Identify chemically diverse, high-quality initial screening hits and scale from compound libraries of several hundred to several billion.
Diverse Workflows for Hit Discovery

Leverage rapid orthogonal virtual screening technologies to accurately screen billions of compounds, with or without protein structures.

Structure-based Virtual Screening

Dock Novel Ligands
Screen compounds accurately with a well-validated, easy to use ligand-receptor docking algorithm.

> Product: Glide

Virtually Screen Billion+ Libraries with Docking and Machine Learning
Rapidly, accurately, and cost-effectively screen billions of purchasable compounds with an automated workflow that combines Glide docking and scoring with the power of machine learning.

> Products: Active Learning Glide, Virtual Screening Web Service

Ligand-based Virtual Screening

Screen using Pharmacophores
Rapidly screen compounds based on the steric and electronic features of molecules known to have biological activity, optionally including receptor information.

> Product: Phase

Screen using 3D Ligand Shape
Screen billions of compounds quickly by optimizing the 3D shape and pharmacophore overlap between known active ligand conformations and library molecules.

> Product: Shape Screening (GPU)

Enrich Hits from Screens
Use advanced sampling and scoring techniques to improve the enrichment of virtual screens and find the most promising hits.

> Products: ABFEP, WScore
Accurate Ligand Preparation

Rapidly generate bioactive ligand structures with accurate ionization and tautomeric states to increase the probability of identifying relevant hits.

**Perform Ligand Preparation**

Easily translate molecular structures from 1D, 2D to 3D while carefully enumerating structural and chemical possibilities to ensure the accuracy of subsequent modeling predictions.

> **Product:** LigPrep

**Predict pKa using a Knowledge-based System**

Predict pKa using a rapid and robust knowledge-base algorithm.

> **Product:** Epik

**Generate Ensembles for Conformation Analysis**

Predict accurate bioactive conformers of ligands in solution and perform efficient conformational searches.

> **Products:** ConfGen, MacroModel

**Screen Prepared Compound Libraries**

Start screening immediately using prepared compound libraries of 10 million to >1 billion from Enamine, MolPort, Sigma Aldrich, WuXi, and Mcule with quick and easy purchase of virtual hits.

*Several commercial prepared libraries available*

**Predict pKa using Quantum Mechanics**

Predict pKa of molecules in novel chemical space using a highly accurate quantum mechanics approach.

> **Product:** Jaguar
## Services For Hit Discovery

Maximize the chances of program success by leveraging Schrödinger’s most advanced technologies at scale.

### Research Enablement Hit Discovery Campaign

Schrödinger scientists will run complementary cutting-edge virtual screening technologies to screen ultra-large libraries followed by advanced re-scoring steps to enable the discovery of potent, diverse and high-quality hits.

**Best suited for companies and teams:**
- In need of burst screening capabilities for hit identification
- With limited in-house computational chemistry capabilities
- Who want to maximize their chance of success by fully leveraging Schrödinger’s platform and expertise

**Best suited for projects where:**
- Molecular strategy is defined and there is sufficient structural target information available

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### Virtual Screening Web Service

Access a cloud-based web service for Schrödinger’s fully-automated ultra-large-scale virtual screening workflow and included burst computing power to screen >1B purchasable compounds in one week.

**Best suited for companies and teams:**
- In need of occasional or one-time large-scale screening
- Lack the compute infrastructure or technical resources to screen in-house efficiently
- Already have access to Schrödinger software to build docking models

**Best suited for projects where:**
- Molecular strategy is defined and there is sufficient structural target information available

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| > Services: Virtual Screening Web Services |

### Scientific and Technical Support

- **Training resources designed for novice and experts users**
  - Vast educational materials and training courses to make you an expert.

- **Expert technical and scientific support included**
  - Self-help, email, and face-to-face from industry-leading scientific and technical support.

- **Cross-platform support for Linux, Windows, Mac, and cloud-based solutions**
  - Designed to work within your computer environment.

**Contact us:** sales@schrodinger.com
**Learn more:** schrodinger.com