Orion Molecule Search: Unlocking Vast Chemical Space with High-Speed 2D/3D Search

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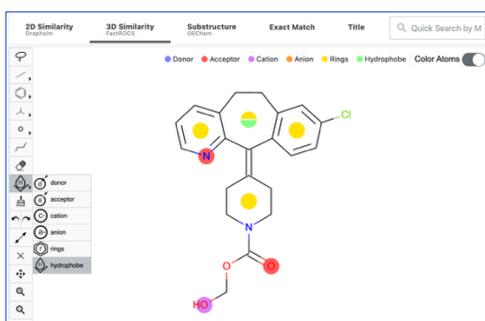*OpenEye, Cadence Molecular Sciences, 9 Bisbee Court Suite D, Santa Fe, NM 87508*

Summary:

- Searches very large vendor libraries in seconds to minutes
- Find analogs and new scaffolds with 2D, substructure, and 3D shape & feature similarity
- Sketch-and-search web interface runs entirely in the cloud with no local compute required
- Integrates seamlessly into downstream modeling workflows

Product Keywords: Virtual Screening, Molecule Search, ROCS®, FastROCS™, Orion®

Abstract:

OpenEye's Orion Molecule Search makes it fast and effortless to explore vast chemical spaces using high-performance 2D and 3D similarity search. Instead of juggling multiple vendor databases or managing your own infrastructure, you can search hundreds of millions of commercially available compounds directly from a web browser. Orion Molecule Search is powered by industry leading shape and chemical feature (color) similarity search (FastROCS) to help you find high-quality hits.
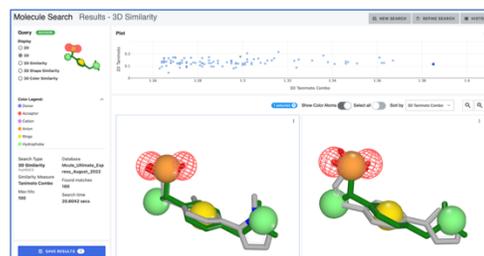

Orion Molecule Search offers unified 2D/3D search across vendor-ready chemical space, powered by industry leading FastROCS, to instantly uncover high-quality analogs.

Submit any query molecule via sketch, SMILES, cut-and-paste, name, or file upload to instantly find close analogs, new scaffolds, or shape-matched candidates using high-speed 2D and 3D similarity search.

The interface provides interactive filtering, ranking, and visualization of hits to simplify decision-making. From the interface, user can move hit lists directly into downstream modeling workflows, from docking to MD to free-energy calculations. This tight integration accelerates hit discovery and hit-expansion campaigns while enabling scalable, reproducible cheminformatics workflows entirely in the cloud, accessed conveniently through a web browser.

Clear and intuitive results. Instantly visualize molecular relationships with intuitive color-coding, making it easy to spot similarities at a glance.

The entire process is scalable, shareable, and reproducible across teams. Orion Molecule Search helps R&D groups accelerate hit discovery and expand chemical diversity, allowing medicinal chemists and computational scientists to focus on designing better molecules rather than managing data or compute resources.