![CONFLEX - HIGH PERFORMANCE Conformation Analysis]

CONFLEX®
Conformation Analysis Consulting

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As an alternative to licensing CONFLEX 7 software, clients can outsource their needs to CONFLEX Corporation by way of its Conformation Analysis Consulting services.

The team of conformational experts at CONFLEX can provide fast turn-around in helping you to solve problems related to molecular conformations.

CONFLEX 7
The service primarily utilizes CONFLEX 7 software. CONFLEX 7 permits fast, accurate, automated conformation searching and analysis critical to drug discovery and chemical engineering.

Unique to CONFLEX 7 is its capability to completely search the conformational space of a flexible molecule to find every optimal structure of chemically significant conformers. CONFLEX 7 is not limited to finding only locally-optimized structures that depend on an initial structure input by the user.

Additionally, CONFLEX 7 can perform crystal search and optimization as well as crystal packing of generated conformers and permits residue substitution.

PARALLEL CONFLEX
PARALLEL CONFLEX performs geometry optimization by distributing to multiple computers the starting structures generated by means of step-wise perturbations to the initial structure. PARALLEL CONFLEX is especially effective for reducing the research time in analyzing
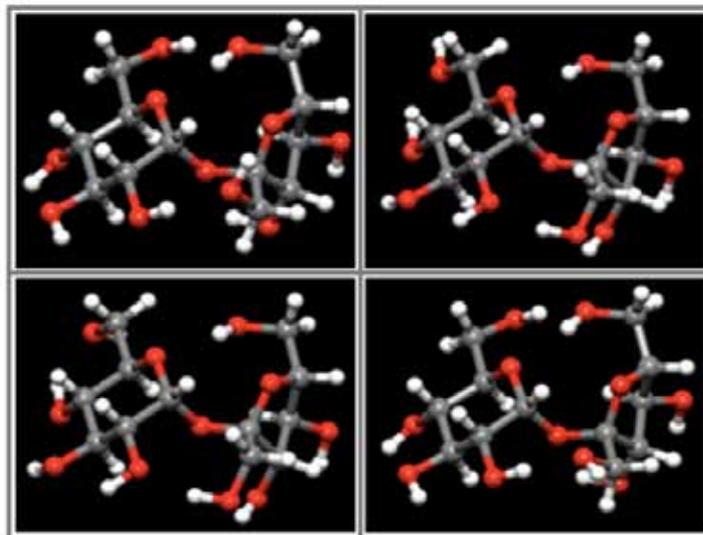
Conformational isomers of sucrose: most stable is upper-left, second is upper-right, third is lower-left, and fourth is lower-right using MMFF94s.

Service Details
1. Conformation generation
2. Conformational analysis
3. Force field calculation details
4. ab initio calculation details
5. AMBER calculation details
6. Various vibration calculations (thermodynamic quantities)
7. Crystal Calculation and Polymorphism Analysis
8. H-NMR 3JHH estimation (classical theory)
9. NMR chemical shift
10. Solvent effect GB/SA model
11. Residue Substitution
12. Examine Electrostatic interactions
13. Analysis of Folding and Reaction Paths

Other Services
- Dedicated machine on annual contract
- Consulting contract
- Project contract

References:
J.Am.Chem.Soc.,1989,111,8950-8951.
J.Chem.Soc., Perkin Trans .2,1993,187-198.