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
Cassandra Fleming, Chalmers University of Technology

An Approach to Capture Pre-reaction 3D Structural Information of Reactive Ligands
Nina Forsgren, FOI

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

Transesterification of sulfonyl carbamates to generate new angiotensin II type 2 receptor (AT2R) ligands
Rebecka Isaksson, Uppsala Universitet

Modelling Permeation of Compounds through the Membrane of Gram-Negative Bacteria
Peter Lind, Collaborative Drug Discovery, Burlingame

Fragment-Based Drug Discovery Data – Hsp90 inhibitors as example of shared and collaborative data usage
Alexander Minidis, Collaborative Drug Discovery, Burlingame

Docking of Macrocycles: Comparing Rigid and Flexible Docking in Glide
Gustav Olander, Uppsala Universitet

HTS Assay Development: an airway mucus microenvironment modelling to be applied on cystic fibrosis drug discovery
Sonja Visentin, University of Torino

Lunch, Poster session & Exhibition

Session Chair: Anna-Lena Gustavsson

Beyond small molecules: harnessing new modalities to drug challenging biological targets
*Eric Valeur, AstraZeneca*

Modifications and conjugations for development of oligonucleotide therapeutics
*Roger Strömberg, Karolinska Institutet*

Coffee, Poster session & Exhibition

Identification of AZD9567, a glucocorticoid receptor modulator with improved side effect profile
*Lena Ripa, AstraZeneca*

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/fruit**

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