

CONFORMERS

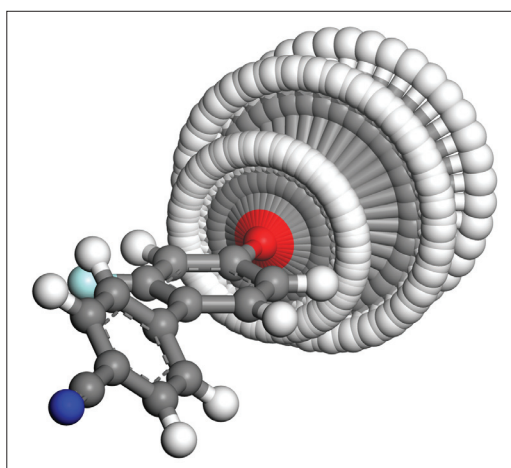
Conformational searching is one of the key applications in the exploration of molecular property-geometry relationships. In combination with powerful analysis techniques, it provides valuable information on the accessible conformational space of a molecule and helps identify low energy conformations.

Conformers provides access to a comprehensive collection of conformational searching and analysis techniques for the exploration of conformational space. It may be used in a variety of applications ranging from simple conformational exploration to complex conformational search problems. Conformers can also be used to average QSAR descriptors that are dependent on 3D geometry.

WHAT CAN CONFORMERS BE USED FOR?

Conformers has been developed to provide a simple way to explore the potential energy surface of a molecule. For a small molecule, the potential energy surface can already be very complex. Conformers allows you to perturb specific torsion angles thus allowing researchers to focus in on key areas of the potential energy surface. There are three main methods for sampling torsion angles:

1. Systematic grid searching – systematically varies torsion angles by a set amount. Systematic grid searching allows researchers to create energy maps of a few crucial torsion angles.
2. Random sampling – stochastic searching by perturbation of specified torsions. Used to search for low energy conformers with multiple searchable torsions.
3. Boltzmann's jump – stochastic searching by random perturbation with selection of conformers based on Metropolis criteria. Applied when there are multiple searchable torsions.



Overlaid structures generated from a systematic grid search showing the sampling of conformational space.

Besides generating different conformations for a molecule, Conformers also provides a set of tools to analyze the generated conformers. The analysis tools allow researchers to predict properties such as dipole moments and cluster the conformers based on the RMS difference of the Cartesian coordinates.

THE MATERIALS STUDIO ADVANTAGE

Conformers uses the study table, one of Materials Studio's core documents, to store results giving a seamless integration with other property prediction tools such as VAMP and DMol3. A wide variety of electronic properties from Fukui functions to accurate dipole moments can be calculated

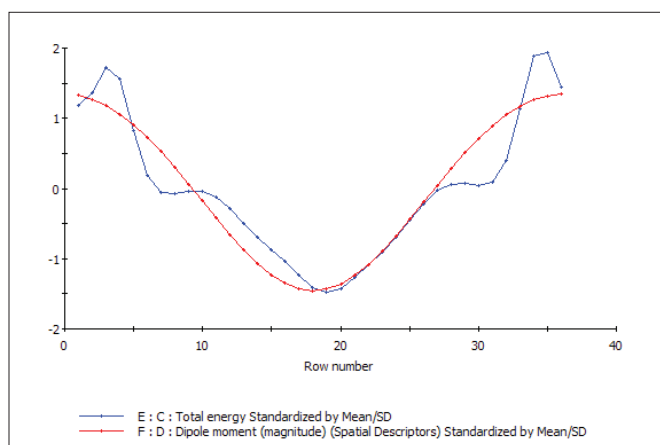
easily using these and other modules. The study table is also at the heart of Materials Studio QSAR modules providing a direct link from Conformer generation to descriptor generation for QSAR.

Materials Studio's integrated structure building and editing tools enable you to quickly build your molecule from pre-defined fragments, polymers, or by simply sketching the atoms. Conformers generated from a calculation can be overlaid and aligned in the collection document, providing a visual comparison of changes in the structures.

HOW CAN CONFORMERS BENEFIT YOU?

Conformers provides a quick and easy way to sample many conformations of a molecule. It allows researchers to locate energy minima, vital for the prediction of properties, and explore simple geometry-property relationships, gaining insight into the properties of a molecule.

Conformers uses simple search set-up procedures for easy identification of conformational minima. Set-up procedures can also be tuned to fit specific needs for expert users. For example, Conformers integrates a wealth of conformation generation techniques such as grid scan, random sampling or Boltzmann jump. Conformers is based on the Forcite energy server providing access to multiple force fields such as Dreiding for small molecules or COMPASS for polymers and materials science applications.



Plot showing the change in scaled dipole moment and energy as a torsion is rotated. For this case, the energy minimum corresponds to the dipole moment minimum.

CONFORMERS FEATURES

Conformer Generation

- Automatically find rotatable torsions in molecule
- Systematic scan of selected torsions
- Random sampling of torsions
- Boltzmann jump sampling of torsions
- Scan ring conformations using ring closures
- Output to trajectory or study table
- Filter on server to ensure diversity
- Geometry optimization of conformers.

Automated setup of energy expression

- Choose forcefield from Universal, Dreiding, COMPASS, pcff or cvff
- Use current charges or calculate charges using Gasteiger or Qeq methods.

Analysis

- Cluster by RMS of Cartesian coordinates
- Calculate RMS differences for Cartesian coordinates and torsion angles
- Calculate dipole moments and radius of gyration for probing geometry-property relationships
- Calculate total energy using specific forcefields for forcefield comparison
- Post optimization of geometry
- Calculate the difference in radial distribution functions for sets of atoms in the conformers.

To learn more about Materials Studio, go to accelrys.com/materials-studio