



Lhasa and Optibrium Enter Research and Product Development Collaboration

Drug discovery software specialists combine expertise to extend studies into drug metabolism modelling

CAMBRIDGE and LEEDS, UK 11 April 2017– Optibrium™ and Lhasa Limited (Lhasa), developers of software for small molecule property prediction, design and optimisation, announced today they have formed a collaborative partnership to research next generation drug metabolism modelling. Results from the work will be used by both organisations in the development of future products with improved and extended metabolism prediction capabilities.

The development of methods to predict metabolism is an important avenue of research and finds application in the development of drugs, cosmetics, nutritional supplements and agrochemicals. It is necessary to understand a compound's pharmacokinetics and ensure that it has sufficient exposure at a target to exert its therapeutic effect. In addition to this, it is important to predict the formation of toxic metabolites, which contributes to the high attrition rates experienced in the development of new chemical entities, the imposition of black-box warnings or even the withdrawal of approved pharmaceuticals. Therefore, the ability to identify potential metabolite issues early is of crucial importance to improving the efficiency and safety of the drug discovery process.

The research project has appointed Dr Mario Öeren as Senior Scientist to lead the study and work with a team of scientists from both Lhasa and Optibrium. As a theoretical chemist who has specialised into computational chemistry, Mario has a PhD in Natural Sciences from Tallinn University of Technology, Estonia where he has since worked as a researcher and lecturer. Mario will be based at Optibrium's headquarters in Cambridge, UK.

Dr. Matt Segall, CEO at Optibrium said: "This R&D collaboration with Lhasa builds on a long-standing relationship and is part of our continued investment in the development of novel technologies to improve efficiency in drug discovery. We welcome Mario to the team and look forward to extending the metabolism modelling capabilities within our combined product portfolio for the mutual benefit of Lhasa members and StarDrop users."

Dr. Chris Barber, Director of Science at Lhasa added: "We are excited by the complementary approaches that Lhasa and Optibrium have applied in the past with Lhasa capitalising on data donated by its member organisations and Optibrium applying theoretical approaches. Both approaches have their advantages but combining and applying them across all stages of development should allow us to provide real benefit to the end user".

In StarDrop, Optibrium has developed a comprehensive suite of integrated software with a highly visual and user-friendly interface. It 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 drug discovery process. Seamlessly connecting with other models, informatics methods and databases, StarDrop provides user-friendly access to resources making project management quicker and simpler.

Lhasa specialises in the development of transparent *in silico* models together with supporting databases in the fields of toxicology, metabolism, degradation and organic synthesis. The company is considered a pioneer in the production of knowledge-based systems and Meteor Nexus, the expert knowledge-based system for the prediction of metabolism, is used extensively within the pharmaceutical and related industries.

For further information on Optibrium and StarDrop, please visit www.optibrium.com/stardrop/ or contact info@optibrium.com.

For further information on Lhasa, please visit www.lhasalimited.org or contact info@lhasalimited.org.

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About Optibrium Ltd

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, US. 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 Lhasa Limited

Lhasa is an active, scientific research organisation working to promote the use of computer aided reasoning in chemistry and the life sciences. Its areas of specialisation include the development of transparent in silico models together with supporting databases in the fields of toxicology, metabolism, degradation and organic synthesis. Working closely with its members and the broader scientific community, Lhasa continues to draw on over 30 years of experience to create user-friendly, state-of-the-art in silico prediction and database systems.

Lhasa was founded on the basis of data and knowledge sharing. Building on its reputation as the eponymous 'honest broker', Lhasa has continued to work on the basis of 'shared knowledge, shared progress' for more than 30 years. Over this time, Lhasa has regularly been trusted with proprietary data and this can be seen in the many successful consortia that it continues to be involved in. The sustained success of such consortia is demonstrative of how working with Lhasa has a positive impact on the research and development process of its members.

Lhasa's products include the Derek Nexus expert system for predicting toxicity, Sarah Nexus, a transparent statistical system for predicting mutagenicity, Vitic Nexus for managing chemical data and information, Meteor Nexus for predicting metabolic fate and Zeneth for predicting forced degradation pathways. More recently, Lhasa Limited has worked with members on the development of Mirabilis, a tool for assessing the relative purging of mutagenic impurities.