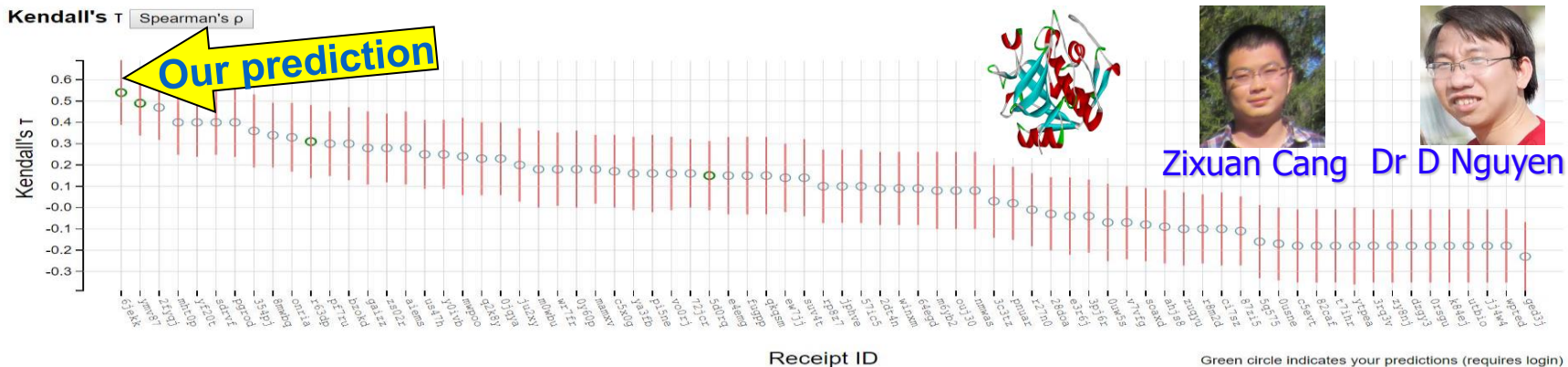


D3R Grand Challenges are a communitywide competition series in computer-aided drug design, with components addressing pose-prediction, affinity ranking, binding free energy, and active/inactive predictions. The most recent competition, D3R Grand Challenge 3, involves Cathepsin S (CatS) and five different kinases, and is separated into five subchallenges, some of which involve multiple protein targets. There was a total of 26 predictive tasks (<https://drugdesigndata.org/about/grand-challenge-3-evaluation-results>).

Our predictions were ranked 1st in 10 of the 26 predictive tasks (see detail at http://users.math.msu.edu/users/wei/Wei_Team.pdf).

Grand Challenge 3 - Affinity Ranking for Cocrystalized Ligands - Cathepsin S (Stage 2)



Grand Challenge 3 - Affinity Ranking For Cocrystalized Ligands - Cathepsin S (Stage 1A)

