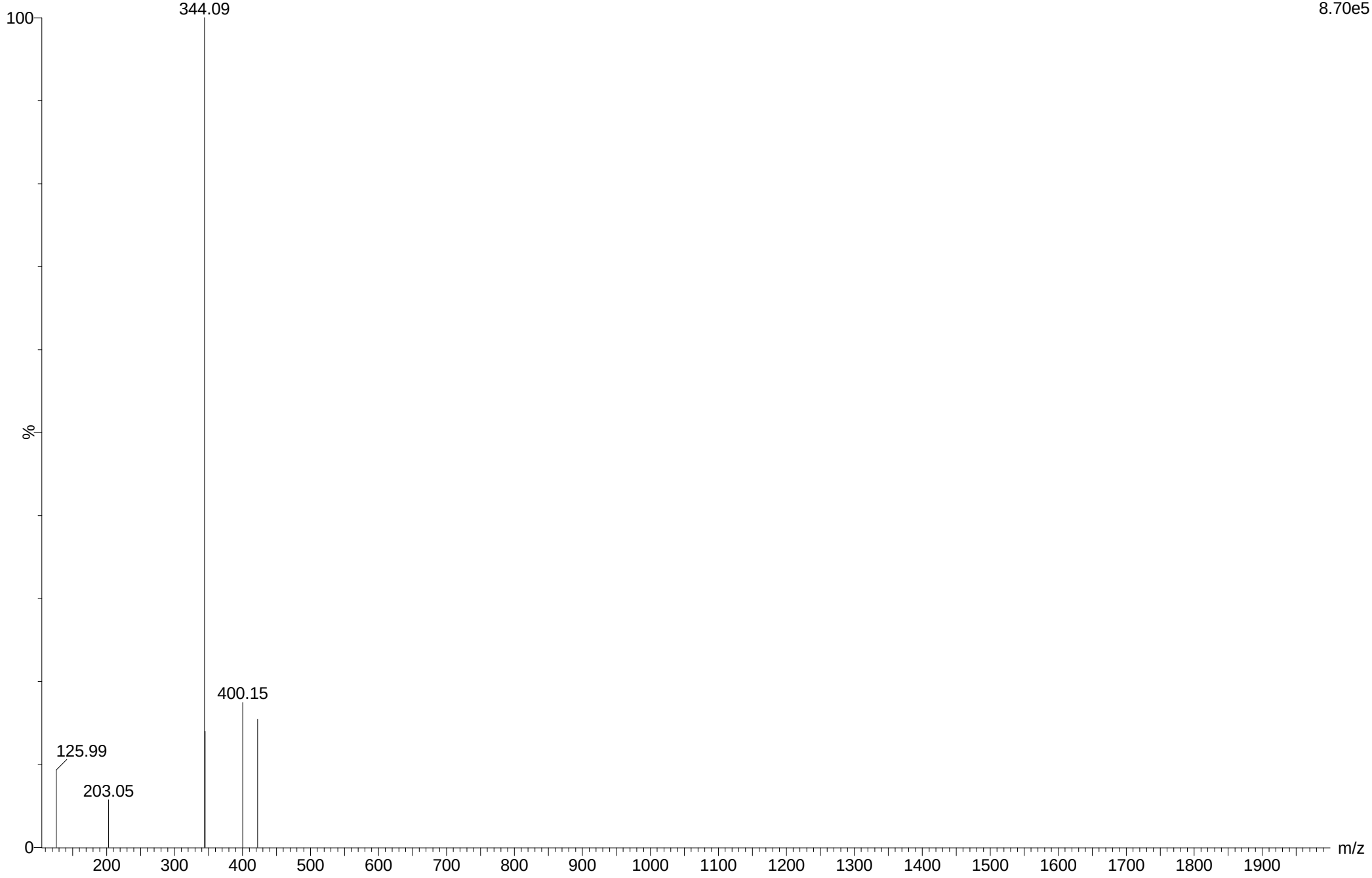
LNB0367-050-P C17H25N3O6S MW=399
Methanol
LRC-DXK-3UTAF-ESI-Pos-1 9 (0.648) AM2 (Ar,30000.0,0.00,0.00); ABS

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

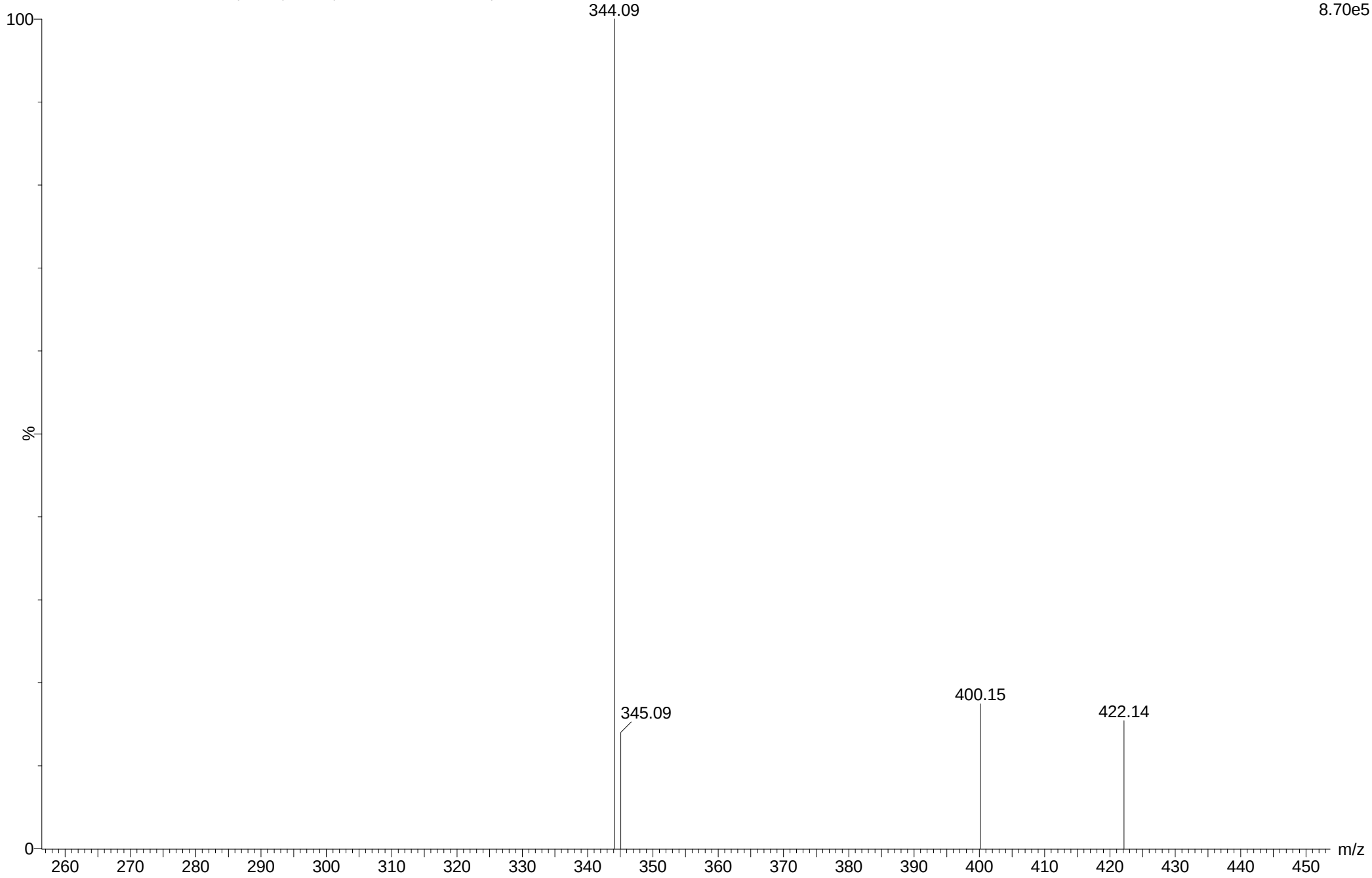
Daniel Kovari
11-Dec-2020 22:33:55
1: TOF MS ES+
8.70e5



LNB0367-050-P C17H25N3O6S MW=399
Methanol
LRC-DXK-3UTAF-ESI-Pos-1 9 (0.648) AM2 (Ar,30000.0,0.00,0.00); ABS

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Daniel Kovari
11-Dec-2020 22:33:55
1: TOF MS ES+
8.70e5



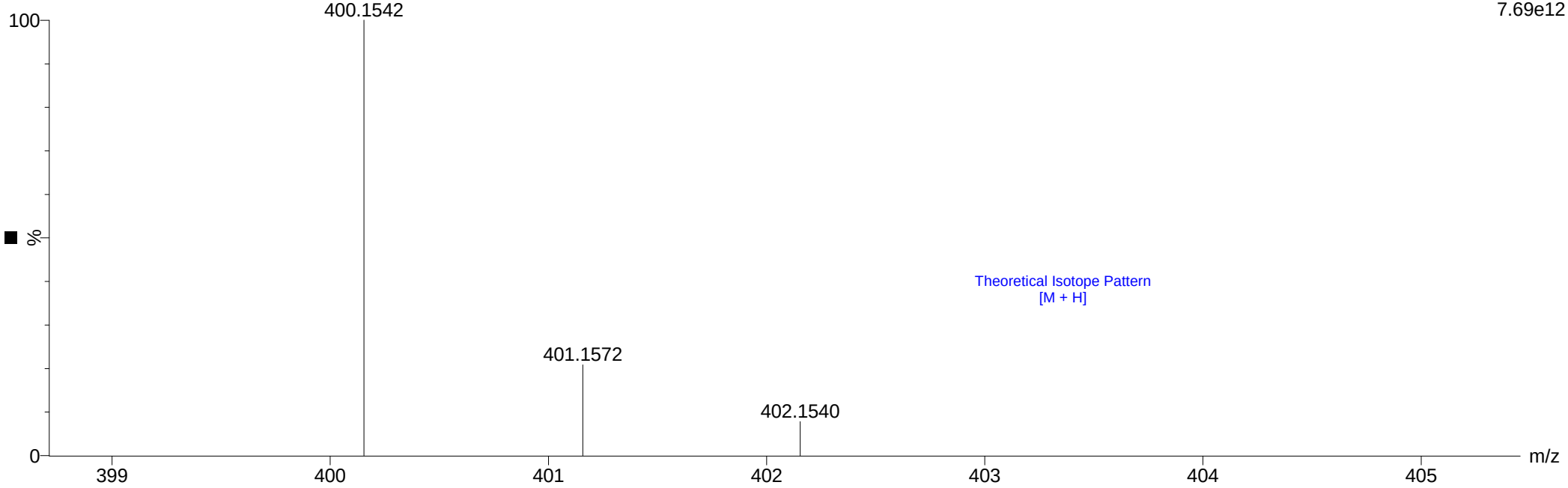
LNB0367-050-P C17H25N3O6S MW=399
Methanol

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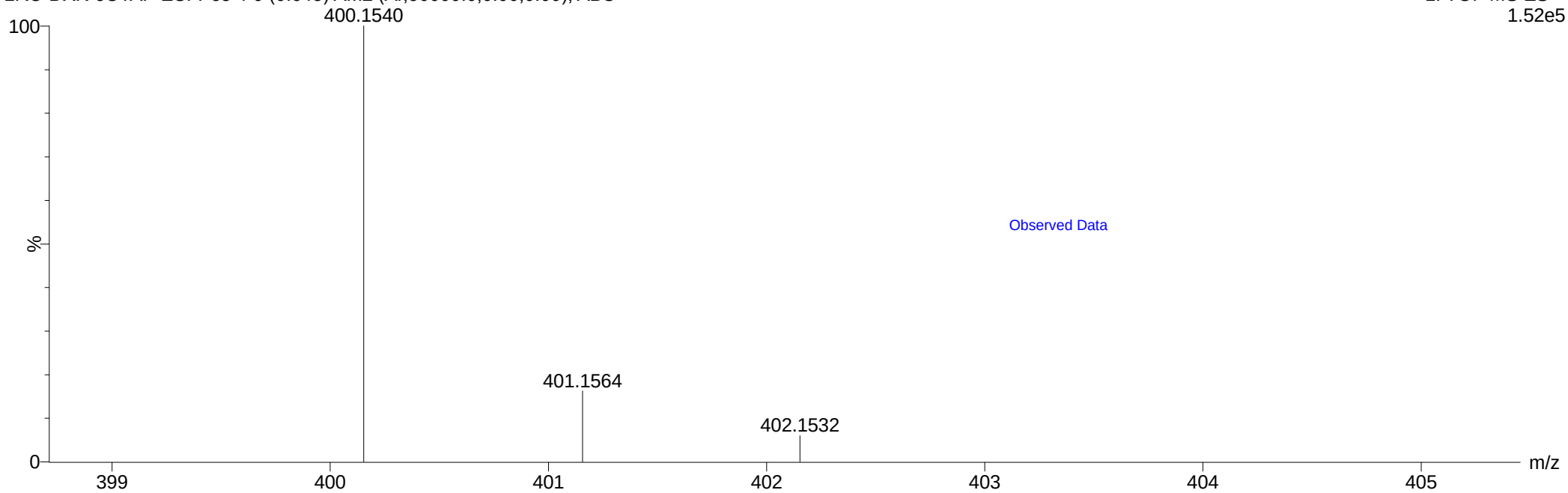
LRC-DXK-3UTAF-ESI-Pos-1 (0.062) Is (1.00,0.01) C17H25N3O6S H

1: TOF MS ES+
7.69e12



LRC-DXK-3UTAF-ESI-Pos-1 9 (0.648) AM2 (Ar,30000.0,0.00,0.00); ABS

1: TOF MS ES+
1.52e5



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
592 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-60 N: 0-10 O: 0-10 S: 1-1

Minimum:				-10.0				
Maximum:		5.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
400.1540	400.1542	-0.2	-0.5	6.5	37.7	0.213	80.82	C17 H26 N3 O6 S
	400.1556	-1.6	-4.0	11.5	39.1	1.651	19.18	C18 H22 N7 O2 S