



**Drug Design  
Data Resource**

## **D3R Workshop Agenda**

### **Wednesday, March 9 @ La Jolla Shores Hotel**

6:00 – 8:00 PM Check-in and Welcome Reception @ La Jolla Shores Hotel

### **Thursday, March 10 @ UCSD Faculty Club**

8:15 AM Shuttle(s) from La Jolla Shores Hotel to UCSD Faculty Club

8:30 AM Arrivals – Continental Breakfast

9:00 – 9:40 AM Vicki Feher/Mike Gilson/Rommie Amaro, UCSD, D3R  
“Welcome and Introduction to D3R”

9:40 – 9:45 AM Peter Preusch, NIH NIGMS

9:45 – 10:15 AM Heather Carlson, University of Michigan  
“CSAR Lessons Learned”

10:15 – 10:30 AM BREAK

10:30 – 11:15 AM Pat Walters, Vertex  
“Evaluation Overview of Grand Challenges”

11:15 – 11:45 AM Antonia Mey, University of Edinburgh  
“Successes and Failures of Docking and Relative Free Energy  
Calculations on HSP90”

11:45 – 12:45 PM LUNCH

12:45 – 1:15 PM Xinjun Hou, Pfizer  
“Potency Prediction: What Do Pharma Practitioners Wish For?”

1:15 – 1:45 PM Xiaoqin Zou, University of Missouri – Columbia

1:45 – 2:15 PM David Mobley, UC Irvine  
“SAMPL5 Overview”

2:15 – 2:45 PM BREAK

2:45 – 3:15 PM John Chodera/Bas Rustenburg, SKMCC  
Bruce Gibb, Tulane University

3:15 – 3:45 PM Andreas Klamt, COSMOlogic  
“Prediction Distribution Coefficients and with COSMO-RS: General Performance and Special Issues with Extreme Ends”

3:45 – 4:15 PM Emilio Gallicchio, CUNY Brooklyn  
“A Combined Hydration Site Analysis and Implicit Solvation Alchemical Approach For the Modeling of Host-Guest Binding”

4:15 – 6:00 PM Poster Session & Liquid Refreshments

6:00 – 7:30 PM DINNER @ Faculty Club

7:30 PM Shuttles back to La Jolla Shores Hotel

**Friday, March 11 @ UCSD Faculty Club**

8:15 AM Shuttle(s) from La Jolla Shores Hotel to UCSD Faculty Club

8:30 AM Arrivals – Continental Breakfast

9:00 – 10:00 AM D3R Community Feedback Discussion  
Datasets – Attributes, Types, Size, Number/Challenge  
Challenges & Workshops - Timing, Type, Frequency  
Challenge Evaluations – Metrics, Statistics & Website posting  
CELPP/Grand Challenges/SAMPL Feedback

10:00 – 10:30 AM Torsten Schwede, University of Basel  
“Integration of CAMEO with CELPP and International Collaborations”

10:30 – 10:45 AM Group Photo

10:45 – 11:00 AM BREAK

*PROTEIN LIGAND TRACK – morning*

11:00 – 11:30 AM Zhaofeng Ye, University of Pittsburgh

11:30 – 12:00 PM Nanjie Deng, Temple University  
“Large Scale Binding Free Energy Screening of HSP90 Ligands”

12:00 – 12:30 PM David Koes, University of Pittsburgh

*SAMPL TRACK – morning*

11:00 – 11:30 AM Frank Pickard,  
TBA

11:30 – 12:00 PM Stefano Bosiso,  
TBA

12:00 – 12:30 PM Stefan Kast,  
TBA

12:30 – 1:30 PM LUNCH

*PROTEIN LIGAND TRACK – afternoon*

1:30 – 2:00 PM Stephen Burley, Rutgers UCSD RCSB

2:00 – 2:30 PM Hanneke Jansen, Novartis  
“TDT & D3R: progress towards fully enabled state-of-the-art  
workflows for drug discovery”

2:30 – 3:00 PM Vicki Feher, UCSD, D3R  
“Upcoming Challenges”

*SAMPL TRACK – afternoon*

1:30 – 2:00 PM Florintina Tofoleanu,

2:00 – 2:30 PM Kenny Merz,

2:30 – 3:00 PM Ulf Ryde,

3:00 – 3:30 PM BREAK

3:30 – 4:15 PM Cathy Peishoff, GlaxoSmithKline, retired  
“Computational chemistry looking forward: how can we as a  
community improve our field?”

4:15 – 4:30 PM Terry Stouch, JCAMD  
“JCAMD Special Issues Publication Details”

4:30 – 4:45 PM Wrap-up & Conclusions

5:00 PM Workshop Concludes; Shuttles back to La Jolla Shores Hotel