

D3R Grand Challenge 4 (2018-2019)



Pose Predictions

BACE Stage 1A

[Pose Predictions \(Partials\)](#)



BACE Stage 1B

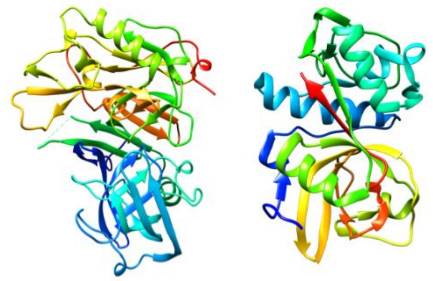
[Pose Prediction \(Partials\)](#)



Affinity Predictions

Cathepsin Stage 1

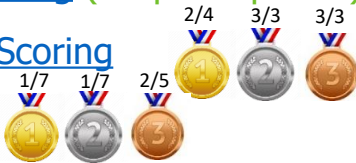
[Combined Ligand and Structure Based Scoring](#)



[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](#)



D3R Grand Challenge 3 (2017-2018)

Pose Prediction

Cathepsin Stage 1A

[Pose Predictions \(partials\)](#)

Affinity Rankings excluding Kds > 10 μM

Cathepsin Stage 1

[Scoring \(partials\)](#)

[Free Energy Set](#)

VEGFR2

[Scoring \(partials\)](#)

JAK2 SC3

[Scoring](#)

[Free Energy Set](#)



Active / Inactive Classification

VEGFR2

[Scoring \(partials\)](#)

JAK2 SC3

[Scoring](#)

[Free Energy Set](#)



Affinity Rankings for Cocrystallized Ligands

Cathepsin Stage 1

[Scoring \(partials\)](#)

[Free Energy Set](#)



Cathepsin Stage 1B

[Pose Prediction](#)

Cathepsin Stage 2

[Scoring \(partials\)](#)

[Free Energy Set](#)

JAK2 SC2

[Scoring \(partials\)](#)

TIE2

[Scoring](#)

[Free Energy Set 2](#)



JAK2 SC2

[Scoring \(partials\)](#)

TIE2

[Scoring \(partials\)](#)

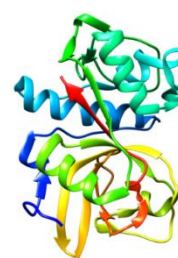
[Free Energy Set 1](#)



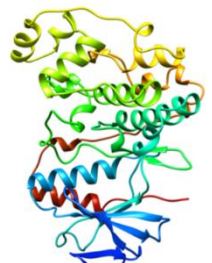
Cathepsin Stage 2

[Scoring \(partials\)](#)

[Free Energy Set](#)



Cathepsin 5



Kinase: p38-α

p38-α

[Scoring](#)

ABL1

[Scoring \(partials\)](#)



p38-α

[Scoring \(partials\)](#)

ABL1

[Scoring \(partials\)](#)

D3R Grand Challenge 2 (2016-2017)

Stage 1

[Pose Predictions \(partials\)](#)

[Scoring \(partials\)](#)

[Free Energy Set 1 \(partials\)](#)

[Free Energy Set 2 \(partials\)](#)

Stage 2

[Scoring \(partials\)](#)

[Free Energy Set 1 \(partials\)](#)

[Free Energy Set 2 \(partials\)](#)

