

Accelerating Drug Discovery Through Computational Molecular Design

SCIENCE | SPEED | SCALE

Science: Use physics-based design and machine learning to advance

- Hit identification, hit-to-lead, and lead optimization
- Binding affinity and molecular dynamics simulations
- Membrane permeability pathway modeling
- Quantum chemistry calculations
- Pharmaceutical formulations

Speed: Delivered the way you need with

- Orion's web-based cloud native modeling platform
- Desktop and Linux applications for local hardware
- Cheminformatics and development toolkits
- Expert consulting services

Scale: Perform extreme-scale search and screening on

- Billions-sized libraries using ligand (2D/3D) and structure-based (3D) methods
- Millions of sequences from Next Generation Sequencing antibody data
- Hundreds of thousands known and putative protein-ligand binding sites for off-target effects
- Your proprietary libraries using combined physics-based and data-driven approaches

In Virtual Screening against the Enamine *REAL*[®] Database

2D ligand
similarity in

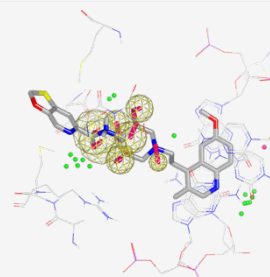
Seconds

3D ligand
similarity in

Minutes

3D ligand-protein
docking in

Hours



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