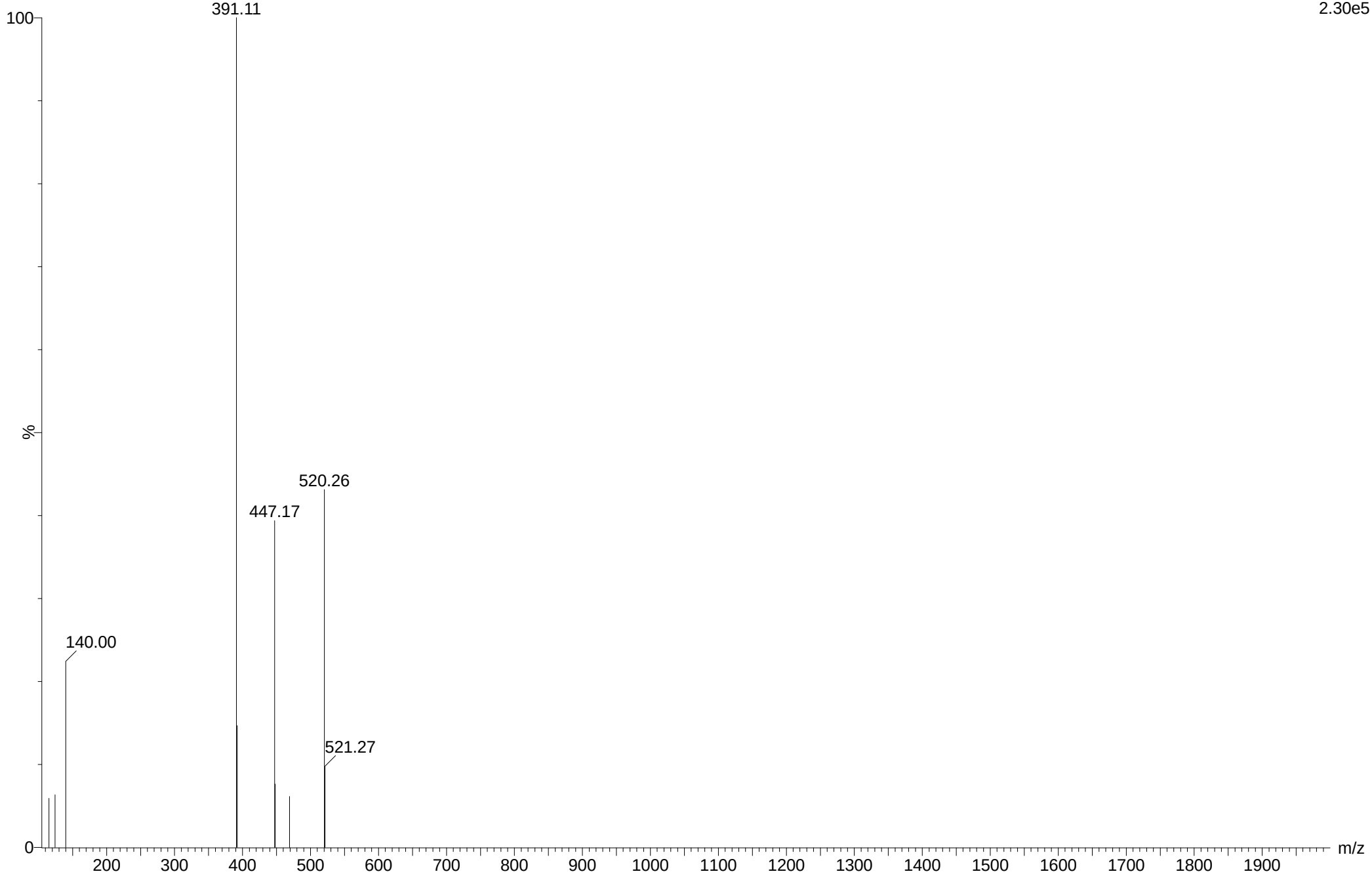
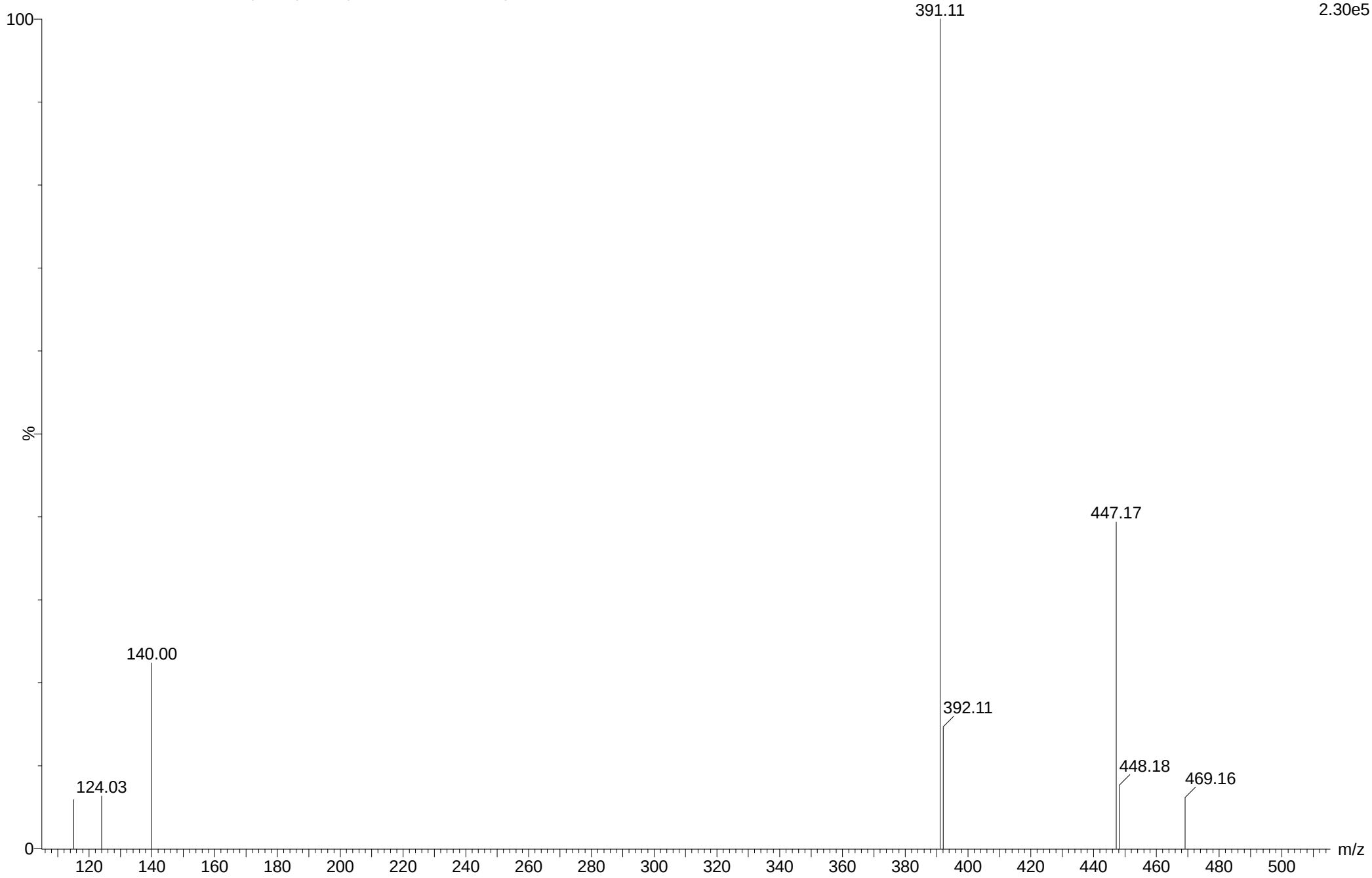
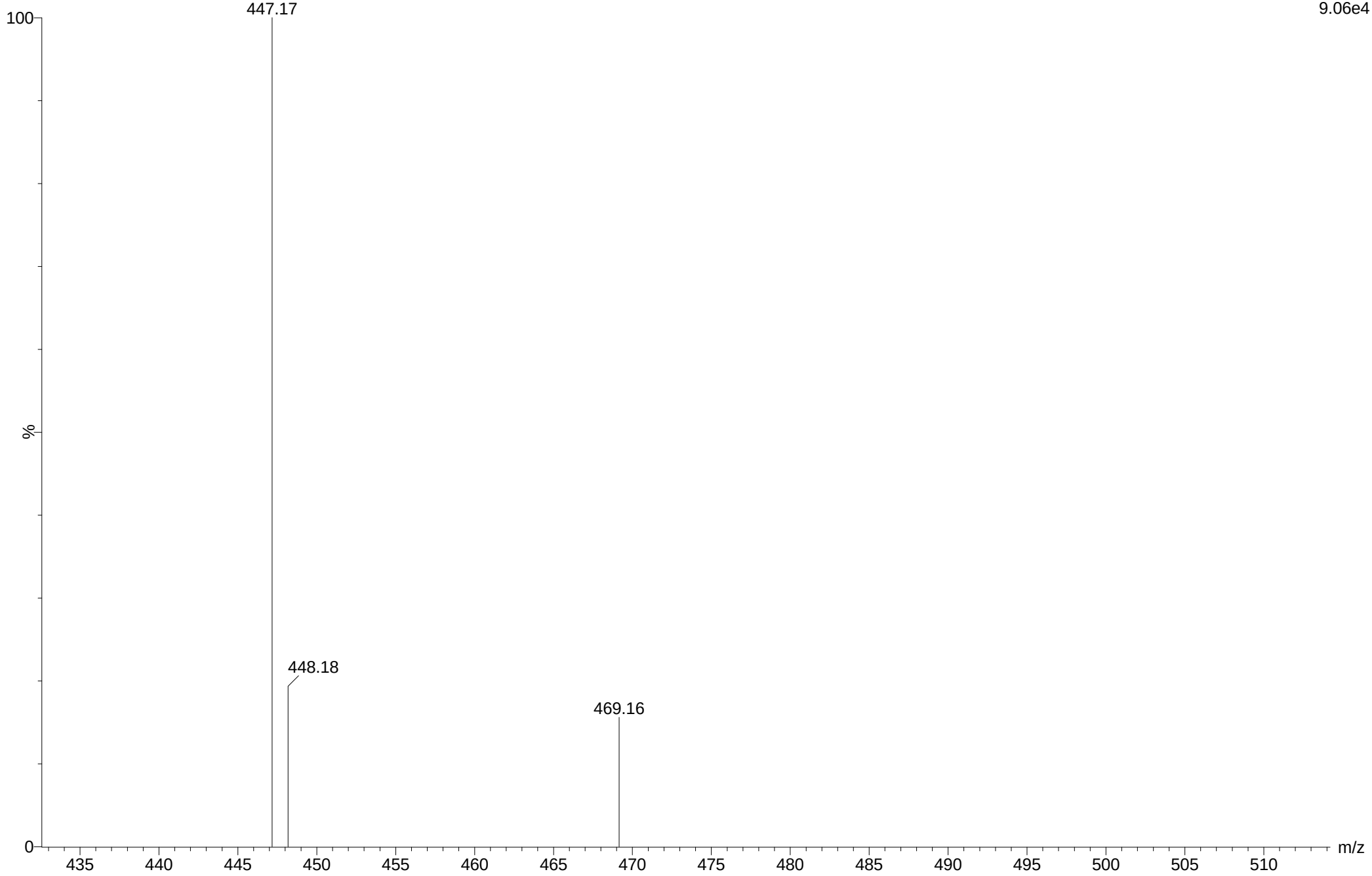
LNB0367-126-P C20H25F3N2O6 MW=446 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 20:09:25
LRC-DXK-3UCAR-ESI-Pos-1 15 (1.078) AM2 (Ar,30000.0,0.00,0.00); ABS 1: TOF MS ES+
2.30e5



LNB0367-126-P C20H25F3N2O6 MW=446 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 20:09:25
LRC-DXK-3UCAR-ESI-Pos-1 15 (1.078) AM2 (Ar,30000.0,0.00,0.00); ABS 1: TOF MS ES+
2.30e5

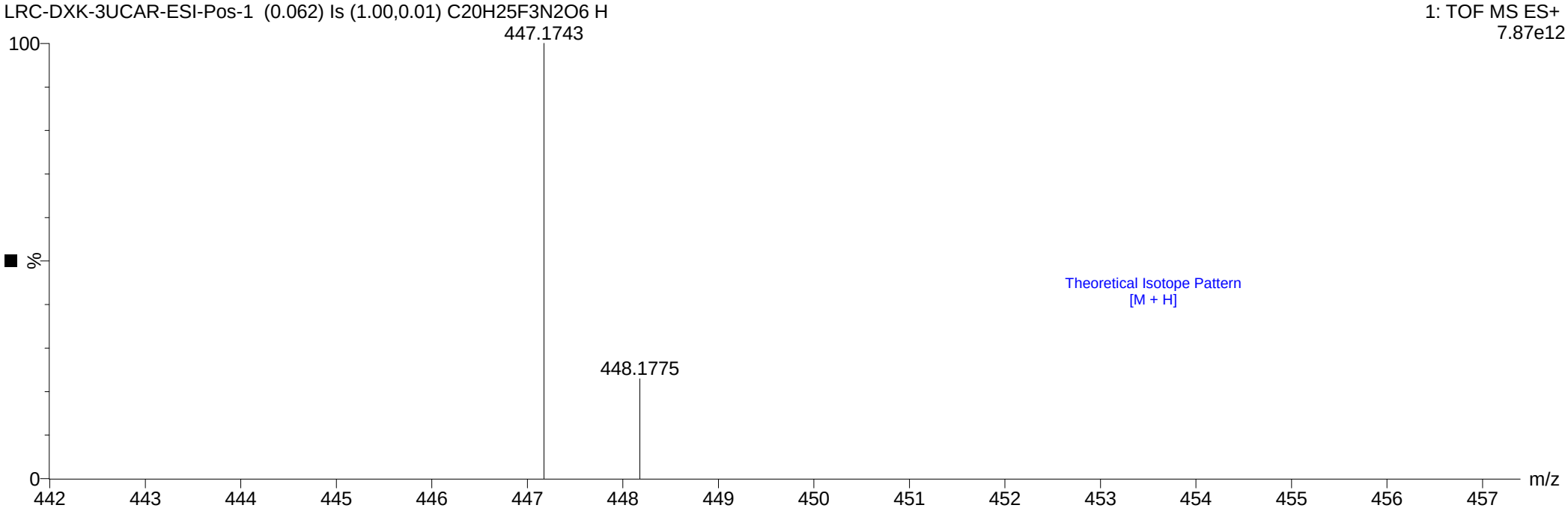


LNB0367-126-P C20H25F3N2O6 MW=446 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 20:09:25
LRC-DXK-3UCAR-ESI-Pos-1 15 (1.078) AM2 (Ar,30000.0,0.00,0.00); ABS 1: TOF MS ES+
9.06e4

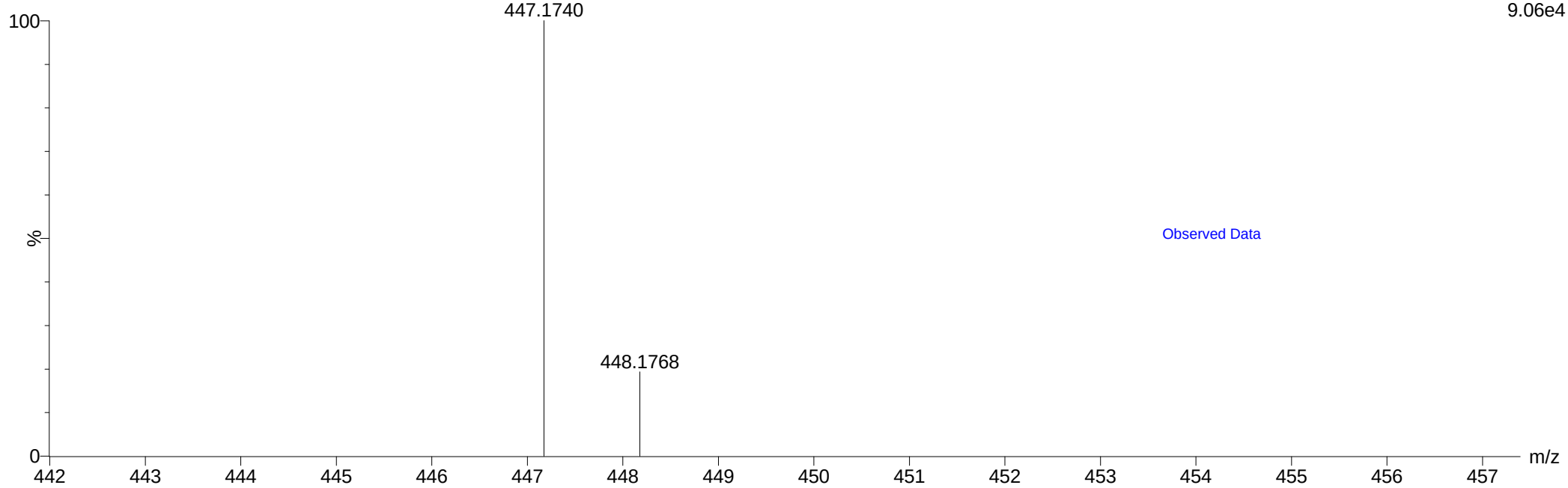


LNB0367-126-P C20H25F3N2O6 MW=446 University of Birmingham, School of Chemistry Daniel Kovari
Methanol Waters Xevo G2-XS 11-Dec-2020 20:09:25

LRC-DXK-3UCAR-ESI-Pos-1 (0.062) Is (1.00,0.01) C20H25F3N2O6 H



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



Single Mass Analysis

Tolerance = 2.0 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
2453 formula(e) evaluated with 6 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 F: 0-3

Minimum:				-10.0				
Maximum:		5.0	2.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
447.1740	447.1741	-0.1	-0.2	11.5	38.5	1.018	36.11	C18 H23 N8 O6
	447.1743	-0.3	-0.7	7.5	39.2	1.746	17.44	C20 H26 N2 O6 F3
	447.1745	-0.5	-1.1	16.5	39.2	1.679	18.66	C24 H21 N6 O F2
	447.1733	0.7	1.6	20.5	39.4	1.919	14.67	C27 H20 N6 F
	447.1732	0.8	1.8	11.5	39.7	2.193	11.16	C23 H25 N2 O5 F2
	447.1749	-0.9	-2.0	23.5	41.4	3.935	1.95	C34 H23 O