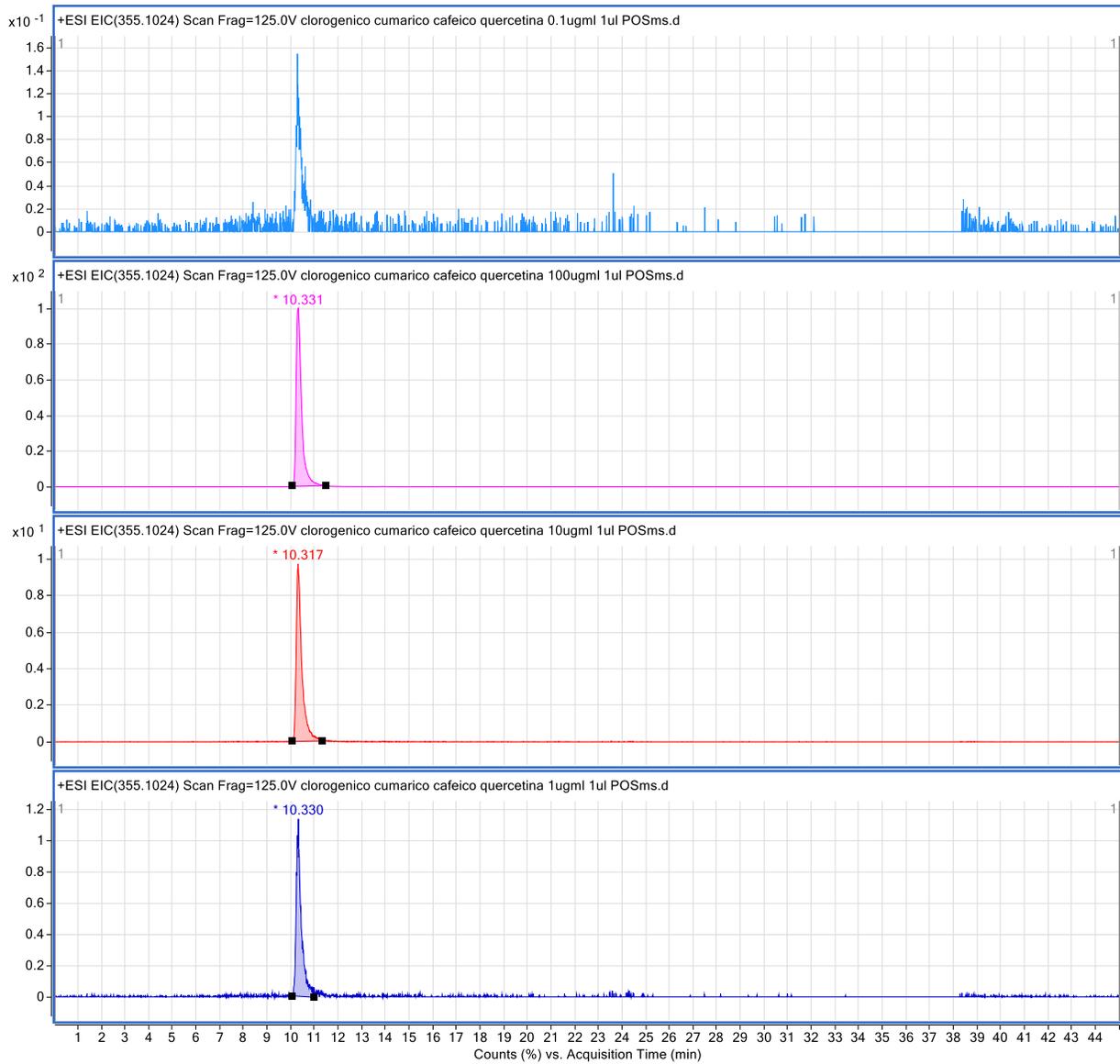


**Supplementary material S1.** Examples of chromatograms and MS spectrum results for standards and samples from different outlets. All measurements were performed in triplicate. Samples 1-3: Sale point 4 in the manuscript; samples 4-6: Sale point 3 in the manuscript; samples 7-9: Sale point 5 in the manuscript; samples 10-12: Sale point 1 in the manuscript; samples 13-15: Sale point 2 in the manuscript.

**STANDARD MULTIPLE (CHLOROGENIC ACID, CUMARIC ACID, CAFFEIC ACID AND QUERCETIN)**

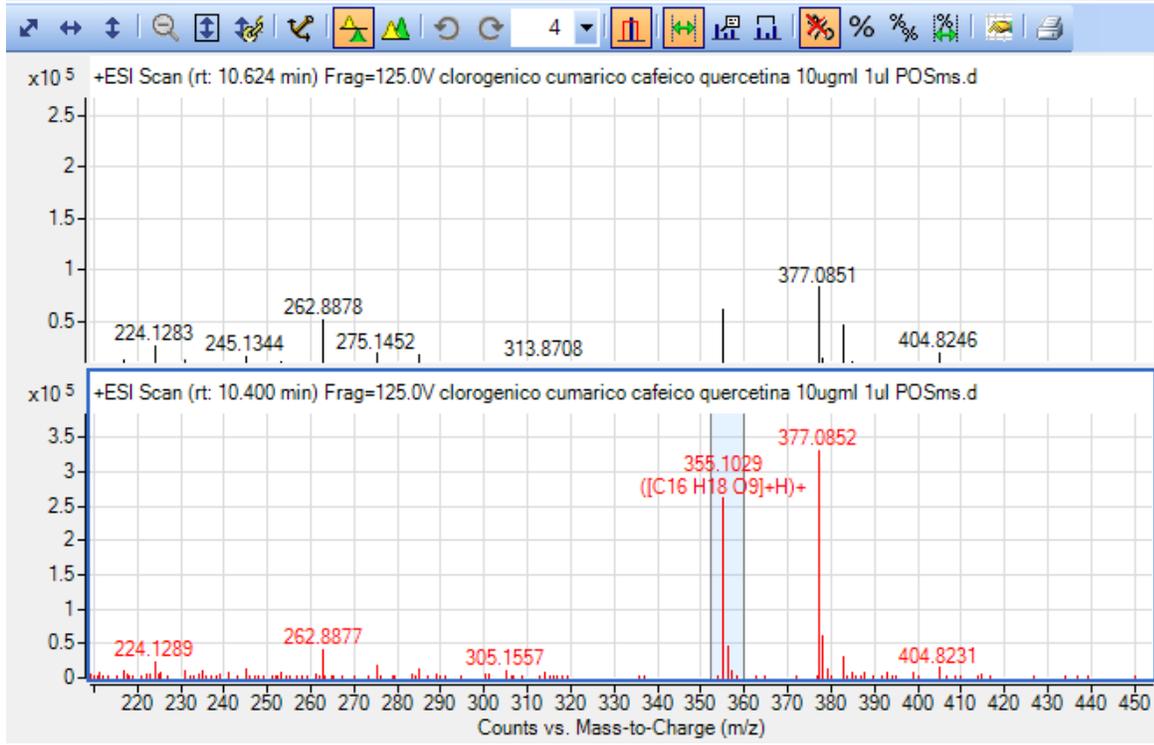
**CHLOROGENIC ACID STANDARD (355.10)**



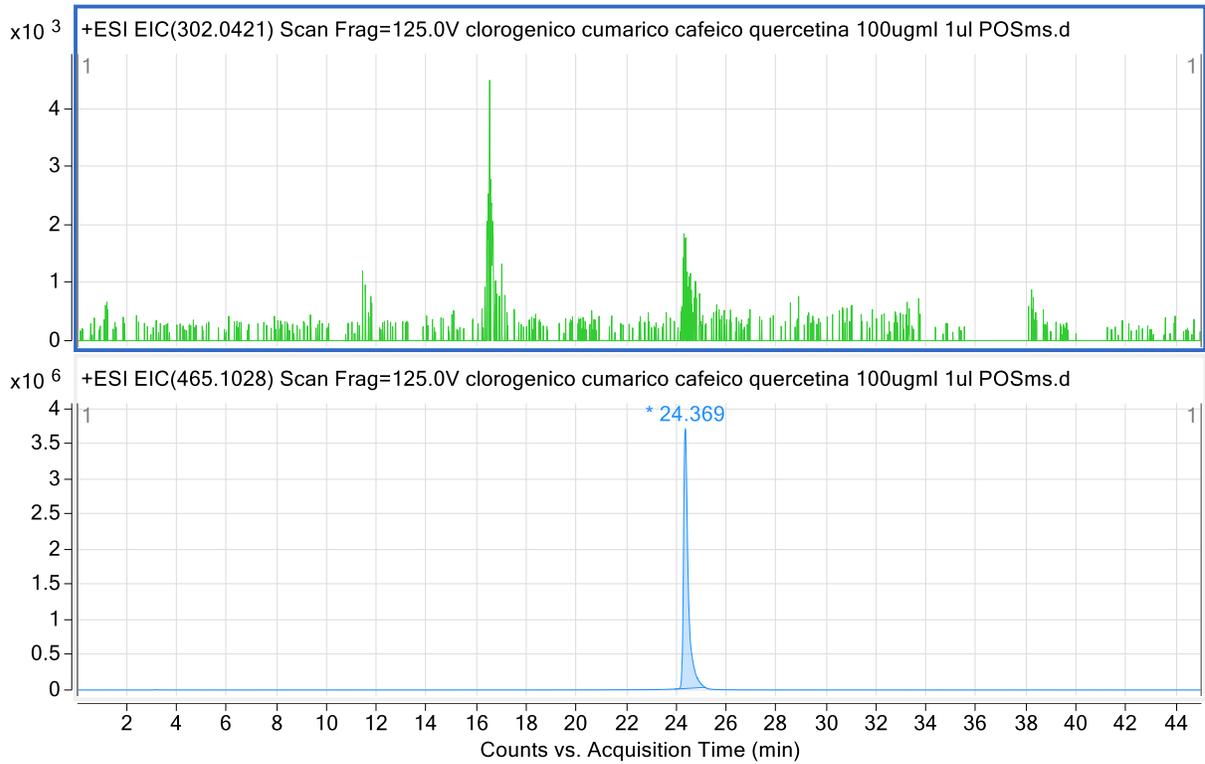
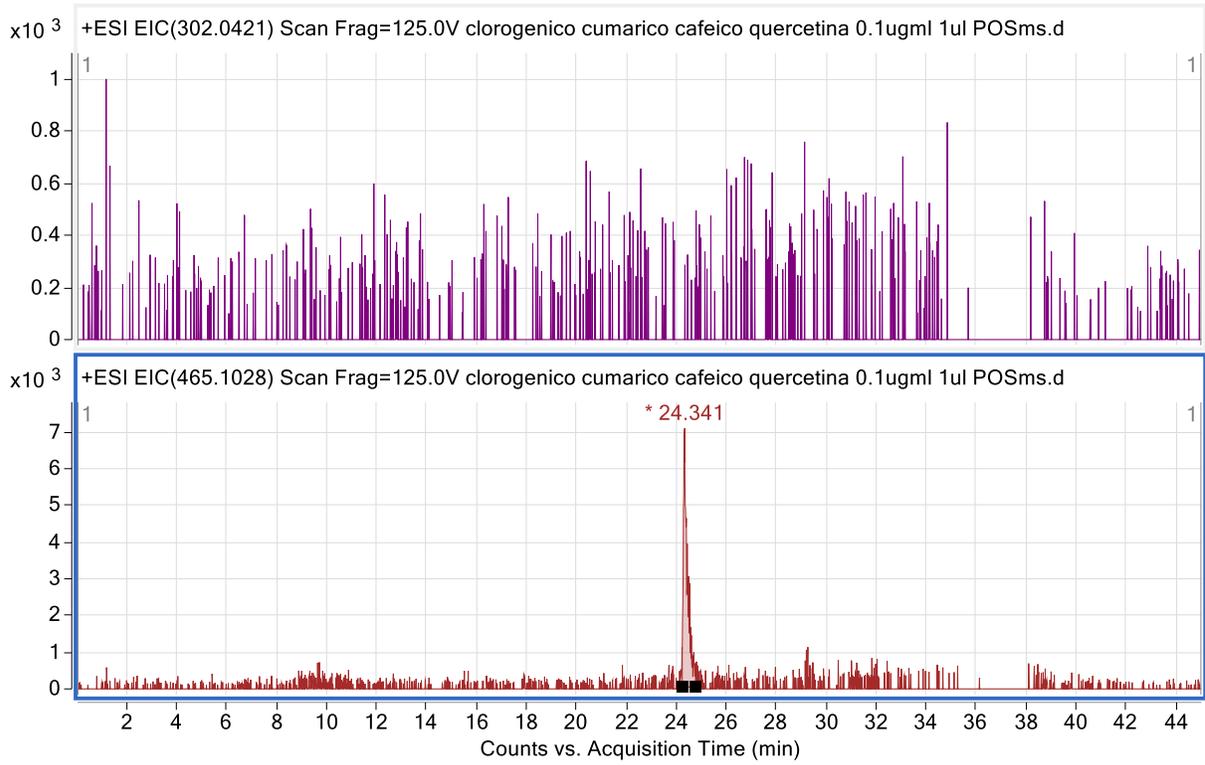
| Best | ID Source | Name | Formula          | Species | m/z      | Score | Score (RT) | RT |
|------|-----------|------|------------------|---------|----------|-------|------------|----|
| ●    | MFG       |      | C16 H18 O9       | (M+H)+  | 355.1029 | 99    |            |    |
| ○    | MFG       |      | C15 H12 N7 O4    | (M+H)+  | 355.1029 | 96.22 |            |    |
| ○    | MFG       |      | C17 H14 N4 O5    | (M+H)+  | 355.1029 | 95.75 |            |    |
| ○    | MFG       |      | C14 H16 N3 O8    | (M+H)+  | 355.1029 | 89.35 |            |    |
| ○    | MFG       |      | C9 H18 N6 O7 S   | (M+H)+  | 355.1029 | 87.05 |            |    |
| ○    | MFG       |      | C10 H14 N10 O3 S | (M+H)+  | 355.1029 | 87.01 |            |    |
| ○    | MFG       |      | C11 H20 N3 O8 S  | (M+H)+  | 355.1029 | 85.99 |            |    |
| ○    | MFG       |      | C13 H10 N10 O3   | (M+H)+  | 355.1029 | 85.22 |            |    |
| ○    | MFG       |      | C23 H16 N O S    | (M+H)+  | 355.1029 | 84.44 |            |    |
| ○    | MFG       |      | C19 H16 N O6     | (M+H)+  | 355.1029 | 84.34 |            |    |
| ○    | MFG       |      | C17 H22 O4 S2    | (M+H)+  | 355.1029 | 83.39 |            |    |
| ○    | MFG       |      | C18 H10 N8 O     | (M+H)+  | 355.1029 | 81.84 |            |    |
| ○    | MFG       |      | C15 H20 N3 O3 S2 | (M+H)+  | 355.1029 | 78.47 |            |    |
| ○    | MFG       |      | C18 H18 N4 S2    | (M+H)+  | 355.1029 | 77.35 |            |    |
| ○    | MFG       |      | C12 H16 N7 O4 S  | (M+H)+  | 355.1029 | 77.23 |            |    |
| ○    | MFG       |      | C21 H14 N4 S     | (M+H)+  | 355.1029 | 76.75 |            |    |
| ○    | MFG       |      | C13 H22 O9 S     | (M+H)+  | 355.1029 | 75.05 |            |    |
| ○    | MFG       |      | C12 H14 N6 O7    | (M+H)+  | 355.1029 | 73.49 |            |    |

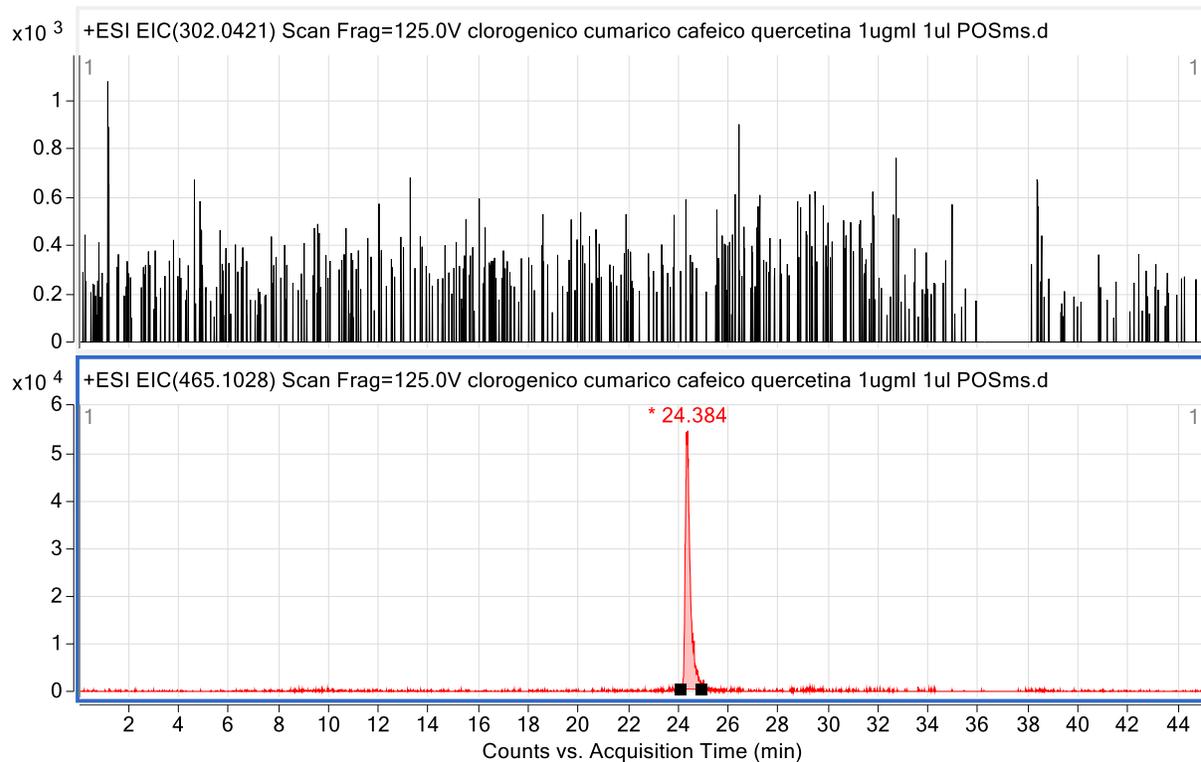
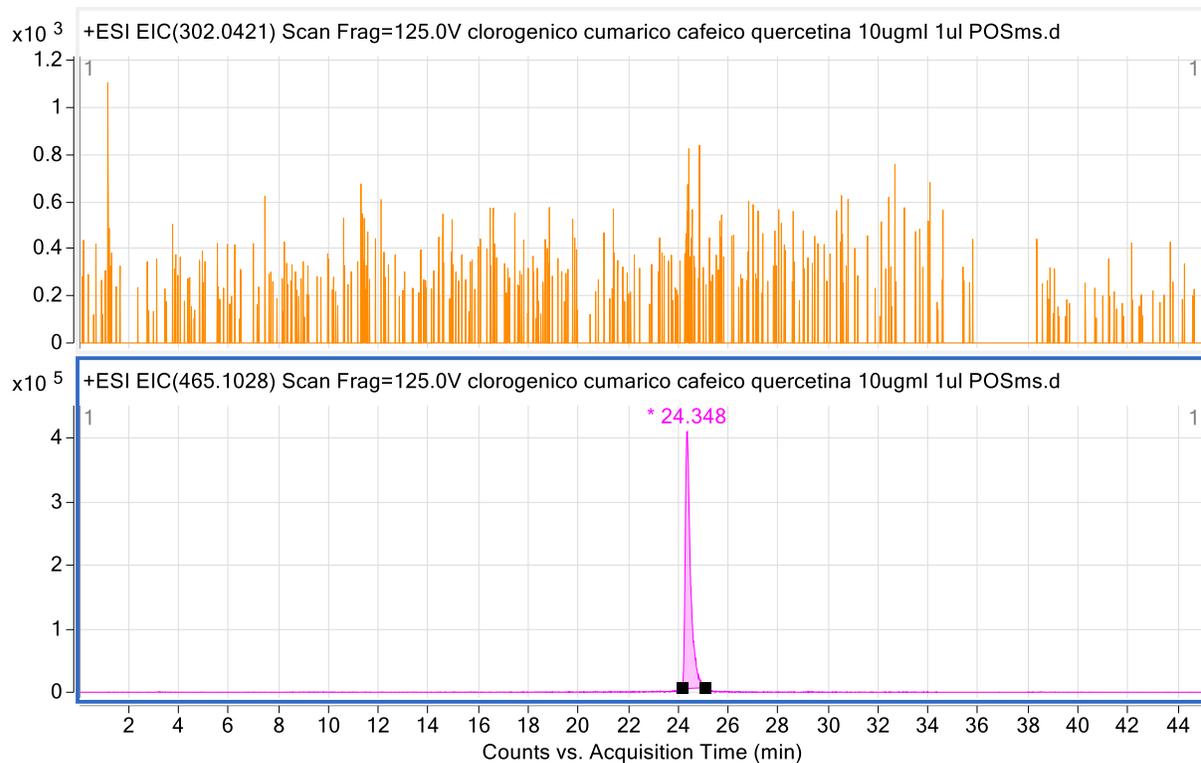
Chromatogram Results Spectrum Identification Results: + Scan (rt: 10.400 min)

MS Spectrum Results



### QUERCETIN-3-GLUCOSIDE (465.1028) AND QUERCETIN (302.0421) STANDARDS

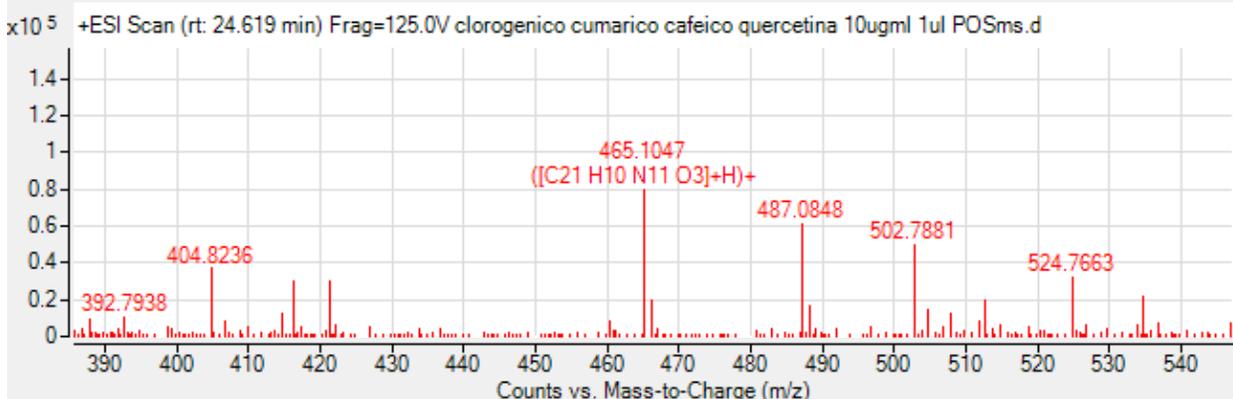
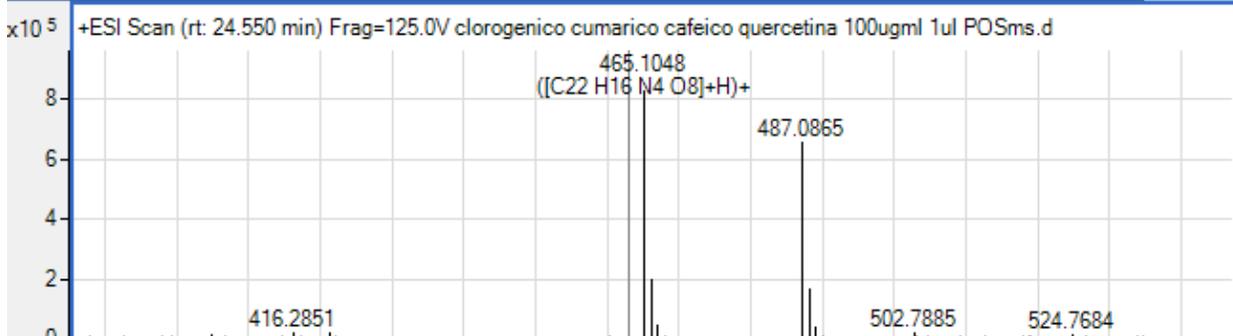




| Best | ID Source | Name | Formula          | Species | m/z      | Score | Score (RT) |
|------|-----------|------|------------------|---------|----------|-------|------------|
| ●    | MFG       |      | C22 H16 N4 O8    | (M+H)+  | 465.1048 | 96.32 |            |
| ○    | MFG       |      | C15 H16 N10 O6 S | (M+H)+  | 465.1048 | 95.5  |            |
| ○    | MFG       |      | C16 H12 N14 O2 S | (M+H)+  | 465.1048 | 95    |            |
| ○    | MFG       |      | C21 H10 N11 O3   | (M+H)+  | 465.1048 | 94.94 |            |
| ○    | MFG       |      | C17 H18 N7 O7 S  | (M+H)+  | 465.1048 | 93.03 |            |
| ○    | MFG       |      | C24 H18 N O9     | (M+H)+  | 465.1048 | 93.01 |            |
| ○    | MFG       |      | C16 H22 N3 O11 S | (M+H)+  | 465.1048 | 92.63 |            |
| ○    | MFG       |      | C23 H12 N8 O4    | (M+H)+  | 465.1048 | 92.56 |            |
| ○    | MFG       |      | C21 H20 O12      | (M+H)+  | 465.1048 | 91.28 |            |
| ○    | MFG       |      | C20 H14 N7 O7    | (M+H)+  | 465.1048 | 90.78 |            |
| ○    | MFG       |      | C18 H24 O12 S    | (M+H)+  | 465.1048 | 88.91 |            |
| ○    | MFG       |      | C14 H20 N6 O10 S | (M+H)+  | 465.1048 | 86.96 |            |
| ○    | MFG       |      | C23 H20 N4 O3 S2 | (M+H)+  | 465.1048 | 86.72 |            |
| ○    | MFG       |      | C29 H14 N5 S     | (M+H)+  | 465.1048 | 85.45 |            |
| ○    | MFG       |      | C18 H14 N11 O3 S | (M+H)+  | 465.1048 | 85.45 |            |
| ○    | MFG       |      | C21 H18 N7 O2 S2 | (M+H)+  | 465.1048 | 83.98 |            |
| ○    | MFG       |      | C22 H24 O7 S2    | (M+H)+  | 465.1048 | 82.96 |            |
| ○    | MFG       |      | C19 H20 N4 O8 S  | (M+H)+  | 465.1048 | 82.77 |            |

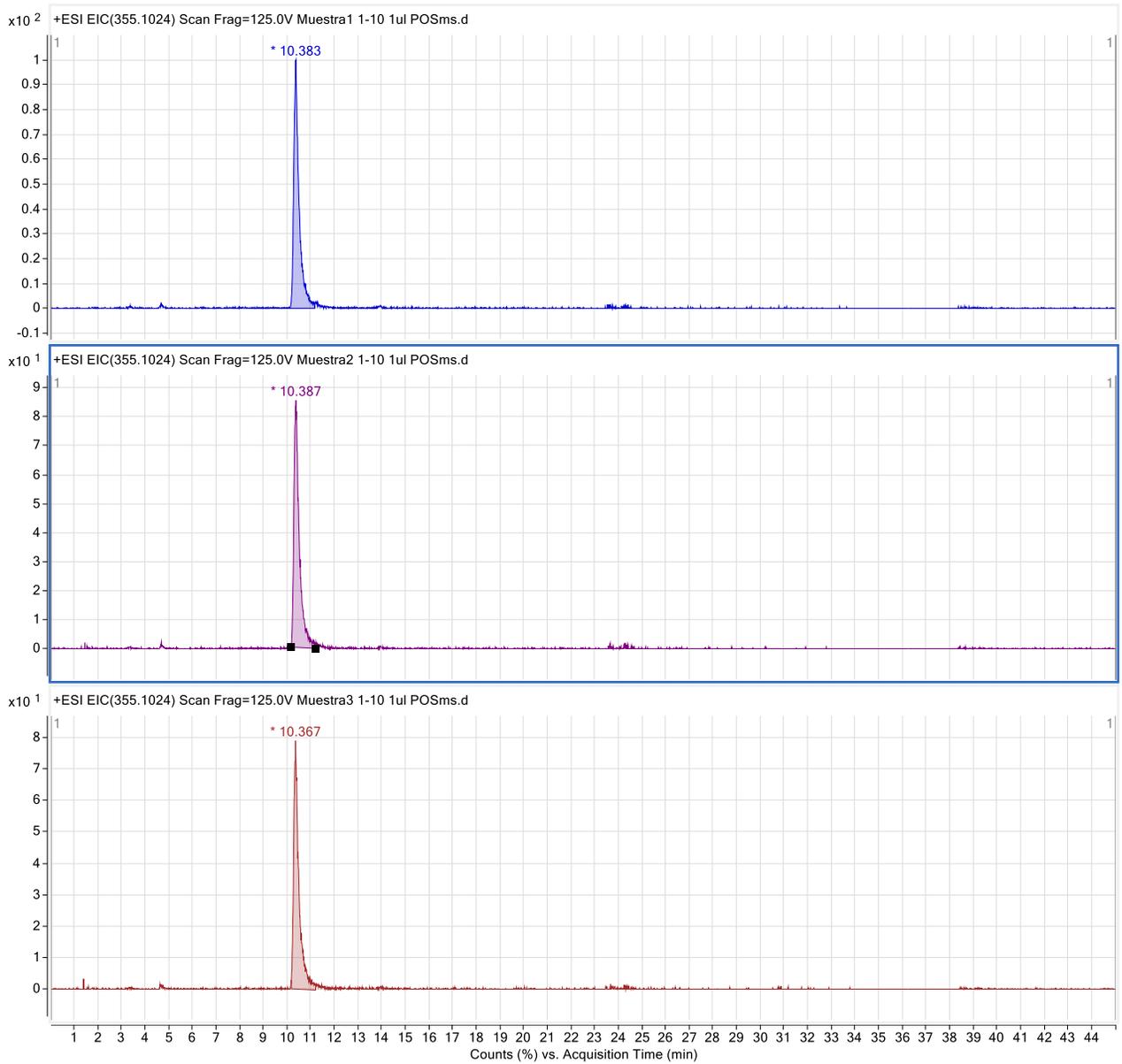
Chromatogram Results Spectrum Identification Results: + Scan (rt: 24.550 min)

**MS Spectrum Results**

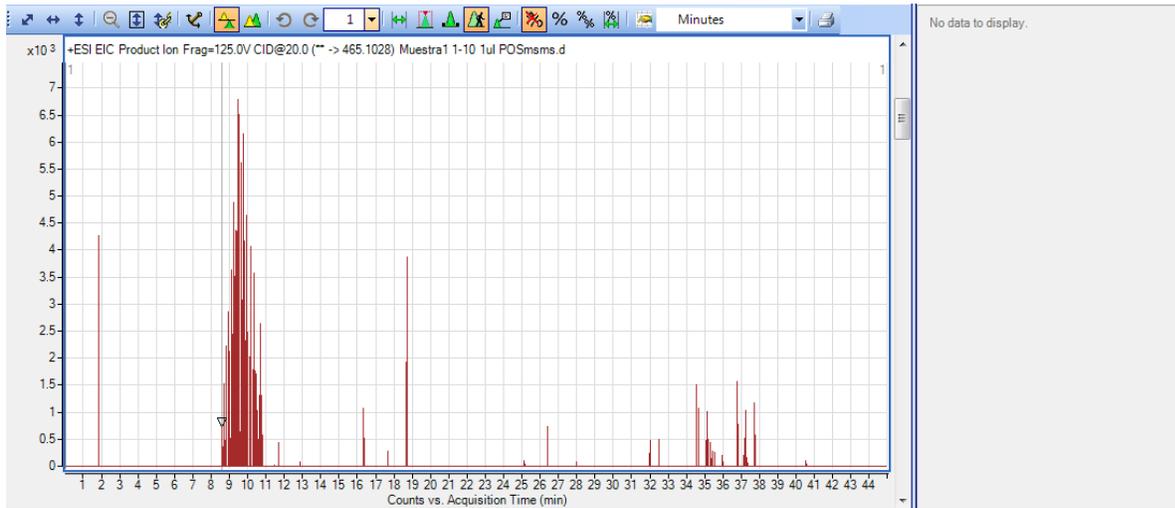
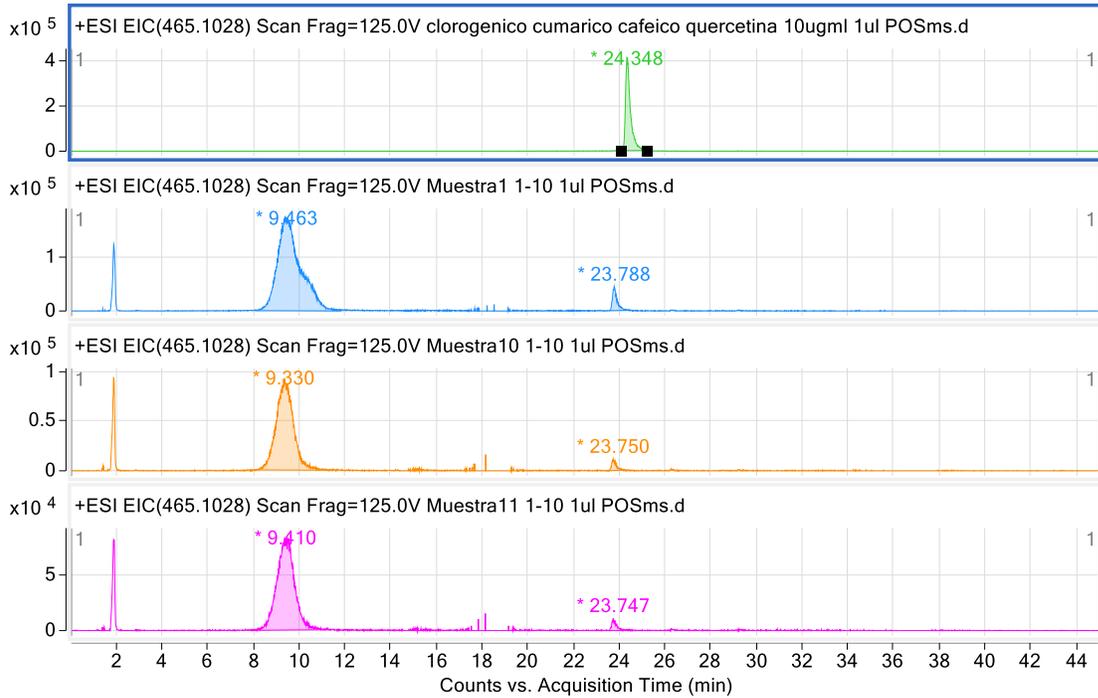


# CHLOROGENIC ACID IN SAMPLES

## SALE POINT 4 (TRIPLICATE)

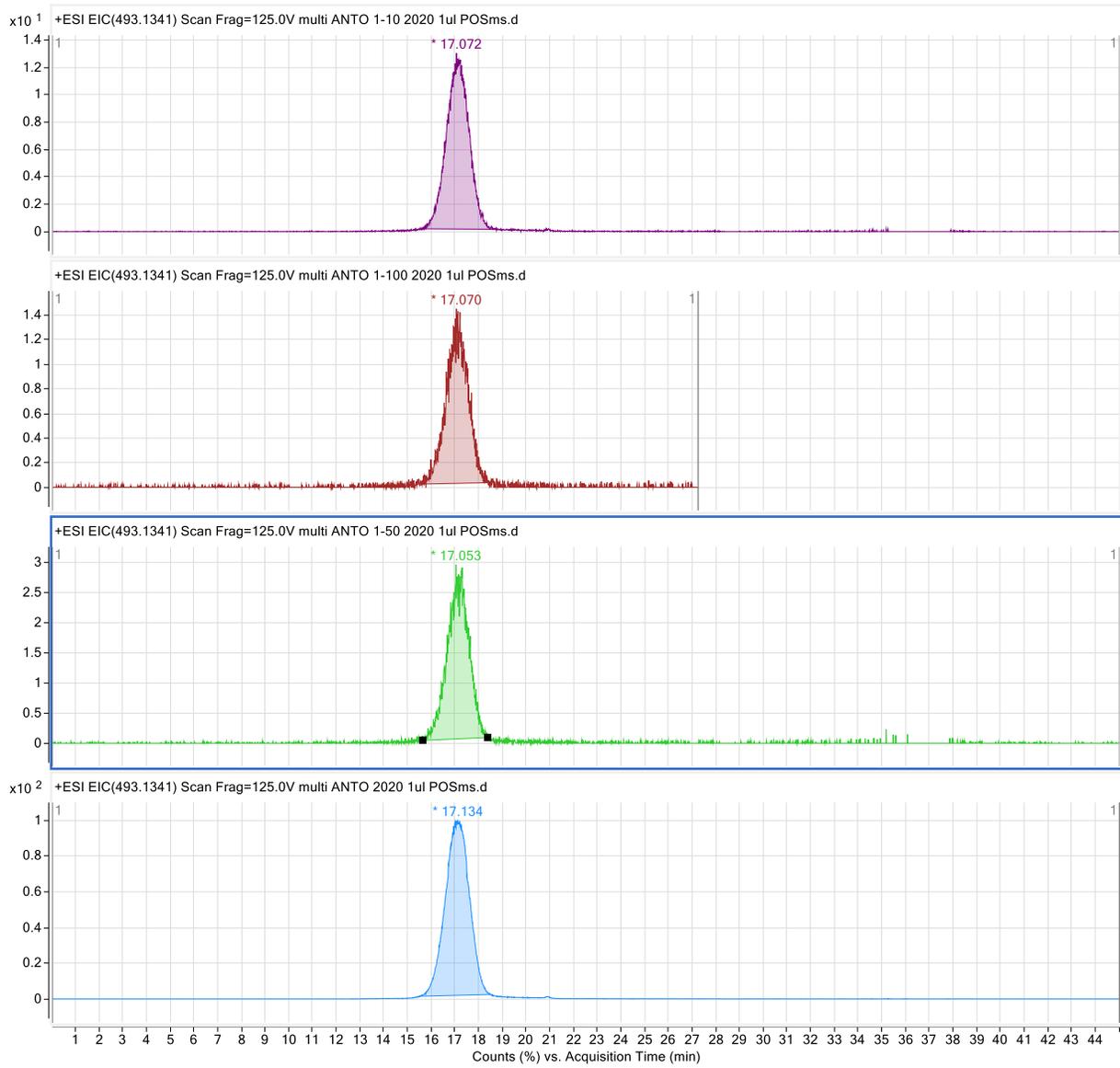


## DELPHINIDIN 3-PYRANOSIDE (465.1028) IN SAMPLES



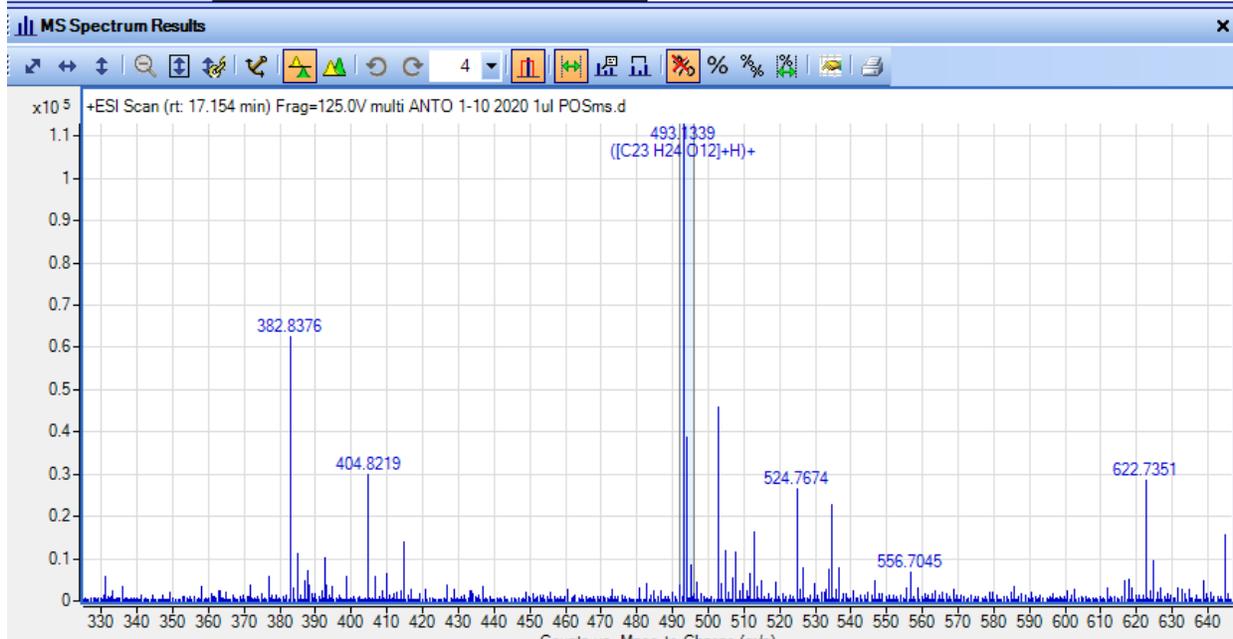
# STANDARD SOLUTIONS

## 1. Malvidin-3-glucoside (493.1341)

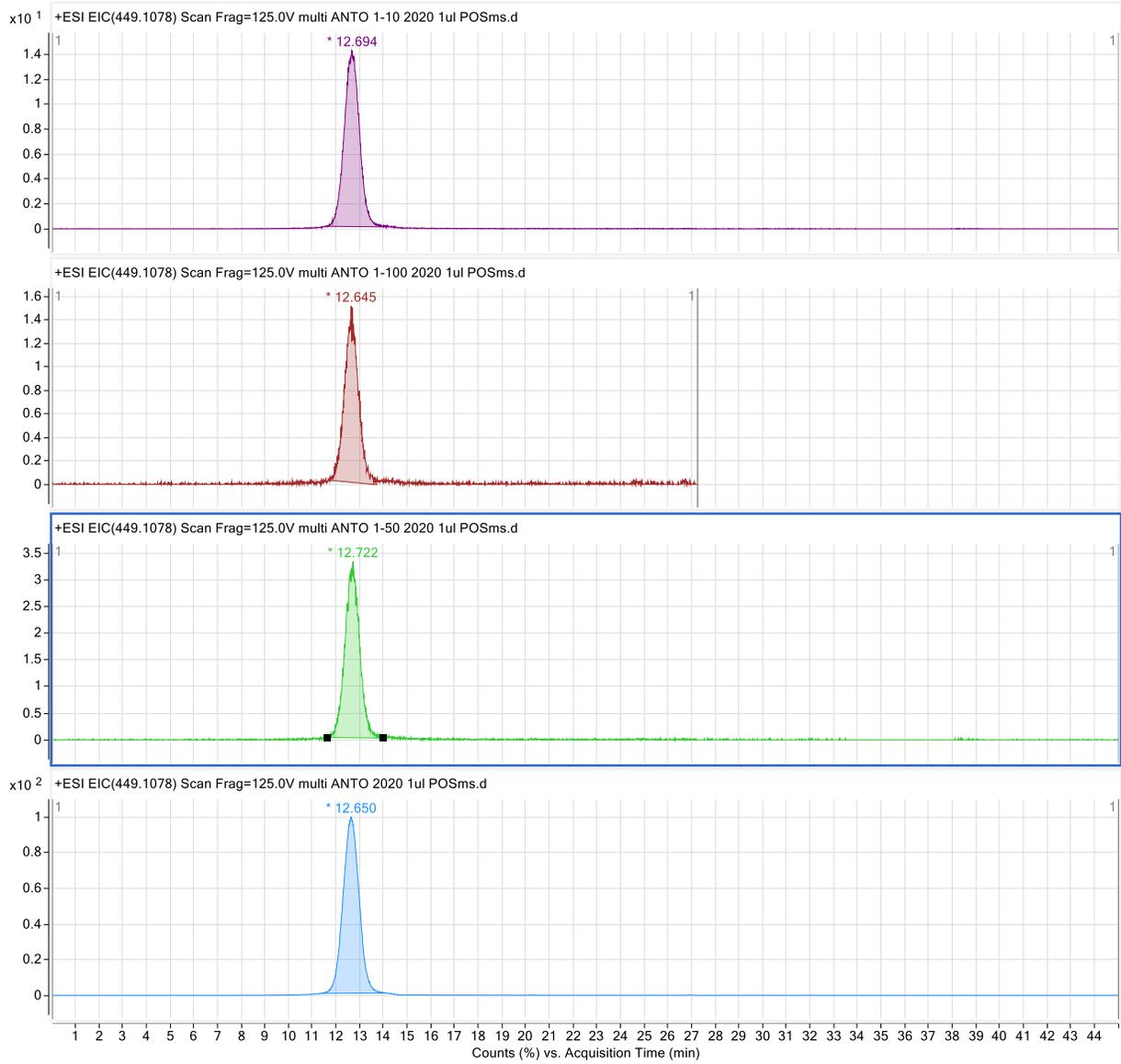


| Best | ID Source | Name | Formula          | Species | m/z      | Score | Score (RT) | RT Diff | Diff (ppm) | Score (Lit) |
|------|-----------|------|------------------|---------|----------|-------|------------|---------|------------|-------------|
| ●    | MFG       |      | C23 H24 O12      | (M+H)+  | 493.1339 | 98.67 |            |         | -0.06      |             |
| ○    | MFG       |      | C22 H18 N7 O7    | (M+H)+  | 493.1339 | 98.09 |            |         | -0.37      |             |
| ○    | MFG       |      | C24 H20 N4 O8    | (M+H)+  | 493.1339 | 95.79 |            |         | 2.5        |             |
| ○    | MFG       |      | C21 H12 N14 O2   | (M+H)+  | 493.1339 | 95.72 |            |         | -0.69      |             |
| ○    | MFG       |      | C23 H14 N11 O3   | (M+H)+  | 493.1339 | 94.36 |            |         | 2.2        |             |
| ○    | MFG       |      | C21 H22 N3 O11   | (M+H)+  | 493.1339 | 93.17 |            |         | -2.94      |             |
| ○    | MFG       |      | C20 H16 N10 O6   | (M+H)+  | 493.1339 | 91.65 |            |         | -3.27      |             |
| ○    | MFG       |      | C30 H22 N O4 S   | (M+H)+  | 493.1339 | 89    |            |         | -0.12      |             |
| ○    | MFG       |      | C26 H22 N O9     | (M+H)+  | 493.1339 | 86.36 |            |         | 5.37       |             |
| ○    | MFG       |      | C28 H20 N4 O3 S  | (M+H)+  | 493.1339 | 85.65 |            |         | -2.98      |             |
| ○    | MFG       |      | C25 H16 N8 O4    | (M+H)+  | 493.1339 | 85.47 |            |         | 5.08       |             |
| ○    | MFG       |      | C15 H18 N13 O5 S | (M+H)+  | 493.1339 | 84.52 |            |         | 0.1        |             |
| ○    | MFG       |      | C36 H16 N2 O     | (M+H)+  | 493.1339 | 84.5  |            |         | -1.09      |             |
| ○    | MFG       |      | C16 H24 N6 O10 S | (M+H)+  | 493.1339 | 83.28 |            |         | 0.48       |             |
| ○    | MFG       |      | C31 H18 N5 S     | (M+H)+  | 493.1339 | 83.17 |            |         | 2.48       |             |
| ○    | MFG       |      | C17 H20 N10 O6 S | (M+H)+  | 493.1339 | 82.59 |            |         | 3.03       |             |
| ○    | MFG       |      | C23 H22 N7 O2 S2 | (M+H)+  | 493.1339 | 81.9  |            |         | 0.74       |             |
| ○    | MFG       |      | C19 H20 N6 O10   | (M+H)+  | 493.1339 | 80.9  |            |         | -5.83      |             |

Chromatogram Results Spectrum Identification Results: + Scan (rt: 17.154 min)



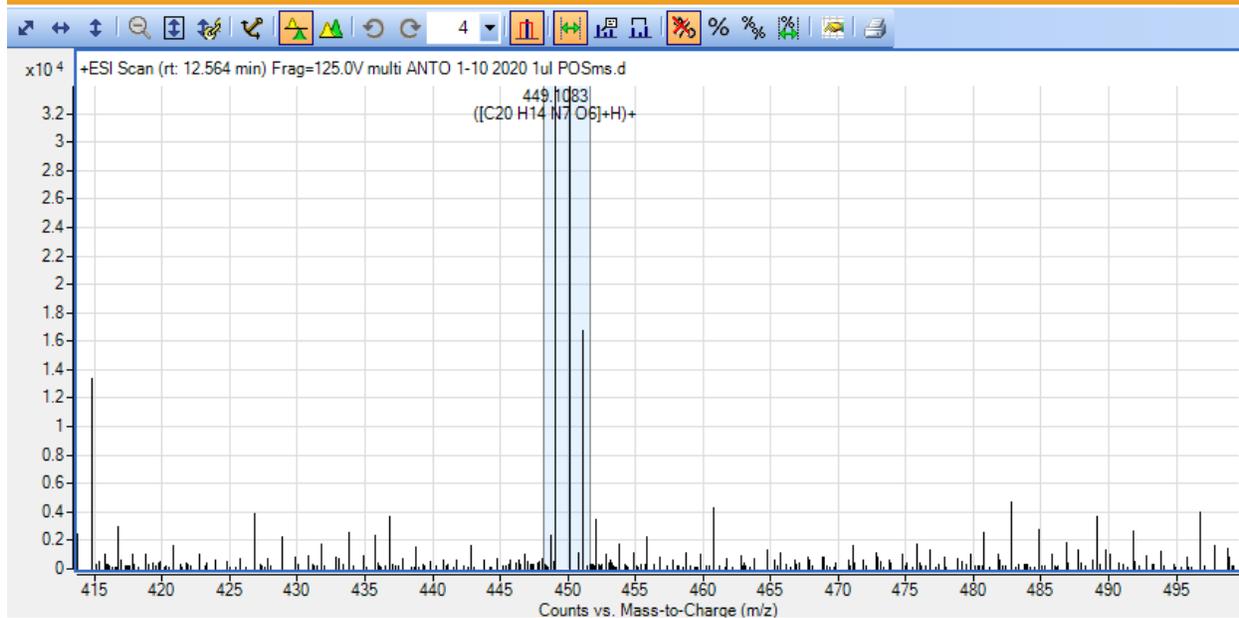
## 2. Cyanidin-3-glucoside (449.1078)



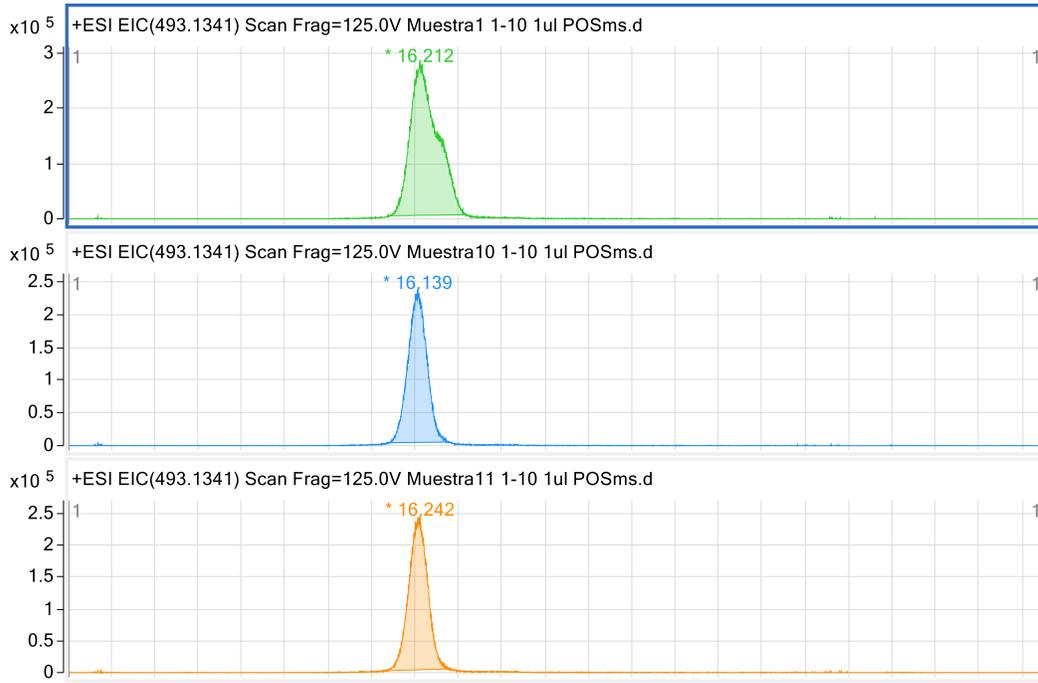
| Best                             | ID Source | Name | Formula          | Species | m/z      | Score | Score (RT) | RT Diff | Diff (ppm) | Score (Lit) |
|----------------------------------|-----------|------|------------------|---------|----------|-------|------------|---------|------------|-------------|
| <input checked="" type="radio"/> | MFG       |      | C20 H14 N7 O6    | (M+H)+  | 449.1083 | 97.88 |            |         | -0.74      |             |
| <input type="radio"/>            | MFG       |      | C21 H20 O11      | (M+H)+  | 449.1083 | 97.68 |            |         | -0.42      |             |
| <input type="radio"/>            | MFG       |      | C22 H16 N4 O7    | (M+H)+  | 449.1083 | 94.07 |            |         | 2.41       |             |
| <input type="radio"/>            | MFG       |      | C21 H10 N11 O2   | (M+H)+  | 449.1083 | 93.45 |            |         | 2.1        |             |
| <input type="radio"/>            | MFG       |      | C19 H18 N3 O10   | (M+H)+  | 449.1083 | 92.94 |            |         | -3.57      |             |
| <input type="radio"/>            | MFG       |      | C18 H12 N10 O5   | (M+H)+  | 449.1083 | 92.32 |            |         | -3.91      |             |
| <input type="radio"/>            | MFG       |      | C14 H20 N6 O9 S  | (M+H)+  | 449.1083 | 91.73 |            |         | 0.26       |             |
| <input type="radio"/>            | MFG       |      | C15 H16 N10 O5 S | (M+H)+  | 449.1083 | 91.04 |            |         | 3.07       |             |
| <input type="radio"/>            | MFG       |      | C16 H22 N3 O10 S | (M+H)+  | 449.1083 | 87.23 |            |         | 3.45       |             |
| <input type="radio"/>            | MFG       |      | C28 H18 N O3 S   | (M+H)+  | 449.1083 | 86.58 |            |         | -0.44      |             |
| <input type="radio"/>            | MFG       |      | C12 H18 N9 O8 S  | (M+H)+  | 449.1083 | 86.35 |            |         | -2.95      |             |
| <input type="radio"/>            | MFG       |      | C21 H18 N7 O S2  | (M+H)+  | 449.1083 | 85.74 |            |         | 0.58       |             |
| <input type="radio"/>            | MFG       |      | C22 H24 O6 S2    | (M+H)+  | 449.1083 | 83.99 |            |         | 0.88       |             |
| <input type="radio"/>            | MFG       |      | C19 H16 N10 S2   | (M+H)+  | 449.1083 | 83.9  |            |         | -2.57      |             |
| <input type="radio"/>            | MFG       |      | C13 H24 N2 O13 S | (M+H)+  | 449.1083 | 83.66 |            |         | -2.52      |             |
| <input type="radio"/>            | MFG       |      | C26 H16 N4 O2 S  | (M+H)+  | 449.1083 | 83.21 |            |         | -3.57      |             |
| <input type="radio"/>            | MFG       |      | C20 H22 N3 O5 S2 | (M+H)+  | 449.1083 | 83.05 |            |         | -2.26      |             |
| <input type="radio"/>            | MFG       |      | C16 H12 N14 O S  | (M+H)+  | 449.1083 | 82.64 |            |         | 5.91       |             |

Chromatogram Results Spectrum Identification Results: + Scan (rt: 12.564 min)

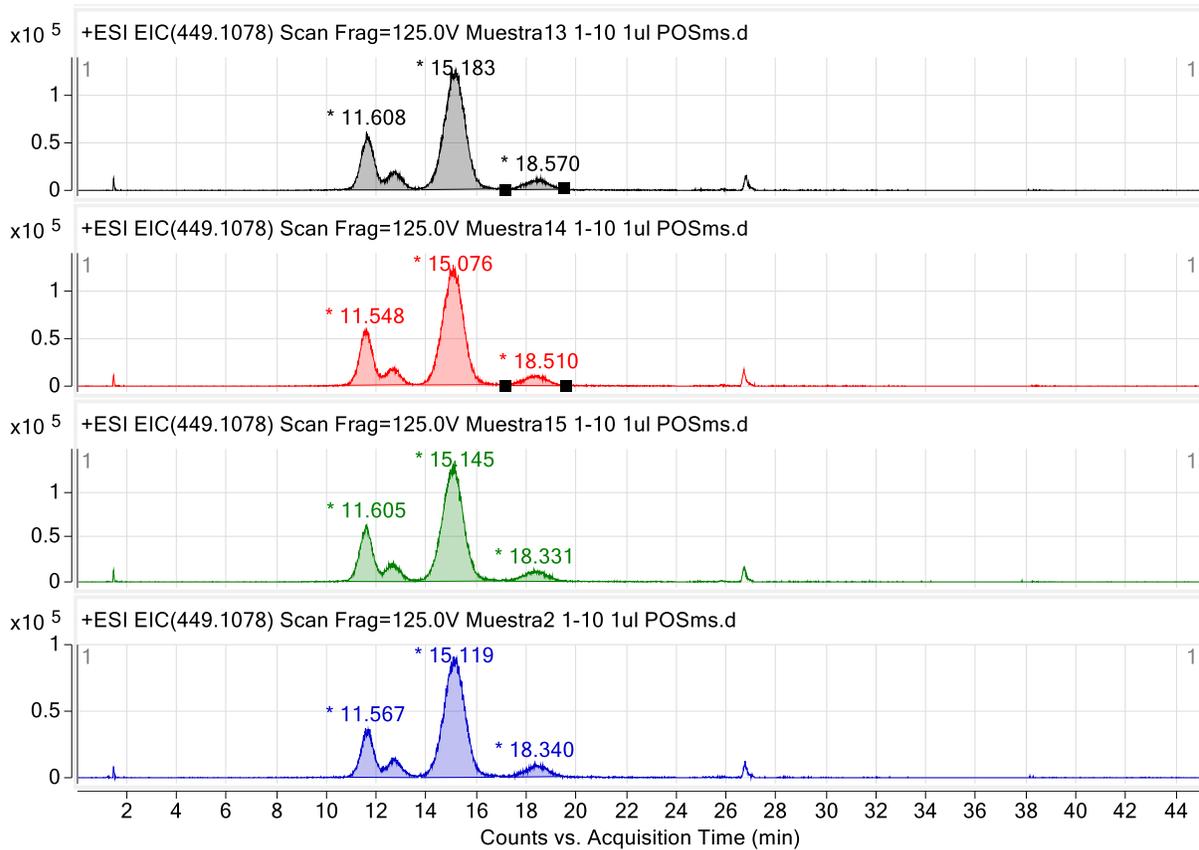
MS Spectrum Results

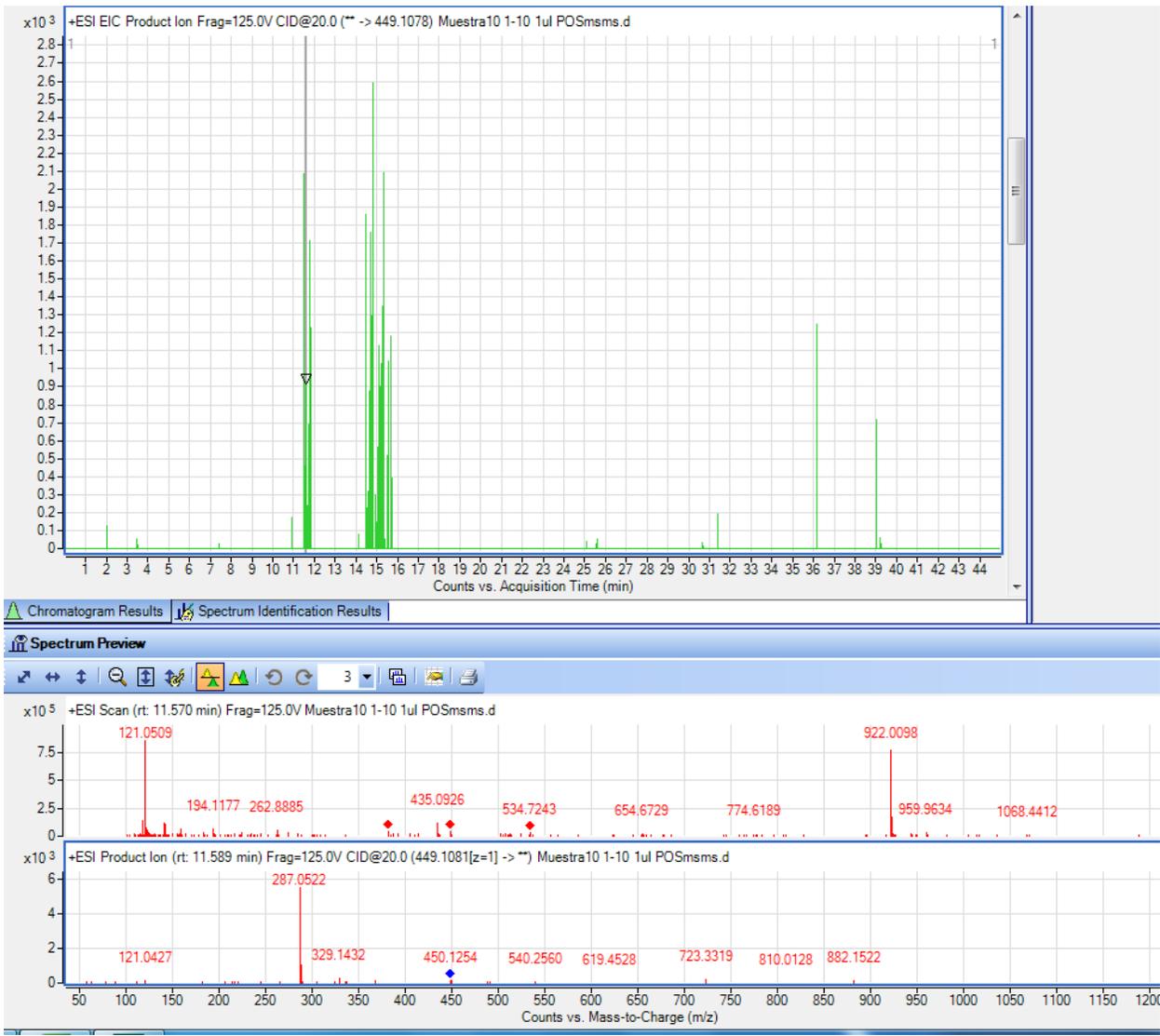


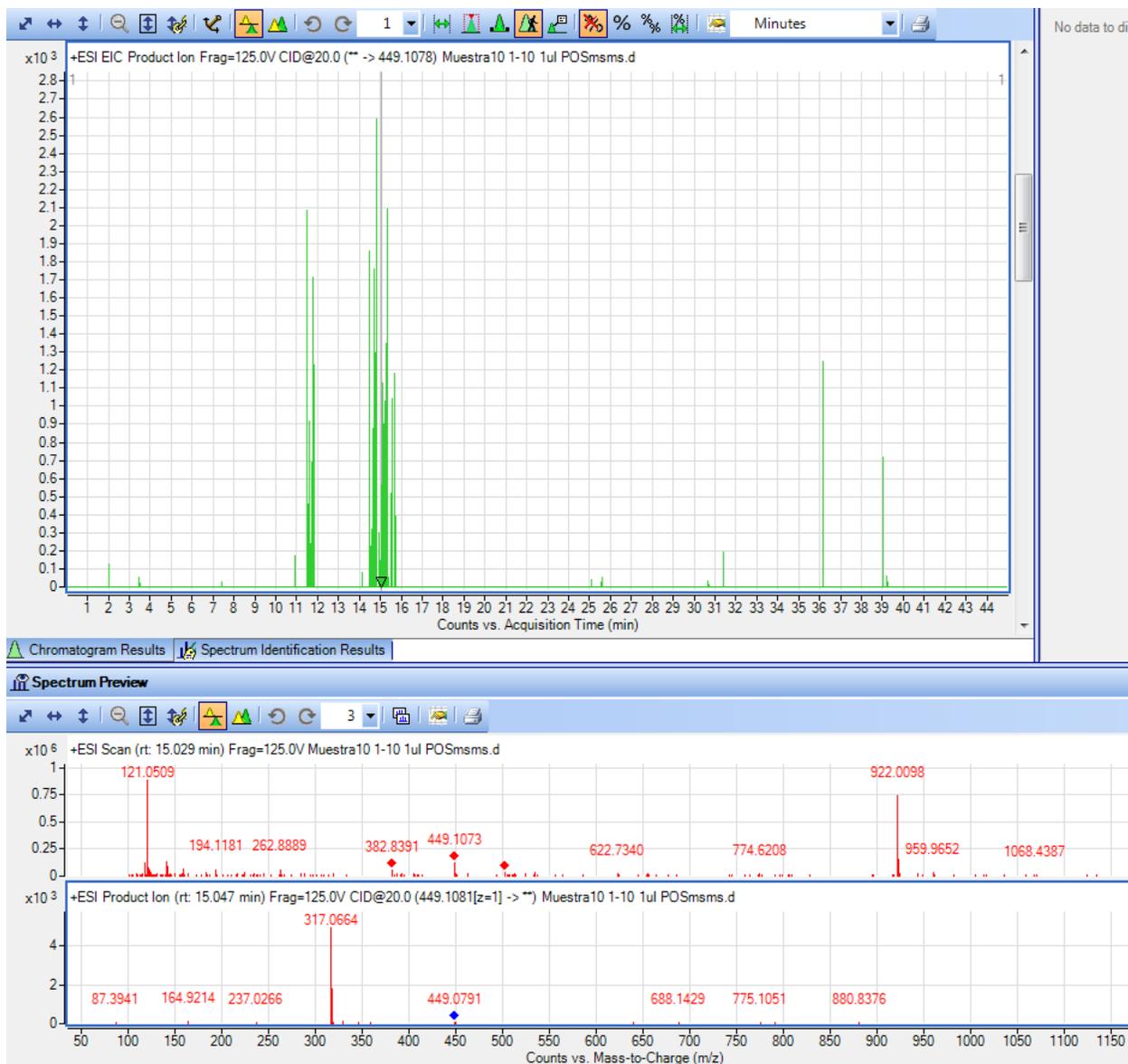
### MALVIDIN 3-GLUCOSIDE (493.1341) IN SAMPLES



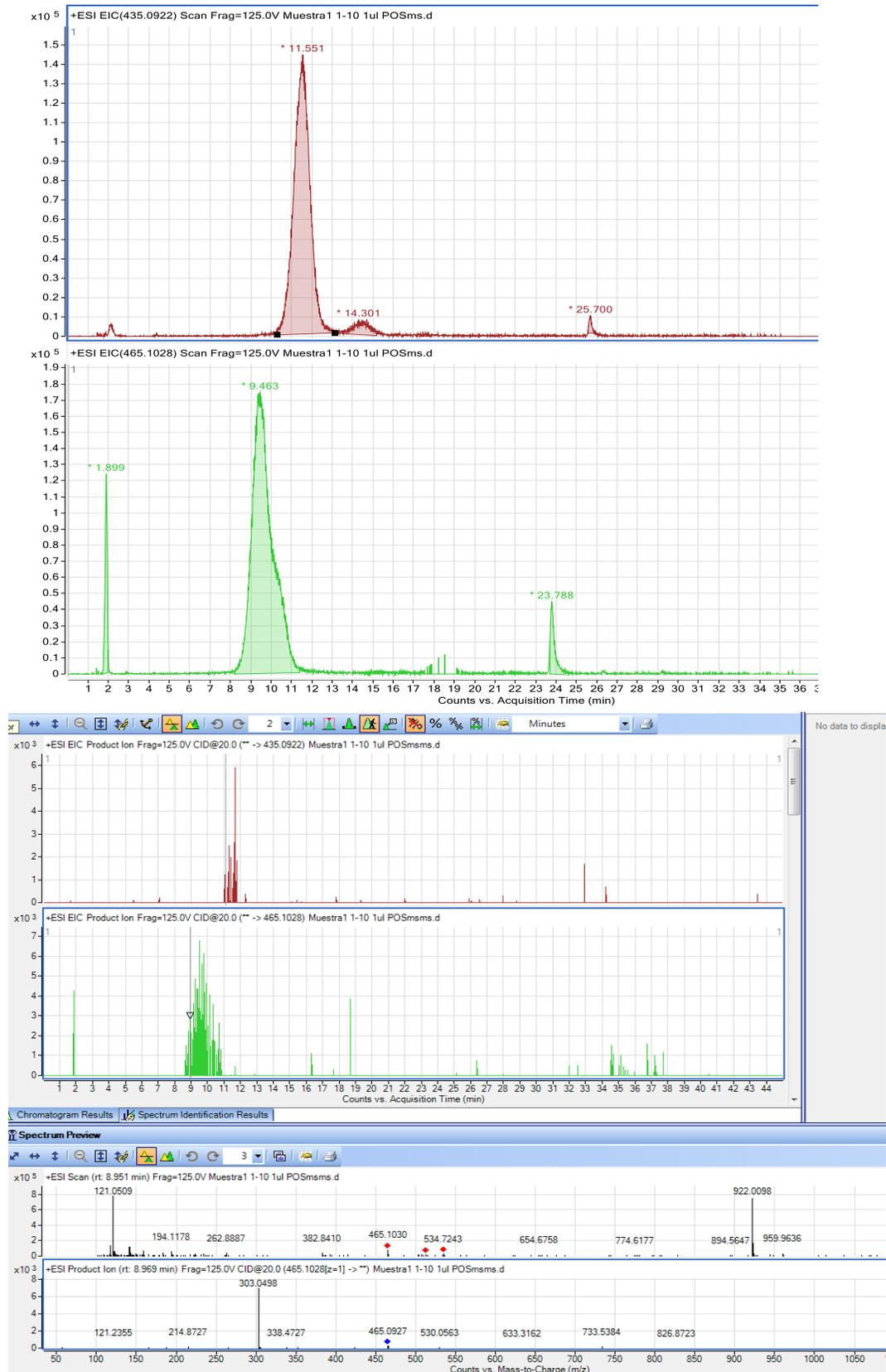
### CYANIDIN-3-O-GLUCOSIDE (449.1078) IN SAMPLES



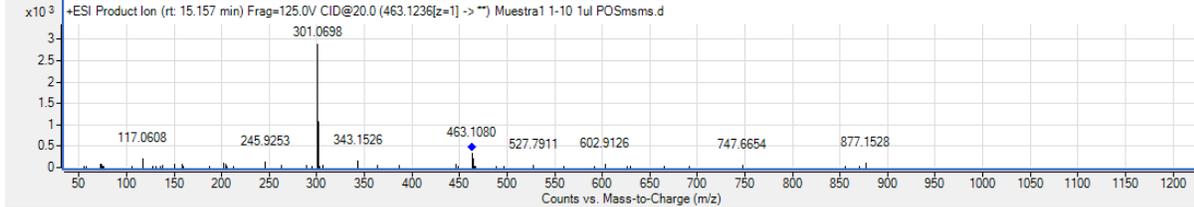
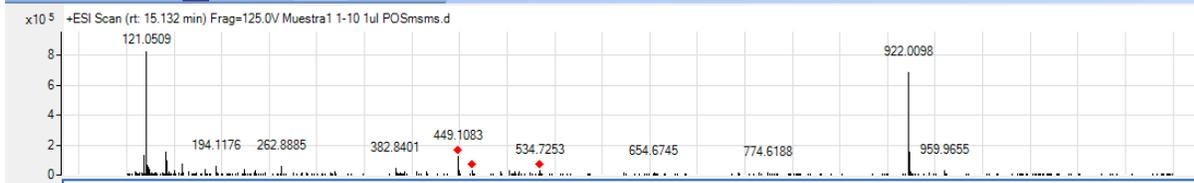
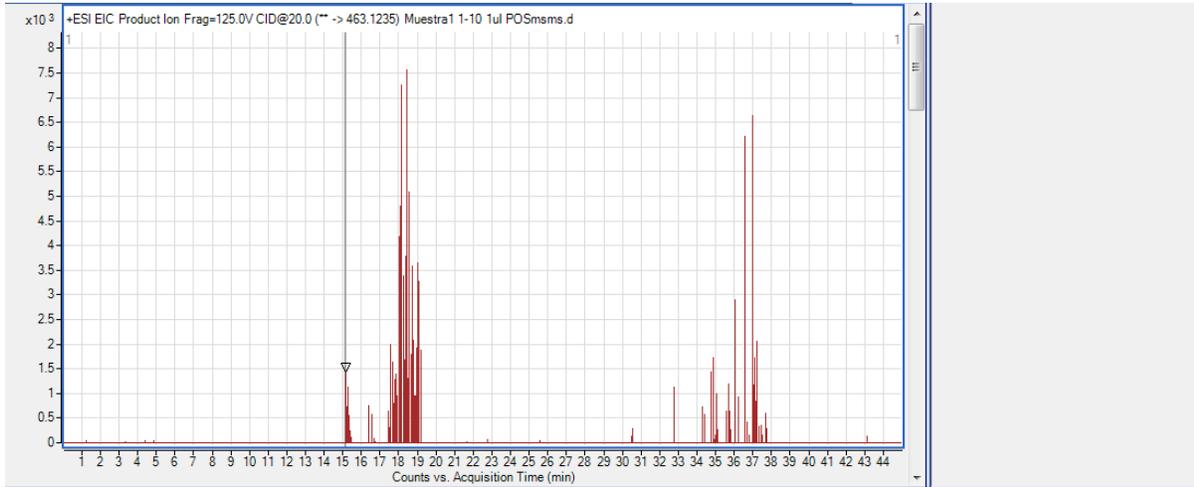
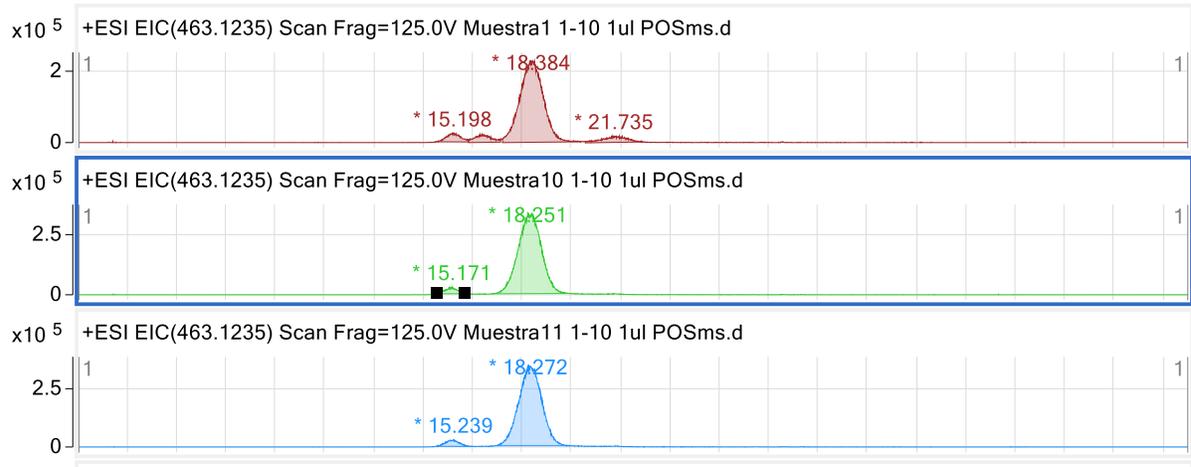


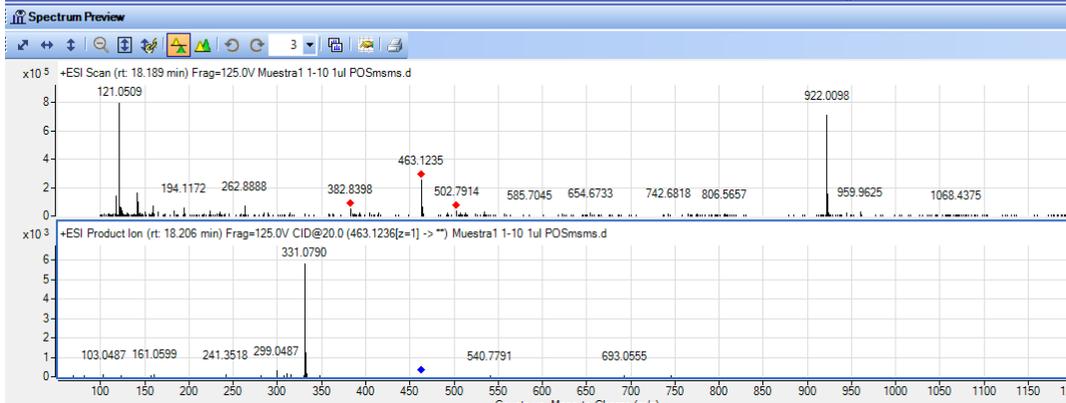
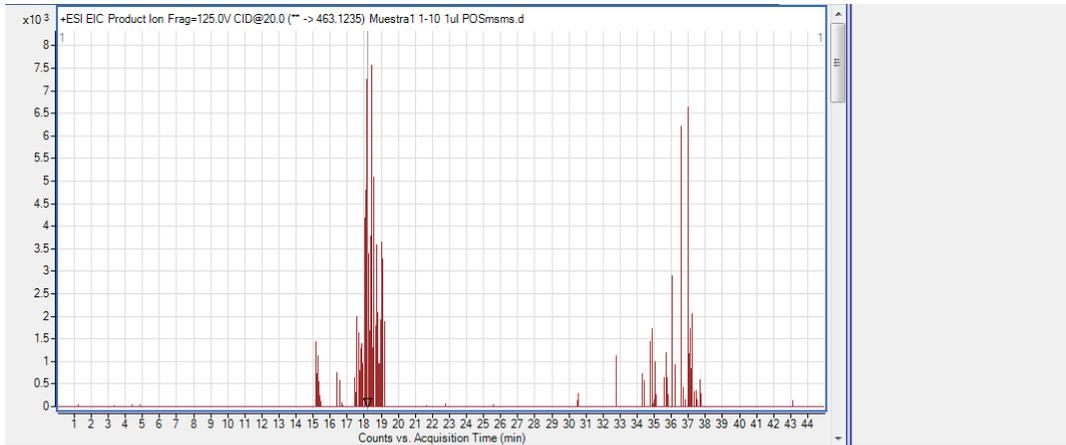
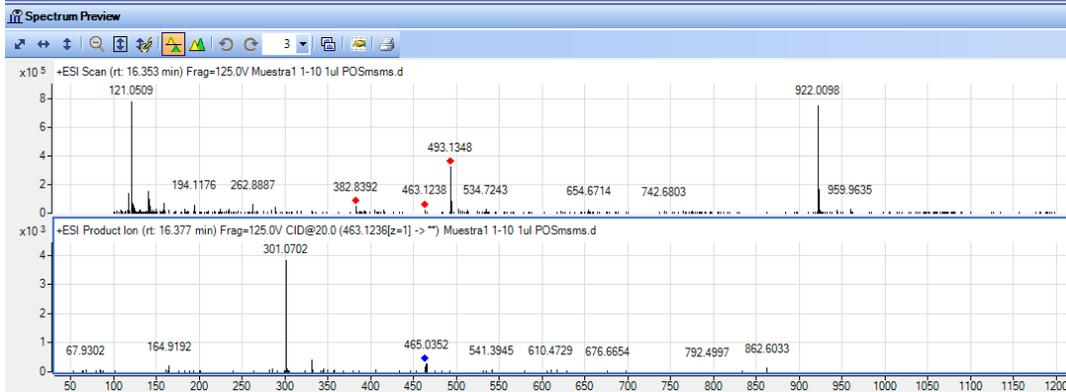
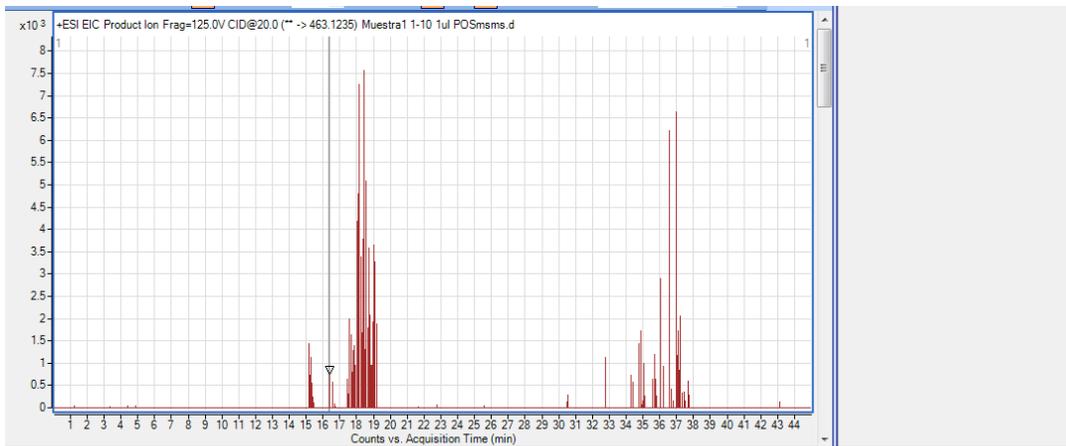


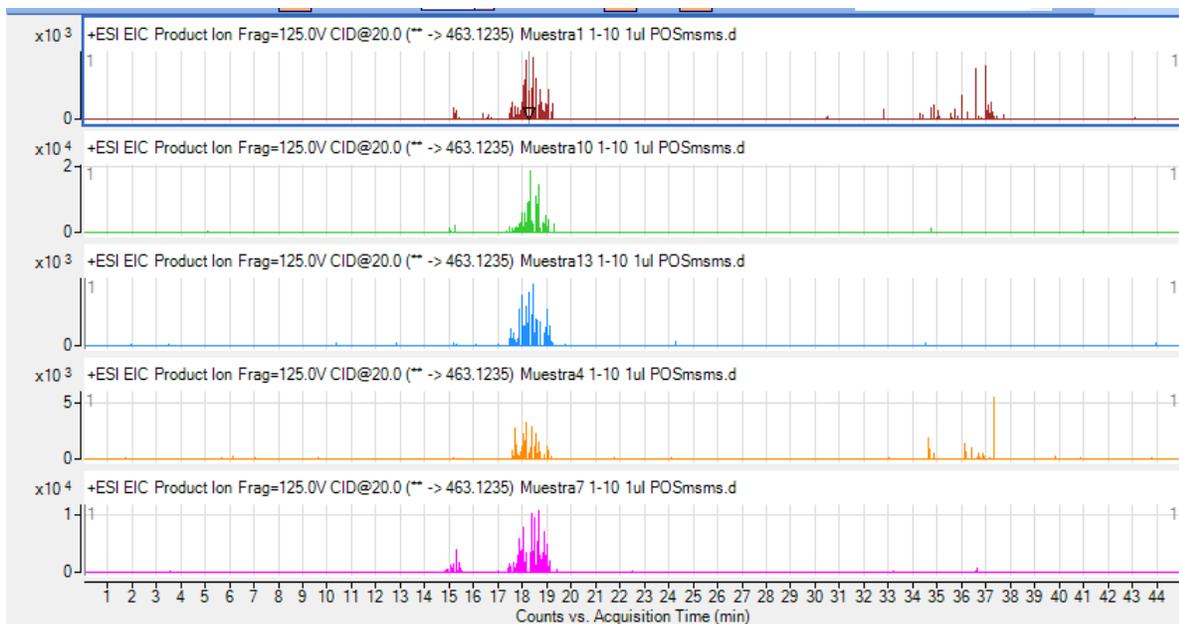
# DELPHINIDIN 3-ARABINOSIDE (435.0922) AND 3-PYRANOSIDE (465.1028) IN SAMPLES



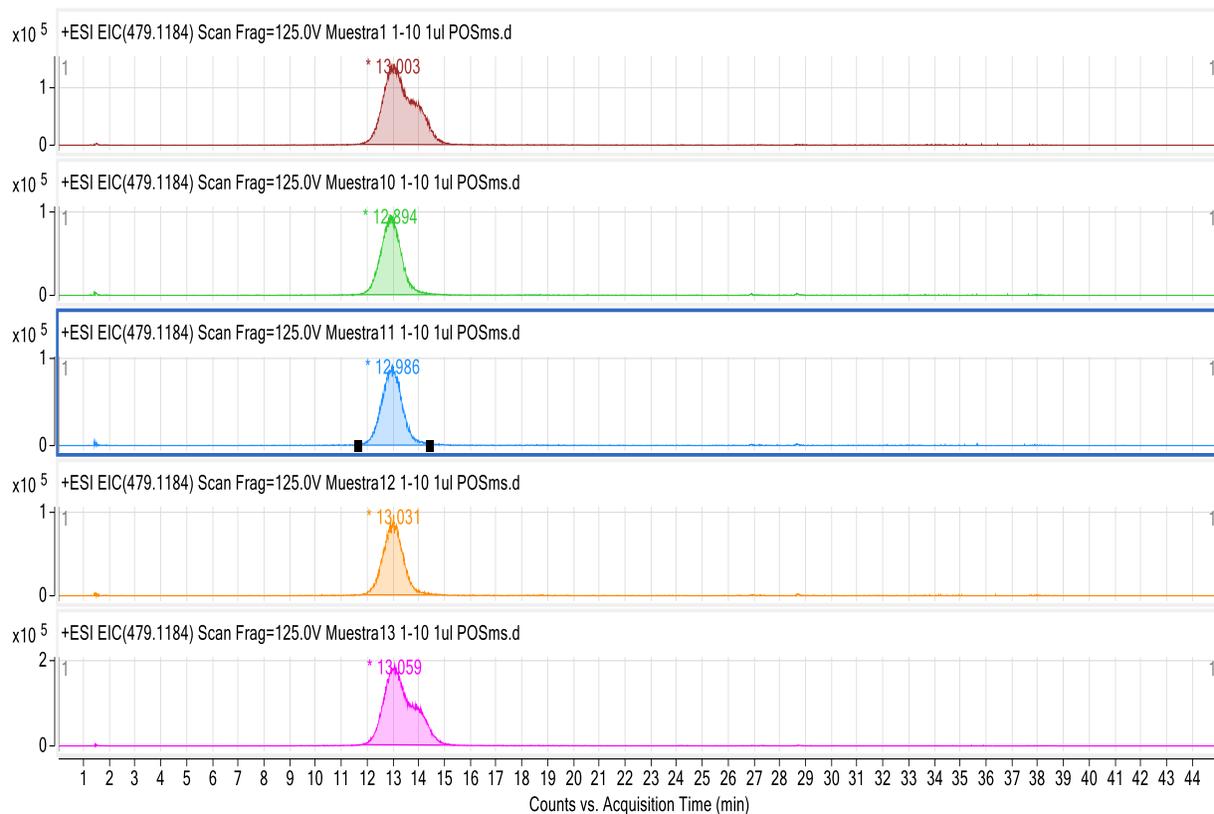
### MALVIDIN-3-ARABINOSIDE (463.1235) AND PEONIDIN 3-PYRANOSIDE (463.1235) IN SAMPLES



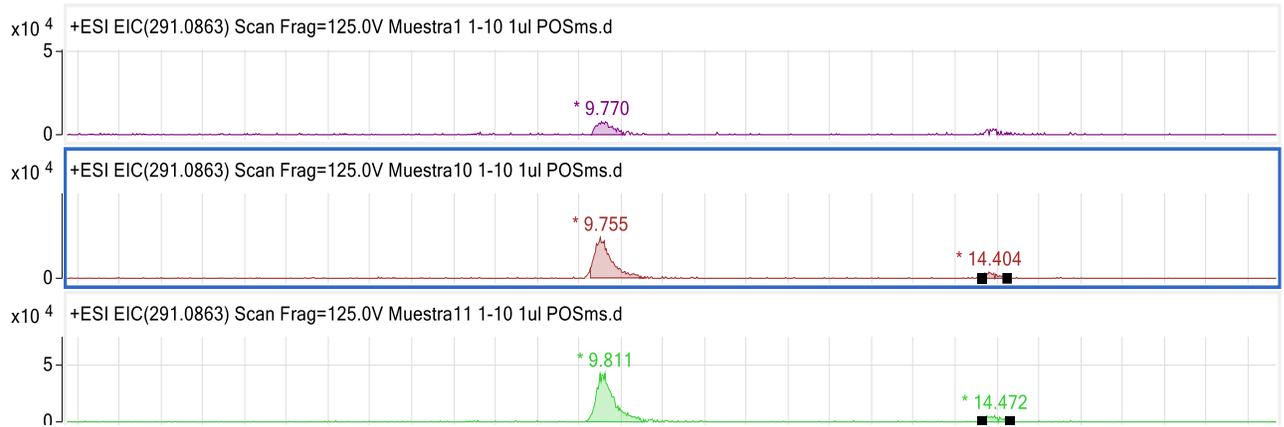




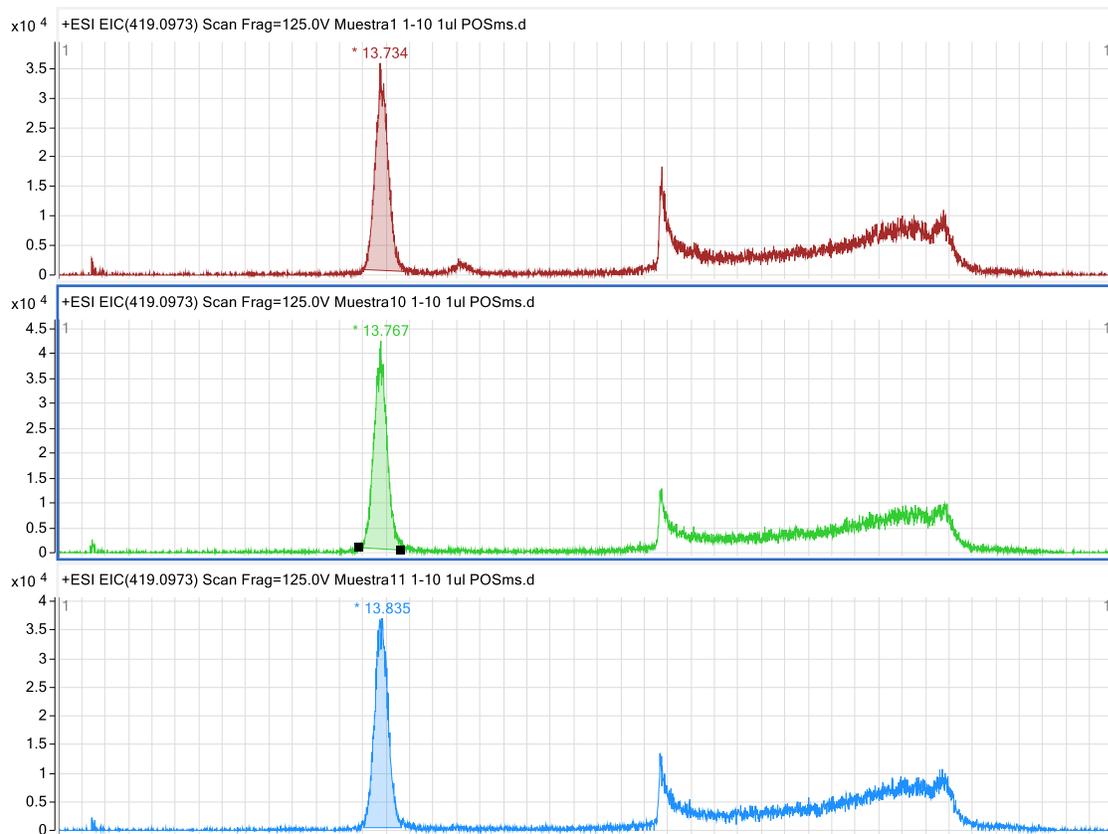
### PETUNIDIN-3-PYRANOSIDE (479.1184) IN SAMPLES



### CATECHIN/EPICATECHIN (291.0863) IN SAMPLES



### CYANIDIN 3-ARABINOSIDE (419.0973) IN SAMPLES



| Best | ID Source | Name | Formula          | Species | m/z      | Score | Score (RT) | RT Diff | Diff (ppm) | Score (Lib) |
|------|-----------|------|------------------|---------|----------|-------|------------|---------|------------|-------------|
| ●    | MFG       |      | C20 H18 O10      | (M+H)+  | 419.0972 | 99.1  |            |         | -0.17      |             |
| ○    | MFG       |      | C19 H12 N7 O5    | (M+H)+  | 419.0972 | 97.47 |            |         | -0.55      |             |
| ○    | MFG       |      | C21 H14 N4 O6    | (M+H)+  | 419.0972 | 94.89 |            |         | 2.84       |             |
| ○    | MFG       |      | C18 H16 N3 O9    | (M+H)+  | 419.0972 | 92.38 |            |         | -3.56      |             |
| ○    | MFG       |      | C17 H10 N10 O4   | (M+H)+  | 419.0972 | 89.69 |            |         | -3.97      |             |
| ○    | MFG       |      | C27 H16 N O2 S   | (M+H)+  | 419.0972 | 88.97 |            |         | -0.29      |             |
| ○    | MFG       |      | C25 H14 N4 O S   | (M+H)+  | 419.0972 | 84.43 |            |         | -3.66      |             |
| ○    | MFG       |      | C13 H18 N6 O8 S  | (M+H)+  | 419.0972 | 84.13 |            |         | 0.41       |             |
| ○    | MFG       |      | C23 H16 N O7     | (M+H)+  | 419.0972 | 84.01 |            |         | 6.22       |             |
| ○    | MFG       |      | C14 H14 N10 O4 S | (M+H)+  | 419.0972 | 82.89 |            |         | 3.4        |             |
| ○    | MFG       |      | C20 H16 N7 S2    | (M+H)+  | 419.0972 | 82.84 |            |         | 0.75       |             |
| ○    | MFG       |      | C21 H22 O5 S2    | (M+H)+  | 419.0972 | 82.58 |            |         | 1.1        |             |
| ○    | MFG       |      | C22 H10 N8 O2    | (M+H)+  | 419.0972 | 82.25 |            |         | 5.88       |             |
| ○    | MFG       |      | C15 H20 N3 O9 S  | (M+H)+  | 419.0972 | 81.05 |            |         | 3.86       |             |
| ○    | MFG       |      | C19 H20 N3 O4 S2 | (M+H)+  | 419.0972 | 80.35 |            |         | -2.28      |             |
| ○    | MFG       |      | C16 H14 N6 O8    | (M+H)+  | 419.0972 | 78.15 |            |         | -6.98      |             |
| ○    | MFG       |      | C12 H22 N2 O12 S | (M+H)+  | 419.0972 | 77.44 |            |         | -2.53      |             |
| ○    | MFG       |      | C11 H16 N9 O7 S  | (M+H)+  | 419.0972 | 76.7  |            |         | -3.07      |             |
| ○    | MFG       |      | C24 H18 O5 S     | (M+H)+  | 419.0972 | 76.42 |            |         | -6.69      |             |
| ○    | MFG       |      | C22 H18 N4 O S2  | (M+H)+  | 419.0972 | 76.21 |            |         | 4.13       |             |

Chromatogram Results Spectrum Identification Results: + Scan (rt: 13.169-14.420 min)

MS Spectrum Results



x10<sup>5</sup> +ESI Scan (rt: 13.169-14.396 min, 105 scans) Frag=125.0V Muestra8 1-10 1ul POSms.d



x10<sup>5</sup> +ESI Scan (rt: 13.169-14.396 min, 105 scans) Frag=125.0V Muestra8 1-10 1ul POSms.d



x10<sup>5</sup> +ESI Scan (rt: 13.169-14.420 min, 107 scans) Frag=125.0V Muestra9 1-10 1ul POSms.d

