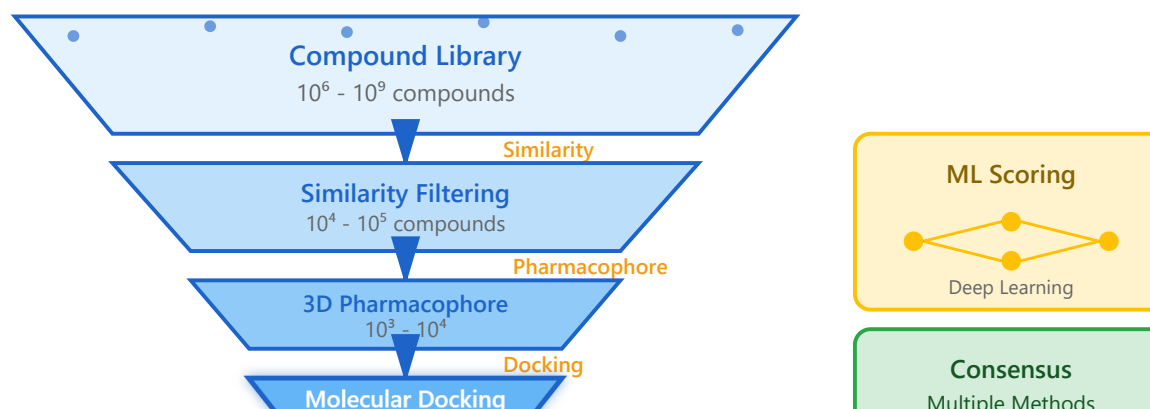


Virtual Screening



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