

# the Analytical Scientist®



Meet the 60 human health heroes, planet protectors, and instrumental innovators changing the world – for the better

10





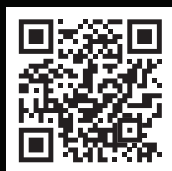
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# Still Invisible?

*Why we must continue to work hard to ensure the achievements of industrial scientists are not forgotten*

One of our big themes for 2024 has been to showcase analytical science’s tremendous impact on the world. The inclusion of an Instrumental Innovators category in The 2024 Power List reflects the fact that fundamental improvements in analytical methods and technology are the foundation of transformative work in cancer research, environmental monitoring, and other important applications. It’s also true that the individuals working in this area – especially those outside of academia – often go under the radar.

This point was made by Terry Berger back in 2019: “There is incredible analytical talent in instrument companies that is generally not acknowledged,” he said. Terry sadly passed away on May 5 earlier this year – but his words still ring true. (See page 7, for Caroline West’s tribute to Terry.)

This year’s Instrumental Innovators category was, in part, an attempt to carve out a space for “invisible” scientists within The Power List, without leaving out the academics whose achievements also deserve recognition. But given the fact that just four out of our 20 Instrumental Innovators work in industry, it seems we have more work to do. With that in mind, in addition to sincerely congratulating the 60 impactful analytical scientists featured on this year’s Power List, I’d like to reiterate Terry’s closing remarks from 2019, and encourage readers to bear in mind everyone who contributes to the field when placing their nominations for the next year, so that we may celebrate the achievements of scientists across all sectors of our community.

**James Strachan,**  
Editor




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### General enquiries:

www.texerepublishing.com |  
info@theanalyticalscientist.com  
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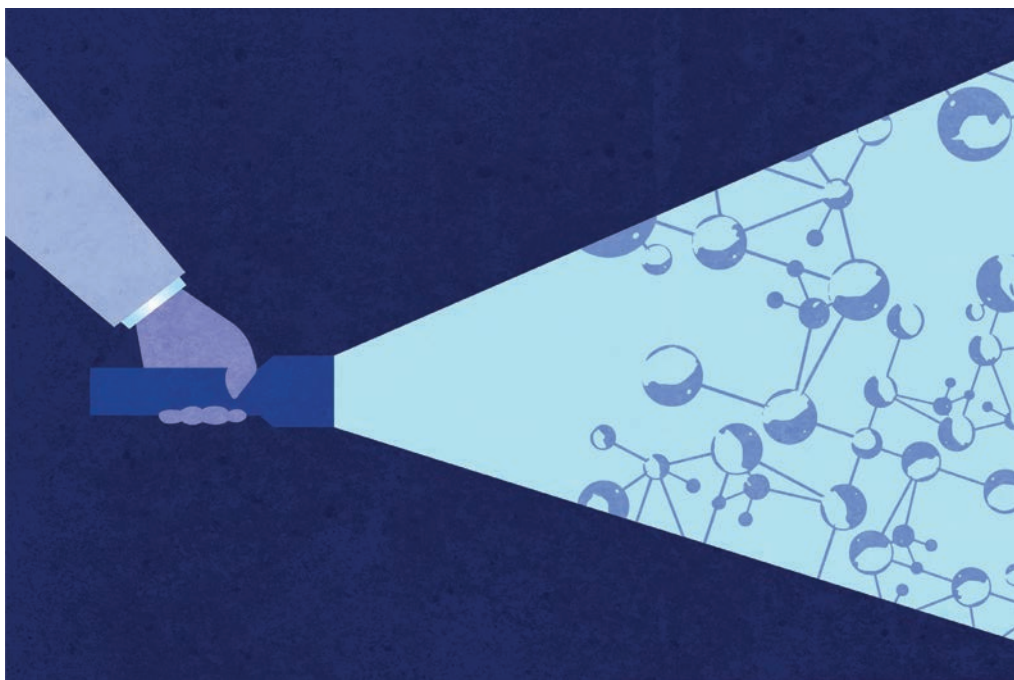
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## The Dark Metabolome: A Figment of Our Fragmentation?

*In-source fragmentation accounts for over 70 percent of the peaks observed in typical LC-MS/MS metabolomic datasets, suggests research from Leiden–Scripps collaboration*



Mass spectrometry, specifically liquid chromatography–tandem mass spectrometry (LC-MS/MS), has revealed hundreds of thousands to millions of metabolites that still need to be characterized. This unknown and extensive collection has been dubbed the “dark metabolome” and it represents more than 98 percent of observed LC-MS/MS spectra. On the face of it, we appear to be far from fully describing the human metabolome. But what if this discrepancy can be explained not by biology but by technology?

The latter may be closer to the truth according to research from Martin Giera – Center for Proteomics and Metabolomics, Leiden University Medical Center, The Netherlands – and Aries Aisporna, Winnie Uritboonthai, and Gary Siuzdak – all from the Scripps Center of Metabolomics and Mass Spectrometry, USA (1).

Several groups have observed a phenomenon called in-source fragmentation (ISF), which relates to the fragmentation of analytes during the initial ionization process within the electrospray ionization (ESI) source and hence before the collision cell. “ISF basically generates a forest from a tree, in other words a single analyte can be presented as a molecular ion and one or many fragments,” write the authors in their *Nature Metabolism* Correspondence paper.

“The employed mass analyzer will blindly isolate and fragment (again) whatever is being sent into the collision cell.” Given this fact, it appeared plausible to the researchers that ISF might partially be responsible for the dark metabolome.

To test their hypothesis, the team mined the METLIN MS/MS database – consisting of more than 930,000 molecular standards – at 0 eV, an energy designed to simulate the fragmentation observed in ISF. They found that ISF could account for over 70 percent of the peaks observed in typical LC-MS/MS metabolomic datasets.

Siuzdak and Giera believe the findings could have important implications for anyone doing MS-based analysis of small molecules.

“Mass spectrometry practitioners need to be more rigorous in verifying the identity of the molecules they detect,” they say. “For example, when multiple peaks share identical retention times and peak shapes, the smaller (lower  $m/z$ ) ions should be scrutinized as potential in-source fragments. This approach will help distinguish real molecules from fragments, ultimately reducing the perceived complexity of LC/MS data.”

The authors believe that by implementing these identification steps, researchers can avoid misinterpretations

and focus on the true molecular species present in their samples.

And it’s not just LC-MS. “It is also worth noting that, since matrix-assisted laser desorption/ionization (MALDI) is generally considered a higher energy ionization source, as compared to electrospray, MALDI-based imaging will also be subjected to significant ISF of small molecules.”

The findings could be particularly important for researchers in the metabolic networking field, which involves mapping out the complex interactions and pathways of metabolites within biological systems. “Previously, the assumption was that all detected peaks represented intact molecules (as most networking approaches do). This leads to erroneous network interpretations due to the inclusion of data from these in-source fragments artifacts,” say Siuzdak and Giera. “Our study highlights the necessity for more selective data interpretation, ensuring that only real molecules are considered. This shift will enhance the accuracy of metabolic networks, avoiding distortions from non-existent molecules and providing a clearer, more reliable map of metabolic interactions.”

### Reference

1. M Giera et al. *Nat Metab*, online (2024). DOI: 10.1038/s42255-024-01076-x.

## A Matter of Minutes

*Mass spectrometry provides forensic toxicologists with a reliable and rapid answer to drug screening*



A team of Japanese researchers have developed a reliable method – dubbed RaDPi-U – that can detect 40 forensically significant drugs in urine in less than three minutes. Unlike many mass spec methods, RaDPi-U requires only three relatively straightforward steps. First, 10 microliters of urine are mixed with an internal standard in ethanol for approximately one minute. Second, the resulting solution is pipetted onto a sample plate. Third, the plate is inserted into the probe electrospray ionization and tandem mass spectrometry (PESI-MS/MS) instrument for analysis. The results are automatically reported through an integrated software.

“Rapid and reliable analytical techniques are imperative for forensic toxicologists,” explains corresponding author Kei Zaitzu, “We’re also planning to expand RaDPi-U to include blood analysis – potentially naming it RaDPi-B – which would be instrumental in therapeutic drug monitoring.”

### Reference

1. K Hisatsune et al., *Anal Bioanal Chem*, 416 (2024). PMID: 38523158.



## World’s Oldest Wine Discovered

In 2019, archeologists uncovered an ash urn – roughly 2,000 years old – in a Roman mausoleum in Carmona, southern Spain. Surprisingly, the urn contained liquid of a reddish hue... Researchers from the University of Cordoba, Spain, analyzed the liquid using ICP-MS and HPLC-MS and found a distinctive mineral salt profile, which allowed them to identify the liquid as white wine – the oldest wine ever discovered.

Credit: Juan Manuel Roman

### QUOTE of the month

*“All ecosystems are complex networks of organisms interacting with each other and their abiotic surroundings. We tend to simplify, divide and conquer, but in the process, we lose valuable information about how the system works, ability to predict and ultimately control biology. Addressing the complexity challenge requires not only quantum leaps in measurement science, but also effective collaboration across disciplines.”*

Ljiljana Paša-Tolić (page 24)



## The Work–Life Balance Myth

*What do high-performing scientists have in common?  
Their work is their main hobby.*

By Isabelle Kohler, Assistant Professor at the Division of Bioanalytical Chemistry at the Vrije Universiteit Amsterdam, The Netherlands; and Founder of NextMinds

Nature recently published the results of a global survey conducted among postdocs – reporting that 31–40 years old are “less happy in their career” and “more negative about job prospects, job security and work–life balance” than their younger peers (1). What could be going on here?

The transition between a postdoc fellowship and the next step of the academic ladder is a challenging one: there are way more postdocs interested in pursuing an academic career than the positions actually available – let alone positions offering a permanent contract or tenured positions. Thus, making the so-called “postdoc blues” a global trend that concerns not only the analytical world, but academia in general.

Those who really want an academic career might have to enter a never ending cycle – extending their postdoc years for as long as possible, jumping from one postdoc position to another, with the hope of broadening their skills, their network, and opportunities of finding a fixed position. However, for most this means remaining a postdoc with a temporary contract in their mid-thirties, while their prospects of a tenure position are decreasing at an alarming rate.

Compensation is not the only factor feeding into the problem. Many young scientists embark on a PhD journey being excited about spending a few years doing research, but without having a clear idea of what they’ll do after their PhD.



If universities offered (mandatory) career development training during master’s studies and PhDs, young scientists would be able to prepare effectively and choose the most suitable career path – avoiding career dissatisfaction later on.

Today, the pressure from online communities and social media also intensifies the problem. Many online accounts have started focusing on just the negative aspects of academia, which can lead into a storm of negative emotions – with people constantly comparing themselves and their work to others. This creates and sustains a cloud of negativity and self-doubt, breaking any boundaries between work and personal life.

All of these things remind me of a saying: “There is no way to have a relaxed life in science.” But how true is that? Is it crazy to dream of work–life balance in our careers?

Some time periods are naturally more stressful because of tight deadlines at work, while others might call for more focus on our personal lives. I think that it all depends on everyone’s perception about what a “relaxed life” means. I belong to the category of people who are not very resilient

to stress (physically and mentally). Because of this, I admire the accomplished and high-achieving analytical scientists in our community, who seem to go through their career in a very relaxed yet productive way.

I had the chance to co-organize the IMSC2022 conference in Maastricht, so I spent quite some time working closely with the Chairs Ron Heeren, Albert Heck, and Manfred Wuhrer – some of the top analytical scientists in The Netherlands. To me at least, they all look like they have managed to secure a somewhat relaxed life in science – running multiple projects and a big lab in parallel. Surely, this must be quite stressful, and yet they undoubtedly – overtly – enjoy their work and their community. I believe I came to understand what they all have in common: they consider their work as their main hobby!

There is no key to work–life or life–work balance; rather, it is a combination of different approaches that can bring us a satisfactory balance.

### Reference

1. Nature Research, “Nature Post-Doctoral Survey 2023.” Available at: <https://bit.ly/3WQttiw>.



## Lessons Learned from Terry Berger (1946–2024)

*The father of modern supercritical fluid chromatography, Terry Berger, sadly passed away on May 5, 2024. Here, I reflect on his contributions to the field – and to me personally.*

By Caroline West, Full Professor, Institute of Organic and Analytical Chemistry, University of Orléans/CNRS, Orléans, France



The news of Terry Berger's passing hit me hard. I hugely admired his work and had much affection for the man. For those of you who do not know, Terry was considered "the father of modern supercritical fluid chromatography" (SFC). I have practiced SFC for over 20 years, so you can perhaps understand my emotion.

This description was well deserved; he really made SFC enter a new era – transitioning from the less satisfying neat-CO<sub>2</sub> capillary SFC to the modified-CO<sub>2</sub> packed-column SFC. This feat was achieved through his significant contribution to instrument development, fundamental studies that increased general understanding of supercritical fluid behavior, and many application

papers, where he aptly demonstrated the interest of the technique for a broad range of application domains.

I started SFC when I was only a baby chromatographer during my PhD years, and I had read all his papers early on in my career – several times. I had of course learnt a lot of science from reading these papers. But apart from the content, they also taught me what a good, convincing paper should look like; I learnt to be straightforward, to not embarrass myself with long sentences to get to my point, and to recognize that a good figure is always better than a long page of text.

But this is not the only thing I learnt from Terry. To understand what else he taught me, although quite involuntarily, I would like to share two personal stories.

When I was still a PhD student, I was fortunate to attend a conference on supercritical fluids in Pittsburgh, USA. Terry gave a lecture on the last day of the conference. I had seen him from a distance, but I would never have dared to approach him – I was rather young and shy. Mind you, he was pretty impressive: tall, burly, with his long gray hair held in a ponytail. There was something of a rock-star about him. When he came on stage for his lecture, the title appearing on the first slide was not the one indicated in the program. He started saying that he had completely changed his mind about his talk as a result of the previous days' conversations, which had generated new ideas that he wanted to share. I was rather flabbergasted at his nerve and panache.

However distant, this first encounter left a lasting impression on me, because I am also that sort of person, who cannot stick to an old idea too long. I hate writing an abstract six months before an intended talk, because I have no idea what will be on my mind six months later. (By the way, don't ever read my abstracts, they are pretty boring.) I am also the sort of person who will always change their slides at the last minute, not because I was not

*“Science is moving.  
It is not meant to  
be gospel truth.  
What is true today  
will be wrong  
tomorrow.”*

ready but because new ideas keep popping into my mind. When I heard that lecture, I understood that it was OK to not stay on track with the intended program, as long as you have something interesting to share. Indeed, I have puzzled some of my audience several times this way!

Six years after first seeing him, I had the chance of meeting Terry again at the HPLC conference in Boston, USA. As I had grown into an assistant professor, I felt confident enough to approach him. When introductions were made, I remember that the first thing I said was: “You know, you are a sort of SFC-God to me.” Terry laughed and said: “That scares the hell out of me!” This brilliant man was also modest. Perhaps he was also suffering from “impostor syndrome,” which I know quite well.

Looking back on this moment, I believe I now know what he meant. Continuing my journey with SFC and improving my understanding of the technique, I have sometimes allowed myself to disagree with some of Terry's views. (Terry, wherever you are, I hope you can forgive this!) Science is moving. It is not meant to be gospel truth. What is true today will be wrong tomorrow. I have no problem admitting that I was wrong about the things I have previously believed to be true, as long as I receive a sound proof of my error.

I hope I can transfer some of this philosophy to my students, as Terry – whether or not he was conscious of it – transferred much of his philosophy to me.

## Diagnostics’ Biosensor Backbone

*How multidisciplinary collaboration is taking biosensor technology to the next level for early disease diagnosis*

By Luisa Torsi, Professor of Analytical Chemistry, University of Bari; and President, Regional Center on Single-Molecule Digital Assay, Italy



Advances in biosensor technology have provided a fruitful avenue for analytical chemistry to positively affect clinical research – particularly in enabling early diagnosis. However, this progress must coincide with the discovery of new and specific biomarkers. With this in mind, we must take a comprehensive approach, encompassing both nucleic acid and antigen (protein) biomarkers. Improvement in performance levels of sensing devices is particularly notable in immunoassays as their performance is lower in comparison to molecular assays.

Today, we’re seeing a plethora of proposed assay technologies for improved

diagnostic and clinical research. For example, for many years, we’ve been working with electronic devices, particularly bioelectric transistors, to enable ultra-high-performance levels – not only in terms of low detection limits, but also in high reliability. We are perhaps best known for our “Single-Molecule with a Large Transistor” (SiMoT) technology, which is being developed at technology readiness level 6 (TRL6). SiMoT can uniquely detect both antigens and oligonucleotides at extremely low concentrations with an accuracy of 96 percent. It’s particularly suitable for point-of-care testing, especially for screening asymptomatic individuals, providing fast, reliable, and cost-effective identification of illness. SiMoT can be used for various diseases – we proved its effectiveness in detecting SARS-CoV-2 in saliva (1) and diagnosing pancreatic cancer from a blood test (2, 3).

SiMoT devices consist of a reusable reader and a compact disposable cartridge tailored for early disease diagnosis, offering ultra-portability and handheld convenience. The affordable cartridges work alongside smartphones or tablets, so they can be used anywhere, and the simple nature of the technology makes it suitable for untrained users – even in home settings or in resource-constrained environments. Array technology, on the other hand, is better suited to trained personnel in clinical facilities or smaller laboratories.

Another analytical technology stepping into the clinical spotlight is CRISPR/Cas biosensing, which employs precision gene editing to identify specific oligonucleotide sequences within a sample. This technique harnesses CRISPR’s inherent capacity to pinpoint and target genetic sequences within an organism genome or biomarker. It’s also been tailored for diverse diagnostic and detection applications. CRISPR systems hold great promise for accurately and sensitively detecting pathogen-specific

nucleic acids, which could potentially transform on-site diagnostic and genotypic applications.

One notable advancement is the use of CRISPR-based paper biosensing platforms, which offer an innovative approach to pathogen detection evidence in recent work to detect mycoplasma pneumoniae (4). This newly developed test firstly amplifies the target gene with specific primers before using the CRISPR/Cas9 system for precision recognition, which reduces false negative results. This method is highly sensitive, detecting as few as three DNA copies, thanks to the efficient amplification and ability of the CRISPR/Cas9 system to work at a relatively low temperature of 39 °C.

Of course, these highly performing sensing devices would not be possible without multidisciplinary collaboration. When a project is tackled solely by specialists in one area, it can lead to imbalances in development. For example, focusing only on device performance level may result in a device with limited reliability. The SiMoT project in particular shows the importance of collaboration with other fields.

Looking into the future of diagnostic and clinical research, it’s crucial that we stay resilient in the face of challenges and setbacks in our push for innovation. To my colleagues and fellow researchers, both experienced and new to the field, I propose that we advocate for ourselves and others across the scientific community. Without collaboration, we are destined for failure. But together, we can contribute clinical and diagnostic research that paves the way for future generations.

### References

1. E Macchia et al., *SciAdv*, 8, 27 (2022). DOI: 10.1126/sciadv.abe0881.
2. E Genco et al., *AdvMater* (2023). DOI: 10.1002/adma.202304102.
3. E Macchia et al., *AdvMater* (2024). DOI: 10.1002/adma.202309705.
4. R Zhu et al., *Anal Chim Acta* (2023). DOI: 10.1016/j.aca.2023.341175.





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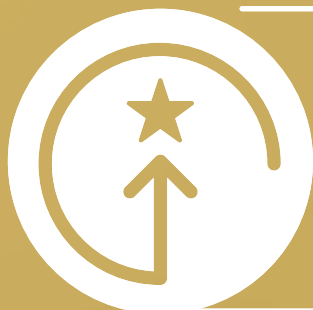
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the Analytical Scientist

# POWER List

*Meet the 60 leaders and influencers in analytical science whose work is transforming the world around us – for the better*



What are the biggest challenges facing humanity in 2024? From improving our health and wellbeing to clean water and clean energy, analytical science is playing a crucial – but often underappreciated – role. And that's why the The Analytical Scientist 2024 Power List is all about *impact*. We are recognizing individuals who are having a real impact in the three

categories: Human Health Heroes, Planet Protectors, and Instrumental Innovators. There are 20 nominees per category – each with a ranked Top 10.

Of course, no list is definitive – and we recognize that many of the individuals on this year's list deserve recognition for their impact across several areas. We hope you'll join us to celebrate

the achievements of the 60 impactful analytical scientists featured in the 2024 Power List.

Scan the QR code to view this list, with additional content, online





# Human Health Heroes



## 1 / Matthias Mann

*Professor of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Germany; and Director at the NNF Protein Research Center, Denmark*

Matthias Mann has been at the forefront of the mass spectrometry-based proteomics field for almost three decades. So far this year, the Mann Lab has: helped to uncover the role of proteomic shift in migraine, used deep visual proteomics to tailor cancer therapy to specific cell types, developed an open-source DIA search engine – just to name a few recent breakthroughs.

## 4 / Jonathan V. Sweedler

*James Eisner Family Endowed Chair of Chemistry, Professor of Bioengineering, Neuroscience, Physiology and Medicine, University of Illinois at Urbana Champaign, USA*

*Spending a \$1 billion research grant...*  
This funding level could enable a new national effort (think the human genome project) where I would be helping to lead one of the thrusts. I support Neil Kelleher's idea to create a comprehensive proteoform atlas and tie this unmatched protein detail to the



## 2 / R. Graham Cooks

*Distinguished Professor of Chemistry, Purdue University, USA*

*Most memorable advice?*

"If you worry about tenure then you don't deserve it," said to me by H. C. Brown in 1969 when he was visiting Kansas State University where I was an Asst. Prof. of organic chemistry. I was so successful at not worrying that the next year I took a non-tenure track position at another university – by chance, Purdue University.

*Missing from the analytical toolbox?*

The same item that has been missing for two decades: a powerful portable commercial mass spectrometer for point-of-care measurements. It must privilege speed over other parameters and must have MS/MS for chemical specificity.

small molecule repertoire within cells. Can we use this chemical information to predict cell physiology and activity in health and disease?

*Most memorable advice?*

One of my professors in graduate school made the following comment about collaborations. If you are ever unsure if a collaborator has done enough to be a coauthor on your manuscript, rest assured they are not in doubt that they belong. The professor went on to encourage us to have the difficult conversations that many avoid about co-authorship as the questions arise.



## 3 / Perdita Barran

*Director of the Michael Barber Centre for Collaborative Mass Spectrometry, The University of Manchester, UK*

*Main research aims?*

To use mass spectrometry to solve problems of societal importance that cannot be readily understood with other methods and to train people to "think like ions" so that they can optimize the mass spectrometry experiment, or even make a new instrument. To measure the conformational landscapes adopted by proteins with disordered regions, and to diagnose Parkinson's disease from swabbed sebum with quantitative MS.

*How to transform disease diagnosis and treatment...*

We need to work fast – we need to keep up with the predictive power offered by machine learning and we need to test their hypotheses. When we have robust markers there will be two types of assay, to develop: point-of-use and point-of-care. Both are based on analytical science. We also need to keep both accessible. MRM assays for biomarkers in the clinic remain the most affordable way to provide results, especially for non-infectious disease.





**5 / Livia Schiavinato Eberlin**  
Associate Professor and Vice-Chair  
for Research, Department of Surgery,  
Baylor College of Medicine, USA

*Qualities of an innovative thinker?*  
If I had to pick two, it would be  
creativity and fearlessness. Innovators  
have to be creative and think about  
clever solutions to problems in novel  
and disruptive ways – that is a given.  
But the most successful innovators  
and inventors that I know were also  
incredibly bold and fearless. They  
knew people would likely doubt them  
and criticize them for their creative  
ideas, and regardless of these  
challenges they believed  
in their invention and  
pushed forward with  
confidence until  
others started to  
realize the potential  
and novelty of  
what they had  
created.

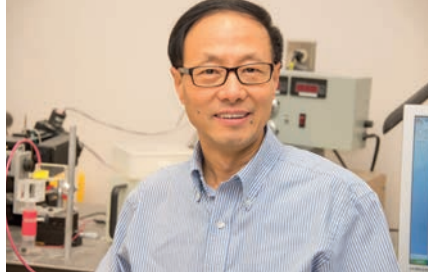


**8 / Ying Ge**  
Vilas Distinguished  
Achievement  
Professor,  
Department of Cell  
and Regenerative  
Biology, Department  
of Chemistry, and  
Director of the Human  
Proteomics Program, University  
of Wisconsin-Madison, USA



*Main research aims?*  
To advance top-down mass  
spectrometry-based proteomics to  
understand human diseases at the  
molecular level and identify new  
targets for diagnosis and treatment.

*Spending a \$1 billion  
research grant...*  
I would establish a world-leading  
interdisciplinary research institute.



**6 / X. Chris Le**  
Distinguished University Professor and  
Director, Analytical and Environmental  
Toxicology Division, Faculty of Medicine and  
Dentistry, The University of Alberta, Canada

Chris Le's interdisciplinary research  
focuses on the development and  
applications of analytical techniques  
for studies of human health effects  
arising from environmental exposure.  
His team develops chemical speciation  
techniques that enable characterization  
of arsenic species, assessment of  
human exposure, and understanding  
of molecular mechanisms of arsenic  
toxicity. His development of DNA-  
protein binding assays, isothermal and  
signal amplification techniques, and  
improvements in CRISPR techniques,  
advance studies of DNA damage and  
repair, environmental carcinogenesis,  
gene editing, and molecular interactions.

**7 / Robert Kennedy**  
Hobart Willard Distinguished Professor,  
Department of Chemistry, University of  
Michigan, USA

*An exciting frontier in human health?*  
Something that I feel is still barely  
tapped is developing analytical methods  
for better understanding the brain. The  
brain has many layers of organization so  
that single cell, small regions, circuits and  
the whole brain all represent interesting  
analytical challenges. We are seeing  
important advances in many aspects  
including imaging of neurotransmitters  
(via receptor interactions) and direct  
measurements by sensors and sampling.



**9 / Albert Heck**  
Chair, Biomolecular  
Mass Spectrometry  
and Proteomics,  
Utrecht University,  
The Netherlands;  
and Scientific Director,  
Netherlands  
Proteomics Center



*Main research aims?*  
I am trying to understand life – by  
studying all facets of all proteins and  
how they function. I do this through  
the glasses of a mass spectrometer.

*Making personalized medicine  
a reality...*  
In the short term, analytical science  
could be used to much better monitor  
drug effects and optimize doses/  
treatments, thereby avoiding the  
misuse of drugs and adverse effects.

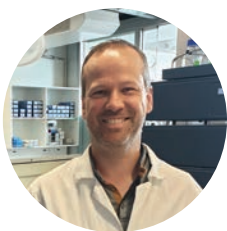
**10 / Zoltan Takats**  
Professor of Analytical Chemistry, Faculty  
of Medicine, Imperial College London, UK

Zoltan Takats has produced  
breakthroughs in desorption  
electrospray ionization (DESI), as well  
as rapid evaporative ionization mass  
spectrometry (REIMS) – which is at  
the heart of the iKnife, the technology  
Takats is perhaps best known for. The  
iKnife is a “smart scalpel” that surgeons  
can use to determine whether a tissue  
being removed is cancerous or not.



## Davy Guillaume

Senior Lecturer  
and Research  
Associate (MER),  
University of Geneva, Switzerland



### Main research aims?

My research focuses on developing advanced liquid chromatography and mass spectrometry methods to analyze and characterize new drug modalities, including mAbs, oligonucleotides, and cell and gene therapy products.

### Most exciting trend today?

The most exciting development in analytical science today is the integration of advanced technologies such as ultra-high performance liquid chromatography, high-resolution mass spectrometry, artificial intelligence, and machine learning to enhance the performance and predictive capabilities of analytical methods.

## Michal Holčápek

Professor  
of Analytical  
Chemistry,  
Department of Analytical Chemistry,  
Faculty of Chemical Technology,  
University of Pardubice, Czech Republic



### Main research aims?

Lipidomic analysis of biological samples using a combination of advanced mass spectrometric and chromatographic techniques with applications in the discovery and translation of cancer biomarkers for clinical screening.

### How to transform disease diagnosis and treatment...

I hope for improvements in high-throughput quantification of many biomolecules, which will be correlated with the prediction and diagnosis of serious human diseases.



## Neil Kelleher

Walter and Mary E. Glass Professor  
of Molecular Biosciences; Director,  
Northwestern Proteomics; Director,  
Chemistry of Life Processes Institute;  
Northwestern University, USA

Neil Kelleher is known for his work on the development of electron capture dissociation and is considered a proteome pioneer, working towards the completion of the Human Proteoform Project – to map and define the human proteome. His research is focused on top-down proteomics, chromatin biology, and natural product biosynthesis and discovery using mass spectrometry.

## Lingjun Li

Vilas Distinguished Achievement Professor of Chemistry  
and Pharmaceutical Sciences, Charles Melbourne Johnson  
Distinguished Chair in Pharmaceutical Sciences, School of  
Pharmacy and Department of Chemistry, University of  
Wisconsin-Madison, USA

### Main research aims?

My research program is centered around the development of novel mass spectrometry-based technologies and enabling tools to study challenging and significant neuroscience and biomedical problems that are relevant to human health.

### Making personalized medicine a reality...

I believe that with the rapid development of more sensitive and high-resolution and precision measurement tools, analytical science can make personalized medicine a reality.



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### Jeremy Nicholson

Director, Australian National Phenome Center; Professor of Medicine, Murdoch University, Australia

*Main research aims?*

Elucidating the systemic metabolic signatures of gene-environment-microbiome interactions to discover new diagnostic and prognostic biomarkers and models for disease diagnosis and predictive outcomes in personalized and preventive medicine.



*Making personalized medicine a reality...*

This requires measuring and modeling human populations at large scale with multiple analytical technologies and combining those data to discover new predictive risk biomarkers.

### Jürgen Popp

Chair for Physical Chemistry, Friedrich Schiller University Jena; and Scientific Director Leibniz Institute for Photonic Technologies e.V., Germany



of a wide range of disciplines, such as chemists, physicists, physicians, computer scientists, engineers, etc. One of the most important lessons we have learnt as technologists over the last 20-25 years is the need to involve the end user, i.e. the medical profession, in research from the outset. There is no point in researching a “cool” optical analytical method that is not needed clinically.

*A problem that could be tackled interdisciplinarily...*

Optical health technologies is a prime example of interdisciplinary research and requires the interaction



### Koen Sandra

CEO and Co-owner, RIC Group, Kortrijk, Belgium; and Visiting Professor, Ghent University, Belgium

*Main research aims?*

We strive to be a key contributor to the ever-evolving domain of life sciences. We embrace the unknown, think outside-the-box and passionately follow our own path.

*An exciting frontier in human health?*

Without a doubt, mass spectrometry. I cannot imagine what our research and the field in general would look like without this dazzling technology.

### Gary Siuzdak

Professor and Director, Scripps Center for Metabolomics and Mass Spectrometry, USA

*Biggest challenge facing the field right now?*

Filtering out artifactual (in-source fragmentation) mass spectrometry data from datasets.

*Most exciting trend today?*

The most exciting development is the advent of subcellular quantitative imaging of metabolites at the organelle level. A technology being spearheaded by Michael Kurczyk (AstraZeneca and University of Gothenburg).



### Renā Robinson

Professor of Chemistry, Dorothy J. Wingfield Phillips Chair, University of Pittsburgh, USA

*Main research aims?*

My research aims to increase equity in Alzheimer’s disease research and biomarker discovery efforts in disparate populations using proteomics and lipidomics.

*Spending a \$1 billion research grant...*

I would build a highly diverse and multidisciplinary team to establish cutting edge proteomics research.



### Jennifer Van Eyk

Professor, Cardiology and Basic Medical Sciences, Director of Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, USA

*Main research aims?*

Changing and democratizing medical practice.

*Making personalized medicine a reality...*

Analytical science can help us achieve this through the accurate, precise and high throughput quantification of proteins in all of their forms and functional configurations, especially if linked to remote blood sampling devices.





# Planet Protectors

## 1 / *Damià Barceló Cullerès*

*Honorary Adjunct Professor,  
Chemistry and Physics Department,  
University of Almeria, Spain*

### *Main research aims?*

My work focuses on wastewater based-epidemiology (WBE) using environmental proteomics and high resolution mass spectrometry, as well as analysis, fate and advanced removal technologies of emerging contaminants and micro/nanoplastics in aquatic and agroecosystems.



## 2 / *Susan Richardson*

*Arthur Sease Williams  
Professor of Chemistry,  
Department of Chemistry and Biochemistry,  
University of South Carolina, USA*

### *Main research aims?*

My main research revolves around making drinking water safer. I think we have good water, but I think we can do better. I focus mostly on understanding disinfection by-products (DBPs) that are formed when we disinfect our water, working with toxicologists to determine which are harmful, and working with engineers to develop new treatments that can be used to minimize their formation and make water safer.



## 3 / *Derek Muir*

*Research Scientist,  
Environment and  
Climate Change  
Canada*

Derek's focus is mainly on persistent organic chemicals and, more recently, emerging contaminants. When asked about the future of environmental analysis in 2021, he said: "We need to look towards more artificial intelligence-based approaches for analyzing and collecting data [...] There's also room for improved analytical methods."

### *Biggest challenge in environmental analysis?*

Non target analysis and bioinformatics seem to be the necessary tools for the future, but an old problem still remains in the field of environmental analysis: the lack of standards of newly identified chemicals, such as transformation products of emerging contaminants. With high resolution MS we are able to discover large amounts of new chemical compounds, but many of them can only be identified tentatively due to the lack of commercially available standards.



## 4 / *Teresa Rocha-Santos*

*Principal Researcher with Aggregation,  
Centre for Environmental and Marine  
Studies (CESAM) and Department of  
Chemistry, University of Aveiro, Portugal*

### *Main research aims?*

Development of novel methods, fit for purpose, and study of organic contaminants and microplastics, fate and behavior in the environment, and the use of fungi for the biodegradation of microplastics.

### *Missing from the analytical toolbox?*

Screening devices for fast laboratory and on-site determinations of emerging contaminants are lacking. Specifically for microplastics, there is a need for instrumentation for the quick and easy identification and quantification of polymeric particles.



## 5 / *Thomas Ternes*

*Head of Department, Qualitative  
Water Science, Federal Institute  
of Hydrology, Germany*

Specializing in aquatic ecosystems, Thomas Ternes combines expertise in chemistry, ecotoxicology, microbiology, and radiology to study pollutants in rivers and coastal waters. His work

includes investigating the occurrence and effects of these pollutants, providing expert reports, and advising governmental bodies such as the BMDV and BMUV. Ternes' research aims to understand and mitigate the impacts of anthropogenic pollution on water quality, using data from extensive monitoring networks to inform public awareness and policy decisions.



**7 / Torsten C. Schmidt**

*Professor, Instrumental Analytical Chemistry and Centre for Water and Environmental Research (ZWU), University of Duisburg-Essen, Germany*

*Main research aims?*

Our research mainly aims to provide a more comprehensive understanding of the occurrence, effects, fate and abatement of organic contaminants in aquatic systems.

*Most exciting emerging technology?*

There is a lot of exciting work trying to uncover more of the exposome, like the total human exposure and associated diseases in a broader One Health concept. This perfectly aligns with strengthening the links between environmental analysis, hygiene and epidemiology in using wastewater as a source of health-related information in the population.

**Andrew Ault**

*Associate Professor, Department of Chemistry, College of Literature Science and the Arts, University of Michigan, USA*

*Main research aims?*

To use advanced analytical instrumentation and novel methods to understand the impact of atmospheric aerosols from a wide variety of sources on human health and global climate.

*Biggest challenge in environmental analysis today?*

Inhaled pollutants are critical to understand, as our lungs are much less adept at handling novel toxins and pollutants in comparison to exposures to our gut or skin.



**6 / Mark Strynar**

*Senior Physical Scientist, US EPA, Research Triangle Park, USA*

Mark has developed analytical methods for the measurement of PFAS and other chemicals in environmental and biological samples. When recently asked about the role of the analytical scientist in the broader PFAS problem, he said: “At the EPA, our mission is to protect human health and the environment. Real

and concrete regulatory decisions are made based on analytical data, and I believe it’s our responsibility to help alleviate past PFAS contamination while looking to the future for new issues that may arise.”



**8 / Diana Aga**

*SUNY Distinguished Professor, and Director of RENEW Institute, University at Buffalo, USA*

*Main research aims?*

My research involves investigating the fate, transport, treatment, and toxicity of environmental contaminants, including persistent organic pollutants, pharmaceuticals and



personal care products, and PFAS in environmental and biological samples.

*Most critical environmental issue?*

The identification and quantification of currently “unknown” contaminants and their transformation products that are toxic, even at trace levels – they are highly challenging especially when they occur in complex mixtures.

**9 / Gangfeng Ouyang**

*Professor, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, China*

Gangfeng Ouyang specializes in environmental analytical chemistry and has published over 110 scientific

articles and five books on the fundamental studies and applications of microextraction technology. Ouyang has previously been honored with the National Science Fund for Distinguished Young Scholars of China and the title of Fellow of the Royal Society of Chemistry (FRSC).

**10 / Juliane Hollender**

*Senior Scientist, Eawag & Adjunct Professor, Department Environmental Systems Science, ETH Zurich, Switzerland*

*Most critical environmental issue?*

Analytical scientists should support necessary changes due to climate change, such as the energy transition, so that they are efficient and do not create new problems.



### Michael Gonsior

Professor, University of Maryland Center for Environmental Science, USA



#### Main research aims?

The discovery of structures of deep ocean dissolved organic matter (DOM) molecules, so that we can use them as reactivity tracers to better constrain marine organic carbon turnover.

#### The moral responsibilities of analytical scientists...

Environmental science would be dead in the water (pun intended) without analytical scientists and experts in analytical chemistry are largely driving the discovery of fundamental biogeochemical processes today.

### Stefan van Leeuwen

Senior Scientist, Wageningen Food Safety Research, Wageningen University & Research, The Netherlands



#### Most critical environmental issue?

I believe society needs to re-think on what basis chemicals are allowed on the market. The speed of designing new chemicals is enormous, and environmental scientists cannot keep up.

#### Main research aims?

I focus my work on PFAS, and how these pollutants move through the environment and how they impact food safety. I want to unravel this complex group of chemicals, and design comprehensive measurement strategies.

### Paul Mayewski

Distinguished Professor and Director, Climate Change Institute, University of Maine, USA



Paul Mayewski played a key role in one of the most important modern discoveries concerning our interaction with the environment: the concept of abrupt climate change. He is the first person to develop and lead prominent climate research programs at the "three poles." During the pandemic, he focused on the Colle Gnifetti Historical Ice Core Project to explore the intricate interactions between humans and the environment using laser ablation inductively coupled plasma-MS.

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### Janusz Pawliszyn

Professor, Department of Chemistry,  
University of Waterloo, Canada

#### Main research aims?

My main research objective over my whole career as an independent researcher has been to develop sustainable analytical technologies, in particular eliminating solvents from sample preparation and on-site sampling strategies.



*Spending a \$1 billion research grant...*  
Continue the development of reliable and sustainable on-site and high throughput analytical screening technologies.

### Katherine Peter

Research Scientist, Center for Urban Waters, University of Washington, USA

Katherine's work is focused on water quality and contaminant fate in both natural and engineered systems,

specifically urban stormwater and vehicle-derived pollution. She is also working on the development of non-targeted analysis by high-resolution mass spectrometry for contaminant monitoring, as well as designing tools to improve data analysis quality and interpretation.

### Emma Schymanski

Full Professor, Environmental Cheminformatics, Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Luxembourg

#### Main research aims?

The identification of known and unknown chemicals in our environment and their effect on health and disease,



primarily with open source cheminformatics approaches coupled with high resolution mass spectrometry.

#### Most memorable advice?

Actually for me it's two pieces of advice that combine to be both memorable and recurrent; I use them repeatedly either in combination or separately – "gather the data" and "pick your battles."

### Kim Prather

Distinguished Professor and Distinguished Chair in Atmospheric Chemistry, Scripps Institution of Oceanography, USA

Kim focuses on developing and conducting measurements for aerosol chemistry. When asked about her motivation, she said: "Making a difference for our planet. Our research on aerosol impacts on clouds can help explain why we are seeing a sudden increase in weather-related disasters." She once discovered that dust from 12,000 miles away in Africa (and ocean microbes) affects snowfall over California – her most rewarding moment.

*Credit: Anna Thorbjörnsdóttir*



### Charlotta Turner

Professor of Analytical Chemistry, Lund University, Sweden; and Chair, Analytical Chemistry Division, Swedish Chemical Society

Charlotta's research focuses on green analytical chemistry and sustainable development by enhancing the value of renewables such as lignin, seaweed and food waste. She once "made (inter)national headlines by freeing her doctoral student and his family from an Islamic State warzone," as highlighted by a nominator.



**Marek Tobiszewski**  
Associate Professor, Analytical Chemistry Department, Faculty of Chemistry, Gdańsk University of Technology, Poland

#### Main research aims?

My work focuses on making analytical chemistry more green – connecting our technological advancements to society.

#### The moral responsibilities of analytical scientists...

Everyone has a responsibility to society. Every professional and every scientist has the moral obligation to make a lower impact on the environment in their field.



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# Instrumental Innovators

## 1 / Alexander Makarov

Director Global Research LSMS, Thermo Fisher Scientific, Germany; Professor of High-Resolution Mass Spectrometry, Utrecht University, The Netherlands; and Fellow, Royal Society, UK

*Making analytical instruments accessible...*

This goal could be facilitated by national funding agencies, especially if several of them are working together and involve vendors.

*Missing from the analytical toolbox?*

A technique to “see” a single molecule with atomic resolution directly and rapidly.

*Spending a \$1 billion research grant...*

I would create a massively parallelized high-resolution mass spectrometer on a chip!

*Biggest challenge facing the field?*

I think the biggest challenge is translation of analytical methods to clinics – it happens too slowly...

*Most memorable advice?*

Actually, there were several: “It is quality of people that defines success, not the quality of machines they run” (Lidia Gall, Institute for Analytical Instrumentation of Russian Academy of Sciences); “Never copy!” (Reinhold Pesch, R&D Director in Finnigan MAT); “Only the paranoid survive” (Andy Grove, CEO Intel).



## 2 / Gert Desmet

Full Professor and Department Head, Vrije Universiteit Brussel, Belgium

*Main research aims?*

Using advances in micro-fabrication techniques (etching, 3D printing) to develop improved liquid chromatography supports and devices, and using smart algorithms to improve liquid chromatography methods.

*Biggest challenge facing the field?*

I fear this is the rapidly declining training level of the average analyst starting today in industry, augmented by the fact that the samples they are confronted with are ever more complex and need to meet ever stricter regulations. Hopefully, instrument manufacturers see this as an opportunity to stuff their instruments with tons of artificial intelligence to make them much smarter than they are now.



## 3 / Ron Heeren

Distinguished Professor, Maastricht University; Director, M4i, The Maastricht MultiModal Molecular Imaging Institute; Member of the Dutch Academy of Arts and Sciences, The Netherlands

*Missing from the analytical toolbox?*

Accessible artificial intelligence tools that bring together morphological and molecular imaging data with the aim to facilitate easier clinical diagnostics.

*Spending a \$1 billion research grant...*

I would establish a center for innovative translational medical technologies, to make the time to market of MedTech innovations substantially shorter. The center would consist of a unique analytical infrastructure, imaging facility, and engineering infrastructure.



## 4 / J. Michael Ramsey

Goldby Distinguished Professor of Chemistry, Professor of Biomedical Engineering, Professor of Applied Physical Sciences, The University of North Carolina at Chapel Hill, USA

*Main research aims?*

Our group utilizes micro- and nano-fabrication strategies to develop devices for eliciting chemical and biochemical information with time and cost efficiencies. Our primary focus is on life sciences related needs.

*Spending a \$1 billion research grant...*

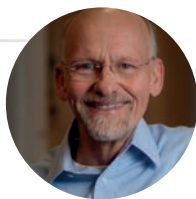
Managing such a huge research grant would be very exciting and a huge responsibility. I would prefer that the \$1 billion award was an endowment that could fund analytical R&D activities in perpetuity and that it was intended to have an international impact.





**5 / Richard Smith**

*Battelle Fellow and Chief Scientist, Biological Sciences Division, Pacific Northwest National Laboratory, USA (Recently Retired)*



Dick Smith's career has been characterized by, in his words, a desire to "contribute to society by developing separation and mass spectrometry technologies that are applicable to routine applications, particularly in areas of biological and biomedical importance." At a recent ASMS session held in Smith's honor, Joseph Loo described Smith as a "master inventor of new analytical technologies," which have included: the electrodynamic ion funnel in 1999, and more recently, structures for lossless ion manipulations' (SLIM). Earlier this year, after more than 47 years at PNNL, Dick Smith announced his retirement.

**6 / Ruedi Aebersold**

*Professor (Emeritus) of Molecular Systems Biology, ETH Zürich, Switzerland*



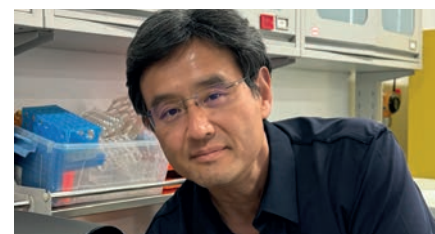
*Biggest challenge facing the field?*

The biggest challenge in the analytical sciences applied to biology and medicine is the lack of a paradigm to position

measured analytes such as nucleic acids, proteins, metabolites and lipids in the context of living systems. Progress in the analytical sciences has catalyzed amazing progress in detecting, quantifying and identifying biomolecules as chemical entities to a degree that essentially any biomolecule can be detected, many even from single cells. Yet, a collection of molecules is not sufficient to create and sustain a living cell.

**7 / Zheng Ouyang**

*Professor, State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, China*



*Main research aims?*

Develop analytical tools enabling fundamental research and biomedical applications.

*Spending a \$1 billion research grant... To launch the "Human Lipidome*

Project," which would be highly complementary to the Human Genome Project and the Human Proteome Project. It's the last missing part in human omics!

**8 / Chad Mirkin**

*Director, International Institute for Nanotechnology; George B. Rathmann Professor of Chemistry, Professor of Chemical and Biological Engineering, Northwestern University, USA*

*Main research aims?*

We synthesize new forms of matter at the nanoscale, delineate the unique properties that distinguish these structures from all other forms of matter, and use this knowledge to develop

technologies that advance medicine, clean energy, optics and photonics, manufacturing, and other fields.

*Most memorable advice?*

At the start of my journey at MIT, I was initially intimidated by the aura of the institution and many of my peers, but, as a friend of mine put it, "Everyone here puts their pants on one leg at a time; no one jumps off the dresser!"

**9 / Frances S. Ligler**

*Eppright Chair and University Distinguished Professor of Biomedical Engineering, Texas A&M University, USA*

*Spending a \$1 billion research grant... Set up a virtual institute with a 10-year lifetime to create, manufacture*

and deploy sensors that can measure complex toxic components in aquatic species, animals, plants and people over diverse parts of the earth. Analytics would be developed to provide data on the impact of manufacturing, energy creation, agricultural practices, climate change and human habitation.



## 10 / Daniel W. Armstrong

*R.A. Welch Distinguished Professor,  
Department of Chemistry and Biochemistry,  
University of Texas at Arlington, USA*

### *Most exciting trend today?*

Clearly artificial intelligence (AI) is attracting a lot of attention, although its actual contributions to chemistry

research have been limited thus far. One of the exciting aspects of AI in measurement science is using chatbots to implement ideas and solve task-specific problems by posing targeted questions. Can the chatbot complete the assignment with minimal human direction or



data input (which we refer to as unguided) or can it complete complex tasks with a bit more human direction (which we refer to as guided)? In

other words, can AI complete some scientific tasks that take researchers months to years to complete, in a matter of minutes to perhaps days?

## Erin Baker

*Associate Professor, Chemistry  
Department, The University of North  
Carolina at Chapel Hill, USA*

### *Main research aims?*

My research group is examining how chemical exposure affects human health by studying the exogenous chemicals we are exposed to in our daily lives and the endogenous molecules they affect.

### *Most memorable advice?*

“You can’t make everyone happy, but you can make everyone angry.”

This has helped me worry less about people who criticize my efforts even when I am trying my hardest.



## Purnendu (Sandy) Dasgupta

*Hamish Small Chair,  
University of Texas at  
Arlington, USA*



### *Instrument you couldn't live without?*

A high-resolution digital microscope.

### *In another life...*

The near-impossible – trying to make a living writing poetry!



## Martin Gilar

*Research Fellow, Separations R&D,  
Waters Corporation, USA*

### *Main research aims?*

I am fortunate to participate in research of LC instruments, columns, and analytical techniques at Waters. I enjoy developing the methods for analysis of biomolecules such as peptides and oligonucleotides.

### *Spending a \$1 billion research grant...*

With a \$1 billion research grant, I could apply the proteomic and genomic methods to study the most primitive forms of bacteria, their molecular machinery, and metabolism.

## Gunda Köllensperger

*Professor, Institute of Analytical  
Chemistry, Faculty of Chemistry,  
University of Vienna, Austria*

### *Main research aims?*

My current research aims at advancing small scale omics-type of analysis by mass spectrometry. My ultimate goal is the analysis of single cells in a spatial biology context.

### *Most exciting trend today?*

These are exciting times for multidisciplinary analytical science. There are many prime examples of emerging technologies that go beyond instrumental and procedural development of a single measurement principle. I am really excited about research on multimodal analysis of single entities, such as cells and particles at high throughput.



## Wim De Malsche

*Professor (Group Leader)  $\mu$ Flow group,  
Chemical Engineering Department,  
Bioengineering Sciences Department; Director  
MICROLAB, Microfabrication Core  
Facility; Vrije Universiteit Brussel, Belgium*

### *Main research aims...*

To gain full control of liquid flow profiles in flow devices and of trajectories of molecules and (bio)particles within these liquids, enabling the highest possible resolution batch and continuous separations.

### *Making analytical instruments accessible...*

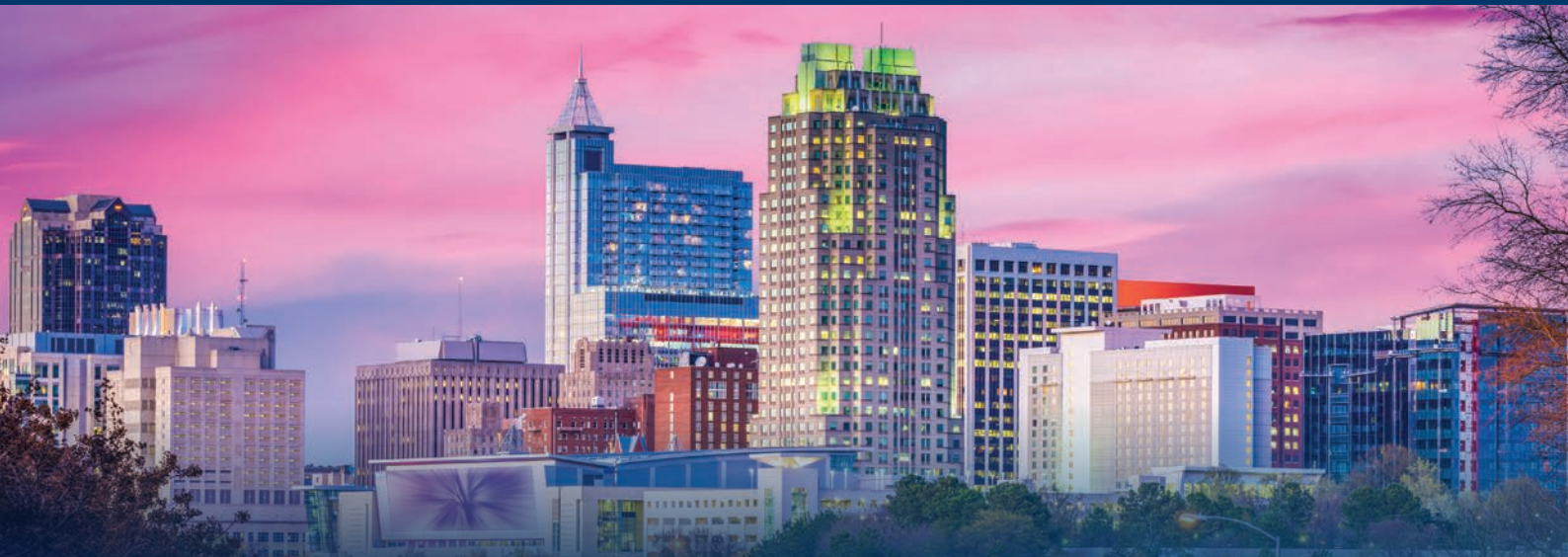
Current HPLC instrumentation is too bulky and expensive. Recent developments in optics, more general detection devices, and in pumping allow for shoe-box compatible solutions.



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**Ljiljana Paša-Tolić**

Laboratory Fellow and Lead Scientist, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, USA

*Main research aims?*

The most recent focus of our research involves technology development to enable multiomic measurements of single cells derived directly from tissues (or other natural sources) for medical and environmental research.

*A problem that could be tackled interdisciplinarily...*

All ecosystems, including human, are complex networks of organisms interacting with each other and their abiotic surroundings. We tend to simplify, divide and conquer, but in the process, we lose valuable information about how the system works, ability to predict and ultimately control biology. Addressing the complexity challenge requires not only quantum leaps in measurement science

(throughput, sensitivity, depth of coverage, real-time and in-situ measurements, etc.), but also effective collaboration across disciplines.



**Jeanne E. Pemberton**

Regents Professor, John and Helen Schaefer Professor of Chemistry, BIO5 Faculty Member, Department of Chemistry and Biochemistry, University of Arizona, USA

*Most exciting trend today?*

The increasing use of cheminformatics, an umbrella term that I define to

include chemometrics, machine learning, and artificial intelligence methods.

*Most memorable advice?*

Many years ago, my undergraduate research adviser once told me when lauding the breadth of areas that Al Bard's research had impacted in electroanalytical chemistry (even by that time): "It's relatively easy to be a specialist; it's far more difficult to be a generalist." My take-away from that was: learn as much as you can about as many things as you can and seek to become a generalist. In retrospect, I can clearly see the impact that this advice had in guiding many of my choices throughout my career!

**David H. Russell**

MDS Sciex Professor of Mass Spectrometry, Texas A&M University, USA

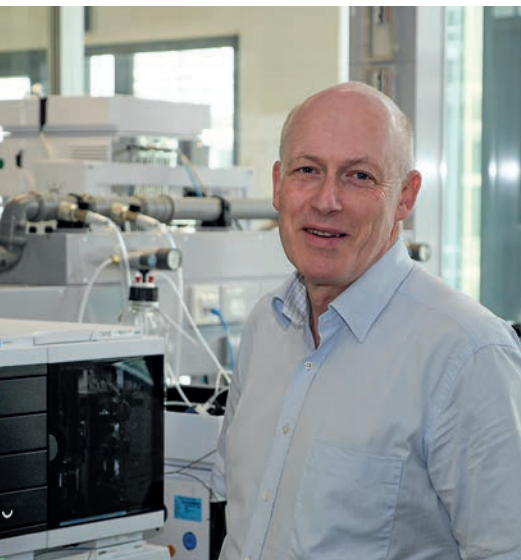
*Main research aims?*

My research focuses on the development of ion mobility-mass spectrometry for studies of structure(s), stabilities and dynamics of large protein complexes, including roles of metal ions and water on each of these properties.



**Konstantin Shoykhet**

Principal R&D Scientist, Agilent Technologies, Germany



*Missing from the analytical toolbox?*

Although we have versatile instrumentation which can successfully take a sample from the input and produce numbers as an output, there is significant room for improving the data interpretation and validation. For example, intelligent estimation of the quality of a result, and flagging. Also understanding of the entire workflow from sample taking and preparation, through the possible interferences during the analysis itself, to the adequate interpretation of analytical data results in a global context, requires more attention with increasing complexity of the workflows.

**Lloyd M. Smith**

W. L. Hubbell Professor of Chemistry, Department of Chemistry, University of Wisconsin – Madison, USA



*Main research aims?*

We develop new mass spectrometric technologies for the comprehensive identification and quantification of proteoforms in complex systems, by means of improved strategies and tools for bottom-up, top-down, and intact mass proteomics.

## Fast Lipidomic Analysis with High Resolution of the Molecular Species

The analysis of lipidomes deals with many isomeric compounds, making comprehensive separation essential to generate a biologically informative dataset. To achieve sufficient separation, the analysis times with standard methods, commonly using C18 stationary phases, tend to be longer than 20 min. This example uses human plasma samples to demonstrate that separations under 10 minutes are also possible with real samples

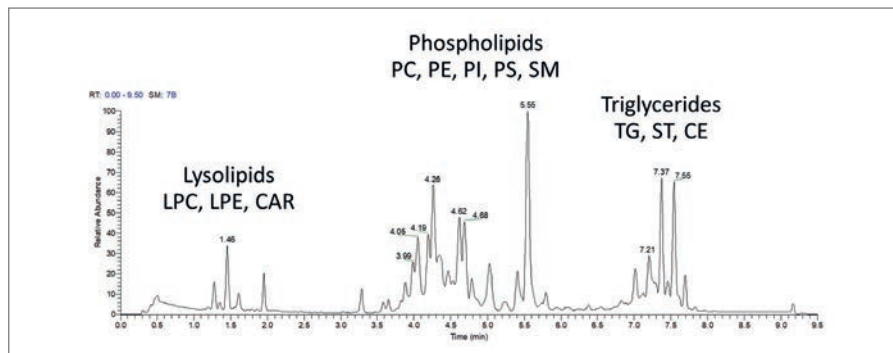


Figure 1: Successful lipidomic analysis of a human plasma sample using a YMC Accura Triart C8 column.

using a less hydrophobic YMC Accura Triart C8 column with bioinert coating to facilitate higher levels of sensitivity and recovery.




Figure 1 shows a well-defined separation between classes of lysolipids, phospholipids and triglycerides – typical for reversed-phase lipidomic analysis. Even with the less hydrophobic YMC-Triart C8 modification, molecular species of complex lipids can be feasibly separated

in a fast run. Hence, around 700 distinct molecules can be reliably determined.

Full method details can be accessed here:  
<https://ymc.eu/d/brDqg>

\* Application data by courtesy of Sergey Girel, Institute of Pharmaceutical Sciences of Western Switzerland (University of Geneva), Geneva, Switzerland.

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*“Pay attention to your data – not just from the perspective of the planned publication, but also for what can be learnt from the data.”*



## LC Sommelier

*Sitting Down With...*  
*André de Villiers, Professor*  
*of Chemistry and Polymer*  
*Science, Stellenbosch University,*  
*Stellenbosch, South Africa*

### Did you always want to be a scientist?

To be frank, I was never sure about what direction I wanted to take. In fact, I planned on becoming a veterinarian after university. However, after a rather momentous discussion with Pat Sandra and Henk Lauer in my fourth year, I decided to take separation science as a postgraduate. And I've never looked back.

### What sparked your interest in chromatography?

As I delved into separation science, I became particularly interested in wine chemistry. After discussions with wine researchers at Stellenbosch, the importance of analytical chemistry in this area was evident. I was very fortunate to complete both my MSc and PhD degrees under the supervision of Pat Sandra, who introduced me to experts across the chromatography field. To this day, I continue to work with these scientists, focusing my research on wine phenolic chemistry, improved separation, and characterization of tannins. The complexity of wine tannins make it an ideal application for testing the performance of the liquid chromatography (LC) and 2D-LC-MS methods my research group develops.

### What's the most significant change or development in separation science that you have seen during your career?

One noteworthy development that precedes my introduction to the field is capillary electrophoresis (CE), which became the focus of my MSc degree. Despite this, there are two developments

in particular that stand out: ultra high pressure liquid chromatography (UHPLC) and multidimensional LC. I was fortunate enough to be involved in HPLC research as a postdoc fellow at Pfizer Analytical Research Centre (PARC) just as commercial UHPLC instrumentation was introduced. Today, this technology is commonly used, and I think the paradigm-shift we've seen in performance as a result isn't appreciated enough – neither are some of the lessons learned surrounding extra-column dispersion and frictional heating. Even today, many of our LC-MS methods don't optimally exploit the available chromatographic performance due to instrumental constraints.

Additionally, despite being developed many years ago, multidimensional LC has rapidly developed over the past 20 years – specifically in terms of fundamental concepts, instrumentation, methodologies, and applications. I was also first introduced to multidimensional LC during my time at PARC – and, since 2006, 2D-LC has been a main focus of my research groups activities.

I must also mention the rapid advancements in MS technology and hyphenated chromatography-MS methods. These standout developments have provided us with more robust, flexible, faster, sensitive, and higher-resolving MS detection systems for high-resolution chromatography – allowing us to investigate compositions of complex samples in much more detail. Moreover, ion mobility spectrometry (IMS) has added additional value to LC-MS workflows. With data analysis becoming even more essential and progressively more complex within the chromatographic protocol, these advancements have been crucial in allowing us to extract relevant information.

### What is the biggest challenge facing the field today?

The training of suitably qualified

chromatographers. Though chromatography is used extensively in research and industrial environments, it's often in the context of an “analytical tool” and so relatively few users of advanced chromatography and mass spec systems are experts. Much of this can be overcome by on-the-job training, but the increasing complexity of our technology requires genuine expertise to extract optimal performance. I believe that too few highly experienced PhD and postdoc fellows are trained in chromatography. Maybe because the field isn't considered “sexy enough” compared with other avenues.

### What are you currently working on?

Our work currently focuses on the use of MS – particularly with cyclic IMS (cIMS) – in combination with one and two-dimensional LC for complex natural product analysis. The emphasis in MD-LC is on developing tools for improved method development and data analysis. All of this is tied to particular applications, such as analysis of tannins, cannabis, and South African plants.

### What are your hopes for the future?

I'd like our field to receive more recognition as an independent research area. Often chromatography in particular is taught at undergraduate level primarily from the aspect of an analytical tool, which doesn't reflect the exciting research and career opportunities within the field.

### What advice do you have for the next generation of analytical scientists?

Pay attention to your data – not just from the perspective of the planned publication, but also for what can be learnt from the data. Often, “failed” experiments are the most interesting and can lead to further exciting research avenues. They can certainly contribute to our understanding of the tools we use. Apart from this, be curious, work hard, and make the best of the opportunities that come your way.

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