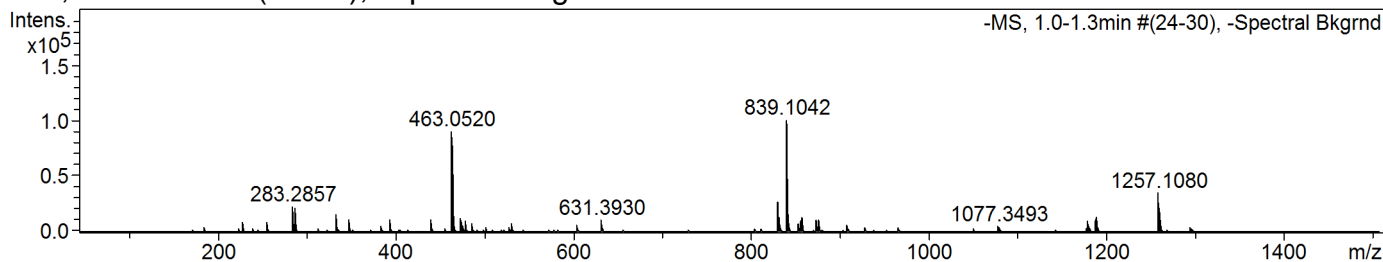


Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo178	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo178_353299_33_01_58910.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to1500 loop inj.m	Acquisition Date	13/09/2017 10:48:36
Ionisation Mode	negative electrospray (ESI)		

-MS, 1.0-1.3min #(24-30), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	283.2857	22671	22.6	708	2784.1
2	287.0993	21341	21.2	717	2525.3
3	463.0520	90119	89.7	4685	2590.1
4	464.0543	20046	20.0	1126	570.6
5	829.0783	26954	26.8	2793	722.0
6	839.1042	100467	100.0	10818	2308.8
7	840.1086	43200	43.0	4581	978.8
8	841.1068	17057	17.0	1815	381.2
9	1257.1080	34865	34.7	5529	1734.2
10	1258.1121	21106	21.0	3603	1043.8

Generate Molecular Formula Parameters

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

Expected Formula C35 H29 F3 O16 S

Adduct(s): H, Na

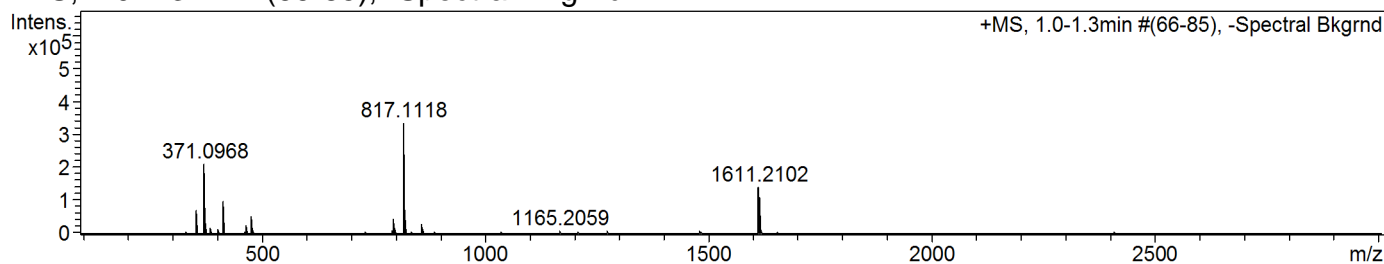
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo178	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo178_353299_33_01_58912.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to1500 loop inj.m	Acquisition Date	13/09/2017 10:58:31
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(66-85), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	353.0844	72467	21.5	2689	5425.3
2	371.0968	211242	62.7	8774	14418.3
3	413.0999	96558	28.7	3259	7009.9
4	477.1001	50820	15.1	2598	5504.8
5	817.1118	336712	100.0	22714	14335.0
6	818.1088	139840	41.5	11384	5988.3
7	819.1056	60464	18.0	5452	2604.5
8	1611.2102	142803	42.4	19478	10893.0
9	1612.2123	110717	32.9	17690	8500.9
10	1613.2076	72131	21.4	11603	5574.5

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	795.1212	795.1201	1.40	0.0298	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