FOR IMMEDIATE RELEASE

CHEMICAL COMPUTING GROUP RELEASES THE NEW VERSION OF ITS PROTEIN STRUCTURE DATABASE SYSTEM - PSILO 2012.11

MONTREAL, Canada, December 7, 2012 - Chemical Computing Group (CCG) announces the release of PSILO 2012.11. PSILO is a protein structure database and visualization system that provides an easily accessible, consolidated repository for macromolecular and protein-ligand information. It offers research organizations a means to systematically track, register and search both experimental and computational macromolecular data. A web-browser interface facilitates the searching and accessing of public and private structural data. New and enhanced features in PSILO 2012.11 include:

- **Domain Motif Search**
- **Non-redundant BLAST summary report**
- **Automatic GPCR annotation**
- **Interactive protein:ligand interaction diagrams**

A key focus for the new release was the addition of the new Domain Motif Search which identifies similar 3D arrangements of secondary structure elements to find distantly related homologues. “These sequence-independent queries make possible the detection of remote homologues and analogs for drug repurposing and more thorough analysis of potential off-target effects,” mentioned Paul Labute, President and CEO of CCG.

The non-redundant BLAST summary report is another important feature included in PSILO 2012.11. This new page displays BLAST sub-query results in an interactive graphical format that includes a phylogenetic tree with matching multiple sequence alignments. BLAST hits can be browsed to better identify clusters of related hits. Clicking individual branches on the tree highlights corresponding points of sequence similarity whereas clicking on the sequence will highlight the protein position in the phylogenetic tree.

PSILO 2012.11 automatically detects, classifies and annotates GPCR sequences. It identifies the transmembrane helices and classifies the sequences into GPCR families and subfamilies. “Many clients who work on GPCR targets expressed interest in more advanced tools that cater to the specific, and often challenging, properties of GPCRs. This was one of the motivations behind developing automatic GPCR detection and annotation protocols in PSILO,” explained Paul Labute. He also added, “Automatic protocols have been added to generate and maintain clustered and aligned kinases, antibodies, and GPCRs, to be used in conjunction with MOE's specialized modeling tools for these families.

For additional information about PSILO 2012.11 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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