**Sunday, July 24, 5:00pm to 6:30pm**

**All-Telluride Science Meet and Greet at Phoenix Bean (221 W Colorado Ave.)**

**DAY 1**

**Monday, July 25, 2022**

**Session 1**

**Chair: Robert Jernigan**

9:00a.m. – 9:30a.m. **Florence Tama– RIKEN/ Nagoya University**

Integrative modeling approaches to characterize dynamics of biomolecules: application to Atomic Force Microscopy and X-ray Free Electron Laser data– V

9:30a.m. – 10:00a.m. **Jarek** **Meller – University of Cincinnati**

Structural Alphabets for Efficient Retrieval and Clustering of Protein & RNA Structures– IP

10:00a.m. – 10:30a.m. **Jia Kejue – Iowa State University**

New amino acid substitution matrix brings sequence alignments into agreement with structure matches – IP

10:30a.m. – 11:00a.m. **Julie C. Mitchell– Oak Ridge National Laboratory**

Machine Learning Approaches to Biophysics– V

11:00a.m. – 11:20a.m. **BREAK**

**Session 2**

**Chair:** **Jarek** **Meller**

11:20p.m. – 11:50a.m. **Dzmitry Padhorny – Stony Brook University**

Simulation of multi-protein systems – IP

11:50a.m. – 12:20p.m. **Ilya Vakser - The University of Kansas**

Docking-based simulation of cell-size protein systems -IP

12:20p.m. – 12:50p.m. **Discussion** – Can we survive without MSFD Study Section?

**DAY 2**

**Tuesday, July 26, 2022**

**Session 3**

**Chair: Ilya Vakser**

9:00a.m. – 9:30a.m. **Kei-ichi Okazaki– Institute for Molecular Science, Japan**.

Coarse-grained simulations of curvature induction and sensing of the F-BAR protein Pacsin1 on lipid membranes -v

9:30a.m. – 10:00a.m. **Sergei Kotelnikov–** **Stony Brook University**

From fragments to molecules: fast giga-size library screening– V

10:00a.m. – 10:30a.m. **Marina** **Guenza – University of Oregon**

Dinuleotides as simple models of the base stacking-unstacking component of DNA ‘breathing’ mechanisms – V

10:30a.m. – 11:00a.m. **Jie Liang – University of Illinois at Chicago**

Driver Interactions and Many-Body Units of 3D Genome Folding from Coarse Grained Simulation – IP

11:00a.m. – 11:20a.m. **BREAK**

**Session 4**

**Chair: Andrzej Kloczkowski**

11:20p.m. – 11:50a.m. **Mubasher Hassan – Nationwide Children’s Hospital**

Exploration of Potential Ewing Sarcoma Drugs from FDA-Approved Pharmaceuticals through Computational Drug Repositioning approaches – V

11:50p.m. – 12:20p.m. Dima **Kozakov – Stony Brook University**

TBA – IP

12:20p.m. – 12:50p.m. **Sayantan Mondal – Boston University**

Membrane remodeling by polyelectrolyte condensates – V

6:30p.m. – 7:30p.m. **TOWN TALK:** **Viewpoints Matter: How diverse perspectives bring about scientific progress:** Korana Burke, University of California Davis

Peter Salamon, San Diego State University, Dontarie Stallings, University of California San Diego

Location: The Telluride Depot, 300 S Townsend Street, Town of Telluride

**DAY 3**

**Wednesday, July 27, 2022**

**Session 5**

**Chair: Dima Kozakov**

9:00a.m. – 9:30a.m. **Jin Wang – Stony Brook University**

Chromosome structural conformation dynamics of cell fate decision making – V

9:30a.m. – 10:00a.m. **Jeffrey Skolnick – Georgia Institute of Technology**

Insights into biochemical pathways from predicted protein complexes –V

10:00a.m. – 10:30a.m. **Robert Jernigan – Iowa State University**

Entropies Derived from Single Protein Structures – IP

10:30a.m. – 11:00a.m. **Shi-Jie Chen – University of Missouri-Columbia**

Graph deep learning locates magnesium ions in RNA – V

11:00a.m. – 11:20a.m. **BREAK**

**Session 6**

**Chair: Jie Liang**

11:20a.m. – 11:50a.m. **Daisuke Kihara – Purdue University**

Validating protein structure models from cryo-EM maps using deep learning – V

11:50a.m. – 12:20p.m. **Tobin Sosnick – University of Chicago**

Prediction of a Protein’s Free Energy Surface With Validation Using Hydrogen/Deuterium Exchange – V

12:20p.m. – 12:50p.m. **Xiaoqin Zou - University of Missouri-Columbia**

A DeepConvolution Neural Network for Protein-Protein Structure Prediction -v

5:30pm - 7:30pm **All Telluride Science Picnic at the Depot (300 S. Townsend Street)**

**DAY 4**

**Thursday, July 28, 2022**

**Session 7**

**Chair: Dzmitry Padhorny**

9:00a.m. – 9:30a.m. **Adam Liwo – University of Gdansk**

Origin of through-sequence correlations between local conformational states of amino-acid residues and their role in shaping protein structures and in allostery– V

9:30a.m. – 10:00a.m. **Cristian Micheletti – SISSA - International School for Advanced Studies**

Nonequilibrium unzipping of DNA and RNA using nanopore translocation – IP

10:00a.m. – 10:30a.m. **Silvina Matysiak – University of Maryland**

Coarse-Grained Protein Model with Polarizablity and Transferability –V

10:30a.m. – 11:00a.m. **George Stan – University of Cincinnati**

Translocation of proteins through AAA+ nanopores initiated at internal sites – V

11:00a.m. – 11:20a.m. **BREAK**

**Session 8**

**Chair:** **Cristian Micheletti**

11:20p.m. – 11:50a.m. **George Rose – Johns Hopkins University**

Protein Folding: conformational entropy induces pre-organization – V

11:50a.m. – 12:20p.m. **Andrzej Kloczkowski - Nationwide Children’s Hospital**

Prediction of the effects of protein mutations– IP

12:20p.m. – 12:50p.m. **DISCUSSION –** Alpha-Fold and the future of computational structural biology

**DAY 5**

**Friday, July 29, 2022**

**FREE TIME**

**INFORMATION FOR VIRTUAL PARTICIPANTS**

Zoom meeting

Topic: Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules

Time: This is a recurring meeting Meet anytime

Join Zoom Meeting

[https://us06web.zoom.us/j/81274851691?pwd=WTVBUkxaQ25iZ1c4akNlTkRZaENzQT09](https://urldefense.com/v3/__https:/us06web.zoom.us/j/81274851691?pwd=WTVBUkxaQ25iZ1c4akNlTkRZaENzQT09__;!!NiUAmZJ8c1GNWg!W1I91kajnkSAwLdFr2ERxS56yNsxxInGK_ZzXii5CMslDyKbTtHmqVkiTQVRMzssWCR-thpW4Ff37UD0DPRLHcXP3WQvk3UogztIwKbY$)

Meeting ID: 812 7485 1691

Passcode: 030602

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