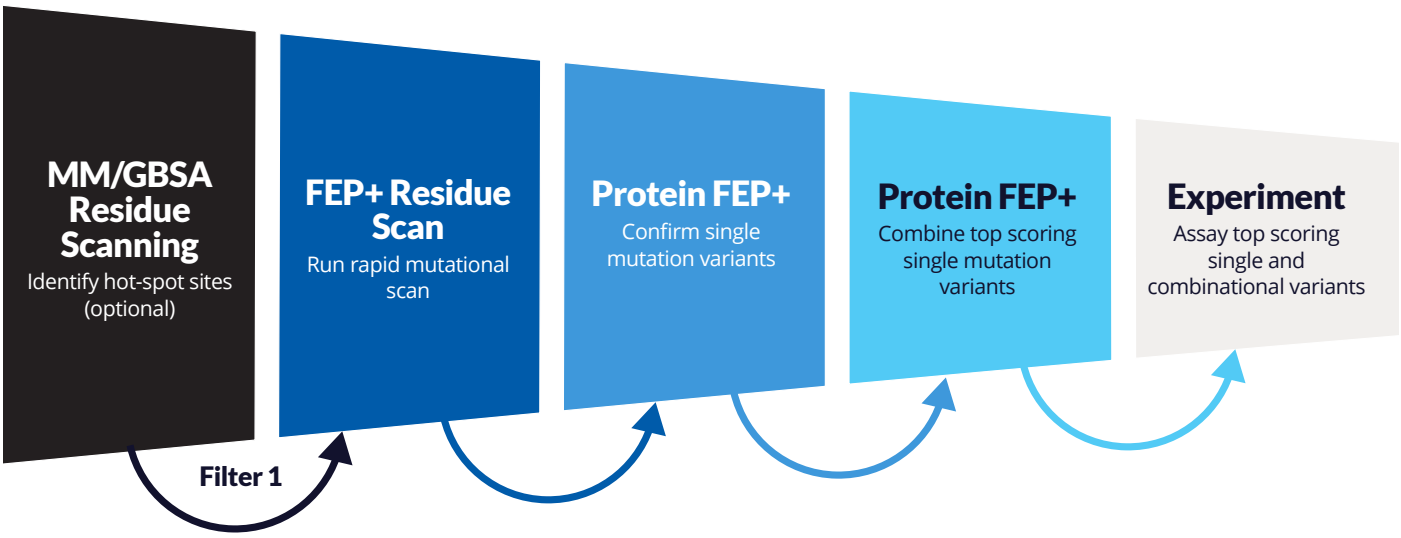
Engineer better proteins, faster with *in silico* workflows powered by FEP+

Schrödinger's protein engineering workflow combines the proven principles of structure-based rational design with advanced computational methods, enabling precise, efficient *in silico* protein design and multi-parameter optimization.

Reduce time-to-results from months to weeks by discarding irrelevant mutations early, as well as quickly generating and iterating through new ideas and follow-up designs

Lower protein optimization costs compared to traditional directed evolution wet lab protocols by running fewer cycles and assaying fewer variants

Identify better quality candidates through simultaneous optimization of multiple parameters to facilitate more rapid testing and triaging of ideas



Schrödinger's customizable protein engineering workflow leverages FEP+ Residue Scan and Protein FEP+ technologies to enable precise and efficient exploration of protein mutations to simultaneously optimize stability, binding affinity, specificity, pH-dependent binding, and cross-reactivity.

Schrödinger

Key Capabilities

Accurately predict the impact of residue substitution on stability, binding affinity, specificity, pH-dependent binding, and cross-reactivity

Benefit from a **7X improvement in accuracy** with FEP+ Residue Scan over MM/GBSA and up to **20X speedup** compared to Protein FEP+

Refine protein candidate selection using Protein FEP+ with an accuracy that reproduces experimentally determined relative free energies to within ~1 kcal/mol

FEP+ Residue Scan offers significant improvements in accuracy over MM/GBSA and speedup over Protein FEP+

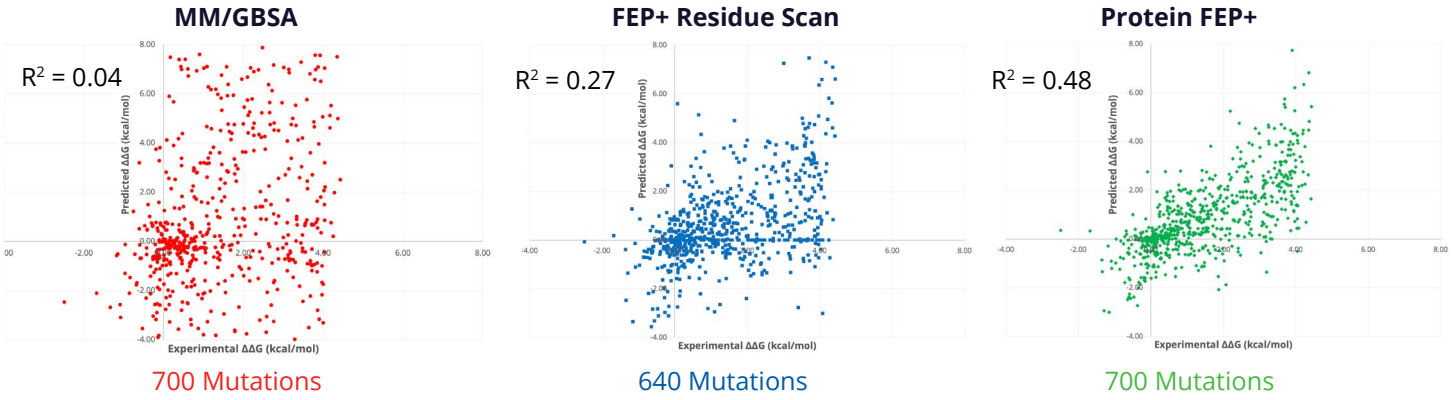


Figure: Correlation plots between MM/GBSA, FEP+ Residue Scan and Protein FEP+ calculations (y-axis), and relative experimental affinity measurements (x-axis), shown in kcal/mol. All calculations performed on the same system, mutations to and from proline currently excluded from FEP+ residue scan results. Pearson correlation coefficient (R2) shown at top left of each plot.

Software and services to meet your organization's needs

Industry-Leading Software
Deploy digital biologics discovery workflows using a comprehensive and user-friendly platform for molecular modeling, design, and collaboration.

Modeling Services
Leverage Schrödinger's team of expert computational scientists to advance your protein design with structure-based modeling.

Scientific and Technical Support
Access expert support, educational materials, and training resources designed for both novice and experienced users.

Contact us: ls-sales@schrodinger.com
Learn more: www.schrodinger.com/platform/products/fep

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Speak with an expert to get started