

CLEARLY
BETTER



Agilent 6460

Table 1 HPLC and MS analytical conditions for UK-C18

HPLC				MS			
Instrument	:	Agilent1200 series Binary Pump (G1312B) MicroDegasser (G1379B) High Performance Autosampler (G1367E) Column Compartment (G1316C)		Instrument	:	Agilent 6460	
Column	:	Unison UK-C18 (4.6x 150mm, 3 μ m)		Mass range	:	30 ~500 (m/z)	
Mobile phase	:	A:0.2% HCOOH aq. B: CH ₃ OH		Polarity	:	Negative	
Flow	:	0.2 ml/min		Ionization	:	ESI(Jet Stream)	
Gradient	:	min	B%	ml/min	Nebulizer	:	N ₂ (50 psi)
		0.00	5.0	0.200	Drying gas	:	N ₂ (10L/min)
		20.00	65.0	0.200	Drygas temp.	:	250 °C
		23.00	98.0	0.200	Sheath temp.	:	275 °C
		28.00	98.0	0.200	Sheath flow	:	N ₂ (6L/min)
		28.10	98.0	1.500	Fragmentor	:	50V
		31.00	98.0	1.500	MRM	:	MCAA
		32.00	5.0	1.500			Precursor m/z 93
		42.00	5.0	1.500			Product m/z 35
		42.10	5.0	0.200			Collision 4eV
	Stop time 43min					DCAA	
						Precursor m/z 127	
						Product m/z 83	
						Collision 4eV	
						TCAA	
						Precursor m/z 161	
						Product m/z 117	
						Collision 4eV	
Oven temp.	:	40°C		試薬: ギ酸(関東化学 HPLC用 1ml x5 ,16233-96)			
Injection vol.	:	50, 75, 100 μ l		メタノール(関東化学 LCMS用 1L, 25185-79)			
				水(MilliQ 超純水)			
Sample	:	STD: 2, 4, 10, 20, 40, 100, 200 ng/ml Sample: Tap Water+2ppb spiked		ハロ酢酸(関東化学 ハロ酢酸混合標準原液4種 水質試験用 2mlx5, 18150-96, 1mg/ml)			
				標準液の調整:ハロ酢酸混合標準原液(10mg/Lメタノール溶液)を超純水で希釈して 検量線用標準品を調整			

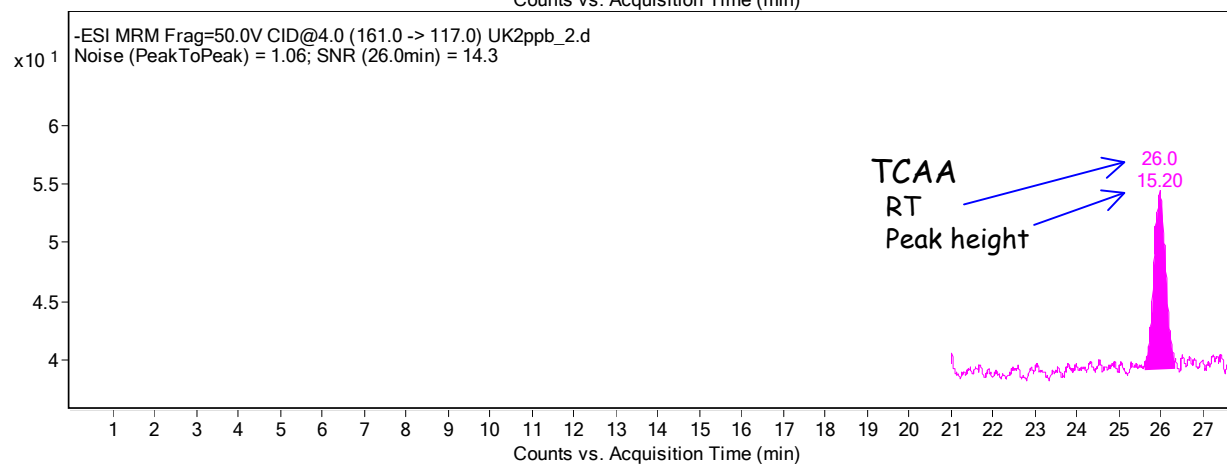
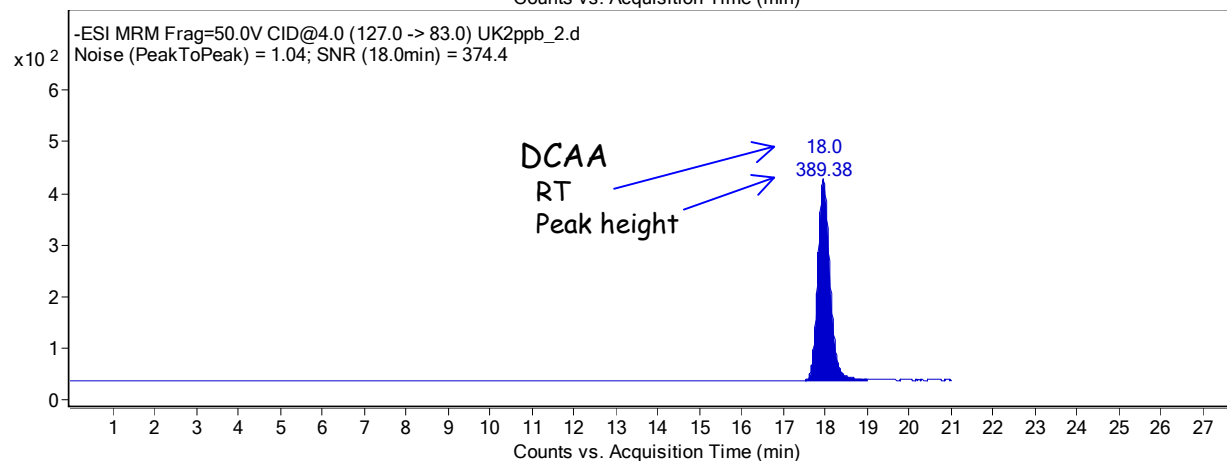
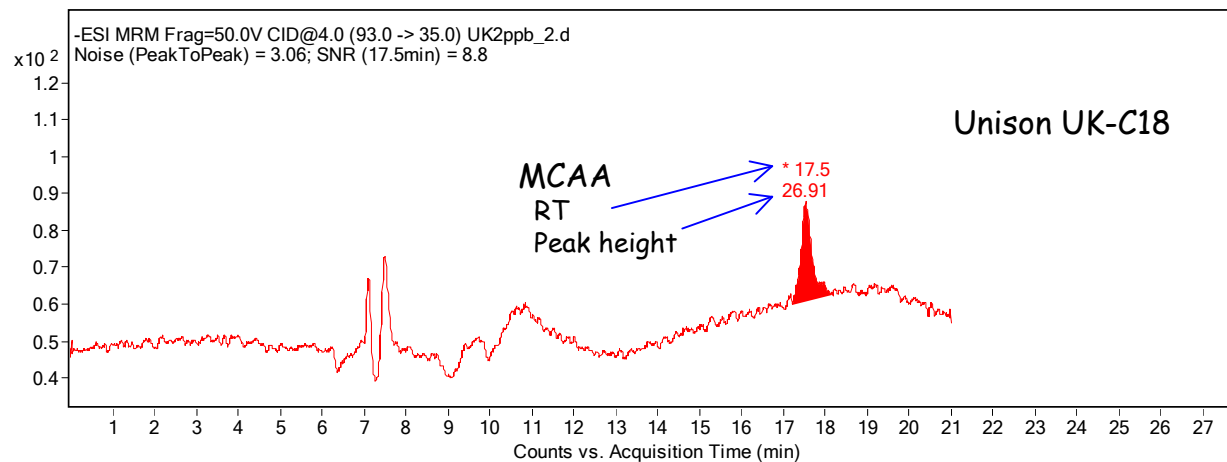


Fig.1 MRM chromatograms of halogenated acetic acids (Unison UK-C18 50 μ L each 2ppb)

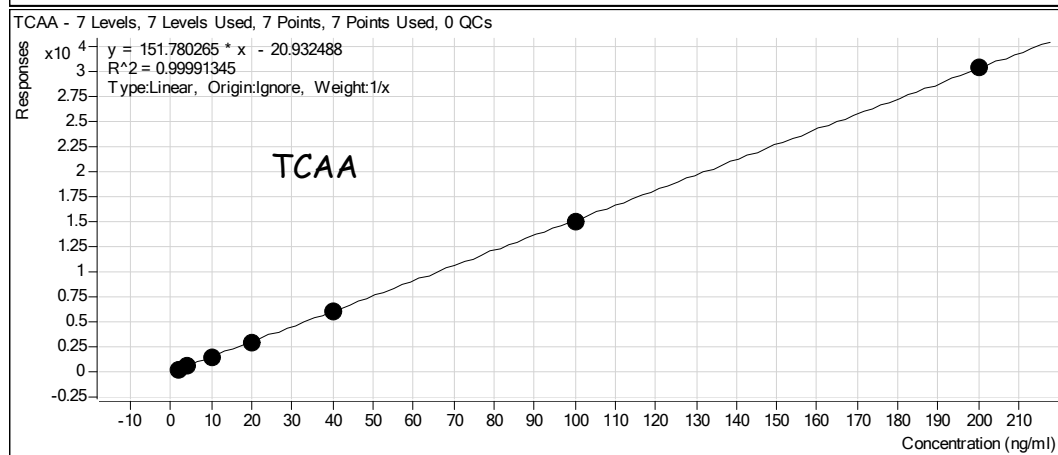
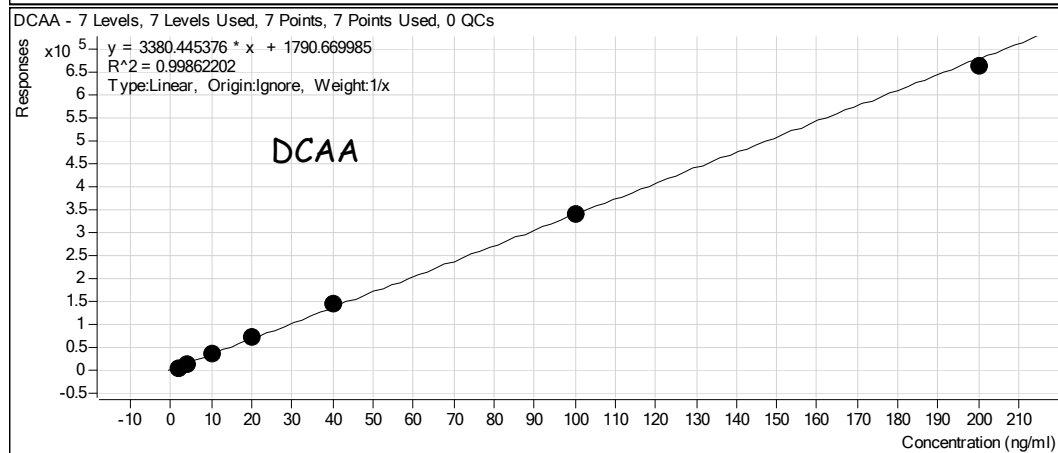
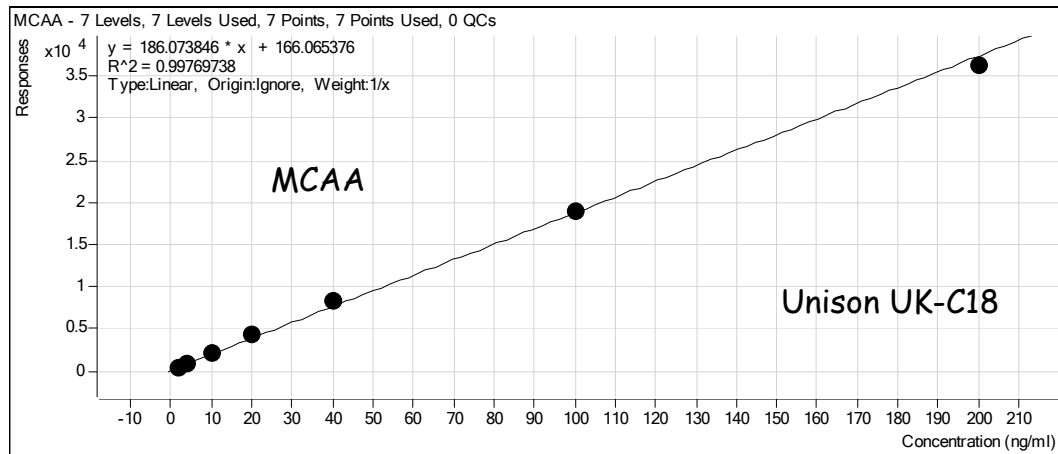


Fig.2 Calibration curves of halogenated acetic acids (Unison UK-C18 50 μ L 2-200ppb)

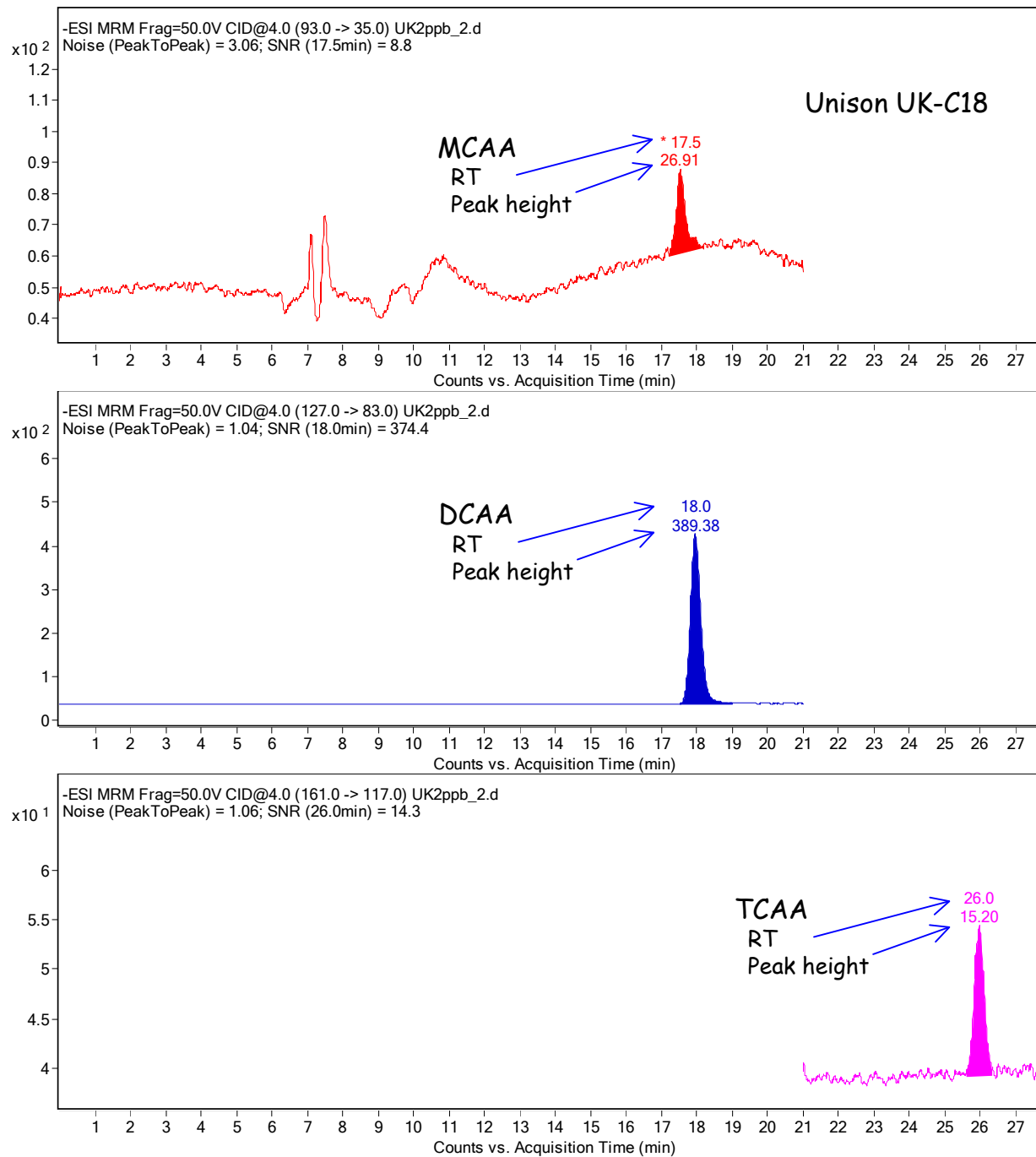


Fig.3 MRM chromatograms of halogenated acetic acids in 2ppb spiked tap water (Unison UK-C18 50 μ L each 2ppb)

Table 2 Quantitative results of Halogenated acetic acid with Unison UK-C18 (50 μ L)

Sample	MCAA Results				DCAA Results				TCAA Results			
Name	RT	Final Conc.	Area	Accuracy	RT	Final Conc.	Area	Accuracy	RT	Final Conc.	Area	Accuracy
2ppb	17.536	1.66349597	475.6	83.1748	17.957	1.7400545	7672.83	87.00272	25.988	2.03232379	287.53	101.6162
4ppb	17.546	3.87502037	887.11	96.87551	17.967	3.91641958	15029.9	97.91049	26.008	4.0653501	596.11	101.6338
10ppb	17.526	10.443053	2109.2	104.4305	17.967	10.3272135	36701.3	103.2721	25.988	9.82760735	1470.7	98.27607
20ppb	17.526	21.7947079	4221.5	108.9735	17.977	21.308574	73823.1	106.5429	26.008	19.4464524	2930.7	97.23226
40ppb	17.536	43.4574243	8252.4	108.6436	17.987	42.7497258	146304	106.8743	26.028	40.5259986	6130.1	101.315
100ppb	17.526	101.037825	18967	101.0378	17.987	100.83692	342664	100.8369	26.038	99.7511849	15119	99.75118
200ppb	17.526	193.728473	36214	96.86424	17.997	195.121093	661387	97.56055	26.048	200.351083	30388	100.1755
TW+2ppb	17.455	1.42066838	430.41		17.865	2.88871602	11555.8		25.877	6.23555008	925.5	

MCAA

DCAA

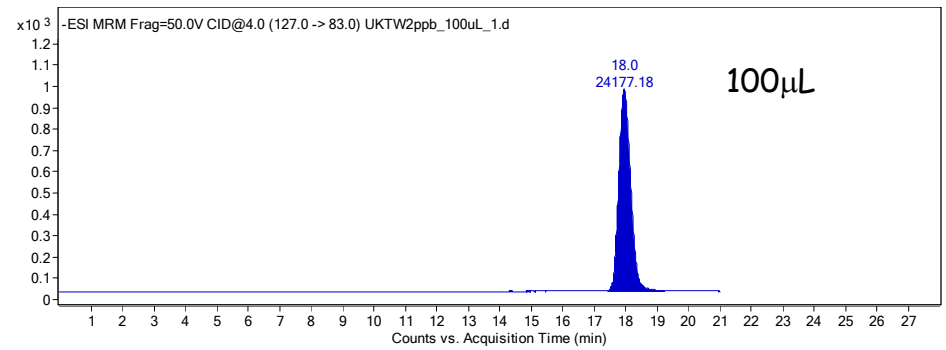
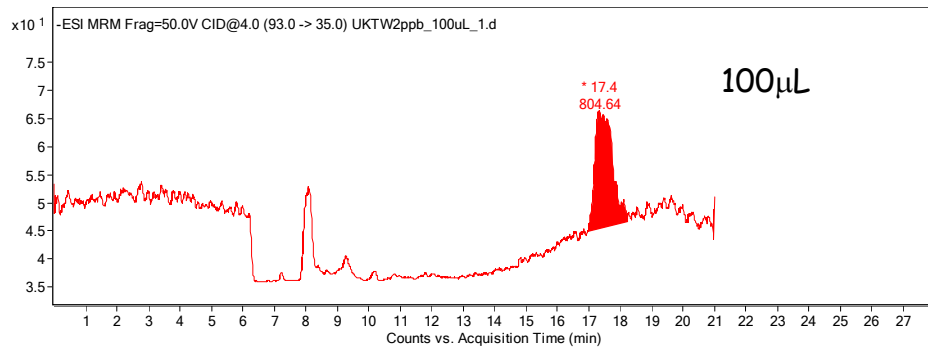
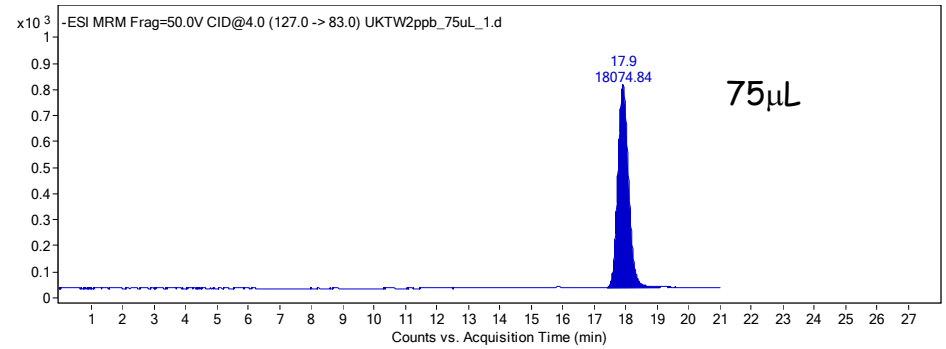
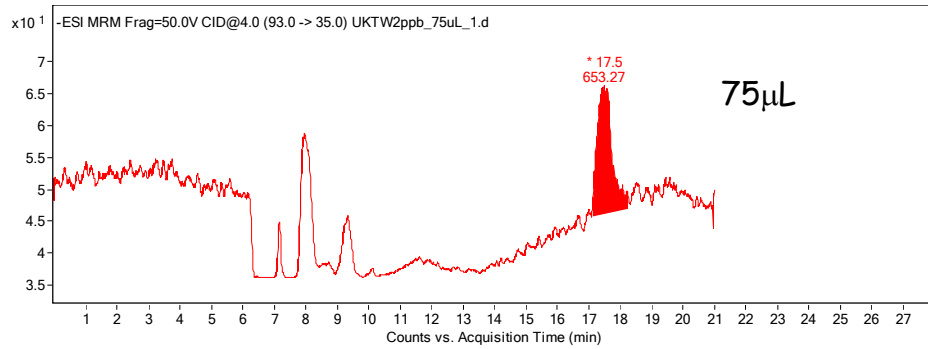
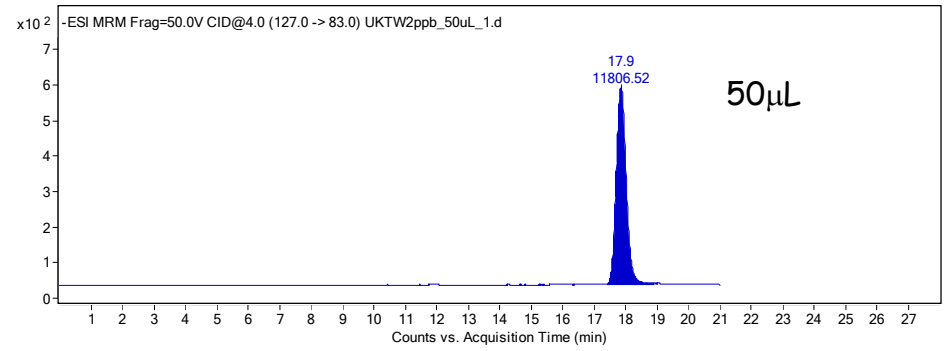
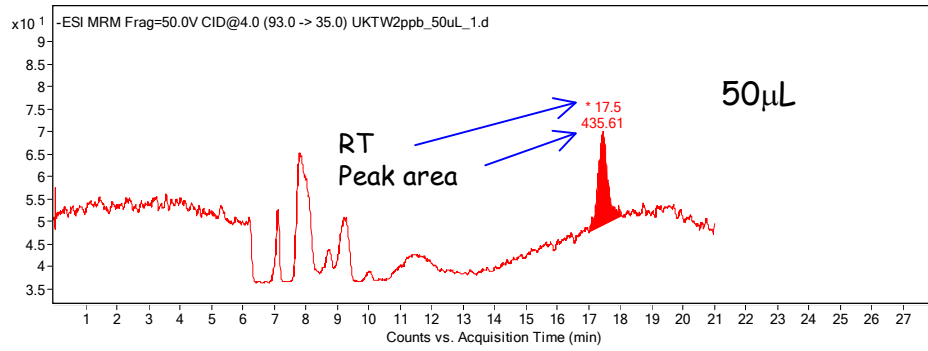


Fig.4 MRM chromatograms of 2ppb spiked Tap Water (Unison UK- C18)

TCAA

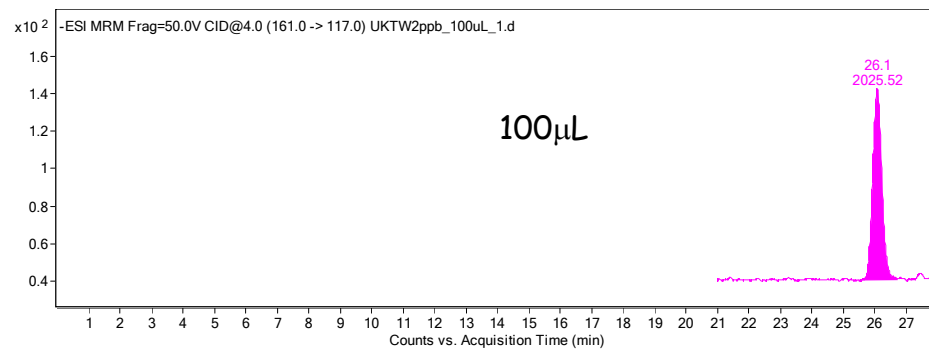
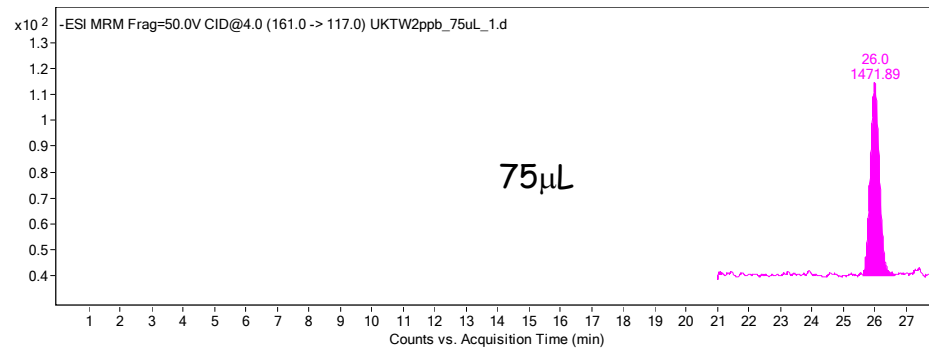
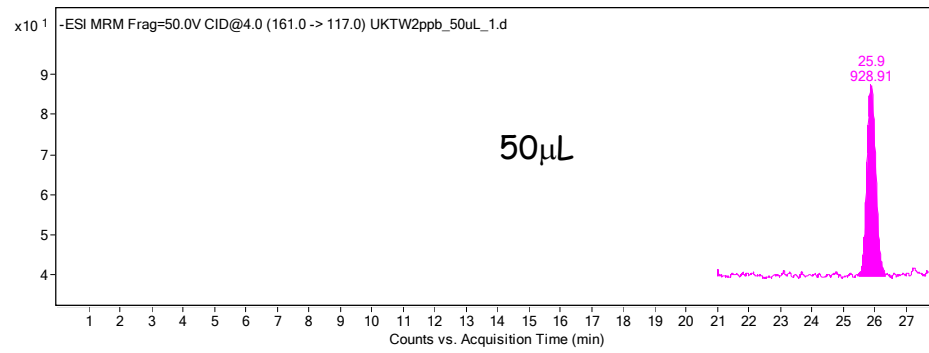


Fig. 5 MRM chromatograms of 2ppb spiked Tap Water (Unison UK- C18)