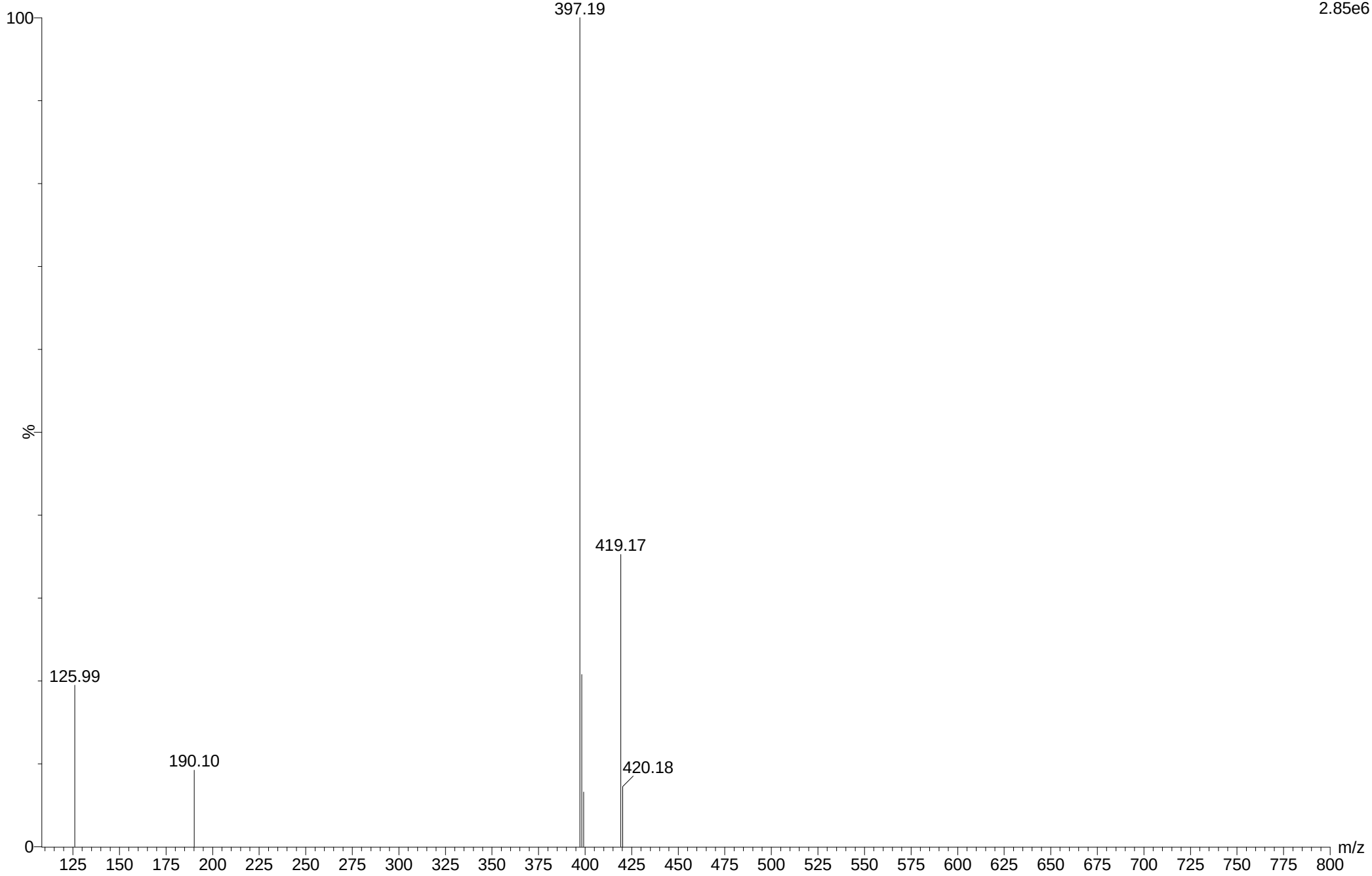
NAT384-652801 C18H28N4O4S MW=397
Methanol:Water
LRC-HVA-4U3V4-ESI-Pos-1 22 (1.156) AM2 (Ar,27500.0,0.00,0.00); ABS

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

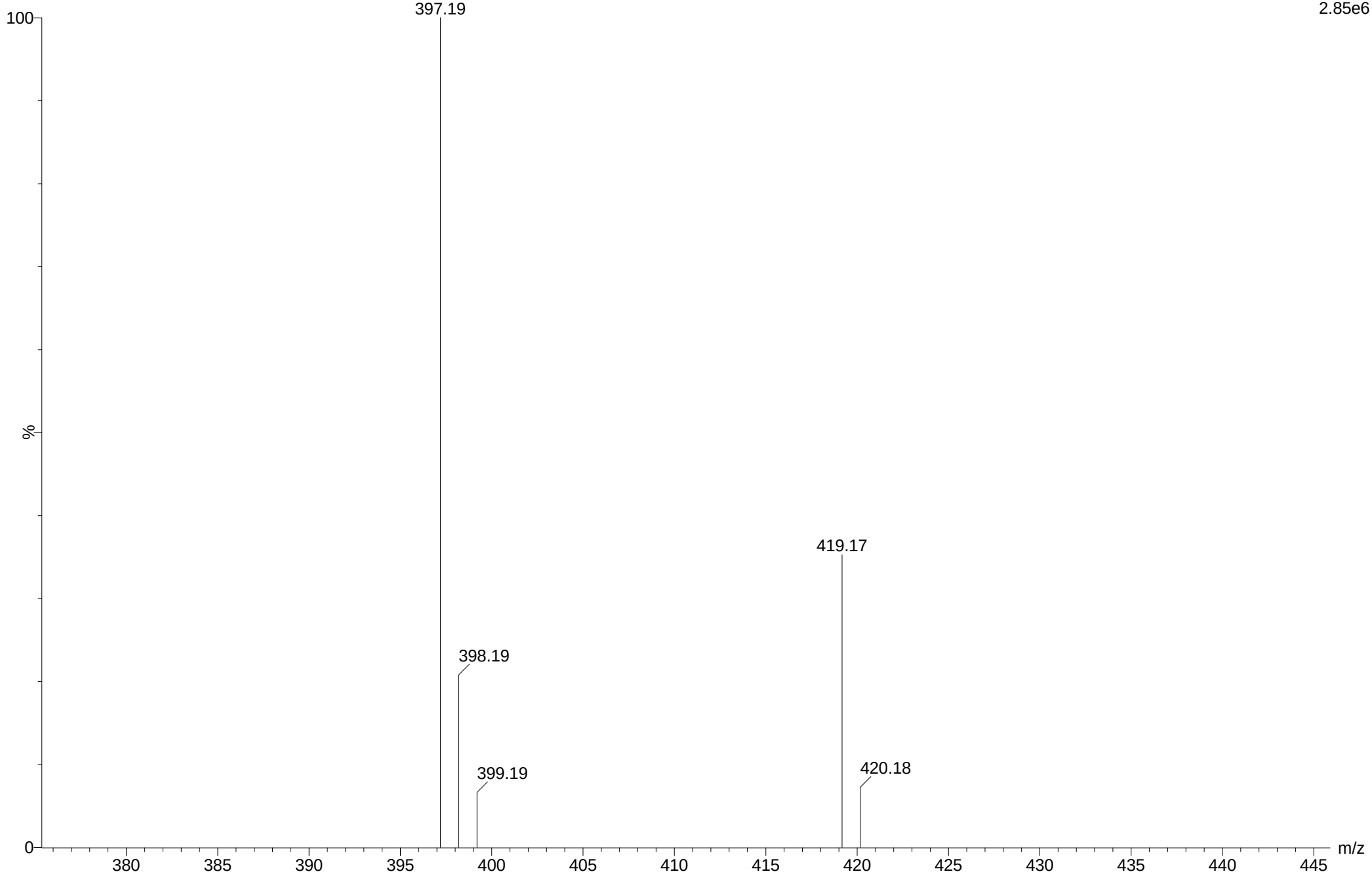
Holly Adcock
16-Apr-2021 17:45:21
2: TOF MS ES+
2.85e6



NAT384-652801 C18H28N4O4S MW=397
Methanol:Water
LRC-HVA-4U3V4-ESI-Pos-1 22 (1.156) AM2 (Ar,27500.0,0.00,0.00); ABS

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

Holly Adcock
16-Apr-2021 17:45:21
2: TOF MS ES+
2.85e6



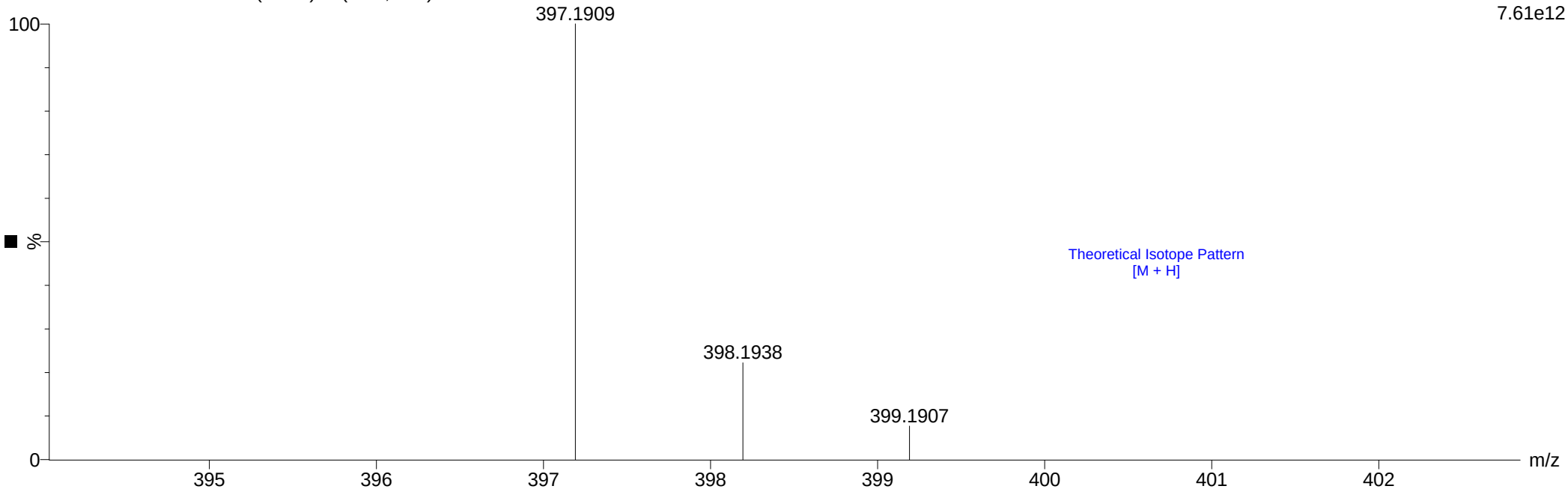
NAT384-652801 C18H28N4O4S MW=397
Methanol:Water

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

Holly Adcock
16-Apr-2021 17:45:21

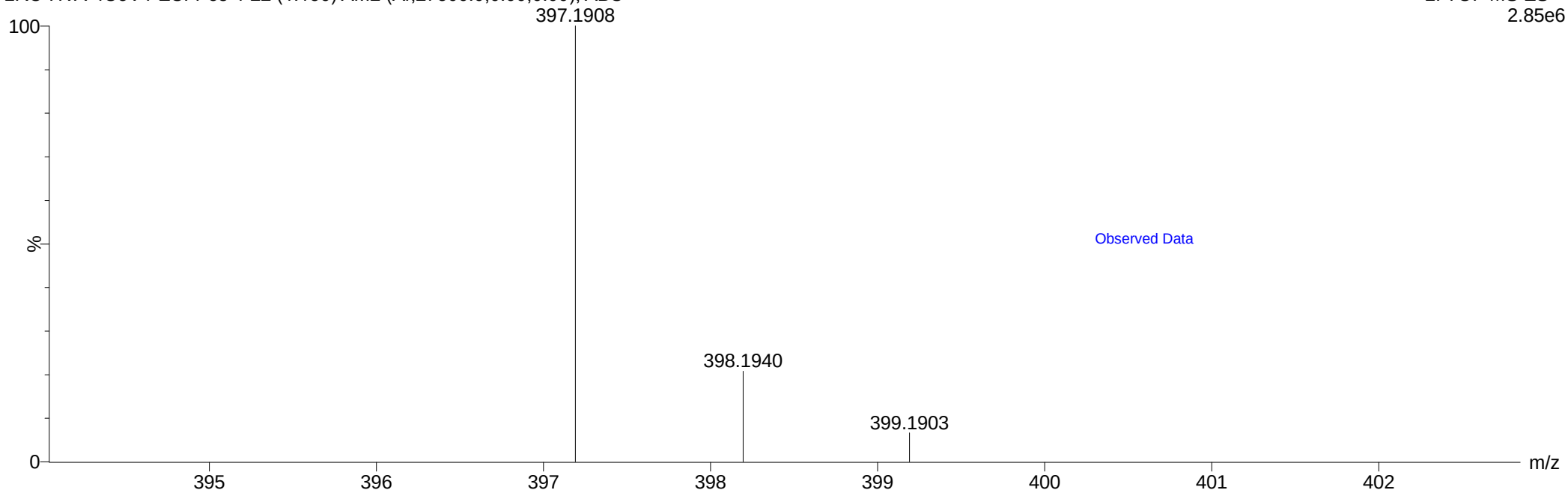
LRC-HVA-4U3V4-ESI-Pos-1 (0.290) Is (1.00,0.01) C18H28N4O4S H

2: TOF MS ES+
7.61e12



LRC-HVA-4U3V4-ESI-Pos-1 22 (1.156) AM2 (Ar,27500.0,0.00,0.00); ABS

2: TOF MS ES+
2.85e6



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
1545 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
397.1908	397.1908	0.0	0.0	3.5	40.0	14.125	0.00	C10 H25 N10 O7
	397.1910	-0.2	-0.5	6.5	25.9	0.059	94.25	C18 H29 N4 O4 S
	397.1903	0.5	1.3	-2.5	36.9	11.068	0.00	C10 H33 N6 O6 S2
	397.1916	-0.8	-2.0	15.5	40.9	15.091	0.00	C26 H25 N2 O2
	397.1916	-0.8	-2.0	2.5	35.9	10.002	0.00	C11 H29 N10 O2 S2
	397.1896	1.2	3.0	1.5	28.7	2.856	5.75	C17 H33 O8 S