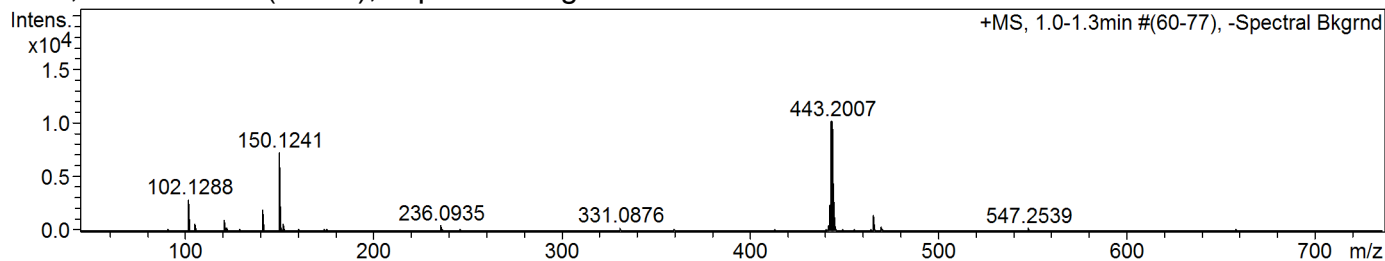


Confirmation of Expected Formula

Sample-ID acs_sdb_ACS307 Submitter Adam Sedgwick
 Analysis Name acs_sdb_ACS307_345890_88_01_50508.d Supervisor Steve Bull
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 15/12/2015 09:45:40
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	102.1288	2933	28.9	51	10425.1
2	105.0708	671	6.6	9	2202.5
3	121.0745	984	9.7	14	2241.9
4	141.0903	1902	18.7	51	3070.1
5	150.1241	7257	71.5	254	10348.7
6	152.1049	671	6.6	17	933.1
7	442.2057	2292	22.6	212	719.1
8	443.2007	10153	100.0	868	3245.1
9	444.2043	2829	27.9	246	921.9
10	465.1816	1423	14.0	111	779.3

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 C26 H27 B N2 O2 S

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