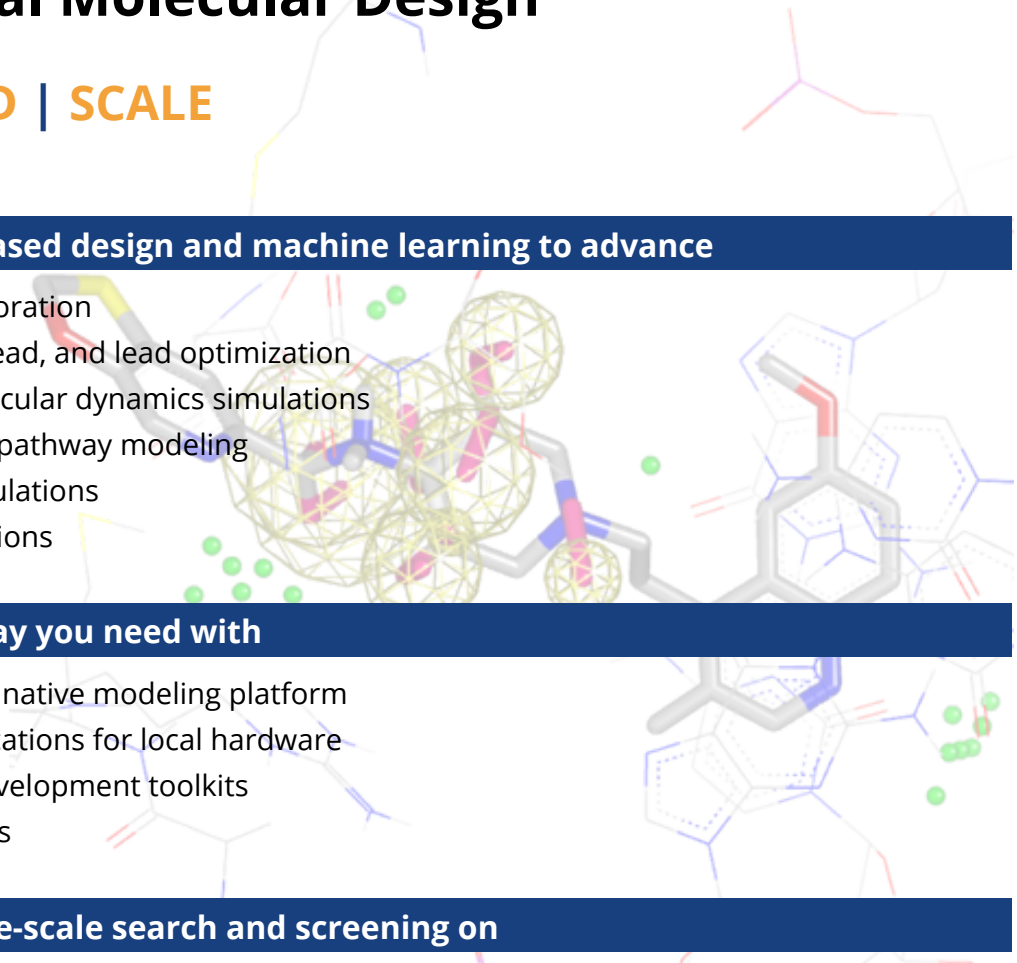
Accelerating Drug Discovery Through Computational Molecular Design

SCIENCE | SPEED | SCALE

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

- Biomolecular target exploration
- 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	3D ligand similarity in	3D ligand-protein docking in
Seconds	Minutes	Hours

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