

## Optibrium's Quantum Mechanics and Machine Learning Methods Predict Routes of Drug Metabolism

*Peer-reviewed study published in Xenobiotica describes an innovative new method that predicts the routes and products of Phase I and II metabolism with high sensitivity and greater precision than other approaches*

**CAMBRIDGE, UK, 07 December 2023** – Optibrium, a leading developer of software and AI solutions for drug discovery, today announced the publication of its peer-reviewed study in *Xenobiotica*, 'Predicting routes of phase I and II metabolism based on quantum mechanics and machine learning'<sup>1</sup>. In the paper, the team demonstrate a new method that better determines the routes of metabolism and metabolites in early drug discovery.

Unexpected metabolism can lead to late-stage drug candidate failure, or even the withdrawal of approved drugs. Early *in silico* prediction of the dominant routes of metabolism is therefore vital to improve a drug's chance of success.

The paper first describes the development and validation of Optibrium's WhichEnzyme™ model, which accurately predicts the enzyme families most likely to metabolise a drug candidate. The team then combine this new model with Optibrium's previously published models. These include regioselectivity models for key Phase I and Phase II drug metabolising enzymes, which use quantum mechanical simulations with machine learning methods to predict sites of metabolism and the resulting metabolites. Additionally, the WhichP450 model, which predicts the Cytochrome P450 isoform(s) responsible for a compound's metabolism.

Based on the combined model outputs, Optibrium showcase a new method to determine the most likely routes of metabolism and metabolites to be observed experimentally. The paper demonstrates that this method delivers high sensitivity in identifying experimentally reported metabolites, as well as higher precision than other methods for predicting *in vivo* metabolite profiles. It enables researchers to identify compounds with greater metabolic stability and better safety profiles, and underpins Optibrium's recently launched StarDrop Metabolism module.

*"Our latest study is the result of six years of focused research, delivering a practical model that allows users to predict metabolic pathways for a wide range of drug-like compounds. Thanks to our carefully curated datasets and our signature reactivity-accessibility approach, we have managed to build accurate isoform-specific regioselectivity models for the important Phase I and II enzyme families"* **Dr Mario Öeren, Principal Scientist, Optibrium said.** *"Using that very same data, we've trained models that predict the likely enzyme families and isoforms which metabolise a compound. And then by combining these models, we've trained and validated a 'model of models' that predicts the full metabolism pathway for a given compound."*

For further information on Optibrium or the StarDrop Metabolism module, please visit <https://optibrium.com/metabolism-module>, contact [info@optibrium.com](mailto:info@optibrium.com) or call +44 1223 815900.

1: Mario Öeren, Peter A. Hunt, Charlotte E. Wharrick, Hamed Tabatabaei Ghomi & Matthew D. Segall (2023) Predicting routes of phase I and II metabolism based on quantum mechanics and machine learning, *Xenobiotica*, DOI: [10.1080/00498254.2023.2284251](https://doi.org/10.1080/00498254.2023.2284251)

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**Notes to Editors:**



**Dr Mario Öeren, Principal Scientist, Optibrium**

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**About Optibrium**

Optibrium develops exceptional software and AI solutions that help scientists advance their discovery projects. Cutting-edge science, backed up by rigorous research, underpins their intuitive software for compound design, optimisation and data analysis. Optibrium's comprehensive in silico platform improves the speed, efficiency, and productivity of the discovery process and supports a worldwide customer base, including leading pharma, biotech, agrochemical and flavouring companies and not-for-profit and academic groups.

Optibrium was founded in 2009 and is headquartered in Cambridge, UK, with a US subsidiary, Optibrium Inc., based in Cambridge MA.

For further information, visit [www.optibrium.com](http://www.optibrium.com).