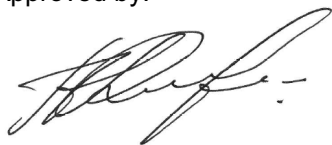


| | |
|---------------------------|---|
| Name: | Lithocholic Acid-D4 |
| Lot#: | GR-19-063 |
| Test Date: | 02/12/2024 (re-test date: 02/12/2029) |
| CAS No.: | 83701-16-0 |
| MF: | C ₂₄ H ₃₆ D ₄ O ₃ |
| MW: | 380.60 |
| Appearance: | White solid |
| Purity: | >97% by NMR; TLC – one spot (eluent 30% Acetone in Hexanes) |
| ¹H-NMR: | Conforms |
| MS-ESI (-) | Conforms (shows peak at m/z = 379.32 [M-H] ⁻) |
| Storage | Store at -18°C in a dry place away from direct sunlight |

Approved by:

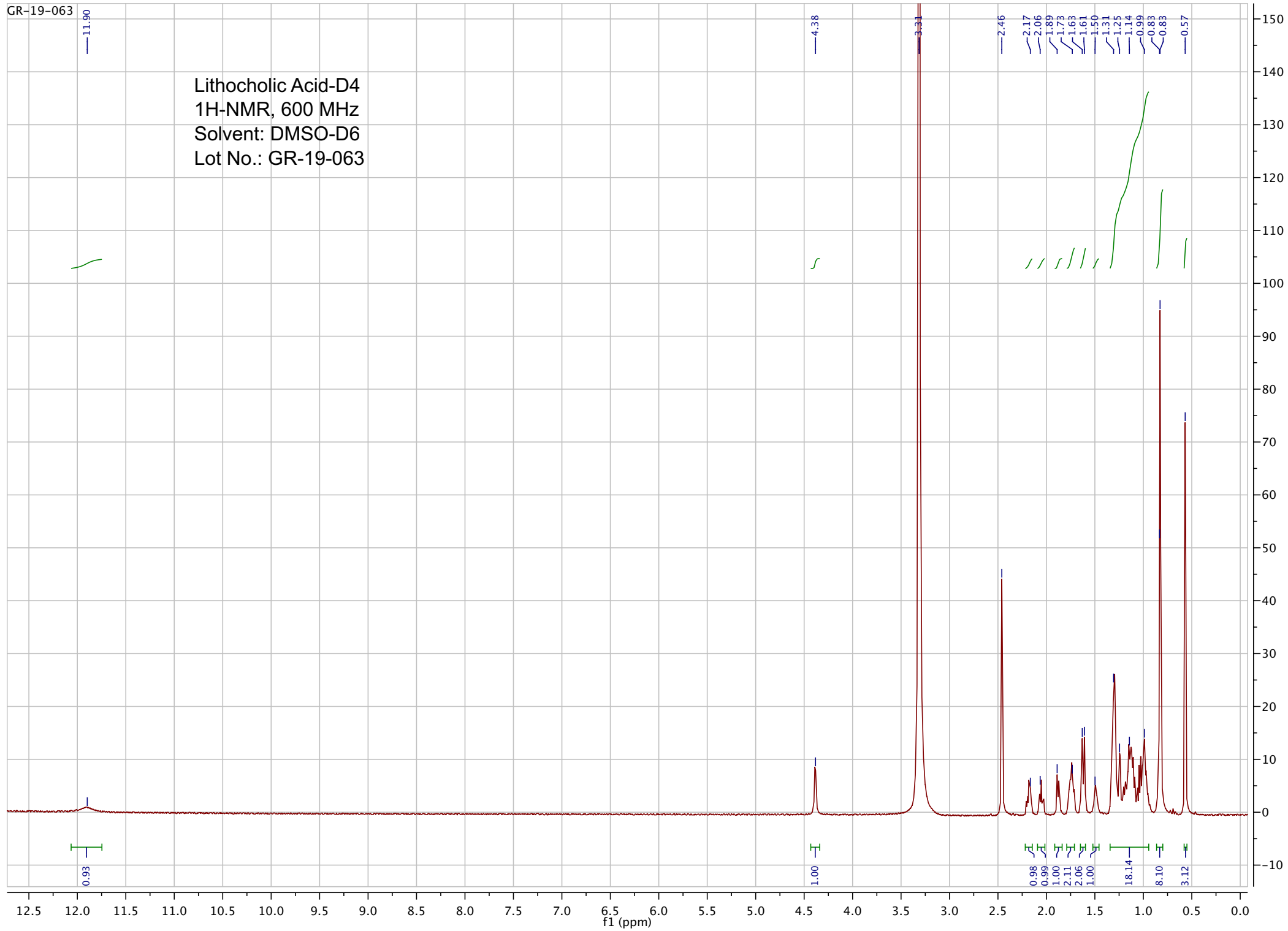
Date: 02/12/2024



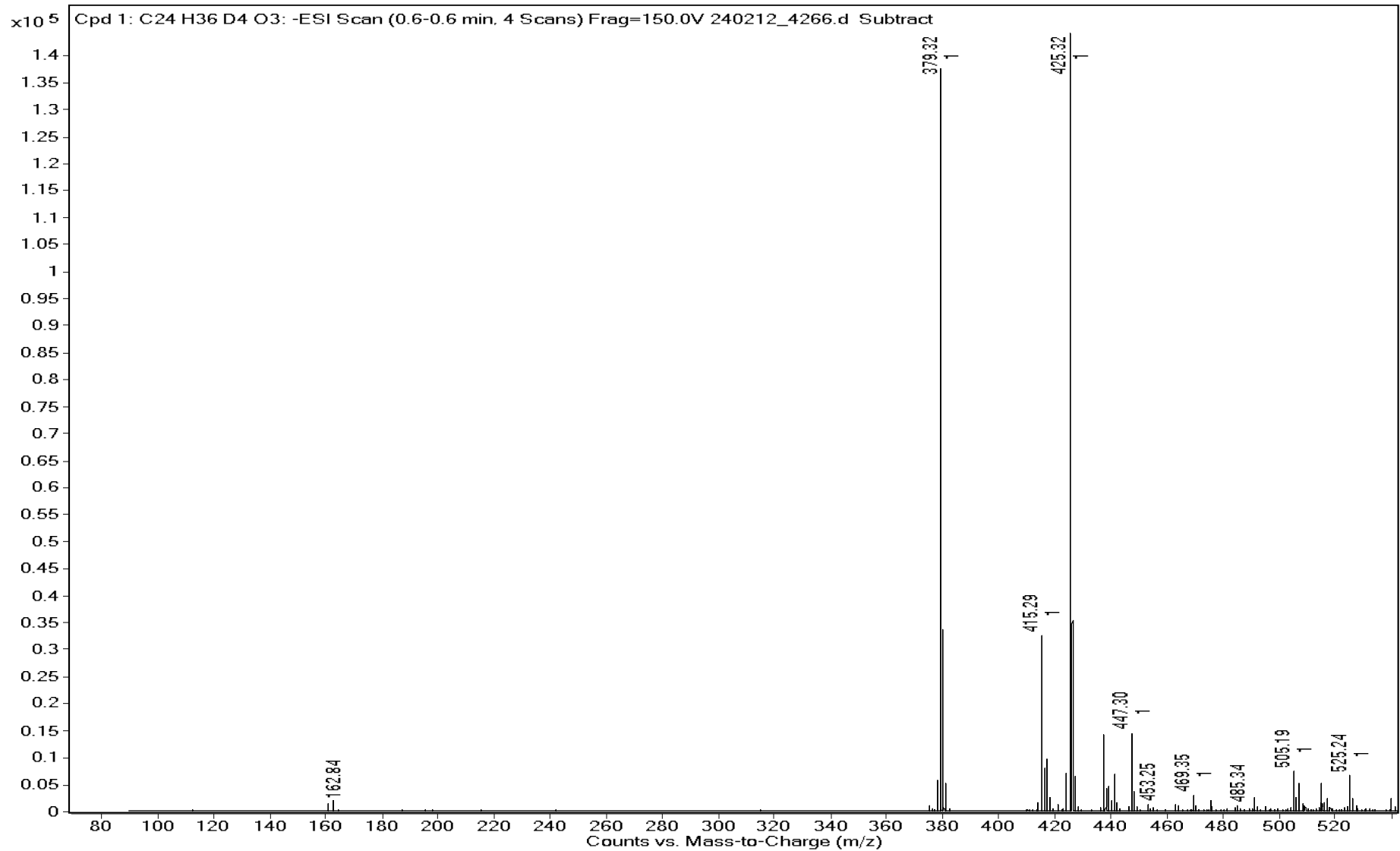
Viorica Rusu, QC/QA Manager

GR-19-063

Lithocholic Acid-D4
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-063



| | | | | | |
|--------------------|----------------------|-------------------|------------------|-----------------------|-----------------------|
| Sample Name | GR-19-063 | Data File | 240212_4266.d | Acq Method | HRMS_Negative.m |
| DA Method | AIMS_Accurate_Mass.m | Instrument | Agilent 6538 UHD | Acq Date, Time | 12/02/2024 1:29:11 PM |
| Comment | ESI- | | | | |



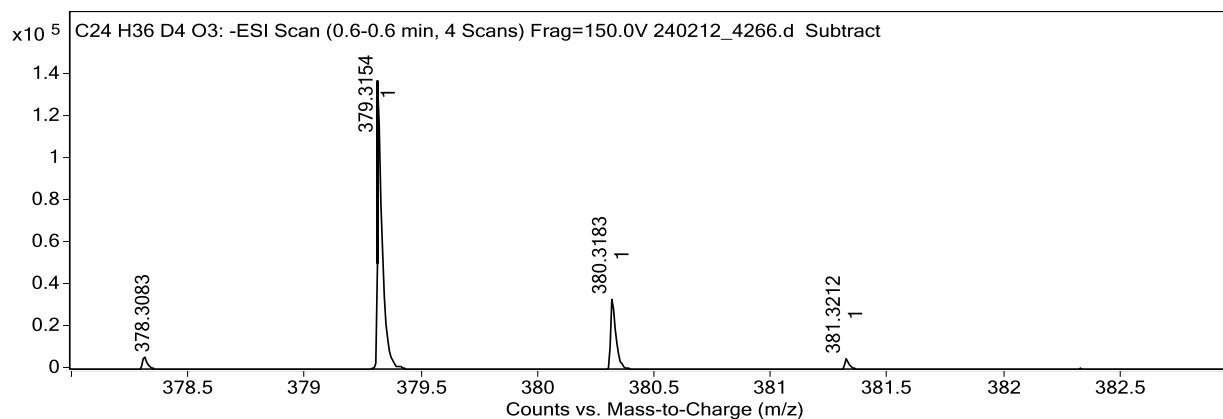
| | | | |
|--------------------|------------------|-----------------------|-----------------------|
| Sample Name | GR-19-063 | Data File | 240212_4266.d |
| Acq Method | HRMS_Negative.m | DA Method | AIMS_Accurate_Mass.m |
| Instrument | Agilent 6538 UHD | Acq Date, Time | 12/02/2024 1:29:11 PM |
| Comment | ESI- | | |

Target Ion Species

| Ion Species | m/z | Ionic Formula |
|--------------------|----------|---|
| (M-H) ⁻ | 379.3154 | C ₂₄ H ₃₅ D ₄ O ₃ |

MFG Calculator Results

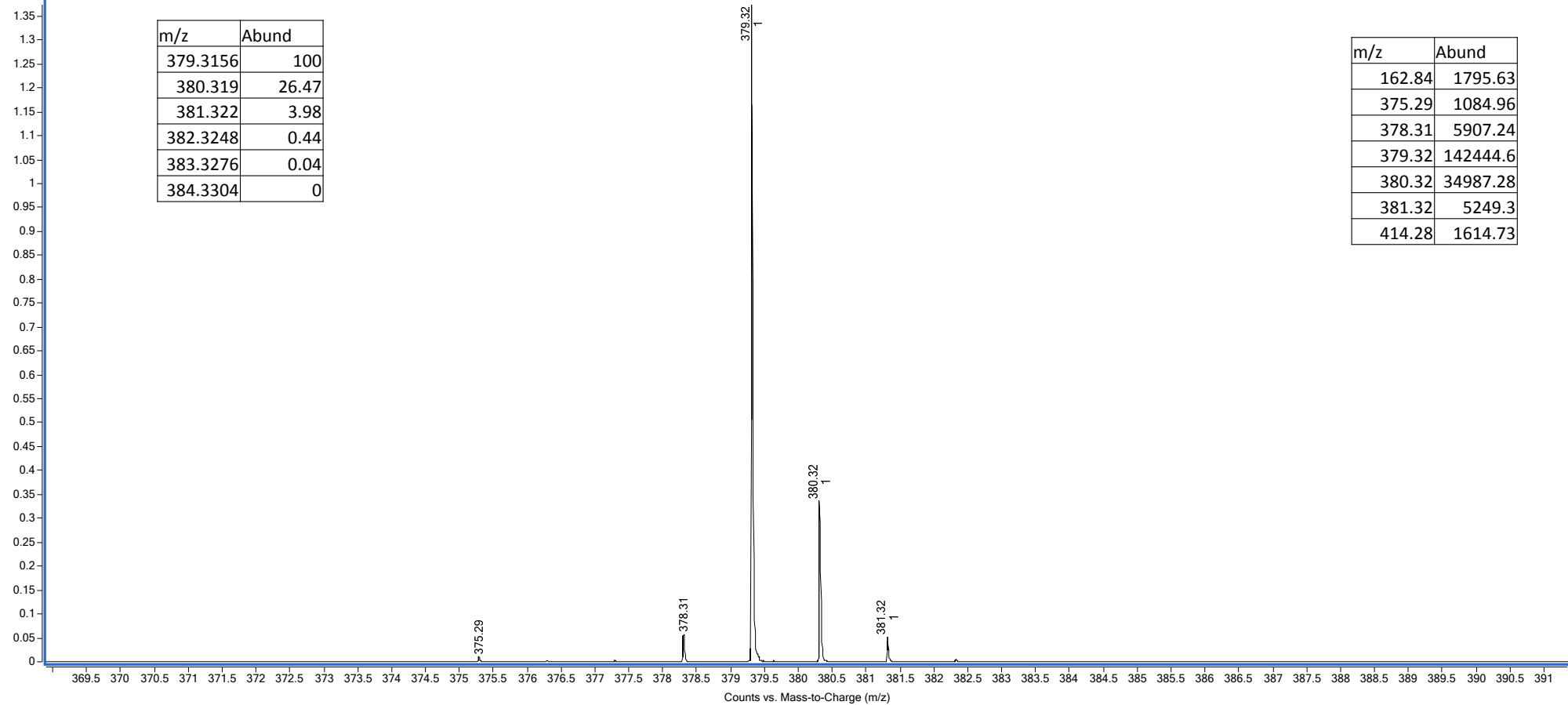
| Target m/z | Ionic Formula | Calc m/z | +/- (mDa) | +/- (ppm) | DBE | MFG Score |
|------------|--|----------|-----------|-----------|-----|-----------|
| 379.3154 | C ₂₄ H ₃₅ D ₄ O ₃ | 379.3156 | -0.2 | -0.5 | 5.0 | 98.78 |
| 379.3154 | C ₂₀ H ₃₁ D ₄ N ₆ O | 379.3129 | 2.5 | 6.6 | 6.0 | 84.72 |
| 379.3154 | C ₁₉ H ₃₅ D ₄ N ₂ O ₅ | 379.3116 | 3.8 | 10.0 | 1.0 | 70.99 |



Predicted Isotope Match Table

| Isotope | m/z | Calc m/z | Diff (mDa) | Abund (%) | Calc Abund (%) | +/- |
|---------|----------|----------|------------|-----------|----------------|-----|
| 1 | 379.3154 | 379.3156 | -0.2 | 100.0 | 100.0 | 0.0 |
| 2 | 380.3183 | 380.3190 | -0.7 | 24.6 | 26.5 | 1.9 |
| 3 | 381.3212 | 381.3220 | -0.8 | 3.7 | 4.0 | 0.3 |

x10⁵ Cpd 1: C24 H36 D4 O3: -ESI Scan (0.6-0.6 min, 4 Scans) Frag=150.0V 240212_4266.d Subtract



| m/z | Abund |
|----------|-------|
| 379.3156 | 100 |
| 380.319 | 26.47 |
| 381.322 | 3.98 |
| 382.3248 | 0.44 |
| 383.3276 | 0.04 |
| 384.3304 | 0 |

| m/z | Abund |
|--------|----------|
| 162.84 | 1795.63 |
| 375.29 | 1084.96 |
| 378.31 | 5907.24 |
| 379.32 | 142444.6 |
| 380.32 | 34987.28 |
| 381.32 | 5249.3 |
| 414.28 | 1614.73 |