Optibrium and Lhasa Limited Collaborate to Bring High Level, Expert Toxicity Prediction to Chemists' Desktops

New Derek™ module for StarDrop™ facilitates the efficient design and selection of safe, efficacious compounds in early drug discovery

CAMBRIDGE and LEEDS, UK, February 5th, 2013 – Optibrium and Lhasa Limited, providers of software for compound design, selection and property prediction, today announce a technology collaboration agreement. Lhasa's Derek Nexus™ platform for knowledge-based prediction of compound toxicity will be integrated as an optional plug-in module for Optibrium's StarDrop software, that guides the design and selection of high quality compounds in drug discovery. The combination of these technologies will enable chemists to intuitively balance the reduction of toxicity risk with the other requirements for a successful, safe and efficacious drug in hit-to-lead and lead optimisation. An easy-to-use reporting feature will facilitate collaboration between chemists and expert toxicologists to interpret and understand the relevance of a potential liability, enabling effective, early decision-making regarding the prioritisation of chemistries early in the drug discovery process.

Toxicity of drug candidates is a major cause of expensive, late-stage failure in pre-clinical and clinical development. Lhasa's Derek Nexus technology uses data from published and donated (unpublished) sources to identify structure-toxicity relationships and alert scientists to the potential for compounds to cause toxicity.

Optibrium's StarDrop software platform intuitively guides decisions on the design and selection of compounds with a high chance of success against a drug discovery project's objectives. StarDrop's unique probabilistic scoring approach to multi-parameter optimisation allows predicted and experimental data to be given appropriate weights when balancing the many requirements for a high quality lead or candidate compound. These include potency against the therapeutic target(s), selectivity against off-targets, and appropriate absorption, distribution, metabolism, elimination and toxicity (ADMET) properties.

The new Derek Nexus module in StarDrop will provide chemists with a prediction of the likelihood of a compound causing toxicity in over 40 endpoints, including mutagenicity, hepatotoxicity and cardiotoxicity. Furthermore, the region of a compound triggering an alert will be highlighted using StarDrop's Glowing Molecule™ visualisation, helping to guide the redesign of compounds to avoid the potential toxic liability. StarDrop's interactive design capabilities and Glowing Molecule™ visualisation guide the exploration of strategies to redesign compounds and improve their overall balance of properties. Combined with interactive chemical space visualisation, R-group analysis and data analysis, StarDrop provides a comprehensive platform for the design and selection of compounds, supported by additional plug-in modules providing: ADME QSAR models; prediction of P450 metabolism; robust generation and validation of QSAR models; 3D structure-activity relationships using Cresset's Field technology; and rapid exploration of virtual chemistry using medicinal chemistry transformations, precedented bioisostere replacements and virtual library enumeration.

Matthew Segall, CEO of Optibrium, commented, "Prediction of toxicity is a key requirement for our users and a major challenge for the industry. We are very happy to be working with the leading experts in the field of knowledge-based toxicity prediction to bring this state-of-the art technology to our users' desktops. In addition to this new agreement with Lhasa, our ongoing collaborations with Cresset and Digital Chemistry demonstrate our commitment to provide access to the best computational methods through our user-friendly StarDrop environment. We continue to explore new collaborations with leading groups to further this goal."

David Watson, CEO of Lhasa, added, "Scientists are under unprecedented pressure to increase efficiency through compound design and selection. We are excited by this collaboration which presents scientists with high level toxicity predictions at an early stage in compound development, in an interface that supports their workflow and enables effective decision-making."

The new Derek Nexus module for StarDrop will be available later this year. For a preview of this exciting new technology integration, please visit Lhasa's stand (#1228) at the upcoming Society of Toxicology meeting in San Antonio, Texas from March 10 - 14 or Optibrium's stand (#708) at the American Chemical Society Spring National Meeting in New Orleans, Louisiana from April 7 to 11.

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

For further information on Derek Nexus or Lhasa's other products and services, please visit www.lhasalimited.org, contact info@lhasalimited.org or call +44 113 394 6060.

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About Optibrium Ltd.

Optibrium (www.optibrium.com) is dedicated to providing software to guide decisions involving complex, uncertain data in an intuitive way. Based in Cambridge, UK, Optibrium has a global customer base ranging from top-ten pharmaceutical companies to biotechs and academic groups. Our mission is to continue to develop new technologies that will optimise project strategy, reduce wasted molecules and experiments, shorten timelines and improve the quality of candidate compounds for our clients. Optibrium's primary product, StarDrop, is focused on the drug discovery industry, helping guide scientists to make decisions in the design and selection of high quality drug candidates. Visit the online community at http://www.optibrium.com/community for further discussions on improving the productivity of drug discovery.

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About Lhasa Ltd.

Lhasa Limited is a not-for-profit organisation that facilitates collaborative data sharing projects in the pharmaceutical, cosmetics and chemistry-related industries. A pioneer in the production of knowledge-based systems for forward thinking scientists, Lhasa Limited continues to draw on over twenty five years of experience to create user-friendly, state of the art in silico prediction and database systems.

We believe in 'Shared Knowledge, Shared Progress'. Our not-for-profit, member driven status is designed to facilitate collaborative working and confidential data sharing between organisations. We run collaborative projects with industry, academia and regulatory bodies to continually enhance all our products.

Lhasa's products include Derek Nexus for predicting toxicity, Vitic Nexus for managing chemical information, Meteor Nexus or predicting metabolic fate and Zeneth for predicting forced degradation pathways.