

Media Briefings 2020

#4 Partnership & Collaboration: Igniting Innovation

Catherine Kaye
EMEA PR Manager

12 May 2020

Media Briefing Series

‘Igniting Innovation’ a catalyst for the advancement of science and technology.

Showcasing the drivers of **Innovation** in today’s world:

- **Product innovation** advances in technology offering new approaches that work smarter and faster for the lab of the future
- **Sustainability** of the lab and operations
- **Collaborations and partnerships** that advance science



#4 Partnership & Collaboration: Igniting Innovation

Today's Agenda

Speaker	Presentation
 <p>Prof. Dr. Oliver Schmitz University of Duisburg Essen</p>	<p>Igniting Innovation Through Partnership Showcasing the Teaching and Research Center for Separation, and some of the successful research being done by Duisburg-Essen</p>
 <p>Kaj Petersen Marketing Manager, GERSTEL GmbH & Co.KG</p>	<p>Partnering for Innovation The relationship with Agilent, and innovations which have helped customers move science forward.</p>
<p>Closing remarks session</p>	<p>Audience Q&A and briefing recap</p>

Igniting Innovation Through Partnership

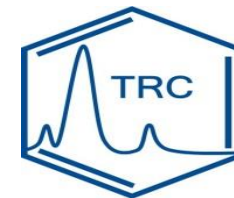
Professor Dr. Oliver Schmitz
University of Duisburg Essen



At moment

- two secretaries,
- one technical staff,
- two senior scientists,
- three postdocs,
- 11 internal PhD students,
- five external PhD students,
- one bachelor student,
- four master students and
- one Alexander-von-Humboldt Fellower

from Bangladesh, China, Germany, South Korea, Spain, Syria and Vietnam are working in my group.



- Teaching and Research Center for Separation: One of Agilent's Center of Excellence
- Collaboration between Agilent and TRC at University of Duisburg-Essen
 - 2D-LC (Agilent, Waldbronn, Germany)
 - IM-MS (Agilent Santa Clara, USA)
 - GC-APCI (Agilent Santa Clara, USA)
- Global partnerships of the TRC at University of Duisburg-Essen



A State-of-the-art Laboratory



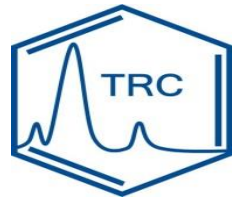
Further information:

www.uni-due.de/aac

www.trc-separation.com

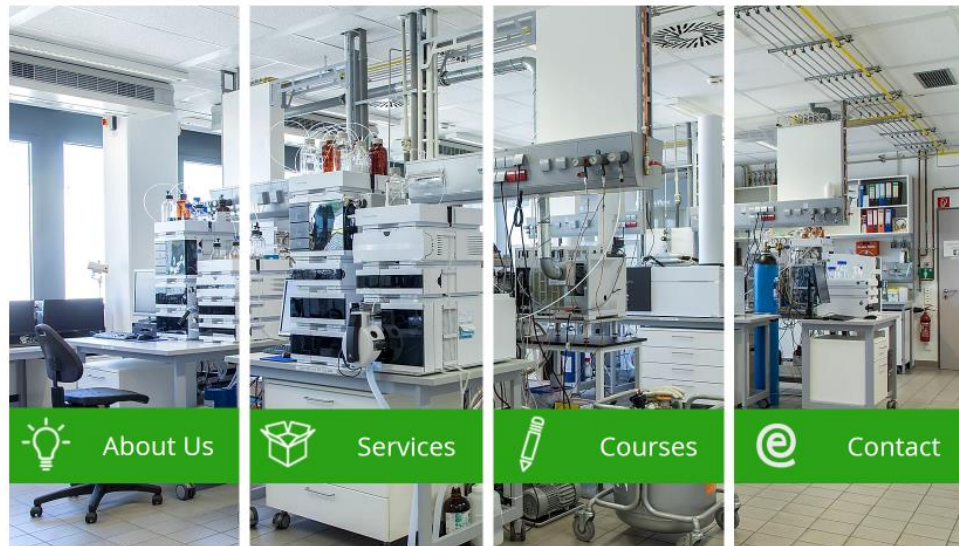
www.oliver-schmitz.net

www.igentrax.com



Teaching and Research Center for Separation

We offer courses in separation techniques (chromatography, electrophoresis) and mass spectrometry as well as high-quality practical courses with latest technology.



Disclaimer & Datenschutz

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To provide comments or feedback on this website, please email: 1979schmitz@gmx.de

Course 1
Basic Course Liquid Chromatography

Course 2
Advanced Course Liquid Chromatography

Course 3
1- and 2D Gas Chromatography

Course 4
GC-MS

Course 5
LC-MS

Course 6
ICP-OES, ICP-MS and CE

1.5 days theory (from me) and
1.5 days practical course (from my team)



- Ion source development
- Multidimensional chromatography
- Ion mobility - mass spectrometry
- Metabolomics/Lipidomics
- Origin-of-Life



nature
chemical biology

ARTICLES

Identification of *Chaoborus* kairomone chemicals that induce defences in *Daphnia*

Linda C. Weiss¹, Basile Albada^{1,2}, Sina M. Becker³, Sven W. Meckelmann⁴, Julia Klein¹, Martin Meyer⁵, Oliver J. Schmidt¹, Ulf Sommer⁶, Markus Lecl⁷, Johannes Zaggerman⁸, Nils Metzler-Nolte⁹ and Ralph Tollrian¹⁰

Invertebrates play important roles in aquatic ecosystems. They were mostly food web interactions, such as by inducing defence in prey. In one case, but still not fully understood example, the planktonic freshwater crustacean *Daphnia pulex* forms specific morphological defences (such as helmets) 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, we report here the chemical identity of the *Chaoborus* kairomone. The biologically active form consists of fatty acids conjugated by the active group of glutamine via the N-terminus. These cues are involved in *Chaoborus* digestive processes, which explains why they are constitutively released despite the disadvantage for its emitter. The identification of the kairomone may allow to design studies on multiple aspects of this inducible defence system.

Information transfer to aquatic ecosystems is highly dependent on chemical cues. Species can acquire information to find food, potential mating partners and predators via chemical signals. For organisms with poor vision, or in turbid environments, chemical cues are indispensable as they can transmit location and temporal and spatial values. These 'infectious' signals affect inter- and intraspecific processes like development, growth, fat storage and reproduction in many aquatic organisms. In consequence, chemical cues are greatly affected by a network of chemical cues. This substantially challenges our current understanding of trophic interactions. It is therefore obligatory to use such double-traited interactions per se to also identify the underlying agents. Treatment examples are: phytochemical cues released by predators that induce the development of defence features in prey organisms. These are called kairomones because of the efficiency of the predator. 'Heavily affecting the dynamics of entire food webs'.

Such interactions have been well studied in microorganisms of the genus *Yersinia*. Ecologically, this bacterium is a keystone species for freshwater habitats, as it is an important link between primary producers and higher trophic levels. Levels of intricate ecological processes, in combination with its exposure to grasses, non-rodent *Daphnia* is a novel model that is highly sensitive to environmental changes and highly sensitive to chemical-dependent phenotypes. Under an increased predation risk, indicated by increasing kairomone concentrations in the environment, modelled biological defences, for example, stressors of stress, spines, helmets, crests, or mouthparts can be developed by the 'chironomid species'. The model predator-prey relationship between the phantom midge larva (*Chaoborus*) and *D. pulex* (*Chaoborus*) allowed dissection of the involved costs and the resulting benefits in relation to the ecology and evolution of inducible defences. Several *D. pulex* induced to *Chaoborus* predator (Fig. 1) resulting benefits include: (Fig. 1) metabolic morphology (Fig. 1), detectability

Results. Chemical identification of putative kairomone agents. For the initial identification of the main compounds, we analysed water in which juveniles of *D. pulex* were subjected to predation

nature
COMMUNICATIONS

ARTICLE

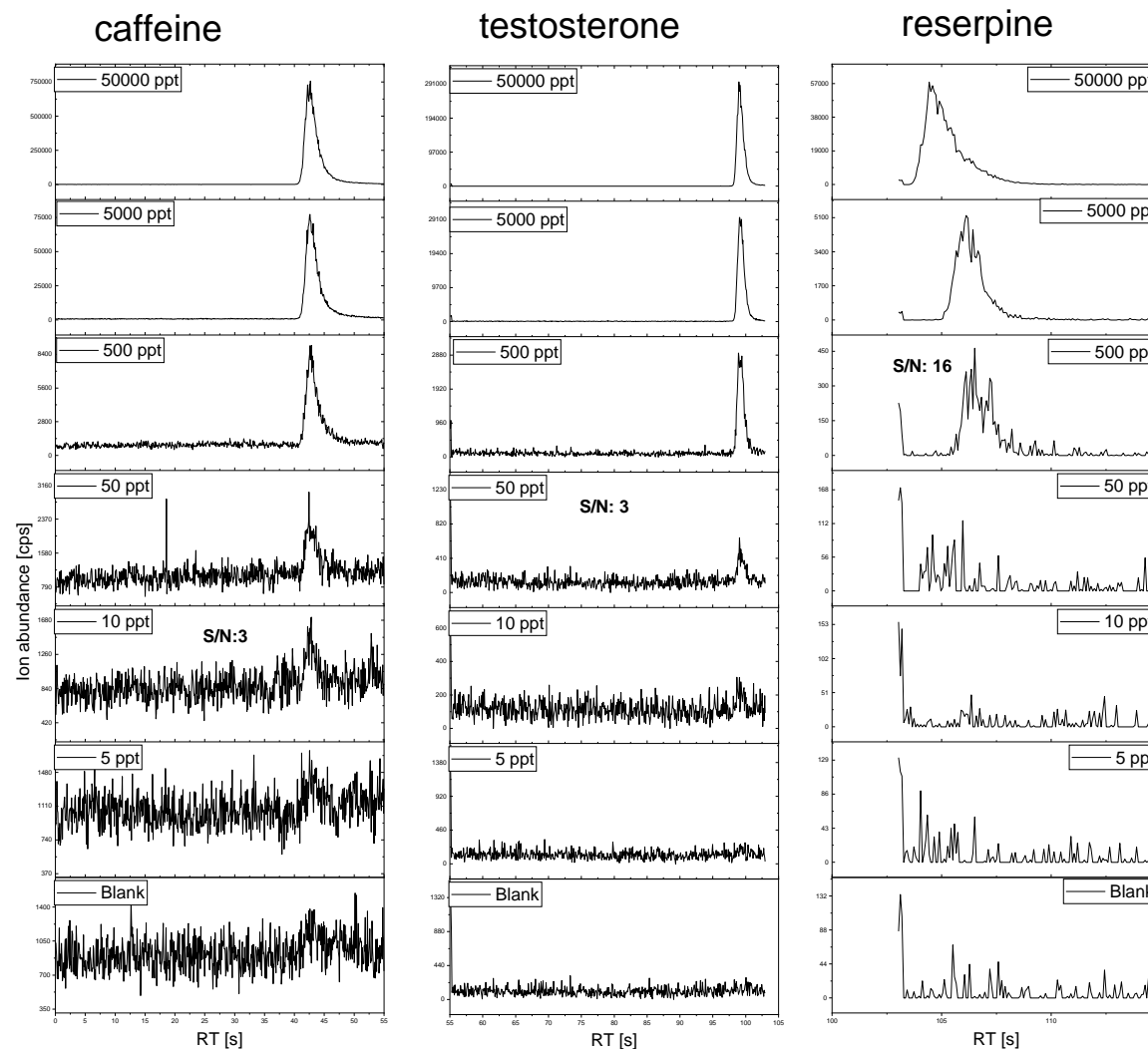
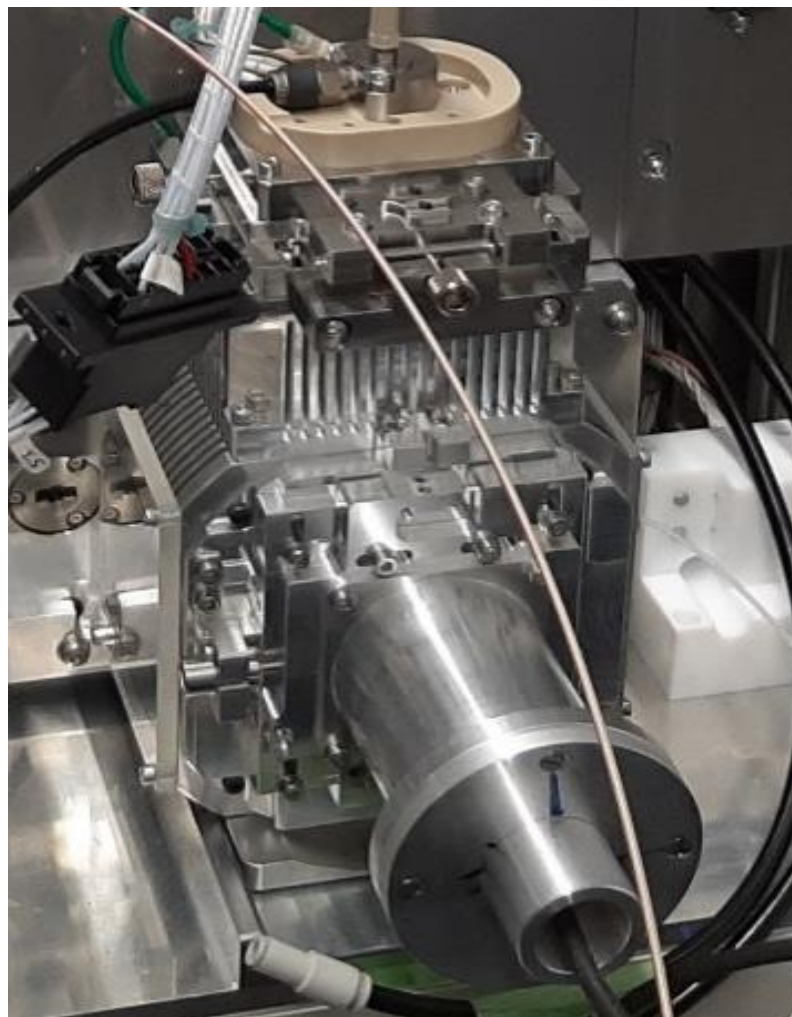
LipidCreator workbench to probe the lipidomic landscape

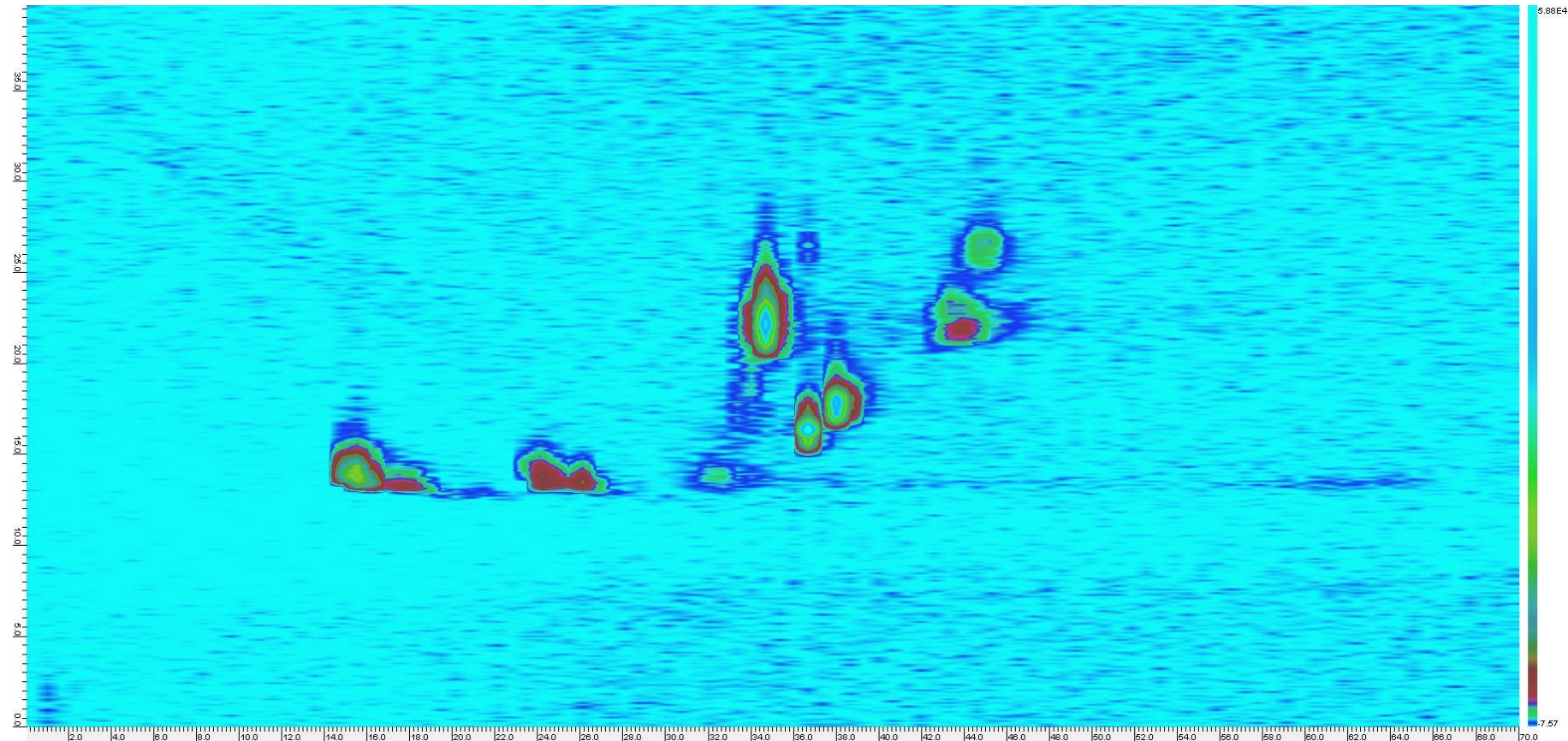
Bing Peng^{1,2,3}, Dominik Kopycynski^{1,8}, Brian S. Pratt³, Christa S. Eising^{1,5}, Bo Barla⁴, Martin Himmerson^{4,7}, Peter Inze Borker⁴, Seth Howe^{1,10}, Mark Y. Chan^{10,11}, Federico Torta¹, Dominik Schwaiblmair^{1,12,14}, Sven W. Meckelmann¹, Cristina Coman^{1,5}, Oliver J. Schmidt¹, Brendan MacLean¹, Mark-Christin Meier¹, Oliver Bors¹, Markus R. Wenk^{1,6}, Nils Hoffmann¹ and Robert Altmann^{1,13,14}

Mass spectrometry (MS)-based lipidomics enables the robust quantification of selected lipids under various biological conditions but comprehensive software tools to support such analysis are lacking. Here we present LipidCreator, a software that fully supports targeted lipidomics analysis development. LipidCreator offers a comprehensive framework to compare MS/MS fragment masses for over 60 lipid classes. LipidCreator provides a mechanistics model to define fragments, merge subtle feature finding, optimize carbon energy and generate in silico spectra. We validate LipidCreator across complex, naturally and synthetically derived lipid samples that it is capable to generate large targeted experiments to analyze lipid and to detect lipid-synthesizing signals such as human lipoproteins.

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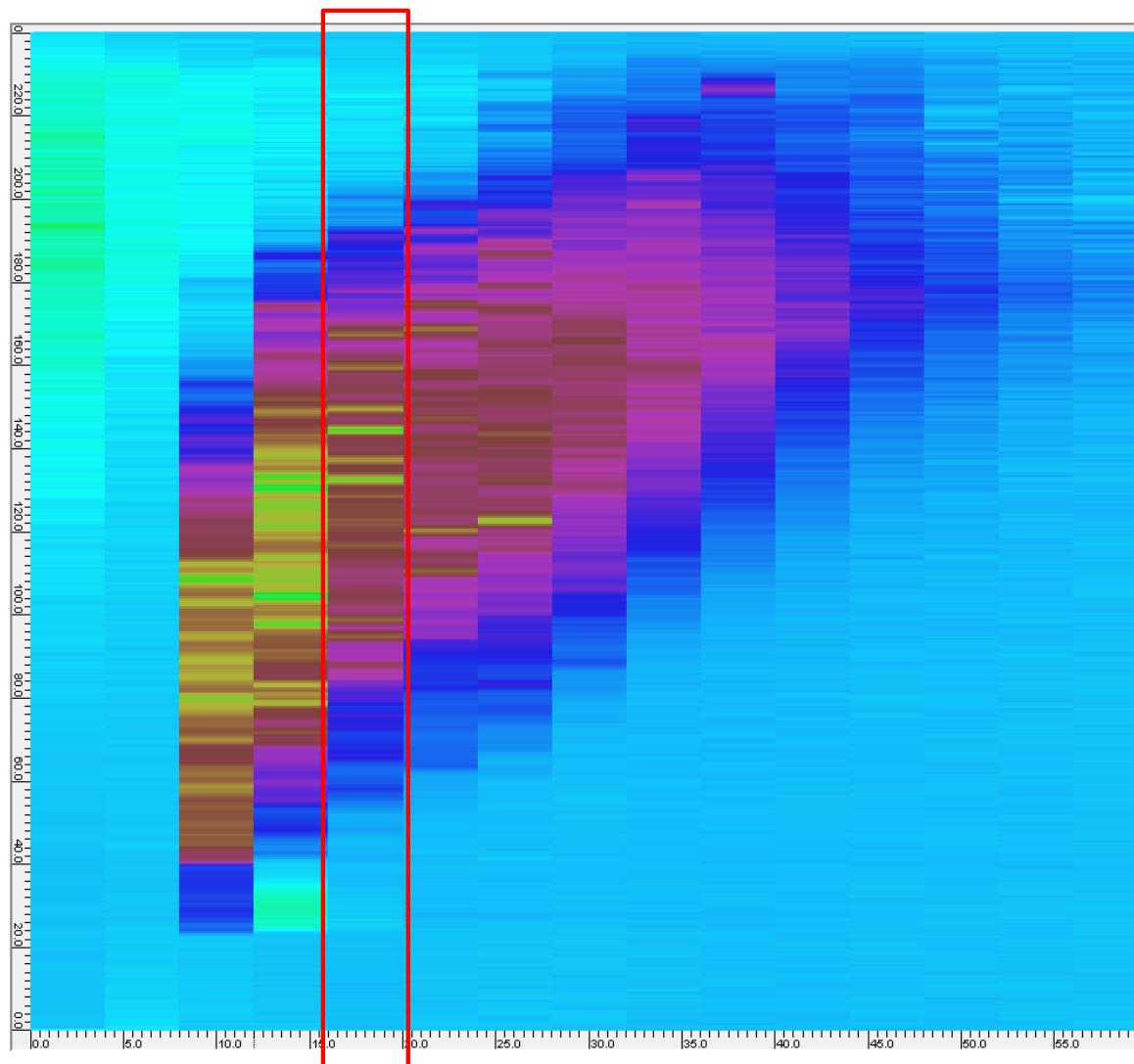
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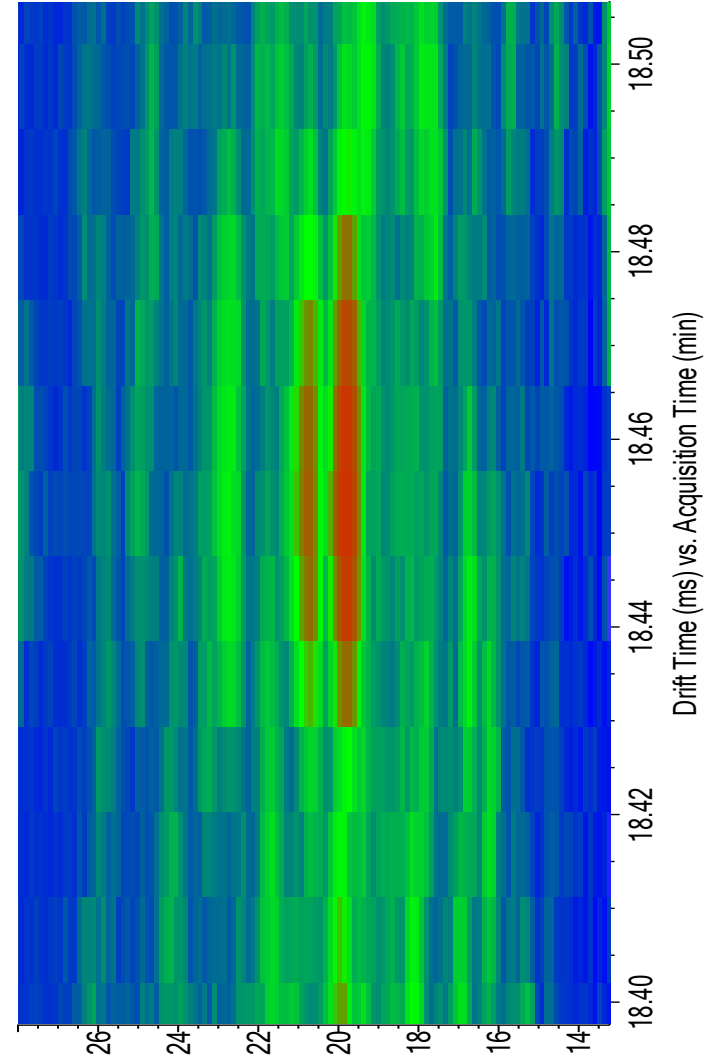
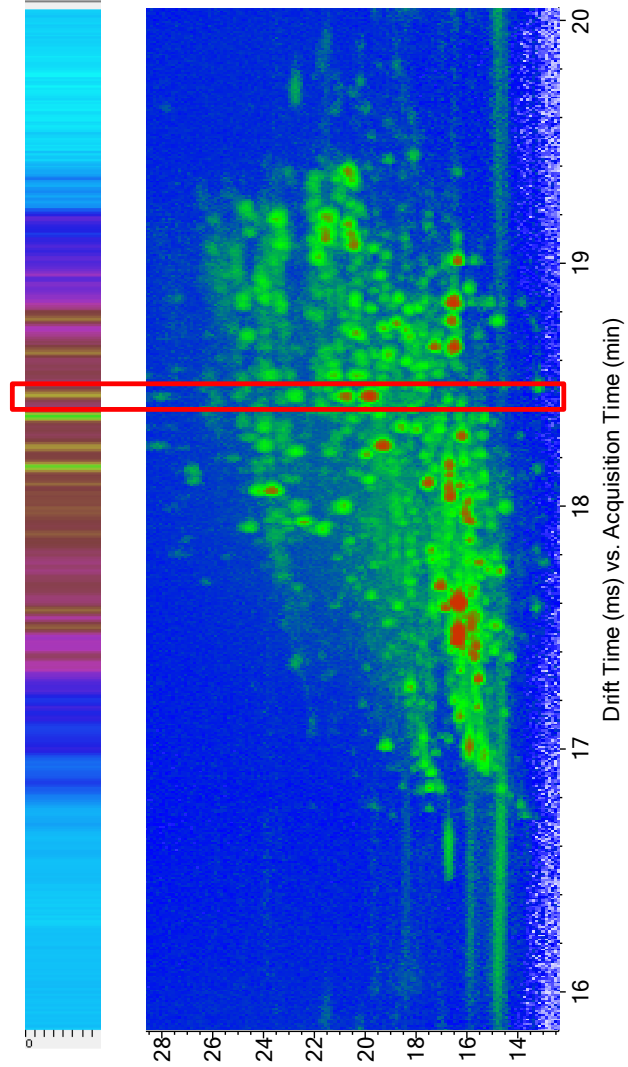


Lubricants in fuel

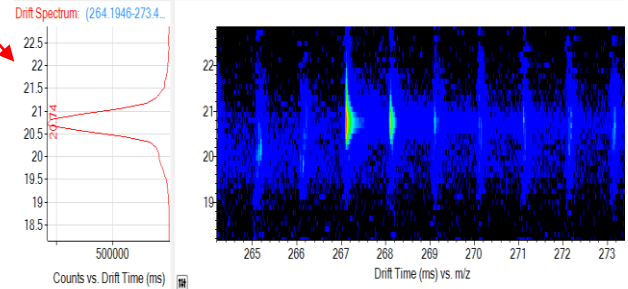
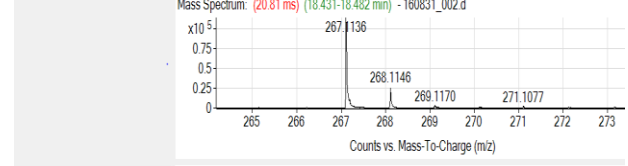
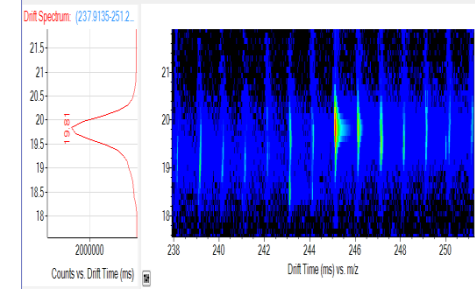
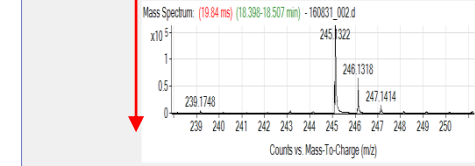
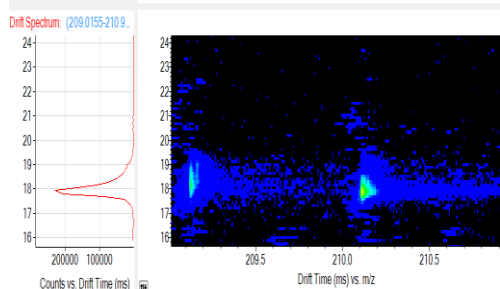
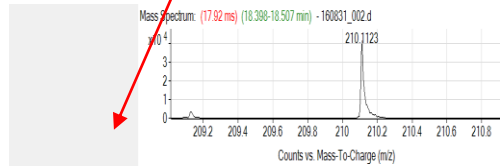
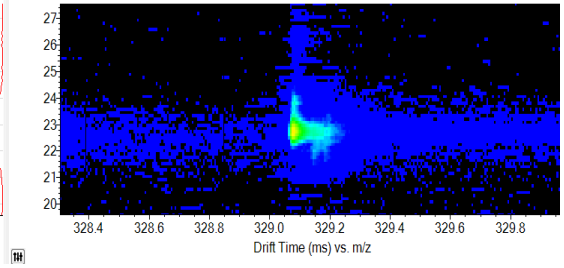
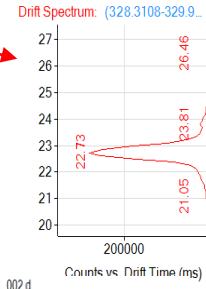
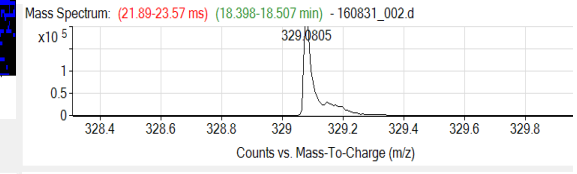
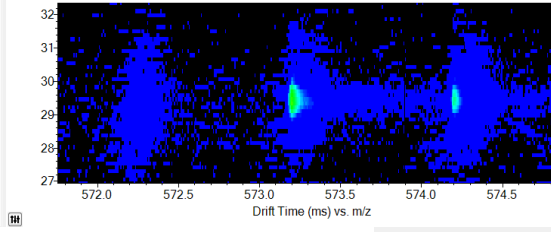
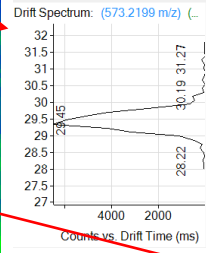
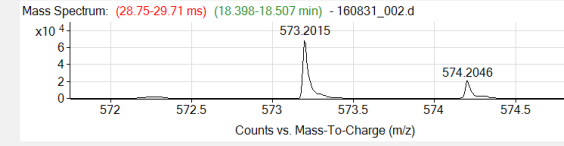
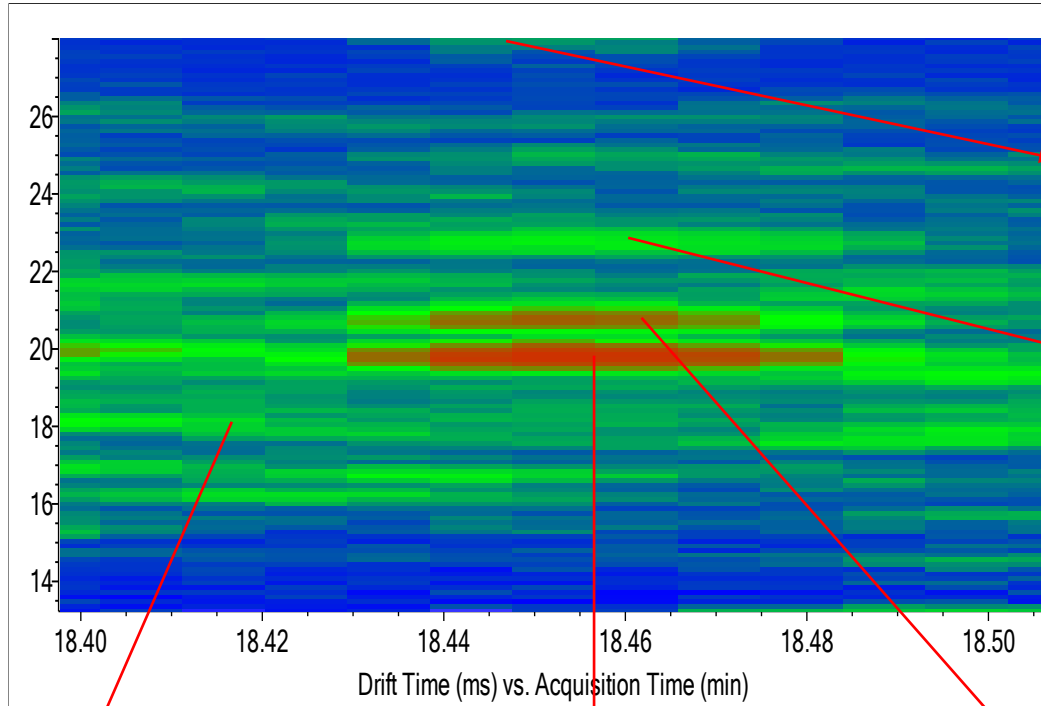
Bio Coal (HTC – Hydrothermal Carbonisation) analyzed with LC+LC-IM-TOF-MS in 60 min



Fraction: 16 and 20 min



Fraction: 6 s (18.40 – 18.50 min)



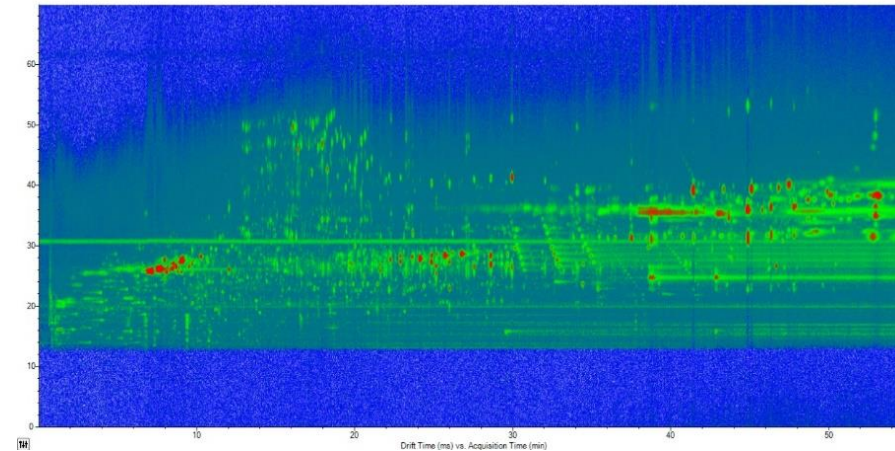
Expeditions into the jungle to understand the active ingredients of herbal prescriptions



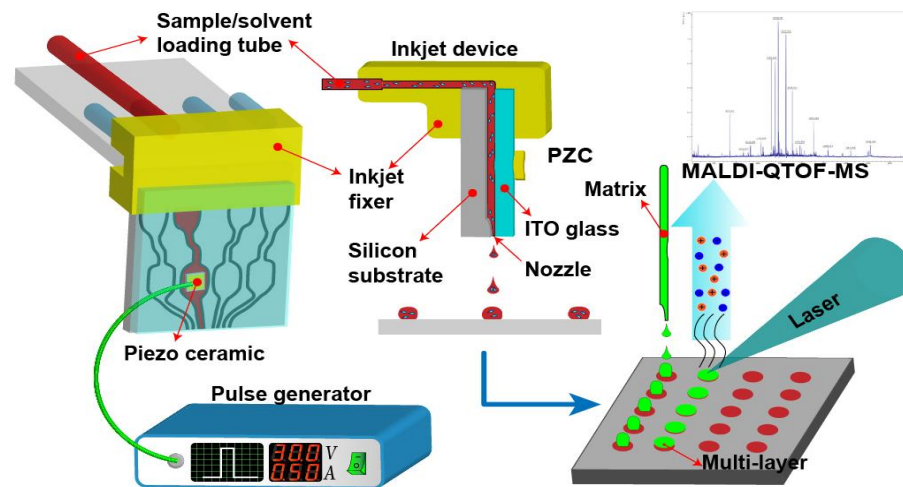
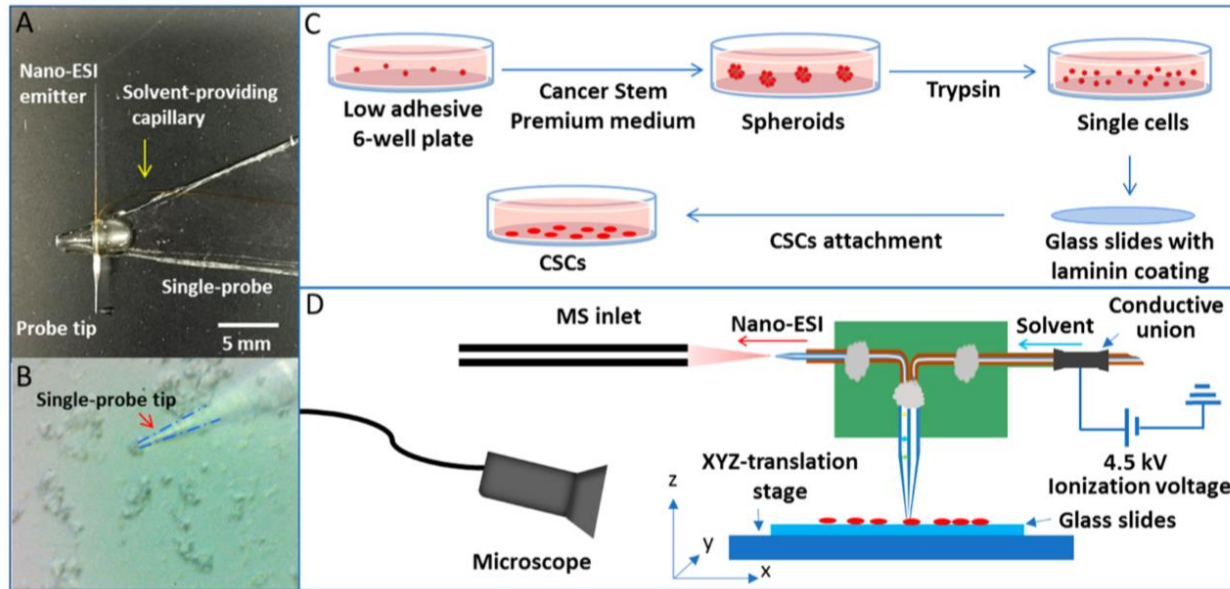
According to the World Health Organization (WHO), 70-80% of the world population, i.e. approximately 5 billion people living mainly in developing countries, are treated with herbal medicines as primary care.

The search for active ingredients against liver diseases began with a survey of 69 practitioners and patients in the northwestern regions of Vietnam, covering 30 ethnic groups of 9 million people.

147 herbal prescriptions used to treat liver disease were collected, and after careful sorting and *in-vitro* and *in-vivo* testing two promising recipes are identified.



HPLC-IM-qTOF-MS analysis of
Gynostemma pentaphyllum



Cooperation with good friends:

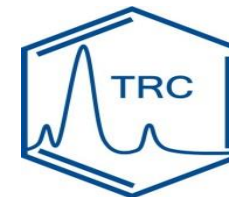
Prof. Guowang Xu, Dalian Institute of Chemical Physics

Prof. Jin-Ming Lin, Tsinghua University, Beijing

What do all research topics have in common?



INNOVATION



ARTICLE



<https://doi.org/10.1038/s41467-020-15960-z>

OPEN

LipidCreator workbench to probe the lipidomic landscape

Bing Peng^{1,2,18}, Dominik Kopczynski^{1,18}, Brian S. Pratt³, Christer S. Ejsing^{4,5}, Bo Burla⁶, Martin Hermansson^{4,7}, Peter Imre Benke⁸, Sock Hwee Tan^{9,10}, Mark Y. Chan^{9,10,11}, Federico Torta⁸, Dominik Schwudke^{12,13,14}, Sven W. Meckelmann¹⁵, Cristina Coman^{1,16}, Oliver J. Schmitz¹⁵, Brendan MacLean³, Mailin-Christin Manke¹⁷, Oliver Borst¹⁷, Markus R. Wenk^{6,8}, Nils Hoffmann¹ & Robert Ahrends^{1,16}✉

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"... At present, there are 52 universities in Germany with departments or faculties of chemistry and only 43% have the subject "Analytical Chemistry" according to an analysis of the GDCh; in about half of the cases it is linked to the subject "Inorganic Chemistry", since traditionally the chemistry beginners were introduced to the subject chemistry by means of simple analytical laboratory tasks.

Such a wrong classification or subordination is detrimental to an interdisciplinary discipline like Analytical Chemistry with increasing research tasks in the entire field of materials science, life sciences and medicine..."

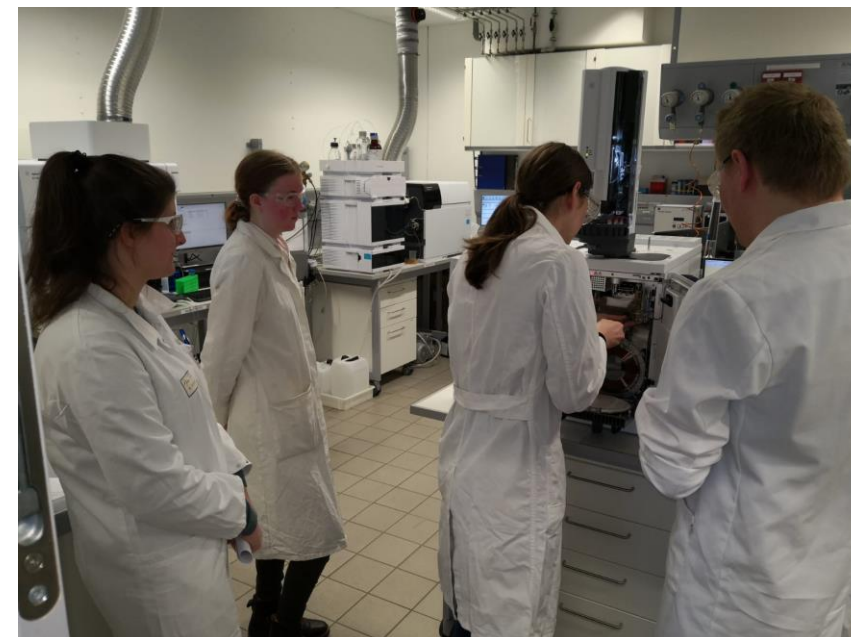
"...The current European Survey for European Chemists 2017, like the previous one in 2015, shows that among the four major disciplines (in addition to inorganic, organic and physical chemistry) analytical chemistry is the only one that produces significantly fewer graduates than the job market requires.

Despite clear warnings and appeals over the last two decades, many professorships and institutes for analytical chemistry in Germany have not been reoccupied, closed or assigned to other disciplines, as is currently happening in Saarbrücken..."



Dr. Joachim Richert
Competence Center Analytics,
BASF, Ludwigshafen

Editorial by Dr. Joachim Richert in *Nachrichten aus der Chemie* 7/8 2018
(translated into English by Oliver J. Schmitz)



Students at the TRC



1. Innovation and Partnership to improve Training

- TRC try to improve the quality of analytical education in Europe
- Spring school Industry for Analytical Chemistry in Germany
- Annual PhD seminar in Hohenroda partly sponsored by industry
- We need more cooperation between industry and university in education, not only in research



2. Innovation and Partnership to improve Research

- New ways in industrial research at universities to realize synergistic effects (a joint project team from industry and university)



3. Innovation and Partnership to improve Talent

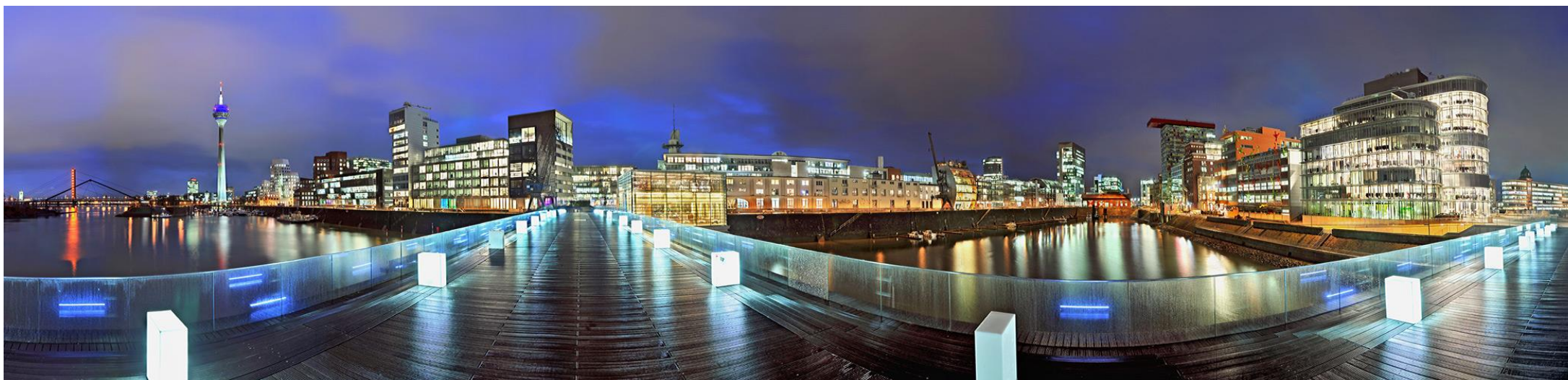
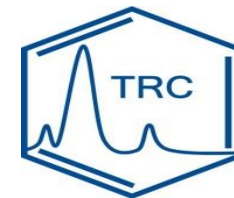
- Talent transfer and shared knowledge with talent transfer between academia and industry



Thank you very much and see you in Düsseldorf 2021!

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HPLC 2021 20–24 JUNE 2021
DÜSSELDORF GERMANY

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HPLC2021



GERSTEL: Partnering for Innovation

Kaj Petersen M.Sc. Chem. Eng.
Marketing Manager
GERSTEL GmbH & Co.KG

GERSTEL: Customer focused solutions

- ▷ Founded in 1967 in Mülheim an der Ruhr, Germany
- ▷ Family owned and operated
- ▷ 5 subsidiaries and >70 distributors
 - 220 employees world-wide
 - 30 employees in R&D, incl. 10 for Software
 - 13 Ph.D. Scientists, 1 Ph.D. Student.
- ▷ Worldwide customers and partners
- ▷ Focus:
 - Automation and sample preparation
 - Extraction and clean-up
 - Analyte concentration
 - Sample Introduction
 - Solutions for GC/MS and LC/MS



Research & Development

The collage features several patent certificates:

- Australia:** Letters patent No. 762611, STANDARD PATENT, dated 2006-05-11.
- Canada:** Brevet canadien / Canadian Patent, dated 2014-05-28.
- United States:** United States Patent, granted to John Doll, dated 2005-05-26.
- Germany:** Urkunde über die Erteilung des Patents Nr. 10 2014 004 57, dated 2015-05-28.
- China:** 发明专利证书 (Invention Patent Certificate), No. ZL 2005 1 0073883.X, dated 2008-10-15.

Central Text Overlay: more than 100 patents held or pending

Bottom Right: Japanese Patent Office (JPO) certificate, dated 2008-08-29, signed by Commissioner 鈴木隆史 (Ryuji Suzuki).

GERSTEL - Agilent partnership

- ▶ 1984: GERSTEL PTV: Cooled Injection System CIS (1984)
- ▶ 1986: Agilent Value Added Reseller (VAR)
- ▶ 1996: HP PTV (OEM)
 - >20,000 installed World-Wide
- ▶ 2000: Agilent Premier Solution Partner
 - Delivering Sample Prep Automation
 - Complete solutions / customized solutions
 - Service and Support



GERSTEL CIS 4
OEM Product
HP-PTV

GERSTEL - Agilent partnership

▶ Automation, Sample Preparation and Analysis Systems

MPS

GERSTEL

Dynamic
Headspace DHS



TDU 2 Thermal Desorption
and PYROlysis



Solid Phase
Extraction SPE



MPS for GC & GC/MS



ATEX Thermal
Extraction in µVials



TD3.5+ for larger
3,5" sorbent tubes



SPME & automated
SPME fiber exchange



Headspace



ALEX Automated
Liner EXchange



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MPS

GERSTEL

Evaporative
Concentration ^mVAP



Extraction
Derivatization
Addition of Standards



Solid Phase
Extraction SPE



MPS for LC & LC/MS



Cold storage
of samples



Disposable Pipette-
Extraction DPX



MASE Membrane
Assisted Extraction



Dried Blood Spot
Autosampler DBS-A



Online-SPE SPE²



www.gerstel.com

AGILENT PARTNER

GERSTEL Partnering for Innovation

▷ Academia and Public Research Institutes

- Development or implementation of new methods and technologies
 - ▷ Example shown: Microplastics TED-GC/MS
- Implementation of GERSTEL automation
 - ▷ Examples: Metabolomics Research, Pharmacokinetics, Stability Assays

▷ Health & Safety, Food, and Forensic Toxicology Laboratories

- Automated and traceable complex sample preparation
- Automating and implementing new Sampling Techniques, DBS shown.
- Complete analysis methods/solutions for THC, Opioids, metabolites
 - ▷ Example shown: THC and metabolites in hair

GERSTEL Partnering for Innovation

- ▷ Industry and Contract Laboratories
 - Technical Solutions and Digitalization project examples:
 - ▷ Automated Liner Exchange (ALEX) for pesticides in tea (QuEChERS)
 - ▷ Automated sequence setup from barcode/LIMS information
 - Automation with GERSTEL technology to meet customer needs
 - ▷ Sample Preparation Methods customized to partner specifications
 - ▷ Miniaturization (savings on sample, solvents and logistics)
- ▷ Agilent Technologies – GERSTEL partnership since 1986
 - Cooperative projects and integrated solutions.
 - ▷ Example shown: EU-WFD surface water analysis without DCM

Innovation Project With Government Institute

Microplastics in the Environment

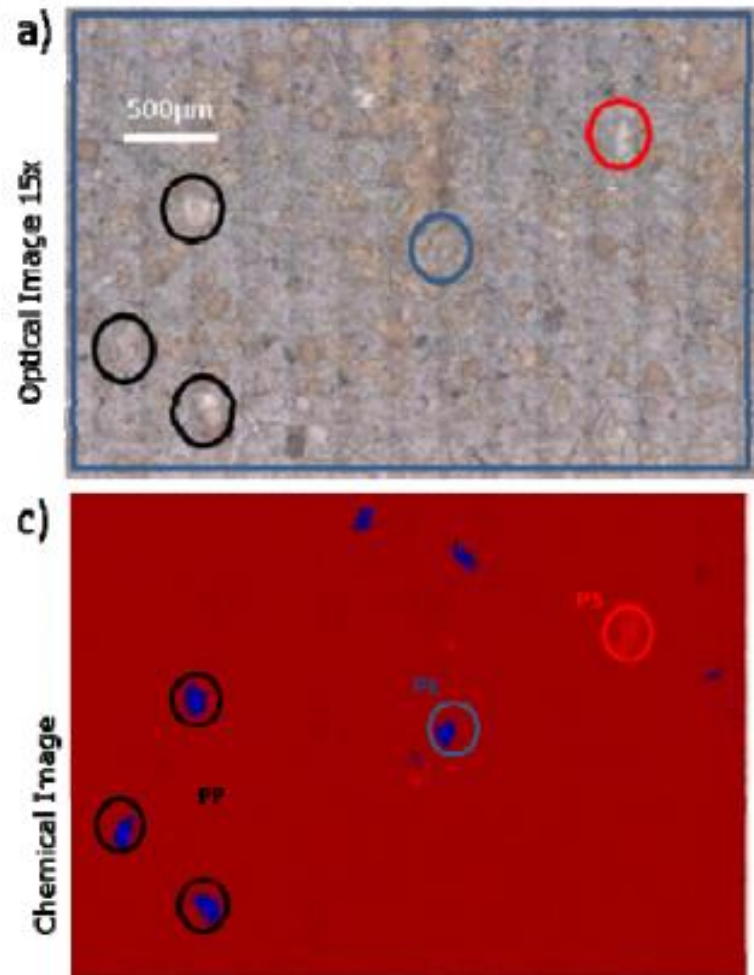
- Analyze this!

GERSTEL



Source: BAM

Spectroscopic Analysis - Imaging (μ -FTIR or μ -Raman – “particle picking”)



- ▷ Identification of plastic types possible
- ▷ Non-destructive
- ▷ Number of particles and size can be determined

But...

- ▷ Time-consuming with regard to measurement and Sample preparation
- ▷ No basis for limit value, no conversion from particle number to mass

Thermal **E**xtraction-**D**esorption Gas**c**hromatography-**M**ass **S**pectrometry

-

TED-GC/MS developed by

BAM

Bundesanstalt für
Materialforschung
und -prüfung

Ulrike Braun, Ph.D.
Erik Dümichen, Ph.D.

Paul Eisentraut
et al.

TED-GC/MS

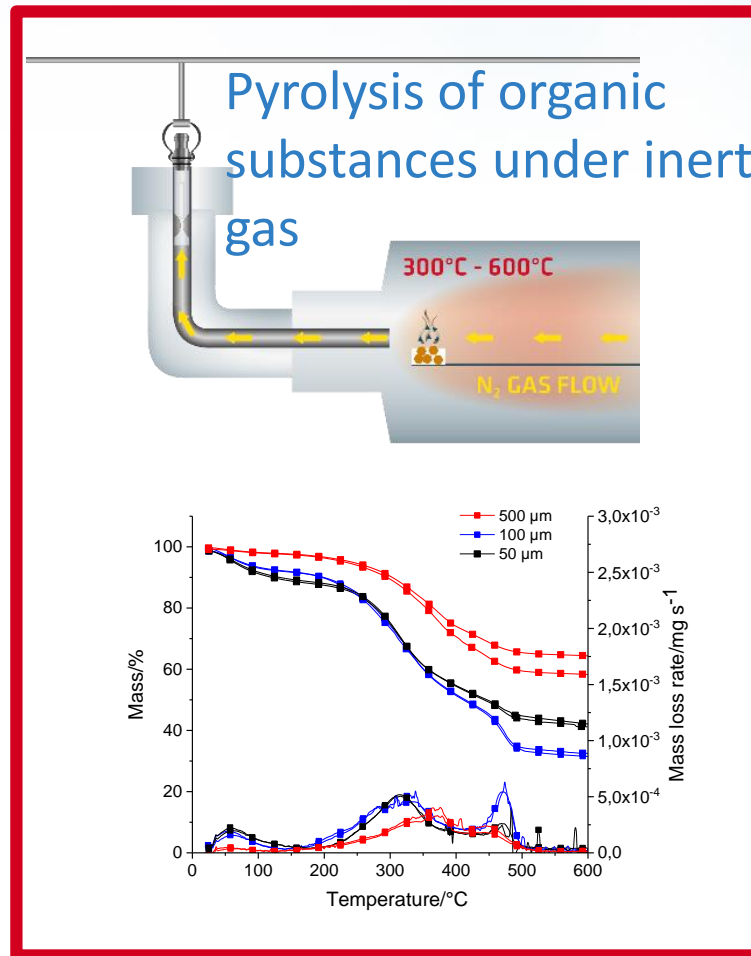
1st step: Thermal Extraction

GERSTEL



Environmental sample:
Sediment, Soil, Sand, Filter
= Matrix + Microplastics

Sample up to 100 mg



Thermogravimetric Analyzer (TGA)

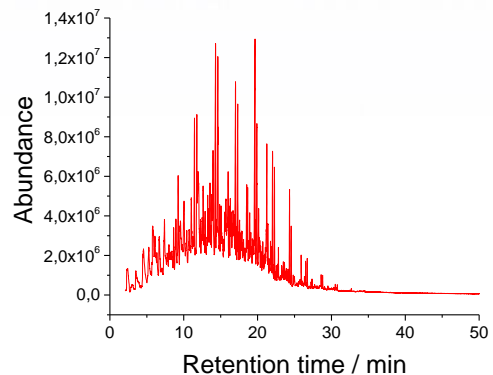


Collection of pyrolysis products on Polydimethylsiloxane (PDMS), e.g. GERSTEL Twister

TED-GC/MS

GERSTEL

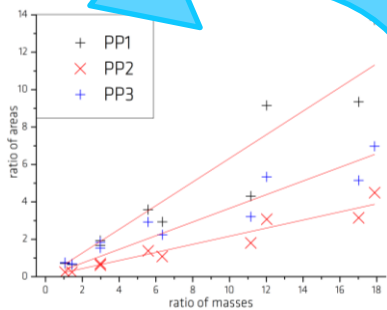
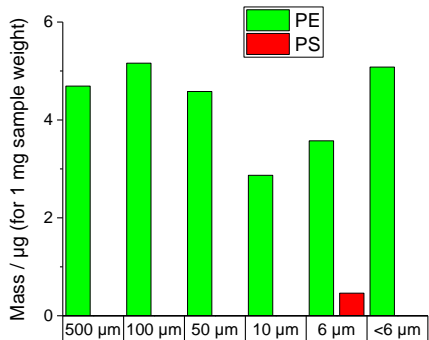
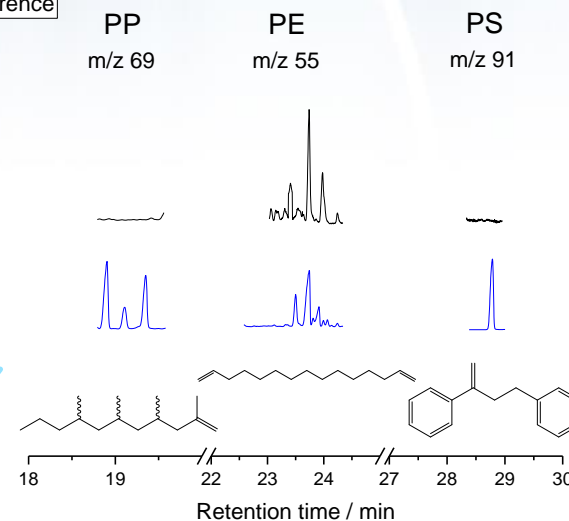
2nd Step: Determination of pyrolysis products



Thermal Desorption GC-MS

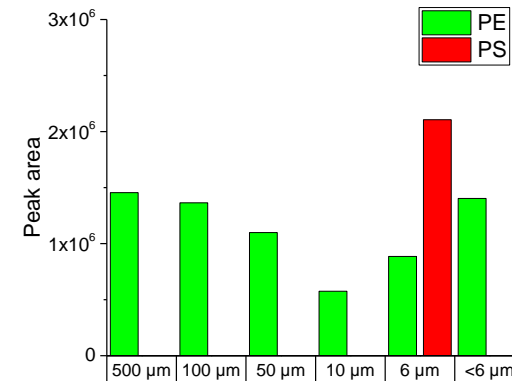
Marker-Compounds Identification

Sample
Reference



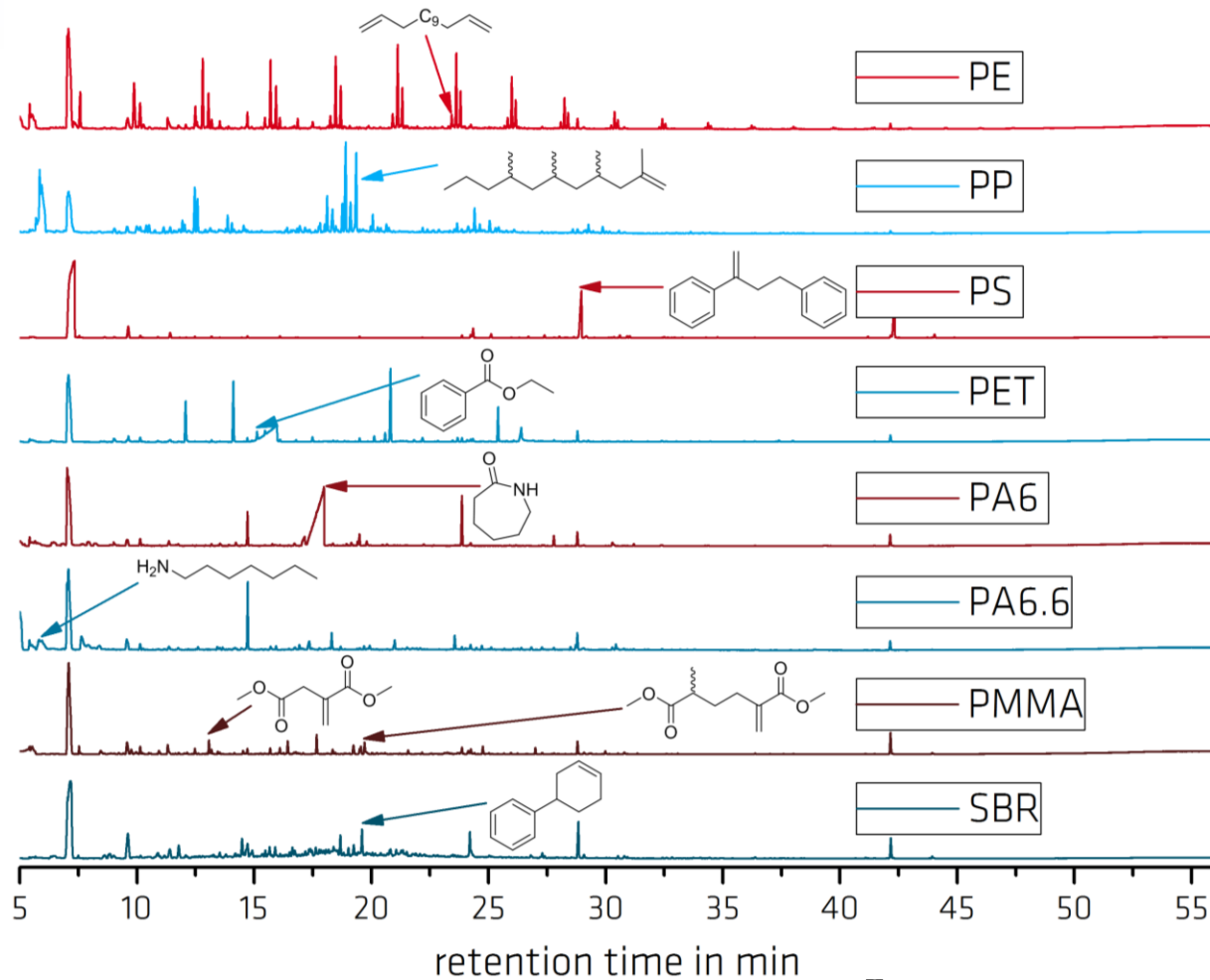
Polymer Quantification

Polymer Identification



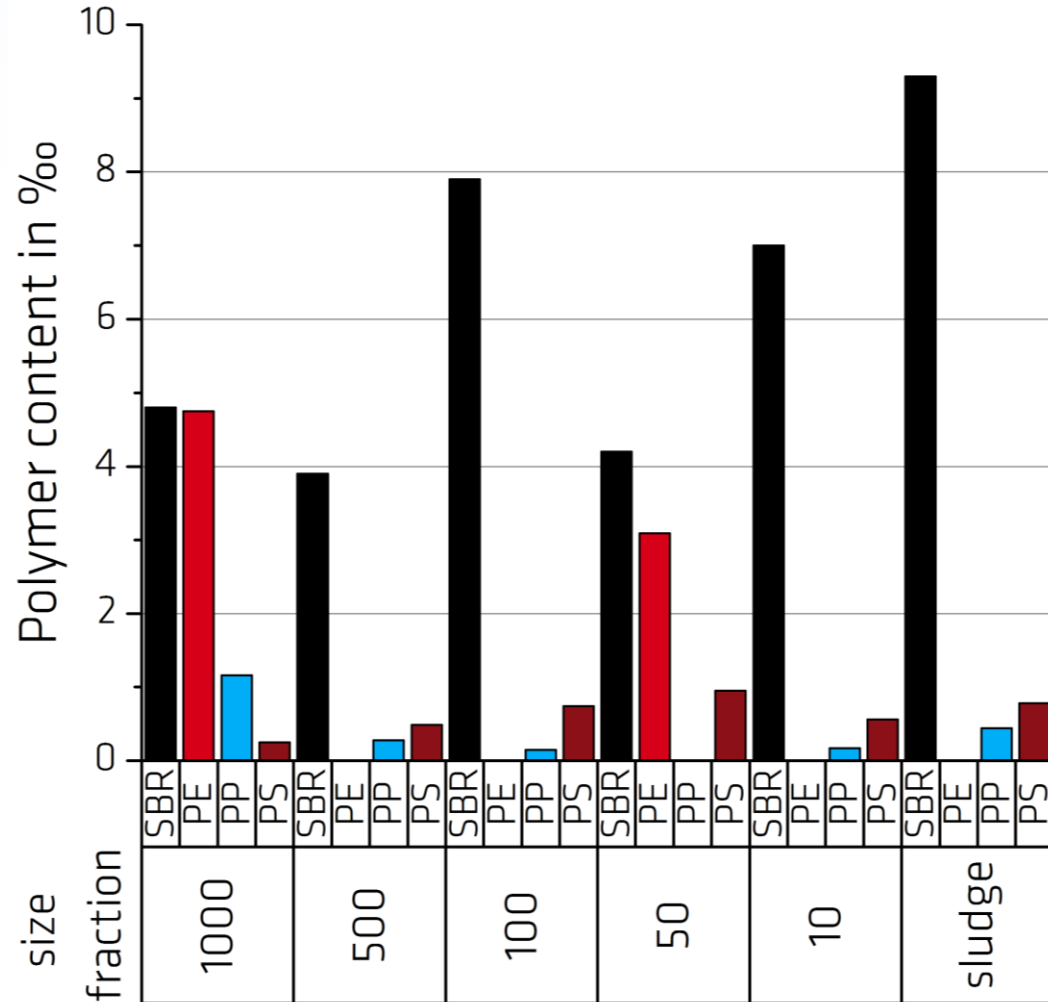
TED-GC/MS

Specific pyrolysis polymer markers

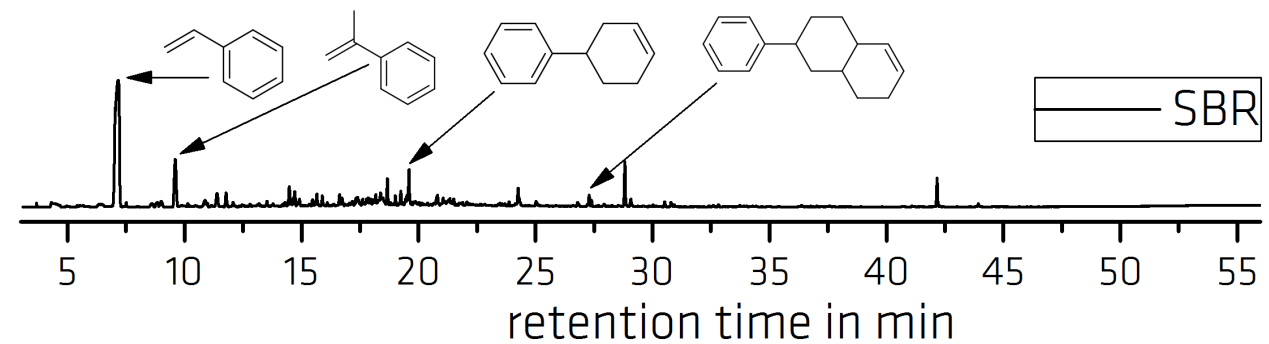


Polymer	LOD in μg
PE	2.2
PP	0.14
PS	0.08
PET	0.24
PA6	0.24
PA 6.6	3.4
PMMA	0.12
SBR	0.06

Application example: Road run-off



Styrene-Butadiene rubber
(SBR, tire abrasion) 4-10 %



P. Eisentraut , E. Dümichen, A. S. Ruhl, M. Jekel, M. Albrecht, M. Gehde, U. Braun, *Environ. Sci. Technol. Lett.*, 2018, 5, 10 608-613.



Contents lists available at ScienceDirect

Journal of Chromatography A

journal homepage: www.elsevier.com/locate/chroma

Automated thermal extraction-desorption gas chromatography mass spectrometry: A multifunctional tool for comprehensive characterization of polymers and their degradation products

E. Duemichen^{a,*}, P. Eisentraut^a, M. Celina^b, U. Braun^a^a Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany^b Sandia National Laboratories, Organic Materials Science Dept. 1853, Albuquerque, NM, 87185-1411, USA

Water Research 85 (2015) 451–457



Contents lists available at ScienceDirect

Water Research

journal homepage: www.elsevier.com/locate/watres

Analysis of polyethylene microplastics in environmental samples, using a thermal decomposition method

Erik Dümichen^a, Anne-Kathrin Barthel^a, Ulrike Braun^{a,*}, Claus G. Bannick^b, Kathrin Brand^{b,c}, Martin Jekel^c, Rainer Senz^d^a BAM Federal Institute for Material Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany^b UBA Umweltbundesamt, Wörlitzer Platz 1, 06844 Dessau-Roßlau, Germany^c Technical University of Berlin, Water Urban Area, Strasse des 17. Juni, 10623 Berlin, Germany^d Beuth University of Applied Sciences, Luxemburger Straße 10, 13353 Berlin, Germany

Environmental Pollution xxx (2017) 1–9



Contents lists available at ScienceDirect

Environmental Pollution

journal homepage: www.elsevier.com/locate/envpol

Comparison of different methods for MP detection: What can we learn from them, and why asking the right question before measurements matters?*

Anna M. Elert^{*}, Roland Becker, Erik Duemichen, Paul Eisentraut, Jana Falkenhagen, Heinz Sturm, Ulrike Braun

Federal Institute for Material Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany

GERSTEL

Chemosphere 174 (2017) 572–584



Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

Fast identification of microplastics in complex environmental samples by a thermal degradation method

Erik Dümichen^{a,*}, Paul Eisentraut^a, Claus Gerhard Bannick^b, Anne-Kathrin Barthel^b, Rainer Senz^c, Ulrike Braun^a^a BAM Bundesamt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany^b UBA Umweltbundesamt, Corrensplatz 1, 14195 Berlin, Germany^c BHT Beuth University of Applied Sciences, Luxemburger Straße 10, 13353 Berlin, Germany

ENVIRONMENTAL
Science & Technology
LETTERS

Letter

Cite This: *Environ. Sci. Technol. Lett.* XXXX, XXX, XXX–XXXpubs.acs.org/journal/estlcu

Two Birds with One Stone—Fast and Simultaneous Analysis of Microplastics: Microparticles Derived from Thermoplastics and Tire Wear

Paul Eisentraut,[†] Erik Dümichen,[†] Aki Sebastian Ruhl,[‡] Martin Jekel,[‡] Mirko Albrecht,[§] Michael Gehde,[§] and Ulrike Braun^{*,†,§}[†]Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany[‡]Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany[§]Technische Universität Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz, Germany

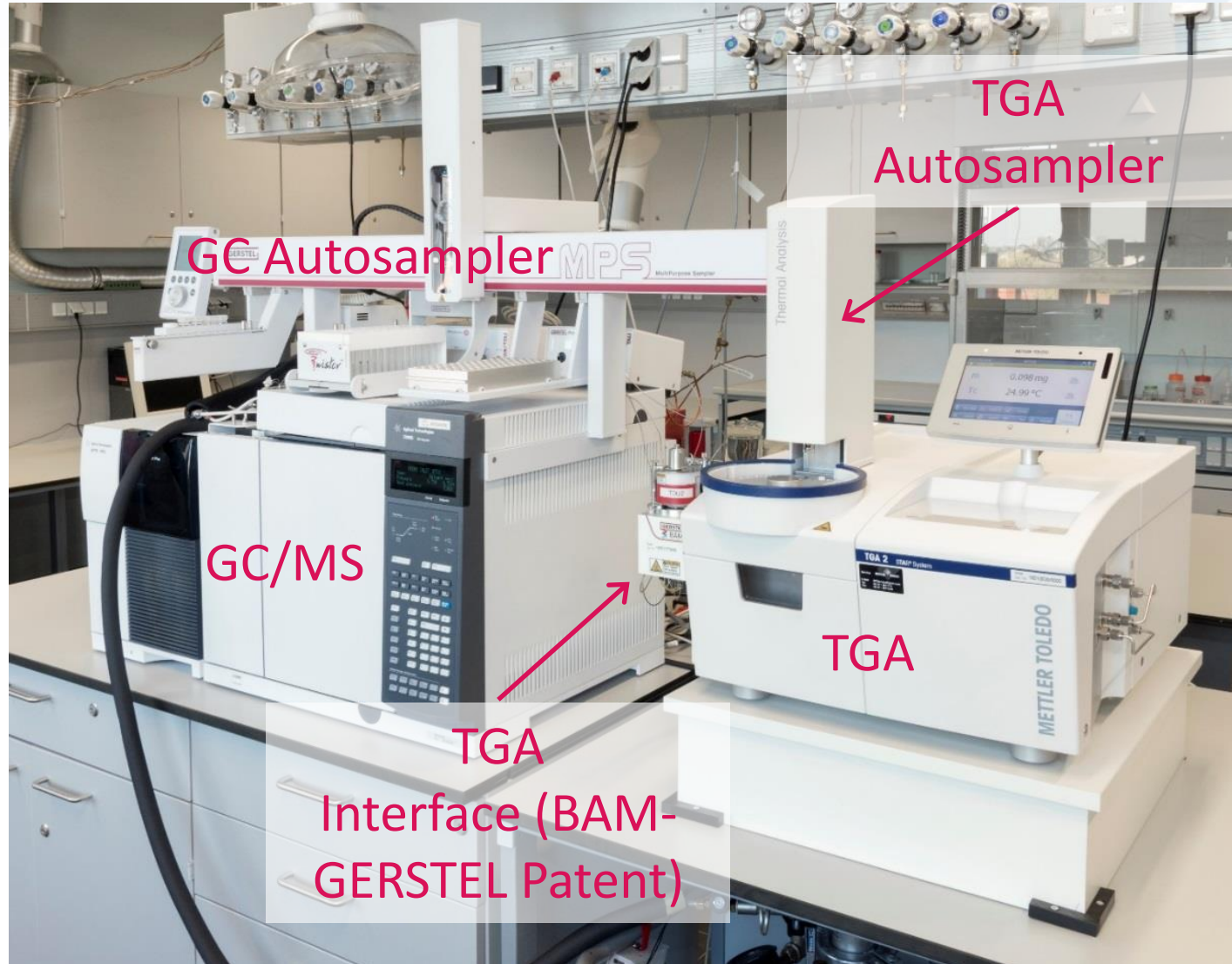
Supporting Information

ABSTRACT: Analysis of microplastic particles in environmental samples needs sophisticated techniques and is time intensive due to sample preparation and detection. Alternatives to the most common (micro-) spectroscopic

Microplastic Analysis using TED-GC-MS



TED-GC/MS Automation



ChromIdent® Software Match Results

Visual display of query chromatogram mirrored with highlighted reference (Results table) and selected peak (Peak List)

The screenshot displays the ChromIdent software interface. On the left is a navigation tree with categories like Polymers, Origins, Samples, and Substances. The main area is divided into several panels:

- Query Chromatogram:** Shows a chromatogram with intensity vs. minutes. A peak is highlighted at approximately 7.88 minutes.
- Summary Report:** An 'Editable Summary Report' table listing marker peaks with their retention times (RT), LP IDs, substance names, and reference sources.
- Results Table:** A table showing similarity indices (uSI, fSI, iSI, rSI) for various substances. The PMMA row is highlighted.
- Peak List:** A table listing identified peaks with their retention times (RT), relative retention times (RRT), relative indices (RI), sample names, and origins.

Annotations include a green box labeled 'Reference overview' pointing to the navigation tree, a red box around the Summary Report table, a red box around the Results table, and a red box around the Peak List table. Arrows indicate the mirroring of the query peak to the reference peak in the Summary Report and the corresponding peak in the Peak List.

Mirrored scan comparison of query peak and reference peak

Sample Peak List with further match results: Relative retention time/index, area%, mass spectrum match result.

4 Similarity indices and numbers of marker, ambiguous and unidentified peaks.

ChromIdent® for TED-GC/MS adapted by LabLicat GmbH, Hamburg Germany

TED-GC/MS Standardization activity

Standard regarding analytical methods:

ISO TC 61 (plastics) / SC 14 (environmental aspects)

ISO/CD 24187

“Principles for the development of standards for investigation procedures of plastics in environmental matrices and related materials”

Stage April 28, 2020: 30.60 Close of voting/ comment period

Stage May, 25, 2020: 30.92 Committee Draft referred back to Working Group

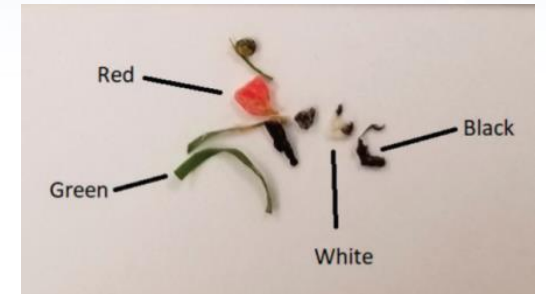
Content: Techniques for visible properties (sizing, distributions) and chemical properties (major components, minor components) incl. **TED-GC/MS** and **Pyrolysis-GC/MS**.

Sampling for water, air, soil, sludge, ...

Source: <https://www.iso.org/committee/6578018/x/catalogue/p/0/u/1/w/0/d/0> (May 25, 2020)

TED-GC/MS Summary

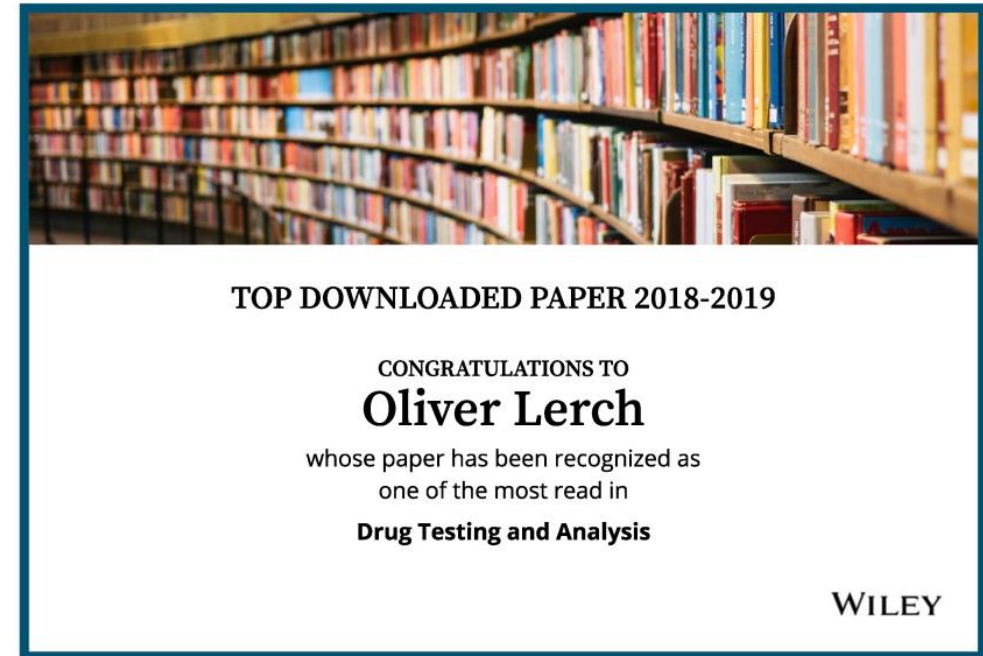
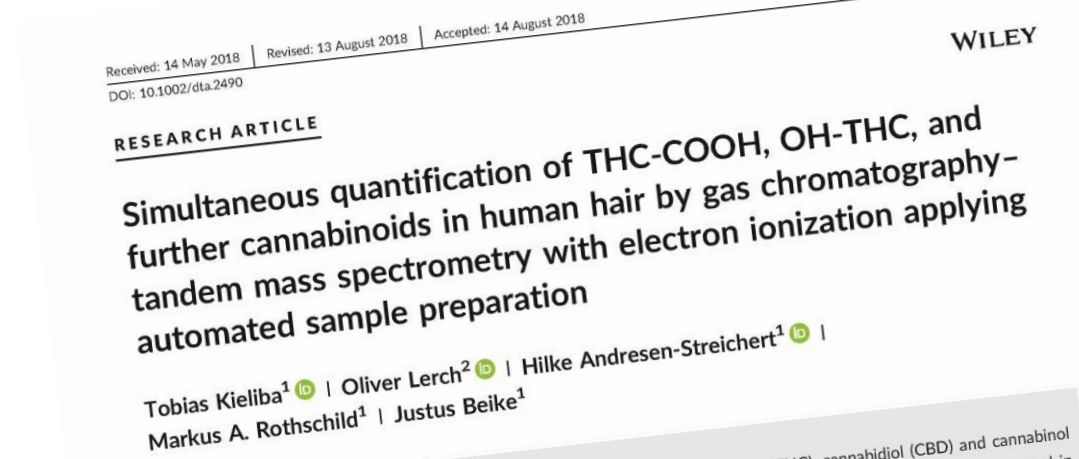
- ▷ Automated chemical determination of microplastics in environmental samples and seafood:
 - Soil and river sediment; Waste water treatment residue; air- or water filtrate; mussels
 - Qualitative and quantitative results
- ▷ Sample amount up to 100 mg for representative sampling
- ▷ Less sample preparation (mainly sample homogenization)
- ▷ Polymer markers identified using ChromIdent[®] software
- ▷ Introduction analytica 2020, several systems installed



Forensic Toxicology: Hair analysis project

Project with Institute of Legal Medicine, Cologne

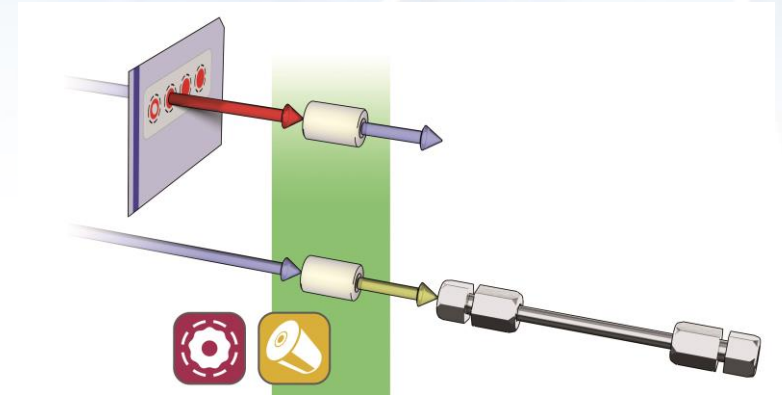
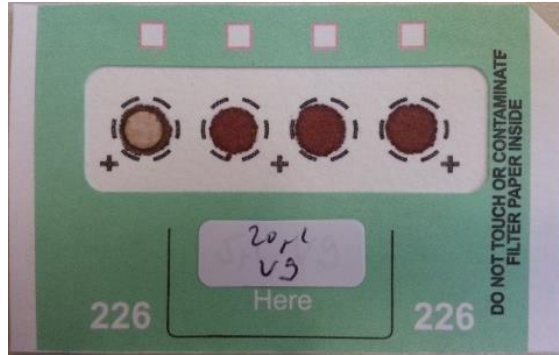
- ▶ New method: THC and metabolites in hair
 - Automated Sample Preparation and analysis
 - Just wash and grind your hair, the rest is automated
 - One extraction, one GC/MS run for all analytes (novelty)
 - Fully validated according to GTFCh rules
 - Method to be implemented in Cologne
 - DTA Publication: DOI: 10.1002/dta.2490



Forensic Toxicology ongoing project:

Determination of Phosphatidylethanol (PEth)
in Dried Blood Spots (DBS) using a
DBS Autosampler (DBSA)

Dried Blood Spots (DBS)



- ▷ Dried Blood Spot = dried blood sample on cellulose card
- ▷ Defined area = defined blood volume
- ▷ HemaXis™ DB10:
 - Accurate and precise volume whole blood sampling
 - @home sampling (= social distancing) and secure shipment
 - Pharmacokinetic Study example: <http://www.gerstel.com/pdf/AppNote-211.pdf>
- ▷ Flow-through desorption, clean-up (SPE) and LC/MS analysis

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Dried Blood Spot Autosampler (DBS-A)

Liquid handling

Card handling

MPS

DBS

Column
oven

MS/MS

SPE^{xos}

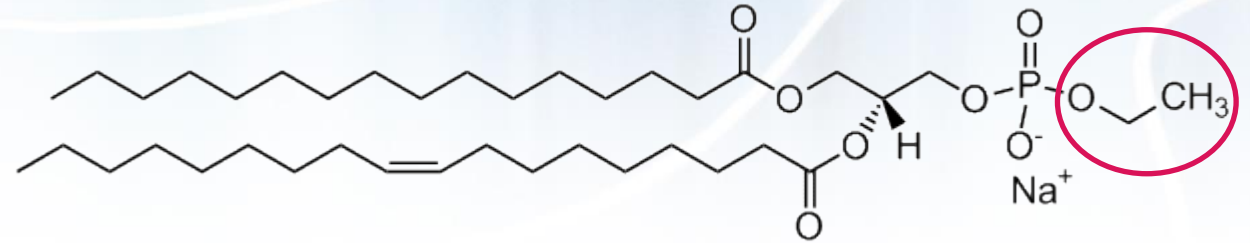
LC pump



Integrated non-destructive hematocrit measurement on DBS cards with NIRFlex N-500 from:



Phosphatidylethanol (PEth)



- ▷ Alcohol consumption marker
- ▷ Proves single alcohol intake up to 12 days after consumption
- ▷ Uses: Driver aptitude test, workplace drug testing
- ▷ DBS is ideally suited: PEth formed/degraded in liquid whole blood
- ▷ Comprehensive analysis method under development

Application of Stir Bar Sorptive Extraction (SBSE)- GC-MS/MS to Water Analysis guided by the EU Water Framework Directive (EU-WFD)

Collaboration with Agilent Technologies

Goal: Eliminating the use of dichloromethane (DCM) extraction
(100 mL per sample).

SBSE Method: Only 100 mL Sample and no DCM



Standard method
Sample Volume 1 L

2 Extractions using
50 mL DCM each

Twister method
100 mL
Extraction with
reusable
PDMS Twister

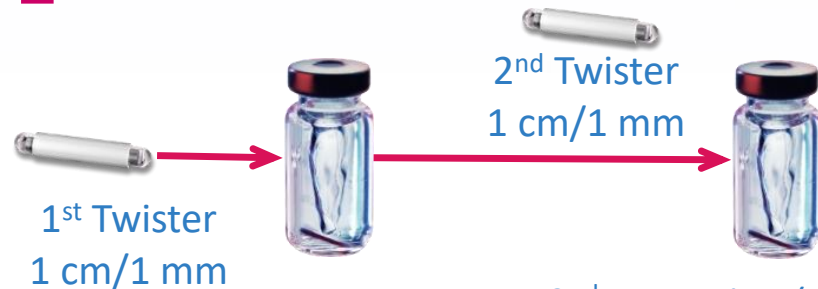


Multi-Sample parallel extraction
for high productivity whole-water
analysis (water and sediment)

SBSE Method: Surface water and sediment

Sample Preparation

1



1st Twister
1 cm/1 mm

2nd Twister
1 cm/1 mm

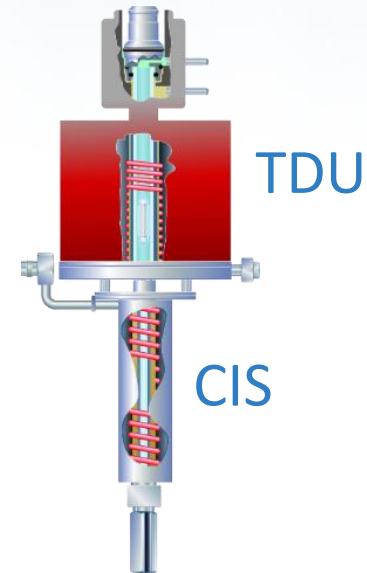
1st Extraction (5h):
100 mL water sample
including ISTD mix

2nd Extraction (17h)
at elevated temperature
with organic modifier



Thermal Desorption

2



TDU

CIS

Thermal Desorption Unit
(TDU): 90 – 300 °C
Cooled Injection System
(CIS): -40 – 300 °C.
Cryofocusing + Injection

GC-MS/MS

3



GC 7890/7010 TripleQuad MS
RTL on chlorpyrifos-methyl
MRM

100 pg/L, 100 mL sample → 10 pg per injection

Limits of Quantification

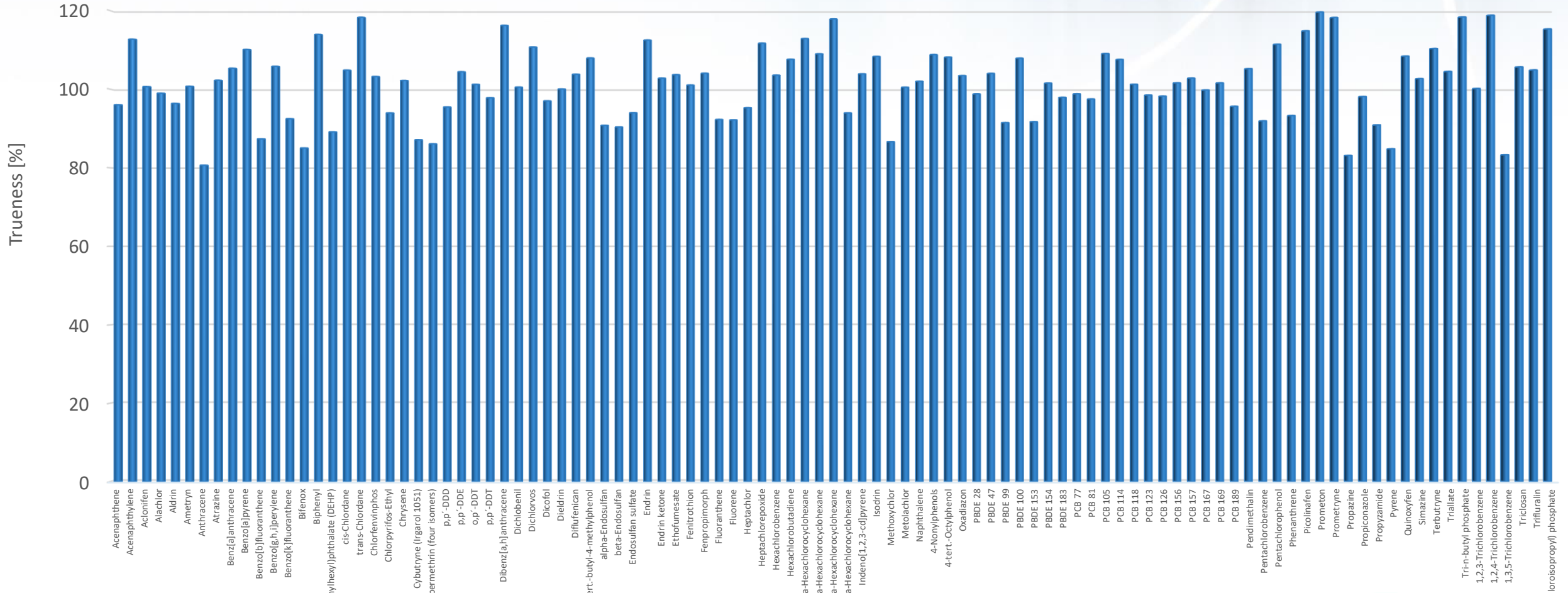
Analyte	LOQ [ng/L]
Acenaphthene	1.0
Acenaphthylene	0.10
Aclonifen	0.56
Alachlor	0.42
Aldrin	0.066
Ametryn	0.069
Anthracene	0.061
Atrazine	0.18
Benz[a]anthracene	0.076
Benzo[a]pyrene	0.033
Benzo[b]fluoranthene	0.078
Benzo[g,h,i]perylene	0.049
Benzo[k]fluoranthene	0.081
Bifenox	0.47
Biphenyl	9,0
Bis(2-ethylhexyl)phthalate (DEHP)	134
Chlordane, cis	0.052
Chlordane, trans	0.026
Chlorfenvinphos	0.084
Chlorpyrifos-Ethyl	0.024
Chrysene	0.027
Cybutryne (Irgarol 1051)	0.030
Cypermethrine (4 isomers)	0.12
p,p'-DDD	0.020
p,p'-DDE	0.017
o,p'-DDT	0.052
p,p'-DDT	0.067
Dibenz[a,h]anthracene	0.073
Dichlobenil	2.1
Dichlorvos	0.073
Dicofol	0.15
Dieldrin	0.034
Diflufenican	0.16
2,6-Di-tert.-butyl-4-methylphenol	5.9

Analyte	LOQ [ng/L]
alpha-Endosulfan	0.070
beta-Endosulfan	0.059
Endosulfan sulfate	0.052
Endrin	0.043
Endrin ketone	0.052
Ethofumesate	0.073
Fenitrothion	0.024
Fenpropimorph	0.13
Fluoranthene	1.0
Fluorene	0.45
Heptachlor	0.052
Heptachlorepoxyde	0.052
Hexachlorobenzene	0.10
Hexachlorbutadiene	0.043
alpha-Hexachlorocyclohexane	0.052
beta-Hexachlorocyclohexane	0.13
gamma-Hexachlorocyclohexane	0.052
delta-Hexachlorocyclohexane	0.052
Indeno[1,2,3-cd]pyrene	0.044
Isodrin	0.16
Methoxychlor	0.083
Metolachlor	0.064
Naphthalene	5.0
Nonylphenol	8.8
Octylphenol	0.46
Oxadiazon	0.082
PBDE 28	0.018
PBDE 47	0.015
PBDE 99	0.050
PBDE 100	0.011
PBDE 153	0.032
PBDE 154	0.020
PBDE 183	0.13
PCB 77	0.041

Analyte	LOQ [ng/L]
PCB 81	0.039
PCB 105	0.043
PCB 114	0.036
PCB 118	0.012
PCB 123	0.037
PCB 126	0.050
PCB 156	0.046
PCB 157	0.047
PCB 167	0.044
PCB 169	0.054
PCB 189	0.054
Pendimethalin	0.094
Pentachlorobenzene	0.075
Pentachlorophenol	3.0
Phenanthrene	2.5
Picolinafen	0.26
Prometon	0.18
Prometryne	0.13
Propazine	0.057
Propiconazole	0.14
Propyzamide	0.35
Pyrene	0.45
Quinoxifen	0.087
Simazine	1.9
Terbutryne	0.1
Triallate	0.084
Tri-n-butyl phosphate	9.7
1,2,3-Trichlorobenzene	0.95
1,2,4-Trichlorobenzene	1.2
1,3,5-Trichlorobenzene	0.18
Triclosan	1.4
Trifluralin	0.19
Tris(2-chloroisopropyl)phosphate (TCPP)	29

More Information:
<http://www.gerstel.com/pdf/AppNote-196.pdf>

Spiked Mineral Water near LOQ (n=6)



Average Deviation from 100 % = 7.2 %

www.gerstel.com

Summary EU-WFD analysis project

- ▷ SBSE successful for EU-WFD guided water analysis (No DCM)
- ▷ Extraction of particle adsorbed compounds confirmed with ref. sediment
- ▷ Analysis method for around 100 relevant compounds, more can be added
- ▷ LOQs of analytes mainly in the low pg/L range
- ▷ Required LOQs for inland surface water achieved for all except heptachlor, heptachlor-epoxide, cypermethrine (notoriously difficult)
- ▷ Sample Prep Solution available: Manual, method description, validation data
- ▷ Systems already installed in Germany (state and private labs)

Why pursue partnerships ?

Partnerships *for Innovation*

- ▷ Academia and Public Research Institutes
 - Development or Implementation/Automation of New Technologies
 - Publication of results
- ▷ Industry and Contract Laboratories
 - Learning about customer needs as well as the latest challenges and trends
 - Implementing Automation/Digitalization using GERSTEL technology and know-how.
- ▷ Public Health and Safety, Food, and Forensic Toxicology Laboratories
 - Automated and traceable complex sample preparation
 - Introduce new sampling techniques (e.g. DBS)
- ▷ Agilent Technologies and GERSTEL Partnership
 - Premier Solution Partner GERSTEL develops Sample Prep and Analysis Solutions
 - Agilent contributes the latest in GC/MS and LC/MS technology

Future Trends – Laboratory Analysis

- ▷ Automation:
 - Improved productivity and efficiency
 - Reduced cost per sample
- ▷ Digitalization, automated analysis setup from sample data / LIMS
- ▷ Environmental sustainability and miniaturization
 - Reduced solvent consumption
 - Reduced Energy consumption
- ▷ Sample Prep Solutions and complete Analysis Systems
 - Chromatography is here to stay – and so is sample preparation
 - You need separation to get the right results from complex samples

Future Trends – Laboratory Analysis

- ▷ Projects are increasingly complex and partnering is a necessity
- ▷ GERSTEL is continually forming Partnerships and entering Collaborations to *accelerate* the innovation process

“Years ago, we were contacting researchers for a chance to collaborate with them. Today, we are being contacted. That is a very nice development”

Ralf Bremer, Managing Director R&D,
Production and Service, GERSTEL

Thank you for your attention to the future.

Questions & Answers

Please use the Q&A chat function or “raise your hand” to ask a question to our panelists.



Thank You!

For more information visit

<https://www.agilent.com/about/newsroom/media-room/ignite.html>