2025 Computational Structural Bioinformatics Workshop

Sunday, October 12, 2025
All times are Eastern Time Zone

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

Workshop Co-chairs: Salim Sazzed and Brian Chen
Each talk will be **25** minutes, consisting of a **20**-minute presentation followed by a **5**-minute Q&A session.

Session 1 (10:00 am - 11:50 am) Protein Mutations & Stability Analysis (4 talks)
10:00 – 10:10 *Opening remarks (10 minutes)*
10:10 – 10:35: Systematic Evaluation of 566 Sequence-Based Features for Predicting Protein Stability Changes Induced by Mutations Using Machine Learning (*Qiaobin Yao, Junyan Li, Dongxiao Liu, Krish Wahi, Shaolei Teng*)
10:35 – 11:00: Red Teaming Generative Proteins with Unsupervised Toxin-Based Risk Embeddings (*Tia Pope, Ahmad Patooghy*)
11:00 – 11:25: Structural Impacts of Insertion Mutations on Protein-Protein Interfaces (*James Tessmer, Logan Day, Bogdan Trigubov, Emilia Galant, Filip Jagodzinski*)
11:25 – 11:50: PRIMRose: Insights into the Per-Residue Energy Metrics of Proteins with Double InDel Mutations Using Deep Learning (*Stella Brown, Nicolas Preisig, Autumn Davis, Brian Hutchinson, Filip Jagodzinski*)

Lunch 12:00 – 1:00

Session 2 (1:00 pm - 2:15 pm) Small Molecule / Ligand Design & Active Learning (3 talks)
1:00 – 1:25: From Contrast to Control: Domain Conditioned Masking for Small Molecule Generation of Quaternary Ammonium Compounds (*Shiva Ghaemi, Rehenuma Tasmin Rodosh, Shahana Shultana, Amarda Shehu, Daniel Barbará*)
1:25 – 1:50: Physics-Guided Active Learning for New Ligand Discovery (*Nikhil Dhiman, Dikshant Sagar, Negin Forouzesh*)
1:50 – 2:15: DyVarMap: An Interpretable, Dynamics-Aware Framework for Missense Variant Classification (*Yiyang Lian, Amarda Shehu*)

Break 2:15 – 2:20

Session 3 – Panel Discussion (2:20 pm – 3:10 pm)
Panel Title: *TBA*
Panelists: • Panelist 1 (TBA) • Panelist 2 (TBA) • Panelist 3 (TBA) • Panelist 4 (TBA)

Break 3:10 – 3:15pm

Session 4 (3:15 pm – 5:05 pm) Protein Structure & Fold Modeling (4 talks)

3:15 – 3:40: ConSOLAE: Learning Smooth and Generalizable Representations for Protein Fold Recognition (*Shraddha Patre, Riya Kanani, Aarnav Tare, Pranavh Vallabhaneni, Fardina Fathmiul Alam*)

3:40 – 4:05: DeepSSETracer 2.0: Improved Deep Learning Model Performance for Protein Secondary Structure Segmentation from Cryo-EM Maps (*Bryan Hawickhorst, Thu Nguyen, Willy Wriggers, Jiangwen Sun, Jing He*)

4:05 – 4:30: A Molecular Dynamics Study of Polyacrylamide Conformational Changes in Ca2+ and Mg2+ Solutions (*Gideon K. Gogovi, Lorcan Cheng*)

4:30 – 4:55: Benchmarking and Consensus Ranking of Inverse Folding Models for Protein-Ligand Interface Design (*Yao Wei, Uliano Guerrini, Ivano Eberini*)

Concluding Remarks 4:55 – 5:05