Accepted Manuscript

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Authors: Nina Hermes, Kevin S. Jewell, Arne Wick, Thomas A. Ternes

PII:	S0021-9673(17)31668-0
DOI:	https://doi.org/10.1016/j.chroma.2017.11.020
Reference:	CHROMA 359004
To appear in:	Journal of Chromatography A
Received date:	12-9-2017
Revised date:	7-11-2017
Accepted date:	12-11-2017

Please cite this article as: Nina Hermes, Kevin S.Jewell, Arne Wick, Thomas A.Ternes, Quantification of more than 150 micropollutants including transformation products in aqueous samples by liquid chromatography-tandem mass spectrometry using scheduled multiple reaction monitoring, Journal of Chromatography A https://doi.org/10.1016/j.chroma.2017.11.020

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Quantification of more than 150 micropollutants including transformation products in aqueous samples by liquid chromatography-tandem mass spectrometry using scheduled multiple reaction monitoring

Nina Hermes, Kevin S. Jewell, Arne Wick, Thomas A. Ternes*

Federal Institute of Hydrology (BfG), Am Mainzer Tor 1, D-56068 Koblenz, Germany

*corresponding author. Thomas A. Ternes, phone: +49 261-1306 5560; fax: +49 261-1306 5363; e-mail: ternes@bafg.de)

Highlights

- A direct injection multi-residue analysis method for 154 compounds was developed
- Quantification of 84 precursors and 70 TPs/metabolites in different water matrices by two chromatographic runs
- Influence of target scan time on dwell time and data points per peak is shown
- Methods can aid the assessment of water quality and water treatment processes

Abstract: A direct injection, multi analytical residue method separated in two chromatographic runs was developed utilizing scheduled analysis to simultaneously quantify 154 compounds, 84 precursors and 70 Transformation products(TPs)/metabolites. Improvements of the chromatographic data quality, sensitivity and reproducibility were achieved by scheduling the analysis of each analyte into pre-determined retention time windows. This study shows the influence of the scan time on the dwell time and the number of data points per peak as well as the effect on the precision of analysis. Lowering the scan time decreased dwell time to a minimal value, however, this had no negative effects on the precision. Increasing the number of data points per peak by decreasing the scan time led to more accurate peak shapes. A final set of parameters was chosen to obtain a minimum of 10 data points per peak to

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