

Wednesday, February 21 at La Jolla Shores Hotel

6:00-8:00 PM Check-in and Welcome Reception at La Jolla Shores Hotel—La Jolla Room + Patio

Thursday, February 22 at Scripps Institute of Oceanography Forum (SIO)

8:15 AM Walk or Ride Share from La Jolla Shores Hotel to SIO
Breakfast on-site

9:00-9:30 AM *Welcome and D3R Update* —
Mike Gilson and Rommie Amaro, D3R, UC San Diego

9:30-9:40 AM *NIH Perspective* — Peter Lyster, NIGMS, NIH

9:40-10:15 AM *Evaluation Overview of GC3* — Mill Lambert & Neysa Nevins, GSK

10:15-10:30 AM BREAK

10:30-10:50 AM *GC3 Participant Talk 1* — Maxim Totrov, MolSoft

10:50-11:10 AM *GC3 Participant Talk 2* — Guo-wei Wei, Michigan State

11:10-11:30 AM *GC3 Participant Talk 3* — David Koes, University of Pittsburgh

11:30-11:50 AM *GC3 Participant Talk 4* — Ashutosh Kumar, RIKEN

11:50-12:10 PM *Open Discussion on Evaluation Metrics* — D3R Moderator

12:10-1:30 PM LUNCH AT SIO

1:30-1:40 PM *SAMPL6 Intro* — John Chodera, MSKCC

1:40-1:55 PM *SAMPL6 Host-Guest Intro and Overview* — Andrea Rizzi, MSKCC

2:00-2:15 PM *SAMPL6 Host-Guest Participant 1* — Michail Papadourakis, Edinburgh (video presentation)

2:15-2:30 PM *SAMPL6 Host-Guest Participant 2* — Marie Laury, Washington University

2:30-2:50 PM *SAMPLing Challenge Overview and Results* — Andrea Rizzi, MSKCC

2:50-3:05 PM BREAK

3:05-3:25 PM *SAMPL6 pKa Intro and Overview* — Mehtap Isik, MSKCC

3:25-3:40 PM *SAMPL6 Participant 1* — Samarjeet Prasad

3:40-3:55 PM *SAMPL6 Participant 2* — Qiao Zeng, NIH

3:55-4:10 PM *SAMPL6 Participant 3* — Marvin Waldman, Simulations Plus

4:15-6:00 PM Poster Session, Sunset (5:30PM) with Snacks and Liquid Refreshments

6:00-7:30 PM DINNER ON THE PATIO AT SIO

7:30 PM Walk or Ride Share Back to La Jolla Shores Hotel

Friday, February 23 at Scripps Institute of Oceanography Forum (SIO)

8:15 AM	Walk or Ride Share from La Jolla Shores Hotel to SIO Breakfast on-site
9:00-9:10 AM	<i>Introduction to Day 2</i> — Mike Gilson and Rommie Amaro
9:10-9:40 AM	<i>A Longitudinal View of the Grand Challenges</i> — Pat Walters, Relay Therapeutics
9:40-10:00 AM	<i>A Longitudinal View of the SAMPL Challenges</i> — David Mobley, UC Irvine
10:00-10:20 AM	<i>D3R Lessons Learned</i> — Alexandre Bonvin, Utrecht U (Video Conference)
10:20-10:40 AM	<i>SAMPL Lessons Learned</i> — Bogdan Iorga, ICSN, CNRS
10:40-11:00 AM	BREAK
11:00-11:20 AM	<i>Continuous Evaluation of Ligand-Protein Predictions (CELPP)</i> - Jeff Wagner, D3R, UC San Diego
11:20-11:40 AM	<i>GC and CELPP: Workflows and Insights</i> —Xiaoqin Zou, U. Missouri
11:40-12:00 AM	<i>MoISSI and Workflows</i> — John Chodera, Memorial Sloan Kettering
12:00-12:30 PM	<i>Open Discussion on Enabling Adoption of Workflows</i>
12:30-1:30 PM	LUNCH AT SIO
1:30-1:45 PM	Group Photo
1:45-2:00 PM	<i>Upcoming D3R and SAMPL Challenges</i> —Mike Gilson, Rommie Amaro, David Mobley
2:00-2:10 PM	<i>GC3 and SAMPL6 Special Issues</i> — Terry Stouch, Journal of Computer Aided Molecular Design
2:10-3:15 PM	D3R Community Feedback Discussion <i>Datasets—Attributes, Types, Size, Number/Challenge Challenges and Workshops—Timing, Type, Frequency Challenge Evaluations—Website Posting Future funding / support of blinded prediction challenges</i>
3:15- 3:30 PM	<i>Wrap-up and Conclusions</i> —Mike Gilson and Rommie Amaro
3:30 PM	Workshop Concludes
4:00-5:00 PM	SAB Meeting (Closed Session)
5:00-5:30 PM	SAB Session with D3R PIs
6:00 PM	SAB Dinner at La Jolla Shores Hotel

