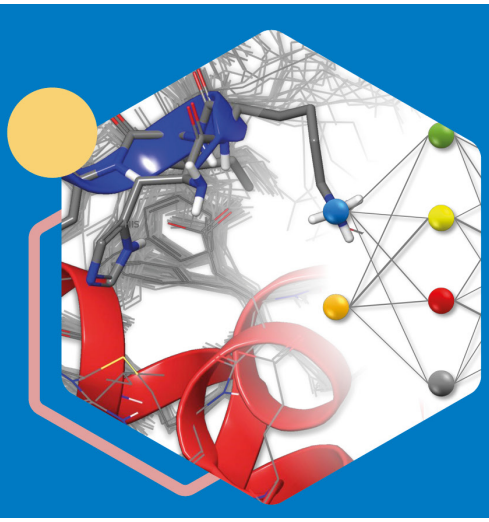
Apotekarsocieteten

The 2nd Nordic Conference on Computational Chemistry

18-19 March 2025



Preliminary program

Tuesday 18th March	
09.15 – 10.00	Registration
10.00 – 10.10	Welcome
10.10 – 12.10 *10.10 – 10.50* *10.50 – 11.30* *11.30 – 12.10*	**Session 1:** Chair: Simone Fulle, Novo Nordisk • **Title to be announced,** Charlotte Deane, Oxford University • **Computational biophysics at the proteome scale,** Kresten Lindorff-Larsen, Copenhagen University • **An integrative approach to study intrinsically disordered proteins: From solution behavior to interaction with surfaces,** Marie Skepö, Lund University
12.10 – 12.40	**Poster Flash presentations**
12.40 – 13.40	**Lunch**
13.40 – 15.00 *13.40 – 14.20* *14.20 – 15.00*	**Session 2:** Chair: Jens Carlsson, Uppsala University • **Current Developments in Chemical Space Exploration and Molecular Design,** Mathias Rarey, University of Hamburg • **Trends in GPCR drug discovery,** David Gloriam, Copenhagen University
15.00 – 15.20	**Selected talk:** **Discovery of small molecule modulators of FZD_7 using in silico docking screens,** Magdalena M. Scharf, Karolinska Institutet
15.20 – 16.20	**Break & poster session**
16.20 – 17.00 *16.20 – 16.40* *16.40 – 17.00*	**Selected talk:** **The ribosome lowers the entropic penalty of protein folding,** Julian O. Streit, University College London **Innovative computational drug design strategies at the intersection of automated molecule generation, machine learning, and free energy calculations,** Aniket Magarkar, Boehringer Ingelheim Pharma GmbH & Co
17.00 – 17.40	• **Structure prediction and design of protein interactions,** Efstathios Nikolaos Vlachos, Stockholm University, SciLifeLab
19.00 –	**Dinner**

Wednesday 19th March	
08.30 – 09.00	Entrance to conference
09.00 – 10.20 *09.00 – 09.40* *09.40 – 10.20*	**Session 3:** Chair: Ruth Brenk, University of Bergen • **Engineering Molecules to Specification with Generative AI,** Rocio Mercado, Chalmers • **Novel Technologies Impacting Drug Discovery across Modalities at Lundbeck,** Henrik Keränen, Lundbeck
10.20 – 11.10	**Break & poster session**
11.10 – 11.50	• **The holy grail of generative AI – from hit to candidate drug,** Eva Nittinger, AstraZeneca
11.50 – 12.10	**Selected talk:** **Bimodal Data Fusion of Compound Structures and Cell Morphology Features for AI-driven Mechanism of Action Prediction in Cancer Drug Discovery,** Osheen Sharma, Karolinska Institutet
12.10 – 13.15	**Lunch**
13.15 – 14.35 *13.15 – 13.55* *13.55 – 14.35*	**Session 4:** Chair: Ola Engkvist, AstraZeneca • **Exploring Chemical Space with Assembly Theory & Chemputation,** Lee Cronin, University of Glasgow • **Computational studies of permeation enhancers for orally administered peptide drugs,** Per Larsson, Uppsala University
14.35 – 15.00	**Poster Award and closing**
15.10 –	**Tour of AstraZeneca**

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