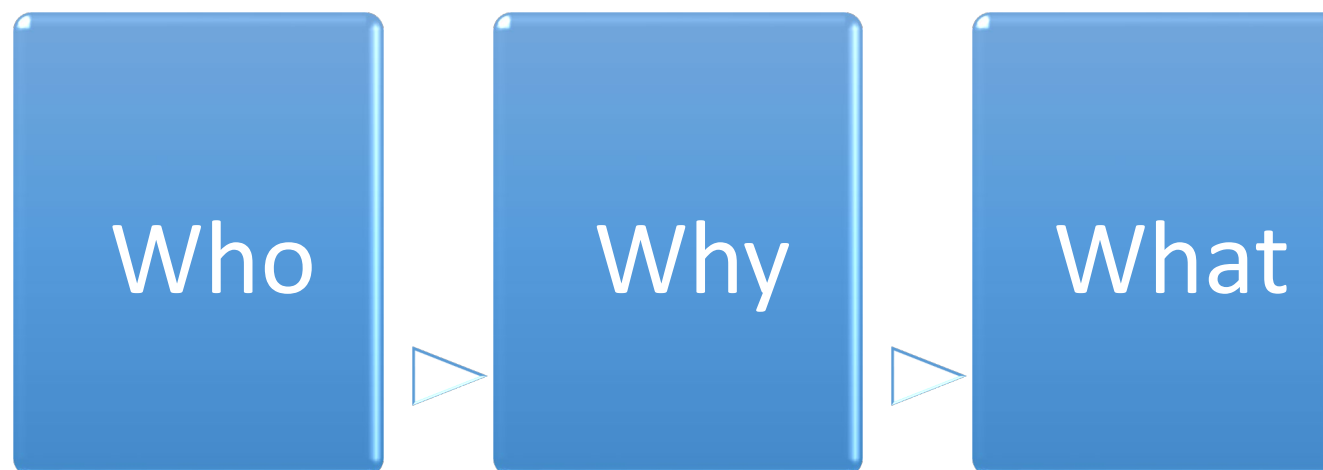




# **A roadmap of harmonization efforts: successes, challenges, and future developments**

**Ruth Marfil-Vega<sup>1</sup>, Christine M. Fisher<sup>2</sup>, Benjamin Place<sup>3</sup>, Elin M. Ulrich<sup>4</sup>  
Shimadzu<sup>1</sup>, US FDA<sup>2</sup>, NIST<sup>3</sup>, US EPA<sup>4</sup>**

*This presentation does not necessarily reflect agency policy*



# 4 years ago, here in Durham...



US EPA held a workshop with the Non-targeted Analysis (NTA) Collaborative Trial (ENTACT) participants and other NTA practitioners.

With leadership of Elin Ulrich (US EPA) and Ben Place (NIST):  
*“a diverse working group consisting of industry, academic and government representatives dedicated to clarifying the definitions and methods for Non-Targeted Analysis by publications and presentations”* was formed.

Some outcomes from ENTACT: <https://doi.org/10.1007/s00216-018-1435-6>.

# BP4NTA Overview - WHO

A consensus-based working group formed to address challenges in Non-Targeted Analysis studies using mass spectrometry.

Chairs:

Christine Fisher

Ruth Marfil-Vega



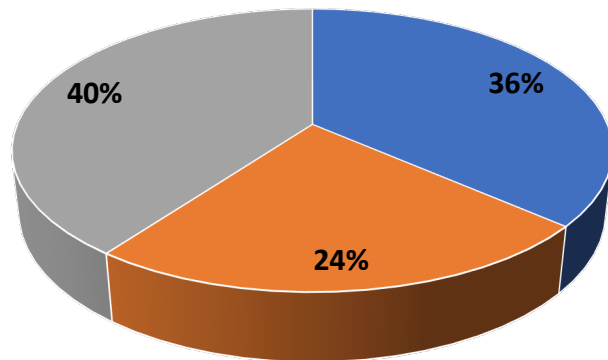
<https://nontargetedanalysis.org/>



# BP4NTA Overview - WHO

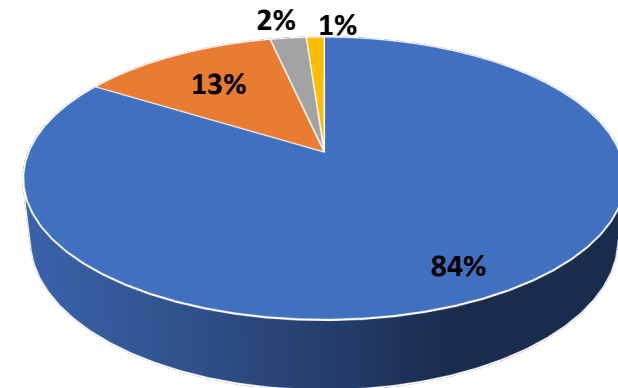
Total Number of Members (as of 5/5/2022): **173**,  
with **40% increase in membership since mid-November 2021**

Distribution by Sector



■ Academia ■ Industry ■ Government

Distribution by (sub-)continent



■ North America ■ Europe ■ Asia ■ Africa

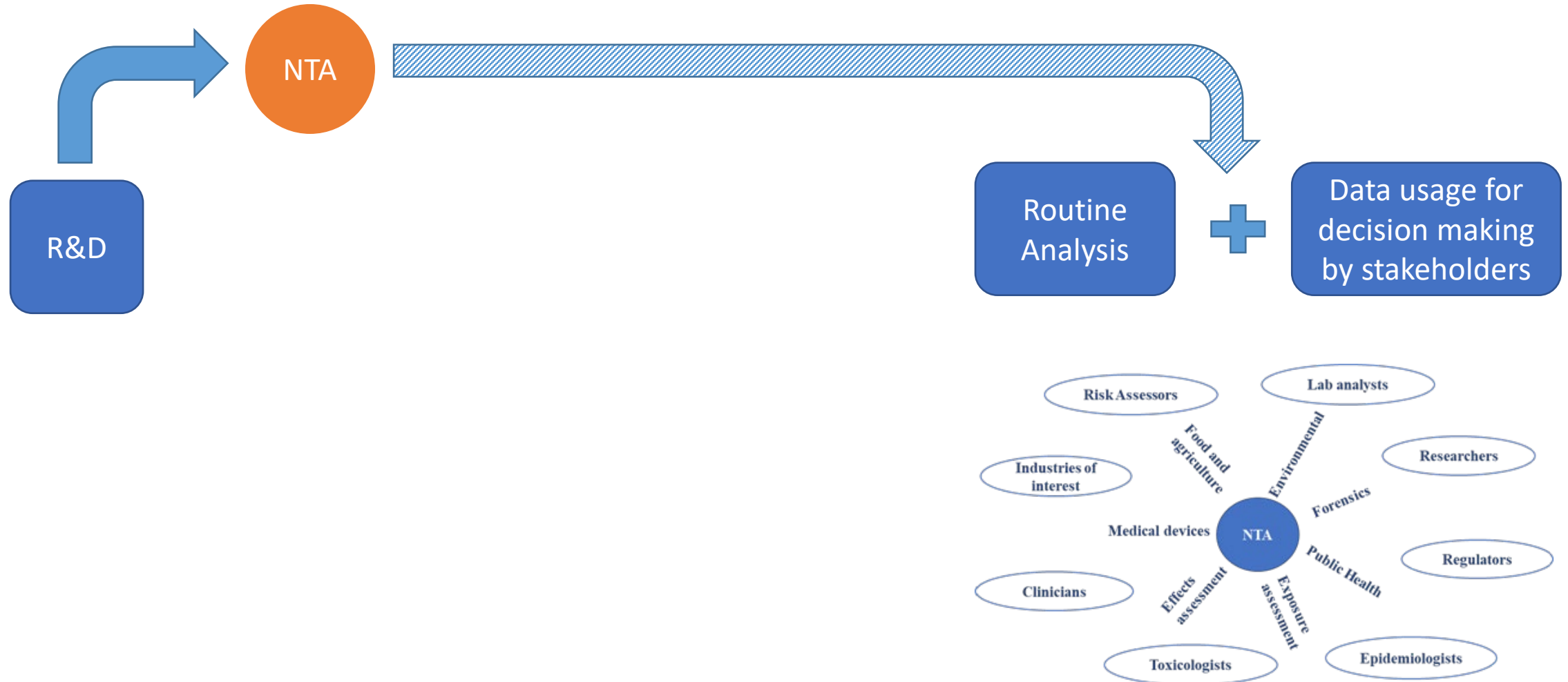
# BP4NTA Overview - WHO

Organized into Sub-committees, with chairs from each group forming the Steering Committee.

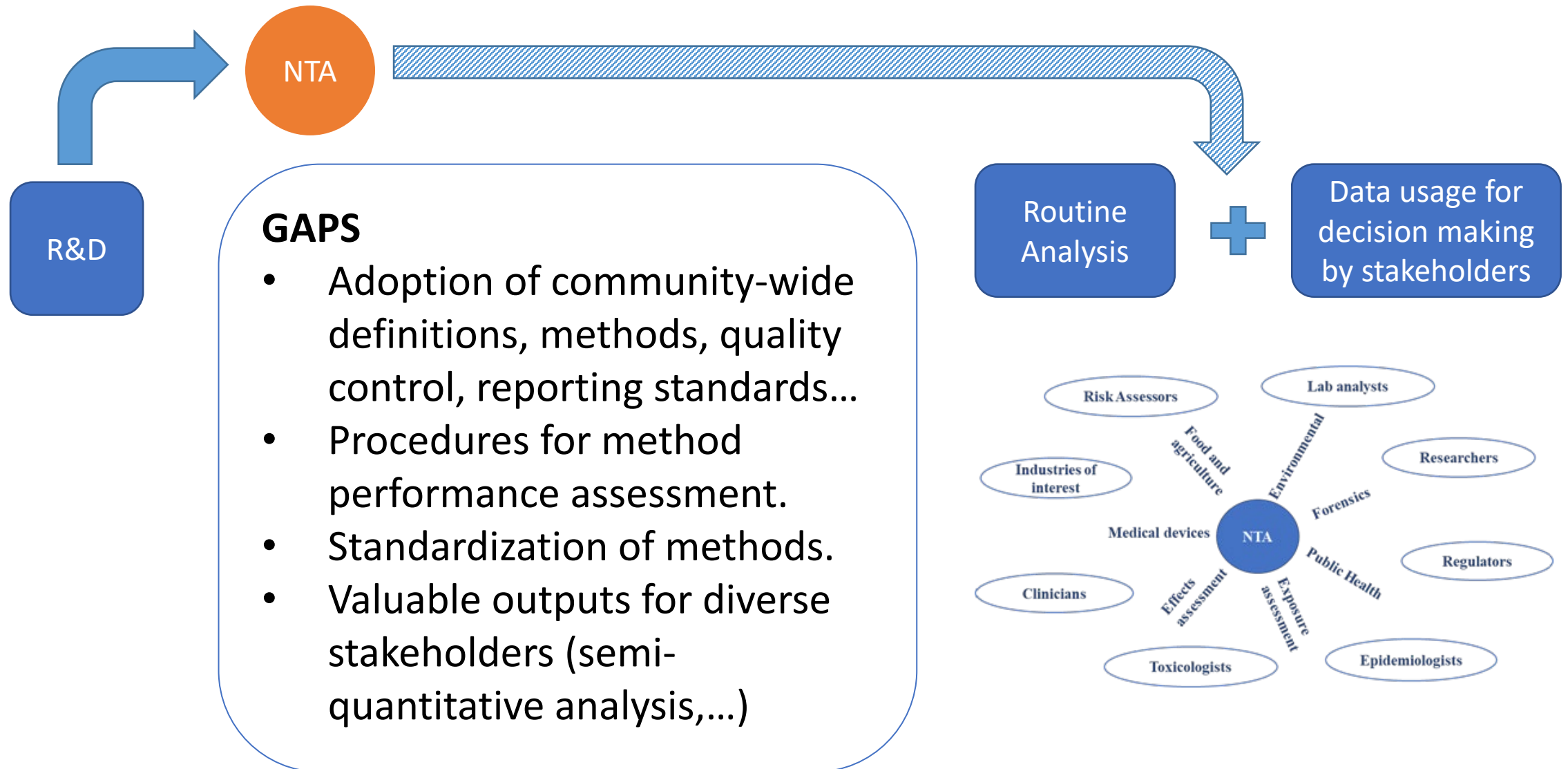


Monthly meetings, alternating business discussions with presentations by NTA practitioners (including non-BP4NTA members), the 3<sup>rd</sup> Tuesday of every month, at 12 pm EST.

# BP4NTA Overview - WHY



# BP4NTA Overview - WHY

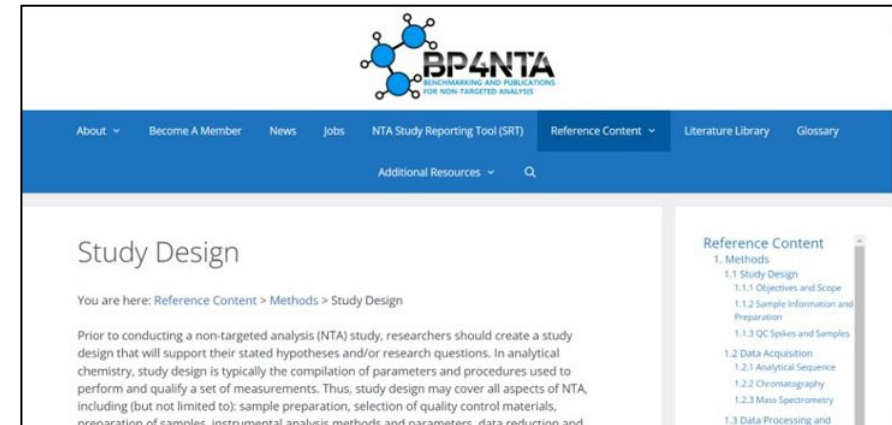




# BP4NTA Overview - WHAT



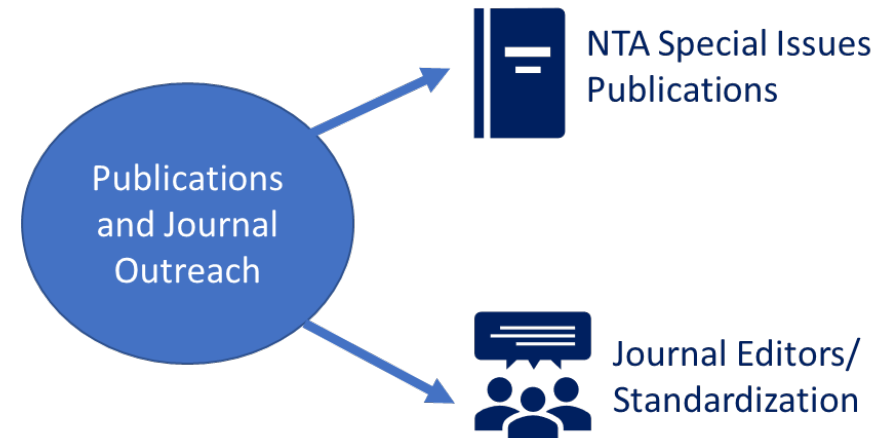
<https://nontargetedanalysis.org/>



Chairs:

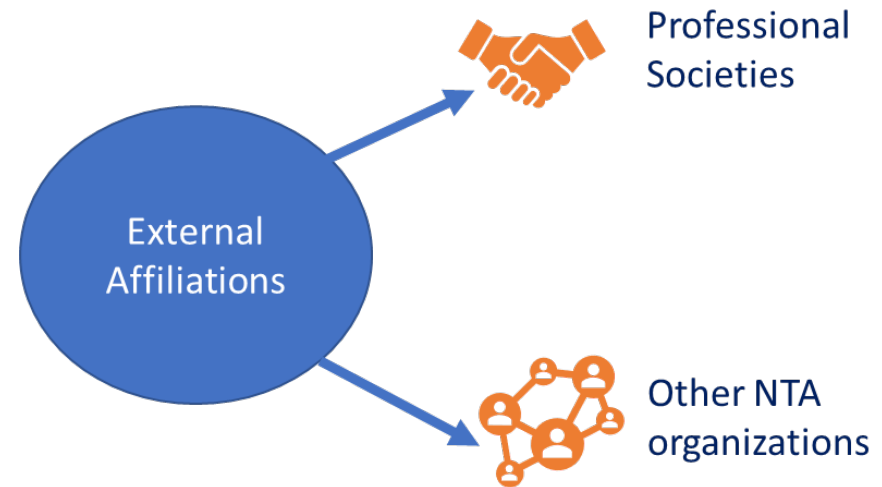
Sara Nason  
Seth Newton

# BP4NTA Overview - WHAT



Chairs:  
Natalia Soares Quinete

# BP4NTA Overview - WHAT



Chairs:  
Elin Ulrich  
Tarun Anumol

# BP4NTA Overview - WHAT



NTA Study Chronology

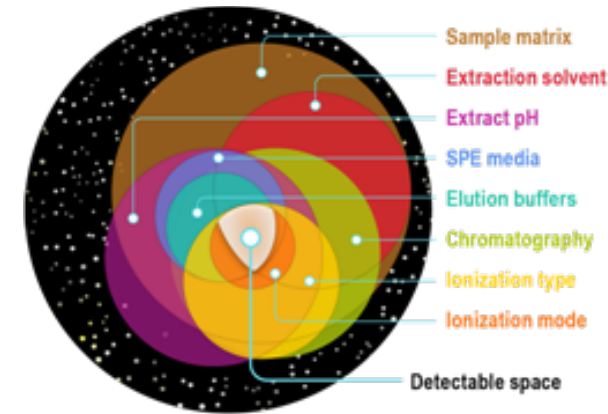
Section	Category	Sub-Category	Example Information to Report	Score	Rationale
Methods	Study Design	Objectives & Scope	• Study goals, hypothesis, scope • Expected chemical coverage	1	Space for reviewer to explain assigned score (i.e., typical peer review rationale)
		Sample Info & Preparation	• Sampling collection, processing • Description, intended use of blanks	2	
		QC Spikes & Samples	• Description of spikes/controls	2	
	Data Acquisition	Analytical Sequence	• Details on order, analytical batches	NA	
		Chromatography	• 3-4 examples of representative information to report for each of the 13 sub-categories.  • Not an exhaustive list – intended to guide researcher/reviewer and relies on expertise/discretion.	0	
		Mass Spectrometry		1	
	Data Processing & Analysis	Data Processing		2	
		Statistical & Chemometric Analysis		3	
		Annotation & Identification			
Results	Data Outputs	Statistical & Chemometric Outputs	• Basic statistical outputs & results of chemometric analyses • Descriptors, new statistical metrics, algorithms, etc.		
		ID & Confidence Levels	• Reported IDs and confidence levels & supporting data • Sample-level data, reported MS/MS spectra	3	
	QA/QC Metrics	Data Acquisition QA/QC	• Method impacts on observable chemical space • Accuracy & precision of chromatography, mass error, abundance	1	
		Data Processing & Analysis QA/QC	• Method impacts on observable chemical space • Performance measures for accuracy, reproducibility of results	0	

## STUDY REPORTING TOOL

Chairs:  
Alli Phillips  
Kathy Peters

**Keynote Presentation Monday May 23 – 10:30**  
Approaches for Assessing Performance of High-Resolution Mass Spectrometry-Based Non-Targeted Analysis Methods  
*K. Peter, University of Washington Tacoma*

# BP4NTA Overview - WHAT



## CHEMICAL SPACE TOOL

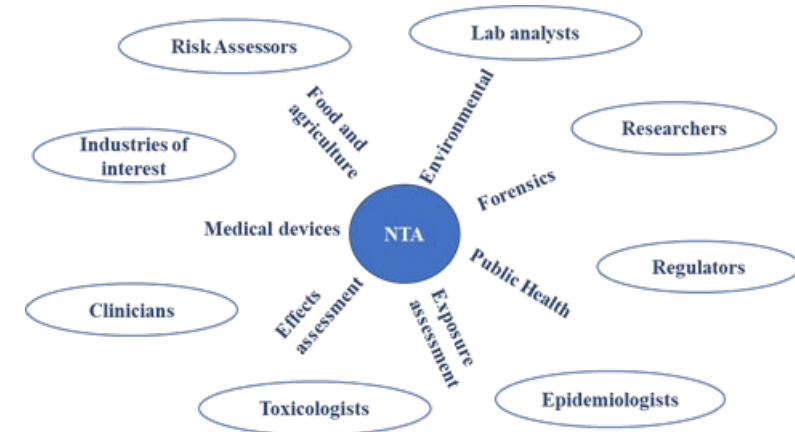
Chairs:

Gabby Black

Charlie Lowe

Interactive Presentation Monday May 23 – 14:55  
Mapping Chemical Space Coverage in Non-Targeted Analysis  
G. Black, University of California, Davis

# BP4NTA Overview - WHAT



## Stakeholders Outreach

### Chairs:

Sara Nason

Yong-Lai Feng

**Oral Presentation Thursday May 26 – 8:50**

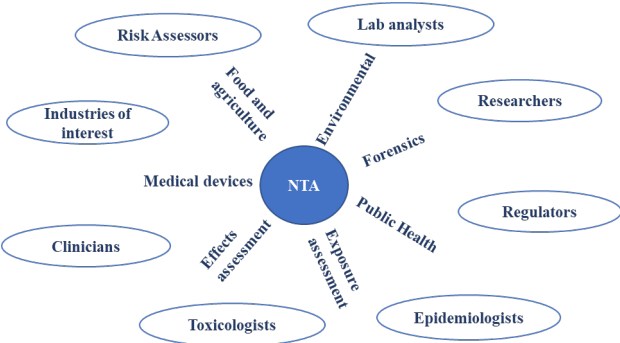
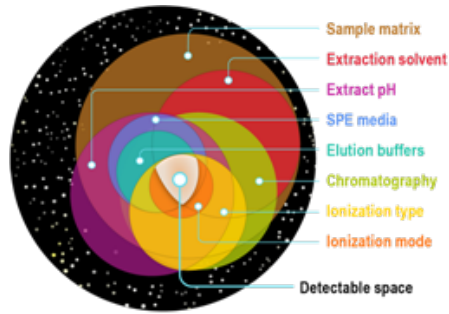
Building Stakeholder Relationships to Facilitate Expanded Application of Non-Targeted Analysis Methods

S.L. Nason, Connecticut Agricultural Experiment Station

# BP4NTA Overview - WHAT



Section	Category	Sub-Category	Example Information to Report	Score	Rationale
NTA Study Chronology	Study Design	Objectives & Scope			
		Sample Info & Preparation			
	Methods	QC Spikes & Samples			
		Analytical Sequence			
		Chromatography			
		Mass Spectrometry			
	Data Processing & Analysis	Data Processing			
		Statistical & Chemometric Analysis			
	Data Outputs	Annotation & Identification			
		Statistical & Chemometric Outputs			
Results	QA/QC Metrics	ID & Confidence Levels			
		Data Acquisition QA/QC			
		Data Processing & Analysis QA/QC			



# Message from Christine?

Message from Christine?



**To learn more about successes, challenges,  
and the future, stop by the poster in the  
interactive part of the session!**

Ruth Marfil-Vega: [rmmarfilvega@shimadzu.com](mailto:rmmarfilvega@shimadzu.com)

Christine Fisher (O'Donnell): [Christine.odonnell@fda.hhs.gov](mailto:Christine.odonnell@fda.hhs.gov)

Social Media and Website:

