Discover better quality molecules, faster with FEP+

FEP+ is Schrödinger's proprietary, physics-based free energy perturbation technology for computationally predicting protein-ligand binding at an accuracy matching experimental methods, across broad chemical space.

Explore vast chemical space and reduce costs

Leverage FEP+ as an accurate, digital binding affinity assay to drive rapid *in silico* design cycles and focus experimental efforts on only the highest quality ideas.

Improve molecular profiles, efficiently

Optimize multiple properties simultaneously, including potency, selectivity, and solubility, to improve the profile and developability of small and large molecules.

Pursue novel chemistry with confidence

Synthesize novel and challenging chemistry with a high degree of confidence through prospective application of FEP+.

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Automated workflows to drive real-world discovery

Access a diverse set of FEP+ workflows that cover design scenarios common in drug discovery programs:

Predict change of affinity and selectivity for structural modifications of small molecules	**Score diverse small molecules to enrich hits in virtual screens**
Predict ligand kinetic and thermodynamic solubility	**Facilitate macrocyclization and fragment linking to improve affinity and selectivity**
Predict selectivity through protein residue mutation between on and off targets	**Engineer biologics for affinity and stability**

Proven impact across a broad range of applications

FEP+ offers industry-leading accuracy, with predicted binding affinities generally within one kcal/mol of experimental values, as demonstrated through numerous published studies.

- Discovery of a Novel Class of D-amino Acid Oxidase (DAO) Inhibitors with the Schrödinger Computational Platform. Tang H, et al. *J. Med. Chem.* 2022, 65(9): 6775-6802.

- Prospective Applications of Free Energy Methods in Drug Discovery Programs. Ozen A, et al. Free Energy Methods in Drug Discovery: Current State and Future Directions. 2021, Chapter 5:127-141.

- Prospective Evaluation of Free Energy Calculations for the Prioritization of Cathepsin L Inhibitors. Kuhn B, et al. *J. Med. Chem.* 2017, 60:2485-2497.

- Enhancing Hit Discovery in Virtual Screening Through Accurate Calculation of Absolute Protein-Ligand Binding Free Energies. Chen W, et al. *ChemRxiv*. 2022, preprint.

- Accurate Prediction of Protein Thermodynamic Stability Changes Upon Residue Mutation Using Free Energy Perturbation. Scarabelli G, et al. *JMB.* 2022, 434:1673-75.

Enabling technology that fits your organization's needs

Industry-Leading Software Platform

Deploy digital drug discovery workflows using a comprehensive and user-friendly platform for molecular modeling, design, and collaboration.

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