

Molsoft ICM Workshop “Protein Structure and Drug Discovery”

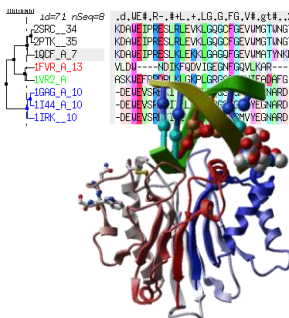
Conducted by:

Prof. Ruben Abagyan (The Scripps Research Institute)

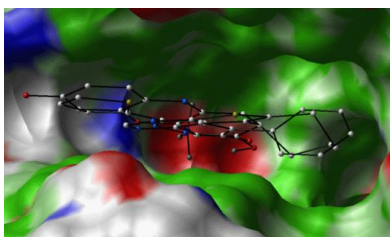
Dr. Maxim Totrov (Principal Scientist, Molsoft LLC)

“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

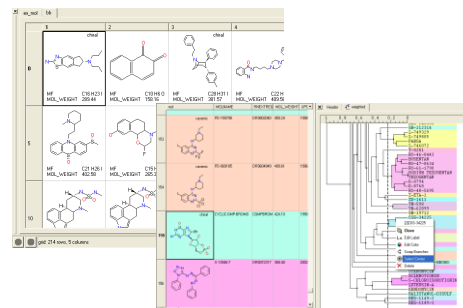
| DAY 1 | |
|---------------|---|
| 9:00 - 10:00 | ICM Methods and Success Stories |
| 10:00 - 10:15 | Break |
| 10:15 - 11:00 | Graphical User Interface and Molecular Graphics |
| 11:00 - 12:00 | Sequence Analysis, Alignments and Bioinformatics Tools |
| 12:00 - 1:00 | Lunch |
| 1:00 - 3:00 | Protein 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

Program content subject to change without notice.

For more details contact:

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