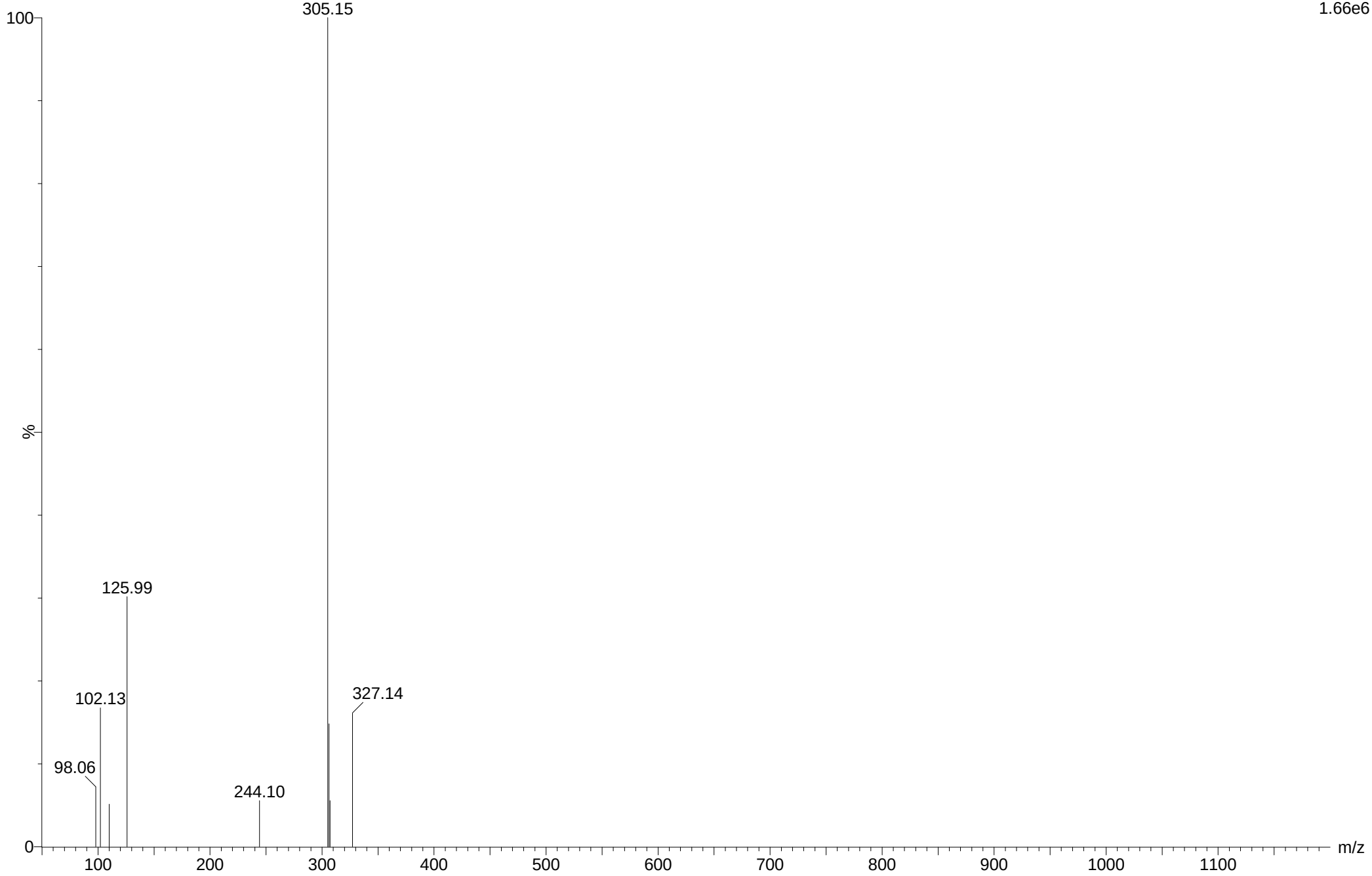
NAT384-652766 C13H24N2O4S MW=304
Methanol:Water
LRC-HVA-4TTTF-ESI-Pos-1 19 (1.037) AM2 (Ar,27500.0,0.00,0.00); ABS

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

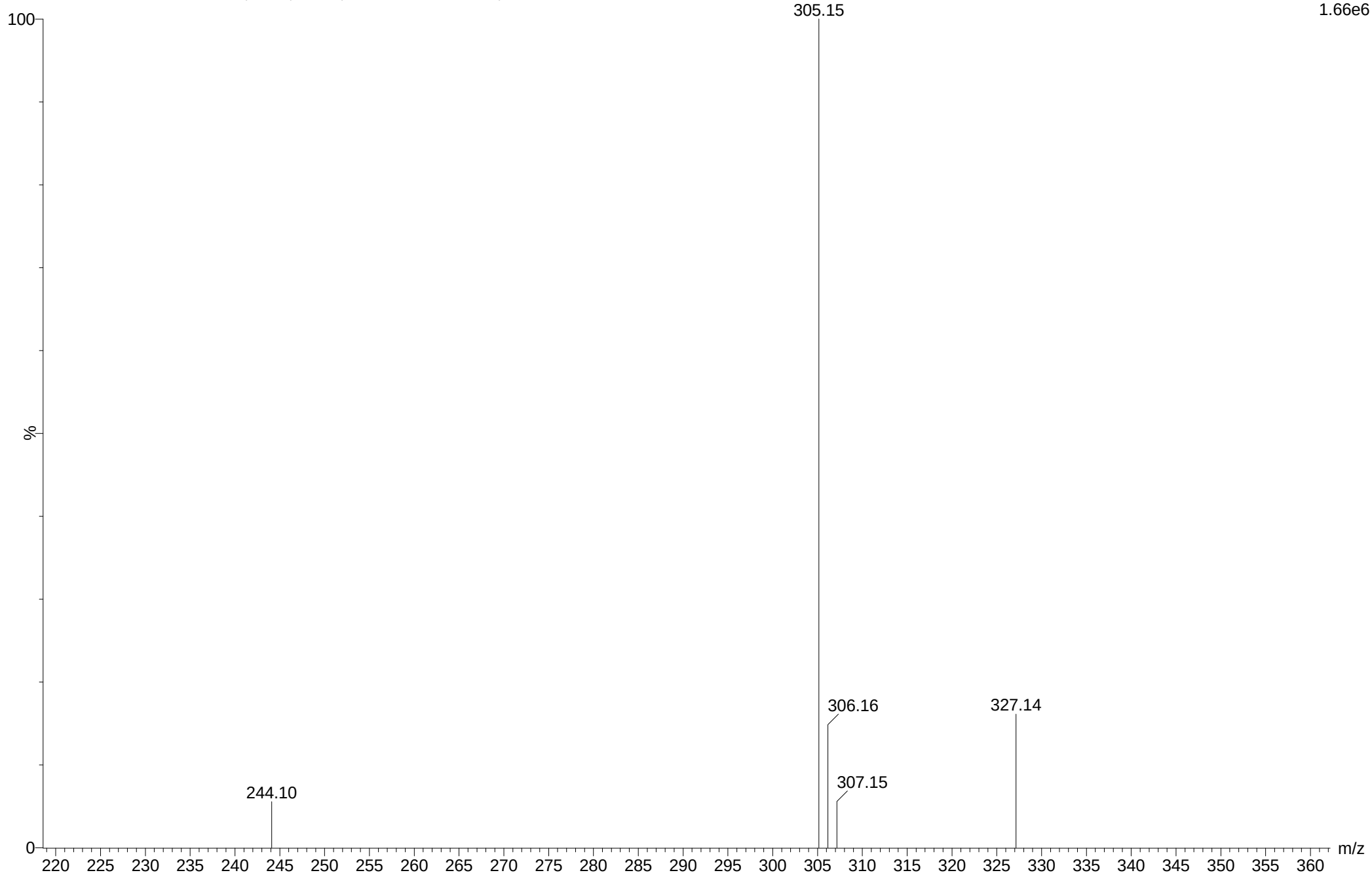
Holly Adcock
16-Apr-2021 14:04:23
3: TOF MS ES+
1.66e6



NAT384-652766 C13H24N2O4S MW=304
Methanol:Water
LRC-HVA-4TTTF-ESI-Pos-1 19 (1.037) AM2 (Ar,27500.0,0.00,0.00); ABS

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

Holly Adcock
16-Apr-2021 14:04:23
3: TOF MS ES+
1.66e6



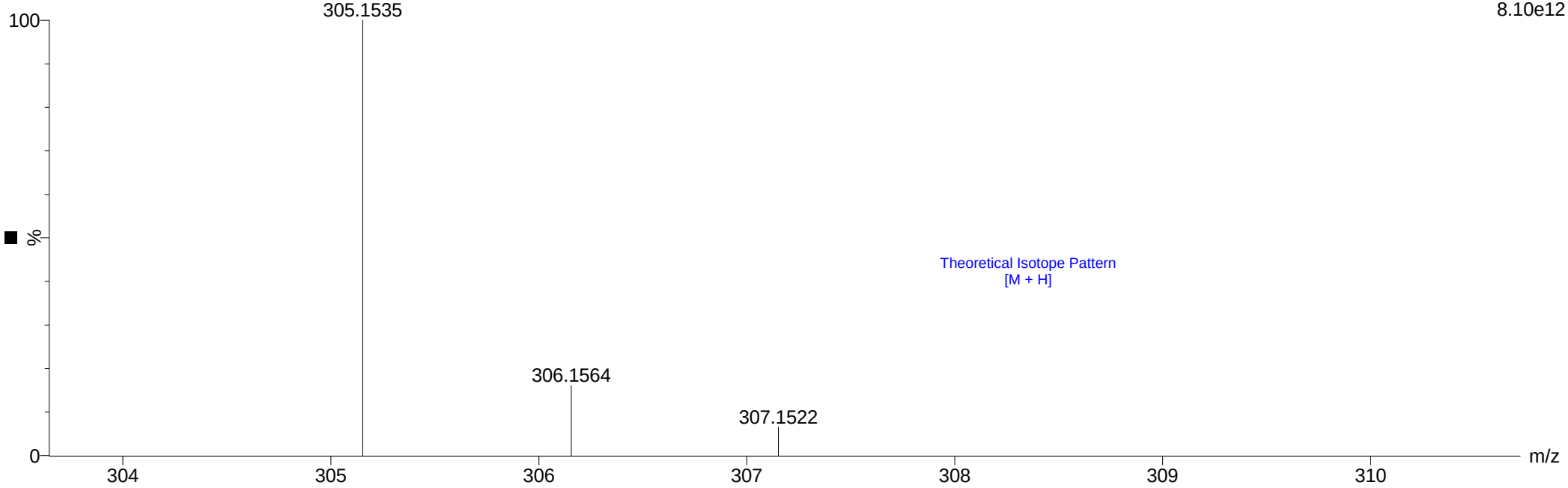
NAT384-652766 C13H24N2O4S MW=304
Methanol:Water

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

Holly Adcock
16-Apr-2021 14:04:23

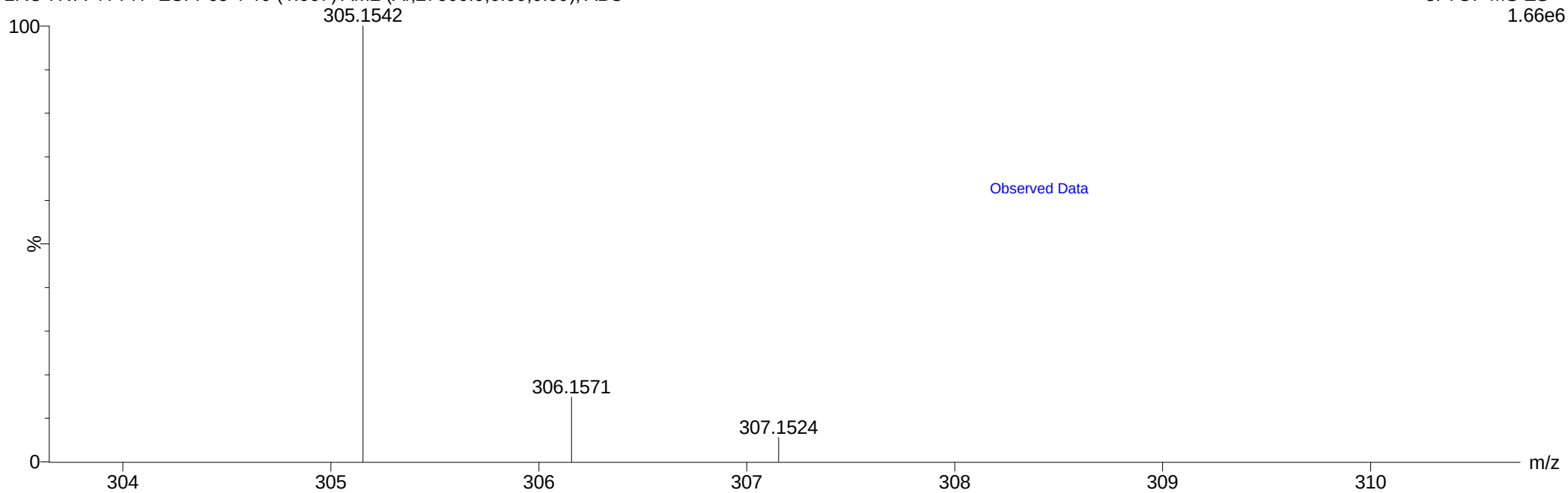
LRC-HVA-4TTTF-ESI-Pos-1 (0.087) Is (1.00,0.01) C13H24N2O4S H

3: TOF MS ES+
8.10e12



LRC-HVA-4TTTF-ESI-Pos-1 19 (1.037) AM2 (Ar,27500.0,0.00,0.00); ABS

3: TOF MS ES+
1.66e6



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
1126 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
305.1542	305.1542	0.0	0.0	11.5	40.7	16.185	0.00	C21 H21 O2
	305.1542	0.0	0.0	-1.5	34.5	10.001	0.00	C6 H25 N8 O2 S2
	305.1548	-0.6	-2.0	7.5	26.6	2.089	12.38	C14 H21 N6 S
	305.1535	0.7	2.3	2.5	24.6	0.132	87.61	C13 H25 N2 O4 S
	305.1533	0.9	2.9	-0.5	39.7	15.169	0.00	C5 H21 N8 O7