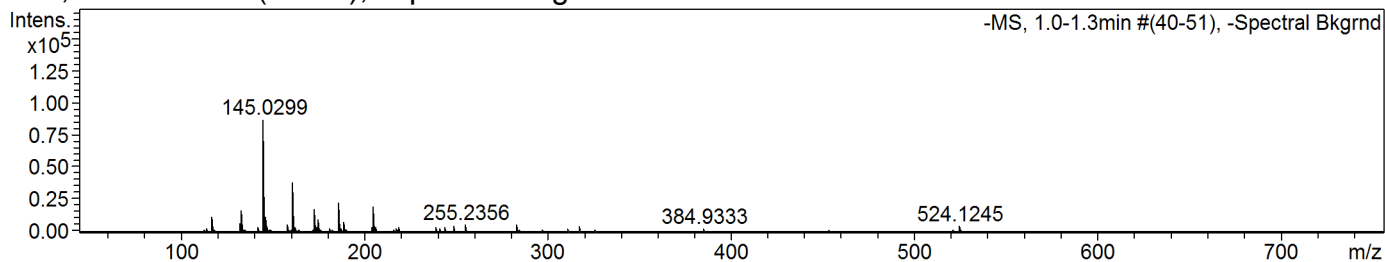


## Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo339	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo339_357797_67_01_64123.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to500 loop inj.m	Acquisition Date	13/07/2018 11:49:10
Ionisation Mode	negative electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	117.0351	11240	13.0	286	3687.9
2	133.0298	16104	18.6	451	1680.8
3	145.0299	86404	100.0	2760	5965.9
4	146.0344	10868	12.6	310	729.7
5	161.0254	38142	44.1	1306	1814.9
6	173.0249	16993	19.7	648	867.0
7	175.0409	9270	10.7	311	484.8
8	186.0204	21742	25.2	854	1317.6
9	189.0254	7578	8.8	299	480.1
10	205.0496	19110	22.1	803	1597.2

### 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** C13 H11 Br O4 **Adduct(s):** H, Na

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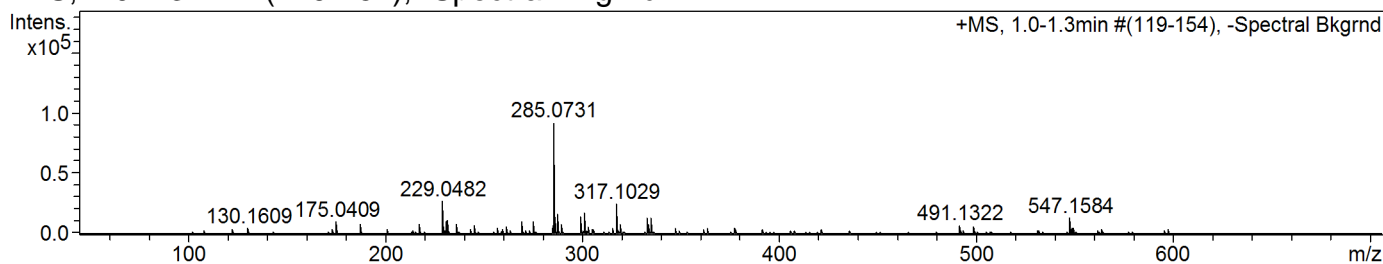
Note: Sigma fits < 0.05 indicates high probability of correct MF.

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

## Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo339	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo339_357797_67_01_64127.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	13/07/2018 12:06:24
Ionisation Mode	positive electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	229.0482	26806	29.1	1261	1185.1
2	285.0731	92204	100.0	4968	1630.1
3	286.0762	14349	15.6	745	250.2
4	287.0568	16201	17.6	957	279.2
5	299.0535	13719	14.9	663	255.6
6	301.0675	17593	19.1	908	332.4
7	317.1029	24536	26.6	1663	521.4
8	332.9737	12922	14.0	715	312.5
9	334.9721	13352	14.5	752	328.2
10	547.1584	12776	13.9	1389	402.1

### 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 H11 Br O4                      **Adduct(s):**    H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	332.9737	332.9733	1.10	0.0180	C 13 H 11 Br 1 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