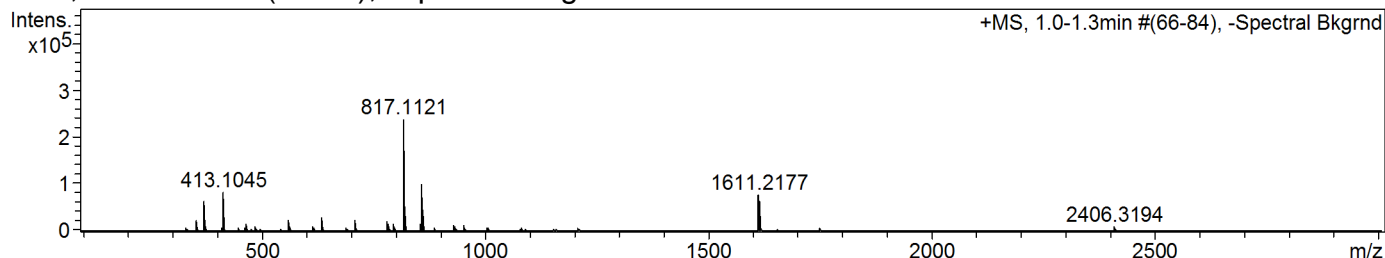


Confirmation of Expected Formula

Sample-ID ug_ja_mo_mlo174 Submitter mlo22 Maria Odyniec
 Analysis Name ug_ja_mo_mlo174_353195_23_01_58781.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 05/09/2017 17:03:36
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(66-84), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	371.0966	64600	27.3	2693	2803.5
2	413.1045	81492	34.5	3261	3428.5
3	817.1121	236448	100.0	17667	4361.6
4	818.1114	106224	44.9	8778	1967.2
5	819.1092	44926	19.0	3964	835.3
6	858.1346	98613	41.7	9401	2168.9
7	859.1369	43487	18.4	4477	961.0
8	1611.2177	76473	32.3	13387	3091.3
9	1612.2211	62244	26.3	11108	2521.7
10	1613.2166	35316	14.9	6803	1433.9

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 C35 H29 F3 O16 S **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	795.1267	795.1201	8.30	0.0077	C 35 H 30 F 3 O 16 S 1

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