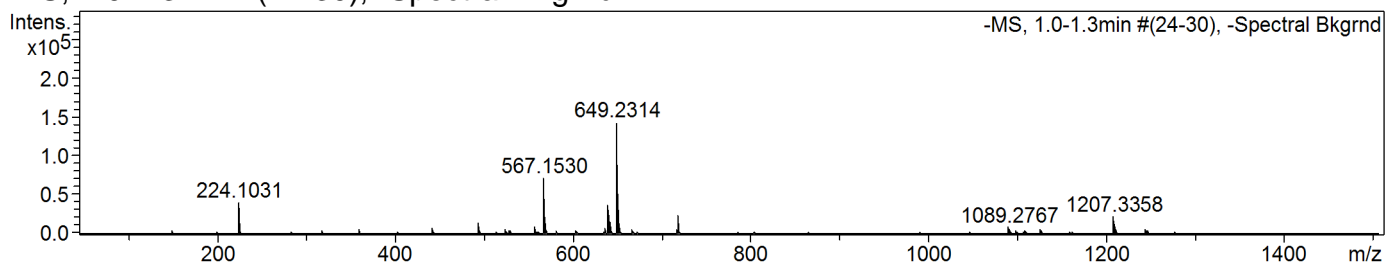


## Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo187	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo187_353574_24_01_59237.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to1500 loop inj.m	Acquisition Date	02/10/2017 15:52:50
Ionisation Mode	negative electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	224.1031	39895	27.9	379	17512.0
2	566.1568	16892	11.8	1133	542.8
3	567.1530	70903	49.6	4977	2260.3
4	568.1565	22101	15.5	1519	698.9
5	639.2022	36129	25.3	2834	701.8
6	648.2336	32734	22.9	2760	605.5
7	649.2314	142952	100.0	11510	2630.6
8	650.2341	51518	36.0	4286	943.1
9	717.2165	23740	16.6	2092	555.0
10	1207.3358	21932	15.3	3221	599.9

### 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
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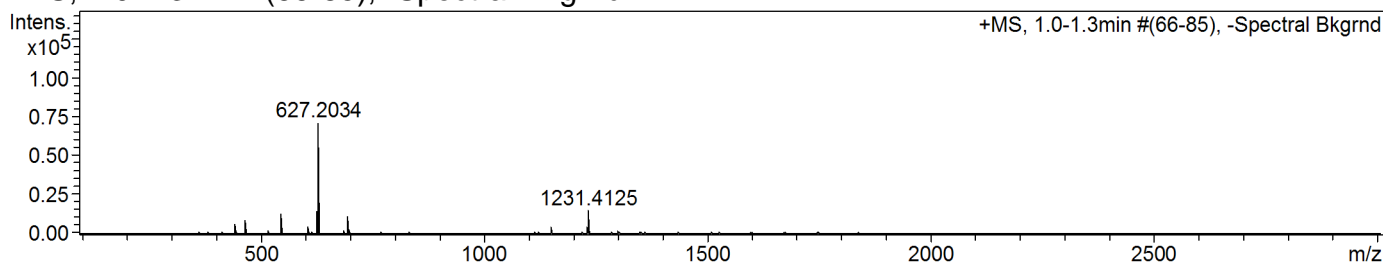
Note: Sigma fits < 0.05 indicates high probability of correct MF.

For formula confirmation the mass error / accuracy at 200 Da should be better than 25 ppm, for 500 Da better than 10 ppm and for 1000 Da better than 5 ppm

## Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo187	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo187_353574_24_01_59239.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to1500 loop inj.m	Acquisition Date	02/10/2017 16:03:15
Ionisation Mode	positive electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	443.1671	6169	8.7	269	2873.3
2	465.1484	8218	11.5	378	3185.2
3	545.1253	12642	17.8	578	3041.3
4	626.2052	14263	20.0	918	3423.2
5	627.2034	71200	100.0	4605	17148.3
6	628.2059	24131	33.9	1544	5832.2
7	695.1881	10777	15.1	728	3406.0
8	1230.4215	4678	6.6	535	588.1
9	1231.4125	14689	20.6	1907	1848.8
10	1232.4142	8735	12.3	1107	1100.7

### 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
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#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	627.2034	627.2014	3.20	0.0170	C 32 H 33 B 1 Na 1 O 11

Note: Sigma fits < 0.05 indicates high probability of correct MF.

For formula confirmation the mass error / accuracy at 200 Da should be better than 25 ppm, for 500 Da better than 10 ppm and for 1000 Da better than 5 ppm