



## Optibrium collaborates with Enamine and BioSolveIT to add REAL Space Search Tool to StarDrop

*New extension enables researchers to explore the REAL Space of 11 billion readily accessible compounds directly from StarDrop*

**CAMBRIDGE, UK., KIEV, UKRAINE and SANKT AUGUSTIN, GERMANY, 19 November, 2019** – Optibrium™, BioSolveIT™ and Enamine™, leading providers of software and services for drug discovery, today announce a three-way collaboration enabling efficient search of Enamine’s REAL Space directly from within Optibrium’s StarDrop™ software. This extension to StarDrop is powered by BioSolveIT’s proprietary Feature Trees (FTrees) technology, to search a gigantic chemical space of over 11 billion readily accessible compounds and identify novel compounds that are similar to a query structure of interest. The resulting chemical structures and data are pre-formatted and ready to evaluate using StarDrop’s comprehensive suite of integrated software for small molecule design, optimisation and data analysis.

REAL Space, developed by Enamine, is a chemical space currently containing over 11 billion compounds that can be quickly synthesised with a high success rate. StarDrop’s new add-on REAL Space Search tool will allow researchers to, for example, investigate the chemical space local to their selected compound, find structurally novel leads with improved properties or avoid patent-protected space. The new extension deploys BioSolveIT’s FTrees technology to rapidly explore the vast space for high quality drug candidates using pharmacophore- and topology-style similarity searching, analogous to REAL Space Navigator, a tool previously developed by BioSolveIT and Enamine.

Dr Matthew Segall, Optibrium’s CEO, said: “The identification of new and promising lead molecules is a highly challenging process and the need for fast access to novel compounds is essential to support the development of chemistry and drug discovery projects. We are delighted to offer this link with REAL Space as a further extension to StarDrop, enabling researchers to quickly find high-quality compounds for their drug discovery projects, improving both productivity and timelines.”

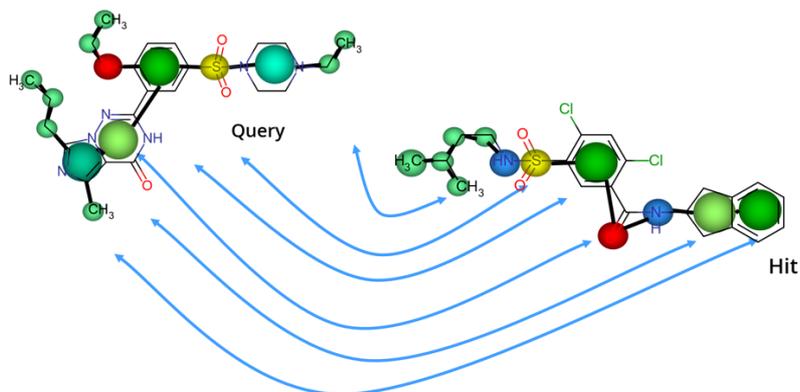
Michael Bossert, Head of Strategic Alliances at Enamine, commented: “Enamine is a world-leading provider of screening compounds and building blocks, driven by a rapidly increasing demand for novel chemical compounds for the discovery of new and more effective drugs. Our collaboration with Optibrium continues our quest to expand the borders of the REAL Space and to provide StarDrop customers with the widest source of commercially available drug-like compounds.”

Christian Lemmen, CEO of BioSolveIT, explained: “Our technology is based on extremely fast tree-based algorithms that avoid visiting every virtual molecule while traversing vast chemistry spaces for interesting hits. We have long standing partnerships with Optibrium and Enamine, and together we strive to consolidate strength and value for drug discovery researchers.”

For further information on StarDrop, please visit <https://www.optibrium.com/stardrop/>, contact [info@optibrium.com](mailto:info@optibrium.com) or call +44 1223 815900.

ENDS

## Notes to Editors:



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### About Optibrium Ltd [www.optibrium.com](http://www.optibrium.com)

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. Optibrium'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. The company's new Augmented Chemistry™ products and services deliver ground-breaking artificial intelligence technologies that continuously learn from all available data to supplement researchers experience and skills.

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](http://www.optibrium.com) or join in discussions on improving the productivity of drug discovery at [www.optibrium.com/community](http://www.optibrium.com/community).

### About Enamine Ltd. [www.enamine.net](http://www.enamine.net)

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: 175,000+ in



stock with 2,000 additions synthesized each month. These research functionalized 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. Enamine's REAL (readily accessible) concept is based on the careful and knowledge-guided design and selection of compounds that can be confidently produced from stock building blocks using over 160 validated reaction procedures.

**About BioSolveIT GmbH** [www.biosolveit.com](http://www.biosolveit.com)

BioSolveIT visualizes drug discovery. The highly innovative company's fast and easy-to-use software enables every chemist to advance their research. Perceptive visualization helps users to understand computational results at a glance. BioSolveIT believes in full transparency, and all the science behind their software is published. The trusted flagship platforms SeeSAR and infiniSee support research in structure-based and ligand-based drug discovery and inspire with new, vivid ideas. BioSolveIT is passionate about the needs of their customers and lives this through the discovery services that they offer. Working together with users in this way helps the organization to stay at the forefront of current research, addressing the questions that chemists are interested in right now. BioSolveIT aspires to develop software that is indispensable to drug discovery and, more importantly, software that is a pleasure to use every day.