CONFLEX 9
Conformation Search program

CONFLEX® permits fast, accurate, automated conformation searching and analysis critical to drug discovery and chemical engineering.
Unique to CONFLEX is its capability to completely search the conformational space of a flexible molecule to find every optimal structure of chemically significant conformers.

CONFLEX Corporation
Shinagawa Center Bldg. 6F
3-23-17 Takanawa, Minato-ku,
Tokyo 108-0074 Japan
TEL: +81-3-6380-8290
FAX: +81-3-6380-8299
Email：info@conflex.co.jp
http://www.conflex.net/

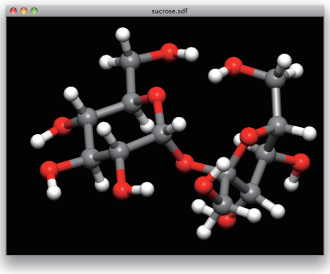
Major Functions

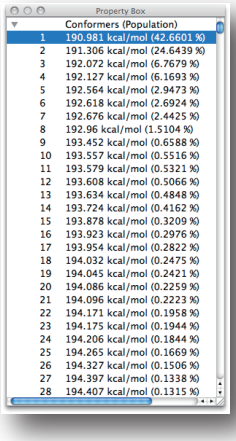
Conformational Space Search

CONFLEX recognizes the molecular structure automatically and identifies a ring and side-chain structures. CONFLEX applies three local perturbation methods to generate new conformations: Corner Flap and Edge Flip for the ring structure, and Stepwise Rotation for the side chains.

CONFLEX employs the reservoir algorithm to generate a new structure from a stable structure at all time and a range of search limit to search conformers.

With these algorithm and limitation, CONFLEX can avoid an explosive growth of conformation number.



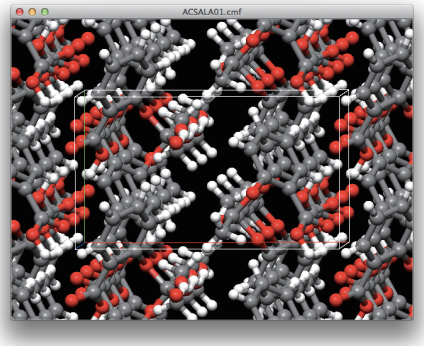


Crystal Structure Calculation and Search

CONFLEX can generate crystal structures automatically from a molecular structure and symmetrical operations defined by the specified space groups.

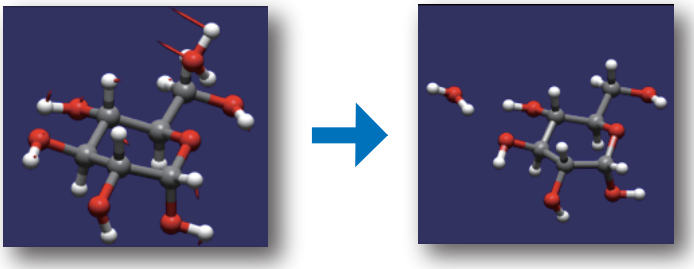
CONFLEX optimizes the crystal structures and search minimum energy structures exhaustively.

Also, CONFLEX can rank the crystal structures according to their crystal energies or simulated powder X-ray diffraction data.



Dynamic Reaction Coordinate (DRC)

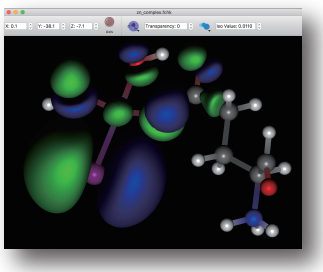
DRC is molecular dynamics calculation method using initial velocity vectors calculated from normal vibrational modes. This feature is applicable to configuration changes between multiple molecules or conformation changes of a large molecule.



Invoke External Gaussian 09/16 Program

If Gaussian program is installed to a computer with CONFLEX program, CONFLEX can invoke Gaussian to optimize and search conformers of a molecule.

With this feature, CONFLEX can handle molecules lacking force field parameter(s) and electronic states which cannot treat by the molecular force field.



CONFLEX File Format

- ○ mol — MDL Mol File
- ○ mol2 — Sybyl mol2 File
- ○ sdf — MDL SD File
- ○ pdb — Protein Data Bank File
- ○ cmf — CIF/MIF File
- ○ cif — Crystallographic Information File

CONFLEX Force Fields

- ○ MM2
- ○ EMM2
- ○ MM3
- ○ MMFF94s
- ○ Amber

System Requirements

OS: Windows
macOS
Linux
Check for detais:
https://www.conflex.net/

1.0GHz Processor & up
40GB Disk Space
Memory 1GB minimum

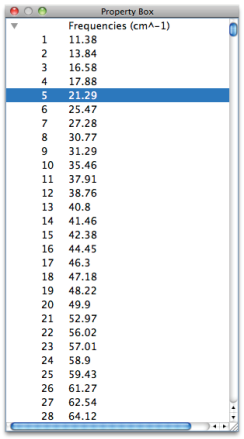
CONFLEX
HIGH PERFORMANCE
Conformation Analysis

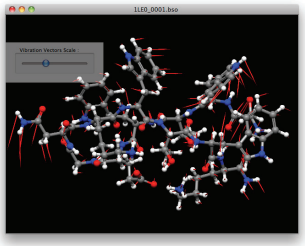
CONFLEX 9

Conformation Search program

Geometry Optimization

CONFLEX performs a normal mode analysis automatically after geometry optimization, and estimates thermodynamic properties such as Gibbs free energy. CONFLEX also permits partially constraining a structure during geometry optimization.





Host - Ligand Coordination Search

CONFLEX has the feature named Host - Ligand coordination search. This is used for specifying energetically stable configurations of complex or molecular cluster.

Solvent Effect

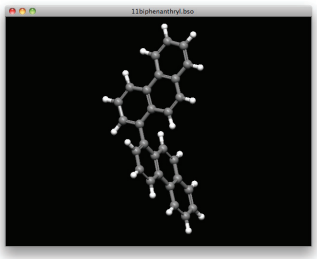
CONFLEX utilizes the GB/SA model for geometry optimization, normal mode analysis, and conformational search, as well as for calculating LogP.

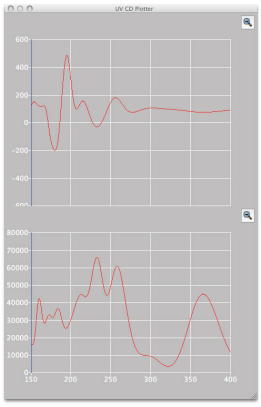
Parameter Configuration

User can customize force field parameter(s) for molecule lacking parameter(s) or modify the existing parameter(s). The user-customized parameters are only for MMFF94s parameter set.

CD/UV/Vis Spectral Analysis

CONFLEX can simulate CD/UV/Vis spectrum with conformers.





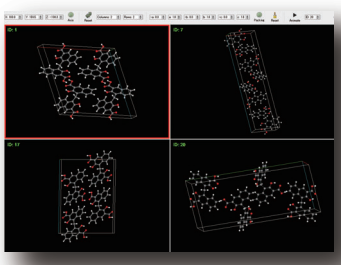
CONFLEX Interface

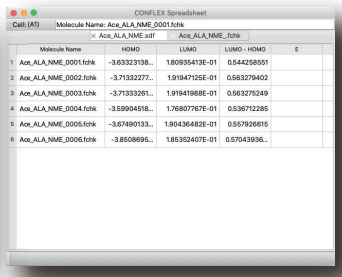
File Formats

- MDL format files: .mol, .sdf
- Sybyl mol2 format
- GAMESS log file
- Firefly log file
- CONFLEX Output file: .bso, .nmr
- Crystallographic Information File format: .cif, .cmf
- Gaussian formatted checkpoint file: .fchk
- Protein Data Bank (PDB) format: .pdb
- Copy & paste from ChemDraw

Molecule, Crystal Structure Display

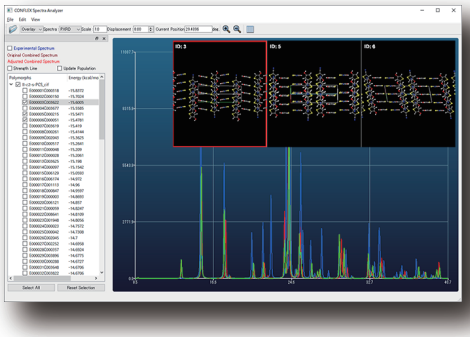
- Display formats: Wire Frame, Ball & Stick, CPK
- 3D rotation and zoom
- Crystal surface display
- Animate normal modes
- Animate sequences of DRC trajectory





Calculation Results Display

- View bond distance, bond angle, and torsion angles
- List conformational isomers
- Vector representation for normal mode analysis
- View spectra for IR, NMR, CD/UV/Vis
- Display molecular orbital surface and electron density surface
- Change surface area width in real time
- IR, UV or VCD (Gaussian) Spectral Synthesis based on conformer population
- CONFLEX Spreadsheet



Calculation Setup & Execution

- Generate calculation input file
- Execute job locally or via network
- Parameter setup for solvent effect
- Easily access frequently used keywords

Third Party Connectivity

Setup and execute jobs for/from:

- Gaussian
- ChemOffice