Hyphenation of high-performance liquid chromatography or supercritical fluid chromatography to mass spectrometry: techniques and data evaluation

## **Abstract**

The hyphenation of highly efficient separation methods such as high-performance liquid chromatography (HPLC) or supercritical fluid chromatography (SFC) to spectroscopic methods that provide structural information, such as mass spectrometry (MS), represents a very powerful tool for chemical and biological analysis. Exploitation of different chromatographic separation modes as well as miniaturization of chromatographic separation are prime prerequisites both to enable the efficient on-line interfacing of HPLC and MS and to facilitate the analysis of femtomol to attomol amounts of analytes present in complex samples.

This workshop will introduce the basic principles of chromatographic separation in liquid and supercritical phase and discuss separation conditions that are suitable for the on-line hyphenation to mass spectrometry by means of atmospheric pressure ionization (including ESI, APCI, APPI).

Moreover, various approaches to data-dependent (DDA) or data-independent (DIA) data acquisition alongside with application in the qualitative and quantitative analysis of complex mixtures will be discussed.

As far as data interpretation is concerned, the workshop will provide some guidelines of systematic data interpretation based on (accurate) intact molecular mass and fragment ion mass data.

Finally, the workshop will discuss some selected examples of application from the analysis of metabolites, drug degradation products, pharmaceuticals, drugs of abuse, and lipids.

## **Biography Gérard Hopfgartner**

Gérard Hopfgartner studied chemistry at the University of Geneva and received his Ph.D. degree in 1991 in the field of organic geochemistry and mass spectrometry. Then he moved to Cornell University as a postdoctoral fellow working on atmospheric pressure ionisation LC-MS/MS. In 1992 he joined the bioanalytical section of F. Hoffmann-La Roche in Basel as the head of the LC-MS group. From 2002 to 2015 he was full Professor for analytical sciences and mass spectrometry in the School of Pharmaceutical Sciences at the University of Geneva and Lausanne. Since August 2015 he is full Professor in the department of Analytical and Inorganic Chemistry of the University of Geneva. His research interests focus on the development of novel mass spectrometry approaches with and without chromatography in the field of life sciences. His scientific interests include separation sciences, mass spectrometry, bioanalysis, metabolism, metabolomics, analytical proteomics, toxicology, multimodal fragmentation and ion mobility spectrometry.

## **Biography Christian Huber**

Christian Huber trained as an analytical chemist at the University of Innsbruck focusing on chromatographic separation methods for biopolymers. After a postdoc in Csaba Horváth's group at Yale University in 1996 focusing on building an instrument for capillary electrochromatography, he obtained lecturing qualification in analytical chemistry at the University of Innsbruck in 1997. As an associated professor of analytical chemistry at the University of Innsbruck from 1997 to 2002, he developed monolithic stationary phases for hyphenating high efficiency nucleic acid-, peptide-, and protein separations to mass spectrometry. From 2002-2008 he held a position as professor for analytical chemistry at Saarland University, where he started working in the field of proteome analysis and data mining of mass spectrometry data. Since 2008, he is a professor of chemistry for biosciences at the University of Salzburg. From 2013 to 2021 he led the Christian Doppler Laboratory for Biosimilar Characterization, which cooperated with Novartis and Thermo Fisher Scientific. His current research interests include proteome and metabolome analysis of biological models for disease as well as in-depth (therapeutic) protein characterization by means of HPLC and MS.