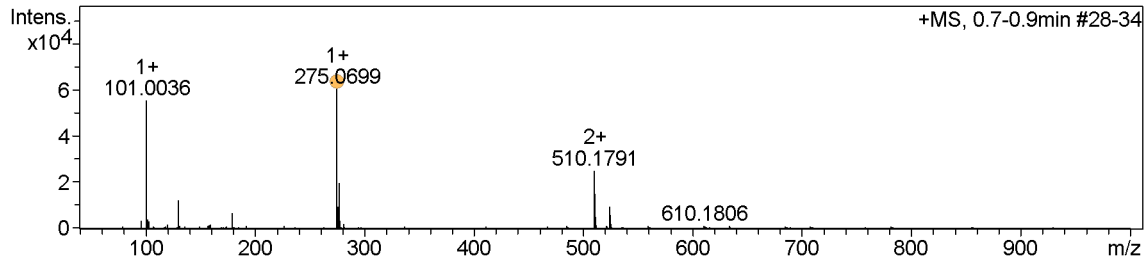
Mass Spectrometry
Analytical Services
School of Chemistry

The University of Nottingham

Sample-ID	pcxtw2_TW113v2	Lab	C13
Submitter	Thomas Weston (pcxtw2)	Supervisor	Luisa Ciano (pczlc1)
Analysis Name	pcxtw2_TW113v2_649356_11_01_130442.d	Acquisition Date	5/15/2023 2:11:27 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #28-34



#	m/z	I %
1	96.0422	5.7
2	101.0036	91.8
3	102.0063	3.0
4	102.1282	6.5
5	103.0000	5.1
6	120.0455	2.9
7	130.1599	20.5
8	158.9644	2.7
9	179.0170	11.1
10	275.0699	100.0
11	276.0725	15.8
12	277.0666	32.8
13	278.0693	5.4
14	281.2013	3.0
15	510.1791	41.5
16	510.6798	25.3
17	511.1821	8.0
18	524.1945	15.9
19	524.6964	9.7
20	525.1969	3.3

Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C13 H11 Cl1 N4 O1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	|Err|[ppm]	Sigma	Formula	Adduct	Adduct Mass
1	275.0699	275.0694	1.70	0.0032	C13H12ClN4O	M+H	1.0078

Note: Sigma fits < 0.05 indicates high probability of correct MF