

**DAY 1: THURSDAY, APRIL 16 2026**

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

## DAY 2: FRIDAY, APRIL 17 2026

9:00 – 10:30	<b>Virtual Ligand Screening and Lead Discovery</b> (Andrew Orry Ph.D.) Advanced Docking Strategies: Mastering induced fit, covalent, template and fragment-based methods. Learn to optimize hitlist analysis and prioritize compounds for experimental follow-up.
10:30 – 11:15	<b>groupGen and LigandAide</b> (Maxim Totrov Ph.D. CTO) AI Ligand optimization and <i>de novo</i> ligand generation via AI Design Evolution
COFFEE BREAK	
11:15 – 12:00	<b>PROTAC Modeling</b> (Andrew Orry Ph.D.) Ternary Complex Modeling: Predicting the structural assembly of the Target-PROTAC-E3 Ligase complex.
LUNCH PROVIDED BY MOLSOFT	
1:00 – 1:45	<b>MolScreen – AI and ML Models</b> (Polo Lam Ph.D. Senior Scientist ) 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	<b>Molecular Dynamics</b> (Andrew Orry Ph.D.) GPU-Powered Simulations and Enhanced MD Snapshot Analysis in ICM
COFFEE BREAK	
2:45 – 4:00	<b>GPU/AI 3D- Structure and Ligand Based Library Screening of Ultra Large Libraries</b> (Eugene Raush, Principal Developer) <ul style="list-style-type: none"><li>• <b>GINGER</b> - Graph Internal-coordinate Neural-network conformer Generator Energy Refinement for Large Chemical Libraries</li><li>• <b>RIDE</b> - Rapid Isostere Discovery</li><li>• <b>RIDGE</b> - Rapid Docking GPU Engine</li><li>• <b>CombiRIDGE</b> – Efficient combinatorial anchored docking for virtual screening</li></ul>
4:00 – 5:00	<b>Q&amp;A Session</b> (Ruben Abagyan Ph.D. MolSoft Founder and MolSoft Team)

Agenda subject to change.