CONFLEX
HIGH PERFORMANCE
Conformation Analysis

CONFLEX®
Computational Background of CONFLEX7

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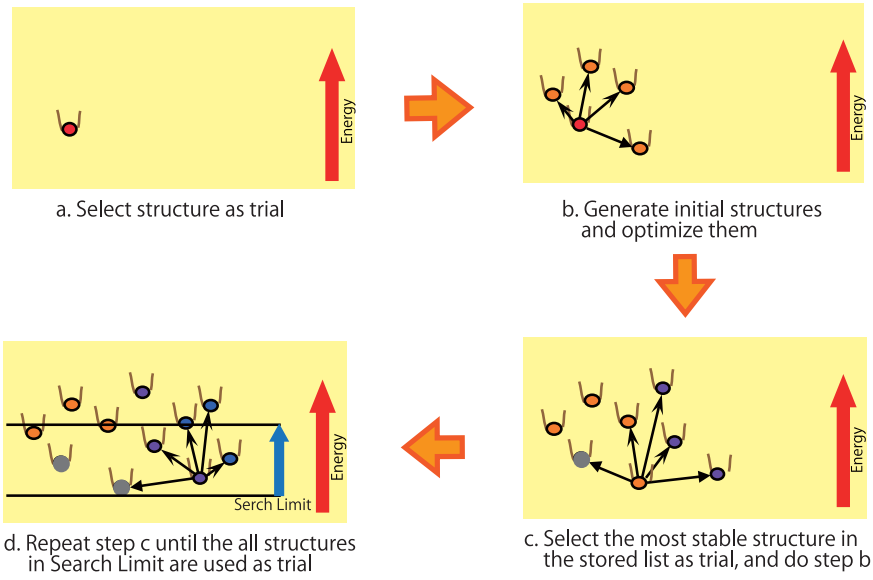
Conformation Search

The basic concept behind CONFLEX is to examine the conformational space of a structure using an exhaustive stepwise approach:

1. The selected structure as trial is perturbed using one of the three perturbation methods (see below)
2. The resulting molecular geometry is optimized using force field. (MMFF94s, EMM2, etc)
3. A comparison is made to determine whether or not to the conformation is a new energy-minimum conformer
4. Steps 1-3 are repeated until all conformers in the range of setting energy relative to the most stable conformer (named 'Search Limit') are selected as trial

Schematic representation of computational steps are indicating on below

Another representation of CONFLEX Algorithm



a. Select structure as trial

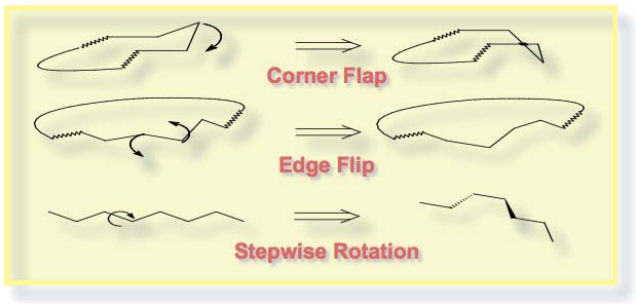
b. Generate initial structures and optimize them

c. Select the most stable structure in the stored list as trial, and do step b

d. Repeat step c until the all structures in Search Limit are used as trial

CONFLEX Perturbation Algorithms

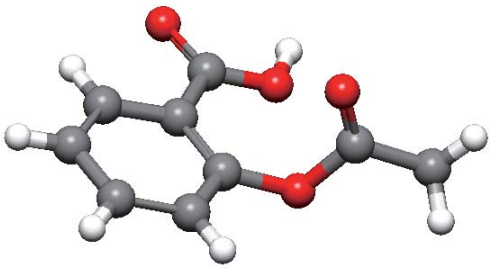
Corner Flap: Move one of the ring-skeleton atoms to the side opposite the average plane of the peripheral atoms
Edge Flip: Flap a pair of adjacent corners simultaneously in opposite directions
Stepwise Rotation: Rotate around bonds in acyclic parts of molecule
These three perturbations mimic thermal vibration of cyclic and acyclic molecules.



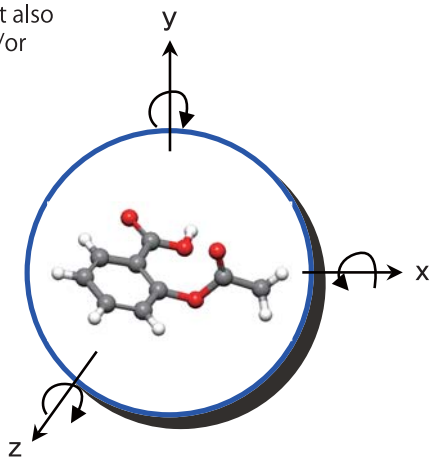
References:
H. Goto and E. Osawa, J. Am. Chem. Soc., 1989, 111, 8950- 8951.
H. Goto and E. Osawa, J. Chem. Soc., Perkin Trans. 2, 1993, 187-198.

Crystal Structure Prediction

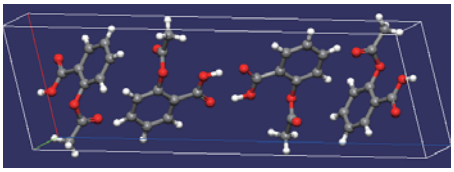
CONFLEX is used to carry out screening of crystal polymorphs by predicting the crystal structure using unique algorithms (see below).
This method is effective in screening not only conformational polymorphism but also packing polymorphism occurring due to the differences in the space group and/or lattice constants.

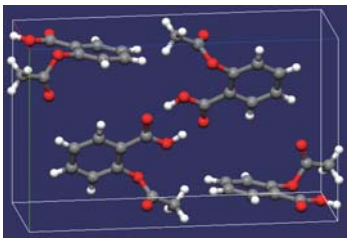


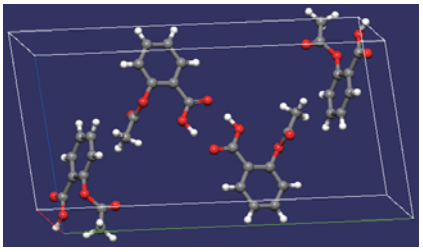
Provide molecular geometries in asymmetric unit (both CIF and MDL-Mol format are available)



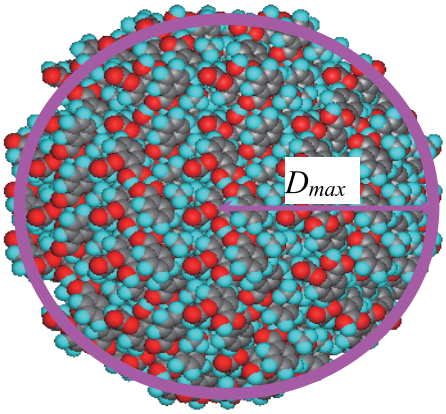
Generate initial orientation in unit cell by rotating around x, y, and z axes.







Set initial molecular crystal structures by orientation and pace group.
The initial value of lattice constants are generated automatically, and multiple space groups are available for setting simultaneously.



Property Box

	Crystals	Space Group
1	36.7098 kcal/mol	P21/C
2	37.4688 kcal/mol	P21/C
3	37.6333 kcal/mol	P21/C
4	37.7415 kcal/mol	P21/C
5	41.4176 kcal/mol	P21/C
6	42.8424 kcal/mol	P21/C
7	43.0809 kcal/mol	P21/C
8	44.2788 kcal/mol	P21/C

Construct spherical crystal structures, optimize, and sort them by energy or similarity diffraction pattern.

References:
S. Obata and H. Goto, J. Comput. Chem. Jpn., 7, 2008, 151-164.
S. Obata and H. Goto, J. Comput. Aided Chem., 9, 2008, 8-16.