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Structural bioinformatics

ConfBuster: Open-source tools for macrocycle conformational search and analysis

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Availability: ConfBuster is freely available at github.com/patricklague/ConfBuster
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Supplementary Material

Table of Content

ConfBuster: installation, dependencies and usage

ConfBuster was designed to work as command lines. The instructions for installation and running ConfBuster are provided for Linux OS, but should work for other OS as long as the dependencies are satisfied.

Dependencies
CORE

- Python 2.7 (https://www.python.org)
- R (≥ 3.0.0) (https://cran.r-project.org/index.html)
- NetworkX (tested with 1.11) (https://networkx.github.io)
- Pymol (≥ 1.8) (https://sourceforge.net/projects/pymol)
- OpenBabel (≥ 2.4.1) (http://openbabel.org/wiki/Main_Page)
  The version of OpenBabel should imperatively be 2.4.1.
  Link to download: https://sourceforge.net/projects/openbabel/files/
  For a clean and functional installation:

  In openbabel-2.4.1 directory:
  $ mkdir build
  $ cd build
  $ cmake ../ -DCMAKE_INSTALL_PREFIX=/path/to/where/you/want
  $ make -j4
  $ make install
  (This is essential for OpenBabel to work properly)

OPTIONAL (VISUALIZATION)

- R package ComplexHeatmap (≥ 3.5) (from bioconductor.org)
  R shell:
  source("http://bioconductor.org/biocLite.R")
  biocLite("ComplexHeatmap")

- R package circlize (≥ 0.4.0)
  R shell:
  install.packages("circlize")

Installation

The most simple way to install ConfBuster is by downloading the official release in the GitHub section “release”. Alternatively, one may clone the ConfBuster repository using git :

$ git clone https://github.com/patricklague/ConfBuster.git

At your choice, put the scripts in a directory present in your $PATH OR add the directory where the scripts are to your $PATH:

export PATH=$PATH:/full-path-here/ConfBuster/

PyMOL and OpenBabel should also be recognized in your $PATH. If you want to install them locally, you should change the headers of the ConfBuster scripts to add their correct respective paths.

ConfBuster tools

- ConfBuster-Single-Molecule-Minimization
  Perform a simple minimization of the given molecule (recommended before all analysis).

- ConfBuster-Macrocycle-Linear-Sampling
  Find the conformation of a cyclic molecule.

- ConfBuster-Rotamer-Search
  Identify rotational isomers of a molecule.

- ConfBuster-Analysis
  Perform post-analyses to visualize a clustering based on RMSD values between the conformations.

Tutorial

A complete step-by-step tutorial is available on the ConfBuster GitHub (https://github.com/patricklague/ConfBuster).
(See also sections below)

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GNU General Public License for more details.

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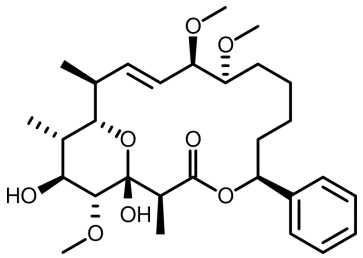
along with this program. If not, see http://www.gnu.org/licenses/.

ConfBuster example of use: macrocycle from PDB 1W96



Macrocycle molecule S1A from PDB 1W96

From the PDB 1W96, the macrocycle molecule (the first segment identified as S1A) was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-1w96.pdb* in the *examples/1w96* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-1w96.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-1w96.pdb
```

This will create the file *macro-1w96.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-1w96.mol2 -n 5 -N
5 -r 0.5
```

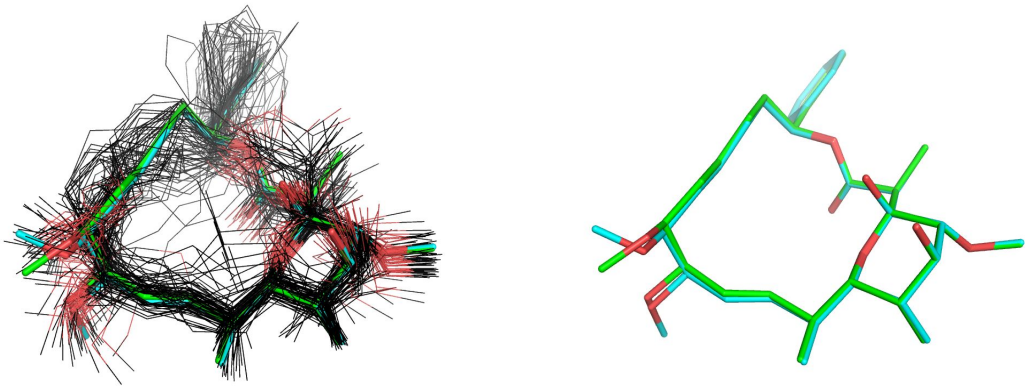
This will create a directory called *macro-1w96* which will contain the solutions from the conformational search, each conformation in a single file.

c. **Viewing and Analyzing results**

To view results go in the *macro-1w96* directory and run the following commands. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-1w96
$ pymol Follow-macro-1w96.py
```

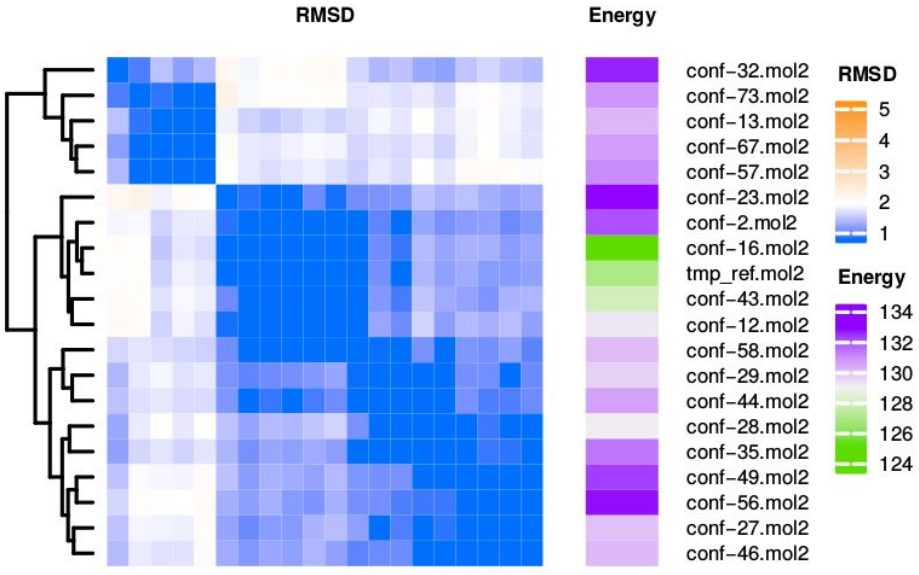
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-1w96.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-16.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-16.mol2 and PDB structure is 0.405 Å over all atoms. All sampled conformations are in black thin lines to show the conformational space of the macrocycle. Results may vary from one search to another.

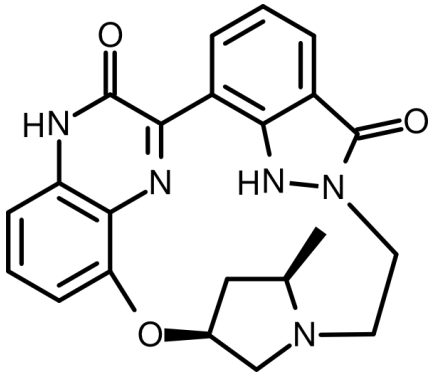
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-1w96 -R macro-1w96.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 1W96. The conformation from the object conf-16.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 2DS1



Macrocycle molecule 1CD from PDB 2DS1

From the PDB 2DS1, one of the macrocycle molecules (the first segment identified as 1CD) was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-2ds1.pdb* in the *examples/2ds1* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-2ds1.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-2ds1.pdb
```

This will create the file *macro-2ds1.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-2ds1.mol2 -n 5 -N
5 -r 0.5
```

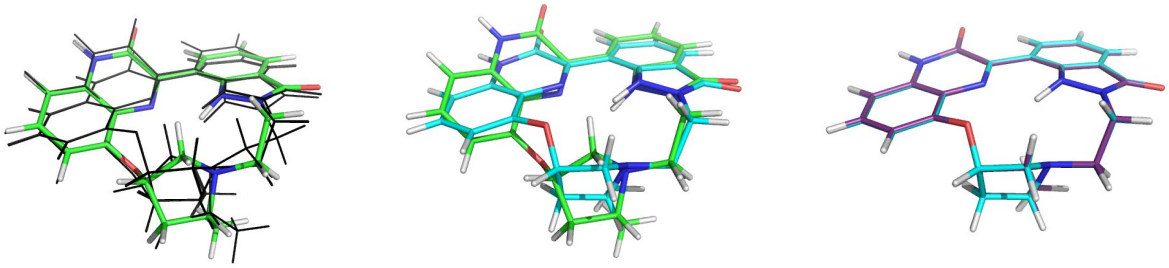
This will create a directory called *macro-2ds1* which will contain the solutions from the conformational search, each conformation in a single file.

c. **Viewing and Analyzing results**

To view results go in the *macro-2DS1* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-2ds1
$ pymol Follow-macro-2ds1.py
```

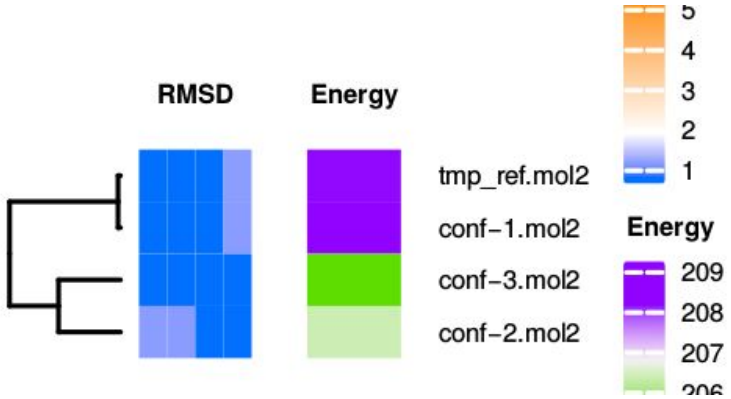
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-2ds1.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-3.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-3.mol2 and PDB structure is 0.893 Å over all atoms. All sampled conformations are in black thin lines to show the conformational space of the macrocycle. Results may vary from one search to another.

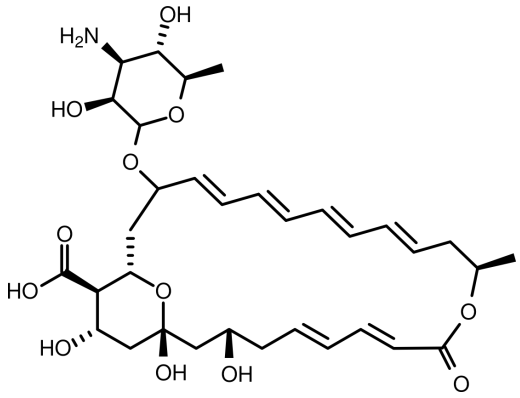
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-2ds1 -R macro-2ds1.mol2 -n 20
```



RMSD matrix between the 3 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 2DS1. The conformation from the object conf-3.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 2XBK



Macrocycle molecule XBK from PDB 2XBK

From the PDB 2XBK, one of the macrocycle molecules (the first segment identified as XBK) was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-2xbk.pdb* in the *examples/2xbk* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-2xbk.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-2xbk.pdb
```

This will create the file macro-2xbk.mol2, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-2xbk.mol2 -n 5 -N
5 -r 0.5
```

This will create a directory called *macro-2xbk* which will contain the solutions from the conformational search, each conformation in a single file.

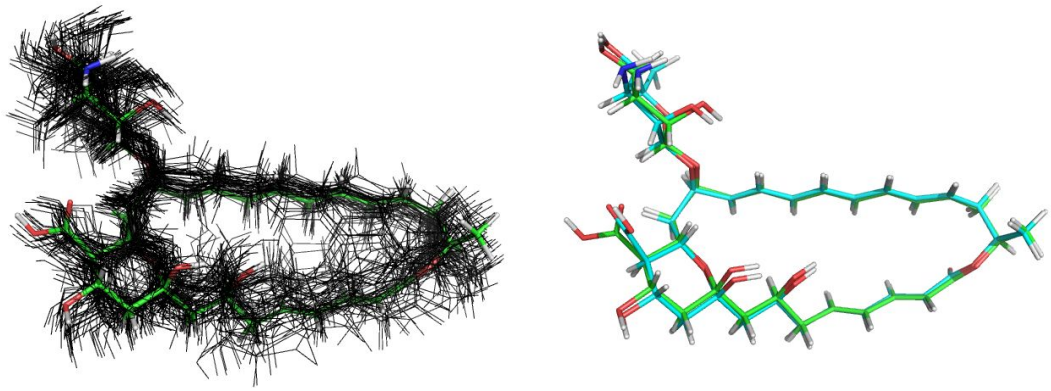
c. **Viewing and Analyzing results**

To view results go in the *macro-2xbk* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-2xbk
$ pymol Follow-macro-2xbk.py
```

In PyMOL, progress may also be followed using the run command:

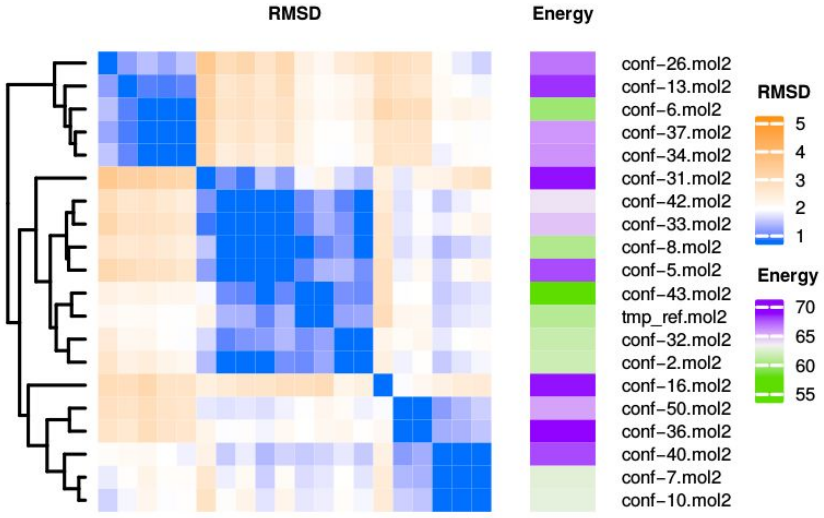
```
(in PyMOL) run Follow-macro-2xbk.py
```



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-43.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-43.mol2 and PDB structure is 0.607 Å over all atoms. All sampled conformations are in black thin lines to show the conformational space of the macrocycle. Results may vary from one search to another.

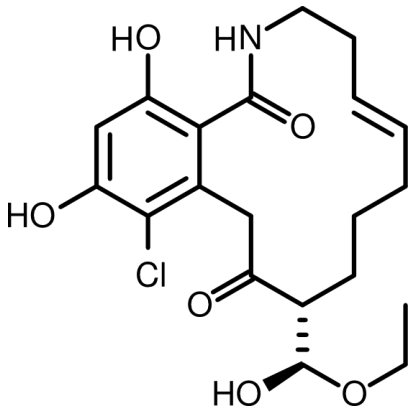
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-2xbk -R macro-2xbk.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 2XBK. The conformation from the object conf-43.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 2XX4



Macrocycle molecule 13I from PDB 2XX4

From the PDB 2XX4, one of the macrocycle molecules (the first segment identified as 13I) was was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-2xx4.pdb* in the *examples/2xx4* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-2xx4.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-2xx4.pdb
```

This will create the file *macro-2xx4.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-2xx4.mol2 -n 5 -N
5 -r 0.5
```

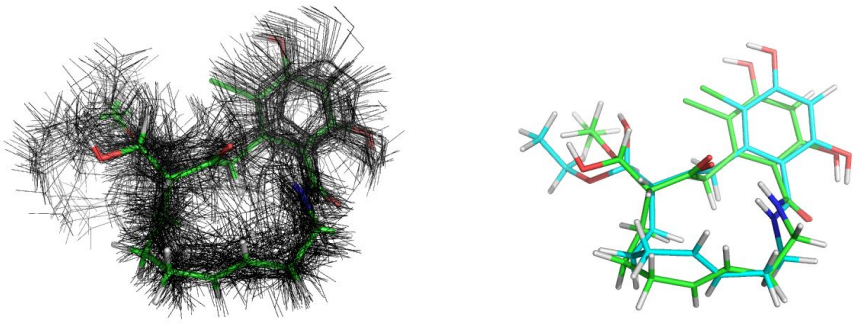
This will create a directory called *macro-2xx4* which will contain the solutions from the conformational search, each conformation in a single file.

c. **Viewing and Analyzing results**

To view results go in the *macro-2XX4* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-2xx4
$ pymol Follow-macro-2xx4.py
```

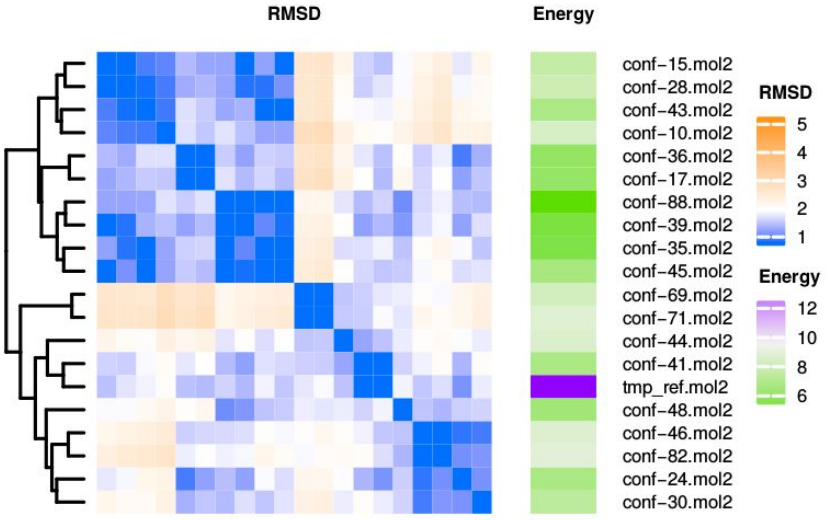
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-2xx4.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-88.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-88.mol2 and PDB structure is of 1.722 Å over all atoms. All sampled conformations are in black thin lines to show the conformational space of the macrocycle. Results may vary from one search to another.

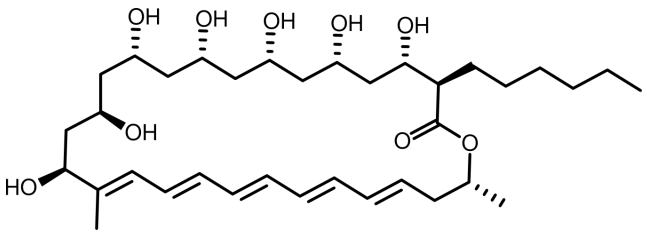
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-2xx4 -R macro-2xx4.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 2XX4. The conformation from the object conf-88.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 3ABA



Macrocycle molecule FLI from PDB 3ABA

From the PDB 3ABA, one of the macrocycle molecules (the first segment identified as FLI) was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-3aba.pdb* in the *examples/3aba* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-3aba.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-3aba.pdb
```

This will create the file *macro-3ABA.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-3ABA.mol2 -n 5 -N
5 -r 0.5
```

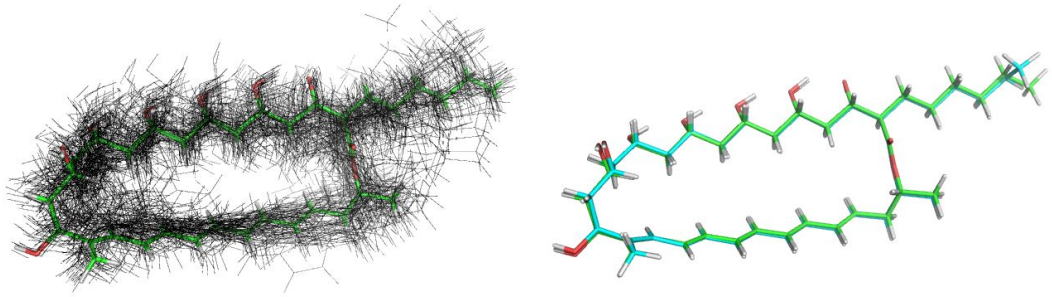
This will create a directory called *macro-3ABA* which will contain the solutions from the conformational search, each conformation in a single file.

c. **Viewing and Analyzing results**

To view results go in the *macro-3ABA* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-3aba
$ pymol Follow-macro-3aba.py
```

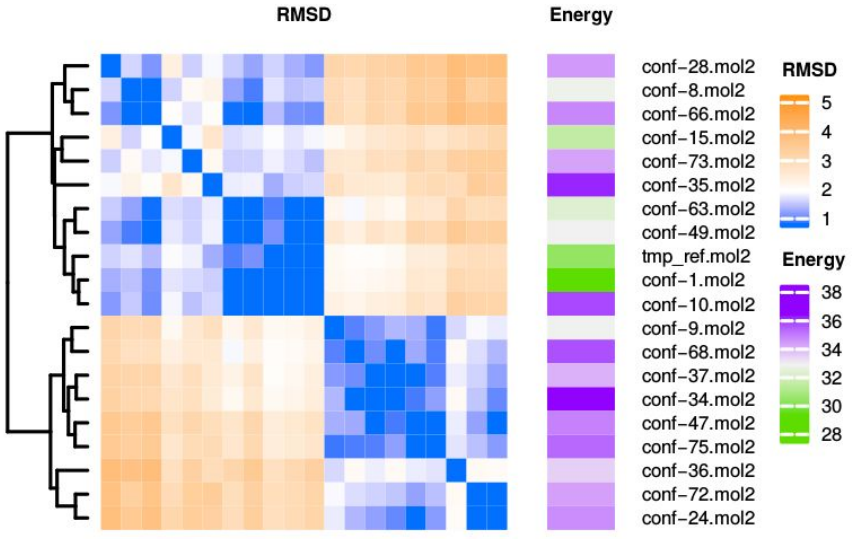
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-3aba.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-1.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-1.mol2 and PDB structure is 0.643 Å over all atoms. All sampled conformations are in black thin lines to show the conformational space of the macrocycle. Results may vary from one search to another.

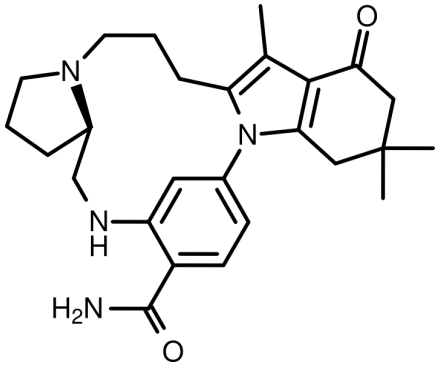
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-3aba -R macro-3aba.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 3ABA. The conformation from the object conf-1.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 3R92



Macrocycle molecule 06J from PDB 3R92

From the PDB 3R92, one of the macrocycle molecules (the first segment identified as 06J) was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-3r92.pdb* in the *examples/3r92* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-3r92.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-3r92.pdb
```

This will create the file *macro-3r92.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-3r92.mol2 -n 5 -N
5 -r 0.5
```

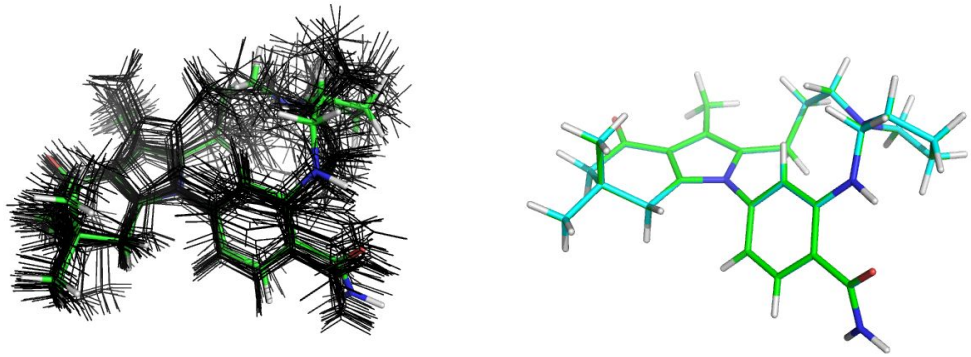
This will create a directory called *macro-3r92* which will contain the solutions from the conformational search, each conformation in a single file.

c. **Viewing and Analyzing results**

To view results go in the *macro-3R92* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-3r92
$ pymol Follow-macro-3r92.py
```

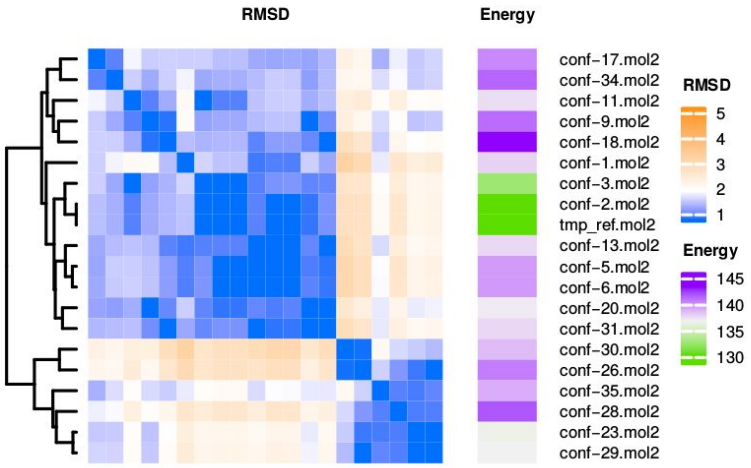
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-3r92.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-2.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-2.mol2 and PDB structure is 0.010 Å over all atoms. All sampled conformations are in black thin lines to show the conformational space of the macrocycle. Results may vary from one search to another.

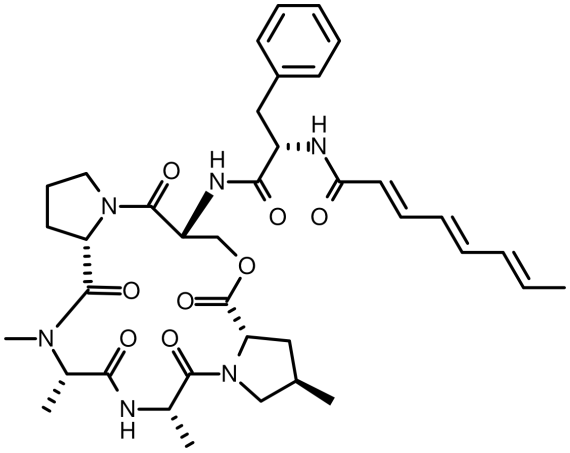
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-3r92 -R macro-3r92.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 3R92. The conformation from the object conf-2.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 3MT6



Macrocycle molecule "OTT FSP MAA A MP8" from PDB 3MT6

From the PDB 3MT6, one of the macrocycle molecules (the first segment identified as "OTT FSP MAA A MP8") was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-3mt6.pdb* in the *examples/3mt6* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-3mt6.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-3mt6.pdb
```

This will create the file *macro-3mt6.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-3mt6.mol2 -n 5 -N
5 -r 0.5
```

This will create a directory called *macro-3mt6* which will contain the solutions from the conformational search, each conformation in a single file.

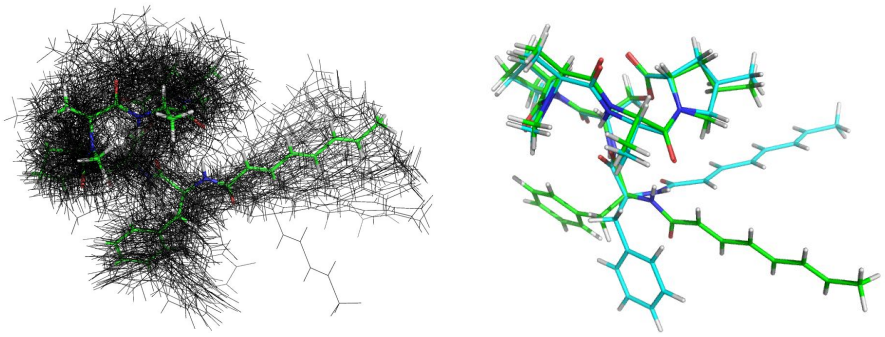
c. **Viewing and Analyzing results**

To view results go in the *macro-3mt6* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-3mt6
```

```
$ pymol Follow-macro-3mt6.py
```

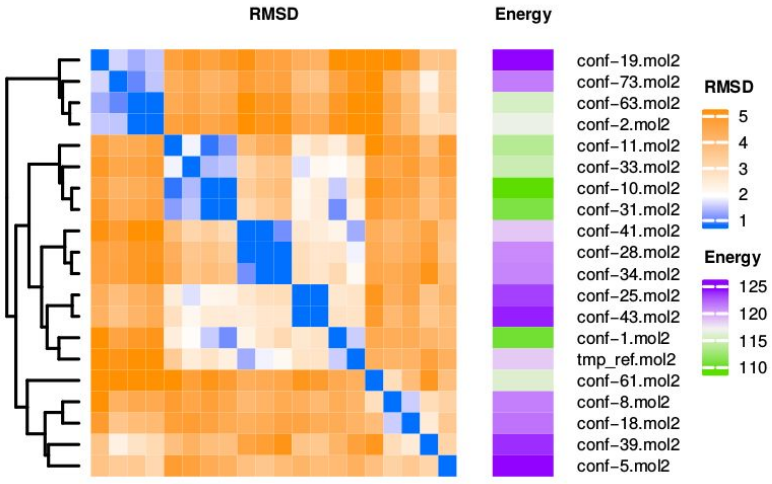
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-3mt6.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-10.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-10.mol2 and PDB structure is 2.728 Å over all atoms. All sampled conformations are in black thin lines to show the conformational range of the macrocycle. Results may vary from one search to another.

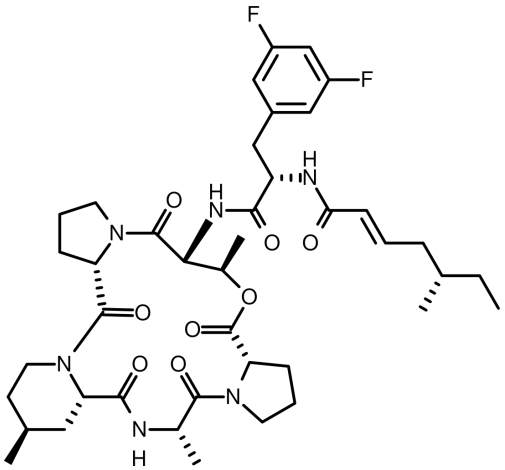
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-3mt6 -R macro-3mt6.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 3MT6. The conformation from the object conf-10.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 4U0G



Macrocycle molecule "39Y WFP TP 3A0 AP" from PDB 4U0G

From the PDB 4U0G, one of the macrocycle molecules (the first segment identified as "39Y WFP TP 3A0 AP") was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-4u0g.pdb* in the *examples/4u0g* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-4u0g.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-4u0g.pdb
```

This will create the file *macro-4u0g.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-4u0g.mol2 -n 5 -N
5 -r 0.5
```

This will create a directory called *macro-4u0g* which will contain the solutions from the conformational search, each conformation in a single file.

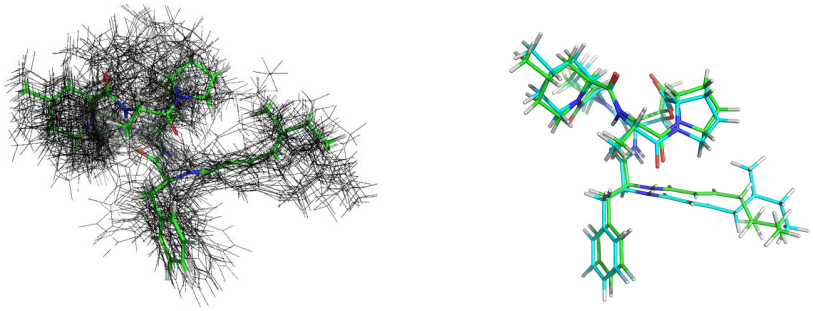
c. **Viewing and Analyzing results**

To view results go in the *macro-4u0g* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-4u0g
```

```
$ pymol Follow-macro-4u0g.py
```

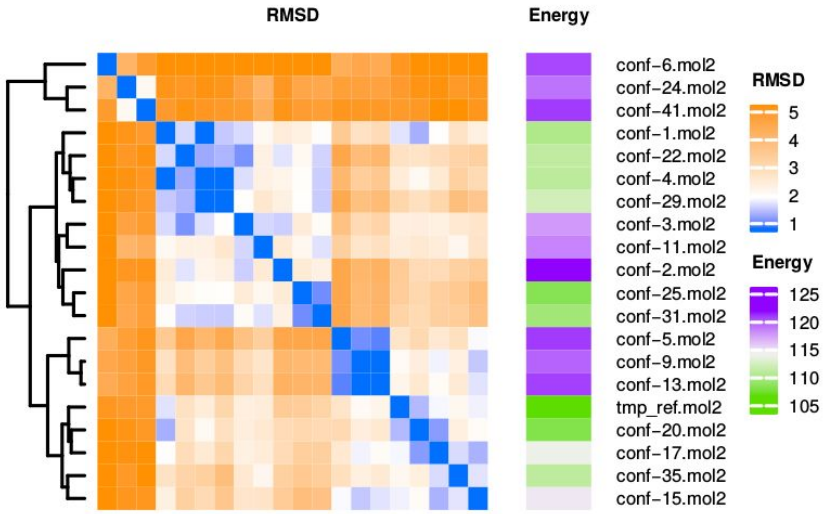
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-4u0g.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-20.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-20.mol2 and PDB structure is 1.541 Å over all atoms. All sampled conformations are in black thin lines to show the conformational range of the macrocycle. Results may vary from one search to another.

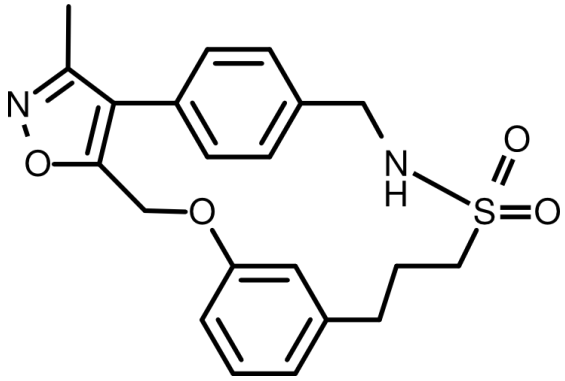
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-4u0g -R macro-4u0g.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 4UG0. The conformation from the object temp_ref.mol2 (reference structure from the PDB) displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 5L7H



Macrocycle molecule 6QG from PDB 5L7H

From the PDB 5L7H, one of the macrocycle molecules (the first segment identified as 6QG) was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-5l7h.pdb* in the *examples/5l7h* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. **Perform a minimization on macro-5L7H.pdb**

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-5l7h.pdb
```

This will create the file *macro-5l7h.mol2*, which is used in the next step.

b. **Start Macrocyclic linear sampling**

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-5l7h.mol2 -n 5 -N
5 -r 0.5
```

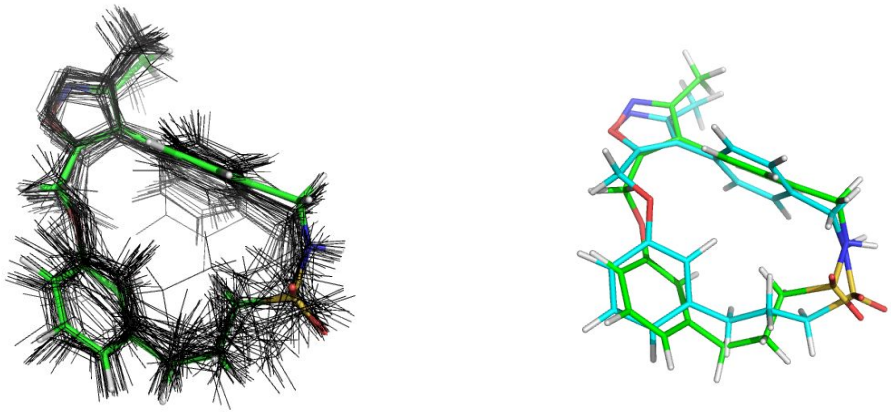
This will create a directory called *macro-5l7h* which will contain the solutions from the conformational search, each conformation in a single file.

c. **Viewing and Analyzing results**

To view results go in the *macro-5l7h* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-5l7h
$ pymol Follow-macro-5l7h.py
```

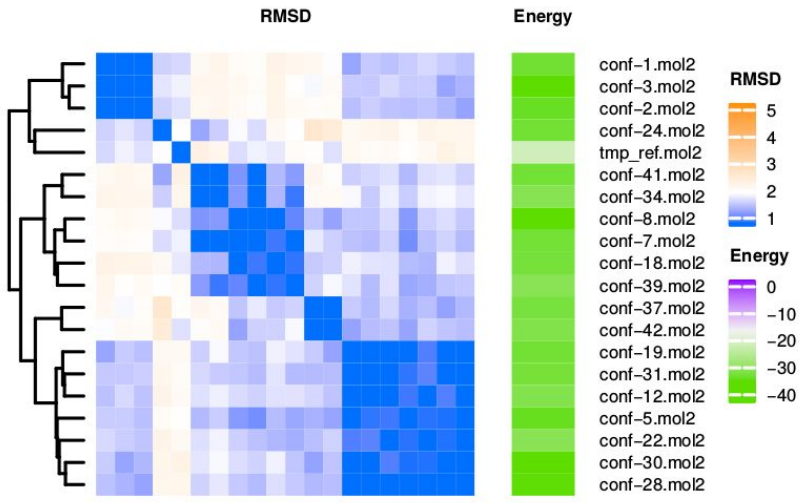
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-5l7h.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-8.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-8.mol2 and PDB structure is 1.785 Å over all atoms. All sampled conformations are in black thin lines to show the conformational range of the macrocycle. Results may vary from one search to another.

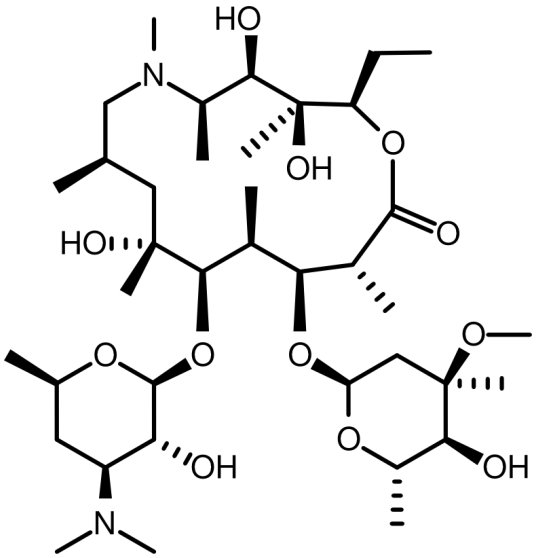
Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-5l7h -R macro-5l7h.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 5l7h. The conformation from the object conf-8.mol2 displays the lowest conformational energy. Results may vary from one search to another.

ConfBuster example of use: macrocycle from PDB 5IGI



Macrocycle molecule ZIT from PDB 5IGI

From the PDB 5IGI, one of the macrocycle molecules (the first segment identified as ZIT) was prepared (correct bond orders and addition of hydrogens) and saved to a file (file *macro-5igi.pdb* in the *examples/5igi* directory of ConfBuster distribution).

The conformational search steps are as follows (command lines are highlighted with a light gray color):

a. Perform a minimization on macro-5igipdb

```
$ ConfBuster-Single-Molecule-Minimization.py -i macro-5igi.pdb
```

This will create the file *macro-5igi.mol2*, which is used in the next step.

b. Start Macrocyclic linear sampling

```
$ ConfBuster-Macrocycle-Linear-Sampling.py -i macro-5igi.mol2 -n 5 -N
5 -r 0.5
```

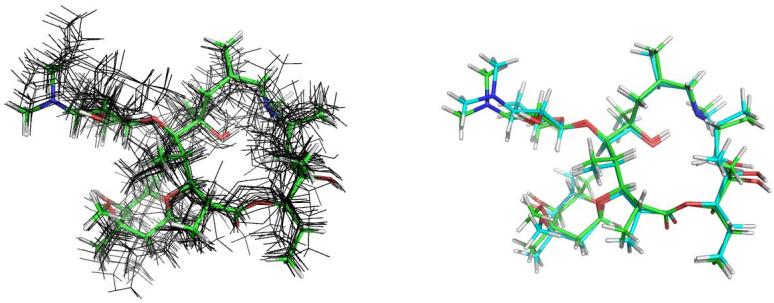
This will create a directory called *macro-5igi* which will contain the solutions from the conformational search, each conformation in a single file.

c. Viewing and Analyzing results

To view results go in the *macro-5igi* directory and run the following command. In the PyMOL window, the best conformation will be the first object loaded at the top of the object list and shown in green sticks.

```
$ cd macro-5igi
$ pymol Follow-macro-5igi.py
```

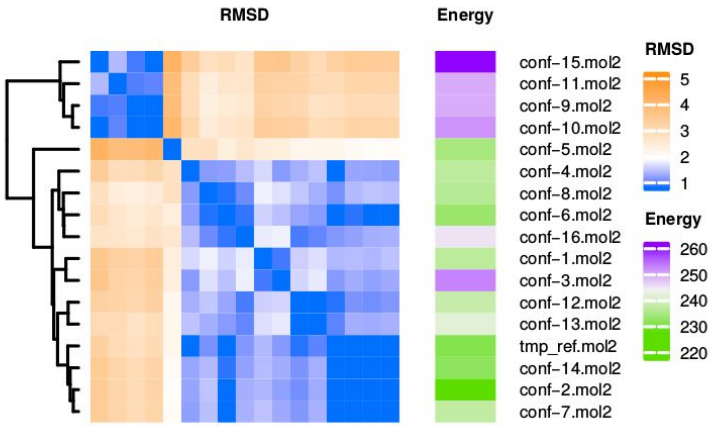
In PyMOL, progress may also be followed using the run command:
`(in PyMOL) run Follow-macro-5igi.py`



Conformational search results, as displayed in PyMOL. Lowest energy conformation is in green (conf-2.mol2 in the matrix below). PDB structure is in cyan. RMSD between conf-2.mol2 and PDB structure is 0.635 Å over all atoms. All sampled conformations are in black thin lines to show the conformational range of the macrocycle. Results may vary from one search to another.

Using the ConfBuster-Analysis.py script allows to compare the *n* best results with a reference or the initial structure. Results are shown as a 2D RMSD matrix of *n* conformations. On the right, an energy bar (from green to purple) between the best and worst energy is displayed:

```
$ ConfBuster-Analysis.py -i macro-5igi -R macro-5igi.mol2 -n 20
```



RMSD matrix between the 20 lowest energy conformations from a ConfBuster conformational search of the macrocycle from PDB 5IGI. The conformation from the object conf-2.mol2 displays the lowest conformational energy. Results may vary from one search to another.