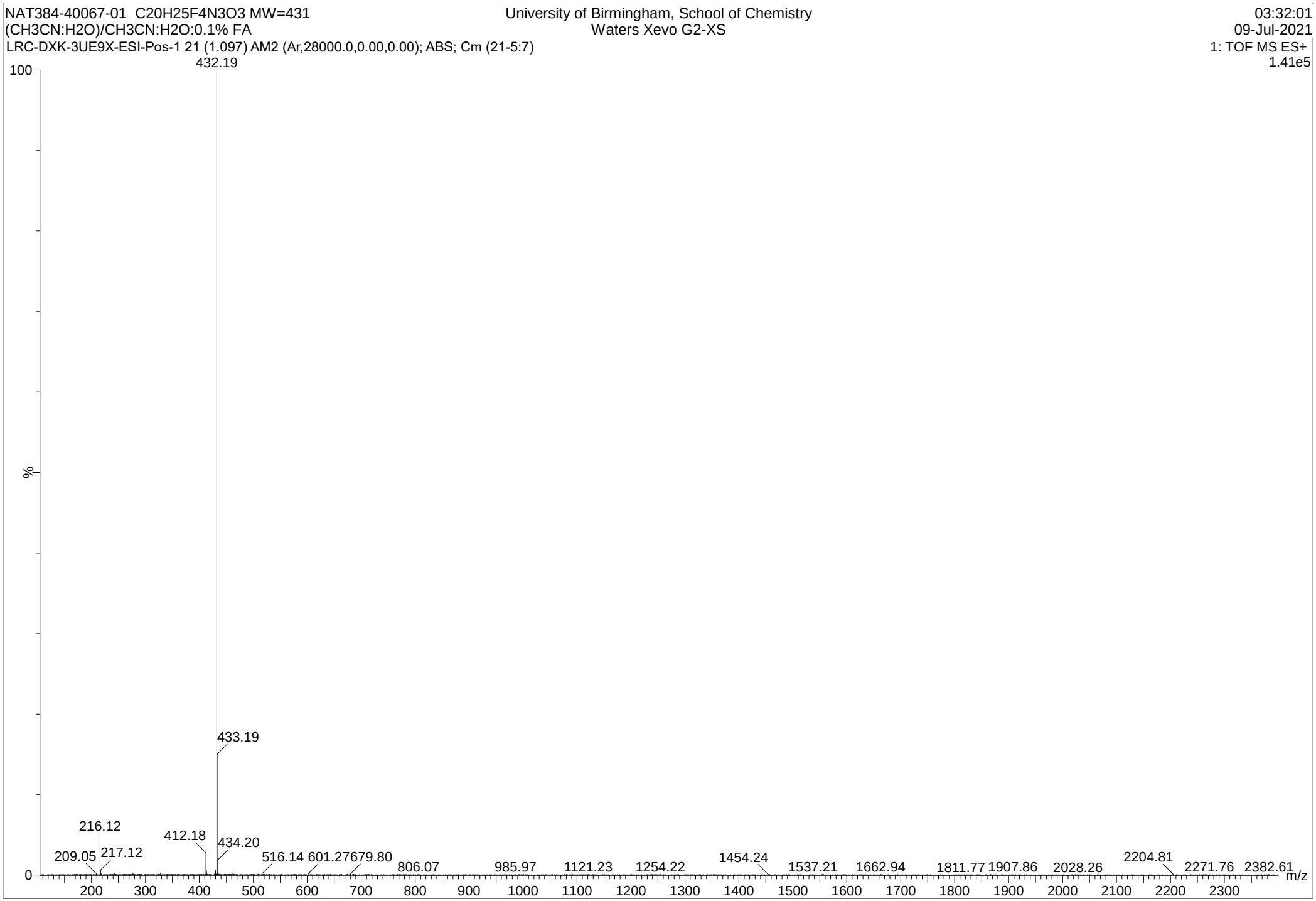
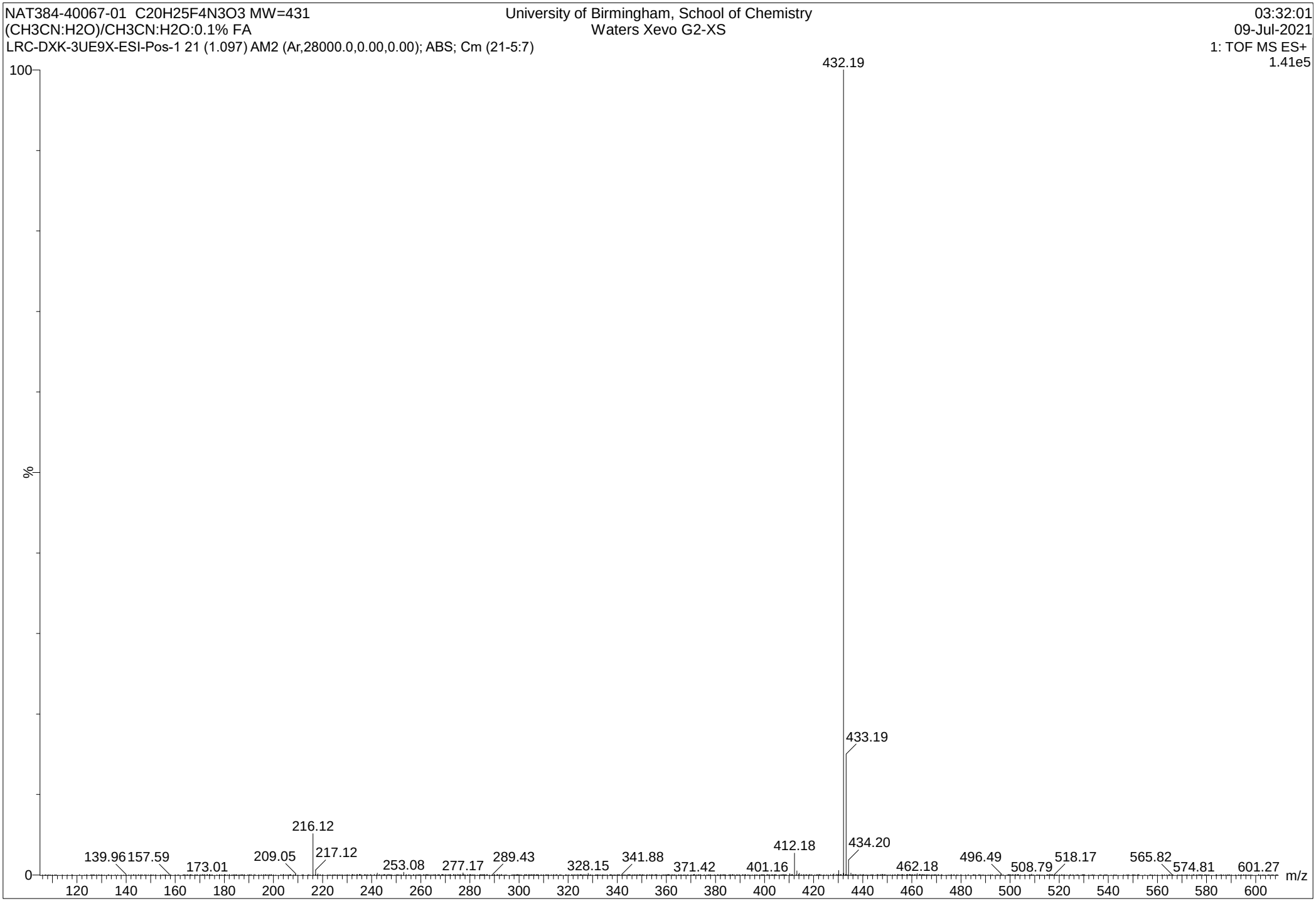
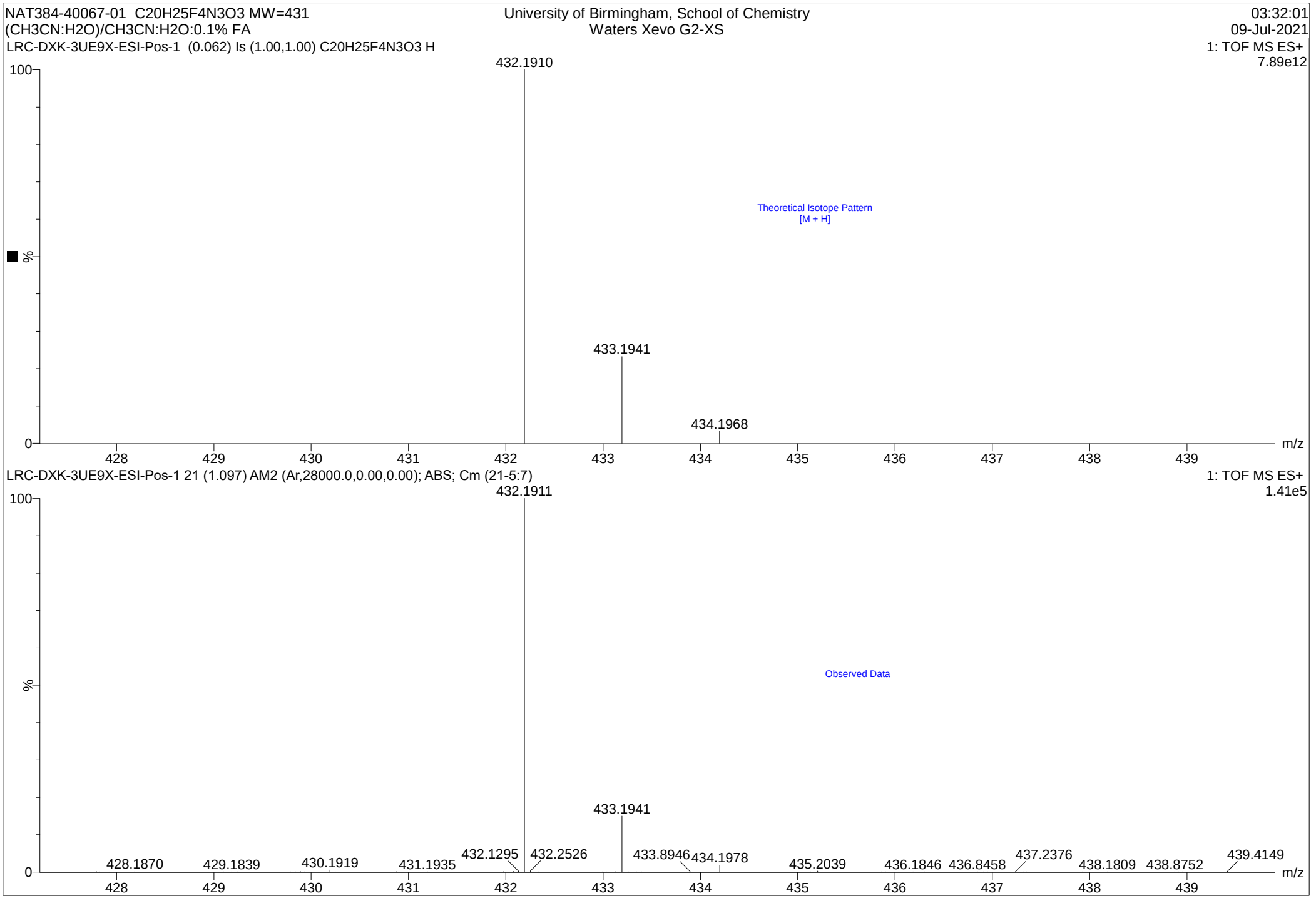

NAT384-40067-01 C20H25F4N3O3 MW=431
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UE9X-ESI-Pos-1 21 (1.097) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (21-5:7)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
03:32:01
09-Jul-2021
1: TOF MS ES+
1.41e5
100
%
0
432.19
433.19
216.12
412.18
434.20
209.05
217.12
516.14
601.27
679.80
806.07
985.97
1121.23
1254.22
1454.24
1537.21
1662.94
1811.77
1907.86
2028.26
2204.81
2271.76
2382.61
m/z
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
2000
2100
2200
2300


NAT384-40067-01 C20H25F4N3O3 MW=431
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UE9X-ESI-Pos-1 21 (1.097) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (21-5:7)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
03:32:01
09-Jul-2021
1: TOF MS ES+
1.41e5
100
%
0
432.19
433.19
434.20
216.12
217.12
412.18
139.96
157.59
173.01
209.05
253.08
277.17
289.43
328.15
341.88
371.42
401.16
462.18
496.49
508.79
518.17
565.82
574.81
601.27
m/z
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600


NAT384-40067-01 C20H25F4N3O3 MW=431
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UE9X-ESI-Pos-1 (0.062) Is (1.00,1.00) C20H25F4N3O3 H
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
03:32:01
09-Jul-2021
1: TOF MS ES+
7.89e12
100
%
0
432.1910
433.1941
434.1968
Theoretical Isotope Pattern
[M + H]
428
429
430
431
432
433
434
435
436
437
438
439
m/z
LRC-DXK-3UE9X-ESI-Pos-1 21 (1.097) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (21-5:7)
1: TOF MS ES+
1.41e5
100
%
0
432.1911
433.1941
428.1870
429.1839
430.1919
431.1935
432.1295
432.2526
433.8946
434.1978
435.2039
436.1846
436.8458
437.2376
438.1809
438.8752
439.4149
Observed Data
428
429
430
431
432
433
434
435
436
437
438
439
m/z

Single Mass Analysis

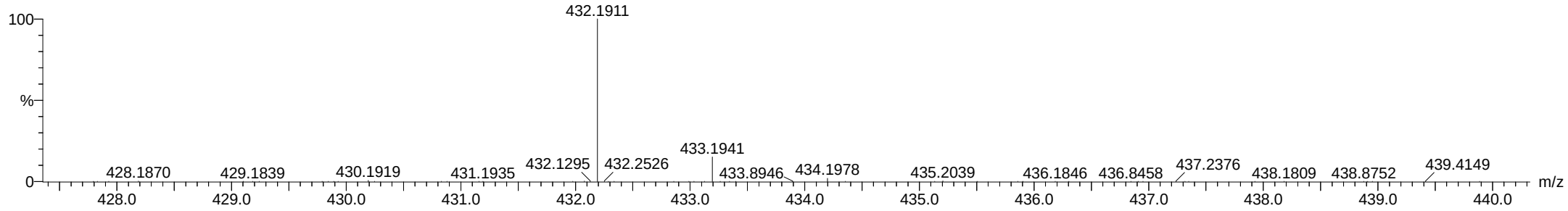
Tolerance = 3.0 PPM / DBE: min = -4.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3953 formula(e) evaluated with 9 results within limits (up to 30 closest results for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-15 O: 0-20 F: 1-4

NAT384-40067-01 C20H25F4N3O3 MW=431
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UE9X-ESI-Pos-1 21 (1.097) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (21-5:7)

University of Birmingham, School of Chemistry
Waters Xevo G2-XS

03:32:01
09-Jul-2021
1: TOF MS ES+
1.41e+005



Minimum:				-4.5				
Maximum:		5.0	3.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
432.1911	432.1910	0.1	0.2	7.5	103.4	3.798	2.24	C20 H26 N3 O3 F4
	432.1908	0.3	0.7	11.5	106.1	6.474	0.15	C18 H23 N9 O3 F
	432.1915	-0.4	-0.9	0.5	105.9	6.294	0.18	C5 H22 N15 O4 F4
	432.1906	0.5	1.2	2.5	103.8	4.182	1.53	C14 H28 N5 O8 F2
	432.1917	-0.6	-1.4	-1.5	102.2	2.534	7.94	C11 H29 N5 O9 F3
	432.1904	0.7	1.6	4.5	99.8	0.142	86.72	C8 H21 N15 O3 F3
	432.1919	-0.8	-1.9	7.5	104.2	4.534	1.07	C15 H24 N9 O4 F2
	432.1902	0.9	2.1	-4.5	107.7	8.090	0.03	C4 H26 N11 O8 F4
	432.1899	1.2	2.8	11.5	106.3	6.631	0.13	C23 H25 N3 O2 F3