Optibrium and Lhasa Limited advance predictive modelling for drug-metabolising enzymes

- *Optibrium and Lhasa Limited publish joint peer-reviewed research in the Journal of Medicinal Chemistry, expanding predictive modelling beyond human Cytochrome P450*
- *Study demonstrates novel predictive models for drug metabolism to improve drug design and reduce toxicity and costs*

CAMBRIDGE and LEEDS, UK 03 November 2022 – Optibrium and Lhasa Limited, two of the leading developers of software and artificial intelligence (AI) solutions for drug discovery and development, today announced the publication of a peer-reviewed study in the Journal of Medicinal Chemistry. In the paper, 'Predicting Regioselectivity of AO, CYP, FMO and UGT Metabolism Using Quantum Mechanical Simulations and Machine Learning', the team combined existing experimental results, quantum mechanics and machine learning to build predictive models for drug metabolism.[1] The research will underpin the development of new capabilities for StarDrop, enabling users to better determine the metabolic fate of drug candidates and further streamline the preclinical drug discovery process.

Unexpected metabolism can cause the failure of many late-stage drug candidates, or even the withdrawal of approved drugs. It is therefore essential to predict metabolism for potential drug candidates. Current predictive models of metabolism usually target the human Cytochrome P450 (CYP) enzyme family, due to its well-characterised role in the metabolism of drug-like compounds. However, there is an increasing need to predict metabolism for other enzymes, such as human Aldehyde Oxidates (AOs), Flavin-containing Monooxygenases (FMOs), and Uridine 5'-diphosphoglucuronosyltransferases (UGTs).

The study demonstrates novel predictive models for AO, FMO, and UGT metabolism, and extends the existing model for CYP metabolism to preclinical species. Expanding the portfolio of predictive models beyond CYPs will enable drug discovery scientists to determine a compound's metabolic fate more accurately, helping to design better drugs and identify toxicity earlier in the project. *In silico* modelling for CYP in preclinical species can also reduce animal testing in toxicology studies, making trials quicker, less expensive, and more ethical.

Dr Mario Öeren, Principal Scientist at Optibrium, said: "We are delighted to see our research published in The Journal of Medicinal Chemistry. Combining quantum mechanical simulations and machine learning has allowed us to successfully expand predictive models of metabolism to new enzymes — a unique undertaking which addresses some of the key preclinical challenges of today. We are confident that this research's demonstrated ability to predict metabolism across a broad range of different metabolic enzymes will provide an invaluable resource for scientists approaching drug discovery."

Dr Matthew Segall, CEO of Optibrium, commented: "A huge congratulations to our team on this achievement. Here at Optibrium, we are always looking to innovate, and we pride ourselves on the scientific rigour behind our portfolio. The research will deliver powerful new capabilities to our StarDrop platform, strengthening our mission to push the boundaries of what's possible within the computer-aided drug discovery space."

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

1. Research Paper: Predicting Regioselectivity of AO, CYP, FMO, and UGT Metabolism Using Quantum Mechanical Simulations and Machine Learning (Mario Öeren et al., J. Med Chem. (2022) DOI: 10.1021/acs.jmedchem.2c01303)

ENDS

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About Optibrium

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 Augmented Chemistry® products and services, including Cerella™, 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 a US subsidiary, Optibrium Inc., based in Cambridge, MA. The company works closely with over 170 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.

About Lhasa Limited

Lhasa Limited is a Leeds based not for profit organisation. At Lhasa, we are driven by our purpose; To enable informed decision making on chemical safety. In line with this purpose, we create forward-thinking software solutions, which have been solving real-world chemical safety assessment problems for almost 40 years. Our technology is designed by scientists, for scientists, in collaboration with industry stakeholders and regulators. We are committed to enabling scientists to make better predictions on the safety of drugs, chemicals and cosmetics by using existing data better and developing computer-aided reasoning and information systems for the advancement of science.

For further information, visit www.lhasalimited.org.