Optibrium and Intellegens achieve further success in Open Source Malaria initiative with *in vitro* validation of *in silico* generated compound

- *StarDrop™ and Augmented Chemistry™ prove a powerful combination in AI-guided design and validation of novel antimalarial drug candidates*
- *In silico designed compound demonstrates potency against pfATP4 protein target in malaria parasite*

CAMBRIDGE, UK, 01 April, 2020 – Optibrium™, leading providers of software and services for drug discovery, and Intellegens™, a spin-out from the University of Cambridge with a unique Artificial Intelligence (AI) toolset, today announced they have reached a further significant milestone in their contribution to the Open Source Malaria (OSM) initiative. The team has successfully completed phase 2 of a global challenge aimed at developing and testing novel antimalarial compounds. During this phase, predictive models from phase 1 were combined with generative methods to design novel compounds. The compounds were subsequently validated by testing their activity against the target. Out of four compounds proposed in this phase, only Optibrium/Intellegens' entry demonstrated potency against the target indicating the powerful combination of StarDrop™, Optibrium's computational platform for small molecule design and optimisation, with the AI-powered technologies of its Augmented Chemistry™ platform.

In the latest phase of the OSM project, the team deployed the *in silico,* generative chemistry capabilities of StarDrop™ to design new compounds predicted to be active against a putative target in *Plasmodium falciparum*, the deadliest species of malaria-causing parasites. In phase 1, Optibrium's Augmented Chemistry™ technologies, which incorporate Intellegens' Alchemite™ [1] deep learning platform, were used to build accurate predictive models for activity against this target. These were applied to guide the design efforts in phase 2. Combining StarDrop™ and Augmented Chemistry™ technologies, the team designed the only compound, out of four submitted by different organisations, for which activity was confirmed using *in vitro* tests, and the measured activity was in strong agreement with the predicted values.

Founded in 2012 by Professor Matthew Todd, Chair of Drug Discovery at University College London, the OSM consortium aims to find new medicines for the treatment of malaria, which is recognised by the World Health Organisation as one of the world's biggest killers. The latest results from the initiative can be found at https://github.com/OpenSourceMalaria/Series4_PredictiveModel/issues/25

Dr Benedict Irwin, Senior Scientist at Optibrium, said: *"Our latest work with the Open Source Malaria consortium is a testament to the power of Optibrium's software. It demonstrates, in an open and transparent way, the impact this dynamic blend of computational chemistry and machine learning can have in supporting drug discovery scientists in tackling these serious diseases."*

Professor Matthew Todd, Founder of the OSM consortium, added: *"It's great to see that the Optibrium/Intellegens' strong modelling results from phase 1 could be complemented with generative methods and held up in in vitro testing. While the use of AI in drug discovery is still in its infancy and in many cases the potential of in silico designed compounds hasn't yet been rigorously validated experimentally, this example can help pave the way and is a valuable contribution to our efforts. I hope to see more from the team in support of our quest to develop effective treatments for malaria."*

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Dr Tom Whitehead, Head of Machine Learning at Intellegens, said: *"This result is a powerful validation of the benefit advanced deep learning methods such as Alchemite™ can bring to chemistry design and optimisation problems. We are looking forward to continuing to support OSM in their pursuit of new treatments for malaria."*

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

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

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

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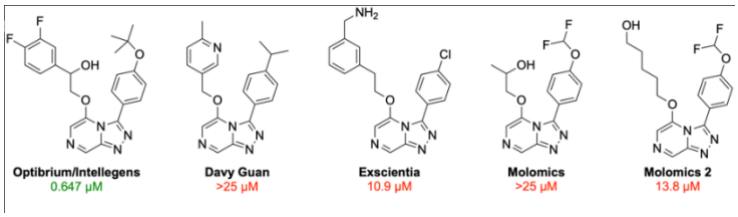
Notes to Editors:

For high resolution images please email sarah.jeffery@zymecommunications.com

Dr Benedict Irwin,
Senior Scientist at Optibrium



Measured activity of 5 in silico generated compounds against pfATP4 assay

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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.

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.