

Optibrium and Enamine collaboration extends commercial compound database access for StarDrop users

- *Partnership expands number of free extensions available through StarDrop*
- *EnamineStore contains over 3.3 million screening compounds, and 7.8 million building blocks*

CAMBRIDGE, UK and KIEV, UKRAINE, 4th September, 2018 – Optibrium™, a developer of software for drug discovery, today announced a collaboration with Enamine, a chemical research organisation and compound supplier. The collaboration provides StarDrop™ users with easy access to EnamineStore, a database of their commercially available screening compounds and chemical building blocks. StarDrop has been developed to connect seamlessly with a wide variety of internal and external informatics systems and this latest partnership further extends the wealth of information available to users through StarDrop and its capabilities for small molecule design, optimisation and data analysis in drug discovery.

StarDrop provides free access to the Enamine database to easily search for commercially available compounds and building blocks. Enamine has over 3.3 million screening compounds and a further library of 7.8 million building blocks available to order from EnamineStore. The link enables users not only to search for specific compounds, but also find those that are structurally similar to their most interesting hits and leads or contain relevant substructures. This provides an invaluable tool for researchers to quickly enrich the understanding of their chemical structure-activity relationships.

Users can apply all of StarDrop's functionality to the compounds returned from Enamine, including *in silico* predictive models and multi-parameter optimisation, guiding the identification of objective-driven, high quality compounds. The extended services are particularly relevant to the latest platform version, StarDrop 6.5, which includes a novel R-group clipping feature, enabling researchers to easily use the building blocks returned in the enumeration of virtual libraries to explore new compound ideas. Associated information, such as stock and cost for each building block, are linked with the enumerated compounds to facilitate ordering for synthesis of the best compounds.

Dr Matthew Segall, Optibrium's CEO, commented: "This partnership with Enamine reflects our collaborative approach to working with leading providers of technology and services for drug discovery and other chemistry fields. With StarDrop's latest capabilities, and seamless connection to additional informatics systems, our customers have all the information they need at their fingertips to make the best decisions for their discovery projects."

Michael Bossert, Head of Strategic Alliances at Enamine, said: "Enamine has become a world leading provider of screening compounds and building blocks driven by a rapidly increasing demand for novel chemical compounds for the discovery of new and more effective drugs. We are excited to be working with Optibrium to provide StarDrop customers with the widest source of publicly available chemistry data."

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 Enamine, visit www.enamine.net

ENDS

Notes to Editors:

Building blocks need to be clipped to be used in virtual library enumeration

Clip R-groups by defining substitution point around a substructure search

SMILES	Fragment1_0	Price	Currency	Quantity	Units
<chem>CN1CC(=O)N1Cc2ccccc2</chem>	<chem>CN1CC(=O)N1Cc2ccccc2</chem>	547			
<chem>CN1CC(=O)N1Cc2ccccc2</chem>	<chem>CN1CC(=O)N1Cc2ccccc2</chem>	443			
<chem>CN1CC(=O)N1Cc2ccccc2</chem>	<chem>CN1CC(=O)N1Cc2ccccc2</chem>	695			

For high resolution image please email sarah.jeffery@zymecommunications.com

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

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 Enamine Ltd.

Established in Kiev, Ukraine in 1991, Enamine is a chemical company producing building blocks and screening libraries of world reputation. The major asset of the company is the world's largest collection of building blocks: 150,000 in stock with 2,000 additions synthesised each month. These research functionalised compounds provide a significant competitive advantage to the company in supplying custom compound libraries particularly in the frame of medicinal chemistry collaborations or compound collection enhancement programs. Custom synthesis and kilogram scale up based both on fee-for-service and FTE models represent another area of business activities provided by Enamine, which are growing significantly in recent years.

For further information visit: www.enamine.net