# Optibrium Adds 3D Structure-Based Design with Introduction of StarDrop 6.3

*Seamless link between 2D and 3D structure-activity relationships guides more efficient compound optimisation*

**CAMBRIDGE, UK, and SANKT AUGUSTIN, GERMANY, 10 March, 2016 –** Optibrium™, a developer of software for small molecule drug discovery and optimisation, today announced the launch of version 6.3 of the StarDrop™ platform. The release introduces a new module providing seamless access to best-in-class structure-based design technologies, based on BioSolveIT's SeeSAR™ package, and follows the companies' recently announced collaboration. The addition of intuitive visualisation of 3-dimensional (3D) protein-ligand interactions to StarDrop results in a fully integrated environment for analysis and visualisation of compound data, coupled with a comprehensive range of ligand- and structure-based design capabilities that guide the optimisation of high-quality compounds.

The new SeeSAR module for StarDrop provides a state-of-the-art and scientifically rigorous approach to understanding the binding of compounds in their protein targets in 3D. Users can import ligand and protein structures, derived from crystal structures or predicted with any docking software, and visualise the key interactions driving potency. This is seamlessly linked to StarDrop's chemoinformatics methods based on 2-dimensional (2D) compound structure and its unique Card View™ approach to interpreting the resulting structure-activity relationships (SAR). This combination enables chemists to better understand and rationalise the SAR within their project chemistry. StarDrop's suite of predictive modelling and *de novo* design capabilities guide further improvements in a truly multi-parameter optimisation environment.

In addition to the new module, StarDrop 6.3 will also bring further enhancements to its existing capabilities, including powerful chemical sub-structure searching, an interactive designer for StarDrop's Card View and updates to both the Derek Nexus™ module for toxicity prediction and the BIOSTER™ database of precedented chemistry transformations.

Dr Matthew Segall, Optibrium's CEO, commented: "We are delighted to announce this exciting new version of StarDrop, including the SeeSAR module developed with our partners at BioSolveIT. In the short time since its announcement, our collaboration has already produced enhancements to both SeeSAR and StarDrop. This latest addition to StarDrop provides users with a complete compound design and optimisation platform in a fully integrated, intuitive user interface."

"We are proud to collaborate with Optibrium on this powerful combination of 2D and 3D worlds. Merging our user-friendly technologies will save project team's time and enable better research as visually informed decisions literally guide scientists to design the best molecules to be synthesised next," commented Dr Christian Lemmen, BioSolveIT's CEO.

A preview of StarDrop 6.3 will be on show at the American Chemical Society National Meeting, 13th-17th March 2016, in San Diego with demonstrations on booth #1227. Attendees at this meeting can also gain 'hands on' experience of these new capabilities during an interactive workshop at 3.30 pm on Monday 14th March; to register, visit http://bit.ly/1TRtrjV.

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

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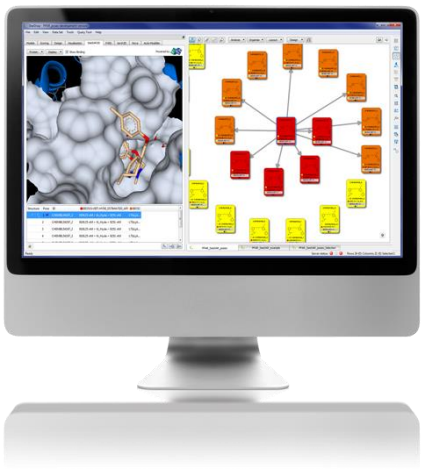

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**About Optibrium Ltd.**

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 www.optibrium.com/community for further discussions on improving the productivity of drug discovery.

**About BioSolveIT GmbH**

BioSolveIT is a globally acting medicinal chemistry informatics company. BioSolveIT is highly renowned for their superior custom software solutions for affinity estimation, structure-based design, docking, flexible molecular alignment, database searching, library design, and analysis. Their visual and fast computational technologies help to innovate pharmaceutical research with a proven track record in almost all big pharma companies, amongst them AstraZeneca, F. A. Hoffmann-LaRoche, BASF, Bayer, Boehringer-Ingelheim, GSK, Novartis, Zealand Pharma, Pfizer, Sanofi, and many others. Their latest portfolio addition, SeeSAR™, roots in co-developments with Bayer, F. A. Hoffmann-LaRoche, and Hamburg University, and helps to predict and visualize binding of therapeutic molecule candidates. Profiting from a radically simple user interface, it addresses computationally inexperienced medicinal chemists and experts alike.

BioSolveIT is based in Sankt Augustin, Germany and entertains a support and sales office in Seattle, USA, and several distribution partner offices in Japan, China, and India.

For further information: www.biosolveit.com

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