Molsoft ICM Workshop
"Protein Structure and Drug Discovery"

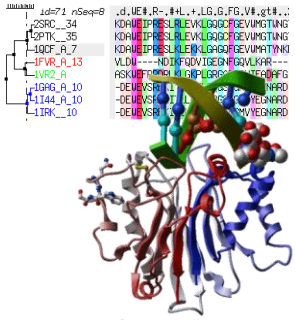
Conducted by:

Prof. Ruben Abagyan (UCSD)

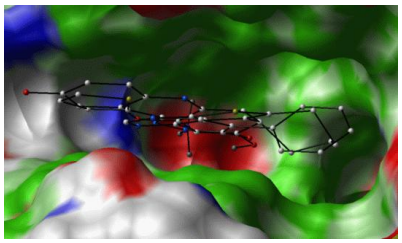
Dr. Maxim Totrov (Principal Scientist, Molsoft LLC)

"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

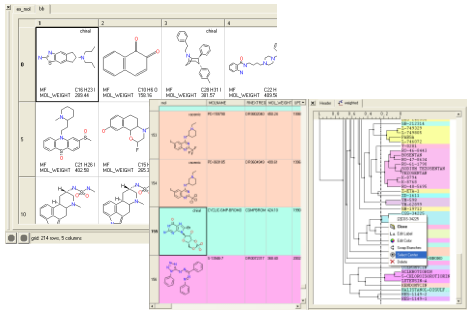
DAY 1	
9:00 - 10:00	ICM Methods and Success Stories
10:00 - 10:15	Break
10:15 – 11:00	Graphical User Interface and Molecular Graphics
11:00 -12:00	Sequence Analysis, Alignments and Bioinformatics Tools
12:00 - 1:00	Lunch
1:00 - 3:00	Protein Structure Analysis and Homology Modeling
3:00 - 3:15	Break
3:15 - 5:00	Structure Refinement and Simulations
DAY 2	
9:00 - 9:30	Cheminformatics Introduction
9:30 - 10:45	Cheminformatics Tools: Chemical drawing, spreadsheets, search, cluster, QSAR…
10:45 - 11:00	Break
11:00-12:00	ICM Ligand Editor
12:00 - 1:00	Lunch
1:00 - 2:00	Small Molecule Docking
2:00 – 3:30	Virtual Ligand Screening
3:30 – 3:45	Break
3:45 - 5:00	Protein-Protein Docking



Sequence and Structure Analysis



Modeling and Docking



Drug Design and Cheminformatics

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