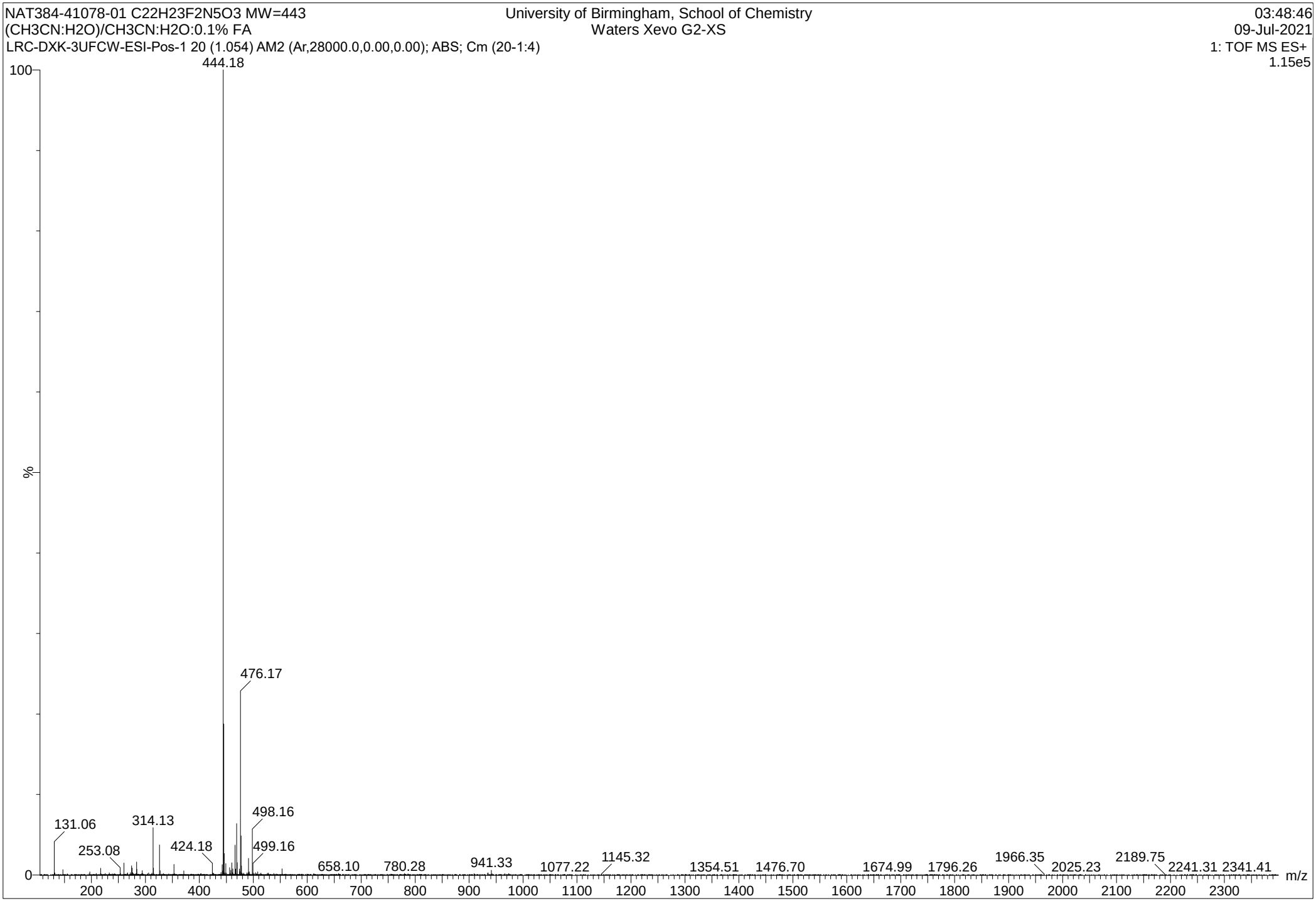
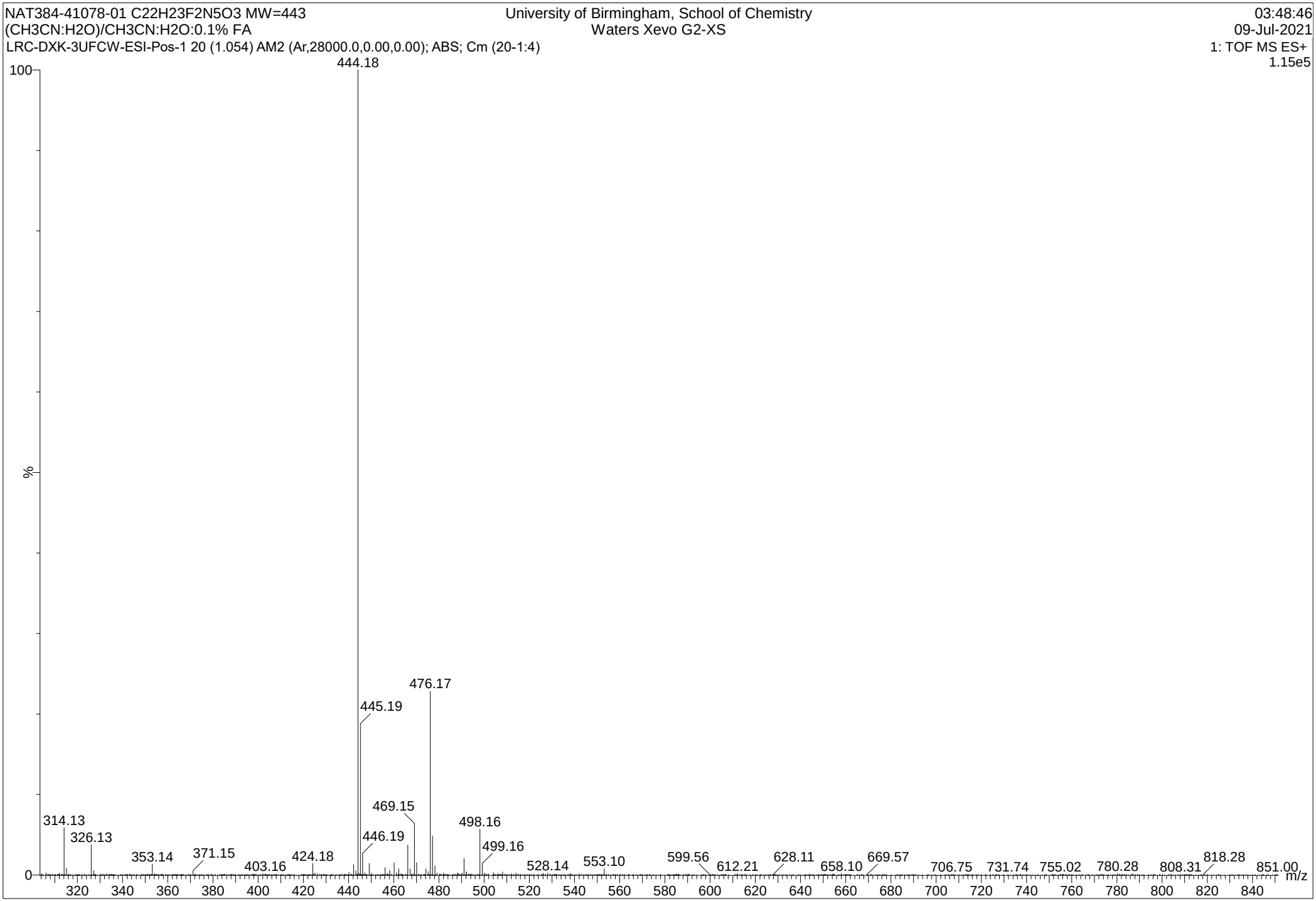
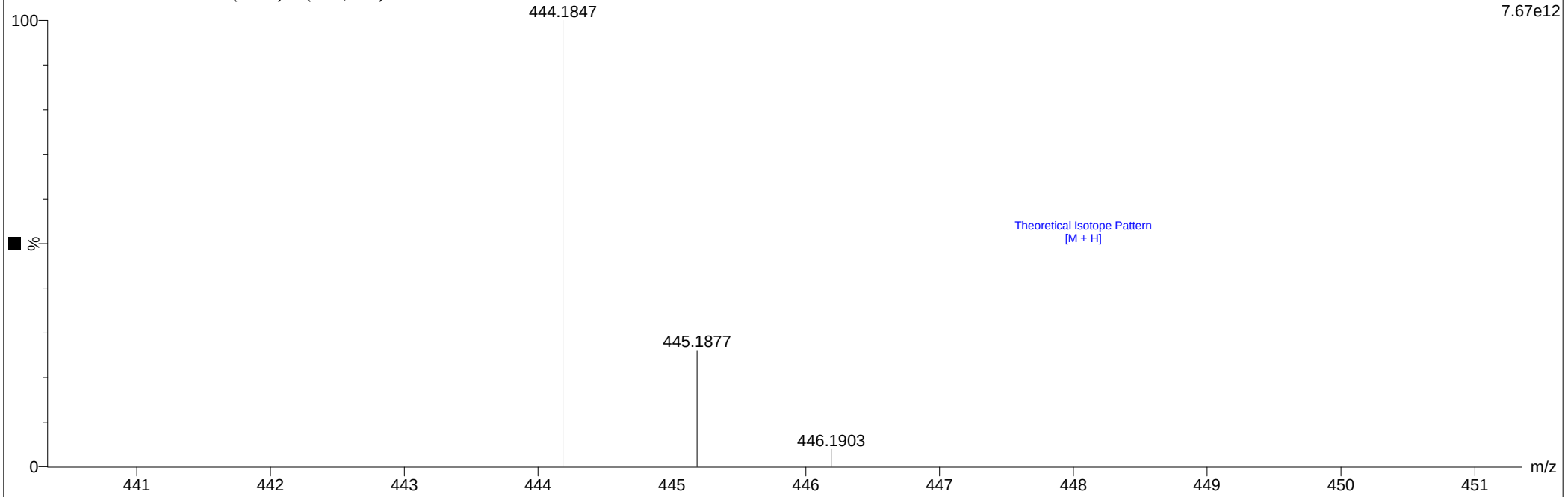

NAT384-41078-01 C22H23F2N5O3 MW=443
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UFCW-ESI-Pos-1 20 (1.054) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20-1:4)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
03:48:46
09-Jul-2021
1: TOF MS ES+
1.15e5
100
%
0
444.18
476.17
498.16
499.16
131.06
314.13
253.08
424.18
658.10
780.28
941.33
1077.22
1145.32
1354.51
1476.70
1674.99
1796.26
1966.35
2025.23
2189.75
2241.31
2341.41
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
2000
2100
2200
2300
m/z


NAT384-41078-01 C22H23F2N5O3 MW=443
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UFCW-ESI-Pos-1 20 (1.054) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20-1:4)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
03:48:46
09-Jul-2021
1: TOF MS ES+
1.15e5
100
%
0
444.18
476.17
445.19
469.15
498.16
446.19
499.16
314.13
326.13
353.14
371.15
403.16
424.18
528.14
553.10
599.56
612.21
628.11
658.10
669.57
706.75
731.74
755.02
780.28
808.31
818.28
851.00
m/z
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
700
720
740
760
780
800
820
840

NAT384-41078-01 C22H23F2N5O3 MW=443
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UFCW-ESI-Pos-1 (0.062) Is (1.00,1.00) C22H23F2N5O3 H

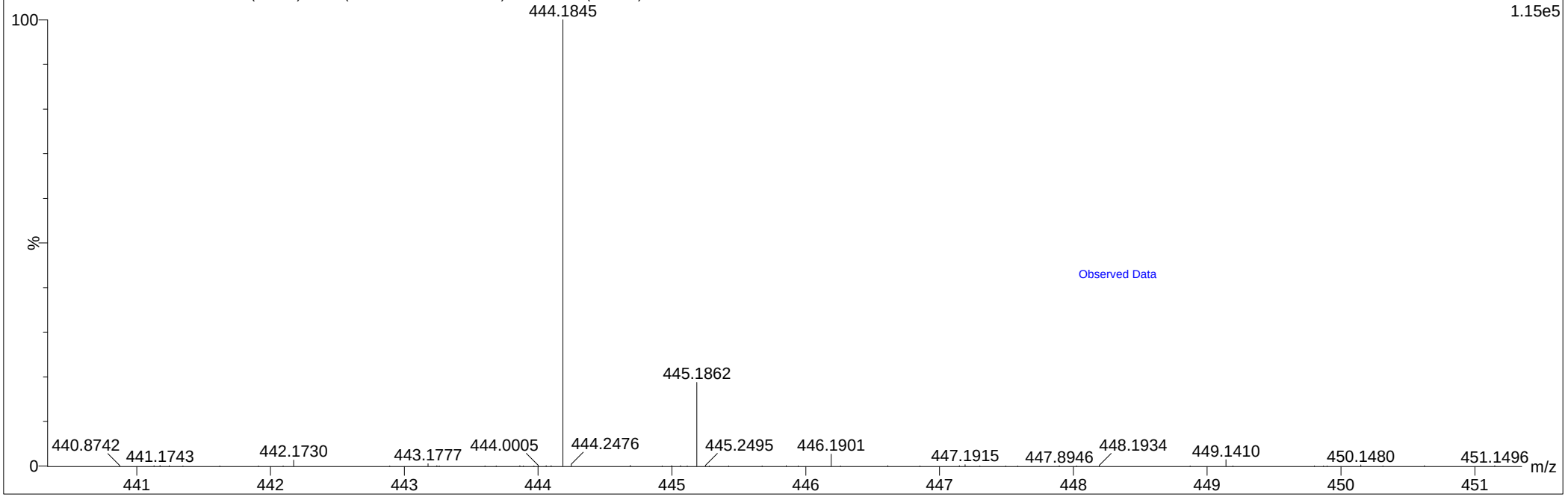
University of Birmingham, School of Chemistry
Waters Xevo G2-XS

03:48:46
09-Jul-2021
1: TOF MS ES+
7.67e12



LRC-DXK-3UFCW-ESI-Pos-1 20 (1.054) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20-1:4)

1: TOF MS ES+
1.15e5



Single Mass Analysis

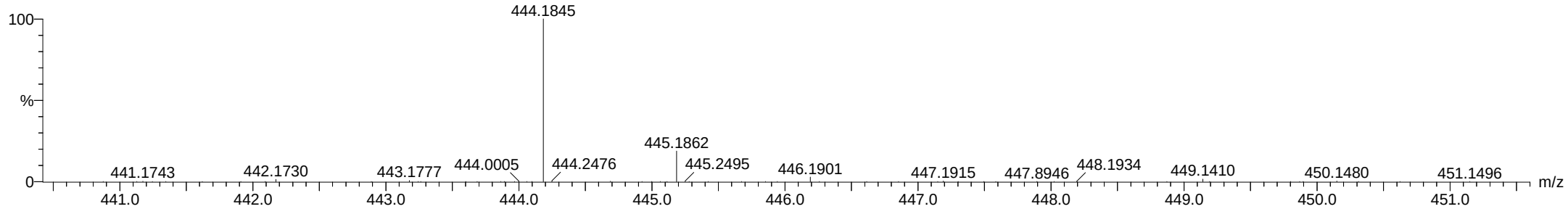
Tolerance = 3.0 PPM / DBE: min = -4.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4175 formula(e) evaluated with 11 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

NAT384-41078-01 C22H23F2N5O3 MW=443
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UFCW-ESI-Pos-1 20 (1.054) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20-1:4)

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

03:48:46
09-Jul-2021
1: TOF MS ES+
1.15e+005



Minimum:				-4.5				
Maximum:		5.0	3.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
444.1845	444.1845	0.0	0.0	3.5	124.1	2.461	8.53	C18 H29 N O8 F3
	444.1847	-0.2	-0.5	12.5	126.6	4.938	0.72	C22 H24 N5 O3 F2
	444.1843	0.2	0.5	5.5	122.7	1.113	32.86	C12 H22 N11 O3 F4
	444.1841	0.4	0.9	-1.5	126.3	4.702	0.91	C12 H31 N3 O13 F
	444.1850	-0.5	-1.1	-3.5	129.6	7.975	0.03	C3 H25 N13 O9 F3
	444.1839	0.6	1.4	0.5	128.6	6.972	0.09	C6 H24 N13 O8 F2
	444.1836	0.9	2.0	16.5	127.6	5.988	0.25	C25 H23 N5 O2 F
	444.1854	-0.9	-2.0	3.5	123.1	1.461	23.20	C13 H27 N7 O9 F
	444.1834	1.1	2.5	7.5	126.3	4.684	0.92	C21 H28 N O7 F2
	444.1857	-1.2	-2.7	-0.5	124.2	2.568	7.67	C15 H30 N O9 F4
	444.1832	1.3	2.9	9.5	123.0	1.394	24.82	C15 H21 N11 O2 F3