

# The Computational Structural Biology Workshop (CSBW 2017)

Co-located with ACM BCB, Boston MA, August 20, 2017

Venue: CONCEPT

08:30-08:45	<b>Opening and Welcome Remarks</b> Chairs: Nurit Haspel, Amarda Shehu, and Kevin Molloy
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<b>Session 1</b> <b>Session Chair: Stephanie Mason</b>	
08:45-09:10	Title: <i>Automated Protein Chain Isolation from 3D Cryo-EM Data and Volume Comparison Tool</i> Authors: Michael Nissenson and Dong Si
09:10-09:35	Title: <i>Gaussian Mixture Models with Constrained Flexibility for Fitting Tomogram Tiltseries</i> Authors: Kasra Manavi, Sahba Tashakkori, and Lydia Tapia
09:35 - 10:00	Title: <i>Geometry Analysis for Protein Secondary Structures Matching Problem</i> Authors: Kamal Al Nasr, Feras Yousef, Christopher Jones, and Ruba Jebril

10:00-10:30	<b>Coffee Break</b>
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<b>Session 2</b> <b>Session Chair: Michael Nissenson</b>	
10:30-10:55	Title: <i>Analysis of <math>\beta</math>-strand twist from the 3-dimensional Image of a protein</i> Authors: Tunazzina Islam, Michael Poteat, and Jing He
10:55-11:20	Title: <i>A Graph Based Method for the Prediction of Backbone Trace from Cryo-EM Density Maps</i> Authors: Peter Collins and Dong Si
11:20-11:45	Title: <i>Investigating Rigidity Properties of Protein Cavities</i> Authors: Stephanie Mason, Brian Chen, and Filip Jagodzinski

12:00-13:30	<b>Lunch (on your own)</b>
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<b>Session 3</b>	
<b>Session Chair: Peter Collins</b>	
13:50-14:15	Title: <i>ProMuteHT: A High-throughput Compute Pipeline for Generating Protein Mutants in silico</i> Authors: Erik Andersson and Filip Jagodzinski
14:15-14:40	Title: Statistical Analysis of Computed Energy Landscapes to Understand Dysfunction in Pathogenic Protein Variants Authors: Wanli Qiao, Tatiana Maximova, Erion Plaku, and Amarda Shehu
14:40-15:05	Title: Geometric Sampling Framework for Exploring Molecular Walker Energetics and Dynamics Authors: Bruna Jacobson, Jon David, Mitch Malone, Kasra Manavi, Susan R. Atlas and Lydia Tapia
15:05-15:30	Title: Evolving Conformation Paths to Model Protein Structural Transitions Authors: Emmanuel Sapin, Kenneth De Jong, and Amarda Shehu

15:30-16:00	<b>Coffee Break</b>
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<b>Session 4</b>	
<b>Session Chair: Bruna Jacobson</b>	
16:00-16:25	Title: <i>Computational Modeling of pH-dependent gp120-CD4 Interactions in Founder and Chronic HIV Strains</i> Authors: Jonathan Howton and Joshua Phillips
16:25-16:50	Title: <i>Feature-Based and String-Based Models for Predicting RNA-Protein Interaction</i> Authors: Donald Adjero, Jun Tan, and Jie Lin
16:50-17:15	Title: <i>Ranking Protein-Protein Binding Using Evolutionary Information</i> Authors: Roshanak Farhoodi, Bahar Akbal-Delibas, and Nurit Haspel

17:15-17:20	<b>Closing Remarks</b> Chairs: Nurit Haspel, Amarda Shehu, and Kevin Molloy
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