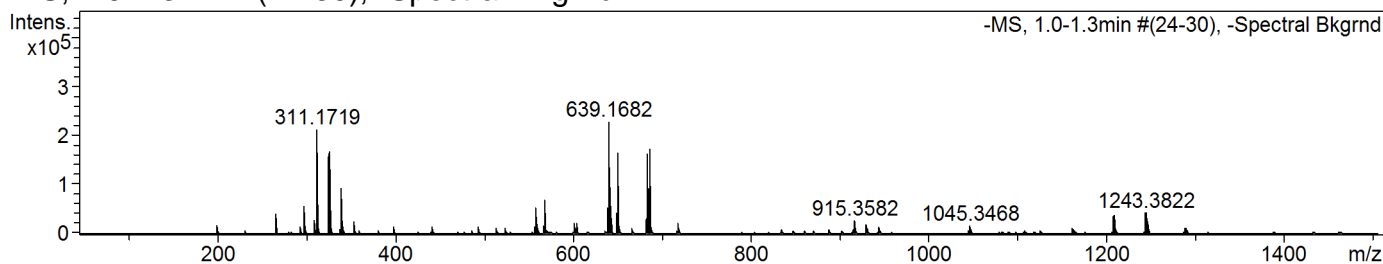


Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo182	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo182_353389_26_01_59018.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to1500 loop inj.m	Acquisition Date	19/09/2017 15:20:57
Ionisation Mode	negative electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	311.1719	212329	93.5	7404	4835.7
2	325.1865	167051	73.6	6448	4041.1
3	339.2017	92011	40.5	3675	2373.4
4	639.1682	227081	100.0	17303	1371.9
5	640.1703	102887	45.3	7995	616.9
6	641.1663	95272	42.0	7614	566.9
7	649.1967	164669	72.5	13163	924.1
8	683.1155	162280	71.5	13287	796.6
9	684.1168	92742	40.8	8001	459.3
10	685.1143	173892	76.6	14052	868.8

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 C32 H33 B O11

Adduct(s): H, Na

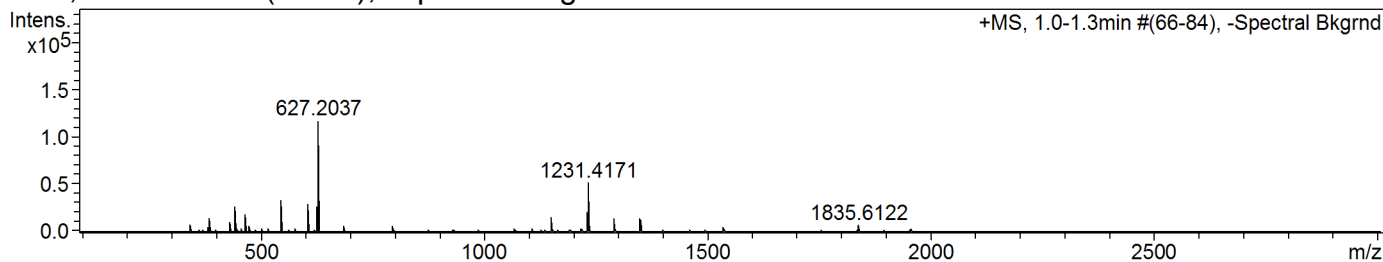
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
---	-----------	-----------	----------	-------	---------

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_mlo182	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo182_353389_26_01_59019.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to1500 loop inj.m	Acquisition Date	19/09/2017 15:27:25
Ionisation Mode	positive electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	443.1669	26504	22.6	1171	3669.5
2	465.1484	18431	15.7	766	2281.2
3	545.1253	32967	28.1	1709	2944.5
4	605.2153	28344	24.2	1644	2491.1
5	626.2036	26748	22.8	1645	2570.0
6	627.2037	117239	100.0	7683	11314.7
7	628.2031	40957	34.9	2579	3970.5
8	1230.4146	20572	17.5	2458	938.9
9	1231.4171	51655	44.1	6900	2366.3
10	1232.4218	36033	30.7	4724	1656.9

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 C32 H33 B O11 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	627.2037	627.2014	3.70	0.0150	C 32 H 33 B 1 Na 1 O 11

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