Optibrium and Digital Chemistry Announce Technology Collaboration to Guide Successful Drug Discovery

Integration of bioisostere database with automatic application and prioritisation will guide the identification of novel, high quality compounds in drug discovery

CAMBRIDGE and SHEFFIELD, UK, December 4th, 2012 – Optibrium and Digital Chemistry, providers of software and database solutions for drug discovery, today announce an agreement to collaborate on the integration of Digital Chemistry's unique BIOSTER™ database of precedented bioisostere replacements with Optibrium's StarDrop™ software suite. This combination will allow drug discovery teams to quickly identify novel, high quality compounds based on the BIOSTER molecular transformations and prioritise these within StarDrop's intuitive environment that guides the design and selection of compounds with an optimal balance of properties.

The BIOSTER database contains over 25,000 bioisostere replacements, hand-curated from the literature by Dr István Ujváry and is distributed exclusively by Digital Chemistry. As part of the collaboration with Optibrium, the BIOSTER database will be converted into transformations that can be applied in StarDrop's Nova™ module, which automatically generates new, chemically relevant compound structures to stimulate the search for high quality chemistry related to initial hit or lead compounds. The combined functionality of Nova and BIOSTER will allow for the application of this comprehensive database of precedented bioisostere replacements to generate novel structures with a high likelihood of biological activity and synthetic accessibility. StarDrop's unique capabilities for multi-parameter optimisation and predictive modelling will allow efficient prioritisation of the resulting compound ideas to identify those with the best chance of achieving the property profile required for a successful drug.

The applications of these technologies extend throughout the drug discovery process, including the rigorous exploration of chemistries around early hits, scaffold hopping to overcome issues with a lead series or to identify diverse back-up series and protection of patent space around a candidate drug.

Matthew Segall, CEO of Optibrium commented, "We are very pleased to announce our collaboration with Digital Chemistry. This furthers our on-going strategy to work with other leading developers of informatics solutions in drug discovery to provide project teams with seamless access to the best technologies to guide the efficient discovery of novel, high quality drugs."

Julian Hayward, Managing Director of Digital Chemistry added, "The deployment of BIOSTER data within a predictive software environment fulfils a long-held ambition to enhance the usefulness of this uniquely valuable database for the discovery of novel active compounds. The ability to generate highly focused libraries of both 'obvious' and 'non-obvious' drug candidates in this manner, will, no doubt, be a welcome addition to the armoury of drug discovery tools."

István Ujváry, Managing Director of iKem and developer of BIOSTER, concluded: "Since its conception two decades ago, BIOSTER has strived to analyse and catalogue historically documented fragment replacement strategies to assist medicinal and pesticide chemists in their quest for new bioactive molecules. The sophisticated Nova module of Optibrium's StarDrop software suite offers an exciting new tool for navigation through the chemical space of sets of bioisosteric and other transformations of this unique database. I am certain that the collaboration between Optibrium and Digital Chemistry will result in a versatile and popular new product."

The results of this collaboration will be available in a future version of StarDrop, expected to be released during 2013.

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 BIOSTER or Digital Chemistry's other products and services, please visit www.digitalchemistry.co.uk, contact info@digitalchemistry.co.uk or call +44 113 2678667.

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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.

For further press information regarding Optibrium please contact: Sarah Morley, The Scott Partnership, 1 Whiteside, Station Road, Holmes Chapel, Cheshire CW4 8AA, UK Tel: + 44 1477 539539 Fax: +44 1477 539 540 E-mail: optibrium@scottpt.com.

About Digital Chemistry Ltd

Digital Chemistry (www.digitalchemistry.co.uk) specialises in cheminformatics software, science & services related to pharmaceutical R&D. We offer a comprehensive range of software tools, that are readily integrated into 3rd-party applications and able to make light work of processing the largest of chemistry databases, stored either as discrete molecules or as concise libraries using our proprietary Markush technology. Recent developments have focused on refinements to our patent Markush searching algorithms, enabling advanced (sub)structure searching of chemical patent databases.

For further press information regarding Digital Chemistry, please contact: Julian Hayward, Digital Chemistry Ltd., 30 Kiveton Lane, Todwick, Sheffield, S26 1HL, UK Tel: +44 (0)113 2678667 Fax: +44 (0)1909 515444 E-mail: Julian@digitalchemistry.co.uk