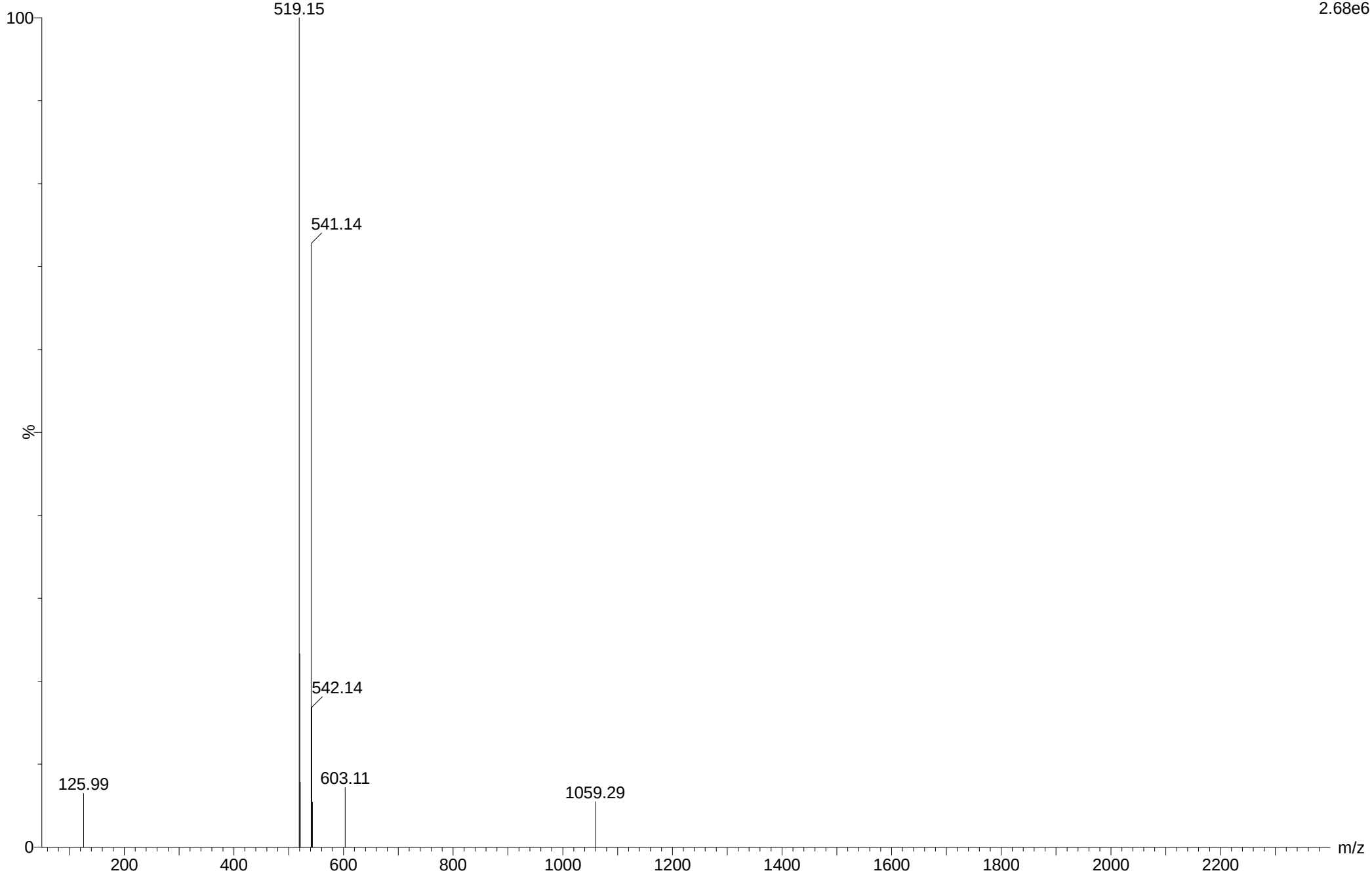
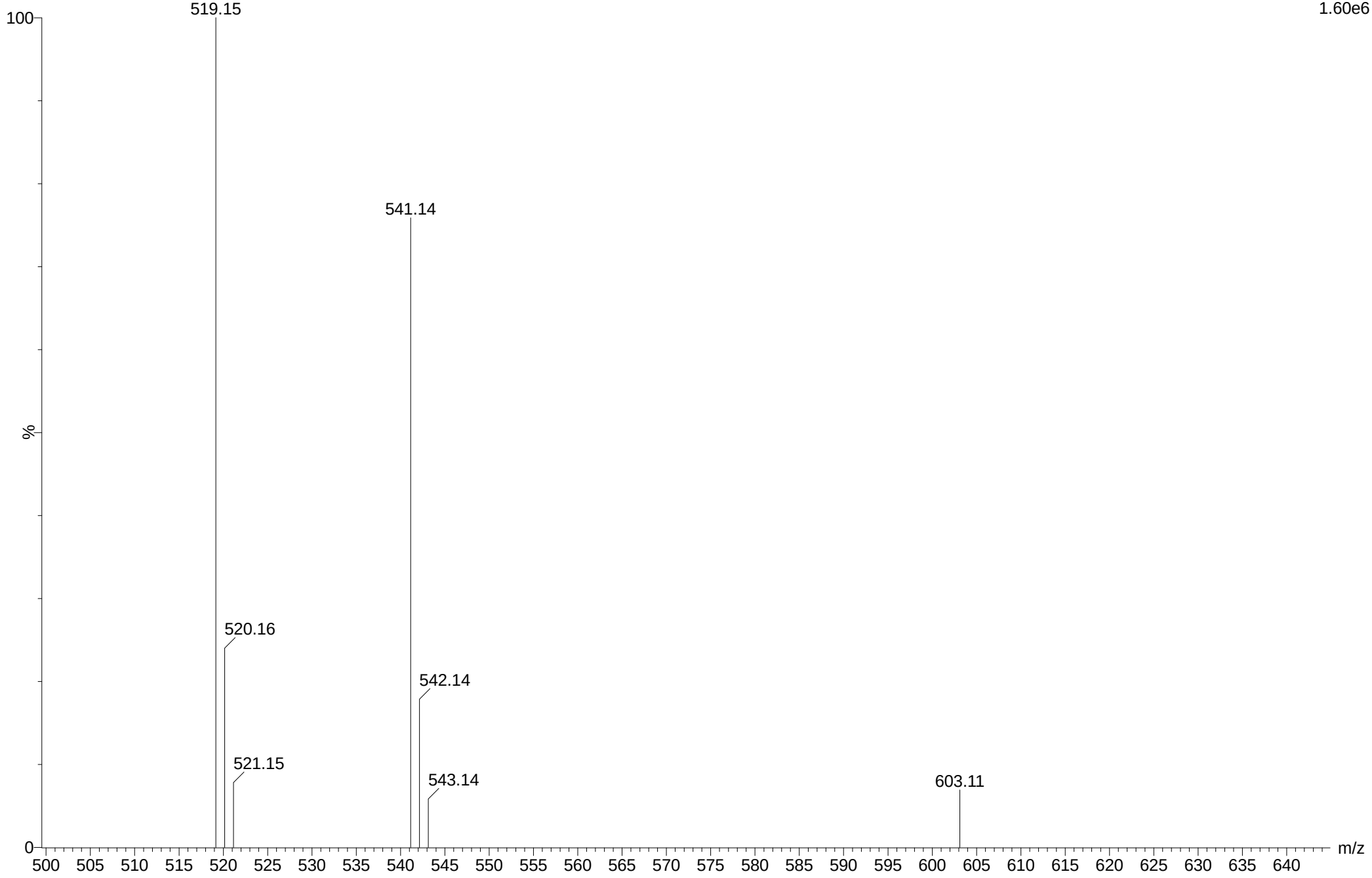
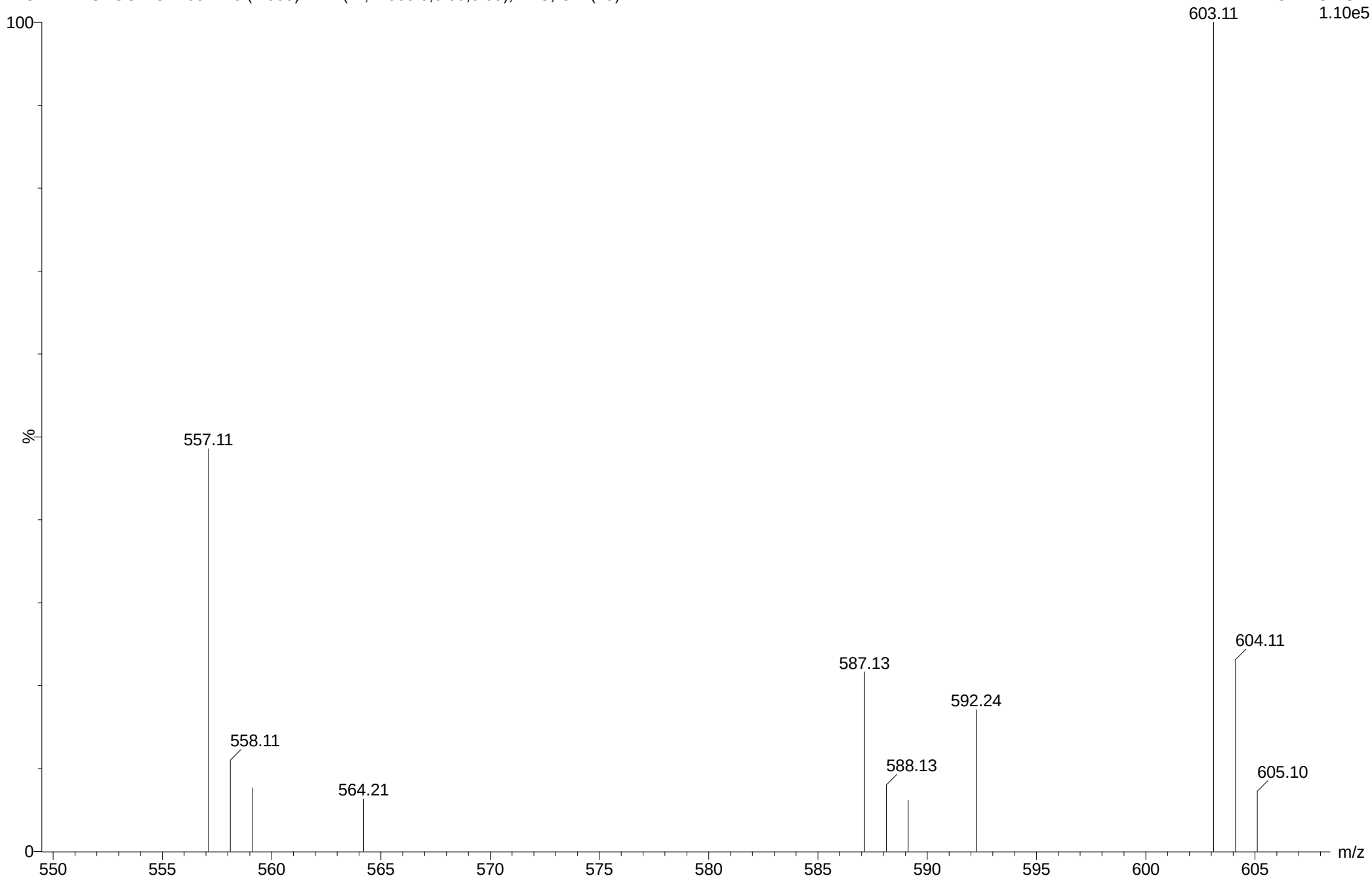
NAT384-652872 C21H25F3N4O6S MW=519 University of Birmingham, School of Chemistry Holly Adcock
Methanol:Water Waters Xevo G2-XS 16-Apr-2021 16:22:30
LRC-HVA-4UEUC-ESI-Pos-1 19 (1.044) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (19) 1: TOF MS ES+
2.68e6



NAT384-652872 C21H25F3N4O6S MW=519 University of Birmingham, School of Chemistry Holly Adcock
Methanol:Water Waters Xevo G2-XS 16-Apr-2021 16:22:30
LRC-HVA-4UEUC-ESI-Pos-1 19 (1.053) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (19) 2: TOF MS ES+
1.60e6



NAT384-652872 C21H25F3N4O6S MW=519 University of Birmingham, School of Chemistry Holly Adcock
Methanol:Water Waters Xevo G2-XS 16-Apr-2021 16:22:30
LRC-HVA-4UEUC-ESI-Pos-1 19 (1.053) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (19) 2: TOF MS ES+



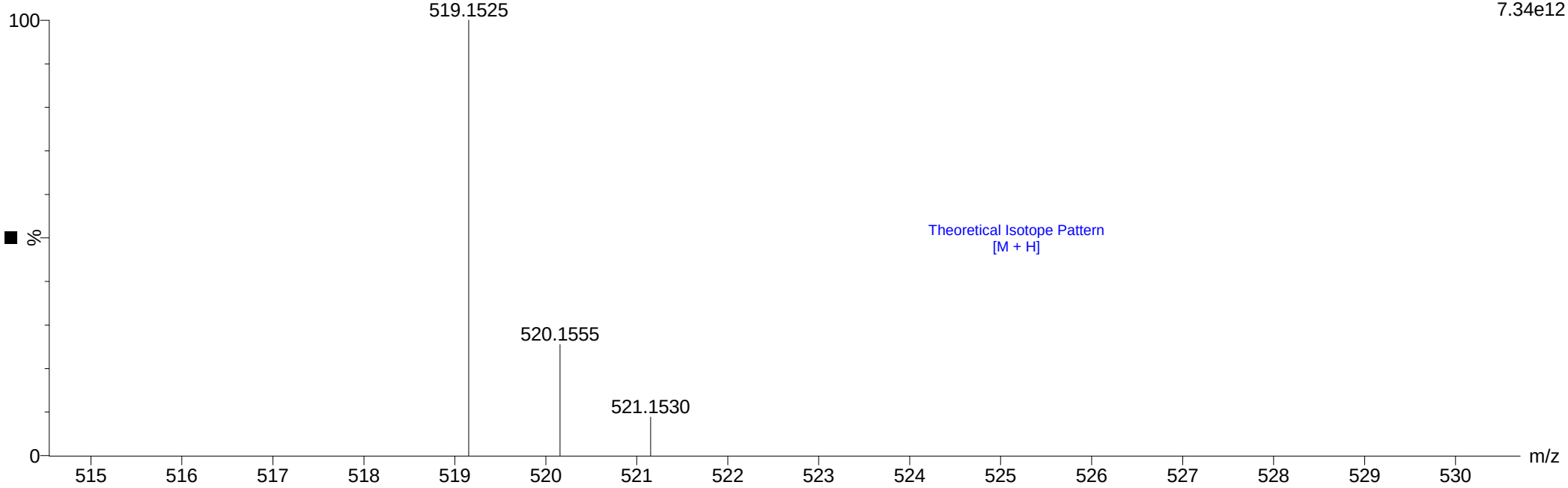
NAT384-652872 C21H25F3N4O6S MW=519
Methanol:Water

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

Holly Adcock
16-Apr-2021 16:22:30

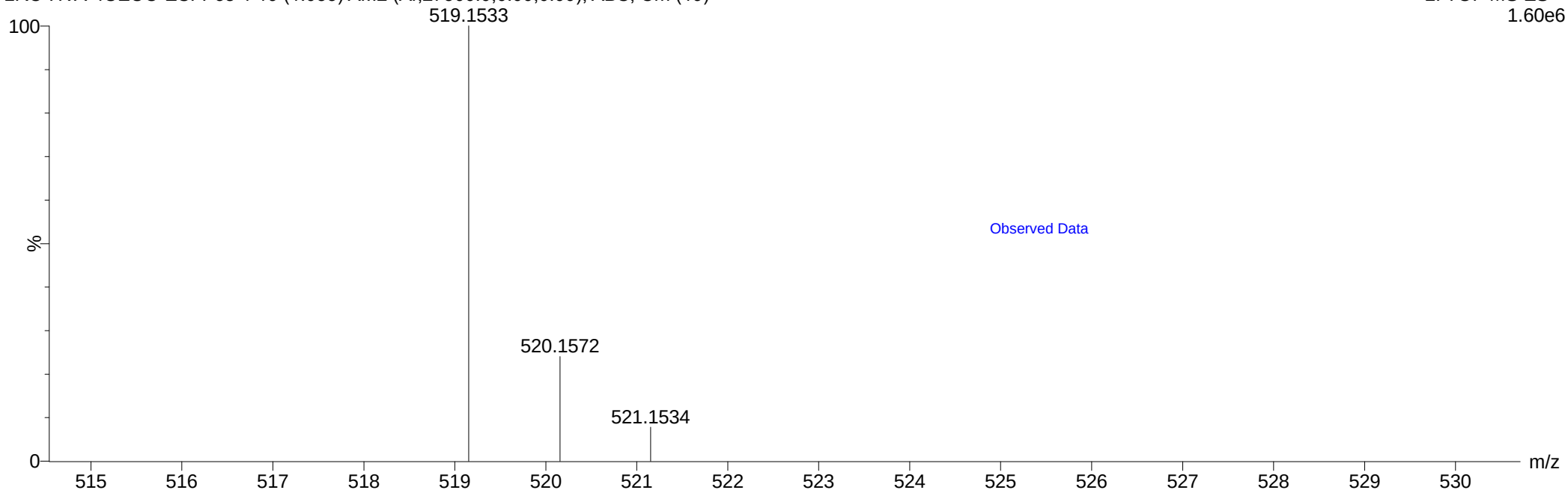
LRC-HVA-4UEUC-ESI-Pos-1 (0.290) Is (1.00,0.01) C21H25F3N4O6S H

2: TOF MS ES+
7.34e12



LRC-HVA-4UEUC-ESI-Pos-1 19 (1.053) AM2 (Ar,27500.0,0.00,0.00); ABS; Cm (19)

2: TOF MS ES+
1.60e6



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
6910 formula(e) evaluated with 27 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 F: 1-4

Minimum:				-4.0				
Maximum:		3.0	3.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
519.1533	519.1534	-0.1	-0.2	9.5	26.9	1.884	15.20	C16 H24 N10 O7 S F
	519.1532	0.1	0.2	5.5	34.3	9.230	0.01	C14 H26 N10 O4 S2 F3
	519.1532	0.1	0.2	18.5	38.3	13.314	0.00	C29 H22 N2 O4 F3
	519.1534	-0.1	-0.2	3.5	31.5	6.518	0.15	C20 H33 O9 S2 F2
	519.1535	-0.2	-0.4	2.5	38.8	13.818	0.00	C10 H23 N10 O10 F4
	519.1536	-0.3	-0.6	12.5	31.8	6.777	0.11	C24 H28 N4 O4 S2 F
	519.1530	0.3	0.6	-3.5	35.8	10.788	0.00	C10 H31 N6 O9 S2 F4
	519.1537	-0.4	-0.8	5.5	25.4	0.374	68.79	C18 H27 N4 O7 S F4
	519.1527	0.6	1.2	13.5	36.0	11.015	0.00	C23 H24 N4 O9 F
	519.1539	-0.6	-1.2	14.5	28.8	3.823	2.19	C22 H22 N8 O2 S F3
	519.1527	0.6	1.2	18.5	32.0	7.019	0.09	C25 H21 N8 O S F2
	519.1539	-0.6	-1.2	9.5	36.1	11.094	0.00	C20 H25 N4 O10 F2
	519.1525	0.8	1.5	9.5	27.1	2.053	12.83	C21 H26 N4 O6 S F3
	519.1541	-0.8	-1.5	18.5	37.2	12.223	0.00	C24 H20 N8 O5 F
	519.1543	-1.0	-1.9	14.5	37.7	12.648	0.00	C26 H23 N2 O5 F4
	519.1543	-1.0	-1.9	1.5	34.8	9.764	0.01	C11 H27 N10 O5 S2 F4
	519.1543	-1.0	-1.9	21.5	36.0	10.976	0.00	C32 H24 N2 O2 S F
	519.1523	1.0	1.9	7.5	33.4	8.422	0.02	C23 H32 O8 S2 F
	519.1523	1.0	1.9	6.5	37.8	12.792	0.00	C13 H22 N10 O9 F3
	519.1545	-1.2	-2.3	-0.5	32.3	7.254	0.07	C17 H34 O10 S2 F3
	519.1521	1.2	2.3	9.5	34.8	9.730	0.01	C17 H25 N10 O3 S2 F2
	519.1545	-1.2	-2.3	23.5	39.3	14.244	0.00	C30 H18 N6 F3
	519.1546	-1.3	-2.5	5.5	30.5	5.442	0.43	C13 H25 N10 O8 S F2
	519.1520	1.3	2.5	22.5	39.1	14.071	0.00	C32 H21 N2 O3 F2
	519.1547	-1.4	-2.7	8.5	32.1	7.105	0.08	C21 H29 N4 O5 S2 F2
	519.1519	1.4	2.7	0.5	35.9	10.854	0.00	C13 H30 N6 O8 S2 F3
	519.1518	1.5	2.9	18.5	34.5	9.521	0.01	C30 H23 N2 S F4