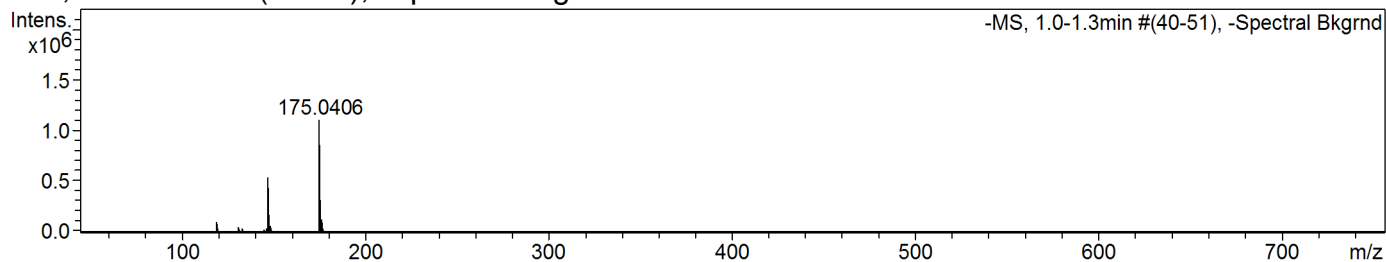


## Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo336	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo336_357799_69_01_64125.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to500 loop inj.m	Acquisition Date	13/07/2018 11:56:20
Ionisation Mode	negative electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	119.0505	98122	8.9	2635	6463.3
2	131.0506	42120	3.8	1243	1259.9
3	133.0298	23831	2.2	703	653.9
4	145.0305	12422	1.1	353	227.1
5	146.0373	26940	2.5	854	479.2
6	147.0456	537253	48.9	18323	9301.8
7	148.0486	53615	4.9	1736	904.4
8	175.0406	1099049	100.0	42806	17609.1
9	176.0438	119867	10.9	4523	1974.4
10	177.0459	12797	1.2	465	216.9

### Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
negative	20 ppm	0.05 m/z	0	3	both	true	0.05

**Expected Formula**      C13 H12 O4      **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.

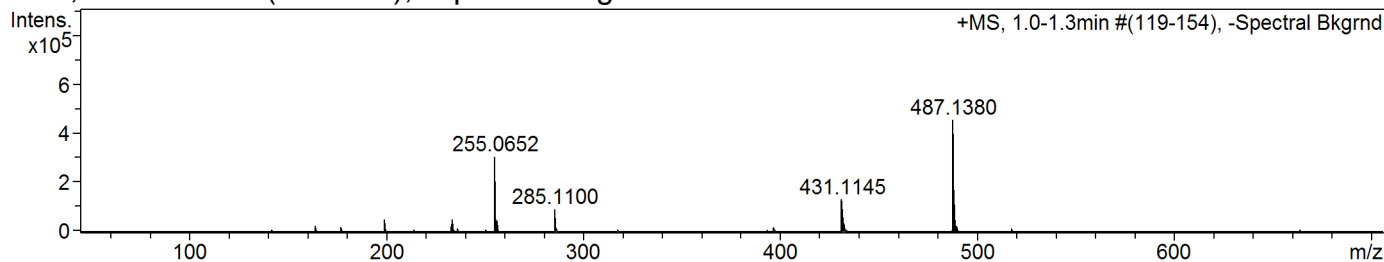
For formula confirmation the mass error / accuracy at 200 Da should be better than 25 ppm, for 500 Da better than 10 ppm and for 1000 Da better than 5 ppm

**Sample concentration too high! Dilute sample by factor 1000.**

## Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo336	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo336_357799_69_01_64129.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	13/07/2018 12:13:25
Ionisation Mode	positive electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	199.0366	46563	10.3	1685	4774.5
2	233.0807	48681	10.8	1912	1526.0
3	255.0652	306313	67.6	14438	9334.4
4	256.0670	44216	9.8	1919	1366.7
5	285.1100	91948	20.3	4614	4867.1
6	431.1145	131873	29.1	11267	4470.9
7	432.1172	32794	7.2	2746	1118.3
8	487.1380	452818	100.0	42970	7360.3
9	488.1412	129277	28.5	11454	2049.0
10	489.1431	24381	5.4	2136	377.0

### 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** C13 H12 O4 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	233.0807	233.0808	-0.70	0.0204	C 13 H 13 O 4
1	255.0652	255.0628	9.40	0.0053	C 13 H 12 Na 1 O 4

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