Optibrium Enhances Compound Design Strategies in Major Upgrade to StarDrop Software

New features include reaction-based library enumeration for novel molecule generation and optimisation, and seamless AI-integration for deeper data analysis

Optibrium Enters Cheminformatics Collaboration with MSD

CAMBRIDGE, CAMBRIDGESHIRE, UNITED KINGDOM, January 19, 2021 /EINPresswire.com/ -- Optibrium™, a developer of software for drug discovery, today announced the release of the newest version of StarDrop™, a comprehensive software platform for small molecule design, optimisation and data analysis. The new release, StarDrop 7.0, further extends the software's compound design strategies, provides enhanced workflows, and seamlessly connects with Optibrium's Cerella™ platform, delivering unique Artificial Intelligence (AI) capabilities to drug discovery scientists. More than 150 organisations worldwide use StarDrop in their research programs - the new features have been developed in close collaboration with key customers and have proven their benefits in identifying optimally balanced, successful and novel compounds faster.

Reaction-based Library Enumeration (RBE) enables chemists to easily enumerate compound libraries and explore optimisation strategies. As a new feature of StarDrop 7.0, RBE delivers a highly-flexible and user-friendly environment to generate new molecules, by applying tractable, robust chemical reactions and linking directly with in-house and commercial building block libraries. Combined with StarDrop's multi-parameter optimisation capabilities, this enables medicinal chemists to target high-quality and synthetically accessible compounds.

StarDrop 7.0 seamlessly integrates with Cerella, Optibrium's newly introduced AI software platform, providing intuitive workflows that leverage Cerella's unique capabilities to accelerate discovery cycles and reduce costs while targeting high-quality compounds. Deploying advanced deep learning methods, Cerella has been demonstrated to extract additional value from compound data, highlighting relationships between structures, activities and other properties on a scale and accuracy unmatched by conventional cheminformatics methods.

Edmund Champness, Optibrium's Chief Scientific Officer, commented, "Having surveyed the available reaction-based enumeration tools, and found no solutions that met their requirements, our collaborators asked us to develop this feature. We thank them for their input, which was instrumental in shaping an industry-leading capability with the elegance and functionality they've come to expect from StarDrop. Added to which, after the successful launch of our AI platform Cerella, we are excited to provide our users with seamless access to a groundbreaking AI system through its integration in StarDrop 7.0."

For further information on Optibrium, StarDrop 7.0 or Cerella, please visit www.optibrium.com, contact info@optibrium.com or call +44 1223 815900.

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