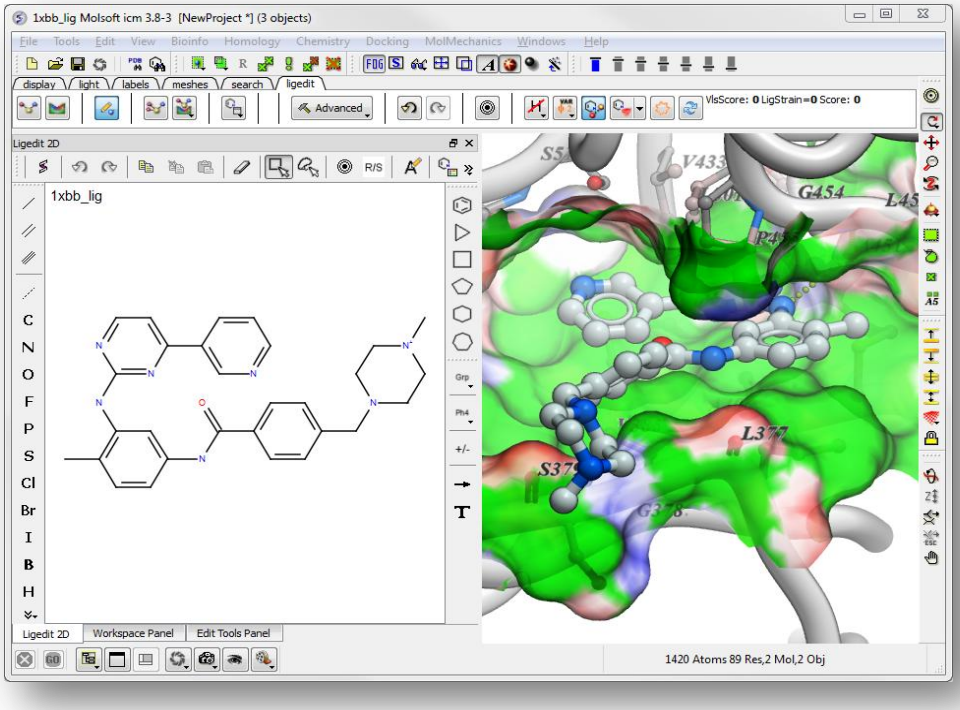
molsoft
molecules *in silico*

ICM Workshop
Protein Structure and Drug Design

Nov 13th

UCL London UK



Workshop Schedule

Workshop hosted by Shozeb Haider Ph.D. (UCL, London)
Presented by Andrew Orry Ph.D. (Senior Scientist, MolSoft LLC)
andy@molsoft.com | 858-625-2000 x108

9:30 – 9:40 Introduction to the ICM Desktop Modeling Software

9:40 – 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 – 10:45 Coffee Break

10:45 – 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 Lunch

1:00-2:00 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.
- Covalent Docking

2:00-2:45 Cheminformatics

- How to use the Molecular Editor

- How to work with Chemical Spreadsheets.
- How to download and work with ChEMBL and SureCHEMBL data
- Chemical searching
- Chemical clustering
- Combinatorial library generation (Markush and Reaction)

2:45-3:00 Break

3:00 - 4:00 Virtual Ligand Screening and MolScreen

- Structure-based virtual ligand screening
- Ligand-based 3D pharmacophore screening
- MolScreen: >900 polypharmacology models

4:00 Question and Answer Wrap Up Session

Schedule is subject to change