Optibrium Introduces StarDrop 6.1 with New Strategies for Selection and Optimisation of High Quality Compounds

Next generation software previews at American Chemical Society's Spring National Meeting

CAMBRIDGE, UK, 19th March, 2015 – Optibrium™, a developer of software for drug discovery, has announced the launch of version 6.1 of its StarDrop™ platform to guide researchers in the design of high quality compounds in drug discovery, agrochemicals and other chemistry fields. The latest release introduces the Matsy™ technology, based on matched molecular series analysis, which proposes strategies for chemical substitutions to optimise compound activity. Also included is a major upgrade to StarDrop's P450 metabolism module that facilitates the design of compounds with improved metabolic stability, in addition to enhancements to the platform's data analysis and management capabilities.

As a result of Optibrium's collaboration with NextMove Software, the addition of the Matsy algorithm extends the capabilities of StarDrop's Nova™ module that automatically generates and prioritises novel compound ideas. Matsy searches databases of matched molecular series to identify chemical substitutions that are most likely to improve target activity. Using data from longer series of matched compounds, instead of the common matched molecular pairs approach, provides additional context and enables more relevant predictions to be made for a chemical series of interest. The combination with StarDrop's unique capabilities for multi-parameter optimisation and predictive modelling enables efficient prioritisation of the resulting ideas to identify high quality compounds with the best chance of success.

StarDrop's P450 module uses quantum mechanical methods to predict the most likely sites of metabolism on a compound by drug metabolising isoforms of Cytochrome P450 and guides the design of compounds to improve metabolic stability. The major upgrade of this module in StarDrop 6.1 offers further improvements in the accuracy of existing isoform models (CYP3A4, CYP2D6, CYP2C9) as well as adding new models (CYP2C8, CYP2C19, CYP2E1, CYP1A2). The corresponding metabolite structures are also predicted to assist analysis of their properties and guide metabolite identification. This research was undertaken as part of the HeCaToS project, funded under the European Union Seventh Framework Programme (grant agreement 602156).

Dr Matthew Segall, Optibrium's CEO, commented: "We are delighted to announce another significant upgrade to StarDrop, further expanding its predictive capabilities and building on the success of StarDrop 6's ground-breaking Card View™. These developments enhance StarDrop's already comprehensive environment for compound design and selection to guide chemistry projects to successful outcomes."

StarDrop 6.1 is previewed at the American Chemical Society National Meeting, 22nd-26th March 2015, in Denver with demonstrations on booth #1219.

For further information on Optibrium and StarDrop, please visit www.optibrium.com/stardrop/, contact info@optibrium.com or call +44 1223 815900.

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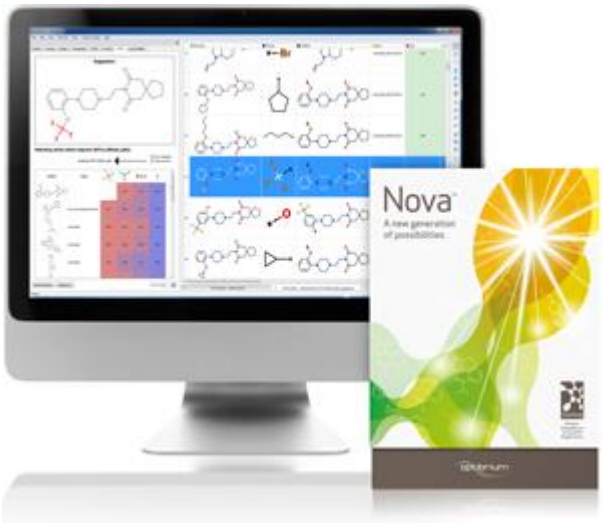

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About Optibrium Ltd.

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. Optibrium's portfolio of products includes:

- StarDrop™, which brings confidence to the selection and design of high quality candidate compounds. StarDrop creates an intuitive, highly visual and flexible environment to facilitate and speed up lead identification and optimisation, quickly targeting effective candidate compounds with a high probability of success downstream.
- Sentira™, an easy-to-use, dynamic data visualisation platform that helps to quickly spot patterns in compound data, analyse structure-activity relationships and elegantly present and report results.
- Asteris™, an iPad app that enables researchers to explore new compound ideas when and where they want, by combining highly intuitive chemistry drawing tools with StarDrop's visually informative predictive modelling.

Founded in 2009, Optibrium continues to develop new products and research novel technologies to improve the efficiency and productivity of the drug discovery process. Optibrium works closely with its broad range of customers and collaborators that include leading global pharma, agrochemical and flavouring companies, biotech and academic groups.

Visit the online community at http://www.optibrium.com/community/ for further discussions on improving the productivity of drug discovery.