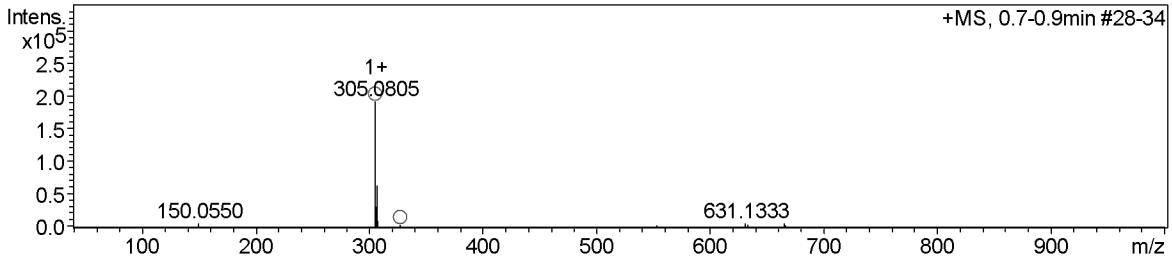
Mass Spectrometry
Analytical Services
School of Chemistry

The University of Nottingham

Sample-ID	pcxtw2_Tw131 V2	Lab	C13
Submitter	Thomas Weston (pcxtw2)	Supervisor	Luisa Ciano (pczlc1)
Analysis Name	pcxtw2_Tw131 V2_653449_26_01_134132.d	Acquisition Date	8/16/2023 2:45:43 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #28-34



#	m/z	I %
1	118.0862	1.0
2	150.0550	2.9
3	261.1315	0.8
4	303.5878	0.8
5	305.0805	100.0
6	305.4827	0.8
7	305.5533	0.9
8	306.0824	17.0
9	307.0773	33.4
10	308.0789	5.6
11	327.0610	2.6
12	329.0588	1.0
13	333.2793	0.8
14	553.4222	1.5
15	609.4812	0.9
16	631.1333	3.2
17	632.1338	1.1
18	633.1312	2.3
19	665.5458	2.8
20	666.5479	1.4

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 C14 H13 Cl1 N4 O2 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	|Err|[ppm]	Sigma	Formula	Adduct	Adduct Mass
1	305.0805	305.0800	1.60	0.0020	C14H14ClN4O2	M+H	1.0078
1	327.0610	327.0619	2.90	0.0142	C14H13ClN4NaO2	M+Na	22.9898

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