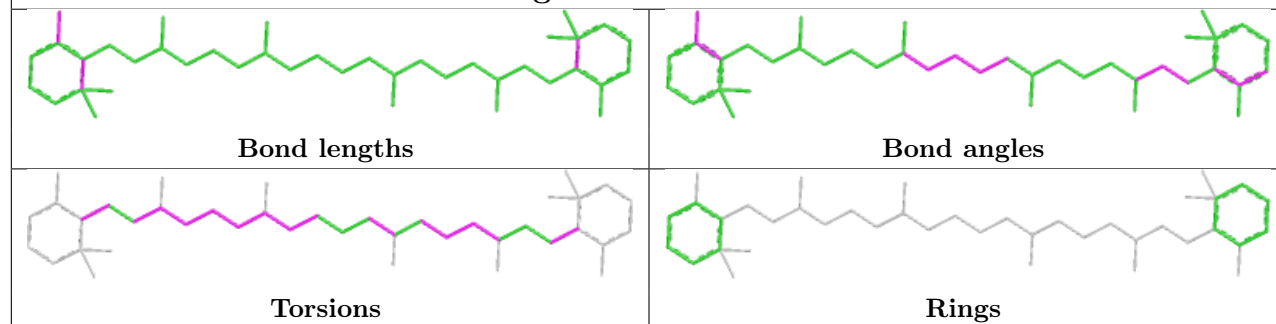


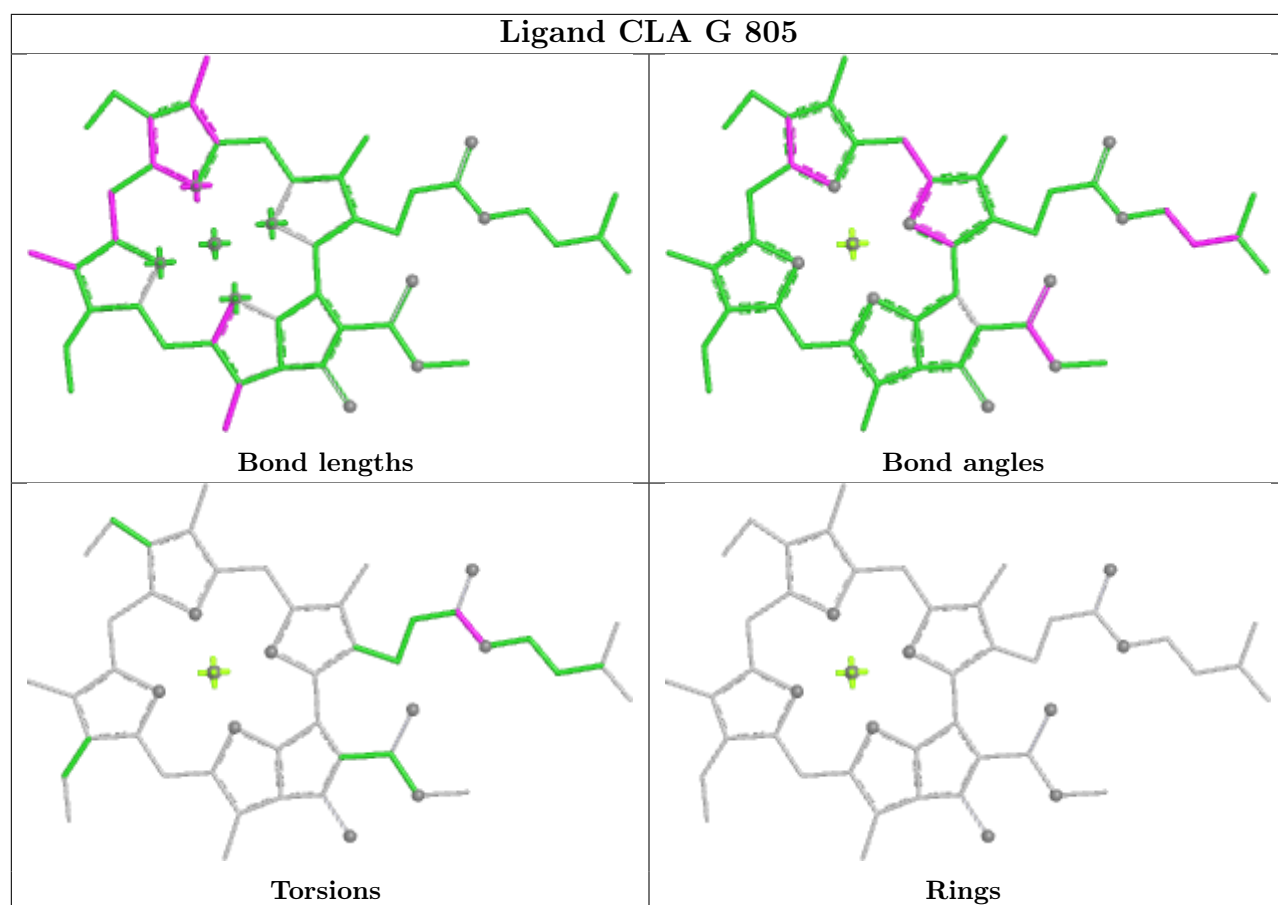


## Ligand CLA b 839

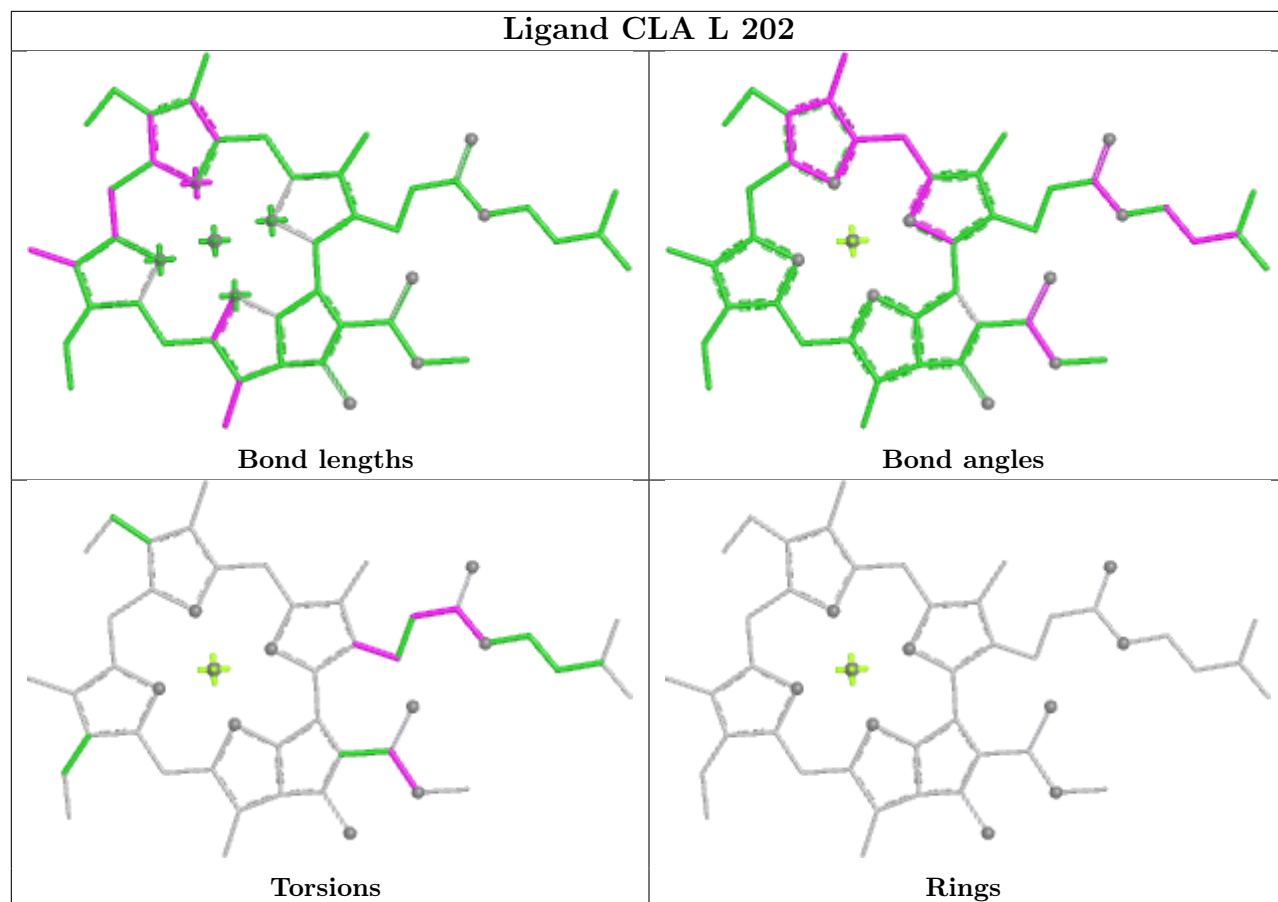


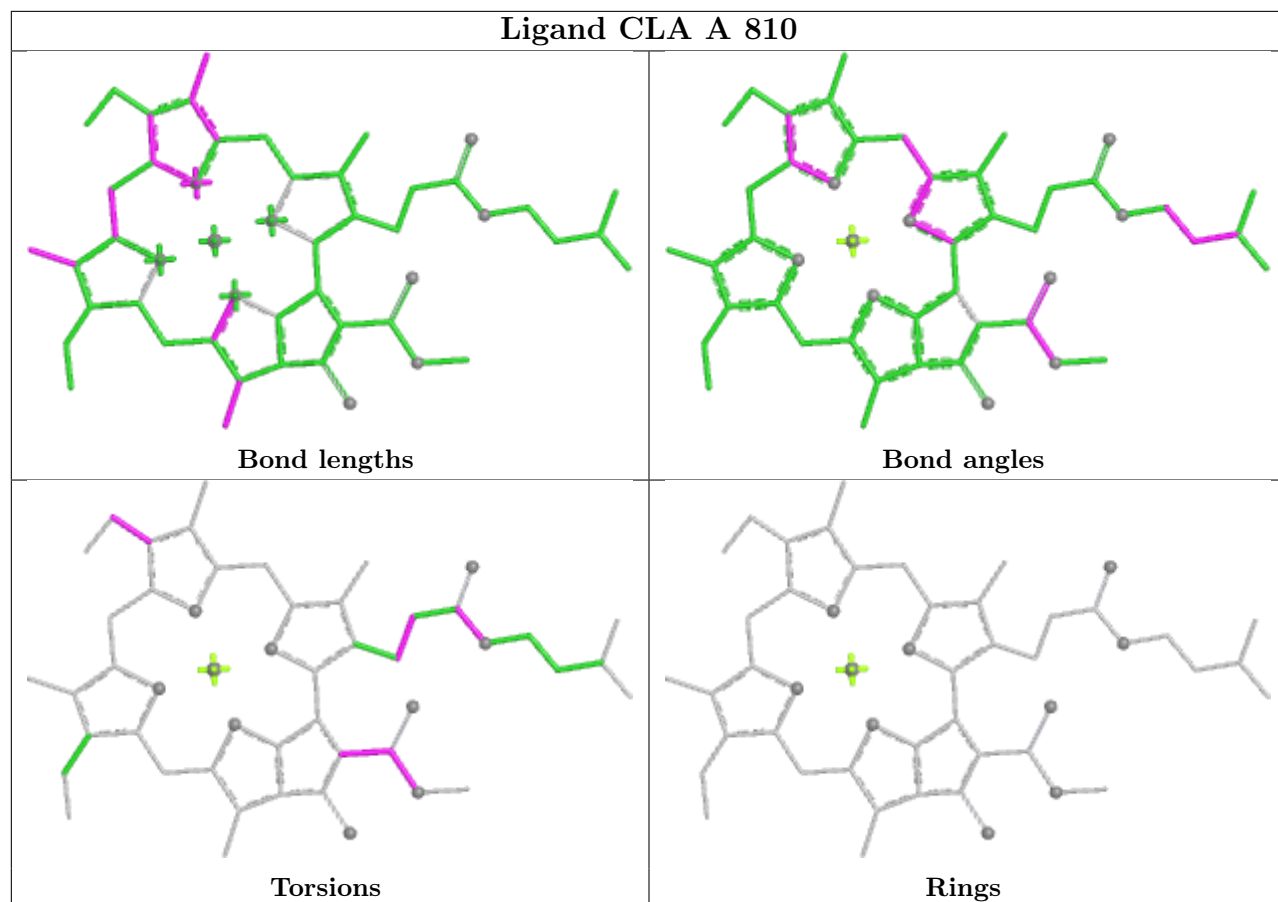
## Ligand BCR b 845



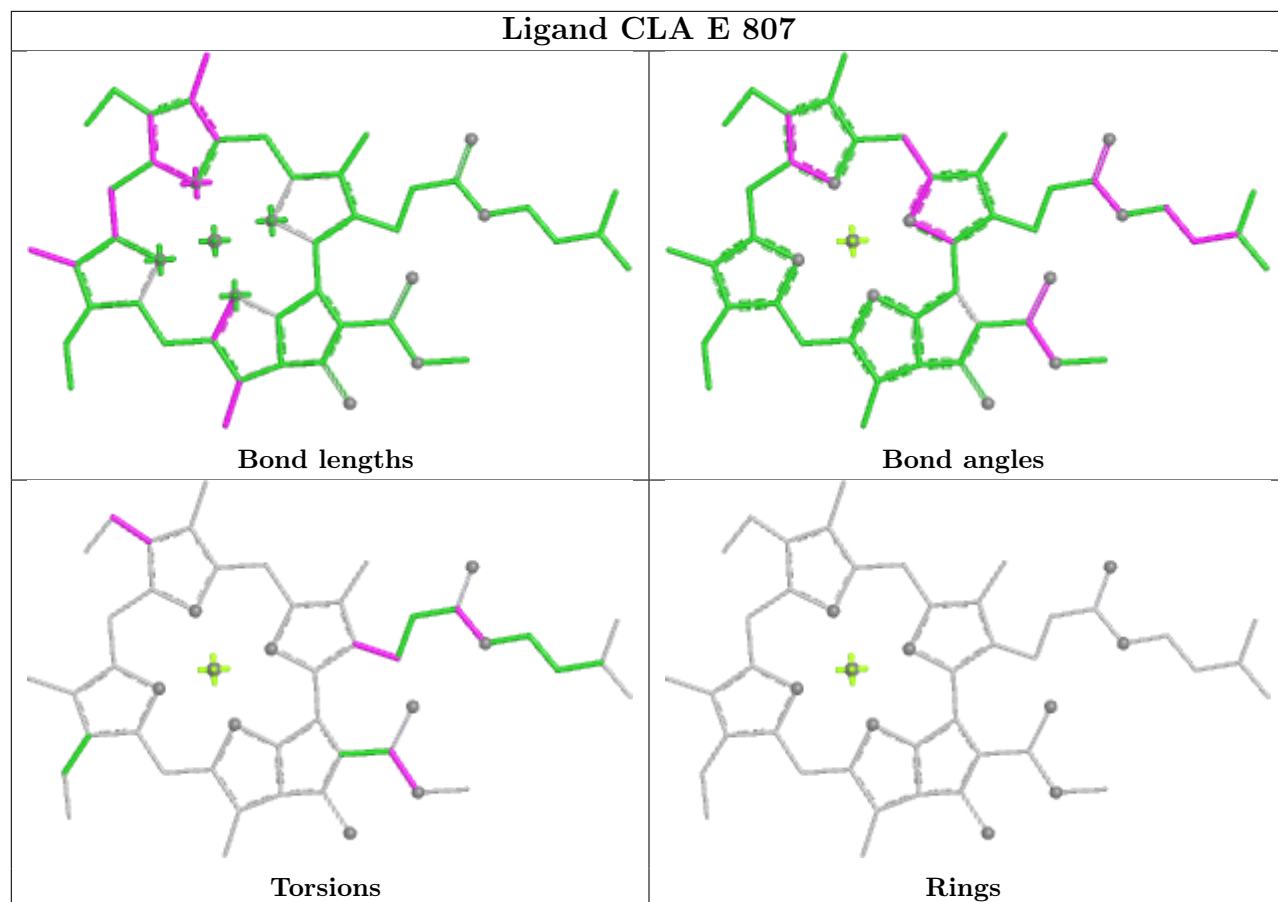


## Ligand CLA L 202



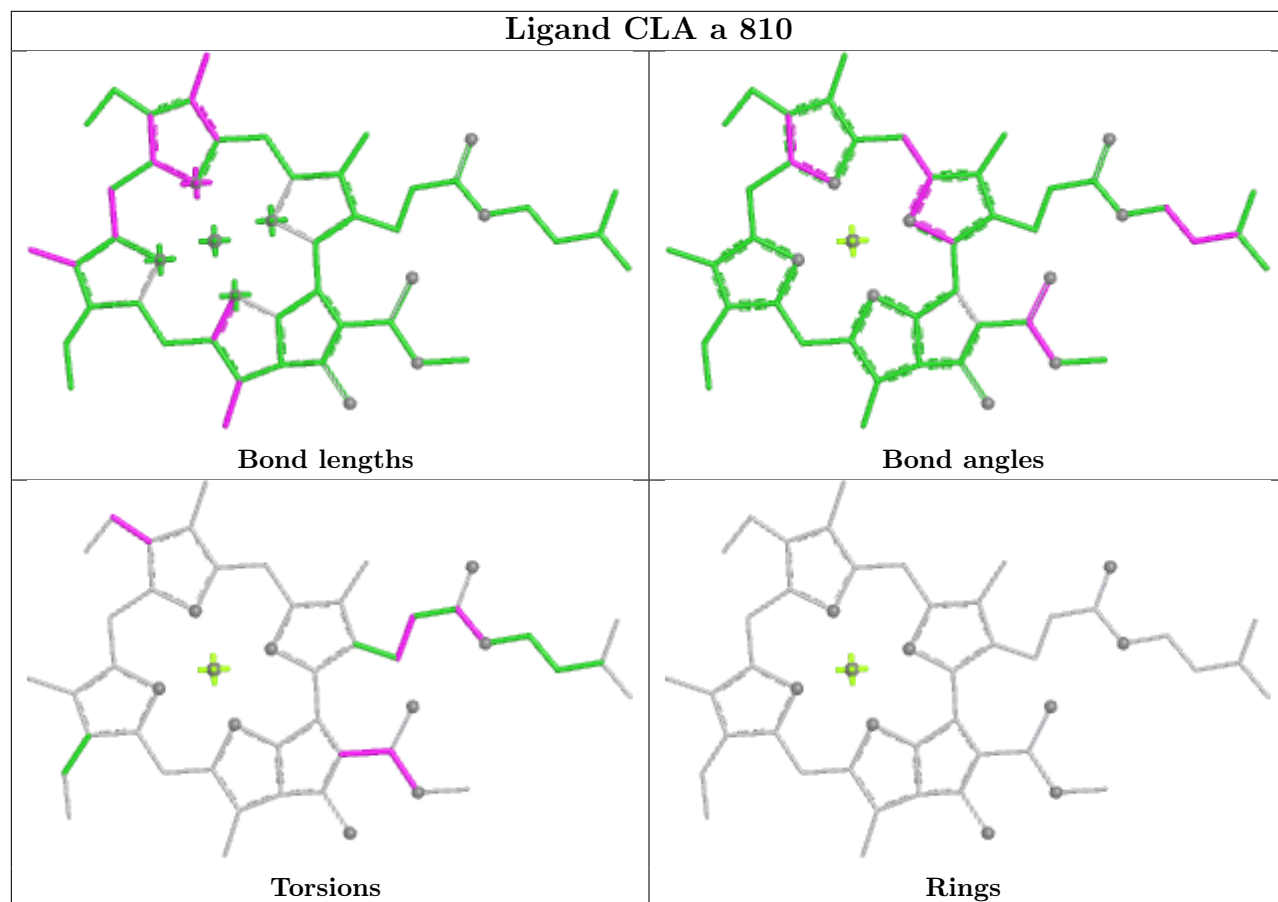


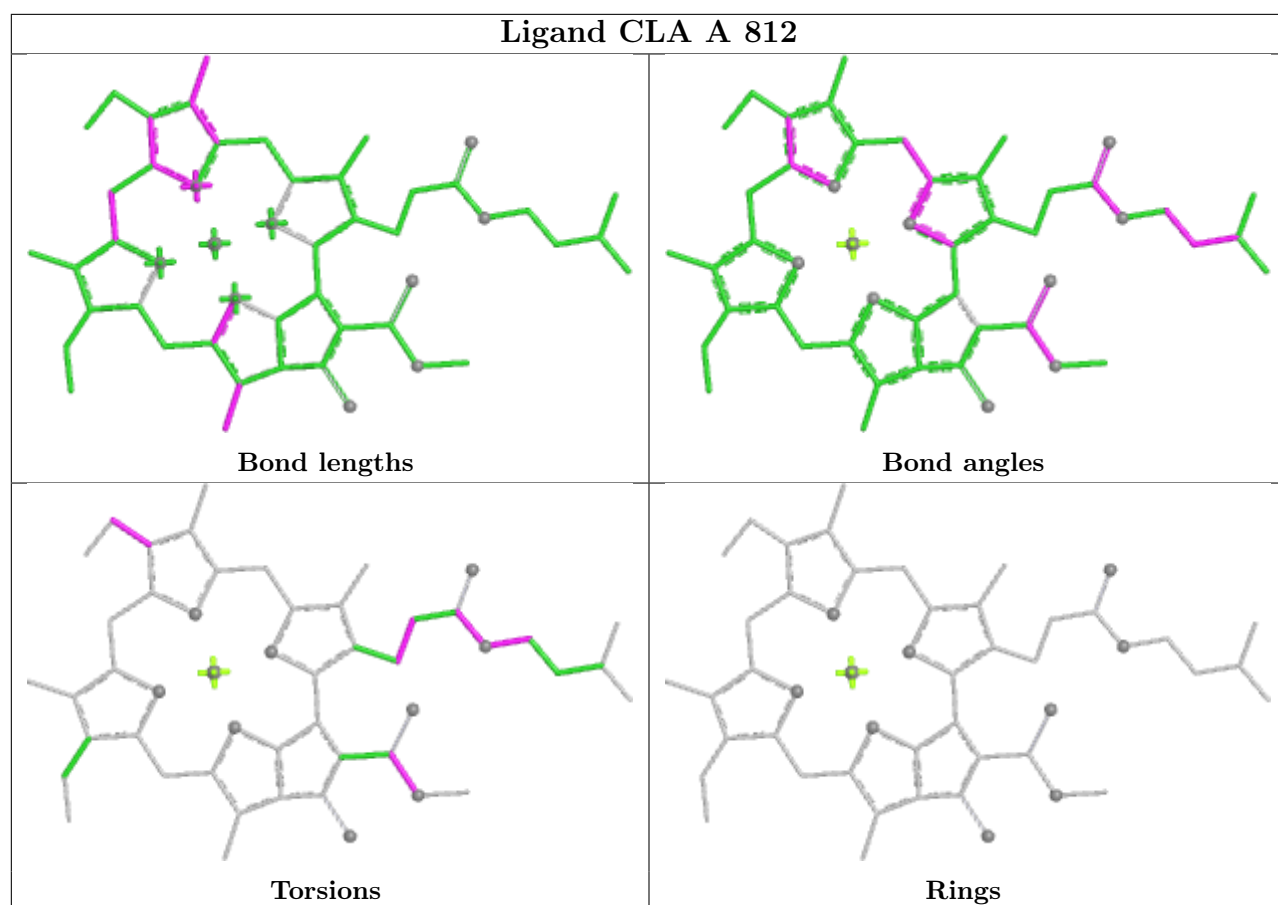
## Ligand CLA E 807



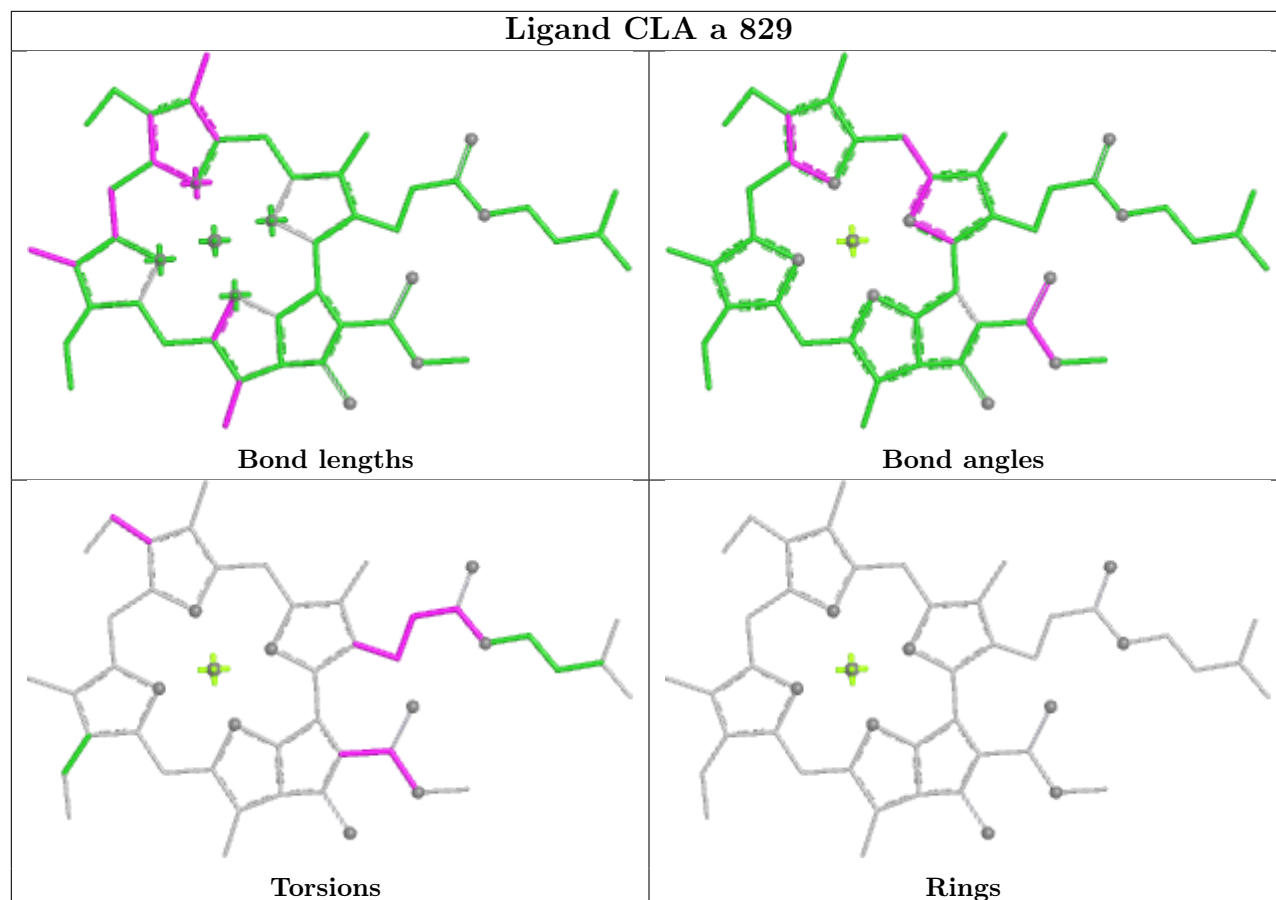


## Ligand CLA a 810

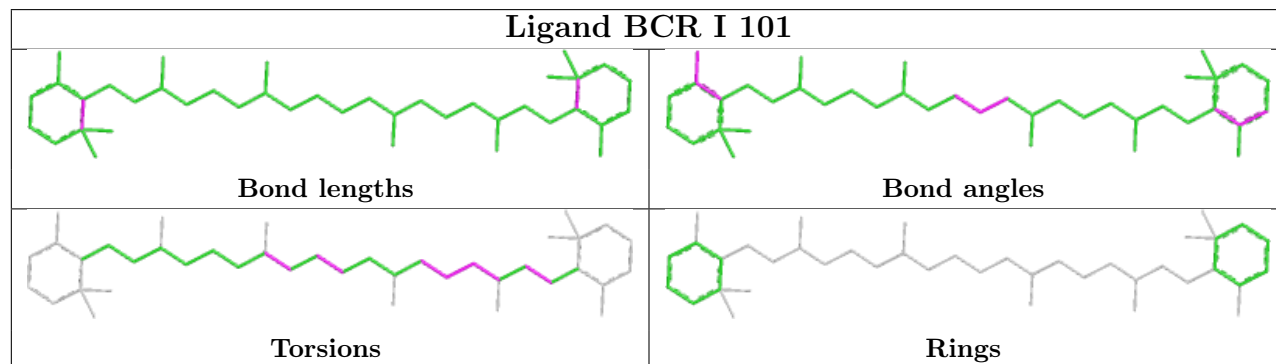




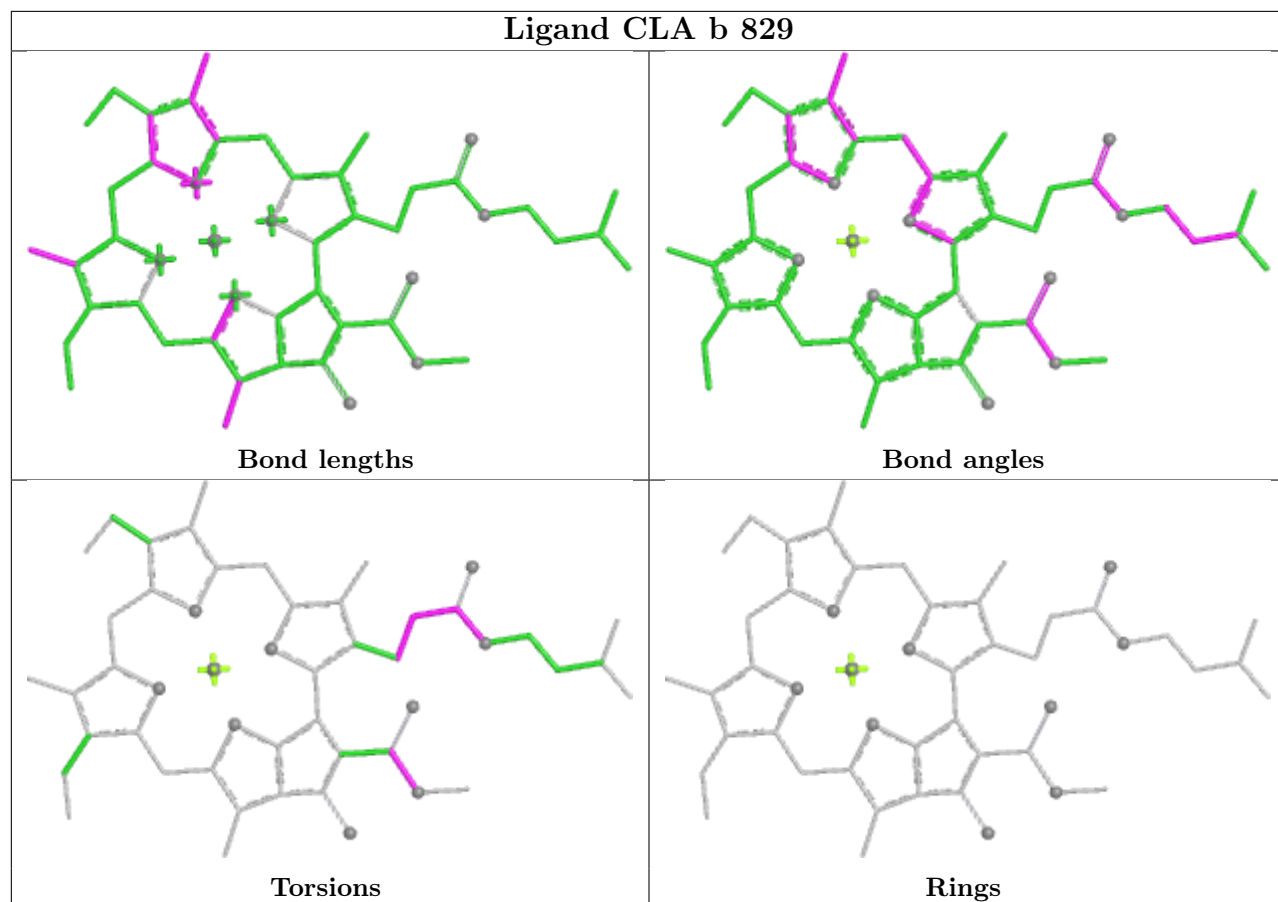
## Ligand CLA a 829

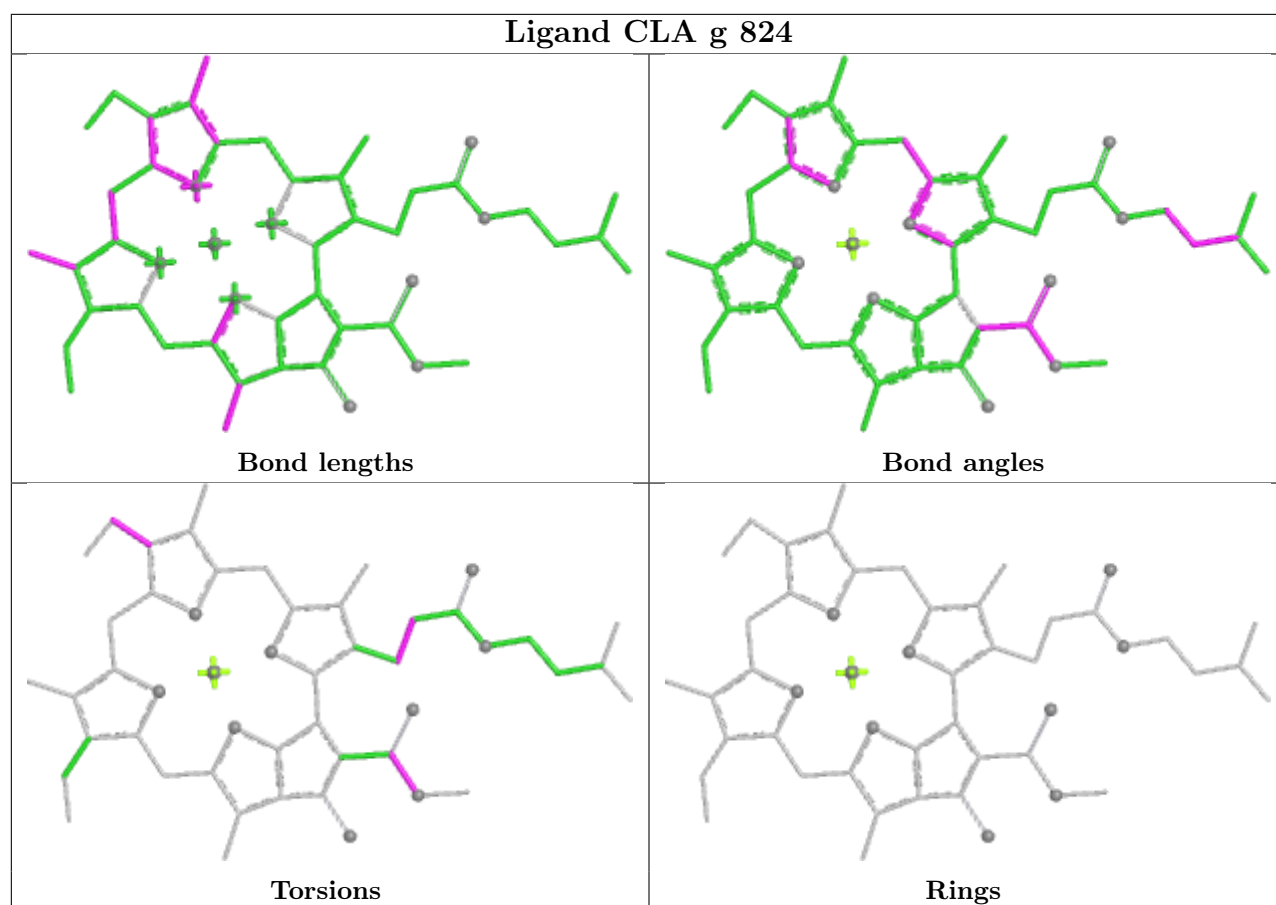


## Ligand BCR I 101

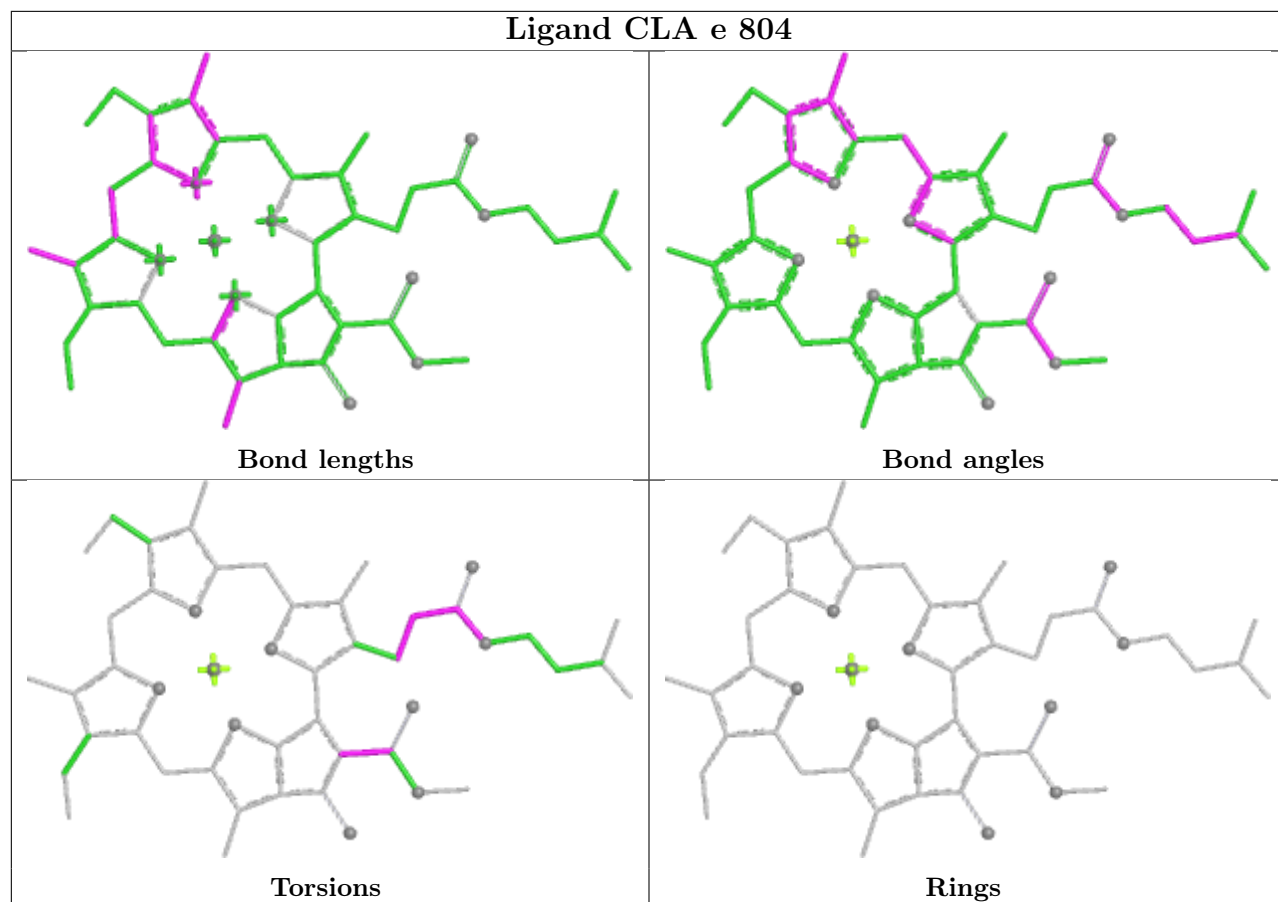


## Ligand CLA b 829

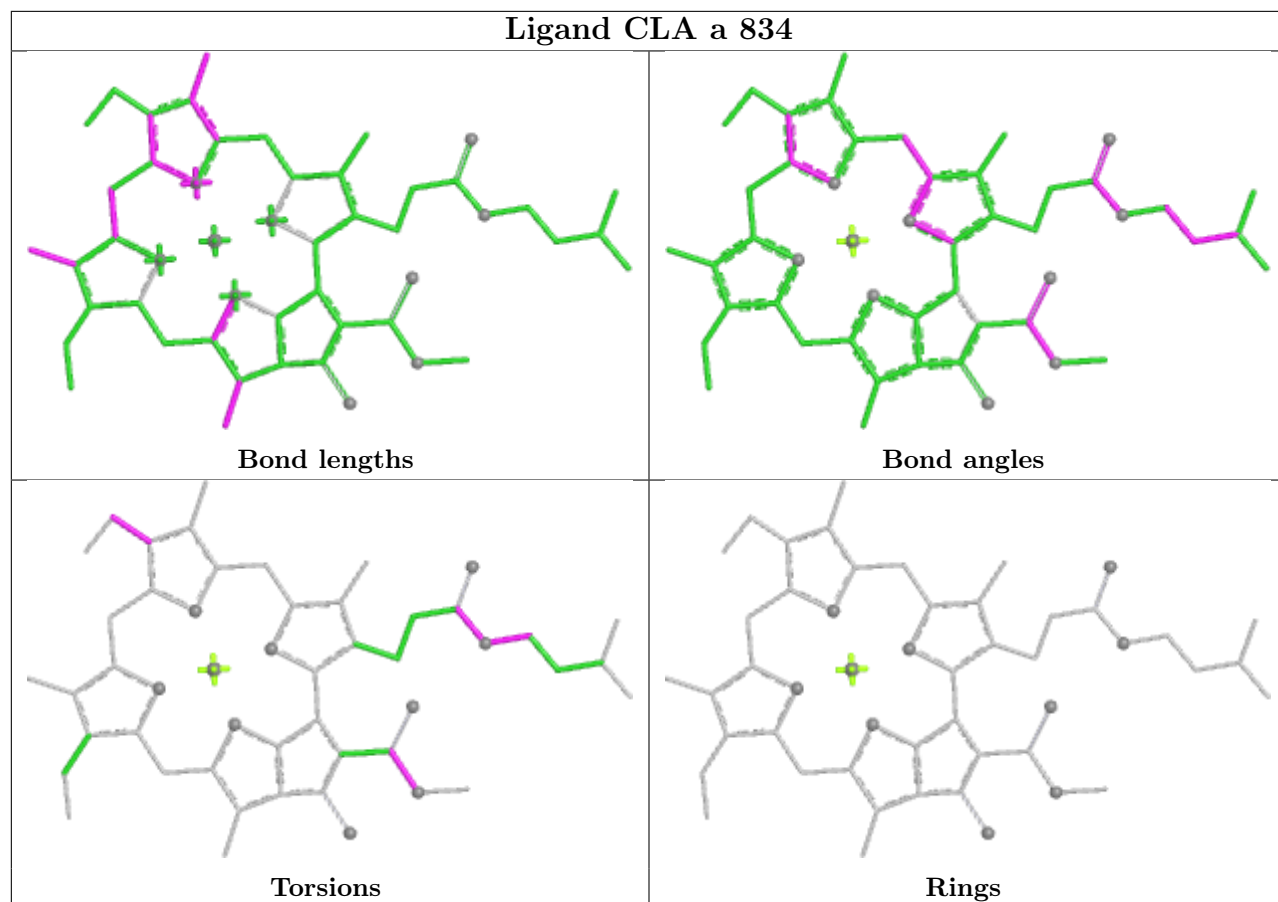




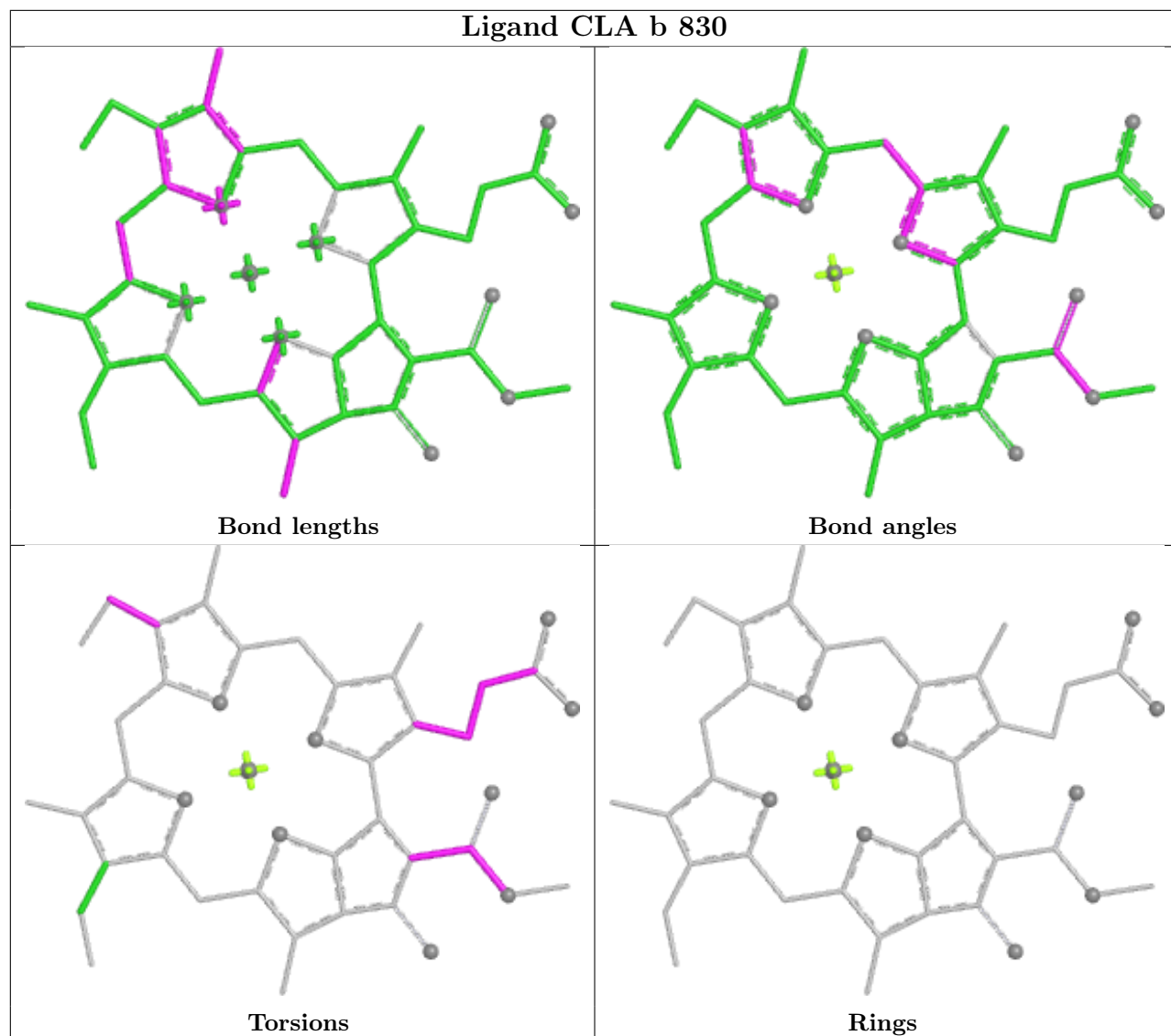
## Ligand CLA e 804



## Ligand CLA a 834

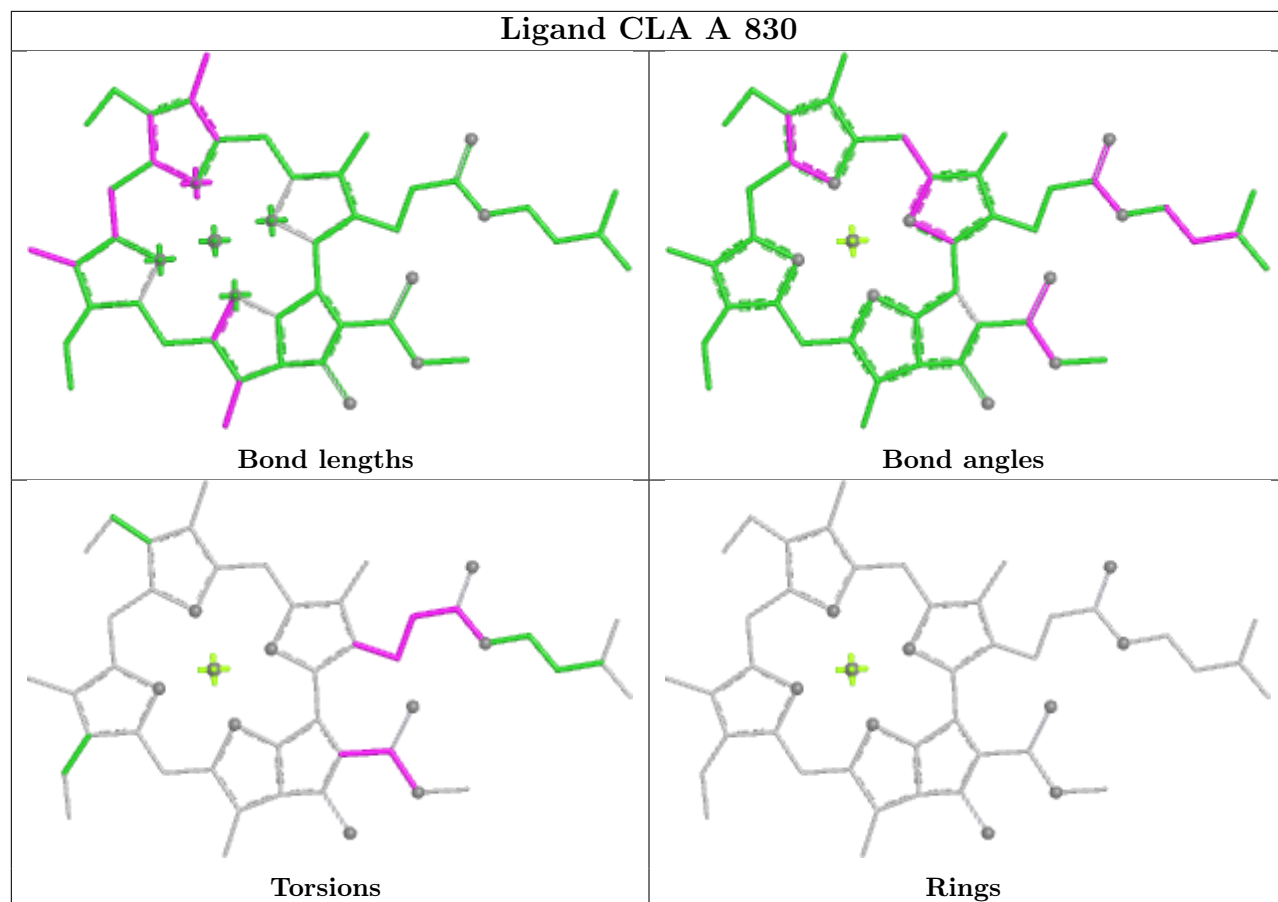


## Ligand CLA b 830

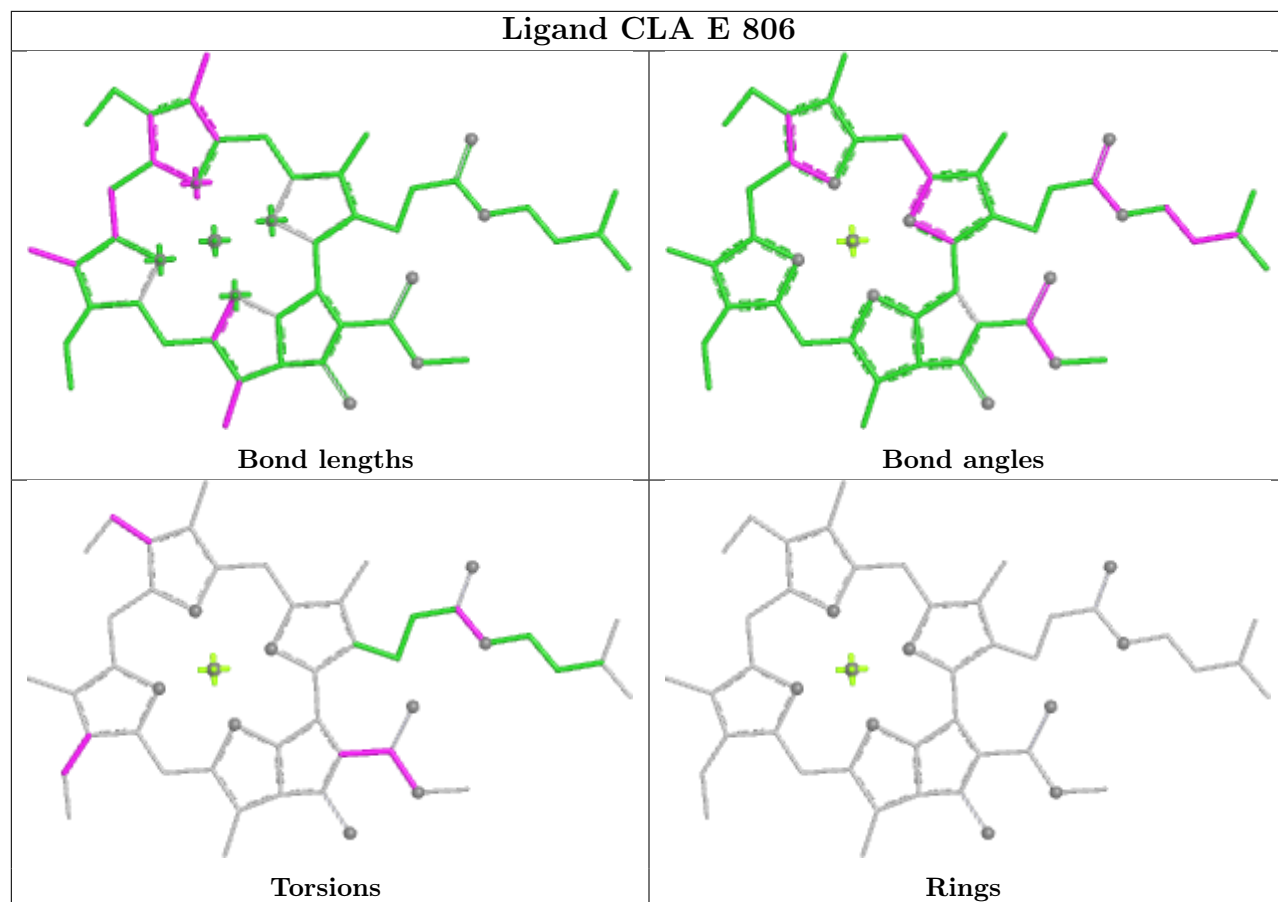




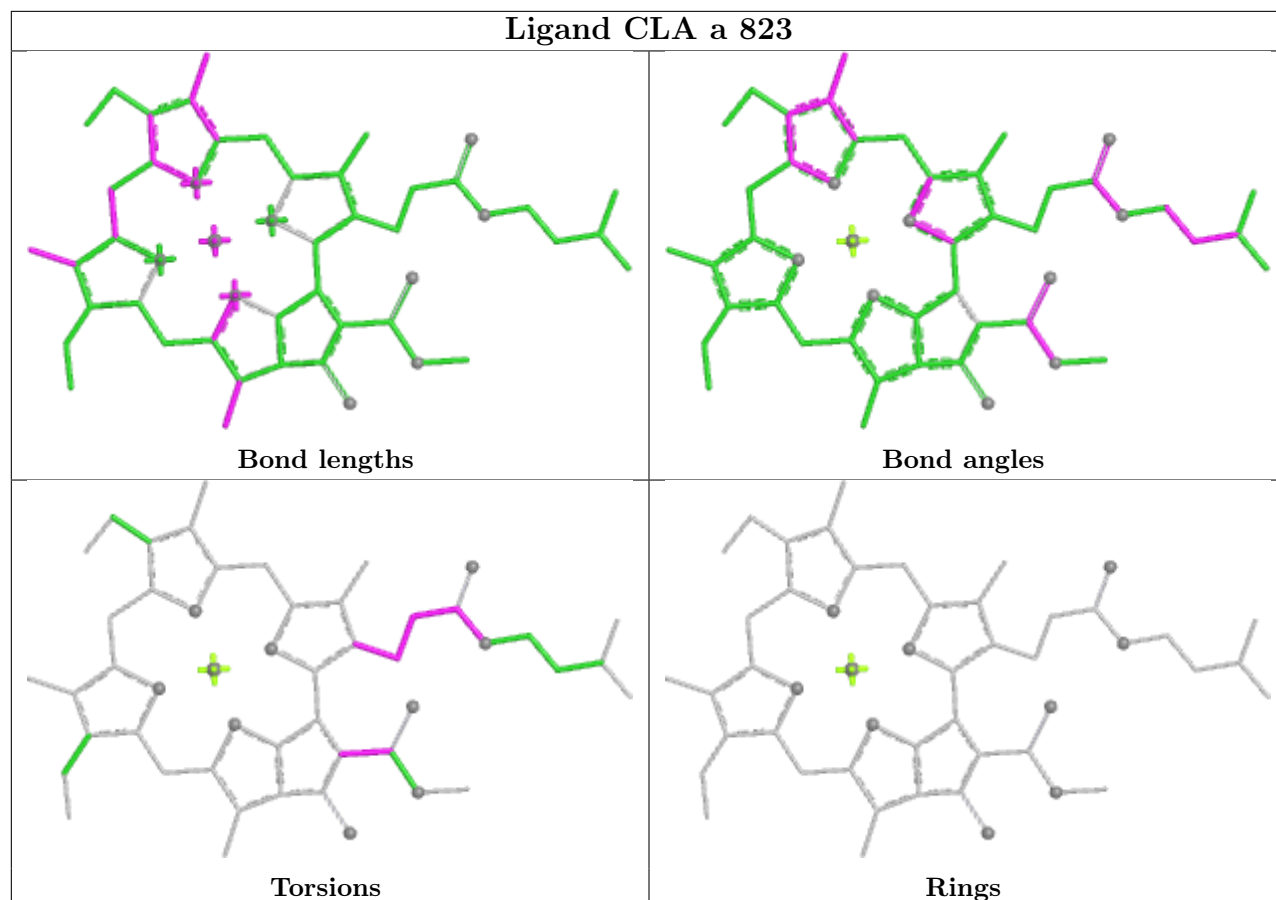
## Ligand CLA A 830



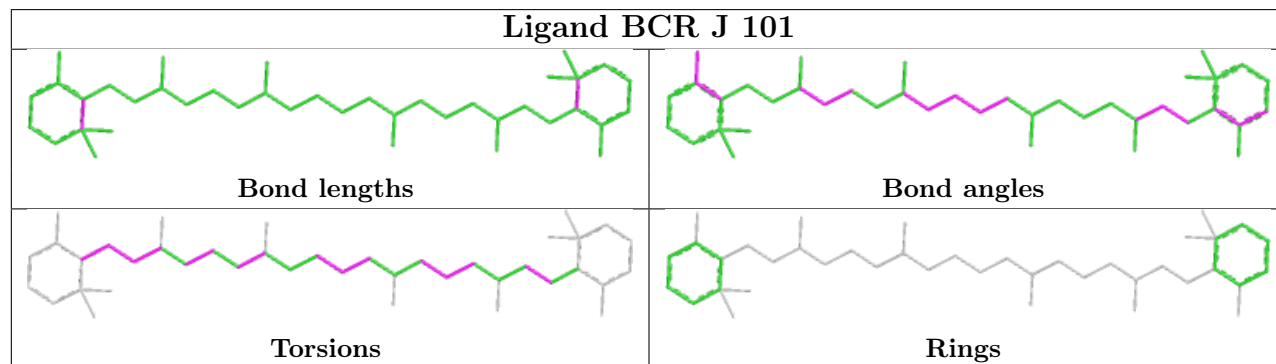
## Ligand CLA E 806

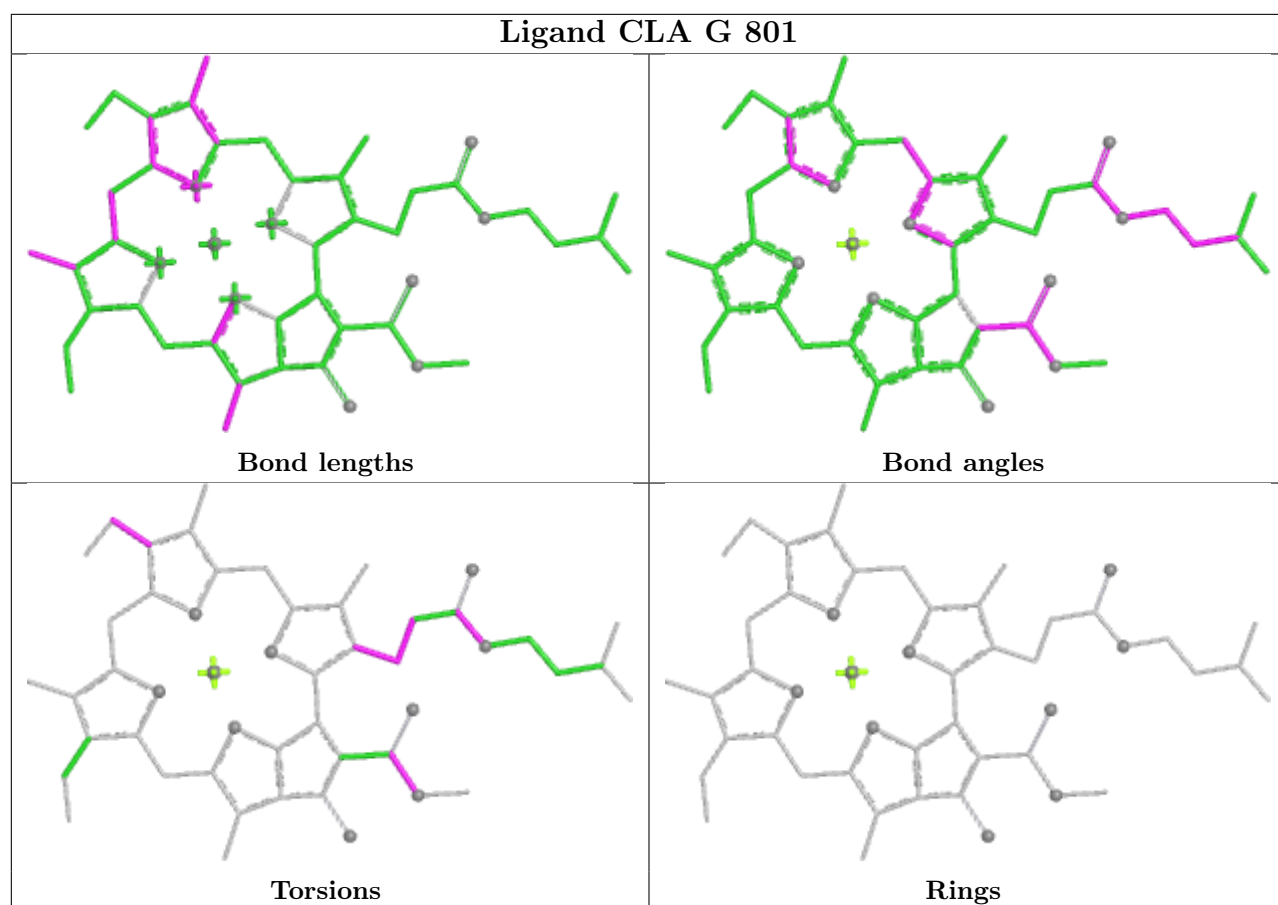


## Ligand CLA a 823

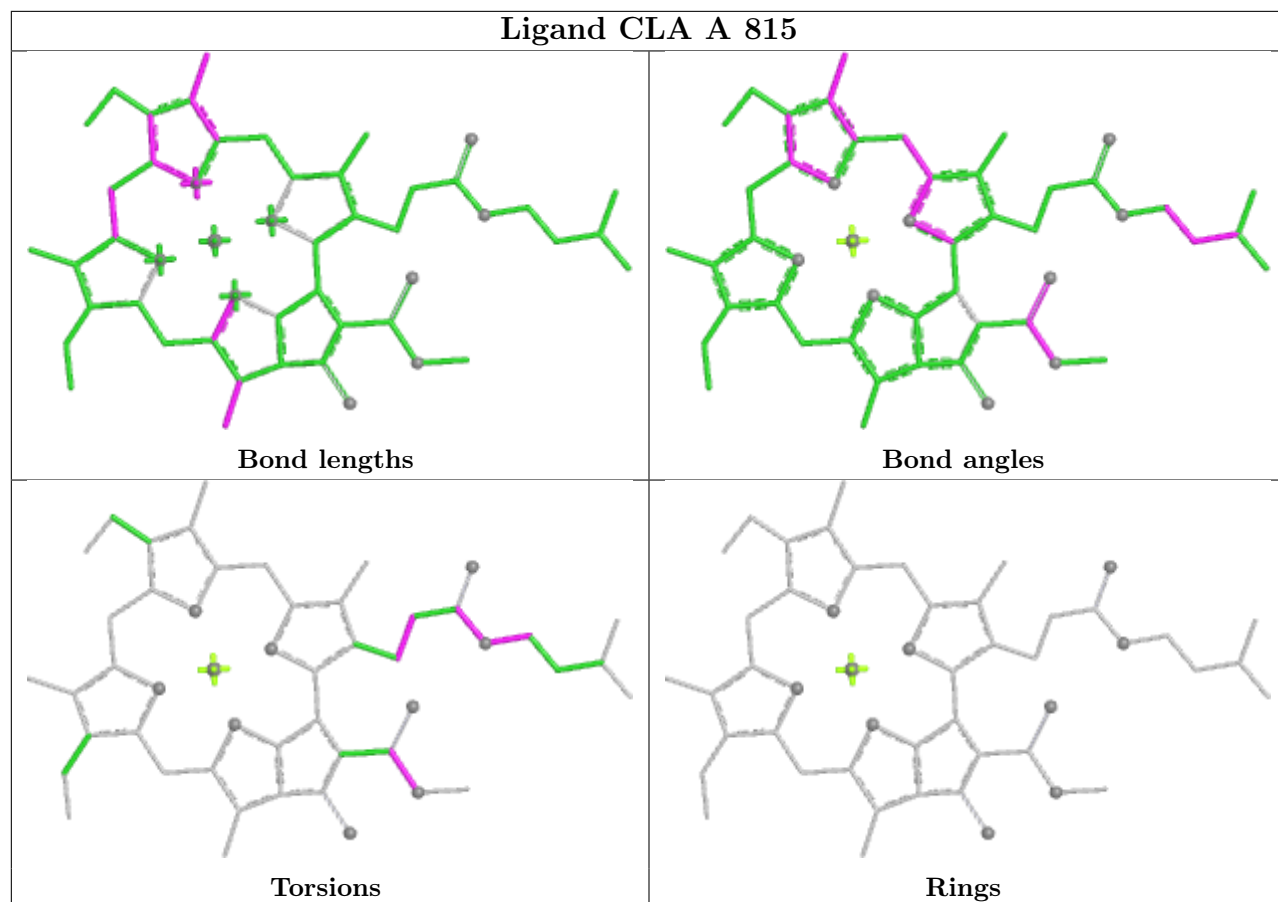


## Ligand BCR J 101

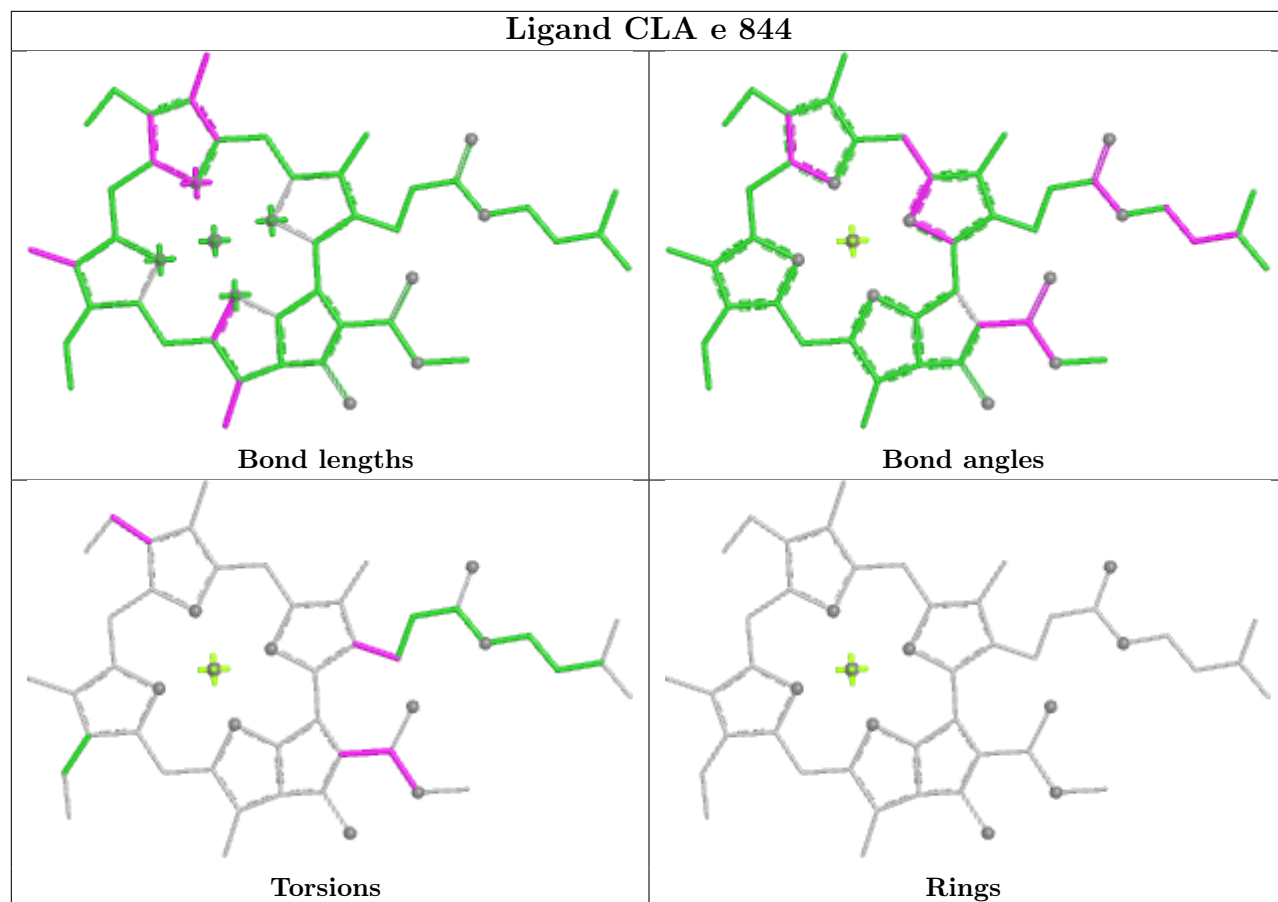




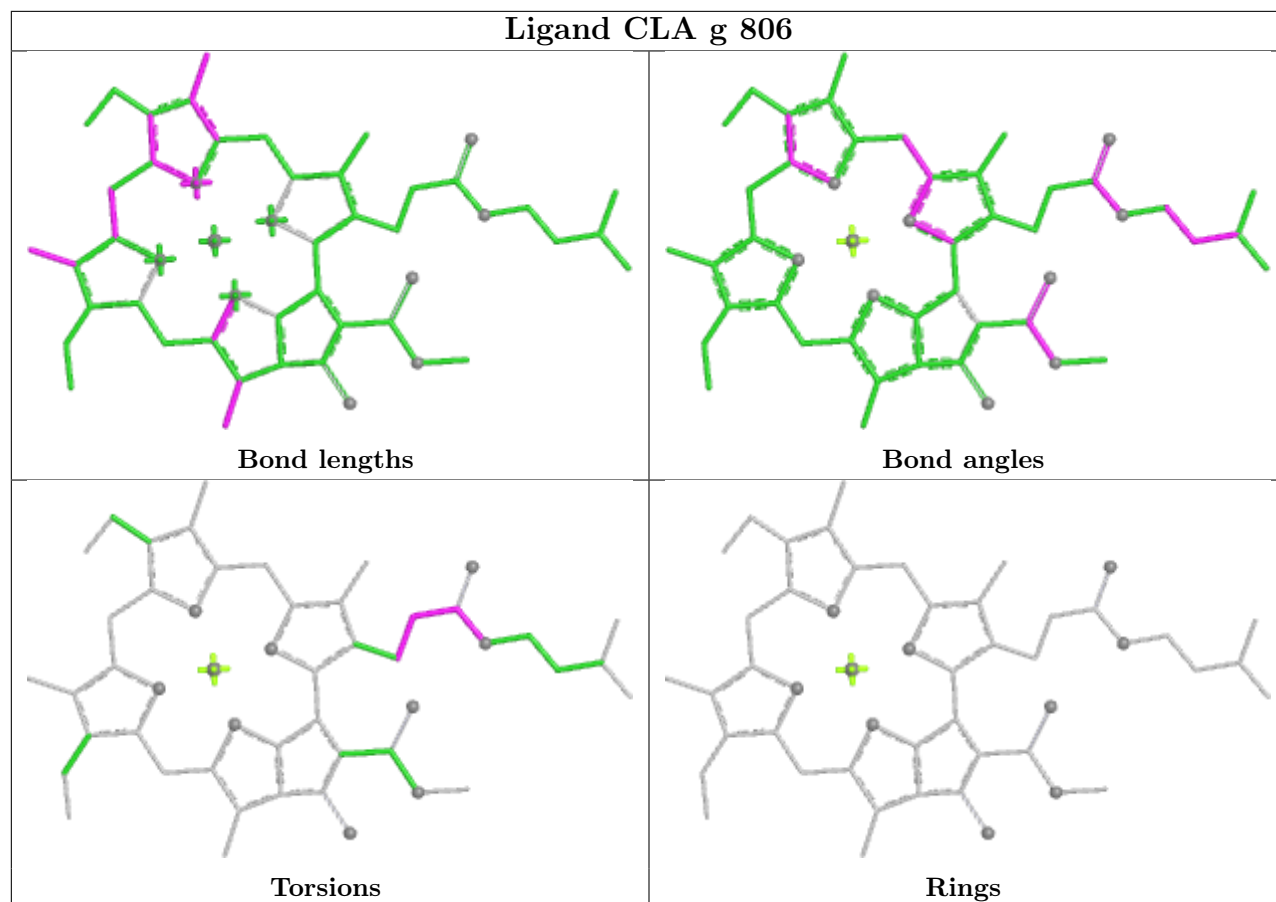
## Ligand CLA A 815



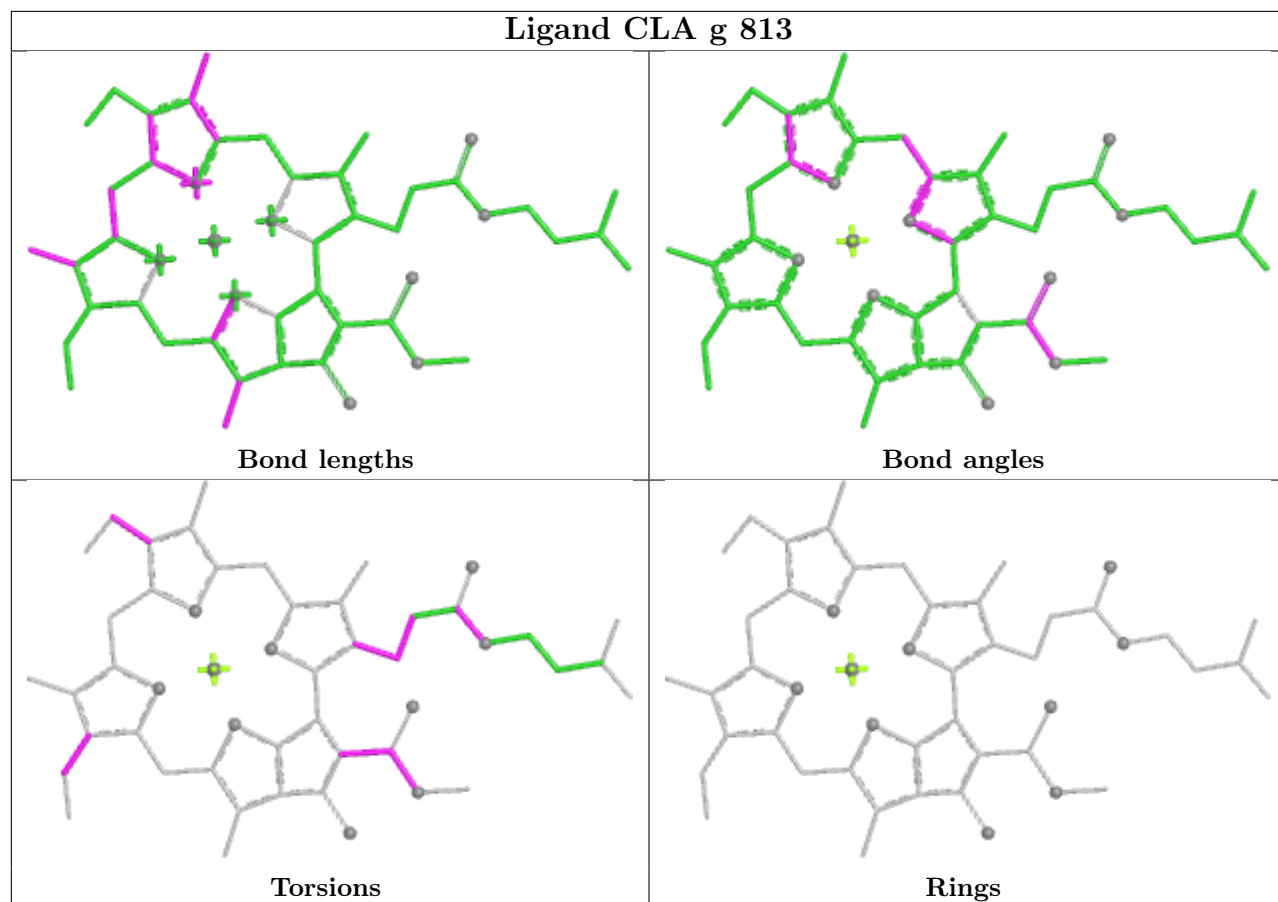
## Ligand CLA e 844



## Ligand CLA g 806

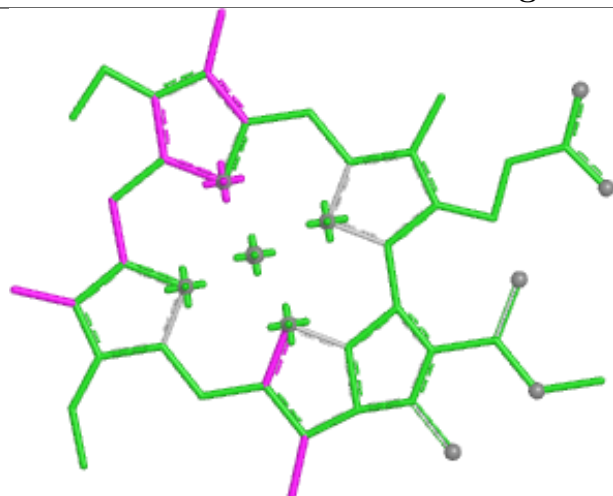


## Ligand CLA g 813

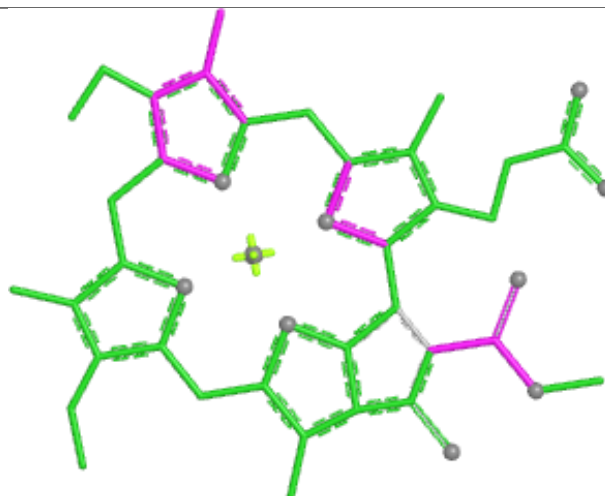




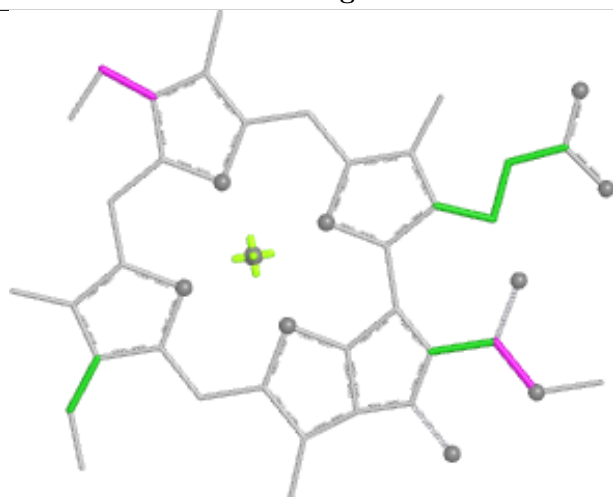
## Ligand CLA e 817



Bond lengths



Bond angles

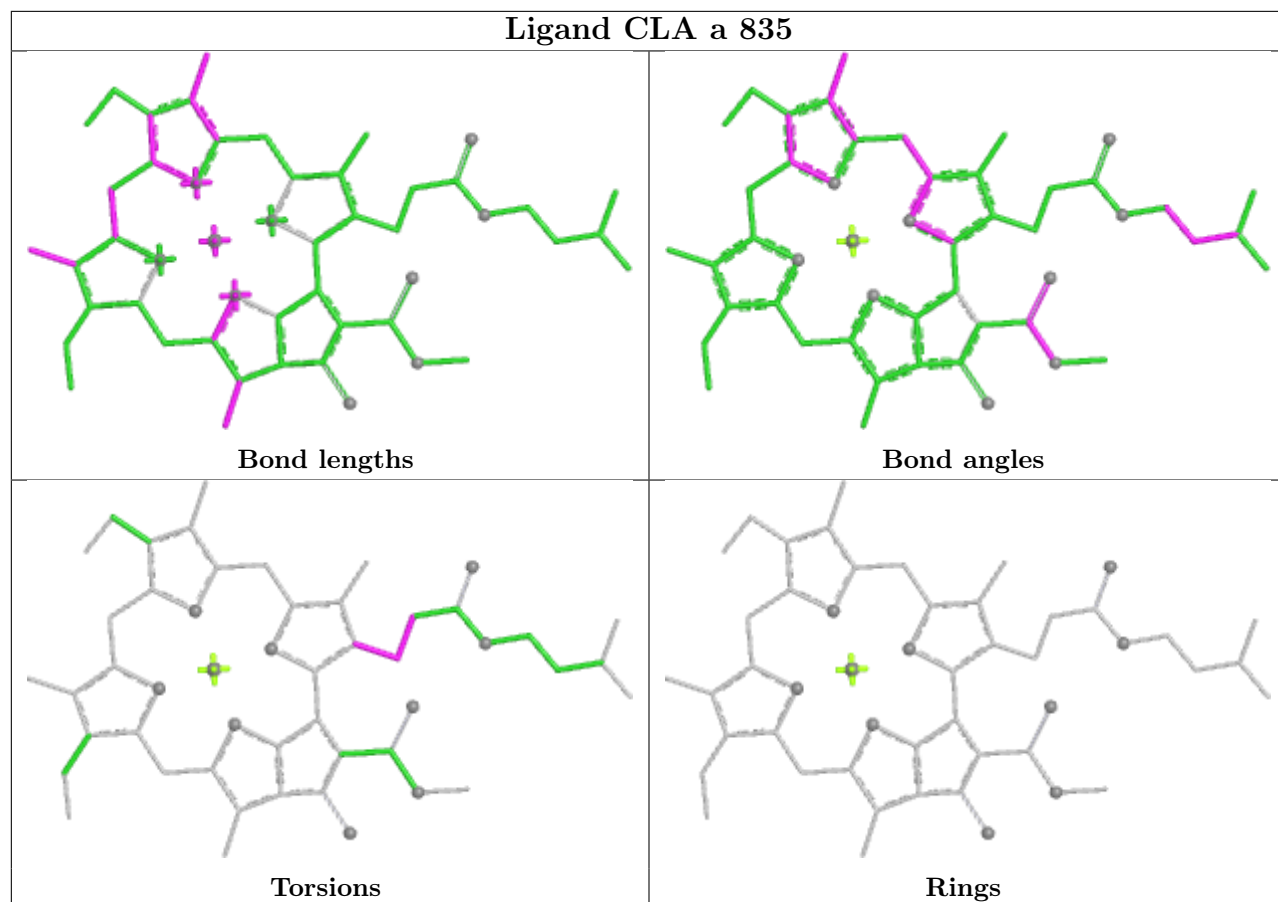


Torsions

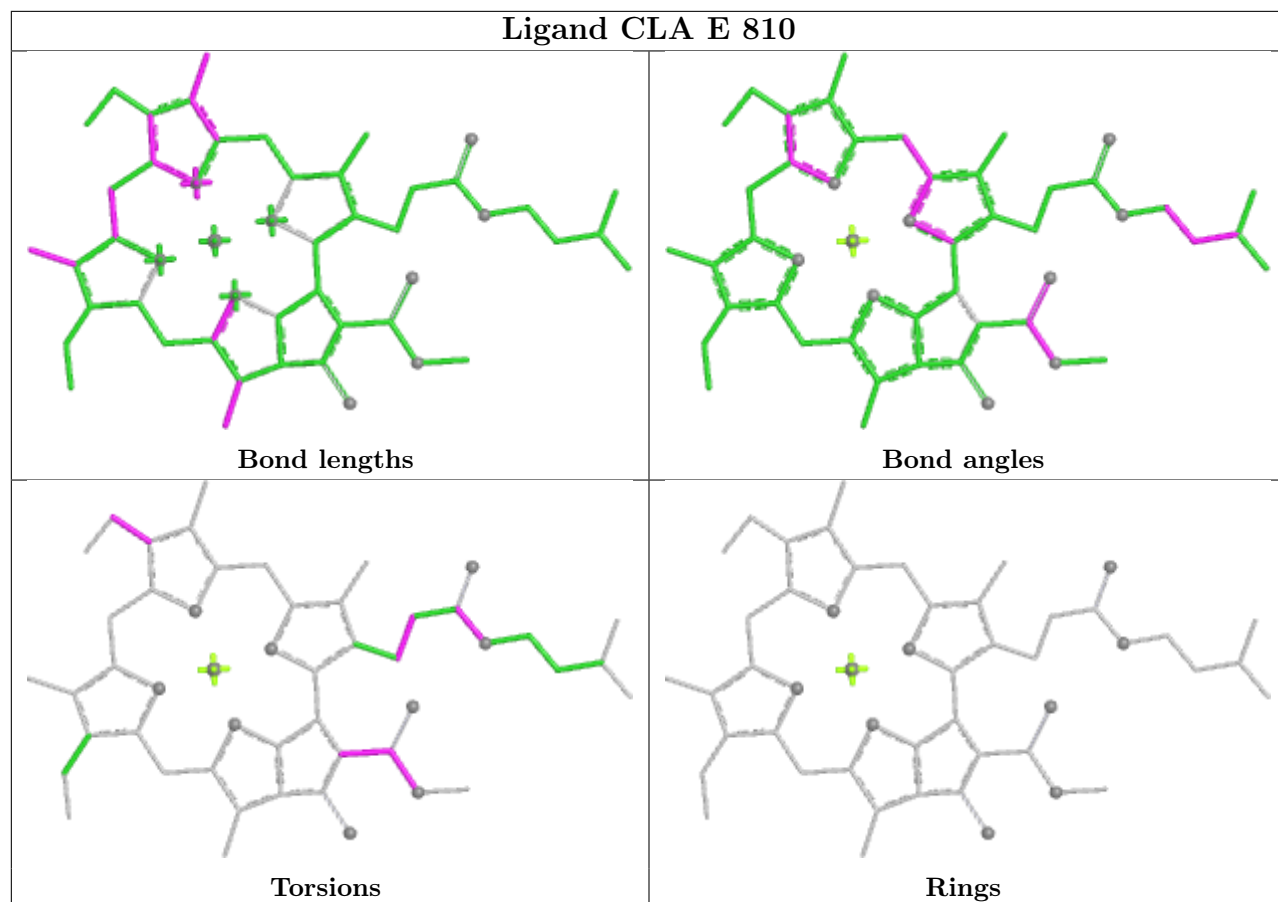


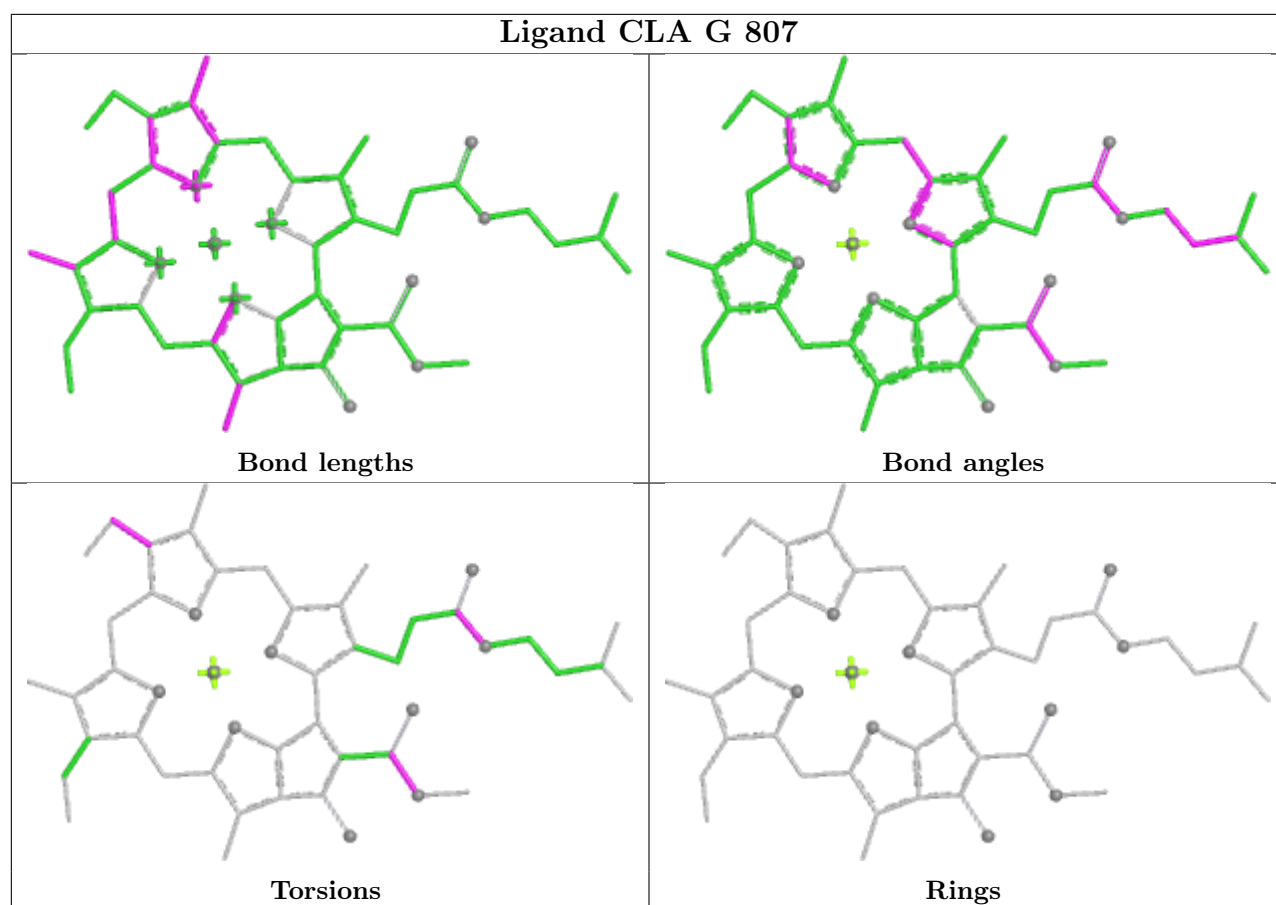
Rings

## Ligand CLA a 835

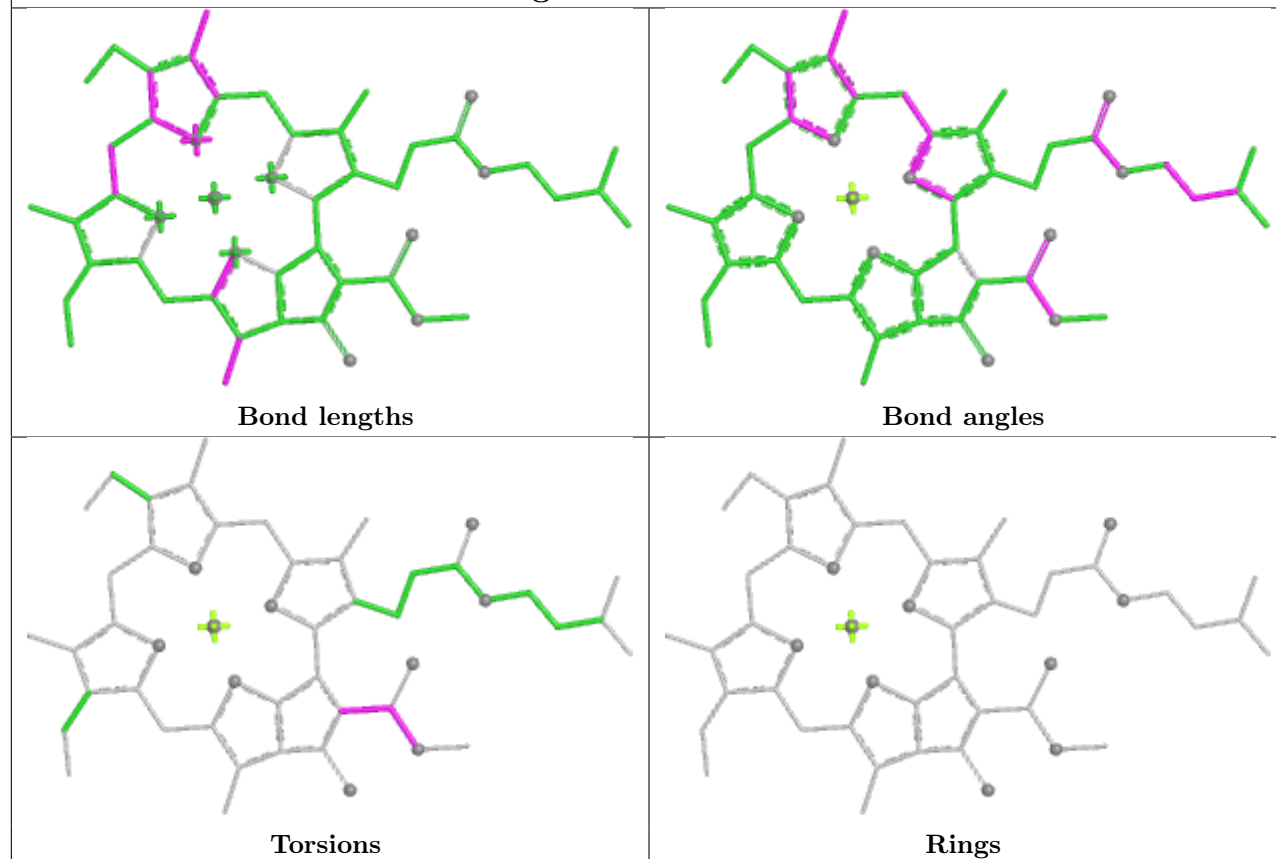


## Ligand CLA E 810

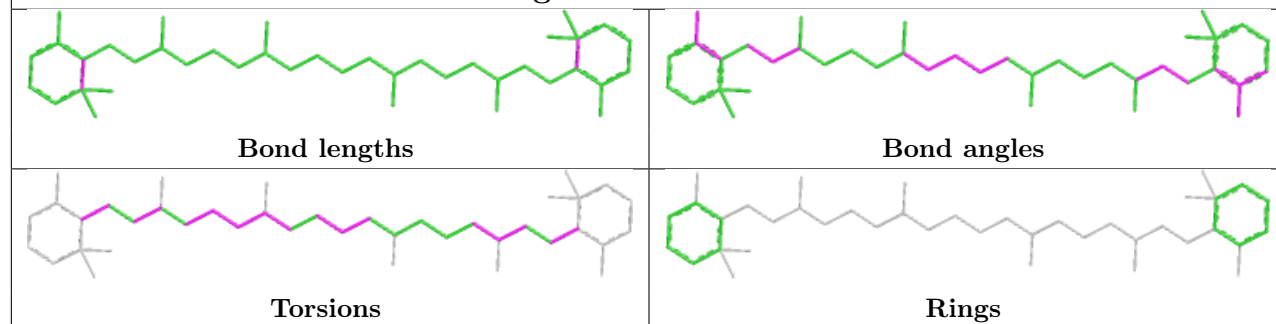




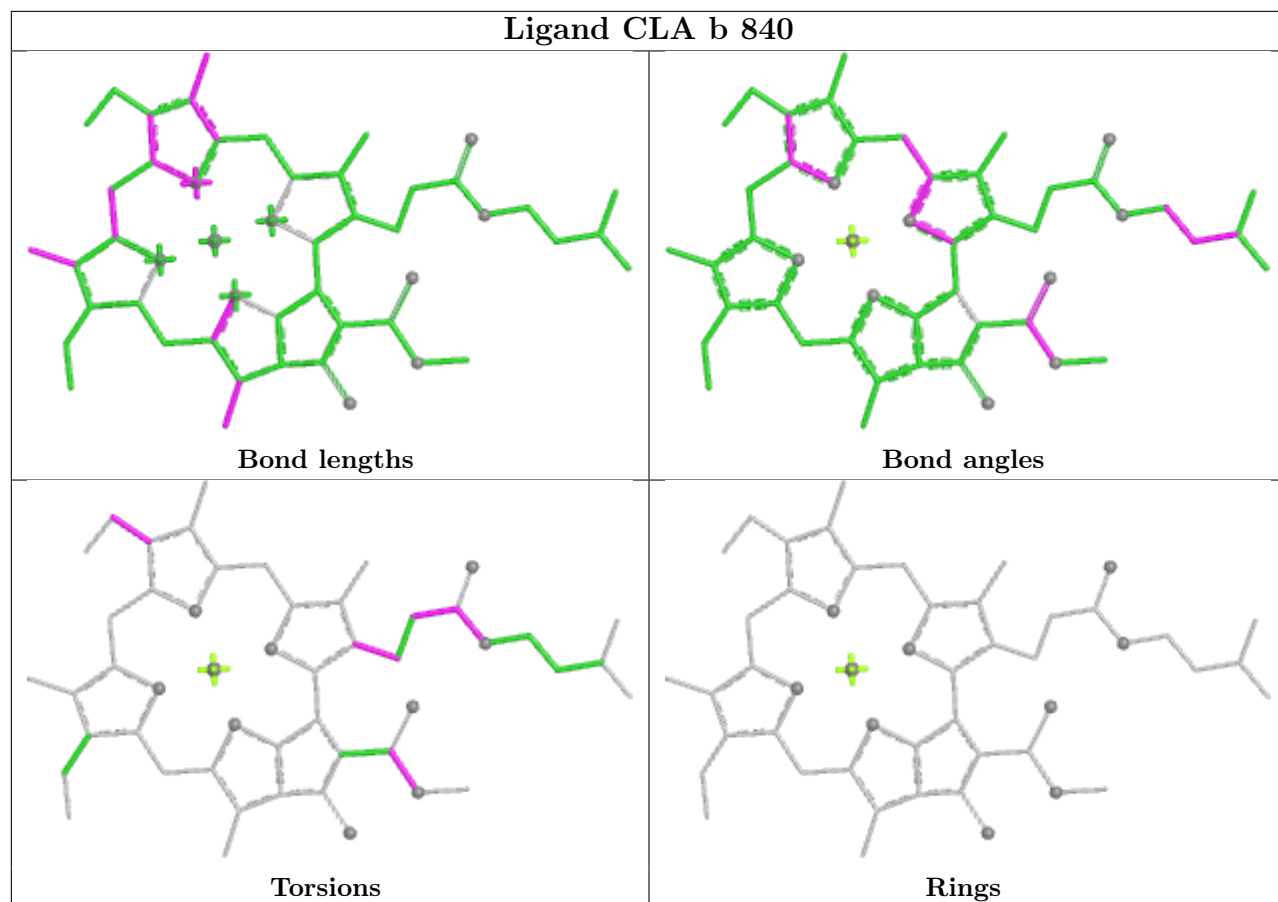
## Ligand CLA B 837



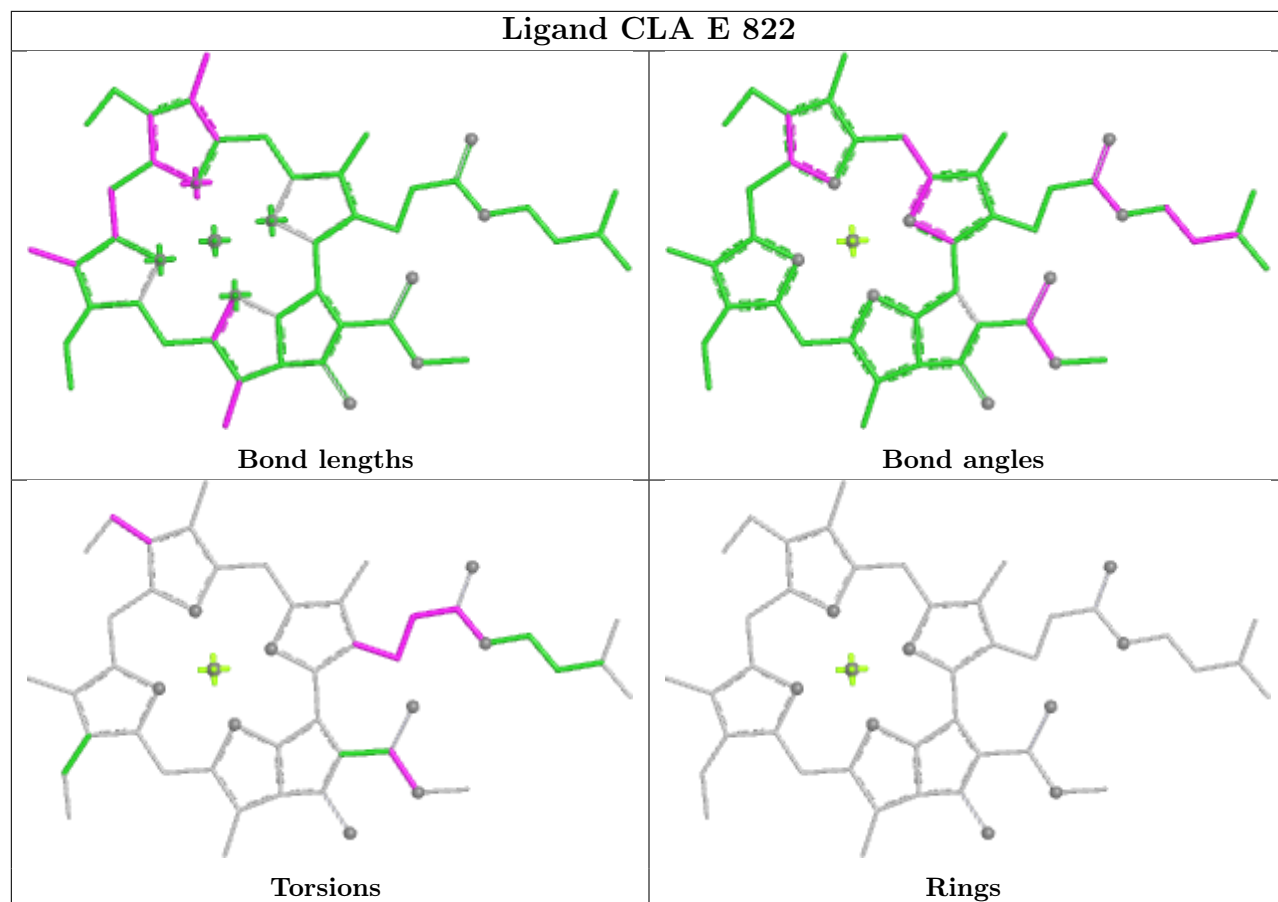
## Ligand BCR b 847



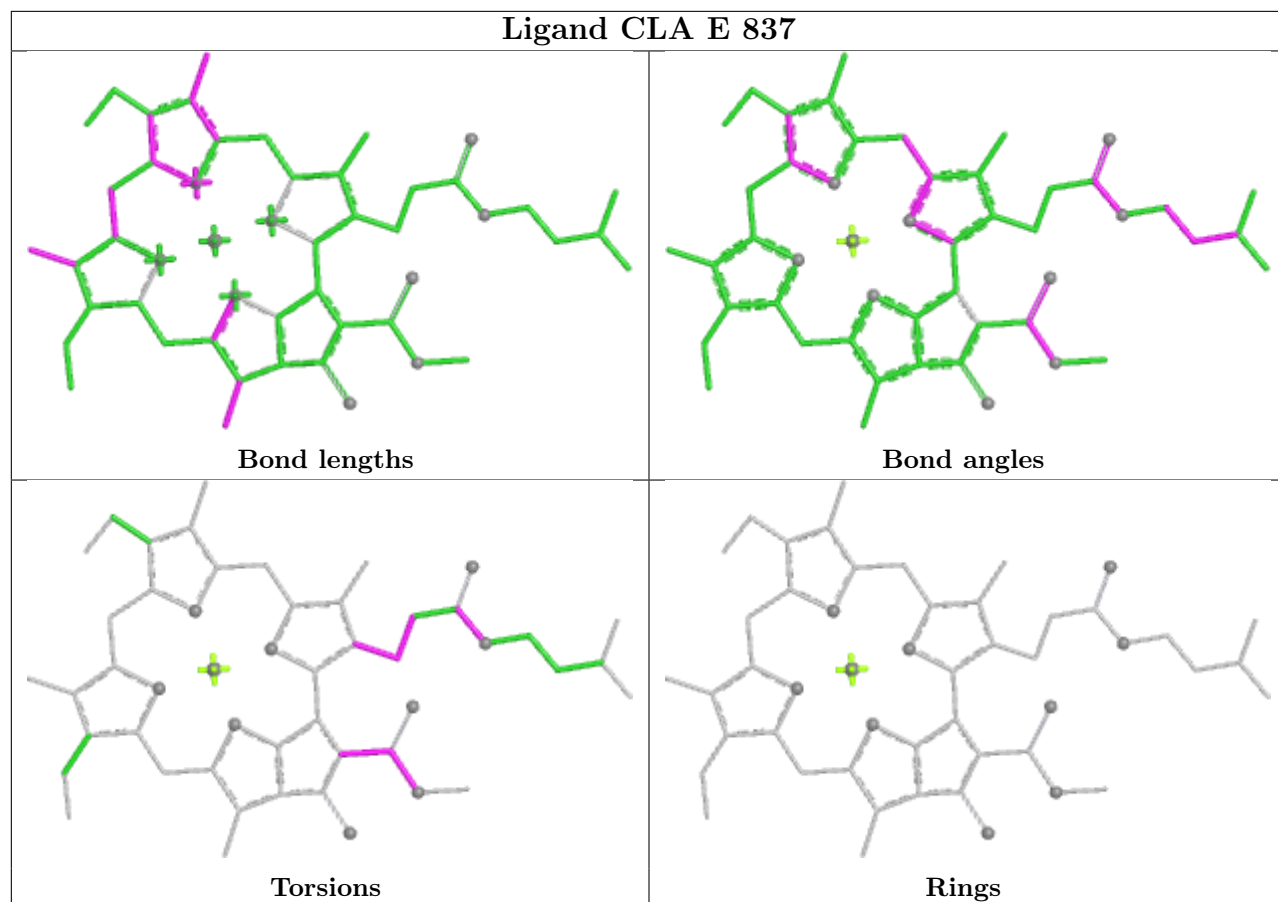
## Ligand CLA b 840



## Ligand CLA E 822

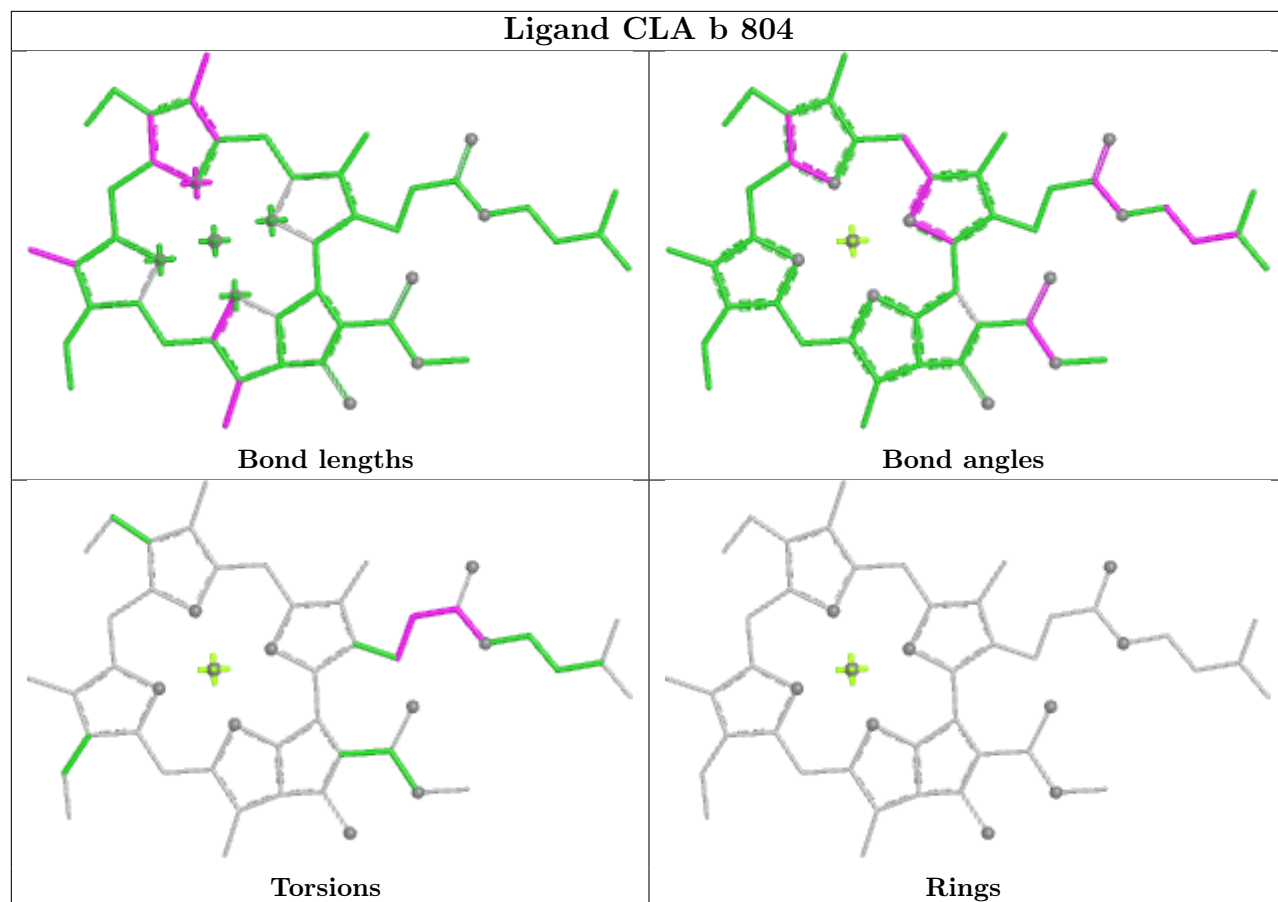


## Ligand CLA E 837

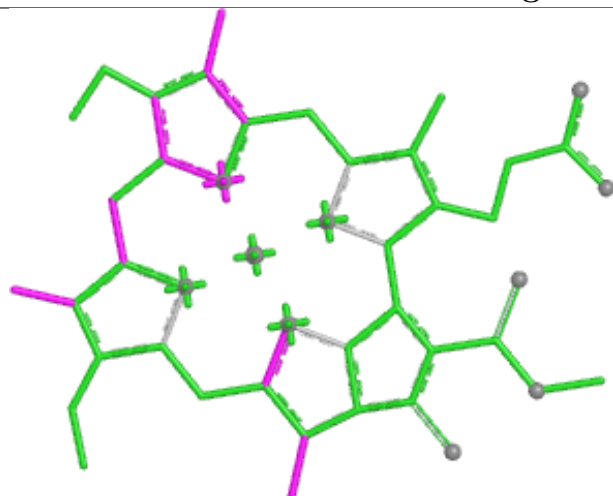




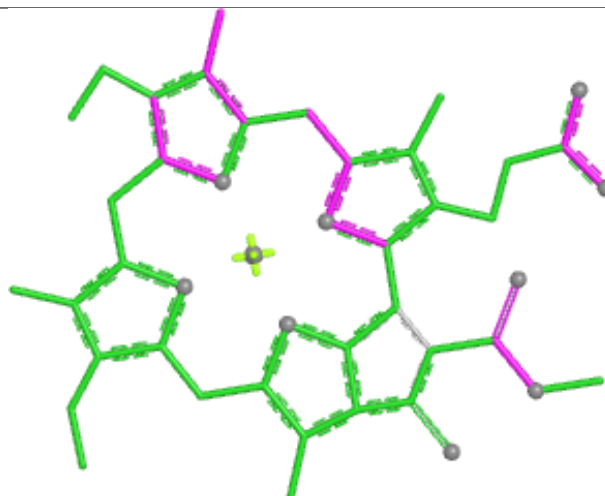
## Ligand CLA b 804



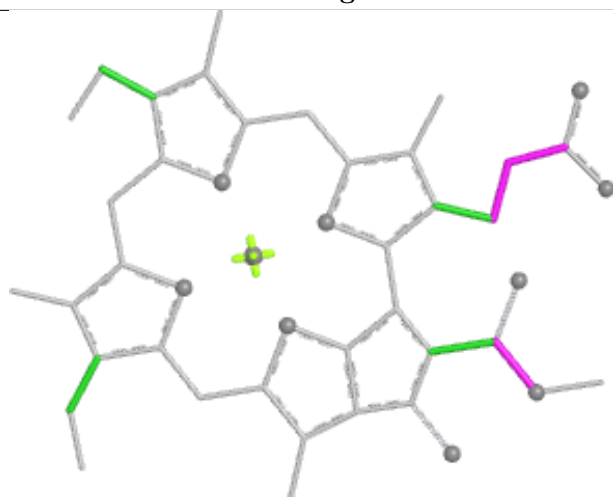
## Ligand CLA 1 204



Bond lengths



Bond angles

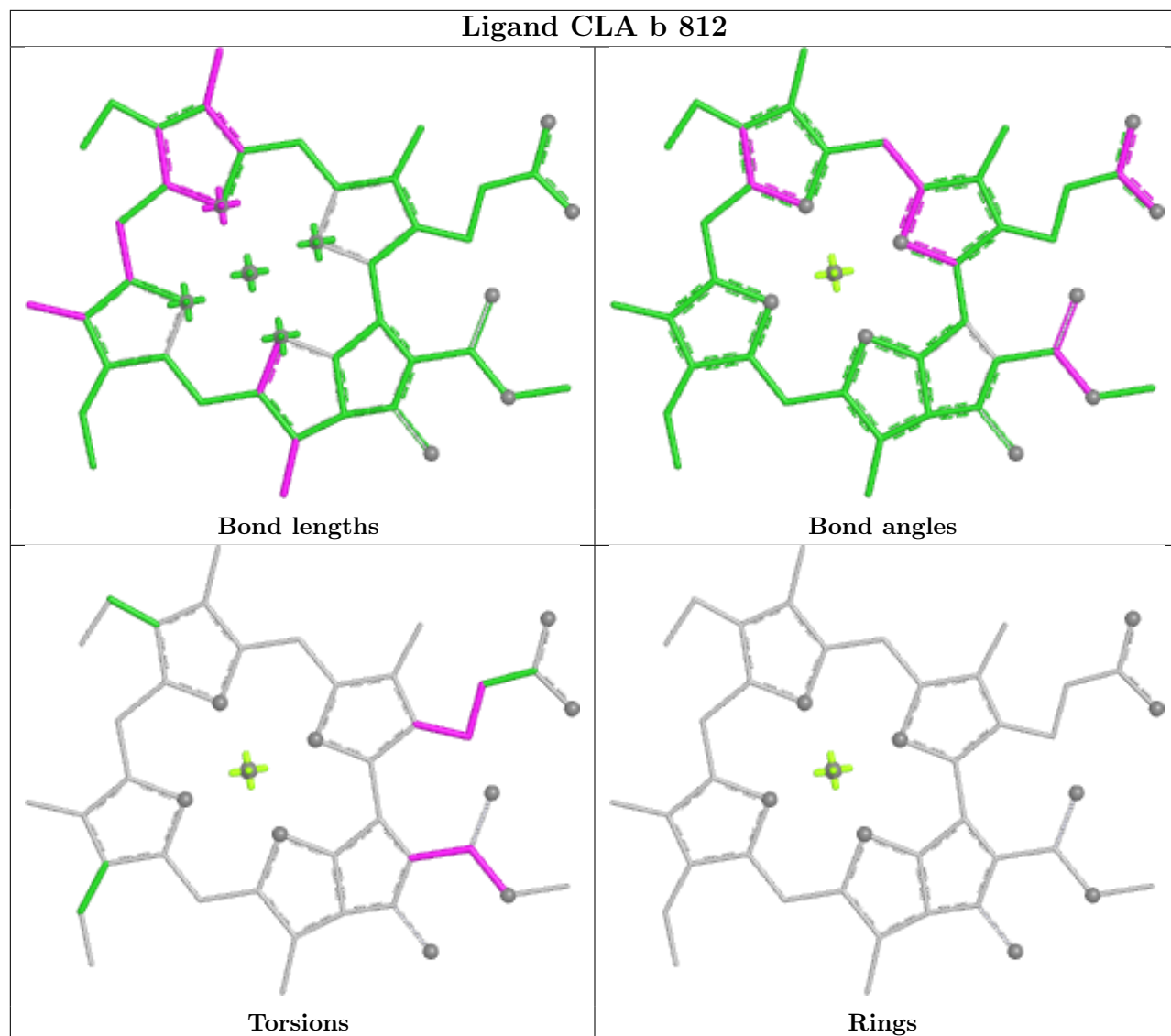


Torsions

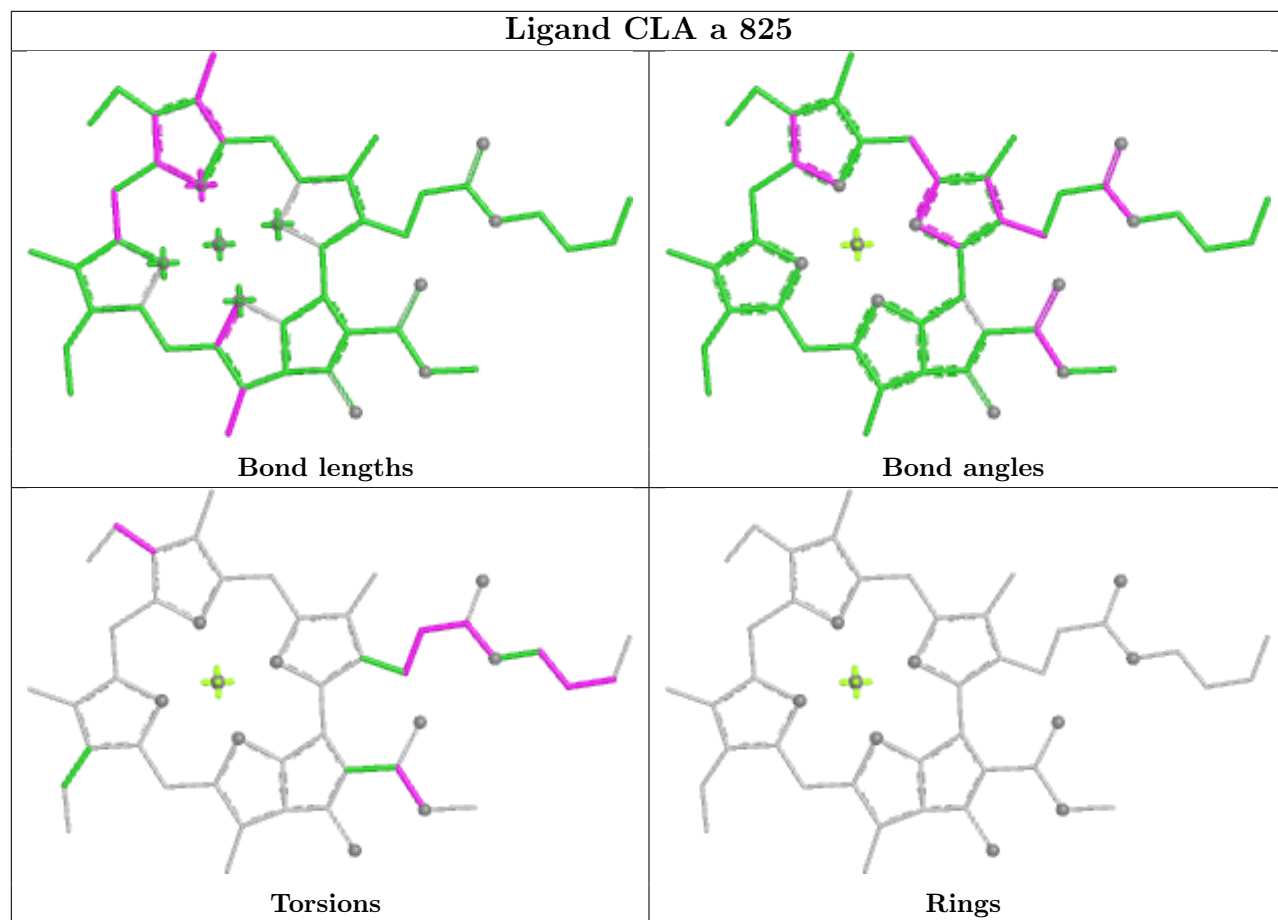


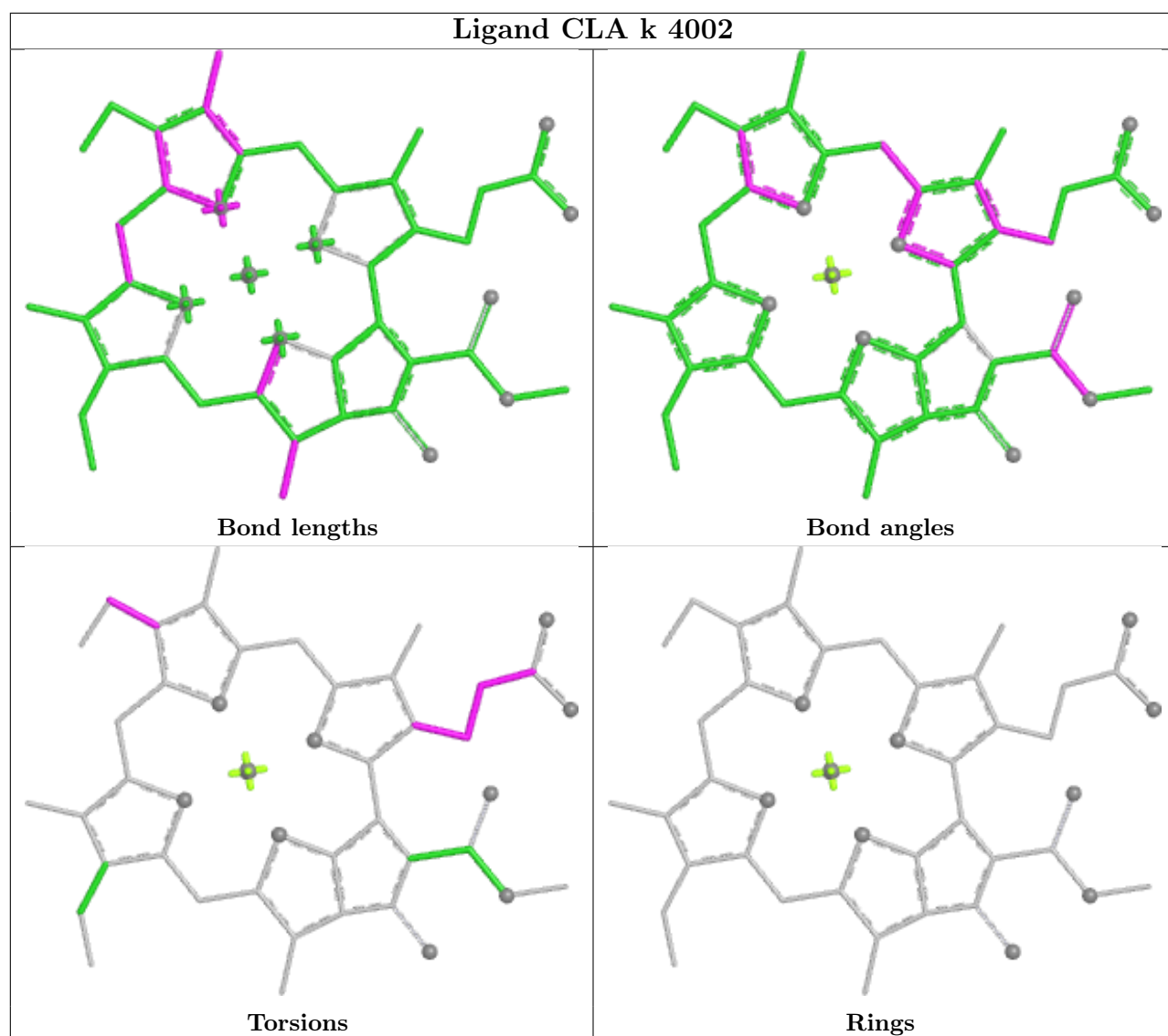
Rings

## Ligand CLA b 812

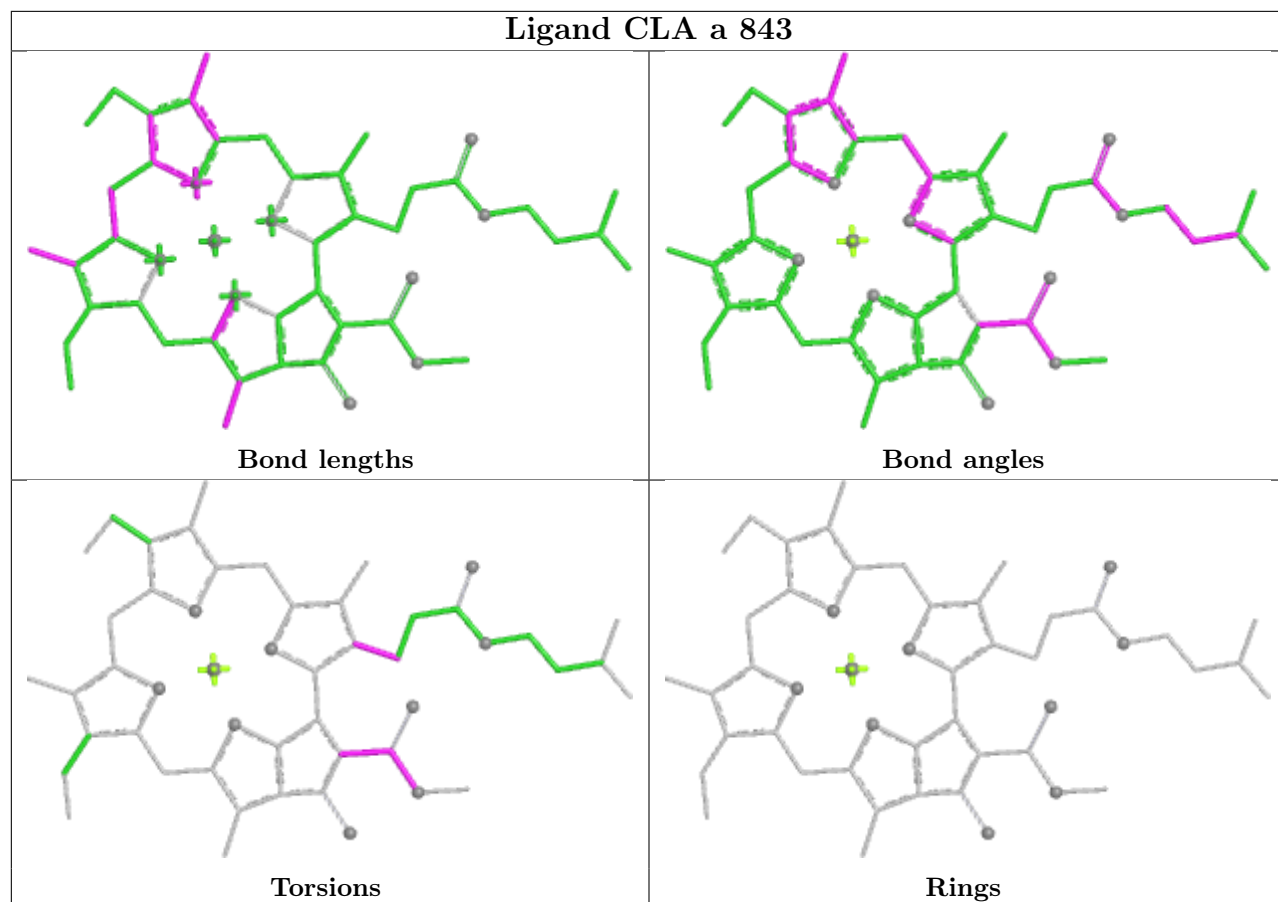


## Ligand CLA a 825

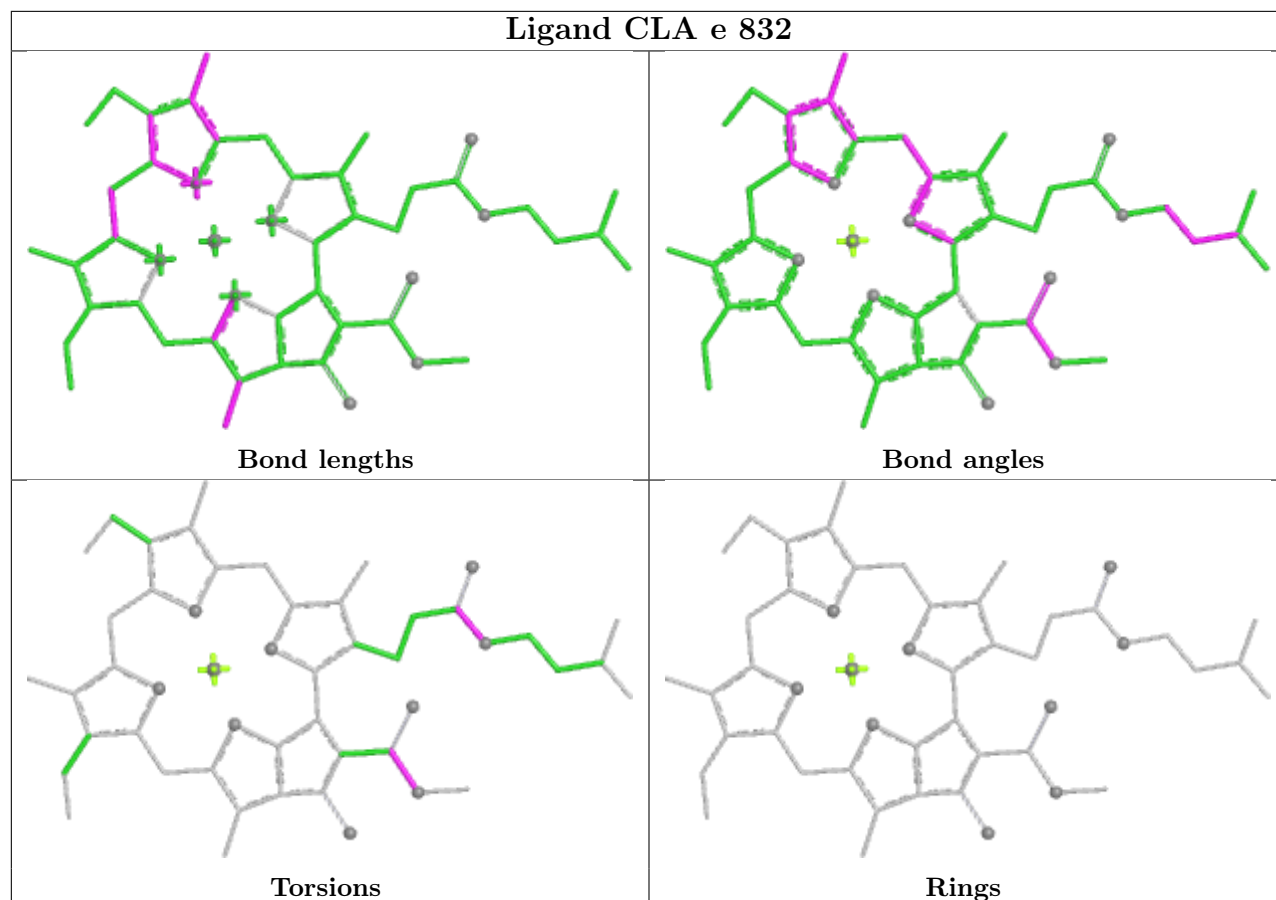




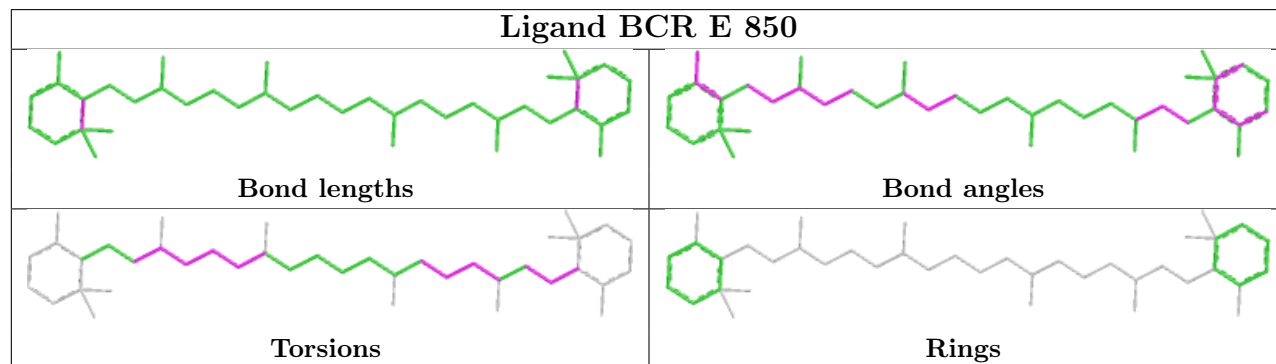
## Ligand CLA a 843

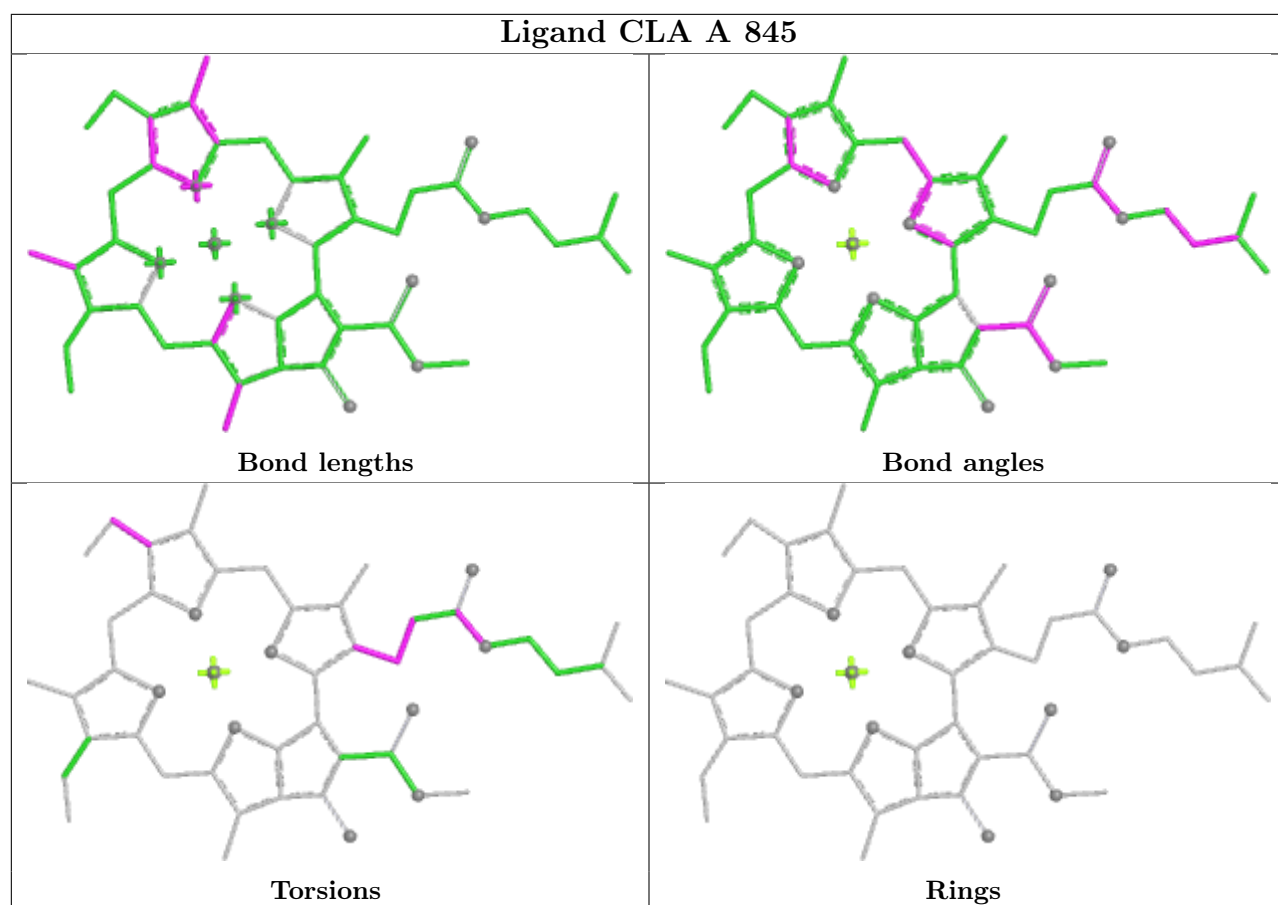


## Ligand CLA e 832

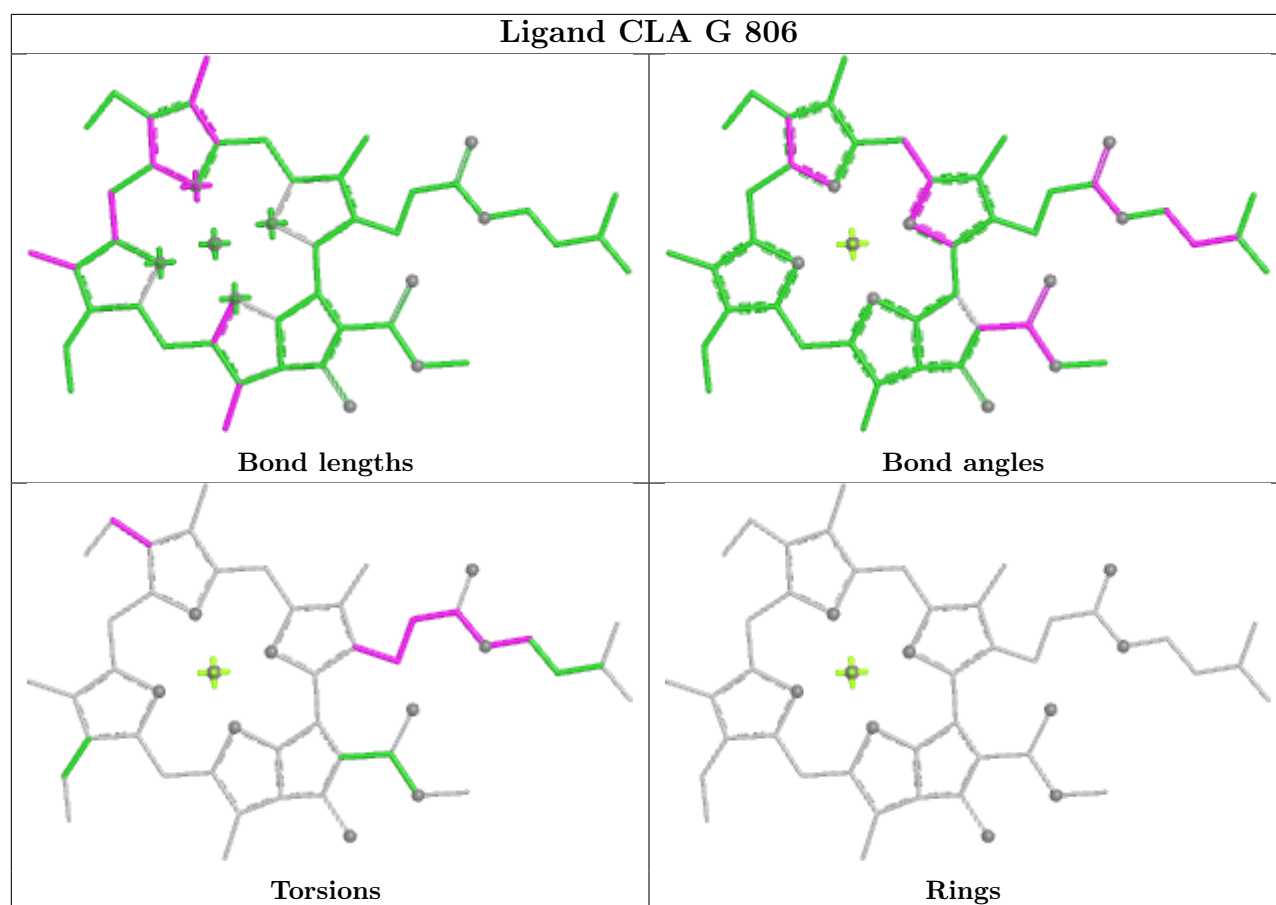


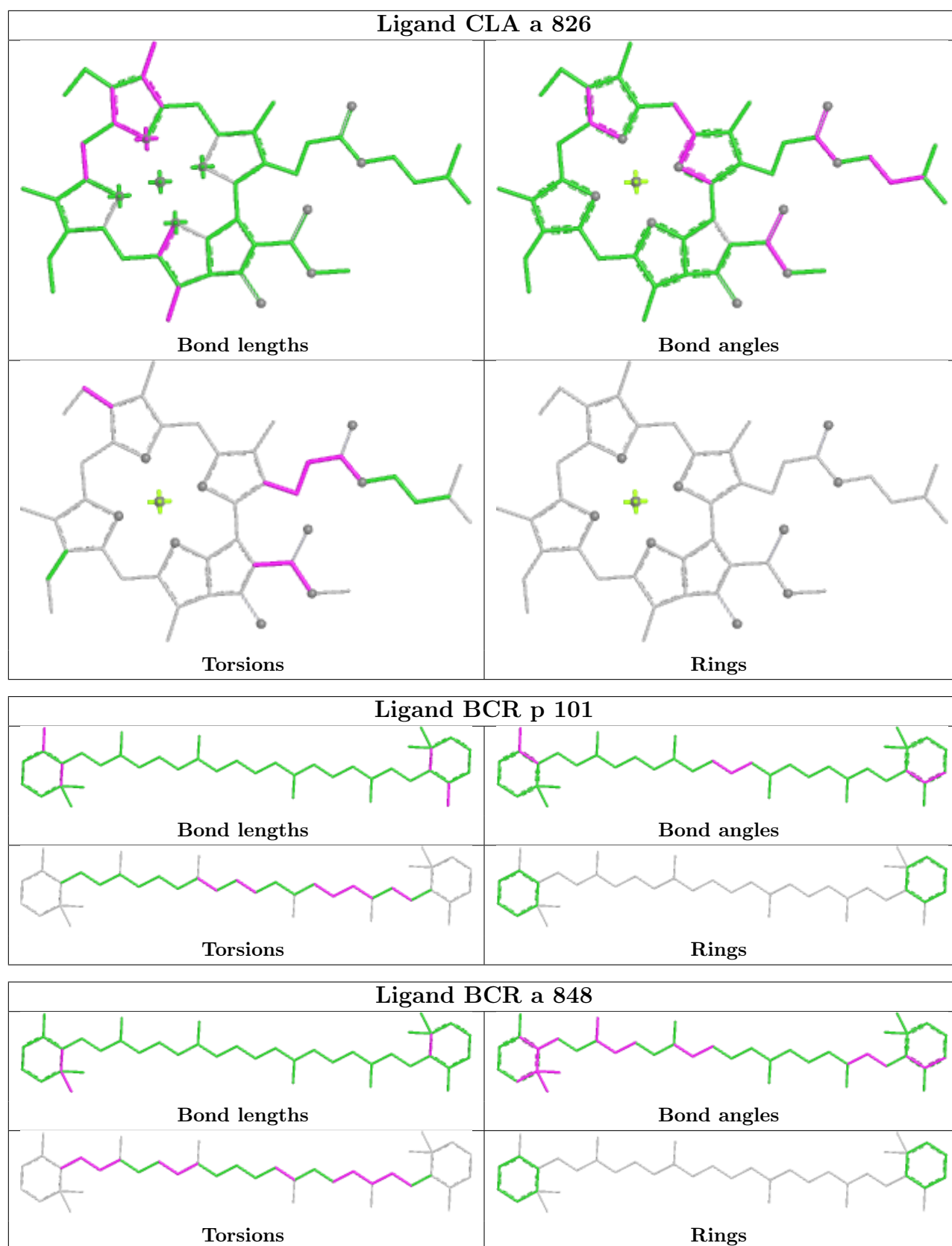
## Ligand BCR E 850



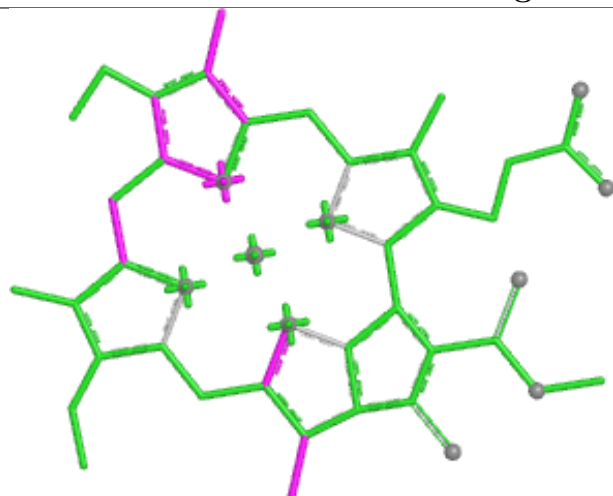




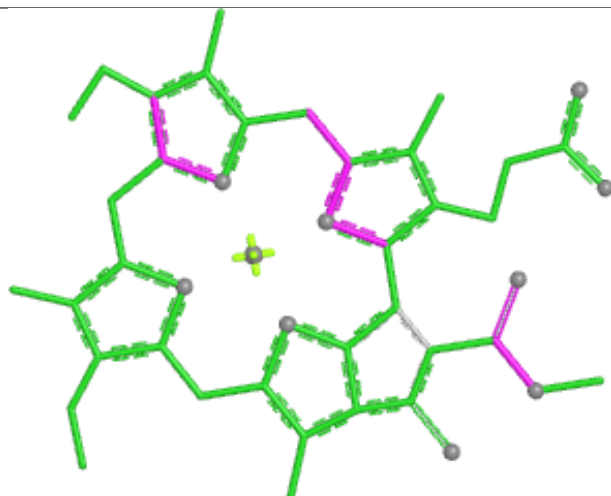




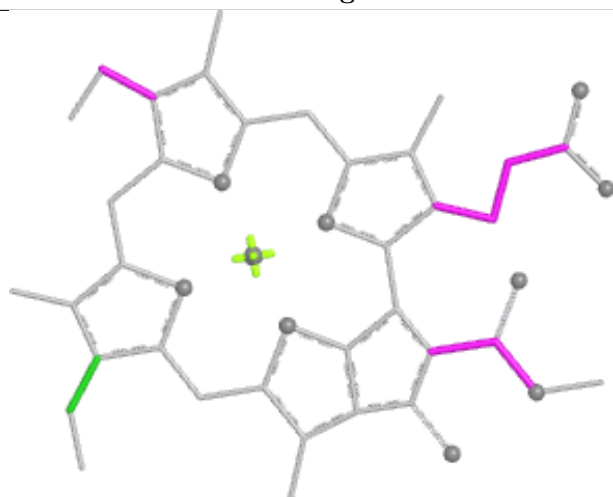
## Ligand CLA B 831



Bond lengths



Bond angles

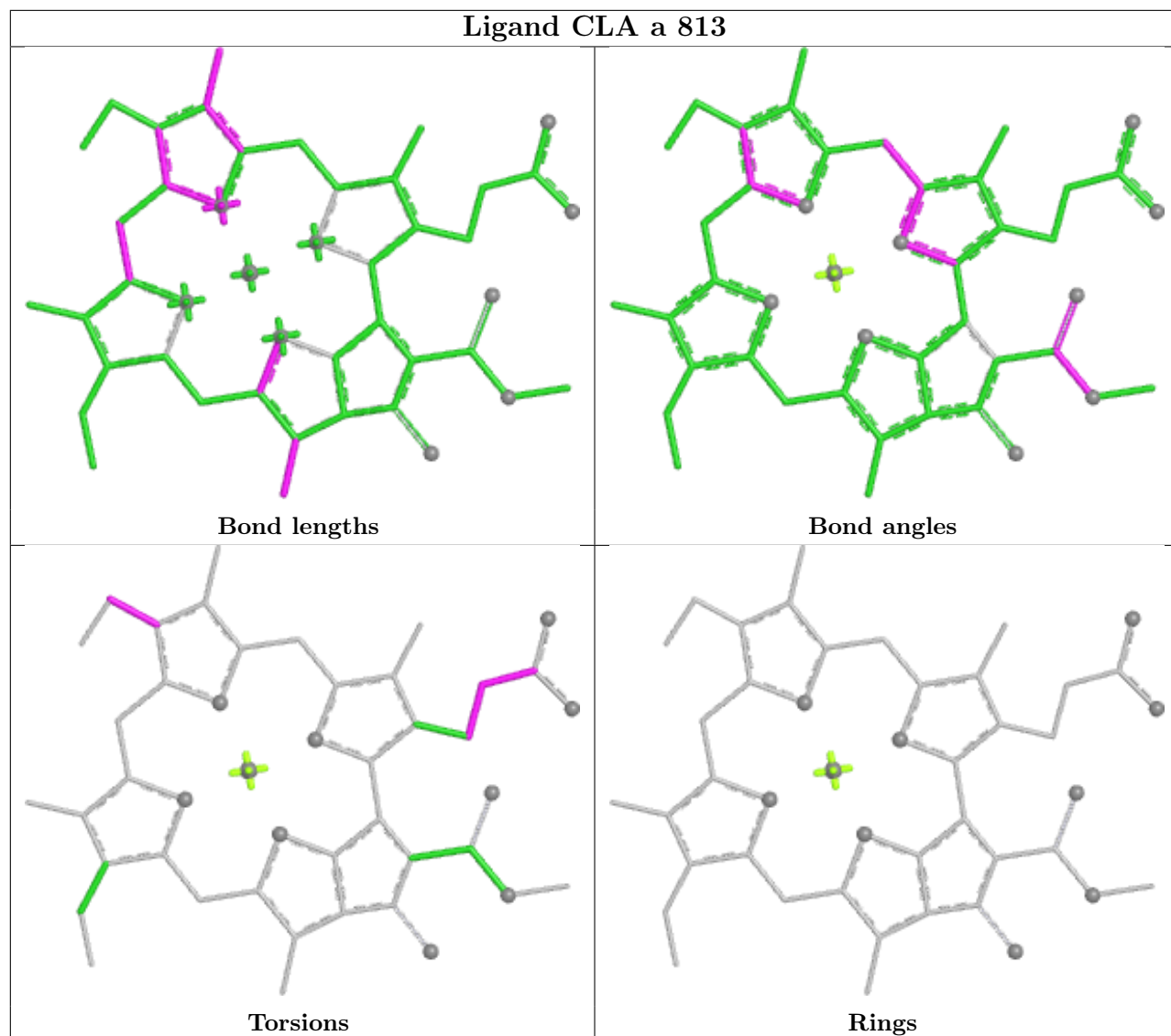


Torsions

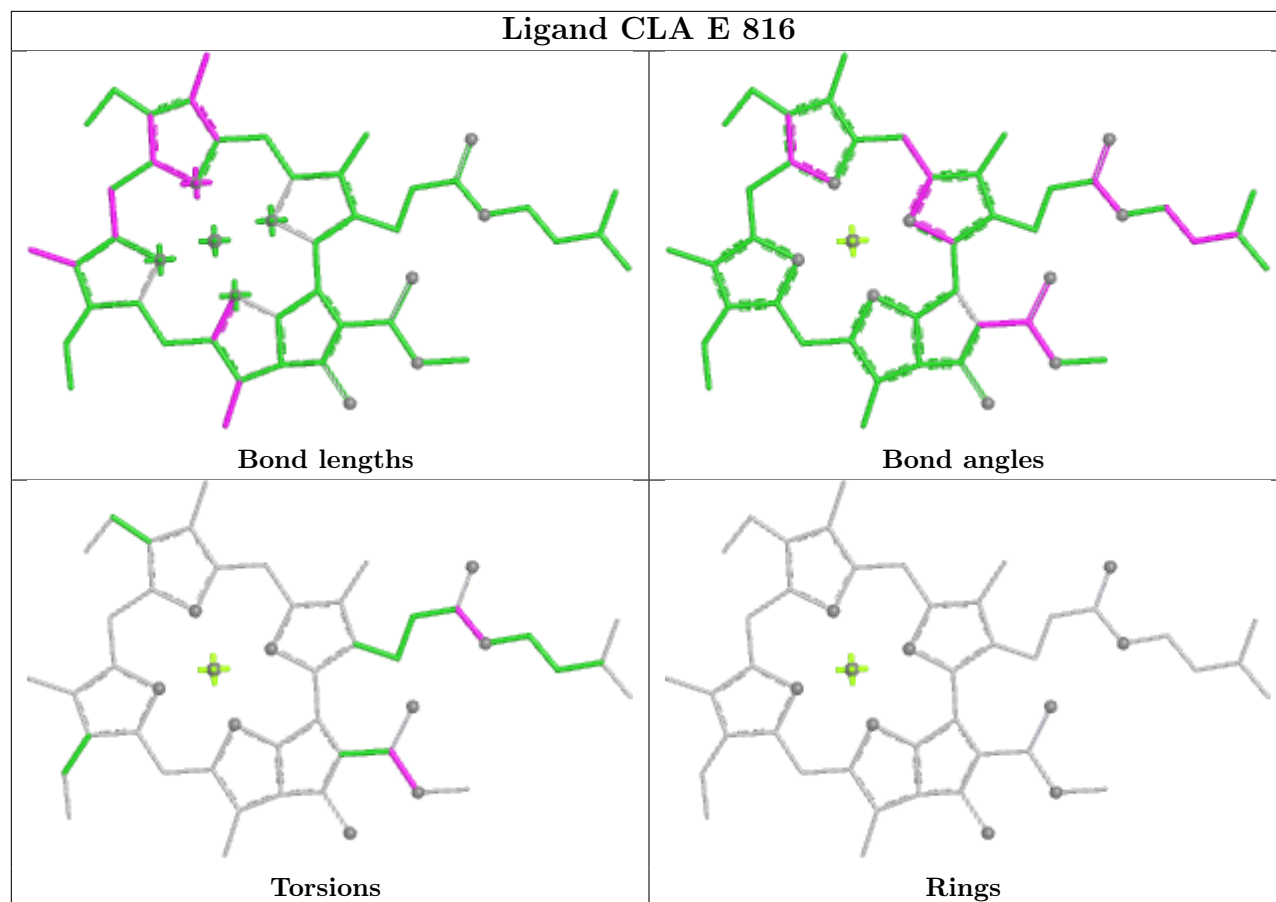


Rings

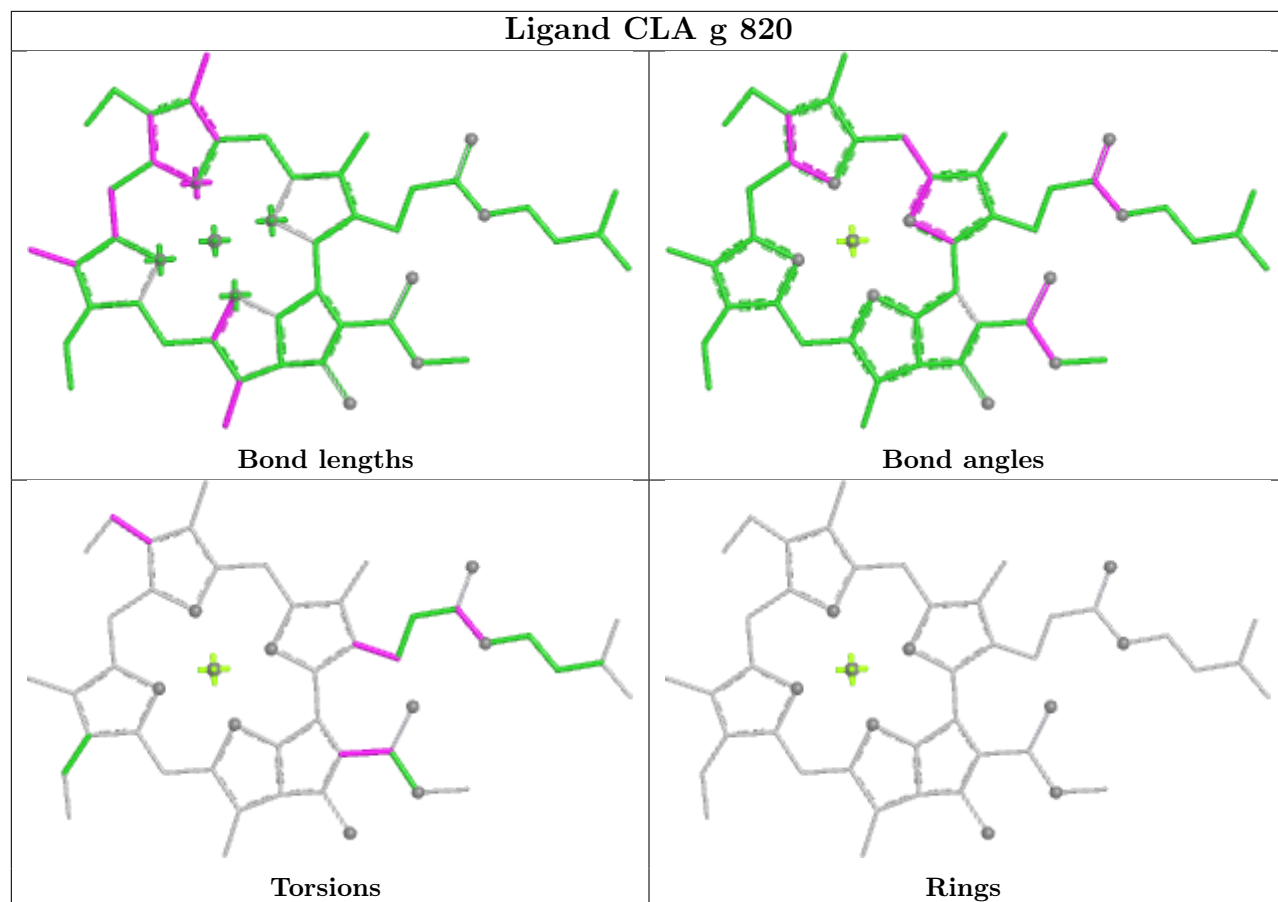
## Ligand CLA a 813

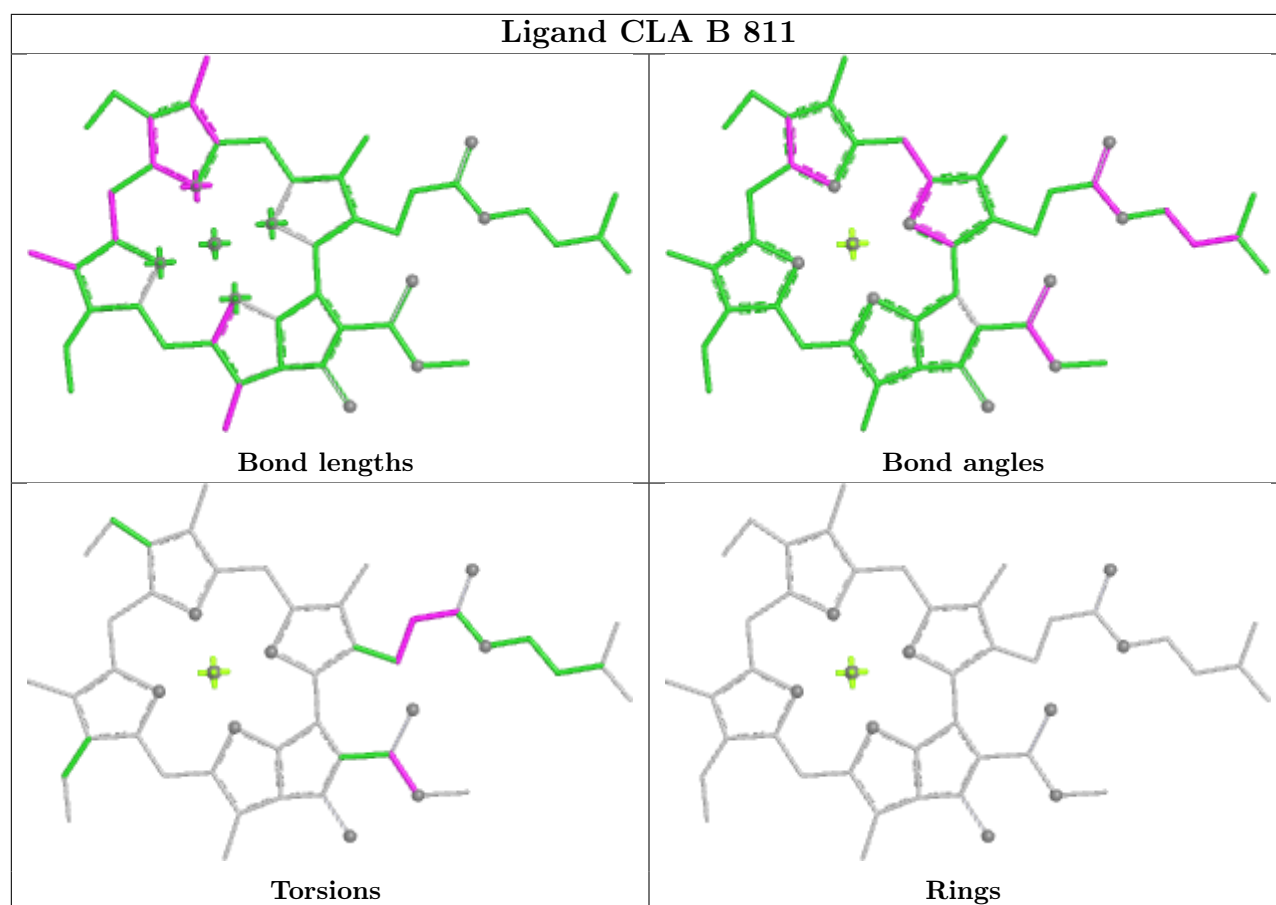


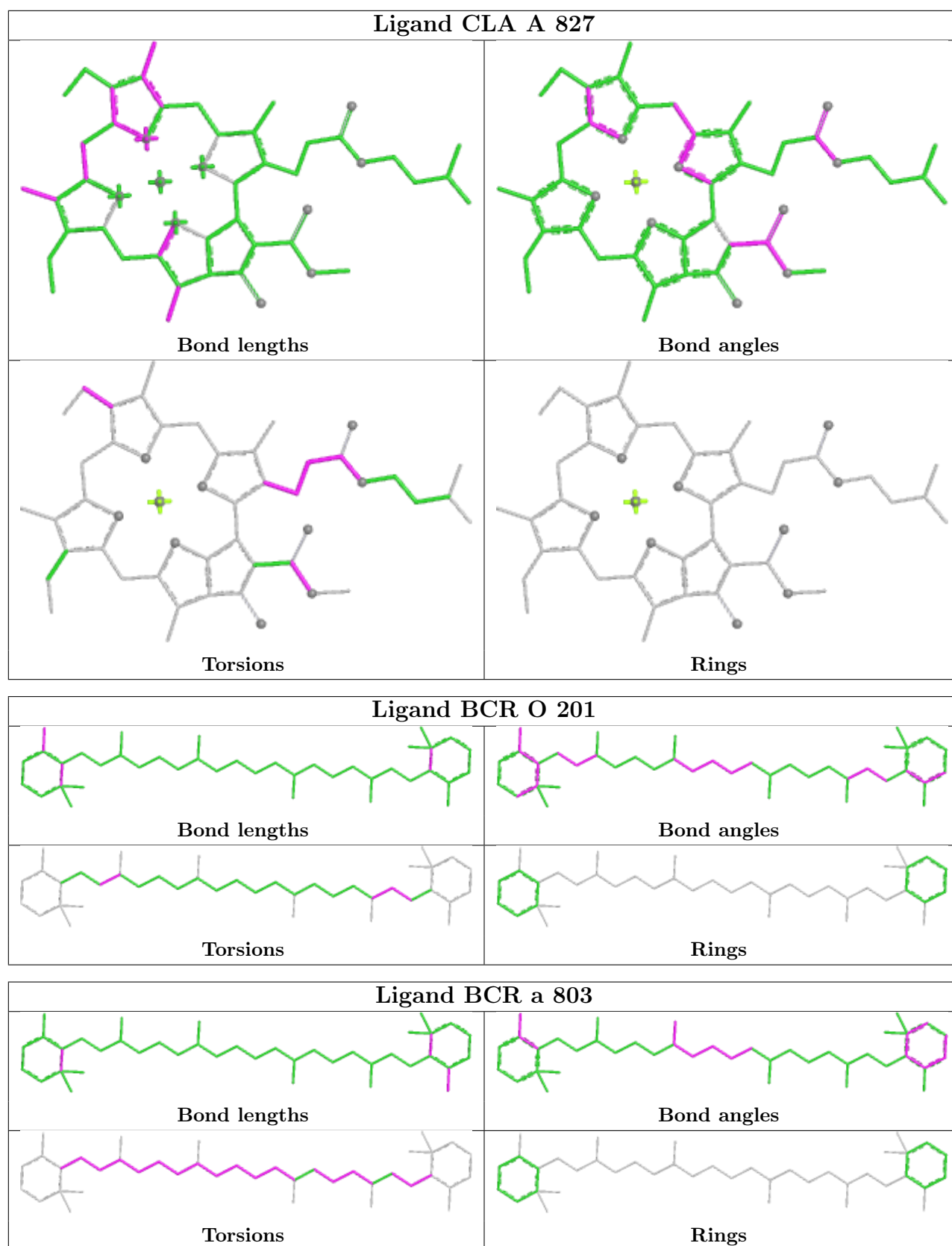
## Ligand CLA E 816



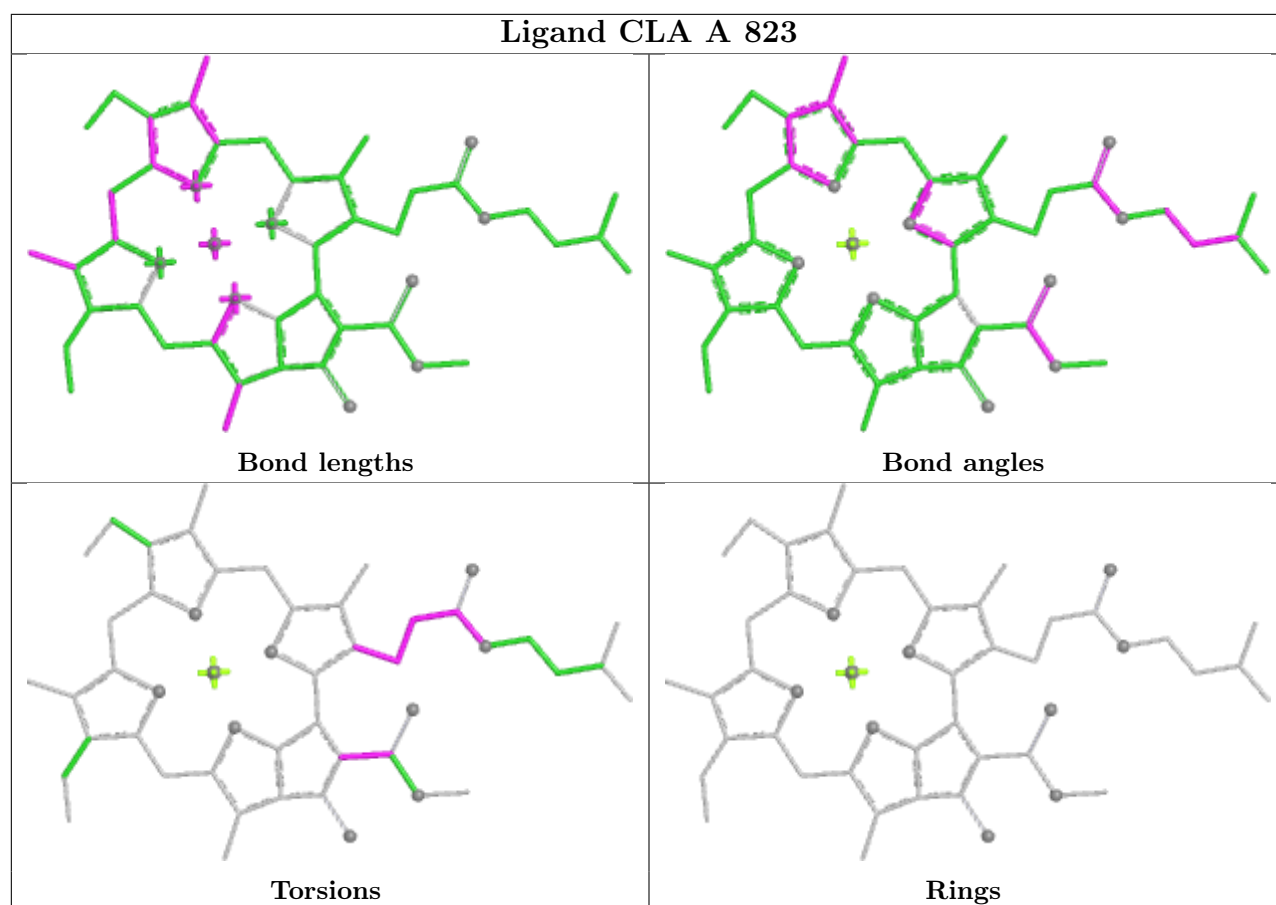
## Ligand CLA g 820

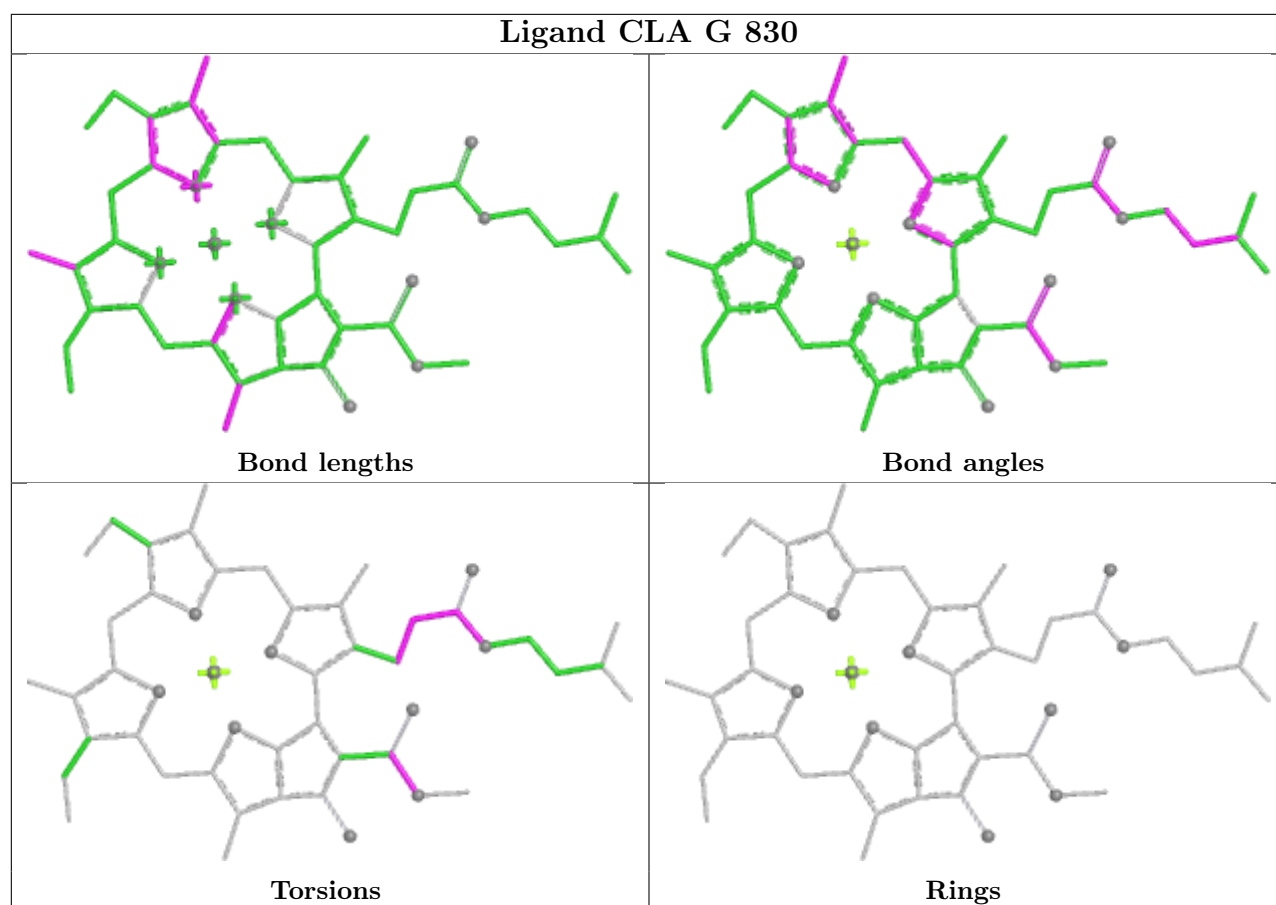


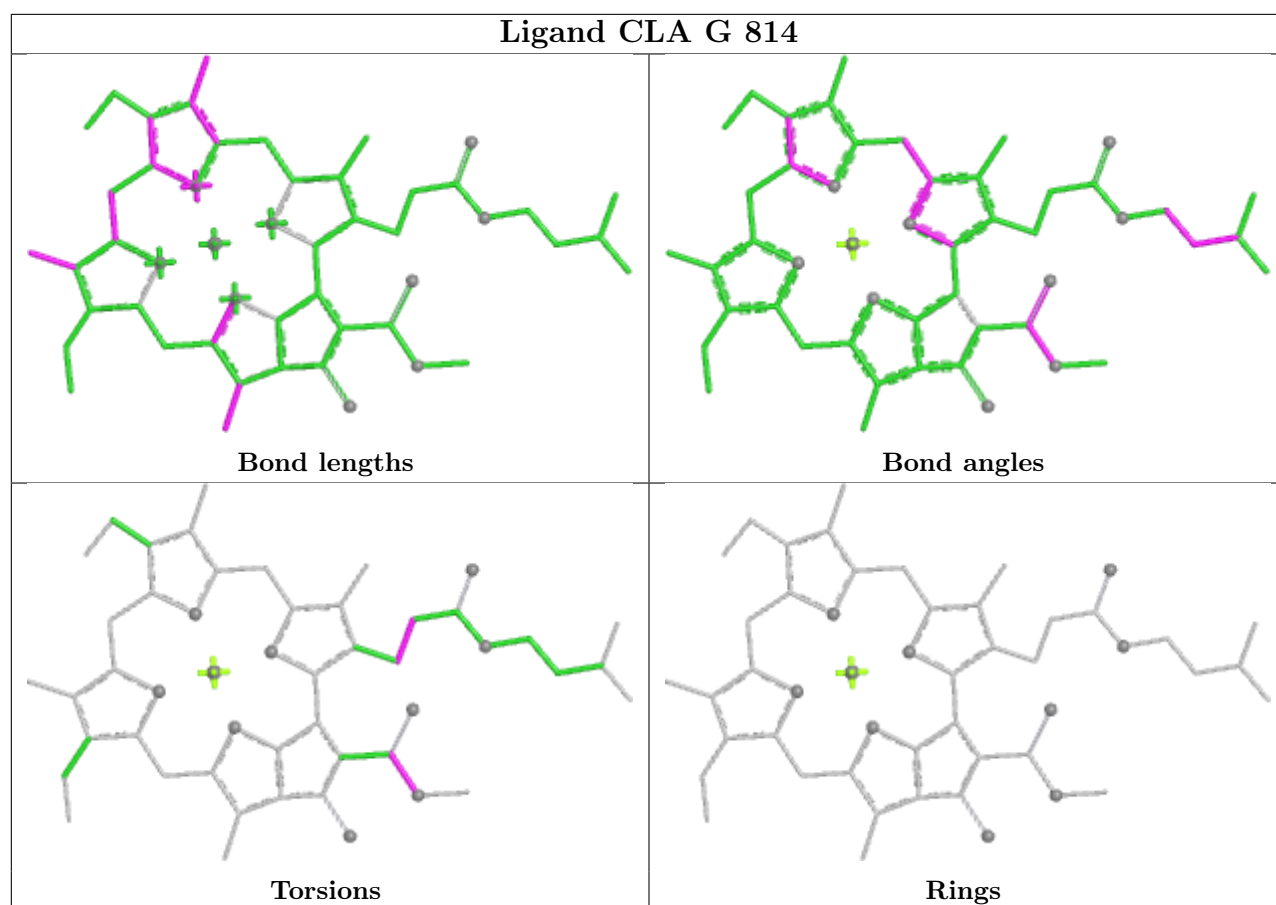




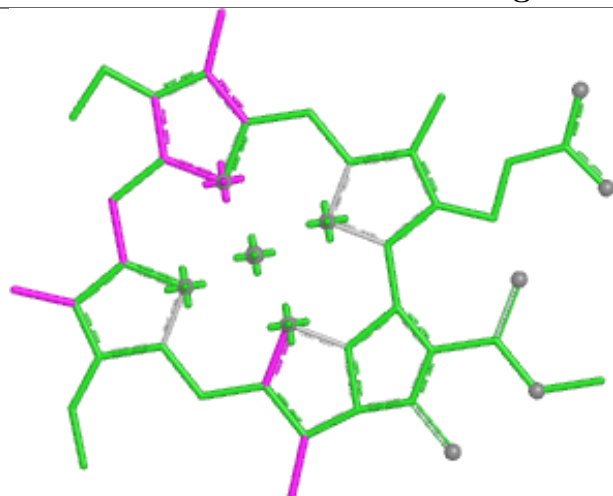




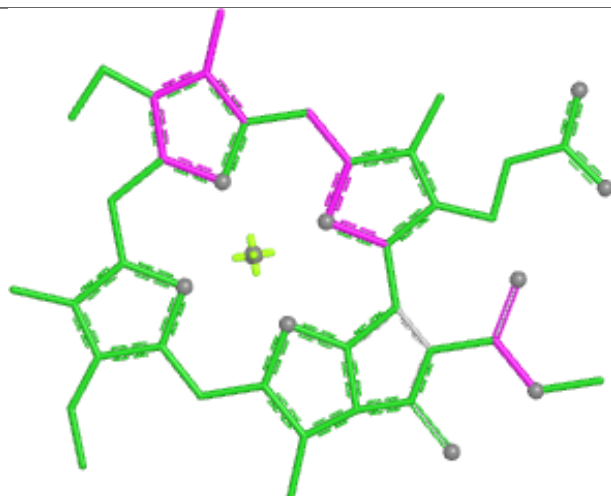




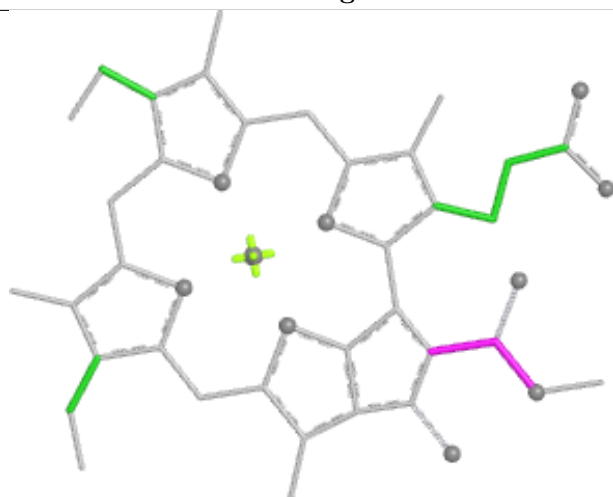
## Ligand CLA G 822



Bond lengths



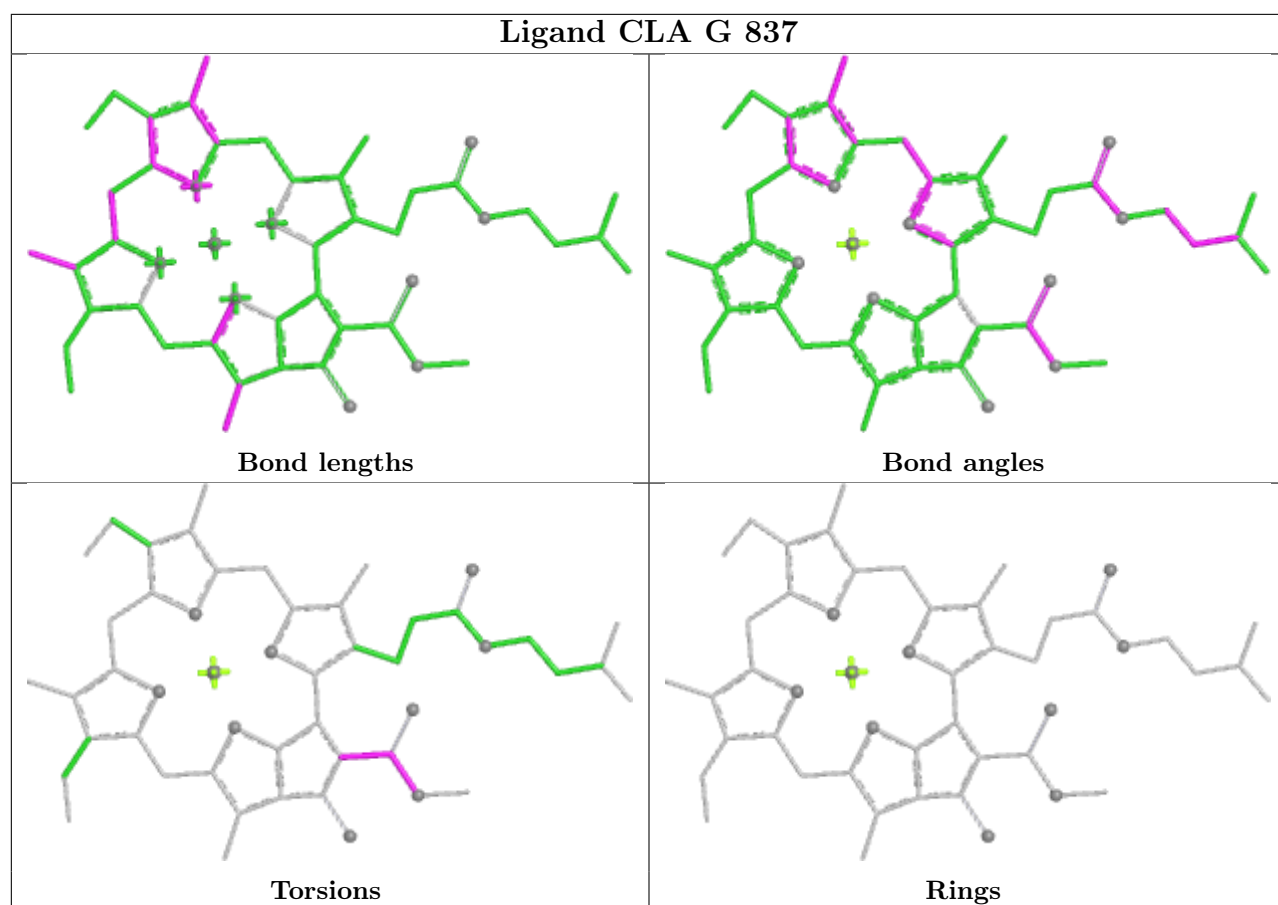
Bond angles



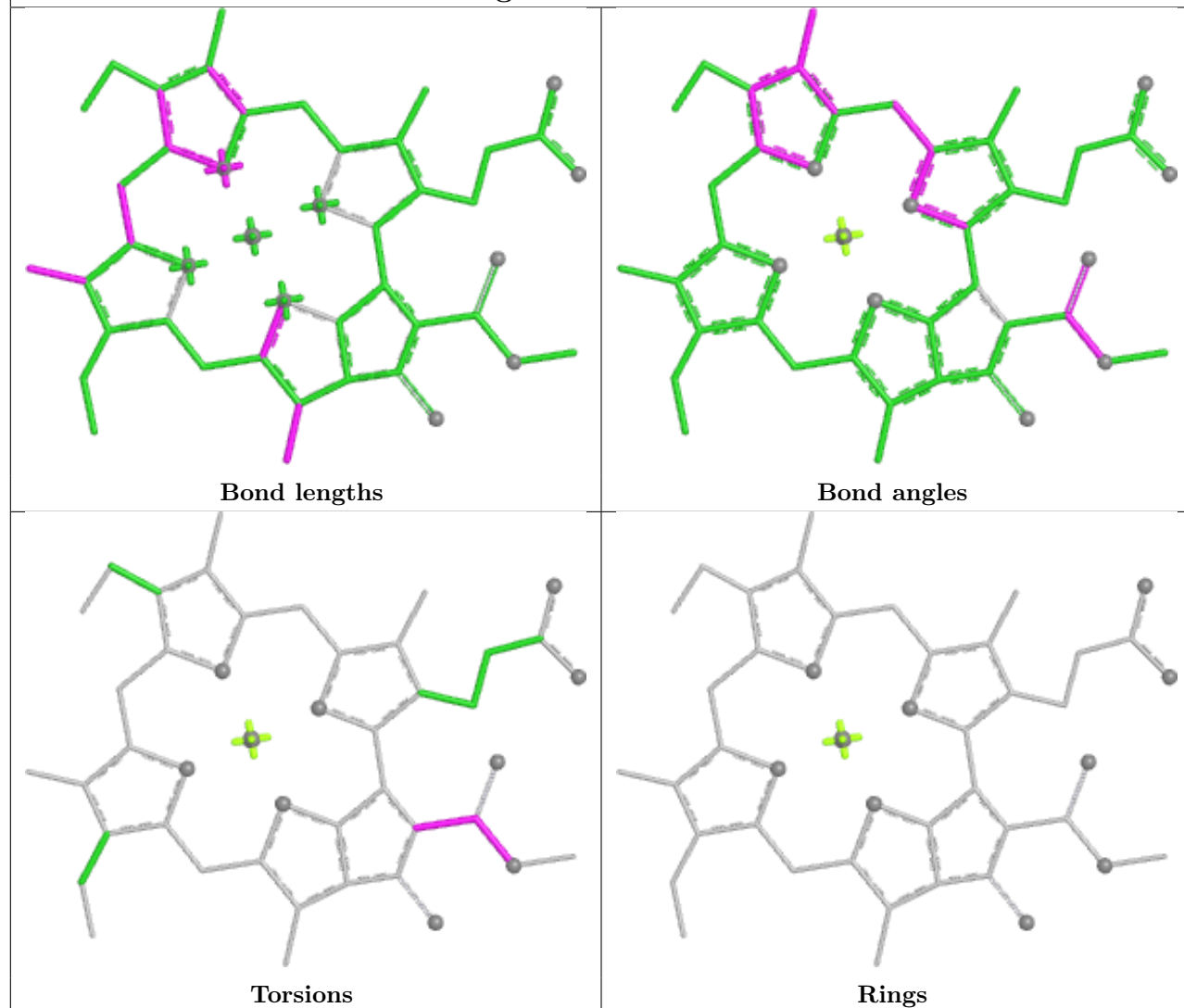
Torsions



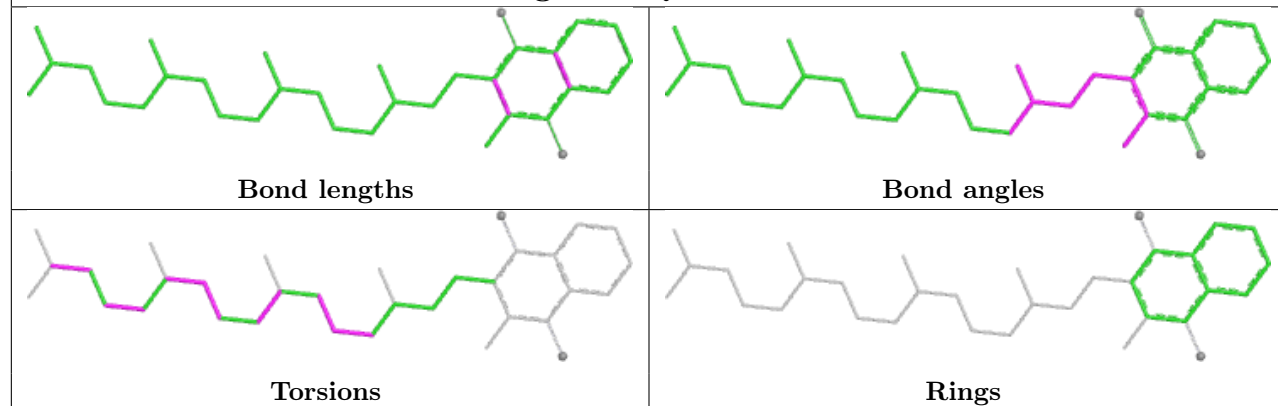
Rings



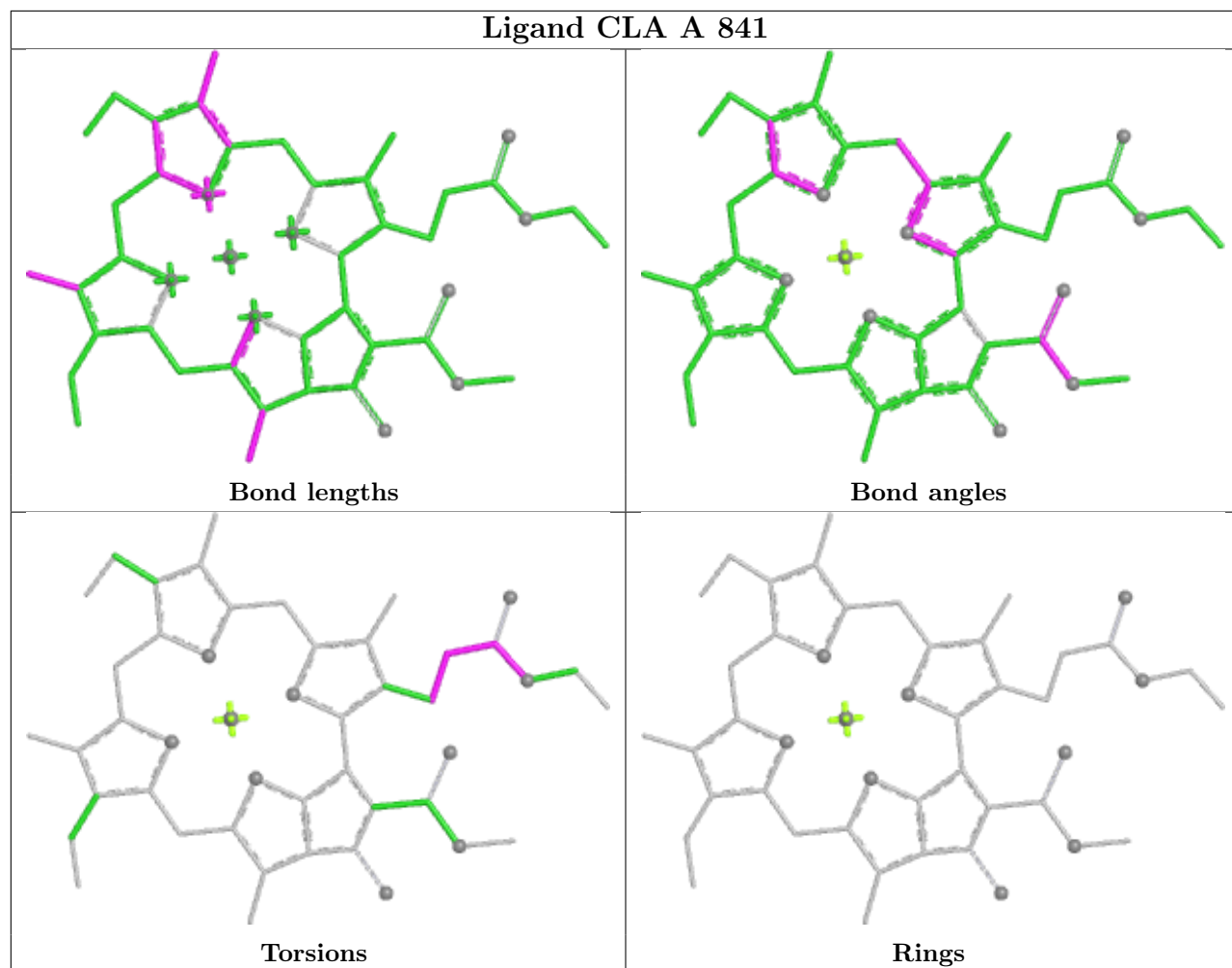
## Ligand CLA b 821



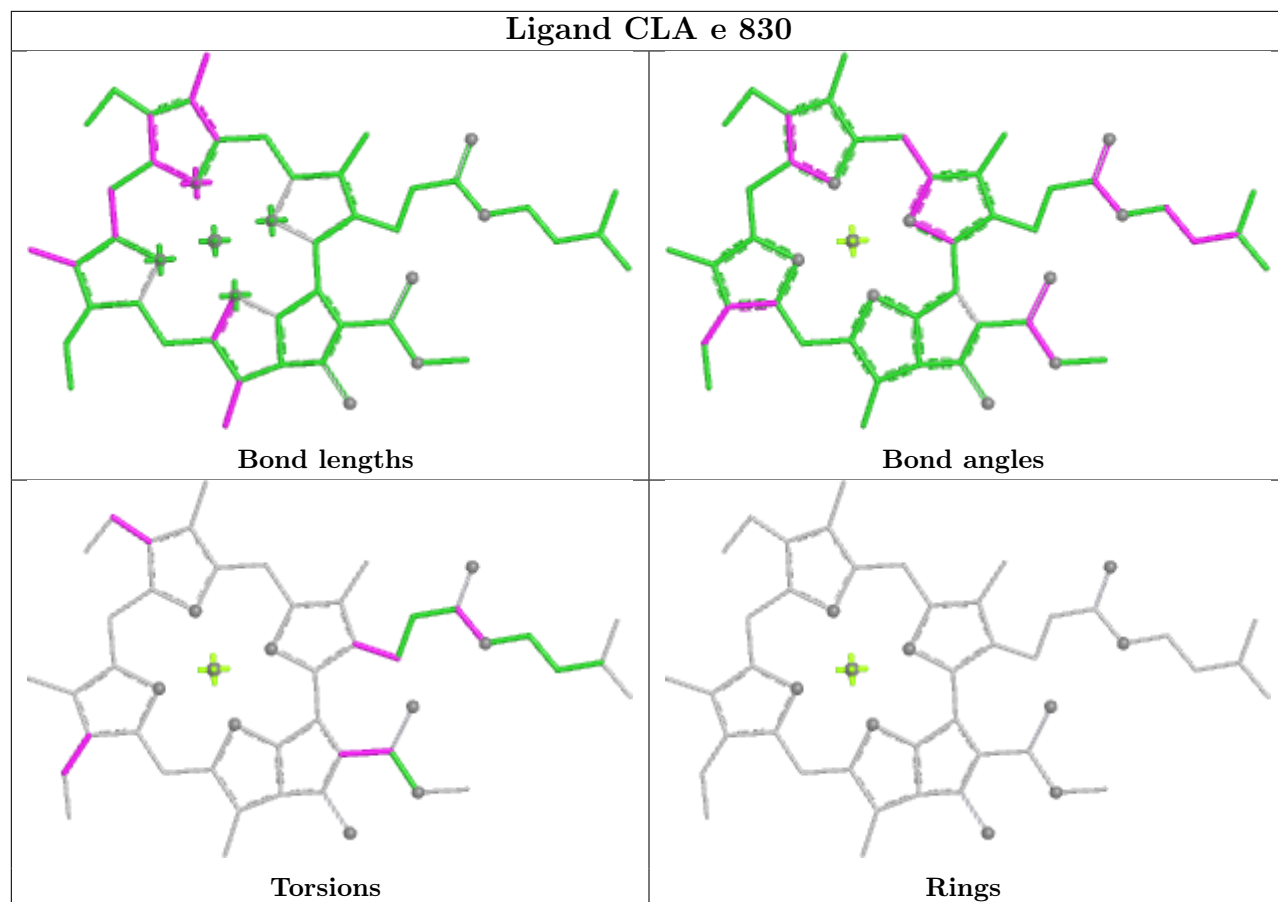
## Ligand PQN a 847



## Ligand CLA A 841

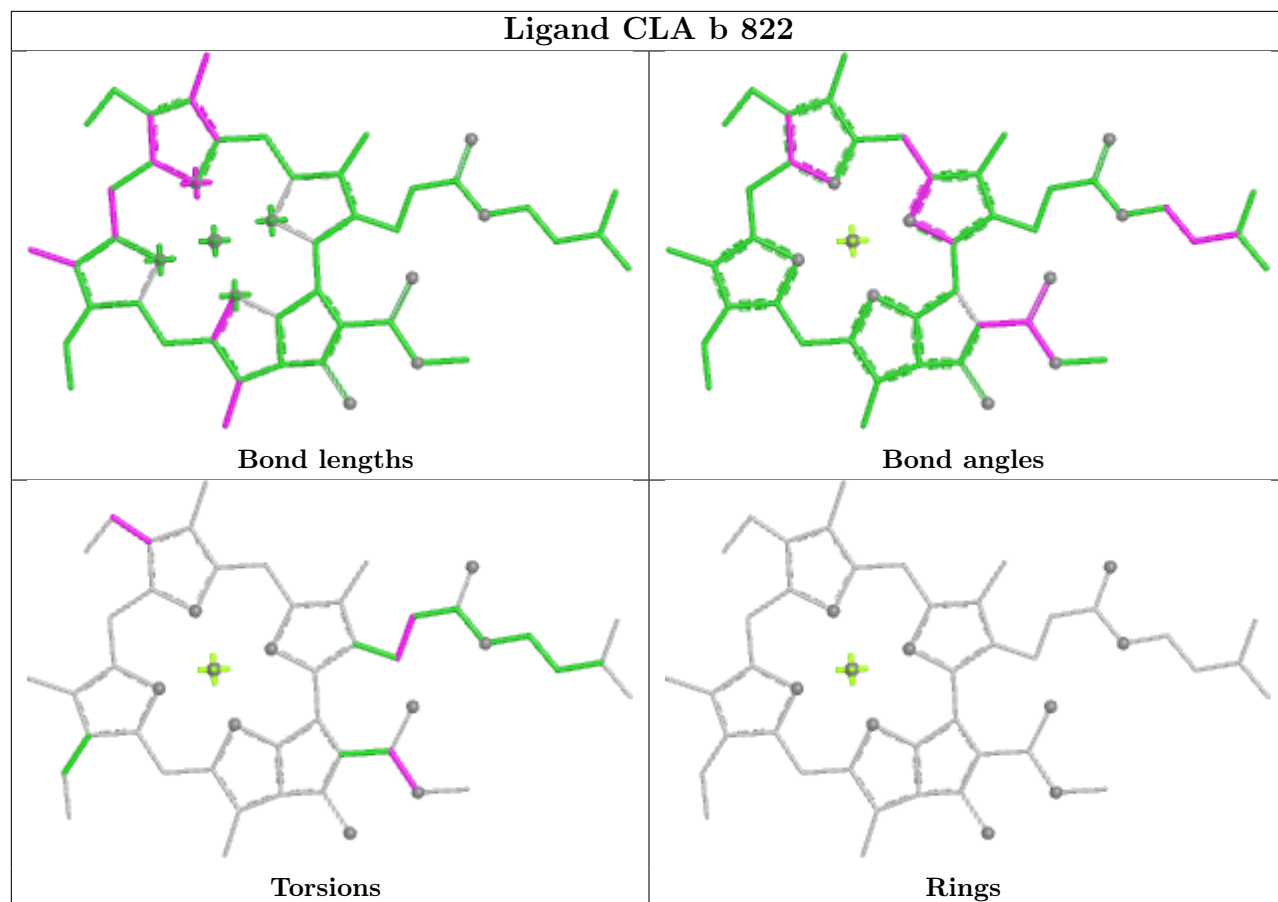


## Ligand CLA e 830

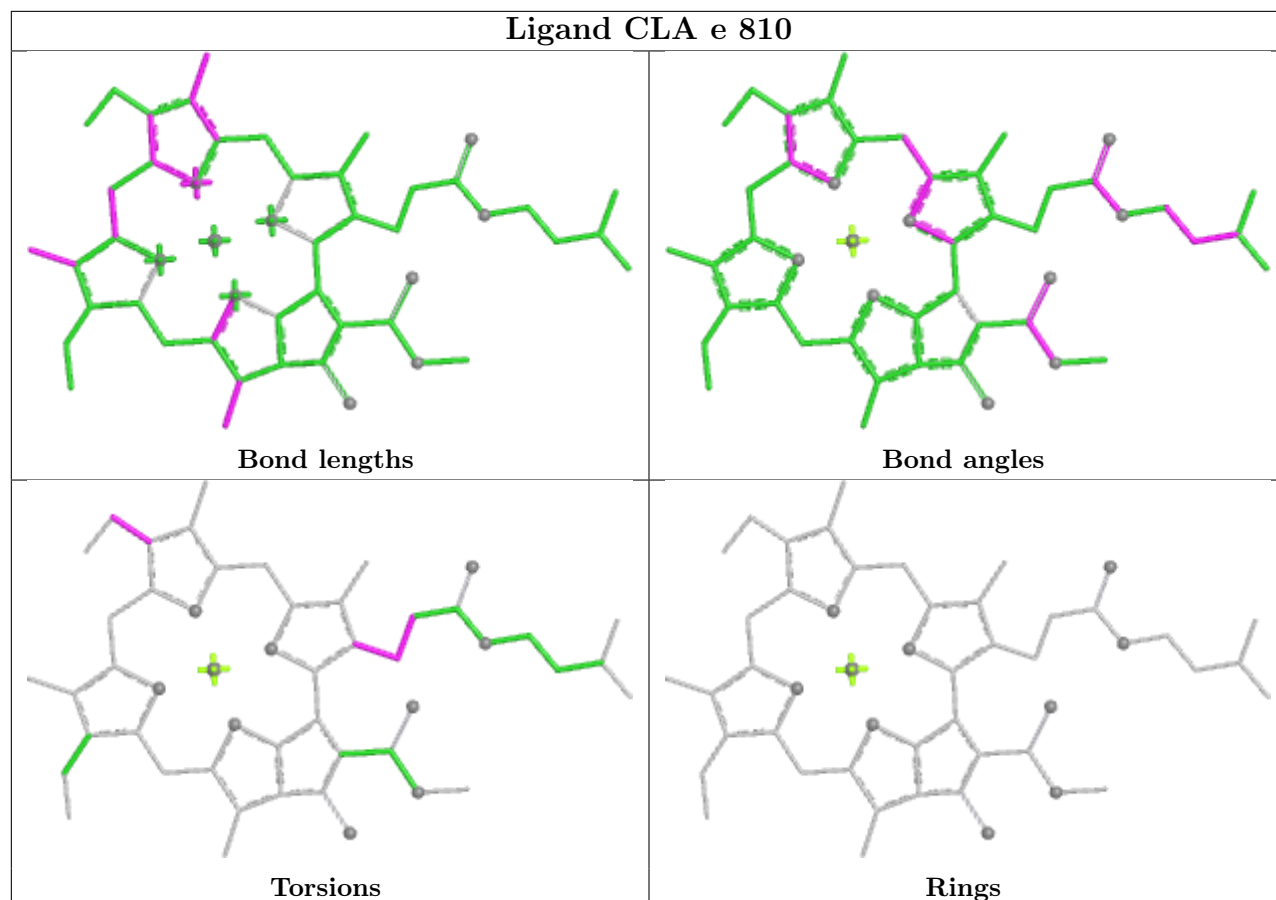




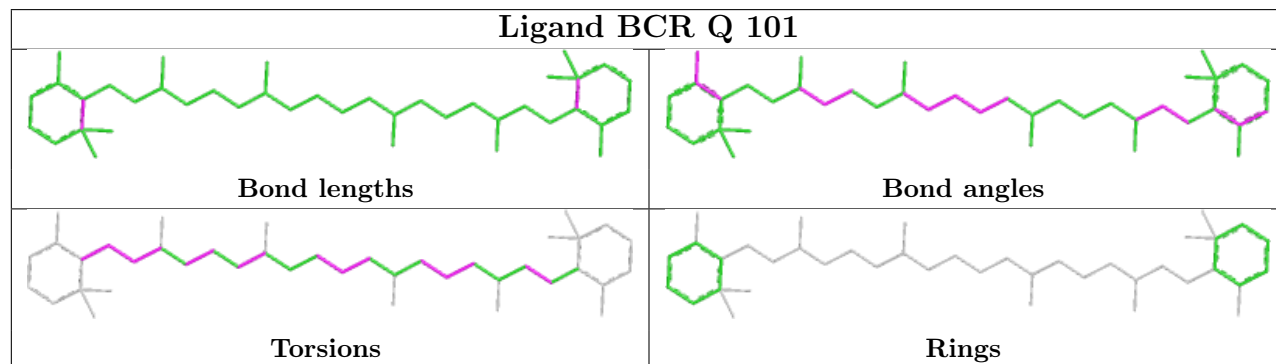
## Ligand CLA b 822



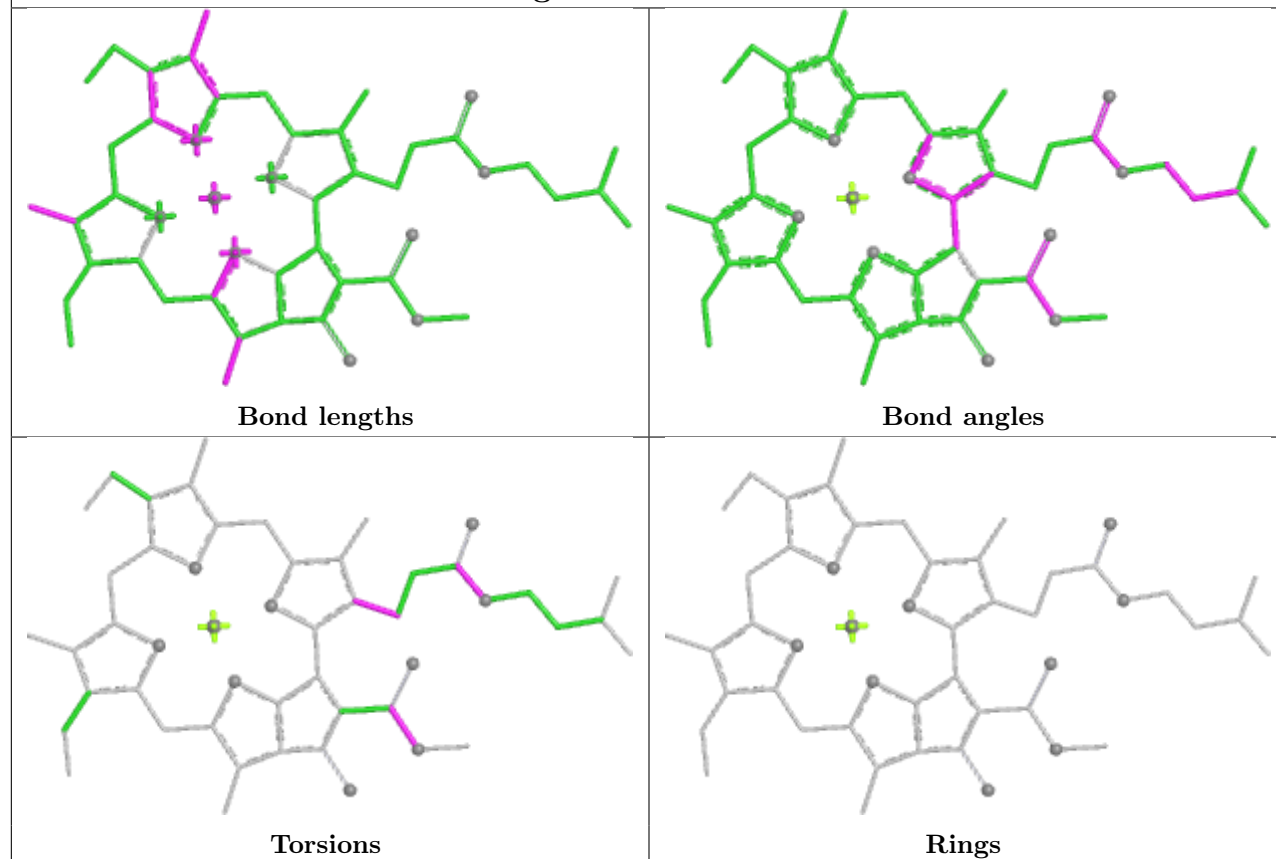
## Ligand CLA e 810



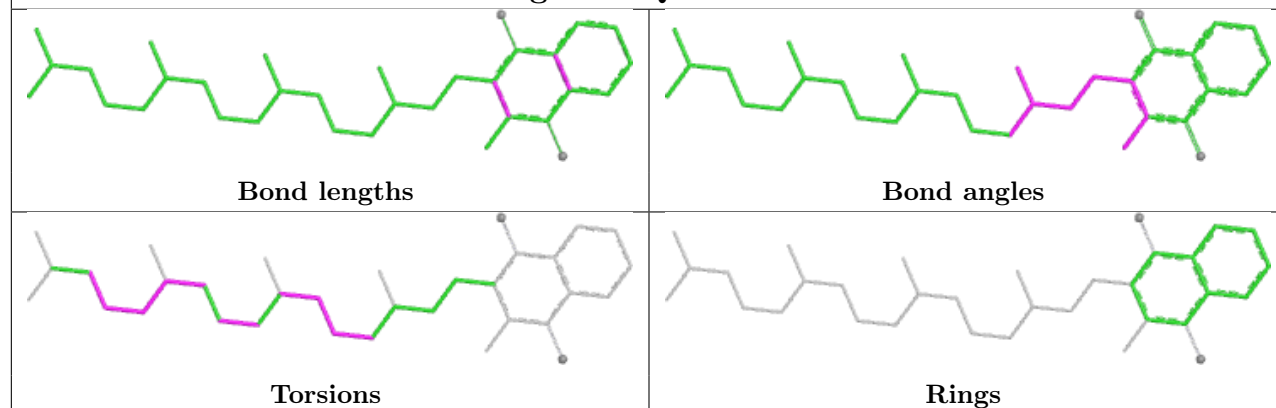
## Ligand BCR Q 101



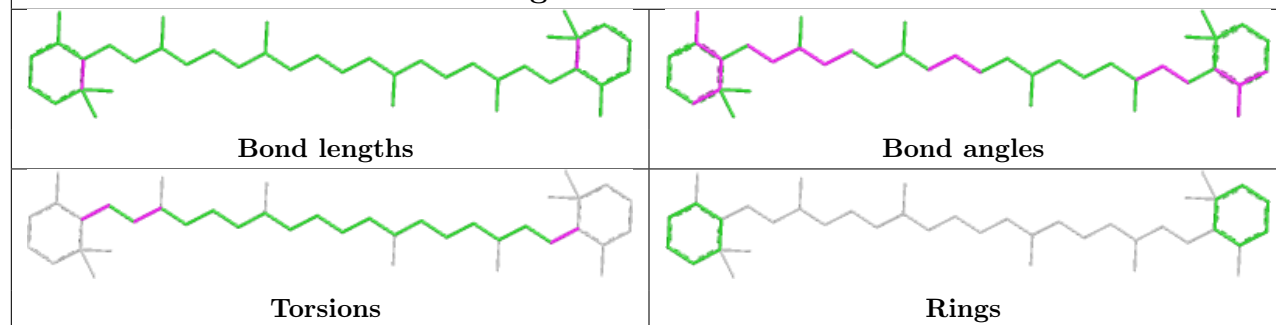
## Ligand CLA E 836



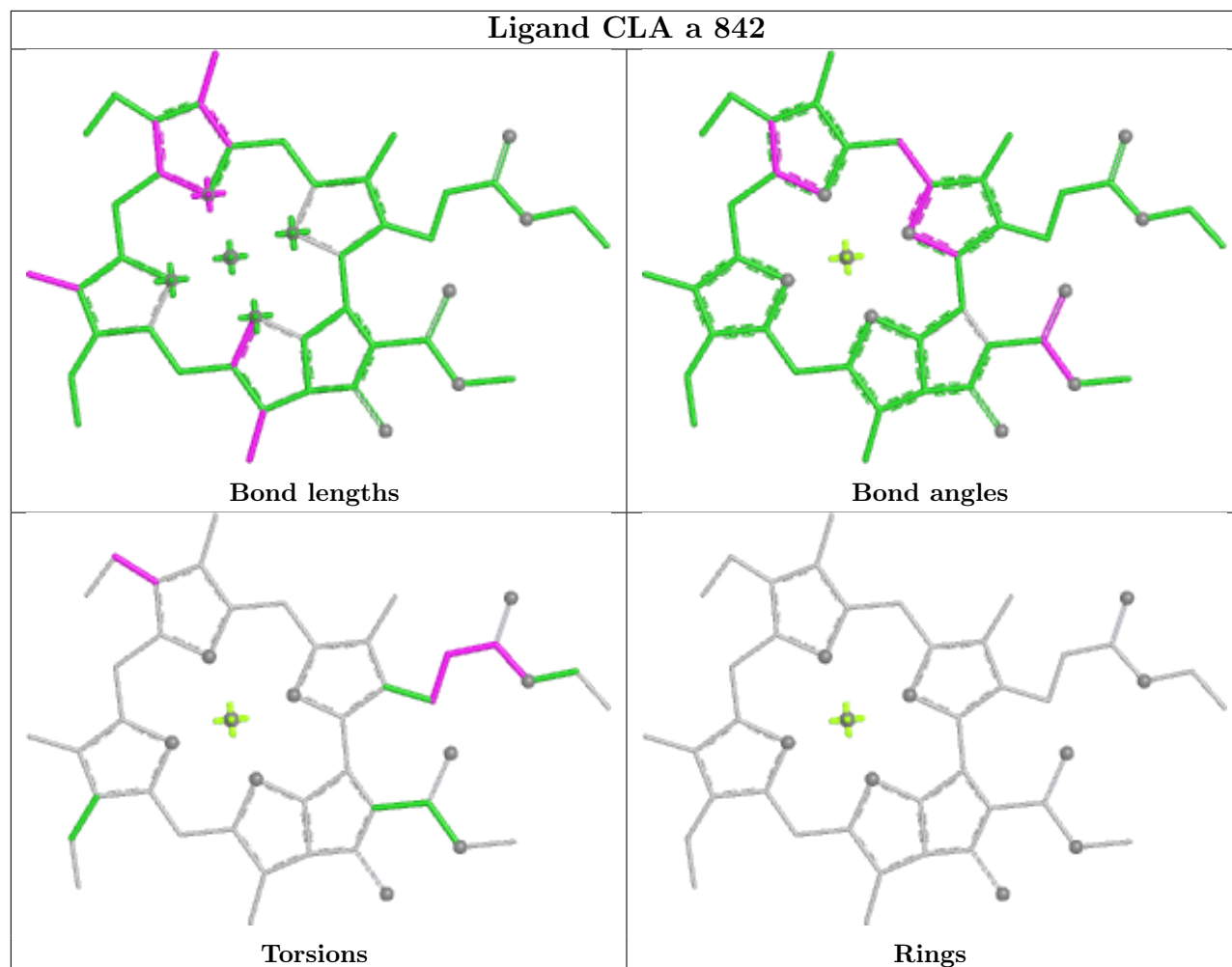
## Ligand PQN B 842



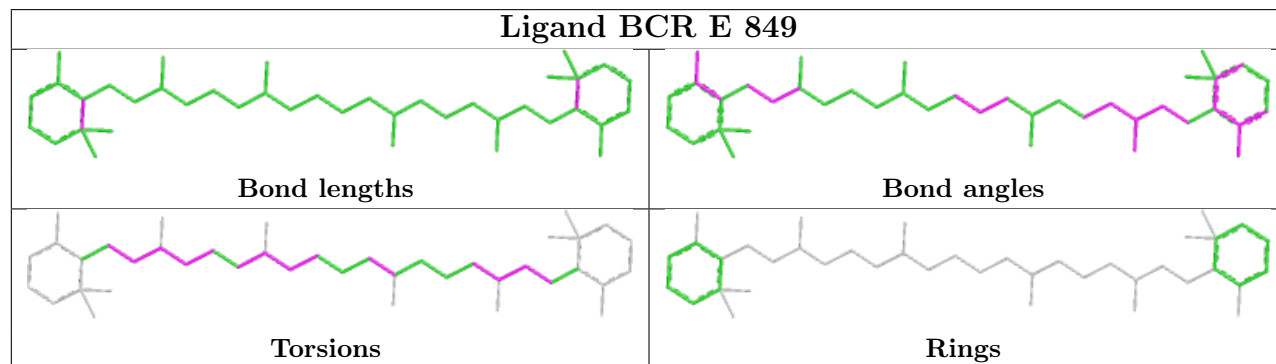
## Ligand BCR A 851



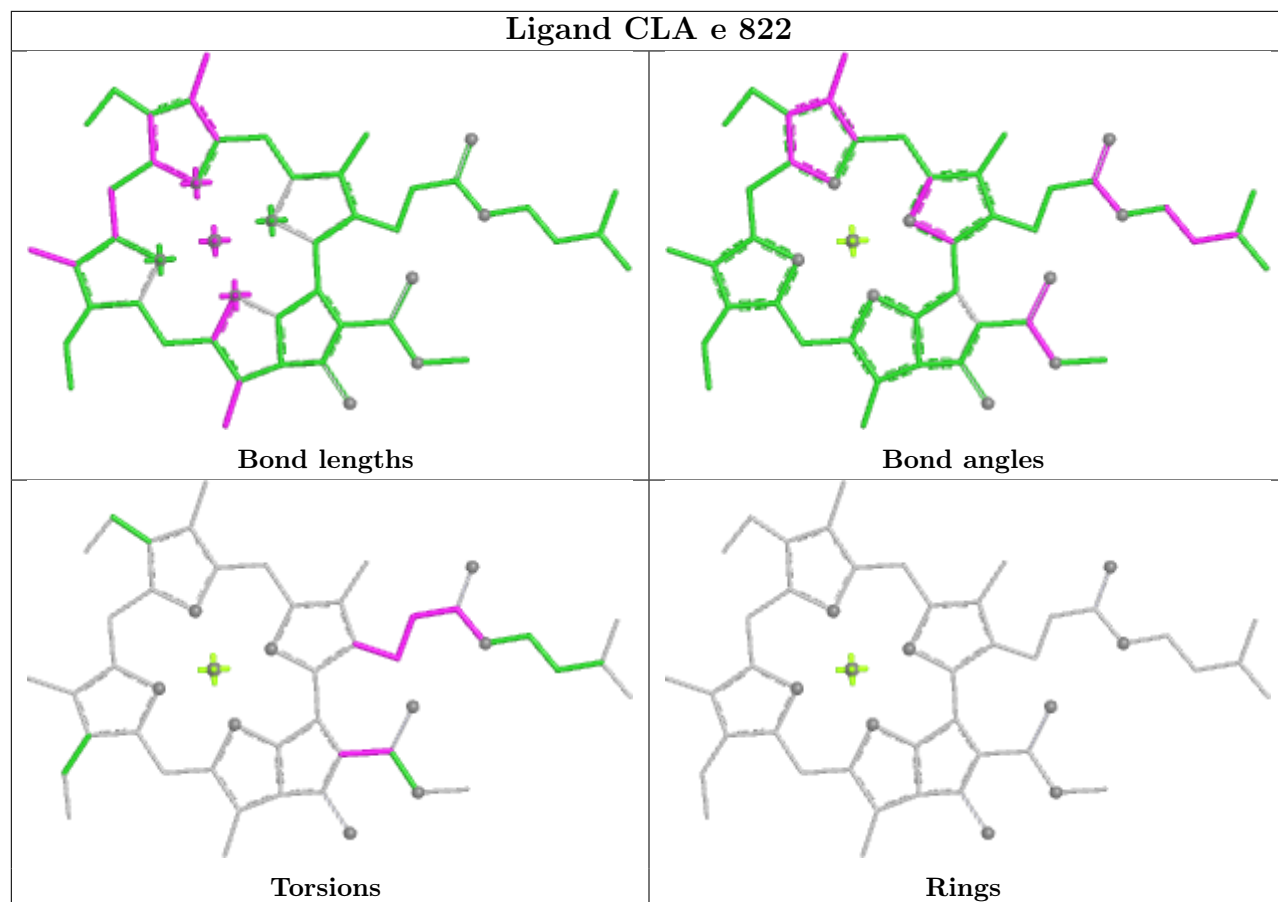
## Ligand CLA a 842

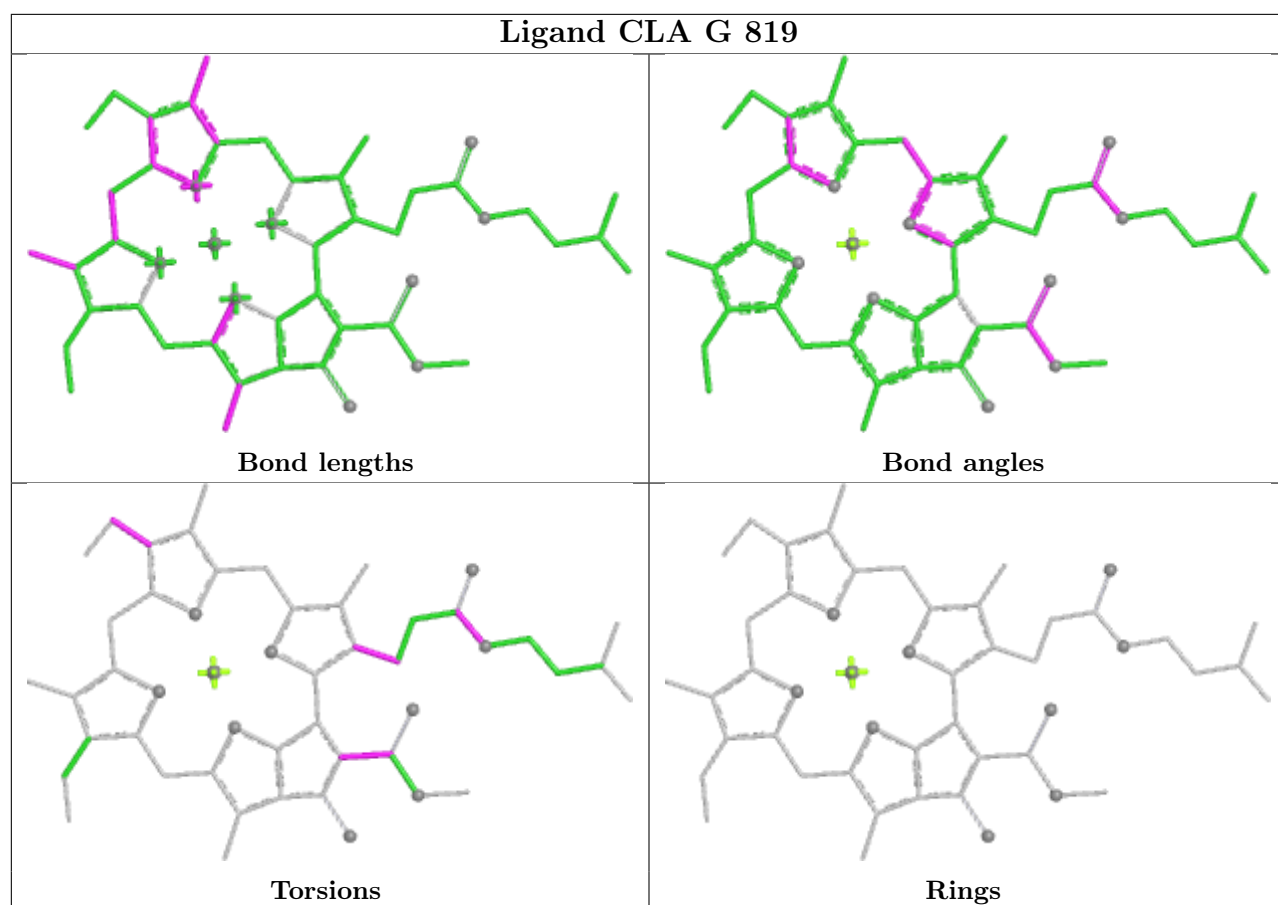


## Ligand BCR E 849

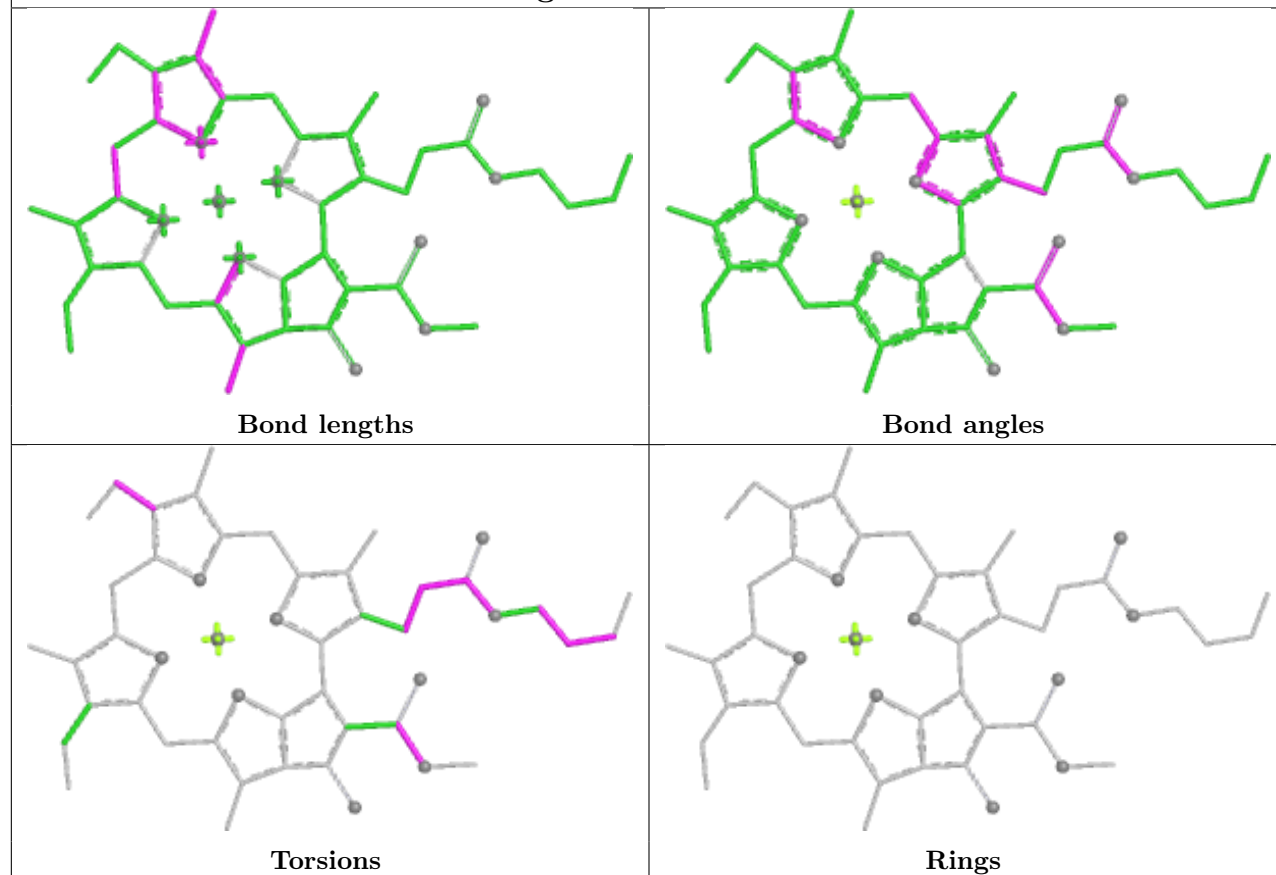


## Ligand CLA e 822

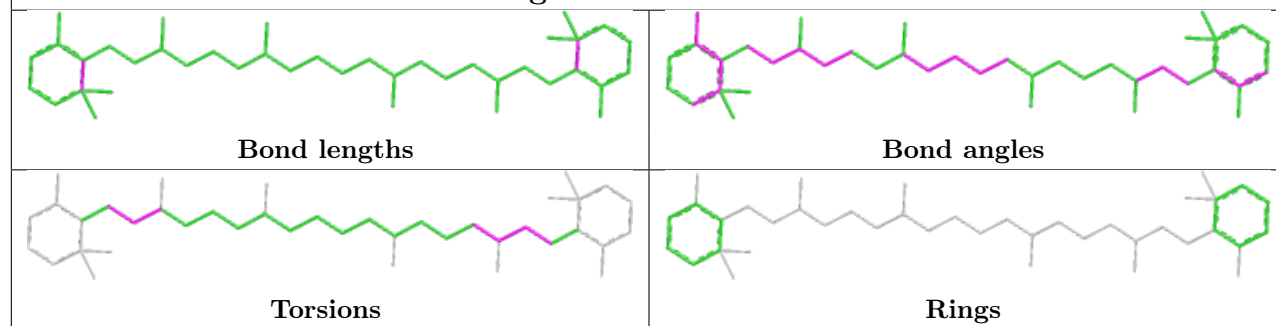




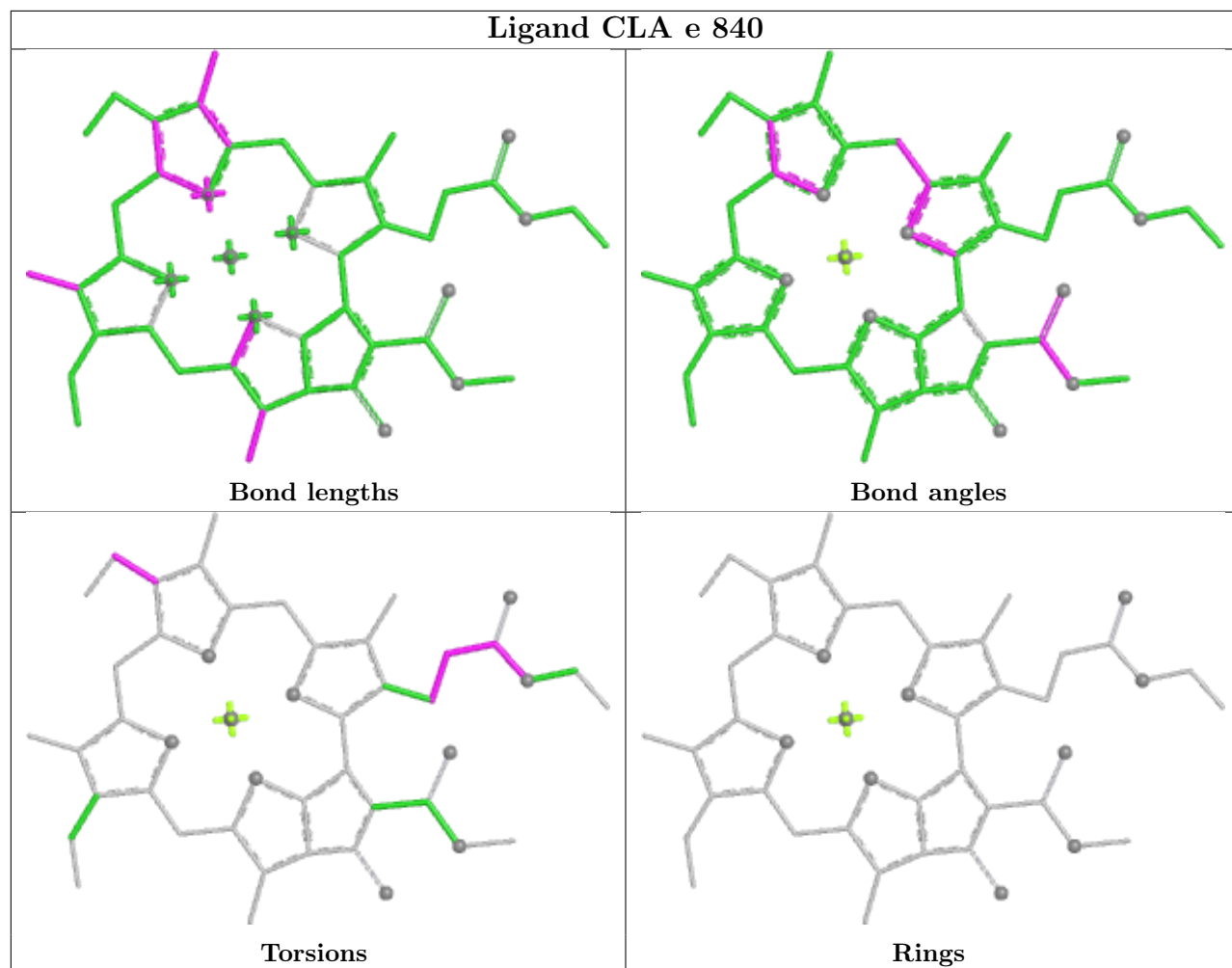
## Ligand CLA e 824



## Ligand BCR G 843

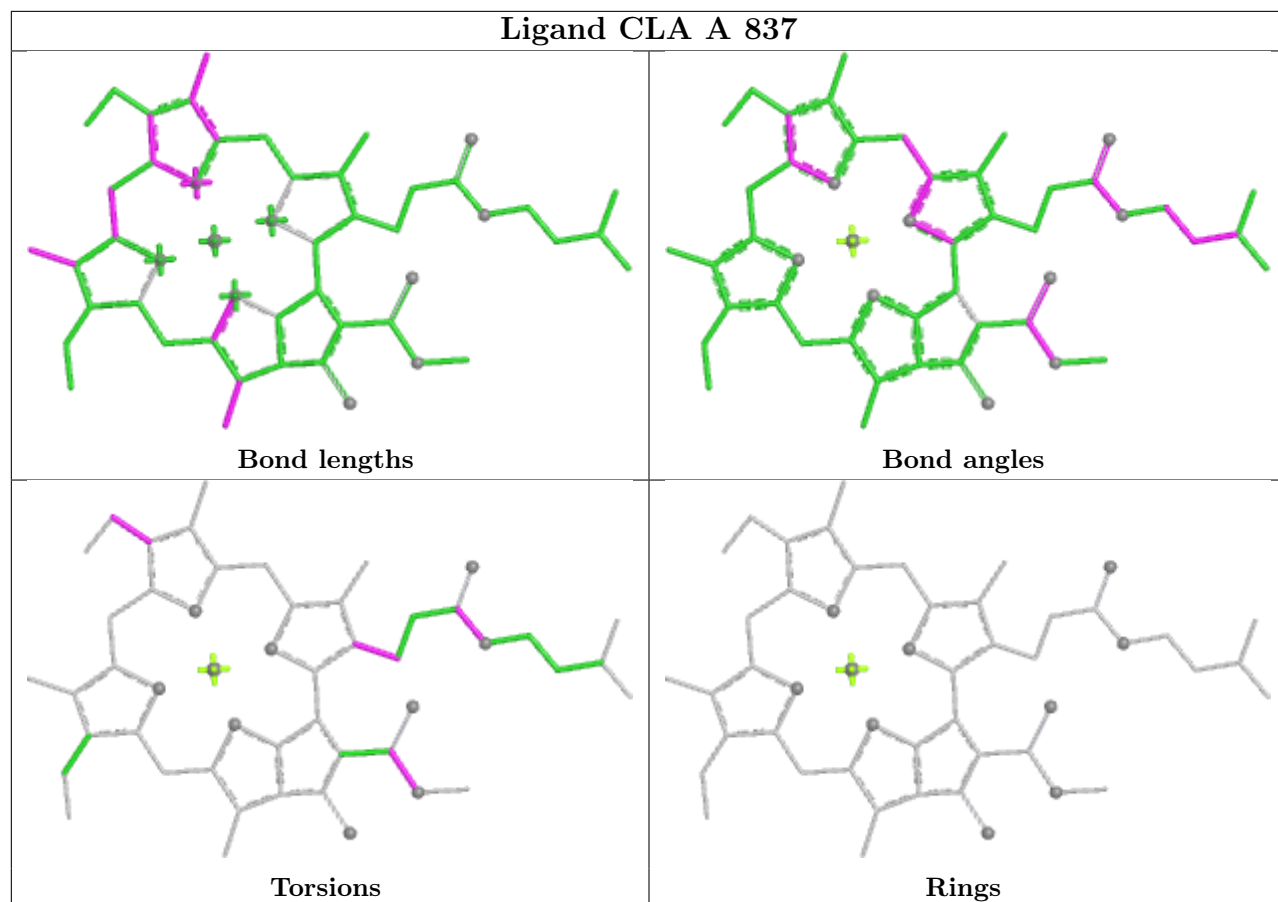


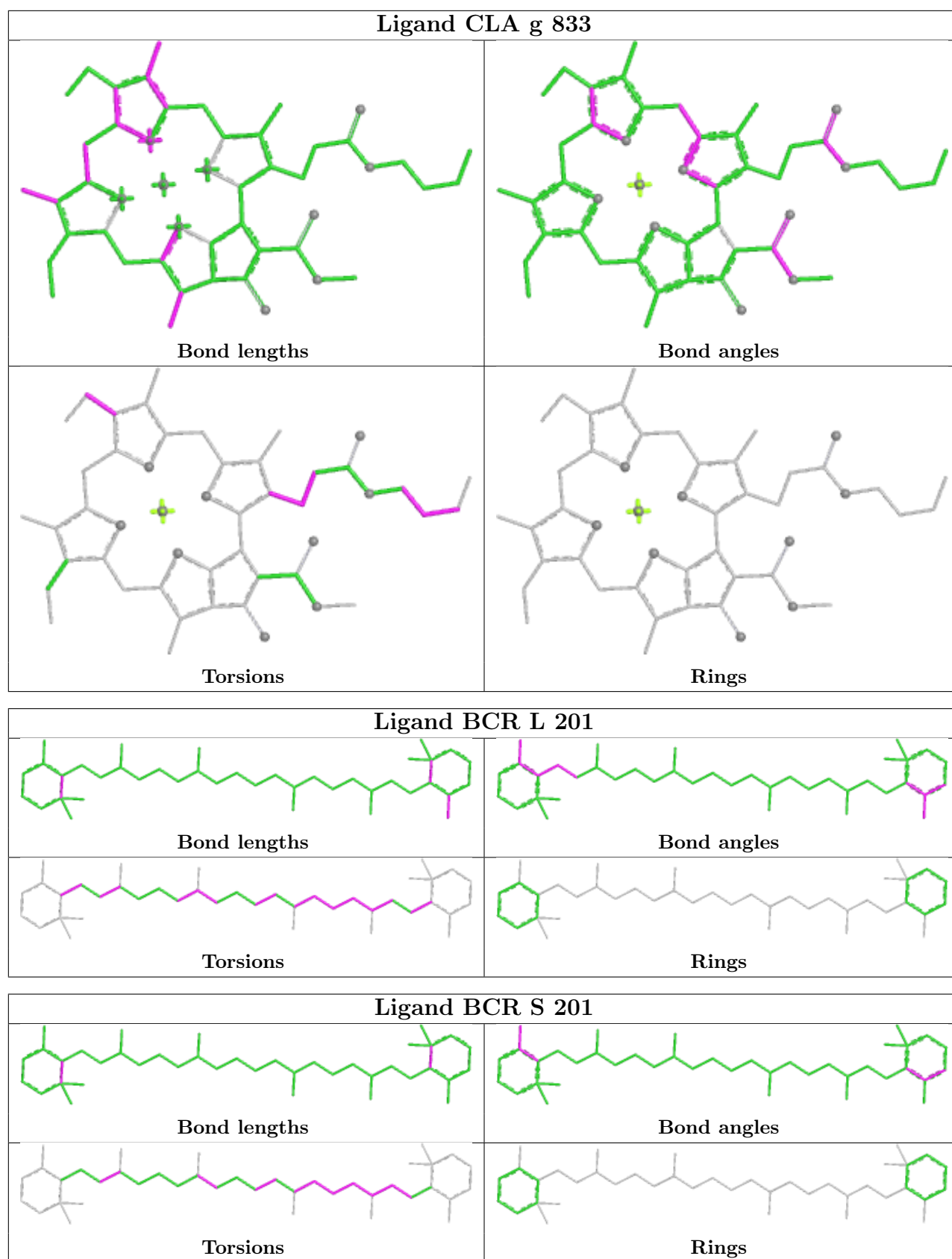
## Ligand CLA e 840



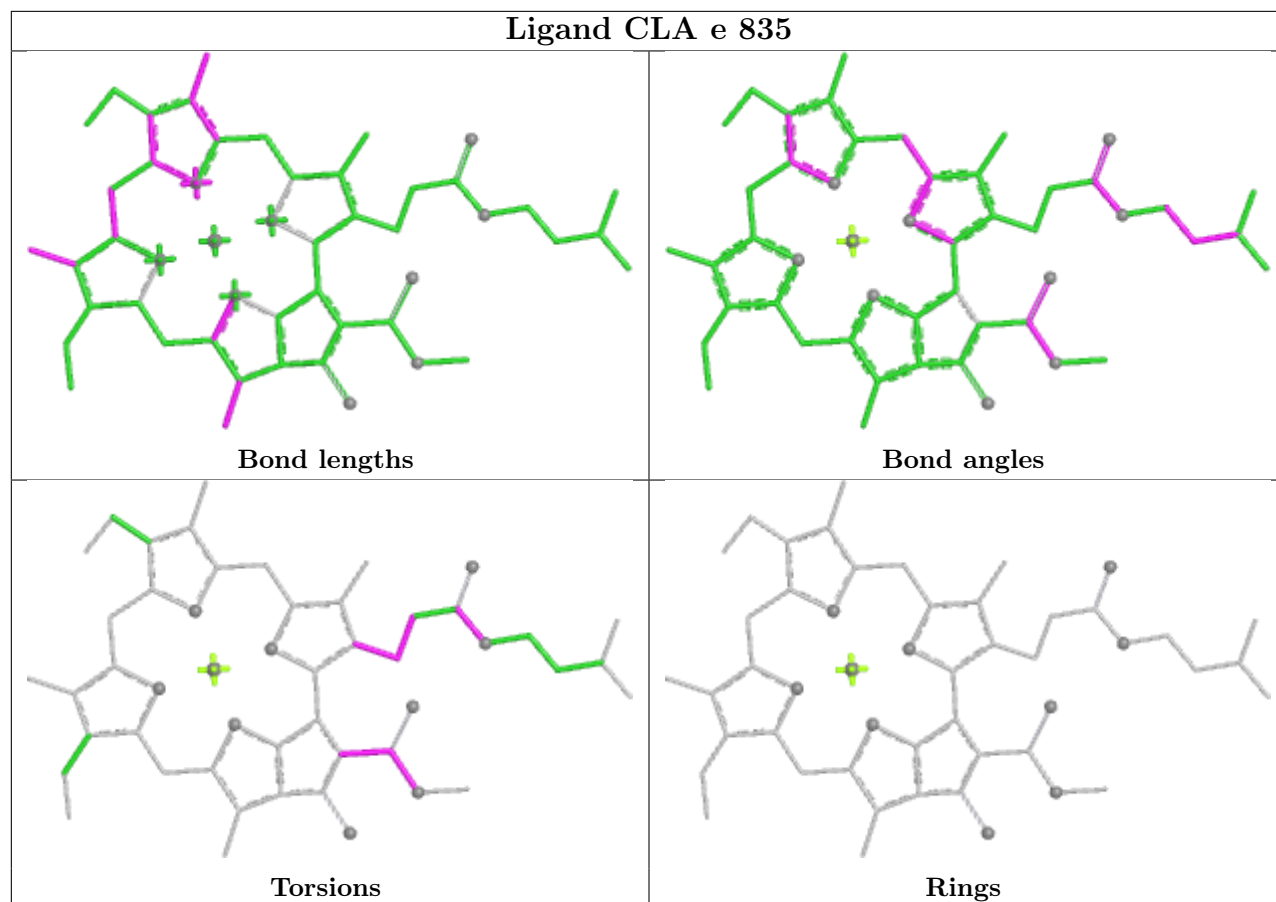


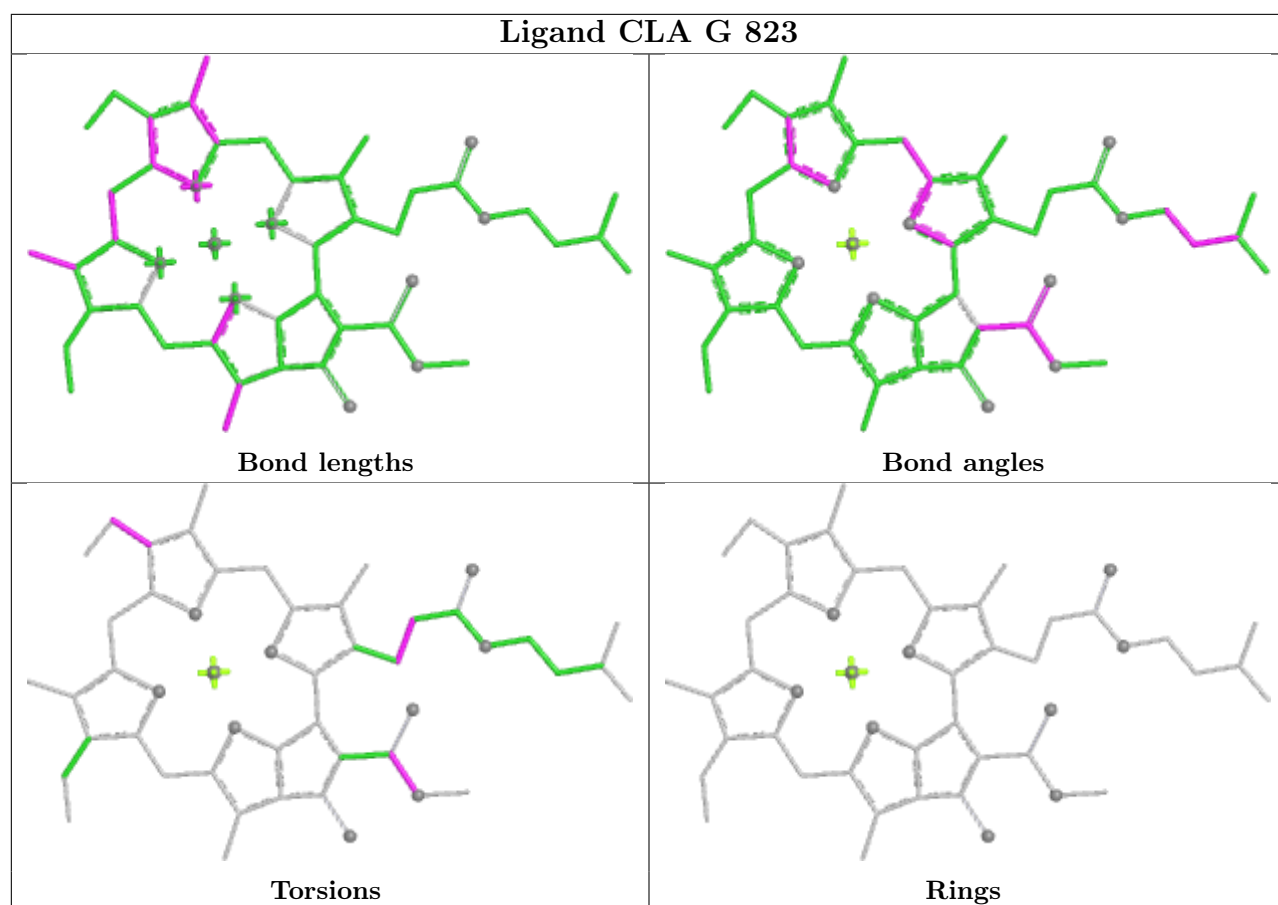
## Ligand CLA A 837



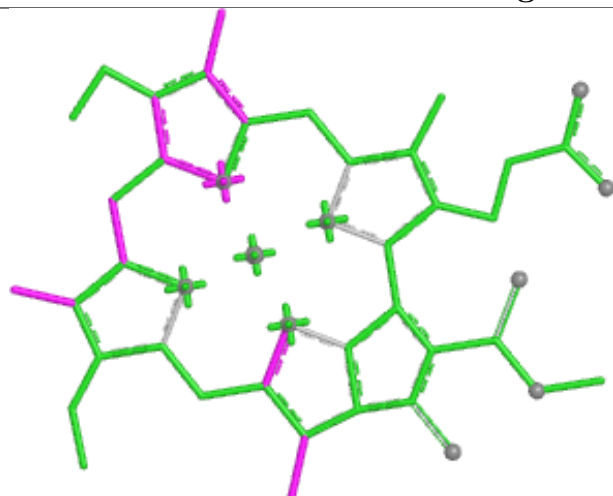


## Ligand CLA e 835

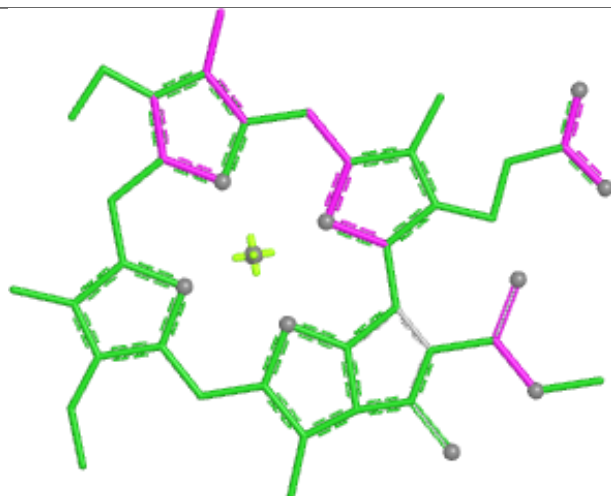




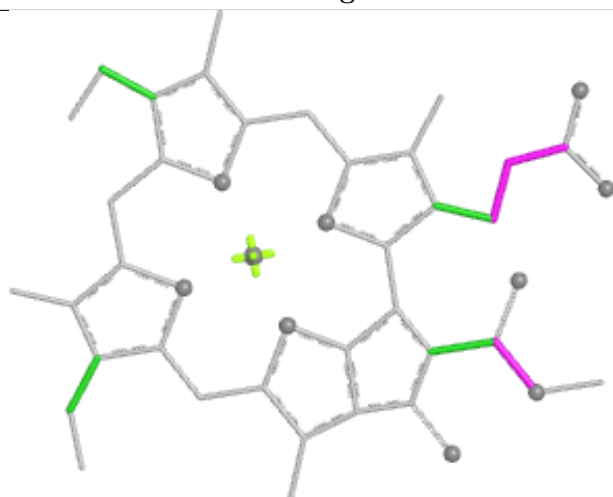
## Ligand CLA S 203



Bond lengths



Bond angles

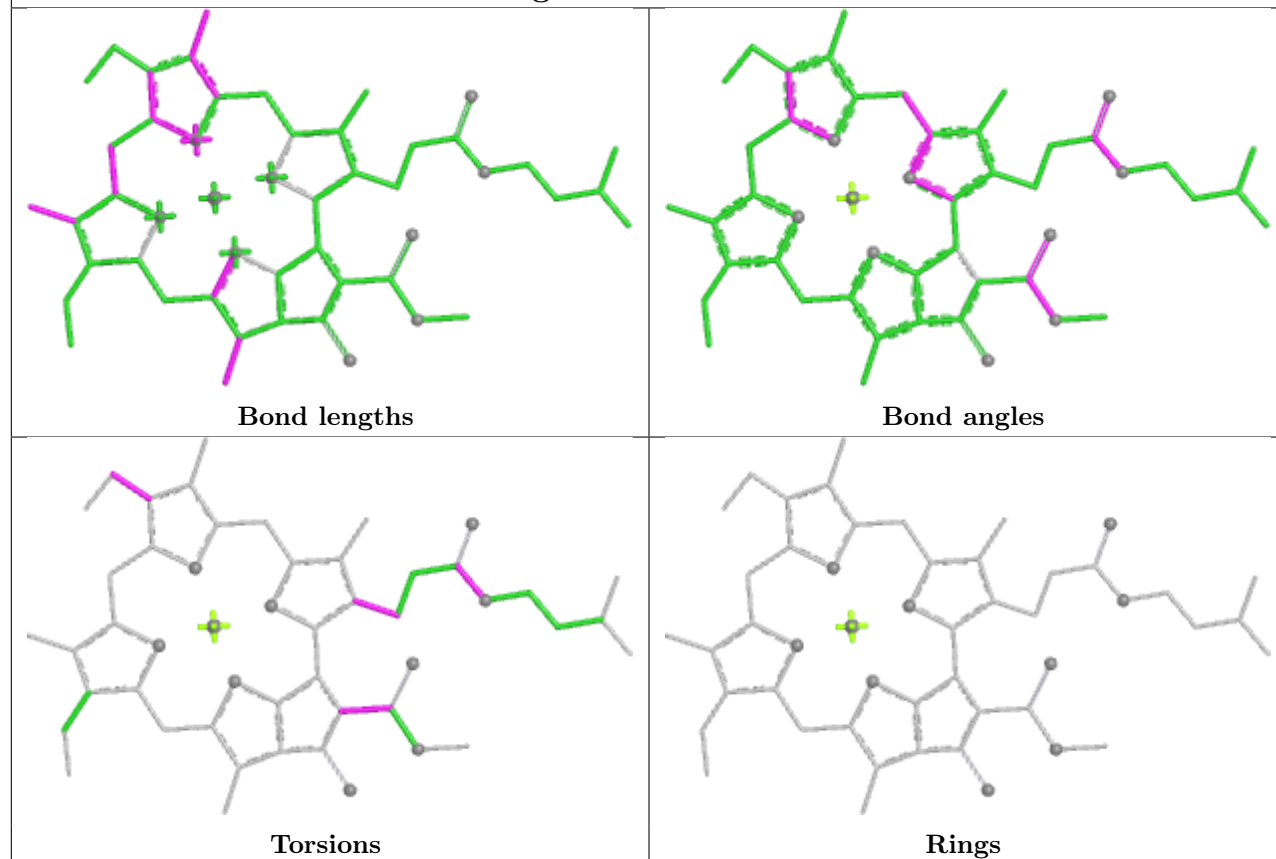


Torsions

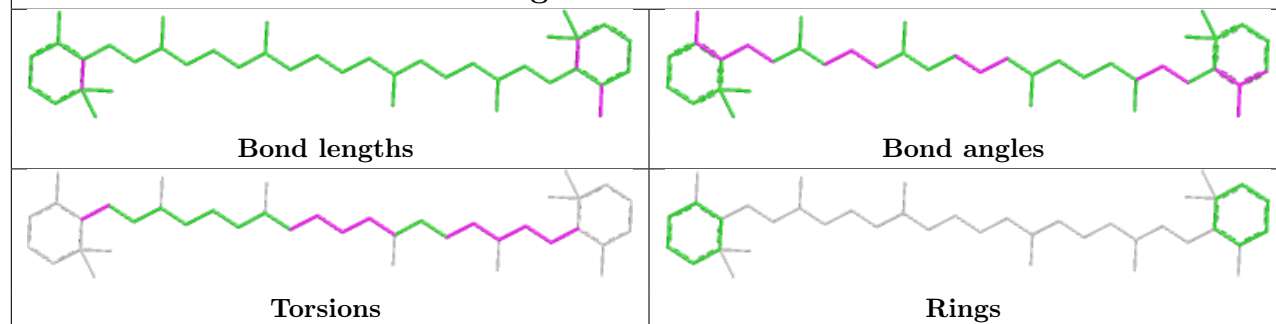


Rings

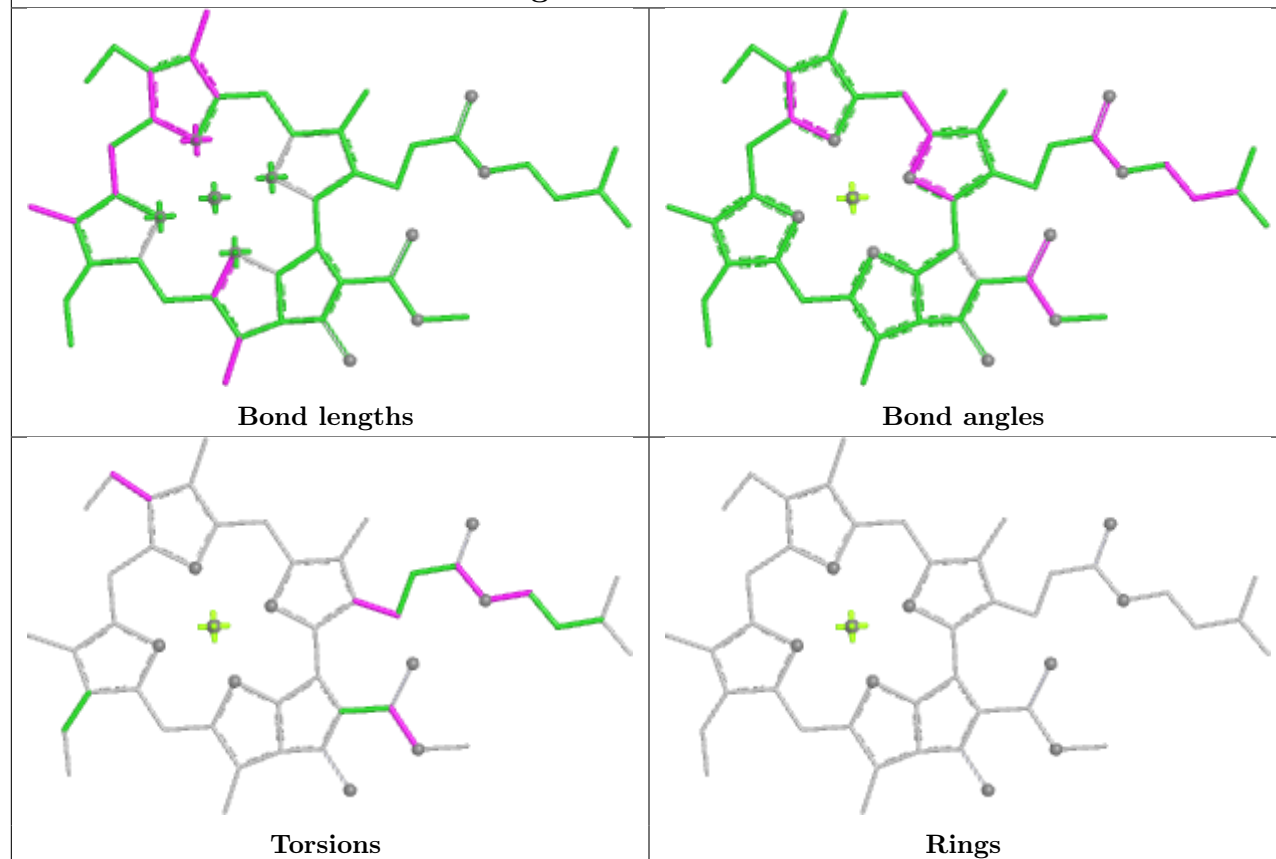
## Ligand CLA B 819



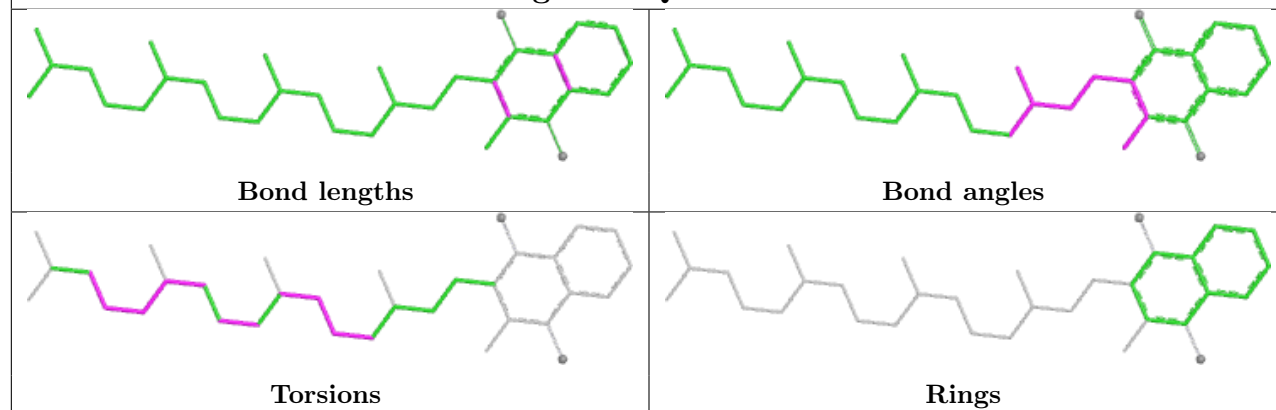
## Ligand BCR B 847



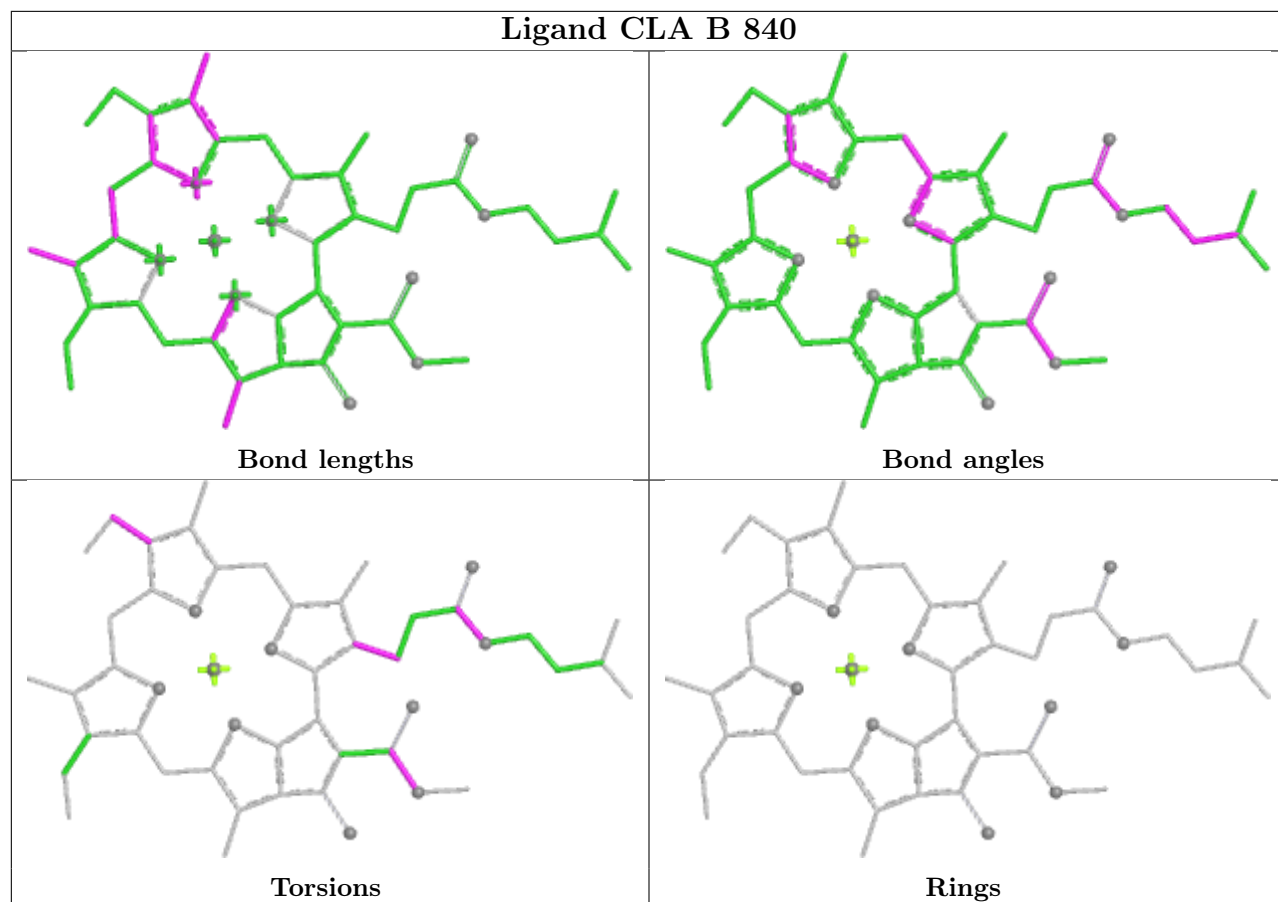
## Ligand CLA G 828



## Ligand PQN b 841

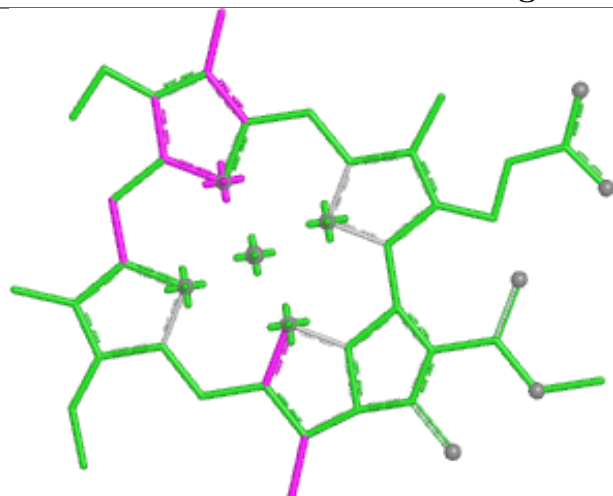


## Ligand CLA B 840

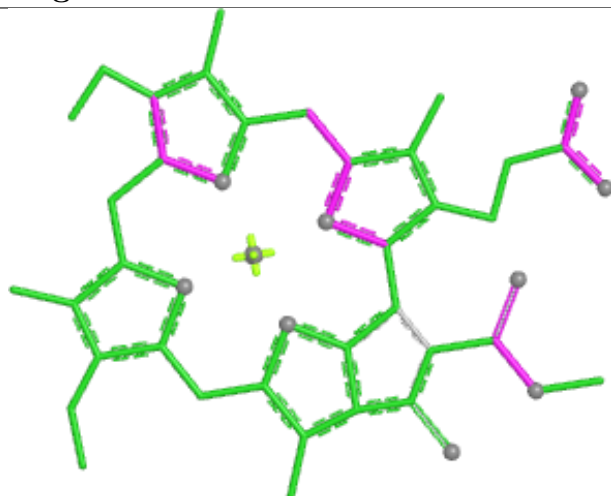




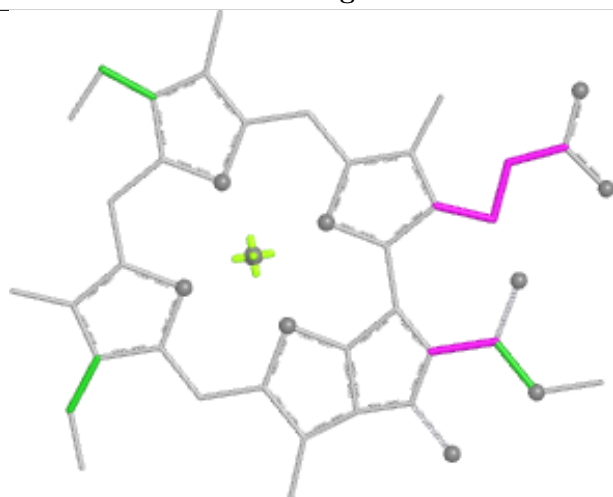
## Ligand CLA g 836



Bond lengths



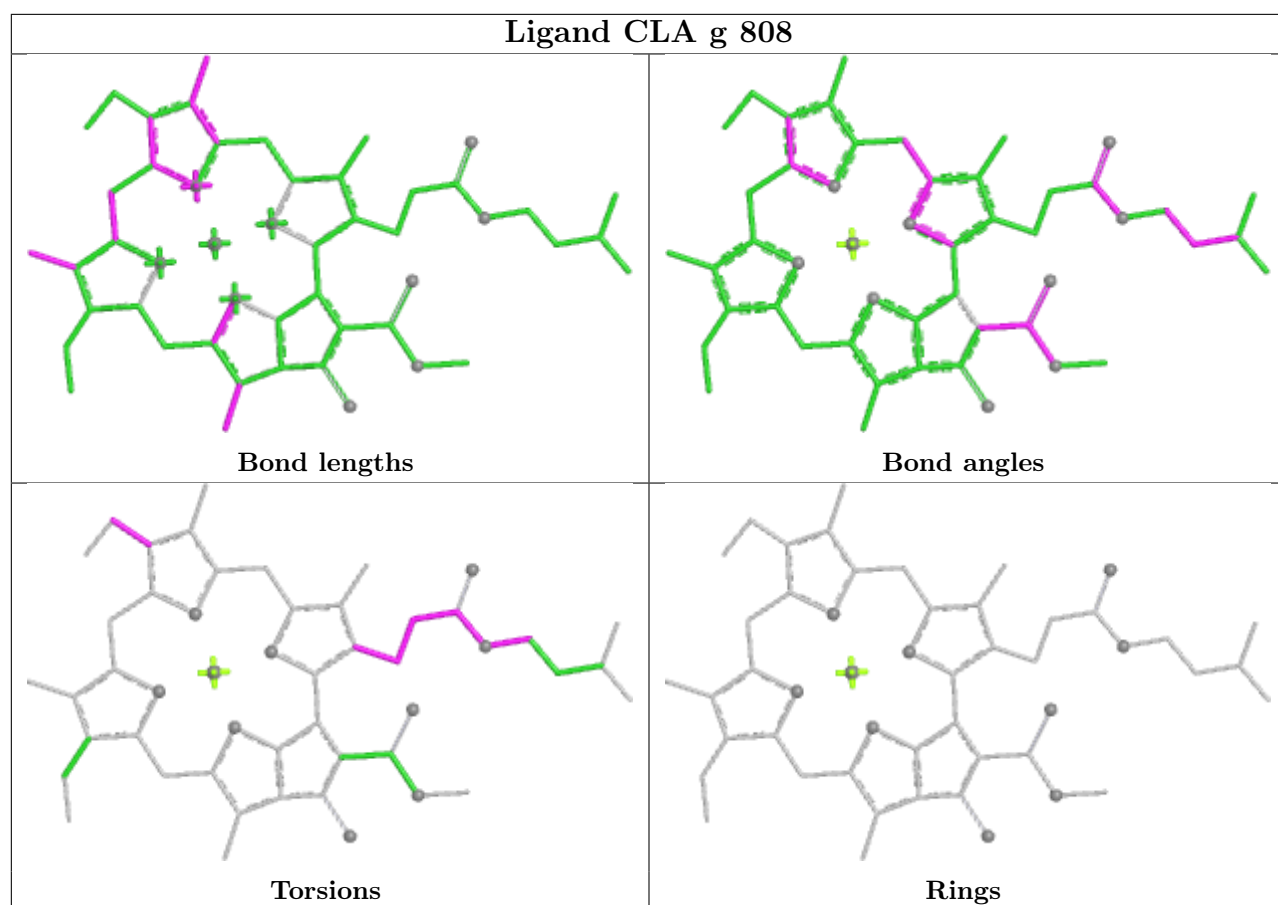
Bond angles



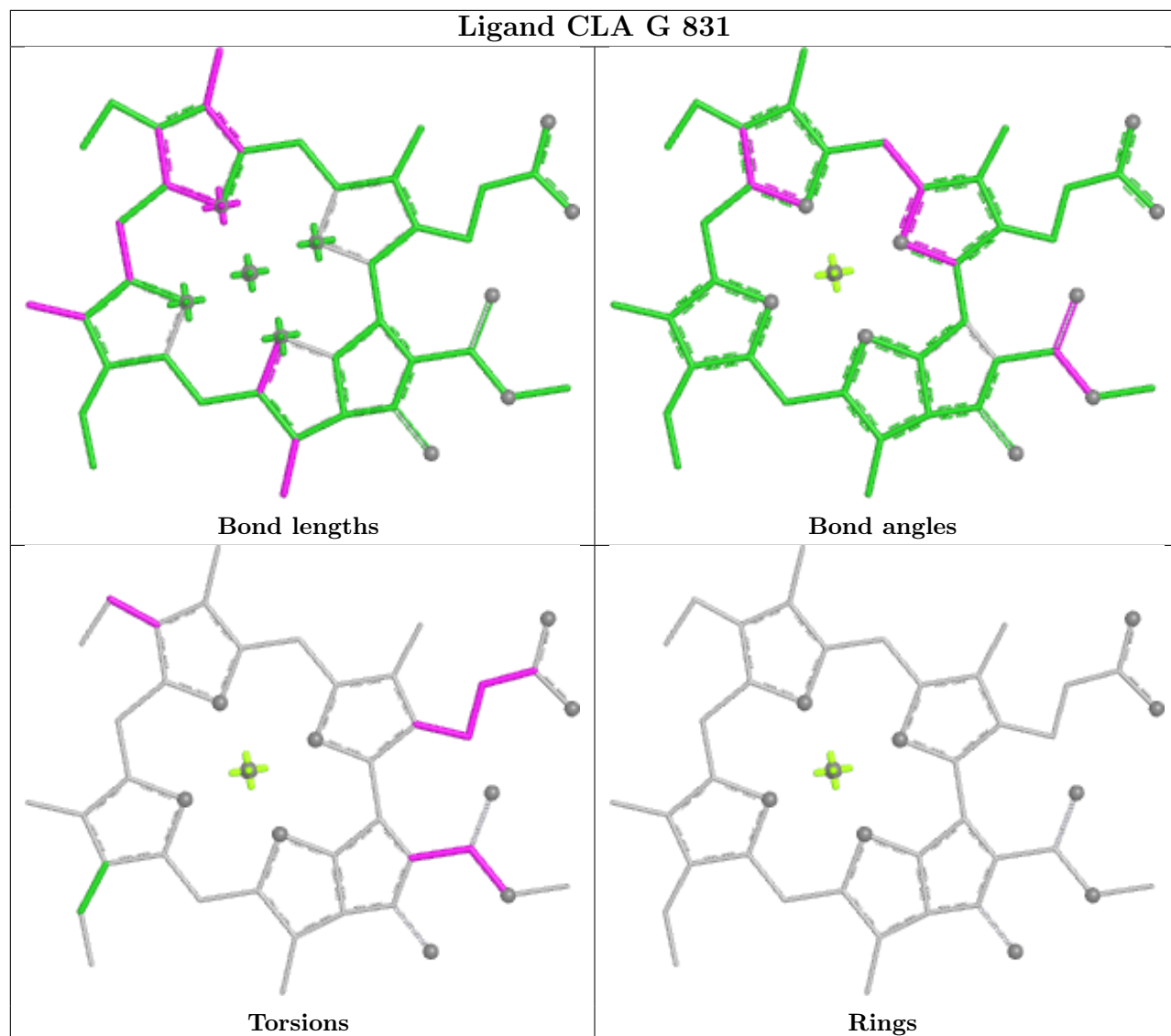
Torsions



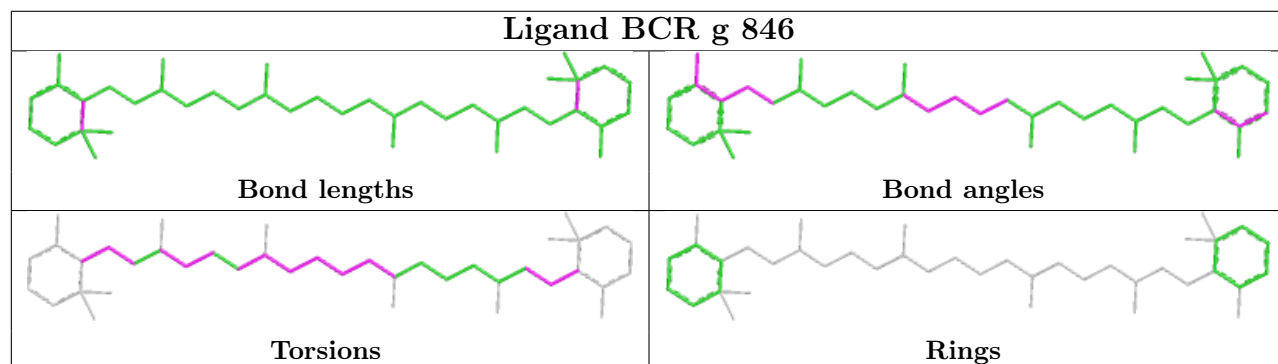
Rings

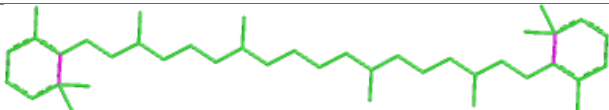
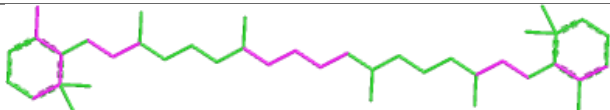
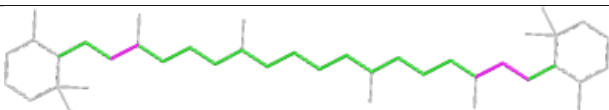
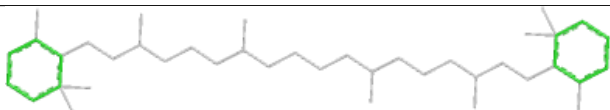


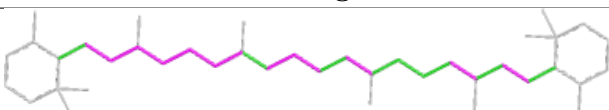
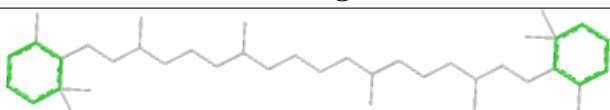
## Ligand CLA G 831



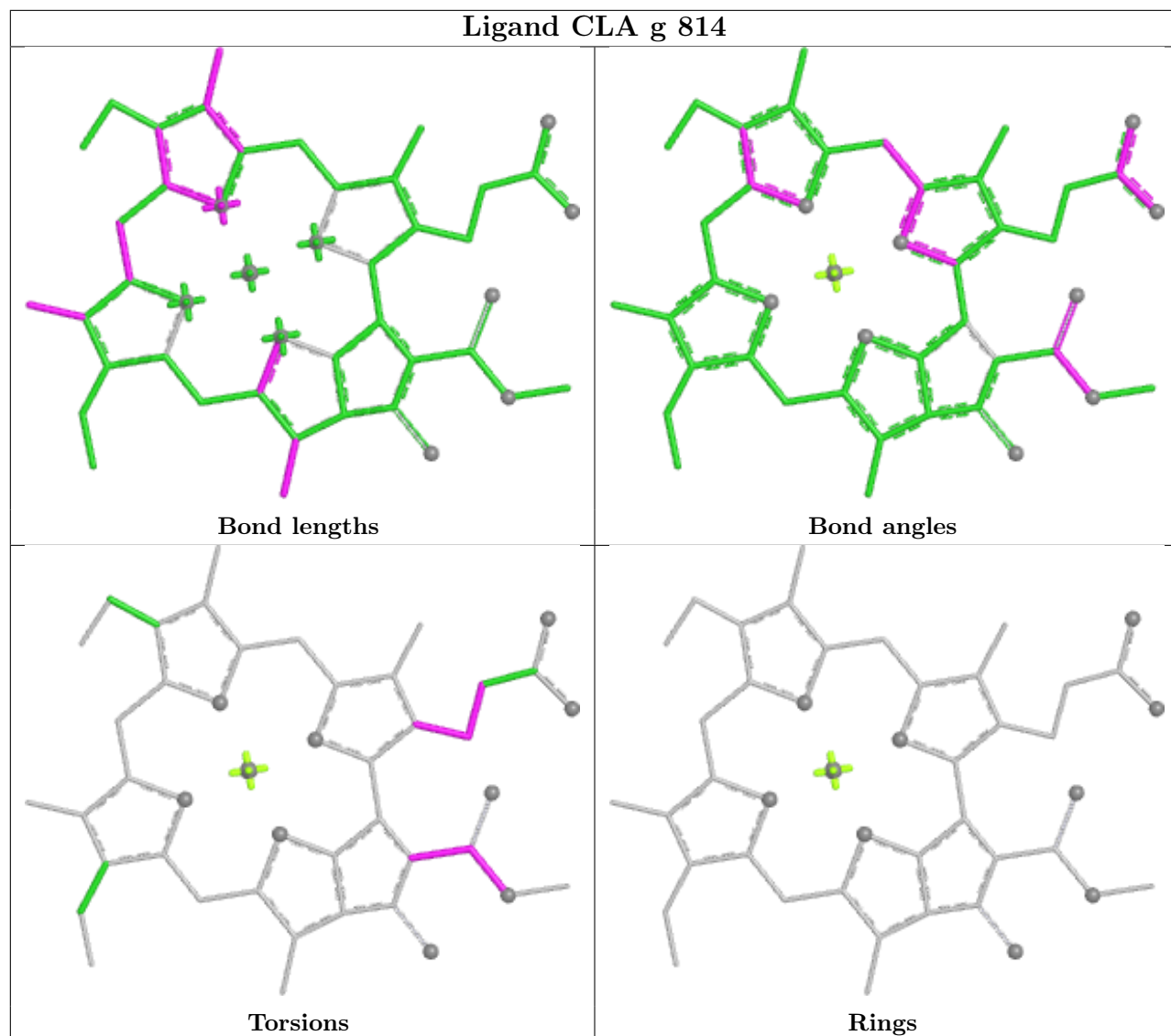
## Ligand BCR g 846



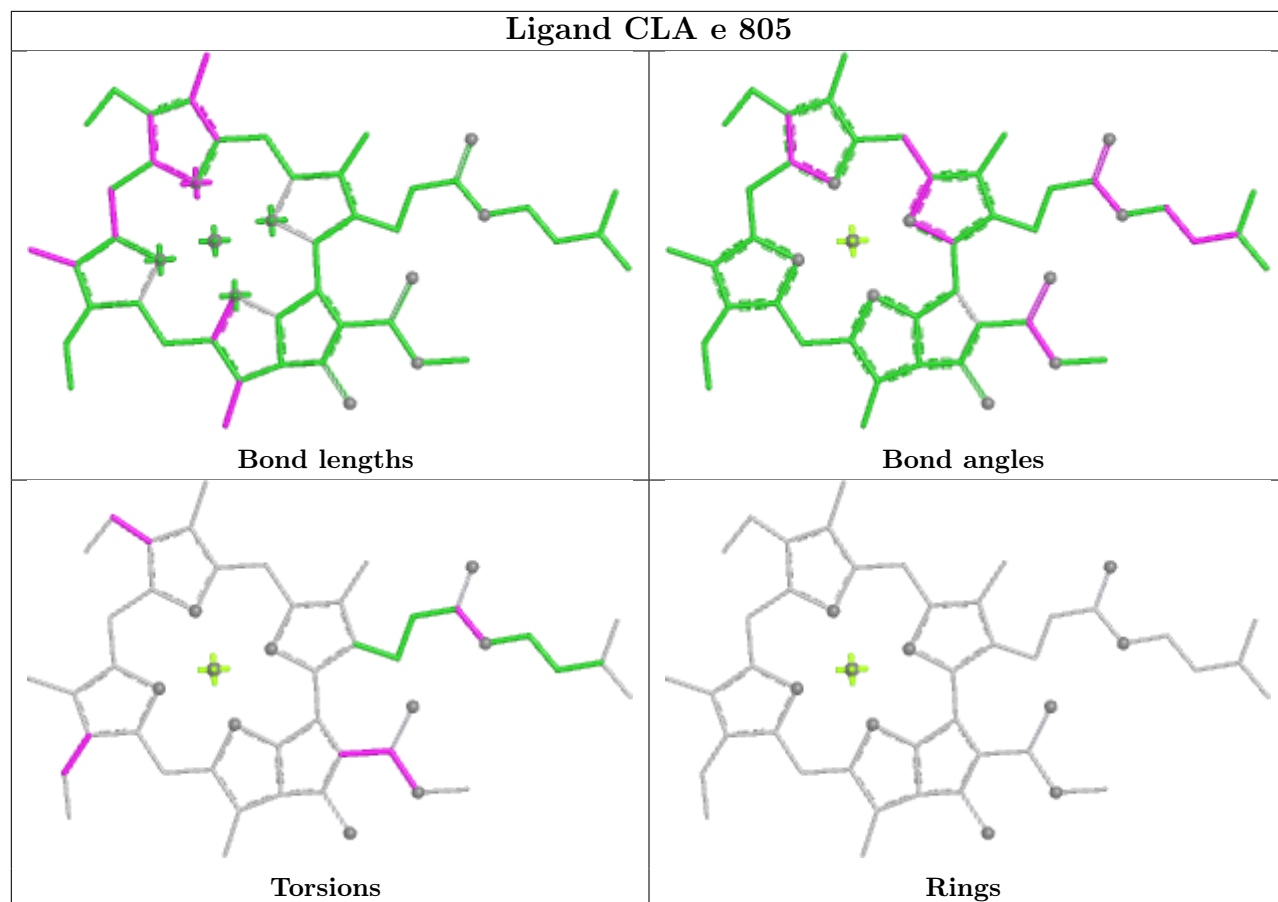
| Ligand BCR F 201                                                                   |              |
|------------------------------------------------------------------------------------|--------------|
|   | Bond lengths |
|  | Bond angles  |
|   | Torsions     |
|  | Rings        |

| Ligand BCR R 101                                                                   |              |
|------------------------------------------------------------------------------------|--------------|
|   | Bond lengths |
|  | Bond angles  |
|   | Torsions     |
|  | Rings        |

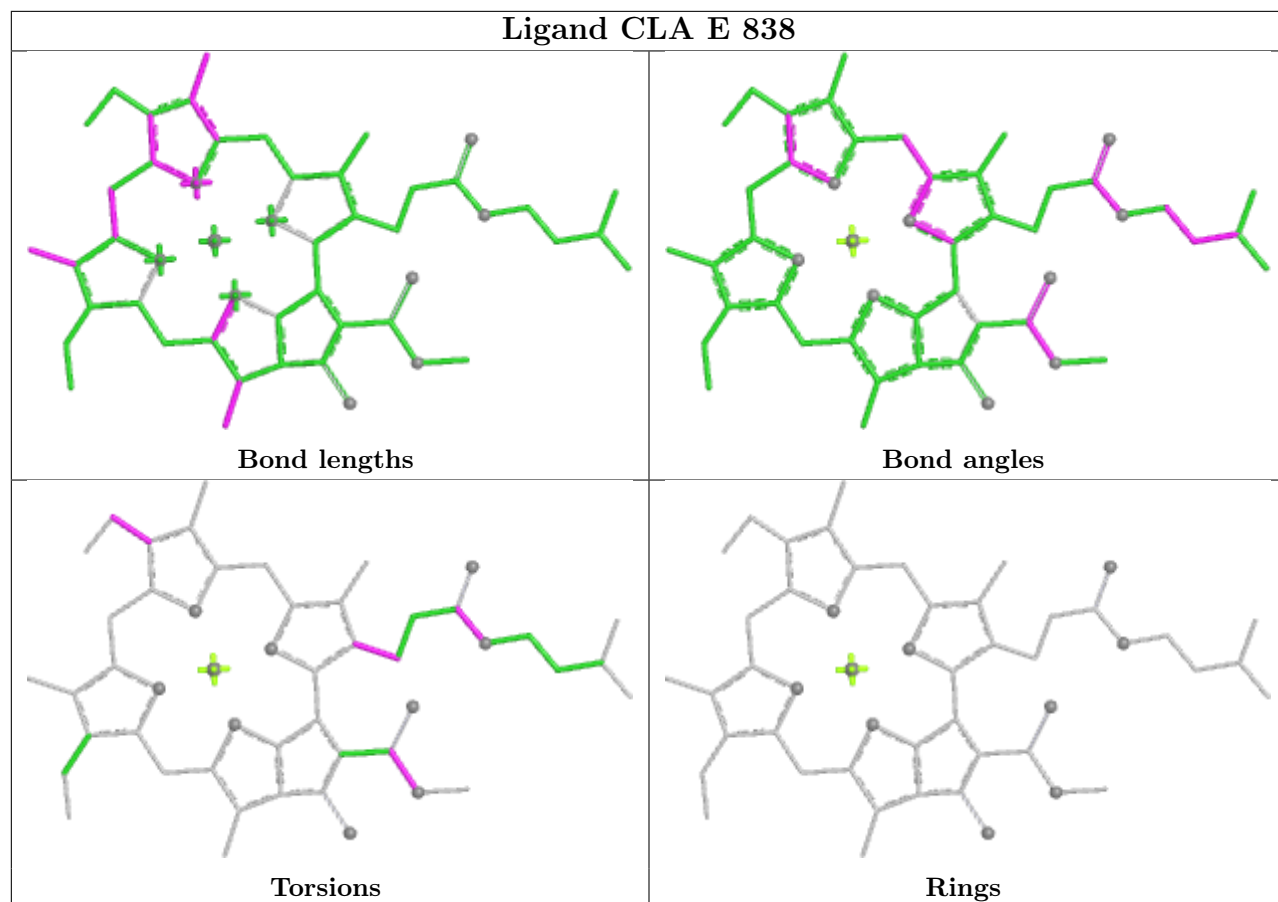
## Ligand CLA g 814



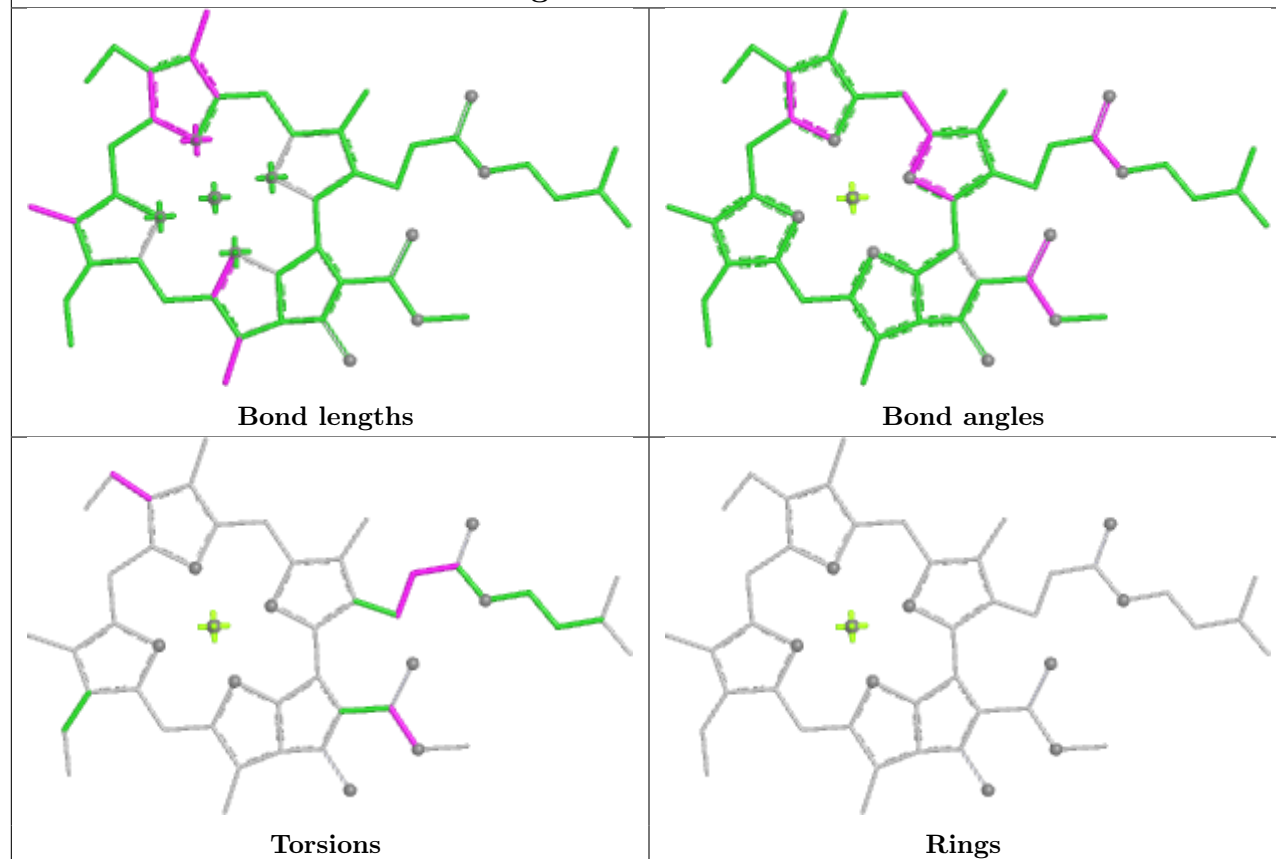
## Ligand CLA e 805



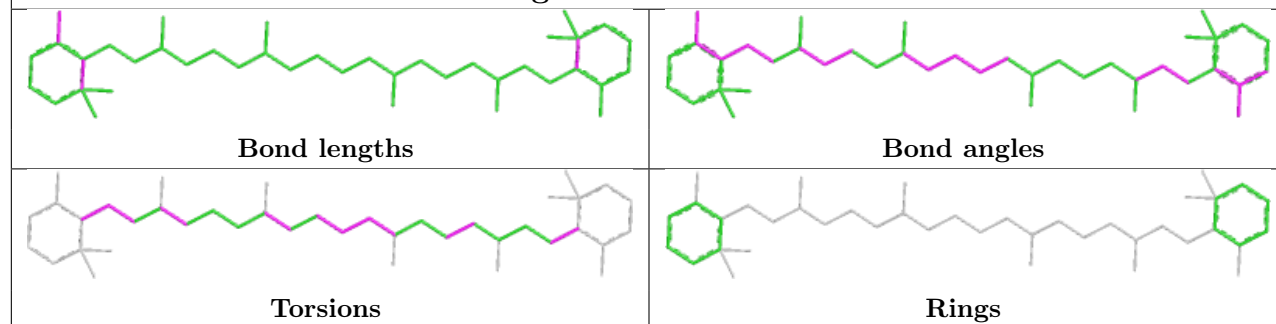
## Ligand CLA E 838



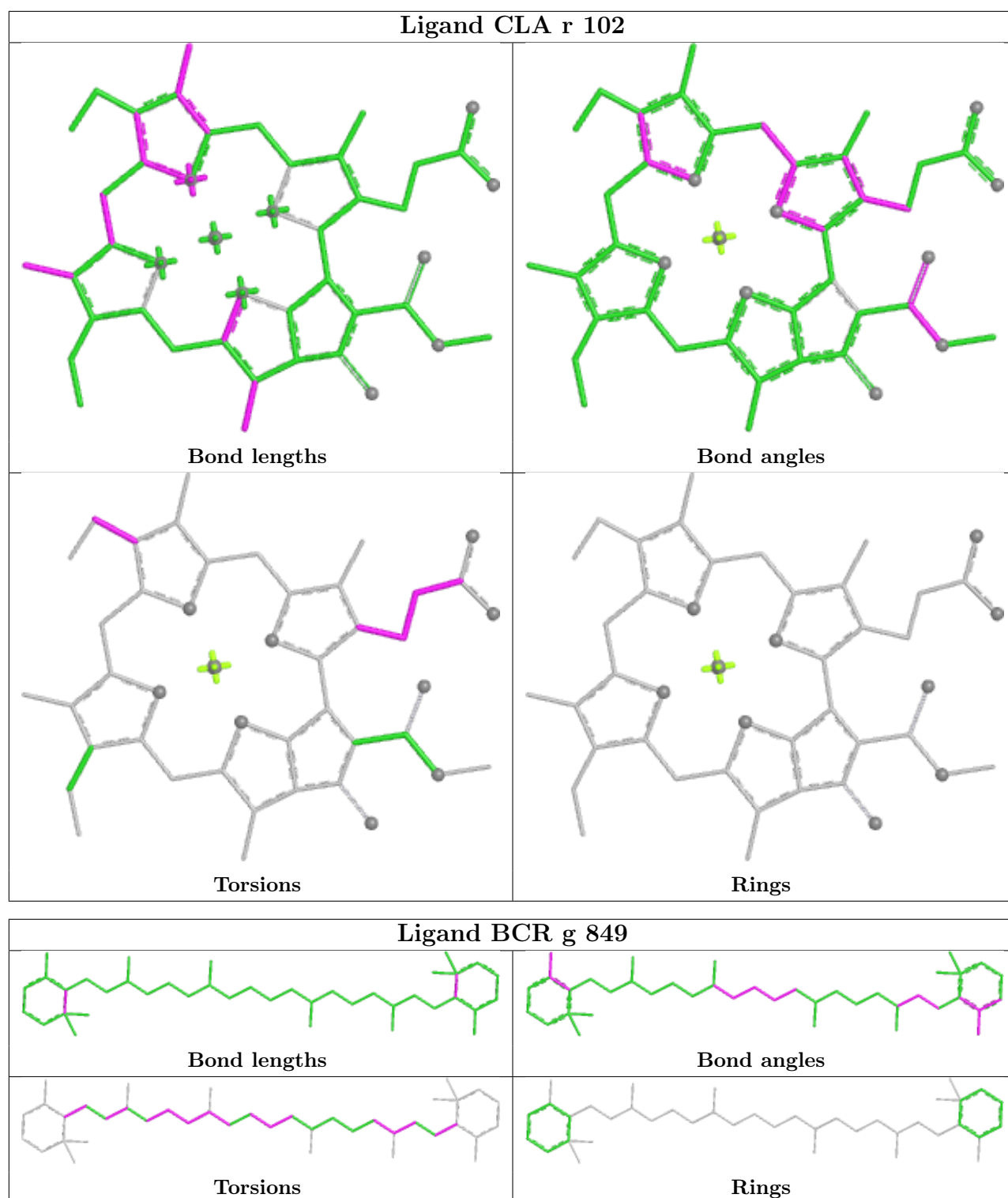
## Ligand CLA G 808



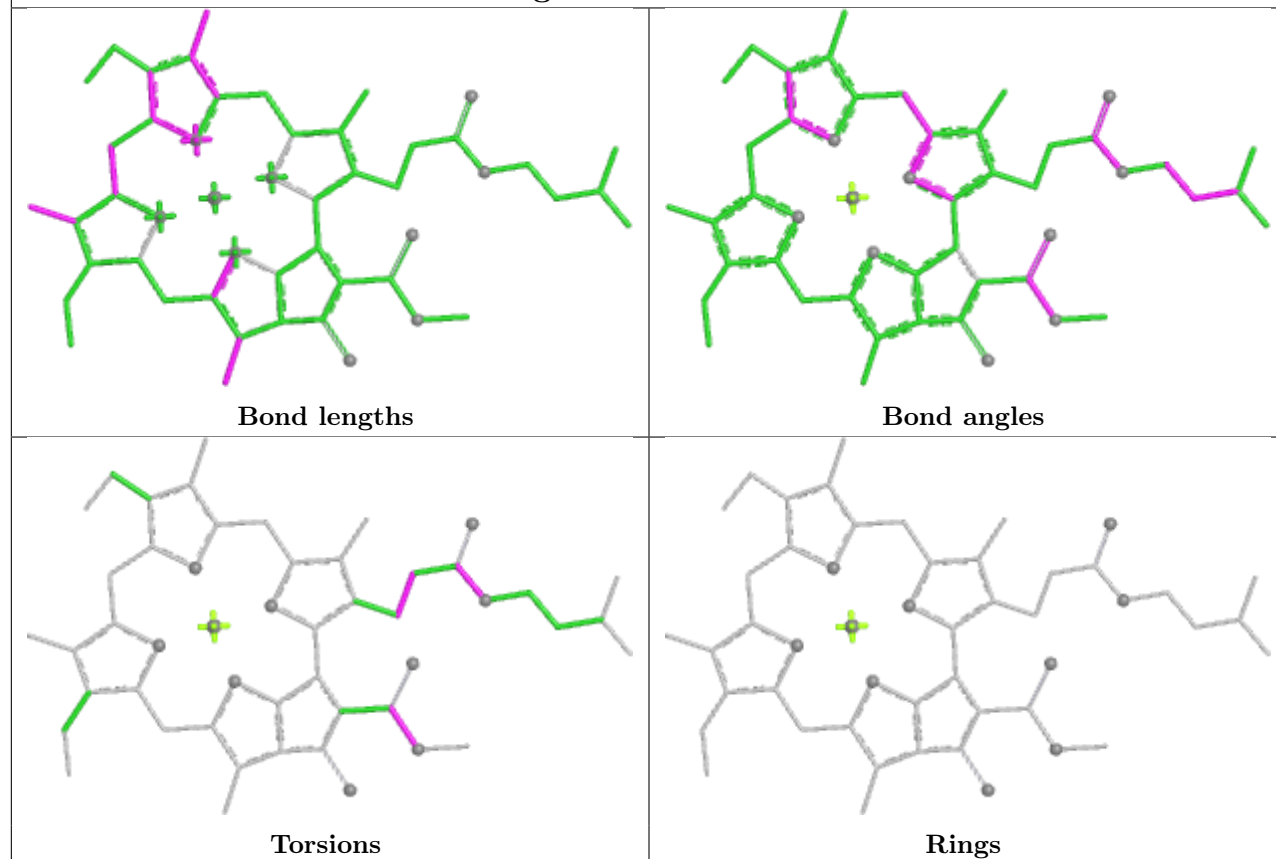
## Ligand BCR E 801



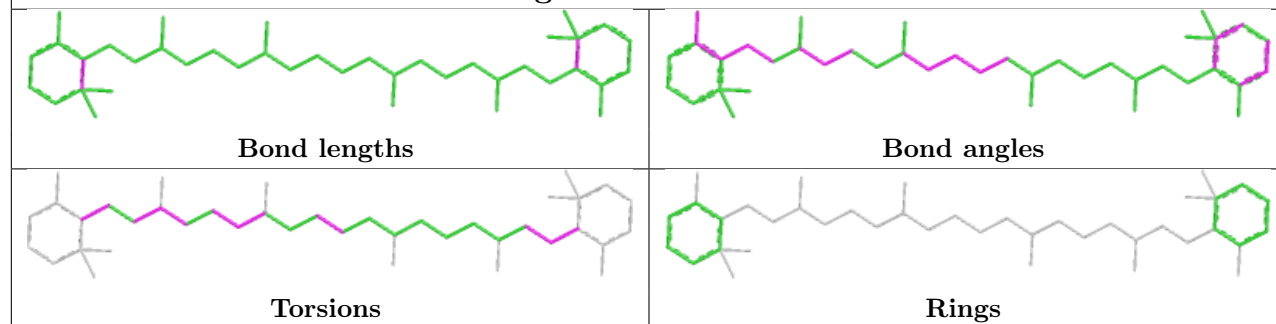




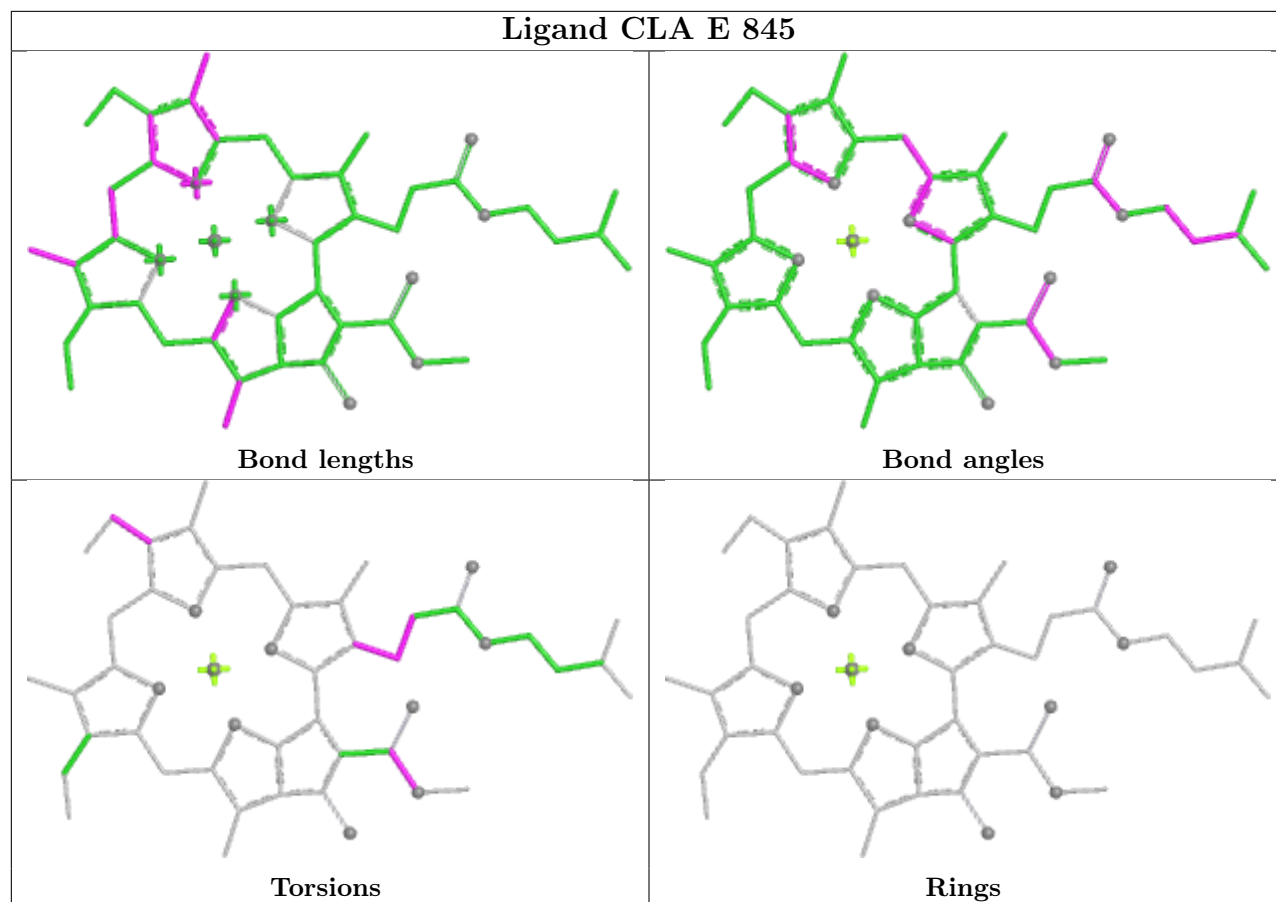
## Ligand CLA E 844



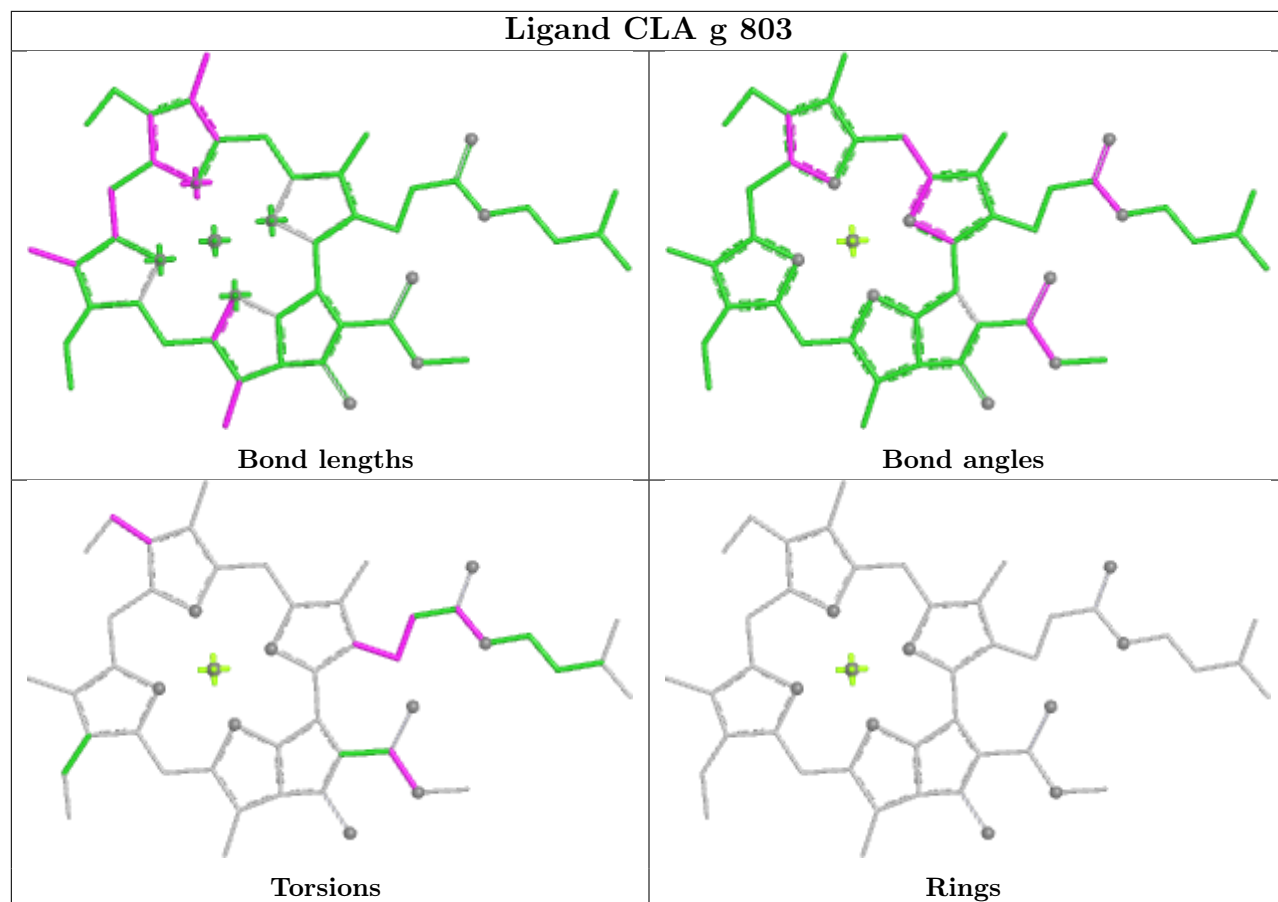
## Ligand BCR a 853



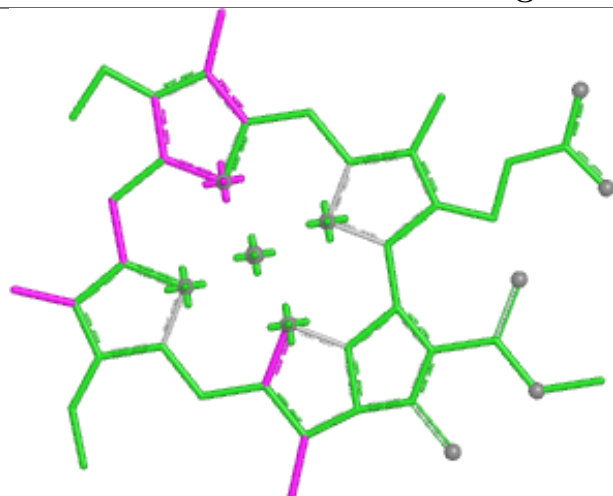
## Ligand CLA E 845



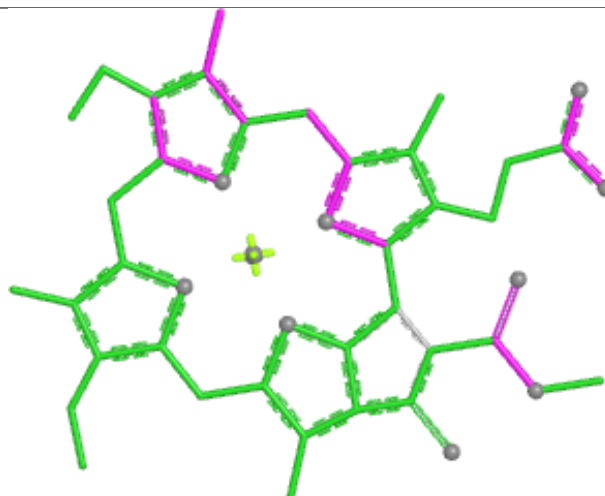
## Ligand CLA g 803



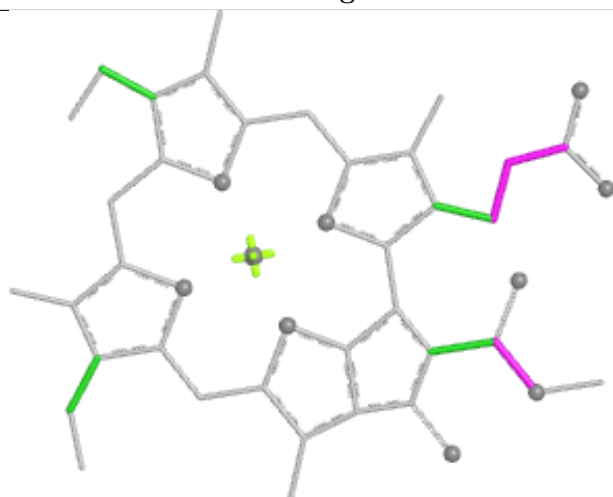
## Ligand CLA L 203



Bond lengths



Bond angles

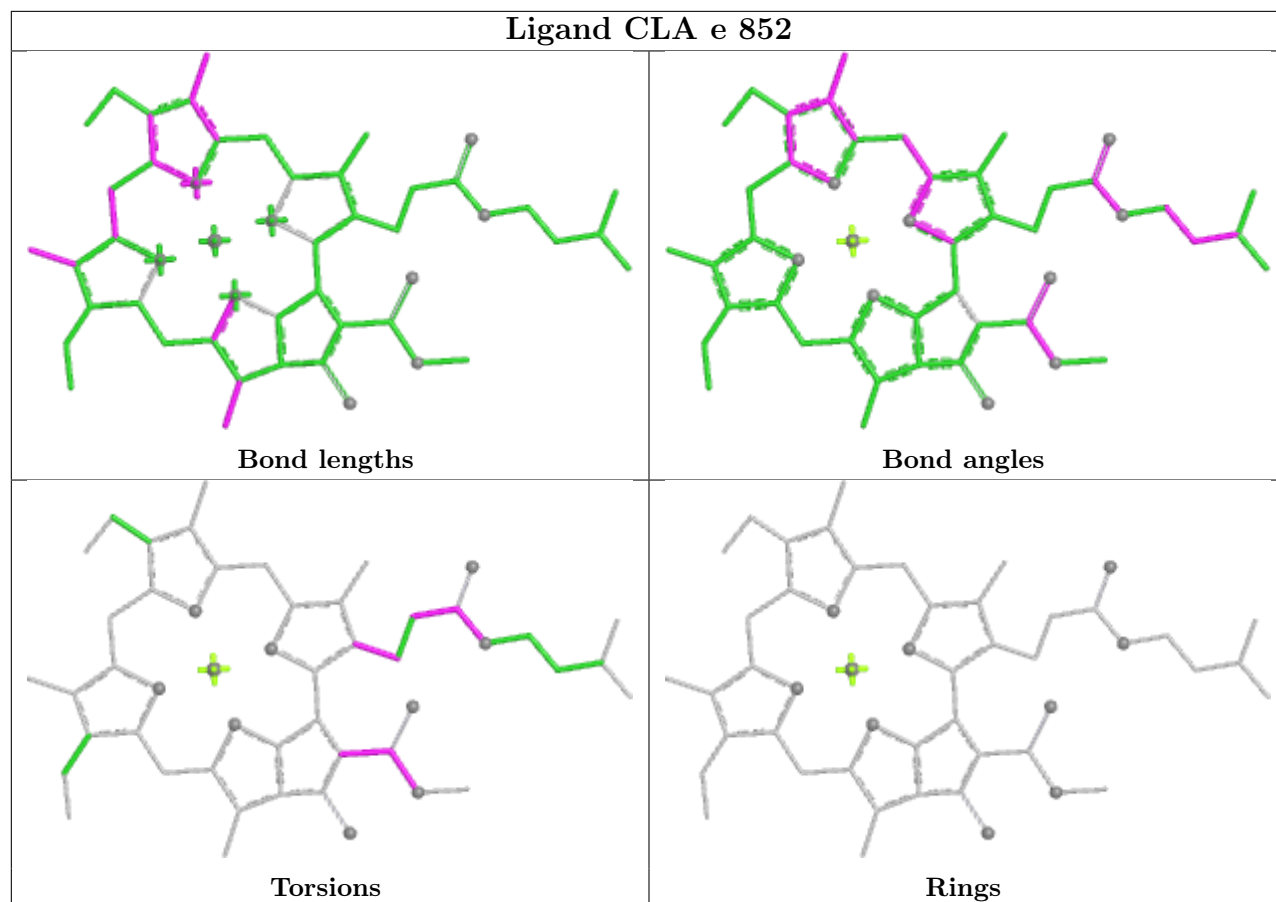


Torsions

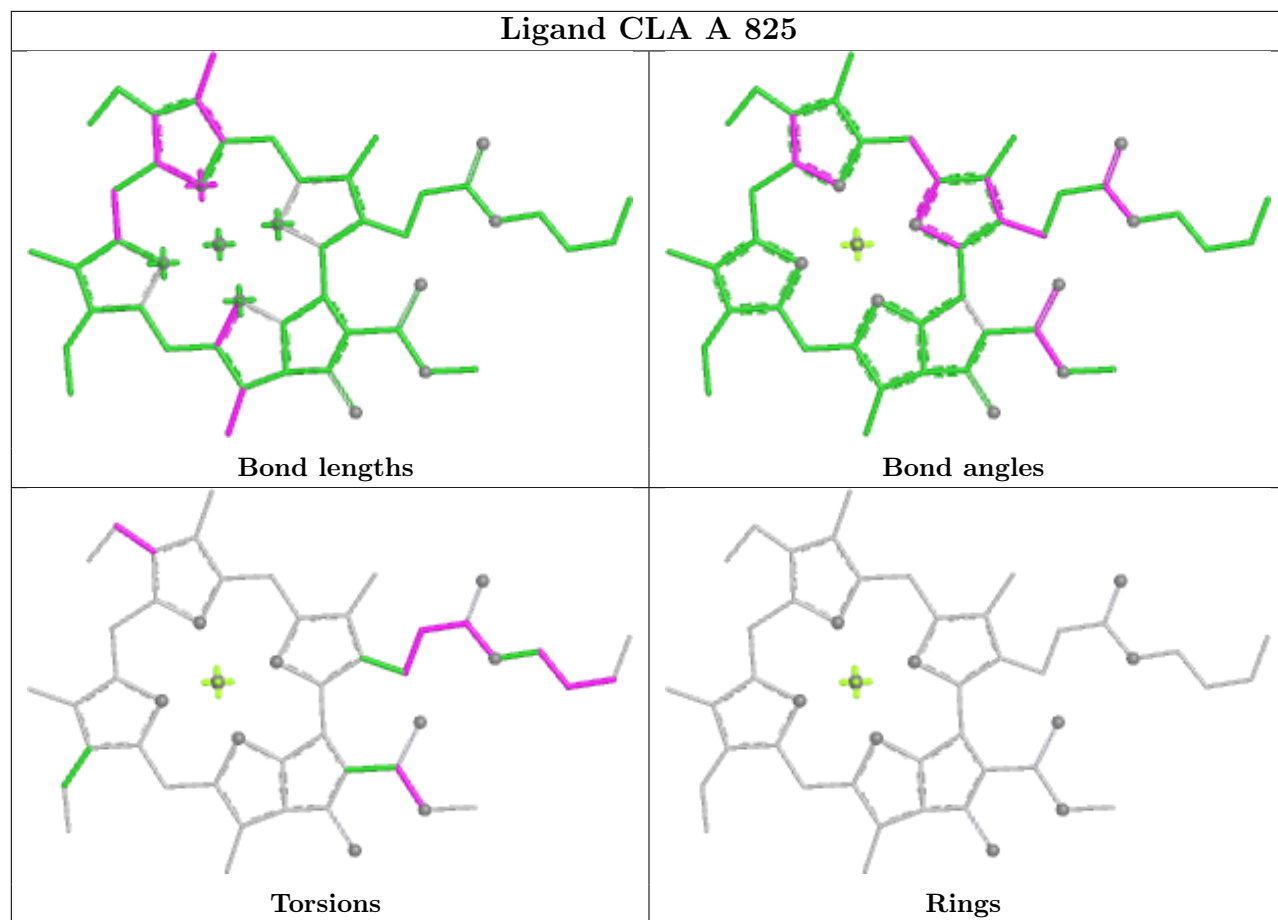


Rings

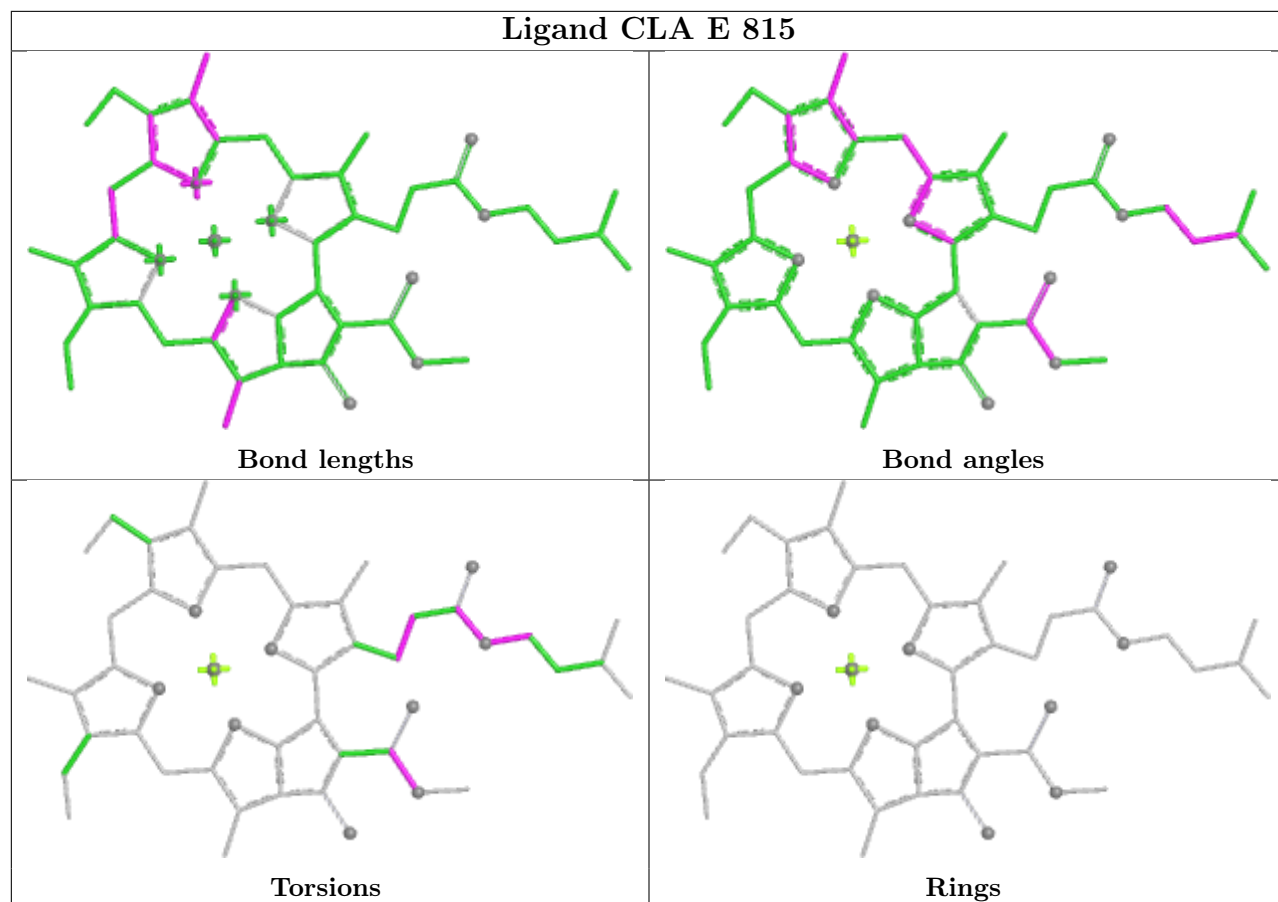
## Ligand CLA e 852



## Ligand CLA A 825

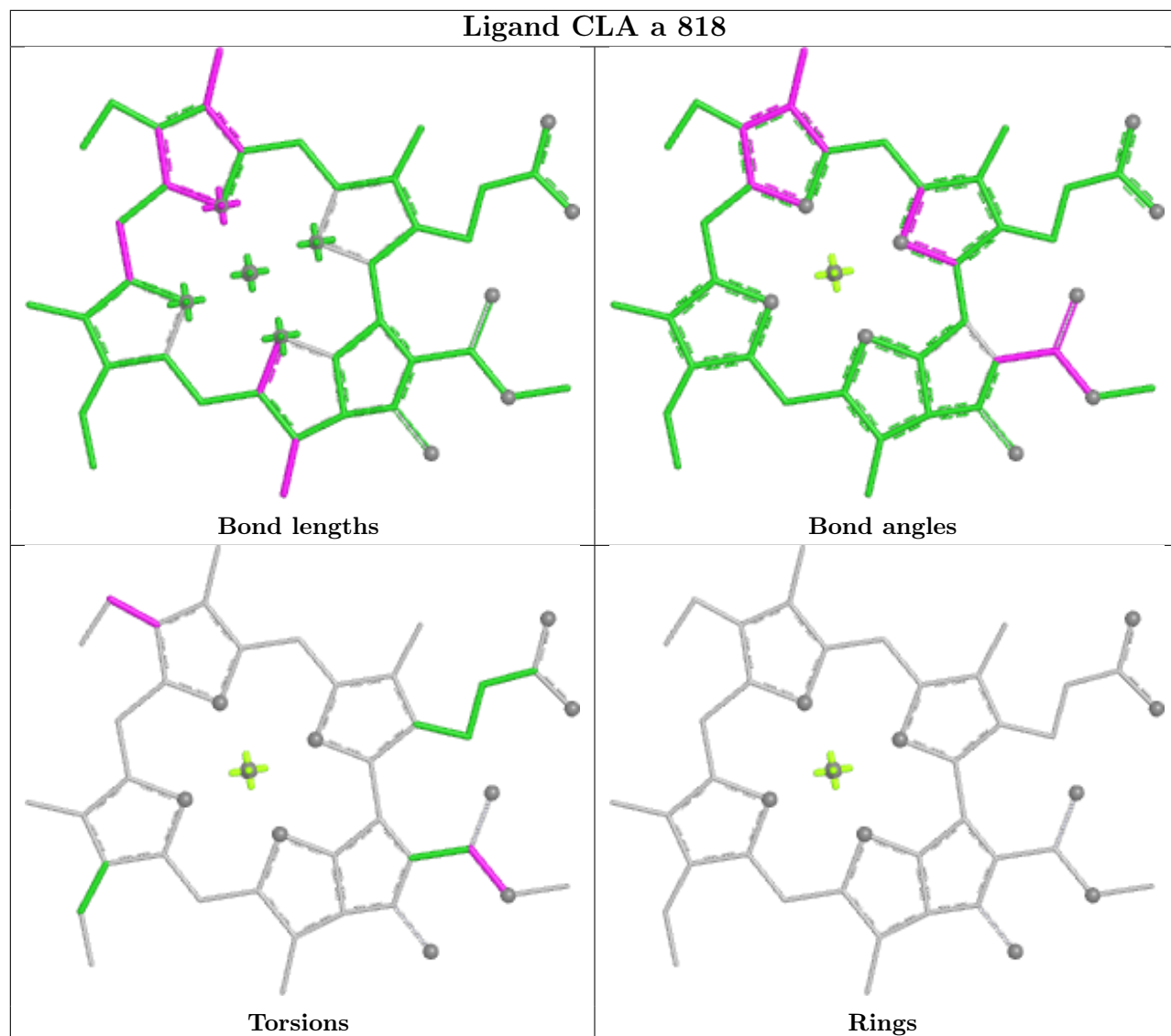


## Ligand CLA E 815

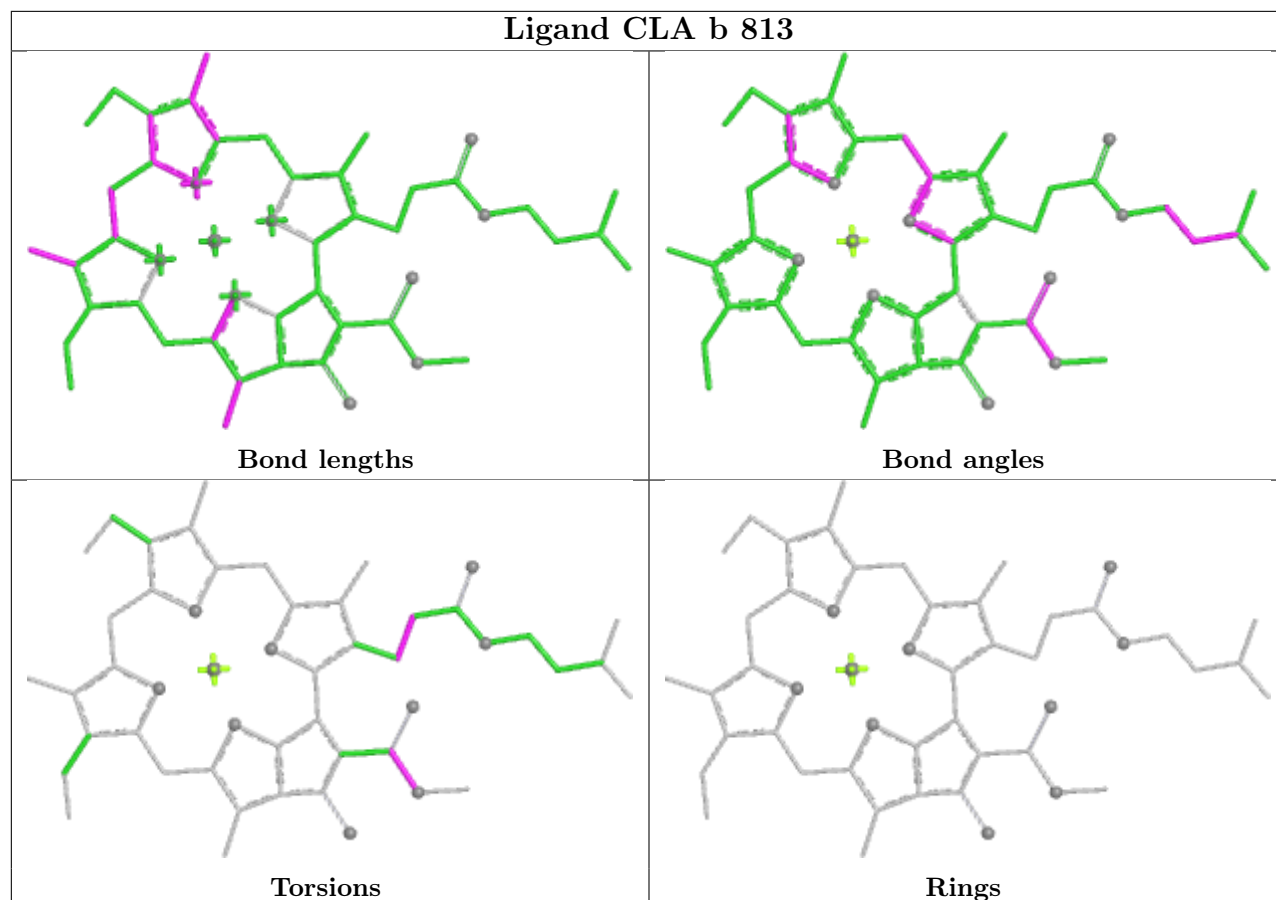




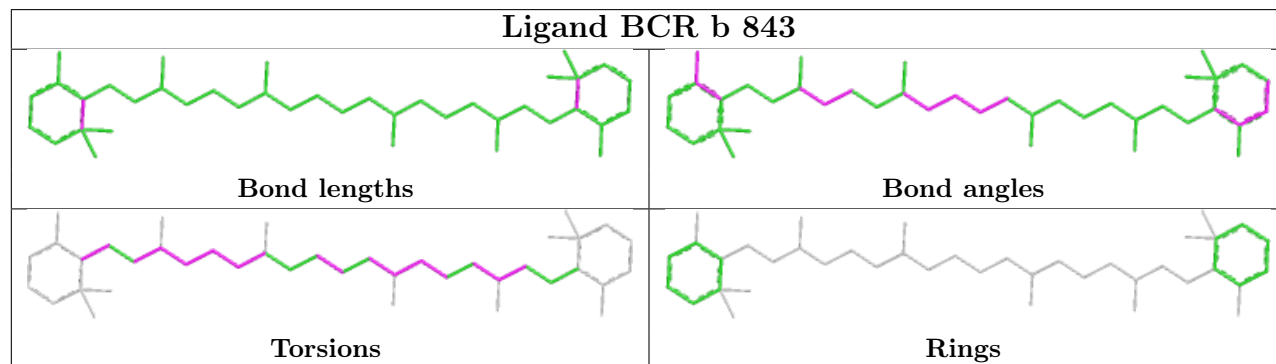
## Ligand CLA a 818



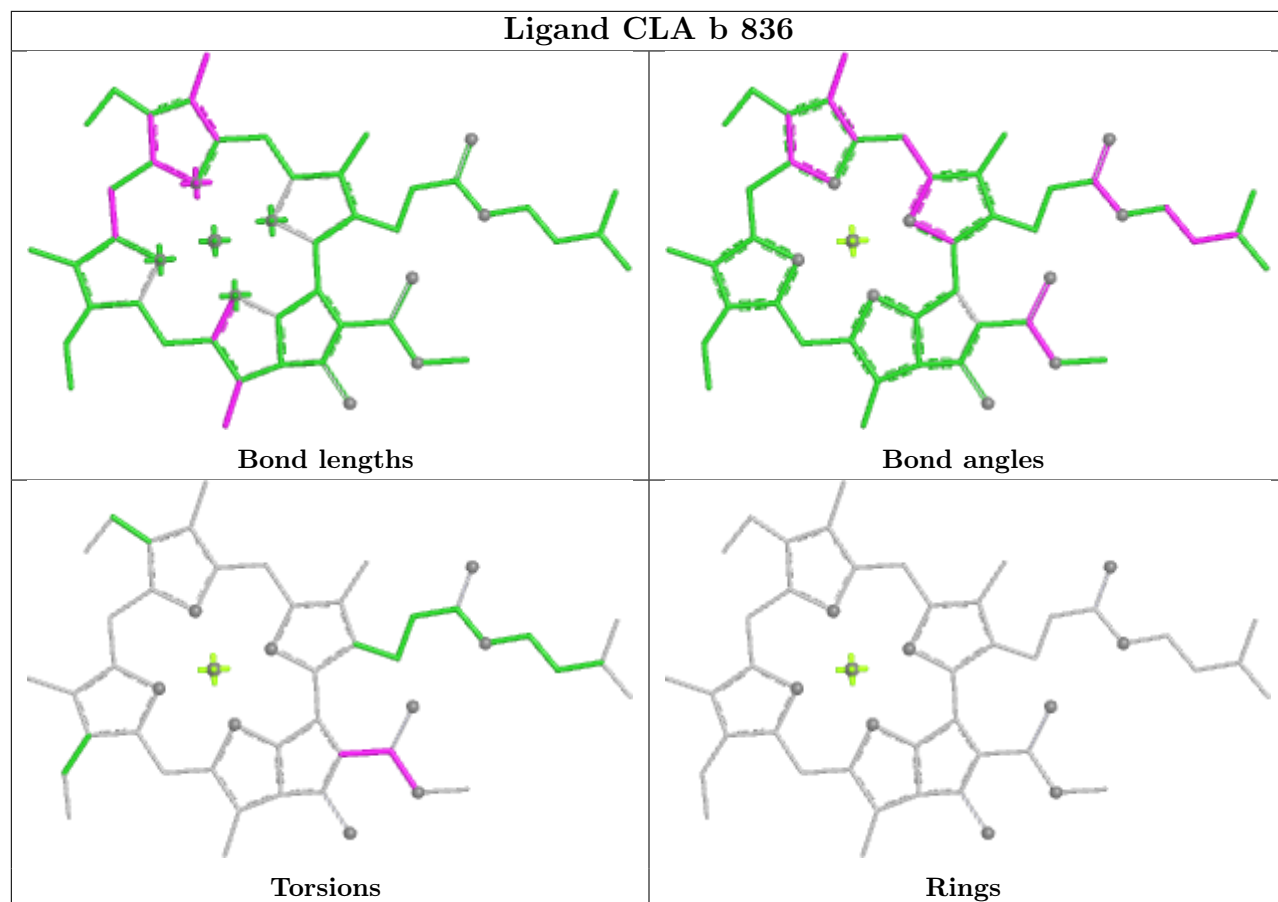
## Ligand CLA b 813



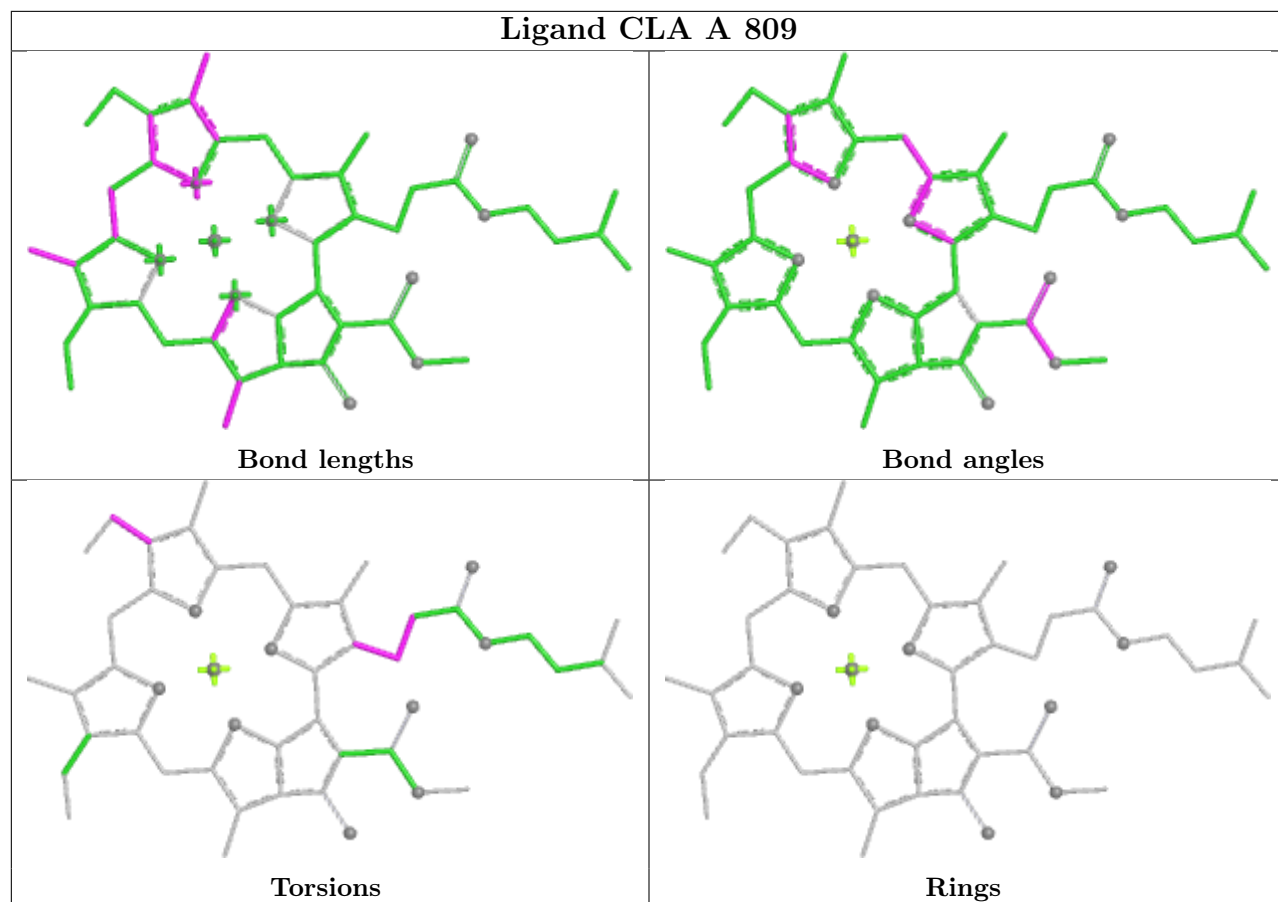
## Ligand BCR b 843

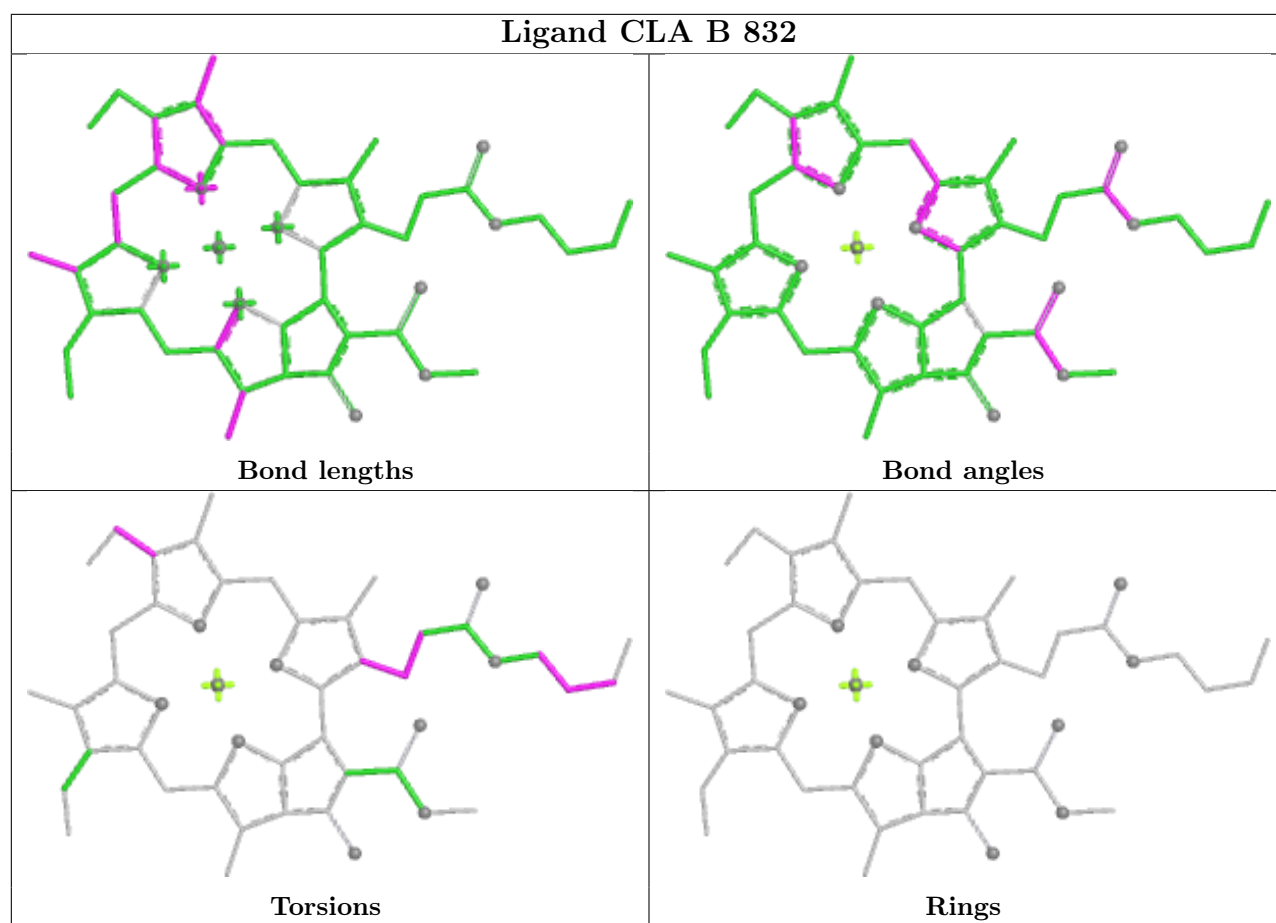


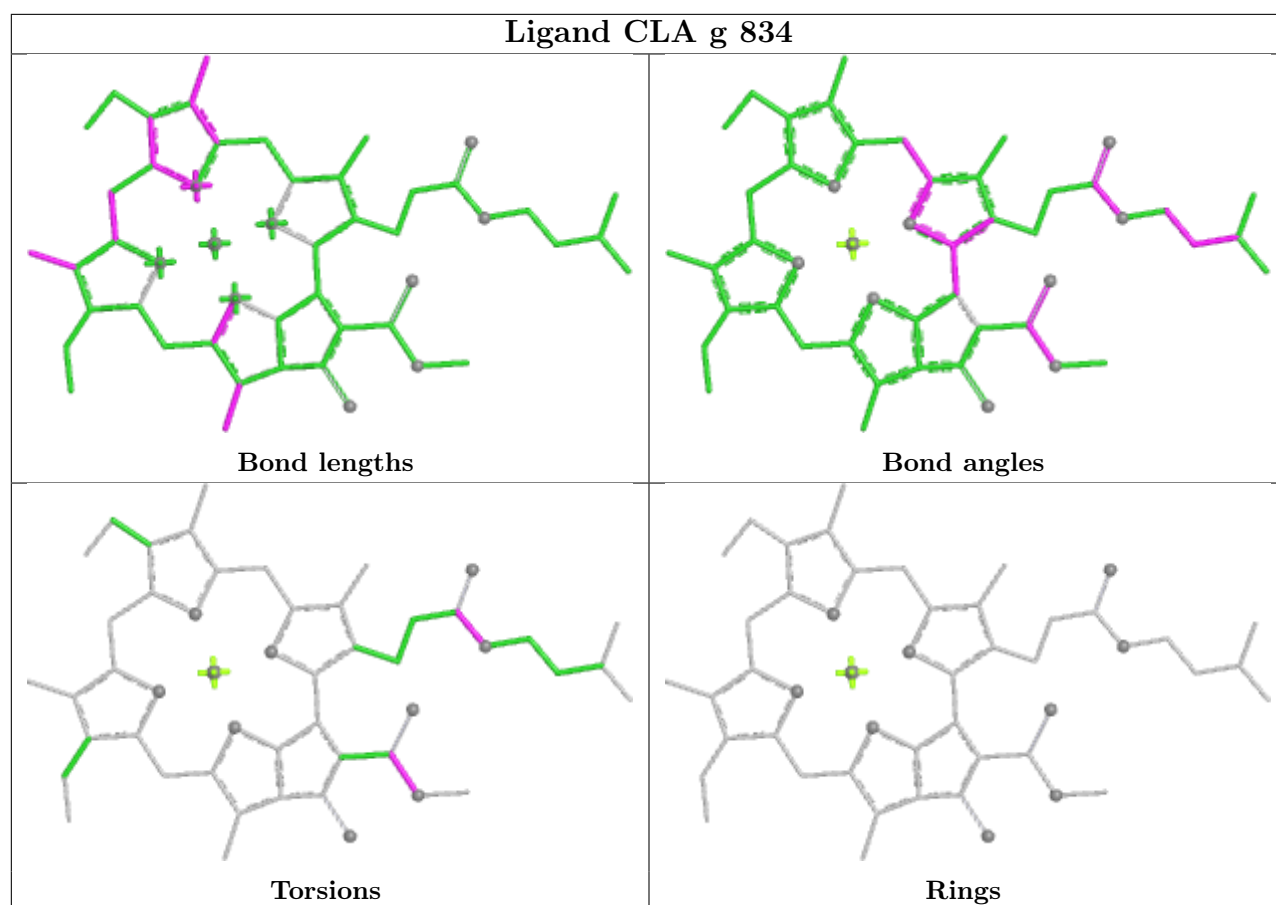
## Ligand CLA b 836



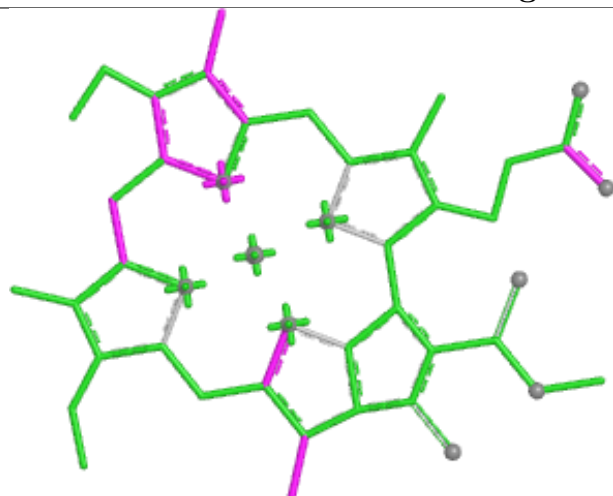
## Ligand CLA A 809



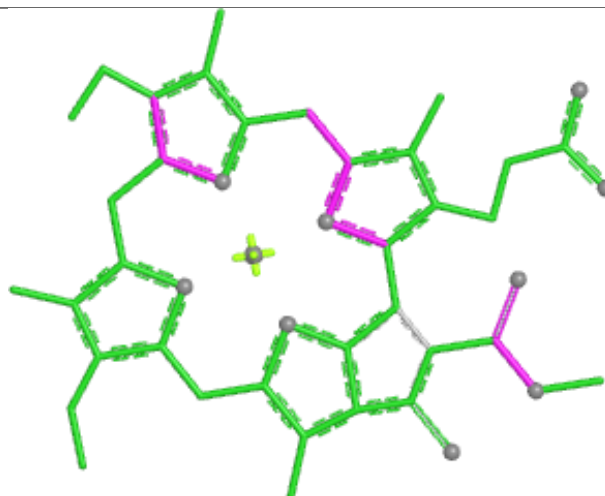




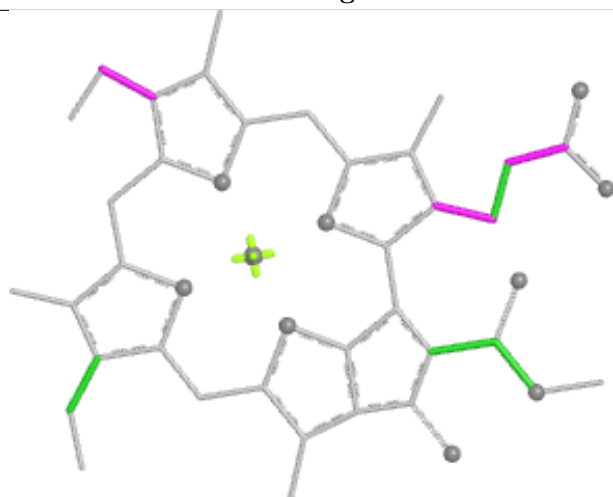
## Ligand CLA e 816



Bond lengths



Bond angles

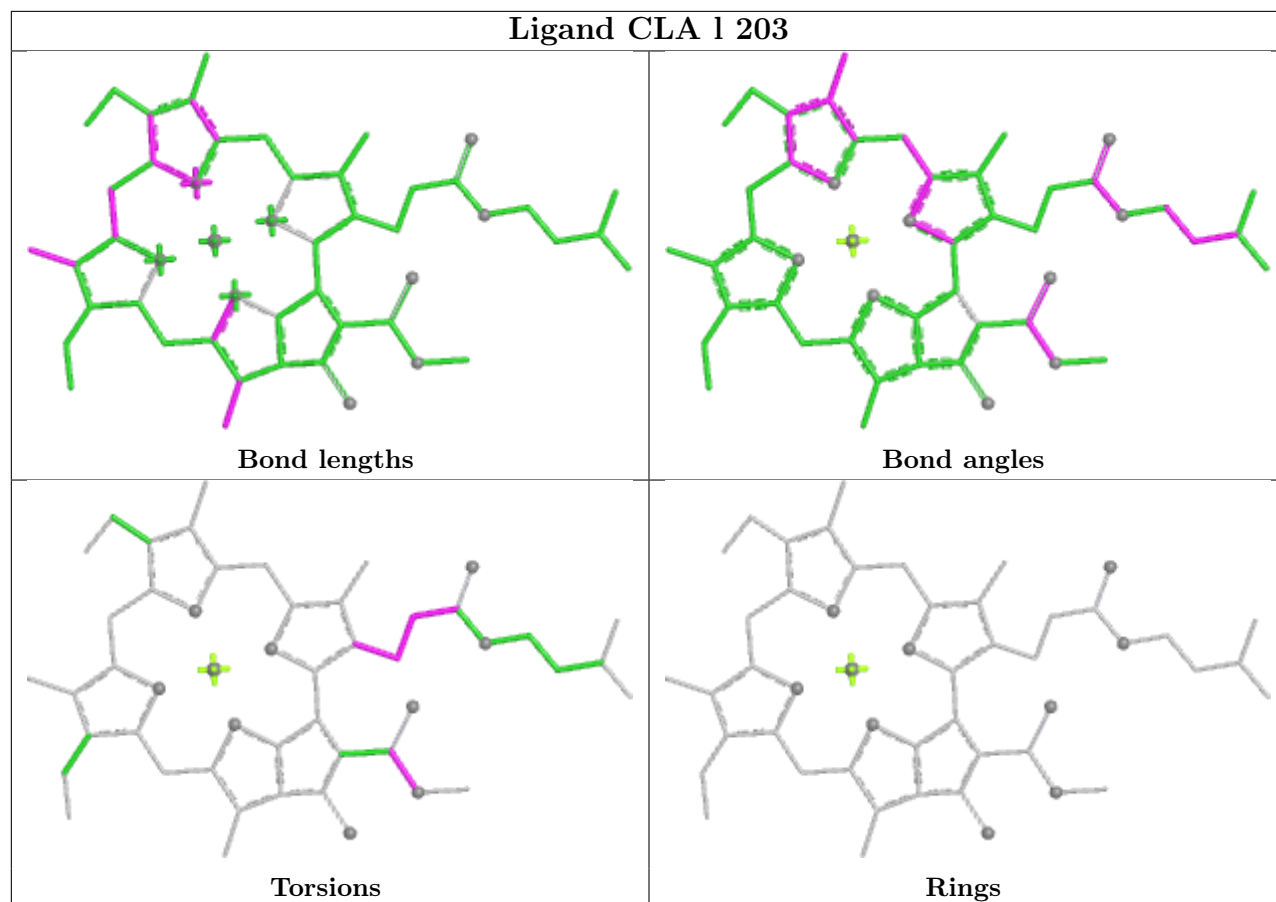


Torsions



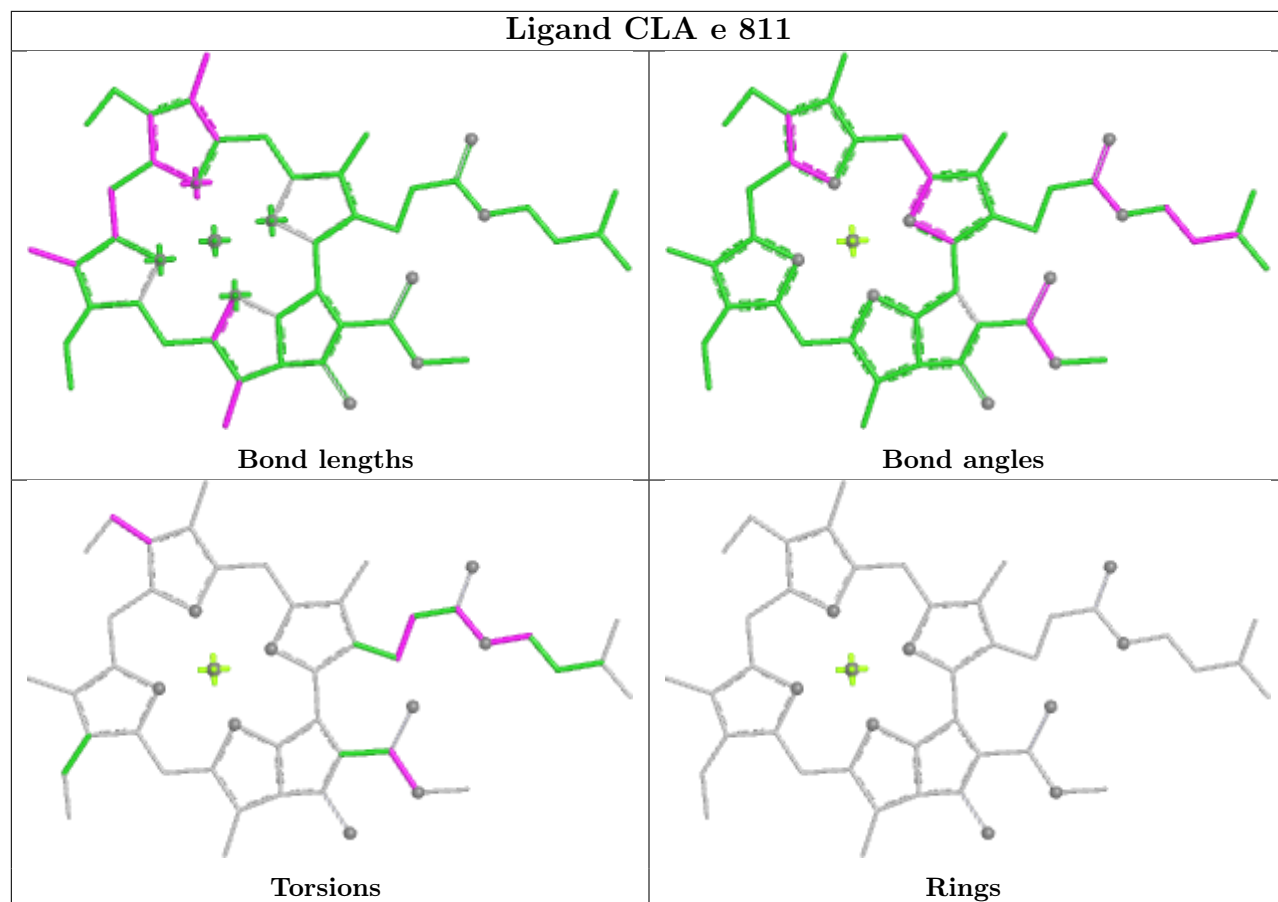
Rings

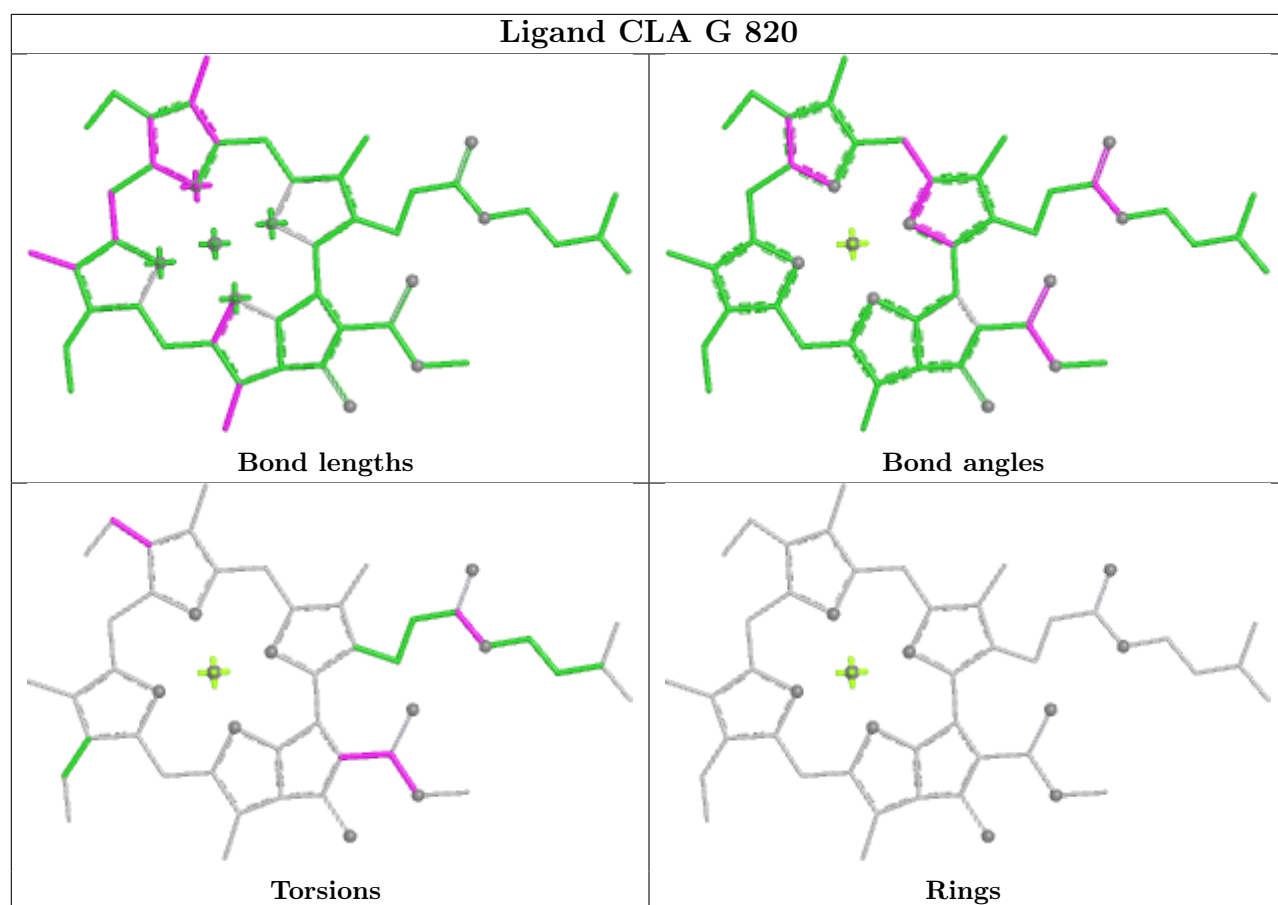
## Ligand CLA 1 203



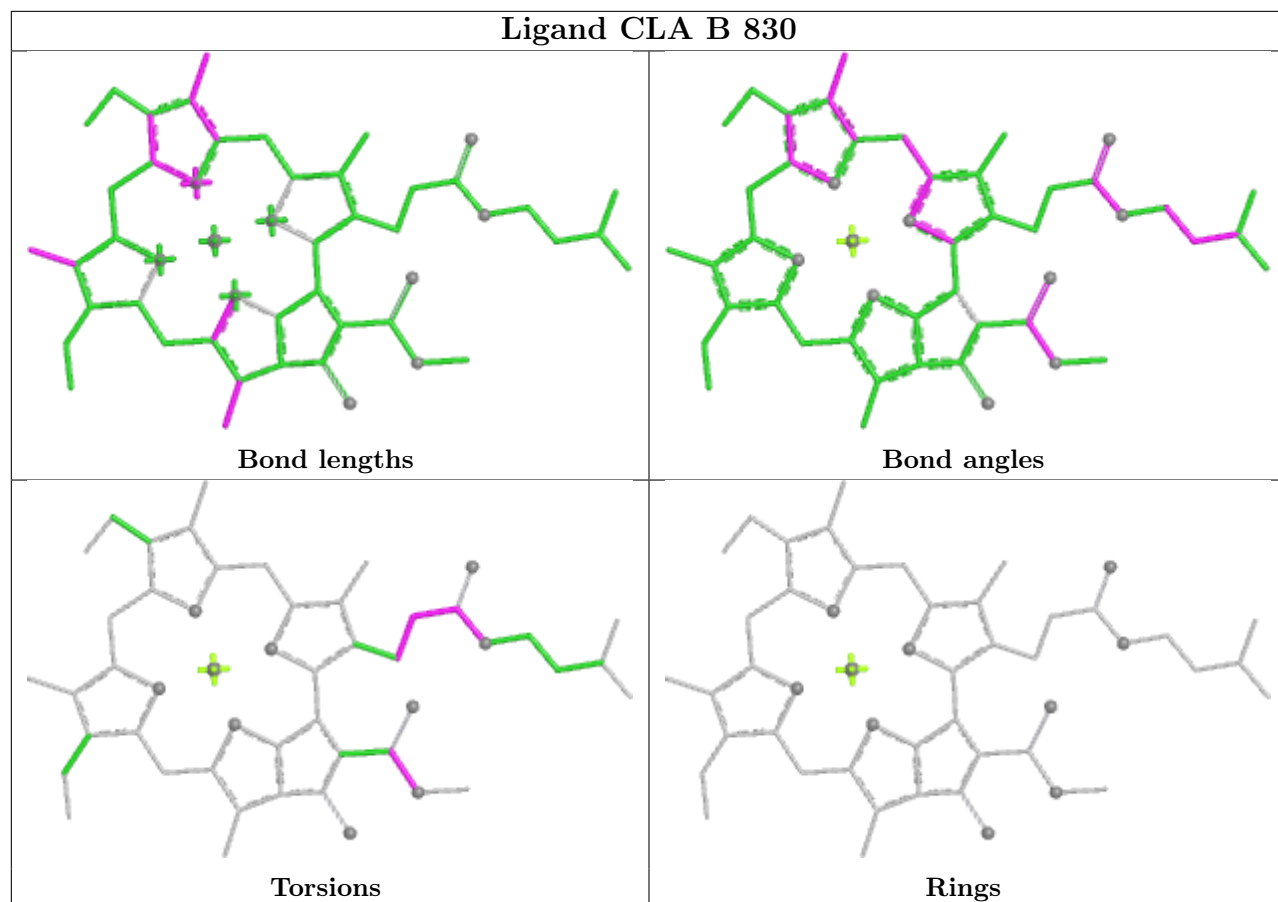


## Ligand CLA e 811

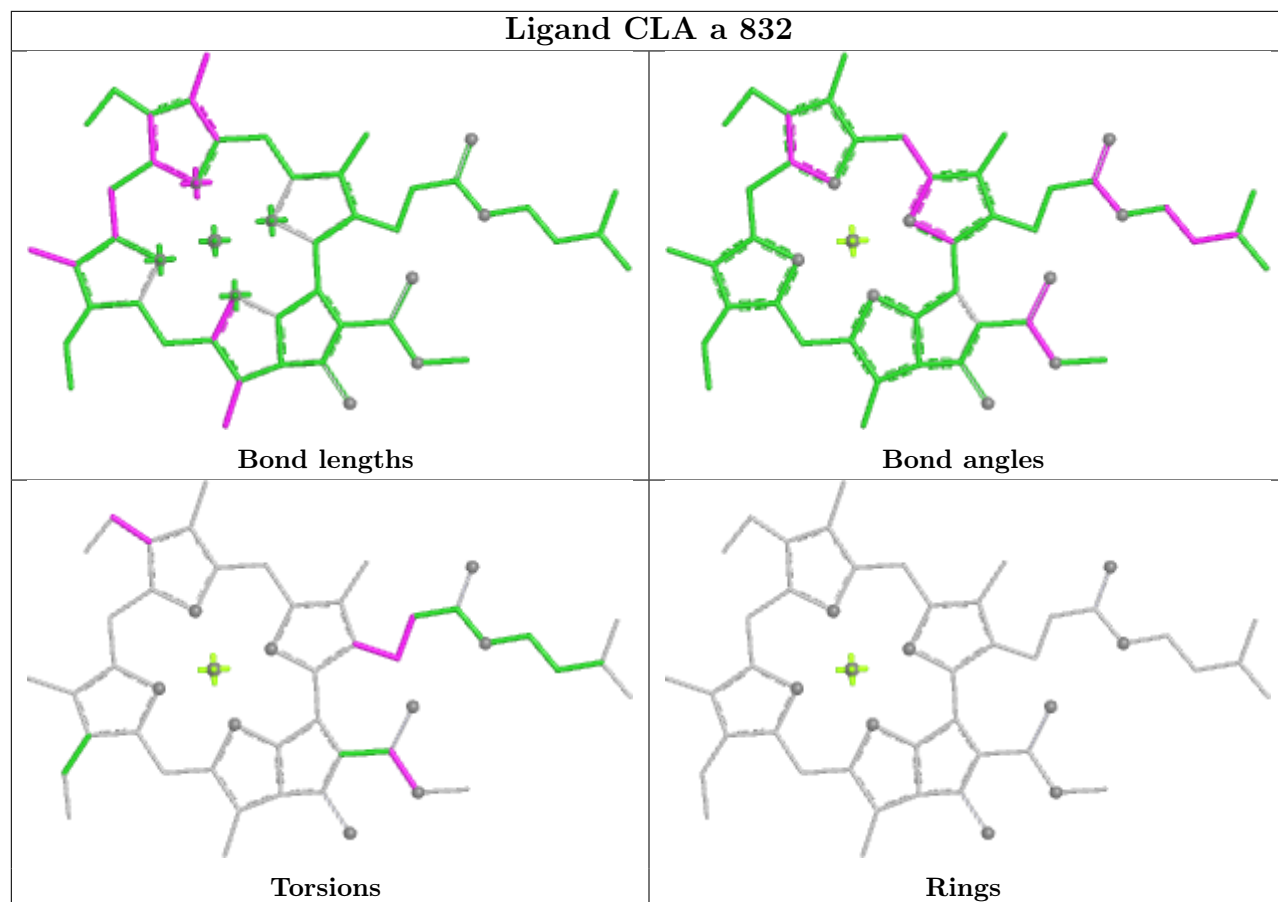




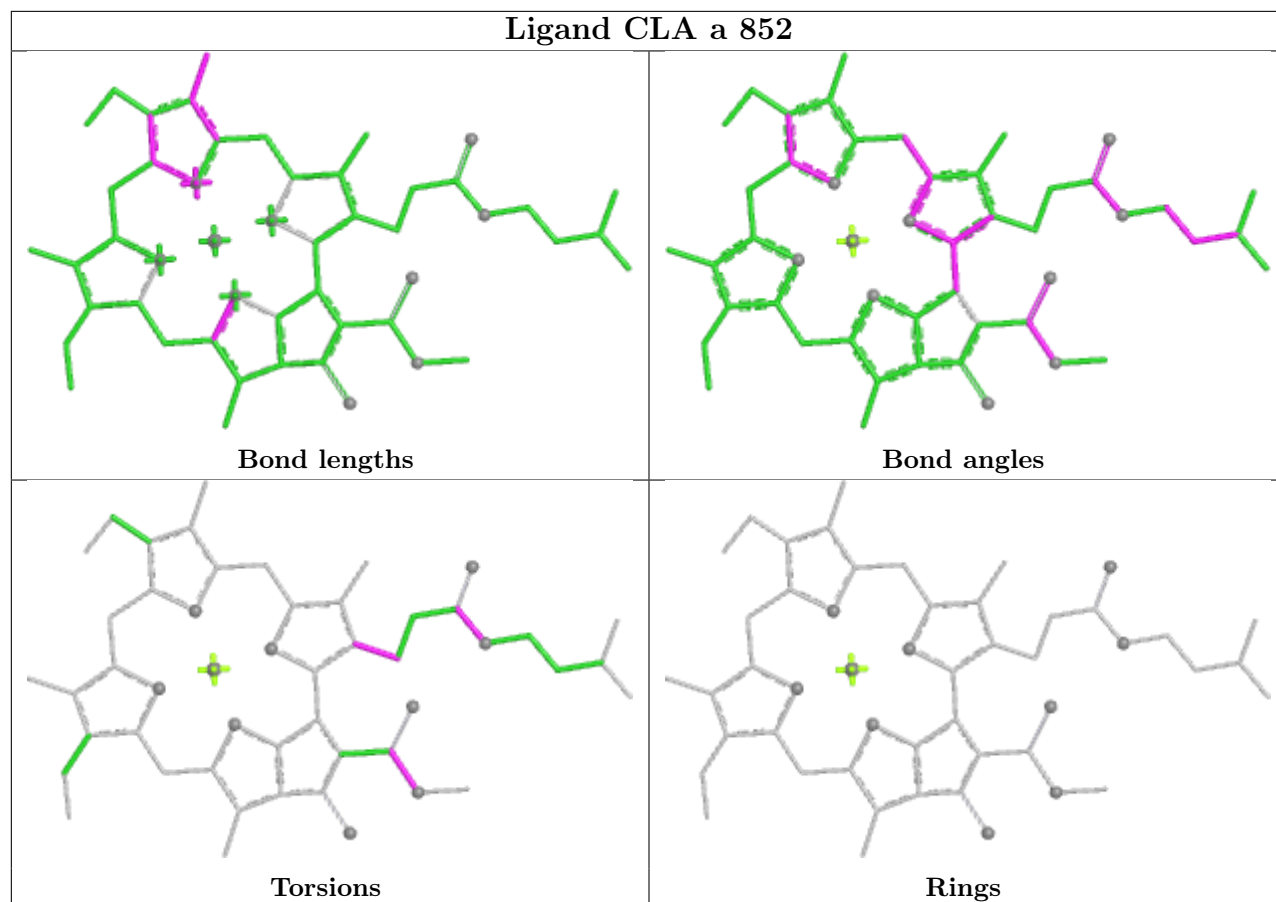
## Ligand CLA B 830



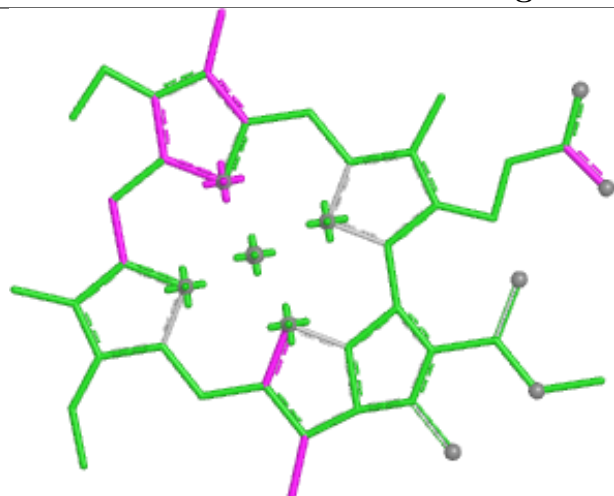
## Ligand CLA a 832



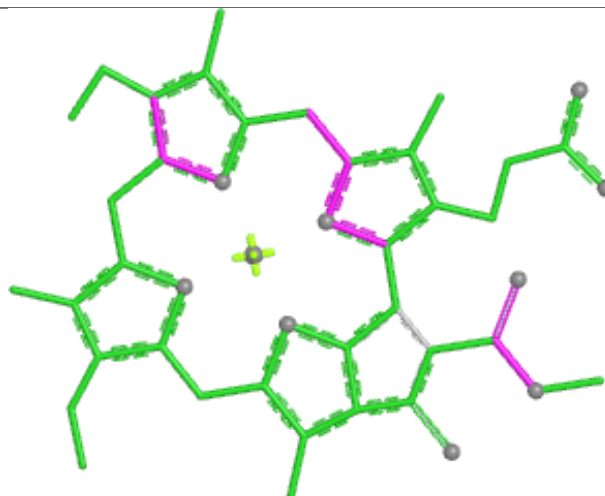
## Ligand CLA a 852



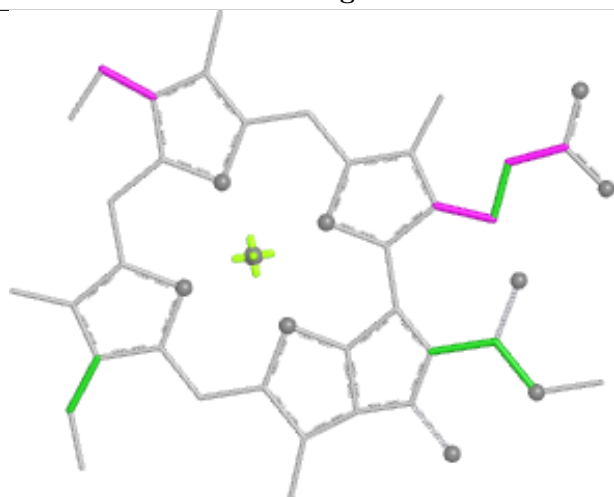
## Ligand CLA E 817



Bond lengths



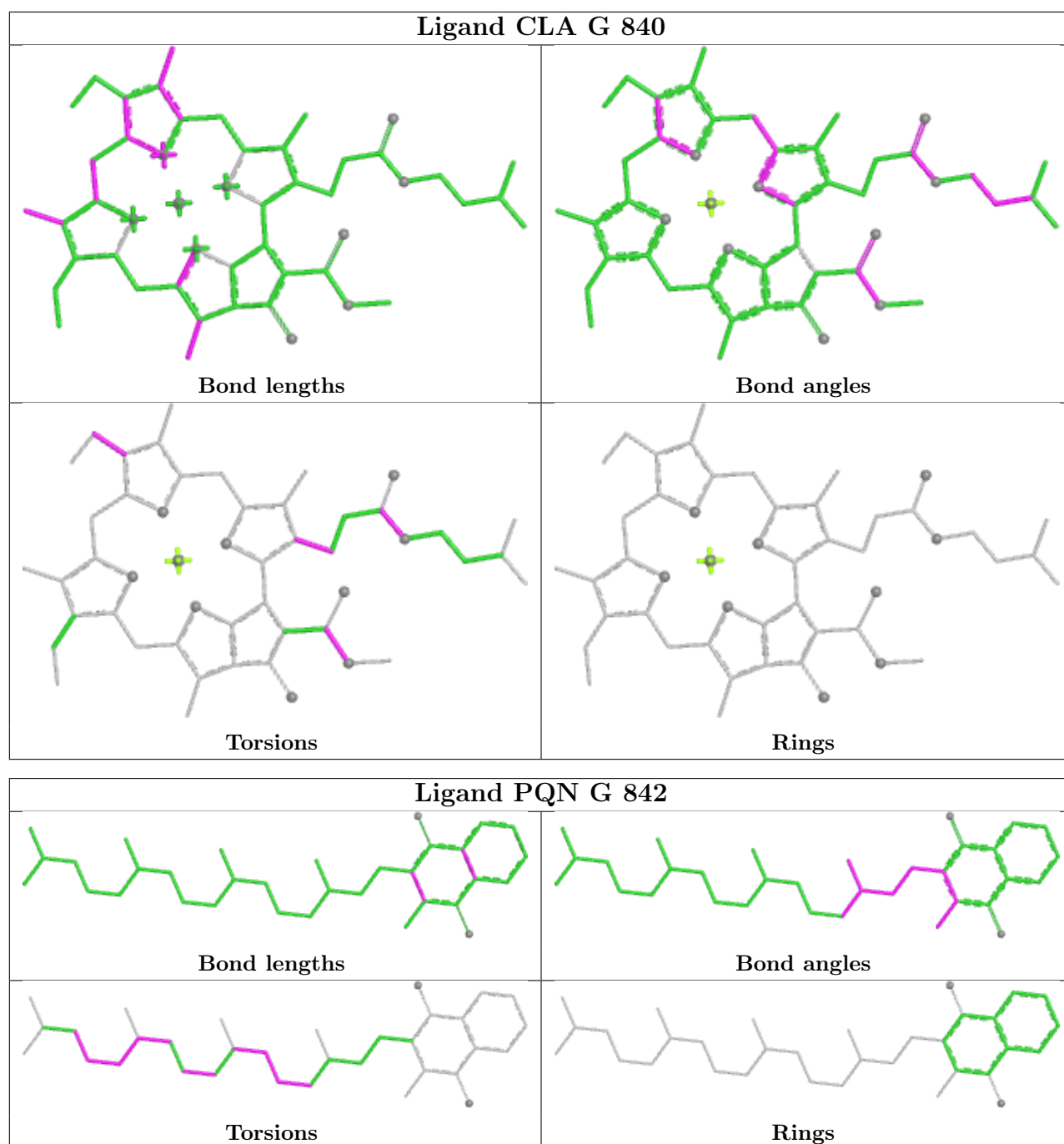
Bond angles



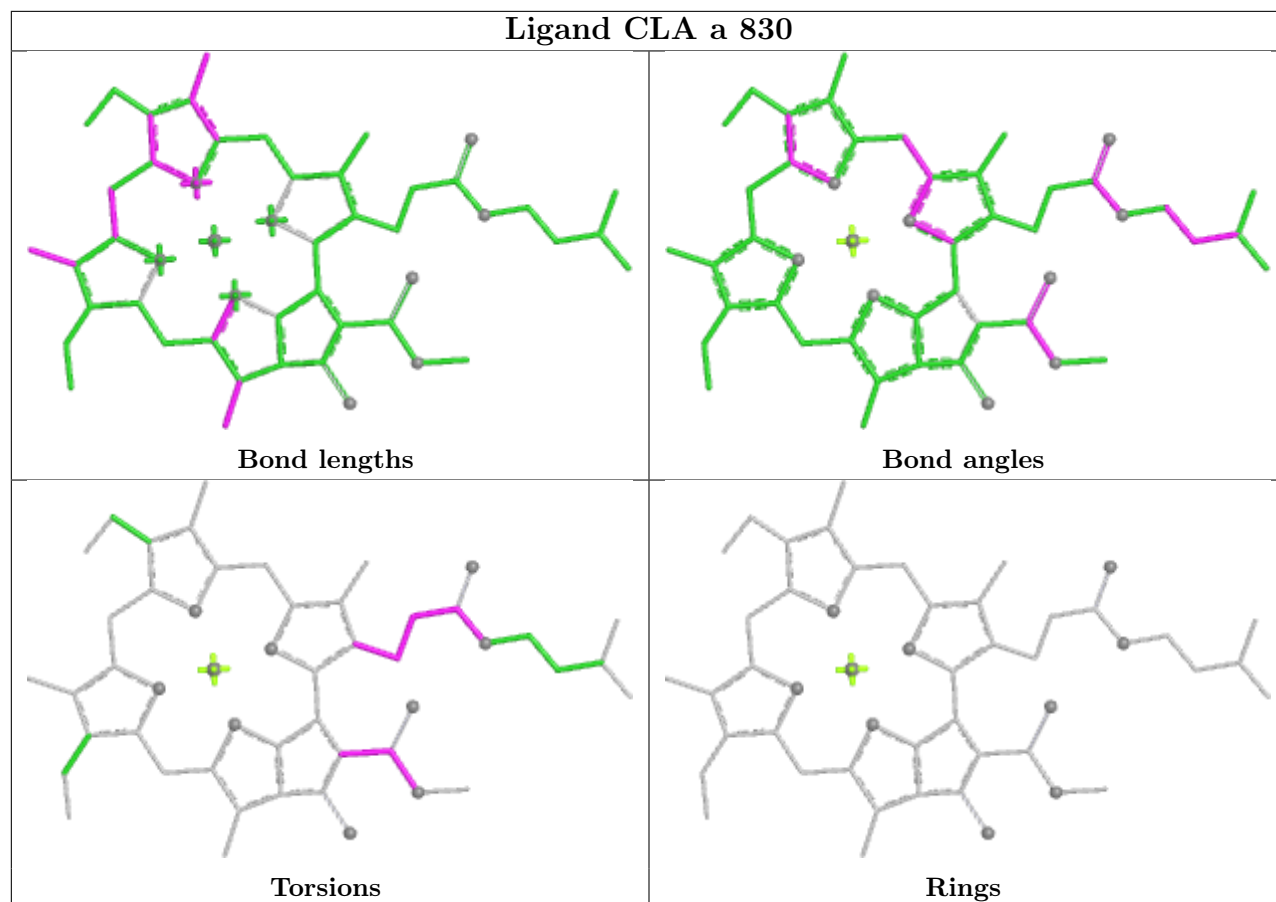
Torsions



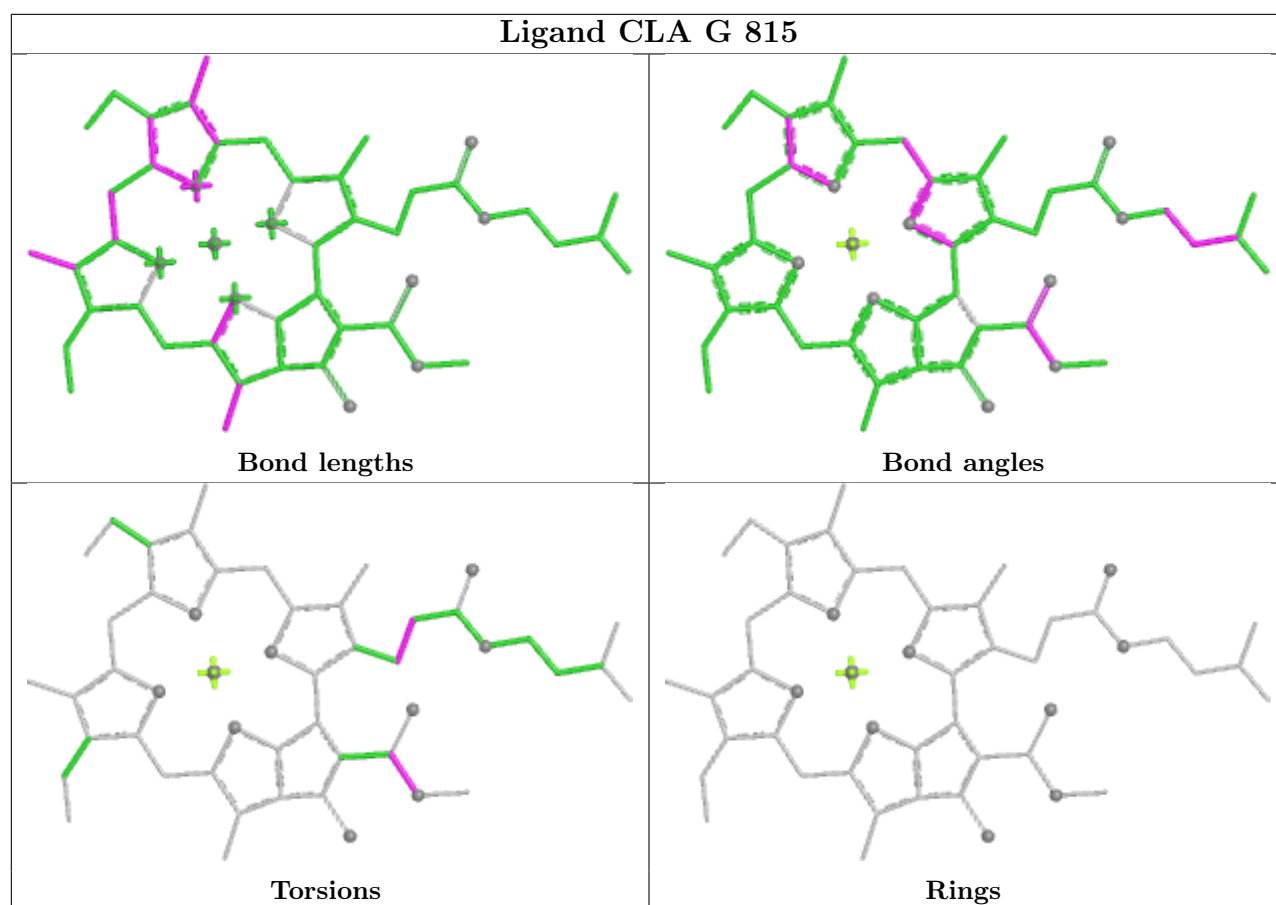
Rings



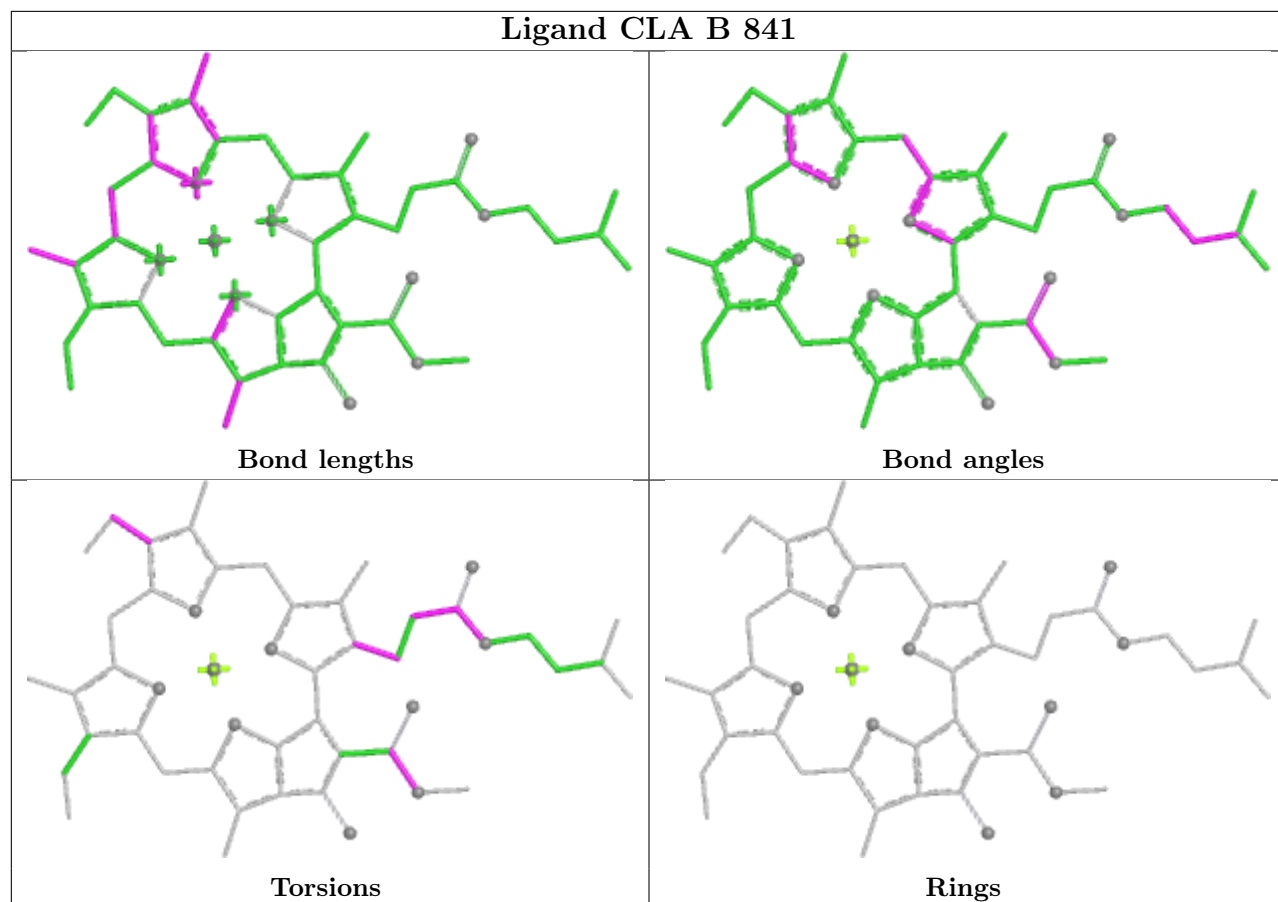
## Ligand CLA a 830



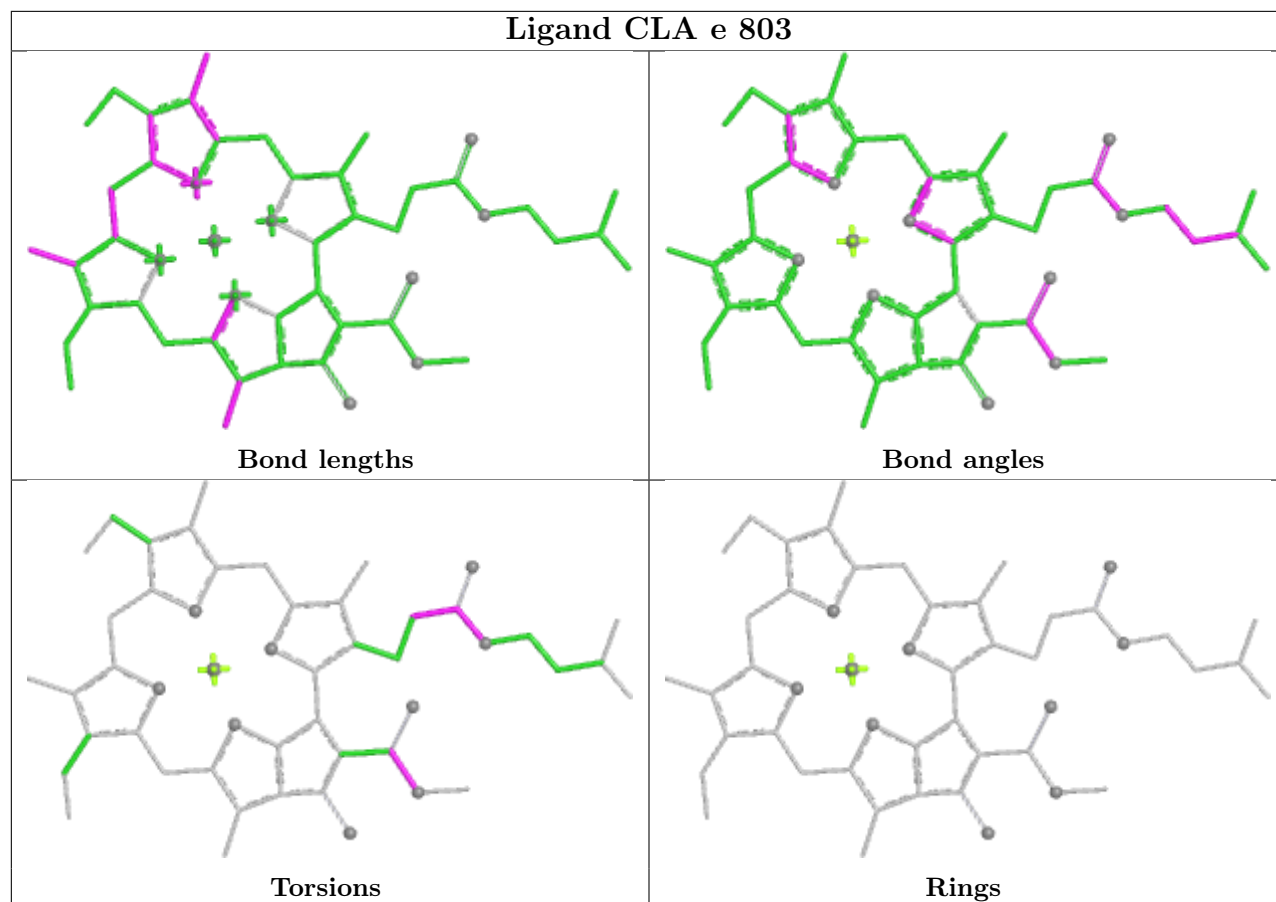


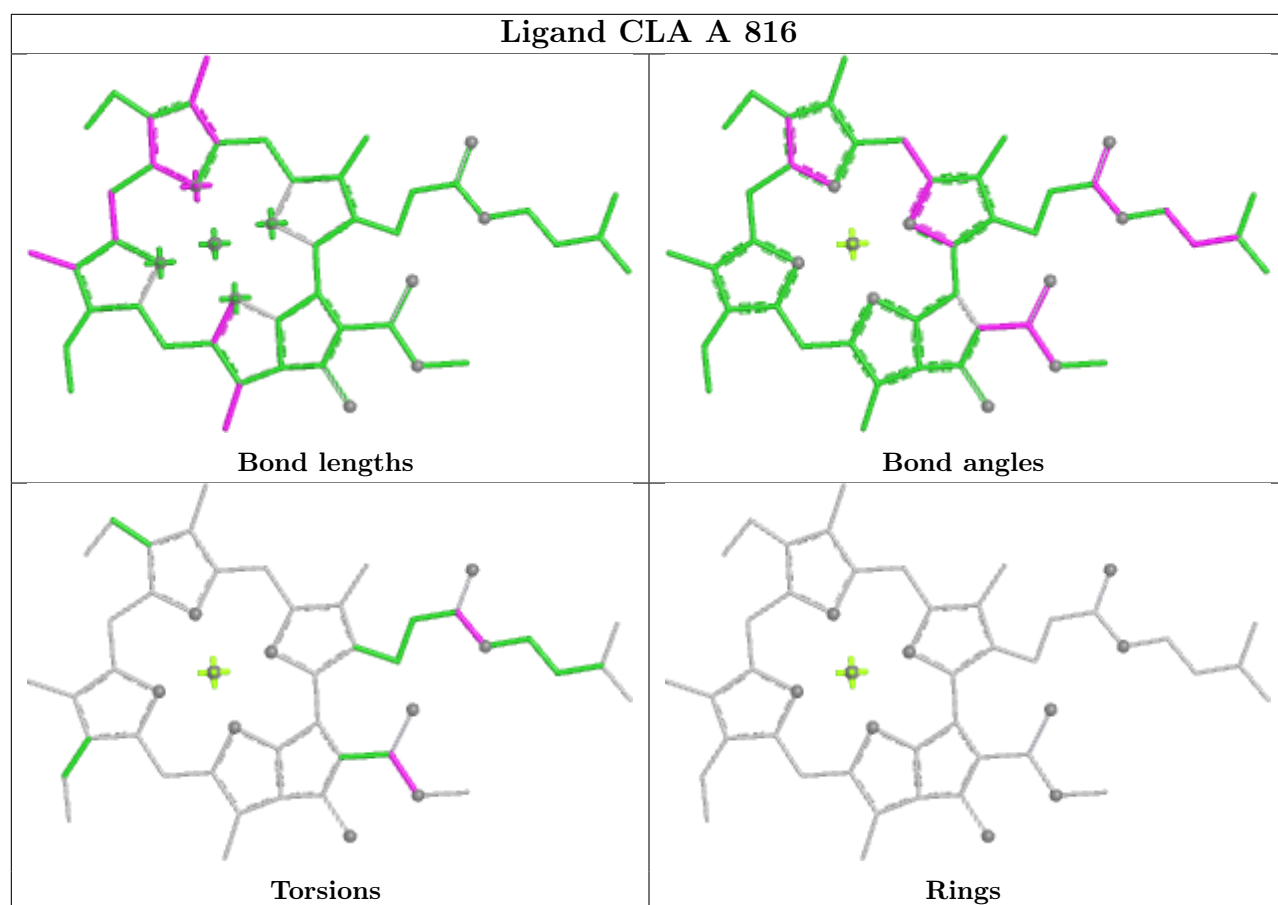


## Ligand CLA B 841

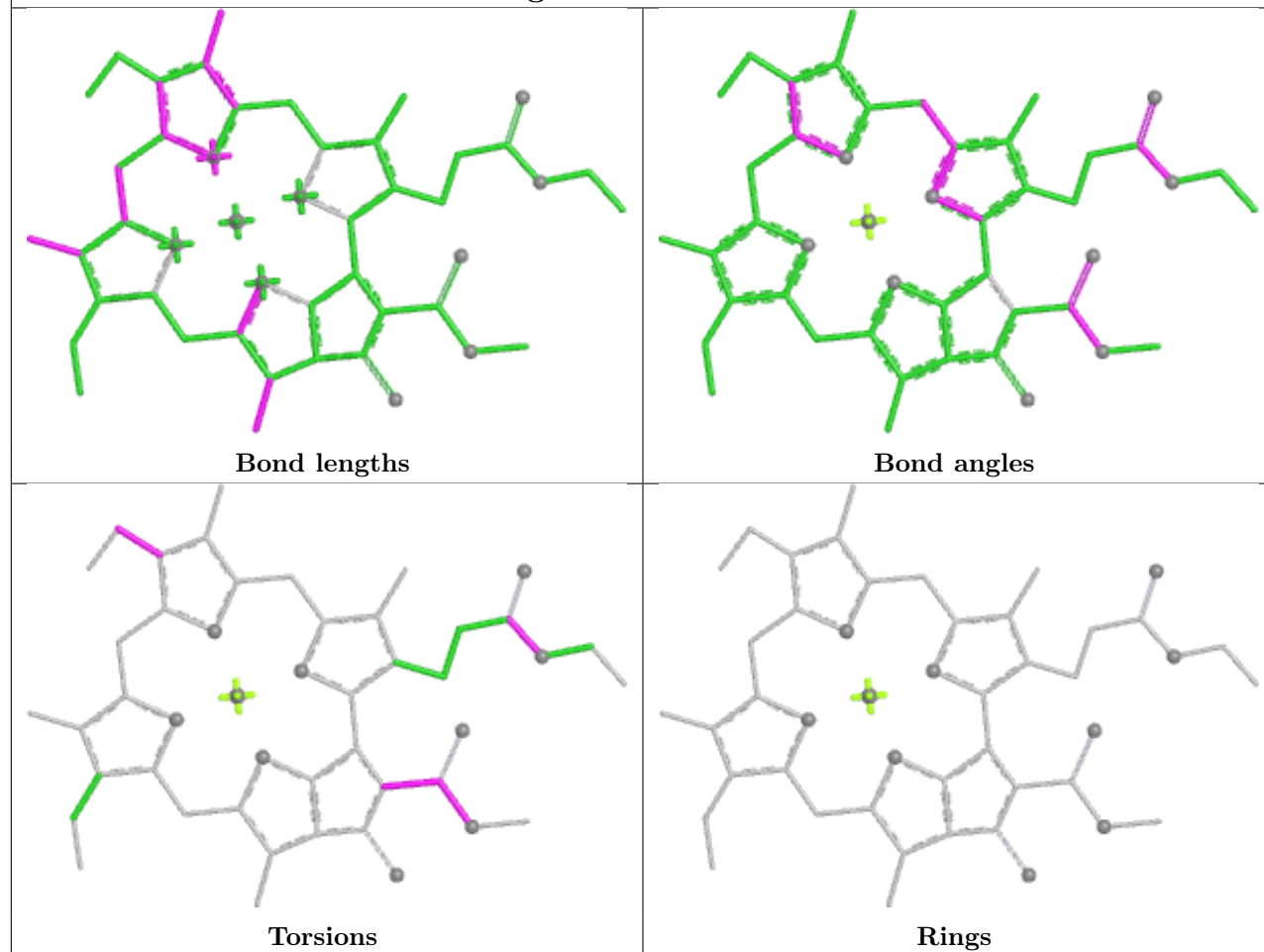


## Ligand CLA e 803

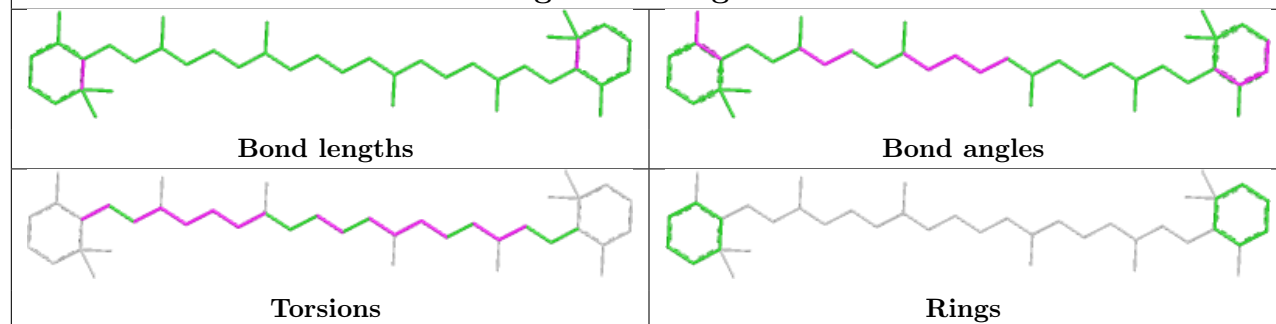




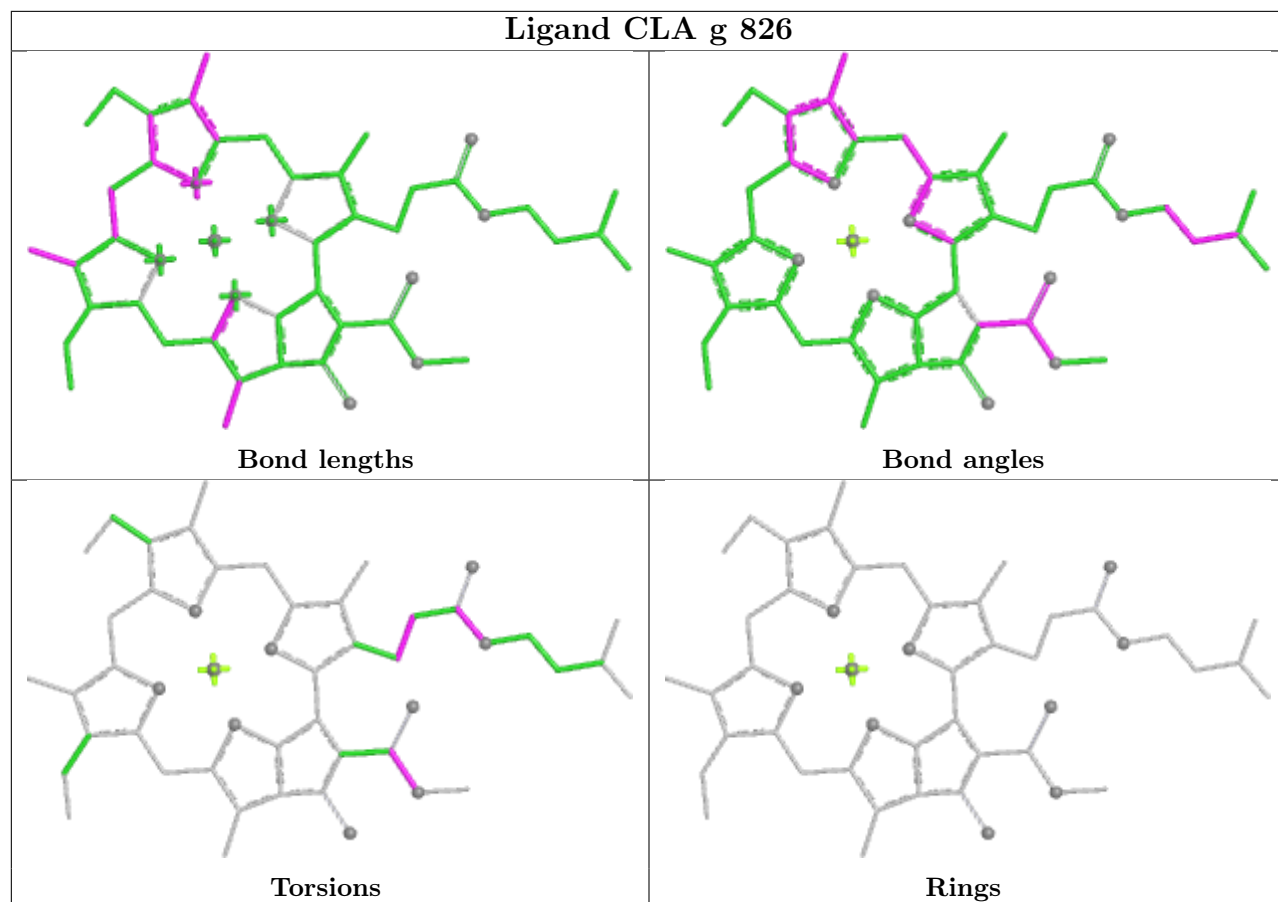
## Ligand CLA B 821



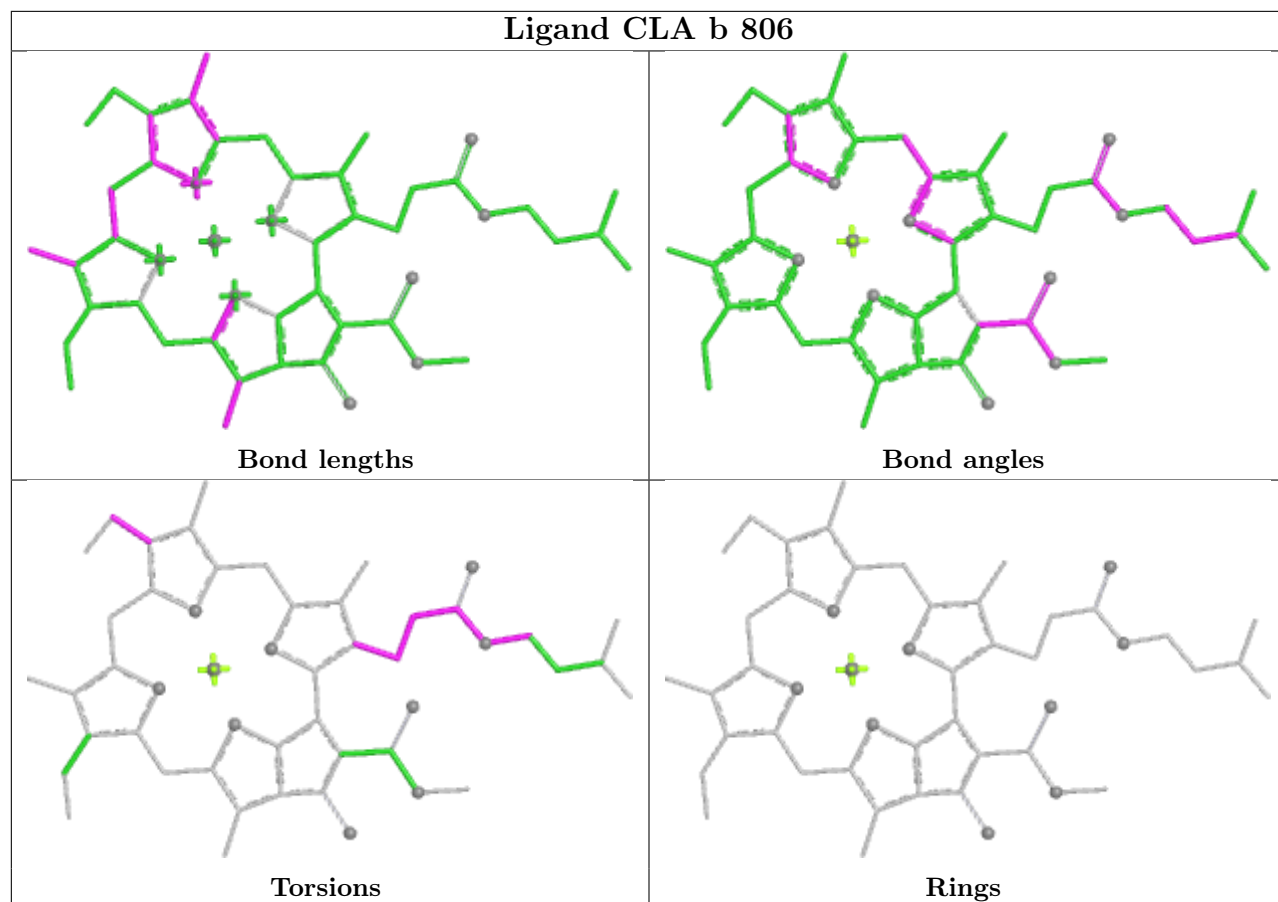
## Ligand BCR g 845



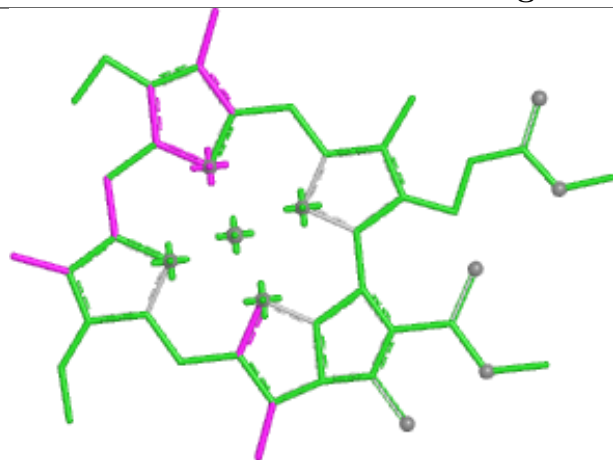
## Ligand CLA g 826



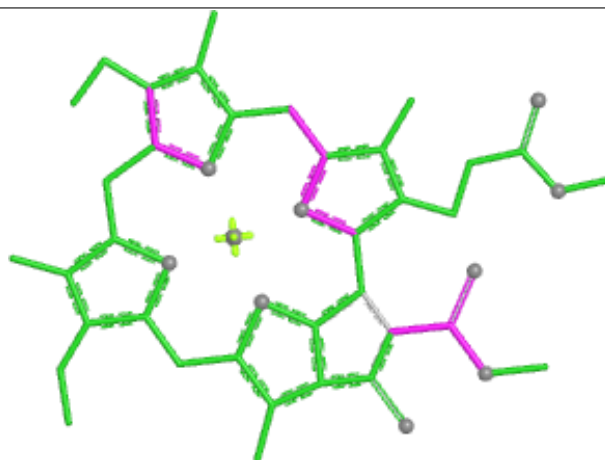
## Ligand CLA b 806



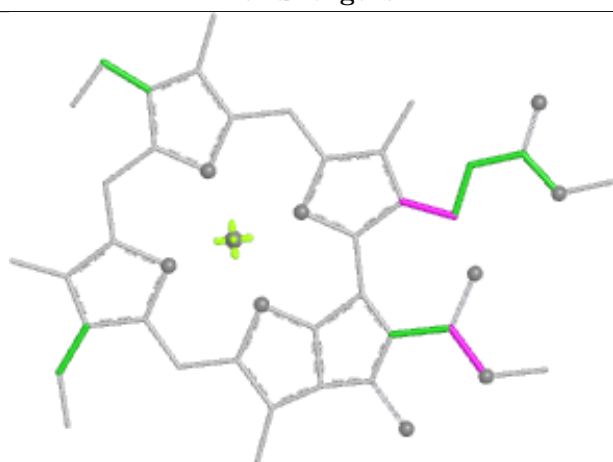
## Ligand CLA b 825



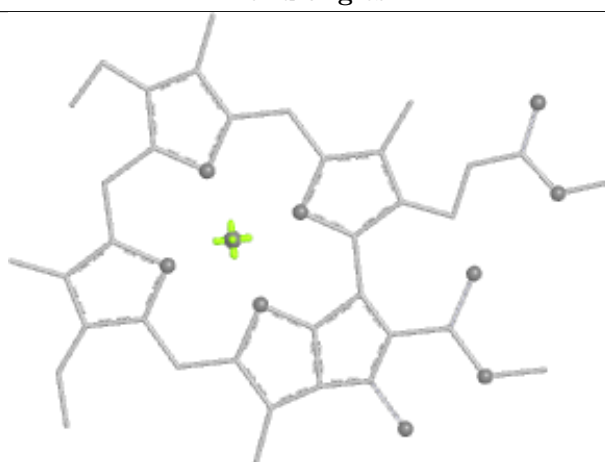
Bond lengths



Bond angles



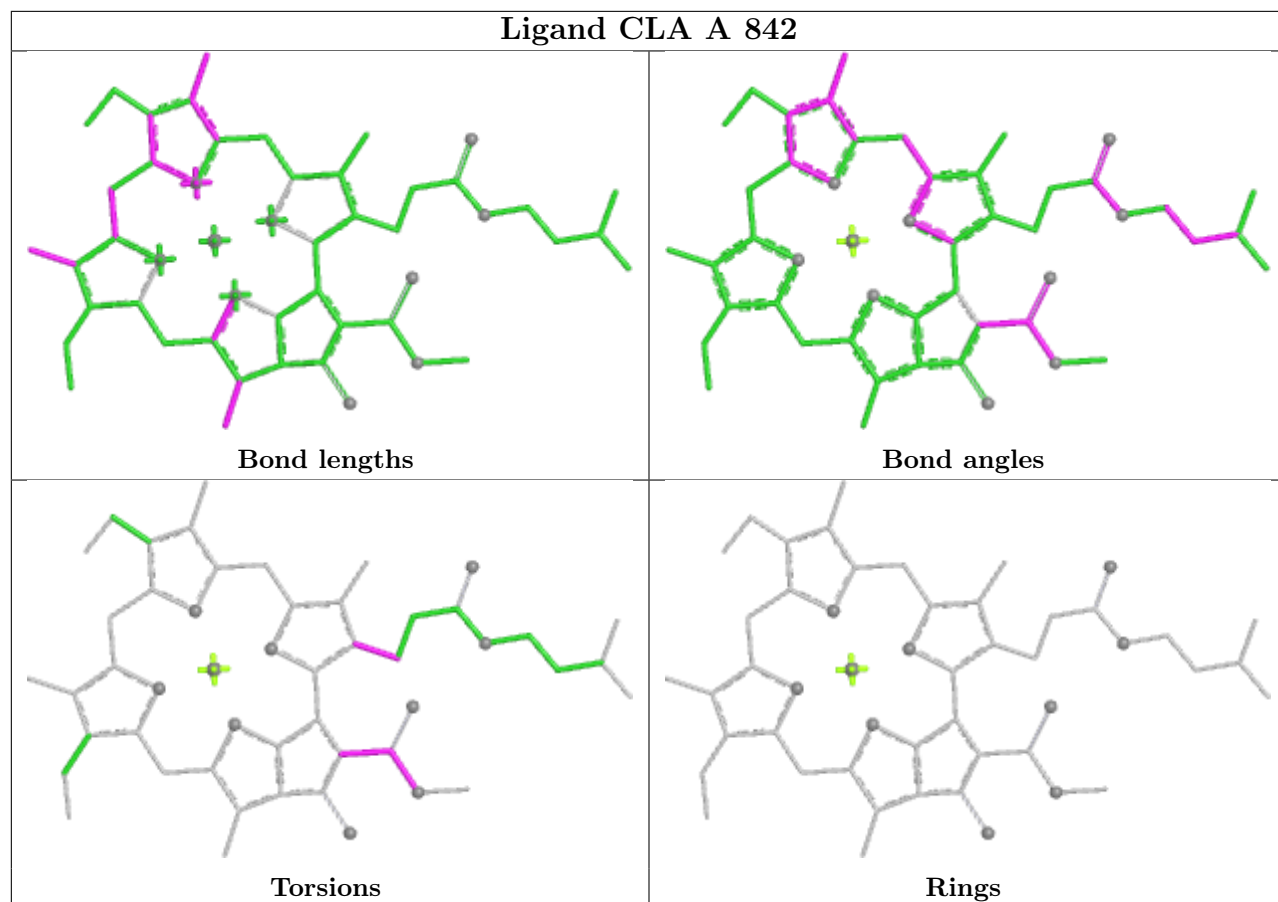
Torsions



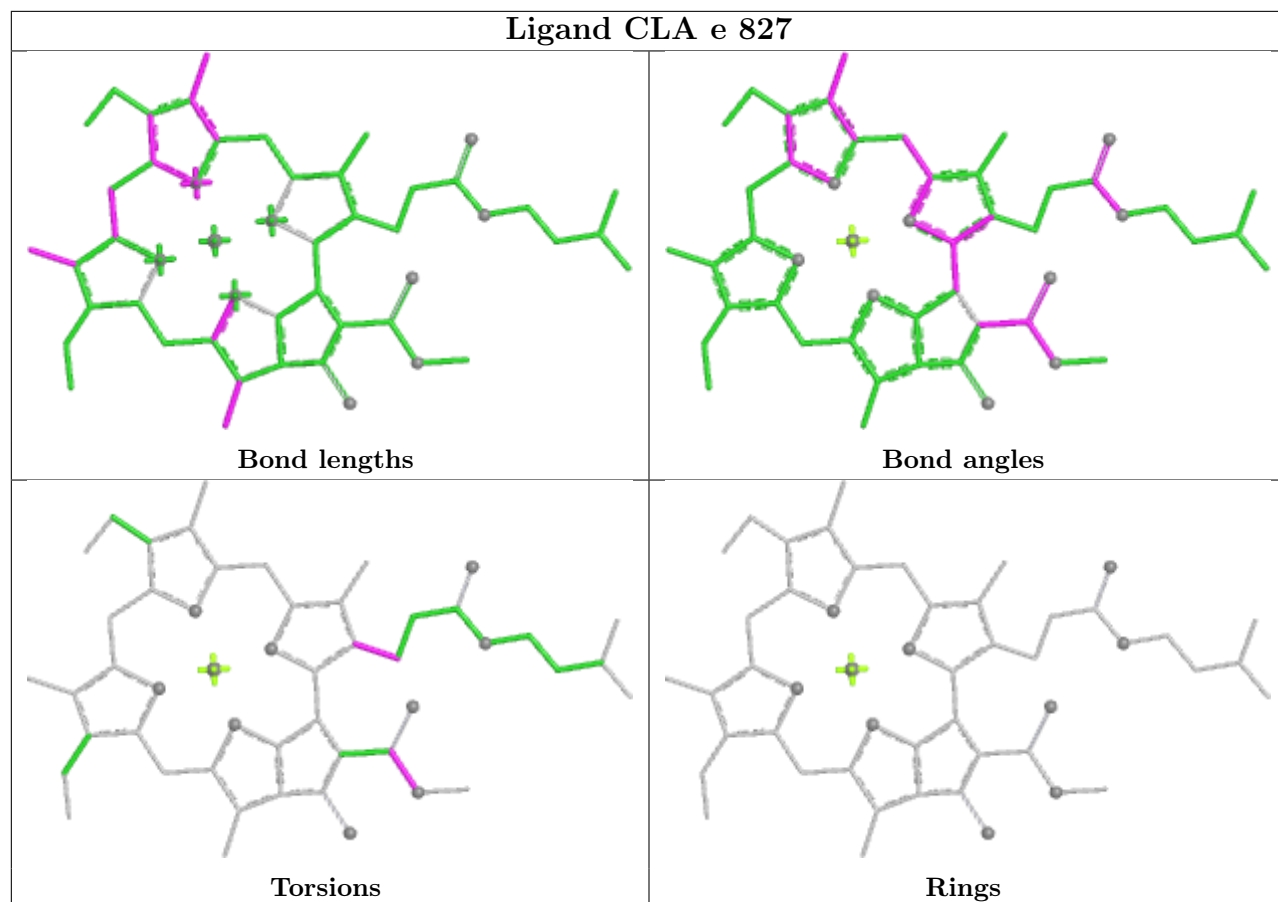
Rings



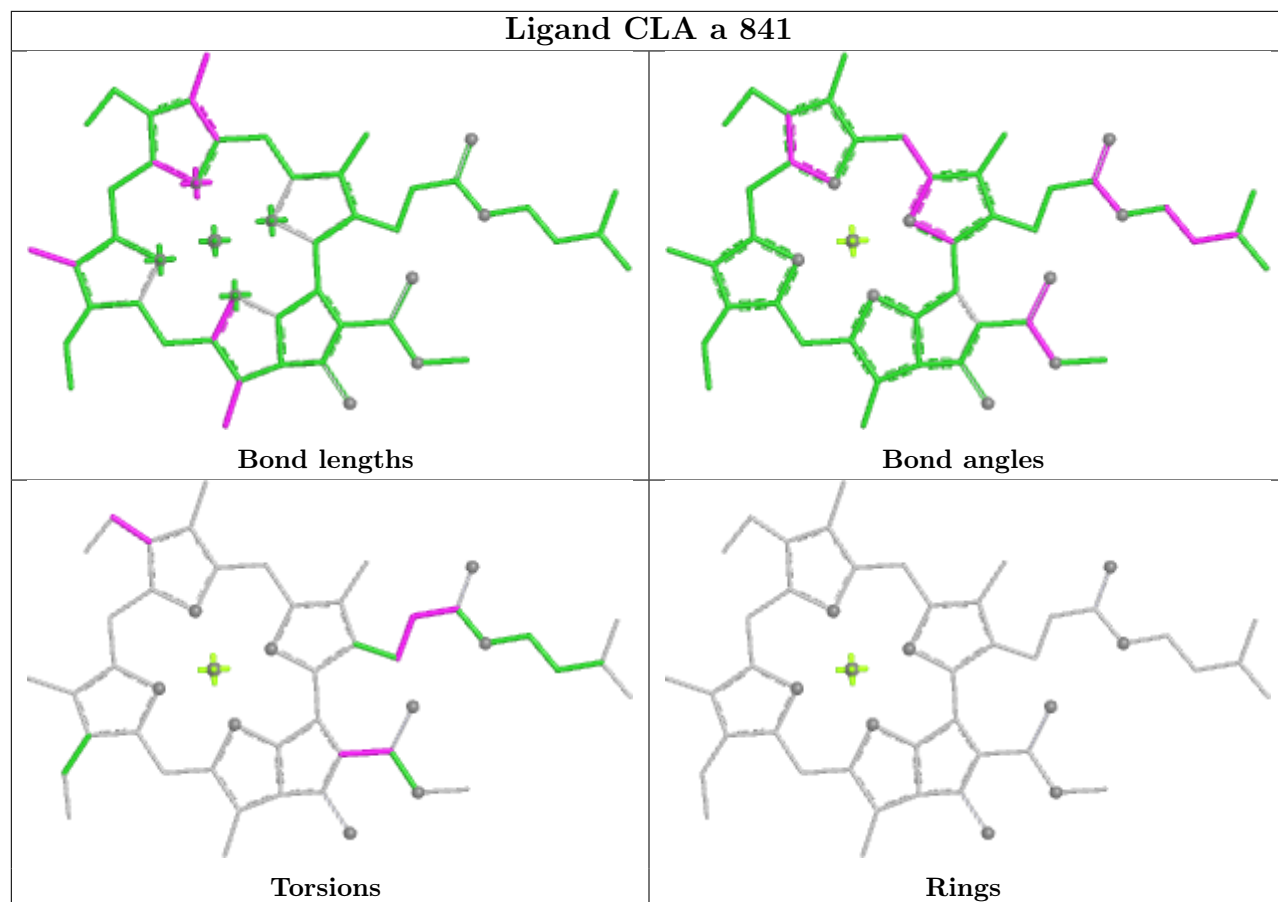
## Ligand CLA A 842



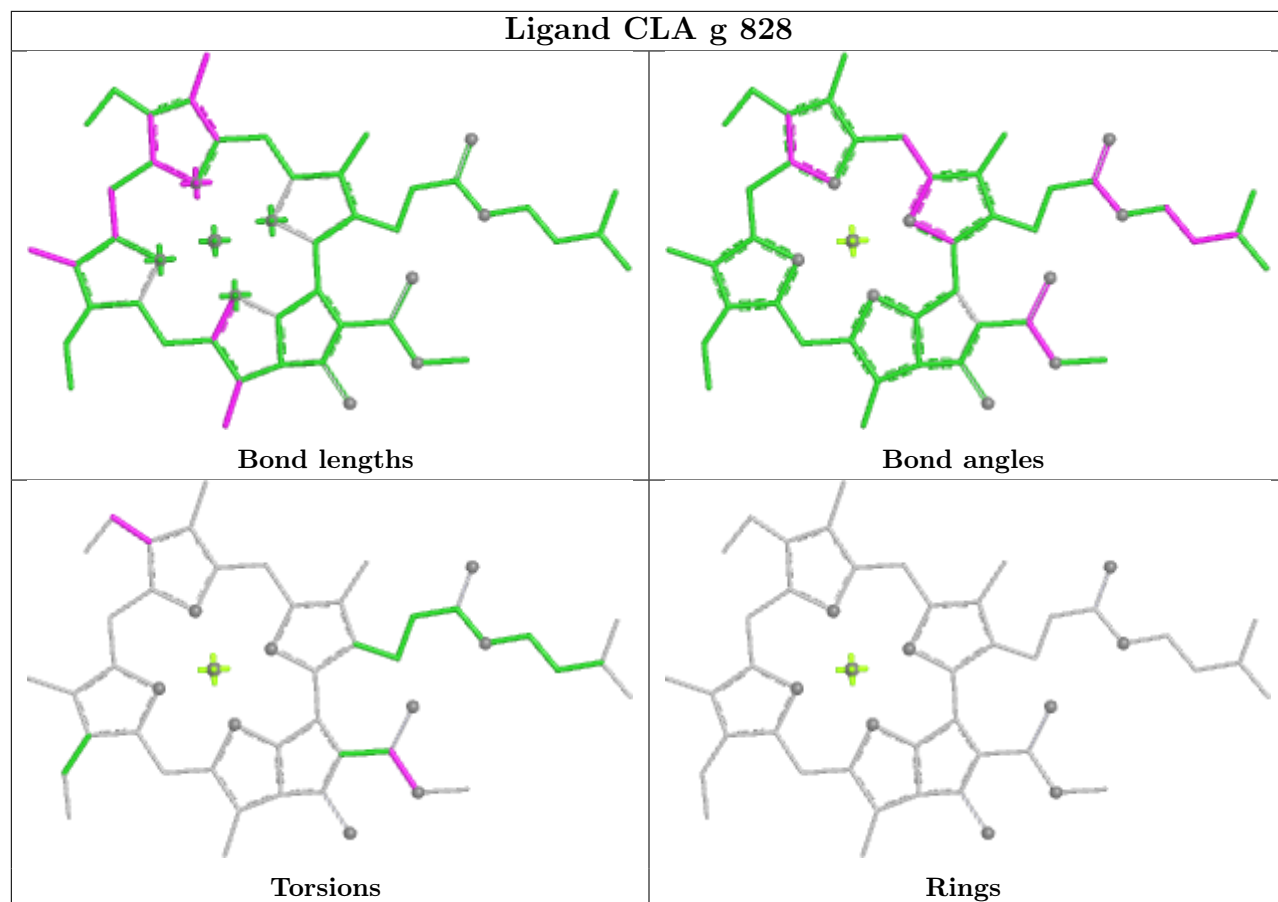
## Ligand CLA e 827



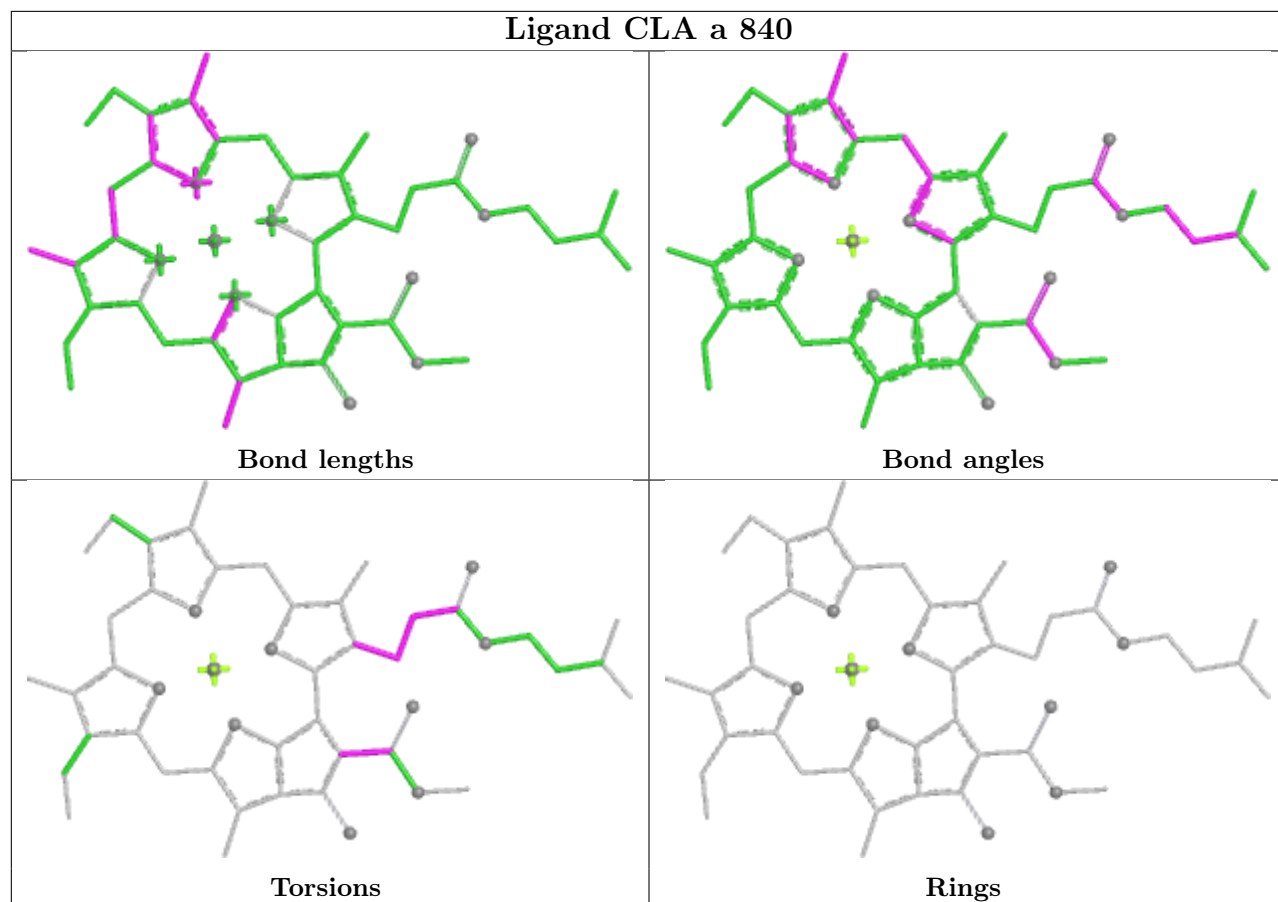
## Ligand CLA a 841



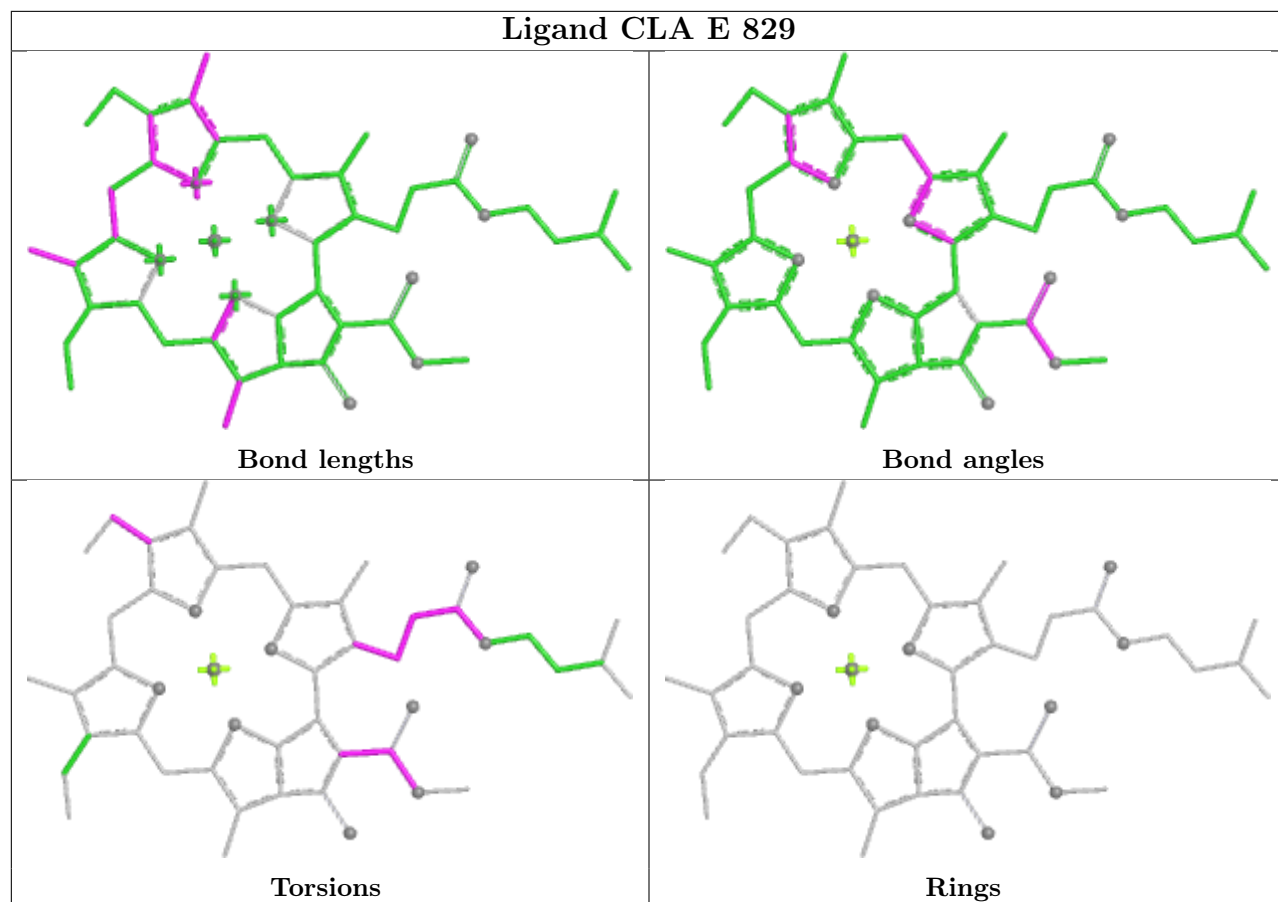
## Ligand CLA g 828



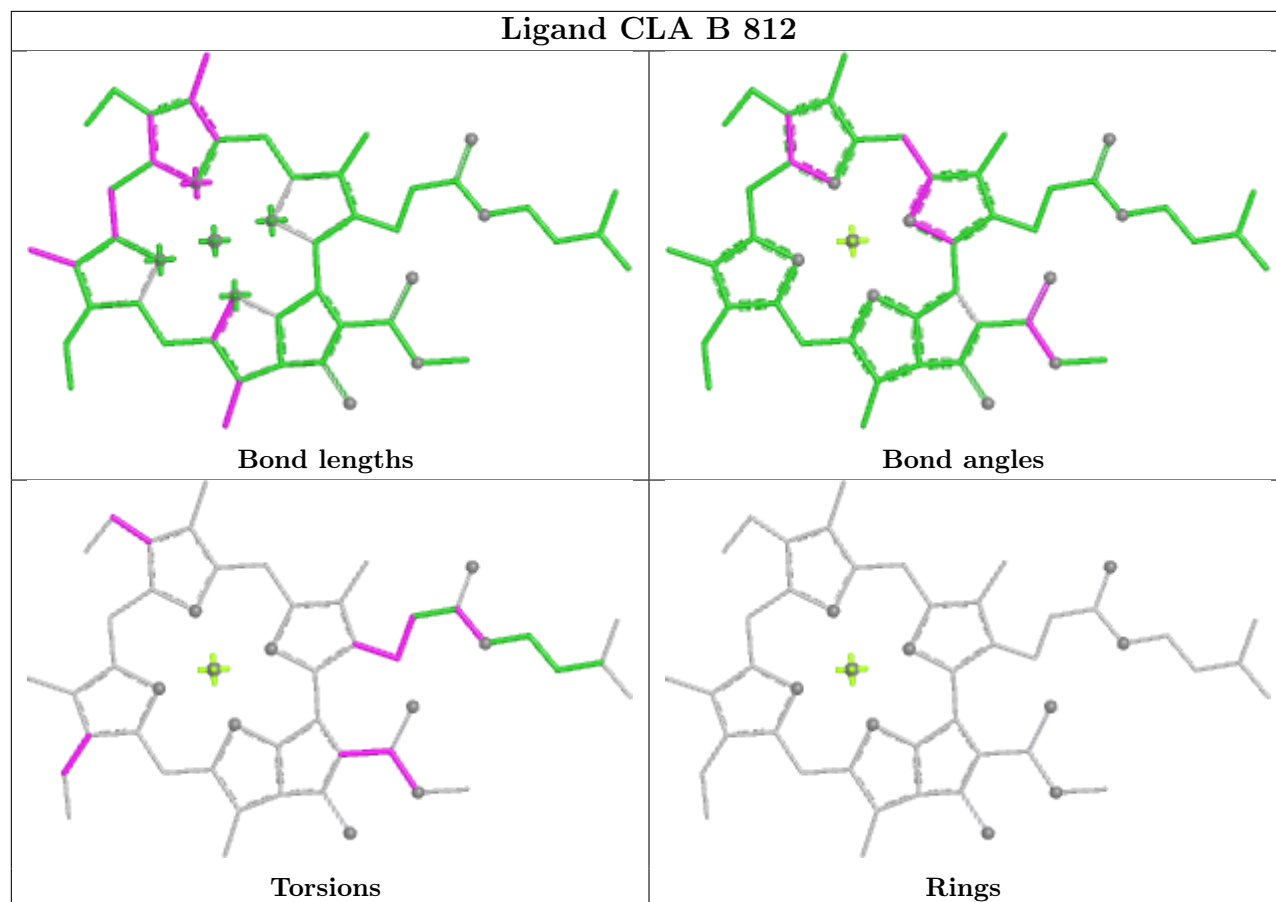
## Ligand CLA a 840



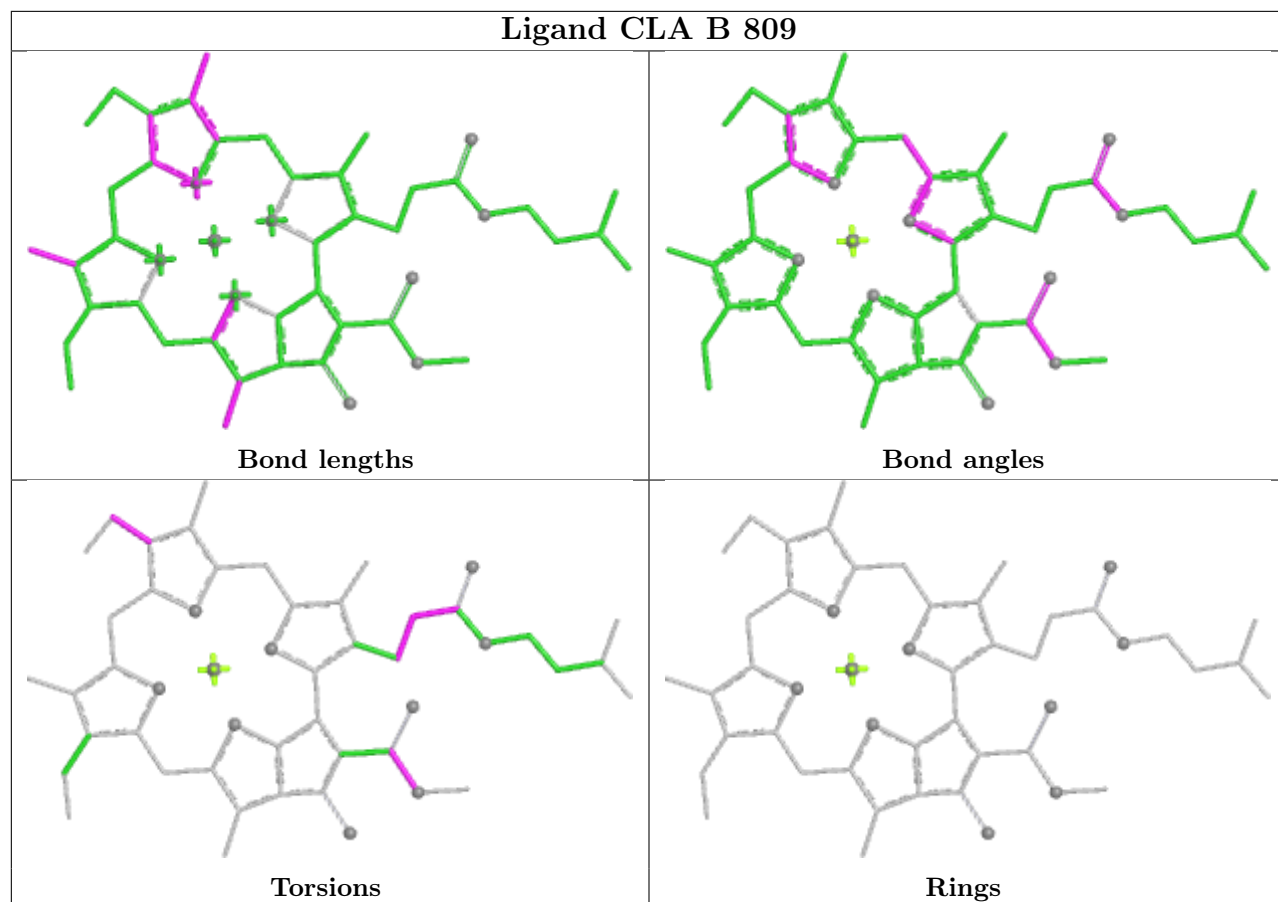
## Ligand CLA E 829



## Ligand CLA B 812

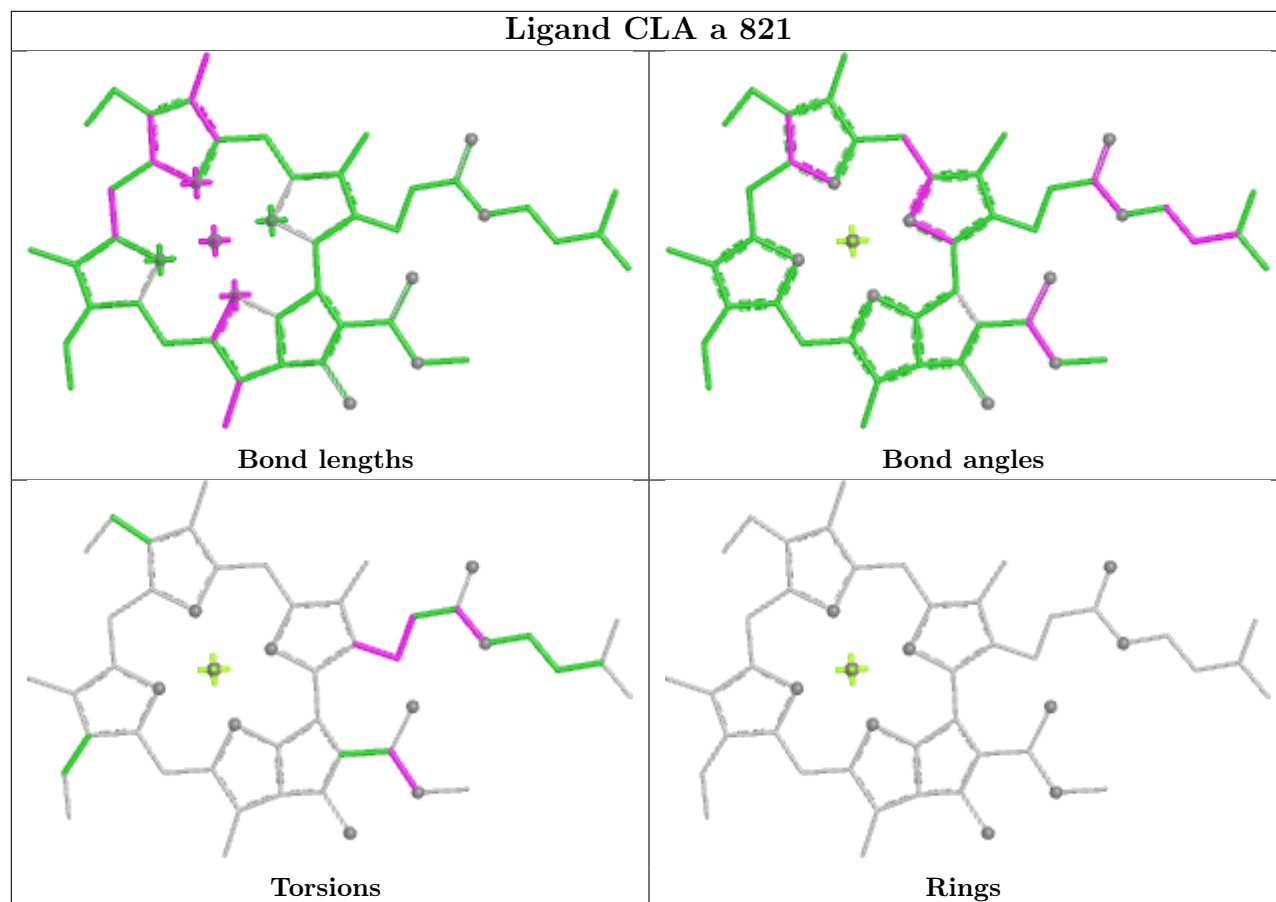


## Ligand CLA B 809

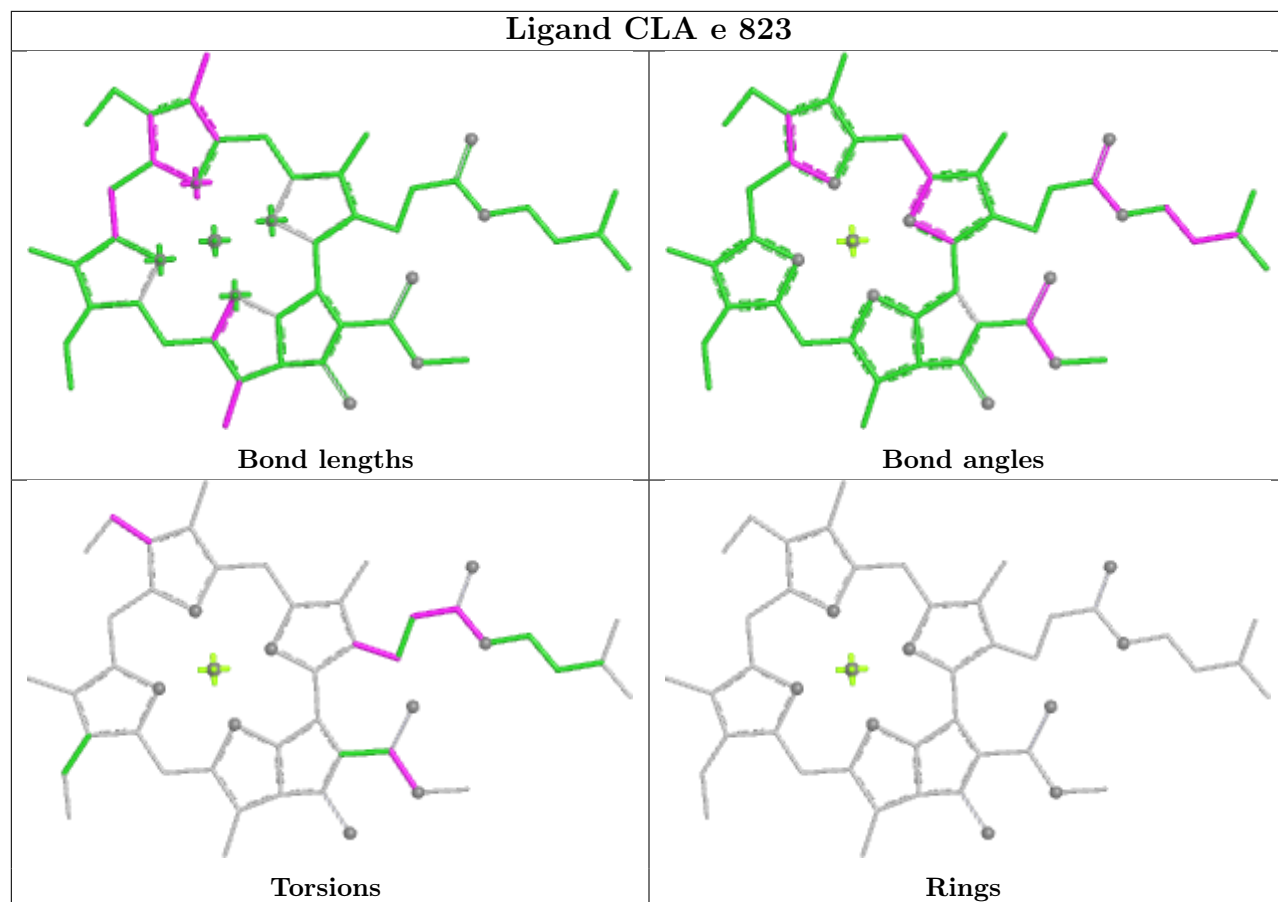




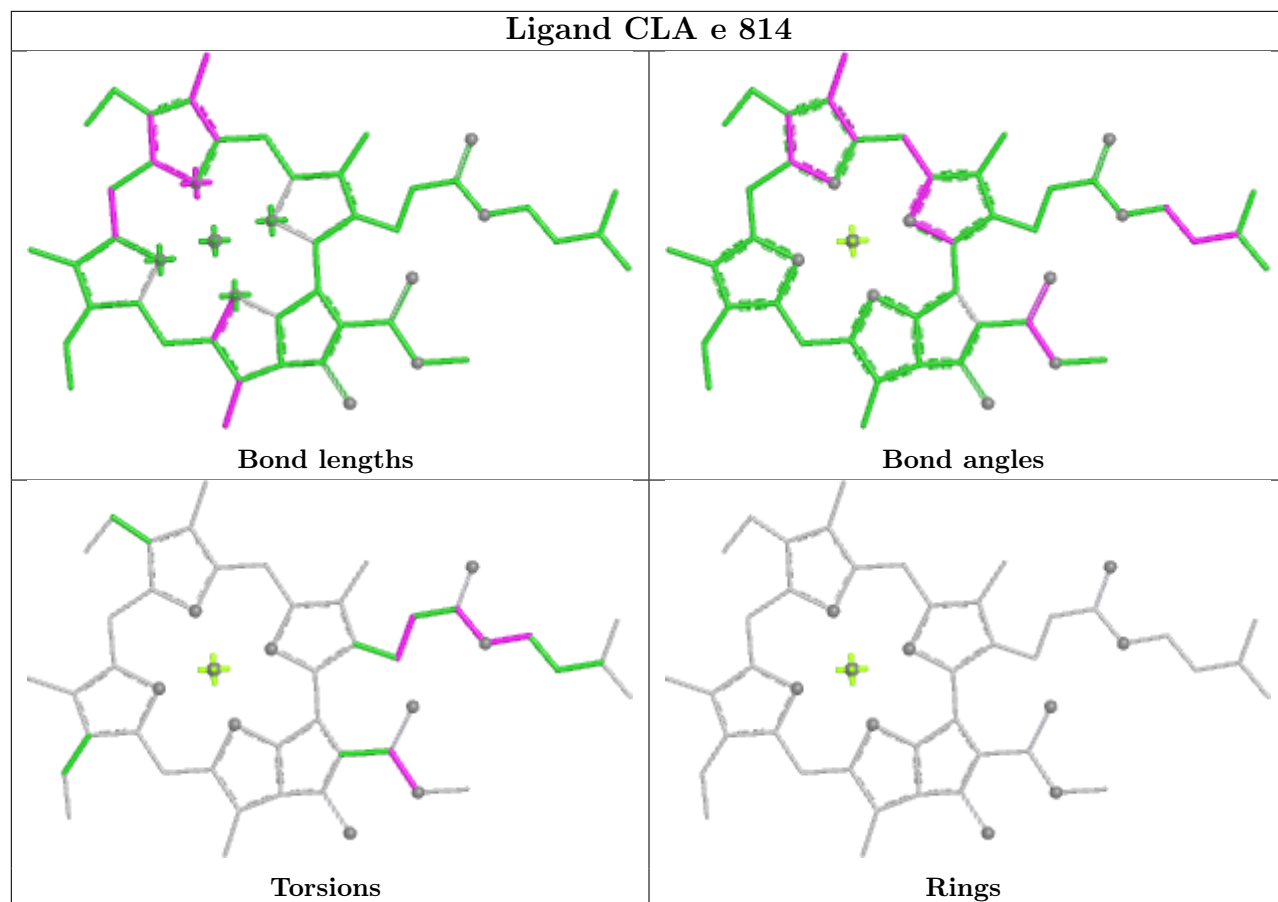
## Ligand CLA a 821



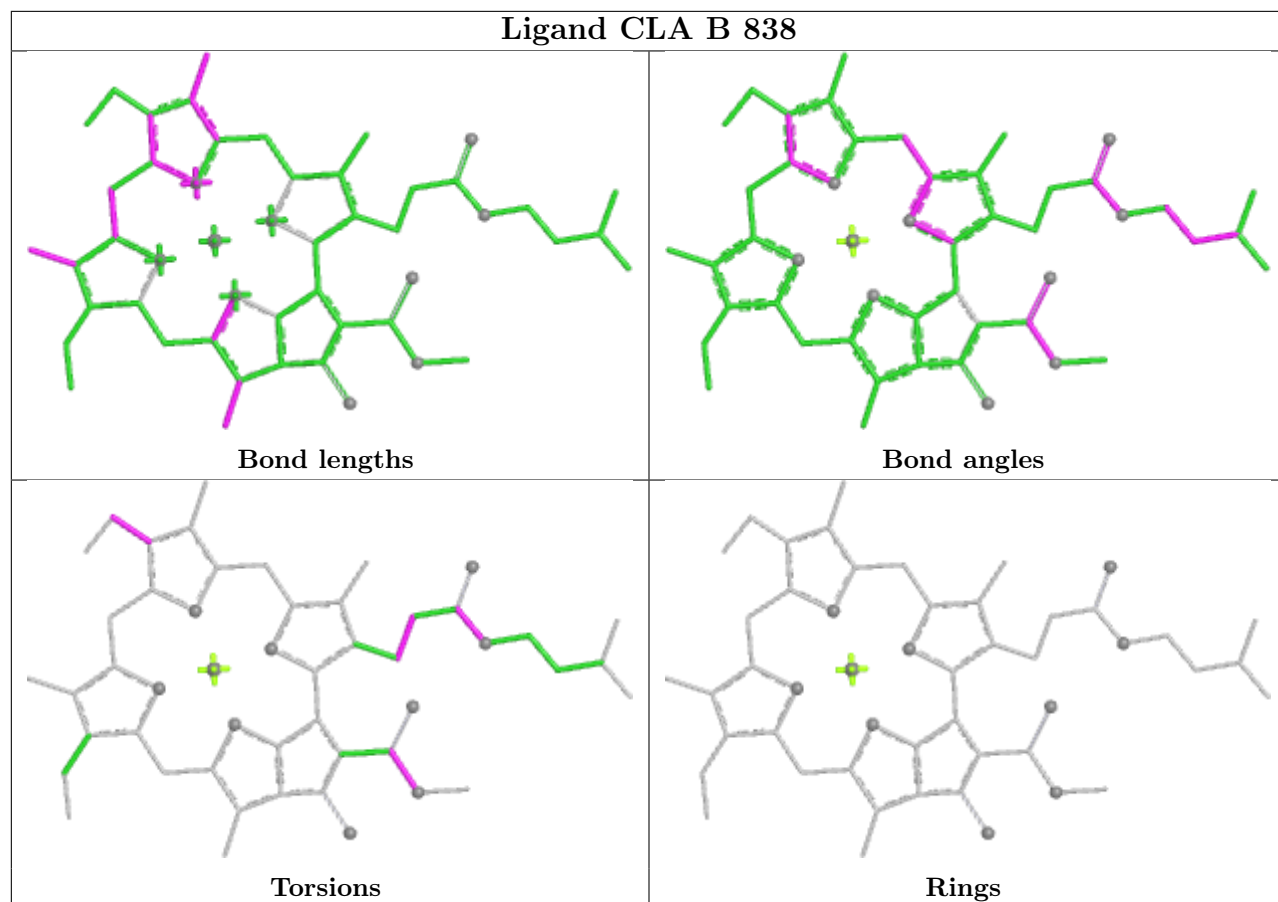
## Ligand CLA e 823



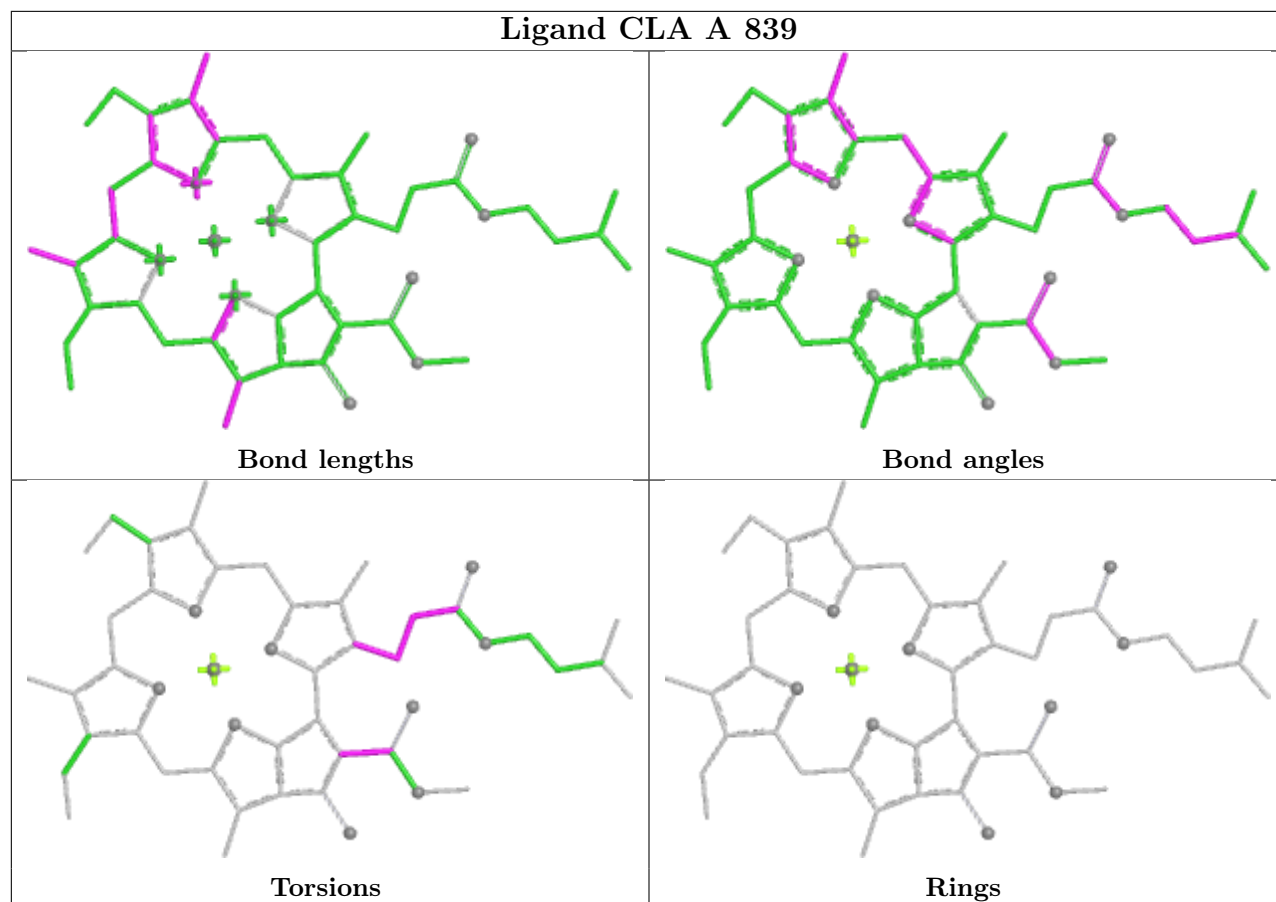
## Ligand CLA e 814



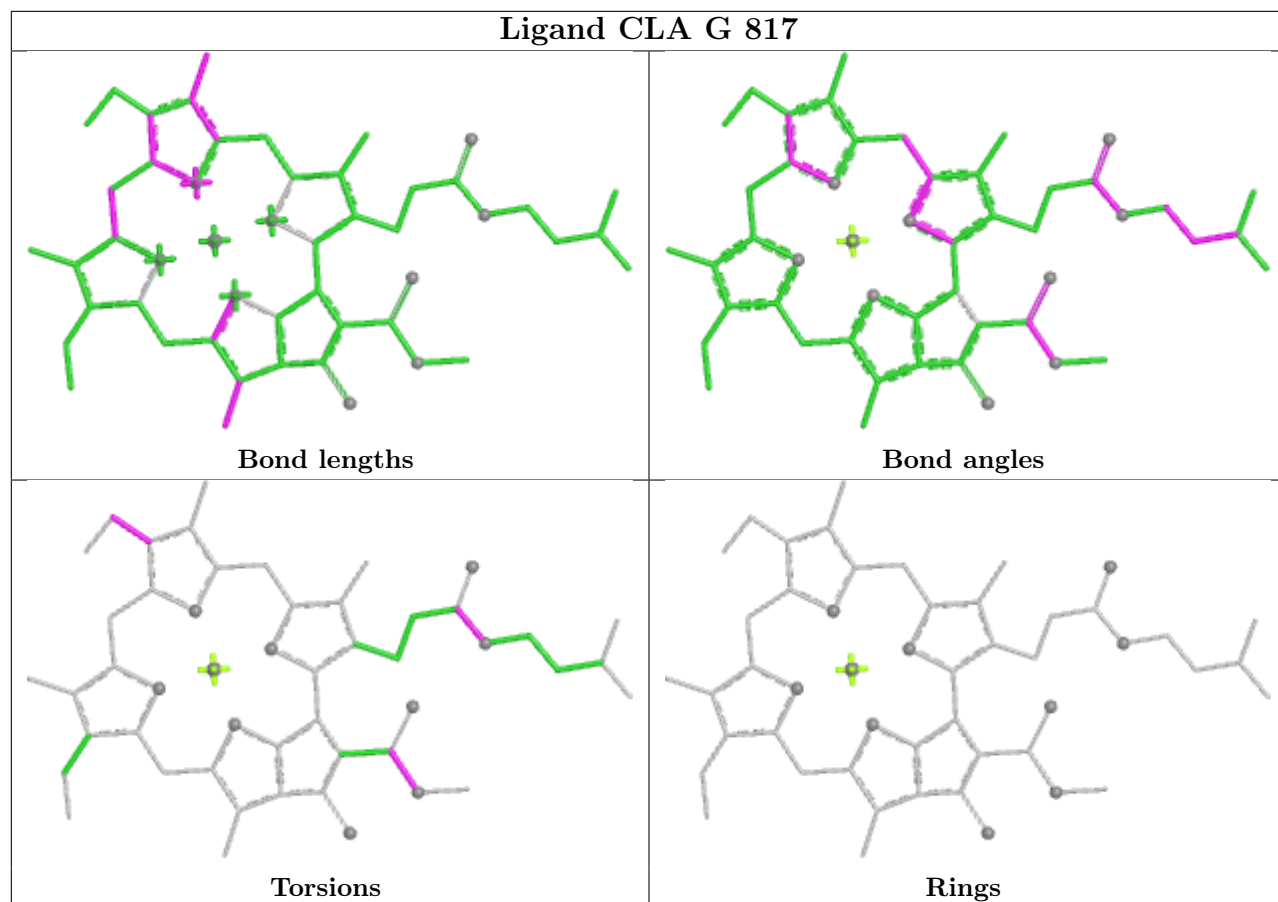
## Ligand CLA B 838



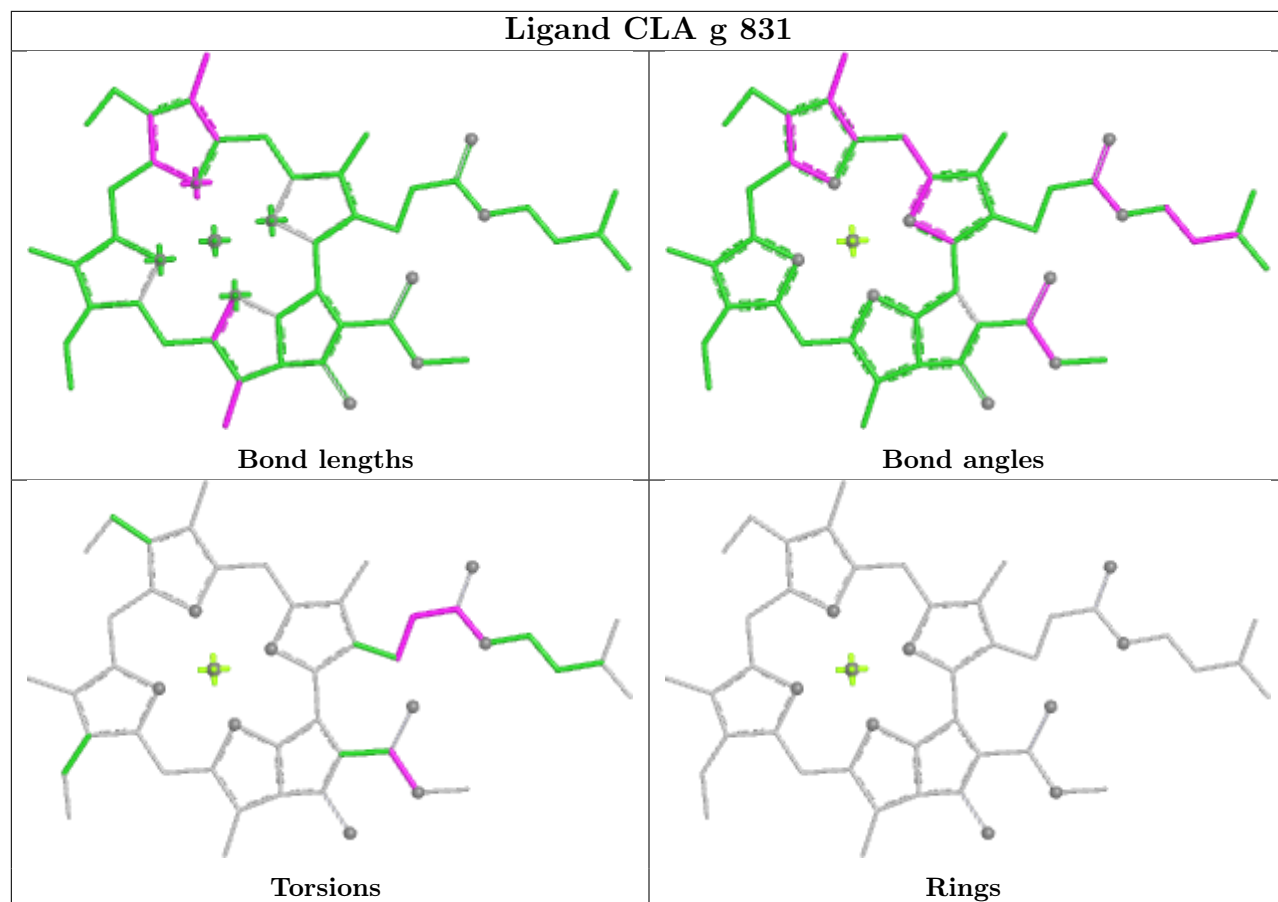
## Ligand CLA A 839



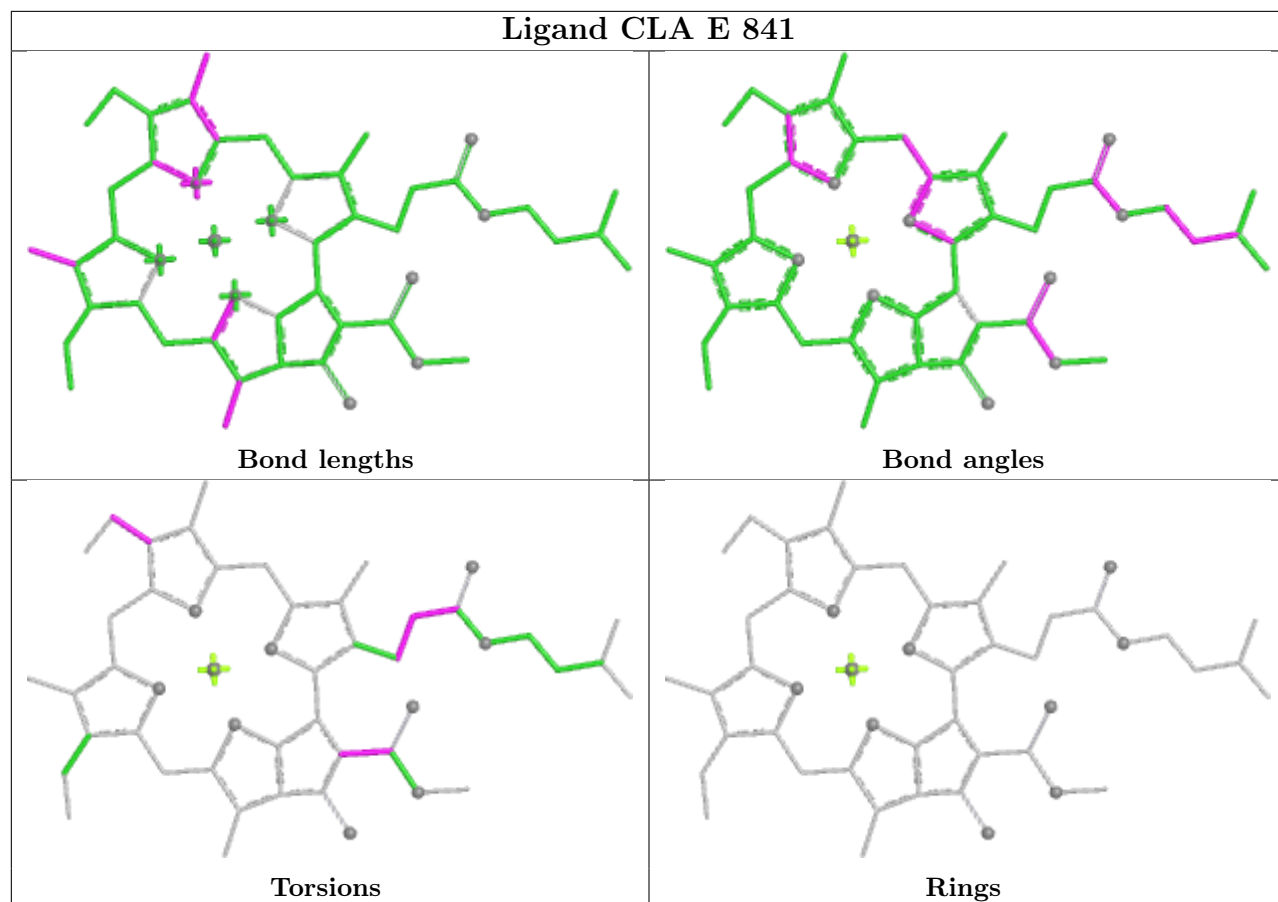
## Ligand CLA G 817



## Ligand CLA g 831

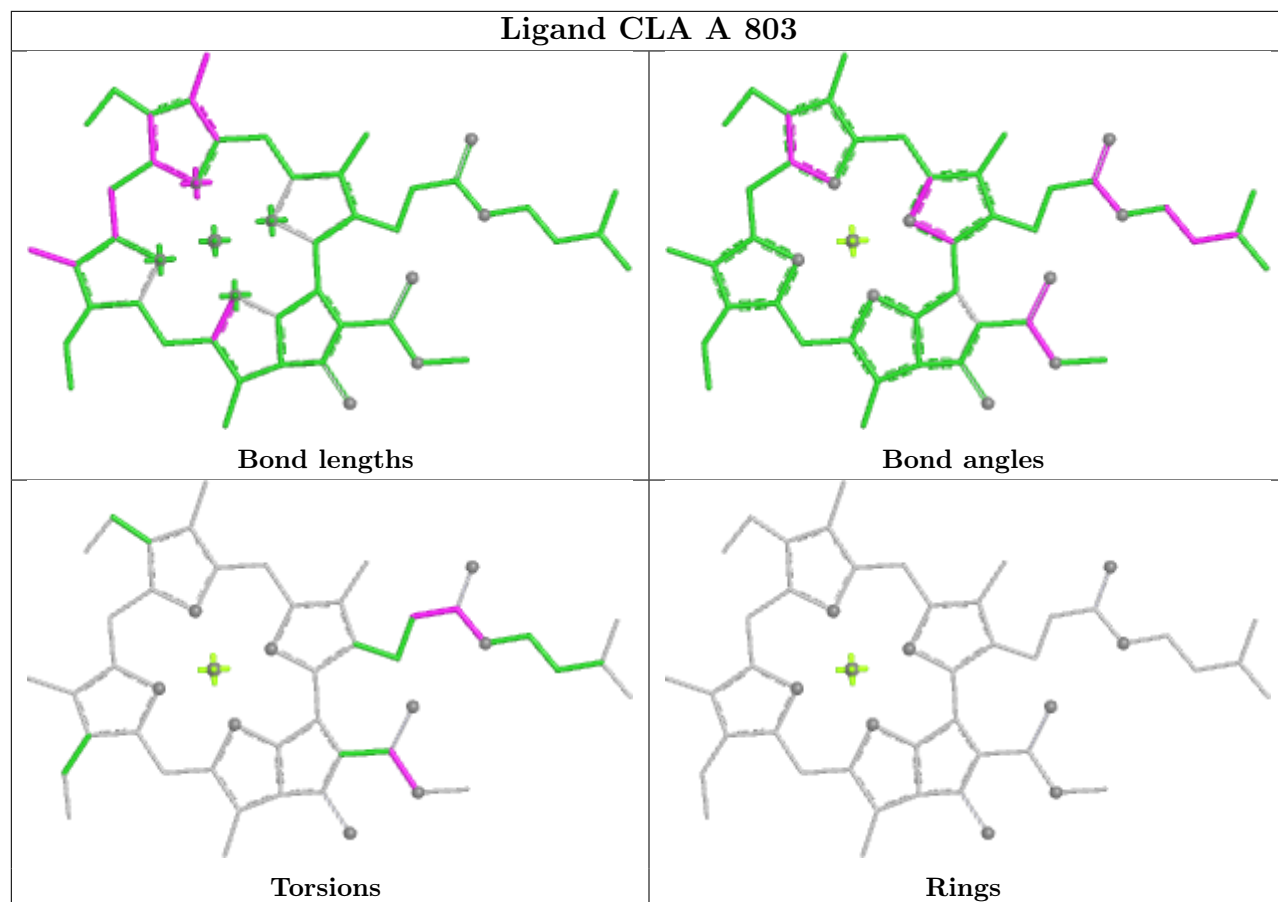


## Ligand CLA E 841

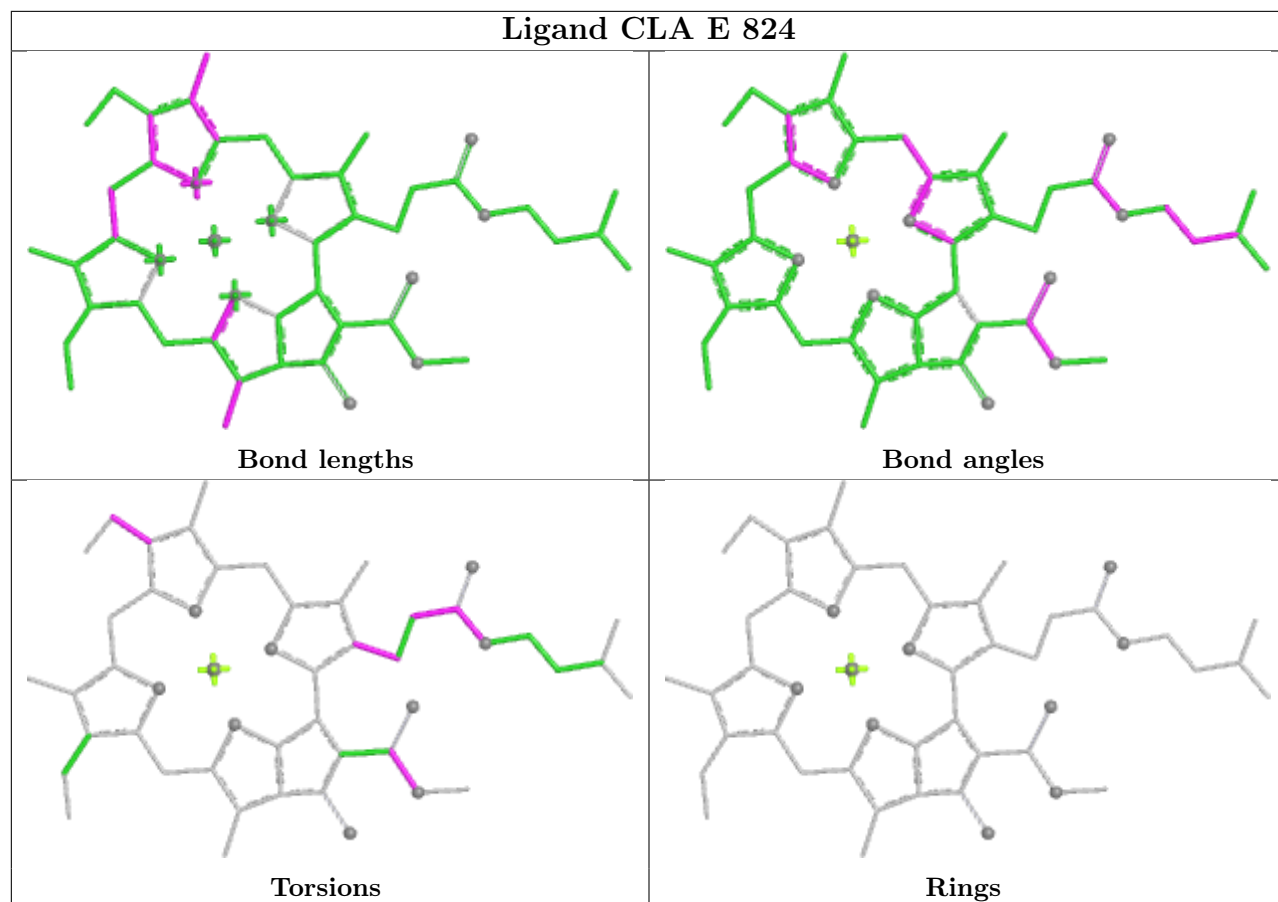




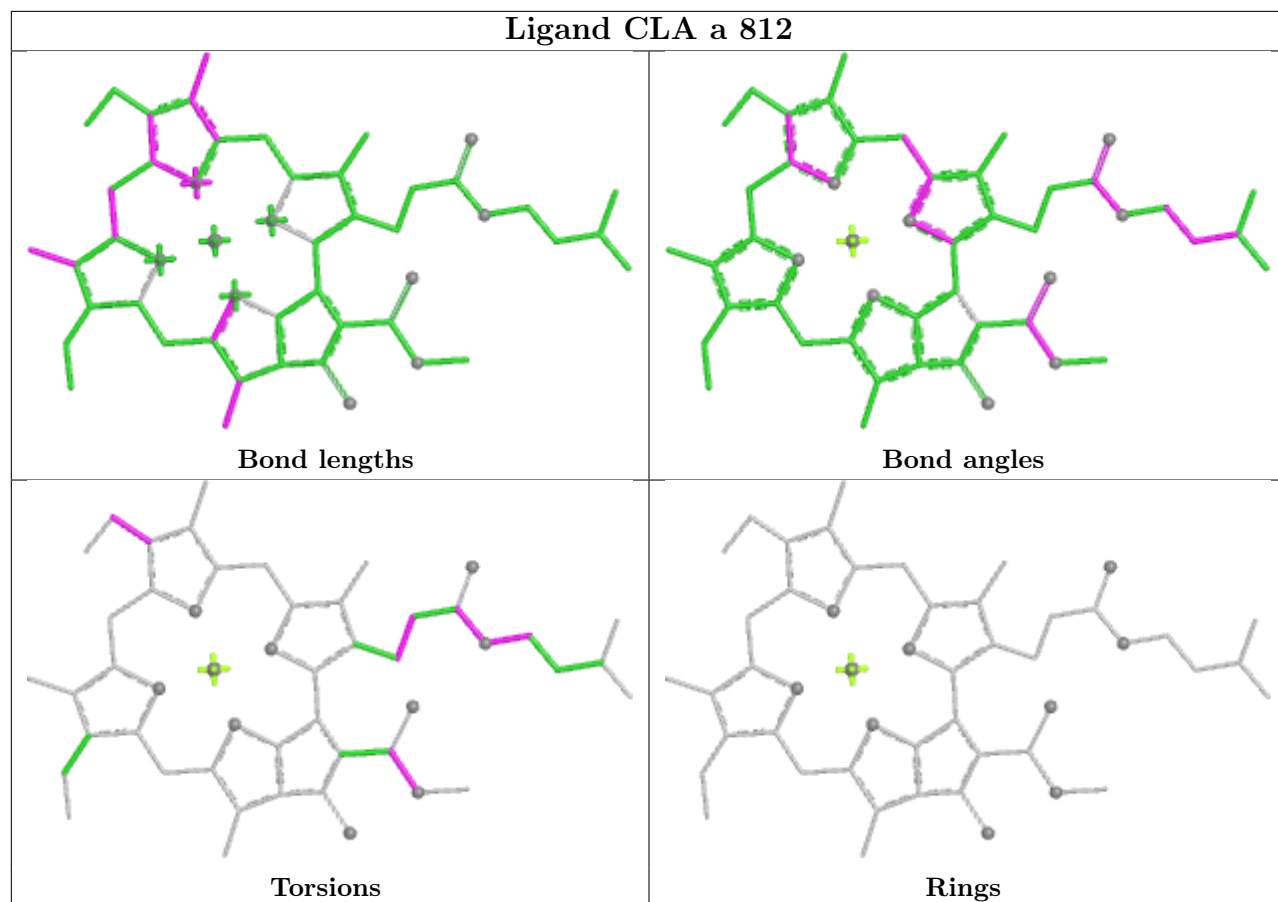
## Ligand CLA A 803



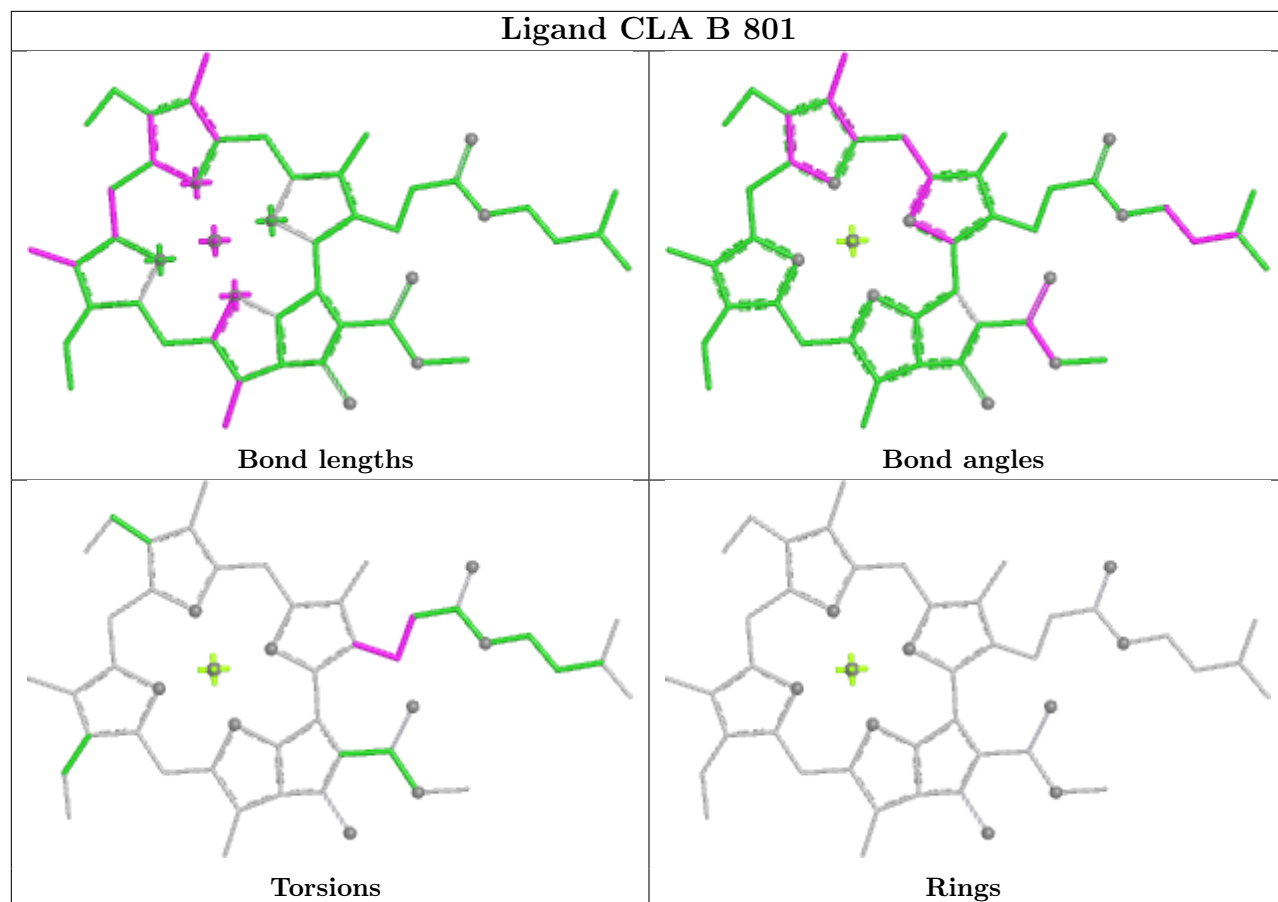
## Ligand CLA E 824



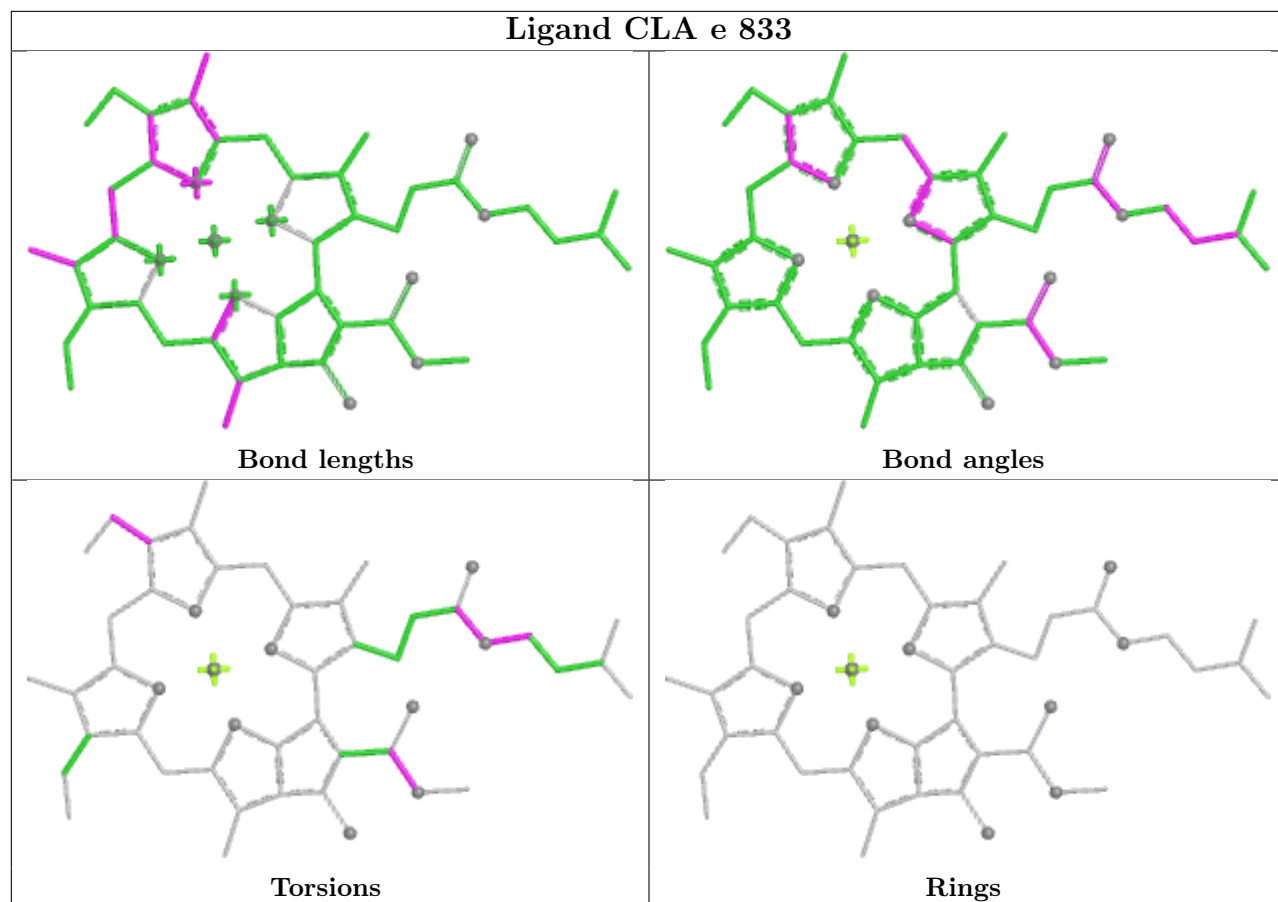
## Ligand CLA a 812



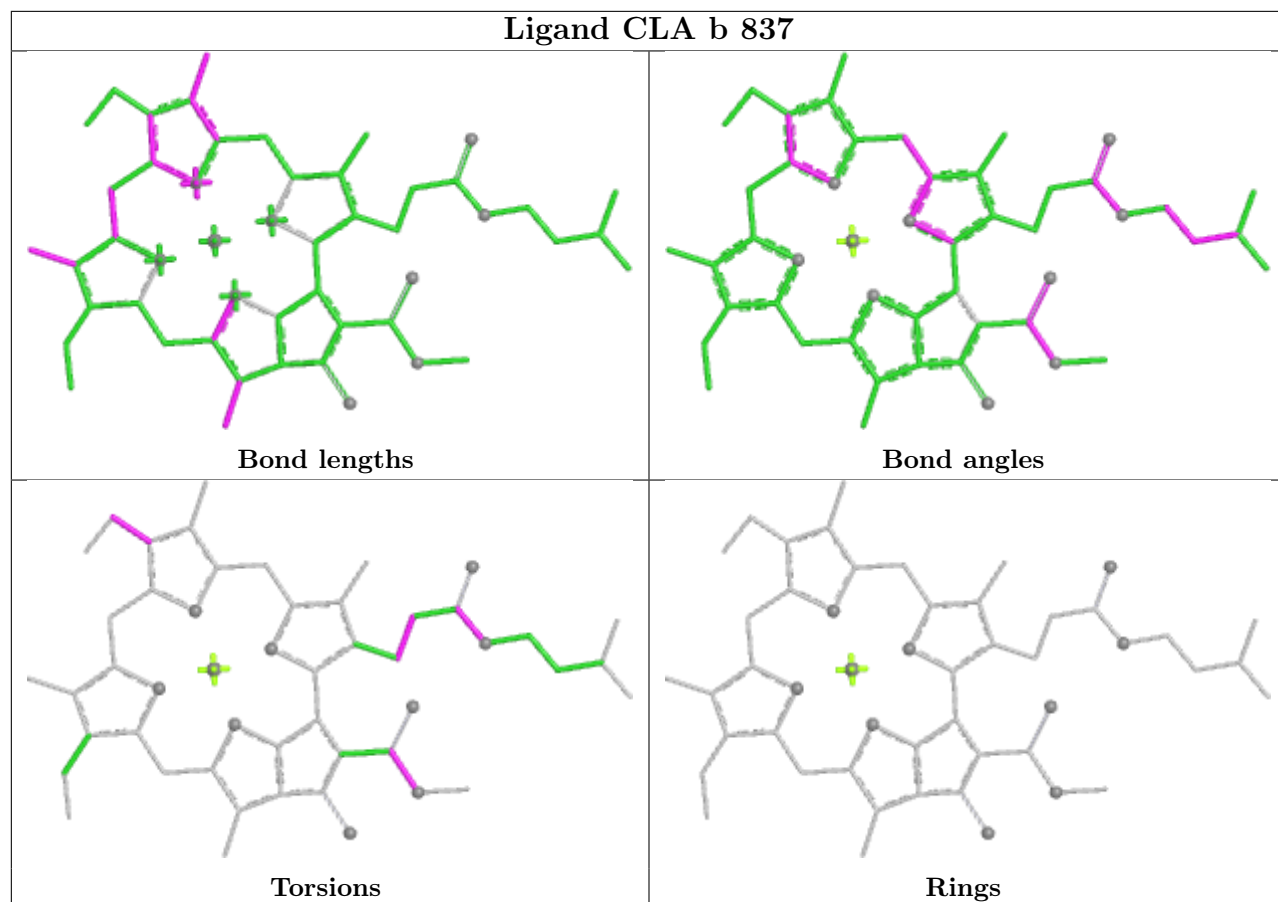
## Ligand CLA B 801



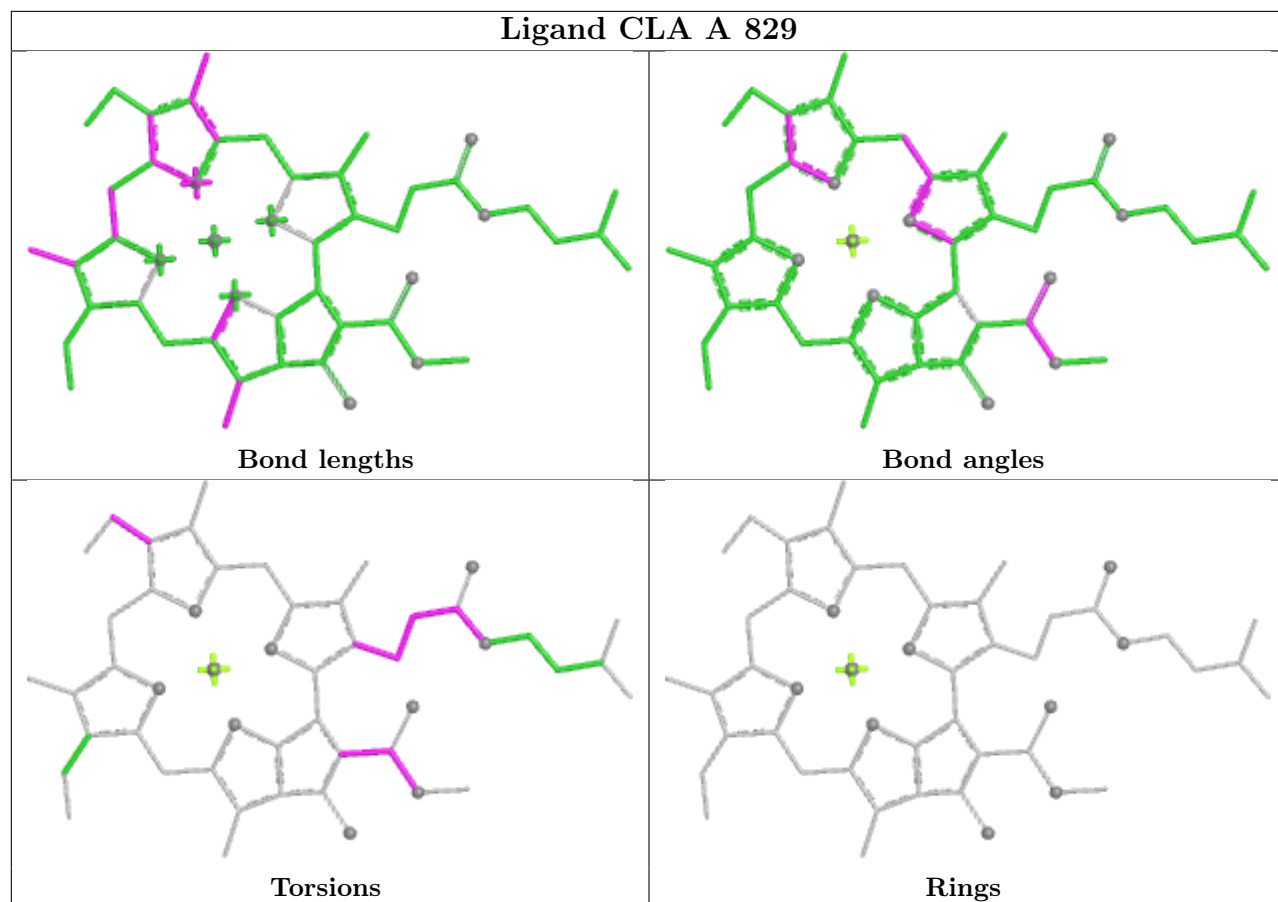
## Ligand CLA e 833



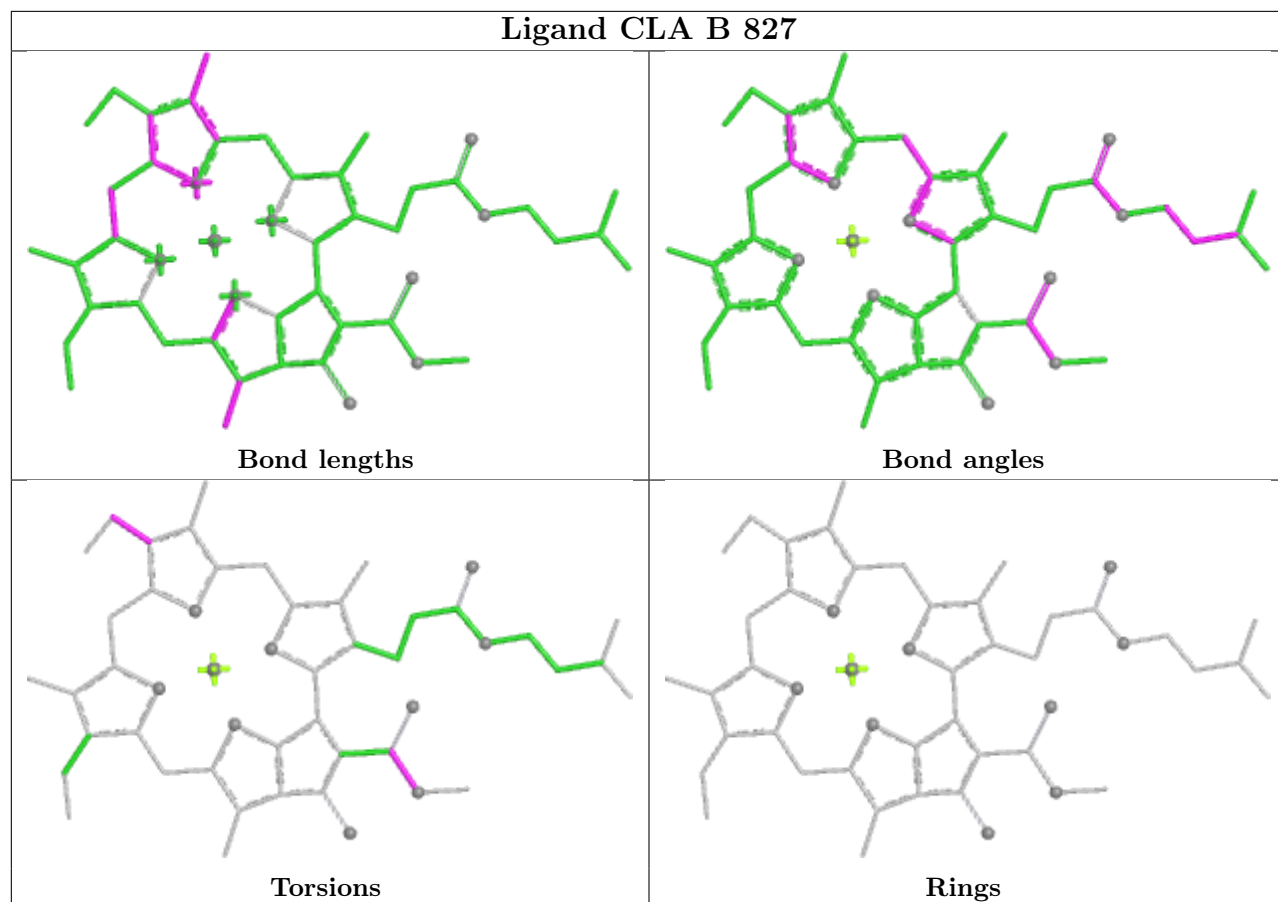
## Ligand CLA b 837



## Ligand CLA A 829

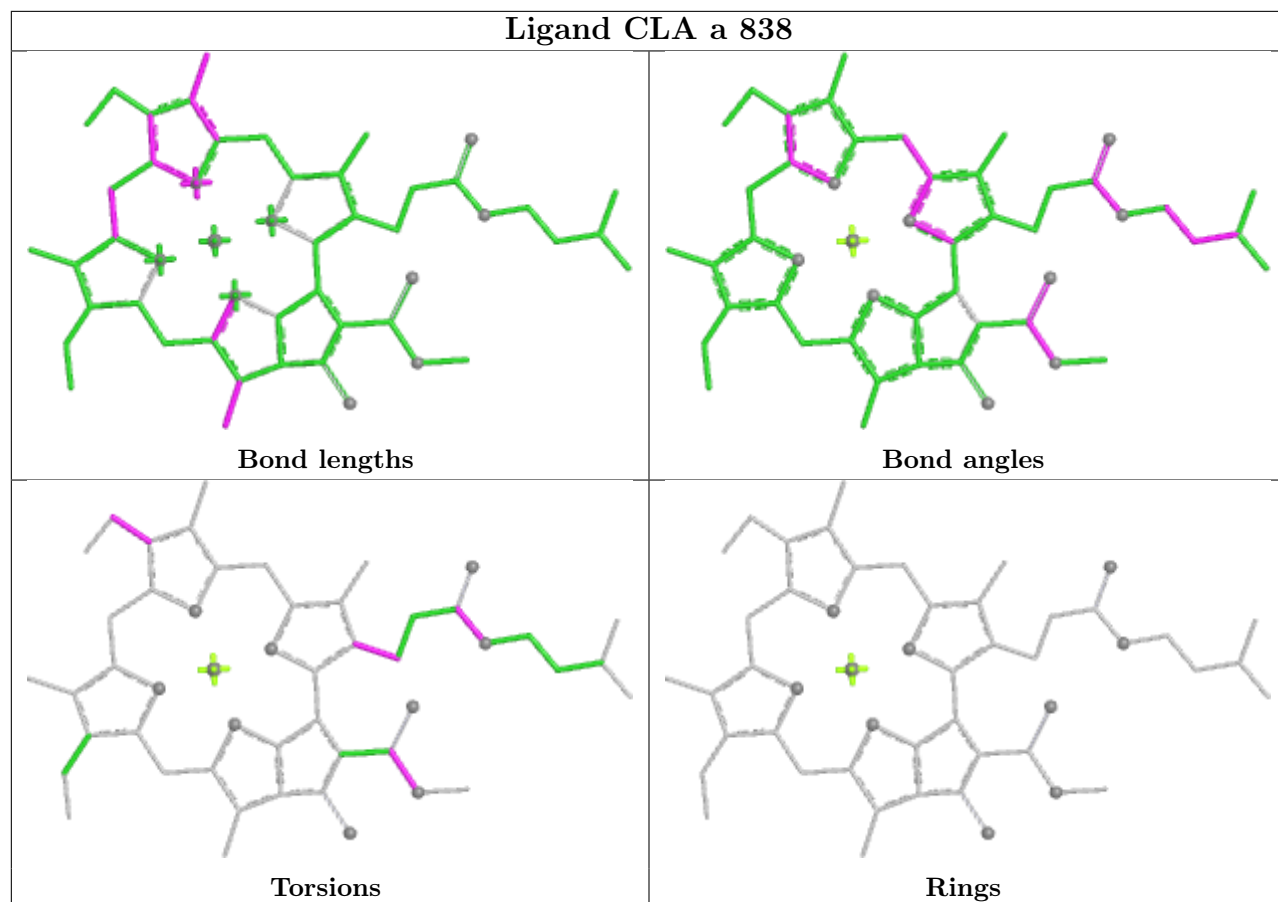


## Ligand CLA B 827

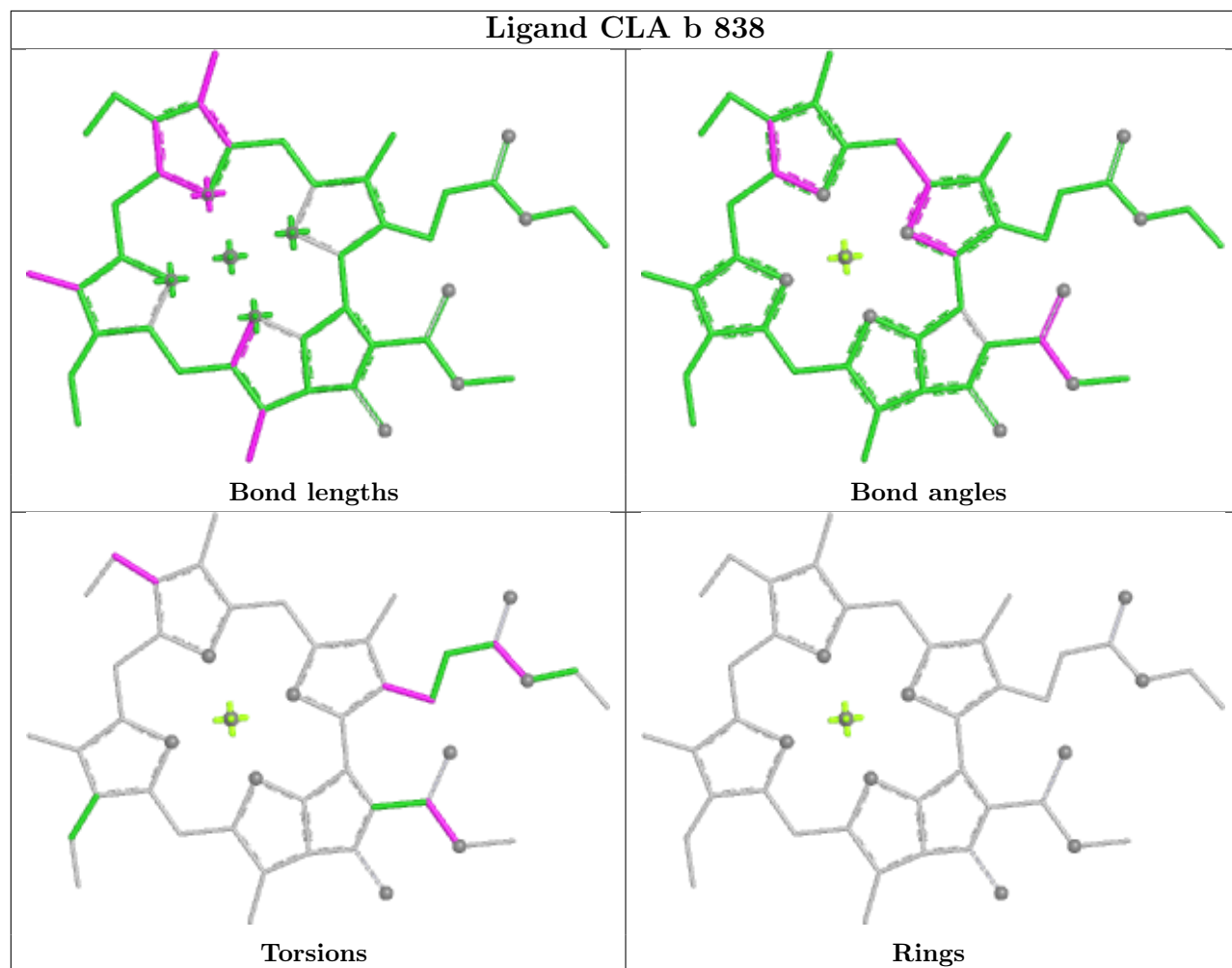




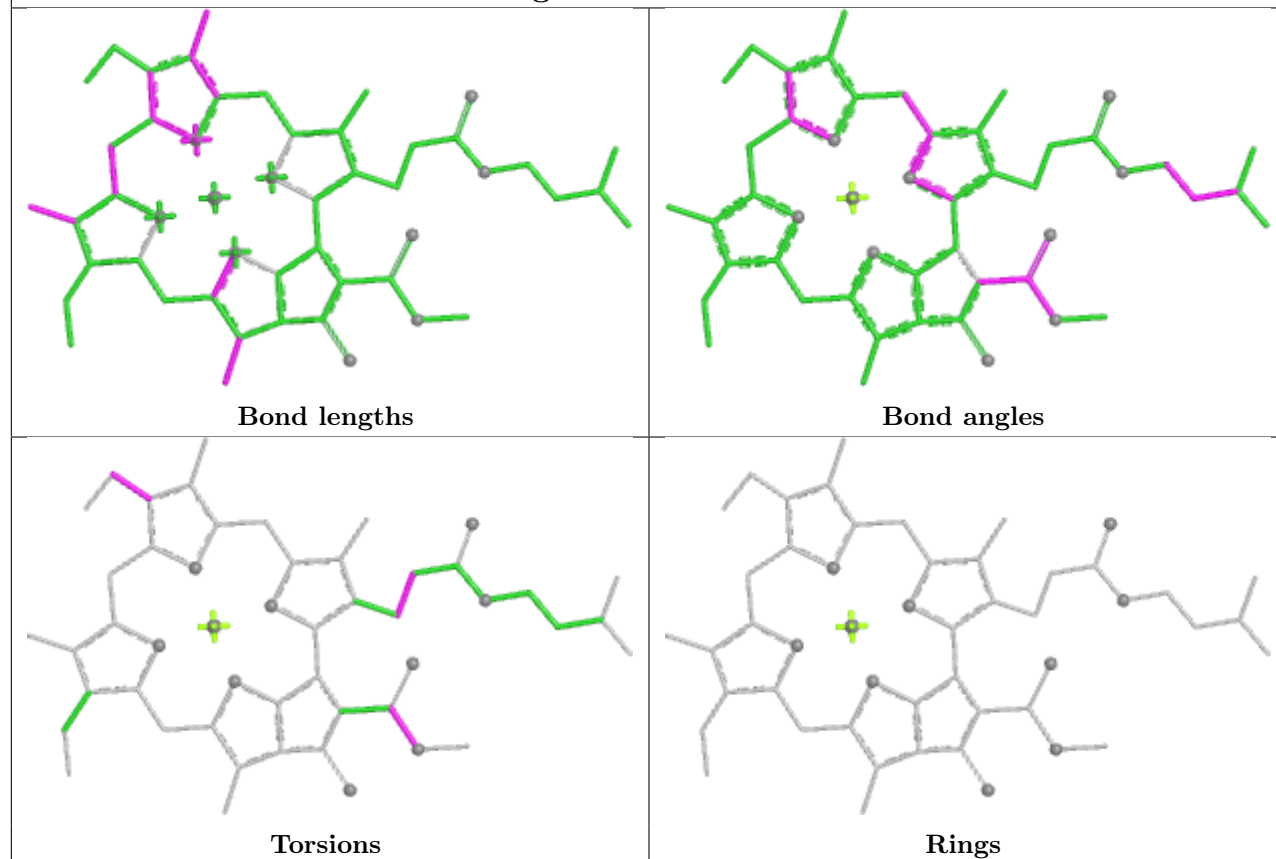
## Ligand CLA a 838



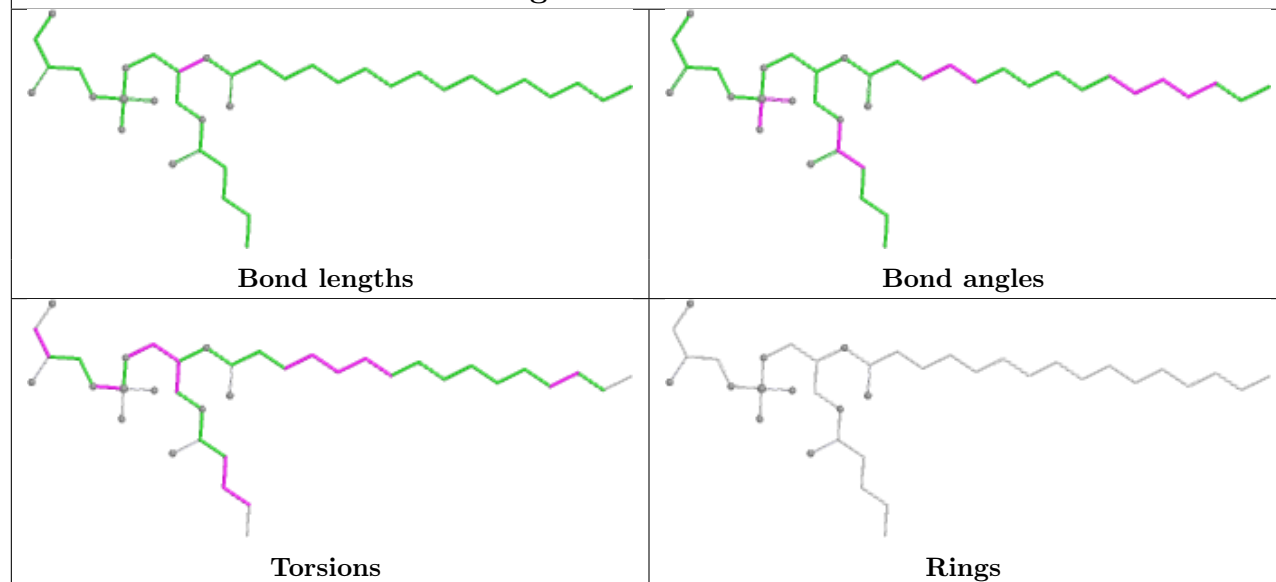
## Ligand CLA b 838

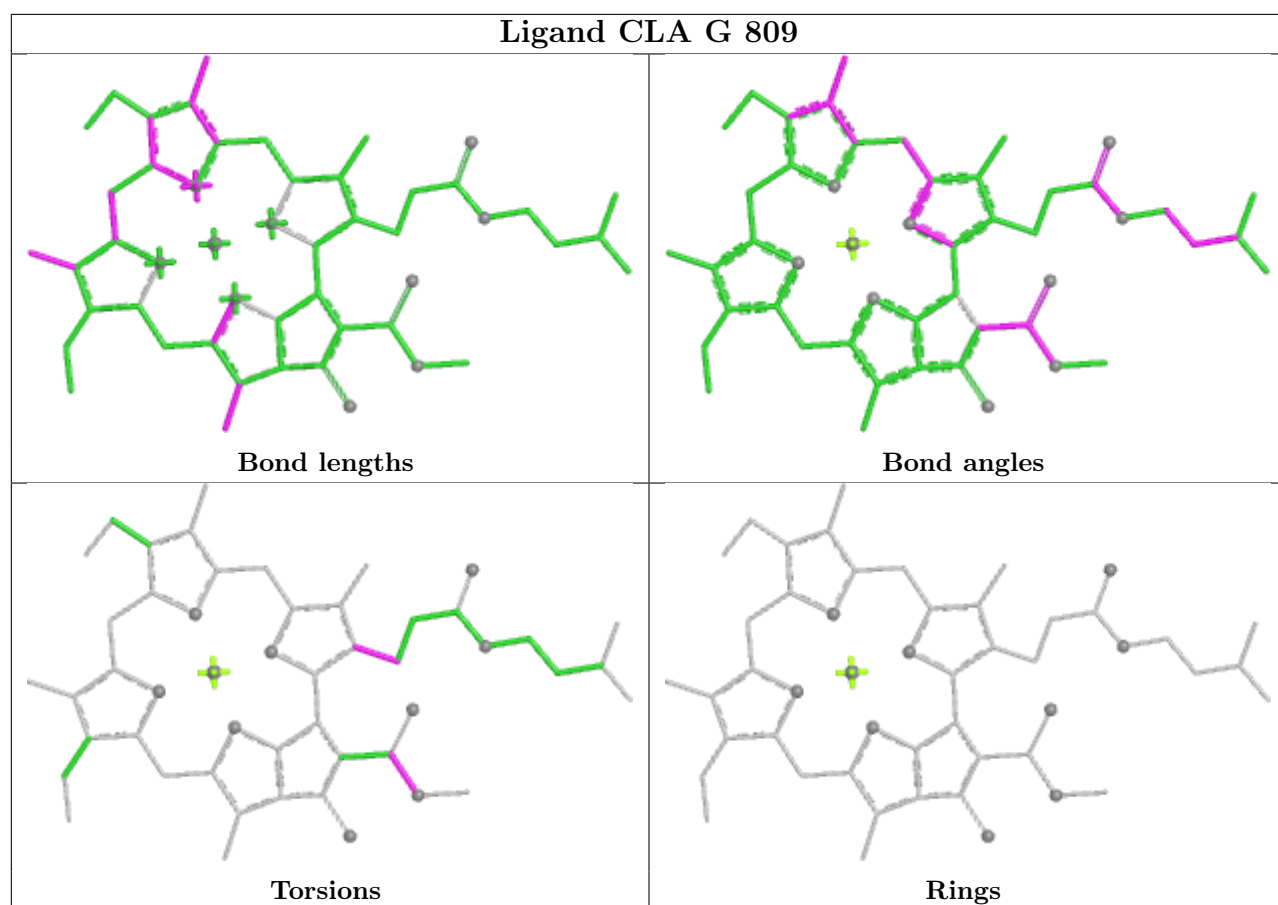


## Ligand CLA B 823

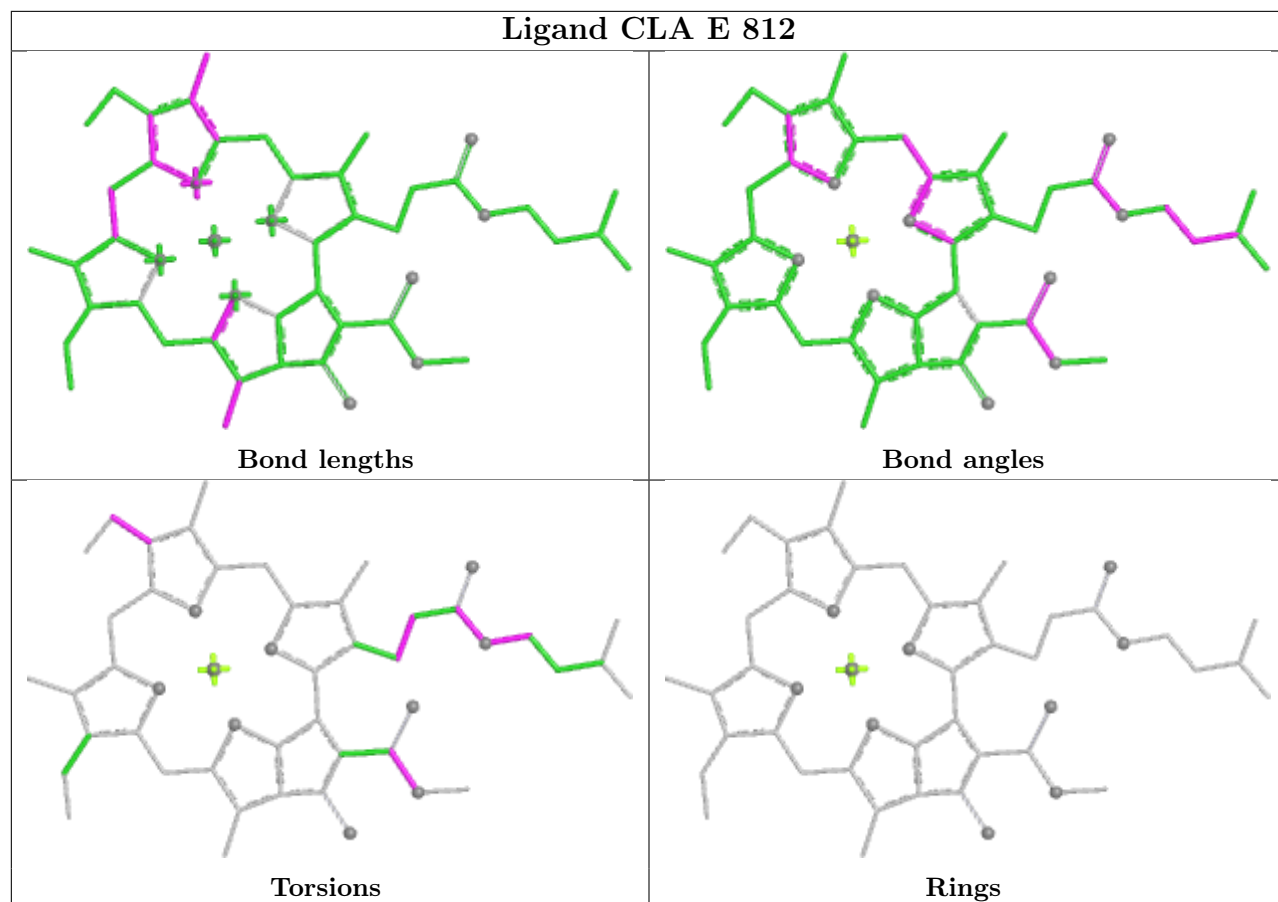


## Ligand LHG A 802

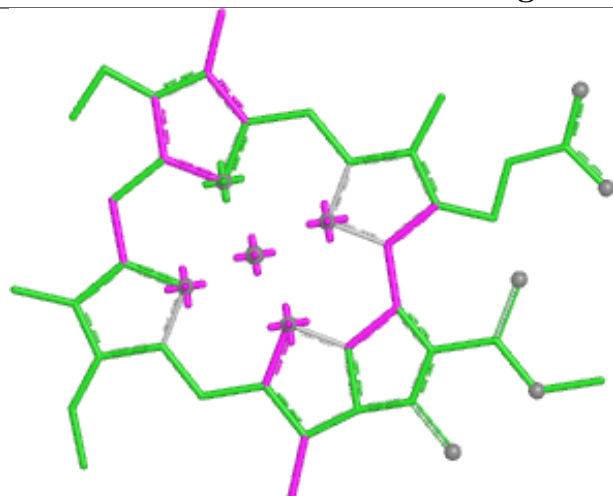




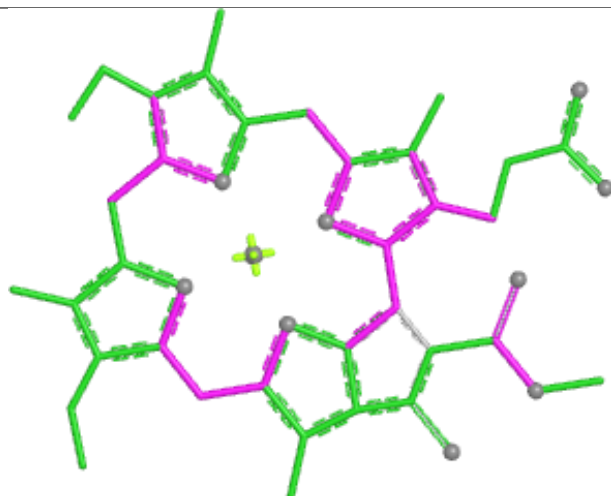
## Ligand CLA E 812



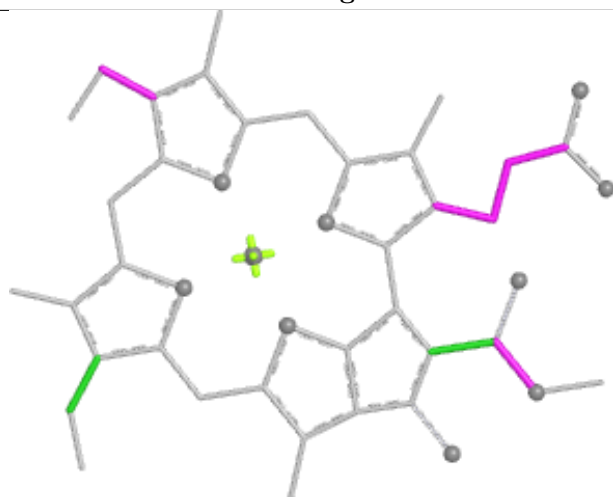
## Ligand CLA S 204



Bond lengths



Bond angles

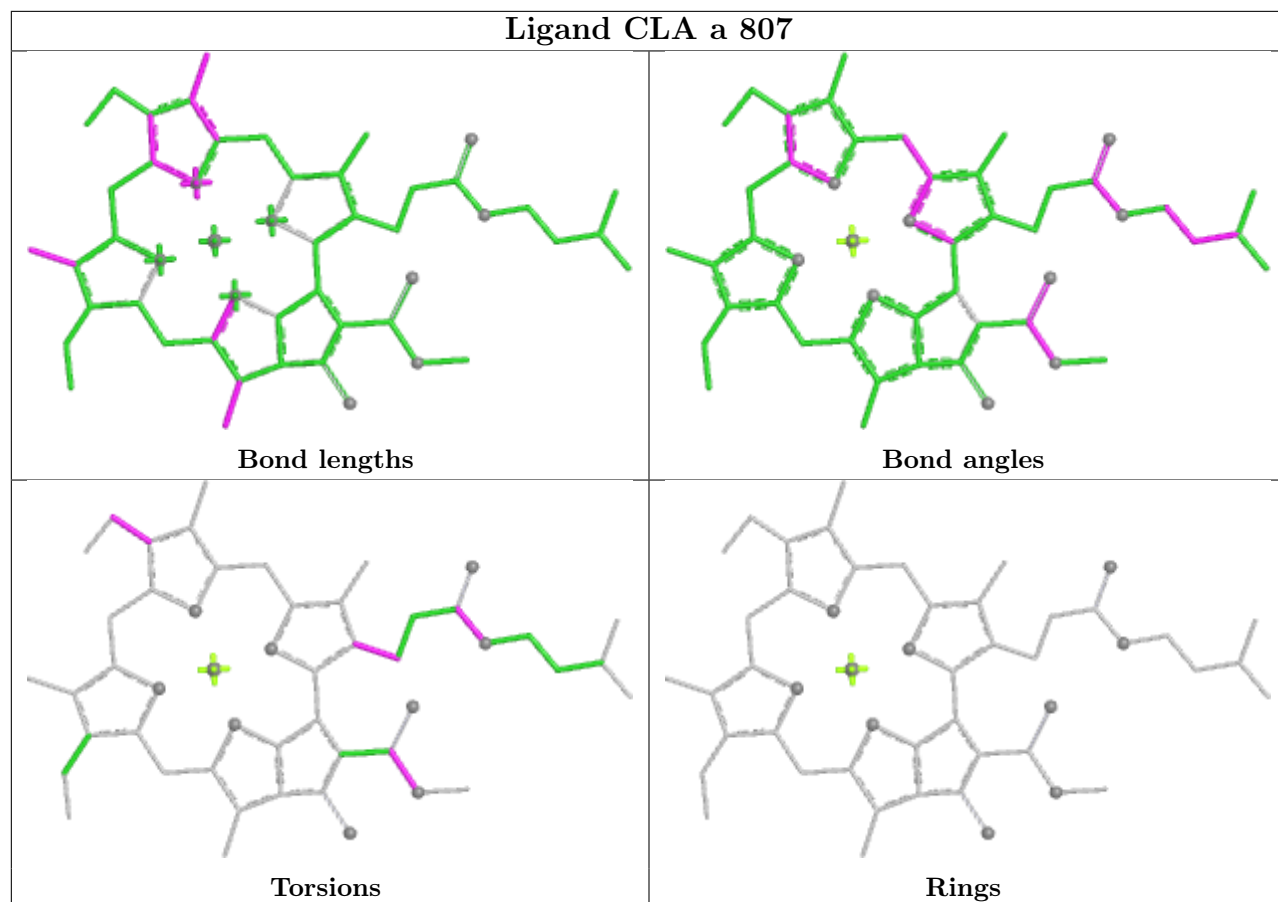


Torsions

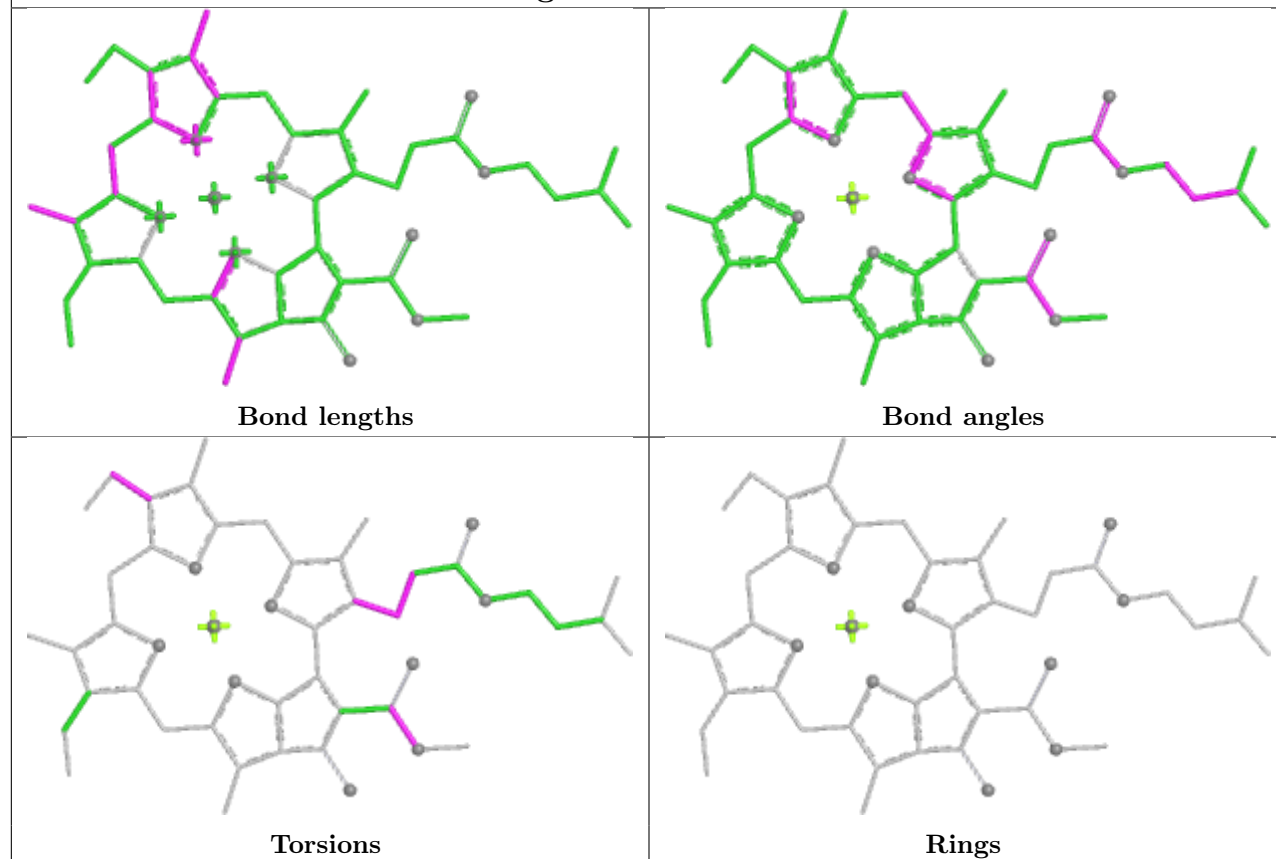


Rings

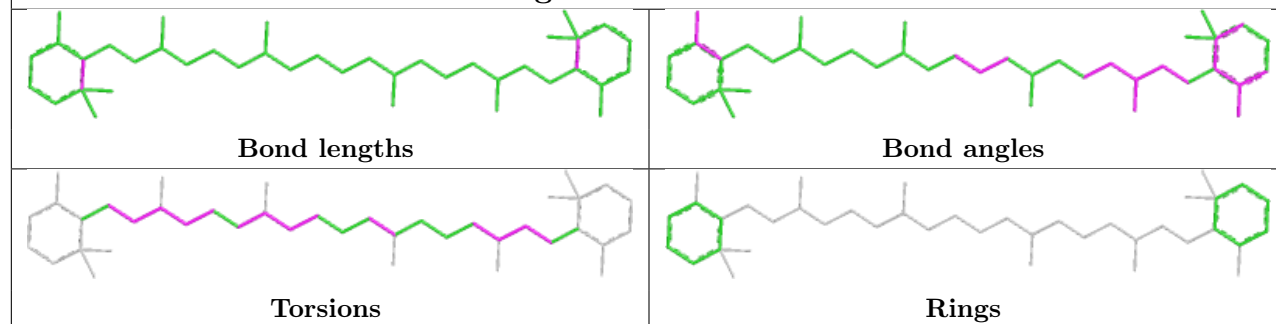
## Ligand CLA a 807



## Ligand CLA e 843

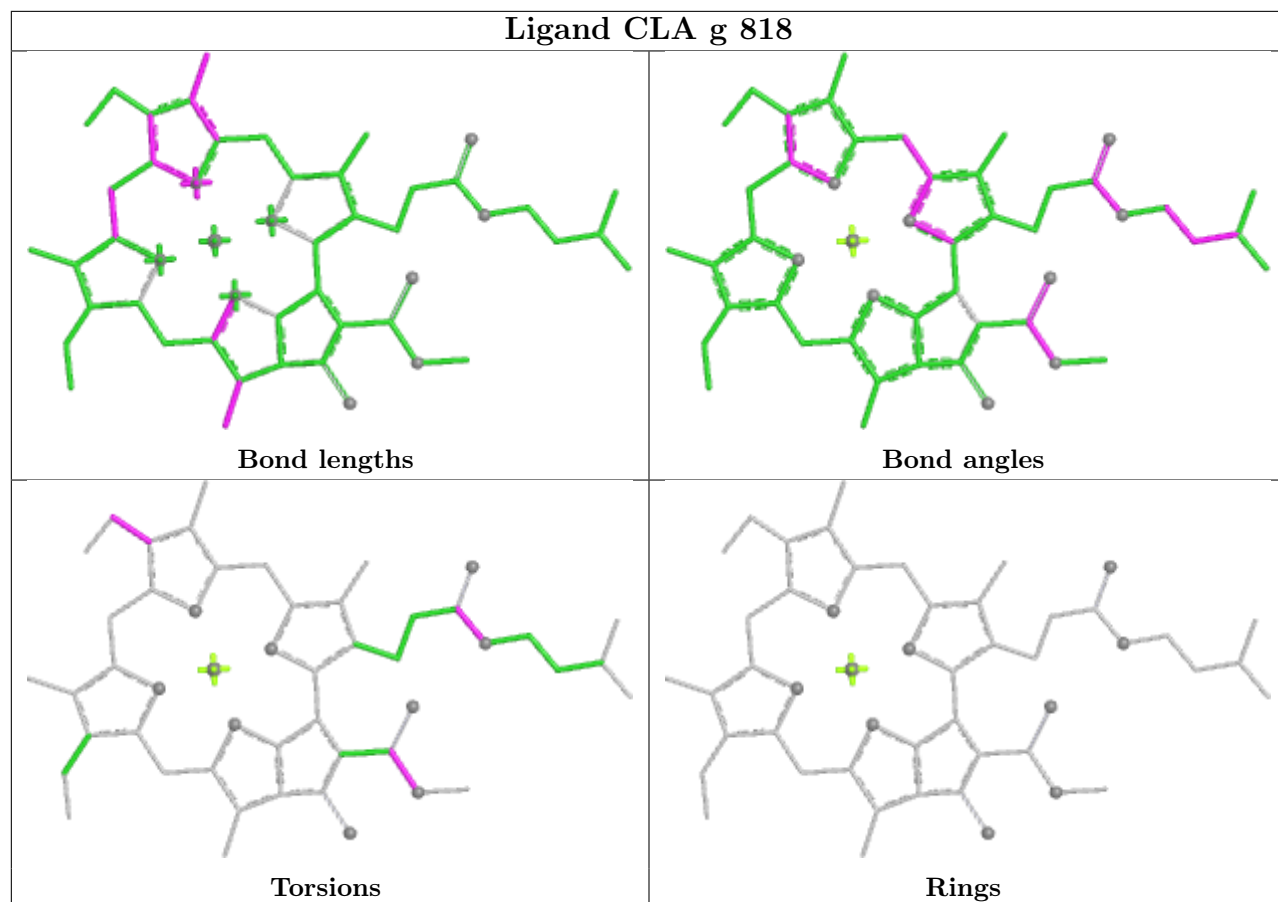


## Ligand BCR a 849

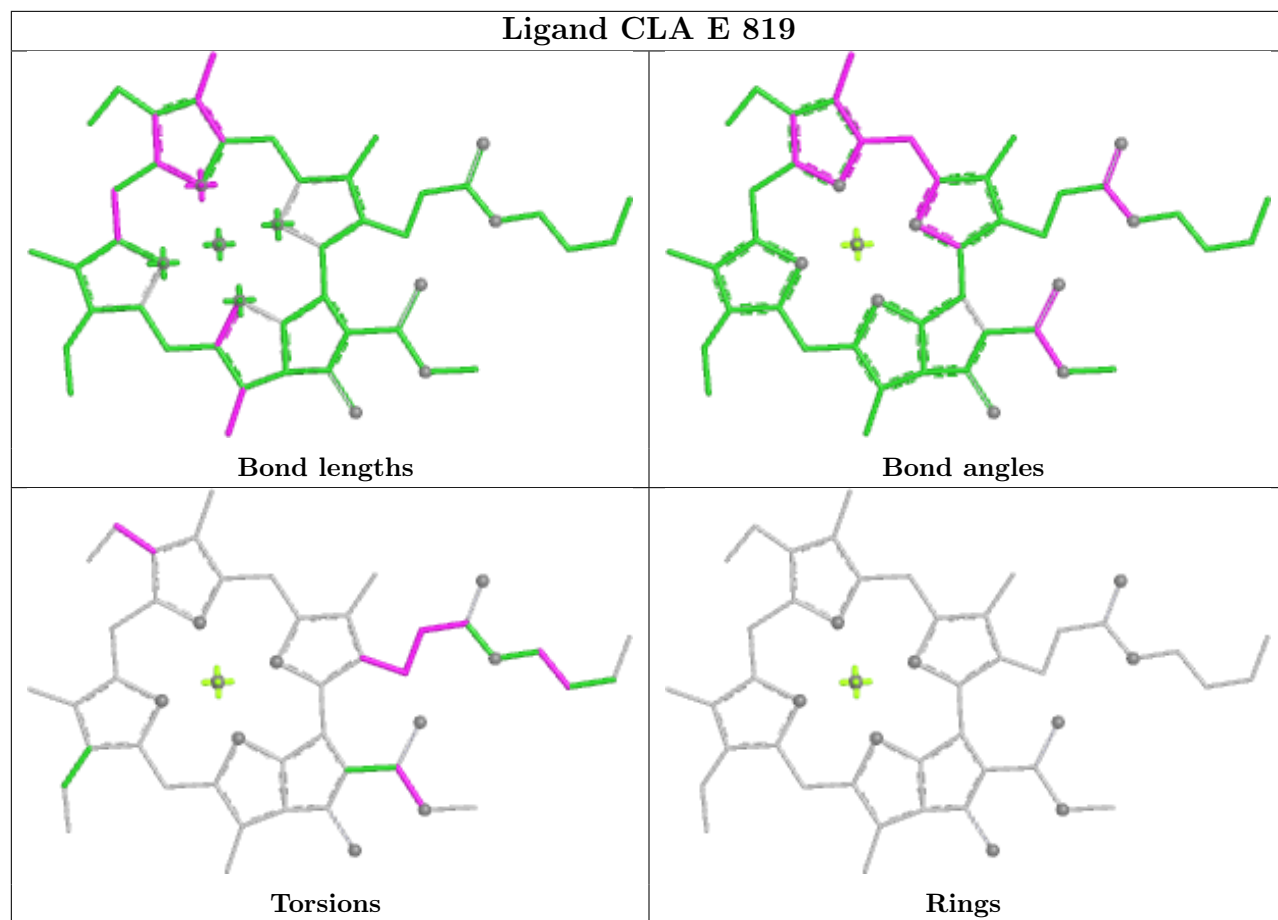




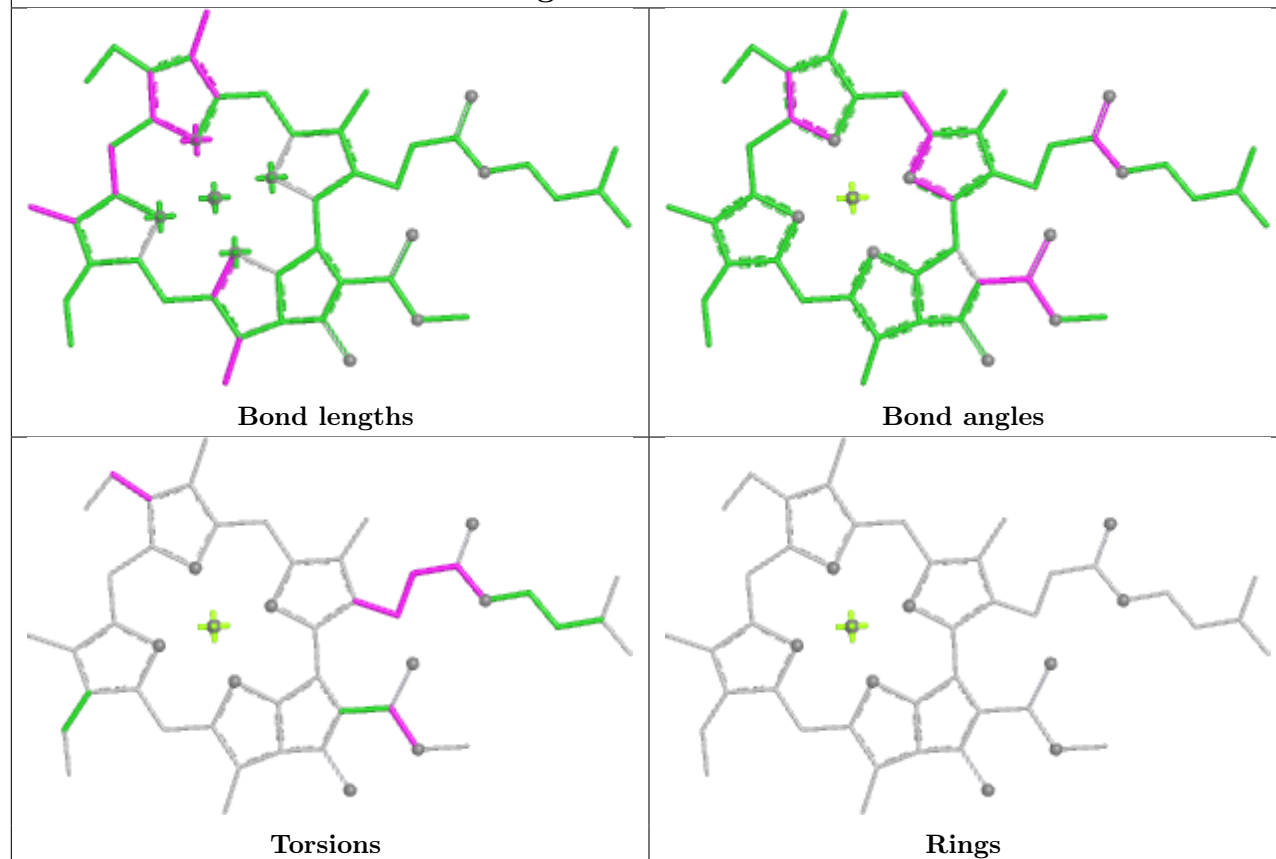
## Ligand CLA g 818



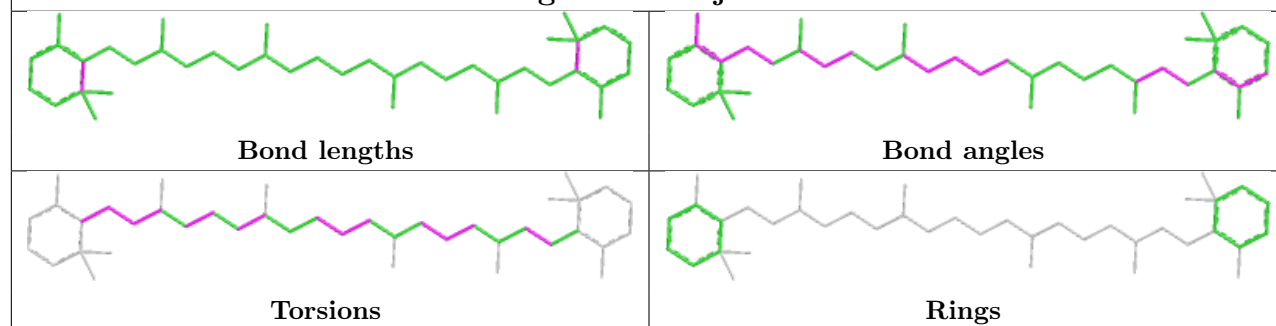
## Ligand CLA E 819



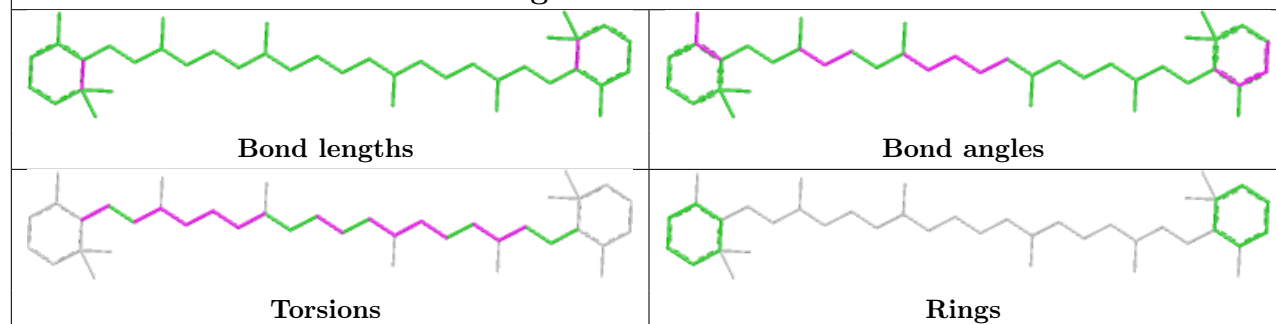
## Ligand CLA e 826



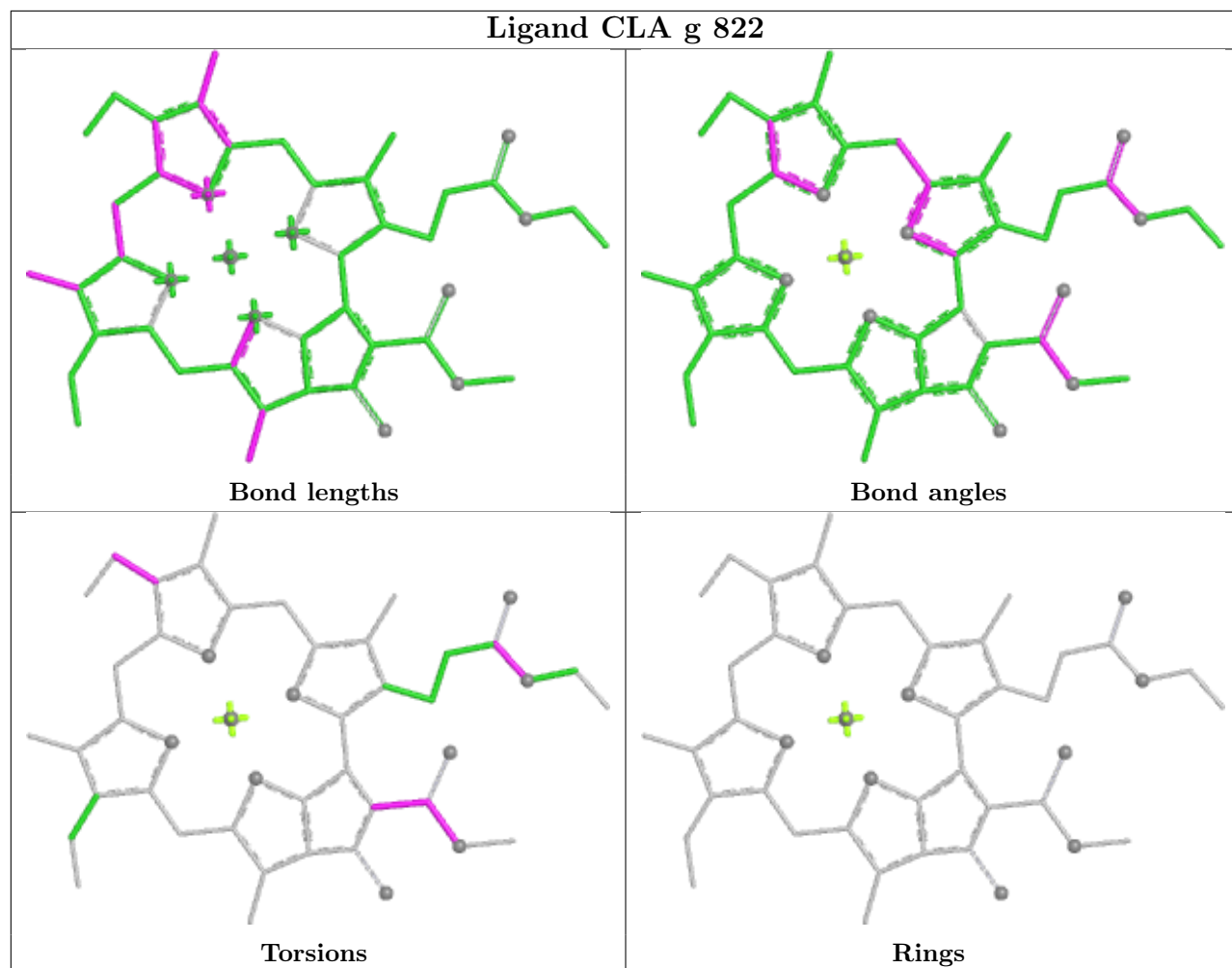
## Ligand BCR j 101



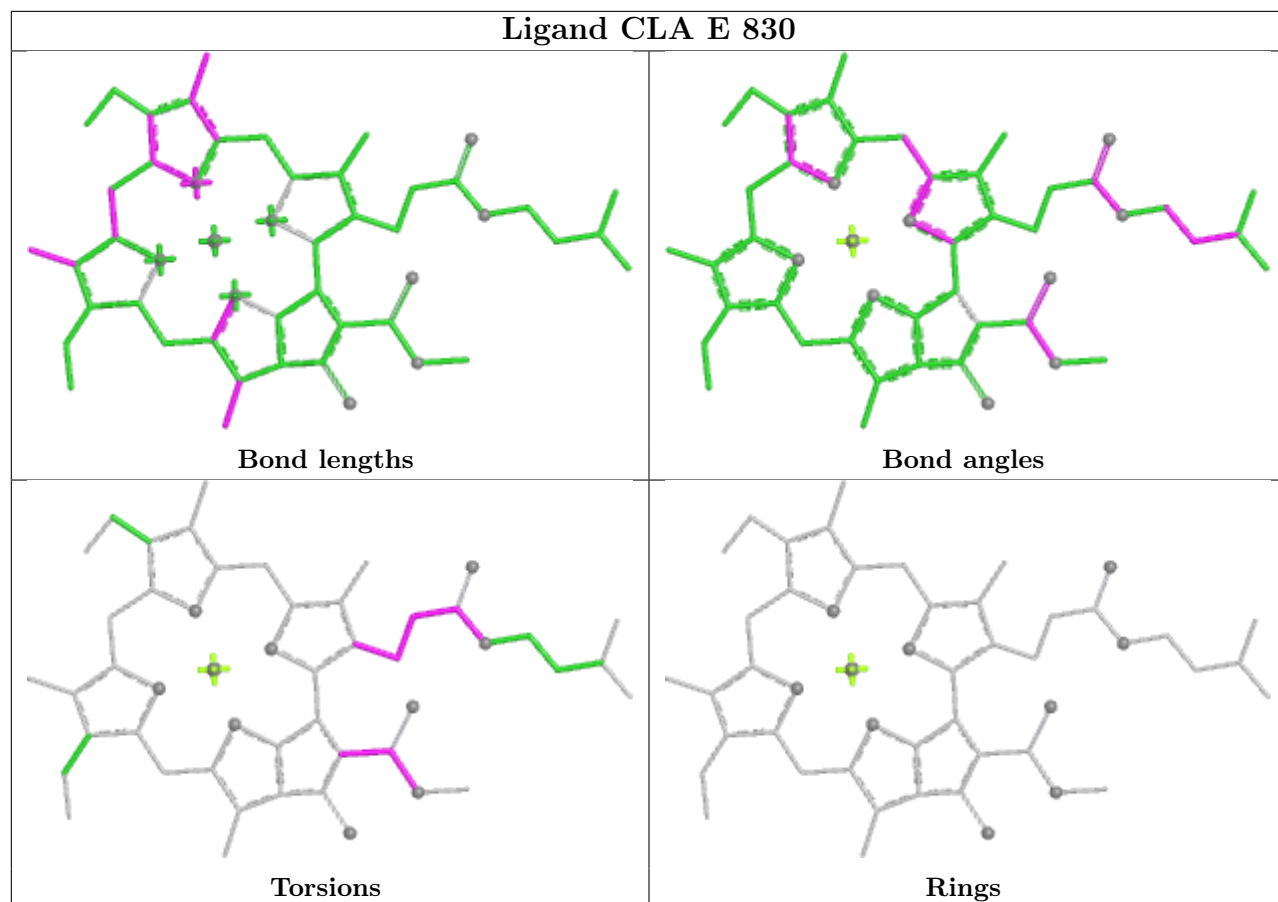
## Ligand BCR B 844

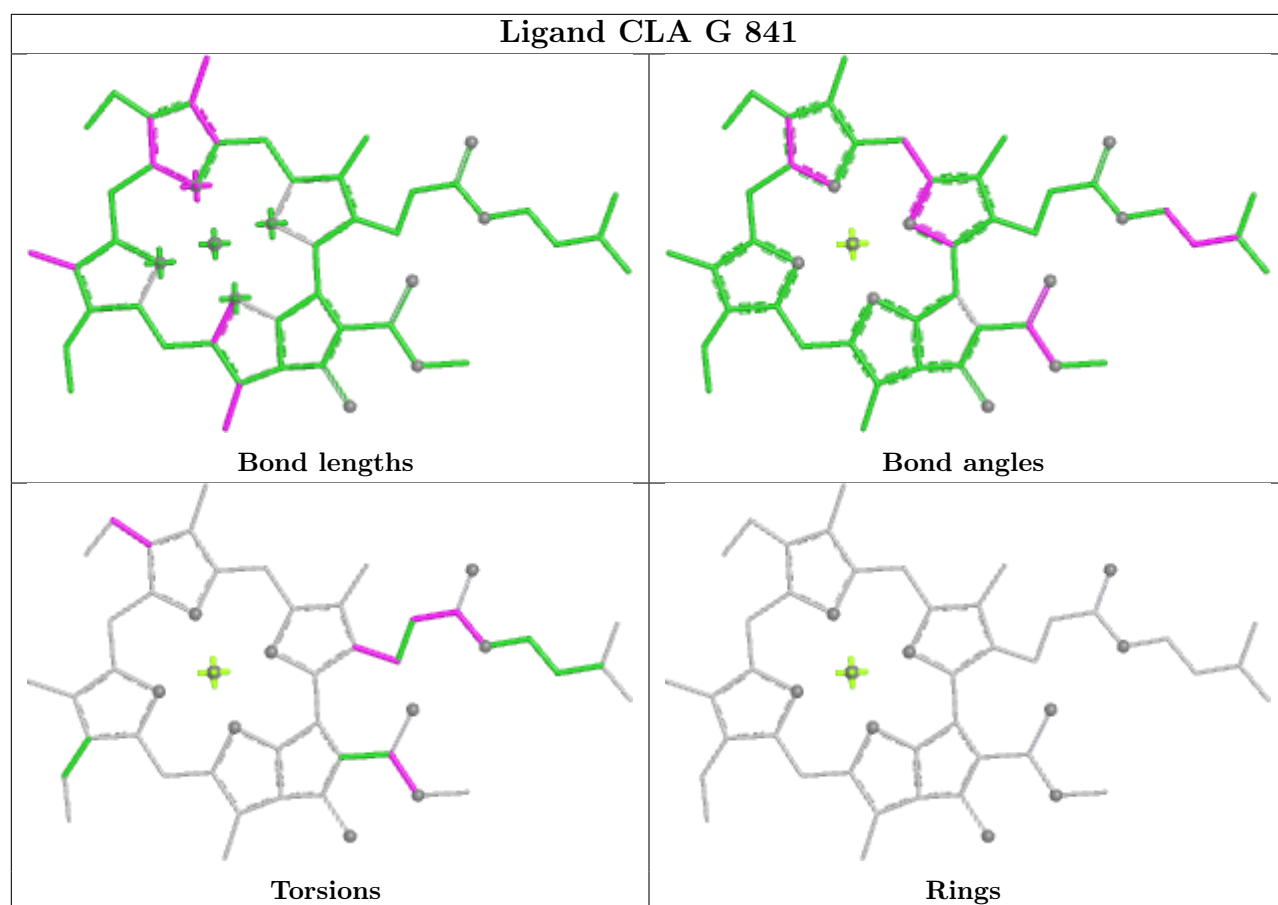


## Ligand CLA g 822

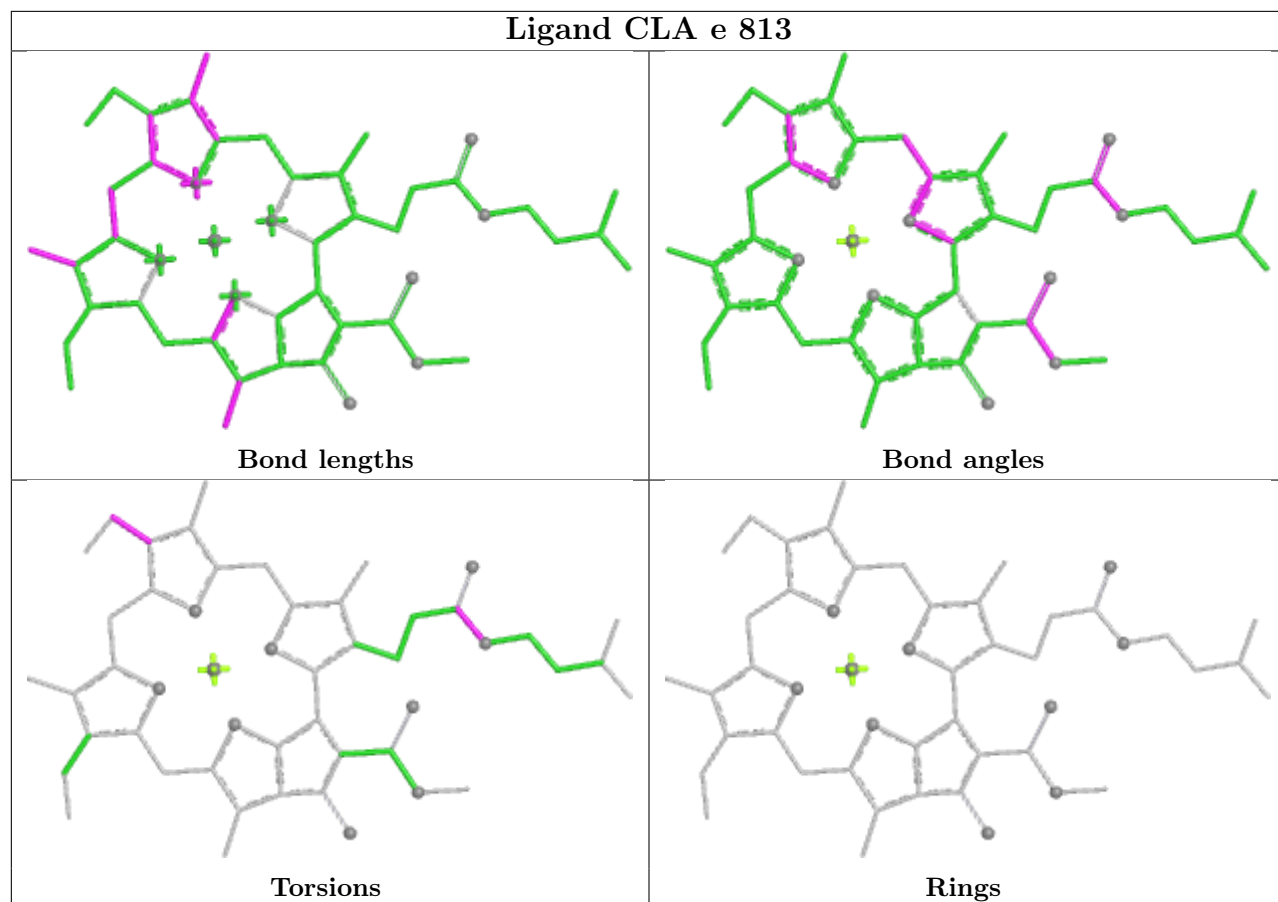


## Ligand CLA E 830

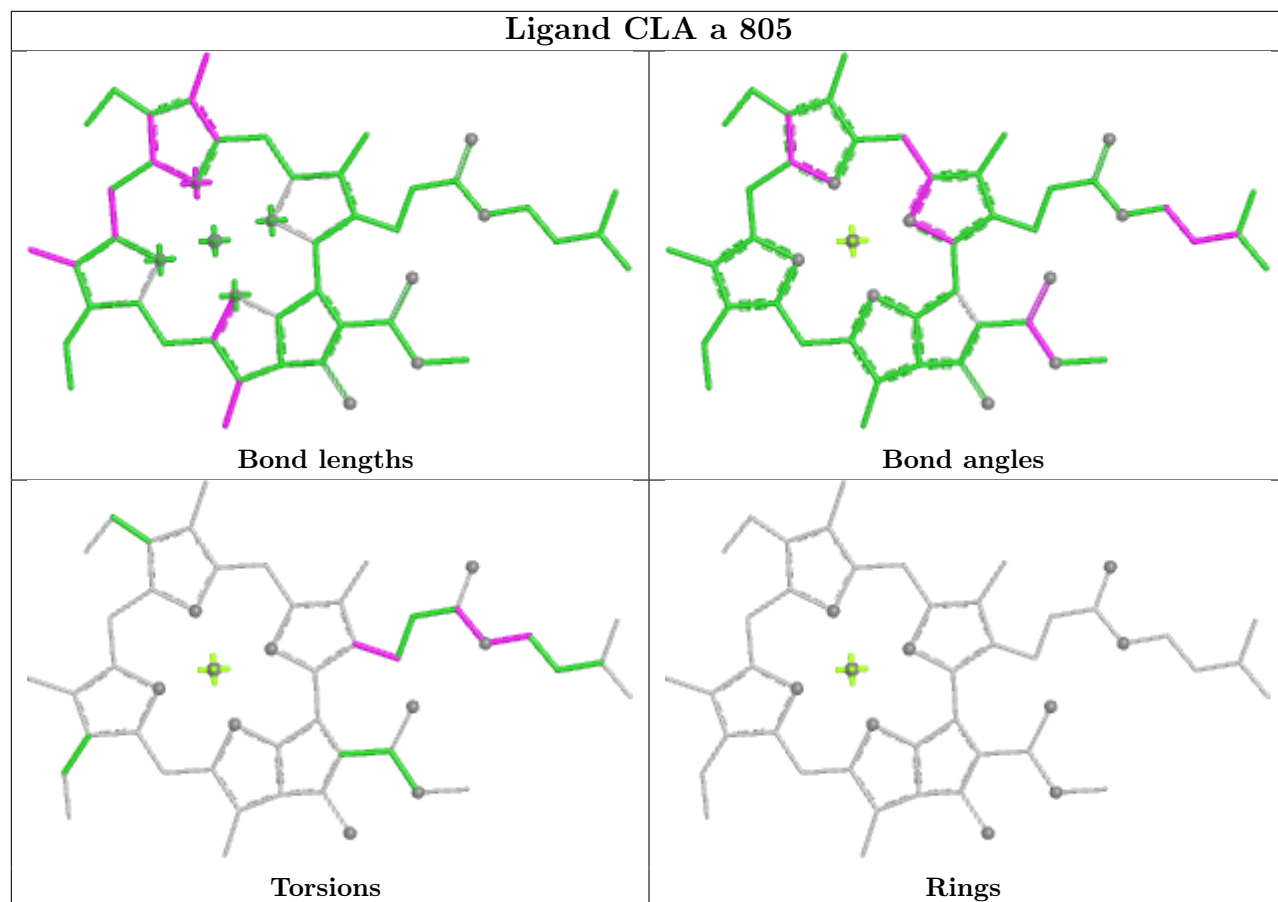




## Ligand CLA e 813

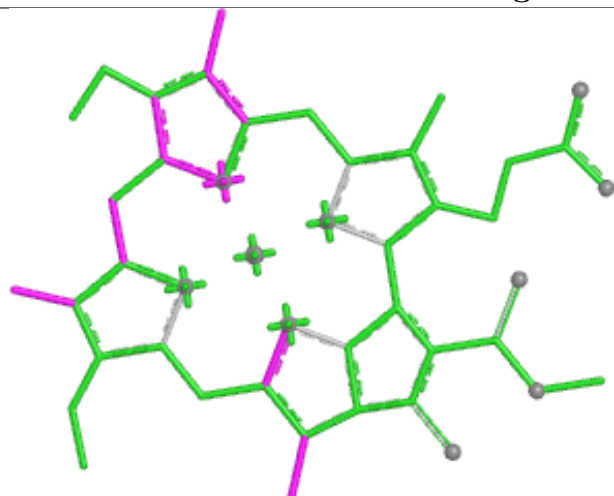


## Ligand CLA a 805

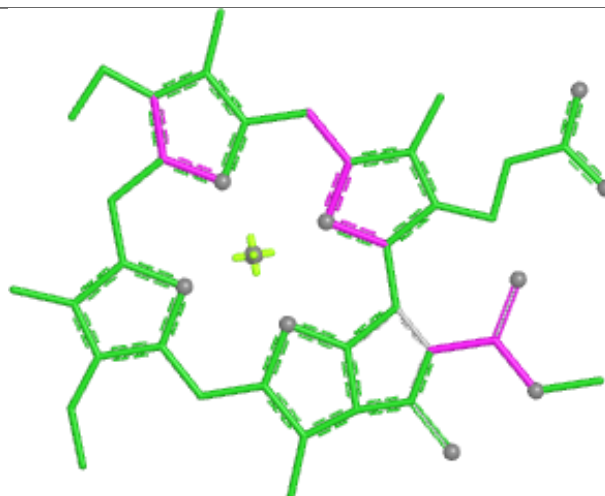




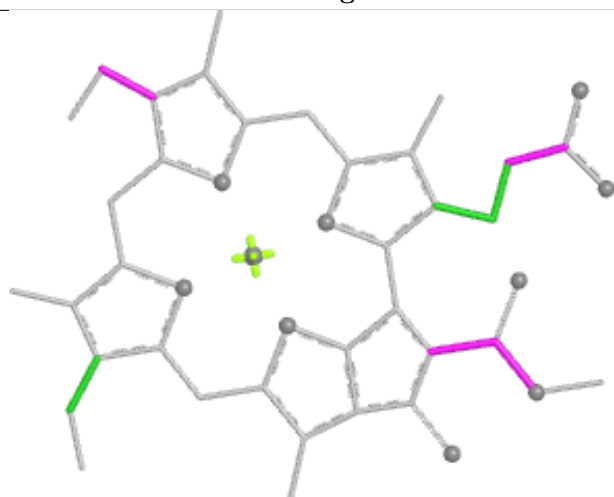
## Ligand CLA G 824



Bond lengths



Bond angles

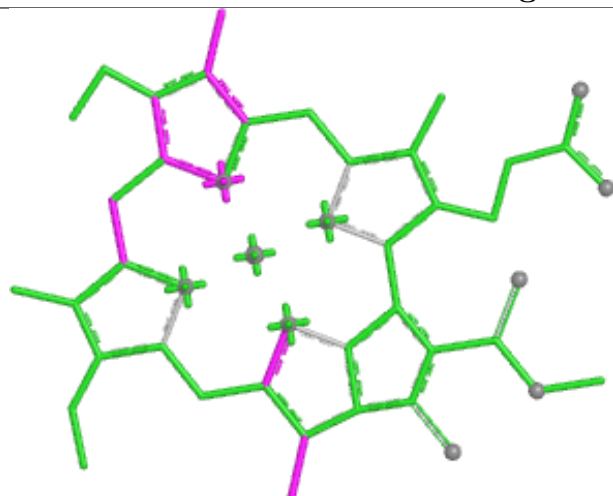


Torsions

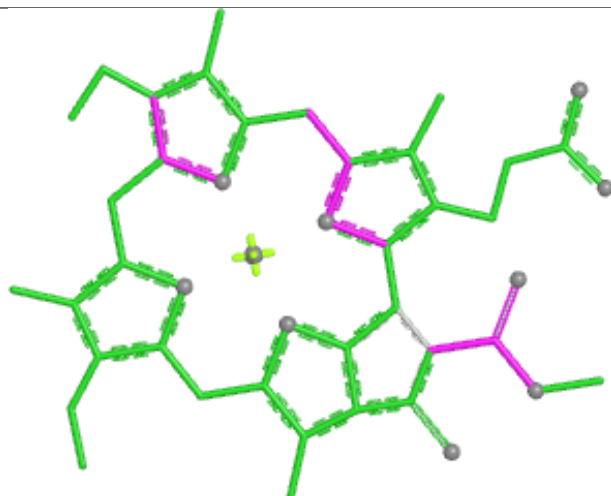


Rings

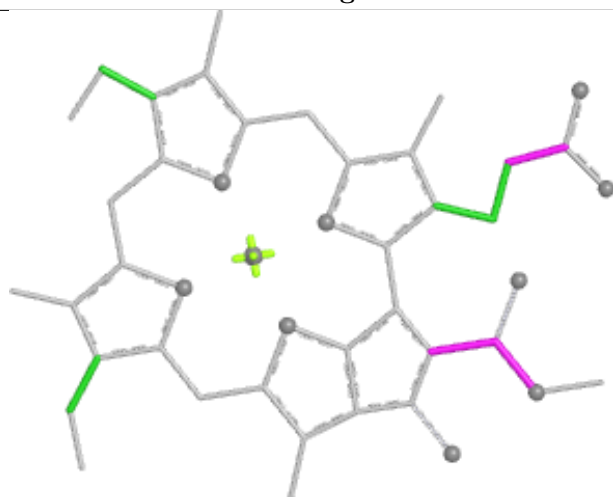
## Ligand CLA e 837



Bond lengths



Bond angles

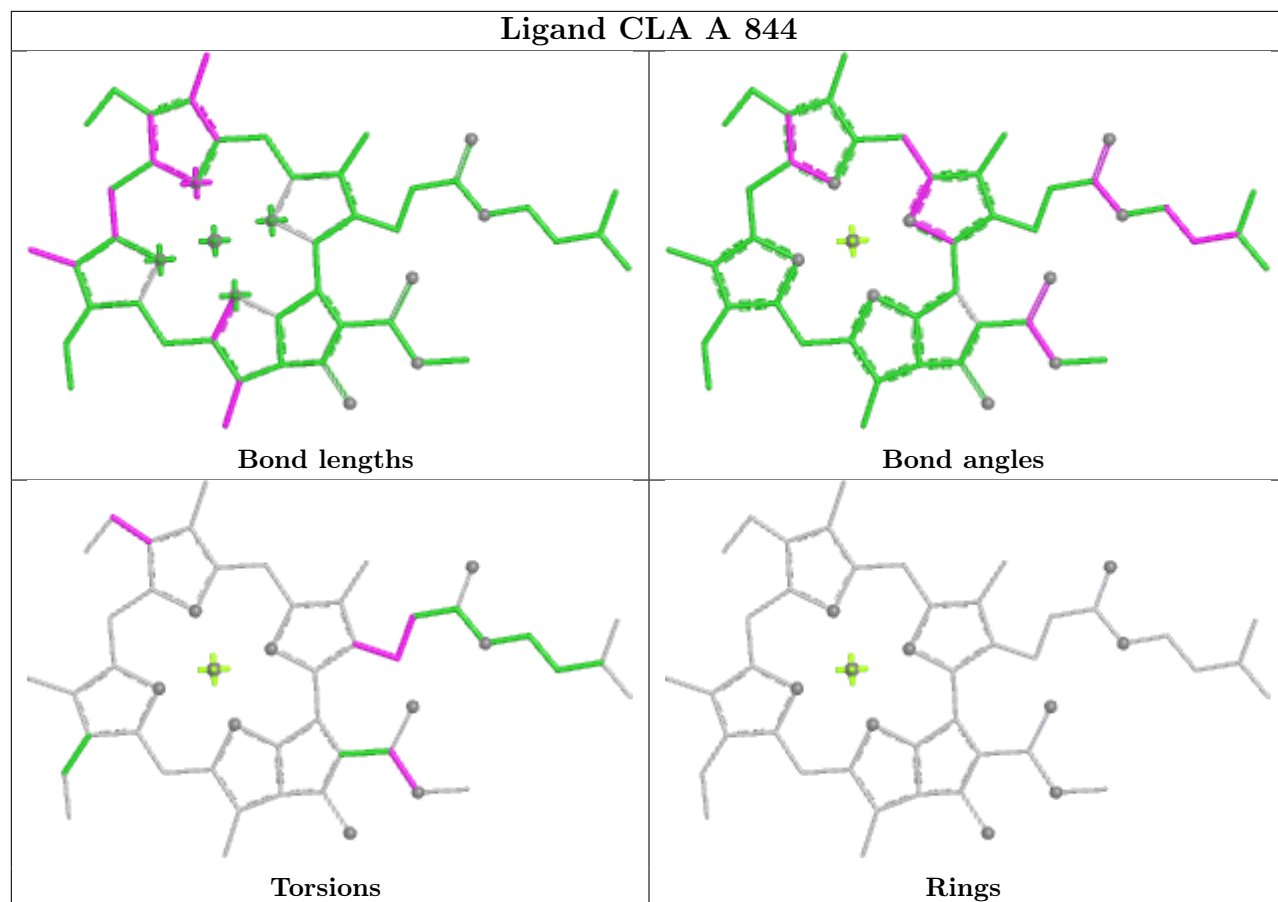


Torsions

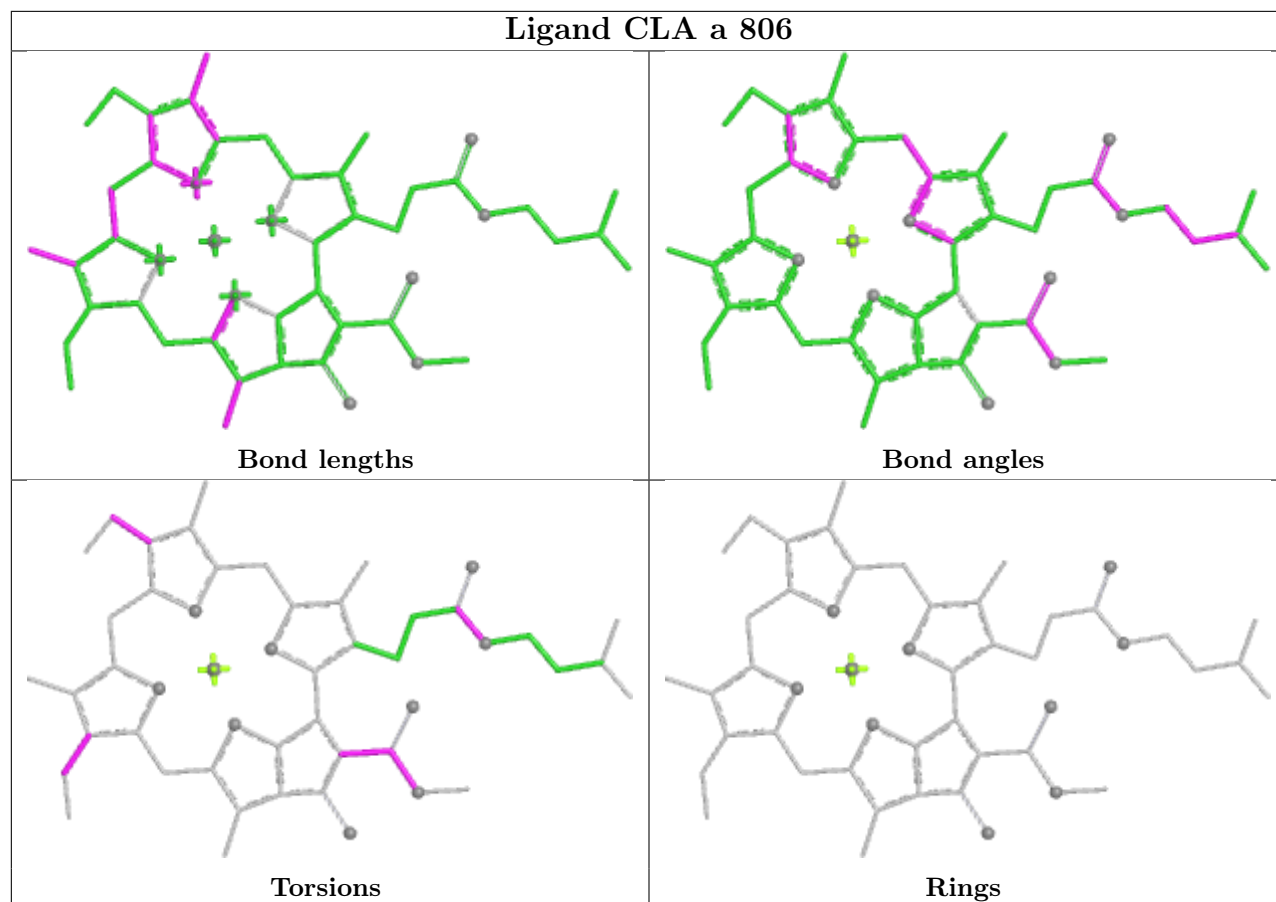


Rings

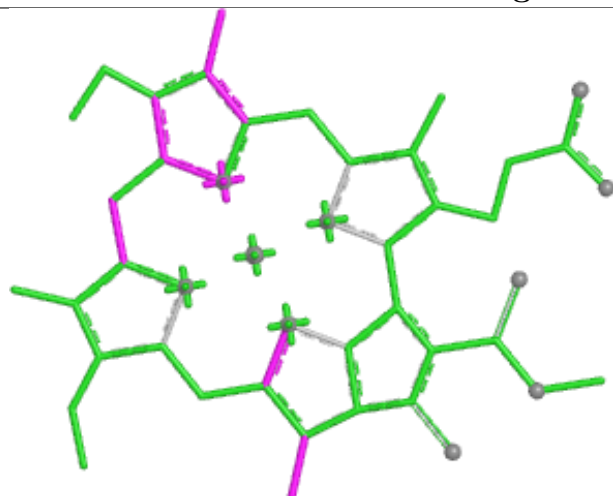
## Ligand CLA A 844



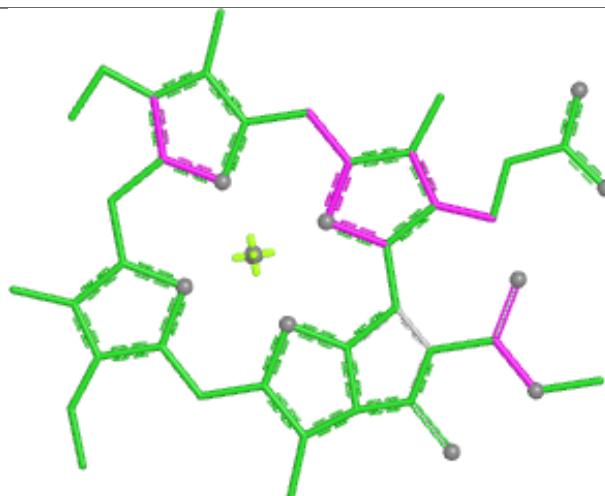
## Ligand CLA a 806



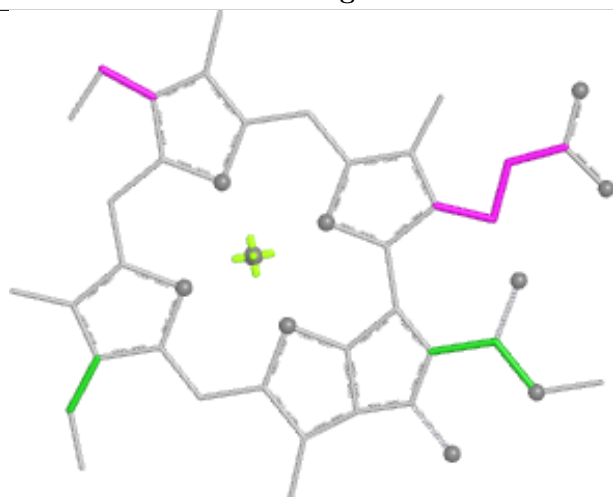
## Ligand CLA K 102



Bond lengths



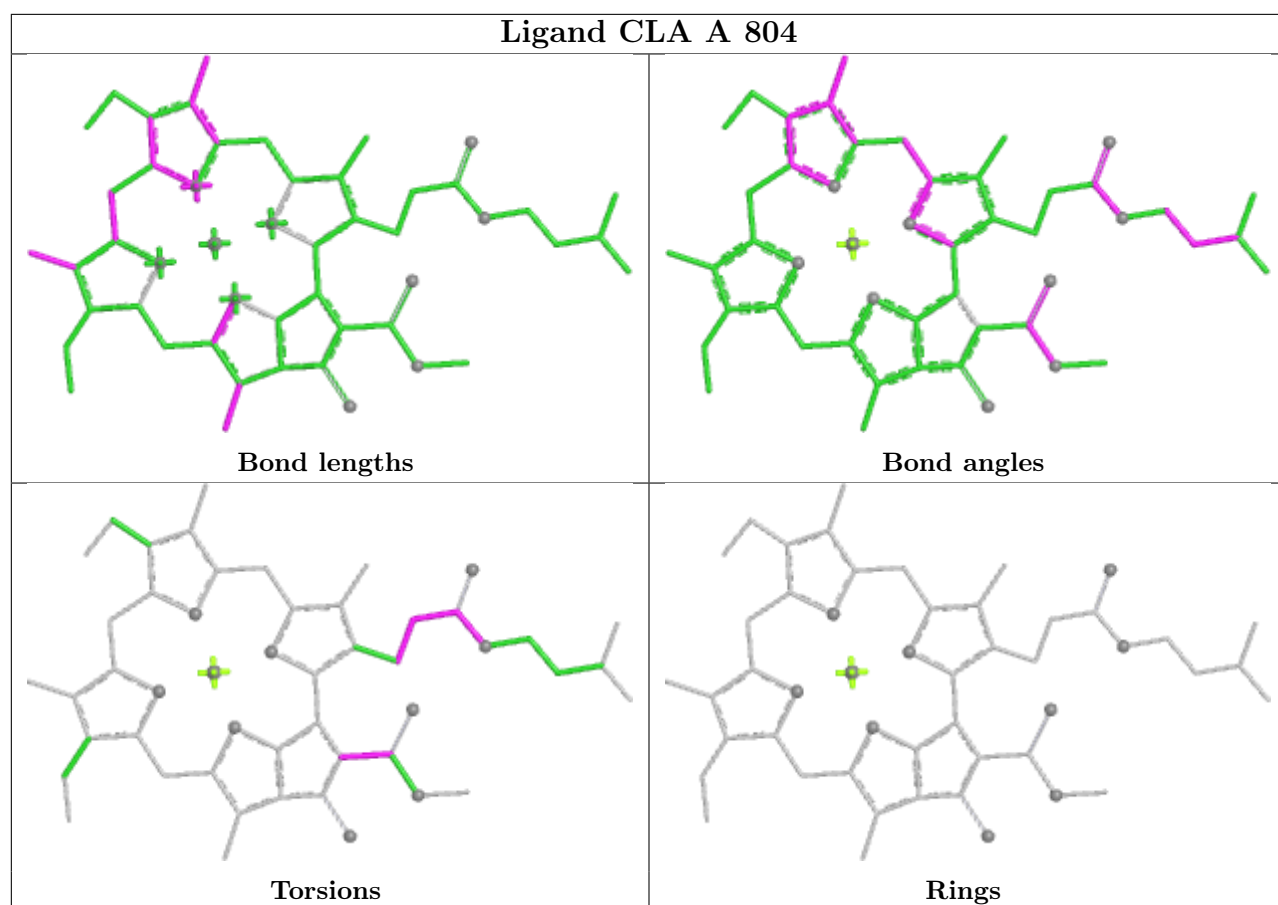
Bond angles



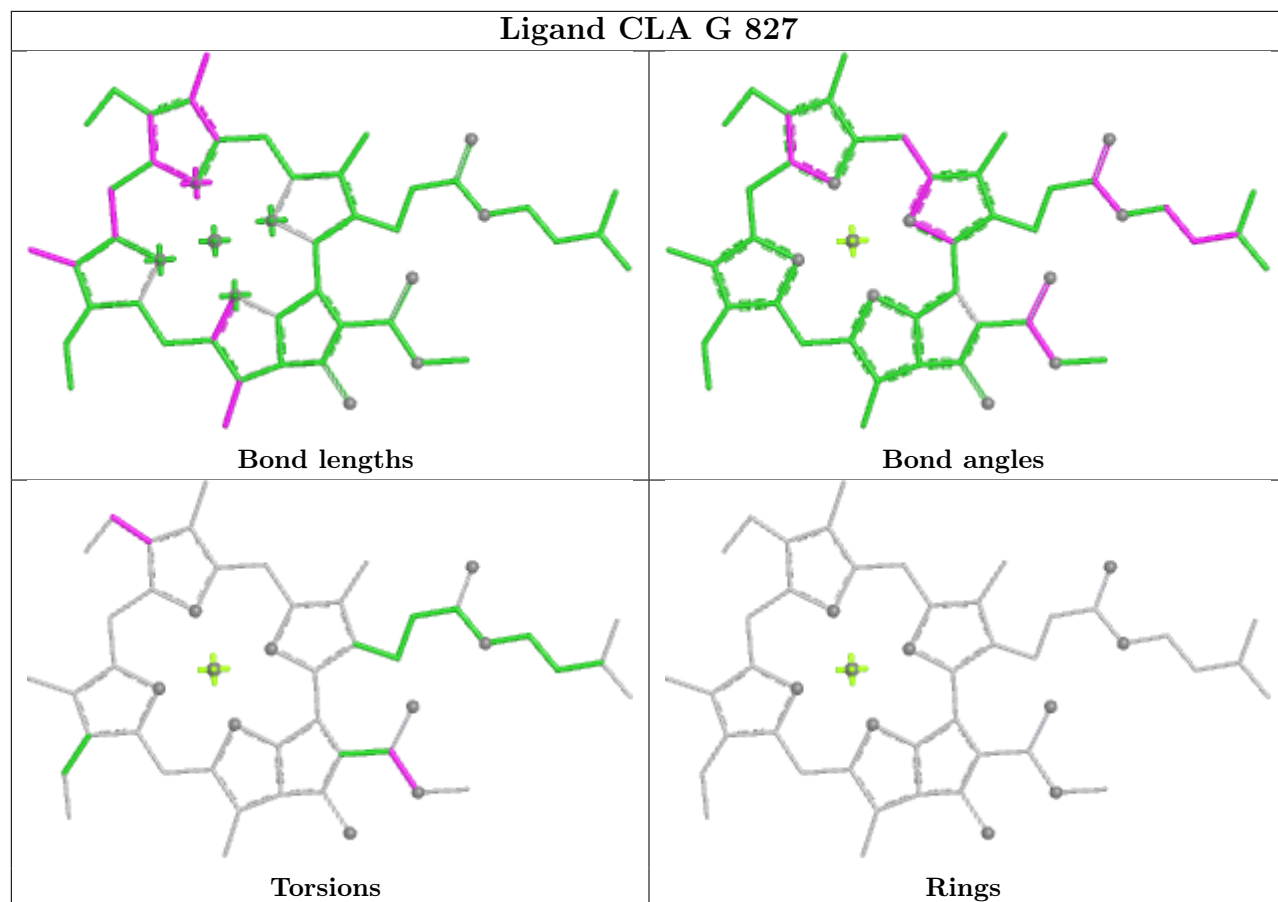
Torsions



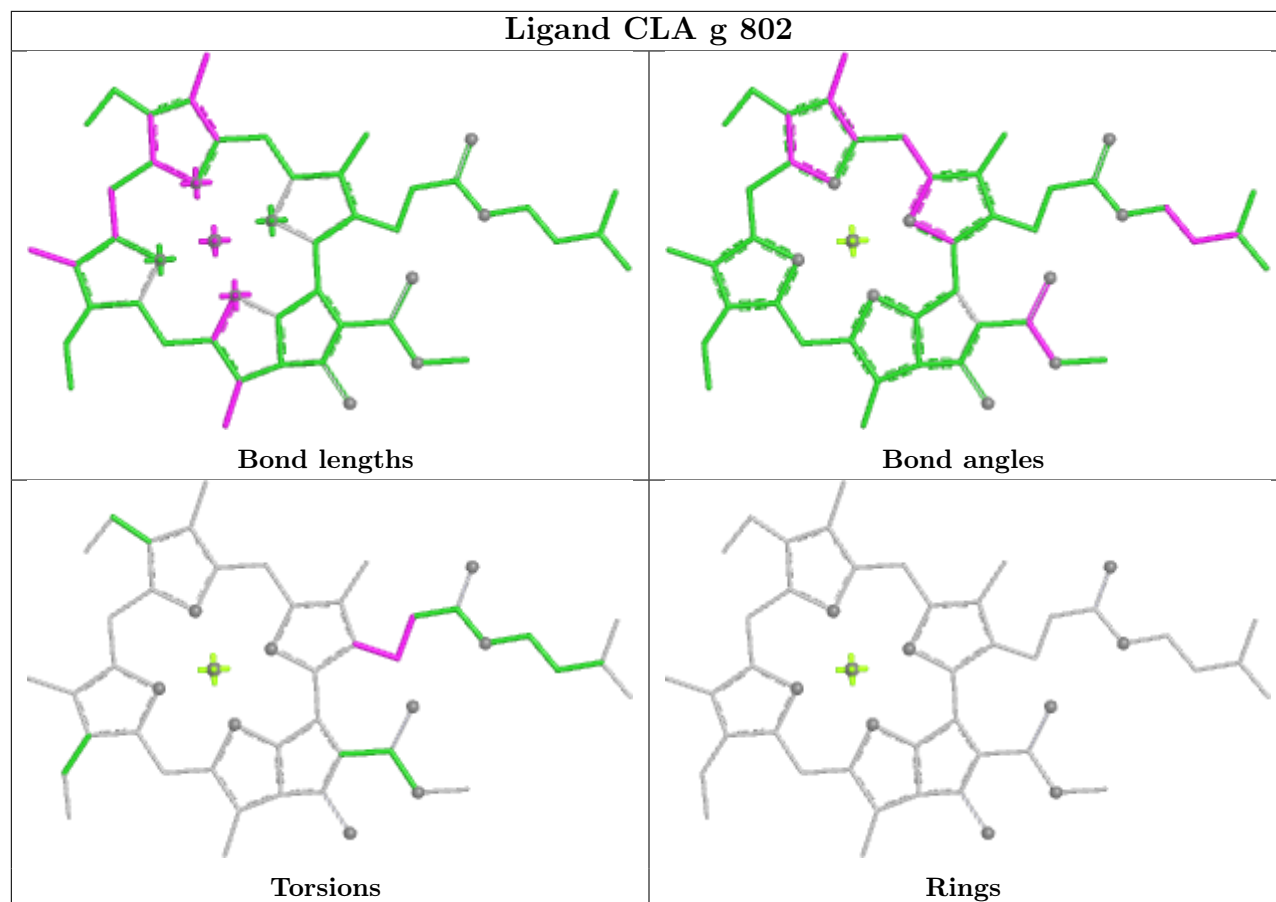
Rings



## Ligand CLA G 827

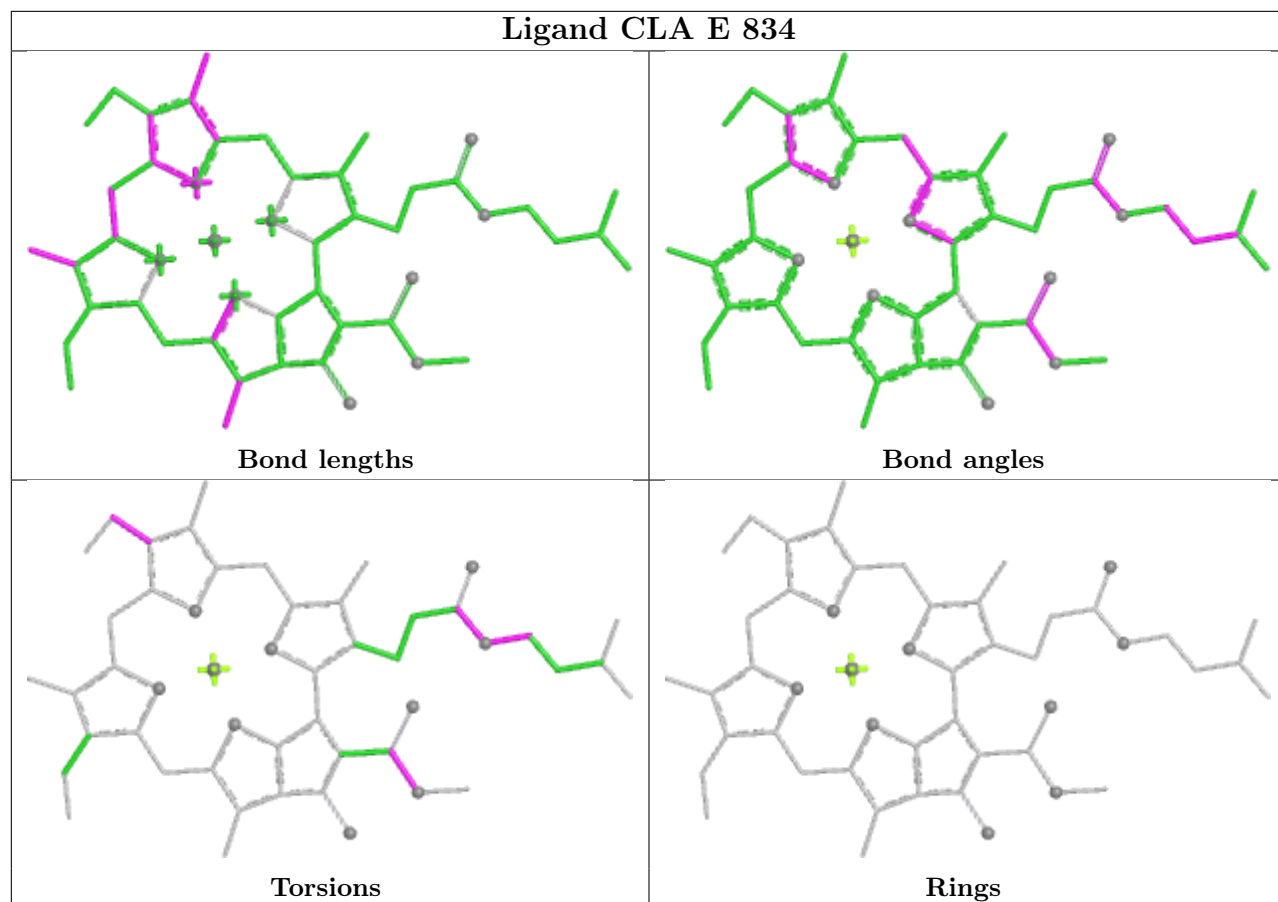


## Ligand CLA g 802

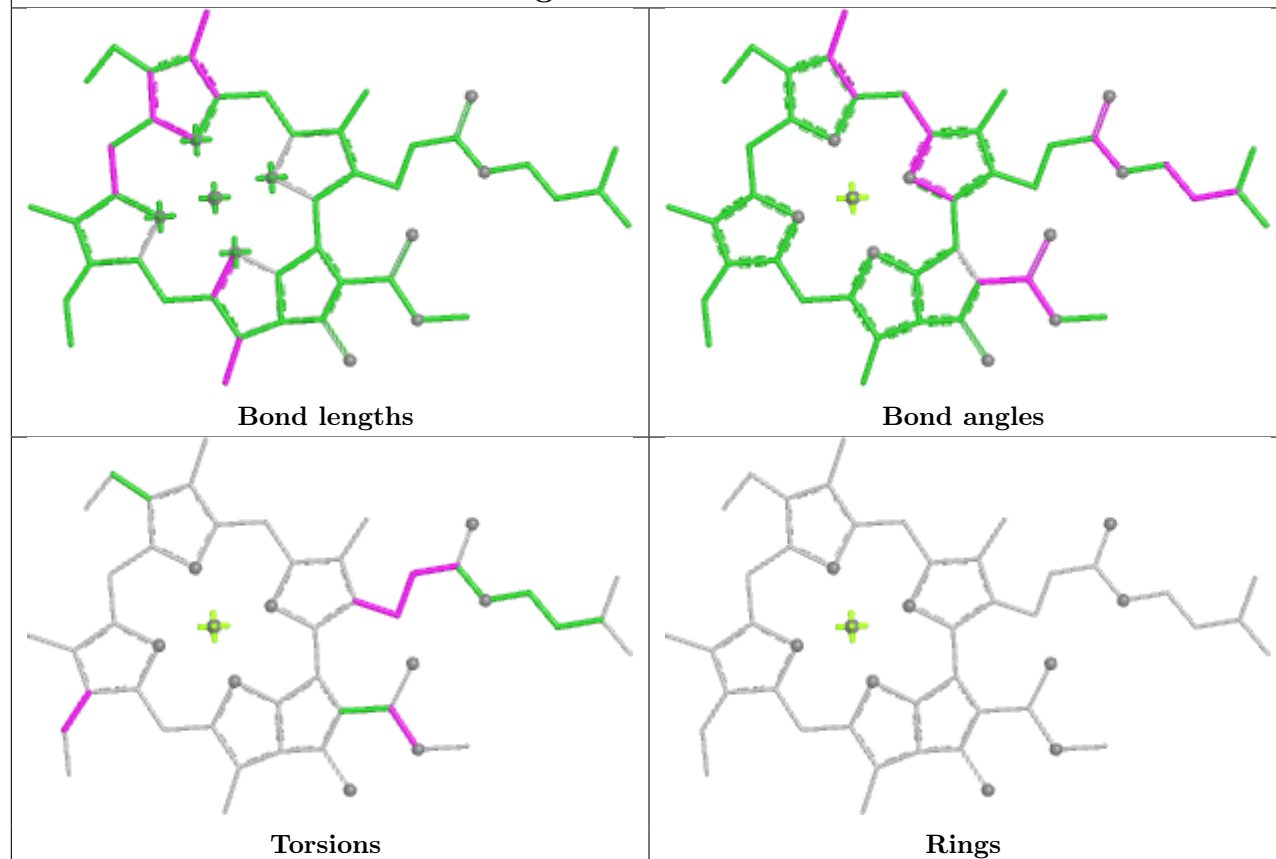




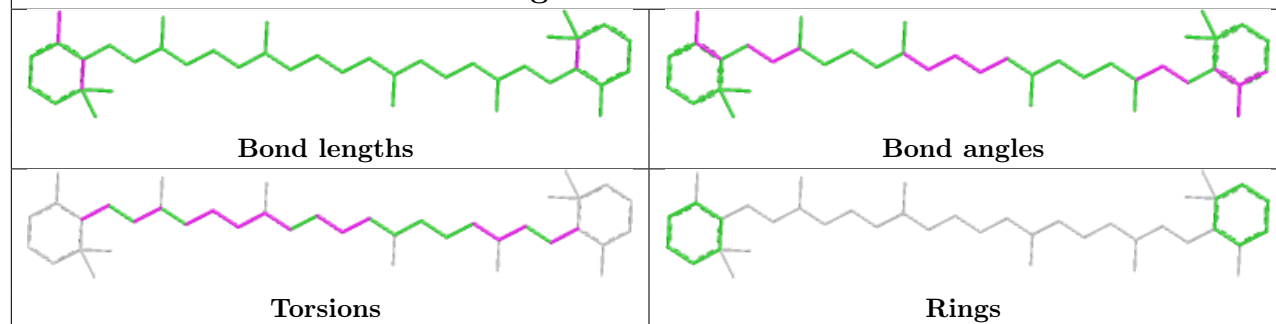
## Ligand CLA E 834



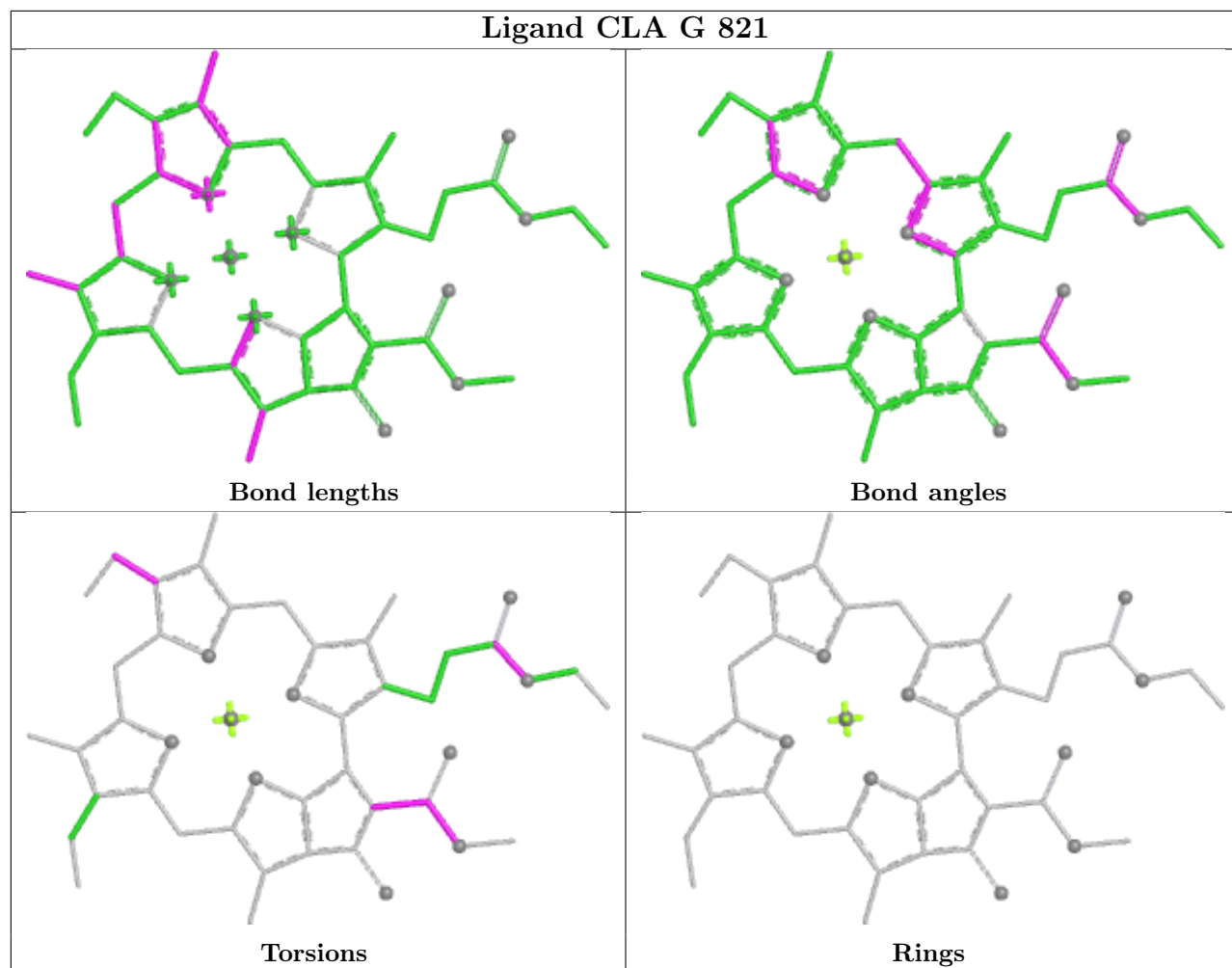
## Ligand CLA b 833

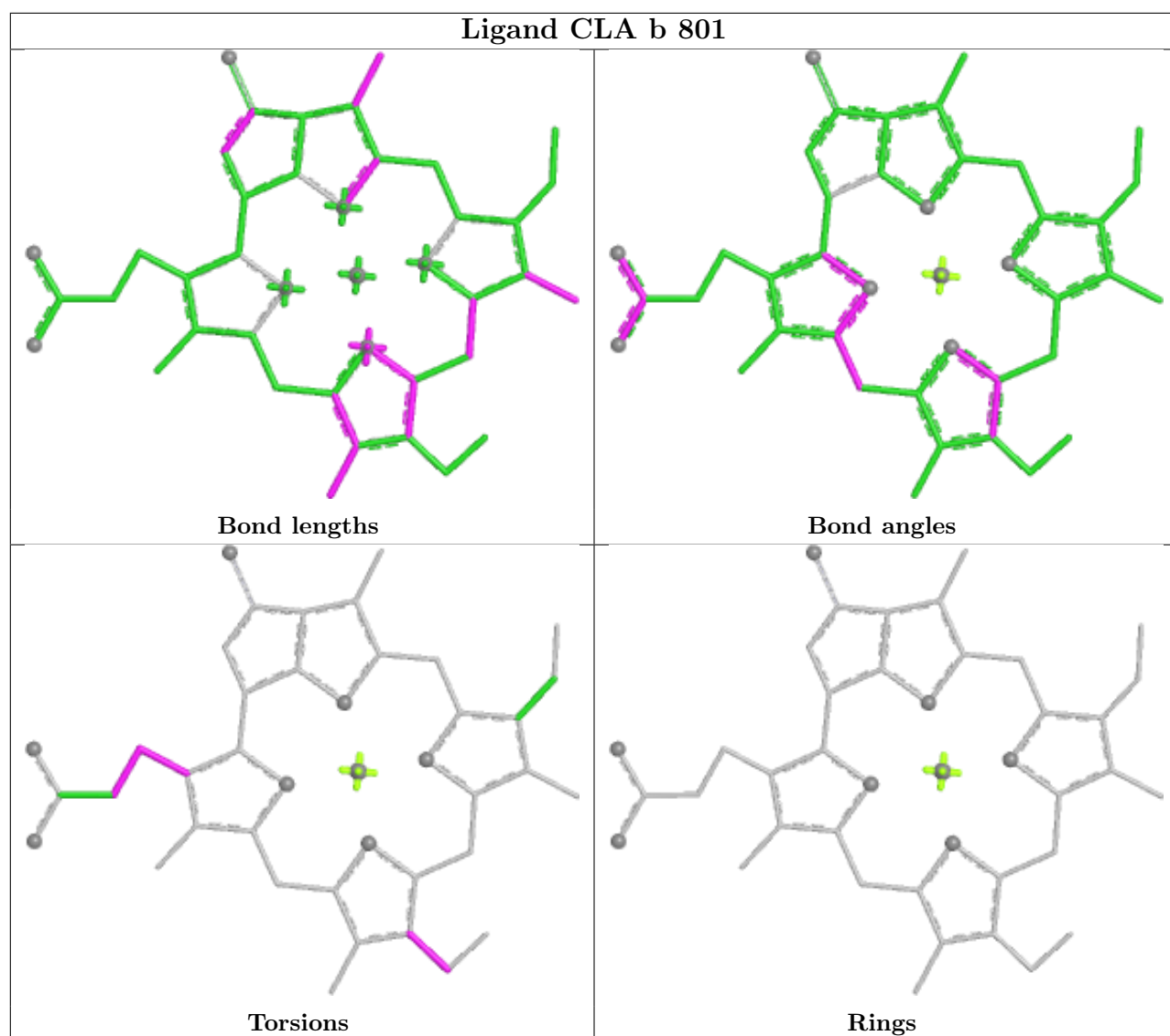


## Ligand BCR B 848

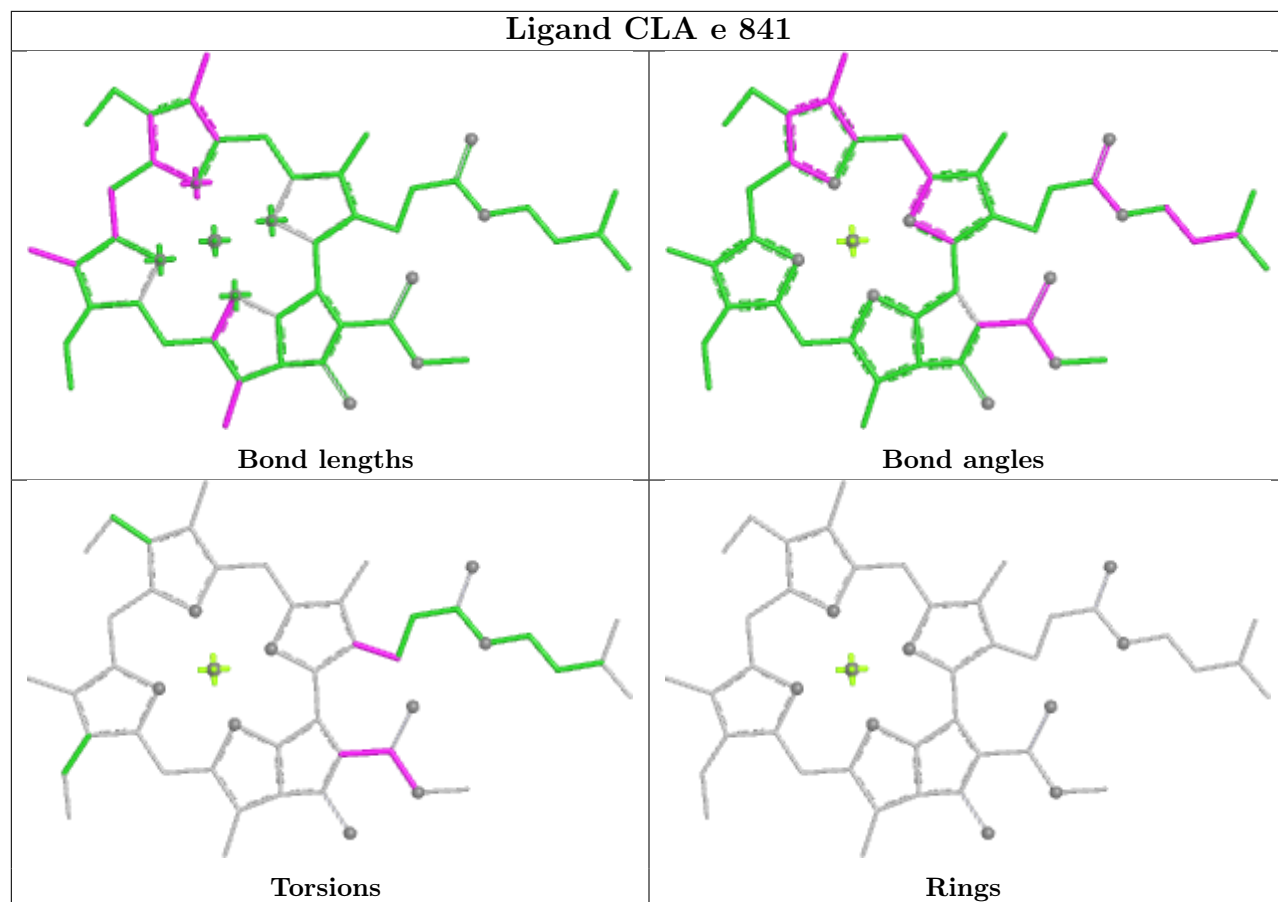


## Ligand CLA G 821

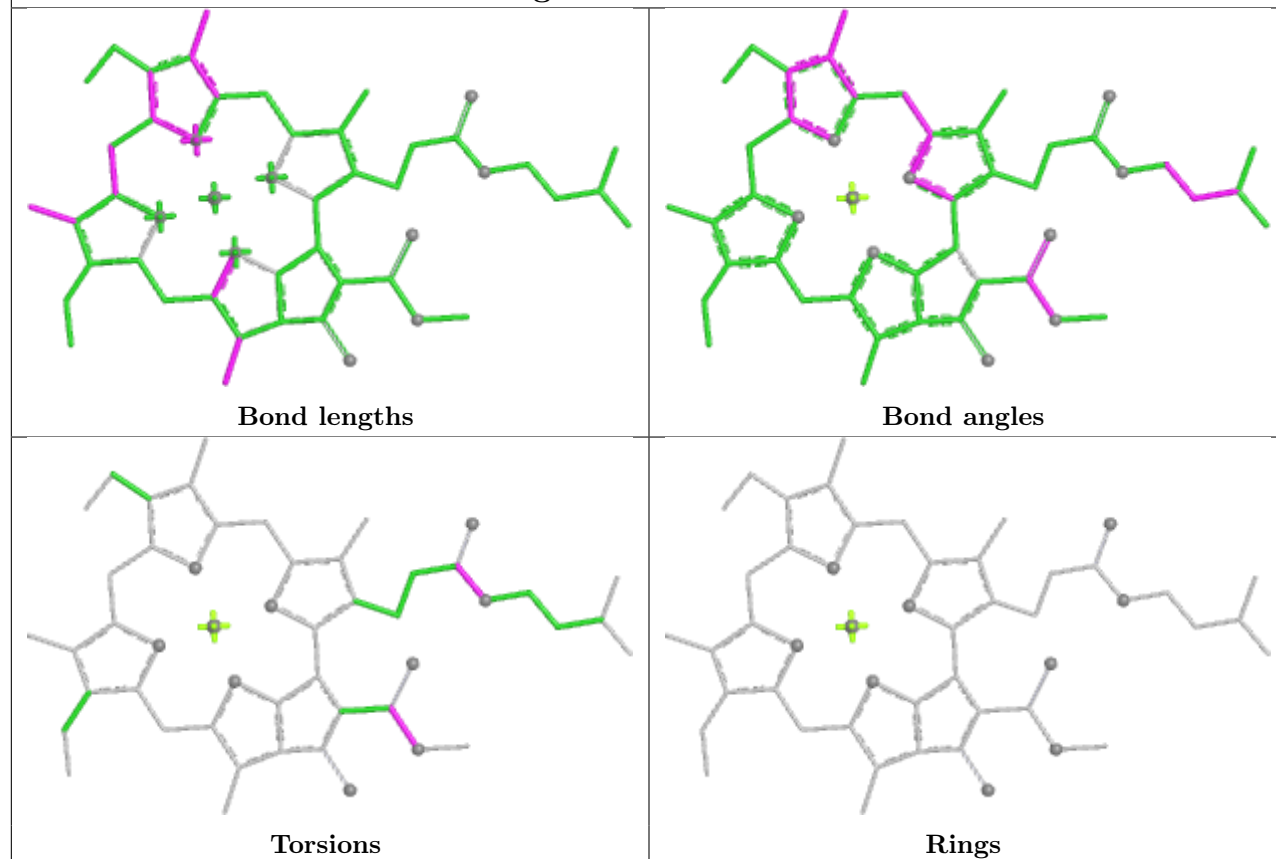




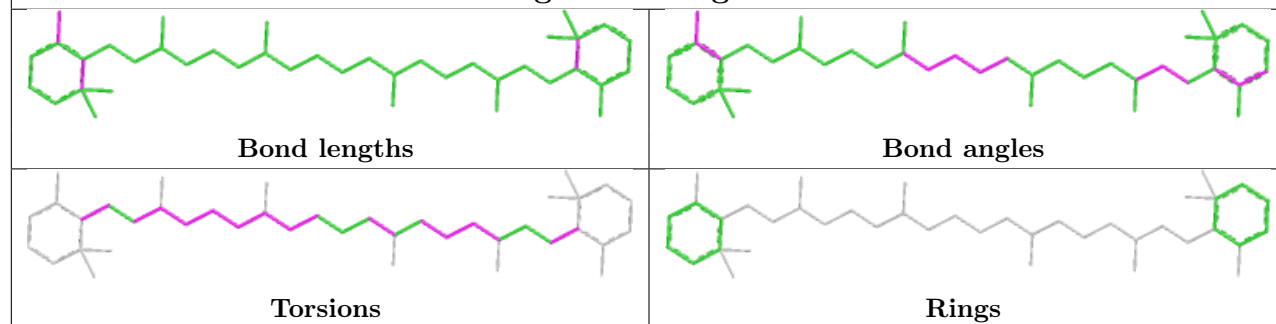
## Ligand CLA e 841



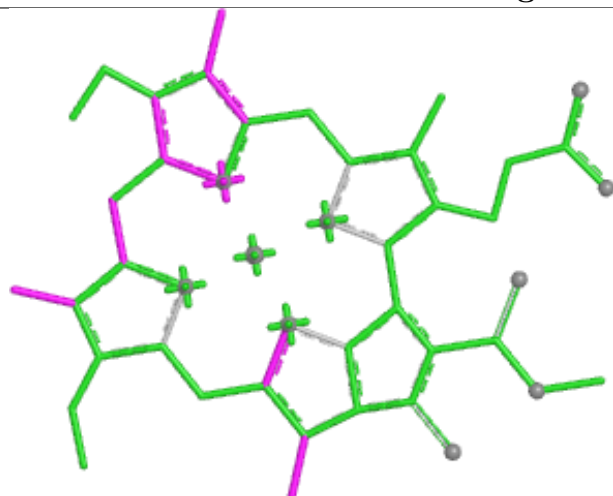
## Ligand CLA E 833



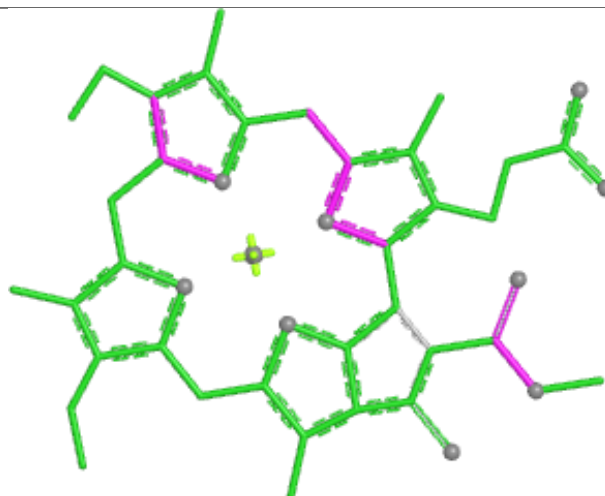
## Ligand BCR g 847



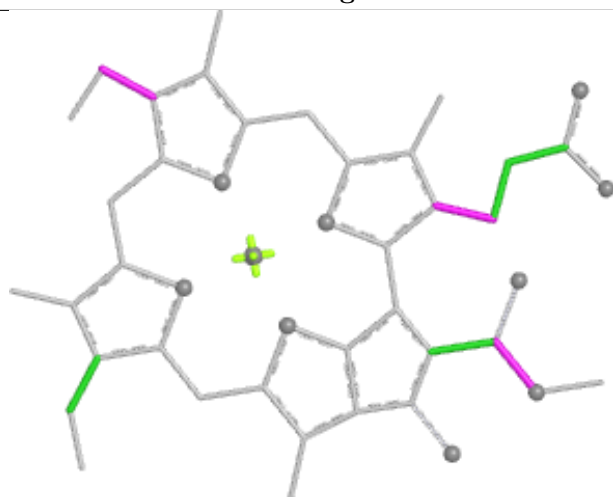
## Ligand CLA b 811



Bond lengths



Bond angles

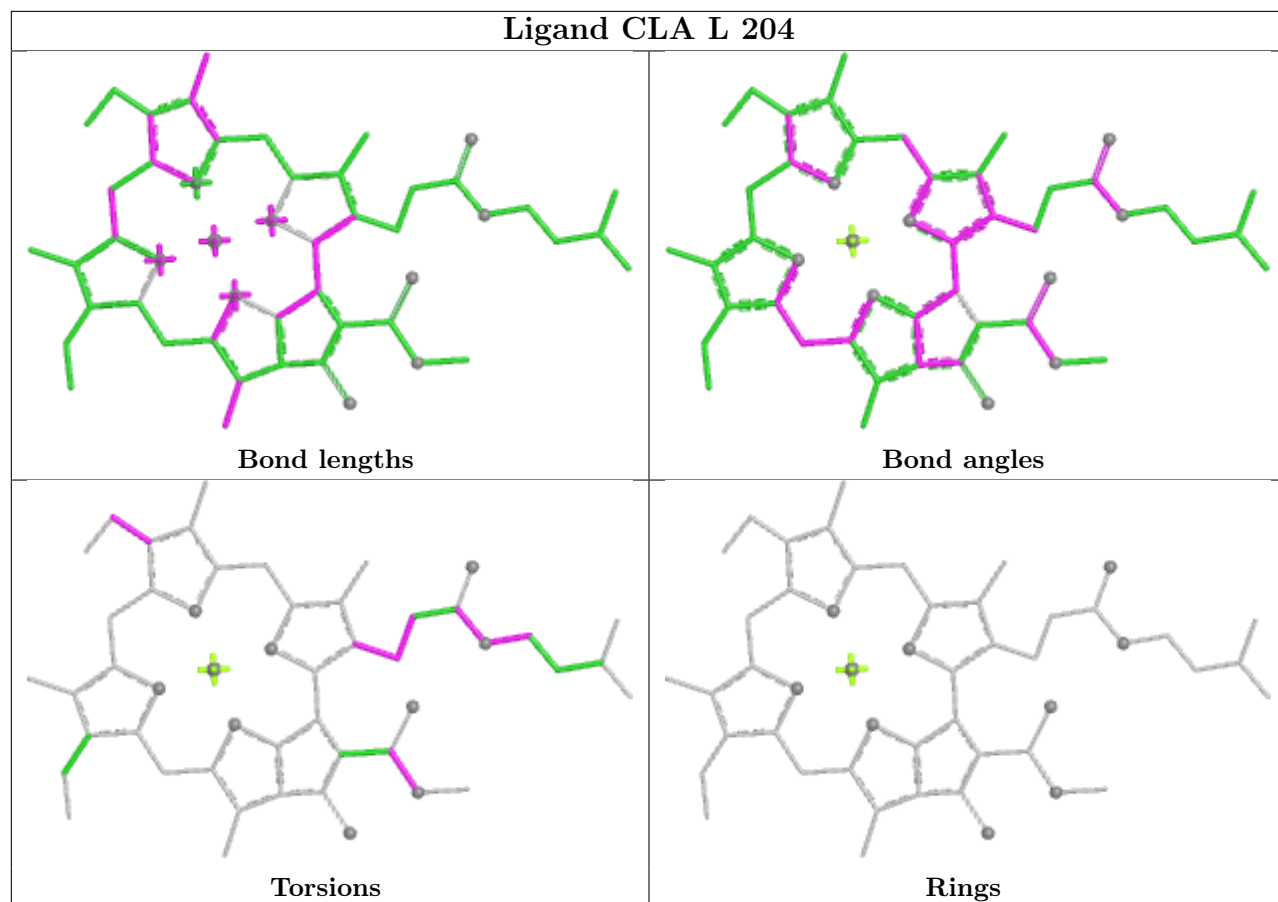


Torsions



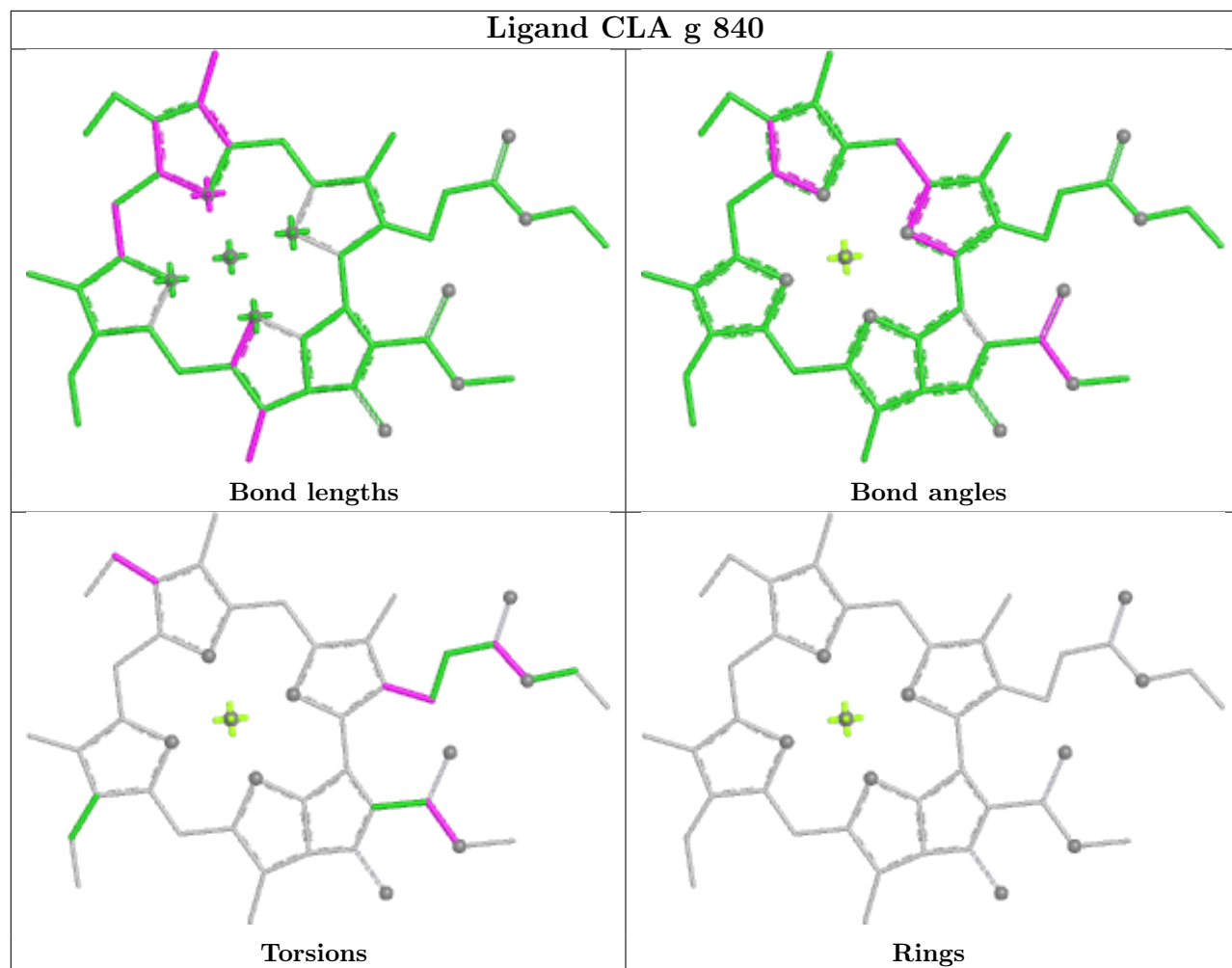
Rings

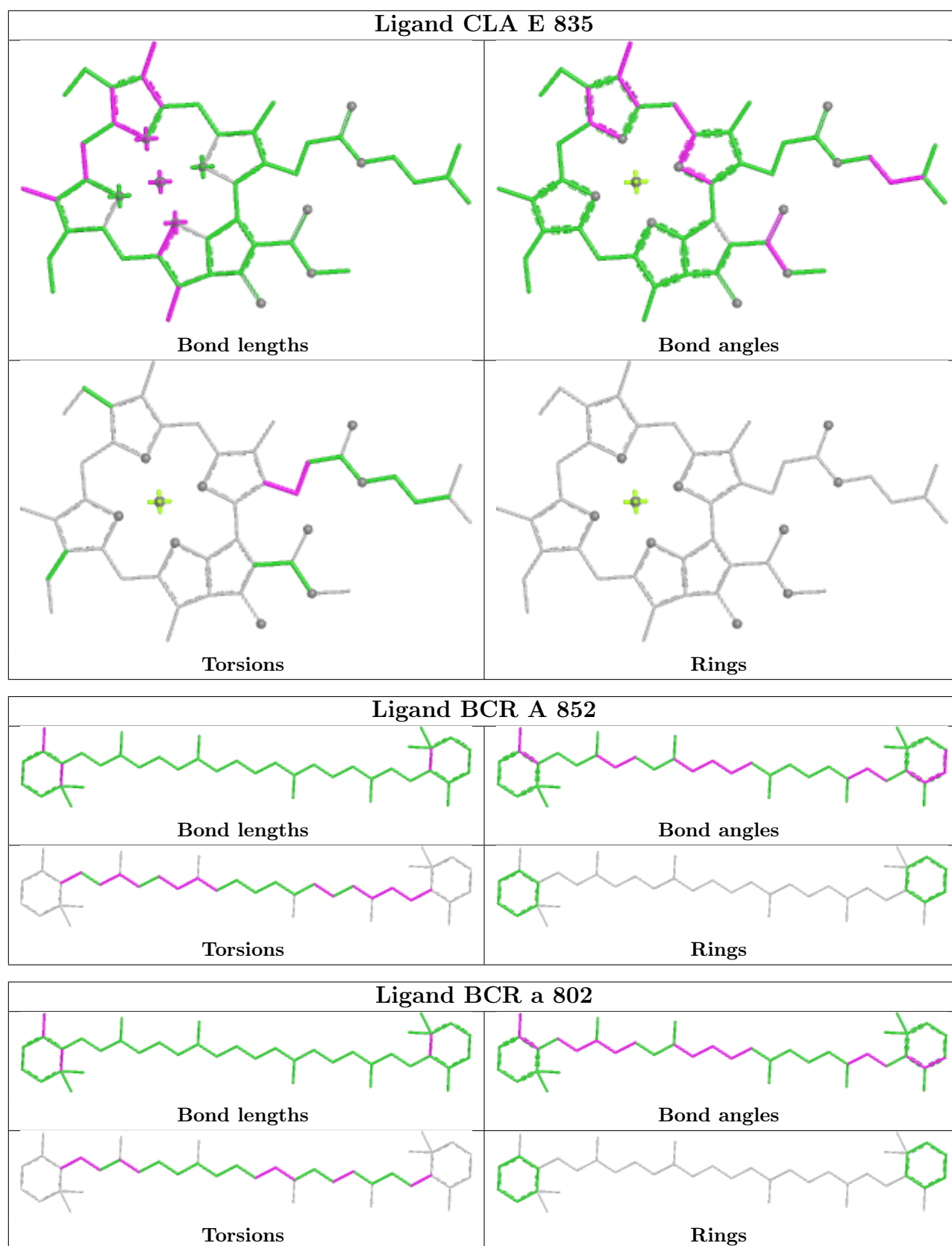
## Ligand CLA L 204



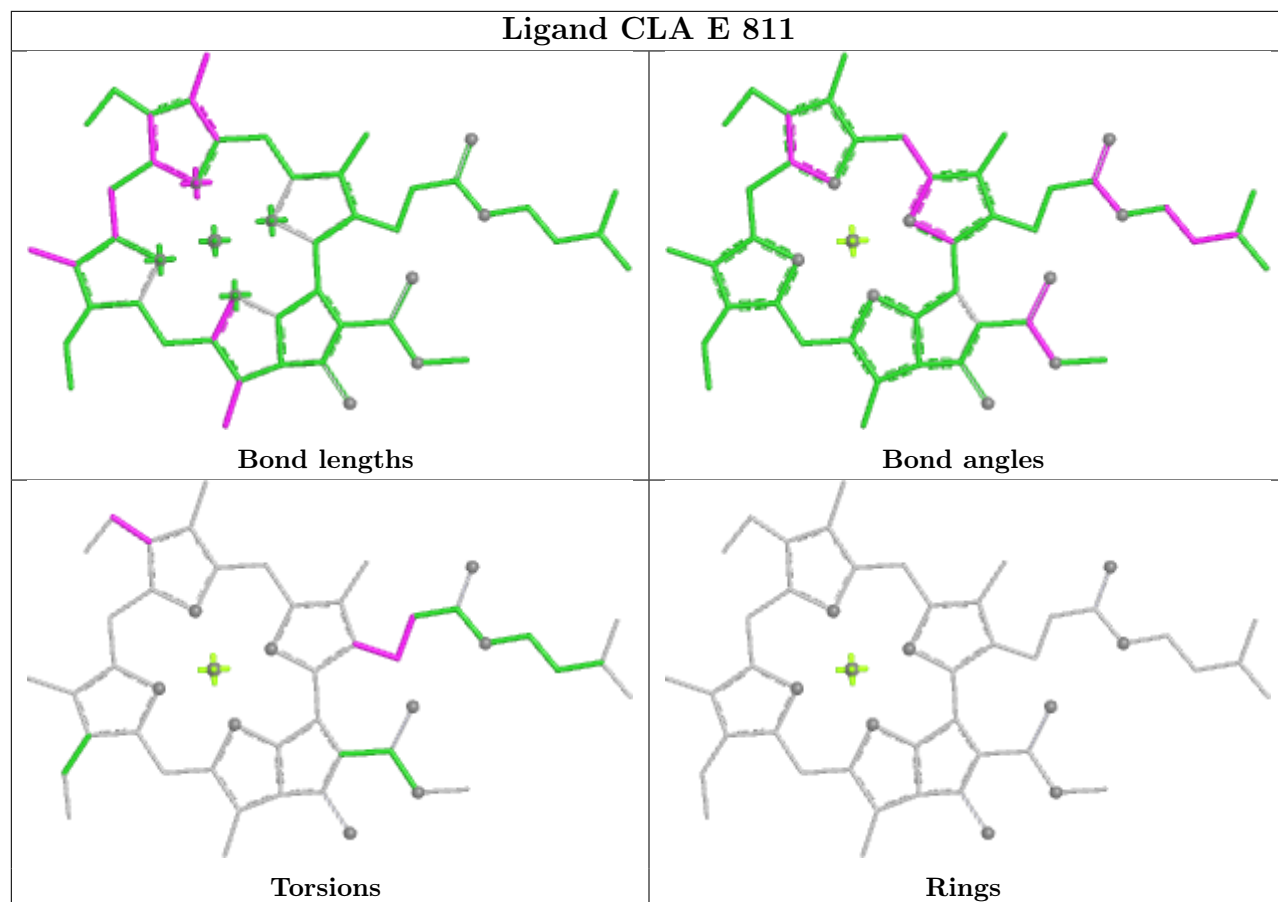


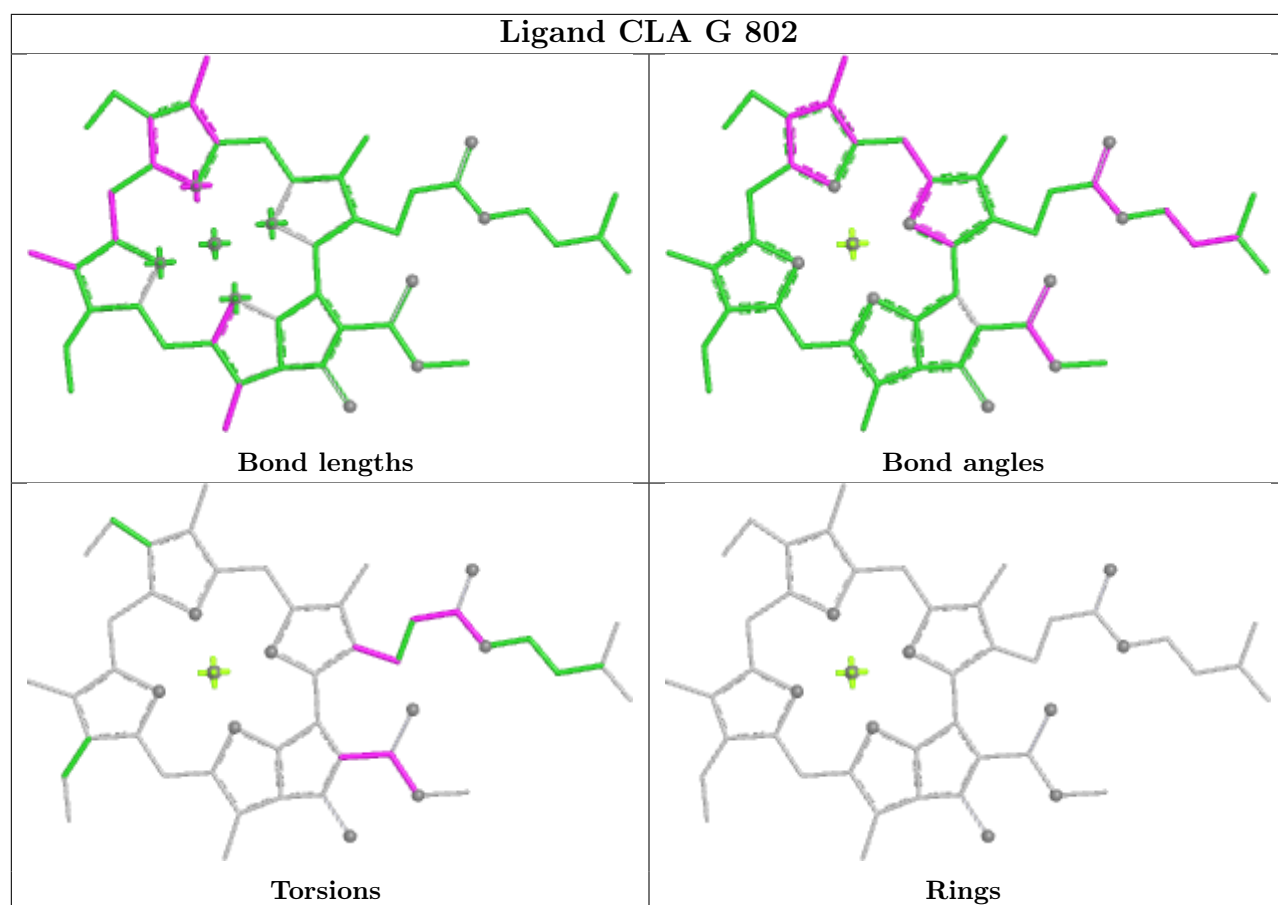
## Ligand CLA g 840



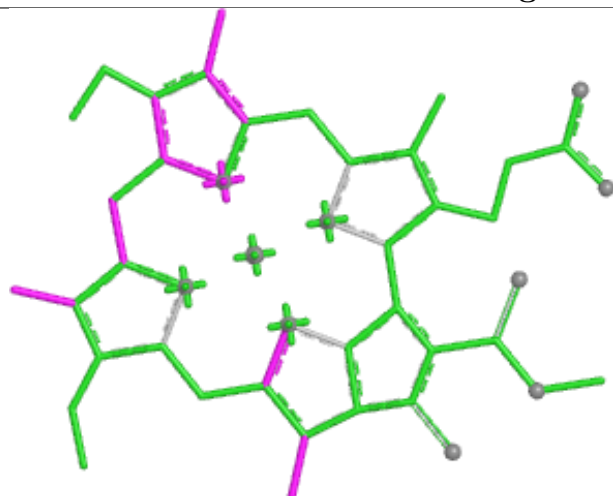


## Ligand CLA E 811

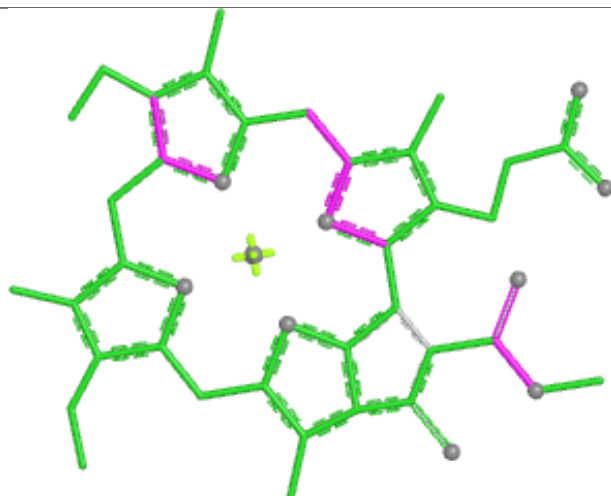




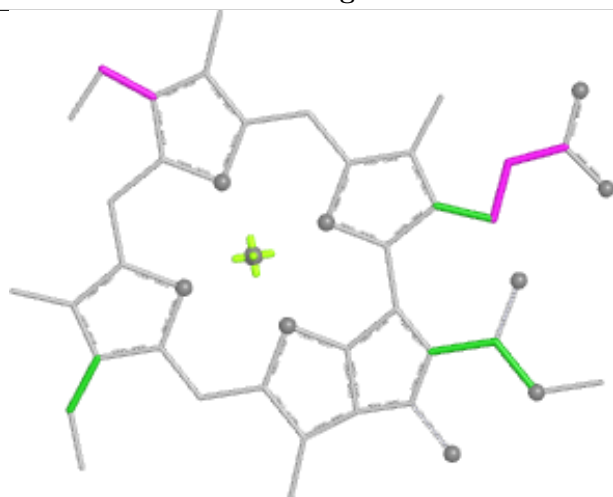
## Ligand CLA e 812



Bond lengths



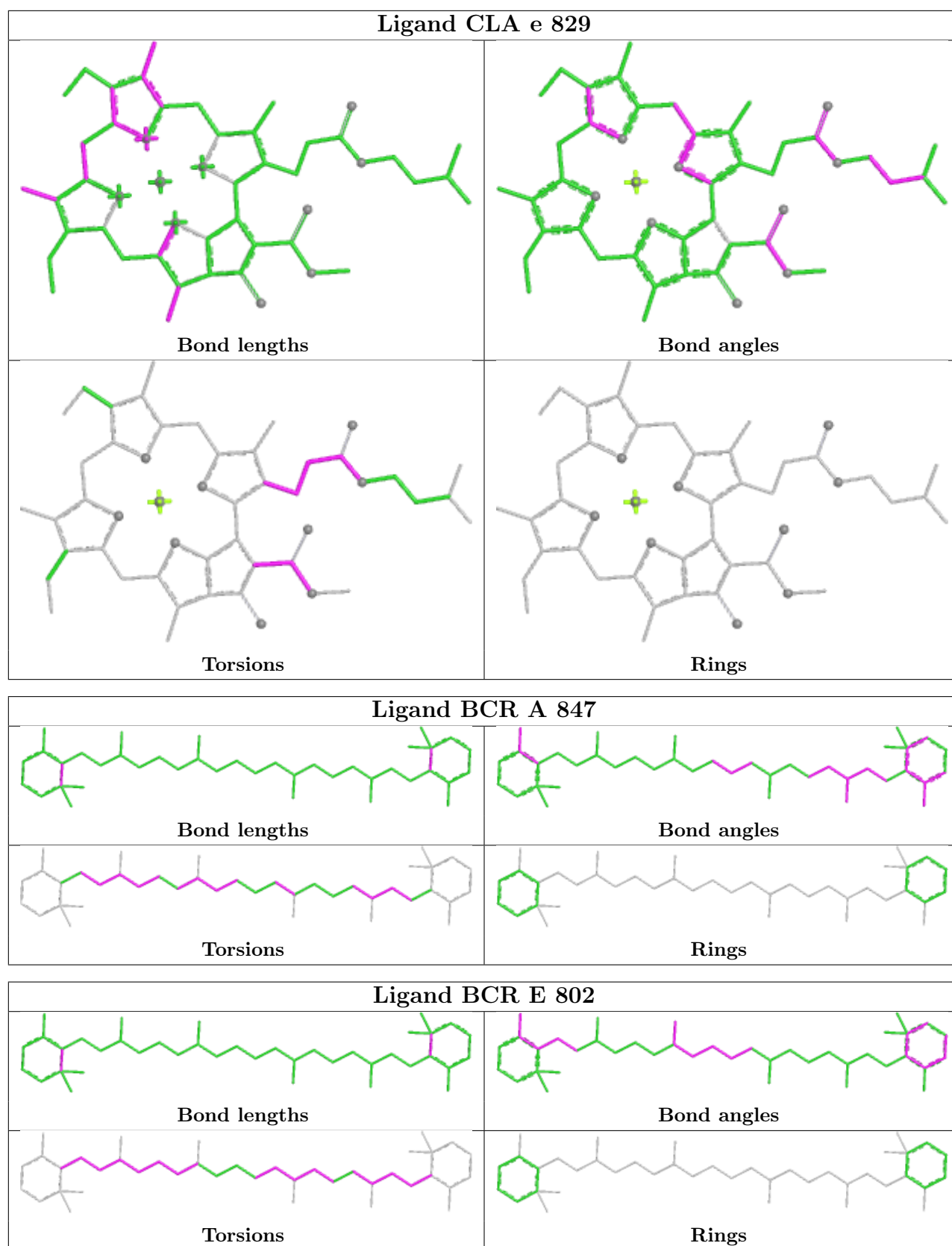
Bond angles

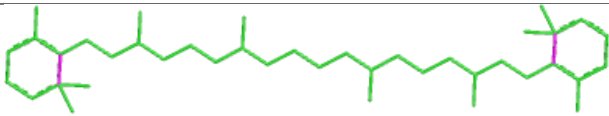
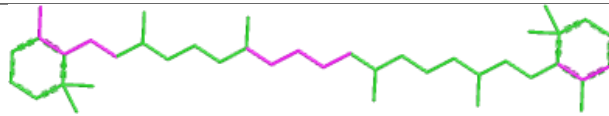
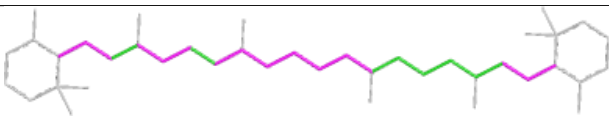
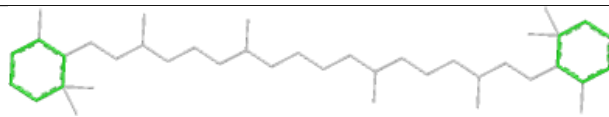


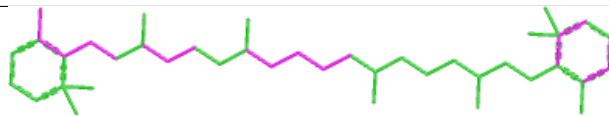
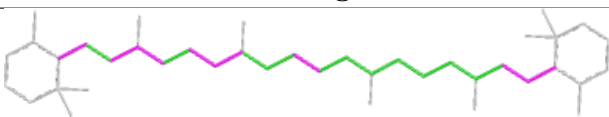
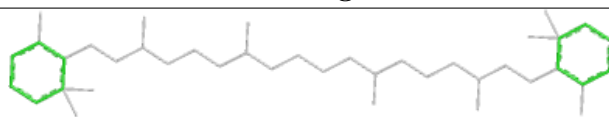
Torsions

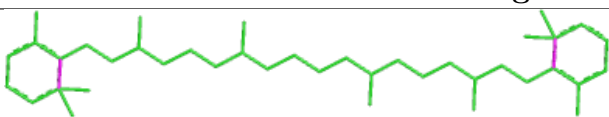
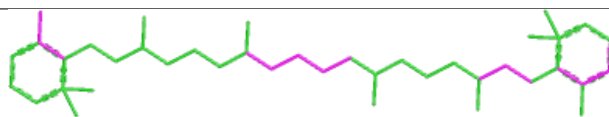
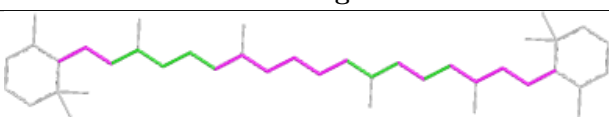
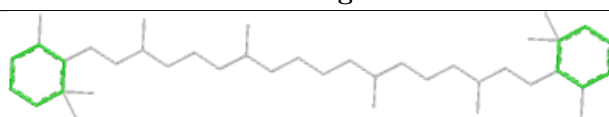


Rings

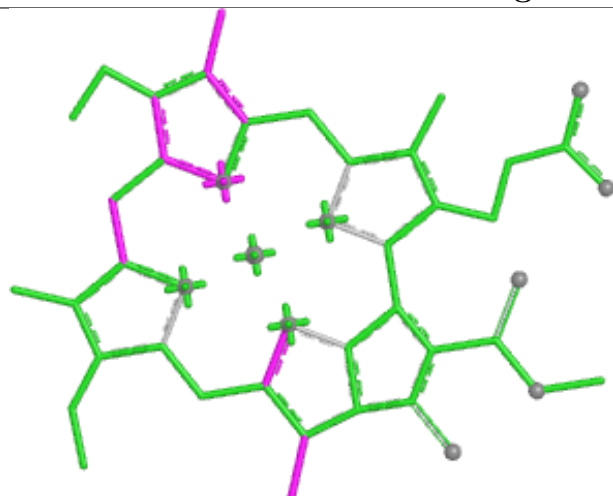


| Ligand BCR b 844                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

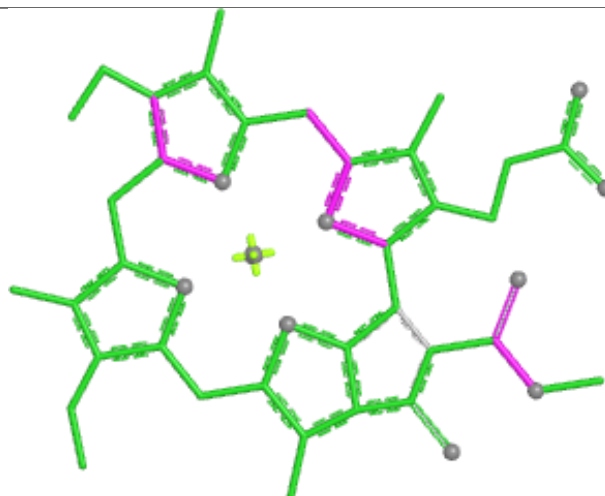
| Ligand BCR J 102                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR e 851                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

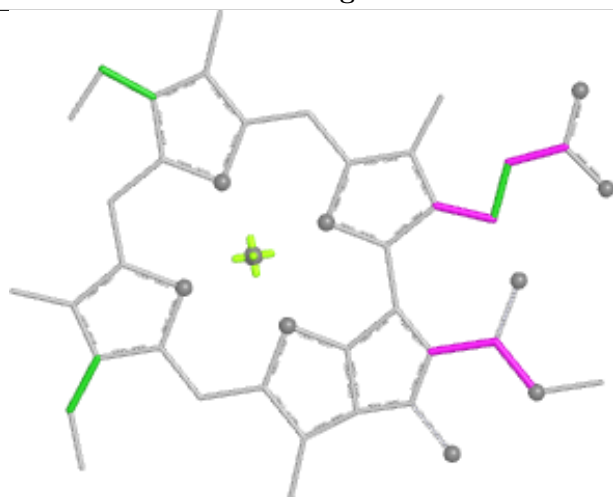
## Ligand CLA B 836



Bond lengths



Bond angles



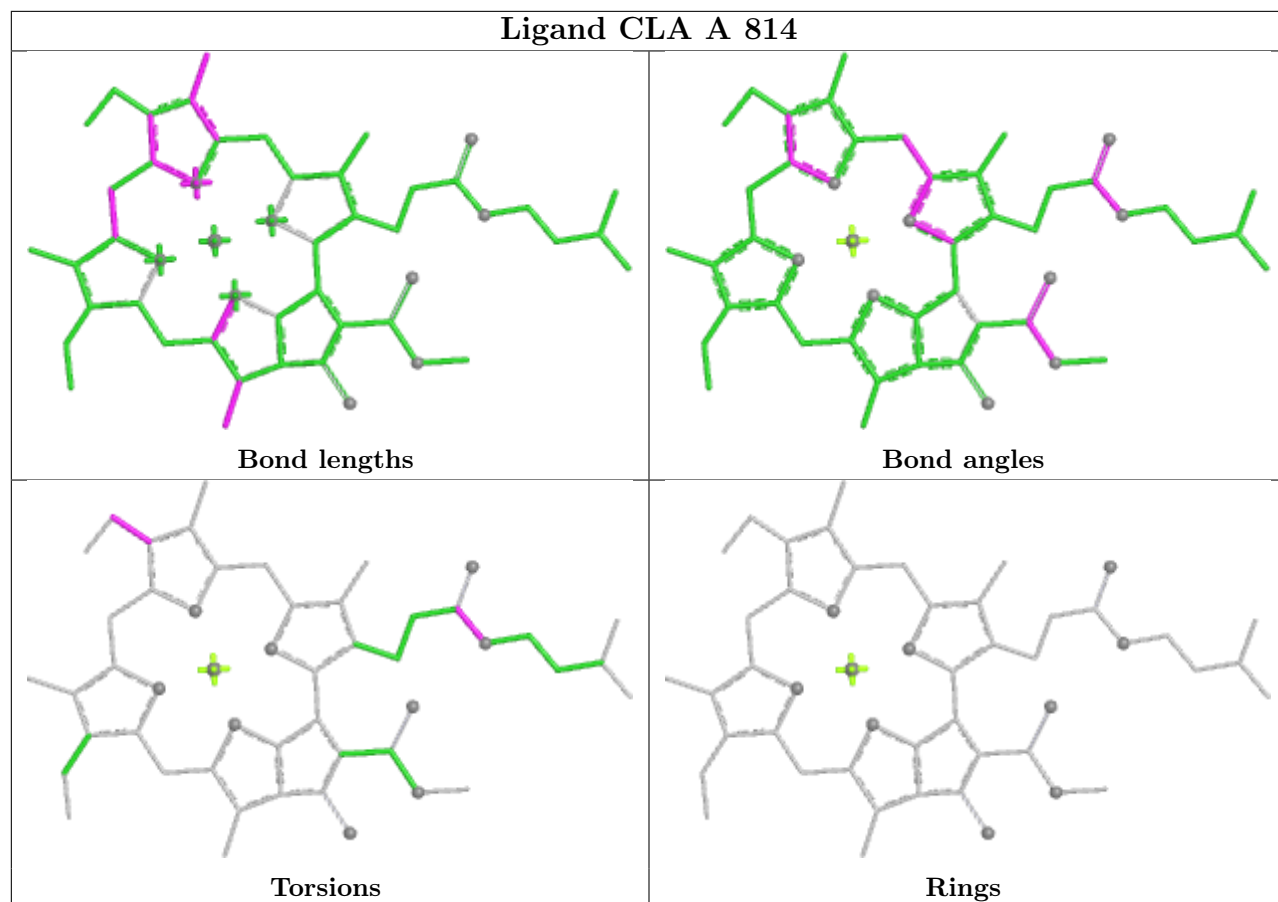
Torsions



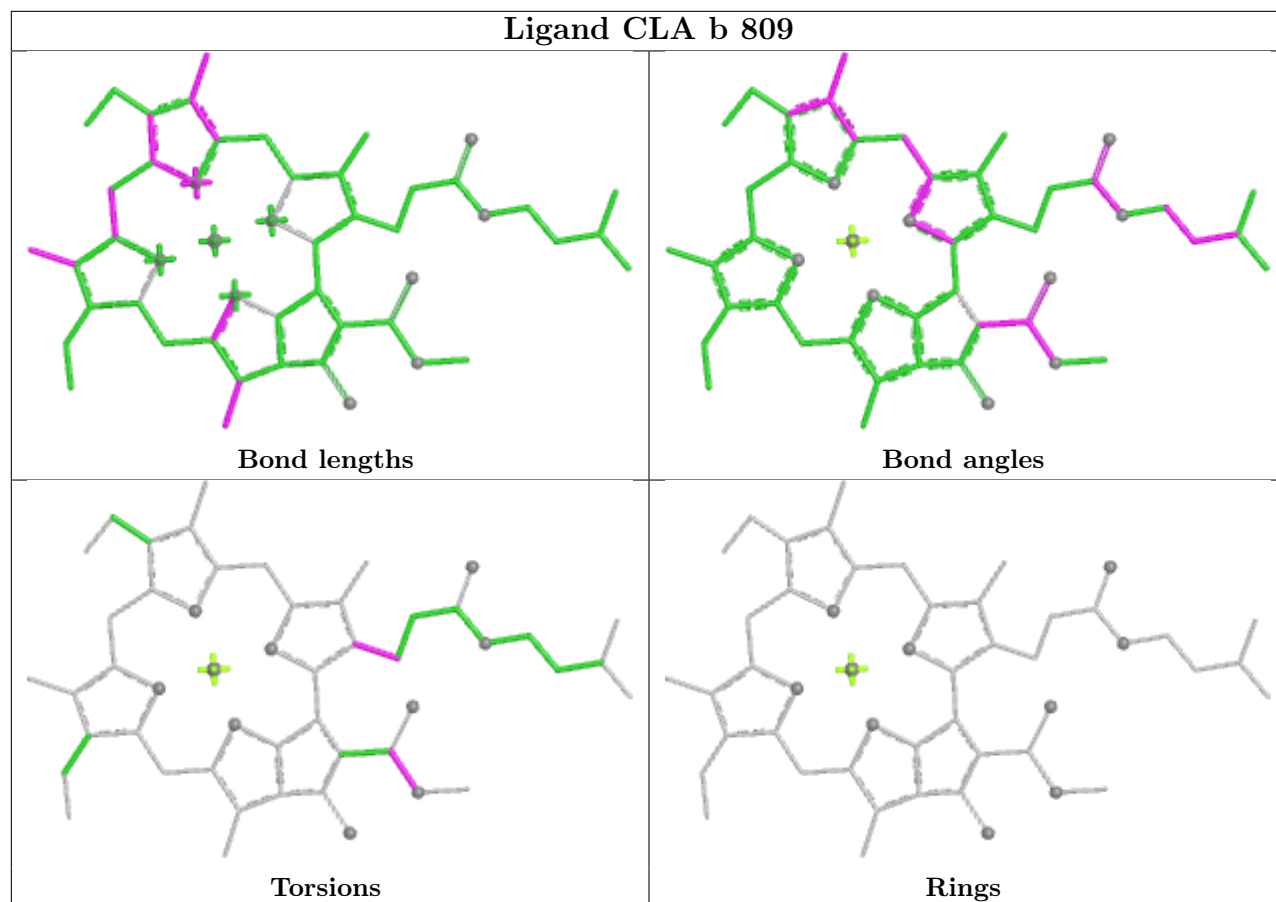
Rings



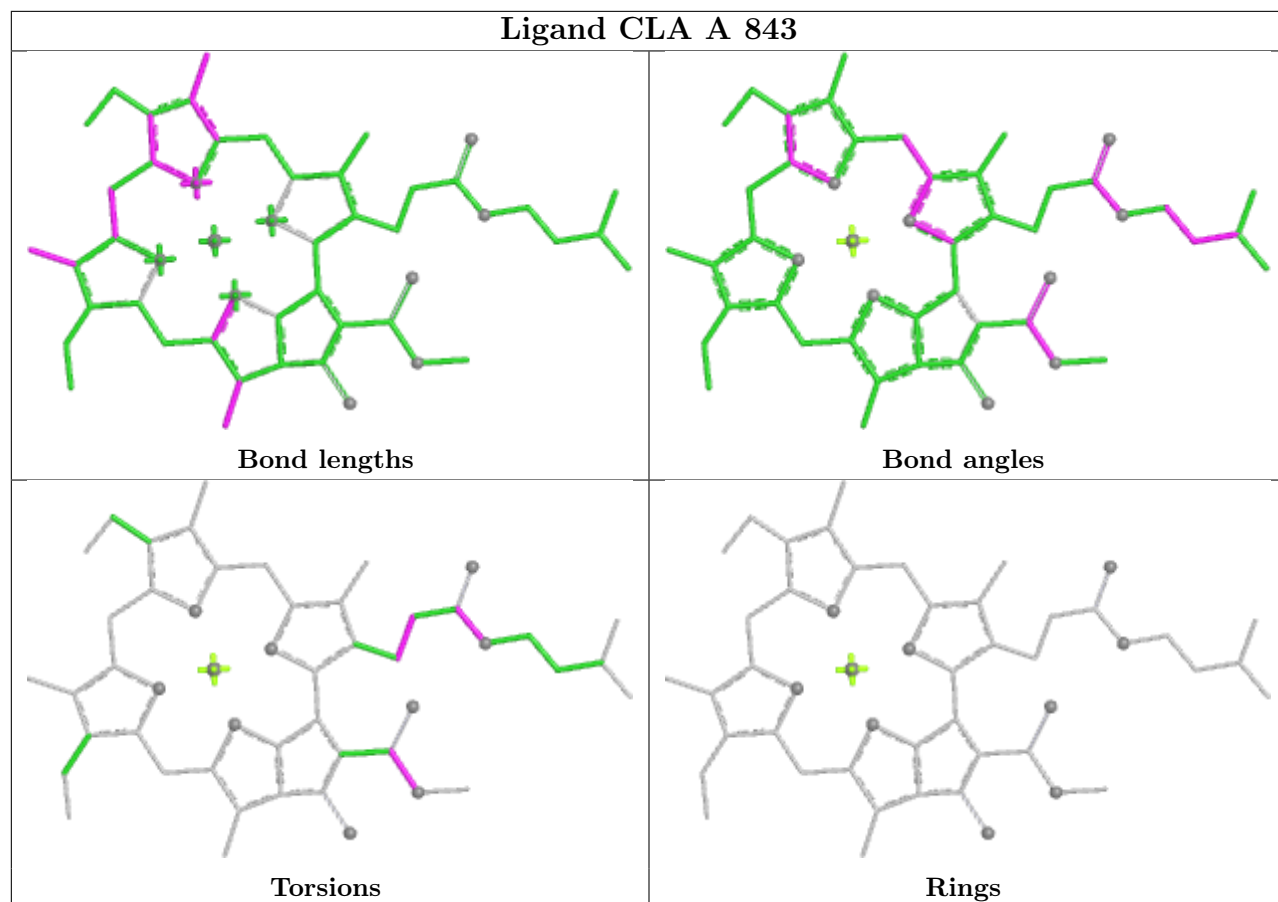
## Ligand CLA A 814



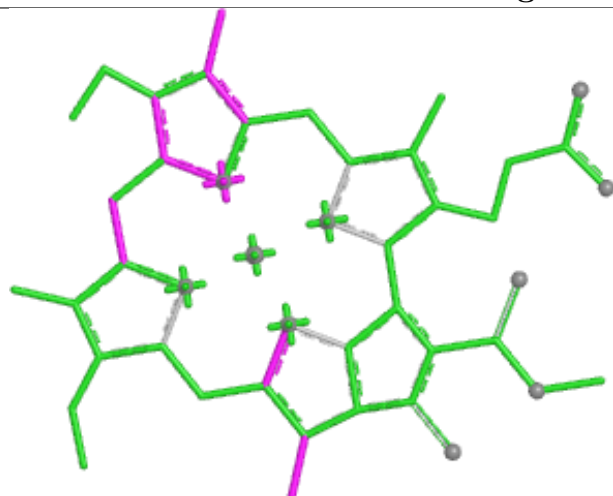
## Ligand CLA b 809



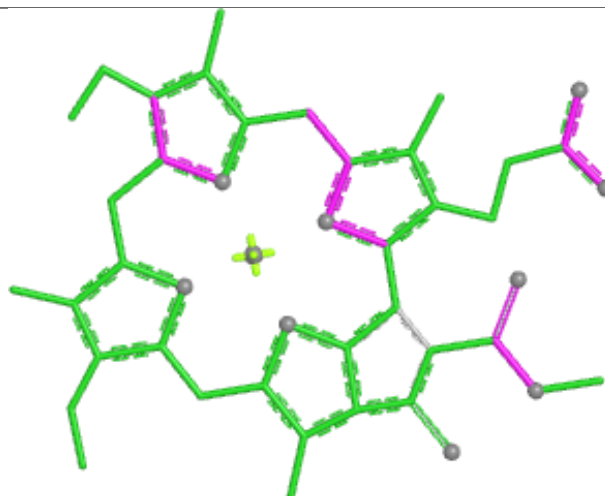
## Ligand CLA A 843



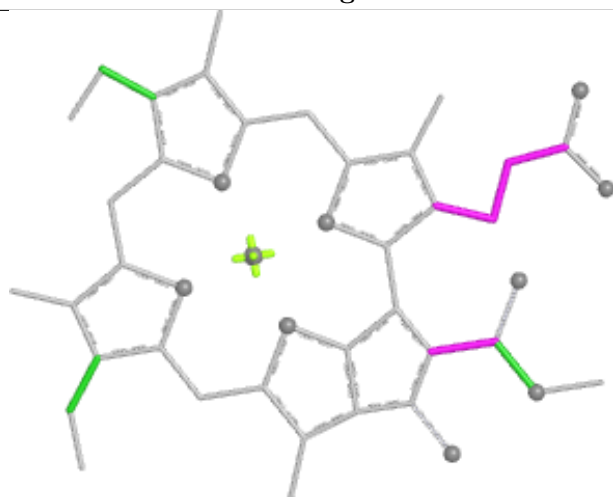
## Ligand CLA b 834



Bond lengths



Bond angles

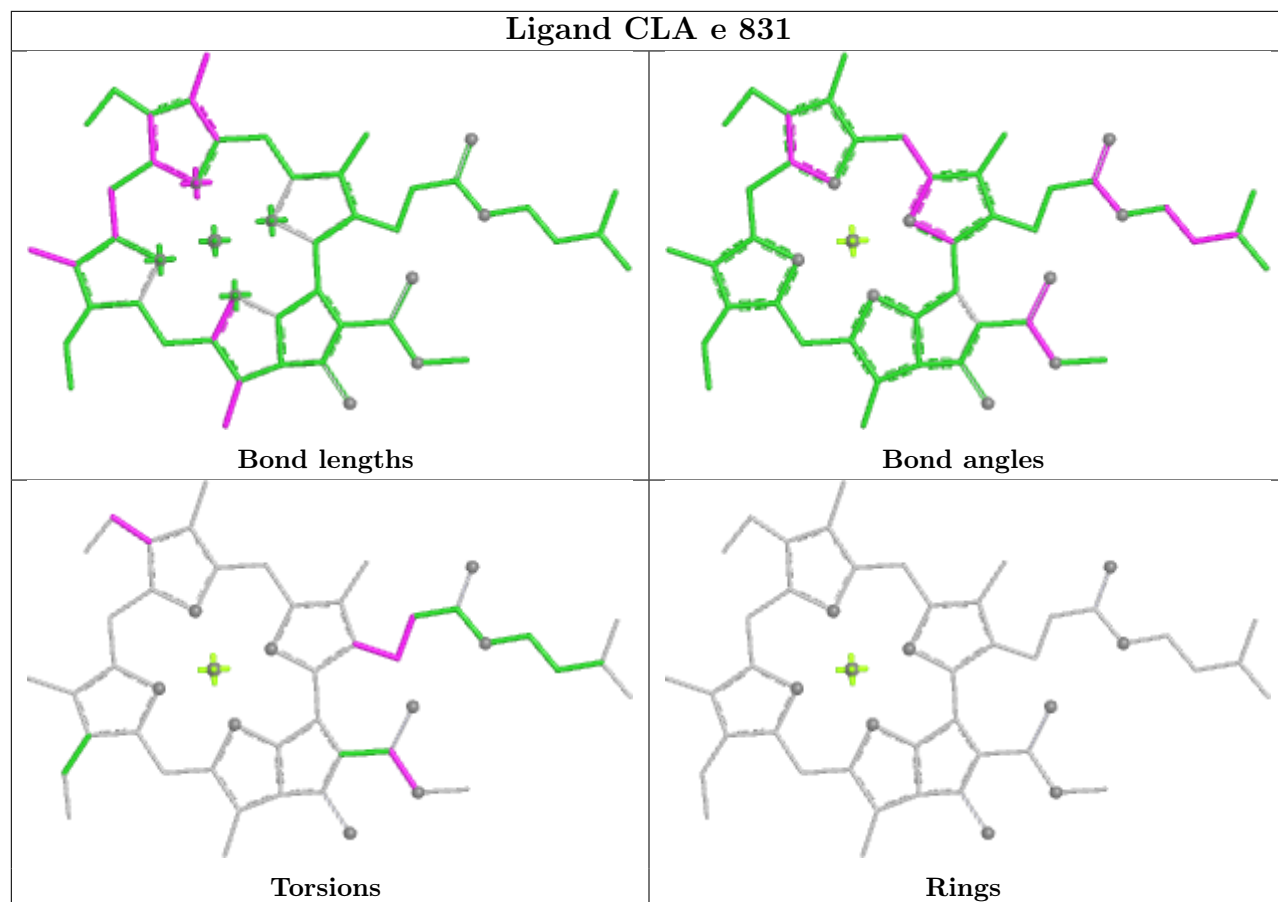


Torsions

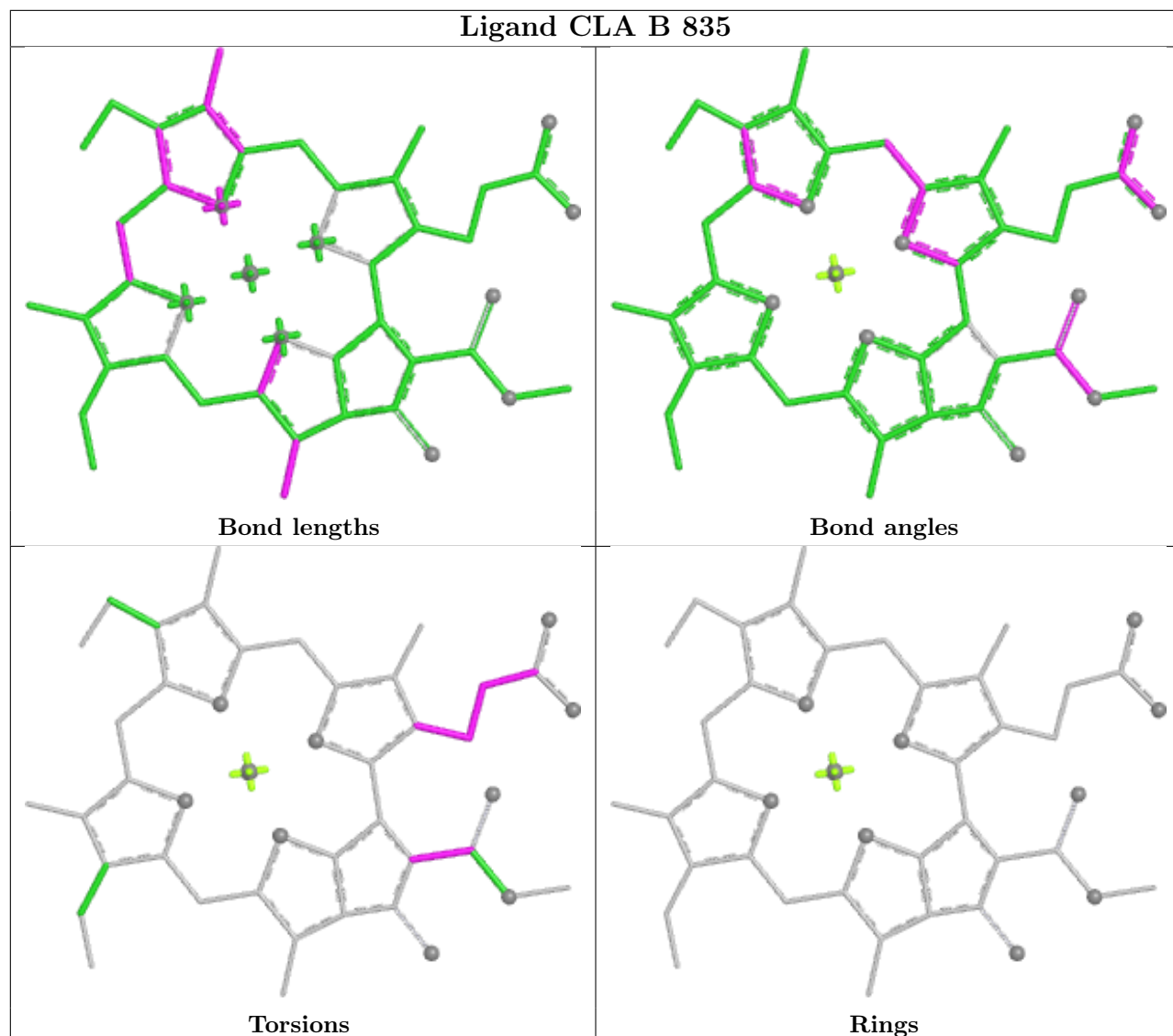


Rings

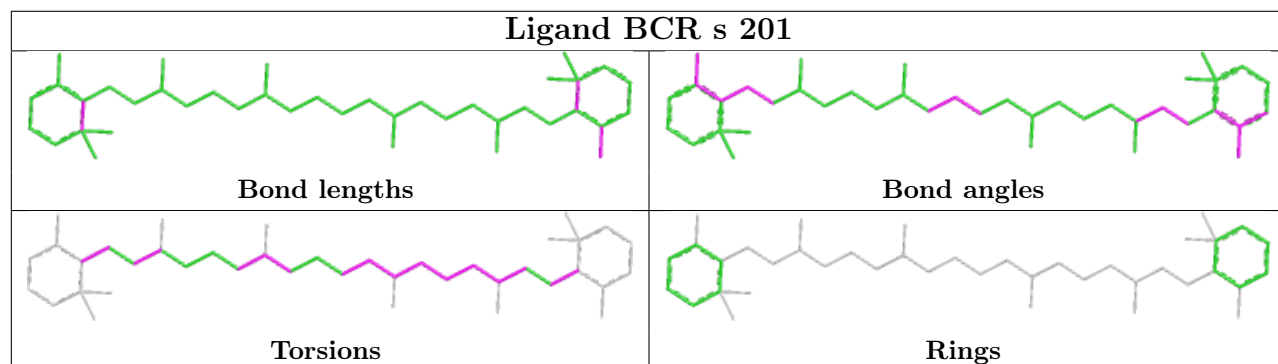
## Ligand CLA e 831



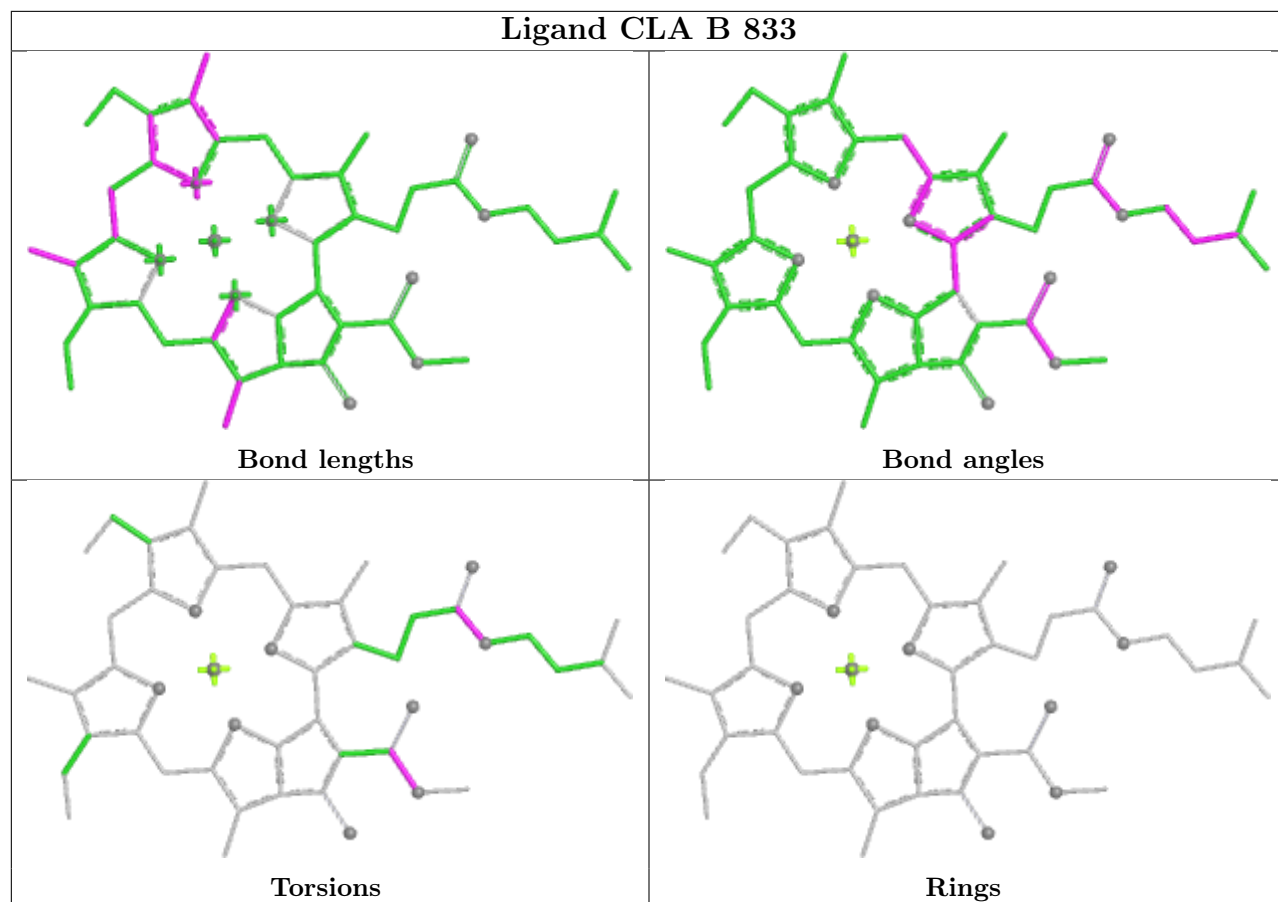
## Ligand CLA B 835



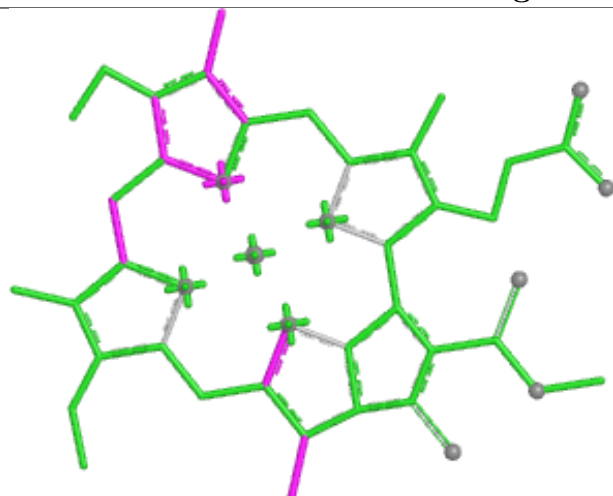
## Ligand BCR s 201



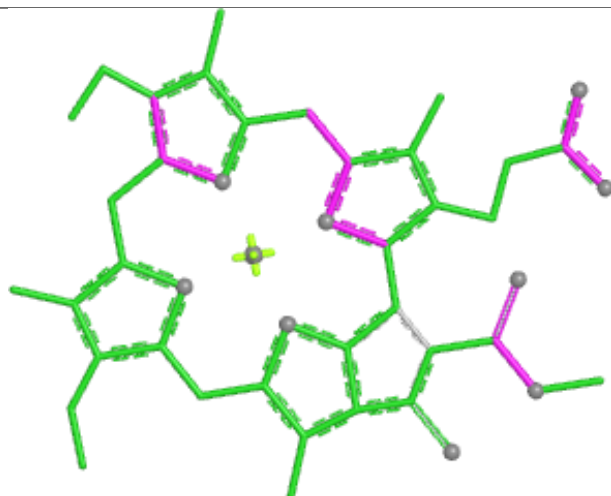
## Ligand CLA B 833



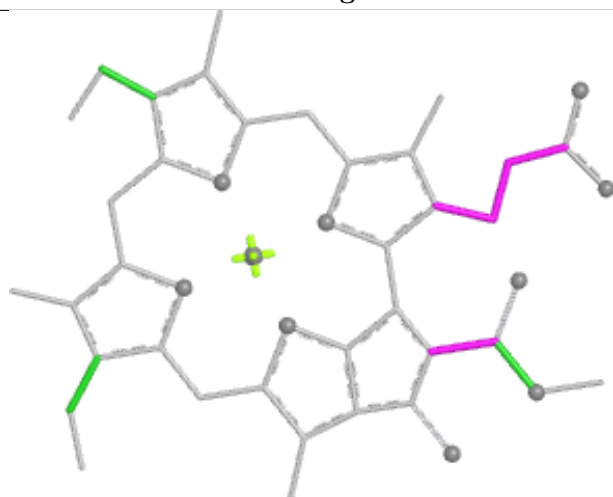
## Ligand CLA G 835



Bond lengths



Bond angles



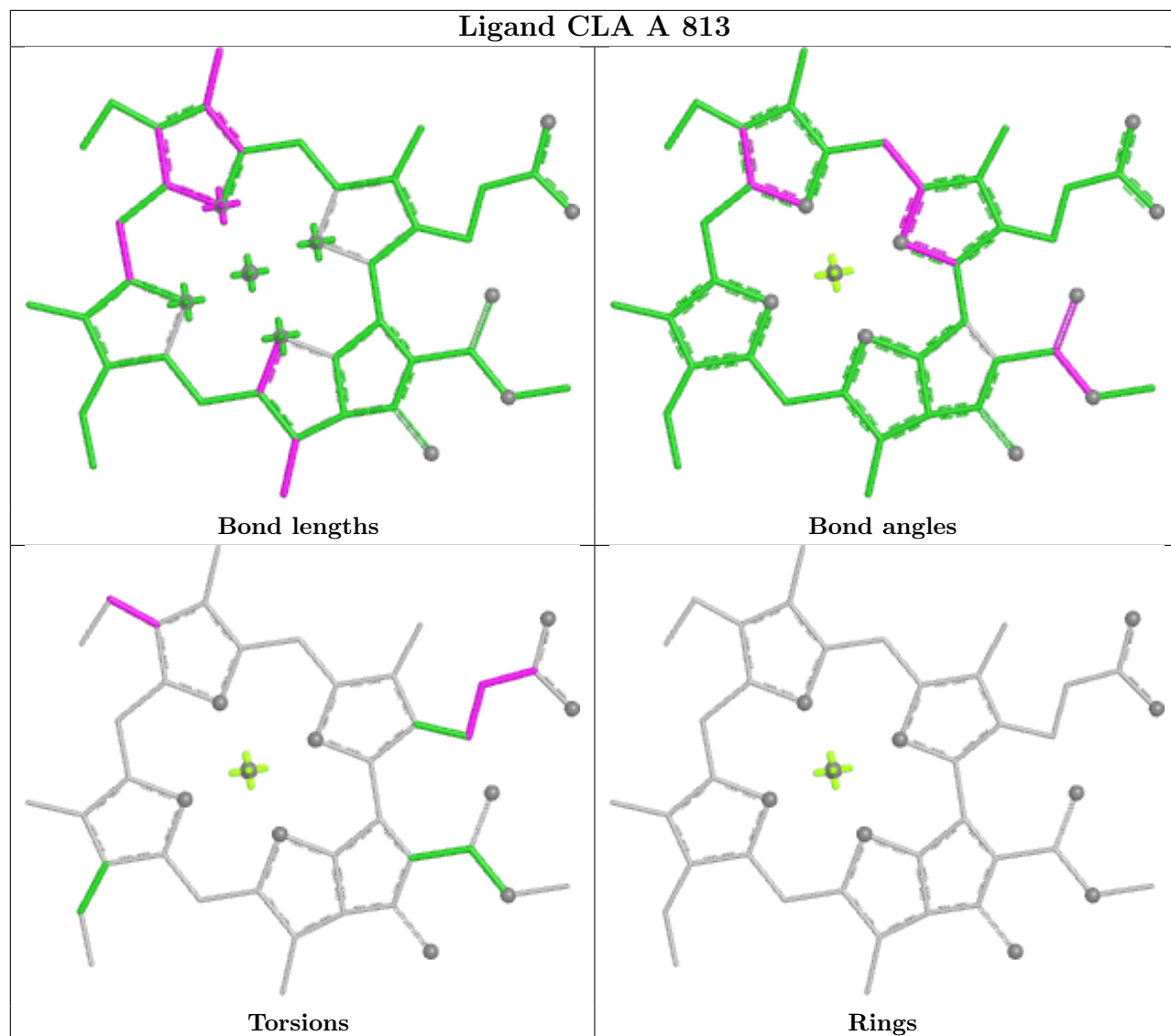
Torsions



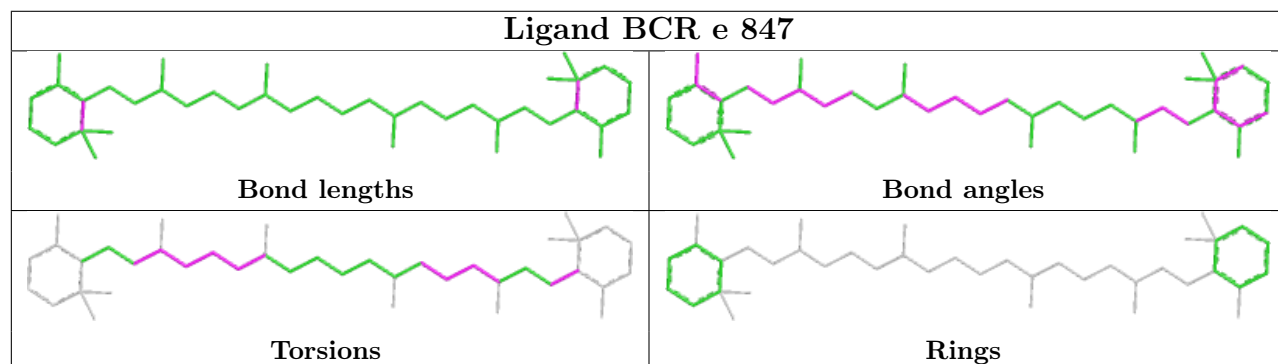
Rings



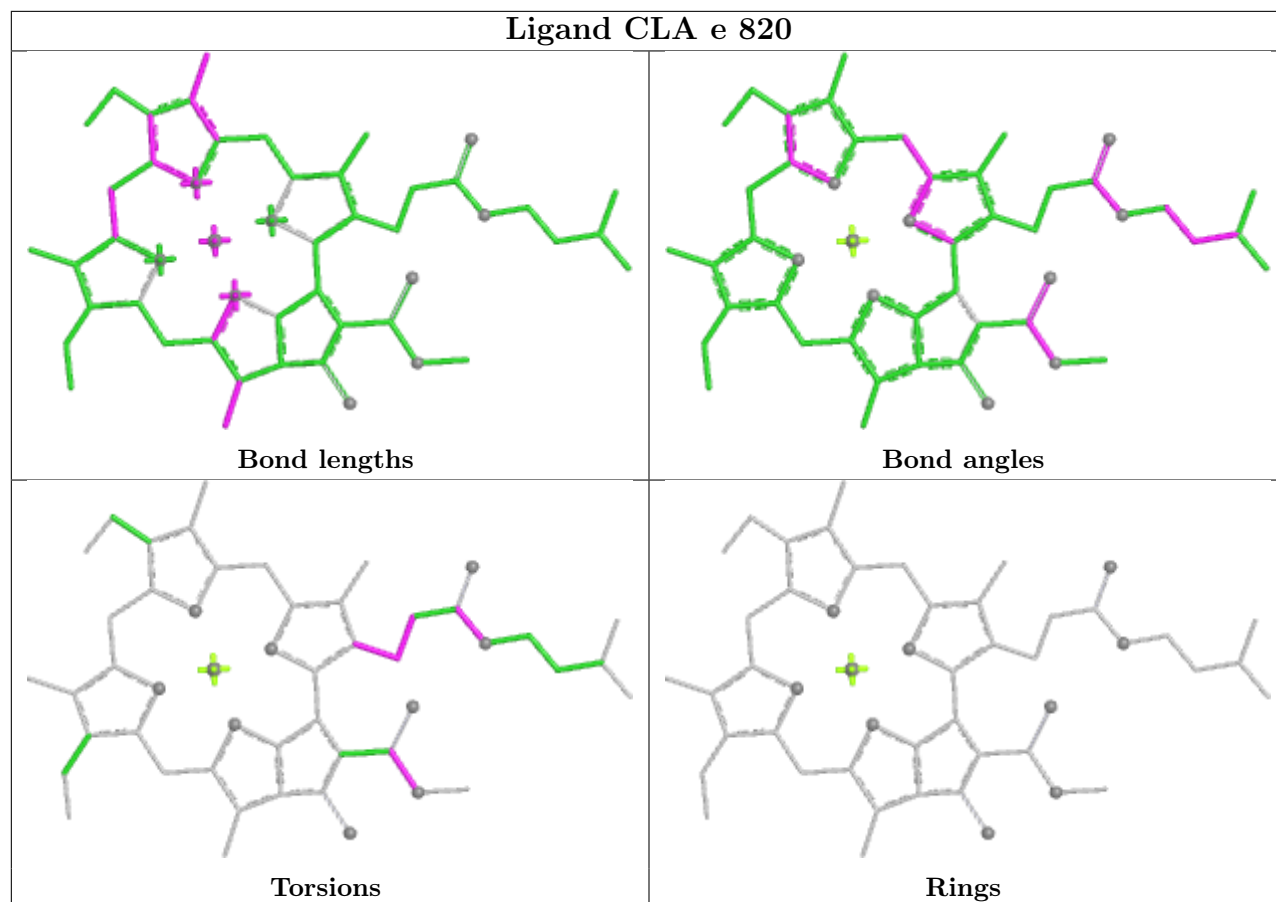
## Ligand CLA A 813



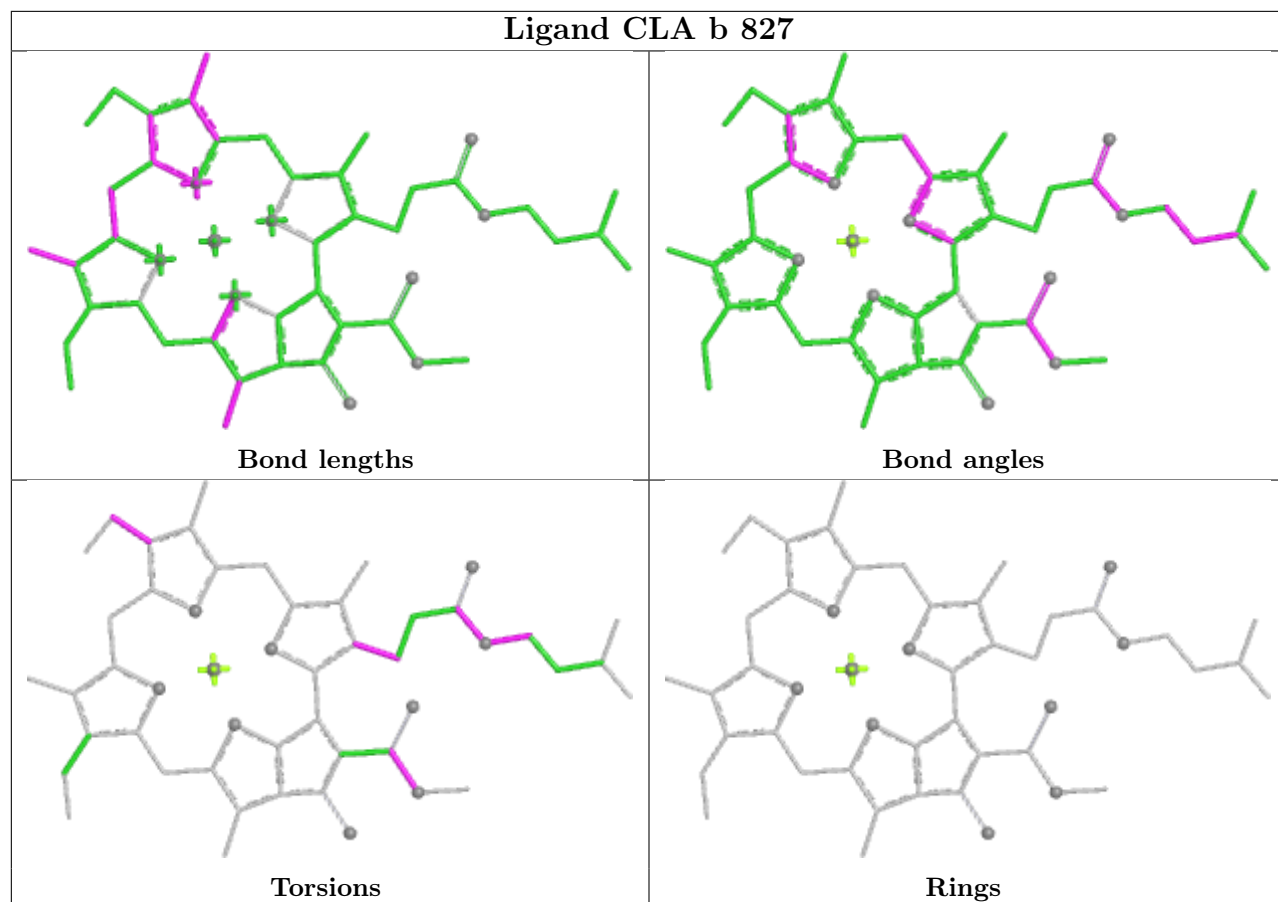
## Ligand BCR e 847

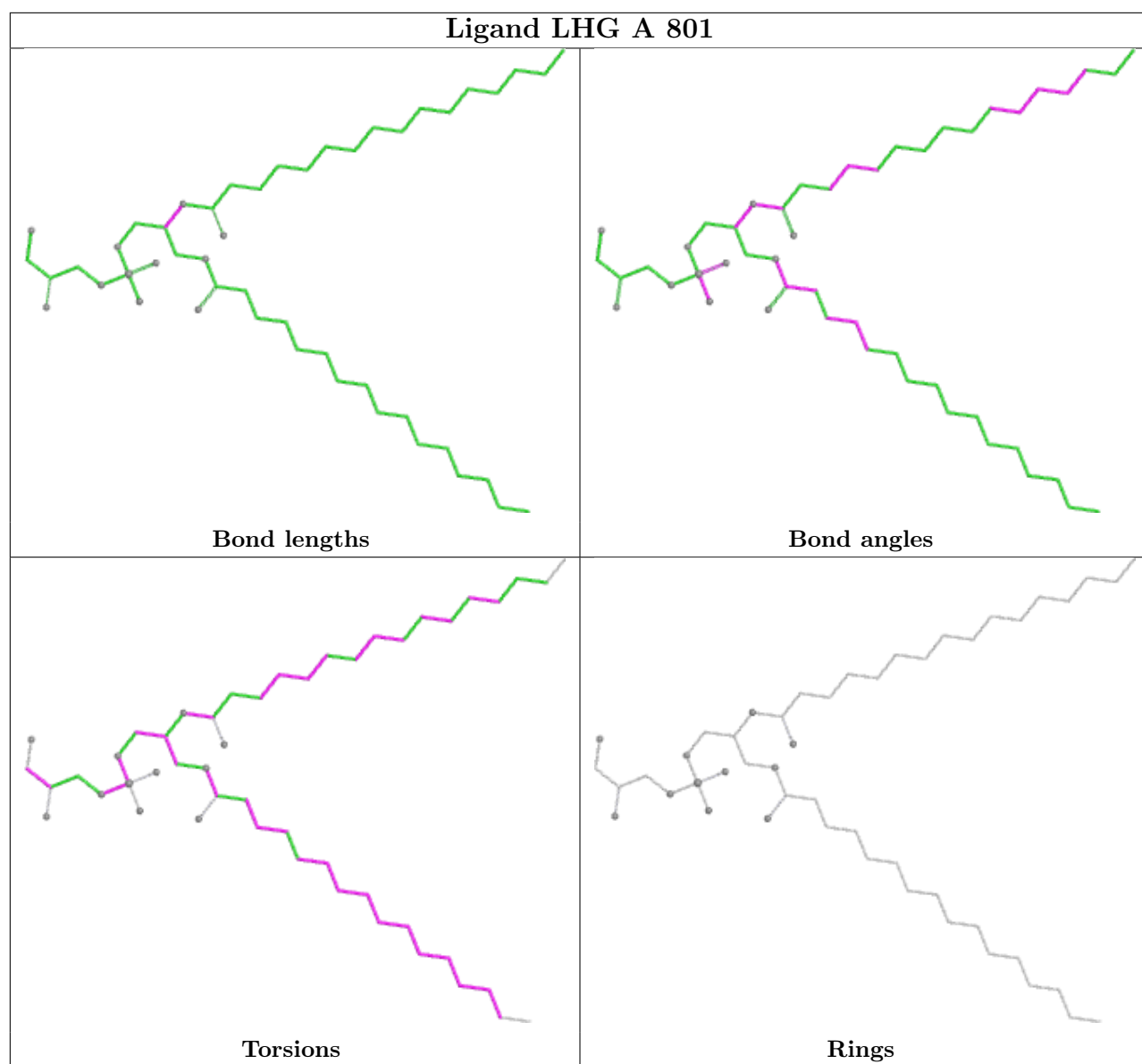


## Ligand CLA e 820

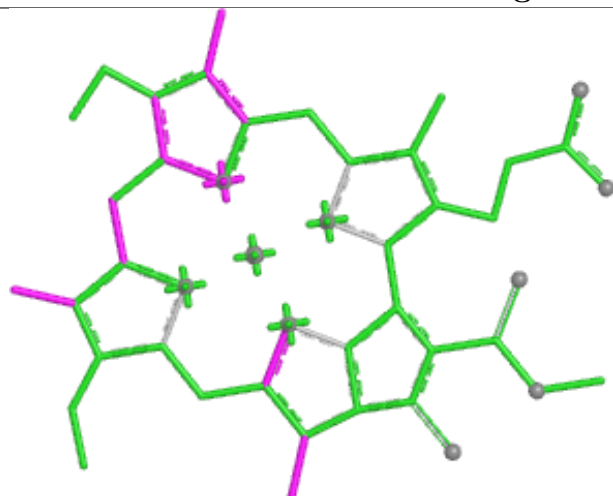


## Ligand CLA b 827

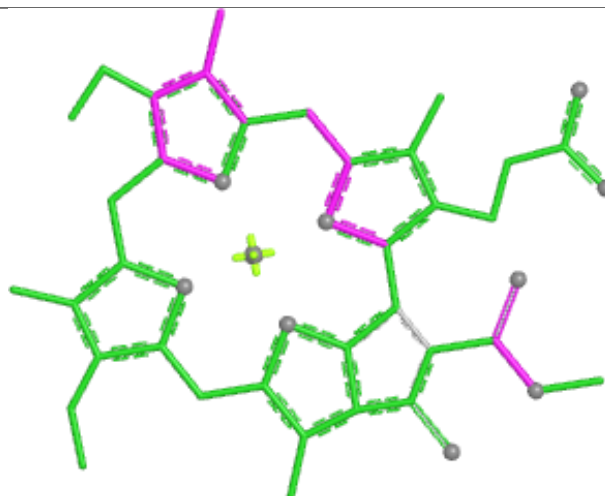




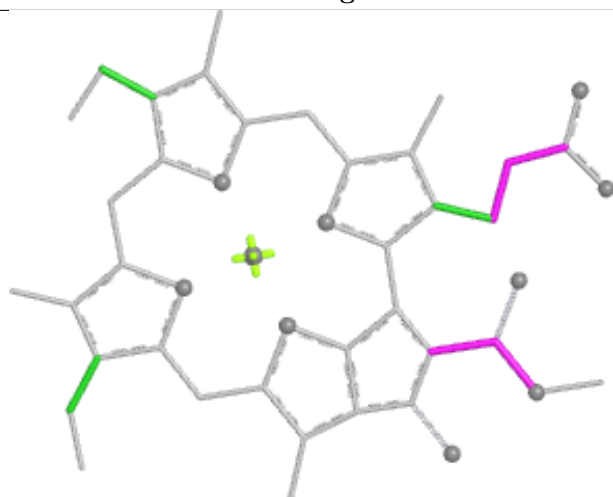
## Ligand CLA O 203



Bond lengths



Bond angles

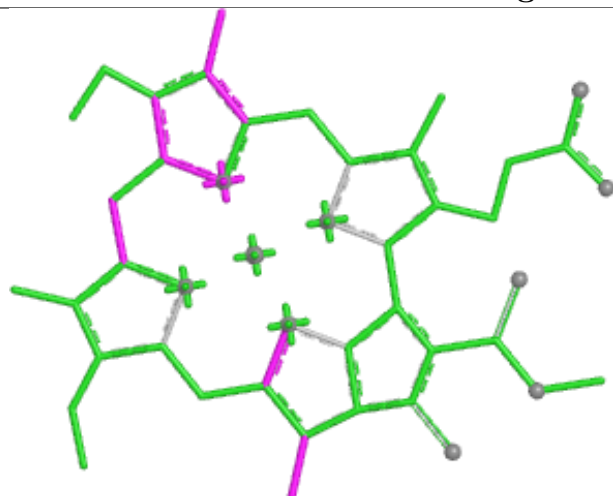


Torsions

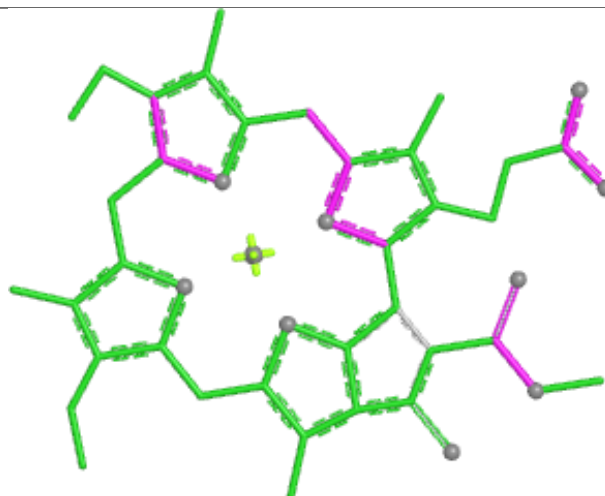


Rings

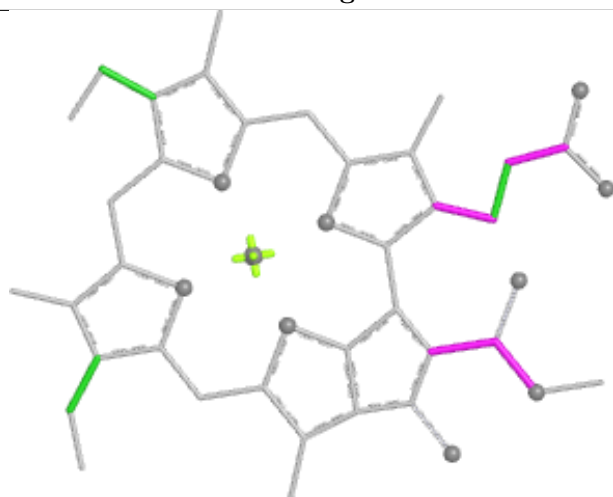
## Ligand CLA b 835



Bond lengths



Bond angles

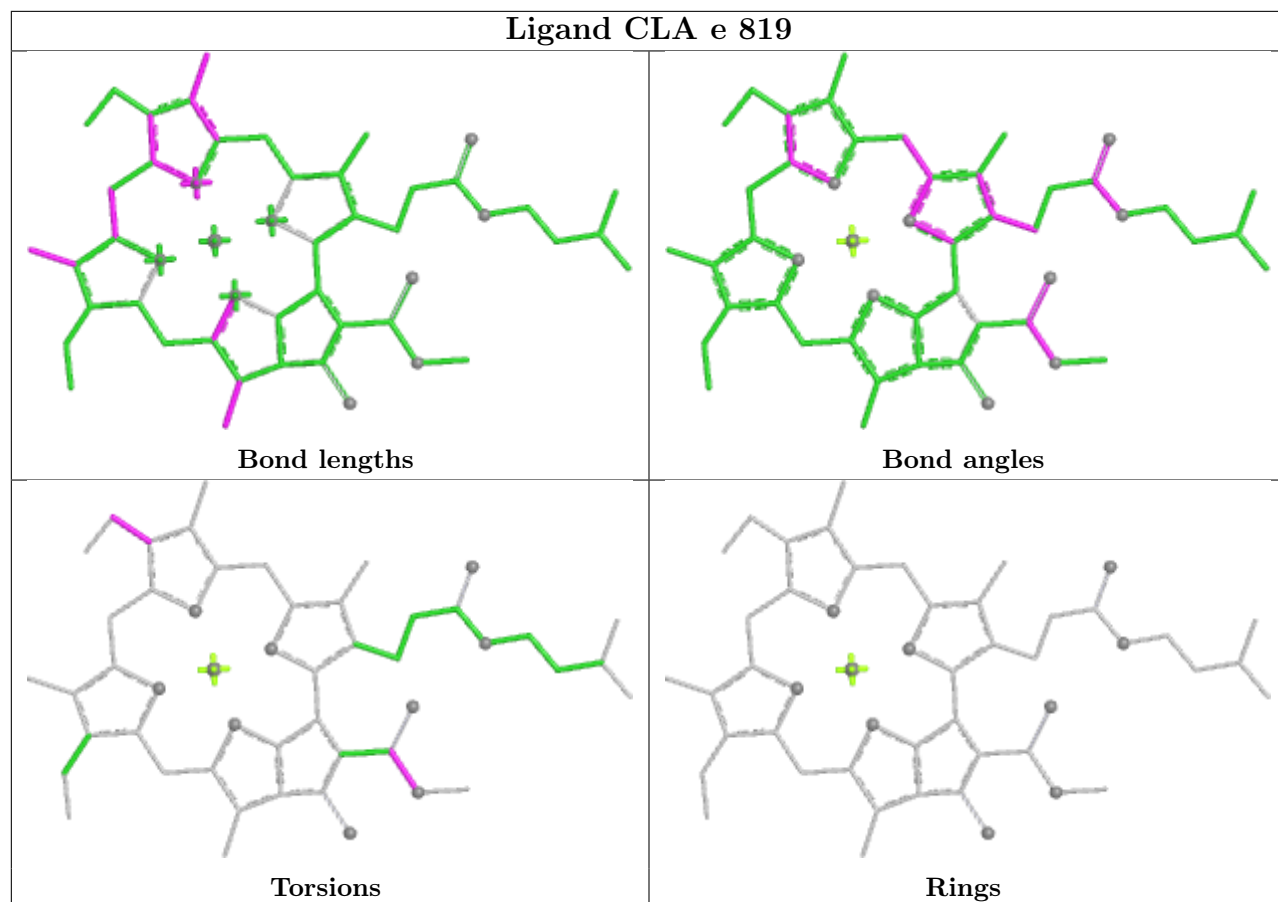


Torsions

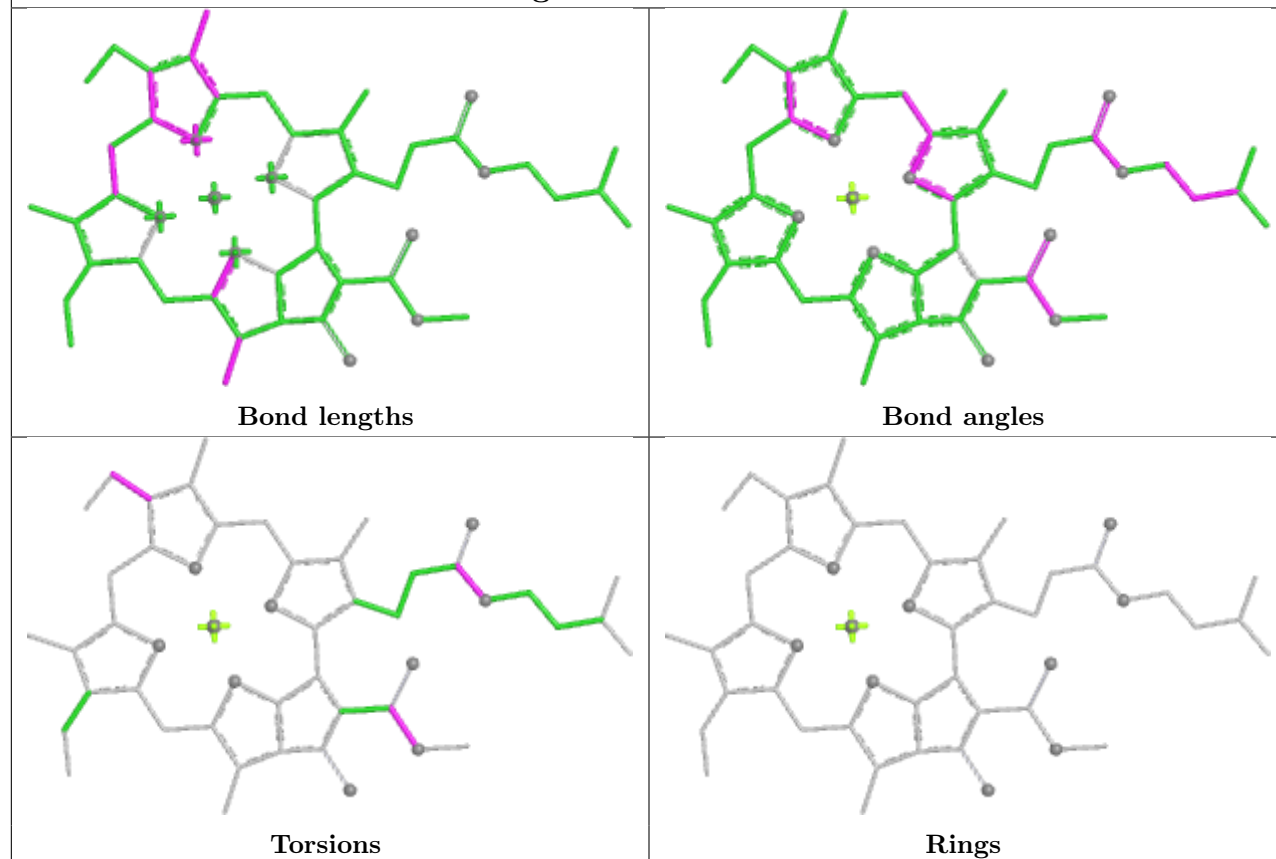


Rings

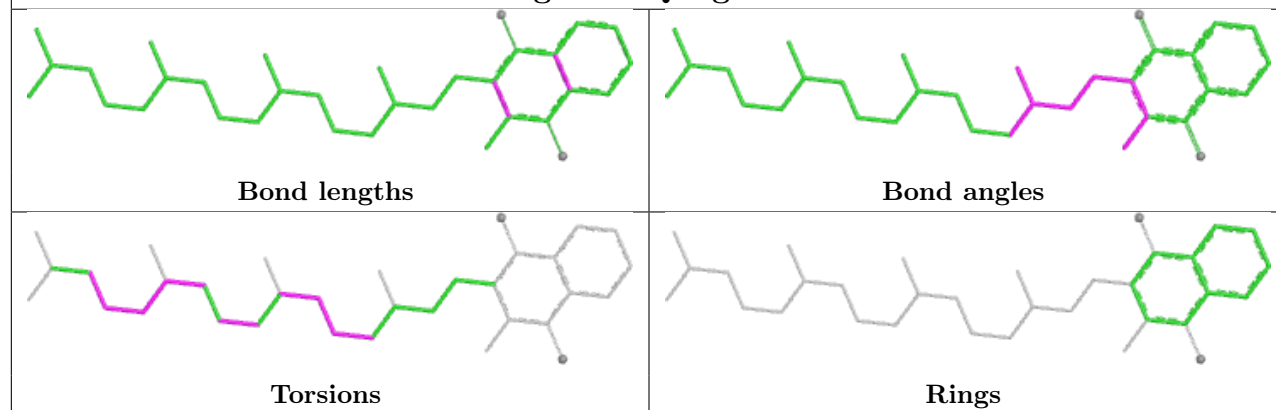
## Ligand CLA e 819



## Ligand CLA B 817

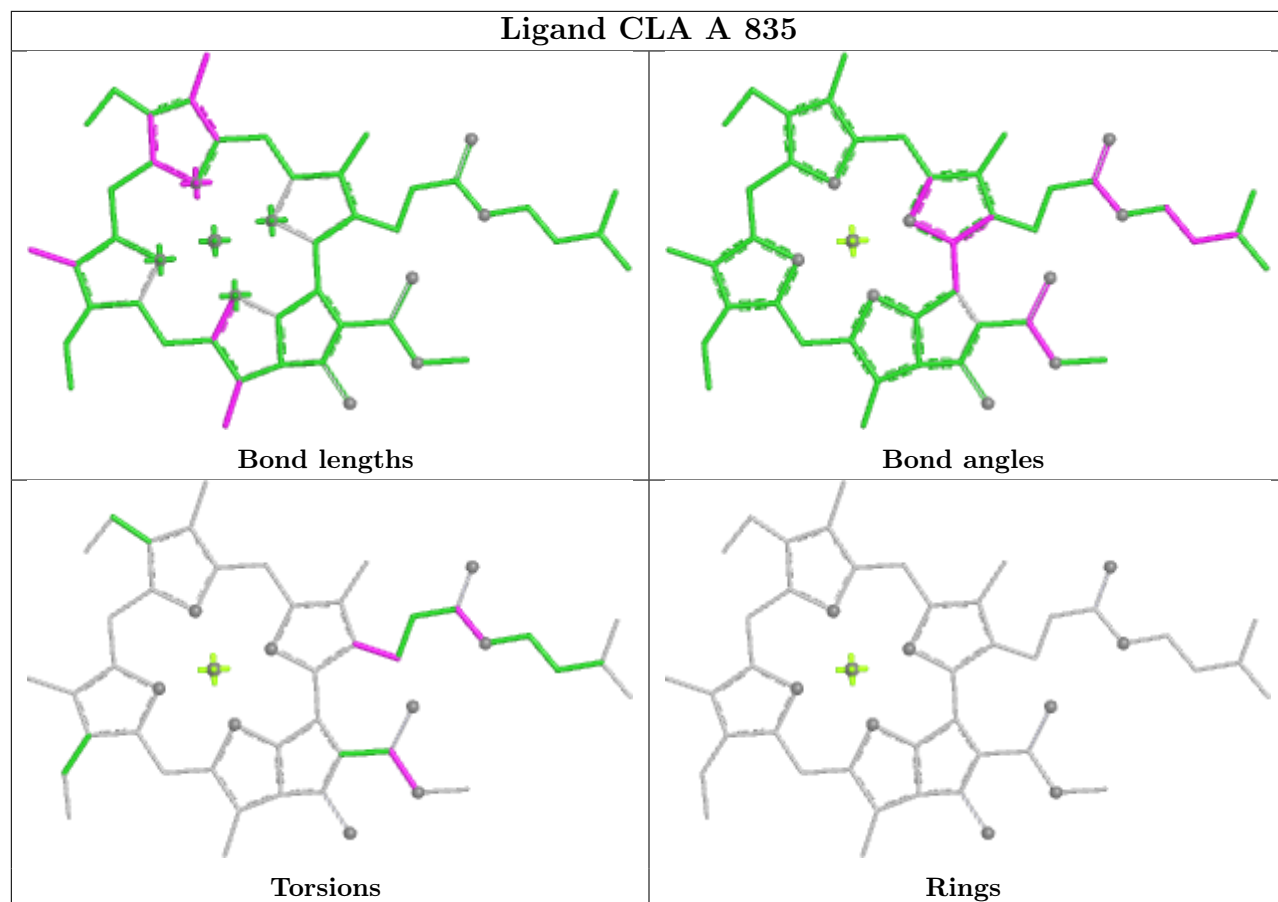


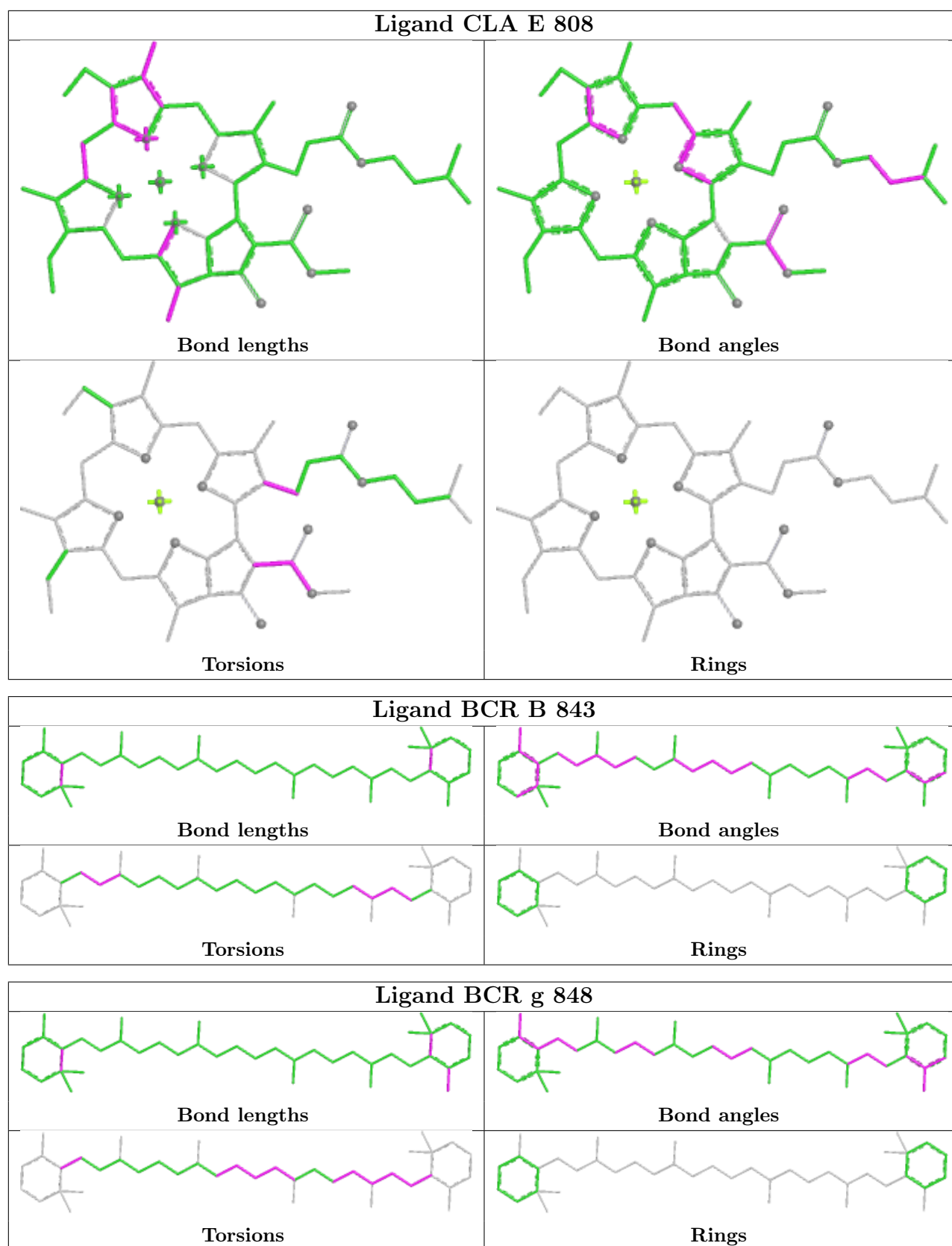
## Ligand PQN g 843

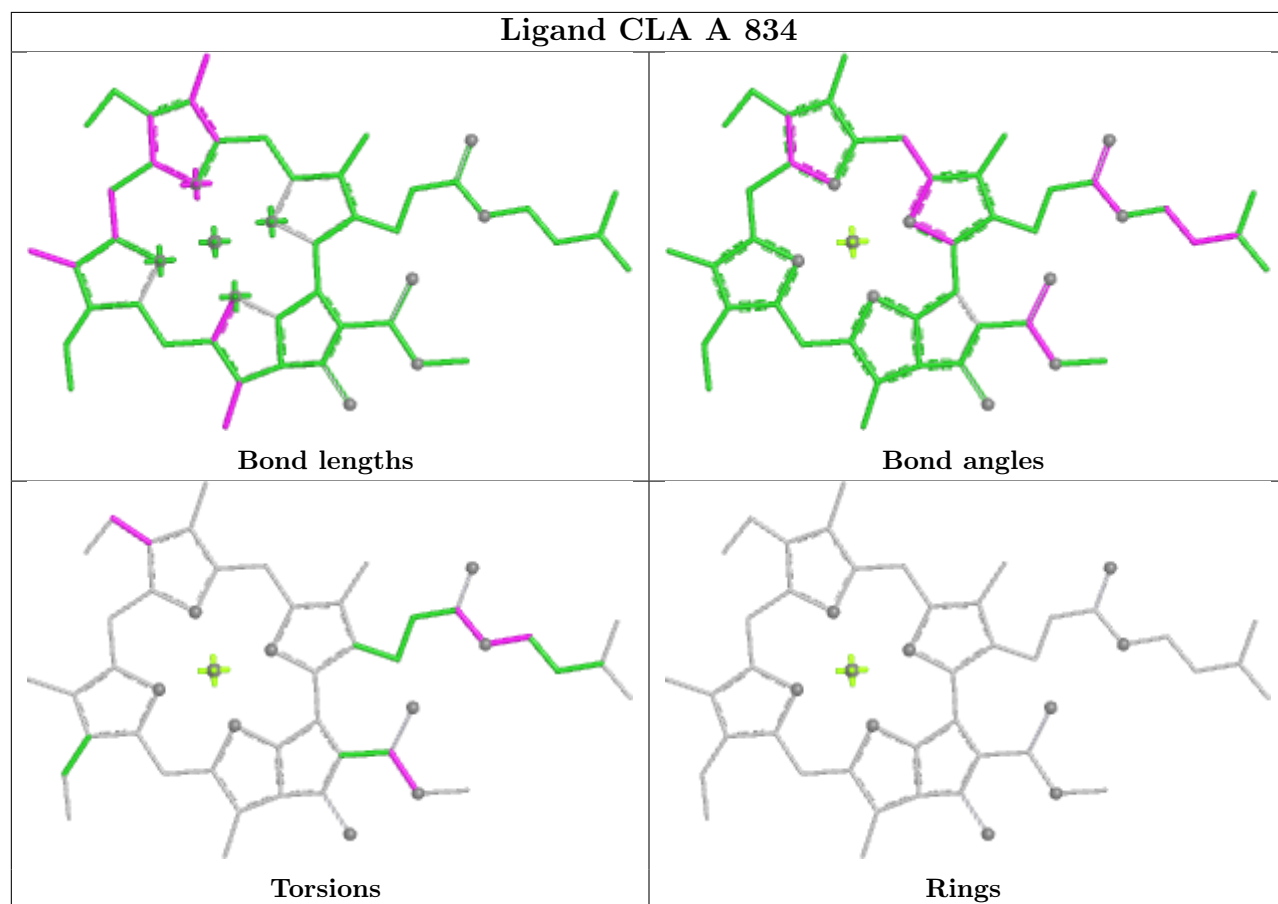
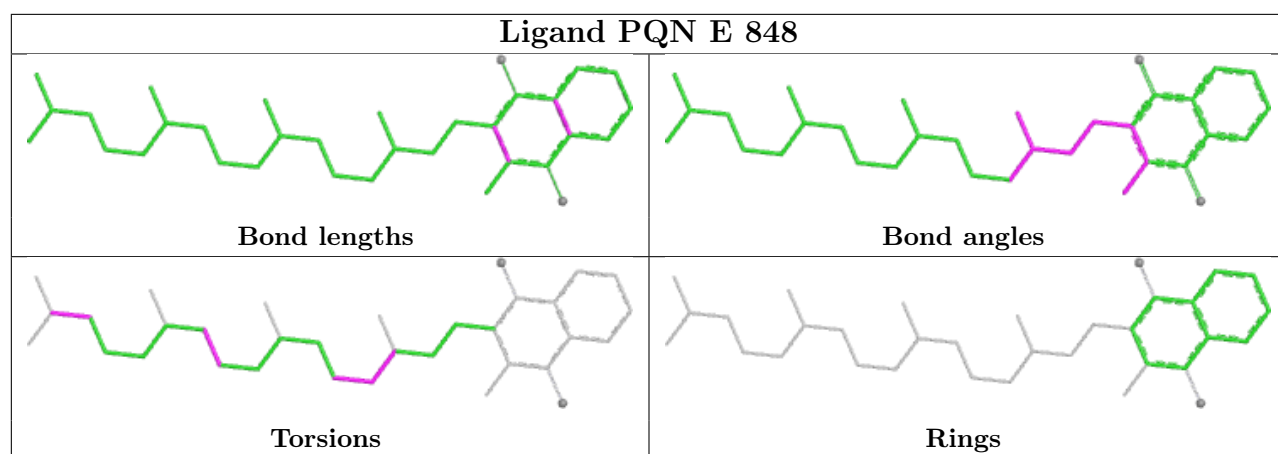




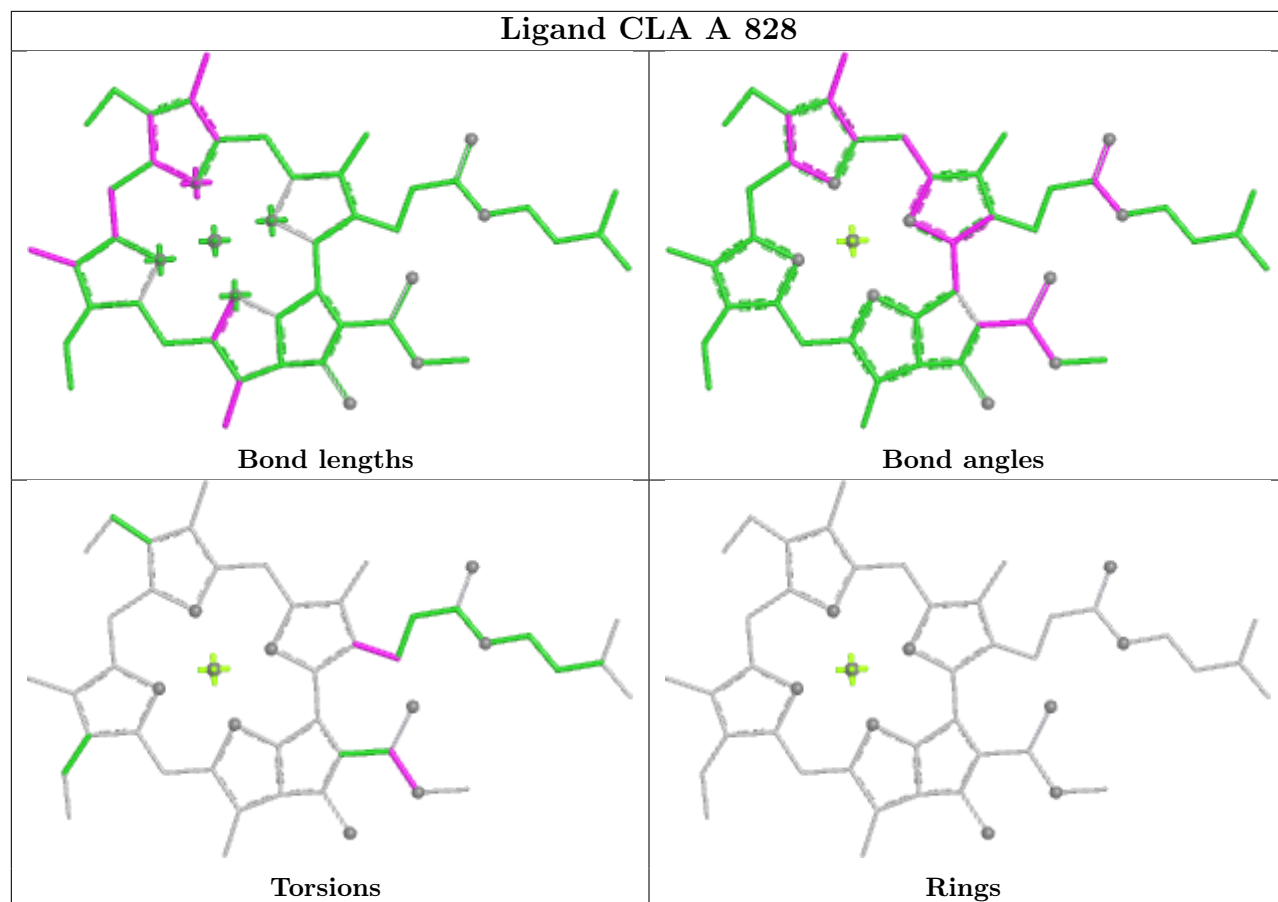
## Ligand CLA A 835



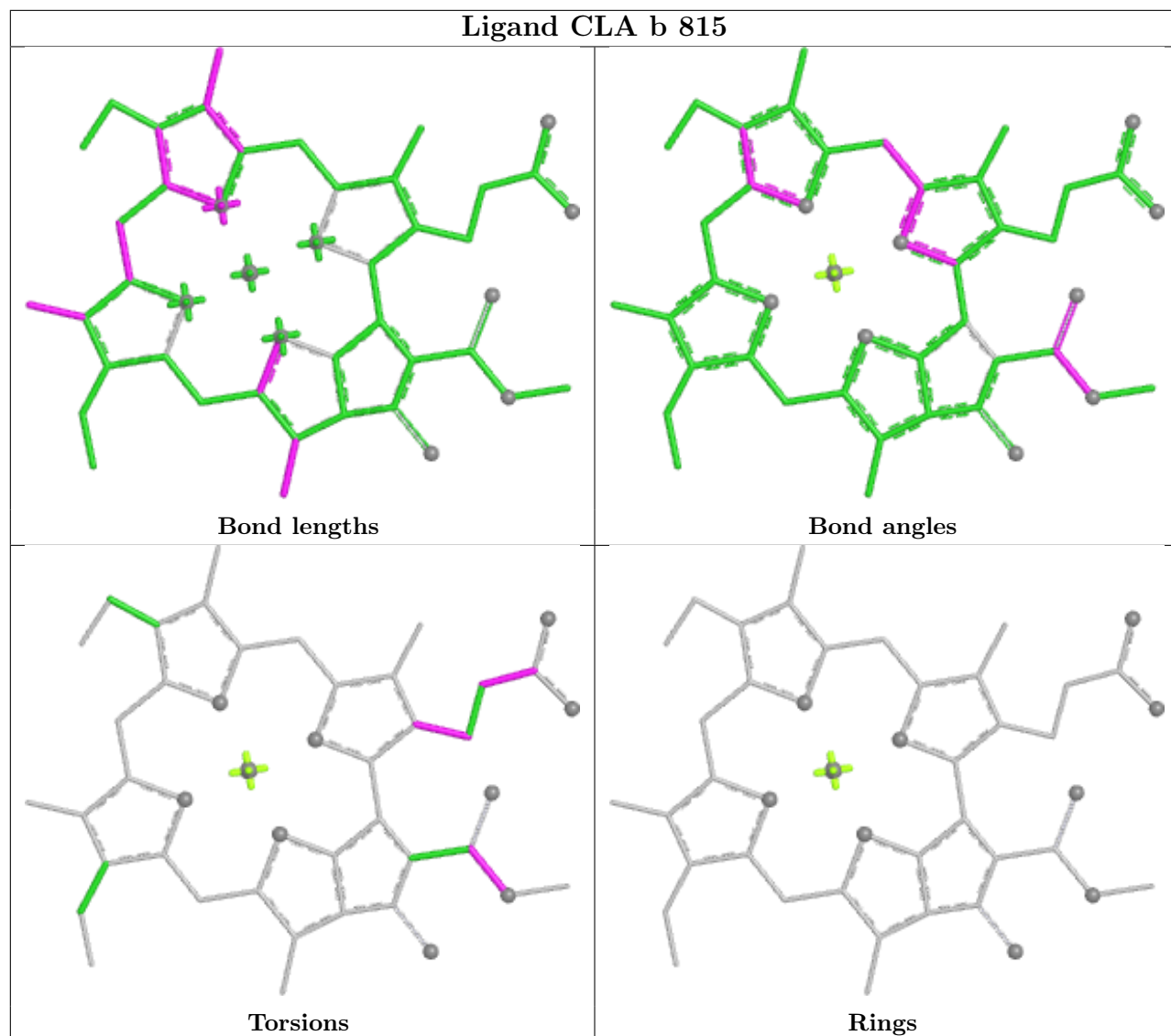




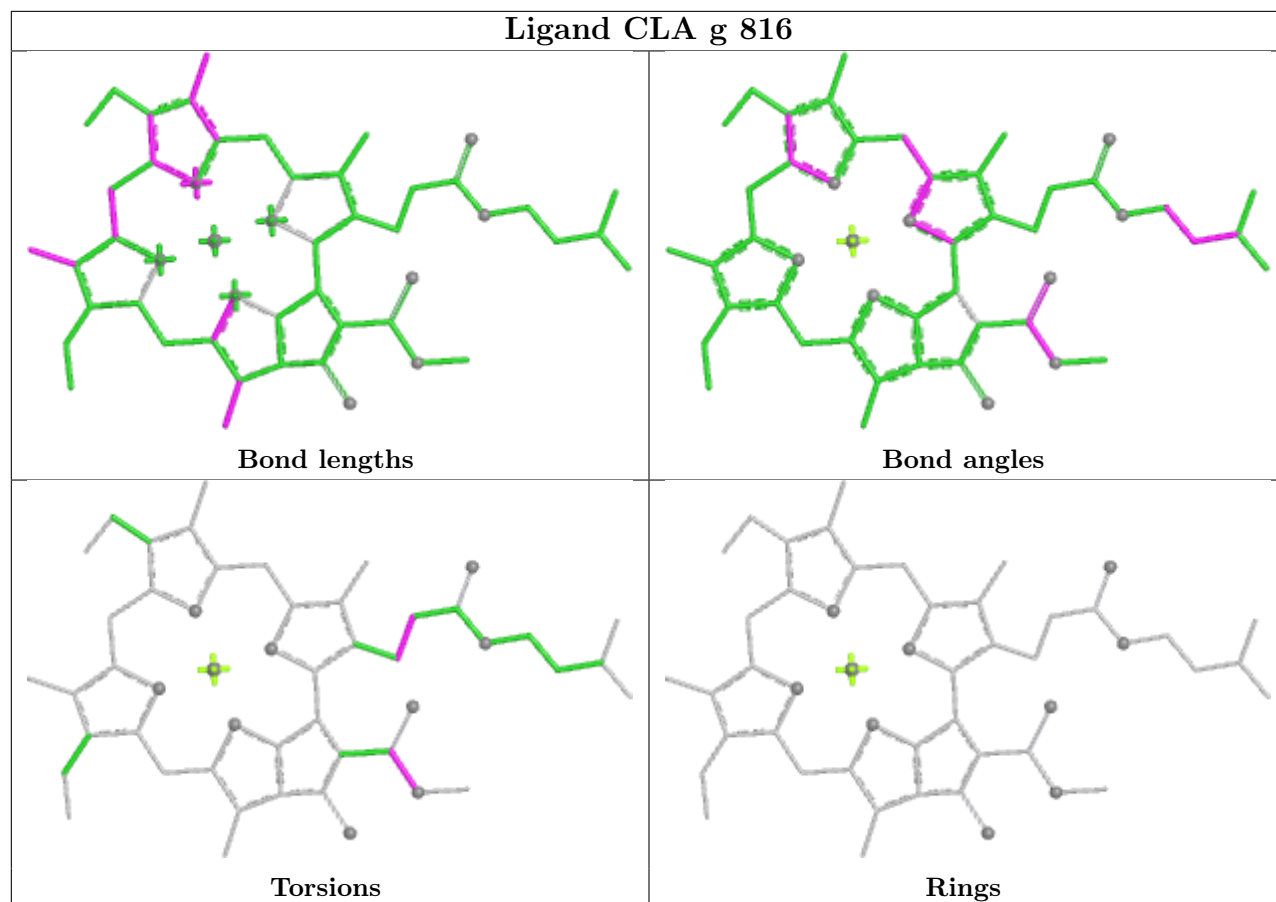
## Ligand CLA A 828

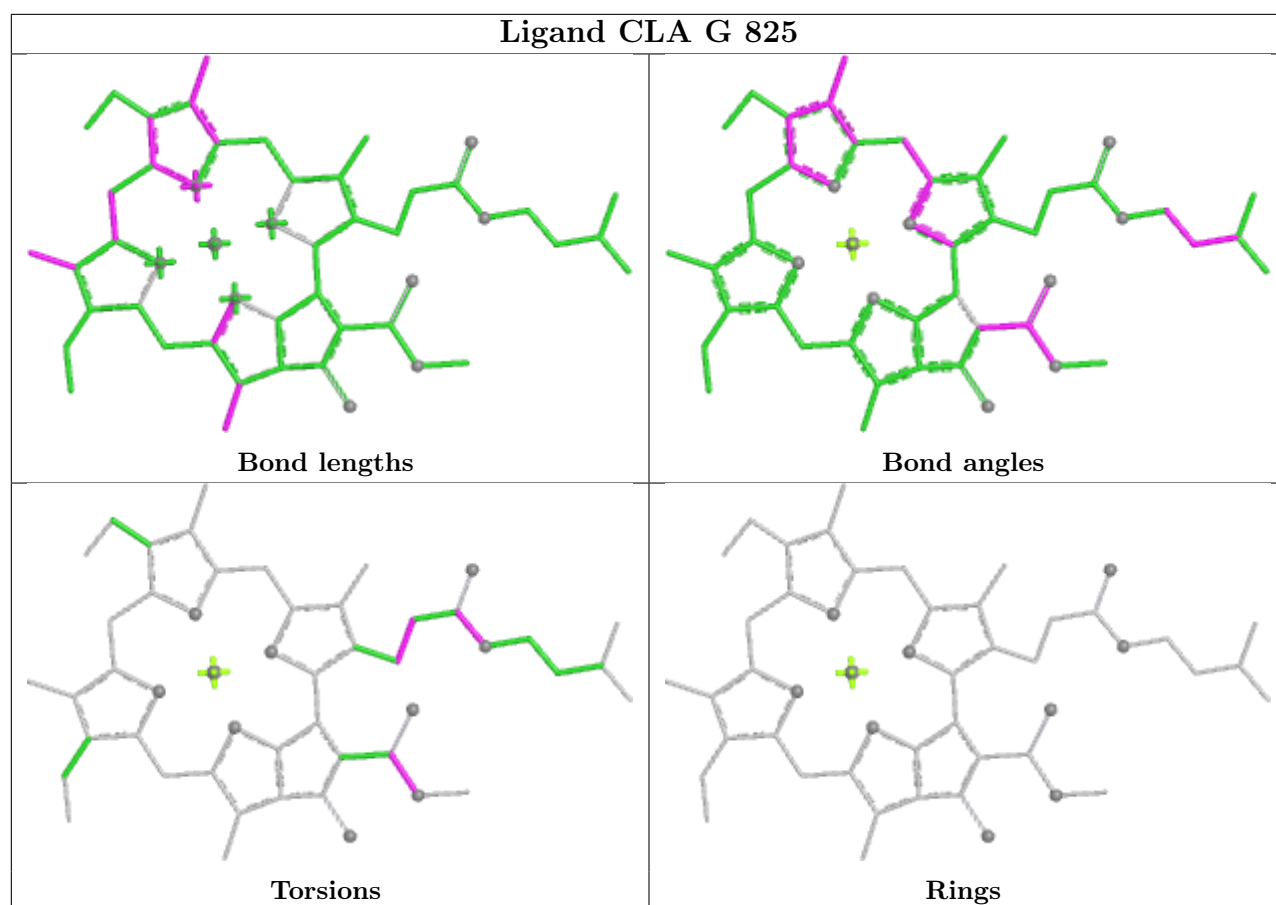


## Ligand CLA b 815

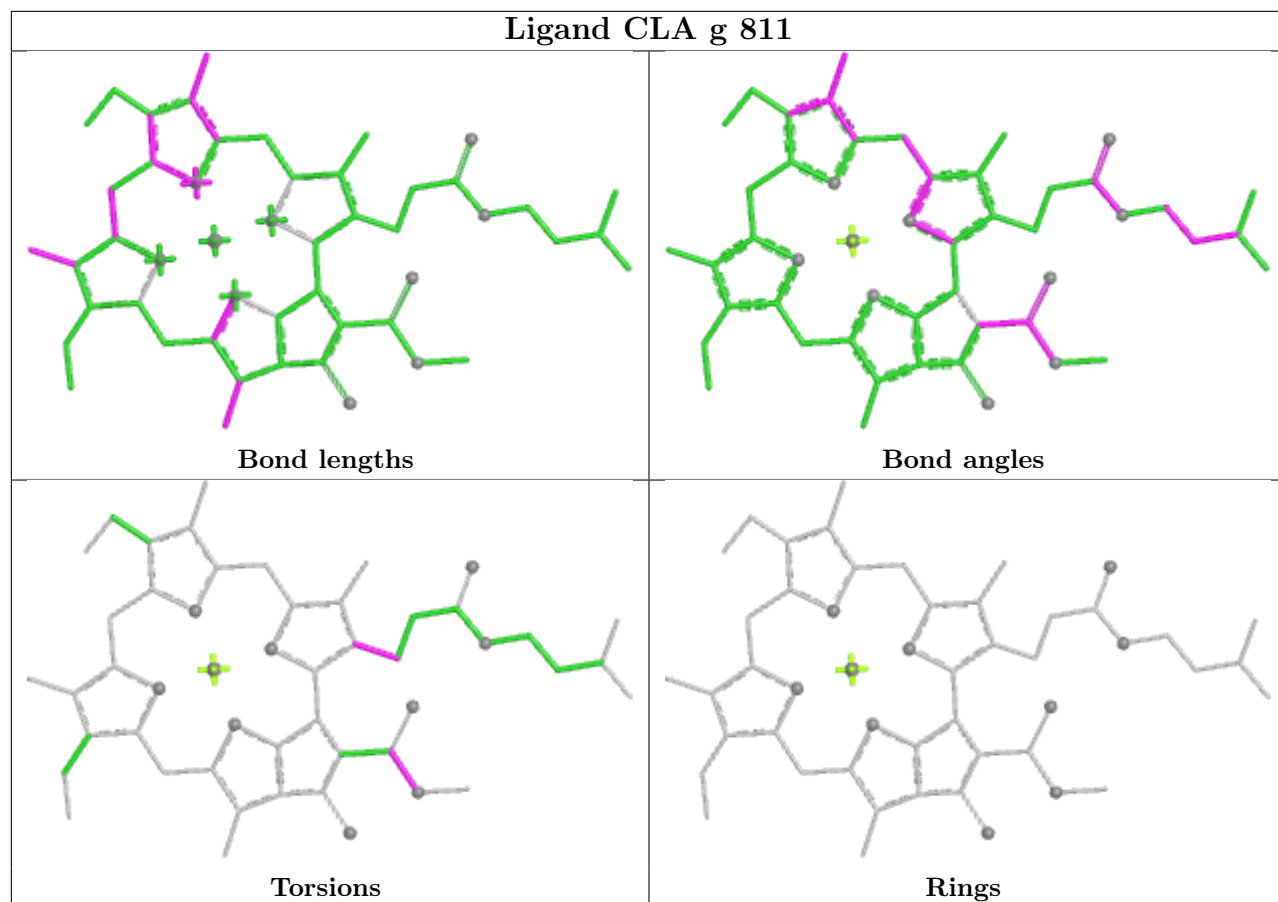


## Ligand CLA g 816



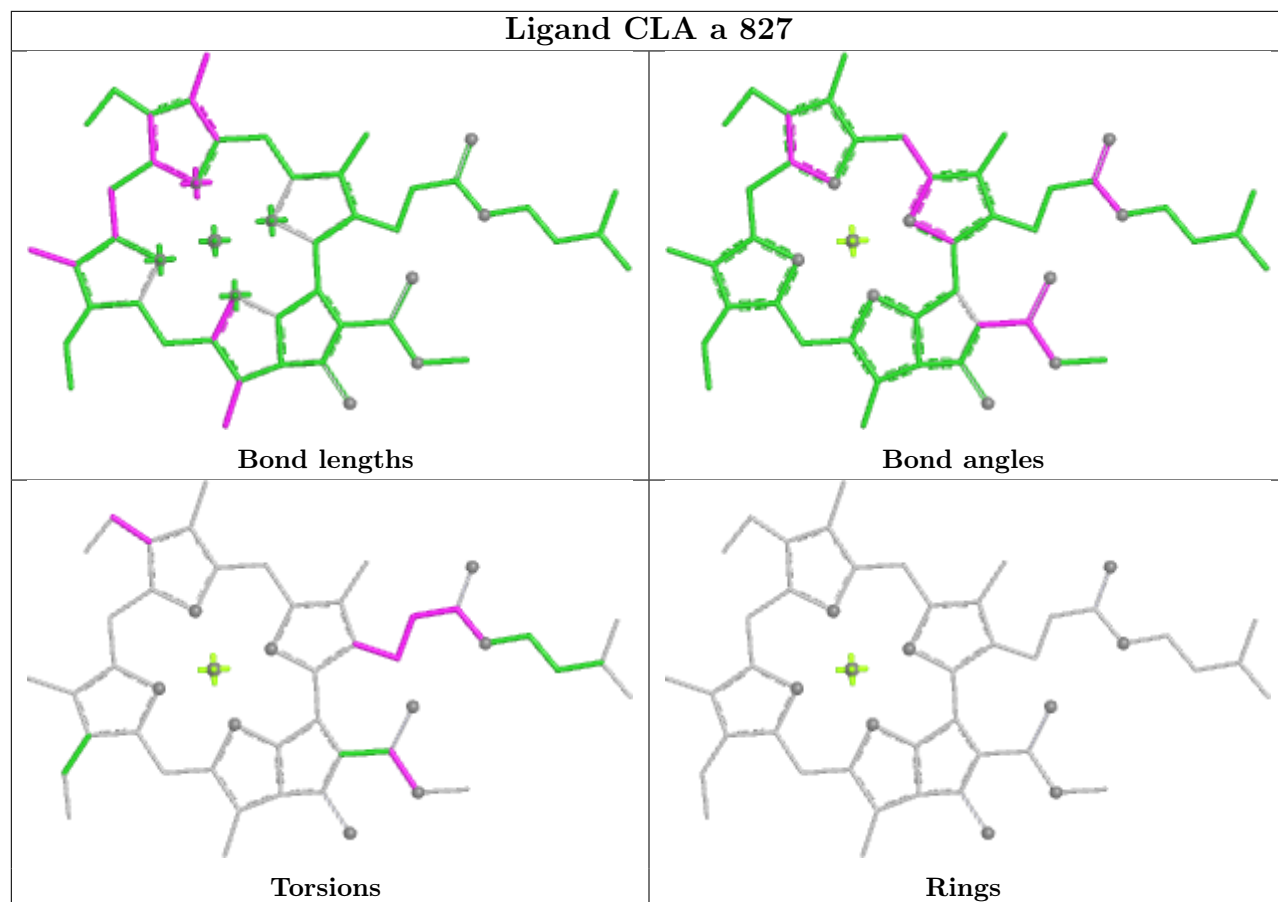


## Ligand CLA g 811

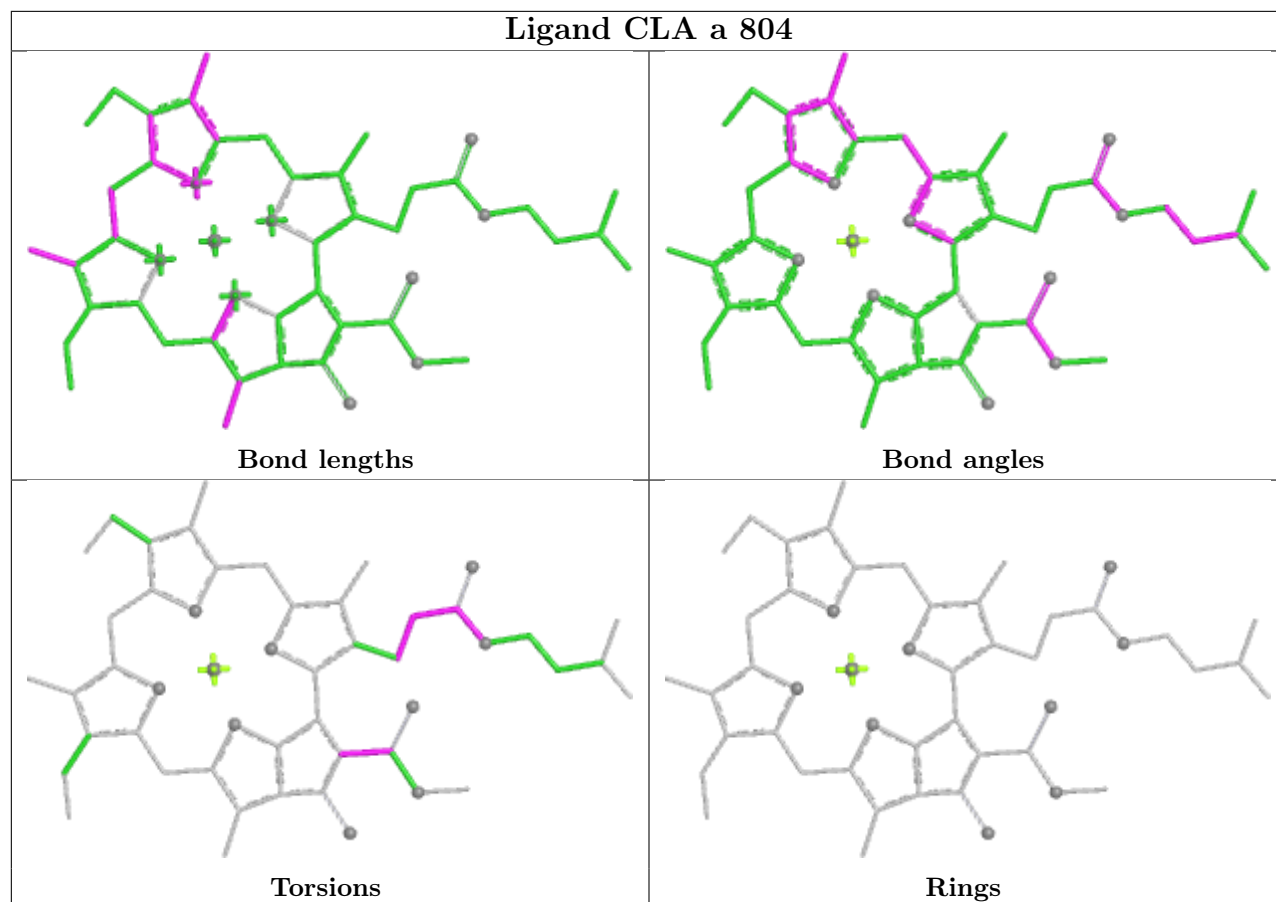




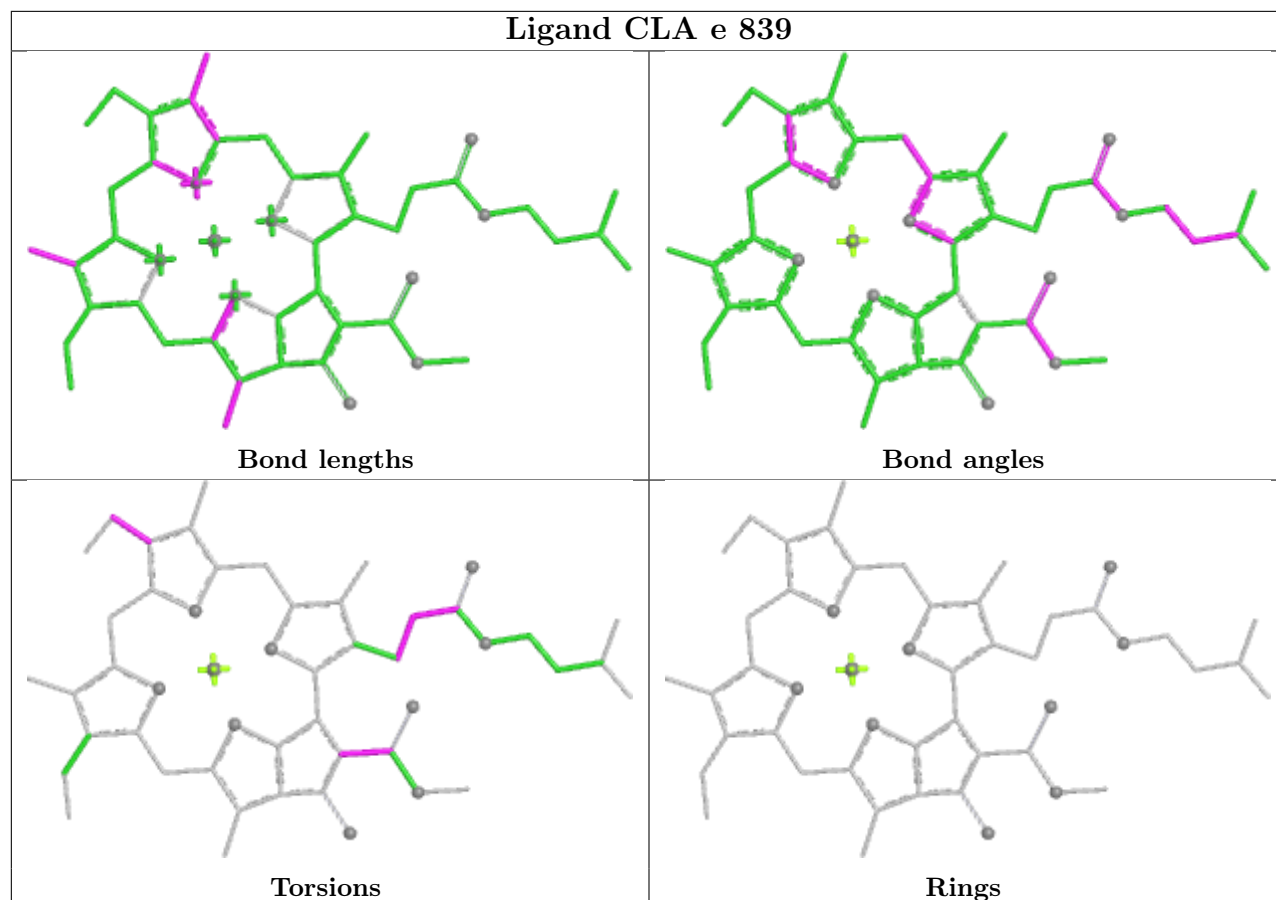
## Ligand CLA a 827



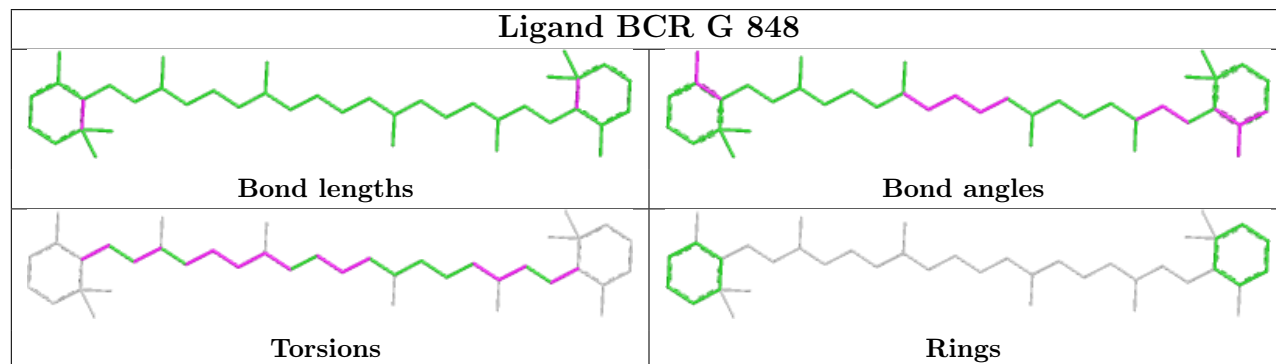
## Ligand CLA a 804



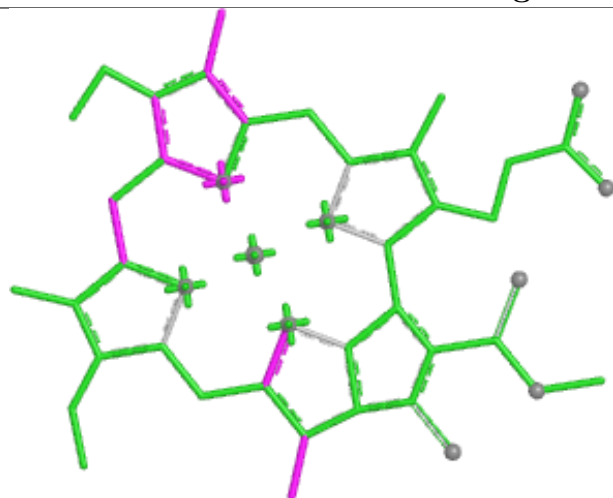
## Ligand CLA e 839



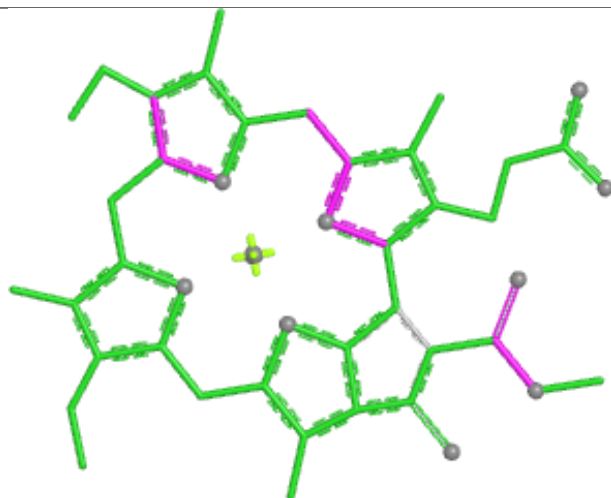
## Ligand BCR G 848



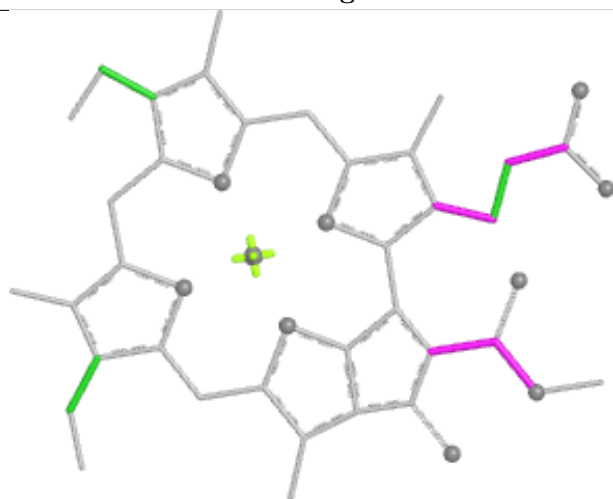
## Ligand CLA G 836



Bond lengths



Bond angles

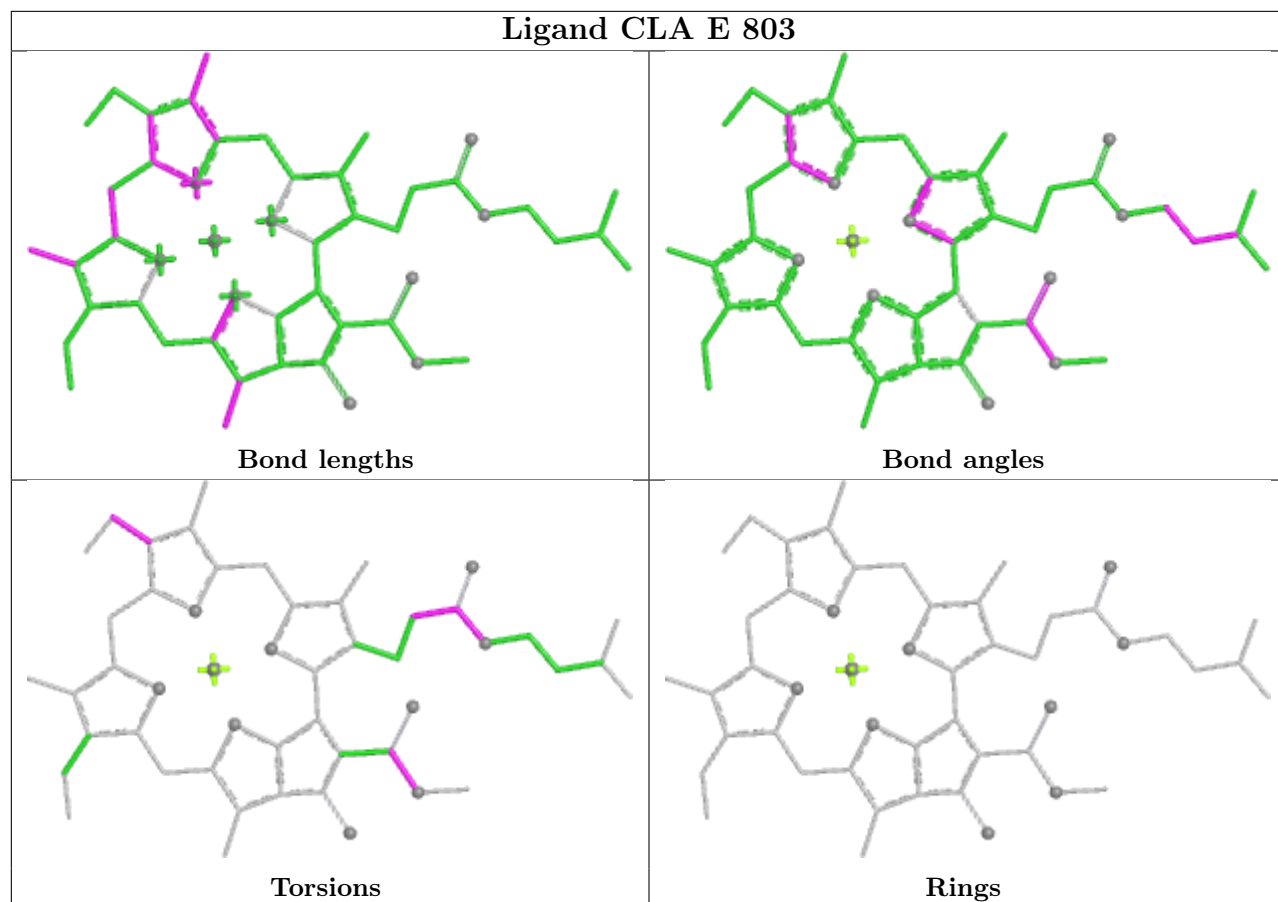


Torsions

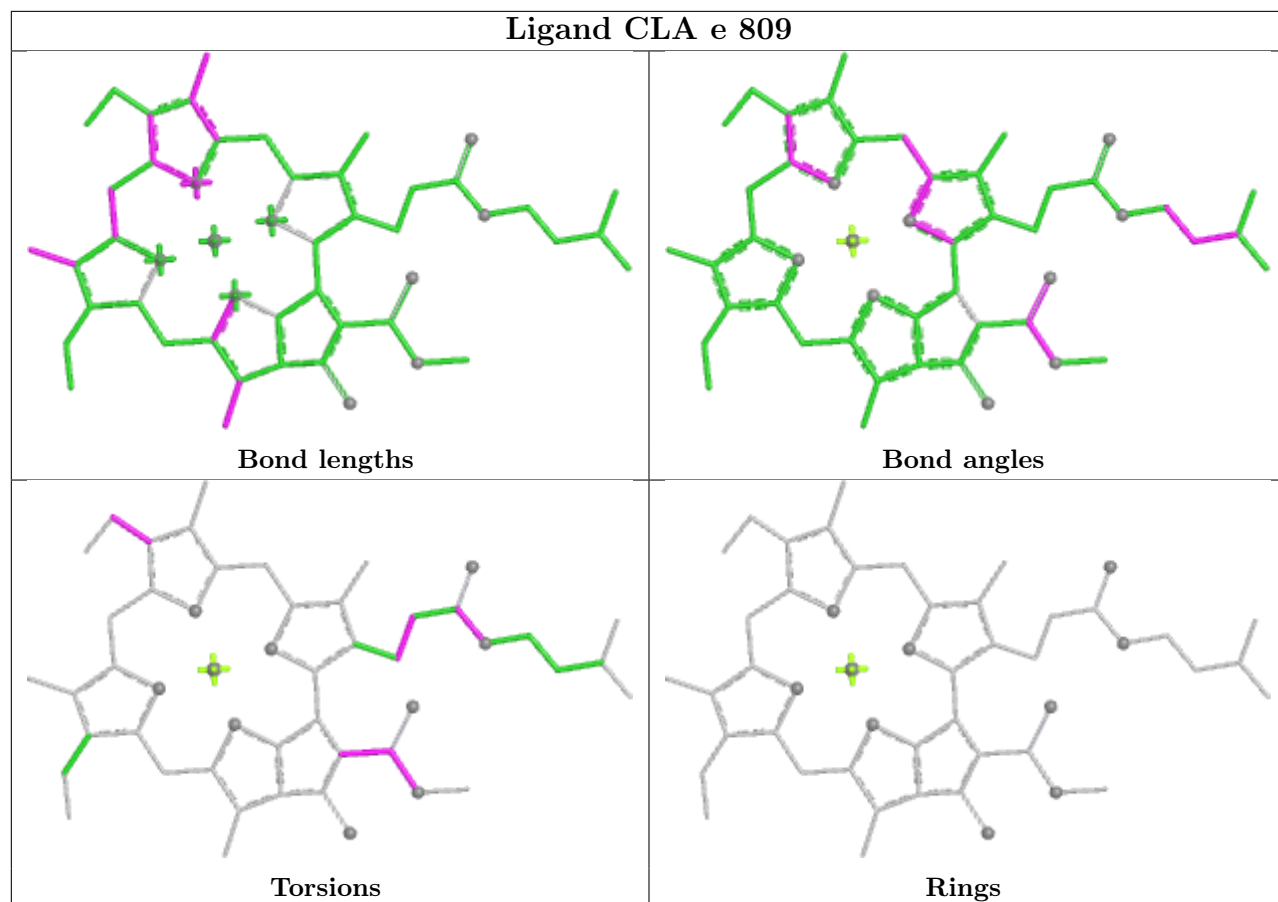


Rings

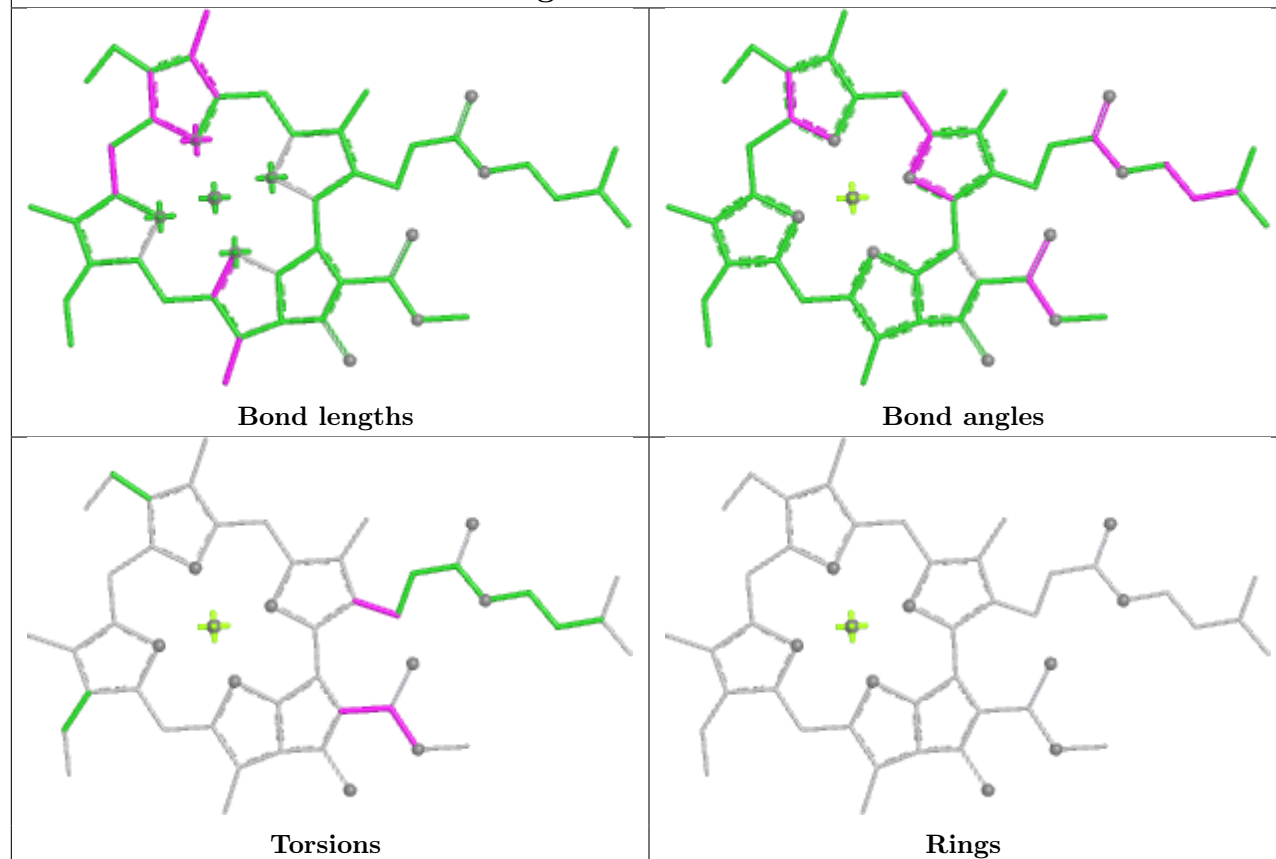
## Ligand CLA E 803



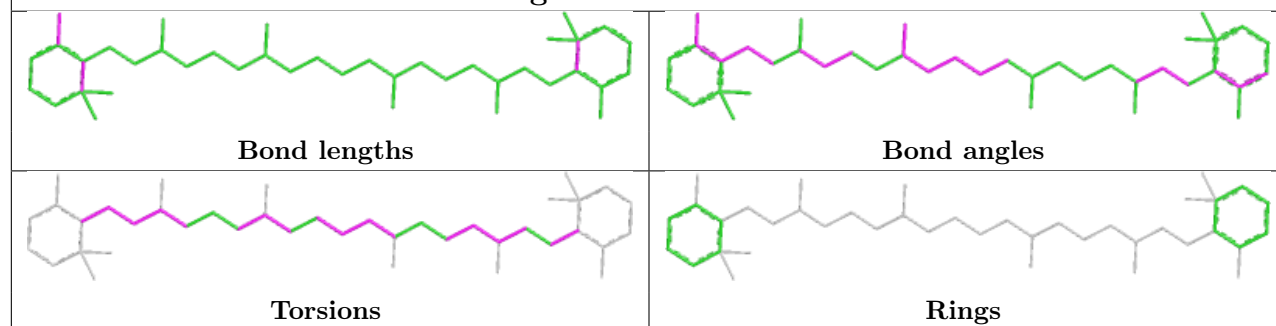
## Ligand CLA e 809



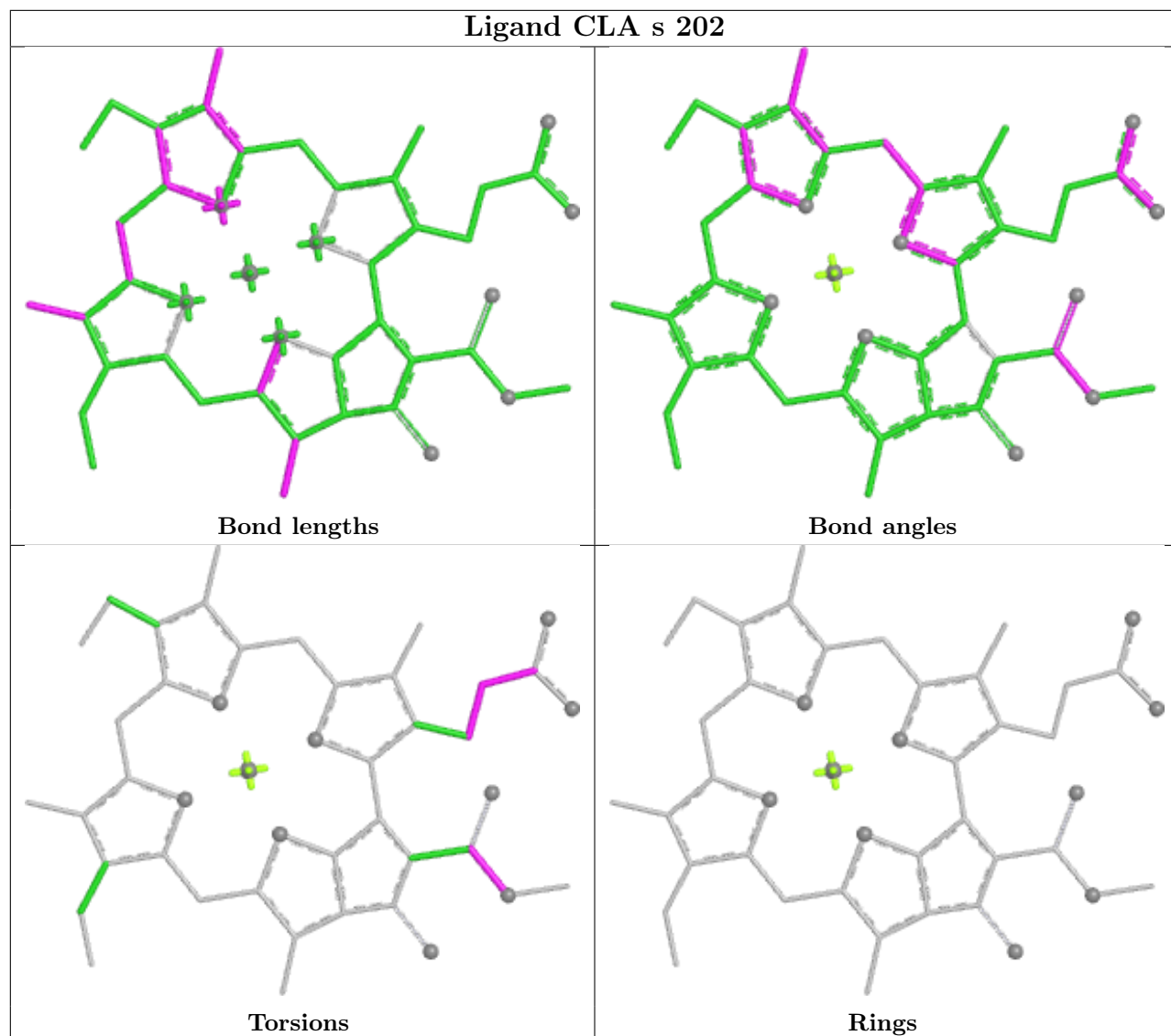
## Ligand CLA e 807



## Ligand BCR A 850

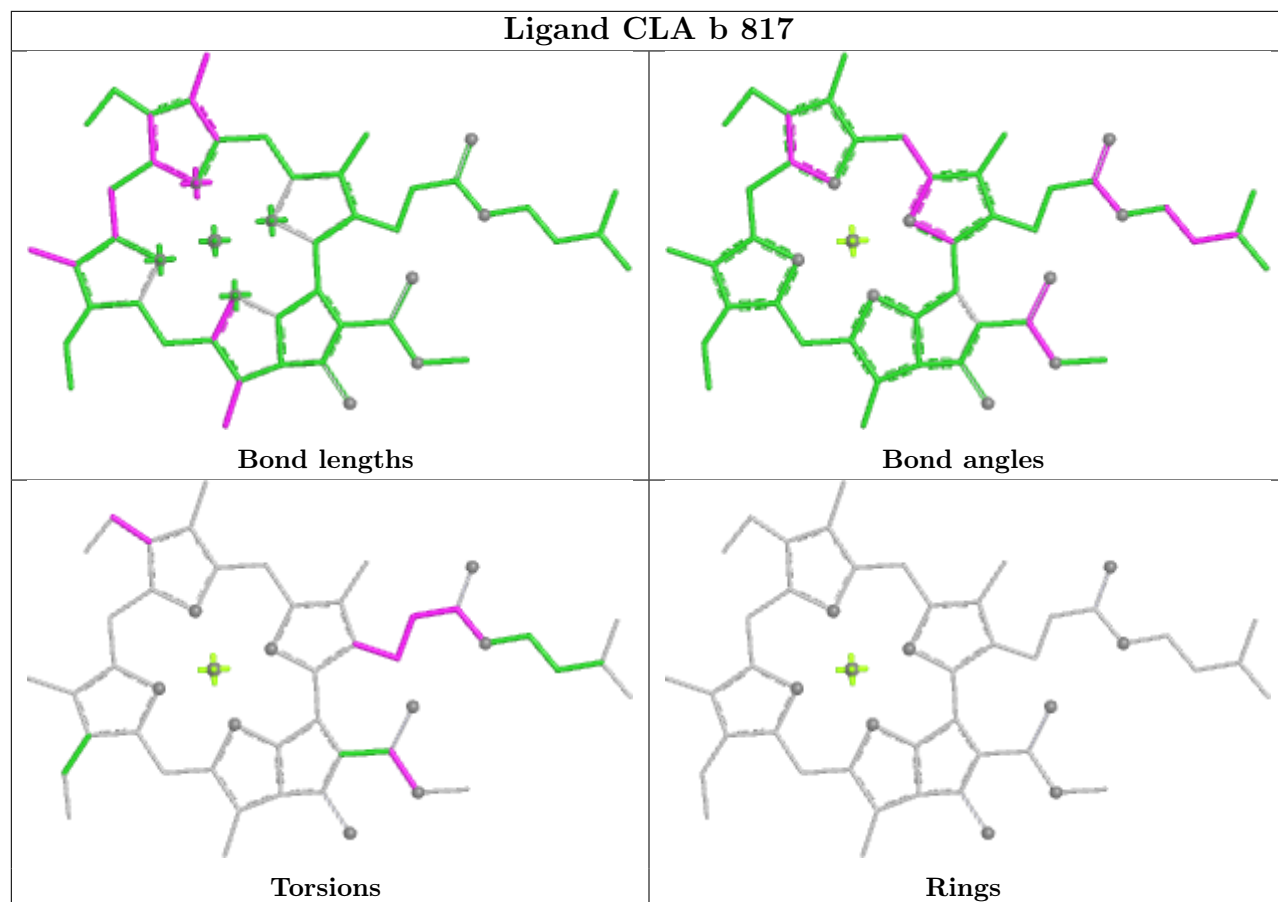


## Ligand CLA s 202

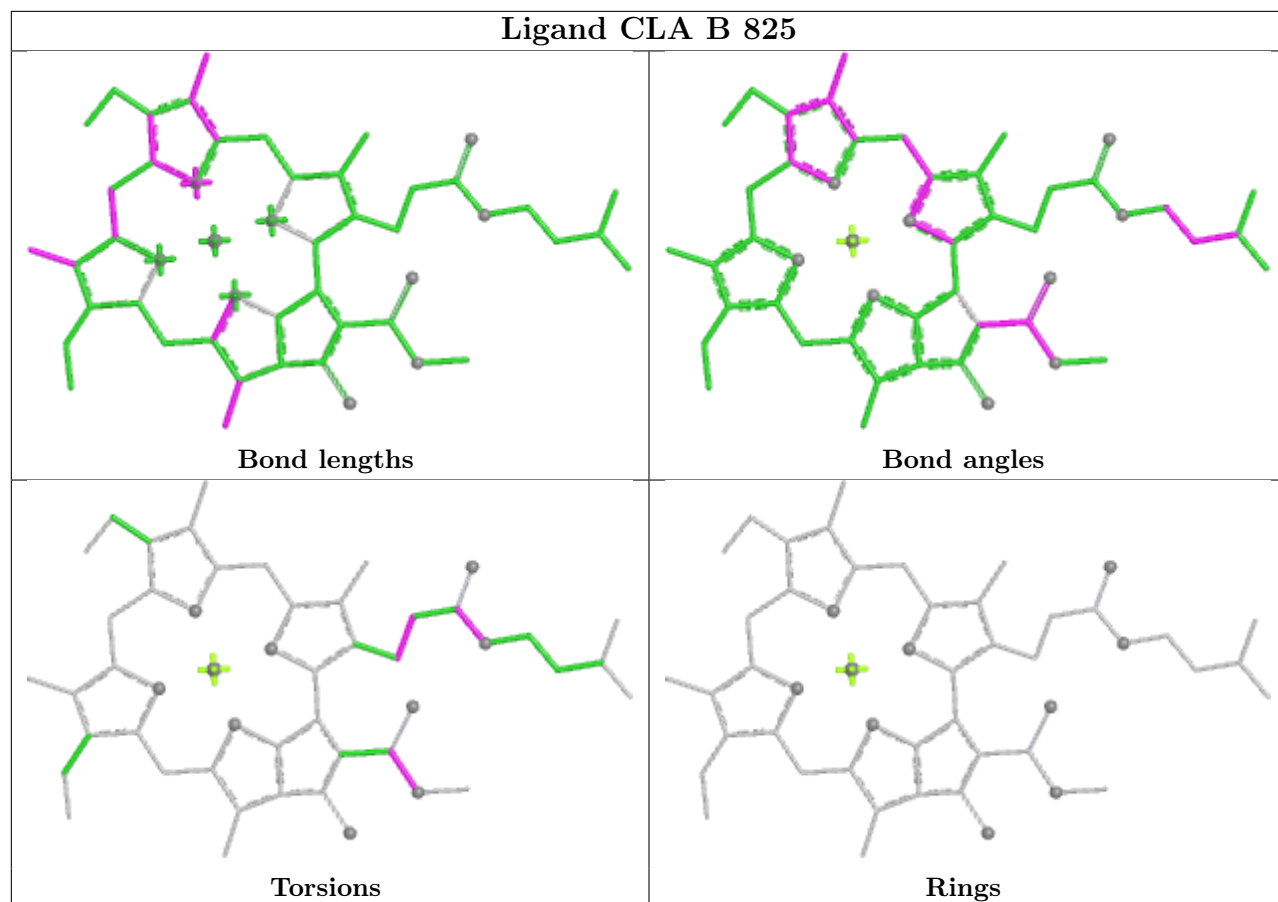




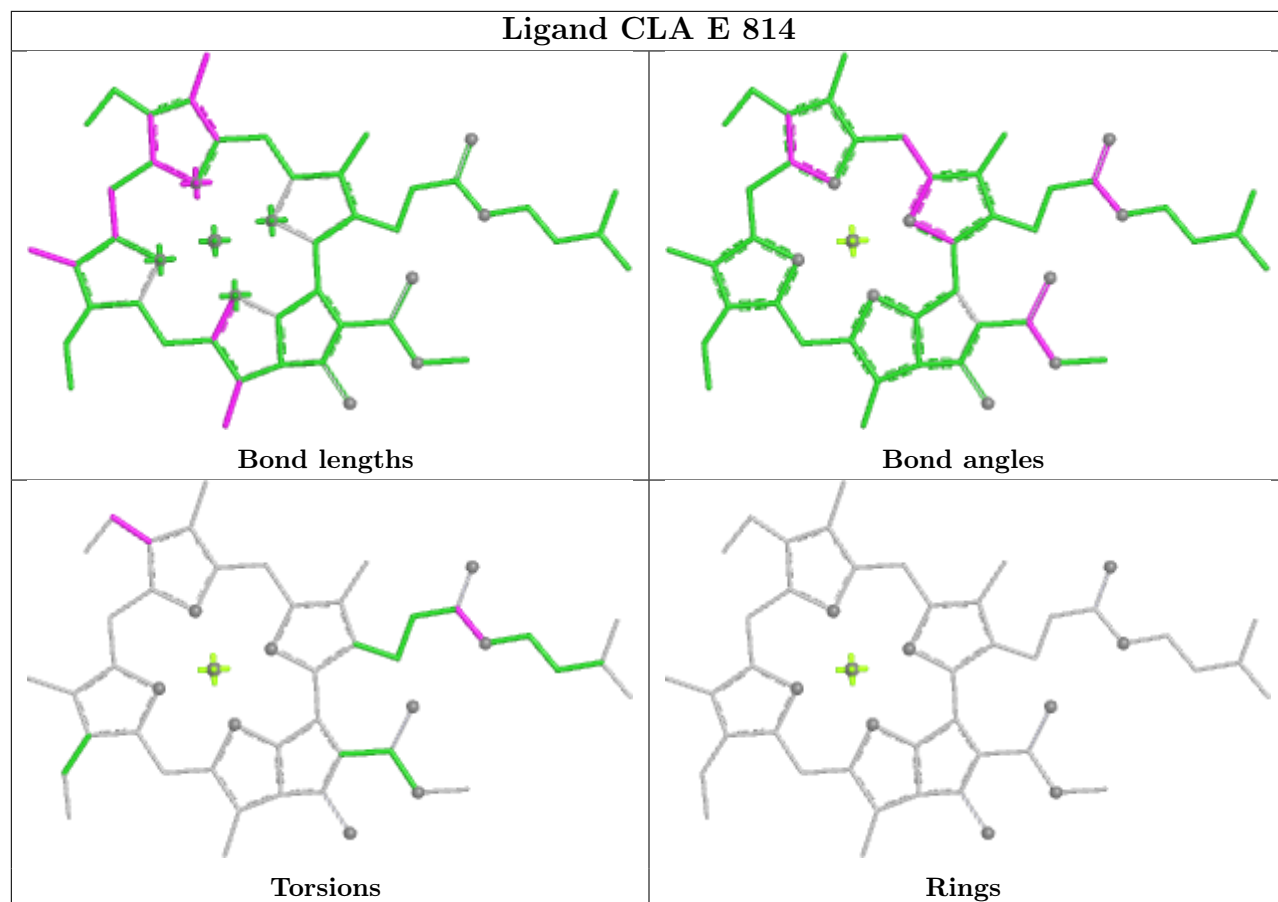
## Ligand CLA b 817



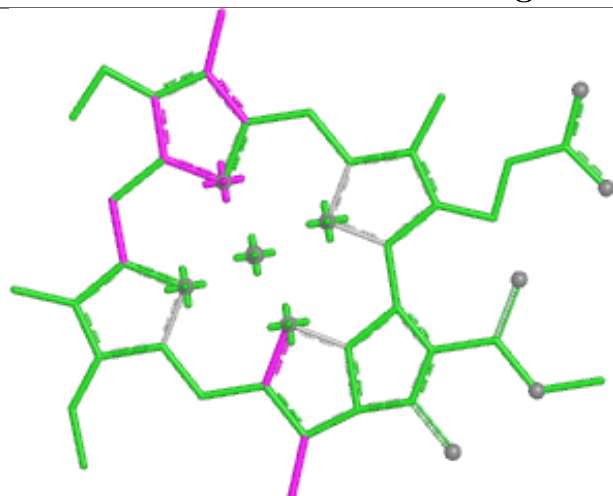
## Ligand CLA B 825



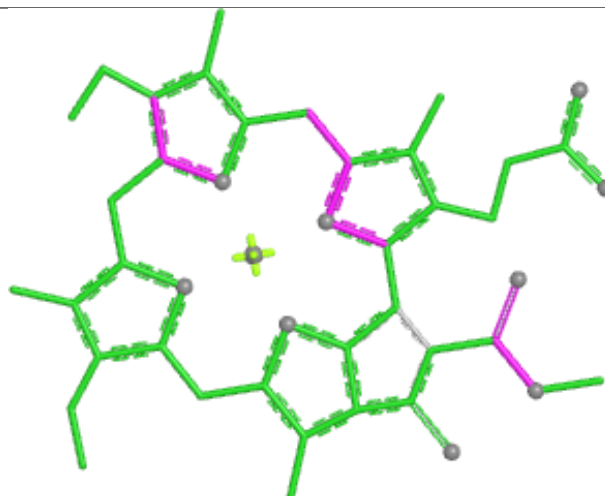
## Ligand CLA E 814



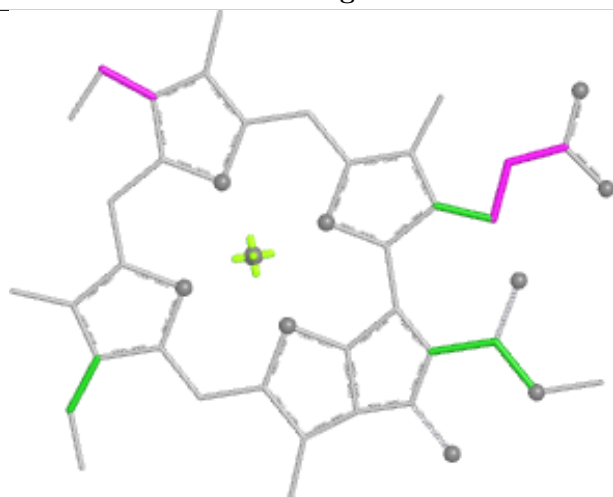
## Ligand CLA E 813



Bond lengths



Bond angles

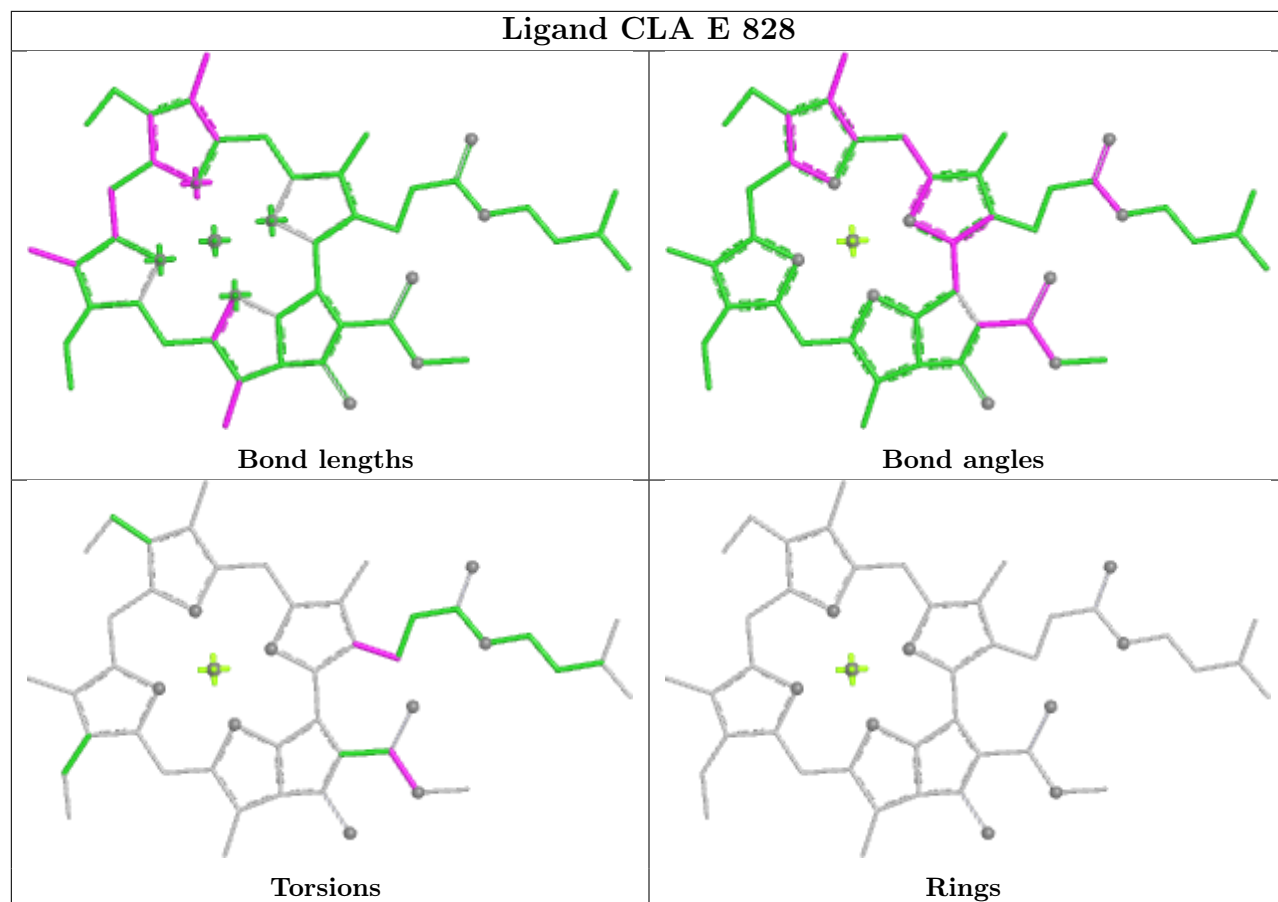


Torsions

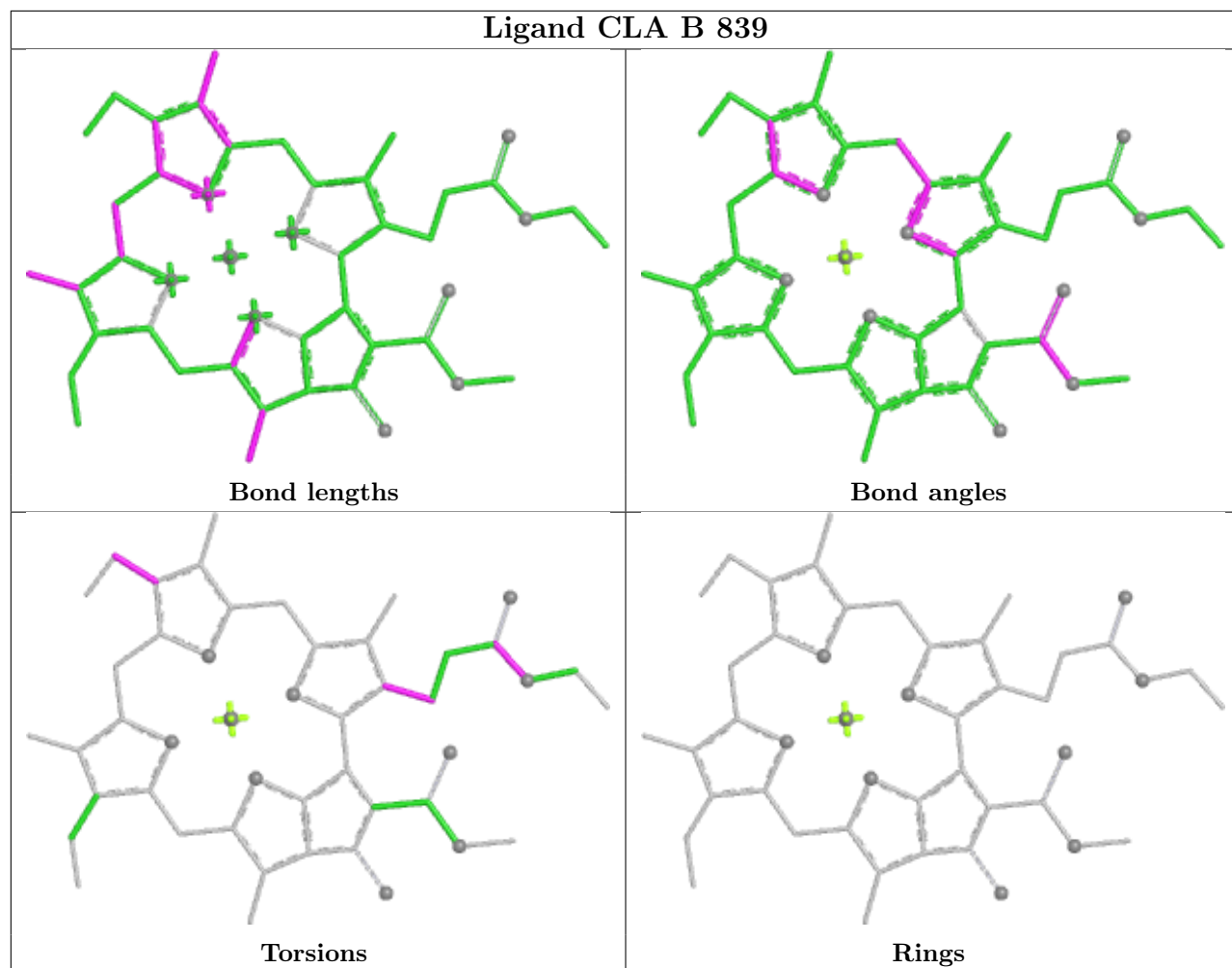


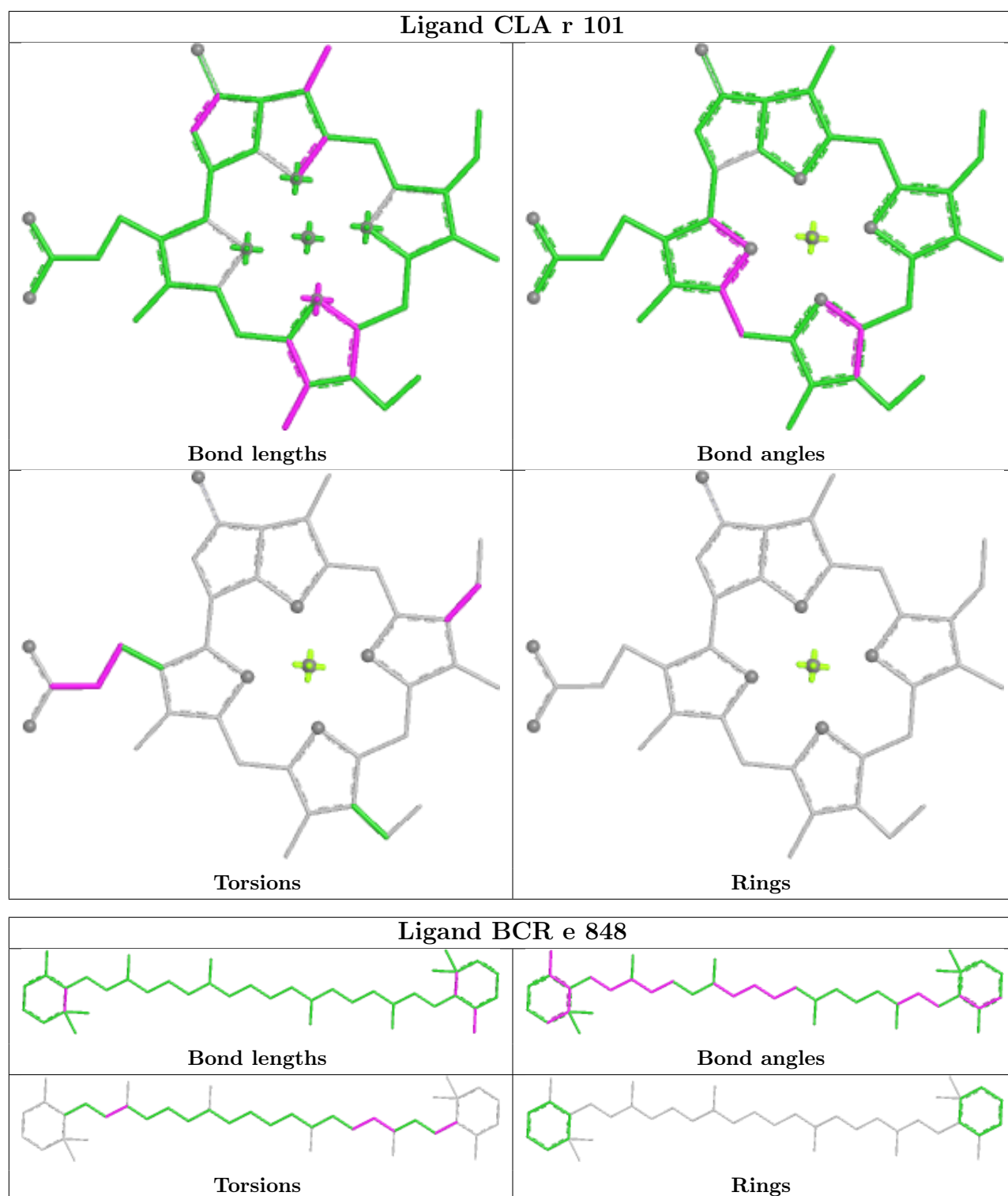
Rings

## Ligand CLA E 828

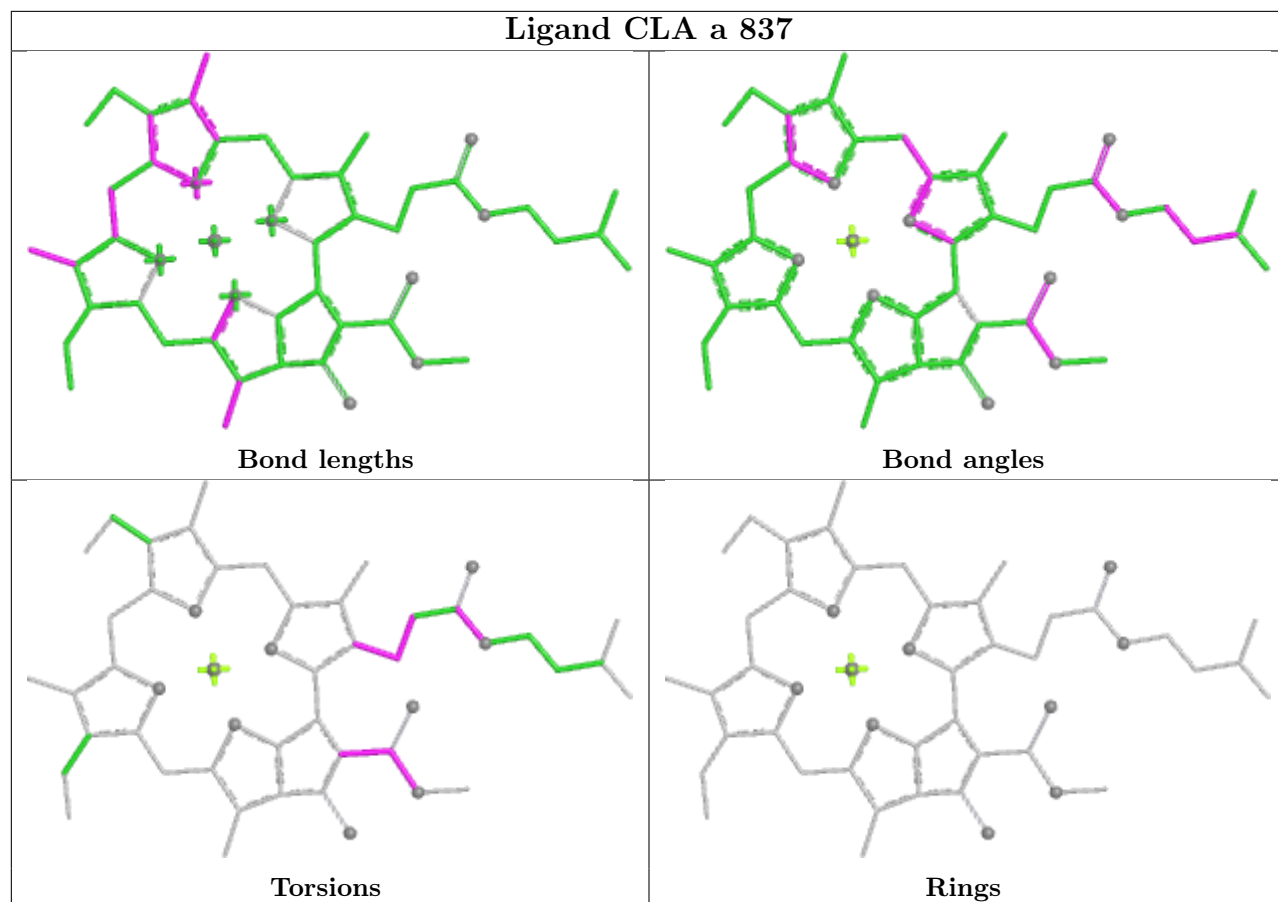


## Ligand CLA B 839



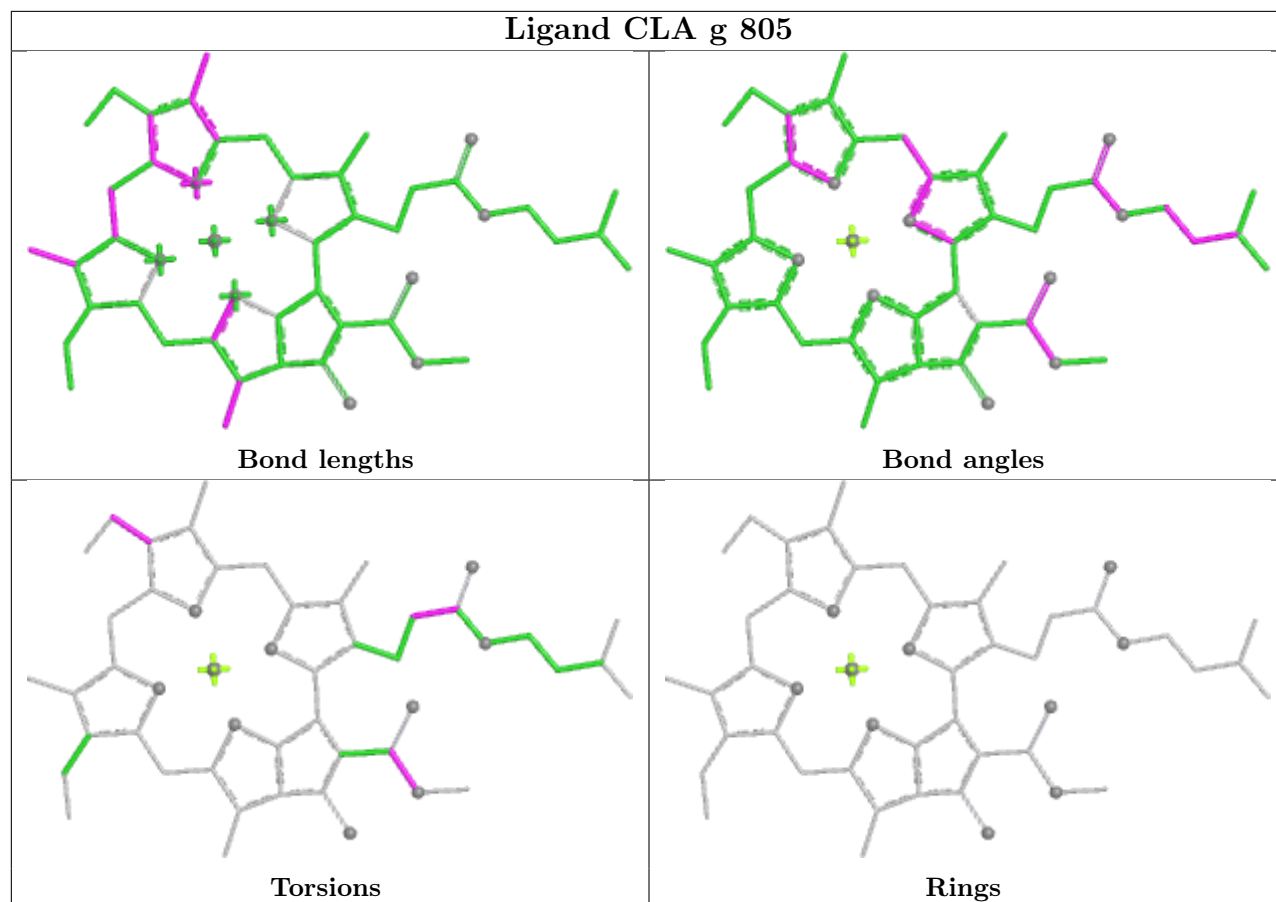


## Ligand CLA a 837

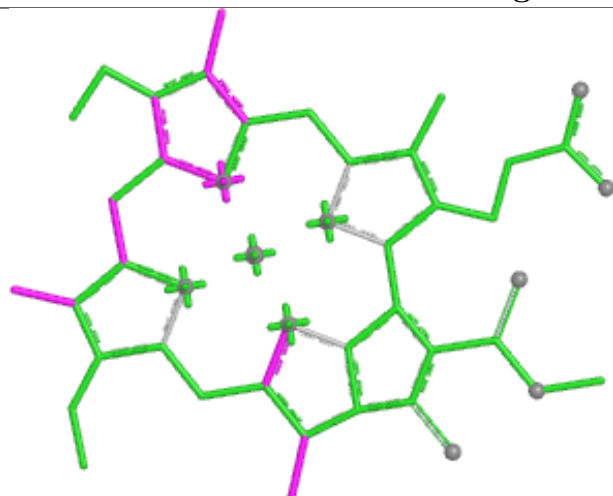




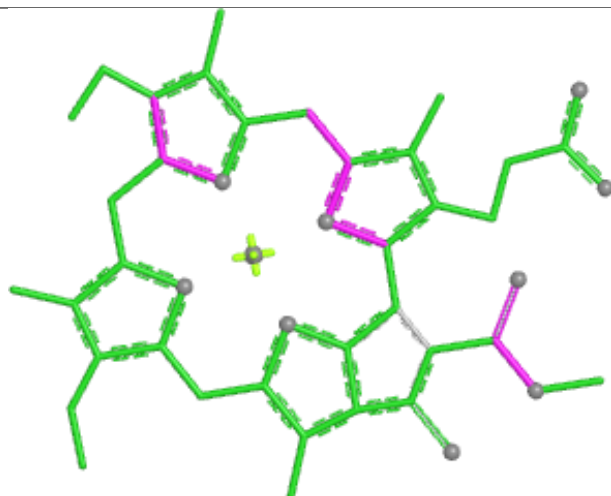
## Ligand CLA g 805



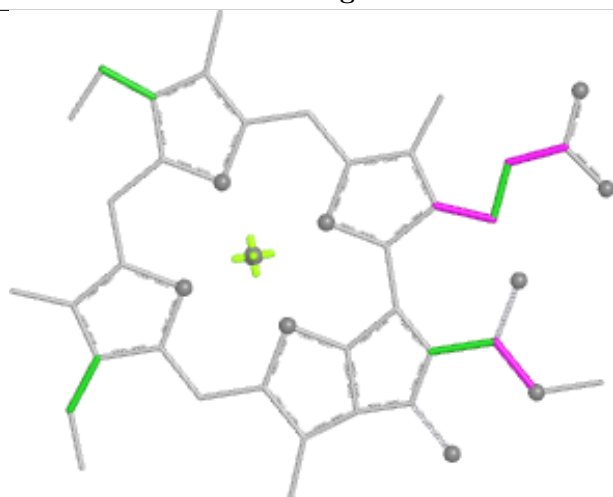
## Ligand CLA G 816



Bond lengths



Bond angles

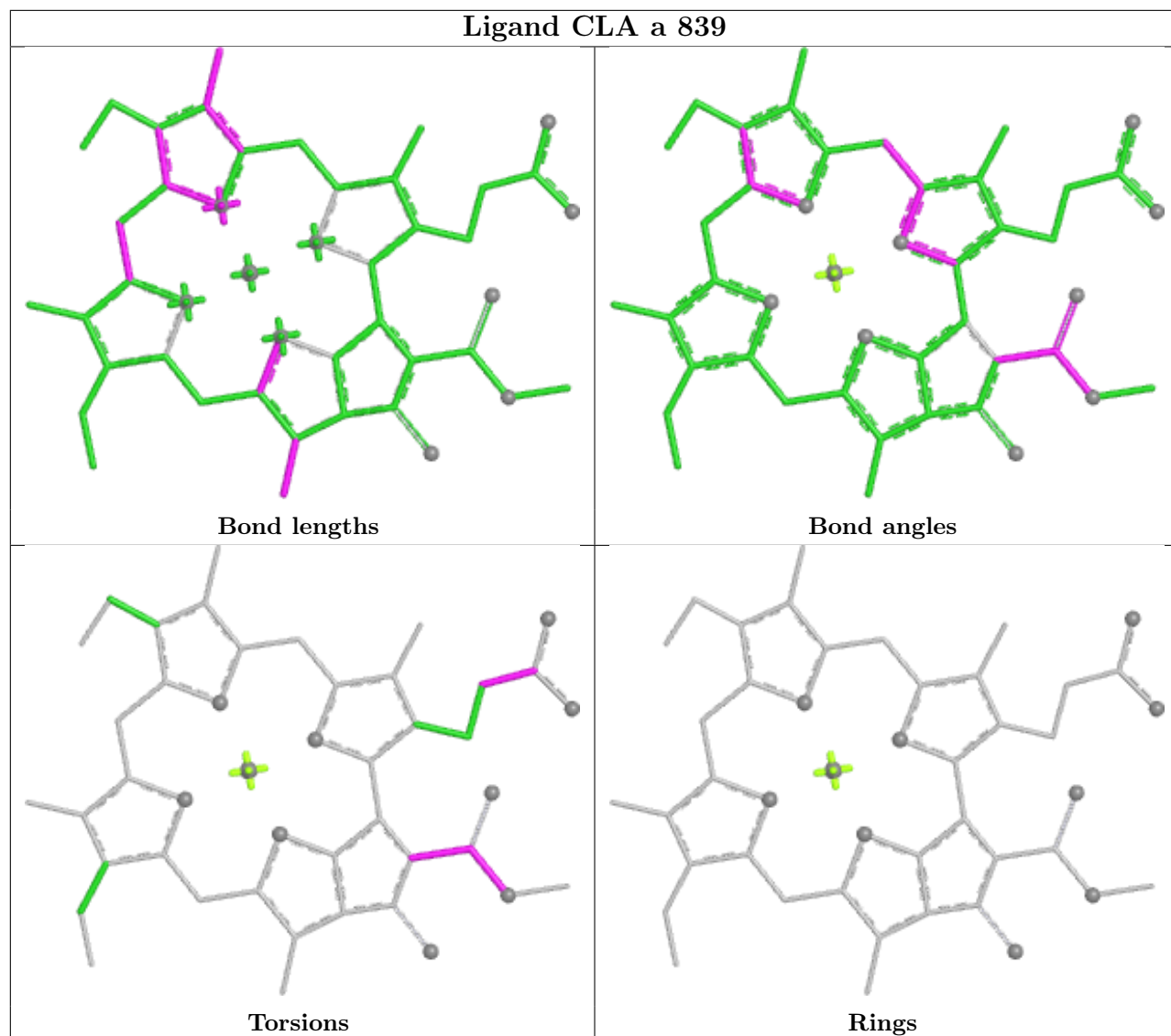


Torsions

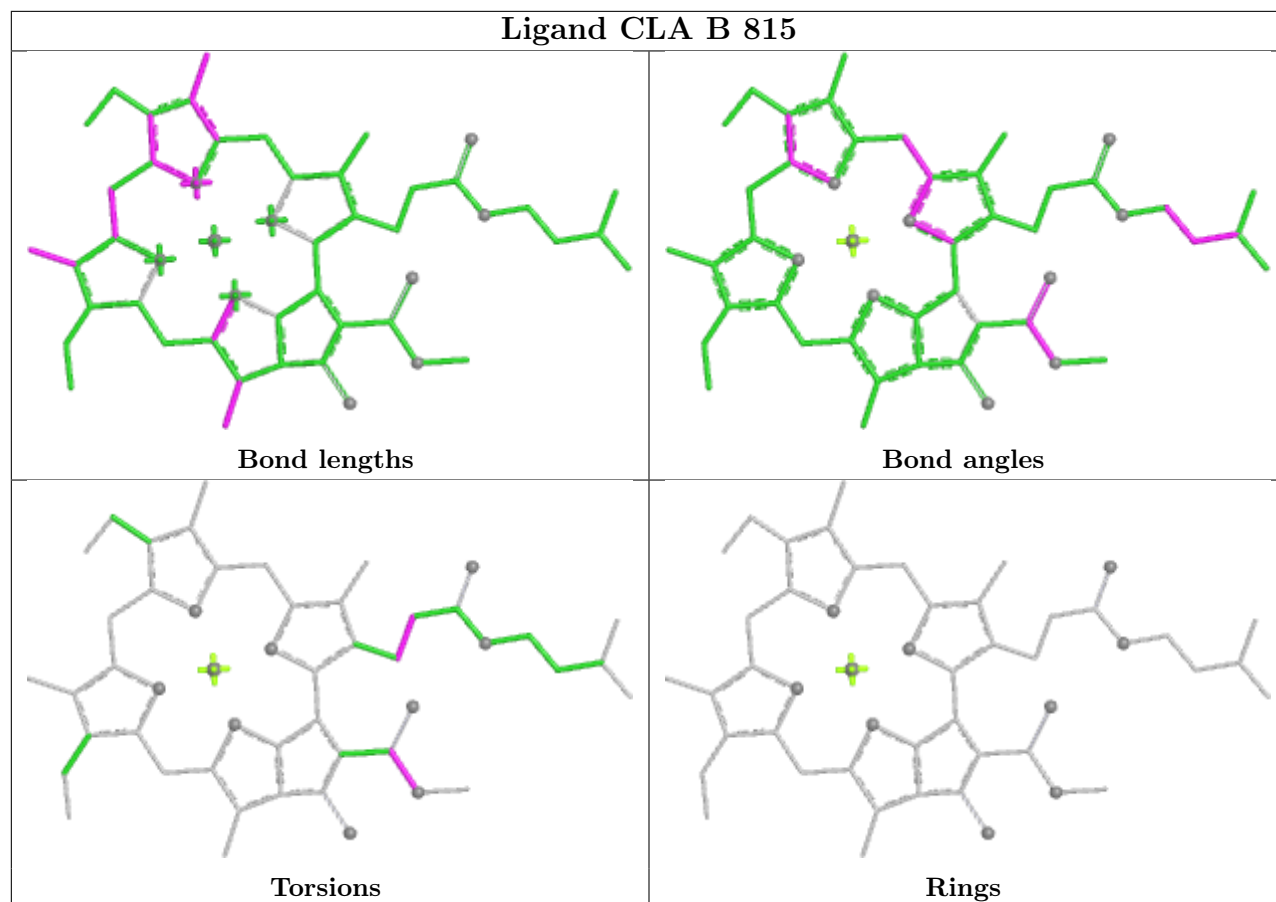


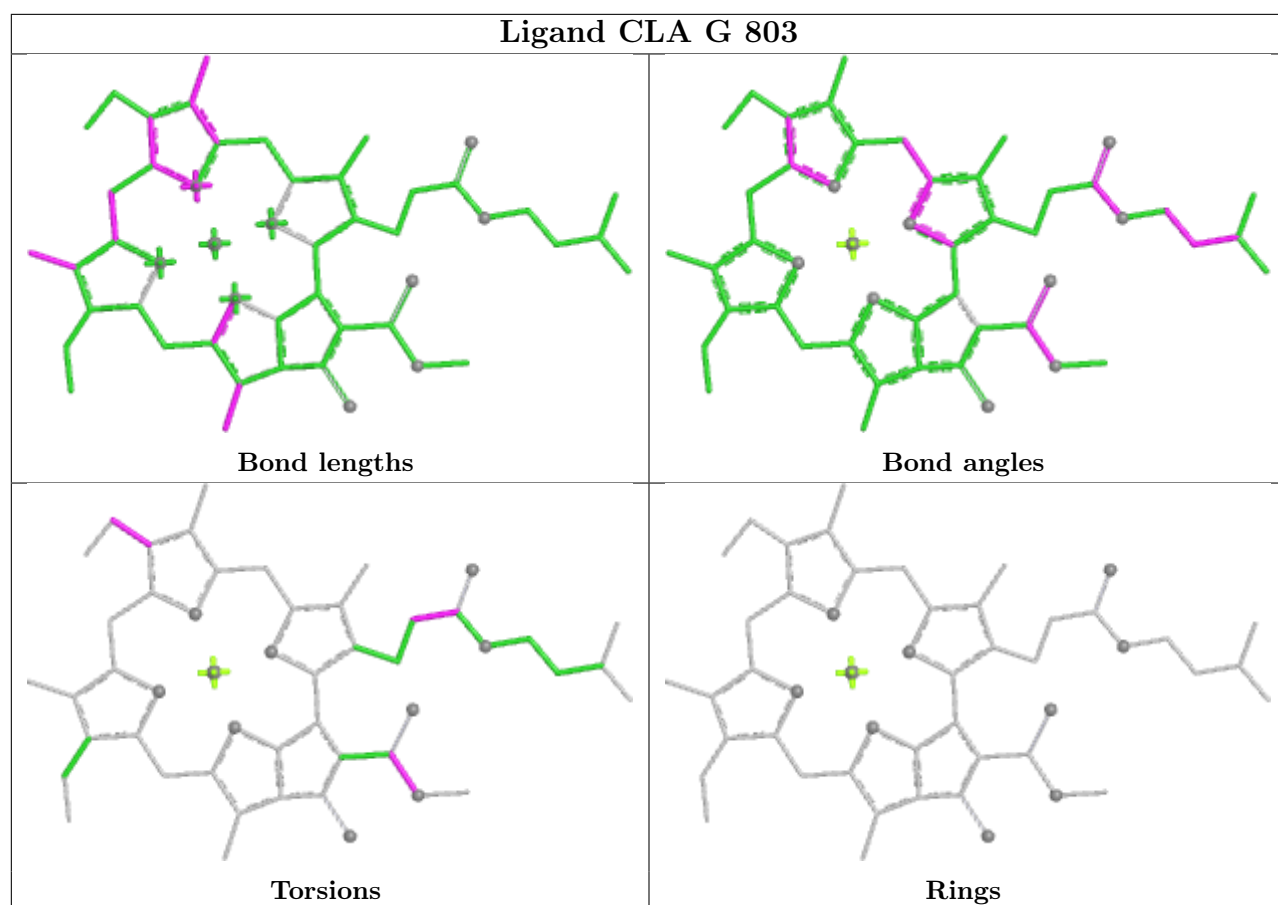
Rings

## Ligand CLA a 839

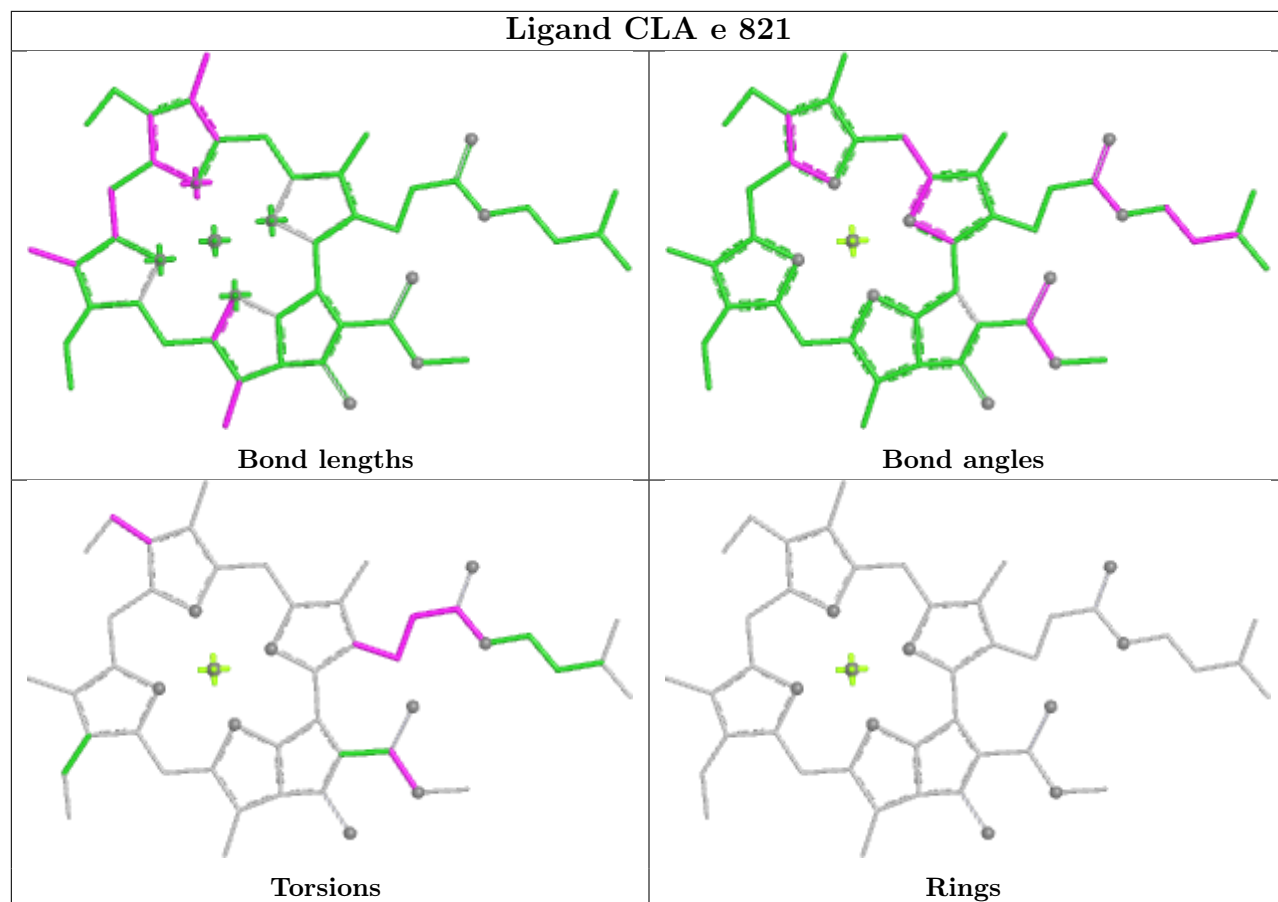


## Ligand CLA B 815

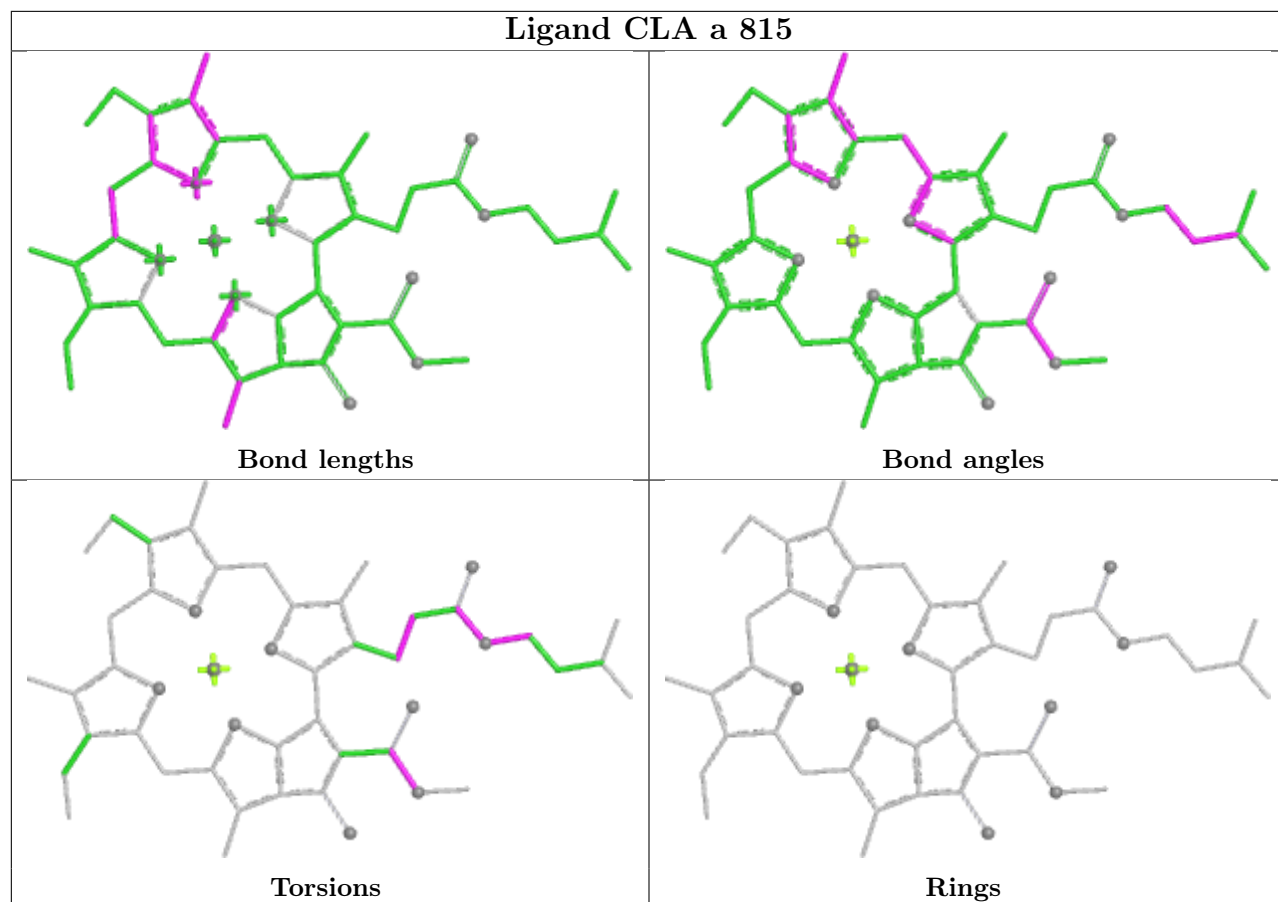




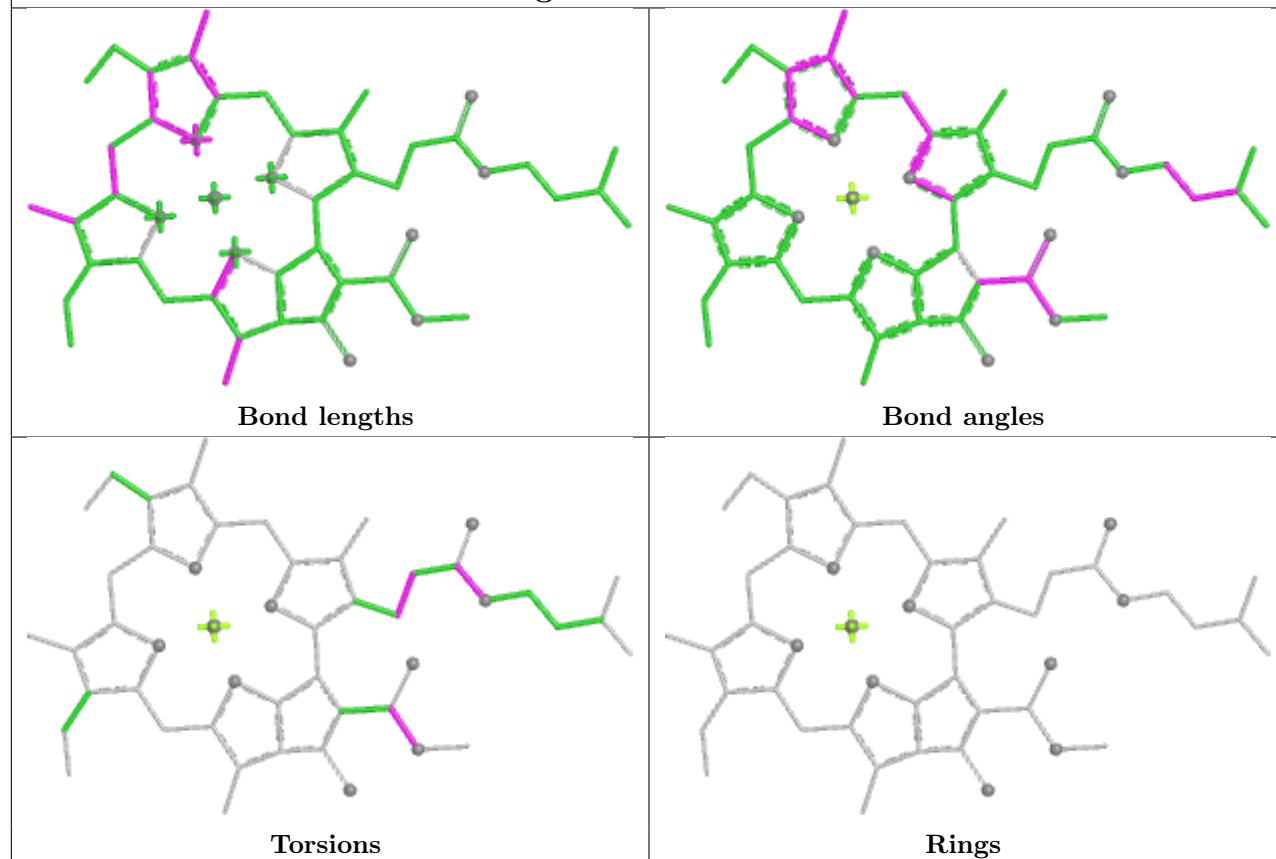
## Ligand CLA e 821



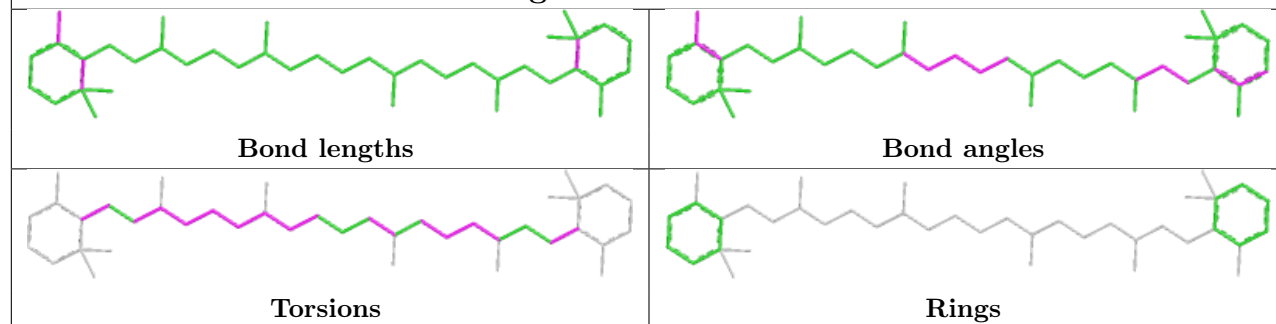
## Ligand CLA a 815



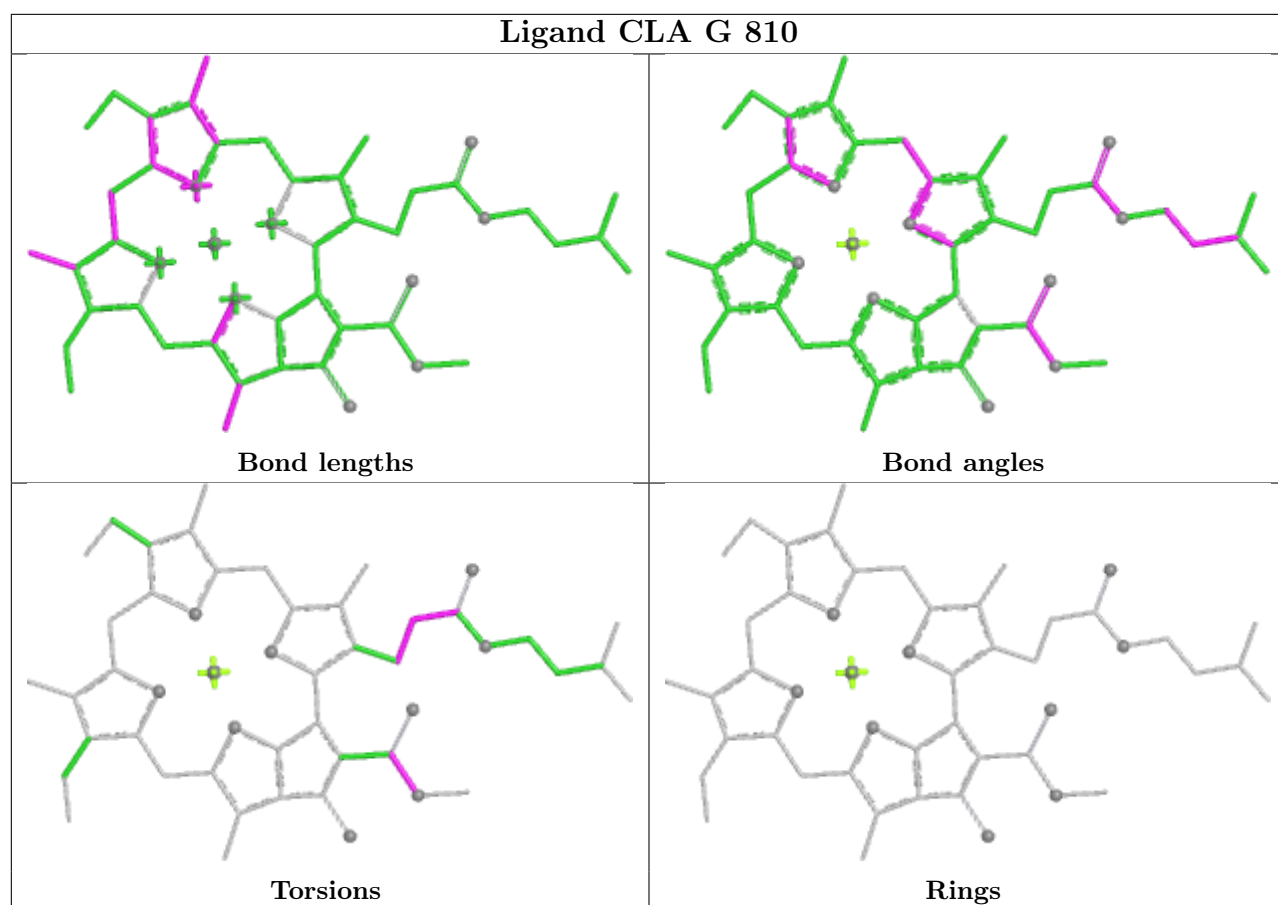
## Ligand CLA b 824



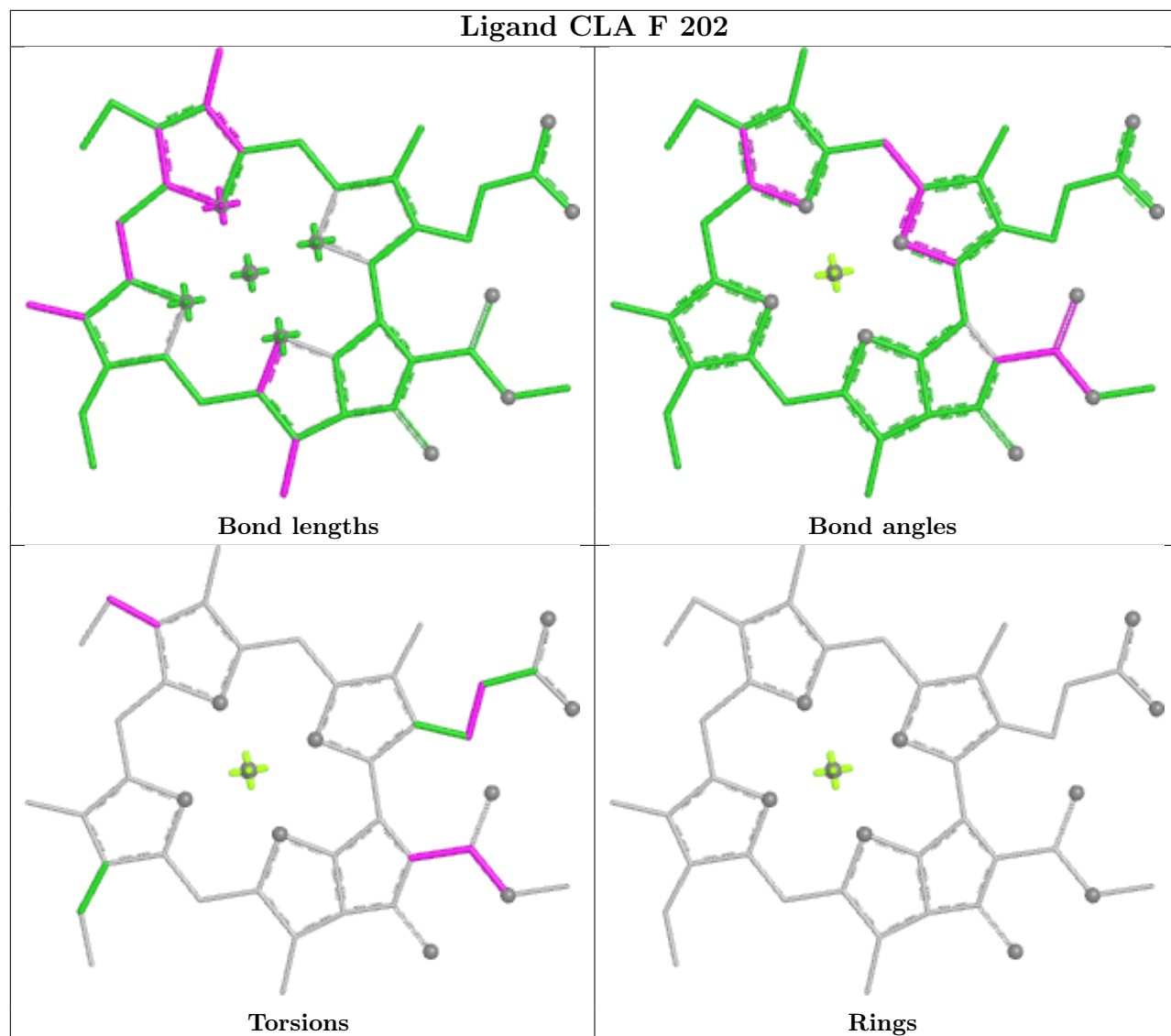
## Ligand BCR G 846

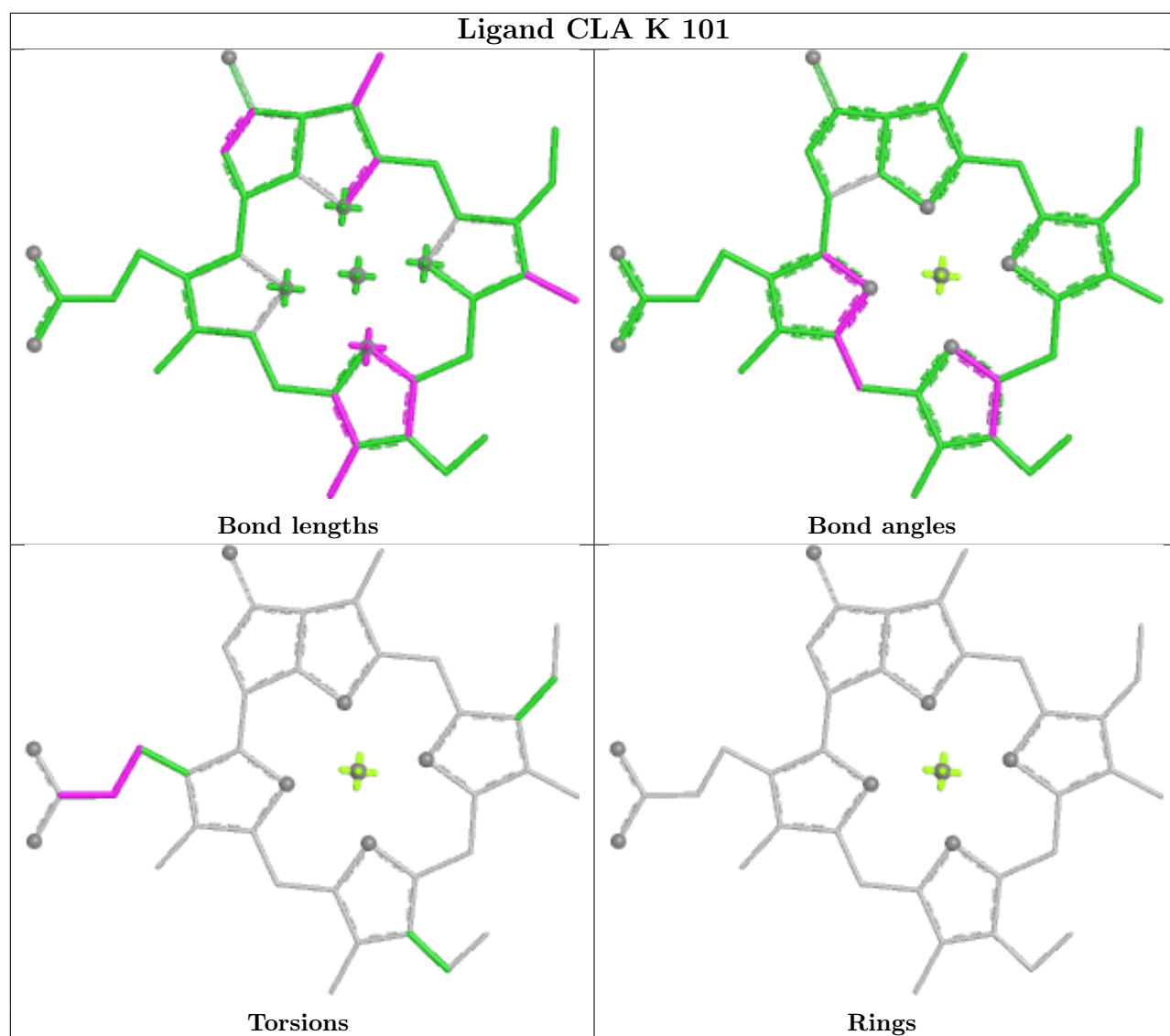




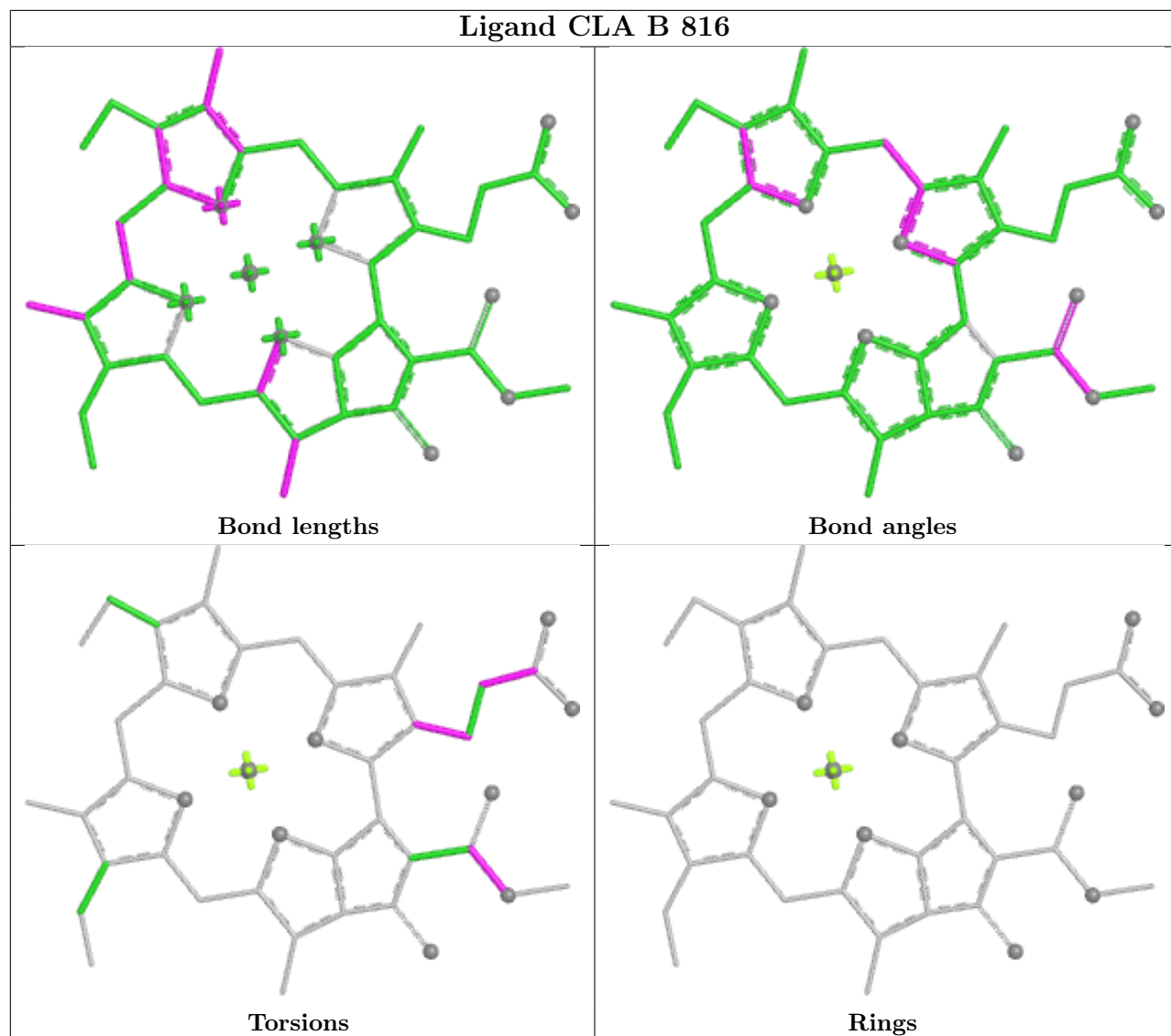


## Ligand CLA F 202

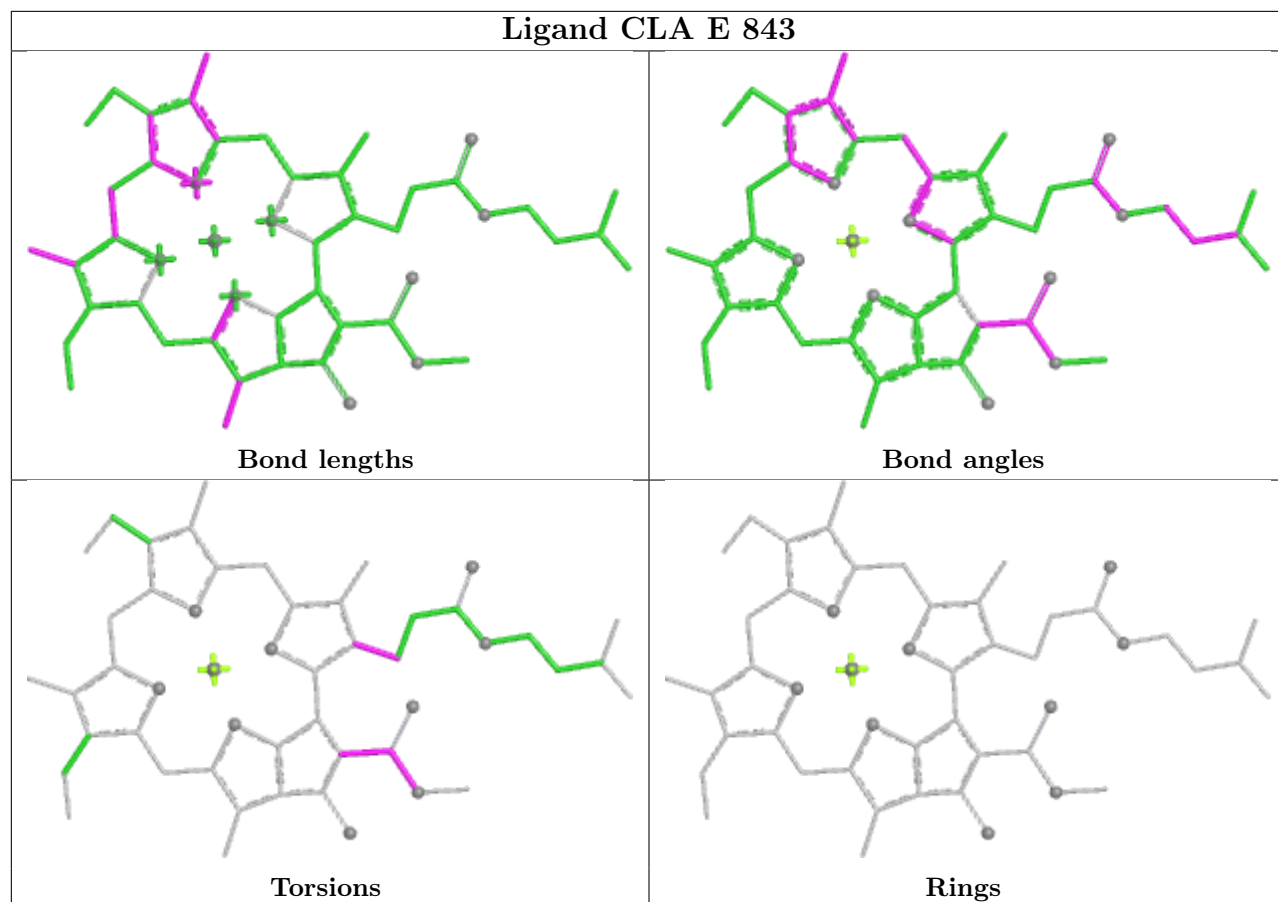


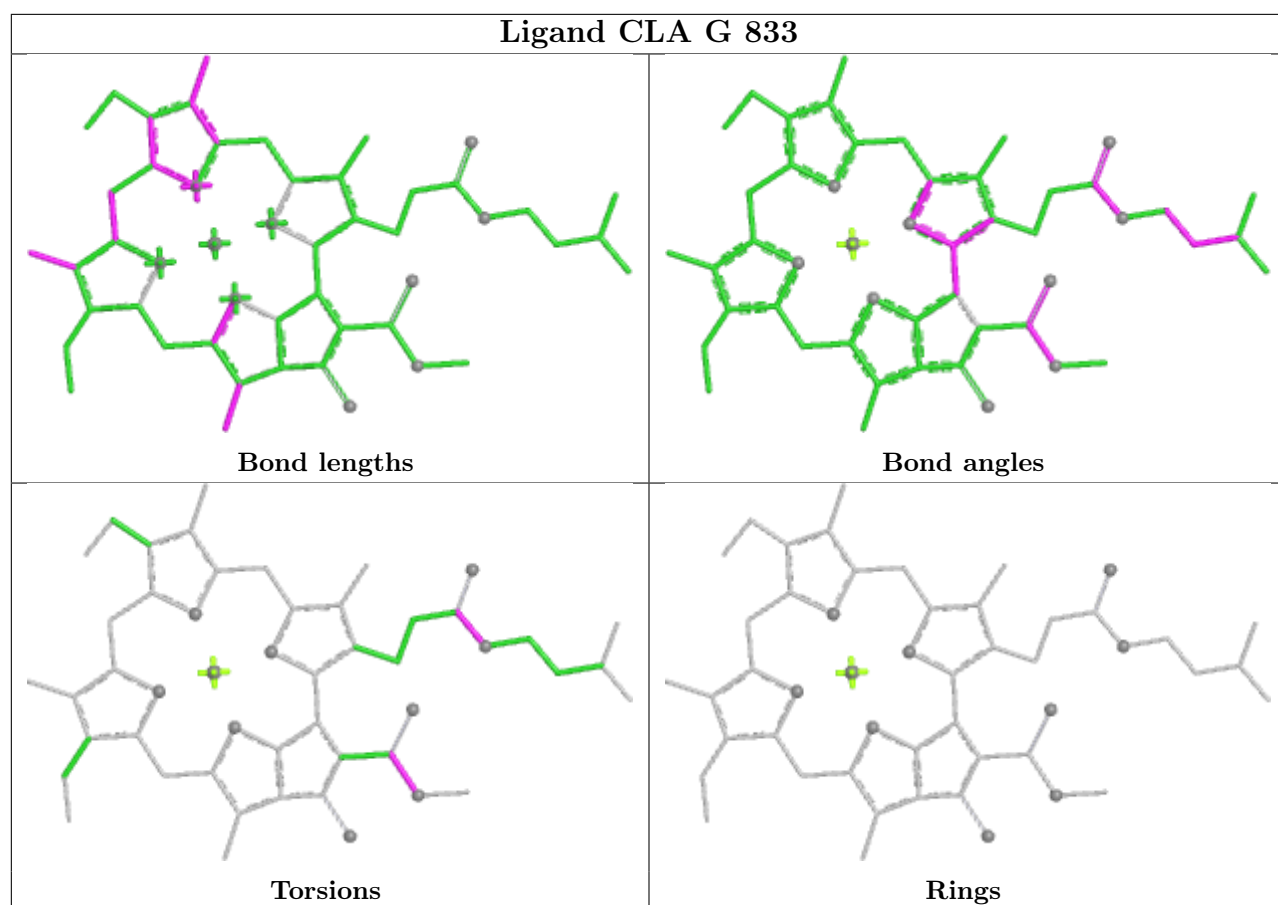


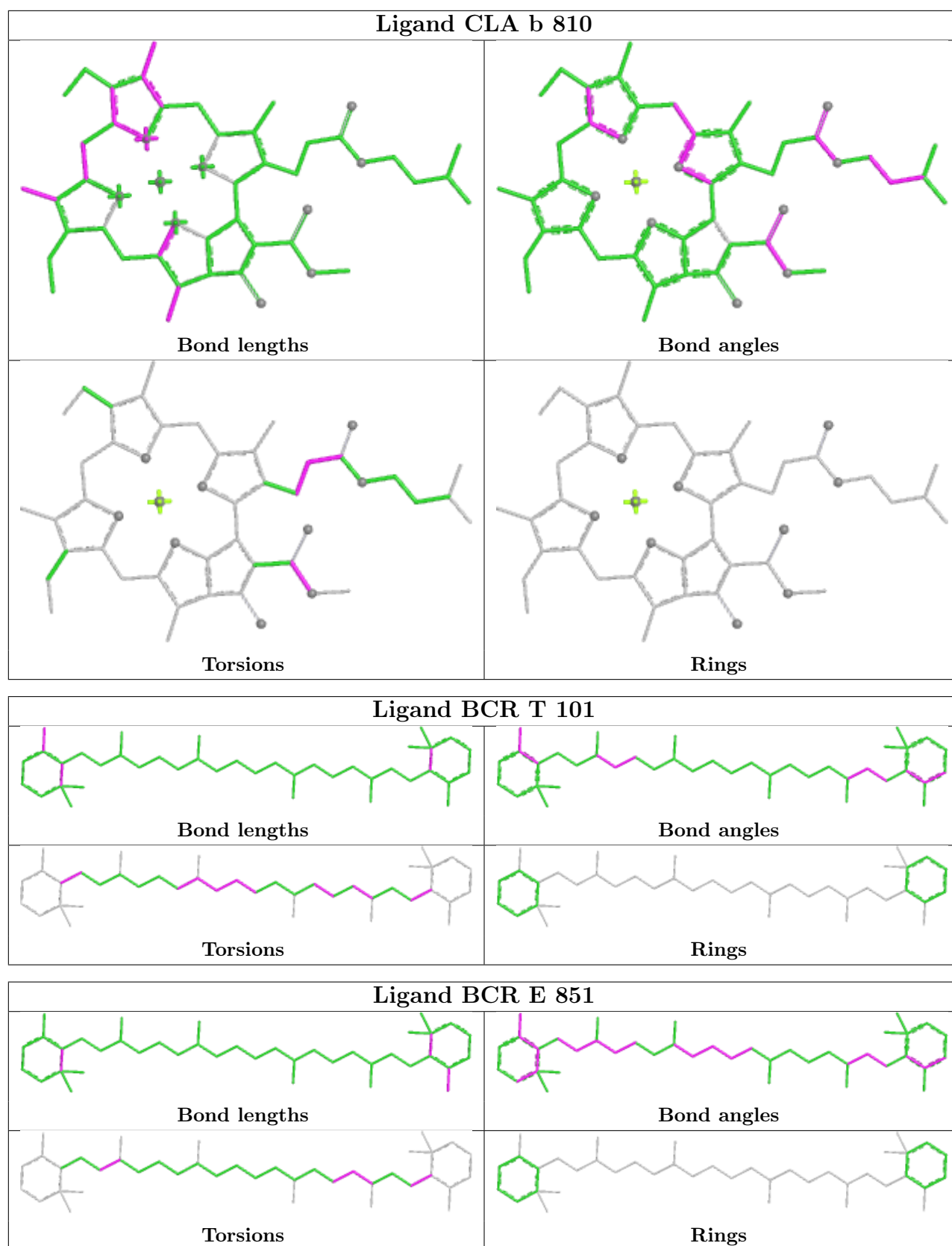
## Ligand CLA B 816



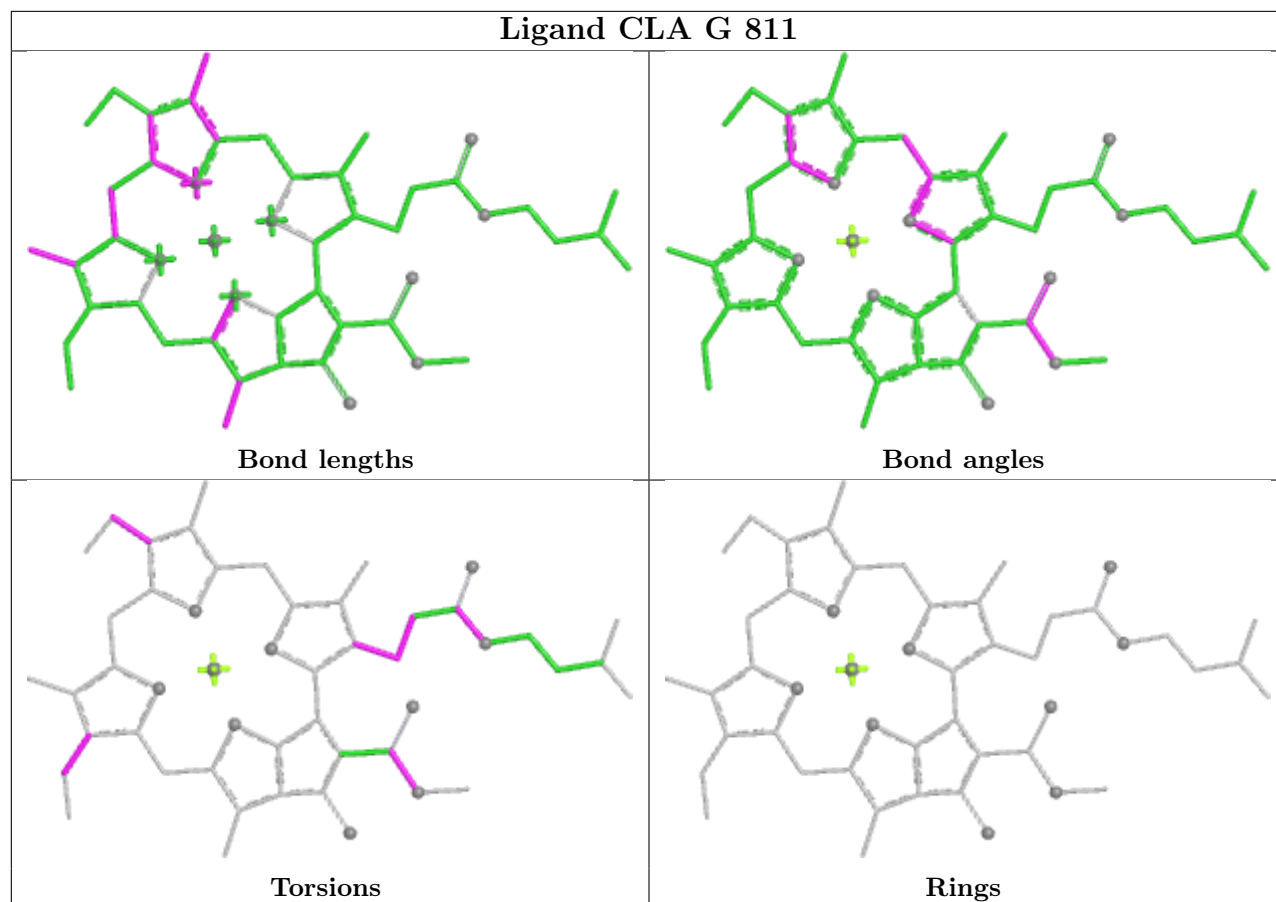
## Ligand CLA E 843





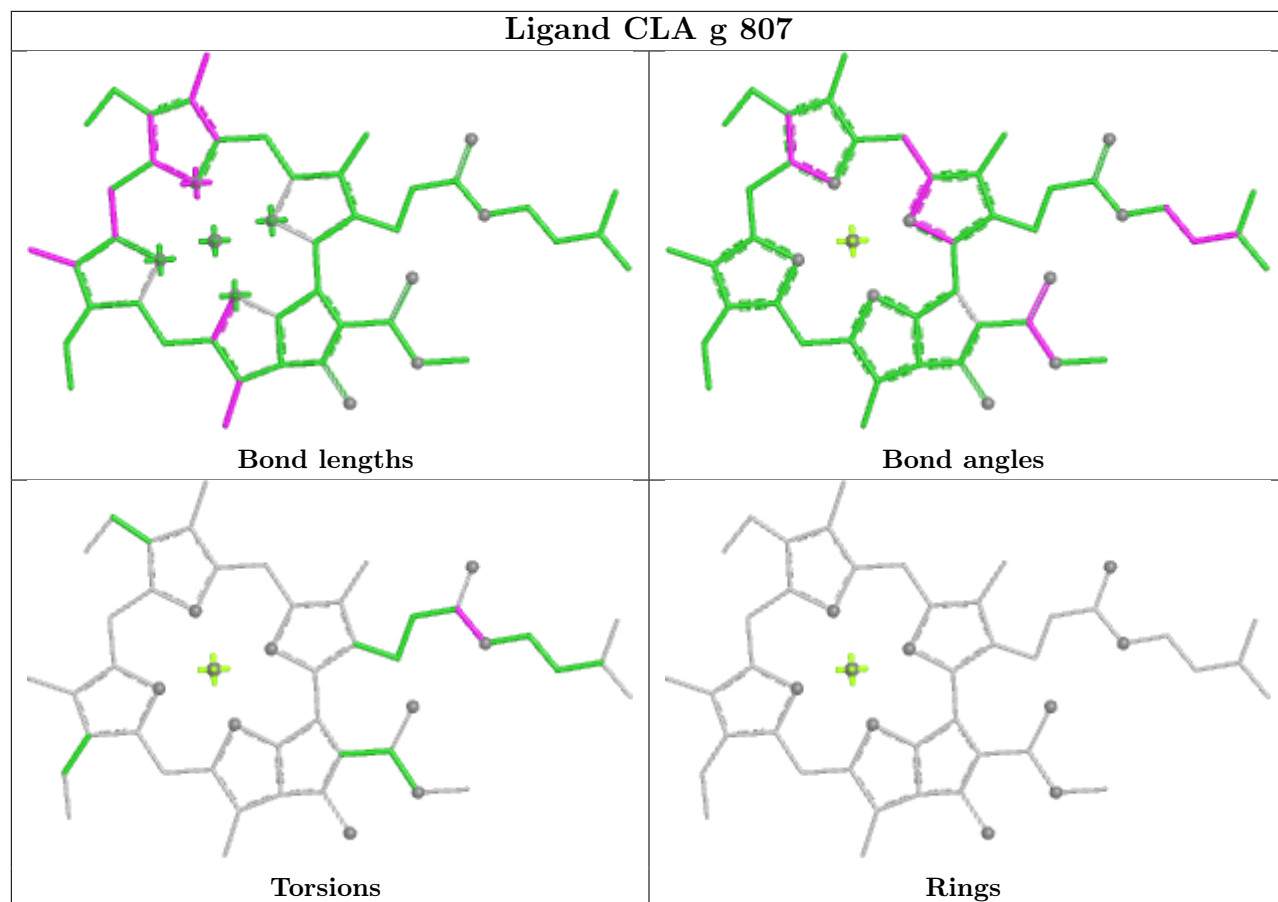


## Ligand CLA G 811

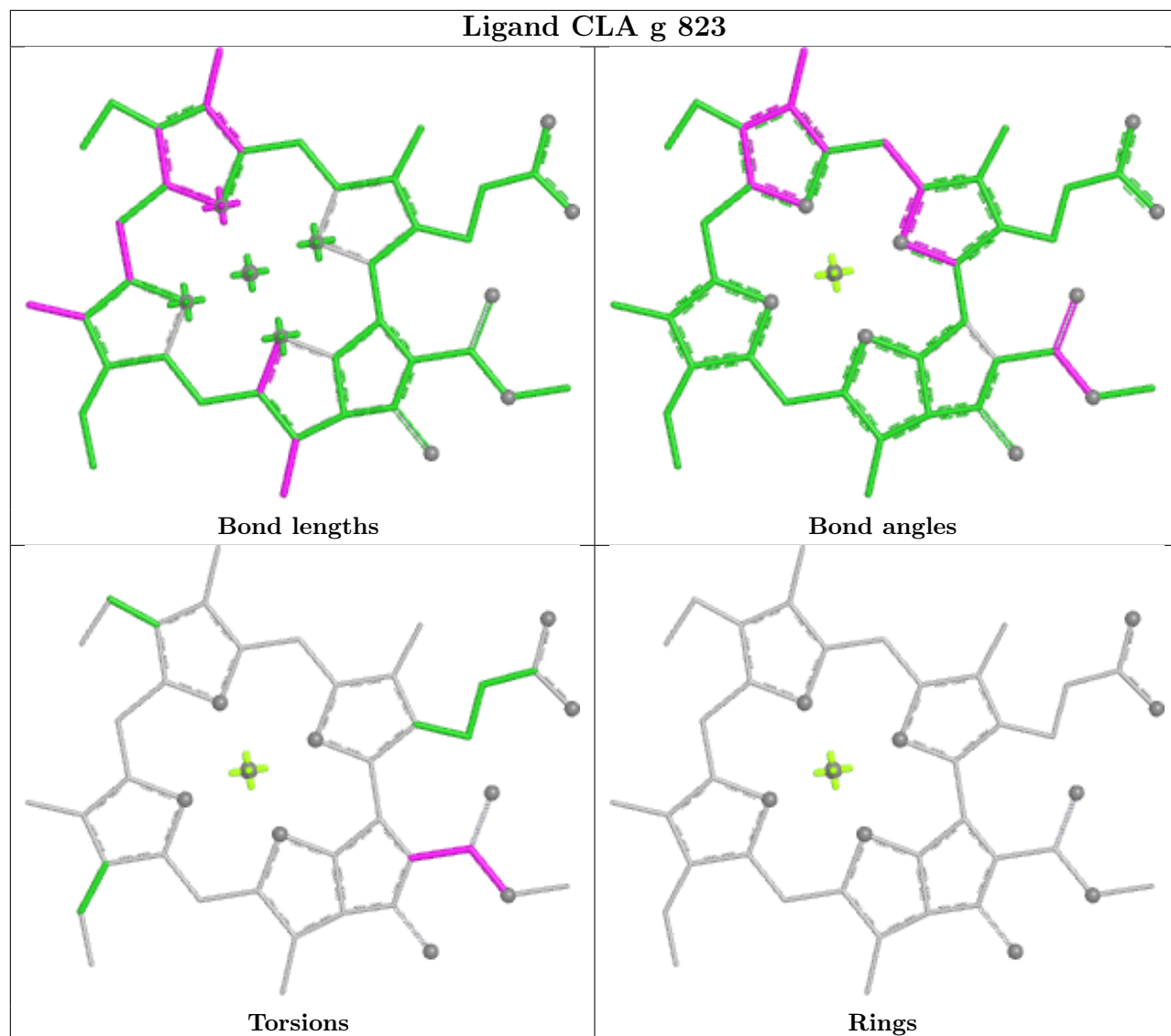




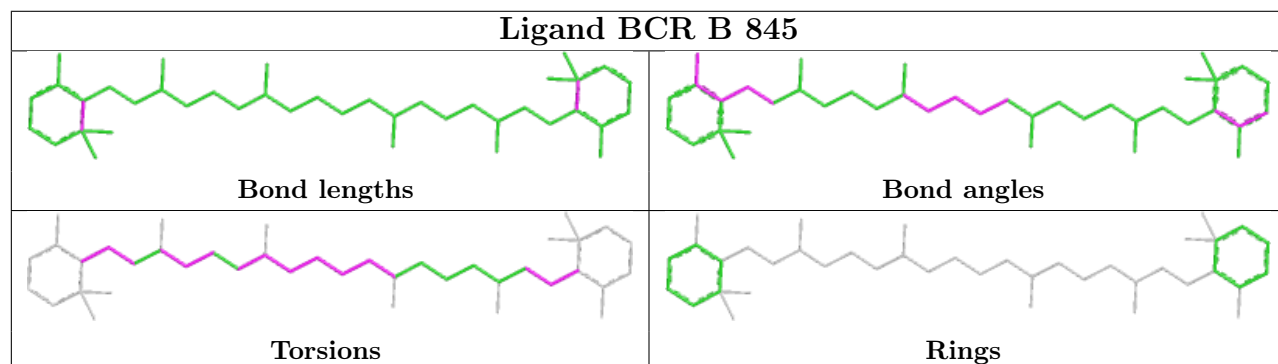
## Ligand CLA g 807

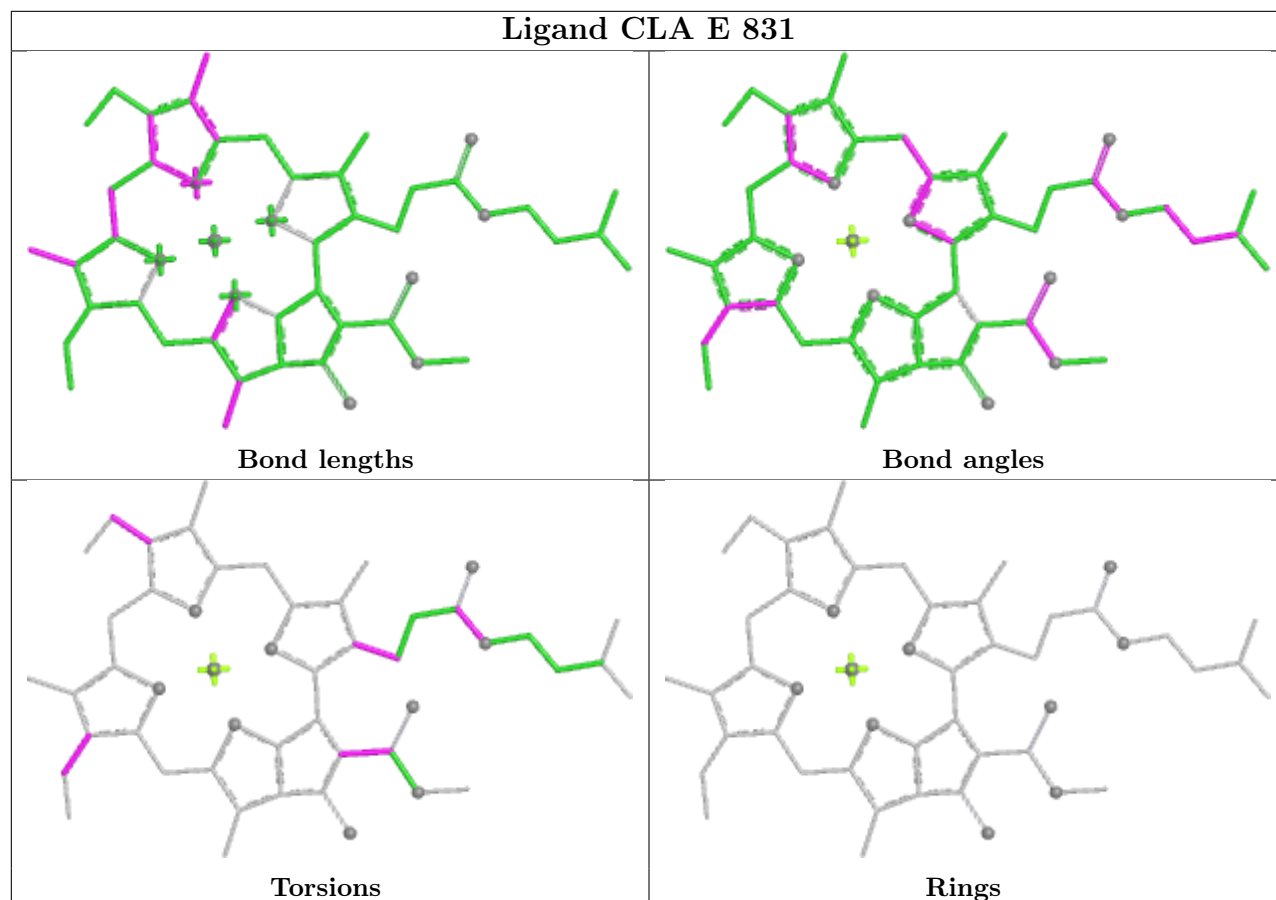
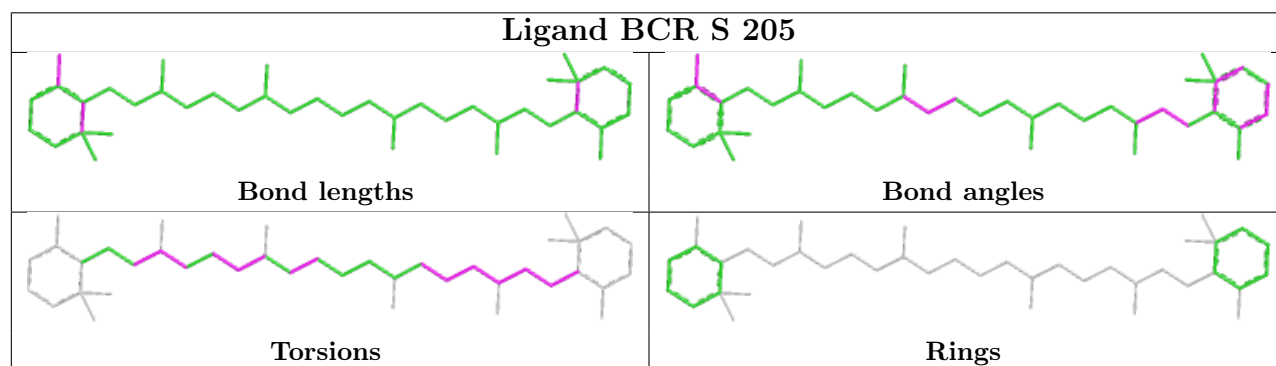
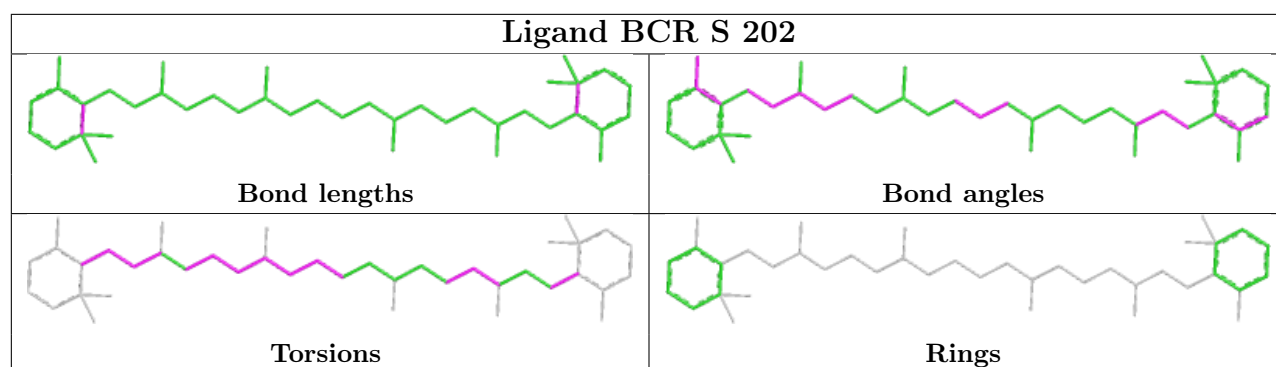


## Ligand CLA g 823

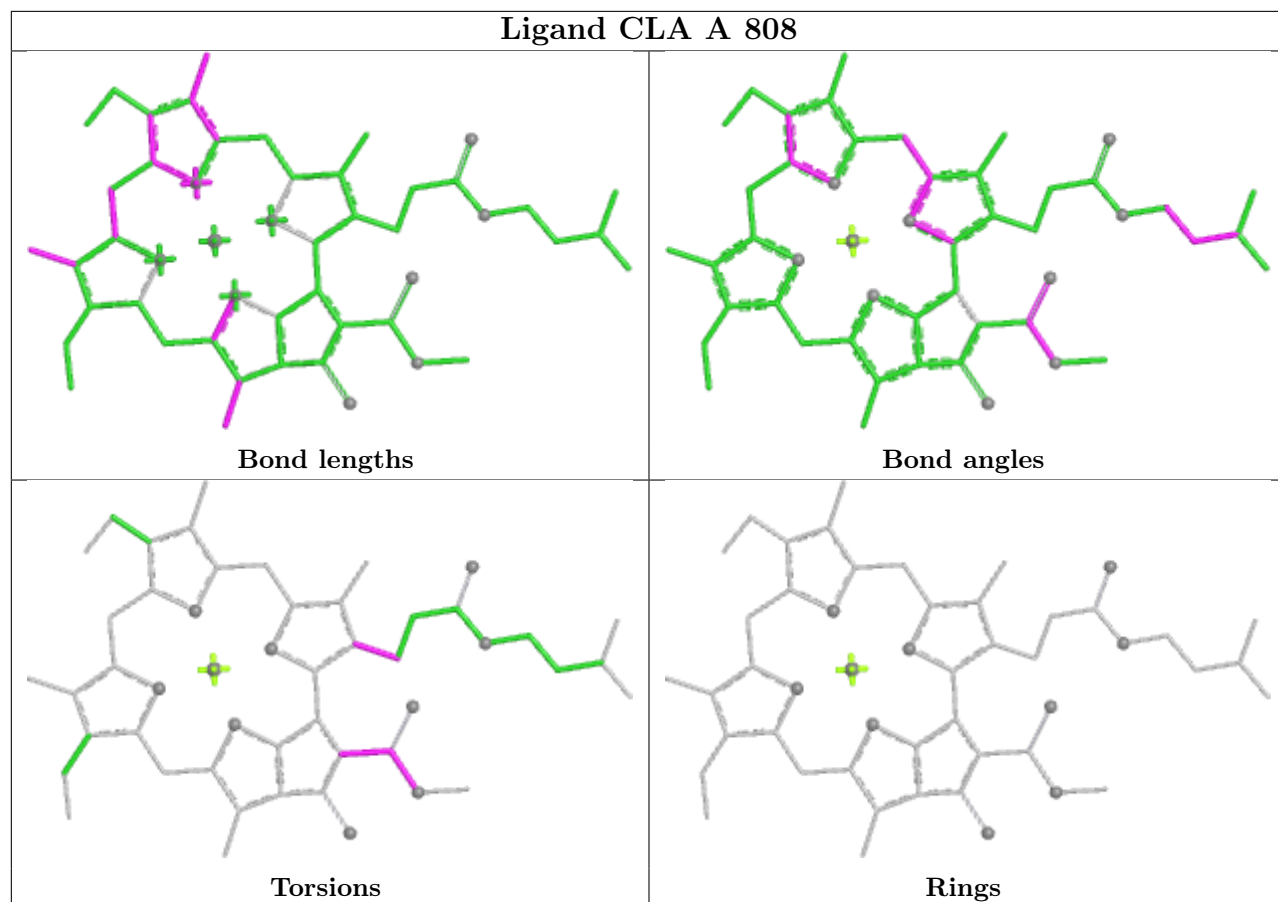


## Ligand BCR B 845

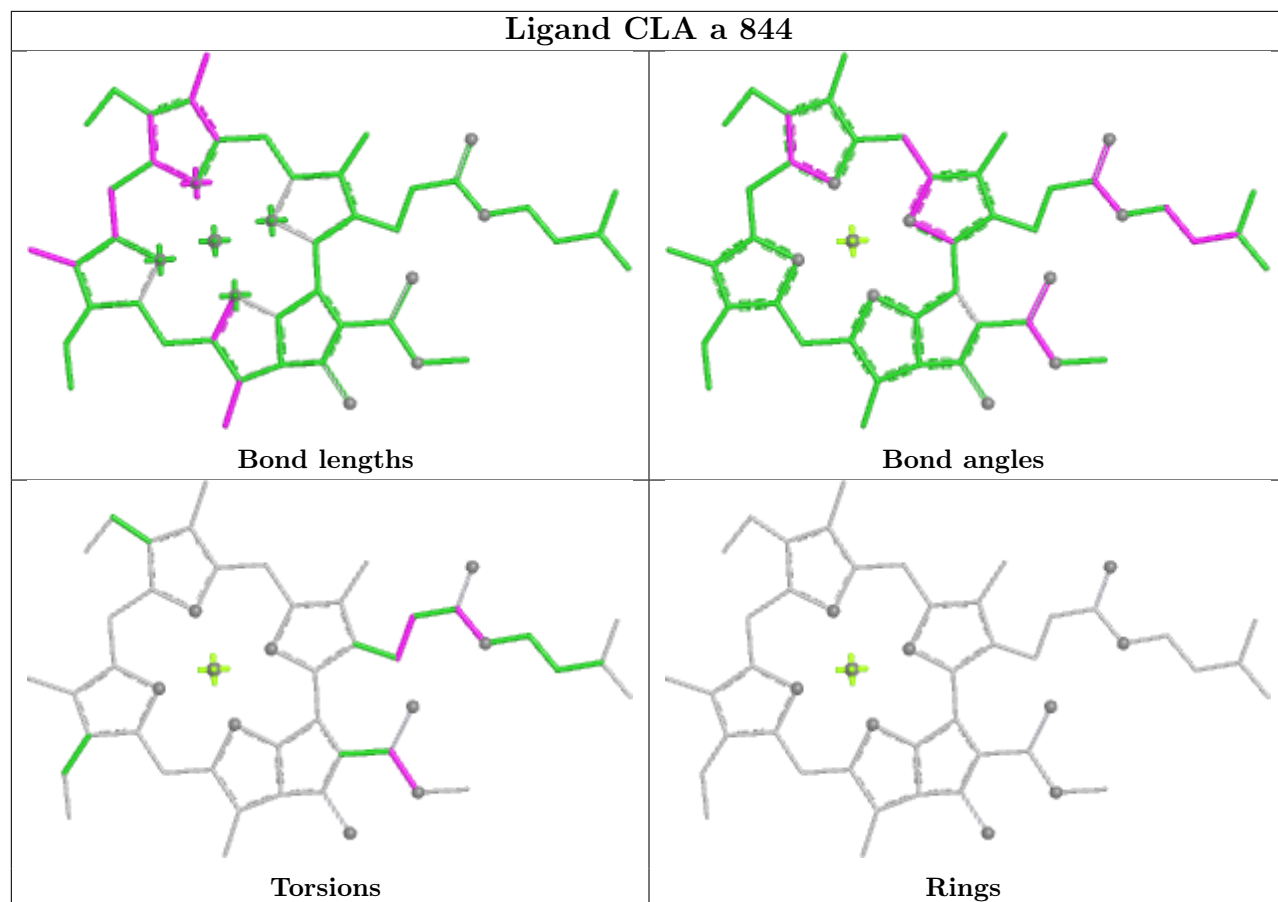




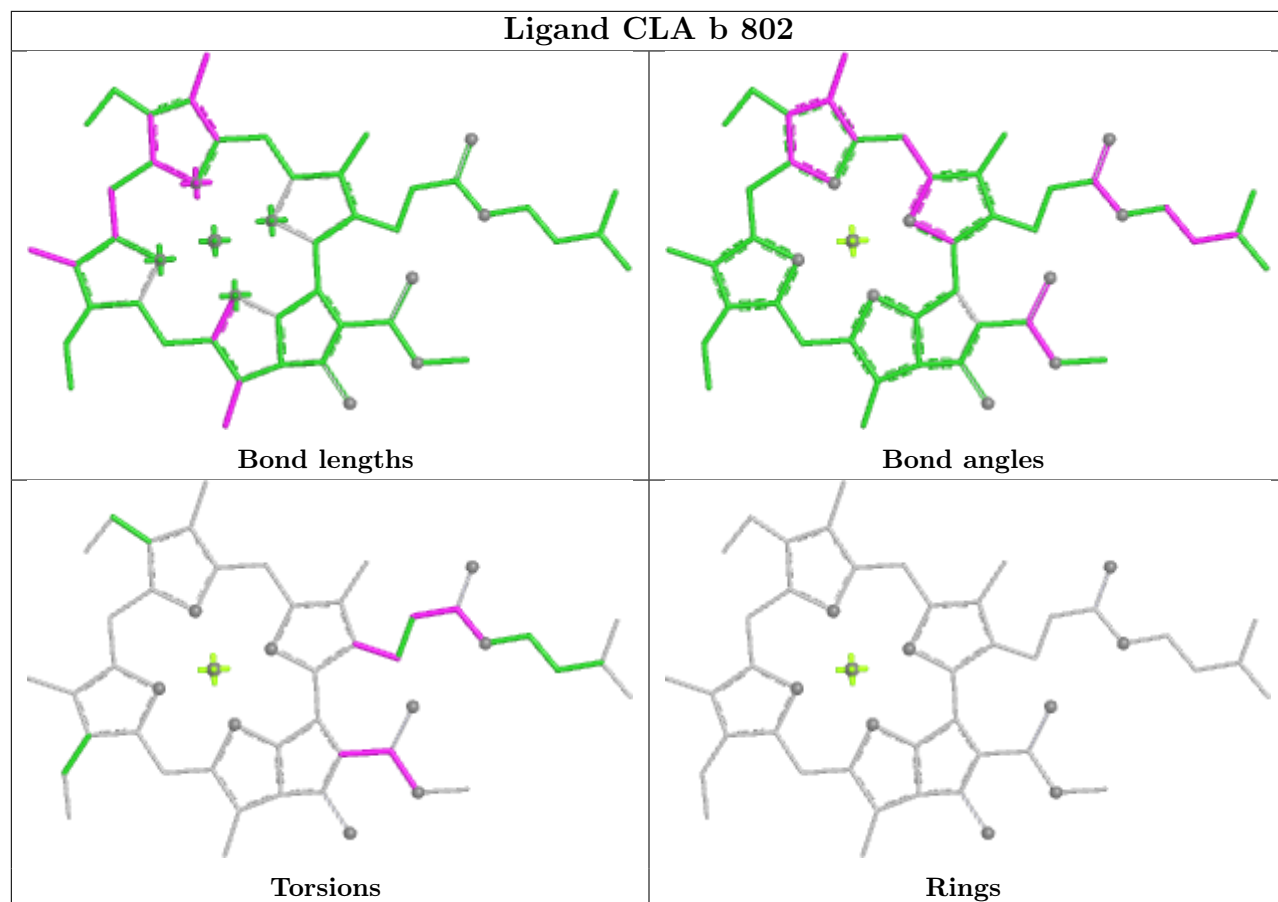
## Ligand CLA A 808



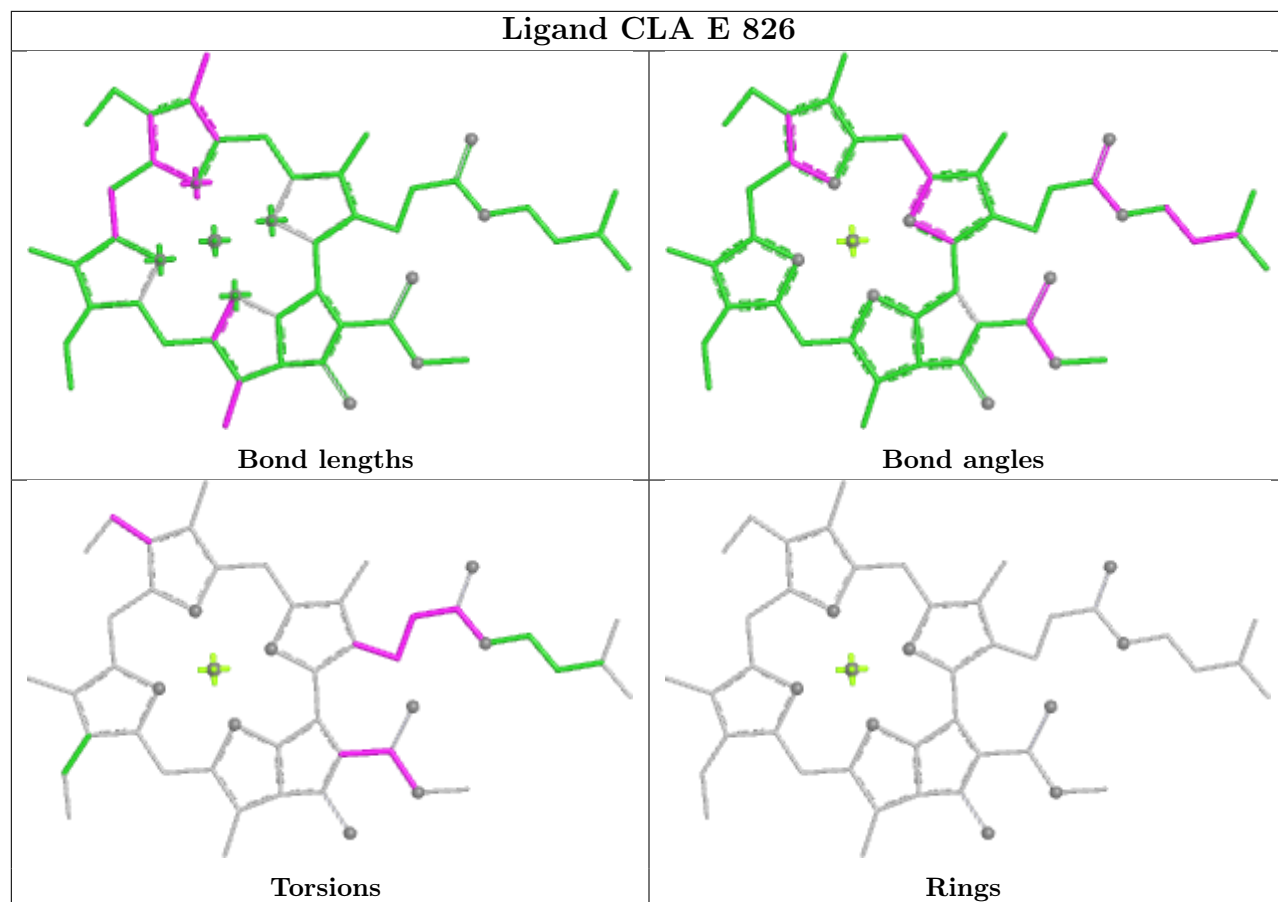
## Ligand CLA a 844



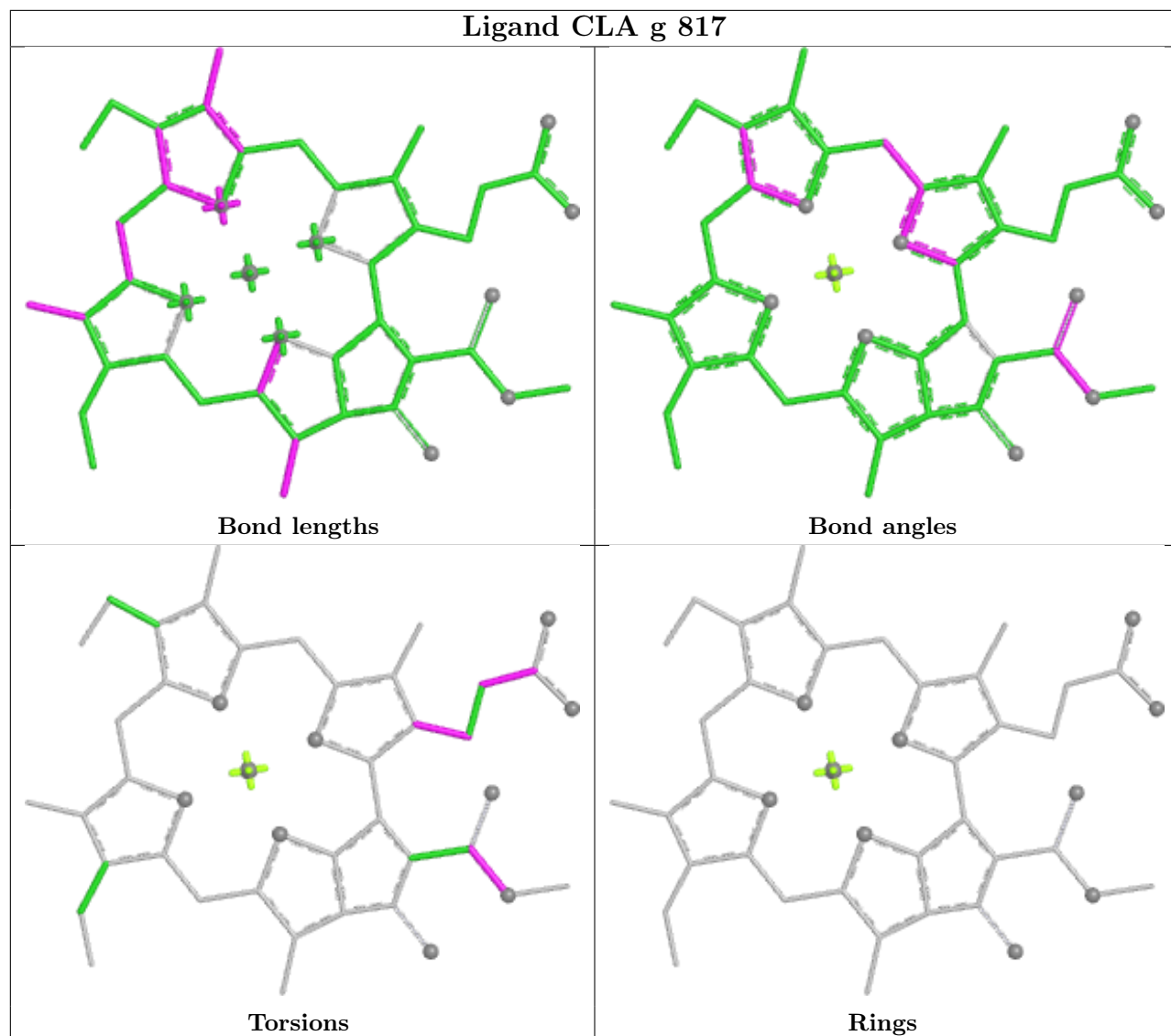
## Ligand CLA b 802



## Ligand CLA E 826

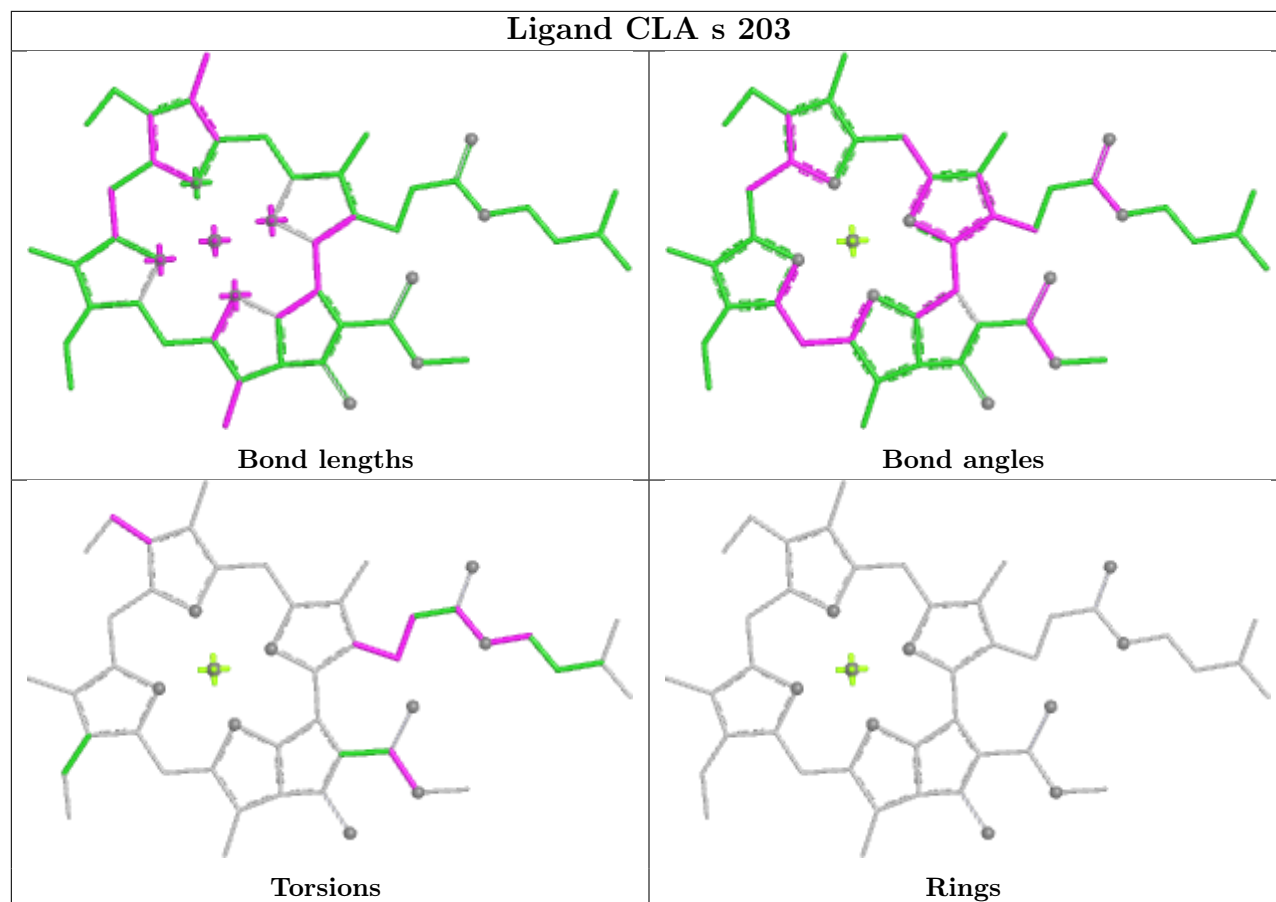


## Ligand CLA g 817

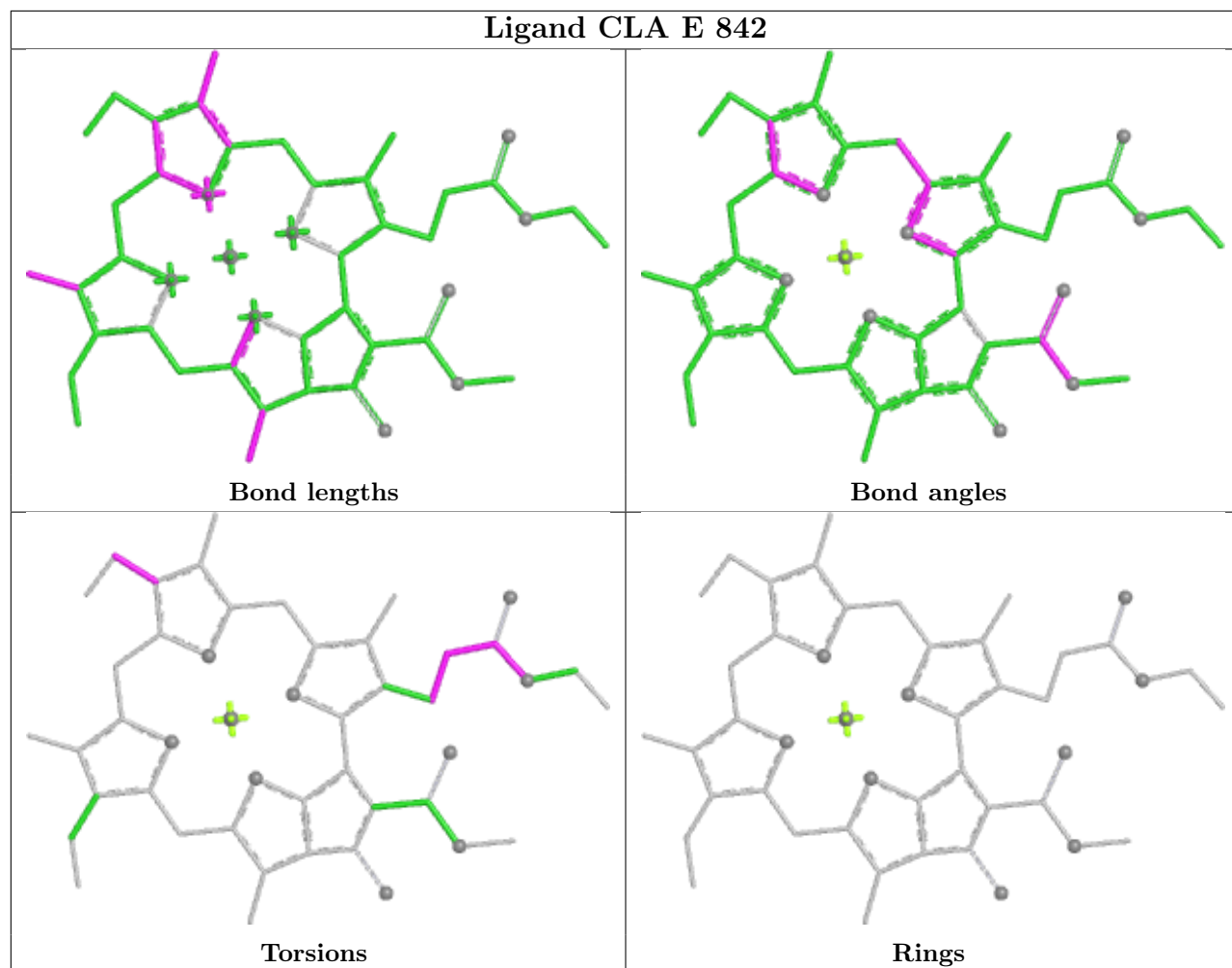




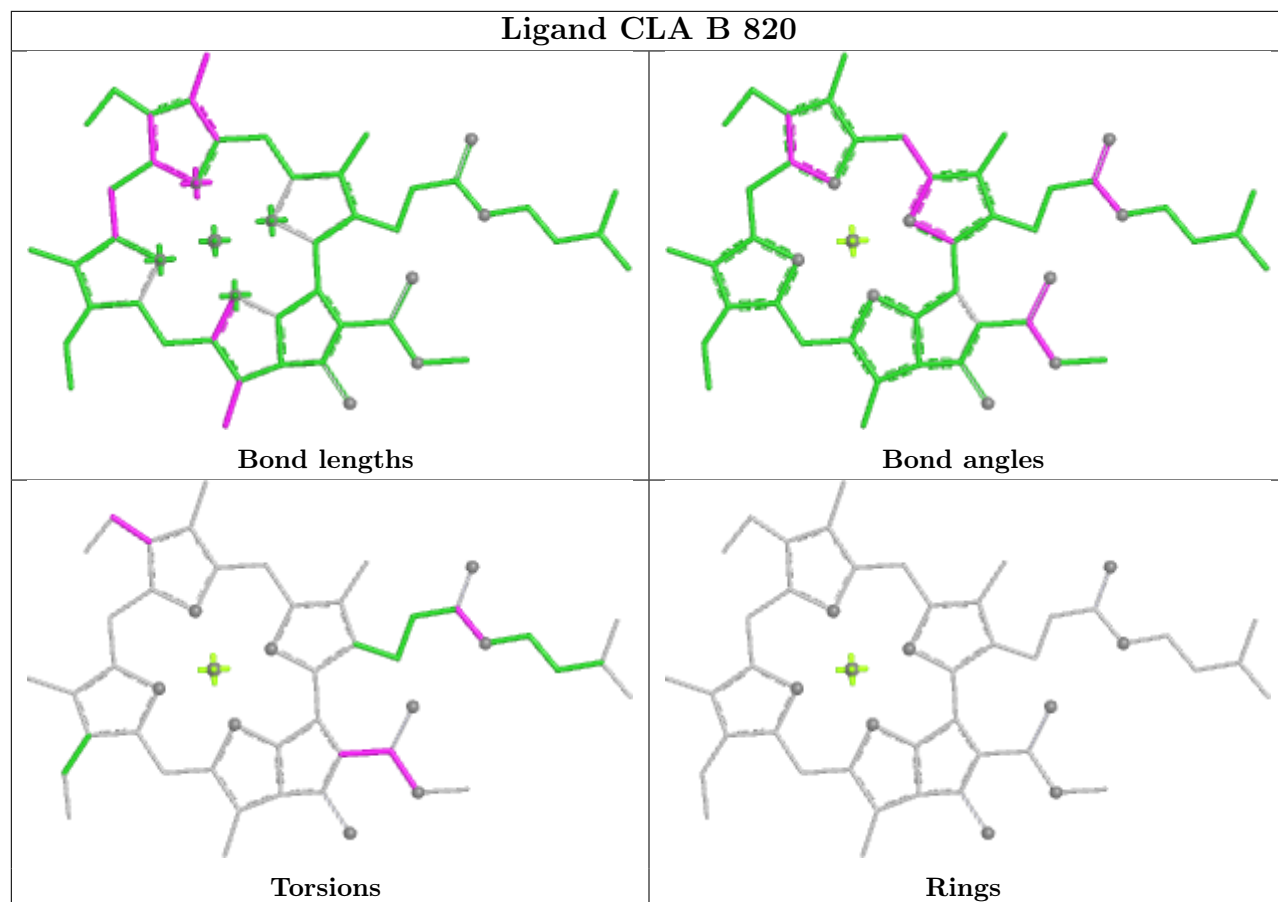
## Ligand CLA s 203



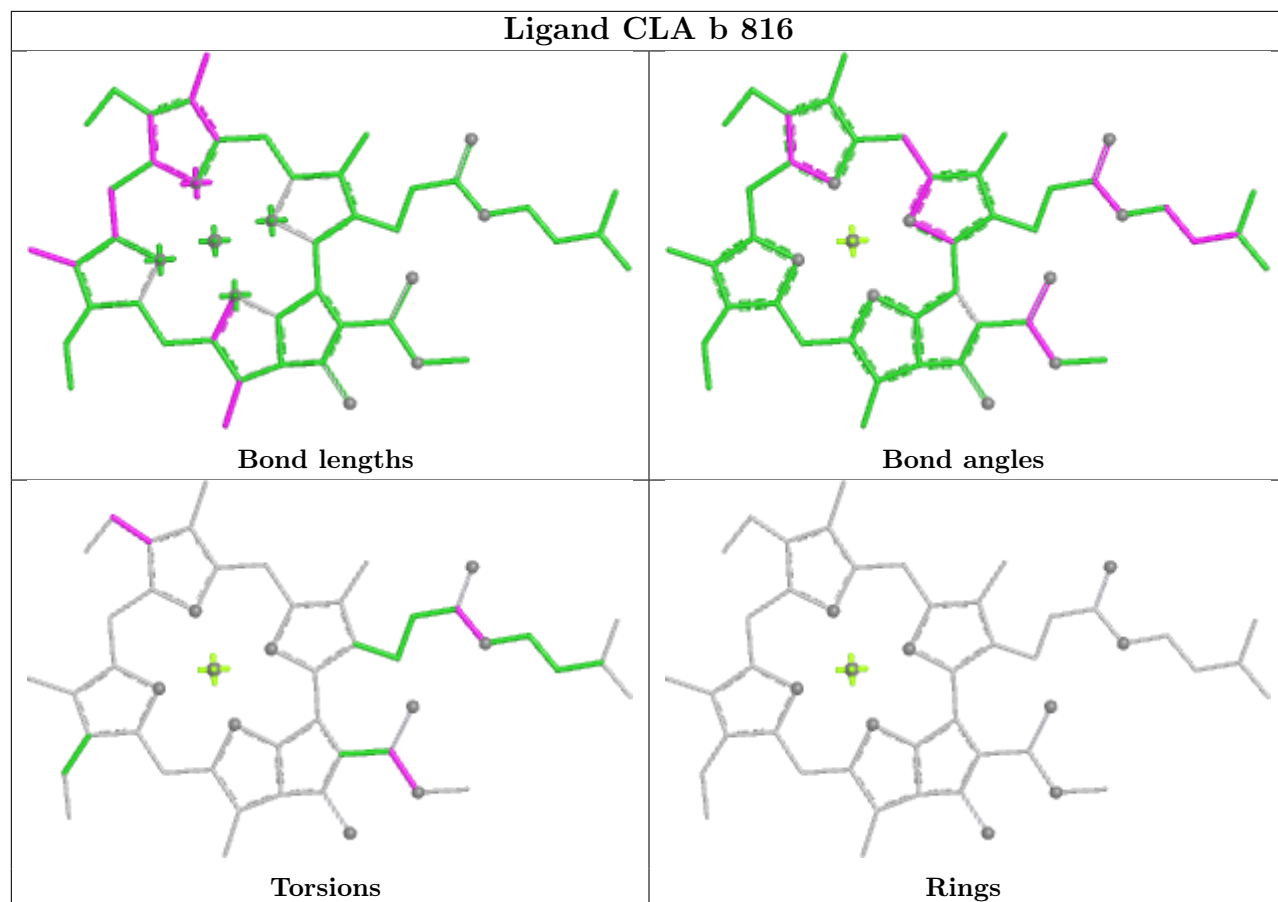
## Ligand CLA E 842

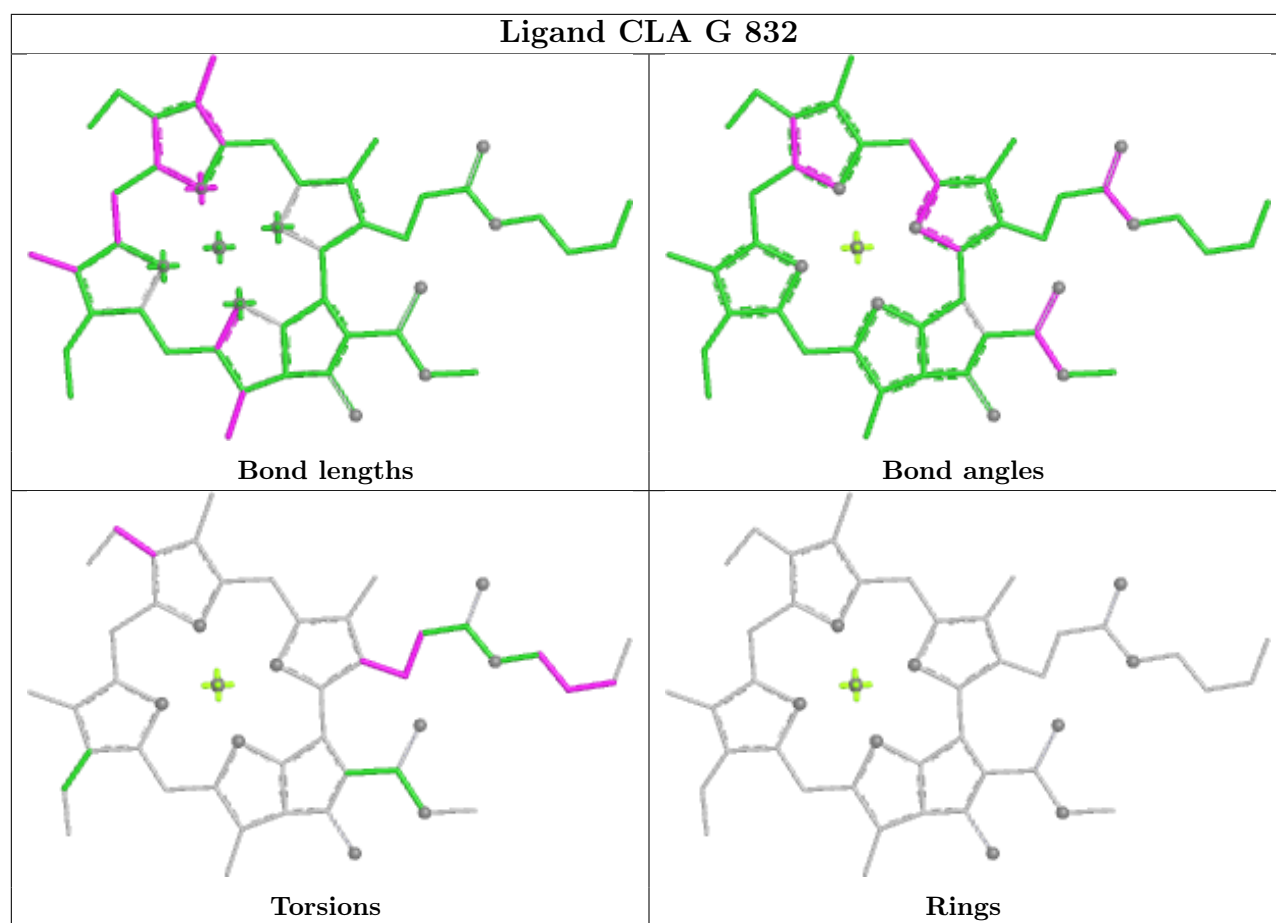


## Ligand CLA B 820

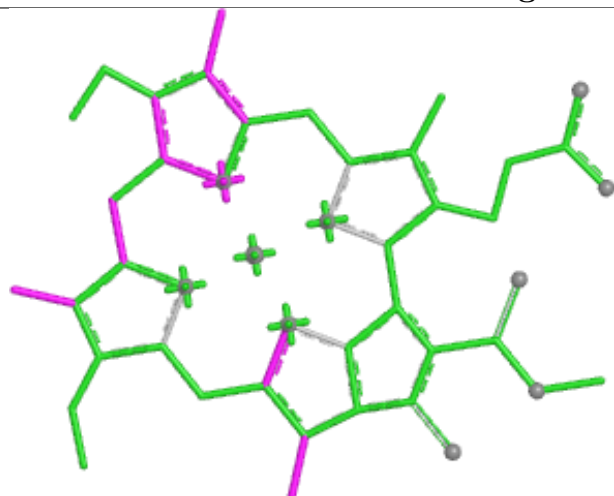


## Ligand CLA b 816

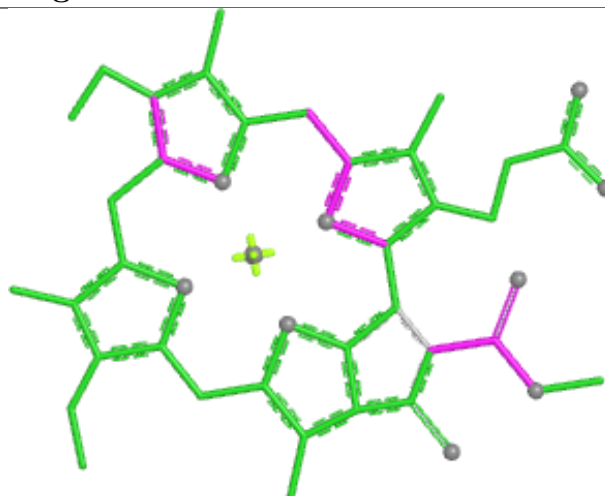




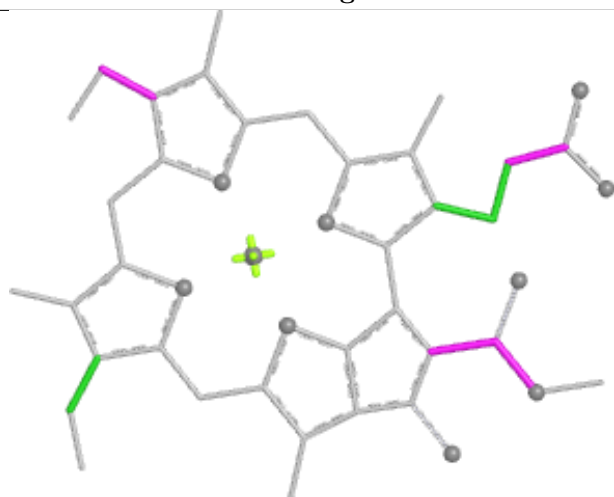
## Ligand CLA g 825



Bond lengths



Bond angles

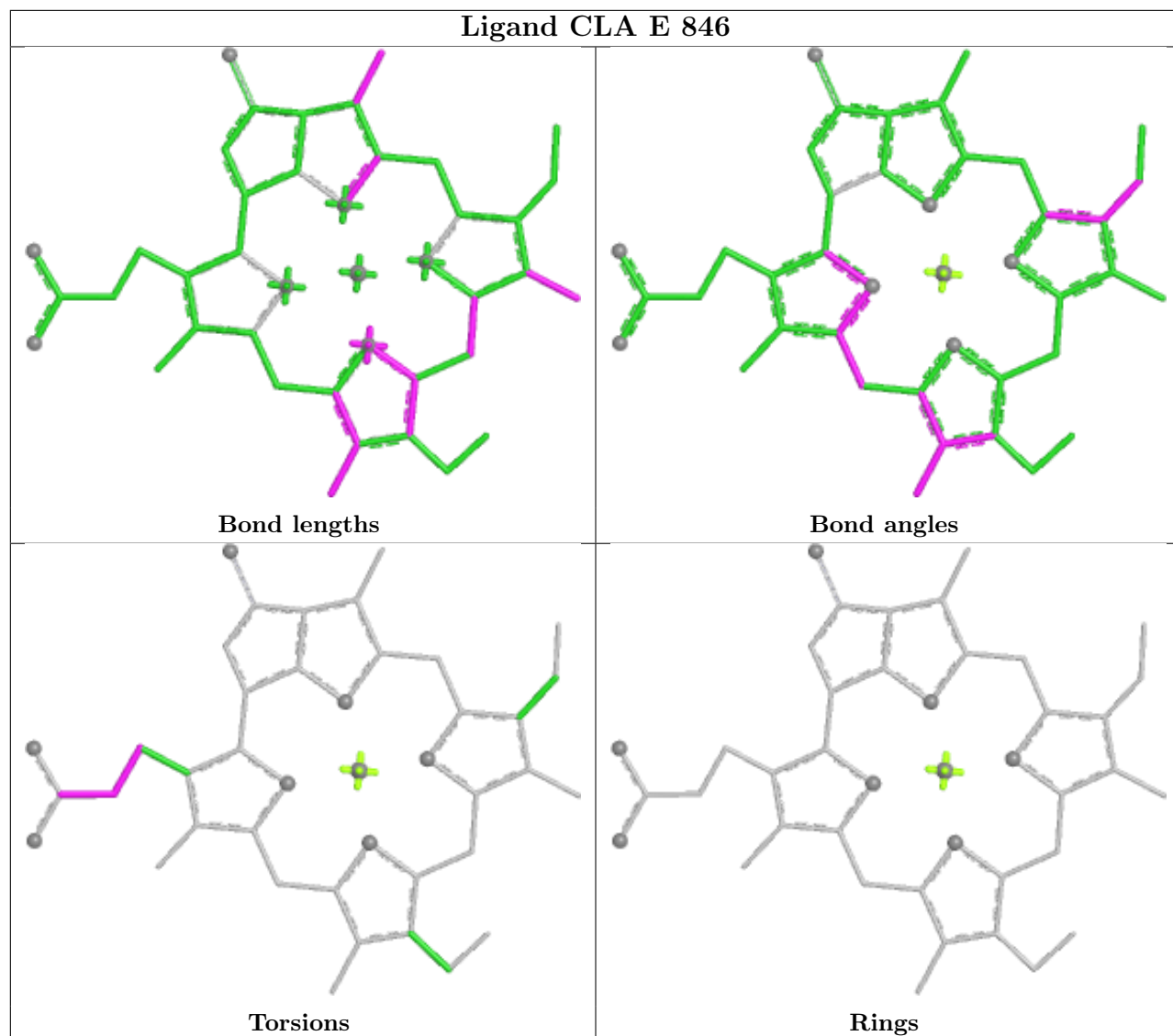


Torsions

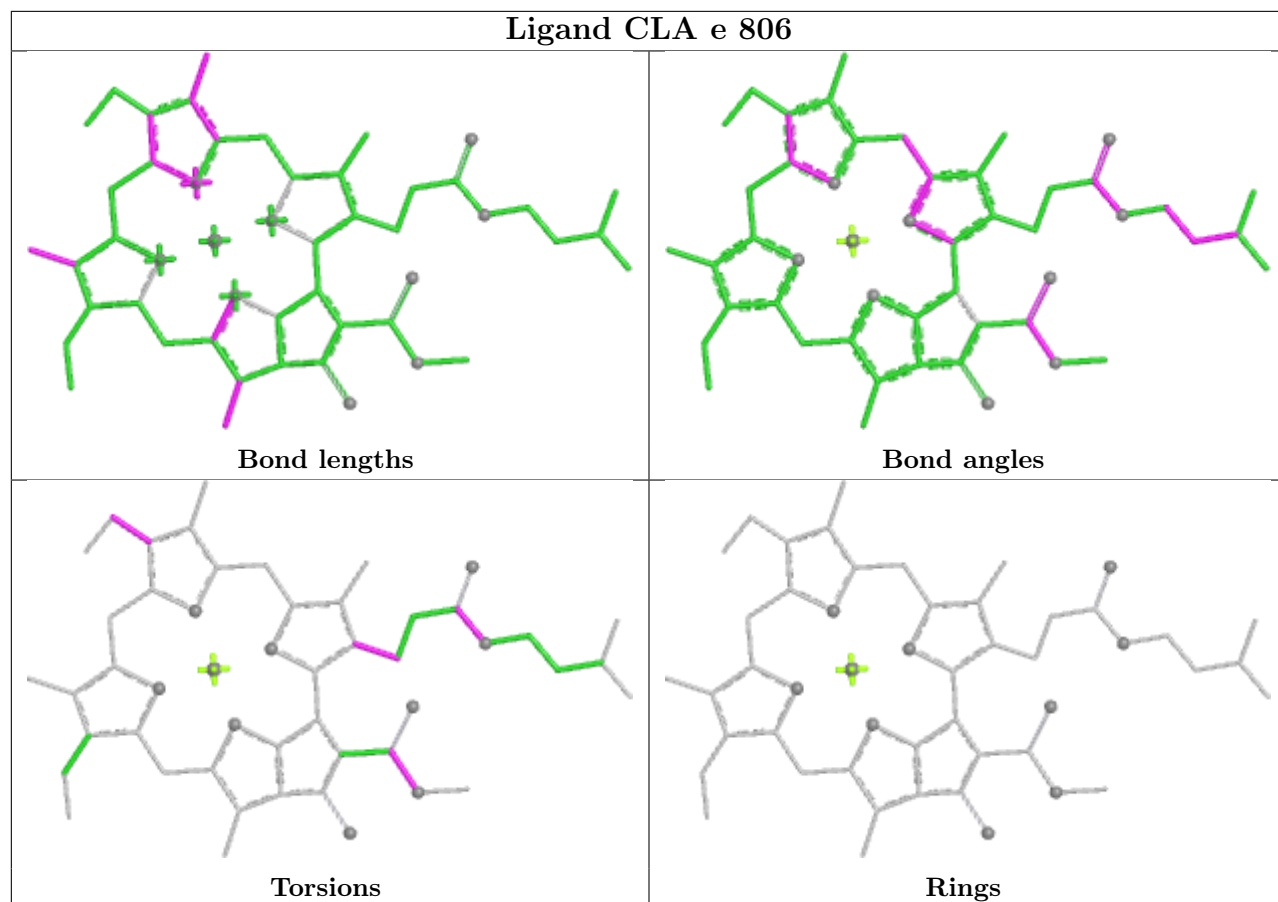


Rings

## Ligand CLA E 846

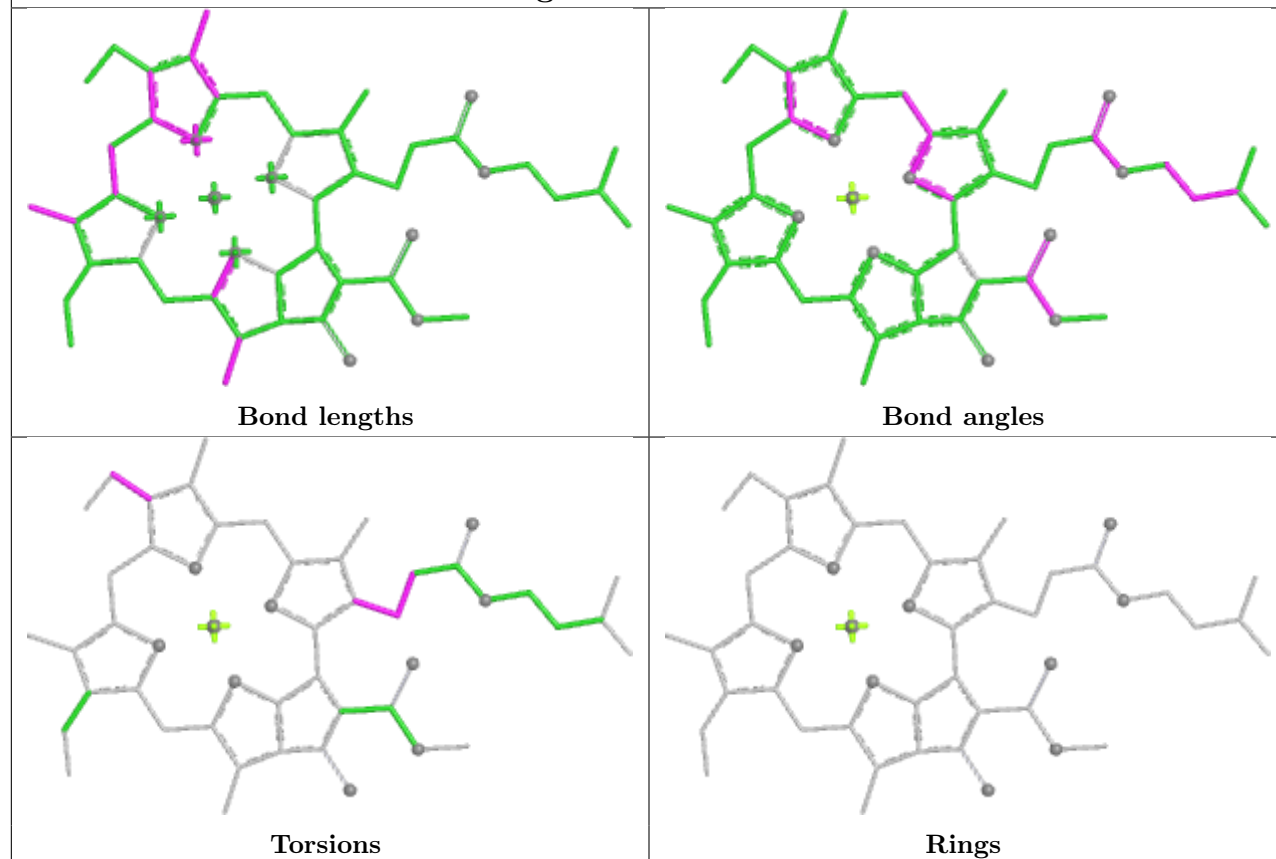


## Ligand CLA e 806

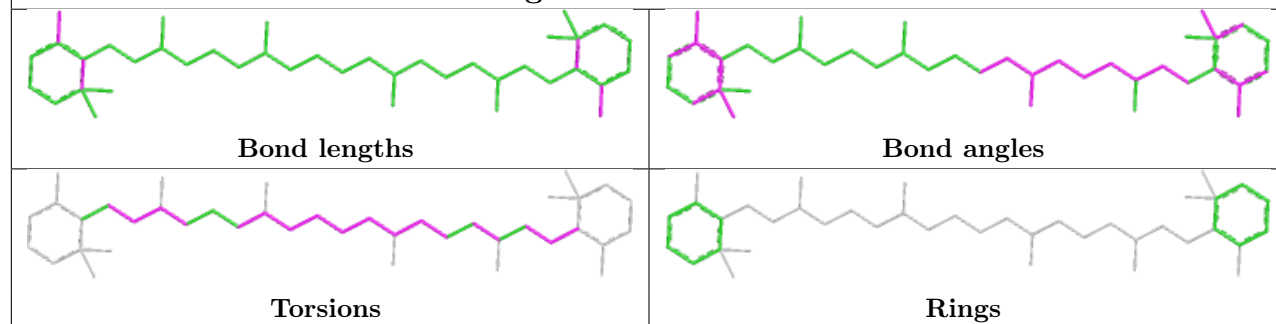


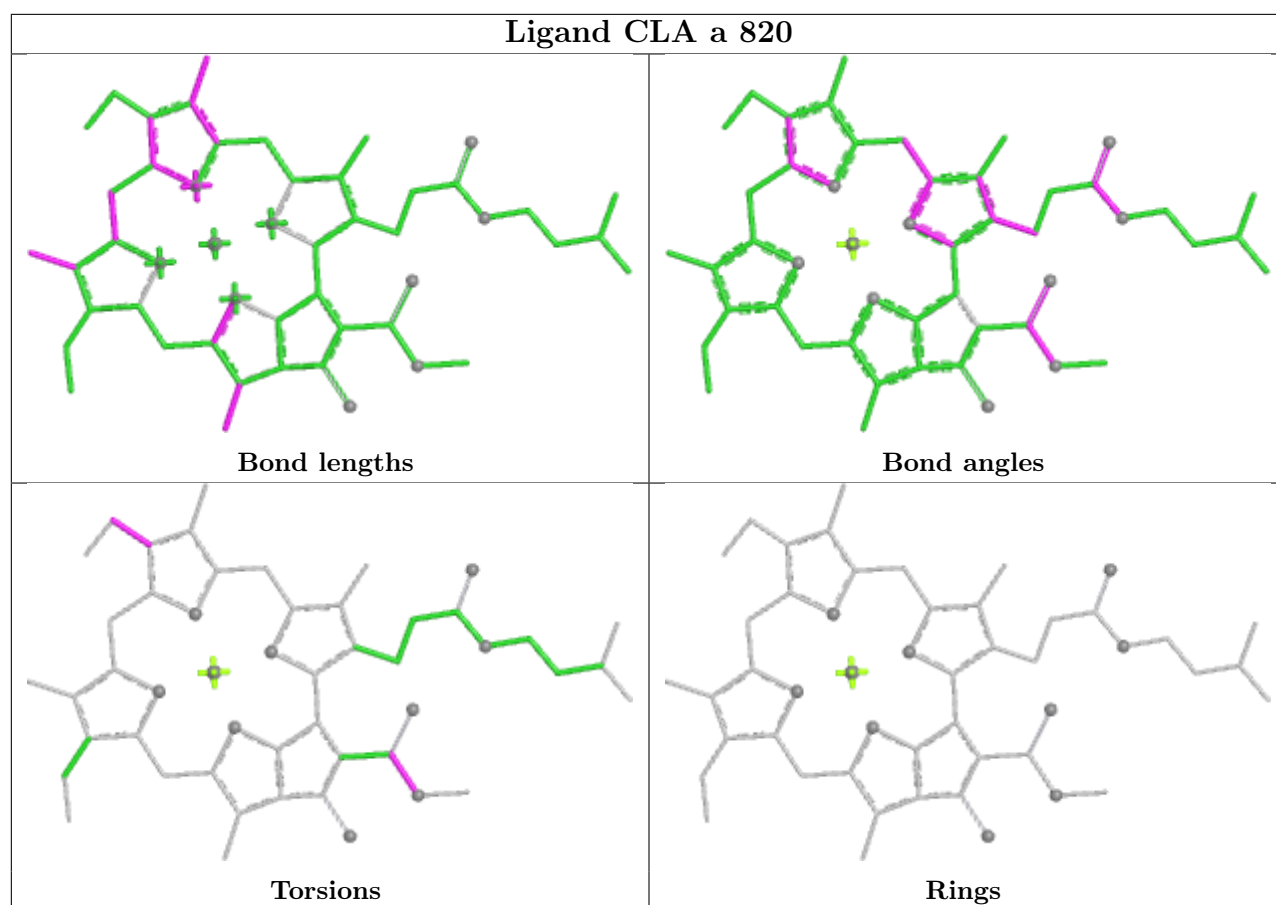


## Ligand CLA a 811



## Ligand BCR k 4001





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

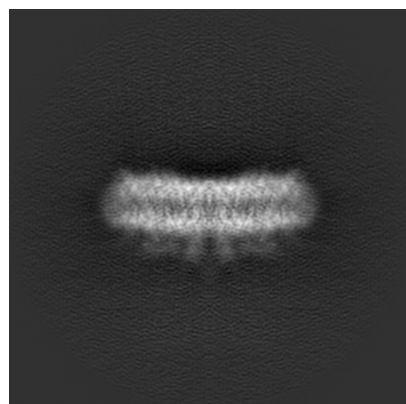
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13898. These allow visual inspection of the internal detail of the map and identification of artifacts.

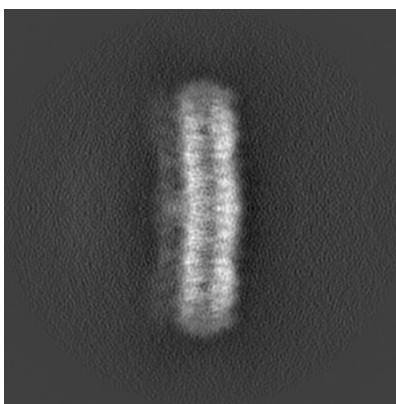
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

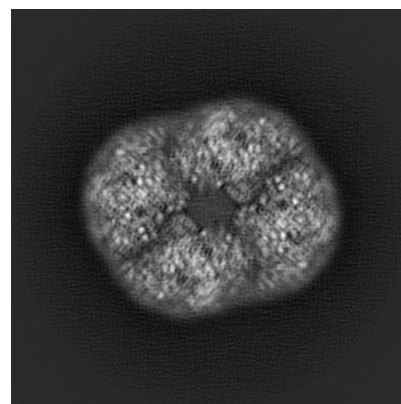
#### 6.1.1 Primary map



X

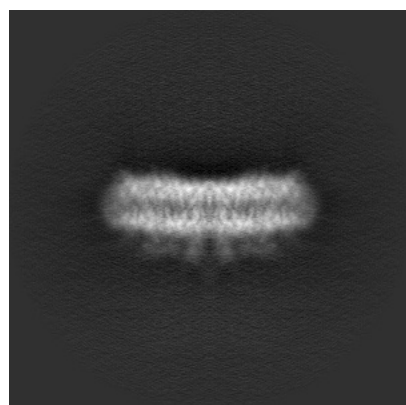


Y

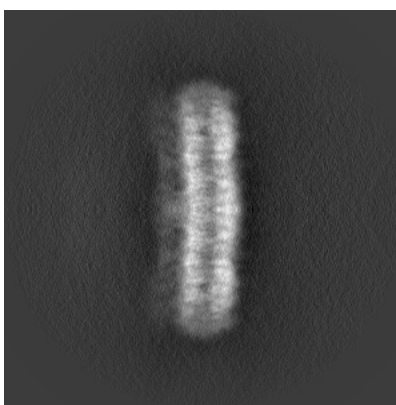


Z

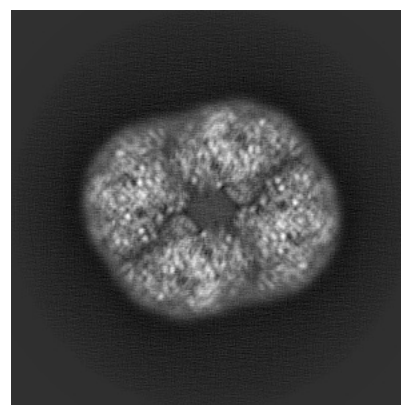
#### 6.1.2 Raw map



X



Y

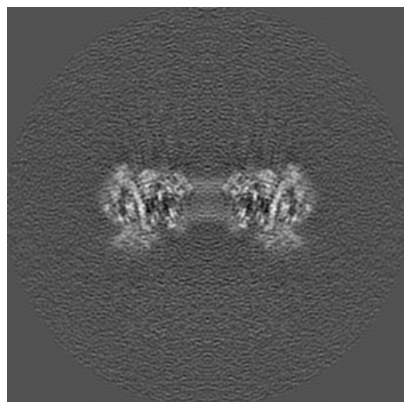


Z

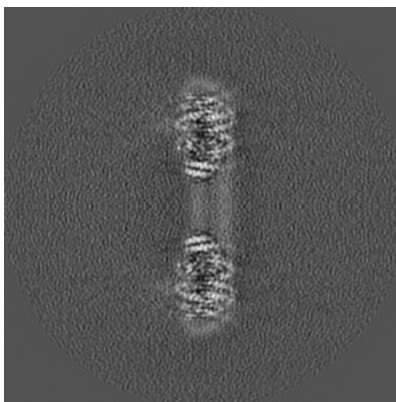
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

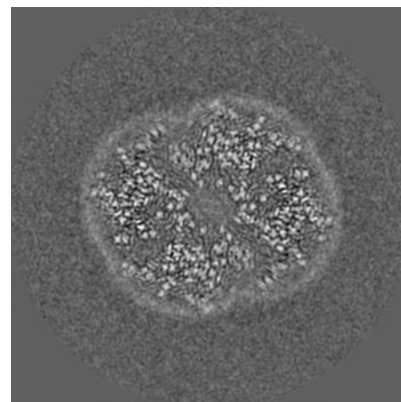
### 6.2.1 Primary map



X Index: 192

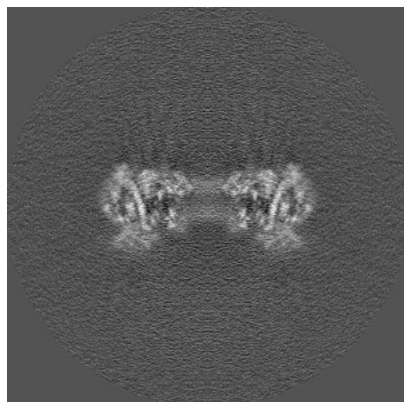


Y Index: 192

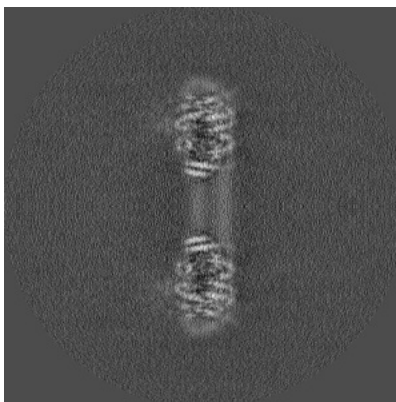


Z Index: 192

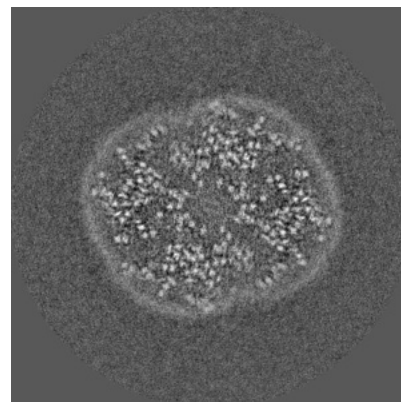
### 6.2.2 Raw map



X Index: 192



Y Index: 192

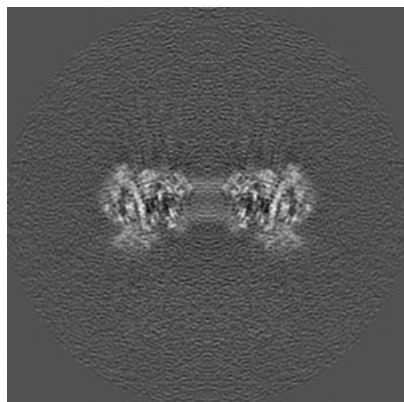


Z Index: 192

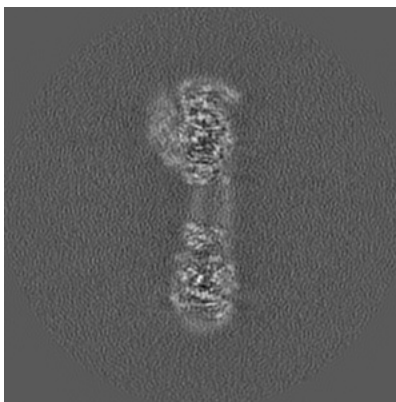
The images above show central slices of the map in three orthogonal directions.

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

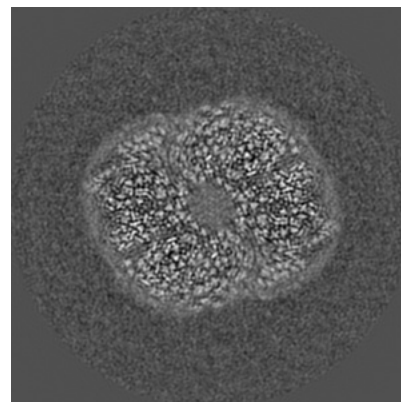
### 6.3.1 Primary map



X Index: 192

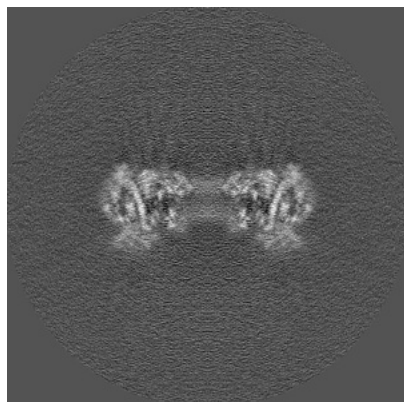


Y Index: 180

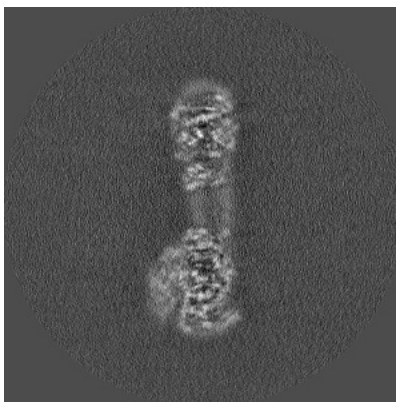


Z Index: 184

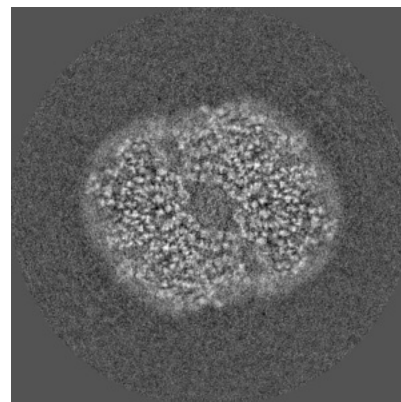
### 6.3.2 Raw map



X Index: 192



Y Index: 204



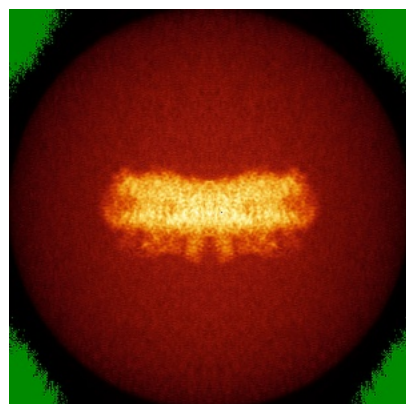
Z Index: 180

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

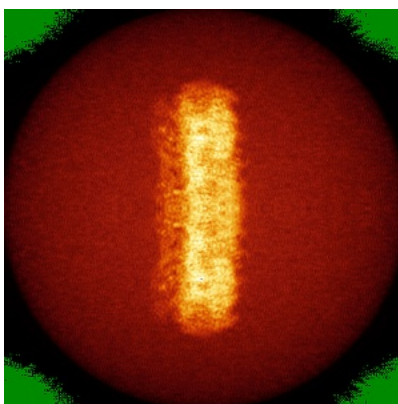


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

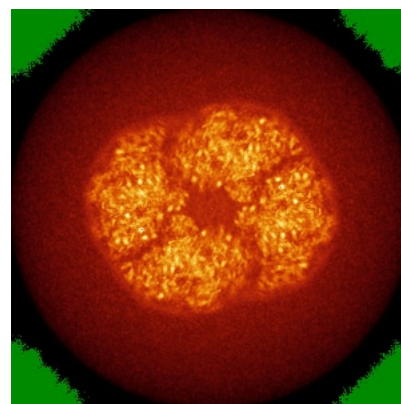
### 6.4.1 Primary map



X

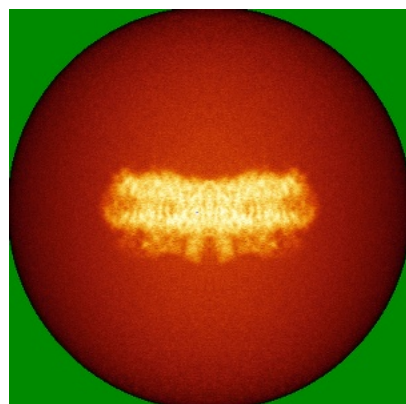


Y

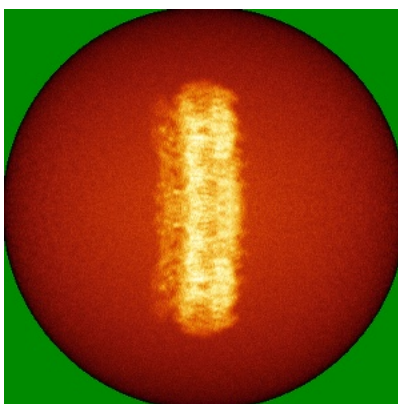


Z

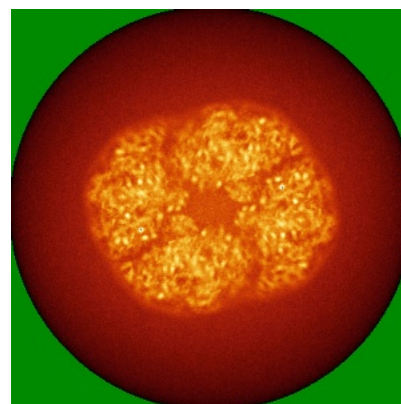
### 6.4.2 Raw map



X



Y

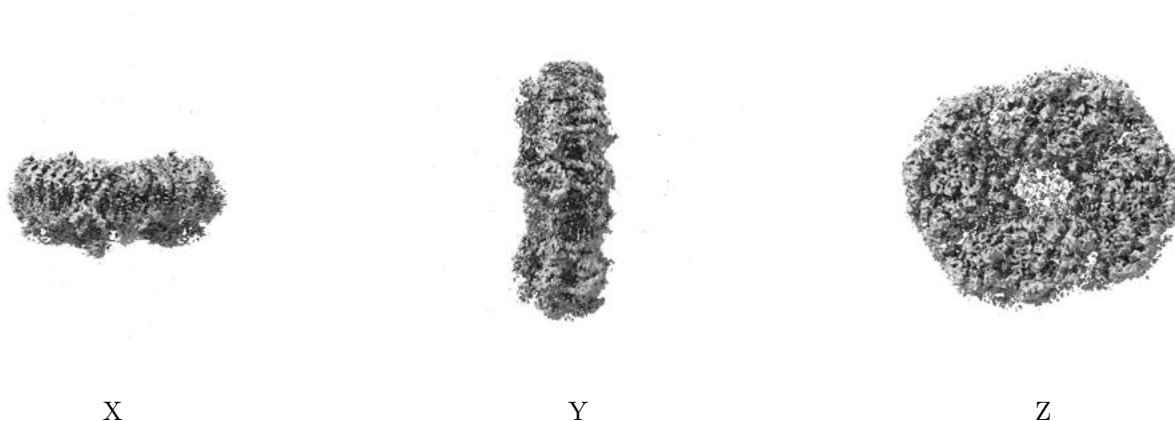


Z

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

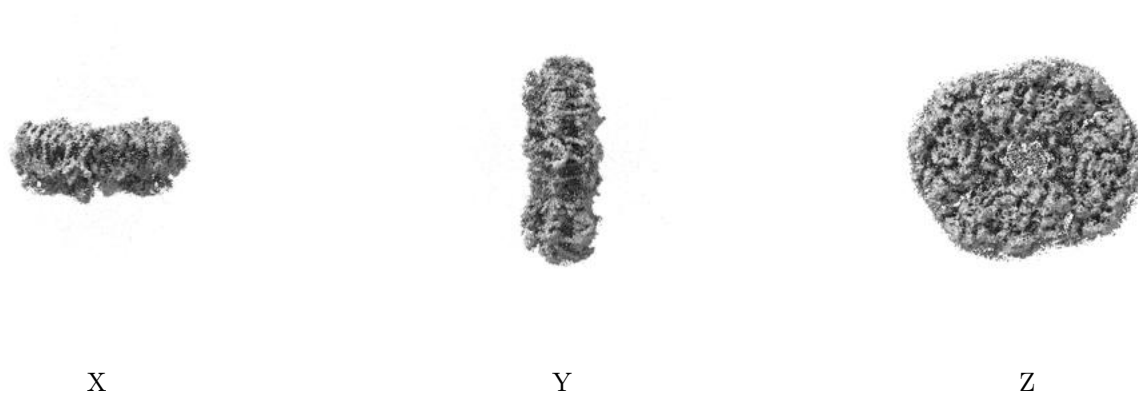
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

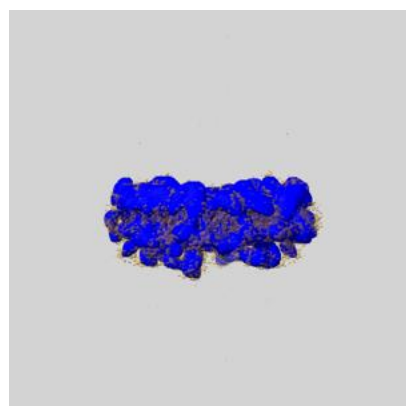
## 6.6 Mask visualisation [i](#)

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

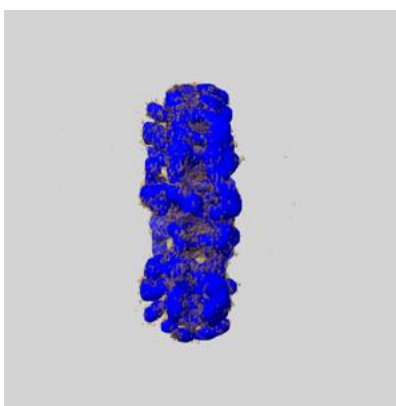
A mask typically either:

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

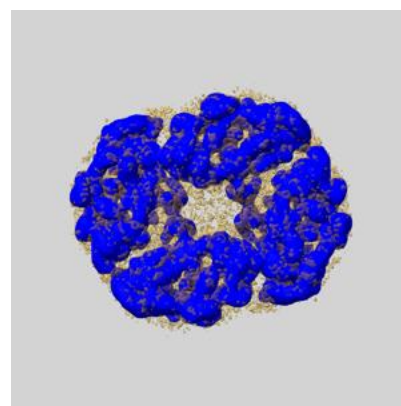
### 6.6.1 emd\_13898\_msk\_1.map [i](#)



X



Y



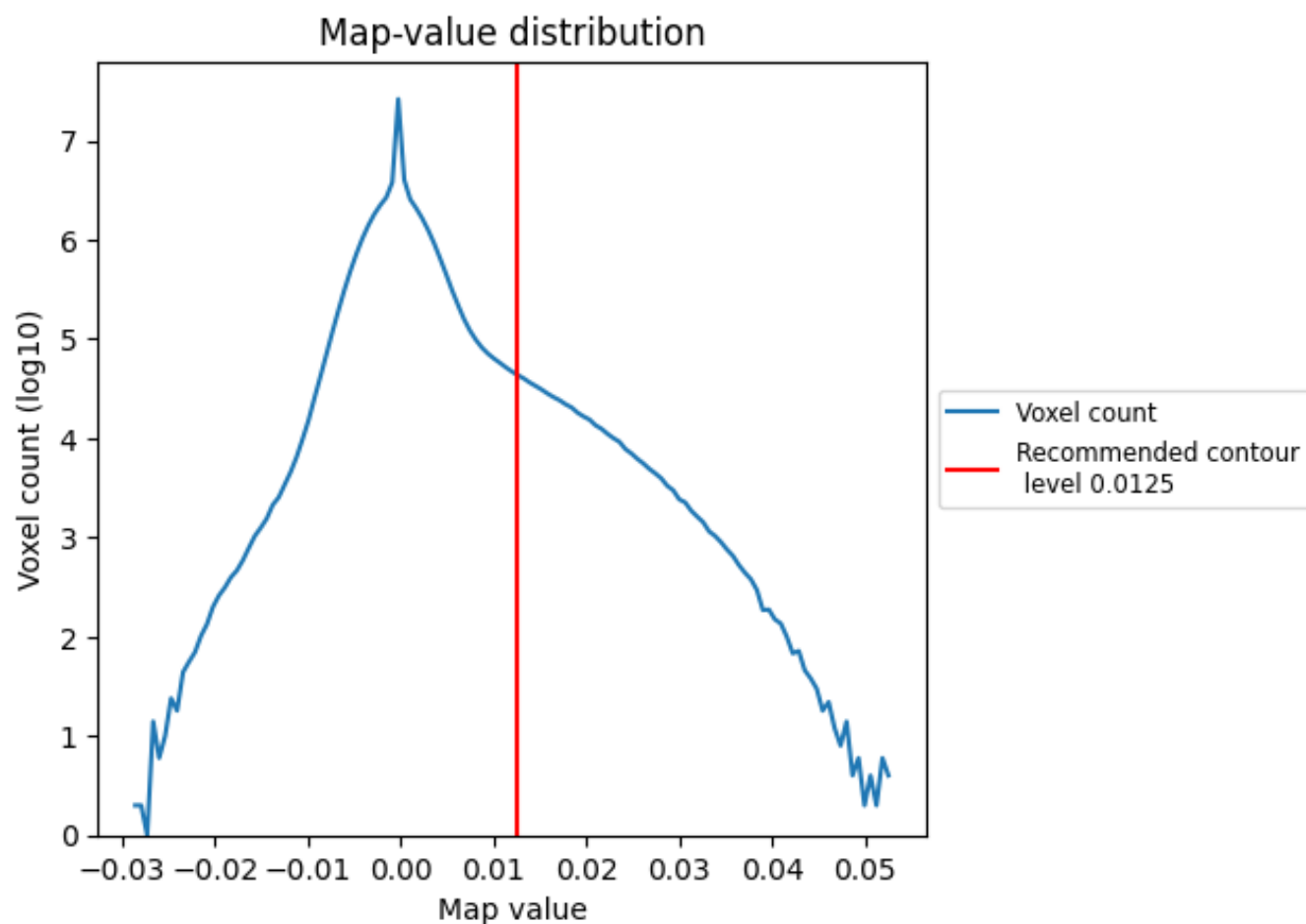
Z



## 7 Map analysis [i](#)

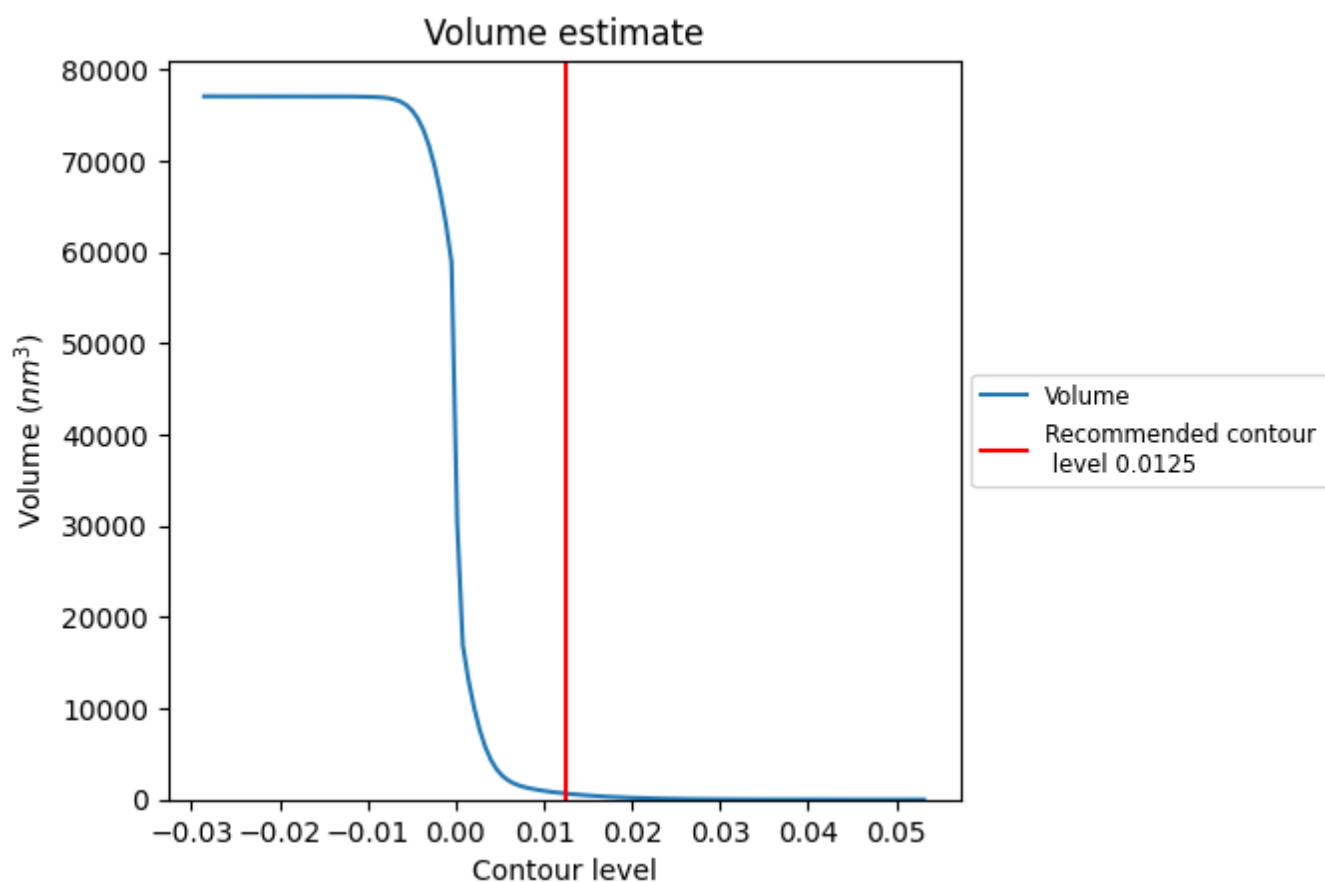
This section contains the results of statistical analysis of the map.

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



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

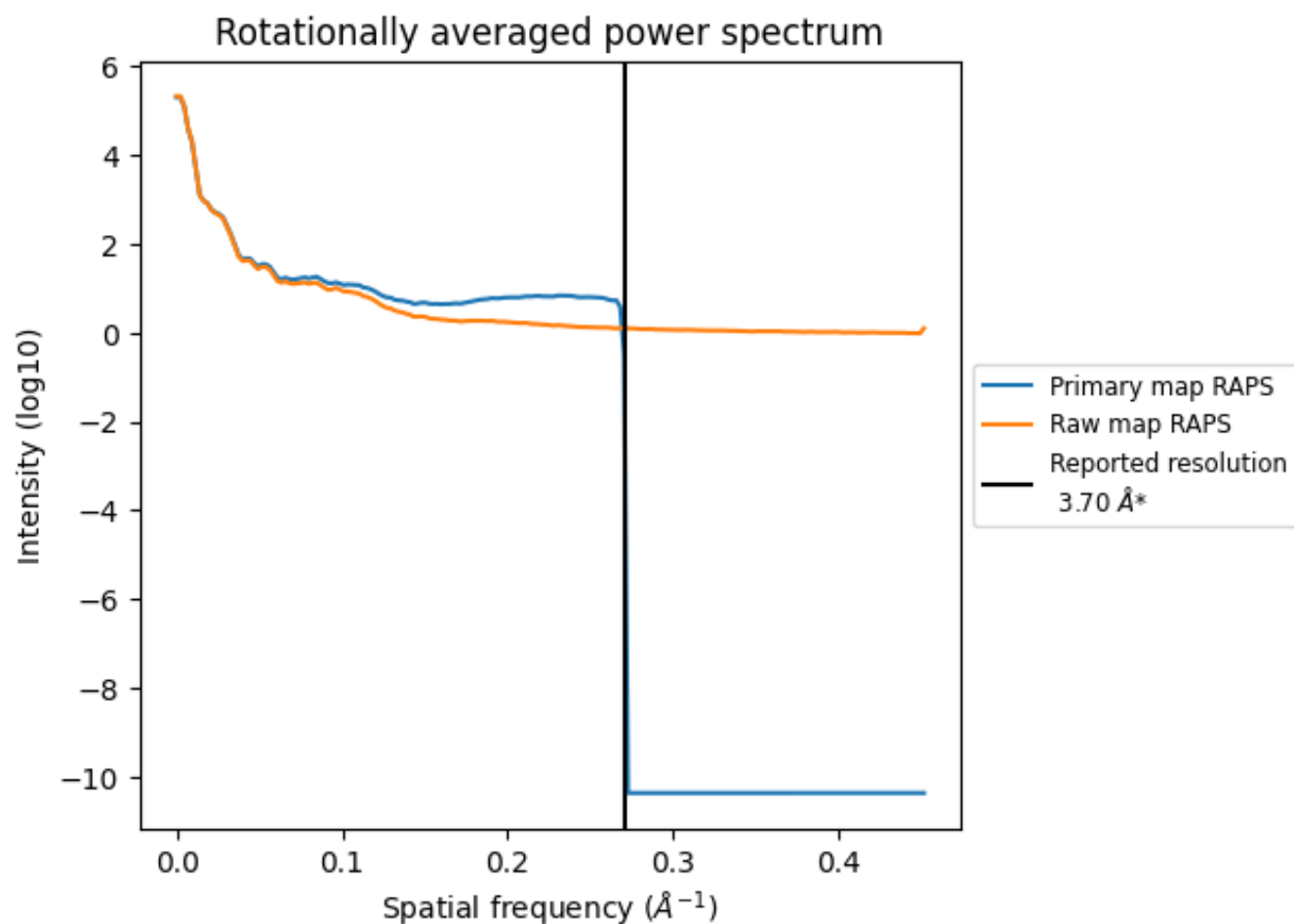
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 658 nm<sup>3</sup>; this corresponds to an approximate mass of 594 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 ⓘ

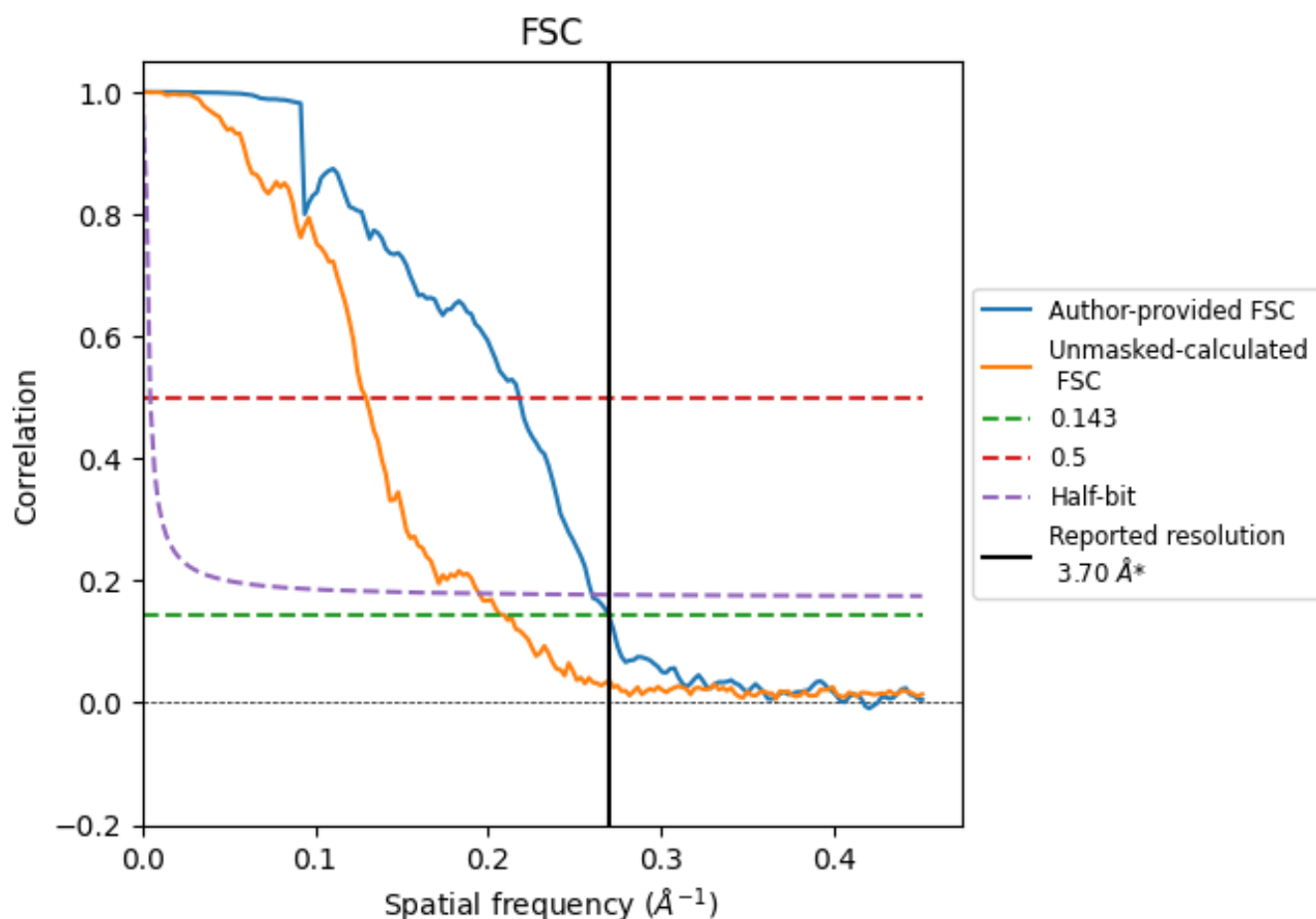


\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.270 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.70                               | -    | -        |
| Author-provided FSC curve | 3.71                               | 4.59 | 3.84     |
| Unmasked-calculated*      | 4.77                               | 7.73 | 5.13     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.77 differs from the reported value 3.7 by more than 10 %

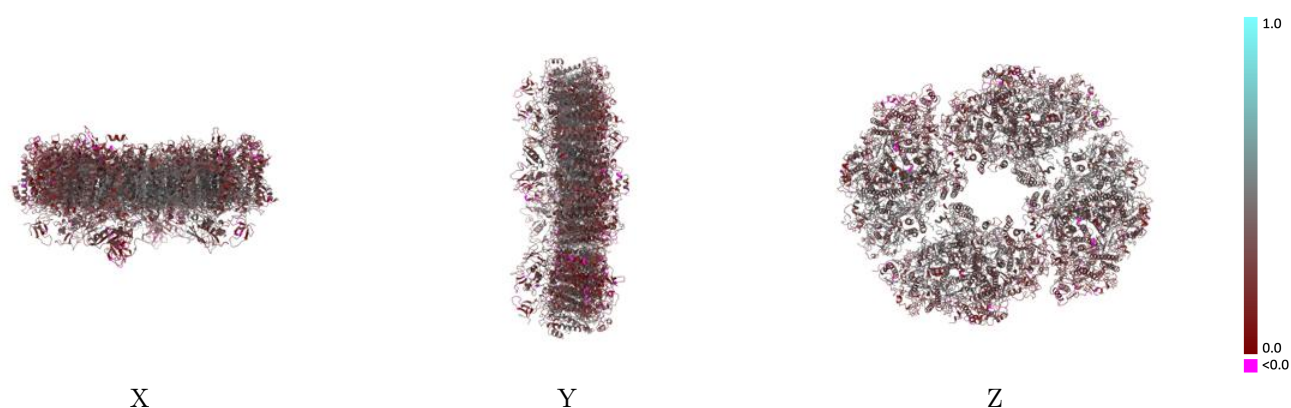
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13898 and PDB model 7QCO. Per-residue inclusion information can be found in section 3 on page 42.

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

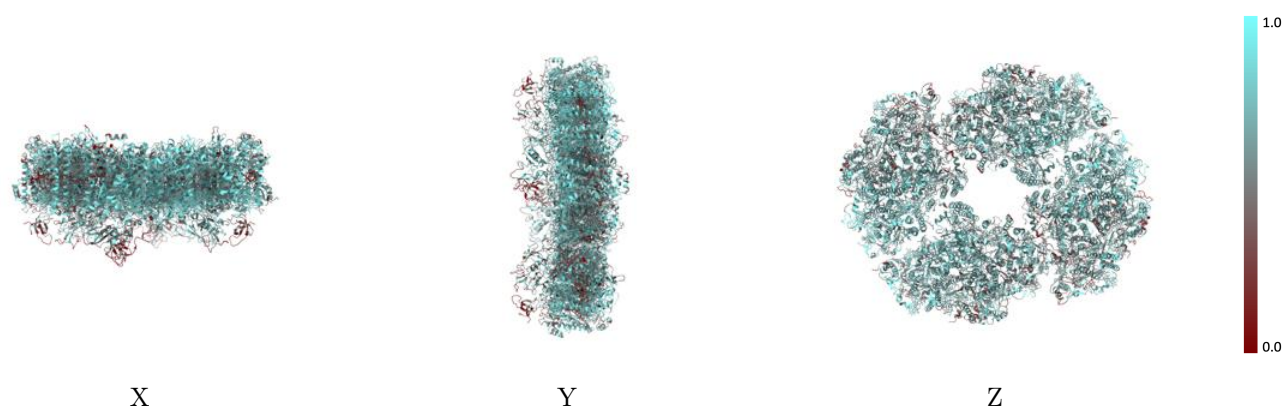
This section was not generated.

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



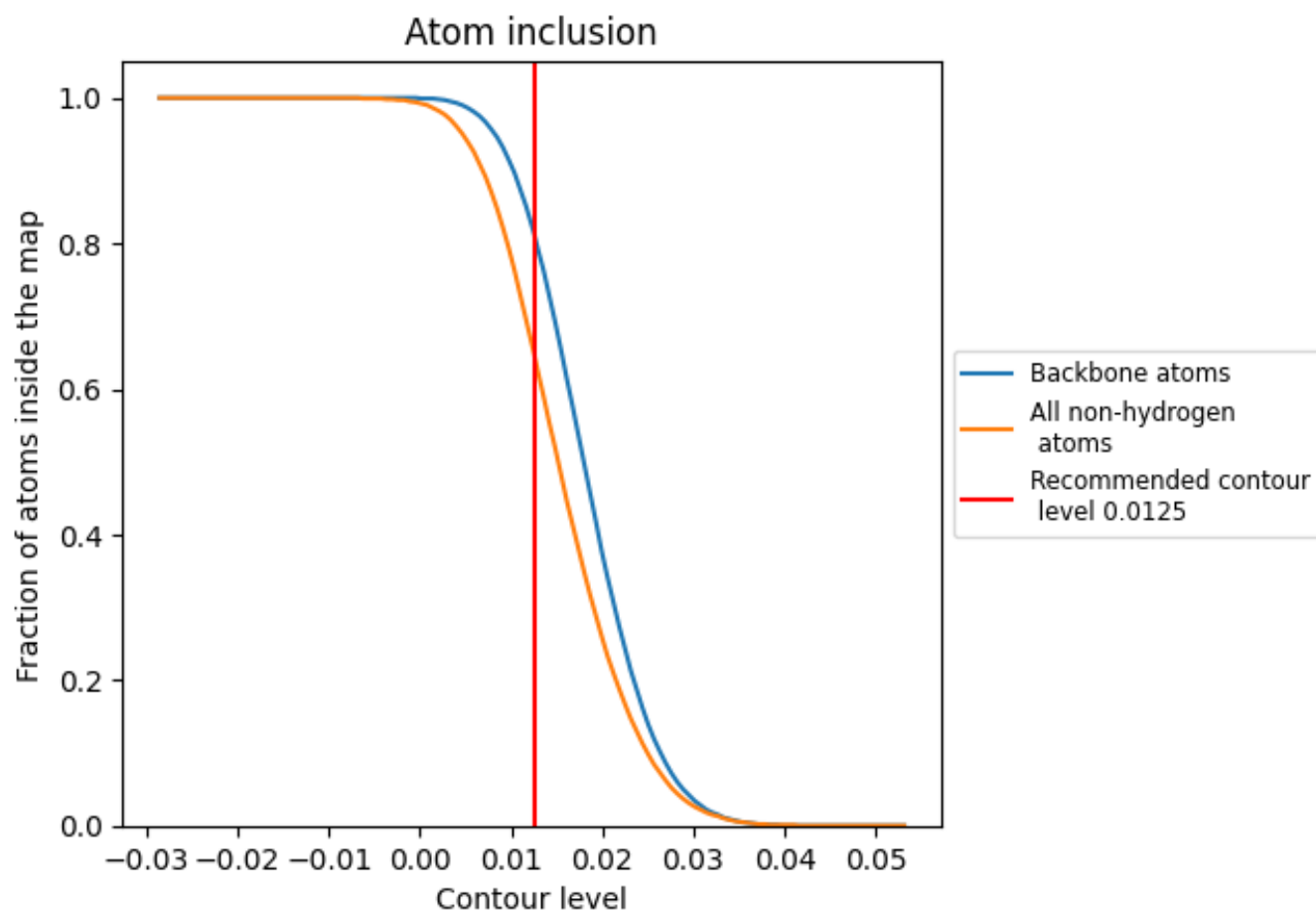
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 65% 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 (0.0125) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6500   |  0.3260   |
| A     |  0.7060   |  0.3530   |
| B     |  0.6540   |  0.3250   |
| C     |  0.6330   |  0.2920   |
| D     |  0.5610   |  0.3410   |
| E     |  0.6410   |  0.2980   |
| F     |  0.6020   |  0.2680   |
| G     |  0.7410   |  0.3840   |
| H     |  0.6010   |  0.2430   |
| I     |  0.5870   |  0.3220   |
| J     |  0.4660   |  0.2660   |
| K     |  0.6510   |  0.2800   |
| L     |  0.7000   |  0.3730   |
| M     |  0.5400   |  0.2970   |
| N     |  0.4420  |  0.3070  |
| O     |  0.5780 |  0.3140 |
| P     |  0.6930 |  0.3780 |
| Q     |  0.4970 |  0.3000 |
| R     |  0.4300 |  0.1660 |
| S     |  0.5970 |  0.3020 |
| T     |  0.6760 |  0.3850 |
| V     |  0.3020 |  0.1980 |
| W     |  0.2600 |  0.1520 |
| a     |  0.6340 |  0.2930 |
| b     |  0.7440 |  0.3820 |
| c     |  0.6000 |  0.2430 |
| d     |  0.4280 |  0.3040 |
| e     |  0.7080 |  0.3510 |
| f     |  0.5790 |  0.3130 |
| g     |  0.6580 |  0.3250 |
| h     |  0.6160 |  0.2860 |
| i     |  0.6870 |  0.3730 |
| j     |  0.5170 |  0.3010 |
| k     |  0.4300 |  0.1650 |
| l     |  0.5960 |  0.3030 |



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*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| m     |  0.6650 |  0.3820 |
| n     |  0.5660 |  0.3430 |
| o     |  0.6020 |  0.2660 |
| p     |  0.5720 |  0.3100 |
| q     |  0.4690 |  0.2620 |
| r     |  0.6460 |  0.2780 |
| s     |  0.6880 |  0.3610 |
| t     |  0.5530 |  0.3010 |
| v     |  0.3650 |  0.2490 |
| w     |  0.2600 |  0.1690 |