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Poly(ethylene terepthalate) oligomers: assessing their migration in foods and food simulants using an UHPLC-qTOF-HRMS method

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Polyethylene terephthalate (PET) is among the most common food contact materials (FCMs). Concerns about the non-intentionally added chemicals (NIAS) present in FCMs that can arise during polymerization have grown over the past few years. Specific migration restrictions for PET cyclic oligomers, which are considered as NIAS, have not yet been established by EU legislation. However, due to the lack of toxicological knowledge, their impact on human health is still unclear. Additionally, *in silico* calculations and evaluation of the Toxicological Threshold of Concern (TTC) established by the European Food Safety Authority (EFSA) show that PET cyclic oligomers are Cramer III toxicity compounds, indicating a potential risk for human health.

This study aims to investigate the migration of these species in common foodstuff, such as tap water and olive oil. For this purpose, an UHPLC-qTOF-HRMS was developed and validated. Due to the complexity of analysing edible oils, a QuEChERS clean-up was applied to facilitate oligomers' extraction, for the first time in the literature**.** The method validated in terms of linearity, sensitivity, accuracy and precision. Calibration curves were constructed using fortified samples, and the limits of quantifications (LOQs) ranged from 10 to 50 μg L^{-1}, while the recoveries ranged between 86.6 and 113%. Thereafter, the study evaluated the migration of PET oligomers from virgin and recycled PET FCMs into virgin olive oil (VOO), tap water and official food simulants. For this purpose, two procedures were performed and compared: 1) test conditions according to Commission Regulation EU No. 10/2011 [1] and 2) storage of VOO and water in household conditions.

The results showed that after a year of storage in room temperature, there is no migration of oligomers in VOO samples or tap water. On the contrary, significant amounts of cyclic and linear PET oligomers were found in food simulants (95% ethanol and 20% ethanol) and in both types of tested PET bottles (virgin and recycled), with the migration of PET cyclic trimer from recycled bottles being the most abundant. Our findings are in accordance with previous studies, which demonstrated that accelerated testing conditions strongly overestimate the migration under room temperature conditions [2,3].

Keywords: polyethylene terephthalate, migration testing, food contact materials (FCMs), QuEChERS clean-up

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