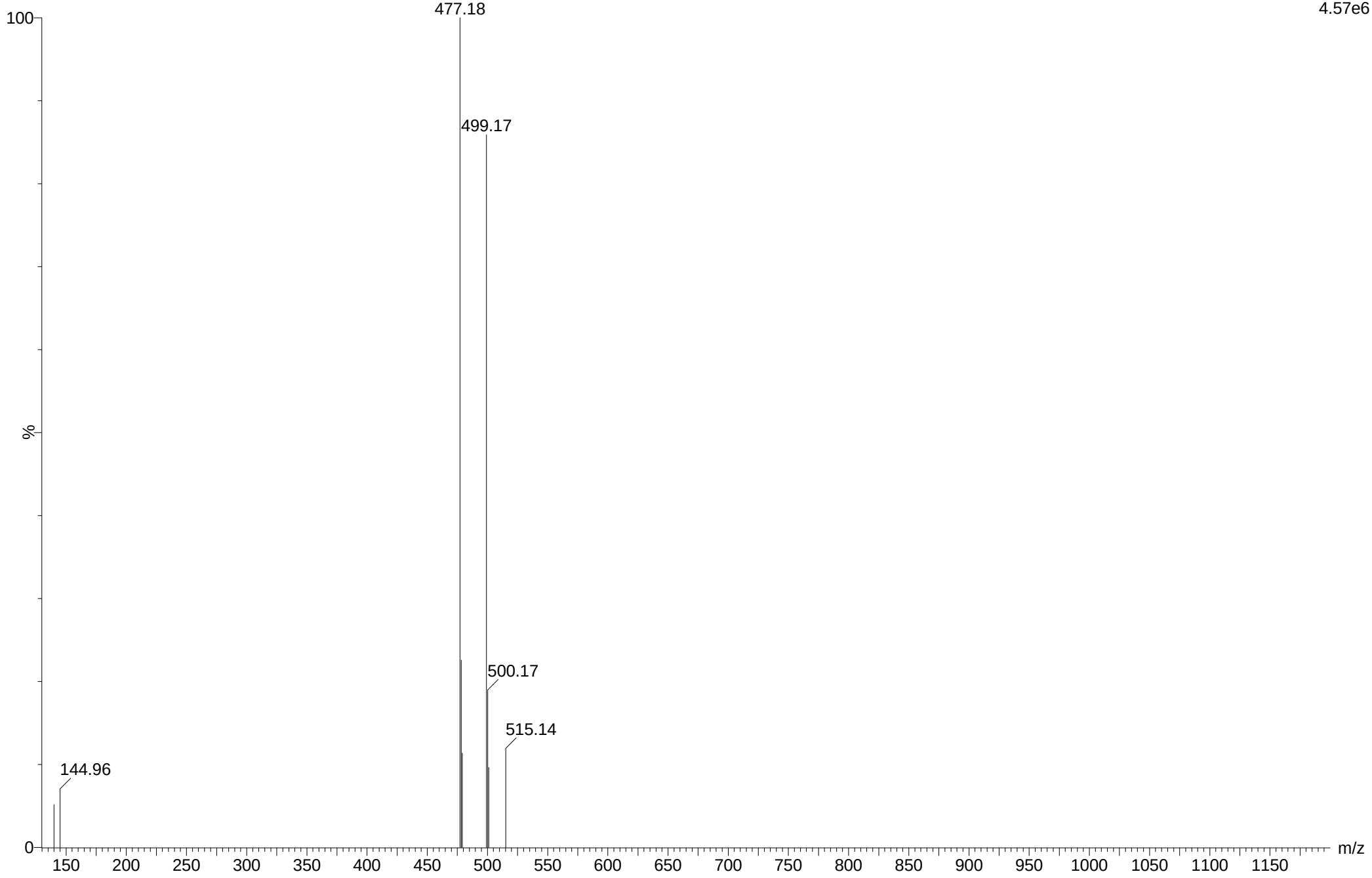
NAT384-652788 C19H32N4O6S2 MW=477
Methanol:Water
LRC-HVA-4TVFH-ESI-Pos-1 13 (0.774) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (12:14)

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

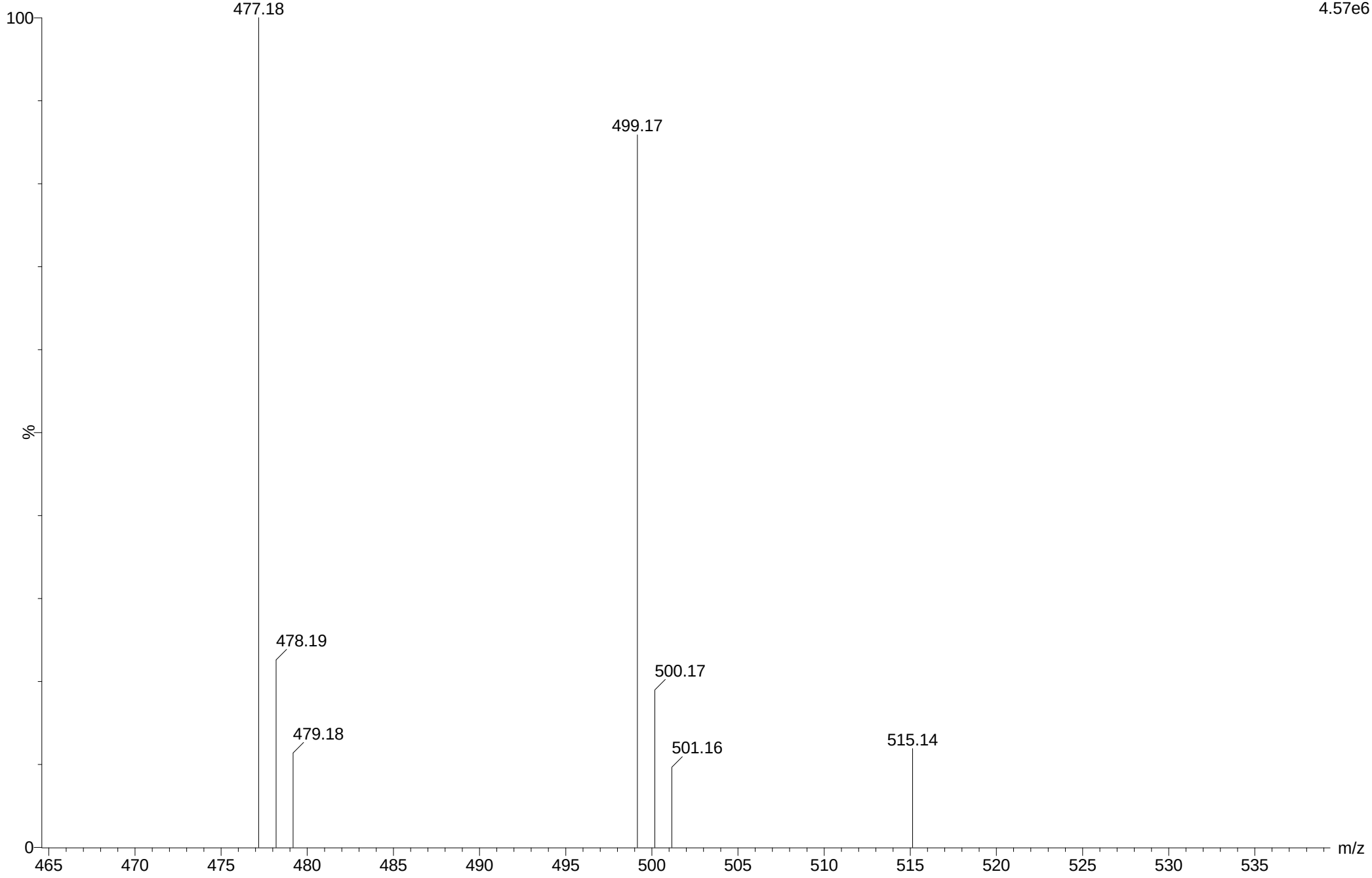
Holly Adcock
16-Apr-2021 18:47:28
2: TOF MS ES+
4.57e6



NAT384-652788 C19H32N4O6S2 MW=477
Methanol:Water
LRC-HVA-4TVFH-ESI-Pos-1 13 (0.774) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (12:14)

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

Holly Adcock
16-Apr-2021 18:47:28
2: TOF MS ES+
4.57e6



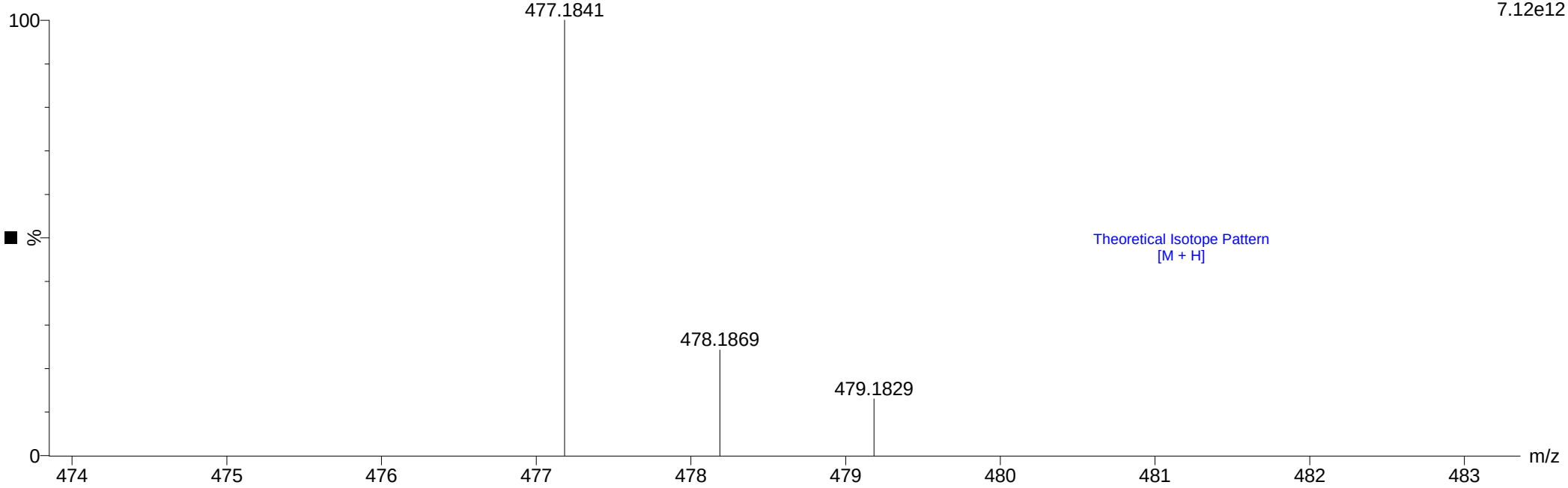
NAT384-652788 C19H32N4O6S2 MW=477
Methanol:Water

University of Birmingham, School of Chemistry
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Holly Adcock
16-Apr-2021 18:47:28

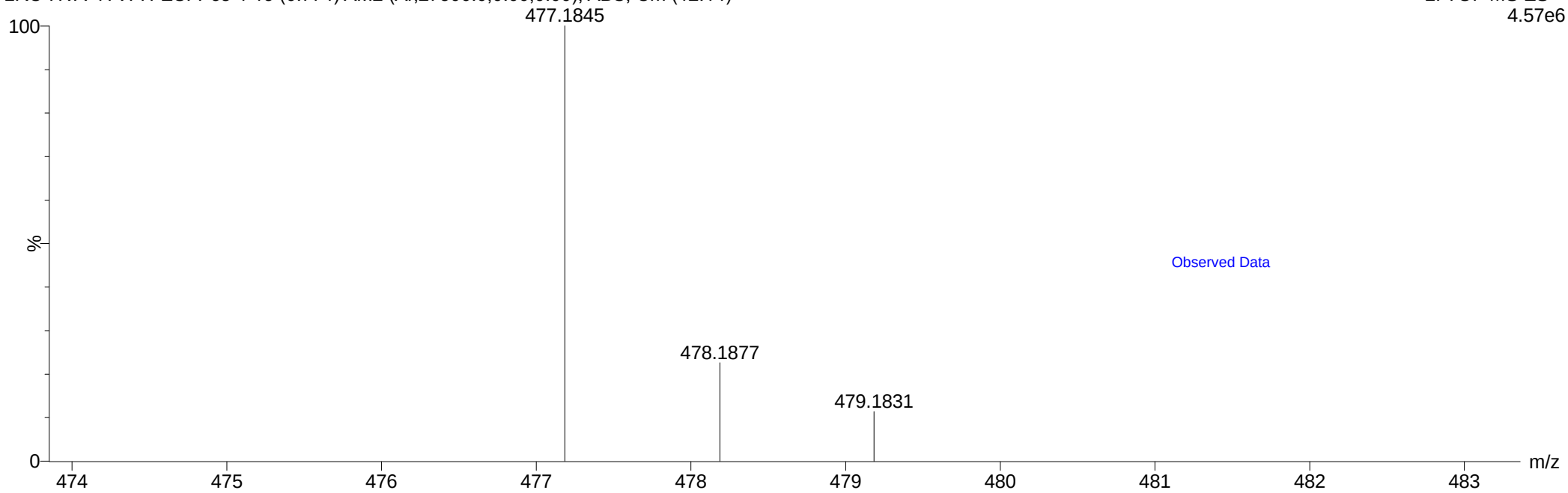
LRC-HVA-4TVFH-ESI-Pos-1 (0.290) Is (1.00,0.01) C19H32N4O6S2 H

2: TOF MS ES+
7.12e12



LRC-HVA-4TVFH-ESI-Pos-1 13 (0.774) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (12:14)

2: TOF MS ES+
4.57e6



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
1777 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
477.1845	477.1846	-0.1	-0.2	11.5	42.9	14.287	0.00	C19 H25 N8 O7
	477.1848	-0.3	-0.6	14.5	38.6	10.014	0.00	C27 H29 N2 O4 S
	477.1842	0.3	0.6	5.5	28.6	0.078	92.48	C19 H33 N4 O6 S2
	477.1840	0.5	1.0	2.5	36.1	7.580	0.05	C11 H29 N10 O9 S
	477.1855	-1.0	-2.1	23.5	45.1	16.544	0.00	C35 H25 O2
	477.1855	-1.0	-2.1	10.5	31.2	2.595	7.47	C20 H29 N8 O2 S2