

Supplementary Information

High Throughput Mass Spectrometry Platform for Prospecting High Value Chemicals from Bioconversion of Glycerin

Diana R. Amazonas,^{id} ^a Augusto L. Souto,^a Flávia S. Vieira,^{a,b} Andréia A. J. Carneiro,^a Rebeca B. Vianna,^a Thaís D. Mendes,^a Karen S. Lima,^a José A. A. Ribeiro,^a Mônica C. T. Damaso,^a Cleilson M. Rodrigues^a and Patrícia V. Abdelnur^{id} ^{,a,b}*

^a*Empresa Brasileira de Pesquisa Agropecuária, Embrapa Agroenergia, W3 Norte, PqEB, Asa Norte, 70770-901 Brasília-DF, Brazil*

^b*Instituto de Química, Universidade Federal de Goiás, Campus Samambaia, 74690-900 Goiânia-GO, Brazil*

Table S1. Cross-validated data of the PCA analysis in the positive mode [ESI(+)-MS] and in the negative mode [ESI(-)-MS]

| Explained X total variance | Positive mode [ESI(+)-MS] | | | Negative mode [ESI(-)-MS] | | |
|----------------------------|---------------------------|---------|---------|---------------------------|---------|---------|
| | PC-1 | PC-2 | PC-3 | PC-1 | PC-2 | PC-3 |
| Calibration | 78.9440 | 91.8752 | 94.3142 | 64.1801 | 76.3004 | 83.8313 |
| Validation | 78.6744 | 91.6541 | 94.0468 | 63.3231 | 71.3340 | 77.9347 |

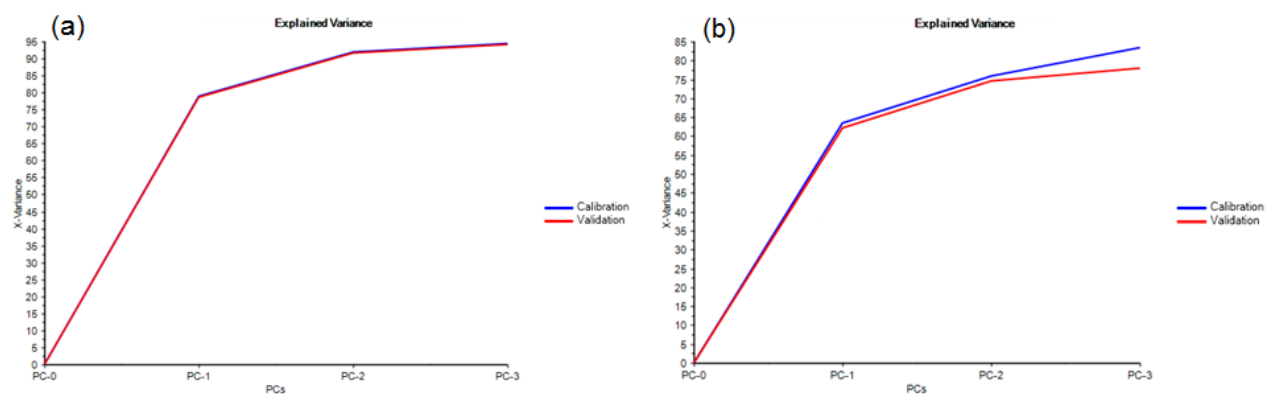


Figure S1. Graph of the cross-validated data of the PCA analysis. (a) In the positive mode [ESI(+)-MS] and (b) in the negative mode [ESI(-)-MS].

*e-mail: patricia.abdelnur@embrapa.br

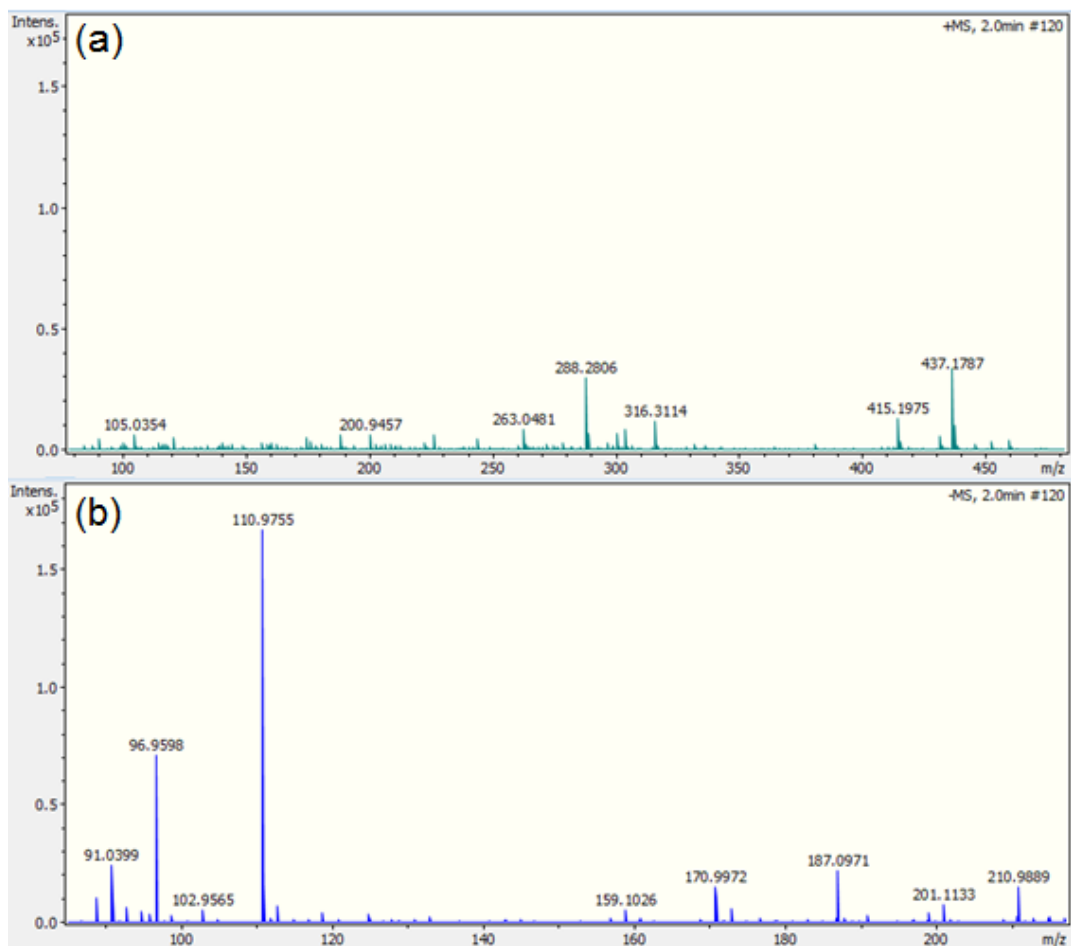


Figure S2. Mass spectra of the microorganism culture medium. (a) In the positive mode [ESI(+)-MS], and (b) in the negative mode [ESI(-)-MS].

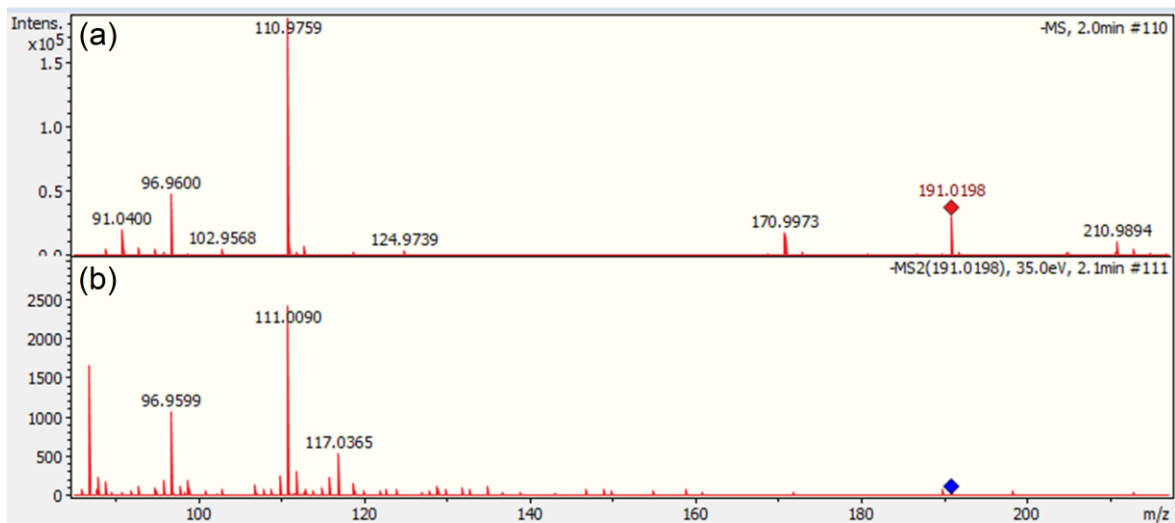


Figure S3. Mass spectra of the sample 2C (a), and tandem mass spectrometry experiment (MS/MS) of the citric acid (b).

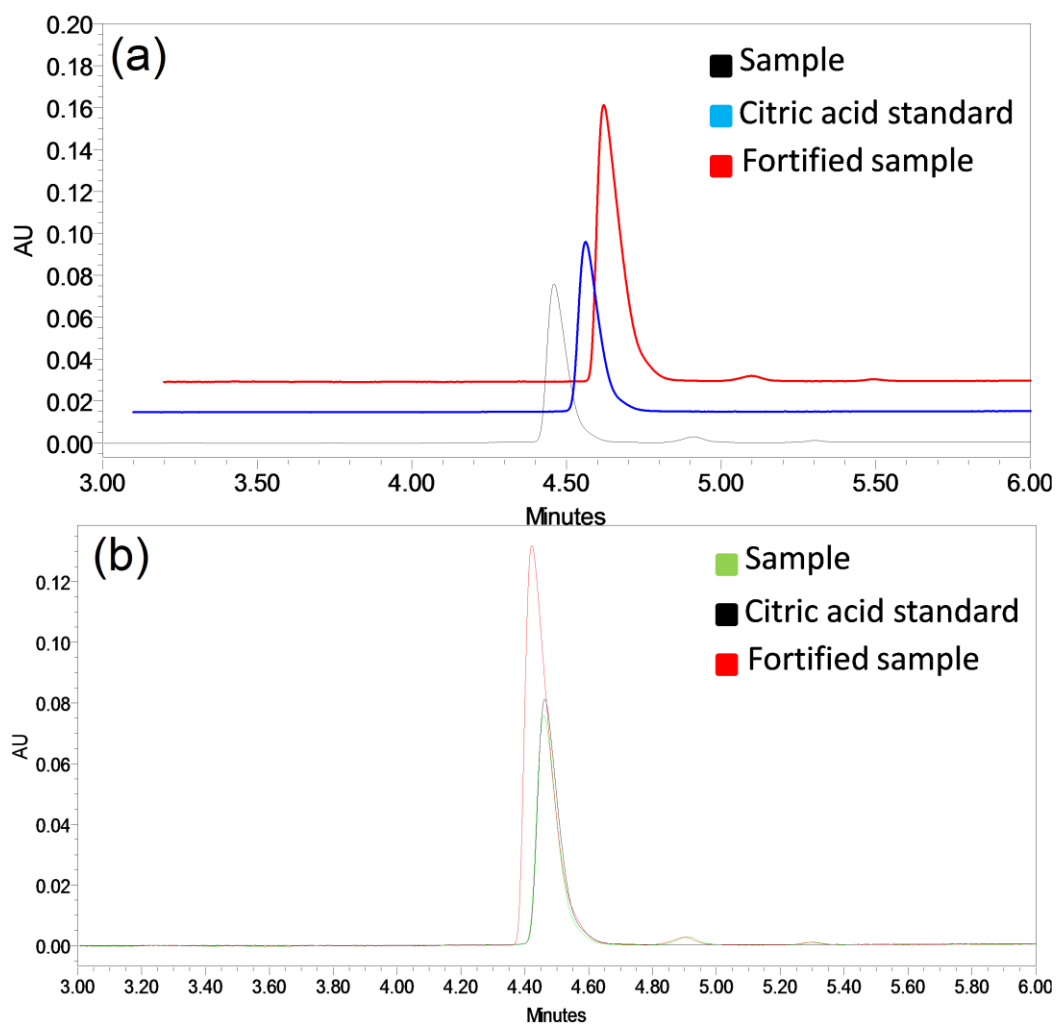


Figure S4. UHPLC-PDA chromatogram of sample 2C, co-injection experiment with citric acid commercial standard acquired at 210 nm, showing 2C sample 20 fold diluted, citric acid at 0.35 g L^{-1} and fortified sample with 0.35 g L^{-1} of citric acid. (a) Stacked peaks, and (b) overlaid peaks.

Table S2. Quantification of citric acid produced by filamentous fungi samples

| Sample | Citric acid concentration / (g L^{-1}) |
|--------|---|
| 2A | 1.0 |
| 2B | 3.9 |
| 2C | 6.2 |

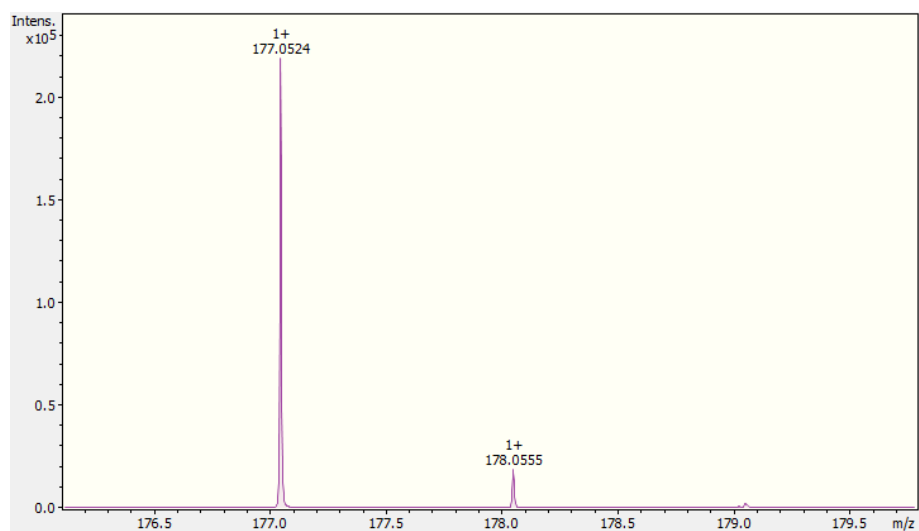


Figure S5. ESI(+)-MS spectrum of ion m/z 177.0524 that was highlighted in sample 5A.

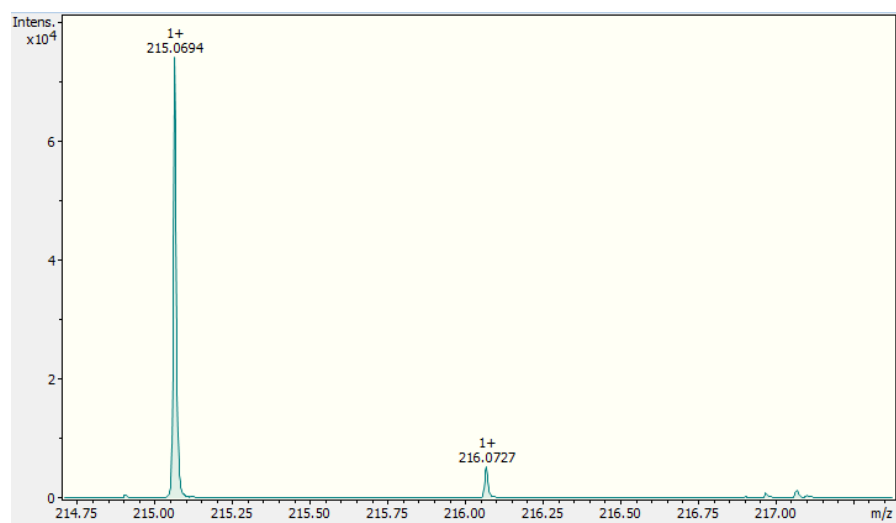


Figure S6. ESI(+)-MS spectrum of ion m/z 215.0694 that was highlighted in sample 8A.

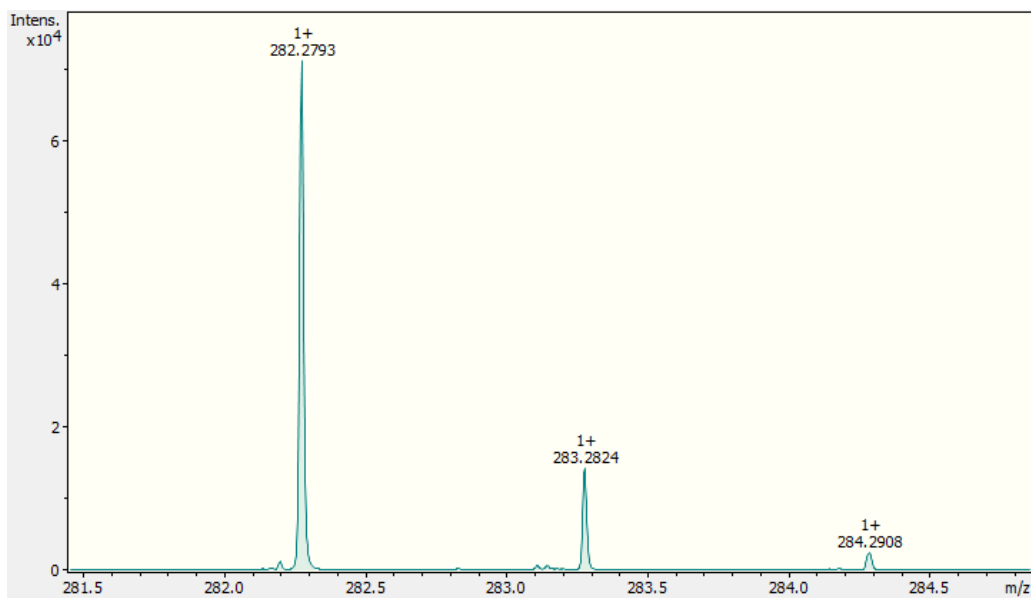


Figure S7. ESI(+)-MS spectrum of ion m/z 282.2793 that was highlighted in sample 8A.

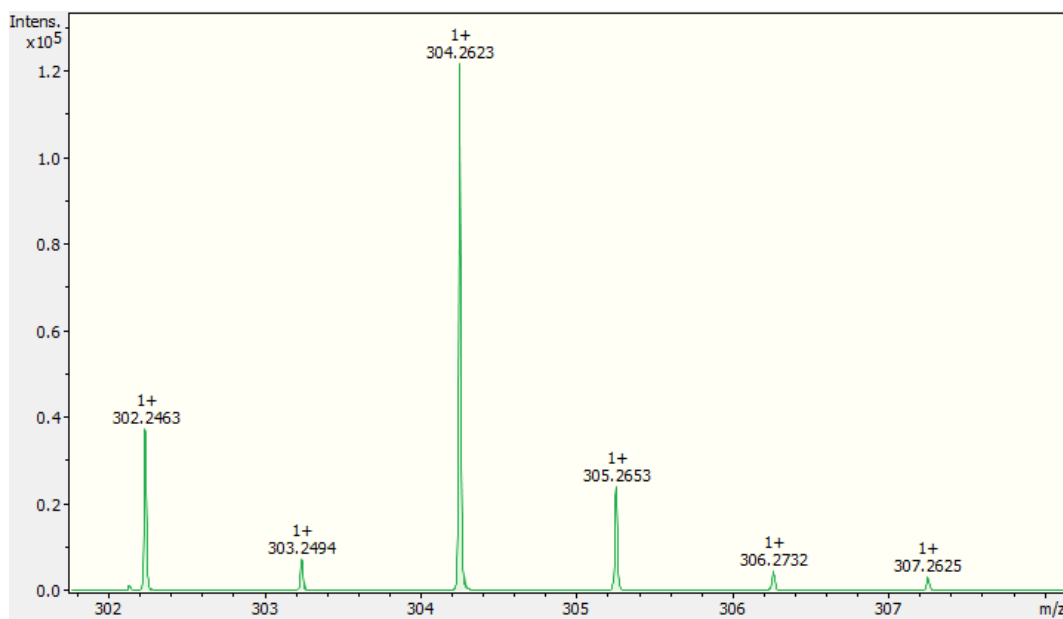


Figure S8. ESI(+)-MS spectrum of ions m/z 302.2463 and m/z 304.2623 that was highlighted in sample 4A.

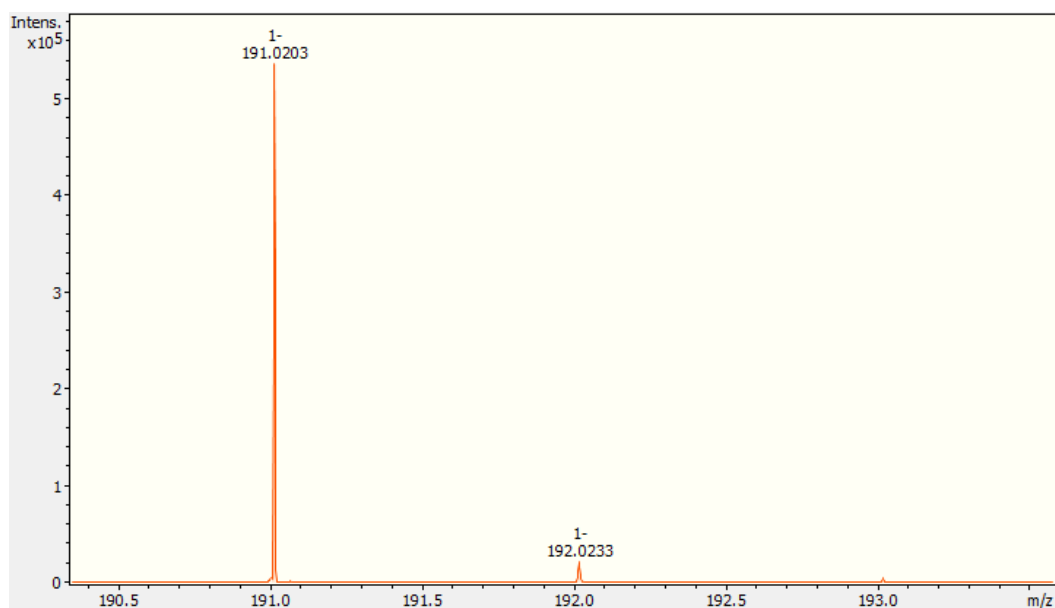


Figure S9. ESI(-)-MS spectrum of ion m/z 191.0203 that was highlighted in samples 2A, 2B and 2C.

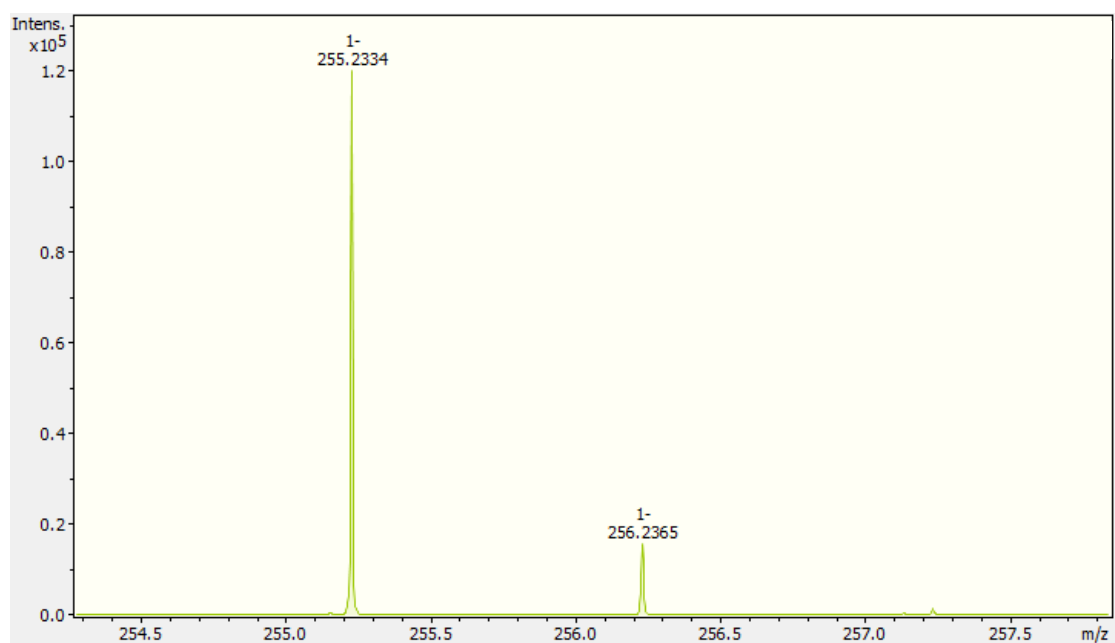


Figure S10. ESI(-)-MS spectrum of ion m/z 255.2334 that was highlighted in samples 1A, 1B, 1C, 3C, 4A, 4B, 4C, 5A, 5B and 6A.

