Establishing universal non-targeted analysis vocabulary and reporting recommendations: An update from the Benchmarking and Publications for Non-Targeted Analysis **(BP4NTA)** working group

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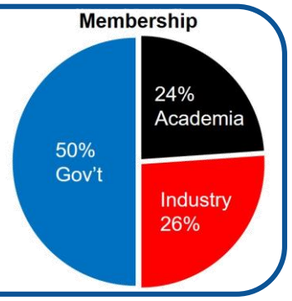
About BP4NTA

As a field, non-targeted analysis (NTA) lacks cohesive vocabulary and universal recommendations for reporting methods and results. We are a tripartite working group focused on addressing these challenges.

- 91 members: 46 gov't, 22 academia, 23 industry; monthly meetings
- Sub-working groups focused on specific NTA topics and outputs



Current Initiatives

- Create a glossary of common NTA terminology
- Provide detailed information about NTA, organized by study chronology, for use by the NTA community (new and current NTA researchers, editors, reviewers, etc.)
- Develop a checklist table for use in evaluation of non-targeted studies (see table at right)
- Host a website as a hub for sharing NTA resources: **NonTargetedAnalysis.org**

Short Term Goals

- Publish a manuscript introducing our working group and website content
- Evaluate the efficacy of the checklist tool for reviewing NTA studies → publish manuscript presenting the tool and validation effort to the community
- Make the checklist, glossary, and additional information available to the wider scientific community via publication on our website
- Distribute the checklist to journal editors/reviewers; promote its use as an evaluation tool

Long Term Goals and Future Directions

- Widespread use of BP4NTA resources and assessment tools by NTA community.
- Develop tools and standards for assessing NTA study quality to move the field of NTA toward proficiency testing (e.g., a mechanism like ASTM/ISO Guidance on Performance and Data Reporting Requirements)
- Develop proficiency levels for suspect screening and NTA, such as expert, competent, etc.

Acknowledgements

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All BP4NTA materials are produced via collaborative effort by many NTA researchers!

Join BP4NTA or let us know your opinions!

Comments box: nontargetedanalysis.org
Email us: BP4NTA@gmail.com

Checklist of Information to be Reported in NTA Studies (DRAFT)

Section	Category	Sub-Category	Examples of Information to Report
Methods	Experimental Design	Objectives & Scope	• Scope of the study with respect to use of NTA / suspect screening • Study goals and hypotheses • Expected chemical coverage of approach and potential limitations
		Sample Information & Preparation	• QA practices related to sample handling and processing • Sample collection, storage, preparation, extraction, and clean-up methods • Development and use of blanks
		QC Spikes & QC Controls	• Development and use of controls & native/labeled standards • Use of isotopically labeled standards and/or RT reference material
	Data Acquisition	Run Order Preparation	• Sample randomization, use of replicate injections, inclusion of blanks/QCs • Single vs. multiple analytical batches
		Chromatography	• Instrument specifications • Method settings (e.g., column/guard, mobile phases, injection techniques)
		Mass Spectrometry	• Instrument specifications; calibration and/or tuning procedures • Acquisition parameters (e.g., polarity, resolution, DDA vs. DIA)
	Data Processing & Analysis	Data Processing	• File type and file conversion information • Software program(s) used • Workflow steps (e.g., peak picking, RT calibration, alignment) and settings • Feature detection thresholds (e.g., replicate criteria; min height, area, or S/N; comparison to blanks) • Data correction or normalization/scaling methods
		Statistical Analyses	• Software program(s) used • Method goals (e.g., prioritize features, classify samples) • Method type (e.g., clustering, classification, hypothesis testing) and settings
		Annotation & Identification	• Software program(s) used • Libraries and databases used (including in-house databases) • Workflow steps (e.g., formula assignment, suspect screening, MS/MS matching) • Workflow methods (e.g., formula prediction method, scoring algorithm) & settings (e.g., mass error/RT tolerances, accepted match scores)
Results	Data Outputs	Identification & Confidence Levels	• Reported IDs and associated confidence levels • Supporting annotated data (e.g., formula match scores, isotope pattern, RT match, MS/MS match, source of MS/MS spectra used to support ID) • For annotated features, proposed structures/other annotated data • (Semi)-quantification data • Exported MS/MS spectra (e.g., as a library, in online database)
		Statistical Outputs	• Visuals/plots (e.g., heatmaps, PCA) and statistical outputs (e.g., p-values) • Reported classifications or groupings of features, IDs, or samples • New statistical packages or code
	QA/QC & Other Performance Metrics	Data Acquisition	• Quality: Deviations from QA practices, results from QC checks for sample prep/data acquisition • Boundary: Observed impact (of prep, chromatography, MS) on chemical space • Accuracy: Reported chromatographic and mass accuracy • Precision: Reported variability of RT, precursor mass error, and abundance
		Data Processing & Analysis	• Quality: Outcomes of QC checks for data analysis workflow • Boundary: (Semi)-quantification of ID'd compounds, limits of detection/ID, impact of database or data analysis method on chemical space • Accuracy: TPR, FPR, etc. for known compounds or samples • Precision: Reproducibility of detection/ID for QCs; FDR, F1 score, etc.