

StarDrop 5.3 Offers Intuitive Virtual Library Design

Optibrium extends StarDrop's capabilities to guide the design of high quality compound libraries for drug discovery

CAMBRIDGE, UK, 20th November 2012 – Optibrium™, developer of software solutions for drug discovery, today announces a new version of its StarDrop™ platform. Version 5.3 introduces new features focused on the design of virtual libraries, guided by StarDrop's unique multi-parameter optimisation capabilities to prioritise compounds with the best balance of properties for synthesis and testing.

Version 5.3 introduces its virtual library design capability as part of StarDrop's Nova™ module, providing flexible and easy scaffold-based enumeration of a virtual library to allow drug discovery teams to rapidly explore new chemistry ideas. After drawing the scaffold on which the library will be based, users can select multiple functional groups, atoms or fragments to vary at each point of modification. These lists may be selected from a user-defined or centrally managed library, or sketched on an individual basis. A fully combinatorial library may be generated for detailed investigation or, alternatively, a subset of compounds can be automatically selected based on a predicted property or StarDrop's unique Probabilistic Scoring algorithm for multi-parameter optimisation.

These new capabilities are supported by further enhancements to StarDrop's core features, including easy-to-use tools for clustering, filtering based on substructure or properties and extensions to its interactive data visualisation. StarDrop offers a comprehensive desktop environment that saves time and reduces costs in drug discovery by guiding compound design and selection to quickly target high quality chemistry. These include plug-in modules providing: rigorously validated ADME QSAR models; quantum mechanical prediction of P450 metabolism; automatic generation of robust QSAR models; compound idea generation; application of 3D SAR based on Cresset's™ Field technology; and the ability to integrate seamlessly with other informatics and modelling platforms.

Matt Segall, CEO of Optibrium, commented, "StarDrop offers a seamless workflow allowing our users to go from design and enumeration of a virtual library, through property prediction to prioritising the resulting compounds against the profile of properties they require for their project objective. Supported by interactive visualisations in StarDrop's intuitive user interface, chemistry teams can quickly identify novel compounds with a high chance of success." Matt goes on to explain, "Many of the enhancements to StarDrop come as a direct result of working collaboratively with our users, which now include over 50 companies world-wide and seven of the top-ten pharma."

For more information and to arrange a free trial of StarDrop, visit www.optibrium.com, contact info@optibrium.com or call +44 01223 815900.

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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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