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**CATAPULT**  
Medicines Discovery

## 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** – The consortium behind the DeepADMET project set up to advance artificial intelligence (AI) technologies for drug discovery, today announced the successful conclusion of this project which was funded by Innovate UK, the UK's innovation agency. Optibrium Limited - a developer of software for drug discovery, Intellegens Limited - 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 and develop a next-generation software platform supporting the design of new drug candidates. In collaboration with global pharma and biotech companies, the consortium demonstrated the ability of its new AI platform, Cerella™, to identify compounds with improved 'on target' properties more efficiently and was proven to reduce costs and shorten discovery cycle times.

The successful project culminated in the release of Cerella™, which leverages Intellegens' unique Alchemite™ deep learning algorithm<sup>[1]</sup>, custom-tailored by the joint research team to the specificities of drug discovery data. The platform complements current drug discovery processes, improving efficiency and productivity by extracting additional value from drug discovery data to make more accurate predictions of compounds' activity and absorption, distribution, metabolism, excretion and toxicity (ADMET) properties. Based on these predictions, it prioritises experimental efforts and increases confidence in decisions<sup>[2,3]</sup>. Cerella™ combines on-premises deployment with cloud computing, providing both data security and scalability, and by connecting directly with a corporate data repository, it automatically updates predictions using the latest data.

**Karen Spink, Innovation Lead- Precision Medicine at Innovate UK:** *"The digital and AI revolution will lead to faster and smarter ways of discovering and developing safe and effective drugs. Applying the diverse expertise within the DeepADMET project consortium, unique solutions to the predictive modelling of drug candidates have been delivered through the Cerella™ platform. Advancements in this exciting area of innovation will ultimately deliver better-targeted medicines with an optimised safety profile more quickly to the patient."*

**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 data needed 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 the 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."*



<sup>[1]</sup> T. Whitehead, B. Irwin, P. S. M. Hunt and G. Conduit, "Imputation of Assay Bioactivity Data Using Deep Learning," *J. Chem. Inf. Model.* (2019) 59(3), pp. 1197-1204.

<sup>[2]</sup> B. Irwin, et al., "Practical Applications of Deep Learning to Impute Heterogeneous Drug Discovery Data," *J. Chem. Inf. Model.* (2020) 60(6), pp. 2848-2857.

<sup>[3]</sup> Irwin et al. "Guiding Drug Optimisation Using Deep Learning Imputation and Compound Generation" *International Pharmaceutical Industry* (2020) 12(2), pp. 28-31

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## 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](http://www.optibrium.com) or join in discussions on improving the productivity of drug discovery at [www.optibrium.com/community](http://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.

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