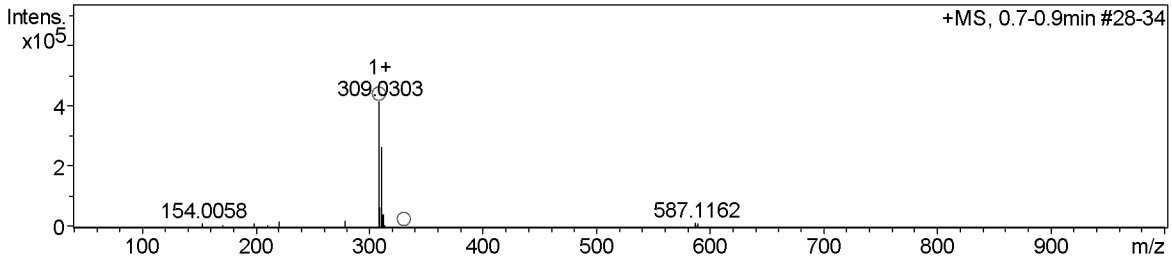
Mass Spectrometry
Analytical Services
School of Chemistry

The University of Nottingham

Sample-ID	pcxtw2_TW133	Lab	C13
Submitter	Thomas Weston (pcxtw2)	Supervisor	Luisa Ciano (pczlc1)
Analysis Name	pcxtw2_TW133_655514_34_01_135945.d	Acquisition Date	10/3/2023 9:12:17 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #28-34



#	m/z	I %
1	139.0074	0.9
2	154.0058	3.1
3	156.0036	1.0
4	171.0983	1.2
5	199.0711	2.9
6	211.0577	1.3
7	221.0529	4.4
8	279.0926	5.5
9	280.0956	1.1
10	309.0303	100.0
11	309.5086	1.1
12	310.0327	15.9
13	311.0273	63.3
14	312.0304	10.2
15	313.0242	10.7
16	314.0279	1.8
17	587.1162	3.8
18	588.1199	1.3
19	589.1134	2.7
20	641.0300	1.1

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 H10 Cl2 N4 O1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	|Err|[ppm]	Sigma	Formula	Adduct	Adduct Mass
1	309.0303	309.0304	0.50	0.0084	C13H11Cl2N4O	M+H	1.0078
1	331.0120	331.0124	1.20	0.0295	C13H10Cl2N4NaO	M+Na	22.9898

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