

# BARISTA™

## Molecular Analysis and Visualization Platform

Conflex Corporation  
AIOS Meguro 6F  
2-15-19, Kami-Osaki  
Shinagawa-ku, Tokyo 141-0021  
Japan  
Tel: +81-3-6380-8290  
FAX: +81-3-6380-8299  
<http://www.conflex.co.jp>

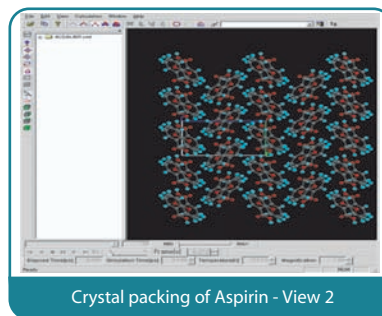
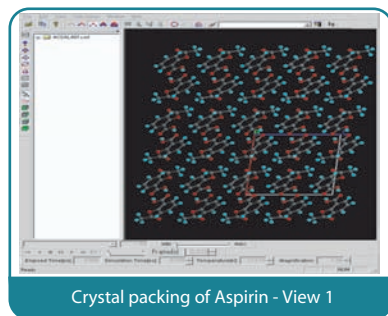
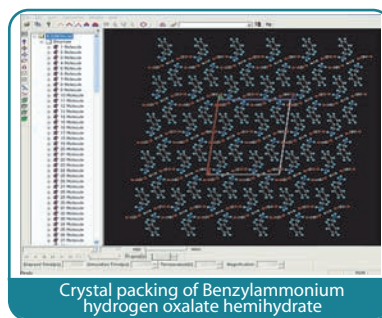
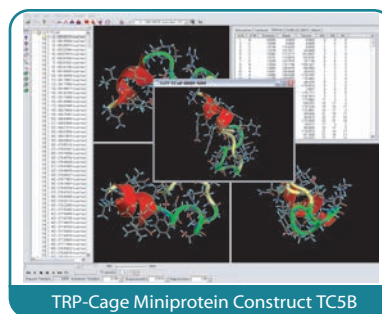
For inquires outside Japan:

Conflex USA  
5631 Palmer Way, Suite C  
Carlsbad, CA 92130  
USA  
Tel: +1 (760) 930-9277  
USA: 1 (800) 298-0054  
Fax: +1 (509) 692-4541  
[info@conflex.us](mailto:info@conflex.us)  
<http://www.conflex.us>

**BARISTA™** is a visualization and analysis platform containing functions for molecular structural analysis, molecular orbital analysis, standard vibrational analysis, and dynamic analysis in addition to proprietary functions for multi-conformational analysis, crystal calculations and polymorphism analysis.

BARISTA visualization functions create, display, and manipulate 3D depictions of molecular structures based on results computed by molecular computation programs such as CONFLEX® 6, and are designed specifically to facilitate the analysis of these results.

- Molecular structural analysis
  - 3-directional, 3-dimensional display
  - Multi-window display
  - Minimal mouse operation
- Multi-conformational analysis
  - Conformational clustering function
  - Prediction of unfolding pathways among multiple conformations
- Molecular orbital analysis
  - 3-dimensional display of electron orbitals by means of isodensity surface display
- Standard vibrational analysis
  - Animation of standard vibration
  - Display of vibration frequency spectra
- Dynamic analysis
  - Animation of dynamic simulation results
  - Graphing of energy conversion
- Crystal Packing and Polymorphism Analysis



### Key Features & Benefits

- Effortlessly submits jobs for CONFLEX 6 processing
- Cherry pick conformers and submit to Gaussian for ab initio analysis
- Directly reads CONFLEX 6 output files for analysis
- Crystal Packing Analysis
- Permits fast browsing and easy selection of conformer structures
- Displays lists in tree view
- Deepens understanding with separate camera views
- Full color, high-resolution display

### New in this Release

- Crystal Packing - explore energies of crystal polymorphism
- Visualization of Normal-Mode Analysis and Conformational Dynamics
- Ribbon, Tube, and Cylinder Views for Peptides and Proteins
- Read and Write PDB Format
- Superimpose Molecules
- Conformational Clustering

### File Formats

BARISTA handles these commonly used file formats:

- bso - Force field output file including normal mode analysis
- cmf - Crystallographic and Molecular Information file
- dat - Coordinates file
- ent - Protein Data Bank file
- mmi - MM2 / MM3 input format
- mol - MDL molfiles
- out - Optimization output file
- pdb - Protein Data Bank file

### System Requirements

#### BARISTA

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

#### CONFLEX 6

Mac OS X 10.2 & up  
Redhat Linux 8 & up  
Windows XP  
1.0 GHz Processor & up  
40 GB Disk Space  
Memory 1 GB minimum