MolSoft ICM Workshop

*In Silico* Drug Design

March 6th, 2018

Hosted by Chapman University

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Workshop Schedule

Presented by: Andrew Orry Ph.D. (Senior Scientist, MolSoft LLC)
Hosted by: Prof. Keykavous Parang Ph.D. (Professor of Medicinal Chemistry and Pharmacology, Chapman University School of Pharmacy)
Location: Room 205, 9501 Jeronimo Road Chapman University Irvine, CA 92618

9:00 – 9:30 Registration

9:30 – 9:45 Introduction to the ICM Software

9:45 – 10:30 3D Molecular Graphics, Documents and Movies

- PDB search and conversion to an ICM object
- Molecular representations, coloring, annotation and labeling
- Ligand binding pocket display and hydrogen bonds
- Graphics effects and high-quality images for publication
- Slides and viewpoints
- Importing fully interactive 3D molecules in PowerPoint and Web
- Molecular movies

10:30 – 12:00 Sequence-Structure Alignments and Protein Modeling

- Sequence alignments, annotation and editing
- BLAST search in ICM
- Link sequence and alignment to structure
- Homology Modeling
- Loop Modeling

12:00 – 1:00 Break for Lunch

1:00 – 2:00 Ligand Docking and Lead Optimization: ICM Fully Interactive Ligand Editor

- Ligand pocket display options.
- Ligand docking and minimization.
- Ligand editing and screening for best replacement group
- Tethering and distance restraints during docking
- Docking to Atomic Property Fields
- Docking to Multiple Receptor Conformations.

2:00 – 2:45 Cheminformatics

- Chemical Sketching
- Working with chemical spreadsheets.
- Chemical substructure and fingerprint searching.
- Chemical clustering
- Chemical superposition
- Virtual library enumeration
- **MolScreen** - a set of high quality 2D fingerprint and 3D pharmacophore models for a broad range of pharmacology and toxicology targets.

2:45 – 3:00 Break

3:00 – 4:00 Virtual Ligand Screening

- Structure-based virtual screening
  - How to prepare databases for screening
  - How to make a hitlist of the results
  - Post-screening analysis
- Fragment screening
- Covalent ligand screening
- Ligand-based screening using Atomic Property Fields

4:00 – 4:40 Methods for incorporating Induced Fit in Docking and Screening

- 4D Multiple Receptor Docking
- Selected Side Chain Hybrid Maps/Explicit Docking

4:40 - Question and Answer Wrap Up Session

Schedule is subject to change