

# Biophysics, Structural and Computational Biology

2015 Retreat  
October 5, 2015

## Poster Presentations

- 1) **Improving the Amber RNA Force Field**  
Asaminew H. Aytenfisu, Aleksandar Spasic, Alan Grossfield, Harry Stern and David H. Mathews
- 2) **Structural/Thermodynamic Investigation of RNA Internal Loops Flanked by GU Base Pairs**  
Kyle Berger, Scott Kennedy and Douglas Turner
- 3) **Bio-Engineered Photocatalytic Systems for Solar Hydrogen Generation**  
Saikat Chakraborty, Banu Kandemir and Kara L. Bren
- 4) **Expression of HIV Envelope Glycoprotein at the Yeast Cell Surface for Vaccine Development**  
Sara Connelly, Elizabeth Mathew, Hong Zhu, Mark Sullivan and Mark Dumont
- 5) **Nucleosome Directed Folding of Linker Histone C-terminal Domain**  
He Fang, Tamara L. Caterino and Jeffrey J. Hayes
- 6) **Using Yeast to Determine the Binding Sites of Small Molecule Modulators of G $\beta$  Signaling**  
Isaac Fisher, Sara Connelly, Mark Dumont and Alan Smrcka
- 7) **Global Analysis of Autophagic Flux in Human Cells**  
Tian Zhang and Sina Ghaemmaghami
- 8) **The URM Mass Spectrometry Resource Facility**  
Sina Ghaemmaghami, Kevin Welle and Jennifer Hryhorenko
- 9) **Improving Nucleic Acid Design Using Biased Sequence Initialization**  
Mohammad Kayedkhordeh, Stanislav Bellaousov and David H. Mathews
- 10) **Initiation Factor 2 Stabilizes the Ribosome in a Semi-Rotated Conformation during Translation Initiation**  
Clarence Ling & Dmitri N. Ermolenko
- 11) **Center for Integrated Research Computing**  
Brendan Mort, Will DiGrazio, Jonathan Carroll-Nellenback, Baowei Liu, Harry Stern, Rob Lemley, Carl Schmidtman and Chris Wilson

# Biophysics, Structural and Computational Biology

2015 Retreat  
October 5, 2015

## Poster Presentations

- 12) **Dynamic Ligand-Protein Interactions Alter Rhodopsin's Conformational Ensemble: Simulations of Rhodopsin and Opsin**  
Letty Salas-Estrada, Nicholas Leioatts, Tod D. Romo, Shairy Azmy Danial and Alan Grossfield
- 13) **Following Structural Dynamics of Elongation Factor G During Ribosomal Translocation**  
Enea Salsi, Elie Farah, Jillian Dann, Zoe Netter and Dmitri N. Ermolenko
- 14) **Characterizing Expression of Type Two Voltage Gated Calcium Channels in Rat Sympathetic Ganglia**  
Mallory Scott and Paul Kammermeier
- 15) **Modeling Sieving Behavior in Silicon Nanomembranes Across Variable Concentrations and Average Pore Sizes**  
Karl J. P. Smith, Joshua D. Winans and James McGrath
- 16) **Examining the Unusual Conformation of the GAGU Internal Loop Using Molecular Dynamics**  
Aleksandar Spasic, Laura Needham and David H. Mathews
- 17) **Understanding the Function of the Cyclic Antifungal Lipopeptide Fengycin Using All-Atom Simulation**  
Sreyoshi Sur, Tod D. Romo and Alan Grossfield
- 18) **Benchmark of AMBER ff12SB Force Field by Comparison of Estimated Hairpin Loop Folding Stabilities to Experiments**  
Zhen Tan, Aleksandar Spasic, Letty Salas-Estrada, Debapratim Dutta and David H. Mathews
- 19) **Investigation of the Mechanism of Antimicrobial Lipopeptides using Coarse-Grained Molecular Dynamics Simulations**  
Dejun Lin and Alan Grossfield