Welcome to the Drug Design Data Resource Webinar

27 March 2017
Opening Remarks

Overview of the Drug Design Data Resource (D3R)

Webinar Agenda

Webinar Rules of Engagement
D3R: NIH-U01 Resource, Unique Purpose

Central Goal: Utilize previously unpublished datasets as benchmarks for developers of protein-ligand modeling technologies

Synergy with Public Databases: Public release of more industrial crystal structures and affinity data

Broader Goals: Utilize blinded datasets to drive improvement of all CADD technologies and to foster training and dissemination of methods

More predictive CADD methods benefit everyone!
Scientific Advisory Board

Aled Edwards  
SGC

Charles Grimshaw  
Takeda

Marti Head  
GSK

David Mobley  
UC Irvine

John Moult  
U Maryland

Adrian Roitberg  
U Florida

Torsten Schwede  
Biozentrum, Basel

Martin Stahl  
Roche
D3R’s Role & Vision

- Unpublished Datasets
- Improved CADD Methods & Workflows
- Workforce Training, Education
- Blinded Challenges
- CADD Community

D3R’s Ultimate Goal to Help Drive Development of New & Safer Medications
We give contestants **63 hours** to predict next week’s new PDB additions

Our program scans the PDB pre-release sequences for entries which:
- Are bound to a druglike molecule
- Have 95%+ homology to an existing PDB structure
- Consist of just one sequence

For each eligible “target” sequence, we select up to 5 “candidate” PDB structures for contestants to perform cross-docking.

[https://drugdesigndata.org/about/celpp](https://drugdesigndata.org/about/celpp)
Find out more @ http://drugdesigndata.org
Find out more @ http://drugdesigndata.org

We’ve added...

• Publications
Find out more @ http://drugdesigndata.org

We’ve added...

- Presentations
Find out more @ http://drugdesignndata.org

We’ve added...

• What we’ve learned
Find out more @ http://drugdesigndata.org

We’ve added...

- Assessment scripts on GitHub
Webinar Goals & Agenda

• Present overview & results for 2016 Protein-Ligand challenge

• Present overview & results for Grand Challenge 2

• Discuss x-ray refinement challenges
Webinar Rules of Engagement

• We will follow the schedule timing closely.
• The webinar will be recorded.
• All questions will be handled via a moderated Q&A session
  – Q&A from 11:55AM – 12:25PM PT **ONLY**
  – As the webinar proceeds, please send your written questions to the D3R team through the Question box
  – Question format should include the name of the speaker to whom you are asking the question
    • SPEAKER NAME: question
  – D3R will collect questions and read them to the group during the Q&A session