62nd

Annual North American Chemical Residue Workshop

July 12-15, 2026

San Antonio, Texas



Keeping with Tradition

On the cover: Black-capped Vireo

The Black-capped Vireo is a small, striking songbird that thrives in the oak juniper scrublands of the Texas Hill Country, including areas around San Antonio. This species favors rocky hillsides with dense, brushy vegetation, especially scrub oak and low shrubs, where it can forage for insects and nest in concealed thickets. It typically arrives in Texas in late March to mid April and remains through the breeding season before migrating south to the Pacific coast of Mexico. The Hill Country provides some of the best remaining habitat for this once endangered bird.

About the photographer: Jack Cochran

Jack Cochran lives in Georgetown, Texas. He is a Texas Master Naturalist in the Good Water Chapter and was recently awarded a Lifetime Achievement Award by President Joe Biden for his 4000 hours of volunteer service on behalf of the Texas Parks and Wildlife Department. Previously he worked as an analytical chemist and served as a Board Member for the North American Chemical Residue Workshop.

Wildlife Photography Inspiration – by Jack Cochran (former NACRW volunteer & FLAG Works, Inc., Board Member)

I have two inspirations for my entry into wildlife photography. The first was my visit to South Africa for Analitika in 2006. The conference itself was "in the bush" at Pilanesberg National Park and the first day at breakfast an elephant came to a waterhole just a few yards away from my table. I had a camera, snapped some photos, and was hooked.
My second inspiration is closely connected to the North American Chemical Residue Workshop (formerly the Florida Pesticide Residue Workshop) through the wildlife photography of its founder, George Fong. For many years, NACRW speakers and volunteers have received one of George's photographs as a thank you gift for their participation. I'm grateful to help carry on that tradition by providing photographs for NACRW to use. Many thanks to the speakers and volunteers who make NACRW so special!

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Welcome to the 62nd Annual NACRW

Dear NACRW Attendees,

We warmly welcome you to the 2026 North American Chemical Residue Workshop. We are delighted to have you with us and look forward to a program filled with engaging, informative, and thought-provoking sessions. This conference has become a favorite event for many members of the organizing committee, and we hope it will be the same for you—whether this is your first time attending or you are a returning participant.

Our agenda features sessions on challenging food matrices, PFAS, method development and validation, innovative analytical approaches, natural toxins, non-targeted analysis, reference materials, and much more. We also encourage you to participate in the lunch seminars hosted by our vendors and to explore the many posters that will be presented throughout the workshop.

As each day concludes, we hope you have the opportunity to enjoy the beautiful River Walk nearby and experience all that San Antonio has to offer. We hope you find the conference valuable and enjoyable, and that you will share your experience with colleagues who may wish to attend in future years.

We look forward to meeting you and sharing this outstanding program together.

Sincerely,

Julie Brunkhorst
2026 NACRW President

Holly Lee & Kelsey Powers
2026 NACRW Program Committee Co-Chairs

The Future of NACRW: A Letter to Our NACRW Community

Dear Friends and Colleagues,

On behalf of the Board of Directors, welcome to the 62nd North American Chemical Residue Workshop. Whether this is your first NACRW or your thirtieth, thank you for being here. Your presence is what makes this workshop what it is.

I want to speak to you plainly, because that is the spirit in which this community has always operated. The past several years have not been easy ones for NACRW. For a range of reasons, we found ourselves stretched, and the path forward was not always clear. What I can tell you is this: we have come through that period, and we have returned to the model that built this workshop in the first place, a fully volunteer-led community of scientists giving their time because they believe in what we do here.

That return is not a retreat. It is a homecoming.

Yes, we are smaller than we once were. But smaller has never meant lesser. It means the hallway conversations run a little longer, the introductions are a little warmer, and the sense that you belong here arrives a little faster. The two things that have always made NACRW dear to us remain fully intact: a technical program of genuine excellence, and a culture that is open, welcoming, and generous to newcomers and veterans alike. Those are not things we are trying to rebuild. They are things we get to protect.

Going forward, you will see a Board that is more present and more engaged. We are committed to building new structure while reviving what has always worked, and to renewing our tradition of mentorship, because NACRW has always been a place where the next generation of scientists finds its footing, and we intend to keep it that way.

Most importantly, I want you to hear this clearly: this is your workshop. Not the Board's, not any single institution's, but yours. The new Board is open to every idea about what this community wants to become. We are listening, and we mean it. If you have a thought, a concern, or a vision for where NACRW should go, we want to hear it.

And you can start right here at this meeting. **Please join us on Tuesday from 5:15 to 6:00 pm for the NACRW Organizing Committee Meeting, which is open to all attendees. Come share your ideas, ask your questions, and help us shape what comes next. There is no better place to begin.**

To everyone who stood by us through this challenging transition, whether you submitted an abstract, sponsored a session, sponsored the workshop, judged a poster, or simply showed up, thank you. You did not have to, and you did anyway. That loyalty is the foundation we are building on.

We cannot do what comes next without you. And we would not want to.

With deep gratitude and real optimism,

Alex Bush
Board Chair
On behalf of the NACRW Board of Directors

Board of Directors & Committees

FLAG Works, Inc. Board of Directors

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Co-Chairs: Holly Lee, SCIEX | Kelsey Powers, Montana Department of Agriculture

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DRE-A50000805AL	LC PestiMix 5 10 µg/mL in Acetonitrile	74
DRE-A50000806AL	LC PestiMix 6 10 µg/mL in Acetonitrile	75
DRE-A50000807AL	LC PestiMix 7 10 µg/mL in Acetonitrile	63
DRE-A50000808AA	LC PestiMix 8 10 µg/mL in Acetonitrile:Acetone	27
DRE-A50000809AL	LC PestiMix 9 10 µg/mL in Acetonitrile	72
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Exhibitors

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Visit Our Exhibitors

Please take time during the conference to visit our exhibitors and sponsors. Their support helps make NACRW possible, and their products, services, and expertise are valuable resources for our community. Stop by the exhibit area, make connections, ask questions, and thank them for supporting NACRW.

- Discover new instruments, technologies, and services relevant to residue analysis.
- Connect directly with technical experts and company representatives.
- Learn about practical solutions for laboratory workflows, method development, and troubleshooting.
- Explore vendor seminars, product resources, and opportunities for follow-up conversations.
- Support the sponsors and exhibitors whose participation helps make NACRW possible.

Get to Know Your Sponsor Quiz

Participate in the "Get to Know Your Sponsor" quiz for a chance to win a prize, iPad. A quiz sheet will be provided in your registration bag. Visit each sponsor booth, get the correct answer, and have the sponsor stamp your quiz. Return completed quizzes to the registration desk no later than Wednesday at 1:30 pm. Winner announced Wednesday afternoon.

Sister Workshops

NACRW is proud to be affiliated with these regional residue workshops





General Information

Wi-Fi

Network: Hyatt Meeting
Password: GHSA2026q2

Registration Desk Hours

Date	Room	Hours
Sunday, July 12, 2026	Prefunction, 4th Floor	1:00 – 6:00 pm
Monday, July 13, 2026	Prefunction, 4th Floor	7:30 am – 5:00 pm
Tuesday, July 14, 2026	Bonham A, 3rd Floor	8:00 am – 4:00 pm
Wednesday, July 15, 2026	Bonham A, 3rd Floor	7:45 am – 12:00 noon

Presentation Numbering Key

Oral Presentations are numbered O-1, O-2, O-3, etc.
Vendor Seminars are numbered V-1, V-2, V-3, etc.
Session A Posters are ODD numbered: P-1, P-3, P-5, etc.
Session B Posters are EVEN numbered: P-2, P-4, P-6, etc.

Poster Sessions

Location: Texas C
Hang posters: Sunday afternoon 3:00–6:00 pm OR Monday morning 7:00–9:30 am
Take down posters: Wednesday after lunch
Posters may be viewed any time the Exhibition Hall is open.

Poster judging will take place during poster sessions listed below:
Poster presenters, please be present at your poster during the following days/times:

Poster Session A (odd # posters):

Monday 10:15–10:35 am and 4:50–6:00 pm

Tuesday 3:00–3:20 pm

Wednesday 9:55–10:15 am

Poster Session B (even # posters):

Monday 3:00–3:20 pm and 4:50–6:00 pm

Tuesday 10:00–10:20 am

Wednesday 9:55–10:15 am

Poster Prizes

Two poster prizes of $250 each will be awarded. The People's Choice Poster Award is determined by popular vote of attendees; the Judges' Choice Poster Award by the poster committee. Criteria: importance of study, quality of science, and presentation. Votes must be placed in the ballot box by Wednesday noon.

Exhibition Hall — Texas C

Sunday: Welcome Reception with food and open bar, 6:00–9:00 pm (see you all there!!)

Monday: 7:45 am – 6:00 pm

Tuesday: 7:45 am – 6:00 pm

Wednesday: 7:45 am – 1:30 pm

Door Prizes

Door prizes will be drawn at the end of each morning and afternoon oral session. You must be **ON TIME** at the beginning of each session to receive a ticket. You must be present at each drawing to win.

Feel free to contribute to a door prize! Drop-off your prize(s) at the designated area at Registration.

Get to Know Your Sponsor Quiz

Participate in the "Get to Know Your Sponsor" quiz for a chance to win a prize. A quiz sheet will be provided in your registration bag. Visit each sponsor booth, get the correct answer, and have the sponsor stamp your quiz. Return completed quizzes to the registration desk no later than Wednesday at 1:30 pm. Winner announced Wednesday afternoon.

Copies of Presentations

Oral Presentations: Following the meeting, oral presentations may be posted on our website if author permission is granted. Files are converted to PDF format. No files will be posted without written speaker permission.

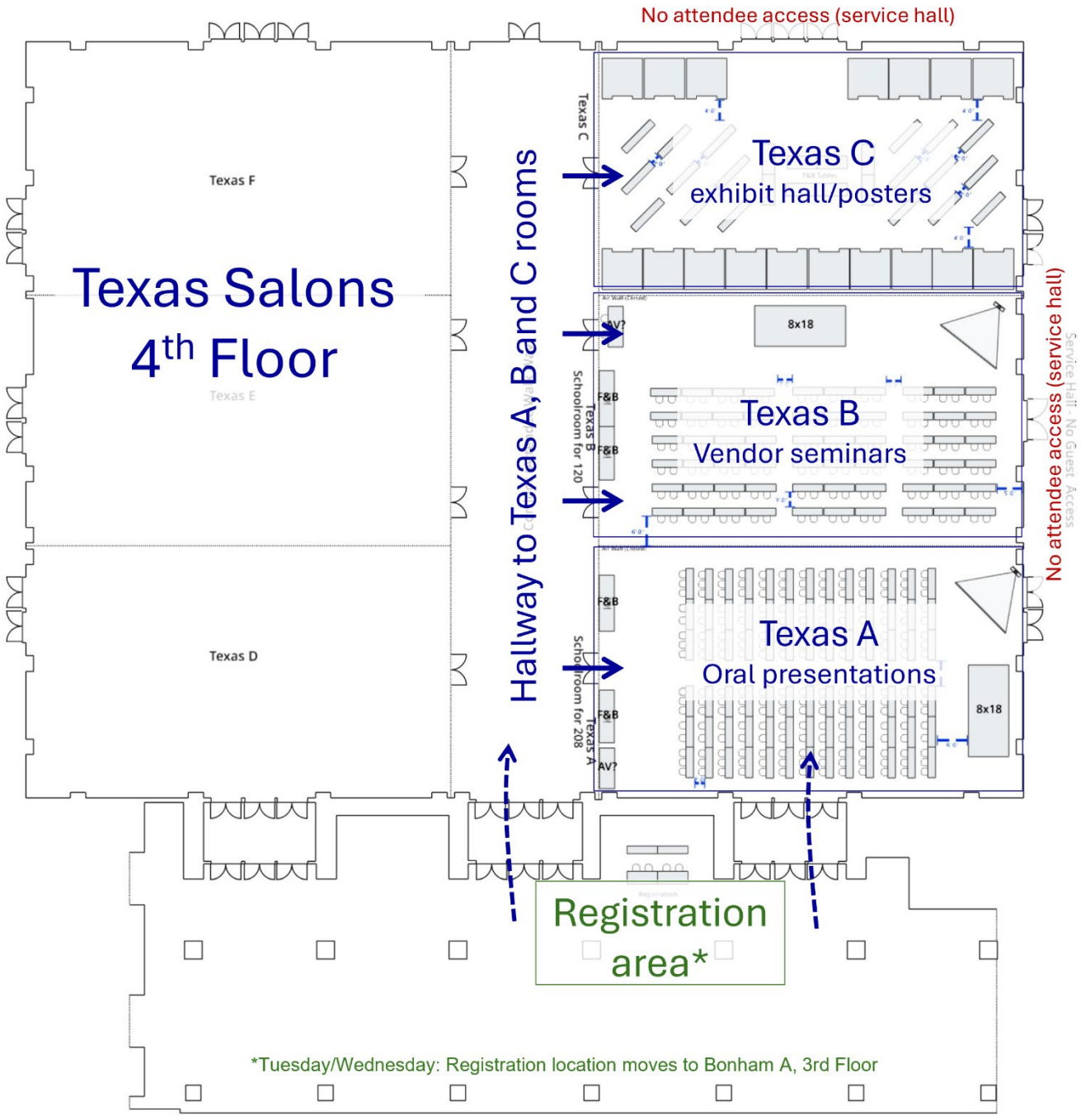
Poster Presentations: Drop your business card in the reprint request envelope at each poster board.

Meeting Website

www.NACRW.org — current and future meetings, archives, and posted presentations.

A BIG THANK YOU TO ALL OF OUR VOLUNTEERS, SPONSORS & EXHIBITORS!

Grand Hyatt San Antonio River Walk — Hotel Map & Rooms

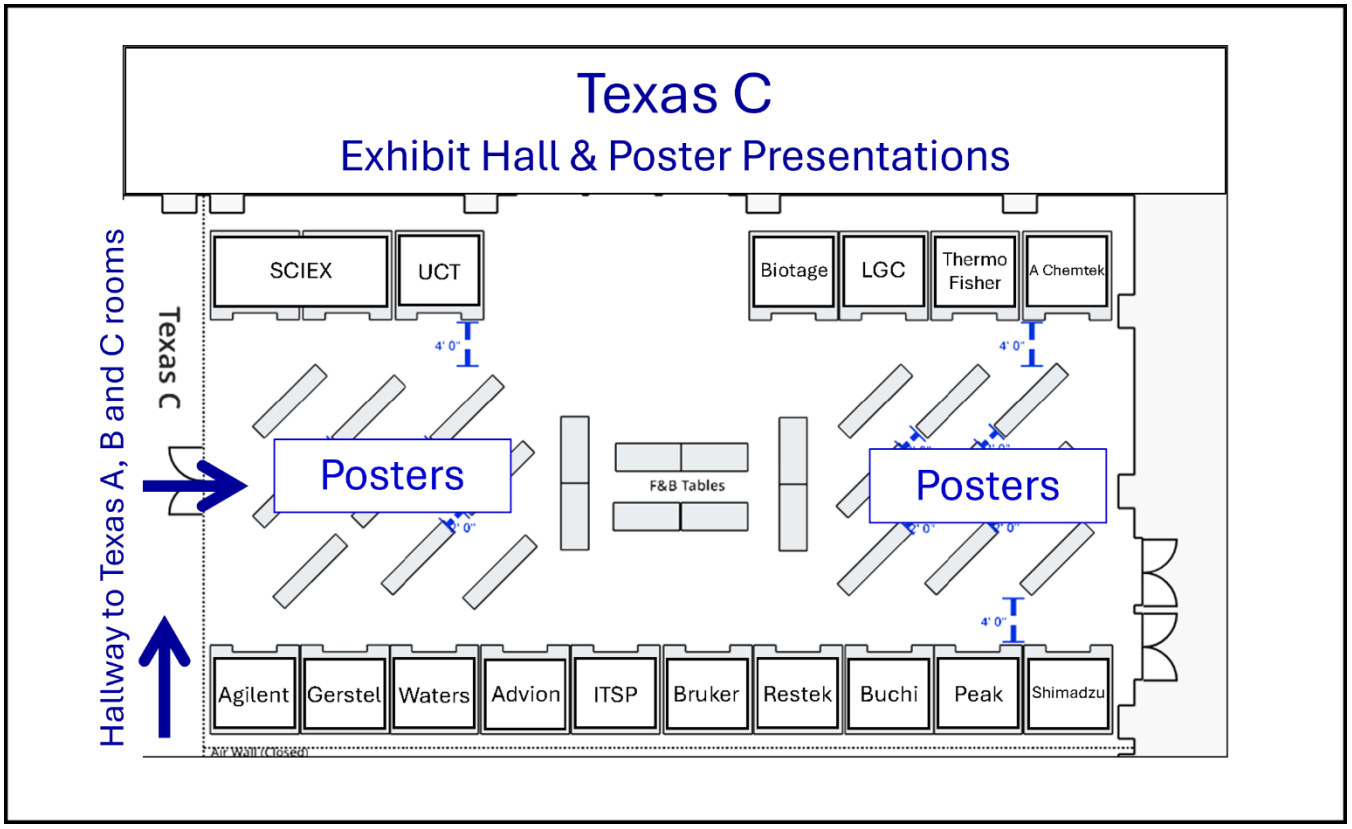


Key Room Assignments

Time	Room	Event / Session
All sessions	Texas A	Main oral session room
Vendor Seminars	Texas B	All vendor seminars (pre-registration required)
Exhibition / Posters / Coffee	Texas C	Exhibition hall, poster boards, coffee breaks
Registration (Sun/Mon)	Prefunction, 4th Floor	Registration desk
Registration (Tue)	Bonham A, 3rd Floor	Registration desk

Location address: Grand Hyatt San Antonio River Walk, 600 E. Market St, San Antonio, TX 78205

Exhibition Hall Floor Plan & Exhibitor Listing



2026 Exhibitors (listed in alphabetical order)

1. A Chemtek
2. Advion
3. **Agilent (Platinum Sponsor)**
4. Biotage
5. Bruker
6. Buchi
7. Gerstel
8. ITSP
9. **LGC (Gold Sponsor)**
10. Peak
11. Restek
12. **SCIEX (Platinum Sponsor)**
13. Shimadzu
14. Thermo Fisher
15. **UCT (Gold Sponsor)**
16. **Waters (Gold Sponsor)**

Vendor Seminars

Food and beverage provided. **PRE-REGISTRATION IS REQUIRED. Please sign up at the registration desk.** Full abstracts and speaker biographies are included in the Abstracts section of this program.

V-1 Monday, July 13, 2026 | 7:15–8:15 am

Waters

Room: Texas B

Improving laboratory efficiency through Simultaneous Quant and Qual Analysis using a Benchtop Multi-reflecting Time-of-flight Mass Spectrometer

Shashank Jain, MS, PhD, Waters Corporation

High-resolution mass spectrometry is increasingly central to regulatory science, enabling confident compound identification, sensitive quantitation, and streamlined workflows across diverse application areas. This presentation highlights the Waters Xevo MRT platform and demonstrates how a single HRMS system can support both qualitative and quantitative analyses across environmental, pharmaceutical, and food safety markets. Practical workflow examples will span PFAS analysis, pharmaceutical impurity profiling, and food contaminant screening, illustrating how HRMS can simplify method development while increasing analytical confidence and laboratory efficiency.

V-2 Monday, July 13, 2026 | 12:15–1:15 pm

SCIEX

Room: Texas B

Is your matcha latte really matcha? Exploring matcha quality and origin using high-resolution mass spectrometry

Kendra Adams, SCIEX

This talk highlights high-resolution LC–MS/MS for evaluating matcha quality, authenticity, and origin in a single workflow. Using a ZenoTOF 7600+ with ZT Scan DIA, comprehensive MS and MS/MS data are generated to enable broad profiling and confident compound identification across commercial matcha samples spanning culinary and ceremonial grades from China and Japan. PCA differentiates samples by grade and origin, while markers such as L-theanine, catechins, and flavonoid glycosides provide chemical context. The workflow demonstrates how HRMS supports efficient, data-rich food analysis through non-targeted discovery for authenticity and quality assessment.

V-3 Tuesday, July 14, 2026 | 7:15–8:15 am

LGC Standards

Room: Texas B

Recent Advances in Reference Materials: Chemicals of Concern

Dan Biggerstaff, LGC Standards

LGC Standards presents *Recent Advances in Reference Materials: Chemicals of Concern* with Dan Biggerstaff, End Market Technical Sales Manager for LGC Standards in the Americas. A look at how the newest developments in certified reference materials support accurate quantitation and defensible QC for the analytes drawing the most regulatory attention today.

V-4 Tuesday, July 14, 2026 | 12:15–1:15 pm

Agilent

Room: Texas B

Strategic Approaches to Complex Sample Analysis in Regulatory Pesticide Samples

Deidre E. Damon, PhD

This presentation reviews the Ohio Department of Agriculture's extraction and detection of over 300 pesticides and how this testing ties into federal government programs. Resulting methods used by the Ohio Department of Agriculture Pesticide Residue laboratory show a lower quantitation limit at or below 10 parts per billion in complex matrices using a QuEChERS extraction paired with GC/MS/MS and LC/MS/MS. This work will summarize difficult cases and testing strategies used to analyze a variety of sample types.

Routine Multiresidue Analysis with Hydrogen Carrier Gas: Sensitivity Improvements by Dual-Layer Injection

Prof. Amadeo Rodríguez Fernández-Alba

The transition from helium to hydrogen carrier gas has become increasingly attractive for routine GC-MS/MS laboratories due to supply, cost, and sustainability considerations. However, sensitivity losses remain one of the main limitations for multiresidue pesticide analysis under hydrogen conditions. This presentation demonstrates how Dual-Layer solvent vent injection can enhance analyte transfer and improve instrumental sensitivity, enabling reliable pesticide residue determination at trace levels. Validation data, real-sample analysis, and EUPT performance results support the suitability of this approach for routine regulatory monitoring.

V-5 Wednesday, July 15, 2026 | 7:15–8:15 am

UCT

Room: Texas B

Doing the Work Before the Work: A Low-Burden Approach to Sample Preparation Screening for Cannabis Pesticide Analysis

Rhiley Schmidt, Method Testing Laboratories; Anthony Repay, Method Testing Laboratories; Julie Kowalski, jkSS, LLC

Cannabis flower is an analytically demanding matrix for pesticide residue analysis, and laboratories face challenges achieving consistent routine performance under production conditions. This presentation introduces a fast, low-burden screening framework for evaluating cleanup performance before committing to resource-intensive recovery and matrix effects studies. The framework uses pigment removal, nonvolatile coextractives removal, volatile coextractives removal, and cannabinoid-specific removal to rank candidate cleanup methods. Applied to cannabis flower, the workflow identified promising cleanup options that outperform the current method while maintaining analytical performance, providing a transferable low-resource approach for sample preparation selection.

Oral & Poster Presenters Index

Alphabetical order by last name. Full abstracts available in the digital program.

Pres. #	Presenter Name	Affiliation
O-S1-1	Jeffrey Sayen	Agilent Technologies
O-S1-2	Holly Lee	SCIEX
O-S1-3	Tiffany Liden	Shimadzu Scientific Instruments
O-S1-4	Lukas Vaclavik	Eurofins Food Chemistry Testing
O-S1-5	Zeyu Han	Mérieux NutriSciences, Silliker Canada Co. Ltd.
O-S1-6	Wiley Hall	USDA-ARS-SJVASC
O-S1-7	Lihini Tharanga Mendis	Shimadzu Scientific Instruments
O-S2-1	Taryn McKnight	Eurofins Environmental Testing
O-S2-2	Margot Lee	Waters Corporation
O-S2-3	Tiffany Liden	Shimadzu Scientific Instruments
O-S2-4	Alicia Stell	CEM Corporation
O-S2-5	Ed George	Thermo Fisher Scientific
O-S2-6	Seyyedhadi Khatami	Bruker
O-S2-7	Michael Buhrman	Eurofins Food Chemistry Testing
O-S2-8	Ashley Griffin & Xun (Ann) Fu	Nestle Quality Assurance Center
O-S3-1	Christian Talavera	FDA
O-S3-2	Julie Kowalski	Intrepid Scientific
O-S3-3	Tiffany Liden	Shimadzu Scientific Instruments
O-S3-4	Evan Walters	Biotage
O-S3-5	Katherine Weddell	Fera Science Limited
O-S3-6	Sue D'Antonio	Agilent Technologies
O-S3-7	Alexis Shelow	Restek
O-S3-8	Jacob Jalali	PerkinElmer
O-S4-1	Andrew Folkerson	SCIEX
O-S4-2	Amadeo R. Fernández-Alba	University of Almeria
O-S4-3	Justin Smolen	Texas A&M University
O-S4-4	Limian Zhao	Agilent Technologies Inc.
O-S5-1	Lukas Vaclavik	Eurofins Food Chemistry Testing
O-S5-2	Julie Brunkhorst	Trilogy Analytical Laboratory
O-S5-3	Makda Araya	Waters Corporation
O-S5-4	Adam DeWilde	Eurofins Food Chemistry Testing
O-S5-5	Stuart Oehrle	Northern Kentucky University / Waters Lab
O-S6-1	Florencia Jesús	University of Almeria
O-S6-2	Jayesh Gandhi	Metrohm USA
O-S6-3	Yufang Zheng	NIST
O-S6-4	Michael S. Young	Cambridge Polymer Group

O-S7-1	Daryl Staveness	ExciPlex, Inc.
O-S7-2	HuiChen Stavros	O2si Smart Solutions / LGC Standards
O-S7-3	Ryan Malone	Trilogy Analytical Laboratory
O-S8-1	Marti Z. Hua	Carleton University / NRC Canada
O-S8-2	Bikram Subedi	Louisiana State University
O-S8-3	Adam R. Wronski	Baylor University
O-S8-4	HyeongYoung Choi	Baylor University
P-1	Oscar Cabrices	G-Flo Scientific / Tyson Foods
P-2	Ming Gao	Meriuex/Silliker
P-3	Oscar G. Cabrices	G-Flo Scientific / Tyson Foods
P-4	María Dolores Hernando	Experimental Station of Arid Zones, Spanish National Research Council (CSIC-EEZA)
P-5	Kendra Adams	SCIEX
P-6	Marti Z. Hua	Carleton University / National Research Council Canada
P-7	Daniel Biggerstaff, PhD	O2si Smart Solutions and LGC Standards Company
P-8	Jacob Jalali	PerkinElmer
P-9	Alexandria Bush	Restek
P-10	Holly Lee	SCIEX
P-11	Manisha Dhanshetty	Technological University Dublin
P-12	Holly Lee	SCIEX
P-13	Ally Fairman	NOW Foods
P-14	Tiffany Liden	Shimadzu Scientific Instruments
P-15	Artem Filipenko	Bruker Scientific
P-16	Cory Lytle	Bruker Scientific
P-17	Jayesh Gandhi	Metrohm USA
P-18	Caroline Mackay	Food and Drug Administration
P-19	Chiquita Price	Mississippi State Chemical Laboratory
P-20	Ingrid Marques	USDA-ARS
P-21	Rhiley Schmidt	Method Testing Laboratories
P-22	Lihini Tharanga Mendis	Shimadzu Scientific Instruments
P-23	Raghvendra Sengar	Bruker Scientific
P-24	Naren Meruva	Waters Corporation
P-25	Dimple Shah	Waters Corporation
P-26	Sara Moayedi	Ohio Department of Agriculture
P-27	Alexis Shelow	Restek
P-28	Zeljka Popovic	Waters Corporation
P-29	Katherine Weddell	Fera Science Limited
P-30	Bryn O. Shurmer	Canadian Food Inspection Agency

Meeting Program

Sunday, July 12, 2026

Time	Room	Event / Session
1:00–6:00 pm	Prefunction, 4th Floor	Registration Open
1:00–5:00 pm	Texas C	Exhibitor Set-Up
3:00–6:00 pm	Texas C	Poster Board Set-Up
5:30–6:00 pm	Texas C	Volunteer Meeting
6:00–9:00 pm	Texas C	Welcome Reception (food and open bar)

Monday, July 13, 2026

Time	Room	Event / Session	Speaker(s)
7:00–9:30 am	Texas C	Poster Board Set-Up (continued)	
7:15–8:15 am	Texas B	V-1 Waters Vendor Seminar (pre-registration required)	
7:30–5:00 pm	Prefunction, 4th Floor	Registration Open	
7:45–8:15 am	Texas C	Early Morning Coffee	
8:20–8:30 am	**Texas A**	**Opening Remarks**	*Alexandria Bush, Chair, FLAG Works, Inc. Board of Directors*
8:35–8:40 am			*Julie Brunkhorst, 2026 NACRW President*
8:40–8:45 am			*Holly Lee & Kelsey Powers, 2026 NACRW Program Co-Chairs*
8:45–10:10 am	**Texas A**	**SESSION 1 – Part 1: Analysis of Chemical Residues in Challenging Food Matrices** **Chairs: Edmund Azah, Ken Kise**	
8:45–8:50 am	Texas A	Agilent 5-min Introduction	
8:50–9:10 am	Texas A	Determination of the Geographical Origin of Spices Using ICP-OES, ICP-MS, and PCA Analysis	*Jeffrey Sayen, Agilent Technologies*
9:10–9:30 am	Texas A	Quantitation of polar pesticides in foods of plant origin	*Holly Lee, SCIEX*
9:30–9:50 am	Texas A	Analysis of Volatile PFAS in Complex Juice Matrices Using a Simplified HS-SPME GC/MS/MS Approach	*Tiffany Liden, Shimadzu Scientific Instruments*
9:50–10:10 am	Texas A	Determination of Mineral Oil Hydrocarbons in Foods: Setup and Validation of an Online-Coupled HPLC–GC–FID Method with Automated Sample Preparation	*Lukas Vaclavik, Eurofins Food Chemistry Testing*
10:15–10:35 am	Texas C	Coffee Break, Exhibition & Posters (authors present: odd # posters)	

10:40–11:40 am	**Texas A**	**SESSION 1 – Part 2: Analysis of Chemical Residues in Challenging Food Matrices** **Chairs: Edmund Azah, Ken Kise**	
10:40 - 11:00 am	Texas A	Analysis of Multi-Class Drug Residues and Glucosamine in Animal Feed	*Zeyu Han, Mérieux NutriSciences, Silliker Canada Co. Ltd.*
11:00 - 11:20 am	Texas A	The Identification and Quantification of Persistent Pesticide Residues Resulting from the Treatment of Museum Display Items	*Wiley Hall, USDA-ARS-SJVASC*
11:20 - 11:40 am	Texas A	Quantitative and Qualitative Analysis of Pyrethroid Residues in Soy Based Choline Supplements Using LC MS/MS with ESI	*Lihini Tharanga Mendis, Shimadzu Scientific Instruments*
11:45–1:30 pm	Texas C	Lunch & Exhibition	(poster authors are NOT required to man poster during lunch break but poster available for viewing)
12:15–1:15 pm	Texas B	V-2 SCIEX Vendor Seminar (pre-registration required)	
1:30–2:55 pm	**Texas A**	**SESSION 2 – Part 1: Analytical and Regulatory Perspectives on PFAS in Food and Food Contact Materials** **Chairs: Lorna De Leoz, John Schmitz**	
1:30–1:35 pm	Texas A	SCIEX Introduction	
1:35–1:55 pm	Texas A	Aligning Analytical Method Options for PFAS with Evolving Regulatory and Compliance Requirements	*Taryn McKnight, Eurofins Environmental Testing*
1:55–2:15 pm	Texas A	Flame-Broiled and Fluorinated: PFAS Analysis in BBQ Foods Using a Reduced QuEChERS Approach	*Margot Lee, Waters Corporation*
2:15–2:35 pm	Texas A	Single-System LC–MS/MS Analysis of PFAS and Cyanotoxins: Evaluation of Method Performance and the Effects of Mobile Phase Additives	*Tiffany Liden, Shimadzu Scientific Instruments*
2:35–2:55 pm	Texas A	Pressurized Extraction and Cleanup in One Automated Process for PFAS Analysis of Food	*Alicia Stell, CEM Corporation*
3:00–3:20 pm	Texas C	Coffee Break, Exhibition & Posters (authors present: even # posters)	
3:25–4:45 pm	**Texas A**	**SESSION 2 – Part 2: Analytical and Regulatory Perspectives on PFAS in Food and Food Contact Materials** **Chairs: Lorna De Leoz, John Schmitz**	
3:25–3:45 pm	Texas A	Automated Extraction Paired with a Dual-LC Orbitrap Workflow for Targeted PFAS Analysis in Food	*Ed George, Thermo Fisher Scientific*
3:45–4:05 pm	Texas A	A Rapid Screening Method for PFAS Analysis (EPA 1633a) Using DART/MS	*Seyyedhadi Khatami, Bruker*
4:05–4:25 pm	Texas A	Setup and Validation of a Sensitive, Robust and High-Throughput LC-MS/MS Method for Determination of Thirty Priority PFAS in Foods, Infant Formula and Dietary Supplements	*Michael Buhrman, Eurofins Food Chemistry Testing*
4:25–4:45 pm	Texas A	Evaluating the Efficacy of PFAS Preventive Controls: A Statistical	*Ashley Griffin & Xun (Ann) Fu, Nestle Quality Assurance Center*

		Comparison of Nestle and FDA Market Basket Data	
4:45–4:50 pm	Texas A	Closing Remarks	*Kelsey Powers, Holly Lee*
4:50–6:00 pm	Texas C	Exhibition & Poster Session B (authors present: ALL POSTERS -odd # & even #)	

Tuesday, July 14, 2026

Time	Room	Event / Session	Speaker(s)
7:15–8:15 am	Texas B	V-3 LGC Standards Vendor Seminar (pre-registration required)	
7:45–8:15 am	Texas C	Early Morning Coffee	
8:00–4:00 pm	Bonham A, 3rd Floor	Registration Open	
8:30–9:55 am	**Texas A**	**SESSION 3 – Part 1: Basic 101 in Method Development, Validation and Troubleshooting Laboratory Challenges** **Chairs: Scott Krepich, Bikram Subedi**	
8:30–8:35 am	Texas A	UCT 5-min Introduction	
8:35–8:55 am	Texas A	Single Laboratory Validation of an LC-MS/MS Method for the Determination of Quaternary Ammonium Pesticides in Food	*Christian Talavera, FDA*
8:55–9:15 am	Texas A	Developing a Practical Pesticide Method Development Handbook for Emerging and Complex Matrices: An AOAC CASP Initiative	*Julie Kowalski, Intrepid Scientific*
9:15–9:35 am	Texas A	Practical Performance Drivers in EPA 1633A: A Case Study in Landfill Leachate	*Tiffany Liden, Shimadzu Scientific Instruments*
9:35–9:55 am	Texas A	Optimizing Sample Preparation Strategies for Antibiotic Residue Analysis in Honey Using LC MS/MS	*Evan Walters, Biotage*
10:00–10:20 am	Texas C	Coffee Break, Exhibition & Posters (authors present: even # posters)	
10:25–11:45 am	**Texas A**	**SESSION 3 – Part 2: Basic 101 in Method Development, Validation and Troubleshooting Laboratory Challenges** **Chairs: Scott Krepich, Bikram Subedi**	
10:25–10:45 am	Texas A	An alternative statistical approach for method development under EU regulation 2021/808	*Katherine Weddell, Fera Science Limited*
10:45–11:05 am	Texas A	QuEChERS Streamlined: Cut a Step, not corners with the Agilent Multisampler	*Sue D'Antonio, Agilent Technologies*
11:05–11:25 am	Texas A	Advancing GC–MS Method Development for Low-Level Analysis: Impacts of Column Chemistry and Modeling Approaches	*Alexis Shelow, Restek*
11:25–11:45 am	Texas A	Cross Matrix Evaluation of a High Throughput Method for 100+ Drugs in Oral Fluid and Hair using QSight LC-MS/MS	*Jacob Jalali, PerkinElmer*

11:45–1:15 pm	Texas C	Lunch & Exhibition	(poster authors are NOT required to man poster during lunch break but poster available for viewing)
12:15–1:15 pm	Texas B	V-4 Agilent Vendor Seminar (pre-registration required)	
1:20–2:45 pm	**Texas A**	**SESSION 4: Analytical Innovation for a Changing World — AI, New Technologies and New Challenges** **Chairs: Amadeo Rodriguez Fernandez-Alba, Dan Biggerstaff**	
1:30–1:35 pm	Texas A	Waters Introduction	
1:35–1:55 pm	Texas A	Maximizing throughput and robustness for long-term food testing on a new generation triple quadrupole mass spectrometer	*Andrew Folkerson, SCIEX*
1:55–2:15 pm	Texas A	Towards more automated, robust and high-throughput workflows for routine multiresidue pesticide analysis	*Amadeo R. Fernández-Alba, University of Almeria*
2:15–2:35 pm	Texas A	Automated Microplastic Identification in Biological and Environmental Samples by Applying Machine Learning to Multimodal Fluorescence and µFTIR Imaging	*Justin Smolen, Texas A&M University*
2:35–2:55 pm	Texas A	Analysis of Ultra Short Chain and Short Chain PFAS in Fresh Produce and Beverages using Novel Mixed-mode LC Column and EMR Passthrough Matrix Cleanup	*Limian Zhao, Agilent Technologies Inc.*
3:00–3:15 pm	Texas C	Coffee Break, Exhibition & Posters (authors present: odd # posters)	
3:20–5:00 pm	**Texas A**	**SESSION 5: The Past, Present and Future of Natural Toxins Analysis** **Chairs: Julie Brunkhorst, Dimple Shah**	
3:20–3:40 pm	Texas A	Development of Standard Method Performance Requirements (SMPR) for Mycotoxin Analysis in Novel Foods and Ingredients: An Update	*Lukas Vaclavik, Eurofins Food Chemistry Testing*
3:40–4:00 pm	Texas A	Mycotoxin Testing: Past to Present, Where Have We Been and Where Are We Now	*Julie Brunkhorst, Trilogy Analytical Laboratory*
4:00–4:20 pm	Texas A	Aflatoxin Immunoaffinity Chromatography with Automated Vacuum Manifold	*Makda Araya, Waters Corporation*
4:20–4:40 pm	Texas A	Quantitative Determination of Cereulide Toxin in Infant Formula and Ingredients Using LC–MS/MS	*Adam DeWilde, Eurofins Food Chemistry Testing*
4:40–5:00 pm	Texas A	Cyanobacterial toxins in recreational waters using a targeted UPLC/MS/MS method and comparison to metagenomics	*Stuart Oehrle, Northern Kentucky University, Waters Lab*
5:05–5:10 pm	Texas A	Closing Remarks	*Kelsey Powers, Holly Lee*
5:15–6:00 pm	Texas C	Exhibition	
5:15–6:00 pm	Texas A	NACRW Organizing Committee Meeting **(open to all attendees)**	

Wednesday, July 15, 2026

Time	Room	Event / Session	Speaker(s)
7:15–8:15 am	Texas B	V-5 UCT Vendor Seminar (pre-registration required)	
7:45–8:15 am	Texas C	Early Morning Coffee	
8:30–9:50 am	**Texas A**	**SESSION 6: Nontargeted Analysis Using High Resolution Mass Spectrometry and Other Technologies** **Chair: Wiley Hall**	
8:30 - 8:50 am	Texas A	Expanding PFAS pesticide monitoring using micro-flow LC-HRMS: a combined targeted and suspect screening approach	*Florencia Jesús, University of Almeria*
8:50 - 9:10 am	Texas A	An Exploration of Sample Prep Techniques for Non-targeted Analysis of PFAS using Combustion Ion Chromatography	*Jayesh Gandhi, Metrohm USA*
9:10 - 9:30 am	Texas A	Expanding EI Mass Spectral Libraries for PFAS: Improved Spectral Quality and New Fragmentation Mechanisms	*Yufang Zheng, NIST*
9:30 - 9:50 am	Texas A	Analytical Strategies to Identify and Quantify Extractable/Leachable Chemical Residues from Implantable Medical Devices: A Comparison with Food Safety Residue Analysis	*Michael S. Young, Cambridge Polymer Group*
9:55 - 10:15 am	Texas C	Coffee Break, Exhibition & Posters (all posters)	
10:20–11:30 am	Texas A	**SESSION 7: Development and Application of Reference and Proficiency Test Materials** **Chair: Ryan Malone**	
10:20 - 10:25 am	Texas A	LGC Standards 5-min Introduction	
10:25 - 10:45 am	Texas A	Total synthesis as a new path toward natural abundance and isotopically labeled natural toxin reference standards	*Daryl Staveness, ExciPlex, Inc.*
10:45 - 11:05 am	Texas A	The Evolution in Designing a Master LC/MS Calibration Solution for Pesticides Containing Over 700 Analytes	*HuiChen Stavros, O2si Smart Solutions / LGC Standards*
11:05 - 11:25 am	Texas A	Toxic Truths: Reference Materials are Non-Negotiable in Mycotoxin Testing	*Ryan Malone, Trilogy Analytical Laboratory*
11:25 - 1:30 pm	Texas C	Lunch & Exhibition	
1:30 - 2:50 pm	**Texas A**	**SESSION 8: Early Career Scientists in Action: Advancing Contaminant and Residue Analysis** **Chairs: Margot Lee, Marti Zhong Hua**	
1:30 - 1:50 pm	Texas A	Introducing PFAS-RAD, a Retrospective Analysis Database for targeted screening of legacy and emerging PFAS in food samples by LC-HRMS	*Marti Z. Hua, Carleton University/National Research Council Canada*

1:50 - 2:10 pm	Texas A	Wastewater Clues in the Drug “Cat and Mouse”	*Bikram Subedi, Louisiana State University*
2:10 - 2:30 pm	Texas A	Towards Precision-based Source Reduction: Development, Validation, and Application of an LC-MS/MS Method for Analysis of Drugs of Abuse and Addiction Interventions in Wastewater	*Adam R. Wronski, Baylor University*
2:30 - 2:50 pm	Texas A	Seasonal Occurrence and Water Quality Hazards of Per- and Polyfluoroalkyl Substances in Estuarine Systems across a Gradient of Effluent Contributions to Base Flow	*HyeongYoung Choi, Baylor University*
3:00 - 3:30 pm	Texas A	Poster Awards and Closing	
3:30 - 4:30 pm	Texas A	NACRW 2026 Feedback Session	

Oral & Poster Abstracts

Full oral and poster presentation abstracts follow below.

Vendor Seminar Abstracts

V-1 — Waters: Improving laboratory efficiency through Simultaneous Quant and Qual Analysis using a Benchtop Multi-reflecting Time-of-flight Mass Spectrometer

Shashank Jain, MS, PhD, Waters Corporation

High-resolution mass spectrometry (HRMS) is increasingly central to regulatory science, enabling confident compound identification, sensitive quantitation, and streamlined workflows across diverse application areas. This presentation highlights the Waters Xevo™ MRT platform and demonstrates how a single HRMS system can support both qualitative and quantitative analyses across environmental, pharmaceutical, and food safety markets. Xevo™ MRT elevates analytical performance by delivering quantitation-grade sensitivity with high-resolution structural clarity in a single injection. With up to 100K FWHM resolving power and sub-ppm mass accuracy, Xevo MRT provides the selectivity required to resolve isobaric interferences that routinely compromise triple quadrupole MRM assays—enabling accurate quantification alongside confident identification, even in complex biological matrices. High MS/MS acquisition rates (>100 Hz) combined with ~2 ms interscan duty cycles preserve sensitivity on fast UPLC gradients, while dual-gain detection delivers over five orders of dynamic range for simultaneous measurement of parent drugs and low-abundance components. Practical workflow examples will be presented spanning PFAS analysis, pharmaceutical impurity profiling, and food contaminant screening. These case studies demonstrate how Xevo MRT integrates high mass accuracy, resolving power, and sensitivity with routine robustness to address evolving regulatory challenges. Emphasis will be placed on harmonized qualitative and quantitative strategies, including targeted and non-targeted screening, confirmatory workflows, and quantitative performance in complex matrices—illustrating how HRMS can simplify method development while increasing analytical confidence and laboratory efficiency.

Speaker Bio: Shashank Jain is the Business Development Manager for Xevo™ MRT at Waters Corporation, supporting the Americas in driving XMRT adoption and customer success. He brings over 10 years of experience in analytical instrumentation, spanning field service, product specialization, and strategic sales in mass spectrometry. Shashank holds a Ph.D. in Analytical Chemistry from the University of Vermont and M.S. in Analytical Chemistry from Western Michigan University.

V-2 — SCIEX: Is your matcha latte really matcha? Exploring matcha quality and origin using high-resolution mass spectrometry

Kendra Adams, SCIEX

This talk highlights high resolution LC–MS/MS for evaluating matcha quality, authenticity, and origin in a single workflow. Using a ZenoTOF 7600+ with ZT Scan DIA, comprehensive MS and MS/MS data are generated to enable broad profiling and confident compound identification across commercial matcha samples spanning culinary and ceremonial grades from China and Japan. PCA differentiates samples by grade and origin, while markers such as L-theanine, catechins, and flavonoid glycosides provide chemical context. Overall, the workflow demonstrates how HRMS supports efficient, data rich food analysis through non targeted discovery for authenticity and quality assessment.

V-3 — LGC Standards: Recent Advances in Reference Materials: Chemicals of Concern

Dan Biggerstaff, LGC Standards

This presentation reviews the Ohio Department of Agriculture’s extraction and detection of over 300 pesticides and how this testing ties into federal government programs. Resulting methods used by the Ohio Department of Agriculture (ODA) Pesticide Residue laboratory show a lower quantitation limit at or below 10 parts per billion in complex matrices using a QuEChERS extraction paired with GC/MS/MS and LC/MS/MS. This work will summarize several difficult cases and testing strategies to overcome and analyze a variety of sample types.

Dan Biggerstaff serves as the End Market Technical Sales Manager for LGC Standards in the Americas. With over three decades of experience in environmental testing and reference material development, Dan is a trusted technical resource for customers, sales teams, and product development groups alike.

He founded o2si Smart Solutions in 1997, a company dedicated to producing high-quality, custom organic solution reference materials for the environmental sector. Under his leadership, o2si expanded into both organic and inorganic reference materials across multiple industries and is now part of LGC Standards.

Dan holds a Ph.D. in Physical Chemistry from the University of Delaware and currently leads initiatives in specialized product development, method innovation, customer support, and technical problem-solving.

V-4 — Agilent: Strategic Approaches to Complex Sample Analysis in Regulatory Pesticide Samples

Deidre E. Damon, PhD

This presentation reviews the Ohio Department of Agriculture's extraction and detection of over 300 pesticides and how this testing ties into federal government programs. Resulting methods used by the Ohio Department of Agriculture (ODA) Pesticide Residue laboratory show a lower quantitation limit at or below 10 parts per billion in complex matrices using a QuEChERS extraction paired with GC/MS/MS and LC/MS/MS. This work will summarize several difficult cases and testing strategies to overcome and analyze a variety of sample types.

Routine Multiresidue Analysis with Hydrogen Carrier Gas: Sensitivity Improvements by Dual-Layer Injection

Prof. Amadeo Rodríguez Fernández-Alba

The transition from helium to hydrogen carrier gas has become increasingly attractive for routine GC-MS/MS laboratories due to supply, cost and sustainability considerations. However, sensitivity losses remain one of the main limitations for multiresidue pesticide analysis under hydrogen conditions. This presentation demonstrates how Dual-Layer solvent vent injection can significantly enhance analyte transfer and improve instrumental sensitivity, enabling reliable pesticide residue determination at trace levels. Validation data, real-sample analysis and EUPT performance results support the suitability of this approach for routine regulatory monitoring.

V-5 — UCT: Doing the Work Before the Work: A Low-Burden Approach to Sample Preparation Screening for Cannabis Pesticide Analysis

Rhiley Schmidt, Method Testing Laboratories; Anthony Repay, Method Testing Laboratories; Julie Kowalski, jkSS, LLC

Cannabis flower is an analytically demanding matrix for pesticide residue analysis. While sample preparation methods have been published for this application, peer-reviewed and independently replicated performance data remains limited. Available publications predominantly demonstrate fit-for-purpose performance through recovery studies, providing little characterization of cleanup performance directly. Laboratories still face significant challenges achieving consistent, routine performance under production conditions, suggesting that recovery alone is insufficient to fully vet a sample preparation method for a highly complex matrix with high cannabinoid and pigment content.

This presentation introduces a fast, low-burden screening framework for systematically vetting cleanup performance of candidate methods under real laboratory constraints, before committing to resource-intensive recovery and matrix effects studies. The framework uses four screening parameters: pigment removal (visual assessment), nonvolatile coextractives removal (gravimetric analysis), volatile coextractives removal (GC-MS, scan), and cannabinoid-specific removal (LC/UV). This enables meaningful ranking and elimination of sample preparation candidates without requiring recovery studies or sophisticated analytical methods. Candidate methods were designed considering extractability and analyte detectability, while targeting an increased sorbent-to-sample ratio benchmarked against our current method to establish a target for cleanup improvement.

Applied to cannabis flower, this screening framework identified promising sample cleanup options that outperform our current method without straining laboratory resources, even when starting from a large pool of candidate cleanup methods. Pesticide recovery and matrix effects studies, generated for the two promising candidate sample preparation options as well as the current method benchmark, confirm that analytical performance is maintained with the selected cleanup options. We demonstrate both an improved sample preparation strategy for cannabis pesticide testing and a transferable, low-resource workflow that any laboratory can deploy early in method development to guide sample preparation selection efficiently.

Speaker Bio: Rhiley Schmidt is currently Assistant Laboratory Director at Method Testing Laboratories in Tampa, Florida, where she supports laboratory operations, analytical testing, and team leadership within the cannabis testing industry. Rhiley's background includes experience in forensic science, analytical chemistry, and regulated laboratory workflows. She earned her Bachelor of Science in Forensic Science from the University of Tampa and has continued to build her career around quality-driven laboratory testing, technical problem-solving, and operational improvement.

Oral Presentation Abstracts

O-S1-1 — Determination of the Geographical Origin of Spices Using ICP-OES, ICP-MS, and PCA Analysis

Jeffrey Sayen, Agilent

Food fraud driven by economic incentives presents a significant challenge to the global food industry, particularly for high-value, origin-specific commodities such as spices. Practices including counterfeiting, substitution, adulteration, and mislabeling often evade detection due to the lack of standardized analytical methods, resulting in economic losses and erosion of consumer trust. Dramatic price increases have further intensified incentives for fraudulent activity. Consequently, there is an increasing need for robust analytical approaches capable of defending geographic origin claims. In this study, elemental profiling was investigated as a tool for determining the geographical origin of spices. Samples with verified country-of-origin information were sourced from a major U.S. spice importer. Following microwave-assisted acid digestion, elemental compositions were measured using inductively coupled plasma optical emission spectrometry (ICP OES) and inductively coupled plasma mass spectrometry (ICP MS). Multielement datasets were evaluated to assess whether statistically meaningful distinctions between spices originating from different countries could be achieved. The results demonstrate that elemental analysis combined with microwave digestion provides a reliable and reproducible means of differentiating spice origins. This work highlights the applicability of ICP based elemental fingerprinting as a practical approach for food authenticity testing and supports its potential use in regulatory, quality control, and supply-chain verification contexts.

O-S1-2 — Quantitation of polar pesticides in foods of plant origin

Holly Lee, SCIEX

Polar pesticides, such as glyphosate, glufosinate and ethephon, are widely used for agricultural crop protection due to their low cost and high effectiveness. Growing concerns about their safety have resulted in stringent maximum residue levels (MRLs) in Europe. Due to their high polarity and hydrophilicity, polar pesticides are analytically challenging for conventional GC and HPLC techniques, which typically require derivatization. The European Reference Laboratory (EURL) quick polar pesticides (QuPPe) method has enabled direct LC-MS/MS analysis as a viable alternative; however, its minimal sample clean-up typically yields extracts containing numerous polar co-extractives. This can lead to significant matrix effects, especially when using reverse-phase chromatography, where polar pesticides are typically poorly retained and not well separated. Novel stationary phases, such as mixed-mode and HILIC chemistries, have emerged with more targeted selectivity for polar pesticides. Here, a HILIC-based LC-MS/MS method was developed to complement the QuPPe-PO extraction for the analysis of 10 polar pesticides in tomato, orange and oats on the SCIEX 7500+ system. HILIC chromatography demonstrated robust and good retention and separation in solvent and matrix. Matrix-matched calibration exhibited r2 ≥0.99, accuracy ±30% and %CV

O-S1-3 — Analysis of Volatile PFAS in Complex Juice Matrices Using a Simplified HS-SPME GC/MS/MS Approach

Tiffany Liden, Shimadzu Scientific Instruments

Per- and polyfluoroalkyl substances (PFAS) pollution is a growing global concern due to their persistence and link with adverse health effects, many of which remain poorly understood. Accurate detection and quantitation are therefore important. While PFAS analysis has conventionally focused on water, attention is also expanding into food and beverages, where testing remains limited despite high stakes and increasing regulations. A recent lawsuit involving PFAS in juice highlighted rising public scrutiny, placing food safety and brand reputation at risk. As regulatory oversight continues to expand, reliable methods for accurately quantifying PFAS in beverages are becoming increasingly critical. This study presents a Headspace Solid-Phase Microextraction–Triple Quadrupole Gas Chromatography/Mass Spectrometry (HS-SPME GC/MS/MS) method for PFAS quantitation in juices. GC/MS enables analysis of volatile PFAS unsuitable for LC/MS, while HS-SPME allows rapid analysis with minimal sample preparation in complex matrices. This study targeted ten PFAS spanning PFI, FTI, FTAC, FTMAC, FTOH, and FASA classes. An eight-point calibration curve (1–2000 ng/L) was prepared in 10 mL of water with isotopically-labeled internal standards and 2% NaCl to enhance extraction efficiency. The calibrators were then vortexed and placed on an AOC-6000 Plus autosampler for GC/MS analysis. The targeted compounds were analyzed using a multiple reaction monitoring (MRM) GC/MS method coupled with HS-SPME to enhance selectivity and sensitivity at ng/L levels. Calibration verification controls were run after the initial calibration and again after an average of 14 samples to evaluate the calibration stability. Method performance was assessed using spiked laboratory control samples (LCS) and four fortified juice matrices (100 ng/L). As part of quality control, an initial evaluation of the system background was performed before calibration and sample analysis. The method blank results showed no detectable interferences. Calibration curves were linear ($R^2 \geq 0.993$), and verification control recoveries met method criteria (70–130%). LCS results (n=4) showed 83–115% recoveries with %RSDs of 0.6–6.8, demonstrating the high accuracy and precision of the method in a clean matrix. Preliminary analysis of the juice samples showed significant matrix effects, highlighting the need for isotopically labeled internal standards. Isotope dilution was applied to each target compound to achieve accurate quantification in complex matrices. For instance, 8:2 FTMAC was accurately quantified only when its corresponding isotopically labeled internal standard (8:2 FTMAC-d5) was used; other internal standards from the same PFAS class did not sufficiently correct for matrix effects for this analyte.

Concentrations of targeted PFAS in replicate analyses of both spiked and unspiked samples (n = 3) were determined using the initial calibration curve. In four juice matrices, recoveries ranged from 69–120% with %RSDs

O-S1-4 — Determination of Mineral Oil Hydrocarbons in Foods: Setup and Validation of an Online-Coupled HPLC–GC–FID Method with Automated Sample Preparation

Lukas Vaclavik, Eurofins Food Chemistry Testing

Mineral oil hydrocarbons (MOH), including mineral oil saturated hydrocarbons (MOSH) and mineral oil aromatic hydrocarbons (MOAH), are receiving increasing attention in food analysis due to their potential presence from processing aids, lubricants, environmental sources, and migration from food-contact materials. Their determination remains analytically challenging because MOSH and MOAH are measured as complex unresolved mixtures and may overlap with naturally occurring hydrocarbons or other non-mineral interferences sharing similar structure. This presentation describes the setup of an online-coupled HPLC–GC–FID method with automated sample preparation for determination of MOSH and MOAH in the C10–C50 range in foods. The method was established for a wide range of matrices including edible oils and fats, milk powder, powdered and ready-to-feed infant formula, and green coffee beans. Sample preparation combines automated extraction with matrix-dependent saponification and epoxidation, with optional online aluminum oxide clean-up to further reduce interferences when needed. While LC–GC–FID is the primary quantification tool, confirmation remains important, particularly for complex or suspect samples. Orthogonal techniques such as comprehensive two-dimensional gas chromatography–mass spectrometry (GC×GC–MS) can provide additional structural insight, help differentiate mineral oil fractions from interfering hydrocarbons, and support interpretation when unusual chromatographic patterns are observed. The talk will highlight practical implementation of the method, key matrix-specific challenges, and performance characteristics supporting its use for routine MOSH/MOAH testing in complex food matrices.

O-S1-5 — Analysis of Multi-Class Drug Residues and Glucosamine in Animal Feed

Zeyu Han, Mérieux NutriSciences, Silliker Canada Co. Ltd.

The analysis of multi-class veterinary drug residues and nutritional additives in animal feed is frequently challenged by high lipid content and matrix complexity, which can lead to significant ion suppression and instrument contamination, etc. This presentation describes two distinct analytical workflows utilizing the Captiva EMR-Lipid SPE column to streamline sample cleanup across diverse matrices of pet food, ensuring enhanced sensitivity, accuracy and repeatability/reproducibility while analysis using LC-MS/MS. The first method focuses on the simultaneous determination of eight analytes, including six ionophore antibiotics (monensin, narasin, lasalocid, salinomycin, nicarbazin, and maduramicin), the beta-agonist (ractopamine), and the streptogramin antibiotic (virginiamicin). This approach was validated in dried animal feed pellets and further verified in canned fish meal. The EMR-Lipid technology provided superior removal of lipids while maintaining high recoveries for the hydrophobic compounds. The second method addresses the quantification of glucosamine in pet food. By implementing the EMR-Lipid cleanup, the workflow effectively attenuated matrix interferences from high-fat pet food formulations, resulting in improved chromatographic peak shape and analytical reliability using LC-MS/MS. These validated methods demonstrate excellent linearity, repeatability/reproducibility, accuracy, and precision, confirming that our laboratory's capability to perform both drug residue and nutritional analysis across a wide range of challenging feed matrices.

O-S1-6 — The Identification and Quantification of Persistent Pesticide Residues Resulting from the Treatment of Museum Display Items.

Wiley Hall, USDA-ARS-SJVASC

Over the last 70+ years, several dozen pesticides have been reported as having been used for the purpose of preventing biodegradation of museum collection items from a variety of pests, including rodents, fungi and insects. The pesticides commonly used in museums, especially for older display items (pre-1980's), tend to be persistent, like DDT; highly toxic, like mercuric chloride; or both, like lead arsenate. They vary in terms of their chemical nature, ranging from low polarity, organic compounds (e.g. – DDT or pyrethroids) to inorganic salts and / or other compounds containing heavy metals (e.g. – lead arsenate, thallium sulfate or hydrogen cyanide). These compounds may have been appropriate for their intended use: protecting items that would only be handled by professionals from a wide variety of potential pests with minimal reapplications (although most of the older pesticides are no longer used); but now there is a push to repatriate some of the items (baskets in this case) to the peoples who first made them. Once repatriated, the baskets may be used according to their original purpose: i.e. - handled by the public, including children, or even used for the preparation or storage of foodstuffs. Thus, it is critical to determine which baskets have detectable levels of residual pesticides on their surface, and, at least, a semi-quantitative assessment of the relative magnitudes of those pesticide residues. The optimization and validation of methods for the extraction of pesticide residues from polyvinyl alcohol wipes followed by their analysis by total reflection fluorescence (TXRF) spectrometry for the presence of heavy metals and by gas chromatography coupled to time-of-flight mass spectrometry (GC-MSToF) is presented.

O-S1-7 — Quantitative and Qualitative Analysis of Pyrethroid Residues in Soy Based Choline Supplements Using LC MS/MS with Electrospray Chemical Ionization

Lihini Tharanga Mendis, Shimadzu Scientific Instruments

Plant based nutraceuticals and dietary supplements are experiencing increased consumer demand. Plants used in supplement manufacturing are often treated with agricultural pesticides and herbicides at various stages of cultivation. Depending on agricultural practices and downstream processing, residues of these compounds may persist in finished dietary supplements. Choline is an essential nutrient associated with reproductive health, neurological function, and lipid metabolism; this nutrient is available in animal-derived and plant-based forms, with plant-based products commonly using soy phosphatidylcholine. As choline extraction involves lipid fractionation of soybeans, there is potential for co extraction and enrichment of lipophilic pesticides. Pyrethroids, a widely used class of synthetic insecticides, exhibit high lipophilicity and therefore pose a potential risk of enrichment during oil based processing. In this study, a targeted LC MS/MS method was developed for the qualitative and quantitative determination of pyrethroid residues in commercially available soy based choline supplements. Ten pyrethroid compounds were analyzed using a LCMS 8045RX triple quadrupole mass spectrometer operated in positive electrospray ionization mode. Chromatographic separation was achieved on a Shim-pack Velox Biphenyl (2.7µm, 2.1×100mm) column using Nexera 40-series UHPLC system. A 15-minute gradient was applied at constant flow with 1µL injections with sample preparation optimized for lipid rich nutraceutical matrices. Multiple reaction monitoring (MRM) transitions were optimized to achieve high selectivity and sensitivity. All analytes were baseline separated under optimized conditions, with calibration curves demonstrating excellent linearity (R^2 \> 0.99) from 1 mg/mL to 0.01 ng/mL. The method enabled reliable detection and quantification of residual pyrethroids using 1 µL injection volumes, demonstrating a robust and sensitive method addressing complex supplement matrices. This work demonstrates the applicability of LC MS/MS for residue monitoring in soy derived nutraceuticals and underscores the importance of targeted pesticide analysis in lipid rich plant-based supplements.

O-S2-1 — Aligning Analytical Method Options for PFAS with Evolving Regulatory and Compliance Requirements

Taryn McKnight, Eurofins Environmental Testing

There has been no shortage of developments over the past few years with regards to legislative and regulatory activity around the management of PFAS chemicals in consumer products, food, and the environment. The U.S. EPA has finalized rules with various reporting requirements under TSCA, TRI, and the National PFAS Testing Strategy. The EU has considered a comprehensive proposal to enact a broad ban on PFAS in products, and the U.S. states have continued to forge ahead with more aggressive approaches to limiting or removing PFAS from products and the environment. All of this has not gone off without a hitch, however. With overwhelming public comments highlighting the essential uses and lack of viable substitutes, and with a litany of litigation challenging adopted rules, legislative and regulatory bodies are grappling with the path forward. In the meantime, a number of these laws have progressed passed the proposed or considered stage and are in effect, which brings us to compliance. In some cases, compliance is a matter of reporting what you know or think you know about PFAS in your processes or products, but ultimately, we see a growing need for generating empirical data to substantiate these claims or assumptions. With environmental regulations far more mature than those in products, testing and compliance protocols in environmental matrices have served as the foundation for how we approach products or food but what questions we are trying to answer about PFAS in any of these media varies. With that, what analytical method options are available to us for demonstrating compliance with these myriad of laws or investigating where PFAS are coming from and ending up in the environment? Is there a solution for every rule or regulation as written? This presentation will inform the listeners about the analytical options for demonstrating compliance, investigating sources, and understanding how representative the data are or are not, and what developments are underway or needed to better align the data with the rules.

O-S2-2 — Flame-Broiled and Fluorinated: PFAS Analysis in BBQ Foods Using a Reduced QuEChERS Approach

Margot Lee, Waters Corporation

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants with increasing evidence of bioaccumulation in the human food chain. Animal-derived proteins such as pork, poultry, and beef, as well as certain fruits and vegetables, represent potential exposure pathways. Contamination may occur through feed, water, soil, or other environmental inputs. In recognition of these risks, the European Union has established maximum levels for four PFAS compounds (PFOA, PFOS, PFNA, PFHxS) in meats and produce, while U.S. regulatory and public health interest continues to expand. To address these emerging concerns, an adaptable and resource-efficient sample preparation and analysis approach was developed for the determination of PFAS in diverse food matrices, focusing on foods commonly consumed at a BBQ. A scaled-down QuEChERS-based approach was evaluated for both animal and plant-based samples, where reduced sample mass and salt content minimized solvent and standard consumption, lowered costs, reduced hazardous waste, and improved overall workflow efficiency. Following extraction, dual-phase SPE GCB/WAX (graphitized carbon black and weak anion exchange) cartridges were then utilized for sample cleanup prior to analysis. Analysis was performed using LC-MS/MS where enhanced sensitivity ensures reliable detection at low concentration levels despite the reduced sample size. The reduced sample and salt quantities improve efficiency and throughput, as there is less material to homogenize and smaller salt packs dissolve more

easily with less clumping for easier handling. The lower sample mass also minimizes co-extraction of lipids and other matrix interferences, as evidenced by reduced turbidity in comparison to traditional 10 g extractions. This results in cleaner extracts, which can enhance SPE performance and reduce matrix effects during LC-MS/MS analysis. Overall, this streamlined workflow supports higher throughput without compromising sensitivity or data quality This work provides insight into PFAS occurrence across a range of food matrices and highlights key differences in contamination profiles between animal-derived and plant-based foods. The approach demonstrates how flexible, scaled sample preparation strategies can support regulatory compliance, reduce laboratory burden, and improve accessibility for PFAS monitoring. Importantly, the method is designed to be transferable, enabling broader adoption across laboratories to support ongoing food safety and public health efforts.

O-S2-3 — Single-System LC–MS/MS Analysis of PFAS and Cyanotoxins: Evaluation of Method Performance and the Effects of Mobile Phase Additives

Tiffany Liden, Shimadzu Scientific Instruments

Per- and polyfluoroalkyl substances (PFAS) and cyanotoxins are regulated drinking water contaminants under the United States Environmental Protection Agency (EPA). Although EPA Method 533, EPA Method 544, and EPA Method 545 rely on LC–MS/MS, they are typically performed using separate systems. This study demonstrates an integrated LC–MS/MS workflow for simultaneous determination of 25 PFAS, six microcystins and nodularin, and cylindrospermopsin and anatoxin-a on a single Shimadzu LCMS-8060RX platform. PFAS were analyzed using negative electrospray ionization in a 15-minute method with an inline delay column to reduce background contamination. Cyanotoxins were measured in positive mode using 8-minute separations. Quantitation was performed by multiple reaction monitoring (MRM). Because PFAS analysis in negative ESI is sensitive to acidic residues, the impact of mobile phase additives was systematically evaluated. Continuous exposure to formic acid–containing mobile phases resulted in significant signal suppression for several PFAS, with compounds such as PFBA and 3:3 FTCA decreasing by up to 40%. Replacing formic acid with acetic acid minimizes PFAS negative mode ion suppression. These results demonstrate that formic acid is detrimental to PFAS analysis, while acetic acid provides a reliable alternative compatible with analyzing PFAS and cyanotoxin on one system. System robustness was assessed through 294 injections simulating frequent switching among Methods 533, 544, and 545. The sequence included calibration sets, continuing calibration checks, and mobile phase rinses between transitions. No carryover or sensitivity loss was observed. All analytes achieved R^2 \> 0.99 within their respective calibration ranges, with acceptable accuracy and precision. These results demonstrate a robust, single-platform solution for integrated PFAS and cyanotoxin analysis in drinking water.

O-S2-4 — Pressurized Extraction and Cleanup in One Automated Process for PFAS Analysis of Food

Alicia Stell, CEM Corporation

The scientific community is very aware of the risks that per- and polyfluoroalkyl substances (PFAS) pose to human health. PFAS are known to bioaccumulate, leading to their presence throughout daily life. The occurrence of PFAS in food is an exposure concern. Food matrices are very diverse and require extraction and cleanup to address matrix interferences, complicating method development, standardization, and data consistency. Methods typically employ a solvent extraction followed by a separate cleanup protocol in order to isolate PFAS analytes of interest. This multi-step process can be time-consuming, inconsistent, and susceptible to human error. To address these limitations, a fully automated protocol was developed for integrated Pressurized Extraction and Cleanup (PEC). This work details the extraction, cleanup, and filtration of food matrices in under fifteen minutes, enabling automated preparation followed directly by LC-MS/MS analysis. To demonstrate performance, fish tissue samples were prepared for automated extraction coupled with in-situ cleanup. LC-MS/MS analysis of the resulting extracts displayed good recoveries and reproducibility for PFAS compounds and internal standards. These results suggest that this method enables a fast, reliable, and scalable workflow suitable for high-throughput PFAS testing laboratories.

O-S2-5 — Automated Extraction Paired with a Dual-LC Orbitrap Workflow for Targeted PFAS Analysis in Food

Ed George, Thermo Fisher Scientific

The analysis of per- and polyfluoroalkyl substances (PFAS) in food and food contact materials remains challenging due to complex matrices and the need for robust targeted methods. This presentation highlights a novel workflow for targeted PFAS determination in food and beverage samples, combining automated dispersive liquid–liquid microextraction (DLLME) with advanced dual-channel liquid chromatography–mass spectrometry. DLLME integrates extraction, cleanup, and concentration into a rapid, low-solvent automated workflow (

O-S2-6 — A Rapid Screening Method for PFAS Analysis (EPA 1633a) Using DART/MS

Seyyedhadi Khatami, Bruker

Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals known as "forever chemicals" because they persist in the environment and accumulate in living organisms. The Environmental Protection Agency (EPA) currently employs liquid

chromatography-tandem mass spectrometry (LC-MS/MS) for PFAS analysis in various matrices. However, high concentrations of PFAS in samples frequently cause carryover in LC-MS/MS, resulting in false-positive peaks in subsequent analyses. Eliminating these contaminants necessitates an extensive cleaning process. This study proposes the use of direct analysis in real time tandem mass spectrometry (DART-MS) to pre-screen samples, thereby avoiding the analysis of high-concentration samples by LC-MS/MS and reducing carryover. Preliminary findings indicate that samples prepared according to EPA Method 1633 can be rapidly analyzed by DART-MS within seconds. These results suggest that DART-MS may serve as an effective screening tool for identifying high-concentration samples prior to LC-MS/MS analysis, thereby minimizing carryover.

O-S2-7 — Setup and Validation of a Sensitive, Robust and High-Throughput LC-MS/MS Method for Determination of Thirty Priority PFAS in Foods, Infant Formula and Dietary Supplements

Michael Buhrman, Eurofins Food Chemistry Testing

Per- and polyfluoroalkyl substances (PFAS) are man-made chemicals that have been widely used in various industries and products. Due to the potential adverse health effects and environmental persistence, there are growing concerns about the widespread exposure to the public. Given their persistence, resistance to degradation, and tendency to accumulate in biological systems, dietary intake is considered a significant contributor to overall human exposure. This underscores the importance of sensitive and reliable analytical methods capable of detecting PFAS at trace levels, in order to support risk assessment, regulatory compliance, and monitoring efforts. A wide range of analytical methodologies is currently available for the testing of food matrices; however, ongoing regulatory developments continue to drive the need for improved performance. In particular, the progressive lowering of maximum limits, coupled with the expansion of matrix scope to include increasingly complex and diverse food products, places greater demands on analytical workflows. As a result, methods that were previously considered fit-for-purpose may no longer provide the required sensitivity, selectivity, or robustness. In this study, an LC-MS/MS method was setup and validated in routine food analysis lab for low-level detection of 30 priority PFAS across a wide range of matrices, including edible oils and fats, powdered and ready-to-eat infant formulae, terrestrial meats, seafood and shellfish, fruits and vegetables, dietary supplements, and related ingredients. Samples were extracted using a modified QuEChERS workflow followed by further extract clean-up on Agilent Technologies enhanced matrix removal (EMR) PFAS Food I and II SPE past-through cartridges. Instrumental analysis was performed using Agilent 1290 Infinity II fitted with PFC-free kit and coupled to 6495D triple quadrupole mass spectrometer. Large volume injections were implemented along with a feed injection port to achieve the required sensitivity while maintaining acceptable peak shape for early eluting analytes. The method validation data generated in this study support the acceptable performance of the method compliant with the AOAC Standard Method Performance Requirements (SMPRs®) 2023.003.

O-S2-8 — Evaluating the Efficacy of PFAS Preventive Controls: A Statistical Comparison of Nestle and FDA Market Basket Data

Ashley Griffin and Xun (Ann) Fu, Nestle Quality Assurance Center

In 2026, the importance of having a food safety plan that includes monitoring and controlling for PFAS contamination cannot be overstated. But how do we know that these controls within our food safety plans are actually limiting human exposure like they are intended to do? At the Nestle Quality Assurance Center in Dublin, Ohio, we have three years of longitudinal data to evaluate these safety frameworks. Through a collaborative effort in 2024, NQAC Dublin worked with the FDA to compare the performance of our two different analytical methods for the determination of PFAS in food. A statistical analysis of results collected on the four regulated compounds showed no bias between the two methods, providing a valid basis for data comparison. By benchmarking results collected at NQAC Dublin against the FDA's Market Basket (Total Diet Study) data, we will explore the differences and similarities and what implications those might have on preventive controls within your food safety plans. We will also explore some trends in PFAS detections and where the science and industry may be headed in the future to ensure that these "forever chemicals" are properly monitored and restricted in the global food chain.

O-S3-1 — Single Laboratory Validation of Quaternary Ammonium Pesticides in Food using LC/MS-MS

Christian Talavera, US Food and Drug Administration

With the discovery of quaternary ammonium compounds as potent contact herbicides in the 1950s, their production and usage worldwide have increased manifold for the control and management of terrestrial and aquatic vegetation. Diquat and Paraquat are the most widely used, but highly toxic to humans. In this study, a single laboratory validated LC-MS/MS method was developed for the quantification of five quaternary amines in six food matrices: Kale, Tomato, Blueberry, Avocado, Soybeans, and Lentils. Commodities with greater than 80% natural moisture (wet) were extracted with 10 mL of acidified methanol at 0.05M HCl. For commodities with less than 80% natural moisture (dry), water was added to the analytical portion to reach a total water content of approximately 10 g. Samples were then extracted with 10 mL of acidified methanol at 0.05 M and 0.5 M HCl. All samples were spiked with an internal standard at 25 ng/g for each of the five quaternary amines. Wet commodities were cleaned up by a 2-step filtration, dry commodities were cleaned with acetonitrile and C18 sorbent. Chromatographic

separation of the five quat amines was performed under acidic conditions (pH 3.7) on a HILIC column using a gradient with a flow rate of 0.4 mL/min. Quantitation was performed using an internal standard calibration prepared in water, 10% acetonitrile. The method was validated by performing spike recoveries at three different levels in triplicate for each matrix. Included in these experiments were method and matrix blanks along a linear curve covering the range from 1.0-1,000 ng/mL, where the LOQ was set to 1.0 ng/mL.

O-S3-2 — Developing a Practical Pesticide Method Development Handbook for Emerging and Complex Matrices: An AOAC CASP Initiative

Julie Kowalski, Intrepid Scientific

Reliable pesticide residue testing depends not only on validated analytical methods but also on a scientifically sound and well-structured method development process. In emerging analytical sectors such as cannabis testing, many laboratories have entered the field without the extensive experience in pesticide residue method development that exists within traditional food and agricultural testing communities. As a result, laboratories attempt to adopt existing methods or vendor methods without fully understanding the analytical considerations required to produce reliable results. To address this gap, a working group within the AOAC Cannabis Analytical Science Program (CASP) is developing a Pesticide Method Development Handbook designed to provide a practical framework for laboratories developing pesticide residue methods. The objective of the handbook is to bridge the gap between guidance documents and experimental laboratory work by outlining a structured, science-based approach to method development. Planned content includes guidance on information gathering prior to method development, evaluation of compound physicochemical properties, matrix considerations, instrumental method selection, calibration scheme design, sample preparation strategies, and planning experiments needed to support future method validation studies. While the initial motivation for the handbook arose from challenges observed in cannabis testing laboratories, the core concepts are broadly applicable to pesticide residue testing across diverse matrices. The intent is therefore to develop a resource that can benefit laboratories working in cannabisnd other complex analytical contexts. An additional distinguishing feature of this project is the planned format of the final deliverable. Rather than a traditional static document, the handbook will be released as a collection of practical resources—including worksheets, checklists, decision frameworks, and reference tables—hosted online and made freely accessible without a paywall. This working session will introduce the origins, objectives, and current progress of the AOAC CASP handbook initiative and invite discussion from the North American Chemical Residue Workshop community. NACRW has long been a gathering place for many of the scientists who have developed, refined, and applied the analytical approaches that define modern pesticide residue testing. The practical expertise represented within the NACRW community, spanning method development, troubleshooting difficult compounds, and translating analytical science into workable laboratory methods, makes this group uniquely positioned to help shape the handbook. Input from NACRW participants is therefore essential to ensure that the resource reflects the collective knowledge and real-world experience of the residue analysis community. Attendees will be invited to provide feedback, suggest practical tools and reference materials, and consider contributing to the ongoing working group as the handbook continues to develop. , food, agricultural, a

O-S3-3 — Practical Performance Drivers in EPA 1633A: A Case Study in Landfill Leachate

Tiffany Liden, Shimadzu Scientific Instruments.

EPA Method 1633A provides a validated framework for PFAS analysis in complex environmental matrices, including landfill leachate. However, successful implementation in real-world laboratories often requires optimization beyond procedural compliance. Landfill leachate is among the most analytically challenging matrices due to extreme chemical heterogeneity, elevated dissolved organic content, and variability between sites and over time. These characteristics frequently lead to variability in recovery, matrix suppression, and inconsistent sensitivity. This work presents a practical approach to method development and troubleshooting within the 1633A framework, using landfill leachate as a case study to illustrate foundational principles. Authentic landfill leachate composite samples were prepared according to EPA 1633A. To evaluate sample preparation performance, commercially available weak anion-exchange (WAX) SPE cartridges were compared using extracted isotopically labeled internal standards (EIS) to assess recovery and reproducibility across PFAS chemistries. Significant differences were observed between cartridges. For example, $^{13}C_2$-6:2 FTS recovery increased from approximately 40% with one cartridge to approximately 100% with another, while D_3-NMeFOSAA improved from \~19% to \~41%. Similar trends were observed across fluorotelomer sulfonates, perfluoroalkyl carboxylates (PFBA–PFDoA), sulfonates, and precursor compounds. In several cases, improved recovery was accompanied by reduced variability, highlighting the importance of cartridge chemistry selection during validation. To distinguish matrix-driven effects from instrumental contributors, chromatographic and MS evaluations were conducted using analytical standards prepared in 1633A diluent. Comparison of multiple C18 columns of identical dimensions revealed measurable differences in retention, peak shape, response, and resolution, demonstrating that column selection can materially influence method robustness and sensitivity even when nominal specifications are identical. Mass spectrometric source parameter screening identified desolvation-related settings, including nebulizing gas flow, interface temperature, and drying conditions, as dominant drivers of signal behavior. Response improvements were compound dependent. Increased nebulizing gas flow enhanced short-chain PFAS response (e.g., \~1.5× increase for PFBA), while elevated desolvation temperature produced substantial gains for longer-chain and precursor compounds; HFPO-DA (GenX) increased more than seven-fold under optimized thermal conditions. These findings underscore the importance of understanding aerosol formation and ion transfer efficiency when troubleshooting sensitivity issues. Collectively, these results

demonstrate that systematic isolation of sample preparation, chromatographic, and source variables enables laboratories to identify root causes of performance variability and improve confidence in quantitative results.

O-S3-4 — Optimizing Sample Preparation Strategies for Antibiotic Residue Analysis in Honey Using LC MS/MS

Evan Walters, Biotage

The determination of antibiotic residues in honey is analytically challenging due to the complexity of the matrix, which can significantly affect extraction efficiency and detection accuracy. This presentation investigates a range of sample preparation approaches aimed at improving matrix removal and analyte recovery prior to LC MS/MS (Liquid Chromatography–Tandem Mass Spectrometry) analysis. Traditional QuEChERS extraction is compared with several solid phase extraction (SPE) techniques to evaluate their performance in terms of cleanliness, recovery, and reproducibility. The work focuses on method development and optimization, assessing parameters such as extraction solvent composition, sample-to-solvent ratios, and clean up sorbent selection. Particular attention is given to balancing high recovery rates with effective matrix removal across a diverse panel of antibiotics commonly found in honey. The evaluation includes the examination of both manual and automatable workflows to support consistent and reproducible results in a routine laboratory setting. The presentation aims to provide practical guidance to laboratories involved in food residue analysis, emphasizing data quality, reproducibility, and operational efficiency rather than specific products or proprietary systems. Insights gained from this comparative study contribute to a broader understanding of how different extraction and clean up strategies influence analytical outcomes for antibiotic residue testing in honey. The findings support the development of more robust, efficient, and reproducible sample preparation methodologies applicable to other complex food matrices as well.

O-S3-5 — An alternative statistical approach for method development under EU regulation 2021/808

Katherine Weddell, Fera Science Limited

The EU regulation 2021/808 for the performance of analytical methods for residues of pharmacologically active substances used in food-producing animals specifies performance parameters that must be demonstrated by analytical methods to ensure the quality of monitoring programs. Due to the vast numbers of veterinary drugs and sample matrices, conventional re-validations to this new regulation is both time consuming and costly. Hence, we developed an alternative, more efficient, validation approach. The value of parameters that describe the relationship between added concentration and each of three quantities: mean measurement result, the uncertainty of the mean result, and within laboratory reproducibility standard deviation are directly estimated by a maximum likelihood fit of a statistical model to measurement results. Hence, the model provides estimates of trueness, relative standard deviation and measurement uncertainty at any concentrations of interest that are within the concentration range investigated. The decision limit for confirmation (CCα) and detection capability for screening (CCβ) are calculated from the estimates of measurement uncertainty at the concentration limit and screening threshold. This model was applied to two separate alternative approaches for validation , using different approaches to data generation. Our first approach used results gathered from spikes added to routine screening batches over the course of approximately one year, which is in contrast to the typical three-day validation regime specified in EU regulation 2021/808. The statistical model was fitted to the results to estimate the method performance parameters. Because this approach used data collected across a large number of analytical batches, carried out by many analysts under a variety of laboratory conditions, the estimates of method performance more accurately reflect routine laboratory use. This also provides ruggedness data, another requirement of EU regulation 2021/808. The estimates of performance given by these validations have been comparable to those gained via the conventional approach. Our second, and most recent, approach is to conduct targeted validation batches which include several species and where the spiking concentrations bracket the levels of interest, rather than those levels being spiked directly. The benefit of this spiking regime was to allow for multi-species validations, where regulatory limits may vary, because the method performance metrics can be calculated at any concentration within the range concentrations spiked. This workflow uses a minimum of three mixed species validations followed by a statistical assessment of whether species effects method performance. Where there is no statistically significant species effect, a single model fitted to the results from all species can be used to estimate the measurement performance (trueness, precision, uncertainty, CCα, CCβ) for each species. This work demonstrates that a statistical, maximum-likelihood–based validation framework can provide a robust and efficient alternative to conventional re-validation under EU Regulation 2021/808. By modelling trueness, precision, and measurement uncertainty as functions of concentration, method performance parameters can be reliably estimated across relevant concentration ranges without extensive, resource-intensive experiments.

O-S3-6 — Quechers Streamlined: Cut a Step, not corners with the Agilent Multisampler

Sue DAntonio, Agilent

QuEChERS remains a widely adopted sample preparation approach for pesticide and contaminant analysis due to its simplicity and robustness; however, traditional workflows often require the manual addition of water at the last steo to ensure good chromatography. This additional step increases hands-on time, introduces variability, and creates opportunities for error. The Agilent Hybrid Multisampler streamlines the QuEChERS workflow by eliminating the need for water addition after sample preparation. Removes any error related to dilution and does not dilute out any contaminants. By reducing sample manipulation

and preparation complexity, this approach improves workflow efficiency, enhances reproducibility, and supports consistent data quality. The elimination of water addition also reduces opportunities for contamination and handling errors, making the method well suited for high-throughput laboratories and routine LC/MS applications. Overall, the Agilent Hybrid Multisampler enables a more streamlined QuEChERS workflow, delivering reliable performance with no dilution step and supporting laboratories seeking increased productivity without compromising chromatographic resolution

O-S3-7 — Advancing GC–MS Method Development for Low-Level Analysis: Impacts of Column Chemistry and Modeling Approaches

Alexis Shelow, Restek

Environmental laboratories are increasingly adopting highly sensitive gas chromatography–mass spectrometry (GC–MS) techniques for low-level analysis, introducing challenges in method performance and development. At trace levels, analyte interactions with reactive surfaces in the GC flow path, arising from residual activity and column deactivation chemistry, can impact peak shape, calibration, and reproducibility. Column phase selection and surface chemistry therefore play a critical role in analytical outcomes. Chromatographic modeling tools are also being leveraged to streamline method development and improve throughput. This work examines the combined influence of column chemistry, surface activity, and modeling-assisted optimization on GC–MS workflows. Findings highlight opportunities to enhance robustness and reduce method development time in low-level analytical applications.

O-S3-8 — Cross Matrix Evaluation of a High Throughput Method for 100+ Drugs in Oral Fluid and Hair using QSight LC-MS/MS instrument

JACOB JALALI, PerkinElmer

The increasing prevalence of emerging psychoactive substances and the expanding scope of forensic toxicology testing have created a critical need for robust, multi analyte methods capable of operating across diverse biological matrices. This study presents the development and validation of a comprehensive analytical workflow for the detection of over 100 target compounds in oral fluid and hair using QSight LC-MS/MS instrument, followed by an in-depth comparison of matrix performance and interpretive outcomes. This work establishes a scalable, high throughput approach for sensitive analyte detection and provides evidence-based guidance for laboratories seeking to optimize matrix selection in complex testing environments.

O-S4-1 — Maximizing throughput and robustness for long-term food testing on a new generation triple quadrupole mass spectrometer

Andrew Folkerson, SCIEX

Large multiresidue panels often contain hundreds to thousands of analytes, which can affect data quality, especially in regions of high MRM concurrency, where the data point density across chromatographic peaks is critical for accurate quantitation. Lengthening the gradient can improve separation and reduce concurrency, but often at the cost of lower sample throughput. This work features ultrafast MRM quantitation of \>500 pesticides in orange juice on a new triple quadrupole mass spectrometer, capable of analyzing up to 1000 transitions/sec. Sub-to-low ms pause and dwell times, coupled with fast polarity switching, enabled initial retention time (RT) discovery of 1411 transitions, including both quantifier and qualifier transition for each pesticide, in a single injection. Fast MRM acquisition supports narrower peaks and faster gradients, enabling shorter runs and increasing sample throughput. The combination of a shorter pause (2 ms) and minimum dwell time (1 ms) allowed for greater MRM concurrency and thereby, the development of a faster 20-min gradient, without sacrificing data quality, as compared to a 30-min method using a pause time of 3 ms and a minimum dwell time of 2 ms. Comparison of sensitivity, matrix effects, ion ratios, limits of quantitation (LOQs), accuracy and precision (%CV) against the SANTE 11312/2021 criteria demonstrated quantitative performance was largely preserved between the 20-min and 30-min methods, resulting in \~30% time savings per sample. The extra data point density from faster cycling of each LC peak enabled the widening of the RT window to 80 sec, strengthening the method’s robustness against RT shifts from column aging, complex food matrices and instrument variability. In addition, the new instrument delivered exceptional robust performance with thousands of consecutive injections of food matrix extracts over 5 weeks of continuous operation, achieving

O-S4-2 — Towards more automated, robust and high-throughput workflows for routine multiresidue pesticide analysis

Amadeo R. Fernández-Alba, University of Almeria

Routine pesticide residue analysis requires workflows capable of combining broad analytical scope, high sensitivity, reliable identification and high sample throughput across diverse food matrices. Although LC-MS/MS, GC-MS/MS and HRMS platforms have greatly improved analytical performance, routine laboratories still depend on labour-intensive sample preparation, matrix-specific clean-up procedures and sample-introduction conditions that may limit reproducibility, sensitivity and operational efficiency. This work brings together three complementary developments aimed at modernising multiresidue pesticide analysis through automation, simplification of manual operations and optimisation of critical analytical steps. The first

development focuses on automation of the clean-up step in LC-MS/MS methods. Conventional dispersive clean-up is often time-consuming, matrix-dependent and prone to losses of reactive or acidic pesticides, particularly when PSA sorbent is used. An automated µSPE clean-up workflow using a PAL-RTC system was compared with manual dispersive clean-up in tomato, orange, avocado, tea and rice. The automated cartridges, containing MgSO4/PSA/C18/CarbonX, provided broadly comparable extract cleanliness and analytical performance while improving recoveries for problematic acidic compounds such as fluazifop, haloxyfop and quizalofop through an additional elution step with acidified acetonitrile. Sulphonylurea pesticides also showed improved behaviour. The automated procedure provided good repeatability, with RSD values below 10%, doubling sample throughput compared with the manual workflow. The second development integrates automated sample preparation with HRMS. The EDGE system was evaluated as an automated extraction platform capable of combining extraction, in-line filtration and rinsing in a single programmed sequence. This reduces manual handling and intermediate steps. Coupling EDGE to LC-QTOF using a ZenoTOF 7600 operated in DIA/SWATH mode provided wide-scope acquisition and improved fragment-ion sensitivity for trace-level confirmation. In a 162-pesticide panel, 82% of compounds reached an LOQ of 5 µg/kg and 95% reached LOQs ≤10 µg/kg. Results obtained in real fruit and vegetable samples were comparable, within measurement uncertainty, to those generated using a validated LC-QqQ/QuEChERS workflow, while maintaining the advantages of HRMS for accurate-mass identification, DIA-based confirmation and retrospective data analysis. The third development addresses optimisation of sample introduction in GC-MS/MS. Acetonitrile is an effective extraction solvent in QuEChERS workflows, but its direct injection in GC can be problematic due to co-extracted interferences, residual water and expansion-volume effects. To improve solvent compatibility and chromatographic performance, QuEChERS extracts were diluted two-fold with ethyl acetate before GC-MS/MS injection. Solvent-vent injection using a 2 mm dimpled liner was optimised in terms of vent flow, pressure and time, initial inlet temperature, and injection volume. Column flow and dwell times were also refined to balance sensitivity, peak shape and analytical speed. The method was validated for 200 pesticides in tomato, orange and avocado, with calibration ranges of 5-200 ppb for several analytes, and was successfully applied to real and proficiency-test samples. Together, these studies show that routine pesticide residue analysis can be significantly improved by targeting critical steps across the analytical chain: clean-up, extraction, HRMS detection and GC sample introduction, thereby reducing manual handling, improving robustness and maintaining sensitivity and regulatory confidence in high-throughput food safety laboratories.

O-S4-3 — Automated Microplastic Identification in Biological and Environmental Samples by Applying Machine Learning to Multimodal Fluorescence and µFTIR Imaging

Justin Smolen, Texas A&M University

The heterogeneity of microplastics (MPs) in size, composition, and degradation state, coupled with high levels of matrix interference, creates a significant analytical bottleneck for detecting these contaminants. This research presents an automated analytical pipeline that integrates fluorescence-guided imaging with micro-Fourier transform infrared (µFTIR) spectroscopy to overcome challenges in particle localization and classification. Central to this method are machine-learning (ML) models that utilize computer vision to rapidly target candidates from large-area fluorescence scans and similarity learning to perform generalized polymer identification. This approach optimizes µFTIR focal plane array (FPA) imaging by focusing acquisition only on high-probability regions, significantly reducing scanning time. To ensure real-world applicability, the procedure was validated using environmentally degraded and weathered microplastics, demonstrating high accuracy across diverse matrices including environmental sediments and bovine and porcine organ tissues. This integration of ML-driven automation and advanced spectroscopy transitions microplastic analysis from a labor-intensive manual task to a standardized, high-throughput protocol capable of assessing plastic accumulation within the agricultural food chain and the broader environment.

O-S4-4 — Analysis of Ultra Short Chain and Short Chain PFAS in Fresh Produce and Beverages using Novel Mixed-mode LC Column and EMR Passthrough Matrix Cleanup

Limian Zhao, Agilent Technologies Inc.

Ultrashort chain (USC; C1–C3) and short chain (SC; C4–C7) per and polyfluoroalkyl substances (PFAS) are highly polar, water soluble compounds that commonly occur in high moisture food matrices such as fresh produce and beverages. Increasing regulatory and scientific interest in these analytes highlights the need for reliable analytical methods capable of accurate and precise determination. However, conventional reversed phase LC columns often exhibit insufficient retention for USC and SC PFAS, resulting in poor chromatographic performance, severe matrix effects, compromised sensitivity, and unsatisfactory quantitation. In addition, traditional weak anion exchange (WAX)–based SPE protocols frequently show poor recovery for USC PFAS due to inefficient retention caused by highly polar co extracted matrix components and ionic strength effects. This study presents a novel analytical workflow that combines an Enhanced Matrix Removal (EMR) pass through matrix cleanup approach with a mixed mode LC column, the Altura Poroshell 120 PFAS LC, for the determination of USC and SC PFAS in high moisture food matrices. Fresh produce samples were extracted using a QuEChERS based method, while beverage samples were prepared by dilution with acidified acetonitrile. The resulting crude extracts were loaded onto EMR PFAS Food I cartridges for pass through cleanup. The EMR eluate was then directly analyzed by LC–MS/MS using the Altura Poroshell 120 PFAS column, coupled with online dilution via feed injection mode on a Hybrid LC Sampler. The highly streamlined sample preparation workflow reduces preparation time and effort while minimizing the risk of PFAS contamination and losses of volatile USC PFAS during sample handling. The EMR mixed mode pass through cleanup approach is compatible with both QuEChERS extraction and direct solvent extraction, providing efficient and selective removal of matrix interferences such as carbohydrates, pigments, and organic acids. The use of feed injection on the Hybrid LC Sampler

enables direct large volume injection of sample extracts with high organic solvent content. The Altura Poroshell 120 PFAS column demonstrated significantly improved chromatographic performance for the analysis of polar USC PFAS. Compared with other mixed mode LC columns designed for USC PFAS analysis, the Altura PFAS column provided substantially enhanced analyte retention, achieving retention factors greater than three for all evaluated USC and SC PFAS analytes without requiring LC gradients starting at extremely low organic mobile phase composition. Improved retention enhanced the separation of target PFAS from food matrix interferences, reduced matrix effects, and increased detection sensitivity for both USC and SC compounds. In addition, the robust retention mechanism enabled direct injection of high organic sample extracts without compromising peak shape for early eluting analytes. Overall, this workflow provides a robust and efficient solution for the accurate identification and quantitation of USC and SC PFAS in complex, high moisture food matrices, offering improved detection sensitivity, selectivity, and quantitative reliability.

O-S5-1 — Development of Standard Method Performance Requirements (SMPR®) for Mycotoxin Analysis in Novel Foods and Ingredients: An Update

Lukas Vaclavik, Eurofins Food Chemistry Testing

The rapid expansion of novel foods and alternative protein sources is reshaping the global food landscape, while simultaneously introducing new analytical challenges for contaminant monitoring. Mycotoxins remain highly relevant in these matrices due to their presence in raw materials, potential concentration during processing, and possible transfer across emerging production systems. At the same time, existing regulatory frameworks and standardized analytical methods were largely developed for traditional food commodities and do not adequately address the complexity and diversity of these new products. AOAC INTERNATIONAL, through its collaborative and stakeholder-driven programs, is addressing this gap by developing a new Standard Method Performance Requirements (SMPR®) document for the determination of mycotoxins in foods and feed, with emphasis on novel foods and ingredients. The SMPR defines consensus-based, performance-oriented criteria to guide method development, validation, and evaluation within the AOAC Official Methods of Analysis℠ framework, ensuring that analytical approaches are fit for purpose across a broad range of applications. The proposed SMPR covers a wide range of matrices, including plant-based protein ingredients and finished products, fermentation-derived materials, insect-based foods, and animal feed. It establishes requirements for multi-analyte methods targeting key regulated and emerging mycotoxins, such as aflatoxins, ochratoxin A, deoxynivalenol, fumonisins, zearalenone, T-2/HT-2 toxins, and Alternaria toxins. Performance criteria include recovery, precision, and limits of quantification aligned with current regulatory expectations and analytical capabilities. In this presentation, the development process of the SMPR will be outlined, including the identification of target analytes and matrices, key analytical challenges, and the rationale behind the proposed performance criteria. Developed by a globally representative working group of experts from academia, industry, and regulatory bodies, this SMPR will support harmonization of analytical methods and enable reliable monitoring of mycotoxins in emerging food systems.

O-S5-2 — Mycotoxin Testing: Past to Present, Where Have We Been and Where Are We Now

Julie Brunkhorst, Trilogy Analytical Laboratory

Mycotoxins are natural toxins and an increasingly large group of organic toxins that are caused by molds. The first of these mycotoxins was discovered 60+ years ago when an unknown disease referred to as turkey “X” was linked to contaminated Brazilian groundnut meal affected by Aspergillus flavus the toxin was named “Aspergillus flavus toxin or Aflatoxin”. This presentation will discuss the journey from the identification of Aflatoxin to the discovery of the mycotoxins that are now well known and regulated. It will go back in time and discuss the initial ways of analysis and how technology has developed throughout the years. The session will talk about TLC, HPLC, GC and various on-site test kit methods and how they evolved. It will also dive into the different purification techniques that have been used over the years and how some are still in use today. The first methods to the present will be mentioned and how these advances have uncovered many different mycotoxins and enabled the analysis of mycotoxin from simple cereals to complex food and feeds.

O-S5-3 — Aflatoxin Immunoaffinity Chromatography with Automated Vacuum Manifold

Makda Araya, Waters Corporation

Mycotoxins are toxic metabolites produced by Aspergillus, Fusarium, and Penicillium fungi that contaminate crops and food products. These compounds are heat stable and persist through cooking and food processing, requiring reliable analytical monitoring to ensure regulatory compliance. They are fat soluble and can accumulate in body tissues, increasing health risks to humans and animals. Aflatoxins are among the most hazardous mycotoxins, commonly found in commodities such as corn, peanuts, and grains, and are classified as Group 1 carcinogens. AOAC Official Method 991.31 describes the extraction of aflatoxins from corn, raw peanuts, and peanut butter using an immunoaffinity column. While highly selective and sensitive, this workflow is traditionally performed manually and requires careful control of column loading and elution rates (≤1 drop per second), making the method labor intensive and potentially susceptible to operator-to-operator variability. Traceable and programmable extraction enabled by advances in processing hardware could improve robustness and reproducibility for aflatoxin testing. In this study, immunoaffinity chromatography was performed using an automated vacuum manifold. Pressure gradients were optimized across the three-step workflow to maintain a loading flow rate of less than one drop per second. With an automated vacuum pump, aflatoxins B1, B2, G1, and G2 spiked in corn were successfully isolated over a concentration

range of 0.1 to 100 ng/g. Integration of an automated vacuum manifold with an audit-trailed software enabled a fully traceable, turnkey workflow that is less hands-on, limiting manual variability while maintaining the selectivity of the AOAC method prior to UHPLC-FLR analysis.

O-S5-4 — Quantitative Determination of Cereulide Toxin in Infant Formula and Ingredients Using LC–MS/MS.

Adam DeWilde, Eurofins Food Chemistry Testing

Recent cases of cereulide toxin contamination in infant formula have underscored the need for monitoring of ingredients and finished products to ensure the safety of foods intended for vulnerable populations. The cereulide toxin, a heat-stable dodecadepsipeptide produced by certain strains of Bacillus cereus, is responsible for emetic food poisoning and can cause severe gastrointestinal symptoms, mitochondrial dysfunction, liver failure, and, in rare cases, death, particularly in infants and young children. In response to the need for testing, an analytical method for the quantification of cereulide using liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) was developed and validated. This method was modified from the ISO 18465:2017 for quantitative determination of emetic toxin (cereulide) using LC-MS/MS. The method was later adapted to meet the European Food Safety Authority acute reference dose limits for infants by implementing QuEChERS sample preparation workflow. This work supports the implementation of a validated LC–MS/MS approach for cereulide analysis in infant nutrition products and ingredients. The method met validation benchmarks for all evaluated matrices, demonstrating mean recoveries within 70–120% and precision better than 20% relative standard deviation (RSD). Quantification was based on the use of stable isotope labeled internal standards to correct for matrix effects. Cereulide identity was confirmed using retention time matching and qualifier to quantifier multiple reaction monitoring (MRM) peak area ratios. The method strengthens analytical preparedness for risk assessment, and regulatory compliance considering increased scrutiny following recent contamination events.

O-S5-5 — CYANOBACTERIAL TOXINS IN RECREATIONAL WATERS USING A TARGETED UPLC/MS/MS METHOD AND COMPARSION TO METAGENOMICS

Stuart Oehrle, Waters Lab

In this paper we investigate the use of smaller column packing (sub 2µm particles) to monitor for many cyanobacterial toxins using a generic gradient method and a targeted Liquid Chromatography/Tandem-Mass Spectrometry (LC/MS/MS). We analyzed various freshwater lake samples from a region in Ecuador for a variety of toxins including microcystins, anatoxin-a, cylindrospermopsin as well as newer toxins, such as euglenophycin, anabaenopeptins and micropeptins. In addition, Metagenomic sequencing and analysis of the samples identified one genomic bin identified tentatively as Planktothrix agardhii, and several genomic fragments of other toxin producing cyanobacteria. Using the genome we examined which genes were present and what toxins were capable of being produced. In this case both the DNA analysis and LC/MS/MS analysis gave results that agreed. Data from both techniques will be presented including the novel detection of various forms of cylindrospermopsin in this sample. Additional work from Ohio River water samples and elsewhere will be discussed as well showing commonalities of toxic productions over several years.

O-S6-1 — Expanding PFAS pesticide monitoring using micro-flow LC-HRMS: a combined targeted and suspect screening approach

Florencia Jesús, University of Almeria

Per- and polyfluoroalkyl substances (PFAS), as defined by the OECD, comprise a broad class of chemicals characterized by the presence of at least one fully fluorinated carbon moiety. In plant protection products (PPP), fluorinated functional groups are intentionally introduced to enhance chemical stability and efficacy. Recently, several PFAS pesticides and their transformation products have gained attention due to their environmental persistence, including degradation to highly persistent and mobile compounds such as trifluoroacetic acid. The increasing number of PFAS pesticides and related metabolites challenges routine residue monitoring, as analytical reference standards are not available for all compounds. High-resolution mass spectrometry (HRMS) enables expanded analytical coverage by combining targeted determination with suspect screening approaches for known and emerging PFAS pesticides and metabolites. Samples were prepared using a citrate-buffered QuEChERS extraction followed by automated micro-solid-phase-extraction clean-up. Analyses were performed using micro-flow liquid chromatography (LC) coupled to a high-resolution Orbitrap Exploris 240 mass spectrometer. Two separate acquisition methods were applied using positive and negative electrospray ionization modes. Data were acquired using a full scan at 90,000 FWHM combined with nine data-independent acquisition MS2 scans at 15,000 FWHM. A targeted method was validated for 50 PFAS pesticides in tomato, orange, and avocado matrices at 0.005, 0.010, and 0.050 mg/kg according to SANTE criteria. The targeted method demonstrated robust analytical performance in tomato, orange, and avocado matrices, fulfilling the validation requirements established in the SANTE guidelines for pesticide residue analysis. The use of micro-flow LC provided sufficient sensitivity for the determination of PFAS pesticides in food matrices, with limits of quantification of 0.005 mg/kg for the majority of compounds. The validated method was applied to more than 190 fruit and vegetable samples. Targeted analysis revealed the occurrence of several PFAS pesticides and metabolites, with the fungicides fluopyram, fludioxonil and fluopicolide among the most frequently detected. Suspect screening was performed using an in-house database containing approximately 100 additional PFAS pesticides and metabolites, including accurate mass

information of precursors and at least one diagnostic fragment ion per compound. Tentative identification was further supported by accurate mass measurements (±5 ppm) and isotopic patterns. In addition to parent compounds, known PFAS pesticide transformation products and metabolites were tentatively identified. These included trifloxystrobin acid and sulfoxaflor metabolite X11719474, which retained key PFAS structural features. The combined targeted and suspect screening workflow enabled comprehensive PFAS pesticide assessment within a single analytical platform, allowing retrospective data analysis as new PFAS pesticides or metabolites emerge, without additional sample preparation or reanalysis.

O-S6-2 — An Exploration of Sample Prep Techniques for Non-targeted Analysis of PFAS using Combustion Ion Chromatography

Dr. Jayesh Gandhi, Metrohm USA

Due to their environmental persistence and potential implications for human health, the analysis of per- and polyfluoroalkyl substances, or PFAS, in the environment remains critical. Targeted analysis using LC-MS/MS has long been the analytical method of choice, due to its high sensitivity and specificity. With more than 3000 potential PFAS-type compounds, targeted analysis does not always allow for the assessment of the total impact of these compounds. Because of this, there has been increasing interest by regulatory committees in non-targeted analysis techniques, such as quantifying total organic fluorine (TOF), as a PFAS impact assessment. Combustion Ion Chromatography, or CIC, allows for the sensitive quantitation of TOF, ranging from single digit ppb to percent levels. In this technique, samples are combusted in an elevated temperature oven, where organofluorine bonds are broken to produce HF, which is subsequently absorbed into solution and analyzed by IC for fluorine. Prior to analysis by IC, inorganic, or free fluoride must be separated from the sample to prevent interference. A variety of techniques exist to accomplish removal of inorganic fluoride, such as the AOF (adsorbable organic fluorine) method (USEPA Method 1621), which captures organofluorine compounds on an activated charcoal bed and allows for removal of free fluoride through a rinsing step. CIC can then analyze the charcoal. Other methods have also been investigated to further improve recovery of TOF, allowing for the non-targeted identification of PFAS compounds ranging from C1-C16+. Most recently Metrohm USA and Markes International collaborated to introduce “Total Fluoride in Air by C-IC.” A complete portfolio of Total Fluorine analysis in Air, Water and Soil will be presented.

O-S6-3 — Expanding EI Mass Spectral Libraries for PFAS: Improved Spectral Quality and New Fragmentation Mechanisms

Yufang Zheng, National Institute of Standards and Technology

Per- and polyfluoroalkyl substances (PFAS) are a large class of environmentally persistent contaminants that present significant analytical challenges due to their chemical stability, structural diversity, and typically low environmental concentrations. Reliable identification of PFAS is therefore highly dependent on comprehensive and high-quality mass spectral reference libraries. In this work, we report an integrated strategy to expand the coverage and improve the quality of electron ionization (EI) mass spectra for PFAS in the NIST Mass Spectral Library. This approach combines computational selection of candidate compounds, targeted acquisition of commercially available PFAS, optimized derivatization methods, and advanced spectral validation tools. An initial list of PFAS candidates was generated from the EPA PFAS Master Database by removing polymers and salts and excluding compounds already represented in the NIST library. This process revealed that the many of PFAS remain absent or underrepresented in current spectral databases. From this screening, a prioritized subset of compounds was selected based on commercial availability, leading to the acquisition and analysis of over 200 PFAS. Depending on functional groups, derivatization strategies including silylation, acetylation, and methylation were applied to improve volatility and chromatographic performance. Both liquid injection GC/MS and headspace sampling techniques were employed to accommodate compounds across a wide volatility range, supported by retention index predictions using an AI-based model. Mass spectra were extracted using AMDIS and evaluated through a combination of MS Interpreter, structure similarity search, and hybrid search algorithms. This workflow enabled confident spectral annotation and identification. Notably, analysis of trimethylsilyl (TMS) derivatives of fluorinated alcohols revealed unusual fragmentation behavior, including the consistent formation of a previously unreported \[M−111\]+ ion. This fragmentation pathway is attributed to fluorine migration to silicon and the formation of a five-membered ring intermediate, followed by loss of a fluorinated silyl group. These findings highlight distinct differences between fluorinated and nonfluorinated analogues and provide new mechanistic insight into PFAS fragmentation patterns. Through this integrated workflow, a total of 322 high-quality EI mass spectra representing 220 PFAS compounds were generated and incorporated into the NIST26 library. The inclusion of retention indices alongside validated spectra further enhances compound identification reliability. Overall, this work not only expands spectral library coverage but also improves understanding of PFAS-specific fragmentation mechanisms, thereby supporting more accurate identification of these critical environmental contaminants in analytical and regulatory applications.

O-S6-4 — Analytical Strategies to Identify and Quantify Extractable/Leachable Chemical Residues from Implantable Medical Devices: A Comparison with Food Safety Residue Analysis

Michael S. Young, Cambridge Polymer Group

A common goal for residue analysis is the determination of potentially toxic substances in materials intended for introduction into the human body. In foodstuffs, the residues of interest are typically pesticides or veterinary pharmaceuticals that were used in food production. Also, other types of residues, PFAS for instance, can leach into foodstuffs from packaging materials. These foodborne residues are introduced into the body by ingestion. The implantation of polymeric medical devices represents a different effective mechanism for introduction of potentially toxic residues to the body. In order to minimize any human risk, the manufacturers of implantable devices are required to identify and quantify extractable/leachable residues in their devices. As in other types of residue analysis, targeted and non-targeted high resolution LC-MS and GC-MS are the primary analytical tools employed in this endeavor. In this presentation the similarities and significant differences in strategies for residue analysis will be discussed, comparing the requirements for food analysis (21 FCR part 109) with requirements for analysis of medical devices (ISO 10993-1B).

O-S7-1 — Total synthesis as a new path toward natural abundance and isotopically labeled natural toxin reference standards

Daryl Staveness, Ph.D., ExciPlex, Inc.

Toxin vigilance in agricultural or environmental monitoring sectors is greatly enabled or hindered by the availability of reference standards. For naturally occurring toxins, a lack of reference standards can be a primary barrier to developing robust analytical methodologies. This supply issue, in many cases, can only be addressed through total synthesis, since there is no guarantee that fermentation techniques or isolation will be viable for a given toxin. ExciPlex is addressing this need using modern synthetic strategies, aiming to facilitate both industrial quantification as well as independent research of pressing natural toxin threats. Mycotoxins are the primary focus, particularly those emerging mycotoxins or mycotoxin metabolites that are not readily supplied in purified form, such as ergot alkaloids, glucuronidated toxins, and NX toxins. Employing modern photochemical techniques and novel design strategies, these toxins can be prepared in quantities needed to match the global demand for new reference materials. These synthetic approaches necessarily create opportunities to introduce unique isotope labeling patterns, offering new internal standard candidates in food and feed analysis. This new-found accessibility to natural abundance and isotopically labeled toxin products is expected to be highly enabling in standardization of mycotoxin testing, our overall mycotoxin traceability capabilities, and most importantly, global mycotoxin management and prevention.

O-S7-2 — The Evolution in Designing a Master LC/MS Calibration Solution for Pesticides Containing Over 700 Analytes

HuiChen Stavros, PhD, O2si Smart Solutions an LGC Standards Company

As laboratories continue to increase the number of analytes that are included in multiple residue monitoring methods, the preparation and maintenance of the calibration and quality control solutions can become a significant task. As a custom reference material manufacturer, we produce approximately 50 new solutions weekly with many of them being pesticide solution reference materials. This places a high demand on generating excellent data quality and high throughput in the quality control laboratory. To facilitate both of these aspects, we have developed a set of LC/MS pesticide reference material solutions containing over 700 analytes which is on the third revision. Rational in the design and revision for each set along with stability data, solvent, pH, and chemistries will be discussed.

O-S7-3 — Toxic Truths: Reference Materials Are Non-Negotiable in Mycotoxin Testing.

Ryan Malone, Trilogy Analytical Laboratory

From corn ethanol protein streams to apple-derived ingredients, the diversity of today's food and feed matrices presents a growing challenge for accurate mycotoxin analysis. Ensuring reliable results across such varied products requires more than advanced instrumentation, it demands the consistent use of well-characterized and repeatable reference materials. Yet, the importance of these materials is often overlooked outside the laboratory. When consumers purchase products like pet food, they inherently trust that safety testing has been performed correctly, but what underpins that confidence? This presentation examines the critical role of mycotoxin reference materials in delivering accurate, reproducible analytical results. It will highlight how these materials support method validation, ensure data integrity, and enable comparability across laboratories and industries. Ultimately, it makes the case that reference materials are not simply a best practice, but a non-negotiable foundation for trustworthy testing in today's complex supply chains.

O-S8-1 — Introducing PFAS-RAD, a Retrospective Analysis Database for targeted screening of legacy and emerging PFAS in food samples by LC-HRMS

Marti Z. Hua, Carleton University / National Research Council Canada

Per- and polyfluoroalkyl substances (PFAS) comprise a vast and structurally diverse universe of thousands of synthetic chemicals which exhibit extreme environmental persistence and bioaccumulative potential, posing multifaceted toxicological risks to both human health and wildlife. The comprehensive characterization of PFAS in complex matrices remains analytically challenging, primarily due to the continuous emergence of novel and replacement compounds that evade traditional targeted screenings. Furthermore, current nontargeted data analysis workflows remain ineffective for PFAS detection at the ultra-trace level in complex matrices. To address this issue, we developed a liquid chromatography–high resolution mass spectrometry (LC–HRMS) workflow based on an expandable compound database. The novel method enables rapid screening and allows retrospective investigation of legacy and emerging PFAS in various agri-food matrices. An in-house PFAS Retrospective Analysis Database (PFAS-RAD) was built analyzing over 170 individual compounds. The full MS ion profile, LC retention time, and 460+ manually curated MS2 spectra of major precursor ions (e.g., in-source fragments) were arranged in a MS1 profile table and a NIST-format MSP file. All agri-food samples from local grocery stores were prepared by acidic acetonitrile extraction, salt-induced phase separation and pass-through solid-phase extraction with Agilent EMR cartridges. The MS spectra of samples and standards were acquired using an Orbitrap Exploris 120 Mass Spectrometer operated in variable data-independent acquisition mode (vDIA). Each cycle (\~1.16 s) comprises a full MS scan (100-1500 Da) and 18 DIA MS2 windows (13 of 50-Da and 5 of 150-Da width). The identification of PFAS in agri-food products was performed using mzmine 4.9.14 software in conjunction with the newly developed PFAS-RAD database. Accurate mass (Δm/z \< 5ppm) of major precursor(s) in MS1, retention time (ΔRT

O-S8-2 — Wastewater Clues in the Drug “Cat and Mouse”

Bikram Subedi, Louisiana State University

The United States continues to face a rapidly evolving overdose crisis driven by polysubstance use and the proliferation of highly potent synthetic opioids. Illicit drug supplies are increasingly characterized by the intermittent emergence of novel synthetic opioids and the adulteration of established substances with new, highly potent agents. In recent years, fentanyl has been widely adulterated with xylazine, followed by the appearance of nitazenes, and more recently cychlorphine. These dynamic changes, combined with limited analytical capabilities to comprehensively monitor drug supply chains and delays in timely reporting, pose significant challenges for public health and law enforcement stakeholders. Unfortunately, individuals who use drugs are often unaware of the composition and potency of the substances they consume, contributing to increased rates of non-fatal overdoses and fatalities. Analysis of residual drug biomarkers in wastewater can provide a comprehensive, non-invasive, and near-real time use of emerging substances in target communities. Using this approach, we report the first detections of xylazine in Kentucky, nitazenes in Louisiana, and cychlorphine in Eastern Tennessee during the early stages of drug-related harm in these regions. This presentation will highlight the analytical challenges associated with identifying newly emerging substances in complex wastewater matrices. It will also discuss the opportunities for wastewater surveillance to serve as an early warning system, enabling more proactive and informed responses to the evolving drug landscape.

O-S8-3 — Towards Precision-based Source Reduction: Development, Validation, and Application of an LC-MS/MS Method for Analysis of Drugs of Abuse and Addiction Interventions in Wastewater

Adam R. Wronski, Baylor University

Although progress has been made in the assessment and management of pharmaceuticals and other emerging environmental contaminants, comparably little environmental research has examined illicit drugs. This presents an important data gap because these drugs act on many of the same highly evolutionarily conserved receptors as pharmaceuticals; neuroactive substances in both groups may elicit behavioral changes in fish at environmentally relevant concentrations. Furthermore, because human behaviors, such as the use of pharmaceuticals or illicit drugs, exist across complex gradients, important questions remain regarding the identification of sites where use, loading, and environmental risks posed by these compounds are elevated. To begin to close these data gaps, we developed a method to extract and analyze 35 illicit drugs, metabolites, addiction intervention treatments, and wastewater tracers in wastewater treatment plant (WWTP) influents by isotope dilution LC-MS/MS. Because the targeted compounds span a broad range of physicochemical characteristics, we developed two solid phase extraction methods (HLB and SCX) to maximize analyte recovery, while nicotine and cotinine were present in influent at sufficient concentrations to allow analysis by direct injection. Compound extraction efficiencies ranged from 83-105%, while method detection limits were below 2.5 ng/L for all compounds except caffeine (7.3 ng/L), cotinine (0.07 µg/L), nicotine (0.29 µg/L), and sucralose (33.9 ng/L). Following development and validation, the method was applied to 24-hour time weighted composite influent samples collected from diverse WWTPs. Specifically, because recent work has demonstrated the influence of community socioeconomic status on the use rates of several classes of pharmaceuticals, we selected sites in communities that exist across a broad gradient of population size, urbanization, and socioeconomic status, with a hypothesis that community socioeconomic status may influence use of illicit drugs or addiction intervention treatments. The wastewater tracer compounds (sucralose, caffeine, carbamazepine) were detected in every sample, as well as 11-nor-9-carboxy-delta9-THC (concentrations ranging from 400-1959 ng/L), amphetamine (194-1380 ng/L), benzoylecgonine (1341-13705 ng/L),

hydrocodone (4-46 ng/L) and methamphetamine (700-4000 ng/L), while delta9-THC, 2-oxo-3-hydroxy-LSD, 6-acetylmorphine, medetomidine, nalmefene, protonitazene, and several benzodiazepines were not detected in any samples. By “thinking upstream” and focusing on the relationships of socioeconomics with illicit drug use, we aim to inform interventions within sewersheds that will lead to source reduction, thereby reducing loading to WWTPs and discharges to the environment.

O-S8-4 — Seasonal Occurrence and Water Quality Hazards of Per- and Polyfluoroalkyl Substances in Estuarine Systems across a Gradient of Effluent Contributions to Base Flow

HyeongYoung Choi, Baylor University

Global estuaries provide diverse benefits to human populations, biodiversity, and ecosystem services. Similar to other coastal systems, Gulf of Mexico estuaries in Texas, USA, experience diverse anthropogenic stress, including base flows that are influenced by upstream wastewater discharges. Given the limited global information for the occurrence and water quality hazards of per- and polyfluoroalkyl substances (PFAS) in estuaries, we employed a hydrological model to examine 14 Texas estuaries across gradients of annual precipitation (\~60-140 cm/yr) and wastewater effluent contribution to base flows. Conventional grab and time-weighted composite samples over a 24-hour period were collected from these 14 estuaries during wetter (Spring) and drier (Fall) seasons of 2024, the hottest year in Texas since 1895. We quantitated surface water concentrations of 24 PFAS via isotope dilution LC-MS/MS. We employed a two-factor generalized linear model and identified sum perfluoroalkyl carboxylic acid (PFCA), long-chain PFAS, and precursors concentrations to significantly ($p \< 0.05$) differ between seasons, with higher mean concentrations detected in spring. Concentrations of perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) did not exceed United States Environmental Protection Agency water quality criteria for aquatic life during either season across the 14 estuaries examined here. However, PFOS levels in these study systems consistently exceeded European environmental quality standards and Australian and New Zealand guideline values during both seasons by

Poster Abstracts

Poster numbers are assigned by presenter. Session A (SA) includes odd-numbered posters; Session B (SB) includes even-numbered posters.

Poster judging will take place during poster sessions listed below:

Poster presenters, please be present at your poster during the following days/times:

Poster Session A (odd # posters):

Monday 10:15–10:35 am and 4:50–6:00 pm

Tuesday 3:00–3:20 pm

Wednesday 9:55–10:15 am

Poster Session B (even # posters):

Monday 3:00–3:20 pm and 4:50–6:00 pm

Tuesday 10:00–10:20 am

Wednesday 9:55–10:15 am

Poster-SA-P-1 — Determination of Carnosic Acid in Chicken Meal and Rendered Chicken Fat by QuEChERS-Based LC-MS/MS: Expanding Residue Surveillance to Antioxidant Additives

Oscar Cabrices, G-Flo Scientific / Tyson Foods

Carnosic acid, a naturally occurring diterpene phenol derived from rosemary (Rosmarinus officinalis) and sage (Salvia officinalis), is widely used as an antioxidant additive in rendered poultry ingredients to retard lipid oxidation and extend shelf life. As a regulated feed additive, its use is subject to labeling requirements and customer-defined inclusion limits, creating a clear analytical need for sensitive and reliable methods capable of monitoring carnosic acid in finished rendered ingredient matrices. Accurate quantification supports dosage verification, label compliance, and supply chain quality assurance — functions increasingly demanded by ingredient purchasers and feed manufacturers alike. While LC-MS/MS methods for carnosic acid have been reported in plasma and plant matrices, no QuEChERS-based approach has been described for rendered poultry ingredient matrices, which present distinct challenges due to their high lipid and protein content. A targeted LC-MS/MS method was developed on a Waters TQ-S Micro for the quantitative determination of carnosic acid in chicken meal and rendered chicken fat. Sample preparation employed a traditional QuEChERS extraction framework with matrix-specific modifications to accommodate the compositional differences between the dry meal and high-fat rendered substrates. Quantitation was performed using matrix-matched calibration to compensate for matrix-dependent ion suppression inherent to these challenging sample types. Method performance was evaluated across multiple fortification levels in both matrices. Mean recoveries ranged from 80–100% in chicken meal and rendered chicken fat, with acceptable precision across all concentration levels. An LOQ of 5 µg/kg was achieved in both matrices, demonstrating the sensitivity of the approach relative to customer-defined action levels. This work describes the first QuEChERS-based LC-MS/MS method for carnosic acid in rendered poultry ingredient matrices and broadens the scope of residue surveillance programs to encompass antioxidant feed additives, a compound class not traditionally addressed by veterinary drug residue platforms. Integration of this capability into a comprehensive rendered ingredient testing portfolio reflects the growing analytical demand for additive monitoring alongside conventional residue surveillance in the rendered poultry supply chain.

Poster-SB-P-2 — PFAS Quantitative testing in Food and Packaging by LC-MS/MS

Ming Gao, Meriuex/Silliker

Per- and polyfluoroalkyl substances (PFAS) are man-made fluorinated compounds recognized for their exceptional resistance to heat and chemical breakdown. Due to their slow degradation, PFAS remain in the environment for long periods, and human exposure can occur through food, drinking water, dust, or dermal contact. Ongoing research has linked certain PFAS to possible health effects such as increased cholesterol, liver impacts, endocrine disruption, and potential associations with cancer. Regulatory agencies have taken steps to reduce exposure. In April 2024, the EPA established the first national drinking water limits for six PFAS, while the FDA has worked with industry to phase out PFAS-based grease-resistant substances used in food packaging. AOAC has also developed Standard Method Performance Requirements (SMPRs) to promote harmonized PFAS analysis in foods and packaging materials. This method outlines a validated LC-MS/MS approach for PFAS determination. Food analysis follows AOAC SMPR 2023.003 covering 30 PFAS compounds, while packaging analysis is based on AOAC SMPR 2025.001. The procedure involves homogenizing the sample, spiking with isotopically labeled internal standards, extracting with acidified acetonitrile, and applying clean-up techniques such as QuEChERS and

solid-phase extraction. Detection is performed using multiple reaction monitoring with retention time confirmation, and quantification relies on calibration curves with dilution and mass adjustments.

Poster-SA-P-3 — A Unified LC-MS/MS Testing Workflow for Broad-Scope Residue Surveillance Across Three Rendered Poultry Ingredient Matrices

Oscar G. Cabrices, G-Flo Scientific / Tyson Foods

Rendered poultry ingredients, including chicken byproduct meal, feather meal, and rendered chicken fat, are widely incorporated into animal feed and pet food formulations. These three matrices present significant analytical challenges for residue monitoring due to their distinct compositional profiles, high lipid and protein content, and associated matrix effects. Despite growing industry demand for broad-scope residue surveillance in rendered ingredients, multi-residue methods covering this matrix class remain limited. A unified antibiotic LC-MS/MS testing workflow was developed on a Waters Xevo TQ Absolute, comprising three complementary analytical workflows targeting 43 residues across five compound categories in all three rendered poultry matrices. The first workflow addresses prohibited dyes: crystal violet, leucocrystal violet, malachite green, leucomalachite green, and brilliant green using a dedicated extraction and LC-MS/MS method optimized for these highly lipophilic colorants. The second workflow targets nitrofuran metabolites (AHD, AMOZ, AOZ, and SEM) via derivatization-based sample preparation. The third and broadest workflow employs a modified QuEChESER Mega-Method for simultaneous determination of avermectins and anthelmintics, phenicol and fluoroquinolone antibiotics, sulfonamides, macrolides, tetracyclines, and the ionophore salinomycin. Modifications to the QuEChESER Mega-Method were introduced to accommodate the high fat and protein burden characteristic of rendered substrates, with extraction and dispersive cleanup conditions optimized separately for dry meal matrices and rendered fat. Column chemistries across the three workflows included a Phenomenex Luna Omega Polar C18, a Restek Inert Biphenyl, and a Restek Inert C18, selected to address the diverse physicochemical properties of the target analyte classes. Target reporting limits were established in alignment with FDA, AAFCO, and customer-driven action levels, with LOQs ranging from 1 to 100 µg/kg depending on analyte class. Method performance across all three workflows was evaluated using matrix-fortified samples prepared in all three rendered matrices, with mean recoveries of 80–115% and acceptable precision, demonstrating analytical suitability across this diverse compound set and challenging matrix class. This workflow represents a purpose-built approach to residue surveillance in rendered poultry ingredients, a sample type historically underserved by available testing methods. By integrating complementary, fit-for-purpose workflows under a common analytical framework, the platform enables comprehensive multi-class residue monitoring aligned with both regulatory requirements and commercial supply chain demands.

Poster-SB-P-4 — Evaluation of the sorption/desorption processes of pesticides in biodegradable mulch films used in agriculture

María Dolores Hernando, Experimental Station of Arid Zones, Spanish National Research Council (CSIC-EEZA)

Microplastics from mulch films can be a source of chemical contamination to agricultural soils. In this context, biodegradable films have been widely positioned as a greener choice. However, their sorption/desorption capabilities, in contrast to the conventional plastic types remain understudied. It is for this reason that objective evaluation of their interactions with residual agricultural contaminants becomes important. Our findings reveal that polyethylene (PE) mulch films retained lower amounts of pesticide residues and demonstrated a higher desorption/release \[median desorption = 71.86 µg/L or about 50%\], while polybutylene adipate terephthalate (PBAT) mulch films retained higher amounts of pesticide residues onto their surface and demonstrated a much lower desorption \[median desorption = 24.27 µg/L or about 17%\] after a spraying event. A higher ambient temperature had no significant effect on final desorption amounts in both PE \[median = 65.27 µg/L at 20 -C and 74.23 µg/L at 40 -C\] and PBAT \[median = 24.26 µg/L at 20 -C and 24.78 µg/L at 40 -C\] mulch films. However, it did favour a faster desorption pace in PE films. Desorption in PBAT and PE plastic types was correlated with the log Kow value \[Spearman's correlation: 0.857 and 0.837 respectively, p \< 0.05\]. However, only a moderate correlation with pKa was observed in PBAT \[Spearman's correlation: 0.478, p \< 0.05\], while none for PE plastic type. Sorption of pesticides onto biodegradable PBAT microplastics were best explained by Elovich \[R2: 0.937–0.959\] and pseudo-second order kinetics \[R2: 0.942–0.987\], suggesting the presence of chemisorption. Furthermore, Weber Morris plots suggested the presence of a multi-step process and Boyd plots indicated that film diffusion or chemical bond formation was the rate-limiting step governing this phenomenon.

Poster-SA-P-5 — From Fry to Fingerprint Non Targeted Food Differentiation Using SCIEX ZenoTOF 7600

Kendra J. Adams, SCIEX

Non targeted liquid chromatography–high resolution mass spectrometry (LC HRMS) enables food characterization and differentiation when analytes of interest are unknown or not fully defined. In this study, a non targeted LC HRMS workflow was applied to commercially available fast food french fry samples to evaluate the ability of high-resolution accurate mass data and multivariate analysis to generate reproducible chemical fingerprints and differentiate products without prior knowledge of marker compounds. Samples from multiple fast food establishments were prepared using a QuEChERS based extraction and analyzed on a SCIEX ZenoTOF™ 7600 qTOF mass spectrometer using Zeno SWATH DIA. This approach enabled comprehensive and unbiased acquisition of MS and MS/MS data across a broad mass range. Data processing, including

feature detection, alignment, and database searching, was performed in SCIEX OS software, while multivariate statistical analysis and feature prioritization were conducted using MarkerView™ software. Principal component analysis (PCA) revealed clear and reproducible clustering of samples by restaurant, demonstrating distinct chemical signatures associated with each product. Independent samples were correctly classified within the established PCA space, confirming workflow robustness. Feature loading analysis combined with accurate-mass MS/MS data enabled tentative identification of compounds related to seasoning components, processing aids, and packaging-associated materials. Compound identities were supported using accurate mass and MS/MS spectral matching utilizing the power of both the SCIEX All-in-One HRMS and NIST 2023 mass spectral libraries. These results highlight the utility of SCIEX non-targeted LC-HRMS workflows for food differentiation and authenticity-focused applications using a single, comprehensive dataset.

Poster-SB-P-6 — Introducing PFAS–RAD, a Retrospective Analysis Database for targeted screening of legacy and emerging PFAS in food samples by LC–HRMS

Marti Z. Hua, Carleton University / National Research Council Canada

Per- and polyfluoroalkyl substances (PFAS) comprise a vast and structurally diverse universe of thousands of synthetic chemicals which exhibit extreme environmental persistence and bioaccumulative potential, posing multifaceted toxicological risks to both human health and wildlife. The comprehensive characterization of PFAS in complex matrices remains analytically challenging, primarily due to the continuous emergence of novel and replacement compounds that evade traditional targeted screenings. Furthermore, current nontargeted data analysis workflows remain ineffective for PFAS detection at the ultra-trace level in complex matrices. To address this issue, we developed a liquid chromatography–high resolution mass spectrometry (LC–HRMS) workflow based on an expandable compound database. The novel method enables rapid screening and allows retrospective investigation of legacy and emerging PFAS in various agri-food matrices. An in-house PFAS Retrospective Analysis Database (PFAS-RAD) was built analyzing over 170 individual compounds. The full MS ion profile, LC retention time, and 460+ manually curated MS2 spectra of major precursor ions (e.g., in-source fragments) were arranged in a MS1 profile table and a NIST-format MSP file. All agri-food samples from local grocery stores were prepared by acidic acetonitrile extraction, salt-induced phase separation and pass-through solid-phase extraction with Agilent EMR cartridges. The MS spectra of samples and standards were acquired using an Orbitrap Exploris 120 Mass Spectrometer operated in variable data-independent acquisition mode (vDIA). Each cycle (\~1.16 s) comprises a full MS scan (100-1500 Da) and 18 DIA MS2 windows (13 of 50-Da and 5 of 150-Da width). The identification of PFAS in agri-food products was performed using mzmine 4.9.14 software in conjunction with the newly developed PFAS-RAD database. Accurate mass (Δm/z \< 5ppm) of major precursor(s) in MS1, retention time (ΔRT

Poster-SA-P-7 — Microplastics and Nanoplastics (MNP)– An Emerging Contaminate of Concern in Our Food Supply

Daniel Biggerstaff, PhD, O2si Smart Solutions an LGC Standards Company

There has been a rapid increase in research surrounding microplastics and nanoplastics (MNP) and their routes of entry in the human body. It has now been well established that MNP’s bioaccumulate in multiple organs including the brain. The National Institute of Health through the Advanced Research Projects Agency for Health (ARPA-H) has initiated the Systemic Targeting of Microplastics (STOMP) to develop a gold standard measurement method for MNP’s in biological materials, identifying direct physiological impacts, understanding routes of entry, and remediation of MNP’s from the human body. The development of labeled MNP’s that can be traced in the food supply, whether plant or animal based, is critical in understanding the level of contamination in our food supply. From a method development perspective, labeled MNP’s can also be distinguished from background ubiquitous contamination aiding in the development of the gold standard method.

Poster-SB-P-8 — Cross Matrix Evaluation of a High Throughput Method for 100+ Drugs in Oral Fluid and Hair using QSight LC-MS/MS instrument

JACOB JALALI, PerkinElmer

The increasing prevalence of emerging psychoactive substances and the expanding scope of forensic toxicology testing have created a critical need for robust, multi analyte methods capable of operating across diverse biological matrices. This study presents the development and validation of a comprehensive analytical workflow for the detection of over 100 target compounds in oral fluid and hair using QSight LC-MS/MS instrument, followed by an in depth comparison of matrix performance and interpretive outcomes. This work establishes a scalable, high throughput approach for sensitive analyte detection and provides evidence based guidance for laboratories seeking to optimize matrix selection in complex testing environments.

Poster-SA-P-9 — PFAS Reference Standards Storage and Handling

Alexandria Bush, Restek

The testing of PFAS in environmental and commercial products has become an increasingly more ubiquitous globally. The high fluorophilicity of many commonly tested PFAS in conjunction with their ionic nature can result in prominent adsorption onto un-deactivated surfaces and micelle formation in solution. If unaccounted for, these effects can lead to erroneous results and shorten shelf-life of standards. This webinar will discuss how specific characteristics of PFAS compounds can lead to complications in the storage and handling of certified reference material and provides recommendations to mitigate these difficulties.

Poster-SB-P-10 — Comprehensive quantitation of water-soluble vitamins in infant formula

Holly Lee, SCIEX

Water-soluble vitamins (WSVs) are essential nutrients that support healthy growth and development during infancy, which include vitamin C and the B complex group comprised of thiamine (B_1), riboflavin (B_2), niacin (B_3), pantothenic acid (B_5), pyridoxine and related forms (B_6), biotin (B_7), folate/folic acid (B_9) and cobalamin (B_{12}). As they are highly water-soluble, WSVs are readily excreted from the body, necessitating recommended dietary allowances (RDAs) to ensure adequate dietary intake across age groups, especially for infants. As an alternative to human breastmilk, infant formula is fortified with water- and fat-soluble vitamins, minerals and other functional ingredients to ensure compliance with nutritional requirements. As such, infant formula is highly regulated and requires accurate vitamin verification in the finished product. Quantitation of WSVs in infant formula is challenging due to their structural diversity, wide range of polarities, multiple vitamers and susceptibility to degradation. Variability in sensitivities among WSVs across detection techniques often requires separate methods to meet the different quantitation criteria specified for each B-vitamin in the AOAC standard method performance requirements (SMPRs). This work describes a combined sample preparation and LC-MS/MS method for the quantitation of 12 water-soluble vitamins (WSVs) in infant formula using the QTRAP 4500 system. Excellent instrument sensitivity was demonstrated by the sub-to-low limits of quantitation (in-vial LOQs, 0.1–10 ng/mL) achieved for most analytes in solvent standards, with average accuracies of 70–118% and

Poster-SA-P-11 — Development and Validation of an Analytical Method for Determination of Nitrosamines in Processed Meat Products Using QuEChERS based Extraction and analysis with Gas Chromatography-Tandem Mass Spectrometry (GC-MS/MS)

Dr. Manisha Dhanshetty, Technological University Dublin, Grangegorman, Dublin 7, Ireland

Nitrites, nitrates, and their salts such as sodium and potassium nitrate and nitrite which are classified as permitted food additives are commonly incorporated into processed meat products to enhance colour and flavour, extend shelf life, and reduce microbial contamination including the growth prevention of Clostridium botulinum. Regulatory authorities, such as European Union, establish and enforce limits on the use of sodium and potassium nitrates and nitrites in cured meat products \[Regulation (EC) 1333/2008\]. However, one of the major concerns regarding nitrites is their contribution to the formation of nitrosamines during the processing of meat products. These compounds are typically formed through the reaction of secondary amines with nitrosating agents such as nitrite, particularly under acidic conditions or during high-temperature processing. These N-nitrosamines are of significant concern in food safety due to their well-documented carcinogenic and mutagenic properties. Many nitrosamines, including include full name (NDMA), have been classified as probable human carcinogens by regulatory agencies. Considering these significant global food safety concerns, this project aims to reduce nitrate and nitrite levels, as well as nitrosamines, in meat and processed products. on the chemical analysis of nitrosamines. This study presents an optimised sample preparation workflow including the extraction of processed meat samples using a QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) based solid-phase extraction protocol and analysis using gas chromatography–tandem mass spectrometry (GC-MS/MS). The method was validated in a range of meat matrices, including bacon, meat rasher and salami. The optimized sample preparation involved extracting meat samples with acetonitrile, followed by QuEChERS salts ($MgSO_4$ and sodium acetate) and a freezing step at −20 °C to remove co-extractives. The extract was then cleaned using dispersive solid-phase extraction, evaporated, and directly analyzed by GC–MS/MS. This approach effectively reduced matrix interferences. Nitrosamines were analysed by GC–MS/MS within a runtime of 15 min. The optimal analytical approach was validated for three product categories in terms of linearity, matrix effects, accuracy, and precision. The limit of quantification (LOQ) was 0.01 mg/kg. The recoveries at LOQ and higher levels ranged between 70% and 120%, with precision-RSDs of \< 20%. Overall, the developed method provided a robust, reliable, and high-throughput analytical tool for the determination of nitrosamines in this complex food matrices- meat. This methodology can be effectively applied for routine surveillance and regulatory monitoring to ensure the safety and quality of food products, as well as to support risk assessment studies related to dietary exposure to nitrosamines.

Poster-SB-P-12 — Targeted quantitation of 28 antibiotics in honey

Holly Lee, SCIEX

Honey is a complex natural product containing bioactive compounds such as sugars, enzymes and proteins, organic acids and polyphenols. Many of these compounds are associated with honey's broad health benefits, including antioxidant, anti-inflammatory, antimicrobial and antiviral properties. However, the use of antibiotics in apiculture can lead to residue contamination in honey, posing potential health risks to consumers. Consequently, antibiotic use in beekeeping has been prohibited in several regions, including the European Union, under Commission Regulation EU 37/2010. Given these regulatory demands, selective and sensitive analytical methods for monitoring antibiotics in honey are needed. The European Union Reference Laboratories (EURL) updated the Minimum Method Performance Requirements (MMPRs) in 2020 for several antibiotic classes in food; however, api-products such as honey are excluded due to a zero-tolerance policy for antibiotic residues. This work features the analysis of 28 antibiotics in honey across seven classes using a simple dilution-based sample preparation procedure, achieving in-sample limits of quantitation (LOQs) of 0.5–10 ng/g without the use of any internal standards. Using the SCIEX QTRAP 4500 system, good quantitative performance was demonstrated in matrix-matched calibration standards with mean LOQ accuracies of 70-130% and mean LOQ precision mainly

Poster-SA-P-13 — Essential Experiments - Automating SPE Extraction of Challenging Oil Matrices for Multi-Residue Pesticide Analysis

Ally Fairman, NOW Foods

At NOW Foods, routine modified QuEChERS extraction for a wide range of botanical matrices supporting a 400+ pesticide panel has been successfully transitioned to a semi-automated workflow, significantly improving laboratory efficiency and sample throughput. However, highly complex, non-polar matrices such as essential oils have remained a critical gap, as they are not readily compatible with the current automated extraction approach. The primary challenge arises during the high-pressure drying step, which forces excess oil through SPE cartridges beyond their retention capacity. Attempts to remove this step without further optimization resulted in inconsistent matrix recovery following the initial extraction phase. While the established manual method remains reliable, it is time-intensive - particularly for preparing matrix-matched calibration curves with spiked samples required for both LC-MS and GC-MS analyses - highlighting the need for a robust automated alternative. This study presents a systematic investigation of key extraction parameters to enable semi-automated SPE cleanup of essential oil matrices. The work outlines observed limitations, experimental modifications, and optimized conditions that improve reproducibility and recovery, supporting the feasibility of automated preparation for multi-residue pesticide analysis in these challenging matrices.

Poster-SB-P-14 — Single-System LC–MS/MS Analysis of PFAS and Cyanotoxins: Evaluation of Method Performance and the Effects of Mobile Phase Additives

Tiffany Liden, Shimadzu Scientific Instruments

Per- and polyfluoroalkyl substances (PFAS) and cyanotoxins are regulated drinking water contaminants under the United States Environmental Protection Agency (EPA). Although EPA Method 533, EPA Method 544, and EPA Method 545 rely on LC–MS/MS, they are typically performed using separate systems. This study demonstrates an integrated LC–MS/MS workflow for simultaneous determination of 25 PFAS, six microcystins and nodularin, and cylindrospermopsin and anatoxin-a on a single Shimadzu LCMS-8060RX platform. PFAS were analyzed using negative electrospray ionization in a 15-minute method with an inline delay column to reduce background contamination. Cyanotoxins were measured in positive mode using 8-minute separations. Quantitation was performed by multiple reaction monitoring (MRM). Because PFAS analysis in negative ESI is sensitive to acidic residues, the impact of mobile phase additives was systematically evaluated. Continuous exposure to formic acid–containing mobile phases resulted in significant signal suppression for several PFAS, with compounds such as PFBA and 3:3 FTCA decreasing by up to 40%. Replacing formic acid with acetic acid minimizes PFAS negative mode ion suppression. These results demonstrate that formic acid is detrimental to PFAS analysis, while acetic acid provides a reliable alternative compatible with analyzing PFAS and cyanotoxin on one system. System robustness was assessed through 294 injections simulating frequent switching among Methods 533, 544, and 545. The sequence included calibration sets, continuing calibration checks, and mobile phase rinses between transitions. No carryover or sensitivity loss was observed. All analytes achieved R^2 \> 0.99 within their respective calibration ranges, with acceptable accuracy and precision. These results demonstrate a robust, single-platform solution for integrated PFAS and cyanotoxin analysis in drinking water.

Poster-SA-P-15 — Sensitive Quantification of a 1,000 Compounds in Single Run with a Novel Triple Quad Approach

Artem Filipenko, Bruker Scientific

Pesticides represent the most frequently analyzed hazardous compounds in food and feed. The analysis of an ever-increasing number of diverse pesticides in a single LC/MS run and the demand for higher sample throughput are key challenges. A rapid LC-TQ quantitative analysis method addressing both throughput and the high number of target pesticides is presented. For the evaluation of the analytical performance, the new method was optimized in a real scenario in common matrices for \> 700 pesticides in positive/negative mode with the focus on how the speed, number of compounds and other parameters influence

the sensitivity and robustness. UHPLC gradients with water (A) and methanol (B) (0.01% FA, 2 mM ammonium formate) at a 15-100% B gradient in 0.5-8min were used at a runtime of 9.2 min with subsequent 2.5 min equilibration. 2 uL sample were injected on an Intensity Solo 2.0 100x2.0 mm column at 45 ºC. A novel triple quadrupole was used in MRM Compound Based Scanning. With a scan time for each compound of 4-11 ms, the method accommodates \>1000 pesticides in fast polarity switching with ≥ 2 transitions in a single run. A probe temperature program reduced the impact for thermolabile compounds. A calibration curve containing 520 pesticides was prepared in pepper matrix (QuEChERS) with five calibration levels at 0.2-50 ppb. The analysis speed fits to generate a high number of data points for each peak to ensure accurate analysis. Statistics demonstrate even with different acquisition speeds and polarity switching a reproducibility of 2.6% within 10 consecutive injections. Calibration curves show R2 \>0.99 for 95% of the compounds with 765 pesticides in a single run with positive/negative switching. Due to the high instrument sensitivity, samples and standards can be diluted to reduce matrix effects, leading to less interference and use of one matrix to calibrate similar samples. Novel electronics and rapid polarity switching ensure consistent intensity and ion ratio regardless of the scan speed. All these parameters indicate robust and reliable screening and quantitation up to 1000 pesticides in a single run. Higher throughput, less maintenance and downtime can be achieved. Finally, 30 real samples prepared with the same extraction method were analyzed afterward to quantify the potential pesticides. Novel Aspect: Novel electronics, rapid polarity switching ensure stable intensity and ion ratios, enabling quantitation of up to 1000 analytes per run.

Poster-SB-P-16 — A NEW ULTRA-SENSITIVE TRAPPED-ION-MOBILITY-QTOF MS METHOD FOR THE ANALYSIS OF PESTICIDES IN FOOD EXTRACTS

Cory Lytle, Bruker Scientific

The maximum residue levels (MRL) permitted for pesticides and other chemical residues in food and feedstuffs are strictly controlled by national and international regulatory bodies. An important aspect of reducing pesticide exposure is monitoring their concentrations in food extracts. An ion-mobility QTOF is an ideal tool for this workflow due to its additional separation apabilities and the use of collisional cross section (CCS) to improve annotation reliability. In this study, we evaluate a novel, small-molecule-focused LC-TIMS QTOF platform (timsMetabo, Bruker) for pesticide screening. We investigated the impact of key instrument hardware and acquisition innovations on sensitivity and mass/mobility range, such as the Mobility Range Enhancement (MoRE) mode, a brighter ion beam, collision energy variation, and the Athena Ion Processor (AIP) system. MoRE utilizes the full length of the dual TIMS tunnel through ion accumulation and mobility separation in successive stages. This expands the effective mobility range per scan and increases ion throughput, particularly in the low m/z range. A glass capillary with a larger inner diameter increases the brightness of the ion beam compared to the previous timsTOF product line. The AIP, an additional RF/DC ion optics stage downstream of the collision cell, dynamically optimizes ion transfer to the TOF analyzer across the entire mass range, while the redesigned TIMS instrument increases ion capacity and transfer. To determine the limits of detection and quantification, orange and tomato QuEChERS extracts were spiked with a mixture of 240 pesticides in a dilution series from 0.1 – 100 ppb. An Elute+ SL UHPLC system (Bruker) equipped with an Intensity Solo 1.8 C18-2 column was coupled to a timsMetabo mass spectrometer (Bruker). The samples were analyzed with a 15 min gradient. Screening and quantification were performed using TASQ 2026B (Bruker) and a TargetScreener database containing 1156 pesticides, including retention times (RT), CCS values, and their fragments as qualification ions. The hardware innovations resulted in a 5 – 10-fold gain in sensitivity compared to previous (TIMS) QTOF MS. Ion mobility spectrometry can be used as an additional filter to obtain significantly purer chromatograms and spectra, even at trace levels in complex matrix. CCS as an additional criterion for pesticide identification helps to increase the reliability of identification and reduce false-positive results, even when using databases with more than 1150 compounds.

Poster-SA-P-17 — Simple direct injection method for analysis of Glyphosate and AMPA using Ion Chromatography coupled with Mass Spectrometry

Dr. Jayesh Gandhi, Metrohm USA

Glyphosate is a widely used, herbicide that kills most plants by blocking essential amino acid production such as enzyme 5-enolpyruvylshikimate-3-phosphate (EPSP) synthase, preventing plants from making necessary proteins for growth. Commercially available formulations contain surfactants and other additives which make agricultural applications easy. Most importantly, Glyphosate will decompose into AMPA due to exposure to sunlight. Both chemicals act like pseudo-amino acids for any living cell having carcinogenic properties. Several global regulatory methods of analysis (e.g.,USEPA Method 547) include extensive sample preparation (derivatization) and require LC-MS/MS instrumentation. Additionally, Glyphosate and AMPA can be analyzed using Pulsed Amperometric Detection (PAD); however, PAD detection is non-specific and prone to errors due to matrix effect. This poster presents a simple, sensitive direct injection method developed by Metrohm and Agilent Technologies for the analysis of glyphosate and AMPA in complex food matrices, including dry grains, raw nuts, and fresh vegetables. The method employs ion chromatography coupled with single quadruple mass spectrometry (IC-MS) for selective detection based on analyte mass-to-charge ratio. Method performance, including limits of detection (LOD) and quantification (LOQ) at the parts-per-billion (ppb) level will be discussed.

Poster-SB-P-18 — Multiresidue Pesticide Detection in Dried Cayenne Pepper: Demonstrating FDA's Analytical Capabilities Across GC-MS/MS, and LC-MS/MS Platforms

Caroline Mackay, Food and Drug Administration

The mission of the US Food and Drug Administration (FDA) is to promote and protect public health through the enforcement of the Federal Food, Drug and Cosmetic Act (FD\&C). Raw agricultural commodities, including spices and other dried foods, are subject to pesticide chemical tolerances and exemptions established by the Environmental Protection Agency (EPA), with enforcement responsibility delegated to FDA to serve the mission. FDA laboratories have developed a harmonized acetonitrile-based extraction method capable of detecting 800+ pesticide residues across multiple analytical platforms: GC-MS, GC-MS/MS, and LC-MS/MS. The method's versatility enables simultaneous screening, identification, and quantitation of pesticide residues. Two dried cayenne pepper samples were collected based on suspicion of adulteration. These two samples highlight the lab's capabilities to confirm multiple residues at once and to detect rarely encountered pesticides, like triflumuron in Sample A. Sample B contained 25+ pesticide residues, ten of which were actionable. Quantitative results for both samples were confirmed through standard addition, single-point calibration, and replicate analysis. These case studies exemplify FDA's analytical aptitude to protect consumers from unsafe pesticide residues in imported and domestic food commodities. The ability to detect rarely seen pesticides and multiple violations at once is a testament to the robustness and effectiveness of the methods used by FDA around the country.

Poster-SA-P-19 — A Student Capstone Project: Workflow-Based Untargeted LC–HRMS Analysis in Soil Extracts

Chiquita Price, Mississippi State Chemical Laboratory

Identification of unknown compounds in complex environmental matrices remains a significant analytical challenge, particularly when spectral library coverage is incomplete. This student capstone project investigated the application of liquid chromatography–high resolution tandem mass spectrometry (LC–HRMS) for the identification of compounds extracted from soil samples using the QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) extraction method. The study focused on developing a practical workflow for unknown identification using currently available laboratory resources, including Thermo Scientific Compound Discoverer, mzVault, and high-resolution MS/MS data interpretation as well as training students and applying these different laboratory techniques. Three students extracted soil samples using a modified QuEChERS procedure and extracts were then analyzed using a generalized LC–HRMS method with positive/negative polarity switching to maximize analyte coverage. Data were acquired in full-scan high-resolution mode with tandem MS fragmentation for structural characterization. Afterwards, using Compound Discoverer, feature detection, retention time alignment, adduct grouping, and molecular formula prediction were performed. Candidate structures were evaluated using accurate mass, isotope pattern distribution, fragmentation behavior, group area intensity counts, and spectral library comparison. Three compounds were successfully identified from the extracted soil matrix. Only one compound produced a confident match within the local mzVault spectral library; however, all three compounds were ultimately identified. This project demonstrated that meaningful compound identification can still be achieved in the absence of comprehensive library matches through a structured workflow emphasizing chemical structure interpretation and LC–HRMS evidence. This work also highlighted both the strengths and limitations of non-target LC–HRMS workflows in environmental analysis and demonstrates the practical value of Compound Discoverer-based unknown screening for laboratories with limited spectral library resources.

Poster-SB-P-20 — Interbrand Variability of SPE Cartridges and Its Impact on PFAS Analytical Performance

INGRID MARQUES, USDA-ARS

The growing demand for accurate and reliable PFAS data requires analytical methods that are not only robust but also critically validated under realistic laboratory conditions. Although multiple commercial SPE cartridges are commonly used in PFAS workflows, limited information is available regarding interbrand analytical variability and its potential impact on data comparability, reproducibility, and harmonization among laboratories. This study evaluated the analytical performance of six commercially available SPE cartridges for PFAS extraction under standardized experimental conditions. Experiments were conducted using Ottawa sand, an EPA reference matrix, fortified at 0.2 µg/kg with native and isotope-labeled PFAS compounds. Following extraction based on EPA Method 1633, cartridge performance was assessed under different storage conditions and holding times, including room temperature and refrigeration, with elution performed immediately after extraction (T0) and after 7, 14, and 28 days. Analyses were performed using LC-ESI-QOrbitrap-MS, within a strict QA/QC framework to ensure traceability and data integrity. In general, most cartridges showed acceptable recoveries, confirming satisfactory initial analytical performance. However, differences between brands became evident over time, with increasing variability in recovery profiles despite identical extraction procedures, matrix composition, and LC-HRMS conditions. Storage time and temperature influenced analytical performance for selected cartridges, with increased variability observed under prolonged storage conditions. Several cartridges maintained acceptable analytical precision, with relative standard deviations (RSDs) generally within common analytical acceptance criteria, while others exhibited increased variability under extended storage conditions. Distinct recovery behaviors were also observed between native and isotope-labeled compounds, suggesting that isotope dilution may not fully compensate for extraction-related variability associated with different SPE sorbents and storage

conditions. These findings highlight SPE cartridge selection and storage conditions as important factors influencing PFAS analytical reliability, reproducibility, and interlaboratory comparability. The study provides practical insight into cartridge robustness during storage and transport prior to LC-MS analysis and contributes to ongoing efforts toward harmonization and standardization of PFAS analytical workflows.

Poster-SA-P-21 — Cannabis Matrix Clean-up on GC-MS Pesticides Analysis

Rhiley Schmidt, Method Testing Laboratories

Cannabis is a highly complex matrix that spans from raw plant material to processed derivatives, this variability presents significant challenges for GCMS pesticide analysis. Having a high throughput of cannabis samples ran on the instrumentation can cause matrix accumulation which leads to increased maintenance and potential impacts to data quality. To combat these issues, effective sample clean up is critical while also maintaining accurate pesticides recovery. In this study, multiple different dispersive solid phase extraction (dSPE) products were evaluated and compared to a current in-house clean up procedure for cannabis flower. The efficiency of clean-up was assessed using gravimetric analysis and visual color evaluation. Top performing products were reassessed through a round of pesticide recovery studies to confirm that the pesticides required for testing were not lost throughout the extraction process. Results indicate there are optimized sorbent combinations that perform a more efficient matrix removal in comparison to the current in-house methodology. The evidence of this was seen in the decreased mass of the extract in the gravimetric analysis and the clearer extracted product seen visually. These findings support the use of optimized clean-up techniques to decrease accumulation of matrix on GC-MS systems used for cannabis pesticides analysis.

Poster-SB-P-22 — Quantitative and Qualitative Analysis of Pyrethroid Residues in Soy Based Choline Supplements Using LC MS/MS

Lihini Tharanga Mendis, Shimadzu Scientific Instruments

Consumer preference for plant-based nutraceuticals has increased significantly, leading to greater reliance on agricultural commodities such as soybeans for supplement production. Choline supplements derived from soy commonly utilize phosphatidylcholine as the active ingredient, which is extracted from soybean oil using nonpolar solvents. This lipid-based extraction process may promote co extraction and enrichment of lipophilic pesticide residues, including pyrethroids. Choline is a commonly used prenatal supplement, yet pyrethroids are known to impact reproductive systems. Pyrethroids are a class of synthetic insecticides with high octanol–water partition coefficients and are widely applied in crop protection. Due to their lipophilicity, these compounds may persist through processing and appear in finished dietary supplements. This study presents the development and application of an LC MS/MS method for detecting pyrethroid residues in soy-based choline supplements. Ten pyrethroids were analyzed using a LCMS 8045 RX triple quadrupole mass spectrometer operated in positive electrospray ionization mode. Chromatographic separation was achieved on a Shim-pack Velox Biphenyl (2.7µm, 2.1×100mm) column using a 15-minute gradient with ammonium formate–modified water and methanol mobile phases. Data were acquired in multiple reaction monitoring (MRM) mode, with transitions optimized based on signal intensity, reproducibility, and specificity. Sample preparation from commercial soy-based choline supplements optimized for lipid rich nutraceutical matrices with alternative solvent and cleanup strategies. Method optimization resulted in adequate chromatographic separation of all analytes and excellent calibration linearity (R^2 \> 0.99). The method demonstrated reliable sensitivity at low injection volumes (1 µL), enabling quantitative determination of pyrethroid residues in complex nutraceutical matrices. The results highlight the suitability of the LCMS for trace level pesticide residue analysis in soy derived supplements and support further application of this approach to other botanical and multivitamin formulations.

Poster-SA-P-23 — Comprehensive Analysis of Pesticide Residues with High-Resolution Mass Spectrometry

Raghvendra Sengar, Bruker Scientific

Pesticide residue analysis plays a critical role in ensuring the safety and quality of food, feed, and environmental samples. As global regulations become more stringent and the list of monitored pesticides continues to grow, methods that offer high sensitivity, selectivity, and the ability to detect a wide variety of chemical structures in complex matrices are required. Ultra High Performance Liquid Chromatography (UHPLC) coupled with high resolution Quadrupole Time-Of-Flight-Mass Spectrometry (QTOF-MS) has emerged as a key technology to meet these demands. QTOF-MS provides accurate mass measurements, with mass errors below 5 ppm. This allows to distinguish target pesticides from matrix interferences, even at trace levels. In this study, fruit samples were extracted following the QuEChERS procedure and analyzed using a multi-component UHPLC-QTOF-MS method for the detection of pesticide residues in food matrices (TargetScreener 2025, Bruker). Therefore, an Elute UHPLC system (Bruker) equipped with an Intensity Solo 1.8 C18-2 column was coupled to an impact II VIP mass spectrometer (Bruker). Data was acquired using the data-independent broadband collision induced dissociation (bbCID) acquisition mode and subsequently processed using the TASQ software together with the TargetScreener database. This database was recently extended and now contains the monoisotopic precursor ion mass, retention time, isotopic pattern and high resolution diagnostic qualifier ions for a total of 1156 pesticides and metabolites. In the analyzed samples up to 16 pesticides and metabolites were detected. Results were confirmed in accordance with the Sante Guideline which requires a mass accuracy below 5 ppm, a retention time deviation smaller than 0.1 min and at least one diagnostic qualifier ion. In

addition, the isotope pattern fit (mSigma) was used as criterion which has to be below 800. A blueberry sample was tested positive for Acetamiprid and its metabolite Acetamiprid IM-2-1 for which the maximum residue level was recently lowered in the EU due to the neurotoxicological effects. The fungicides Boscalid and Pyraclostrobin among their metabolites were detected in a red currant sample. Selected pesticides were also quantified using standard addition successfully demonstrating the quantitation capabilities of this method. The here presented TargetScreener workflow allows to analyze more than 1100 pesticides in a single run. Due to the use of data independent bbCID acquisition this number can be further increased simply by adding new pesticides or metabolites to the database.

Poster-SB-P-24 — Expanding PFAS Analysis from Legacy to Short-Chain Compounds Using LC-MS/MS

Naren Meruva, Waters Corporation

Regulatory PFAS methods such as EPA 533, 537.1, and 1633 have established robust workflows for a defined set of legacy per- and polyfluoroalkyl substances (PFAS); however, growing concern around short-chain, ultra-short-chain, and emerging PFAS highlights the need for broader analytical coverage and simplified sample preparation. This work demonstrates the performance of Waters™ LC-MS/MS solutions using direct-inject methodologies designed to expand PFAS scope while maintaining sensitivity, accuracy, and reproducibility across diverse sample matrices. Optimized chromatographic and mass spectrometric conditions enable reliable detection and quantitation of both regulated and emerging PFAS, including highly polar, early-eluting compounds that are challenging for conventional methods. Results show that direct injection significantly reduces sample preparation time and potential contamination while delivering low-ppt detection limits and robust method performance. These approaches provide laboratories with a flexible, future-ready PFAS analysis strategy that complements existing EPA methods and supports evolving regulatory and monitoring needs.

Poster-SA-P-25 — Increased Confidence in PFAS Detection and Identification in Complex Matrices with High Resolution Mass Spectrometry

Dimple Shah, Waters Corporation

The extensive use and persistent environmental presence of per- and polyfluoroalkyl substances (PFAS) have raised significant concern due to their potential adverse effects on human health. Current regulatory testing methods for PFAS like EPA methods 533 and 537 utilize an LC-MS/MS system and focus on a short list of legacy and emerging PFAS. As the testing for PFAS has expanded beyond drinking water to complex environmental and biological matrices, there is a greater chance of interference in the detection of PFAS with LC-MS/MS. Non-targeted analysis (NTA) with high-resolution mass spectrometry (HRMS) is a promising technique for the detection of known PFAS and identification of new PFAS. The high mass resolving power and excellent mass accuracy (<2ppm) on the Waters Xevo™ MRT mass spectrometer make it a powerful tool for NTA of PFAS in complex samples. As an example of this methodology, seafood samples that had been prepared for EPA method 1633 were analyzed by LC-HRMS.

The analysis of the seafood samples by LC-HRMS revealed three key advantages over traditional LC-MS/MS workflows: 1) greater confidence in identification of PFAS with a single MRM transition, 2) reduction of false positives in PFAS detection caused by interfering ions, and 3) the ability to identify PFAS that are not included in the targeted method. The first advantage of HRMS was demonstrated through the identification of perfluorobutanoic acid (PFBA) in a farm-raised shrimp sample. As PFBA lacks a secondary MRM transition for confirmation, the precise mass accuracy provided by HRMS offered the necessary extra specificity for confident identification. The second advantage - eliminating false positives - was demonstrated with a sample of canned clams. When this sample was analyzed by LC-MS/MS there was a peak detected in the trace for perfluorooctanesulfonic acid (PFOS) that could have corresponded to a branched isomer. Looking at the HRMS data for this sample, when an extracted mass chromatogram of PFOS was generated with a 5ppm mass window, there was no peak to indicate a possible branched isomer. Further investigation showed the signal originated from a lipid compound, not PFOS, highlighting HRMS's ability to distinguish true PFAS signals from background interference. Finally, HRMS enabled the discovery of previously unmonitored PFAS. By applying a data reduction techniques to isolate likely PFAS ions, a series of polyfluorocarboxylic acids with one H in the backbone were identified in the farm-raised shrimp sample – compounds not covered in standard LC-MS/MS methods. Together, these findings demonstrate the power and potential of LC-HRMS as a complimentary technique for PFAS testing in complex samples.

Poster-SB-P-26 — Modified QuEChERS extraction method for detection and quantification of wide range of pesticides and their metabolites in water samples using LC-QQQ mass spectrometry

Sara Moayedi, Ohio Department of Agriculture

Introduction: Toxic chemical contamination, including pesticides into waterways, is a safety concern for both humans and the environment. Many marine animals are sensitive to trace level toxic chemicals even at ppb levels in the environment. Because of this, development of efficient extraction methods capable of accurate detection and quantification is crucial. As a result, this study was conducted to reduce the detection limit of pesticide residues in water samples using modified QuEChERS extraction technique. Once validated, this method will be used for chemical monitoring in surface and groundwater sources in Ohio.

Method: Pure water samples were collected from Milli Q water equipment. These samples were spiked at three different levels including 1, 5, and 50 ppb with a mixture including 88 pesticides. Water samples were extracted using modified QuEChERS method with reduced solvent consumption and eliminated clean-up stage. The extracts were screened for 88 pesticides or their metabolites by LC-QQQ mass spectrometry. Instrument sensitivity was evaluated through measurement of limit of detection (LOD) and limit of quantification (LOQ). The latter is crucial for method development and validation. Results: The results on the extracted spiked samples showed limits of detection ranging from 0.5-50 ng/mL (ppb). 75% of pesticides had LOD of equal and less than 1 ppb. Of the 88 selected pesticides, 48 pesticides were detected with an LOD of 0.5 ppb, while 18 pesticides had LOD equal to 1 ppb. 13 out of 88 pesticides had LOD equal 5 ppb, 4 out of 88 pesticides had LOD equal to 10 ppb, and 5 out of 88 pesticides had LOD equal to 50 ppb. The LOD and LOQ were calculated based on signal to noise ratio (S/N \~ 3 and 10, respectively) compared to a blank sample, indicating high method sensitivity at low ppb levels for 75% of the pesticides. Calibration standards were prepared with concentrations ranging from 0.5-200 ppb, showing excellent linearity with a correlation coefficient (R^2) equal and greater than 0.995 in 86% of samples. High linearity between the analytes' concentration and their responses confirmed that this method of extraction is reliable for quantifying residues down to ppb levels. Also, high R^2 ensured the calculation of the unknown concentrations if they are within the range of calibration curve. The method showed that the retention times (RTs) are approximately consistent (except Etoxazole, Flubendiamide, and Propargite) with well-defined chromatographic peaks that indicate good selectivity and stability. Accuracy was evaluated through calculation of recovery % using spiked samples at multiple concentration levels. All samples showed good extraction efficiency with slightly matrix enhancement at low and high concentrations ensuring reliable quantification at trace levels. The qualifier ratio showed consistency of at least one secondary MRM ion transition, confirming the identity of the target analyte in the matrix. Conclusion: Overall, the modified QuEChERS extraction with the eliminated clean-up stage provided an accurate and sensitive approach for detecting and quantification of the contaminants at ppb levels among majority of samples ensuring suitability for analytical applications.

Poster-SA-P-27 — Comparative Evaluation of SPE Cartridge Performance for PFAS in Automated Workflows

Alexis Shelow, Restek

This study evaluates the performance of multiple solid-phase extraction (SPE) cartridge configurations for PFAS analysis across automated extraction platforms. Replicate blanks and low-level spikes were used to assess recovery, reproducibility, and background contributions under comparable method conditions, with additional consideration given to drying parameters. Observed trends highlight differences in analyte behavior across sorbent types, particularly for later-eluting compounds, as well as the influence of system-specific factors. These results provide practical insight for laboratories optimizing automated SPE workflows for PFAS.

Poster-SB-P-28 — Method Development and Validation for the Determination of Pyrrolizidine Alkaloids in Plant-Based Foods and Honey Using LC-MS/MS

Zeljka Popovic, Waters Corporation

Pyrrolizidine alkaloids (PAs) are naturally occurring toxic secondary metabolites produced by various plant species and are of increasing concern due to their presence in plant-based foods and honey. Chronic exposure to PAs has been associated with hepatotoxicity and potential carcinogenic effects, necessitating sensitive and reliable analytical methods for their determination across diverse food matrices. This study describes the development and validation of a robust liquid chromatography–tandem mass spectrometry (LC-MS/MS) method for the simultaneous determination of multiple PAs in a wide range of plant-based foods and honey. Sample preparation was optimized to ensure efficient extraction and cleanup across complex matrices, including herbal products, teas, and honey. A solid-phase extraction (SPE) protocol was employed to reduce matrix interferences and improve analyte recovery. Chromatographic separation was achieved using reversed-phase liquid chromatography, enabling effective resolution of structurally similar alkaloids and their N-oxide forms. Detection was performed using tandem mass spectrometry in multiple reaction monitoring (MRM) mode, providing high sensitivity and selectivity. The method was validated in accordance with established guidelines, demonstrating excellent linearity over a broad concentration range for all targeted analytes. Limits of quantification were sufficiently low to meet regulatory and monitoring requirements. Method precision and accuracy were assessed through repeatability and recovery studies, yielding consistent results across multiple matrices. Matrix effects were evaluated and effectively mitigated through the optimized sample preparation and calibration strategies. Application of the method to various commercially available plant-based food products and honey samples confirmed its suitability for routine analysis. The method successfully identified and quantified multiple PAs, highlighting the variability of contamination levels across different sample types. The use of SPE cleanup significantly reduced co-extracted interferences, improving overall method robustness and data quality. This validated LC-MS/MS method provides a reliable and sensitive approach for the determination of pyrrolizidine alkaloids in complex food matrices. Its applicability to a wide range of plant-based products and honey supports its use in food safety monitoring and regulatory compliance, contributing to improved risk assessment and consumer protection.

Poster-SA-P-29 — An alternative statistical approach for method development under EU regulation 2021/808

Katherine Weddell, Fera Science Limited

The EU regulation 2021/808 for the performance of analytical methods for residues of pharmacologically active substances used in food-producing animals specifies performance parameters that must be demonstrated by analytical methods to ensure the quality of monitoring programs. Due to the vast numbers of veterinary drugs and sample matrices, conventional re-validations to this new regulation is both time consuming and costly. Hence, we developed an alternative, more efficient, validation approach. The value of parameters that describe the relationship between added concentration and each of three quantities: mean measurement result, the uncertainty of the mean result, and within laboratory reproducibility standard deviation are directly estimated by a maximum likelihood fit of a statistical model to measurement results. Hence, the model provides estimates of trueness, relative standard deviation and measurement uncertainty at any concentrations of interest that are within the concentration range investigated. The decision limit for confirmation (CCα) and detection capability for screening (CCβ) are calculated from the estimates of measurement uncertainty at the concentration limit and screening threshold. This model was applied to two separate alternative approaches for validation, using different approaches to data generation. Our first approach used results gathered from spikes added to routine screening batches over the course of approximately one year, which is in contrast to the typical three-day validation regime specified in EU regulation 2021/808. The statistical model was fitted to the results to estimate the method performance parameters. Because this approach used data collected across a large number of analytical batches, carried out by many analysts under a variety of laboratory conditions, the estimates of method performance more accurately reflect routine laboratory use. This also provides ruggedness data, another requirement of EU regulation 2021/808. The estimates of performance given by these validations have been comparable to those gained via the conventional approach. Our second, and most recent, approach is to conduct targeted validation batches which include several species and where the spiking concentrations bracket the levels of interest, rather than those levels being spiked directly. The benefit of this spiking regime was to allow for multi-species validations, where regulatory limits may vary, because the method performance metrics can be calculated at any concentration within the range concentrations spiked. This workflow uses a minimum of three mixed species validations followed by a statistical assessment of whether species effects method performance. Where there is no statistically significant species effect, a single model fitted to the results from all species can be used to estimate the measurement performance (trueness, precision, uncertainty, CCα, CCβ) for each species. This work demonstrates that a statistical, maximum-likelihood–based validation framework can provide a robust and efficient alternative to conventional re-validation under EU Regulation 2021/808. By modelling trueness, precision, and measurement uncertainty as functions of concentration, method performance parameters can be reliably estimated across relevant concentration ranges without extensive, resource-intensive experiments.

Poster-SB-P-30 — Solving the Semicarbazide Problem – Towards a Unique Marker of Nitrofurazone Use in Meat

Bryn O. Shurmer, Canadian Food Inspection Agency

Accurate detection of nitrofuran residues in food of animal origin is essential for effective enforcement of bans on these veterinary drugs and for protection of public health. Nitrofurazone, a member of the nitrofuran class of antibiotics, was historically used to treat bacterial infections and promote growth in food producing animals but is now prohibited due to toxicological concerns. Following administration, nitrofurazone is rapidly metabolized in vivo, with its reactive metabolites forming covalent bonds with tissue proteins that persist for extended periods. Current regulatory monitoring relies on the detection of semicarbazide (SEM), released from these protein bound residues under harsh acid hydrolysis conditions. However, SEM may also originate from non-nitrofurazone sources, resulting in poor specificity, potential false positives, and reduced confidence in regulatory decision making. The analytical process is further limited by lengthy hydrolysis and derivatization steps. The objective of this work was to identify a specific and unambiguous marker of nitrofurazone exposure by characterizing protein bound metabolites and developing an alternative approach to SEM-based detection. Nitrofurazone metabolism was investigated in vitro using bovine liver S9 fractions and tissue homogenates, coupled with high resolution mass spectrometry. Both native and 13C15N3 labeled nitrofurazone were employed to support structural elucidation and confirm metabolite origin. Pseudo-incurred tissue samples containing protein bound nitrofurazone metabolites were successfully generated and used to evaluate deconjugation and protein substitution reactions aimed at liberating diagnostically informative residues. Mass spectrometric analysis revealed the formation of a previously unreported protein-bound nitrofurazone metabolite. This metabolite could be released from protein binding, forming a thiol conjugate detectable by LC–MS/MS. Isotopic labeling experiments confirmed the direct origin of the conjugate from nitrofurazone metabolism, supporting its specificity. Formation of the conjugate occurred rapidly under optimized conditions, representing a substantial reduction in sample preparation time compared with conventional SEM analysis. Preliminary stability studies indicate that the metabolite–thiol conjugate is sufficiently robust for targeted quantitative analysis. The identification of a specific metabolite conjugate provides a promising alternative to SEM as a definitive marker of nitrofurazone use in meat. This approach has the potential to improve analytical specificity, reduce false positives, accelerate residue analysis, and strengthen regulatory enforcement of nitrofurazone bans in animal derived foods.

Thank you for attending the 62nd Annual NACRW.

We hope to see you at the 63rd Annual NACRW in 2027 in San Antonio, Tx.

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