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CCS Part 2: CONFLEX Corporation

General Consultant for Computational Chemistry (Project Article)

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CONFLEX Corp. mainly sells and supports CONFLEX, the conformation-generation software that was developed at Toyohashi University of Technology and after which the company was named. In addition, the company's consulting service, which handles general computational chemistry, has thrived recently. Of the users who have been analyzing low-molecular-weight molecules by means of semiempirical methods, more and more researchers desire to simulate large molecules by means of molecular dynamics methods and to perform more precise calculations by means of molecular orbital methods, so companies seeking such support increasingly are asking CONFLEX Corp. to apply its specialized know-how.

CONFLEX has spread because it can be used by CAChe, Fujitsu's general-purpose molecular modeling software. Recently, however, CONFLEX Corp. developed BARISTA, dedicated graphics software usable even without CAChe. BARISTA supports the new functionality of the latest version of CONFLEX2000. Because it analyzes while gradually deforming the chemical bonds of flexible molecules, it is able to find all optimized structures of chemically significant conformers. Advanced functionality becomes usable because processing is more automated. For example, 50-member rings and enantiomers are identified automatically.

The company developed a series of flows that allows CONFLEX-generated conformations to be analyzed by means of GAUSSIAN, the standard molecular orbital method. As a result, the number of users utilizing CONFLEX Corp.'s consulting services has increased recently.

The company also supplies a parallel version, and recently began to offer formal support of Linux clusters, in addition to Macintosh. Parallelization is highly efficient because computations are performed by distributing, to each node of a cluster, the multiple starting structures resulting from the perturbation of the original compound. The company offers a free trial service at its dedicated Web site (http://www.conflex.net).

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