Optibrium Launches Cerella, a Novel Artificial Intelligence Platform for Active Learning in Drug Discovery

Cerella™ is proven to accelerate drug discovery and increase confidence in lead optimisation

CAMBRIDGE, UK, 20 October 2020 – Optibrium™ today announced the launch of Cerella™, an Artificial Intelligence (AI) software platform for drug discovery that delivers active learning using advanced deep learning methods. Cerella™ leverages the unique Alchemite™ algorithm [1], which has been demonstrated to extract additional value from drug discovery data to make more accurate predictions, prioritise experimental efforts and increase confidence in decisions [2,3]. It thereby reduces costs and improves cycle times while targeting high-quality compounds.

Cerella™'s novel architecture combines on-premises deployment with cloud computing, providing both data security and scalability. The most sensitive information is processed on-premises, and the cloud-based components work only with encrypted and anonymised data, enabling scaling from individual project data sets to corporate compound repositories containing millions of compounds.

By connecting directly with a corporate compound database, Cerella™ automatically updates models using the latest data to ensure that the predictions and analyses are always based on the latest information.

Cerella™ is powered by Alchemite™, a deep learning method developed by Optibrium's technology partner Intellegens Limited. In collaboration with pharmaceutical and biotechnology partners, Optibrium has rigorously demonstrated Alchemite's unique benefits over conventional modelling methods in peer-reviewed studies [1,2,3], resulting in reductions in cost and time of discovery cycles.

The Cerella™ software is the newest member of Optibrium's Augmented Chemistry™ platform. This brings sophisticated AI technologies that continuously learn from all available data to supplement expert scientists' experience and skills.

Matt Segall, Optibrium's CEO, commented on the launch: *"Our Augmented Chemistry™ platform continues to amaze our collaborators with the unprecedented outcomes it delivers. We are proud to reach this new milestone of launching Cerella™, enabling us to put our technologies directly into the hands of our customers."*

For further information on Cerella™, join the launch webinar on 27 October 2020 and register at bit.ly/cerella_webinar, visit optibrium.com/augmentedchemistry/, or contact info@optibrium.com.

[1] T. Whitehead, B. Irwin, P. S. M. Hunt and G. Conduit, "Imputation of Assay Bioactivity Data Using Deep Learning," J. Chem. Inf. Model. (2019) **59**(3), pp. 1197-1204.

[2] B. Irwin, *et al.*, "Practical Applications of Deep Learning to Impute Heterogeneous Drug Discovery Data," J. Chem. Inf. Model. (2020) **60**(6), pp. 2848-2857.

[3] Irwin *et al.* "Guiding Drug Optimisation Using Deep Learning Imputation and Compound Generation" International Pharmaceutical Industry (2020) **12**(2), pp. 28-31

ENDS

Notes to Editors:

Matt Segall, CEO, Optibrium

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

To opt-out from receiving press releases from Zyme Communications, please email info@zymecommunications.com
To view our privacy policy, please click here

Media contact
Grace Holland
Zyme Communications
Email: grace.holland@zymecommunications.com
Phone: +44 (0)7530 386228

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

Founded in 2009, Optibrium's headquarter is in Cambridge, UK, and Optibrium has regional offices in Boston, MA, and San Francisco, CA, 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.