

# 2012 Workshop on Computational Structural Bioinformatics

Thursday, October 4, 2012 — Hyatt Regency, Philadelphia — Room: Gb-A  
Co-Chairs: Jing He, Amarda Shehu, Nurit Haspel, Brian Chen

<b>8:30 – 10:10 Session 1</b>
Session Chair: Jing He Session Co-chair: Andrew McKnight
<b>Opening Remarks</b>
Bahar Akbal-Delibas and Nurit Haspel, <i>Refining Multimeric Protein Complexes Using Conservation, Electrostatics and Probabilistic Selection</i>
Ibrahim Al-Blawi, Marc Vaisset, Thierry Siméon, and Juan Cortés, <i>Coarse-grained elastic networks, normal mode analysis and robotics-inspired methods for modeling protein conformational transitions</i>
Thomas Evangelidis, Li Xie, Philip Bourne, and Lei Xie, <i>An integrated workflow for proteome-wide off-target identification and polypharmacology drug design</i>
Jim Havrilla and Ahmet Saçan, <i>Meta-analysis of Protein Structural Alignment (short)</i>
Lauro Galvão, Luiz Nunes, Pablo Moscato, and Heitor Lopes, <i>A New Greedy Heuristic for 3DHP Protein Structure Prediction With Side Chain (short)</i>
<b>10:10-10:20 Coffee Break, poster setup</b>
<b>10:20-11:50 Session 2</b>
Session Chair: Brian Chen Session Co-chair: Brian Godshall
Ankur Dhanik, John McMurray, and Lydia Kavraki, <i>AutoDock-based incremental docking protocol to improve docking of large ligands</i>
Andrew McKnight, Kamal Al Nasr, Dong Si, Andrey Chernikov, Nikos chrisochoides, and Jing He, <i>CryoEM Skeleton Length Estimation using a Decimated Curve</i>
Majid Masso, <i>Knowledge-Based Scoring Function Derived from Atomic Tessellation of Macromolecular Structures for Prediction of Protein-Ligand Binding AffinityX</i>
Masood Zamani and Stefan C. Kremer, <i>Protein Secondary Structure Prediction Using Support Vector Machines and a Codon Encoding Scheme (short)</i>
<b>11:40-12:30 poster session 1</b>
<b>12:30-1:30 Lunch (on your own)</b>
<b>1:30-3:30 Session 3</b>
Session Chair: Amarda Shehu Session Co-chair: Irina Hashmi
<b>Keynote Speaker: Roland Dunbrack, Fox Chase Cancer Center</b> <b>“Structural bioinformatics of proteins and protein complexes” (see abstract)</b>
Yajia Zhang and Kris Hauser, <i>Unbiased, Scalable Sampling of Constrained Kinematic Loops</i>
Brian Godshall and Brian Chen, <i>Improving Accuracy in Binding Site Comparison with Homology Modeling</i>
Sameh Saleh, Brian Olson, and Amarda Shehu, <i>A Population-based Evolutionary Algorithm for Sampling Minima in the Protein Energy Surface</i>
<b>3:30-3:50 poster session 2 (coffee: 3:30-3:50)</b>
<b>3:50-5:20 Session 4</b>
Session Chair: Nurit Haspel Session Co-chair: Bahar Akbal-Delibas.

Boyuan Zhang, Daniel Yehdego, Kyle Johnson, Ming-Ying Leung, and Michela Taufer, *A modularized MapReduce framework to support RNA secondary structure prediction and analysis workflows*

Kevin Molloy and Amarda Shehu, *A Robotics-inspired Method to Sample Conformational Paths Connecting Known Functionally-relevant Structures in Protein Systems*

Weiwei Han and Lei Xie, *Structural Basis of Polypharmacological Effects of Metformin (short)*

Bahar Akbal-Delibas, Filip Jagodzinski, and Nurit Haspel, *Towards a Hybrid Method for Detecting Critical Protein Residues (short)*

### **Closing Remarks**

#### **Speaking times:**

18 + 2 minutes for regular papers

15 + 2 minutes for short papers (Bolded)

#### **Posters:**

To promote further discussion, each presenter is encouraged to bring an informal poster to present at the poster session. To confirm your poster, please send an email to [jhe@cs.odu.edu](mailto:jhe@cs.odu.edu). The poster width is limited to 36 inches.

1. "Building the Initial Chain of the Proteins through De Novo Modeling of the Cryo-Electron Microscopy Volume Data at the Medium Resolutions", Kamal Al Nasr, Lin Chen, Dong Si, Desh Ranjan, Mohammad Zubair, Jing He
2. "Sampling Low-energy Protein-protein Configurations with Basin Hopping", Irina Hashmi and Amarda Shehu
3. "Jumping Low, jumping High: Controlling Hopping in the Protein Energy Surface", Brian Olson and Amarda Shehu
4. "Mapping Conformational Pathways between known Functional Protein States", Kevin Molloy and Amarda Shehu
5. "An Evolutionary Framework to Sample Near-native Protein Conformations", Sameh Saleh, Brian Olson, and Amarda Shehu
6. "A Tree-based Search to Bias Sampling of Protein Decoy Conformations", Kevin Molloy and Amarda Shehu
7. "*Towards a Hybrid Method for Detecting Critical Protein Residues*", Bahar Akbal-Delibas, Filip Jagodzinski, and Nurit Haspel
8. "*Refining Multimeric Protein Complexes Using Conservation, Electrostatics and Probabilistic Selection*", Bahar Akbal-Delibas and Nurit Haspel

#### **Keynote Speaker:** Dr. Roland Dunbrack, Fox Chase Cancer Center

Dr. Roland Dunbrack is a Professor in the Institute for Cancer Research of the Fox Chase Cancer Center in Philadelphia. He holds adjunct appointments at the Schools of Medicine of the University of Pennsylvania and Drexel University. He received his A.B. in Chemistry at Harvard College in 1985 and a Ph.D. in Biophysics at Harvard University in 1993. Dr. Dunbrack's research is in structural bioinformatics and methods and applications for prediction of the structures of proteins and protein complexes. He has applied these methods to many proteins of interest in cancer research in collaboration with colleagues in experimental biology and medicine at the Fox Chase Cancer Center. He is a recent recipient of the Senior Research Excellence Award from the Temple University School of Medicine, which Fox Chase Cancer Center joined in July 2012.

## **Structural Bioinformatics of Proteins and Protein Complexes**

### **Abstract:**

The Protein Data Bank (PDB) provides a rich source of information when viewed as a whole. Statistical analysis of structural features from atom-atom contacts to biological and crystallographic interfaces have become a branch of modern bioinformatics and computational biology. We will presents results of several studies that seek to improve our understanding of protein structure and our ability to predict structure from sequence, when an experimental structure is not yet available. We have used modern non- parametric statistical methods including adaptive kernel density estimates and the hierarchical Dirichlet process to produce smooth and differentiable probability density estimates for backbone-dependent rotamer libraries and neighbor-residue-dependent Ramachandran maps. We have employed affinity propagation and a dihedral angle metric to cluster the conformations of the complementarity-determining regions (CDRs) of antibody loops, producing a new classification of these loops for antibody structure prediction and design. Finally, we have examined structures of homologous proteins in different crystal forms to identify likely biologically relevant interfaces. Our database, ProtCID, is a rich source of biological information on the evolution of protein-protein interactions. We have used it to identify previously unrecognized structures of autophosphorylation events of kinases.