FOR IMMEDIATE RELEASE

PSILO

CHEMICAL COMPUTING GROUP

CHEMICAL COMPUTING GROUP RELEASES THE NEW VERSION OF ITS PROTEIN STRUCTURE DATABASE SYSTEM - PSILO 2013.10

MONTREAL, Canada, December 16, 2013 - Chemical Computing Group (CCG) announces the release of PSILO 2013.10. PSILO is a structure database and visualization system that provides an easily accessible, consolidated repository for macromolecular and protein-ligand structural information. It offers research organizations a means to systematically track, register and search both experimental and computational macromolecular structural data. A web-browser interface facilitates the searching and accessing of public and private structural data. New and enhanced features in PSILO 2013.10 include:

- **Improved search and core infrastructure performance**
- **Enhanced alignments using STOVCA criteria**
- **Access a knowledge-based library of small molecule crystallographic data through MOGUL**

The primary focus of the PSILO 2013.10 release has centered on enhanced performance, in terms of search speed and search results management. The user has greater options and flexibility in rapidly examining and evaluating the search hit list. The secondary structure similarity search has also been modified and now uses a lower resolution definition of secondary structure which produces improved results. “We have re-defined the secondary structure based on Cα distances rather than on hydrogen bonding,” said Paul Labute, President and CEO of CCG. “This has the advantage of being independent of other chains in the system while still corresponding to *Dictionary of Secondary Structure of Proteins* (DSSP).”

PSILO 2013.10 can now be integrated with CCDCs MOGUL for structural diagnostics. The new version of PSILO connects to MOGUL and allows access to a knowledge-based library of small molecule geometry, derived from the Cambridge Structural Database (CSD). Assessment of statistical molecular conformations can be directly conducted through PSILO and included as part of the structural Health Report.

Additional important features in PSILO 2013.10 include core infrastructural enhancements relating to streamlined IT deployment. PSILO has been modified so that all calls to MOE are now routed through MOE/web using SOAP calls. This results in more efficient communication between PHP and MOE. This also facilitates the use of certain PSILO functionality, such as electron density calculation, by making SOAP requests to the server. The binaries for PSILO have also been upgraded. PSILO now uses precompiled binaries of PHP, MySQL, Apache, and the other related tools which it relies upon. All of these have been updated to the most recent, stable versions. The change in binaries will make upgrading future versions of PSILO much easier.

For additional information about PSILO 2013.10 please contact: sales@chemcomp.com

About Chemical Computing Group

Chemical Computing Group (CCG) is a leading supplier of software solutions for Life Sciences. Since its inception in 1994, CCG has been providing state-of-the-art applications for drug discovery to pharmaceutical, biotech and academic researchers. CCG’s products and services are used by biologists, medicinal chemists and computational chemists throughout the world. Chemical Computing Group has a proven track record in scientific innovation, consistently releasing new versions and upgrades for all its products. CCG has a very strong reputation for collaborative scientific support, with offices in both North America and Europe. CCG headquarters are in Montreal, Canada. **For more information visit:** www.chemcomp.com

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