

2011 Workshop on Computational Structural Bioinformatics

Saturday, November 12, 2011 — Marriott Atlanta Marquis — Room: International 6
Jing He, Amarda Shehu, Nurit Haspel, Brian Chen, Co-Chairs

8:30 – 10:00 Session 1 (18 minute presentation + 2 minutes questions for each paper) Session Chair: Jing He Co-chair: Abhishek Biswas
Opening Remarks
Refinement of Docked Protein Complex Structures Using Evolutionary Traces Bahar Akbal-Delibas, Irina Hashmi, Amarda Shehu, and Nurit Haspel
A Statistical Model of Overlapping Volume in Ligand Binding Cavities Brian Chen and Soutir Bandyopadhyay
Recursive protein modeling: a divide and conquer strategy for protein structure prediction and its case study in CASP9 Jianlin Cheng, Jesse Eickholt, Zheng Wang, and Xin Deng
P.R.E.S.S. – An R-package for Exploring Residual-Level Protein Structural Statistics Yuanyuan Huang and Zhijun Wu
10:00-10:20 Break, poster setup
10:20-11:50 Session 2 (18 minute presentation + 2 minutes questions for each paper) Session Chair: Nurit Haspel Session Co-chair: Bahar Akbal-Delibas
A Distance and Orientation Dependent Potential Energy Function with cluster energy Lin Chen and Jing He
SCOP Family Fingerprints: An Information Theoretic Approach to Structural Classification of Protein Domains Alberto Casagrande and Francesco Fabris
Protein Docking with Information on Evolutionary Conserved Interfaces Irina Hashmi, Bahar Akbal-Delibas, Nurit Haspel, and Amarda Shehu
Rigid Region Pairwise Sequence Alignment Marko Zivanic, Ovidiu Daescu, and Anastasia Kurdia,
Amino Acid Encoding Schemes for Machine Learning Methods MasoodZamani and Stefan C. Kremer
11:50-12:30 poster session 1
12:30-1:30 Lunch (on your own)
1:30-2:50 Session 3 (18 minute presentation + 2 minutes questions for each paper) Session Chair: Brian Chen Session Co-chair: Seyed Farid Hendi
A symmetry-driven BP algorithm for the Discretizable Molecular Distance Geometry Problem Antonio Mucherino, Carlile Lavor, and Leo Liberti
Protein Conformational Search with Geometric Projections Brian Olson, Farid Hendi, and Amarda Shehu
Using Rigidity Analysis To Probe Mutation-Induced Structural Changes in Proteins Filip Jagodzinski, Jeanne Hardy, and Ileana Streinu
Encoding Protein Structure with Functions on Graphs Promita Bose, Xia Xia Yu, and Robert Harrison

2:50-3:50 poster session (coffee: 3-3:20)
3:50-4:30 Session 4 (18 minute presentation + 2 minutes questions for each paper) Session Chair: Amarda Shehu Session Co-chair: Irina Hashmi
The development of a proteomic analyzing pipeline to identify proteins with multiple RRM s and predict their domain boundaries Kyung Dae Ko, Chunmei Liu, Mugizi Robert Rwebangira, Legand Burge, and William Southerland
Normal mode analysis of protein structure dynamics based on residue contact energy Weitao Sun
4:30-4:35 Closing Remarks

Posters:

1. **Moonlighting Proteins**, Constance Jeffery
2. **Towards accurate modeling of hydrogen bonds for protein rigidity analysis**, Naomi Fox, Ileana Streinu
3. **Application of QM/MM Calculations with Novel Polarized Embedding to Detail Investigation of the Flavoprotein WrbA**, David Řeha, Vasilina Zayats, Rüdiger Ettrich
4. **Protein Conformational Search with Geometric Projections**, Brian Olson, Farid Hendi, and Amarda Shehu
5. **Refinement of Docked Protein Complex Structures Using Evolutionary Traces**, Bahar Akbal-Delibas, Irina Hashmi, Amarda Shehu, and Nurit Haspel
6. **Populating Local Minima in the Protein Conformational Space**, Brian Olson and Amarda Shehu
7. **Assembly of Low-Energy Protein Conformations with Heterogeneous Fragments**, Kevin Molloy and Amarda Shehu
8. **Refinement of Docked Protein Complex Structures Using Evolutionary Traces**, Bahar Akbal-Delibas, Irina Hashmi, Amarda Shehu, and Nurit Haspel.
9. **A Constraint Dynamic Graph Approach to identify the Secondary Structure Topology from cryoEM Density Data in Presence of Errors**, Abhishek Biswas, Dong Si, Kamal Al Nasr, Desh Ranjan, Mohammad Zubair, and Jing He.
10. **On the Energy of Bifurcated Hydrogen Bonds for Protein Structure Prediction**, Sajal Dash and Jack Snoeyink.
11. **A Distance and Orientation Dependent Potential Energy Function with cluster energy**, Lin Chen and Jing He
12. **Using Rigidity Analysis To Probe Mutation-Induced Structural Changes in Proteins**, Filip Jagodzinski, Jeanny Hardy and Ileana Streinu