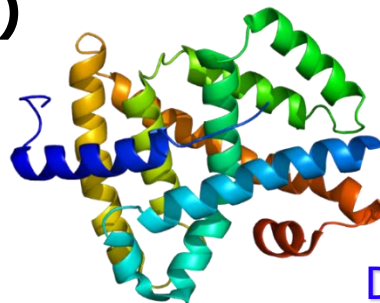


# D3R Grand Challenge 2 (2016-2017)

**Given:** Farnesoid X receptor (FXR) and 102 ligands

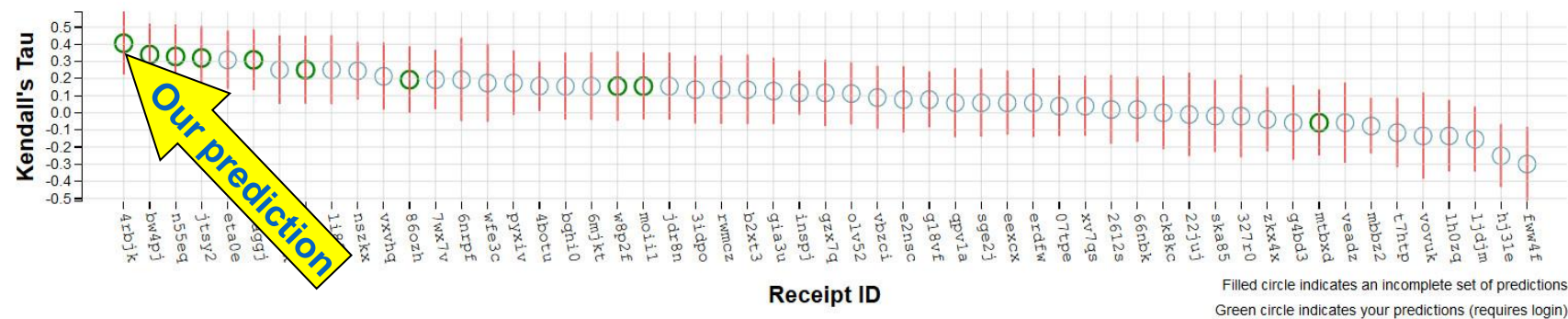
**Tasks:** Dock 102 ligands to FXR, and compute their poses, binding free energies and energy ranking



Dr Duc Nguyen

## Grand Challenge 2

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



## Grand Challenge 2

### Free Energy Set 1 (Stage 1) - RMSD

