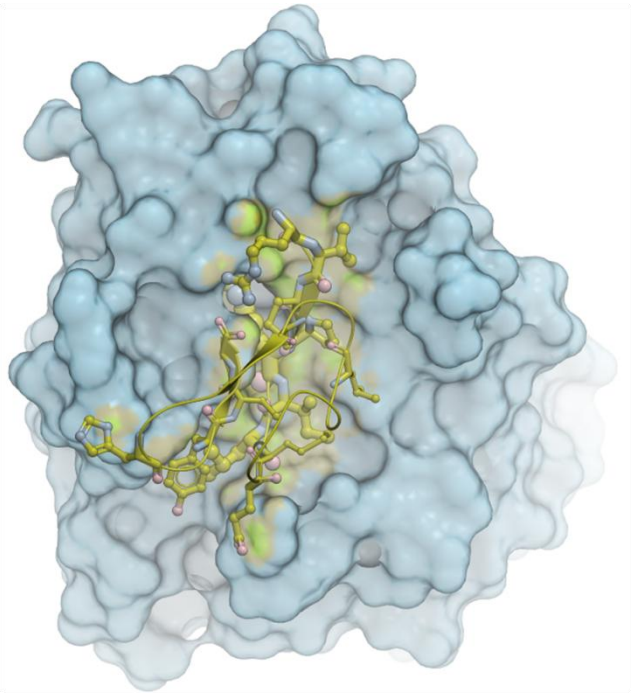
ICM User Group Meeting 2016

San Diego, CA March 17-18 2016,



THURS 17th MARCH MORNING

8:00 - 8:30 Meeting registration.

LATEST ICM DEVELOPMENTS

8:30 - 8:55 **Prof. Ruben Abagyan, Ph.D.**

Professor, University of California San Diego, and MolSoft Founder

Title to be announced

8:55 - 9:20 **Maxim Totrov, Ph.D.**

Principal Scientist MolSoft LLC

Title to be announced

9:20 – 9:*40* **Brian Marsden, Ph.D.**

Principal Investigator, Research Informatics at SGC, University of Oxford

Scarab – Data Capture, Integrator and Miner

9:40 - 9:55 **Break** - Refreshments provided by MolSoft

PROTEIN-PROTEIN INTERACTIONS

9:55 – 10:35 **Stanley Krystek Ph.D.**

Senior Principal Scientist Bristol-Myers Squibb

"Antibody Modeling & Computational Design of Optimized Molecules"

10:35 -11:00 **Xiangpeng Kong Ph.D.**

Principal Investigator, Associate Professor NYU

"ODA analyses of antigen binding sites"

11:00 - 11:25 **Irina Kufareva, Ph.D.**

Project Scientist at University of California, San Diego

"Chemokines and their receptors: structural insights into a key PPI in immunity, inflmation, and cancer""

11:25 - 2:20 **Lunch provided by MolSoft at Torrey Pines State Beach**

Eat, hike and swim. (weather permitting)

THURS 17TH MARCH AFTERNOON

ICM FOR TEACHING

2:25 – 2:50 **Charles Grisham, Ph.D.**

Professor of Chemistry, University of Virginia

"The Protein Structure and Function Exploration Project at the University of Virginia" by Charles Grisham and Julia Moy

2:50 – 3:15 **Katherine Kantardjieff, Ph.D.**

Dean, College of Science and Mathematics at Cal State San Marcos

"ICM as a robust tool to enhance learning in biochemistry"

3:15 - 3:40 **Kimberly Lane Ph.D**

Associate Professor, Radford University

"Molecular modeling of β-glucuronidase: Oligomerization, ligand binding, and drug design"

3:40 – 3:50 **Break** – Refreshments provided by MolSoft

GPCRS

3:50 - 4:15 **Vsevolod "Seva" Katritch, Ph.D.**

Assistant Professor USC

"Computational Modeling of GPCRs: Understanding Receptor Signaling for Biology and Drug Discovery"

4:15 – 4:40 **Ingebrigt Sylte Ph.D.**

Professor UiT

"Screening for new serotonergic compounds"

4:40 – 5:05 **Thomas Coudrat**

Ph.D. Candidate Monash University

"Structure-Based Drug Design Strategies for G Protein-Coupled Receptors"

FRIDAY 18TH MARCH MORNING

LATEST ICM DEVELOPMENTS

8:30 - 8:55 **Eugene Raush, M.Comp.Sc.**

Principal Developer MolSoft LLC

"New features and recent development in the Ligand Editor. ActiveIcmJS - JavaScript implementation of ICM shell and 3D graphics"

8:55 - 9:15 **Brian Marsden, Ph.D.**

Principal Investigator, Research Informatics at SGC, University of Oxford

"***ActiveIcmJS in WONKA & OOMMPPAA."***

CHEMINFORMATICS

9:15 - 9:40 **Valery Polyakov Ph.D.**

Senior Investigator I, Novartis Institute for Biomedical Research

"Clustering large datasets in KNIME for model building and hitlist triaging"

9:40 - 10:05 **Christine Hajdin Ph.D.**

Investigator, Novartis Institute for Biomedical Research

Title to be announced

10:05 - 10:30 **Giovanni Bottegoni Ph.D.**

Scientist Istituto Italiano di Tecnologia

"Ligand- and structure-based approaches to predicting activity"

10:30– 10:45 **Break** – Refreshments provided by MolSoft

CHEMICAL BIOLOGY & DRUG DESIGN

10:45 - 11:10 **Tim Cardozo Ph.D. MD**

Associate Professor, NYU

"***Inhibition of protein-protein interactions by stabilization"***

11:10 - 11:35 **Gennadiy Poda, Ph.D.**

Principal Scientist and Manager Computational Chemistry and Cheminformatics at Ontario Institute for Cancer Research, Toronto

"Structure-Based Design of Inhibitors as Potential Therapeutics for Multiple Myeloma and Leukemia"

11:35 - 12:00 **Lutz Tautz Ph.D.**

Research Associate Professor at Sanford Burnham Prebys Medical Discovery Institute

"Allosteric Inhibition of Protein Tyrosine Phosphatases"

12:00 – 2:30 **Lunch Provided by MolSoft at La Jolla Shores Beach**

Eat, Swim, Volley Ball etc… (weather permitting)

FRIDAY 18TH MARCH AFTERNOON

2:30 – 2:55 **Badry Bursulaya, Ph.D.**

Research Investigator, III at Genome Novartis Foundation

""Development of Mutant Selective Inhibitor of EGFR Kinase"."

2:55 – 3:20 **William Bisson, Ph.D.**

Assistant Professor at Oregon State University

"Computational Chemical Genomics in Cancer Drug Discovery and Prevention: Recent Applications"

3:20 - 3:45 **Shozeb Haider Ph.D.**

Excellence Fellow in Computational Medicinal Chemistry, UCL

"*Defining the architecture of KPC-2 carbapenemase: conditio sine qua non for resistance."*

3:45 – 4:10 **Manuel Rueda Ph.D.**

Senior Bioinformatician, Scripps Translational Science Institute

"ALiBERO: Hands-on session - Ligand-guided receptor optimization"

ROUND TABLE DISCUSSION

4:10 – 4:45 **Questions and answers with MolSoft's developers and scientists.**

followed by **Wine and cheese reception at MolSoft**