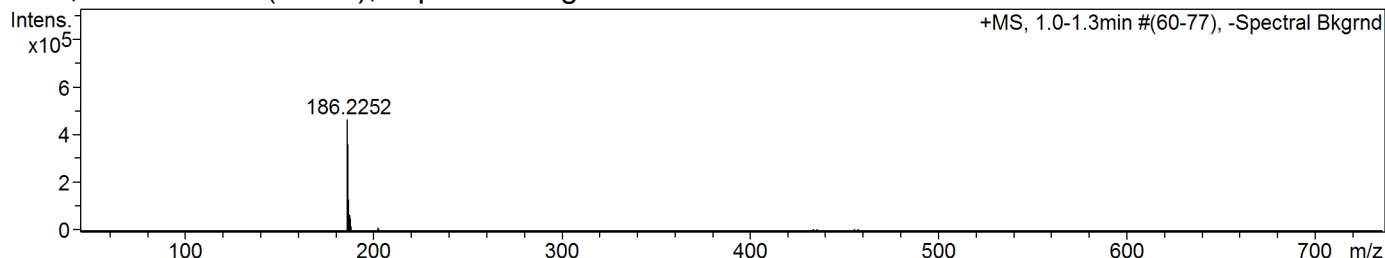


Confirmation of Expected Formula

Sample-ID acs_sdb_acs242 Submitter Adam Sedgwick
 Analysis Name acs_sdb_acs242_344360_25_01_48822.d Supervisor Steve Bull
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 20/07/2015 18:09:55
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	112.0775	4023	0.9	56	4439.6
2	186.2252	462810	100.0	12190	41162.6
3	187.2253	66697	14.4	2448	5728.6
4	202.2165	12077	2.6	516	685.0
5	214.0968	3947	0.9	72	247.3
6	433.0872	9174	2.0	736	816.3
7	434.0904	3693	0.8	327	323.0
8	435.0869	8813	1.9	797	758.0
9	455.0722	5310	1.1	493	689.4
10	457.0685	5800	1.3	495	797.3

Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C20 H20 B Br F2 N2 O **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	433.0872	433.089838	5.70	0.0273	C 20 H 21 B 1 Br 1 F 2 N 2 O 1

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication