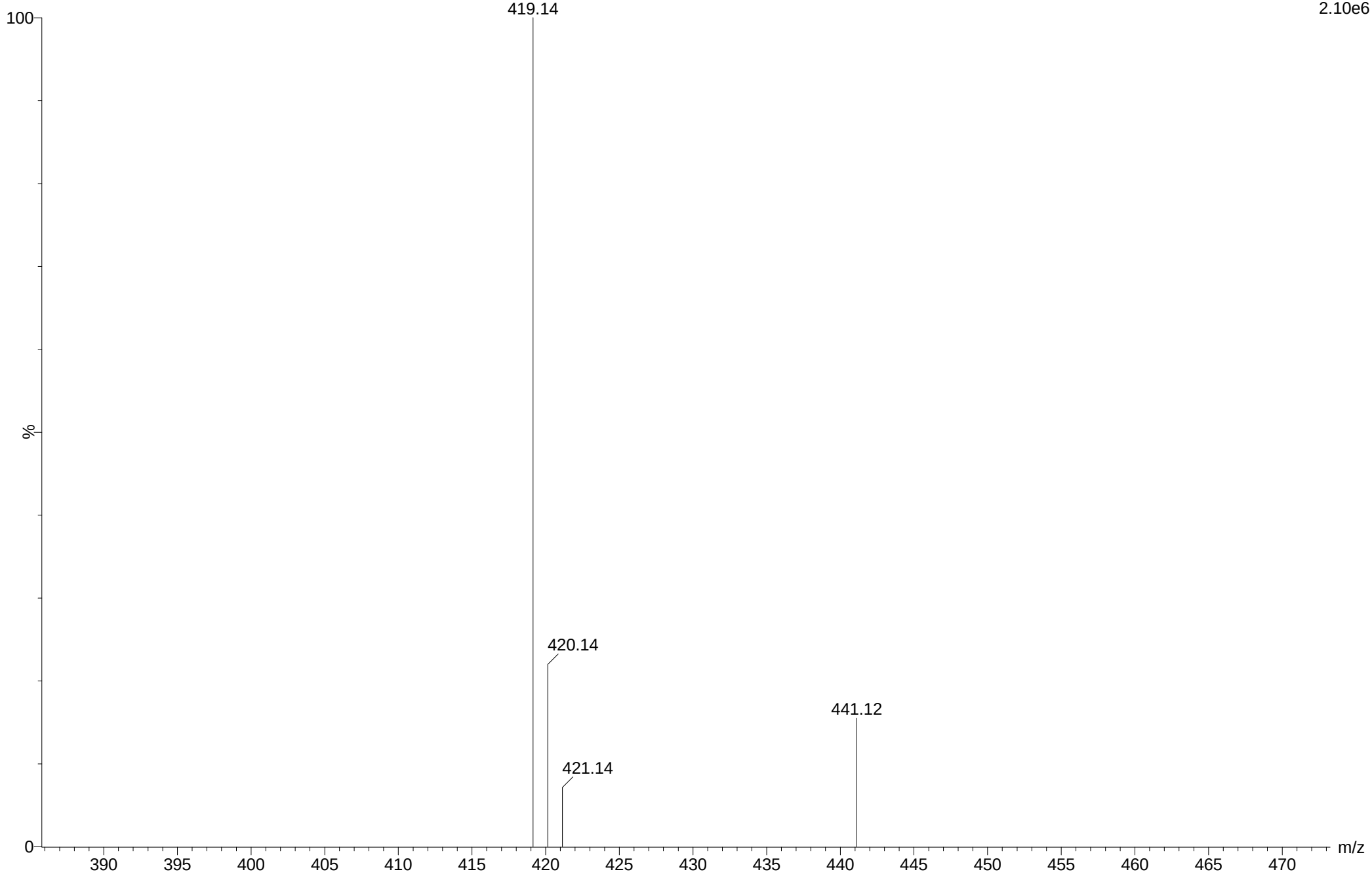
NAT384-653072 C19H22N4O5S MW=418 University of Birmingham, School of Chemistry Holly Adcock
Methanol:Water Waters Xevo G2-XS 16-Apr-2021 16:33:15
LRC-HVA-4TVAP-ESI-Pos-1 20 (1.079) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (20) 1: TOF MS ES+
3.72e6



NAT384-653072 C19H22N4O5S MW=418
Methanol:Water
LRC-HVA-4TVAP-ESI-Pos-1 20 (1.087) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (20)

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

Holly Adcock
16-Apr-2021 16:33:15
2: TOF MS ES+
2.10e6



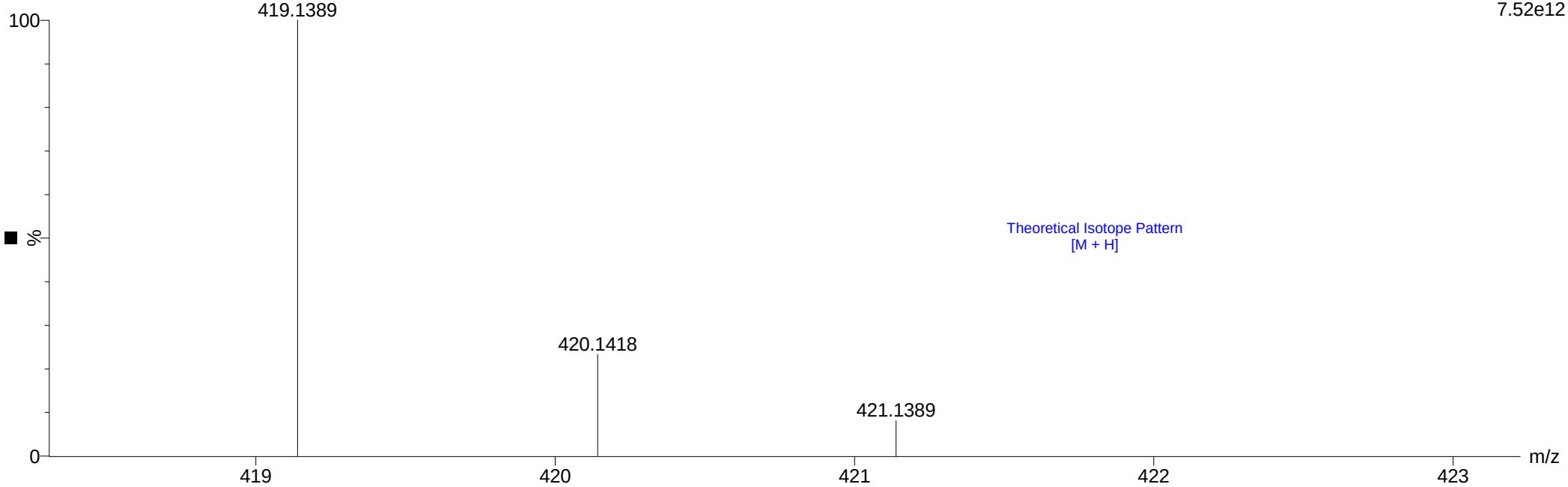
NAT384-653072 C19H22N4O5S MW=418
Methanol:Water

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

Holly Adcock
16-Apr-2021 16:33:15

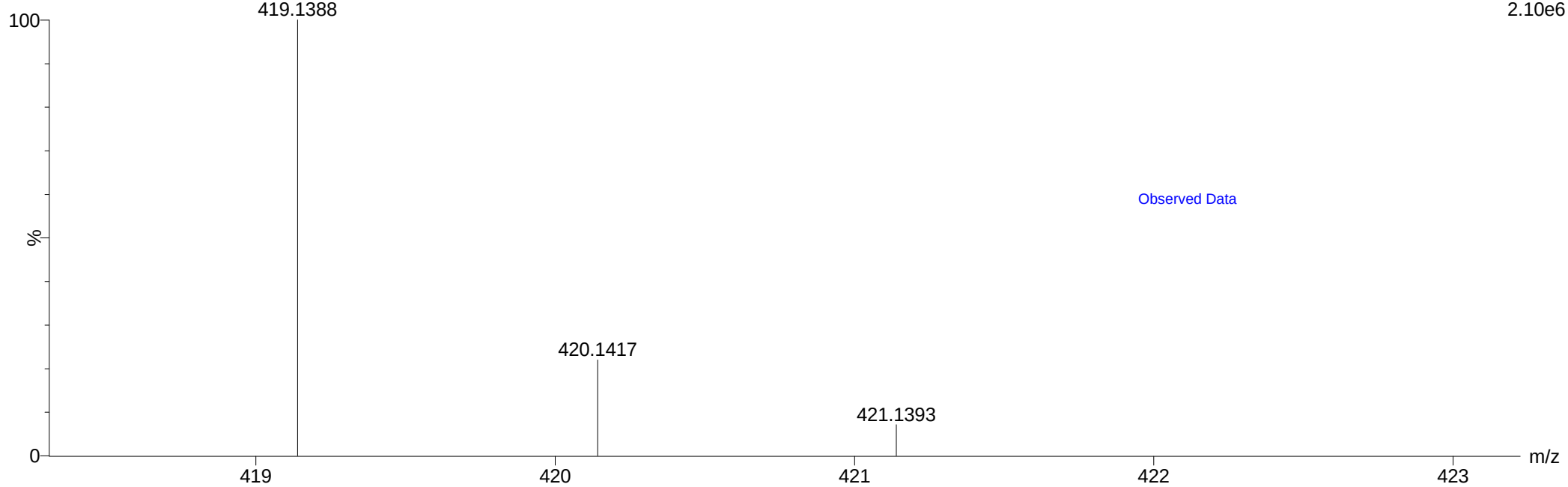
LRC-HVA-4TVAP-ESI-Pos-1 (0.290) Is (1.00,0.01) C19H22N4O5S H

2: TOF MS ES+
7.52e12



LRC-HVA-4TVAP-ESI-Pos-1 20 (1.087) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (20)

2: TOF MS ES+
2.10e6



Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -4.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1635 formula(e) evaluated with 6 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-40 H: 0-60 N: 0-10 O: 0-10 S: 0-2

Minimum:				-4.0				
Maximum:		3.0	3.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
419.1388	419.1387	0.1	0.2	7.5	38.0	13.644	0.00	C11 H19 N10 O8
	419.1389	-0.1	-0.2	10.5	24.4	0.029	97.14	C19 H23 N4 O5 S
	419.1383	0.5	1.2	1.5	36.9	12.523	0.00	C11 H27 N6 O7 S2
	419.1396	-0.8	-1.9	19.5	39.1	14.733	0.00	C27 H19 N2 O3
	419.1396	-0.8	-1.9	6.5	35.8	11.431	0.00	C12 H23 N10 O3 S2
	419.1376	1.2	2.9	5.5	28.0	3.557	2.85	C18 H27 O9 S