




Electronic Supplementary Material

This supplementary material has not been peer reviewed.

Title: Substances of Emerging Concern in Baltic Sea Water – Review on Methodological Advances for the Environmental Assessment and Proposal for Future Monitoring

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Table S 1 Conducted literature searches following the procedure described by Mengist et al. 2020. For this study, 3 review objectives were defined and the specifications of the conducted searches are described in the respective cell columns. The literature searches were performed from April 2020 to July 2021.

| REVIEW OBJECTIVES AND SCOPE OF THE SEARCHES | | |
|--|---|--|
| Which concentrations for contaminants of emerging concern are reported for Baltic Sea surface water? | Which methodological advances are reported for the chemical analysis of contaminants of emerging concern in marine water? | Which effect-based methods exist that could be used for marine water analysis? |
|  |  |  |
| TARGET COMPOUND CLASSES | | |
| pharmaceuticals / UV-filters / estrogens and estrogenic compounds / polar pesticides / per- and polyfluoroalkyl substances / algal toxins | | |
| ADDITIONAL CLASSIFICATION | | |
| chemical analysis / effect-based analysis | sample processing / analytical approaches / passive sampling | <i>in situ</i> field monitoring / <i>in vitro</i> bioassays / effect-directed analysis |
| SEARCH STRATEGY, SOURCES | | |
| • databases Web of Science and HELCOM | • database Web of Science or Science Direct • reports of marine science organizations • reports of water policy working groups | |
| SEARCH KEYWORDS | | |
| pharmaceuticals UV-filter estrogen pesticide perfluoroalkyl PFAS nodularin microcystin polybrominated phenols polybrominated dibenzo-p-dioxins AND Baltic Sea | • sample processing: solid-phase extraction AND pharmaceutical UV-filters UV-stabilizers estrogen pesticide PFAS perfluoroalkyl algal toxins AND seawater marine • analytical approaches: HRMS FT-ICR-MS Orbitrap MS-MS mass-spectrometry multi method AND contaminant AND marine ocean seawater • passive sampling: passive sampling AND seawater • effect-based methods: effect-based in vitro bioassay in vivo bioassay effect-directed analysis AND marine seawater water | |
| INCLUSION CRITERIA | | |
| • within review objective from title and abstract • accessible • English language | • within review objective from title and abstract • accessible • English language • reports not older than 2010 • method applied in seawater or promising for seawater analysis | |
| EXTRACTED INFORMATION | | |
| • Baltic Sea study area • study year • mode of assessment (chemical or effect-based) • method details • surface seawater conc. | • description of the method • reported limitations • example study sites and key findings | |
| ANALYSIS | | |
| • summary or reported data • outlining predominant substances within compound classes for the Baltic Sea • describing methods for chemical and effect-based analysis potentially suitable for analysis of marine water • built recommendations for improved assessment of the state of the Baltic Sea on data | | |

References

- Mengist, W., T. Soromessa, and G. Legese. 2020. Method for conducting systematic literature review and meta-analysis for environmental science research. *MethodsX* 7: 100777. doi:10.1016/j.mex.2019.100777.