Optibrium to Unveil StarDrop 5 and Revolutionary Nova Module at ACS Spring 2011

Offering a New Generation of Possibilities in Guiding Decisions for Drug Discovery

CAMBRIDGE, UK, March, 07, 2011 – Optibrium™, a provider of software solutions for drug discovery, will be officially launching the next generation of StarDrop™ featuring the ground-breaking Nova™ module on booth #1121 at the American Chemical Society (ACS) National Exposition, 27-31 March, 2011, Anaheim, CA. This intuitive platform helps to guide scientists' decisions to quickly identify compounds with a high chance of success for their drug discovery project. Nova is a completely new module within StarDrop 5, helping pharmaceutical and biotech companies to search for high quality drugs by generating new chemistry ideas, prioritised against specific property profile requirements when making critical decisions in drug discovery.

Fast identification of high quality compounds with the best balance of multiple property requirements is a major challenge in making effective drug discovery decisions. Complex, often conflicting requirements, combined with uncertain data, make it difficult to decide with confidence which lines of enquiry to pursue and which compounds to prioritise. So, it's no surprise that most research in drug discovery results in expensive failure.

The revolutionary Nova module stimulates the search for high quality compounds by generating new chemistry ideas, prioritised against defined property profile requirements. It facilitates the search for prospective drug candidates by expanding the chemistry around an initial compound based on medicinal chemistry transformation rules, ensuring that they are chemically feasible. Independent tests proved that more than 94 per cent of generated compound structures were acceptable to medicinal chemists. In addition to an initial library of more than 200 transformations derived from literature and provided with Nova, chemistry knowledge can be transferred between medicinal chemists by defining their own transformation rules, flagging favourites and grouping rules tailored to specific goals. Nova provides the user with complete control of which transformations they wish to apply and enables a rigorous exploration of possibilities while searching for compounds with improved properties. A white paper describing Nova in more detail can be downloaded from http://www.optibrium.com/community/publications/112-a-new-generation-of-possibilities.

Nova ensures a broad exploration for new chemical ideas and, combined with StarDrop's existing probabilistic scoring, chemical space visualisation, Glowing Molecule™ and predictive modelling capabilities, helps to quickly focus on high quality chemistry and speed up hit-to-lead and lead optimisation. Example applications include rigorously exploring the chemistry around new hits to identify those most likely to provide access to good drug-like properties; searching for new chemical strategies to overcoming issues in lead optimisation, including lead hopping; and identifying opportunities for patent busting.

The new Nova module is an addition to the existing suite of plug-in modules for the StarDrop platform, including a suite of predictive ADME QSAR models, quantum mechanics-based models to predict the regioselectivity and vulnerability to P450 metabolism and the Auto-Modeller that automatically generates and validates high quality QSAR models tailored to a project's chemistry and data.

Furthermore, StarDrop 5 provides a comprehensive range of upgrades and significant new features, including enhanced data visualisation and new functionality to perform mathematical calculations within StarDrop, helping users to explore data and produce graphs, histograms and chemical spaces that can be easily included in reports. These build on StarDrop's unique capabilities such as: Glowing Molecule™, which visualizes the influence of different regions of potential drugs to interactively guide the design of improved molecules and; Probabilistic scoring, which allows the user to objectively compare compounds against a weighted profile of required properties to discover the compounds most likely to yield successful results.

"We are very excited about the official launch of StarDrop 5 at ACS Spring 2011", commented Dr. Matthew Segall, CEO of Optibrium. "The revolutionary Nova module and the major improvements to the core of StarDrop are the culmination of a major R&D effort and offer a step change in the ability of StarDrop to help our users to rapidly target high quality chemistry and improve the efficiency and productivity of drug discovery."

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The official launch of StarDrop 5 will be on booth #1121 at the American Chemical Society (ACS) National Exposition in Anaheim, CA, 27-31 March, 2011. Matt Segall will also be giving a talk on Nova at the ACS meeting in the DCOMP session at 11:15am on March 27th in room 213B of the Anaheim Convention Centre. For more information about Nova and StarDrop 5 please visit www.optibrium.com/stardrop5/ , alternatively please call +44 (0) 1223 815 900 or email info@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. Optibrium's primary product, StarDrop, is focused on the drug discovery industry, helping scientists to guide decisions in the design and selection of high quality drug candidates. Optibrium was founded in 2009 as a spin-out of BioFocus DPI (formerly Inpharmatica). The founding group was responsible for the development of StarDrop from 2003 and, prior to this, research and development of related technologies since 1994. Based in Cambridge, UK, Optibrium has a global customer base ranging from top-ten pharmaceutical companies to small biotechs and academic groups.

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