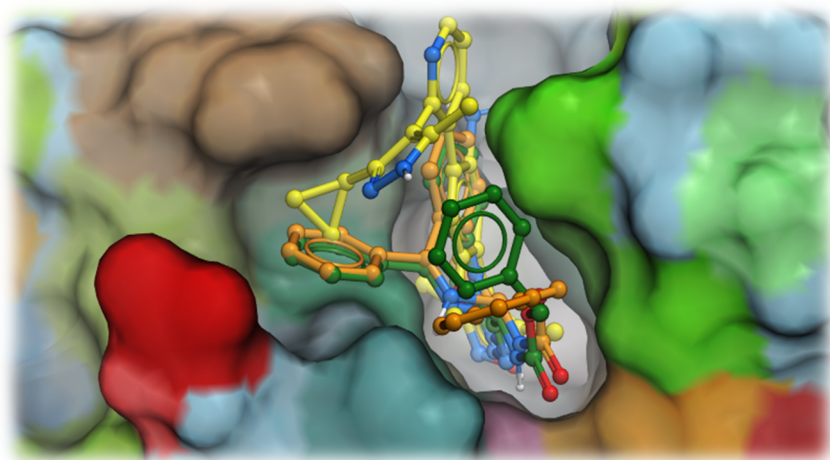# Advances in Physics and AI Methods for Drug Discovery

MolSoft ICM
User Group Meeting

May 17th to 18th 2023

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May 17th 2023

8:00   Welcome and Presentation by **Ruben Abagyan Ph.D.** (UCSD, MolSoft Founder)
       MolSoft ICM: Integrating Physics and AI in a Fast Giga Drug Discovery Pipeline

8:30   **Max Totrov Ph.D.** (CTO, MolSoft)
       New technologies in Molsoft ICM: neural networks and beyond.

9:00   **Brian Marsden Ph.D.** (University of Oxford)
       How Molsoft Scarab helped fight COVID-19 in the UK

9:45   Break

10:00 **Marc Nicklaus Ph.D.** (NCI)
       Mining in the Ultra-Large Library SAVI with the Help of Molsoft Tools.

10:30 **Nadya Tarasova Ph.D.** (NCI)
       Don't blame the software. It is the structure, bro.

11:00 **Wilnelly Martinez Ortiz Ph.D.** (Arrakis Therapeutics)
       Using ICM to target undruggables

11:30 **Evianne Rovers** (SGC, University of Toronto)
       Computational approaches and methodologies in proximity induced pharmacology.

May 18th 2023

8:00   **Eugene Raush** (Principal Developer, MolSoft)
Highlights of recent ICM developments: GPU acceleration, its applications and more

8:30   **Vsevolod "Seva" Katritch Ph.D.** (USC)
Computer Driven Discovery of GPCR Ligands with New Chemotypes and Functional Selectivity

9:00   **Andrea Cavalli Ph.D.** (Ecole Polytechnique Fédérale de Lausanne)
Thermodynamics and kinetics of drug-target binding via molecular simulations

9:30   **Shozeb Haider Ph.D.** (UCL)
Learning about PDC-3 β lactamase: from simulations to covalent docking.

10:00   **Tim Cardozo M.D. Ph.D.** (NYU)
Chemically probing the mechanism of KATP channels

10:30 Break

10:45   **Lutz Tautz Ph.D.** (Sanford Burnham Prebys Medical Discovery Institute)
Fragment-based Ligand Discovery for Protein Tyrosine Phosphatases

11:15   **William Bisson Ph.D.** (OHSU Knight Cancer Institute)
Design and development of intracellular paired agent imaging (iPAI) molecules for quantitative assessment of cancer drug target availability in live cells and tissues.

11:45   **John Dawson Ph.D.** (UCSD)
Using ICM to characterize the molecular determinants of antagonist interactions with chemokine receptors CCR2 and CCR5

12:15   **ICM Future Directions**
Round Table Discussion
Everyone is welcome to participate.