

Optibrium and InfoChem collaborate on retrosynthetic analysis in StarDrop

Collaboration enables drug discovery researchers to generate alternative, novel synthesis pathways for target molecules

Partnership expands number of free extensions available through StarDrop

CAMBRIDGE, UK and Munich, GERMANY, 19 March 2019 – Optibrium™, a developer of software for drug discovery, today announced a collaboration with InfoChem GmbH, a leader in cheminformatics. The collaboration provides StarDrop™ users with easy access to ICSYNTH light, an entry-level version of InfoChem's computer-aided synthesis design (CASD) software to generate synthesis pathways for a target molecule. By stimulating new and unbiased ideas, researchers can explore alternative or novel synthetic routes with the potential to save time and reduce costs.

StarDrop seamlessly connects with a wide variety of internal and external informatics systems, providing users with full support for compound design and optimisation through a single interface. The latest partnership further increases the number of extensions available to StarDrop users, free of charge.

ICSYNTH light uses a transform-based approach to generate synthesis pathways for target molecules, even if these are novel and/or unpublished. The advanced cheminformatics algorithm suggests precursors using chemical rules automatically generated from reaction databases, with machine learning approaches. The results can be explored as a synthetic tree with each step supported by literature citations describing a similar precedented transformation.

StarDrop can access ICSYNTH light to evaluate possible synthetic pathways for new molecules designed in StarDrop's interactive designer or Nova module. This provides an invaluable tool for chemists to easily understand the synthetic tractability of proposed new molecules.

This free extension to StarDrop can be downloaded from URL.

Dr Matthew Segall, Optibrium's CEO, commented: "This partnership with InfoChem continues our collaborative approach to working with leading providers of technology and services for drug discovery and other chemistry fields. We have developed StarDrop to seamlessly connect with a wide range of informatics systems thus giving our customers ultimate choice and flexibility, and providing everything they need for effective compound design and optimisation through a single interface."

Dr Josef Eiblmaier, Managing Director of InfoChem, said: "InfoChem has a long tradition in developing software solutions for the retrieval and handling of structures and reactions. Customers are demanding ever more powerful and innovative tools to process the increasing amount of data arising from the constant progress in scientific knowledge. We are delighted to be working with Optibrium on the integration of both companies' industry leading software, to enhance researchers' own knowledge and expertise by providing the tools to help generate new and balanced ideas."

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

For further information on InfoChem or ICSYNTH, visit www.infochem.de, contact info@infochem.de or call +49 89 2030432410.

ENDS

Notes to Editors:



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Media contact

Sarah Jeffery

Zyme Communications

E-mail: sarah.jeffery@zymecommunications.com

Phone: +44 (0) 7771 730919

Optibrium

Nick Foster

Head of Commercial Operations

E-mail: nick.foster@optibrium.com

Phone: +44 (0) 1223 815900

InfoChem

Valentina Eigner-Pitto

Senior Marketing Manager

E-mail: ve@infochem.de

Phone: +49 (0)89 2030432413

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 and San Francisco, USA. 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.

About InfoChem

Founded in 1989 and based in Munich, Germany, InfoChem has 30 years' experience in the development and integration of sophisticated software tools for the storage and handling of structure and reaction information. Crucial properties of InfoChem products are not only design and performance, required to process the increasing amount of data arising from constant progress in scientific knowledge, but also reliability and flexibility, which enable complete integration in pre-existing infrastructures.

The company main activities involve the production of synthesis planning and reaction prediction solutions and the automatic extraction of scientific information from text and images.

For further information visit www.infochem.de