BioSolveIT and Optibrium™ Sign Collaboration Agreement

Partnership will deliver a link between 2D and 3D design on medicinal chemists' desktops.

St. Augustin, Germany, and Cambridge, UK, October 13, 2015.

Optibrium, providers of software for compound optimisation, and chemoinformatics specialist BioSolveIT, today announced that they will collaborate to create seamlessly integrated data analysis, visualisation and simulation software for drug research.

The two companies are known for their best-in-class prediction tools for selection and optimisation of potential therapeutics, where it is essential to recognise and resolve potential problems as early as possible. Computer software for 'virtual design' of drug candidate molecules prior to synthesis and testing is ubiquitous in medicinal chemistry and an important time-saver in research. As part of the agreement, both companies will exchange their proprietary technologies; the first phase will incorporate a suite of high-quality predictive models of absorption, distribution, metabolism and excretion (ADME) and physicochemical properties from Optibrium's StarDrop™ platform as an optional feature within BioSolveIT's SeeSAR™ package. This will be followed by the integration of SeeSAR's capabilities to work with 3D structural information into StarDrop's unique environment that guides the design of high quality compounds.

Dr. Matt Segall, CEO of Optibrium, commented: "*Our customers tell us that they want to understand the relationship between the SAR in their data and the 3D structures of their compounds and protein targets. BioSolveIT's state-of-the-art and scientifically rigorous approach is unparalleled when it comes to visualizing and predicting 3D binding – it was an obvious first choice to work with them. There is great synergy between our platforms' capabilities that needs seamless integration to*

provide the most value. The strongest binding molecule is of no use if it doesn't achieve sufficient exposure in a patient. Therefore, the discovery of a new drug is a multi-faceted optimization challenge. The adsorption, distribution, metabolism, and excretion (ADME) behaviour, as well as the toxicity of compounds need to be always at the forefront of drug discovery – alongside target inhibition."

BioSolveIT's Director of Application Science, Dr. Marcus Gastreich, said: "*Having an integrated solution for the researcher is like a head-up display: The impact of easy-to-use software accompanying the research process must be non-obstructive but always there: All parameters nicely organized, plus a powerful and minimalistic alerting system are the keys to avoid costly failure!*"

Dr. Christian Lemmen, CEO of BioSolveIT, said: "*Both companies share a passion for intuitive and clean user interfaces – an aspect which is widely neglected in scientific software. Management has realized that users need easily accessible functionality besides scientific value in software. For both, we are proud to have Optibrium as a like-mind partner, their ADME property predictions are highly regarded by the industry.*"

Optibrium are world leaders in the prediction of compound properties, such as solubility, metabolism, or penetration of the blood-brain-barrier, and the use of these predictions alongside experimental data to guide the selection and design of high quality compounds. Optibrium's StarDrop™ platform includes ground-breaking features, such as Card View™, which provides researchers with highly intuitive ways to explore the structure-activity relationships (SAR) in their data and identify new strategies for optimisation.

BioSolveIT is renowned for their extreme speed and accuracy in predicting "inhibition" in 3D – the strength of lock and key-like binding of candidate molecules in their target proteins; their radically simple and visual tools such as SeeSAR™ and LeadIT™ are used worldwide by big pharma and biotech companies.

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

For information on BioSolveIT, SeeSAR and LeadIT, please visit biosolveit.com, contact contact@biosolveit.com, or call +49-2241-2525-0

ENDS

Media contact

Sarah Jeffery
Zyme Communications
E-mail: sarah.jeffery@zymecommunications.com
Phone: +44 (0) 7771 730919

Optibrium

Nick Foster
Director, Business Development
E-mail: nick.foster@optibrium.com
Phone: +44 (0)1223 815900

BioSolveIT

Marcus Gastreich
Director of Application Science
E-mail: marcus.gastreich@biosolveit.com
Phone: +49 2241 25 25 0

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.

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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