

# Schrödinger Software

Schrödinger provides accurate, reliable, and high performance computational technology to solve real-world problems in life science research.

## Small Molecule Modeling and Simulations

### Conformation Generation and Clustering

- MacroModel - gas phase and solution
- ConfGen - bioactive conformation generation
- XCluster - clustering conformations

### Property Generation and Filtering

- QikProp - descriptor generation and ADME/Tox prediction
- Ligand Properties & Filtering

### ID/2D to 3D Structure Generation

- LigPrep
- Epik - fast pKa and tautomer prediction

### Molecular Mechanics

- MM2, MM3, AMBER, AMBER94, MMFF, MMFFs, OPLS, and OPLS-AA Force Fields
- GB/SA Solvation Model
- MacroModel
- Impact
- MINTA - conformational free energies
- Force Field Viewer

### Molecular Dynamics

- Desmond - explicit solvent MD
- Impact - implicit and explicit solvent MD

### Quantum Mechanics

- Jaguar
- Jaguar pKa
- Hydrogen Bond Calculator

## Macromolecular Modeling and Simulations

### Structural Biology – Crystallography

- PrimeX - protein crystal structure refinement
- Protein Structure Analysis

### Protein Modeling and Bioinformatics

- Prime Loop and Side-Chain Prediction
- Prime Sequence Alignment
- Prime Fold Recognition/Threading

### Molecular Mechanics

- MM2, MM3, AMBER, AMBER94, MMFF, MMFFs, OPLS, and OPLS-AA Force Fields
- GB/SA Solvation Model
- Prime
- MacroModel
- Large-Scale Low-Mode (LLMOD) conformational sampling
- Impact
- Force Field Viewer

### Molecular Dynamics

- Desmond - explicit solvent
- Impact - implicit and explicit solvent

### Monte Carlo Simulations

- MCPRO+

### QM/MM

- QSite

## Lead Discovery

### Cheminformatics

- Canvas

### Ligand-Based Discovery

- Phase - pharmacophore modeling
- Phase Shape
- Phase Multiple Binding Mode Predictor
- Phase CAC database
- Flexible Ligand Superposition

### Fragment-Based Discovery

- Glide - docking and scoring
- CombiGlide
- Phase - pharmacophore modeling
- Rule-based Molecule Fragmenting
- Fragment Joining/Linking
- Ligand Efficiency (LE) Metrics
- BREED - ligand hybridization

### Structure-Based Discovery

- Glide - docking and scoring
- Virtual Screening Workflow (VSW)
- SiteMap - protein binding site identification and analysis
- Covalent Docking
- Protein Preparation Wizard
- Protein Structure Alignment
- GPCR Modeling

## Lead Optimization

### Cheminformatics

- Canvas

### 2D/3D QSAR

- Phase - pharmacophore modeling
- Strike - statistical modeling
- QikProp - property generation

### Combinatorial Chemistry

- CombiGlide R-group Evaluator
- CombiGlide Core Hopping

### Fragment-Based Design

- Glide - docking and scoring
- Rule-based Molecule Fragmenting
- Fragment Joining/Linking
- Ligand Efficiency (LE) Metrics
- BREED - ligand hybridization

### Ligand-Based Design

- Phase - pharmacophore modeling

### Structure-Based Design

- Glide - docking and scoring
- Induced Fit Docking
- Prime MM/GBSA
- WaterMap - identification and calculation of free energies of binding site water molecules
- CombiGlide Core Hopping
- CombiGlide Screening
- HERG Modeling with Induced Fit Docking
- SiteMap - protein binding site identification and analysis
- Embrace - post-docking refinement
- Hydrogen-Bond Calculator
- Liaison - linear interaction approximation
- MCPRO+
- QM-Polarized Ligand Docking
- SIFt - Structural Interaction Fingerprints
- QSite - QM/MM
- Ligand Designer

### Absolute and Relative Binding Affinity Prediction

- Glide XP - docking and scoring
- Prime MM/GBSA
- WaterMap
- MCPRO+
- Desmond FEP - molecular dynamics free energy perturbation

## Visualization and Automation

### Molecular Visualization

- Maestro - molecular modeling graphical interface
- Glide XP Visualizer
- 2D Viewer

### Application Deployment Interfaces

- Maestro - molecular modeling interface
- Canvas - cheminformatics
- KNIME Extensions

### Scripting, Methods Development and Deployment

- Python API
- Maestro Command Language

### Workflow/Pipelining

- KNIME Extensions
- Python Pipelining Infrastructure

### Medicinal Chemistry Applications

- 2D Viewer
- 3D Builder
- Glide Web Interface
- Medicinal Chemistry Interface to Minimization, Torsion Scans, Conformational Searches, and ESP Surfaces
- Ligand Designer

