

Conformers Search

When dealing with organic molecules of medium to large size, molecular properties are conformation dependent. *MedeA*¹ *Conformers Search* systematically builds all conformers, or a representative set of conformers for your molecules.

MedeA Conformers Search is part of the standard *MedeA Environment*. It comes with a pre-optimized set of search parameters and algorithms, while also allowing custom search protocols. *MedeA Conformer Search* deploys the versatile UFF94 forcefield and is thus applicable to a wide variety of molecules. The integration with *MedeA* structure lists and flowcharts allows for seamless processing and computations using any of *MedeA*'s compute engines or property modules.

For systematic search, the next conformers in the list are sorted as a function of their conformer energy (UFF94). For the GA search, the following conformers are added according to their similarity with the previous conformers in the list. Similarity is a distance defined as the number of different torsion values with respect to previous conformers. Similarity of 0 means identity. Additional column provides:

- Similarity to first: similarity to the most stable conformer
- Average similarity: average similarity to all other conformers in the list
- Minimum similarity: minimum similarity to all other conformers in the list

Conformer Id	Energy increase	Similarity to first	Average similarity	Minimum similarity
1	0	0	2.42	
2	5.22	4	4.42	
3	5.03	3	4.21	
4	5.04	3	4.32	
5	5.56	3	4.42	
6	4.27	3	4.63	2
7	5.04	3	4	2
8	4.17	3	4.58	3
9	3.75	2	3.74	1
10	3.3	2	3.68	1
11	3.44	2	3.84	2
12	3.41	2	3.95	2
13	3.26	2	3.63	1
14	4.33	2	3.63	2
15	4.67	3	4.21	2
16	5.49	3	4.05	2
17	4.93	3	4	2
18	1.4	1	3.96	1

Context menu options: View conformer(s), Save selected structure list, Export to file

Fig. 2: MedeA Conformer Search Results panel

Key Benefits

- Straightforward generation of molecular conformers
- Integration with other *MedeA* modules
- Conformer structure list storage for use with *MedeA HT-Launchpad*

- *MedeA Environment*

'A simple and efficient module, beautifully integrated!'

Recommended Modules

- *MedeA HT-Launchpad*
- *MedeA LAMMPS*
- *MedeA VASP*
- *MedeA MOPAC*
- *MedeA GAUSSIAN GUI*

Find Out More

Learn more about *MedeA* features and capabilities: Databases, Builders, Compute Engines, Forcefields, Property Modules, Analysis Tools, and High-Throughput.

Watch our Upcoming and Recorded Materials Design webinars on *MedeA* for related topics in computational materials simulation design and materials engineering.

Molecule

Set from MedeA | Set from file

Set from SMILES: | CCCCCCCCCCCCCC

Formula: C14H30

Number of possible conformers: 177147

Search parameters

Number of conformers to create: 20 Find Conformers

☒ Advanced settings ☒ Create molecules in periodic conditions

Choose between the 3 possible approaches:

- Systematic: search all possible conformers, rotating torsions step by step.
- Weighted: randomly rotates around the rotatable bonds in a molecule, the random choice of torsions is reweighted based on the energy of the generated conformer
- Genetic Algorithm (GA): optimize the conformer energy using the UFF94 forcefield and preserve diversity in terms of different torsions values on rotatable bonds (i.e. rotors) using fitness sharing

☐ Systematic ☐ Weighted ☒ Genetic Algorithm

Fig. 1: MedeA Conformers Search Settings panel

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