Protein/Ligand Docking

Cyrus automates the *Rosetta* Ligand Docking pipeline, in combination with other software packages, as an easy-to-use, SaaS offering to deliver the next generation of protein/ligand docking with protein flexibility.

- Unrivaled performance in flexible-backbone ligand docking with realistic sampling of protein flexibility
- Novel, iterative Homology Modeling / Docking method - the next generation of protein/ligand docking
- Industry leading performance in fixed-backbone ligand docking with unlimited cloud computing

The innovator in protein backbone flexibility

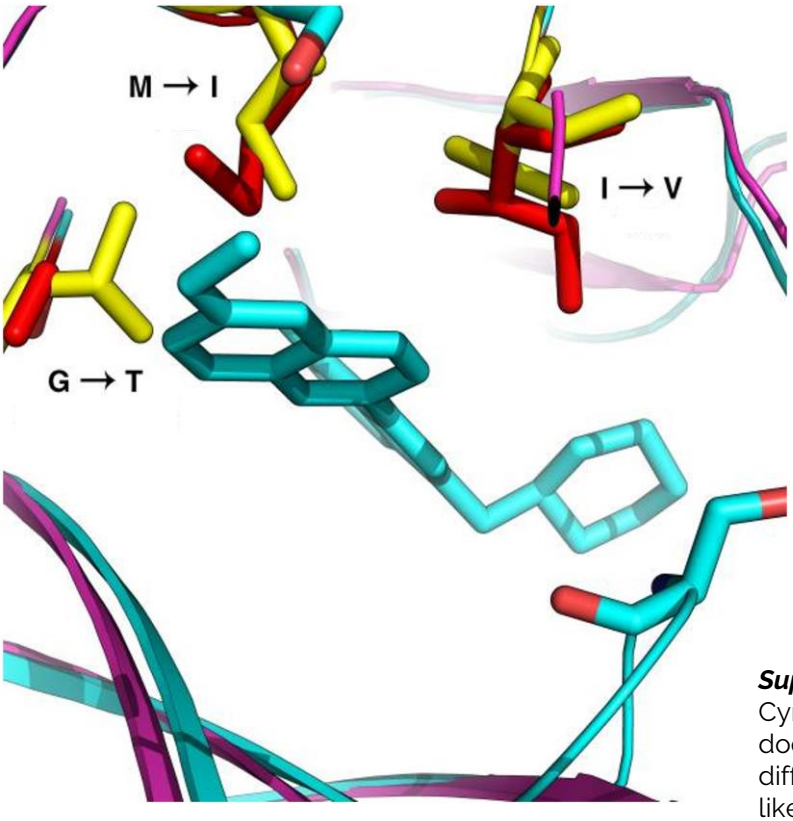
Rosetta yields unrivaled accuracy in protein structure prediction – Cyrus uses these algorithms to deliver high-accuracy docking performance when some backbone motion is necessary to realistically score a ligand.

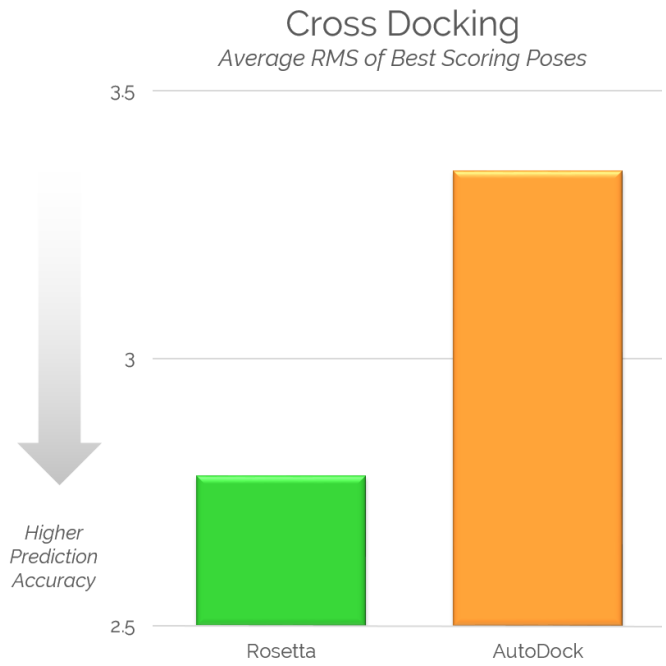
Novel Iterative Modeling/Docking approach

Protein/ligand docking often assumes that the protein backbone is highly rigid, but countless experiments show that structure often changes upon binding. This method can correctly sample larger shifts when needed.

Sample larger conformational shifts: Novel homology modeling with ligand protocol

It is very common for protein backbone to shift upon ligand binding – existing tools sample such changes very poorly. Cyrus's method iteratively combines *Rosetta*'s industry-leading homology modeling with ligand docking to produce higher quality models than ligand docking alone (3).





Superior flexible-backbone docking

Cyrus outperforms AutoDock in cross docking, where a ligand is docked into the crystal structure of the target protein bound to a different ligand, requiring small backbone shifts (1). In a test of drug-like molecules, Rosetta outperforms tools such as Glide (2).

Automated, Integrated Pipeline

Cyrus automates multiple *Rosetta* steps and integrates *RosettaLigand* with several other software packages for small-molecule preparation. Very large amounts of computing are accessible via an easy-to-use, modern web-based GUI, so you can focus on the science.

(1) *Davis, I. et al. "RosettaLigand docking with full ligand and receptor flexibility." J. Mol. Bio. 385 381-392 (2009).*
(2) *Davis I. et al. "Blind docking of pharmaceutically relevant compounds using RosettaLigand". Protein Science 18, 1998-2002 (2009)*
(3) *Keyloun, K. R. et al. "The gatekeeper residue and beyond: homologous calcium-dependent protein kinases as drug development targets for veterinarian Apicomplexa parasites". Parasitology 141, 1499–1509 (2014).*