

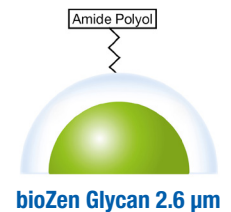
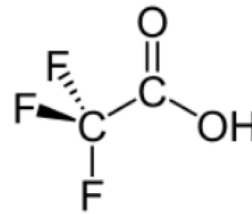
APPLICATIONS

LC-MS/MS Analysis of Trifluoroacetate in Groundwater and Drinking Water using a bioZen® Glycan 2.6 µm 150 x 2.1 mm column

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Introduction

Trifluoroacetate (TFA) is a non-toxic but persistent contaminant of water, including drinking water. Recent research¹⁻³ has indicated that standard wastewater treatment facilities are not able to remove TFA. Some of the processes used at these facilities are possible additional sources of TFA. Since January 2017 TFA is defined by the German Environment Agency (Umweltbundesamt – UBA) as a non-relevant metabolite with a health-oriented guidance value (GOW) of 3.0 µg/L in drinking water. This application note describes an easy, precise, and robust method to determine the concentration of TFA in drinking water and groundwater.



Experimental Conditions

The analyses were performed on an Agilent® 1260 Infinity II system equipped with an Agilent 6475 Series Triple Quad MS-Detector. The MS-detection was done using electrospray ionization in the negative mode (ESI-).

HPLC Parameters

Column: bioZen Glycan 2.6 µm
Dimensions: 150 x 2.1 mm
Part No.: 00F-4773-AN
Mobile Phase: 10 mmol/L NH₄Ac + 0.1 % CHOOH / Acetonitrile (40:60)
Flow Rate: 0.55 mL/min
Injection Volume: 100 µL
Detection: Electrospray Ionization Tandem Mass Spectrometer (ESI-MS/MS)

Mass Spectrometer Parameters

Table 1.
MRM Transitions and Compound Dependent Parameters

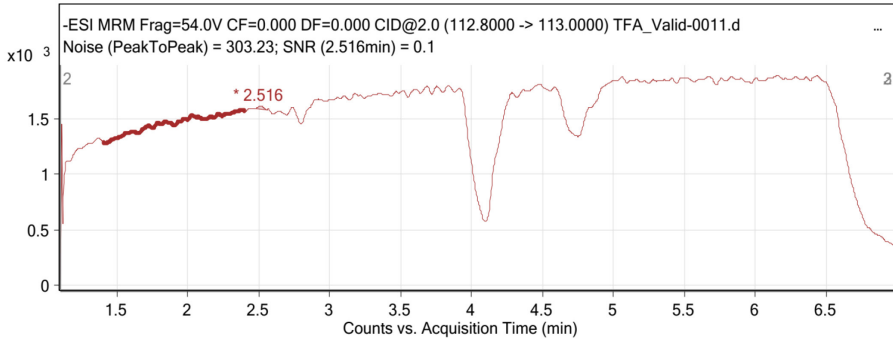
Compound Name	Q1	Q3	Dwell	Frag	CE
TFA- ¹³ C ₂ (ISTD)	115.1	70	40	54	12
TFA	112.8	113	40	54	2
TFA	112.8	69	40	54	11

Table 2.
MS Source Parameters

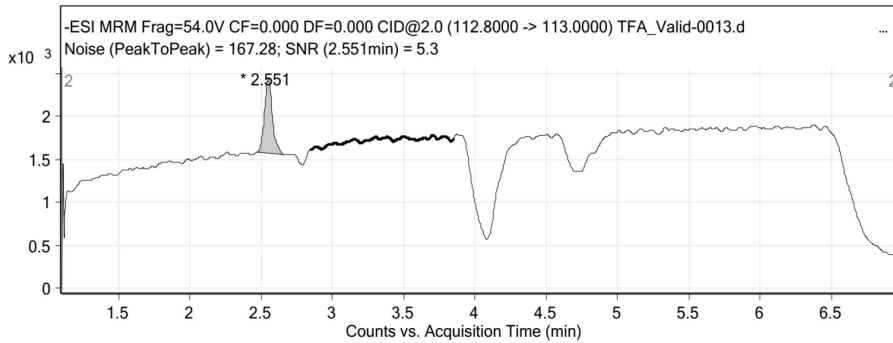
Source Parameter	Setting	
	Value (+)	Value (-)
Gas Temp [°C]	300	300
Gas Flow [l/min]	9	9
Nebulizer [psi]	45	45
Sheath Gas Heater [°C]	350	350
Sheath Gas Flow [l/min]	11	11
Capillary [V]	3,500	3,500
V Charging	0	300

Analyte and Retention Time

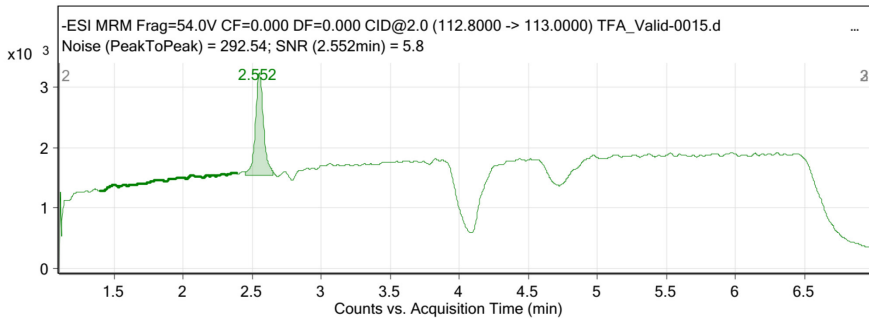
Analyte	RT
TFA	2.55 min



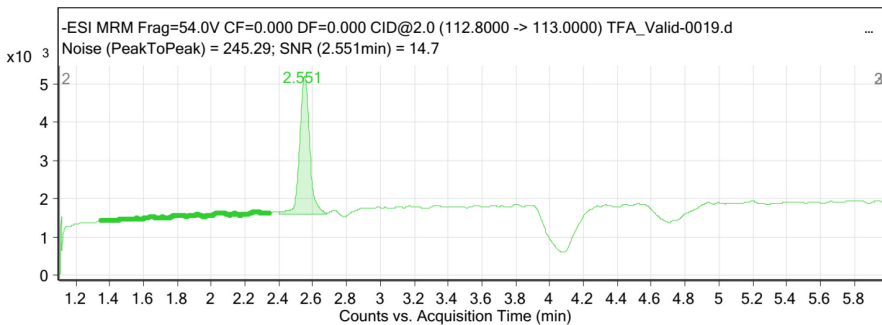
Blank



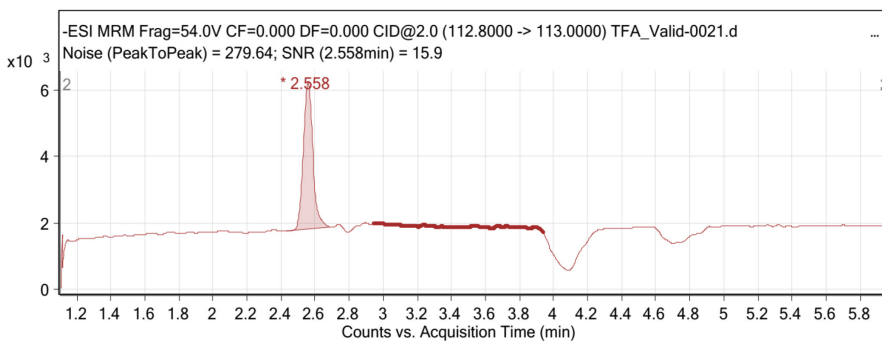
0.05 µg/L



0.10 µg/L

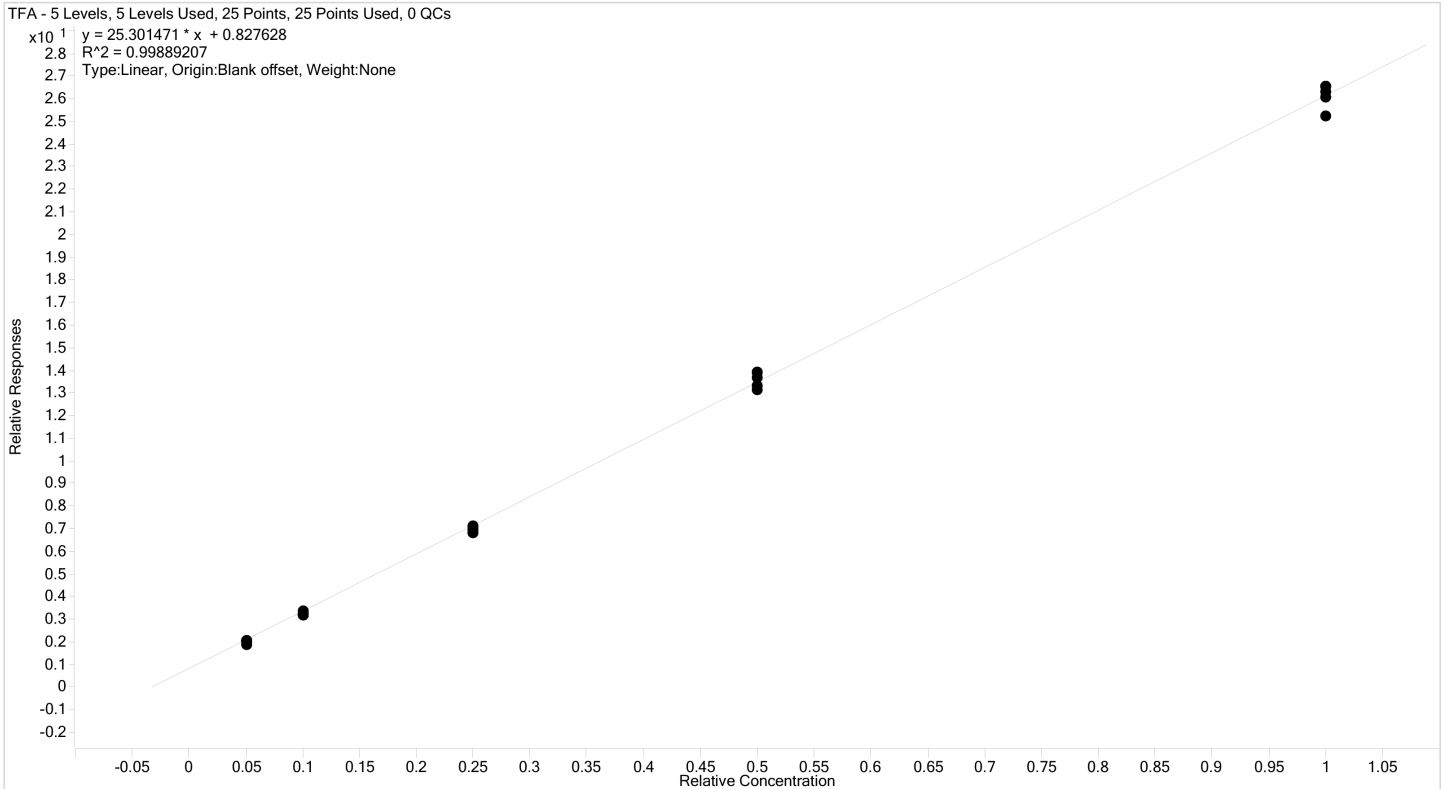


0.20 µg/L



0.25 µg/L

The linearity range of the method was determined by using standard injections with concentrations from 0.05 µg/L - 0.25 µg/L. Each sample was injected 5 times.



Results and Discussion

The presented HILIC method allows a fast and reliable quantification of TFA in groundwater and drinking water samples under isocratic conditions. The LOD according to DIN 32645:2008-11 is 0.0187 µg/L and the LOQ is 0.0495 µg/L.

References

1. Scheurer, M. et. al. Small, mobile, persistent: Trifluoroacetate in the water cycle – Overlooked sources, pathways, and consequences for drinking water supply, *Water Res* 126 (2017), 460-471
2. Brunner, A.M. et. al. Integration of target analyses, non-target screening and effect-based monitoring to assess OMP related water quality changes in drinking water treatment, *Sci. Total Environ.* 705 (2020), online article 135779
3. Janda, J. et. al. Robust trace analysis of polar (C2-C8) perfluorinated carboxylic acids by liquid chromatography-tandem mass spectrometry: method development and application to surface water, groundwater and drinking water, *Env Science and Pollution Res* 26 (2019) 7326-7336

Acknowledgements

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Biocompatible Hardware

Ordering Information

bioZen Columns (mm)	Biocompatible Guard Cartridges			
	50 x 2.1	100 x 2.1	150 x 2.1	for 2.1 mm Holder
bioZen 2.6 µm Glycan	00B-4773-AN	00D-4773-AN	00F-4773-AN	AJO-9800 /3pk AJO-9000 ea

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