

# 1<sup>st</sup> Nordic Conference on Computational Chemistry 2022

August 30-31, Gothenburg, Sweden

## Preliminary program

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### Tuesday, August 30

09:30      **Registration**  
10:00      Welcome and Introduction

#### MD

10:10      *Erik Lindahl*, Stockholm University  
11:10      Selected talk  
11:30      Flash poster presentations  
12:30      *Lunch*

#### Structure based and Ligand based design

13:30      *Anna Linusson*, Umeå University  
14:10      *Jens Carlsson*, Uppsala University  
14:50      Selected talk  
15:10      Posters and coffee  
16:00      **Structure-based design of riboswitch ligands and selective NMT inhibitors**  
*Ruth Brenk*, Bergen University  
16:40      Selected talk  
17:00-17:20 Selected talk  
  
19:00      Dinner

## Wednesday, August 31

### Advances in QSAR and Machine Learning

9:00 *Per-Ola Norrby, AstraZeneca*

10:00 *Nadine Schneider, Novartis*

10:40 Coffee and posters

### Modelling of complex systems

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

13:30 *Simone Fulle, NovoNordisk*

14:10 **De novo design of protein encapsulation system**  
*Ingemar André, Lund University*

14:50 Selected talk

15:10 Concluding remarks and poster prize

15:20 Coffee

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

Sponsor:

