

Abstract of the Master Thesis

„Determination of glyphosate and AMPA in seawater by HPLC-MS/MS – Optimization of an ultratrace method by using a pre-concentration step“

Glyphosate was classified as "probably carcinogenic" by the International Agency for Research on Cancer (IARC) in 2015. This classification and the large quantities applied each year make precise monitoring of the fate of glyphosate and its main metabolite aminomethylphosphonic acid (AMPA) in the environment increasingly important. In this work, a method for the analysis of glyphosate and AMPA in seawater samples using HPLC-MS/MS was investigated and optimised. Since the analytes can be extremely diluted in seawater, the limits of quantification should be as low as possible. In order to achieve very low limits of quantification, it was investigated whether pre-concentration by means of solid phase extraction (SPE) prior to derivatisation with FMOC-Cl is possible. Different elution volumes were investigated and compared. In addition, the influence of using ethylenediaminetetraacetic acid (EDTA) before and after derivatisation with FMOC-Cl to stabilise the derivatives was investigated. Furthermore, it was investigated whether filtration of samples prior to sample preparation retains the target analytes and, consequently, has a negative impact on the absolute recovery rates of the analytes. The investigations showed a clear increase in the absolute recovery rates when EDTA was used after derivatisation. Filtration of the samples before sample preparation significantly ($p < 0.05$) reduced the absolute recoveries of the analytes. Pre-concentration step included to the existing method reduced the limits of quantification from 7 ng/L and 10.4 ng/L for glyphosate and AMPA, respectively, to 0.3 ng/L for both analytes. The optimised method was validated with acceptable relative recoveries between 70 and 120% and a satisfying relative standard deviation (RSD) of $\leq 20\%$ in high purity water according to SANTE/12682/2019. Lastly, seawater samples from Bohai Bay, in China, were reanalysed and the results compared with those already available. By applying the optimised method, traces of glyphosate and AMPA could be detected in the samples that were previously not clearly detectable. In addition, the existing results could be confirmed.

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Date: 20.10.2021