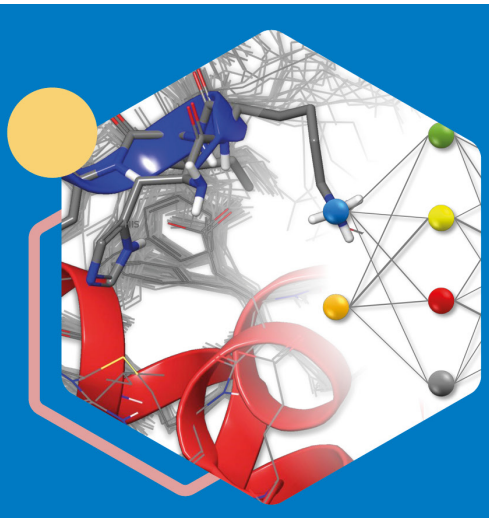
Apotekarsocieteten

# The 2nd Nordic Conference on Computational Chemistry

## 18-19 March 2025



## Program

| Tuesday 18th March | |
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| **09.15 – 10.00** | Registration |
| **10.00 – 10.10** | Welcome |
| **10.10 – 12.10**<br>*10.10 – 10.50*<br>*10.50 – 11.30*<br><br>*11.30 – 12.10* | **Session 1:** Chair: Simone Fulle, Novo Nordisk<br>• **The power and pitfalls of artificial intelligence in the design of new drugs,** Charlotte Deane, Oxford University<br>• **Computational biophysics at the proteome scale,** Kresten Lindorff-Larsen, Copenhagen University<br>• **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**<br>*13.40 – 14.20*<br><br>*14.20 – 15.00* | **Session 2:** Chair: Jens Carlsson, Uppsala University<br>• **Current Developments in Chemical Space Exploration and Molecular Design,** Mathias Rarey, University of Hamburg<br>• **Trends in GPCR drug discovery,** David Gloriam, Copenhagen University |
| **15.00 – 15.20** | **Selected talk:**<br>**Discovery of small molecule modulators of $FZD_7$ using in silico docking screens,**<br>Magdalena M. Scharf, Karolinska Institutet |
| **15.20 – 16.20** | **Break & poster session** |
| **16.20 – 17.20**<br>*16.20 – 16.40*<br><br>*16.40 – 17.00*<br><br><br>*17.00-17.20* | **Selected talk:**<br>**The ribosome lowers the entropic penalty of protein folding,** Julian O. Streit, University College London<br><br>**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<br><br>**Finding better drugs: advice for optimizing multi-parameter optimization scores,** Jenny Viklund, AstraZeneca |
| **19.00 –** | **Dinner** |

| Wednesday 19th March | |
|---|---|
| **08.30 – 09.00** | Entrance to conference |
| **09.00 – 10.20**<br>*09.00 – 09.40*<br>*09.40 – 10.20* | **Session 3:** Chair: Ruth Brenk, University of Bergen<br>• **Engineering Molecules to Specification with Generative AI,** Rocio Mercado, Chalmers<br>• **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:**<br>**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**<br>*13.15 – 13.55*<br>*13.55 – 14.35* | **Session 4:** Chair: Ola Engkvist, AstraZeneca<br>• **Exploring Chemical Space with Assembly Theory & Chemputation,** Lee Cronin, University of Glasgow<br>• **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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