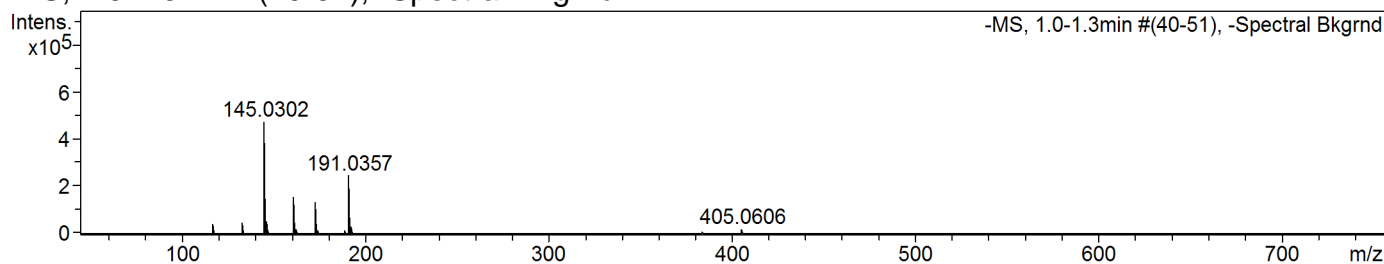


Confirmation of Expected Formula

| | | | |
|-----------------|---|------------------|---------------------|
| Sample-ID | ug_ja_mo_mlo346 | Submitter | mlo22 Maria Odyniec |
| Analysis Name | ug_ja_mo_mlo346_357866_38_01_64199.d | Supervisor | - Tony James |
| Method used | Confirm Formula Negative 50to500 loop inj.m | Acquisition Date | 18/07/2018 14:49:22 |
| Ionisation Mode | negative electrospray (ESI) | | |

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



| # | m/z | I | I % | Area | S/N |
|----|----------|--------|-------|-------|---------|
| 1 | 117.0348 | 39537 | 8.4 | 1005 | 8905.5 |
| 2 | 133.0298 | 47101 | 10.0 | 1387 | 2877.5 |
| 3 | 145.0302 | 471305 | 100.0 | 15840 | 18615.3 |
| 4 | 146.0335 | 49260 | 10.5 | 1531 | 1889.8 |
| 5 | 161.0251 | 154848 | 32.9 | 5487 | 4157.3 |
| 6 | 162.0284 | 15955 | 3.4 | 532 | 419.9 |
| 7 | 173.0251 | 132665 | 28.1 | 4842 | 3857.6 |
| 8 | 191.0357 | 243867 | 51.7 | 9663 | 9361.5 |
| 9 | 192.0389 | 26805 | 5.7 | 1035 | 1047.7 |
| 10 | 405.0606 | 20889 | 4.4 | 1470 | 2622.1 |

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 | C10 H8 O4 | Adduct(s): | H, Na |
|------------------|-----------|------------|-------|

| # | meas. m/z | theo. m/z | Err[ppm] | Sigma | Formula |
|---|-----------|-----------|----------|--------|--------------|
| 1 | 191.0357 | 191.0350 | 3.80 | 0.0011 | C 10 H 7 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

