2016 Press Release

FOR IMMEDIATE RELEASE

CHEMICAL COMPUTING GROUP RELEASES THE NEW VERSION OF ITS PROTEIN STRUCTURE DATABASE SYSTEM - PSILO 2016.10

MONTREAL, Canada, December 01, 2016 - Chemical Computing Group (CCG) announces the release of PSILO 2016.10. 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 2016.10 include:

- **Identify structural issues such as clash score, R_{free}, outliers with the Protein Quality Summary graphic**
- **Perform 3D searches and superpose based on the 3D query for easy structural comparison**
- **Compute weighted electron density maps from raw structure factors (F) for more accurate modeling**
- **Launch COOT directly from PSILO to visualize protein structures**
- **Run large scale searches efficiently with enhanced parallelization using MOE/web**

The PSILO 2016.10 release includes a variety of new features and enhancements for viewing records and for searching and aligning proteins. Geometric protein properties can now be quickly evaluated by consulting the Protein Quality Summary graphic. COOT, a popular 3D visualizer among crystallographers, can now be launched directly from PSILO to visualize and evaluate structures. Additional crystallographic support is available in the form of weighted electron density maps which can now be computed directly from the raw structure factors (F). PSILO now also provides the option to automatically superpose 3D search results relative to the 3D query for pairwise comparison of receptor environments. In addition, the improved parallelization of PSILO using MOE/web introduces enhanced efficiency and scaling of large jobs.

Additional important features in PSILO 2016.10 include: expanded support for sketchers, sorting of ligands by similarity, and a new protocol for handling multi-subunit protein families. The 2016.10 version of PSILO also has enhanced security features for connecting to the MOE/web server over https.

For additional information about PSILO 2016.10 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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