

# D3R Grand Challenge 4 (2018-2019)



## Pose Predictions

### BACE Stage 1A

Pose Predictions (Partials)



### BACE Stage 1B

Pose Prediction (Partials)



## Affinity Predictions

### Cathepsin Stage 1

Combined Ligand and Structure Based Scoring



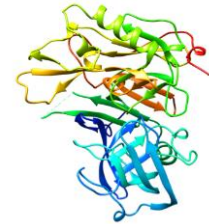
Dr. Kaifu Gao Dr. D Nguyen

Ligand Based Scoring (No participation)

Structure Based Scoring



Free Energy Set



### BACE Stage 1

Combined Ligand and Structure (No participation)

Ligand Based Scoring (Partials) (No participation)

Structure Based Scoring (Partials) (No participation)

Free Energy Set (No participation)

### BACE Stage 2

Combined Ligand and Structure

Ligand Based Scoring (No participation)

Structure Based Scoring (Partials)

Free Energy Set

