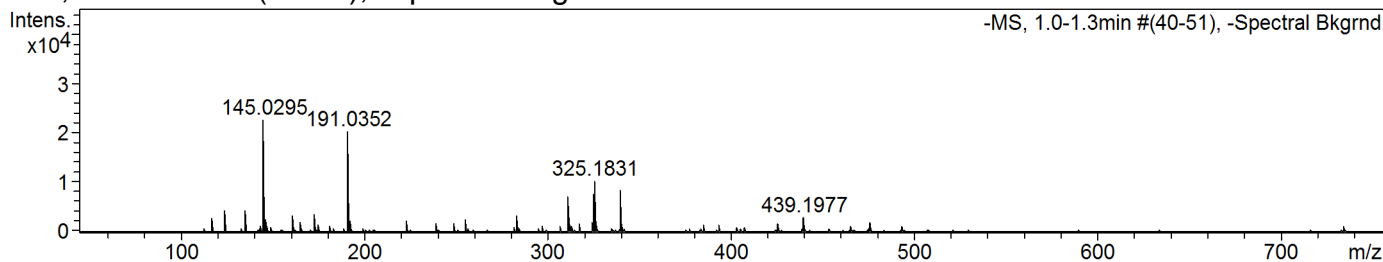


## Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo347	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo347_358061_39_01_64397.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to500 loop inj.m	Acquisition Date	30/07/2018 14:16:32
Ionisation Mode	negative electrospray (ESI)		

### -MS, 1.0-1.3min #(40-51), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	124.0048	4205	18.6	39	3931.8
2	135.0160	4167	18.5	38	2003.6
3	145.0295	22559	100.0	720	7523.3
4	161.0251	3099	13.7	65	693.8
5	173.0245	3540	15.7	118	794.6
6	191.0352	20247	89.8	791	4990.0
7	311.1688	7005	31.1	389	890.4
8	325.0955	7584	33.6	443	1203.0
9	325.1831	10321	45.8	638	1639.9
10	339.2005	8507	37.7	490	1802.2

### 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** C23 H25 B O6 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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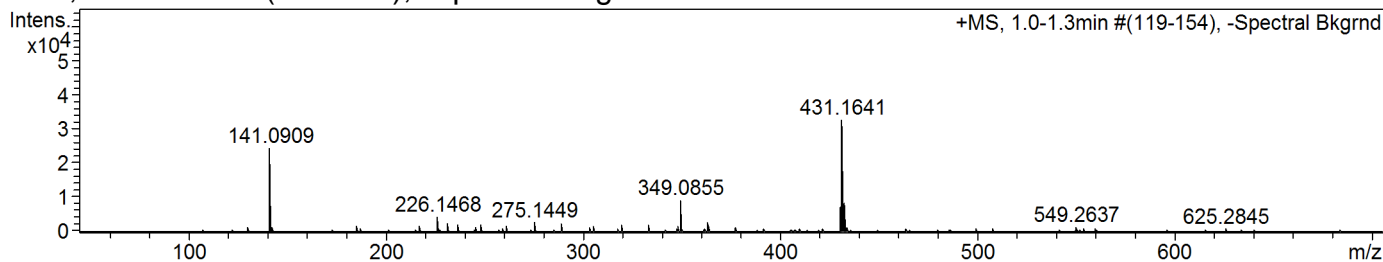
Note: Sigma fits < 0.05 indicates high probability of correct MF.

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_mlo347	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo347_358061_39_01_64404.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	30/07/2018 14:52:14
Ionisation Mode	positive electrospray (ESI)		

### +MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	141.0909	24428	75.1	647	18329.8
2	226.1468	4272	13.1	78	1399.8
3	231.1208	2393	7.4	95	718.8
4	275.1449	2627	8.1	127	874.7
5	289.1539	2209	6.8	124	791.1
6	349.0855	9139	28.1	470	1696.9
7	363.1070	2646	8.1	130	496.1
8	430.1649	7301	22.4	442	603.5
9	431.1641	32546	100.0	2163	2754.1
10	432.1676	8256	25.4	529	715.8

### Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

**Expected Formula** C<sub>23</sub> H<sub>25</sub> B O<sub>6</sub> **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	431.1641	431.1640	0.20	0.0072	C <sub>23</sub> H <sub>25</sub> B O <sub>6</sub>

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