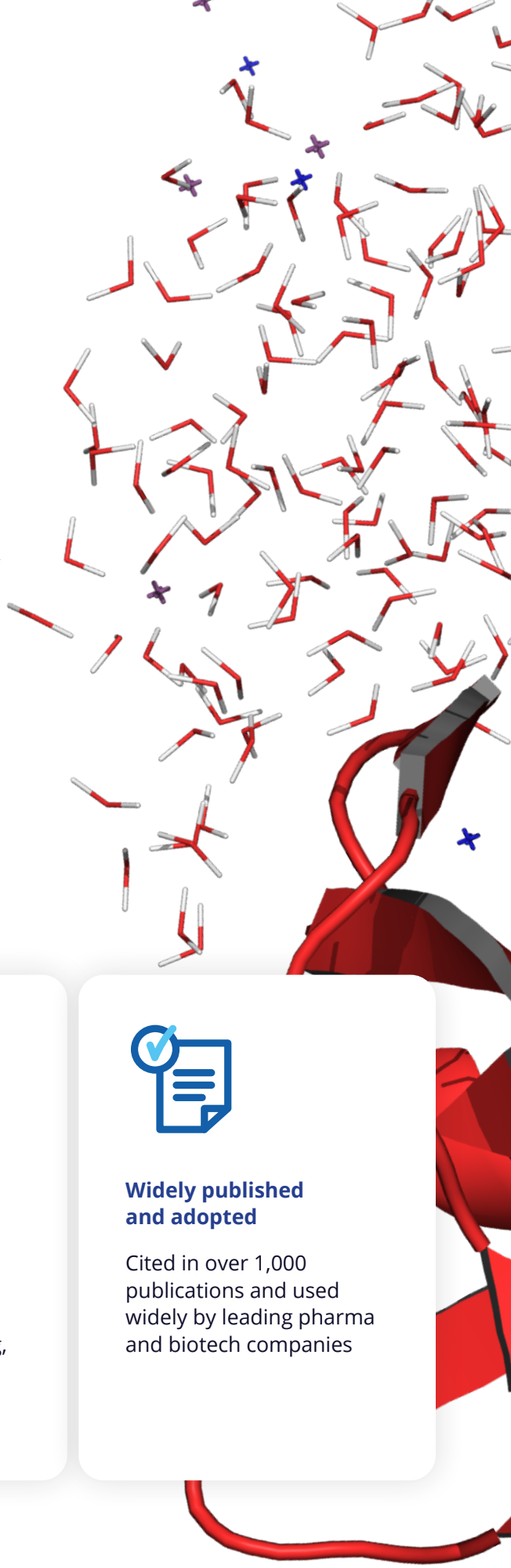
FEP+ for Academic Research



Advance your research with industry-leading technology

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

Schrödinger offers an affordable web-based solution for accessing FEP+ and all required GPU computing for academic researchers performing basic research. FEP+ for Academic Research is intended to promote basic research in chemistry, molecular biology, and related fields, and excludes use for commercial purposes such as drug discovery or other IP generating activities.

Gold standard of accuracy

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Broad domain of applicability

Supports a broad range of calculations and perturbation types including relative binding, absolute binding, solubility, and protein residue mutation FEP

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Apply FEP+ to your chemistry and molecular biology research

- Probe the molecular mechanisms underpinning important molecular biology
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How it works

- Requires access to Schrödinger Small Molecule Discovery Suite for system preparation
- Web-based solution includes all GPU compute resources
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- Restricted to academic research use

Learn how to apply FEP+ to your project with our online certification course, Free Energy Calculations for Drug Design with FEP+

Publications

- The maximal and current accuracy of rigorous protein-ligand binding free energy calculations. Ross GA, et al. *Commun. Chem.* 2023, 6, 222.
- Protein-ligand binding free energy calculations with FEP+. Wang L, et al. *Methods Mol Biol.* 2019, 2022, 201-232.
- Advancing drug discovery through enhanced free energy calculations. Abel R, et al. *Acc. Chem. Res.* 2017, 50, 7, 1625–1632.
- Accurate and reliable prediction of relative ligand binding potency in prospective drug discovery by way of a modern free-energy calculation protocol and force field. Wang L, et al. *J. Am. Chem. Soc.* 2015, 137, 7, 2695–2703.

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