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Suspect screening of halogenated carboxylic acids in drinking water using ion exchange chromatography – high resolution (Orbitrap) mass spectrometry (IC-HRMS)

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Abstract

Retrospective *in silico* screening of analytical data for the identification of new or emerging disinfection by-products in drinking waters could be useful to assess quality and potential hazards, as well as help implement mitigation procedures more rapidly. Herein, the first study coupling ion exchange chromatography (IC) with high resolution mass spectrometry (HRMS) for the determination of halogenated carboxylic acid disinfectant by-products is reported. Separation was achieved using a Metrohm A Supp 5 column and a Na₂CO₃/NaHCO₃ gradient eluent from 1/0.31 to 10/3.1 mM. A variety of solid phase extraction (SPE) sorbents were tested for added selectivity to organic ions and Isolute ENV+ cartridges were selected because of their best overall extraction performance. Method LODs were in the µg L⁻¹ concentration range, with R² ≥ 0.99 for all the analytes, and iso-

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