Computational Structural Bioinformatics Workshop (CSBW 2022) *Workshop Chairs: Bruna Jacobson and Chinwe Ekenna*		
Time	**Title**	**Presenter/Author**
8:45 am	**Welcome**	Bruna Jacobson, Chinwe Ekenna
9:00 am	**Keynote: *"Machine learning and molecular simulation for the design of finely tuned drugs"***	Ron Dror
10:00 am	**Coffee Break**	
10:30 am	S22202: ***"Equivariant Encoding based GVAE (EqEn-GVAE) for Protein Tertiary Structure Generation"***	Taseef Rahman, Fardina Fathmiul Alam, and Amarda Shehu
10:50 am	S22206: ***"Exhaustive In-silico Simulation of Single Amino Acid Insertion and Deletion Mutations"***	Alistair Turcan, Grant Chou, Lilu Martin, Theo Miller, Dylan Thompson, and Filip Jagodzinski
11:10 am	B338: ***"Property-Controllable Generation of Quaternary Ammonium Compounds"***	Bo Pan, Yinkai Wang, Xuanyang Lin, Muran Qin, Yuanqi Du, Shiva Ghaemi, Aowei Ding, Shiyu Wang, Saleh Alkhalifa, Kevin Minbiole, William M. Wuest, Ashley Petersen, Austin Leitgeb, Amarda Shehu, and Liang Zhao
11:30 am	S22203***: "Generation and Characterization of Quaternary Ammonium Compounds via Deep Learning"***	Yinkai Wang, Shiva Ghaemi, Aowei Ding, Yuanqui Du, Bo Pan, Muran Qin, Xuanyang Lin, Ashley Ann Petersen, Austin Leitgeb, Saleh Alkhalifa, Kevin Minbiole, William Wuest, Liang Zhao, and Amarda Shehu
11:50 am	S22209: ***"Molecular Descriptors Property Prediction via a Natural Language Processing Approach"***	Tuan Tran and Chinwe Ekenna
12:10 pm	**Invited talk**	Brian Chen
12:30 pm	**Lunch**	
2:00 pm	B983: **Invited talk:** ***"The Combined Focal Cross Entropy and Dice Loss Function for Segmentation of Protein Secondary Structures from Cryo-EM 3D Density maps"***	Yongcheng Mu, Jiangwen Sun, and Jing He
2:20 pm	S22204: ***"Refinement of AlphaFold2 Models against Experimental Cryo-EM Density Maps at 4-6Å Resolution"***	Maytha Alshammari, Jing He, and Willy Wriggers
2:40 pm	B371: ***"Unsupervised Heterogeneous Cryo-EM Projection Image Classification Using Autoencoder"***	Xiangwen Wang, Yonggang Lu, Jianwei Li, and Zequn Zhang
3:10 pm	S22205: ***"Tracing Randomly Oriented Filaments in Simulated Actin Network Tomograms"***	Salim Sazzed, Peter Scheible, Jing He, and Willy Wriggers
3:30 pm	**Coffee Break**	
4:00 pm	**Panel Discussion**	Jing He, Filip Jagodzinski
4:40 pm	S22210: ***"Calculating the Binding Entropy of Host-Guest Systems with Physics-Guided Neural Networks"***	Alles Rebel, Ali Risheh, Negin Massoudian, and Negin Forouzesh
5:00 pm	B949: ***"A geometric and topological analysis of the binding behavior of Intrinsically Disordered Proteins"***	Aakriti Upadhyay and Chinwe Ekenna
5:20 pm	B521: ***"In silico Screening, Docking, and Redesigning of Traditional Chinese Medicinal Compounds Against Streptococcus pneumoniae Glycosyl Hydrolase GHIP and Peptidoglycan Hydrolase LytB"***	Vince Busania, Denice Millen Canilao, Marla Endriga, and Enrique Jose Frio
5:40 pm	S22207: ***"Computational analysis of Receptor-Binding Domains of SARS-CoV-2 to reveal the mechanism of immune escape"***	Mengxu Zhu, Kongyan Li, and Hong Yan
6:00 pm	B739: ***"Docking-based Multi-objective Molecular Optimization Pipeline using Structure-constrained Genetic Algorithm"***	Yurim Lee, Kyudam Choi, and Cheongwon Kim
6:20 pm	S22208: ***"An Efficient Voxel-Based Deep Learning Approach for Ligand Binding Site Detection"***	Jingbo Liang and Bruna Jacobson
6:40 pm	**Closing Remarks**	