NACRW

NORTH AMERICAN
CHEMICAL RESIDUE WORKSHOP

60th Annual Conference

July 14-17, 2024

Marriott Harbor Beach Resort

Fort Lauderdale, Florida

www.nacrw.org

"Bringing Scientists Together to Develop and Validate Better Methodologies"

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Whether you are a commercial lab or a food manufacturer, the quality of your food testing data is paramount. From residue analysis and authenticity to allergens, cannabinoids, and PFAS testing, SCIEX solutions help you support consumer safety and ensure your product quality standards are met.

Visit us at Booth #16 to learn more

Join our vendor seminar on achieving next-level robustness for PFAS analysis in food
Tuesday, July 16 at 7:15 a.m in Grand Ballroom E

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Future Meeting Dates

2025 July 27-30
Francis Marion Hotel
Charleston, SC

Thank You

to all of our amazing volunteers!

Dear Attendees, Exhibitors, Sponsors and Guests:

Welcome to the 60th North American Chemical Residue Workshop (NACRW)! George Fong founded the precursor to NACRW, the Florida Pesticide Residue Workshop (FPRW) back in 1964. Over its many years of existence, FPRW, and subsequently NACRW, have had huge positive impacts on the professional careers of many and helped nurture numerous life-long friendships. The 2024 meeting celebrates the rich history of 60 years of the working, now covering all sorts of topics related to the analysis of all chemical residues and contaminants in food, feed, and environmental samples. Whether you are a long-time attendee or a first-time participant, we extend a warm greeting to all. We would like to express our sincere gratitude to our Exhibitors and Sponsors for their generous support, which has made this workshop possible while keeping registration fees affordable for attendees. NACRW has become a favorite event for many, are we look forwards to its fantastic technical sessions, interactive poster presentations, and relaxed, informal atmosphere.

We invite you to join us on Sunday, July 14th for the NACRW Veterinary Drugs Working Group meeting. There will also be a fascinating opportunity to be involved in an interactive workshop with Antony Williams from the US EPA on using the EPA Dashboards to support analysis of residues and contaminants. These sessions will feature interesting presentations and an open forum for discussions and questions.

Our Program Committee has put together a marvelous technical program for this year's workshop. It covers a wide range of topics, including advances in analytical technology, pesticide and vet drug residue analysis, toxins and contaminants including PFAS, validations, certifications and regulatory issues, difficult matrices, sampling and method improvements, deficiencies, and expansions. While most attendees are from North America, important international speakers are always included in the Technical Program, and this year we have folk from Europe and South America. Additionally, we have a forum on "Overcoming challenges in the lab - sharing the pain", where attendees can ask questions to the moderators and members of the audience – and hopefully get some answers… We encourage you to attend the poster sessions. The poster authors will be available at designated times to present their posters and talk to you about their work. This is a wonderful opportunity to interact with the authors and ask questions. We are pleased to offer student poster awards, sponsored by FLAG Works, Inc. and the ACS Journal of Agricultural and Food Chemistry. Students will be attending the workshop and will be available at their posters during designated times for a chat. Recipients of student scholarship awards will have the opportunity of presenting their work at a session on Wednesday. We also encourage attendees to visit our exhibitors throughout the workshop and their vendor sessions to learn more about the products and services they offer for all your testing needs.

I would like to express my deepest appreciation to the fantastic volunteers who have made this event a reality. To this year's NACRW Organizing Committee, Program Committee, especially Secretary Jana Hepner, Program Committee Co-Chairs Wendy Young and Wiley Hall, Poster Committee Co-Chairs Brian Eitzer and Susan Genauldi, Student Scholarship Awards Chair, Katie Carlos, and of course our Executive Director Teri Besse, it has been a joy working with you, and I am truly grateful for your patience, time, and dedication to the workshop. I also want to thank NACRW for providing me, a Brit, with the opportunity to be President for 2024; it has been an honor.

We invite you to make the most of your time at NACRW and enjoy all that sunny Florida has to offer. With its warm climate and beautiful beaches, it's the perfect backdrop to enhance your conference experience. Take some time to unwind, soak up the sun, and engage in thought-provoking discussions about residue and contaminant testing. We hope you have a fantastic time at NACRW and make lasting memories both inside and outside the conference venue.

Sincerely,

Simon Hird, 2024 NACRW Organizing Committee President
Wiley Hall and Wendy Young, 2024 NACRW Program Committee Co-Chairs

The George and Wilma Fong Founders Award

In Appreciation for Years of Leadership and Dedication to the
Florida Pesticide Residue Workshop and the North American Chemical Residue Workshop
by Volunteering so many hours that contributed to the Advancement of NACRW

Past Recipients

2011 George and Wilma Fong-Founders

2012 Gail Parker
2013 Pat Beckett
2014 Sherry Garris
2015 Jack Cochran
2016 Amy Brown
2017 Jo Marie Cook
2018 Julie Kowalski
2019 Steven Lehotay
2023 André de Kok

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Jana Hepner,Restek Corporation
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Mark Engel, FDACS
Wiley Hall, USDA-ARS-SJVASC
Holly Lee, SCIEX
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Sherri Turnipseed, US FDA ORA ADRC
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- Cutting-edge research presentations
- Networking with experts
- Interactive workshops

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Buenos Aires

May 4th – 8th, 2025

More information:
www.laprw.com
contacto@laprw.com

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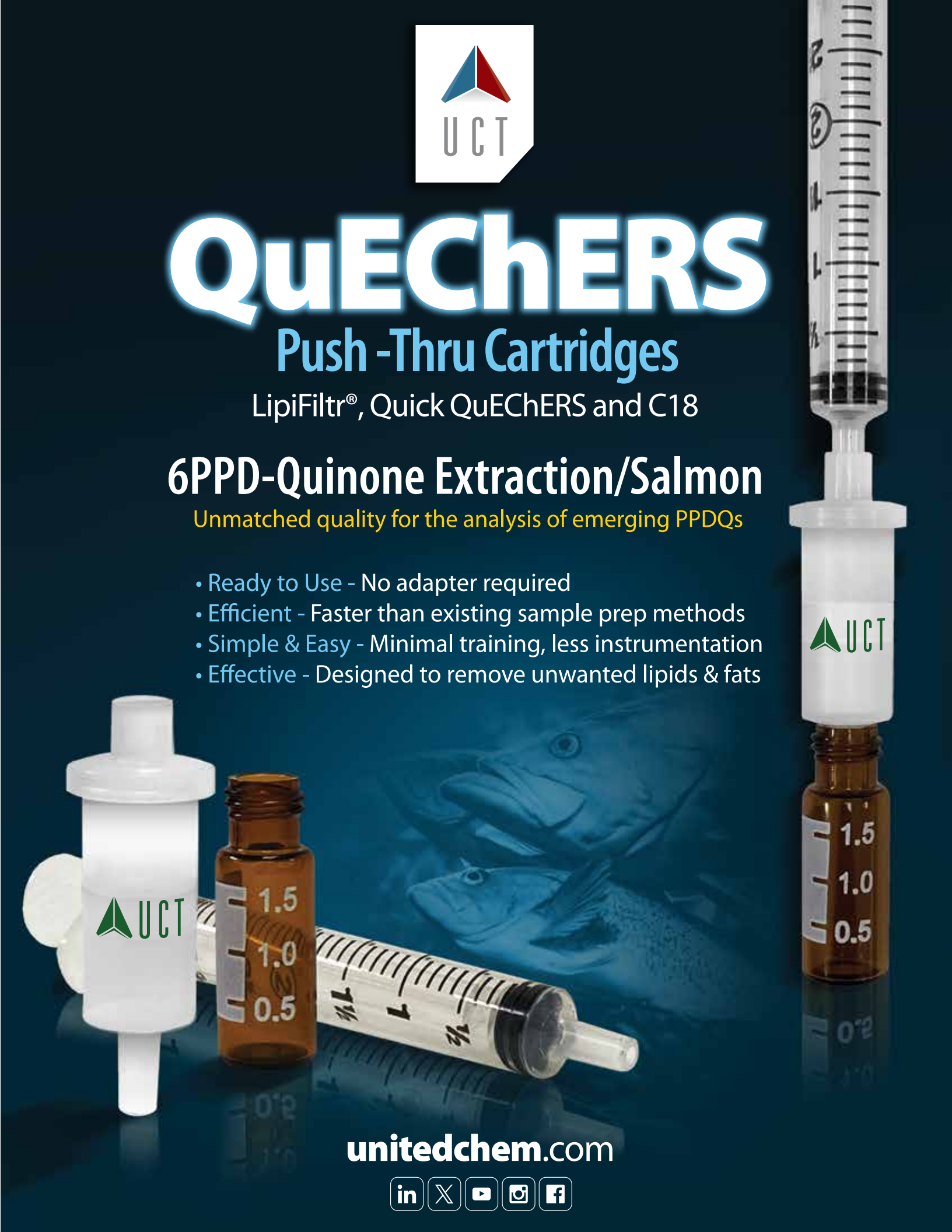

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GENERAL INFORMATION

Registration

Check in once at the registration desk at your earliest opportunity
Sunday - 1:00 pm – 6:00 pm
Monday - 7:30 am – 5:00 pm
Tuesday - 8:00 am – 4:00 pm
Wednesday - 7:45 am – Noon

KEY to Presentation Numbering System

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 (Exhibit Hall, Caribbean Ballroom, 1st level)

Hang posters Sunday afternoon from 3:00 pm to 6:00 pm or Monday morning from 7:00 am to 9:30 am.
Take down posters between 12 noon to 2:00 pm on Wednesday

Posters may be viewed any time Exhibition is open

Poster Session A (odd#) authors must be at their posters from 11:00 am – noon on Monday and 3:10 – 3:55 pm on Tuesday
Poster Session B (even#) authors must be at their posters from 3:10 pm – 3:40 pm on Monday and 11:00 – noon on Tuesday

Poster Prizes

Two poster prizes of $200 each will be awarded this year, and the same poster/author(s) are eligible to win both prizes. The People's Choice Poster Award will be determined by popular vote of attendees, and the Judges Choice Poster Award will be determined by the poster committee. The criteria used in each case will be importance of the study, quality of the science, and its presentation (including oral discussion and abstract). **Attendees must place their votes in the ballot box by noon on Wednesday.** ***Be sure to write your name on the back of your voting ticket for the chance to win a door prize.***

Exhibition (Caribbean Ballroom, 1st level)

Sunday: A welcome reception with light hors d'oeuvres and an open beer and wine bar will be held from 6:30 - 8:00 pm. If you would like to try the **"Strawberry OrbiRITA"** cocktail stop by the ***Thermo Fisher Scientific booth #10*** to get a ticket for a free drink.
Monday: 10 am - 1 pm and 2:30 pm - 4 pm
Tuesday: 10 am - 1 pm and 2:30 pm - 4 pm
Wednesday: 10 am - 12 noon

Coffee and Breaks

Coffee will be available each morning in the Caribbean Ballroom foyer (please refer to the times in the conference program). There will also be mid-morning and afternoon refreshment breaks each day. The Monday and Tuesday mid-morning and afternoon breaks, as well as the Wednesday mid-morning break, will be served in the Exhibition Hall (Caribbean Ballroom). On Wednesday afternoon, the break will be served in the Grand Ballroom foyer.

Announcements

Moderators will make general announcements from the podium. If you need to have an announcement made, please go to the conference registration desk or see the onsite audio-visual team in the meeting room, and give them your annoucement.

Mobile App

Thanks to the Platinum Sponsors we have a mobile app to view the program, see who is attending the meeting, and connect with them via the app. You should have received an email just prior to the conference with a link to download the app to your mobile phone along with a link that will automatically log you in.

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 door prize ticket. You must be present at each drawing to win.

Get to Know Your Sponsor

Participate in the "Get to Know Your Sponsor" quiz and win an Apple iPad tablet. A quiz will be provided to you in your registration bag. Simply take the quiz to each sponsor booth, get the right answer and the sponsor will place a sticker on your quiz. After you have completed the quiz, return it to the registration desk no later than Wednesday, July 17, at 1:30 pm. We will be announcing the winner Wednesday afternoon.

Submission of Manuscripts to *Journal of Agricultural and Food Chemistry*

Oral and Poster presenters are encouraged to contribute original research and/or review articles to the Journal of Agricultural and Food Chemistry for a special section related to the 2023 NACRW. Please inform **Teri Besse (teri@nacrw.org), by September 5, 2024,** if you intend to submit an article. Authors will then be invited by JAFC to submit their manuscripts electronically online through the JAFC website with a deadline of November 29, 2024.

Copies of Presentations

Oral Presentations: Following the meeting, as time and resources permit, oral presentations will be posted on our web site if author permission is granted. There are limitations to what we can post. Absolutely no files will be posted without a speaker's written permission (historically, two thirds of our speakers have given permission). The Power Point files are converted to PDF format. Various security restrictions may be added to the PDF file per speaker's request (such as disabling "copy text" and "print" functions). Some slides containing confidential or proprietary information may be deleted.

Poster Presentations: Drop your business card in the "reprint request" envelope available at each individual poster board. The author should mail/email you a reprint.

Meeting Website

www.NACRW.org - the website includes information on current and future NACRW meetings, as well as archives going back a few years.

Meeting Evaluations

Look for an on-line conference evaluation on the last day of the conference. The evaluation will be emailed to you, so please take a few moments to fill out the online form.

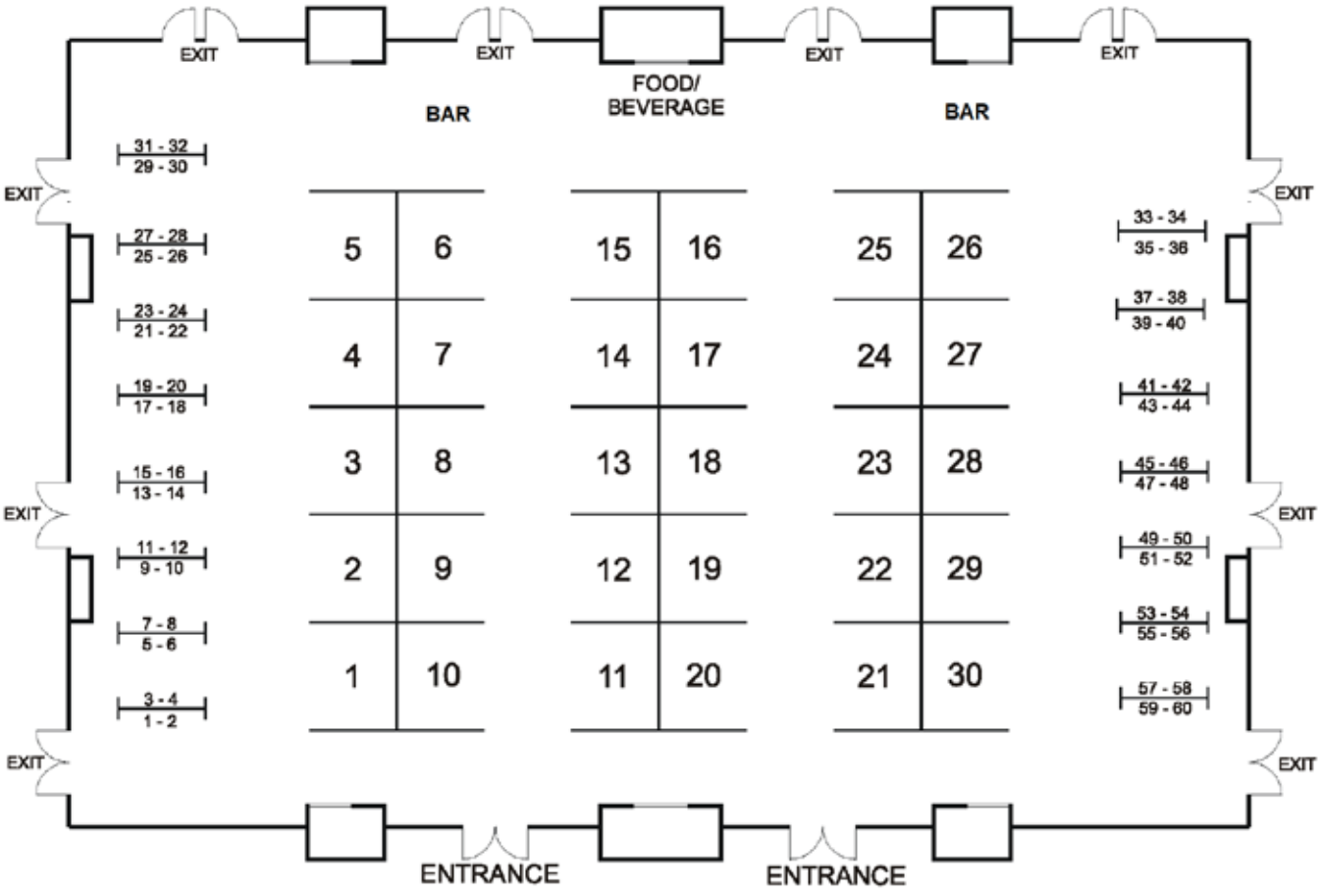
A BIG THANK YOU TO ALL OF OUR VOLUNTEERS, SPONSORS & EXHIBITORS!
The workshop would not be possible without your valuable assistance.

MARK YOUR CALENDAR FOR THE 2025 NACRW

July 27-30 Francis Marion Hotel, Charleston, South Carolina

EXHIBITION HALL
AND
POSTER SESSIONS

Location: Caribbean Ballroom, 1st Level



EXHIBITORS

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Lab Instruments Srl

Booth #2
ITSP Solutions, Inc.

Booth #6
Waters

Booth #8
Perkin Elmer

Booth #10
Thermo Fisher Scientific

Booth #11
Restek Corporation

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Milliporesigma

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Booth #21 and #22
LGC Standards

Booth #23
Providion US

Booth #25
Cambridge Isotope Laboratories

Booth #26
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VENDOR SEMINARS

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(PRE-REGISTRATION IS REQUIRED)

Please sign up at the meeting registration desk

V-1 Monday, July 15, 2024 7:15-8:15 am

Restek Corporation

Location: Grand Ballroom E, 3rd floor

Recent Developments in Emerging and Persistent Contaminants

Colton Myers**, R&D Manager, Sample Preparation, **Restek Corporation

PFAS, mycotoxins, pesticides, and many other compound classes continue to disrupt laboratory workflows due to their chemical nature and difficult matrices, which they persist in. High-throughput laboratories need clean and effective solutions to navigate these challenges, as methods continue to emerge targeting lower limits of detection. Improving areas such as background contamination, analyte behavior, and instrument up-time is critical for accurate quantitation and creating a safer world. These challenges can be mitigated through novel sample preparation and chromatographic products. To be presented are new advancements from the Restek laboratories that showcase innovative LC, GC and sample preparation solutions targeting these emerging compound classes and problematic matrices.

V-2 Monday, July 15, 2024 12:15-1:15 pm

Agilent Technologies

Location: Grand Ballroom E, 3rd floor

Solving Analytical Challenges for PFAS, Pesticides, Mycotoxins, Veterinary Drugs and Other Contaminants in Food

Dana Rothwein**, Technical Director, **IEH Analytical Laboratories
Kyle Heater**, Analytical Chemist 3, **OMIC USA Inc.
Lorna De Leoz**, Director, Global Food Market, **Agilent Technologies
Anastasia Andrianova, GC/MS Applications Scientist, ***Agilent Technologies***

Learn about streamlined workflows and best practices for the analysis of PFAS, patulin, vet drugs, and other contaminants in food. This lunch seminar includes presentations and a panel discussion.

V-3 Tuesday, July 16, 2024 7:15-8:15 am

SCIEX

Location: Grand Ballroom E, 3rd floor

Robustness defined: PFAS in food with the next-generation SCIEX 7500+ system

Holly Lee**, Food LCMS Scientist, Global Technical Marketing, **SCIEX

Residue analysis in food matrices is challenged by the presence of co-extractable compounds that can result in instrument contamination and subsequent system downtime. Come hear how the new SCIEX 7500+ system successfully achieved 6,400 injections of various food extracts under experimental conditions designed to get the system dirty! Performance for various PFAS compounds in salmon, avocado, spice powder and petfood will be presented.

V-4 Tuesday, July 16, 2024 12:15-1:15 pm

Thermo Fisher Scientific

Location: Grand Ballroom E, 3rd floor

From Innovation to Routine: Advances in Targeted and Non-targeted Mass Spectrometry Techniques for Food Control Laboratories

Part 1: High-end chromatography for more efficient mass spectrometry

Professor Amadeo Rodriguez Fernandez-Alba**, **EURL-FV – EU** Reference Laboratory for pesticide residues in Fruits and Vegetables, **University of Almería – Spain

Recent advances in liquid and ion chromatography instrumentation can significantly improve the efficiency and robustness of MS techniques in a routine pesticide residue laboratory. For example, dual-column chromatography with two columns in one LC connected to one MS can improve utilization of the MS time to improve throughput or be used to optimize sensitivity by allowing mobile phase combinations favoring either positive or negative ionization. Another common challenge is a robust and reliable analytical workflow for polar pesticides. An IC-MS/MS workflow was demonstrated for the validation of several food matrices with hundreds of injections, making it ideal for laboratories facing high sample volumes.

continued on next page

Part 2: Non-Targeted Approach for Authentication of Spices and Herbs using GC-Orbitrap MS technology

Ed George, *Vertical Marketing Manager, Environmental and Food Safety,* ***Thermo Fisher Scientific****, San Jose, CA*

Adulteration of spices typically refers to the practice of adding impurities or low-quality substances to spice products, with the intent to deceive consumers and maximize profits. A non-targeted GC-Orbitrap technology workflow using solid phase micro-extraction (SPME) arrow technology and a multivariate statistical analysis was developed to effectively profile intentionally adulterated oregano samples. The workflow includes extraction, deconvolution, and identification of unknown compounds using mass spectral libraries, PCI mode to confirm molecular ions, and additional MS/MS experiments to support the proposed formula.

You will learn:

How dual chromatography can be used routinely to improve productivity and sensitivity.

- How IC-MS/MS meets the challenge of polar pesticides analysis.
- How GC-Orbitrap's high resolution accurate mass system and easy-to-use software can pinpoint adulteration.

V-5 Wednesday, July 17, 2024 7:15-8:15 am

UCT, LLC

Location: Grand Ballroom A-D, 3rd floor

What You Might Not Know About Solid-Phase Extraction

Don Shelly**, Consultant, **UCT

Numerous papers have explored using C18 and HLB sorbents for extraction and purification. However, these papers often overlook a crucial detail - the origin of the sorbents. The manufacturing origin of these sorbents is crucial. This presentation will discuss the differences among C18 produced by 5 different manufacturers and highlight a few underutilized sorbents.

V-6 Wednesday, July 17, 2024 12 noon-1:00 pm

Waters Corp.

Location: Grand Ballroom A-D, 3rd floor

From Trace Quantitation to New Discoveries – A Day in the Life of a Waters MS Applications Scientist

Hosted by:** Narendra Meruva, PhD, MBA, Director, Americas Food & Environmental Markets, **Waters Corporation

Presenter**: **Gordon Fujimoto, PhD**, Chemical Analysis Group Leader, Americas Mass Spectrometry Applications Laboratory, **Waters Corporation

Food and environmental contaminants encompass a wide range of analytes, including pesticides, veterinary drugs, PFAS, mycotoxins, and the unknown. Scientists often specialize in specific contaminant classes or analytical techniques, and instrument vendors seek to collaborate with these experts to develop cutting-edge technologies and enhance laboratory capabilities. Successful partnerships require a shared understanding of industry challenges and opportunities… But who possesses extensive knowledge of both food and environmental matrices, hands-on experience with diverse contaminants and constituents, and deep expertise in trace analysis and discovery? Enter Waters Mass Spectrometry (MS) Applications Scientists! Often described as “jacks of all trades and masters of everything,” these MS Applications Scientists assist current and future collaborators by showcasing how the right analytical tools—whether it’s LC with routine tandem quadrupole MS or APGC with advanced HRMS—can address their specific laboratory needs. From analyzing cucumbers, fish, and water to studying botanicals and soil, no two days are alike for these scientists! Join us for lunch to learn about a day in the life of an MS Applications Scientist at Waters and discover how they contribute to scientific partnerships.

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Oral and Poster Presenters

(alphabetical order by Last Name)

Please note that oral and poster abstracts are available in the mobile app digital program.

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P-6	Carolina Cuchimaque	Florida International University
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P-2	Pushpa Deore	Vasantdada Sugar Institute, Pune
O-08	Luciana Teresa Dias Cappelini	Florida Internacional University
O-21	Amadeo Fernández-Alba	EURL-FV University of Almería
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O-06	Wiley Hall	USDA-ARS-SJVASC
P-14	Zeyu Han	Mérieux Nutrisciences
P-7	Courtney Heath	Florida International University
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P-32, P-33	Jacob Jalali	Perkinelmer
P-31	Kirk Jensen	JEOL USA, Inc
O-11, O-19	Anton Kaufmann	Official Food Control Authority of the Canton of Zurich
O-31, P-1	Lidija Kenjeric	Austrian Competence Centre for Feed and Food Quality, Safety and Innovation
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P-39, P-40	Holly Lee	SCIEX
P-5	Yuki Liang	University of Toronto
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P-4	Madison McMinn	Northeastern University

Please note that oral and poster abstracts are available in the mobile app digital program.

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O-23, P-18	Ederina Ninga	EURL-CF, National Food Institute, Technical University of Denmark
P-10	Joshua Ocheje	Florida International University
P-8	Olutobi Ogunbiyi	Florida International University
O-02	Julien Parinet	ANSES
P-19	Elsie Peprah	FDA CFSAN
P-3	Katherine Poisson	Northeastern University
P-20	Samanta Popol	U.S. Food and Drug Administration
P-30	Zeljka Popovic	GERSTEL Inc
O-01	Carsten Prasse	Johns Hopkins University
P-29	Taylor Prichard	Gerstel
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O-09	Alejandra Rodriguez Haralambides	Universidad De La Republica, Uruguay
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Keynote	Antony Williamson	U.S. Environmental Protection Agency
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P-24	Lawrence Zintek	US EPA R5

2024 - 60th ANNUAL NORTH AMERICAN CHEMICAL RESIDUE WORKSHOP

MEETING PROGRAM

Sunday, July 14, 2024

1:00-6:00 pm	**Registration**	**Caribbean Foyer**
1:00-5:00 pm	**Exhibitor set-up**	**Caribbean Ballroom**
3:00 - 6:00 pm	**Poster Board set-up**	**Caribbean Ballroom**
2:00-3:30 pm	**NACRW Veterinary Drugs Working Group**	**Grand Ballroom E**
2:00-2:25 pm **VDWG-01**	**Anton Kaufmann**, Official Food Control Authority of the Canton of Zürich, Zürich; Switzerland **Comparison of the Low versus High Resolution-based Confirmation Criteria for Veterinary Chemical Residues in Food Control**	
2:25-3:00 pm **VDWG-02**	Robin Kämpf and **Anton Kaufmann**, KLZH, Official Food Control Authority of the Canton of Zurich, Zürich, Switzerland; **Maïwenn Le Floch** and Eric Verdon, ANSES, the French Agency for Food, Environmental and Occupational Health & Safety, Laboratory of Fougeres; France; and **Alejandra Rodríguez Haralambides**, University of the Republic, Montevideo; Uruguay **Progress of the Veterinary Drug Residue Collaborative Study, 2023-2024 (Rounds 1 & 2)**	
3:00-3:15 pm **VDWG-03**	**Eric Verdon**, the French Agency for Food, Environmental and Occupational Health & Safety, Laboratory of Fougeres; France **News on the new EU Implementing Regulation for Analytical Methods Performance for the Veterinary Drug Residue Official Control in Food: CIR (EU) 2021/808**	
3:15-3:30 pm	**Open Forum** **Moderators:** **Jo Marie Cook**, Florida Department of Agriculture, FL, USA, retired; and **Eric Verdon**, The French Agency for Food, Environmental and Occupational Health & Safety, Laboratory of Fougeres; France	
3:30-4:00 pm	**Beverage Break**	**Grand Ballroom Foyer**
4:00-5:30 pm	**Workshop with Antony Williams US EPA** **A Hands-On Experience of Accessing Data from EPA Dashboards to Support Analysis of Pesticides, Veterinary Drug Residues, and other Chemicals in Food, Animal Feed, and Environmental Samples**	**Grand Ballroom E**
6:30 - 8:00 pm	**Welcome Reception (Exhibit Hall)**	**Caribbean Ballroom**

Monday, July 14, 2024

7:00 - 9:30 am	**Poster Board Set-up**	**Caribbean Ballroom**
7:15 - 8:15 am	**Restek Vendor Seminar** *(pre-registration required)*	**Grand Ballroom E**
7:30 am -5:00 pm	**Registration**	**Caribbean Foyer**
7:45- 8:15 am	**Early Morning Coffee**	**Caribbean Foyer**
8:20-8:45 am	**Opening Remarks - NACRW 2024**	**Grand Ballroom F-K**
8:20-8:30 am	**Sherry Garris, Chair, FLAG Works, Inc. Board of Directors**	
8:30-8:35 am	**Simon Hird, 2024 NACRW President**	
8:35-8:40 am	**Wiley Hall and Wendy Young, 2024 NACRW Program Co-Chairs**	

8:40 - 10:45 am	**SESSION 1:** *sponsored by* SCIEX **Progress and Advances in Analytical Technology, Cheminformatics, Monitoring, and Risk Assessment for Hazardous Chemicals in the Environment and Food Supply** **Co-Chairs: Jian Wang and Brian Ng**	**Grand Ballroom F-K**
8:40-8:45 am	**Session Sponsorship – SCIEX**	
8:45-9:40 am **Keynote Speaker**	**Antony Williams**, US EPA, Durham, NC, USA **Accessing Data to Support Pesticide Residue and Emerging Contaminant Analysis from US-EPA Online Dashboards**	
9:45-10:10 am **O-01**	**Carsten Prasse,** Johns Hopkins University, Baltimore, MD, USA **Combining non-targeted analysis with computer-based hazard comparison approaches to support prioritization of unregulated organic contaminants in environmental media**	
10:15-10:45 am **O-02**	**Julien Parinet,** ANSES, Montreuil, France **Strengths & weaknesses to reanalyze by QuEChERS-LC-HRMS/MS (targeted and suspected approaches) a selection of total diet study samples analyzed ten years ago by various LC-MS/MS methods**	
10:45 - noon	**Break - Exhibition and Poster Opening**	**Caribbean Ballroom**
11:00 am - noon	**Poster Session A (authors present for odd #s)**	**Caribbean Ballroom**
12 noon	**Lunch on your own**	
12:15 - 1:15 pm	**Agilent Technologies Vendor Seminar** *(pre-registration required)*	**Grand Ballroom E**
1:30 - 3:10 pm	**SESSION 2:** **Non-Pesticide Residues** **Co-Chairs: Eric Verdon and Jessica Krank**	**Grand Ballroom F-K**
1:30-1:50 pm **O-03**	**Dr. Simon Hird**, Waters Corporation, Wimslow, Cheshire, UK **Determination of nitrofuran metabolites, including nifursol, in shrimp and fish by UPLC-MS/MS: in-house method validation according to Commission Implementing Regulation (EU) 2021/808**	
1:50-2:10 pm **O-04**	**Dr. Jana Hepner,** Restek Corporation, Bellefonte, PA, USA **Exploration of new Low-Pressure GC columns for food and environment emerging contaminants**	
2:10-2:30 pm **O-05**	**Frank Kero,** Bruker, Billerica, MA, USA **A novel approach for monitoring multi-classes of POPs in a single run by GC-Ion Mobility-HRMS**	
2:30-2:50 pm **O-06**	**Dr. Wiley Hall**, US Department of Agriculture, Agricultural Research Service, Parlier, CA, USA **Considerations and Progress in Developing Multiresidue Analysis Methods for the Inorganic Residues of Postharvest and Preplant Fumigants**	
2:50-3:10 pm	**Q & A**	

3:10-3:40 pm	**BREAK- Exhibition & Posters** **Poster Session B** ***(authors present for even #s)***	**Caribbean Ballroom**
3:40-5:00 pm	**SESSION 3:** **Validations, Certifications and Regulatory Issues** **Co-Chairs: Julia Coppin and Kate Mastovska**	**Grand Ballroom F-K**
3:40-4:00 pm **O-07**	**Spencer Walse**, US Department of Agriculture, Agricultural Research Service, Parlier, CA, USA **Regulatory Challenges to the Use of Postharvest Fumigants in the Global Trade of Agricultural Commodities**	
4:00-4:20 pm **O-08**	**Luciana Teresa Dias Cappelini,** Florida International University, North Miami, FL, USA **Occurrence and distribution of emerging contaminants on children's food in Miami-Dade – FL**	
4:20-4:40 pm **O-09**	**Alejandra Rodriguez-Haralambides**, Facultad de Química-IPTP, Universidad de la República-Uruguay, Pando, Canelones, Uruguay **Mapping of Mycotoxins Profiles in Wheat Production Regions of Uruguay**	
4:40-5:00 pm **O-10**	**Thomas Day,** US Food and Drug Administration, Bothell, WA, USA **Detection of C. thevetia Cardiac Glycosides Adulteration in Dietary Supplements utilizing Untargeted High Resolution Mass Spectrometry**	
6:30-9:00 pm	**SOCIAL EVENT (Dinner) – Marriott Harbor Beach**	**Grand Ballroom A-E**

Tuesday, July 16, 2024

7:15-8:15 am	**SCIEX Vendor Seminar** *(pre-registration required)*	**Grand Ballroom E**
8:00 am - 4:00 pm	**Registration**	**Caribbean Foyer**
8:00 am – 8:30 am	**Early Morning Coffee**	**Caribbean Foyer**
8:45 - 10:45 am	**SESSION 4:** ***sponsored by*** Agilent **Residue Analysis in Difficult Matrices** **Co-Chairs: Holly Lee and Julie Brunkhorst**	**Grand Ballroom F-K**
8:45-8:50 am	**Session Sponsorship - Agilent Technologies**	
8:50-9:10 am **O-11**	**Anton Kaufmann,** Official Food Control Authority of the Canton of Zurich, Zurich, Switzerland **Good Chromatography – A Sometimes Neglected Aspect of Modern Multiresidues Methods**	
9:10-9:30 am **O-12**	**Benedict Liu**, CEM Corporation, Matthews, NC, USA **Automated Solvent Extraction Method of PFAS From Difficult Food and Environmental Matrices**	
9:30-9:50 am **O-13**	**Jerry Mueller,** NOW Health Group, Bloomingdale, IL, USA **Effective Sample Preparation for LC-MS and GC-MS Multi-Pesticide Residue Analysis in Essential Oils Using Novel Passthrough Cleanup**	

9:50-10:10 am **O-14**	**Zhihong Wang**, NOAA/NOS National Centers for Coastal Ocean Science, Charleston, SC, USA **Determination of Microcystins and Nodularins in Ambient Freshwater and Seawater by LC-MS**	
10:10-10:30 pm **O-15**	**Kaitlyn Nobles**, Trilogy Analytical Laboratory, Washington, MO, USA **Quantitative Analysis for the Adsorption and Desorption Capabilities of Mycotoxin Deactivators Containing Multiple Biogenic Amines by LC-MS/MS**	
10:30-10:50 am **O-16**	**Shweta Gupta**, ImagoAI, Inc., Milpitas, CA, USA **Quantification of Mycotoxin Levels in Grains Utilizing Hyperspectral Imaging and Artificial Intelligence**	
10:50 am-noon	**Break - Exhibition and Posters**	**Caribbean Ballroom**
11:00-noon	**Poster Session B** ***(authors present for even #s)***	**Caribbean Ballroom**
12 noon	**Lunch on your own**	
12:15-1:15 pm	**Thermo Fisher Scientific Vendor Seminar** *(pre-registration required)*	**Grand Ballroom A-D**
1:30-3:10 pm	**SESSION 5:** ***sponsored by*** ThermoFisher SCIENTIFIC **PFAS Contamination: Looking Beyond Environmental Matrices** **Co-Chairs: Matt Noestheden and Elsie Peprah**	**Grand Ballroom F-K**
1:30-1:35 pm	**Session Sponsorship – Thermo Fisher Scientific**	
1:35-2:00 pm **O-17**	**Amy Rand,** Carleton University, Ottawa, Ontario, Canada **PFAS analysis in house dust across socioeconomic factors using targeted LC-MS/MS and total fluorine approaches**	
2:00-2:25 pm **O-18**	**Ming Gao**, Meriuex/Silliker, Crete, IL, USA **Detection and Quantitation of PFAS Substances in food and packaging with LC-MS/MS**	
2:25-2:50 pm **O-19**	**Anton Kaufmann,** Official Food Control Authority of the Canton of Zurich, Zurich, Switzerland **Fast and easy nontargeted detection of PFAS in complex food matrices**	
2:50-3:15 pm **O-20**	**Thomas Simones**, Maine CDC, Augusta, ME, USA **PFAS Contamination in Agricultural Settings and Assessment of Human Exposure Pathways through Food Products**	
3:15-3:55 pm	**BREAK- Exhibition & Posters** **Poster Session A** ***(authors present for odd #s)***	**Caribbean Ballroom**
4:00-5:00 pm	**SESSION 6:** **FORUM: Overcoming challenges in the lab - sharing the pain** **Moderators: Kendra Adams and Simon Hird**	**Grand Ballroom F-K**
5:05-6:00 pm	**NACRW Organizing Committee Meeting** *open to all attendees*	**Caribbean Ballroom**

Wednesday, July 17, 2024

7:15-8:15 am	UCT, LLC Vendor Seminar *(pre-registration required)*	Grand Ballroom E
7:45 am-noon	Registration	Caribbean Foyer
7:45-8:15 am	Early Morning Coffee	Caribbean Foyer
8:30-10:05 am	SESSION 7: *sponsored by* RESTEK Sampling: Collection, Preparation, and Statistics Co-Chairs: Jana Hepner and Don Shelley	Grand Ballroom F-K
8:30-8:35 am	Session Sponsorship – Restek Corporation	
8:35-8:55 am O-21	**Amadeo Fernández-Alba,** EURL-FV University of Almería, La Cañada de San Urbano, Almería, Spain **Advancements in Miniaturization and Automation for Eco-Friendly Analytical Methods in Pesticide Residue Evaluation in Food**	
8:55-9:15 am O-22	**Alexis Shelow**, Restek, Bellefonte, PA, USA **Reduced Instrument Downtime for Organochlorine Pesticide Analysis by Using an Optimized SPE Cartridge for Sample Extract Cleanup**	
9:15-9:35 am O-23	**Ederina Ninga,** EURL-CF, National Food Institute, Technical University of Denmark, Lyngby, Denmark **Optimization and validation of new sorbents combination in micro solid phase extraction cartridges for the analysis of pesticides in cereals**	
9:35-9:55 am O-24	**Volker Bornemann**, Avazyme, Inc., Durham, NC, USA **New, fully automated analytical method for accurate, extended PFAS screen in water, beverages, and food**	
10:00-10:45 am	Student Scholarship Award Presentations	Caribbean Ballroom
10:45-noon	BREAK (Exhibition & Posters)	Caribbean Ballroom
12:00-1:00 pm	Waters Corp. Vendor Seminar *(pre-registration required)*	Grand Ballroom E
1:05-2:45 pm	SESSION 8: Pesticides: Method Improvements, Deficiencies and Expansions Co-Chairs: Ken Kise and Kyle Heater	Grand Ballroom F-K
1:05-1:25 pm O-25	**Jian Wang,** Canadian Food Inspection Agency, Calgary, Alberta, Canada **Application of nDATA Work Flow for Semi-Quantitative Screening of 1094 Pesticide Residues in Fruits and Vegetables using UHPLC/ESI Q-Orbitrap Full MS/vDIA**	
1:25-1:45 pm O-26	**Greg Mercer,** US Food and Drug Administration, Bothell, WA, USA **Keeping a Regulatory Pesticide Monitoring Program Current: Extension of 38 Analytes to the FDA Harmonized Pesticide Method**	
1:45-2:05 pm O-27	**Leah Ritter**, Bayer, Chesterfield, MO, USA **Residues of Glyphosate in Food and Dietary Exposure**	

2:05-2:25 pm **Anastasia Andrianova**, Agilent Technologies, Wilmington, DE, USA
O-28 **A High-Efficiency Approach to Quantitating 246 Pesticides in Black Tea with GC/MS/MS using a New Electron Ionization (EI) Source for Maximized Uptime**

2:25-2:45 pm **Jon Wong**, US Food and Drug Administration, College Park, MD, USA
O-29 **Evaluation of Complex Food Matrices for Multiresidue Pesticide Analysis using QuEChERS Modificatins and GC- and LC-MS/MS**

2:45-3:15 pm **BREAK** **Grand Ballroom Foyer**

3:15-4:55 pm **SESSION 9:** **Grand Ballroom F-K**
Toxins in Agriculture and Food Safety
Co-Chairs: Kai Zhang and Lukas Vaclavik

3:15-3:40 pm **Hans Mol**, Wageningen Food Safety Research, Wageningen, The Netherlands
O-30 **Mycotoxins: Measuring Body Fluids versus Food to Assess Dietary Exposure**

3:40-4:05 pm **Lidija Kenjeric,** Austrian Competence Centre for Feed and Food Quality,Safety and Innovation FFoQSI GmbH, Tulln an der Donau, Austria
O-31 **Exploring Mass Spectrometer Limits: UHPLC-MS/MS Method for Determination of 1,000 Toxins in 10 Minutes**

4:05-4:30 pm **Krista Thomas,** National Research Council Canada, Halifax, NS, Canada
O-32 **Multi-Class Analysis of Cyanobacterial Toxins using Hydrophilic Interaction Liquid Chromatography–Mass Spectrometry**

4:30-4:55 pm **Jacolin Murray**, National Institute of Standards and Technology, Gaithersburg, MD, USA
O-33 **Development of a Mycotoxin in Animal Feed Reference Material**

4:55-5:10 pm **Poster Awards and Closing** **Grand Ballroom F-K**

5:10 pm **Adjourn**

ORAL PRESENTATION ABSTRACTS

O-Keynote

Accessing Data to Support Pesticide Residue and Emerging Contaminant Analysis from US-EPA Online Dashboards

Antony J Williams, Center for Computational Toxicology and Exposure, U.S. Environmental Protection Agency

In recent years, the growth of scientific data and the increasing need for data sharing and collaboration in the field of environmental chemistry has led to the creation of various software and databases that facilitate research and development into the safety and toxicity of chemicals. The US-EPA Center for Computational Toxicology and Exposure has been developing software and databases that serve the chemistry community for many years. This presentation will focus on several web-based software applications which have been developed at the USEPA and made available to the community. While the primary software application from the Center is the CompTox Chemicals Dashboard which provides access to data for >1.2 million chemicals (https://comptox.epa.gov/dashboard), almost a dozen proof-of-concept applications have been built serving various capabilities. The publicly accessible proof-of-concept Cheminformatics Modules (https://www.epa.gov/chemicalresearch/cheminformatics) provides access to multiple applications in development allowing for hazard comparison for sets of chemicals, structure-substructure-similarity searching, structure alerts and batch QSAR prediction of both physicochemical and toxicity endpoints. A number of other applications, presently in development but not publicly accessible will also be discussed. These include AMOS, the database of Analytical Methods and Open Spectra.

Analytical methods can vary in nature from detailed regulatory methods to more summary in nature. Regulatory method documents can include details of analytes which can be studied, supported matrices, reagents, methodological details, statistical performance, interlaboratory validation and other details. Summary methods provide a general overview of reagents, instrumentation and commonly a short list of analytes. Regulatory bodies including the US Environmental Protection Agency (US-EPA), US Geological Survey (USGS), US Department of Agriculture (USDA) and others provide detailed analytical methods and collections of summary methods from the agrochemical industry, such as the US-EPA Environmental Chemistry Methods (https://www.epa.gov/pesticide-analytical-methods/environmental-chemistry-methods-ecm). Instrument vendors also provide access to many hundreds of application notes which can be considered as summary methods. AMOS presently contains >4,500 methods integrated to their chemical structures and > 230,000 public domain mass spectral data. AMOS allows for filtering of methods based on analyte, chemical class, method source and other related metadata. AMOS is an important facet of the developing Non-Targeted Analysis WebApp presently also in development at the EPA.

This presentation will provide an overview of existing publicly accessible Dashboards and work in progress to support analysis of pesticides, veterinary drug residues, and other chemicals in food, animal feed, and environmental samples.

This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

O-01

Combining non-targeted analysis with computer-based hazard comparison approaches to support prioritization of unregulated organic contaminants in environmental media

Carsten Prasse,[1] Christopher L. Brueck,[1] Matthew N. Newmeyer,[1] Sara N. Lupolt,[1] Qinfan Lyu,[1] Jon Sobus,[2] Antony J. Williams,[2] Keeve E. Nachman;[1]

[1]**Johns Hopkins University,** Department of Environmental Health and Engineering, 2400 N Charles St, Baltimore, MD 21218, USA; cprasse1@jhu.edu; [2]U.S. Environmental Protection Agency, Center for Computational Toxicology and Exposure, Office of Research and Development

Assessing and addressing the risks associated with the exposure to anthropogenic organic compounds is challenging considering the ever-increasing number of chemicals that are produced and emitted into the environment. In addition, many of these chemicals are likely to degrade after their release into the environment, leading to the formation of transformation products for which even less information about potential health risks is available. Advanced analytical approaches, in particular high-resolution mass spectrometry (HRMS), have substantially increased our ability to characterize these complex mixtures. However, a major challenge that remains is determining which compounds need further risk characterization to identify chemicals of highest human

or environmental health concern. To address this challenge, this talk will discuss the combined application of HRMS-based target and non-target analysis (NTA) and risk and hazard assessment approaches to determine the risks and hazards associated with the exposure to known and unknown organic contaminants, respectively. This will be illustrated using two case studies, the first focusing on the presence and human hazards associated with pesticides and other anthropogenic chemicals identified in kale and the second focusing on the identification and prioritization of organic contaminants in biosolids used as agricultural fertilizer. For kale, hazards of detected pesticides were assessed using nationally representative estimates of kale consumption across life stages in the US whereas the US-EPA's Cheminformatics Hazard Module was used for hazard assessment of nontarget compounds in both kale and biosolids samples.
This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

O-02

Strengths & weaknesses to reanalyze by QuEChERS-LC-HRMS/MS (targeted and suspected approaches) a selection of total diet study samples analyzed ten years ago by various LC-MS/MS methods

Julien Parinet[1], Léna Provost[2], Yassine Makni[1], Véronique Sirot[2]

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Food is one of the key components of our external chemical exposome (Wild, 2012). The exposome being all the factors influencing our health. Indeed, foodstuffs are subject to different types of contamination from field to fork. Against this backdrop, the French Agency for Food, Environmental and Occupational Health & Safety (ANSES) mission is to assess diet-related health risks by characterising consumer exposure to substances present in food. To achieve this, ANSES can rely on total diet studies (TDS) which are studies carried out to assess the dietary exposure of populations to substances of public health interest. TDSs are based on standardized method recommended by European and international organizations (WHO, FAO, EFSA). The aim of the present work was therefore to use liquid chromatography hyphenated to a high resolution mass spectrometer (LC-HRMS), here a QTOF, to analyze a selection of samples from two previous French total diet studies. To this end, we have implemented targeted and suspected approaches to search for the presence of contaminants that had not been prioritized at the time TDS was carried out, over ten years ago. Through this study, we aim to highlight the potential benefits of using HRMS and the associated targeted and suspected approaches to be able to broaden the spectrum of contaminants usually sought by more conventional (targeted) approaches employing low resolution. But we also want to confront the difficulties of such analyses after such a long sample retention period, and draw any necessary lessons for future TDSs.

O-03

Determination of nitrofuran metabolites, including nifursol, in shrimp and fish by UPLC-MS/MS: in-house method validation according to Commission Implementing Regulation (EU) 2021/808

Simon Hird,[1] Anoop Krishnan,[2] Venkateswarlu Thelukutla,[2] Anoop Sengar,[2] Archa Vijayan,[2] Sisira Raveendran,[2] Praveen Malekadi,[2] Ravi Shanker,[2] Saskia Sterk,[3] and J. S. Reddy;[4]

[1]**Waters Corporation**, Wilmslow, SK9 4AX, UK; simon_hird@waters.com; [2]Export Inspection Agency-Kochi, Kochi, India; [3]Wageningen Food Safety Research, Wageningen, Netherlands; [4]Export Inspection Council, New Delhi, India

Nitrofurans are broad-spectrum antibiotics that have been widely used in aquaculture to treat disease. Despite being banned in many countries, nitrofurans are still used illegally due to their known effectiveness, low cost, and easy availability. India maintains a national residue monitoring plan and mandatory pre-harvest and pre-export testing programs for aquaculture products intended for the EU market. Veterinary drug residue testing in India must comply with analytical performance and validation requirements set out in Commission Implementing Regulation (EU) 2021/808. The fact that the number of Rapid Alert System for Food and Feed (RASFF) notifications for banned substances in Indian aquaculture products remains low reflects the effectiveness of this testing in preventing the export of non-compliant consignments to the EU.

This presentation will describe the context for veterinary drug testing in India and focus on the development and validation of a method for the determination of nitrofuran metabolites in farmed shrimp and fish. The method was successfully validated in shrimp and fish. The following parameters were assessed: specificity, identification criteria, linearity, matrix effects, trueness, repeatability, within lab reproducibility, the Decision Limit (CCa), and ruggedness. The trueness of the method was determined to be within the

range of 83-118 %, repeatability ≤14% RSD_r, and within lab reproducibility ≤17% RSD_{WR}. The values for CCa (0.32–0.36 µg/kg) were all less than the reference point for action (RPA) of 0.5 µg/kg. The results from this validation showed the method to be suitable for pre-export testing to check compliance with EU regulations.

O-04

Exploration of new Low-Pressure GC columns for food and environment emerging contaminants

Jana Hepner,[1] Whitney Dudek-Salisbury;[1] and Chris English[1]

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The Low-Pressure GC (LPGC technique) has been successfully used in the past for pesticide residues' analysis. However, the technique is very versatile, and it allows for other applications, especially if different column phases are used. So far, the majority of the applications have been using the "5"-type phase (95% dimethylpolysiloxane, 5% diphenyl polymer). To expand on the previous applications, four additional column phases were selected (cyanopropylphenyl dimethylpolysiloxane; 50% dimethylsiloxane, 50% diphenyl; 65% dimethylsiloxane, 35% diphenyl; and trifluoropropylmethyl polysiloxane phases) to analyze various food and environmental contaminants, such as nitrosamines, alkylfurans, phthalates, arylamines and fluorotelomer alcohols. The LPGC techniques provided significant reduction in run times (up to 3.3x faster runs) and helium consumption reduction (up to 81% less helium used), while keeping an acceptable resolution.

O-05

A novel approach for monitoring multi-classes of POPs in a single run by GC-Ion Mobility-HRMS

Frank Kero[1], Arnd Ingendoh[1]; Carsten Baessmann[1]; Javier Lopez[1]; Miguel Angel Perez[1]; Hugo Muller[2]; Gauthier Eppe[3], Artem Filipenko, Ph.D.

[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [2]Mass Spectrometry Laboratory, MolSys Research Unit, Chemistry Department, University of Liège, Liege, Belgium; [3]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium

Polychlorinated dioxins and furans are bio-accumulative molecules formed during combustion and industrial manufacturing processes. Their analysis is complex due to low regulatory exposure limits and difficult sample matrices. They are persistent organic pollutants (POP), widely found in environmental samples. Severe consequences, even at low exposure concentration, include cancer, reproduction and growth issues, immune system diseases and endocrine effects. Dioxins and furans are mainly quantified in natural matrices by high-resolution sector field MS. Proposed here is a novel workflow involving ion mobility as an orthogonal criterion for identification and quantification, coupled to a high-resolution sensitive QTOF mass spectrometer. The benefit is a high flexibility for separating and analyzing various classes of compounds all in a single GC run with high sensitivity.

O-06

Considerations and Progress in Developing Multiresidue Analysis Methods for the Inorganic Residues of Postharvest and Preplant Fumigants.

Wiley A. Hall, 4th[1*]

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Enforcing the proper use of fumigants through MRLs can be complicated, due in part to their high volatility. By the time a regulatory body collects a sample, there may be no residue of the parent compound even if it was used improperly. In some cases, where the fumigant degradation results in the formation of an inorganic salt, this problem is addressed by setting the fumigants residue definition to the inorganic degradation product (e.g. – bromide, iodide and fluoride). This can present a whole new set of challenges, however, as the inorganic degradant may also be attributable to many sources (including those that are naturally occurring) and their analysis is often challenging. For example: fluoride is difficult to detect using common method of analysis such as LC-MS, and ICP-MS due to (respectively) its low molecular weight, and high ionization potential. Ion selective electrodes (ISEs) can be used, but are time

consuming, have low sensitivity (especially when a high level of dilution is required to reduce matrix effect) and can only be used for the analysis of one analyte at a time. Ion chromatography seems like a likely option, but interference from food matrices often renders it ineffective. Capillary electrophoresis (CE) offers an alternate separation that is automated, sensitive, and flexible while generating minimal waste. The quantitative analysis of fluoride in variety of stored products using capillary electrophoresis coupled to a contactless conductivity detector (CE-C4D) is presented here along with its potential to be expanded to include other inorganic degradants.

O-07

Regulatory Challenges to the Use of Postharvest Fumigants in the Global Trade of Agricultural Commodities

Spencer Walse[1*]

[1]**USDA-ARS-SJVASC**, 9611 S. Riverbend Ave; Parlier, CA 93648, USA; spencer.walse@usda.gov

Postharvest fumigants are a critical part of the international trade in agricultural commodities, allowing food to be transported across the world without spreading invasive pests and diseases. Despite their ubiquity and importance, registration and residue test guidelines do not accommodate the realities of their use patterns and physiochemical characteristics. Regulatory challenges include: pesticide labels that lack specificity with regards to variables that are critical to obtaining reproducible residue testing results (i.e. – when to collect residue samples after treatment, and how to store and transport those samples); residue definitions that are deharmonized across major markets so that one market requires the analysis of the highly volatile parent compound, while another requires the analysis of the non-volatile degradation product; and a general lack of familiarity with the nuances of fumigant behavior and analysis amongst regulators. Presented here are case studies where the differences between fumigants and more traditional pesticides has led to regulatory challenges detrimental toward global registrations and use.

O-08

Occurrence and distribution of emerging contaminants on children's food in Miami-Dade - FL

[1]Luciana Teresa Dias Cappelini, [1]Olutobi Daniel Ogunbiyi, [2]Vinícius Guimarães Ferreira, [1]Emily Mejias, [1]Monica Perez, [1]Piero Gardinali, [1]Daniel Bagner, [1]Natalia Quinete.

[1]**Florida International University**, 3000 NE 151st St, North Miami, FL 33181, USA; ldiascap@fiu.edu; [2]Faculdade de Saúde Publica da USP, Departamento de Saúde Ambiental- São Paulo – SP Brazil

The presence of organic compounds in foods across Miami-Dade varies significantly due to industrial activity, traffic, and land use. This is relevant when considering the vulnerability of children, who may be more adversely affected by these chemicals in their food due to their developing bodies and metabolism. Stringent safety standards are needed for food products taking into consideration the presence of a wide diversity of chemicals, not always regularly monitored or regulated. This study aims to identify chemicals in daily children's food samples from 43 families collected from May 2022 to February 2024. Each of the 99 samples were homogenized, spiked with an internal standard, and analyzed using a modified QuEChERS extraction method. A non-targeted analysis (NTA) approach was conducted using a Q-Exactive Orbitrap MS and Compound Discoverer. The mobile phase consisted of water, methanol, acetonitrile, and 0.1% formic acid, with the analytes separated and identified in positive and negative modes over a 100.0 - 800.0 m/z range and resolution of 140,000, followed by MS2 data dependent. A linear regression log Kow model helped minimize false positives. Data analysis was carried out in Python, using univariate and multivariate statistical models, such as t-test, ANOVA, PCA, and PLS-DA. Our data suggested that most children are exposed to emerging contaminants, such as 4-Dodecylbenzenesulfonic acid, Dodecyl sulfate, and Methenolone, which can potentially lead to health problems. Understanding and managing the distribution of these contaminants are vital for food safety and public health, necessitating controls to reduce exposure and associated risks.

O-09

Mapping of Mycotoxins Profiles in Wheat Production Regions of Uruguay

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Toxins produced by fungi in food and feed are a serious health risk. The challenges associated with the monitoring and risk management of mycotoxins include the chemical diversity of their structures and their persistence in food matrices even after processing. Among the mycotoxins produced by Fusarium (the pathogen causing Fusarium head blight in wheat), zearalenone (ZEA) and type B trichothecenes deoxynivalenol (DON), 3-acetyldeoxynivalenol (3ADON), 15-acetyldeoxynivalenol (15ADON) and nivalenol (NIV) are the most relevant. Not all these mycotoxins have defined maximum concentrations in food matrices, but growing concern about their toxicity and their co-occurrence in food have led to wider scope analytical approaches.

In this study, we used LC-MS/MS on a triple quadrupole instrument for the quantification of DON, its acetylated forms, NIV and ZEA in samples from wheat producing regions of Uruguay collected in the field during the 2018 growing season. The analytical method consisted of a modified QuEChERS extraction, followed chromatographic separation and detection by positive and negative ion MS/MS. Following SANTE guidelines, quantitative method validation showed acceptable performances with recoveries of 70-120% and <20% RSD for the 5 analytes. The mycotoxins profile of the samples was evaluated for the production regions and different cultivars. The most detected mycotoxin was DON (66% of the samples), followed by NIV (12.7%) and ZEA (8.5%), whereas co-occurrence of mycotoxins was observed in 18% of the samples.

O-10

Detection of *C. thevetia* Cardiac Glycosides Adulteration in Dietary Supplements utilizing Untargeted High Resolution Mass Spectrometry

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Dietary supplements are an area of significant consumer interest, with estimated global value of over $353 billion in 2019. More than 2/3 of US adults are overweight or obese, and the market for weight loss supplements is valued at over $30 billion. A challenge in testing dietary supplements is the wide range of potential analytes. Untargeted analysis helps in this regard when looking for undeclared additives, or in this case unknown toxins present in the product. An adverse health event in Maryland triggered an FDA investigation into supplements labeled variously as containing Brazil nuts, Candle Nuts, or Tejocote Root. In this study, UHPLC-MS on an Orbitrap instrument was used for the identification of cardiac glycoside produced by yellow oleander (*Cascabela thevetia*) in weight loss dietary supplement samples. The UHPLC-MS provided high mass accuracy with untargeted analysis, enabling identification without commercial standards with a high degree of certainty. Fortification and recovery experiments results using FERN Poison/Toxin Screening by LC/HRMS methodology achieved overall recoveries 30-90% and <30% RPD for 3 characteristic *Thevetia* glycosides in a blank matrix at 2 spiking levels. In a qualitative assessment, a variety of dietary supplements were analyzed for the presence of cardiac glycosides, where sample extracts were compared to commercial standards and extracts of authentic oleander for confirmation of masses and retention times. The FERN method provided reliable and precise identification of cardiac glycosides in seeds and powder samples. Here we present modifications to the FERN method, challenges, and future work to support enforcement actions.

O-11

Good chromatography a sometimes-neglected aspect of modern multiresidue methods

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Regarding modern multiresidue methods, chromatography has received significantly less attention than mass spectrometry. Yet, chromatography is the basis for obtaining reliable analytical results. This became obvious when analyzing a "new matrix" namely ovine liver with a multiresidue method validated for bovine liver and many other food matrices. A significant number of compounds eluted in the form of split peaks. In addition, some analytes showed prolonged retention times which moved the peak out of the pre-defined MRM detection window.
A thorough investigation led to the finding, that the elevated levels of taurocholic acid, as found in ovine liver, was responsible for these observations. Better analyte peak shapes could not be obtained by employing alternative stationary, but mobile phases (higher formic acid concentration). There is a loss of analyte signal abundance, yet many analytes actually show improved detectability. This is due to a significantly better chromatographic peak shape.
Even in the absence of matrix, a higher formic acid concentration improves the peak shape of many analytes (e.g. quinolones, penicillin's etc.). This is due to the suppression of analyte metal chelates interactions. The flow path (e.g. frits) of LC system appears to be the source of these metals (Fe and Ti). Finally, the addition of medronic acid to the injected sample solution was investigated. This metal complexing modifier improves chromatographic peak shapes more strongly than EDTA. In addition, medronic acid can easily by rinsed from an LC system and produces limited signal suppression in the MS interface.

O-12

Automated Solvent Extraction Method of PFAS From Difficult food and Environmental Matrices

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There is increasing concern of Per- and Polyfluoroalkyl Substances (PFAS) in our environment as a whole, due to their persistent nature. More and more regulation regarding PFAS is being implemented. Having a harmonized method to accurately determine the PFAS content in food as well as other matrices is important to this industry. The extraction of PFAS can be challenging given the susceptibly to contamination and the low levels in which these compounds are present. Existing techniques are predominately manual methods that are not rapid, simple, and efficient. In this study, an automated solvent extraction system, the EDGE PFAS is explored. This method offers efficient extraction of PFAS from any challenging food and environmental matrices in less than 10 minutes in one simple process, where the final extract is filtered and ready for further cleanup and analysis. Excellent extraction recovery and reproducibility of PFAS from variety of matrices including vegetables and fish is presented. The EDGE PFAS method offers a rapid, simple, and efficient solvent extraction solution for PFAS testing.

O-13

Effective Sample Preparation for LC-MS and GC-MS Multi-Pesticide Residue Analysis in Essential Oils Using Novel Passthrough Cleanup.

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Throughout history, essential oils have been cherished for their diverse applications in food preparation, medicine, personal care, and religious rituals. The widespread popularity of essential oils underscores the need for monitoring their quality, including pesticide residue levels. However, extracting and recovering pesticide residues from an essential oil is challenging due to the complex matrix of the botanical materials. Furthermore, limited research has been conducted on pesticide analysis in essential oils, resulting in sparse data in scientific literature. To address this gap, a novel preparation method was developed to accurately detect and quantitate pesticide residues in essential oils. This innovative approach builds upon our in-house QuEChERS extraction method, which is currently used to test over 400 pesticide residues in botanical dietary supplements using LC-MS/MS and GC-MS/MS. The key step in

essential oil cleanup is utilizing a novel SPE sorbent designed to remove lipid content as a pass-through to remove as many terpenes, sesquiterpenes, and their derivatives as possible without reducing residue recovery. Further cleanup is achieved by an additional cartridge containingC18E and Carbon S sorbents to remove any remaining matrix components from the essential oil extract. All monitored residues met the SANTE linearity, precision, and recovery guidelines. This method allows for the necessary flexibility and robustness in pesticide residue analysis in essential oils and for streamlining the process to introduce essential oil testing without major disruptions to the overall workflow.

O-14

Determination of Microcystins and Nodularins in Ambient Freshwater and Seawater by LC-MS

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Matrix effects are common issues associated with analyte quantification by liquid chromatography-mass spectrometry (LC-MS); they can be resolved by sample cleanup, adjustment of LC-MS conditions, matrix-matched standards (MMS), stable-isotope labeled internal standards (SIL-IS), or standard addition. We evaluated cyanobacterial cell lysis methods, monitored toxin extraction process, and quantified toxins for about 300 microcystins (MCs) and nodularins (NODs) including those without standards available in freshwater and seawater by LC-MS/MS. Our approaches included solid phase extraction (SPE) to cleanup toxins from seawater and freshwater, MMS to adjust LC gradients and evaluate toxin extraction efficiency, and SIL-IS (MC-RR-$^{15}N_{13}$, MC-LR-$^{15}N_{10}$, and MC-LA-$^{15}N_{7}$ to represent MCs containing 2, 1, and 0 arginine residues, respectively) . Two brands of reversed-phase SPE cartridges preformed comparably to desalt seawater and concentrate toxins in freshwater and seawater. Trizma instead of acid was used as an ion pairing reagent to increase retention of MCs without arginine residues on Strata X SPE. Toxin elution from Oasis HLB SPE was complicated by hydrophilic interactions coupled with hydrophobic interactions between toxins and HLB sorbent. Average recoveries of toxins in lake water and seawater using the HLB sorbent with LC-MS/MS analysis ranged from 90 to 109% except MC-WR & LW (71 to 87%) with limits of detection from 1.3 to 24.9 ngL^{-1}. The average recoveries of MMS against toxin standards in 50% methanol accompanying the validation sample runs ranged from 95 to 107% for all toxins, with most very close to 100%, indicating reduction of matrix effects to minima.

O-15

Quantitative Analysis for The Adsorption and Desorption Capabilities of Mycotoxin Deactivators Containing Multiple Biogenic Amines by LC-MS/MS

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Mycotoxin deactivators are commonly used as additives in animal feeds to minimize the absorption of mycotoxins by the animal. There are many different forms of these deactivators, some are bentonites, zeolites, yeast cell walls, charcoal, algae, and others. Typical analysis of these analyzes for mycotoxin adsorption and desorption, however this study was to see how mycotoxin deactivators work on binding biogenic amines. A quantitative liquid chromatography with tandem mass spectrometry method was developed for the detection of biogenic amines in mycotoxin deactivators. An evaluation was conducted to determine if biogenic amines could be removed effectively. Putrascine, Cadaverine, Histamine, Tryptamine, Tyramine, Spermine, Phenethylamine and Sperimidine were prepared in ruminant fluid and added to a recommended dosage of each deactivator with biogenic amine concentrations that represented the average concentrations found in TMR (total mixed rations). The fortified solutions were then analyzed for adsorption and desorption using pH 3 for adsorption and pH 6.5 for desorption. The adsorption was performed for 3 hours followed by desorption for an additional 3 hours to simulate the digestion of dairy cattle. The desorption percentage was then subtracted from the adsorption percentage and an overall percent efficiency was calculated. The analysis was performed by LC-MS/MS utilizing an QualiT Pure QP1100 SPE purification step. Overall, the deactivators that were analyzed had very low percent adsorption and desorption, but a couple had greater than 93% efficiency for Spermine and several others had greater than 30% efficiency for Spermidine.

O-16

Quantification of Mycotoxin Levels in grains utilizing Hyperspectral Imaging and Artificial Intelligence.

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Near-infrared (NIR) spectroscopy has long been employed to assess grain quality factors like fat or protein content. Grains often harbor mycotoxin contaminants, typically at very low levels (e.g., parts per million or billion), posing challenges in detecting them. Prior efforts using NIR to estimate mycotoxin concentrations have seen limited success. ImagoAI, Inc. has introduced the "*Galaxy by ImagoAI for Mycotoxins"* test, specifically engineered to quantify mycotoxins—Aflatoxins B1, B2, G1, and G2 (AFLA), Deoxynivalenol (DON), Fumonisins B1, B2, and B3 (FUM), and Zearalenone (ZEA)—simultaneously in ground corn. This test leverages Artificial Intelligence (AI) and Hyperspectral Imaging (HSI) that combines digital imaging and spectroscopy to provide spectral data for each pixel location. The Galaxy's workflow is straightforward: a hyperspectral image is scanned and then input into the AI-driven Galaxy software. Within 30 seconds, Galaxy analyzes the image and presents precise AFLA, DON, FUM, and ZEA levels in parts per billion (ppb), without requiring any chemicals or reagents. Galaxy is designed for use by laboratory analysts, plant operators, or farmers, with no specialized training needed.In AOAC quantitative validation, acceptable performances were achieved with overall recoveries 90-105% and <11% RSD for all four mycotoxins. Validation was done with HPLC or LC-MS/MS as reference methods.

O-17

PFAS analysis in house dust across socioeconomic factors using targeted LC-MS/MS and total fluorine approaches

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PFAS are used extensively in products designed for indoor use, such as stain-resistant coatings for carpet and furniture, and have been found in household dust at high concentrations. Dust sampling has found PFOA and PFOS and other PFAS, including relatively large amounts of precursor PFAS like the polyfluoroalkyl phosphates (PAPs). Yet current evaluations may be underestimating total indoor exposure to PFAS from dust across subpopulations. A primary objective of this study was to explore the relationships between PFAS exposures and socioeconomic status (SES; e.g., education, income), because some researchers have suggested that SES may contribute to exposure disparities. We collected settled dust and handwipe samples from n=40 residences having different socio-economic backgrounds in Ottawa, Ontario, Canada. Dust samples were subsampled to receive both total fluorine analysis by particle-induced gamma ray emission (PIGE) spectroscopy and targeted PFAS (n=25) analysis using LC-MS/MS. Targeted PFAS were chosen based on those of interest as listed on the 2022 Canadian Chemicals Management Plan (e.g., PFOS, PFOA), in addition to precursor PFAS. Preliminary results show that the 6:2 diPAP was present on all participants hands. PFAS was also detected in all homes, with PFOS and PFHxS present at highest concentrations (214 and 242 ng/mL) respectively. Of the PAPs, the 6:2 diPAP ranged from <LOD to 280 ng/mL. Total fluorine levels ranged from <LOD to 1440 ng/mg. Examining the levels of both targeted PFAS and total fluorine in these samples will lead to a greater understanding of the impact of dust ingestion and inhalation on human exposure.

O-18

Detection and Quantitation of PFAS Substances in food and packaging with LC-MS/MS

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Merieux NutriSciences

Perfluoroalkyl compounds (PFAS) are a subset of fluorinated substances widely utilized since the 1950s due to their unique properties, such as high thermal and chemical stability. PFAS are commonly found in various products like fabrics, paper coatings, non-stick cookware, and firefighting foams. Due to their stability, PFAS persist in the environment, contaminating soil, air, and water sources, potentially exposing populations through food ingestion, inhalation, or direct contact. Human studies on PFAS exposure have shown mixed health effects, including potential associations with elevated cholesterol, uric acid levels, liver issues, hormone disruption and even potential links to cancers. Regulatory agencies, like the FDA, are taking steps to limit human exposure.

While there's no federal ban on PFAS in food packaging, some states have enacted regulations. Recently, the FDA announced the discontinuation of PFAS-containing grease-proofing substances in food contact materials. This method outlines the analysis of PFAS in food items and packaging materials for human consumption using LC-MS/MS technology. The procedure involves homogenizing the sample, fortifying it with isotopically labeled surrogates, and extracting PFAS using acetonitrile and formic acid. Clean-up techniques like QuEChERS and solid phase extraction may be necessary for complex samples. LC-MS/MS is then used for analysis, identifying PFAS compounds through multiple reaction mode transitions and retention time matching. Quantitation is achieved by comparing response ratios to calibration standards, with adjustments made for dilution and starting sample mass. In sum, this method provides an approach to accurately assess PFAS levels in food and packaging samples, ensuring consumer safety and regulatory compliance.

O-19

Fast and easy nontargeted detection of PFAS in complex food matrices

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There is a high interest in non-targeted techniques for the detection of PFAS compounds in the environment and food.
However, it is the absence of fluorine isotopes which makes the mass spectrometry based nontargeted detection of PFAS difficult. Yet, each hydrogen replaced by a fluorine atom not only increases the mass defect, but also makes the molecule heavier. Therefore, the idea was conceived that not the mass (*m/z*) or the mass defect (md) of a particular ion should be studied, but that these measurement-based values should be divided (normalized) by the number of carbons (C) present in the studied ion. The number of carbons present in an ion can be readily estimated by comparing the ion abundance of the first isotopic peak versus the ion abundance of the monoisotopic peak.
Plotting md/C versus *m/z*/C strongly discriminates exogenous PFAS from endogenous compounds. This was demonstrated by analyzing fish tissues (muscle and liver). The high-resolution mass spectrometry based chromatograms were deconvoluted and the two mentioned parameters were calculated for each of the thousands of extracted chromatographic peaks (features). The nontargeted methodology detected PFAS down to sub µg/kg levels.
Unlike other techniques, the simple approach does not rely on fragmentation data, neutral losses, assumption of homologous series or the availability of spectra libraries. The proposed methodology is not only simple to use but has already been integrated into a commercially available ms data processing software and has been independently evaluated by a number of recent peer reviewed papers.

O-20

PFAS Contamination in Agricultural Settings and Assessment of Human Exposure Pathways through Food Products

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Historical land application of biosolids resulted in per- and polyfluoroalkyl substances (PFAS) soil contamination on agricultural land in Maine. Multiple human exposure pathways to PFAS have been identified from contaminated farmland including through cow's milk, beef, vegetables, backyard chicken eggs, and consumption of wildlife such as fish, deer, and turkey. Sampling by Maine state agencies has found elevated PFAS levels in farm products and wildlife on and around PFAS-impacted farms. As PFAS measurement in foods was not a common matrix for commercial laboratories, Maine worked with the Food and Drug Administration (FDA) Center for Food Safety and Applied Nutrition laboratory to perform interlaboratory comparisons of PFAS measurement in a variety of foods including grass and corn forage crops, cow's milk, beef, and deer and turkey. There was generally good agreement in the measurement of PFOS, the predominant PFAS detected in most media sampled, with an average relative percent different (RPD) <20% between laboratories. An evolving issue for PFOS/PFAS measurement in forage crops and foods is the ability to lower detection limits to both assist in determining what plants have low PFOS/PFAS uptake when grown in contaminated soil and to meet potentially low food action guidelines or standards. The Maine Center for Disease Control and Prevention derived draft action levels for several foods using PFAS toxicity values from the Agency of Toxic Substances and Disease Registry. These action level values are similar to the European Union maximum levels for PFAS in certain foods and are currently near commercial laboratory reporting limits.

O-21

Advancements in Miniaturization and Automation for Eco-Friendly Analytical Methods in Pesticide Residue Evaluation in Food

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Food control laboratories specializing in pesticide residue detection have made considerable progress, expanding their analytical scope and refining their limits of quantification (LOQs) through the use of improved mass spectrometry instrumentation to comply with stringent food safety regulations. Although speed and quality have been the primary goals of our laboratories, it is now imperative to look beyond, striving to enhance these objectives while simultaneously embracing cleaner and more environmentally friendly methodologies.
In our research, we explore and discuss the latest advancements in analytical tools that are either newly introduced or on the verge of being implemented. These developments are particularly focused on automation and miniaturization, often serving a dual purpose in certain contexts. This examination highlights the innovative direction of analytical methodologies, emphasizing their evolution towards more efficient and eco-friendly approaches.
We have categorized the examples into three distinct phases. First, we focus on the automation of sample extraction, utilizing analytical tools like EDGE® or Extreva®, with a special emphasis on dry commodities. Next, we address cleanup procedures that concentrate on Micro-SPE for both multi-residue and single-residue methods. Finally, we delve into chromatography, specifically examining supercritical fluid chromatography and microflow chromatography.
The critical evaluation of these procedures is guided by the specific requirements that food control laboratories face in terms of accreditation, in accordance with ISO 17025 standards, and aims at significantly reducing organic waste.

O-22

Reduced Instrument Downtime for Organochlorine Pesticide Analysis by Using an Optimized SPE Cartridge for Sample Extract Cleanup

Jason Thomas, Alexis Shelow

Some of the most commonly encountered problems experienced by those analyzing environmental samples for organochlorine pesticides are instrument downtime and shortened calibration periods both due to the deleterious effects of coextracted matrix components that are introduced into the analytical instrument during sample injection. In addition to this, chromatographic interferences complicating identification and quantification have also made life difficult for environmental analysts. Although there are cleanup options provided such as Florisil, silica gel, and alumina, these normal phase solutions often do not adequately remove the less polar and high molecular weight compounds that are responsible for diminishing instrumental performance and sample path inertness.
In this presentation, a cartridge is introduced that is designed specifically to be utilized exactly like the frequently employed Florisil cartridge, but to a much superior effect for highly pigmented and inlet degrading samples. What this means for the analyst is the ability to consistently generate calibration curves that can be maintained longer and reduced instrument maintenance, ultimately leading to higher sample throughput.

O-23

Optimization and validation of new sorbents combination in micro solid phase extraction cartridges for the analysis of pesticides in cereals

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The QuEChERS citrate buffer method, prepared according to EN 15662 followed by dispersive PSA (dPSA) clean-up, is the most commonly used method for the pesticides residues analysis in cereals and feedingstuff (72% in the last EU proficiency test organized

by the European Reference Laboratory in 2022). Despite its effectiveness, this method is associated with manual work and thereby potential human errors. Miniaturized and robotic analytical techniques have gained popularity in official laboratories all over Europe in recent years. This study aims to gain more knowledge about the possibilities for transferring the dPSA method into automatization. A preliminary evaluation on wheat and oat extract was conducted to assess the effect of different amounts of PSA introduced in µSPE cartridges (5, 10, 15 and 20 mg combined with 20 mg $MgSO_4$) on matrix removal efficiency, pesticides recoveries and RSD. The assessment included two proficiency test materials, EURL-CF11 (oat) and CF17 (wheat), both of which contained incurred and spiked pesticides. Based on the evaluation the most optimal sorbent combination, containing 10 mg PSA and 20 mg $MgSO_4$ was selected. Cartridges containing this combination, as well as two other combinations, 20 mg Zsep/20 mg $MgSO_4$ and 12 mg PSA/12 C18/ 1 mg GCB/ 20 mg $MgSO_4$, were used in a validation study for the analysis of pesticides in cereal. Data obtained from analysis using GC-MS/MS and LC-MS/MS will be presented.

O-24

New, fully automated analytical method for accurate, extended PFAS screen in water, beverages, and food

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A new and fast-growing concern is centered around the man-made per- and polyfluoroalkyl substances (PFAS), which are a diverse group of thousands of chemicals used in hundreds of types of products. PFAS in the environment can enter the food supply through plants and animals grown, raised, or processed in contaminated areas, as well as seafood in contaminated watersheds. PFAS are also a concern in drinking water, ground water, wastewater, as well as irrigation water.

We have adapted methodology that was originally developed at NC based universities and the local EPA/ORD laboratory into a new, fast, fully automated, accurate LC-MS/MS based method for various types of water and various beverages and fruit juices. The limits of quantitation (LOQ) are below ppt levels for 57 PFAS analytes (including all analytes that are part of current EPA methods, including EPA method 1633}. The only manual step is transfer of sample into a 96 well plate, yielding high accuracy and speed. Our method captures basic, acidic, and neutral PFAS analytes. It can be adapted to additional PFAS analytes as needed and as reference standards become available. It can be adapted for other matrices, e.g., food and feed, and be applied to evaluate effectiveness of remediation and removal technologies.

O-25

Application of nDATA Work Flow for Semi-Quantitative Screening of 1094 Pesticide Residues in Fruits and Vegetables using UHPLC/ESI Q-Orbitrap Full MS/vDIA

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Cost-effective multi-residue pesticide methods with a large detection scope are desired for both routine monitoring programs and risk identification. These methods are complex especially when using targeted methods to analyze several hundred pesticides. The aim of this study was to validate a nDATA (non-target data acquisition for target analysis) workflow using UHPLC/ESI Q-Orbitrap for semi-quantitative screening of 1094 pesticides in fruits and vegetables fortified at 10 and 100 µg/kg. Pesticides were extracted using a QuEChERS procedure, and non-target data acquisition was achieved using UHPLC/ESI Q-Orbitrap Full MS scan and variable data independent acquisition (vDIA). Data were processed using a Compound Database (1094 pesticides) and a one-point standard calibration with internal standards. Data processing criteria were based on either the retention time (± 0.5 min) and the mass accuracy of a precursor ion (± 5 ppm) (RTP by Full MS) or the retention time (± 0.5 min) and the mass accuracy of a precursor ion (± 5 ppm) and that of its fragment ion (± 10 ppm) (RTFI by Full MS/vDIA). RTP found 1010 and 1094 pesticides at 10 and 100 µg/kg, respectively, whereas RTFI identified 906 and 1029 pesticides at the same respective concentrations. The nDATA workflow was further verified by analyzing proficiency testing (PT) samples. The method identified all 30 LC amenable pesticides in eight PT samples. The validated nDATA workflow using UHPLC/ESI Q-Orbitrap Full MS/vDIA proved to be a comprehensive detection method for semi-quantitative screening of up to 1094 pesticides in fruits and vegetables.

O-26

Keeping a Regulatory Pesticide Monitoring Program Current: Extension of 38 Analytes to the FDA Harmonized Pesticide Method

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The FDA Pesticide program monitors a targeted list of pesticides using GC-MS/MS and LC-MS/MS technologies. This list must be updated periodically to reflect the changing worldwide uses and the introduction of new products. The FDA completed a large multi-lab validation study of its pesticide methods in early 2021. Since that time, roughly 25 "QuEChERS-amenable" pesticides have had or are in the process of having new tolerances established with the US EPA. Pesticides with new tolerances plus some additional residues recommended by FDA's Center for Food Safety and Applied Nutrition (CFSAN) were evaluated for incorporation into the FDA harmonized procedure. This presentation will describe the evaluation process, changes in scope of analysis, and present study results.

O-27

Residues of Glyphosate in Food and Dietary Exposure

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Glyphosate (N-(phosphonomethyl)glycine), one of the most widely used herbicide around the world, and its metabolite aminomethylphosphonic acid (AMPA) are not typically included in multiresidue pesticide monitoring methods due to their polarity and ionic nature creating challenges in residue analytical methodology. The lack of multiresidue methods has led to the development of an array of residue method platforms, most commonly LC-MS/MS and LC-FLD, but in recent years ELISA has also been applied. The analytical figures of merit of the three techniques applied to glyphosate residue analysis will be discussed. Glyphosate residues, using these variety of methods are commonly reported in the literature from industry or government labs, academic labs, non-government agencies and citizen science efforts.
Understanding the context in terms of risk assessments and analytical figures of merit is important when examining this large and diverse set of literature. To achieve this goal, glyphosate residue data in raw agricultural commodities and processed foods generated either as part of the normal regulatory processes and testing conducted by university researchers and nongovernmental agencies were summarized. These data were placed into context of European maximum residue limits (MRLs) or U.S. Environmental Protection Agency tolerances. These data were then coupled with measurements of glyphosate in urine, to calculate an estimate of ingested glyphosate exposure of <3% of the current European ADI for glyphosate, which is 0.5 mg glyphosate/kg body weight.

O-28

A High-Efficiency Approach to Quantitating 246 Pesticides in Black Tea with GC/MS/MS using a New Electron Ionization (EI) Source for Maximized Uptime

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Tea is among the most common non-alcoholic beverages consumed worldwide. Assessing pesticide levels in tea is essential for evaluating its safety and required by many regulatory bodies, including the US EPA and the European Commission. The developed and validated complete GC/MS/MS workflow solution for accurate and reliable analysis of 246 volatile and semi-volatile pesticides in black tea demonstrated LOQs as low as 0.01 ppb for 34% of the targets, at or below 0.1 ppb for 74% of compounds, and below 2 ppb for 96%. Matrix-matched calibration allowed for excellent accuracy over a wide dynamic range, spanning up to five orders of magnitude over 0.01-1,000 ppb in a complex black tea extract. Method ruggedness was demonstrated through maintaining measurement accuracy with good precision (RSDs<20% for 176 compounds) for black tea extract spiked at 2 ppb sequentially analyzed over 800 runs spanning over 17 days of continuous analysis. Sample preparation efficiency and precision were validated at 10 and 50 ppb in black tea matrix with excellent recoveries between 70 and 120% and RSDs below 20%. The key components for a robust and rugged workflow discussed in this presentation include a combination of the efficient sample preparation and cleanup,

the GC hardware, functionality, GC supplies, the novel electron ionization (EI) source technology with HES 2.0, and lastly the built-in GC/TQ intelligence and new software functionality.

O-29

Evaluation of Complex Food Matrices for Multiresidue Pesticide Analysis using QuEChERS Modifications and GC- and LC-MS/MS

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The analysis of approximately 250 and 275 pesticides by QuEChERS and GC-MS/MS and LC-MS/MS, respectively, in over fifty agricultural matrices will be described. Modifications of the QuEChERS procedure were validated based on different types of complex matrices such as animal products, lipid-rich foods, agricultural products, low moisture commodities (botanicals, spices, and cereal grains), and beverages. These modifications include a decrease in sample size, hydration or dilution of the sample with water, and removal of lipids and matrix interferants using different types of dispersive solid-phase sorbents. Recovery studies were performed by fortifying food matrices with pesticides at concentrations of 10, 25, 50, and 100 µg/kg in (n = 4), resulting in average recoveries between 80-120% and relative standard deviations < 20% for the majority of target pesticides. Lower (< 80%) and higher (>120%) recoveries were most likely from complications of pesticide polarity and matrix interferences that led to increasing the 10 µg/kg minimum level of quantitation for pesticides. Despite many improvements made to sample preparation and hardware and software technology over the last twenty years, there are still challenges that need to be addressed, such as the analysis of highly nonpolar pesticides in high lipid foods or botanical materials that contain high levels of essential oils.

O-30

Mycotoxins: measuring body fluids versus food to assess dietary exposure

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Dietary exposure of mycotoxins is typically assessed based on analysis of various raw agricultural commodities and food consumption data. Closer to actual intake is analysis of duplicate diets. An alternative to food analysis is human biomonitoring (HBM), i.e. analysis of body fluids. HBM provides information on the internal exposure. Analytical methods based on LC-MS/MS were developed and applied to determine several mycotoxins (deoxynivalenol, zearalenone, T2-toxin/HT-2 toxin, fumonisins, ochratoxin, aflatoxins) in urine and/or blood. The use of immuno-affinity based cleanup was needed to achieve sufficiently low LOQs (ranging from 0.005-0.25 ng/mL). An in-depth study was done for deoxynivalenol (DON) and zearalenone (ZEN) for which the highest detection frequencies were observed. These were measured in duplicate diets and 24h urine samples collected from the same persons on the same day. Quantitative relationships of the mycotoxins and their corresponding urinary biomarkers were investigated. For deoxynivalenol 80% (median) of the intake was excreted as total DON in urine. ZEN was only found as such in the duplicate diet and excreted as (conjugates of) ZEN, α-zearalenol (αZEL) and β-zearalenol (βZEL). In contrast to DON, the ratio of urinary excretion of ZEN biomarkers vs. dietary intake showed a much higher variance. To gain a better understanding of the ADME for ZEN, a human volunteer study was conducted in which 19 subjects ingested ZEN (@ 75% TDI) and urine was collected. A median ratio urinary excretion vs ZEN intake of 30% was observed. The data are highly useful to support the establishment of urinary biomonitoring equivalents.

O-31

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Our in-house method is fully validated and capable of quantifying over 1000 fungal metabolites and plant toxins in 40 minutes, with 2 injections in positive/negative ionization modes, 20 minutes each. To explore the extent to which the method can be accelerated without compromising accuracy and precision, we applied fast polarity switching (FPSW) alongside with scheduled multiple reaction monitoring (sMRM).
Nine (9) different setups were tested to compare the applicability of HPLC & UHPLC columns, to explore variations in method performance between FPSW and positive/negative polarity, as well as the impact of accelerated gradients, ranging from 20 minutes measurement time to 10 minutes measurement time.
To determine whether the implementation of these accelerated methods is feasible without significant deterioration of data quality, all 9 methods were validated according to SANTE 11312/2021(V2). Validation was carried out on 5 distinct samples of oats and muesli. Samples spiked on high concentration levels (pre- and post-extraction) were tested to determine both repeatability as well as intermediate precision, matrix effects, and recoveries of the extraction. Additionally, three low concentration levels were employed to determine the limits of detection (LOD) and quantification (LOQ). Final analysis of the validation data is pending due to the extensive number of validated setups. Results retrieved so far indicate that matrix effects are not significantly affected by FPSW, while repeatability and intermediate precision still comply with official criteria. However, applying a fast UHPLC-gradient on top of FPSW severely compromises data quality especially on lower concentration levels.

O-32

Multi-Class Analysis of Cyanobacterial Toxins using Hydrophilic Interaction Liquid Chromatography–Mass Spectrometry

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Cyanobacteria produce diverse classes of toxins including microcystins (MCs), anatoxins (ATXs), cylindrospermopsins (CYNs), and saxitoxins (STXs). These vary widely in toxicity, polarity and molecular weight, generally requiring multiple extraction and analytical techniques for evaluation. Here we present a single LC–MS/MS method for the simultaneous detection and quantitation of the aforementioned toxin classes.

A comprehensive liquid-solid extraction method for freeze dried cyanobacteria was developed using 75% MeCN/water (0.1% HCOOH) providing >74% recovery for all classes present. A HILIC gradient elution was used with detection by selected reaction monitoring on a triple quadrupole MS with positive/negative polarity switching. Confirmatory transitions, product ion ratios, and retention time matching with standards were used for identification. Recoveries were determined by spiking freeze-dried *Aphanizomenon sp*. samples. In-house validation demonstrated good performance of the method including selectivity, precision (1.5% (MC-LA) to 5.8% (GTX2) RSD), and detection limits (0.2 (ATX) and 2.7 (GTX3) ng/mL).

This method was applied to evaluate cyanobacterial cultures for use in the development of a cyanobacterial matrix certified reference material. It was also utilized for the analysis of environmental field-study samples of benthic and planktonic cyanobacteria, as well as shellfish, therefore demonstrating suitability for screening and quantitation of a range of sample matrices. The method can be extended to the analysis of other noteworthy toxin classes, including *Lyngbya wollei* toxins, guanitoxin, domoic acid and tetrodotoxin, which demonstrates an even broader future utility including applications in estuarine environments impacted by both marine and freshwater phycotoxins.

O-33

Development of a Mycotoxin in Animal Feed Reference Material

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Distiller's dried grains with solubles (DDGS) is a co-product of ethanol production from corn. Due to its high protein content, DDGS is used as animal feed. High levels of mycotoxins can be present in DDGS, especially if stored under warm or humid conditions. Thus, there is a need to measure mycotoxins in animal feed. Interlaboratory studies have shown significant variability among laboratories when measuring mycotoxins in DDGS. The availability of reference materials may help improve measurement comparability and determine the sources of the variability. The National Institute of Standards and Technology (NIST) and the Instituto Nacional de Tecnología Industrial (INTI) are collaborating to produce a naturally contaminated reference material for mycotoxins in DDGS. Bulk DDGS candidate material was obtained, and preliminary screening using LC-MS/MS showed measurable amounts of deoxynivalenol, zearalenone, and fumonisin. Results from other studies of the bulk material concluded that the bulk material did not require further milling, and irradiation of the material at doses between 10 kGy to 20 kGy ensures microbiological stability. The bulk material was homogenized, irradiated, and packaged into 60 g aliquots. The packaged material was characterized for five mycotoxins, and the homogeneity of the material was evaluated over the entire production lot. In addition to measurements at NIST, the material will be evaluated in collaborating laboratories and through an interlaboratory study.

POSTER ABSTRACTS

P-01

Extension and interlaboratory comparison of an LC-MS/MS multi-class method for the determination of 15 different classes of veterinary drug residues in milk and poultry feed

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The continuous utilization of veterinary drugs on livestock gives rise to various concerns, such as the need for residue monitoring, cumulative risk evaluation, antimicrobial resistance, and environmental pollution. Hence, veterinary drugs and reliable methods for their determination are not a fading concern. The objective of this study was to evaluate the applicability of a previously established LC-MS/MS multiclass method [1] for analyzing various food and feed matrices, including expansion of veterinary drugs scope.
To challenge the robustness and accuracy of the method, five different samples with potential differences in matrix effects were assessed. Findings of which were then proved through the validation of the method across two laboratories. Method validation for >140 analytes was conducted according to the SANTE validation guideline [2]. The majority of the analytes in milk and chicken feed met the SANTE routine laboratory criteria for accuracy, with a range of 80- 90% for milk and 50-60% for chicken feed, with apparent recovery range between 60-140%. Limits of quantification for all analytes with an existing MRL in milk were below the related MRL. Intermediate precision complied with the SANTE criterion of RSD <20% for almost 90% of the analytes for both matrices. In the interlaboratory comparison, analysis of twenty-nine samples of milk and chicken feed found no veterinary drug residues in the milk but detected elevated levels of nicarbazin, salinomycin, and decoquinate in the feed samples.

P-03

Sample Preparation, Nontarget and Suspect Screening of Persistent and Mobile Organic Contaminants in Drinking Water

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Persistent mobile organic contaminants (PMOCs) are a class of small molecule contaminants and transformation products whose high polarity enables them to persist in aquatic environments. These contaminants enter waterways by way of household, industrial, and agricultural waste, encompassing many use classes such as pharmaceuticals, pesticides, industrial chemicals, and short- and ultra-short-chain PFAS. Due to their hydrophilicity, PMOCs do not sorb well to sediments, soils or biomaterials, allowing them to slip through common water treatment and occur in drinking water. In addition to this protection gap, high polarity makes these compounds difficult to analyze by conventional means, posing an analytical gap and leaving PMOCs under-monitored, understudied, and undiscovered. To enable PMOC analysis, evaporative concentration and multilayer SPE methods were developed and assessed for recovery for 22 model PMOC standards, including known PMOCs metformin, melamine, and trifluoroacetic acid. These methods were then employed to enrich PMOCs in drinking water samples with high recovery versus conventional enrichment methods. Targeted zwitterionic hydrophilic interaction liquid chromatography (HILIC) methods were developed for model standards and paired with electrospray ionization high resolution mass spectrometry using an Orbitrap Exploris 240. These methods were then expanded to suspect and nontarget analysis of PMOCs in drinking water, revealing unmonitored organic contaminants. This study reinforces that conventional means of enrichment and chromatographic separation are often not amenable to highly polar analytes and tailored analytical methods are necessary to perform broad screening of this emerging class of contaminants.

P-04

Targeted Quantitation and Suspect Screening of Additives in Artificial Turf Crumb Rubber using High Resolution Mass Spectrometry

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In the United States alone, around 5 million tons of end-of-life tires (ELTs) are generated annually. Crumb rubbers from ELTs are of interest as a potential source of environmental toxicants due to its widespread commercial use, such as artificial turf which is made from recycled car tires. Crumb rubbers contain a complex mixture of chemicals, and people are unknowingly exposed to these potentially toxic compounds when playing on artificial turf fields and playgrounds. Anecdotal links between crumb rubber exposure and cancers in athletes have been documented, but current testing may not identify risk due to the complexity and unknown nature. To address this knowledge gap, we aimed to investigate both the chemical composition of crumb rubber when subjected to different sample preparation methods (extraction, leaching, and bioaccessibility), as well as investigate trends based on the age of the artificial turf field. High-Performance Liquid Chromatography-High Resolution Mass Spectrometry (HPLC-HRMS) was utilized to determine the concentration of known tire additives of concern by Parallel Reaction Monitoring. Quantitation was performed for 19 compounds (1,3-Diphenylguanidine, 6PPD-quinone, benzothiazole) using an internal standard method. Crumb rubber was collected from 11 artificial turf fields in the Northeast United States, with installation dates ranging from 2009 to 2024. The relative abundance of other additives and transformation products in the crumb rubber samples was assessed by a suspect screening approach. Preliminary results indicate differences in chemical composition between tire and newly installed turf fields, turf fields aged 2-3 years, and turf fields installed for 5+ years.

P-05

Analysis of Potentially Unrecognized Fluorine-Containing Compounds in Environmental Samples using LC-MS and 19F NMR

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Per- and polyfluoroalkyl substances (PFAS) have gained attention in the scientific community with their ubiquity in manufactured products, leading to contamination in the environment. Because some PFAS are resistant to degradation processes, these chemicals can be found in biosolids (post-treatment sewage sludge fertilizer) and bioaccumulated in organisms. With rising concerns regarding elevated PFAS levels, robust techniques to detect, identify, and quantify PFAS are needed. In this research, I use nuclear magnetic resonance (NMR) spectroscopy with the fluorine nucleus (19F) to screen biosolids for novel fluorinated chemicals and create human exposure profiles of different areas in Ontario, Canada. Since C-F bonds are largely devoid in the environment, 19F NMR offers a unique advantage in providing unbiased analyses (e.g. no matrix effects) when searching and quantifying total PFAS. Complementary to NMR spectroscopy, liquid chromatography mass spectrometry (LC-MS) is used as a tool to confirm the presence, identities, and concentrations of PFAS in both biosolids and soil samples. Additionally, these results can provide information on the potential migration of known PFAS from biosolids to soil and crops. Preliminary NMR data shows high levels of fluorinated aromatic compounds present in different biosolid samples, suggesting possible pharmaceutical exposure. For LC-MS, there were minimal differences in levels of various PFAS between pre and post application of biosolids on farm soils and the control soils (background PFAS levels from rainwater deposition). It is hypothesized that further investigation of new soil samples from the same land will show variations in PFAS concentration following greater dispersion of the biosolids.

P-06

Assessment of Per- and Polyfluoroalkyl Substances (PFAS) in Tap Waters from Miami-Dade and Palm Beach, South Florida

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Per- and poly-fluoroalkyl substances (PFAS) are a class of synthetic chemical compounds widely used in various industrial and commercial products due to their unique properties, including resistance to heat, water, and oil, which make them useful in a wide range of applications, such as non-stick cookware, water-resistant textiles, and firefighting foams. However, their persistence in the environment and the human body has led to concerns about their potential health effects. Exposure to PFAS has been associated with various adverse health outcomes, including developmental delays, reduced immune system function, and an increased risk of certain cancers. One of the most concerning routes of exposure to PFAS is through drinking water contaminated with these chemicals. Drinking water contaminated with PFAS has become a growing public health concern in recent years, and there is a need for more data on the prevalence of these chemicals in different regions. To address this concern, this study aims to determine the levels of PFAS in 70 tap water samples collected between March and June 2023 (dry season) from nineteen zip code areas in Miami Dade County, and 30 tap water samples collected between April and May 2024 (dry season) from Palm Beach County. Samples are processed using Solid Phase Extraction (SPE) and liquid chromatography-tandem mass spectrometry (LC-MS/MS). This PFAS assessment contributes to the expansion of knowledge of the PFAS distribution and insights about human health risks by evaluating compliance with the recent PFAS National Primary Drinking Water Regulation issued by the Environmental Protection Agency (EPA).

P-07

Presence and Quantification of Per- and Polyfluoroalkyl Substances (PFAS) in Marshes and Canals in the Miccosukee Reservation

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It is well established that per- and poly- fluoroalkyl substances, (PFAS) are present in the environment as “forever chemicals” due to their stable, persistent, and accumulative properties. While some PFAS, such as perfluorooctanesulfonic acid, (PFOS) and perfluorooctanoic acid, (PFOA), were phased out in the U.S., new alternatives are being produced and these shorter-chain PFAS can be as persistent and toxic as the previously banned compounds. PFAS are of environmental and health concern in both the urban coastal environment of the city, but also in the wetlands of the Everglades, potentially impacting agriculture, and wildlife. By invitation of the Miccosukee tribe and their water resources representatives, 12 exploratory samples were collected for the first time from the Miccosukee Reservation’s marshes and canals. Solid phase extraction (SPE) was performed for 250 mL of water samples using Strata-XL Cartridges. Samples were dried down under nitrogen gas and reconstituted to 500 µL then analyzed by liquid chromatography tandem mass spectrometry (LC-MS/MS) following EPA Method 1633. The characterization of PFAS levels in the surface water from the Everglades canals and wetlands around the Miccosukee Reserve would provide a comparison, or baseline values, to compare to the tributaries in the urban environment. Understanding the presence and concentration of specific compounds will be important for the continued efforts creating a thorough monitoring map of PFAS in South Florida and to determine hotspots of potential pollution point sources in the water bodies of the Miccosukee community.

P-08

Targeted and non-targeted analysis using LC-Orbitrap-HRMS for screening of novel Per-and polyfluoroalkyl substances (PFAS) in recreational fisheries

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Per-and polyfluoroalkyl substances (PFAS) are group of anthropogenic contaminants ubiquitous in all environmental compartments. Hence, their persistent, bioaccumulative and toxic characteristics pose human and ecological health concerns. Therefore, the aim of this research is to characterize and quantify for 30 targeted PFAS compounds using LC-(-ESI)-MS/MS in tissue samples of recreational fisheries such as Blackfin tuna (*Thunnus atlanticus*), (N=30) and Lobsters (*Homarus americanus*), (N=30) that are commonly consumed among South Florida's residents. An alkaline based extraction followed by dispersive solid phase extraction (dSPE) was used for extraction and clean-up step, respectively. ΣPFAS body burden range from 0.15 - 3.40 ng/g ww in blackfin tuna samples and 0.37- 5.15 ng/g ww in lobster samples, respectively. PFOS (0.047 ± 0.021 ng/g ww) was the highest of all PFAS in tuna being a pelagic fish species while N-MeFOSAA (0.65 ± 0.86 ng/g ww) was reported highest in lobster samples due to preferential sediment-sorptive interactions for longer chain PFAS. Furthermore, we implemented a non-targeted analysis (NTA) workflow for the holistic screening of PFAS in the tissue samples using a liquid chromatography (LC)- Q-Exactive Orbitrap HRMS system followed by data processing and identification using Compound Discoverer v 3.1, as a complementary approach to screen for novel PFAS in recreational fisheries. A total of 3073 and 1417 annotated chemical features were obtained from tuna and lobster samples, respectively, after application of additional manual filters. Van Krevelen and Kendrick mass defect suggests that majority of chemical features identified are polyfluorinated with increasing O:C content in their structure.

P-09

High throughput method and trace levels detection of per- and polyfluoroalkyls substances (PFAS) by online SPE-LC-HESI-MS/MS, including 1633 EPA compounds list

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PFAS are water soluble and resistant to biodegradation due to the exceptional stability of C-F bonds. The physicochemical properties inherent to their structures have made them attractive to be used in many industrial applications. Their inability to be removed by traditional water treatments and the health risks associated with exposure to PFAS have brought the need to better understand its fate and transport in the environment. Once these compounds are released into the environment, they enter the water cycle and follow different transport mechanisms toward the groundwater and surface water, which are usually sources of drinking water. The Environmental Protection Agency recently defined the Final PFAS National Primary Drinking Water Regulation. This emphasizes the need for faster analysis time, high sensitivity, accuracy, and high throughput methods. Here we developed a new method involving the injection of 10 mL of sample in an online solid phase extraction (SPE) system using a weak anion exchange (WAX) column, followed by PFAS detection in an Altis Plus liquid chromatography-tandem mass spectrometry (LC-MS/MS). We have optimized the method for the analysis of PFAS analytes listed in the EPA method 1633, and isotopically labeled standards were used for quantification. The method was validated in terms of linearity, detection limit, precision, and accuracy, with an instrument detection limit as low as 0.5 ppt.

P-10

Development of A Sensitive Method for the Determination of Per and Polyfluoroalkyl Substances (PFAS) in Biosolids Leachates

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Per and polyfluoroalkyl substances (PFAS) are recalcitrant environmental contaminants of global concern. They are widely used in household and industrial products and are commonly found in the environment and humans. PFAS are extremely persistent and not removed by traditional wastewater treatment processes. In wastewater treatment plants (WWTPs), biodegradation is limited, and PFAS can be adsorbed on suspended solids during activated sludge process, leading to accumulation in biosolids. Land application of biosolids is a sustainable agricultural method of disposing treated sludge. However, limited studies have investigated the presence and quantity of PFAS in biosolids and their potential impact on agricultural lands. The uptake of PFAS from soil to crops could constitute a significant exposure pathway to humans and animals via food chain. Therefore, evaluating the quality of biosolids produced at WWTPs and their impact on the environment for PFAS content is crucial.
In this study, biosolids samples were collected from the South and Central District WWTPs in Miami Dade County, and leaching experiments were conducted for one day. A method based on semi-automated solid phase extraction(SPE) was developed and tested, followed by the analysis of PFAS using high-performance liquid chromatography-tandem mass spectrometry(HPLC-MS/MS).
The method focused on the determination of 40 legacy PFAS using isotopic labeled standards consistent with EPA method 1633. The preliminary results of this study demonstrate a sensitive method for assessing PFAS levels and composition in biosolids leachate, which could inform recommendations for appropriate biosolids testing, land application practices, and the potential risks associated with PFAS contamination in Florida.

P-11

Application of Ambient Ionization Mass Spectrometry for the Detection of Pesticide Contaminants in Cannabis Plant Materials

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In recent years, ambient ionization mass spectrometry (AIMS) has become more prevalent due to its targeted/non-targeted capabilities and the ability to rapidly screen for trace level contaminants. One area that would benefit from leveraging these advantages is pesticide residue analysis of *Cannabis sativa* plant materials. This study utilized a common AIMS technique known as direct analysis in real time – high-resolution mass spectrometry (DART-HRMS) to investigate 113 pesticides commonly screened during *Cannabis* testing. A DART ion source coupled to an ion trap mass spectrometer was operated in positive- and negative-ion modes at 350 °C. In positive-ion mode, the masses of 102 pesticides were detected, while 64 pesticides were detected in negative-ion mode. In total, 107/113 pesticides were detected by DART-HRMS. Analysis of a range of concentration levels revealed that most of the pesticides were detectable down to a concentration of 0.01 ppm by this approach. These concentrations are comparable to the action levels listed in the method performance requirements by the Association of Official Analytical Chemists (AOAC). Subsequent experiments in this study included: (1) examination of a subset of pesticides to determine potential interferences with cannabinoids; (2) investigation of pesticide-spiked *Cannabis* plant material to study matrix effects; and (3) analysis of hemp plants that had been treated with pesticides. The results of this study reveal the ability of DART-HRMS to successfully screen for pesticide residues on *Cannabis*, as well as the potential widespread applicability in other areas, such as food safety and natural products.

P-12

Ensuring Safety Beyond Application: Monitoring Off-Target Exposure in Veterinary and Agrochemical Products

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In recent years, off-target exposure to products used in veterinary and agrochemical applications has emerged as a significant and pressing concern, prompting manufacturers to demonstrate safety in previously overlooked areas. Particularly noteworthy is the unintentional human and environmental exposure to residues of pesticides, veterinary medicines, and related transformation products. Given the biological activity of these compounds, their use poses a high safety risk, with off-target effects that are often challenging to predict. It is crucial, therefore, to monitor and control their release through various means and understand the potential formation of transformation products with additional toxicological implications. This concern has led to the issuance of new guidance by the European Food Safety Authority (EFSA) and European Chemicals Agency (ECHA) on assessing the impact of water treatment processes (e.g., chlorination, ozonation) on active substances and their metabolites. This document contributes to a growing collection of regulatory guidance aimed at addressing the complex issue of off-target exposure, emphasizing the importance of comprehensive evaluations to ensure the safety and efficacy of these chemicals throughout their lifecycle. Our poster examines various routes of environmental release and discusses methods for monitoring to ensure product safety beyond application. This includes examples of analysis of treatment plant effluent from manufacturing, assessing operator exposure, and investigating leeching of biocides (e.g. from paint). Additionally, we present example methodologies capable of trace level detection and quantitation of a popular over-the-counter flea treatment medication for companion animals, in support of human exposure studies.

P-13

Determination of Natamycin in Food by HPLC

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Natamycin, also known as pimaricin or tennectin, is a polyene macrolide antimycotic utilized as an antifungal preservative in various food products. This study presents the development and validation of a reverse-phase HPLC method for the analysis of natamycin in common food matrices. Natamycin extraction from samples involved methanol and water, followed by analysis using a C18 column and UV detection at 305nm. The method exhibited linearity ($R^2 > 0.99$) within the concentration range of 0.01-10 ppm. Validation involved spiking natamycin standards into American cheese, sausage, yogurt, soft cheese, and hard cheese. Precision, with RSD values ranging from 1-10.8%, and method recovery were evaluated. The Limit of Quantification (LOQ) was determined to be 1 ppm, while the Limit of Detection (LOD) was 0.25 ppm. Repeatability and reproducibility data met performance expectations (<20% at LOQ level, <10% at other levels). The method's uncertainty was calculated to be 4.3%. This validated method offers a reliable means for quantifying natamycin levels in food products, ensuring compliance with safety regulations and facilitating efficient food preservation strategies to extend shelf life and reduce food waste.

P-14

Determination of 3-MCPD and Glycidol in Oils, Fats and Other Food with High Fat Contents by GC-MS/MS

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Esters of 3-Monochloropropane-1,2-diol (3-MCPD) and glycidol are contaminants found in refined oils. 3-MCPD esters are formed from naturally occurring acylglycerols in the presence of chlorinated compounds during high-temperature deodorization processes. Studies show that the 3-MCPD esters and glycidyl esters can hydrolyzed to toxic 3-MCPD and glycidol in the gastrointestinal tract,

which are carcinogenic and can cause damage to kidneys. Therefore, the levels of the 3-MCPD and glycidyl esters in foods must be controlled.
This method permits the determination of 3-MCPD and glycidyl esters (expressed as free 3-MCPD and glycidol, respectively) in edible oils, fats and other foods with high fat contents by GC-MS/MS. The LOD is 30µg/kg and the LOQ is 50µg/kg, expressed as free 3-MCPD and glycidol.
In this method, esters of 3-MCPD and glycidol in the samples were hydrolyzed, extracted and derivatized using phenylboronic acid. The extracts were analysed on an Agilent GC-MS Triple Quad system.
This method has been validated in extra virgin olive oil together with ruggedness and selectivity studies. The recoveries of the target analytes are in the range of 80-110%. The precision, expressed as the relative standard deviation (RSD), is in the range of 3-9%.
The extension of matrices was also verified in lard, spread and salted butter. The overall results demonstrated excellent linearity, repeatability, accuracy and precision, indicating this method to be suitable to simultaneously detect and quantify 3-MCPD and glycidol esters.

P-15

Survey on the presence of mycotoxins in commercial bee pollen sourced from different countries

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Bee pollen is one of the most valued natural products, appreciated because of its high content in macro-, micronutrients and bioactive compounds. However, there are still a number of questions regarding the safety of this beekeeping product. Mycotoxins are a family of molecules for which no legal restrictions are set in bee pollen. The presence of five mycotoxins - aflatoxin B1 (AFB1), ochratoxin A (OTA), zearalenone (ZEN), deoxynivalenol (DON), and toxin T2 - was evaluated in 80 samples from 28 countries. AFB1 had the highest incidence rate (98.75%), followed by DON (66.25%), ZEN (55%) and OTA (28.75%). From the multiple comparisons carried out among samples coming from different climatic areas and sub-areas, it was not possible to observe any significant difference in terms of single and total mycotoxins concentration. No significant differences in terms of single and total mycotoxins' content were found by comparing organic and conventional production. The comparison between mono and multifloral samples revealed that the total mycotoxins' concentration was significantly higher in the multifloral samples than in monofloral ones. In the three types of processing, a positive correlation between moisture content and total mycotoxin concentration was found. The results were used to assess the risk associated with single and multiple mycotoxin exposure due to bee pollen consumption by calculating the respective hazard quotients and margins of exposure. In 28% of the analyzed cases, DON exceeded the safe limits, while AFB1, because of its generally high concentration, resulted of high health concern in 84% of the considered cases.

P-16

Investigating Per- and Poly-Fluoroalkyl Substances (PFAS) Interferences in Food Matrices with High-Resolution Mass Spectrometry

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The widespread use and stability of per- and poly-fluoroalkyl substances (PFAS) has led to their detection in the environment and certain PFAS can bioaccumulate in the food chain. Targeted methods using triple quadrupole mass spectrometers are commonly used for quantification of known PFAS compounds due to their low detection limits and high-throughput capabilities. However, their unit mass resolution can be insufficient to differentiate some PFAS compounds from potential interferences, which can lead to false positives or overestimation of PFAS concentrations. This is particularly challenging for complex matrices, such as foods, and for short-chain PFAS compounds with only one transition. In this study, we utilized the mass accuracy (<5 ppm) and resolution of HRMS to

differentiate PFAS compounds from matrix interferents. For example, we found an interferent for 4:2 fluorotelomer (4:2 FTS) in corn snaplage spiked for method validation that is within the ± 1 Da window of the precursor ion (*m/z* 327.2180 vs *m/z* 326.9743), which also produced interfering product ions for both the quantification (*m/z* 307.1907 vs *m/z* 306.9681) and confirmation (*m/z* 81.0355 vs *m/z* 80.9652) transitions. Using HRMS to differentiate 4:2 FTS from the interferent prevented overestimation of the concentration of 4:2 FTS. We have also observed other PFAS interferences in other matrices including PFPeA interference in chocolate chip cookies. More suspected interferences are being discovered as we test additional matrices, and add additional PFAS compounds to the targeted method, making this HRMS confirmation approach important for ensuring accurate reporting of PFAS concentrations in food.

P-17

Exploring sorption of pesticides in microplastics derived from plastic mulch films used in modern agriculture

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The sorption and vector effect of microplastics on the transfer of pesticides, as well as its impact on agriculture remain largely unexplored. This comparative study is first to investigate the sorption behavior of different pesticides at environmentally realistic concentrations by model microplastics and microplastics derived from polyethylene mulch films. Sorption was found to be up to 90% higher in microplastics derived from mulch films as opposed to pure polyethylene microspheres. For microplastics from mulch films, the sorption for pesticides in media containing $CaCl_2$ were reported to be: pyridate (75.68% and 52.44%), fenazaquin (48.54% and 32.02%), pyridaben (45.04% and 56.70%), bifenthrin (74.27% and 25.88%), etofenprox (82.16% and 54.16%) and pyridalyl (97.00% and 29.74%) at 5 µg/L and 200 µg/L respectively. Sorption was influenced by the octanol-water partition coefficient (log Kow) and ionic strength. Kinetics in the sorption of pesticides were best explained by pseudo-first order kinetic model (R2 between 0.90 and 0.98) while the best fitting isotherm model was Dubinin-Radushkevich (R2 between 0.92 and 0.99). Results suggest the presence of surface level physi-sorption through a micropore volume filling mechanism and the role of hydrophobic and electrostatic forces. Pesticide desorption data in polyethylene mulch films indicate that pesticides with high log Kow were almost completely retained in mulch films, while those with lower log Kow were desorbed rapidly into the surrounding media. Our study highlights the role of microplastics from plastic mulch films as vectors for pesticide transport at environmentally realistic concentrations and the factors that influence it.

P-18

Validation of QuEChERSER mega-method in Insect Samples

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The QuEChERSER method, which stands for “quick, easy, cheap, effective, rugged, safe, efficient, and robust,” was developed in 2019 and has proven to be highly effective in high-throughput residue analysis in several difficult matrices, such as catfish, lamb, beef and hemp. This study was conducted to extend the applicability of the QuEChERSER method in the analysis of insects, which are known to be particularly challenging samples. Two grams of homogenized insect samples were extracted with a 4/1 (v/v) acetonitrile/water solution for 5 minutes by shaking, followed by centrifugation for 3 minutes. In contrast to original QuEChERSER method, where a small portion is transferred into a clean vial and run into LC-MS/MS without further cleanup, we transferred all the extract into a tube for the salting out step. After phase separation 1.5 mL of the extract was transferred into a sample vial, 300 µL of which undergoes clean-up by micro-solid-phase extraction (µSPE). After the clean-up through a ITSP µSPE cartridges the extract was injected in both GC-MS/MS and LC-MS/MS. Finding on the validation and ongoing validation, including two different insects’ samples (black soldier fly and mealworm larvae) will be presented. A comparison of the results obtained by the same batch of spike samples cleaned-up in ITSP and Pal µSPE cartridges will also be included.

P-19

Improvements in Chromatography and Sample Preparation for Resolving Cholic Acid Interferents in Food

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In the analysis of PFAS in foods, the presence of cholic acids can impact the accurate quantification of perfluorooctane sulfonic acid (PFOS) in certain food commodities, such as eggs and seafood. In research ongoing at the FDA, the goals are to optimize the chromatography separation of cholic acids from PFOS and to investigate prototype cartridges for the complete removal of cholic acids from the matrix during sample preparation. This research focuses on testing a variety of mobile phase conditions to monitor their effect on the separation and response of PFOS and cholic acid interferences when analyzed by LC-MS/MS. Additionally, two different prototype GCB-WAX solid phase extraction (SPE) cartridges were tested to determine their ability to remove cholic acids from the sample matrix prior to instrumental analysis. Initial results indicate that modifications to the solvent selection of the organic mobile phase can completely resolve cholic acids separation from PFOS. The prototype SPE cartridges also offer a promising alternative for cholic acid removal.

P-20

Validation of Enhanced Matrix Removal Method for the Analysis of Per-and Polyfluoroalkyl Substances in Priority Food Matrices

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The current FDA method for the analysis of per-and polyfluoroalkyl substances (PFAS) in food and feed was designed to accommodate a wide range of matrices and thus includes several sample clean-up steps. These clean-up steps ensure that the method can reliably be used to analyze nearly any food matrix. An additional simplified method specifically for the analysis of PFAS in milk, egg, fish, and animal tissue matrices is currently undergoing a single-lab validation. This method employs the recently released PFAS EMR II pass-through cartridge by Agilent which contains enhanced matrix removal (EMR) technology as well as additional cleanup sorbents. Preliminary data suggests that the PFAS EMR II cartridge effectively removes lipids from the sample while keeping the recovery ranges for animal tissue between 82-127% for a 50 ppt spike for all 30 PFAS analytes in the current FDA method. Matrix effects were calculated and determined to be negligible. Further recovery and LOQ testing will be discussed for all matrices.

P-21

A Suite of Four LC-MS/MS Assays for Analysis of Pharmaceutical Adulterants in Dietary Supplement Products

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There has been increased scrutiny of dietary supplements in recent years. Particularly when dealing with high-value and widely-used products, specifically in the genre of weight loss, male sexual enhancement, sports nutrition, and joint wellness and pain management supplements. In each of these categories there are numerous pharmaceutical adulterants of interest that may be added illicitly to develop or enhance the advertised health effect. Weight loss supplements may contain anorectic drugs, such as fluoxetine, phenolphthalein, sibutramine, and others. Male enhancement products are frequently adulterated with phosphodiesterase-5 inhibitors including sildenafil, tadalafil, vardenafil along with their structural analogs. Sports nutrition materials may contain various anabolic steroids, beta agonists, SARMs, or growth hormones. Adulterants potentially present in joint health products include NSAIDs, analgesic agents, or muscle relaxants. In each of these instances it is beneficial to testing labs to have aligned method for extraction, dilution, and analysis. The goal of this project was to harmonize all methodologies for adulterant

classes mentioned above while providing reasonably low reporting limits in the range of 1 to 50 ppm in each product. Each analyte class provided its own challenges, including poor ionization, increased matrix effects, need for use of negative ionization mode, isomer coelutions, or poor/excessive retention. We will present data outlining the use of common laboratory reagents and consumables to produce one method for each analyte category and how they are being used together to analyze a variety of relevant dietary supplements representing various dosage forms.

P-22

Determination of Ergot Alkaloids in Commercially Available Cereal-based Food Products using LC-MS/MS

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Ergot alkaloids is a fungal disease caused by fungi of the *Claviceps* genus and is most common in cereal grains such as rye, wheat, barley, and oats. The fungus infects the developing grain or seed as a dark colored crescent shape known as sclerotium, which contains the toxic ergot alkaloid content. In this study, a single laboratory validated LC-MS/MS method was implemented for the quantification of six most prominent EAs and their corresponding epimers in 60 commercially available cereal grain products. Samples were extracted using acetonitrile and water containing 200 mg/L ammonium carbonate (85:15, v/v) and cleaned up using a MycoSep 150 Ergot SPE column. Chromatographic separation of the EAs was conducted using mobile phases under alkaline conditions (pH 9) on a high pH resisted C18 column. Quantitation was performed using an external standard calibration prepared in matrix. The performance of the method was assessed according to quality assurance and quality control processes executed throughout the study. At least one EA was detected in 25 of the 60 products with a range of 0.3-231.2 µg/kg for an individual EA. Ergocristinine was the most detected EA in all analyzed products (23 of 60 products). Total EA concentrations (sum of the 12 monitored EAs) ranged from 0.4-755.0 µg/kg in tested products, with a median total EA concentration of 7.7 µg/kg. Notably, rye-based products had the highest EA occurrence and concentrations, consistent with literature findings, highlighting rye as the main contributor to the EA contamination in cereal-grain products.

P-23

Research and Development of Reference Materials for Cyanobacterial Toxins at the National Research Council of Canada

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The limited availability of cyanotoxin certified reference materials (CRMs) has impeded development and validation of methods required to support cyanotoxin regulation and monitoring programs. Traceable CRMs prepared in compliance with laboratory testing quality standards (e.g. ISO 17025) ensure comparability between measurements carried out at different times or in different laboratories. An understanding of the chemistry and stability of the toxins is required to produce fit-for-purpose CRMs. The large number of toxin variants within each cyanotoxin class makes this a significant challenge.

The National Research Council of Canada (NRCC) has produced a number of publicly-available cyanotoxin CRMs including microcystins (MC-LR, [Dha7]MC-LR, MC-RR, MC LA), nodularin, cylindrospermopsin, anatoxin-a, lyngbyatoxin, as well as several saxitoxins. New CRM projects are selected to expand the range of CRMs available for the analogs that are relevant in the environment. Recent efforts have focused on the preparation of calibration solution CRMs for homoanatoxin-a (hATX-a), [Leu^{1}]MC-LY and MC-YR. These CRMs in-turn play a vital role in the characterization of new dietary supplement matrix CRMs prepared using the non-toxic cyanobacteria *Aphanizomenon flos-aquae* (Cyano A), and *Aphanizomenon flos-aquae* blended with a variety of toxic cultured cyanobacterial species (Cyano-T).

A summary will be provided on the production of cyanotoxin CRMs, outlining key steps in their preparation including algal culturing, toxin isolation, CRM preparation, stability testing, and accurate quantitation. Certified values for these materials are assigned providing traceability to the International System of Units.

P-24

ASTM D8421- Standard Test Method for Determination of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Matrices by Co-solvation followed by Liquid Chromatography Tandem Mass Spectrometry (LC/MS/MS).

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ASTM conducted an inter-laboratory study (ILS) to determine the precision of test method ASTM D8421. EPA Region 5 assisted in preparation and distribution of ILS samples. Eight volunteer laboratories tested eleven different matrices for sixty-eight compounds. Every test result represents an individual determination of samples processed directly in the sample vial according to the method. Each participant received and reported two replicate tests for each material. Additionally, participants were instructed to not dilute and reanalyze off-scale detections since the method was only validated inside the range of the method. This was done to ease the burden on the volunteer laboratories. ASTM Practice D2777 was followed for the interlaboratory design and analysis of the data. This poster will elaborate on the ILS results including precision and bias from the study. This method will be submitted for inclusion in the upcoming Methods Update Rule to 40 CFR part 136.

P-25

PFAS Reference Material Optimization on LC – High Resolution Accurate Mass Spectrometry

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With the EPA finalizing legally enforceable Maximum Contaminant Levels (MCL) for multiple PFAS compounds in drinking water at low ng/L concentrations, it is crucial to understand how different PFAS analytes in reference materials react to solvents and surface interactions. Using the HALO 90 Å PFAS 2.7um x 2.1mm x 100mm column, we explored parameters that could impact data integrity with the analytes in EPA Method 1633, UCMR 5 and EU DWD. The method was developed on ThermoFisher Scientific Vanquish UPLC with Exploris 120 HRAMS, emphasizing the influence of solvent on sample stability and surface effects. Various solvents, blends, and modifiers were evaluated, along with investigating interactions between the reference material ampule and sample vial surfaces and PFAS response factors for designing optimal reference materials. Ratioing response factors against concentrations helped determine suitable concentrations that give similar responses. After the individual analytes were optimized, the response factors were ratioed against the concentrations to give the appropriate concentration for similar response factors.

P-26

Ultra-Fast Multiresidues Accurate Mass Screening Strategy

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In the area of mass food production and global goods exchange, it is crucial to develop ultra-fast screening to assure raw material food safety. Annually in Europe more than 88,000 samples are analyzed for the presence of pesticide residues. It is crucial to develop rapid methods to facilitate swift safety assessment. High resolution accurate mass spectrometry offers a unique opportunity to employ an ultra-fast chromatographic gradient to improve on reliable residue detection in complex matrices. A ballistic short reverse-phase chromatography (4 minutes) was developed with an Agilent Revident LC/Q-TOF system. Broccoli, celery, and strawberry matrices were extracted with QuEChERS and spiked with a pesticide mixture of over 150 compounds and 4 heavy labeled internal standards. A calibration curve was generated from 8 different concentrations (1 to 100 ng/ml) and all injections were completed in triplicate. Initial data were analyzed using embedded screening software, after which they were automatically reinjected in the

case of a non-compliant result using a longer LC/MS method, including identifying fragment information, without interjection by the analyst. With the first pass, over 150 compounds were identified in complex matrices in the calibration range based only on mass accuracy and matching retention time. The review of results was assisted by a commercially available software with 90% of the detected compounds with a match score higher than 90.0 and 96% with a mass accuracy less than 1 ppm independent of concentration. The majority of identified compounds showed good linearity with R^2 values above 0.99.

P-27

End-to-end Workflow for Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Meat, Seafood, Eggs, and Milk

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Per- and polyfluoroalkyl substances (PFAS) comprise a large group of synthetic chemicals used in industrial and consumer products. The dietary exposure to PFAS substances through foods draws more and more attention, calling for the reliable analytical methods for PFAS determination in food. AOAC released a new standard with the limits of quantification (LOQ) at lower to mid part per trillion level for typical animal-origin food matrixes [1]. The ultra-low LOQs and high complexity of animal-origin food matrices pose challenges on the PFAS testing workflow, from sample preparation to LC/MS/MS detection.
In this study, we developed a method using QuEChERS extraction, enhanced matrix removal (EMR) mixed-mode passthrough cleanup using Captiva EMR PFAS Food II cartridges, and LC/MS/MS detection for PFAS analysis in typical animal-origin food matrices. Pre-homogenized food sample was extracted using QuEChERS followed by pass through clean on the EMR PFAS Food II cartridges. Sample analysis was performed using an Agilent 6495D LC-MS system, with the modified LC system using a PFC-free conversion kit. Method calibration was based on neat calibration curve standards with the use of isotopic internal standards. The method was demonstrated to provide below or equal LOQs and acceptable method recovery and reproducibility according to AOAC SMPR 2023.003. The sample preparation method demonstrated a simplified but reliable workflow saving time and effort, and improved lab productivity for food sample analysis.

P-28

Detecting PFAS beyond the Current Regulative Request: a Comprehensive Overview of the Contamination in Water by UPHLC-Ion mobility-HRMS Arnd Ingendoh1; Carsten Baessmann1; Javier Lopez1; Miguel Angel Perez1; Hugo Muller2; Gauthier Eppe3
Presenter: Frank Kero, Ph.D.

Arnd Ingendoh[1]; Igor Nikitin[1]; Carsten Baessmann[1]; Andrea Kiehne[1]; Eva-Maria Niehaus[1]

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PFAS are quite present in the public news as true threat to mankind and nature as “forever chemicals” due to their persistent, bio-accumulative, toxic (PBT) properties and ubiquitous presence in the environment and organisms. The US EPA estimates 15,000 PFAS species as manufactured, precursor and degradation products. This makes their systematic and comprehensive environmental monitoring extremely challenging. Due to the group size, there is a lack of reference standards or spectral libraries, and there are many isomers. Adding trapped ion mobility spectrometry (TIMS) to UHPLC-HRMS allows for comprehensive monitoring of PFAS in environmental matrices without using reference libraries. Here, water samples were analyzed and PFAS identified by the data matching with the NIST PFAS suspect list containing 5,000 entries.

P-29

Automated Sugaring-Out Assisted Liquid-Liquid Extraction and Determination of Neonicotinoids in Honey Samples using a Robotic Autosampler and LC-MS/MS Platform

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Honeybees are experiencing high mortality in both the United States and worldwide. Neonicotinoids, a prevalent class of insecticides, have been detected in honey samples, indicating exposure of bees and other pollinators to these hazardous chemicals. Pesticide exposure is recognized as a significant stressor contributing to this mortality and potentially leading to colony collapse disorder. This research presents a robotic sampling approach to streamline the extraction and analysis of neonicotinoid compounds from honey samples. Sugaring-out assisted liquid-liquid extraction (SULLE) was employed to facilitate the separation of neonicotinoids. By automating the entire extraction process using the GERSTEL MPS roboticPRO sampler, including syringe transfer, controlled mixing, and centrifugation, high-throughput analysis via LC-MS/MS was achieved. The study demonstrated the successful application of the automated liquid-liquid extraction method for various neonicotinoids in honey samples. The extracted analytes were then analyzed using an Agilent Ultivo LC-MS/MS instrument. The recovery rates for different neonicotinoid compounds ranged from 81.5% to 104%, with accuracy averaging 105% and precision averaging 2.28% RSD. These findings underscore the efficacy of the automated extraction technique for accurately quantifying neonicotinoids in honey samples, providing valuable insights into pesticide exposure levels in bee populations.

P-30

Determination of Persistent Organic Pollutants Using an Automated Sample Preparation Workflow

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Persistent organic pollutants (POPs) are toxic chemicals that adversely affect human health and the environment around the world. They persist for long periods of time in the environment and can accumulate and pass from one species to the next through the food chain. To ensure the quality and safety of foods and animal feed, for example, samples are tested for a variety of contaminants like polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F) as well as dioxin-like and non-dioxin-like polychlorinated biphenyls (PCBs). The extraction of POPs from the samples involves tedious, time consuming, and potentially hazardous extraction steps. Modern analytical labs are looking to automation to help increase sample throughput and ensure the safety of workers, while ensuring the resulting data is of the highest quality.
In this study we show the automated workflow for the sample preparation of POPs like PCDD/Fs, PCBs, polychlorinated naphthalenes (PCNs), and polybrominated diphenyl ethers (PBDEs). This includes the extraction of these compounds from food/feed and environmental samples with pressurized fluid extraction, the automated multi-column clean-up using the DEXTech instrument, as well as the concentration of the extracts simultaneously with the D-EVA evaporator instrument. In addition, the DEXTech instruments can perform a variety of clean-up and fractionation methods, including the simultaneous clean-up of PCBs, PBDEs, PCDD/Fs and PCNs in one clean-up run as well as the clean-up of all 209 PCBs separated from the PCDD/Fs.

P-31

Pesticide Residue Analysis of Honey Samples Using a Gas Chromatograph and a Triple-Quadrupole Mass Spectrometer Equipped with a Short Collision Cell

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The use of pesticide agents to increase crop yields is necessary to help meet the food needs of the population. Consequently, regulatory testing of pesticide residues in foods has also become a mainstay to ensure food safety. In addition to concerns about pesticides that are toxic to humans, other important flora and fauna, particularly bees, can also be affected. Bees pollinate crops for us, but if those crops have too much pesticide content, colony collapse and pesticide-related bee deaths are possible. Gas chromatography-tandem mass spectrometry is a common technique for measuring pesticides that can be volatilized. Recently, short collision cell technology has been developed to improve MS/MS analysis by allowing up to 1,000 channels/s for SRM measurement, which translates into more channel time for each pesticide. Several honey samples were collected from different producers and tested for pesticide content. A honey matrix was spiked with 54 pesticides to test the effectiveness of the technique. All samples were processed using a modified QuEChERS technique with an additional dSPE step to mitigate sugar content. Recovered analytes were then measured using a triple-quadrupole GC-MS/MS equipped with a short collision cell. All 54 of the pesticides spiked into the honey matrix were observed at 600 ppb, and 40 of those 54 were observed at 1 ppb or less. Clofentazine and cabaril, as well as a few fungicides, were observed in some of the honey samples. Cabaril is particularly alarming as it is highly toxic to bees.

P-32

Analysis of PFAS in Surface Water and Wastewater Samples by Automated Solid Phase Extraction and QSight LC-MS/MS Based on US EPA Method 1633

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Per- and polyfluoroalkyl substances (PFAS) are a group of human-made fluorinated organic compounds. Due to their unique chemical properties, long-term persistence in environment, and associated risks for human health, PFAS have been classified as persistent organic pollutants and have become the current hot topics around the world. Due to their inert nature, PFAS are very persistent and have been found to accumulate throughout the environment. Originally considered biologically inactive, recent research has revealed their toxicity to humans and wildlife leading to stricter global regulations restricting their levels in food, water, air and soil. US EPA Method 1633 is a widely used method for the determination of selected PFASs in drinking water by solid phase extraction and liquid chromatography/tandem mass spectrometry. Since surface waters are the primary sources of drinking water in many areas around the world, there have been many studies on PFAS exposure in these water resources and the PFAS concentrations were found in the range from low ng/L to µg/L levels. In this study, seven surface water samples collected in Toronto Lakeshore area (Lake Ontario, Humber Bay River, Mimico Creek, and Grenadier Pond) and eight wastewater samples from Ontario, Canada were analyzed using automated SPE and QSight LC-MS/MS based on US EPA1633 method.

P-33

A comprehensive Multi-residue Analysis of Near 400 Pesticides in Tea & 500+ Pesticides in Fruit and Vegetables By QSight LC-MS/MS

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As the most consumed beverage globally, the global tea crop has immense cultural and economic importance. As with any crop, growers use pesticides to ensure high harvest yields and quality resulting in consumer exposure via the brewing process. Pesticides

are frequently found in teas, with 41% of samples reported with at least one residue detected and 10% of samples with a residue above the maximum regulatory limit according to the 2019 European Union report on pesticide residues in food. In some regions a positivity rate of over 6% with a mean concentration of 138 ng/g can be found for chlorpyrifos, which was recently banned in the EU due to increased neurological damage risk in children. The European Commission (EC) has set maximum residue limits (MRLs) for pesticide residues in or on food and feed of plant and animal origin, as detailed in legislative framework Regulation (EC) 396/2005. MRLs vary for given pesticides and food products, but generally, the MRLs are set at 0.01 mg/kg for many fruits and vegetables. Regulatory and testing laboratories face a challenge as consumer preference in organic products increase, pesticide screening lists broaden, and global tea trade and consumption grow. These laboratories rely on mass spectrometry techniques such as GC/MS/MS and LC/MS/MS to quantify pesticide targets, often requiring both instrument platforms to fully cover their target lists. The APCI source in QSight's Dual Source technology can substitute for GC/MS/MS for the analysis of some nonpolar compounds which can reduce cost and complexity for routine analysis laboratories.

P-34

Fast and Robust Analysis of Anionic and Cationic Polar Pesticides Using a New Mixed Mode Column.

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Polar pesticides play a significant role in modern agriculture due to their affordability and high efficiency.
However, their widespread use raises concerns as these pesticides are associated to the food chain through various pathways. Glyphosate, one of the most extensively discussed polar pesticides, has been found in numerous studies to be present in soil, crop products, animals that consume these products, humans, and even in freshwater sources. The emergence of concerns regarding their toxicity and
potential carcinogenic effects highlight the importance of developing accurate and sensitive analytical methods to detect and quantify these compounds. Furthermore, it is particularly challenging to analyze polar pesticides due to their unique physicochemical properties, which encompass both anionic and cationic groups, making them an extremely difficult group of molecules study. Traditionally, two different separation modes are employed to analyze the positive and negative groups,
necessitating the use of multiple columns. In this study, we present two integrated fast and robust methods for separating a suite of anionic and cationic pesticides using a single column. The Luna polar pesticides column is employed for analyzing anionic/negative polar pesticides in a reversed phase mode; while it is utilized for analyzing cationic/positive polar pesticides in a hydrophilic interaction liquid chromatography (HILIC) mode. Additionally, we demonstrate the equilibration time for each method and the impact of switching between the negative and positive modes on the precision and reproducibility of the analysis. By simplifying the analytical process and minimizing the need for multiple columns, our method offers a practical solution for accurately detecting and quantifying anionic and cationic pesticides.

P-35

Method Performance using Dual WAX/GCB and GCB/WAX formats for EPA 1633.

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The US EPA recently released Method 1633 "Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous, Solid, Biosolids, and Tissue Samples by LC-MS/MS".This method involves a two-step sample prep approach using a weak anion exchange (WAX) SPE cartridge and graphitized carbon black (GCB) clean-up in a powder format, known as dispersive Solid Phase Extraction (dSPE). For water samples, GCB is added after WAX extraction, but for soil samples the GCB is added before the WAX SPE step. The purpose of the additional GCB clean-up step is to eliminate matrix that can cause interference and reduce bias. GCB has been shown to remove organic acids (such as humic and cholic acids), which can suppress ionization and lead to low bias on the recoveries (especially for PFOS). However, limitations of using GCB are well known in that this media can bind to longer chain PFAS compounds and lead to lower recoveries. This is stated in the EPA Method 1633, "…It is important to minimize the time the sample extract is in contact with the carbon." Besides these practical limitations, adding GCB in a dSPE step is very labor intensive and therefore not practical due to the extra time needed to add, mix, and centrifuge for each sample, especially in high throughput laboratories. In addition, due to the vague guidelines on using GCB for dSPE listed in the 1633 Draft Method, this step can also lead to higher RSD values. To sort out

this challenge, Strata™ PFAS cartridges were developed as a single cartridge stacked with Strata-X-AW and Strata GCB sorbents that function as a traditional SPE cartridge with a built-in polishing step to meet the method guidelines. We have demonstrated the utility of the Strata PFAS stacked SPE format for PFAS analysis following DOD QSM 5.2/Table B15 for various water matrices. We have shown that using a single, stacked WAX/GCB is cheaper, easier, and ultimately yields better recoveries for PFAS analytes from various water samples. PFAS compounds are not all the same and include differences in carbon length and additional functionality. For example, PFAS compounds include PFCA's from C4-C18, PFSA's from C4-C10, Perfluorooctane Sulfonamide and Derivatives (PFOSA, FOSEs, FOSAs, and FOSAAs), Fluorotelomer sulfonates(FTS) , Fluorotelomer carboxylic acids(FTCA), Perfluoroalkyl ether carboxylic acids (PFECA), Chlorinated Polyfluoroalkyl Ether Sulfonic Acids (Cl-PFESAs) plus four additional compounds Nonafluoro-3,6-dioxaheptanoic acid (NFDHA), Perfluoro(2-ethoxyethane) sulfonic acid (PFEESA), Perfluoro-3-methoxypropanoic acid (PFMPA), Perfluoro-4-methoxybutanoic acid (PFMBA). This poster will present a comparison of SPE cartridges varying in functionality for the extraction of a wide range of PFAS compounds in water. Data will show spike recovery comparisons between WAX + dSPE and a WAX/GCB stacked column.

P-36

Simultaneous Determination of Alternaria Toxins, Ergot Alkaloid Epimers, and Other Major Mycotoxins in Various Food Matrices by LC-MS/MS

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Food commodities are vulnerable to different types of fungal pathogens and could be contaminated with differential classes of mycotoxins. It is ideal to implement a generic method for simultaneous determination of multi-mycotoxins in different food matrices or agricultural products. In this study, a simplified sample preparation procedure and a reliable LC-MS/MS analytical method was developed for comprehensive measurement of 37 regulated and emerging mycotoxins including 5 *Alternaria* toxins, 6 major ergot alkaloids and their corresponding epimers. Four different food matrices (baby wheat cereal, peanut, tomato puree, and blended flour) were chosen for method validation to demonstrate the applicability of this analytical method to a wide range of food types. Chromatographic analysis was performed using MS-friendly acidic mobile phases and completed with a short 11-minute cycling time for proper separation of ergot alkaloid epimers. The recoveries of all mycotoxins (except citrinin) in fortified samples were from 70% to 120%, and the relative standard deviation was less than 20%. The established workflow was simple and fast for multi-mycotoxin determination with a unique benefit of simultaneous analysis of *Alternaria* toxins and ergot alkaloids. Furthermore, a novel inert Biphenyl LC column demonstrated the high degree of Non-Specific Binding (NSB) that occurs between the column's stainless-steel hardware and certain mycotoxins. The implementation of the inert column offers a robust and improved chromatographic performance as it mitigates the NSB for highly adsorptive analytes (e.g. Fumonisins, Aflatoxins, and Tenuazonic acid) leading to better sensitivity and peak shapes without the need of mobile phase additives or sample passivation.

P-37

Method Development for PFAS Analysis Using a Virtual Method Development Tool

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Development and optimization of liquid chromatography (LC) separations can be time consuming and costly, often requiring many steps including literature research, column selection, method scouting, development, and optimization. To mitigate instrument downtime for the method development process, reduce costs and save time, an instrument-free software modeling tool was developed. This free software allows users to select compounds from a database and instantly model separations by adjusting parameters such as instruments/system effects (dwell and extra column volume), temperature, and mobile phase additives, the modeler delivers a fast, no-cost starting point. The current PFAS library contains 57 PFAS compounds and three bile acids, encompassing most analytes for major methods. This work demonstrates how selected methods were virtually developed and transferred to an LC-MS/MS. To determine the software's ability to model separations, acceptance criteria was chosen based on a retention time window of ±15 seconds, selected to represent half a typical MRM window. Results show this virtual tool can be used to develop PFAS methods quickly and accurately with an improved turnaround time, optimize existing methods for the addition of new PFAS compounds, offer an on-demand consultative user experience, and greener solutions for method development.

P-38

Acrylamide Quantitation in a Diverse Range of Food and Beverage Matrices

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Acrylamide is a substance that has been classified as a probable human carcinogen and can form naturally as a byproduct during high-temperature cooking of starch rich foods. Currently, there are no regulations concerning acrylamide in food however, sensitive, accurate and robust testing methods are necessary for food safety and the protection of human health. In this research, a quantitative LC-MS/MS testing method was developed using a SCIEX QTRAP 4500 to measure acrylamide in a diverse range of food and coffee matrices. The AOAC SMPR 2022 006 provides performance criteria for these measurements which can be met by the method presented herein. This testing method boasts a limit of quantitation of 1 ng/mL in neat solution with a linear dynamic range from 1-500 ng/mL and an r^2 value of 0.999. Several food matrices were tested for background contamination of acrylamide and results show high levels in potato chips, biscuits, bread, and baby food. Matrix spike experiments were performed with varying spike levels (20, 50 and 3000 ug/kg) depending on background concentrations (n=6). Mean absolute recoveries of acrylamide in spiked in food matrix ranged from 77-100% demonstrating good method recovery and achieving the AOAC recovery criteria. This method also provides good robustness showing a %CV of 4.1% across 20 replicate injections of extracted potato chip and showing no loss in sensitivity.

P-39

Combined qualitative and quantitative analysis of food packaging materials using the ZenoTOF 7600 system

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Extractable and leachable (E&L) compounds have long been a safety concern, with EU Commission Regulation 10/2011 being in place for over a decade to enforce prohibitions or limit their levels in food contact materials. However, the current regulated list is not exhaustive, which necessitates further characterization of food packaging for other unknown compounds. These components are considered non-intentionally added substances (NIAS) and must be identified to ensure they are controlled to an acceptable level. Here, we explored the combined use of suspect screening, non-targeted screening and MRM^{HR} quantitation on the ZenoTOF 7600 system for the analysis of food packaging materials. The combined workflows demonstrated the benefits of each acquisition mode to fully characterize and quantify compounds in a food contact material. Spectral MS/MS libraries were used to streamline the data processing workflow, reducing the number of compounds that required manual review. For unknown screening, the Formula Finder and ChemSpider tools within SCIEX OS software reduced the time required for compound identification. Further, using the optimized compound-specific parameters in MRM^{HR} acquisition, limits of quantitation (LOQs) as low as 0.1 µg/L were achieved for some compounds. These workflows highlight the ability to perform quantitative and qualitative analyses on the ZenoTOF 7600 system.

P-40

Sensitive quantitation of nitrosamines in multiple foodstuffs using the SCIEX 7500 system

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Nitrosamines are chemical substances that can form in food during processing and cooking. These chemicals have been discovered in various foods, including cured meat products, processed seafood and vegetables, cereals, chocolate, milk and dairy products and beer and other alcoholic beverages. Some nitrosamines have been demonstrated to have genotoxic and carcinogenic effects, specifically N-nitrosodimethylamine (NDMA) which is used as a marker for other nitrosamines. In the United States, there are limits

for NDMA or total nitrosamines in some cured meat products, but no regulatory limits have been established yet for N-nitroso compounds (NOCs) in foods in Europe. Here, a sensitive LC-MS/MS method using the SCIEX 7500 system was developed for the quantitation of 15 nitrosamines in malt, sausage and fish. Limit of quantitation (LOQ) values as low as 0.01 µg/L in solution were achieved for multiple compounds due to the sensitivity of the system used, with linear ranges spanning up to 4 orders of magnitude. Samples were spiked post-extraction at 0.05, 0.5 and 5 µg/kg concentrations, and accuracies between 70% and 130% and %CV values <10% were observed for most compounds analyzed.

P-41

Evaluation of PFAS Levels in Infant Formula based on the AOAC Draft SMPR

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Despite approximately 22 years of research, quantifying the major PFAS exposure routes to humans remains unresolved. Interest in PFAS food analysis as increased in recent years. In the European Union, maximum levels of specific PFAS (PFHxS, PFOS, PFOA, PFNA and sum of the 4 PFAS), in some foods (e.g., meat, eggs, fish, seafood and shellfish) were implemented in January 2023. Further, the AOAC has established as working to develop criteria for PFAS analysis in food. This poster describes a method to analyze 34 PFAS in baby food using a high-end mass spectrometer. 5 g of baby food was extracted with a Quechers method and dispersive SPE. Chromatographic separation was performed using a PS C18 column (150 mm length, 3 µm particle size). Mobile phases were comprised of "A": water with 10mM ammonium acetate and "B": acetonitrile. Gradient conditions were used with a flow rate of 0.8 mL/min and run time of 13 min. The injection volume was 20 µL and column oven was set to 40oC. Two transitions per analyte were monitored except for those analytes which did not have stable secondary transitions. Analyte responses were normalized to their appropriate mass-labelled internal standard response. Method detection limits were determined following the protocol described in 40 CFR Part 136. MDLs were generally within the range of 1-10 pg/g with the exception of 6:2 FTS, PFBA, PFODA and PFPeS which were in the 10s of pg/g. The results demonstrate that low part-per-trillion detection limits in baby food were achieved with the Quechers method and high-end triple quadrupole mass spectrometer.

P-42

Improved laboratory productivity with a single GC-MS/MS configuration for multipurpose environmental analysis

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Analytical testing laboratories play a pivotal role in monitoring common contaminants in different environmental matrices. For volatile and semi volatile substances, gas chromatography is the method of choice for separating compounds including pesticides, polyaromatic hydrocarbons (PAHs), flame retardants such as polybrominated diphenyl ethers (PBDE´s) among others. It is essential that these laboratories meet requirements of established regulations such as U.S. EPA methods or European standards. These laboratories must also overcome other challenges including producing consistent data, maintaining productivity and meeting sample turn-around times. Ensuring these challenges are overcome is essential to ensure laboratories maintain a good reputation.

Due to existing methodologies laboratories need to use different instrument configurations, with either specific consumables including the analytical column or a dedicated detector. This leads to multiple protocols and potential instrument setups required to be operated in a laboratory. Utilizing Gas chromatography coupled with triple quadrupole systems provide the selectivity needed to effectively leverage Selected Rection Monitoring (SRM) as a tool for method consolidation to existing workflows. Laboratories can reduce their need for instrument-specific consumables and components on-hand to reduce costs and complexity with a single instrument configuration. This poster will demonstrates the use of a single hardware configuration for the analysis of different environmental contaminants.

P-43

Accurate and reliable multielement analysis of alternative protein foods using ICP-MS

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Plant-based, protein-rich foods and other alternatives to conventional meat and meat-based food products have long been a part of the human diet—termed here as "alternative protein foods." Historically, foods like soy and other beans, lentils, non-dairy milks like almond milk, locally available edible insects, etc. have been consumed traditionally in many parts of the world and in smaller amounts as "alternative" options elsewhere. In recent times, an exponential increase of the plant-based alternatives has been seen globally due to increasing concerns of the impact of conventional and industrial meat production on the global climate and the environment, as well as ethical concerns and the effects of over-consumption of animal-derived products on human health.
The Commission Regulation (EU) 2023/915121, lays down guidelines on permitted levels of contaminants, including toxic metals, in many different foods including some alternative options. For example, the prescribed limits for Cd in pulses and proteins from pulses in this regulation are 0.040 $mg \cdot kg^{-1}$ and 0.10 $mg \cdot kg^{-1}$, respectively, and analytical techniques must be able to accurately determine such low concentration levels in relevant samples.
For comprehensive multielement analysis of alternative foods, a highly sensitive technology with large linear dynamic range such as inductively coupled plasma mass spectrometry (ICP-MS) is required for low level detection of toxic elements as well as high level detection of nutrients like K and Ca.
In this presentation, a method based on single quadrupole ICP-MS was developed for accurate, fast, and reliable multielement analysis of ten different alternative protein food samples.

P-44

Screening for PFAS by determining AOF with pyrohydrolytic combustion IC: Our lab's results from EPA 1621 Collaboration Study

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Per-fluoroalkyl and poly fluoroalkyl substances (PFAS) are synthetic compounds containing multiple CF2 bonds. PFAS compounds are used in many products and found extensively across nearly all industries. PFAS compounds are persistent and bioaccumulate, and therefore are an environmental contamination concern. A wide range of health concerns have been reported, from mild to acute toxicity, to reproductive and development toxicity. Additionally, public awareness and concerns have grown as PFAS compounds have been reported in various foods. Therefore, screening analytical methods are needed. Pyrohydrolytic combustion – ion chromatography (C-IC) has been demonstrated as a method that eliminates the sample matrix and converts all halogens to halide anions and organosulfur compounds to sulfur species. The ions are then analyzed by ion chromatography with suppressed conductivity. The C-F2 bond in PFAS provides a nearly unique opportunity to use C-IC directly on granular activated carbon (GAC) columns loaded with PFAS-containing water. In this poster, results of the U.S. EPA draft Method 1621 collaboration study by our lab are shown, including method validation tests, analysis of wastewater samples, and recovery results of PFAS standards. In the method, 100 mL of wastewater is adsorbed onto GAC, pyrolyzed under inert gas at 1050 °C, hydrolyzed with oxygen and water vapor, aerated into deionized water (DI). Fluoride is separated from the water dip and other anions by an electrolytically-generated hydroxide gradient on IonPac AS24 anion-exchange column and detected by suppressed conductivity detection. Results showed the method was accurate, 80-120% recoveries, and sensitive, 2.5 µg/L MDLs.

P-45

Meeting the challenges of Dioxin analysis with GC-Orbitrap high mass resolution capabilities

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Polychlorinated dibenzo-*p*-dioxins/furans (PCDD/F) have been a global issue for over six decades. Magnetic sector mass spectrometry has been the gold standard over the past few decades providing the required mass resolution for global compliance. In this study, we evaluated the performance of a GC Orbitrap high mass resolution spectrometer operating at 60,000 mass resolution (200 m/z full width at half maximum (FWHM) to deliver trace analysis of PCDDs / following EPA method 1613. Linear calibration response was observed across all PCDD/F congeners spanning over three orders of magnitude (0.05 – 100 pg/µL) with response deviation being less than 6 %. Average relative response factor was observed to deviate no more that 20% across all calibration points. Analysis run time (i.e., 45 min) was also significantly reduced using the TG-Dioxin column compared to conditions outlined in EPA 1613 using a DB-5 stationary phase without loss in chromatographic resolution efficiency.

At a mass resolution setting of 60,000, this criterion was achieved all targeted analytes across the entire mass range. Simulating the required mass resolution for OCDD under EPA 1613, a mass resolution of approximately 23,000 is needed. At a mass resolution setting of 60,000, a resolving power of approximately 40,000 was achieved, surpassing the criteria needed for EPA 1613 compliance. Quantified results from the analysis of a soil extract spiked with PCDD/F (congener concentration range: 30 – 3000 fg/µL) were in good agreement with spike concentrations.

P-46

Automated targeted and non-targeted LC-Orbitrap MS workflow for analysis of more than 40,000 PFAS compounds in environmental samples

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Per- and polyfluorinated alkyl substances (PFAS) are a class of bioaccumulative, often toxic small molecules featured in environmental targeted methods. However, these labor-intensive solid phase extraction (SPE) methods only measure a handful of the thousands of known PFAS compounds due to a lack of standard availability and compatibility with SPE sorbents. This work describes an automated dispersive liquid-liquid microextraction (DLLME) method applied to water samples to reduce solvent consumption, cost-per-sample, and sample contamination. These extracts were analyzed using a targeted quantitative and non-targeted screening LC-Orbitrap MS method. Non-targeted results were compared against a 40,000+ PFAS compound library including a new in silico predicted transformation library. For this method, a panel of 53 PFAS compounds of interest to both North American and European regulatory bodies was quantified alongside untargeted analysis across multiple environmental matrices. Quantitative results show limits of quantitation down to part per trillion levels for most analytes. The automated DLLME method provides a cleaner, more concentrated sample than direct injection approaches while providing some of the sensitivity gains seen from solid phase extraction. Untargeted data generated from this experiment includes a list of suspected compounds detected along with their confidence level for each sample matrix. This overall workflow provides an automated solution to both quantify known PFAS and explore potential unknown PFAS with confidence.

P-47

An Integrated GC-MS/MS and LC-MS/MS Workflow for Quantitative Analysis of Pesticides with Cross-confirmation using a Single Chromatography Data System Software

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According to the World Health Organization, more than one thousand different pesticides are used to protect crops from pests to increase yields and to minimize deterioration of agricultural products during storage and transportation. Consequently, laboratories are tasked to develop methods with a broad scope to detect, correctly identify, and quantitate hundreds of different pesticides and their transformation products in diverse sample matrices, and often at levels well below maximum residue levels (MRLs) set by regulatory bodies.

Careful optimization of over 700 pesticide residues was performed on LC-MS/MS and GC-MS/MS triple quadrupole platforms. Sampe preparation was based on QuEChERS method AOAC 2007.01. It was discovered that approximately 48% of the residues tested were amenable to both techniques. As a result, an integrated workflow was developed within a chromatography data system software package that allowed merging of results from each analysis into one convenient UI for data acquisition and processing. This allowed for cross-confirmation between the two techniques, where both GC and LC results are visualized side-by-side and reports were generated with pre-configured templates checking compliance against quality control criteria such as the EC SANTE guidelines. The developed methods and cross-confirmation approach were applied to the quantitative analysis of performance test (PT) samples of green beans and wheat. The results for all the pesticides in the PT test were all within the minimum and maximum values with z-scores mostly below 1. Other figures of merit along with examples showing the benefits of cross-confirmation visualization in the UI will also be shown.

P-48

A Novel Ion Chromatograph for Fast Anion Analysis in Drinking Water with Built-in Flexibility to Adapt to New Regulations

Terri Christison [1] and Ed George[2]; **Thermo Fisher Scientific**, Sunnyvale, CA[1]; San Jose CA[2]

Ion Chromatography (IC) has been an extremely useful tool in many environmental applications over the years. From common anions in drinking water to perchlorate analysis to hexavalent chromium, IC is a key technology to meet existing and emerging regulations. Recently, the State of California has passed a new regulation stating municipalities must measure hexavalent chromium instead of total chromium, down to a limit of 0.02 ppb. The rule is the first in the nation to specifically target chromium-6, and the regulation is expected to reduce the number of cancer and kidney disease cases from long-term ingestion.

Along with achieving resolution and sensitivity requirements, labs require an IC system which must operate in a robust manner and allow optional accessories that can be swapped in and out of the instrument by the user very rapidly for extended application capabilities as their needs change. This novel platform is easily tailored to meet current analytical requirements, and at the same time, allow for cost-effective extension of IC capabilities into new workflows that may emerge.

This poster presents a new, flexible platform which can quickly run the seven common anions in drinking water in under 5 minutes according to the US EPA 300 and 300.1 and perchlorate according to US EPA 314.0 and ISO 19340. This new system has also demonstrated the analysis of hexavalent chromium using post-column reaction and UV/VIS detection in accordance with US EPA 218.7.

P-49

A Robust Extraction Method For Monitoring 6PPD-Q and Other PPD-Quinones in Fish Tissue

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6PPD-quinone (6PPD-Q) is an ozonation by-product of the tire antioxidant 6PPD, which emerging research shows poses a significant threat to aquatic ecosystems. Other PPD quinones are also created through tire degradation, with toxicities yet to be evaluated. Since the focus is currently on measuring levels of these contaminants in water, not many studies have been published concerning testing in other matrices. As the primary toxicity is known to affect aquatic organisms, this poster explores the extraction of fish tissue using a QuEChERS approach combined with UCT's dual-phase cartridge clean-up for extraction of 6PPD-Q and other PPD-Qs with commercially available reference standards. A matrix-matched internal standard calibration is performed, followed by LOD and LOQ studies to determine detection limits. The extracts are analyzed using UCT's SelectraCore C18 HPLC column using LC-MS/MS in positive ionization mode. 6PPD-Q, the compound of most interest, is quantitated using isotope dilution, with the remaining PPD-Qs quantitated using an extracted internal standard model. A deuterated 6PPD-Q measures instrument performance as an instrumental internal standard. Recoveries are optimized for 6PPD-Q to be between 70 – 130 % at low and medium levels of the calibration curve. This method demonstrates a robust extraction and fast analysis method for analyzing these emerging contaminants in fish tissue without complex procedures.

P-50

Analysis of PFAS in Food using SPE concentration and cleanup with determination using LC-MS/MS – Part 1: Vegetable, Fruit and Baby Food

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This study introduces an optimized LC-MS/MS methodology for the comprehensive analysis of Per- and Polyfluoroalkyl Substances (PFAS) in vegetable, fruit, and baby food. The method demonstrates an exceptionally low limit of quantification, reaching 0.0005 µg/kg for some compounds in matrix, while accurately detecting and quantifying the PFAS compounds listed in the Commission Recommendation (EU) 2022/1431. The combination of enhanced sensitivity of the Xevo™ TQ Absolute MS System, with the increased clean-up efficacy of a prototype bilayer dual-phase GCB/WAX SPE cartridge gave excellent recoveries, between 87 and 116% for the mandatory PFAS, and between 65 and 131% for the majority of the recommended compounds along with repeatability (RSD_r) ≤10%.

P-51

Identification of short chain per and polyfluorinated alkyl substances (PFAS) using ion ratios with low mass product ions

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As the environmental impact and health hazards of legacy long chain (≥C8) PFAS emerged, they started to be substituted for short (C4-C7) and ultrashort chain (≤3) PFAS in manufacturing. The belief was these would have less of an impact but initial evidence suggests

that there are still concerns regarding their effects. The analysis of the carboxylate PFAS with chain lengths C3-C4 is problematic in terms of positively identifying the analyte due to the lack of a second product ion with suitable intensity to use for ion ratio calculations to meet common identification criteria. The use of m/z 19 is possible and this response can be significantly improved using a modified high performance tandem quadrupole mass spectrometer.
For a number of short and ultrashort chain PFAS, predominately carboxylates with a carbon chain length of 5 or less (PFPrA, PFBA, PFPeA), there has been no mass product ion (m/z ≥50) identified to use to create ion ratios. Initial work has been carried out on a high performance negative ion tandem quadrupole mass spectrometer to show that the detection of a fluoride ion (m/z 19) was possible using the standard configuration, but the ion ratios measured were between 0.001 to 0.002. By modifying the mass spectrometer improved sensitivity for the fluoride ion was achieved, and initial results show the increase in response was 2 orders of magnitude. Using this modified system, the ion ratios measured were between 0.054 and 0.074 making confirmation of analyte identity by ion ratio a realistic possibility.

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Direct injection screening method for Per-and-polyfluoroalkyl substances in drinking water using a prototype benchtop multi-reflecting Time-of-flight

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The widespread use of Per and polyfluoroalkyl substances (PFAS) in industrial processing and manufacturing over the last decades has led to global environmental and health concerns. As the number of these compounds continues to increase, it is becoming a challenging task to monitor PFAS using the traditional targeted methods. Screening workflows using High Resolution Mass Spectrometry (HRMS) is an ideal bridge for monitoring the regulated PFAS and detecting non-regulated PFAS. In this study, samples and standards were directly injected and analyzed using an ACQUITY™ Premier UPLC™ system coupled to a prototype benchtop multi-reflecting time-of-flight (MRT) mass spectrometer.
The screening workflow is based on accurate mass, fragment ion information, isotopic matching and mass defect, this coupled with high mass resolution, fast scan speeds and exceptional levels of mass precision of the prototype MRT significantly reduces false positives and enables rapid and confident assignment and identification of PFAS. The UNIFI™ screening workflow within waters_connect along with the PFAS libraries (in-house and the online version of CompTox library), enabled the identification of multiple PFAS compounds in the spiked drinking water samples with typical mass measurements and mass resolution within 200 ppb and 100,000 (FWHM) respectively. A variety of the PFAS components were readily identified, including the short-chain PFAS's, perfluorobutane sulfonic acid (C4, PFBS) and perfluorohexane sulfonic acid (C6, PFHxS). The work described demonstrates the exceptional mass accuracy, sensitivity, high mass resolution, and dynamic range of the prototype MRT for non-targeted PFAS screening.

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Confirmation of Dioxins and Dioxin-like Substances at Sub-Femtogram Levels Using Atmospheric Pressure Gas Chromatography (APGC) MS/MS

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Polychlorinated dibenzo-dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs) are a group of chemically related compounds that are toxic and persistent organic pollutants (POPs). These compounds are restricted internationally under the Stockholm Convention. Since they are bioaccumulative, it is essential to monitor them at ultra-trace levels in food and environmental samples. Traditionally

these compounds have been analyzed using magnetic sectors with electron ionization (EI) sources, requiring expert users to obtain consistent results. As there is a growing concern for the analysis of Dioxins, more accessible technology is essential for sample analysis. Results from the APGC-MS/MS testing showed excellent linearity of 2,3,7,8-TCDD between 100 ag to 100 pg on column with an R2 of 0.998. At 100 ag on-column for TCDD, the signal to noise was calculated at 5.7 while at 250 ag the signal to noise was 20.7. These limits far surpass the required regulatory values for limit of detection and limit of quantitation. An on-column standard of 2,3,7,8-TCDD at 100 fg was injected over 20 days to assess reproducibility of the system. The RSD over 1000 injections during the 20 days was 9.2% with no internal standard correction. The isotope ratio stability of the same 100 fg sample over the 1000 injections was better than +/- 10%. Atmospheric Pressure Gas Chromatography (APGC) coupled to a highly sensitive tandem quadrupole mass spectrometer allows analysis of sub-femtogram levels of dioxins surpassing regulatory requirements traditionally set for magnetic sectors.

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Quantitation of PFAS in Salmon Tissue Using LC-MS/MS and Dual-Phase SPE to Meet EPA Method 1633 Requirements

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In January 2024, the US Environmental Protection Agency (EPA) finalized Method 1633, an LC-MS/MS method for the detection of 40 per- and polyfluoroalkyl substances (PFAS) in various aqueous matrices. Data resulting from this methodology serve as a crucial indicator of PFAS contamination in aquatic environments and could also extend to seafood. At the time of publication, EPA Method 1633 stands as the only multi-laboratory validated method for quantifying PFAS in fish tissue.
This "performance-based" method allows for modifications that enhance performance, so Oasis™ GCB/WAX for PFAS dual-phase SPE cartridges were used instead of dispersive graphitized carbon black. Salmon samples were spiked with mixed internal standards before and after solvent extraction, concentration, and SPE cleanup. An ACQUITY™ Premier UPLC™ System and Xevo™ TQ Absolute Mass Spectrometer were used for sample analysis.
The 11-minute LC-MS/MS method achieved experimental percent recoveries and relative standard deviations (% RSDs) within acceptable ranges for the extracted internal standards, with the mean extracted internal standards recovery being 85% with a %RSD of 9.2%. Additionally, the target PFAS analytes fell within acceptable ranges. Notably, the detection and calibration ranges resulting from the ACQUITY Premier UPLC System and Xevo TQ Absolute Mass Spectrometer were significantly lower than those presented in EPA Method 1633. This presents an opportunity to reduce sample size and expedite sample preparation for higher throughput laboratories.

P-55

Determination of chlormequat chloride residues in cereals by LC-MS/MS

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Recent reports from the US show residues of the growth regulator, chlormequat chloride, in a range of cereal products, despite the lack approval other than for imported cereals. Waters previously developed a LC-MS/MS method for the determination of highly polar and cationic pesticides and growth regulators in various food commodities. The method is based upon extraction with the established Quick Polar Pesticides method (QuPPe) using the BEH™ Amide Column. This application brief shows the evaluation of the performance of this method for chlormequat chloride, in a representative cereal sample, using an ACQUITY™ UPLC™ I-Class Plus System and Xevo™ TQ-S cronos Tandem Quadrupole Mass Spectrometer. Sample of different cereal flours were spiked at 0.05 mg/kg. The accuracy of the method, using an internal standard, was evaluated and apparent recovery found to be within the range 94 to 102% and repeatability (RSDr) < 4% RSD. Additional verification of performance was obtained from the analysis of QC reference materials, the results from which compared well with the assigned values. This demonstrated that the method could be suitable for checking compliance with any MRLs/tolerances and has the potential for determination at much lower concentrations, for example in the absence of any MRLs/tolerances and for food business operators' due diligence testing and brand protection.

P-56

Determination of glyphosate, aminomethylphosphonic acid (AMPA), and glufosinate in drinking water using direct analysis by LC-MS/MS

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Reliable analytical methods are needed for detection, quantification, and identification of glyphosate, aminomethylphosphonic acid (AMPA), and glufosinate in drinking water. Accurate and reliable methods are required to monitor these widely used pesticides in drinking water from different sources. This work describes a simple direct analysis method, based on liquid chromatography coupled to tandem mass spectrometry (LC–MS/MS), which avoids the need for lengthy and laborious derivatization and solid-phase extraction (SPE). Samples of water were injected directly into the LC-MS/MS (ACQUITY™ Premier System with Xevo™ TQ Absolute Tandem Mass Spectrometer System) using the Anionic Polar Pesticide Column. The performance of the method was successfully evaluated in three different types of drinking water. The extremely high sensitivity of the Xevo TQ Absolute System was demonstrated with reliable detection for all three analytes at concentrations as low as 10 ng/L (0.01 µg/L). The performance of the method was evaluated in-house and by an inter-laboratory study using spiked water samples. Results from both studies showed that the trueness of the method was between 82 and 110%. Close agreement was observed with the repeatability, within laboratory reproducibility, and between laboratory reproducibility, all being <16% RSD. The method is considered sensitive, specific, accurate, and suitable for the determination of these challenging analytes in a range of different types of drinking water, for checking compliance with regulatory limits, and to support studies focusing on human exposure.

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Adapting GC-HRMS Analysis of Organochlorine Pesticides to GC-APCI MS/MS Using Nitrogen Carrier Gas

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Organochlorine pesticides (OCPs) continue to be an important class of contaminants to monitor for in environmental samples such as biota and sediment because of their persistence in the environment beyond their initial use. It is also noteworthy, and perhaps surprising, that even though most OCPs are banned by regulations and treaties worldwide, annual global production of DDT in 2020, for instance, has still been estimated at 1,071 tons. Furthermore, their tendency to bioaccumulate contributes to their toxicity in living organisms. When combined with their ready transport through the environment the importance of continued monitoring becomes evident.

Due to the rigorous requirements of monitoring for these analytes at trace levels in complex matrices, electron ionization (EI) high resolution mass spectrometry (HRMS) has often been applied to this work in the past. However, the barriers to implementing and maintaining magnetic sector based EI GC HRMS instruments and methods have only increased across time. Meanwhile, gas chromatography atmospheric pressure ionization (GC-APCI) combined with tandem mass spectrometry (MS/MS) has increasingly been successfully applied to challenging analyses, such as dioxins, while meeting or exceeding the stringent quality control criteria of even the most rigorous methods. In this study we investigate the conversion of an EI GC-HRMS reference method targeting 39 OCPs based on helium carrier gas to a method using GC-APCI MS/MS and nitrogen carrier gas. Comparison of the quantification results, sensitivity and chromatographic separations between the two techniques will be presented.

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