Contaminants of Emerging Concern Identified by Suspect and non-target Screening in Marine Environment: A Scoping Review

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PhD student (PRORISK ESR 3): Kelsey Ng (527416@muni.cz / ng@ei.sk)
Supervisor: Dr. Jaroslav Slobodnik (EI)
Co-supervisors: Dr. Ludek Blaha(MU), Dr. Knut Erik Tollefsen (NIVA)

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Background

- Numerous contaminants of emerging concern (CECs) and transformation products (TPs) in the marine environment → often overlooked by target screening as reference standards (RSs) are not always available
- Advances in high-resolution mass spectrometry (HRMS) and tandem Mass Spectrometry (MS/MS)→ suspect and non-target screening (SNTS) made possible → wide-scope screening of these compounds without RSs
- Potential for regulatory implementation of SNTS

Aims of the study

1. **Retrieve CECs & their TPs detected in marine environments (seawater, sediment, biota) by SNTS studies**
2. **Identify various strategies adopted in the 4 steps of non-target screening (NTS) workflow by the scientific community**
3. **Address gaps, challenges, and future outlook for application of NTS in the regulatory monitoring and framework**

Scoping review process

Scopus database search

- Search for "marine", "non-target" and "high-resolution" in title, abstract and keywords
- Potentially relevant articles retrieved (n=175)

Study selection (SNTS on marine samples)

- Screen titles & abstracts for relevance (n=175) → articles selection (n=25)
- Screen their references → additional relevant articles identified (n=5)

30 Articles retained for detailed evaluation

CECs & TPs in marine samples detected by SNTS

- In the 30 articles, **1,567 CECs & TPs** were detected in marine environment of **23 countries/regions** in Europe, Asia, Oceania, North & South America
- Anthropogenic origin e.g., industrial chemicals, pesticides, pharmaceuticals
- 24 of them were **first reported in P. oceanica**
- 51 of them were considered as **posing significant environmental risk**

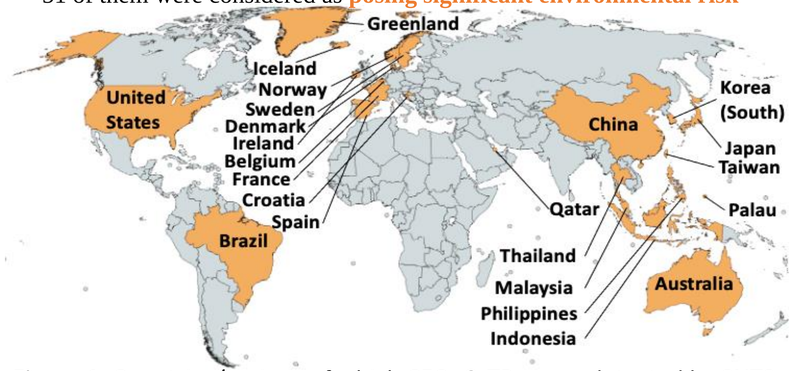

Figure 1. Countries/regions of which CECs & TPs were detected by SNTS

The NTS workflow and strategies adopted

Sample extraction

No harmonized approach, treatment preferred: as exhaustive as possible

SPE | GPC | QuEChERS

Matrix/analyte specific: e.g., activated Cu to remove sulfur in sediment

Component list generation

Different criteria sets on various parameters adopted for peak selection

S/N ratio | Mass error | Signal counts

Peak area/height/width

Peak prioritization

Various statistical tools/protocols used
→ depend on analytical instruments & analytes' properties

$^{79}Br/^{81}Br$ or $^{35}Cl/^{37}Cl$ peak pairs selected for CECs with Br/Cl

$-CF_2-$, $-CH_2CF_2-$, $-C_2F_4-$ mass differences as indicators of PFAS

Signal elucidation

Many elucidation tools available to identify prioritized CECs

Often complimentary to analytical instruments

Lack standardized protocols/quality requirements

Gaps, challenges and future outlook for NTS

Challenge: NTS analytical protocols lack standardization

- Standards in sample extraction, analytical & validation procedures
- Special technical protocols to target CEC groups (matrix specific)

Gap: harmonization in NTS methodological framework

- Distinct criteria on identification, terminology, QA/QC actions, etc.
- To maintain quality & consistency of outputs from NTS workflows

Development: data sharing/dissemination strategies

- Joint evaluation by wider scientific community → create synergy
- Initiatives by NORMAN: MassBank & Digital Sample Freezing Platform

Advancement: computational & knowledge exchange tools

- Advanced tools enhance essential knowledge exchange
- To facilitate the optimization & automation of NTS workflows

Discussion & Conclusion

- Scoping review: **30 SNTS studies** retrieved, revealing **1,567 CECs & TPs** in marine environment of **23 countries/regions in five continents**
- 75 compounds were first reported/posing significant environmental risk
- Major challenges: **lack of harmonization in NTS analytical protocols & methodological framework**
- Future outlook: development in **computational tools and data exchange** platforms → accelerates **harmonization & automation** of the NTS workflow → fosters **regulatory application of SNTS** in marine samples

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