BioSolveIT and Optibrium™ Release First Integrated 2D and 3D Software for Medicinal Chemists

Partnership quickly delivers integrated software that combines 3D structure-based design with ADME predictions to guide high quality compound design

SANKT AUGUSTIN, GERMANY and CAMBRIDGE, UK, 24th November 2015. German chemoinformatics specialist BioSolveIT and Optibrium, developer of software for small molecule discovery and optimisation, today announce the release of the first software resulting from their recently-announced collaboration. The newly enhanced version of BioSolveIT's popular SeeSAR software adds an entirely new capability – to predict absorption, distribution, metabolism, and excretion (ADME) properties – seamlessly integrated within SeeSAR's, simple and minimalistic design. This helps medicinal chemists to consider these important properties side-by side with SeeSAR's structure-based design capabilities, thereby guiding the efficient design of potent, high quality drug candidates.

The key to efficiently find good therapeutic compounds is often an X-Ray crystal structure or 3D model of the 'target', a protein centrally involved in a disease mechanism. Researchers aim to design molecules that interact with the target to achieve effects such as blocking a movement, inhibiting interactions of certain molecules in the body with the target protein, or closing a channel. The key to optimising potent drug candidates is a deep understanding of these interactions in 3D. Addressing this challenge is a core specialty of BioSolveIT who have a 15-year track record in global pharma, biotech, and academic research, providing tools that both predict and visualise these key interactions - a unique combination in the field.

However, achieving target potency is not the only goal of lead optimisation. To achieve efficacy and avoid safety issues, a high quality drug candidate must have an appropriate profile of ADME properties. For example, an orally administered drug for a target in the central nervous system must be soluble, absorbed through the intestine, survive metabolic attack and penetrate the blood-brain-barrier, while avoiding off-target interactions that lead to toxicity. Therefore, accurate predictions of these compound properties, while considering new 'virtual' compounds, can guide the design process toward compounds that achieve a balance of potency with these other requirements, reducing the risk of late-stage failures that can cost R&D departments millions of Euros. Development and application of these models have been a strength of Optibrium's team for over 15 years. "We have given a preview to selected users in Big Pharma, and we are happy to say that the feedback has been entirely enthusiastic", comments Dr Christian Lemmen, BioSolveIT's CEO.

Given today's pace of research, scientists seek to minimise the need to switch between complex software packages. "An integrated solution has an enormous appeal to users and management - besides being an obvious time-saver. Today, Optibrium and BioSolveIT deliver a platform that is unparalleled in speed, predictive power, and ease of use", says chemist Dr. Marcus Gastreich, Director Application Science, who acts as the interface between BioSolveIT's customers and software engineers. The new SeeSAR package targets high quality compounds by elegantly displaying the relevant properties, calculated with Optibrium's rigorously validated models. "The speed and quality with which we have achieved this first step demonstrates our common development approaches and commitment to delivering value to our users", comments Dr Matt Segall, CEO of Optibrium.

The new SeeSAR package can be obtained directly from BioSolveIT's website at www.biosolveit.de/SeeSAR.

Contact:

BioSolveIT

Marcus Gastreich

Director of Application Science

E-mail: marcus.gastreich@biosolveit.com

Phone: +49 2241 25 25 0

Optibrium

Nick Foster

Director, Business Development

E-mail: nick.foster@optibrium.com

Phone: +44 (0)1223 815900

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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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.