2021 Computational Structural Bioinformatics Workshop

Saturday, December 11, 2021 (virtual) All times are Eastern Time Zone

CSBW Website: http://cs.wwu.edu/csbw

Workshop Co-chairs: Negin Forouzesh, Kamal Al Nasr

Each recorded video talk is 10-15 minutes; 10-15 minute (group) QA session for each session

Time (EST)	Title
10:00-10:05 AM	Opening and Introduction
10:05-11:00 AM	Keynote Speech (live presentation+ live Q&A) Speaker: Jens Meiler, Vanderbilt University
11:00 AM-12:15 PM	Session I: Docking, Mutations, and Protein Binding (recorded videos + live Q&A)
12:15-12:30 PM	Break
12:30-1:30 PM	Session II: Machine Learning-Based Approaches (recorded videos + live Q&A)
1:30-2:30 PM	Lunch Break
2:30-3:10 PM	Panel (live discussion + live Q&A) Topic: Industry and Academic Careers in Bioinformatics: Current Trends and Prospects for the Future Chairs: Kamal Al Nasr Panelists: - Amarda Shehu, George Mason University, and NSF III/IS - Xia Ning, Ohio State University - Negin Forouzesh, California State University- Los Angeles
3:10-3:40 PM	Research Highlight I (live presentation+ live Q&A) Speaker: Lukasz Kurgan, Virginia Commonwealth University
3:40-4:10 PM	Research Highlight II (live presentation+ live Q&A) Speaker: Xia Ning, Ohio State University
4:10-4:30 PM	Break
4:30-5:30 PM	Session III: Protein/RNA Structure and Function (recorded videos + live Q&A)
5:30-5:45 PM	Break
5:45-6:45 PM	Session IV: Cryo-EM and Structural Modeling (recorded videos + live Q&A)
6:45- 7:00 PM	Closing Remark

Keynote Speech:

Speaker: Dr. Jens Meiler, Vanderbilt University
Title: Computational Structure Prediction and Therapeutic Design with Rosetta
Time: 10:05-11:00 AM (EST)

Bio: Jens Meiler studied Chemistry Leipzig University in Germany before he obtained his PhD working in the laboratory of Christian Griesinger at the Goethe University in Frankfurt developing new computational methods for biomolecular NMR spectroscopy. In 2001 he moved to Seattle to work with David Baker creating the protein modeling software Rosetta. In 2005 he joined the faculty at Vanderbilt University. In his research Dr. Meiler fuses computational and experimental efforts to investigate proteins, the fundamental molecules of biology, and their interactions with small molecule substrates, therapeutics, or probes. He develops computational methods with three major ambitions in mind: to enable protein structure elucidation of membrane proteins, design proteins with novel structure and/or function, and understand the relation between chemical structure and biological activity for drug-like small molecules. His research team in Nashville consists of around 30 undergraduate, graduate, and post-graduate students as well as staff scientists. He co-authored more than 250 peer-reviewed publications (H-index >50). Jens Meiler received several honors including the Chancellor Faculty Award at Vanderbilt University and the Friedrich-Wilhelm-Bessel Award of the Humboldt Foundation. In January 2020, with an Alexander von Humboldt Professorship, Jens Meiler became director of the newly founded Institute for Drug Discovery at Leipzig University. Simultaneously, he continues in his role as Professor at Vanderbilt University.

Research Highlight I:

Speaker: Dr. Lukasz Kurgan, Virginia Commonwealth University
Title: Prediction of intrinsic disorder in the post-AlphaFold era
Time: 3:10-3:40 PM (EST)

Bio: Dr. Kurgan is the Endowed Professor of Computer Science at the Virginia Commonwealth University. His research interests include development and applications of bioinformatics methods and resources for the analysis of sequences and functions of proteins. He serves as the Associate Editor-in-Chief of Biomolecules, Associate Editor of Bioinformatics, and editor of several other journals and conferences. More details can be found on the website of his lab (http://biomine.cs.vcu.edu/) and on his Google Scholar profile (http://scholar.google.com/citations?user=zXw_54AAAAAJ).

Research Highlight II:

Speaker: Dr. Xia Ning, Ohio State University
Title: A Deep Generative Model for Molecule Optimization via One Fragment Modification
Time: 3:40-4:10 PM (EST)

Bio: Dr. Xia Ning is a tenured Associate Professor in the Biomedical Informatics Department and Computer Science and Engineering Department, The Ohio State University. She co-directs the Computational Health and Life Sciences Community of Practice at the Translational Data Analytics Institute (TDAI) at OSU. Dr. Ning received her Ph.D. from University of Minnesota, Twin cities, in 2012. From 2012 to 2014, she worked as a research staff member at NEC Labs, America. From 2014 to 2018, she was an Assistant Professor in the Computer and Information Science Department, Indiana University – Purdue University Indianapolis. She joined OSU in July 2018. Ning's research is on Artificial Intelligence and Machine Learning with applications in Biomedicine. In specific, Ning's research focuses on developing scalable AI/ML models and computational methods to derive knowledge from heterogeneous Big Data via modeling, ranking, classification and prediction, etc., and ultimately to solve critical and high-impact problems. Specific research topics include information retrieval from electronic medical records, drug candidate prioritization for drug discovery, cancer drug selection for precision medicine, etc. Dr. Ning is a fellow of American Medical Informatics Association (AMIA).

Session 1: Docking, Mutations, and Protein Binding
Time: 11:00 AM- 12:15 PM (EST)
Chair: Kamal Al Nasr

1- [S13214] Assessing the Effects of Amino Acid Insertion and Deletion Mutations, Muneeba Jilani, Alistair Turcan, Nurit Haspel, and Filip Jagodzinski. Time: 11:00- 11:12 AM (EST).
2- [S13208] Allosteric Modulation of Small Molecule Drugs on ACE2 Conformational Change upon Binding to SARS-CoV-2 Spike Protein, Duen-Shian Wang, Hamed S Hayatshahi, Vindi M. Jayasinghe- Arachchige, and Jin Liu. Time: 11:12- 11:22 AM (EST).
3- [S13209] Discovering SARS-CoV-2 genes and mutations adapted for humans in 2594 genomes, Weitao Sun. Time: 11:22- 11:34 AM (EST).
4- [B229] pH Dependent Binding Energies of Broadly Neutralizing Antibodies, Scott Morton and Joshua Phillips. Time: 11:34- 11:46 AM (EST).
5- [B644] Understanding the binding of the same ligand to GPCRs of different families, Kwabena Owusu Dankwah, Jonathon E Mohl, Khodeza Begum, and Ming-Ying Leung. Time: 11:46- 11:58 AM (EST)

Live Group Q&A: 12:00 - 12:15 PM (EST)

Session 2: Machine Learning-Based Approaches
Time: 12:30- 1:30 PM (EST)
Chair: Kamal Al Nasr

1- [S13203] Generating Physically-Realistic Tertiary Protein Structures with Deep Latent Variable Models Learning Over Experimentally-available Structures, Fardina Fathmiul Alam and Amarda Shehu. Time: 12:30- 12:45 PM (EST).
2- [S13219] Assignment of Protein Secondary Structure Elements from Cα Backbone Trace: An Ensemble of Machine Learning Approaches, Kamal Al Nasr and Ali Sekmen. Time: 12:45- 12:57 PM (EST).
3- [B610] Deep Learning for Assignment of Protein Secondary Structure Elements from Cα Coordinates, Kamal Al Nasr, Ali Sekmen, Bahadir Bilgin, Christopher Jones, and Ahmet Bugra Koku. Time: 12:57- 1:07 PM (EST).
4- [S13218] Calculation of Protein-Ligand Binding Free Energy Using a Physics-Guided Neural Network, Sahar Cain, Ali Risheh, and Negin Forouzesh. Time: 1:07- 1:19 PM (EST).

Live Group Q&A: 1:20- 1:30 PM (EST)

Session 3: Protein/RNA Structure and Function
Time: 4:30- 5:30 PM (EST)
Chair: Negin Forouzesh

1- [S13202] Antigen Binding Reshapes Antibody Energy Landscape and Conformation Dynamics, Kazi Lutful Kabir, Ruth Nussinov, Buyong Ma, and Amarda Shehu. Time: 4:30- 4:43 PM (EST).
2- [S13205] Designing a Survey of Structural Trends in Intermolecular Bond Formation, Justin Tam, Talulla Palumbo, Julie M. Miwa, and Brian Y. Chen. Time: 4:43- 4:56 PM (EST).
3- [S13216] Characterizing the Behavior of Mutated Proteins with EMCAP: the Energy Minimization Curve Analysis Pipeline, Matthew Lee, Bodi Van Roy, and Filip Jagodzinski. Time: 4:56- 5:11 PM (EST).
4- [B773] RNA Secondary Structure Database, Analysis Tool-Set, and Case-Study Results on SARS-CoV-2, Abdullah N. Arslan, Mutlu Mete, and Anjali Kumari. Time: 5:11- 5:26 PM (EST)

Live Group Q&A: 5:26-5:30 PM (EST)

Session 4: Cryo-EM and Structural Modeling
Time: 5:45- 6:45 PM (EST)
Chair: Negin Forouzesh

1- [S13207] A Conical Representation of Hydrogen Bond Geometry for Quantifying Bond Interactions, Chesphongphach Buranasilp and Brian Chen. Time: 5:45- 5:58 PM (EST)
2- [S13212] TomoSim: Simulation of Filamentous Cryo-Electron Tomograms, Peter Scheible, Salim Sazzed, Jing He, and Willy Wriggers. Time: 5:58- 6:08 PM (EST).
3- [S13210] Tracing Filaments in Simulated 3D Cryo-Electron Tomography Maps Using a Fast Dynamic Programming Algorithm, Salim Sazzed, Peter Scheible, Jing He, and Willy Wriggers. Time: 6:08- 6:20 PM (EST).
4- [S13213] A study on the impact of the distance types involved in protein structure determination by NMR, Simon Hengeveld, Therese Malliavin, Jung-Hsin Lin, Leo Liberti, and Antonio Mucherino. Time: 6:20- 6:35 PM (EST).

Live Group Q&A: 6:35-6:45 PM (EST)