

## THURSDAY 9<sup>TH</sup> APRIL - MORNING SESSION

8:00am - 8:30am Meeting registration.

8:30am - 9:05am **Welcome by Prof. Ruben Abagyan, Ph.D.**

**Professor, The Scripps Research Institute, and MolSoft Founder**

*“ICM – Past, Present and Future”*

9:05am - 9:40am **Keynote Speaker: Maxim Totrov, Ph.D.**

**Principal Scientist, MolSoft LLC**

*“Atomic Property Fields (APF): methodology for ligand and receptor superposition and comparison”*

### ***PROTEIN STRUCTURE MODELING AND ANALYSIS***

9:40am – 10:05am **Irina Kufareva, Ph.D. (The Scripps Research Institute)**

*"Identification, characterization, and targeting of protein kinase exosites"*

10:05am - 10:25am **Break** - Refreshments provided by MolSoft

10:25am -11:00am **Keynote Speaker: Prof. Michael Sundström, Ph.D.**

**Managing Director, Novo Nordisk Foundation Center for Protein Research,  
University of Copenhagen**

*“Chemical bioprobes for structural and functional studies of medically relevant proteins”*

11:00am - 11:25am **Timothy Cardozo, M.D., Ph.D. (NYU)**

*"Deciphering conserved structures in dynamic or unstable protein surfaces."*

11:25am - 11:50am **Bengt Persson, M.D., Ph.D. (Linköping University & Karolinska Institute)**

*"Prediction of mutant severity using structural calculations in ICM"*

11:50am - 2:30pm **Lunch provided at Del Mar Powerhouse Park**

## THURSDAY 9<sup>TH</sup> APRIL AFTERNOON SESSION

2:30pm – 2:55pm **Lutz Tautz, Ph.D. (Burnham Institute for Medical Research)**

*“Structure-based design of tyrosine phosphatase inhibitors”*

2:55pm – 3:30pm **Keynote Speaker: Brian Marsden, Ph.D.**

**Structural Genomics Consortium, University of Oxford, UK**

*“Structural Biology Data Visualization for the Masses”*

## MEMBRANE PROTEIN MODELING AND DRUG DESIGN

3:30pm - 3:55pm **Aina Westrheim Ravna, Ph.D. (University of Tromso)**

*“Molecular modeling and docking studies of drug transporters using ICM”*

3:55pm - 4:10pm Break – Refreshments provided by MolSoft

4:10pm – 4:35pm **Lars Brive, Ph.D. (University of Goteburg)**

*“A hybrid receptor/ligand-based approach for dopamine receptor agonist selectivity.”*

4:35pm - 5:00pm **Vsevolod “Seva” Katritch, Ph.D. (The Scripps Research Institute)**

*“Structure based selectivity profiling for GPCR ligands”*

5:00pm - 5:25pm **Polo Lam, Ph.D. (MolSoft LLC)**

*“Modeling the Secretin Receptor”*

Evening **Sundowner Reception at MolSoft LLC**

## FRIDAY 10<sup>TH</sup> APRIL MORNING SESSION

7:00am- 8:15am Early morning walk at Torrey Pines State Reserve for early birds and jet lagged people! See flyer for more details.

### *CHEMICAL BIOLOGY AND CHEMINFORMATICS*

- 8:30am - 9:05am **Keynote Speaker: Dr. Eric Martin, Ph.D.**  
**Novartis Institute for Biomedical Research**  
*“Interactive Drug Design Using the ICM 3D Ligand Editor”*
- 9:05am- 9:30am **Valérie Campagna-Slater, Ph.D. (Structural Genomics Consortium, Toronto)**  
*“Out of the box computational chemistry -> Outside the box applications”*
- 9:30am - 9:55am **Olga Lomovskaya Ph.D. (MPex Pharmaceuticals)**  
*“Overcoming multi-drug resistance in bacteria”*
- 9:55am - 10:10am Break – Refreshments provided by MolSoft
- 10:10am - 10:45am **Keynote Speaker: Donovan Chin, Ph.D.**  
**Novartis Institute for Biomedical Research**  
*“FOCUS: A Software Platform For Virtual Medicinal Chemistry”*
- 10:45am - 11:10am **Professor Katherine Kantardjieff, Ph.D. (Cal State University - Fullerton)**  
*“Exploiting Structural Information for Modeling and Simulation: Guiding Principles from Chemistry”*
- 11:10am - 11:35pm **Eugene Raush, M.Sc. (MolSoft LLC)**  
*“Overview and recent development of Molsoft ActiveICM.”*
- 11:35pm - 1:30pm **Lunch on your own**

**FRIDAY 10<sup>TH</sup> APRIL AFTERNOON SESSION**

***PROTEIN-PROTEIN DOCKING***

- 1:30pm – 1:55pm **Juan Fernandez-Recio Ph.D. (Barcelona Super Computing Center )**  
*"Protein-protein docking with ICM and beyond: current and future challenges"*
- 1:55pm – 2:20pm **Andrew Bordner, Ph.D. (Mayo Clinic)**  
*"Peptide-MHC docking with ICM for epitope prediction".*

***STRUCTURE BASED DRUG DESIGN***

- 2:20pm - 2:45pm **Jianghong An, Ph.D. (BCGSC)**  
*"Discovery of a novel small-molecule inhibitor of the avian influenza H5N1 virus"*
- 2:45pm - 3:00pm Break – Refreshments provided by MolSoft
- 3:00pm - 3:25pm **Giovanni Bottegoni Ph.D. (Istituto Italiano di Tecnologia)**  
*"The Challenge of Receptor Flexibility in Molecular Docking Studies"*
- 3:25pm - 3:50pm **Edmond Ma, Ph.D. (University of Hong Kong)**  
*"Computer-Aided Drug Design and Lead Optimization: Small Molecule Inhibitor of Beta-Lactamase"*
- 3:50pm - 4:15pm **Colin Smith, Ph.D. (University of California at San Francisco)**  
*"Identifying druggable sites in protein structures and virtual screening-based discovery of PfENR inhibitors"*

***CLOSING PRESENTATION***

- 4:15pm – 5:15pm **Prof. Ruben Abagyan, Ph.D.**  
**Professor, The Scripps Research Institute, Founder, MolSoft LLC**
- Evening **Wine and cheese reception – Abagyan Lab - TSRI**