ICM Computational Drug Discovery Workshop
Agenda

April 4-5, 2024
San Diego, CA

Thursday April 4th, 2024

9:00 – 9:45 Introduction to ICM (Ruben Abagyan Ph.D.)
- Basic ICM Principles
- Molecular Graphics
- ICM Objects and Documents

9:45 – 10:30 Protein Structure Analysis

10:30 – 10:45 Break

10:45 – 12:00 Sequence-Structure Alignments and Protein Modeling

12:00 – 1:00 Lunch provided by MolSoft

1:00 – 2:30 Cheminformatics
- Chemical Search and Clustering
- Property Prediction and MPOs
- SAR Analysis
- Library Enumeration by Markush and Reaction

2:30 – 2:45 Break

2:45- 3:30 3D Pharmacophore – Atomic Property Fields

3:30-4:30 Lead Optimization and Design using ICM 3D Ligand Editor
Developed with Medicinal Chemists at Novartis
- How to setup the Receptor and Ligand
- Visualizing Ligand-Receptor Interactions
- Ligand Editing
- Scaffold Hopping
- Core Replacement

4:30 – 5:00 Q&A

Friday April 5th, 2024

9:00 – 10:30 Docking and Virtual Ligand Screening (Andrew Orry Ph.D.)

- Induced Fit
- Template
- Fragment
- Post Screening Analysis

10:30 – 10:45 Break

10:45 – 11:15 Covalent Docking

11:15 – 12:00 PROTAC Modeling and Docking

12:00 – 1:00 Lunch provided by MolSoft

1:00 – 1:45 MolScreen – Combining Deep Learning with Docking (Polo Lam Ph.D)

- How to screen chemicals against the MolScreen panel
- Drug Target Panel
- ADMET Panel
- Model preparation example.

1:45 – 2:30 Molecular Dynamics in ICM using OpenMM (Max Totrov CTO Ph.D.)

2:30 – 2:45 Break

2:45 – 4:00 GPU-Based Ultra Large Library Screening (Eugene Raush Principal Developer)

- RIDE - Rapid Isostere Discovery Engine
- RIDGE – Rapid Docking GPU Engine
- GigaScreen – Deep Learning

4:00 – 5:00 Q&A with MolSoft's ICM Developers

Agenda Subject to Change