Applied Analytical Chemistry (AAC)

Annual Report 2018

AAC
applied analytical chemistry

Applied Analytical Chemistry

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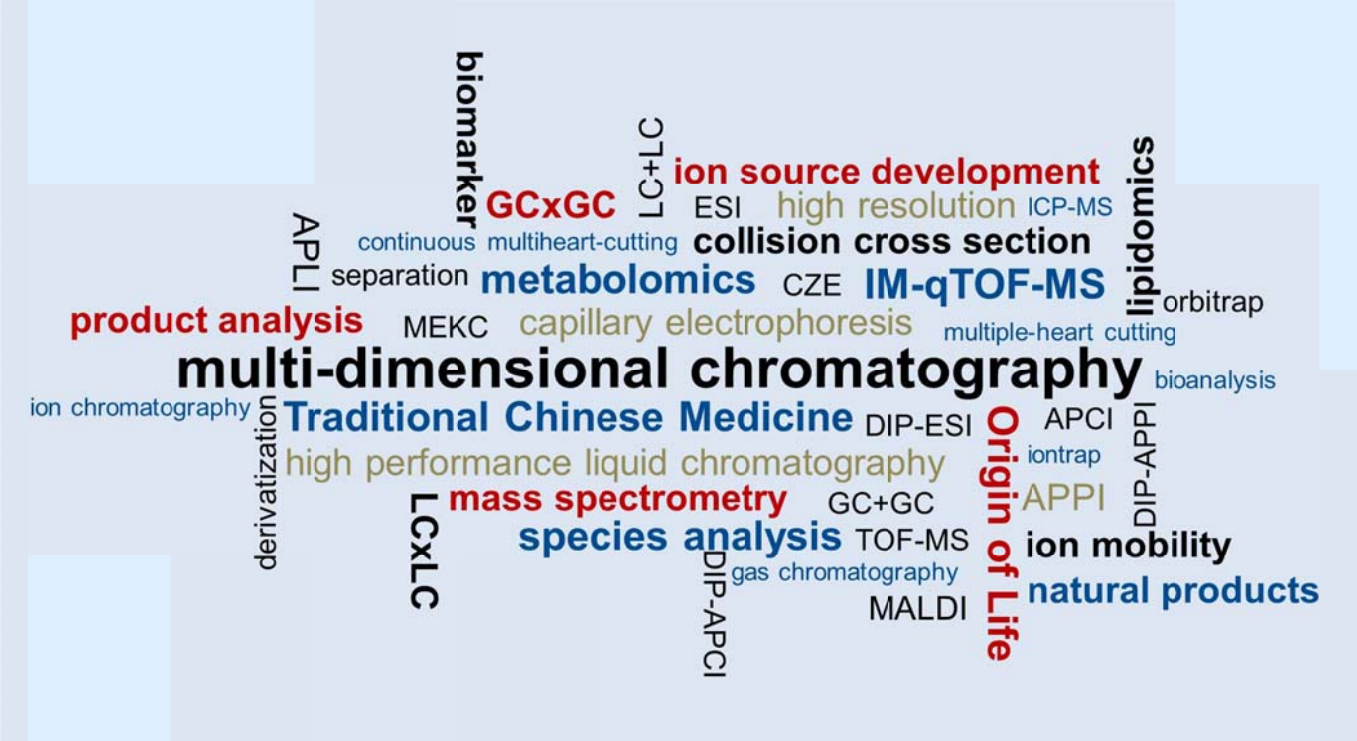

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Faculty of Chemistry
Applied Analytical Chemistry
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Applied Analytical Chemistry

The Applied Analytical Chemistry (AAC) is part of the Faculty of Chemistry at the University of Duisburg-Essen (UDE). The AAC exists since September 2012 with the main focus on the development of novel ion-sources for mass spectrometry, the non-target analysis of complex samples by multi-dimensional separation techniques in combination with ion mobility and high-resolution mass spectrometry and the metal(oid) species analysis by ICP-MS in combination with gas chromatography (GC) or liquid chromatography (LC).

Prof. Dr. Oliver J. Schmitz
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2018 was the sixth year of the Applied Analytical Chemistry research group at the University of Duisburg-Essen and a very successful one.

The most important topic in 2018 was that Agilent Technologies has formed a collaboration agreement with the University of Duisburg-Essen and the AAC to found an Agilent-sponsored Teaching and Research Center for Separation (TRC) in the laboratories of AAC. Fortunately, with BASF an additional sponsor of the Teaching and Research Center has been found.

In addition, 10 scientific papers in peer-reviewed journals – including one in Nature Chemical Biology – and 12 posters at national and international conferences with two poster awards were published. Several third-party funds were successfully raised and further national and international industrial cooperations were newly founded or extended. Many colleagues have contributed to an exciting year of research, teaching and last but not least to shouldering many other tasks.

This time I would like to thank especially Dr. Sven Meckelmann, who was indispensable in organizing the research group and in managing all smaller and bigger problems in the labs.

During 2018 we started several new projects, e.g. the development of a new ESI/APCI combi source, LCxLC-MS for petrochemical products, investigation of extracellular polymeric substances in *Sulfolobus acidocaldarius* etc. In the future – because of our outstanding equipment (many thanks to Agilent) – we will not only deal with device and method development, but also work in the fields of effect-based analysis, metabolomics and lipidomics.

Nevertheless, my group has, for the third time, organized the PhD seminar of the Working Group Separation Science of the Section for Analytical Chemistry of the GDCh in Hohen-

roda. Many thanks to Julia Klein and Junjie Li for organizing this very successful and inspiring conference with 146 participants and 28 lectures.

As mentioned last year, it is a pleasure and honor that the Permanent Scientific Committee of HPLC has commissioned Prof. Dr. Michael Lämmerhofer (University of Tübingen, Germany) and me with the organization of the 51st International Symposium on High Performance Liquid Phase Separations and Related Techniques (HPLC 2021), which will be held from June 20 to 24, 2021 in Düsseldorf, Germany. It will be the fourth HPLC symposium in Germany, after Baden-Baden in 1983, Hamburg in 1993, and Dresden in 2009. This year we updated our website www.hplc2021.com and continued to promote the conference in order to make HPLC 2021 successful. Mark your calendar! We look forward to your participation.

I want to take this opportunity to thank all co-workers for their excellent work in 2018 as well as the many collaborators in- and outside the University of Duisburg-Essen for pleasant and efficient collaborations.

In case you see possibilities for future collaborations, I would be happy to discuss them with you.

I wish you all the best, good health, happiness, and success for the year 2019.

Essen, December 15, 2018

Applied Analytical Chemistry – Staff

Regular Staff

Prof. Dr. Oliver J. Schmitz	Head
Dr. Martin Sulkowski	Senior Researcher
Dr. Sven Meckelmann	Senior Researcher
Maria Madani	Technician / Lab Assistant
Birgit Wöstefeld	Secretary

Post-Docs

Dr. Yingzhuang Chen, Dr. Lidia Montero, Dr. Florian Uteschil

Ph.D. Students

University Duisburg-Essen	External
Maha Alhasbani	Susanne Brüggen
Dominik Brecht	Annika Doell
Amela Bronja	Wiebke Mehwald
Lin Gan	Niklas Danne-Rasche
Simeon Horst	Dinh Lien Chi Nguyen
Julia Klein	Bing Peng
Timo Köhler	Dominic Mähler
Claudia Hellmann	Ruzanna Mnatsakanyan
Claudia Lenzen	
Junjie Li	
Christian Lipok	
Martin Meyer	
Kristina Rentmeister	
Alexandra von Trotha	

M.Sc. Students

Martin Meyer, Harley Simpson, Rezaul Karim Chowdhury

B.Sc. Students

Tharsiha Kandasamy, Tatiana Kiltau, Janina Nagel, Ina Obrock, Annika Schubert, Kevin Schulz

Guest Scientists

Juan Francisco Ayala Cabrera (University of Barcelona), Thanh D. Hoang (Vietnam National University, Hanoi)

Apprentices

Julia Banken, Christian Müller, Gina Paulus

Major News 2018

Teaching and Research Center for Separation

There is a great need to catch up in the university education, specifically in the field of HPLC, gas chromatography and mass spectrometry. Since there are only few analytical working groups at German universities, they cannot educate enough analytical scientists in order to meet the growing demand for qualified analysts. I believe that we are heading for a serious problem, because analytical skills are extremely important for product control and the export nation Germany needs highly qualified specialists. Dr. Joachim Richter mentioned this problem in his wake-up call in Chemistry News (Nachrichten aus der Chemie) 7/8 2018: "The current European Survey for European Chemists 2017 shows, as did the previous one in 2015, that analytical chemistry is one of the four major disciplines (besides inorganic, organic and physical chemistry) and is the only one that produces significantly fewer graduates than the labor market requires."

Therefore, Agilent Technologies has formed a collaboration agreement with the University of Duisburg-Essen and the AAC. As part of the collaboration, Agilent has supported the AAC with a broad range of instruments to equip a new Agilent-sponsored Teaching and Research Center for Separation (TRC). The center focuses on teaching separation science and training students and industry employees (from technicians to managers, graduates to postdocs) in the use of modern analytical equipment. Agilent is developing a global network of world-class Centers of Excellence that can be linked together to broaden scientific collaborations. Now, the University of Duisburg-Essen is the fifth university to join this network.

The next teaching courses will be given on:

11. – 15.03.2019 about 1D- and 2D-GC

08. – 12.04.2019 about GC-MS

16. – 20.09.2019 about LC-MS and Ion mobility-MS

23. – 27.09.2019 about ICP-OES, ICP-MS and CE

04. – 08.11.2019 about Basic Course Liquid Chromatography (Theory and HPLC)

18. – 22.11.2019 about Advanced Course Liquid Chromatography (2D-LC, LCxLC, SFC)

For more information visit our website www.trc-separation.com

HPLC 2021 in Düsseldorf, Germany

It is a great pleasure to announce that the 51st International Symposium on High Performance Liquid Phase Separations and Related Techniques (HPLC 2021) will be held at June 20-24, 2021 in Düsseldorf, Germany. Prof. Michael Lämmerhofer from the University of Tübingen and Prof. Oliver J. Schmitz from the University of Duisburg-Essen are chairmen of this conference.

The HPLC symposium series is known as the world leading conference on liquid phase separations and related technologies. Its program covers all aspects of separation sciences in liquid and supercritical fluid phases as well as hyphenation with advanced detection technologies in particular mass spectrometry. The program will span from fundamentals and theory of chromatographic separations and detection principles, over methodological and technological advances including separation materials, column technologies and instruments, to applications in various fields and quality assurance aspects. The symposium will feature workshops and tutorials, plenary and keynote lectures from the leading scientists in the field. Yet, the majority of lectures will be selected from submitted abstracts to make sure that participants can share and discuss their newest results with the audience. Besides, HPLC 2021 will have a big exhibition and vendor seminars in which attendees can see the latest innovations from the leading vendors in the field.

Mark your calendar! We look forward to your participation.

For more information visit our website www.hplc2021-duesseldorf.com

Hero of the Year 2018

Without the outstanding help of **Dr. Sven Meckelmann** the year 2018 would not have been ended so successfully. In addition to countless assistance in the area of procurement, Sven has significantly redesigned the laboratories of the AAC and, thus, contributed to the successful launch of the Teaching and Research Center for Separation. Furthermore, he was scientifically very successful and has published six peer-reviewed papers (including Nature Chemical Biology) and hold two talks at international conferences.

List of Projects 2018

(Abstracts of these projects within the next pages)

Effect-based analysis
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Julia Klein

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Lidia Montero

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Martin Meyer

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Lipidomic profiling of pancreatic cancer cells and corresponding liver metastases
Sven W. Meckelmann

Analysis of complex natural substances: Marijuana and Cannabinoids with GC+GC-APCI-IM-MS
Christian Lipok

Characterization of the metabolome of P. aeruginosa in biofilm as a lung infection model
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Dominik Brecht, Florian Uteschil

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Susanne Brüggen

Development of an ESI and APCI dual ionization source
Dominik Brecht, Florian Uteschil

Molecular Evolution in a Peptide-Vesicle System
Amela Bronja

Ozone Stress Effect on the Intracellular Metabolites from *Cobetia marina* measured by GCxGC-MS
Junjie Li

How to deal with mercury in sediments?
A short summary about the aspects of mercury speciation in sediments.
Claudia Hellmann

New developments in chemical ionization at atmospheric pressure
Christian Lipok

Capillary zone electrophoresis coupled to drift tube ion mobility-mass spectrometry for the analysis of native and APTS-labeled N-glycans
Julia Klein, Sven Meckelmann

Effect-based analysis

Sven W. Meckelmann, Julia Klein, Martin Meyer

Our group is also focused on metabolomics and, very recently, effect-based analysis. One of our first projects in this field was the analysis of *Chaoborus* kairomone chemicals that induce defences in *Daphnia*. Infochemicals play important roles in aquatic ecosystems. They even modify food web interactions, such as by inducing defenses in prey. In one classic but still not fully understood example, the planktonic freshwater crustacean *Daphnia pulex* forms specific morphological defenses (neckteeth) induced by chemical cues (kairomones) released from its predator, the phantom midge larva *Chaoborus*.

On the basis of liquid chromatography, mass spectrometry, and chemical synthesis, the chemical identity of the *Chaoborus* kairomone was done. The biologically active cues consist of fatty acids conjugated to the amino group of glutamine via the N terminus. These cues are involved in *Chaoborus* digestive processes, which explains why they are consistently released despite the disadvantage for its emitter. The identification of the kairomone may allow in-depth studies on multiple aspects of this inducible defense system.

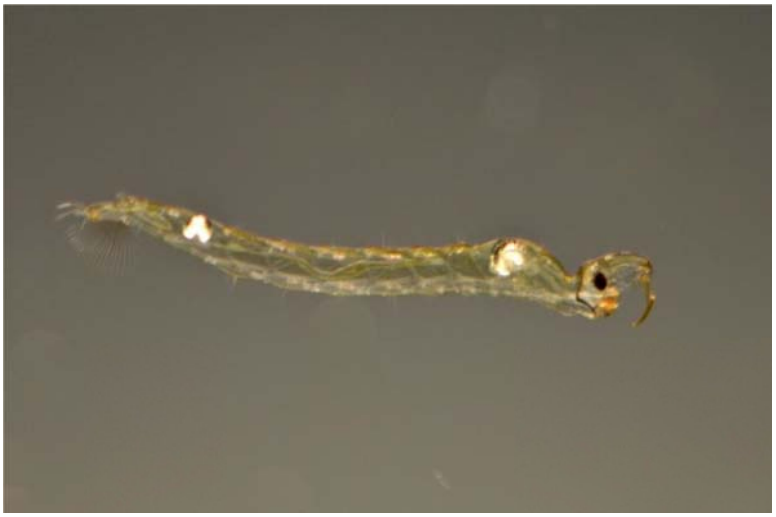


Figure: Larva *Chaoborus*

From an analytical point of view, these kairomones were very difficult to analyse because of their surface activity and, therefore, recovery problems by using any sample preparation techniques. The abandonment of any form of sample preparation and the use of the extremely sensitive Agilent 6495B triple quadrupole mass spectrometer leads to the published results [Nature Chemical Biology (2018) 14:1133-1139].

Collaborative Project – Project Partner: Ruhr University Bochum (Germany), Wageningen University (The Netherlands), University of Birmingham (UK)

Funded by: Agilent Technologies (Santa Clara, USA)

Analysis of complex samples using multidimensional separation and detection techniques

Julia Klein

For non-target approaches, liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS) is a powerful tool for the analysis of complex samples. However, there are limitations when analyzing very complex matrices, as for example ion suppression during the ionization process due to many coeluting compounds. In addition, coelution of isobaric compounds that cannot be separated by HRMS or tandem mass spectrometry (MS/MS) in case of similar fragmentation can occur.

One possible approach to increase separation power is increasing the number of separation dimensions, for example by using comprehensive two-dimensional liquid chromatography (LCxLC) or a two-dimensional liquid chromatography based on a continuous multi-heart-cutting approach (LC+LC). The introduction of ion mobility spectrometry (IMS) offers the possibility of an additional separation dimension by separating compounds according to their shape-to-charge ratio. Beside this, IMS allows the identification of compounds according to their collision cross sections (CCS). Coupling two-dimensional liquid chromatography to ion mobility quadrupole time-of-flight mass spectrometry (LCxLC- or LC+LC-IM-qTOF-MS) provides a powerful four-dimensional separation method. To evaluate the performance of different LC-HRMS techniques, three complex sample matrices (extract of Traditional Chinese Medicine plants, waste water and biocoal) were analyzed under comparable conditions using LC-, LCxLC- and LC+LC-IM-qTOF-MS.

As a result, in comparison to LC analysis, ion suppression was drastically reduced by using LCxLC and LC+LC. Furthermore, ion mobility allowed the identification of isobaric compounds after chromatographic separation according to their CCS, which would not be possible by accurate masses only.

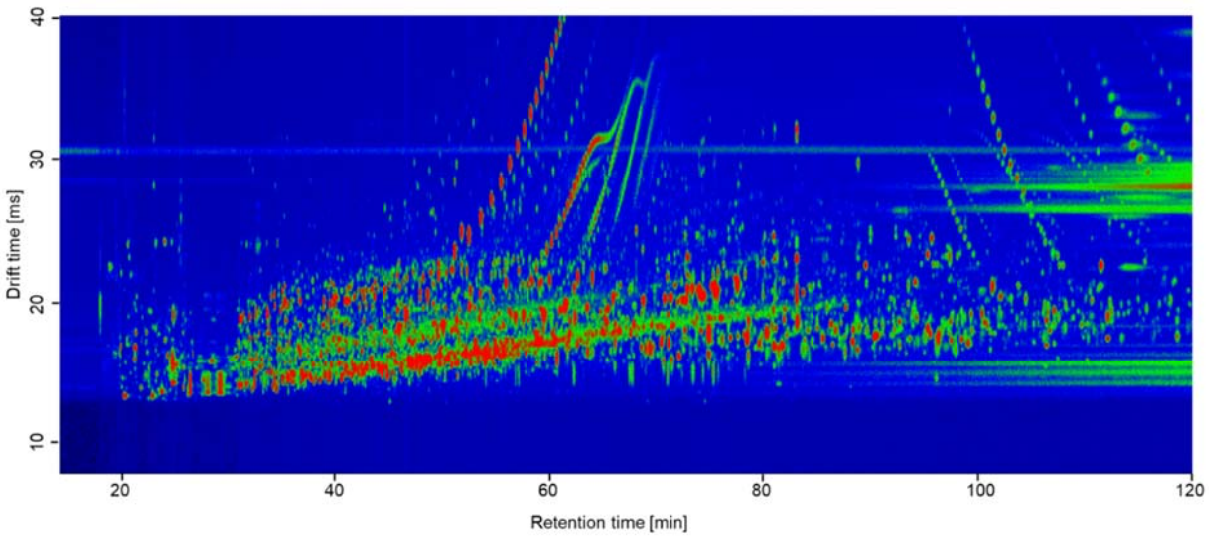


Figure: Heat map of a biocoal analysis with LC-IM-qTOF-MS.

Funded by: Agilent Technologies, Santa Clara, USA

At column dilution (ACD) modulator developing for flexible and precise control dilution factors to overcome mobile phase incompatibility in comprehensive two-dimensional liquid chromatography

Yingzhuang Chen, Junjie Li

With the combination of different separation mechanisms, two-dimensional liquid chromatography has brought the revolutionary changes compared to the traditional one-dimensional separation, which dramatically improves the peak capacity in separation and meets the ever-increasing demand for the analysis of the complex sample in different research fields, such as chemistry, medicine, biology, etc.

However, the incompatibilities between two columns due to the transport of the large sample volume and solvent effect always limit the widespread use of two-dimensional liquid chromatography. To resolve this problem, a new interface, at-column dilution (ACD), was established to overcome the solvent incompatibility in the orthogonal combination within the comprehensive two-dimensional liquid chromatography. This interface is modified from normal two-dimensional interface by additional injection pump, which realize the at-column dilution without splitting during the transportation. Moreover, with the control of the flows in the injection pump and two dimension gradient pump, it is able to precisely regulate the at-column dilution factor and conveniently optimize the separation conditions in both dimensions.

In this work, systematic research has been done between the setups with/without the at-column interface in the combination of RPLCxHILIC and HILICxRPLC, which proved that the at-column interface is able to resolve the solvent conflicting problem very well. Furthermore, the red ginseng root was chosen as a real sample, which offers further proof for the applicability of at-column dilution in the construction of comprehensive two-dimensional chromatography with high orthogonality in the future.

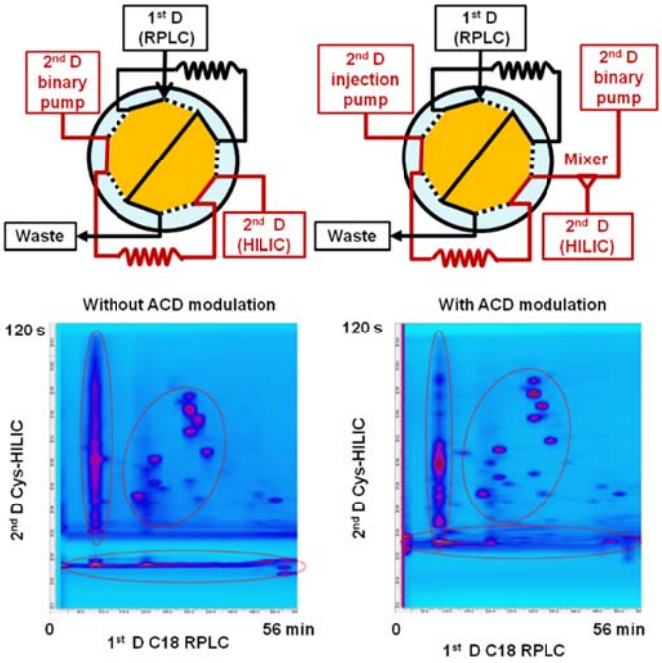


Figure: Contor plot with and without ACD modulation.

Funded by: Agilent (Germany) and Chinese Chemical Society

µLC+LC-IM-qTOF-MS for a four-dimensional proteome analysis

Lidia Montero

Proteomics is one of the branches of the omics sciences that studies the state of the cells through the analysis of the proteome. However, this ambitious aim involves the analysis of biological samples, which present an enormous complexity level. Therefore, analytical techniques able to provide with the needed separation power and resolution are required.

In this regard, a four-dimensional separation method was employed for achieving the maximum separation of three different peptide samples, that is, BSA, yeast and E. coli samples. The four dimensions were constituted by the on-line coupling of two-dimensional liquid chromatography to ion mobility mass spectrometry (IM) and high resolution mass spectrometry (µLC+LC-IM-qTOF-MS). Specifically, the two-dimensional liquid separation employed was a µLC+LC method using reversed phase separation in both dimensions. The orthogonality between the two dimensions was achieved modifying the pH of the mobile phases of the first and the second dimension. Concerning the other two separation dimensions, IM separated the peptides according to their structures since the separation is based in the shape-to-charge ratio. And finally, the fourth dimension separation was achieved by MS which provided a further separation of the peptides as a function of their mass-to-charge ratio.

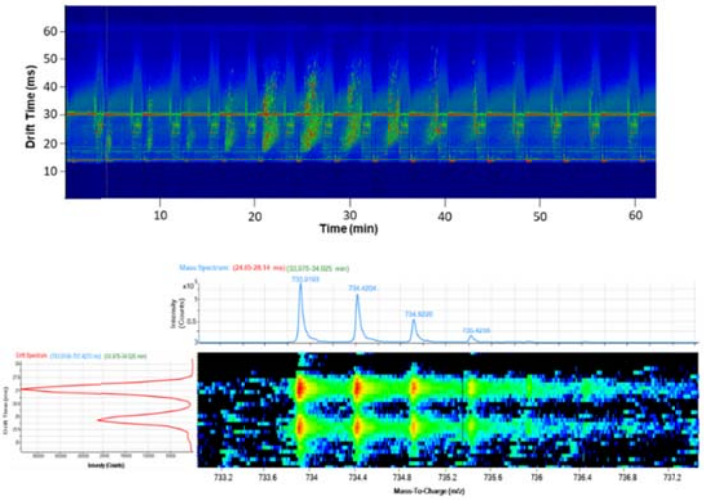


Figure:
A) Separation of E. coli peptides using the four dimensional µLC+LC-IM-qTOF-MS developed method.
B) Ion mobility separation of two isobaric peptides with the same m/z value.

This method provides a huge separation power, as can be observed in Figure A, where the drift time of each previous separated E.coli peptides by µLC+LC are separated according to their structure in IM. Nevertheless, the great advantage of this method is that the separation of isobaric peptides, with exactly the same m/z value but different structure, is also possible, as shown in Figure B.

Collaborative Project – Project Partner: Dr. Stephan Buckenmaier, Agilent Technologies
Funded by: Agilent Technologies, Inc. Research Project Grant

Optimization of SPE protocols for the enrichment of phenolic compounds

Martin Meyer

Phenolics are among the most common phytochemicals and are produced in varying numbers and variability in all plants for protection against microbiological pathogens, solar radiation etc. by biosynthesis. The chemical properties of various phenolic compounds suggest an antioxidant effect of these compounds, thus this class of compounds can be used in a variety of therapies or general health-conscious nutrition. Increased health awareness over the past 20-30 years has created a greater interest in food ingredients, in both private and scientific field. Many different methods of extraction and analysis have been developed and applied so that today many different approaches to this field of analytical chemistry are available. For quantification, the emphasis is usually placed on the extraction and analysis of individual substances. In the characterization of phytochemicals, such as phenolic compounds, the focus is instead on being able to extract as many substances of interest as possible from samples for analysis.

For non-target or suspected-target analyses of the phytochemicals contained in foods by means of e.g. LC-IM-MS, the latter approach is of greater importance. For this, an optimal SPE protocol has to be found in a series of experiments based on DoE, which allows the enrichment of as many phenolic / aromatic substances as possible with the highest possible recovery. The evaluation of experimental data by multivariate statistics showed that due to large differences in polarity, molecular size, acidity and other chemical properties in the broad spectrum of naturally occurring phenols, solid-phase extraction with a single commercially available phase is usually not possible in a satisfactory manner. Rather, a grouping of similar substances, roughly divisible into acids, mono- and polyaromatics, each showing high recoveries on certain phases. Based on the PCA (shown in figure on the left), optimal parameters for the SPE were determined for the individual groups, followed by further SPE experiments on specially prepared multiple phases from Macherey-Nagel with these optimum parameters. These phases showed a good agreement of the predicted and obtained recoveries for all substances. Overall, with the optimized SPE protocol, recoveries of at least 50% and enrichment factors between 10 to 25 were achieved for the substances tested (with a few exceptions). This opens the possibility for non-target or suspected-target analysis to extract and enrich the broadest possible spectrum of phenolic and aromatic substances in a single sample preparation step.

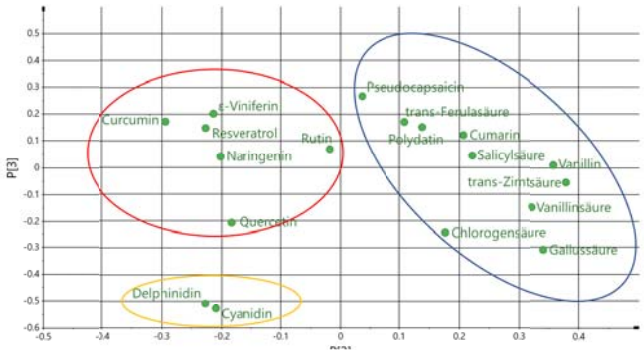


Figure: PCA of 128 SPE-experiments based on DoE shows grouping of chemically similar substances.

Funded by: Macherey-Nagel, Düren, Germany

Characterization of the plasma lipidome using LC-IM-qTOF-MS/MS

Kristina Rentmeister, Sven W. Meckelmann

There are at least two big challenges in analyzing lipids. On one hand, there are about 100,000 lipids estimated to occur in nature but only 40,000 lipids are reliably identified and reported in the biggest database (LipidMaps). On the other hand, there is a large number of isobaric lipids, which are difficult to separate by liquid chromatography. Ion mobility spectrometry (IMS) is an additional separation dimension, which allows the separation of coeluting isobaric compounds in the gas phase according to their size-to-charge ratio leading to an increased separation power. Furthermore, the collision cross section (CCS) can be easily determined using a drift-time IMS, which is useful as an additional parameter for the identification of lipids in complex biological samples such as human plasma.

We are using a three-dimensional lipidomics approach with a high separation power by coupling liquid chromatography to the Agilent 6560 IM-qTOF-MS. For the chromatographic separation a long 60 minutes gradient with a mixture of water/acetonitrile and acetonitrile/isopropanol on a C18 column is used. The described method shows low LODs below 100 nM (2 pmol on column) for most lipid classes in human plasma, which was determined doing a matrix match calibration of deuterated standards from 12 lipid classes.

Currently, we can detect about 3,000 lipid features with our method and identify roughly 1,000 of them on species level. For this we use an in house build database, including retention times, CCS values and m/z values of the most abundant adducts in ESI positive and negative ionization mode. For further identification, MS/MS spectra for all lipids are obtained with the data independent MS/MS acquisition mode of the instrument. Since fragmentation takes place after the drift tube fragment ions have the same drift time as their precursor ions and can be easily assigned. Furthermore, one gets MS/MS spectra with low background because of the prior separation by drift time.

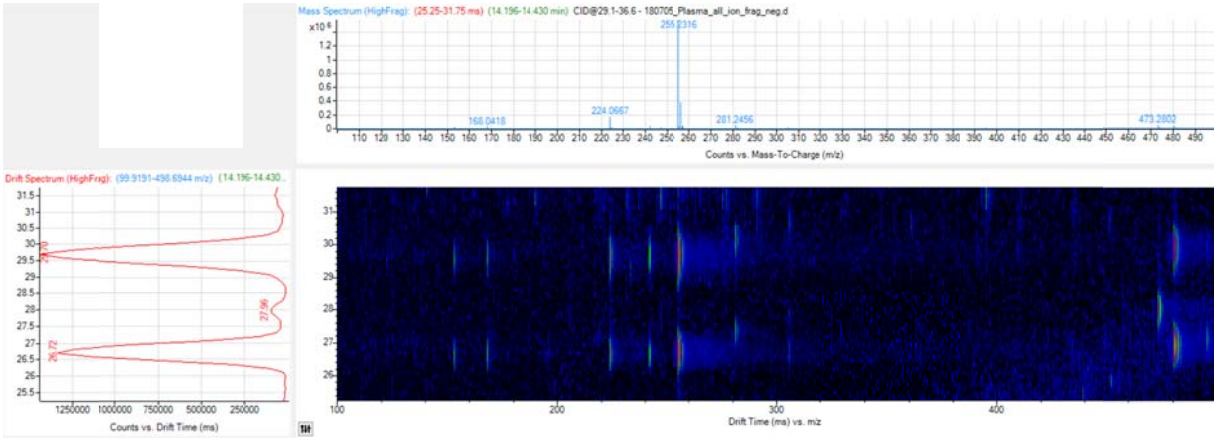


Figure: 2D plot (drift spectra vs. mass spectra) of LPC (16:0) (m/z = 480.3090) measured in ESI negative mode using data independent MS/MS acquisition.

Collaborative Project – Project Partner: Dr. John Fjeldsted, Agilent Technologies (Santa Clara, USA)

Lipidomic profiling of pancreatic cancer cells and corresponding liver metastases

Sven W. Meckelmann

People diagnosed with pancreatic cancer have a very poor prognosis. After diagnosis, only 25% survive the first year, because there are usually no symptoms of the disease in early stage. Only in later stages, symptoms are specific enough to suggest pancreatic cancer and by that time the cancer has often spread into other parts of the body. One of the first target for the development of metastases is the liver. However, the underlying biological process of metastasis is yet poorly understood.

In a recently started research project in cooperation with the University Hospital Essen (working group Barbara Grüner), we have profiled the lipidome of isolated pancreatic cancer cells and compared these with the matching cells of a liver metastasis. Both cell types were from a mouse model established in the group of Barbara Grüner. Cells from the primary tumor as well as from the corresponding metastases from the same animal were harvested and further grown in culture to acquire a sufficient amount of cells. Afterwards, lipids from the cells were extracted and analysed using the established lipidomics workflow by means of LC-IM-qTOF-MS.

Even from the obtained raw data, distinct differences between both cell types can be seen. After feature extraction, the data were cleaned up using LipidFinder. First statistical data analysis using univariate and multivariate (PCA and PLS) approaches revealed significant differences for various lipid classes allowing a complete classification of the different cell types.

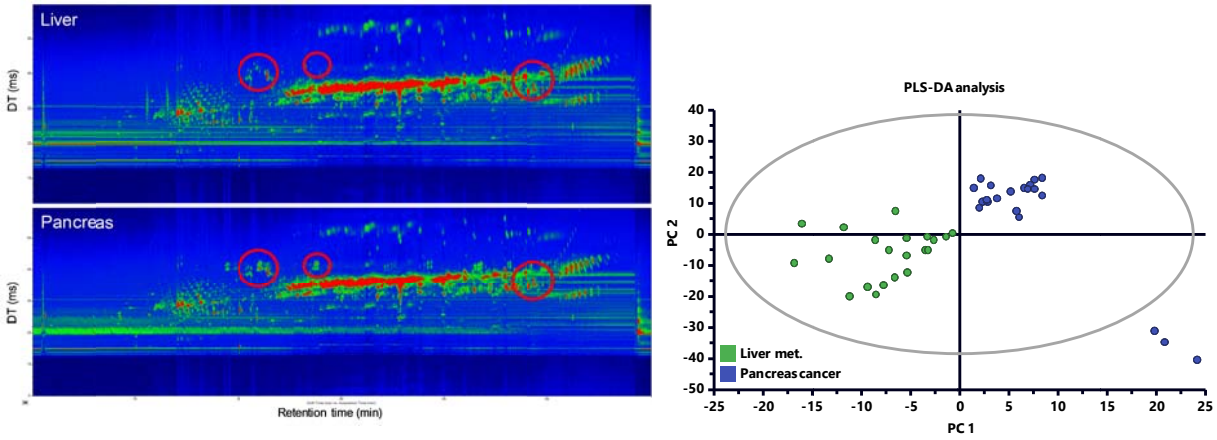


Figure:
Left: 2D-Heat map of the obtained LC-IM-qTOF-MS data for a pancreatic cancer cell extract and of the corresponding cells from a liver metastases.
Right: PLS-DA analysis of the data after feature extraction and data clean-up allowing a complete classification of the primary tumor cells and the metastases.

Collaborative Project – Project Partner: Dr. Barbara Grüner (Molecular Tumorpathology, Hospital Essen)

Analysis of complex natural substances: Marijuana and Cannabinoids with GC+GC-APCI-IM-MS

Christian Lipok

The analysis of marijuana and the determination of all ingredients is a subject of growing interest, but the determination of all compounds in natural samples such as marijuana is very challenging. On one hand, Marijuana is used as an illegal psychoactive drug and the complete profile of the drug can help to identify where the plant has grown and to identify the producer but on the other hand, Marijuana is used as an medicinal drug and there are strict legal regulations.

The complexicity of natural samples, such marijuana has led to the development of multidimensional chromatography techniques as comprehensive two dimensional gas chromatography (GCxGC), with a higher peak capacity compared to one-dimensional GC. Furthermore the coupling of 1D- or 2D-GC with ion mobility-mass spectrometry (IM-MS) should drastically increase the peak capacity. But GCxGC-IM-qTOF-MS is hard to realize because no software is available, which can simplify the four-dimension data into a readable plot and the peak width after the second dimension (100-600 ms) is to narrow for IM-MS, because data acquisition of this instrument is too low. To overcome this and simplify data evaluation, a 2D-GC method with a longer modulation time (20 s) and a longer column (7 m) in the second dimension was developed.

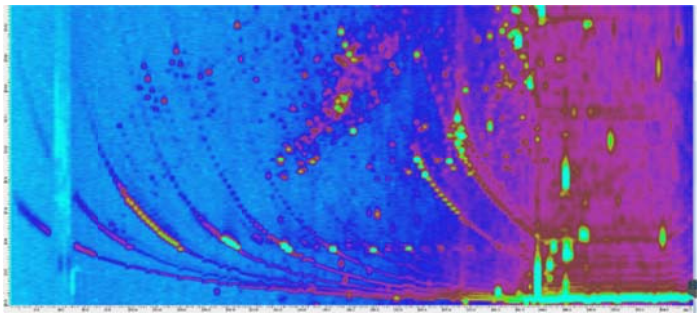


Figure 1. Analyse of an ethanol extract of marijuana with GC+GC-IM-qTOF-MS.

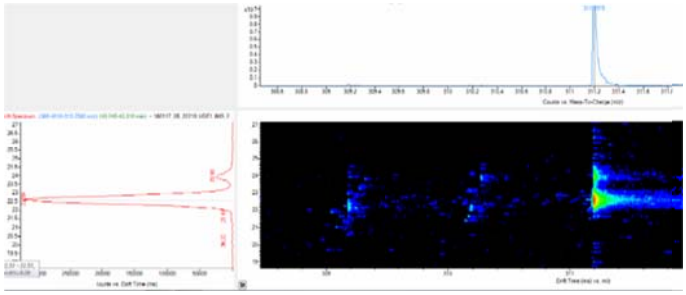


Figure 2. Separation of two isobaric compounds with m/z 311.1978. Possible cannabinoids: cannabinodiol (CBND-C5), cannabinol (CBN-C5).

Thererfore, GC+GC-APCI-IM-MS was used to analyse an ethanol extract of marijuana. Figure 1 shows the contour plot of the GC+GC-APCI-IM qTOF-MS measurement. An Agilent 6560 Ion Mobility Quadrupole Time-of-Flight Mass Spectrometer was used in combination with a 6890N GC from Agilent and a four-jet modulator from Leco. About 100 spots have been detected. Furthermore, Figure 2 shows the separation of isobaric compounds, which could not be separated with 2D-chromatography and MS. To sum up, the GC+GC APCI-IM-qTOF-MS method works as a continuos multi-heartcutting approach with an outstanding separation power and allows the separation of compounds based on boiling point, polarity, size (shape)-to-charge and mass-to-charge ratio.

Funded by: International Restek Academic Support Program

Characterization of the metabolome of P. aeruginosa in biofilm as a lung infection model

Timo Koehler

Pseudomonas aeruginosa is an opportunistic pathogenic germ, which leads to nosocomial infection. Especially the lung of cystic fibrosis patients is mostly colonized by this bacterium, in form of a biofilm, and leads to fatal lung infections, which causes the early death of cystic fibrosis patients due to raspatory failures. The expected life time of cystic fibrosis patient is increased from about 8 years in 1974 to about 40 years nowadays but this was achieved by an intensive treatment with antibiotics. The drawback of this treatment is the increasing resistance of the bacterium against the antibiotics. To reduce the therapy with antibiotics and allow another extension of increase the life time of cystic fibrosis patients a non-invasive early detection technique is necessary, but still not developed.

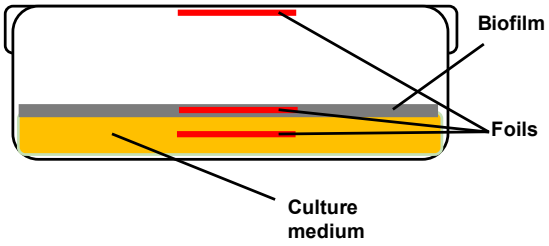


Figure: schematic overview of the biofilm system for P. aeruginosa as lung infection model.

In this project such a detection technique should be developed. Therefore, a biofilm system under adapted lung conditions was planned and tested. This three-phase approach, shown in the left figure, is a biofilm system, where the metabolites are going to be sampled using thin film microextraction (TFME) with PDMS films. The advantage of this model is that in addition to the metabolites of the biofilm, the substances of the nutrient and the headspace can be collected and analyzed. This allows a differentiation of the detected and characterized substances in substrates and metabolites.

In the first step of the project, a suitable film material and manufacturer was selected. Thereafter, the cleaning process for the selected film was optimized with the aim of minimal initial contamination. A suitable separation and detection technique for the loaded films, using a thermo desorption system (TDS A2, Gerstel GmbH, Muelheim, Germany) with a GC-MS (Agilent Technologies Inc., Santa Clara, USA) was developed. The development of the TD-GC-MS method was carried out using an aqueous solution consist of twelve standards. The standards were potential metabolites of P. aeruginosa and are already published in scientific journals. With the developed method we are able to identify and quantify several of these possible metabolites down to nanomolar concentrations in a matrix of the nutrient. Furthermore first TFME experiments using liquid cultures of three different strains of P. aeruginosa shows that several metabolites, produced by P. aeruginosa can be detected with the developed method. At the moment we are optimising the developed method with the aim of lower LODs for the potential metabolites and higher peak capacity.

Collaborative Project – Project Partner: PD Dr. Ursula Telgheder (UDE) and Dr. Jost Wingender (UDE)
Funded by: German Research Foundation (DFG), Bonn, Germany

Thermogravimetry atmospheric pressure photoionization mass spectrometry (TG-APPI-MS) as analytical tool for the analysis of pharmaceutical tablets

Dominik Brecht, Florian Uteschil

The reliability of pharmaceutical formulations is an important issue in the industrial and even more important in developing countries. Therefore, a trusted analysis of produced tablets or suspected falsified drugs is very important. At the moment the product control in the industry and the investigation of falsified drugs is done by DSC analysis which only gives the information of physical properties like the melting or boiling point of an analyte. Hyphenated techniques like GC-MS and LC-MS are other methods which are used for the analysis of pharmaceuticals. These methods go hand in hand with a long sample preparation like the extraction of the analytes from the tablet matrix and in some cases also require derivatization. In the analysis of tablets described before the TG-APPI-MS shows an advantage in the sample preparation which is very easy and consists of grinding the tablet to a homogeneous powder. The use of the TG-APPI-MS simplifies the analysis of tablets. When using an APPI-MS as a detector for the evolved gas of the thermogravimetry additional information about the molecule masses are required. This is caused by the soft ionization of the APPI. Additionally, the TG is often equipped with a DTA analysis which also can increase the knowledge about the physical properties of the sample.

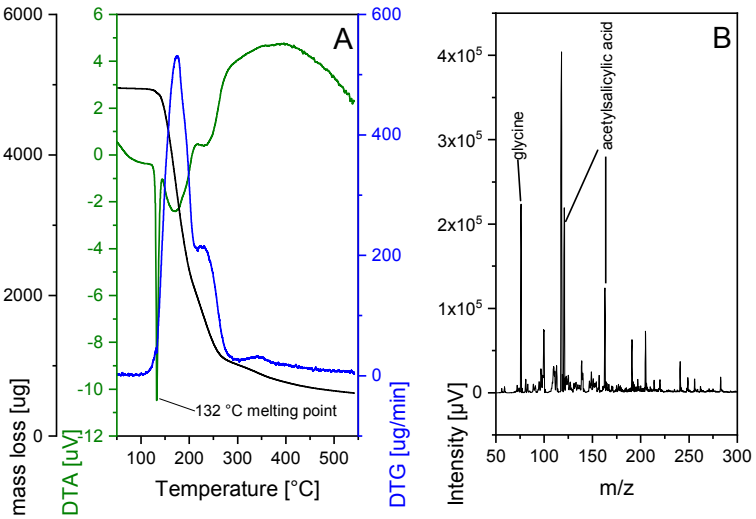


Figure: A: Thermogravimetric analysis of an acetylsalicylic acid tablet with the TG-APPI-MS; B: Mass spectrum averaged over the whole analvsis time.

The presented figure shows the information which can be collected by the analysis of an acetylsalicylic acid (ASA) tablet by the TG-APPI-MS. Figure A is the TG analysis of 4 mg of the ground tablet. It shows a sharp peak of the DTA signal at 132 °C which is the melting point of the acetylsalicylic acid in the formulation with the excipients. The melting point of the pure ASA is 136 °C. One excipient can be detected which is shown in figure B. Here a signal for the m/z 76 presents the protonated molecule of glycine. So, the TG-APPI-MS can identify excipients in the pharmaceutical formulations. Also, the fragmentation of acetylsalicylic acid is observed with the m/z values of 121 and 163. These abilities to identify the active substance as well as the excipients, makes the TG-APPI-MS a powerful instrument for the product control and identification of falsified drugs with less sample preparation.

Funded by: Hitachi High-Tech Corporation, Mito, Japan

A modern concept for regulatory water monitoring via High-Performance Liquid Chromatography coupled to high-resolution mass spectrometry or how less can be more

Susanne Brüggen

Water monitoring is understood as the registration of chemical, physical and biological properties of a water body over a longer period of time to observe its development and quality. The basis of water monitoring is the European Water Framework directive (WFD), which has the main ambition to significantly improve the quality of surface waters and groundwater throughout Europe to achieve a good ecological condition.

At the moment water samples are measured in many different LC-MS/MS methods classified mostly into substance classes for e.g. drugs, pesticides, industrial chemicals etc., which leads to a high effort of measurements and quality assurance (QA). This leads to the question if the established methods should not be reconsidered and can replaced by goal-oriented and innovative solutions to get more information and have less measuring effort.

A combined approach of target, suspected target and non-target screening using liquid chromatography high resolution mass spectrometry (LC-ESI-HRMS) in one analytical run was used to open up a new concept for water monitoring.

(1) Target Analysis

Quantitative analysis of 100 target compounds selected by e.g. the WFD

(2) Suspect Target Analysis

Quantitative Screening with a database of 3,000 substances, positive results are reported

(3) Non Target Analysis

Peak picking results in a large number of features (m/z with RT). Various evaluation strategies depending on the analytical question, e.g. creation of time profiles

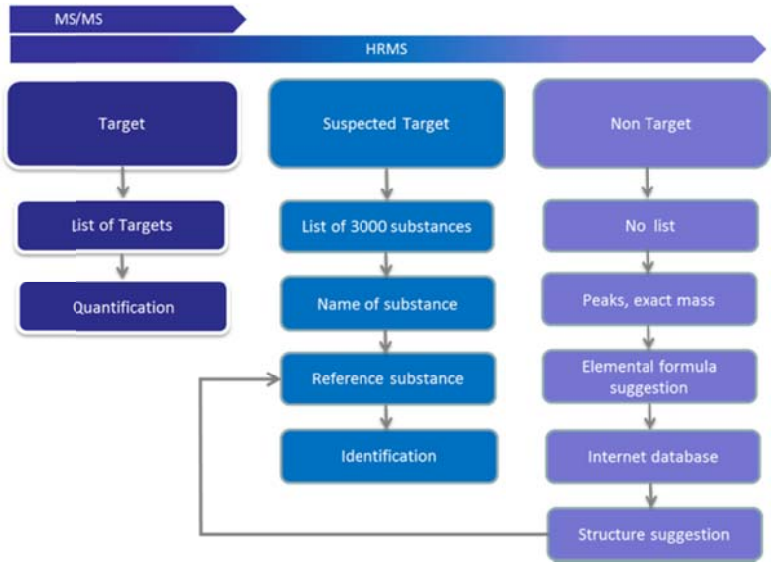


Figure: Survey of the three different evaluation strategies

With the new concept it is possible to detect 100 target compounds without losing accuracy. Furthermore a suspect target screening can be performed to get broader qualitative information about the water samples. In addition the non-target screening offers the possibility to identify unknown micropollutants. This concept could change the water monitoring and assessment and make it much more efficiently, without losing any information. There is a chance to measure less but learn more about the water bodies.

Development of an ESI and APCI dual ionization source

Dominik Brecht, Florian Uteschil

The demand on high throughput methods for LC-MS is a growing market in the analytical chemistry. Therefore, our group is working on solutions to increase the sample throughput in chromatographic analyses hyphenated with mass spectrometer. Here, we focused our research on the development of new ion sources for mass spectrometry. In this work an ion source should be created which is capable to ionize the analyte molecules with electrospray ionization (ESI) or atmospheric pressure chemical ionization (APCI). Our first attempt to realize such a source is to combine the ESI and the APCI probe in one ion source housing with two entrances for the effluent of the HPLCs. The high sample throughput is realized by connecting two HPLCs with a six-port switching valve which switches between the two HPLCs and the two probes of the ion source. The challenge of this project is to create an ion source which is comparable to single probe ion sources, but compromises must be made because ESI and APCI ionization relies on different ionization mechanism. ESI ionization takes place in the liquid phase and APCI in the gas phase, therefore, there is a challenge to find the right temperature to use both probes as efficient as it is possible. This new ion source shall reduce the delay time of a mass spectrometer to increase the efficiency of mass spectrometric analyses.

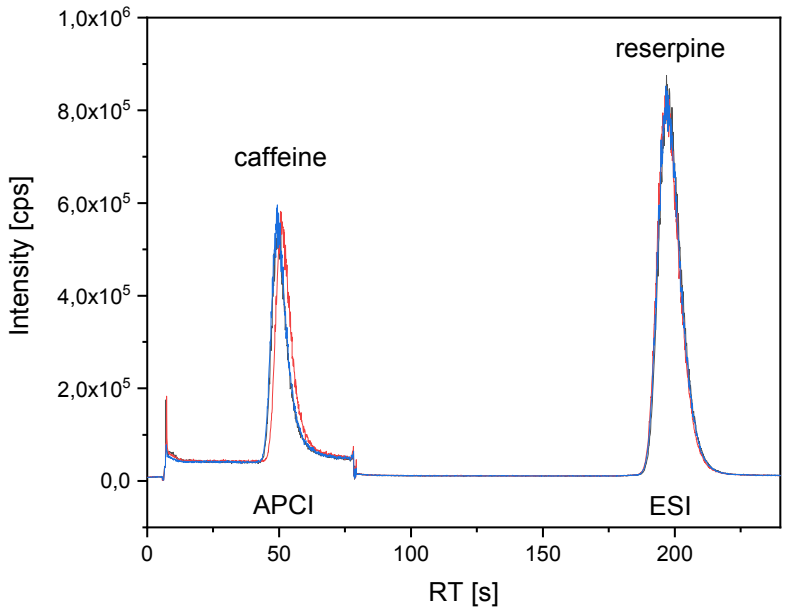


Figure: Chromatographic analyses of a caffeine solution (HPLC 2) and a reserpine solution (HPLC 1) by the ESI-APCI- dual probe ion source.

The figure presents one of the first analysis with the new developed dual probe ion source. One sample of caffeine (50 ppb) is injected in HPLC 2 and one sample of reserpine (50 ppb) is injected in HPLC 1. Both HPLCs are started at the same time. The chromatogram is divided in two parts the first is the detection of caffeine using the APCI probe (HPLC 2). After that the six-port valve switches between the two probes and the effluent of the HPLC 1 is directed into the ESI probe. Reserpine and caffeine are detected as protonated molecule ion with a mass of 609 Da and 195 Da, respectively. The first experiments show promising results as it presented here. Especially the short equilibration time of the ESI ion source after the switching of the valve supports a high throughput method, in which analyses can be done by ESI or APCI in one LC run.

Funded by: Hitachi High-Tech Corporation, Mito, Japan

Molecular Evolution in a Peptide-Vesicle System

Amela Bronja

Based on the model "*origin of life in deep-reching tectnic faults*", an efficient and stable system undergoing structural reproduction, self-optimization, and molecular evolution is proposed. This system is being formed under early earth conditions by the interaction of two cyclic processes, one of which offers vesicles as the structural environment, with the other supplying peptides from a variety of amino acids. The main mechanism is the stabilization of the peptides by the vesicles and of the vesicles by the peptides together with a constant production and selection of both. Figure 1 is illustration three possible scenarios which formed peptides can be exposed to. On the left side peptide chains formed by hydrophilic amino acids (blue circles) will undergo little interaction with vesicles and remain in the aqueous phase where they undergo hydrolysis. On the right side peptide chains formed by hydrophobic amino acids (red circles) will eventually be eluted by scCO2. Whereas amphiphilic peptides (center) will accumulate in the bilayer membrane and remain partially protected against hydrolysis and elution. In order to simulate conditions given in depths between 1 and 7 km of the earth's crust a high pressure phase equilibrium apparatus containing lipid vesicles and 11 amino acids was used. In order to accelerate the peptide formation cycle and to induce selection pressure on the vesicles, the temperature inside the cell is kept at 120°C during the whole experiment. The pressure is repeatedly switched between 100 bar and 70 bar every 30 min. During each pressure cycle, a phase transition from supercritical scCO2 to gaseous gCO2 and vice versa is induced. The solid products from the aqueous solution were analyzed with LC-qTOF-MS.

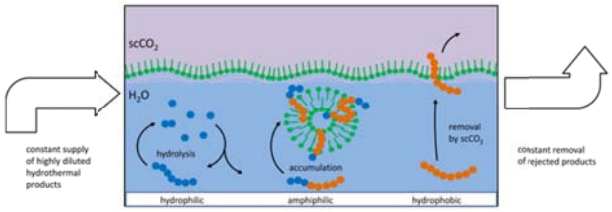


Figure 1: Mechanism of peptide selection and accumulation in the presence of vesicles.

Figure 2 is showing the EIC's of a possible hexapeptide with the possible amino acid combinations: GASDDE, GGTDDE, GGSDEE, VTLLKK, SLLLKK. They contain hydrophilic as well as hydrophobic amino acids and have the potencial to act as amphiphiles. Most probably, this peptide has been accumulated and preserved from hydrolysis in a selection process induced by the presence of membrane vesicles.

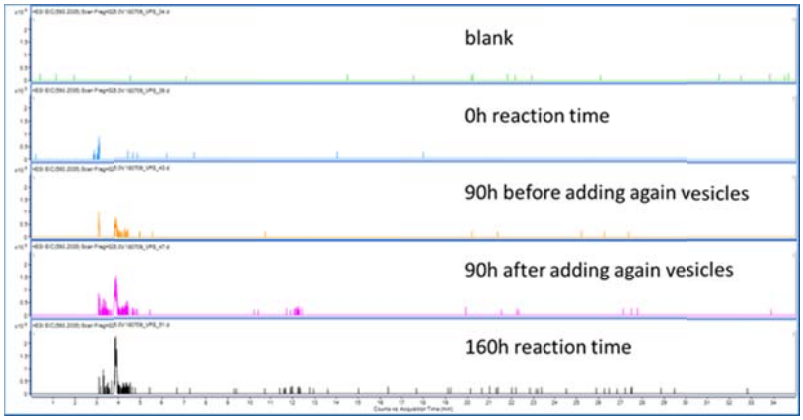


Figure 2: EIC's of a possible hexapeptide with the m/z $[M+H]^+$: 593.2035.

Collaborative Project – Project Partner: Prof. Ulrich Schreiber (UDE), Prof. Christian Mayer (UDE)

Ozone Stress Effect on the Intracellular Metabolites from *Cobetia marina* measured by GCxGC-MS

Junjie Li

Cobetia marina, a Gram-negative marine bacterium, was first proposed in 1971 by Cobet et al. Considerable research over past few decades has indicated its feasible features as a bio-fouling model system in marine or similar circumstance. The previous studies, especially in the last decade, barely focused on metabolites aspect – the unique chemical fingerprints regarding to certain cellular processes.

Ozone treatment, known as a sufficient disinfection method, has been modified to stress the *Cobetia marina* in different extent. Different amount of ozone was spiked to observe the stress effect. After extraction, the derivatized samples were determined with a GCxGC-MS according to the orthogonality formed by two columns, Rxi-5sil MS and Rxi-17sil.

After spiking, as shown in Fig. b, the number of metabolites was obviously decreased due to the ozone stress with the 600 µM dosage. As comprison with GasPedal in Fig. c, the overlayed patterns (in yellow) indicate that the majority of the compounds from ozone spiked sample could be found in the normal state one. On the other hand, a large number of metabolites (in red) was decreased or disappeared because of the ozone stressing condition, eg. Ethandiamine, Glucopyranoside, Pyrrolidionone, Azelaoyl Chloride, Hexanedioic acid, Undecanoic acid, Tetradecanoic acid and Myristic acid amide (1-8).

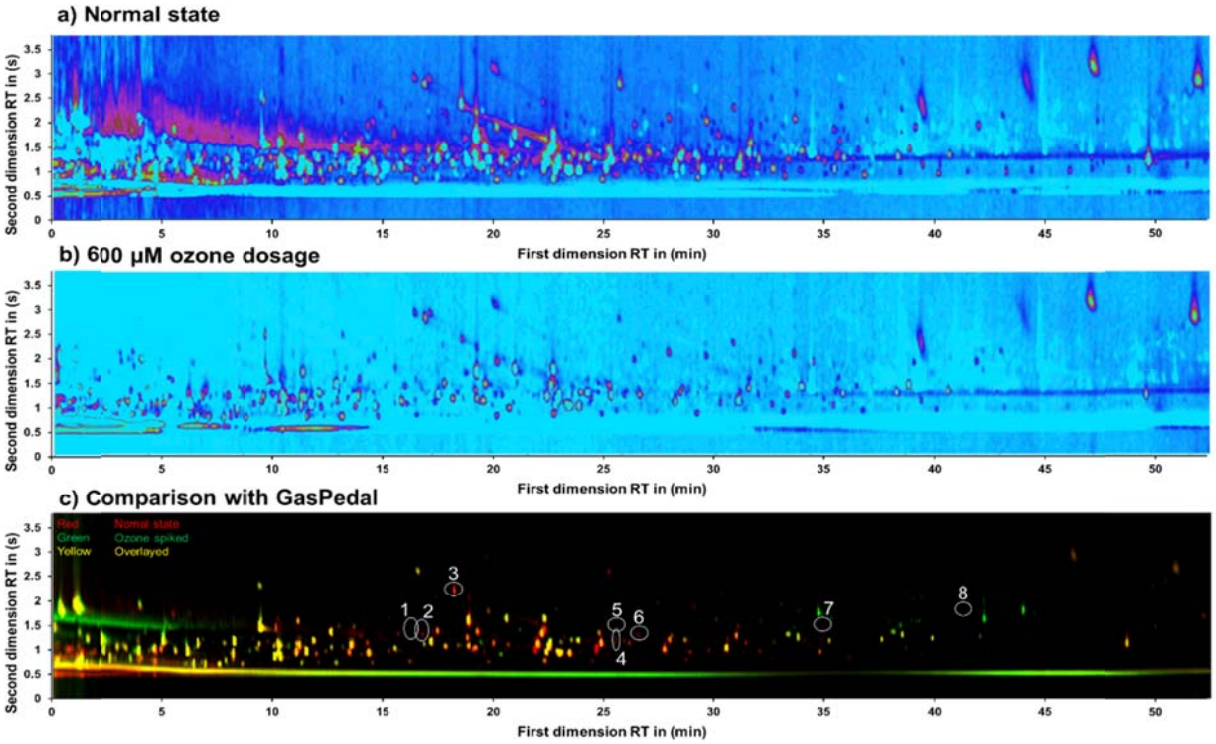


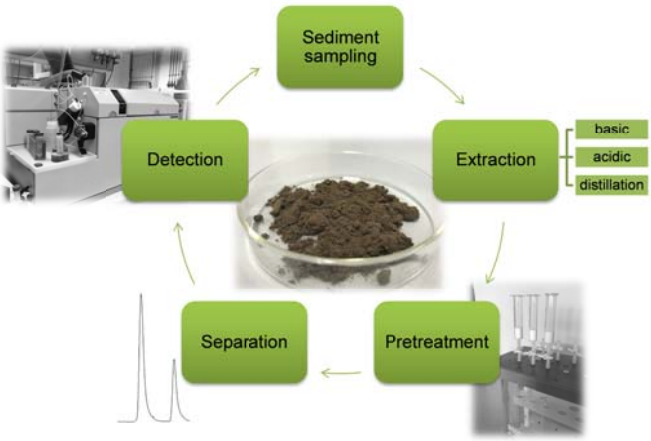
Figure: Contour plots of intracellular metabolites of *Cobetia marina* from GCxGC-MS a) normal state, non-spiked b) spiked with 600 µM ozone dosage c) comparison visualized by GasPedal

Collaborative Project – Project Partner: Profs. T. Schmidt (UDE), A. Rosenhahn (RUB), W. Schuhmann (RUB)
Funded by: Mercator Research Center Ruhr GmbH (MERCUR) , Essen, Germany

How to deal with mercury in sediments?
A short summary about the aspects of mercury speciation in sediments.

Claudia Hellmann

According to the World Health Organization, mercury is one of the most dangerous substances. The reason for this is the occurrence of mercury in different species, which differ in their degree of toxicity. Due to this fact, a speciation is indispensable for the evaluation of the environmental condition. The speciation can be divided into several sub-sections, which are defined by extraction, enrichment, separation and detection.



Sediments serve as an indicator of the state of the environment, as they reveal, anthropogenic influences (e.g. industry) over time. The knowledge about the composition of sediments, in particular by the speciation, helps in the assessment of the environmental situation. Therefore speciation of mercury in sediments is still being discussed and continues to pose a great challenge for analytical chemists. Above all, sediments, in which the methylmercury concentration is only 0.1-1% of the total mercury content, must be treated with special caution.

For the extraction of sediments mainly acidic, alkaline or distillative methods are used. However, the acidic extraction is one of the most common techniques and is used in various modifications. Due to the very low content of methylmercury, a separation or enrichment after the extraction is necessary. For the enrichment of mercury species solid phase extraction is a very frequently used method and provides a number of different phases, e.g. thiol-containing compounds with a high affinity for mercury. After a successful enrichment, the separation of the species with a suitable separation method takes place. HPLC and GC are very frequently used methods for this purpose. For the detection a lot of methods are discussed in the literature, while (CV)-AFS and ICP-MS are the most common.

Due to the complexity of the speciation of mercury in sediments and the resulting high number of publications in this field the goal is to find a working, robust standard method that is suitable for different sediments.

Funded by: Federal Institute of Hydrology, Koblenz, Germany

New developments in chemical ionization at atmospheric pressure

Christian Lipok

Gas chromatography (GC) coupled to mass spectrometry (MS) is usually done with electron impact ionization (EI). This technic produces mass spectra with a high degree of fragmentation. This fragmentation allows the identification via a database comparison. However, for a high degree of agreement with these databases, it is necessary that the mass spectra of the analytes do not overlap. Complex samples show very often coelution which complicate the identification of the analytes.

Chemical ionization at atmospheric pressure (APCI) offers a way out of this problem. The soft ionization with APCI provides mainly the molecule peak and causes no or very little fragmentation. Coupled with a high-resolution mass spectrometer it is possible to determine the molecular formula of the molecule. Furthermore, because of no fragmentation, very sensitive analysis by quadrupole tandem MS/MS are possible.

GC-APCI is not the ion source of choice for GC-MS and all commercial sources can still be improved. One common problem of commercially available sources is poor reproducibility, because of non constant conditions in the gas phase inside the ion source. Therefore, a closed APCI source was developed (Fig. 1) which is isolated from the surrounding room air. This source is characterized by a very small reaction chamber and enables the exact settings of humidity, temperature, gas flows, pressure, position of corona needle and GC column. The new construction for GC-APCI already shows an improved reproducibility. The relative standard deviation of 5 different test substances (low to high polar) was between 1-10% (inter-day). However, not all possible settings are optimized yet and there should be room for further improvement.

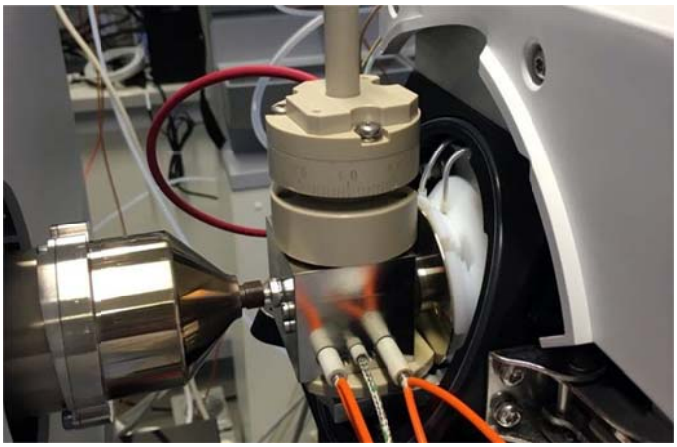


Figure 1: New developed GC-APCI source.

Collaborative Project – Project Partner: Dr. Terry Sheehan, Agilent Technologies (Santa Clara, USA)

Capillary zone electrophoresis coupled to drift tube ion mobility-mass spectrometry for the analysis of native and APTS-labeled N-glycans

Julia Klein, Sven Meckelmann

Capillary zone electrophoresis (CZE) based on electrophoretic mobility in the liquid phase and ion mobility spectrometry (IMS) based on mobilities in the gas-phase are both powerful techniques for the separation of complex samples.

Protein glycosylation is one of the most common post translational modification being associated with a wide range of biological functions and human diseases. Due to their high structural variability, the analysis of glycans still represents a challenging task, especially if one-dimensional separation is applied.

In this work, the first on-line coupling of CZE with drift tube ion mobility mass spectrometry (DTIM-MS) has been perfomed to further improve separation capabilities for the analysis of native and 8-aminopyrene-1,3,6-trisulfonic acid (APTS)-labeled *N*-glycans. In this way, a complexity of glycan signals was revealed which could not be resolved by these techniques individually, shown for both, native and APTS-labeled glycans. Each individual glycan signal separated in CZE exhibited an unexpected high amount of peaks observed in the IMS dimension. This observation could potentially be explained by the presence of isomeric forms, including different linkages, and/or gas phase conformers.

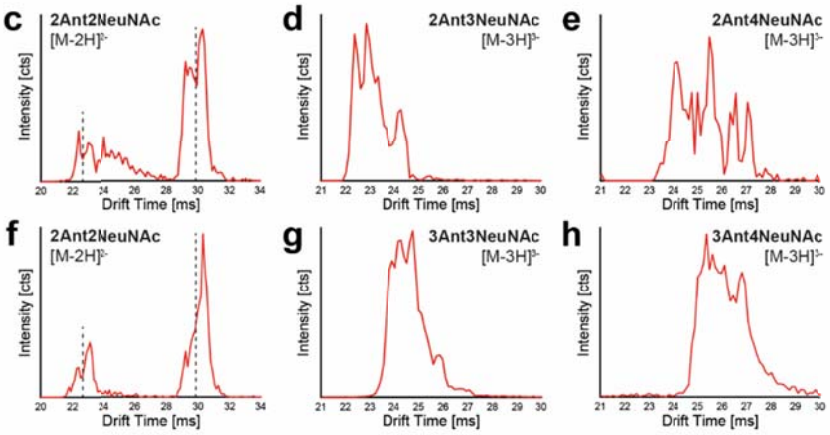


Figure: DT spectra of AGP (c – e) and Fetuin (f – h) glycans associated with the major peaks separated by CZE.

In addition, the type of sialic acid attached to glycans has a significant impact on the obtained drift time profile.

Furthermore, the application of α2-3 Neuraminidase enabled the partial assignment of peaks in the DTIMS spectra considering their sialic acid linkages (α2-3/α2-6). This work is a showcase for the high potential of CZE-DTIM-MS, which is expected to find various applications in the future.

Collaborative Project – Project Partner: Prof. Christian Neusüß and Dr. Kevin Jooß (Aalen University, Germany)

Doctoral Theses accomplished 2018

Simeon Horst

Development and use of an ambient ionization method based on atmospheric pressure photo ionization

This thesis demonstrates, that the use of photoionization enlarges the applications of the direct inlet probe towards nonpolar compounds which are poorly ionizable with APCI or ESI. By optimization, it was possible to achieve a comparable sensitivity as with DIP-APCI and DIP-ESI leading to good signal intensities even with a sample volume of 1 µL. In consequence, no chemical and time intensive sample preparation was needed. Due to this and abdication of chromatographic separation, this method reduces the operating costs as well as the need of chemicals.

By application onto different real samples the potential of the new ion source is demonstrated. Thereby the DIP-APPI shows an increased sensitivity for the compounds of the EPA 8720 mix compared to DIP-APCI. Due to ion mobility spectrometry, it was possible to achieve a separation and detection even of isobaric compounds within a total analysis time of 5 min.

Because of the reduced ion suppression of the DIP-APPI in comparison to the DIP-APCI, it was possible to quantify different bisphenols nearly without sample preparation out of recycled papers. In this case the DIP-APPI offers an alternative to the classical analytical methods that use extensive clean-up and separation steps.

For the determination of alteration of olive oils by other eatable oils the results point out the DIP-APPI to be a fast alternative to classical analytical methods. The DIP-APPI is able to determine alterations up to 15% in contrast to the DIP-APCI where the alteration is only detectable higher than 25%. This is achieved by the calculation of a sum parameter that contains 41 compounds for APPI and only 20 compounds for APCI. Due to the higher number of compounds, the APPI sum parameter showed better standard deviations and therefore reduced the threshold value of the system.

Master Theses accomplished 2018

Hayley Sherlee Simpson
Analysis of Cannabis sativa with a four dimensional separation method based on Continuous Multi-Heart Cutting Gas Chromatography, Ion Mobility and High Resolution Mass Spectrometry

Martin Meyer
Development of a SPE protocol for enrichment of phenolic/aromatic compounds

Bachelor Theses accomplished 2018

Tharsiha Kandasamy
Comparison of different Collision Cross Section determination methods using DTIM-qTOF-MS

Tatiana Kiltau
Optimization of SPE protocols for the enrichment of phenolic / aromatic compounds

Janina Nagel
Characterization of the ingredients of various liquors

Ina Obrock
Origin of Life: High Pressure Simulation and Analysis of Vesicular Peptide Systems

Annika Schubert
Establishment of a CCS database for lipids

Kevin Schulz
Further development of an LC-IM-qTOF-MS/MS method for the determination of lipids in biological samples and foods

Accepted and/or Published Scientific Publications 2018

Original Paper / Peer-reviewed

S. Brüggen, O. J. Schmitz **A new concept for regulatory water monitoring via high-performance liquid chromatography coupled to high-resolution mass spectrometry**, accepted in Journal of Analysis and Testing

C. Koch, M. Nachev, J. Klein, D. Koester, O. J. Schmitz, T. Schmidt, B. Sures **Degradation of the polymeric brominated flame retardant "Polymeric FR" by heat and UV**, accepted in Environmental Science & Technology

K. Jooß, S. W. Meckelmann, J. Klein, O. J. Schmitz, C. Neusüß **Capillary zone electrophoresis coupled to drift tube ion mobility-mass spectrometry for the analysis of native and APTS-labeled N-glycans**, accepted in Analytical and Bioanalytical Chemistry as Paper in Forefront

L. C. Weiss, B. Albada, S. M. Becker, S. W. Meckelmann, J. Klein, M. Meyer, O. J. Schmitz, U. Sommer, M. Leo, J. Zagermann, N. Metzler-Nolte, R. Tollrian **The scent of predation: Identification of an aquatic infochemical – the Chaoborus kairomone**, Nature Chemical Biology (2018) 14:1133-1139

C. Hellmann, O. J. Schmitz **How to deal with mercury in sediments ? A critical review about used methods for the speciation of mercury in sediments**, Chromatographia (https://doi.org/10.1007/s10337-018-3625-y)

V. Hinnekamp, J. Klein, S. Meckelmann, P. Balsaa, T. Schmidt, O. J. Schmitz **Comparison of CCS Values Determined by Traveling Wave Ion Mobility Mass Spectrometry and Drift Tube Ion Mobility Mass Spectrometry**, Analytical Chemistry (2018) 90:12042-12050

C. Mayer, U. Schreiber, M. J. Dávila, O. J. Schmitz, A. Bronja, M. Meyer, J. Klein, S. W. Meckelmann **Molecular Evolution in a Peptide-Vesicle System**, Life (2018) 8: 16 open access (https://doi.org/10.3390/life8020016)

C. Lipok, J. Hippler, O. J. Schmitz **A four dimensional separation method based on continuous heart-cutting gas chromatography with ion mobility and high resolution mass spectrometry**, Journal of Chromatography A (2018) 1536:50-57

M. Aldrovandi, S. Banthiya, S. Meckelmann, Y. Zhou, D. Heydeck, V.B. O'Donnell, H. Kuhn **Specific oxygenation of plasma membrane phospholipids by Pseudomonas aeruginosa lipoxygenase induces structural and functional alterations in mammalian cells,** Biochim Biophys Acta Mol Cell Biol Lipids 1863 (2018) 152-164

E. Fahy, J. Alvarez-Jarreta, C.J. Brasher, A. Nguyen, J.I. Hawksworth, P. Rodrigues, S. Meckelmann, S.M. Allen, V.B. O'Donnell **LipidFinder on LIPID MAPS: peak filtering, MS**

searching and statistical analysis for lipidomics, Bioinformatics (2018) 10.1093/ bioinformatics/bty679

Poster Presentations

T. Koehler, J. Klein, O. J. Schmitz, S. W. Meckelmann, **Characterization of the human plasma lipidome using LC-IM-qTOF-MS**, Regionalverbandstagung NRW der Lebensmittelchemischen Gesellschaft (Essen, Germany) March 2018

L. Montero, K. Rentmeister, S. W. Meckelmann, O. J. Schmitz, S. Buckenmaier, **A novel 4D-analytical platform for Omics Sciences**, Agilent Science Fair Posters, March 2018

T. Koehler, O. J. Schmitz, S. W. Meckelmann, **Characterization of the human plasma lipidome using LC-IM-qTOF-MS**, analytica Munich conference (Munich, Germany) April 2018

C. Lipok, J. Klein, F. Uteschil, S. W. Meckelmann, O. J. Schmitz, **Determination of complex natural samples: Marijuana & Cannabinoids with GC+GC-APCI-IM-MS**, analytica Munich conference (Munich, Germany) April 2018

D. Brecht, F. Uteschil, O. J. Schmitz, **Investigation of drugs using a novel thermogravimetry atmospheric pressure photo ionization mass spectrometry coupling (TG-APPI-MS)**, analytica Munich conference (Munich, Germany) April 2018

K. Rentmeister, T. Kriegsmann, J. Klein, S. W. Meckelmann, A. H. Duong, V. H. Pham, O. J. Schmitz, **Analysis of Vietnamese herbs and formulations by means of LC-IM-qTOF-MS**, analytica Munich conference (Munich, Germany) April 2018

C. Lipok, O. J. Schmitz, **A generic method for the analysis of complex natural substances: Marijuana and Cannabinoids with GC+GC-APCI-IMS**, 42nd International Symposium on Capillary Chromatography (Riva, Italy) May 2018 **Analytical Method Poster Prize**

J. Klein, S. W. Meckelmann, V. Hinnenkamp, T. C Schmidt, O. J. Schmitz, **Collision cross section: Influences and comparability**, ASMS 2018 (San Diego, USA) June 2018

S. Stow, R. Kurulugama, G. Stafford, J. Fjeldsted, J. Klein, O. J. Schmitz, T. Causon, S. Hann, **Achieving Highly Accurate CCS Measurements in LC-IM-MS Analyses**, ASMS 2018 (San Diego, USA) June 2018

K. Rentmeister, L. Montero, S. W. Meckelmann, S. Buckenmaier, O. J.Schmitz, **A novel 4D-analytical platform for Omics Sciences**, 47th HPLC 2018 (Washington, USA) August 2018

J. Li, O. J. Schmitz, **Ozone Stress Effect on the Intracellular Metabolites from Cobetia Marina by Two-dimensional Gas Chromatography with Mass Spectrometer**, 9th analytica Conference (Shanghai, China) October 2018 **The Best Poster of the Symposium**

K. Rentmeister, T. Köhler, O. J. Schmitz, S. W. Meckelmann, **Characterization of the human plasma lipidome using LC-IM-qTOF-MS**, Lipidomic-Forum (Dortmund, Germany) November 2018

Invited Lectures / Oral Presentations

Prof. Oliver J. Schmitz

µLC+LC-IM-qTOF-MS for complex samples such as lipidome or proteome
Analytica China conference, Shanghai, China, October 2018

Five-dimensional analysis (LC+LC-IM-qTOF-MS) for complex samples such as metablome, lipidome or proteome
International Symposium on Metabolic diseases and translational medicine, Dalian, China, October 2018

LC+LC- and GC+GC-IMS-qTOF-MS as a generic analytical platform and first results with a new GC-APCI ion source
Tsinghua University, Beijing, China, October 2018

Thousands of separated signals in a four-dimensional separation approach: How can we manage the data
SECyTA 2018, 18th meeting of the Spanish Society of Chromatography and Related Techniques, Granada, Spain, October 2018

From one- to five-dimensional analysis platform: pros and cons
2nd 2D-LC / GC Symposium**: User meeting for multidimensional chromatography Frankfurt, Germany, September 2018**

Multidimensional Chromatography coupled with Ion-Mobility Mass Spectrometry: Enough is enough
Analytica conference, Munich, Germany, April 2018

LC+LC- and GC+GC-IMS-qTOF-MS in combination with a CCS data base as a generic analytical platform
University of Graz, Graz, Austria, March 2018

Einsatz der Ionenmobilitäts-Massenspektrometrie für suspected und non-target Fragestellungen: Ein kritischer Überblick
IUTA, Duisburg, Germany, March 2018

LC+LC- and GC+GC-IMS-qTOF-MS as a generic analytical platform
Dow-Chemicals, Stade, Germany, January 2018

Multidimensional Chromatography coupled with Ion Mobility - Mass Spectrometry: Hype or Ripe?
4th International Ion Mobility Spectrometry (IMS) Meeting, Uetrecht, The Netherlands, January 2018

Dr. Sven Meckelmann

LC-MS based Lipidomics: From QqQ to IM-qTOF
Analytik Seminar at the University Muenster, Muenster, Germany, July 2018

Characterization of the Human Plasma Lipidome using LC-IM-qTOF-MS
47th International Symposium on High Performance Liquid Phase Separations and Related Techniques, Washington DC, USA, August 2018

Julia Klein

Collision Cross Section: Comparability of DTIMS and TWIMS and influences of source parameters
ASMS 2018, San Diego (USA), June 2018

Miscellaneous

Conference Organization

Prof. Oliver J. Schmitz, Chairman (together with Prof. Jin-Ming Lin, Tsinghua University, Beijing, China) of the 8th analytica China conference in Shanghai, China, October 31th – November 1st 2018

Prof. Oliver J. Schmitz, Chairman of the Session "Ion Mobility - Mass Spectrometry: Hype or Ripe? Theory and Application" at the analytica Munich conference

Prof. Oliver J. Schmitz (together with Julia Klein and Junjie Li), Organization of the 28th PhD seminar of the Working Group "Separation Science" of the Section for Analytical Chemistry of the GDCh in Hohenroda

Guest Editor

The first issue of this journal was published in February 2017 and it is extremely exciting to be involved in the development of this first English-language Analytical Chemistry Journal in China from the very beginning. This year I was the guest editor for a special issue about Food Chemistry.

Editorial Tasks by Prof. Oliver J. Schmitz

Advisory Board member of Chromatographia

Editorial Board member of Journal of Pharmaceutical Analysis

Associate Editor-in-Chief of Journal of Analysis and Testing

Member of the "Fachbeirat" of analytica Munich

Member of the DAAD selection committee (Foreigners from Asia and Oceania)

Member of the DAAD selection committee (Project-related people exchange with India)

Member of the committee for the Eberhard-Gerstel-Price

Member of the committee for the Ernst-Bayer-Price

Deputy Chairman of the Working Group Separation Science of the Section for Analytical Chemistry of the GDCh

Awards

In January 2018, during the 28th PhD seminar of the Working Group "Separation Science" of the Section for Analytical Chemistry of the GDCh in Hohenroda, Dr. Susanne Stephan was awarded with the Ernst-Bayer-Award 2017 for her publication "Contaminant screening of wastewater with HPLC-IM-qTOF-MS and LC+LCIM-qTOF-MS using a CCS database", Analytical and Bioanalytical Chemistry (2016) 408:6545-6555.

In May 2018, during the 42nd International Symposium on Capillary Chromatography in Riva, Italy, Christian Lipok was awarded with an Analytical Methods Poster Prize.

In October 2018, during the 9th analytica conference in Shanghai, China, Junjie Li was awarded with the Prize for the best poster of the symposium.

Institute Colloquium

(in cooperation with the research group of Prof. Torsten Schmidt)

Prof. Dr. Jules Griffin from the Cambridge visited the Applied Analytical Chemistry (AAC) at University of Duisburg-Essen. He was one of the speakers at the Analytical Chemistry-Colloquium held in cooperation with the research group of Prof. Torsten Schmidt (IAC).

We would also like to thank all our other guests who participated in our colloquium:

Prof. Dr. Jules Griffin, Department of Biochemistry, University of Cambridge, UK, From 5000 people to 50 µm: studying fatty liver disease using high resolution mass spectrometry, 22.01.2018

Dr. Jochen Türk, IUTA, Duisburg, Germany, Instrumentelle und wirkungsbezogene Analytik bei der erweiterten Abwasserreinigung zur Spurenstoffelimination, 29.01.2018

Dr. Michael Maiwald, BAM Berlin, Germany, Aktuelle Herausforderungen für die Prozessanalytik – von der Online-NMR-Spektroskopie im Feld bis zum Plasmaspektrometer auf dem Acker, 23.04.2018

Prof. Dr. Michael Elsner, TU München, Germany, Advancements in Compound-specific Isotope Analysis (CSIA): Perspectives for Studying Reaction Mechanisms in Complex Systems, 28.05.2018

Prof. Dr. Jin-Ming Lin, Tsinghua University, Beijing, China, Droplet Generation for Cell Analysis on Microfluidics and Mass Spectrometry, 01.06.2018

PD Dr. Bernd Kammerer, University of Freiburg, Germany, Massenspektrometrische Metabolomanalysen in der medizinischen Forschung, 02.07.2018

Prof. Dr. Hans-Gerd Janssen, Unilever and University of Amsterdam, The Netherland, Optimization of Column Formats and Flow Conditions in Comprehensive GC×GC, 08.10.2018

Prof. Dr. Karl Speer, TU Dresden, Germany, Authentizität von Sortenhonigen, 03.12.2018

Teaching

Chemistry (B.Sc. / M.Sc.)

Lecture Analytical Chemistry I (in German, Prof. Dr. O. J. Schmitz)

Tutorial Analytical Chemistry I (in German, Dr. S. Meckelmann)

Lecture Anaytical Chemistry II (in German, Prof. Dr. O. J. Schmitz)

Tutorial Analytical Chemistry II (in German, Dr. S. Meckelmann)

Water Science (B.Sc. / M.Sc)

Lecture Analytical Chemistry I (in German, Prof. Dr. O. J. Schmitz)

Tutorial Analytical Chemistry I (in German, Dr. S. Meckelmann)

Lecture Anaytical Chemistry II (in German, Prof. Dr. O. J. Schmitz)

Tutorial Analytical Chemistry II (in German, Dr. S. Meckelmann)

Lecture Applied Analytical Chemistry (in English, Prof. Dr. O. J. Schmitz)

Tutorial Applied Analytical Chemistry (in English, Prof. Dr. O. J. Schmitz)

Lecture Environmental Chemistry: Pollutants (in English, Prof. Dr. O. J. Schmitz)

Tutorial Environmental Chemistry: Pollutants (in English, Prof. Dr. O. J. Schmitz)

Exercise Environmental Chemistry: Soil and Waste (in English, Dr. M. Sulkowski)

Environmental Toxicology (M.Sc.)

Lecture Applied Analytical Chemistry (in English, Prof. Dr. O. J. Schmitz)

Tutorial Applied Analytical Chemistry (in English, Prof. Dr. O. J. Schmitz)

Lecture Environmental Chemistry: Pollutants (in English, Prof. Dr. O. J. Schmitz)

Tutorial Environmental Chemistry: Pollutants (in English, Prof. Dr. O. J. Schmitz)

Magisterium

Lecture Environmental Chemistry: Soil (in German, Dr. M. Sulkowski)

Seminar

Analytical-chemical seminar
(in German/English, Prof. Dr. O. J. Schmitz in cooperation with Prof. Dr. T. Schmidt)

Practical courses

Practical course analytical chemistry

Research practical courses

Teaching and Research Center for Separation

Course 1: Basic Course Liquid Chromatography (in German, Prof. Dr. O. J. Schmitz)

Course 2: Advanced Course Liquid Chromatography (in German, Prof. Dr. O. J. Schmitz)

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2018