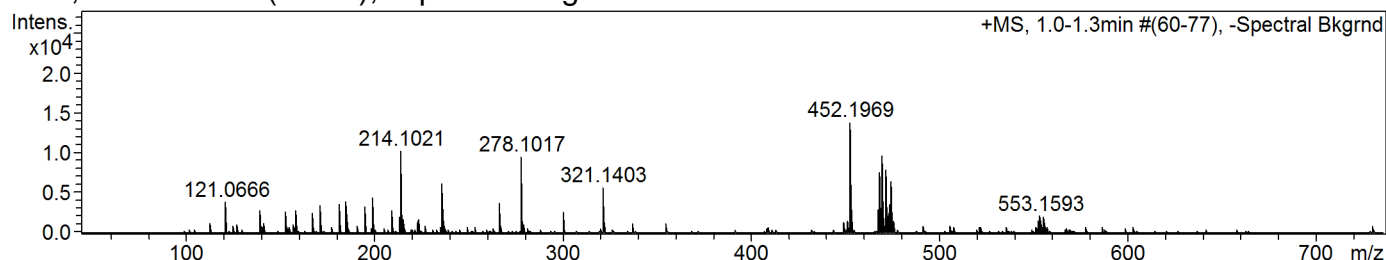


Confirmation of Expected Formula

Sample-ID acs_sdb_acs253 Submitter Adam Sedgwick
 Analysis Name acs_sdb_acs253_344533_9_01_49028.d Supervisor Steve Bull
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 06/08/2015 10:16:47
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	199.1815	4420	32.0	165	665.5
2	214.1021	10209	73.8	199	1393.7
3	236.0812	6076	43.9	213	811.8
4	278.1017	9520	68.9	496	1310.2
5	321.1403	5677	41.1	338	960.6
6	452.1969	13825	100.0	1210	1345.0
7	468.1065	7574	54.8	699	606.9
8	469.1047	9653	69.8	934	765.1
9	471.1045	7820	56.6	731	606.5
10	474.1743	6437	46.6	612	483.3

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 C24 H24 B F2 N3 O3

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication