Optibrium Launches a Metabolism Prediction Software Platform Tailored to DMPK Scientists

Semeta™ offers high sensitivity and superior precision for the prediction of Phase I and II metabolic routes, sites, products and liabilities in early drug discovery

CAMBRIDGE, UK, 27 February 2024 – Optibrium, a leading developer of software and AI solutions for drug discovery, today announced the launch of Semeta™, a metabolism prediction platform tailored specifically for drug metabolism and pharmacokinetics (DMPK) scientists. Fundamental to improving a drug's chance of clinical success, Semeta allows the accurate prediction of Phase I and II metabolic routes, sites, products and liabilities in early drug discovery, with superior precision to comparable software.

DMPK scientists are responsible for interpreting metabolite-ID experiments, a task which can be made easier with sensitive and precise *in silico* metabolite prediction. However, many of the currently available tools suffer from significant metabolite overprediction, resulting in wasted time, effort and resources as researchers have to filter through predicted metabolites that are then not reported experimentally. Tackling this key challenge, Optibrium's Semeta offers high sensitivity and superior precision to improve workflow efficiency.

Semeta enables more precise metabolite prediction across the key enzymes involved in human Phase I and II metabolism. It also includes models for rat, mouse and dog cytochrome P450 (CYP), the most important enzyme family involved in drug metabolism. This enables comparison between human, rat, mouse and dog predictions, supporting selection of the most appropriate preclinical species for *in vivo* efficacy, PK, and toxicology studies. Semeta employs models that are based on a fundamental understanding of the reaction mechanisms leading to drug metabolism, using quantum mechanics and machine learning to indicate potential sites of metabolism for each compound by each enzyme. In addition, classification models give a fast indication of which enzymes or isoforms are most likely to metabolise a compound. In Semeta, these models are integrated in a user-friendly, intuitive, cloud-based environment, with a range of tools to support data management and sharing. The software allows users to surface powerful metabolism data to improve their likelihood of compound success.

Dr Peter Hunt, Director of Computational Chemistry at Optibrium, said: *"Semeta is the culmination of years of extensive peer-reviewed metabolism research, and we are delighted to offer this accurate and robust new software to the DMPK community. We believe Semeta is excellently placed to tackle the many challenges of drug metabolism, and provide an accurate picture of Phase I and II metabolism."*

For further information on Optibrium or Semeta, please visit https://optibrium.com/semeta, contact info@optibrium.com or call +44 1223 815900.

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Notes to Editors:

Dr Peter Hunt, Director of Computational Chemistry at Optibrium

Semeta logo

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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.