

Optibrium and eMolecules Collaborate on Chemistry Data Integration in StarDrop

Combines eMolecules' collection of commercially available chemicals with StarDrop's data analysis and compound design capabilities in drug discovery

CAMBRIDGE, UK and CALIFORNIA, USA, 12 January, 2017 – Optibrium™, a developer of software for small molecule design and optimisation today announced a collaboration with eMolecules, the provider of a comprehensive chemical sourcing database. The collaboration provides StarDrop™ users with seamless access to eMolecules' extensive collection of screening compounds and chemical building blocks, further extending StarDrop's capabilities to guide compound selection and design.

eMolecules is a world-leading provider of screening compounds and building blocks for the pharmaceutical, biotechnology and chemical industries. eMolecules collates compounds from a network of over 100 trusted global suppliers, so that researchers can easily and quickly search one single source, saving valuable research time and cost. The database contains more than 7 million unique chemical structures and 1.5 million building blocks.

StarDrop users are now provided with direct access to eMolecules' database via a free extension, so that they can quickly search for commercially available screening compounds. This enables users to easily enrich their understanding of structure–activity relationships in their project's chemistry. Researchers can apply all StarDrop's capabilities to the compounds returned from eMolecules, including *in silico* predictive models and multi-parameter optimisation, guiding the selection of high quality compounds for their project's specific objectives. Users can also select eMolecules building blocks with which to design new compounds using StarDrop's Nova module. Imported building blocks are available in Nova's flexible and user-friendly library enumeration tool, enabling the rapid exploration of new, synthetically accessible chemistry ideas.

Dr Matthew Segall, CEO of Optibrium, commented: "StarDrop has been developed to connect with a wide variety of both internal and external informatics systems, giving users access to everything they need through a single, intuitive interface. We are pleased to be partnering with eMolecules to offer its comprehensive collection of chemicals and chemistry data with which to guide the design of new, high quality compounds."

Dr Niko Gubernator, CEO of eMolecules said: "eMolecules maintains a highly curated data set of true commercially available compounds which is increasingly being selected as a resource for internal and external informatics tools. We are excited to be working with Optibrium making our data integral in the design specification of new compounds and giving chemists access to our data and supply chain solutions."

For further information on Optibrium and StarDrop, please visit www.optibrium.com/stardrop/stardrop-integration.php or contact info@optibrium.com.

For further information on eMolecules, please visit www.emolecules.com or contact lester@emolecules.com.

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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.

About eMolecules

eMolecules is driven to enable scientists to accelerate their research to find the cures. To achieve this eMolecules provides business intelligence data and integrated ecommerce software for screening compound, chemical building blocks and primary antibody supply chains. These tools combined with their acquisition, aggregation and analytical services greatly empower drug discovery researchers working in the pharmaceutical, biotechnology, academia, CRO and agrochemical industries. A privately owned company, eMolecules was founded in 2005 at its San Diego headquarters and has offices in Boston and London employing over 40 people across the three sites. www.emolecules.com.