Virtual Screening

Compound Library
10^6 - 10^9 compounds

Similarity

Similarity Filtering
10^4 - 10^5 compounds

Pharmacophore

3D Pharmacophore
10^3 - 10^4

Docking

Molecular Docking

ML Scoring

Deep Learning

Consensus
Multiple Methods
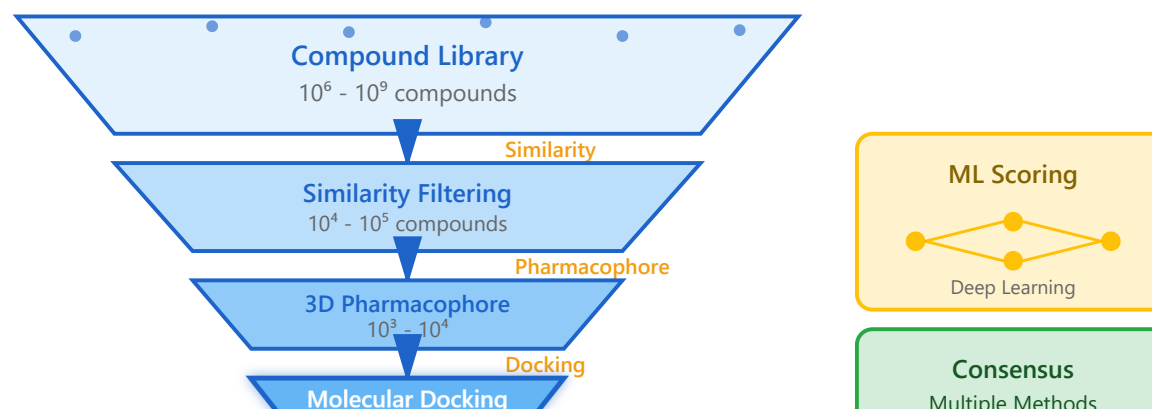
Similarity searching
Finding similar active compounds

Pharmacophore modeling
3D feature-based screening

Docking scores
Protein-ligand binding prediction

ML scoring functions
Learning-based scoring

Consensus approaches
Combining multiple methods