StarDrop Auto-Modeller Wins Environmental Toxicity Prediction Challenge

CAMBRIDGE, United Kingdom, September 22, 2009 – Optibrium successfully demonstrated that its technology for automatically building predictive models of molecule properties can match 'hands-on' modelling approaches by generating the equal-best model in a competition organised by ICANN'09[1], ENNS[2] and CADASTER. The entry by Olga Obrezanova, Principal Scientist at Optibrium, came out joint winner in a challenge to build a model that can predict the environmental toxicity of new molecules.

Ed Champness, CSO of Optibrium, said "I'd like to congratulate Olga and the StarDrop team on an excellent result in a difficult challenge that attracted 80 international participants. This demonstrates the power of the modern machine learning techniques in StarDrop to generate high quality, robust models, making predictive modelling more accessible to all research scientists."

Olga's recent work focused on combining the Gaussian Processes modelling method with StarDrop's Auto-Modeller. This automatic framework gives both novice and expert users access to the tools needed to thoroughly analyse data and produce validated, predictive models to guide the design of new molecules in drug discovery. For non-experts, the Auto-Modeller can automatically generate models using multiple advanced modelling techniques and the built-in validation process rigorously tests and compares the resulting models to identify the most appropriate model to apply to new compounds. Alternatively, expert users can manually adjust modelling methods, data sets and descriptors to fine-tune the process. For more information on StarDrop and the Auto-Modeller, visit www.optibrium.com.

For details of the CADASTER competition and the results, visit http://www.cadaster.eu/node/65.

About Optibrium. Optibrium (www.optibrium.com) is dedicated to providing software to guide decisions involving complex, uncertain data in an intuitive way. Optibrium's primary product, StarDrop, is focused on the drug discovery industry, helping scientists to guide decisions in the design and selection of potential drug molecules. Optibrium was founded in 2009 as a spin-out of BioFocus DPI (formerly Inpharmatica). The founding group was responsible for the development of StarDrop from 2003 and, prior to this, research and development of related technologies since 1994. Based in Cambridge, UK, Optibrium has a global customer base ranging from top-ten pharmaceutical companies to small biotechs and academic groups.

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[1] International Conference on Artificial Neural Networks

[2] European Neural Network Society