

DAY 1: THURSDAY, APRIL 16 2026

9:00 – 9:45	Introduction to ICM Core ICM principles, molecular graphics, visualization, and working with ICM objects.
9:45 – 10:30	Drug Target Analysis Structure quality assessment and preparation, binding pocket identification.
COFFEE BREAK	
10:45 – 12:00	Protein Modeling and Engineering Linking structure to sequence alignments, protein and loop modeling workflows and predict effect of mutation.
LUNCH PROVIDED BY MOLSOFT	
1:00 – 2:30	Chemical Structure Analysis SAR and Library Design Cheminformatics: chemical spreadsheets, clustering, search, property prediction, MPOs, SAR & Activity Cliff analysis, and library enumeration.
COFFEE BREAK	
2:45 – 3:30	3D Pharmacophore Modeling Atomic Property Fields (APF) methodology. Ligand-based superposition, screening and scaffold hopping.
3:30 – 4:30	Lead Optimization, Design and AI Decoration ICM 3D Ligand Editor – ligand editing, docking, R-group search, core replacement and AI decoration.
4:30 – 5:00	Q&A Session ICM discussion and technical questions.

DAY 2: FRIDAY, APRIL 17 2026

9:00 – 11:15	Virtual Ligand Screening and Lead Discovery Advanced Docking Strategies: Mastering induced fit, covalent, template and fragment-based methods. Learn to optimize hitlist analysis and prioritize compounds for experimental follow-up. LigandAide <i>de novo</i> ligand generation via AI Design Evolution
COFFEE BREAK	
11:15 – 12:00	PROTAC Modeling Ternary Complex Modeling: Predicting the structural assembly of the Target-PROTAC-E3 Ligase complex.
LUNCH PROVIDED BY MOLSOFT	
1:00 – 1:45	MolScreen – AI and ML Models Combining Deep Learning with Docking: Millions of preclinical activity data points incorporated into >2500 AI models for drug targets and ADMET prediction.
1:45 – 2:30	Molecular Dynamics GPU-Powered Simulations and Enhanced MD Snapshot Analysis in ICM
COFFEE BREAK	
2:45 – 4:00	GPU/AI 3D- Structure and Ligand Based Library Screening of Ultra Large Libraries <ul style="list-style-type: none">• GINGER - Graph Internal-coordinate Neural-network conformer Generator Energy Refinement for Large Chemical Libraries• RIDE - Rapid Isostere Discovery• RIDGE - Rapid Docking GPU Engine• CombiRIDGE – Efficient combinatorial anchored docking for virtual screening
4:00 – 5:00	Q&A Session with MolSoft's Scientists and Developers.

Agenda subject to change.