Innovate UK Funded Project Produces Next-Generation AI Drug Discovery Platform

Optibrium, Intellegens and Medicines Discovery Catapult combine their expertise in drug discovery and AI research

CAMBRIDGE, and MACCLESFIELD, UK, 3 December 2020 – DeepADMET, a consortium set up to advance AI technologies for drug discovery, today announced the successful conclusion of a project funded by Innovate UK, the UK's innovation agency. Optibrium - a developer of software for drug discovery, Intellegens - an AI company, and Medicines Discovery Catapult (MDC) - the UK's catapult centre for medicine research and innovation, partnered to harness the power of AI for drug discovery research and developed a next-generation software platform supporting the design of new drug candidates. The consortium demonstrated how their software supports drug discovery teams in identifying compounds with improved 'on target' properties more efficiently in case studies with pharma and biotech companies.

Utilising Optibrium's small molecule design, optimisation and data analysis software, StarDrop™, and leveraging Intellegens' unique Alchemite™ deep learning algorithm, the joint research team custom-tailored their algorithms to the specificities of drug discovery data. The resulting software platform complements current drug discovery processes and improves efficiency and productivity. The project reached its successful conclusion, demonstrating the strength of their prototype's prediction of drug candidate's absorption, distribution, metabolism, excretion and toxicity (ADMET) properties on live industry data.

Optibrium continued to develop this prototype into a commercial product, Cerella™, a platform that directly integrates with a customer's in-house research database to generate models based on the customer's proprietary data automatically. Models and predictions continue to update as new data becomes available, resulting in increasingly accurate predictions.

Matthew Segall, CEO at Optibrium: *"We appreciate the support received from Innovate UK, enabling us to advance the development of our AI platform, Cerella™. As proven by several case studies, Cerella™ fills a critical need in modern drug discovery, with collaborators' research and development teams eager to exploit its capacity to accelerate their discovery of novel breakthrough treatments. We are grateful for Innovate UK's initiatives that enable collaborations like ours, and will continue to work with Intellegens and MDC to further the UK's role in drug discovery."*

Ben Pellegrini, CEO at Intellegens: *"This project represents a significant step forward for Intellegens. Through this collaborative project, we have validated the underlying science with some of the biggest pharma companies in the world, and more importantly, wrapped it up in a robust, deployable platform. We look forward to building on this technology and continuing our collaboration with Optibrium."*

John P. Overington, Chief Informatics Officer at Medicines Discovery Catapult: *"The power that comes from discovering and preparing the needed data for medicines research cannot be overstated. This project is unequivocal in its demonstration of how quality data can refine, direct and expedite drug discovery, resulting in faster and flexible routes to clinic, while minimising overall project costs."*

"It has been an extremely rewarding venture working with Optibrium and Intellegens during this project; a collaboration which will enable a more streamlined and efficient approach to drug discovery and be able to see future applications in other key business areas."

ENDS

Notes to Editors:

Matt Segall, CEO, Optibrium

Ben Pelligrini, CEO at Intellegens

John P. Overington, CIO at Medicines Discovery Catapult

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About Optibrium Ltd

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. Optibrium's flagship 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 deliver ground-breaking artificial intelligence technologies that continuously learn from all available data to supplement researchers experience and skills.

Founded in 2009, Optibrium's headquarter is in Cambridge, UK, and Optibrium has regional offices in Boston, MA, and San Francisco, CA, 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.

About Intellegens https://www.intellegens.co.uk/

Intellegens is a spin-out from the University of Cambridge with a unique Artificial Intelligence (AI) toolset that can train deep neural networks from sparse or noisy data. The technique, created at the Cavendish Laboratory, is encapsulated in Intellegens first commercial product, Alchemite™. The innovative deep learning algorithms that Alchemite™ is based on can see correlations between all available parameters, both inputs and outputs, in fragmented, unstructured, corrupt or even noisy datasets. The result is accurate models that can predict missing values, find errors and optimise target properties. Capable of working with data that is as little as 0.05% complete, Alchemite™ can unravel data problems that are not accessible to traditional deep learning approaches. Suitable for deployment across any kind of numeric dataset, Alchemite™ is delivering ground breaking solutions in drug discovery, advanced materials, patient analytics and predictive maintenance – enabling organisations to break through data analysis bottlenecks, reduce the amount of time and money spent on research, and support better, faster decision-making.

About the Medicines Discovery Catapult

The Medicines Discovery Catapult is a national centre of applied Research and Development expertise, uniquely designed to promote and support innovative, fast-to-patient drug discovery in the UK through collaborative projects.

It is one of a network of elite, not-for-profit technology and innovation centres established by Innovate UK as a long-term investment in the UK's economy. The Medicines Discovery Catapult will work with industry, academic teams, technology experts, charities, regulators and others.

It provides unique scientific capabilities and act as a gateway to specialist facilities, technology and expertise within the UK, supporting SMEs to drive the development of new approaches for the discovery and early development of new medicines. Helping to transform ideas into commercial products and services for the wider health and wealth of the country.

By developing and validating new ways of discovering new medicines, and promoting key talent and expertise across sectors, it can help the UK maintain its heritage position as a global leader in this key industry.

https://md.catapult.org.uk/ @MedDiscCat