Towards the development of a framework for applying non-target chemical analysis data within exposure and risk assessment

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Introduction

- Chemical risk assessment (Risk = Exposure/Effect) relates the bioavailable fraction of a chemical (i.e. freely dissolved concentration (Cfree)) to a toxicological effect.
- Exposure assessment can use a wide range of tools to quantify Cfree (**Figure 1**), which include both chemical analytical and environmental mass balance fate models.
- An increasing trend towards multi-targeted analysis and non-target screening methods to increase the number of analytes monitored in biomonitoring and environmental samples.
- NTA is often preceded by exhaustive extraction techniques, which may/may not adequately represent a potential for exposure, i.e., "bioavailability".
- There is no framework for interpreting and using non-target analysis (NTA) data to inform exposure and risk
- Guidance is thus needed to provide a strategy that allows for an efficient mechanism to couple NTA data with an accurate characterization of the chemical exposure potential.

Objectives

- Review the peer-reviewed literature reporting results associated with NTA and compile a database that captures the sample matrices that have been investigated, the extraction methods used, and the analytical technique employed to identify unknown chemicals in complex matrices.
- Based on state-of-the-art for NTA, propose a framework to guide the appropriate use of NTA data to inform exposure assessment.

Methods

Compile and evaluate available monitoring data collected using a non-target chemical analysis method.

(**Figure 2**)

Identify and evaluate key challenges certain matrices present for NTA for assessing exposure, either as a screening and prioritization tool and/or for risk assessment.

(**Figure 3**)

Apply a proposed framework that couples NTA data with an environmental fate mass balance model, aimed at an improved understanding of exposure potential for chemicals of emerging concern.

(**Figure 4, Poster MO74**)

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Results and Discussion

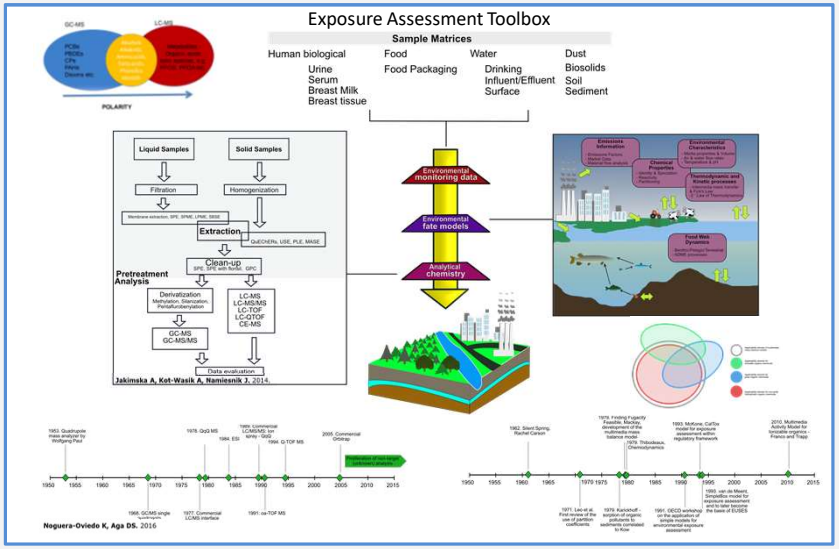

Figure 1: Illustrative representation of tools used to characterize exposure.

- **Figure 2:** Summary of analytical approaches adopted for targeted, suspect screening, and non-targeted analysis and key observations obtained from literature review.
- **Figure 3:** A conceptual approach illustrating the importance of the extraction method in assessing exposure potential.
- **Figure 4:** A proposed framework that couples NTA data with an environmental fate model.
- **Figure 5:** Key elements of the US EPA Chemistry Dashboard, and its use in linking NTA data with toxicity.

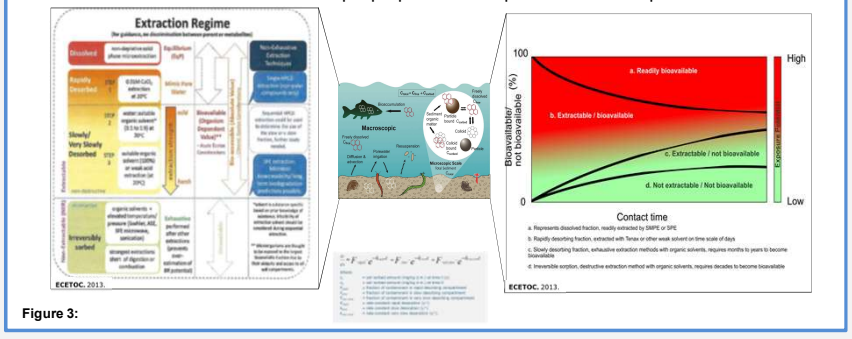

Figure 3:

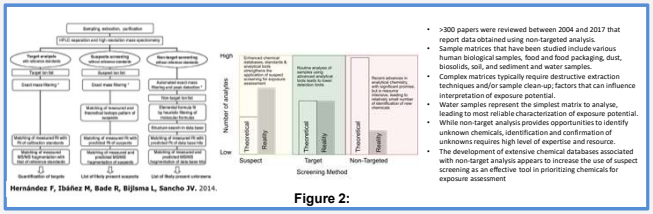

Figure 2:

- >300 papers were reviewed between 2004 and 2017 that report data obtained using non-targeted analysis.
- Sample matrices that have been studied include various human biological samples, food and food packaging, dust, biosolids, soil, and sediment and water samples.
- Complex matrices typically require destructive extraction techniques and/or sample clean-up; factors that can influence interpretation of exposure potential.
- Water samples represent the simplest matrix to analyse, leading to most reliable characterization of exposure potential.
- While non-target analysis provides opportunities to identify unknown chemicals, identification and confirmation of unknowns requires high level of expertise and resource.
- The development of extensive chemical databases associated with non-target analysis appears to increase the use of suspect screening as an effective tool in prioritizing chemicals for exposure assessment

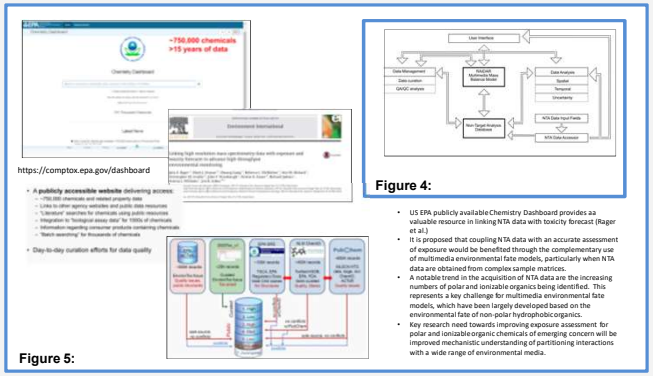

Figure 5:

Figure 4:

- US EPA publicly available Chemistry Dashboard provides aa valuable resource in linking NTA data with toxicity forecast (Rager et al.)
- It is proposed that coupling NTA data with an accurate assessment of exposure would be benefited through the complementary use of multimedia environmental fate models, particularly when NTA data are obtained from complex sample matrices.
- A notable trend in the acquisition of NTA data are the increasing numbers of polar and ionizable organics being identified. This represents a key challenge for multimedia environmental fate models, which have been largely developed based on the environmental fate of non-polar hydrophobic organics.
- Key research need towards improving exposure assessment for polar and ionizable organic chemicals of emerging concern will be improved mechanistic understanding of partitioning interactions with a wide range of environmental media.

- Exposure assessment requires accurate characterization of the bioavailable fraction, quantification of which depends on the complexity of the sample matrix being investigated.
- Careful consideration of the extraction method is important.
- Exhaustive extraction techniques can lead to large number of analytes detected. Identification of NTA requires significant resource, with accurate identification requiring confirmation against an analytical standard.
- Suspect screening methods that utilize extensive databases, such as the U.S. EPA Chemistry Dashboard, provide opportunities to identify and confirm the presence of a far larger number of analytes in samples as opposed to standard target analysis.
- Multimedia mass balance models coupled with analytical data can provide an effective framework for integrating the data for exposure assessment.
- A modelling platform that would couple NTA data with models such as RAIDAR, is proposed to help guide regulatory activities, both for screening and prioritization based on exposure and risk assessment.

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