

## CCG and BioSolveIT Integrate FlexX Docking Into Life Science Modeling Suite MOE

Users of cutting-edge life science modeling suite MOE will benefit from intuitive interface of premier protein ligand docking technology FlexX.

(Montreal and St. Augustin, September 5th, 2006) Chemical Computing Group (CCG) and BioSolveIT announce the introduction of a graphical interface to BioSolveIT's high speed/high precision docking program FlexX™ within CCG's leading-edge life science modeling software MOE™. Both companies collaborated closely to create an intuitive interface that allows users to optimally benefit from the synergy between the two packages.

While the two software programs constitute independent executables, the integration will appear seamless to end users: MOE's strengths on the preparation and analysis side for ligands and proteins plus its variety of intermolecular interaction energy computations and informatics applications can be used directly before and after FlexX docking calculations. Both companies believe that multiple computational techniques and strategies will be required to address what is known in the community as the "scoring problem" - the prediction of binding affinity from docked structures. By integrating MOE and FlexX, a unique environment is created for exploring possible methodologies for solving this problem. In addition, the interface in MOE is carefully designed to allow easy access to FlexX's essential parameters but leaves the experienced user with full control over the broad range of configuration options that FlexX offers. Also FlexX add-on modules such as the Pharm extension to exploit a priori know-how about protein specifics will be supported, the companies declared.

BioSolveIT's CEO, Dr. Christian Lemmen, is particularly pleased with this collaboration. "Not only was development possible in record time due to the modular architecture of both systems, but also the first prototype already revealed the wealth of synergies between CCG's fantastic piece of software and our FlexX engine. Certainly, new ideas keep emerging all the time", Dr. Lemmen comments, "but I am certain that we have achieved our major goal which was to broaden the scope of application of both suites for the user's benefit!".

MOE's broad functionality is further augmented by direct access to the long-standing industry standard FlexX, originally authored by Professor Matthias Rarey, which is known for its high accuracy and speed. Paul Labute, CCG's CEO, said "Our customers will benefit greatly from the integration of FlexX and MOE. A key strength of MOE is its flexibility in allowing users to maximize their use of computational drug discovery software. With the integration of FlexX, users will be able to far better exploit this outstanding technology, with MOE bringing important data preparation and results analysis capabilities." He went on to say that "I am also pleased to see that both CCG and BioSolveIT share the same commitment to high quality and standards, in both the engineering and scientific domains. It certainly helped make this collaboration a success and will be an important factor in future collaborations."

The new interface will be presented to the general public for the first time at this year's Fall National Meeting of the American Chemical Society in San Francisco from September 10-14<sup>th</sup>.

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### About Chemical Computing Group

Chemical Computing Group (CCG) Inc. provides computational applications for drug discovery and design. CCG's product is the Molecular Operating Environment (MOE), a comprehensive system that combines visualization, simulation and methodology development in one software package. MOE's integrated suite of powerful and intuitive chemistry software include tools for HTS, Structure-based Design, Molecular Modeling, Protein and Homology Modeling as well as an embedded programming language (the Scientific Vector Language) for the rapid prototyping of scientific methods. MOE runs on a range of computer hardware so it is accessible to experts and occasional users. CCG's headquarters are in Montreal, Canada, with offices in Cologne, Germany, Cambridge, UK, and Bangalore, India.

### About BioSolveIT

BioSolveIT, the developer of FlexX, is a globally operating cheminformatics and bioinformatics software company. BioSolveIT provides superior custom software solutions for structure-based design, flexible molecular alignment, database searching, library design, and analysis. Its breakthrough computational technologies help to innovate pharmaceutical research — transforming ideas into success stories.