



Optibrium introduces Augmented Chemistry™ services to guide successful drug discovery

Incorporating AI technologies that highlight the most confident, accurate compound predictions to enable effective project decision-making

CAMBRIDGE, UK, 10 October, 2019 – Optibrium™, a developer of software for drug discovery, today announced the introduction of its Augmented Chemistry™ services, which provide collaborators with novel artificial intelligence technologies to supplement their skills and experience, enabling them to make more effective decisions and advance their drug discovery projects.

In discovery projects, it is important to base decisions on reliable data to avoid wasted effort pursuing incorrectly selected compounds or missing opportunities by inappropriately discarding potentially valuable compounds. Augmented Chemistry™ services are built on a unique deep learning capability for data imputation, Alchemite™, which has been developed in collaboration with Intellegens Limited. Alchemite™ has been demonstrated to outperform traditional predictive models, both in benchmarking studies [1] and in partnerships with global pharma and biotech research organisations. Unlike conventional machine learning approaches, Alchemite™ learns simultaneously across all experimental endpoints in a project or corporate database, even based on limited data. The resulting model can automatically highlight the most confident, and therefore accurate, predictions on which to base experimental decisions, including the identification of new or previously overlooked high-quality compounds.

Dr Matthew Segall, Optibrium's CEO, said: "Optibrium has an extensive track record of successfully introducing and delivering cutting-edge technologies to drug discovery, and our intimate knowledge of the unique challenges of drug discovery and the underlying data enable us to go beyond the hype and deliver results that make a difference. After successfully demonstrating its capabilities in collaboration with our partners, we're excited to now be able to bring Augmented Chemistry™ services to our global customer base."

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

[1] Whitehead *et al.* J. Chem. Inf. Comput. Model. (2019) **59**(3) pp. 1197-1204

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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 is headquartered in Cambridge, UK with offices in Boston and San Francisco, 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.