



Analysis of Difluoroacetic Acid and Trifluoroacetic Acid in Drinking Water Sources Using a Luna™ Omega 3 µm PS C18 HPLC Column

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Overview

Trifluoroacetic Acid (TFA) and Difluoroacetic Acid (DFA) are ultra-short-chain Polyfluoroalkyl Substances (PFAS) that have been found to be breakdown products of many pesticides. Pesticides, and therefore TFA, have the potential to contaminate drinking water supplies as they are applied to farmlands, gardens, and lawns making their way into groundwater and surface water systems.

The German Federal Environment Agency (UBA) issued a guidance value for TFA in drinking water of 60 µg/L and a target value of 10 µg/L.¹ In this application note we show a robust and reliable method for the determination of TFA from drinking water and mineral water well sources, using a Luna Omega 3 µm PS C18 column, by LC-MS/MS. Interestingly, by changing the conditions of the mobile phase from 5 % B to 10 % B, sharper peaks are attained without affecting the retention times (Figures 1 and 2). TFA was detected as low as 0.55 µg/L in drinking water (Figure 3) and 0.005 µg/L in mineral water (Figure 4), both well below the target value set forth by the UBA.

LC Conditions

Column: Luna Omega 3 µm PS C18

Dimension: 150 x 2.1 mm

Part No.: [00F-4758-AN](#)

Mobile Phase: A: 10 mM Ammonium Acetate with 0.1 % Acetic Acid in Water
B: Acetonitrile

Gradient:	Figures 1, 3, 4		Figure 2	
	Time (min)	%B	Time (min)	%B
	0	5	0	10
	5	95	5	95
	7	95	7	95
	8	5	8	10
	12	5	12	10

Flow Rate: 0.4 mL/min

Injection Volume: 20 µL – Figures 1, 3, 4
40 µL – Figure 2

Temperature: 30 °C

Instrument: Shimadzu® Nexera®

Detection: MS/MS

Detector: Shimadzu LCMS-8050

MS/MS Conditions

ESI Voltage: -1 V

Nebulizing Gas Flow: 3 L/min

Drying Gas Flow: 5 L/min

Heating Gas Flow: 15 L/min

Heat Block Temperature: 300 °C

Interface Temperature: 150 °C

Desolvation Line Temperature: 150 °C

CID: 270 kPa

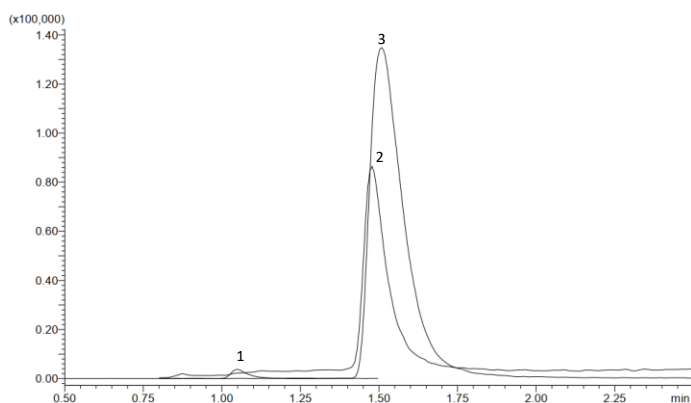
Dwell Time: 20 ms

Table 1. MRM Transitions

Analyte	Precursor (m/z)	Product (m/z)
Difluoroacetic Acid	95.2	51.1
Trifluoroacetic Acid	113.1	69, 94.95, 77
C ¹³ -Trifluoroacetic Acid	115.3	70

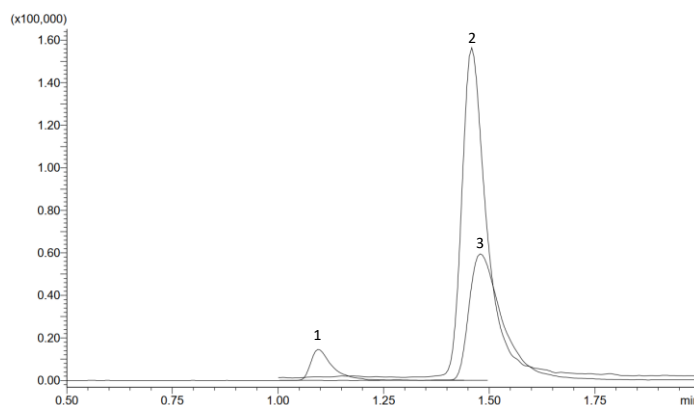


Figure 1. 0.5 µg/L Trifluoroacetic Acid and 0.5 µg/L Difluoroacetic Acid Standards with 1.0 µg/L C¹³-Trifluoroacetic Acid Internal Standard.



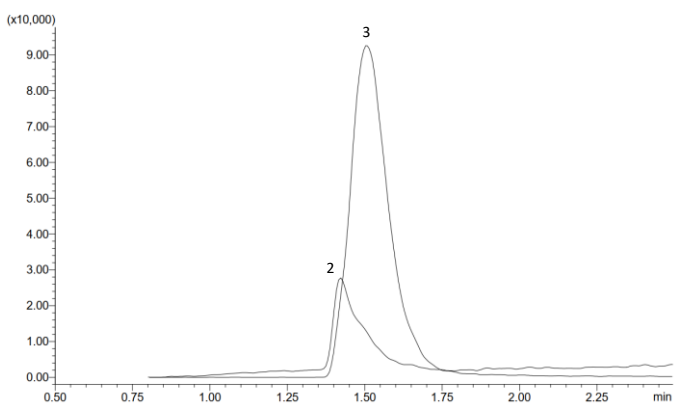
Peak No.	Analyte	Retention Time (min)	Area	Concentration (µg/L)
1	Difluoroacetic Acid	1.048	14644	0.535
2	Trifluoroacetic Acid	1.477	440612	0.586
3	C ¹³ -Trifluoroacetic Acid	1.508	962918	1.00

Figure 2. 1.0 µg/L Trifluoroacetic Acid and 1.0 µg/L Difluoroacetic Acid Standards with 1.0 µg/L C¹³-Trifluoroacetic Acid Internal Standard.



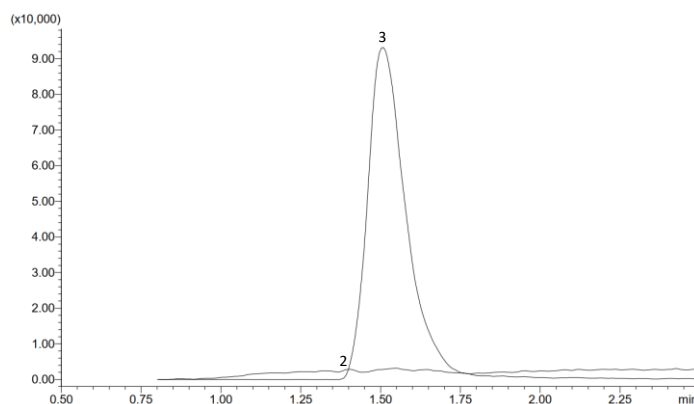
Peak No.	Analyte	Retention Time (min)	Area	Concentration (µg/L)
1	Difluoroacetic Acid	1.096	53185	2.91
2	Trifluoroacetic Acid	1.458	588005	1.17
3	C ¹³ -Trifluoroacetic Acid	1.479	321098	1.00

Figure 3. Difluoroacetic Acid and Trifluoroacetic Acid in Drinking Water with 1.0 µg/L C¹³-Trifluoroacetic Acid Internal Standard.



Peak No.	Analyte	Retention Time (min)	Area	Concentration (µg/L)
1	Difluoroacetic Acid	-	-	N.D. Peak
2	Trifluoroacetic Acid	1.422	168710	0.548
3	C ¹³ -Trifluoroacetic Acid	1.505	789084	1.00

Figure 4. Difluoroacetic Acid and Trifluoroacetic Acid in Mineral Water with 1.0 µg/L C¹³-Trifluoroacetic Acid Internal Standard.



Peak No.	Analyte	Retention Time (min)	Area	Concentration (µg/L)
1	Difluoroacetic Acid	-	-	N.D. Peak
2	Trifluoroacetic Acid	1.402	1350	0.005
3	C ¹³ -Trifluoroacetic Acid	1.507	759723	1.00

References

1. Umweltbundesamt (UBA) (2021, November). *Reducing the Input of Chemicals into Waters: Trifluoroacetate (TFA) as a Persistent and Mobile Substance with Many Sources.* (EPA 821-D-22-002). German Federal Environment Agency.



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