ANALYTIKER-RINGEN
Sektion af Danmarks Farmaceutiske Selskab

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Selskabet for Analytisk Kemi
The Danish Society of Analytical Chemistry
SAK

Cordially invite you to a seminar on topics in Analytical Chemistry

Expending the Hyphenation of Separation Sciences and Mass Spectrometry for the Analysis of Pharmaceuticals and Metabolites in Biological Samples

by

Gérard Hopfgartner

Life Sciences Mass Spectrometry, Department of Inorganic and Analytical Chemistry
University of Geneva, 24 Quai Ernest Ansermet, CH-1211 Geneva 4

The seminar takes place

Thursday, November 22, 2018, 15:00 - 18:00

University of Copenhagen, Dept. of Pharmacy, Auditorium 4

Universitetsparken 2, 2100 København Ø.

Program

15:00-15:50	Possibility to visit the new research and teaching labs related to analytical activities at the Dept. of Pharmacy
15:55-16:05	We meet in Aud. 4 – welcome by Analytikerringen, SAK and IF
16:05-16.50	Presentation by Gérard Hopfgartner
16:50-17:00	Discussion
17:00-18:00	We walk over to the Atrium of the Pharma Science Building for drinks and snacks and networking

*Everybody interested is welcome to attend (registration before **Nov 15** is mandatory)*
To register, please follow this link:
http://farmaceutisk-selskab.dk/arrangementer/expending-the-hyphenation-of-separation-sciences/
Or https://tinyurl.com/y7kjf5g9

Abstract and Short Bio

Expending the Hyphenation of Separation Sciences and Mass Spectrometry for the Analysis of Pharmaceuticals and Metabolites in Biological Samples

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Accurate and precise identification and quantification of pharmaceuticals, endogenous metabolites and lipids in biological samples relies mostly on the combination of separation sciences and mass spectrometric detection. One of the major challenges is the chemical space and the dynamic range of the analytes of interest and calls for improved analytical workflows Supercritical fluid chromatography (SFC) has experienced a renaissance in the last decade offering an additional separation dimension to reversed phase chromatography. In LC-MS the ionization conditions are predominantly controlled by the mobile phase composition, whereas in SFC-ESI/MS, the ionization can be tuned using the addition of a liquid make-up, which is independent of the chromatographic conditions. The control of adduct formation in electrospray ionization has become a major issue for quantitative and qualitative analysis.

Current instrumental improvements in high resolution mass spectrometry (HRMS) have enabled data independent information acquisition (DIA) schemes, such SWATH using multiple Q1 windows of typically 25 Da. With SWATH a collision induced MS/MS spectra can be generated for every precursor ion from a given Q1 mass window enabling simultaneous quantitative and qualitative analysis (QUAL/QUANT). MS/MS database or the use of in-silico fragmentation tools enables multi-analytes quantification post-acquisition.

Ion mobility has demonstrated its potential to enhance the selectivity of quantitative LC-MS assays and for the separation of isobaric and isomeric compounds. Peak capacity and selectivity of the analytes can further be improved with the use of organic modifiers (e.g. alcohols, toluene) in differential mobility spectrometry (DMS) opening new tuning possibilities in multi-dimensional LC-MS separations.

Electron induced fragmentation (ExD) has been largely described for peptides analysis but far less for the analysis of low molecular weight compounds as singly charged analytes, in particular on an LC time scale. Recently, a chimeric collision cell (CID and EXD) mounted on a QqTOF platform has been described opening new possibilities in metabolites structural characterization.

In the present talk the benefits to apply multiple separation techniques (LC, SFC) with multiple MS and MS/MS techniques (SMR^3, DIA, IMS, ExD) will be presented with focus on bioanalysis, drug metabolomics and multi-omics.

Gérard Hopfgartner received his Ph.D. degree in 1991 in the field of organic geochemistry and mass spectrometry at the University of Geneva. From 1991 to 1992 he was postdoctoral fellow with Prof. Jack Henion at Cornell University, Ithaca, NY and worked in the field of atmospheric pressure ionisation mass spectrometry. From 1992 to 2002 he was in heading the LC-MS group and the bioanalytical section in the DMPK Department of F. Hoffmann-La Roche in Basel. In 2002 he joined the University of Geneva as a full Professor for Analytical Sciences and Mass Spectrometry in the School of Pharmaceutical Sciences. Since 2015 he is full Professor in the Department of Analytical and Inorganic Chemistry of the University of Geneva working in the field of life sciences around the development and application of novel mass spectrometry approaches with and without separation techniques for the analysis of pharmaceutical, metabolites and proteins. His current scientific focus includes hyphenated mass spectrometry, ion mobility spectrometry, electron induced fragmentation and mass spectrometry imaging. He acts also as an editor for Analytical Bioanalytical Chemistry.