Application of QSAR models for screening of sea-dumped munition and related chemicals: The Paardenmarkt as a case study

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Vast quantities of conventional and chemical munitions were dumped in the marine environment after World War I and World War II, with the coastal areas of the countries directly involved in such conflicts being particularly impacted. Due to decades of corrosion, several munition-related chemicals have been detected in environmental samples. Despite their lasting legacy, considerable data gaps still exist with regards to environmental properties and toxicity to human and environmental health of such chemicals. Here, Quantitative Structure-Activity Relationship (QSAR) models compiled under EPI Suite and OECD QSAR Toolbox were applied to screen and prioritize an array of seven chemical warfare agents and related chemicals (CWA&RC), i.e. sulphur mustard, 1,4-oxathiane, 1,4-dithiane, thiodiglycol, Clark I, diphenylarsinic acid and bis(diphenylarsinyl) oxide, and eight conventional explosives and related chemicals (E&RC), i.e. TNT, 2-ADNT, 4-ADNT, tetryl, picric acid, 1,3-DNB, 2,4-DNT, 2,4-DANT. These chemicals were specifically selected due to their particularly relevant to the Paardenmarkt, a WW I dumpsite located approximately 1.5 km from the Belgian coast where 35 000 tons of conventional and chemical munitions were reportedly dumped. Specifically, the assessment of the chemicals' environmental properties show that only Clark I and bis(diphenylarsinyl) oxide are excepted to bioaccumulate in aquatic organisms, even though field studies also report the presence of TNT, 2-ADNT and 4-ADNT in the tissues of marine biota collected in the vicinity of munition dumpsites. Additionally, following European guidelines, all screened E&RC as well as the CWA&RC sulphur mustard were deemed persistent, suggesting that the former tend to be, as a group, more persistent in the environment. With regards to toxicity to aquatic organisms, the screened E&RC are expected to be acutely as well as chronically more toxic than the CWA&RC. Furthermore, parent compounds present higher toxicity than their respective degradation production in both groups of chemicals. Interestingly, the trends observed in toxicity to aquatic organisms are transversal to the human health hazard assessment. Overall, the gathered data shows that QSAR models can generate conservative and reliable estimations useful for the prioritization of munition-related chemicals to further investigation, essential given the safety measures associated with the performance of experimental work on E&RC and CWA&RC. Hence, based on their persistence, bioaccumulation potential and human and environmental toxicity, sulphur mustard, Clark I and bis(diphenylarsinyl) oxide were prioritized among the screened chemical warfare agents and 1,3-DNB, 2-ADNT, 4-ADNT, 2,4-DNT, tetryl and TNT among the conventional explosives.

Keywords
QSAR Models; Paardenmarkt Dumpsite; Munition-Related Chemicals; (Eco)Toxicity, Environmental Properties