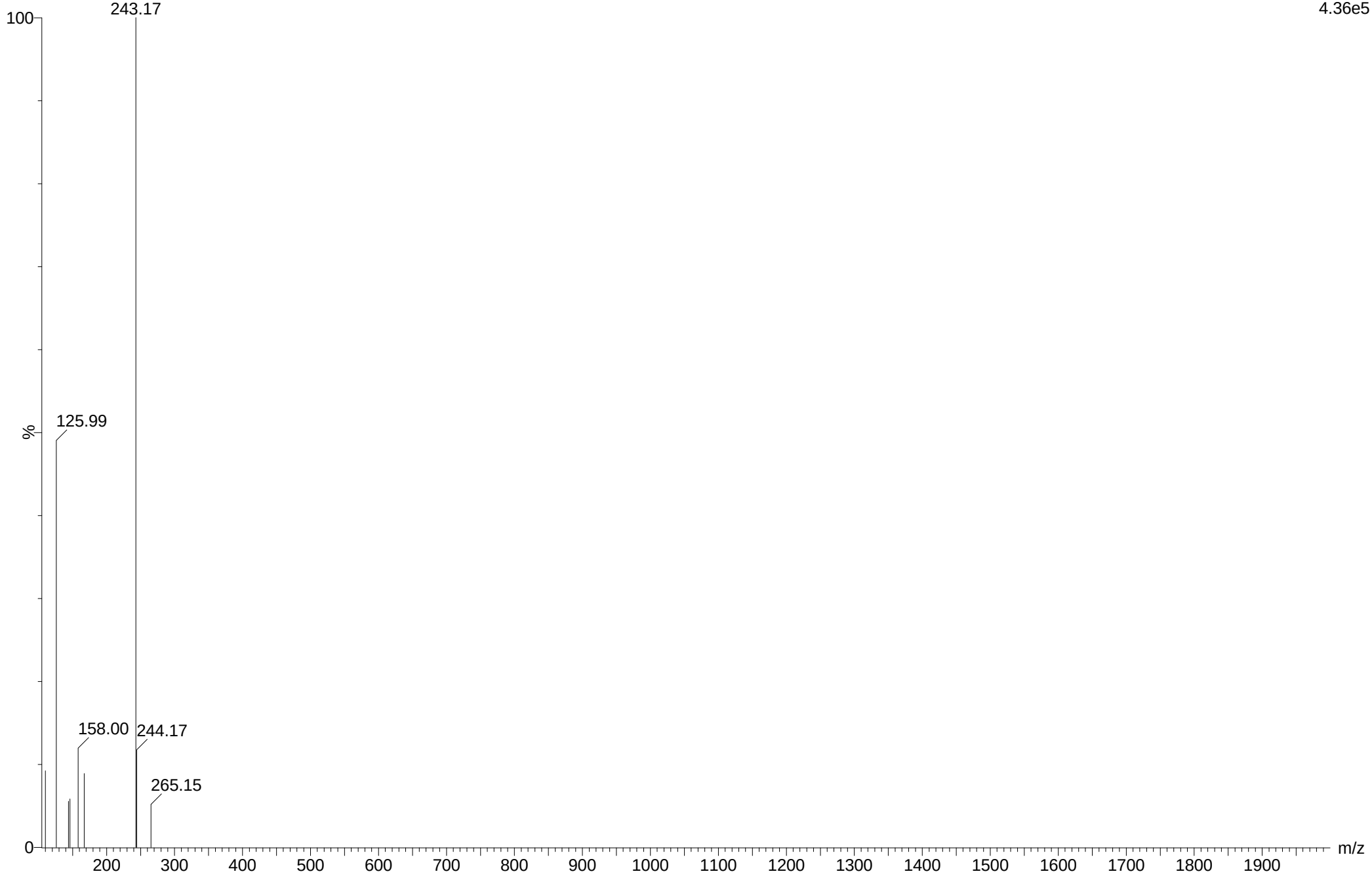
LNB0367-127-P C12H22N2O3 MW=242
Methanol
LRC-DXK-3TRKJ-ESI-Pos-1 7 (0.518) AM2 (Ar,30000.0,0.00,0.00); ABS

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

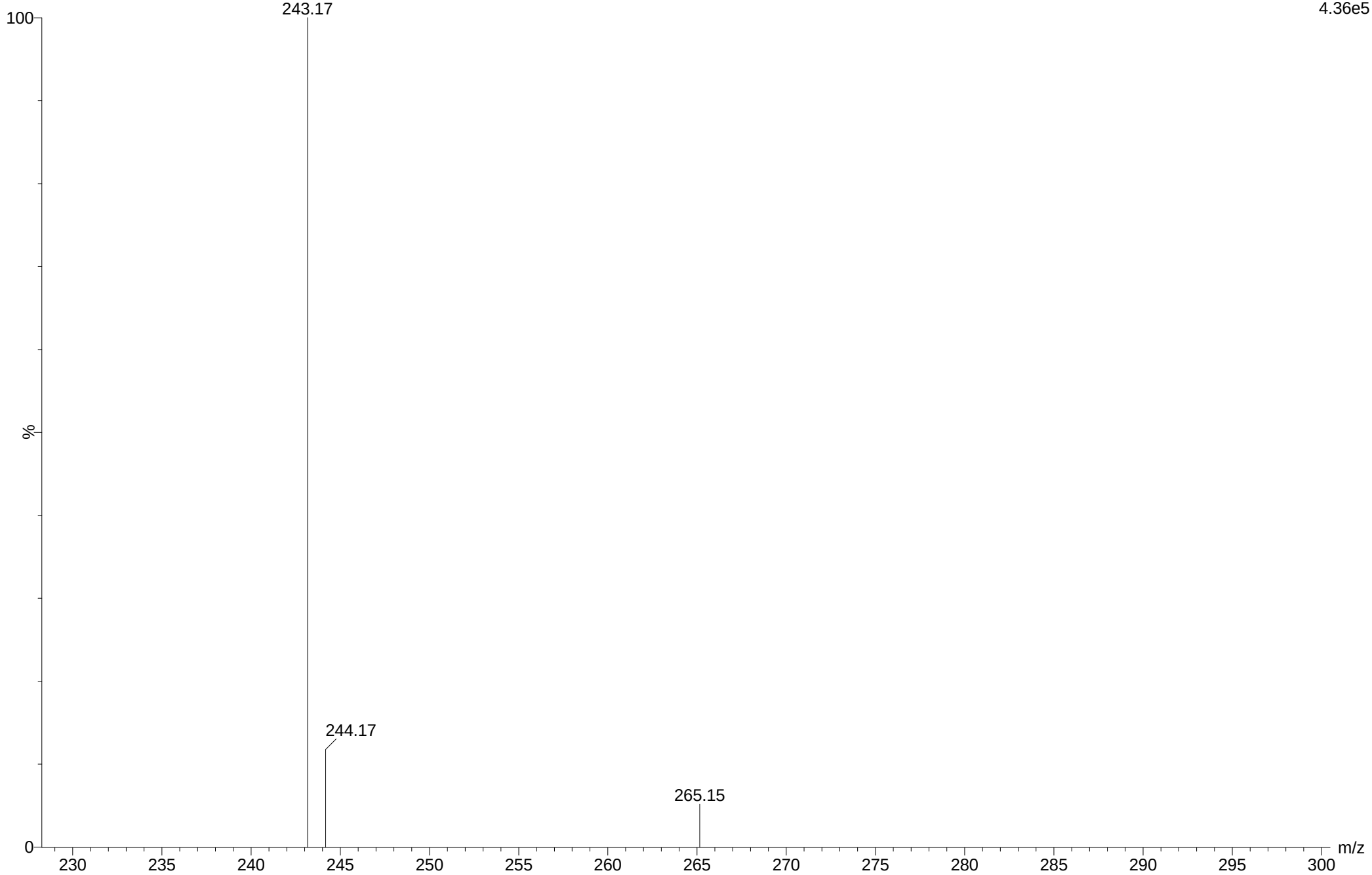
Daniel Kovari
11-Dec-2020 23:58:22
3: TOF MS ES+
4.36e5



LNB0367-127-P C12H22N2O3 MW=242
Methanol
LRC-DXK-3TRKJ-ESI-Pos-1 7 (0.518) AM2 (Ar,30000.0,0.00,0.00); ABS

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3: TOF MS ES+
4.36e5



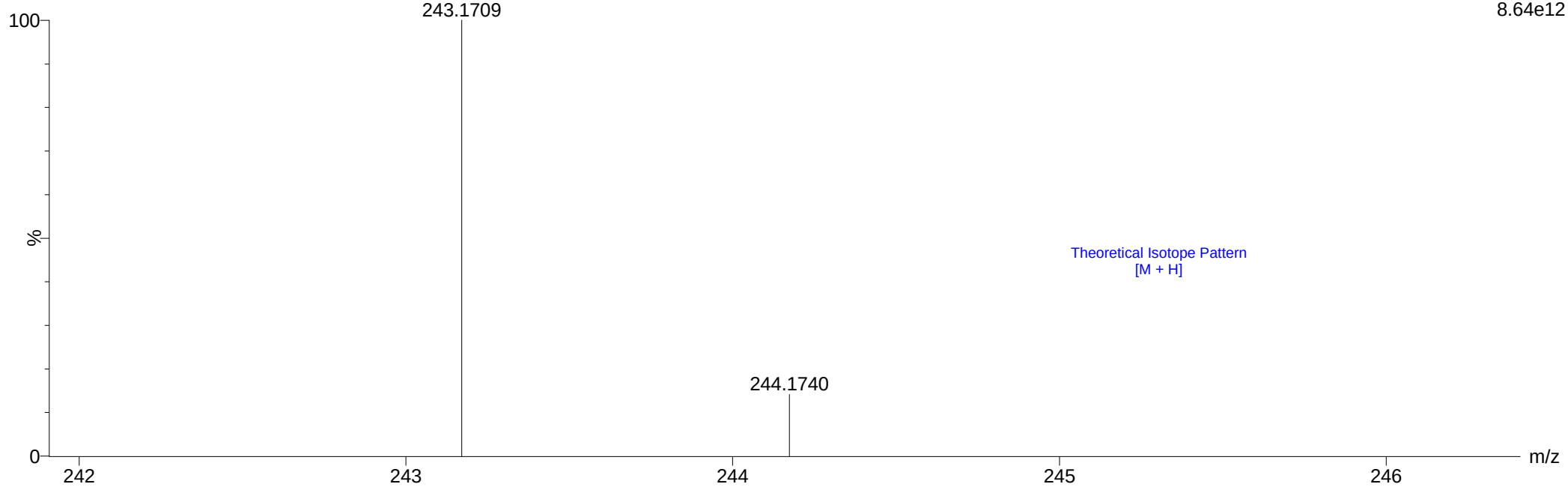
LNB0367-127-P C12H22N2O3 MW=242
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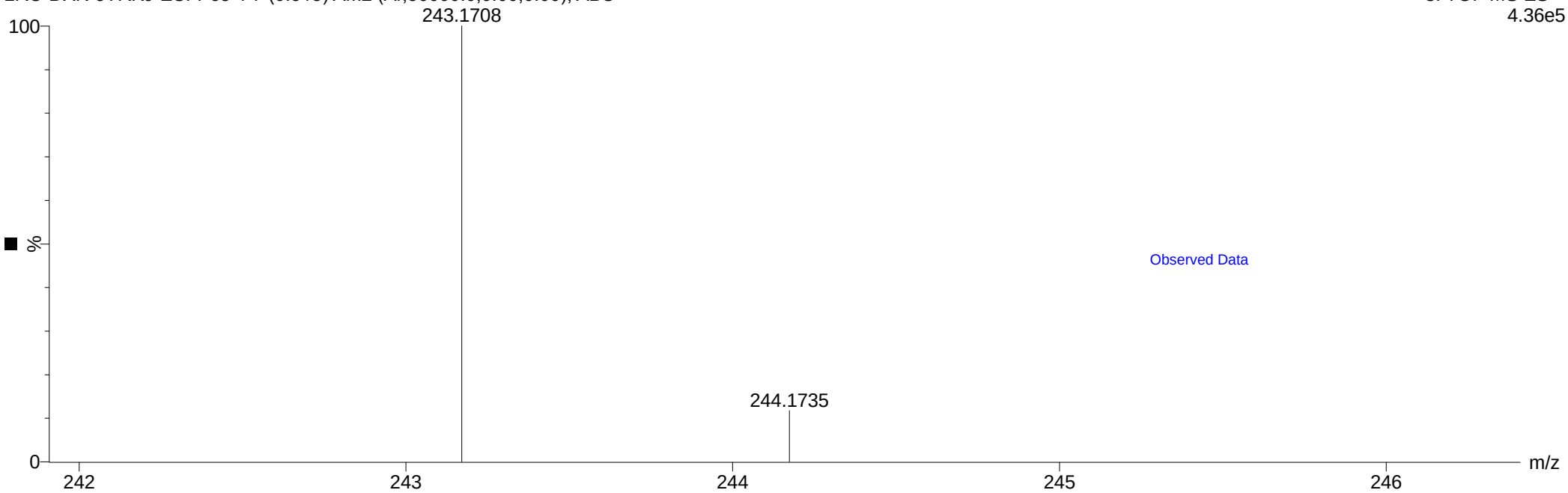
LRC-DXK-3TRKJ-ESI-Pos-1 (0.087) Is (1.00,0.01) C12H22N2O3 H

3: TOF MS ES+
8.64e12



LRC-DXK-3TRKJ-ESI-Pos-1 7 (0.518) AM2 (Ar,30000.0,0.00,0.00); ABS

3: TOF MS ES+
4.36e5



Single Mass Analysis

Tolerance = 10.0 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
1001 formula(e) evaluated with 3 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: 0-2

Minimum:				-10.0				
Maximum:		5.0	10.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
243.1708	243.1709	-0.1	-0.4	2.5	42.2	0.035	96.53	C12 H23 N2 O3
	243.1702	0.6	2.5	-6.5	45.8	3.623	2.67	C4 H27 N4 O5 S
	243.1716	-0.8	-3.3	-1.5	47.0	4.825	0.80	C5 H23 N8 O S