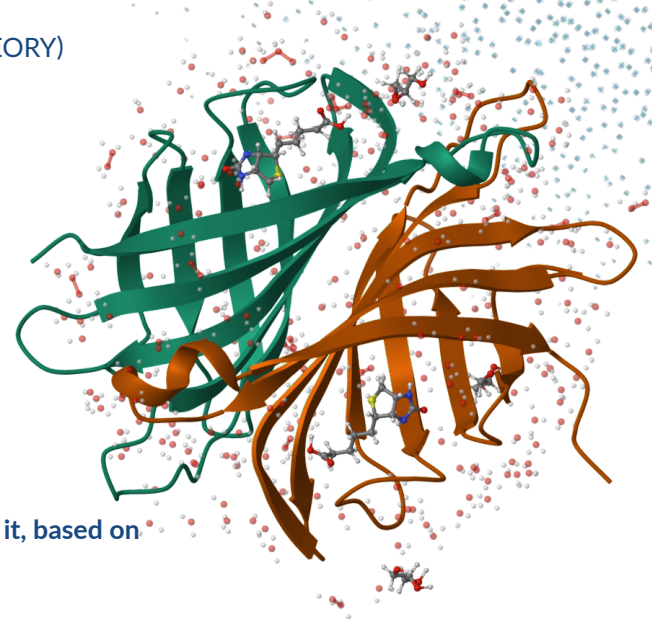
Promethium

UNBLOCK DRUG DISCOVERY

WITH **INTERACTIONMAP** POWERED BY F-SAPT
(FUNCTIONAL-GROUP SYMMETRY ADAPTED PERTURBATION THEORY)

WHAT IS INTERACTIONMAP?

Promethium's proprietary InteractionMap workflow utilizes F-SAPT methodology to provide a quantum-accurate, functional group level breakdown of non-covalent interactions. With InteractionMap, medicinal chemists now have a direct line of sight into *why* ligands bind the way they do. It moves beyond heuristics and docking scores, offering quantitative, interpretable insights that accelerate lead optimization.



Streptavidin-Biotin complex

INTERACTIONMAP DELIVERS POWERFUL INSIGHT

1. **Discover which functional groups drive binding and which hinder it, based on quantitative interaction energies in kcal/mol, broken down into:**
   - Electrostatics
   - Exchange (steric repulsion)
   - Induction
   - Dispersion
2. **Automated Protein-Ligand Setup**
   Promethium automates sample preparation for protein-ligand complexes, reducing setup time and eliminating fragmentation errors.
3. **Comparative Analysis across Ligand Series**
   Evaluate how interaction patterns change across congeneric series, essential for understanding SAR and guiding R-group modifications.
4. **Visual, Color-Coded Insights**
   Promethium provides intuitive visualization and full access to rich, downloadable numerical data, making it easy to communicate findings **across teams.**

SUPERCHARGE YOUR LEAD OPTIMIZATION FUNNEL

Step One: **Filter** with QC Score

- Quantum chemical scoring of docked poses
- Geometry optimization of ligand + active site
- Fragmented interaction energy ranking
- Fast (5-15 min/ligand and scalable to hundreds of ligands in parallel)

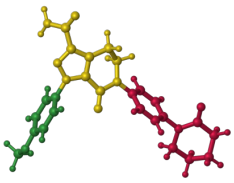
Step Two: **Fix** using InteractionMap

- Deep-dive into functional-group contributions
- Identify fragments to strengthen, replace or re-design
- Understand *why* binding energies differ between ligands
- Supports rational design decisions grounded in quantum mechanics

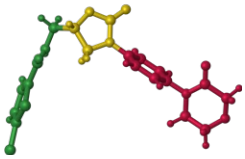
CASE STUDY: FACTOR Xa INHIBITORS

FROM FILTER TO FIXER

Using QC Score the binding site geometries were optimized and the relative affinities were compared between apixaban and rivaroxaban at the ωB97X-D3/def2-svp level of theory. Promethium's One-click push to InteractionMap was then used to explore the differences between the affinities by highlighting specific functional-group/residue interactions.

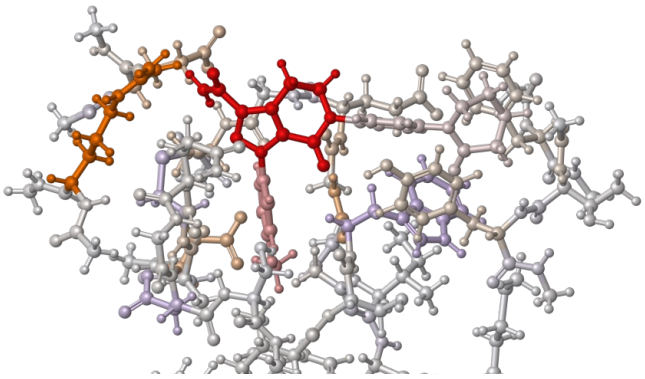


Apixaban



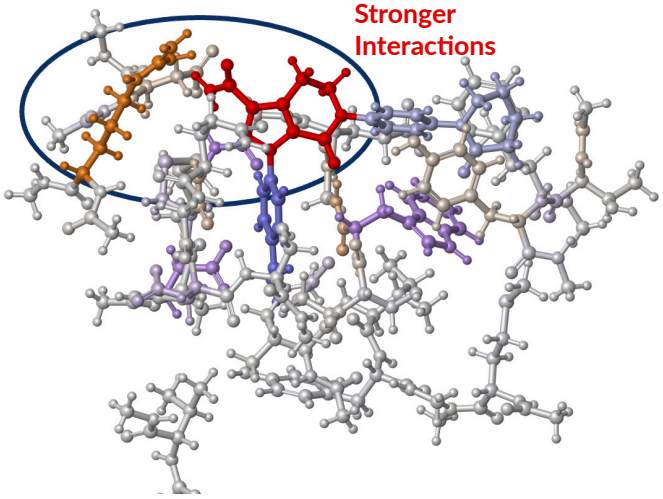
Rivaroxaban

Promethium's point-and-click interface makes it easy to partition molecules into equivalent groups



Electrostatic interactions color-coded for Apixaban in the Factor Xa binding site.

InteractionMap's visual interface makes it clear that the dominant interaction is that between the arginine residue and the pyrazolopyridine.



Interaction Difference Map highlights functional groups that have stronger interactions for apixaban (red) or rivaroxaban (blue)

- Apixaban's higher affinity arises from stronger electrostatic interactions between the pyrazolopyridine and the nearby arginine residue.
- Dispersion, steric and electrostatic maps highlight residue-specific hotspots that can be targeted for optimization.

This type of mechanistic clarity is impossible to obtain from docking, MM/GBSA, or even Free Energy Perturbation.

THE PROMETHIUM ADVANTAGE

- GPU-accelerated quantum chemistry
- Automated workflows from QC Score to InteractionMap
- Drag-and-drop interface
- Enterprise-grade encryption
- Designed for medicial chemists, not quantum chemists

READY TO ACCELERATE YOUR DISCOVERY?

Perfect for:

- Medicinal chemistry teams
- Computational chemistry groups
- AI/ML modelers needing high-quality quantum labels
- Structure-based drug design programs

READY TO LEARN MORE?