

Wei Team's Performance at D3R Grand Challenge 3 (2017-2018)

Pose Prediction

Cathepsin Stage 1A

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

Affinity Rankings excluding Kds > 10 μ M

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 Cocrystalized Ligands

Cathepsin Stage 1

[Scoring \(partials\)](#)



[Free Energy Set](#)

Cathepsin Stage 1B

[Pose Prediction](#)

Affinity Rankings excluding Kds > 10 μ M

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](#)

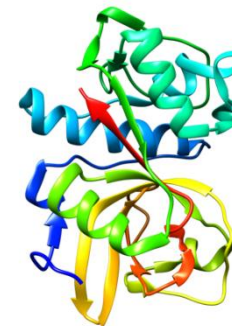


Cathepsin Stage 2

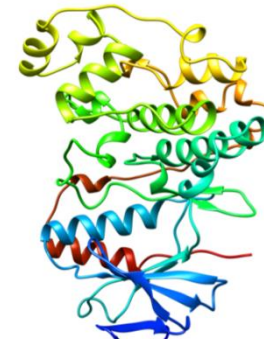
[Scoring \(partials\)](#)



[Free Energy Set](#)



Cathepsin S



Kinase: p38-α

p38-α

[Scoring](#)

ABL1

[Scoring \(partials\)](#)



p38-α

[Scoring \(partials\)](#)

ABL1

[Scoring \(partials\)](#)



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