Computational Approaches

Quantum Computing
Next-gen simulations

Structure-based
Protein structures

- Molecular docking
- MD simulations
- Homology modeling

Ligand-based
Known actives

- QSAR modeling
- Pharmacophore
- 3D-QSAR

HPC

GPU

AI/ML
Hub

Cloud

Big Data

Systems
Network-based

- Pathway analysis
- Target networks
- Drug synergy

ML Integration
AI-powered

- Deep learning
- Graph neural nets
- Transfer learning

Integrated Platform Benefits
10x faster • 50% cost reduction • Higher success rate