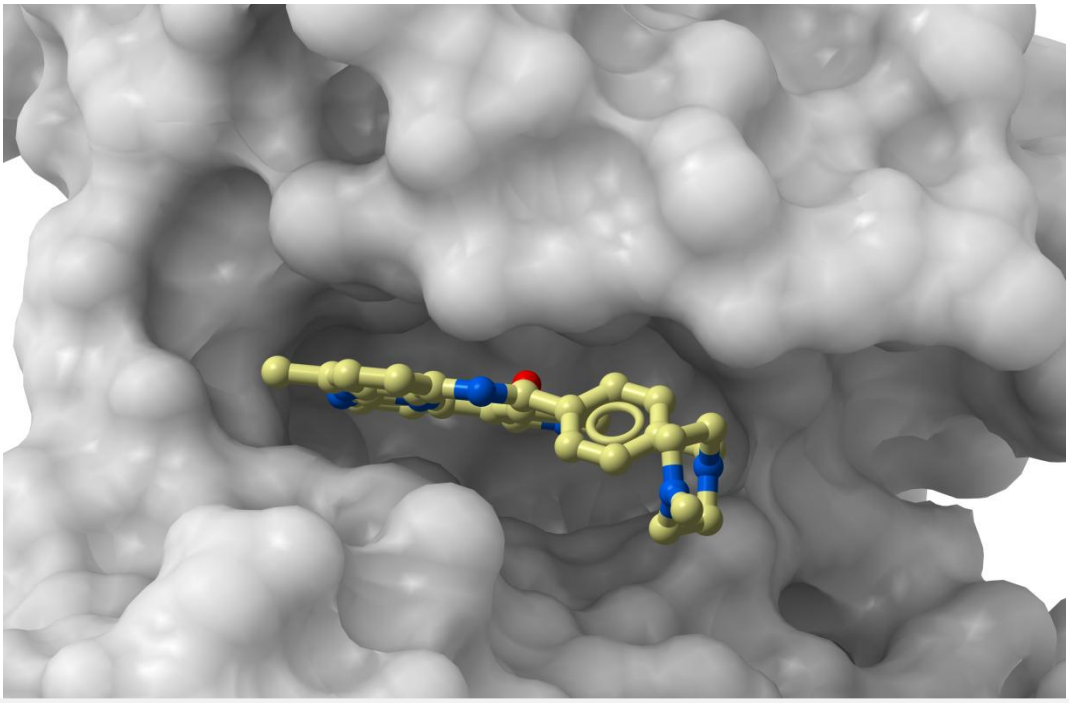
San Diego, CA



MOLSOFT WORKSHOP

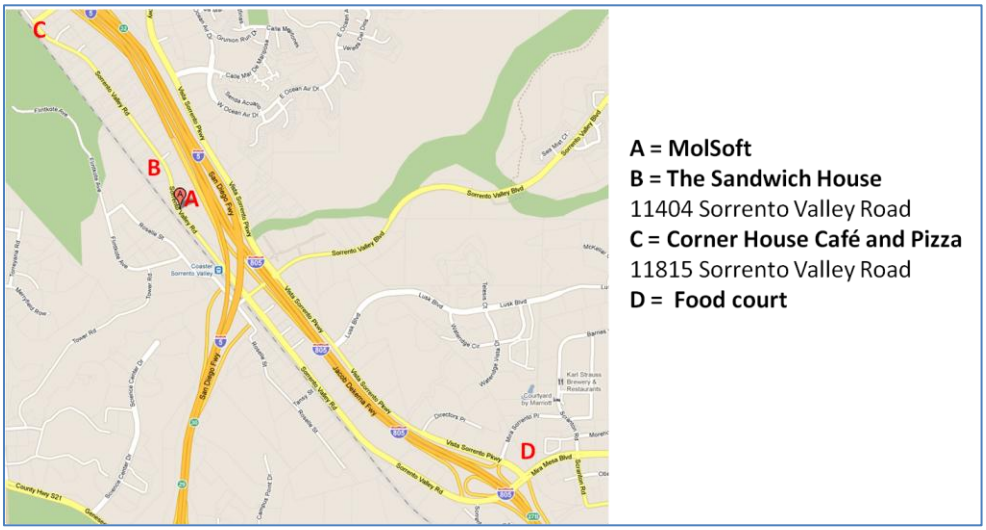
PROTEIN STRUCTURE & DRUG DESIGN

www.molsoft.com | info@molsoft.com

General Instructions

Thank you very much for attending the ICM workshop “Protein Structure and Drug Design”. We hope you enjoy the workshop and find it useful for your research projects. All workshop tutorials and presentations can be downloaded from out ftp site (the address will provided at the start of the workshop).

Coffee and snacks will be provided during the breaks and the workshop will close with a wine and cheese reception. There are a number of nearby restaurants for lunch (see map below) and if you want to you can bring lunch back to MolSoft to eat in the meeting room or foyer. We request lunch is not eaten in the computer training room.



If you have any questions during or after the workshop please contact:

Andrew Orry Ph.D. – E-mail: andy@molsoft.com Call: 858-625-2000 x108

Instructors

Ruben Abagyan Ph.D. MolSoft Founder and Professor UCSD

Max Totrov Ph.D. Principal Scientist, MolSoft LLC

Andrew Orry Ph.D. Senior Research Scientist, MolSoft LLC

Polo Lam Ph.D. Senior Research Scientist, MolSoft LLC

Day 1

9:00 - 10:15	**ICM Methods and Success Stories** **Presentation by Ruben Abagyan Ph.D. (RA)**
10:15 - 10:30	**Break**
10:30 – 11:20	**Molecular Graphics, Movies, and Documents** **Hands-on examples guided by Andrew Orry Ph.D (AO).** • Molecule selection and representations • Graphics coloring, labeling and annotation • Stereo viewing • Molecular slides and documents • Molecular documents in PowerPoint and the Web • Publication quality images • Molecular movies.
11:20 -12:00	**Sequence Analysis, Alignments and Bioinformatics** **Hands-on examples guided by AO.** • Importing sequences and extract sequences from PDB files • BLAST search • Making an alignment • How to use the alignment editor • How to link sequence to structure
12:00 - 1:00	**Lunch**
1:00 - 2:30	**Protein Structure Analysis** **Hands-on examples guided by AO.** • PDB structure preparation • Crystallographic data analysis • Measuring distances and angles • Ramachandran plot • Calculating contact and surface areas • Protein superposition • RMSD calculation • Prediction of ligand binding pockets and cavities • Prediction of protein-protein interaction sites

2:30 - 2:45	**Break**
2:45 - 3:45	**Homology Modeling, Refinement, and Simulations** **Presentation by RA**
3:45 – 5:00	**Modeling Examples** **Hands-on examples guided by AO and RA** • Building a homology model • Homology model analysis – checking for errors • Loop modeling and optimization • Side-chain refinement • How to incorporate modeling restraints. • How to work with stacks of conformations • Predicting the effect of a mutation
4:45-5:00	**Questions & Answers Session.**

Day 2

9:00 - 10:00	**Cheminformatics** **Hands-on examples presented by AO** • Chemical Sketching • Working with chemical spreadsheets. • Chemical substructure and fingerprint searching. • Chemical clustering • Chemical superposition • Virtual library enumeration
10:00 - 10:30	**MolScreen** **Presented by Polo Lam Ph.D (Senior Research Scientist, MolSoft).** MolScreen is a set of high quality 2D fingerprint and 3D pharmacophore models for a broad range of pharmacology and toxicology targets.
10:30- 10:45	**Break**
10:45 – 11:15	**Small molecule docking: principles, strategies and pitfalls.** **Presented by Max Totrov Ph.D. (Principal Scientist, MolSoft) (MT)**
11:15 – 12:00	**Ligand Docking Examples** **Hands-on examples guided by MT**
12:00 - 1:00	**Lunch**
1:00 - 1:20	**Key concepts and methodology of Virtual Ligand Screening.** **Presentation by MT**
1:20 – 2:00	**Structure-based Virtual Ligand Screening Example** **Hands-on examples guided by Max Totrov Ph.D.**
2:00 – 3:00	**Advanced topics in docking: techniques for induced fit simulations and covalent docking.** **Hands-on examples guided by MT**

3:00 – 3:15	**Break**
3:15 – 3:30	**Protein-Protein Docking Presentation** **Presentation by MT**
3:30 – 3:45	**Protein-Protein Docking Example** **Hands-on examples guided by MT**
3:45 – 5:00	**ICM Interactive Ligand Editor** **Hands-on examples presented by AO** • Ligand and receptor setup • Pocket display options • Docking and Minimization • Ligand editing • Replacement group screening • Fragment linking • Docking distance restraints and tethers • Induced fit docking • Covalent docking • Ligand-based docking using Atomic Property Fields
5:00	**Questions & Answers followed by wine and cheese reception.**

Schedule is subject to Change