

Benchmarking and Publications for Non-Targeted Analysis Working Group (BP4NTA)



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Mention of product or trade names does not indicate endorsement.

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ENTACT Workshop (August 2018)

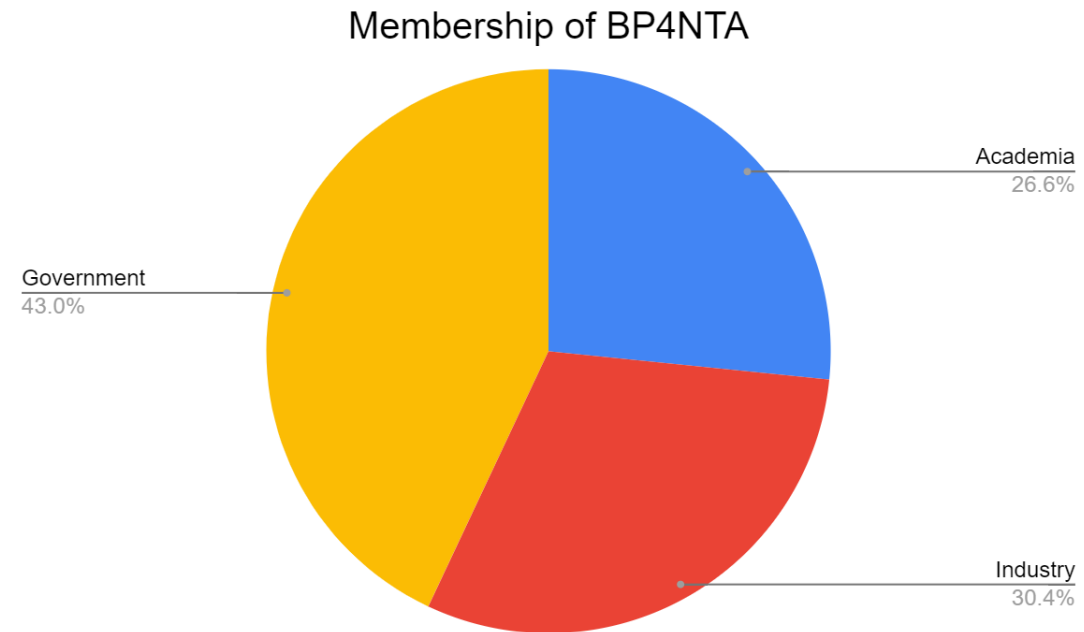
- The EPA's Non-Targeted Collaborative Trial (ENTACT) was an interlaboratory comparison of nontargeted analytical methods with nearly 30 participants (DOI: <https://doi.org/10.1007/s00216-018-1435-6>).
- In August 2018, the US EPA held a workshop with ENTACT participants (and other NTA practitioners) in RTP.
- During the workshop, smaller discussion groups were formed with specific topics of interest.
 - Two different groups (Benchmarking/Proficiency Testing and Publications/Peer Review Standards groups) were merged together based on mutually-shared interests.

BP4NTA Working Group

- The perspective of the group at the workshop was: the NTA community, peer-reviewers, and journal editors need to use a common language when reporting NTA methods and results.
 - Shared terms and definitions can lead to better comparison of methods and results.
 - We can determine benchmark performance only once methods and results reporting are more harmonized.
 - Once benchmarks set, can then tackle concepts like “proficiency testing” for NTA measurements.
- Formed the Benchmarking and Publications for Non-Targeted Analysis (BP4NTA) Working Group.

Working Group Members

- Currently, the working group is ~80 international members.
- Membership based on interest in NTA.
 - Wide range of experience with NTA, from relative beginners to experts.
- Primarily focused on environmental/exposure non-targeted analysis.
 - Some members represent food analysis and metabolomics.
 - Focused on exogenous chemicals, and usually from a bottom-up (source) perspective.



Working Group Operation

- Monthly phone calls.
- Use of Google Drive to create collaborative documents and post useful information for the group.
- Currently not affiliated with a larger organization, but are investigating that option.
- Nine subgroups ($N = 5-10$) have taken on the bulk of current efforts.

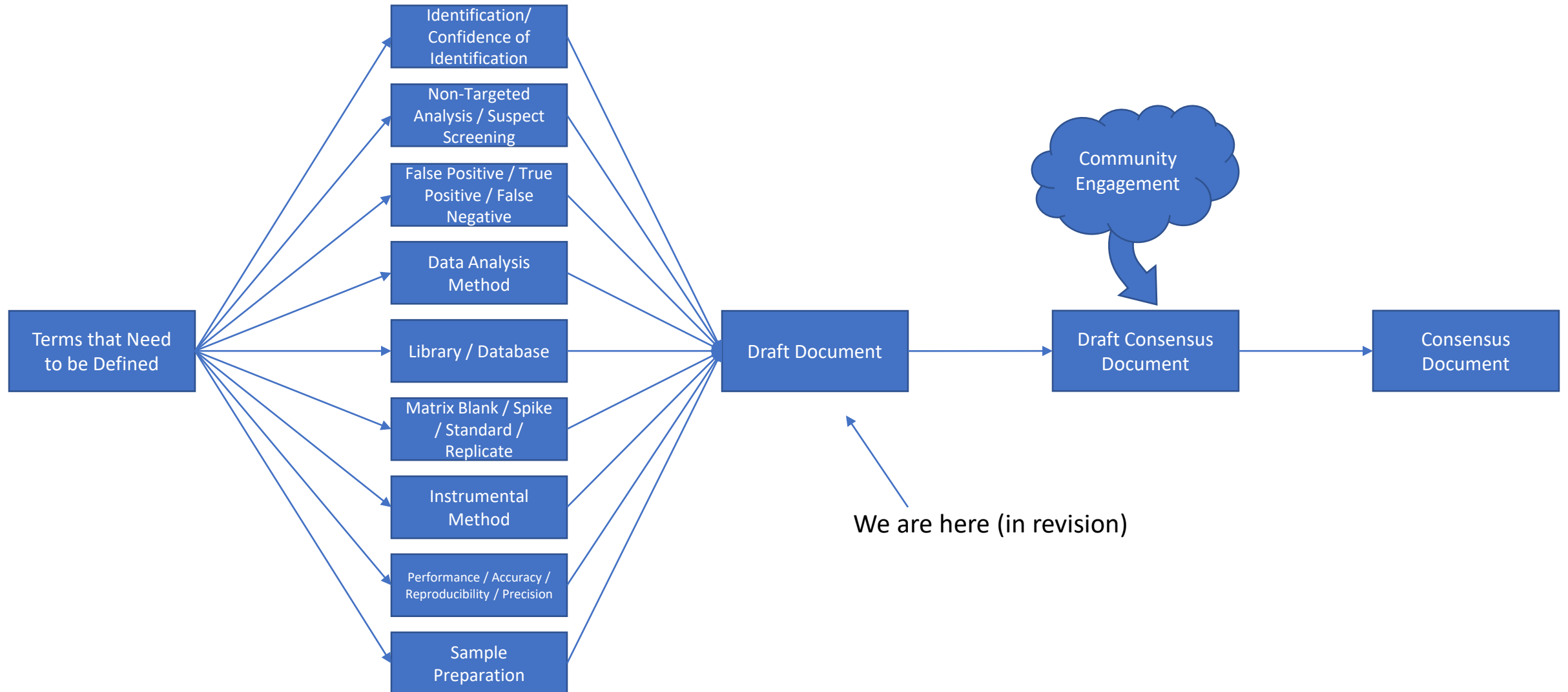
Short-Term Working Group Objective

- Create a list of commonly-used NTA terms, concepts, and performance calculation and provide definitions/equations.
 - Publish guidance document that shares these terms, based on community consensus and feedback.
 - Audience broad, including new NTA researchers, journal reviewers/editors, and expert users.
- Reporting recommendations and scientific best practices to promote transparency and reproducibility.
 - Further dialogue with journal editors to encourage the use of reporting recommendations as related to the defined terms.

Long-Term Working Group Objective

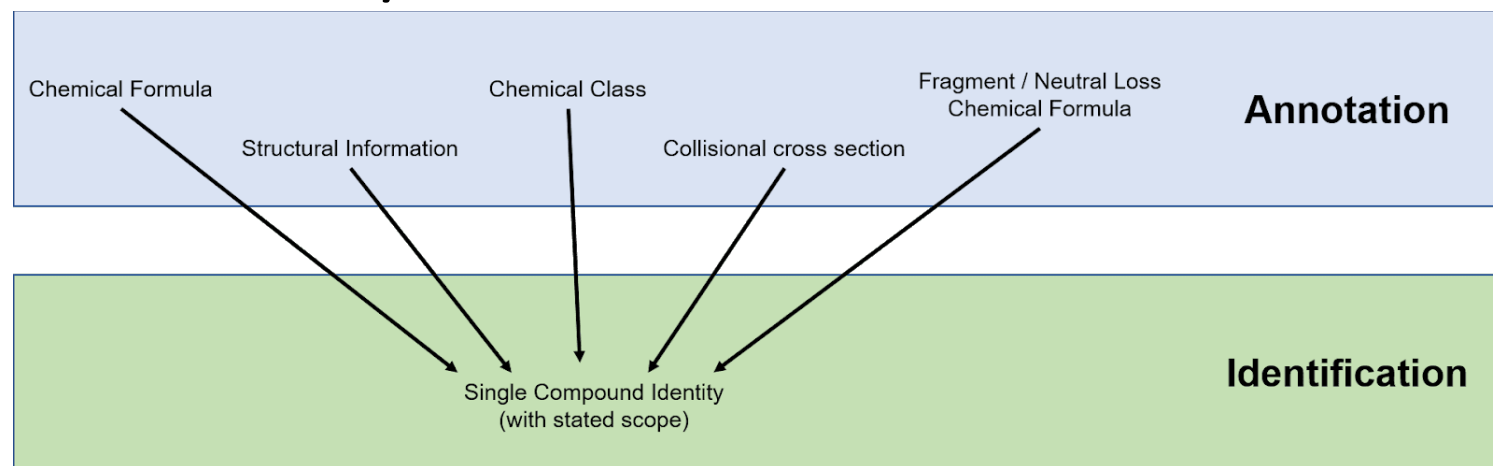
- Move the field of NTA toward proficiency testing, using a mechanism like ASTM/ISO Guidance on Performance and Data Reporting Requirements. Define proficiency levels for SSA, NTA, expert, competent, etc. This is likely 10 years out.
- Build and maintain coalitions/communications with other groups that have similar interests including metabolomics, NORMAN, mQACC.

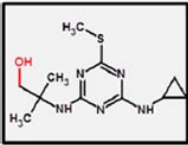
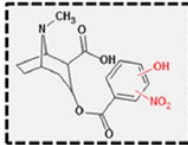
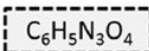

Consensus-building process



Examples of definitions- Confidence of Identification/Identification

Annotation	Attribution of one or more compound-identifying properties to a detected feature. These properties may not provide enough evidence to identify a single compound.
Identification	The case where the annotated compound-identifying properties provide enough evidence to attribute a specific compound within a stated scope to the measured feature
Confidence of Identification /Annotation	The data evidence and/or statistical foundation that supports the proposed identification. The determination of confidence should be presented in a clear and concise fashion.



Example	Identification confidence	Minimum data requirements
	Level 1: Confirmed structure by reference standard	MS, MS ² , RT, Reference Std.
	Level 2: Probable structure a) by library spectrum match b) by diagnostic evidence	MS, MS ² , Library MS ² MS, MS ² , Exp. data
	Level 3: Tentative candidate(s) structure, substituent, class	MS, MS ² , Exp. data
	Level 4: Unequivocal molecular formula	MS isotope/adduct
	Level 5: Exact mass of interest	MS

“Schymanski scale”

<https://doi.org/10.1021/es5002105>

Examples of definitions- Instrumental Method

- Instrumental methods comprise a detailed list of conditions and parameters that are set or used for the acquisition of (high resolution) mass spectrometry raw data files (to include separations) used in suspect screening and/or non-targeted analysis. Settings, conditions, and parameters generally fall into broad categories including but not limited to: instrument, chromatography column(s), mobile phase, injection, sample, ion mobility, mass spectrometry (general and specific), tuning/mass calibration, and lock/reference mass.

LC	GC	Location in publication
Column manufacturer, part #, lot #	Column manufacturer, part #, lot #	Main
Stationary phase	Stationary phase	Supplemental
Length	Length	Main
Particle size	Film thickness	Main
Pore size		Supplemental
ID	ID	Main
Column startup, conditioning, shutdown method		Supplemental
Guard column and dimensions	Retention gap/pre-column and dimensions	Main

Path forward

- Decide on format and outlet for draft document(s). Thoughts?
- Complete draft document for community review. Publish.
- Reach out to other NTA working groups/consortia that have similar goals and objectives.
 - Identify ways to collaborate and complement efforts.
- Reach out to journal editors to start conversation on creating reporting standards for NTA research.