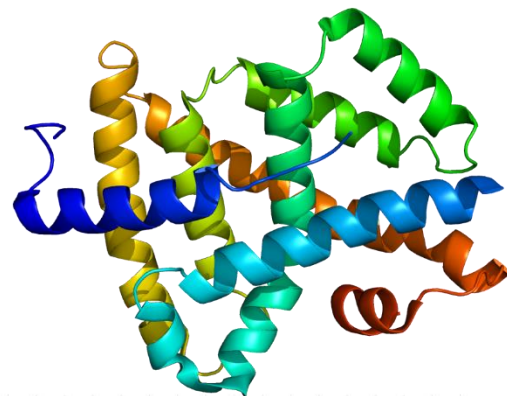


In D3R Grand Challenge 2, our prediction of free energy ranking was ranked 1st for Set 1 (Stage 2)

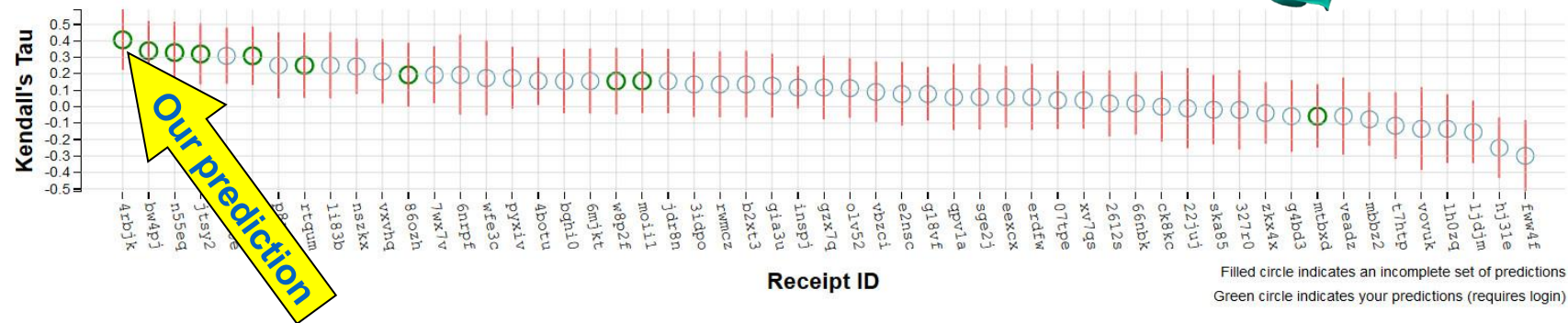
(<https://drugdesigndata.org/php/d3r/gc2/combined/free-energy/index.php?component=443&q=rmsd&set=1>)

Given: Farnesoid X receptor (FXR) and 102 ligands
Tasks: Dock 102 ligands to FXR, and compute their poses, binding free energies and energy ranking



Grand Challenge 2

Free Energy Set 1 (Stage 2) - Kendall's Tau



Free Energy Set 1 (Stage 2) - RMSEc

