

BP4NTA Newsletter

A mixture of business, social, and news

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From the Chair

Dear BP4NTA Members,

It is my pleasure to introduce myself as the newly elected chair of BP4NTA. Over the coming year I hope to continue to support the exceptional efforts of our

committees and members in advancing NTA activities across scientific fields. You can see other newly elected steering committee members and chairs on page 3 and learn more about them by visiting our website <https://nontargetedanalysis.org/about/leadership/>.

As the chair of BP4NTA, I would like to extend a warm invitation to participate in our committees and learn from our [webinars](#) and educational materials. Non-Targeted Analysis is a rapidly maturing field with huge opportunities for environmental and public health - but it needs all of our expertise to guide its growth. Whether you are a seasoned expert looking to share your knowledge, organize a committee on an NTA project, or collaborate with other experts - or a new NTA user looking for guidance, scientific talks, or to contribute to ongoing NTA efforts - BP4NTA has a place for you.

If you are interested in getting involved, please consider become a member. You can seek out the leadership of our existing subcommittees to see how you can participate or approach me or any other members of the steering committee if you have an interest in starting a new subcommittee for a project or interest area.

Cont'd on pg. 2

From the Chair cont'd

Cont'd from pg. 2

Our newest technical committee (page 4) focused on PFAS is less than a year old! And as always, please enjoy our monthly webinars and the content available on the BP4NTA website. We anticipate making some updates to the website throughout the year to better support membership and content delivery.

I look forward to an exciting year ahead, and hope to see you all along the way!

James McCord, PhD
Chair, BP4NTA (2024-2025)

Visit our website:
nontargetedanalysis.org



Meet BP4NTA's Chair

James McCord, U.S. EPA

Employment & Outside Positions: Chemist, US Environmental Protection Agency, Office of Research and Development, Research Triangle Park, North Carolina

Current Research or Employment Focus: My non-targeted analysis work is focused on novel-compound elucidation, technical support investigations of manufacturing facilities, and methods standardization for NTA to support decision making.

Any Career Highlights? Our work in PFAS elucidation identified several new classes of PFAS that are now part of routine PFAS monitoring and regulations (e.g. GenX & Nafion by-products in NC, CIPPEACAs in NJ).

Educational Background: I received my PhD in Chemistry at NC State University where I did proteomics research. My undergraduate BS is also in Chemistry, from the University of North Carolina – Chapel Hill; although I was interested in teaching and also completed an Education program.

Past Involvement with/Contributions to BP4NTA: Prior to my position as Chair I worked on the Stakeholders committee due to my interests in spreading NTA techniques and identifying research needs for NTA adoption.

What excites you most about NTA/Why does NTA matter? Non-targeted analysis has the potential to be the perfect synthesis of measurement methods over the past 50 years. If you can measure thousands of chemicals and link them to thousands of other data points it's giving you access to the raw firmament of chemical interactions; you can look at co-exposures, find new chemicals, and unravel relationships in biology and environmental systems.

What do you think is our biggest scientific challenge in the next 100 years? I think the biggest challenge is going to be dealing with complexity. I feel like it's common for every scientific generation to feel like the "low-hanging fruit" is already plucked, but we are dealing with exponentially increasing levels of new understanding in basically every field. No more "Renaissance Men," we have to figure out communication strategies and ways to get information to flow between different complex domains and address really complicated interconnected problems.

What are your hobbies? I rock climb and backpack as much as I can. I love being outdoors and it gives me a feeling of place. I also bake a lot of bread.

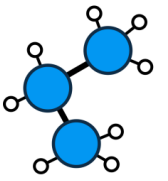
What's the best piece of advice you've ever been given? There is a quote often attributed to Hemingway that there is no virtue in being superior to your fellow man, only in being better than your former self. I think as a life philosophy that is good to keep in mind; we should try to make ourselves and our work better rather than worry about comparison.

What's the weirdest food you've ever eaten? I was served a flower of *Acmella oleracea*, which is in the Daisy family but makes your mouth tingle and go numb. Definitely a weird experience.

What is the most interesting thing in your workspace (laboratory, office space, home office)? I like to hang posters and vintage advertisements around where I work to give me a little temporal perspective. I have an old ad touting the benefits of leaded gasoline, one implying that failure to provide adequate bathroom tissues leads to communism, and another that reminds me that working towards platonic ideals is being a moth drawn into flame.



BP4NTA Has a New Charter!



Charter Approval

In January 2024, BP4NTA members voted to approve an official charter for the organization. Adopting the charter is the first official step towards BP4NTA becoming a legal nonprofit organization. The synthesis of the charter, which outlines a new organizational structure for BP4NTA, was initiated by past-chairs Christine Fisher (O'Donnell) and Ruth Marfil-Vega with significant input from Robert Young, Elin Ulrich, and Kathy Peter.

With the new operating structure, the BP4NTA Steering Committee is led by an elected Chair and supported by a Vice Chair, Past Chair(s), Secretary, Treasurer, Technical Liaison and Operations Liaison. The Technical Liaison interacts directly with subcommittees for the development of technical scientific products (current technical subcommittees: stakeholder, PFAS, Study Reporting Tool (SRT), and Study Planning Tool (SPT)). These technical committees are expected to change overtime as products are developed and new products are in progress. The operations subcommittees include Outreach, Awards, Elections, and Membership.

Looking Ahead...

Once we achieve official nonprofit status, BP4NTA is planning to implement a new tiered membership system where members can pay a small annual fee to have voting rights and hold committee positions. Voting members will have the opportunity to participate in any future decisions reached via a consensus procedure as outlined in the charter. Membership fees are an undesirable but necessary step to address administrative needs for BP4NTA, such as the maintenance of the BP4NTA website, and we hope they can improve the quality and accessibility of BP4NTA products by funding more open access content such as publications and educational media. Non-voting members (no fee) will still reap the many benefits of public BP4NTA events.

BP4NTA welcomes and encourages new ideas for tools and products that fit this mission! If you have ideas that could benefit from leveraging the BP4NTA network please let the technical and/or operations liaison know.

The Charter is [available to view](#) on the members-only BP4NTA Teams channel. Please reach out to James McCord if you have trouble accessing it or have further questions.

Meet BP4NTA's Secretary

Robert B. Young, CSIRO

Employment & Outside Positions: I am a Senior Research Scientist for CSIRO, Australia's national science agency, working in the Contaminants and Mitigation group of Industry Environments, and based in Adelaide, South Australia. In addition to my role as BP4NTA Secretary, I'm an elected member of the NSF-funded National High Magnetic Field Laboratory (NHMFL) Ion Cyclotron Resonance (ICR) Facility User Advisory Committee.

Current Research or Employment Focus: I have been using high resolution mass spectrometry-based non-targeted analysis methods to detect and identify per- and polyfluoroalkyl substances (PFAS) in groundwater, and toxic compounds in produced water from oil and gas development. These projects have produced exciting collaborations with the US EPA, the NHMFL ICR Facility, the US Naval Facilities Engineering and Expeditionary Warfare Center (NAVFAC EXWC), and members of the New Mexico Produced Water Research Consortium (NMPWRC), as well as my current (CSIRO) and previous (New Mexico State University) employers. I also work with the NHMFL ICR Facility to characterize complex organic mixtures like dissolved organic matter, petroleum hydrocarbons, and biofuels.



Any Career Highlights? NMSU University Research Council Team Award for Exceptional Achievements in Creative Scholarly Activity (January 2024)

Educational Background: Ph.D., Environmental Chemistry, Colorado State University (2014); J.D., Columbia University (1991); B.B.A., Finance, University of Texas (1988)

What excites you most about NTA/Why does NTA matter? For me, the most exciting thing about NTA is the ability to screen environmental samples for a range of contaminants, by-products, and other characteristic chemicals without predetermining what to target. The better we are at identifying whatever is present in a sample, the less likely we are to miss something important, and the easier it will be for us to develop relevant targeted methods.

If you were a wrestler what would be your entrance theme song? Enter Sandman, by Metallica. (It has been used as an entrance theme song by a couple of baseball players, and it's very effective!)

If you could have lunch with anyone (past or present) who would it be and what would you talk about? Chuck Leavell. He's a mostly self-taught musician who was a member of the Allman Brothers Band at their commercial peak, and keyboardist and musical director of the Rolling Stones for decades when touring. He's an award-winning Georgia tree farmer and conservationist, and a friend of Jimmy and Rosalynn Carter. To top it off, he's been married to the same woman for more than 50 years. Chuck Leavell seems to excel at everything and stay down to earth. He must have some interesting experiences and life lessons to share!

If you could choose to have any superpower, what would you choose and why? Ability to learn by osmosis or Matrix-style download. I like learning, but am interested in so many things that it's difficult to learn fast enough!

If you weren't a scientist, what would you be doing? Software developer. I hated computer science and chemistry in high school and college. Now I love them both.

BP4NTA Organizational Structure

STEERING COMMITTEE



Chair
James McCord



Vice-Chair
Sara Nason



Past Chair
Christine Fisher (O'Donnell)



Past Chair
Ruth Marfil-Vega



Secretary
Robert B. Young



Treasurer
Stephan Baumann



Technical Liaison
Jon Sobus



Operational Liaison
Gabby Black

OPERATIONS COMMITTEES



Elections and Awards Committee
Chair
Elin Ulrich



Membership Committee
Chair
Marci Smeltz



Outreach Committee
Chair
Esra Mutlu



Outreach Committee
Content Lead
Allison Phillips



Outreach Committee
Website Manager
Anna Feerick

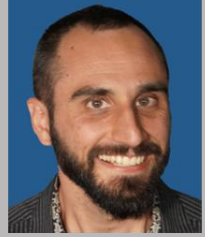


Outreach Committee
External Affiliations Liaison
Drew Szabo



Outreach Committee
Journals/Events Lead
Keaton Nahan

BP4NTA Technical Committees



Stakeholder Committee
Chair
Sara Nason

Study Planning Tool
Co-Chair
Niti Shah

Study Planning Tool
Co-Chair
Heather Whitehead

PFAS Working Group
Co-Chair
Jacqueline Bangma

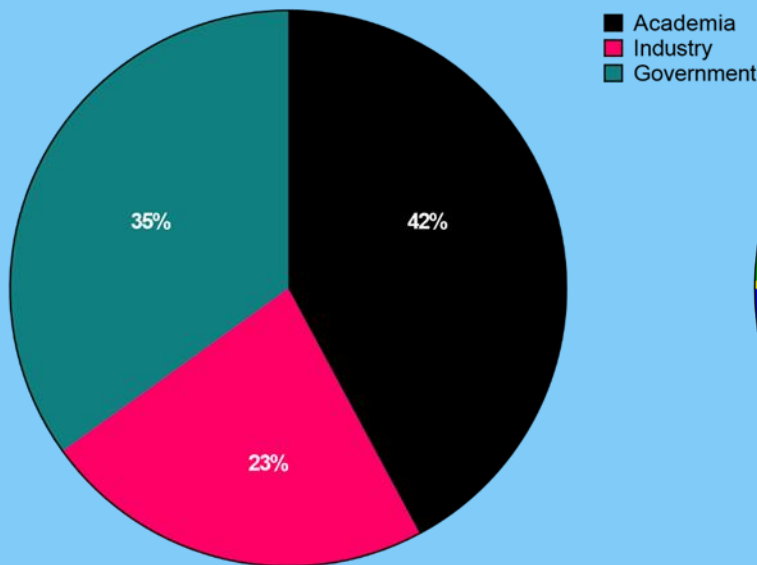
PFAS Working Group
Co-Chair
Jeremy Koelmel

Become a Member!

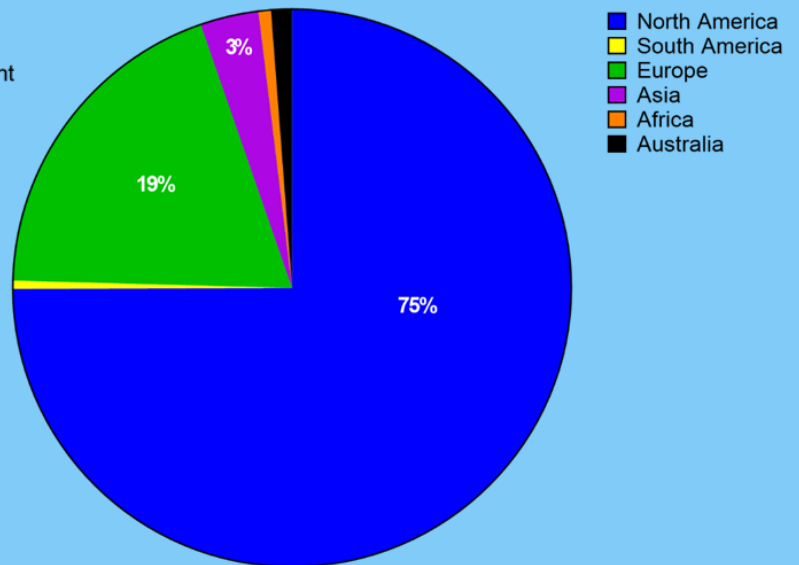
<https://nontargetedanalysis.org/become-a-member/>

As of April 15, 2024, BP4NTA has **415 individuals** that have requested interest in our working group. This large, diverse group has worldwide coverage with a large distribution of affiliations in government, academia, and industry (including research institutes and consultants).

Distribution by Sector



Distribution by Continent

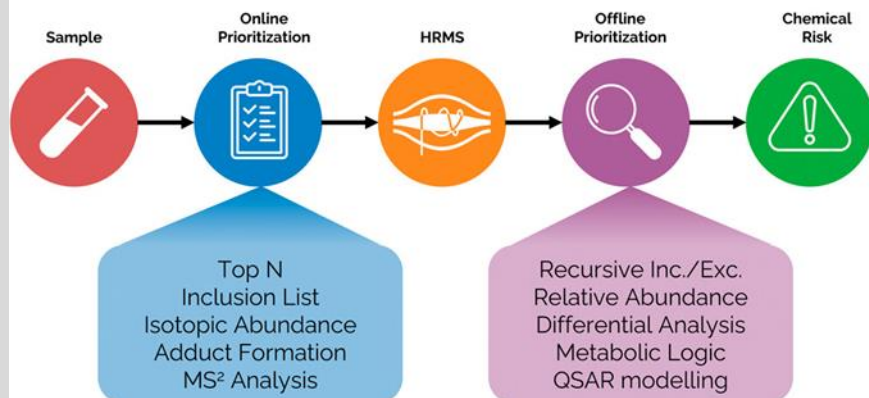


Under the Operational Committees, the Membership Chair manages all active participants in BP4NTA. We are currently working to streamline requests for membership by adding their email address to our listserv as well as providing access to our Teams page if requested. In the future, this role will be responsible for recruiting new members as well as maintaining our large membership.

If you are experiencing any issues with receiving emails or cannot access the Teams page, please reach out to the current Membership Chair, Marci Smeltz (smeltz.marci@epa.gov).

Publications & Presentations

HRMS Prioritization



Online and Offline Prioritization of Chemicals of Interest in Suspect Screening and Non-targeted Screening with High-Resolution Mass Spectrometry, Drew Szabo, Travis M. Falconer, Christine M. Fisher, Ted Heise, Allison L. Phillips, Gyorgy Vas, Antony J. Williams, and Anneli Krueve, *Anal. Chem.*, February 21, 2024, 96, 9, 3707–3716, DOI: 10.1021/acs.analchem.3c05705.

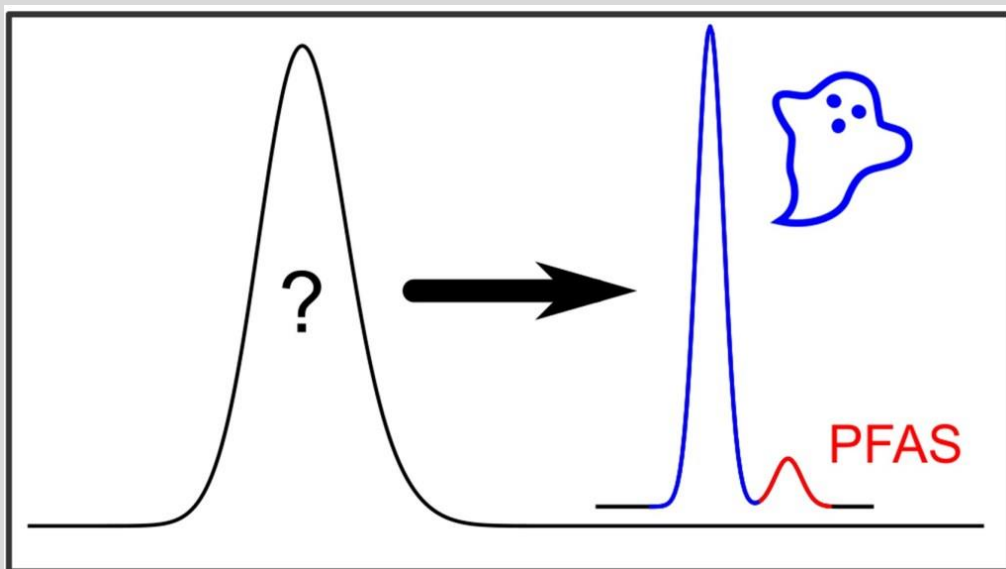
<https://pubs.acs.org/doi/10.1021/acs.analchem.3c05705>

Establishing performance metrics for quantitative non-targeted analysis: a demonstration using per- and polyfluoroalkyl substances, Shirley Pu, James P McCord, Jacqueline Bangma, and Jon R Sobus, *Anal Bioanal Chem.*, 2024 Feb;416(5):1249-1267. doi: 10.1007/s00216-023-05117-4. Epub 2024 Jan 30.

<https://www.ncbi.nlm.nih.gov/pmc/articles/38289355/>

Quantitative Targeted Analysis			Quantitative Non-Targeted Analysis	
Approach 1:	Approach 2:	Approach 3:	Approach 4:	Approach 5:
- Targeted Acquisition	- Targeted Acquisition	- Non-Targeted Acquisition	- Non-Targeted Acquisition	- Non-Targeted Acquisition
- Calibration Curve	- Calibration Curve	- Calibration Curve	- Expert-Selected Surrogates	- Global Surrogates
- IS Normalization	- No IS Normalization	- No IS Normalization	- No IS Normalization	- No IS Normalization

Accuracy, Certainty & Reliability	?	Generalizability
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PFAS ghosts: how to identify, evaluate, and exorcise new and existing analytical interference, Jacqueline Bangma, Kitrina M Barry, Christine M Fisher, Susan Genualdi, Theresa C Guillet, Carin A Huset, James McCord, Brian Ng, Benjamin J Place, Jessica L Reiner, Anna Robuck, and Alix E Rodowa, *Anal Bioanal Chem.*, 2024 Mar;416(8):1777-1785. doi: 10.1007/s00216-024-05125-y. Epub 2024 Jan 27.

<https://www.ncbi.nlm.nih.gov/pmc/articles/38280017/>

Email BP4NTA Outreach Chair, Esra Mutlu (Mutlu.esra@epa.gov), to have your publication featured on BP4NTA social media or in our next newsletter!

Recent and Upcoming Webinars

BP4NTA holds monthly meetings, alternating business discussions with presentations by Non-Targeted Analysis practitioners (including non-BP4NTA members). Join us the 3rd Tuesday of every month, at 12 p.m. EST!



March 19: “Periodic Table of Foods Initiative (<https://foodperiodictable.org/>) – developing standardized analytical approaches and centralized data processing to characterize food supplies.”

Steve Watkins, PhD | Founder & Director, Verso Biosciences; CEO, BCD Bioscience

April 16: “Linking NTA and Toxicity/Methods Information.”

Tony Williams, PhD | Scientist, U.S. Environmental Protection Agency



May 21: “The use (and challenges) of NTA to drive regulatory actions.”

Sin Urban, PhD | Chief, Environmental Sciences at the Maryland Public Health Laboratory



June 18: “Ion mobility spectrometry paired with NTA.”

Erin Baker, PhD | Associate Professor, University of North Carolina



July 16: “Knowing Known Unknowns: A Vision for Non-Targeted Analysis Product Offerings.”

Sarah Choyke, PhD | Technical Director, Eurofins Environmental Testing

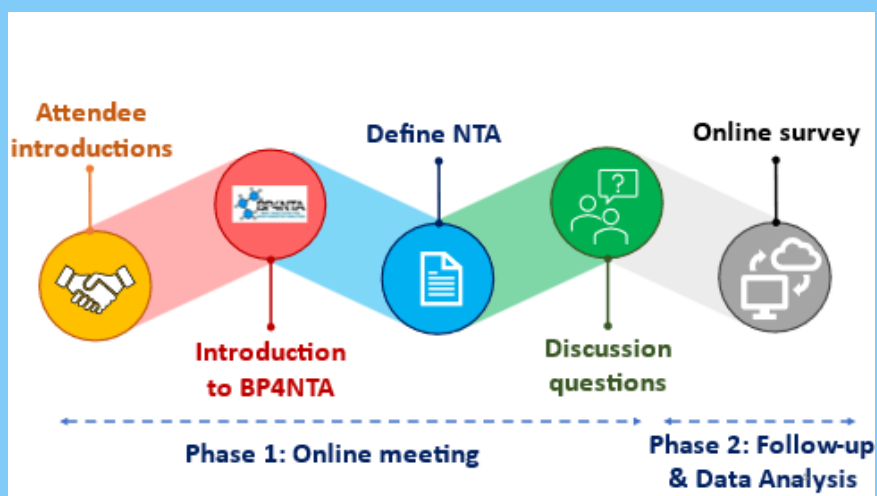


Access these presentations and other past BP4NTA webinars [HERE](#).

The next BP4NTA webinar is on August 19, 2024 (12 p.m. EST) and the speaker will be David Schiessel of Babcock Laboratories.

Committee Spotlight: Stakeholders

The BP4NTA Stakeholder committee was founded in 2021 based on the idea that as an organization, we should not only be creating products aimed at the existing NTA research community, but also reaching out to folks who may not be actively engaged in NTA but could benefit from increased knowledge or application of NTA. In early 2022, we began our current effort of holding focus group interviews with stakeholders whose work has the potential to benefit from improvements in NTA. In total, we have met with 9 diverse stakeholder groups who include both data producers (e.g., food and agricultural chemists, environmental labs) and data end users (e.g., regulatory risk assessors, epidemiologists) as well as those who frequently use NTA data (e.g., medical devices industry consultants) and those with minimal NTA experience (e.g., emergency response labs). We also requested that meeting attendees fill out an exit survey with follow up questions about barriers and opportunities for NTA. We presented results from the meetings and surveys at the February BP4NTA meeting and are currently in the final stages of editing a manuscript which will be submitted to *Analytical Chemistry* as a perspectives article.



The results from stakeholder committee efforts have already started to influence BP4NTA's overall activities. Multiple participants from the stakeholder meetings have joined BP4NTA, and working group efforts such as the Study Planning Tool have been influenced by the needs expressed in stakeholder discussions. Additionally, we have been considering topics of interest to stakeholders when planning the BP4NTA monthly meetings.

As the focus group effort wraps up, we plan for the Stakeholder Committee to transition its focus to generating some of the educational materials that are in high demand from stakeholders. Materials will potentially include short courses, case studies, fact sheets, and short videos. We will be recruiting new members and are actively looking for new committee leadership as we make this transition! Please reach out to Sara and James (sara.nason@ct.gov and mccord.james@epa.gov) if you are potentially interested, and we will be in touch.

Meet BP4NTA's Vice Chair



Sara Nason, Connecticut Agricultural Experiment Station

Employment & Outside Positions: Research Scientist, Departments of Environmental Science and Forestry and Analytical Chemistry, Connecticut Agricultural Experiment Station, New Haven, CT; Adjunct Research Scientist, Department of Plant Science and Landscape Architecture, University of Connecticut; Adjunct Lecturer, Department of Environmental Health, Yale School of Public Health

Current Research or Employment Focus: I work in a unique environment that combines regulatory science and research. I contribute to a wide range of projects, mainly focused on molecules that can be detected using LC-MS. My current interests include PFAS, wastewater derived contaminants, and biological signaling molecules in plants and bacteria. I lead projects focused on phytoremediation, reclaimed wastewater use for irrigation, and monitoring of PFAS in agricultural soils.

Educational Background: B.A., 2012, Princeton University, Geosciences, minor in Environmental Studies; Ph.D., 2017, University of Wisconsin, Madison, Environmental Chemistry and Technology; Postdoc, 2018-2019, Johns Hopkins Bloomberg School of Public Health, Environmental Health

Past Involvement with/Contributions to BP4NTA: I joined BP4NTA in 2018. I helped with the creation of the BP4NTA website, and have continued to assist with maintenance. In 2022, I became a co-chair of the BP4NTA Stakeholder Outreach Committee, and I have led our current effort featuring focus group meetings with stakeholders to help determine priorities for increasing effectiveness and accessibility of NTA.

How did you first get involved with NTA? I started using NTA as a post doc, on a project investigating contaminant degradation in anaerobic digestion systems. The LC-orbitrap experience I gained as a postdoc was a key factor in being hired for my current job, where I have continued to use NTA.

What excites you most about NTA/Why does NTA matter? There is a lot of untapped potential for NTA to be used across many fields. Finding solutions to current issues with accessibility, replicability, and transparency in NTA work has the potential to change monitoring strategies across the fields of environmental safety and human health protection.

What's the best piece of advice you've ever been given? You can be a valuable team member just by reliably showing up and committing. (given to me as a hopelessly bad young little league player)

If you weren't a scientist, what would you be doing? Probably teaching grade school.

What's your favorite trip that you've been on? I really enjoyed visiting Serbia. We spent time in Belgrade and in Subotica, a smaller city that was a common local tourist spot, but not a big international destination. There were a lot of interesting sites to see, and things were quite accessible. It didn't feel overly touristy like some of the other European cities I have visited. Lots of inexpensive food and spa treatments!

BP4NTA @ ASMS



BP4NTA members meet up for a social in Anaheim at the annual meeting of the American Society for Mass Spectrometry in June. Pictured from left to right (top row): Andrew McEachran, Emir Nazdrajic, Mike Thurman, Imma Ferrer, Ruth Marfil-Vega, Emma Rennie, Jeremy Koelmel, David Schiessel, Anna Boatman, Kirsten Overdahl, Samantha Wickramesekara, Brian Ng; (bottom row): Sonja Klee, Rachael Smolinski, Christine Fisher, Gabby Black, Karen Butler.

BP4NTA members Ruth Marfil-Vega, Christine Fisher, and Gabby Black presided over an evening workshop titled "Non-Targeted Analysis: Building bridges among mass spectrometrists." Pictured from left to right: Jonathan Martin, Benedikt Warth, Nina Zhao, Christine O'Donnell, Gabby Black, Ruth Marfil-Vega, and Pablo Gago Ferrero.



Kudos & Congrats...

Anna Feerick passes qualifying exam

Anna Feerick, our BP4NTA webmaster, passed her qualifying exam “Enhancing Chemical Monitoring Through Non-Target Analysis: Methods for Prioritizing and Increasing Confidence in Non-target Features” and moved on to candidacy. She is excited to continue her work in building quantitative structure relationships and hopes to publish her first paper on non-target prioritization techniques this year.

Drew Szabo MSCA Postdoctoral Fellow

Drew Szabo (BP4NTA Outreach Committee), was successful in his Marie Skłodowska-Curie Postdoctoral Fellowship application. This Fellowship will be funded by the UK Research & Innovation to the University of York, United Kingdom. The project aims to develop new prioritization strategies for non-targeted workflows.

...Special Topic Issues

Non-Targeted Analysis of the Environment

A joint Special Issue of ES&T and ES&T Letters is seeking papers detailing new developments and applications of cutting-edge NTA. BP4NTA members Seth Newton and Jon Martin are Guest Editors and the submission deadline is November 28, 2024. [MORE DETAILS HERE!](#)

Non-Targeted Analysis for Exposure Monitoring and Assessment of Human, Food, and Environmental Samples

A Special Issue of the Journal of AOAC International is seeking papers related to NTA. BP4NTA member Yong-Lai Feng is a Guest Editor and the deadline for submission is October 31, 2024.

Email your accomplishment to the BP4NTA Outreach Committee (Esra Mutlu; mutlu.esra@epa.gov) to have it featured in the next BP4NTA newsletter.

See you at SETAC!



**SETAC NORTH AMERICA
45TH ANNUAL MEETING**
20-24 OCTOBER 2024 ★ FORT WORTH, TEXAS
[FORTWORTH.SETAC.ORG](https://fortworth.setac.org)

BP4NTA members are chairing sessions that are NTA-related! More information here:

4.17 Quantitative Non-Targeted Analysis (qNTA): Bridging the Gap Between Characterization and Quantitation

Chairs: James McCord, Jon Sobus, Anneli Kruve

Monday, October 21 10:00 a.m. – 12:00 p.m.

4.20 The Practicalities of Non-Targeted Analysis To Support Decision Making

Chairs: James McCord, Heather Whitehead, Gabrielle Black

Monday, October 21 1:30 p.m. – 3:30 p.m.

4.22 Understanding the Ecological Effects and Rolling Out Solutions for Tire Road Wear Particles and Related Chemicals

Chairs: Rachael Lane, Austin Baldwin, Prarthana Shankar, Gabrielle Black

Monday, October 21 10:00 a.m. – 12:00 p.m. & 1:30 p.m. – 3:30 p.m.

4.05 Challenges in PFAS Analyses and Detection

Chairs: Lilit Ispiryan, Helmer Jonathan Korb

Wednesday, October 23 10:00 a.m. – 12:00 p.m. & 1:30 p.m. – 3:30 p.m.

OTHER UPCOMING CONFERENCES:

- National Environmental Monitoring Conference. Garden Grove, CA. August 5-9, 2024
- International Mass Spectrometry Conference. Melbourne, Australia. August 17-23, 2024
- American Chemical Society Fall Meeting. Denver, CO. August 18-22, 2024
- International Symposium of Chromatography. Liverpool, UK. October 6-11, 2024
- International Society of Exposure Science. Montreal, CAN. October 20-24, 2024
- British Mass Spectrometry Society Super Meeting. Warwick, UK. September 4-6, 2024
- Pittcon Conference and Exposition. Boston, MA. March 1-5, 2025.
- Society of Environmental Toxicology and Chemistry. Vienna, Austria. May 11-15, 2025
- International Conference on Non-Target Screening. Erding, Germany. October, 13-16 2025