Optibrium Announce the Release of StarDrop™ 6.6

Novel features include a unique pK_a model, combining quantum mechanics and machine learning methods, and extended capabilities in structure-based design.

CAMBRIDGE, UK, 28 October, 2019 – Optibrium™, a developer of software for drug discovery, today announced the introduction of StarDrop™ 6.6, the latest version of this comprehensive software platform for small molecule design, optimisation and data analysis. The enhanced software will introduce new *in silico* modelling approaches, ensuring scientists can easily link two- and three-dimensional structural information, identify potential liabilities and design new compounds with the highest chance of success.

The acid dissociation constant (pK_a) has an important influence on molecular properties that are crucial to compound synthesis, formulation and optimisation of absorption, distribution, metabolism and excretion properties. StarDrop's new pK_a model, featured in StarDrop's ADME QSAR module, integrates quantum mechanics and machine learning to make accurate predictions for a wide range of compounds. Rigorously validated, this model shows excellent on external benchmark datasets specifically created to assess pK_a prediction methods.

StarDrop 6.6 also includes an extended suite of SeeSAR™ modules that enhance StarDrop's capabilities for structure-based design. Developed in collaboration with BioSolveIT GmbH, SeeSAR View enables researchers to visualise ligands in their protein environment to identify the key interactions driving binding affinity. SeeSAR Affinity uses the award-winning HYDE scoring method to analyse a ligand's binding affinity, related to free energies with visual atomic contributions, and view torsion angle heat maps to assess docked poses. SeeSAR Pose generates docked compound poses for virtual screening and interactive 3D design. The combination of these modules within StarDrop will enable researchers to better understand 2D and 3D structure-activity relationships and design compounds with a higher chance of downstream success.

Dr Matthew Segall, Optibrium's CEO, said: "We're continuing to invest in cutting edge research to deliver high-quality science and new functionality that is accessible within StarDrop's intuitive user interface, addressing the needs of our global user base. The launch of StarDrop 6.6 further demonstrates our ongoing commitment to providing best-in-class technologies across a comprehensive range of *in silico* modelling and compound design capabilities."

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

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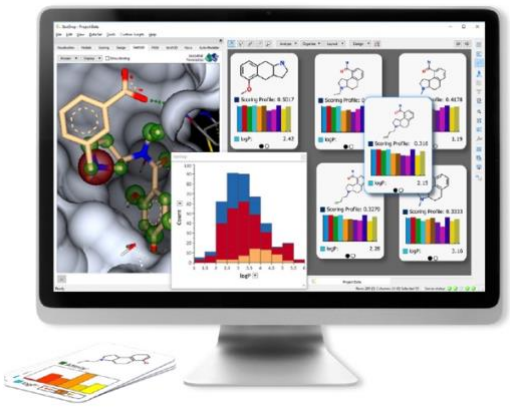

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About Optibrium Ltd

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. Optibrium'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. The company's new Augmented Chemistry™ products and services deliver ground-breaking artificial intelligence technologies that continuously learn from all available data to supplement researchers experience and skills.

Founded in 2009, Optibrium is headquartered in Cambridge, UK with offices in Boston and San Francisco, USA. 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.