Workshop I: Design of Drugs and Chemicals that Influence Biology

Monday April 4, 2011

8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*

9:00–9:15 *Welcome and Opening Remarks*

9:15–10:45 **William Jorgensen** (Yale University)
Overview of Computer-Aided Drug Discovery

10:45–11:15 *Break*

11:15–12:05 **Ursula Roethlisberger** (École Polytechnique Fédérale de Lausanne (EPFL))
Integrating Computational Methods to Retrofit Enzymes to Synthetic Pathways

12:15–2:00 *Lunch (on your own)*

2:00–2:50 **Rich Friesner** (Columbia University)
Incorporating the Effects of Water Structure, Ligand Strain, and Protein Reorganization into the Prediction of Protein-Ligand Binding Affinity

3:00–3:30 *Lightning Poster Presentations*

3:30–4:00 *Break*

4:00–4:50 **Charles Brooks** (University of Michigan)
Methods and molecules for interrogation and control of biological processes

5:00–7:00 *Reception and Poster Session (Hosted by IPAM)*

Tuesday April 5, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Dimitris Agrafiotis** (Johnson & Johnson Pharmaceutical Research & Development, LLC)
Self-organizing algorithms in data mining and computational drug design

10:00–10:15 *Break*

10:15–11:05 **Anastassia Alexandrova** (University of California, Los Angeles (UCLA))
Multi-scale approaches in description and design of enzymes

11:15–11:30 *Break*

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11:30–12:20 **Maria Ramos** (University of Porto)
Computational Enzymology and Drug Design

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Jiali Gao** (University of Minnesota, Twin Cities)
Quantum Mechanical Approaches to Biomolecular Simulations: From a Single Electron to Fully Solvated Proteins

3:30–4:00 *Break*

4:00–4:50 **Robert Rizzo** (SUNY Stony Brook)
Molecular Dynamics and Docking Approaches to Characterize Drug Resistance and Assist Lead Discovery

Wednesday April 6, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Brian Kuhlman** (University of North Carolina)
Computational Design of Protein Structures and Interfaces

10:00–10:15 *Break*

10:15–11:05 **Amy Keating** (Massachusetts Institute of Technology)
Modeling and Designing Protein-Protein Interaction Specificity

11:15–11:30 *Break*

11:30–12:20 **Elisa Fadda** (National University of Ireland, Galway)
Quantifying the standard binding free energy of highly conserved water molecules in proteins binding sites: how important is the choice of water model?

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Kendall Houk** (University of California, Los Angeles (UCLA))
Design of Enzymes for Non-natural Reactions

3:30–4:00 *Break*

4:00–4:50 **William Jorgensen** (Yale University)
Recent Progress on Discovery of Drug Candidates

Thursday April 7, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Cecilia Clementi** (Rice University)
Prediction of protein functional states by multi-resolution protein modeling

10:00–10:15 *Break*

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10:15–11:05 **Jeffery Saven** (University of Pennsylvania)
Engineering structure and function with theoretical protein design

11:15–11:30 *Break*

11:30–12:20 **William DeGrado** (University of Pennsylvania)
De novo protein design

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Robert Glen** (University of Cambridge)
Drug discovery: a multi-objective optimization problem

3:30–4:00 *Break*

4:00–4:50 **Gagerin Papoian** (University of Maryland)
Exploring Protein Energy Landscapes with Simulations: Applications to Histone Tails and Allosteric Transitions

Friday April 8, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Michele Parrinello** (University of Lugano)
Well-tempered metadynamics: theory and applications

10:00–10:15 *Break*

10:15–11:05 **Shaomeng Wang** (University of Michigan)
Design of small-molecule drugs to target protein-protein interactions in the apoptosis pathways

11:15–11:30 *Break*

11:30–12:20 **Alexandre Tkatchenko** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Weak van der Waals interactions: How well can we treat them and how relevant are they for peptides and proteins?

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Andrej Sali** (University of California, San Francisco (UCSF))
Virtual Ligand Screening Against Comparative Protein Structure Models

3:30–4:00 *Break*

4:00–4:50 **Parag Mallick** (Stanford University)