Peer-reviewed Study by Optibrium Demonstrates the Value of Deep Learning for Imputation of Drug Discovery Data

Collaboration with Constellation Pharmaceuticals highlights the value of deep learning imputation to exploit heterogeneous drug discovery data.

CAMBRIDGE, UK: 8 September 2020 – Optibrium™, leading providers of software and services for drug discovery, today announced a peer-reviewed publication, 'Practical Applications of Deep Learning to Impute Heterogeneous Drug Discovery Data', in the Journal of Chemical Information and Modeling [1]. This paper is testament to the unique ability of the Alchemite™ deep learning algorithm to extract additional value from experimental data in the context of an evolving drug discovery project. In collaboration with the clinical-stage biopharmaceutical company Constellation Pharmaceuticals and technology partner Intellegens, Optibrium's Augmented Chemistry™ technologies were demonstrated to more accurately guide compound optimisation to target high-quality compounds.

The study showed that, whereas conventional quantitative structure-activity relationship methods struggle with the inherently noisy and sparse experimental data in drug discovery, the Augmented Chemistry™ platform, powered by Intellegens' Alchemite™ method, provides robust, high-quality predictions. Its ability to exploit correlations between different measurements and explicitly estimate uncertainties in each prediction enables confident decision-making to prioritise experimental work and expedite drug discovery project cycles.

Optibrium's Augmented Chemistry™ family of innovative products and services enhance decision making in drug discovery using Artificial Intelligence technologies. These supplement project scientists' experience and skills by learning from all available data, updated continuously with the latest data generated in discovery project iterations. Having demonstrated the value of the Augmented Chemistry™ platform in many successful collaborations with global pharma and biotech companies, Optibrium is releasing this ground-breaking technology as a deployable product that will support and enhance pharmaceutical research and development.

Julian Levell, Vice President of Drug Discovery, Constellation Pharmaceuticals, said: *"The fact that each prediction was provided with a confidence level opened up substantial opportunities for our projects. For example, this study demonstrated that we could have avoided synthesising at least 10% of the compounds in our discovery project. Those compounds predicted to be inactive with high confidence, were confirmed to be inactive – with a negligible rate of false negatives. Furthermore, some experimental data were flagged up as outliers based on these confidence levels. Investigating these data points further confirmed that many were measured false negatives in assays and potentially missed opportunities or missed liabilities. Overall, the Augmented Chemistry™ platform brings something truly new to the table."*

Matthew Segall, Optibrium's CEO, added: *"We very much enjoy working with Constellation Pharmaceuticals in this close collaboration. The truly outstanding results corroborate the tremendous potential we have seen in joint projects with other pharmaceutical companies and biotechs, and we are excited to be releasing Augmented Chemistry™ products later this year to make this technology widely available."*

Gareth Conduit, Intellegens' CTO, said: *"We were delighted that the Alchemite engine could add so much value to the Constellation Pharmaceuticals data set, outperforming traditional QSAR methods. Moreover, the confidence predictions of Alchemite allowed us to drill down on those predictions most important for Constellation Pharmaceuticals, focusing their efforts on the most promising compounds."*

The companies continue to work closely together to leverage future opportunities to advance their respective projects and invest in the innovative technologies that enhance their work.

For further information on Augmented Chemistry, please visit http://www.optibrium.com/augmentedchemistry/, contact info@optibrium.com or call +44 1223 815900.

[1] Irwin *et al.* J. Chem. Inf. Model. (2020), **60**(6) pp. 2848–2857

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Notes to Editors:

Matt Segall, CEO, Optibrium

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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.