

# Computational Structural Bioinformatics Workshop (CSBW) UMass Boston, November 16, 2024

Workshop Chairs: Nurit Haspel and Kevin Molloy

Location: Y03-3350 (University Hall, third floor, room 3350).

Time	Title	Presenters/Author(s)
10:15 AM	Coffee and Meet and Greet	
10:30 AM	CSBW Opening Remarks	Nurit Haspel and Kevin Molloy
10:35 AM	Decoys Reveal Multiple Basins of Attraction for Cryo-Electron Microscopy Flexible Fitting	Willy Wriggers, Jing He and Maytha Alshammari
10:50 AM	SuperFoldAE: Enhancing Protein Fold Classification with Autoencoders	Shraddha Patre, Riya Kanani and Fardina Fathmiul Alam
11:15 AM	Using Molecular Dynamics to Assess How Two Insertion Mutations Affect Protein Structure	Changrui Li, Katie Christensen, Sarah Coffland and Filip Jagodzinski
11:40 AM	Automatically Explaining Binding Mechanisms: A Preliminary Study	Justin Tam, Yangying Liu, Dhruv Jain and Brian Chen
12:05 PM	Lunch	
1:00 PM	Using Autoencoders to Explore the Conformational Space of the Cdc42 Protein	Fatemeh Afrasiabi, Ramin Dehghanpoor and Nurit Haspel
1:25 PM	Predicted Multimers using Alphafold-3 and Detected Secondary Structure Elements from Cryo-EM maps – Case Studies	Changrui Li, Thu Nguyen, Willy Wriggers and Jing He
1:50 PM	Enhancing Drug Discovery via Physics-Guided Deep Generative Models	Dikshant Sagar, Ari Jasko and Negin Forouzesh
2:15 PM	Coffee /Break	
2:30 PM	Planning Session for CSBW 2025	Nurit Haspel and Kevin Molloy
3:00 PM	Workshop completes	