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1 Swedish Medicinal Chemistry Symposium
September 13-14, Stockholm, Sweden

Program

Wednesday, September 13

Session Chair: Peter Sjö

08:45 Registration

09:15 **Housekeeping - Opening remarks changing drug discovery environment**
Peter Sjö, AstraZeneca

09:45 **Drug discovery beyond the rule of 5 – Insight into design of cell permeable ligands for difficult targets**
Jan Kihlberg, Uppsala Universitet

10:15 **Function and pharmacology of cyclotides**
Ulf Göransson, Uppsala Universitet

10:45 *Coffee/fruits*

11:15 **The possibilities and challenges of small molecules that stabilise G-quadruplex DNA structures**
Erik Chorell, Umeå Universitet

11:45 **Are carbohydrate binding targets druggable: A case with Galectin 3**
Fredrik Zetterberg, Galecto Biotech

Poster flash presentation

12:15 **An unusual mode of inhibition of acetylcholinesterase: cooperative binding of crystal violet**
Anders Allgardsson, Totalförsvarets forskningsinstitut

12:20 **IAM chromatography: information provided and relevance in the prediction of permeability**
Giulia Caron, Univeristy of Turino

12:25 **Validated structural alerts for reactive metabolites**
Alf Claesson, Awametox AB

12:30 **Computational chemistry input to the development of highly potent and selective prevention of activation (POA) MK2 inhibitors**
Emma Evertsson, AstraZeneca

- 12:35 **Towards the Development of *Release-and-Report* Kinase Inhibitors as Molecular Tools for Investigating Neurodegenerative Diseases.**
Cassandra Fleming, Chalmers University of Technology
- 12:40 **An Approach to Capture Pre-reaction 3D Structural Information of Reactive Ligands**
Nina Forsgren, FOI
- 12:45 **What can be learnt from the testing of over 6 million compounds in antimalarial phenotypic whole parasite high throughput screens?**
Thomas Hansson, Medicines for Malaria Venture
- 12:50 **Transesterification of sulfonyl carbamates to generate new angiotensin II type 2 receptor (AT2R) ligands**
Rebecka Isaksson, Uppsala Universitet
- 12:55 **Modelling Permeation of Compounds through the Membrane of Gram-Negative Bacteria**
Peter Lind, Collaborative Drug Discovery, Burlingame
- 13:00 **Fragment-Based Drug Discovery Data – Hsp90 inhibitors as example of shared and collaborative data usage**
Alexander Minidis, Collaborative Drug Discovery, Burlingame
- 13:05 **Docking of Macrocycles: Comparing Rigid and Flexible Docking in Glide**
Gustav Olander, Uppsala Universitet
- 13:10 **HTS Assay Development: an airway mucus microenvironment modelling to be applied on cystic fibrosis drug discovery**
Sonja Visentin, University of Torino
- 13:15 **Lunch, Poster session & Exhibition**
- Session Chair:** Anna-Lena Gustavsson
- 14:45 **Beyond small molecules: harnessing new modalities to drug challenging biological targets**
Eric Valeur, AstraZeneca
- 15:15 **Modifications and conjugations for development of oligonucleotide therapeutics**
Roger Strömberg, Karolinska Institutet
- 15:45 **Coffee, Poster session & Exhibition**
- 16:15 **Identification of AZD9567, a glucocorticoid receptor modulator with improved side effect profile**
Lena Ripa, AstraZeneca
- 16:45 **Mingle with Poster Session, Exhibition & Cocktails**
- 18.00

Thursday, September 14

Session Chair: Mikael Elofsson

09:00 **Housekeeping**

09:15 **From phenotypic screen in primary cells to identification of selective CDK8/19 inhibitors as potential treatment of Diamond-Blackfan Anemia (DBA)**

Anna-Lena Gustavsson, Chemical Biology Consortium Sweden

09:45 **Creation of a Novel Class of Potent and Selective MTH1 Inhibitors Using Fragment-Based Screening and Structure-Based Drug Design**

Jenny Viklund, SprintBioscience

10:15 *Coffee/fruits*

10:45 **Computational chemistry in modern drug discovery**

Jens Carlsson, Uppsala Universitet

11:15 **Thermodynamics of binding interactions**

Johan Ulander, AstraZeneca

11:45 **Lunch, Poster Session & Exhibition**

13:00 **Award ceremony 2017 Medicinal Chemistry Prizewinner**

Session Chair: Anders Karlén

13:15 **Tailoring hit identification and qualification methods for targeting protein-protein interactions**

Björn Walse, SARomics Biostructures

13:45 **Chemical Warfare Agents: Structure, Mechanism and Design of Novel Antidotes**

Fredrik Ekström, Totalförsvarets forskningsinstitut (FOI)

14:15 **Concluding remarks – End of Symposium**

-14:30

Exhibitors

