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.

Key Benefits

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

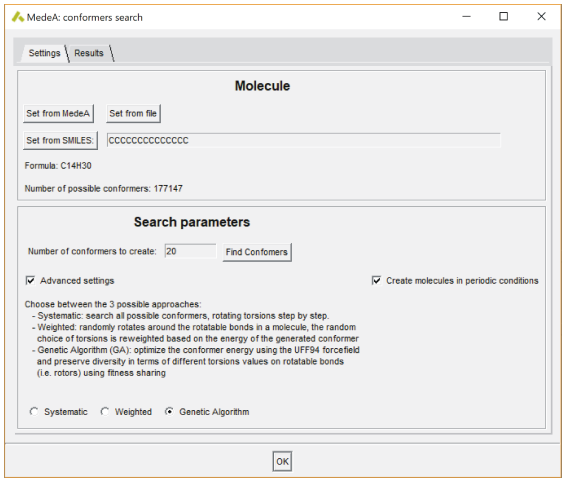

Fig. 1: MedeA Conformers Search Settings panel

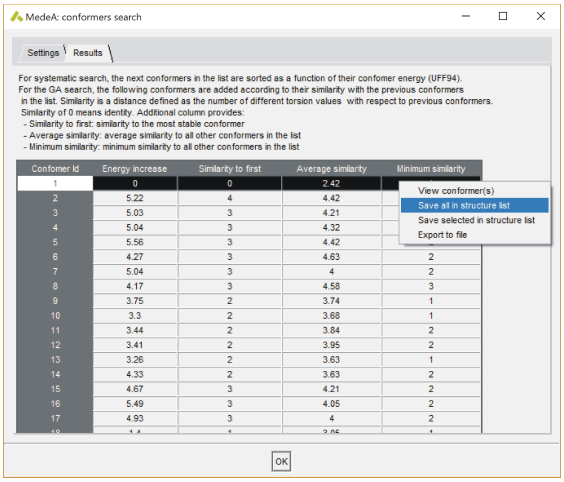

Fig. 2: MedeA Conformer Search Results panel

Required Modules

- *MedeA Environment*

'A simple and efficent 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.

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