# Enzymatic synthesis of a novel pterostilbene α-glucoside by the combination of cyclodextrin glucanotransferase and amyloglucosidase

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**Figure S1:** ESI-MS spectrum (positive mode) of the isolated pterostilbene monoglucoside.

**Figure S2:** ESI-MS spectrum (negative mode) of the isolated pterostilbene diglucoside.

**Figure S3:** NMR Spectra (600 MHz, DMSO-d6, 298 K) for pteroestilbene 4'-O-α-D-glucopyranoside: (a) $^1$H spectrum; (b) COSY; (c) HSQC- edited; (d) NOESY 500 ms.

**Figure S4:** HRMS and elementary composition calculation for pterostilbene 4'-O-α-D-glucopyranoside.

**Figure S1.**

ESI-MS spectrum (positive mode) of the isolated pterostilbene monoglucoside.

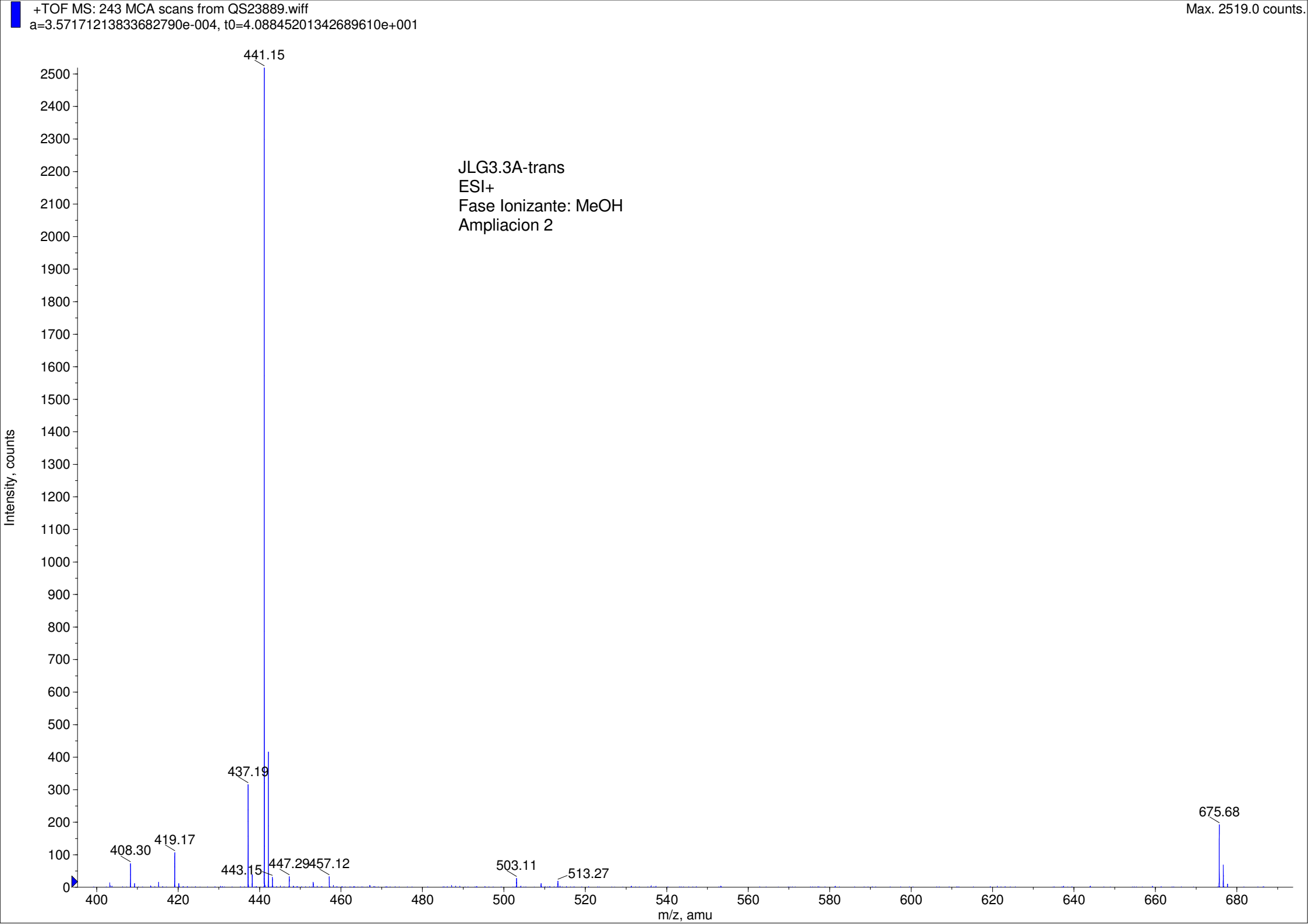

+TOF MS: 243 MCA scans from QS23889.wiff
a=3.57171213833682790e-004, t0=4.08845201342689610e+001
Max. 2519.0 counts.
441.15
JLG3.3A-trans
ESI+
Fase Ionizante: MeOH
Ampliacion 2
437.19
675.68
419.17
408.30
443.15
447.29
457.12
503.11
513.27
Intensity, counts
m/z, amu

**Figure S2.**

ESI-MS spectrum (negative mode) of the isolated pterostilbene diglucoside.

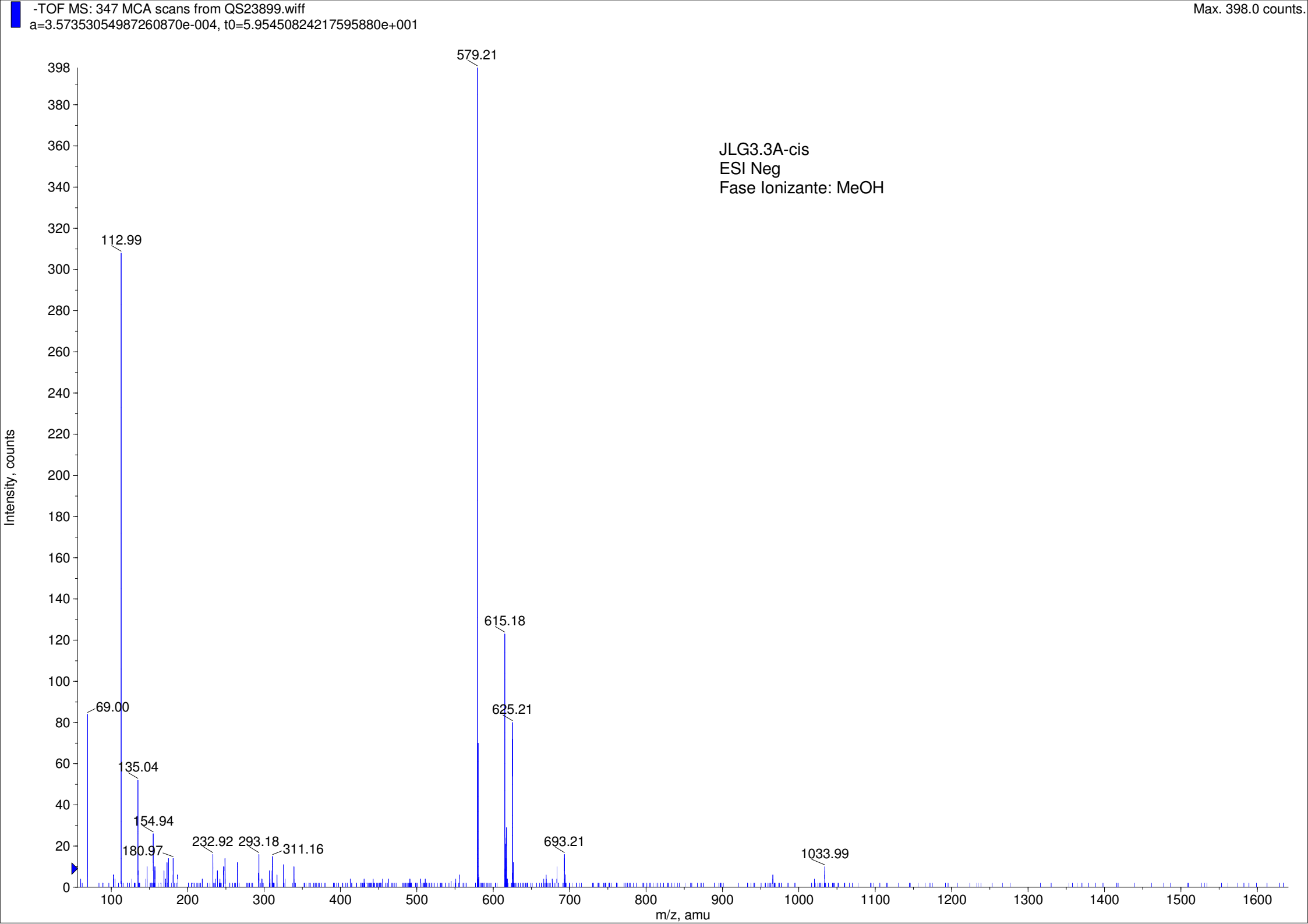
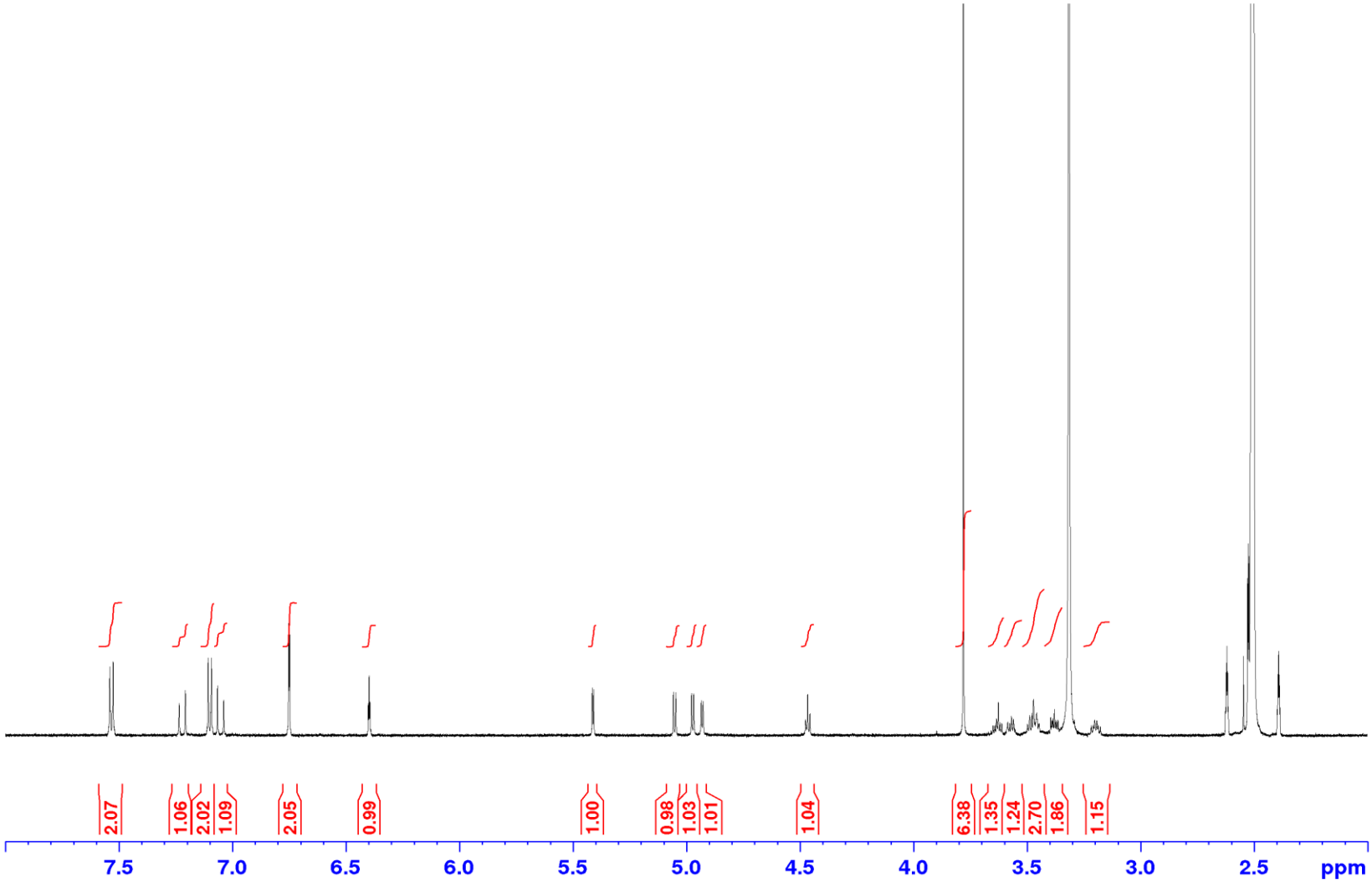

-TOF MS: 347 MCA scans from QS23899.wiff
a=3.57353054987260870e-004, t0=5.95450824217595880e+001
Max. 398.0 counts.
JLG3.3A-cis
ESI Neg
Fase Ionizante: MeOH
579.21
112.99
615.18
625.21
69.00
135.04
154.94
180.97
232.92
293.18
311.16
693.21
1033.99
Intensity, counts
m/z, amu

**Figure S3.**

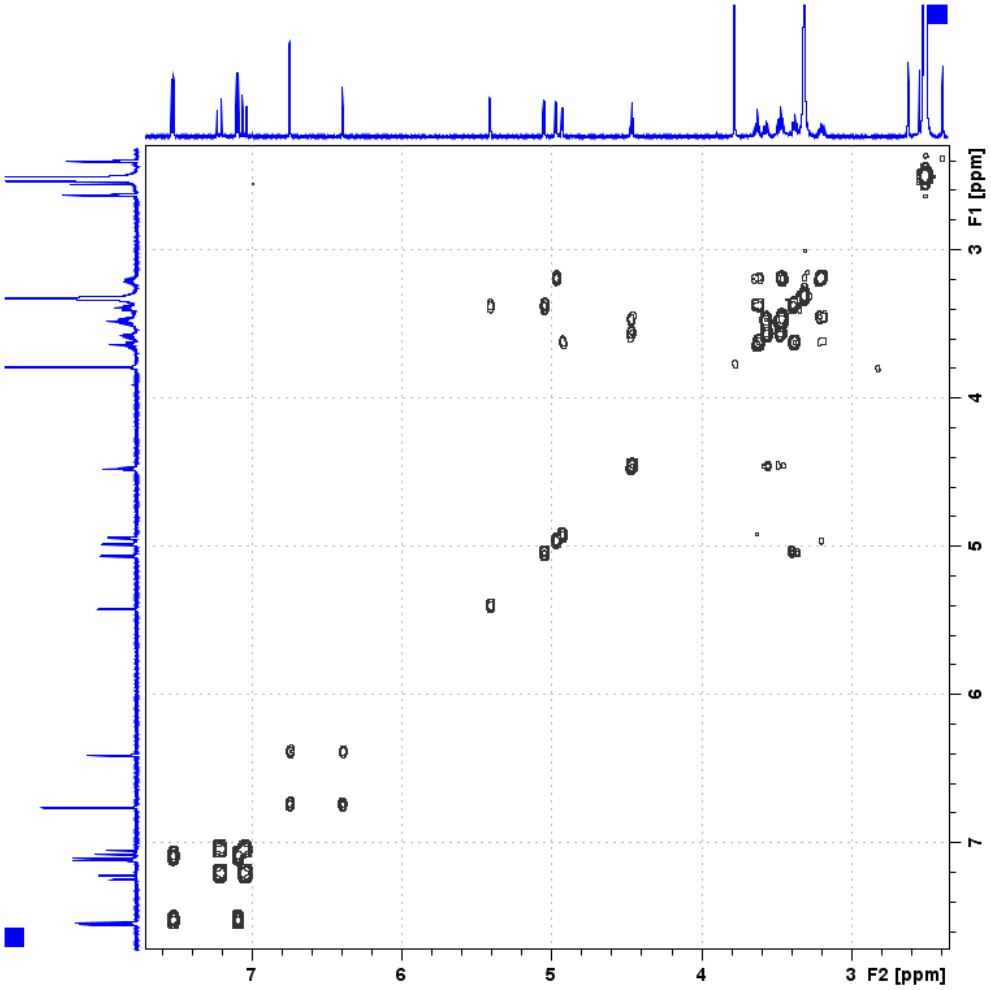
NMR Spectra (600 MHz, DMSO-d6, 298 K) for pteroestilbene 4'-O-$\alpha$-D-glucopyranoside: (a) $^{1}$H spectrum; (b) COSY; (c) HSQC- edited; (d) NOESY 500 ms.

**NMR Spectra (600 MHz, DMSO-$d_6$, 298K) for pteroestilbene 4'-O-α-D-glucopyranoside**

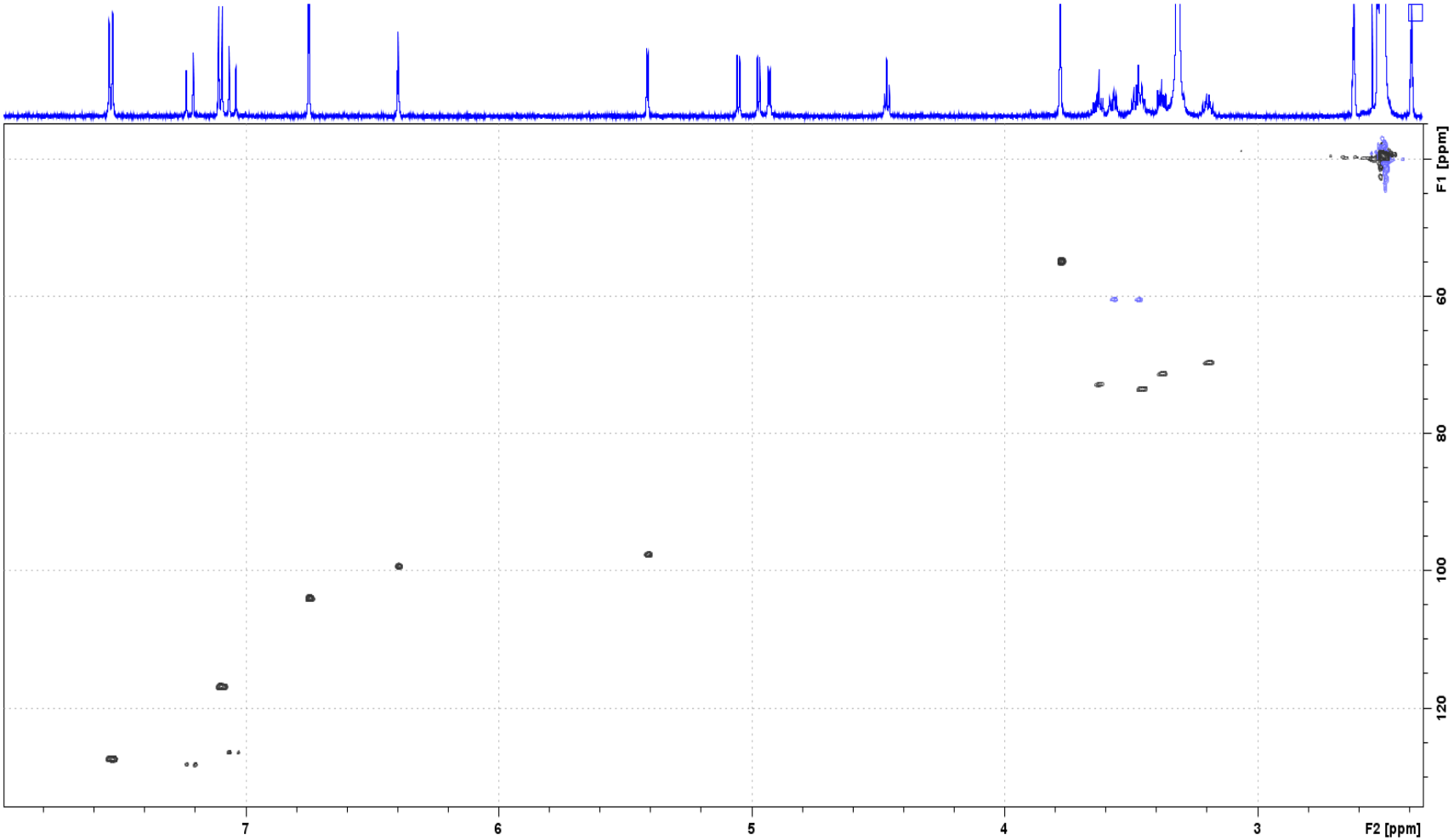
**(a) $^1$H spectrum**



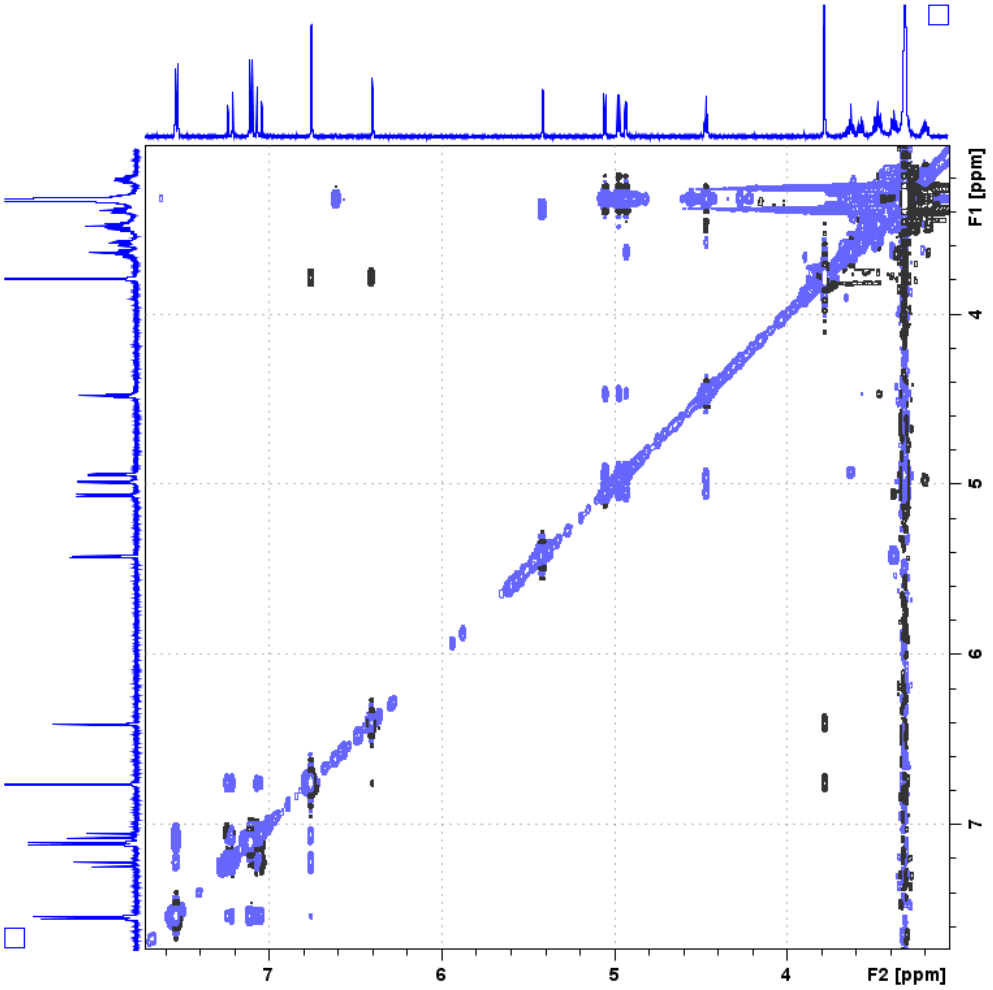
**(b) COSY**



**(c) HSQC- edited**



**(d) NOESY 500ms**



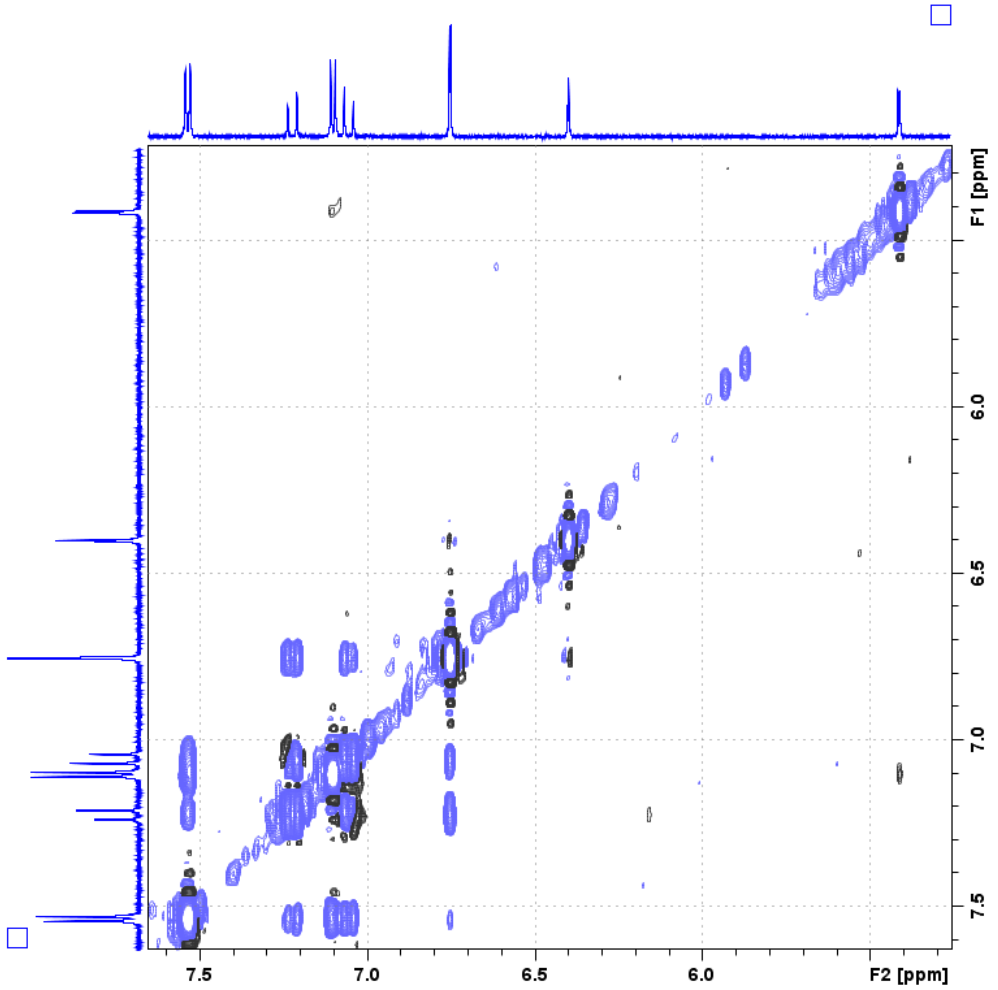
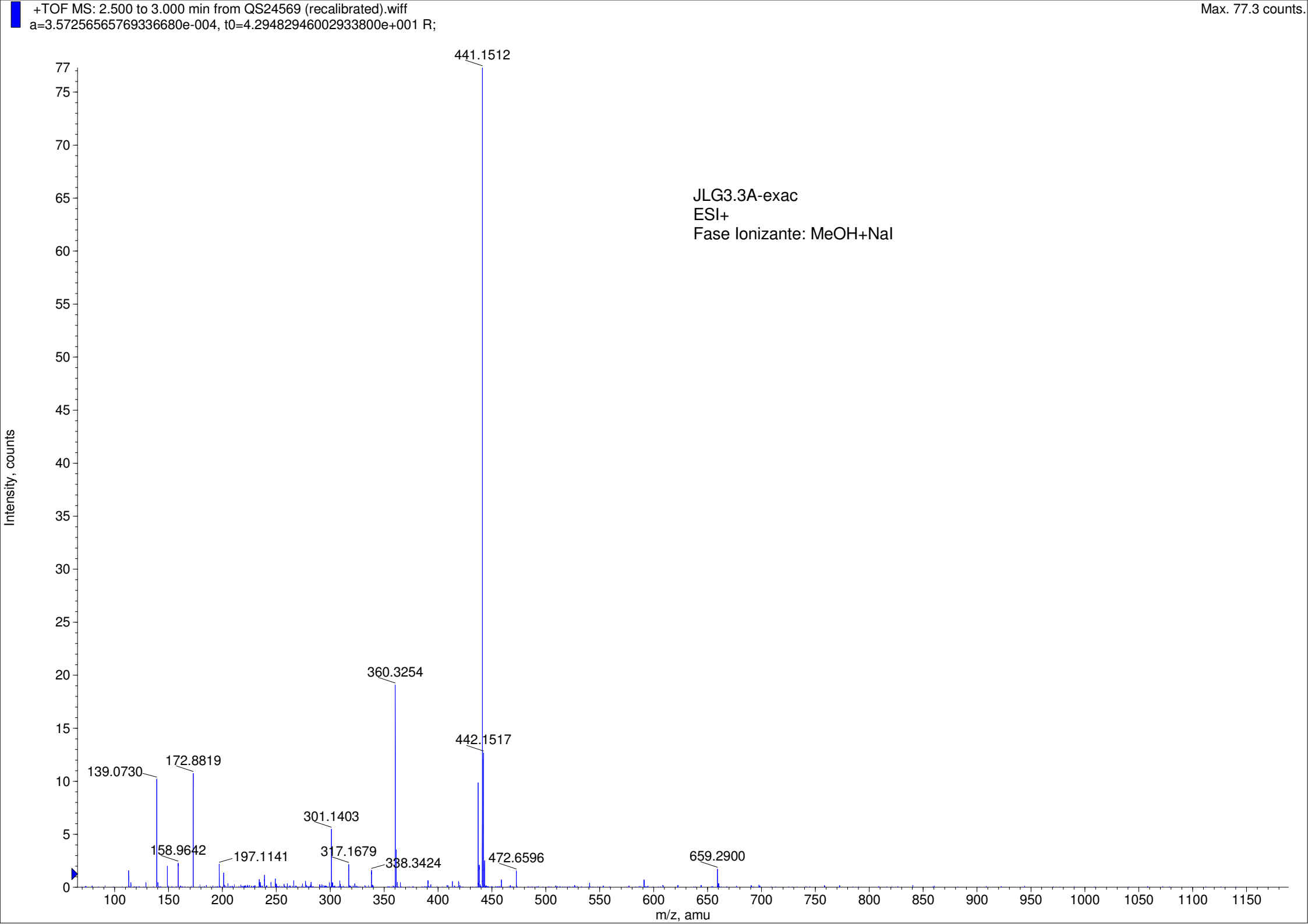
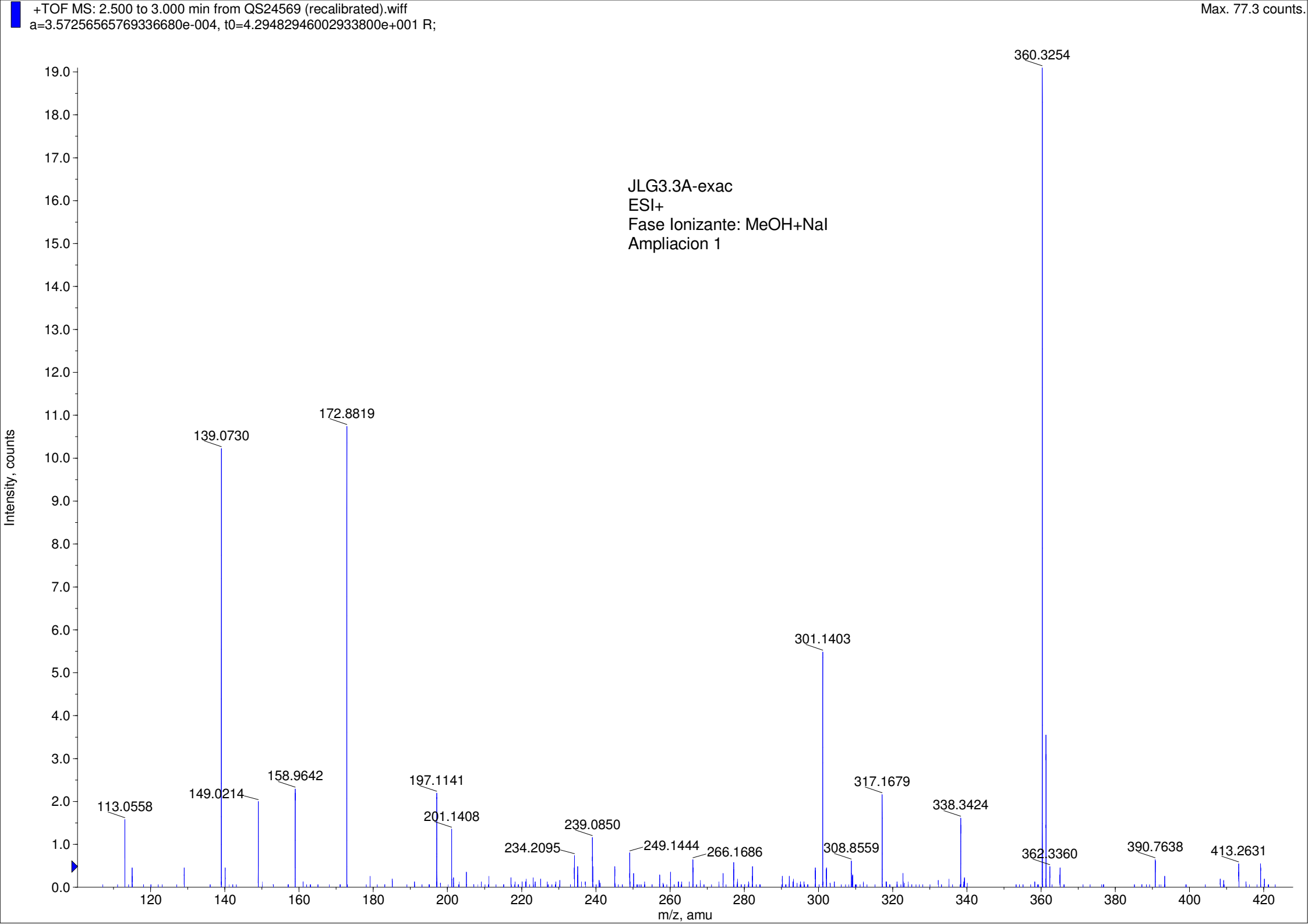
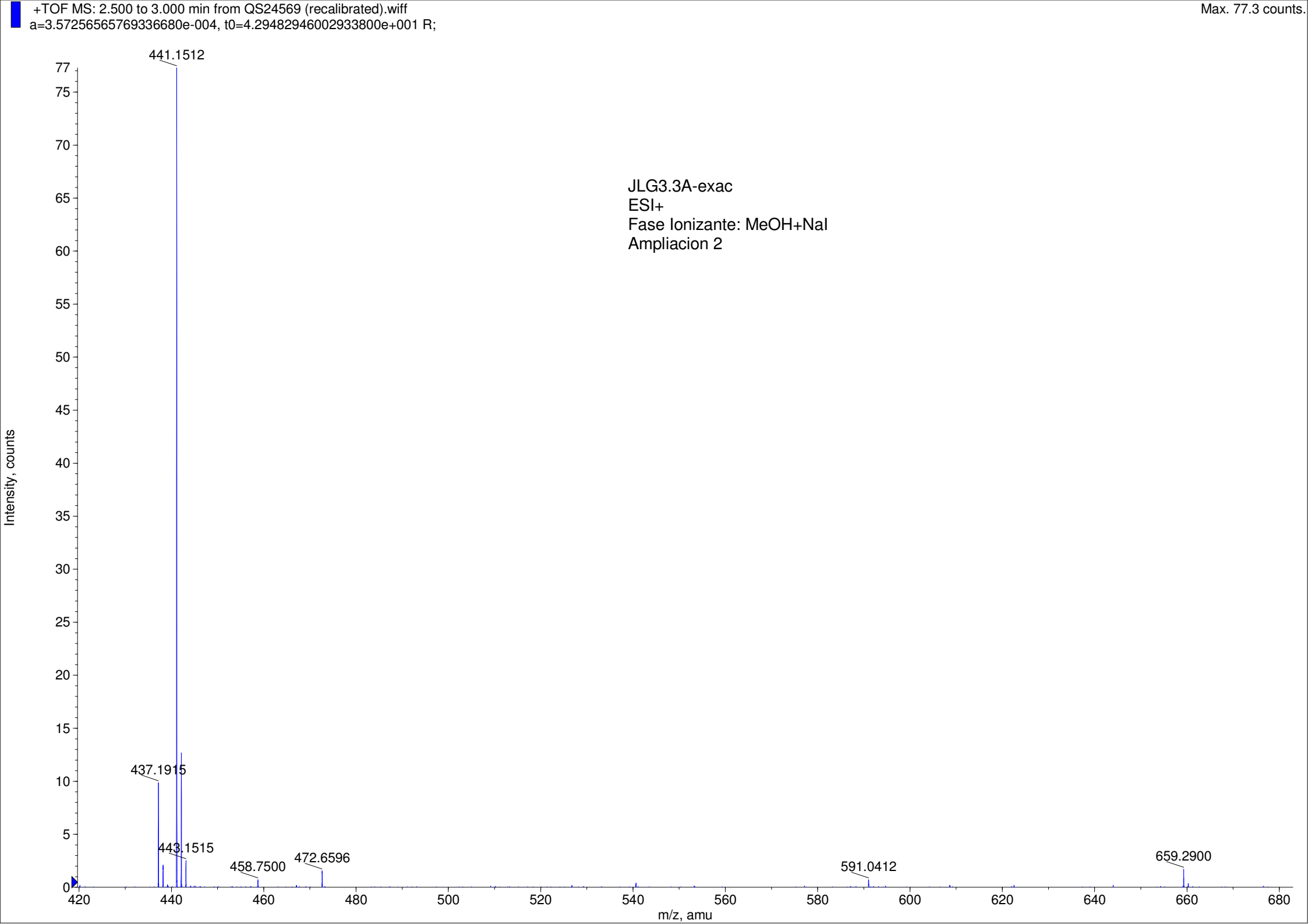



**Figure S4.**

HRMS and elementary composition calculation for pterostilbene 4′-O-*α*-D-glucopyranoside.

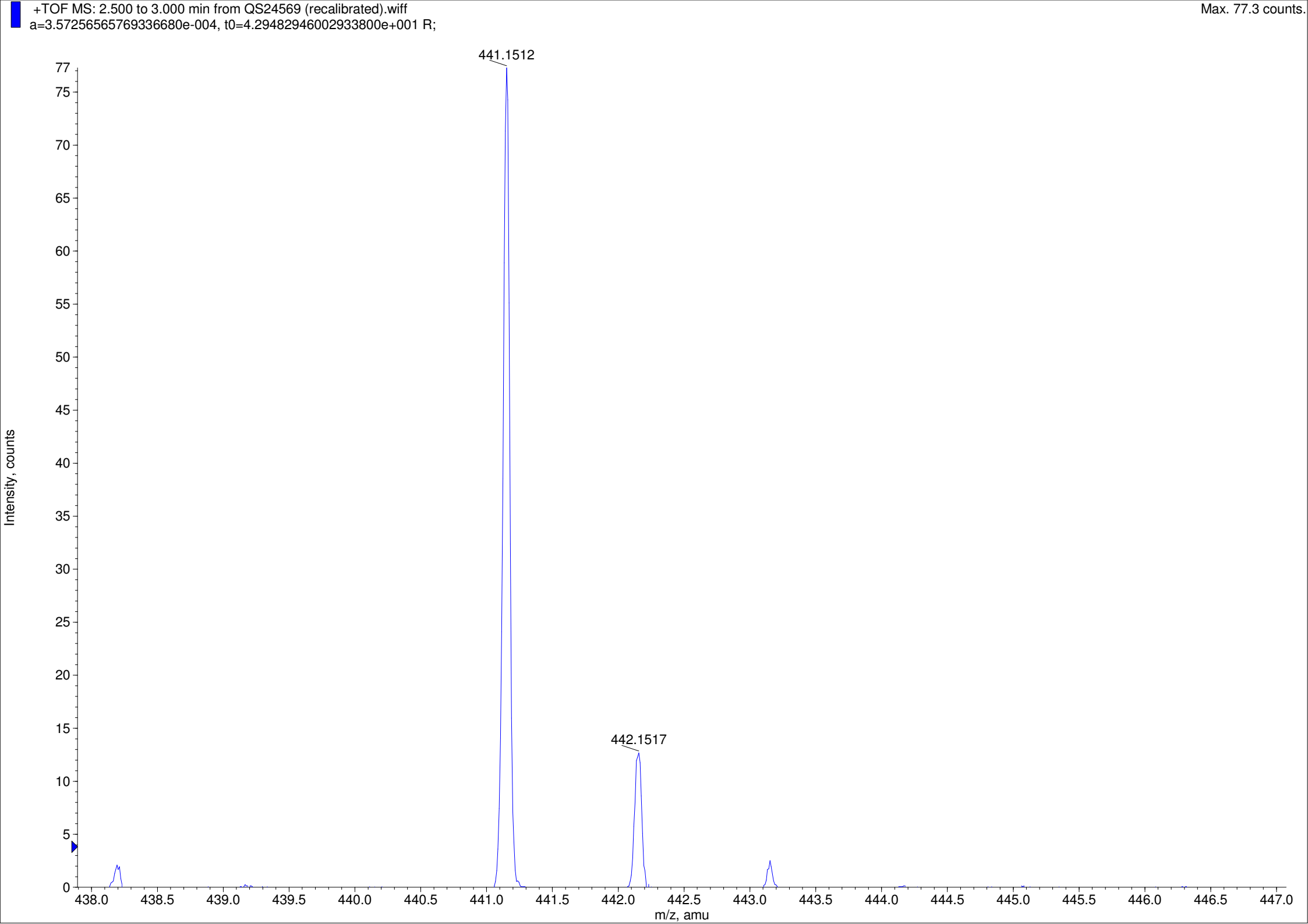

+TOF MS: 2.500 to 3.000 min from QS24569 (recalibrated).wiff
a=3.57256565769336680e-004, t0=4.29482946002933800e+001 R;
Max. 77.3 counts.
441.1512
JLG3.3A-exac
ESI+
Fase Ionizante: MeOH+NaI
360.3254
442.1517
172.8819
139.0730
301.1403
158.9642
197.1141
317.1679
338.3424
472.6596
659.2900
Intensity, counts
m/z, amu

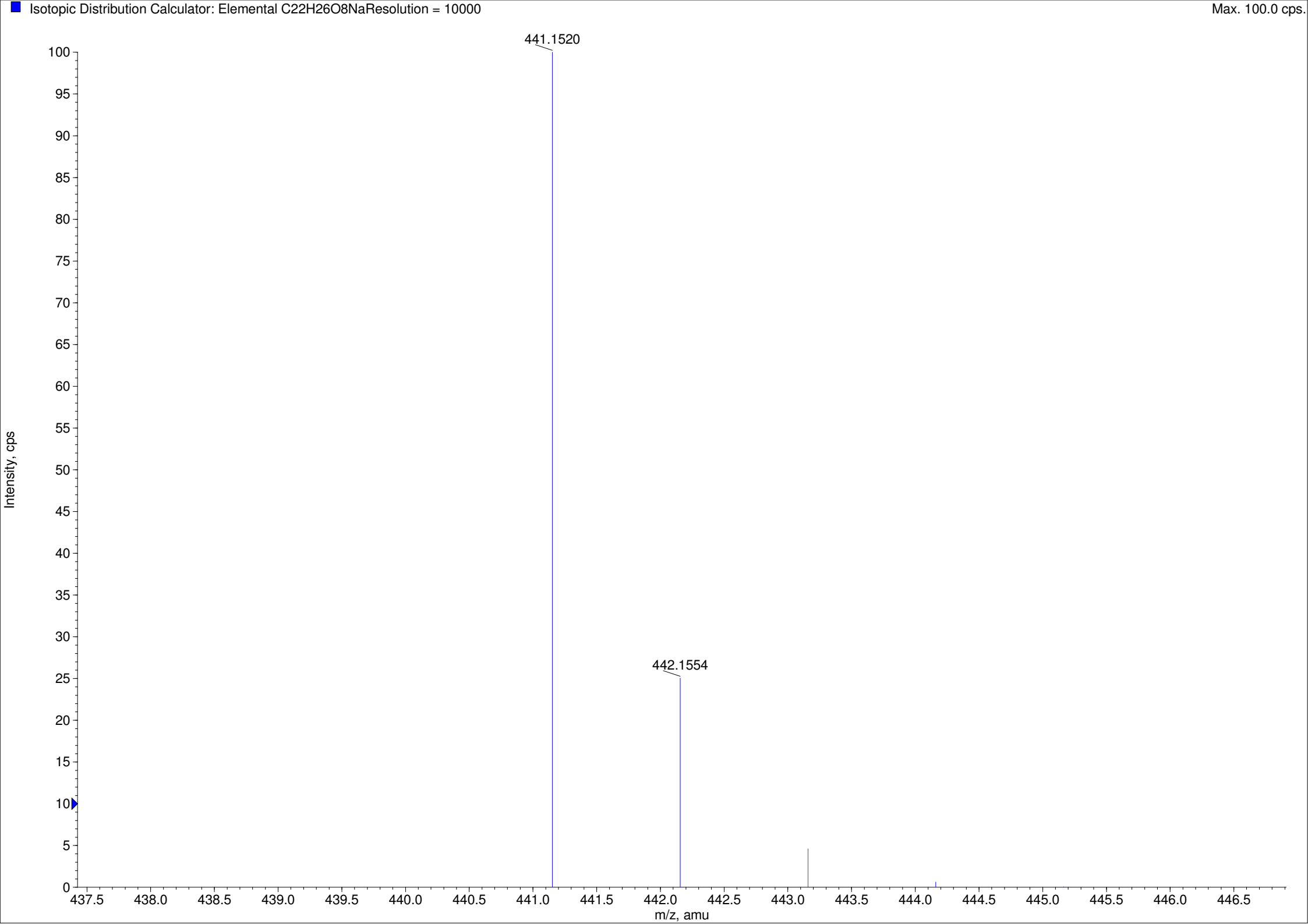

+TOF MS: 2.500 to 3.000 min from QS24569 (recalibrated).wiff
a=3.5725656576933668e-004, t0=4.2948294600293380e+001 R;
Max. 77.3 counts.
JLG3.3A-exac
ESI+
Fase Ionizante: MeOH+NaI
Ampliacion 1
Intensity, counts
m/z, amu
360.3254
172.8819
139.0730
301.1403
158.9642
149.0214
197.1141
317.1679
338.3424
113.0558
201.1408
239.0850
234.2095
249.1444
266.1686
308.8559
362.3360
390.7638
413.2631


+TOF MS: 2.500 to 3.000 min from QS24569 (recalibrated).wiff
a=3.57256565769336680e-004, t0=4.29482946002933800e+001 R;
Max. 77.3 counts.
441.1512
437.1915
443.1515
458.7500
472.6596
591.0412
659.2900
JLG3.3A-exac
ESI+
Fase Ionizante: MeOH+NaI
Ampliacion 2
Intensity, counts
m/z, amu
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
77
420
440
460
480
500
520
540
560
580
600
620
640
660
680

Peak List for " +TOF MS: 2.500 to 3.000 min from QS24569 (recalibrated).wiff□a=3.57256565769336680e-004, t0=4.29482946002933800e+001 R;"

| | Centroid mass (amu) | Centroid intensity | Charges | %Intensity |
|---|---|---|---|---|
| 1 | 113.0558 | 1.8280 | Undefined | 2.0451 |
| 2 | 139.0730 | 12.1720 | Undefined | 13.2304 |
| 3 | 149.0214 | 2.5269 | Undefined | 2.5876 |
| 4 | 158.9642 | 2.7634 | Undefined | 2.9633 |
| 5 | 172.8819 | 16.4731 | Undefined | 13.8982 |
| 6 | 197.1141 | 2.6667 | Undefined | 2.8381 |
| 7 | 201.1408 | 1.3548 | Undefined | 1.7529 |
| 8 | 234.2095 | 0.6183 | Undefined | 0.9599 |
| 9 | 235.0948 | 0.3978 | Undefined | 0.6260 |
| 10 | 239.0850 | 1.3871 | Undefined | 1.5025 |
| 11 | 245.0788 | 0.6022 | Undefined | 0.6260 |
| 12 | 249.1444 | 0.7742 | Undefined | 1.0434 |
| 13 | 266.1686 | 0.6989 | Undefined | 0.8347 |
| 14 | 277.1427 | 0.7204 | Undefined | 0.7513 |
| 15 | 282.2085 | 0.4731 | Undefined | 0.6260 |
| 16 | 301.1403 | 8.4785 | Undefined | 7.0952 |
| 17 | 308.8559 | 0.5645 | Undefined | 0.7930 |
| 18 | 317.1679 | 2.9194 | Undefined | 2.7963 |
| 19 | 338.3424 | 2.3226 | Undefined | 2.0868 |
| 20 | 360.3254 | 30.5914 | 1 | 24.7078 |
| 21 | 361.3284 | 5.7634 | 1 | 4.5910 |
| 22 | 362.3360 | 0.5430 | Undefined | 0.6260 |
| 23 | 390.7638 | 1.0000 | Undefined | 0.8347 |
| 24 | 413.2631 | 0.6613 | Undefined | 0.7095 |
| 25 | 419.1647 | 0.8172 | Undefined | 0.7095 |
| 26 | 437.1915 | 17.1398 | 1 | 12.7713 |
| 27 | 438.1961 | 3.3978 | 1 | 2.7129 |
| 28 | 441.1512 | 140.1828 | 1 | 100.0000 |
| 29 | 442.1517 | 26.4516 | 1 | 16.4023 |
| 30 | 443.1515 | 3.3978 | 1 | 3.2554 |
| 31 | 458.7500 | 1.0161 | Undefined | 0.9182 |
| 32 | 472.6596 | 2.2366 | Undefined | 2.0033 |
| 33 | 591.0412 | 1.1183 | Undefined | 0.9182 |
| 34 | 659.2900 | 2.2688 | Undefined | 2.2120 |


+TOF MS: 2.500 to 3.000 min from QS24569 (recalibrated).wiff
a=3.57256565769336680e-004, t0=4.29482946002933800e+001 R;
Max. 77.3 counts.
441.1512
442.1517
Intensity, counts
m/z, amu
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
77
438.0
438.5
439.0
439.5
440.0
440.5
441.0
441.5
442.0
442.5
443.0
443.5
444.0
444.5
445.0
445.5
446.0
446.5
447.0


Isotopic Distribution Calculator: Elemental C22H26O8NaResolution = 10000
Max. 100.0 cps.
441.1520
442.1554
Intensity, cps
m/z, amu
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
437.5
438.0
438.5
439.0
439.5
440.0
440.5
441.0
441.5
442.0
442.5
443.0
443.5
444.0
444.5
445.0
445.5
446.0
446.5

# Elemental composition calculator

Target m/z: +441.1512 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 20
Min DBE: -2.0000 Max DBE: +100.0000
Electron state: Even
Num of charges: 1
Add water: N/A
Add proton: N/A

| | Elements | Min Number | Max Number |
|---|---|---|---|
| 1 | C | 0 | 100 |
| 2 | H | 0 | 100 |
| 3 | O | 0 | 10 |
| 4 | Na | 1 | 1 |

| | Formula | Calculated m/z (amu) | mDa Error | PPM Error | DBE |
|---|---|---|---|---|---|
| 1 | C22 H26 O8 Na | 441.1519 | -0.7892 | -1.7891 | 9.5 |