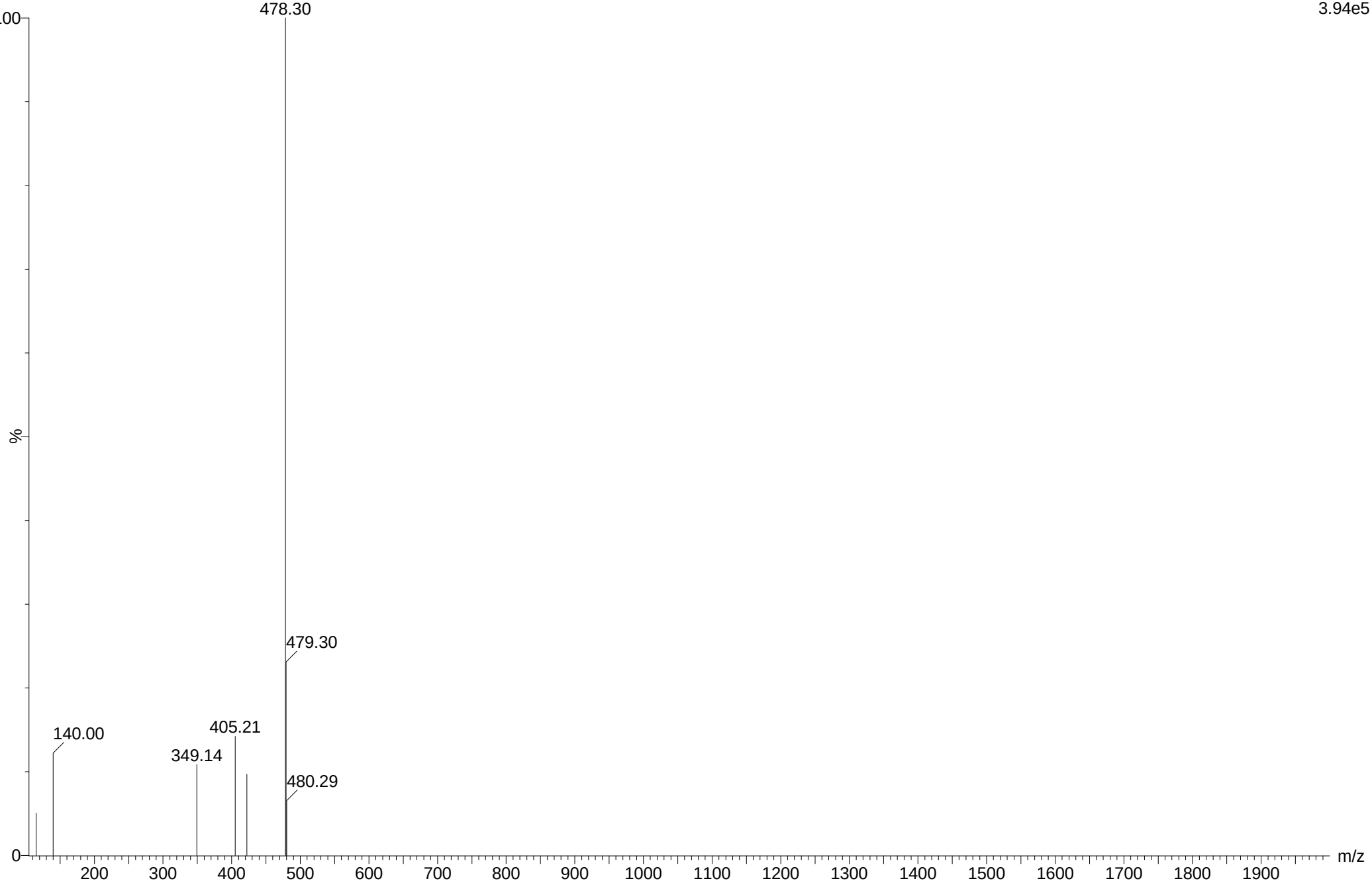
LNB0367-100-P C18H32N2O6S MW=404
Methanol

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

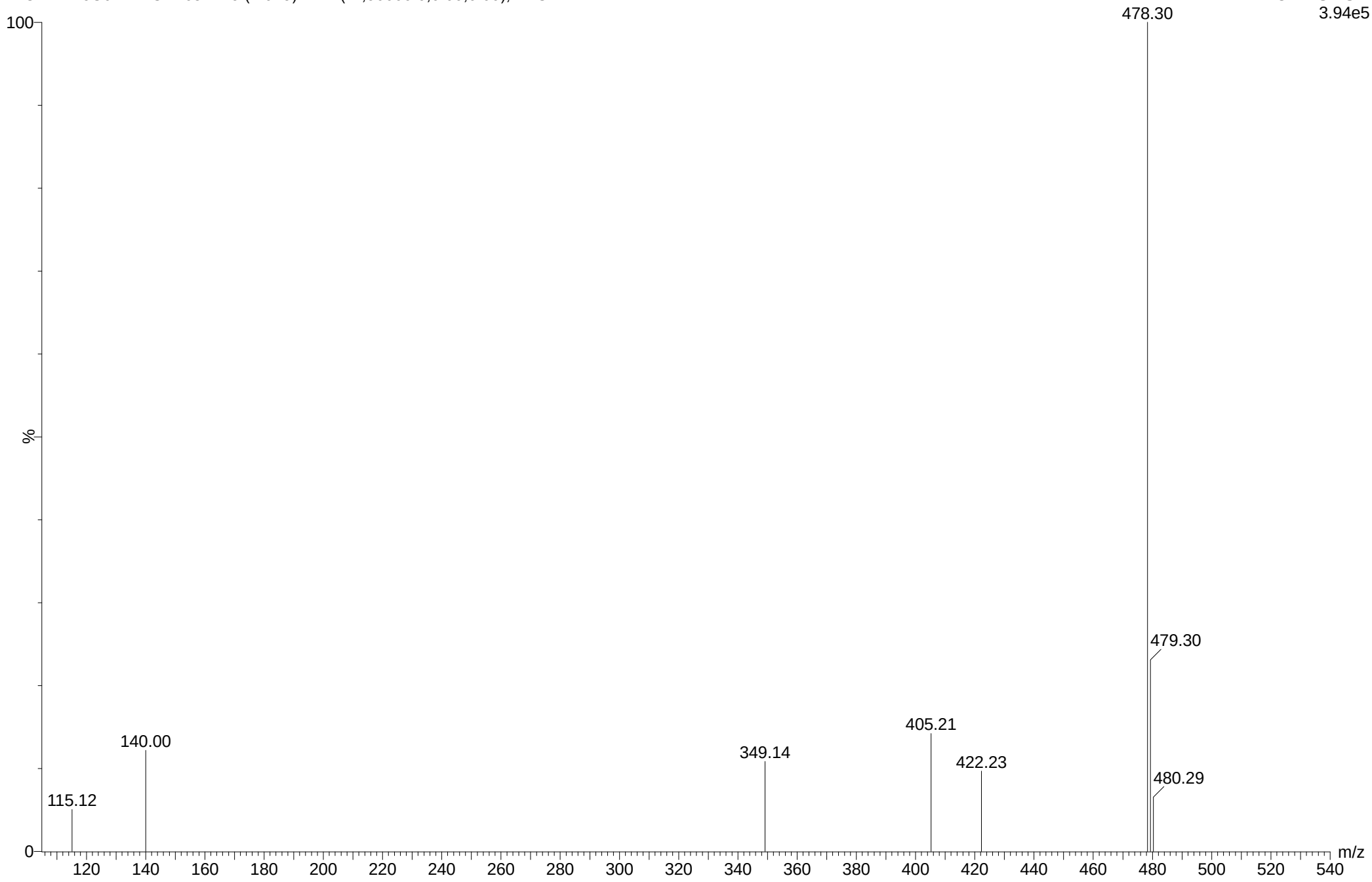
Daniel Kovari
11-Dec-2020 19:41:02

LRC-DXK-3U9VK-ESI-Pos-1 15 (1.078) AM2 (Ar,30000.0,0.00,0.00); ABS

1: TOF MS ES+
3.94e5



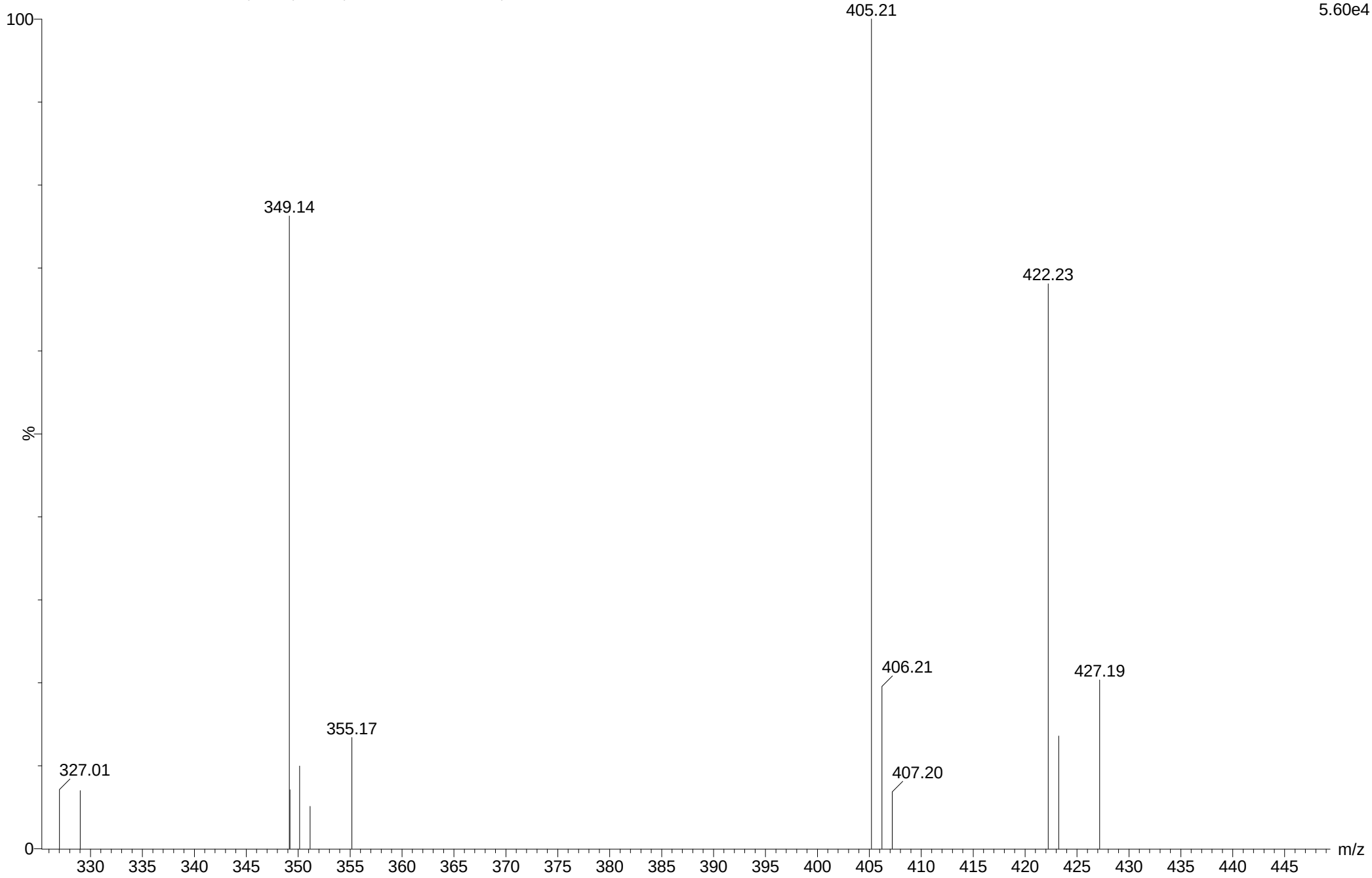
LNB0367-100-P C18H32N2O6S MW=404 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 19:41:02
LRC-DXK-3U9VK-ESI-Pos-1 15 (1.078) AM2 (Ar,30000.0,0.00,0.00); ABS 1: TOF MS ES+



LNB0367-100-P C18H32N2O6S MW=404
Methanol
LRC-DXK-3U9VK-ESI-Pos-1 15 (1.078) AM2 (Ar,30000.0,0.00,0.00); ABS

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

Daniel Kovari
11-Dec-2020 19:41:02
1: TOF MS ES+
5.60e4



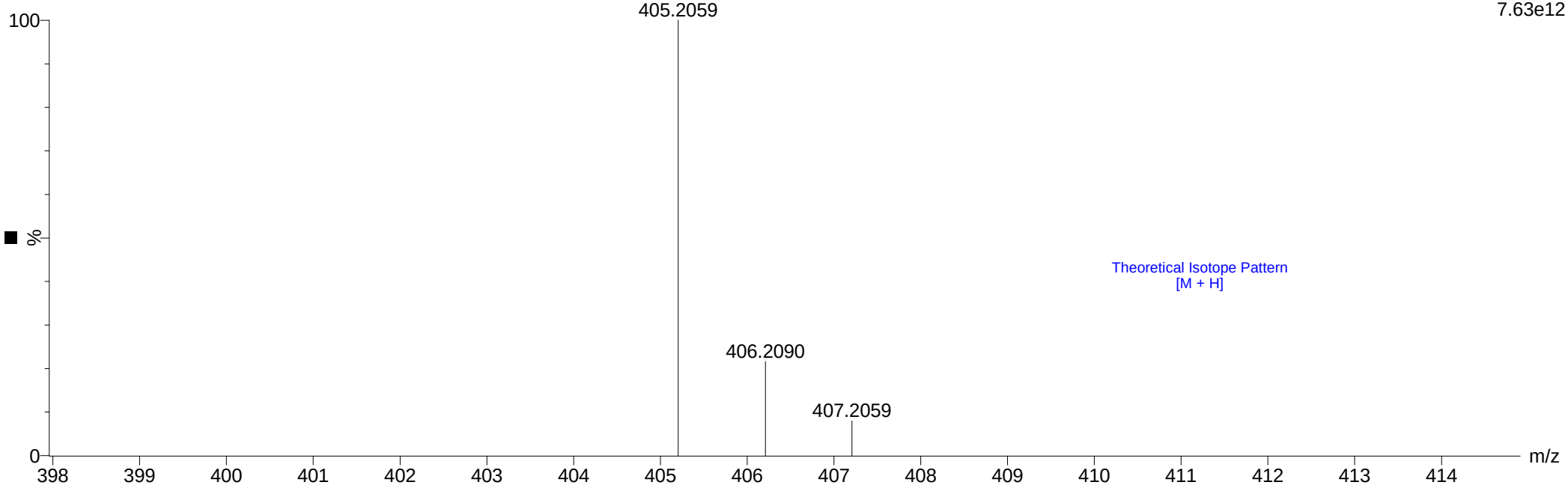
LNB0367-100-P C18H32N2O6S MW=404
Methanol

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

Daniel Kovari
11-Dec-2020 19:41:02

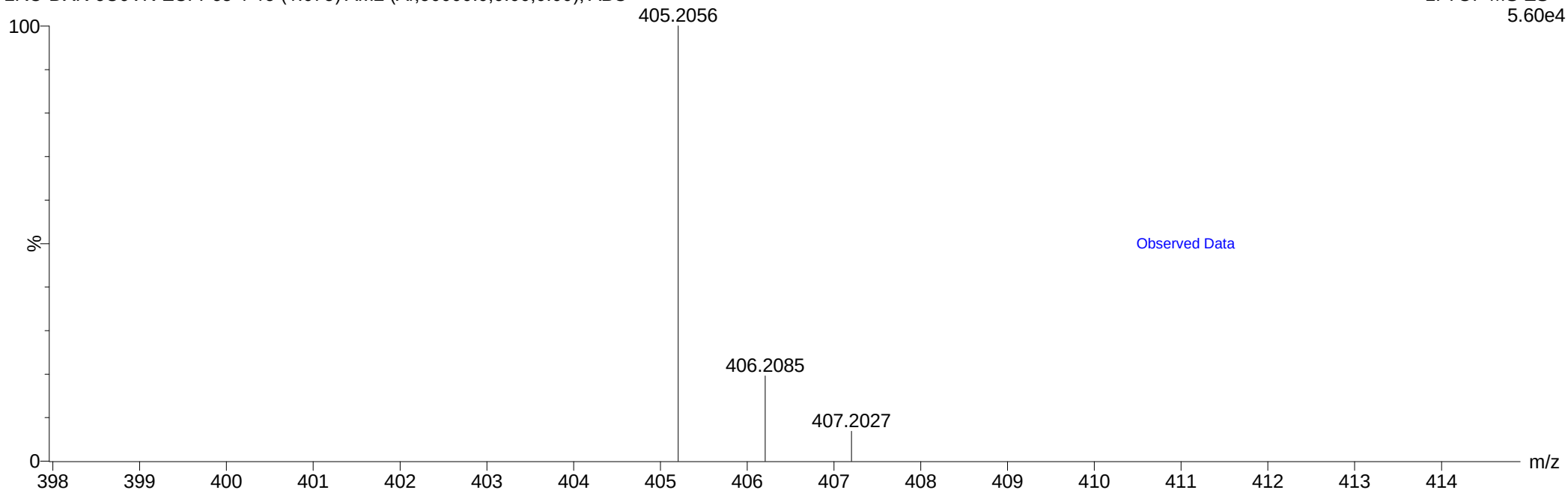
LRC-DXK-3U9VK-ESI-Pos-1 (0.062) Is (1.00,0.01) C18H32N2O6S H

1: TOF MS ES+
7.63e12



LRC-DXK-3U9VK-ESI-Pos-1 15 (1.078) AM2 (Ar,30000.0,0.00,0.00); ABS

1: TOF MS ES+
5.60e4



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
595 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
405.2056	405.2059	-0.3	-0.7	3.5	39.2	0.603	54.69	C18 H33 N2 O6 S
	405.2073	-1.7	-4.2	8.5	39.4	0.792	45.31	C19 H29 N6 O2 S