



PRESS RELEASE

For further information or to arrange interviews please see contact details below for Optibrium, Intellegens and Medicines Discovery Catapult.

Novel deep learning drug discovery platform gets £1 million innovation boost

Optibrium™, Intellegens and Medicines Discovery Catapult awarded funding to apply machine learning in drug discovery

Funding to support Artificial Intelligence (AI) in drug discovery takes a significant step forward today as Optibrium, Intellegens, and Medicines Discovery Catapult secure a grant from Innovate UK to fund a £1 million project.

The program will see Optibrium, which creates software to improve the efficiency and productivity of drug discovery, and Intellegens, a spin out from the University of Cambridge which is focused on a specific form of AI called ‘deep learning’, work with Medicines Discovery Catapult over the next two years.

The aim is to harness the power of AI to learn from complex data and guide scientists in the design and testing of potential new drugs. Drug discovery generates a huge quantity of complex biological, chemical, clinical and safety information that needs to be collected, analysed and presented in a way that it can be best used to make evidence-based decisions.

The research partners are seeking a means of providing better insights into how a drug interacts with the body, improving the efficiency and productivity of drug discovery. The project will use novel deep learning methods to create a next generation platform that will better predict the absorption, distribution, metabolism, excretion and toxicity (ADMET) of new drug candidates.

Building on Optibrium’s existing software offering (StarDrop™) and an Intellegens’ deep learning toolkit (Alchemite™), the project will develop and apply novel AI methods across ADMET. By developing DeepADMET technology the aim is to improve the scope and reliability of drug design parameters, currently inaccessible or unavailable, for the first time.

Each partner in the collaboration brings a unique skill set.

Matthew Segall, Chief Executive Officer of Optibrium, says:

“We are delighted to lead this project in collaboration with Medicines Discovery Catapult and Intellegens. We will apply cutting edge deep learning methods and new data to address important challenges in drug optimisation. The funding from Innovate UK is important validation of our project team’s expertise and the impact it will have on the industry’s efficiency and productivity. We look forward to making these models available to researchers through the StarDrop platform.”

Professor John Overington, Chief Informatics Officer of the Medicines Discovery Catapult, says:



“At Medicines Discovery Catapult we apply innovation, working alongside UK SMEs to drive the development and adoption of new approaches for the discovery and early development of new medicines. This collaborative R&D activity will allow us to do just that and the grant from Innovate UK represents an important milestone for the advancement of informatics and data science.”

Ben Pellegrini, Chief Executive Officer of Intellegens, says:

“Intellegens is extremely excited to be part of this collaboration and looks forward to applying our novel deep learning techniques to help build a next generation platform to improve the drug discovery process.”

Currently, high failure rates mean that 9 out of 10 potential drugs fail somewhere between phase 1 trials and regulatory approval, greatly adding to the costs of creating new medicines.

The growth in computer-processing power, availability of large data sets, development of advanced algorithms and major improvements in machine learning presents a great opportunity for drug discovery.

The technology and models created as a result of this project will help guide the selection and design of compounds early in the discovery process, to more quickly identify candidate drugs with a higher chance of success and lower development risk.

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Notes to Editors:

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.



We provide 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](#)

About Optibrium

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. The company'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.

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

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About Intellegens

Intellegens is a spin-out from the University of Cambridge that has developed a unique Artificial Intelligence (AI) toolset for training neural networks from sparse or noisy data.

The technique, developed at the Cavendish Laboratory in the Department of Physics, has been encapsulated in Intellegens first commercial product Alchemite where it is solving problems in drug discovery, advanced materials, patient analytics and predictive maintenance.

Intellegens provides a combination of consultancy and software to understand and solve these high value data analysis bottlenecks where traditional deep learning approaches do not work.

For more information, please visit www.intellegens.ai or contact us at info@intellegens.ai

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