



Molsoft ICM Workshop

“Protein Structure and Drug Discovery”

Conducted by:

Prof. Ruben Abagyan (UCSD)

Dr. Maxim Totrov (Principal Scientist, Molsoft LLC)

“The objective of this training course/workshop is to help computational chemists and biologists to solve challenging problems in the area of drug discovery by efficient use of the science and technology present in ICM molecular modeling tools.” Ruben Abagyan, Molsoft Co-Founder

Program content subject to change without notice.

DAY 1	
9:00 - 10:00	ICM Methods and Success Stories – Talk by Ruben Abagyan
10:00 - 10:15	Break
10:15 – 11:00	Graphical User Interface and Molecular Graphics <ul style="list-style-type: none">• Molecule selection, representations, coloring, labeling and annotation.• How to make molecular slides and documents.• How to display molecular documents in PowerPoint and the Web.• How to make publication quality images and movies.
11:00 -12:00	Sequence Analysis, Alignments and Bioinformatics Tools <ul style="list-style-type: none">• How to import sequences and extract sequences from PDB files.• How to make 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 and Homology Modeling <ul style="list-style-type: none">• How to prepare a protein a structure from the PDB.• How to analyze crystallographic data.• How to measure distances and angles.• How to make an interactive Ramachandran plot.• How to calculate contact and surface areas.• How to superimpose proteins.• How to calculate RMSD.• How to predict ligand binding pockets and cavities.• How to predict protein-protein interaction sites.
2:30 - 3:00	Break
3:00 - 4:45	Homology Modeling, Structure Refinement, and Simulations <ul style="list-style-type: none">• How to build an homology model.• How to check for errors in a model.• How to build and optimize loops.• How to refine side-chains.• How to incorporate modeling restraints.• How to work with stacks.
4:45-5:00	Questions & Answers.

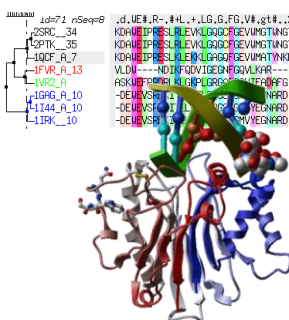
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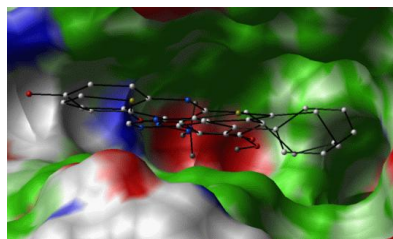
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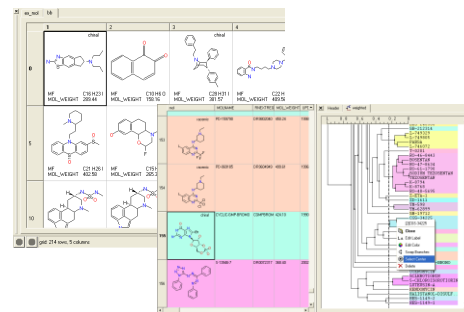
DAY 2	
9:00 - 9:30	Cheminformatics Introduction – Talk by Ruben Abagyan
9:30 - 10:45	Cheminformatics Tools <ul style="list-style-type: none"> • How to use the Molecular Editor. • How to work with chemical spreadsheets. • How to perform chemical substructure and fingerprint searching. • How to perform pharmacophore searching. • How to generate 3D conformers, tautomers, and stereoisomers. • How to perform chemical clustering. • How to perform chemical superposition. • How to build compound libraries. • MolCart and Local Databases.
10:45 - 11:00	Break
11:00-12:00	ICM 3D Interactive Ligand Editor <ul style="list-style-type: none"> • How to setup ligand and receptor. • How to display the binding pocket. • How to redock and minimize the ligand. • How to edit the ligand. • How to find the best replacement group. • How to insert a linker. • How to impose restraints to the ligand. • How to incorporate flexibility into the receptor.
12:00 - 1:00	Lunch
1:00-1:45	Docking Introduction – Talk by Max Totrov
1:45 - 2:30	Small Molecule Docking Examples <ul style="list-style-type: none"> • Re-dock biotin to the streptavidin receptor. • Re-dock an inhibitor to the ricin receptor. • Methods for incorporating induced fit upon ligand binding.
2:30 – 2:45	Break
2:45 – 3:00	Virtual Screening Introduction – Talk by Max Totrov
3:00 - 4:00	<ul style="list-style-type: none"> • Screening a small database of compounds to the ricin receptor. • Virtual screen a database of COX inhibitors to the cyclooxygenase receptor. • Screen a focused Markush library.
4:00 - 4:20	Protein-Protein Docking Introduction – Talk by Max Totrov
4:20 – 5:00	<ul style="list-style-type: none"> • Docking serine proteinase-protein inhibitor complex example.
5:00	Questions & answers followed by wine and cheese reception.



Sequence and Structure Analysis



Modeling and Docking



Drug Design and Cheminformatics

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