

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

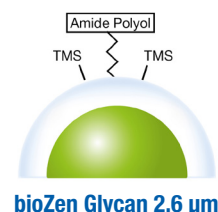
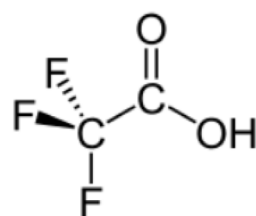
Peer Ziese¹, Julia Engel², Jörg Baute² and Dirk Hansen²

¹Umwelt Control Labor GmbH, Köpenicker Straße 59, 24111 Kiel, Germany

²Phenomenex Ltd, Zeppelinstraße 5, 63741 Aschaffenburg, Germany

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

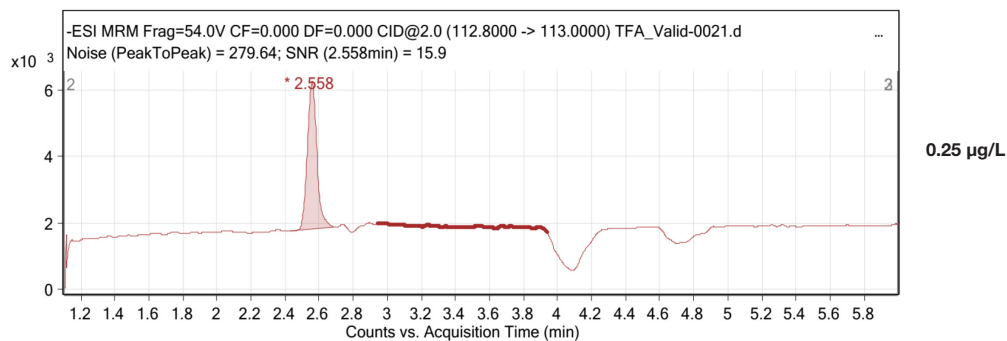
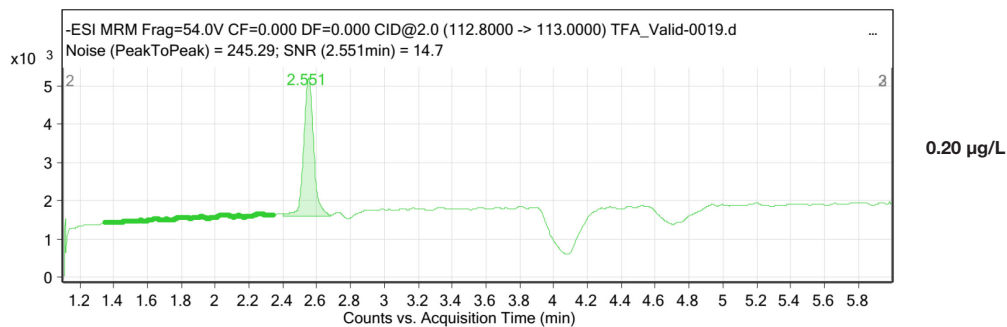
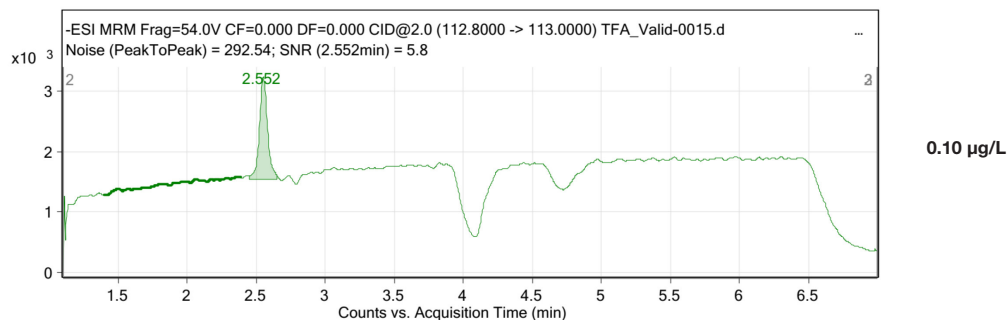
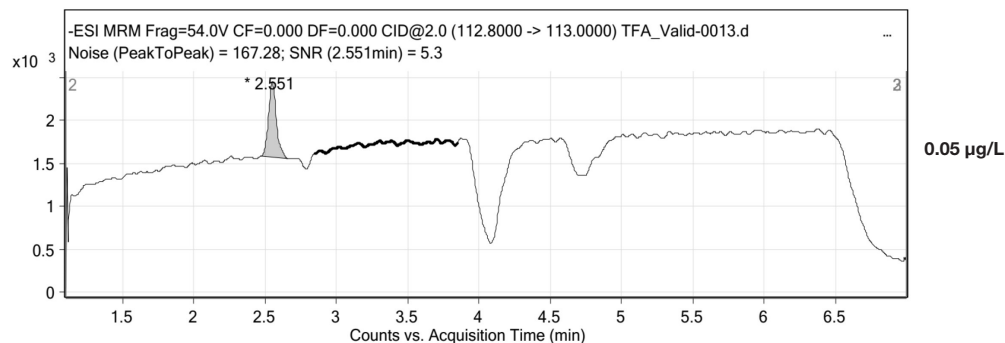
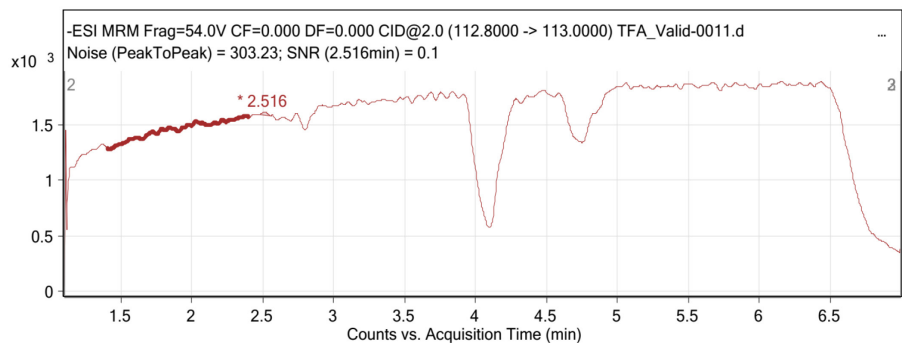
Compound Name	Q1	Q3	Dwell	Frag	CE
TFA- ¹³ C ₂ (ISTD)	115.1	70	40	54	12
TFA	112.8	113	40	54	2
TFA	112.8	69	40	54	11

Table 2.
MS Source Parameters

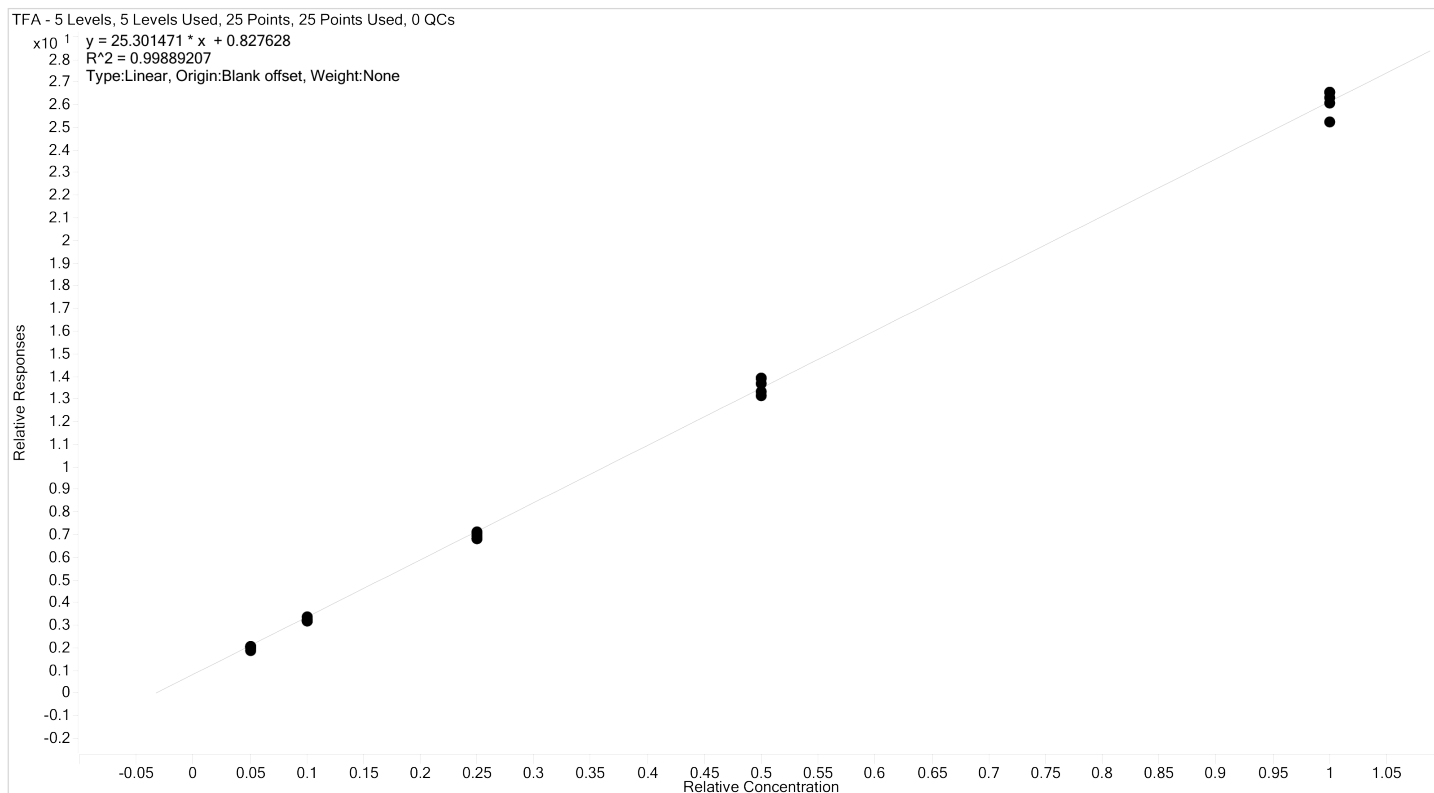
Source Parameter	Setting	
	Value (+)	Value (-)
Gas Temp [°C]	300	300
Gas Flow [l/min]	9	9
Nebulizer [psi]	45	45
Sheath Gas Heater [°C]	350	350
Sheath Gas Flow [l/min]	11	11
Capillary [V]	3,500	3,500
V Charging	0	300

Analyte and Retention Time

Analyte	RT
TFA	2.55 min



The linearity range of the method was determined by using standard injections with concentrations from 0.00 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

Special thanks to Peer Ziese and to Umwelt Control Labor GmbH for contributing this method.



bioZen[®] Products - Powered by BioTi[™] 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	/3pk	ea
				AJO-9800	AJO-9000

Australia

t: +61 (0)2-9428-6444
auinfo@phenomenex.com

Austria

t: +43 (0)1-319-1301
anfrage@phenomenex.com

Belgium

t: +32 (0)2 503 4015 (French)
t: +32 (0)2 511 8666 (Dutch)
beinfo@phenomenex.com

Canada

t: +1 (800) 543-3681
info@phenomenex.com

China

t: +86 400-606-8099
cninfo@phenomenex.com

Denmark

t: +45 4824 8048
nordicinfo@phenomenex.com

Finland

t: +358 (0)9 4789 0063
nordicinfo@phenomenex.com

France

t: +33 (0)1 30 09 21 10
franceinfo@phenomenex.com

Germany

t: +49 (0)6021-58830-0
anfrage@phenomenex.com

Ireland

t: +91 (0)40-3012 2400
indiainfo@phenomenex.com

Italy

t: +39 051 6327511
italiainfo@phenomenex.com

Luxembourg

t: +31 (0)30-2418700
nlinfo@phenomenex.com

Mexico

t: 01-800-844-5226
tecnicomx@phenomenex.com

The Netherlands

t: +31 (0)30-2418700
nlinfo@phenomenex.com

New Zealand

t: +64 (0)9-4780951
nzinfo@phenomenex.com

Norway

t: +47 810 02 005
nordicinfo@phenomenex.com

Poland

t: +48(12) 881 0121
pl-info@phenomenex.com

Portugal

t: +351 221 450 488
ptinfo@phenomenex.com

Singapore

t: +65 800-852-3944
sginfo@phenomenex.com

Spain

t: +34 91-413-8613
espinfo@phenomenex.com

Sweden

t: +46 (0)8 611 6950
nordicinfo@phenomenex.com

Switzerland

t: +41 (0)61 692 20 20
swissinfo@phenomenex.com

Taiwan

t: +886 (0) 0801-49-1246
twinfo@phenomenex.com

United Kingdom

t: +44 (0)1625-501367
ukinfo@phenomenex.com

USA

t: +1 (310) 212-0555
info@phenomenex.com

All other countries/regions

Corporate Office USA
t: +1 (310) 212-0555
info@phenomenex.com

BE-HAPPY[™]
guarantee

Your happiness is our mission. Take 45 days to try our products. If you are not happy, we'll make it right.

www.phenomenex.com/behappy

Terms and Conditions

Subject to Phenomenex Standard Terms and Conditions which may be viewed at www.phenomenex.com/TermsAndConditions.

Trademarks

Phenomenex bioZen is a registered trademark and SecurityGuard, BioTi, and BE-HAPPY are trademarks of Phenomenex. Agilent is a registered trademark of Agilent Technologies, Inc.

Disclaimer

Phenomenex is no way affiliated with Agilent Technologies, Inc.

FOR RESEARCH USE ONLY. Not for use in clinical diagnostic procedures.

© 2020 Phenomenex, Inc. All rights reserved.

www.phenomenex.com

Phenomenex products are available worldwide. For the distributor in your country/region, contact Phenomenex USA, International Department at international@phenomenex.com