Agilent InfinityLab

InfinityLab LC Virtual Scientific Conference

June 22-23, 2021 | Virtual Event eBook

Agilent
Trusted Answers

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Welcome

Agilent is excited to welcome you to the first virtual **InfinityLab LC scientific conference**, held on 22- 23 June, 2021.

This fully online LC conference will provide you with the opportunity to stay up-to-date with the latest trends and developments in the field of high-performance liquid phase separations.

Virtual sessions include:

- The Power of 2DLC Part 1
- Current Developments in LC and LC-MS for Food and Environmental Applications
- Trends in Biopharmaceutical Analysis Trends in Biopharmaceutical Analysis
- Innovations and Novel Insights in Liquid Chromatography

In this first-of-its-kind virtual conference, don't miss the opportunity to hear and speak with top scientific leaders and application experts. Ask each speaker questions in the real-time Q&A session following each live broadcast. Virtually meet, chat, and exchange ideas with all participants, as well as with Agilent experts, from the comfort of your laboratory or office.

Thank You to Our Guest Speakers

We are also excited to welcome our guest speakers for each of the sessions. This conference would not be made possible without their contributions and invaluable support. Information about each of the speakers and their sessions can be found in this eBook.

Lastly, this is a conference for you. Feel free to get involved, ask questions, make suggestions and be a part of the InfinityLab LC Community.

We look forward to "seeing" you virtually in June.

Sincerely,
The Agilent InfinityLab LC Virtual Conference Team

A Tribute to Prof. K.-P. Hupe, Scientist and Entrepreneur

Gerard P. Rozing*, Fred Strohmeier, Günter Nill, Agilent Technologies emeritus

Agilent Technologies is a worldwide leader in life sciences, diagnostics and applied chemical markets. The company provides laboratories worldwide with instruments, services, consumables, applications and expertise, enabling customers to gain the insights they seek. Agilent's expertise and trusted collaboration give them the highest confidence in their solutions.

As an essential part of this portfolio, Agilent Technologies today is a well-established supplier of liquid phase analysis instrumentation and systems and provides solutions for (bio)analysis in chemical, pharmaceutical, and biotech industries and many research fields in academia, institutions, and industry. Agilent is a technology leader in liquid phase separation methods, in spectrophotometric, and mass-spectroscopic detection, and in many essential engineering disciplines which form the basis for the development and manufacturing of these systems.

The core of Agilent's research, development, and manufacturing activities in liquid phase separation technology (chromatography and electrophoresis) is based at their high-tech, innovative campus in Waldbronn, Germany. One may ask, though, why this Agilent center is based in Waldbronn?

It all started with Hewlett-Packard's 1973 acquisition of a small company, Hupe + Busch, based in Karlsruhe, Germany, founded by **Prof. Klaus-Peter Hupe**.

In 2021 Prof. Hupe received the highly prestigious Pittcon Heritage Award for his lifetime achievements.

This presentation intends to illustrate how Prof. Hupe has brought science and engineering into solving demanding questions for the separation and isolation of natural compounds. His keen drive to develop such solutions into products that help others and which formed the basis for industrial manufacturing and international distribution of these products.

Professor Hupe's scientific work and the connection with his company and later Hewlett-Packard will be illustrated, especially how he has influenced Hewlett-Packard's business development of instrumental liquid phase analysis.

Program at a Glance

First Agilent InfinityLab LC Virtual Scientific Conference

Program at a Glance

Day 1 - 22 June 2021

08:50 a.m. – 09:00 a.m. CEST	Welcome and introduction *Jacob Thaysen, Senior Vice President,* *Life Sciences and Applied Markets Group,* *Agilent Technologies*
09:00 a.m. – 09:05 a.m. CEST	Session: The Power of 2DLC Part 1 Chair: *Oliver J. Schmitz,* *University of Duisburg-Essen, Germany*
09:05 a.m. – 09:30 a.m. CEST	Maximizing Two-Dimensional Liquid Chromatography Peak Capacity for the Separation Of Complex Industrial Samples *Gert Desmet, Vrije Universiteit Brussel, Belgium*
09:30 a.m. – 09:55 a.m. CEST	The Power of On-line RPLC x RPLC *Sabine Heinisch, University of Lyon, France*
09:55 a.m. – 10:20 a.m. CEST	Advanced Separation Tools for Chemical Structure Characterization *Matthias Pursch, Dow Chemical, Germany*
10:20 a.m. – 10:50 a.m. CEST	Break
10:50 a.m. – 10:55 a.m. CEST	Session: The Power of 2DLC Part 2 Chair: *Oliver J. Schmitz,* *University of Duisburg-Essen, Germany*
10:55 a.m. – 11:20 a.m. CEST	What Can 2DLC Offer in Food Applications? *Lidia Montero, University of Duisburg-Essen, Germany*
11:20 a.m. – 11:45 a.m. CEST	The Power of Comprehensive Two Dimensional Liquid Chromatography to Characterize Very Complex Food Related Samples *Miquel Herrero, Institute of Food Research, Spain*
11:45 a.m. – 12:10 p.m. CEST	2DLC a Powerful Extension in (Bio)Pharmaceutical Analysis *Michael Lämmerhofer, University of Tuebingen, Germany*
12:10 p.m. – 13:10 p.m. CEST	Break

Program at a Glance

Day 1 - 22 June 2021

13:10 p.m. – 13:15 p.m. CEST	Session: Current Developments in LC and LC-MS for Food and Environmental Applications Part 1 *Chair: Imma Ferrer, University of Colorado, USA*
13:15 p.m. – 13:40 p.m. CEST	Sensitive, Automated Determination of Pesticide Residues in Wine Samples by On-line SPE LC-MS/MS *Leticia Pérez-Mayán,* *University of Santiago de Compostela, Spain*
13:40 p.m. – 14:05 p.m. CEST	Not Only Dilution Is a Solution: Tools for Correcting the Matrix Effect in Environmental Samples for Reliable Non-Target LC-ESI-MS Analysis *Selina Kornelia Tisler, Copenhagen University, Denmark*
14:05 p.m. – 14:30 p.m. CEST	LC-HRMS Screening of Per- and Polyfluorinated Alkyl Substances (PFAS) in Food Contact Paper and Contaminated Soils *Boris Bugsel, University of Tuebingen, Germany*
14:30 p.m. – 15:00 p.m. CEST	Break
15:00 p.m. – 15:05 p.m. CEST	Session: Current Developments In LC and LC-MS for Food and Environmental Applications Part 2 *Chair: Imma Ferrer, University of Colorado, USA*
15:05 p.m. – 15:30 p.m. CEST	A Ubiquitous Tire Rubber–Derived Chemical Induces Acute Mortality in Coho Salmon *Zhenyu Tian, University of Washington, USA*
15:30 p.m. – 15:55 p.m. CEST	Fast and Highly Sensitive Determination of 11-Nor-9-Carboxy-Δ9-Tetrahydrocannabinol in Hair Using Liquid-Chromatography-Multistage Mass Spectrometry ($LC\text{-}MS^3$) *Petra Hehet, Ludwig Maximilian University of Munich, Germany*

Program at a Glance

15:55 p.m. – 16:20 p.m. CEST	Determination of Micropollutants Metabolisation in Biofilms by HPLC-MS *Kai Bester, Aaurhus University, Denmark*
16:20 p.m. – 16:40 p.m. CEST	A Tribute to Prof. Klaus-Peter Hupe, Scientist and Entrepreneur *Stefan Schuette, Vice President Liquid Phase Separations Division, Agilent Technologies and Gerard Rozing, Emeritus Agilent Technologies Research Fellow*

Day 2 - 23 June 2021

09:00 a.m. - 09:05 a.m. CEST	Session: Trends in Biopharmaceutical Analysis Part 1 *Chair: Koen Sandra, RIC Group, Belgium*
09:05 a.m. - 09:30 a.m. CEST	Targeted Bottom-up Characterization of Recombinant Monoclonal Antibodies by Multidimensional LC/MS *Cinzia Stella, Genentech, CA, USA*
09:30 a.m. - 09:55 a.m. CEST	2D-LC in the Pharmaceutical Industry: From the Characterization of Complex Drug Modalities to High Throughput Analysis *Alexandre Goyon, Genentech, USA*
09:55 a.m. - 10:20 a.m. CEST	Coupling Non Denaturing Chromatographic Techniques with Mass Spectrometry for Biopharmaceuticals Characterization *Davy Guilarme, Geneva University, Switzerland*
10:20 a.m. - 10:50 a.m. CEST	Break
10:50 a.m. - 10:55 a.m. CEST	Session: Trends in Biopharmaceutical Analysis Part 2 *Chair: Koen Sandra, RIC Group, Belgium*
10:55 a.m. - 11.20 a.m CEST	Exploring the Chemical Space of Modifications in Therapeutic Proteins Employing Chromatography, Mass Spectrometry, and Bioinformatics *Christian Huber, University of Salzburg, Austria*

Program at a Glance

Day 2 - 23 June 2021

11:20 a.m. - 11:45 a.m. CEST	Bioanalysis of Therapeutic Proteins *Rainer Bischoff, Univeristy of Groningen, The Netherlands*
11:45 a.m. - 12:10 p.m. CEST	Challenges in Analytical Characterization of Biosimilars *Anurag Rathore, Indian Institute of Technology, India*
12:10 p.m. - 13:10 p.m. CEST	Break
13:10 p.m. - 13:15 p.m. CEST	Session: Innovations and Novel Insights in Liquid Chromatography Part 1 Chair: Ken Broeckhoven, Vrije Universiteit Brussel, Belgium
13:15 p.m. - 13: 40 p.m. CEST	Rationalisation of Peak Shapes of Peptides and mAbs in Reversed-Phase LC Using a Variety of Mobile Phase Additives *David McCalley, UWE Bristol, United Kingdom*
13:40 p.m. - 14:05 p.m. CEST	Comparison of HILIC and RP Approach in the Multiplex Analysis of Antivirals to Tackle Drug-Drug Interactions *Lucie Nováková, Charles University, Czech Republik*
14:05 p.m. - 14:30 p.m. CEST	Implementing Miniaturized Separation Platforms into Pharmaceutical Workflows *James Grinias, Rowan University, USA*
14:30 p.m. - 15:00 p.m. CEST	Break

Program at a Glance

Day 2 - 23 June 2021

15:00 p.m. – 15:05 p.m. CEST	Session: Innovations and Novel Insights in Liquid Chromatography Part 2 Chair: Ken Broeckhoven, Vrije Universiteit Brussel, Belgium
15:05 p.m. – 15:30 p.m. CEST	Shedding Light on Mechanisms Leading to Convex-Upward Van Deemter Curves on a Cellulose Tris (4-chloro-3-methylphenylcarbamate)-Based Chiral Stationary Phase *Martina Catani, University of Ferrara, Italy*
15:30 p.m. – 15:55 p.m. CEST	Innovations in Temperature Responsive Liquid Chromatography *Frederic Lynen, University of Gent, Belgium*
15:55 p.m. – 16:20 p.m. CEST	Design Aspects of a Microfluidic Device for Comprehensive Satial Three-Dimensional LC *Sebastiaan Eeltink, Vrije Universiteit Brussel, Belgium*

This is a meeting for you – feel free to get involved, ask questions, make suggestions and be a part of the Agilent InfinityLab LC Community.

Presentations

First Agilent InfinityLab LC Virtual Scientific Conference

Presentations

Session 1, The Power of 2DLC

22 June 2021

Maximizing Comprehensive Two-Dimensional LC Peak Capacity for the Separation of Complex Industrial Samples

Gert Desmet, Vrije Universiteit Brussel, Belgium

With the ever-increasing complexity of samples in the chemical industry, such as trace organic analysis in complex matrix or oligomer analysis, 1-D LC often doesn't have the resolving power to separate peaks of interest. Mass Spectrometry in selective ion monitoring mode could de-convolute analytes but it is very challenging in some cases to obtain accurate quantitation results due to well-known matrix effects. In contrast, 2-D LC, especially operated in comprehensive mode, can dramatically improve the overall peak capacity, which is the multiplication of peak capacities from each dimension assuming the 1st and 2nd dimension separation mechanism is orthogonal.

In the present contribution, we report on a study on the use of 2D-LC in industry wherein we maximized the peak capacity by serially coupling up to six 15cm long columns in the 1st dimension. For the considered aromatic amine oligomer sample, the combination of reverse phase F5 columns in the 1st and a more retaining reverse phase PAH column in the 2nd dimension proved to give the highest orthogonality as 0.82. Whereas a 1D run on a single column revealed around 120 compounds, the optimized 2D LC system revealed around 900 compounds. To achieve this, flow splitting to improve the peak capacity in the 1st dimension and shifting gradients in the 2nd dimension were used. The overall peak capacity of the system was calculated to be 53427 and 10674, respectively, without and with correction for orthogonality and undersampling. Total analysis time with the 6-column system was around 20 hrs.

Presentations

Session 1, The Power of 2DLC

22 June 2021

The Power of On-Line RPLC x RPLC

Sabine Heinisch, Institut of Analytical Sciences, University of Lyon, France

It is now well accepted that the separation power is much higher in on-line LC x LC than in 1D-LC. Here, it will be theoretically and experimentally shown that a critical analysis time exists above which RPLC x RPLC becomes more attractive in term of peak capacity than RPLC. It is also often thought that a larger peak capacity should be obtained at the expense of a higher dilution (lower peak intensity). From a theoretical approach, it will be proved that both demands (higher peak capacity and higher peak intensity) can go hand-in-hand in on-line RPLC x RPLC, with increasing gains as analysis time increases. As illustrative example, a RPLC x RPLC separation of a protein digest in 40 min will show that the peak capacity can be increased by a factor of 3 while increasing the peak intensities by a factor of 5 compared to the optimal RPLC separation.

Presentations

Session 1, The Power of 2DLC

22 June 2021

Advanced Separation Tools for Chemical Structure Characterization

Matthias Pursch, Dow Chemical, Germany

Multidimensional Liquid Chromatography (LC) is an important research and application area for complex sample analysis. In recent years much progress has been made on instrumentation and software, including enhancing compatibility between the two separation dimensions. As such, several separation modes, such as (multiple) heart-cutting, high-resolution sampling and comprehensive 2D-LC are available to meet the researcher's needs. In this talk, examples will be provided showing the power of multidimensional chromatography for various separation problems. These include (i) the target analysis of small molecules in complex polymeric matrices or natural products, (ii) the characterization of oligomeric compounds such as surfactants and polyols, (iii) copolymer analysis, and (iv) the versatility of using UV, ELSD and accurate mass MS detectors for these separation challenges.

Presentations

Session 1, The Power of 2DLC

22 June 2021

What Can 2DLC Offer in Food Applications?

Lidia Montero, Applied Analytical Chemistry,
University of Duisburg-Essen, Germany

Nutritional and organoleptic characteristics of a food product are important properties that the consumers are interested in. However, nowadays, other properties are increasing their importance when a product should be selected. For instance, the fact that a product is safe and free of contaminants, or the importance of products produced in a specific geographical region with characteristic qualities, or even products that enhance or promote the health of the consumers. Therefore, a big effort should be done to ensure all these valuable characteristics of food products.

In this regard, food safety, food authenticity, food traceability, and food bioactivity are four important branches in food analysis that can be responsible for obtaining the required information.

Usually, LC-MS and GC-MS have been employed as analytical tools to develop methods for food applications. However, foods are usually very complex matrices, and it is difficult to obtain complete separation and identification of all the analytes present in the sample. For this reason, new analytical techniques able to offer higher resolution power and confidence in the determination of the food profile are needed. Among these techniques, 2DLC can offer significant advantages in comparison to one-dimensional techniques since the sample is analyzed by two different but complementary separation mechanisms, allowing to obtain much higher separation power. Therefore, 2DLC can provide reliable and valuable information about contaminants, potential markers of origin, or potential health promoter ingredients.

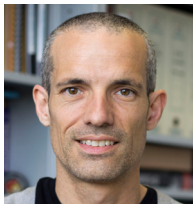
However, 2DLC is complex and has some limitations related to the compatibility of the two dimensions employed for the separation. Consequently, improvements in the 2DLC configuration are essential for increasing the power of this technique.

In this presentation, 2DLC applications for the mentioned food analytical branches as well as a new development for improving the performance of comprehensive 2DLC will be introduced.

Presentations

Session 1, The Power of 2DLC

22 June 2021



The Power of Comprehensive Two-Dimensional Liquid Chromatography to Characterize Very Complex Food-Related Samples

Miguel Herrero, Institute of Food Research, Spain

The study of the relationship between food and health is at the core of modern Food Science research. Within this topic, the chemical characterization of food and food-related products is of utmost importance to precisely know the food constituents that would be responsible for the health beneficial effects. Nevertheless, foods are often very complex matrices, making this characterization very challenging.

Although liquid chromatography (LC) coupled to mass spectrometry (MS) is a very robust and useful tool to chemically characterize food bioactive components, there are lots of samples that are simply too complex to be analyzed by conventional one-dimensional approaches. The use of comprehensive two-dimensional liquid chromatography (LC×LC) is able to provide with the additional separation power required in those cases. LC×LC is based on the use of two independent and complementary (thus, orthogonal) separation mechanisms through which the whole sample is analyzed. By using this approach, resolving power is greatly enhanced as, theoretically, the peak capacity attainable in each dimension can be combined.

Moreover, the combination of LC×LC with MS increases the capabilities of this analytical tool to characterize samples composed by a great variety of closely related unknown compounds. In this work, different applications devoted to the separation and elucidation of the secondary metabolite pattern of several food-related complex matrices are described, including different couplings and modifications at the modulator level in order to solve some important problems and limitations in LC×LC practice.

Presentations

Session 1, The Power of 2DLC

22 June 2021

2D-LC a Powerful Extension in (Bio-) Pharmaceutical Analysis

Michael Lämmerhofer, University of Tuebingen, Germany

The concept of two-dimensional liquid chromatography was promoted already more than 40 years ago, e.g. by Erni and Frei (1978), and since then fascinated separation scientists. However, in these early days such 2D-LC separations were most often reserved to experts in research labs. The technology received a push with the introduction of UHPLC with sub2-µm and core-shell particle column technology which allows superfast separations in the second dimension in the sub-minute time scale that allows now to fully exploit the power of 2D-LC technology. With the introduction of robust instrumentation and user-friendly software support, 2D-LC has found its way also into more routine applications in the pharmaceutical analysis quality control lab. There are numerous separation challenges in pharmaceutical sciences which can be more elegantly, faster or more adequately solved with 2D-LC. In this presentation, possibilities of 2D-LC in pharmaceutical analysis and biopharmaceuticals characterization will be demonstrated by selected applications.

2D-LC has a long tradition in enantioselective analysis. Chiral columns often fail to completely separate chiral compounds with more than one stereogenic centers into all possible stereoisomers. On the other hand, achiral columns cannot separate enantiomers. The combination of achiral and chiral column on the other hand allows to deal with such problems with short development time on a routine basis. More complex mixture like a full separation of all amino acid enantiomers are also still challenging even by 1D-LC-MS. Especially the simultaneous enantiomer separation of isomeric amino acids like the Thr, allo-Thr, homo-Ser as well as Leu, Ile, allo-Ile enantiomer pairs along with all other amino acids is still not a trivial task. In this presentation with show a multiple heart-cutting approach for the comprehensive separation of all proteinogenic amino acids in a single analysis within around 60 min including a full separation of all isobaric threonine and leucine analogs. The method is utilized for the determination of the enantiomer composition in lipocyclopeptides from natural chiral pool.

Presentations

Session 1, The Power of 2DLC

22 June 2021

2D-LC a Powerful Extension in (Bio-) Pharmaceutical Analysis

Michael Lämmerhofer, University of Tuebingen, Germany

continued

2D-LC further turned out to be extremely powerful for impurity profiling and the comprehensive characterization of therapeutic peptides, proteins and oligonucleotides. Impurity profiling in pharmaceutical industry often employs MS incompatible mobile phases, e.g. phosphate buffers, due to their high UV transparency at low wavelength. If impurities show up at levels higher than the identification threshold (typically > 0.1%), they must be structurally clarified. MS cannot be simply directly coupled. Development of a new MS compatible method is time consuming and the correlation to the original impurity gets easily lost and may be difficult to reestablish. With a 2D-heart cutting method such analytical challenges are easy to solve. Therapeutic peptides, proteins and oligonucleotides often have a multitude of impurity or proteoform peaks. Multiple heart cutting but also full comprehensive 2D-LC methodologies are then methods of choice for a convenient and comprehensive characterization of these structures. Chromatographic separation modalities for these biopharmaceuticals are often ESI-MS incompatible. In order not to lose the correlation to the original separation, the coupling of an MS compatible complementary chromatographic mode leads to a powerful separation which increases the information about structural characteristics and impurities in advanced therapeutics.

Presentations

Session 2, Current developments in LC and LC-MS for food and environmental applications

22 June 2021

Sensitive, Automated Determination of Pesticide Residues in Wine Samples by On-Line SPE LC-MS/MS

Leticia Pérez-Mayán, University of Santiago de Compostela, Spain

Presence of fungicide and insecticide residues in wine is a well-documented issue, and a matter of concern for consumers and wine producer organizations. Despite these evidences, specific regulations limiting the maximum residues (MRLs) of pesticides in commercial wines are still exceptional. Setting specific MRLs for wine requires a deep knowledge of background levels of pesticides existing in wine. Furthermore, the added market value of ecological wines must be supported by a rigorous control of the product before its distribution.

Whilst LC-MS/MS is the gold standard for the determination of fungicides and insecticides in wine, no agreement exists regarding the extraction step. Thus, QuEChERS and off-line SPE coexist with different microextraction approaches, and even with LLE. Some drawbacks of the above approaches are the use of moderate volumes of organic solvents, cost of disposable sorbents and/or automation limitations.

This presentation shows an automated method, based on on-line SPE and LC-MS/MS, to determine around 50 compounds in wine samples. Sample throughput, matrix effects during ESI ionization, accuracy and sensitivity are compared with those achieved in the off-line method. The presentation also discusses analysis costs, sorbents durability, and the effect of the injection volume on peak shapes and method´s LOQs.

Presentations

Session 2, Current developments in LC and LC-MS for food and environmental applications

22 June 2021

Not Only Dilution is a Solution: Tools for Correcting the Matrix Effect in Environmental Samples for Reliable Non-Target LC-ESI-MS Analysis

Selina Kornelia Tisler, Copenhagen University, Denmark

This study describes a three-step method to evaluate and compensate the matrix effect in LC-ESI-MS. As a first step, the “dilute and shoot” approach was used to determine the optimal dilution of wastewater extracts to obtain a residual matrix effect of on average 15% at a relative enrichment factor (REF) of 10 for influent and REF of 50 for the effluent samples. However, the exponential loss of non-target compounds with dilution leads to the need for a correction of the matrix effect for reliable analysis of more up-concentrated samples. As a second step, the observed matrix effect at higher REF was corrected by the retention time dependent matrix effect. A new scaling (TiChri scale) of the matrix effect was introduced, which demonstrates that the total ion chromatogram (TIC) can be used to predict the matrix effect: the average median matrix effect for 67 micropollutants was improved from -65 to 1% for influent (REF 100) and from -46% to -2% for effluent (REF 250). As a final step, the residual structure specific matrix effect was predicted and corrected by quantitative structure-property relationship. In conclusion, a comprehensive procedure has been developed that allows compensation of the matrix effect for known and unknown compounds in environmental samples.

Presentations

Session 2, Current developments in LC and LC-MS for food and environmental applications

22 June 2021

LC-HRMS Screening of Per- and Polyfluorinated Alkyl Substances (PFAS) in Food Contact Paper and Contaminated Soils

Boris Bugsel, University of Tuebingen, Germany

The class of per- and polyfluorinated substances comprises more than 3000 individual compounds which have a broad application area from the use in industrial processes to consumer products. PFAS are persistent, toxic and bioaccumulating and may form persistent transformation products (TPs).

The contamination of agricultural soils on several millions of square meters on a site in southwest Germany goes back to the application of compost and paper sludge from impregnated paper products.

We used liquid chromatography coupled to high resolution mass spectrometry (LC-HRMS) and Kendrick mass analysis to screen for major contaminants in soil samples from the contaminated area. Dialkylated polyfluorinated phosphate esters (diPAPs), N-ethyl perfluorooctane sulfonamido ethanol phosphate diesters (diSAmPAPs) and TPs of those two substance classes have been identified (Bugsel and Zwiener 2020). We further used LC-HRMS screening to corroborate the hypothesis that contaminated paper sludge led to the soil contamination. For that purpose, 14 impregnated paper samples and 14 contaminated soil samples were screened for PFAS. In addition to diPAPs and diSAmPAPs, the substance class of fluorotelomer mercapto alkyl phosphates (FTMAPs) was detected in a soil sample and in various paper samples. Comparison of soil and paper samples was based on PFAS patterns by principal component analysis and by the distribution of carbon chain length of diPAPs, diSAmPAPs, FTMAPs and their main TPs and allowed further conclusions on the fate of PFAS and prevalent environmental processes.

Bugsel, B. and C. Zwiener (2020) LC-MS screening of poly- and perfluoroalkyl substances in contaminated soil by Kendrick mass analysis. Anal.Bioanal. Chem. 412: 4797-4805.

Presentations

Session 2, Current developments in LC and LC-MS for food and environmental applications

22 June 2021

A Ubiquitous Tire Rubber–Derived Chemical Induces Acute Mortality in Coho Salmon

Zhenyu Tian, University of Washington, USA

In U.S. Pacific Northwest coho salmon (Oncorhynchus kisutch), stormwater exposure annually causes unexplained acute mortality when adult salmon migrate to urban creeks to reproduce. By investigating this phenomenon, we identified a highly toxic quinone transformation product of N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD), a globally ubiquitous tire rubber antioxidant. Retrospective analysis of representative roadway runoff and stormwater-affected creeks of the U.S. West Coast indicated widespread occurrence of 6PPD-quinone at toxic concentrations. These results reveal unanticipated risks of 6PPD antioxidants to an aquatic species and imply toxicological relevance for dissipated tire rubber residues.

Presentations

Session 2, Current developments in LC and LC-MS for food and environmental applications

22 June 2021

Fast and Highly Sensitive Determination of 11-Nor-9-Carboxy-Δ9- Tetrahydrocannabinol in Hair Using Liquid-Chromatography-Multistage Mass Spectrometry (LC-MS^3)

Petra Hehet, Ludwig Maximilian University of Munich, Germany

The medical and recreational use of cannabis are discussed in politics and in society around the world, resulting in various regulations by different countries and states. Simultaneously, cannabis and its components are encountered increasingly, among others, in food and health products. In hair analysis, identification of 11-nor-9-carboxy-Δ9-tetrahydrocannabinol (THC-COOH), one of the major endogenously formed metabolites of the psychoactive cannabinoid tetrahydrocannabinol (THC) in blood, is considered as an unambiguous proof of cannabis consumption. Due to the complex matrix and low target concentrations of THC-COOH in hair, this kind of investigation represents a great analytical challenge. The aim of this work was the establishment of a fast, simple and reliable LC-MS^3 routine method for sensitive detection of THC-COOH in hair samples. Hair sample preparation prior to detection of THC-COOH was based on digestion of the hair matrix under alkaline conditions followed by an optimized liquid-liquid extraction (LLE) procedure. A significant analytical detection improvement was introduced by the multistage fragmentation (MS^3) leading to enhanced specificity and low limit of quantification (0.1 pg/mg). Application of the validated method to 981 authentic hair samples from cannabis users resulted in THC-COOH concentrations ranging from 0.1 to >15 pg/mg hair.

Presentations

Session 2, Current developments in LC and LC-MS for food and environmental applications

22 June 2021

Determination of micropollutants metabolisation in biofilms by HPLC-MS

Kai Bester, Aarhus University, Denmark

Micropollutants are contained in a lot of polluted waters (including municipal wastewater) and need removing. An especially elegant (as green & energy friendly) way to reach this is by using biofilm reactors. A special format it the moving bed biofilm reactor that is especially interesting for science as reactors can easily be parallelized and subsamples can easily be taken for mass spectral determination.
Our work flow is constituted by taking a subsample of the biomass after targeted adapted to special conditions, transfer into a micro-reactor and systematically manipulate its functions by modifying the substrate (aka aqueous phase).

As the biomass is in the biofilm and the to be analyzed parents and metabolites stay mostly in the aqueous phase, the aqueous phase can usually be sampled and analyzed directly by means of HPLC-MS/MS.

Three approaches are followed:

1) metabolic studies (known compounds and metabolites): analysis of enantiomeric composition under different loading of easily degradable compounds using enantioselective HPLC with MS/MS.

2) Biosynthesis of metabolite standards of tensides relevant in wastewater with the parents not ionizing in ESI with detection of HR-MS.

3) Identification of biofilm metabolites that are classified as inherently non-degradable by means of ESI –HRMS/MS.

Presentations

Session 3, Trends in Biopharmaceutical Analysis

23 June 2021

Targeted Bottom-Up Characterization of Recombinant Monoclonal Antibodies by Multidimensional LC/MS

Cinzia Stella, Genentech, CA, USA

On-line bottom-up approaches have recently emerged as promising alternatives to standard off-line processes for characterizing post-translational modifications (PTMs) of therapeutic monoclonal antibodies (mAbs). The benefits of on-line processing include reductions in required sample amount and sample handling, as well as reducing the overall turnaround time. However, shortening digestion time for the on-line approach of an intact mAb can cause incomplete peptide cleavages, leading to low sequence coverage and poor repeatability of analyses. For the first time, we describe a novel, automated targeted bottom-up strategy consisting of reducing the complexity of intact mAb by digesting the product into small ~25 kDa fragments, followed by an on-line peptide mapping analysis of each fragment. For this purpose, a four-dimensional-liquid chromatography/mass spectrometry (^{4}D-LC/MS) method was developed using an immobilized *IdeS*-high-performance liquid chromatography (HPLC) column as a first dimension (^{1}D) for on-line digestion, followed by a (^{2}D) on-column reversed-phase liquid chromatography (RPLC) for reduction and fragments separation. Then, only one fragment was selected for digestion using a (^{3}D) immobilized trypsin cartridge and, finally, the obtained peptides were analyzed by (^{4}D) RPLC-MS. This strategy considerably improved the on-line digestion efficiency with higher sequence coverages (LC and HC >97%), thus allowing various PTMs including oxidation, deamidation, and isomerization located in the complementarity-determining regions (CDRs), as well as N-glycans present on the Fc/2 fragment, to be monitored with similar sensitivity to those obtained with standard off-line approaches. Additional investigations at a middle-up level were also performed via a three-dimensional-LC/MS (3D-LC/MS) approach within the same system, demonstrating the feasibility to achieve a multilevel comprehensive characterization of mAbs.

Presentations

Session 3, Trends in Biopharmaceutical Analysis

23 June 2021

2D-LC in the Pharmaceutical Industry: From the Characterization of Complex Drug Modalities to High Throughput Analysis

Alexandre Goyon, Genentech, USA

The pharmaceutical landscape is getting more diverse with the investigation of new drug modalities such as oligonucleotides and protein degraders as well as the characterization of drug delivery systems such as lipid nanoparticles. These new drug modalities and delivery systems present increased analytical challenges to determine the multiple quality attributes. 2D-LC has proved value for the coupling of non-MS compatible LC separations to MS, matrix interference removal and the assessment of peak purity. In this presentation, various recent 2D-LC method development and applications are showcased. In particular, the simultaneous characterization and desalting by 2D HILIC of antisense oligonucleotide impurities separated by 1D ion-pairing RPLC is described. The high-resolution separation of oligomeric impurities by selective comprehensive 2D-LC and insights on the manufacturing process is discussed. Finally, a high throughput achiral-chiral single heart-cutting 2D-LC method applied for the analysis of > 2,000 samples is presented.

Presentations

Session 3, Trends in Biopharmaceutical Analysis

23 June 2021

Coupling Non Denaturing Chromatographic Techniques with Mass Spectrometry for Biopharmaceuticals Characterization

Davy Guilarme, Geneva University, Switzerland

The goal of this presentation will be to highlight some recent advances in non-denaturing liquid chromatography, in terms of innovative stationary phase and mobile phase conditions. Various chromatographic modes will be discussed, such as ion exchange chromatography (IEX), size exclusion chromatography (SEC) and hydrophobic interaction chromatography (HIC), to allow coupling with mass spectrometry (MS), for the direct identification of peaks and detailed characterization of various biopharmaceutical products (mAbs, ADCs, bispecific mAbs, fusion proteins…).

Presentations

Session 3, Trends in Biopharmaceutical Analysis

23 June 2021

Exploring the chemical space of modifications in therapeutic proteins employing chromatography, mass spectrometry, and bioinformatics

Christian Huber, University of Salzburg, Austria

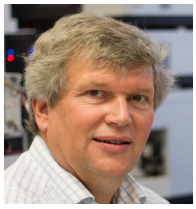
Current research into the structure and function of different protein isoforms reveals an eminent role of protein variants in the function and regulation of practically all biological processes. Recent estimates of the total number of human protein isoforms are within the several millions. Advanced analytical strategies including top-down and middle-up HPLC-MS approaches have become powerful alternatives to classical bottom-up analysis for the characterization of protein isoforms. In spite of the high-resolution capabilities both of HPLC and MS, both techniques have principal limitations with respect to the revelation of very small structural differences: while minor sequence variations may lead to relatively small mass differences that are unresolvable by MS, the molecular recognition mechanism chromatography can lead to a separation of variants. On the other hand, posttranslational modifications such as glycosylation may facilitate a distinction of protein variants by mass that frequently coelute in HPLC.

We show here that a combination of chromatographic separation with mass spectrometric measurements often is the method of choice to reveal very small structural differences in protein isoforms. Using this approach, we present an analytical workflow for analyzing the glycoforms in therapeutic monoclonal antibodies (e. g. Rituximab, Bevacizumab). Extensive glycoform profiling, based on the computational integration of intact molecular mass data, subunit molecular mass data, and glycopeptide data was evaluated as a tool for the comprehensive glycoform profiling in the biopharmaceutical chorionic gonadotropin (OvitrelleTM or PregnylTM), which is utilized as hormone substitute in the treatment of infertility.

Presentations

Session 3, Trends in Biopharmaceutical Analysis

23 June 2021



Bioanalysis of Therapeutic Proteins by LC-MS

Rainer Bischoff, Univeristy of Groningen, The Netherlands

The quantification of proteins in complex biological samples is central to many areas of research as well as to industrial and clinical applications. Especially the development of novel biologics requires the accurate and precise quantification of proteins in blood (serum, plasma), other body fluids or tissue. Furthermore, clinical chemistry laboratories use quantitative protein assays on a daily basis to assist in medical decision making. While quantitative protein assays rely to a large part on ligand binding assays (LBAs) and in particular on immunoassays, we experience the advent of liquid chromatography – mass spectrometry (LC-MS) assays as an alternative to LBAs. In this lecture, I will delineate the advantages and shortcomings of LBAs and LC-MS assays with the goal of showing that there is no single approach that can answer every question. I will notably address the point that proteins do not exist as single molecular entities and that we must refer to proteins as families. Interpreting the results of quantitative protein determinations must therefore take the measurement principle into account, be it an LBA or an LC-MS assay, since we only measure a small portion of any given protein (e.g. an epitope or a signature peptide). It is thus not surprising that results between LBAs and LC-MS may differ, since each method measures a different, partially overlapping part of a given protein family.[1] I will highlight the possibilities of LC-MS using the example of Trastuzumab, a monoclonal antibody used in treating HER-2-positive breast cancers, where we study in vivo biotransformation.[2] I will further elaborate briefly on the use of LC-MS to quantify anti-drug antibodies[3], a concern when developing biopharmaceuticals for long-term use, and end with an LC-MS assay at the protein level that does not require antibodies for enrichment.[4]

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[4] M.S. Pratt, M. van Faassen, N. Remmelts, R. Bischoff, I.P. Kema, Analytical and Bioanalytical Chemistry, 2021, 413, 2035-2044.

Presentations

Session 3, Trends in Biopharmaceutical Analysis

23 June 2021

Challenges in Analytical Characterization of Biosimilars

Anurag Rathore, Indian Institute of Technology, India

The ever-increasing cost of healthcare together with our improving understanding of biotech therapeutic drugs have fuelled the rise of biosimilars. Discussion and resolution of the various scientific and regulatory factors that play a role in approval of biosimilars is arguably one of the most significant events over the last decade for biotechnology. Key scientific factors include the complexity of biotech products and processes, use of complex raw materials that are not always well characterized, and our relatively limited understanding of how the numerous quality attributes that define a biotherapeutic impact the product's safety and/or efficacy in the clinic. A key step towards achieving successful development of a biosimilar is to establish analytical comparability with the innovator drug. This is necessary for the biosimilar manufacturer to avail of the significant reduction in clinical data required for achieving regulatory approval. This talk will discuss key developments that have occurred in the past decade with a focus on addition of more sophisticated platforms to our analytical armoury for characterization of biologics. Limitation of our ability to accurately measure significant quality attributes for a biotech product during production culture in real time will also be discussed. Finally, technology drivers that can alleviate the above mentioned gaps will be discussed.

Presentations

Session 4, Innovations and novel insights in Liquid Chromatography

23 June 2021

Rationalisation of Peak Shapes of Peptides and Mabs in Reversed-Phase LC Using a Variety of Mobile Phase Additives

David McCalley, UWE Bristol, United Kingdom

Peptides and proteins are notorious for giving poor peak shape in RP-LC. Basic peptides give particularly poor peak shape when formic acid (favoured in LC-MS applications) is used as mobile phase additive, compared with phosphate buffer, ammonium formate and trichloracetic acid. The effect is often attributed to the presence of acidic ionised silanols on the silica column surface. However, the contributory factors may be more complex, considering that similar results are obtained on totally polymeric (polystyrene divinylbenzene) stationary phases. Studies were performed to ascertain whether findings with these peptides could be extrapolated to monoclonal antibodies (mAbs) when analysed on superficially porous RP columns. These proteins require additional considerations due to their size and require large pore packings and higher temperatures, needed to prevent irreversible adsorption or carry-over of the solute.

Presentations

Session 4, Innovations and novel insights in Liquid Chromatography

23 June 2021

Comparison of HILIC and RP Separation Modes in the Complex Analysis of Current Antivirals to Tackle Drug-Drug Interactions

Lucie Nováková, Charles University, Czech Republik

Simultaneous administration of multiple drugs can result in drug-drug interactions (DDI) and hence in altered plasma levels leading to therapy failure or toxic effect. Well-designed bioanalytical methods are thus of key importance to support evaluation of new drugs, drug-drug interactions, drug repurposing, and optimization of combination therapy, which is very common for example in cases of antivirals in complex HIV and HCV treatment. A unique multianalyte method targeting multiple antivirals in a single run is desirable although typical combinations involve two to three antivirals and thus it is unlikely that numerous antivirals can be simultaneously present in one biological sample. However, multianalyte methods allow direct analysis of new combinations without carrying out often tedious optimization of dedicated methods and enable switching among these combinations and testing different compounds for DDI.

Simultaneous analysis of multiple antiviral drugs from different groups remains challenging due to the large structural diversity. Indeed, they involve highly hydrophilic compounds, such as tenofovir and its metabolites, zidovudine, and didanosine, as well as highly lipophilic, such as ledipasvir, velpatastvir, ritonavir, and rilpivirin with log P values ranging within -3.44 to 6.71 and various acid-base properties. In our study, two ultra-high performance liquid chromatography (UHPLC) methods with tandem mass spectrometry detection (MS/MS) were optimized. Selected 21 current antivirals and their metabolites were analyzed in Hanks balanced salt media (pH 7.4 and 6.5) used in experiments to evaluate the membrane transport. The focus was put on each step of bioanalytical method including sample preparation step using micro-solid phase extraction in pipette tips, LC separation conditions including RP and HILIC, and tandem mass spectrometry detection. Although enhanced separation selectivity was achieved in RP-UHPLC-MS/MS, substantially higher sensitivity was observed in HILIC-UHPLC-MS/MS. Moreover, the latter also exhibited superior method validation results indicating HILIC mode to be more suitable for our multianalyte method.

Presentations

Session 4, Innovations and novel insights in Liquid Chromatography

23 June 2021

Implementing Miniaturized Separation Platforms into Pharmaceutical Workflows

James Grinias, Rowan University, USA

The importance of UHPLC in pharmaceutical analysis continues to grow, although many applications still rely upon outdated column/instrument technology that is slow and generates larger amounts of chemical waste. In this presentation, technical strategies designed to reduce the cost and/or volume of various aspects of pharmaceutical workflows will be described. Compact liquid chromatography instrumentation that utilizes capillary-scale columns enables effective analysis with a 1000-fold reduction in solvent consumption relative to standard HPLC methods. This methodology has been applied to impurity, metabolite, and dissolution testing in both over-the-counter and prescription analgesic drugs. Progress towards coupling this compact instrumentation directly to reagent flasks for real-time synthetic reaction monitoring will also be described.

Automated workflows have simplified many of the aspects related to pharmaceutical drug testing. However, most commercial platforms are extremely expensive and require significant laboratory space. The advent of open-source microcontrollers and single-board computers, along with low-cost robotic hardware enabled through the expansion of 3D printers, has provided an opportunity for simplified systems that are smaller and more affordable. An autosampling mechanism, various pumping strategies, an antibiotic screening tool, and open-source approaches to components of chromatographic separations have all been designed and will be presented.

Presentations

Session 4, Innovations and novel insights in Liquid Chromatography

23 June 2021

Shedding Light on Mechanisms Leading to Convex-Upward Van Deemter Curves on a Cellulose Tris(4-Chloro-3-Methylphenylcarbamate)-Based Chiral Stationary Phase

Martina Catani, University of Ferrara, Italy

This work reports about an unusual but not rare behaviour that is the occurrence of convex-upward van Deemter curves in chiral chromatography. They were observed for the more retained enantiomer of a chiral sulfoxide (2-(benzylsulfinyl)benzamide) on a cellulose tris(4-chloro-3-methylphenylcarbamate)-based chiral stationary phase (CSP), prepared on silica particles of 1000 Å pore size. In contrast, the firstly eluted enantiomer of the same molecule exhibited the traditional convex-downward van Deemter curve.

A detailed kinetic and thermodynamic investigation has revealed that this unusual phenomenon originates when the adsorption of the compound is very strong, and the solid-phase diffusion is negligible. Overall, this translates into very little longitudinal diffusion (b-term of van Deemter curve) accompanied by high solid-liquid mass transfer resistance (c-term). In addition, the comparison with another, differently-substituted chiral sulfoxide (whose enantiomers both exhibited convex-downward van Deemter curves) has allowed to correlate these findings to specific structural properties of the molecules.

Presentations

Session 4, Innovations and novel insights in Liquid Chromatography

23 June 2021

Innovations in temperature responsive liquid chromatography

Frederic Lynen, University of Gent, Belgium

Temperature responsive liquid chromatography (TRLC) has originally emerged as an alternative HPLC mode allowing for the separation of organic solutes under purely aqueous conditions. The concept is based on the stimuli-responsive nature of e.g. acrylamide based polymers such as poly[N-isopropylacrylamide] (PNIPAAm), which gradually becomes more hydrophobic or hydrophilic at temperatures above and below 32°C, respectively. When such polymers are anchored to a silica supporting material, and packed into columns, the phenomenon becomes exploitable in HPLC. TRLC allows for a number of novel developments in HPLC including 1) a relatively broadly applicable type of green reversed phase liquid chromatography which can be operated with either 100% aqueous conditions or (if whished) with aqueous/organic mobile phases; 2) a simple isocratic type of HPLC whereby solvent gradients are not necessary paving the way for more universal quantitation; 3) a novel tool for the protein, peptides, pharmaceutical or e.g. natural product analyses; 4) a superior first dimension separation mode (in terms of modulation) in LCxLC allowing for optimal refocusing in between the separation dimensions. During this presentation an overview is presented of the developments by the Separation Science Group during the last decade in the light of these aspects, together with a critical assessment of the pros and cons of this separation mode. The potential of various temperature responsive polymers is compared in terms of the fundamental chromatographic performance they can offer in HPLC. Finally, new approaches for column temperature control are proposed to allow for enhanced exploitation of temperature gradients on such phases in HPLC.

Presentations

Session 4, Innovations and novel insights in Liquid Chromatography

23 June 2021

Design Aspects of a Microfluidic Device for Comprehensive Spatial Three-Dimensional LC

Sebastiaan Eeltink, Vrije Universiteit Brussel, Belgium

In spatial comprehensive three-dimensional chromatography (3D-LC) components are separated within a three-dimensional separation space that can lead to unprecedented resolving power, in terms of peak capacity and peak-production rate. The maximum peak capacity is the product of the peak capacities achieved in the individual dimensions when orthogonal retention mechanisms are incorporated. The parallel development of the second- and third-dimension separation stages overcomes the fundamental limitation of conventional multi-dimensional approaches, in which sampled fractions are analyzed sequentially. General considerations for chip design are discussed and possibilities and prospects to establish spatial comprehensive 3D-LC analysis are presented.

Guest Speakers

First Agilent InfinityLab LC Virtual Scientific Conference

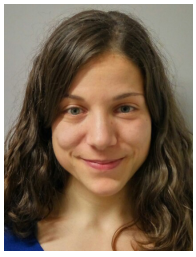
Guest Speakers

Session 1, The Power of 2DLC

Gert Desmet

Vrije Universiteit Brussel, Belgium

Gert Desmet has a Master's degree and PhD in chemical engineering from the Vrije Universiteit Brussel (VUB), Brussels, Belgium, where he currently is a full professor in chemical engineering. His research mainly focuses on the miniaturization and automation of separation methods, as well as on the investigation and the modeling of flow effects in chromatographic systems. He is a past chair of the Chemistry Panel of the Flemish National Science Fund and currently is the Deputy-director of the Solvay Institute for Chemistry. He currently also is an Associate Editor for the journal "Analytical Chemistry" and holder of an ERC Advanced Grant. In 2008, he received the "Emerging Leader in Chromatography"-award from LC-GC. In 2009, he received the Silver Jubilee Medal of the Chromatographic Society of the UK. In 2019, he received the American Chemical Society Award for Chromatography. He is currently also a member of the permanent scientific committee of the international HPLC and ISC conference series.



Lidia Montero

University of Duisburg-Essen

Dr. Lidia Montero obtained the Master degree in Agricultural Chemistry and Novel Foods (2012) and the PhD. in Biology and Food Science (2017) in the University Autónoma of Madrid. Since 2018, she is a postdoctoral researcher in the department of Applied Analytical Chemistry in the University of Duisburg-Essen. Her main research interests are, on one hand, the application of different advanced extraction techniques for the extraction of bioactives from complex natural and food matrices (pressurized liquid extraction (PLE) or supercritical fluid extraction (SFE)). And, on the other hand, the development and application of new analytical methodologies based on chromatographic technologies like multidimensional LC and LC coupled analytical techniques like HRMS and ion mobility for the analysis and characterization of complex biological and food samples.

Guest Speakers

Session 1, The Power of 2DLC

Matthias Pursch

Dow Deutschland Anlagen GmbH

Matthias Pursch is a R&D Fellow at Dow, currently located in Wiesbaden/ Germany. His research interests involve Separations and Spectroscopy, with an emphasis on Liquid Chromatography and related techniques. Most recent focus is on new developments and applications of multi-dimensional LC (2D-LC). He is author of 55 publications and has given 50 external presentations. He is an extended board member in the Separation Science subdivision within the German Chemists Society (GDCh).

Michael Lämmerhofer

University of Tübingen, Germany

Michael Lämmerhofer is Full Professor (W3) for Pharmaceutical (Bio-)Analysis at the University of Tübingen, Germany (since 2011). He graduated in Pharmaceutical Sciences in 1992 and earned his PhD in Pharmaceutical Chemistry in 1996 at the University of Graz, Austria (Supervisor: Prof. Wolfgang Lindner). Between 1997 and 2011 he was assistant professor and since 2002 associate professor at the University of Vienna, Department of Analytical Chemistry. From 1999-2000 he spent a year of research as post-doc at the Department of Chemistry of the University of California, Berkeley with Prof. Frantisek Švec. Since 2007, he is associate editor of Journal of Separation Science.

His research interests include the development of functionalized separation materials (chiral stationary phases, mixed-mode phases, chemo- & bioaffinity materials, nanoparticles, monoliths), metabolomics and lipidomics, pharmaceutical analysis (impurity profiling, enantioselective analytics), multidimensional separations and biopharmaceuticals analysis (peptides, oligonucleotides, proteins, plasmids).

Guest Speakers

Session 1, The Power of 2DLC

Miguel Herrero

Institute of Food Science Research (CIAL, CSIC-UAM)

Dr. Miguel Herrero is a Research Scientist at the Institute of Food Science Research (CIAL-CSIC) of the Spanish National Research Council, in Madrid, Spain. He holds a PhD in Food Science and Technology from the University Autonoma of Madrid (2006) and carried out a two-year postdoctoral research stage at the University of Messina, Italy. His main research interests are aimed to the study and characterization of new functional ingredients including the development of new advanced extraction and analytical methods to obtain and characterize interesting food-related compounds. Particularly, on the development of new methods and applications using comprehensive two-dimensional liquid chromatography (LC x LC) coupled to mass spectrometry. Scopus author ID: 7102420113.

Guest Speakers

Session 1, The Power of 2DLC

Oliver J. Schmitz

University of Duisburg-Essen

In 2009 Oliver J. Schmitz got a full professor in Analytical Chemistry at the University of Wuppertal (BUW). Between 2010 and 2012 he was the chair of the Analytical Chemistry department at BUW. Since 2013 Schmitz has been a full professor at the University of Duisburg-Essen and is the chair of the Institute of Applied Analytical Chemistry.

2009 he cofounded the company iGenTraX UG which develops new ion sources and units to couple separation techniques with mass spectrometers. In 2011 he was one of the founding directors of the Interdisciplinary Centre for Pure and Applied Mass Spectrometry, University of Wuppertal. In 2018, together with Agilent Technologies, he founded the Teaching and Research Center for Separation (TRC).

The research fields of Prof. Schmitz are the development of ion sources, use and optimization of multi-dimensional LC and GC, ion mobility-mass spectrometry and coupling analytical techniques with mass spectrometers. Furthermore he is working about origin of life and metabolomics. Prof. Schmitz was awarded the scholar-in-training award of the American Association for Cancer Research in 2003, the Gerhard-Hesse Prize for chromatography in 2013 and the Waksmundzki Medal Award for Analytical Chemistry of the Polish Academy of Sciences in 2018.

Guest Speakers

Session 1, The Power of 2DLC

Sabine Heinisch

Institute of Analytical Science; University of Lyon

Sabine Heinisch is a research team leader at ISA (Institute of Analytical Science; University of Lyon). She is interested in the fundamentals and applications in liquid chromatography. Her primary research topic is on the development of on-line LCxLC-HRMS for the separation of pharmaceuticals, peptides or therapeutic proteins. Her research interests also cover the development of LC x SFC for chiral compounds or biomass by-products. She has published more than 70 referred articles, 5 book chapters and has given more than 150 oral presentations.

Guest Speakers

Session 2, Current developments in LC and LC-MS for food and environmental applications

Boris Bugsel

Eberhard Karls Universität Tübingen

Boris Bugsel is a PhD student at the Center for Applied Geosciences, University of Tübingen. His research focuses on the application of high resolution mass spectrometry screening approaches to identify per- and polyfluoroalkyl substances (PFAS).

In lab experiments, he studies the photochemical and electrochemical transformation behavior of PFAS precursors which have the potential to form persistent transformation products.

Guest Speakers

Session 2, Current developments in LC and LC-MS for food and environmental applications

Imma Ferrer

University of Colorado

Imma Ferrer completed her Ph.D. on the development of LC-MS techniques for the detection of pesticides in environmental samples at the University of Barcelona (Catalonia, Spain) in 1999. Afterwards, she did a post-doc with the U.S. Geological Survey at the National Water Quality Laboratory in Denver, Colorado for 3 years, where she worked on tandem mass spectrometric techniques for the analysis of pharmaceuticals in the environment. She then worked as an Assistant Professor at the University of Almeria for 5 years, where her main focus was the development of advanced LC-MS methodologies for the analysis of pesticides in food samples, specially the use of time-of-flight techniques using accurate mass identification. In 2008, she moved back to the U.S. where she is currently an Associate Research Scientist and one of the co-founders of the Center for Environmental Mass Spectrometry at the University of Colorado in Boulder (USA). She has more than 24 years experience on developing methods for emerging contaminants using LC-MS techniques. She is author of more than 100 peer review papers (h-index of 50) and chapters and has co-edited 4 books on LC-MS and GC-MS applications for the analysis of organic contaminants in the environment. She was recently appointed as an Associate Editor of Trends in Environmental Analytical Chemistry.

Guest Speakers

Session 2, Current developments in LC and LC-MS for food and environmental applications

Kai Bester

Aaurhus University, Denmark

Kai Bester focusses on water technology to remove organic micropollutants from water. In this connection, KB has a double qualification: A) on water technologies, especially biofilm technologies B) on analytical and environmental chemistry. This crossover allows to follow processes important for innovative water technology in detail with tailor made analytical methods such as advanced mass spectrometry and sophisticated chromatography as KB is able to determine enantiomeric fractions of chiral pollutants at ultratrace concentrations. KB currently runs 20 laboratory and 7 pilot reactors for removing micropollutants from contaminated waters.

Guest Speakers

Session 2, Current developments in LC and LC-MS for food and environmental applications

Leticia Pérez-Mayán

University of Santiago de Compostela, Spain

My research career has been developed in the Chromchem research group (University of Santiago de Compostela), coordinated by Prof. Rafael Cela. My academic training and research experience to date have provided me with an excellent background in chromatographic separation coupled to mass spectrometry. In addition, I enhanced my knowledge on several sample preparation techniques during my predoctoral research.For my graduate and master training, I conducted research with Prof. Isaac Rodriguez on the development of amultianalyte method for the determination of pesticides in wine, which gave me an insight into Solid Phase Extraction (SPE) and Triple Quadruple (QqQ) – Mass Detectors. This resulted in a co-authorship publication in the Analytical and Bioanalytical Chemistry journal. For my initial predoctoral research, a Fabric Phase Sorptive Extraction (FPSE) was optimized for fungicides and insecticides in the same matrix, wine. Next research project was carried out using Supercritical fluid chromatography coupled to quadrupole-time-of-flight detection (SFC-QTOF), applied to a set of concerning insecticides. Vineyard soil was the second environmental matrix used in my research since it is closely related to wine production. Presence and distribution of pesticides were studied in consecutive wine production campaigns in order to draw a conclusion regarding compounds accumulated in environmental compartments. For this purpose, Pressurized Liquid Extraction (PLE) for a set of 50 compounds and detection, using Ultrahigh Performance Liquid Chromatography coupled to tandem-mass spectrometry (UHPLC-MS/MS), were optimized. Additionally, five chiral compounds were studied to understand their enantiomeric/ non-enantiomeric degradation in soil. Overall, analytical methodologies are necessary to adapt quality control to foodstuff consumed nowadays.Different methodologies have been developed so as to improve accuracy and sensibility in pesticide detection. Furthermore, reduction in organic solvent usage is a key factor to guide research to an environmentally-friendlyresearch process.

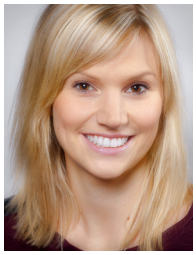
Guest Speakers

Session 2, Current developments in LC and LC-MS for food and environmental applications

Petra Hehet

Ludwig Maximilian University of Munich

Petra Hehet is a doctoral research scientist at Ludwig Maximilian University of Munich, working in cooperation with the Forensic Science Institute of Bavarian State Police Office in Munich. Her PhD research includes hair analysis in forensic toxicology, forensic analysis and method development for the detection of explosives and new psychoactive substances (NPS). Her area of expertise also includes analytical techniques like LC-MS/MS, GC-MS/MS, LC-QTOF as well as different sample preparation methods (SPE, LLE) for environmental and biological matrices. She is an active participant of the EU project SYSTEM.



Selina Tisler

University of Copenhagen

Selina Tisler is a postdoctoral researcher in the analytical chemistry group, University of Copenhagen. She has here main focus in non-target screening of the aquatic environment (mainly wastewater and drinking water). She is developing non-target screening workflows on SFC- and LC-HRMS systems for the identification of high risk compounds for a safe water environment. She received her Ph.D. from University of Tübingen, Germany, studying the formation of transformation products of pharmaceuticals in wastewater and surface water.

Guest Speakers

Session 2, Current developments in LC and LC-MS for food and environmental applications

Zhenyu Tian

Center for Urban Waters, University of Washington Tacoma

Zhenyu Tian is a postdoctoral research scientist at the Center for Urban Waters, University of Washington Tacoma, applying non-target screening to identify emerging contaminants in stormwater, marine water, and biota, and to evaluate engineered treatment systems. He received his Ph.D. from University of North Carolina in 2018, studying the transformation products and co-occurring pollutants of PAHs in contaminated soil.

Guest Speakers

Session 3, Trends in Biopharmaceutical Analysis

Alexandre Goyon

Genentech

Dr Alexandre Goyon is a Scientist in the Small Molecule Pharmaceutical Science organization of Genentech. He received a Ph.D. degree in Pharmaceutical Analytical Chemistry in 2019 from the University of Geneva, Switzerland. His team supports early & late stage research. He authored 30 journal articles, including 21 as first author.

Anurag S. Rathore, Ph. D.

Indian Institute of Technology, Delhi, India

Anurag S. Rathore is an Institute Chair Professor at the Department of Chemical Engineering, Indian Institute of Technology, Delhi, India. He is also the Coordinator for the DBT COE for Biopharmaceutical Technology. His previous roles included management positions at Amgen Inc., Thousand Oaks, California and Pharmacia Corp., St. Louis, Missouri. His areas of interest include process development, scale-up, technology transfer, process validation, biosimilars, continuous processing, process analytical technology and quality by design. He has authored more than 500 publications and presentations in these areas. He is presently serving as the Editor-in-Chief of Preparative Biochemistry and Biotechnology and Associate Editor for Journal of Chemical Technology and Biotechnology. He also serves on the Editorial Advisory Boards for Biotechnology Progress, Electrophoresis, BioPharm International, Pharmaceutical Technology Europe and Separation and Purification Reviews. Dr. Rathore has edited books titled Novel Bioprocessing Technology for Production of Biopharmaceuticals and Bioproducts, Preparative Chromatography for Separation of Proteins and Peptides, Quality by Design for Biopharmaceuticals: Perspectives and Case Studies (2009), Elements of Biopharmaceutical Production (2007), Process Validation (2005), Electrokinetic Phenomena (2004) and Scale-up and Optimization in Preparative Chromatography (2003). He has a Ph.D. in Chemical Engineering from Yale University. Prof. Rathore is presently serving as Dean, Corporate Relations, at IIT Delhi.

Guest Speakers

Session 3, Trends in Biopharmaceutical Analysis

Christian Huber

University of Salzburg, Austria

Christian Huber trained as an analytical chemist at the University of Innsbruck focusing on chromatographic separation methods for biopolymers. After a PostDoc in Csaba Horváth's group at Yale University in 1996, he obtained lecturing qualification in analytical chemistry at the University of Innsbruck. From 2002-2008 he held a position as professor for analytical chemistry at Saarland University. He is currently a professor of chemistry for biosciences at the University of Salzburg. He also leads the Christian Doppler Laboratory for Biosimilar Characterization, which cooperates with Novartis and Thermo Fisher Scientific. His research interests include proteome and metabolome analysis as well as in-depth protein characterization by means of HPLC and MS.

Cinzia Stella

Genentech

Dr Cinzia Stella received her Ph.D. in Pharmaceutical Analytical Chemistry from the University of Geneva (Switzerland), after her Master's Degree in Pharmaceutical Sciences from the University of Pavia (Italy). Following a post-doctoral fellowship at Imperial College London (UK) on Metabolomics funded by Unilever, she held a position at the University of Geneva in the School of Pharmacy, where she was responsible for the development and optimization of protein based pharmaceutical formulations in collaborations with industrial partners. She is currently a Sr Scientist and Functional Leader at Genentech and she is responsible for the development and implementation of analytical platforms to support the pipeline.

Guest Speakers

Session 3, Trends in Biopharmaceutical Analysis

Davy Guillarme

University of Geneva, Switzerland

Davy Guillarme holds a Ph.D. degree in analytical chemistry from the University of Lyon, France. He is now senior lecturer and research associate at the University of Geneva in Switzerland. He authored more than 270 journal articles related to pharmaceutical analysis. His expertise includes HPLC, UHPLC, HILIC, LC–MS, SFC, SFC-MS, multidimensional LC, analysis of proteins, mAbs and ADCs.

He is an associate editor of Journal of chromatography B and editorial advisory board member of several journals (Trends in analytical chemistry, Journal of Chromatography A, Journal of Separation Science, LC–GC North America…). He was the recipient of the LC-GC emerging leader award in chromatography in 2013 and the jubilee medal from the chromatographic society in 2018. He was also elected as one of the world's most influential analytical scientists by "Analytical Scientist" magazine in in 2013, 2014, 2015, 2017, 2019 and 2020.

Last, he is also widely involved in teaching and education activities, such as training courses, seminars, and conferences on HPLC, SFC, biopharmaceuticals analysis…

Koen Sandra

RIC Group

Koen Sandra received a PhD degree in Biochemistry from the Ghent University, Belgium in 2005. After his PhD, he joined Pronota, a molecular diagnostics company where he was active in developing analytical platforms for disease biomarker discovery and in setting up external collaborations. In 2008, he joined RIC, a company that provides chromatographic, electrophoretic and mass spectrometric support to the chemical, life sciences and pharmaceutical industries, where he holds the position of CEO. As a non-academic scientist, Koen Sandra is author of over 50 highly cited scientific papers and has presented his work at numerous conferences as an invited speaker.

Guest Speakers

Session 3, Trends in Biopharmaceutical Analysis

Rainer Bischoff

Univeristy of Groningen, The Netherlands

Rainer Bischoff obtained his Ph.D. in chemistry from the University of Göttingen (Germany) with practical work performed at the Max-Planck-Institute for Experimental Medicine. After a postdoc at Purdue University (USA) he joined the biotechnology company Transgene S.A. (Strasbourg, France), where he worked in a team that brought the first therapeutic protein developed in Europe to the market. He joined AstraZeneca (Lund, Sweden) as Head of the Target Development section and became professor and Head of the Analytical Biochemistry Department (www.biomac.nl) at the University of Groningen (the Netherlands) in 2001.

Guest Speakers

Session 4, Innovations and novel insights in Liquid Chromatography

David Victor Mccalley

University of the West of England, Coldharbour

David McCalley is Professor of Bioanalytical Science at the University of the West of England, U.K. In 2019, 2015 and 2013, he was named as one of the world's 100 most influential analytical scientists by 'Analytical Science' magazine. He was awarded the Silver Jubilee medal of the Chromatographic Society in 2008. He serves on the Editorial Board of the Journal of Chromatography A and the magazine LC.GC, and has been a member of the Scientific Committee of a number of conferences including the HPLC 2013 symposium in Amsterdam and the 2016 ISC symposium in Cork. In the past five years, he has given invited lectures in Cannes, Cambridge MA, Princeton, Geneva, Helsinki, London, San Francisco, Cork, Paris, Prague, Lake Balaton and Sandefjord. Professor McCalley's research is directed towards the understanding of the fundamental mechanisms of separation that occur in liquid and gas chromatography. These studies in LC have included the effects of pressure and temperature on retention and efficiency, mixed mechanisms for strongly basic compounds, performance of superficially porous packings, and overloading effects in both reversed-phase and hydrophilic interaction chromatography. Applications have included monoclonal antibodies, peptides, natural products, steroids, pharmaceuticals and clinically relevant compounds using both UV detection and mass spectrometry. His h index is 42.

Guest Speakers

Session 4, Innovations and novel insights in Liquid Chromatography

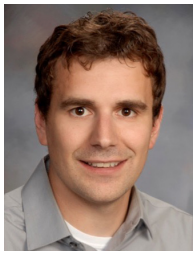
Frederic Lynen

University of Gent, Belgium

Frederic Lynen (°1974) began his academic career at Ghent University in Belgium, where he obtained his PhD under the supervision of Prof. Pat Sandra in 2002. He then moved to the university of Stellenbosch in South Africa for postdoctoral research and returned in 2004 to Ghent University with the start-up of the Pfizer Analytical Research Centre (PARC). Since 2011 Dr. Lynen is associate professor, in charge of the Separation Science Group in the Department of Organic and Macromolecular Chemistry, at Ghent university. His research interests span a broad range of activities from fundamental (electro-) chromatographic performance predictions, improved predictive chromatographic modeling through Stationary Phase Optimize Liquid and Supercritical Fluid Chromatography (SOS-LC and SOS-SFC), stationary phase synthesis and column design for HPLC, SFC, GC and CEC, purely aqueous green temperature responsive liquid chromatography, the development various alternative 2-D LCxLC, LC-LC, LCxCE and GCxGC approaches, the design of enhanced separation and quantitation approaches specifically for medium sized and large molecules, matrix effects studies in mass spectrometry, immobilized artificial membrane chromatography, universal detection, natural product and complex pharmaceutical analysis, and also biomarker discovery in the framework of biomedical, art-historical and archeological research projects. Prof. Lynen has published over 140 papers, has given more than 40 presentations at international conferences and has a research group that comprises 8 PhD researchers. Over 10 PhD and postdoctoral researchers in the group have been honoured with poster awards at major chromatographic conferences in recent years. In 2012 Frederic was also awarded the Silver medal during the Method Development Olympics. He is a member of the editorial board of Journal of Chromatography A, and was chair of various editions (2012, 2014, 2016) of the International Conferences in Hyphenated Techniques in Chromatography (HTC) and Hyphenated Techniques for Sample Preparation (HTSP).

Guest Speakers

Session 4, Innovations and novel insights in Liquid Chromatography



James Grinias

Rowan University in Glassboro, NJ

James Grinias is currently an Associate Professor in the Department of Chemistry & Biochemistry at Rowan University in Glassboro, NJ. His research interests include improving the throughput and efficiency of chromatographic separations and the miniaturization of chemical measurement techniques. He received his Ph.D. from the University of North Carolina at Chapel Hill in 2014 and the moved onto a postdoctoral fellowship at the University of Michigan until the end of 2016. James has received a number of awards for his work to date, including the HPLC 2013 Csaba Horváth Award, the 2020 Young Investigator Award from the Chinese American Chromatography Association, a National Science Foundation CAREER grant, and the 2021 American Chemical Society Satinder Ahuja Young Investigator in Separation Science Award. He was also named to The Analytical Scientist's "Top 40 Under 40" Power List in 2018. To date, he has published over 30 articles and given over 80 oral/poster presentations.

Guest Speakers

Session 4, Innovations and novel insights in Liquid Chromatography

Ken Broeckhoven

Vrije Universiteit Brussel

Ken Broeckhoven is an associate professor at the Vrije Universiteit Brussel (VUB) in Belgium since February 2017, in the departments of Chemical Engineering and Bioengineering Sciences. He teaches courses on Chemical Process Technology, Modelling of Biomedical Systems, Heat and Mass transfer and Technology projects on Environmental Engineering. His research focusses on fundamental aspects of chromatography and the optimization aspects of separation performance in both liquid and supercritical fluid chromatography. He is the author of more than 80 research papers with more than 1300 citations and presented over 40 oral presentations at international conferences. He was part of the “Top 40 Under 40” by The Analytical Scientist in both editions (2014 and 2018) and the recipient of the LCGC magazine’s “Emerging leader in chromatography” award in 2019. One of his paper was voted as ‘Landmark Paper for 2015’ by the Analytical Scientist magazine. During his PhD, his poster was ranked nr. 1 at the Best Poster Award competition at HPLC2008 in Boston (MA, USA) and afterwards his PhD students obtained numerous poster awards at different international conferences. He is also part of the organizing and scientific committee of the biennial HTC-conference series (Hyphenated Techniques in Chromatography) and member of the ChiMiC consortium, grouping 5 leading groups in chromatographic techniques in Belgium. Since 2014, he is a member of the Editorial Board of Journal of Pharmaceutical Analysis and since 2018 of the advisory editorial board of Journal of Chromatography and LCGC.

Guest Speakers

Session 4, Innovations and novel insights in Liquid Chromatography

Lucie Nováková

Charles University, Czech Republik

Lucie Nováková is a Full Professor in Analytical Chemistry at the Charles University, Faculty of Pharmacy in Hradec Králové, Department of Analytical Chemistry, the Czech Republic since 2019. She received her Ph.D. from Pharmaceutical Analysis at the same university in 2005 followed by an Associate Professor degree in 2011. Her research is focused on separation techniques, including ultra-high performance liquid chromatography, supercritical fluid chromatography, and their coupling to mass spectrometry, and also on the sample preparation, where the focus is put on the current trends enabling facilitation, miniaturization, and reduction of time and sample requirements. She is involved in a wide scope of research projects focused on pharmaceutical analysis, doping control, plant analysis, and bioanalytical methods. She extended her scientific experience during the fellowships at world-recognized universities, such as the University of Geneva and Vrije Universiteit Brussel, beyond others. She authored two books on HPLC theory and practice and 9 book chapters. She published over 120 peer-reviewed scientific articles and review papers with more than 3800 citations and an h-index of 34. She is also widely involved in teaching and education activities, such as HPLC and SFC training courses, seminars, and conferences. Currently, she is a principal team manager of the STARSS project.

Guest Speakers

Session 4, Innovations and novel insights in Liquid Chromatography

Martina Catani

University of Ferrara, Italy

Martina Catani received the PhD in Chemical Sciences cum laude from the University of Ferrara (Italy) in 2018. She is currently working as a research associate/assistant professor at the same University. Her research activities revolve around fundamentals of liquid chromatography, in particular for what regards the impact of kinetics and thermodynamics, particle geometry (fully porous vs core-shell) and their physico-chemical characteristics on the performance of achiral and, especially, chiral columns. More recently, she has started working also on the separation of cannabinoids by means of HPLC and SFC and on the development of purification methods for therapeutic biomolecules by means of both single-column and continuous multicolumn preparative liquid chromatography.

During the PhD she has spent research periods as visiting PhD student at the VUB Brussels (Belgium) in the group of Prof. Gert Desmet and at the University of Pécs (Hungary) under the supervision of Prof. Attila Felinger. In 2019 she spent a period as a post-doctoral research fellow at ETH Zurich (Switzerland) working on continuous purification techniques in the group of Prof. Massimo Morbidelli.

In 2018 she won the “Csaba Horváth Young Scientist Award” at HPLC2018 Washington and in 2020 the “Young Researcher Award” assigned by the Interdivisional Group of Separation Science of the Italian Chemical Society.

Guest Speakers

Session 4, Innovations and novel insights in Liquid Chromatography

Sebastiaan Eeltink

Vrije Universiteit Brussel

Sebastiaan Eeltink received his PhD degree in Analytical Chemistry in 2005 from the University of Amsterdam, The Netherlands. From 2005-2007 he conducted two years of post-doctoral research at the University of California, Berkeley, USA and he was a guest scientist at The Molecular Foundry in the Lawrence Berkeley National Laboratory. Here, he developed novel column formats, including coated capillary columns and monolithic structures in microfluidic chips. In 2007 he joined Dionex (currently Thermo Fisher Scientific) and conducted research on packed and monolith column technology and bioanalysis. In 2009, Sebastiaan received an Odysseus award from the Research Foundation Flanders to establish his research group at the Vrije Universiteit Brussel. He is now full professor leading a research team focusing on development and characterization of novel column structures for liquid chromatography, design of novel microfluidic chip solutions for multi-dimensional separations, and advancement of LC-MS workflows to characterize contemporary biopharmaceutical and life-science mixtures. He is author of more than 100 scientific publications, 3 book chapters, and 3 patent applications on spatial three-dimensional liquid chromatography.

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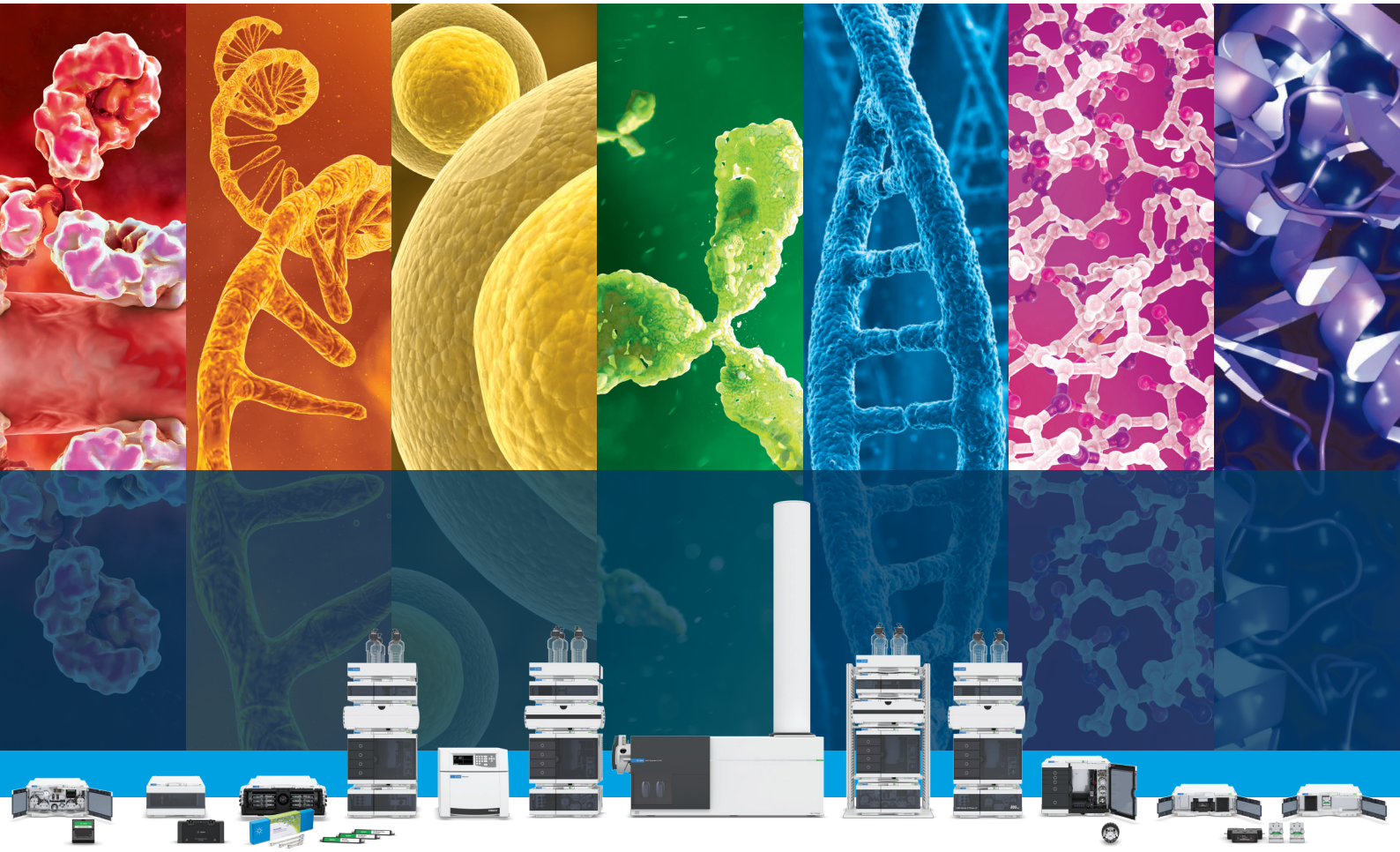

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