Optibrium Introduces StarDrop 6.4 with Universal Pose Generation Interface

Adds seamless link to compound structure assessment in 3D docking and alignment models

CAMBRIDGE, UK, 27 June 2017 – Optibrium, a developer of software for small molecule drug discovery, today announced the launch of version 6.4 of the StarDrop™ platform. The latest release includes a universal Pose Generation Interface, which seamlessly links expertly prepared docking and alignment models with StarDrop's comprehensive environment for small molecule design, optimisation and data analysis. The integration of this 3-dimensional (3D) information with analyses based on 2-dimensional (2D) structure, ensures that scientists can quickly understand structure-activity relationships, identify potential liabilities and design new compounds with the highest chance of success.

The new Pose Generation Interface in StarDrop 6.4 supports collaboration between computational and medicinal chemists, making routine 3D modelling accessible to all decision makers, leading to better decisions and shorter project timelines. Medicinal chemists can evaluate multiple iterations of designs in real time and inspect returned poses to give an understanding of important binding interactions, while also considering data from experiments and other predictive methods in a single, elegant environment. Computational chemists can make their validated 3D models available to colleagues via StarDrop's Pose Generation Interface, giving them greater opportunity to focus on expert computational design and model building rather than routine calculations. Only the most relevant compounds will then go on for further specialist computational evaluation, having a positive impact on project efficiency and progression.

StarDrop's Pose Generation Interface is compatible with software from major computational chemistry providers including; BioSolveIT, Cambridge Crystallographic Data Centre, Chemical Computing Group and OpenEye Scientific.

Other improvements in StarDrop 6.4 will make it even easier for users to prepare presentations and reports based on their analysis in StarDrop and work with large high-throughput or virtual screening data sets.

Dr Matthew Segall, Optibrium's CEO, commented: "We recognise that scientists often have preferred software with which to perform docking and alignment calculations. We have developed StarDrop 6.4 to be 'open' and not restricted to any specific method. This latest release further shows StarDrop's capability to support discovery projects from end-to-end, fully integrating into a client's computational chemistry and informatics infrastructure."

In StarDrop, Optibrium has developed a comprehensive suite of integrated software with a highly visual and user-friendly interface. It enables a seamless flow from the latest data through to predictive modelling and decision-making regarding the next round of synthesis and research, improving the speed, efficiency, and productivity of the drug discovery process. Seamlessly connecting with other models, informatics methods and databases, StarDrop provides user-friendly access to resources, making project management quicker and simpler.

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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About Optibrium Ltd.

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. The company's lead product, StarDrop, is a comprehensive suite of integrated software with a highly visual and user-friendly interface. StarDrop enables a seamless flow from the latest data through to predictive modelling and decision-making regarding the next round of synthesis and research, improving the speed, efficiency, and productivity of the discovery process.

Founded in 2009, Optibrium is headquartered in Cambridge, UK with offices in Boston, US. 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.

For further information visit www.optibrium.com or join in discussions on improving the productivity of drug discovery at www.optibrium.com/community.