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

May 29, 2020
#4 Partnership & Collaboration: Igniting Innovation

Today’s Agenda

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<thead>
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<td>Igniting Innovation Through Partnership</td>
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<tr>
<td>University of Duisburg Essen</td>
<td>Showcasing the Teaching and Research Center for Separation, and some of the successful research being done by Duisburg-Essen</td>
</tr>
<tr>
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<td>Partnering for Innovation</td>
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<tr>
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</tr>
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Igniting Innovation Through Partnership

Professor Dr. Oliver Schmitz
University of Duisburg Essen
The Team

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.
Building Better Science and Education Through Partnership

- 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
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)
Research Topics

- Ion source development
- Multidimensional chromatography
- Ion mobility - mass spectrometry
- Metabolomics/Lipidomics
- Origin-of-Life
Cooperation with Hitachi Japan: LC-LTP-QQQ
Cooperation with Total France: 2D-LC

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
Real Single-Cell Analysis

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
LipidCreator workbench to probe the lipidomic landscape

Bing Peng1,2,18, Dominik Kopczynski1,18, Brian S. Pratt3, Christe S. Eising4,5, Bo Burla6, Martin Hermansson4,7, Peter Imre Banko8, Sock Hwee Tan9,10, Mark Y. Chan9,10,11, Federico Torta8, Dominik Schwudke12,13,14, Sven W. Meckelmann15, Cristina Coman1,16, Oliver J. Schmitz15, Brendan MacLean3, Mailin-Christin Manke17, Oliver Borst15, Markus R. Wenk6,8, Nils Hoffmann1 & Robert Ahrends1,16,19

Mass spectrometry (MS)-based targeted lipidomics enables the robust quantification of selected lipids under various biological conditions but comprehensive software tools to support such analyses are lacking. Here we present LipidCreator, a software that fully supports targeted lipidomics assay development. LipidCreator offers a comprehensive framework to compute MS/MS fragment masses for over 60 lipid classes. LipidCreator provides all functionalities needed to define fragments, manage stable isotope labeling, optimize collision energy and generate in silico spectral libraries. We validate LipidCreator assays computationally and analytically and prove that it is capable to generate large targeted experiments to analyze blood and to dissect lipid-signaling pathways such as in human platelets.
"... 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…"

Editorial by Dr. Joachim Richert in Nachrichten aus der Chemie 7/8 2018
(translated into English by Oliver J. Schmitz)
What Do Innovation and Partnership Mean to Me?

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!

Find us on Facebook and Instagram:

[Facebook logo] HPLC2021 [Instagram logo]
GERSTEL: Partnering for Innovation

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

more than 100 patents held or pending
GERSTEL - Agilent partnership

- 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 - Agilent partnership

► Automation, Sample Preparation and Analysis Systems
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!

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 Extraction-Desorption
Gas chromatography-Mass Spectrometry

TED-GC/MS developed by

Ulrike Braun, Ph.D.
Erik Dümichen, Ph.D.
Paul Eisentraut et al.
TED-GC/MS

1\textsuperscript{st} step: Thermal Extraction

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

Sample up to 100 mg

Pyrolysis of organic substances under inert gas

Thermogravimetric Analyzer (TGA)

Collection of pyrolysis products on Polydimethylsiloxane (PDMS), e.g. GERSTEL Twister
TED-GC/MS

2nd Step: Determination of pyrolysis products

Thermal Desorption GC-MS

Marker-Compound Identification

Polymer Quantification

Polymer Identification

Sample
Reference
PS
m/z 91
PE
m/z 55
PP
m/z 69

Retention time / min
18 19 22 23 24 27 28 29 30

Mass / µg (for 1 mg sample weight)

500 µm 100 µm 50 µm 10 µm 6 µm <6 µm
0
2
4
6

Peak area

500 µm 100 µm 50 µm 10 µm 6 µm <6 µm
0
1x10^6
2x10^6
3x10^6
TED-GC/MS
Specific pyrolysis polymer markers

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Application example: Road run-off

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

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

E. Dümenichen a,*, P. Eisenraut b, M. Celina c, U. Braun c


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

Erik Dümenichen a,*, Anne-Kathrin Barthel b, Ulrike Braun c, Claus G. Bannick c, Kathrin Brand b,*, Martin Jekel b, Rainer Senz a

Water Research

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

Erik Dümenichen a,*, Paul Eisenraut b, Claus Gerhard Bannick c, Anne-Kathrin Barthel d, Rainer Senz e, Ulrike Braun f

Chemosphere 143 (2016) 372–384

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

Anna M. Elett a, Roland Becker a, Erik Dümenichen a, Paul Eisenraut b, Jana Falkenhagen a, Heinz Strum b, Ulrike Braun c

Environmental Pollution 217 (2016) 1–8

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

Paul Eisenraut a, Erik Dümenichen a, Aki Sebastian Ruhl a, Martin Jekel a, Mirko Albrecht a, Michael Gehde a and Ulrike Braun a

Environmental Science & Technology LETTERS

Microplastic Analysis using TED-GC-MS

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
TED-GC/MS Automation

GC Autosampler

GC/MS

TGA Autosampler

TGA

TGA Interface (BAM-GERSTEL Patent)
ChromIdent® Software Match Results

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

Reference overview

Editable Summary Report

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 LabLicate 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](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

*HemaXis is a Trademark of DBS Systems SA
Integrated non-destructive hematocrit measurement on DBS cards with NIRFlex N-500 from:

DBS

LC pump

SPE\textsuperscript{xos}

Column oven

Card handling

Liquid handling

MPS

MS/MS

Dried Blood Spot Autosampler (DBS-A)
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
1st Twister 1 cm/1 mm
1st Extraction (5h): 100 mL water sample including ISTD mix

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

2nd Twister 1 cm/1 mm

Thermal Desorption

1st Twister 1 cm/1 mm

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

TDU

CIS

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

GC-MS/MS

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

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

www.gerstel.com
## Limits of Quantification

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<td>Pentachlorophenol</td>
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</tr>
<tr>
<td>Phenanthrene</td>
<td>2.5</td>
</tr>
<tr>
<td>Picolinfen</td>
<td>0.26</td>
</tr>
<tr>
<td>Prometon</td>
<td>0.18</td>
</tr>
<tr>
<td>Prometryne</td>
<td>0.13</td>
</tr>
<tr>
<td>Propazine</td>
<td>0.057</td>
</tr>
<tr>
<td>Propiconazole</td>
<td>0.14</td>
</tr>
<tr>
<td>Propyzamide</td>
<td>0.35</td>
</tr>
<tr>
<td>Pyrene</td>
<td>0.45</td>
</tr>
<tr>
<td>Quinoxyfen</td>
<td>0.087</td>
</tr>
<tr>
<td>Simazine</td>
<td>1.9</td>
</tr>
<tr>
<td>Terbutryne</td>
<td>0.1</td>
</tr>
<tr>
<td>Triallate</td>
<td>0.084</td>
</tr>
<tr>
<td>Tri-n-butyl phosphate</td>
<td>9.7</td>
</tr>
<tr>
<td>1,2,3-Trichlorobenzene</td>
<td>0.95</td>
</tr>
<tr>
<td>1,2,4-Trichlorobenzene</td>
<td>1.2</td>
</tr>
<tr>
<td>1,3,5-Trichlorobenzene</td>
<td>0.18</td>
</tr>
<tr>
<td>Triclosan</td>
<td>1.4</td>
</tr>
<tr>
<td>Trifluralin</td>
<td>0.19</td>
</tr>
<tr>
<td>Tris(2-chloroisopropyl)phosphate (TCP)</td>
<td>29</td>
</tr>
</tbody>
</table>
Trueness

Spiked Mineral Water near LOQ (n=6)

Average Deviation from 100 % = 7.2 %

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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

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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!

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