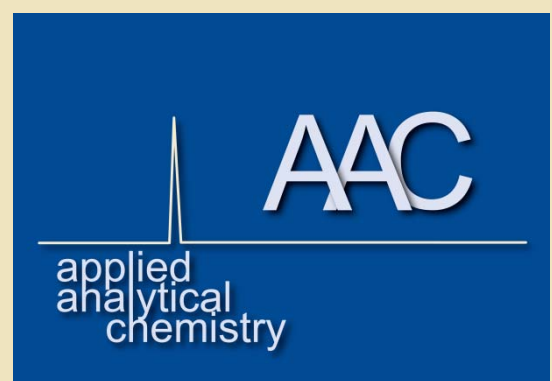


UNIVERSITÄT
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**Applied Analytical Chemistry
(AAC)**

Annual Report 2016



Content

Applied Analytical Chemistry	4
Applied Analytical Chemistry – Staff	6
Major News 2016	7
Hero of the Year 2016	8
List of Projects 2016	9
Contaminant screening of wastewater with HPLC-IM-qTOF-MS and LC+LC-IM-qTOF-MS using a CCS database	10
Development of a GC+GC-System for coupling to an IM-qTOF-MS.....	11
Build up a CCS data base	12
Origin of Life – Analysis of liquid inclusions in quartz samples	13
Determination of Intracellular Metabolites from <i>Cobetia Marina</i> by GCxGC-MS	14
Quantitative analysis of bisphenol A in recycled paper with a novel DIP-APPI-IonTrap-MS	15
Analysis of different pharmaceutical with the further developed DIP-ESI-MS.....	16
Speciation of mercury (II) and methylmercury in sediments by HPLC-ICPMS	17
Determination of Nicotine and Cotinine in Human Blood by Dried Blood Spot-LC-Orbitrap MS Technique	18
Doctoral Theses accomplished 2016	19
Bachelor Theses accomplished 2016	19
Master Theses accomplished 2016.....	19
Accepted and/or published scientific publications 2016	20
Invited Lectures / Oral Presentations	23
Miscellaneous.....	25
Institute Colloquium.....	26
Teaching.....	27

Applied Analytical Chemistry

The Applied Analytical Chemistry (AAC) is part of the Faculty of Chemistry at the University of Duisburg-Essen. 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 (e.g. metabolome) 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), liquid chromatography (LC) or laser ablation.

2016 was the fourth year of the Applied Analytical Chemistry research group at the University of Duisburg-Essen and up to now the most successful one. 13 scientific papers in peer-reviewed journals, 10 posters at national and international conferences (one Best Poster Award), several successful grants, strong industrial cooperations and all finished PhD students in job.

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. Jörg Hippler, who was indispensable in organizing the research group and to manage all smaller and bigger problems in the labs. As from 2017 Jörg Hippler will start his industrial career at Agilent and, therefore, we wish him all the best for the future and as much success as he had at the University of Duisburg-Essen.

During 2016 several new projects are approved, e.g. construction of a combi ion source for clinical approaches, peptid synthesis at prebiotic conditions as an molecular evolution system and development of a novel two-dimensional gas chromatographic separation method. In addition, several cooperations with Agilent, Hitachi and Phenomenex were continued to further increase industrial related research.

In addition, the third edition of the successful textbook "Analytische Chemie" from Prof. Georg Schwedt was published in December 2016 with Prof. Torsten Schmidt and me as additional authors.



Prof. Dr. Oliver J. Schmitz
(Head of the Research Group)

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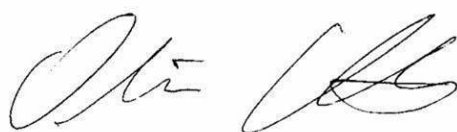
Email: oliver.schmitz@uni-due.de

web: www.uni-due.de/aac
www.oliver-schmitz.net

I want to take this opportunity to thank all co-workers for their excellent work in 2016 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 2017.

A handwritten signature in black ink, consisting of two distinct parts. The first part is a stylized, cursive 'A' followed by a horizontal line. The second part is a more complex, cursive signature that appears to be 'G' followed by several loops and a final flourish.

Essen, December 19, 2016

Applied Analytical Chemistry – Staff

Regular Staff

Prof. Dr. Oliver J. Schmitz	Head
Dr. M. Sulkowski	Senior Researcher
Dr. J. Hippler	Senior Researcher
M. Madani	Technician / Lab Assistant
B. Wöstefeld	Secretary



Post-Docs

Dr. Sven Meckelmann, Florian Uteschil

Ph.D. Students

University Duisburg-Essen

Ahmad Abu awwad
Amela Bronja
Maxim Diel
Lin Gan
Simeon Horst
Julia Klein
Claudia Kowalczyk
Claudia Lenzen
Junjie Li
Pia Rosendahl
Susanne Stephan
Alexandra von Trotha

External

Susanne Brügger
Annika Doell
Wiebke Mehwald
Niklas Danne-Rasche
Dinh Lien Chi Nguyen
Bing Peng

M.Sc. Students

Nitesh Babu (external), Christian Lipok, Simon Schade, Pratima Shrestha

B.Sc. Students

Stefanie Bettin, Jens Dreschmann (external), Alexander Haupt, Robert Kalnins, Tim Kriegsmann, Martin Ohrt, Carolin Wolff

Guest Scientists

Prof. Abdalla A. Elbashir (Karthoum University, Sudan), Jessica Pandohee (RMIT University, Melbourne, Australia), Dr. Ousmane Ilboudo (University of Ouagadougou, Burkina Faso)

Apprentices

Julia Banken, Miriam Brosch

Major News 2016

Industrial Cooperations

In 2016 we increased our cooperation with industrial companies in the field of analytical chemistry. This allows us to expand our analytical equipment and, therefore, optimize the education of students and improve our possibility to solve analytical problems. At moment we have fantastic working conditions in our labs and looking forward to use this equipment for many interesting and important applications.



HPLC 2021 in Düsseldorf, Germany



The HPLC conference series is the most renowned symposium series with focus on separation science and its application in various fields of research, quality assurance, diagnostics and monitoring. It has a clear vision and structure and is, therefore, attractive to attendees from various branches of science and industries.

While other meeting series have shown declining participation numbers, the HPLC congress series has maintained its attractiveness for participants and exhibitors or even gained attendees and companies with interest to showcase their newest products in recent years.

In 2021, Prof. Michael Lämmerhofer (University of Tübingen) and Prof. Oliver J. Schmitz (University of Duisburg-Essen) will be the chairmen of the 51st International Symposium on High-Performance Liquid Phase Separations and Related Techniques, HPLC 2021, in Dusseldorf, Germany. The conference will be organized under the auspices of the "Working Group for Separation Science" (AK Separation Science). This is a working group within the "Division Analytical Chemistry" (*Fachgruppe Analytische Chemie*) of the German Chemical Society (GDCh). The legally authorized entity is the "Division Analytical Chemistry", which will, therefore, be indirectly the official hosting organization.

Hero of the Year 2016



In 2016 Dr. Susanne Stephan was very successful.

She published the first three papers about LC+LC, a new two-dimensional chromatography method in combination with ion mobility and high-resolution mass spectrometry, as first author. Two other papers as co-author about photocatalytic transformation of acesulfame and the analysis of degradation products of polymeric brominated flame retardants are also published. Another manuscript as a co-author about anaerobic naphthalene degradation is submitted.

In addition, she finished her PhD thesis with summa cum laude and starts her first job position at Agilent in Waldbronn.

List of Projects 2016

(Abstracts of these projects within the next pages)

Contaminant screening of wastewater with HPLC-IM-qTOF-MS and LC+LC-IM-qTOF-MS using a CCS database

S. Stephan

Development of a GC+GC-System for coupling to an IM-qTOF-MS

C. Lipok

Build up a CCS

J. Hippler, S. Stephan, T. Köhler, S. Schade

Origin of Life – Analysis of liquid inclusions in quartz samples

A. Bronja

Determination of intracellular metabolites from *Cobetia Marina* by GCxGC-MS

J. Li

Quantitative analysis of bisphenol A in recycled paper with a novel DIP-APPI-IonTrap-MS

S. Horst

Analysis of different pharmaceutical with the further developed DIP-ESI-MS

C. Lenzen

Speciation of mercury (II) and methyl mercury in sediments by HPLC-ICP-MS

C. Kowalczyk

Determination of nicotine, cotinine, nicotine-N-oxide in human blood, plasma, urine, semen and sperm by LC-orbitrap-MS

A. Abu awaad

Contaminant screening of wastewater with HPLC-IM-qTOF-MS and LC+LC-IM-qTOF-MS using a CCS database

Susanne Stephan, Jörg Hippler, Timo Köhler, Ahmad Deeb

Non-target analysis has become an important tool in the field of water analysis since a broad variety of pollutants from different sources are released to the water cycle. For identification of compounds in such complex samples, liquid chromatography coupled to high resolution mass spectrometry is often used. The introduction of ion mobility spectrometry provides an additional separation dimension and allows determining collision cross sections (CCS) of the analytes as a further physicochemical constant supporting the identification. The CCS database developed in our group was expanded in the last year and contains now more than 500 standard substances including drug-like compounds and pesticides. This database was used for contaminant screening of a wastewater sample.

The analysis was initially performed with high performance liquid chromatography (HPLC) coupled to ion mobility-quadrupole-time of flight mass spectrometer (IM-qTOF-MS). A database search including exact mass (± 5 ppm) and CCS ($\pm 1\%$) delivered 22 different compounds. Furthermore, the same sample was analyzed with LC+LC-IM-qTOF-MS.

This four dimensional separation platform revealed 53 different compounds, identified over exact mass and CCS, in the examined wastewater sample. It was also demonstrated that the CCS database can also help to distinguish between isobaric structures exemplified for cyclophosphamide and ifosfamide as shown in the figure below, where an extracted ion chromatogram of the $[M+Na]^+$ -adduct of ifosfamide and cyclophosphamide ($m/z = 283.0140$) shows two peaks eluting close together. The first of these peaks has a slightly higher drift time,

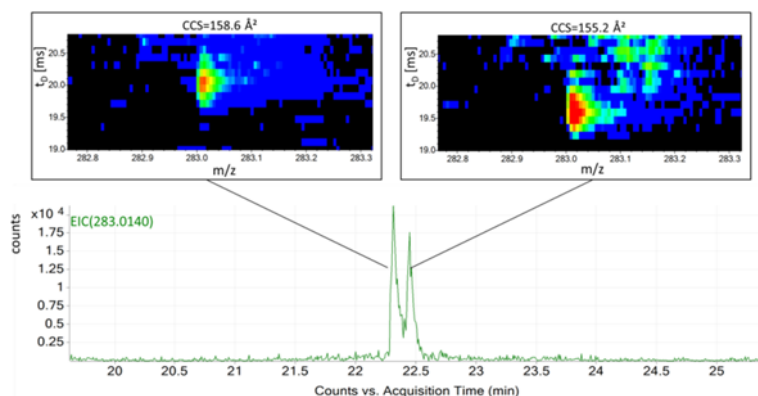


Figure: Extracted ion chromatogram for the $[M+Na]^+$ -adduct ($m/z = 283.0140$) of ifosfamide and cyclophosphamide. For both chromatographic peaks, the extracted 2D plot (drift time versus m/z) and the resulting CCS value are shown.

resulting in a calculated CCS value of $\Omega = 158.6 \text{ \AA}^2$, than the second peak with $\Omega = 155.2 \text{ \AA}^2$.

This difference enables to identify the first peak as ifosfamide (database value is $\Omega([M+Na]^+) = 158.7 \text{ \AA}^2$), whereas the second peak must be cyclophosphamide (database value is $\Omega([M+Na]^+) = 155.2 \text{ \AA}^2$).

Funded by: Agilent Technologies R & D Mktg. GmbH & Co KG (Waldbronn, Germany)

Development of a GC+GC-System for coupling to an IM-qTOF-MS

Christian Lipok, Jörg Hippler

One dimensional gas chromatography (1D-GC) and comprehensive two-dimensional gas chromatography (GCxGC), each coupled with mass spectrometer (MS) are often used analytical platforms for analyzing the metabolome of plants and humans. In the last years more and more high-resolution mass spectrometer (HRMS), not only in combination with liquid chromatography, but also coupled with GC and GCxGC are used to analyze thus complex samples. But there are four major problems in the analysis of complex samples with GC-MS, which make a fast analysis very difficult. At first, with HRMS a powerful mass resolution with high accurate mass is possible, which allows us to calculate a molecular formula of an analyte. But the molecular formula is not the structure and normally more as one, often tens or hundreds of compounds show the same molecular formula, which do not allow an identification of the analytes in the sample. Secondly, the separation power of a 1D-GC – and for really complex samples also of GCxGC – is often not enough for a baseline separation of complex samples. This leads to coelution, which means that several, often tens or more, compounds are in the ion source at the same time. Because of this coelution ion suppression happens, especially with an atmospheric pressure ion sources such as APCI or APPI in combination with GC, which is increasingly used in the last years, which complicate a quantitative analysis. The third problem is that the coelution leads to mixed MS spectra and, therefore, problems with the qualitative analysis appears. The fourth problem is that the method development for complex samples is very difficult and takes time.

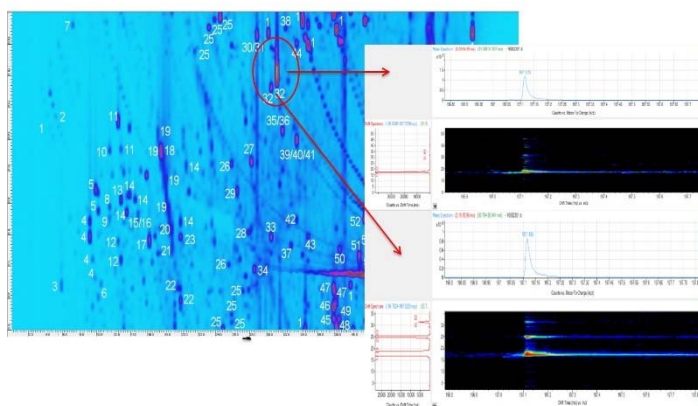


Figure: Analysis of *Calendula officinalis* with GC+GC-APCI-IM-qTOF-MS

Here we are working on a four-dimensional separation method with an outstanding peak capacity, which allows a generic approach for totally different complex samples. The powerful separation will be realized by a two-dimensional chromatography (2D-LC), which is based on a continuous multi-heartcutting approach.

After the chromatographic separation an orthogonal gas phase electrophoretic separation, the ion mobility in a Drift-tube (DTIMS), is followed. The measured drift time allows the calculation of the collision cross section (CCS) by the Mason-Schamp equation. As a fourth separation dimension and the final detector a high-resolution time-of-flight mass spectrometer (qTOF-MS) was used. With the help of a data base in which the m/z and CCS values are listed, an identification of the signals is possible and, therefore, a suspected target analysis of complex samples can be easily realized.

Build up a CCS data base

Jörg Hippler, Susanne Stephan, Timo Köhler

The request to qualify and quantify as many compounds as possible in very complex samples leads to more complex and powerful analytical platforms. For this purpose, comprehensive two-dimensional chromatographic techniques (e.g. LCxLC) are coupled to modern ion mobility-high resolution mass spectrometers (IM-TOF-MS).

The introduction of ion mobility (IM), separating compounds according to their shape-to-charge ratio, provides an additional separation dimension and allows the calculation of the collision cross sections (CCS) as a further physicochemical constant. Unfortunately, this combination of a two dimensional chromatographic system combined with IM-TOF-MS (as 3rd and 4th dimension) leads to a separation in four dimensions – resulting in very complex data sets. Thus data evaluation is a big challenge and currently no available software can simplify this data into a readable plot, including 2D retention times, drift times (respectively CCS), m/z ratio and signal intensity (peak area). To overcome this problem we developed a data analysis software, including LCxLC demodulation after feature analysis (MassHunter IM-MS browser, Agilent Technologies Inc.), m/z matching and CCS Database search. Up to now several hundred CCS values for standard compounds have been measured and included into the CCS database.

 <p>Figure: Home-made CCS data base</p>
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 <p>Collaborative Project – Project Partner: Prof. Thomas Moritz (Swedish Metabolomics Center, Umeå, Sweden)
Funded by: Agilent Technologies (Santa Clara, USA)</p>
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Origin of Life – Analysis of liquid inclusions in quartz samples

Amela Bronja

The origin of life is still an unsolved mystery in science. Hypothetically, prebiotic chemistry and the formation of protocells may have evolved in the hydrothermal environment of tectonic fault zones in the upper continental crust, an environment where sensitive molecules are protected against degradation induced e.g. by UV radiation.

The composition of fluid inclusions in minerals such as quartz which have grown in this environment during the Archean period might provide important information about the first organic molecules formed by hydrothermal synthesis.

We are analyzing organic compounds which were preserved in fluid inclusions of Archean quartz minerals from Western Australia. We found a variety of organic compounds such as alkanes, halocarbons, alcohols and aldehydes which unambiguously show that simple and even more complex prebiotic organic molecules have been formed by hydrothermal processes.

Stable-isotope analysis confirms that the methane found in the inclusions has most likely been formed from abiotic sources by hydrothermal chemistry. Obviously, the liquid phase in the continental Archean crust provided an interesting choice of functional organic molecules. We conclude that these organic substances could have made an important contribution to prebiotic chemistry which might eventually have led to the formation of the first living cell.

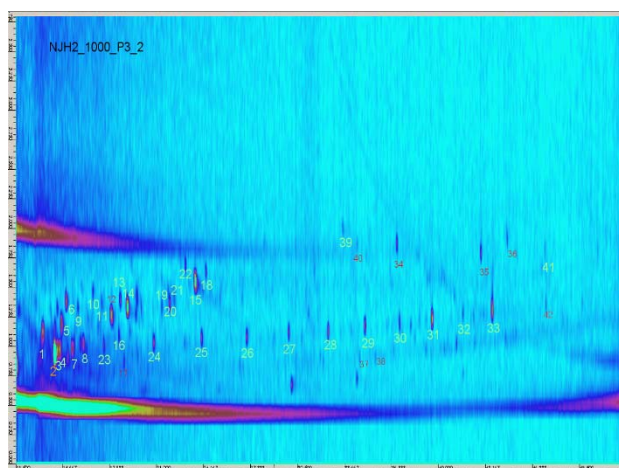


Figure: GCxGC-MS analysis of liquid inclusions

Collaborative Project – Project Partner: Prof. Ulrich Schreiber (UDE), Prof. Christian Mayer (UDE), Prof. Heinz F. Schöler (Ruprecht Karls University Heidelberg)

Determination of Intracellular Metabolites from *Cobetia Marina* by GCxGC-MS

Junjie Li

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

A comprehensive method, utilizing a Shimadzu GCxGC coupled to MS, has been developed to investigate the instantaneous physiological state of *Cobetia Marina* via intracellular metabolites. A quenching method with cold physiological saline was adopted to stop the metabolic activity, which results in less cell membrane damage than normal method and avoided the usage and pollution of organic solvent in the meantime.

To illuminate the contamination of extracellular metabolites, factually reveal the inner cellular state, a cleaning strategy was arranged directly after quenching with phosphate buffered saline as washing agent. The mixture of methanol/water/chloroform was utilized in the followed two-phase extraction. As a result, the upper-phase extract containing polar metabolites was then lyophilized with freezing dryer and derivatized by silylation.

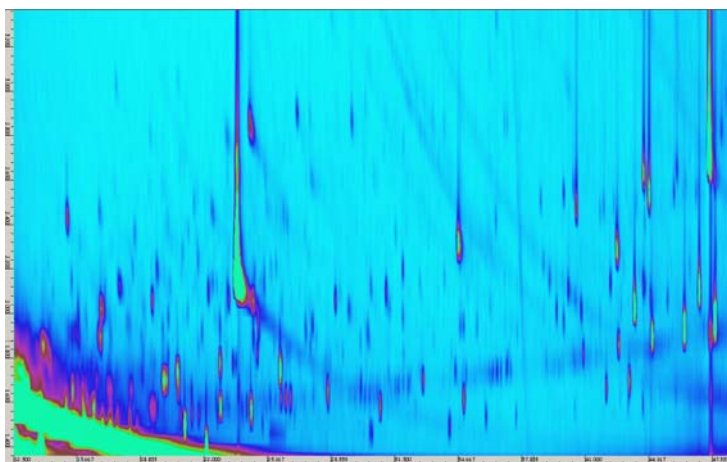


Figure: The 2D contour plot with intracellular metabolites from *Cobetia Marina* separated on GCxGC-MS after derivatization

As shown in the figure, the derivatized sample was separated and determined with GCxGC-MS according to the orthogonality formed by two columns – ZB-5MSi and ZB-50. Finally, among 100 metabolites, 37 metabolites were identified including 8 fatty acids from C_{14:0} to C_{22:0} and 5 amino acids such as Glutamic acid, etc.

Once the solid-water interface, where bacteria are growing and adhering at, is electrochemically activated, the identified metabolites above are supposed to be the potential biomarkers for evaluating the anti-biofouling treatment in the future.

Collaborative Project – Project Partner: Prof. A. Rosenhahn (RUB), Prof. Torsten Schmidt (UDE), Prof. W. Schuhmann (RUB)

Funded by: Mercator Research Center Ruhr

Quantitative analysis of bisphenol A in recycled paper with a novel DIP-APPI-IonTrap-MS

Simeon Horst

A new ambient ion source was developed and its application to real samples has been demonstrated. This ion source is based on a previously build ion source using chemical ionization under atmospheric pressure and electrospray ionization (DIP-APCI/ESI).

To enhance the range of analytes we added to this ion source a photo ionization lamp to enable also photo ionization, which allows the possibility to analyze polar (ESI), middle (APCI) and non-polar (APPI) analytes with the same source and with no or only a small change of the setup. In comparison with DIP-APCI this ion source reaches similar analytical limits but shows better sensitivity for some aromatic and nonpolar analytes.

The analysis of bisphenol A from extracts of recycled paper demonstrates the use of this ion source for real samples. Quantification was possible by the use of a deuterated internal standard that was added to the papers before extraction.

Here atmospheric pressure chemical ionization leads to bad results due to ion suppression whereas atmospheric pressure photo ionization shows results that fit to literature values.

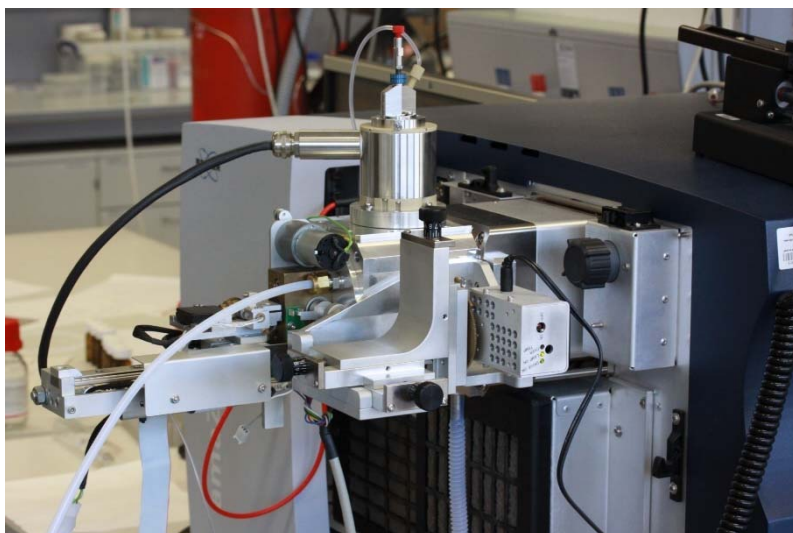


Figure: Picture of the new DIP-APPI ion source

Analysis of different pharmaceutical with the further developed DIP-ESI-MS

Claudia Lenzen

Since the invention of ambient ionization technologies in 2004 this field of analytical chemistry is rapidly grown. The great advantage of ambient mass spectrometry over other analytical procedures is that no or less sample pre-treatment is necessary. The samples can be introduced into the instrument without any modification. Therefore it simplifies and shortens the analytical procedure. The great disadvantage of ambient ionization methods is that there might be problems by matrix components which would not occur if the sample is cleaned in front of the measurement. To overcome this disadvantage a temperature controlled desorption is achieved by the direct inlet probe-atmospheric pressure chemical ionization (DIP-APCI) interface developed by our group.

2015 we had develop the direct inlet probe-electrospray ionization (DIP-ESI) based on the DIP-APCI. It was coupled to an ion trap mass spectrometer (MS) for the detection of more polar compounds such as degradation products from pharmaceuticals.

The enhancement of the DIP-ESI was going on in 2016 and different pharmaceuticals in its tablet forms were analysed with the DIP-ESI and compared with the DIP-APCI and with established analytical methods as HPLC-DAD and HPLC-ESI-MS. One of these drugs is Amlodipine besylate. Using the example of the eight possible known impurities in tablets that are listed in the European Pharmacopoeia, some advantages and disadvantages of the DIP-ESI could be shown. Six substances have been identified as known impurities.

But it turned out that two of them were incorrectly identified by overlapping with other impurities. Additionally, with the DIP-ESI eleven impurities or degradation products were found which are not described in the literature. These impurities were further investigated. For two of these substances structures were proposed, which are based on MS² and MS³-studies.

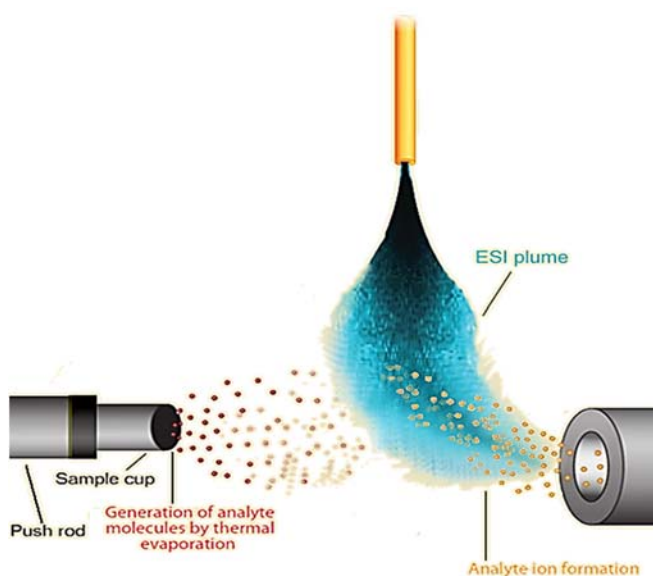


Figure: Scheme of the new ion source

Speciation of mercury (II) and methylmercury in sediments by HPLC-ICPMS

Claudia Kowalczyk

Mercury has several species that differ in their availability, mobility and toxicity. By biotic and abiotic processes natural transformation of these species occurs in the environment. The high mobility and toxicity of methylmercury (MeHg^+) is one reason for the particular interest in this species. Due to the low concentration of methylmercury in sediments and possible species transformation the determination of these species is still a challenge. Furthermore the significance for accumulation of these low concentration for exceeding the EU thresholds (Water Framework Directive) is still not understood.

In the literature, there are a variety of methods for the extraction of mercury species, including acidic and alkaline extraction methods. However, a best practice advice is still not available. The goal is to find the optimal extraction method and to improve it for different sediments.

In this study speciation of mercury (II) (Hg^{2+}) and methylmercury was performed by HPLC-ICPMS. L-cysteine and 2-mercaptoethanol are two common used additives for the extraction and determination of mercury species. Because of the harmful effect of 2-mercaptoethanol investigations were undertaken with L-cysteine. In the present experiments acidic extractions with different L-cysteine concentrations were carried out, to check if it has a positive effect on the recovery of both species.

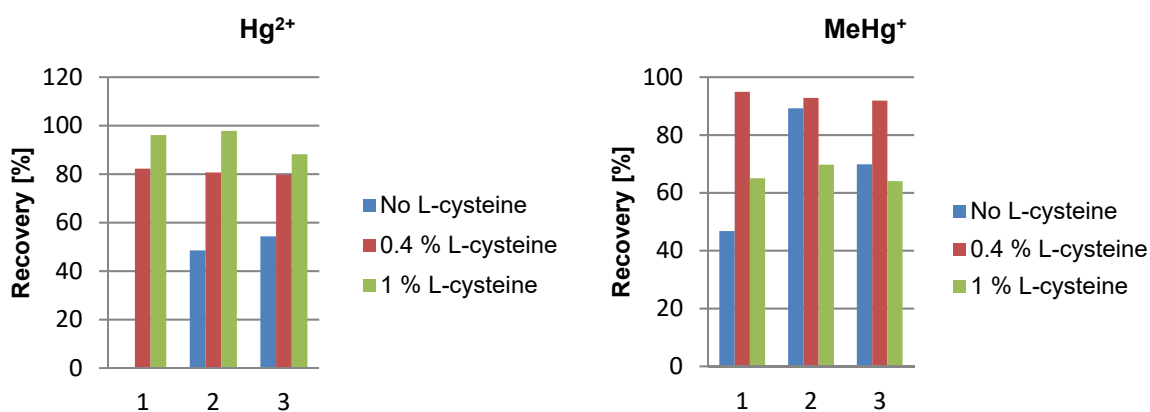


Figure: Influence of the L-cysteine content on the extraction efficiency of Hg^{2+} and MeHg^+

The results show that the content of L-cysteine has a decisive influence on the extraction efficiency, thereby making the usage of 2-mercaptoethanol unnecessary. The recoveries of Hg^{2+} improve with increasing L-cysteine content, whereas the recovery of MeHg^+ appears to be the best at 0.4%. This is the reason to consider this concentration level as the best for the extraction of Hg^{2+} and MeHg^+ .

Determination of Nicotine and Cotinine in Human Blood by Dried Blood Spot-LC-Orbitrap MS Technique

Ahmad Abu-awwad

A simple, robust and economic bioanalytical method for simultaneous determination of nicotine (Nic) and cotinine (Cot) in human blood was developed and validated using dried blood spots (DBS) and LC-Orbitrap MS technique. The DBS was punched at 6.35 mm diameter and extracted by 10% w/v of trichloroacetic acid solution, containing Nic-d3 as an internal standard (IS). The extracted samples were then injected into a Kinetex-C18 column and eluted by mobile phase of methanol:water:formic acid (10:90:0.001, v/v/v).

Nic, Cot and IS were detected accurately by Orbitrap-MS using heated-ESI source at positive ions m/z of 163.1235, 177.1028 and 166.1423, respectively. The developed method was validated according to European and American guidelines for bioanalytical method validation.

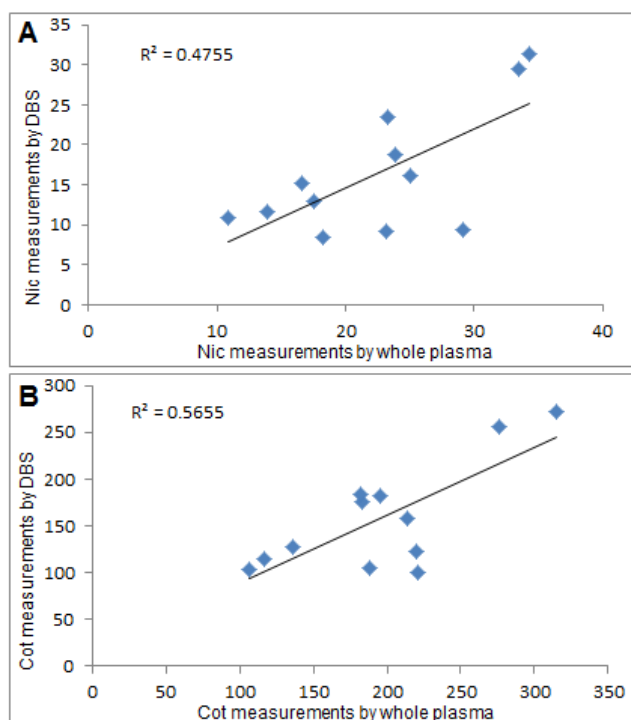


Figure: Correlation between DBS measurements with their corresponding measurements from whole plasma for Nic (A) and Cot (B).

The chromatographic effect of DBS was investigated by decentralized disk punching (peripheral area). The established calibration ranges for Nic and Cot were linear between 5-250 ng/mL and 10-500 ng/mL, respectively. Within- and between-run measurements accuracy for Nic and Cot were all higher than 80% for LLOQ and 85% for QC levels. Within- and between-run measurements precision for Nic and Cot were all within 15%.

Doctoral Theses accomplished 2016

Pia Rosendahl

GC-MS as an alternative diagnostic method for identification of ruptured silicone gel-filled breast implants

Susanne Stephan

Development of a four-dimensional separation method for the analysis of complex samples

Bachelor Theses accomplished 2016

Stefanie Bettin

Analysis of extracts from Calendula officinales with GCxGC-MS

Jens Dreschmann (external)

Qualitative and Quantitative Determination of Polar and Nonpolar Organic Pollutants in Avian Scavengers

Alexander Haupt

GC-APPI-MS

Robert Kalnins

Determination of CCS values of lipids from a cell disruption with LC-IM-qTOF-MS

Tim Kriegsmann

Quantitative determination of Zn with Laser-Ablation-ICP-MS

Martin Ohrt

Analysis of various standards using DIP-ESI/APPI/APCI

Master Theses accomplished 2016

Nitesh Babu (external)

Investigating the effect of contaminated carbon source on activated sludge process in laboratory scale leachate water treatment plant for optimization of an industrial scale plant

Christian Lipok

Development and optimization of GC+GC-APCI-IM-qTOF-MS

Pratima Shrestha

Pesticide analysis of Chinese drugs with LC-IM-qTOF-MS

Simon Rene Schade

Formation of a CCS data base for lipids and its use for the analysis of real samples

Accepted and/or published scientific publications 2016

Original Paper / Peer-reviewed

S. Stephan, J. Hippler, T. Köhler, D. Brecht, O. J. Schmitz*, **A powerful four-dimensional separation method for complex samples**, accepted in Journal of Analysis and Testing

C. Koch, A. Dundua, J. Aragon-Gomez, M. Nachev, S. Stephan, S. Willach, M. Ulbricht, O.J. Schmitz, T. Schmidt, B. Sures **Degradation of polymeric brominated flame retardants: Development of an analytical approach using PolyFR and UV irradiation**, accepted in Environmental Science & Technology

S. Scherer, E. Wollrab, L. Codutti, T. Carlomagno, S. Gomes da Costa, A. Volkmer, A. Bronja, O. J. Schmitz, A. Ott **Chemical analysis of a "Miller-type" complex prebiotic broth Part II: gas, oil, water and the oil/water-interface**, Origins of Life and Evolution of Biospheres, DOI 10.1007/s11084-016-9528-8

A. Abu awwad, T. Arafat, O. J. Schmitz* **Study the Influence of Licorice and Pomegranate Drinks on Nicotine Metabolism in Human Urine**, Journal of Pharmaceutical and Biomedical Analysis 132 (2017) 60-65

S. Stephan, J. Hippler, T. Köhler, A. Deep, T. Schmidt, O. J. Schmitz* **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

M. M. A. Omar, A. A. Elbashir , O. J. Schmitz* **Capillary Electrophoresis Method with UV-detection for Analysis of Free Amino Acids concentrations in Food**, Food Chemistry, DOI: 10.1016/j.foodchem.2016.07.060

A. Abu awwad, T. Arafat, O. J. Schmitz* **Simultaneous determination of nicotine, cotinine and nicotine N-oxide in human plasma, semen and sperm by LC-Orbitrap MS**, Analytical and Bioanalytical Chemistry (2016) 408:6473-6481

T. Arafat, B. Arafat, A. Abu awwad, O. J. Schmitz **Determination of Fenofibric Acid in Human Plasma by LC-MS/MS and LC-UV**, Chromatography DOI 10.1007/s10337-016-3080-6016-3080-6

C. Lenzen, G. A. Winterfeld, O. J. Schmitz **Comparison of Piracetam measured with HPLC-DAD, HPLC-ESI-MS, DIP-APCI-MS and a newly developed and optimized DIP-ESI-MS**, Analytical and Bioanalytical Chemistry (2016) 408:4103-4110

S. Stephan, C. Jakob, J. Hippler, O. J. Schmitz **A novel four-dimensional analytical approach for complex samples**, Analytical and Bioanalytical Chemistry (2016) 408:3751-3759

P. Rosendahl, J. Hippler, O. J. Schmitz, O. Hoffmann, P. Rusch **Cyclic volatile methylsiloxanes in human blood as markers for ruptured silicone gel-filled breast implants**, Analytical and Bioanalytical Chemistry (2016) 408:3309–3317

A. Li, O. J. Schmitz, S. Stephan, C. Lenzen, P. Y.-K. Yue, K. Li, H. Li, K. S.-Y. Leung, **Photocatalytic transformation of acesulfame: transformation products identification and embryotoxicity study**. Water Research (2016) 89:68-75

D. Klink, O. J. Schmitz, **SFC-APLI-(TOF)MS – a novel hyphenation of Supercritical Fluid Chromatography to Atmospheric Pressure Laser Ionization Mass Spectrometry**, Analytical Chemistry (2016) 88:1058-1064

Book/ Book Chapters/ Mics. Publications

Georg Schwedt, Torsten Schmidt, Oliver J. Schmitz Hrsg. **Analytische Chemie**, Wiley-VCH (2016)

Stavros Kromidas Hrsg. **The HPLC-Expert – Possibilities and Limitations of Modern High Performance Liquid Chromatography**, (Chapter 1.1), Wiley-VCH (2016)

Stavros Kromidas Hrsg. **The HPLC-MS Handbook for Practitioners**, (Chapter 1.1), Wiley-VCH (2016)

Stavros Kromidas Hrsg. **Das HPLC-MS-Buch für Anwender**, (Chapter 1.1), Wiley-VCH (2016)

S. Stephan, C. Jakob, J. Hippler, O. J. Schmitz **A Novel Four-Dimensional Analytical Approach For Analysis of Complex Samples**, Agilent Application Note

Poster Presentations

D. El-Zeihery, O. J. Schmitz, C. Zongwei, H. H. Schmeiser, **A link between aberrant methylation level and AA-adducts: Fact or coincidence**, World Congress on Chromatography (Amsterdam, Netherlands), October 2016, [Best poster award](#)

J. Li, O. J. Schmitz, **Determination of Intracellular Metabolites from *Cobetia Marina* by Two-dimensional Gas Chromatography with Mass Spectrometer**, analytica conference China (Shanghai, China), October 2016

C. Kowalczyk, J. Hippler, L. Düster, O.J. Schmitz, **Speciation of mercury (II) and methyl mercury in sediments by HPLC-ICPMS**, TRACESPEC 2016: 15th Workshop on Progress in

Trace Metal Speciation for Environmental Analytical Chemistry, Dansk (Poland), September 2016

C. Lenzen, O. J. Schmitz, **Development of a DIP-ESI-MS for drug analysis, 64th ASMS Conference**, San Antonio (Texas, USA), June 2016

S. Horst, O. J. Schmitz, **Development of a DIP-APPI-IM-qTOF-MS, 64th ASMS Conference**, San Antonio (Texas, USA), June 2016

J. Hippler, S. Stephan, T. Köhler, O. J. Schmitz, **Development of a software solution for the evaluation of multi-dimensional LC-systems coupled to an IM-qTOF-MS**, 44th HPLC, San Fransisco (USA), June 2016

C. Lenzen, O. J. Schmitz, **Development of DIP-ESI-MS**, analytica conference Munich (Germany), May 2016

S. Horst, O. J. Schmitz, **Quantification of Bisphenol A from recycled papers with DIP-APPI-IonTrap-MS**, analytica conference Munich (Germany), May 2016

C. Lipok, O. J. Schmitz, **Development of a GC-APCI coupling to an IM-qTOF-MS**, analytica conference Munich (Germany), May 2016

Invited Lectures / Oral Presentations

Prof. Oliver J. Schmitz

The four separation dimensions of 2D-LC-IM-qTOF-MS as an optimal tool for non-target analysis

Novia-Analytiktag, Bad Soden, Germany, November 2016

A novel multi-dimensional separation approach for Lipidomics

10th analytica Anacon conference in Hyderabad, India, October 2016

LC+LC- and GC+GC-IM-qTOF-MS as a potential tool in non-target analysis

8th Shanghai International Symposium on analytical Chemistry in Shanghai, China, October 2016

Ion mobility spectroscopy as a powerful separation dimension in LC-MS

18th International Symposium on Advances in Extraction Technologies & 22nd International Symposium on Separation Sciences, Torun, Poland, July 2016

The four separation dimensions of 2D-LC-IM-qTOF-MS as an optimal tool for non-target analysis

Agilent Lunch seminar at 40th International Symposium on Capillary Chromatography and 13th GCxGC Symposium, Riva del Garda, Italy, June 2016

GC-IM-QTOF-MS – A new hyphenated separation technique for the analysis of complex samples

40th International Symposium on Capillary Chromatography and 13th GCxGC Symposium, Riva del Garda, Italy, June 2016

Ion Mobility Spectrometry as a Powerful Separation Dimension in LC-MS

Analytica conference, Munich, Germany, May 2016

Ion Mobility Spectrometry as a Powerful Separation Dimension in LC-MS

Agilent 6560 Ion Mobility Q-TOF LC/MS Workshop, Shanghai, China, April 2016

Ion Mobility Spectrometry as a Powerful Separation Dimension in LC-MS

Agilent 6560 Ion Mobility Q-TOF LC/MS Workshop, Beijing, China, April 2016

Panel discussion with Christian Minz (Eurofins) and Dr. Alexander Schiffer (Sanofi-Aventis)

Agilent meeting "Win as one" in Berlin, Germany, March 2016

The four separation dimensions of 2D-LC-IM-qTOF-MS as an optimal tool for non-target analysis

DPhG-lecture at University of Freiburg, Freiburg, Germany, February 2016

2D-LC-IM-MS as the ultimate tool in non-targeted analysis

2nd European IM-MS User Meeting, Waldbronn, Germany, January 2016

Dr. Susanne Stephan

Development of a continuous multiheart-cutting LC-System (LC+LC) for coupling to an IM-qTOF-MS

44th International Symposium on High Performance Liquid Phase Separations and Related Techniques, San Fransisco, USA, June 2016

Prof. Abdalla El-Bashir

Capillary Electrophoresis and Molecular Modeling as a Complementary Technique for Chiral Recognition Mechanism of Baclofen and Ofloxacin enantiomers

CE-Forum 2016, Regensburg, Germany, October 2016

Miscellaneous

Conference organization

Prof. Oliver J. Schmitz, Chairman (together with Dr. Ashes Ganguly, Indian Analytical Instruments Association) of the 10th analytica Anacon conference in Hyderabad, India, October 20-21th 2016

Prof. Oliver J. Schmitz, Chairman (together with Prof. Dr. Jin-Ming Lin, Tsinghua University, Beijing, China) of the 8th Shanghai International Symposium on analytical Chemistry in Shanghai, China, October 10-12th 2016

Prof. Oliver J. Schmitz, Chairman of the Session "Separation techniques: How many dimensions are enough?" at the analytica Munich conference

Prof. Oliver J. Schmitz (together with Amela Bronja and Simeon Horst), Organization of the 26th PhD seminar of the Working Group "Separation Science" of the Section for Analytical Chemistry of the GDCh in Hohenroda

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" der analytica Munich

Member of the DAAD selection committee

Member of the committee for the Eberhard-Gerstel-Price

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

Institute Colloquium

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

Prof. Dr. Boguslaw Buszewski from the University of Torun (Poland) 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. Boguslaw Buszewski, University of Torun, Poland, Modified surfaces in determination of biologically important compounds by hyphenated separation techniques, 18.01.2016

Prof. Dr. Christain Neusüß, Aalen University, Germany, Glycan and intact protein analysis: from CE-MS to CE-CE-MS, 18.04.2016

Prof. Dr. Wolfgang Schrader, MPI Mülheim (Ruhr), Germany, Energieforschung und Analytik – Ein chemisches Puzzle in einer Million Teile, 04.05.2016

Prof. Dr. Michael Lämmerhofer, University of Tübingen, Germany, Lipidomic workflows and pharmaceutical and bioanalytical applications, 23.05.2016

Prof. Dr. Patrick Höhener, Aix-Marseille Université, France, Stable isotopes in organic groundwater contaminants and their use for the study of processes at contaminated sites, 13.06.2016

Dr. Stefan Lamotte, BASF Mannheim, Germany, Bridges over troubled water: Strategies for method development of complex samples in HPLC, 27.06.2016

Dr. John Fjeldsted, Agilent, Santa Clara, USA, Highly Accurate Collision Cross Section Measurements for Comprehensive High Throughput Applications, 29.06.2016

Prof. Dr. Astrid Gjelstad, University of Oslo, Microextraction from aqueous samples based on supported liquid membranes – recent trends and new applications, 04.07.2016

Dr. Hans Peter Arp, Norwegian Geotechnical Institute, Polarity, Products and Particles – Emerging Issues in Environmental Organic Contaminant Science, 14.11.2016

Dr. Stephan Buckenmaier, Agilent, Waldbronn, Germany, Multiple Heart Cutting 2D-LC – theory and applications, 05.12.2016

Teaching

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

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

Tutorial Analytical Chemistry I (in German, Dr. J. Hippler)

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

Tutorial Analytical Chemistry II (in German, Dr. J. Hippler)

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

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

Tutorial Analytical Chemistry I (in German, Dr. J. Hippler)

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

Tutorial Analytical Chemistry II (in German, Dr. J. Hippler)

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

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