

# the Analytical Scientist®

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## The Hidden “Me” in Team

*As we prepare to celebrate 100 issues of The Analytical Scientist, we recognize that we couldn't have done it without you. “Me?” you ask. Yes, you.*

Editorial



Some of us – and hopefully a good many of you – can remember Issue #01 of The Analytical Scientist...

Thank you to the pioneering contributors and interviewees in our inaugural issue: Samuel Kounaves, Ian Jardine, Caroline West, Luigi Mondello, Peter Tranchida, Norman Dovichi, Amanda Hummon, Barbara Bojko, Janusz Pawliszyn, Alun Cole, Liz Woolfenden, Marco Koenen, Eric Yeatman, Terry Berger, Razi Imam, Hans Versnel, Willem van Raalte, and Fasha Mahjoor.

And thank you to our first commercial partners: AkzoNobel, Tosoh, Thermo (Fisher) Scientific, Shimadzu, Leco, Markes International, HPLC (2013!), Pittcon (2013!), and PSS.

January 2013 seems like a very long time ago now – possibly because some of us have been intimately involved in the 98 issues of The Analytical Scientist that followed. Apologies, but we don't have the space to name all those who contributed editorially or commercially to issues 2–98 – but our eternal thanks is yours.

We launched The Analytical Scientist with a bold mission: to record, scrutinize, and celebrate all endeavors in the analytical sciences. And we've been doing it ever since. How? By listening to as many of you as possible; by seeking out the opinions of (vocal) leaders in the field; by keeping our ears to the ground for the latest challenges; and by keeping our eyes open to the future. Having dedicated over 5000 pages to a very special bunch of scientists, we can honestly say that we could not have done it without you.

And so, if Rich Whitworth ever states (undoubtedly, tongue in cheek): “It was all me” – you have our permission to knowingly smile or tut-tut. Equally, as you become familiar with a new face at The Analytical Scientist – a big welcome to Editor James Strachan – you can rest assured that it's not all him either.

Next month, we look forward to welcoming everyone to our 100th issue, which we hope will be a true celebration of analytical scientists everywhere. In particular, we'll pay tribute to 100 individuals in The Power List – all of whom would say, if asked, that they could not have done it alone, before genuinely acknowledging the great efforts of their own excellent teams.

And so, though we can unequivocally agree that there is no “I” in team, there are plenty of you(s).

**Best wishes,**  
*Team TAS*



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The Hidden “Me” in Team,  
by The Analytical Scientist  
editorial team

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*Physical events are back! Are  
you ready for lanyards, business  
cards – and SciX 2021?  
Rhode Island Photo by Craig  
Fildes / CC BY*

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Distribution: The Analytical Scientist (ISSN 2051-4077),  
is published monthly by Texere Publishing Limited, Booths  
Park 1, Chelford Road, Knutsford, Cheshire, WA16 8GS, UK.  
Single copy sales \$15 (plus postage, cost available on request  
info@theanalyticalscientist.com). Non-qualified annual  
subscription cost is available on request.

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## Marrying Up Proteins using Molecular Glues

**New research uses MS to identify new drugs that “glue” proteins together**

Protein interactions underpin every function of the human body. When they go awry, disease results. At present, drugs that can sever these interactions – and therefore halt disease – do exist. But that’s only half the story.

In some cases, absent or malformed protein interactions are the root of the problem and could benefit from drugs that serve as “glue” to bind relevant proteins together, restoring the correct balance of protein-protein interactions. Joint research undertaken by the Universities of Leicester and Birmingham in the UK explores this concept further.

Aneika Leney, lecturer in biological mass spectrometry at the University of Birmingham says, “Richard Doveston, the other lead author on this work, is my husband, so [our departments] were a logical connection! The project largely stopped under lockdown because we were unable to enter the labs so could not perform any experiments, but we

made the most of a difficult situation. It started with a conversation between my husband and I over a drink. We realized that a huge challenge in the ‘molecular glues’ field (his area of expertise) could be overcome using modern native MS technology.”

Using mass spec, Leney and colleagues separated out single proteins, protein-protein complexes, and any “glues” present. By monitoring what

happened when adding a mixture of potential glues to the proteins, the team was able to identify which offered the best performance from within a single mass spectrum.

What’s next? Leney believes that pharma companies can employ mass spectrometry as a screening tool to search for even more glues that can slow down disease progression or perhaps even treat disease.



### TIMELINE

## A Timeline of (Jim) Waters

**Looking back at select milestones in the life of this pioneer – and of his legacy: the Waters Corporation**

the Analytical Scientist

1925

James (Jim) Logan Waters was born in Nebraska, USA on October 7, 1925

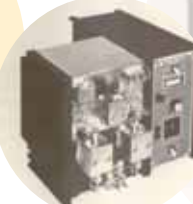


1958

After stints as a university math teacher, Naval officer, project engineer, and entrepreneur, Jim launches Waters Associates in the basement of Framingham Police Department, MA

1963

Waters debuts its first gel permeation chromatography instrument, the GPC 100



1967

The ALC 100 launches, setting Waters on the path to becoming “The Liquid Chromatography People”





## BUSINESS IN BRIEF

*Our round up of the latest business news – from FTIR spectroscopy for COVID-19 diagnosis to the first LC-Raman system*

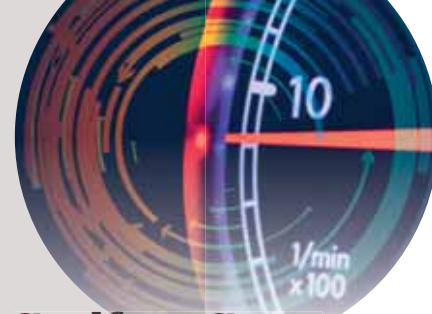
- MOBILion systems has launched its first commercial product based on SLIM (Structures for Lossless Ion Manipulation) technology developed by Richard Smith at Pacific Northwest National Laboratory. MOBIE, a high-resolution ion mobility (HRIM) product, aims to address characterization challenges faced during biopharmaceutical drug development (1).
- Honey fraudsters beware – Bruker has just released its latest NMR honey-profiling module that expands the database of reference honey samples and enables more advanced analysis of authenticity (2).
- Using an Agilent Cary FTIR Spectrometer, researchers have developed a rapid method for identifying those COVID-19 patients expected to develop severe symptoms. The technology, which is based on analyzing the infrared spectra of blood plasma, aims to free up healthcare resources (3).



- COXEM Co Ltd and Bruker Nano have together released the world's first tabletop scanning electron microscope (SEM) with energy dispersive spectroscopy (EDS) and electron backscatter diffraction (EBSD) systems. The aim is to provide a low-cost product for entry-level users of SEM, with the added advantages of EDS and EBSD (4).
- Shimadzu and HORIBA have come together to launch the first LC-Raman system. The unique combination of separation and visualization technologies strives to increase the accuracy and efficiency of measurements, while enabling detection of unknown components (5).

### References

1. MOBILion Systems (2021). Available at: <https://bit.ly/3B66DH4>
2. Bruker (2021). Available at: <https://bit.ly/2WpCdk7>
3. Agilent (2021). Available at: <https://bit.ly/3sT4xav>
4. Azo Materials (2021). Available at: <https://bit.ly/2Y1nWuD>
5. Shimadzu (2021). Available at: <https://bit.ly/3mBWspM>



## Swifter Spec

### Taking measurement into the ultrafast range with spectral vector beams

Many advances have been made in spectroscopy over recent decades, namely by manipulating the complexity of the light field in question. In a recent paper, researchers have developed a viable method for high-speed spectroscopic measurements with GHz readout rates by generating “spectral vector beams” (SVBs) – beams with different polarization states for each wavelength (1).

“Our work shows a simple way to have different polarizations for all color components of the laser. By using this light as a probe, we can simply measure the polarization to gain information about changes in the color spectrum,” explains Lea Kopf, lead author of the study (2).

SVBs enable measurements to be made using only polarization, making the process easier than conventional spectroscopy. The authors even propose the method could be used with supercontinuum light sources to enable measurements over the entire NIR or IR spectrum.

### References

1. Lea Kopf et al., *Optica*, 8, 930 (2021). DOI: 10.1364/OPTICA.424960
2. Tampere University (2021). Available at: <https://bit.ly/3zczylL>

1972

Jim uses the ALC 100 to help Nobel Laureate Robert Woodward's chief post doc isolate and purify vitamin B12

1980

The company merges with Millipore Corporation and expands globally

1996

Waters introduced the Alliance HPLC System at Pittcon, just as MS was emerging as a detector

2004

ACQUITY UPLC launches at Pittcon, fundamentally changing separation science

2017

Waters Corp establishes the Jim Waters Society in his honor to recognize employees for scientific achievement

2021

Jim passes away at 95



Credit: Barbara Wier



## Small Molecule Discovery – and Make It Snappy!

### An MS-based algorithm could transform natural product drug discovery

Researchers across the life sciences face the crucial challenge of correctly identifying small molecules in a sample. Historically, natural product drug discovery has been a low-throughput process that depends a lot on luck – just think of how penicillin was discovered! Though recent decades have shown significant advances in genomics and high-throughput MS-based data collection, trawling databases for this information is difficult and takes time. To add to this, existing approaches are based on chemical domain knowledge and often fail to explain many of the peaks found in mass spectra.

Now, a team of researchers from Pittsburgh's Carnegie Mellon University and Russia's St. Petersburg State University have created an MS-based algorithm that can quickly and accurately identify whether a particular molecule is truly

new or has previously been discovered.

"When we started this study, efficient and accurate methods for identification of small molecules from their mass spectra were not available," says Hosein Mohimani, part of the research team. "We had previously developed scalable methods (such as Dereplicator and Dereplicator+) for identifying small molecules, but they failed to correctly identify a large portion." MolDiscovery builds on these previous attempts by combining machine learning and expert knowledge to create theoretical MS fragmentation patterns from the molecular structures and scoring these against query mass spectra.

"Our results showed that molDiscovery outperforms state-of-the-art methods in accuracy and efficiency. Additionally, unlike existing machine learning methods, molDiscovery generalizes well to unseen data," says Mohimani. In fact, the paper reports that molDiscovery identified six times more unique small molecules than previous methods.

But the researchers don't plan to stop there. They are already working on various extensions to molDiscovery and plan to incorporate expert knowledge from analytical chemistry literature into their model to further improve accuracy. "We are also working on more complex models that automatically learn unknown small molecule fragmentation rules. We also plan to integrate molDiscovery and its derivatives into our computational pipelines for high-throughput natural products discovery from multi-omic data, such as NRPminer and MetaMiner," says Mohimani. "We believe molDiscovery and its derivatives will play a crucial role in shaping the future of data-driven natural product drug discovery."

#### Reference

1. L. Cao et al., *Nat Comms*, 12, 3718 (2021). DOI: 10.1038/s41467-021-23986-0.

## Stashed Skull, Hidden Dragon (Man)

### Once stowed away in an abandoned well, analysis of a Hominin fossil suggests we've found a long-lost sister lineage

A team of researchers from Hebei GEO University, China, have recently published

findings that suggest a human fossil known as the Harbin cranium represents a new lineage in the *Homo* family tree – and potentially our closest relatives (1, 2, 3).

One of the best preserved human fossils, the Harbin cranium was discovered in the 1930s near the Songhua River in Northeastern China – but it has raised questions ever since. To confirm the provenance of the skull, the team analyzed the concentrations of rare earth elements and the strontium isotopic ratio via ICP-MS, followed by XRF fluorescence spectroscopy to determine the distributions

of these elements. The results confirmed the fossil does indeed hail from the Harbin area, with direct uranium-series dating placing it in the late Middle Pleistocene era.

Based on further morphological evidence, the authors suggest the Harbin skull should be recognized as a new sister species in itself – the *Homo longi* or "Dragon Man." Though still up for debate among scientists, such a classification would disrupt our current understanding of human evolution.

References can be found online





## IMAGE OF THE MONTH

### *Positively Medieval*

A group of windows from Canterbury Cathedral may be the oldest stained glass windows in England, according to a team of scientists from UCL and conservators from Canterbury Cathedral. The researchers used X-ray fluorescence spectrometry – specifically, a portable version of the technique, customized with a 3D-printed attachment – to date the windows.

Would you like your photo featured in Image of the Month?  
Send it to [lauren.robertson@texerepublishing.com](mailto:lauren.robertson@texerepublishing.com)

## QUOTE OF THE MONTH

*"One of my former students was asked if he had learned a lot about chemistry from me. He said, 'Chemistry? That came easily. We learnt how to drink beer, how to travel around the world, how to stay up late entertaining people and still get up the next day to give a lecture at 8am. We learnt from Professor McNair how to live and enjoy life!'"*

Harold McNair – a titan of gas chromatography – back in 2016.  
Harold passed away on June 27, 2021. <https://bit.ly/3Bhks5E>.

## Putting Pen to Tumor

**The MassSpec Pen looks set to transform cancer surgery with encouraging new results**

Many of you will already be well aware of the MassSpec Pen, a handheld MS device capable of nondestructively diagnosing human cancer tissues. In fact, we covered the technology back in 2017 when it began to make headlines. Now, the first diagnostic results have just been published (1) – and they're pretty exciting.

In case you need a refresher, the device works by dissolving the metabolites from a tumor's microenvironment in a droplet of water and then analyzing them via MS. The aim is to make surgical cancer removal easier for clinicians by offering a faster, more accurate alternative to tumor margin evaluation than traditional frozen section analysis.

After the pandemic called a halt to testing of the device in surgeries, the team are now back in operating rooms and have used the pen in more than 150 human surgeries so far.

"These results show the technology works in the clinic for surgical guidance," said lead author Livia Schiavinato Eberlin in a press release (2). "Surgeons can easily integrate the MasSpec Pen into their workflow, and the initial data really supports the diagnostic accuracy we were expecting to achieve."

The current study in pancreatic cancer surgery is the first to have results published, but the team plan to continue testing the pen in other cancers, with results expected to be published soon.

### References

1. Mary E King et al., PNAS, 28, e2104411118 (2021). DOI: 10.1073/pnas.2104411118.
2. UTNews (2021). Available at: <https://bit.ly/2TFH7rY>.

## We Need to Talk About Clinical Representation

**Alzheimer's research should benefit all, regardless of ethnicity or race**

*By Renā Robinson, Associate Professor of Chemistry, Dorothy J. Wingfield Phillips Chancellor's Faculty Fellow, Department of Chemistry, Vanderbilt University, and Department of Neurology, Vanderbilt University Medical Center; Leader of Outreach, Recruitment, and Engagement, Vanderbilt Memory and Alzheimer's Center; Training Faculty, Vanderbilt Brain Institute, Vanderbilt Institute of Chemical Biology, Vanderbilt University, Tennessee, USA; NOBCCbE President-Elect*

As of today, there is no cure for Alzheimer's disease (AD). Historically, Black people and other ethnic minorities have been underrepresented in clinical research. We have a duty to ensure that our greatest advances in scientific research are for the benefit of all. These statements, at least in my view, are simple facts. Therefore, excluding minority groups from Alzheimer's research is not only a disservice to them, but to the entire population, because it means we do not have a complete understanding of the disease. If we want to get serious about finding a cure for AD, we need to ensure we're including representative samples in our clinical studies.

Of course, this holds true across many different research areas, but our group's focus – and my expertise – is in AD. In recent months, we've focused a lot of effort on understanding the proteomic and lipidomic influences of AD across underrepresented groups



### In My View

*Experts from across the world share a single strongly held opinion or key idea.*

– and it has become apparent that we have many challenges still to overcome in ensuring that clinical research is truly representative.

First, we need to ensure that everyone values true representation in their study populations. This may seem obvious to some, but the lack of diversity still seen in many cohorts would suggest that not all research communities agree. To start with, we should look at cohorts' diversity and ask whether they are inclusive. Some progress has been made with certain funding agencies, such as NIH, recognizing the importance of this work and trying to move toward equity in research – but there is still much more

*“We’ve focused a lot of effort on understanding the proteomic and lipidomic influences of AD across underrepresented groups.”*

to be done to understand how systemic racism impacts our ability to perform outstanding clinical research.

I believe it is imperative that diversity, inclusion, and equity are built into the peer review process. We might have trainees from diverse backgrounds, but we need to ensure that work that is creating inclusive studies is valued and supported. We also need to recognize that there is some way to go to rectify issues of the past (for instance, current discrepancies with the level of funding and support available to researchers interested in doing diversity and inclusion work). To support this effort, I believe there should be more accountability within these processes; we should be asking people to justify the lack of diversity in their cohorts and to contribute to making their studies more representative.

Second, even if you do want to have diverse cohorts, you need to identify enough biospecimens from minority groups. I'm involved in encouraging research participation among different population groups – African Americans in particular. We need to improve educational awareness and share with our communities the importance of research overall, but especially with respect to disparities faced by particular communities.

One way we are trying to do this is through sharing positive messaging around research participation within the African American community. Until now, we've focused mostly on negative messaging and the barriers to research and not on facilitating that research. To counteract this, we try to capture authentic (and positive) messages from

people who have participated in studies, and highlight why they did so. We then include these stories in resources that are handed out at various centers recruiting participants for clinical research. We are also running a social media campaign and have created videos that can be used in outreach events, community settings, doctors' offices, and more. The idea behind all of this is to see whether this particular approach to storytelling is more effective than traditional (passive) approaches to recruiting people.

Clearly, much work still remains to ensure that the research community is undertaking truly inclusive studies and to fully understand the disparities present in AD. It's simply not possible to see the complete picture of this disease if we don't understand how it works – in everyone.



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## (NA)DES: Delivering on a Green Promise?

**Could (NA)DES help the field deliver on the 2013 Green Analytical Chemistry (GAC) principles?**



*By Lourdes Ramos, research scientist, Department of Instrumental Analysis and Environmental Chemistry, the Institute of Organic Chemistry (CSIC), Madrid, Spain*

The 12 principles of Green Chemistry were introduced by Anastas and Warner in 1998 (1). The aim of these principles is to reduce the chemical-related impact

on human health and the environment by designing customized, more efficient, and more sustainable chemical products and processes. However, only the 11th principle, aimed at developing real-time processes, was directly related to analytical chemistry, which led to the definition of 12 Green Analytical Chemistry (GAC) principles in 2013 (2).

Most of the GAC principles refer directly or indirectly to sample preparation, pointing towards the minimization or, whenever possible, complete elimination of this step of the analytical process. Yet, despite efforts over the past few decades, direct determination of specific sample components (by spectroscopy combined with chemometrics, for example) is only feasible for a rather limited number of applications. In practice, most sample-analyte combinations still require sample treatment before instrumental analysis – regardless of the technique selected for final separation and detection.

As a result, a plethora of novel miniaturized techniques have been developed in recent years – some of which have become well-accepted strategies for robotized and automatic treatment of gaseous and liquid matrices. Although equivalent developments for solid samples are still lacking, advances achieved in this research field over the years have been rapidly adopted by the analytical laboratories and commercial companies, thus contributing to the incorporation of GAC principles into analytical practice.

Nevertheless, other issues highlighted by the GAC principles have yet to be adequately addressed; for example, the need to simplify waste management (principle 7), the (already pressing) demand to avoid using hazardous chemicals in analytical chemistry (principle 11), and related to this, the

need to minimize analyst exposure (principle 12). In the late 1990s, research in this area benefited from the synthesis of room-temperature ionic liquids (ILs). ILs were introduced as a green alternative to conventional volatile organic solvents (VOSs) from fossil sources because of their negligible volatility, chemical and thermal stability, and low flammability over a relatively wide range of temperatures. Their tunable physico-chemical properties and tailored selectivity led to their rapid acceptance as green solvents in a variety of research areas, including the analytical field. Later on, their inherent toxicity and limited degradability led to their exclusion from the category of green solvents, thus promoting the development of a new generation of solvents, the deep eutectic solvents (DESs).

DESs were introduced in 2001 as eutectic mixtures prepared by mixing two/three accessible bulk, cheap, and non-toxic chemicals. Similarly to ILs, DESs are chemically and thermally stable, have low vapor pressures and flammability, while also exhibiting high viscosities, which limit their practical implementation in certain application

*“In practice, most sample-analyte combinations still require sample treatment before instrumental analysis.”*



areas. Additional concerns regarding the safety of some of these mixtures prompted a shift to the use of natural components as alternative ingredients for the synthesis of eutectic mixtures.

The first “natural deep eutectic solvent” (NADES) was synthesised in 2011. NADESs were initially used for the extraction of bioactive compounds from natural sources. However, during the last decade, the practicality of these green and non-toxic solvents has been gradually demonstrated in a variety of research areas, including pharmaceutical- and bio-orientated applications, food and environmental studies, and the development of new materials – again thanks to their tunable properties. The introduction of hydrophobic water-stable NADESs (hNADESs) in 2015 enabled application

to non-polar analytes not amenable by previously described DES – and promising results are increasingly published involving these solvents.

It is evident from these considerations that (NA)DESs are opening up a wide variety of new analytical possibilities that should be carefully considered and evaluated. More importantly, the results also point to (NA)DESs as an invaluable alternative to address the largely overlooked GAC principles concerning the nature and toxicity of the reagents used in the analytical practice and, in particular, for sample preparation.

Now, it is our responsibility as analytical chemists to increase the greenness of analytical methodologies and processes as much as possible, and to demonstrate our commitment

to reducing our potential impact on human health and the environment.

*The Sample Preparation Study Group and Network belongs to the Division of Analytical Chemistry of the European Chemical Society (DAC-EuChemS) and includes three working groups (WG): 1. Science and Fundamentals, 2. Automation, Innovation and Entrepreneurship, 3. Information Exchange and Networking.*

*The Sample Preparation Network welcomes new European and non-European regular members. Membership is open to individuals who subscribe to the objectives of the network and who are professionally engaged in or associated with sample preparation.*

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# P(r)aying for Authorship: Integrity in Publishing

**With authorship in journals for sale, we must all do our bit to maintain integrity in scientific publishing**



*By Victoria Samanidou, based at the Laboratory of Analytical Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece*

I recently received a message from a connection on social media who isn't an actual acquaintance. It read, "Hi Dr! We are submitting a research article to the [name of journal]. We wonder if you are interested to be added as co-author and can contribute an [X] USD amount in APC upon acceptance." I replied to point out that this way of publishing is unethical and not for me. A response. Apparently they were requesting not just my APC contribution, but also wanted me to proofread and review the manuscript for substantial revisions...

I denied the presumably misleading offer (the word "substantial" was a giveaway, because it appears in many guidelines for academic publishing). It did, however, highlight some of

the pertinent issues in scientific publishing. Article authorship, as we know, influences tenure, funding, and promotions. But what happens when undeserved instances of authorship become more commonplace? One should only be included as an author if they have contributed significantly to the work described in the paper.

Acknowledging specific contributions to a paper is not a simple task. It is impossible to quantify individual author contributions. Luckily, nobody is asking for that – but authorship should indicate a distinct contribution. Accordingly, authorship criteria should be clear from the early stages of a research project. No one should be added at the writing stage unless new data or expert interpretations are required.

The Committee on Publication Ethics (COPE) provides resources for authors and editors to support and ensure authorship integrity. Though there is no universal definition of authorship, COPE say that an "author" is generally considered to be anyone who has made a significant intellectual contribution to the research or study (1). According to the guidelines for authorship established by the International Committee of Medical Journal Editors (ICMJE), "All persons designated as authors should qualify for authorship, and all those who qualify should be listed." They also provide four criteria that must be met for an individual to be credited as an author (2):

- Substantial contribution to the study conception and design, data acquisition, analysis, and interpretation
- Drafting or revising the article for intellectual content
- Approval of the final version
- Agreement to be accountable for all aspects of the work related to the accuracy or integrity of any part of the work

Contributors who supplied assistance (technical, linguistic, reagent supply) but do not meet these criteria should be mentioned in the Acknowledgement section – not listed as an author.

Moreover, there are three types of authorship that are considered unacceptable. These are "ghost" authors, who contribute substantially but are not acknowledged; "guest" authors, who make no distinct contribution but are listed to help increase the chances of publication acceptance due to their stature; and "gift" or "courtesy" authors, whose contribution is based solely on a questionable affiliation with a study (such as a senior faculty staff member or head of project).

In my opinion, there should be a new addition to these unacceptable contributions: solely sharing APC in open-access journals. Because open-access publications continue to emerge and publication fees increase with a journal's reputation and impact factor, this problem will only become more prominent. This will be especially true for developing countries with low budgets and funding rates.

Fortunately, all journals and publishers – as well as institutes and organizations – have basic policies on publication ethics and on what they consider authorship. This is often stated in the journal's "information for authors" section. Confirmatory statements are also requested of authors prior to publication, as stated clearly in the journal's information for authors.

Responsibility for maintaining ethical standards in scientific publishing falls to each of us as individuals. We must all do our bit to ensure that the good name of "author" is not soiled for generations to come. How can we start? In my experience, be careful of authorship offers on social media, for one!

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# SciX: A NEW WORLD

As we take small steps to re-opening our world, SciX prepares to take a giant leap with the greatest scientific exchange in quite some time

That's right. After many months away from our favorite events (and friends), we are finally (somewhat) free to meet once more. SciX 2021 – the first physical event for analytical chemists in the pandemic world – represents a welcome milestone. And so we wanted to explore its offerings ahead of time to make sure you're all just as excited as we are! Grab your things, quick! We don't want to miss the keynote speaker in action...







## KEYNOTE SPEAKER: DAVID WALT

Hello! I'm David Walt – a Professor at Harvard Medical School. My research is largely focused on the development of diagnostic technologies to address unmet needs in clinical medicine. My lab has successfully translated multiple technologies into the marketplace – many through start-ups that I played a key role in establishing. The most famous of these is undoubtedly the microarray, which has now found a place in exciting applications the world over. That discovery also landed me a spot in the USA Inventors Hall of Fame alongside names as big as Thomas Eddison!

With SciX 2021 on the horizon, I wanted to excite and inspire with a sneak preview of my keynote speech. The topic: how to create a successful business in science. There's no formula for a successful company because every technology is different – and every company is different. Think of it like

raising kids – no two kids are the same, and what works for one may not work for the next. But there are some key considerations that remain for any business, namely the people and the different skills that they bring to the table. Scientists have a tendency to think that they can do everything themselves because science itself is so complicated. The reality of the matter is often entirely different.

I plan to talk attendees through a couple of my entrepreneurial journeys, as well as the lessons learned each time. What worked? What didn't? And why? The two that I've chosen to speak about turned out to be quite successful. Illumina is now the most successful genetic analysis and sequencing company in the world. The other, Quanterix, focuses on ultra-sensitive protein detection by capitalizing on technologies developed in my lab. It's been incredible to see some of our technologies make a real difference in the world. I want to help the next generation of scientists to do that, too!

I look forward to seeing you there!

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## ORALS ARE BACK! MEET THE SPEAKERS

Here, we catch up with a few of the speakers to cover just some of the depth and breadth you can expect to find at SciX 2021.

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## SURFACE-ENHANCED RAMAN SPECTROSCOPY (SERS)

*Laura Fabris, Associate Professor, Department of Materials Science and Engineering, Rutgers University, Piscataway, New Jersey, USA*

I'm looking forward to giving my talks on SERS – an area that I've been passionate about since my postdoc work. I

will cover how SERS can be translated from the lab to the clinic, our work detecting viruses with SERS, and how the interactions between target molecules and metal surfaces affect the SERS response – and how the SERS signal can also be used to understand these interactions!

SERS has many key characteristics, most importantly selectivity and sensitivity, that allow it to act as an excellent diagnostic tool. I would love to see SERS applied in such ways in the clinic – and with recent technological developments (a key example being portable equipment) this goal feels more within our reach than ever before! Our group works alongside clinicians and biologists to help push the technique forward and we're particularly proud of our work in virology. But that's not to say we haven't overcome many challenges along the way... Our vision is an advantage in the face of these challenges: we believe in what we are doing and are dedicated to seeing our vision realized.

I see a lot of work being published in this area that gives me



confidence that we are headed in the right direction. Many groups are collaborating with clinicians and biologists to address complex, long-term goals – which is very exciting! There's a way to go yet, but new tools like integrated AI will likely play a pivotal role in our success.

Our return to SciX marks not only the reprise of conferences, but also a return back to our normal, free lives. I've missed many friends dearly and SciX will be a great opportunity to be reunited with a number of them. In addition to the friendly atmosphere, I'm looking forward to the event for its great social events (the gala, for one!), insightful talks, and engaging discussions – it's a great opportunity for everybody, but particularly young scientists! I'll also have the opportunity to see many long-term friends and colleagues receive well-earned awards – and that will be lovely.

## IONIZATION TECHNIQUES

*Steven Ray, Winkler Assistant Professor of Chemistry, State University of New York at Buffalo, New York, USA*

I will be speaking about our work in microwave-enhanced ionization techniques for MS at SciX this year. As is the case for many, this will be my first in-person conference since the pandemic began. I'm excited to get back at it!

Microwaves are appealing for chemistry and plasma spectrochemistry applications for many reasons, and there is a large body of expertise available in microwave engineering. We thought it was time to exploit that expertise in our own field! After quite a learning curve we have reached the point where we can simulate, build, and tailor new microwave waveguides



for specific analytical chemistry applications.

We started by developing microwave plasma excitation and ionization sources for atomic spectrometry – several such sources are now commercially available! Now we have started to investigate how microwave fields can influence ionization sources for molecular MS and chemical kinetics... In the future, such systems may help us address challenging analytical problems, such as the determination of fluorinated-materials at ultra-low concentrations!

SciX is a conference that serves a community. It brings excellent science to an atmosphere that fosters conversation, fruitful debate, and networking. And, this year (as always), the research looks top notch.



## COVID-19 DIAGNOSTICS

*Katherine Hollywood,  
Senior Experimental Officer,  
Manchester Synthetic Biology  
Centre, SYNBIOCHEM,  
Manchester Institute of  
Biotechnology, University of  
Manchester, UK*

My SciX presentation is titled “COVID-19 Diagnostic and Prognostic Analysis using Mass Spectrometry: Weighing Viruses and Consequential Metabolic Response.” The focus: my recent involvement in two COVID-related projects. The first evaluated MS as a viral detection method for eventual clinical applications (see our recent feature: Putting MS to the COVID Test), and the second used proteomics and metabolomics analyses to identify additional prognostic markers.

The onset of COVID-19 placed a huge burden on national testing regimes, which relied heavily on RT-PCR. Our alternative viral detection method has multiple benefits. MS allows for viral detection with comparable sensitivity and specificity, but with the added benefit of multiplexing. Samples can be analyzed for COVID alongside other dominant viral loads, such as the winter respiratory virus panel. It also allows for the detection of mutations within the protein sequence. And, though infection rates are declining and vaccine uptake is increasing, population testing remains paramount.

We were lucky to be supported by partners in both the National Health Service (NHS) and the Department of Health and Social Care to make this project a resounding success. There are multiple rewarding and beneficial outputs from this work – like the potential translation of our method into the NHS – and it’s all incredibly exciting! I can’t wait to see what happens next. Want to know more? Come along to the talk – it’d be great to see you all there!

I’m presenting in the Charles Mann Awards session for Roy Goodacre (my PhD supervisor many years ago and the person who introduced me to metabolomics and MS) – a great honor. I’m also due to be a co-chair for the biopharma section of the conference, alongside John Wasylyk. I imagine the talks there will be just as wonderful as elsewhere.

Overall, SciX is a wonderfully friendly place that gives opportunities to so many people at crucial (and often early) stages in their careers. It’s a great place to gather ideas to really push analytical research forwards. After such a long time away from the conference hall, it’ll also be great to see some of the faces behind the many emails we have been exchanging!



## GEOCHEMISTRY

*Richard Hark, Department of Chemistry, Juniata College, Huntingdon, PA, USA*

SciX will be my first in-person meeting (as I'm sure it will for many others, too) since the end of 2019. I have given several virtual talks (all of which were fine), but the chance to interact with something substantially bigger than a 2" x 2" square on a screen is something I am looking forward to. One of the great things about SciX is the eclectic mix of talks and the opportunity to mingle with scientists working in multiple analytical fields.

I will be giving two invited talks, both involving the application of laser-induced breakdown spectroscopy (LIBS) – an atomic emission spectroscopic unique that's attractive in research on topics from forensics to cultural heritage object and space exploration. The two NASA rovers operating



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"THERE ARE MANY EXCITING TALKS AND POSTER PRESENTATIONS SCHEDULED FOR SCI-X AND I AM EXCITED TO TAKE IN AS MANY OF THEM AS I CAN!"

on Mars have LIBS units because it is essentially the only technique that can perform elemental analysis at standoff distances of up to tens of meters. All elements (hydrogen through uranium) have emission lines in the typical range that LIBS spectrometers operate (~200 to 900 nm) and the technique has very high throughput. Plus, commercial laboratory and handheld instruments are available, and analysis can be performed without sample preparation, making the technique especially useful for in-situ field work!

Most of my publications are focused on geochemical analysis, with a couple of papers devoted to the use of LIBS to identify the source of so-called "conflict minerals." I am also one of several authors on a review paper with over 250 citations on the application of LIBS for geochemical and environmental analysis. Unsurprisingly, my talks at SciX will be on similar topics: "Analysis of Geological Sample Suites with Laser-induced Breakdown Spectroscopy" and "Identification of Mahogany and Lookalike Wood Samples Using Laser-induced Breakdown Spectroscopy."

There are many exciting talks and poster presentations scheduled for SciX and I am excited to take in as many of them as I can! The plenary talks are always very interesting and allow me to learn about other areas of analytical science that could have potential applications in my current position. I look forward to meeting with old friends and making new ones. The annual meeting of the North American Society for Laser-Induced Breakdown Spectroscopy is also held at SciX; I am a member and officer of that group, and that makes me even more excited!



## ELECTROPHORESIS

*Susan Lunte, Director, Adams Institute for Bioanalytical Chemistry, University of Kansas, USA*

Lisa Holland and I are organizers of the sessions for the AES Electrophoresis Society. Among our duties is to hand out awards for a distinguished mid-career scientist (Nathan Swami, who has been a leader in the development of methods for separating cells via dielectrophoresis) and a lifetime achievement award (Juan Santiago, a pioneer in the field of electrophoretic separations responsible for much of the theory used today), which should be great fun!

Lisa and I have been involved in electrophoresis research since the early 1990s. In my case, this started with capillary electrophoresis and then later with microchip electrophoresis-based separations. Electrophoretic methods are very important and are used to separate everything from amino acids to neurotransmitters to whole cells and recombinant proteins. The challenge is to finetune these separations to give better resolution (for example, of cell types) more quickly (which is important in monitoring applications).

SciX will be my second in-person conference since the pandemic started, ACS being the first. It will definitely be good to see people and chat to them in person about their research. As for what to look out for at the conference, specialized groups like the AES are able to deliver their own symposia – so there's sure to be something relevant. I'm really excited for the one that we're running; a lot of leaders in the field are due to speak!

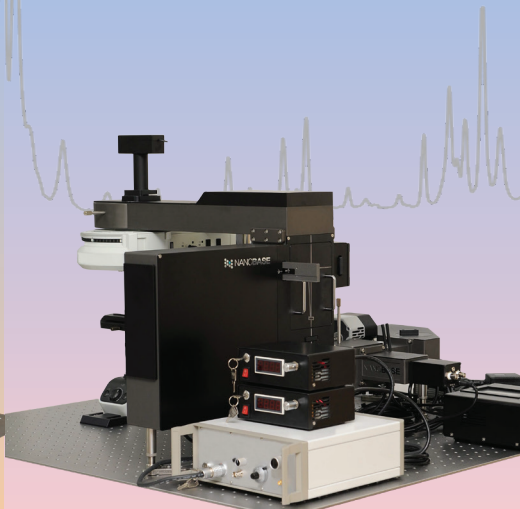
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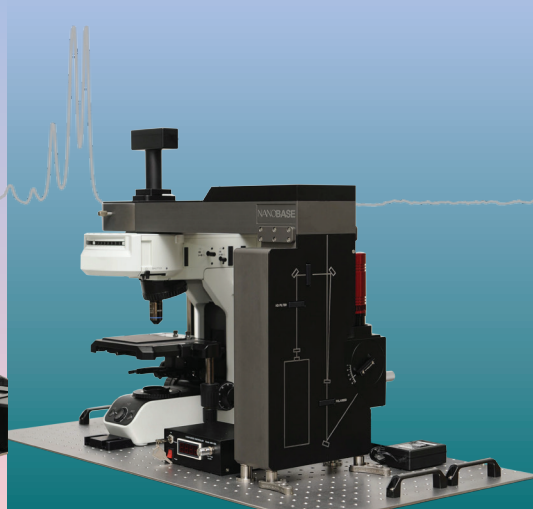
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## BIOMEDICINE

*Fay Nicolson, Research Fellow at Dana-Farber Cancer Institute  
& Harvard Medical School, MA, USA*

I'll be speaking about using SESORS (surface-enhanced spatially offset Raman spectroscopy) for the detection of cancer in mouse models. I don't want to give too much away (it's not published just yet), but hopefully you can get the general gist. If we can detect cancer earlier, and if we can gain a deeper understanding at a molecular level, then we can enhance patient treatment – hopefully improving the length and quality of their life.

With Raman, you can conduct multiplexed imaging (simultaneously detect multiple signatures, for example, surface markers). Another advantage: the technique is very precise, with high resolution that allows us to detect tumors on the micron scale, which is essential – especially in surgical removal, as even the smallest amount of remaining tumor can lead to regrowth of the cancer. And another advantage: the technique is non-destructive! All of these advantages should help us tackle the clinical translation hurdle in the not-too-distant future.

I first attended SciX in Minneapolis in 2016 and I can't wait to get back in the conference hall! It's an amazing place to network; I've made so many great connections there – many of whom have become close friends and collaborators. I'm co-chair of the Biomedical and Bioanalytical section with Karen Esmonde-White and Jürgen Popp – it's shaping up nicely! There are sessions on nanotheranostics, multimodal

“IT'S AN  
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COLLABORATORS”



imaging technologies, and biophotonics in point of care – and I will chair a session on “Vibrational Spectroscopy for Cancer Screening and Diagnosis”. I'm also co-chairing a session on “Spatially Offset Raman Spectroscopy” with Sara Mosca.

Then there's my work with the Society for Spectroscopy early career interest groups. We will be running a networking event on Monday night, which will be our first ever activity together. I'm super excited to launch that – and to have an informal networking session. We hope that this will give early-career scientists a chance to discuss paths and learn from others. Sound helpful? Come along – everybody is welcome!



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## Talking Photonics

In “Analytical Talks,” experts from Hamamatsu Photonics take us on an exciting video tour of the technologies, the evolving application space, and the latest developments in the diverse world of optoelectronics

*Hamamatsu Photonics’ “Analytical Talks” series is now available to view on demand: <https://bit.ly/3yKrdMm>.*

### Episode 1: Water Analysis – Photometry in the UV and VIS

*Presenter: Jennifer Padberg*

Why is Hamamatsu so active in water analysis?

The UNESCO World Water Assessment Program reported that two million tons of human waste are discarded into watercourses every day; clearly, keeping tabs on water quality remains critical – and we’re keen to play our part.

How does Hamamatsu serve this field?

We offer many different products suitable for water analysis applications – from simple photodiodes to sophisticated integrated spectrometer solutions. Notably, many of our customers in this space are OEM manufacturers of water analysis instruments – and we are passionate about using our expertise and insight to help find the right solutions for their specific applications.

Please tell us about a couple of recent innovations...

One standout product is our new – very compact – UV spectrometer.

Despite its small size, it contains the latest CMOS image sensor to provide high sensitivity, high resolution, and robust UV measurements. Our small XeF modules are also worth a special mention because they include all necessary components (lamp, high-voltage power supply, trigger socket), which makes them really easy to use.

### Episode 2: LIBS – Remote Analysis with the O-O-I Principle

*Presenter: Dominik Kunert*



For the uninitiated, what is LIBS?

Laser-induced breakdown spectroscopy (LIBS) uses a short pulse beam laser to create a micro-plasma. Within the plasma, electrons recombine with the ionized atoms and generate a unique spectrum, which allows substances to be identified at the element level. By combining such complex element information with artificial intelligence (AI) technology, it is possible to acquire highly accurate analytical information.



And the O-O-I principle?

O-O-I stands for “online, onsite, insitu,” which highlights the clear benefit of LIBS: high-speed, non-contact, in-line inspections across a diverse range of substances, such as plastics, metals, and glass.

What are the key application areas?

LIBS is a promising technique for in-line inspections at many kinds of manufacturing sites. Some examples: i) in nuclear or thermal plants where exemplary rapid identification and measurement of hydrogen and other light isotopes is

required; ii) in steel and iron manufacturing processes, where analytical equipment could not traditionally be installed nearby due to the extreme heat; iii) even in the recycling field, where accurate identification of mixed waste materials drives more efficient recycling.

### Episode 3: Compact and Sophisticated – Mini-spectrometers Doing Big Business

*Presenter: Christoph Wöhl*

You introduce MOEMS in your Analytical Talk...

Micro-opto-electro-mechanical systems – MOEMS – combine optical technology (including opto-semiconductor devices) and MEMS technology. Crucially, it makes it possible to integrate the components of a typical spectrometer into a compact module.

You also share details of TOKUSPEC...

That’s right. TOKUSPEC supports our mini spectrometer portfolio – and it’s free of charge for all customers. It can operate multiple devices simultaneously and its modern modular design allows the user to customize sections, such as the live data view, measurement settings, or the results window with multiple spectra. Additional functions, such as time lapse, background or reference image acquisition, and setting the calculation method round out the package.

### Episode 4: IR Sources – Hopping Through Technologies

*Presenter: Dominik Kunert*

Could you provide us with a brief IR 101? Infrared radiation (IR) is categorized as IR-A (780 nm–1.4 μm), IR-B (1.4–3 μm), and IR-C (also known as far-IR; 3 μm–1 mm). IR sources radiate measurable quantities of energy in the

infrared region of the electromagnetic spectrum by applying electrical energy. Some molecules have unique vibrational interactions and therefore produce a spectral fingerprint. These tight absorption bands allow high-sensitivity measurements with high resolution down to ppt concentrations.

And what is Hamamatsu working on in the IR space?

We've got a lot going on in IR, but I can mention a handful of exciting developments. First, we have a new window glass material that shifts the cutoff wavelength of traditional XeF farther into the mid-infrared region. Second, we've developed an innovative graphene light source, which has high pulsing rate, low power consumption, and high brightness. Third, our new butterfly package for quantum cascade lasers – the premium class of IR source – reduces the financial burden.

#### **Episode 5: Beyond Human Vision**

*Presenter: Moritz Fischer*

You focus on InGaAs in your Talk – what are they and why are they important?

InGaAs is a compound semiconductor of indium, gallium, and arsenide. Many of you will know that silicon is the material of choice for near-ultraviolet to near-infrared, but longer wavelengths of light cannot create an electric signal in silicon. This gap can be filled by InGaAs, which is capable of detecting light in the near-infrared range (900 to over 2,500 nm).

What are the main applications of InGaAs sensors?

Near-infrared image sensors are often employed in advanced process analytical technology, which is an increasingly important tool in many modern production plants.

Notably, for analytical applications, high sensitivity and low dark signal are critical – but these are usually weak points of



InGaAs detectors. However, Hamamatsu's experience in this area makes us one of the highest quality suppliers of InGaAs detectors on the market today.

#### **Episode 6: Low Light Measurement – Fluorescence in the Analytical Field**

*Presenter: Jennifer Padberg*

You focus on the challenges presented by fluorescence signals in your Talk – could you elaborate?

In general, fluorescence signals are weak and typically have a lifetime of several nanoseconds. To detect weak signals, optical sensors must be highly sensitive – sometimes even necessitating photon counting. Furthermore, sensors should have low dark counts, a wide dynamic range, and be fast enough to detect rapid signals.

And how is Hamamatsu rising to the analytical challenge?

We have a number of different optical sensors and light sources for fluorescent applications. But when it comes to the aforementioned challenge of weak and rapid signals, our avalanche photodiodes, multi-pixel photon counters, and photomultiplier tubes all really shine (no pun intended!) Hamamatsu has a broad portfolio and excels in providing customization options, so we are able to help our customers find the right sensor – whatever their specific application or challenge.

#### **Episode 7: With(out) a Trace - We Help You Find and Resolve Raman Signals**

*Presenter: Moritz Fischer*

What are the main trends in Raman spectroscopy?

One important trend in Raman spectroscopy is miniaturization – to the point where it is now being introduced into application specific handheld devices. The optics in handheld devices are much smaller than in their lab-scale counterparts, but they still enable high-precision Raman spectroscopy wherever you need it!

That said, one challenge in Raman spectroscopy – and a running theme in our Analytical Talk series – is the need to capture faint signals with sufficient signal-to-noise ratio. Furthermore, the spectral sensitivity must be sufficient to resolve narrow spectroscopic features.

And what is Hamamatsu's solution?

We've been busy developing semiconductor sensors and high-performance spectroscopic modules (with integrated excitation lasers) that enable our customers to quickly create Raman devices specifically for their measurement task. In short, we make it easy to design a Raman optical system!

*Get the full tour from Hamamatsu's expert team by watching "Analytical Talks" – now available on demand: <https://bit.ly/3yKrdMm>.*



# WHY PITTCON STANDS FOR

*Philanthropy and  
Collaborative  
Science*

*By Lauren Robertson and Frank van Geel*

The Pittsburgh Conference went virtual in 2021 (for obvious reasons), but it will be back to its full glory for Atlanta 2022. But what makes Pittcon different? And what lies in its future? We spoke with its organizing committee to find out.

Most (if not all) of you reading this will be aware of the allure of the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy – almost universally referred to simply as “Pittcon.” Every year, the best and brightest in our field attend to talk and hear about the latest advances in analytical research and instrumentation, as well as to network and take part in a wide range of activities to bolster their careers.

But perhaps fewer of you will be aware that over 90 percent of the net profit generated by Pittcon goes to funding primary and secondary education, scholarships, lab improvements, and outreach activities that fund the future of analytical science.

Put simply, the real Pittcon difference is philanthropy, and The Analytical Scientist team decided that an exploration of the Pittcon mission was long overdue. Here, key organization committee members – Neal Dando, Helen Boylan, Eli Absey, Penny Gardner, Jonell Kerkhoff, and Melinda Stephens – tell us all about Pittcon’s education and outreach activities, the lessons they’ve learned, and why Pittcon continues to stand out from the crowd.





## Meet the Pittcon Organizing Committee

**Helen:** Hi! My name is Helen Boylan, and I'm Co-chair of the Marketing Committee for Pittcon. I have a BS in environmental science from Westminster College and a PhD in analytical/environmental chemistry from Duquesne University. I am a Professor of chemistry and environmental science and Director of the Center for the Environment at Westminster College. On top of this, I am currently the PI on a National Science Foundation Improving Undergraduate STEM Education grant, where I get to focus on my passion for hands-on, experiential learning and providing innovative learning experiences for students. This initiative brings together STEM students and business, giving them the opportunity to learn environmental science, project management, and leadership skills and then apply those to real-world problems at the intersection of environmental science and business.

**Neal:** My name is Neal Dando, and I am the Pittcon 2021 President. I have an MS and PhD from the University of Delaware in analytical chemistry. My industry career spans 33 years, during which I worked for DuPont, PPG and Alcoa. I have 15 patents to my name and was recognized with Alcoa's highest corporate award for team accomplishment three times – something I'm very proud of. My major career focus was the deployment and use of sensor technologies to reduce manufacturing process losses and improve process recovery. I have been a member of the Pittcon organizing committee since 1987 and a member of the Society for Analytical Chemists of Pittsburgh (SACP) and the Spectroscopy Society of Pittsburgh (SSP) since 1984.

Melinda: I'm Melinda Stephens, and I am the President-Elect for Pittcon 2024 in San Diego. I earned my BS in chemistry from Geneva College and my PhD in analytical chemistry from the

University of Pittsburgh. In 1998, I was appointed to Geneva College as a faculty member in the chemistry department, primarily teaching analytical and organic chemistry. Almost 10 years later, I transitioned into administrative work – first serving as Faculty Development Coordinator, then as Academic Dean. In 2015, I assumed the role of Chief Academic Officer, and I am currently serving as the Provost – although I still occasionally get to teach as a Professor of chemistry! Outside of Geneva, I like to stay active in my discipline by participating in the SACP and the SSP. I've been a volunteer of the organizing committee for Pittcon since 2000.

**Jonell:** My name is Jonell Kerkhoff, and will be the President for Pittcon 2023 in Philadelphia. I received my PhD in analytical chemistry from the University of Florida. My industry career spans 32 years with Alcoa and Arconic, and I have held a number of roles during this time, from Worldwide Supply Chain Manager (Alcoa Chemicals), to Site Director and Program Director (Alcoa Technical Center). A highlight of my career was working as Program Director for a breakthrough technology materials program with the goal of dramatically reducing carbon emissions in the smelting process.

**Penny:** My name is Penny Gardner, and I am currently Co-chair of Committee Arrangements for Pittcon 2023. I graduated from the University of Pittsburgh with a BS in chemistry. My entire career has been in environmental chemistry, and I started off in the local county health department preparing and testing samples of various matrices for pesticides, polychlorinated biphenyls (PCBs), and herbicides. From there, I moved to a contract laboratory and

worked in the organics department analyzing samples for pesticides and PCBs under the Contract Laboratory Program for EPA Superfund sites. I left there to set up a contract laboratory program at another laboratory where, at the age of 30, I became the first female manager in the company when I was promoted to Laboratory Director. I eventually "retired" from the laboratory in 1992 when my son was born, but I continued to participate in the SACP, SSP and Pittcon. In 2016, I went back to work part-time as a Senior Quality Assurance Chemist for Environmental Data Quality, Inc. (EDQI). At EDQI, my responsibilities include review and validation of inorganic and organic data using EPA Guidelines, database management, data entry tabulation, and report writing.

**Eli:** I'm Eli Absey, and I am looking forward to representing Pittcon 2022 as President. I received my BA in biology/chemistry from Hofstra University in Hempstead, New York, USA. I retired from Waters Corporation as a Senior Account Manager in 2019. Before Waters, I was an Account Manager for Dionex and Brinkmann Corporations, and a Laboratory Manager with Von Roll Corporation. At Von Roll I was responsible for developing an Analytical Testing Laboratory for a new Hazardous Waste Facility in East Liverpool, Ohio. I worked closely with the Ohio and US EPAs. I enjoyed my years with these companies and was fortunate to meet some great people. Since the 1980s, I have been involved with the Society for Analytical Chemists of Pittsburgh (SACP) and the Spectroscopy Society of Pittsburgh (SSP). I was also an active member and past President of the Laboratory Information Management System Institute (LIMS).

## *What drives you to dedicate your time and talent to Pittcon as a volunteer?*

**Helen:** I enjoy my role as Co-chair of the Marketing Committee for many reasons. We (the volunteers) get to work closely with the marketing team in the office; we get to brainstorm and be creative. Pittcon 2021 was certainly a challenge for the marketing team in the transition to a virtual show. We wanted to offer our attendees some engaging opportunities in the virtual platform, and I think we did a good job of that. Now, as we move back to an in-person show, we need to think about new ways to engage our participants. I personally enjoy the challenge that my role at Pittcon brings.

**Neal:** I enjoy working on the Pittcon organizing committee because it offers a range of opportunities for personal growth – I have the chance to get involved in leading scientific conference/event management activities that are different from and complement actual work experiences.

**Melinda:** I agreed to serve as President-Elect for 2024 in San Diego because I am excited about being able to launch Pittcon on the West Coast in a beautiful city. I have been involved with Pittcon since 1994, serving as a student aide while a graduate student at the University of Pittsburgh and transitioning through several leadership roles to this point. I believe in the mission of the Pittsburgh Conference and see the fruit of the use of the funds received through Pittcon in science outreach initiatives at all levels of education – elementary through higher education.

**Jonell:** I first became a member of the Pittcon organizing committee in 1986 and a member of the SACP and SSP in 1984. Because of Alcoa work commitments and family, I took a leave of absence in 1991 but have now been active in Pittcon since 2015. Being a part of SACP, SSP, and Pittcon has been a wonderful opportunity to give back to the scientific community, as well as to students and teachers at all levels. Pittcon offers a range of opportunities to network with equipment vendors, educators, and researchers while at the same time generating funds to support the education and outreach efforts of the SACP and SSP. It is thrilling to be a part of an effort of this scale.

**Penny:** In my current position as Co-chairman of Committee Arrangements, my responsibility is to “take care of the needs” of the volunteer committee. I have done this particular job before and enjoy the creativity and fun it brings. I decided to do this job again because Jonell asked me to work with her on creating a fun and enjoyable environment for the Pittcon 2023 organizing committee. As volunteers, many with full-time jobs, we spend hours and hours helping to organize Pittcon every year. Committee Arrangements provides food, relaxation, and an opportunity for team building within the committee. Also, having been the President of Pittcon in 2011, I feel it is my responsibility to help future Pittcon Presidents wherever they may need me. I believe in mentoring and teaching new committee members about the

“I attended my first Pittcon in 1986 in Atlantic City with my husband, and I’ve been involved in every Pittcon since 1988.”

organization and helping them understand its history.

**Eli:** In the early 1980s I became involved with the SACP and SSP. Their contributions to promote scientific outreach has always intrigued me. I especially enjoy working with children, from kindergarten to high school level, to teach them about the wonders of science. My philosophy is we need to expose children to science at an early age. After all, they are our future scientists.

## *What first inspired you to take up a role in the Pittcon organization?*

**Helen:** My inspiration to get involved in the SSP/SACP and then Pittcon was the late Edward Ladner. I got to work with Ed at the National Energy Technology Lab (NETL) when I was an undergraduate student doing an internship there. Ed became a mentor and friend to me, encouraging me to get involved in the SSP, to take leadership positions within the SSP, and ultimately inviting me to get involved with the Pittcon committee.

**Neal:** For me, it’s a chance to give back to our community. Pittcon, as the sole funding source of the SACP and SSP, offers an amazing opportunity to “pay back” for the wealth of positive experiences and scientific contributions I’ve enjoyed by pursuing a career in science.

**Jonell:** As Neal says, Pittcon has been the sole funding source enabling the SACP and SSP to support and promote science awareness and science education locally, nationally, and internationally. It is extremely gratifying to be able to devote my time and energy to this science-based, non-profit organization.

**Penny:** I attended my first Pittcon in 1986 in Atlantic City with my husband, and I’ve been involved in every Pittcon since 1988. I remember walking into the convention center and feeling like a kid in a candy store. I had never seen so many exhibitors, instruments, and equipment in my career! Attending the meetings was a wonderful way to learn about what was happening in the industry through the technical program speakers and a great way to network with fellow chemists. It was my husband who was first involved in the organizing committee, but as his spouse I was

also asked to participate in some aspects. In 1991, I was asked to become a committee member myself. Participating in the societies and Pittcon is something we enjoy as a couple.

### *What is it about Pittcon in particular that appeals to you?*

**Helen:** The mission of science education is what appeals to me the most. I've had the chance to see the benefits of this first-hand – when I got to attend Pittcon as a student aide, and now when I get to take my own students. They are always blown away by the experience, just like I was. For most students, this is their first professional conference, and the experience is such a positive one for them. It makes me proud to be part of the committee. For some students, attending Pittcon is even life-changing. Many of my students have gotten their first jobs through Pittcon's Employment Bureau – a somewhat under-appreciated aspect of the conference.

Secondary to the education mission is the people of Pittcon. The relationships that exist among the committee members, the office staff, and the Pittcon attendees are what makes it so special. We get to work together and have fun together, in working toward

the goal of supporting science education. It's like a big family.

**Neal:** Like Helen, I personally identify with the mission of Pittcon and the SACP and SSP. I too have directly experienced some of the impacts that they have on people's life trajectories. For example, I first came to Pittsburgh for a position I received through Pittcon's Employment Bureau. I met my wife (also a PhD scientist) while at a society-sponsored event – judging a local science fair. My children have also participated (for several years) in science fairs sponsored by the SACP and SSP. I have no doubt these experiences impacted their decisions to become engineers.

**Melinda:** I have spent over twenty years volunteering for Pittcon in various capacities. Each year that I attend, I see the value of this forum for the dissemination of current scientific research and novel scientific instrumentation. And it provides a great opportunity for multi-generational engagement.

Although I have moved into administration now in my regular duties, I have more responsibility for budget and purchasing. I understand how important it is to invest in the development of your faculty and staff. I think that Pittcon is a great way for individuals from many different arenas (academia and industry) to interact with each other and to develop new knowledge and skills

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# Getting to Know Pittcon

What is Pittcon? How did it start?  
And what are some examples of its outreach activities?

The Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, referred to as Pittcon, is a non-profit educational organization that organizes and holds an annual Conference and Exposition on laboratory science. Pittcon is comprised of two volunteer scientific societies: the Spectroscopy Society of Pittsburgh (SSP) and the Society for Analytical Chemists of Pittsburgh (SACP).

Since its inception in 1950, Pittcon's mission has been to support science education. Its current mission reads: "Advancing and enriching scientific endeavor by connecting scientists worldwide, facilitating the exchange of research and ideas, showcasing the latest in laboratory innovation, and funding science education and outreach."

Why Pittsburgh?

Pittcon started as a small technical conference and exposition that was first held in the William Penn Hotel in Pittsburgh, Pennsylvania, USA in February, 1950. The first 18 annual conferences were held in Pittsburgh, before expanding to larger venues.

Pittsburgh has always been blessed as a birthplace of major companies with large science divisions, such as US Steel, PPG, Alcoa, Westinghouse, and Koppers together with several large universities. In the early to mid-1940s, two volunteer

societies, the SACP and SSP, were formed to encourage regular, informal discourse (and meetings) between industrial and academic scientists in the Pittsburgh area.

The Pittsburgh Conference was a logical outgrowth of these meetings, including laboratory equipment and instrumentation developers, so that expanding local industries could quickly adopt new laboratory technologies and equipment, while suppliers could get first-hand feedback from users and potential customers.

How is it organized?

Pittcon is planned and executed by an organizing committee of around 100 volunteers together with a staff of conference/exposition/tradeshows professionals. The net income generated by Pittcon – approximately \$1,000,000 annually – is allocated to the two Societies (SACP & SSP) each year for distribution in the form of equipment grants, scholarships, and education outreach (direct and indirect) programs, and in support of STEM oriented institutions (libraries, museums, and science fairs).

Examples of national outreach

- Grants of Foldscope® microscopes to middle schools and high schools.
- Support of Stem & Buds, which is a peer-based tutoring, mentoring and summer STEM program for middle school and high school students.
- The Undergraduate Analytical Research Program, which provides

research funding for professors and chemistry undergraduate students.

- The Pittcon National College Grant Program, which provides grants to small college science departments to purchase scientific equipment and other teaching aids and materials for undergraduate students.
- The Starter Grants, which are provided to new chemistry professors to encourage high-quality, innovative research and to promote the training and development of graduate students in analytical chemistry.

Examples of local outreach

- The Pittcon Planetarium offers an in-school astronomy program by driving a portable, inflatable planetarium to schools within 200 miles of Pittsburgh.
- The Elementary School Science Olympiad Program (ESSOP) training sessions, where attendees can qualify to apply for grants of complete ESSOP modules that enable them to hold their own in-school science Olympiads.
- K-12 Equipment Grants to teachers and schools for the purchase of equipment and supplies to promote science and chemistry in the classroom.
- Science Fair competition grants to support science enrichment for middle school and high school students.

through our technical program, short courses and exposition.

Jonell: There's so much that appeals to me! Like the others, I am fully invested in Pittcon's science education mission – but it's those personal experiences that stick with me. I went to my first Pittcon as a graduate student with the University of Florida. The conference offered me a significant opportunity to network with other students and to meet and talk with analytical chemistry professors and researchers from different universities, colleges and R&D centers to discuss the latest research and instruments. I don't think this is an experience anyone would forget easily. But I also have other great memories; while finishing up graduate school, I took advantage of the

Pittcon Employment Bureau and got my position with Alcoa. And my husband and I met while judging as society committee members at the Pennsylvania Regional Science and Engineering Fair.

Penny: As the others have mentioned, it's the core mission of science education that really appeals to me. The money that Pittcon has made over the years continues to allow the SACP/SSP to promote science education in the Western Pennsylvania region through various teacher and student awards, as well as grant programs for elementary, middle, and high schools, colleges, and beginning university professors. My favorite part of the year is the annual awards banquet held by the SACP and SSP to honor and celebrate all of



“Besides the outreach initiatives, Pittcon appeals to me in so many other ways. It allows me to travel to cities and meet people I would not normally get to meet.”

the awardees who received grants from the various programs for the year. I enjoy sitting with students and their parents who have received scholarships and grants. The energy, enthusiasm, and optimism from these young, up-and-coming scientists is exhilarating!

When I was chairman of the SSP, in 2005-2006, I started the Elementary School Science Olympiad Program (ESSOP). Essentially, the ESSOP is a hands-on program designed for students of all abilities aged 9-12 years old to excite, inspire, challenge and foster an appreciation for the fun side of science. Pittcon further supports this through their Science Week program, which invites elementary/middle school students from the host city to visit the convention center and participate in several hands-on activities. Through Pittcon Science Week, we are able to promote the ESSOP program and provide seed money to schools within the host city in which our conference is being held. I strongly believe we need to get students interested in science at the elementary school level. Often, children think science is too hard, but by allowing them to experience the fun, hands-on side of science it makes it less scary and less daunting to understand.

Besides the outreach initiatives, Pittcon appeals to me in so many other ways. It allows me to travel to cities and meet people I would not normally get to meet. I have met international scientists and Nobel Prize-winning chemists, and have networked with many people in the chemistry field. The week of Pittcon is like being in your own world. You are immersed in science and technology for an entire week. You get to experience jobs and tasks you would never get to do in your “real life” job. It is one week of the year where you are working but having fun with people who share your passion and commitment to the conference and to science education.

*Eli:* What doesn't appeal? Pittcon is a comprehensive technical conference with a dynamic exposition. The venue allows you to examine the latest advances in research and scientific instrumentation. Over the past 72 years, Pittcon has showcased the latest in analytical

instrumentation, data processing and scientific software, and supplies and column companies all in one place. It is a great place to exchange ideas and information. An attendee can participate in the technical programs, attend short courses, and participate in networking discussions. You can even look for professional opportunities through the aforementioned Employment Bureau.

### *What are some of the challenges today – and what are the solutions?*

*Helen:* I think all organizations, including Pittcon, are trying to figure out what the new normal will look like post-pandemic. The pandemic forced us to figure out ways to do things virtually. Some things work well in a virtual setting and others are simply OK, but there are some aspects where face-to-face interaction cannot be replaced. As an organization, I think the challenge is to offer the best face-to-face experience we can. Beyond that, Pittcon has been offering some year-round programming outside of conference week (online short courses, online coffee breaks, and some other programs in the works). I would like to see our organization continue this and be more relevant to the scientific community outside of conference week.

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Another goal is to promote our mission. I think there are many Pittcon attendees who are not aware that over 90 cents of every dollar spent at Pittcon goes to science education. With that in mind, I think people can feel really good about coming to Pittcon. (Plus, it's still great value!)

**Melinda:** COVID-19 significantly impacted the trade show industry. We remain committed to offering an in-person experience for attendees and exhibitors. We want to attract a larger number of attendees by offering quality programs and provide more ROI for exhibitors by giving them a forum to generate more leads.

**Neal:** In a similar vein to what Melinda has mentioned, my intermediate and long-term goal is to help Pittcon navigate a path that best serves our exhibitors and attendees. This path will continually evolve based on factors both within and outside of our control.

**Jonell:** I agree. A significant challenge for in-person venues is to provide value that cannot be obtained from an online-only experience. Based on feedback, we know that exhibitors and attendees prefer in-person conferences and exhibitions over virtual.

**Eli:** Pittcon 2021 has been a challenge with the COVID-19 pandemic, but as one says – the show must go on! I am proud of all the hard work our organizing committee did to put on a first

class virtual conference despite the challenges. Of all the virtual conferences I visited, none of them met the Pittcon standards.

I, like the others, am also really excited to return to a face-to-face conference in 2022 at the Georgia World Congress Center in Atlanta. Talking to many of our exhibitors and potential attendees, the overall response is that they cannot wait to meet everyone again. We are expecting international travel to resume and are anxious to see our international friends again.

### *What are some of the lessons learned over the last year or so?*

**Melinda:** I was the Chair of Short Courses for Pittcon 2021. I observed that, although a course can be offered in an online format, the experience is not as valuable as an in-person one that allows for informal conversations and networking to occur during coffee breaks. Although we offered a high-quality virtual show, attendance was lower than an in-person conference. In part, because individuals were experiencing significant “Zoom fatigue” and, I believe, yearned for an in-person experience.

**Penny:** I couldn't agree more. Of course, Pittcon 2021 was

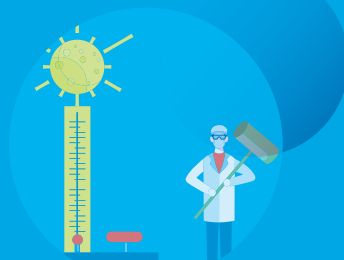
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“I believe a hybrid show of some sort that will allow both in-person and virtual attendance is a real possibility.”

an amazing show, and there are advantages and disadvantages to both in-person and virtual events. I think we need to try and combine the advantages of a face-to-face conference with that of a virtual show. Even before the pandemic, Pittcon was looking for new ways to attract attendees and exhibitors. We started offering short courses throughout the year instead of just the week of the show, and I believe continuing to have the conference in different cities is important to allow more people to attend.

I foresee Pittcon 2022 being a great success. So many people want to get out and see others properly again. People are tired of interacting with others over a computer screen. There is no substitute for actually touching equipment and talking to a person about your laboratory issues.

**Neal:** We've made a number of significant findings from pivoting to a virtual conference in 2021. We now know how to pivot from face-to-face to virtual to hybrid as needed, and when required by expected or unexpected circumstances. I truly believe this will be an invaluable lesson for the future. We've also learnt that, given a choice, both exhibitors and attendees prefer a face-to-face experience. Why? Because creating the opportunity for serendipitous – “Ah-ha” – moments is a significant challenge for virtual-only venues.

**Jonell:** Yes. In a world that is becoming increasingly “virtual,” Pittcon must provide platforms that encourage in-person connectivity and interaction, whether they are vendor-customer, teacher-student, or researcher-researcher.

**Helen:** I find myself drawing parallels between trade shows/professional conferences and higher education. Both are facing real challenges, including budget issues, reduced attendance, and a question of relevance. In both areas, we can't continue to do things the way that they have always been done. We need to continue to innovate. We need to be scientific about it, too. We need to experiment with new ideas/approaches/strategies. We need to see what works and what doesn't. Then we need to tweak the model and run the experiment again. Science continues to evolve and the way that we network with

one another and communicate about science and technologies needs to evolve as well.

**Eli:** 2021 was a challenge. Pittcon did put on an excellent virtual conference, but as Melinda mentioned, people were certainly experiencing “Zoom fatigue.” Virtual does not offer the same benefits as a face-to-face conference. I believe this could have affected the virtual attendance.

### *What do you see (or want to see) in Pittcon's future?*

**Helen:** This is a tricky question. I am not on the board or in line for president, and they are the real decision-makers. But, in my role as a committee member, I will continue to push for innovation, to push for attendee engagement (both during and outside of conference week), and to push for making our mission front and center.

**Neal:** We will continually work to improve integration/harmonization of our technical program and short courses to remain a “one-stop-shop” for technologies, training, and scientific discourse regarding laboratory sciences.

**Eli:** Our staff are dedicated to offering a top-notch program and exposition. We need to make sure we address the scientific areas our customers want to help increase our attendance. Also, we must communicate well with our exhibitors about their advancements to help them receive a good ROI. As long as we promote all aspects of Pittcon (for example the all-inclusive exposition, technical program, short courses, networking opportunities, and employment services) I am extremely optimistic in Pittcon's future.

**Melinda:** I hope we retain our regular attendees and attract new attendees to the conference. We want to grow the number of exhibitors and increase the lead counts per company. We also want to keep costs low for exhibitors so that they can have a significant ROI.

**Jonell:** We have a number of goals for the future. We are working to accelerate our ability to adapt and evolve our technical content, short courses, and networking content. We also want to address the changing needs of our exhibitors and attendees so that we can provide the best value available!

**Penny:** I don't know what Pittcon will look like in the future, but I am excited to help Pittcon evolve. I believe a hybrid show of some sort that will allow both in-person and virtual attendance is a real possibility. As the face-to-face show's dynamic keeps changing, we will be able to fit into even more convention centers and host cities. This will allow us to reach more scientists, especially the bench chemists working in the laboratories. A virtual presence will allow for more international visitors to attend the show. The Pittcon committee's strength lies in our diversity, creativity, and passion to continue to make this the premier international conference and exposition it has always been. Pittcon is very much open to new and exciting possibilities!



## Your GMP Partner in Pharma

**The pandemic has underscored the importance of efficiency – without compromising safety – in pharmaceutical quality management; consistency, flexibility, responsiveness, and experience are key**

*By Kate Monks, Head of Quality and Laboratory at KNAUER*

The pandemic has had the world holding its breath. Normal life has been suspended as we waited – and hoped – for pharmaceutical and biopharmaceutical companies to develop and mass-produce life-saving vaccines. The speed at which this has happened is remarkable and everyone involved deserves great credit – as do other drug developers working hard to ensure the patients they serve do not miss out as a result of COVID-19. The urgency of the task and the constraints placed upon companies during the pandemic has underscored the importance of efficiency. How can we do things faster without sacrificing safety?

This is especially true for GMP, which refers to guidelines that govern quality assurance of the processes and environment in the production of pharmaceuticals and active ingredients, as well as cosmetics, food, and feed. In pharmaceutical production, quality assurance plays a central role, as quality deviations can have a direct impact on the health of the consumer. Quality is something that cannot be rushed – here, lives are at stake.

We work with pharmaceutical companies to provide GMP-Ready HPLC equipment (instruments, parts, and systems) and to help them with GMP, where we offer consultation, engineering, instrument and software qualification, training, maintenance contracts, and technical documentation –

the “great mountains of paper.” Over the years, we’ve learned the importance of flexibility and responsiveness, as well as the recipe for good GMP-compliant products.

From the initial contact to a system installation and qualification, a “GMP project” can take months of intense teamwork. During that time, our partners are allocated a technical engineer to accompany and coordinate the project. We have found that consistency in support is key to the smooth handling of any project.

Typically, a GMP project starts with our partners sharing a list of requirements (the User Requirement Specification). These documents are usually lengthy and detailed, including the functional, technical, and regulatory specifications that must be met, as well as the services and procedures required. The KNAUER team then meticulously works through those requirements and puts together a proposal for a technical solution. Once the customer is happy with the proposal, the project moves forward and we manufacture the instruments, produce the necessary documentation, and – together with the customer – qualify the system.

This generally takes place in two stages: the first qualification happens at the KNAUER site (a factory acceptance test, FAT) and the second occurs at the customer site after installation (a site acceptance test, SAT). Next, those individuals responsible for operating the equipment must be trained. Only at that point is the system ready for integration into its

true production environment, which is handled by our partners.

Another significant service we provide is material documentation.

When supplying equipment to a regulated environment, every component within a system that comes into contact with a pharmaceutical product during production (wetted parts), needs to have the necessary quality while also complying with the necessary regulations. KNAUER

provides a range of documentation including material statements, TSE/BSE certificates, USP Class VI certificates, FDA statements of compliance... The list is long and ever growing.

Of course, it’s crucial that our own staff are fully versed and trained in GMP guidelines. And we have established “GMP Champions” who regularly review regulatory affairs and can be called into play when needed. They also regularly train our staff through our own internal training system, which ensures colleagues working on GMP projects are well aware of the expectations required of them. But our greatest teachers are our customers. We learn continuously from their needs and challenges.

We are now expanding our GMP compliant product portfolio from LC systems to other areas, such as Impingement Jets Mixing Skids for high-flow production of nanoparticles (LNPs, microemulsions, and so on) and other dosing applications. It’s an exciting development, but we’re sure the foundational quality principles we’ve established in LC can be applied anywhere – and we’re very excited.

Overall, we’re passionate about carrying the GMP burden for our customers so they have more time – especially given the past 18 months – to do what they do best: manufacture safe and effective drugs.



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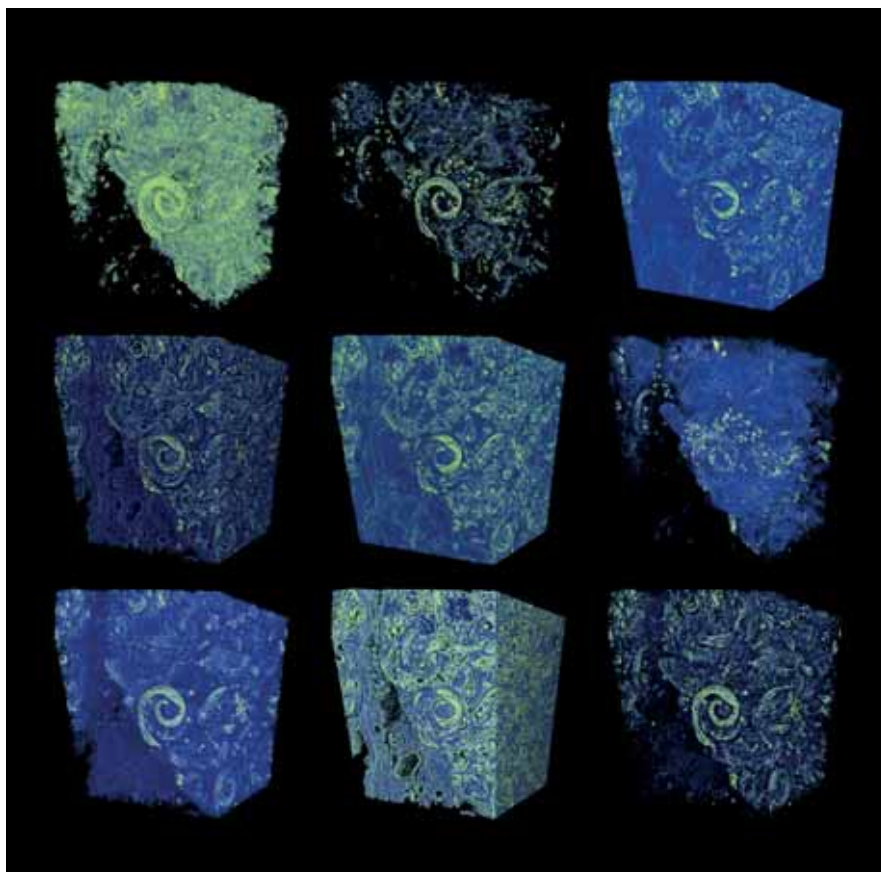
# A Worm's-Eye View

A new approach – based on MALD-MSI and micro-CT – aims to bring unprecedented levels of detail to the study of host-microbe interactions, starting with the earthworm

*By Lauren Robertson*

Charles Darwin was perhaps the most famous proponent of the importance of the humble earthworm – and they've more recently been touted as the most influential species in the history of our world... Unarguably, earthworms play a vital role in our ecosystem – increasing nutrient availability, improving drainage, and contributing to more stable soil structure.

Despite our fascination and nods of approval, methodological challenges have prevented researchers getting a good understanding of the internal workings of an earthworm – including the microbes that colonize it and the associated metabolites they produce. Enter Benedikt Geier and his team at the Max Planck Institute for Marine Microbiology, who set out to accurately image the fundamental interactions between small symbiotic animals and associated microbes in an ecosystem (1). Their recent paper introduces chemo-histo-tomography (or CHEMHIST) – a method for visualizing the metabolic interactions in small animal symbioses,





which is based on MALDI-MS imaging and micro-computed X-ray tomography (micro-CT). Their unique approach outperforms similar methods (developed for medical research in mice) by up to two orders of magnitude. We spoke to Benedikt to find out more.

What inspired you to conduct this research?

Our team has been working with MS to visually explore how metabolites are distributed in tissues colonized by microbial symbionts. What our research (very quickly) showed us was that we can only understand the chemical images if we know the underlying histology of the host. In other words, we need to know which organs, tissues, and cells of the host animal are associated with symbiotic partners (microbes

and parasites) to then assign chemical signals to individual partners.

With this in mind, we set out to create an approach that allowed us to see all this information at once: the host animal's anatomy in 3D, the associated microbes and parasites that live in the tissues, and most importantly, the metabolites they produce.

Why is your research important?

Chemical interactions have allowed bacteria to enter symbioses with organisms across all domains of life. These interactions are critical for the health of individuals as well as whole ecosystems – from deep-sea habitats to our own bodies. The problem is, we know next to nothing about the distribution of metabolites and other small molecules in these associations.

*“Chemical interactions have allowed bacteria to enter symbioses with organisms across all domains of life.”*

CHEMHIST addresses this knowledge gap by linking the identity of tissues and individual cells in complex tissues to their metabolome – independent of

A photograph of a LECO Pegasus BT chromatography system positioned on a road that stretches into the distance, flanked by trees with autumn foliage. The image is used to illustrate the speed and efficiency of the equipment.

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mutualistic or pathogenic associations.

We used an environmental sample – the earthworm – to showcase our technique, because it allowed us to provide a glimpse of the complexity that exists in even the simplest of organisms. Though we have a newfound appreciation for earthworms, our focus is on combining high-resolution MALDI-MSI and micro-CT to enable correlative chemical imaging on a new level. In fact, it was particularly important for us to design an approach that was culture-independent – not only to study symbioses between elusive animals and their microbes, but also to come up with a workflow that would enable the study of human/medical tissue samples. Our approach could also offer new insights into the anatomy and metabolomes of samples



Benedikt Geier uses MALDI-MSI to study the earthworm in unprecedented detail.

*“3D imaging is not only important to understand anatomic and cellular features that might change throughout the animal, but also sheds light on metabolites that indicate certain functions.”*

that focus on medical studies, such as tissue punctures of pathogen infections.

What challenges did you need to overcome?

One major challenge was looking for the associated partners in the host tissues, which can be distributed throughout the whole animal. And that's not easy when you consider that a small animal host may be measured in 10s of millimeters, whereas bacteria are around one micrometer; the resulting four orders of magnitude in size difference is comparable to looking for a Tic Tac mint in an aircraft carrier!

Therefore, we created a multi-scale 3D imaging approach: first we screen the animal at spatial resolutions just large enough to detect where bacteria or parasites are hidden in the animal tissue, and then we follow up on specific regions with high-resolution MALDI-MSI.

Another challenge was to visualize the broad array of targets from the same animal host: microanatomy to understand the anatomic architecture

of the host animal, fluorescence labeling to detect the microbes hidden in the animal's tissues, and ultimately MS imaging to study what each of the partners produce. Because each molecular imaging tool requires different processing steps of the sample that are not necessarily compatible with each other, we had to find a new way of combining all of them at once.

You also integrated metagenomics into the imaging workflow – why? By analyzing DNA, we include two very important aspects that reach beyond knowing the taxonomy of the associated partners: Firstly, once we know who is there, we can design specific fluorescence probes for FISH to label each species of microbe individually and reveal their community composition within the host tissues. Secondly, because metagenomics sequencing provides information on the genomic potential of the associated partners, we can check “who can do what.” In other words, we can learn which metabolites each partner is capable of

producing; by screening the genomes of the associated partners, we can provide essential background information on the metabolite distributions that we record with MALDI-MSI. We described this approach in a paper building up to this publication (2).

Could you tell us about your selection process for appropriate analytical techniques?

MALDI-MSI is extremely powerful because it can deliver both the chemical composition of a sample (like a normal MS) and the spatial distribution of the compounds (like a molecular microscope). On top of that, MALDI-MSI is label-free and allows us to directly observe an animal in its natural habitat, shock-freeze it, and image its body chemistry. As mentioned above, the trickiest part is to understand the chemical images MALDI-MSI produces.

Small symbiotic animals often have complex anatomical structures and even specialized organs or cells that house the symbiotic bacteria – looking in 2D makes it difficult to recognize every structure. This is why we wanted to integrate MALDI-MSI with an approach that would allow us to resolve the detailed 3D anatomy of these tiny host animals at a (nearly) cellular resolution. Although there are fluorescence microscopy techniques capable of 3D imaging, they require tissue clearing approaches for the fluorescence light to illuminate the sample. On the other hand, X-rays pass through any type of biological sample, so we chose micro-CT (an X-ray 3D imaging approach) to resolve and understand the anatomy behind the chemical images that we recorded with MALDI-MSI.

Can you give us specific examples as to how the combination of techniques facilitates discovery?

In the MALDI imaging data, we always saw certain molecules that appeared as large blobs towards the end of the earthworm. We could not explain these chemical signals simply from the 2D tissues sections that we recorded. And then we looked at the micro-CT data, which revealed that the blobs were actually cross sections through cysts that contained parasitic nematodes, which had their own specific chemical composition – possibly related to an immune response of the earthworm against these nematodes. This one example showed us that 3D imaging is not only important to understand anatomic and cellular features that might change throughout the animal, but also sheds light on metabolites that indicate certain functions from immune responses (Figure 3 in the paper) to digestive processes along the gut (Figure 1 in the paper).

Where will your research take you next?

The diverse set of applications that we envision for CHEMHIST is reflected in the different paths that we have decided to pursue. I am looking

forward to taking up my new position as a postdoc at Stanford University, California, where I will transfer my knowledge in correlative chemical 3D imaging to organoid-infection models to better understand human pathogenesis through biomedical research. Manuel Liebeke, one of the key members of our team, is Head of the Metabolic Interactions Group at the MPI for Marine Microbiology in Bremen, Germany, and just recently received a new MALDI imaging setup for faster and higher resolution imaging, which he will use to further push the boundaries of imaging symbiotic interactions. In particular, he will be using a specific MALDI-MSI workflow that enables imaging of glycans – cell surface molecules that are involved in the metabolic interactions at the host-microbe interface.

We are convinced that correlative chemical imaging – as presented in our CHEMHIST study – will lead to more work on host-microbe interactions. In terms of a technical outlook, the increasing speeds, spatial resolutions, and sensitivities of imaging setups will allow scientists in the future to not

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Benedikt Geier hard at work in the lab.

only create a multimodal 3D atlas of one animal, but maybe even a whole time series of different infection or life stages. CHEMHIST is designed as a framework that future scientists can adapt to their needs for studying any symbiotic/host-microbe system.

How would you like to see your research applied in the future? We would love to see CHEMHIST applied as broadly as possible! For example, to specific medical questions

where scientists want to know what metabolites the pathogens, parasites, or maybe even beneficial microbes (for example, in the gut microbiome) produce within their host niche.

One aspect in particular that we wanted our study to highlight is the value of discovery-driven research; for example, observing a system from a different angle and generating hypotheses on the interactions taking place in front of one's eyes. When Darwin studied the Galapagos Islands,

*“One aspect in particular that we wanted our study to highlight is the value of discovery-driven research.”*

he would first observe and describe what he saw before trying to explain it. In a similar way, seeing the distribution of metabolites and the animal and bacterial cells that produce them embedded in the anatomic 3D “world” of the host’s body is like discovering a micrometer-scale ecosystem. New imaging methods enable new observations – similar to discovering an unknown island – which allows us to first observe nature and from there create hypotheses that we can test, discuss, and begin to explain. As Thomas Bosch said in his commentary on our work (3): “How excited Charles Darwin would have been if he had found out that the earthworm’s behavior might be the result of such complex multiorganismic interactions.”

#### References

1. B Geier et al., “Connecting structure and function from organisms to molecules in small-animal symbioses through chemo-histo-tomography,” *PNAS*, 118, e2023773118 (2021). DOI: 10.1073/pnas.2023773118
2. B Geier et al., “Spatial metabolomics of in situ host–microbe interactions at the micrometre scale,” *Nat Microbiol*, 5, 498 (2020). DOI: 10.1038/s41564-019-0664-6
3. T Bosch, “Taking a microscale look at symbiotic interactions—and why it matters,” *PNAS*, 118, e2110874118 (2021). DOI: 10.1073/pnas.2110874118



# Quantitative Sample Recollection by the CDS 7550S Automated Thermal Desorber

By Michael Apsokardu, Xiaohui Zhang

Gas chromatography (GC) commonly adopts direct liquid injection to introduce sample onto the GC column. However, in many situations, the analytes are not compatible for GC analysis and have to be introduced through other GC sample introduction techniques. One such technique, thermal desorption, involves heating a thermal desorption sample tube to release volatile organic compounds (VOCs) adsorbed on the sorbent surface into the vapor phase to reach the GC for separation and detection. To prevent column overload, the sample is often split in the instrument to reduce the amount of analyte reaching the GC inlet. The split sample could be recollected for the purpose of further validation.

A CDS 7550S automated thermal desorber with the sample split/sample saver option was used. The portion of the sample split going to the vent was recollected on a clean sample tube. For the rest of the sample, VOCs were adsorbed by a secondary focusing trap, which was electronically cooled by a Peltier module. Sample adsorbed inside the focusing trap was then transferred to the GC inlet. The 7550S parameters are listed:

Valve oven: 245 °C  
Tube Rest temp.: 37 °C

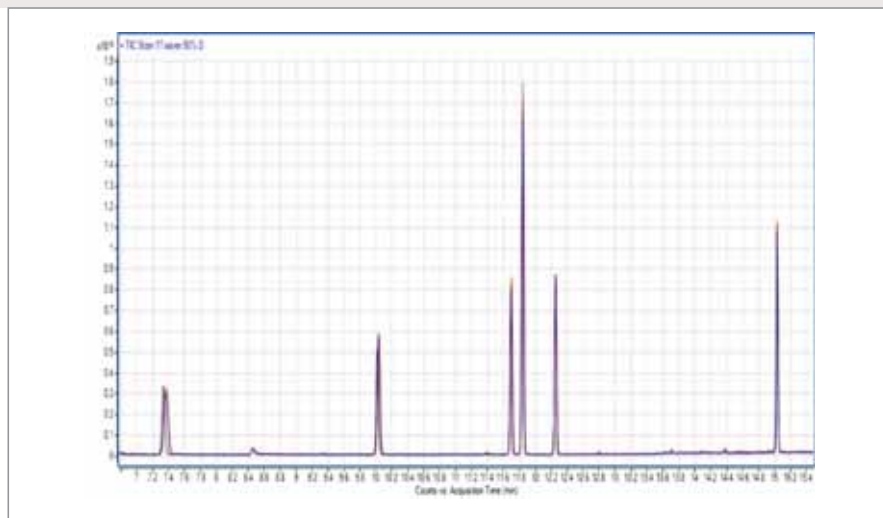


Figure1: TIC overlay of 3 runs at 50% split ratio

	Split Percent (n=3)					
	50%		75%		95%	
Compounds	Acc (%)	RSD (%)	Acc (%)	RSD (%)	Acc (%)	RSD (%)
benzene	103.8	2.2	100.3	0.4	99.3	0.8
Toluene	100.1	0.5	99.0	0.1	98.8	0.1
ethylbenzene	100.1	0.5	98.8	0.3	98.7	0.2
m,p-xylene	99.8	0.5	98.6	0.3	98.6	0.2
o-xylene	99.5	0.4	98.5	0.5	98.5	0.2
Naphthalene	100.1	0.2	99.2	0.1	99.1	0.1

Table 1: Reproducibility from 3 runs at 50%, 75%, and 95% split ratios.

Trap Rest temp.: -20 °C with Peltier  
Tube Desorb temp.: 330 °C  
Tube Desorb time: 8 min  
Trap Desorb temp.: 300 °C  
Trap Desorb time: 2 min  
Trap Type: Tenax TA

Benzene, toluene, ethylbenzene, m,p-xylene, o-xylene and naphthalene standards were mixed and diluted in methanol to a final concentration of 400 mg/L for each component of the stock solution. 1 µL of the stock solution was injected onto a pre-conditioned thermal desorption sample tube. The methanol was removed by purging the sample tube with nitrogen at 110 mL/min for 1 min. This thermal desorption tube was then loaded into the autosampler rack of the 7550S for analysis.

Reproducibility was tested by obtaining % Accuracy (Acc) and %RSD for each of the peaks at a fixed split ratio through multiple runs. Figure 1 is the total ion chromatogram (TIC) overlay from 3 runs at 50% split ratio as an example. Table 1 shows the %Acc and %RSD for each from the three different split percents tested, where the data accuracy is within 98.5%–103.8%, as well as precision below 2.2%. These results indicate that, not only is sample quantitatively split, but is also quantitatively captured by the sample saver tube.

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Dana Arnold  
610-998-4059

# Molecular Weight Determination of VLPs Using LenS3 Multi-Angle Light Scattering Detector

**Combining size exclusion chromatography and multi-angle light scattering determines molecular weight and size of a parvovirus VLP.**

Virus-like particles (VLPs) are multimeric protein structures that mimic viruses but are non-infectious. VLPs are potential candidates in new vaccines and gene therapy products. Robust analytical techniques ensure quality of final products and also provide data for informed decision-making during the development process.

Size-exclusion chromatography (SEC) provides results on the size and purity of macromolecules. When coupled with multi-angle light scattering (MALS), it offers both molecular weight (MW) and radius of gyration (Rg or size). Importantly, A280 detection is only concentration-dependent, whereas MALS corresponds to both concentration and molecular weight. Thus, the large molecular weight of VLPs provides MALS with a strong scattered light response and detects VLPs in a dilute solution well below A280 detection limit.

## Experimental conditions

**Instrument:** Thermo Scientific UltiMate® 3000 with multiple

wavelength UV detector and Shodex RI-504 semi-micro RI detector  
**MALS:** LenS3 MALS detector  
**Columns:** TSKgel® GMPWXL, 13 µm, 7.8 mm ID × 30 cm  
**Mobile Phase:** 0.145 mol/L NaCl, 0.01 mol/L HEPES, 0.05% sodium azide, pH 7.4  
**Flow Rate:** 0.3 mL/min  
**Sample:** Parvovirus VLP (MVM-MVP) (Cygnus Technologies), stock 1 × 10<sup>12</sup> particles/mL (15 µL injection), (dn/dc = 0.19)  
**MALS Calibrant:** BSA, 5 mg/mL (dn/dc = 0.185)

In this application, parvovirus VLP was analyzed on a TSKgel GMPWXL SEC column coupled with the LenS3 MALS detector. RI served as concentration detector and was used with the right-angle light scattering signal (RALS) to measure MW. Extreme low angle (LALS), right angle, and extreme high angle (HALS) signals were used to plot angular dissymmetry and to determine Rg. The MALS detector was calibrated with BSA prior to sample

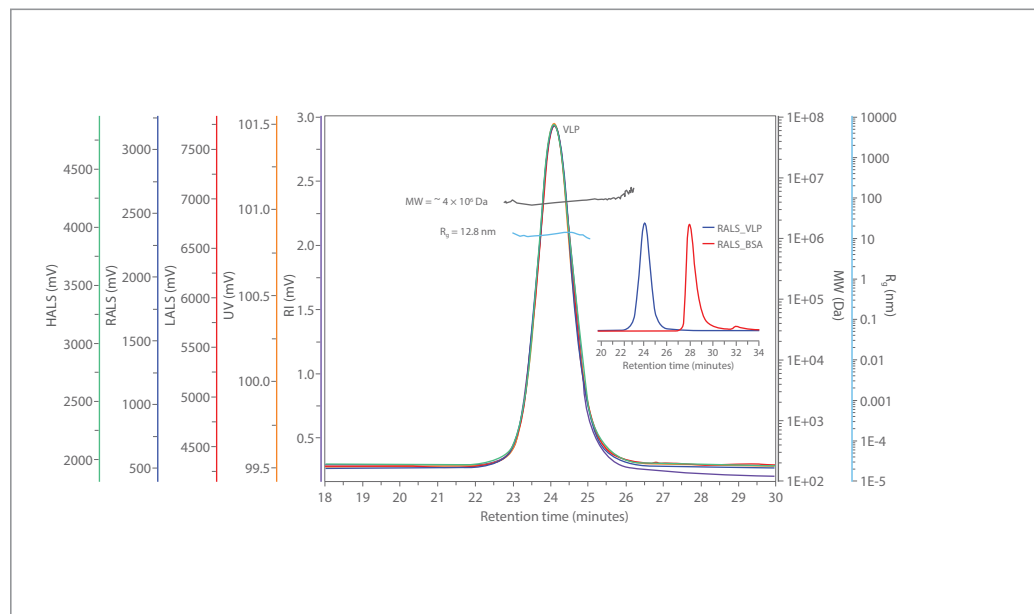


Fig. 1 Analysis of parvovirus VLP and BSA on TSKgel GMPWXL mixed bed pore size SEC column.

analysis and all data were analyzed by SECview® software.

Analysis of parvovirus VLP by SEC-MALS using the TSKgel GMPWXL column revealed a MW of ~4 megadaltons and Rg of 12.8 nm (Figure 1). These results closely align with reported values for this VLP.

## Conclusion

Mass spectrometry is the most common method previously used for VLP size determination, but is costly and impractical for frequent analysis. Inclusion of SEC-MALS to determine the MW and Rg is a preferred alternative and allows for both routine analysis and process monitoring. The wide range in pore sizes and separation ranges of TSKgel PWXL SEC columns overcomes challenges where separations of large macromolecules require a larger pore sized stationary phase. Combining these columns with the greatly enhanced sensitivity of Tosoh Bioscience's LenS3 MALS detector provides fast and easy analysis of MW and Rg with an improved level of detection (LOD).

## Avantor® Chromatography Solutions for the Analysis of Nitrosamines

Nitrosamines have become an increasingly prominent concern as they are highly potent genotoxic impurities which may inadvertently be formed during the manufacture and processing of various consumer goods. The recent detection of nitrosamines in, and recall of, some pharmaceutical products has further increased concern over the presence of these compounds. Additionally, environmental contamination through the release of nitrosamines, along with their

formation during treatment processes (e.g., water treatment), are also areas of concern. Nitrosamines are a class of organic compound containing a nitroso group bonded to an amine (Figure 1) and are typically formed by reaction of a nitrosating agent, such as nitrite, with various amines. Due to many nitrosamines being classified as probable human carcinogens, it is

essential to establish and quantify their presence in a broad range of products and sample matrices. This technical note details several chromatographic solutions that can be applied to the determination of nitrosamines.

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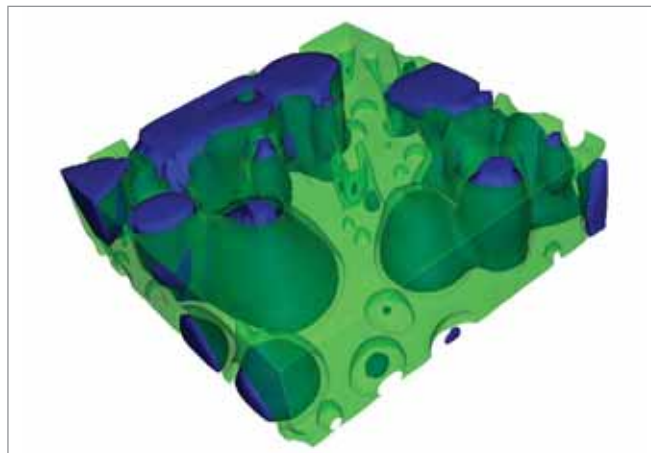


## Food Analysis with Confocal Raman Microscopy

In the food industry, various ingredients and additives such as emulsifiers, stabilizers or thickeners are commonly used to optimize the texture or flavor of food. Their distribution and microstructure strongly influence the properties of the final product. Therefore, research and development, as well as quality control, require powerful analytical methods for studying the distribution of compounds in food.

Confocal Raman microscopy is a versatile tool for analyzing the chemical composition of samples on the sub-micrometer scale that is well suited to analyses in food science.

This survey shows how Raman imaging can characterize samples such as honey, chocolate and fat spreads to help understand the products and production processes. It also features correlative Raman measurements, including: 3D Raman imaging of conventional and spreadable butter, topographic Raman imaging of frosted gingerbread, and



Raman-based automated particle analysis of a mixture of baking ingredients.

See the Application Note here:

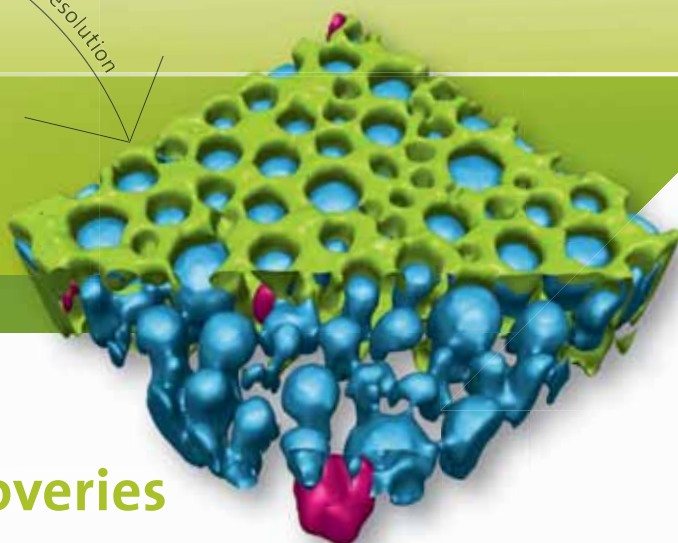
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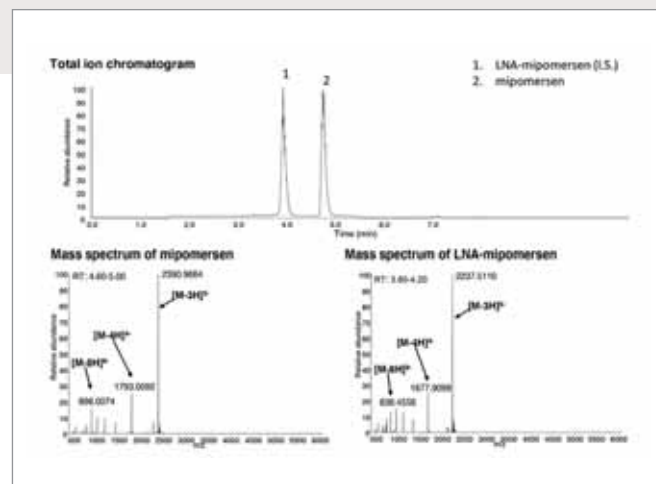


## LC-HRMS Analysis of the Antisense Oligonucleotide Mipomersen Using a Bioinert YMC-Triart Column

Antisense oligonucleotides (ASOs) have outstanding therapeutic potential, since they are used in genetic disease therapy. Several gapmer ASOs have been clinically approved in 2020, including mipomersen (Kynamro®).

Despite their promising therapeutic potential, bioanalytical methods for ASOs have not been well developed and require further optimization. Also, fully validated LC-HRMS methods are yet to be established. Y. Sun et al. have recently reported the development of a sensitive LC-HRMS method for mipomersen in rat plasma as a model compound for 2'-MOE gapmers [1].

In this application note based on the study by Y. Sun et al, a bioinert YMC-Triart C8 metal-free UHPLC column was used. The use of a metal-free column proved crucial, as the use of a standard stainless-steel column showed severe carry-



over. The resulting method showed potential for measuring preclinical samples of very low ASO concentrations and for future analyses of gapmer ASOs.

### Reference

1. Y. Sun, *Bioanalysis*, 12(24),1739–1756 (2020).

Download the application note with the full method details here [www.ymc.de/mipomersen](http://www.ymc.de/mipomersen)

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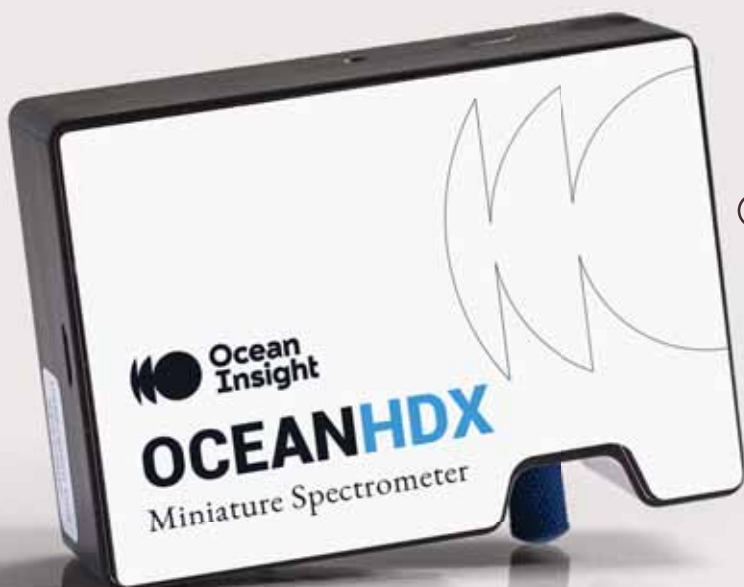
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# Public Service Spectroscopy

Sitting Down With... Ramon Barnes,  
Professor Emeritus of Chemistry, University  
of Massachusetts, Amherst, USA

How did you become interested in spectroscopy?

Howard V. Malmstadt at the University of Illinois was a big influence during my PhD research – which was on the basic concepts of time-resolved spark spectroscopy – he really got me interested in analytical and measurement sciences. I then spent some time at NASA while in the Army, continuing with spark studies of refractory alloys, followed by some plasma work on pre-inductively coupled plasma (ICP) discharges, which, to be honest, I found rather unsatisfactory. But then I read articles by Stanley Greenfield and Velmer Fassel on ICP and immediately realized it was a winner. I actually spent some time with Fassel at Iowa State – and this was a pioneering time for ICP. Then, at the University of Massachusetts, where I eventually became a tenured professor, we built our own ICP sources and continued to develop the technique in terms of fundamentals, computer simulations, applications, and instrumentation.

What excited you about ICP then – and does it still hold its own?

As Fassel pointed out many years back, ICP is sensitive, fast, has relatively few matrix effects – especially in optical emission spectroscopy – and covers the entire periodic table simultaneously. Today, ICP is used everywhere: anything that needs trace analysis uses either ICP emission spectroscopy or ICP-MS, depending on the concentration levels and other criteria. It's very popular in clinical, geochemical, environmental, forensic, pharmaceutical, and industrial analysis. Though it isn't as portable as X-ray fluorescence or as high resolution as nanoSIMS, it complements other technologies and has become central to elemental analysis. Today with laser ablation ICP-MS bioimaging,

single cell nanostructures, and mass cytometry are pushing new frontiers of elemental measurements. Combined with separation and fractionation techniques, ICP detection has advanced speciation analyses significantly as well.

You've worked with some giants of spectrochemical analysis – what made them special?

Both Fassel and Malmstadt were innovative, creative thinkers. In particular, they had a knack for spotting areas of need for development and creating new concepts and ways of applying instrumentation. Malmstadt really encouraged us to think about first principles of instrumentation and measurement – really, he was a measurement scientist. Just glance through the list of people who grew from his research programs: Jim Winefordner, John Walters, Willard Harrison, Gary Hieftje, Gary Horlick, Bonner Denton, Stan Crouch, and their “second-generation” students just to name a handful. He inspired the whole community – students and colleagues.

Please tell us about the Plasma Spectroscopy/Spectrochemistry Winter Conference

I look at my career as one of public service – be it academic, industrial, or educational. Back in the 1970s, the ICP mission was growing, but Fassel had to work hard to battle opposition and convince instrument makers; it was almost 10 years between the technique being described in the literature to the development of the first commercial instrumentation. The big question was whether focusing on ICP was worthwhile, especially when atomic absorption and other techniques were doing so well – they were solving problems and making progress, but not without limitations. Leo de Galan decided to organize two discussion

workshops in Holland in the mid 1970's to gather a small group of both basic researchers and instrumentation developers together to discuss the possibilities and uses of ICP. I felt that the discussions needed to continue, so we set up another workshop as well as a larger conference in San Juan, Puerto Rico, early January 1980, when around 150 people participated. And that worked very well in terms of answering the burning questions at the time and charting the direction of ICP. Some of the first ICP-OES instruments were exhibited. That grew into the Winter Conference on Plasma Spectrochemistry, which has been going for 40 years in North America followed by sister meetings in Europe and Asia-Pacific countries.

Speaking of public service, you also continue to publish the ICP Information Newsletter...

Yes, the newsletter – in combination with the Winter Conference – is a great way to highlight new problems and developments in the field. Both are classified as non-profits entities, which means any revenue we generate must go to support science education, spectrochemical developments, and other activities to help encourage plasma-spectrochemistry through research and travel grants, for example.

Is there anything else you'd like to share?

Yes, I'd like to mention my wife, Dorothy. We've been married for over 50 years, after meeting as graduate students at the University of Illinois. She's much smarter than I am and certainly much more of a people-person! I've learned a great deal from her, and I appreciate all her encouragement and patience over the years. Without her, I think I'd not be doing what I'm doing. She deserves plenty of credit!

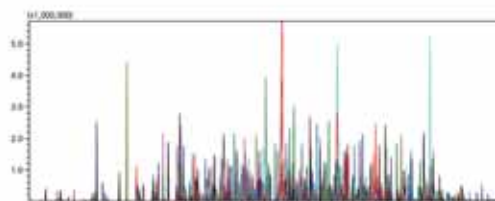




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