

The Non-Targeted Analysis Study Reporting Tool (SRT): A Framework to Improve Research Transparency and Reproducibility

Katherine T. Peter¹⁺, Allison L. Phillips²⁺, Ann M. Knolhoff³, Piero R. Gardinali⁴, Carlos Manzano^{5,6}, Kelsey E. Miller², Manuel Pristner⁷, Lyne Sabourin⁸, Mark Sumarah⁸, Benedikt Warth⁷, **Jon R. Sobus²**

¹NIST; ²US EPA; ³US FDA; ⁴Florida International University; ⁵University of Chile; ⁶San Diego State University; ⁷University of Vienna; ⁸Agriculture and Agri-Food Canada;

⁺Indicates equal contributions; Emails: ktpeter@uw.edu; Phillips.Allison@epa.gov



Agriculture and Agri-Food Canada

THE GAP: NTA REPORTING STANDARDS

- NTA does not have universally-accepted reporting standards
- Lack of standards yields lack of transparency and reproducibility in NTA studies & proposals, as well as inconsistent research reviewing
- Barrier to entry for new NTA researchers

THE SOLUTION: NTA STUDY REPORTING TOOL

- Standardized framework for reviewing quality of NTA reporting (see table)
- Aids NTA study design and review (manuscripts & proposals)
- Sufficiently flexible for use in many NTA research domains

THE FACILITATOR: BP4NTA WEBSITE

www.nontargetedanalysis.org

- Fillable PDF & Excel versions available for download
- Information structure complements detailed reference content
- Comment box for feedback -- annual updates by SRT Committee

THE SRT EVALUATION**

- **Eleven NTA practitioners** reviewed **eight published articles** covering environmental, food, and health-based exposomic applications*
- **Three study types**: NTA performance evaluation (n=2), NTA method development (n=2), NTA application (n=2 GCxGC-TOFMS, n=2 LC-HRMS)
- Considered 3 scoring systems, led to **final hybrid color-coded/numeric system** (red = 0, orange = 1, yellow = 2, blue = 3, gray = NA)

		Papers #1-5							Papers #6-8								
Section	Category	Category Reviewers						3 Complete Reviews per Paper	Full SRT Reviewers			3 Complete Reviews per Paper					
		A	B	C	D	E	F	G	R1	R2	R3	H	I	J	R1	R2	R3
Methods	Study Design	✓	-	✓	-	✓	-	-	A	C	E	✓	✓	✓	H	I	J
	Data Acquisition	-	✓	✓	-	-	✓	-	B	C	F	✓	✓	✓	H	I	J
	Data Processing & Analysis	-	✓	-	✓	-	-	✓	B	D	G	✓	✓	✓	H	I	J
Results	Data Outputs	-	-	✓	✓	-	✓	-	C	D	F	✓	✓	✓	H	I	J
	QA/QC Metrics	✓	✓	-	-	✓	-	-	A	B	E	✓	✓	✓	H	I	J

GET IN TOUCH

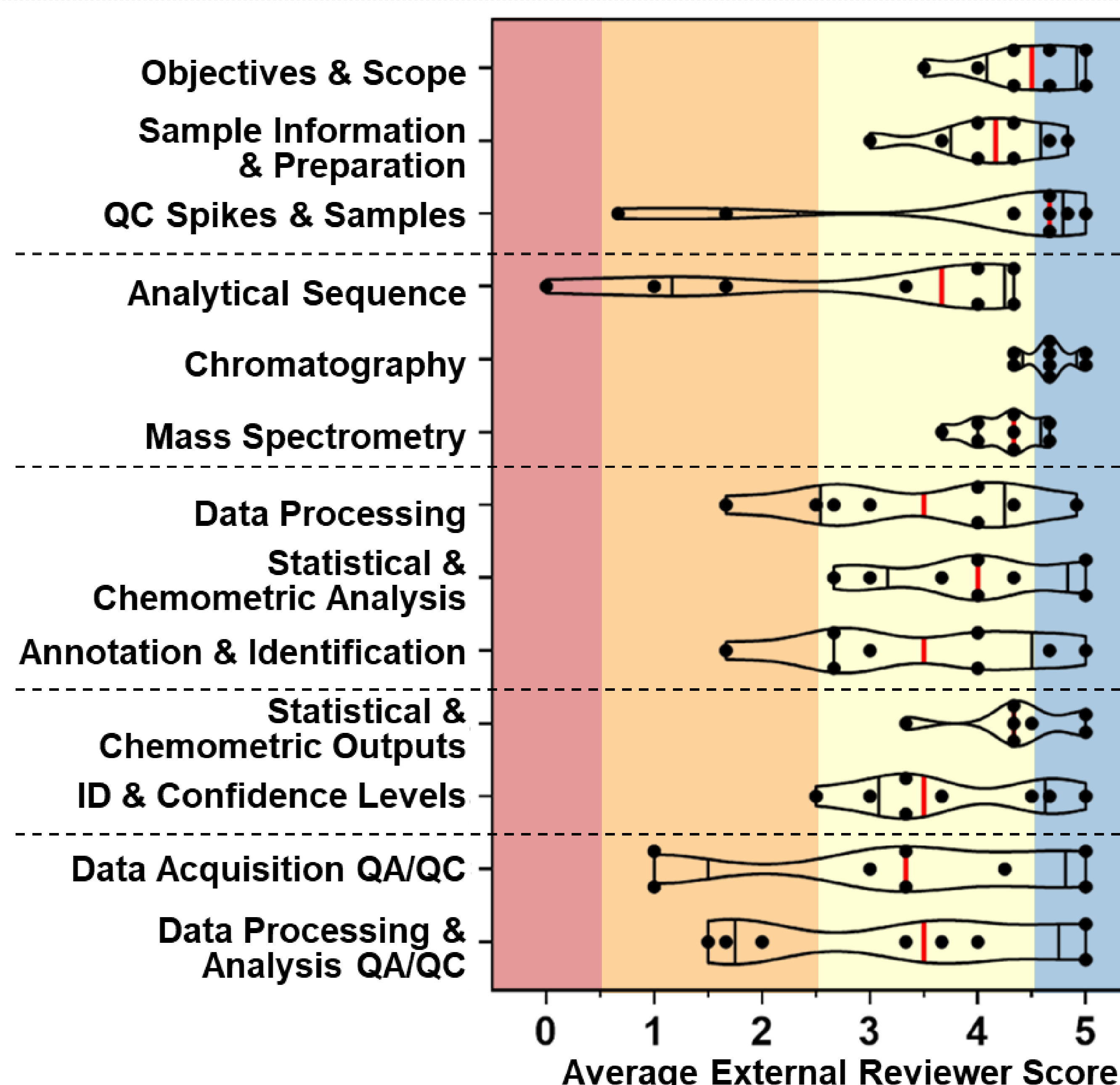
To join BP4NTA and/or provide feedback about the SRT, email us at BP4NTA@gmail.com or leave a comment at www.nontargetedanalysis.org/srt.

ACKNOWLEDGEMENTS

We thank all the BP4NTA members (<https://nontargetedanalysis.org/members/hip-list/>), and especially Seth Newton, Elin Ulrich (EPA), Ben Place (NIST), and Sara Nason (CAES). All BP4NTA materials are produced via collaborative effort.

*Evaluated Articles: Knolhoff et al. *Anal Chim Acta* 2019; Sobus et al. *Anal Bioanal Chem* 2019; Warth et al. *Anal Chem* 2017; Manzano et al. *ES&T* 2017; McCord et al. *ES&T* 2019; Tran et al. *Chemosphere* 2020; Renaud et al. *Anal Chem* 2017; Peter et al. *ES&T* 2018.

**Results: Peter & Phillips et al. doi: 10.1021/acs.analchem.1c02621



Summarized results of SRT evaluation (from initial 0 – 5 scale, NA excluded). Red line shows median of article-specific average scores; black lines show 25th/75th percentile.

THE RESULTS

- Overall, sub-category scores were consistent across reviewers
- High scores for **Study Design** aspects & **Chromatography** and **MS** method reporting – indicated good existing practices
- Highlighted areas for reporting improvement
 - **Analytical Sequence** (batch & run-order information)
 - **Data Processing & IDs** (method settings, MS² reporting)
 - **QA/QC** (lack of universal best practices)

VISION FOR THE SRT

- SRT offers a functional and valid framework to guide study design, manuscript writing & evaluation of reporting quality
- Widespread adoption of SRT will drive universal improvements to NTA reporting, supporting assessment of best practices.
- **Download the SRT at:** www.nontargetedanalysis.org/SRT



NTA Study Reporting Tool						
Section	Category	Sub-Category	Example Info to Report		Score	Rationale
Methods	Study Design	Objectives & Scope	<ul style="list-style-type: none">Study goals, hypotheses, scopeExpected chemical coverage	<ul style="list-style-type: none">Examples of representative information to report for each sub-categoryNon-exhaustive lists – intended to guide reviewer and relies on expertise/discretion	Scores selected from dropdown menu for each sub-category	Space for reviewer to explain assigned score in each sub-category
		Sample Info & Preparation	<ul style="list-style-type: none">Sampling collection, processingDescription, intended use of blanks			
		QC Spikes & Samples	<ul style="list-style-type: none">Description of QC spikes/samples			
	Data Acquisition	Analytical Sequence	<ul style="list-style-type: none">Sample run order, analytical batch(es)			
		Chromatography	<ul style="list-style-type: none">Instrument specs & method settings			
		Mass Spectrometry	<ul style="list-style-type: none">Instrument specs & method settingsCalibration and tune info			
	Data Processing & Analysis	Data Processing	<ul style="list-style-type: none">Software program(s); Workflow steps and settings;Feature detection thresholds; Data correction/normalization methods			
		Statistical & Chemometric Analysis	<ul style="list-style-type: none">Software programs/packagesMethod goals, type, assumptions, and settings/threshold for basic statistical analyses and/or chemometric analyses			
		Annotation & Identification	<ul style="list-style-type: none">Software programs/manual effortsWorkflow steps, methods, and settingsDescription of libraries and databases			
	Results	Data Outputs	Statistical & Chemometric Outputs	<ul style="list-style-type: none">Basic statistical outputs & results of chemometric analysesVisuals/plots, new statistical metrics, algorithms, etc.		
ID & Confidence Levels			<ul style="list-style-type: none">Reported IDs and confidence levels & supporting data (Semi)-quant data; exported MS/MS spectra	3		
QA/QC Metrics		Data Acquisition QA/QC	<ul style="list-style-type: none">Method impacts on observable chemical spaceAccuracy & precision of chromatography, mass error, abundance			
		Data Processing & Analysis QA/QC	<ul style="list-style-type: none">Method impacts on observable chemical spacePerformance measures for accuracy, reproducibility of results			

The views expressed in this presentation are those of the author(s) and do not necessarily represent the views or policies of the US EPA, US NIST, US FDA, or AAFC.