Apotekarsocieteten
Swedish Pharmaceutical Society

1st Nordic Conference on Computational Chemistry

August 30-31 2022, Gothenburg, Sweden

Program

Tuesday, August 30

09:30 **Registration**

10:00 **Welcome and Introduction**
Emma Evertsson, AstraZeneca

MD
Chair: *Werngard Czechtizky*, AstraZeneca

10:10 **Adventures in understanding gating and allosteric modulation of ion channels from experiments and simulations**
Erik Lindahl, Stockholm University

11:10 **Unraveling allosteric cross-talk between co-activator peptide and ligand binding site in glucocorticoid receptor**
Giuseppina La Sala, AstraZeneca, Gothenburg

11:30 **Markov state models of proton- and pore-dependent activation in a pentameric ligand-gated ion channel**
Cathrine Berg, KTH Royal Institute of Technology and SciLifeLab, Solna

11:50 Flash poster presentations

12:30 *Lunch*

Structure based and Ligand based design
Chair: *Eva Nittinger*, AstraZeneca

13:30 **Enzyme Dynamics Determine Potency and Selectivity of Inhibitors Targeting Disease-Transmitting Mosquitoes**
Anna Linusson, Umeå University

14:10 **Structure-based ligand discovery targeting GPCRs and enzymes**
Jens Carlsson, Uppsala University

14:50 **Estimating ligand-binding affinities with quantum-mechanical methods**
Ulf Ryde, Lund University

15:10 Posters and coffee

16:00 **Hit Discovery for RNA Ligands**
Ruth Brenk, Bergen University

16:40 **Semiempirical Quantum Mechanical Scoring in Structure-based Drug Design**
Martin Lepšík, Czech Academy of Sciences, Prague

17:00-17:20 **Computer-based solubility predictions of poorly water-soluble compounds in dog intestinal fluids administered with lipid-based formulations**
Aleksei Kabedev, Uppsala University

19:00 Dinner

Wednesday, August 31

08:30 Coffee/tea

Advances in QSAR and Machine Learning
Chair: *Anna Linusson*, Umeå University

9:00 **Predicting reactions selectivity**
Per-Ola Norrby, AstraZeneca

10:00 **De-novo design 2.0: challenges and opportunities**
Nadine Schneider, Novartis

10:40 Posters and coffee

Modelling of complex systems
Chair: *Anna Linusson*, Umeå University

11:10 **Conformational Landscapes of Membrane Proteins**
Lucie Delemotte, SciLifeLab

11:50 **Data-driven modeling of the liquid-liquid phase behavior of disordered proteins**
Giulio Tesei, University of Copenhagen

12:30 Lunch

Protein and peptide design
Chair: *Christian Tyrchan*, AstraZeneca

13:30 ***In silico* peptide & protein design**
Simone Fulle, NovoNordisk

14:10 **Enhancing Weak Affinity Chromatography (WAC™) fragment-based drug discovery for targeted hit expansion by integrating computational chemistry towards a novel hit-to-lead drug design platform**
Ricardo Ferreira**,** Red Glead, Lund

14:30 **De novo protein design of protein assembly platforms for protein display and delivery**
Ingemar André, Lund University

15:10 **Concluding remarks and poster prize**
Anna Linusson (representing the Pharmaceutical Society)
and Emma Evertsson

15:20 Coffee

15:40-16.40 Tour of the AstraZeneca site with the amazing journey