Analytica Virtual 2020: Update
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Intelligent auto-diagnostics and auto-recovery features
e.g. real-time mobile phase level monitoring, auto-recovery from air bubbles and management of consumable consumption

Efficient process automation and fast, reliable performance
from startup to shutdown providing automated workflow, maximized throughput and dramatically increased analysis capacity

Compact design
offering ease-of-operation on a reduced footprint

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Analytica Virtual 2020

This year, Messe München is hosting the world’s leading trade fair for laboratory technology, analysis and biotechnology as a virtual event. The new format Analytica Virtual 2020 will enable exhibitors to book digital trade fair booths from October 19 to 23, 2020. The virtual event will also offer customers additional opportunities for exchange and networking. Large parts of the lecture, conference and supporting programme will also be available in digital form. The entire fair will be open 24 hours daily to allow participants from all over the world to visit. Visitors will participate free of charge.

From doping control to the detection of antibiotic-resistant germs to artificial intelligence (AI) in the laboratory, the Analytica Virtual 2020 conference reflects the entire spectrum of modern analysis. Attention will be focused on the increasing role of digitization because this drives all the analytical disciplines: What do materials scientists use artificial intelligence methods for? How do physicians handle the increasing flood of data? What digital techniques can be used to optimize the monitoring of industrial processes? These and many other questions will be discussed by renowned researchers from around the world.

Doping and Drugs
In addition to the overarching focus on digitization, the conference agenda covers a wide range of other current topics. One year before the Olympic Summer Games in Tokyo, Japan, the subject of doping control will not be missed out. As a result of the wide variety of performance-enhancing substances—ranging from small inorganic substances to large biomolecules—doping control officers need sophisticated analytical techniques. The symposium “Emerging Topics in Analytical Toxicology, Forensics and Doping Control” organized by toxicologist Hans H. Maurer from Saarland University, Germany, will highlight which methods are the most productive.

Chromatography-on-a-Chip
The basis of the Analytica conference continues to be the numerous new developments in instrumental analysis. There are dedicated sessions on chromatography and mass spectrometry (MS), spectroscopy, microscopy, and electroanalysis.
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The multifaceted programme invites participants to look beyond their own horizons and let themselves be inspired by colleagues from other analytical disciplines. In the age of digitization and digitalization, this is more important than ever. Despite the many digital techniques and extremely helpful methods of artificial intelligence, the knowledge, inventiveness, and, last but not least, intuition of experienced analysts will remain irreplaceable in the future. The challenge is to combine human know-how with the capabilities of machines.

The Digital Laboratory: Live and Tangible
Visitors to Analytica Virtual 2020 can experience the laboratory of the future in a special show, created by partners from science and industry, who have joined forces to demonstrate device networking, collaborative robotics, and user interaction, using the example of eight workflows from real-world applications. In the associated forum, experts will give lectures on the current state of digitization in the laboratory. From laboratory planning through sample logistics to data management, digital technologies will revolutionize the laboratory world. However, the new opportunities that this change will actually open up often remain vague, even for industry experts. In the special show “Digital Transformation”, Analytica will demonstrate in specific terms how daily work in the laboratory will change through a combination of real workflows and a forum.

Visitors to Analytica Virtual 2020 can experience the laboratory of the future in a special show, created by partners from science and industry, who have joined forces to demonstrate device networking, collaborative robotics, and user interaction.
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Trends and Developments

A snapshot of key trends and developments in separation science according to selected panelists from the chromatography sector.

**LC/LC–MS**

**LCGC: What trends do you see emerging in LC or LC–MS?**

**Robert Buco:** Analytical liquid chromatography (LC) has been used as a tool in making decisions for quite a while, and as the need to improve the efficiency, defensibility, and clarity of critical decision-making processes continues to grow, there is an increasing focus on the question the scientist is asking, the analytical data they need, and ultimately the decision they are trying to make. This is driving a shift in LC users’ requirements of their systems, where the advances of technical specifications used to be the most important consideration, it has now been surpassed by reliability, reproducibility, and most importantly, usability. There are many trends in technology that are associated with this high-level need, including the increased desire for automated workflows encompassing pre-analytical, data acquisition, data processing, and reporting components as a way to help minimize the variability of results generated by different users, but I think the more important trend is in the user population. LC separation technology that was once only accessible to expertly trained scientists is now routinely used by a new generation that trusts and expects the technology to function for their purpose so they can focus on the results and what they mean.

**Carsten Paul:** I see a couple of key trends in the industry. First is the increasing utilization of ultrahigh-performance liquid chromatography (UHPLC) applications, with HPLC instruments remaining as the leading instruments in the market. In discovery and research, UHPLC is more prominent. However, as methods are transitioned to routine laboratories, the technology used is typically more “fit-for-purpose” HPLC. Second, the growing importance of mass spectrometry to characterize more complex biotherapeutic molecules, with implementation moving more into routine laboratories. The increasing shift in focus of pharmaceutical companies towards novel biologic medicines will direct the future development of analytical equipment to fulfil the complex characterization needs of these advanced therapies.

**Stephane Moreau:** Ultra-fast mass spectrometry (UFMS) improves the workflow and speed of analysis for routine testing laboratories. With the introduction of tandem LC–MS with fast polarity switching and
The growing importance of mass spectrometry to characterize more complex biotherapeutic molecules, with implementation moving more into routine laboratories.
instruments and interpret the data. I would envision that in the future, an operator of any experience can easily run an analysis and the software can automatically report the results needed — regardless of whether that is a structural characterization, the location of a post-translation modification, or the quantification of a toxic compound. **Stephane Moreau**: In the clinical field, there is clearly an increase in the switch from immunoassays to LC–MS technologies. The better selectivity, sensitivity, and accuracy of analysis coupled with multiplexing capabilities and less risk of cross-reactions give LC–MS/MS a clear advantage in therapeutic drug monitoring as well as for toxicology and forensic applications. The penetration was somehow limited by the lack of automated sample preparation systems, but the recent launch of automated LC–MS systems is opening the door for a switch. The next step is to move for a more compact system fully automated and connected to an automated laboratory system. A similar tendency will also come to food safety analysis. **Rohit Shroff**: We should see continued miniaturization of chromatography systems to increase sensitivity and separation efficiency at lower volumes. As systems get more affordable, increasing adoption should be seen for routine analysis. Demand from bioprocessing would drive innovation in prepacked, disposable columns as well as membrane technology. There will likely be continued development of novel stationary phases, such as miniaturized monolithic columns, unique bonded-silica phases, and polymeric stationary phases that offer better separations in high-throughput analyses. The need for faster analyses, particularly in pharmaceutical research, will drive further developments and commercialization in the near future. Downstream processing in biopharmaceuticals will continue to drive improvements in two-dimensional (2D)-LC as well as continuous chromatography technology. Overall, LC–MS will continue to see innovation driven by biotherapeutic research and industry needs.

**LCGC**: What is the LC or LC–MS application area that you see growing the fastest?

**Robert Buco**: Certainly, there are trends that point towards the need for more comprehensive solutions in the analysis of biopharmaceuticals. The analysis of intact proteins and oligonucleotides, monoclonal antibody subunits, released N-Glycans, and peptide mapping/multi-attribute monitoring (MAM) applications are all growing quickly. However, I think there are other application needs that are growing quickly and more quietly, particularly in materials science where there is a clear need for better characterization tools for complex polymer systems. **Carsten Paul**: As already seen over the past couple of years, there is a tremendous shift in the pharmaceutical industry away from small molecule based active ingredients and towards biologic therapies, especially complex formats such as multispecific antibodies, drug conjugates, oligonucleotide-based, as well as cell and gene therapies. These will require various characterization technologies, which
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need to be transferrable from the initial development stage through to manufacturing. **Stephane Moreau:** The biggest one remains in food analysis, where the needs are mainly driven by the new regulations or the change of existing guidelines such as the Direction Générale de la Santé et des Consommateurs (DG-SANCO). The political pressure linked to random and/or recurrent scandals also boost development of applications in those fields. We have seen, for example, many interests for pyrrolizidine alkaloids recently, but multiresidue pesticides remain the mainstream. The second one would be the clinical field with penetration of MS technologies, not only LC–MS, for many areas, such as therapeutic drug monitoring, oncology, microbiology, and more. **Rohit Shroff:** Biotherapeutic characterization in research as well as the biopharmaceutical industry is currently the fastest growth driver for LC and LC–MS technologies. Advances in columns, stationary phases, detectors, injection devices, as well as the improvements in chromatography methodology, are all leading to an exceeding number of applications, particularly in the pharmaceutical and biopharmaceutical sectors. Examples include: monoclonal antibody characterization, antibody–drug conjugates, DNA/RNA detection and modifications, quality control and process, or analytical technology in bioprocessing applications.

**LCGC:** What obstacles stand in the way of LC or LC–MS development?

**Robert Buco:** One of the technical obstacles relates to the compromise that often exists between the size of an instrument and its technical performance. If analytical LC instruments are to become fully integrated into automated processes and enable real-time decision-making that impacts process control, they must be located in very close proximity to the point of analytical need, which in turn imposes restrictions on the physical size of the system as well as its robustness to be used in manufacturing environments. Developing an easy-to-use LC system that is sufficiently small, preserves the chromatographic capabilities of traditional systems, and offers an unparalleled level of usability while reliably running in continuous operation environments is a significant challenge, but I believe it is one our customer base is calling for and one our industry is ready to accept.

**Carsten Paul:** Some of the challenges are simply moving advanced detection and characterization methods, such as mass spectrometry, into a more routine usage. The instrument-to-instrument reproducibility, analytical precision, and accuracy tend to have wider tolerances than optical detectors, such as UV or DAD. In addition, transitioning mass spectrometry from a high-end research tool to a routine characterization method will require a great deal of simplicity in how the users interact with and optimize the methodologies that require this powerful technique. In addition, many questions remain unanswered when considering LC–MS application in highly regulated environments. This includes, for example, transferability between different instruments and vendors, data handling, product support,
and product life cycle, as well as connectivity into a compliant ready, software network. Steps are being taken to address these challenges today, but will continue to take some time before they are fully embraced within the regulated laboratory environment.

Stephane Moreau: Currently, there are not so many improvements in sensitivity as a result of the difficulties for suppliers to improve the ionization efficiency. Thus, most developments are focused on the other bottlenecks mentioned earlier, that is, automation, easy reviewing/reprocessing using artificial intelligence software, and improved robustness. The request for more compact systems is also challenging because it leads to a compromise between sensitivity and size. For the clinical field, the future in vitro diagnostic regulation (IVDR) regulation is likely to transform the landscape.

Rohit Shroff: Speed of analysis continues to be a limiting factor for chromatography-based hyphenated techniques, particularly in high-throughput drug discovery applications. Although considered a highly sensitive technique, for large molecule applications LC–MS sensitivity can be challenging compared with traditional ligand binding techniques. The high costs of chromatography instruments and reagents continues to be a deterrent for laboratories to invest in expensive equipment, unless the end product is of high value, such as a biotherapeutic. Coelution, sample adsorption, performance over a wide pH range, matrix complexity, robust method development for novel therapeutics, and high-skill requirements for efficiently running LC–MS laboratories are other obstacles.

**LCGC: What was the biggest accomplishment or news in 2019/2020 for LC or LC–MS?**

Robert Buco: For me, the biggest news was the ICH Q12 Guideline on Technical and Regulatory Considerations for Pharmaceutical Product Life Cycle Management and its annexes reaching step 4 of the ICH Process. There has been an increased focus on life cycle management for analytical methods in recent years from the industry's regulatory bodies, resulting in a more harmonized approach to technical and regulatory considerations for method life cycle management. When paired with analytical quality by design (AQbD), method life cycle management is set to change the way the pharmaceutical industry brings products to market, by ensuring the development of more robust analytical methods that result in more consistent, reliable, and high-quality data. The eventual implementation of Q12 will promote innovation and continual improvement in the biopharmaceutical sector, strengthen quality assurance, and improve the reliability of product supply.

Carsten Paul: With the analytical demands of scientists, who are often working with challenging analytes in complex sample matrices, the implementation of advanced LC and LC–MS instrumentation through 2019/2020 has helped to meet their needs and expanded their capabilities. This continual improvement is crucial to ensure scientists are able to conduct their
work, uninhibited by their equipment. **Rohit Shroff**: 2019 saw continued focus on developing stationary phases/column chemistries, particularly to meet the needs in pharmaceutical, biopharmaceutical analysis, and quality control (QC). For small molecule separations, numerous reverse-phase and HILIC chemistries on both superficially porous particle (SPP) and fully porous particle (FPP) architectures were developed. Stationary phases for large molecules had a focus on reversed-phase SPP architecture. Another interesting trend was the introduction of aromatic stationary phases that offered increased sensitivity and could be used with highly aqueous mobile phases for the analysis of polar compounds. 2019 also saw the continued development of new, compact, and hybrid LC–MS systems from key vendors.

**Robert Buco** is the Director of Global Product Management of LC Systems at Waters Corporation.

**Carsten Paul** is a UHPLC Product Marketing Manager at Thermo Fisher Scientific.

**Rohit Shroff** is the Senior Director of LC–MS Strategy and Portfolio Management at VWR, Part of Avantor.

**Stephane Moreau** is a LC–MS and Life Sciences Manager at Shimadzu Europa.

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**GC/GC–MS**

**LCGC: What trends do you see emerging in GC or GC–MS?**

**Christophe Clarysse**: The global trends we are seeing and working on with our customers are a desire for miniaturization, flexibility, and faster results. For example, full automatization of sample preparation and multiple detection channels are helping to address the need for more specific and confident results with shorter turnaround times. In the areas of food safety and environmental health, the number of samples as well as regulatory requirements are always increasing, so this demands a focus on targeted and non-targeted molecules. User-friendly data handling solutions that are combined with smart instruments and approaches, including artificial intelligence, are helpful in preventive maintenance, lowering the cost of ownership, and simplifying workflows — essentially bringing turnkey solutions for QA/QC or analytical laboratories.

**Eric Denoyer**: One trend is the development of smart connected functionality to improve and streamline the user experience. Functions, such as automatic leak checks and troubleshooting diagnostics, allow operators to achieve better results faster, with fewer mistakes. Also, proactively guiding users through preventative maintenance steps helps reduce unplanned downtime and sample reruns, greatly improving productivity. There is a clear trend to cross-train operators...
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and a requirement for them to stay connected with what’s happening in several laboratories simultaneously, even when they are not physically in any given one. Remote connectivity is a future trend as an “Industry 4.0” digital transformation sweeps across analytical laboratory enterprises worldwide, driving resource deployment optimization. Smart functionality and remote connectivity are also invaluable when optimizing laboratory operations during a pandemic, especially when laboratory access is limited. Green chemistry and sustainable operations are also clear trends, and many new instruments are being designed to use less power, water, helium, and other natural resources. We are seeing increased use of recently introduced, cost-efficient oil-free GC–MS pumps, that run much quieter and cleaner, and eliminate oil spills. Moving applications to smaller, greener, and faster GC systems with efficient direct heating technology, is also a growing trend.

Matthew Edwards: We are seeing an increase in discovery-based approaches, where workflows that are typically seen in the ‘omics’ fields are now expanding to other application areas. Analysts no longer want to simply comply with regulated methods, but also want to see what else is present in their samples. For example, in the automotive industry, manufacturers must adhere to Vehicle Interior Air Quality (VIAQ) regulations, but now also want to be able to monitor other potentially harmful compounds and those which may contribute to malodours.

Chris Rattray: Recent emerging trends in GC and GC hyphenated with MS include an increase in the use of mass spectrometers, especially triple quadrupole instruments, instrument miniaturization, and the migration towards multiclass methods of analysis. The upward trend in the adoption of triple quadrupole instruments is a result of the increased sensitivity and selectivity requirements of challenging multiclass methods, improvements in MS sensitivity, and the reduction in MS pricing. In some cases, detector sensitivity is outpacing instrument and analytical column designs, which should prompt further research and subsequent improvements. Miniaturization of instruments, and the trend toward “black-box” applications continue to surface. These instruments are generally intended to cater to field applications and highly routine operations.

Christophe Clarysse: There is still work to be done around capabilities for increasingly lower detection limits and in the chromatography process itself. Miniaturization and the need for faster analysis is creating opportunities for chips technology or low thermal mass

Full automatization of sample preparation and multiple detection channels are helping to address the need for more specific and confident results with shorter turnaround times.
systems together with new micro-detectors and mass spectrometers. Portable GC–MS with on-field sampling techniques is the most important growth driver in GC and brings immediate results in various fields such as air pollution or soil analysis.

In classical GC, we observe a global trend towards hyphenated technologies, such as thermal gravimetry combined with infrared (IR) and GC–MS, to characterize advanced materials and microplastics. This “best of both worlds” approach brings more information-rich data to scientists and technicians in a single run.

**Eric Denoyer:** GC is not going away any time soon. While it is a mature technology, there are still many important applications that depend on GC, such as monitoring climate change, supporting petrochemical processing, and assuring purity of pharmaceuticals from residual solvent residues. However, especially for many food and environmental applications, the future will see more and more GC systems coupled to mass spectrometers. Notably, triple quadrupole GC–MS will be deployed more and more routinely.

In the future, micro-GC will continue to be valued for its convenient small form factor and rapid cycle times. This makes it ideal for “going to the sample”, for example in reaction gas monitoring — an application that is growing, especially as alternative biofuel research is increasingly funded. Also, as natural gas grows in popularity as a fuel source, micro-GC is being used more and more to verify calorific value as a measure of quality and economic valuation.

**Matthew Edwards:** With the use of GC×GC becoming routine, we are seeing a resurgence in the use of single-channel detectors, such as the simple, robust flame ionization detector (FID) or highly sensitive and selective detectors like sulphur chemiluminescence detectors (SCD). Quality control laboratories that would have previously resorted to MS in an attempt to deconvolve complex samples now benefit from the enhanced separation of GC×GC coupled with single-channel detectors, while in discovery applications, parallel detection is on the rise for fully automated qualitative MS and quantitative FID workflows.

In the cannabis industry, the analysis of terpenes by GC–MS has been particularly problematic. The extreme diversity of the terpene and terpenoid classes, as well as their similar spectra, result in deconvolution difficulties and poor data quality, but physical separation by GC×GC allows confidence in results even with simple FID, as well as a wide dynamic range and robust quantitation.

**Chris Rattray:** The future of GC and GC–MS will continue to focus on platform miniaturization, reduced analysis times, increased sensitivity, and more rugged chemistries in the sample pathway. For example, electrical and mechanical advances will continue to reduce the size of GC ovens and MS detectors. Reduced analysis times will come by the way of shorter and/or narrower bore columns coupled with a more maintenance-friendly option to thermally-resistive column heating, a technology the market as a whole has been unwilling to adopt. MS will continue to increase in sensitivity, such as lower detection limits, through...
We are seeing an increase in discovery-based approaches, where workflows that are typically seen in the ‘omics’ fields are now expanding to other application areas.

more efficient generation and transfer of ions. Instrument uptime will be maximized through the development of more rugged surface chemistries and easily replaceable guard assemblies. We also expect to see greater adoption of tandem mass detectors as their price and footprint continues to drop. Ultimately, the future of GC or GC–MS may be uncertain with the potential adoption of ambient/atmospheric pressure ion sources such as desorption atmospheric pressure photoionization (DAPPI), desorption electrospray ionization (DESI), and/or direct analysis in real time (DART). These ionization techniques are currently applied without the use of a GC system. The future is unclear as to whether or not these ionization techniques will be incorporated with the use of a GC or eliminate the need for a GC system. Until that time, instrument manufacturers will continue to innovate in all the aforementioned areas.

**LCGC: What is the GC or GC–MS application area that you see growing the fastest?**

**Christophe Clarysse:** This tends to depend on which geographies you are talking about. Emerging markets such as India or China see their regulations growing rapidly especially in air and water monitoring, and also in food quality due to globalization, so this is driving GC and GC–MS demand. Furthermore, pharmaceutical companies have invested a lot in production plants (especially in China, India, and Israel to lower production costs) and require routine QA/QC systems under GMP-regulated environments. In more mature markets, such as North America and Europe, cannabis and hemp markets also continue to be a growth enhancer for GC as well as food safety and QA/QC laboratories that are expanding their GC and GC–MS use faster than say the academic or R&D service areas. High-throughput systems or fully automated sample handling devices are also in higher demand and generally GC–MS systems have become accepted as an important tool globally as a result of their more specific and sensitive detection capabilities and simplified use.

**Eric Denoyer:** Detecting nitrosamines in pharmaceuticals by GC–MS has grown sharply this past year as pharmaceutical companies race to assure their products are free of these contaminants. Air and water quality continue to be recognized as critical, not only to human health, but also to the health of the planet as a whole. This is a growing application area especially in markets such as China and India. As new materials are developed and more commonly used, their presence in air and water are increasing. Detection of perfluorinated alkanes (PFAS) in water is a major growing concern. Microplastics finding their way into waterways and associated biota is also a rapidly growing area of research and regulation development.
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The recently approved Senate Bill 1422 in the State of California specifies funding for developing analytical methods for measuring microplastics with an intention to set appropriate regulatory levels over the next several years. The growing legalization of cannabis worldwide is driving rapid demand for purity and potency analysis. GC–MS Triple Quad (TQ) is an especially popular technique to determine pesticides in plant materials, and demand for this application is growing rapidly. Recent legalization of harvesting hemp as a multipurpose raw material is also driving a growing need to verify its authenticity and freedom from THC using GC–MS.

Matthew Edwards: An obvious one is the cannabis industry, and this is expected to increase further when regulated testing methods are enforced. We have also seen a rapid increase in biomarker discovery — from samples such as breath, urine, and saliva — in an effort to develop non-invasive diagnostic tests. Both application areas will benefit from the adoption of routine, robust, fully automated workflows that encompass everything from sample preparation to data handling and reporting. They deal with high numbers of samples, and automation could help to develop standardized approaches across these industries.

Chris Rattray: Emerging contaminants in the environment as well as the expanding legalization of cannabis are two areas that have seen growth and change in analytical approaches and techniques. While the risk to human health has not been determined for emerging contaminants, scientists, and regulatory agencies support research to document these compounds, most notably in drinking water. The brominated flame retardants have gained notoriety given their ubiquitous use in products and persistence in the environment. While cannabis potency is best performed by LC; GC is most suitable for residual solvents and terpene analysis. Cannabis concentrate products such as tinctures, edibles, and oils are extracted in solvents and those products must be analyzed by GC to verify they are free of solvents prior to human consumption. Terpenes are a class of compounds responsible for the flavours and aromas in cannabis. Cannabis growers are interested in determining the ratio of terpenes in different strains for their possible therapeutic effects.

LCGC: What obstacles stand in the way of GC or GC–MS development?

Christophe Clarysse: We often say that virtually nothing is impossible in GC. Initially designed for small volatile and non-polar molecules, recent column developments have brought GC and GC–MS into the extended application ranges of polar or larger molecules analysis. As an example, the recent development of thermally-resistant polar stationary phases, such as ionic liquids, removes traditional barriers. Hence, GC development can no longer be considered in a silo and should be developed together within the application need — including consumables, sample matrix handling, and software solutions. Many of the recent developments in GC have
also brought specific solutions to specific needs or constraints in niche markets such as multidimensional analysis or LC–GC for mineral oil saturated hydrocarbons/ mineral oil aromatic hydrocarbons (MOSH/MOAH) analysis. From a GC-solution-provider standpoint like ours, there is no limitation around GC's technical capabilities. The challenge is more around seeing research and development return on investment (ROI) for GC solutions that are created to address small/niche markets and realities around what customers are able and willing to invest in terms of innovation.

Eric Denoyer: The ever-increasing complexity of materials needing to be analyzed by GC or GC–MS poses a real challenge to technology and instrument development. Advanced composite materials are increasingly used in new product design. Just compare today’s tennis racket, road bike, or airplane wing to those of 30 years ago. The complex composition of new materials imparts finely tuned performance characteristics that have to be maintained within tight tolerances. This means that analytes have to be separated from a complex matrix of concomitant material. These more difficult separations require even better chromatography, and place a real constraint on instrument-size reduction, or throughput improvements. However, the growing use of MS/MS techniques greatly simplifies data for complex mixtures, improving specificity and certainty.

Matthew Edwards: The global shortage of helium has meant that new laboratories struggle to secure helium gas cylinders, so there is a desperate need to develop GC–MS technology that is fully compatible with a hydrogen carrier — ideally with the performance levels we’ve come to expect when using helium.

Chris Rattray: There are some complications in the development of the GC–MS platform, especially if you consider tandem mass analyzers. The past decade has seen the refinement of the gas chromatograph as a platform. Improvements in flow control and rapidly responding thermocouples and heating elements have greatly increased retention time reproducibility for methods with complex temperature programmes. On the other hand, detector sensitivity has been improving by an order of magnitude every few years. There are now single quadrupole instruments available from multiple vendors with sources that are so efficient at generating and delivering ions to the mass analyzer that their sensitivity has greatly outpaced improvements in the inertness of the sample pathway, so most end users are not able to take advantage of this leap in sensitivity. The inert sample pathway is one major challenge for the consumables vendors. Short narrow columns could be used to reduce the analyte residence time on-column, which reduces the probability of degradation or adsorption. Faster run times are always desired, however, this raises its own issues. Column selectivity is temperature-dependent, so to preserve the separations we are used to, we would need to be capable of very fast ramp rates,
and fast ramp rates require very fast and accurate electronic pressure control.

**LCGC: What was the biggest accomplishment or news in 2019/2020 for GC or GC–MS?**

**Christophe Clarysse:** We have already reached next generation GC–MS. From my point of view, the biggest recent accomplishments in GC have been focused on sample pretreatment before the GC analysis, such as thermal desorption, online analysis, and on-site sampling devices. New detection systems, such as plasma detectors, have also become more popular while many traditional GC–MS/MS applications are beginning to move towards LC–MS/MS as a result of new ionization techniques. The latest data handling systems have also brought together GC, GC–MS, LC, and LC–MS/MS under the same software platform, making the workflow inside laboratories much more flexible and easier to operate by “generalist” chromatographers. 

**Eric Denoyer:** By far the biggest achievement in 2019/2020 was smart-connected technology, developed originally for cutting-edge next-generation systems, now being extended to mainstream GC and GC–MS systems. The fact that this enabling technology is now available in market-leading mainstream systems, across high-end, mid-range, and micro-GC platforms, means it will get into the hands of far more people. This is an inflection point in terms of productivity improvement and resource deployment that will have a huge lasting impact on efficiency gains in the analytical industry. As importantly, laboratories are returning to work in split shifts to minimize on-site staff numbers during the COVID pandemic. This means expertise on-site during a single shift is unlikely to be available on all three extended shifts. Smarter instruments help troubleshoot faster to get up and running sooner. Remote connectivity helps connect a remote expert to the on-site instrument. These smart connected functions are invaluable as laboratories return to work in a pandemic. 

**Matthew Edwards:** Modern GC–MS and GCxGC–MS instruments allow us to gain greater insight into sample compositions than ever before. Until now, data analysis has remained a challenging prospect. The rise in untargeted ‘discovery-based’ workflows has finally put pressure on instrument manufacturers to develop software that can tackle these huge volumes of data. New software tools are now available to extract meaningful results using all of the raw data, without resorting

Emerging markets like India or China see their regulations growing rapidly especially in air and water monitoring, and also in food quality due to globalization, so this is driving GC and GC–MS demand.
to hours of manual pre-processing or complicated statistics - making discovery workflows more amenable to routine labs.

Oliver Lerch: From the perspective of a product manager for automated sample preparation, I see that a number of established, effective, and rugged sample preparation techniques are still performed manually by many laboratories worldwide — even though they could be automated with existing means. Automation is definitively still on the rise, contract laboratories and the chemical industry want to automate as many manual workflows as reasonably possible and this applies to all types of chemical analysis, not just LC– and GC–MS applications. This means that instrument manufacturers need to invest more in the development of innovative hardware and especially software solutions. I see the trend of coupling diverse instruments from different manufacturers under one communication protocol. This could give the analytical world a boost similar to what we experienced during the “golden years” after GC–MS and LC–MS had first emerged.

Coupling or hyphenating instruments requires new soft- and hardware interfaces. Establishing generic communication/ interface standards such as the standardization in laboratory automation (SiLA 2) or open platform communications unified architecture (OPC UA) could be a valuable first step. Our efforts should result in the availability of a toolbox of techniques that “just” need to be connected to gain significant new benefits for the user. Mobile robots delivering samples from the refrigerator to a pipetting robot and finally to an analysis system are not just a dream any more. The future

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of analytical chemistry will increasingly be the domain of software/firmware programmers — like most areas in the our future life. Accordingly, laboratory staff will need a higher level of training.

**Mihir Thakar:** Sample preparation in the proteomics field is one of the most critical and under-focused areas as a result of the meticulous research that is required before upgrading conventional procedures. While the research may be time-consuming, the impact to the results are substantial, such as speed, reproducibility, sustainability, and cost-effectiveness. Some examples of these advances are trypsin spin columns for quick peptide mapping, rapid glycan analysis tools for digestions, labelling, and clean-up, and specialized spin cartridges/columns for complex post-translation modification analysis. As the goal of sample preparation is to balance time savings and the integrity of results, developing high-throughput workflows while minimizing protein modification helps to achieve this.

**Stig Pedersen-Bjergaard:** I think sample preparation is going “micro”. Microextraction has been around for 30 years, so it is definitely not new. A lot of microextraction is published in the scientific journals, but implementation into routine laboratories is slow. I also think the next generation of analytical chemists will be much more concerned about the use of hazardous chemicals, and they will prefer microextraction for environmental reasons. This generation are also born with smartphones in their hands, and will use them as much as they can for chemical measurements. Of course, this requires sample preparation, not with separation funnels, but with microextraction integrated into devices compatible with smartphones!

**LCGC:** In your opinion, what is the future of sample preparation?

**Marisol Cárdenas:** We should emphasise that although sample preparation is very often identified as a bottleneck, sometimes it is an unavoidable step. Bearing this in mind, reduced sample manipulation, either by automation or the design of selective extractant phases that could isolate the target analyte or family of analytes is essential. Additionally, the integration of these extraction units with the instrumental techniques, and specifically high-resolution mass spectrometry is a clear trend in sample preparation.

**Oliver Lerch:** Generally, I see a bright future for sample preparation. Questions of cost for each sample, miniaturization, and sustainability are gaining importance. In my opinion, microscale sample preparation techniques that can be combined and automated will have a promising future.

A good example is the analysis of microplastics in different compartments of the environment. Currently, the analysis is performed predominantly manually using spectroscopic methods or even counting particles under a microscope after sample pretreatment. These approaches are extremely tedious and result in a throughput of only a couple of samples a day. The combination of pyrolizing a complex soil or
filter sample in a thermogravimetric oven, collecting the evolved breakdown products, and analyzing them for characteristic compounds by thermal desorption GC–MS offers a quick screening tool (TED-GC–MS) for microplastics in complex samples.

Moreover, microsampling and analysis techniques for blood are gaining importance. In this context dried blood spot (DBS) sampling and volumetric absorptive microsampling (VAMS) play an important role because they enable safe and simple self-sampling in any location on the world. This translates to more frequent analysis of important blood parameters and ultimately better patient care, a more effective fight against doping and drug abuse, and more meaningful pharmaceutical study results, respectively.

Mihir Thakar: Currently, with the technology that exists on the market, proteomic scientists can easily analyze protein modifications with moderate time and minimal errors. In the future, with improvements to the current workflow, it would make it possible to save even more time, including resources and human errors, while maximizing automation to increase output. Innovations in sample preparation automation equipment will lend to increases in productivity that all laborotories can process samples in a fast-paced laboratory environment for quicker and more reliable results.

Stig Pedersen-Bjergaard: As I mentioned before, future sample preparation will be based on microextraction, tailor-made for smartphones and other hand-held devices. Microextraction will also be implemented in biomedical research to assist soft extraction. In this way we can do extractions in living biological systems, without disturbing biochemical equilibria.

**LCGC: What one recent development in the area of sample preparation would you say is the most important?**

Marisol Cárdenas: It is not easy to choose one, but in my field of expertise, I would say that the use of nanostructured materials and new extractant phases such as supramolecular solvents (SUPRAS) or metal-organic frameworks (MOFs) have clearly contributed to increase the efficiency of sample preparation and to reduce the sample volume/chemicals making sample preparation more sustainable.

Oliver Lerch: In my view there has been no single ground-breaking new development. Nevertheless, combining different existing techniques will catalyze significant advances in the area of sample preparation and analysis overall. Reinventing the wheel for individual techniques is not as likely to make a difference as just combining established techniques.
Mihir Thakar: One of the most important recent developments in sample preparation is rapid glycan clean-up. Traditionally this workflow would take over two days of preparation and subsequent analysis. In order to get the results, the protocol required a daily glycan digestion followed by a tedious protein removal, 4-hour-long fluorophore tagging, and eventually led to clean-up by solid phase extraction prior to the LC–fluorescence detection (FLR) or LC–MS analysis. With improvements to this method, the workflow has been optimized to only a 30 min sample preparation procedure while still leading to accurate results.

Stig Pedersen-Bjergaard: From my perspective, which is from a pharmaceutical and biomedical angle, I think recent research on in-vivo SPME and LPME/EME are very important, but I am probably a little biased.

LCGC: What obstacles do you think stand in the way of sample preparation development?

Marisol Cárdenas: One difficulty that needs to be solved is the difficulty associated with the validation of analytical processes that implement new tools at the sample preparation level. The time required to modify official or reference methods always makes the advances proposed at the R&D step obsolete, even if eventually they are approved.

Oliver Lerch: Analytical chemistry and sample preparation in particular only get limited attention in chemical research. This is illustrated by the relatively small number of professorships for analytical chemistry and the low impact factors of analytical chemistry journals. I think this is one key factor that slows down new developments.

Manufacturers of sample preparation tools and systems have invented numerous new techniques over the past years. Nevertheless, many users take a lot of convincing and stick to tried and trusted products and concepts, which in many cases are of course methods that have been validated and proven over years.

From the manufacturers’ point of view, regulations also slow down innovation. This is especially seen in the field of clinical diagnostics. Instruments and tests need to be developed and manufactured according to in-vitro diagnostic legislation. After having passed such a complex and costly process successfully, the manufacturer of an in-vitro diagnostic test has no interest in changing anything in the workflow or instrumentation because this would result in the need for a recertification. The outcome is most clearly seen in clinical laboratories worldwide where LC–MS techniques have arrived with a delay of 10 to 15 years compared to other application areas, such as food safety analysis. The in-vitro diagnostic legislation is a barrier against using calibration-based techniques such as LC–MS and GC–MS, which are solely calibrated by the end user and not by the instrument manufacturer. Assuming that the instrument and the method are generally "fit for purpose", the quality of results is much more dependent on the quality of the work performed in the laboratory than on the instrument being manufactured according
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to IVD guidelines. Case in point: Personally, I would rather have my hormone levels determined by a validated non-IVD LC–MS test in an accredited clinical laboratory than by an IVD immunoassay in the same laboratory. Whatever the IVD regulations require, in my view a mass spectrum says more than an immunoassay. In my perspective, IVD legislation is the main impediment to the implementation of state-of-the-art techniques in the clinical laboratory and also slows down the development of innovative techniques, especially in small innovative companies.

Mihir Thakar: What we commonly see as a hurdle for sample preparation is not only a knowledge barrier around complete solutions but also having to work with analytes that are constantly changing, such as biologics in drugs development that are diversified in advanced segments of discovery biology. It is difficult to have a deep and extensive understanding for all of the biological workflows for diverse analytes that also have different clean-up and analysis requirements.

Stig Pedersen-Bjergaard: Analytical methods used in routine analysis are validated, and this is a big advantage in the way that we then know the data are accurate. Validation takes time and costs money, and therefore routine laboratories prefer to use their existing methods, including the sample preparation methods. Although a lot of new sample preparation methods are published in the scientific literature, they are implemented into routine analysis to a very small extent.

LCGC: What was the biggest accomplishment or news in 2019/2020 for sample preparation?

Marisol Cárdenas: After several years of evaluation of novel extractant phases and (micro)extraction formats, we have been able to catch the interest of the scientific community with sample preparation. This can be visualized through the consolidation of dedicated international conferences on this topic. Also, the proposal of thematic networks that join scientists working on sample preparation for sharing knowledge and providing visibility to the topic. The EuChemS Sample Preparation Task Force and the Spanish Network on Innovation in Miniaturized Sample Treatment exemplify this.

Oliver Lerch: Analytical chemists are increasingly focused on the sustainability of their laboratory operations, their techniques, and their methods. Guidelines for rating analysis methods with regard to environmental friendliness and sustainability have already been established over the past couple of years. Becoming aware of this was my personal highlight of the last year. For example, I listened to a presentation from a member of the “Green Analytical Project”. Analytical chemists have started to feel responsible for the future in terms of reducing the environmental impact of their activities, partly driven by young activists that make their voices heard all over the globe. That has impressed me and I propose that we as analytical chemists should strive for greener and more sustainable
analysis techniques. For example, the liquid–liquid extraction (LLE) with 50 mL of toxic dichloromethane is still widely used, but completely outdated and often unnecessary. We as a community should fix that as a helping hand to future generations.

**Mihir Thakar:** From analytical to large molecule sample preparation, some of the biggest accomplishments have come from coupling multi-functional sample preparation products with automation. The advantages of using multi-well products that can clean-up, extract, concentrate, remove matrix effects in parallel, while also using semi-automation or automation to speed up the method is a big achievement. Even using something as simple as a high-throughput magnetic separation device for immunocapture using magnetic beads has massive implications for improving on traditional ELISA methods.

**Stig Pedersen-Bjergaard:** I think it is very difficult to select a single accomplishment. I think the accumulated sample preparation efforts are the biggest accomplishment, to establish this as a scientific discipline and attract the attention of analytical chemists.

**DATA HANDLING**

**LCGC:** What is currently the biggest problem in data management for chromatographers?

**Shawn Anderson:** The biggest current challenger for chromatographers in managing data is integrating chromatography results into a larger data ecosystem. While there are a variety of different scenarios, a common example is where a lab manager would like the laboratory information management system (LIMS) connected to a chromatography data system (CDS). The sheer number of vendors, platforms, and IT environments in this solution space can be daunting. Fortunately, some options are now available that enable this CDS–LIMS connection with a few straightforward configuration steps.

**Darren Barrington-Light:** Data security and integrity, and ensuring this during the data’s entire life cycle, are key concerns for many chromatographers. This permeates to nearly all laboratories where data is
relied on for product release or any form of quality control. In compliant laboratories, the most recent focus is on data integrity and demonstrating control of processes by ensuring appropriate reviews of data are taking place. This is not about simply viewing audit trails and trying to identify anomalies but really understanding what events occurred in the system during the data life cycle that could affect results; such as manual changes on an instrument during an injection or manual integration of a chromatogram. Chromatography data systems that can highlight these incidents make it easy for reviewers to discover whether they did or, importantly, did not occur and investigate accordingly.

Another challenge we consistently hear from our customers and industry leaders is lack of integration between and across systems because of proprietary data formats or software incapability. For example, mass spectrometry (MS) usage in routine laboratories is becoming more prevalent and many software packages are not optimized for compliance or networking of these instruments leading to siloed data with inherent backup and archiving risks. This “siloing” ultimately limits the value of the data collected. A laboratory-wide CDS that is designed to support both chromatography and MS in a network environment can connect these workflows and deliver compliance with a common data format stored in one central location.

Proprietary data formats also lead to data silos but through more widespread implementation of open standards for data, we can begin to realize the full value of chromatography data.

**Graham A. McGibbon:** Productivity is a prime goal of chromatographers, so a major daily challenge is to rapidly and easily collect, compare, and interpret data to deliver results — from a collection of different instruments, CDSs, and methods — for multiple samples and injections. Even with “enterprise-scale” systems there will surely be heterogeneity in hardware and software versions, detectors, methods, various metadata, and digital data formats that can complicate rapid results assembly for decision-making. Some may face difficulties innovating to enhance quality while satisfying compliance requirements.

**Stephen McDonald:** Our focus has been in the laboratory performing routine analyses where chromatography data systems are the most actively used tools to generate data. The most important requirement that we gathered was that any solution used in these types of laboratory-based businesses must be able to be in an operating state that complies with local regulatory requirements. Beyond the requirements of compliance, one must then resolve the issues facing chromatographers, which currently focus on consistent and accurate integration of complex chromatograms, particularly for analyses such as impurity and stability evaluation. Second is the ability to pool and access large data sets, which can then be used for comparative trend analysis for the purpose of understanding.
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how to achieve better quality — currently a challenge because most businesses generate data in multiple data formats. This is particularly important in companies that see the value of method life cycle management as part of the adoption of new ICH guidelines such as Q12, and Q14 for method development. Traditionally the documentation supporting method development was considered outside the realm of “regulated data” but these new paradigm shifts, to include knowledge gathered during method development and include in a regulatory submission, move that line of “compliance”. These emerging expectations require tools that can store large amounts of data, extract and compare across multiple data formats, and finally store information over long periods of time whilst making it readily available for review and reporting.

**LCGC: What is the future of data handling solutions for chromatographers?**

**Shawn Anderson:** We feel the future of data handling goes beyond CDS and LIMS products. Our customers are telling us that they want (and need) to interrogate their data in new ways rather than the traditional “how pure is my sample” question. For example, can they extract causal relationships between product purity and yield, and any number of external factors such as raw material source, synthesis step variation, and even shift productivity. To do this, they need access to a much larger data lake which contains all of this information, including the chromatography results.

**Darren Barrington-Light:** I see three main trends: First, the adoption of cloud and deployment of the CDS as software as a service (SaaS). This provides on-demand data handling across the laboratory and delivers the highest levels of data security while driving down operational costs for in-house administration and capital expenditure for server hardware. Second, I envisage an ecosystem of connected applications that would allow laboratories to build their own solutions based on their workflows. Furthermore, the adoption of cross-supplier standards for data, such as those supported by the Pistoia Alliance, have the potential to transform the laboratory by enabling cross-technique and cross-supplier review of data, enabling a truly connected digital ecosystem that offers collaboration and helps to accelerate scientific discovery, drive productivity, and minimize risk.

Third, many companies are establishing company-wide pools for all laboratory or even all analytical data, also referred to as “data lakes”. This data can then be associated with data managed in relational databases, like chromatography data. These organizations hope to use data lakes to improve data access and overcome silos. Data lakes would also

“Data security and integrity, and ensuring this during the data’s entire lifecycle, are key concerns for many chromatographers.”
enable artificial intelligence (AI), machine learning (ML), and deep learning (DL) to extend the value of data.

**Graham A. McGibbon:** A shift and transformation of technologies to support a wide range of cyber-resilient, enterprise-scale, virtualized, distributed, and services-based data handling solutions is already taking place for all data analysts, including chromatographers. Innovative and sophisticated chromatographic instruments and CDS software will still require some proprietary technologies for optimal control, data acquisition, and pre-processing. Future systems will simply or automatically and seamlessly be able to transfer captured data and results to other software systems.

**Stephen McDonald:** We hear that scientists need tools that can improve peak integration and automated creation of results for better accuracy and consistency, store large amounts of data in an accessible and open format, and extract and compare information over long periods of time and across multiple or unified data formats.

These tools will need to be able to share this information over large geographies and operate at performance levels that do not inhibit the use of those applications. The future tools must be “easy to use” and provide a guided workflow just like those we use today for banking and shopping online.

**LCGC: What one recent development in “Big Data” is most important for chromatographers from a practical perspective?**

**Shawn Anderson:** Plainly put, it’s the cloud. The value of having instantly scalable storage without having to negotiate with an overburdened IT department cannot be underestimated. There are many additional benefits such as simplified back-up/restore and connectivity across globally dispersed laboratories. Many software solutions now support cloud integration for these very reasons. Some vendors offer a stepwise approach based on comfort level and organizational flexibility. For example, a less flexible laboratory may only want to store data in the cloud, keeping other essential components on-premise, while an organization more open to change might want a fully cloud-based solution.

**Darren Barrington-Light:** Leveraging the power of the cloud has recently been made possible for chromatographers through support for infrastructure as a service (IaaS) in CDS and LIMS software. Uplifting central network resources, such as servers, databases, and file storage, to the cloud can deliver both cost-savings and performance gains. Using the elasticity of cloud computing, laboratories only need to pay for what they use and can quickly ramp up or down resources to meet local, regional, or global demands. This eliminates the need to spec servers for peak usage and can deliver extra compute power should it be required at peak times potentially delivering “workstation-like” performance in the network, even for large data sets like MS.

**Graham A. McGibbon:** We are so familiar with the term *Big Data* that it may be used
when it wouldn’t apply — most organizations’ own chromatography data is not considered “Big Data”. It may come from a variety of sources and each may contain many data points, but unlike genomic data, for example, the scale of data is not truly large, and data processing to a much smaller useful set of peaks is typically straightforward using traditional methods. Nevertheless, some big data technologies may be used to store and transfer chromatographic data more effectively or to assess the performance and usage of chromatographic equipment and data at an organizational asset level to help make educated decisions about future capital investments in hardware and software.

Stephen McDonald: The biggest development in “Big Data” is the speed at which we have seen its application multiply, today there are so many new applications being explored by so many. The number of players has dramatically increased and the sheer number of people and companies driving/collaborating on “Big Data” solutions has increased exponentially. Proposals for the application of “machine learning” to solve some of those challenges of complex integrations, and improvement and expediting for design of experiments (DOE) are some of the exciting things we are seeing.

A stepping stone on the path of “Big Data” is “automated system integration”, allowing data to flow safely and traceably, between” best-in-class” applications. This opens the door to innovation and leveraging the data a scientist may already have to create smarter and more timely insights, whether this is in QC or in discovery of new molecules.

LCGC: What obstacles do you think stand in the way of chromatographers adopting new data solutions?

Shawn Anderson: The bad news is there are many obstacles. The good news is that they can all be overcome with an open attitude and a bit of persistence. One common barrier that we encounter is a reluctance to change what has always worked well in the past. While another is an often unfounded fear of increased complexity and cost. Vendors in the industry share the responsibility with customers to make the future accessible, by streamlining adoption steps, proving equivalent functionality, and reducing validation costs.

Darren Barrington-Light: For many chromatographers the biggest obstacles to adopting new solutions are compliance, (re)validation, and previous investments into legacy systems with proprietary data formats. The big challenge is adopting new technology capabilities while preserving existing information and capabilities of current systems. Aligning the various stakeholders in large organizations with complex structures and competing goals is another. IT may want to place all new applications in the cloud, but the laboratory may be hesitant to store their valuable data, and quite possibly intellectual property, in the cloud due to perceived security risks and uncertainty around validation requirements. Fortunately, these concerns can be mitigated through appropriate contracts with internet service provider (ISP) and cloud providers. Still, for many users
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just the idea of redeploying and revalidating their systems is unpalatable and can outweigh any potential benefits they may see. Companies can provide validation services and documentation that alleviate these pains, streamlining the process and enabling chromatographers to take advantage of the latest data handling solutions available.

Graham A. McGibbon: Chromatographers will continue to value getting reliable results faster and more simply and being able to design effective experiments to characterize and understand materials. So, to rapidly and consistently exchange methods, data, and results, they need to have simple but extensive programmatic application programming interfaces (APIs) and user interfaces (UIs) that allow easy connections between the CDS and other software systems and informatics tools. The consequent challenge will be to work collaboratively using those other systems so their key results — namely assigned and integrated peaks having properties such as relative area and widths that are the deciphered outputs of the chromatographic data — can be examined and understood in larger contexts, such as making quality materials.

Stephen McDonald: For most of our customers the need to be compliant and to maintain a strong data integrity position is the first hurdle any new technology must clear before being accepted. Currently the barrier to adopting an improved software update, instrument, or analytical method is the hurdle of qualifying, verifying, or validating that change.

There is a big drive to work with regulatory agencies and expert groups to change this stagnating paradigm in the regulatory space, and then provide tools, data, and services that customers can leverage to properly risk-manage changes to make their laboratory processes faster and more automated. This, at the same time, will help make their products safer. These concepts are being promoted by the FDA’s center for medical devices (CDRH), such as the case for quality computer software assurance (CSA) guidance, and are being promulgated to reduce the barriers to innovation and improving quality and safety, without introducing new risks.
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