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Improved Determination of Fluorotelomer Alcohol Compounds Based on EN 17681-1:2025

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Introduction

To align with the latest EU PFAS regulations , the EN 17681-1:2025 was officially implemented in 2025. Within this standard the use of alkaline extraction significantly enhances the extraction efficiency of fluorotelomer alcohol compounds (hereinafter referred to as FTOHs, see Figure 1). However, this approach also leads to increased matrix complexity of the samples.

In addition, The standard provides only one product ion for FTOHs, compared with the other compounds in the standard that have two or more product ions available (e.g., PFOS & PFHxS), therefore the qualitative confirmation reliability of FTOHs is lower. These adverse factors render the testing and confirmation of FTOHs more challenging and cumbersome.

Therefore, we developed a method, using $[M-H]^-$ as the precursor ion and incorporating four product ions for FTOHs. **The method more effectively handles complex matrix interferences and enables confirmation of positive results**

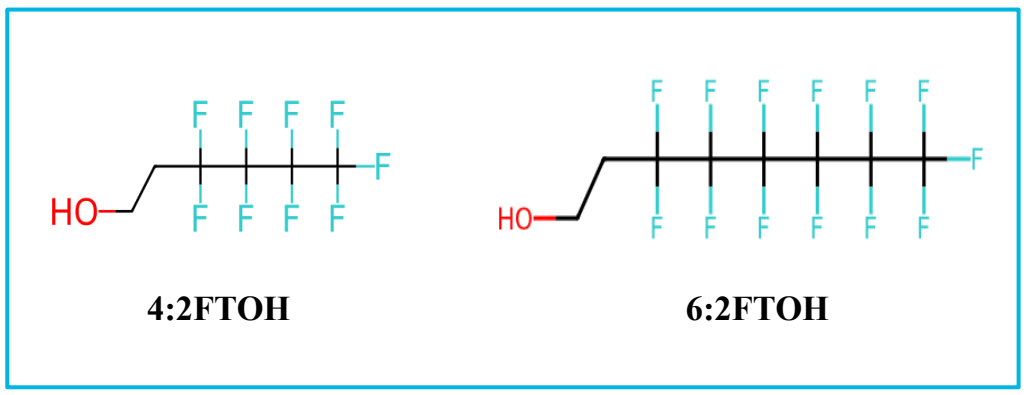

Figure 1. Structure of 4:2FTOH and 6:2FTOH

Figure 2. Agilent 6495 LC/TQ

Experimental

Standard and sample preparation

In the study, the standard and sample preparation is strictly in accordance with the requirements of the alkaline extraction method specified in EN 17681-1:2025.

Instrument Conditions

MRM conditions

Compound Name	Prec.Ion [m/z]	Prod. Ion [m/z]	Frag. (V)	CE (V)	Polarity
4:2FTOH	203*	155**	166	12	-
	223*	155	166	16	-
	263	203	166	6	-
	263	223	166	2	-
5:1FTOH	299	119.1**	166	20	-
	299	193	166	21	-
	299	258.9	166	13	-
	299	279	166	13	-
6:2FTOH	363	255	166	23	-
	363	283	166	13	-
	363	302.9**	166	4	-
	363	323	166	1	-
8:2FTOH	463	317	166	28	-
	463	355	166	21	-
	463	403**	166	6	-
	463	423	166	1	-
10:2FTOH	563	454.9	166	24	-
	563	482.9	166	21	-
	563	503**	166	8	-
	563	523	166	4	-
12:2FTOH	663	554.9	166	24	-
	663	583.1	166	24	-
	663	603**	166	10	-
	663	623	166	4	-

* The precursor ion generated via in-source fragmentation
** Quantifier ion.

Experimental

LC conditions

HPLC system	Agilent 1290 Infinity III Binary Pump UHPLC
Analytical column	Agilent Poroshell120 EC-C18 (3.0 x100mm 2.7μm)
Delay column	Agilent PFC Delay Column (4.6 x 30mm)
Mobile phase	Phase A: H2O Phase B: Methanol
Gradient program	0min, 40%B; 1min, 85%B; 4min, 95%B; 5.5min, 95%B; 5.51min,40%B; 7min,40%
Injection volumn	2μL
Flow rate	0.4mL/min
Stoptime	7min
Posttime	Off

MS conditions

Mass System	Agilent 6495 LC/TQ
Ion Source & Polarity	AJS ESI, Negative
Gas Temp.	100℃
Gas Flow	16L/min
Nebulizer	60psi
Sheath Gas Temp.	250℃
Sheath Gas Flow	12L/min
Capillary Voltage	2500V
Nozzle Voltage	2000V

Results and Discussion

Mobile phase & in-source fragmentation

In this study, systematic investigation was carried out on the mobile phase. The main findings are as follows:

- When trace ammonium acetate, e.g., 5 mmol/L, was added into any mobile phase channel, FTOHs analyzed by LC/TQ yielded only one MRM transition $[M+59]^-$ > 59, m/z59 refers to the acetate ion.
- With water and methanol as the mobile phase, 4:2 FTOH yields the $[M-H]^-$ precursor ion of m/z263, accompanied by in-source fragmentation, forming ions at m/z 203 and m/z 223 in Scan mode(Figure 3) .
- With water and methanol as the mobile phase, FTOHs analyzed by LC/TQ formed the $[M-H]^-$ precursor ion, which can be fragmented into multiple product ions (Figure 4) .
- When the mobile phase methanol was replaced with acetonitrile, the $[M-H]^-$ ion response of FTOHs decreased significantly:4:2 FTOH and 6:2 FTOH decreased by about 90-fold and 50-fold, respectively (Figure 5) .

Results and Discussion

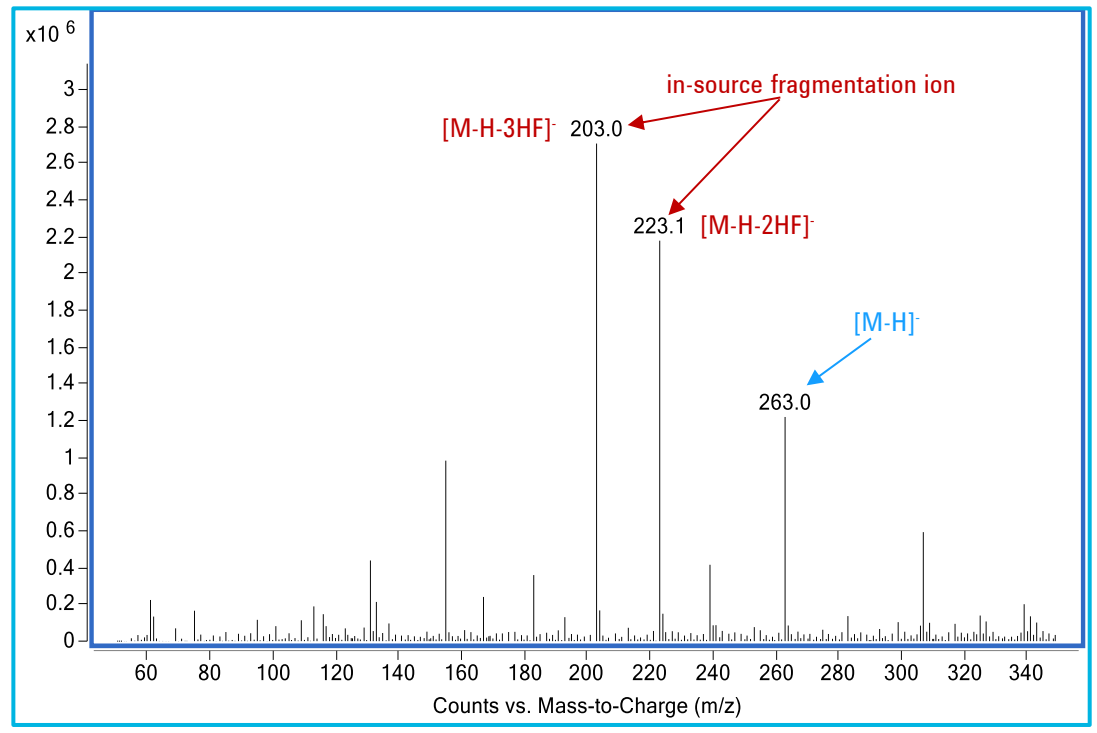

Figure 3. Scan mass spectrum of 4:2 FTOH with water and methanol as mobile phase

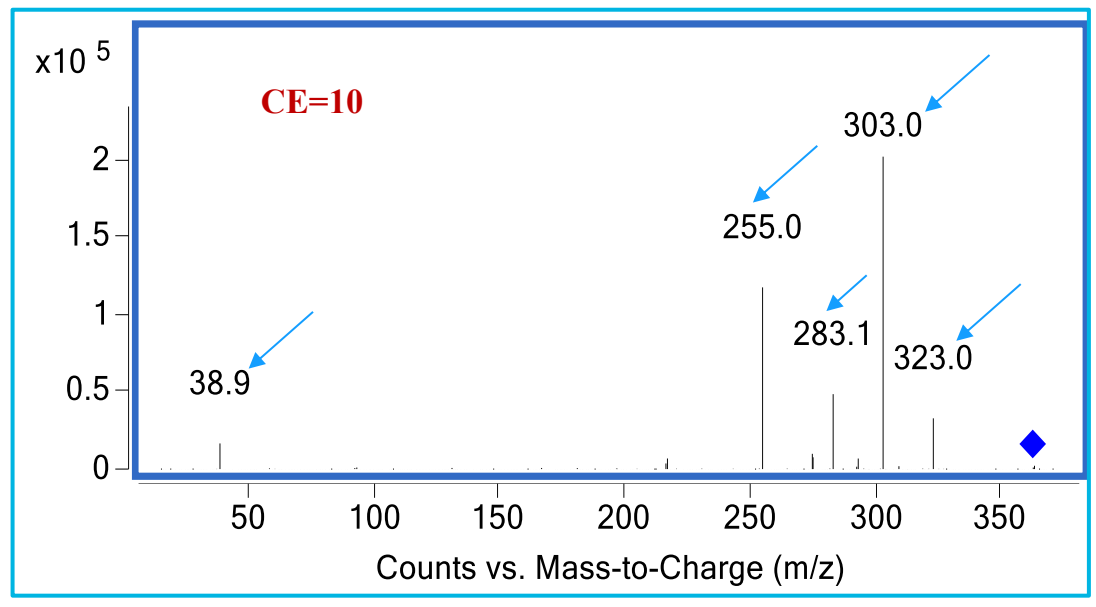

Figure 4. Product ion scan mass spectrum of m/z363 for 6:2 FTOH with water and methanol as mobile phase :

Multiple product ions were yielded

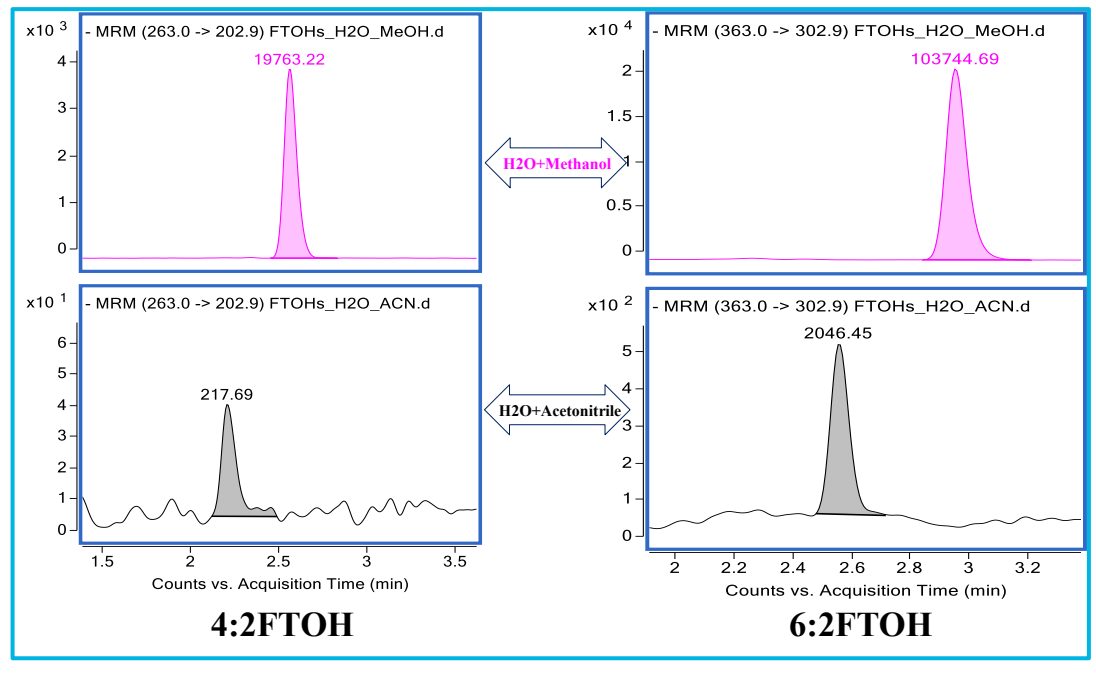

Figure 5. Replacing methanol with acetonitrile in the mobile phase resulted in a significant reduction for the $[M-H]^-$ ion response of FTOHs

Results and Discussion

Method sensitivity, precision and linearity

The sensitivity, precision and linearity of 6495 LC/TQ were assessed by analyzing mixed standard solution of six FTOHs.

- Figure 6 showed that six analytes exhibited excellent sensitivity: the signal-to-noise ratio (S/N) of the quantifier ion at the limit of quantification (LOQ) of 1 ng/mL was 31~234.
- Figure 7 showed that six analytes had good precision: ten consecutive injections at 10 ng/mL, the RSD% of peak area all less than 3.5%.
- The analytes showed good linearity with $1/x^2$ weighting, and the R^2 values of six calibration curves are 0.994 ~ 0.998 with 80%~120% accuracy of curve readback for each level. Calibration levels ranged from 1 ng/mL to 100 ng/mL for all analytes. Figure 8 showed the good results of calibration curves.

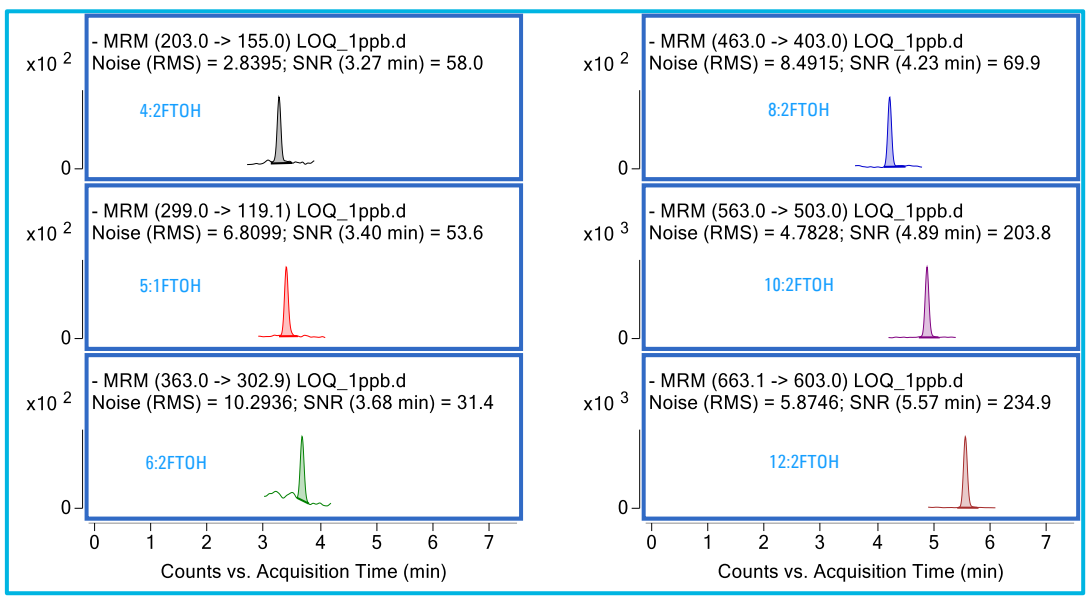

Figure 6. S/N ratio results of quantifier ion for six FTOHs at 1ng/mL (LOQ)

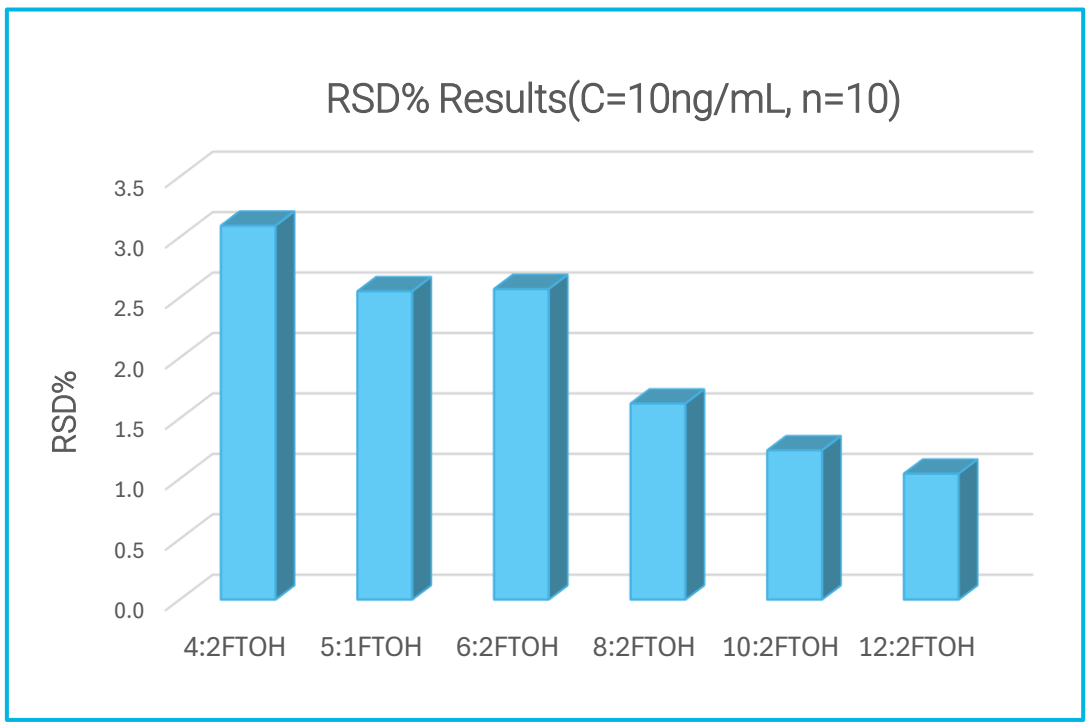

Figure 7. The results of RSD% of quantifier peak for 10 replicate injections of six FTOHs at 10ng/mL

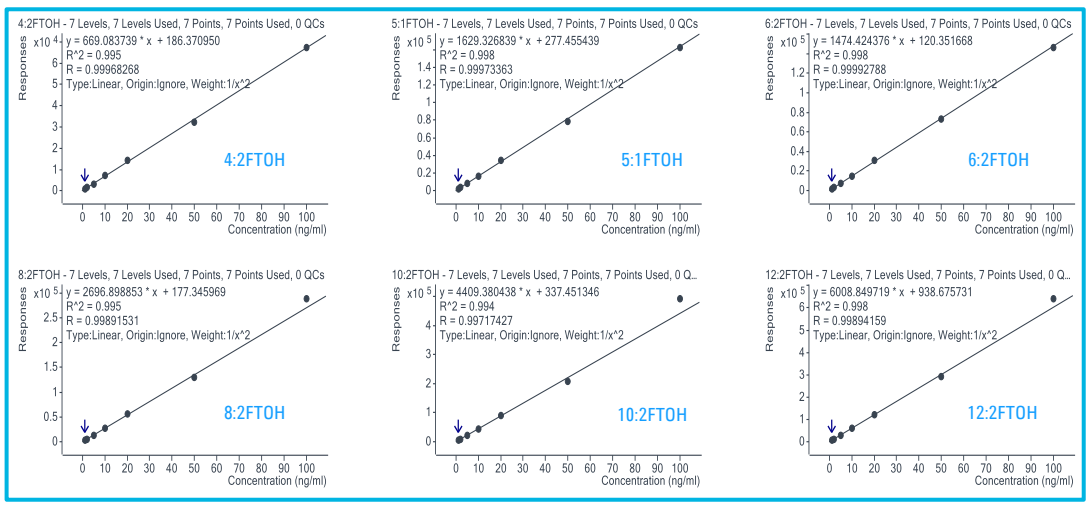

Figure 8. Calibration curves from 1 ng/mL to 100 ng/mL for six FTOHs

Authentic Sample Test

To evaluate the practicality of the developed method, a 5:1FTOH suspected sample previously analyzed in accordance with EN 17681-1:2025 was subjected to confirmatory testing in this study. The test result confirmed that the sample was negative, which further demonstrates that the method possesses very important practical value (Figure 9) .

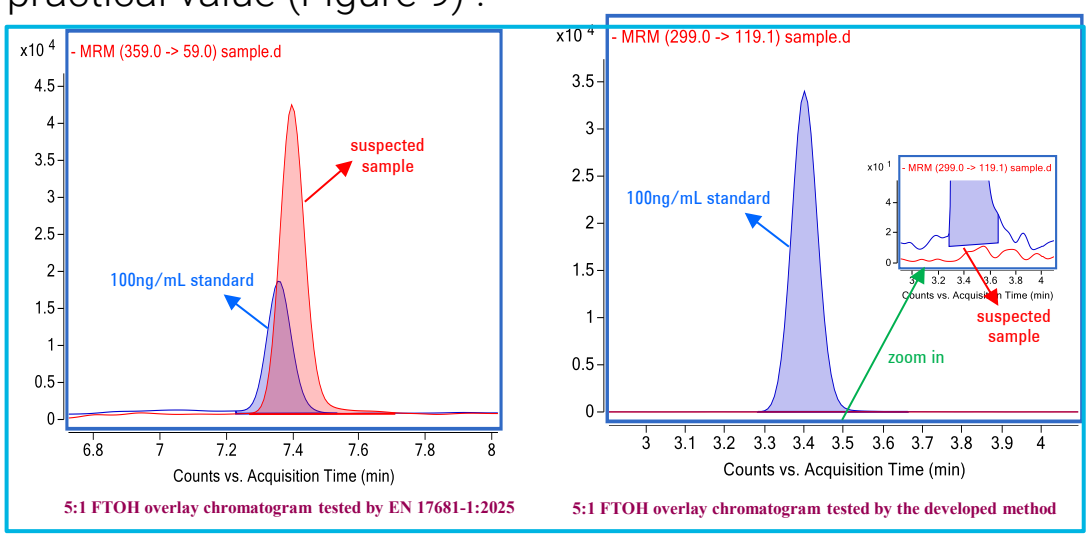

Figure 9. Confirmatory testing for 5:1 FTOH suspected sample by the developed method

Conclusions

We have demonstrated a rapid, highly sensitive and accurate LC/TQ method for quantitative, qualitative and confirmatory analysis of six FTOHs using the Agilent 6495 LC/TQ.

- In contrast to EN 17681-1:2025, which provides only one MRM transition for each FTOH, the developed method adopts $[M-H]^-$ as the precursor ion and offers four product ion fragments for each FTOH, thereby improving the quantitative and qualitative reliability.
- The results of methodological validation are as follows.
  - Sensitivity: LOQ=1ng/mL
  - Precision: RSD < 3.5% (C=10ng/mL, n=10)
  - Linearity: R^2=0.994 ~ 0.998 (from 1 to 100 ng/mL)

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