A detailed illustration in shades of blue and green, depicting various elements of aquatic science and environmental research. It includes a diver, a large fish, a chemical structure, a flask, a boot, a buoy, and a stack of pipes, all set against a background of water and reeds.

Bridging the gap between regulatory agencies and academic research for non-target screening studies in a Swedish context

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Report 2025:14
2026-04-01

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Publisher:	Department of Aquatic Sciences and Assessment, SLU
Year of publication:	2026
Place of publication:	Uppsala
Copywrite:	All images are used with the permission of the author.
Title of report series:	Rapport / Institutionen för vatten och miljö, SLU
Keywords:	Non-target screening; Suspect screening; High Resolution Mass Spectrometry; HRMS; Regulatory – academic collaboration

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Sammanfattning

Förutsättningslös (non-target) och bred, riktad (suspect) masspektrometri (MS)-screening (NTS och SS) av miljöföroreningar används i allt större utsträckning för att upptäcka ett brett spektrum av kemiska ämnen i exponerade matriser. Skillnader i förväntningar mellan tillsynsmyndigheter och forskare kan dock begränsa användningen av den information som erhålls genom sådana uppdragsstudier. Denna rapport sammanfattar resultaten av en workshop organiserad av Toxikologiska rådet (2024) som syftade till att förbättra samarbetet och anpassa förväntningarna mellan tillsynsmyndigheter och forskare involverade i NTS- och SS-studier.

Deltagare från tillsynsmyndigheter, forskningsinstitutioner och andra intressenter identifierade viktiga utmaningar och rekommendationer i fyra steg av uppdragsstudier: projektdesign, implementering, rapportering och tolkning av resultat samt kommunikation efter projektet. Tidiga och transparenta diskussioner framhölls som viktiga för att tydligt definiera de regulatoriska frågeställningarna, fastställa realistiska förväntningar och avgöra om riktad analys (targeted analysis), SS eller NTS, alternativt en kombination av dessa, är den lämpligaste metodiken.

Workshopen betonade också vikten av en kontinuerlig dialog under projektgenomförandet, robusta kvalitetssäkringsförfaranden, transparent rapportering av konfidensnivåer och detektionsgränser samt strategisk arkivering av analytiska data för framtida retrospektiv analys. Att stärka kommunikationen och anpassa förväntningar identifierades som viktiga steg för att öka det regulatoriska värdet av NTS och SS inom miljöövervakning och hantering av kemiska risker.

Nyckelord: non-target screening (NTS); suspect screening (SS); högupplösande masspektrometri (HRMS); regulatoriskt – akademiskt samarbete

Abstract

Non-target and suspect mass spectrometry screening (NTS and SS) are increasingly used to detect a broad range of chemical contaminants in exposed matrices. However, differences in expectations between regulatory authorities and academic researchers can limit the effective use of the information obtained by such commissioned studies. This report summarizes the outcomes of a 2024 workshop organized by the Swedish Toxicological Council that aimed to improve

collaboration and align expectations between regulators and researchers involved in NTS and SS projects.

Participants from regulatory agencies, research institutions, and other stakeholders identified key challenges and recommendations across four stages of commissioned studies: project design, study implementation, reporting and interpretation of results, and post-project communication. Early and transparent discussions were highlighted as essential to clearly define regulatory questions, establish realistic expectations, and determine whether targeted analysis, SS or non-target screening, alternatively a combination of them, is the most appropriate approach.

The workshop also emphasized the importance of continuous dialogue during project execution, robust quality assurance procedures, transparent reporting of confidence levels and detection limits, and the strategic archiving of analytical data for future retrospective analysis. Strengthening communication and aligning expectations were identified as key steps to enhance the regulatory value of NTS and SS in environmental monitoring and chemical risk management.

Keywords: non-target screening (NTS); suspect screening (SS); high resolution mass spectrometry (HRMS); regulatory – academic collaboration

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1. Introduction

In the ever-changing field of screening of small organic molecules in complex matrices, the evolution of screening techniques over recent years is outstanding (Menger et al., 2020; Mohammed Taha et al., 2022; Schymanski et al., 2015; Yang et al., 2023). The distinct instrumental configurations available in the market (triple quadrupole mass analysers, quadrupole time-of-flight, orbitrap, ion mobility, etc.) as well as their variety of working modes (data (in)dependent acquisition, sequential window acquisition, etc.) occasioned the rise of numerous approaches, each of them with their own goals, advantages and drawbacks. On top, the numerous possibilities for the chromatographic analysis of the sample (liquid chromatography, reverse phase, hydrophilic interaction, gas chromatography, etc.) multiply the possibilities to achieve even more comprehensive screening approaches. However, this creates a limitation in the full understanding of what each technique has to offer and what its limitations are.

Yet, independently of the technique of choice for the analysis, the overarching concepts and strategies for the analysis of small molecules in complex matrices remain intact. In brief, the different screening analyses could be grouped in: (i) target screening (TS), when performed directed towards the analysis of a specific list of chemicals (limited number) for which analysts have reference standards and an optimized methodology for their robust analysis (often quantitative); (ii) suspect screening (SS), when the screening is also directed towards a list of chemicals but for which no reference standards are available and a more generic analysis method is applied considering that SS is often scoping a relative large list of chemicals; and (iii) non-target screening (NTS) where no lists or chemicals of interest is a priori selected and the final goal is to identify the chemical structure of (virtually) all the chemical signals observed in the sample (Hollender et al., 2017; Krauss et al., 2010). Nonetheless, each strategy provides insights into different aspects of the chemical space, aligned with the specific goals of the analysis.

Considering the wide range of possibilities for conducting screening studies of organic molecules in complex matrices, commissioning such studies by authorities and regulators to academic institutes can sometimes lead to misunderstandings or misaligned expectations regarding capabilities and outcomes. In the scientific literature, NTS and SS is often described as valuable tools for regulating chemicals.

However, when commissioning such studies, it has been the experience of several authorities and members in the Toxicological Council that the results did not meet the regulatory needs, but instead often only being able to report legacy substances with high enough certainty, many times due to method limitations such as sample collection, sample extraction, chromatographic technique, the chromatographic column as well as the mass spectrometer design. With this in mind, the Toxicological Council (www.kemi.se/en/about-the-swedish-chemicals-agency/organisation/the-toxicological-council) identified the need for a discussion forum where researchers and regulators could work together for a better understanding of each other's needs and limitations. In this document, we would like to highlight the main ideas, lessons and suggestions learned from a thorough workshop-based discussion for bridging the gap between academics and authorities. The purpose of the workshop and the current document is to improve the performance of commissioned NTS/SS studies and to produce a document serving as a foundation for a follow-up guidance for both regulatory agencies and academic researchers for meaningful and comprehensive understanding in commissioned suspect and non-target screening analyses.

2. Lessons learned from the workshop. Recommendations for a robust collaboration between researchers and regulators

The ‘Workshop for improved regulatory non-target and suspect screening of chemicals’, held in 2024, was organized as a discussion forum in which both researchers and regulators could express their needs, limitations and suggestions to facilitate understanding between the different parts involved in the process of designing, commissioning, performing and reporting studies.

A total of 32 people attended the workshop, consisting of 17 representatives from research institutions and 15 representatives of stakeholders, agencies, and authorities in Sweden. This balanced audience of academics and regulators helped steer the discussions towards practical priorities and mutual understanding relevant to both groups. Starting with some introductory talks to lay the fundamental concepts on the table and followed by some presentations on real cases in which commissioned studies (partly) failed at delivering the expected information due to miscommunication between regulators and researchers, attendees got an overview of the scenario and the goals of the workshop. Later, breakout rooms with small discussion groups were set to suggest ideas, provide clear information and propose actions for improvement in the context of commissioned suspect and non-target screening studies. The results of the discussions are summarized and discussed in the coming sections. Although this discussion serves as a list of recommendations, it is important to highlight that this is not a checklist; there may still be recommendable actions that are missing from the list depending on each project’s nature.

Overall, the workshop identified four key stages in which close and continuous communication is essential to ensure the success of commissioned projects (Figure 1). The following discussion outlines the main lessons learned, recommendations and topics to be addressed at each of these stages.



Figure 1. Identified main stages in which clear communication should be established during commissioned non-target and suspect screening projects.

2.1 Project design: Setting the foundation

The planning and design of a commissioned project is the stage where most of the potential later issues could be solved without impacting on the development of the project or its associated costs. A clear definition of the regulators' expectations as well as the analytical or instrumental limitations faced by researchers should be thoroughly discussed so that the project can be adapted to achieve its aims. In this sense, probably the most critical question to be discussed is whether non-target or suspect screening is the best approach to deal with the commissioned needs or, contrarily, evidence suggests that a targeted analysis, although more limited and focused, is the best strategy. For this discussion, transparent communication from both researchers and regulators about analytical capabilities and limitations is essential, even if it means acknowledging constraints that could potentially affect the feasibility of the collaboration.

Upholding scientific integrity at this early stage ultimately strengthens trust and leads to more realistic and successful outcomes. On top, the potential commission of follow-up projects to deal with the identified challenges and cover the aspects which were previously hindered by analytical or instrumental limitations could be explored.

Additionally, the establishment of clear goals as well as managing the expectations from the project from the start is critical for commissioned projects. Following, some other aspects to consider when initiating a collaboration.

- A. Define the scope and requirements of the project
 - i. Clarify the regulatory task or question in a detailed way.
 - ii. Understand whether the project is exploratory or requires confirmatory data that meets regulatory confidence standards. It is important to highlight that

not all regulatory applications require the highest levels of confidence in the findings, for example in an early warning system for identifying new emerging contaminants, a low to medium confidence could be accepted, while for prioritization for risk management actions a medium to high confidence is needed and for actual use as evidence for restricting a substance high confidence is needed. Therefore, setting these expectations early prevents overpromising. For exploratory purposes, tentative identifications might already meet the expectations of the commissioned project, while in other cases leading to regulation formulation confirmatory data to support the directive should be available.

- iii.* Establishing clear goals and interests within the commissioned project is essential for the appropriate selection of sample collection and storage conditions depending on the scope of the suspect screening.

B. Ensure mutual understanding of goals and limitations

- i.* Prioritize early, open and honest discussions about project goals, study limitations, analytical methods (*e.g.* are the chemicals, in the case of a suspect screening-study, within the chemical domain), and what outcomes can realistically be achieved. Scientists should communicate at this stage whether the regulators' expectations are realistic with the available technologies, especially concerning limitations in non-detects (*e.g.* whether a non-detect with high confidence can be interpreted as if the substance is not present in the matrix above a certain concentration or possibly only indicate that the substance is not within the chemical domain) and analytical sensitivity, or the use of existing sample extracts (from previously pretreated samples) or archived data for retrospective analyses.
- ii.* Discuss whether it might be more suitable to apply targeted methods instead of NTS/SS, especially if certain regulatory standards need specific detection limits or confirmatory results. For example, a limited number of chemicals of interest, very low concentration levels expected or the need for environmental concentrations information could also be examples when targeted methods could be efficient than NTS/SS.
- iii.* Ensure complete understanding of contractual agreements. Contracts with the regulatory organizations (Swedish EPA, HaV and KemI) are in Swedish and this can represent a limitation when non-Swedish speaking experts are involved. Considering the fact that Swedish law requires public contracts to be written in Swedish, a translated copy of the agreement, or essential parts thereof, attached as an Appendix would be of great help. Otherwise, there is a high risk of misunderstanding, lack of clarity and confusion. This hinders communication and understanding in an international academic world.

Key aspects for the pre-collaboration stage:

- Is non-target or suspect screening the most appropriate method for the question in hand? May targeted methods yield more suitable information?
- Mutual understanding of the project goals and analytical limitations. Are both in agreement for the correct accomplishment of the commissioned task?
- What are the limitations of this study, and how will they be communicated to all stakeholders?
- Do project timelines, data archiving, and feature prioritization align with the objectives?
- Ensure complete understanding of contractual agreements. Is there a possibility of having a translated copy of the contract? Consider data archiving plans for future retrospective analysis.

2.2 Collaboration stage: Adapting and executing the study design

Designing and executing an effective NTS/SS study involves flexible adaptation to regulatory needs, effective use of data processing tools, and thorough quality control. While at this stage of the project, the biggest work burden is already on the researchers' side, a continuous discussion with the commissioners to follow up on the appropriateness and comprehensiveness of the study can improve the outcome of the project. Such discussions could cover the following topics, although not exclusively.

A. Adapt study design to regulatory needs and instrumental limitations

- i.* When focusing on suspect screening studies, decide on prioritization strategies that help meet the commissioners' expectations (if this has not already been done in the preparatory phase). As an example, prioritizing hazardous substances or compounds with known temporal trends (systematic signal increase in former studies), or compounds with specific physico-chemical properties, such as persistent, mobile (PM) or persistent, bioaccumulative (PB), or with a specific toxicological profile, e.g., endocrine disruptors.

- ii.* Prepare and curate suspect lists that are compatible with the study's analytical methods. Tailor these lists according to sampling, sample preparation, chromatographic technique, and ionization method requirements. Researchers should be aware of the limitations of the selected methodologies and communicate them. With them in mind, it could either be decided to limit the scope of the NTS/SS study or to split the study into sub-studies by using multiple analytical methodologies.
- iii.* Design quality controls strategy by means of matrix-matched quality controls (QCs) as well as isotopically labelled internal standards (ILIS) to ensure appropriate method performance and chemical domain coverage.
- iv.* Foster continuous dialogue between stakeholders and researchers during the decision-making process during the study. Should any setback happen during the study period, a thorough discussion with the commissioner to overcome the unexpected limitations should be established.

B. Implement rigorous data collection and interpretation practices

- i.* Use reproducible workflows with robust quality control, including standards and controls that can validate findings and serve as benchmarks in the data processing pipeline. Implement widely accepted quality control and quality assurance strategies in all the steps along the study.
- ii.* Use of standardized data interpretation and reporting tools for transparency purposes.
- iii.* In case high confidence levels are needed for regulatory use, treat NTS/SS as a preliminary screening tool and compliment with targeted methods if necessary.

C. Data archiving for future access

- i.* Consider digital archiving of raw data to allow retrospective analysis. Archived data can be valuable for identifying trends over time, especially for legacy contaminants that may not warrant current focus but are worth investigating retrospectively. Additionally, archived data can help identifying previously overlooked new emerging contaminants retrospectively or even increase confidence in the findings when new evidence is available in online databases such as, e.g., MassBank.
- ii.* Establishing national or centralized raw data repositories accessible for such retrospective screenings can enhance regulatory value over time. Although this surpasses the boundaries of individual commissioned projects, its benefits are remarkable for retrospective analyses.

Key aspects for the collaboration stage:

- Continuous dialogue and discussion during project implementation are highly encouraged. Especially if any setback should happen.
- Prepare and curate the list of chemicals of interest thoroughly to meet both project requirements as well as method limitations. Explore the possibility of applying multiple methodologies in case the scope of the study required to do so.
- Implement robust quality control and assurance strategies to validate the findings and support the implications of the non-detections.
- Consider data archiving plans for future retrospective analysis.

2.3 Reporting and interpretation of results: Building confidence and clarity

Effective reporting and interpretation of the results ensures that the outcomes of commissioned NTS/SS studies are relevant and actionable for regulators. While there are reporting strategies for NTS/SS widely accepted among researchers, those are not always fulfilling the regulatory understanding and needs. Hence, researchers and commissioners should also be flexible in their adaptation to the regulatory reporting needs. The following guidelines emphasize clarity, confidence, and transparency in data interpretation and reporting.

A. Confidence levels and reporting standards

- i.* Clearly communicate the confidence levels associated with detected compounds, using standardized frameworks like the Schymanski levels, or agreed terms to fit the regulatory needs. If the latter, a clear definition and explanation of each concept used should be included in the report. However, avoid arbitrary use and communicate uncertainties transparently to ensure clarity on reliability.
- ii.* Discuss thoroughly the meaning of a chemical being reported as ‘non detected’. Suspect screening limit of detection (SS-LOD), or in other words instrumental limit of detection (IDL) evaluate which is the lowest concentration in which the NTS/SS methodology would be able to detect a present chemical; indicating that a chemical below such concentration would not be spotted with the applied NTS/SS and end up reported as ‘non-detected’. To this end, linking the SS-LOD, or IDL, to toxicological

thresholds such as the Predicted No-Effect Concentrations (PNEC) in that particular matrix analysed can help to contextualize findings for regulatory risk assessment. While a reported 'non detection' does not necessarily mean that the chemical is not present in the sample but might be at concentration levels not monitorable by the selected analytical methodology, having SS-LODs or IDLs lower than PNEC values ensures that the chemical would not be at hazardous concentrations levels in the sample. In addition, clear indication of the chemical domain covered by the approach (based on physico-chemical characteristics of the analytical methodology) used in the study would greatly benefit the interpretation of non-detection results.

- iii.* Reporting templates flexibility. While the conventional quantitative analyses usually share a common reporting template to the centralized archiving repository of SGU data base for environmental pollutants, the reporting of NTS/SS commissioned studies should be more flexible. So far, this has not yet been achieved and reporting of SS and NTS studies is not yet feasible. It is also very relevant to raise concern about the need for the inclusion of study meta data in the database.

B. Reporting detected compounds and how to handle potential false positives or negatives

- i.* Evaluate and report compounds included as quality controls (QC) in the study to account for potential false results. Additionally, the use of isotopically labelled internal standards (ILIS) added to the individual samples before extraction could be explored. This helps to clarify whether a non-detect truly implies absence or is a methodological limitation.
- ii.* As stated before, be explicit about the limitations of NTS/SS in advance, particularly around false negatives for well-known substances. While the possibility of reporting false negatives or positives is not negligible due to instrumental limitations or artifacts, transparency on the methodology LOD facilitates the understanding of the potential implications of such false reporting.

C. Guidelines for reporting detections and non-detections

- i.* Define and communicate the meaning of "non-detected" within the context of regulatory relevance and the particular commissioned project.
- ii.* Confirm that the manner in which estimated concentrations are reported is meaningful for the regulatory needs, often focused on a compound not exceeding certain concentration values.
- iii.* Link findings to regulatory thresholds with appropriate concentration ranges if quantification is challenging. As an alternative, offer semi-quantitative data to support decision-making. However, the uncertainty in the semi-quantitative data must also be communicated and discussed.

Key aspects for the reporting stage:

- Agree on a reporting guideline that meets both research and regulatory needs to ensure clear and transparent understanding from both parties.
- Discuss thoroughly the meaning of ‘non-detection’ in relation to the methodology limits of detection and the potential implications of false negatives in relation to toxicological thresholds.
- Implement robust quality control and quality assurance strategies in the commissioned NTS/SS studies to ensure the reliability of the reported information.

2.4 Ongoing communication and post-study recommendations

Maintaining open dialogue during and after the study is essential to translating scientific results into practical regulatory applications. Furthermore, discussions after a commissioned project has been completed can result in improvement suggestions for the forthcoming commissioned tasks. Thus, it is pivotal to foster the dialogue between regulators and researchers. The following are some key recommendations highlighted during the workshop.

A. Continuous dialog and iterative feedback

- i.* Hold regular meetings to review data, assess project progress, and address any emerging challenges or setbacks. This helps to align priorities and ensure both parties agree on limitations and findings. This can also help to the flexibility of the project.
- ii.* Consider end-of-project workshops to present results and interpret findings collectively, promoting transparency and shared understanding.

B. Recommendations for future work and data integration

- Provide recommendations for regulators to integrate findings into long-term monitoring, especially when using NTS as a pre-screening tool.
- If confidence levels support it, recommend specific compounds or compound groups identified in NTS for targeted follow-up monitoring.

- Consider involving regulators throughout the study to guide prioritization of results, ensuring continued relevance of findings and efficient use of resources.

Key aspects for the reporting and aftermath stage:

- Hold regular meetings between researchers and regulators to review data, assess project progress and address any setbacks. This helps reacting if any modification to the study design should be made. End-of-project workshops could be greatly helpful for common understanding of the findings.
- Learn lessons from the projects and suggest improvement actions for the forthcoming commissioned tasks

3. The decision-tree for a screening study

Based on the lessons learned in the workshop as well as the expertise of the attendees, a clear and transparent decision process in the preparatory phase of the commissioned project is needed to fulfil the requirements of the partners involved. Figure 2 describes a workflow that should be carefully considered by both the authorities and researchers at the preparatory stage of the project.

In brief, after thoroughly identifying the problem that needs to be addressed e.g., chemical pollution responsible for increased biota mortality, chemical pollution of raw drinking water, or even the need to identify the chemical composition of a spill in natural water bodies; the key question to be answered is whether there is information on which chemical(s) could be responsible. If there is clear evidence of which chemical(s) is/are responsible, targeted methods should be applied. However, in many cases, there is no such information available. In such cases, we should investigate whether there is suspicion of a potential group of chemical(s) or chemical families that could be of interest. If not, we should then apply a pure NTS method to try to identify the corresponding pollutants. If we have a reason, we should decide if transformation products are of interest. If they are, we should apply NTS if no prior information is available on transformation pathways. If there is such information available (suspect lists), both on the suspects as well as their transformation products, we should investigate whether there is a need for quantitative data or not. If there is need for quantitative data, we should decide to apply targeted quantitative methods. However, if there is no need for such data and depending on the potential use of the results in a regulatory context, we could decide to go for suspect screening with a large list of chemicals or to targeted methodologies.

Although Figure 2 aims to guide authorities and researchers when discussing the better fit for the commissioned project, there may be a need to modify and include additional questions/decision point due to the nature of the project might arise. Thus, both authorities and researchers should also be flexible in adapting the suggested scheme when needed.

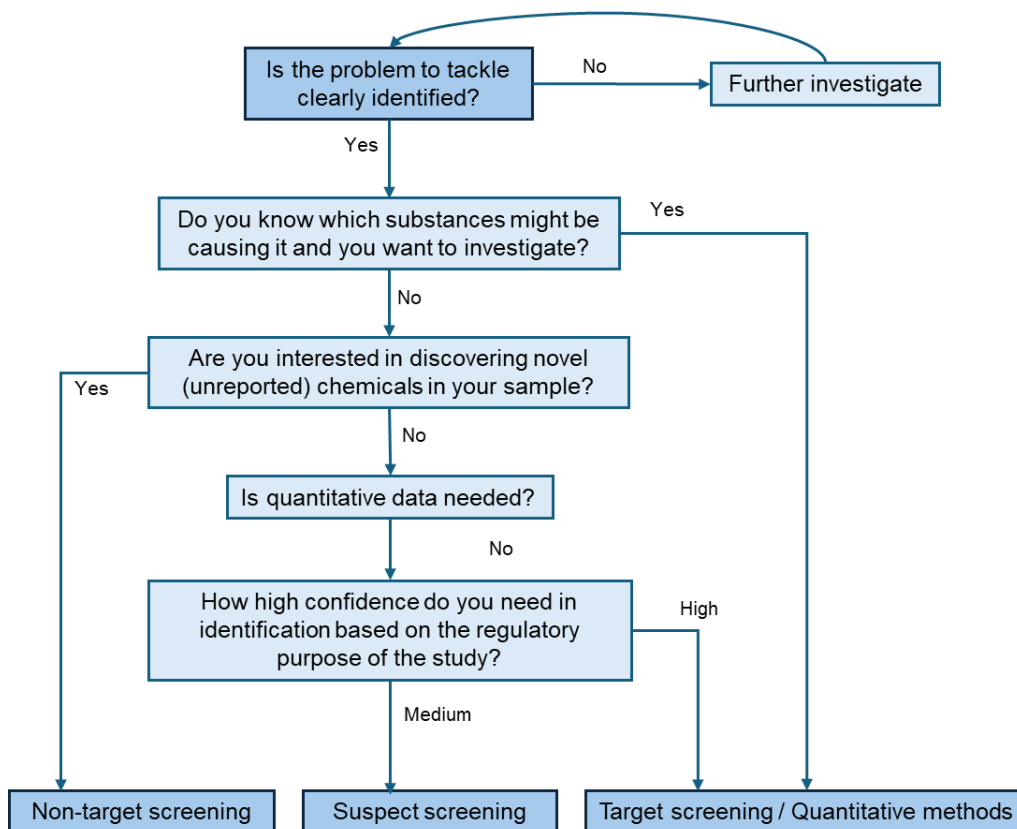


Figure 2. Decision tree for non-target, suspect and target screening studies.

4. Scientific community efforts in guiding and explaining non-target screening studies

While not specifically defined in any of the conclusions from the workshop previously described in this document, the overarching message in the discussions was the need to better understand the possibilities available for non-target studies and their limitations. The scientific community and more especially the NORMAN network has previously developed a guidance document providing a comprehensive and harmonized framework for conducting suspect and NTS within environmental monitoring programs.

The so-called “NORMAN guidance on suspect and non-target screening in environmental monitoring” (Hollender et al., 2023) explains that NTS encompasses two complementary strategies: suspect screening, which focuses on compounds already known or expected to occur based on existing databases or product information, and non-target screening, which aims to identify entirely unknown substances without prior assumptions. Both approaches rely heavily on high-resolution mass spectrometry (HRMS), typically coupled with liquid or gas chromatography, to obtain full-scan data that can be interrogated using reference libraries, predictive models, or retrospective analysis. This data-driven approach allows researchers not only to discover new contaminants but also to revisit historical datasets to trace the occurrence and evolution of emerging compounds over time.

A central message of the paper is the need for methodological consistency and quality across all stages of the NTS workflow—from sample collection and preparation to data processing and interpretation. Because NTS must address a vast range of chemical properties, analytical methods should be as generic as possible while maintaining robustness and reproducibility. The authors discuss in detail how different environmental matrices such as water, soil, sediment, air, and biota require tailored extraction and cleanup strategies to ensure representative chemical coverage and minimal contamination. For instance, solid-phase extraction is often used for trace-level water analysis, while pressurized liquid extraction or QuEChERS methods are more suitable for solids. In biological matrices, additional

cleanup steps are often required to minimize interferences without losing analytes. Passive sampling is also highlighted as a complementary technique for integrating pollutant accumulation over time, offering valuable insights into temporal trends of trace contaminants.

Chromatographic separation and ionization techniques play a crucial role in determining the range of detectable substances. Most NTS studies rely on reversed-phase liquid chromatography coupled with electrospray ionization (RPLC–ESI), which is effective for semi-polar and polar compounds. To extend coverage to more hydrophilic or volatile substances, alternative approaches such as hydrophilic interaction chromatography (HILIC), supercritical fluid chromatography (SFC), gas chromatography (GC), or atmospheric pressure chemical ionization (APCI) are recommended. The authors emphasize that understanding the chemical domain of each method (the set of substances effectively extracted, separated, ionized, and detected) is vital for interpreting analytical results and identifying gaps in chemical coverage.

The authors recognize that data processing and interpretation remain major challenges due to the sheer volume and complexity of HRMS data. The guidance outlines a typical sequence of data-processing steps (feature detection, background subtraction, alignment across samples, and database searching) and stresses the importance of clearly communicating identification confidence. To this end, the paper endorses a five-level confidence scale, ranging from confirmed identification with an authentic standard (Level 1) to tentative mass-only information (Level 5). Open-access databases and spectral libraries, such as the NORMAN SusDat, MassBank Europe, and PubChem, are identified as crucial tools for supporting identification efforts, though expert manual review remains indispensable for high-confidence results. The authors also advocate for open data sharing in accordance with FAIR (Findable, Accessible, Interoperable, Reusable) principles to enhance transparency, reproducibility, and collaboration among laboratories.

Because many substances detected through NTS lack available reference standards, quantification is inherently more uncertain than in traditional analyses. The guidance discusses semi-quantitative approaches that rely on surrogate standards, predicted ionization efficiencies, or relative response factors, while emphasizing that such methods should be interpreted with caution. Robust quality assurance and quality control (QA/QC) are therefore fundamental to NTS, requiring the consistent use of blanks, replicates, and internal standards, as well as detailed documentation of metadata, instrumental settings, and data-processing parameters. Participation in interlaboratory comparison studies is further encouraged to promote harmonization and confidence in reported results.

Overall, the authors position suspect and non-target screening as an essential advancement in environmental monitoring, marking a transition from narrowly focused chemical testing to comprehensive, data-driven chemical surveillance. NTS enables the discovery of previously unrecognized contaminants, supports the study of complex chemical mixtures, and provides early warnings of emerging environmental risks. Yet, for NTS to gain full regulatory acceptance, continued efforts toward harmonizing analytical protocols, data-processing workflows, and reporting formats remain critical. By articulating best practices and fostering open collaboration, the NORMAN guidance establishes a foundation for the global standardization of NTS, paving the way for its integration into future chemical monitoring and management frameworks.

While this comprehensive and detailed summary of the NORMAN guidance document serves as an indication of the content and discussions therein hold, the guidance should serve as a consulting document for better founding the decisions, discussions and interpretations of commissioned projects. The full document is freely available at <https://enveurope.springeropen.com/articles/10.1186/s12302-023-00779-4>.

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