

S2C2 CryoEM Map Modeling and Validation Workshop

September 8-10, 2021

Agenda

Wednesday, September 8, 2021

Time	Title	Speaker
8:00 AM	Phenix tools for improving maps, and building, refining, and validating models	Paul Adams Pavel Afonine Christopher Schlicksup
9:30 AM	Using AlphaFold predicted structures in ChimeraX for cryoEM modeling	Tom Goddard
10:30 AM	Break	
10:45 AM	Model fitting and assessment in CryoEM maps with Segger, SegFit, and Q-scores	Grigore Pintilie
12:15 PM	Deposition, Validation, and Biocuration at the wwPDB	Jasmine Young Justin Flatt
1:25 PM	End of Day	

Thursday, September 9, 2021

Time	Title	Speaker
8:00 AM	Coot Tools for Cryo-EM Model-building, Refinement, Validation and Analysis	Paul Emsley
9:00 AM	Interactive physics-based model building with ISOLDE	Tristan Croll
10:00 AM	Break	
10:15 AM	Secondary structure annotation of reconstruction maps with Haruspex	Maximilian Edich Jola Mirecka
11:15 PM	Macromolecular models automatically built into cryo-EM maps and how to use them	Grzegorz Chojnowski
12:15 PM	CryoEM model validation, to avoid or correct errors at various resolutions	Jane Richardson
1:45 PM	End of Day	

Friday, September 10, 2021

Time	Title	Speaker
8:00 AM	Improving and validating map/model fits with TEMPy	Tristan Cragolini
9:30 AM	Virtual Torsion Plots to Validate Coarse RNA Conformation	Brinda Vallat
10:30 AM	Break	
10:45 AM	Model comparisons	Andriy Kryshtafovych
11:45 AM	Cryo-EM validation from the perspective of the EMDB and EMPIAR archives	Arjan Patwardhan

12:45 PM	Molecular dynamics flexible fitting extended: structures, ensembles and free energy of proteins and small molecules	Abhishek Singharoy + colleagues
2:00 PM	Close of Meeting	