Optibrium Releases Powerful Metabolism Prediction Capability in Next Generation StarDrop Software

- *Backed by six years' research, the new StarDrop Metabolism module combines quantum mechanics and machine learning to better predict the metabolic fate of drug candidates*
- *The module launches within a larger StarDrop update, which also sees additional features, including high-performance 3D virtual screening capabilities available on desktop*

CAMBRIDGE, UK, 25 September 2023 – Optibrium, a leading developer of software and AI solutions for drug discovery, today launched the latest version of its drug discovery platform, StarDrop 7.5, introducing a powerful module for drug metabolism prediction. The culmination of six years' research and development, the new StarDrop Metabolism module uniquely combines quantum mechanics and machine learning to better predict the metabolic fate of drug candidates. The module covers a broad range of drug-metabolising enzymes with greater precision than comparable methods.

Late-stage drug failures can often be attributed to issues relating to drug metabolism, such as poor metabolic stability resulting in low bioavailability of the active compound, unforeseen drug–drug interactions, or the formation of reactive or toxic metabolites. Early-stage predictive modelling of drug metabolism is therefore critical to overcome these challenges and save time, costs, and resources in the long-term.

Optibrium's new StarDrop Metabolism module covers 80% of Phase I and 60% of Phase II human metabolism, building on the Company's 25 years of experience modelling metabolism by cytochrome P450s. The module spans a range of key drug-metabolising enzymes: cytochrome P450s (CYPs), aldehyde oxidases (AOXs), flavin-containing monooxygenases (FMOs), uridine diphosphate glucuronosyltransferases (UGTs), and sulfotransferases (SULTs). The module includes regioselectivity models for these enzymes, enabling users to predict which atomic sites are most likely to be metabolised and the resulting metabolites. Combining these with models that predict which enzyme families and isoforms will metabolise a compound allows users to identify, with precision, which metabolites are most likely to be observed *in vivo,* design compounds with improved metabolic stability and reduce the risk of drug-drug interactions. Furthermore, models for CYP metabolism in rat, mouse, and dog help researchers select the best species for preclinical studies.

The models have been rigorously validated, as exemplified through recent peer-reviewed publications[1-6], including '*Predicting Regioselectivity of AO, CYP, FMO and UGT Metabolism Using Quantum Mechanical Simulations and Machine Learning*' in the *Journal of Medicinal Chemistry* and '*Predicting Regioselectivity of Cytosolic SULT Metabolism for Drugs*' in the *Journal of Chemical Information and Modeling*. Balanced accuracy values of up to 98% were achieved across this research.

To learn more about the StarDrop Metabolism module, please visit https://optibrium.com/metabolism.

Dr Matthew Segall, Chief Executive Officer, Optibrium, said: "Predicting CYP metabolism has been a mainstay of Optibrium's StarDrop platform, and it has long been our ambition to answer a broader range of drug metabolism challenges that our customers face. After extensive research, over many years, we are delighted to launch the Metabolism module, bringing our unique approach based on detailed mechanistic understanding of a broad range of drug-metabolising enzymes. This enables greater precision than other approaches to predicting metabolism and the resulting *in vivo* metabolites."

Dr Mario Öeren, Principal Scientist, Optibrium, said: "The release of the Metabolism module is the culmination of six years of peer-reviewed research, underscoring the universal applicability of our framework for training metabolism models. The module includes a wide variety of models for Phase I and II enzyme families and seamlessly presents complex metabolic data. Thus, the research of our clients is enriched with comprehensive metabolic data, enabling more informed decisions."

Alongside the new Metabolism module, StarDrop 7.5 also includes enhanced virtual screening with Surflex eSim3D, providing a high-performance desktop experience compared to other methods requiring servers. The StarDrop Metabolism module will replace StarDrop's P450 module, with all previous features integrated into the new module.

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

References

1 - M. Öeren et al., *article submitted.*
2 - M. Öeren, S. C. Kaempf, D. J. Ponting, P. A. Hunt, and M. D. Segall, J. *Chem. Inf. Model.,* **2023**, 63, 11, 3340–3349.
3 - M. Öeren, P. J. Walton, J. Suri, D. J. Ponting, P. A. Hunt, and M. D. Segall, *J. Med. Chem.,* **2022**, 65, 20, 1406–1408.
4 - M. Öeren, P. J. Walton, P. A. Hunt, D. J. Ponting, M. D. Segall, *J. Comput.-Aided Mol. Des.*, **2021**, 35(4), 541-555.
5 - P. A. Hunt, M. D. Segall & J. D. Tyzack, *J. Comput.-Aided Mol. Des.,* **2018**, 32, 537–546.
6 - J. D. Tyzack, P. A. Hunt, and M. D. Segall, *J. Chem. Inf. Model.,* **2016**, 56, 11, 2180–2193.

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Notes to Editors:

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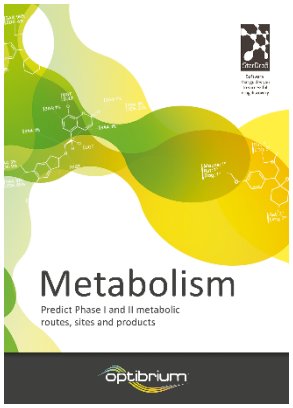

Optibrium's StarDrop Metabolism module

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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 180 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.