Innovation Summit

Agenda

Advancing Analytical Science | 19–21 October 2021

The latest in the Innovation Summit series, join us for the Pharma and Biopharma interactive sessions.

Using a live and on-demand approach you can literally organize your own agenda that it fits in with your schedule. We have many leading industry speakers and Thermo Fisher Scientific experts that will be on hand to answer questions if and when they arise.

The event has been carefully planned, so that current industry issues are tackled with streams that cover hot topics in pharma and biopharma as well as IT, the Lab, Compliance and Mass Spectrometry during the Chromeleon Symposium sessions, in the additional track. This in turn will lead to discussions that will resonate with many of the attendees and will give the opportunity for us all to learn.

With resource libraries and interactive booths there is also a host of useful pieces of collateral that can be accessed freely, whenever it's convenient.

Tuesday, 19 October 2021

11.00–12.30 CEST | Accelerating pharmaceutical characterization

- Capturing process characterization data for mRNA-1273 scale-up during a pandemic lockdown—*Joseph Schariter, Moderna*
- Confidence in process: A fully automated solution for nitrosamine impurity analysis applicable to LC-MS and GC-MS—*Giorgio Blom, Senior Scientist, Astra Zeneca*
- Cutting edge gene therapy analytics – the Vanquish Horizon UHPLC System—*Patrick Hoering, Scientist, Analytical Sciences, Pharmaron Biologics*

14.30–16.00 CEST | Advanced analytical solutions

- Determination of dimethylamine and nitrite in pharmaceuticals by ion chromatography to assess the likelihood of nitrosamine formation—*Jingli Hu, Senior Application Chemist, Thermo Fisher Scientific*
- Systematic investigation LC-MS miniaturization to increase sensitivity in wide-target LC-MS-based trace bioanalysis of small molecules – considerations for practical implementation—*Veronika Fitz, Department of Analytical Chemistry, University of Vienna*
- New approaches to analgesic monograph methods using chromatographic analysis—*James Grinias, Associate Professor, Rowan University*

Registration and additional details can be found **here**

Wednesday, 20 October 2021

11.00–12.30 CEST | Advances in large biomolecules analysis

- Platforms comparison for multi-attribute method implementation—*Sara Carillo, Application Development Team Leader, National Institute of Bioprocessing Research and Training (NIBRT)*
- Microflow SEC for enhanced native MS of proteins and complexes—*Andrea Gargano, Assistant Professor, University of Amsterdam*
- Rapid analysis of biotherapeutics using protein A chromatography coupled to Orbitrap mass spectrometry—*Craig Jakes, PhD Researcher, National Institute of Bioprocessing Research and Training (NIBRT)*

14.30–16.00 CEST | Chromatography with advanced detection methods

- Quality attributes of therapeutic proteins determined by chromatography and/or mass spectrometry: Who senses the difference?—*Christian Huber, Paris Lodron University Salzburg, France*
- The 2D-LC system of your dreams – The Innovative Take on Vaccine Research—*Alexander Schwenger, CureVac and Frank Steiner, Thermo Fisher Scientific*
- How to achieve a confident identification of volatile and semi-volatile extractables and leachables from pharmaceutical packaging by HRAM GC-MS—*Dujuan Lu, PhD., E&L Manager/Global Leader, SGS Health Science*

Thursday, 21 October 2021

11.00–12.30 CEST | Micro-flow proteomics and poster session

- Robust, reproducible and quantitative analysis of more than 40,000 proteomes by micro-flow LC-MS/MS—*Yangyang Bian, College of Life Science, Northwest University, China*

Poster session

- Synthesis and characterization of barium carbonate nanoparticles—*Mohsen Mhadhbi, Laboratory of Useful Materials, National Institute of Research and Physicochemical Analysis, Ariana, Tunisia*
- Development and validation of a new HPLC analytical method for the determination of Sildenafil (Viagra) in an energy drink—*Chathura Dhananjaya Fernando, Laboratory LVR- Clinic Viersen, Germany*
- Advancing analytical workflows with automation solutions—*Sudharshan Rangarajan, Lab Automation, Thermo Fisher Scientific*
- Embracing digital transformation and greater connectivity with the Thermo Scientific™ Momentum™ Workflow Scheduling Software—*Dean Mulyk, Lab Automation, Thermo Fisher Scientific*

14.30–16.00 CEST | Mass Spectrometry and Automation

- Use and reuse of retention time information in metabolite identification in LC-MS-based metabolomics—*Michael Witting, Deputy Head & Scientific Manager Metabolomics and Proteomics Core, Helmholtz Zentrum München*
- Automated, connected & intelligent laboratories—*Melanie Vig, Automated Platforms and Robotic Movers, Lab Automation, Thermo Fisher Scientific*
- Nitrosamine impurities analysis using the Triple Quadrupole Mass Spectrometer—*Lisa Dowse and Wael Elmasri, Pharma Services Group, Thermo Fisher Scientific*

Registration and additional details can be found **here**

Accelerating pharmaceutical characterization

October 19, 2021: 11.00–12.30 (CEST) 10.00–11.30 (EDT)

Joseph Schariter, Moderna—

Capturing process characterization data for mRNA-1273 scale-up during a pandemic lockdown

Abstract

During the lockdown in Massachusetts in the winter of 2020, Moderna had to scale up a phase 1 process to support a phase III and an eventual EUA for the mRNA-1273 COVID-19 vaccine. There was a significant amount of uncertainty on COVID-19 transmission so stringent cleaning procedures and social distancing were employed for critical businesses. As the Technical Development organization was located in Cambridge at the time, it led to significant issues to continue rapid scale-up development while keeping personnel safe from COVID. Social distancing in laboratory environments are difficult in expensive real-estate areas such as Cambridge, so laboratory time was scheduled during off hours to keep the amount of personnel overlap to a minimum. Consequently, cloud based tools for both collaboration, raw data capture, and data analysis were critical for this work stream and help enable the process characterization activities required for mRNA-1273 scale-up.

Giorgio Blom, Astra Zeneca

Confidence in process: A fully automated solution for nitrosamine impurity analysis applicable to LC-MS and GC-MS

Abstract

Since 2018 Nitrosamine analysis in drug products such as Metformin have a been a highly discussed topic following an announcement from regulatory bodies world-wide that every product destined for human-use should be assessed for nitrosamine impurities. Challenges with sensitivity, complex matrices and maintaining regulatory compliance are nothing new, however here scale is also a challenge. The imposed requirements meant that testing is mandatory for any product deemed at risk to contain nitrosamines, including all large-scale production of existing products. By combining the right instrumentation and tools the sensitivity and selectivity requirements can be met, but in order to make this scale manageable in established QC laboratories new technology can be assessed to automate the sample preparation process. Not only does this provide a higher throughput capability, but mitigates against human error and inconsistency. Furthermore, being able to process samples with both an LC-MS and GC-MS endpoint with ether on-line or off-line extraction can have a dramatic impact on consistency and productivity, quickly making the product assessment, and determining the validity of the result, mitigating against false positive results.

Patrick Hoering, Pharmaron Biologics

Cutting edge gene therapy analytics – the Vanquish Horizon UHPLC System

Abstract

From empty: full analysis of Drug Substance to challenging assessment of residuals, the Vanquish Horizon with its sensitive FLD and CAD can improve the analysis of viral DS and the detection limit of residual impurities for optimal quality and safety of the product. The lengthy process of Gene Therapy manufacture introduces many potential impurities, but many of these can be detected using the Vanquish UHPLC helping manufacturers to optimize the toxic profile of their product as shown on the examples of PEI (toxic, non-biodegradable) and PDMS (poorly soluble, biostable).

Furthermore, assessment of the empty: full ratio of Gene Therapy products is a major factor for a functional product. Separation of empty and full AAV capsids has been achieved using standard buffers with a simple gradient.

Registration and additional details can be found **here**

Advanced analytical solutions

October 19, 2021: 14.30–16.00 (CEST) 13.30–15.00 (EDT)

Jingli Hu, Senior Application Chemist, Thermo Fisher Scientific

Determination of dimethylamine and nitrite in pharmaceuticals by ion chromatography to assess the likelihood of nitrosamine formation

Abstract

Since July 2018 several drugs have been recalled due to contamination with N-nitrosodimethylamine (NDMA), a probable human carcinogen. Dimethylamine (DMA) and nitrite are precursors in the formation of NDMA. Ion chromatography (IC) methods were developed for the determination of these two precursors in drug substances and drug products. Dimethylamine was determined by a cation exchange separation with suppressed conductivity detection using one of two methods, depending on the chemical nature of the drug substance. Nitrite was determined by coupling an anion exchange separation with UV absorbance detection. The developed methods were successfully applied to DMA and nitrite determinations in five drug products including metformin, losartan, ranitidine, Nytol, and Benadyrl, and two drug substances (APIs), losartan potassium and metformin hydrochloride. Some samples contained nitrite and DMA at detectable levels. The developed methods should be useful for the rapid screening and quantification of nitrite and DMA in pharmaceuticals and in-process sample to assess the likelihood of NDMA formation. The methods for DMA should be applicable to other amines to assess the likelihood of the formation of other nitrosamines in pharmaceutical products.

Veronika Fitz, Department of Analytical Chemistry, University of Vienna

Systematic investigation LC-MS miniaturization to increase sensitivity in wide-target LC-MS-based trace bioanalysis of small molecules – considerations for practical implementation

Abstract

Systematic investigation LC-MS miniaturization to increase sensitivity in wide-target LC-MS-based trace bioanalysis of small molecules – considerations for practical implementation. The wide dynamic range and physicochemical diversity of analytes found in biological samples calls for sensitive analysis platforms that cope with minimal sample preparation and provide convenient system adaptability for method development. Miniaturization of ESI-MS promises to improve sensitivity and hence detection limits and identification without introducing selectivity. This is especially valuable in wide-targeted exploratory studies. Practical implementation of miniaturization faces technical challenges that curb its theoretical benefits. The presented study compares three platforms (nano-, micro and analytical flow regime) on a technical basis and discusses their merits and downsides.

James Grinias, Rowan University

New approaches to analgesic monograph methods using chromatographic analysis

Abstract

One of today's most widely used analytical tools is ultra-high pressure liquid chromatography (UHPLC). Compared to traditional HPLC techniques, UHPLC enables higher chromatographic efficiency and reduced method times, but requires two- to four-fold increases in system pressure. The use of superficially porous particles (SPPs) and quasi-adiabatic thermal environments can help maintain high efficiency as mobile phase velocity is increased, although broadening due to extra-column effects and viscous friction can still impact separation performance. The impact of these effects in various application areas will be explored in this presentation. A comparison of SPP columns of varying dimensions containing different particle sizes that was made to determine the best approach for reducing the analysis time of pharmacopeial monograph methods for over-the-counter analgesic drugs will also be discussed. System suitability parameters (resolution and peak asymmetry) and temperature changes across the axial length of the column were monitored at conditions near column or system pressure limits. Multiple methods were found to see a 10-to-20-fold improvement in throughput utilizing UHPLC, including a 20 second cycle time method for the separation of four compounds (two active pharmaceutical ingredients, one impurity, and one internal standard) maintaining a baseline resolution of 1.5 between all peaks. Considerations for the qualification of these high-throughput methods and other approaches to improved analysis of analgesic compounds will also be discussed.

Registration and additional details can be found **here**

Advances in large biomolecules analysis

October 20, 2021: 11.00–12.30 (CEST) 10.00–11.30 (EDT)

Sara Carillo, National Institute of Bioprocessing Research and Training (NIBRT)

Platforms comparison for multi-attribute method implementation

Abstract

The need for more informative data to better and deeply characterize monoclonal antibodies is leading LC-MS (liquid chromatography – mass spectrometry) based workflows into the quality control (QC) environment, posing not only a challenge in terms of increased throughput of these methods, but also in terms of reproducibility and transferability across different laboratories and different analytical platforms. The Multi-Attribute Method (MAM) workflow is the best example of this challenge, being based on peptide mapping analysis that requires precise and reproducible high performance in terms of LC separation. The MAM approach is meant to replace multiple assays in QC laboratories, but the lengthy chromatographic gradients required do not correspond to the need for enhanced high-throughput.

In this study, we present the comparison of different uHPLC platforms employed for MAM workflow. Thermo Scientific™ Vanquish™ Duo for Tandem LC, Thermo Scientific™ Vanquish™ Horizon™ and Thermo Scientific™ Vanquish™ Flex™ were used in combination with Thermo Scientific™ Acclaim™ C18 column for the analysis of Nist mAb tryptic digest in a MAM workflow. A Thermo Scientific™ Q Exactive hybrid quadrupole Orbitrap MS was used for analysis in full MS mode of the tryptic digest. We were able to monitor the behavior of the different platforms across the different systems with a processing method created within a compliant environment using Thermo Scientific™ Chromeleon™ CDS software. The processing method used LC-MS/MS data generated using only one of the platform in this study. Repeatability was also evaluated performing two twin data sets 14 days after the first analysis. Several parameters were evaluated, such as variation of retention times, peak area and asymmetry and peak width. As well, a list critical quality attributes, necessary to monitor the suitability of the platform for MAM workflow, were monitored; these include lysing clipping, deamidation, glycation and succinimide formation. Overall, excellent reproducibility of the data was observed within the differences expected by the fluidics present on the platforms used in this study. This proved suitability of Vanquish UHPLC family for MAM workflow and for easy seamless transferability of instrument and processing methods across different platforms.

Andrea Gargano, University of Amsterdam

Microflow SEC for enhanced native MS of proteins & complexes

Abstract

In our work, we investigate the advantages of a low flow SEC (≤15 µL/min) system coupled online to nMS for characterization of proteins, labile protein complexes and their higher-order structures. The internal diameter of the SEC column was reduced to 1 mm ID and the employed flowrate was 15 µL/min. Lowering the elution flowrate to the microESI regime, provided a significant increase in the MS sensitivity and signal-to noise ratio allowing detection of low abundant impurities and higher-order species up to 280 kDa. Furthermore, with this approach the salt tolerance of the MS was much improved. High ionic strength conditions of volatile salts (200–400 mM) can be used to ensure almost interaction-free SEC analysis of proteins. This is particularly useful for biotherapeutics, such as monoclonal antibodies that the non-specific chemical interactions between them and the silica-based stationary phase can induce chromatographic peak tailing and/or significant adsorption. Additionally, more efficient solvent evaporation can be achieved at these low flowrates using softer MS conditions (lower activation energy) that ensure no (or little) structural alterations or denaturation of the proteins and their higher-order structures.

Craig Jakes, National Institute of Bioprocessing Research and Training (NIBRT)

Rapid analysis of biotherapeutics using protein a chromatography coupled to Orbitrap mass spectrometry

Abstract

Protein A capture chromatography is routinely used in the purification of biopharmaceuticals before undergoing characterization. This, however, can result in a number of hours before product characteristics are understood, and traditional characterization procedures can result in artificially induced modification. In this study we outline the use of coupling protein A chromatography technique directly to high resolution mass spectrometry for protein characterization with a high level of mass accuracy that requires no previous treatment of the sample. Method development, robustness and application are outlined demonstrating the universal nature of the approach for the characterization of a wide variety of mAb products using as little as 0.5 µg of protein. The present approached represents a simplified approach that is impactful, rapid, and robust that is based on accurate intact mass profiling. The reported method represents a considerable advance for biopharmaceutical characterization that will complement existing native LC-MS applications and can be easily adapted for online process analytical technologies (PAT).

Registration and additional details can be found **here**

Chromatography with advanced detection methods

October 20, 2021: 14.30–16.00 (CEST) 13.30–15.00 (EDT)

Christian Huber, Paris Lodron University Salzburg, France

Quality attributes of therapeutic proteins determined by chromatography and/or mass spectrometry: Who senses the difference?

Abstract

The commercial use of therapeutic proteins has revolutionized modern medical treatment of a variety of diseases including cancer, (auto)immune diseases, or blood disorders. High-performance liquid chromatography (HPLC), first developed for the separation of small molecules, could later be tailored to enable the efficient chromatographic separation of macromolecules through the development of stationary phase configurations enabling very high efficiency such as sub-2 µm particles, superficially porous particles, or monolithic phases. Likewise, progress in mass spectrometry (MS) technologies, especially electrospray ionization (ESI) for biopolymers, as well as high-resolution mass analyzers have significantly contributed to the success of bioanalytical methods in pharmaceutical and biomedical research. Nevertheless, 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. This lecture discusses the potential, challenges, and achievements of HPLC-ESI-MS methods in the analysis of high-molecular pharmaceutical compounds. Emphasis will be on confirming the identity and purity of the drug compounds and on the characterization of post-translational modifications. Examples of application will include the structural confirmation and analysis of posttranslational modifications in therapeutic proteins produced by recombinant biotechnology, such as monoclonal antibodies, protein hormones, growth factors, and fusion proteins.

Alexander Schwenger, CureVac and Frank Steiner, Thermo Fisher Scientific

The 2D-LC system of your dreams – the innovative take on vaccine research

Abstract

Learn how to overcome current and future challenges in vaccine research with two-dimensional liquid chromatography (2D-LC). This webinar will give an overview of several 2D-LC setups and explain how innovative solutions help to speed up research projects at a real-life example. Revolutionary science needs tailored solutions – learn how we approach personalized vaccine development and production.

Dujuan Lu, SGS Health Science

How to achieve a confident identification of volatile and semi-volatile extractables and leachables from pharmaceutical packaging by HRAM GC-MS

Abstract

Extractables and leachables (E&L) from pharmaceutical packaging, medical devices, and process equipment can potentially pose risks to the safety, efficacy, and stability of pharmaceutical or medical products. As part of safety risk assessment, it is very important to confidently identify those E&L compounds. However, the confident identification of extractables and leachables can be challenging due to the diverse chemical structures and properties of polymer additives found in the manufacturing and packaging components, and medical devices. This presentation will go through the levels of identification confidence illustrated in USP <1663> and strategies to achieve a confident identification. A few case studies will be discussed focusing on identification of volatile and semi-volatile E&L compounds by HRAM GC-MS.

Registration and additional details can be found **here**

Micro-flow proteomics and poster session

October 21, 2021: 11.00–12.30 (CEST) 10.00–11.30 (EDT)

Yangyang Bian, College of Life Science, Northwest University, China

Robust, reproducible and quantitative analysis of more than 40,000 proteomes by micro-flow LC-MS/MS

Abstract

Nano LC–MS/MS was widely used for Proteomics analysis due to its high sensitivity. However, nano LC-MS/MS has limitations particular regarding sample throughput and robustness, which are the bottlenecks for large cohorts of samples. Here, we built a micro-flow LC-MS/MS system using a 1.0 mm i.d. × 150 mm chromatographic column operating at 50 ml/ml coupled to either a Thermo Scientific™ Q Exactive HF-X or Thermo Scientific™ Orbitrap Fusion Lumos mass spectrometer for proteomic analysis. Despite the 177 times higher of flow rate, only about 5–10× more sample was required on the micro-flow compared to the nano LC system when using a 28 Hz MS method. The micro-flow LC-MS/MS reached similar proteome depth to nano LC for both single shot and offline multiple dimensional liquid chromatography analysis of tissue, cell line and body fluid samples. Very high reproducibility of chromatographic retention time (<0.3% CV) and protein quantification was obtained (<7.5% CV) based on data from >2,000 samples. The micro-flow LC column showed hihg separation efficiency, the median full peak width at half maximum varied from 3 to 8 seconds for 10 to 90 min gradients. The median peak width of the same column kept almost the same after running about 15,000 samples within 20 months, and more than 40,000 samples has been measured by two micro-flow LC-MS/MS systems in the last two years. Collectively, we show that standard proteomic analysis should no longer be confined to expert laboratories, which will definitely move the technology into routine clinical applications, and projects with large-scale samples.

Poster session

Mohsen Mhadhbi, Laboratory of Useful Materials, National Institute of Research and Physicochemical Analysis, Ariana, Tunisia

Synthesis and characterization of barium carbonate nanoparticles

Abstract

In this work, barium carbonate nanoparticles with composition $BaCO_3$ were synthetized by using auto-combustion process. Thus, the obtained barium carbonate nanoparticles were calcined at various temperatures (700, 800, and 900 °C). The structural changes of the powders were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared spectroscopy (FTIR). The crystallite size was estimated from the broadening of XRD peaks using Scherrer's formula. The effect of calcination temperature and the possible formation mechanism of the nanocrystallites were also discussed. It was observed that the presence of $BaCO_3$ phase depletes significantly the infrared to visible up-converted luminescence efficiency of the final nano-powders. The particles size of the final product was about 30 nm.

Chathura Dhananjaya Fernando, Laboratory LVR- Clinic Viersen, Germany

Development and validation of a new HPLC analytical method for the determination of Sildenafil (Viagra) in an energy drink

Abstract

In the Clinical-Toxicology laboratory of the LVR-Clinic in Viersen/Germany, as a standard, serum and urine samples are analyzed. As a special service, suspected drug samples from all over Germany can be send in and they are checked for relevant drugs. Therefore, different analytical technologies such as GCMS, LCMS and HPLC are used. Through this drug-checking channel a food sample (energy drink) arrived in the lab. After consumption of the drink, the subjects experienced weird side effects. Using an HPLC, Sildenafil (Viagra) is detected in the sample. After analyzing the energy drink, the lab ordered more food samples from the same resource to check, if illicit drugs are added. Three different kind of food samples (Energy drink, Instant Coffee and Chocolate) and their matrix had to be taken under consideration. A quantitative method is developed utilizing HPLC-PDA detection. The challenge for the lab is the sample preparation of the food matrix.

The results violate the pharma and also the food regulations. On the homepage, a Ginseng extract is advertised for an active agent to improve sexual activity. However, the different samples showed pharmaceutical quality Sildenafil as well as Tadalafil and as an addition Acetaminophen.

The presentation will show a complete workflow for different food matrices including sample preparation, analytical method, detection and quantification for the three prescription drugs.

Registration and additional details can be found **here**

Micro-flow proteomics and poster session

October 21, 2021: 11.00–12.30 (CEST) 10.00–11.30 (EDT)

Poster session continued

Sudharshan Rangarajan, Lab Automation, Thermo Fisher Scientific

Advancing analytical workflows with automation solutions

Abstract

One of the biggest challenges preventing end-to-end automation in the analytical science lab is the lack of a robust sample preparation platform that can be connected to downstream processes. Accelerated by the recent pandemic, strategic discussions on how to embrace automation and digital transformation have consumed the industry and highlighted the need for diverse and connected solutions. It gave rise to new improvements in the field to ensure business continuity without compromising on productivity and data reproducibility. Take your analytical science one step further with the Thermo Scientific™ Vanquish™ UHPLC Loader. Automate your entire workflow creating an end-to-end solution with little to no human intervention. Achieve seamless integration between upstream sample preparation and downstream analysis.

Thermo Fisher Scientific has a solution that gets you one step closer, in the form of an automated UHPLC Loading device. The "Vanquish Loader" works exclusively on the Thermo Scientific™ Vanquish™ UHPLC instrument controlled by both Thermo Scientific™ Momentum™ Workflow Scheduling software and Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software. This platform enables you to work with samples in a high-throughput manner improving productivity, reproducibility as well as data tracking - benefiting the user by shifting the focus on data rather than sample handling. The sample information is seamlessly passed from upstream sample prep through to LC-MS and then finally leading to results through the interaction of Momentum and Chromeleon. The Momentum workflow scheduling software combines ease-of-use with advanced functionality providing users the ability to schedule automation on their analytical workflows with minimal effort and time invested. Overall, the future to automating analytical science is here and the Vanquish Loader provides the missing link to end-to-end automation.

Dean Mulyk, Lab Automation, Thermo Fisher Scientific

Embracing digital transformation and greater connectivity with the Thermo Scientific™ Momentum™ Workflow Scheduling Software

Abstract

The labs are rapidly changing as it undergoes a digital transformation to become the smart lab of the future. Classical Laboratory automation where a robot connects to one or more automation friendly devices and uses "simple" file-based hand-offs to connect to LIMS is evolving to incorporate collaborative robots, smarter devices, and deep dynamic digital connectivity to an organization's software ecosystems. The data demands of the lab are similarly evolving. Data without context is not as actionable as harmonized data (formatted for long term re-usability) and stored in a data lake in context with metadata (data about data). Thermo Scientific Laboratory Automation products can be used by labs to automate their workflows and to easily connect to their digital ecosystem. Thermo Scientific™ Momentum™ Workflow scheduling software is a dynamic event-based scheduling software that connects robots and devices into scientific workflows. Momentum's Unite module enables labs to seamlessly connect Momentum systems to their digital ecosystems to provide real-time, bi-directional, flexible and autonomous data integration. Unite supports REST API, SOAP, .net binaries, SQL and other technologies. Data transform tools within Unite can format data so it can be passed between Momentum and external services (e.g., LIMS, enterprise scientific software, etc) or used within the Momentum workcell to be applied in dynamic machine logic decision driven workflows. Momentum and Unite can capture and provide both result data and user defined metadata for incorporation into an organizations data lake. Momentum is used across a wide range of small and large molecule workflows (e.g., screening, synthetic biology, HCS, cell culture, sample prep, nucleic acid extraction, PCR/qPCR, and many more). These new connectivity and data tools will be shown in the context of the Thermo Fisher Scientific™ Amplitude™ solution. The Thermo Fisher Scientific Amplitude Solution featuring Thermo Scientific's Momentum workflow software, a highly automated molecular diagnostic testing solution that can analyze up to 8,000 COVID19 specimens in 24 hours. This poster and oral session will provide:

- An overview of the Amplitude Solution, along with the critical data tracking and automated data interpretation that is required for diagnostic workflows.
- Details about the simple to use dashboard style interface which enables novice automation lab technicians to operate the system with minimal hands-on time and direction.

Registration and additional details can be found **here**

Mass Spectrometry and Automation

October 21, 2021: 14.30–16.00 (CEST) 13.30–15.00 (EDT)

Michael Witting, Helmholtz Zentrum München TBC

Use and reuse of retention time information in metabolite identification in LC-MS-based metabolomics

Abstract

Metabolite identification in LC-MS based metabolomics requires several orthogonal parameters, such as *m/z*, fragmentation pattern and retention times. While the sharing and (re-)use of MS^1 and MS^2-MS^n data is common practice, retention time information is only used at later stage in metabolite identification, typically when comparing against reference standards. However, retention time information gives valuable insights about the polarity of metabolites and some other properties and can be used to filter or re-rank candidates in library searches or in-silico tools. Still, sharing of retention times is not widespread. We identified that the quality of chromatographic metadata associated with retention times can become a bottleneck for the (re-)use. Based on data from EBI Metabolites and NIH Metabolomics Workbench we investigated the quality of metadata, which allowed us to propose a "minimum set" of information required to make retention times useful in metabolite identification workflows. Furthermore, we started to set up a public retention time repository based on GitHub and continuous integration as well as a standardized nomenclature for metadata to facilitate the sharing of retention time information.

Melanie Vig, Automated Platforms and Robotic Movers, Lab Automation, Thermo Fisher Scientific

Automated, connected & intelligent laboratories

Abstract

Scientific and technological advancements continue to emphasize the importance of automation, both in the physical and digital world. Given recent discussions about the lab of the future, the benefits have expanded to highlight how automation can support greater connectivity between data and workflows, paving the way to a 'smarter lab'. A fully integrated robotic platform with software control systems can help you seamlessly connect workflows and data effectively providing a common missing piece to the analytical advancement puzzle, thereby supporting you on your digital transformation journey and leading to accelerated scientific discoveries. This presentation will discuss how technology-driven strategies can promote success and how automated science is a key driving factor and help researcher's future-proof their laboratories.

Lisa Dowse and Wael Elmasri, Pharma Services Group, Thermo Fisher Scientific

Nitrosamine impurities analysis using the Triple Quadrupole Mass Spectrometer

Abstract

A brief background of the regulatory impact of Nitrosamines in drug products and a discussion on how the Vanquish Triple Quadrupole Mass Spectrometer supports our efforts to perform nitrosamines analysis

Registration and additional details can be found **here**

Useful Information

Connect with your peers and Thermo Fisher Scientific specialists to get help, share expertise and grow your scientific brainpower at **AnalyteGuru**.

Stay up to date with the latest news, applications, events, and more by **signing up for one of our communities**.

Registration and additional details can be found **here**