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Electronic Supplementary Information

Direct Coupling of Desorption Electrospray Ionization Mass Spectrometry to Thin-Film Microextraction and its Application to Wastewater Analysis

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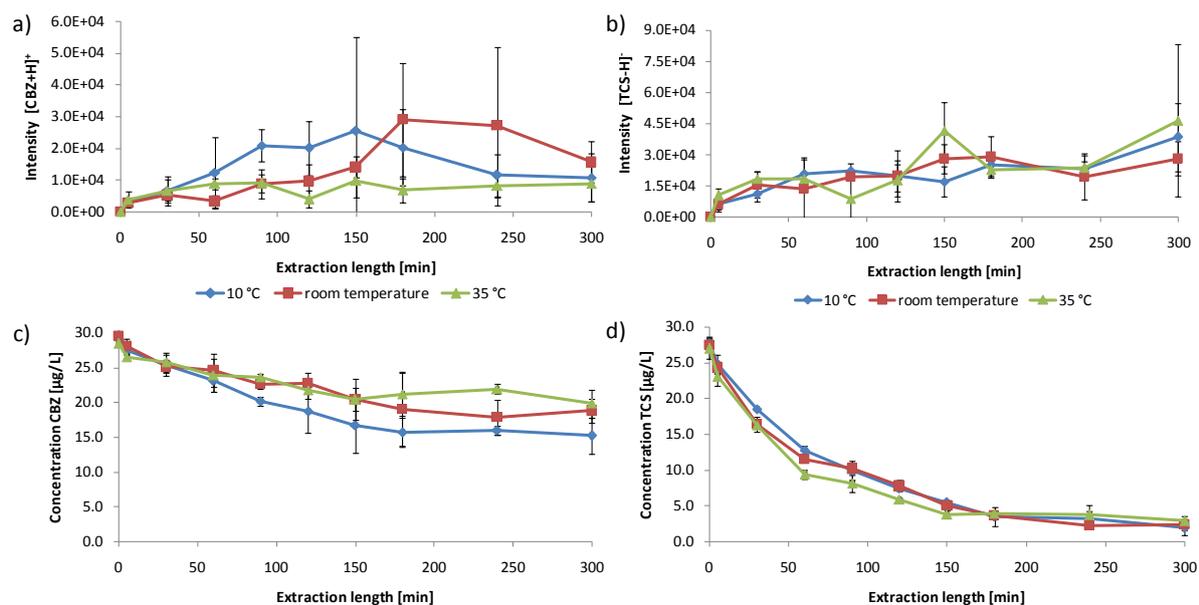


Fig. S1 TFME/DESI-MS data for a) carbamazepine and b) triclosan compared to direct LC-MS analysis (calibrated) of the extracted sample solutions after adding ISTD for c) carbamazepine and d) triclosan; extraction was performed using different temperatures.

Table S1 Amount of extracted triclosan and carbamazepine using equilibrium extraction at different temperatures showing more pronounced temperature dependence for less hydrophobic carbamazepine.

analyte	amount of analyte extracted at different temperatures		
	10 °C	room temperature	35 °C
carbamazepine	49 %	36 %	30 %
triclosan	93 %	91 %	89 %

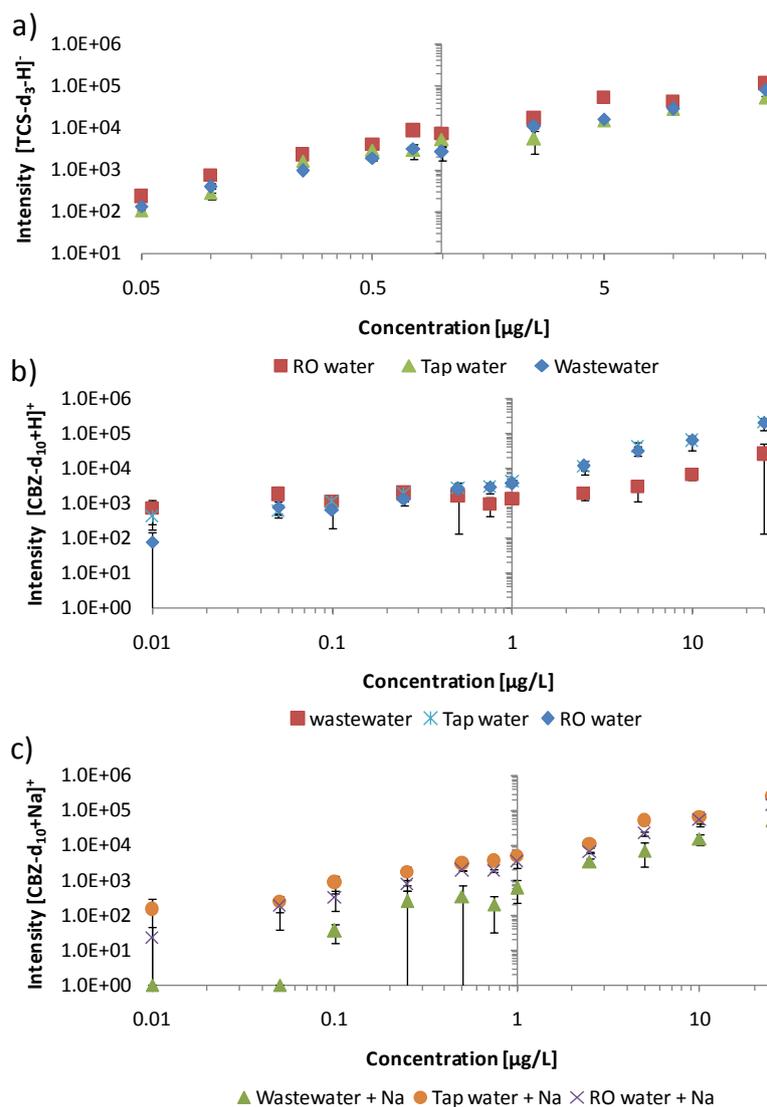


Fig. S2 Figures displaying matrix dependency for a) triclosan and b+c) carbamazepine; b) data analysis performed using protonated molecular species showing constant values for concentrations below 1 μg L⁻¹ because of disturbing isobaric peak; c) data analysis performed using sodium adduct which is not disturbed by isobaric peaks and thus shows further decrease in signal intensity below 1 μg L⁻¹. Signal reduction in wastewater approximately 90 % and 50 % for carbamazepine and triclosan respectively, but still detection limits as low as 10-50 ng L⁻¹ are achieved.

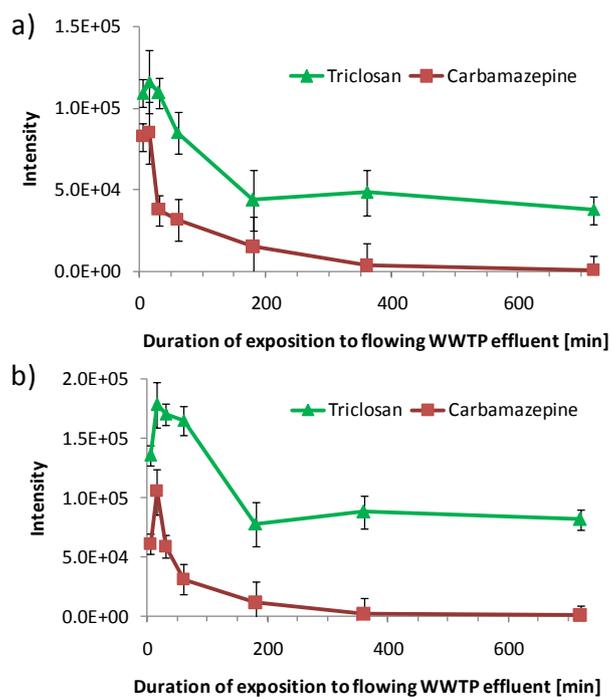


Fig. S3 Absolute intensity of carbamazepine and triclosan in TFME/DESI-MS as function of length of exposure to flowing WWTP effluent after applying a temporarily high analyte concentration; triclosan intensity stays relatively constant at 30 % of the original value after 3 h have passed whereas carbamazepine intensity further reduces; recorded using a) normal scan mode (see Fig 2) and b) continuous scan mode displaying same trend but reduction of intensity about 30 %.

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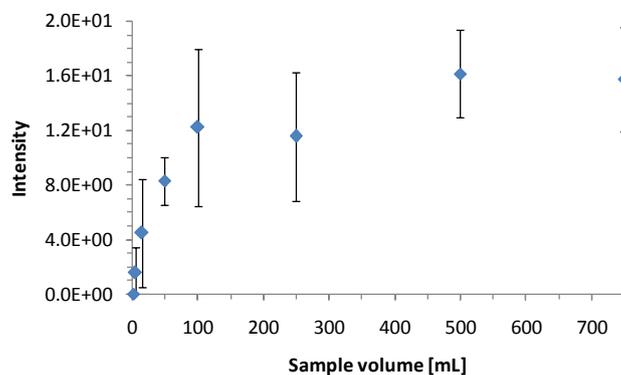


Fig. S4 Intensity of antidepressant sertraline (m/z [M+H]⁺ = 306.0816) as a function of WWTP effluent sample volume extracted; reliably detected in triplicate only using enhanced extraction volumes \geq 50 mL.

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