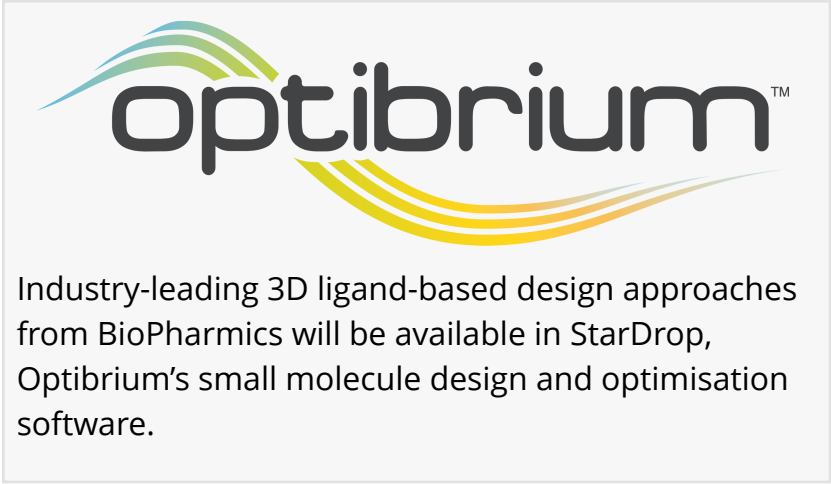
Optibrium and BioPharmics Enter Partnership on Computational Drug Design

Industry-leading 3D ligand-based design approaches from BioPharmics will be available in StarDrop, Optibrium's small molecule design and optimisation software.



CAMBRIDGE, CAMBRIDGESHIRE, UNITED KINGDOM, May 20, 2021 /EINPresswire.com/ -- Optibrium Ltd and BioPharmics LLC, leading providers of software and computational solutions for drug discovery, today announce their partnership. The collaboration will combine industry-leading computational design solutions with advanced interactive user interfaces, engaging with experimental and computational drug discovery experts alike. The first outcome will be a new module for StarDrop™, Optibrium's small molecule design, optimisation and analysis software, used by more than 160 organisations worldwide, including five of the top ten global pharmaceutical companies. The new Surflex eSim 3D module, planned for the 3rd quarter of 2021, will leverage BioPharmics' three-dimensional (3D) ligand-based design approaches, offering exceptional virtual screening and compound design capabilities for targets without available 3D structure information.

BioPharmics develops algorithms and software for computational drug design. The company's peer-reviewed molecular similarity method, eSim, utilises electrostatic field and molecular surface-shape comparisons and directional hydrogen-bonding preferences, combined with their rigorously validated ForceGen conformational search algorithm. This combination results in higher accuracy and performance than approaches reliant on heuristic molecular feature types to represent molecular electrostatics or atom-centric techniques to model molecular shape. In extensive studies, BioPharmics technology has proven its ability to predict active ligand conformations starting from known actives, even in the absence of 3D structure information for ligands or target.

Optibrium develops comprehensive solutions and deep learning methods for computational drug discovery. StarDrop is Optibrium's suite of integrated software for small molecule design,

optimisation, and data analysis, improving the speed and productivity of the discovery process. Optibrium works closely with its broad range of customers and collaborators that include leading global pharma, agrochemical and flavouring companies, biotechs and academic groups. The collaboration with Biopharmics will greatly enhance StarDrop's capabilities for 3D ligand-based design, extending its comprehensive range of in silico modelling and de novo design features.

Dr Matthew Segall, CEO at Optibrium, said: "We are excited to partner with BioPharmics and work with Drs. Ajay Jain and Ann Cleves, who are industry leaders in computational drug design methods. Our collaboration continues our commitment to offering best-in-class technologies to the pharmaceutical industry and further expand our comprehensive StarDrop software."

Dr Ann E. Cleves, Director of Applied Science at BioPharmics, said: "The BioPharmics team is delighted to see the eSim-3D technology integrated with the StarDrop platform. The collaboration will deliver ligand-based design into the hands of medicinal chemists, allowing direct use of state-of-the-art 3D computations from within an elegant and user-friendly interface."

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

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