**6th International Conference on Mathematical and Computational Medicine
(HYBRID)**
TIMES LISTED ARE MOUNTAIN TIME
JUNE 11 – 15, 2022

DAY 1

Saturday, June 11, 2022

12:30p.m. – 12:35p.m.   **OPENING REMARKS** – Jayajit Das, PhD

**Session 1
Chair: Jayajit Das**

12:35p.m. – 1:05p.m.   **Shi-Jie Chen – University of Missouri**
Predicting RNA targeting by small molecules - v

 1:05p.m. – 1:35p.m.   **Shili Lin – The Ohio State University**
CaTCHing TADs by Random Walks on Single-Cell Hi-C Data — Reality or
Fiction - v

 1:35p.m. – 2:05p.m.   **Jarek Meller – University of Cincinnati**
Improving Drug Discovery and Repurposing by Combining Transcriptional
Signature Connectivity with Biophysical Complementarity - v

 2:05p.m. – 2:35p.m.   **Karissa Sanbonmatsu – Los Alamos National Laboratory** - v

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DAY 2

Sunday, June 12, 2022

Session 2
Chair: George Stan

9:00a.m. – 9:30a.m.	**Gaurav Chopra – Purdue University** Neural networks for selection and validation of small molecule immunomodulators – V
9:30a.m. – 10:00a.m.	**Samuel Handelman – Eli Lilly** A mechanistic dynamical systems model of polarized macrophage feedback in nociceptive pain – IP
10:00a.m. – 10:30a.m.	**Andrzej Joachimiak – Argonne National Laboratory** Time-Resolved β-lactam Cleavage by L1 Metallo-β-Lactamase – IP
10:30a.m. – 11:00a.m.	**Ruxandra Dima – University of Cincinnati** Microtubule severing enzymes oligomerization and allostery: a tale of two domains – V
11:00a.m. – 12:30p.m.	**BREAK**

Session 3
Chair: Ruxandra Dima

12:30p.m. – 1:00p.m.	**Mubasher Hassan – Battelle Center for Mathematical Medicine, Nationwide Children's Hospital Research** Mechanistic insights into MADD death domains in Alzheimer's disease through molecular dynamic analysis – V
1:00p.m. – 1:30p.m.	**Daisuke Kihara – Purdue University** Protein structure modeling from cryo-EM maps using deep learning – V
1:30p.m. – 2:00p.m.	**George Stan – University of Cincinnati** Allosteric mechanisms in protein remodeling mediated by AAA+ nanomachines – V
2:30p.m. – 3:00p.m.	**Andrzej Kloczkowski - Battelle Center for Mathematical Medicine, Nationwide Children's Hospital Research** Accessible Surface Area and the Prediction of the Phenotypes of Missense Mutations – V

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DAY 3

Monday, June 13, 2022

Session 4
Chair: Anton Zilman

9:00a.m. – 9:30a.m.	**Indrani Nayak - Battelle Center for Mathematical Medicine, Nationwide Children's Hospital Research** Modeling CD16 signal kinetics reveals the role of adaptor CD3ζ in NK cell signaling in humans and mice – IP
9:30a.m. – 10:00a.m.	**Juilee Thakar – University of Rochester** Discrete-state modeling identifies dysregulated signaling underlying atherosclerosis in people living with HIV – IP
10:00a.m. – 10:30a.m.	**Darren Wethington - Battelle Center for Mathematical Medicine, Nationwide Children's Hospital Research** Mathematical modeling dissects maturation pathway of natural killer cells in response to murine cytomegalovirus infection – IP
10:30a.m. – 11:00a.m.	**Jayajit Das - Battelle Center for Mathematical Medicine, Nationwide Children's Hospital Research** Harnessing the power of immunity – IP
11:00a.m. - 12:30p.m.	**BREAK**

Session 5
Chair: Juilee Thakar

12:30p.m. – 1:00p.m.	**Sid Goyal – University of Toronto** Statistical dynamics of tumor initiation and progression – V
1:00p.m. – 1:30p.m.	**Vitaly Ganusov – University of Tennessee – V**
1:30p.m. – 2:00p.m.	**Anton Zilman – University of Toronto** Modes of ligand discrimination in cross-wired signaling pathways – IP
2:30p.m. – 3:00p.m.	**Harinder Singh – University of Pittsburgh – V**
5:30p.m. – 7:00p.m.	**Telluride Science Picnic (in the tent behind the school)**

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DAY 4

Tuesday, June 14, 2022

Session 6
Chair: Patricia Jennings

9:00a.m. – 9:30a.m.	**Wladek Minor – University of Virginia** Evaluating the impact of Covid-19 vaccinations using U.S. county-level public data – IP
9:30a.m. – 10:00a.m.	**Patricia Jennings – University of California San Diego** – V
10:00a.m. – 10:30a.m.	**Oliver Lichtarge – Baylor College of Medicine** Mutations Obey the Equipartion Theorem – V
10:30a.m. – 11:00a.m.	**Steffen Lindert – The Ohio State University** Free Energy Simulations and Computer-Aided Drug Discovery on Cardiac Troponin C – IP
11:00a.m. – 12:30p.m.	**BREAK**

Session 7
Chair: Paola Malerba

12:30p.m. – 1:00p.m.	**Lyle Muller – Western University** Spatiotemporal dynamics shape perceptual and cognitive processes: computational methods and mathematical models – V
1:00p.m. – 1:30p.m.	**Giri Krishnan – University of California San Diego** Neural basis of resting-state activity: Role of ion dynamics and neuromodulation – V
1:30p.m. – 2:00p.m.	**Hamid Niknazar – University of California Irvine** Slow oscillations promote long range effective communication: the key for memory consolidation in a broken down network – V
2:00p.m. – 2:30p.m.	**Paola Malerba – Nationwide Children's Hospital Research Institute** Differentiating the space-time profiles of sleep slow oscillations – V
6:30p.m. – 7:30p.m.	**Presenter: Jayajit Das, Nationwide Children's Hospital** Town Talk at the Telluride Conference Center in Mountain Village

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DAY 5

Wednesday, June 15, 2022

Session 8
Chair: Andrzej Kloczkowski

9:00a.m. – 9:30a.m.	**Jin Wang – Stony Brook University** Quantifying ligand binding specificity and virtual screening of lead compounds - V
9:30a.m. – 10:00a.m.	**Xiaoquin Zou – University of Missouri-Columbia** A Deep Convolution Neural Network for Protein-Protein Binding Mode Prediction - V
10:00a.m. – 10:30a.m.	**Planning for the next International Conference for Mathematical and Computational Medicine conferences**
10:30a.m. - 10:40a.m.	**CLOSING REMARKS** – Paola Malerba, PhD

DEPARTURE