Intellegens and Optibrium success in global challenge to find novel antimalarial compounds

- **Team deploy Alchemite™ deep learning platform to predict active compounds for malarial drug discovery.**
- **Successful models selected by Open Source Malaria consortium will be progressed through to design novel compounds for synthesis and testing.**

CAMBRIDGE, UK, 3rd December, 2019 – Intellegens, an artificial intelligence (AI) start-up, and Optibrium, leading providers of software and services for drug discovery, today announced joint success in the Open Source Malaria (OSM) global initiative aimed at identifying the best predictive models for antimalarial compounds. Together, the companies developed one of the top models, deploying a cutting-edge deep neural network algorithm[1], Alchemite™, to accurately predict active compounds with novel mechanisms of actions that could be critical to future malaria control and elimination. As one of four prizewinning models selected, the project will now progress through the next phase of the initiative that includes the proposal of new compounds that are predicted to be active, for synthesis and testing against the malaria parasite.

Founded in 2012 by Professor Matthew Todd, Chair of Drug Discovery at University College London, the OSM consortium aims to find a new medicine for the treatment of malaria, which is formally recognised as a neglected tropical disease by the World Health Organisation. Over the past six years, OSM has brought together an international team of researchers who design, synthesise and test new antimalarial candidates that they hope will demonstrate potent activity against Plasmodium falciparum, the deadliest species of the malaria-causing parasite, in vitro and in vivo. The work is published in an open access online platform https://github.com/OpenSourceMalaria/Series4_PredictiveModel/issues/18

In the latest phase of the initiative, Intellegens' predictive modelling platform Alchemite™, applied by Optibrium, has been commended for its ability to predict active compounds with a novel mechanism of action. Alchemite™ has shown to significantly improve the

accuracy of the predictions and outperform conventional quantitative structure-activity relationship (QSAR) models and other well-known approaches, thereby reducing research and development costs associated with the unneeded synthesis of inactive compounds.

Dr Tom Whitehead, Machine Learning Scientist at Intellegens, commented:

> "Alchemite™ demonstrates real-world applicability and has the potential to provide accurate predictions for problems in drug discovery, such as finding active compounds that can counteract tropical diseases like Malaria."

Dr Benedict Irwin, Senior Scientist at Optibrium, said:

> "In order to combat the increasing incidences of resistance to antimalarial medication, it is essential to discover new compounds with novel mechanisms of action. We have previously seen that the Alchemite™ method can add significant predictive value across a range of projects and data sets both large and small. The Open Source Malaria data set was a new challenge and we are thrilled that our partnership with Intellegens has been recognised by the consortium and we look forward to progressing to the next phase of the initiative."

Professor Matthew Todd, Founder of the OSM consortium, added:

> "It's frequently the case in infectious disease drug discovery that we're working without knowledge of the mechanism of action. This so called phenotypic drug discovery can make it a challenge to see the patterns in the data in order to predict what to make next. I hope that new developments in AI and machine learning (ML) can help us to make our research more predictive and hence more efficient. The recent competition in Open Source Malaria, where teams openly contributed models to improve a promising series of antimalarials, suggests that new AI/ML technologies have enormous promise. Congratulations to the Optibrium/Intellegens team for contributing one of the best models, using Alchemite™. We're excited by the new molecules that were suggested because they are not ones that we would necessarily have thought of ourselves. We're now making them in the lab."

For more information on the Alchemite™ engine or Intellegens, go to: https://intellegens.ai or email: ben@intellegens.ai

For further information on Optibrium, please visit www.optibrium.com, contact info@optibrium.com or call +44 1223 815900.

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

Media contact

Sarah Jeffery

Zyme Communications

E-mail: sarah.jeffery@zymecommunications.com Phone: +44 (0) 7771 730919

Optibrium

Nick Foster

Head of Commercial Operations E-mail: nick.foster@optibrium.com Phone: +44 (0)1223 815900

Intellegens

Jamie Smith

Commercial Director

E-mail: jamie@intellegens.ai Phone: +44 (0) 1223 337005

About Optibrium Ltd

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. Optibrium's lead product, StarDropTM, is a comprehensive suite of integrated software with a highly visual and user-friendly interface. StarDropTM 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 ChemistryTM 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

About Intellegens https://www.intellegens.ai

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.