Optibrium Adds Augmented Intelligence for Compound Design to its StarDrop Small Molecule Drug Discovery Software

- *New Inspyra™ module combines chemists' expertise with exploratory capabilities of automated compound design*
- *Inspyra™ provides drug designers direct access to powerful AI capabilities, supporting established workflows*

CAMBRIDGE, UK, 1 March 2022 – Optibrium Ltd, a leading developer of software for drug discovery, today announced the release of the latest version of StarDrop™, its comprehensive software platform for small molecule design, optimisation and data analysis. More than 160 organisations currently use StarDrop, including many of the world's leading pharmaceutical companies. The new release introduces Inspyra™, a module that dynamically learns from chemists' expert knowledge and feedback to guide automated compound design methods, creating a powerful 'augmented intelligence' to accelerate the discovery of high-quality drug candidates.

The impact of 'generative chemistry' algorithms for automated compound design is often limited in practice by a lack of alignment with chemists' existing workflows and know-how, resulting in irrelevant compound suggestions. StarDrop's new Inspyra™ module addresses this limitation by combining exploratory capabilities of automated compound design with chemists' expertise, helping to focus on the most relevant chemistry spaces and suggest optimisation strategies with the highest potential for a project.

Inspyra™ has been developed in collaboration with global pharmaceutical companies, and has already been applied successfully across several hit-to-lead and lead optimisation projects. The module leverages StarDrop's predictive modelling and data visualisation capabilities, multi-parameter optimisation, and 2D and 3D structure-activity-relationship (SAR) analysis, delivering a comprehensive solution for small molecule optimisation that reduces cost and time while increasing the chance of successful drug discovery.

Dr Peter Hunt, Director of Computational Chemistry at Optibrium, said: *"Having led groups at Novartis and MSD, access to an intuitive tool like the new Inspyra module for StarDrop would have been invaluable. While I am a firm believer in the benefits of automated compound idea generation, time and time again, colleagues were frustrated looking at compound suggestions that were not relevant to them for one reason or another. Inspyra is the first approach to address this challenge, and we are proud to release this new StarDrop version with unprecedented automated compound design support."*

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

ENDS

Notes to Editors:

Dr Peter Hunt,
Director of Computational Chemistry at Optibrium

For high-resolution images, please email sarah.jeffery@zymecommunications.com

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Media contact
Sarah Jeffery
Zyme Communications
Email: sarah.jeffery@zymecommunications.com
Phone: +44 (0) 7771 730919

Optibrium
John Norman
Head of Marketing
Email: john@optibrium.com
Phone: +44 (0)1223 815903

About Optibrium Ltd

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 proven artificial intelligence technologies that continuously learn from all available data to supplement researchers experience and skills.

Optibrium was founded in 2009 and is headquartered in Cambridge, UK, with offices in Boston, MA, and San Francisco, CA. The company works closely with over 160 customers and collaborators worldwide, including leading global pharma, biotech, agrochemical and flavouring companies and not-for-profit and academic groups.

For further information, visit www.optibrium.com