

BP4NTA - A roadmap of harmonization efforts : successes, challenges, and future developments

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Since the Benchmarking and Publications for Non-Targeted Analysis (BP4NTA) working group was established in 2018 to address challenges in Non-Targeted Analysis studies using mass spectrometry, we have established multiple working groups (Figure 1) and achieved the following

SUCCESSES:

- Publication of two peer-reviewed manuscripts introducing the group¹ and the Study Reporting Tool (SRT)².
- Two more peer-reviewed publications near completion focused on chemical space and performance assessment of NTA methods.
- Publication of website (nontargetanalysis.org) featuring NTA-focused content generated by BP4NTA members: comprehensive reference content for conducting NTA studies, the SRT, an NTA literature library, news about upcoming conferences and events, job postings, and a BP4NTA membership list.
- Creation of supporting deliverables (e.g., videos, flyers) to promote group's outcomes via scientific conferences and social media.
- Established a seminar series to disseminate NTA knowledge from various fields to group members.
- 40% growth in membership within 6 months (since November 2021).

We are currently working on addressing these

CHALLENGES:

- Grassroots group with diverse membership across fields, affiliations and geographies with no current steady source of funding.
- Limited established guidelines within the group to identify, review and update existing and future products/tools, to ensure succession planning and to maintain and grow membership.

SRT – Accelerate the adoption of the published SRT by the community; examine the impact of the SRT on reporting quality in the NTA community; and develop a SOP for tool updates as feedback is received and advances occur that can also be applied for new tools developed within BP4NTA.

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			
Data Acquisition	Chromatography	Chromatography			
		Mass Spectrometry			
	Data Processing	Statistical & Chemometric			
		Annotation & Identification			
Data Processing & Analysis	Data Outputs	Statistical & Chemometric			
		ID & Confidence Levels			
	QA/QC Metrics	Data Acquisition QA/QC			
		Data Processing & Analysis QA/QC			

Placeholder
QR code –
SRT tool

SCAN THE QR CODE
TO DOWNLOAD THE
SRT!

WEBSITE – Manage website (nontargetanalysis.org), email and social media accounts, and NTA-focused content generated by BP4NTA members: Blog entries, job postings, news about upcoming conferences and events, membership list, and additions to our NTA literature library and resources pages.

EXTERNAL AFFILIATIONS – Coordinate interactions with external organizations to establish official/unofficial affiliations and collaborations, including professional societies (e.g., SETAC, ACS, ASMS) and NTA relevant organizations (e.g., mQACC, NORMAN...).

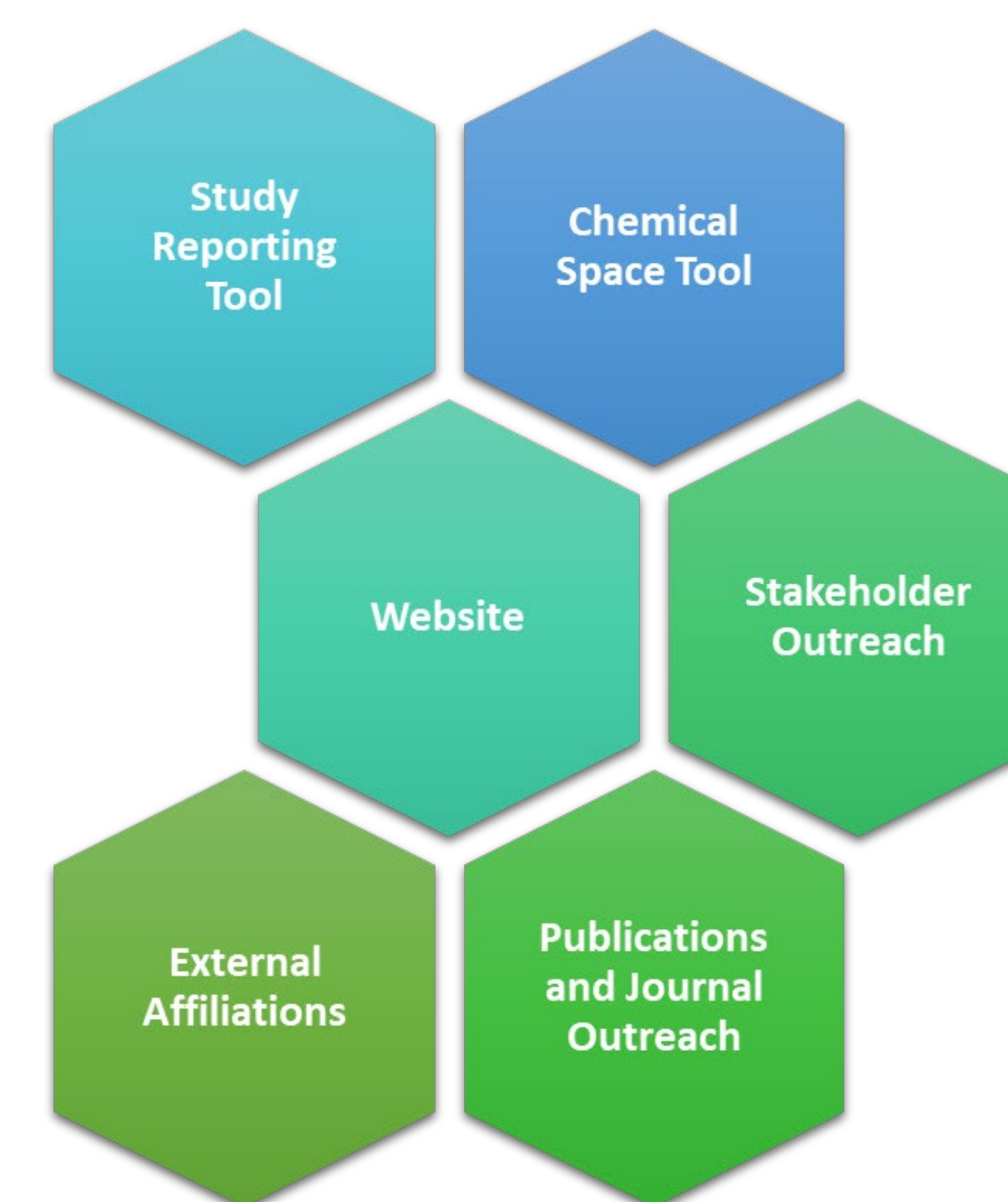
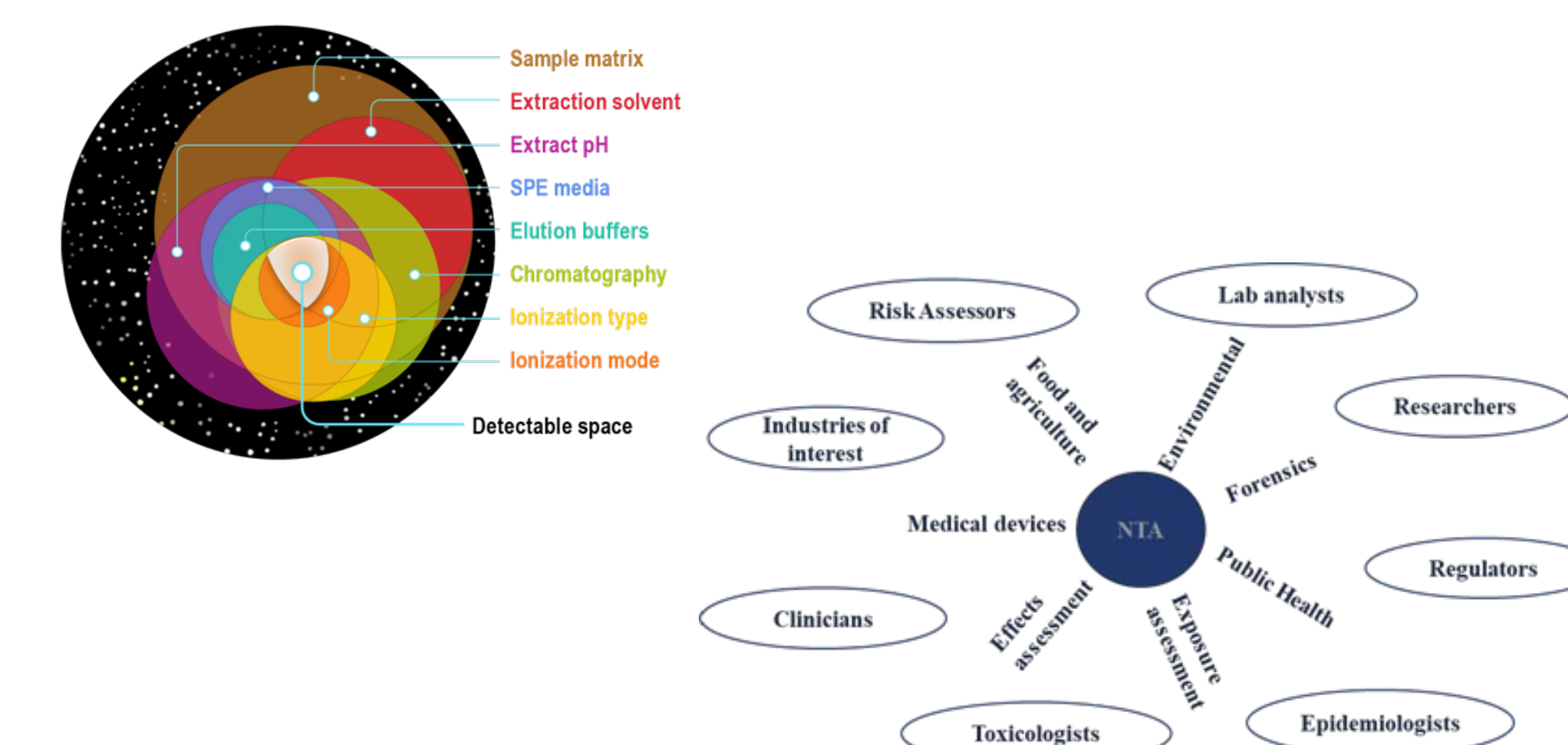


Figure 1. Subcommittees with current goals and activities

SCAN THE QR CODE TO BECOME A MEMBER!



CHEMICAL SPACE – Develop the framework for a tool that can define the region of chemical space detectable by a selected (or planned) NTA method using a suite of chemometric and predictive tools, leveraging the use of existing tools and the creation of new ones to address current barriers for chemical space tools.



STAKEHOLDERS – Engage with stakeholders who could benefit from using NTA workflows or NTA data in their organization to 1) understand their roadblocks to more widespread use of NTA and 2) prioritize needs for addressing gaps, with the ultimate goal of supporting the development of actionable solutions.

FUTURE:

- Determine a viable option for the group to support its vision and growth, through partnering with another working group or society, or establishing it as a non-profit organization.
- Continue addressing scientific challenges through the activities from the current and emerging subcommittees (Figure 1).

This poster aims to open a discussion and strengthen collaborations with other like-minded scientists and organizations across the globe.

¹<https://doi.org/10.1021/acs.analchem.1c02660>

²<https://doi.org/10.1021/acs.analchem.1c02621>