NAT384-652791 C22H33N3O6S MW=468
Methanol:Water

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

Holly Adcock
16-Apr-2021 16:53:35

LRC-HVA-4U99A-ESI-Pos-1 15 (0.871) AM (Cen,3, 50.00, Ar,10000.0,0.00,0.00); Sm (SG, 10x2.00); Cm (15-1:4)

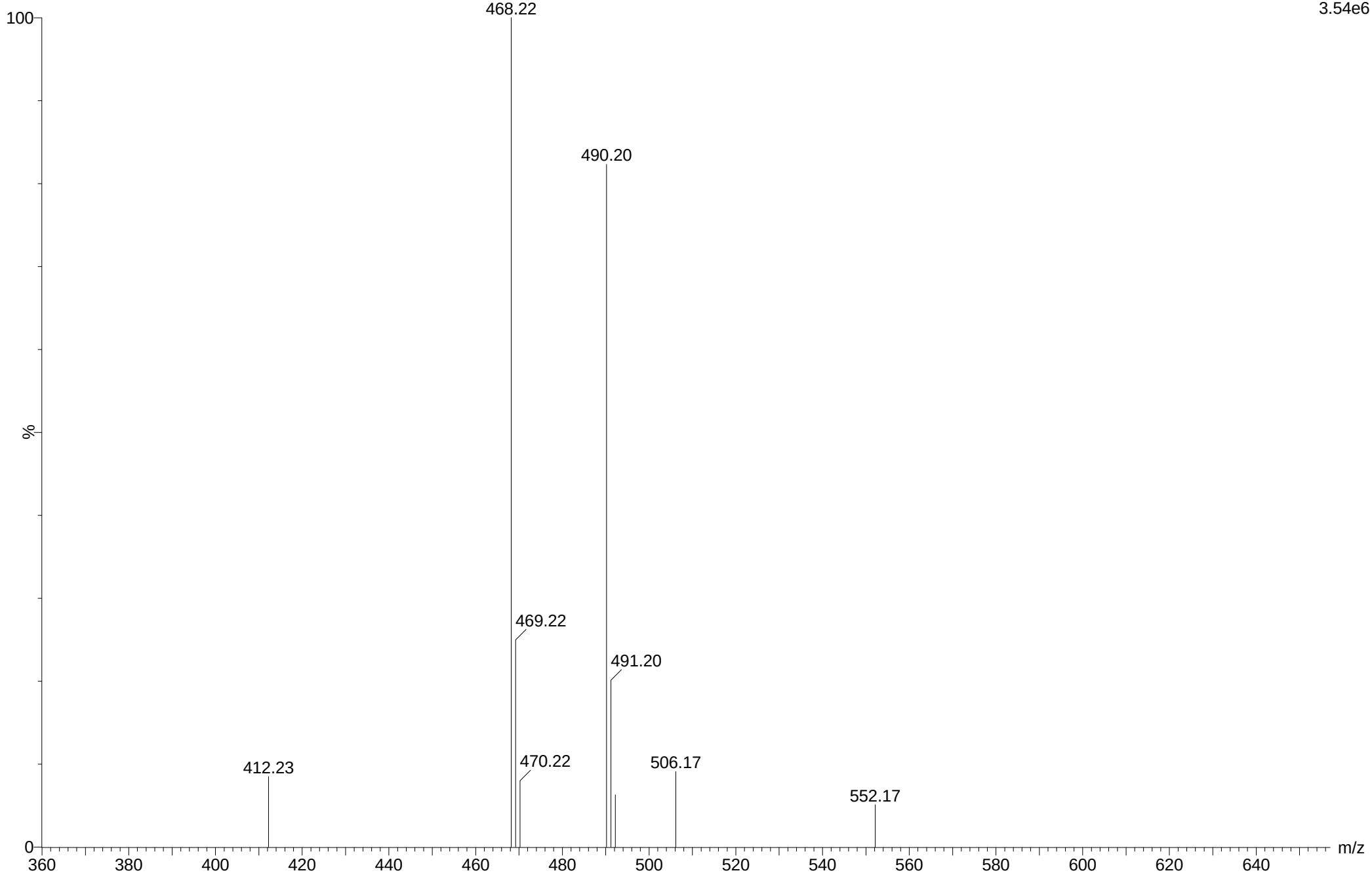
1: TOF MS ES+
3.54e6



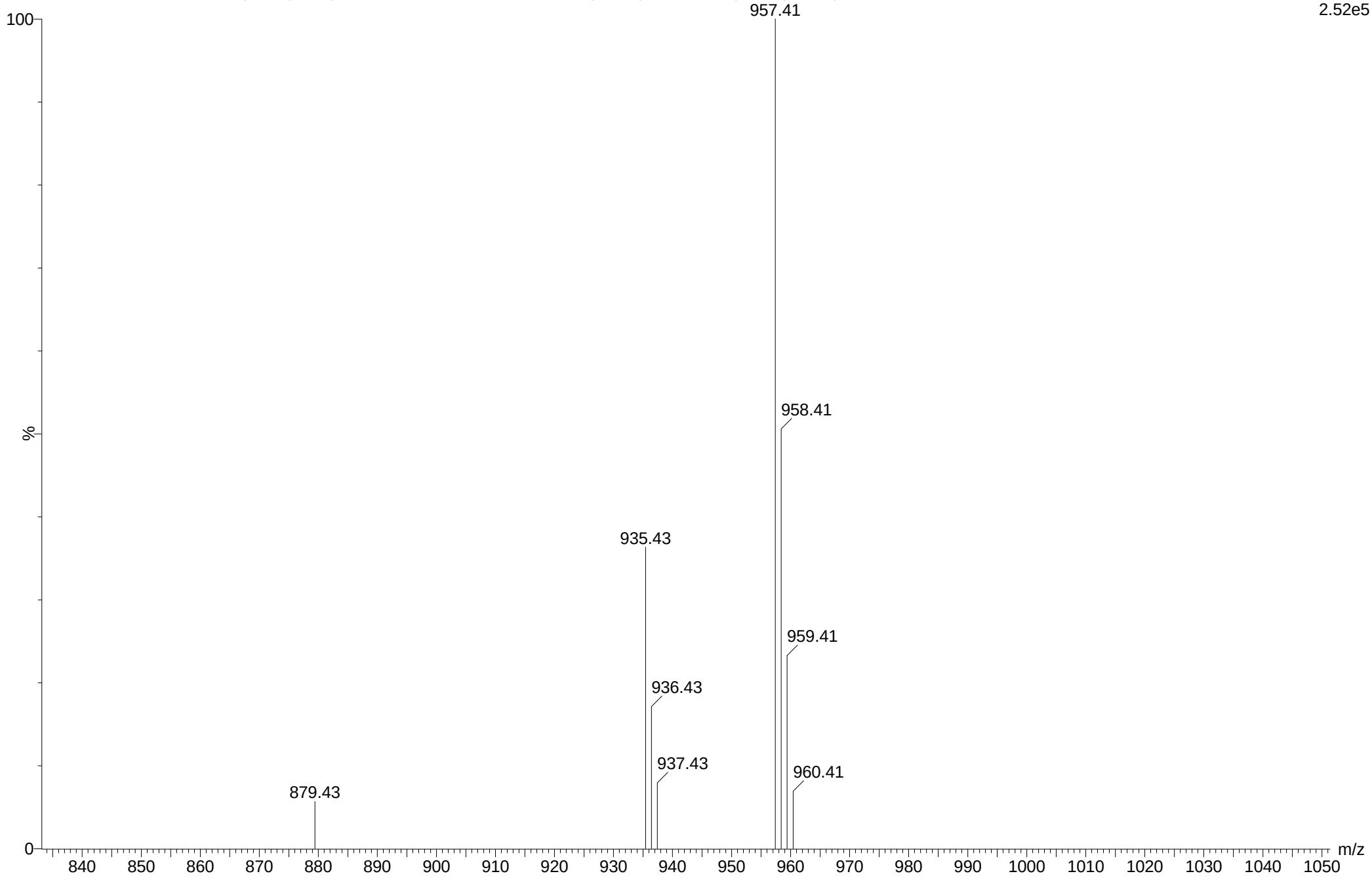
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Methanol:Water Waters Xevo G2-XS 16-Apr-2021 16:53:35
LRC-HVA-4U99A-ESI-Pos-1 15 (0.871) AM (Cen,3, 50.00, Ar,10000.0,0.00,0.00); Sm (SG, 10x2.00); Cm (15-1:4) 1: TOF MS ES+
2.52e5



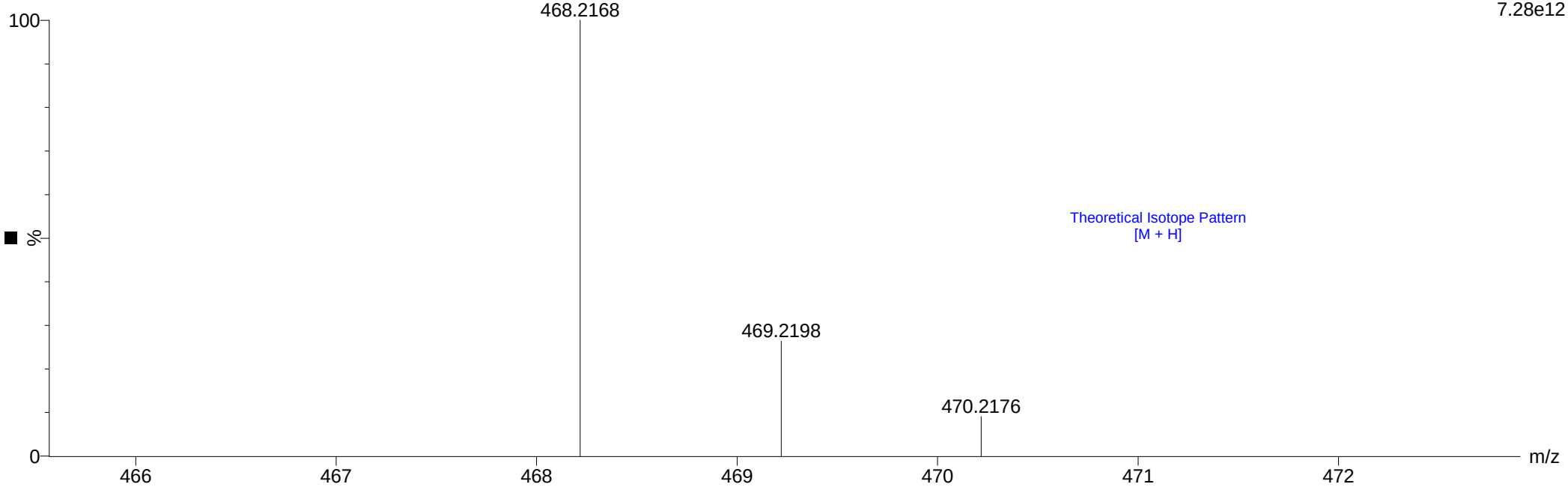
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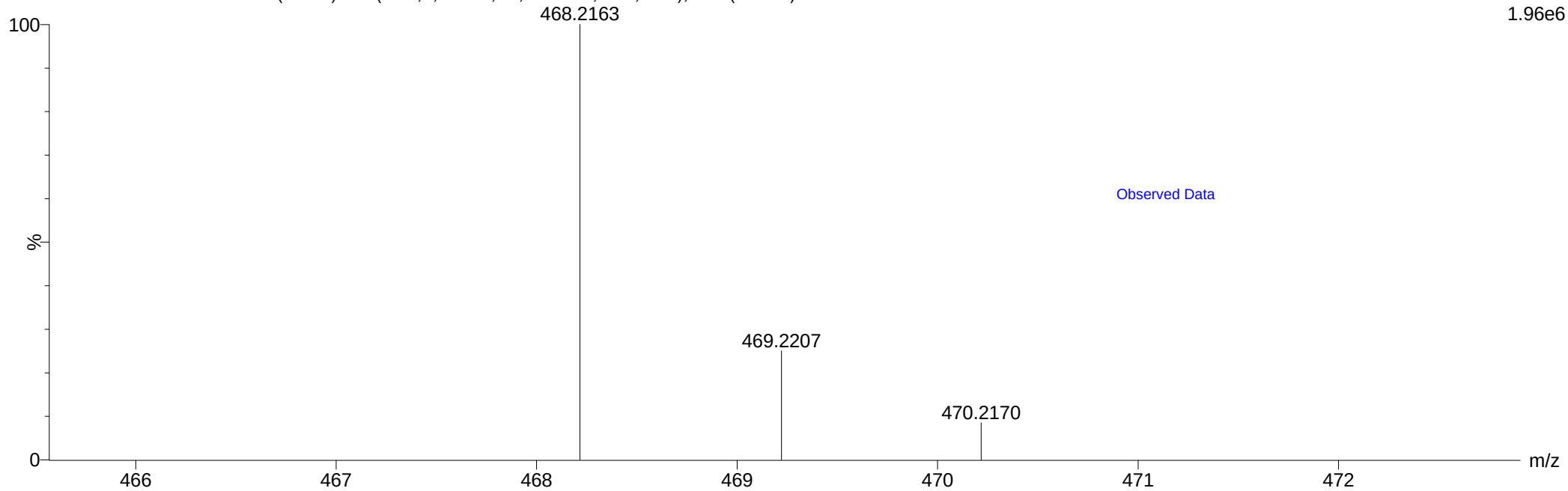
LRC-HVA-4U99A-ESI-Pos-1 (0.290) Is (1.00,0.01) C22H33N3O6S H

2: TOF MS ES+
7.28e12



LRC-HVA-4U99A-ESI-Pos-1 15 (0.879) AM (Cen,3, 50.00, Ar,10000.0,0.00,0.00); Cm (15-1:4)

2: TOF MS ES+
1.96e6



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
1757 formula(e) evaluated with 5 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
468.2163	468.2162	0.1	0.2	-1.5	35.7	9.960	0.00	C14 H38 N5 O8 S2
	468.2166	-0.3	-0.6	4.5	38.7	12.975	0.00	C14 H30 N9 O9
	468.2168	-0.5	-1.1	7.5	25.7	0.000	99.98	C22 H34 N3 O6 S
	468.2175	-1.2	-2.6	16.5	39.2	13.438	0.00	C30 H30 N O4
	468.2175	-1.2	-2.6	3.5	34.6	8.815	0.01	C15 H34 N9 O4 S2