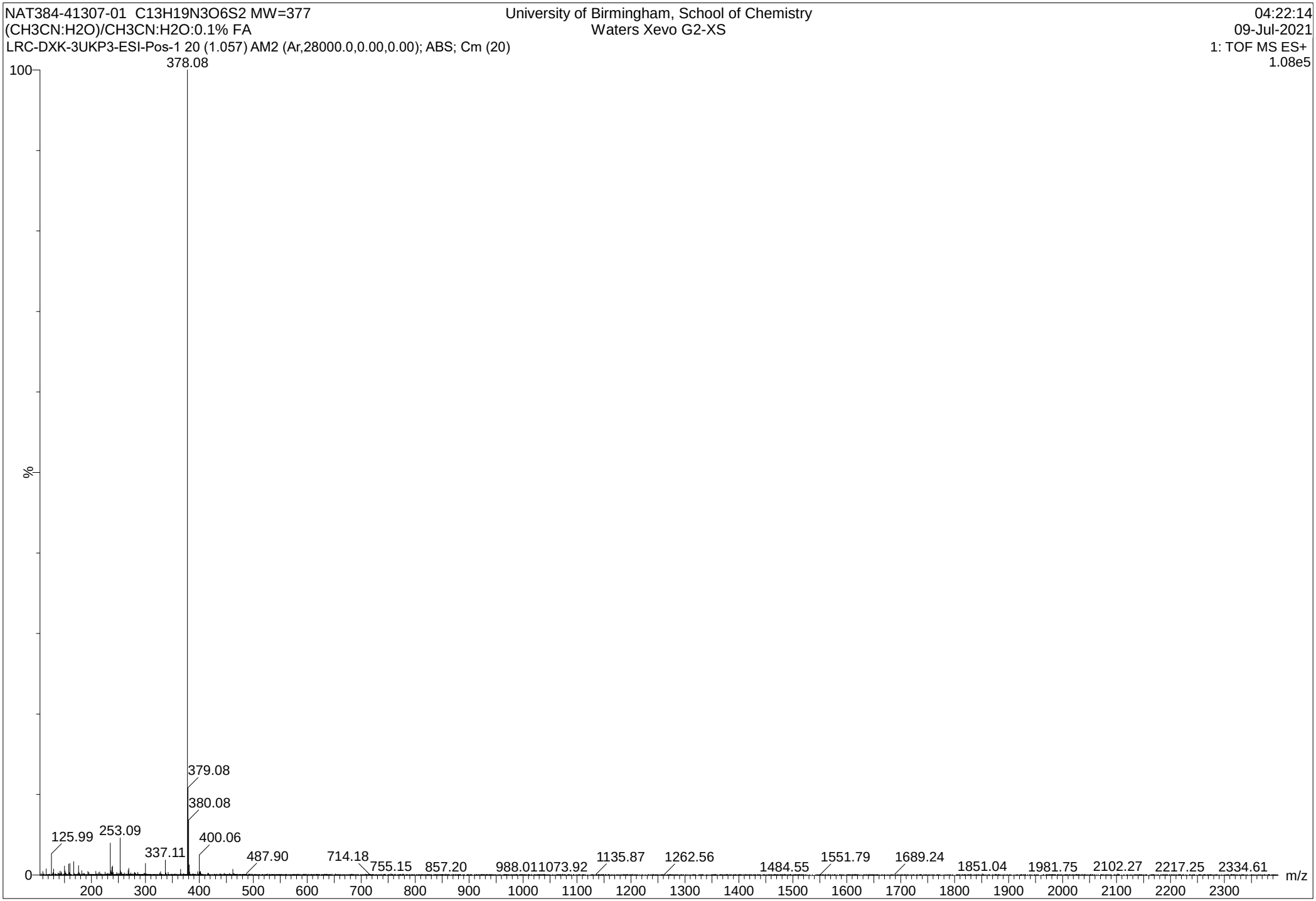
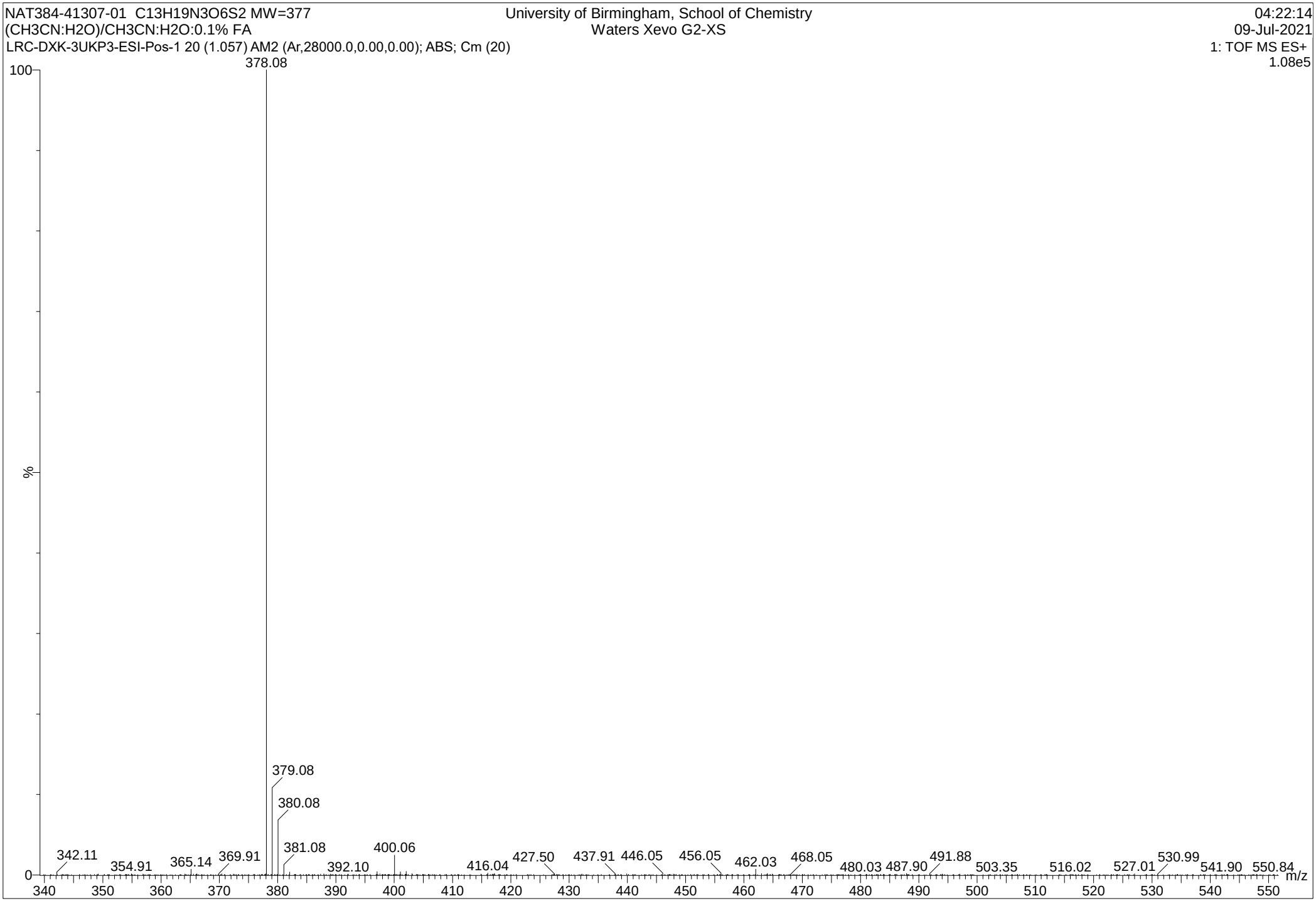
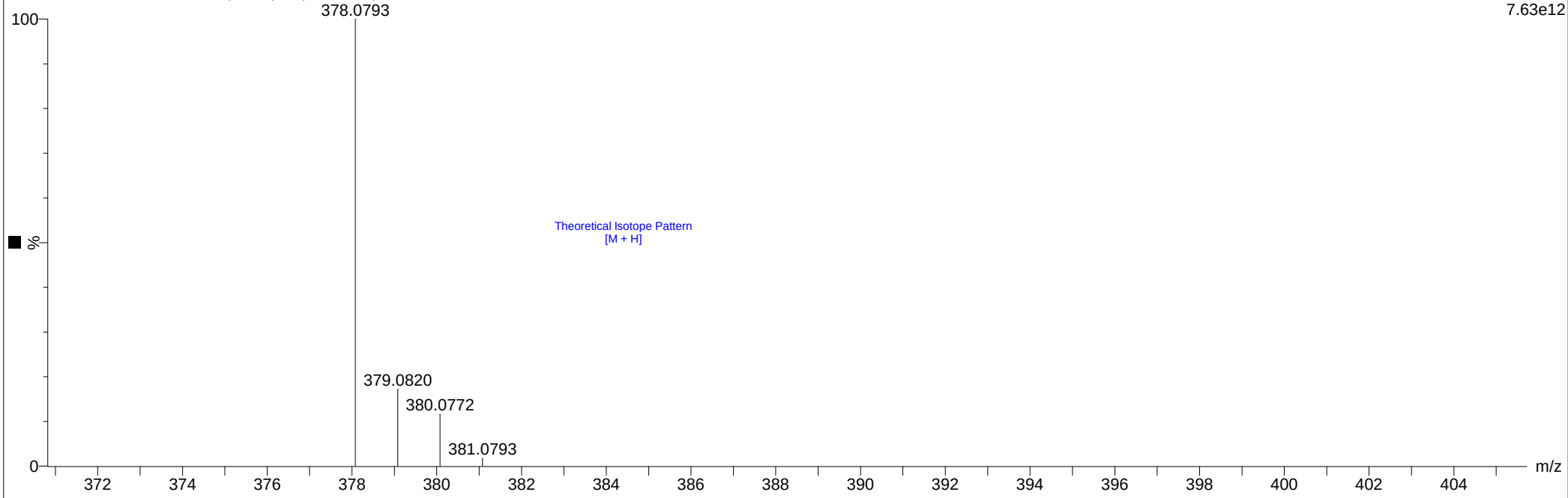

NAT384-41307-01 C13H19N3O6S2 MW=377
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UKP3-ESI-Pos-1 20 (1.057) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
04:22:14
09-Jul-2021
1: TOF MS ES+
1.08e5
100
%
0
378.08
379.08
380.08
125.99
253.09
337.11
400.06
487.90
714.18
755.15
857.20
988.01
1073.92
1135.87
1262.56
1484.55
1551.79
1689.24
1851.04
1981.75
2102.27
2217.25
2334.61
m/z
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
2000
2100
2200
2300


NAT384-41307-01 C13H19N3O6S2 MW=377
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UKP3-ESI-Pos-1 20 (1.057) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20)
University of Birmingham, School of Chemistry
Waters Xevo G2-XS
04:22:14
09-Jul-2021
1: TOF MS ES+
1.08e5
100
%
0
m/z
378.08
379.08
380.08
381.08
342.11
354.91
365.14
369.91
392.10
400.06
416.04
427.50
437.91
446.05
456.05
462.03
468.05
480.03
487.90
491.88
503.35
516.02
527.01
530.99
541.90
550.84
340
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
500
510
520
530
540
550

NAT384-41307-01 C13H19N3O6S2 MW=377
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UKP3-ESI-Pos-1 (0.062) Is (1.00,1.00) C13H19N3O6S2 H

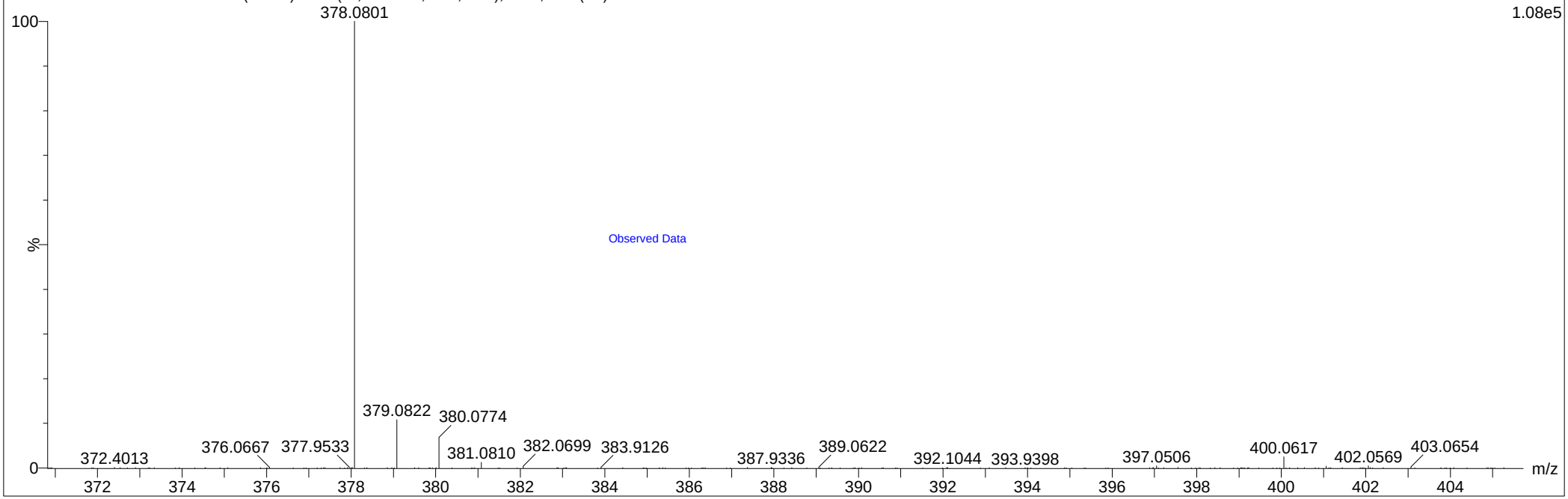
University of Birmingham, School of Chemistry
Waters Xevo G2-XS

04:22:14
09-Jul-2021
1: TOF MS ES+
7.63e12



LRC-DXK-3UKP3-ESI-Pos-1 20 (1.057) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20)

1: TOF MS ES+
1.08e5



Single Mass Analysis

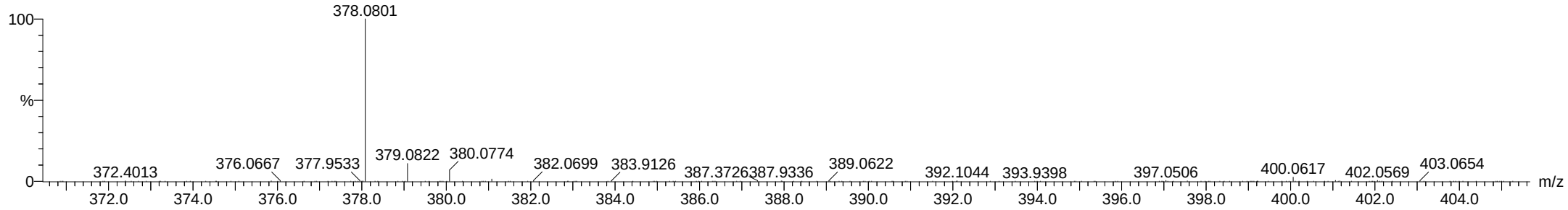
Tolerance = 5.0 PPM / DBE: min = -4.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2519 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-15 O: 0-20 S: 0-2

NAT384-41307-01 C13H19N3O6S2 MW=377
(CH3CN:H2O)/CH3CN:H2O:0.1% FA
LRC-DXK-3UKP3-ESI-Pos-1 20 (1.057) AM2 (Ar,28000.0,0.00,0.00); ABS; Cm (20)

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

04:22:14
09-Jul-2021
1: TOF MS ES+
1.08e+005



Minimum:				-4.5				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
378.0801	378.0800	0.1	0.3	14.5	112.6	11.941	0.00	C21 H16 N O4 S
	378.0798	0.3	0.8	11.5	115.0	14.378	0.00	C13 H12 N7 O7
	378.0805	-0.4	-1.1	7.5	103.2	2.542	7.87	C6 H12 N13 O5 S
	378.0807	-0.6	-1.6	10.5	105.6	4.979	0.69	C14 H16 N7 O2 S2
	378.0794	0.7	1.9	5.5	105.5	4.882	0.76	C13 H20 N3 O6 S2
	378.0792	0.9	2.4	2.5	100.8	0.133	87.52	C5 H16 N9 O9 S
	378.0812	-1.1	-2.9	16.5	115.9	15.197	0.00	C14 H8 N11 O3
	378.0813	-1.2	-3.2	19.5	113.3	12.646	0.00	C22 H12 N5 S
	378.0785	1.6	4.2	6.5	113.9	13.217	0.00	C12 H16 N3 O11
	378.0817	-1.6	-4.2	-1.5	115.6	14.892	0.00	C H16 N9 O14
	378.0819	-1.8	-4.8	1.5	104.1	3.453	3.17	C9 H20 N3 O11 S