CYRUS BIOTECHNOLOGY

Crystallography Accelerated

Cyrus automates the *Rosetta* molecular replacement software protocols (*MR-Rosetta*) as a set of easy-to-use, SaaS offerings to solve structures more rapidly, or to phase otherwise impossible structures in conjunction with established crystallography software,

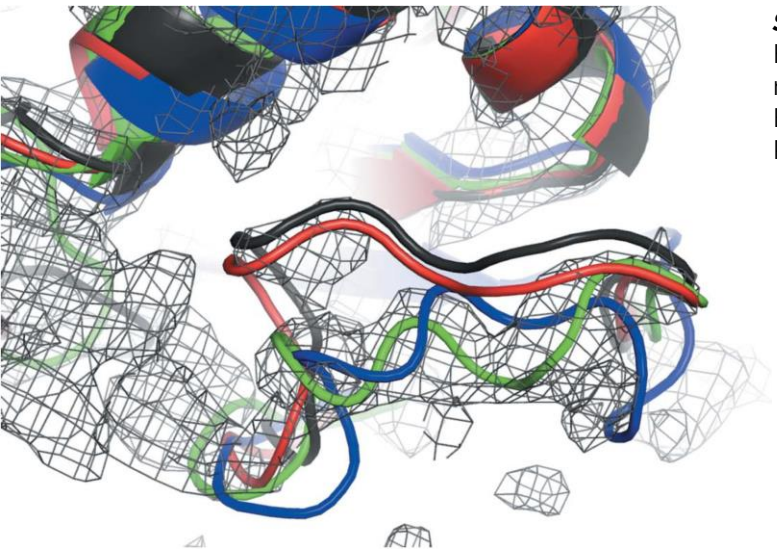
- Save weeks of manual refinement time with high-accuracy homology models
- Phase poor-resolution structures to atomic-resolution with less crystal screening time
- Solve otherwise impossible phasing problems from existing data.

Expand your radius of convergence

Cyrus Bench Homology can generate hundreds of high-quality models to run through phasing independently. This works with any crystallography software suite, and can drastically accelerate molecular replacement.

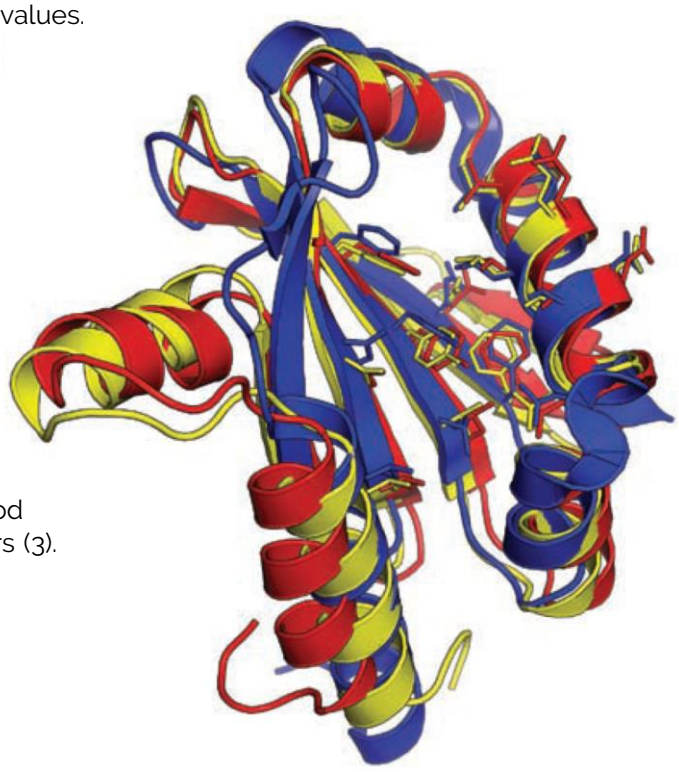
Solve structures from low-resolution datasets

Rosetta scientists collected a set of unsolved phasing problems from leading crystallography labs around the world. 60% of those were solvable using *MR-Rosetta*, the pipeline now available in Cyrus Bench.



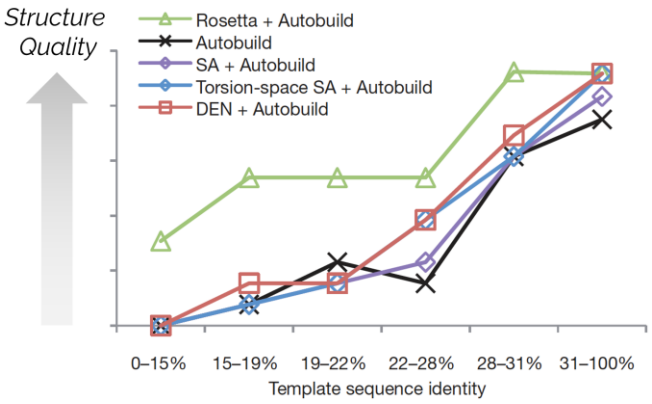
Save weeks of time with better homology models

High accuracy models from Cyrus Bench Homology can solve molecular replacement where a simple homolog structure fails (1). Even when traditional MR succeeds, better models generate lower R-free values.



Solve otherwise impossible structures

Iterative model-building from density, guided by Cyrus Homology Modeling, solves structures in the 3Å resolution range (2). This method solves otherwise impossible structures from expert crystallographers (3).



Accelerate Structure solving: Solve structures from low-resolution datasets

MR-Rosetta in Cyrus can converge to higher map correlations than any other method (3). These higher-quality models can provide a shortcut to structures from lower-quality crystals, or help guide protein engineering during a screen for better crystals (e.g. by removing a flexible loop).

(1) Khatib, F. et al. "Crystal structure of a monomeric retroviral protease solved by protein folding game players." Nature Structural & Molecular Biology 18 1175- 1177 (2011).
(2) DiMaio, F. "Advances in Rosetta structure prediction for difficult molecular-replacement problems". Acta Cryst. Sect. D. vol. D69 2202-2208 (2013).
(3) DiMaio, F. et al. "Improved molecular replacement by density- and energy-guided protein structure optimization". Nature vol. 473, 540–545(2011).