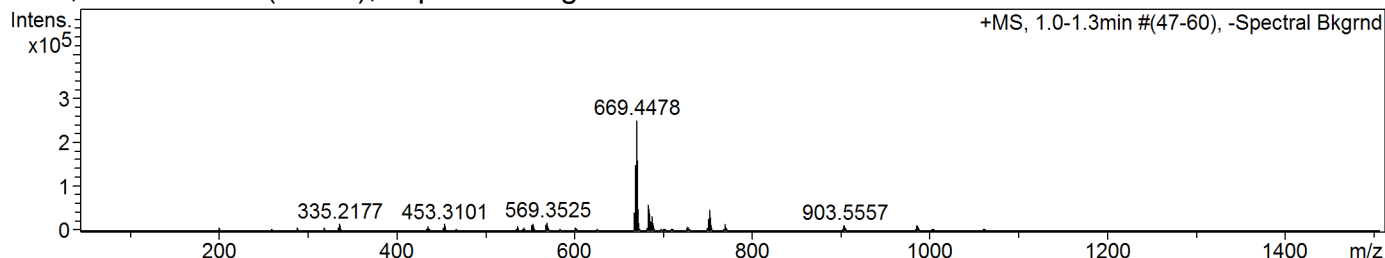


Confirmation of Expected Formula

Sample-ID acs_sdb_acs286 Submitter Adam Sedgwick
 Analysis Name acs_sdb_acs286_345356_76_01_49899.d Supervisor Steve Bull
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 27/10/2015 15:36:30
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(47-60), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	667.4439	40397	16.1	6079	428.8
2	668.4482	147532	58.8	15817	1555.0
3	669.4478	250767	100.0	16091	2624.7
4	670.4436	94088	37.5	12350	978.0
5	682.4573	30059	12.0	4917	310.0
6	683.4533	50212	20.0	7870	522.0
7	686.4229	25344	10.1	3774	269.9
8	687.4222	31381	12.5	4901	337.0
9	750.5210	26572	10.6	4909	599.9
10	751.5184	45706	18.2	7854	1050.2

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 C₃₁ H₄₈ B₂ N₂ O₄

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	535.3869	535.387844	2.70	0.0110	C ₃₁ H ₄₉ B ₂ N ₂ O ₄

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