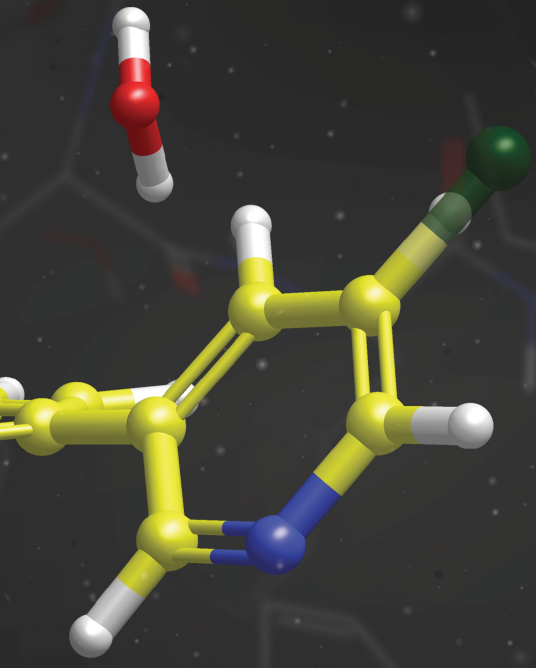
FEP+

High-performance free energy calculations for drug discovery



ACCELERATE RESEARCH AND DEVELOPMENT

- Make synthesis decisions more confidently through the scientific accuracy of Schrödinger's proven FEP+ methodology
- Extend your knowledge base by leveraging the experience of over 200 PhD research scientists at Schrödinger with expertise across computational research areas
- Highly-trained support experts always ready to tackle your scientific and technical challenges
- Stay up-to-date with the latest scientific advances with quarterly updates

SPEED-UP DEVELOPMENT TIMELINES

- Find highly potent binders, while maintaining a host of other ligand properties required for safety and biological efficacy
- Quickly impact lead optimization projects with meaningful comparisons to experimental binding affinities
- Drive projects forward with consistent, easy-to-use simulations, and GPU-enabled computational power

MAXIMIZE THE VALUE OF YOUR COMPUTATIONAL SOFTWARE

- Derive benefits quickly through basic and advanced training with Schrödinger scientists, locally on-site or online across the globe
- Conveniently access a comprehensive library of videos, documentation, and step-by-step online training materials
- Enjoy the support of highly-trained support experts, always ready to tackle your scientific and technical challenges

SCHRÖDINGER®

STATE-OF-THE-ART FORCE FIELD OPLS3E

- Accurate parameters for proteins and nucleic acids
- Improved conformational analyses
- Greater accuracy for free energy predictions

INTUITIVE GUI

- Easily set up the desired perturbations without expert knowledge
- Visualize and examine the computed results

ENHANCED SAMPLING

- Incorporate REST (replica exchange with solute tempering) enhanced sampling methodology
- Detailed-balance-preserving simulation of a selected subsystem at higher effective temperatures
- Focus sampling efforts efficiently traverse the relevant phase space

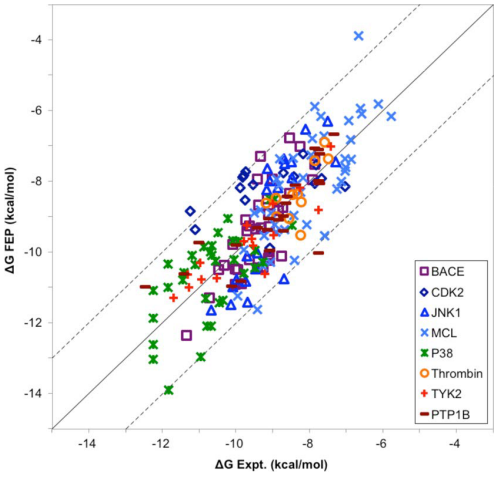
ERROR ESTIMATES

- Elucidate the network of transformations with the FEP Mapper interface
- Analyze consistency and convergence of the simulation results
- Calculate error estimates from individual simulations

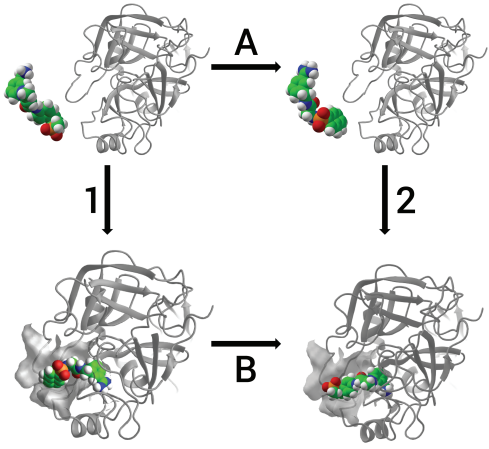
GPU-ENABLED

- Takes full advantage of the Desmond GPU MD engine
- Score 2 to 4 ligands per day on a relatively inexpensive 4 GPU server

Predicted vs. Experimental Binding Energies



Thermodynamic Cycle



$$\Delta\Delta G_{bind} = \Delta G_2 - \Delta G_1$$
$$= \Delta G_B - \Delta G_A$$

FIND THE SOLUTIONS YOU'RE LOOKING FOR:

DRUG DISCOVERY
Comprehensive solutions, validated across hundreds of targets, to accelerate lead discovery and optimization.

MATERIALS SCIENCE
Integrated solutions for atomic-scale simulation of chemical systems to design novel polymers and other products essential to modern life.

ENTERPRISE INFORMATICS WITH LIVEDESIGN
Breaks down traditional silo walls to unleash the power of real-time collaborative design and project management.

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