2020 Computational Structural Bioinformatics Workshop

Monday, September 21, 2020 (virtual)
All times are Eastern Time Zone

CSBW Website: http://cs.wwu.edu/csbw
Virtual Platform: https://acm-bcb-virtual.org
QA Zoom: https://acm-org.zoom.us/j/92007899873?pwd=WnlUZGJlMVY2Y3c0NWozRFRLWGZadz09

Workshop Co-chairs: Filip Jagodzinski, Kevin Molloy
Each video talk is 20 minutes; 10 minute (group) QA session for each section

9:00-10:10 am – Session 1 – Cryo-EM Chair/moderator: Kevin Molloy
1. *A Divide and Conquer Algorithm for Electron Microscopy Segmentation,* Ruba Jebril, Yingde Zhu, Wei Chen and Kamal Al Nasr
2. *Combine Cryo-EM Density Map and Residue Contact for Protein Structure Prediction – A Case Study,* Maytha Alshammari and Jing He
3. *Segmentation based Feature Extraction for Cryo Electron Microscopy at Medium Resolution*, Lin Chen, Ruba Jebril and Kamal Al Nasr
Question and Answer (10 minutes, 10:00-10:10am)

Break 10:10-10:20

10:20-11:30 am – Session 2 – Machine Learning-based approaches Chair/moderator: Kevin Molloy
4. *From Interatomic Distances to Protein Tertiary Structures with a Deep Convolutional Neural Network*, Yuanqi Du, Anowarul Kabir, Liang Zhao and Amarda Shehu
5. *ProLanGO2: Protein Function Prediction with Ensemble of Encoder-Decoder Networks,* Kyle Hippe, Sola Gbenro and Renzhi Cao
6. *Efficient Exploration of Protein Conformational Pathways using RRT* and MC,* Fatemeh Afrasiabi and Nurit Haspel
Question and Answer (10 minutes, 11:20-11:30am)

Break 11:30-11:50

11:50am – 12:30pm – Session 3 – Panel Chairs/moderators: Filip Jagodzinski, Kevin Molloy
7. *Industry and Academia Careers in Bioinformatics: Current Trends and Prospects for the Future*
• Naomi Fox, Clinical Science Software Lead, Invitae • Kameron Decker Harris, Western Washington University • Anna Ritz, Reed College • Amarda Shehu, George Mason University, and NSF III/IS

Break 12:30-1:30pm

1:30-3:00 pm – Session 4 – Protein Structure and Function Chair/moderator: Filip Jagodzinski
8. *Using Guided Motion Planning to Study Binding Site Accessibility,* Diane Marie Bernard Uwacu, Abigail Ren, Shawna Thomas and Nancy M. Amato
9. *HMMeta: Protein Function Prediction using Hidden Markov Models*, Sola Gbenro, Kyle Hippe and Renzhi Cao
10. *Interpretable Molecule Generation via Disentanglement Learning*, Yuanqi Du, Xiaojie Guo, Liang Zhao and Amarda Shehu
11. *Impactful Mutations in Mpro of the SARS-CoV-2 Proteome,* Gideon Wolfe, Othmane Belhoussine, Anais Dawson, Maxwell Lisaius and Filip Jagodzinski (short paper, 12 minutes)
Question and Answer (10 minutes, 2:50-3:00pm)

Break 3:00-3:20

3:20-4:40 pm – Session 5 – Docking, Mutations, and Protein Binding Chair/moderator: Filip Jagodzinski
12. *Binding Free Energy of the Novel Coronavirus Spike Protein and the Human ACE2 Receptor: An MMGB/SA Computational Study,* Negin Forouzesh
13. *Using Curriculum Learning in Pattern Recognition of 3-dimensional Cryo-electron Microscopy Density Maps,* Yangmei Deng, Yongcheng Mu, Salim Sazzed, Jiangwen Sun and Jing He
14. *Assessing Drug Resistance Due to Mutations via Energy Minimization Profiles*, Edward Thompson, Tess Thackray, Cecilia Kalthoff, Ryan Rapoport and Filip Jagodzinski
15. *Using player generated data to elucidate molecular docking,* Torin Adamson, Selina Bauernfeind, Bruna Jacobson and Lydia Tapia (poster, 5 minutes)
Question and Answer (10 minutes, 4:30-4:40pm)