**DAY 1**

**Monday, July 24, 2023**

**Session 1**

**Chair: Robert Jernigan**

9:00a.m. – 9:10a.m. **Mark Kozak – Telluride Science Research Center**

Introduction

9:10a.m. – 9:40a.m. **Laura** **Orellana – Karolinska Institute**

Studies of the EGF receptor with ENMs and MD

9:40a.m. – 10:10a.m. **Domenico Scaramozzino – Karolinska Institute**

Elucidating the conformational transitions of large protein systems with an improved coarse-grained algorithm

10:10a.m. – 10:40a.m. **Jin Wang – Stony Brook University**

TBA

10:40a.m. – 11:00a.m. **BREAK**

**Session 2**

**Chair:** **Jeffrey Skolnick**

11:00a.m. – 11:30a.m. **Tugba Ozturk – Lawrence Livermore National Laboratory**

Mitigation of membrane morphology defects explain stability and orientational specificity of CLC dimers

11:30a.m. – 12:00p.m. **Adam Liwo – University of Gdansk**

Long-Time Dynamics of Selected Molecular-Motor Components Using a Physics-Based Coarse-Grained Approach

**DAY 2**

**Tuesday, July 25, 2023**

**Session 3**

**Chair: Jarek Meller**

9:00a.m. – 9:30a.m. **Marina** **Guenza – University of Oregon**.

Coarse-Grained Dynamics of Biological Macromolecules: Friction Coefficients and Other Stories

9:30a.m. – 10:00a.m. **Jayanth Banavar – University of Oregon**

A simple coarse-grained framework for thinking about proteins

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

Coarse-grained modeling of RNA cotranscriptional folding kinetics

10:30a.m. – 10:50a.m. **BREAK**

**Session 4**

**Chair:** **Daisuke Kihara**

10:50a.m. – 11:20a.m. **Mubasher Hassan – Nationwide Children’s Hospital**

Pharmacoinformatics Analysis of Drug Leads for Alzheimer’s Disease from FDA-Approved Dataset through Drug Repositioning Studies

11:20a.m. – 11:50a.m. **Xiaoqin Zou - University of Missouri-Columbia**

Predicting protein-peptide interactions: Structure, large-scale peptide screening and application

11:50a.m. – 12:20p.m. **Jarek Meller – University of Cincinnati**

TBA

**DAY 3**

**Wednesday, July 26, 2022**

**Session 5**

**Chair: Marina Guenza**

9:00a.m. – 9:30a.m. **Robert Jernigan – Iowa State University**

Using Information from Protein Language Models

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

Some deep learning-based insights into outer membrane protein biogenesis in bacteria

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

Allosteric coupling via long distance communication of disorder-to-order transitions

10:30a.m. – 10:50a.m. **BREAK**

**Session 6**

**Chair: Xiaoqin Zou**

10:50a.m. – 11:20a.m. **Daisuke Kihara – Purdue University**

Structure modeling for cryo-EM using deep learning

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

Efficient Identification of the Pathogenicity of Human

and Non-Human Missense Mutations

11:50a.m. – 12:20p.m. **Discussion**

TSRC Workshop1 is inviting you to a scheduled 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/85313111452?pwd=SFJYNldGNkhWL0t4cmlsZHFJVG0rQT09](https://urldefense.com/v3/__https:/us06web.zoom.us/j/85313111452?pwd=SFJYNldGNkhWL0t4cmlsZHFJVG0rQT09__;!!NiUAmZJ8c1GNWg!QWYrgdzGpK4LHgtUGqbSLcrwTt-3FRsWB9jlLTSHEtkdpq8mECabFdBtdcC-z83tgQw02lDOC-8CSf88zng79TEyhUX2XpfYm0a0ZN-s$)

Meeting ID: 853 1311 1452

Passcode: 652192

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