

# Department of Chemistry

## Departmental Seminar Series: Analytical Chemistry

You are cordially invited to a face-to-face lecture presented by



**Prof. Dr. Dr.h.c. Ralf Zimmermann**

University of Rostock and Helmholtz Centre Munich, Germany

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**Date:** Wednesday, 18 January 2023  
**Time:** 11h30  
**Venue:** The Orbital (Room 3-1 Chemistry Building)

### Coffee roasting and Cannabis smoke: Photoionisation mass spectrometry for studying of complex vapors

A rugged photoionization mass spectrometer (PIMS) for on-line, real-time process monitoring and optimization was developed. The use of VUV-based single-photon ionization (SPI) and resonance-enhanced multiphoton ionization (REMPI) time of-flight mass spectrometry (TOFMS) covers a broad range of compounds, including flavour compounds, toxicants or antioxidants. The benefits of PIMS are demonstrated by reporting on on-line analysis of coffee roasting off-gases and cannabis smoke vapours. a) Coffee roasting: In a chemically highly complex process, green coffee beans are turned into the starting product of one of the most popular beverages. On-line process monitoring of the coffee roasting process enables a better control of the product quality, in particular the flavour profile and likely also antioxidant capacity. Statistical data analysis such as non-negative matrix factorization (NMF) was applied on the PIMS results (four factor solution) allow us to recognize roasting phases which represent 'evaporation', 'early roast', 'late roast' and 'over-roast' status. Each roasting phase features a different molecular fingerprint, which was further investigated due to the high selectivity and softness of the ionization process, simplifying the interpretation of the factor loadings. Validity of the NMF results was proven by recovering known markers in the NMF loadings, e.g. pyridine for over-roast. The newly developed process mass spectrometer has been designed for industrial applications and was applied at large industrial coffee manufacturing plants. b) Cannabis vapours: As a second application the improved PIMS technology was applied for on-line, real-time detection of cannabinoids such as THC, CBD, CBN in the smoke/vapour of smokeable cannabis products (e-cigarette, thermal vaporizers, joint etc.). This technology can be used to e.g., develop new devices/products for legal recreational or medical cannabis application (i.e. minimize health risks of smoking/vaping devices), perform quality control, and ensuring compliance with current and future legislation.

#### Profile

Ralf Zimmermann is full professor of Analytical Chemistry at the University of Rostock and director of the research unit CMA at the Helmholtz Zentrum Munich. Furthermore, he is the speaker of the Department Life, Light & Matter of the Interdisciplinary Faculty of the University of Rostock and is heading the Competence Centre for Mass Spectrometry in the Department. He studied Chemistry and Physics and holds a PhD degree in Physical Chemistry. Among others activities he applies and develops novel (laser) mass spectrometric methods for on-line characterization of aerosols, process- and pyrolysis-gases and is interested in the comprehensive characterisation of ultra-complex molecular mixture using high resolution mass spectrometric technologies as well as multidimensional separation approaches. Recently he is focusing on the interdisciplinary investigation of the composition, toxicology and health impact of ambient aerosols and combustion emissions. He is heading the German-Israeli *aeroHEALTH* research initiative (*Helmholtz International Lab*).

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