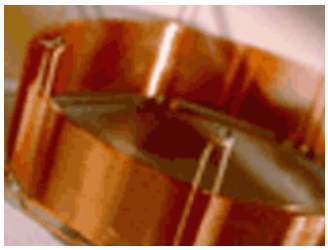
RAFA 2021 BOOKLET

Virtual event highlighting current Trends & Views

RECENT ADVANCES IN FOOD ANALYSIS

November 3–4, 2021



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PROGRAM

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Trends & Views

RECENT ADVANCES IN FOOD ANALYSIS

November 3–4, 2021

Organized by

Department of Food Analysis and Nutrition
University of Chemistry and Technology, Prague (UCT Prague)
Czech Republic

&

Wageningen Food Safety Research (WFSR), part of Wageningen University & Research
The Netherlands

MINISTRY OF AGRICULTURE OF THE CZECH REPUBLIC

RAFA 2021 is held under auspices of the Minister of Agriculture of the Czech Republic, Miroslav Toman.

Wednesday - November 3, 2021 Chairs: Jana Hajslova (UCT Prague) & Michel Nielen (WFSR)			
9:00-13:00	**Series of vendor webinars I**		
13:45-14:00	**Welcome at RAFA 2021**		Jana Hajslova & Michel Nielen, RAFA chairs
Session 1	**Analytical challenges I**		
14:00-14:20	L1	**Fighting food frauds exploiting chromatography-mass spectrometry & infrared technologies: scientific literature vs real industrial approaches**	**Michele Suman** Barilla G. R. F.lli SpA, Advanced Laboratory Research, Parma, Italy
14:20-14:40	L2	**How can we measure and tackle the world wide occurrence of mycotoxins in view of climate change?**	**Rudolf Krska** University of Natural Resources and Life Sciences, Vienna, IFA-Tulln, Austria
14:40-15:00	L3	**Potential of imaging mass spectrometry in characterisation of food crops**	**Chiara Dall´Asta** University of Parma, Parma, Italy
15:00-15:20	L4	**Dimensional Chromatography with Quadruple Parallel Mass Spectrometry, LC3MS4, for Infant/Adult Formula Analysis**	**Craig Byrdwell** U.S. Dept. of Agriculture, Agricultural Research Service, Beltsville Human Nutrition Research Center, USA
15:20-15:30	L5	**Towards decentralized food safety: a FoodSmartphone perspective**	**Georgina Ross** Wageningen University & Research, Wageningen, The Netherlands
15:30-15:40	*Chat discussion with speakers L1-L5*		Led by Jana Hajslova & Michel Nielen
15:40-16:00	*Refreshment break*		
Session 2	**Metabolomics**		
16:00-16:20	L6	**Metabolomics and lipidomics approaches to advance food Science and nutrition research**	**Alejandro Cifuentes** National Research Council of Spain, Madrid, Spain
16:20-16:40	L7	**Deciphering the gut microbiota function by LC/GC-MS metabolomics approaches**	**Josep Rubert** Wageningen University & Research, Wageningen, The Netherlands
16:40-17:00	L8	**Confidence in metabolite annotations from high-resolution MS/MS in food digestion along the human GI tract**	**Oliver Fiehn** UC Davis West Coast Metabolomics Center, Davis, USA
17:00-17:20	L9	**One class modelling, a simple approach to botanical authentication**	**James Harnly** U.S. Dept. of Agriculture, Agricultural Research Service, Beltsville Human Nutrition Research Center, USA
17:20-17:40	*Chat discussion with speakers L6-L9*		Led by Jana Hajslova & Michel Nielen
17:40-18:30	*Opportunities for networking*		

Thursday - November 4, 2021 Chairs: Jana Pulkrabova (UCT Prague) & Stefan van Leeuwen (WFSR)			
Session 3	**Food fraud & authentication**		
09:00-09:20	L10	**From targeted to non-targeted analysis for food authentication: challenges of change**	**Carsten Fauhl-Hassek** Federal Institute for Risk Assessment, Berlin, Germany
09:20-9:40	L11	**Diving into the beer metabolome and discover signatures of materials, technologies and reactions**	**Michael Rychlik** Technical University of Munich, Freising, Germany
09:40-10:00	L12	**Alternative proteins for conventional animal products in China: regulatory process**	**Yongning Wu** China National Center for Food Safety Risk Assessment, Beijing, China
10:00-10:10	L13	**Wine varietal identification: solution of an uneasy task**	**Leos Uttl** University of Chemistry and Technology Prague, Prague, Czech Republic
10:10-10:20	L14	**The story of a leaf: a 2-tiered system for tea authenticity**	**Di Wu** Queen's University Belfast, Belfast, United Kingdom
10:20-10:40	L15	**Food authenticity from a regulatory science perspective**	**Franz Ulberth** European Commission, Joint Research Centre, Geel, Belgium
10:40-11:00	*Chat discussion with speakers L10-L15*		Led by Jana Pulkrabova & Stefan van Leeuwen
11:00-11:20	*Refreshment break*		
Session 4	**Analytical challenges II**		
11:20-11:40	L16	**Comparison of analytical methods and results: "Devil is in the details"**	**Katerina Mastovska** Eurofins Scientific, USA
11:40-12:00	L17	**Scientific and regulatory challenges and developments for EU Reference Laboratories in food safety areas**	**Piotr Robouch** European Commission, Joint Research Centre, Geel, Belgium
12:00-12:20	L18	**Transition to a circular economy: analytical challenges for contaminants in the food chain**	**Stefan van Leeuwen** Wageningen Food Safety Research (WFSR), part of Wageningen University & Research, The Netherlands
12:20-12:30	L19	**Smartphone-based pesticide residue screening: goals achieved & challenges to be faced**	**Aristeidis Tsagkaris** University of Chemistry and Technology Prague, Prague, Czech Republic
12:30-12:50	L20	**Determining the source of our soya using an analytical toolbox**	**Christopher Elliott** Queen's University Belfast, Belfast, United Kingdom
12:50-13:10	*Chat discussion with speakers L16-L20*		Led by Jana Pulkrabova & Stefan van Leeuwen
13:10-13:20	**Summary of RAFA 2021, Trends & Views**		**Michele Suman** Barilla Food Research Labs, Parma, Italy
13:20-13:30	**Announcement of RAFA 2022**		Jana Hajslova & Michel Nielen, RAFA chairs
13:30-18:30	**Series of vendor webinars II**		

L1

FIGHTING FOOD FRAUDS EXPLOITING CHROMATOGRAPHY-MASS SPECTROMETRY & INFRARED TECHNOLOGIES: SCIENTIFIC LITERATURE VS REAL INDUSTRIAL APPROACHES

Michele Suman [1, 3] *, **Daniele Cavanna** [2], **Giuseppe Sammarco** [1, 2], **Francesca Lambertini** [1], **Cecilia Loffi**[2]

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Fraud in food commodities is very common in all regions of the globe and today occurs at different places of the supply chain: the demand for rapid and confirmatory analytical methods has increased in recent years.

This presentation intends to illustrate a comparison between chromatography-mass spectrometry (mainly) & infrared technologies (few other examples) solutions to detect food fraud suggested in scientific literature and practices actually implemented by food companies.

This will be done taking into consideration several different types of matrixes/food chains (wheat/cereals, fruits, nuts and nut products, eggs & egg products,…) and integrating the information about industrial behaviour, directly collected through informal interviews and official open days & workshops; executed during FoodIntegrity European Funded Project.

The academic and food industry worlds are not aligned thus far and should interact better, in particular revolving around the flexibility and performances of chromatography-MS solutions.

References:

[1] Suman et al.
Fighting food frauds exploiting chromatography-mass spectrometry technologies: Scenario comparison between solutions in scientific literature and real approaches in place in industrial facilities
Trends in Analytical Chemistry 142 (2021) - https://doi.org/10.1016/j.trac.2021.116305

[2] McGrath et al.
The potential of handheld near infrared spectroscopy to detect food adulteration: Results of a global, multi-instrument inter-laboratory study
Food Chemistry 353 (2021) - https://doi.org/10.1016/j.foodchem.2020.128718

[3] De Girolamo et al.
Tracing the Geographical Origin of Durum Wheat by FT-NIR Spectroscopy
Foods 8 (2019) - https://doi.org/10.3390/foods8100450

[4] Suman et al.
Hazelnut and apple products traceability through Near Infrared spectroscopy approach
Proceedings of Sensor Fint 2021 - Smart Spectral Sensors for Agri-Food Quality and Process Control Workshop – Porto (Portugal) 30/09/21-01/10/21

L2

HOW CAN WE MEASURE AND TACKLE THE WORLD WIDE OCCURRENCE OF MYCOTOXINS IN VIEW OF CLIMATE CHANGE?

Rudolf Krska [1,2] *

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[2] *Institute for Global Food Security, School of Biological Sciences, Queens University Belfast, University Road, Belfast, Northern Ireland, United Kingdom*
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The Food and Agriculture Organization (FAO) estimated the global food crop contamination with mycotoxins to be 25%. In order to assess the rationale for this figure which dates back to prior 1985, the relevant literature was reviewed and data of around 500 000 analyses from the European Food Safety Authority and large global survey for aflatoxins, fumonisins, deoxynivalenol, T-2 and HT-2 toxins, zearalenone and ochratoxin A in cereals and nuts were examined by M. Eskola et al. 2019. Using different thresholds, i.e., limit of detection, the lower and upper regulatory limits of European Union (EU) legislation and Codex Alimentarius standards, the mycotoxin occurrence was estimated. Impact of different aspects on uncertainty of the occurrence estimates presented in literature and related to our results are critically discussed. Current mycotoxin occurrence above the EU and Codex limits appears to confirm the FAO 25% estimate, while this figure greatly underestimates the occurrence above the detectable levels (up to 60-80%). The high occurrence is likely explained by a combination of the improved sensitivity of analytical methods and impact of climate change. The latter leading to unexpected occurrence patterns and a shift of pathogens towards the poles. It is of immense importance that the detectable levels are not overlooked as through diets, humans are exposed to mycotoxin mixtures which can induce combined adverse health effects. Hence, both, sensitive and fully validated LC-MS-based methods as well efficient integrated strategies to mitigate the mycotoxin issue along food and feed chains are needed. This presentation will summarize the state-of-the-art and recent developments in tackling these global challenges.

L3

POTENTIAL OF IMAGING MASS SPECTROMETRY IN CHARACTERISATION OF FOOD CROPS

Laura Righetti [1], Sara Tortorella [2], Chiara Dall'Asta [1] *

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Mass Spectrometry Imaging (MSI) is a technique used to visualize the spatial distribution of biomolecules such as peptides, proteins, lipids or other organic compounds by their molecular masses.

By collecting mass spectra spot by spot, the sample is scanned and the MS data is used to map the distribution of selected compounds across the sample. This results in pictures of the spatially resolved distribution of a compound pixel by pixel. Most common ionization technologies in the field of MSI are DESI imaging and MALDI imaging. This approach has been used so far mainly in to study the spatial distribution of biomolecules within tissues, and other biological media.

Sample ionization is a major challenge of the technique, especially when the target is on small molecules. In addition, data mining is often cumbersome, due to the size of the generated dataset. Therefore, dedicated, and user-friendly software may be of great support for interpretation.

Although often applied in clinical science, MSI can be of great support in understanding the effect of biotic and abiotic stressors in crops. Plant response to environmental factors may not always end up in an over/under accumulation of specific metabolites, but it more often gives rise to change in their spatial distribution.

We have recently applied MSI for elucidating the spatial distribution of secondary metabolites in plants, following mycotoxin contamination. Atmospheric-pressure scanning microprobe matrix-assisted laser desorption/ionization (AP-SMALDI) MSI, for instance, is versatile enough to cover a broad range of plant metabolites, allowing simultaneous localization clues about the putative activation and the spatial, histological distribution of specific metabolic pathways. In this regard, modern metabolomics coupled with MSI may allow a proper insight into the interplay between plants and mycotoxins, highlighting potential variations and correlations between multiple metabolites.

In this talk, the opportunities and the limitation offered by MSI will be discussed, with a particular focus on the mapping of small molecules in crops.

Acknowledgements: LR and CDA are grateful to Prof. Bernhard Spengler and Dr. Dhaka Ram Bhandari, Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen (Germany) for the scientific and technical support in the MSI analysis as well as for the fruitful collaboration and discussion. LR acknowledges the German–Italian Research Short-Term Scholarship (DAAD-2019, ID:91714320) funded by the German Academic Exchange Service (DAAD).

L4

THREE DIMENSIONAL CHROMATOGRAPHY WITH QUADRUPLE PARALLEL MASS SPECTROMETRY, LC3MS4, FOR INFANT/ADULT FORMULA ANALYSIS

William Craig Byrdwell [1] *, **Hari Karin Kotapati** [1]

[1] *U.S. Dept. of Agriculture, Agricultural Research Service, Beltsville Human Nutrition Research Center, Methods and Application of Food Composition Lab*
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Two-dimensional liquid chromatography (2D-LC) is becoming less exotic and more mainstream as commercially available instruments proliferate. Despite the impressive capabilities of 2D-LC, there are times when even 2D-LC is not sufficient for an adequate separation. One-dimensional reversed-phase HPLC is not adequate to completely resolve all milk (or infant formula) triacylglycerol (TAG) molecular species, which are highly complex, and contain many isomers of TAGs, especially TAGs with short-chain fatty acids. Even conventional 2D-LC is not completely satisfactory. A new approach was developed, in which two second dimensions were used simultaneously for dual parallel comprehensive 2D-LC, giving three dimensions of chromatography, with quadruple parallel (x4) mass spectrometry. A pair of contact-closure (CC) controlled UHPLC switching valves were coupled to a timed CC circuit to allow the second 2D separation, ^{2}D(2). The first second dimension, ^{2}D(1), used the commercially available system, in which conventional 2D-LC improved the separation of components, and all components eluted in the first modulation period from a 50 mm C30 column. The ^{2}D(2), which employed a 100 mm C30 column, produced an even better separation of components, but required more than one modulation period to elute, resulting in multi-cycle chromatography or “controlled wraparound” chromatography. Electrospray ionization (ESI) mass spectrometry (MS) was used in parallel with atmospheric pressure photoionization (APPI) MS for LC1MS2 to monitor the first dimension RP-HPLC, while ESI-MS monitored the 50 mm C30 UHPLC (LC1MS1) and ESI-MS also monitored UHPLC using the 100 mm C30 column (LC1MS1), to produce LC1MS2 x (LC1MS1 + LC1MS1) = LC3MS4.

L5

TOWARDS DECENTRALISED FOOD SAFETY: A FOODSMARTPHONE PERSPECTIVE

Georgina Ross [1] *

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Until recently, food safety was considered a job for governments and industry. However, as consumers become more aware about food safety and the associated risks, we are witnessing a rise in user-friendly food safety tests, such as lateral flow immunoassays (LFIAs) which will allow for affordable and sensitive on-the-go food testing - that's where *FoodSmartphone* comes in. We believe that smartphones have the potential to transform food analysis, allowing consumers to test foods in their kitchen and producers to test crops in the field (step 1). The *FoodSmartphone* approach can also reduce laboratory costs, as high-end analytical instruments, such as mass spectrometry (MS), will be reserved for suspect samples which have been initially screened by end-users with a smartphone-based method (step 2). All that is needed is a portable assay able to detect a target compound or a specific class of compounds, a smartphone and, in some cases, lightweight 3D-printed, auxiliary parts for optimised image capture. This talk will give an overview of the *FoodSmartphone* project, touching on a step 1 integrated device for LFIA based total allergen detection by end-users and an innovative step 2 method for direct analysis of LFIAs for mycotoxin detection by MS. We envision that the concepts and techniques presented here will pave the way for the *FoodSmartphone* approach by combining on-site screening and lab-based confirmation of a range of food safety applications.

L6

METABOLOMICS AND LIPIDOMICS APPROACHES TO ADVANCE FOOD SCIENCE AND NUTRITION RESEARCH

A. Valdés [1], R. Gallego [1], J.D. Sánchez-Martínez [1], Z. Suárez-Montenegro [1], B. Socas-Rodríguez [1], M. Herrero [1], E. Ibáñez [1], G. Alvarez-Rivera [1], A. Cifuentes [1] *

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The main objective of this presentation is to present the latest results obtained in our research group (Foodomics Lab) regarding the use of metabolomics and lipidomics techniques based on LC-HRMS and GC-HRMS to investigate the neuroprotective activity of bioactive compounds obtained from different natural sources (including algae, plants, by-products of the olive oil and orange juice industry, etc.) combining green extraction processes, a systematic study of the chemical composition using advanced analytical techniques (GC-QTOF-MS/MS and LC-QTOF- MS/MS), with in vitro models and cellular models of Alzheimer's disease. The conclusion of this work is that metabolomics and lipidomics techniques help to identify biomarkers related to the neuroprotective activity of the most active natural compounds found in model cells.

L7

DECIPHERING THE GUT MICROBIOTA FUNCTION BY LC/GC-MS METABOLOMICS APPROACHES

Josep Rubert [1] *

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Dietary patterns, or the food we eat, are the sum of many small molecules foreign to the body. After being ingested and digested, nutrients are altered by the trillions of microorganisms that inhabit our gastrointestinal (GI) tract, shaping the chemical structures of such compounds and thus modifying the lifespan, bioavailability, and biological effects. In this context, dietary patterns modulate the gut microbiome (community) and alter its functions by modulating the production of different gut microbial metabolites (GMMs). To date, an array of *in vitro* and *in vivo* models have been proposed to study gut microbiota functionality. In most cases, 16S rRNA has been predominantly used to define which microorganisms are present. On a few occasions, metagenomics has also been employed to resolve differences in the functional potential of microbial communities. However, metagenomics alone offers little information on which microbial traits contributed to human physiology. Since genes predicted from metagenomes may not necessarily be expressed. For this reason, the combination of multi-omics data revealing metabolic activities is highly required to decipher diet-gut microbiota interactions and the intestinal ecosystem.

During this presentation, I will discuss my vision of the diet-gut microbiota field and what we can achieve in the future. Preliminary data will accompany this presentation. First, the function of two distinct gut microbiota compositions, from obese and lean healthy subjects, fed with different foods (apple, apple pectin, and cellulose) will be compared. In this project, the metagenomic analysis revealed differences at the taxonomical level, and then the microbiome's functional activity was investigated in-depth by different pipelines. A further goal of this project is to measure metabolic outcomes of lean and obese gut microbiotas. Because metabolomics directly measures metabolites, these end-products may act as signaling markers at the local level (gut epithelium-gut microbiota) and promote gut health. We paid particular attention to the biotransformation of dietary fibers and phytochemicals, such as proanthocyanidins. Lastly, we investigated gut epithelium responses to specific gut microbial metabolites.

L8

CONFIDENCE IN METABOLITE ANNOTATIONS FROM HIGH-RESOLUTION MS/MS IN FOOD DIGESTION ALONG THE HUMAN GI TRACT

Jacob Folz [1], **Oliver Fiehn** [1] *

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The human small intestine remains an elusive organ to study due to the difficulty of retrieving samples in a non-invasive manner. Stool samples as a surrogate do not reflect events in the upper gut intestinal tract. As proof of concept, this study investigates time-series samples collected from the upper gastrointestinal tract of a single healthy subject. Samples were retrieved using a small diameter tube that collected samples in the stomach and duodenum as the tube progressed to the jejunum, and then remained positioned in the jejunum during the final 8.5 hours of the testing period. Lipidomics and metabolomics liquid chromatography tandem mass spectrometry (LC-MS/MS) assays were employed to annotate 828 unique metabolites using accurate mass with retention time and/or tandem MS library matches.

However, False Discovery Rates (FDR) for LC-MS/MS annotations remain poorly studied. Which adduct species should we expect? At which (relative) retention time should a compound be found? How many alternative isomers and isobar molecules should we consider? We work on integrated workflows using 19 published databases and software packages to assist in structural characterizations, including MassBank.us with more than 650,000 public MS/MS spectra. Here, we show how these packages were employed, with extensions for (1) NIST hybrid search to yield chemical class information on all unknown compounds that did not have direct hits in experimental or in-silico MS/MS libraries; (2) "Entropy Similarity" as measure for MS/MS matching to improveo FDR over classic dot-product similarity matching ; (3) retention time libraries for both HILIC and RP liquid chromatography methods for more than 4,000 metabolite standards, used for retip.app retention time prediction; (4) hydrogen/deuterium exchange data to limit the chemical search space by the number of acidic protons in MS/MS spectra.

Annotated metabolites were clustered based on correlation to reveal sets of biologically related metabolites. Typical clusters included bile metabolites, food metabolites, protein breakdown products, and endogenous lipids. Acylcarnitines and phospholipids were clustered with known human bile components supporting their presence in human bile, in addition to novel human bile compounds 4-hydroxyhippuric acid, N-acetylglucosaminoasparagine and 3-methoxy-4-hydroxyphenylglycol sulfate. Food metabolites were observed passing through the small intestine after meals. Acetaminophen and its human phase II metabolism products appeared for hours after the initial drug treatment, due to excretion back into the gastrointestinal tract after initial absorption. This exploratory study revealed novel trends in timing and chemical composition of the human jejunum under standard living conditions.

L9

ONE CLASS MODELLING, A SIMPLE APPROACH TO BOTANICAL AUTHENTICATION

James Harnly [1] *

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One-class modelling is a non-targeted approach based on principal component analysis (PCA) for authentication of foods or botanical materials. Neither an adulterant nor a specific component (marker compound) needs to be specified. A one-class non-targeted method employs only the data for the samples of the authentic material and any other material is potential adulterant. Non-targeted data are generally comprehensive chromatographic or spectral data that encompasses as many of the samples chemical properties as possible. For example, flow injection mass spectrometry will generally yield a nominal mass spectrum (profile) of around 1000 ions (e.g., m/z 100 to 1000 m/z) or variables. Since neither an adulterant or marker compound is specified, adulteration can only be detected if one or more of the variables of the unknown sample are statistically different from that of the authentic profile. Thus, the emphasis has shifted from what is the adulterant to simply examining deviations in the variables.

PCA provides two statistical values that express the fit of a sample to the model. The Hotelling T^2 statistic provides the sample variance within the model and the Q statistic that provides the distance of the sample from the model. The latter is the best means for determining subtle variations between a sample and the model. In addition, pre-processing with autoscaling (division of all the data for each variable by the standard deviation of the variable) provides normalization of the variance of each variable to a value of 1.0. This reduces the impact of variables with large intensities and places equal emphasis on all variables. Thus, the Q statistic for PCA with autoscaling is very sensitive to differences in intensities. This sensitivity is increased if the intensity of the model variable is small. Thus, adulteration, which presents a new signal at a variable that was previously at the baseline level, is readily observable. Adulteration based on an increase in an existing peak is less easily detected in terms of absolute intensity but equally detectable in terms of relative intensity change.

The relative sensitivity of the Q statistic for any variable can be easily predicted. *In silico* modelling can be used to predict the sensitivity of any variable. With the pure spectra of any adulterant, *in silico* modelling can predict the limit of detection. Thus, one-class modelling using principal component analysis with autoscaling pre-processing and analysis of variance using the Q statistic is a powerful tool for detecting adulteration and predicting limits of detection.

L10

FROM TARGETED TO NON-TARGETED ANALYSIS FOR FOOD AUTHENTICATION: CHALLENGES OF CHANGE

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It is scientifically agreed that non-targeted analytical methods for food and feed authentication have the potential to strengthen official control. In particular, because these methods are able to uncover unknown adulterations in addition to the detection of already known fraudulent practices. The investigation of the complete spectrum or chromatogram of a product sample in question in comparison to appropriate reference data allows its comprehensive characterisation (like a fingerprint) and enables the detection of any deviation from typical product properties.

However, the ongoing process to implement non-targeted analysis alongside targeted analysis is accompanied by various challenges throughout the entire analytical process, from sampling to data handling. From our perspective, three aspects need further attention and will be taken into account in this presentation:

A) Adulteration: Development of innovative approaches for the detection of unknown additions/anomalies,

B) Standardization & Quality Assurance: Efforts with regard to comparability and validation of fingerprinting methods, and

C) Digitalization: Creation of user-friendly solutions for data management, exchange & evaluation.

L11

DIVING INTO THE BEER METABOLOME AND DISCOVER SIGNATURES OF MATERIALS, TECHNOLOGIES AND REACTIONS

Michael Rychlik [1] *, **Stefan Pieczonka** [1], **Philippe Schmitt-Kopplin** [1]

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* *E-mail: michael.rychlik@tum.de*

The last years have seen a tremendous development all fields within food analysis and the generic field of foodomics [1]. In particular for food metabolomics, the number of identified and quantified metabolites has dramatically increased [2]. Therefore, metabolomics is a promising concept to unravel the complex metabolome of beers.

In this study, the compositional space of a diverse set of beer samples is uncovered by a single analytical approach using direct injection Fourier Transform Ion Cyclotron Mass Spectrometry (FTICR-MS) for the first time. The unrivaled resolution on mass measurements combined with mass accuracy and compositional networks uncovers and assigns structural information to thousands of yet unknown metabolites in the beer matrix [3]. Multiple statistical models enable the assignment of different molecular fingerprints to certain beer attributes such as the beer type, the grain used, the use of specialty dark malts or the type of fermentation. The annotation of sum formulae provides information in excess of the m/z-space and reveals the nature of discriminating features as beers from barley, wheat, rice and corn can be differentiated from each other by sets of discriminating markers [4]. For instance, benzoxazinoid hexosides deriving from the wheat's secondary metabolism are uncovered as significant markers for the use of whole wheat grains, which raises the potential of FTICR-MS for quality control and inspection purposes. The detection of fingerprints for light versus dark and top versus bottom fermented beers reinforces the role of FTICR-MS in fundamental studies revealing Maillard reaction patterns [5].

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L12

ALTERNATIVE PROTEINS FOR CONVENTIONAL ANIMAL PRODUCTS IN CHINA: REGULATORY PROCESS

Yongning Wu [1] *

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The globe demand for protein is changing, creating opportunities in the agricultural and food market for several alternative sources of protein s such as cell-based meat and plant-based meat, as well as fermentation protein bases meat. The presentation will address the range of alternative proteins from perspective of science, food safety, technology and regulatory aspects. It offers an opportunity to discuss the novel technology of plant-base and cultivated meat. With the proliferation of new alternative proteins, food safety authorities need to be prepared to regulate new food categories. Understanding the technology and the process behind the alternative proteins production is essential to create regulation that will protect the safety of consumers and will allow them to make choices.

L13

WINE VARIETAL IDENTIFICATION: SOLUTION OF AN UNEASY TASK

Leos Uttl [1] *, **Kamila Bechynska** [1], **Vaclav Kadlec** [1], **Zbynek Dzuman** [1], **Mona Ehlers** [2], **Carsten Fauhl-Hassek** [2], **Jana Hajslova** [1]

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One of the major challenges in wine analysis [1] is authentication of grape variety from which the wine is produced. Here, we have developed and validated an authentication method based on metabolomic fingerprinting, using ultra-high-performance liquid chromatography coupled with quadrupole orbitrap high resolution mass spectrometry (U-HPLC-HRMS/MS). In total, 101 red and 97 white wines, five varieties in each group (all authentic), were analysed within our study. Filtered samples, without any other processing, were directly injected into system. After the data mining and data pre-treatment steps, principal component analysis (PCA) was used to explore the data structure. The obtained unsupervised PCA models revealed a notable clustering according to the grape varieties. Subsequently, orthogonal partial least squares discriminant analysis (OPLS-DA) was used to create supervised binary models. To obtain the best models possible, an in-house R script for optimization of data filtration parameters was developed and implemented. From over 85 000 models calculated, those with the highest prediction abilities were chosen, validated, and arranged into a Rooted Binary Decision Directed Acyclic Graph (RBDDAG), which was used for wine variety authentication. In case of white wines, 96 % of samples in positive (ESI+) and 94 % of samples in negative ionization mode (ESI-) were correctly classified. Regarding red wines, 95 % of samples in ESI+ and 94 % of samples in ESI- were correctly classified. Worth mentioning that the aforementioned accuracies are calculated for the whole RBDDAG structure. Multiple individual binary models achieved prediction ability as high as 100%, however, for some of the binary models present in the RBDDAG structure, correct classification of the grape variety appeared to be more problematic due to a higher genetic (and therefore metabolomic) similarity between varieties. The results obtained within our study indicate the potential suitability of the developed method for official control purposes.

References:

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L14

THE STORY OF A LEAF: A 2-TIERED SYSTEM FOR TEA AUTHENTICITY

Di Wu [1] *, Chris Elliott [1], Yicong Li [1]

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Tea is the world's most popular beverage and have been traded worldwide for centuries, with an annual market worth $200 Bn (2019) with >10% growth rate. Its difference in geographic origin, quality, and taste leads to a huge variance in its price (With more than >50 folds for certain GI products). Recent studies and reports have also revealed the potential fraud issues in developing countries and tea extract drinks. The vulnerability of the global tea supply chain and its safeness have therefore become as major concerns for consumers and technical challenges towards regulation inspections. As an extension and forward program for EU-China collaboration schemes, we aim to develop a 2-Tiered analytical toolbox under the global network and platform of IGFS and integrate with artificial intelligence and machine learning to enhance its performance. Eventually to provide solutions for end users of deferent application levels.

L15

FOOD AUTHENTICITY FROM A REGULATORY SCIENCE PERSPECTIVE

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The fight against food fraud has been explicitly mentioned in the European Green Deal as a policy priority ('… actions to combat food fraud, including strengthening enforcement and investigative capacity at EU level…'). International collaboration on food safety research is already well established, while for food authenticity this is not yet the case. Therefore, the fight against food fraud calls for an international and systemic approach involving cooperation and consultation among all stakeholders at all levels of the food chain. There is a great need for international harmonization in order to be able to detect and, what is more important, prevent or at least minimize fraud. To bridge this gap and support European Commission services regulating the feed-food chain as well as Member States authorities, the EC Knowledge Centre for Food Fraud and Quality was created and installed at the Joint Research Centre. The main remit of its operation is to provide validated knowledge for addressing the issue in a holistic manner, such as the design principles of early warning systems, horizon scans, vulnerability assessment tools and appropriate analytical methods, which are among the critical elements for equipping regulatory agencies as well as industry in the fight against food fraud.

L16

COMPARISON OF ANALYTICAL METHODS AND RESULTS: "DEVIL IS IN THE DETAILS"

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When comparing analytical methods, even small, seemingly insignificant details or parameters may have considerable impact on the reported results. Official or standard methods try to address these issues but their implementation might not be easy or practical if there are too prescriptive in terms of the employed equipment or products. Therefore, a balancing act is needed to allow the use of equivalent instruments or items, without significantly affecting the method performance and results. System suitability and data acceptability criteria are very important in that respect in addition to highlighting critical method steps, parameters or issues, such as potential interferences.

This presentation will explore various examples of details, method parameters and analytical approaches that could play an important role in the overall analysis and lead to differences in analytical results. For instance, many details should be considered in the initial preparation of the received samples, which is commonly a critical step in the overall process, yet often only marginally described in the actual methods. The use of mass spectrometry for analyte detection reduced the need for highly optimized chromatographic separations and opened door to faster analytical runs, but there are cases where chromatographic resolution of certain peaks (may not be only our target analytes) are important for accurate results even when mass spectrometric detection is used. And details behind calibration approaches or the way that the result is expressed as represent another set of examples of potential pitfalls that could be encountered in the analytical practice.

L17

SCIENTIFIC AND REGULATORY CHALLENGES AND DEVELOPMENTS FOR EU REFERENCE LABORATORIES IN FOOD SAFETY AREAS

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After the food incidents of the 90's the European Commission adopted the General Food Law, GFL (Regulation (EC) No 178/2002) setting the general principles, requirements and procedures related to all stages of food and feed production and distribution. Many legal acts were regularly adopted, setting for example new maximum limits for substances in various food or feed commodities. While the GFL is still relevant twenty years later, it needs to address better new challenges and issues such as food sustainability, novel foods, nutrition labelling or recycling of food contact materials. How will this impact our analytical work? Concrete examples from several EURLs will be presented and discussed.

L18

TRANSITION TO A CIRCULAR ECONOMY: ANALYTICAL CHALLENGES FOR CONTAMINANTS IN THE FOOD CHAIN

Stefan van Leeuwen [1] *

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The circular economy rapidly develops in all parts of society, and the need to go circular is also expressed for food and feed production. At national and international level numerous initiatives towards the circular economy are established, both at the policy (e.g. EU's Green Deal), research and technology level. However, the food safety in a circular economy -crucial for the societal acceptance- does not receive the required attention yet. There are several examples where hazardous chemical substances show up in circular products, such as food and feed, but also in food contact materials like plastics. These substances may be present from previous applications, or generated during the recycling process. Clearly, there is a need to address the safety by state-of-the-art chemical analysis to unravel new contaminant sources, to determine exposure levels and support effective circular economy policies in the food chain. The aim of this talk is to demonstrate some examples of safety issues in the circular food production chains, and provide examples of testing strategies that can adequately address the needs for safety testing in these circular agrochains. Analytical challenges will be addressed and some examples will be provided where food safety is compromised by contaminants in circular food production.

L19

SMARTPHONE-BASED PESTICIDE RESIDUE SCREENING: GOALS ACHIEVED & CHALLENGES TO BE FACED

Aristeidis S. Tsagkaris [1]*, **Jana Pulkrabova** [1], **Jana Hajslova** [1]

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The ever-increasing demand for food production, unfortunately, still requires a widespread use of pesticides to prevent pests and boost agricultural productivity. Among them, carbamate (CM) and organophosphate (OP) insecticides are widely applied due to their global availability as well as their minimum environmental persistence. Nevertheless, CMs and OPs show relatively high acute toxicity and their residues in food may result in chronic or even acute toxicity incidents. The toxicity of CMs and OPs arises from the inhibition of cholinesterases, a vital enzyme family in the neural system of insects and mammals including humans. To monitor pesticide residues, chromatographic methods are predominantly utilized. Although they provide selectivity, low limits of detection (LODs) and wide linear ranges, chromatographic methods are also costly and time-consuming requiring highly skilled personnel. To counter these limitations and provide an innovative solution as part of the EU-funded "FoodSmartphone" project, we have been working on a novel approach for CM and OP screening, which combined enzyme recognition to smartphones and 3D-printing technology.

Briefly, acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) assays with smartphone readout were developed and validated in various matrices including fruits, vegetables and human serum. In the first case, the assays can be used for rapid (within 10 min) OP and CM screening utilizing an in-house lab-on-a-chip (LOC) prototype device with certain autonomous features. In detail, *(i)* samples and reagents can be injected using silicone finger pumps eliminating the need of pipettes; *(ii)* acceptance/rejection of each measurement based on its dynamic response using a principal component analysis (PCA) of smartphone-generated data. The cost per prototype was estimated about 0.30 € and the attained detectability (LOD=0.050 mg kg^{-1} for carbofuran) was enough to monitor highly contaminated samples as those reported in the EU Rapid Rapid Alert System for Food and Feed (RASFF). Regarding the application in human serum samples, acute intoxication incidents due to neurotoxic OP insecticides have been occasionally reported. To enable rapid monitoring at an early intoxication stage, a microfluidic paper-based analytical device (µPAD) able to screen for chlorpyrifos-oxon, the toxic chlorpyrifos metabolite was developed. Impressively, the µPAD was pocket-size, cost-efficient (0.70 € per device), required minimal sample preparation (just a sample dilution) and attained robust results.

Undoubtedly the above-mentioned achievements significantly progressed the field, however, there are still challenges that need to be faced. Firstly, the use of multistep lab-based sample preparation protocols remains a bottleneck reducing the portability potential of smartphone-based methods. Another aspect that can significantly improve the current status is the development of smartphone apps for a specific assay providing real-time "one-click" results. Last but not least, large scale commercialization of smartphone-based methods will be achieved only if the result interphone variation will be adjusted. All in all, within this project, a paradigm shift towards portable food contaminant analysis has been initiated and at-home analysis can be realistically considered in the upcoming years.

L20

DETERMINING THE SOURCE OF OUR SOYA USING AN ANALYTICAL TOOLBOX

Brain Quinn, Yunhe Hong, Chris Elliott [1] *

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Food fraud is a growing and the problem for consumers, the food industry and regulators. Criminals will exploit any opportunity to gain economic advantages by cheating on the way that food is produced and false claims made about it. A new opportunity is emerging for fraudsters in terms of the strong desire of consumers to purchase sustainable food. This is turn has put pressure on the markets to deliver this. One of the most controversial crops harvested in the world is soya but to the strong links it has with sustainability and rainforest destruction. Many claims are now being made that soya being sold into the markets is sustainable yet data would show that only about 25% of the world's production is sustainably produced. A major research project is now underway to determine the origin of soya being sold into the markets in terms of the country and region of the country the soya was grown. In addition evidence of the soya being grown on recently deforested land will be sought. A wide range of analytical tools will be employed in the project provided as part of the Agilent Thought Leaders award made to the Institute for Global Food Security.

PROGRAM: Vendor webinars

November 3, 2021

9:00-9:45 (CET)

LECO EMPOWERING RESULTS	Multiple Analytical Challenges for Food Safety Laboratories - Solved by One Solution
phenomenex ...breaking with tradition	Advances in GC Column Selectivity for Fast Analysis of PAH, PCBs, Dioxins in Food Sample
RESTEK Pure Chromatography	New Concepts to Speed up Pesticides Residue Analysis

10:00-10:45 (CET)

Agilent Trusted Answers	From Research to Routine - Analysis of Titanium Dioxide Nanoparticles in Food by Single Particle ICP-MS
SepSolve Analytical	Uncovering Chemical Markers of Food Quality and Authenticity
SHIMADZU Excellence in Science	Pitfalls in the Analysis of Mineral Oil Residues in Food
ThermoFisher SCIENTIFIC	Toxicity and Authenticity Testing of Foods with Trace Elemental and Stable Isotope Analysis

11:00-11:45 (CET)

Agilent Trusted Answers	Analysis of Ethylene Oxide and 2-Chloroethanol Residues in Sesame and Other Food Commodities by GCMS/MS
AXELSEMRAU	Automated Solutions for the Analysis of MOSH/MOAH and Mycotoxins in Food
SCIEX The Power of Precision	Advancements for Food and Environmental Testing with the ZenoTOF 7600 System
ThermoFisher SCIENTIFIC	How PCR Has Revolutionized Food Testing?

12:00-12:45 (CET)

Agilent Trusted Answers	A Novel Workflow to Determine over 1000 Pesticide Residues in Compliance with SANTE 12682/2019 Guidelines in Various Food Matrices
PerkinElmer For the Better	PerkinElmer Technologies for Food Testing: Advancement in the Determination and Confirmatory Analysis of PFAS in Food Matrices Using QSight LC/MS/MS

November 4, 2021

13:30-14:15 (CET)

BÜCHI SWITZERLAND	How to Boost Efficiency in Nitrogen Analysis – Kjeldahl Masterclass for Food Samples
syft Technologies GmbH	High-Throughput Analysis of Freshness Markers in Various Food Samples by SIFT-MS
r-biopharm	Sample Preparation & Quality Assurance Tools for Mycotoxin Analysis
Waters THE SCIENCE OF WHAT'S POSSIBLE.™	Waters Presents Our Recent Advances in Food Analysis at RAFA 2021: A simple, easy, and efficient way to process and review data for large multi residue methods using the MS Quan app within the new waters_connect software

14:30-15:15 (CET)

Agilent Trusted Answers	Per- and Polyfluoroalkyl Substances (PFAS): Analytical Strategies to Identify and Quantify the Next Emerging Contaminant in Food & Beverage
BRUKER	Use timsTOF Ion Mobility Technology to Improve Results in Food Analysis
RESTEK Pure Chromatography	New Methods Targeting Emerging Food Contact Materials

15:30-16:15 (CET)

MILESTONE HELPING CHEMISTS	Microwave Assisted Solvent Extraction: A Powerful Tool to Tackle Sample Preparation Challenges
ThermoFisher SCIENTIFIC	Taking Advantage of the Latest Developments in GC- and LC- High Resolution Accurate Mass MS for Both Quantitative and Non-Target Analysis in Food Safety
Waters THE SCIENCE OF WHAT'S POSSIBLE.™	Waters Presents Our Recent Advances in Food Analysis at RAFA 2021: Enhancing analysis of foods using the ACQUITY™ Premier solution, Vitamin B, Organic Acids and beyond

16:30-17:15 (CET)

phenomenex® ...breaking with tradition℠	Analysis of PFAS Compounds from Food and Food Contact Material

17:30-18:15 (CET)

phenomenex® ...breaking with tradition℠	Determination of Ionic Pesticides, Chlorate and Perchlorate in Various Food Matrices

November 3, 2021 (9:00–9:45, CET)

VENDOR WEBINAR:

Multiple Analytical Challenges for Food Safety Laboratories - Solved by One Solution

Multiple Analytical Challenges for Food Safety Laboratories - Solved by One Solution

Tomáš Kovalczuk[1], Nick Jones[1], Sebastiano Panto[1], Michal Stupák[2], Giorgia Purcaro[3]

[1] LECO European Application and Technology Center Biotechpark, Berlin, Germany
[2] University of Chemistry and Technology, Prague, Faculty of Food and Biochemical Technology, Department of Food Analysis and Nutrition, Prague, Czech Republic
[3] University of Liege, Gembloux Agro-Biotech, Belgium

The trend of the last decade in analytical chemistry is clear – to analyze as many analytes as possible in a single run, utilizing a fast and simple sample preparation step. This demand using modern analytical instrumentation is desired to significantly boost both (i) sample throughput together with (ii) sensitivity – This has shaped the analytical strategies of the last decade.

The routine workflows of today in food safety labs provide a variety of challenges. Although, the analytical approaches are fully validated and greatly optimized, issues related to sample preparation, sample introduction and/or analyte determinations can often be observed, typically due to sample matrix complexity.

The Time-of-flight mass spectrometers (TOF MS) offering the advantages of (i) full mass spectral information collected at fast acquisition rates, across wide concentration ranges, (ii) non-skewed high-quality spectra for each individual analyte and (iii) high level of data robustness due to a unique "open-source design" enabling significantly reduced maintenance/instrument downtime needed for source cleaning.

The comprehensive two-dimensional gas chromatography (GC×GC) offers dramatic improvements over traditional GC, especially in the analysis of complex mixtures. This is due to significantly increased chromatographic resolution and improved analytes' detectability.

A hyphenation of TOF MS with GCxGC is an ideal solution for challenging applications in offering all the benefits of GCxGC and TOF MS techniques. All the benefits of both hyphenated techniques can be only fully utilized when an appropriate data processing software is employed.

All these advantages will be demonstrated in this webinar, summarizing the use of LECO's BT4D GCxGC-TOF MS system in challenging food applications, such as:

- MOSH/MOAH
- Pesticides is difficult matrices
- Ethylene oxide

November 3, 2021 (9:00–9:45, CET)

VENDOR WEBINAR:

Advances in GC Column Selectivity for Fast Analysis of PAH, PCBs, Dioxins in Food Sample

Advances in GC Column Selectivity for Fast Analysis of PAH, PCBs, Dioxins in Food Sample

Ramkumar Dhandapani, Ph.D.

Modern regulations emphasize analytical methods capable of separating critical analyte pairs, for identification as well as quantitation. In order to meet separation goals and to exceed regulatory requirements, new and unique gas chromatography (GC) column selectivities are now essential. In this presentation, we will explore advances in GC column selectivity and method development tips that help provide solutions to challenging chromatographic problems in food analysis. A variety of important Persistent organic pollutants like PAH, PCBs, Dioxins will be explored in this presentation. In addition to method optimization tips and tricks, fast and high throughput analysis, critical pair separation, robustness with dirty samples will be explored for each class of POPs.

November 3, 2021 (9:00-9:45, CET)

RESTEK
Pure Chromatography

VENDOR WEBINAR:

New Concepts to Speed up Pesticides Residue Analysis

Low Pressure GC – InLine Sample Preparation – Fast Polar Pesticide Analysis

Jaap de Zeeuw, Restek Netherlands
Jan Pschierer, Restek Germany
Emanuele Ceccon, Restek Italy

Jaap de Zeeuw from Restek Netherlands is going to report about a new concept for speeding up GC-MS analysis of Pesticides residue analysis, using short 0.53mm capillary columns (directly connected at the MS inlet), connected to a restriction column at the inlet, enabling a high vacuum inside the 0.53mm analytical column. The technique is known as LPGC (Low Pressure Gas Chromatography) or sometimes called "Vacuum GC". Under the conditions created, very fast separations were performed as the optimal carrier gas velocity is a function of the actual pressure inside the capillary, and typically 3x shorter run times are obtained by using this concept in Pesticides residue analysis.

Jan Pschierer from Restek Germany is going to report about Restek Revive ILSP – a new method for an automated removal of matrix components for the analysis of residual pesticides. Revive ILSP selectively retains matrix components from the sample extract and can be utilized as a standalone workflow or integrated into an existing QuEChERS workflow. ILSP was applied to multiple challenging commodities representing a wide range of compositions for the analysis of 61 pesticides.

Emanuele Ceccon from Restek Italy is going to report about a new Hybrid phase, optimized for small screening methods for polar pesticides, without having the disadvantages of HILIC methods. Such a small screening method for ESI negative polar Pesticides was recently added to the QuPPe panel of the European Reference Lab. But the potential of this phase is beyond this, also solving short chain PFAS and underivatized Amino Acid Analysis issues.

November 3, 2021 (10:00–10:45, CET)

Agilent

Trusted Answers

VENDOR WEBINAR:

From Research to Routine - Analysis of Titanium Dioxide Nanoparticles in Food by Single Particle ICP-MS

From Research to Routine - Analysis of Titanium Dioxide Nanoparticles in Food by Single Particle ICP-MS

Katrin Loeschner, Associate Professor, National Food Institute, Technical University of Denmark

The food color E171 (titanium dioxide) is known to contain a fraction of nanoparticles and has been investigated both, in the context of labelling of food for the content of engineered nanomaterials as ingredients and in the context of risk assessment.

It was recently decided to ban the use of E171 in Europe. A single particle ICP-MS method was developed for the determination and characterization of TiO_2 NPs in foods based on ICP-MS/MS. To check the effectiveness of the method, two different TiO_2 NPs were spiked to milk.

The method was further tested in a study that compared the performances of both high-resolution ICP-MS and ICP-MS/MS in single-particle mode for characterization of TiO_2 NPs in food. Finally, the method was applied in an interlaboratory study among seven experienced European food control and food research laboratories.

November 3, 2021 (10:00–10:45, CET)

SepSolve Analytical

VENDOR WEBINAR:

Uncovering Chemical Markers of Food Quality and Authenticity

Finding the needle in the haystack: Non-target GC×GC–TOF MS workflows for food quality and authenticity evaluation

Dr. Laura McGregor, SepSolve Analytical, UK

Reliable analysis of foods and beverages is vital for quality control, new product development and in authenticity studies.

In this presentation, we will describe the use of automated sample extraction and enrichment combined with GC×GC–TOF MS for comprehensive non-target screening of aroma volatiles from food and beverages.

Additionally, we will demonstrate the use of simple data analysis workflows to automatically discover significant differences between complex aroma profiles and allow meaningful conclusions to be drawn in quality and authenticity studies.

Comprehensive volatilome profiling by TD–GC×GC–TOF MS for the determination of fruit quality

Dr. Natasha Spadafora, University of Calabria, Italy

The fruit quality (FRUITY) project aims to provide new predictive technologies and a better understanding of physiological changes in fruit for objective quality assessment of fruit quality during post-harvest storage.

The project uses a multi-trait approach - including sensory profiling, monitoring of the volatile organic compounds (VOCs) produced by the fruit and investigation of biochemical reactions - with the overall goal of providing the industry with diagnostic kits for the evaluation of fruit quality during post-harvest storage

In this presentation, we will focus on the VOC profiles from peach cultivars. Here, the enhanced separation and high sensitivity of TD–GC×GC–TOF MS enabled 115 VOCs to be identified, 15 of which were used to distinguish between the peach cultivars. We will also show how individual cultivars reacted differently to cold storage, with different changes in VOC profiles seen after seven days of storage (the typical time taken for shipping from southern Italy to northern Europe).

November 3, 2021 (10:00–10:45, CET)

SHIMADZU
Excellence in Science

VENDOR WEBINAR:

Pitfalls in the Analysis of Mineral Oil Residues in Food

Pitfalls in the Analysis of Mineral Oil Residues in Food

Andrea Hochegger, Claudia Koraimann, Erich Leitner
TU Graz, Institute of Analytical Chemistry and Food Chemistry, Graz, Austria

The discussion on mineral oil hydrocarbons (MOH; divided into mineral oil saturated hydrocarbons (MOSH) and mineral oil aromatic hydrocarbons (MOAH) started already in the 1990's when publications reported the possible migration from a food contact material into the packed good. The debate on those findings broadened afterwards and is continuing till today, dealing with the still remaining knowledge gaps of analysis, exposure assessment, hazard characterisation and risk assessment[1,2].

This talk will focus on mainly on the still present pitfalls of the analysis. Although there had been significant advancements, the analysis is still a huge challenge. There is a lack of validated and standardized analytical methods for the whole sample preparation procedure to allow generation of reliable occurrence data for the complex and highly variable matrix "food". State-of-the-art analysis is done using the online-coupling of LC-GC-FID, but analysis reveals only unresolved humps with unknown origin. Therefore, confirmatory techniques using multi-dimensional chromatography, e.g. 2D-comprehensvie GC×GC with various detector types, are used to allow for an adequate substance class identification, recognition of false-positive values and therefore correct quantification of the generated humps. Furthermore, toxicological studies on the identified individual substance classes are needed to fully understand and allow for the health risk assessment for consumers[3].

References:
[1] https://doi.org/10.2903/j.efsa.2012.2704
[2] https://doi.org/10.1021/jf901375e
[3] https://doi.org/10.1016/j.tifs.2021.03.021

November 3, 2021 (10:00–10:45, CET)

ThermoFisher SCIENTIFIC

VENDOR WEBINAR:

Toxicity and Authenticity Testing of Foods with Trace Elemental and Stable Isotope Analysis

Using triple quadrupole ICP-MS to improve the speed, sensitivity, and accuracy of the analysis of toxic and nutritional elements in baby foods

Dr. Sukanya Sengupta, Application Specialist, Thermo Fisher Scientific

Food and food supplements supply the human body not only with energy, but also essential macro- and micronutrients for a long and healthy life. While several elements are essential nutritional building blocks, exposure to heavy metals, like arsenic, mercury, and lead, potentially present in food as contaminants may lead to serious negative effects on health. An especially vulnerable group susceptible to different illnesses and potential lifelong neurological damage through exposure to toxic heavy metals are infants and young children. In this presentation we are going present a simple and fast analytical method based on the combination of triple quadrupole ICP-MS with oxygen as the only collision / reaction cell gas used for highly accurate and sensitive analysis of both nutritional and toxic elements in different types of baby foods.

Addressing authenticity of fish oils by online coupling of GC-IRMS with an organic mass spectrometer

Dr. David Psomiadis, Chief Business Officer, Imprint Analytics GmbH
Dr. Mario Tuthorn, Senior Product Marketing Specialist, Thermo Fisher Scientific

As fish oils become a popular and precious source of omega-3 fatty acids, the risk of mislabeling and adulteration has risen significantly. The fatty acid profiles of different fish oils do not often allow the discrimination between different sources and geographical origins. In this study, the compound specific multi-isotope analysis of fatty acids allowed the discrimination of fish oils from different provenance, following risk-based comparisons from market experience. In the light of emerging cases of food fraud, we present how GC-MS-IRMS advanced technology can tackle these problems for addressing authenticity of fish oils.

November 3, 2021 (11:00–11:45, CET)

Agilent

Trusted Answers

VENDOR WEBINAR:

Analysis of Ethylene Oxide and 2-Chloroethanol Residues in Sesame and Other Food Commodities by GCMS/MS

Analysis of Ethylene Oxide and 2-Chloroethanol Residues in Sesame and Other Food Commodities by GCMS/MS

Tatiana Cucu, PhD, Senior Scientist/Project Manager, Research Institute for Chromatography (RIC Group), Kortrijk, Belgium

The unauthorized presence of ethylene oxide (ETO) and 2-chloroethanol (2CE) in food is a new emerging food safety issue. To ensure that foods are safe for consumption, food industry and enforcement agencies need reliable and robust methods. For their determination a combination of a QuEChERS sample preparation method and a GC-MS/MS analytical method was proposed by the EU Reference Laboratories for Residues of Pesticides. However, several challenges are encountered when it comes to the analysis of ETO and 2CE. QuEChERS extracts often contain high amounts of non-volatile material which can accumulate in the inlet liner and column, affecting the accuracy and robustness of the analysis. Integration of the Automated Liner Exchange (ALEX) option and pre-column backflush allows to perform analysis of ETO and 2CE with minimal downtime related to inlet maintenance, frequent analytical column exchange or source maintenance.

November 3, 2021 (11:00–11:45, CET)

AXELSEMRAU

VENDOR WEBINAR:

Automated Solutions for the Analysis of MOSH/MOAH and Mycotoxins in Food

Development & Advances for MOSH MOAH Analytics

Michael Koch, IKB/ Institute Kirchhoff Berlin part of Mérieux NutriSciences, Berlin, Germany

Saturated and aromatic hydrocarbons, the so-called "MOSH MOAH contaminants", have been the focus of sustained public interest for some time. These contaminants are now considered undesirable in food, consumer goods and cosmetics. As a result, a relevant analytical test point has been established and manifested. The basic method for this was published in 2017 in the form of EN method 16995. With this method, it is possible to analyse MOSH/MOAH in vegetable oils and foods based on vegetable oils with the LOQ of 10 mg/kg. Then, in December 2020, a new standard method (DGF C-VI 22 (20)) was established by the German Society for Fat Science (DGF), based on an extensive interlaboratory comparison and proficiency test. With this method, an LOQ of 1 mg/kg can be achieved. Two main techniques have been established for routine practice. First, that always preceding online LCGC/FID test method for indexing and quantification. The other is the GCxGC/TOF-MS technique, which is used in the event of a positive finding via the LCGC/FID procedure. This technique verifies the findings for marker compounds as well as confirmed or false positive. In addition, this analytical system allows the characterization of the sample components. In order to be able to make a qualified and profound statement with both technical procedures, it is essential and important to carry out the sample preparation steps relevantly, precisely and with high quality. With the development of analytical methods and the corresponding automation of the various work steps, there is a strong interest in constantly optimizing these individual steps as well as the entire workflow.

In this short lecture, the effects of application and technical innovations in terms of optimization on analytics will be highlighted. Case studies on the matrices edible oils, chocolate products & milk powder will show potential advances. Specifically, the focus will be on a new, m-cpba-free epoxidation process and the current generation of GCxGC/TOF-MS measurement technology.

A New Online System for the Analysis of Mycotoxins in Food

Elizabeth Manning, International Sales & Business Development Manager, R-Biopharm Rhône Ltd

Busy laboratories with high numbers of analyses to perform (greater than 10 analyses per day) are often under pressure to provide results sooner for their customer or for internal release of manufacturing produce. This can lead to mistakes at the bench resulting in reduced quality and performance of analysis. Laboratories are often tasked to improve efficiency without increasing headcount or reducing the quality of results and putting additional pressure on staff and resources
The benefits of the new CHRONECT Symbiosis RIDA®CREST system, a fully automated clean up system which uses IMMUNOPREP® ONLINE affinity cartridges for testing a range of mycotoxins from sample extraction to final detection. The system offers a front-end solution with a versatile software - CHRONOS Symbiosis which is compatible with the majority of mainstream detector systems including FLD, UV and mass spectrometry. CHRONOS organises processes in parallel and combines sample preparation and analysis in one user interface providing results sooner. Different modules can be selected to meet the requirements of any busy laboratory. Each affinity cartridge is suitable for up to 15 analyses, saving space and offering the possibility to include a QC check or sample blank to meet the strictest accreditation standards. The system with IMMUNOPREP®ONLINE affinity cartridges is shown to remove sample interference leading to improved chromatography and better sensitivity. Previous manual steps are precisely controlled decreasing analytical error and significantly reducing data variability leading to improved performance and greater laboratory efficiency.

The new system CHRONECT Symbiosis RIDA®CREST has been tested using methods for Aflatoxin and Ochratoxin A meeting performance requirements recommended by CEN and AOAC.

November 3, 2021 (11:00–11:45, CET)

The Power of Precision

VENDOR WEBINAR:

Advancements for Food and Environmental Testing with the ZenoTOF 7600 System

Advancements for food and environmental testing with the ZenoTOF 7600 system

Daniel McMillan, Snr. Market Development Manager, Food and Environmental, SCIEX

The ever-growing global demand for food supply has led farmers and producers to focus on optimizing yields, frequently using pesticides and other synthetic chemicals, which will unavoidably end up in the food chain. In order to ensure consumer safety and food integrity, testing for adherence to regional and international requirements is necessary to monitor for chemical residues, including pesticides in addition to natural fungal toxins and microbiological hazards. Traditionally, residue analysis has been performed by triple quadrupole mass spectrometry, due to its sensitivity and quantitative power, and most food laboratories are accustomed to the ease of use and high performance of such instruments. Accurate mass instruments can offer additional levels of confirmation; however, they have traditionally suffered from a lack of sensitivity and precision, especially when performing MS/MS experiments to meet the testing requirements for the regulatory guidelines. The new ZenoTOF 7600 system is set to remove these limitations and open up the technique to labs wishing to increase coverage and confidence in food testing.

This webinar will cover:

- Novel MS technologies to elevate accurate mass sensitivity for MS/MS
- The potential of a new fragmentation option for confirmation and identification
- Examples of the application to pesticide residue screening and confirmation

November 3, 2021 (11:00–11:45, CET)

ThermoFisher SCIENTIFIC

VENDOR WEBINAR:

How PCR Has Revolutionized Food Testing?

How PCR has revolutionized food testing?

Sandra Fréville - Regional Tactical Manager Microbiology - Industries, Thermo Fisher Scientific
Paul In't Veld - Senior Scientist, Netherlands Food and Consumer Product Safety Authority

More than 35 years ago now, the first Polymerase Chain Reaction (PCR) has been successfully experimented. This discovery has been the starting point of a fantastic revolution in the world of analytical testing. From R&D to routine analysis, PCR is now, and especially since the world is facing the COVID pandemic crisis, an unavoidable master piece of molecular diagnostic testing in all laboratories. In this interactive webinar, our experts will highlight how PCR especially revolutionized the food testing world. Sandra Fréville, Marketing Tactical Manager at Thermo Fisher Scientific will focus on major PCR technologies applied to food testing which guarantee high reliability and continuous access to the benefits of cutting-edge technology. An exclusive interview of Paul In't Veld, Senior Scientist at Netherlands Food and Safety Authority, about this revolution to meet the routine testing, standardization and regulations requirements applied to pathogen food testing, will be also presented.

November 3, 2021 (12:00–12:45, CET)

Agilent

Trusted Answers

VENDOR WEBINAR:

A Novel Workflow to Determine over 1000 Pesticide Residues in Compliance with SANTE 12682/2019 Guidelines in Various Food Matrices

A Novel Workflow to Determine over 1000 Pesticide Residues in Compliance with SANTE 12682/2019 Guidelines in Various Food Matrices

Marcus Chadha, Applications Specialist, Agilent Technologies, Cheadle, UK

In Europe, pesticide testing laboratories adhere to the SANTE 12682/2019 guidelines pertaining to the maximum residue level (MRL) legally permitted in or on food or animal feed. Ensuring that foods are free of pesticide residue contamination can involve multiple analytical approaches and heavy technician workloads. Both lead to high operating costs and slow turnaround times. We present a comprehensive, joint LC-MS and GC-MS workflow for the simultaneous quantitation of >1000 pesticide residues in fruits and cereals of varying water and fat content. Details of sample preparation procedures and instrumentation set up will be discussed in conjunction with the data analysis parameters enabling the quantification and confirmation of pesticide residues according to the SANTE 12682/2019 guidelines.

November 3, 2021 (12:00–12:45, CET)

VENDOR WEBINAR:

PerkinElmer Technologies for Food Testing: Advancement in the Determination and Confirmatory Analysis of PFAS in Food Matrices Using QSight LC/MS/MS

Advancement in the determination and confirmatory analysis of PFAS in food matrices using QSight LC/MS/MS

Prof. Ovokeroye A. Abafe, PhD, Agricultural Research Council-OVR, Residue Analysis Laboratory, Pretoria, South Africa
Dr. Ignazio Garaguso, Sr. Principal Regional Segment Leader, Germany, PerkinElmer

Per- and polyfluoroalkyl substances (PFAS) are classified as persistent organic pollutants that are resistant to biodegradation, with half-lives of over fifteen years in humans. Human exposure to these compounds through ingestion, inhalation and dermal contact has been linked to cancer, dermal allergies, low infant birth weight, infertility and increased risks of obesity, among others. Challenges in the analysis of PFAS in biological matrices have been widely reported in the literature.

In this webinar Prof. Abafe will share recent results of his works on the development and validation of sensitive methods for determination and unambiguous confirmation of residues of PFAS in breastmilk, retail milk, infant formulas and human serum. The methods developed demonstrate good linearity, high recovery with acceptable matrix effects and were validated in accordance to the requirements of Commission Decision 657/2002/EC with slight modifications.

November 4, 2021 (13:30–14:15, CET)

VENDOR WEBINAR:

How to Boost Efficiency in Nitrogen Analysis – Kjeldahl Masterclass for Food Samples

How to boost efficiency in Nitrogen analysis – Kjeldahl Masterclass for food samples

Mr. Res Odermatt, Product Manager Kjeldahl Solutions
Mr. Eduard Wiedenbeck, Product Manager Kjeldahl Solutions

Journey through the latest Kjeldahl workflow:

- Sample homogeneity makes the difference
- Digestion secrets unveiled
- State of the art steam distillation
    - Pains and gains
    - Efficiency booster: Reaction detection sensor
    - Automation possibilities

November 4, 2021 (13:30–14:15, CET)

VENDOR WEBINAR:

High-Throughput Analysis of Freshness Markers in Various Food Samples by SIFT-MS

High-Throughput Analysis of Freshness Markers in Various Food Samples by SIFT-MS

A. Ingendoh[1], C. Pfaff[1], M. Perkins[2], V. Langford[3]
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[3] Syft Technologies Ltd, 68 St Asaph St, Christchurch 8011, New Zealand

Consumer acceptance and food safety are key for wholesalers and retailers of fresh fruit, vegetable, fish or meat products. Although consumers provide the ultimate feedback on quality, suitable instrument-based methods can provide rapid analysis, objectivity and low costs per sample, which are not always possible using human subjects.

During ripening, fruits emit a diverse range of low molecular weight compounds arising from various hormonal and metabolic processes. The relative abundances of these volatiles change over time and are detected, quantified and monitored in a high-throughput manner by SIFT-MS.

SIFT-MS (Selected Ion Flow Tube Mass Spectrometry) is a very rapid, direct, and sensitive technique with detection limits matching those of human olfactory system and minimal samples preparation. Therefore, it is ideal for detecting spoiling of food at an early stage and for a wide-scale and high-throughput freshness screening.

SIFT-MS uses soft, precisely controlled chemical ionisation coupled with MS detection to rapidly quantify VOC down to pptv concentrations. For this study, it was combined with a headspace autosampler (Gerstel). Since no front-end separation but a direct analysis of all samples is performed, the setup provides a robust, easy to operate solution for sensitive, quantitative screening of hundreds of samples per day.

November 4, 2021 (13:30–14:15, CET)

VENDOR WEBINAR:

Sample Preparation & Quality Assurance Tools for Mycotoxin Analysis

Sample preparation & quality assurance tools for mycotoxin analysis

Carrie Maune, Trilogy Analytical Laboratory, USA
Ronald Niemeijer, R-Biopharm, Germany

Mycotoxin contaminations of food and feed have a huge economic impact. Mycotoxin contaminations of crops are unavoidable, but mycotoxins can be managed. During the entire process from field to food or feed critical steps can be identified to monitor mycotoxins.

It is well known that sampling plays an important role in the reliability of your result. Less well known is the influence of the sample preparation: Sample grinding and sample size may have a big effect on the variabilities in you result. We will show results from different studies with cereal samples containing Aflatoxin, DON and Zearalenone.

To eliminate matrix effects a clean-up of the sample is necessary. For some samples a simple extraction is sufficient, but for other samples solid phase extraction / immunoaffinty extraction can make a big difference.

But that is just one part of the story. You want to be sure you are making the correct decisions as well. QualiT™ is a toolbox developed by Trilogy Analytical Laboratory for quality control in mycotoxin analysis. QualiT™ offers (certified) reference materials, both as pure material and as well as naturally contaminated materials, quality control materials and analytical standards. Besides that, Trilogy offers additional useful tools for sample preparation and sample clean-up and knowledge database, collecting 20 years of experience as an (ISO 17025 accredited) food testing lab, specialised in mycotoxin, allergen mycotoxin binder testing.

November 4, 2021 (13:30–14:15, CET)

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

VENDOR WEBINAR:

Waters Presents Our Recent Advances in Food Analysis at RAFA 2021

A simple, easy, and efficient way to process and review data for large multi residue methods using the MS Quan app within the new waters_connect software

Dimple Shah, MS, Principal Scientist, Food & Environmental Business Operations, Waters Corporation

Running a targeted method for quantitation of hundreds of analytes, across many batches of different samples, presents food testing laboratories with several challenges. Issues associated with developing, managing, and curating error-free acquisition and data processing methods and the review of data can be both time-consuming and cumbersome. To help overcome these daily challenges, we are showcasing the new MS Quan app that is included within the new waters_connect software platform. We will demonstrate the usability of the software by generating a processing method from acquired data, efficiently process, and review the quantitative data with a focus on a workflow utilizing exception focused review. We will demonstrate the easy of setting up batch QC criteria such as calibration correlation, residuals, QC check, blanks, internal standard response, ion ratio and retention time tolerances, as per documented guidelines (e.g. SANTE/12682/2019) or bespoke values. A batch dashboard immediately gives the user an overview of the health of the batch and highlight potential areas that require user intervention to aid laboratory efficiency. There are many enhancements that allow users to view each chromatogram, but this is also made easier with the ability to view many chromatograms on one screen at once. Come and join use for a glimpse of this new user-friendly software.

November 4, 2021 (14:30–15:15, CET)

Agilent

Trusted Answers

VENDOR WEBINAR:

Per- and Polyfluoroalkyl Substances (PFAS): Analytical Strategies to Identify and Quantify the Next Emerging Contaminant in Food & Beverage

Per- and Polyfluoroalkyl substances (PFAS): Analytical strategies to identify and quantify the next emerging contaminant in Food & Beverage

Tarun Anumol, PhD, Director, Global Environment & Food Applied Markets, Agilent Technologies, Santa Clara, CA, USA

Per- and polyfluoroalkyl substances (PFAS) are a class of >4,000 man-made compounds used since the 1940s. However, their persistence has only recently raised concern of their presence in food & beverages. Analysis of PFAS in the sub part per billion range in foods is challenging and requires robust sample extraction, rigorous quality control to prevent background contamination and sensitive analytical approaches typically involving LC/MS. Furthermore, several of the PFAS present in food & the environment are currently unidentified and do not have analytical standards hence require high-resolution mass spectrometry techniques like quadrupole time of flight instrumentation for their analysis. This presentation will detail strategies for both targeted quantification and identification of legacy & emerging PFAS in food & beverage.

November 4, 2021 (14:30–15:15, CET)

VENDOR WEBINAR:

Use timsTOF Ion Mobility Technology to Improve Results in Food Analysis

Using VIP-HESI and Trapped Ion Mobility Spectrometry to improve confidence in identification

Dr. Carsten Baessmann, Bruker Daltonics GmbH & Co. KG, Bremen, Germany

In the past years, ion mobility has matured into an extremely valuable addition to high-resolution mass spectrometry. Trapped Ion Mobility (TIMS) technology ensures high resolution and highly accurate collisional cross section (CCS) values. Thus, this 4th dimension is able to filter out the chemical background and separate isobaric co-eluting compounds. The associated CCS values for all detected compounds can be used as an additional criteria for the identification of both knowns and unknowns. As ion mobility becomes more and more common, the number of CCS references values in libraries and databases is growing rapidly. When used in a targeted approach, as an additional criteria, CCS values help to increase the reliability of identification and reduce the number of false positives, especially speeding up the review of large sample sets. If TIMS is used in combination with the increased sensitivity obtained from a VIP-HESI source then positive identifications is possible at very low level concentrations. With a duty cycle of 100%, no changes to chromatographic gradients are required allowing this unique combination to provide analytical reporting with greater confidence.

Workflow for setting up and controlling food authenticity analysis

Noud van der Borg, Bruker Nederland BV, Leiderdorp, Netherlands

Food adulteration and authenticity has a greater interest with the public in general and developments in hardware provides better sensitivity, and more accuracy, in elucidating these topics. Historically, the complexity of the workflow made these analyses a task for specialists. However, due to developments in software workflows, 'ready-to-go' solutions have been developed to determine

authenticity markers and subsequently use them in a routine process. By having additional separation power provided by Trapped Ion Mobility Spectrometry (TIMS) and better calculation algorithms, minor differences in the food 'fingerprint' between different regions of authenticity, or lower levels of adulteration become easier to rapidly discern allowing large numbers of samples to be screened.

Positioning of high through put MALDI and high separation HRMS will be explained within this presentation.

November 4, 2021 (14:30–15:15, CET)

RESTEK
Pure Chromatography

VENDOR WEBINAR:

New Methods Targeting Emerging Food Contact Materials

New Methods Targeting Emerging Food Contact Materials: MOSH/MOAH and PFAS

Giorgia Purcaro, University of Liège, Belgium
Milica Jovanovic, Technical University Graz, Austria

Prof. Giorgia Purcaro from University of Liège is going to demonstrate the use of a comprehensive platform, namely LC-GC×GC-ToFMS/FID, for the quantitative and confirmatory analysis of MOSH and MOAH in Food samples. This platform, which is routinely used, is herein proposed for more detailed profiling of the compound distribution into the UCM and easily detect the presence of interference avoiding false positive reported due to the presence of interferences, such as terpenoids, carotenoids, and olefin, which cannot easily be detected without the use of an informative detector as MS. Potentiality and challenges will be discussed.

Mrs. Milica Jovanovic from Technical University in Graz is going to present her work about PFAS in paper cardboards as a possible source for PFAS contamination in Food. Although PFAS are not present in fresh paper fibers, they can end up in paper and board food contact materials through a recycling process. Furthermore, papers can be coated with layers containing PFAS, to increase their hydrophobicity.

In this presentation, the targeted approach for detecting and quantifying PFAS in paper and board matrices using high-performance liquid chromatography coupled with triple quadrupole mass spectrometry is shown. Additionally, we present the possible challenges associated to PFAS analysis, and potential solutions.

November 4, 2021 (15:30–16:15, CET)

MILESTONE
HELPING CHEMISTS

VENDOR WEBINAR:

Microwave Assisted Solvent Extraction: A Powerful Tool to Tackle Sample Preparation Challenges

Tackling extraction bottlenecks with microwave sample preparation
Diego Carnaroglio, PhD, Milestone Srl

Microwave assisted extraction and saponification for food quality and safety
Prof. Giorgia Purcaro, Gembloux, Agro-Bio Tech, University of Liège, Belgium

Microwave extraction in action! Live demonstration of microwave-assisted total fat determination
Roberto Boschini, MSc, Milestone Srl

Sample preparation is a routine step in many analyses, but it's often underestimated. Choosing the right sample preparation step is important, as it can prevent contamination, improve accuracy, and minimize the risk of skewing the results. Despite that, most of the methods applied to fats and oils sample preparation are still tied to traditional, time- and solvent-consuming procedures. The complexity of the food matrices led to challenging sample preparation, for example, the time-consuming saponification. Over the years traditional techniques have been improved, but they are still relying on ancient technologies, so now laboratories are seeking new approaches to ensure fast, rugged, and reproducible analysis of food.

Microwave assisted solvent extraction (MASE) and microwave assisted saponification (MAS) offer a reliable and efficient approach to sample preparation. Several processes can take advantages from microwave heating, reducing time and solvent consumption, enabling the lab to have a greener and more cost-effective approach. In this section some examples will be reported ranging from extraction of contaminants (MOAH and MOSH), to saponification and extraction of DAKs and sterols, to fatty acid methyl ester profile determination from foodstuff.

November 4, 2021 (15:30–16:15, CET)

ThermoFisher SCIENTIFIC

VENDOR WEBINAR:

Taking Advantage of the Latest Developments in GC- and LC-High Resolution Accurate Mass MS for Both Quantitative and Non-Target Analysis in Food Safety

Taking advantage of the latest developments in GC- and LC- High Resolution Accurate Mass MS for both quantitative and non-target analysis in Food Safety

Charles Yang, Senior Marketing Specialist for Environmental and Food Safety, Thermo Fisher Scientific
Giulia Riccardino, Senior Applications Specialist, Thermo Fisher Scientific

The first section of the presentation will demonstrate the benefits of high resolution accurate mass and the analytical flexibility provided by Thermo Scientific™ Orbitrap Exploris™ GC coupled with solid phase micro-extraction (SPME) with Arrow technology to assess the volatile profile of intentionally adulterated and native oregano samples. Full scan non-targeted analysis combined with powerful informatics opens up new possibilities for detecting food fraud.

The second section of the presentation will describe the multi-residue analysis of a target pesticides in extracts of garlic and cumin using the Thermo Scientific™ Orbitrap Exploris™ 120 Mass Spectrometer within Full scan, MS2 and with Thermo Scientific™ AcquireX background exclusion for cleaner spectral while using software with built-in workflows for streamlining method development. The same acquired data was successfully used to screen for unexpected compounds. The presentation will also include information how new features provide improved robustness, sub ppm mass accuracy and easier maintenance in a compact system.

November 4, 2021 (15:30–16:15, CET)

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

VENDOR WEBINAR:

Waters Presents Our Recent Advances in Food Analysis at RAFA 2021

Enhancing analysis of foods using the ACQUITY™ Premier solution, Vitamin B, Organic Acids and beyond

Jinchuan Yang, PhD, Principal Scientist, Scientific Operations, Waters Corporation

Waters recently launched ACQUITY™ Premier LC systems and columns that utilize the novel MaxPeak™ High Performance Surface (HPS) technology, which has been developed to mitigate metal analyte interactions in liquid chromatography. We have evaluated the performance of the ACQUITY™ Premier LC and columns for analysis of multiple B vitamins and organic acids and compared the results with those obtained using the conventional stainless-steel components. We demonstrate significantly improved performance in analyte peak area, limit of quantification, and carry-over using the MaxPeak™ HPS technology in the analysis of not only the phosphorylated B vitamins, but also the non-phosphorylated B vitamins. Significant improvement in peak area was also observed in organic acid analysis. Our results suggest that this novel technology brings a clear advantage over the conventional stainless-steel in the analysis of B vitamins and organic acids. This MaxPeak™ HPS technology has a high potential to improve the LC based analysis for a wide range of compounds in food testing.

November 4, 2021 (16:30–17:15, CET)

VENDOR WEBINAR:

Analysis of PFAS Compounds from Food and Food Contact Material

Analysis of PFAS Compounds from Food and Food Contact Material

Richard Jack

This webinar will give an overview of the PFAS workflows from foods and food contact material by focusing on PFAS extraction and analysis from various food samples, include eggs, fish, butter and Food contact material. We will present a two-step extraction procedure of 23 PFAS analytes from butter, making use of QuEChERS followed by Solid Phase Extraction and analyzed by LCMS/MS. The high resolution and unique mixed-mode selectivity of a Luna Omega 1.6 µm PS C18 LC column results in excellent chromatography in a very short 4-minute run. In addition, further analysis of milk, eggs, and fish tissue were also validated using the method. Results from various butter sources indicate that different packaging results in differences in the PFAS compounds present.

November 4, 2021 (17:30–18:15, CET)

VENDOR WEBINAR:

Determination of Ionic Pesticides, Chlorate and Perchlorate in Various Food Matrices

Determination of Ionic Pesticides, Chlorate and Perchlorate in Various Food Matrices

Richard Jack

This webinar will describe the performance of a new column, Venusil Hilic for the separation of ionic pesticides and inorganic anions chlorate and perchlorate. We will demonstrate the excellent resolution and robustness is a variety of water and food matrices using reversed phase LC-MS/MS detection. The new columns shows excellent peak shape using standard chromatographic conditions. As recommended by Sante Guidelines, the column shows excellent linearity, specificity, repeatability for the full range of analytes and wide range of matrix extracts.