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A Strong Sense of Community

Celebrating EPRWs past and present – as well as the people who make the pesticide residue field so special.

My first experience of the European Pesticide Residue Workshop was in 2014 – in Dublin. I was immediately struck by the strong sense of community within the conference. I witnessed a group of passionate scientists, working together to solve challenges in a highly complex analytical field – eager to learn from each other and pass on stories of successes (and failures) that could benefit others.

Inspired by the "buzz" at the EPRW 2014 – and Lutz Alder's entertaining lecture on the history of pesticides – I set about planning The Analytical Scientist's first foray into pesticide residue analysis (www.theanalyticalscientist.com/issues/0914/gurus-of-pesticide-residue-analysis). Three gurus – Finbarr O'Regan, André de Kok and Lutz Alder himself – shared their views on the regulatory landscape and the challenges and techniques that will dominate the future. Notably, high-resolution accurate mass spectrometry (HRAM-MS) featured prominently in the discussion...

Four years later, EPRW finds itself back in Germany – this time in Munich – for yet more international exchange of insight and experience. And I've thoroughly enjoyed collecting the thoughts of seven pesticide residue scientists for this companion compendium to EPRW 2018, brought to you in collaboration with Thermo Fisher Scientific. It's also been a great pleasure working closely with Richard Fussell. Well known to many of you, Richard is clearly passionate about the field that he's been intimately involved in for many years, and he was a real driving force in gathering our experts together.

In many ways, our compendium is a celebration of EPRWs past and present, as well as the advances made by a community of scientists always keen to push the limits. Lutz Alder takes us back to the inception of a conference that has been more successful than most could have imagined – "a wise decision in a Dutch restaurant." Our other contributors consider the current challenges for the field, discuss the technology most likely to help meet those challenges, and sing the praises of the essential conference that will be there to support them.

Richard and I hope you find the contents of our compendium insightful. And I urge you to share the digital version with colleagues not lucky enough to end up with a printed "collector's" edition: tas.txp.to/0518/EPRW2018

Rich Whitworth
Content Director,
The Analytical Scientist

Contents

The electronic version of this compendium includes: historic photos from EPRW (courtesy of André de Kok), Susanne Ekroth's Top Five screening papers, additional figures, application notes and other resources...
Download here:
http://tas.txp.to/0518/EPRW2018

EPRW: the Origins Story

The Austrian wine scandal, wine-fueled conversations, the rise of computers, and a wise decision in a Dutch restaurant… I recollect a long and rewarding career, take you back 22 years to the inception of the European Pesticide Residue Workshop, and look forward to a future as rich in progress as the past.

By Lutz Alder

Do you remember the Austrian wine scandal of 1985 – when wineries were caught adulterating wine with diethylene glycol to make it sweeter and more full-bodied? Back then, the Chemical Institute of the Humboldt University of Berlin was one of very few places in East Germany able to perform the necessary confirmatory analysis using GC-MS. I happened to be the Head of the mass spectrometry laboratory at the time, and so took my first step into food chemistry. A year later, the Central Hygiene Institute of the German Democratic Republic (GDR) asked for assistance in acquiring a suitable GC-MS system for future analyses – but they also needed someone to operate it. And so, in 1986, I found myself working for the GDR as a residue analyst. It was the start of a long career safeguarding food.

A preference for pesticides

I cannot say exactly what led to me work exclusively in pesticide residues analysis, but I do remember that I considered the challenge attractive – especially as it was a highly regulated environment with political and public impact. (I've been involved in a number of high-profile food scandals over the years.). And despite pesticide residues analysis being considered somewhat "routine," it is far from it; the target list grows each year, the challenges never seem to diminish, and the technology advances rapidly. Additionally, there was (and still is) plenty of scope for interesting scientific exploration; I remember colleagues questioning my logic in the early 2000s when I created a solution containing 300 pesticides: "You cannot do that!" they said. "The compounds will react with each other..."

By 1996, I had worked my way up to become the Head of the Pesticide Residue Unit of what was then called the Federal Health Office (BGA) but is now called the BfR (the Federal Institute for Risk Assessment), where I remained until my retirement in 2013. So whether I found pesticides, or pesticides found me – it ended up being the right choice.

During my time at the BGA, I was tasked with leading a working group of about 20 analytical chemists from all over Germany with the goal of "filling the gaps" in pesticide residues analysis. The working group had many successes over the next 10–15 years, and created many official methods for Germany. But I would like to relay what I found to be my most amusing contribution. My laboratory had acquired an LC-MS/MS system ahead of other members of the group, and so we subsequently developed a method for the simultaneous determination of 100 compounds. We hosted a meeting to demonstrate the method to the group, and invited all attendees to secretly spike a small tomato with a single pesticide (at one of three concentration levels – 10, 20 and 50 ppb) before we began the meeting. During lunch, one of my colleagues shared the findings of his analysis on the notice board. I remember how surprised everyone was that he had found all of the compounds – and how impressed they all were with the capability of LC-MS/MS. This meeting essentially kickstarted the use of LC-MS/MS for pesticide residues analysis in the official testing laboratories of Germany.

Birth of EPRW

I remember getting a telephone call from the Netherlands in 1995. The person on the other end of the line? André de Kok – someone I had met before one or two times in Brussels, when we participated in a EU collaborative trial for the determination of pesticides in cereals. He discussed the potential of organizing a pesticide residue workshop. I asked for two days of thinking time during which my colleagues warned me that it would be a lot of extra work with no extra pay. Fortunately, the vice president of my institute was more supportive and could see the benefit. Later, I called André and gave him my short answer: I am interested!

André, Head of the Pesticide Analysis Department at the Food Inspection Service based in Alkmaar at the time, invited me to the Netherlands to talk further. I remember arriving in the afternoon for a tour of the facility; he showed me his instrumentation, including several good GC-MS systems, and described some of their specialized methods. That evening, we went to a restaurant where we began our discussions of a workshop in earnest. André told me how he had been to the Californian Pesticide Residue Workshop a couple of times with Arne Andersson (Swedish National Food Administration). On one flight back to Europe, sitting side-by-side and drinking wine, André and Arne had mused over the possibility of a European workshop. They decided that they needed a scientific organizing committee with representatives from France, Germany, Italy, Spain, and the UK.

I gave my formal "yes" in the restaurant that night. It was probably one of the most important and best decisions of my professional life. I could see real value in such a meeting – and I was excited! In 1996, André chaired the inaugural EPRW in Alkmaar.

22 Years, 12 workshops

In the beginning, my expectations of the European Pesticide Residue Workshop were relatively humble. When Antonio Valverde organized the second EPRW in Almeria (Spain) fortunately many (but not all) teething troubles had already been

Lutz Alder's MS lab in Humboldt University, 1985. The instrument on the left had a chart recorder. The GC-MS (right) had a computer running with Basic language – a thermo printer was used instead of a monitor

Members of the Scientific Organizing Committee at EPRW 2008 in Berlin

"Laboratories with sufficient tandem mass spectrometry capability should be looking to introduce HRAM MS as a next step."

overcome. Today, EPRW attracts visitors from over 50 countries across all continents (apart from Antarctica) – and I believe it is the leading conference in the world. I could never have expected that we would play such an important role and have such an impact. Quality control procedures created in Europe are represented in the SANTE guidance document, which influences the world; authors from as far afield as China may find it important to state: "We fulfill the SANTE requirements for validation." These guidelines, drafted for the first time by Alan Hill and colleagues in the UK were permanently discussed at – and improved by – the EPRW community of scientists. I feel proud to have played a role.

There have been many EPRW high points over the years, but I'll share a couple of stand out moments. Rome 2002 was a big meeting. Steve Lehotay presented the QuEChERS method for the first time, and it was fascinating to hear why and how the various steps had been chosen by him and Michelangelo Anastassiades. A couple of hours later, a colleague from my group shared – also for the first time – our method for 100 pesticides by LC-MS/MS.

EPRW in Berlin (2008) was also a highlight, partly because I chaired that conference. It was entirely organized by me and my group of around 12 people, all of whom had special tasks. There was so much to do and think about. It was great fun – I've never had such exciting times!

Technology milestones

When I think about milestones over the years, the first thing that comes to mind may surprise some of you (especially younger members of the community): the rise of the computer. In the early days in my mass spec lab, we used chart recorders – so hyphenation with GC or LC was simply not possible; there was too much data. In the early 1980s, mass spectrometry was pretty well developed – but we had no way of accessing the potential. Connection to computers opened up a new world of hyphenation and had a huge impact on analytical chemistry, which, of course, continues to this day.

I would consider a second major milestone for our field to be the introduction of LC-MS/MS. I was at a small Bayer symposium in 1998 when I first saw the potential of LC-MS/MS. Bayer, as part of the pesticide registration process, had to develop analytical methods for pesticide residues, and recognizing that GC-MS was not always sensitive enough to detect residues at the lowest concentration levels, they investigated LC-MS/MS, and shared some of the work with us. It was totally clear to me that we needed such an instrument. As soon as we received our own LC-MS/MS system in 2000, we set about acquiring LC-MS/MS data from our large stock of pesticides to acquire individual parameter sets. Once we'd assessed the data within the working group, we shared everything on our webpage (another reason I am well known, I guess!). Nowadays, instrument manufacturers supply such data sets, but in the beginning it was an important contribution.

The agenda for next 12 workshops?

Right now, I see two main challenges facing the field of pesticide residues analysis.

The first challenge is the need for methods without limits. LC-MS/MS is powerful, but it has a limitation: it is difficult to measure more than 300 compounds in a single analytical run. However, we have over 800 pesticides sold at present and another 700 "old" pesticides, produced in the past. With high-resolution accurate mass (HRAM) MS systems, we can break out of this limit; and so further development of HRAM MS systems will be a key direction of the future. Two technologies compete for this space – Time-of-Flight (TOF) and Orbitrap technology. I've worked with both, and I have to say that the more promising of the two is Orbitrap because of its higher resolution. It seems clear to me that laboratories with sufficient tandem mass spectrometry capability should be looking to introduce HRAM MS as a next step.

The second challenge is the need to make data evaluation a more efficient process. Right now, data evaluation requires more time than measurement, and we all spend too much time in front of those computers I originally loved so much! I heard a clinical analyst say recently: "When will we get an instrument that gives us a simple answer of 'yes' or 'no.' I don't want lectures about matrix effects, better extraction, chromatographic integration or data evaluation. I want a black box!" I think this is the direction analytical chemistry will and must go. It's a shame for scientists who want to learn and delve into the complexity. But routine analysis – whether in food safety or the clinic – demands ease-of-use and robust measurements. Powerful software and comprehensive databases that support full applications – in other words, complete solutions – are going to become increasingly important.

Happily, I think we are all slowly moving in the right direction.

As for me? I'm sure I'll find time to keep up with the world of pesticide residues analysis – and you may even see me at future EPRW conferences (I'm in the local organizing committee for Munich). However, I'm also looking forward to spending more time with my three grandchildren – happy with the knowledge that the food they eat is safeguarded by the next generation!

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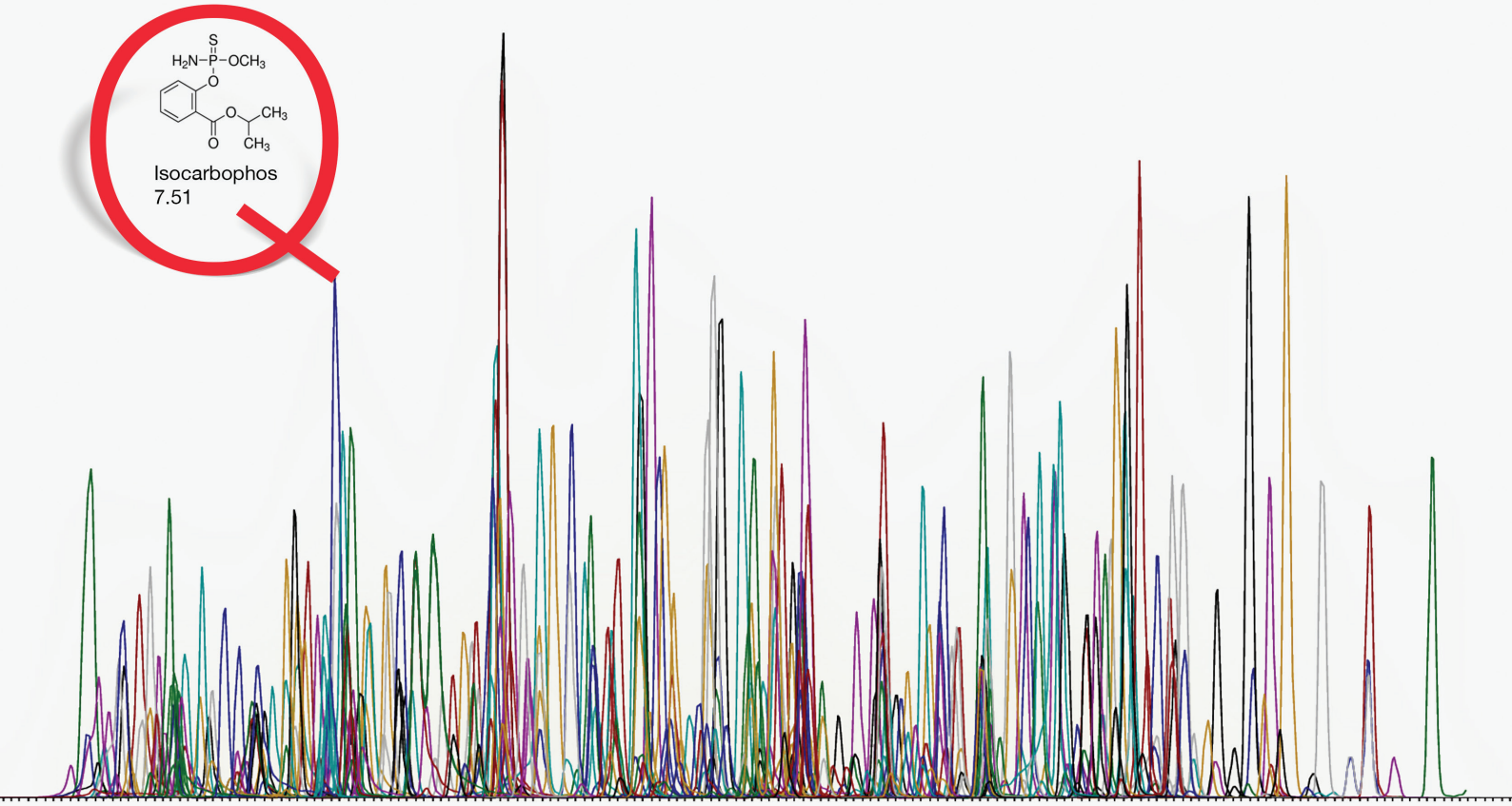

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Protecting Consumers – and Wildlife

How to stay "in the game" when it comes to pesticide residue analysis.

By Kirsty Reid and Mike Taylor

Mike Taylor is passionate about protecting wildlife – from the magnificent golden eagle down to the humble bumble bee.

Pesticide residue analysis is a complex field that evolves quickly, and we think it's fair to say that if you're not up-to-date, then you're out of the game. And that doesn't just apply to instrumentation – it's also about the skillset of your staff and the knowledge base within an organization. In that regard, we're lucky to have the European Pesticide Residue Workshop (EPRW), which is more than a meeting – it's a community that serves several roles. First, it allows essential information exchange – perhaps pointing the way towards a better solution to a current or upcoming problem. Second, it's a "sanity check"; when presenting at EPRW, you not only share your work, but also open yourself up to (friendly) scrutiny, which can be a daunting but fulfilling process (assuming your methods stand up!). Importantly, EPRW also presents an opportunity to compare your own laboratory and efforts with those of the world's leading practitioners. Are barriers being broken? Are people moving into previously uncharted territory that we're interested in? In a fast-paced field, all laboratories need to stay at the top of their game!

The appliance of pesticide science

A good chunk of the work that we do within the Chemistry Branch at Science and Advice for Scottish Agriculture (SASA; a Division of the Scottish Government's Agriculture, Rural and Economy Directorate) feeds into annual UK and EU surveillance programs. As many of you will know, these rolling programs monitor multiple pesticide residues in the main food groups through specific commodity surveys on samples collected within calendar years – and that makes method development a continual challenge. Complexity is added by the need to validate individual commodities in addition to commodity categories; for example, in legumes, you might expect peas and beans to behave similarly – alas no! Thiodicarb converts to methomyl in peas (without pods) but not beans (in pods)...

All the work we do at SASA is applied, but we find it is far from routine given the challenging nature of pesticide/commodity combinations (where "one method fits all" is rarely the case) and the need for rapid turnaround times. Fortunately, we embrace the perpetual challenge – it ensures that our jobs remain exciting. And when we invariably solve problems and hit deadlines, we can bask (for a moment) in the success...

Our ongoing participation in proficiency testing schemes allows us to directly monitor our laboratory's performance against others across Europe – in other words, we can check that we're still "in the game" and if we're winning! The results speak for themselves. Such proficiency tests can also be helpful in informing technology or method choice by indicating where gains can be made. That said, different labs use different methods and instrumentation (often through necessity) – so, ultimately, it's important to decide what works best within your own lab. Here, the level of staff

Find Kirsty Reid at EPRW 2018 in Munich to learn more about the work SASA do.

experience and knowledge is perhaps an under-discussed part of the equation; even the most cutting-edge instrumentation doesn't guarantee the right result in the wrong hands.

Workhorse technology – now and into the future

We would describe our tandem mass spectrometry (MS/MS) systems – both LC and GC – as our lab workhorses. We're now able to look at many more transitions in a more specific and targeted way, which has made life a great deal easier than 15–20 years ago. Being able to screen and confirm several hundred target analytes in a single experiment represents a significant breakthrough. And that's why, for our applications, we can see modern triple quadrupole systems continuing to serve us well. High-resolution accurate mass systems are certainly alluring, but we would consider them a "luxury" – for now...

Where we do feel we can make gains today is at the separation end of our systems; we're looking at ion chromatography and micro-flow LC as inlets, for example – both of which have been subject to technological improvement, making them compatible with our current mass spec portfolio. IC-MS/MS presents a realistic solution for analysis of 'difficult-to-analyze' polar pesticides. A previous evaluation of micro-flow LC-MS/MS indicated significant savings in solvent consumption, dilution of adverse matrix effects and reduction in experimental cycle times.

Whatever the technology, pesticide residue analysis pushes the limits – and the goalposts are not rooted to the spot; the target list is constantly growing and shifting, as is the variety of matrices. But as advanced instrumentation meets the increasing analytical challenges, the volume of data also increases; data handling and analysis represent the real challenges of the future.

Peers = mentors

As noted, pesticide residue analysis is challenging, which is why it's so great to have an engaged community to watch and actively take part in – that's most likely a key reason for EPRW's success over the years.

Most scientists in the field, including us, keenly follow the work of the European Reference Laboratories (EURLs); for example, we've recently seen some intriguing work coming out of the University of Almeria on the use of SFC – something we'll be watching closely. At the same time, we recognize that it's important for us to contribute where we can. To that end, we try to be early adopters where possible – hence our interest in ion chromatography and micro-flow LC-MS for multi-residue analysis in food and wildlife. We actively publish the work that we consider most relevant and will continue to share our explorations into these areas at EPRW and beyond.

One recent game changer for us in GC-MS was our move to a programmable temperature vaporizing (PTV) injector, incorporating a de-activated baffled liner and associated experimental optimization. Previously, we were using cool on-column

The beautiful game

Mike Taylor's route into analytical chemistry was far from the norm. "When I left school, I played professional football for Middlesbrough FC. It was a career that ended more abruptly than I expected, so I used some basic science qualifications as the foundation for joining Imperial Chemical Industries (ICI) – a company that had a huge impact on Teesside," says Mike. Placed – somewhat at random – in the analytical lab, Mike found an aptitude and eagerness for problem solving.

"It's fair to say the transition from professional footballer to analytical chemist was jarring – one minute I had dreams of lifting trophies, the next I was in a lab fixing gas chromatographs!" Back then, several emerging (and now high impact) techniques were being newly applied, so there was no defined "rulebook" as such – and that afforded Mike a degree of analytical creativity and freedom that has been a feature throughout his career. "I found myself continually pushing the limits of mass spectrometry to answer the questions presented to me; that too has been an ongoing feature of my career," Mike says. "Over the years, I've applied cutting-edge techniques to samples as diverse as high performance engine oil, pineapples, sausage rolls – and golden eagle livers..."

Are there any similarities between professional football and applied analytical chemistry? "Well, every analysis or football match represents a singular challenge that demands a top performance – both individually and as a team. And you always strive for the best result possible."

injection with a retention gap, which was being changed before every batch analysis – quite time consuming (a couple of hours analyst/maintenance time per batch). Since introducing PTV, setup is faster and more straightforward. Moreover, when dealing with tricky target compounds that are susceptible to degradation (captan, folpet and metabolites, for example), we've noticed significantly improved stability in many different matrices with the above PTV injector configuration. We've published a poster on that topic (1), and there's a peer-review publication underway.

At EPRW 2018, we'll be presenting another poster: "The quantitative analysis of over 300 pesticides in crude QuEChERS extracts from various fruit and vegetable matrices with high acid and water content using LC-MS/MS and polarity switching."

Where eagles dare not

One area where SASA sets itself apart from most pesticide residue labs is our involvement in the Wildlife Incident Investigation Scheme (WIIS). Set up in the 1970s, WIIS began as a proactive investigation into the adverse effects of legitimate pesticide use on wildlife. Over the years, the scheme has expanded to cover the illegal use of pesticides (which is to say, wildlife crime) – so we've become involved in cases where wildlife and domestic animals have been deliberately poisoned. It's clearly a global issue, but we would argue that Scotland is at the forefront of this field – and we at SASA actively develop and refine analytical approaches to best support this great effort.

The work extends out from pesticides to include anticoagulant rodenticides (rat poison), another class of substances that can enter the food chain accidentally or intentionally. And we've also developed methods looking at veterinary medicines in wildlife; animals may scavenge on dead animals that may have been treated, which is another route of exposure. Essentially, we act as the analytical arm of a forensic investigation into these wildlife incidents.

Certain cases draw more attention than others – those involving endangered species for example. One sad and startling case from 2014 involved the mass poisoning of 16 birds of prey in the Black Isle region of Scotland. The perpetrators remain at large, but we do know that banned carbamate pesticides – aldicarb, carbofuran and carbosulfan – were used.

In some ways, the WIIS work is a natural extension from pesticide residues in foods; the analytical tools and many of the challenges are the same. But in WIIS work, the concentration range is huge – from trace levels of residues in a liver sample to visible contamination in the stomach contents! One specific challenge is that forensic samples are finite in nature – very often we've only got one shot. And that's why our methods need to be extremely robust.

When we tell friends and family about our endeavors at SASA, stories about golden eagles being poisoned certainly grab more attention than those describing how maximum residue levels were (or were not) breached in a bag of frozen peas... But clearly, we consider both the monitoring of pesticide residues in foods and our investigations into wildlife poisoning to be of critical importance both for the community and internationally. And we love what we do.

Reference

1. *KB Reid, KJ Viezens, LM Melton, and MJ Taylor, "The use of a deactivated (baffled) PTV injector liner and GC-MS/MS method for the quantitative determination of Captan, Folpet and their metabolites in ethyl acetate extracts of fruit samples." www.sasa.gov.uk/content/use-deactivated-baffled-ptv-injector-liner-and-gcmsms-method-quantitative-determination*

Kirsty Reid is a Senior Analyst at SASA, with responsibility for the overall management of the Pesticide Residues in Food (PRiF) team. Mike Taylor is Head of Chemistry at SASA.

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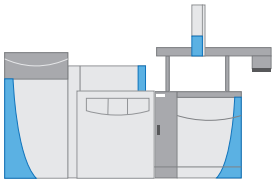

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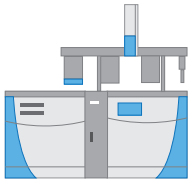

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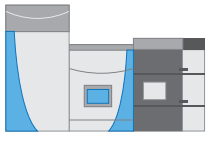

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Fast routine analysis of polar pesticides in foods by suppressed ion chromatography and mass spectrometry

Katerina Boušová[1], Cees Bruggink[2], Michal Godula[1]
[1]Thermo Fisher Scientific, Special Solutions Center, Dreieich, Germany
[2]Thermo Fisher Scientific, Special Solutions Center, Breda, Netherlands

Overview:
The presence of very polar ionic pesticides in surface and drinking water, as well as food and beverages, has become a controversial issue in recent years. The development of genetically modified crops tolerant to glyphosate and glufosinate, for example, promoted the use of these broad-spectrum herbicides. However, the analysis of glyphosate and other polar compounds presents a difficult analytical challenge. Their polarity does not allow easy analysis by reversed-phase HPLC, so alternative methods need to be applied. Recent developments in ion chromatography and mass spectrometry offer many advantages for the analysis of very polar substances. Ion chromatography (IC) is the preferred separation technique for polar ionic analytes, such as anions, cations or small polar analytes (metabolites), and sugars. Triple quadrupole mass spectrometry systems offer low detection limits and high detection selectivity when operated in selected reaction monitoring (SRM) mode. The system robustness allows the analysis of food and environmental samples.

Method:
Homogenized samples of lettuce, oranges, and wheat flour were extracted. The sample extracts were centrifuged and after filtration through syringe filters injected into the IC-MS/MS system. The instrument system comprised a metal-free Thermo Scientific™ Dionex™ Integrion™ HPIC™ System and a Thermo Scientific™ Dionex™ AS-AP Autosampler coupled to a Thermo Scientific™ TSQ Endura™ Triple Quadrupole MS. The chromatographic separation was carried out using a polymer-based Thermo Scientific™ Dionex™ IonPac™ AS24 analytical column (2 × 250 mm, p/n 064153) and Thermo Scientific Dionex IonPac AG24 Guard column (2 × 50 mm p/n 064151). The hydroxide eluent was prepared in-situ using an eluent generator, the Thermo Scientific™ Dionex™ EGC KOH Eluent Generator, and a Thermo Scientific™ Dionex™ CR-ATCII, preventing the use of external chemicals. The analytical data were acquired and processed the Thermo Scientific™ Chromeleon™ Chromatography Data System.

Conclusion:
The reported in-house validated method enables the quantification of ten polar ionic compounds or four ionic pesticides and their metabolites in different food matrices by coupling ion chromatography to a triple quadrupole mass spectrometer at levels significantly below EU MRL definitions. This method is recommended as a reliable and cost-effective solution for any routine lab dealing with the determination of polar pesticides and their metabolites in food samples.

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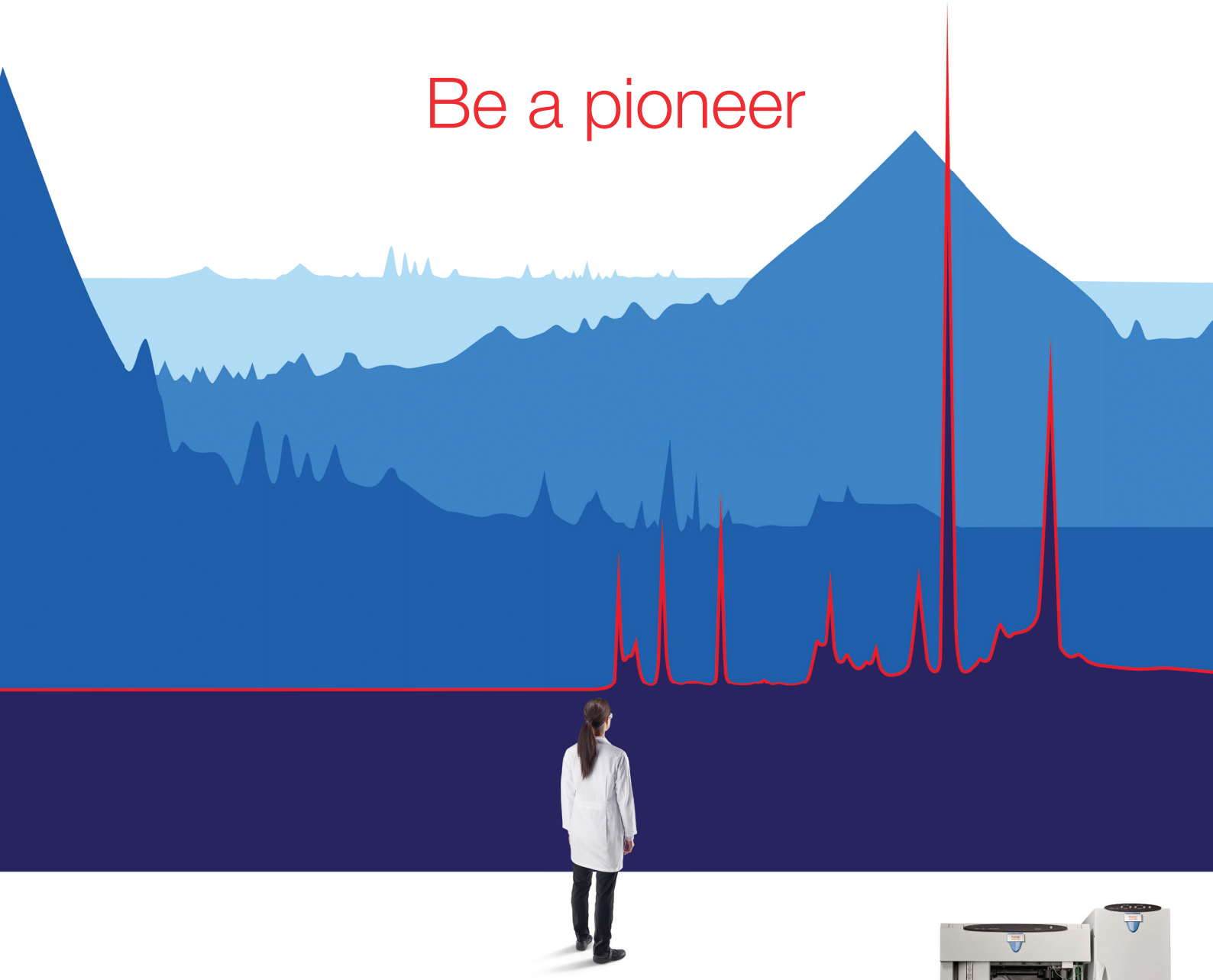

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Full of Promise

What's on the horizon for pesticide residue determination technology? Jim Garvey, from the Department of Agriculture, Food and the Marine and The Pesticide Control Laboratory, Dublin, Ireland, shares his insights – and explains the role that EPRW plays in the advancement of the field.

Walk us through the main changes you've seen during your years in pesticides...

When I joined in 1999, we were analyzing a small number of pesticides – approximately 80 – using non-selective detectors (such as ECDs and PFPDs), which meant that we had to make up a large number of standards to ensure that co-elutions did not affect our analyses. In some cases, it could take us a significant time – sometimes two weeks from extraction to results! In 2000, we started moving to single quadrupole mass spectrometry – and that increased our scope dramatically. The number of standards required was reduced because co-elution was not a problem, as long as we had unique data. Around 2005–2007, we introduced triple quadrupole MS and have operated with those ever since. They've served us very well, but in the last year or so, we've seen another big change: a move to high-resolution accurate-mass (HRAM) MS systems.

So, for you, the major milestones have been technological?

Exactly. In our field, you are limited by the technology you have available at a particular time. When we look back at the work we did on single quad MS, it was the best technology we had, but clearly we were limited in scope. When triple quads came along, we were able to do more in terms of sensitivity and selectivity – but once again, the technology is not without limits. And now HRAM technology opens new doors and allows us to do even more. Having said that, a laboratory that does not have sufficient resources to adopt HRAM systems can still do a great deal of good work using triple quad systems. As with many other areas of analytical science, there is a balance between technology and resources.

Do you sense frustration from those who do not have access to the latest technology?

I think everyone wants to be working with the most modern tools available – especially when you consider that legislation is demanding more from us; the need to cover many more pesticides and metabolites – and at lower concentration levels – ramps up the pressure. In some cases, you really need to be using triple quad MS systems, if not HRAM systems, to cope with what's being asked.

Would you say that legislation is also driven by technological advances?

My answer here could be controversial: I don't think there's any connection between legislation and technology! Often, the scientists in the lab are kept at a distance until the legislation is actually in place – and that can be a problem; sometimes we don't have the sensitivity to achieve what is required. Nevertheless, there appears to be a belief that, if something is written into legislation, the technology will catch up. And that can feel like we're always playing catch up.

What are the main analytical challenges in pesticide residue determination right now?

The multi-residue methods we have tend to be very good, and so the challenges surface in the area of single-residue methods. Tricky compounds that don't fit into multi-residue methods, such as anionic pesticides (for example, glyphosate and glufosinate, chlorates and perchlorates) may demand the use of specific technology. HPLC technology is not always consistent and so there's a debate within our group as to whether we should be switching to ion chromatography (IC). It is our single biggest problem at the moment. We have evaluated different types of multi-mode columns, but getting them to work day in, day out is a challenge. We are now assessing IC as a potential solution for our laboratory

– but that's not to say everybody will go that way. In our field, the advances we have seen so far have been incremental rather than dramatic. We're still waiting for the "lightbulb moment" when we think, "This is going to solve all our problems!"

Why do you feel ion chromatography has promise?

We're only at the start of our assessment of the technology, so it's difficult for me to say whether it will be successful yet, but from the data I've seen so far, it seems to provide more stable retention times with more stable matrix effects. The peak shapes appear to be a little broad, compared with reversed phase liquid chromatography (RPLC) – but peak shapes with other columns are not great either, so that's not really an issue. The main thing that drew me to ion chromatography was the stability and consistency of the system. With current HPLC columns, you have to stabilize your system for a long time to get good data, and you can disturb that stabilization very easily. Our plan is to combine IC with HRAM mass spectrometry to gain real benefits from both.

What does HRAM MS bring to the field?

We started using HRAM technology – Orbitrap™ – with our LC systems, and our original plan was to confine it to pesticide screening approaches. However, it very quickly became clear to us that these systems allowed quantitative analysis, and when we then ran them in parallel with our triple quad systems, we found there was no difference in terms of quantitation; exactly the same sample preparation techniques could be used for both systems, and results were pretty much identical. We had all the advantages of the quantitation but with full scan data, which was new to us; the high mass accuracy fragmentation gives us more certainty in our results.

Could you share a little about your work in pesticide formulations – does it help with pesticide residue determination?

When you work with both, as I do, it's clear that the information we get from formulation work can be very useful for residues determination; for example, if you find positives that you're not expecting. We found herbicides in milk a couple of years ago and, because of our formulations background, we were able to pin it down to the actual product, which allowed us to give useful information to enforcement bodies. One big issue in the formulation world right now is all the illegal and counterfeit pesticides flooding the system – there is no concerted way of dealing with them. Our lab uses profiling methods; essentially, we take the philosophy used in the likes of metabolomics, and transfer it to product analysis. We use whatever technology is most appropriate – at present, FTIR or GC-MS – to "fingerprint" a product; if we know what the authentic product looks like, we can compare it with suspicious products and look for differences.

Given the way that our work in formulations informs our efforts in pesticide residues, I don't think there is enough of a connection between the two in most laboratories. I gave a talk on formulations at the EPRW years ago, which people found interesting because it was something they hadn't even considered. In the last year or so, the European Commission has started to take a big interest in formulations, and over the next 5-10 years I think we're likely to see a more visible formulation aspect to the work we do in the EU. And I think that can only help the residues community.

What value does the EPRW bring to the field of pesticide residue determination?

EPRW is where you get to learn about the cutting-edge work that's going on – it's like an early warning system! For 2018 in Munich, I expect to see HRAM featuring heavily; there's an enormous amount of work going on in this area that is going to dictate the direction pesticide residue analysis takes over the next ten years.

EPRW is very niche conference, which seems to result in a strong community vibe…

Very much so. Pesticides is ahead of many other disciplines in that sense. The group that met in Athens in 1999 (when I first joined the field) really stays together, and essentially dictates policy within Europe. New people join the group and become accepted; there is very much an atmosphere that people are part of a group. We might have different ways of achieving results – but we all have the same goals and challenges.

It's a hugely complex and challenging field in which to work – what keeps you motivated?

Ensuring that we stay up-to-date with technology is probably the core of my work; I have to make sure that, if I retire tomorrow, the lab is future-proofed and the technology we have will survive the next ten years. We're always looking for new technology and new methods – and we spend a great deal of our time trying to plug the gaps – areas where we don't have optimal technology or methods. Our main current focus is the transition to HRAM MS systems; it's important for us to get our methods developed – and to get the transition right. And that's what's driving me forward right now!

Using Advanced Analytical Tools to Accelerate Discoveries – in Coffee

How the latest LC-HRAM-MS technology helped us to get to the bottom of a pesticide mystery in a curious coffee case.

By Thierry Delatour

Analytical chemistry is a fascinating area of science – you need to constantly adapt your tools to the questions you are asking, so there is always a new challenge. Adding to that fascination are the many exciting technologies that are able to provide highly accurate information in a very short timeframe. Looking specifically at pesticide residue analysis, a common approach is to use simple, nonspecific – but speedy – sample preparation ahead of highly sophisticated analytical systems, such as LC/MS-MS or LC-HRAM-MS, which can generate data within just 10 or 20 minutes. The bottleneck? We now struggle to analyze our data as efficiently as we can generate it. Fortunately, we have seen great improvements in software in the last few years – and there is still plenty of room for new advances and opportunities.

The cost of quality

The Nestlé Research Centre carries out a significant portion of Nestlé's research in two major fields: product innovation and food safety & quality. It is also where we develop analytical methods that go on to be implemented in our quality control laboratories – we have 25 Nestlé quality assurance centers, which carry out routine testing for our factories, ensuring that key parameters are analyzed and that our products are compliant with regulations.

When creating analytical methods, our main aim is, of course, to demonstrate compliance – doing our best to eliminate false positives and negatives in the process. But the major challenge is definitely cost. Guaranteeing quality has a certain cost, but we work in a very competitive industry with price expectations from consumers, so we need to constantly challenge our analytical methods, focusing on increasing efficiency and turnaround time. We must always deliver reliable data, but being cost effective for the company and ultimately the consumer is also important. A final challenge is to make methods more environmentally friendly by reducing waste, solvent use, and so on.

What's in your coffee cup?

Back at EPRW 2016, we presented the interesting outcome of our work in food analysis. A few years ago, there was some concern around the pesticide chlormequat being found in high quantities in some raw food materials, causing various labs and food regulators to increase their control of chlormequat. When performing a multiresidue analysis on roasted coffee, one lab found not chlormequat, but mepiquat – a different pesticide. Not only was this a potential compliance issue, but it was also confusing; our coffee plants are never treated with mepiquat! It was a mystery – and one that we needed to solve promptly and definitively.

"This was a unique case of a pesticide being generated by heat from components naturally present in a raw food material."

At Nestlé, we have a great deal of experience in the chemistry of coffee, so we were able to hypothesize the presence of natural precursors of mepiquat in green coffee beans that might decompose during the normal process of coffee roasting to give rise to mepiquat. First, we incubated these precursors in a model system, and demonstrated with LC-HRAM-MS that both mepiquat and some intermediates are formed during decomposition. We then ran a trial on an industrial scale to further confirm our model under real-world conditions. We used green beans initially shown to be free of mepiquat, processed them, and measured for mepiquat again in the same samples after roasting. And indeed, we showed that mepiquat was present. To the best of my knowledge, this was a unique case of a pesticide being generated by heat from components naturally present in a raw food material.

Our study showed that meqiquat can arise not only from pesticide use, but also from heat applied during processing

– or even from cooking at home. In that case, its presence in roasted coffee is not a contamination issue, but could the mepiquat levels in roasted coffee pose a risk to health? We calculated that if you are a heavy coffee drinker (consuming between 5–7 cups of coffee per day), you would be exposed to just 0.2 percent of the tolerable daily intake (TDI) of mepiquat, ruling out any safety issue.

The pesticide residue community at ERPW were very interested in this story, because it's so unusual. But I think the development of new multiresidue methods and the trend towards less targeted analyses – screening methodologies (highlighted by Susanne Ekroth on page 16) will lead to similar cases in future.

My colleague will be attending EPRW 2018 with another very interesting story to tell, regarding folpet and phthalimide. It is known that the pesticide folpet can decompose and produce phthalimide, but it's also generated from other precursors unrelated to pesticides, so it's important to pay careful attention to how it is measured to avoid overestimations.

Community spirit

Attending EPRW is always a great way to share information, and to maintain and develop your network. But, as "the curious case of the non-compliant coffee" shows, it's also a place to highlight findings that have a wider impact. When you're working in your own lab, it can often feel that you are the only one facing a particular issue. Then, when you go to a conference like EPRW, all of a sudden you realize you're not alone; many people have the same issues and challenges.

For example, it's becoming relatively straightforward to measure one particular analyte using simple sample preparation and sophisticated LC-MS platforms. But if you have a method for the determination of 800 pesticides, the complexity quickly stacks up; even preparing your stock solution could take weeks (if every month you need to prepare a stock solution that takes three weeks, you're not going to be very efficient). EPRW is a great platform for discussing these problems, and it often allows you to benefit from other people's experiences. In short, being able to learn from each other and find new ways to improve is invaluable in the complex world of pesticide residues.

Thierry Delatour is Group Leader at the Nestlé Research Centre, Lausanne, Switzerland.

Variety: the Spice of Life

The field of pesticide residue determination is constantly growing and evolving – just like the environment in which we operate. Here, I describe how well-developed screening approaches – with high-resolution accurate mass instrumentation and comprehensive software – allow us to meet current and upcoming challenges in food safety and security.

By Susanne Ekroth

My path to pesticide residue research is a story of constant discovery. In school, I had an excellent chemistry teacher who showed me that it doesn't matter how much you learn about chemistry – you will never know it all. There will always be more things to discover. I kept discovering new layers and finding that I needed to learn more and more. And that's what made it the most interesting subject I had ever encountered – and that's what has kept me going.

Growing up with a father who was a chemist and following him to work was a strong influence on my career choice as well. Hearing him talk about the fascinating work he was doing was a great inspiration!

Analytical chemistry in particular caught my attention because I was – and still am – so intrigued by the instrumentation. All chemists need equipment. All chemists need to analyze samples. To me, analytical chemistry seemed like the gateway to all chemistry.

Pursuing pesticides

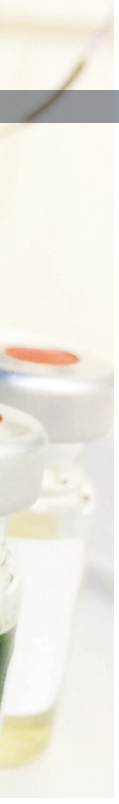
At the start of my career, I explored a range of job opportunities. I was in the pharmaceutical sector; I was a chemistry teacher; and, finally, I took a position at the Swedish National Food Agency – my first introduction to pesticide residue determination. I found immediately that the work never stayed static; it was constantly changing and evolving; the job that I got over 20 years ago is not the same one I had five years ago – and today it's different again.

The technologies and methods we use and develop also need to evolve to stay abreast of the ever-increasing scope of our field. There are many things to take into consideration: the nature of the analyte (polar or non-polar) the low concentration levels, the variety of matrices (fatty or non-fatty...). Even after you've accounted for all of these parameters, your method still has to accommodate about 500 different pesticides. It comes down to having a good analytical method and a good workflow to support it.

At the moment, the LC triple quad MS and GC triple quad MS systems are the workhorses of the pesticide laboratory. Most labs in Europe still use these technologies more than any other. But there's a trend toward implementing high-resolution accurate mass (HRAM) technology, because we're no longer satisfied with just finding the analytes we're expecting to see in our samples; now, we want to see everything (or at least as much as possible). In other words, there is a steady move away from targeted analysis.

The evolution of screening

Screening – as the name suggests – allows us to discover what is in our samples with less bias – at odds with simply looking for what we already suspect is present. Not only does it require advanced instrumentation, it also demands good software; for example, the Thermo Scientific™ Compound Discoverer™ small molecule identification software – a statistical tool that can handle large numbers of features within a single dataset. You can also connect to online databases to search for additional compounds – drugs, chemicals, additives, pesticides, contaminants, and so on. It does take time (about 10 hours per run of 5–10 samples) but, if you combine a generic extraction



method with this kind of multi-class analysis, the result obtained is a "complete" answer.

Perhaps unsurprisingly, screening is trickier than it sounds. Receiving "no hits" on a sample does not necessarily mean that there's nothing present; it may simply mean that your extraction method isn't suitable for all compounds – or that your screening method itself is fallible. If you don't know what you're expecting to see, you have to be sure that your methods work on all analytes of interest in a given sample. In short, that's the main obstacle to adopting a (successful) screening approach. You must know all potential pitfalls in advance.

When screening works, it provides impressive insight. Recently, our analyses of rice samples picked up an aflatoxin, for example. In fact, we found three different compound classes in the same sample: aflatoxin B1, a pesticide called buprofezin , and dibutyl sebacate, which is a plasticizer. Where did it come from? We can't be sure of its origins without further work, but we know it's there and that could be cause for concern. What else are we not looking for? We performed a similar analysis in fig samples and, once again, confirmed hits in a number of compound classes. Being able to distinguish so many species is unusual, but often useful.

Road to EPRW

The European Pesticide Residue Workshop (EPRW) was started by a dear colleague, Arne Andersson with a few other guiding lights in the field who organized the first event in the Netherlands in 1996 (see page 04 for Lutz Alder's origins story). When the EPRW conference was held in Stockholm in 2004, I was a member of the local organizing committee. Each workshop has been a great experience for all attendees but, in the early days, they were particularly valuable because they were the only times all of the European pesticide labs got together to exchange knowledge.

Nowadays, as a member of the Scientific Organizing Committee, my EPRW colleagues and I work hard to maintain the high level of scientific discourse – something most attendees tell me is special to our workshop. We hold a brainstorming meeting before each conference to decide which speakers to invite, what sessions to hold, and the latest "hot topics" in the field. Our core subjects recur each year, of course, but beyond that, we try to think outside the box – otherwise, we might risk boring our guests! In the end, our goal is to feature a wide variety of interesting talks and events that cover every area of pesticide research – allowing our community to exchange ideas and debate the future direction we might take.

The rise of high-resolution techniques in multiresidue methods

Within the pesticide community, we strive to develop methods and techniques to fit the high demands of multiresidue analysis. Therefore, I think we all appreciate that we can benefit from a very friendly but professional fellowship. For example, in my work, I have had valuable help from the groups of Hans Mol and André de Kok from Holland, Jim Garvey from Ireland (see page 14), and Amadeo Fernández-Alba from Spain. Another, perhaps slightly lesser-known researcher is Lukasz Rajski, a member of Amadeo's research group at the University of Alméria, Spain. He is a brilliant researcher specializing in Orbitrap™ technology – and not only that, he's extremely helpful and approachable.

And I must say that all of the major instrument manufacturers have amazing application chemists. We are fortunate that there is close collaboration between instrument and software manufacturers and experts in the field – this is true of many areas of analytical science. Manufacturers are always eager to hear our opinions – and they regularly update their software in accordance with our needs. "This is because a customer told us about a particular need of theirs, so it should make life easier for you as well," they may say. Anything that simplifies the process makes our lives better – and in that regard there is plenty more to collaborate on! Over the years, I've found that an eagerness to learn on both sides benefits the wider pesticide analysis community.

An evolving field

I'm intrigued by what the future may hold for pesticide research. For one thing, climate change looms ever larger; 15 years from now, it will be interesting to see the effect of that transition. If it gets warmer in traditionally cold regions, will we use more pesticides to manage our crops? What kinds of diseases will a warmer climate bring?

Our animal husbandry and consumption is changing, too. Insects are the hot new protein source – but what kinds of regulations will we have to put into place to "harvest" insects? What kinds of analysis will we be required? What unknown problems will we face when we begin working with insects on a large scale? Eventually, these are all questions that will need answers.

In the meantime, I think the future of analysis will involve more and more screening – which also means trying to make screening methods as reproducible, efficient, and effective as possible. It's not an easy task, and there are a number of potential pitfalls but, if you fully understand your sample, your extraction methods and your workflow, those pitfalls can be avoided – and that's when screening becomes a powerful ally for any analytical scientist.

Susanne Ekroth is an analytical chemist at the National Food Agency (Livsmedelsverket), Uppsala, Sweden.

For Susanne Ekroth's Top Five Picks from the screening literature, download the digital supplement: http://tas.txp.to/0518/EPRW2018

The quantitative power of high-resolution GC-Orbitrap mass spectrometry for the analysis of pesticides and PCBs in food

Dominic Roberts[1], Jim Garvey[2], Richard Law[1] and Paul Silcock[1]
[1]Thermo Fisher Scientific, Runcorn, United Kingdom
[2]Department of Agriculture, Food and the Marine, County Kildare, Ireland

Overview:
Confident determination of pesticide residues and polychlorinated biphenyls (PCBs) in food is challenging because of the large number of compounds and diversity of sample types involved. The sensitivity requirements for these compounds are also demanding. The coupling of a high-resolution Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS system is a valuable alternative to triple quadrupole techniques but with additional analytical advantages. With high-resolution accurate-mass (HRAM) mass spectrometry, the default acquisition mode is untargeted (full-scan) meaning that all the ions are acquired with high selectivity at the same time across a specified mass range, making the acquisition simple to manage and giving the analyst the flexibility to decide which pesticides to search for and to quantify. The objective of this study was to evaluate the quantitative performance of the Exactive GC Orbitrap system for the analysis of pesticides and PCBs in food matrices with varying complexity.

Method:
Grape and onion samples were obtained from the market and pesticides extracted. Automatic sample injection was performed using a Thermo Scientific™ TriPlus™ RSH™ autosampler, and chromatographic separation was performed using a Thermo Scientific™ TRACE™ 1310 GC system fitted with a Thermo Scientific™ TraceGOLD™ TG-5SilMS 30 m × 0.25 mm I.D. x 0.25 µm film capillary column with a 5 m integrated guard (P/N 26096-1425). Finally, a Thermo Scientific Exactive GC Orbitrap mass spectrometer was used for accurate mass measurements in full-scan mode.

Conclusion:
The results of this study demonstrate that the Exactive GC Orbitrap HRAM mass spectrometer, in combination with Thermo Scientific™ TraceFinder™ software, offers an excellent solution that simplifies the analysis of pesticides in food commodities and delivers sensitive quantitative performance for pesticide analysis in fruits and vegetables.

Ultra-low level quantification of pesticides in baby foods using an advanced triple quadrupole GC-MS/MS system

Richard Law, Aaron Lamb, Paul Silcock, and Cristian Cojocariu, Thermo Fisher Scientific, Runcorn, UK

Overview:
The high sensitivity and selectivity of GC-MS/MS enables the detection and identification of residues of prohibited compounds, in compliance with regulatory guidelines. An ultra-sensitive, selective, reliable, and robust GC MS/MS system is required to address the challenges of routine high-throughput determination of pesticide residues at trace concentrations. In this study, the quantitative performance of the Thermo Scientific TSQ™ 9000 triple quadrupole GC-MS/MS system, fitted with the Advanced Electron Ionization (AEI) source, was assessed for the analysis of >200 pesticides in baby food at ultra-low concentrations (as low as 0.025 µg/kg).

Method:
Samples of baby food were extracted using the citrate-buffered QuEChERS protocol using Thermo Scientific™ HyperSep™ dispersive solid phase extraction (dSPE) products. Liquid injections of the sample extracts were performed using a Thermo Scientific™ TriPlus™ RSH™ autosampler, and chromatographic separation was achieved by a Thermo Scientific™ TraceGOLD™ TG-5SilMS column (P/N 26096-1425). A TSQ 9000 triple quadrupole GC-MS/MS system equipped with an AEI source and coupled with a Thermo Scientific™ TRACE™ 1310 GC system was used and data acquired, processed, and reported using Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software.

Conclusion:
In this work it has been demonstrated that by using QuEChERS with HyperSep dSPE and a direct injection of acetonitrile extracts, the TSQ 9000 AEI system delivers outstanding quantitative performance for low-level pesticide residue analysis in baby food. The results of this study establish the TSQ 9000 triple quadrupole GC-MS/MS system, in combination with Chromeleon CDS software and HyperSep dSPE, as the ideal solution for the routine analysis of pesticides in baby food, providing unprecedented sensitivity, robustness, ease of use, cost effectiveness, and reliability.

GC-HRAM for the Win

Nuria Cortés-Francisco and colleagues at Laboratori de l'Agència de Salut Pública de Barcelona (LASPB) won a best poster award at EPRW 2016. Two years on, we catch up with Nuria to find out more about the lab's award-winning work – and how the method they developed has proven itself.

Tell us about your award-winning poster…

Currently, pesticide analysis is most commonly carried out using LC or GC coupled with triple quadrupole mass spectrometry (QqQ-MS). Though the sensitivity of QqQ-MS is excellent, it can be affected by matrix effects, so a second, confirmatory method is sometimes needed. Our goal was to develop a new method for the confirmation of pesticides in all kinds of food, taking advantage of the superior performance of high-resolution accurate mass (HRAM)-MS. With help from our talented student, Meritxell Castelló, we built a compound database of mass spectra for 150 pesticides, updated from the existing NIST database. Next, we checked all 150 standards in solvent to confirm these theoretical spectra. Finally, we carried out a third step, where we spiked nine different matrices with the 150 standards, to confirm that the previously selected ions were adequate and would not suffer from matrix interference. We were also trying to test the sensitivity of the instrument, testing the pesticides at different levels – not only the MRL of around 10ppb but also 1, 3 and 5 ppb.

Sounds like a significant endeavor…

Yes, especially as we completed the entire process in six months! It was a lot of work, but now we have all the data validated, so if we need to confirm the result of a suspicious sample, we can be confident of our findings. We don't run all samples through our Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system – only those that give inconclusive results from GC-QqQ-MS, and that means we need to fully trust our GC-HRAM method

We were very proud to get the award; to be recognized for our hard work at an international conference was incredible. And it was a total surprise – we are a contract lab, not a research institution or university, so we can sometimes feel like outsiders at academic conferences. A real highlight was when Hans Mol – one of the poster judges and a real guru of pesticide analysis – said he was impressed with our work.

Did the judges say why they chose your poster?

It was because nothing else had been done in such detail in the pesticides area. Hans Mol had been working in the same space, of course, but had not delved into all the different concentration levels in all kinds of matrices or applied different working modes. The judges commended the amount of work we had done in a short space of time, and the detail and depth we had gone into with such a new approach. Hans asked many questions about our experiences, particularly with tea, as that's something his group were starting some work on.

How did the five-minute award presentation go?

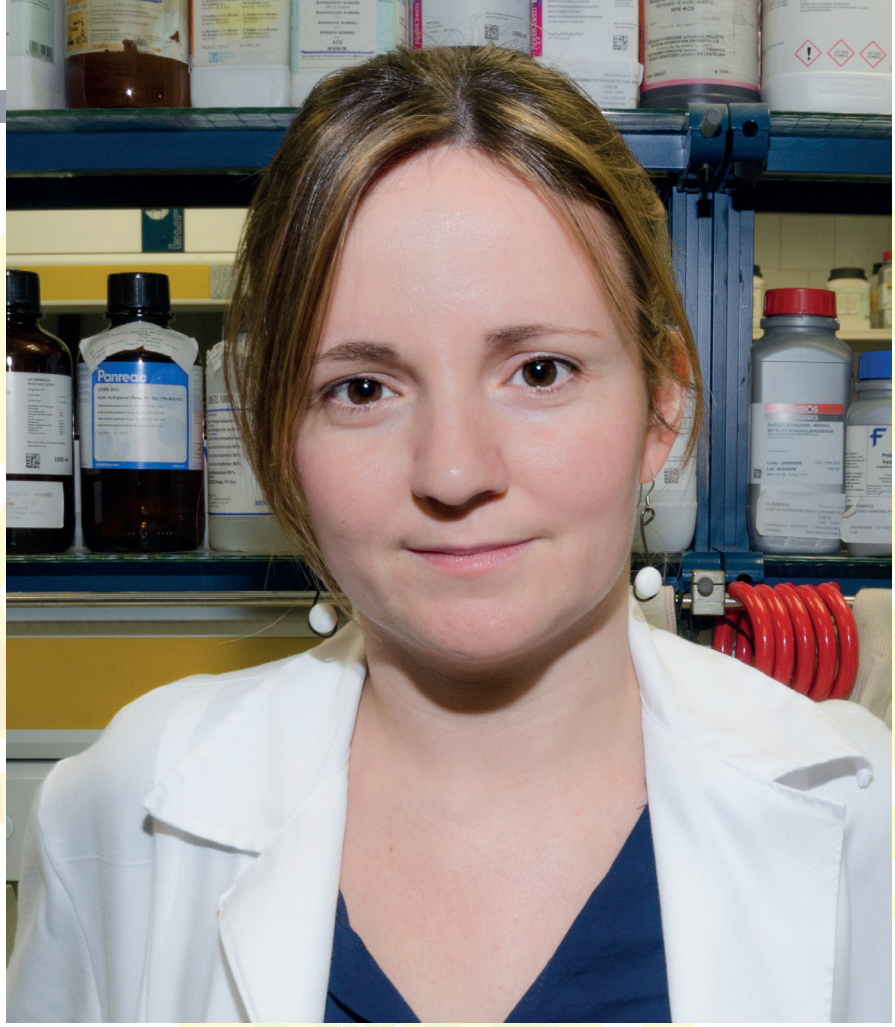
As well as summarizing the method, I discussed the example in tea, which provided a neat illustration of how the GC-Orbitrap itself works. It's a excellent technology, but you really need to know how it works to make the most of it. Of course, if full scan works for you, go ahead – but in some situations, you need to understand what's going on in the C-trap, and in the ion source, and you may need to develop some MS/MS experiments.

Two years on – EPRW 2018 in Munich – how has your work progressed?

The work we put in last year is really paying off. It's so fast to set up the method, because you have all the info in the lab; in five minutes, you have your method. And with a single run taking 35 minutes, you can get your results in half a day. The method really proved itself during the recent fipronil egg crisis in Europe – our lab was receiving eggs from all over the world. We were already looking for fipronil, but in this case the concern included a metabolite that was new to us – one that isn't heavily regulated. Regulators didn't know how significant the metabolite was until the alert, so we didn't even have standards for it. We bought the standards and ran the samples through the triple quad, and in parallel through the Orbitrap. We found that many samples tested positive using QqQ-MS, but we wanted to confirm this finding, as we knew so little about the metabolite. Using the Orbitrap method gave us the confidence to confirm positive results – this compound does not fragment completely in the ion source, which gives you the molecular information, the accurate mass of the compound and also the fragments. At the beginning, we were testing the eggs, but regulators soon realized that the compound was probably accumulating in chickens too. Sure enough, we found the compound in chicken fat and so we started investigating soya, a component of chicken feed. Every day, we had a new matrix to deal with, looking for a compound that we had little experience with – but we still needed to provide a result as soon as possible. Every sample that tested positive in QqQ-MS was confirmed with GC-Orbitrap to give us the confidence that we had a true positive.

Is your database publicly available?
We are happy to share the database, and we encourage others working in this field to contact us. Others will build their own database – its's not difficult, but it's time-consuming. I know other groups in Spain are analyzing pesticides with GC-Orbitrap.

What do you think will be the main talking points at EPRW 2018?
For us, the hottest topic is single residue methods. Another approach that we want to explore in future is screening, to reduce the number of samples that you need to quantify: for example, if eight out of 10 samples are completely negative, we can focus on the two positive – that saves time and money when you have many compounds to quantify! And that's a more realistic endeavor now that we have HRAM MS.



A photo of Nuria Cortes taken by Meritxell Cortes (her sister), as part of a photo essay on "women in science."

What drives your lab to be an early adopter of new technology?
It's really driven by our need to respond to food alerts – we have to be up to date and able to adapt quickly, as the fipronil crisis showed. Our lab director, Francesc Centrich, loves chemistry and always keeps an eye on new technology and upcoming challenges. He's been in the lab for 40 years (he's retiring next month) – he knows we have to be responsive, and that if you want to be responsive you have to have the latest technology. He has fought for funding and to get the right people in place – not always easy as we're publically owned.

Being at the forefront can be difficult; you have to be very sure of your ideas and be prepared to defend them – but we're scientists, so we're prepared for that! The EPRW award gave us validation that we were doing a good job – it showed us that people were interested in the work, and that's the most you can ask for. When you're working more hours than you can count, it's easy to lose sight of what you're achieving... but something as simple as an award helps you remember that your work is valued.

What keeps you motivated?
I consider my job and the work we do here to be highly valuable – and when that's the case, you're not looking at your watch all the time. The management here are also very supportive, allowing us to go to conferences or present reports. The work we are doing can even have relevance outside of food safety. Recently, we got a call from a toxicology institution in Madrid, which does forensics. They contacted us because they knew we had Orbitrap technology, and they wanted me to give a short course on how to apply it properly. It was late in the afternoon, and they should have been heading home, but they were all there until the last possible minute, because they wanted to know more – that was very rewarding! It doesn't matter if the sample is blood or hair or apple – you can still learn a great deal from each other's experiences.

Where are the unmet needs in instrumentation?
One issue for pesticide analysis in particular is how we can combine different GC columns. For example, the Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS system produces "dual data" – they have two GCs connected to the same magnetic sector. If we could access that kind of GC power with Orbitrap technology, it would be extremely useful. In LC, automated column switching is possible – but it takes time and expertise to change GC columns. An automated column switcher for GC would allow us to run multiple analyses overnight and so design workflows to be more productive. Whatever industry you are in, higher throughput and more efficient workflows are always on the agenda!

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