StarDrop 5.2 Adds New FieldAlign Plug-in Module

Optibrium unveils the first output from its collaboration with Cresset

CAMBRIDGE, UK, 21st March 2012 – Optibrium, developer of software solutions for drug discovery, today announces a new version of its StarDrop™ platform. StarDrop 5.2 features a new plug-in module that provides users with access to Cresset's FieldAlign™ technology, which offers a unique, 3-dimensional insight into the biological activity of their compounds. This new development is the first result of the technology exchange, between Optibrium and Cresset, announced earlier this yearand adds another powerful tool to StarDrop that will enable chemists to understand the 3D structure activity relationship (SAR) of their chemistry in order to optimise their compounds.

Achieving a combination of potency with appropriate ADME and safety properties is essential to the discovery of high quality drug candidates. Optibrium's StarDrop platform helps to identify compounds with a good balance of properties by integrating *in silico* and experimentally measured data using a unique multi-parameter optimisation approach, chemical space visualisation and intuitive data analysis. StarDrop's interactive designer with Glowing Molecule™ visualisation guides the exploration of compound design strategies with instant feedback on the impact of changes on a compound's predicted properties. These core features can be extended with plug-in modules to predict key ADME properties and P450 metabolism, build and validate robust QSAR models of in-house compounds and data, and automatically generate new, relevant compound ideas. The new FieldAlign module in StarDrop adds a powerful 3D view of compound interactions that will complement StarDrop's existing 2D QSAR models.

FieldAlign provides a unique insight into the biological activity, properties and interactions of molecules. Using fields, biologically meaningful comparisons can be made that are not limited by two-dimensional structure. FieldAlign is a powerful molecular design and 3D SAR tool that allows the molecular fields of multiple compounds to be compared in their bioactive conformations. By highlighting both similarities and differences between molecules, FieldAlign shows where and how lead molecules bind to their protein target. This enables regions of active molecules that can be replaced, to be quickly identified, to perfect the design of a new lead compound. Furthermore, given the 3D structure of an active molecule and a series of 2D compound structures, FieldAlign will generate the best 3D alignment for the compounds, scored and ranked according to their field similarities with the known active. With this information, small compound libraries can be screened to look for novel series with greater structural diversity, and the design of focused libraries can be optimised for synthesis or initial screening.

Version 5.2 also introduces new enhancements of StarDrop's core capabilities, in particular a flexible tool for performing automatic R-group analysis. This new feature analyses a chemical series to interactively visualise the impact of variations to R-groups, linkers, atoms or fragments on compound properties to help chemists to further understand the SAR of their chemistry and identify new optimisation strategies. StarDrop can also enumerate the full, combinatorial library to explore the properties of compounds that have not yet been synthesised and identify potential missed opportunities.

Matt Segall, CEO of Optibrium, commented "We are excited to be able to provide a great range of new features to our users, continuing to extend StarDrop's seamlessly integrated environment that helps to guide the efficient identification of high quality compounds. We are particularly pleased that our new collaboration with Cresset has so quickly yielded an important new capability for the StarDrop platform and look forward to continuing to work with Cresset on further joint projects."

StarDrop 5.2 will be launched at the upcoming American Chemical Society Spring Meeting and Exposition in San Diego, CA, March 25-29. Visit Optibrium's stand (#1419) for a first sight of this exciting new release. Further information on StarDrop can also be found at www.optibrium.com or by calling +44 1223 815900.

7226 Cambridge Research Park
Beach Drive, Cambridge
CB25 9TL, UK

Tel: +44 1223 815900
Fax: +44 1223 815907

Email: info@optibrium.com
Website: www.optibrium.com

About Optibrium Ltd

Optibrium (www.optibrium.com) is dedicated to providing software to guide decisions involving complex, uncertain data in an intuitive way. Based in Cambridge, UK, Optibrium has a global customer base ranging from top-ten pharmaceutical companies to small biotechs and academic groups. Our mission is to continue to develop new technologies that will optimise project strategy, reduce wasted molecules and experiments, shorten timelines and improve the quality of candidate compounds for our clients. Optibrium's primary product, StarDrop, is focused on the drug discovery industry, helping guide scientists to make decisions in the design and selection of high quality drug candidates. Visit the online community at http://www.optibrium.com/community/ for further discussions on improving the productivity of drug discovery.

For further press information please contact: Sarah Evans, The Scott Partnership, 1 Whiteside, Station Road, Holmes Chapel, Cheshire CW4 8AA, UK Tel: + 44 1477 539539 Fax: +44 1477 539 540 E-mail: optibrium@scottpr.com.