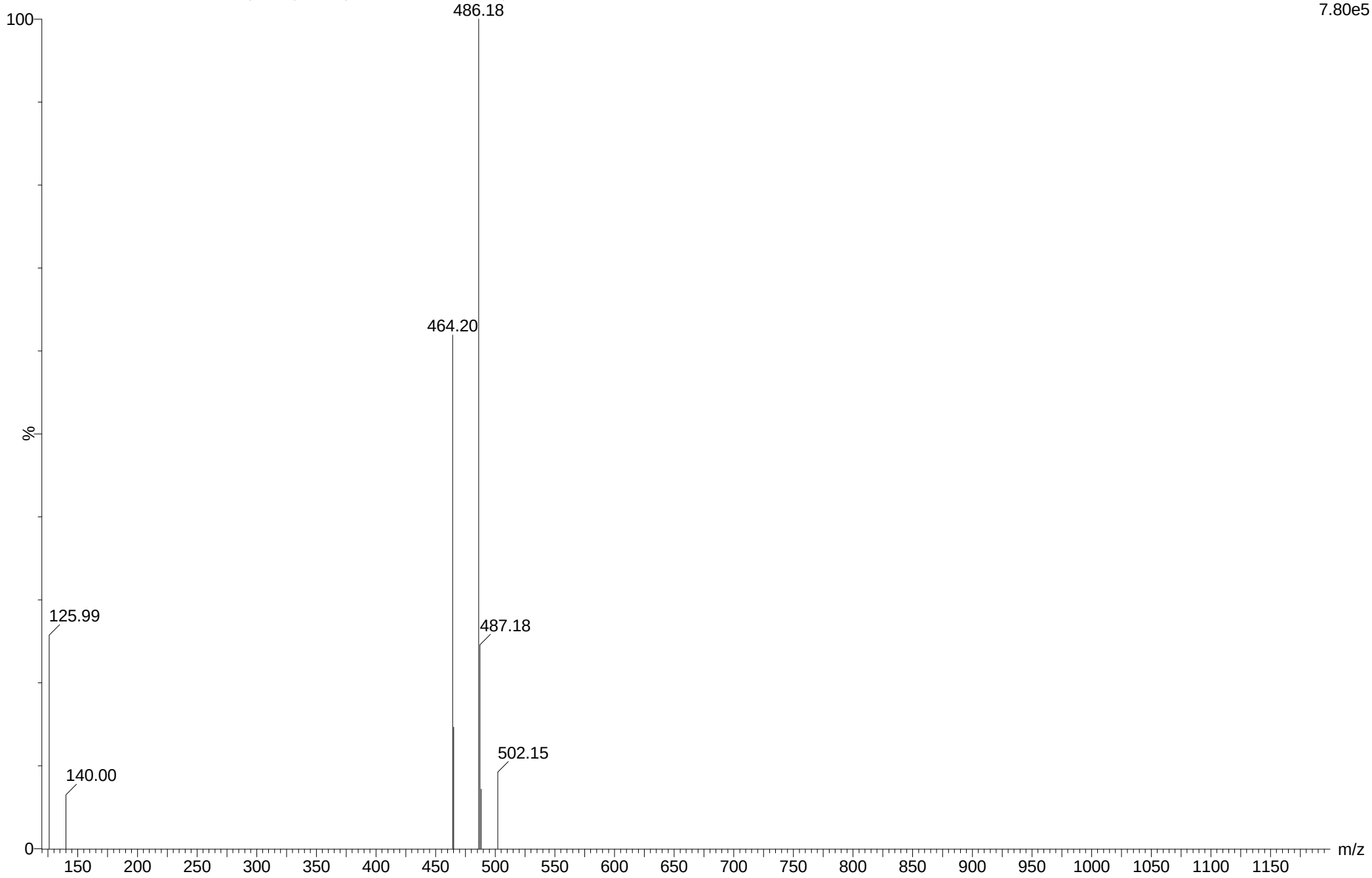
NAT384-652914 C21H29N5O5S MW=464
Methanol:Water
LRC-HVA-4AURX-ESI-Pos-1 29 (1.250) AM2 (Ar,27500.0,0.00,0.00); ABS

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

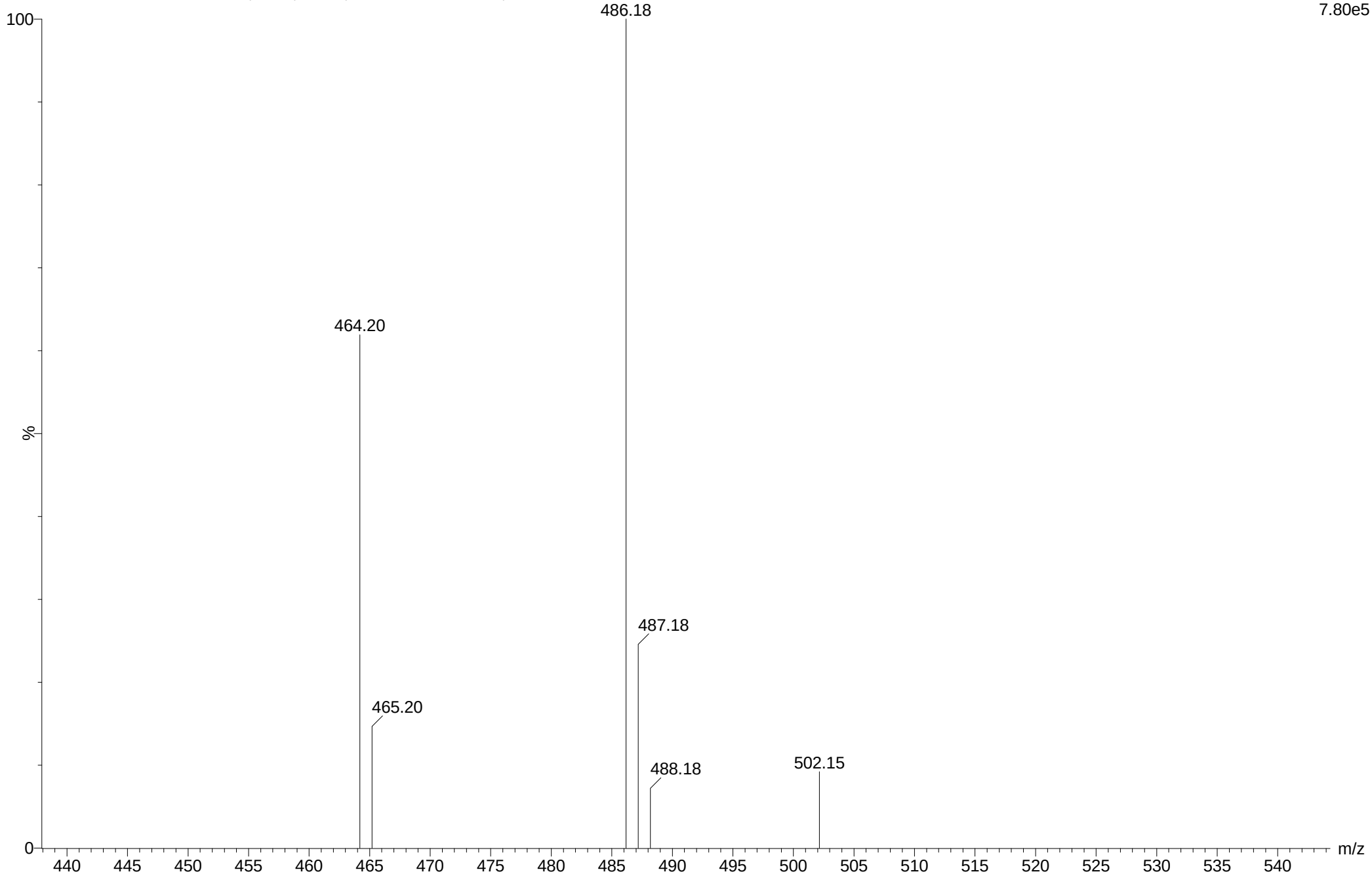
Holly Adcock
16-Apr-2021 15:12:14
2: TOF MS ES+
7.80e5



NAT384-652914 C21H29N5O5S MW=464
Methanol:Water
LRC-HVA-4AURX-ESI-Pos-1 29 (1.250) AM2 (Ar,27500.0,0.00,0.00); ABS

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

Holly Adcock
16-Apr-2021 15:12:14
2: TOF MS ES+
7.80e5



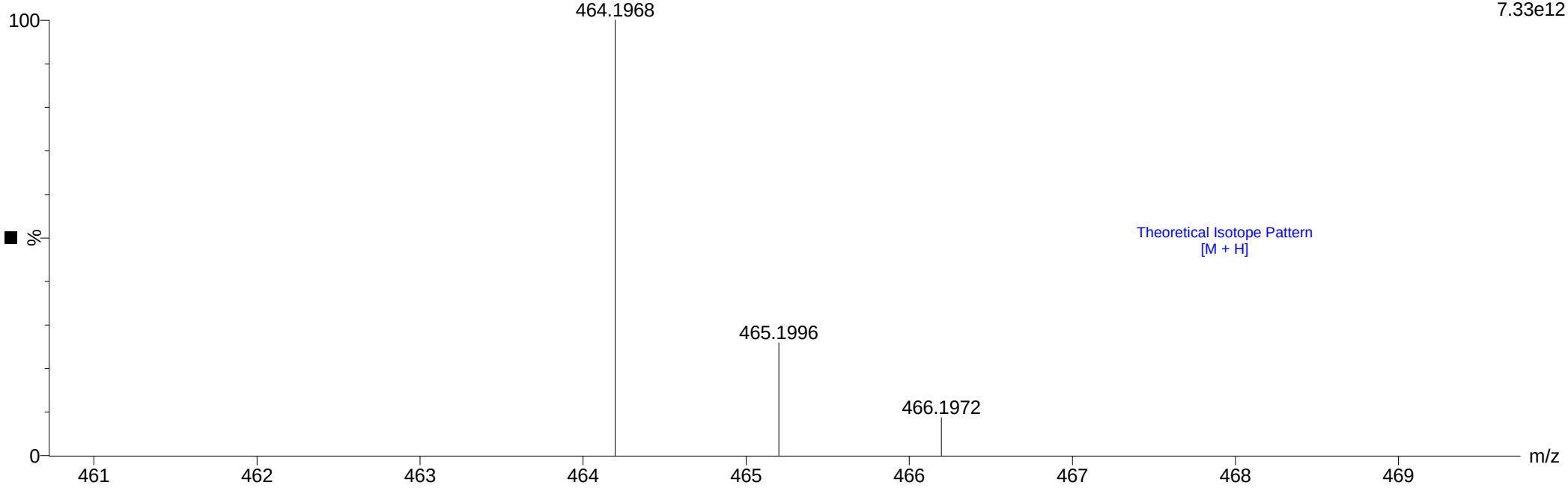
NAT384-652914 C21H29N5O5S MW=464
Methanol:Water

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

Holly Adcock
16-Apr-2021 15:12:14

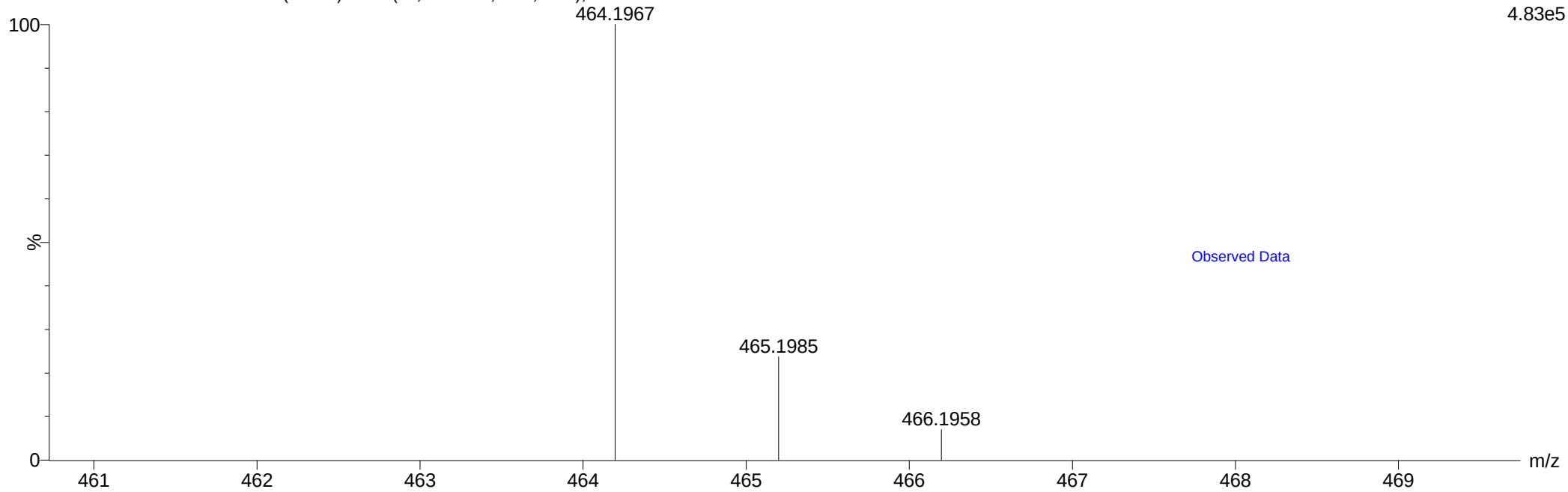
LRC-HVA-4AURX-ESI-Pos-1 (0.070) Is (1.00,0.01) C21H29N5O5S H

2: TOF MS ES+
7.33e12



LRC-HVA-4AURX-ESI-Pos-1 29 (1.250) AM2 (Ar,27500.0,0.00,0.00); ABS

2: TOF MS ES+
4.83e5



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
1741 formula(e) evaluated with 4 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
464.1967	464.1968	-0.1	-0.2	9.5	25.2	0.578	56.08	C21 H30 N5 O5 S
	464.1961	0.6	1.3	0.5	30.0	5.367	0.47	C13 H34 N7 O7 S2
	464.1974	-0.7	-1.5	18.5	35.2	10.523	0.00	C29 H26 N3 O3
	464.1954	1.3	2.8	4.5	25.5	0.834	43.45	C20 H34 N O9 S