

SCHEDULE (last updated 2016-06-15, 18:00)

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25th Organikerdagarna & 23rd Analysdagarna

Aula Nordica and Universum, Umeå University Campus 14-17 June 2016

TUESDAY 14 JUNE

14.00- ARRIVAL & REGISTRATION & POSTER MOUNTING & COFFEE

16.00-16.30 **N430** Annual meeting/Årsmöte Division of Organic Chemistry/ Sektionen för organisk kemi

N440 Annual meeting/Årsmöte Division of Analytical Chemistry/Analytiska sektionen

16.30-17.00 OPENING OF CONFERENCE

17.00-18.00 **Aula Nordica** Chair: Charlotta Turner & Jonas Bergquist

Torbern Bergman Award lecture: Mass spectrometry of membrane proteins – The lipid connection
Carol Robinson, Oxford University, UK

18.00-19.00 **Aula Nordica** Poster pitch (1 slide, 2 minutes presentation) **Analysdagarna and Organikerdagarna**

19.00- GET-TOGETHER



WEDNESDAY 15 JUNE

08.30-09.20	Aula Nordica Chair: Berit Olofsson New strategies for catalytic C–H activation of aliphatic molecules Mathew Gaunt, University of Cambridge, UK				
09.20-10.00	COFFEE				
	<i>Organikerdagarna</i>			<i>Analysdagarna</i>	
10.00-12.00	N320 Seminar 1 Chair: Lukasz Pilarski	N360 Seminar 2 Chair: Christine Dyrager	N420 Seminar 3 Chair: Carl Johan Wallentin	N430 Seminar 4: Forensic analysis Chair: Yvonne Nygren	N440 Seminar 5: Chromatography I (SFC) Chair: Knut Irgum
10.00-10.30	<i>Paramagnetic ligand tagging to identify protein binding sites</i> , Mate Erdelyi, University of Gothenburg, Sweden	<i>The ruthenium-catalyzed click reaction in the synthesis of foldamers</i> , Nina Kann, Chalmers University of Technology, Sweden	<i>Identification and synthesis of compounds targeting specific G-quadruplex DNA structures</i> , Erik Chorell, Umeå University, Sweden	<i>Chemical attribution warfare agents</i> , Karin Höjer Holmgren, Swedish Defence Research Agency (FOI), Sweden	[10.00-10.15] <i>Ultra-high performance supercritical fluid chromatography – selectivity and speed</i> , Margareta Sandahl, Lund University, Sweden [10.15-10.30] <i>A novel targeted analysis of endogenous steroids by supercritical fluid chromatography coupled to tandem mass spectrometry</i> , Neil De Kock, Uppsala University, Sweden
10.30-10.45	<i>Development of oxophilic bitopic porphyrin host-guest systems</i> , Sandra Olsson, Uppsala University, Sweden	<i>Enhanced activity of cancer stem cell selective agents traced in ionophore properties</i> , Björn Borgström, Lund University, Sweden	<i>Redox-neutral coupling of sulfoxides and organometallic nucleophiles</i> , Kilian Colas, Stockholm University, Sweden	<i>Microextraction of nerve agent markers with hollowfiber-chemosorption</i> , Anders Östin, Swedish Defence Research Agency (FOI), Sweden	<i>Understanding the interplay between peripheral and central oxysterols by ultra-performance convergence chromatography with mass spectrometric detection</i> , Kumari Ubhayasekera, Uppsala University, Sweden

10.45-11.00	<i>Orientation effect of carboxyl ester groups in iron porphyrins for electrochemical CO₂ reduction to CO</i> , Ram Ambre, KTH Royal Institute of Technology, Sweden	<i>Synthesis, characterization and reactivity of vinyl benziodoxolones</i> , Elin Stridfeldt, Stockholm University, Sweden	<i>A one-pot four-component assembly of OTHOs using ionic liquids as carbene catalyst precursors</i> , Linda Ta, Chalmers University of Technology, Sweden	<i>Affinity enrichment and LC-MS as tools in forensic analysis of bioterrorism relevant toxins</i> , Tomas Bergström, Swedish Defence Research Agency (FOI), Sweden	<i>Screening of stationary phases for lipid profiling using ultra-high performance supercritical fluid chromatography</i> , Said Al-Hamimi, Lund University, Sweden
11.00-11.10	PAUSE	PAUSE	PAUSE	PAUSE	PAUSE
11.10-11.25	<i>New safe methods of determine presence of additive on dissolving grade pulp for Viscose production</i> , Hans Grundberg, Domsjö Fabriker, Sweden	<i>Ring-fused 2-pyridones inactivate the virulence regulator PrfA of Listeria monocytogenes</i> , Martina Kulén, Umeå University, Sweden	<i>Diglyme substitution strategies based on Hansen solubility parameters applied to coating reactions</i> , Hanno Priebe, Thermo Fisher Scientific, Norway	<i>A systematic approach to identify drugs</i> , Robert Waldebring, Nationellt Forensiskt Centrum - NFC, Sweden	<i>Peak deformations in supercritical fluid chromatography due to co-solvent adsorption</i> , Emelie Glenne, Karlstad University, Sweden
11.25-11.40	<i>Synthesis of multi ring-fused 2-pyridones – Modulators of alfa-synuclein amyloid aggregation</i> , Dan Adolfsson, Umeå University, Sweden	<i>Selective syntheses of heterocycles using Lewis acid catalysis</i> , Nicklas Selander, Stockholm University, Sweden	<i>Luminescent lanthanide complexes for multicolor imaging</i> , Eszter Borbas, Uppsala University, Sweden	<i>Non-destructive analysis of contaminated and ageing latent fingerprints – A Raman and fluorescence spectroscopy study</i> , Per-Ola Andersson, Swedish Defence Research Agency (FOI), Sweden	<i>What's in your food?</i> , Daniel McMillan, Sciex, Sweden
11.40-11.55	<i>3-(3,4-ethylenedioxythiophene)prop-1-yne (pyEDOT) – A new versatile building block for functionalized PEDOTs</i> , Xiao Huang, Uppsala University, Sweden	<i>Ruthenium catalyzed C-H silylation of unprotected gramines, tryptamines and their congeners</i> , Karthik Devaraj, Uppsala University, Sweden	<i>Design and synthesis of novel sialic acid conjugates as inhibitors of host cell attachment by sialic acid recognizing viruses</i> , Emil Johansson, Umeå University, Sweden		
12.00-13.00	LUNCH	LUNCH	LUNCH	LUNCH	LUNCH

Organikerdagarna

13.00-14.20

Aula Nordica Seminar 6

Chair: Nina Kann

13.00-13.40

Design and synthesis of chromone and chromane-4-one-based somatostatin mimetics and sirtuin inhibitors

Kristina Luthman, Gothenburg University, Sweden

13.40-14.20

Total synthesis of arctic marine natural products

Annette Bayer, University of Tromso, Norway

14.20-16.15

POSTER SESSION AND COFFEE

Organikerdagarna

16.15-18.10

N320 Seminar 8

Chair: Mate Erdelyi

N360 Seminar 9

Chair: Eszter Borbas

N420 Seminar 10

Chair: Erik Chorell

16.15-16.45

Boryl (hetero)aryne precursors – Synthesis via C-H activation and orthogonal reactivity, Lukasz Pilarski, Uppsala University, Sweden

Engaging carboxylic acids and derivatives in SET based catalysis, Carl Johan Wallentin, University of Gothenburg, Sweden

Efficient arylations with diaryliodonium salts, Berit Olofsson, Stockholm University, Sweden

16.45-17.00

Covalent protein labeling by enzymatic phosphocholination, Philipp Ochtrop, Umeå University, Sweden

Tuning potentials in quinone-based polypyrroles – Understanding pendant group effects on conducting redox polymers, Hao Huang, Uppsala University, Sweden

Direct chemoselective functionalization of carbohydrates via an ionic liquid mediated three-component reaction, Anton Axelsson, Chalmers University of Technology, Sweden

Analysdagarna

Hall A Seminar 7

Chair: Margareta Sandahl & Peter Spégel

Chromatographic and mass spectrometric methods in metabolomics

Tuulia Hyötyläinen, Örebro University, Sweden

Analysing pharmaceuticals in environmental samples

Jerker Fick, Umeå University, Sweden

POSTER SESSION AND COFFEE

Analysdagarna

N430 Seminar 11: Environmental analysis I

Chair: Fredrik Aldaeus

N440 Seminar 12: Chromatography II (CE & LC)

Chair: Anders Colmsjö

[16.15-16.30]
Isothiocyanates as potent skin sensitizers in rubber and model compounds to study molecular mechanisms behind skin allergy, Ulrika Nilsson, Stockholm University, Sweden

[16.30-16.45]
Discovery of novel ion-channel active peptide toxins in a North Sea ribbon worm, Håkan Andersson, Linnaeus University, Sweden

Microfluidic isoelectric focusing of amyloid beta peptides followed by micropillar-MALDI-MS, Åsa Emmer, KTH Royal Institute of Technology, Sweden

Target and suspect screening of OH-PAHs and other polar organic compounds in wood smoke particles, Rozanna Avagyan, Stockholm University, Sweden

Impact of elevated pressure on the adsorption mechanism in ultra-high pressure liquid chromatography, Dennis Åsberg, Karlstad University, Sweden

17.00-17.15	<i>Chiral anion directed asymmetric carbocation catalysis</i> , Shengjun Ni, KTH Royal Institute of Technology, Sweden	<i>Is spatial arrangement of carbohydrates an important factor in biological interactions?</i> , Brian Timmer, KTH Royal Institute of Technology, Sweden	<i>High-throughput screening for inhibitors of Pseudomonas aeruginosa ADP-ribosylating Exotoxin S</i> , Michael Saleeb, Umeå University, Sweden	<i>Chlorinated pesticides and natural brominated compounds in air at three northern Baltic stations</i> , Terry Bidleman, Umeå University, Sweden	<i>Analysis of polyvinyl alcohol microbubbles in human blood plasma using capillary electrophoresis</i> , Leila Josefsson, KTH Royal Institute of Technology, Sweden
17.15-17.25	PAUSE	PAUSE	PAUSE	PAUSE	PAUSE
17.25-17.40	<i>Photoaffinity labeling approach towards binding site identification of chroman-4-one based sirtuin 2 inhibitors</i> , Tina Seifert, University of Gothenburg, Sweden	<i>Glycerol valorisation using borrowing hydrogen methodology</i> , Anna Said Stålsmeden, Chalmers University of Technology, Sweden	<i>SP1-7 amide related peptides with anti-allodynic effect in spared nerve injury mice after systemic administration</i> , Anna Skogh, Uppsala University, Sweden	<i>Application of analytical methods in studies on mercury biogeochemical processes</i> , Liem Nguyen Van, Umeå University, Sweden	<i>Comparison of core shell columns from six vendors based on separation behavior and physical properties</i> , Henrik Svennberg, Teknolab Sorbent AB, Sweden
17.40-17.55	<i>Synthesis of aryl ketones and β-keto phosphonates by palladium(II) catalyzed addition reactions to nitriles</i> , Bobo Skillinghaug, Uppsala University, Sweden	<i>Metal-free C-arylation of nitro compounds with diaryliodonium salts</i> , Erik Lindstedt, Stockholm University, Sweden	<i>Counterion Influence on The N-I-N Halogen bond</i> , Alavi Karim, University of Gothenburg, Sweden	<i>LC-MS/MS analysis of antimicrobial compounds in sewage sludge and wastewater</i> , Marcus Östman, Umeå University, Sweden	<i>Facile synthesis of melamine-formaldehyde molecularly imprinted monolithic capillary columns for highly specific recognition and selective separation of phosphopeptides</i> , Mingquan Liu, Umeå University, Sweden
17.55-18.10	<i>Design and synthesis of benzothiadiazole derivatives for specific imaging of hypoxia-associated hallmarks in cancer</i> , Christine Dyrager, Linköping University, Sweden	<i>Bioinspired and biocoupled hydrogen production from methanol or formaldehyde</i> , Jan Deska, Aalto-universitetet, Finland	<i>Construction of organized materials through self-assembly of amyloid fibrils</i> , Niclas Solin, Linköping University, Sweden		

18.30 **BUS DEPARTURE** (from outside Aula Nordica)

19.00- CONFERENCE DINNER

The dinner and the midnight sun lecture will take place at a restaurant in the open air.

Dress code: Comfortable clothing and shoes that can handle the slightly chilly northern evening temperatures. Do not forget to bring your umbrella!

~~**Midnight sun lecture: Navigating the chemistry-biology interface – From new enantioselective CH activation to new biology**~~

~~Herbert Waldmann, Max Planck Institute of Molecular Physiology, Germany. **Cancelled due to the SAS pilot conflict.**~~

23.00 **FIRST BUS DEPARTURE BACK TO UMEÅ**

THURSDAY 16 JUNE

08.30-09.20	<p>Aula Nordica Chair: Charlotta Turner & Jonas Bergquist ChemPubSoc Europe lecture: Continuous green chemistry Martyn Poliakoff, University of Nottingham, UK</p>				
09.20-10.00	COFFEE	COFFEE	COFFEE	COFFEE	COFFEE
	Organikerdagarna			Analysdagarna	
10.00-12.00	<p>N320 Seminar 13 Chair: Daniel Strand</p>	<p>N360 Seminar 14 Chair: Luke Odell</p>	<p>N420 Seminar 15 Chair: Kenneth Wärnmark</p>	<p>N430 Seminar 16: Environmental analysis II Chair: Jerker Fick</p>	<p>N440 Seminar 17: MS for health I Chair: Åsa Emmer</p>
10.00-10.30	<p><i>Discovery of AZD1979 – An MCHR1 antagonist combining cardiac safety and free CNS exposure, Anders Johansson, AstraZeneca, Sweden</i></p>	<p><i>Synthetic mucin core glycopeptides to decipher lectin and antibody binding recognition events, Ulrika Westerlind, ISAS, Sweden</i></p>	<p><i>Boosting the antibacterial effect of salicylidene acylhydrazides by gallium complexation, Madeleine Ramstedt, Umeå University, Sweden</i></p>	<p><i>Targeted and untargeted MS and NMR metabolomics protocols in air pollution exposure studies, Malin Linder Nording, Umeå University, Sweden</i></p>	<p><i>Affinity-capture based methods for N-glycan analysis of serum and CSF proteins, Gunnar Thorsén, Stockholm University, Sweden</i></p>
10.30-10.45	<p><i>Synthesis and evaluation of spiro-oxindole dihydroquinazolinone based insulin-regulated aminopeptidase (IRAP) inhibitors identified by high-throughput screening, Karin Engen, Uppsala University, Sweden</i></p>	<p><i>NMR investigations of weak interactions in solution using β-hairpin peptides, Emma Danelius, University of Gothenburg, Sweden</i></p>	<p><i>Synthesis of beta-configured CuAAC clickable FDGs as novel [18F]fluoroglycosylation tools for PET in vivo imaging, Mathias Elgland, Linköping University, Sweden</i></p>	<p><i>Analysis of OH-PBDEs and OH-PCBs in coagulated seal blood, Dennis Lindqvist, Stockholm University, Sweden</i></p>	<p><i>Mass spectrometry imaging of mouse embryo implantation sites using nanospray desorption electrospray ionization, Ingela Lanekoff, Uppsala University, Sweden</i></p>
10.45-11.00	<p><i>Copper-mediated para-selective halogenation of nitrosoarenes, Angela Van Der Werf, Stockholm University, Sweden</i></p>	<p><i>A new Bargellini-Wittig hybrid reaction, Daniel Wiktelius, Swedish Defence Research Agency (FOI), Sweden</i></p>	<p><i>Macrocyclic peptides as inhibitors of human LSD1, Jie Yang, Uppsala University, Sweden</i></p>	<p><i>Selective detection of BTEX in air – Quinoxaline cavitands as novel solid-phase microextraction coatings, Nicolò Riboni, Stockholm University, Sweden</i></p>	<p><i>Analytical strategies for MS-based physicochemical characterisation of targeted drug delivery nanomedicines, Anna Nordborg, SINTEF, Norway</i></p>
11.00-11.10	PAUSE	PAUSE	PAUSE	PAUSE	PAUSE

11.10-11.25	<i>The Nordic Academic Compound Collection (NACC)</i> Mikael Elofsson, Chemical Biology Consortium Sweden & Umeå University, Sweden	<i>Structural insights into HI-6-assisted reactivation of acetylcholinesterase inhibited by sarin</i> , Lotta Berg, Umeå University, Sweden	<i>Pincer-iridium catalysts containing electron deficient ligands</i> , Oleksandr Kovalenko, Lund University, Sweden	<i>Direct analysis of free amino acids in soil solution via mixed-mode chromatography tandem mass spectrometry</i> , Ana Paola Vilches, Mid Sweden University, Sweden	<i>Influence of culture conditions on porphyrin production in oral bacteria</i> , Jonas Fyrestam, Stockholm University, Sweden
11.25-11.40	<i>Biphenyl-based arsine and arsole systems – Coordination chemistry and catalytic performance</i> , Andreas Orthaber, Uppsala University, Sweden	<i>Horner-Wadsworth-Emmons meets phosphorus</i> , Sascha Ott, Uppsala University, Sweden	<i>Development of bright fluorescent multi-cyclic adenine analogues</i> , Morten Grøtli, University of Gothenburg, Sweden	<i>Analysis of environmental and biomedical samples in investigations of alleged use of chemical weapons</i> , Jenny Rattfelt Nyholm, FOI, Sweden	<i>Novel applications of mass spectrometry in organic synthesis, purification and detection</i> , Vijay Gupta, Advion Ltd, United Kingdom
11.40-11.55	<i>Immobilisation of ruthenium metathesis catalysts in metal organic frameworks</i> , Jurjen Spekrijse, Chalmers University of Technology, Sweden	<i>Multienzymatic, one-pot cascade synthesis of enantiopure lamivudine precursor (2R, 5R)-1,3-oxathiolane</i> , Yansong Ren, KTH Royal Institute of Technology, Sweden	<i>Towards new insecticides for vector control – Characterization of acetylcholinesterase-1 from mosquito and identification of selective, non-covalent inhibitors by HTS</i> , Cecilia Engdahl, Umeå University, Sweden		
12.00-13.00	LUNCH	LUNCH	LUNCH	LUNCH	LUNCH
13.00-14.20	<i>Organikerdagarna</i>			<i>Analysdagarna</i>	
13.00-14.20	Aula Nordica Seminar 18 Chair: Rolf Carlson			Hall A Seminar 19 Chair: Gunnar Thorsén	
13.00-13.40	Studies of dehaloperophoramidine - Evolution of a total synthesis Peter Somfai, Lund University, Sweden			Chemometrics and multivariate analyses in analytical chemistry applications Johan Trygg, Umeå University, Sweden	
13.40-14.20	Complexity-generating reactions for screening library production Mads Hartvig Clausen, DTU, Denmark			Microfluidic electrochemical arrays for biosensing and organ-on-a-chip applications Jenny Emnéus, DTU, Denmark	
14.20-16.15	POSTER SESSION AND COFFEE			POSTER SESSION AND COFFEE	

	Organikerdagarna			Analysdagarna	
16.15-18.10	N320 Seminar 20 Chair: Anders Johansson	N360 Seminar 21 Chair: Ulrika Westerlind	N420 Seminar 22 Chair: Madeleine Ramstedt	N430 23: Chemometrics & Spectroscopy Chair: Jean Pettersson & Irene Rodriguez-Meizoso	N440 24: MS for health II Chair: Jörg Hanrieder & Margareta Ramström
16.15-15.45	<i>The making and breaking of amides</i> , Hans Adolfsson, Stockholm University, Sweden	<i>Imaging and control of protein activity by chemical probes</i> , Yaowen Wu, Max Planck Institute of Molecular Physiology, Germany	<i>Controlling the topology of self-assembly by covalent and supramolecular perturbations: Molecular belts, capsules and tubes</i> , Kenneth Wärnmark, Lund University, Sweden	<i>The use of principal component analysis for interpretation of ICP-MS and ICP-AES data</i> , Jean Pettersson, Uppsala University, Sweden	<i>Probing Aβ-plaque pathology in transgenic Alzheimer's disease mice using hyperspectral chemical imaging</i> , Jörg Hanrieder, University of Gothenburg, Sweden
16.45-17.00	<i>Synthesis and in vitro evaluation of 5-substituted benzovesamicol ligands for the vesicular acetylcholine transporter</i> , Sara Roslin, Uppsala University, Sweden	<i>Synthesis of porphyrin-oligothiophene conjugates for potential use in photodynamic therapy</i> , Katriann Arja, Linköping University, Sweden	<i>Development of photoswitchable kinase inhibitors</i> , Cassandra Fleming, Chalmers University of Technology, Sweden	<i>Studying supercritical fluid extraction kinetics by means of on-line detection and inverse modeling</i> , Victor Abrahamsson, Lund University, Sweden	<i>Analytical tools in viral proteomics and phosphoproteomics</i> , Sara Lind, Uppsala University, Sweden
17.00-17.15	<i>Heterocycle acrobatics – a 1,2-oxazole rearrangement applied to a concise total synthesis of siphonazole B</i> , Filip Paulsen, Lund University, Sweden	<i>Functionalization of fullerenes via metal catalysed hydroarylation</i> , Michael Nordlund, Uppsala University, Sweden	<i>Dynamic covalent catalysis: Screening, self-sorting and self-regulation in adaptive catalytic systems</i> , Fredrik Schaufelberger, KTH Royal Institute of Technology, Sweden	<i>The true colours of diabetes</i> , Andras Gorzsas, Umeå University, Sweden	<i>Mass spectrometry-based strategies for accurate protein quantification in multi species</i> , Margareta Ramström, Uppsala University, Sweden
17.15-17.25	PAUSE	PAUSE	PAUSE	PAUSE	PAUSE
17.25-17.40	<i>Palladium and nickel precatalysts in cross couplings</i> , Mikael Friberg, Merck, Sweden	<i>Mild deoxygenation of aromatic ketones and aldehydes over Pd/C using polymethylhydrosiloxane as the reducing agent</i> , Alexey Volkov, Stockholm University, Sweden	<i>Enzymes as valuable tools in organic processes</i> , Staffan Karlsson, AstraZeneca, Sweden	<i>Solubility in supercritical carbon dioxide: in situ studies by Raman spectroscopy and application on purification technology</i> , Irene Rodriguez-Meizoso, Lund University, Sweden	<i>Orbitrap and why resolution matters</i> , Anas Kamleh, ThermoFisher, Sweden

17.40-17.55	<i>A metal-free strategy for C-H functionalization of arenes via diaryliodonium salts, Marcus Reitti, Stockholm University, Sweden</i>	<i>Some mechanistic deliberations from the third row: iridium(I) catalysed cycloadditions based on C-C bond rupture, Daniel Strand, Lund University, Sweden</i>	<i>Sulfonyl azides as carbonylation precursors: Development of new multicomponent reactions, Luke Odell, Uppsala University, Sweden</i>	<i>Solubility of a high molar absorptivity compound in gas-expanded liquids using UV-vis technique, Larissa Cunico, Lund University, Sweden</i>	<i>A new approach to metabolomics - Using Seahorse XF analyzers and Agilent mass spectrometers, Dennis Buurman, Agilent, Sweden</i>
17.55-18.10		<i>A resistively heated reactor for continuous flow chemistry, Jonas Rydfjord, Uppsala University, Sweden</i>	<i>Modified glycopeptides targeting arthritis associated class II MHC DR4 proteins result in an altered T-cell epitope and response, Cecilia Lindgren, Umeå University, Sweden</i>		

FRIDAY 17 JUNE

	<i>Organikerdagarna</i>			<i>Analysdagarna</i>	
9.00-10.20	Aula Nordica Seminar 25 Chair: Hans Adolfsson			Hall A Seminar 26 Chair: Ulrika Nilsson	
09.00-09.40	Mechanistic insights into organocatalytic reactions Petri Pihko, University of Jyväskylä, Finland			HILIC Has come of age Knut Irgum, Umeå University, Sweden	
09.40-10.20	Charting the unknown - Novel targets and oral bioavailability beyond the rule of 5 Jan Kihlberg, Uppsala University, Sweden			Mass spectrometry analysis of metabolites in modern biology - From targeted trace analysis to untargeted profiling and flux analysis Thomas Moritz, SLU, Sweden	
10.20-10.50	COFFEE	COFFEE	COFFEE	COFFEE	COFFEE
10.50-11.40	Aula Nordica Chair: Hans Adolfsson Necessity is the mother of invention: Natural products and the chemistry they inspire Sarah Reisman, California Institute of Technology, USA				
11.40-12.00	Aula Nordica CLOSING REMARKS AND AWARDS				