

3rd Nordic Conference on Computational Chemistry

Preliminary Program March 17

09.30 *Registration with coffee/tea and sandwich*

Chair: TBD

10.00 **Introduction**

10.10 **Integrating rational, computational, and AI-based protein design**

Dek Woolfson, University of Copenhagen

10.50 **Functional Peptide Design Beyond Natural Chemistry**

Patrick Bryant, Stockholm University, SciLifeLab

11.20 **Selected talk**

11.40 **Sequence and structure-based computational approaches for discovering microbial immune systems**

Gemma Atkinson, Lund University

12.20 **Poster flash presentation**

12.40 *Lunch & Exhibition & Posters*

Chair: TBD

13.50 **TBD**

Francesca Grisoni, Eindhoven University of Technology

14.30 **AI Co-Chemist: From Soloist to Conductor**

Lakshidaa Saigiridharan, AstraZeneca

Anna Tomberg, AstraZeneca

15.10 **Selected talk**

15.30 *Coffee/tea, exhibition and poster session*

16.15 **Selected talk**

16.35- **Practical exploration of chemical reaction space**

17.05 *Jan Halborg Jensen, University of Copenhagen*

19.00 *Dinner*

Preliminary Program March 18

Chair: *TBD*

09.00 **Blending biology, chemistry and AI to enable systems pharmacology**

Patrick Aloy Calaf, IRB Barcelona

09.40 **Exploring chemical space with foundation models**

Andreas Lutten, Karolinska Institutet, SciLifeLab

10.10 **Poster flash presentation**

10.30 *Coffee/tea, exhibition and poster session*

11.20 **TBD**

Ainoleena Turku-Metsänen, Orion Pharma

11.50 **Selected talk**

12.10 **Selected talk**

12.30 Lunch & Exhibition

Chair: *TBD*

13.30 **Molecular mechanisms of lipid shuttling: how lipid transfer proteins extract and release membrane lipids**

Nathalie Reuter, University of Bergen

14.00 **TBD**

Anna Linusson, Umeå University

14.30 **Panel discussion**

Francesca Grisoni, Eindhoven University of Technology, Dek Woolfson, University of Copenhagen, Patrick Aloy Calaf, IRB Barcelona, Simone Fulle, Novartis and Ola Engkvist, AstraZeneca, Chalmers

15.10 **Concluding remarks and poster award announcement**

15.20 Tour of AstraZeneca, amazing journey