

|                           |                                                                |
|---------------------------|----------------------------------------------------------------|
| <b>Name:</b>              | <b>Glycocholic Acid-D4</b>                                     |
| <b>Lot#:</b>              | GR-20-029                                                      |
| <b>Test Date:</b>         | 01/12/2026 (re-test date: 01/12/2031)                          |
| <b>CAS No.:</b>           | 1201918-15-1                                                   |
| <b>MF:</b>                | C <sub>26</sub> H <sub>39</sub> D <sub>4</sub> NO <sub>6</sub> |
| <b>MW:</b>                | 469.65                                                         |
| <b>Appearance:</b>        | White solid                                                    |
| <b>Purity:</b>            | ~97% by NMR; TLC – one spot (eluent acetone); 99% atom D       |
| <b><sup>1</sup>H-NMR:</b> | Conforms                                                       |
| <b>MS-ESI (-)</b>         | Conforms (shows peak at m/z = 468.33 [M-H] <sup>-</sup> )      |
| <b>Storage</b>            | Store at -18°C in a dry place away from direct sunlight        |

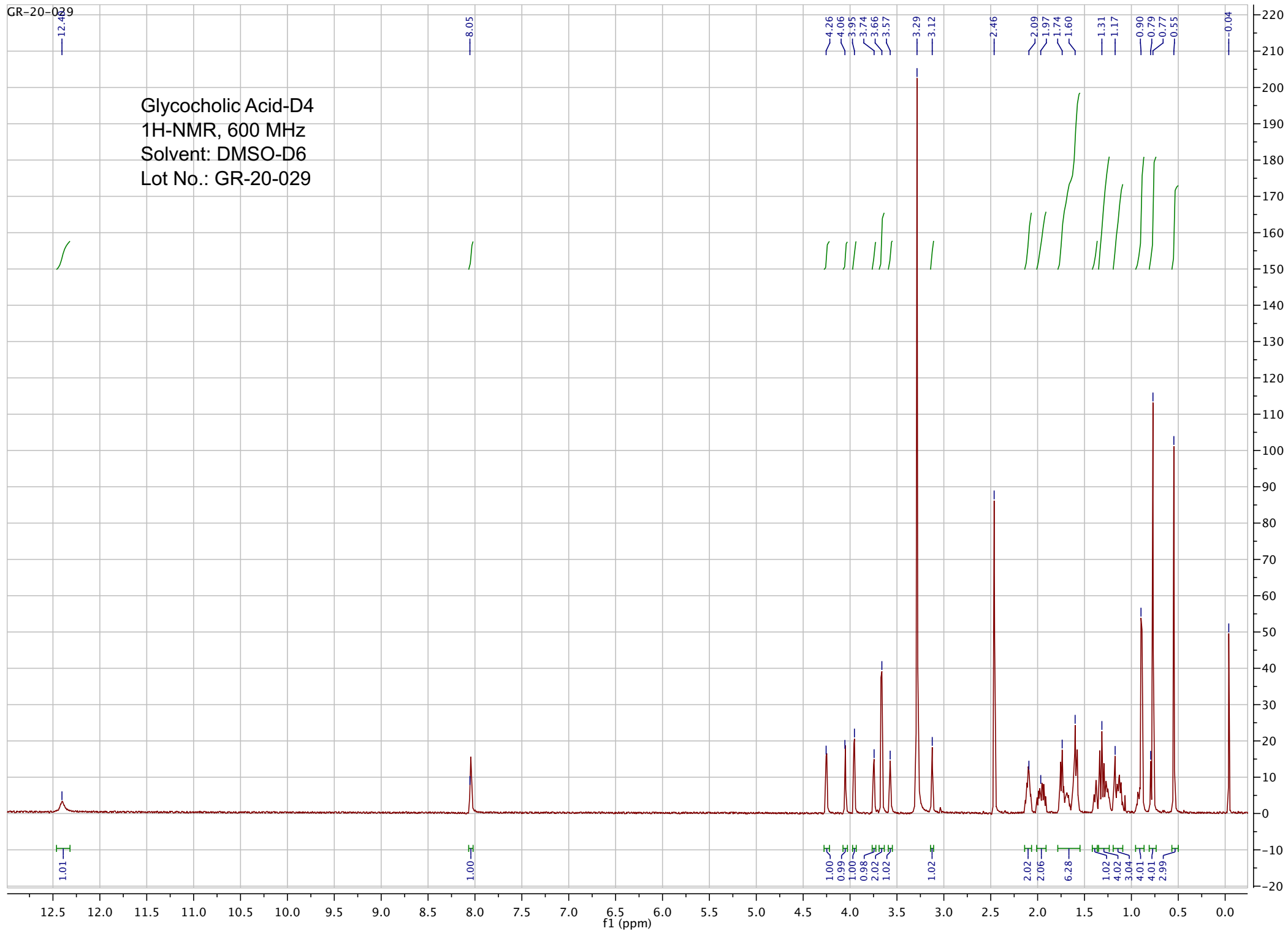
Approved by:

Date: 01/13/2026

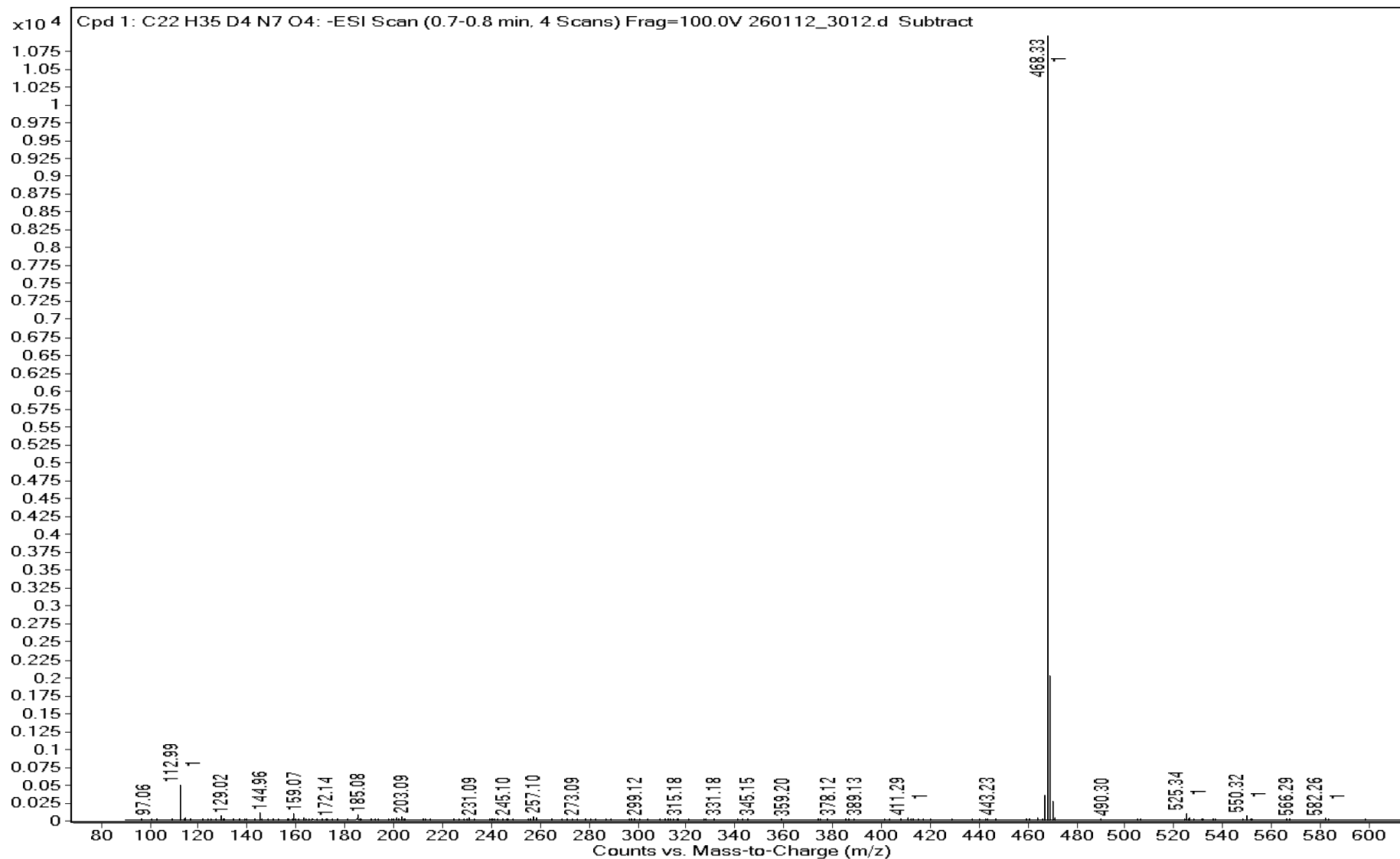
Viorica Rusu, QC/QA Manager

GR-20-029

Glycocholic Acid-D4  
1H-NMR, 600 MHz  
Solvent: DMSO-D6  
Lot No.: GR-20-029



|                    |                      |                   |                  |                       |                       |
|--------------------|----------------------|-------------------|------------------|-----------------------|-----------------------|
| <b>Sample Name</b> | GR-20-029            | <b>Data File</b>  | 260112_3012.d    | <b>Acq Method</b>     | HRMS_Negative.m       |
| <b>DA Method</b>   | AIMS_Accurate_Mass.m | <b>Instrument</b> | Agilent 6538 UHD | <b>Acq Date, Time</b> | 12/01/2026 2:49:33 PM |
| <b>Comment</b>     | ESI-                 |                   |                  |                       |                       |



# ESI-MS Report

## Molecular Formula Generation (MFG)

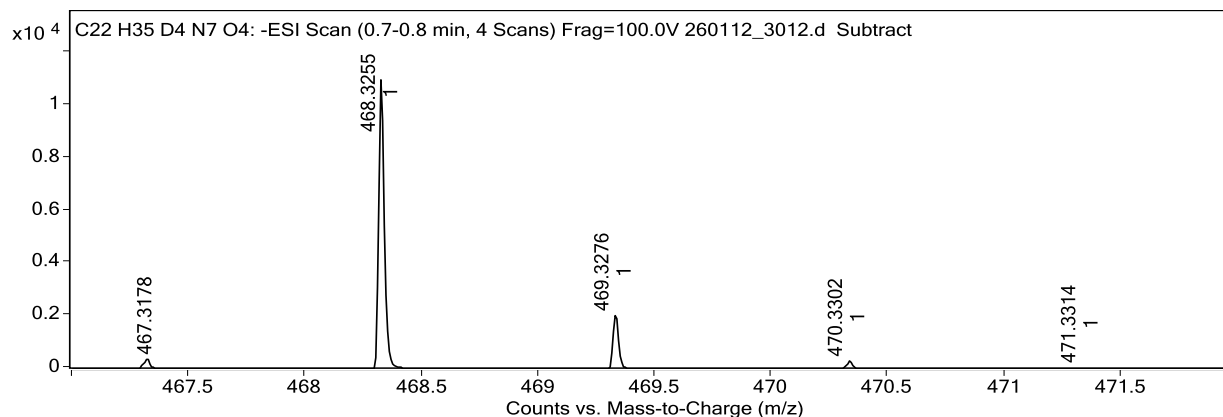
**Sample Name** GR-20-029 **Data File** 260112\_3012.d  
**Acq Method** HRMS\_Negative.m **DA Method** AIMS\_Accurate\_Mass.m  
**Instrument** Agilent 6538 UHD **Acq Date, Time** 12/01/2026 2:49:33 PM  
**Comment** ESI-

### Target Ion Species

| Ion Species        | m/z      | Ionic Formula    |
|--------------------|----------|------------------|
| (M-H) <sup>-</sup> | 468.3255 | C22 H34 D4 N7 O4 |

### MFG Calculator Results

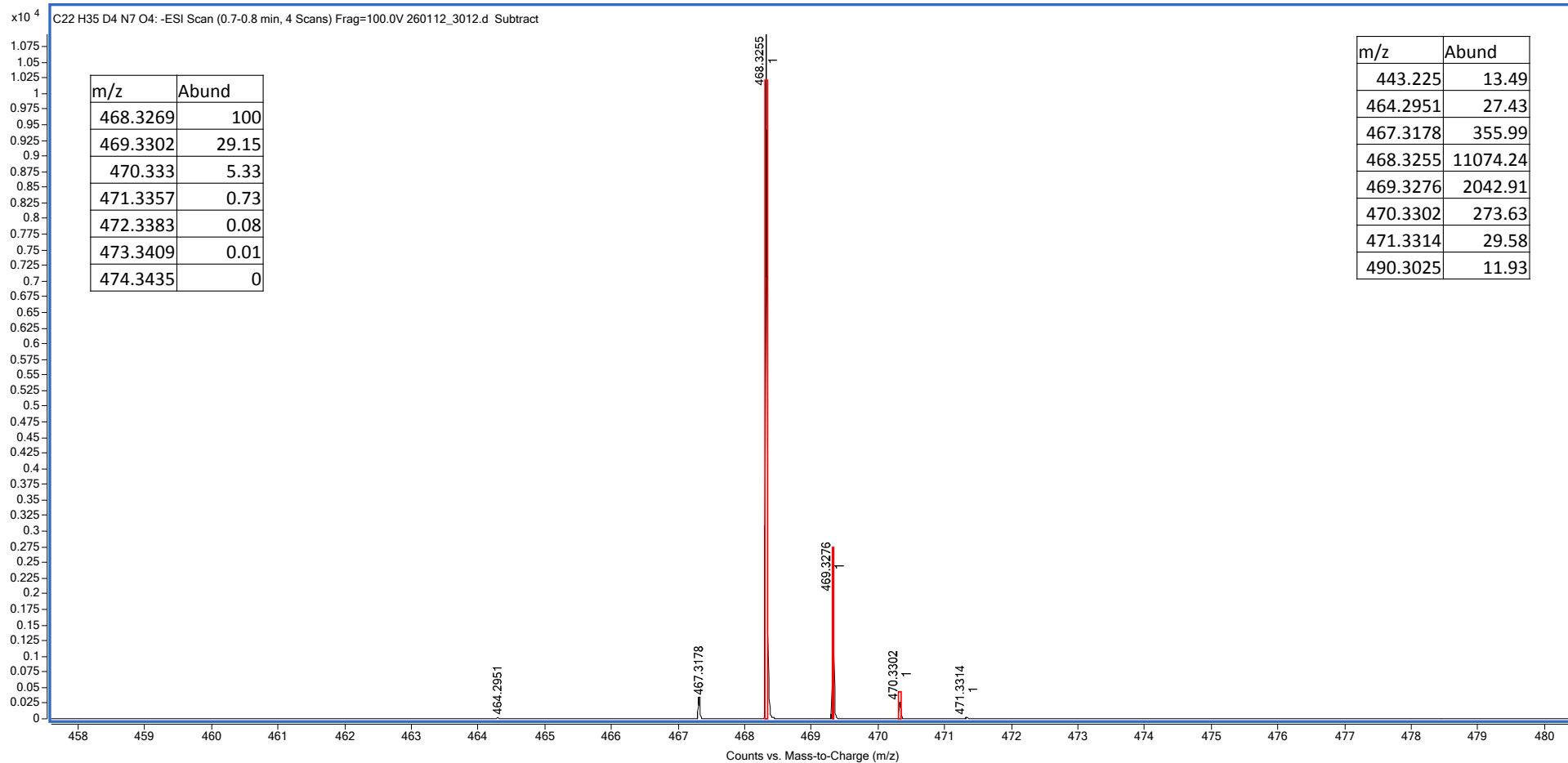
| Target m/z | Ionic Formula    | Calc m/z | +/- (mDa) | +/- (ppm) | DBE  | MFG Score |
|------------|------------------|----------|-----------|-----------|------|-----------|
| 468.3255   | C22 H34 D4 N7 O4 | 468.3242 | 1.3       | 2.8       | 7.0  | 85.35     |
| 468.3255   | C21 H38 D4 N3 O8 | 468.3228 | 2.7       | 5.8       | 2.0  | 80.46     |
| 468.3255   | C26 H38 D4 N O6  | 468.3269 | -1.4      | -3.0      | 6.0  | 77.73     |
| 468.3255   | C27 H34 D4 N5 O2 | 468.3282 | -2.7      | -5.8      | 11.0 | 64.50     |



### Predicted Isotope Match Table

| Isotope | m/z      | Calc m/z | Diff (mDa) | Abund (%) | Calc Abund (%) | +/- |
|---------|----------|----------|------------|-----------|----------------|-----|
| 1       | 468.3255 | 468.3242 | 1.3        | 100.0     | 100.0          | 0.0 |
| 2       | 469.3276 | 469.3270 | 0.6        | 18.4      | 26.9           | 8.5 |
| 3       | 470.3302 | 470.3295 | 0.7        | 2.5       | 4.3            | 1.8 |

C22 H35 D4 N7 O4: -ESI Scan (0.7-0.8 min, 4 Scans) Frag=100.0V 260112\_3012.d Subtract



| m/z      | Abund |
|----------|-------|
| 468.3269 | 100   |
| 469.3302 | 29.15 |
| 470.333  | 5.33  |
| 471.3357 | 0.73  |
| 472.3383 | 0.08  |
| 473.3409 | 0.01  |
| 474.3435 | 0     |

| m/z      | Abund    |
|----------|----------|
| 443.225  | 13.49    |
| 464.2951 | 27.43    |
| 467.3178 | 355.99   |
| 468.3255 | 11074.24 |
| 469.3276 | 2042.91  |
| 470.3302 | 273.63   |
| 471.3314 | 29.58    |
| 490.3025 | 11.93    |