**Molecular Recognition**

Organizers: David Mobley, Piotr Setny

TSRC Hosts: Nana Naisbitt, 970-708-0004 and Rory Sullivan, 970-708-4542

Telluride Intermediate School, 725 W Colorado

Unless otherwise noted, all events are at Telluride Intermediate School.

**Sunday, August 1o, 2014:**

* 6:00 – 8:00pm: Meet and greet, cash bar at Arroyo Wine Bar Gallery at 220 E. Colorado Avenue. Family and guests welcome. TSRC staff member present to pass out badges and answer any questions

**Monday, August 11, 2014:**

(session chair David Mobley)

* 8:00: Breakfast on tented soccer field of school
* 8:30-9:15: “Beyond Affinity: How Thermodynamic and Structural Analysis Provide Deeper Insights into Molecular Recognition in Protein-Ligand Complex Formation”, Gerhard Klebe
* 9:15-10:00: “Free energy calculations in prospective drug discovery”, Robert Abel
* 10:00-10:30: Coffee break
* 10:30-11:15: “Molecular recognition in protein-protein and protein-ligand interactions”, Bert de Groot
* 11:15-12:00: “Modeling intermolecular forces in molecular recognition”, Qiantao Wang
* 12:00-13:30: Lunch on tented soccer field of school
* 17:00-17:45: “MD-based ensemble docking in 'difficult' targets: looking for the magic snapshot”, Jerome Baudry
* 17:45-18:30: The Dark Energy of Proteins Comes to Light: Motion and Conformational Entropy in Molecular Recognition by Proteins”, Joshua Wand

**Tuesday, August 12, 2014:**

(session chair Piotr Setny)

* 8:30-9:15: “Interesting examples of entropy and protein evolution in the dynein motor protein complex”, Justin Hall
* 9:15-10:00: “FEP-Guided Lead Optimization”, Bill Jorgensen
* 10:00-10:30: Coffee break
* 10:30-11:15: “Exploring the drug binding ensemble with simulations visiting multiple thermodynamic ensembles”, Michael Shirts
* 11:15-12:00: “Computational study of the selectivity of BMP type-I receptor inhibitors”, Lyna Luo
* 12:00-13:30: Lunch on tented soccer field of school
* 14:00-16:30: Optional group hike
* 18:00-19:15: Town Talk at Conference Center in Mountain Village

**Wednesday, August 13, 2014:**

(session chair David Minh)

* 8:00: Breakfast on tented soccer field of school
* 8:30-9:15: “Multivalent interactions in the adhesion between biological surfaces:  A simple model and its application to influenza infection”, Huafeng Xu
* 9:15-10:00: “Bridging the gap between explicit and implicit solvent models: a novel approach to modeling of biomolecular hydration”, Piotr Setny
* 10:00-10:30: Coffee break
* 10:30-11:15: “Rate constants and mechanisms of protein-ligand binding”, Huan-Xiang Zhou
* 11:15-12:00: “Exploring the binding of benzamidine to trypsin and of barstar to barnase with Markov state models”, Nuria Plattner
* 12:00-13:30: Lunch on tented soccer field of school
* 13:30-dinner: Free
* 18:00-21:00 Picnic dinner on tented soccer field of school (Family and guests welcome free of charge)

**Thursday, August 14, 2014:**

(session chair Huafeng Xu)

* 8:00: Breakfast on tented soccer field of school
* 8:30-9:15: “Calculations of free energy, entropy and enthalpy, for host-guest and protein systems”, Michael Gilson
* 9:15-10:00: “Efficient free energy calculation methods using molecular dynamics simulations”, Zhixiong Lin
* 10:00-10:30: Coffee break
* 10:30-11:15: “What we've learned about molecular recognition from binding free energy calculations”, David Mobley
* 11:15-12:00: “Using Theory to Reconcile Experiment: The Search for Certainty in an Uncertain World”, Alan Mark
* 12:00-13:30: Lunch on tented soccer field of school
* 17:00-17:45: “Binding Free Energies on a Large Scale, Replica Exchange, and Solvent Models”, Ron Levy
* 17:45-18:30: “Binding free energy, enthalpy and entropy – from a toy system to the real thing”, Chris Oostenbrink

**Friday, August 15, 2014:**

(session chair Michael Gilson)

* 8:30-9:15: “Protein-ligand binding free energies using implicit ligand theory,” David Minh
* 9:15-10:00: “Considering protein flexibility in ligand discovery”, Marcus Fischer
* 10:00-10:30: Coffee break
* 10:30-11:15: “Finding novel anticancer and antibacterial drug leads using CADD - Farnesyl diphosphate synthase (FPPS) and undecaprenyl diphosphate synthase (UPPS) inhibitors from in silico screening”, Steffen Lindert
* 11:15-12:00: “Tackling complex problems in small molecule recognition using computation and automated biophysical experiment”, Sonya Hanson