

# 2015 Workshop on Computational Structural Bioinformatics

Monday, Nov 9, 2015

Hyatt Regency, Bethesda M.D. — Room: Judiciary Suite

Co-chairs: Jing He, Amarda Shehu, Nurit Haspel, Brian Chen

<b>9:00 – 10:30 Session 1</b>
Session Chair: Jing He    Co-chair: Irina Hashmi
<b>Opening Remarks</b>
Roshanak Farhoodi, Bahar Akbal-Delibas and Nurit Haspel. <i>Accurate Prediction of Docked Protein Structure Similarity Using Neural Networks and Restricted Boltzmann Machines</i>
Jing He, Stephanie Zeil, Hussam Hallak, Kele McKaig, Julio Kovacs and Willy Wriggers. <i>Comparison of an Atomic Model and Its Cryo-EM Image at the Central Axis of a Helix</i>
<b>9:40-10:40 Keynote Talk</b>
Willy Wriggers. <i>Multi-Scale Modeling and Visualization of Macromolecular Architecture</i>
<b>10:40-11:00 Coffee Break, poster setup</b>
<b>11:00-12:20 Session 2</b>
Session Chair: Brian Chen    Session Co-chair: Brian Godshall
Rachel Okun and Brian Chen. <i>A Statistical Model of Electrostatic Isopotential Variation in Serine Protease Binding Cavities</i>
Siqi Sun, Jianzhu Ma, Sheng Wang, and Jinbo Xu. <i>Predicting Diverse M-best Protein contact maps</i>
Anastasia Novinskaya, Didier Devaurs, Mark Moll and Lydia Kavraki. <i>Improving Protein Conformational Sampling by Using Guiding Projections</i>
Wen Cheng and Changhui Yan. <i>Mining Graph Patterns in the Protein-RNA Interfaces</i>
<b>12:30-13:30 Lunch (on your own)</b>
<b>13:30-14:50 Session 3</b>
Session Chair: Amarda Shehu    Session Co-chair: Stephanie Zeil
Ziyi Guo and Brian Chen. <i>Predict Protein-Ligand Binding Specificity Based on Ensemble Clustering</i>
Yang Li and Tetsuo Shibuya. <i>Malphite: A Convolutional Neural Network and Ensemble Learning Based Protein Secondary Structure Predictor</i>
Sara E. Hernández-Ayón and Carlos A. Brizuela. <i>Designing Rotamer Libraries Based on Pairs of Consecutive Residues: A Preliminary Analysis</i>
Bijan Afsari, Jin Seob Kim and Gregory S. Chirikjian. <i>Cross-Validation of Data in SAXS and Cryo-EM</i>

**14:50-16:00 Poster Session, (Coffee: 15:30-16:00)**

**16:00-16:30 Session 4**

Session Chair: Nurit Haspel Session Co-chair: Roshanak Farhoodi

Masood Zamani and Stefan Kremer, *A Multi-stage Protein Secondary Structure Prediction System Using Machine Learning and Information Theory*

**Closing Remarks**

**Speaking times:**

17 minutes presentation+ 3 minutes for questions. Additional discussion is the best to carry out during the poster session. Everyone is encouraged to take a poster. It does not have to look nice. You can bring a copy of your presentation slides if you want.