## Supplementary information

# Cytotoxic and antimicrobial indole alkaloids from an endophytic fungus *Chaetomium* sp. SYP-F7950 of *Panax notoginseng*

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**Table S1.**

| Position | Compound 3 | | Position | Compound 5 | |
|---|---|---|---|---|---|
| | **$\delta$ C, type** | **$\delta$ H (*J* in Hz)** | | **$\delta$ C, type** | **$\delta$ H (*J* in Hz)** |
| 1 | 165.6 C | - | 1 | 167.5 C | - |
| 2 $NCH_3$ | 28.7 $CH_3$ | 2.91, s, 3H | 2 $NCH_3$ | 28.5 $CH_3$ | 2.78, s, 3H |
| 3 | 72.6 C | - | 3 | 75.7 C | - |
| 3 $SCH_3$ | 12.5 $CH_3$ | 2.14, s, 3H | 3 $SCH_3$ | 8.59 $CH_3$ | 0.48, s, 3H |
| 4 | 164.5 C | - | 4 | 165.0 C | - |
| 5 NH | - | 9.03, s, 1H | 5 NH | - | 9.04, s, 1H |
| 6 | 64.9 C | - | 6 | 82.3 C | - |
| 6 $SCH_3$ | 13.9 $CH_3$ | 2.29 s, 3H | 6 OH | - | - |
| 7 | 34.5 $CH_2$ | 3.20, d, 1H, 12 | 7 | 35.3 $CH_2$ | 2.99, d, 1H, 12 |
| | | 3.69, d, 1H, 12 | | | 3.56, d, 1H, 12 |
| 8 | 107.7 C | - | 8 | 108.3 C | - |
| 9 | 124.3 CH | 7.16, d, 1H | 9 | 125.2 CH | 7.03, s, 1H |
| 10 NH | - | 10.84, s, 1H | 10 NH | - | 10.85, s, 1H |
| 10a | 135.5 C | - | 10a | 135.7 C | - |
| 11 | 111.0 CH | 7.28, d, 1H, 6 | 11 | 110.9 CH | 7.23, d, 1H, 6 |
| 12 | 120.7 CH | 7.02, d, 1H, 6 | 12 | 120.6 CH | 6.99, d, 1H, 6 |
| 13 | 118.1 CH | 6.94, d, 1H, 6 | 13 | 118.2 CH | 6.92, d, 1H, 6 |
| 14 | 118.7, CH | 7.59, d, 1H, 6 | 14 | 119.2, CH | 7.74, d, 1H, 6 |
| 14a | 127.8, C | - | 14a | 128.0, C | - |
| 15 | 63.1 $CH_2$ | 3.54, d, 1H, 12 | 15 | 62.9 $CH_2$ | 3.39, d, 1H, 12 |
| | | 3.72, d, 1H, 12 | | | 3.68, d, 1H, 12 |

## Table S2.

| Position | Compound 6 | | Position | Compound 13 | |
|---|---|---|---|---|---|
| | $\delta_C$ | $\delta_H$ (*J* in Hz) | | $\delta_C$ | $\delta_H$ (*J* in Hz) |
| 1 | 165.8 C | - | 1 | 165.9 C | - |
| 2 $NCH_3$ | 30.6 $CH_3$ | 3.17, 3H, s | 2 $NCH_3$ | 28.7 $CH_3$ | 2.76, 3H, s |
| 3 | 76.3 C | - | 3 | 72.9 C | - |
| - | - | - | 3 $SCH_3$ | 13.3 $CH_3$ | 1.98, 3H, s |
| 4 | 163.3 C | - | 4 | 164.3 C | - |
| 5 | 80.3 CH | 6.12, 1H, s | 5 | 81.6 CH | 6.10, 1H, s |
| 6 | | 5.30, 1H, brs | 6 | - | 5.38, 1H, brs |
| 6a | 148.5 C | - | 6a | 149.9 C | - |
| 7 | 111.4 CH | 6.80, 1H, d, 6.0 | 7 | 110.4 CH | 6.73, 1H, d, 6.0 |
| 8 | 131.5 CH | 7.33, 1H, t, 6.0 | 8 | 124.7 CH | 7.24, 1H, t, 6.0 |
| 9 | 120.9 CH | 7.04, 1H, t, 6.0 | 9 | 119.6 CH | 6.83, 1H, t, 6.0 |
| 10 | 126.1 CH | 7.42, 1H, d, 6.0 | 10 | 130.9 CH | 7.32, 1H, d, 6.0 |
| 10a | 126,9 C | - | 10a | 134.2 C | - |
| 10b | 73.9 C | - | 10b | 73.6 C | - |
| 11 | 42.4 $CH_2$ | 3.02, 4.40, 2H, d, 12 | 11 | 44.1 $CH_2$ | 4.24, 3.86, 2H, d, 12 |
| 11a | 73.7 C | - | 11a | 68.4 C | - |
| - | - | - | 11a $SCH_3$ | 15.8 $CH_3$ | 2.29, 3H, s |
| 12 | 60.7 $CH_2$ | 4.26, 4.35, 2H, d, 12 | 12 | 64.3 $CH_2$ | 3.16, 3.32, 2H, d, 12 |
| 1’ | 166.0 C | - | 1’ | 165.8 C | - |
| 2’ $NCH_3$ | 29.3 $CH_3$ | 2.75, 3H, s | 2’ $NCH_3$ | 29.3 $CH_3$ | 3.08, 3H, s |
| 3’ | 71.5 C | - | 3’ | 72.8 C | - |
| 3’ $SCH_3$ | 13.5 $CH_3$ | 2.13, 3H, s | 3’ $SCH_3$ | 13.5 $CH_3$ | 2.08, 3H, s |
| 4’ | 165.5 C | - | 4’ | 166.6 C | - |
| 5’ $NCH_3$ | 29.3 $CH_3$ | 3.19, 3H, s | 5’ $NCH_3$ | 30.7 $CH_3$ | 3.15, 3H, s |
| 6’ | 72.8 C | - | 6’ | 71.6 C | - |
| 6’ $SCH_3$ | 14.5 $CH_3$ | 2.30, 3H, s | 6’ $SCH_3$ | 14.5 $CH_3$ | 2.20, 3H, s |
| 7’ | 32.6 $CH_2$ | 3.16, 3.87, 2H, d, 12 | 7’ | 32.4 $CH_2$ | 3.57, 3.75, 2H, d, 12 |
| 8’ | 107.4 C | - | 8’ | 107.0 C | - |
| 9’ | 126.3 CH | 6.88, 1H, s | 9’ | 125.8 CH | 6.97, 1H, s |
| 10’a | 134.0 C | - | 10’a | 127.8 C | - |
| 11’ | 111.3 CH | 7.08, 1H, d, 6.0 | 11’ | 111.8 CH | 7.08, 1H, d, 6.0 |
| 12’ | 122.8 CH | 7.13, 1H, t, 6.0 | 12’ | 122.5 CH | 6.95, 1H, t, 6.0 |
| 13’ | 120.5 CH | 7.13, 1H, t, 6.0 | 13’ | 119.9 CH | 6.85, 1H, t, 6.0 |
| 14’ | 120.1 CH | 7.63, 1H, d, 6.0 | 14’ | 119.5 CH | 7.55, 1H, d, 6.0 |
| 14’a | 130.0 C | - | 14’a | 129.6 C | - |
| 15’ | 64.0 $CH_2$ | 3.17, 3.83, 2H, d, 12 | 15’ | 63.8 $CH_2$ | 3.14, 3.80, 2H, d, 12 |

**Table S3.**

| Position | Compound 7 | |
|---|---|---|
| | $\delta_C$ | $\delta_H$ (*J* in Hz) |
| 1 | 18.2 $CH_3$ | 1.74, 3H, dd, 6.7, 1.3 |
| 2 | 129.5 CH | 5.70, 1H, dq, 14.8, 6.7 |
| 3 | 130.9 CH | 6.03, 1H, ddd, 12.0, 10.5, 1.5 |
| 4 | 133.3 CH | 6.16, 1H, dd, 15.0, 14.8 |
| 5 | 128.3 CH | 5.43, 1H, dd, 15.0, 14.8 |
| 6 | 51.6 CH | 2.85, 1H, dddd, 8.2, 8.1 |
| 7 | 81.6 CH | 3.76, 1H, dd, 7.3, 2.7 |
| 8 | 84.8 CH | 4.11, 1H, m |
| 9 | 133.4 CH | 5.73, 1H, m |
| 10 | 131.6 CH | 6.36, 1H, dd, 12.0, 6.0 |
| 11 | 136.2 CH | 6.33, 1H, ddd, 12.0, 6.0 |
| 12 | 118.3 $CH_2$ | 5.25, 5.12, 2H, dd, 15.6, 8.7 |
| 13 | 71.1 $CH_2$ | 4.13, 3.71, 2H, dd, 9.0, 8.7 |

**Table S4.**

| Position | Compound 8 | | Position | Ergosterol (Kwon et al. 2002) | |
|---|---|---|---|---|---|
| | $\delta_C$ | $\delta_H$ (*J* in Hz) | | $\delta_C$ | $\delta_H$ (*J* in Hz) |
| 1 | 38.5 $CH_2$ | | 1 | 39.0 $CH_2$ | |
| 2 | 32.1 $CH_2$ | | 2 | 32.6 $CH_2$ | |
| 3 | 70.6 CH | 3.64, 1H, m | 3 | 71.1 CH | 3.65, 1H, m |
| 4 | 40.9 $CH_2$ | | 4 | 41.4 $CH_2$ | |
| 5 | 141.5 C | - | 5 | 142.0 C | - |
| 6 | 119.7 CH | 5.57, 1H, m | 6 | 120.2 CH | 5.57, 1H, m |
| 7 | 116.4 CH | 5.38, 1H, m | 7 | 116.9 CH | 5.38, 1H, m |
| 8 | 139.9 C | - | 8 | 140.7 C | - |
| 9 | 46.3 CH | | 9 | 46.9 CH | |
| 10 | 37.1 C | - | 10 | 37.7 C | - |
| 11 | 21.2 $CH_2$ | | 11 | 21.8 $CH_2$ | |
| 12 | 28.4 $CH_2$ | | 12 | 28.9 $CH_2$ | |
| 13 | 42.9 C | - | 13 | 43.5 C | - |
| 14 | 55.8 CH | | 14 | 56.4 CH | |
| 15 | 21.2 $CH_2$ | | 15 | 21.8 $CH_2$ | |
| 16 | 39.2 $CH_2$ | | 16 | 39.7 $CH_2$ | |
| 17 | 54.7 CH | | 17 | 55.2 CH | |
| 18 | 12.2 $CH_3$ | 0.63, 3H, s | 18 | 12.5 $CH_3$ | 0.63, 3H, s |
| 19 | 16.4 $CH_3$ | 0.95, 3H, s | 19 | 16.9 $CH_3$ | 0.95, 3H, s |
| 20 | 40.5 CH | | 20 | 41.1 CH | |
| 21 | 19.8 $CH_3$ | 1.03, 3H, d, 6.0 | 21 | 20.3 $CH_3$ | 1.04, 3H, d, 7.0 |
| 22 | 135.7 CH | 5.19, 2H, m 15.5, 7.5 | 22 | 136.2 CH | 5.20, 2H, m 15.5, 7.5 |
| 23 | 132.1 CH | 5.22, 1H, dd, 15.5, 7.0 | 23 | 132.6 CH | 5.22, 1H, dd, 15.5, 7.0 |
| 24 | 42.9 CH | | 24 | 43.5 CH | |
| 25 | 33.2 CH | | 25 | 33.7 CH | |
| 26 | 20.1 $CH_3$ | 0.82, 3H, d, 6.0 | 26 | 20.6 $CH_3$ | 0.82, 3H, d, 6.5 |
| 27 | 23.1 $CH_3$ | 0.84, 3H, d, 6.0 | 27 | 23.7 $CH_3$ | 0.84, 3H, d, 6.5 |
| 28 | 17.7 $CH_3$ | 0.92, 3H, d, 6.0 | 28 | 18.3 $CH_3$ | 0.92, 3H, d, 6.0 |

Reference: Kwon HC, Zee SD, Cho SY, Choi SU, Lee KR. 2002. Cytotoxic ergosterols from *Paecilomyces* sp. J300. Arch Pharm Res. 25:851–855.

**Table S5.**

| Position | Compound 4 | |
|---|---|---|
| | ***δ* C, type** | ***δ* H (*J* in Hz)** |
| 1 | 165.8 C | - |
| 2 NH | - | 8.44, s, 1H |
| 3 | 65.3 C | - |
| 3 $SCH_3$ | 12.8 $CH_3$ | 2.31, s, 3H |
| 4 | 165.6 C | - |
| 5 NH | - | 8.91, s, 1H |
| 6 | 65.9 C | - |
| 6 $SCH_3$ | 13.5 $CH_3$ | 2.13 s, 3H |
| 7 | 33.9 $CH_2$ | 3.16, d, 1H, 12 |
| | | 3.64, d, 1H, 12 |
| 8 | 107.9 C | - |
| 9 | 124.3 CH | 7.19, s, 1H |
| 10 NH | - | 10.86, s, 1H |
| 10a | 135.5 C | - |
| 11 | 111.0 CH | 7.28, d, 1H, 6 |
| 12 | 120.7 CH | 7.02, t, 1H, 6 |
| 13 | 118.2 CH | 6.94, t, 1H, 6 |
| 14 | 118.8, CH | 7.60, d, 1H, 6 |
| 14a | 127.7, C | - |
| 15 | 65.0 $CH_2$ | 3.37, d, 1H, 12 |
| | | 3.51, d, 1H, 12 |

**Table S6.**

| Position | Compound 9 | | Compound 10 | | Compound 11 | | Compound 12 | |
|---|---|---|---|---|---|---|---|---|
| | $\delta_C$ | $\delta_H$ (*J* in Hz) | $\delta_C$ | $\delta_H$ (*J* in Hz) | $\delta_C$ | $\delta_H$ (*J* in Hz) | $\delta_C$ | $\delta_H$ (*J* in Hz) |
| 1 | 166.4 C | - | 169.5 C | - | 167.7 C | - | 165.7 C | - |
| 2 $NCH_3$ | 27.7 $CH_3$ | 3.17, 3H, s | 28.0 $CH_3$ | 3.25, 3H, s | 29.4 $CH_3$ | 3.00, 3H, s | 28.4 $CH_3$ | 3.16, 3H, s |
| 3 | 76.0 C | - | 75.4 C | - | 79.3 C | - | 76.6 C | - |
| 4 | 163.1 C | - | 165.2 C | - | 167.1 C | - | 163.4 C | - |
| 5 | 80.5 CH | 6.11, 1H, s | 79.7 CH | 6.03, 1H, s | 82.6 CH | 6.23, 1H, s | 80.2 CH | 6.21, 1H, s |
| 6 | - | 5.42, 1H, brs | - | 5.51, 1H, brs | - | 5.17, 1H, brs | - | 5.32, 1H, brs |
| 6a | 148.2 C | - | 149.5 C | - | 148.7 C | - | 148.5 C | - |
| 7 | 110.8 CH | 6.81, 1H, d, 6.0 | 111.0 CH | 6.84, 1H, d, 6.0 | 110.1 CH | 6.66, 1H, d, 6.0 | 111.5 CH | 6.80, 1H, d, 6.0 |
| 8 | 131.3 CH | 7.25, 1H, t, 6.0 | 131.7 CH | 7.24, 1H, t, 6.0 | 131.4 CH | 7.20, 1H, t, 6.0 | 131.6 CH | 7.30, 1H, t, 6.0 |
| 9 | 120.9 CH | 6.86, 1H, t, 6.0 | 120.7 CH | 6.78, 1H, t, 6.0 | 120.5 CH | 6.81, 1H, t, 6.0 | 120.7 CH | 6.81, 1H, t, 6.0 |
| 10 | 124.4 CH | 7.10, 1H, d, 6.0 | 124.6 CH | 6.99, 1H, d, 6.0 | 124.9 CH | 7.18, 1H, d, 6.0 | 125.2 CH | 7.35, 1H, d, 6.0 |
| 10a | 127.3 C | - | 126.1 C | - | 127.6 C | - | 127.4 C | - |
| 10b | 73.8 C | - | 71.8 C | - | 72.7 C | - | 76.2 C | - |
| 11 | 43.8 $CH_2$ | 4.36, 3.10, 2H, d, 12 | 50.1 $CH_2$ | 3.37, 4.04, 2H, d, 12 | 48.7 $CH_2$ | 3.33, 3.93, 2H, d, 12 | 42.8 $CH_2$ | 3.00, 4.35, 2H, d, 12 |
| 11a | 73.5 C | - | 78.1 C | - | 74.6 C | - | 74.9 C | - |
| 12 | 60.7 $CH_2$ | 4.37, 4.27, 2H, d, 12 | 62.2 $CH_2$ | 4.28, 3.99, 2H, d, 12 | 62.1 $CH_2$ | 4.40, 3.93, 2H, d, 12 | 60.8 $CH_2$ | 4.43, 4.28, 2H, d, 12 |
| 1’ | 167.7 C | - | 167.7 C | - | 168.0 C | - | 167.0 C | - |
| 2’ $NCH_3$ | 29.3 $CH_3$ | 3.04, 3H, s | 29.6 $CH_3$ | 3.10, 3H, s | 29.1 $CH_3$ | 3.10, 3H, s | 27.6 $CH_3$ | 2.96, 3H, s |
| 3’ | 78.1 C | - | 78.1 C | - | 78.1 C | - | 73.6 C | - |
| 4’ | 168.0 C | - | 167.9 C | - | 168.8 C | - | 165.6 C | - |
| 5’ $NCH_3$ | 29.4 $CH_3$ | 3.18, 3H, s | 29.4 $CH_3$ | 3.14, 3H, s | 29.9 $CH_3$ | 3.14, 3H, s | 27.5 $CH_3$ | 3.20, 3H, s |
| 6’ | 77.3 C | - | 76.8 C | - | 77.5 C | - | 73.9 C | - |
| 7’ | 30.4 $CH_2$ | 4.14, 3.43, 2H, d, 12 | 30.5 $CH_2$ | 4.15, 3.44, 2H, d, 12 | 30.2 $CH_2$ | 4.10, 3.41, 2H, d, 12 | 32.6 $CH_2$ | 3.10, 3.89, 2H, d, 12 |
| 8’ | 109.1 C | - | 109.2 C | - | 109.2 C | - | 107.8 C | - |
| 9’ | 122.7 CH | 7.25, 1H, s | 122.2 CH | 7.28, 1H, s | 123.2 CH | 7.10, 1H, s | 126.6 CH | 7.19, 1H, s |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 10’a | 135.1 C | - | 135.2 C | - | 135.2 C | - | 134.1 C | - |
| 11’ | 111.6 CH | 7.32, 1H, d, 6.0 | 111.6 CH | 7.41, 1H, d, 6.0 | 111.7 CH | 7.08, 1H, d, 6.0 | 111.3 CH | 6.95, 1H, d, 6.0 |
| 12’ | 120.5 CH | 7.13, 1H, t, 6.0 | 120.4 CH | 7.10, 1H, t, 6.0 | 120.6 CH | 7.06, 1H, t, 6.0 | 123.0 CH | 7.23, 1H, t, 6.0 |
| 13’ | 123.3 CH | 7.13, 1H, t, 6.0 | 123.3 CH | 7.11, 1H, t, 6.0 | 123.2 CH | 7.02, 1H, t, 6.0 | 120.5 CH | 7.23, 1H, t, 6.0 |
| 14’ | 119.1 CH | 7.56, 1H, d, 6.0 | 118.9 CH | 7.51, 1H, d, 6.0 | 119.3 CH | 7.58, 1H, d, 6.0 | 119.3 CH | 7.67, 1H, d, 6.0 |
| 14’a | 129.5.0 C | - | 129.3 C | - | 129.4 C | - | 130.5 C | - |
| 15’ | 62.6 $CH_2$ | 4.47, 4.06, 2H, d, 12 | 62.6 $CH_2$ | 4.56, 4.15, 2H, d, 12 | 62.6 $CH_2$ | 4.39, 4.03, 2H, d, 12 | 61.4 $CH_2$ | 3.08, 3.72, 2H, d, 12 |

**Figure S1**

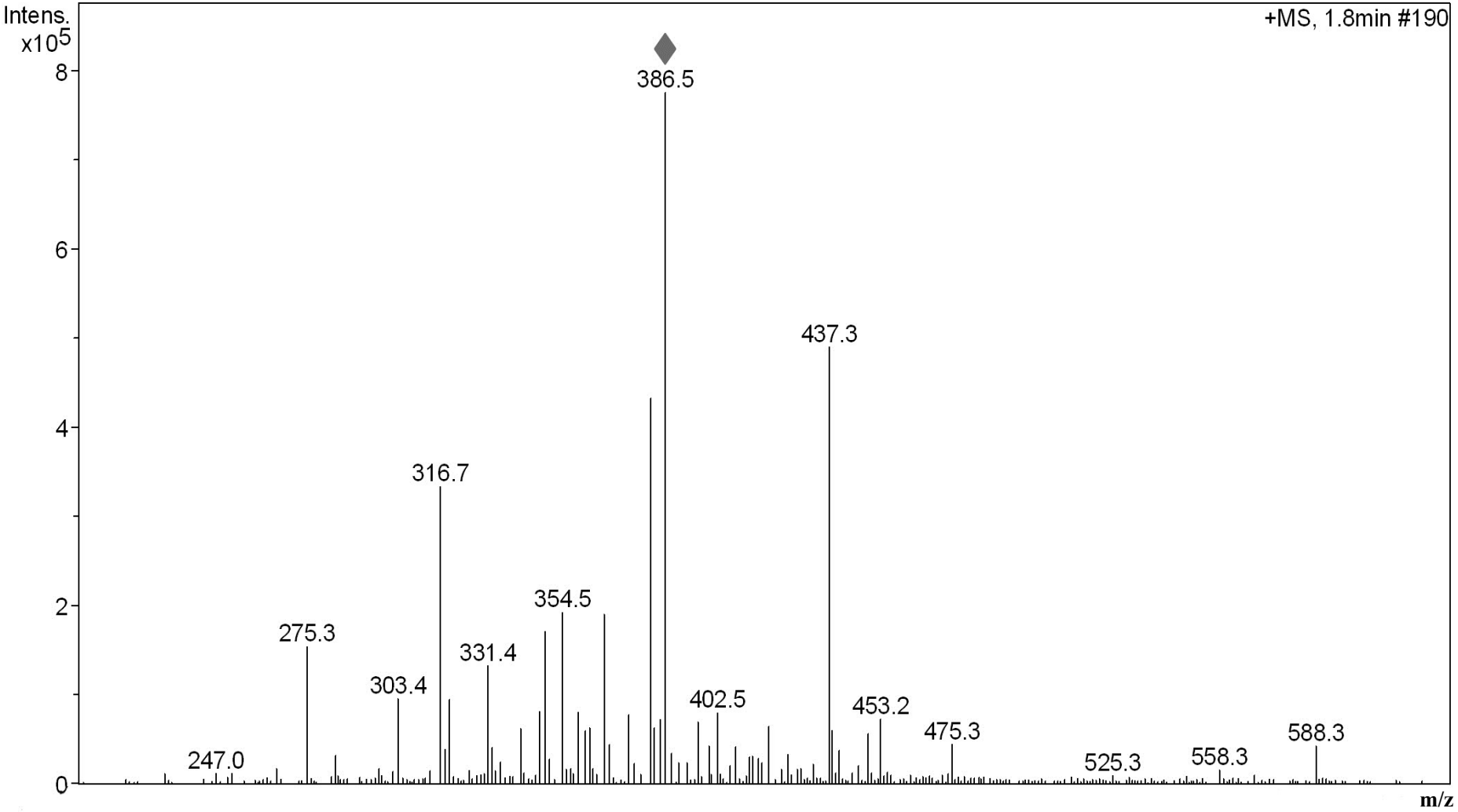
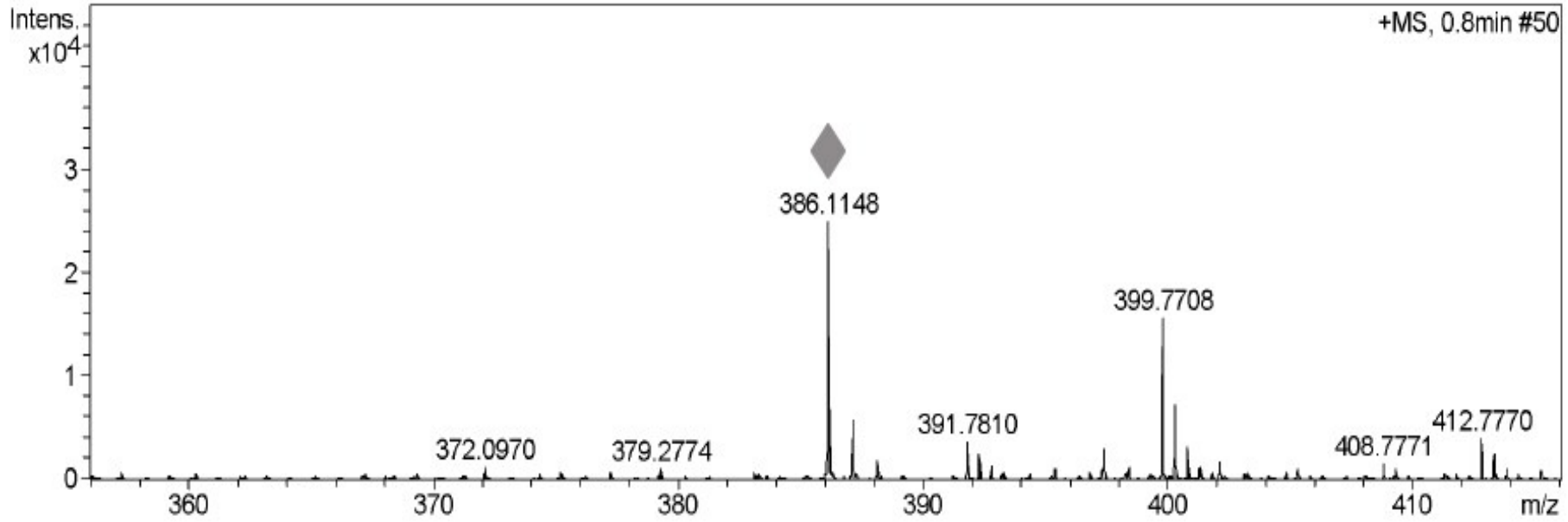

Intens.
x10^5
8
6
4
2
0
+MS, 1.8min #190
386.5
437.3
316.7
354.5
275.3
331.4
303.4
402.5
453.2
475.3
588.3
247.0
525.3
558.3
m/z

**Figure S2**




| Meas. m/z | # | Formula | m/z | err [ppm] | Mean err [ppm] | rdb | N-Rule | e⁻ Conf | mSigma | Std I | Std Mean m/z | Std I VarNorm | Std m/z Diff | Std Comb Dev |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 386.1148 | | | | | | | | | | | | | | |
| | 1 | C 17 H 21 N 3 Na O 4 S | 386.1145 | -0.8 | 0.3 | 8.5 | ok | even | 15.16 | 0.0288 | 0.0009 | 0.0099 | 0.0018 | 0.8427 |

**Figure S3**

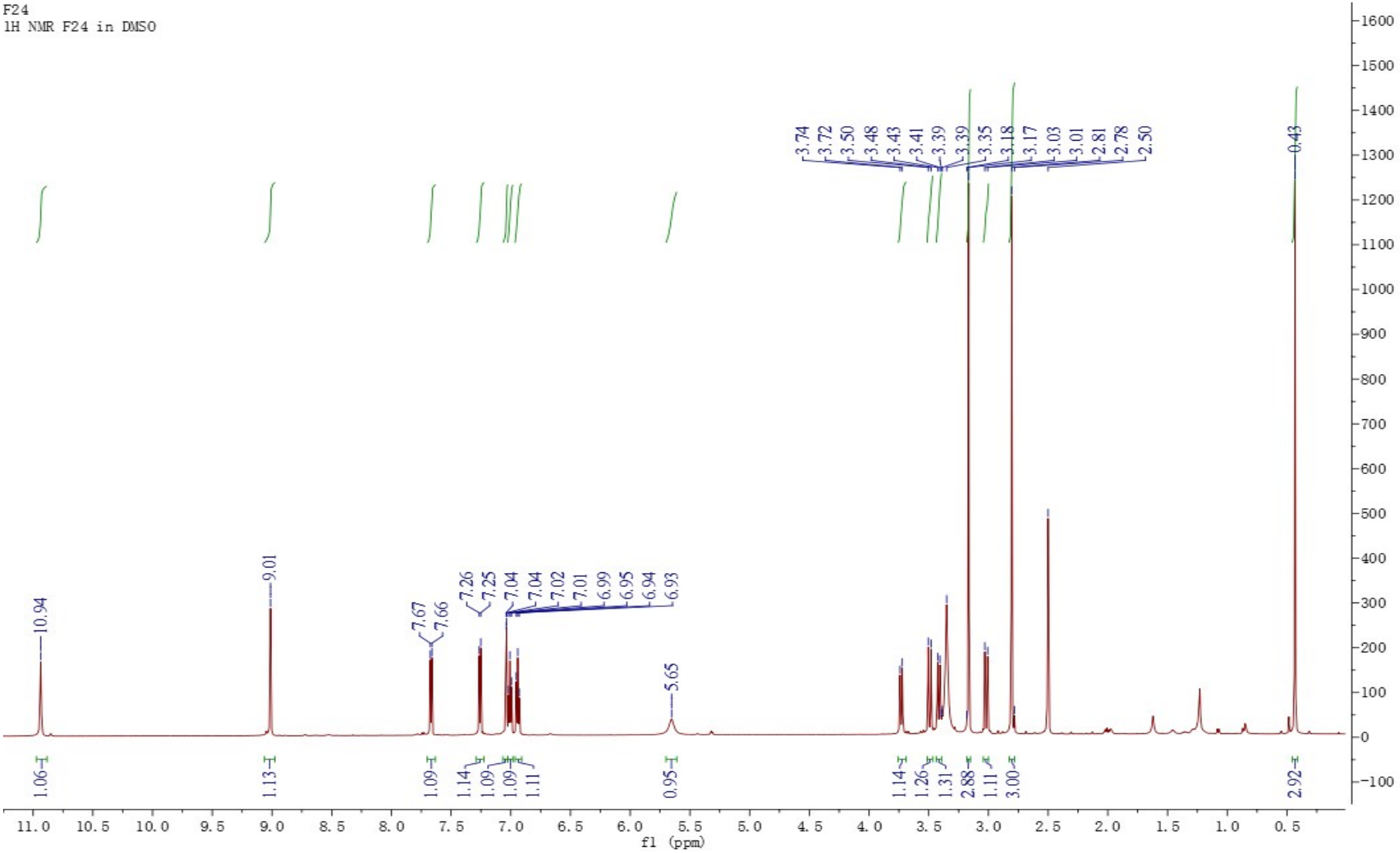

F24
1H NMR F24 in DMSO
10.94
9.01
7.67
7.66
7.26
7.25
7.04
7.04
7.02
7.01
6.99
6.95
6.94
6.93
5.65
3.74
3.72
3.50
3.48
3.43
3.41
3.39
3.39
3.35
3.18
3.17
3.03
3.01
2.81
2.78
2.50
0.43
1.06
1.13
1.09
1.14
1.09
1.09
1.11
0.95
1.14
1.26
1.31
2.88
1.11
3.00
2.92
f1 (ppm)

**Figure S4**

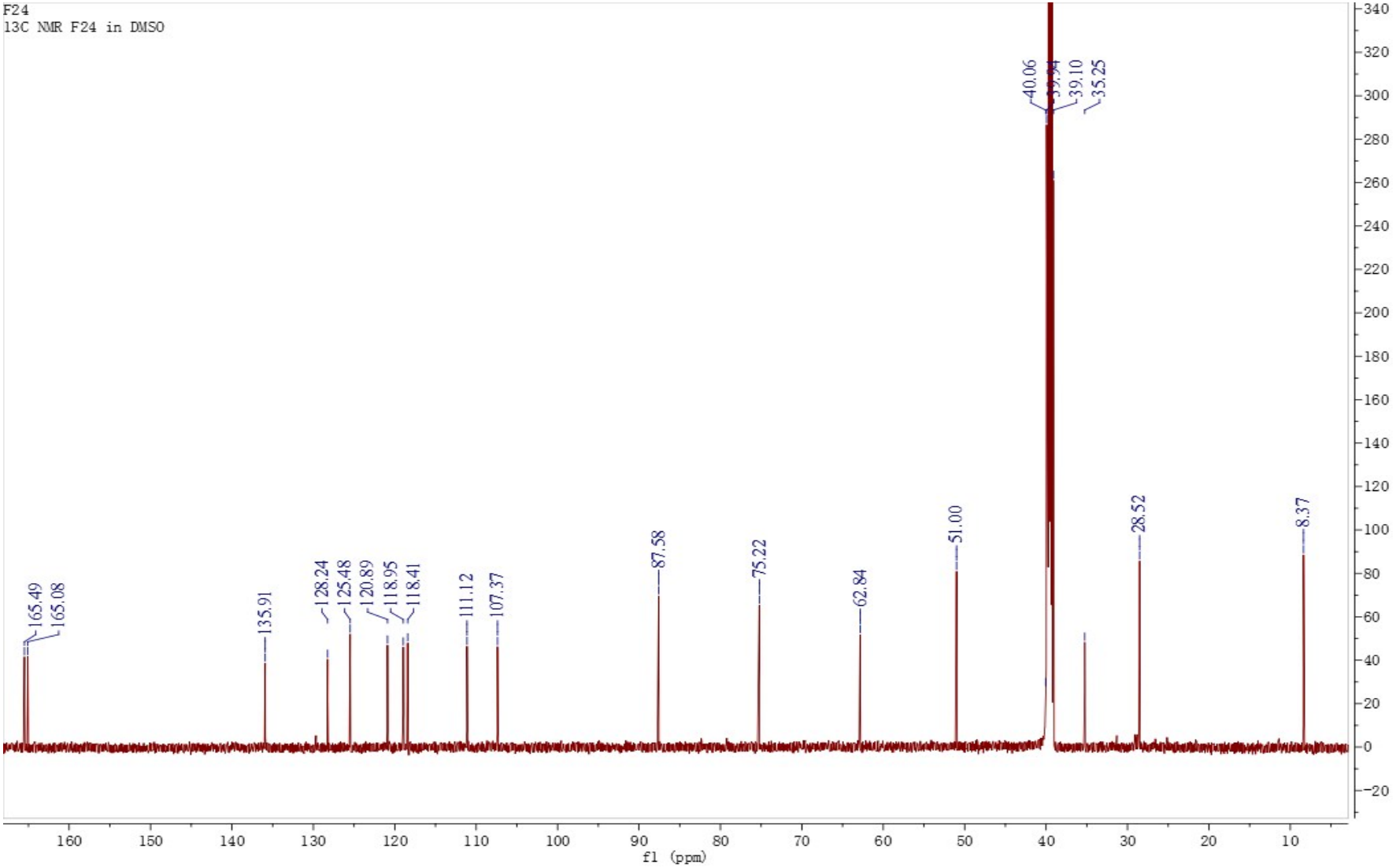

F24
13C NMR F24 in DMSO
165.49
165.08
135.91
128.24
125.48
120.89
118.95
118.41
111.12
107.37
87.58
75.22
62.84
51.00
40.06
39.94
39.10
35.25
28.52
8.37
f1 (ppm)

**Figure S5**

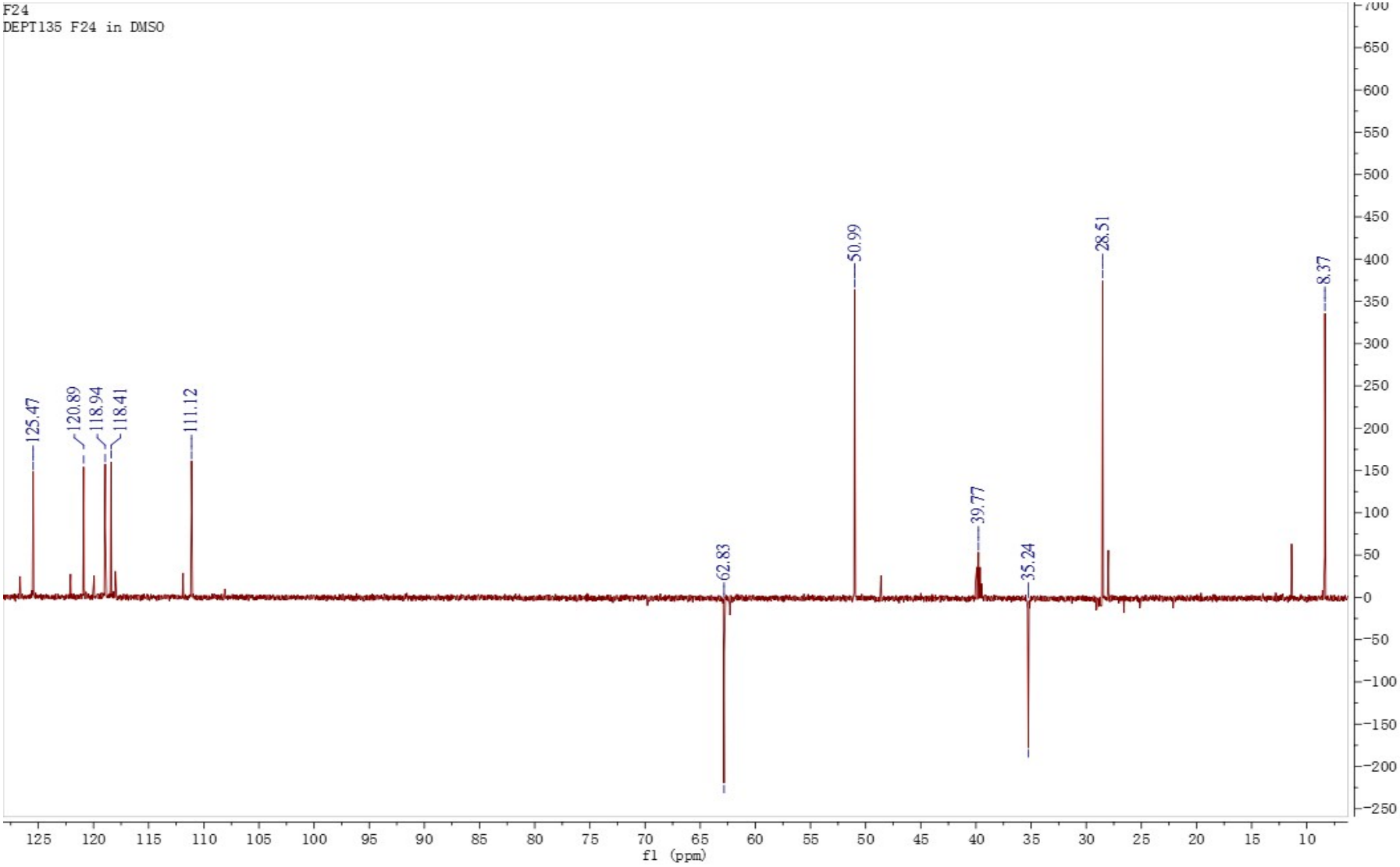

F24
DEPT135 F24 in DMSO
125.47
120.89
118.94
118.41
111.12
62.83
50.99
39.77
35.24
28.51
8.37
f1 (ppm)

**Figure S6**

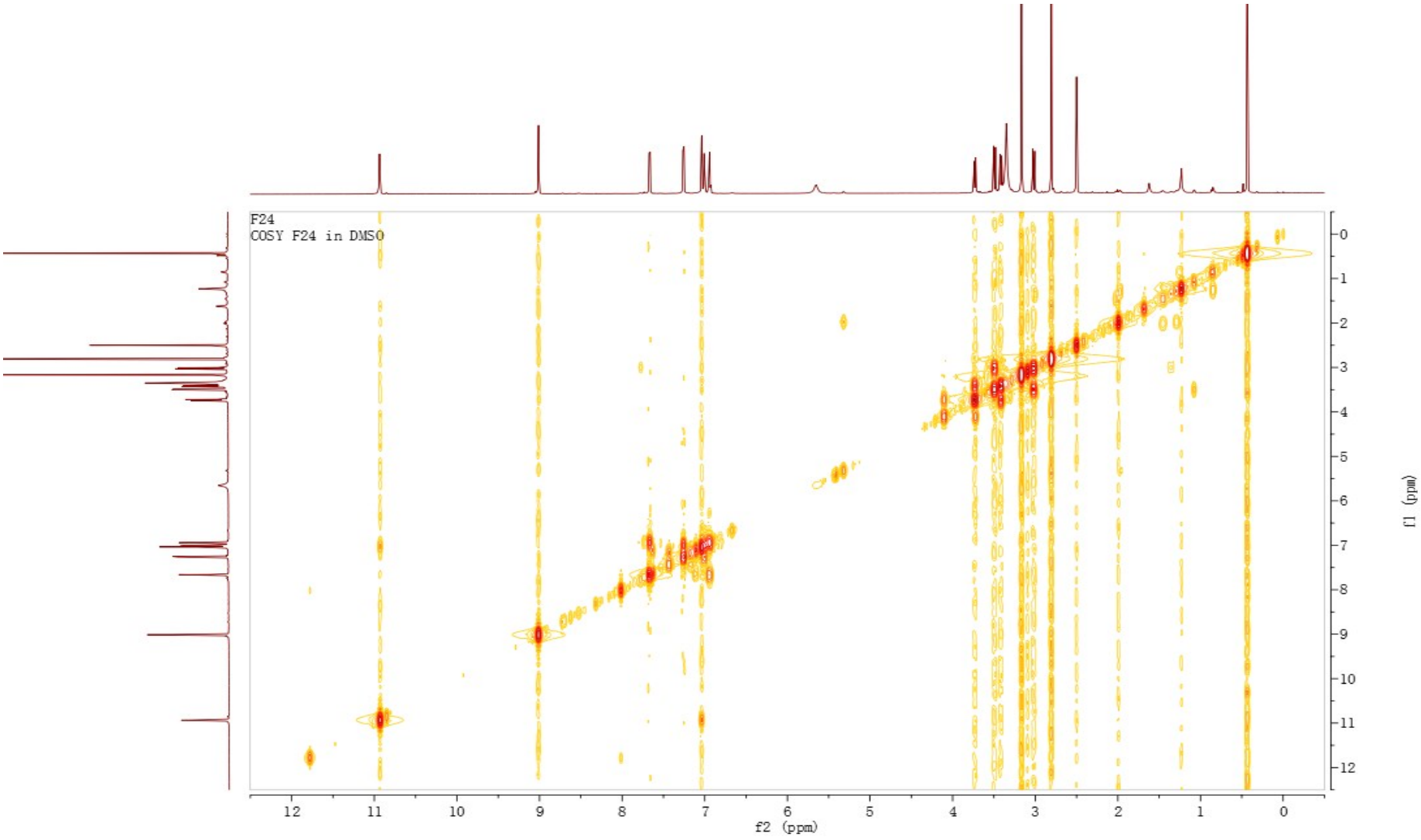


**Figure S7**

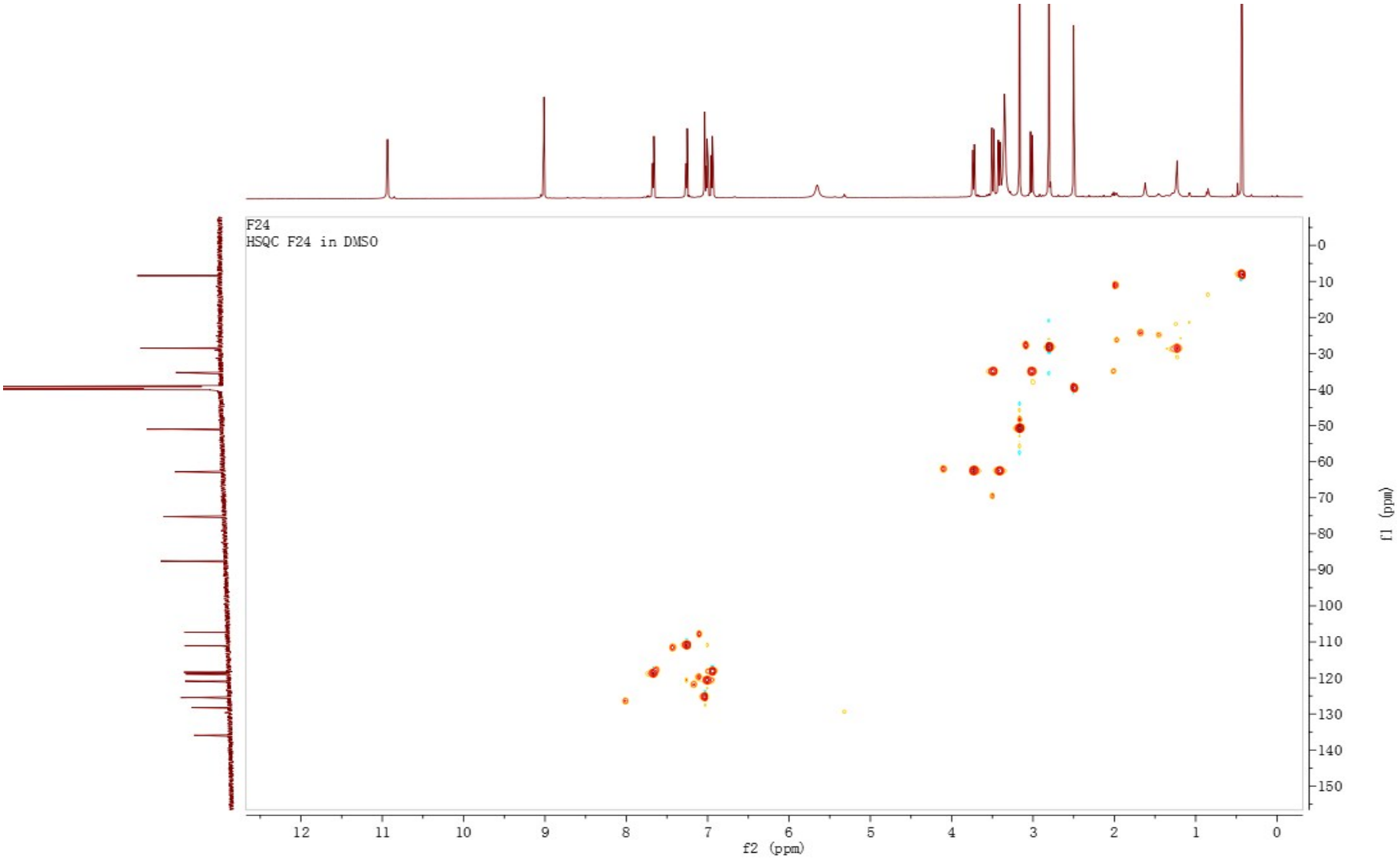


**Figure S8**

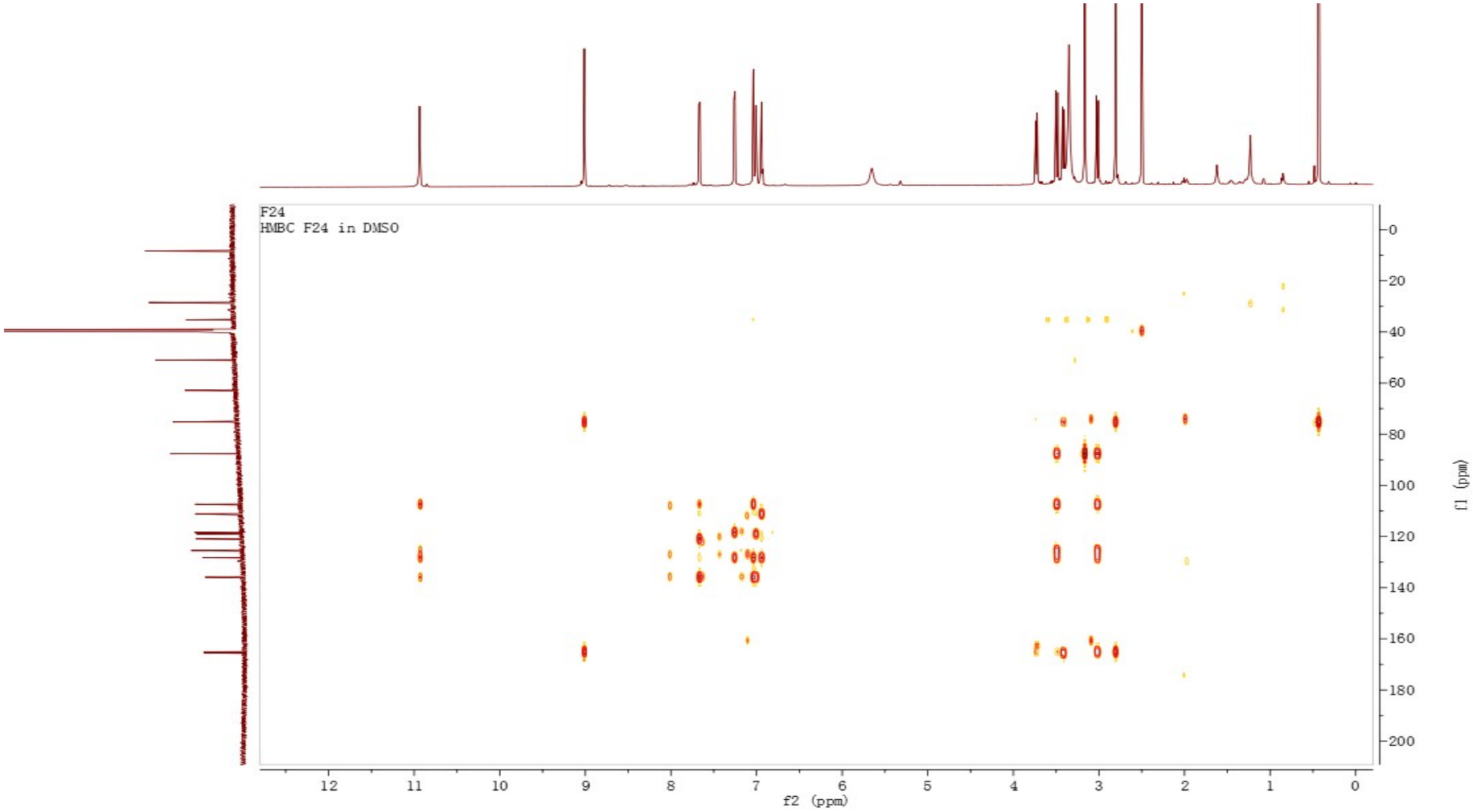


**Figure S9**

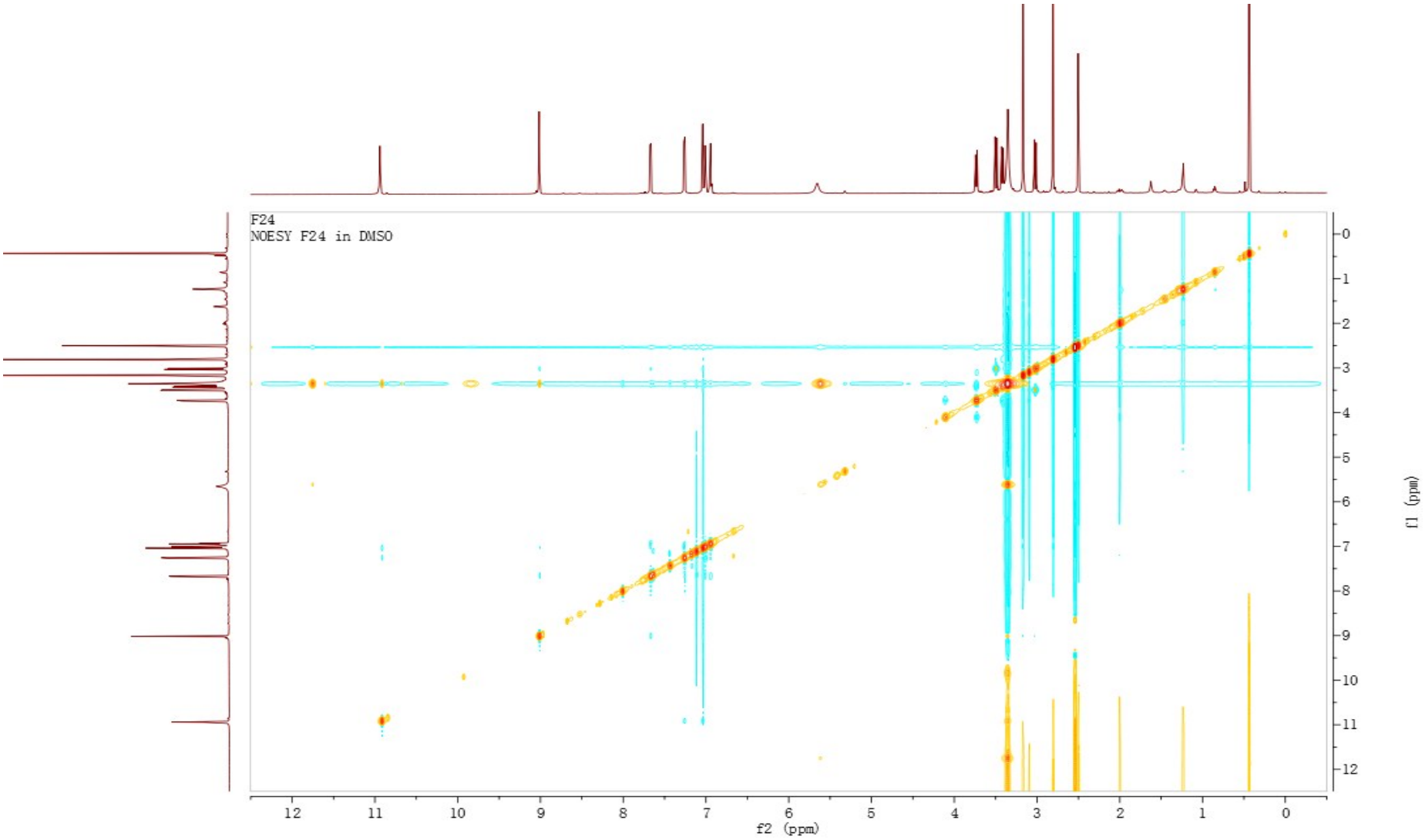


**Figure S10**

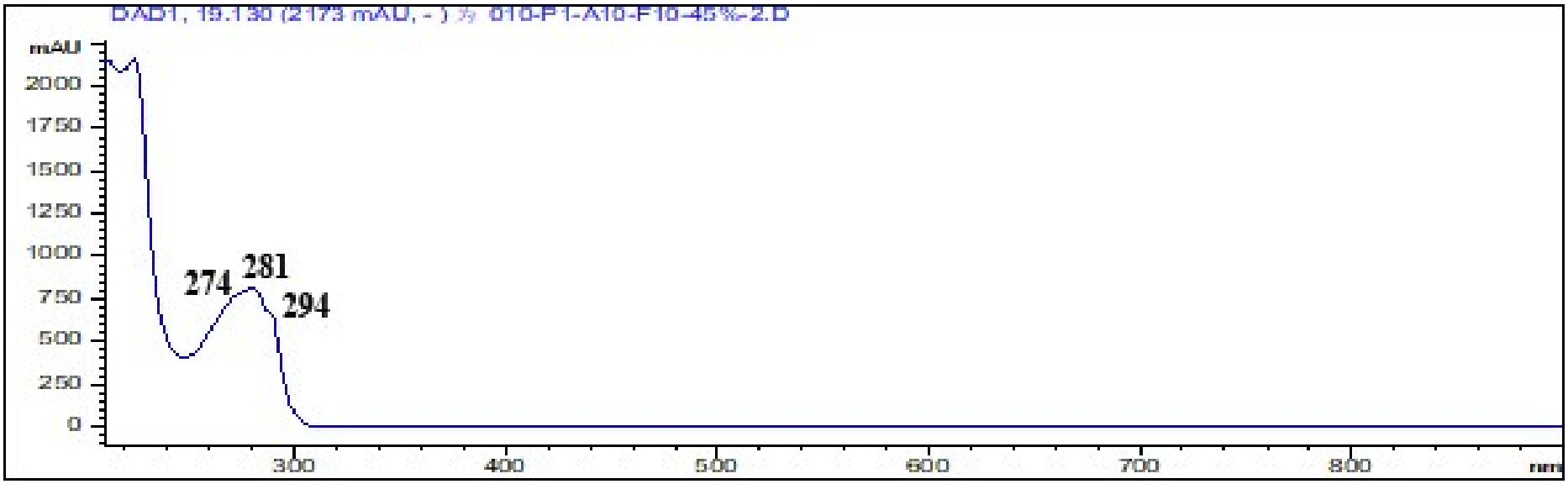

DAD1, 19.130 (2173 mAU, - ) 010-P1-A10-F10-45%-2.D
mAU
2000
1750
1500
1250
1000
750
500
250
0
274
281
294
300
400
500
600
700
800
nm

**Figure S11**

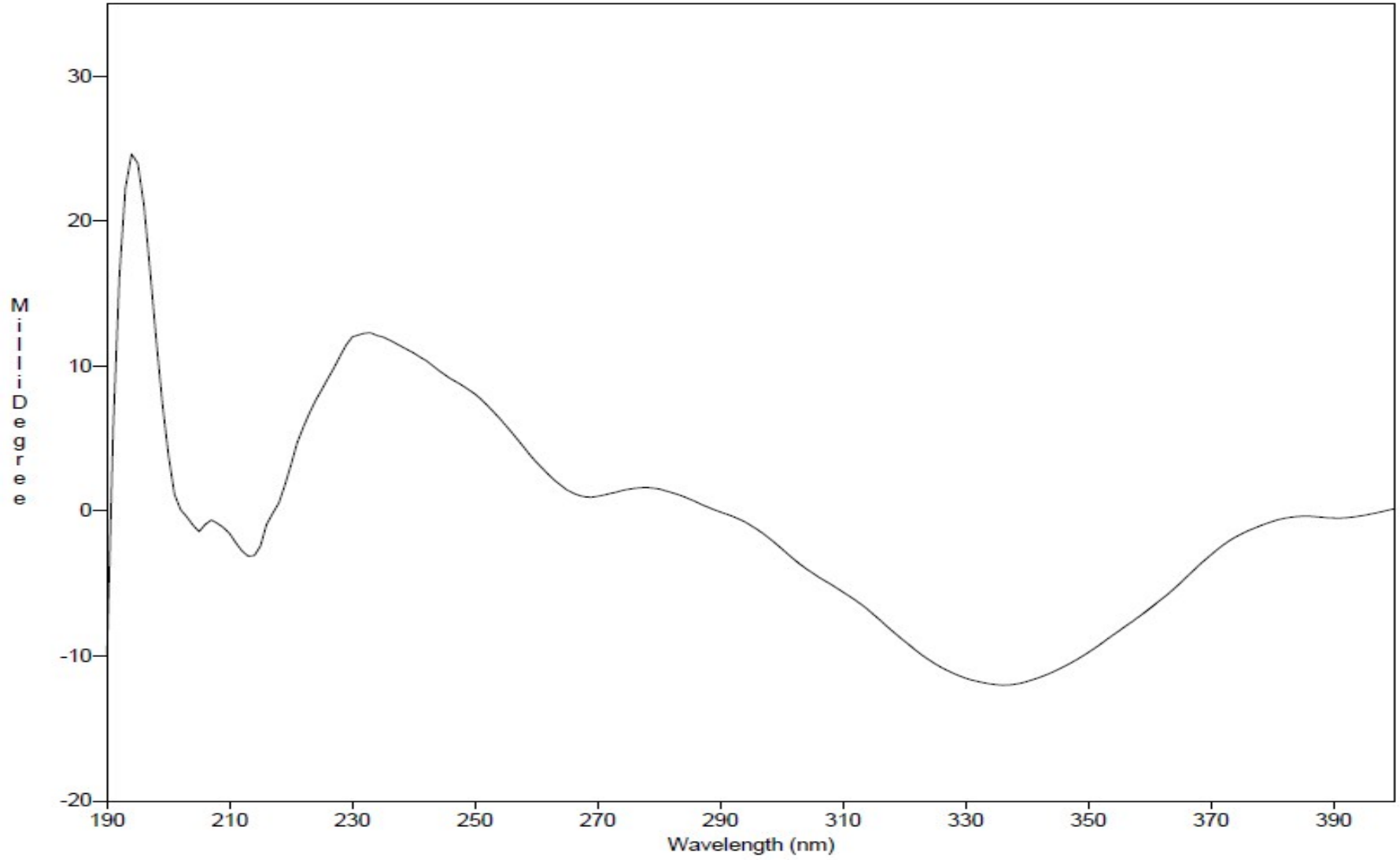

30
20
10
0
-10
-20
MilliDegree
190
210
230
250
270
290
310
330
350
370
390
Wavelength (nm)

**Figure S12**

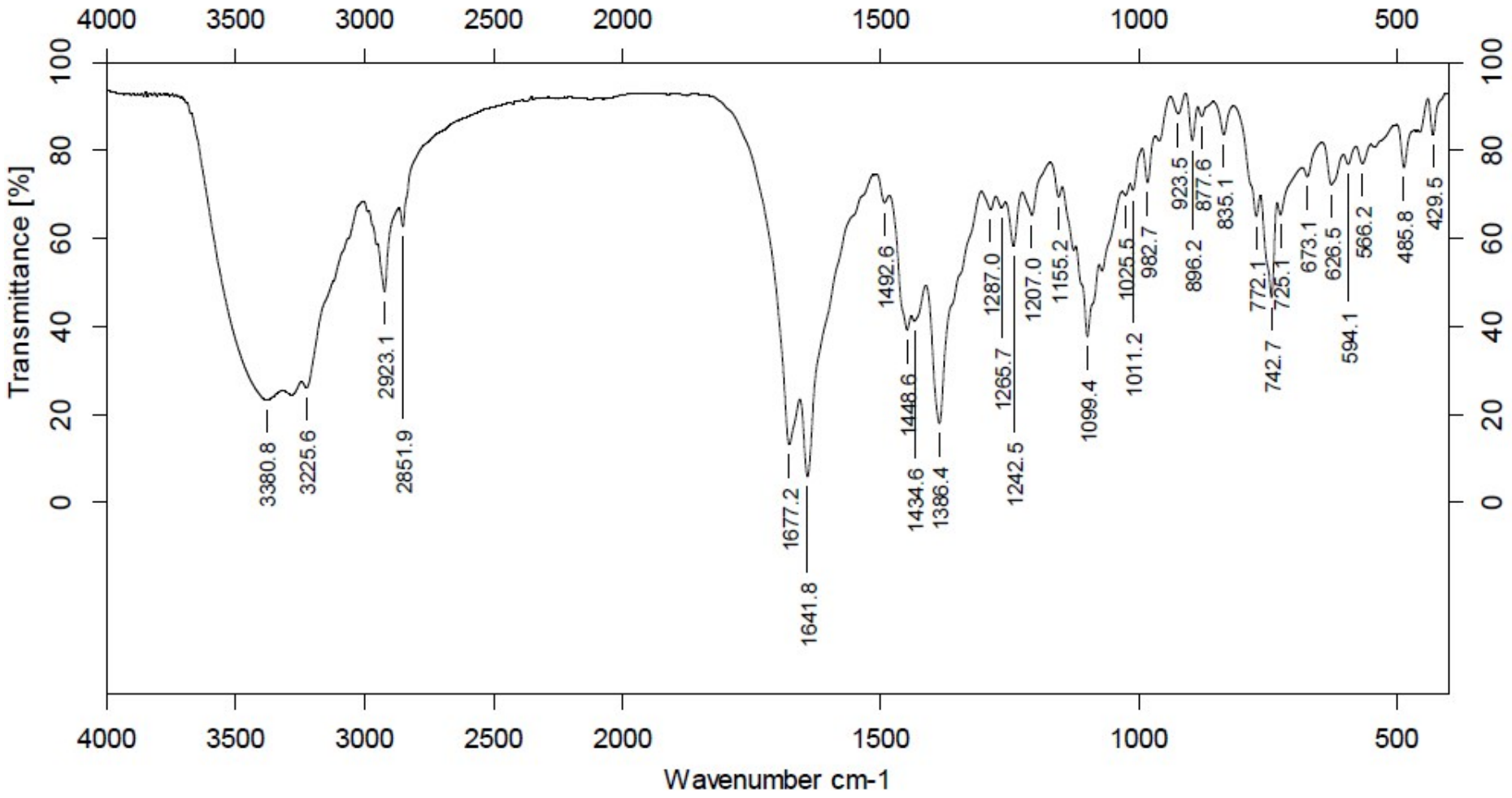

Transmittance [%]
Wavenumber cm-1
4000
3500
3000
2500
2000
1500
1000
500
0
20
40
60
80
100
3380.8
3225.6
2923.1
2851.9
1677.2
1641.8
1492.6
1448.6
1434.6
1386.4
1287.0
1265.7
1242.5
1207.0
1155.2
1099.4
1025.5
1011.2
982.7
923.5
896.2
877.6
835.1
772.1
742.7
725.1
673.1
626.5
594.1
566.2
485.8
429.5

**Figure S13**

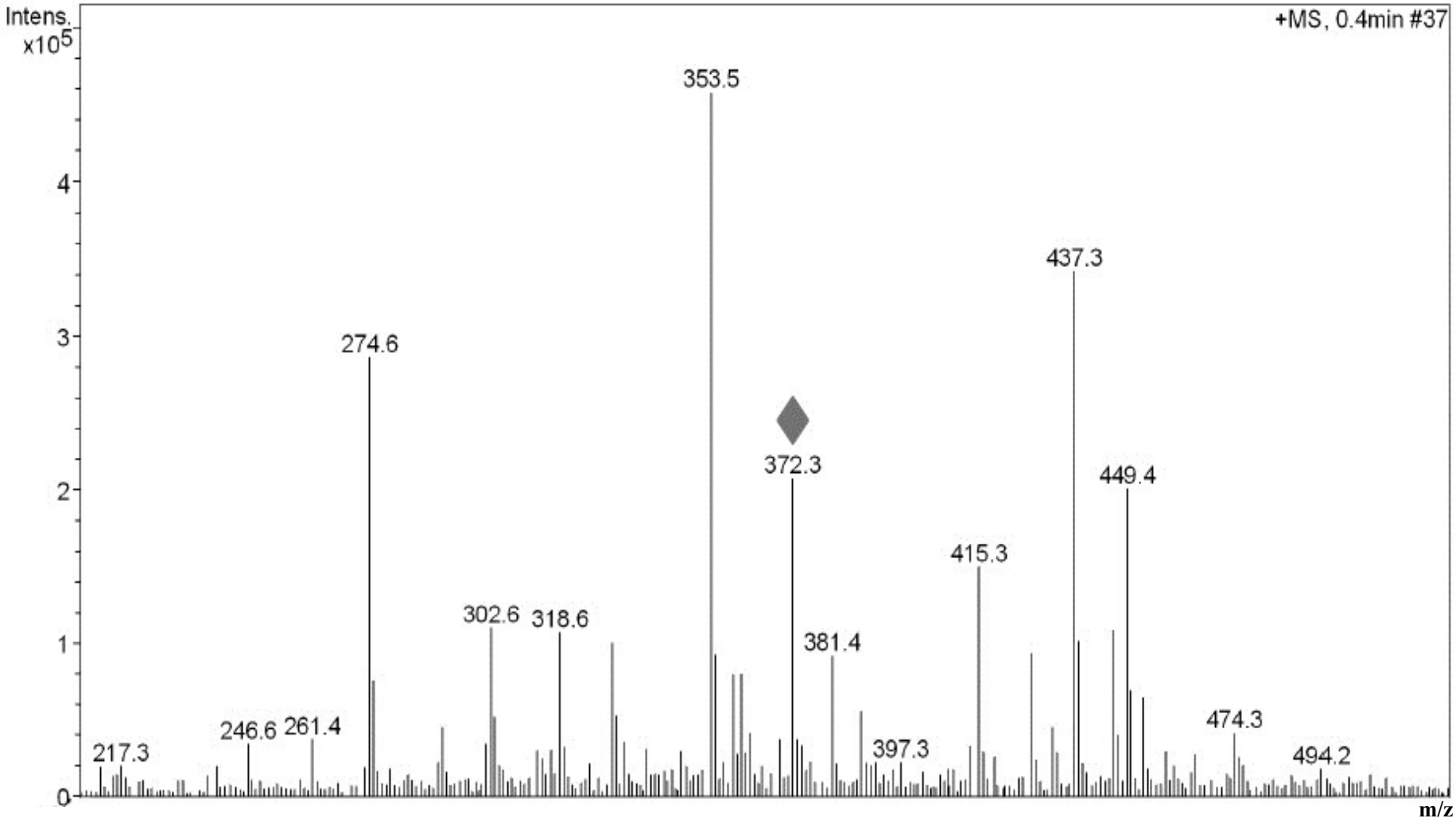
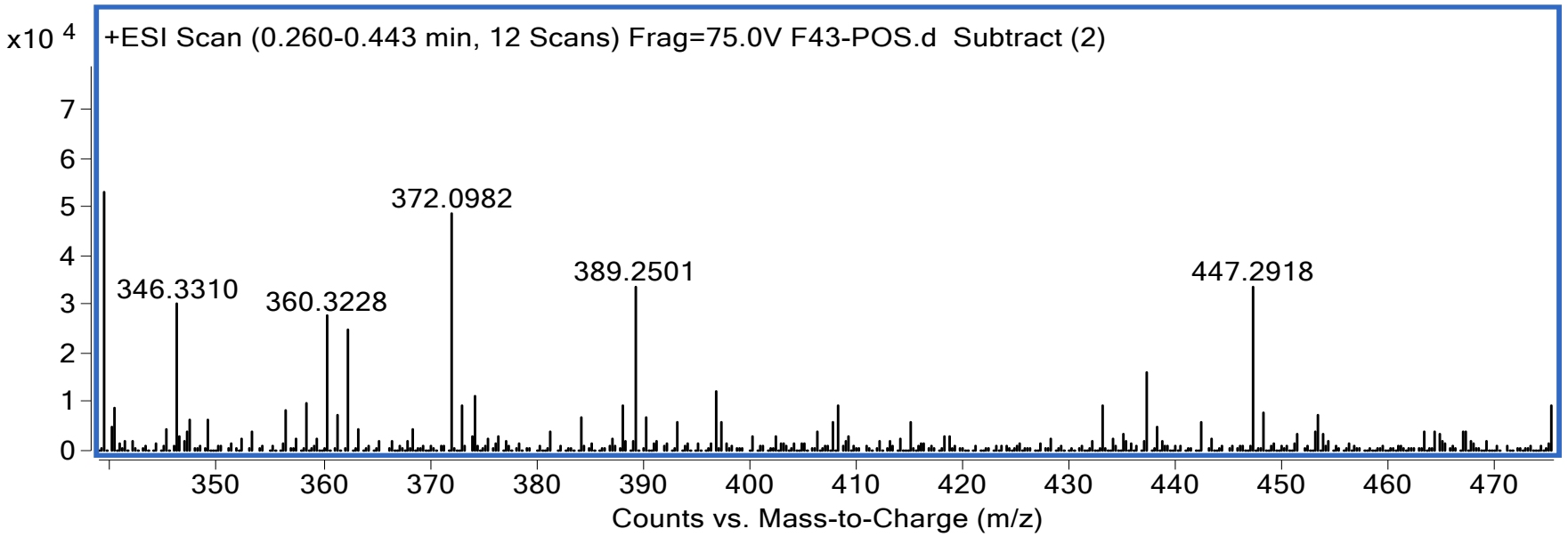

Intens.
x10^5
+MS, 0.4min #37
353.5
437.3
274.6
372.3
449.4
415.3
302.6
318.6
381.4
474.3
246.6
261.4
397.3
494.2
217.3
m/z

**Figure S14**




**Formula Calculator Results**

| Formula | Best | Mass | Tgt Mass | Diff (ppm) | Ion Species | Score |
|---|---|---|---|---|---|---|
| C16 H19 N3 O4 S | TRUE | 349.11 | 349.1096 | 1.85 | C16 H19 N3 Na O4 S | 94.31 |

**Figure S15**

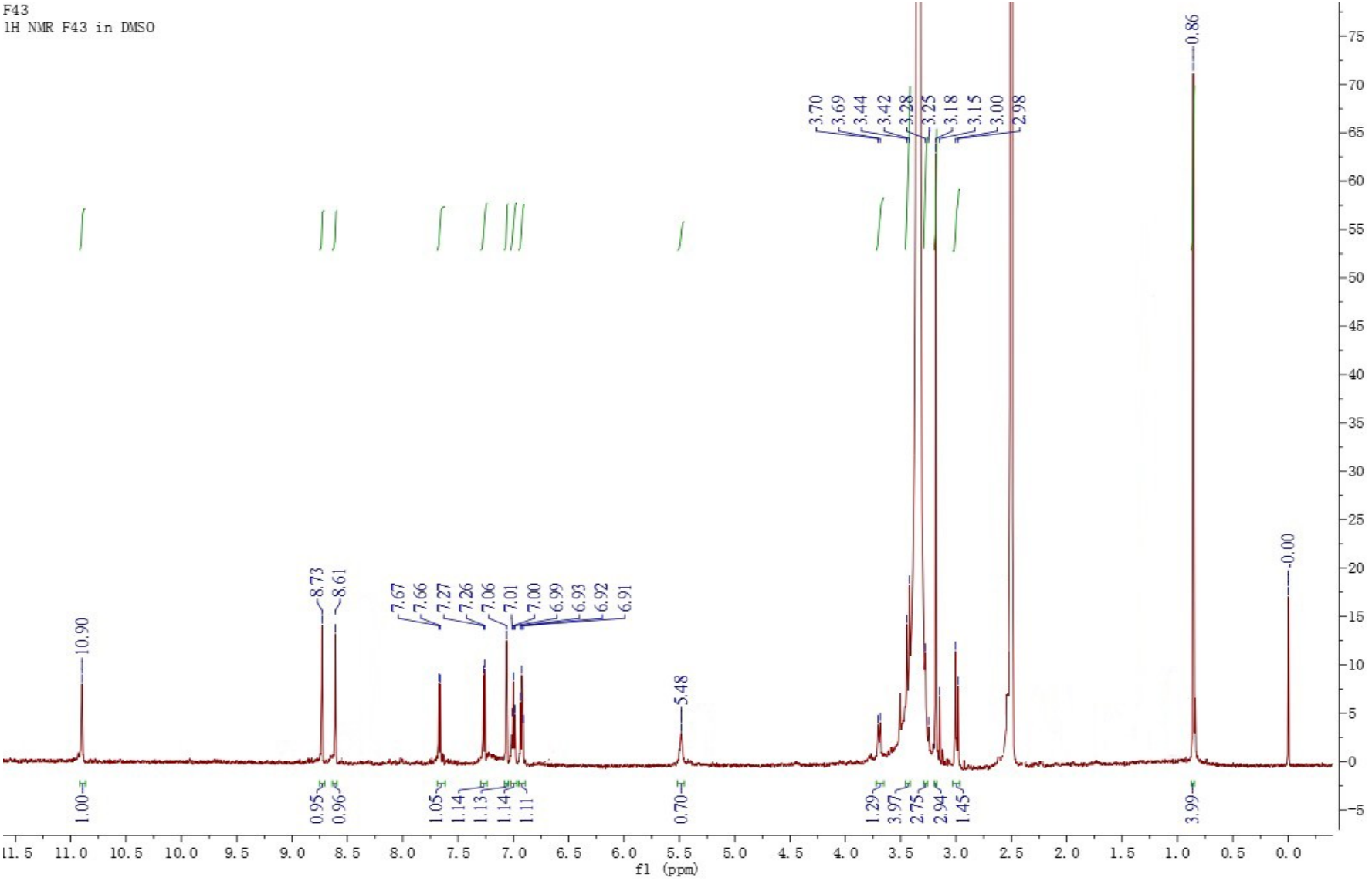

F43
1H NMR F43 in DMSO
10.90
8.73
8.61
7.67
7.66
7.27
7.26
7.06
7.01
7.00
6.99
6.93
6.92
6.91
5.48
3.70
3.69
3.44
3.42
3.28
3.25
3.18
3.15
3.00
2.98
0.86
-0.00
1.00
0.95
0.96
1.05
1.14
1.13
1.14
1.11
0.70
1.29
3.97
2.75
2.94
1.45
3.99
f1 (ppm)

**Figure S16**

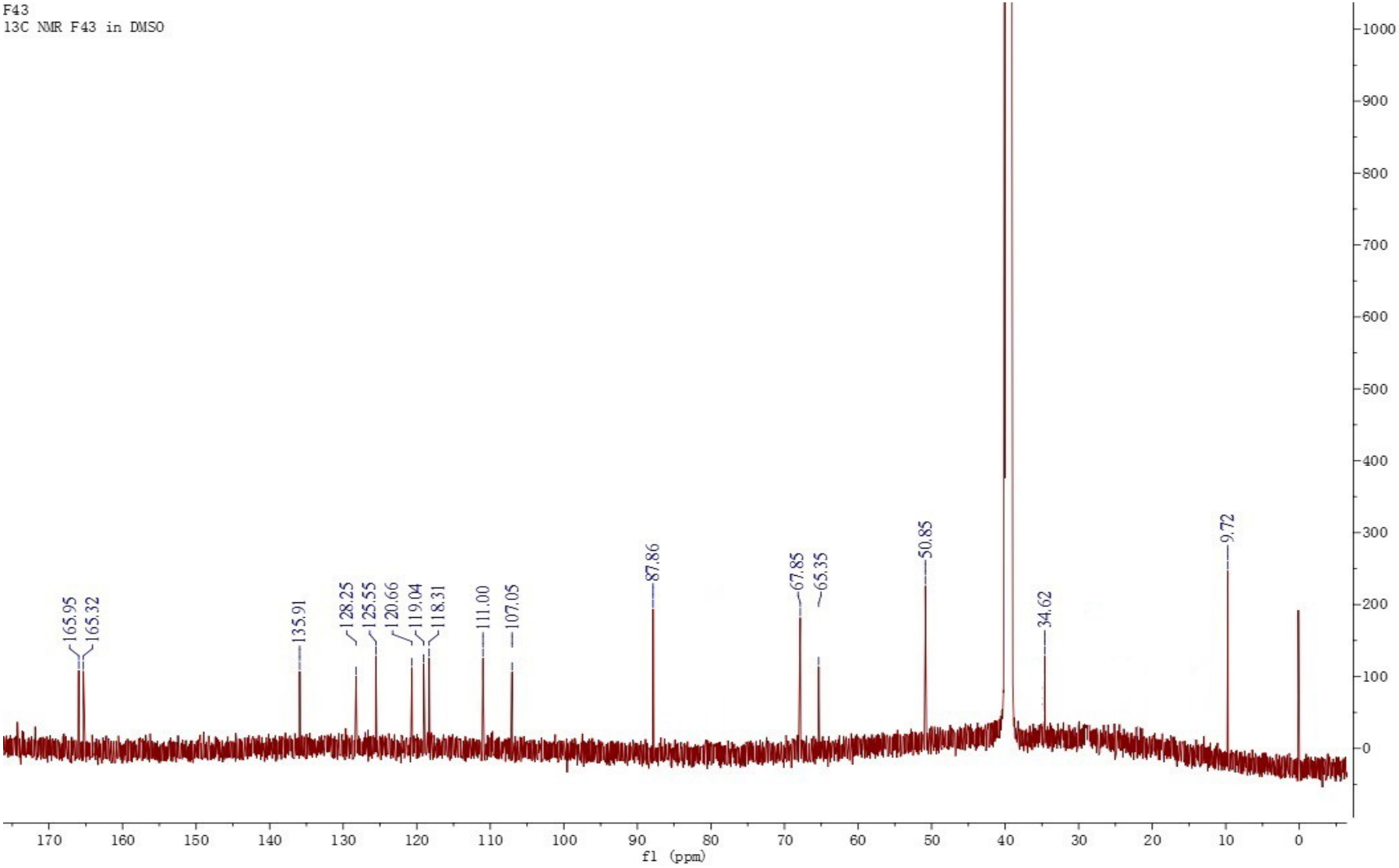

F43
13C NMR F43 in DMSO
165.95
165.32
135.91
128.25
125.55
120.66
119.04
118.31
111.00
107.05
87.86
67.85
65.35
50.85
34.62
9.72
f1 (ppm)

**Figure S17**

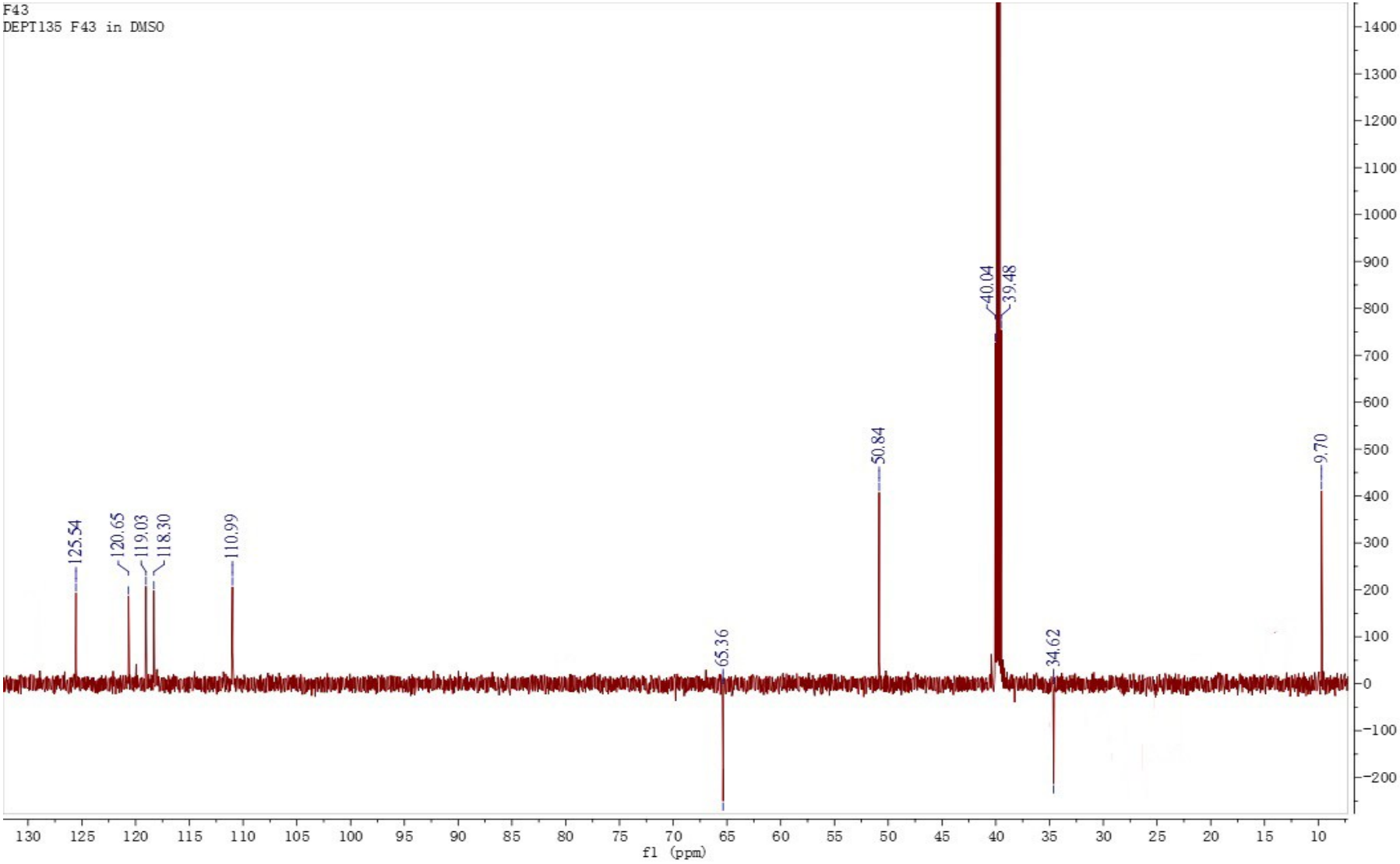

F43
DEPT135 F43 in DMSO
125.54
120.65
119.03
118.30
110.99
65.36
50.84
40.04
39.48
34.62
9.70
f1 (ppm)

**Figure S18**

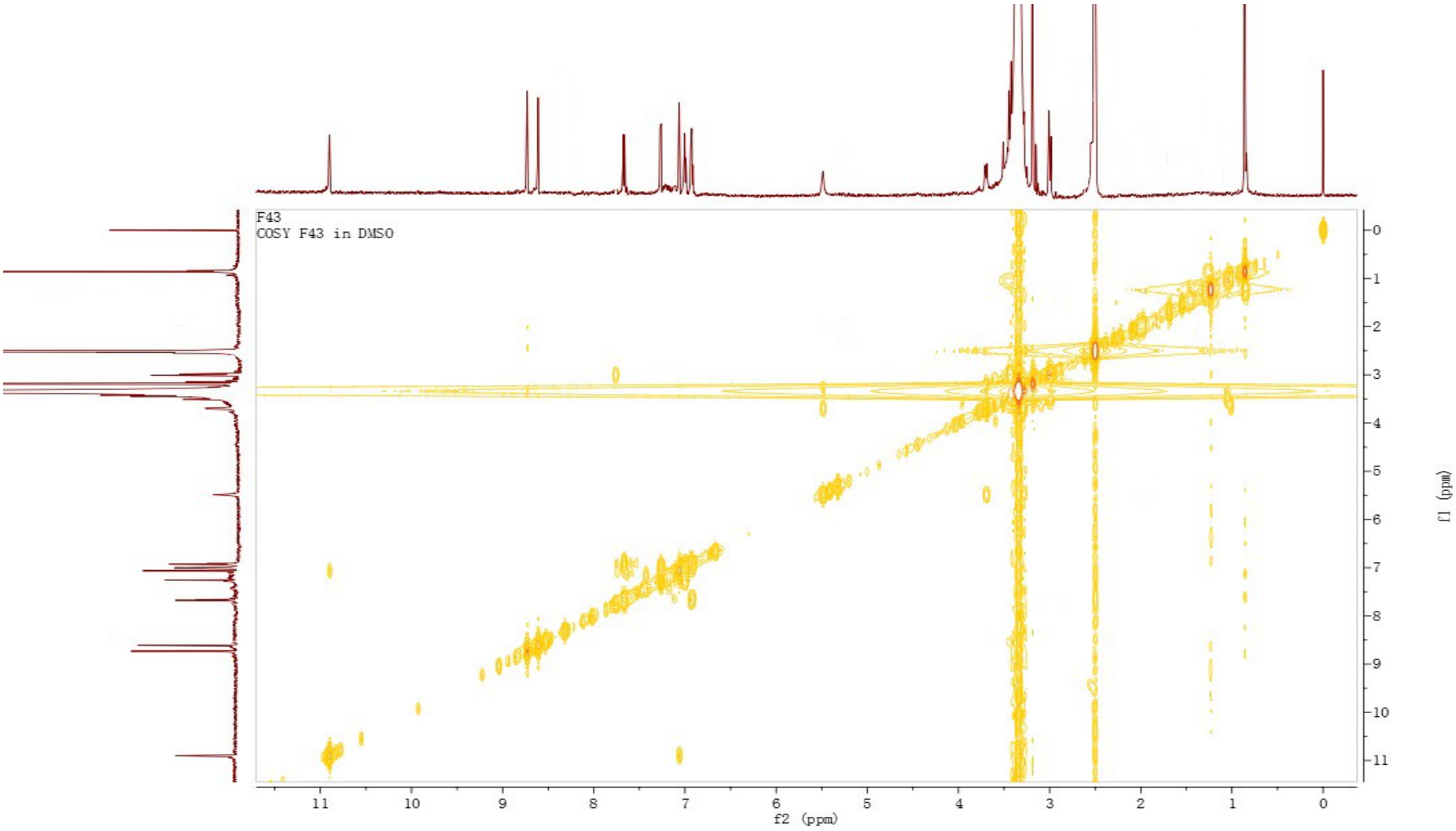


**Figure S19**

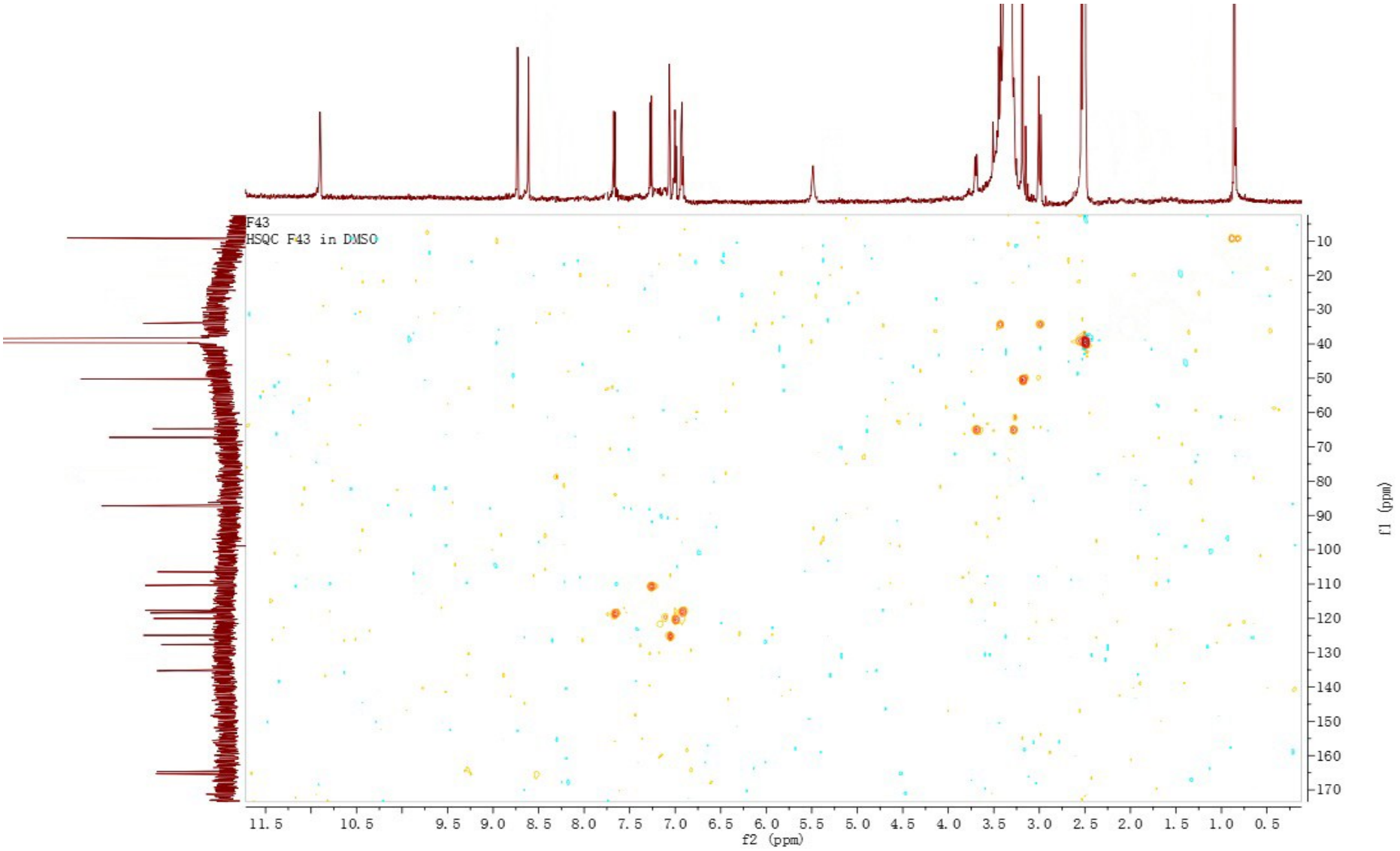

F43
HSQC F43 in DMSO
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)

**Figure S20**

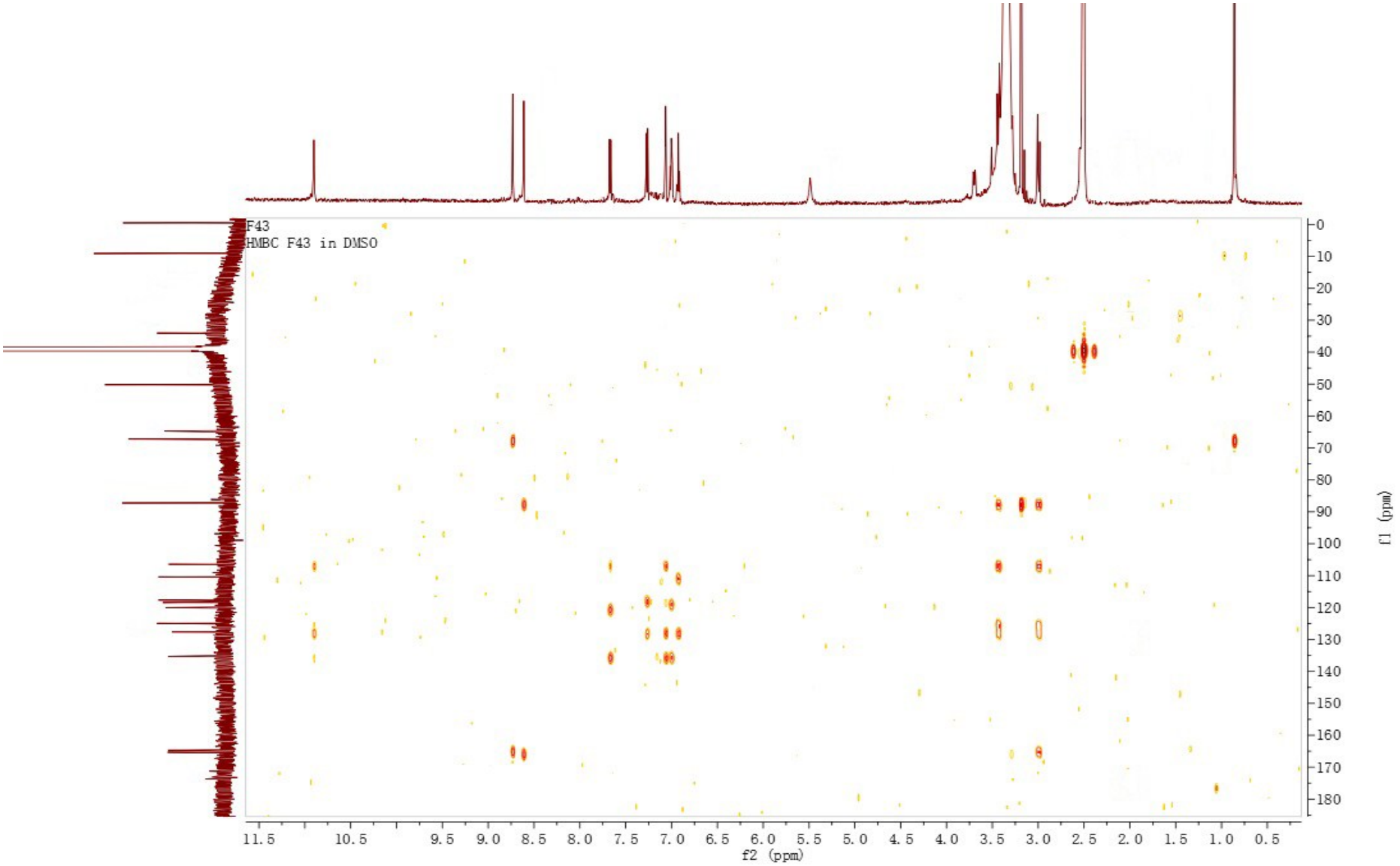


**Figure S21**

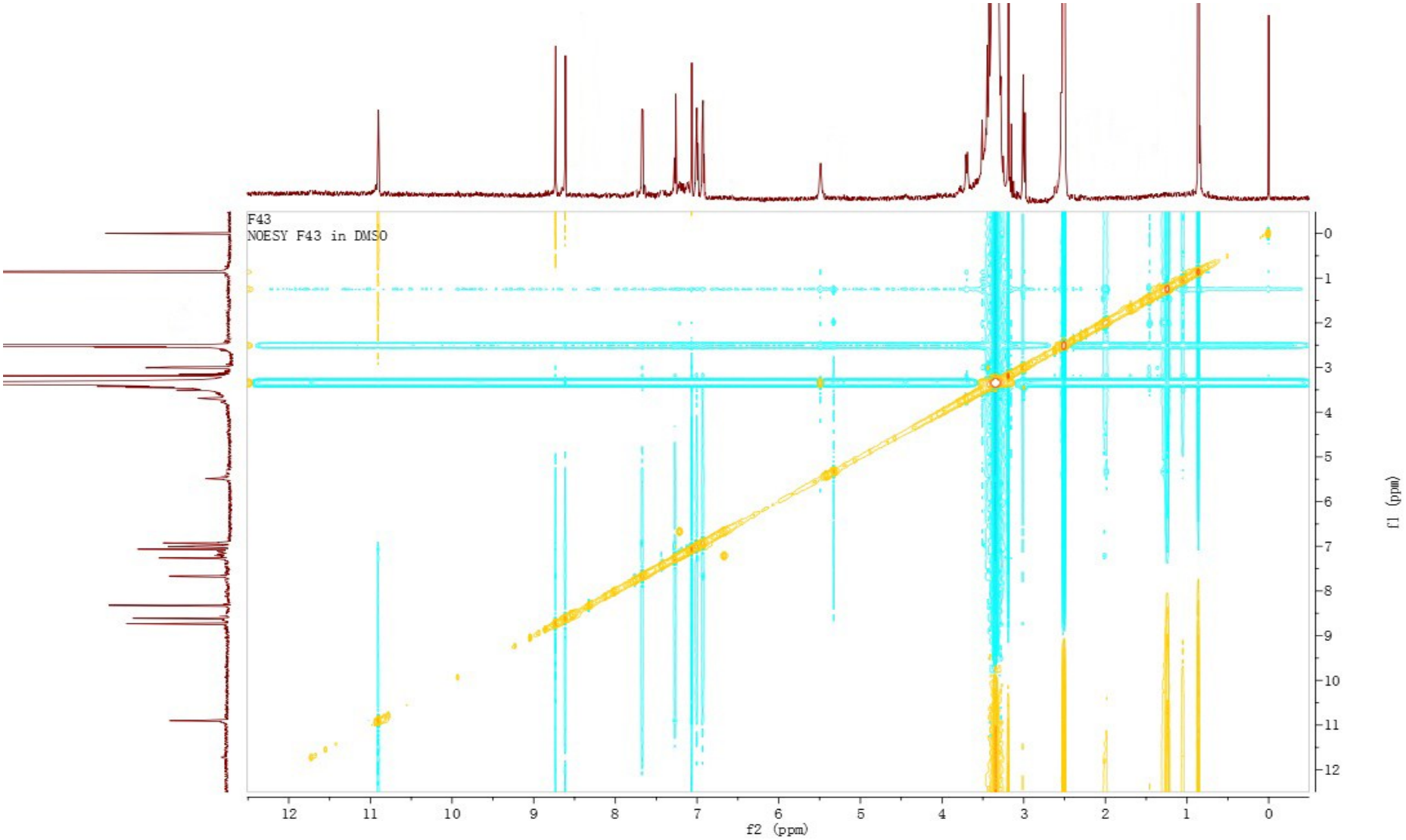


**Figure S22**

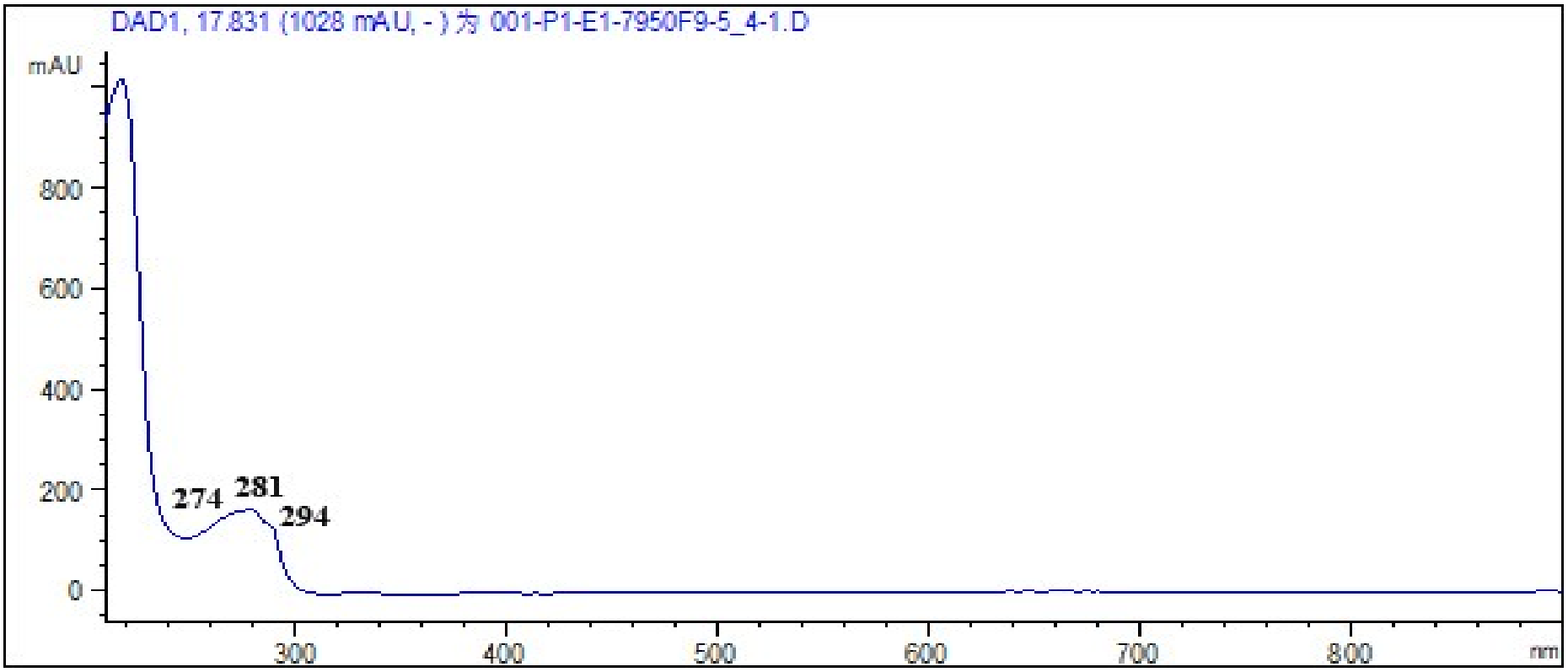

DAD1, 17.831 (1028 mAU, - ) 方 001-P1-E1-7950F9-5_4-1.D
mAU
800
600
400
200
0
274
281
294
300
400
500
600
700
800
nm

**Figure S23**

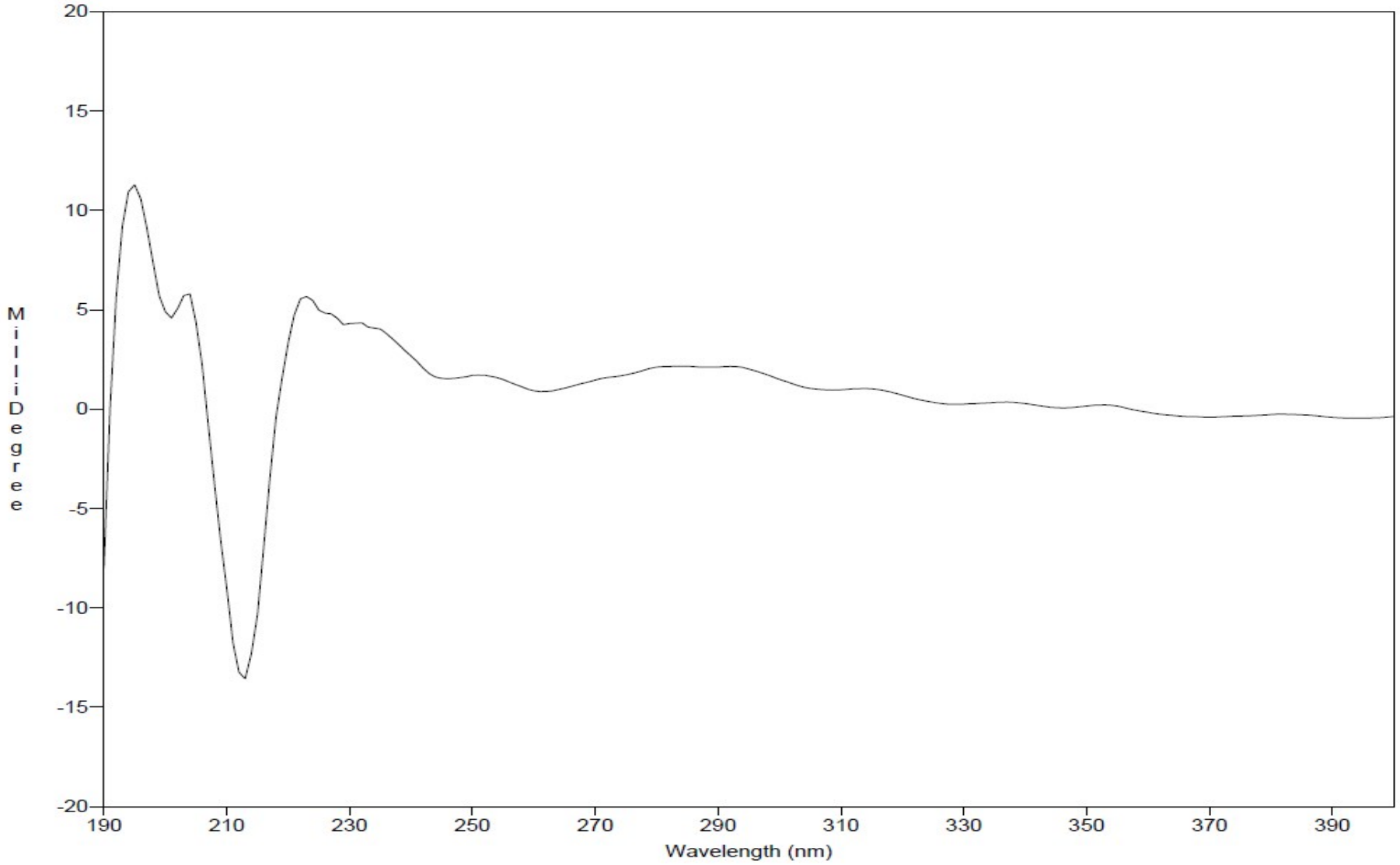

20
15
10
5
0
-5
-10
-15
-20
MilliDegree
190
210
230
250
270
290
310
330
350
370
390
Wavelength (nm)

**Figure S24**

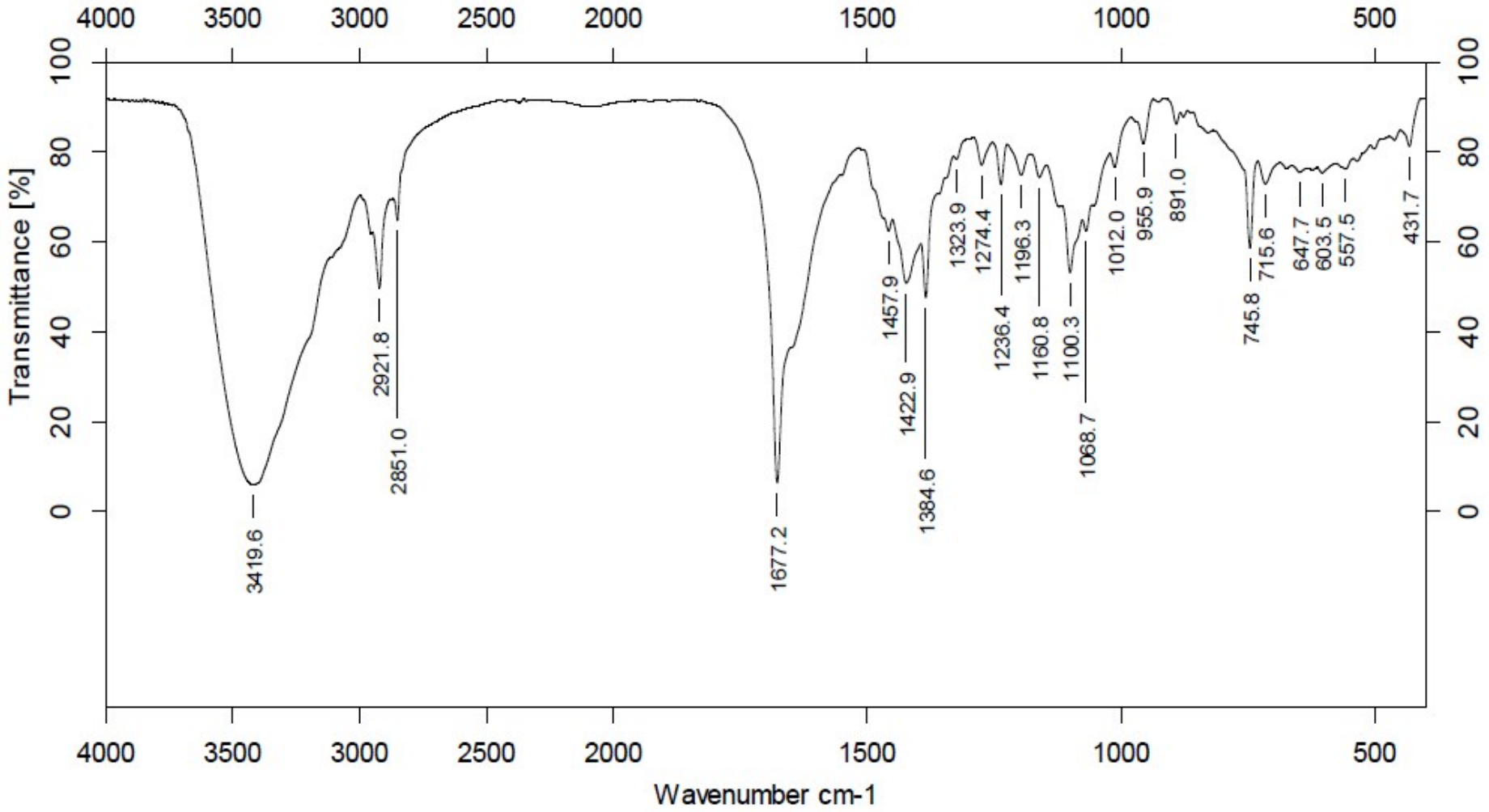

Transmittance [%]
Wavenumber cm-1
4000
3500
3000
2500
2000
1500
1000
500
0
20
40
60
80
100
3419.6
2921.8
2851.0
1677.2
1457.9
1422.9
1384.6
1323.9
1274.4
1236.4
1196.3
1160.8
1100.3
1068.7
1012.0
955.9
891.0
745.8
715.6
647.7
603.5
557.5
431.7

**Figure S25**

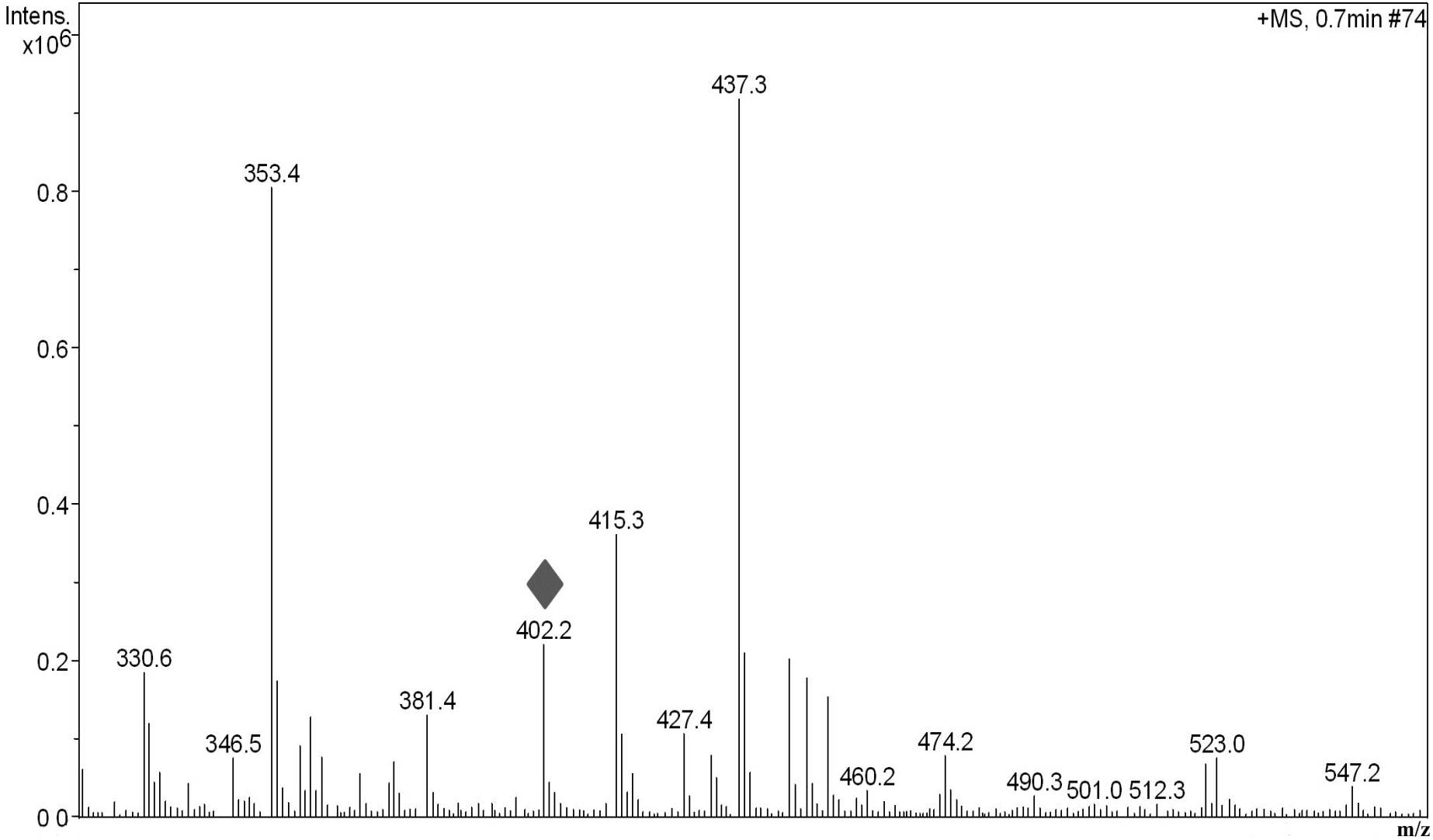

Intens.
x10^6
+MS, 0.7min #74
0.8
0.6
0.4
0.2
0 0
437.3
353.4
415.3
402.2
330.6
381.4
427.4
346.5
474.2
523.0
460.2
547.2
490.3
501.0
512.3
m/z

**Figure S26**

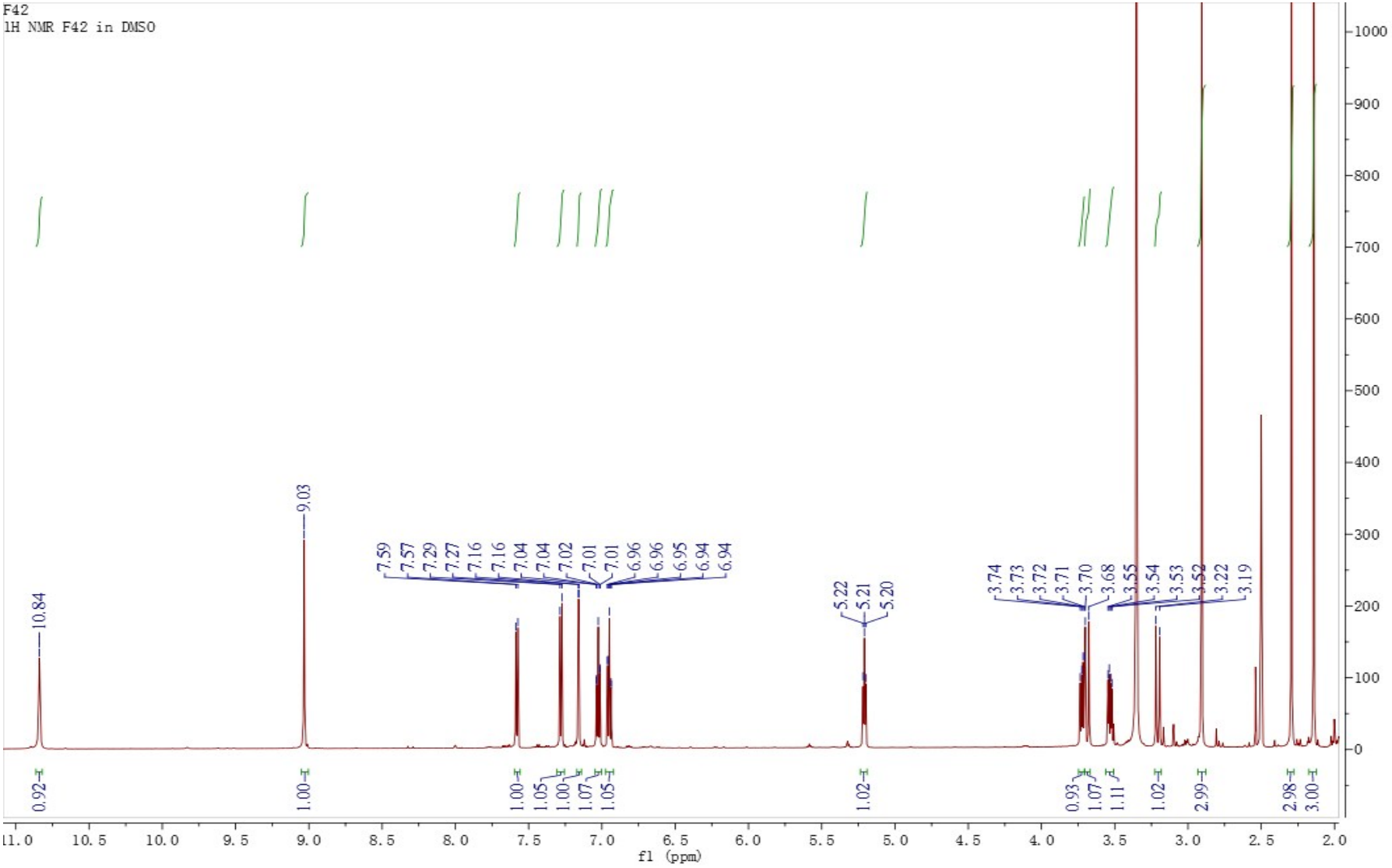

F42
1H NMR F42 in DMSO
10.84
9.03
7.59
7.57
7.29
7.27
7.16
7.16
7.04
7.04
7.02
7.01
7.01
6.96
6.96
6.95
6.94
6.94
5.22
5.21
5.20
3.74
3.73
3.72
3.71
3.70
3.68
3.55
3.54
3.53
3.52
3.22
3.19
0.92
1.00
1.00
1.05
1.00
1.07
1.05
1.02
0.93
1.07
1.11
1.02
2.99
2.98
3.00
f1 (ppm)

**Figure S27**

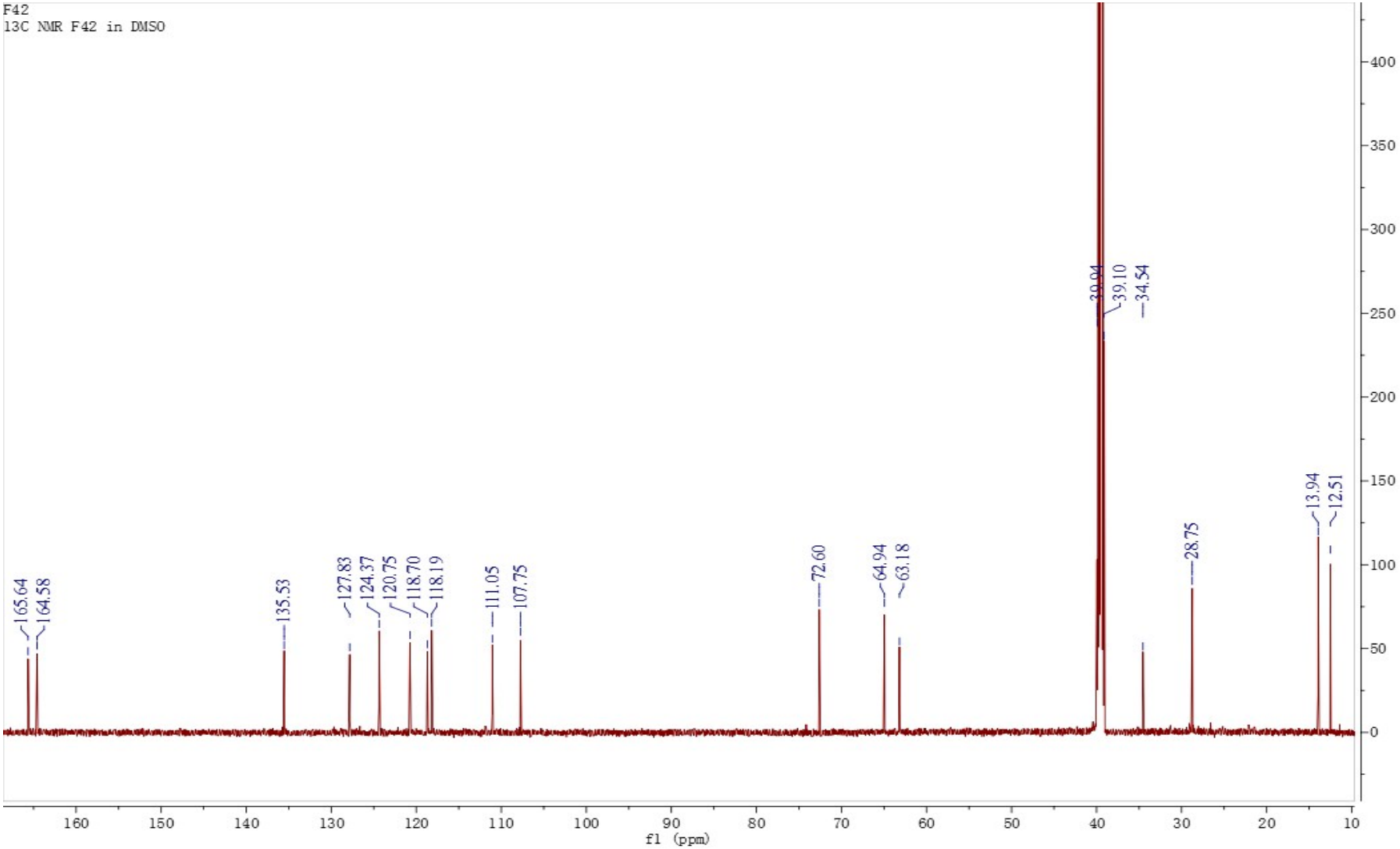

F42
13C NMR F42 in DMSO
165.64
164.58
135.53
127.83
124.37
120.75
118.70
118.19
111.05
107.75
72.60
64.94
63.18
39.94
39.10
34.54
28.75
13.94
12.51
f1 (ppm)

**Figure S28**

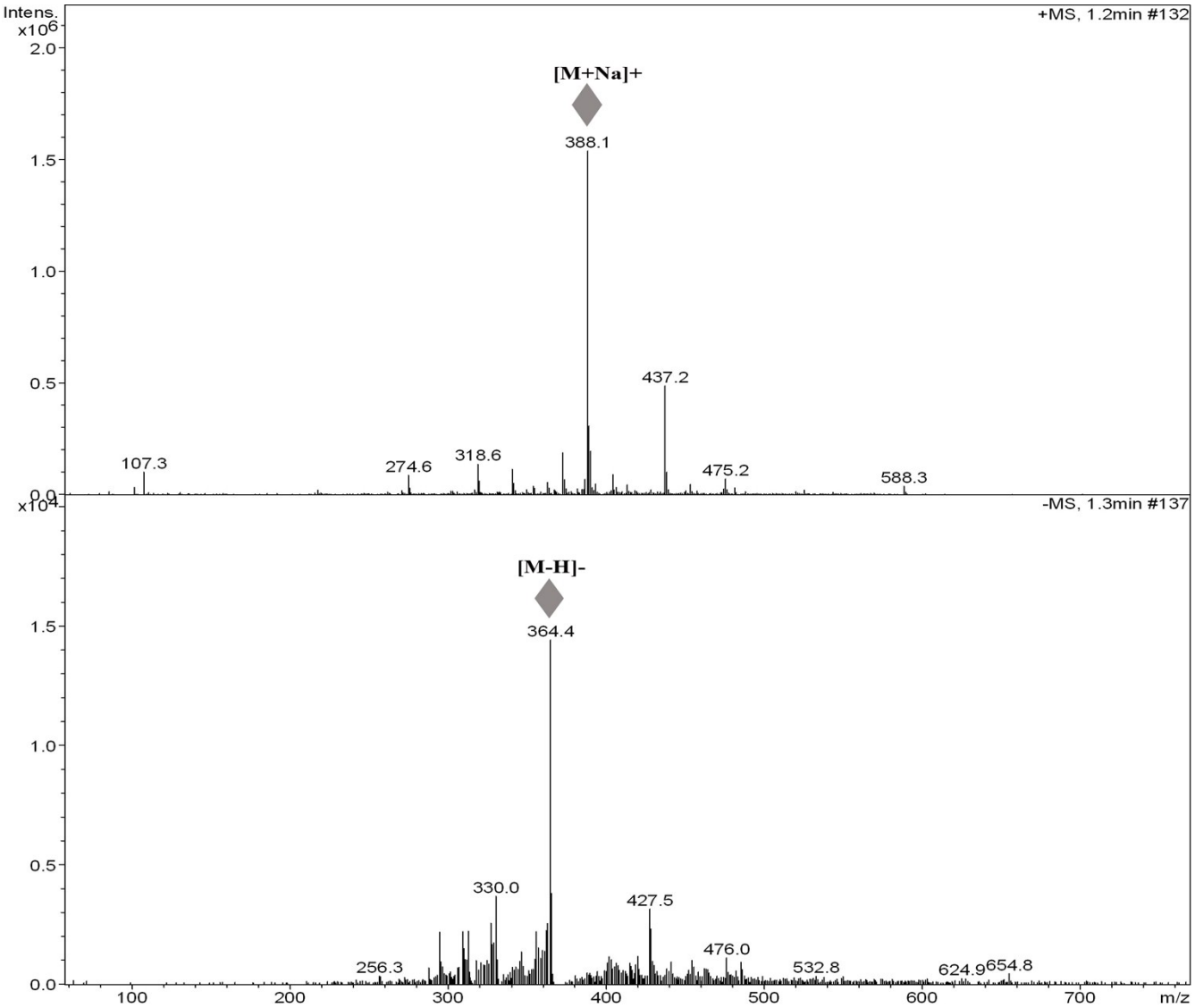

Intens.
x10^6
2.0
1.5
1.0
0.5
0.0
+MS, 1.2min #132
[M+Na]+
388.1
437.2
107.3
274.6
318.6
475.2
588.3
x10^4
1.5
1.0
0.5
0.0
-MS, 1.3min #137
[M-H]-
364.4
330.0
427.5
256.3
476.0
532.8
624.9
654.8
100
200
300
400
500
600
700
m/z

**Figure S29**

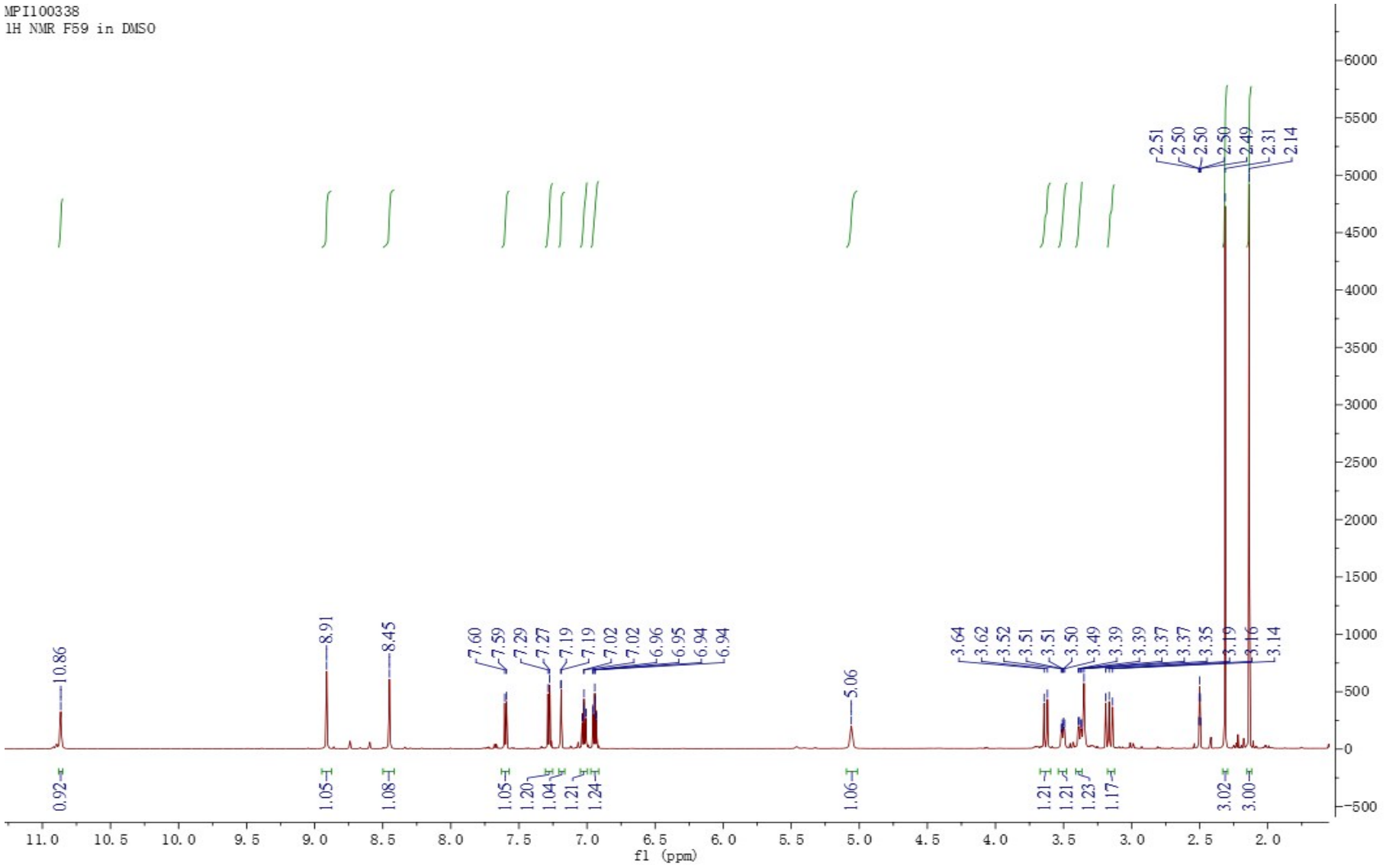

MPI100338
1H NMR F59 in DMSO
10.86
8.91
8.45
7.60
7.59
7.29
7.27
7.19
7.19
7.02
7.02
6.96
6.95
6.94
6.94
5.06
3.64
3.62
3.52
3.51
3.51
3.50
3.49
3.39
3.39
3.37
3.37
3.35
3.19
3.16
3.14
2.51
2.50
2.50
2.50
2.49
2.31
2.14
0.92
1.05
1.08
1.05
1.20
1.04
1.21
1.24
1.06
1.21
1.21
1.23
1.17
3.02
3.00
f1 (ppm)

**Figure S30**

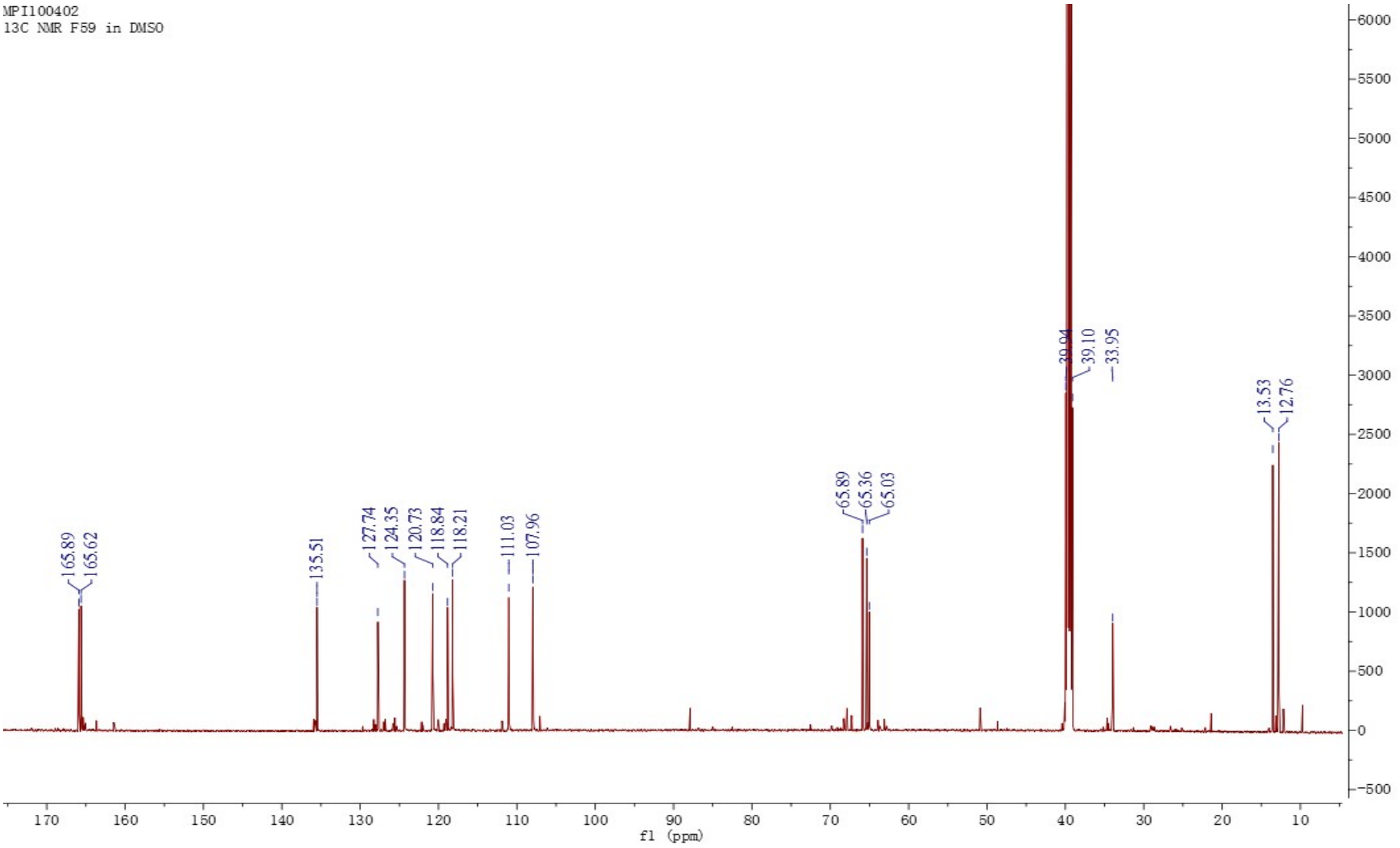

MPI100402
13C NMR F59 in DMSO
165.89
165.62
135.51
127.74
124.35
120.73
118.84
118.21
111.03
107.96
65.89
65.36
65.03
39.94
39.10
33.95
13.53
12.76
f1 (ppm)

**Figure S31**

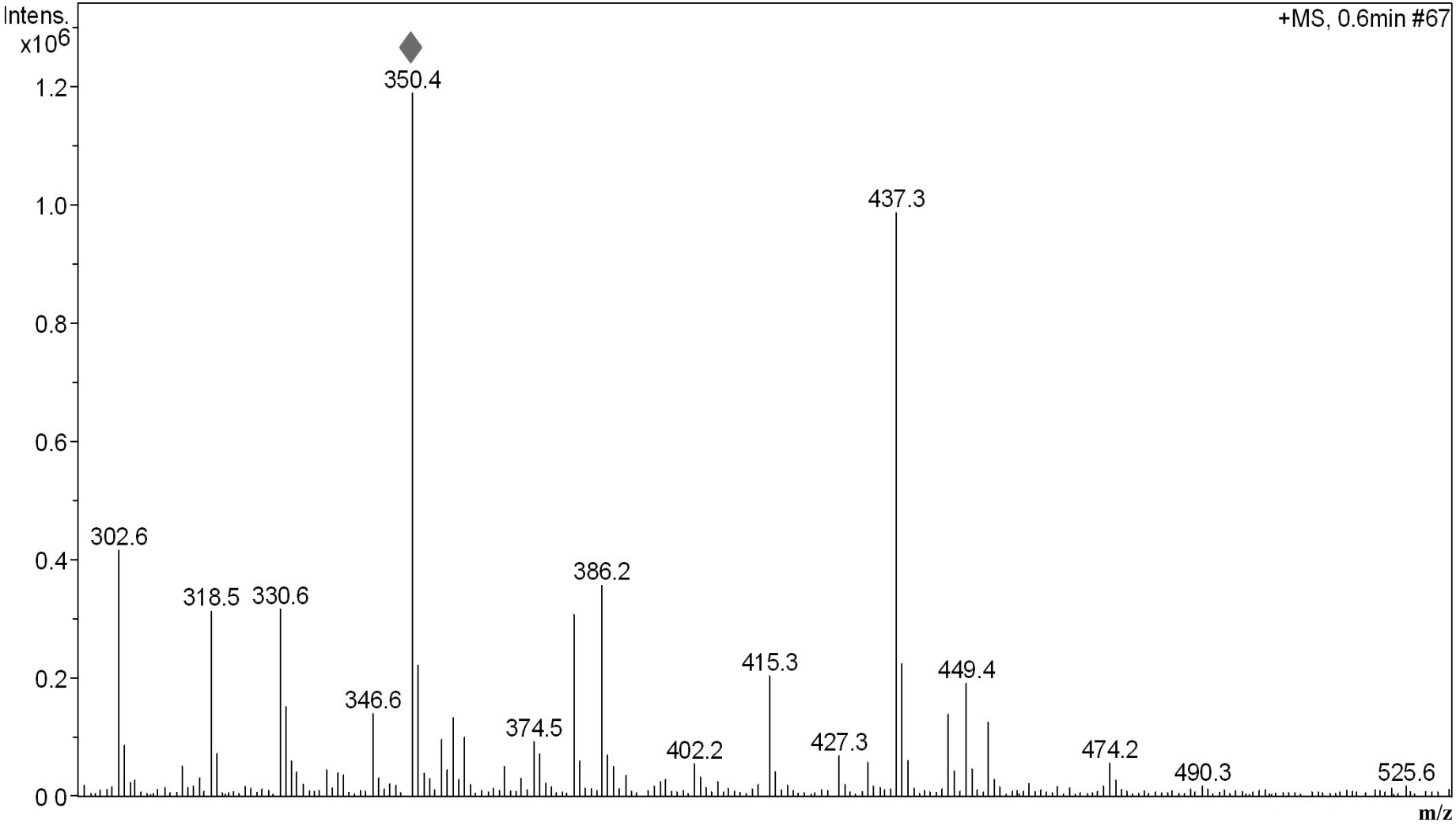

Intens.
x10^6
+MS, 0.6min #67
1.2
1.0
0.8
0.6
0.4
0.2
0 0
350.4
437.3
302.6
318.5
330.6
386.2
346.6
415.3
449.4
374.5
402.2
427.3
474.2
490.3
525.6
m/z

**Figure S32**

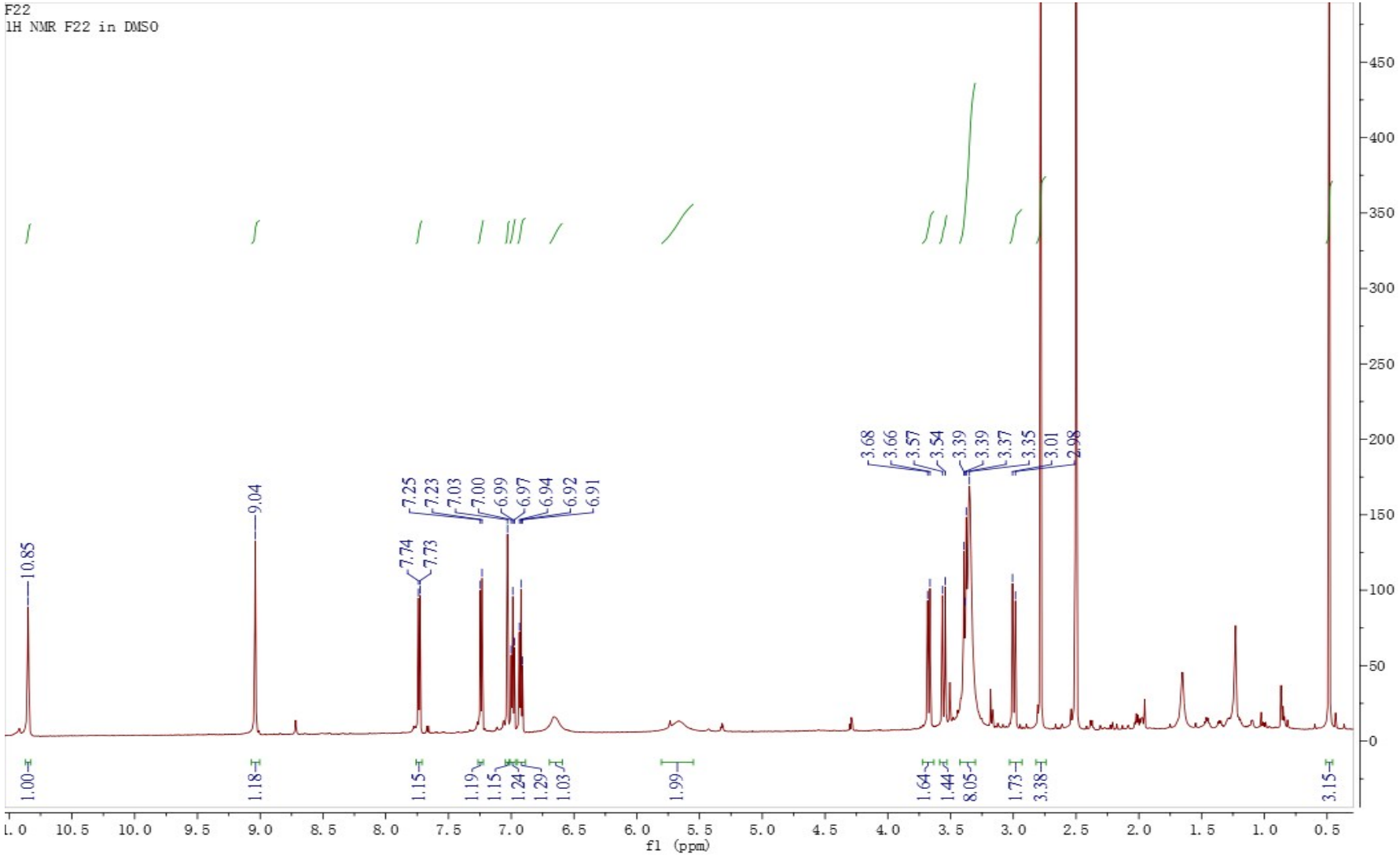

F22
1H NMR F22 in DMSO
10.85
9.04
7.74
7.73
7.25
7.23
7.03
7.00
6.99
6.97
6.94
6.92
6.91
3.68
3.66
3.57
3.54
3.39
3.39
3.37
3.35
3.01
2.98
1.00
1.18
1.15
1.19
1.15
1.24
1.29
1.03
1.99
1.64
1.44
8.05
1.73
3.38
3.15
f1 (ppm)

**Figure S33**

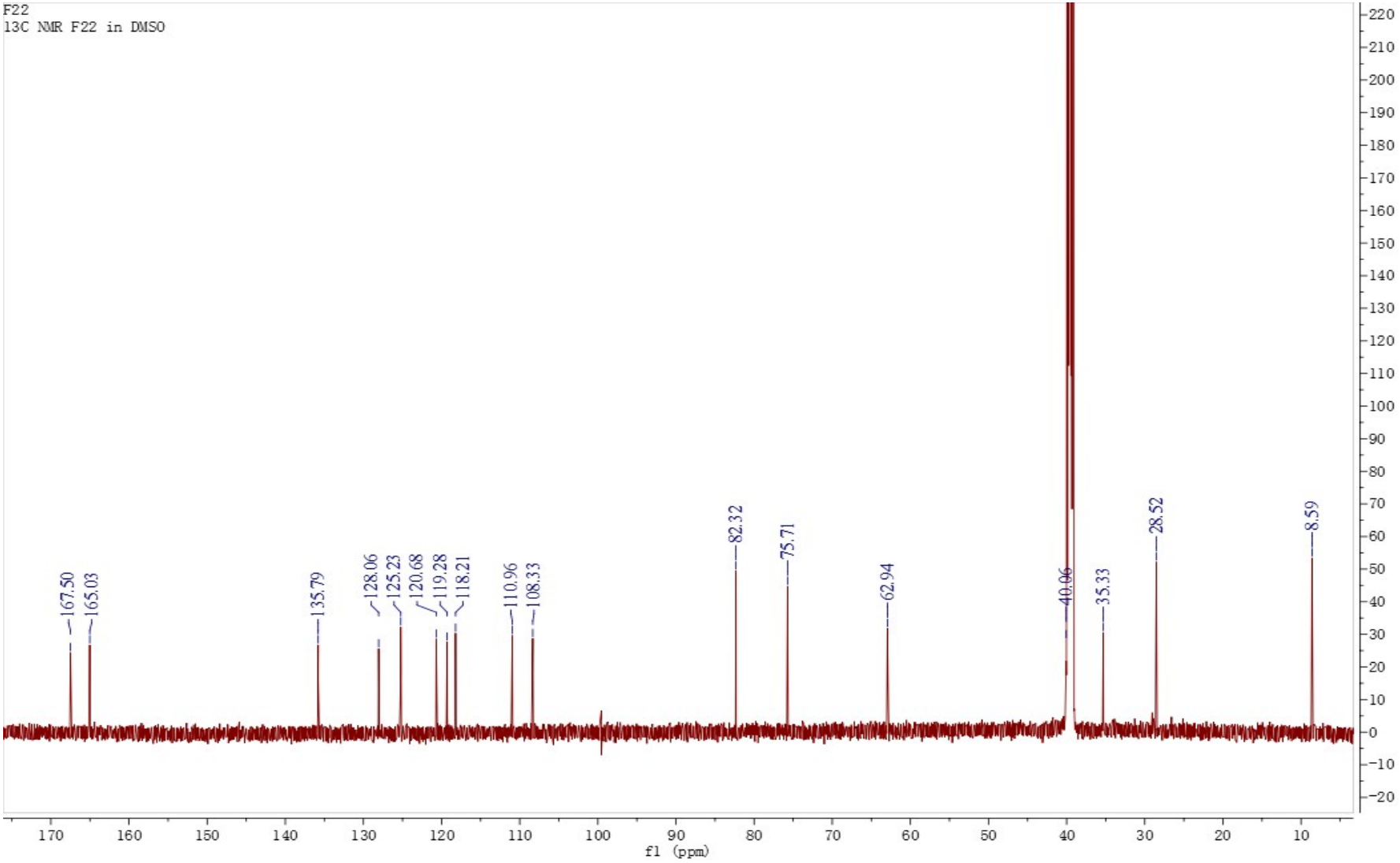

F22
13C NMR F22 in DMSO
167.50
165.03
135.79
128.06
125.23
120.68
119.28
118.21
110.96
108.33
82.32
75.71
62.94
40.96
35.33
28.52
8.59
f1 (ppm)

**Figure S34**

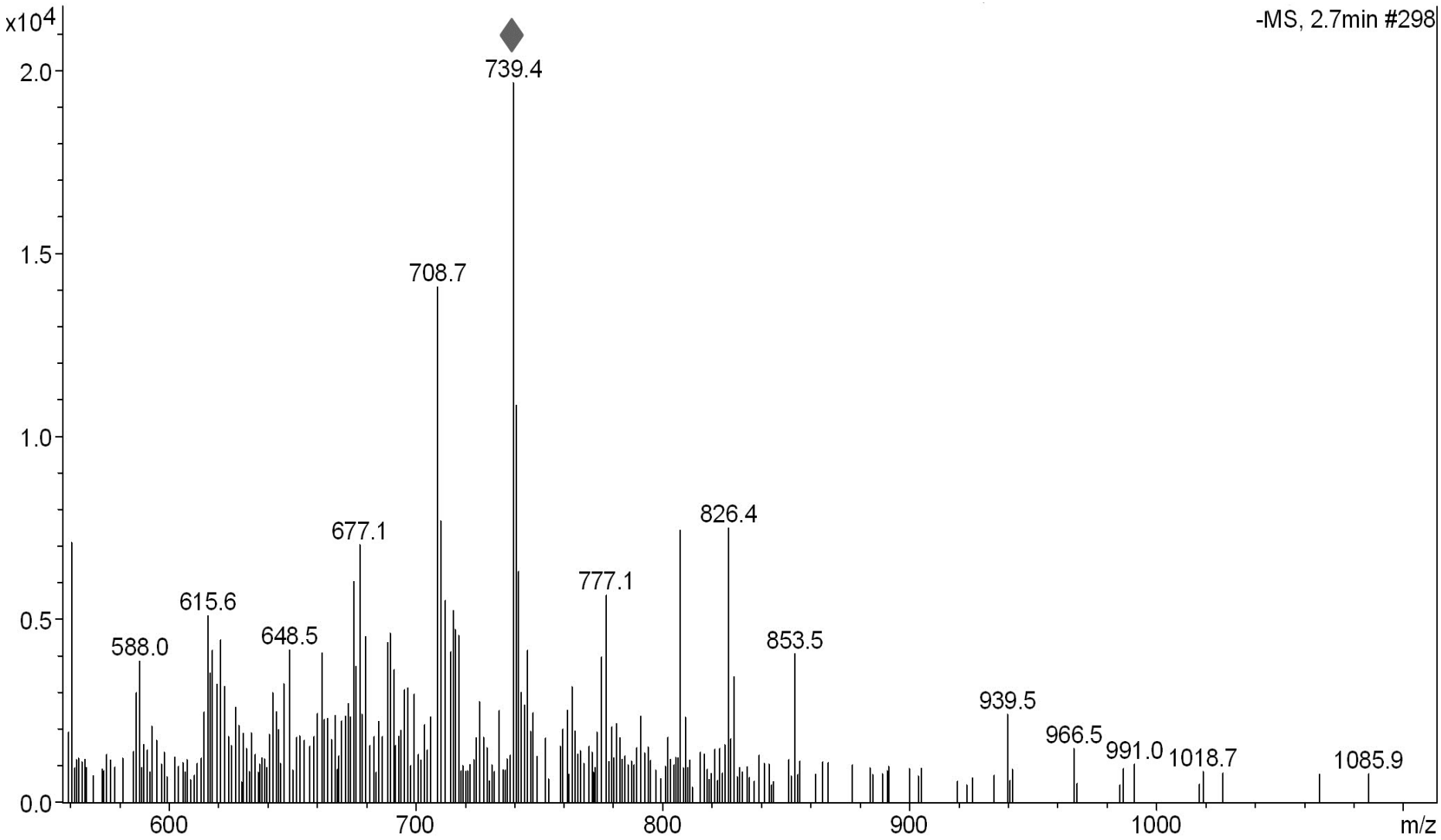

x10^4
-MS, 2.7min #298
2.0
1.5
1.0
0.5
0.0
739.4
708.7
677.1
826.4
777.1
615.6
588.0
648.5
853.5
939.5
966.5
991.0
1018.7
1085.9
600
700
800
900
1000
m/z

**Figure S35**

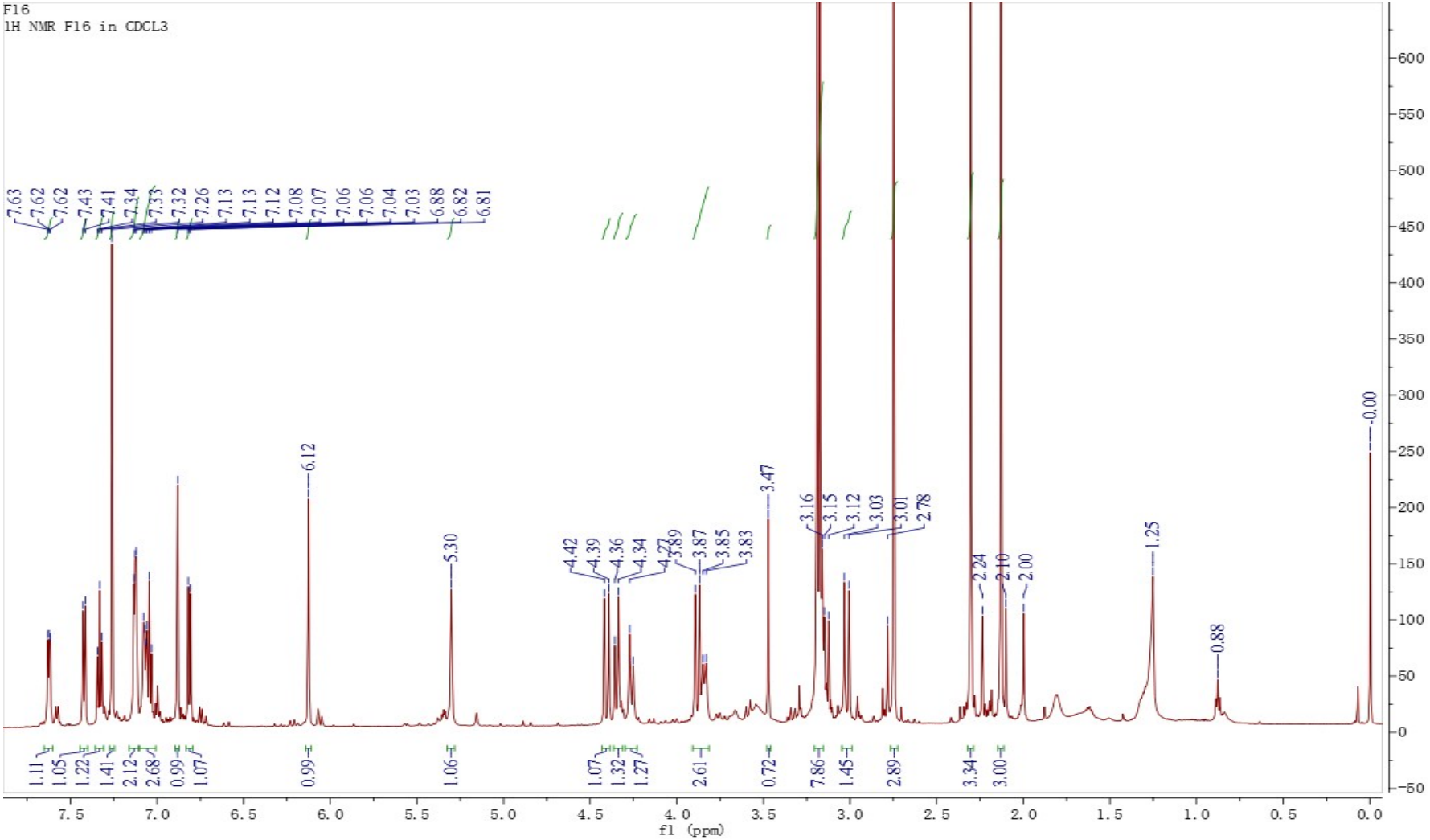

F16
1H NMR F16 in CDCL3
7.63
7.62
7.62
7.43
7.41
7.34
7.33
7.32
7.26
7.13
7.13
7.12
7.08
7.07
7.06
7.06
7.04
7.03
6.88
6.82
6.81
6.12
5.30
4.42
4.39
4.36
4.34
4.27
4.25
3.87
3.85
3.83
3.47
3.16
3.15
3.12
3.03
3.01
2.78
2.24
2.10
2.00
1.25
0.88
-0.00
1.11
1.05
1.22
1.41
2.12
2.68
0.99
1.07
0.99
1.06
1.07
1.32
1.27
2.61
0.72
7.86
1.45
2.89
3.34
3.00
f1 (ppm)

**Figure S36**

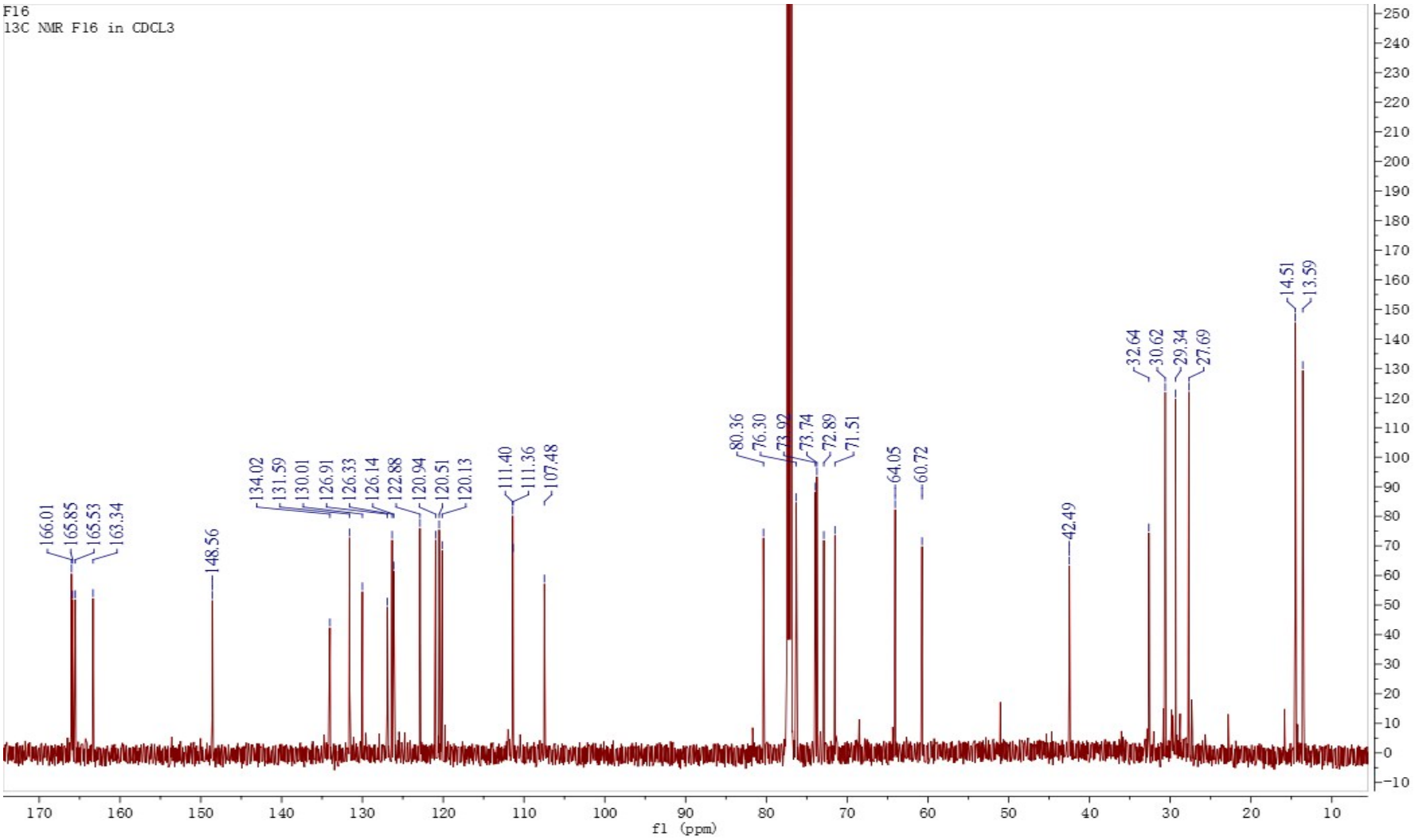

F16
13C NMR F16 in CDCL3
166.01
165.85
165.53
163.34
148.56
134.02
131.59
130.01
126.91
126.33
126.14
122.88
120.94
120.51
120.13
111.40
111.36
107.48
80.36
76.30
73.74
72.89
71.51
64.05
60.72
42.49
32.64
30.62
29.34
27.69
14.51
13.59
f1 (ppm)

**Figure S37**

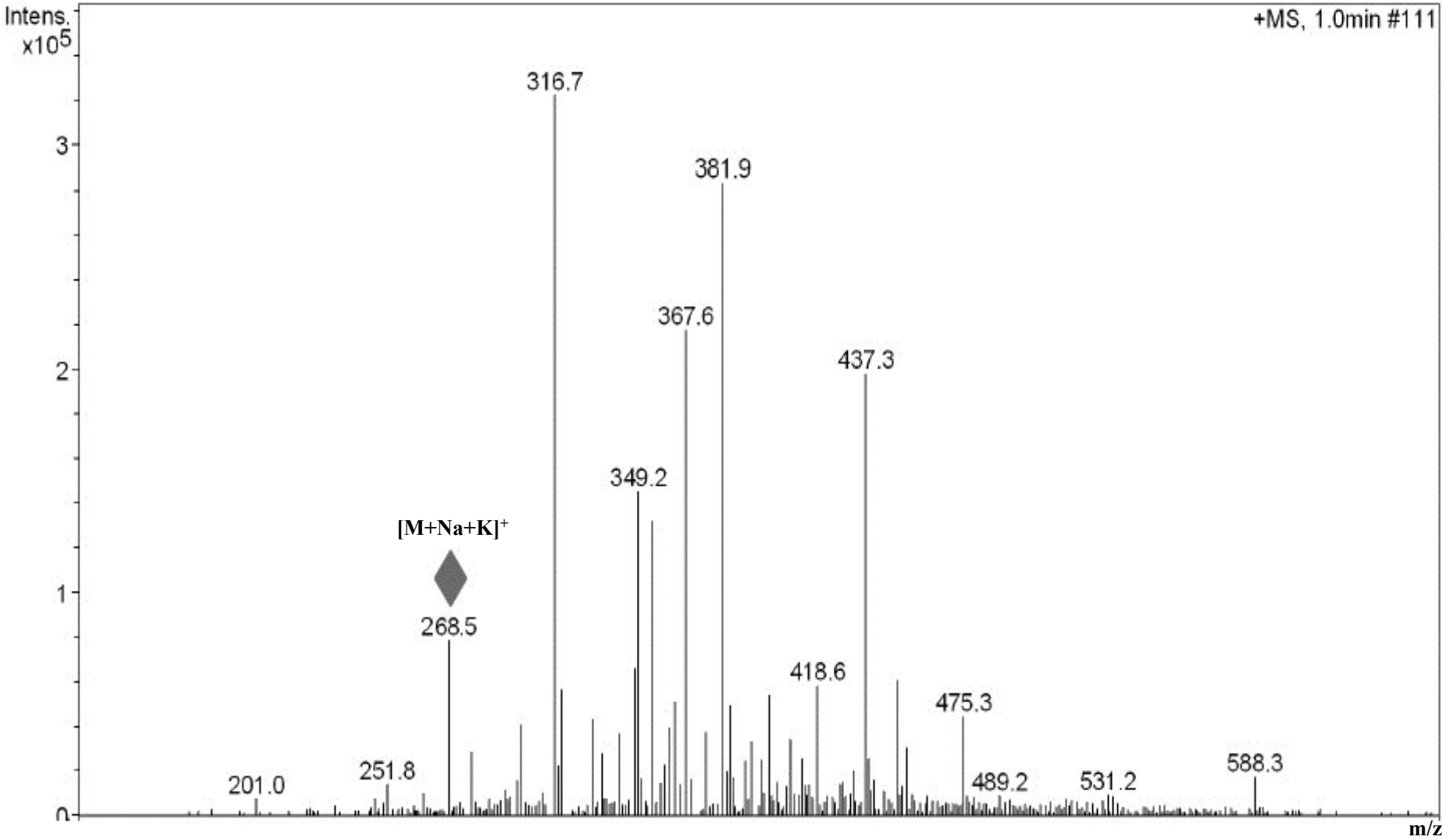

Intens.
x10^5
+MS, 1.0min #111
316.7
381.9
367.6
437.3
349.2
[M+Na+K]+
268.5
418.6
475.3
588.3
201.0
251.8
489.2
531.2
m/z

**Figure S38**

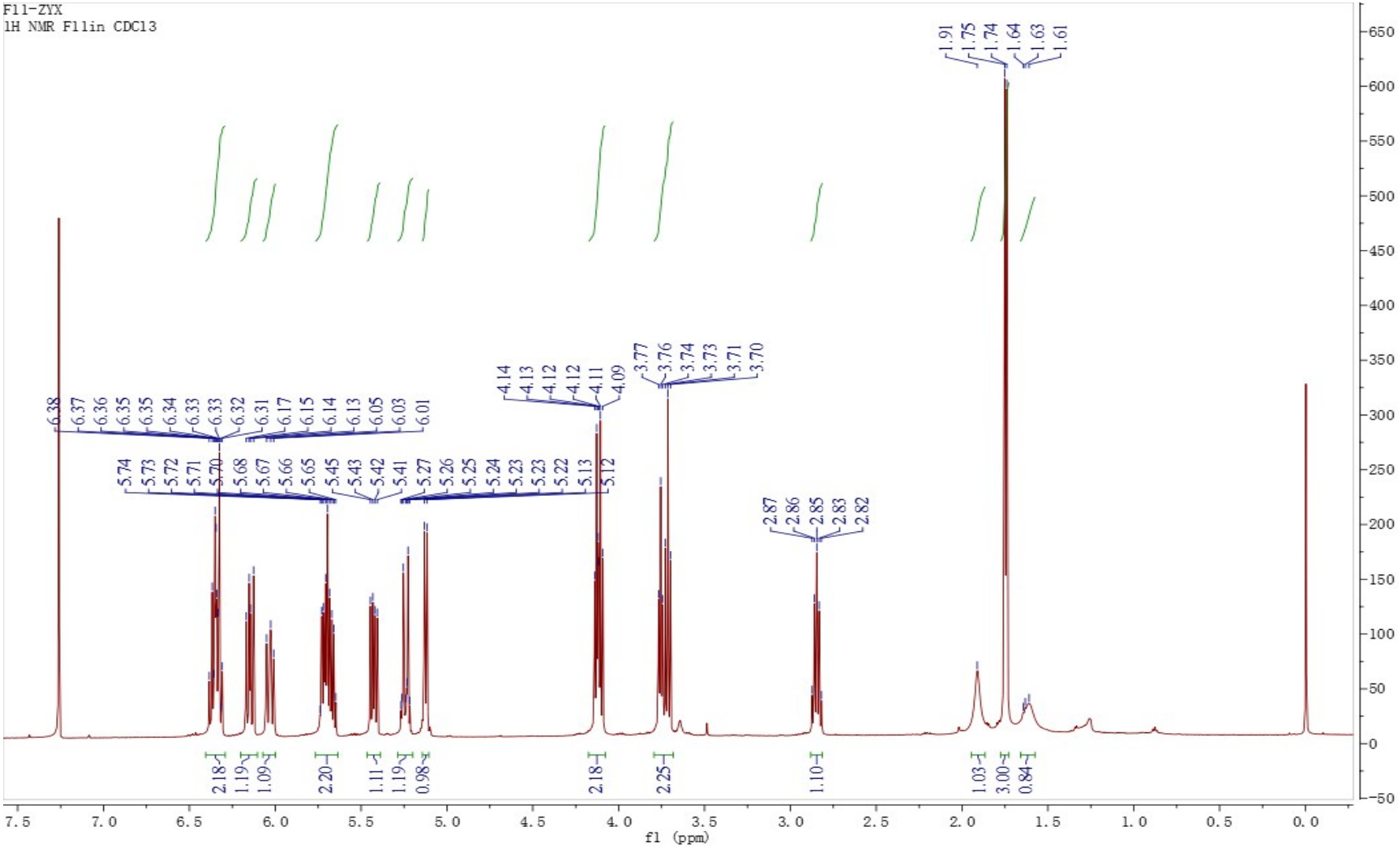


**Figure S39**

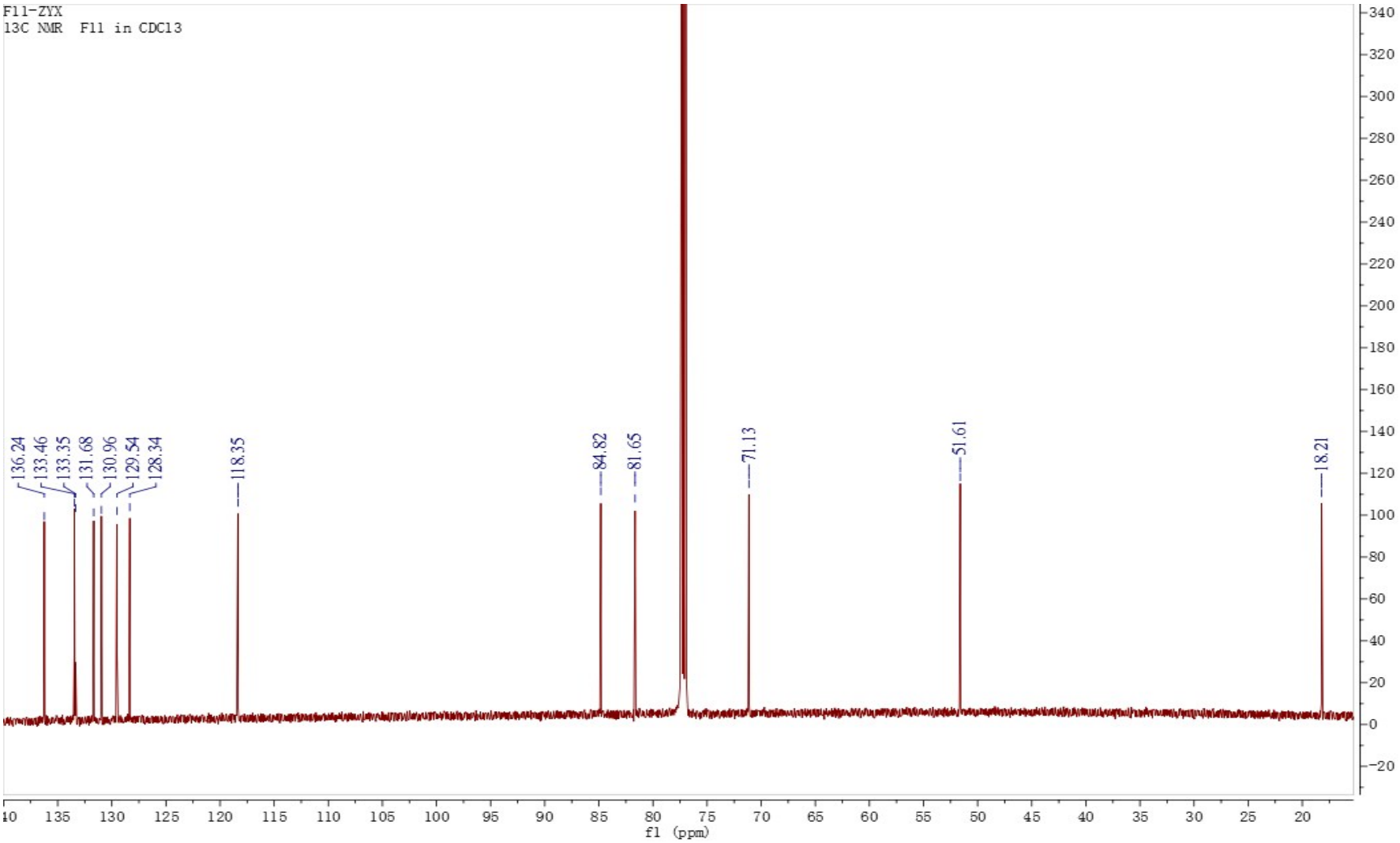

F11-ZYX
13C NMR F11 in CDCl3
136.24
133.46
133.35
131.68
130.96
129.54
128.34
118.35
84.82
81.65
71.13
51.61
18.21
f1 (ppm)

**Figure S40**

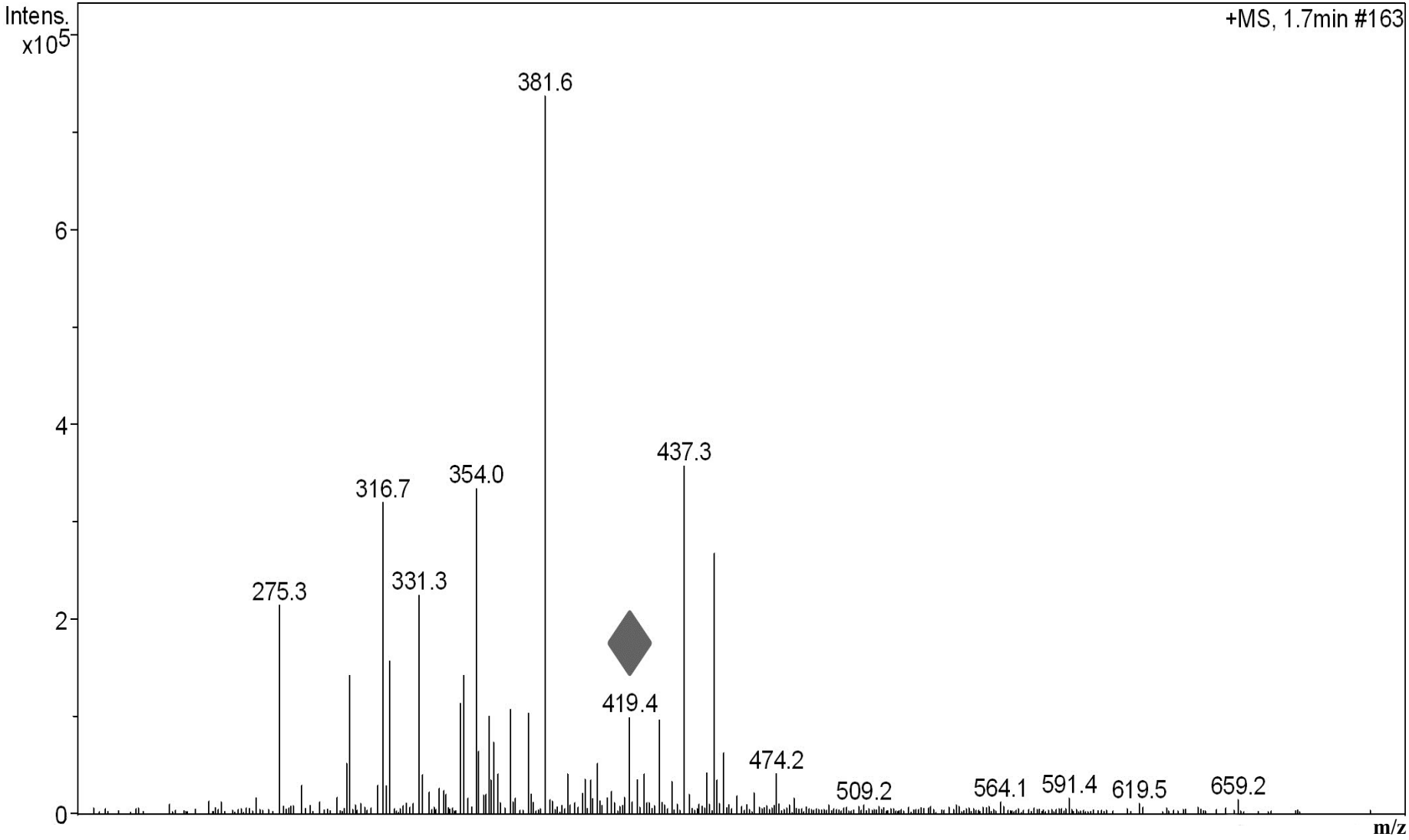

Intens.
x10^5
+MS, 1.7min #163
6
4
2
0
381.6
437.3
354.0
316.7
331.3
275.3
419.4
474.2
509.2
564.1
591.4
619.5
659.2
m/z

**Figure S41**

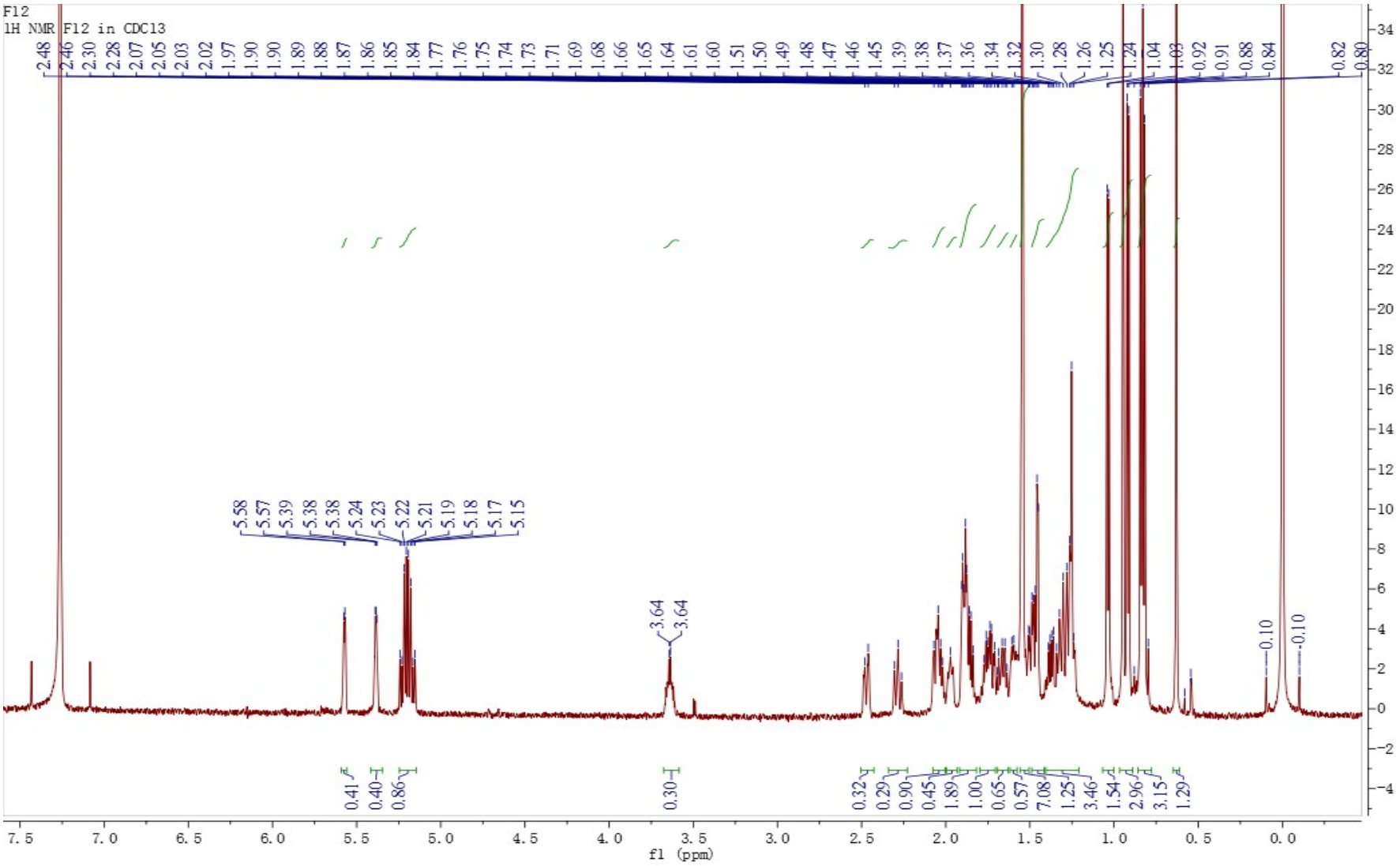


**Figure S42**

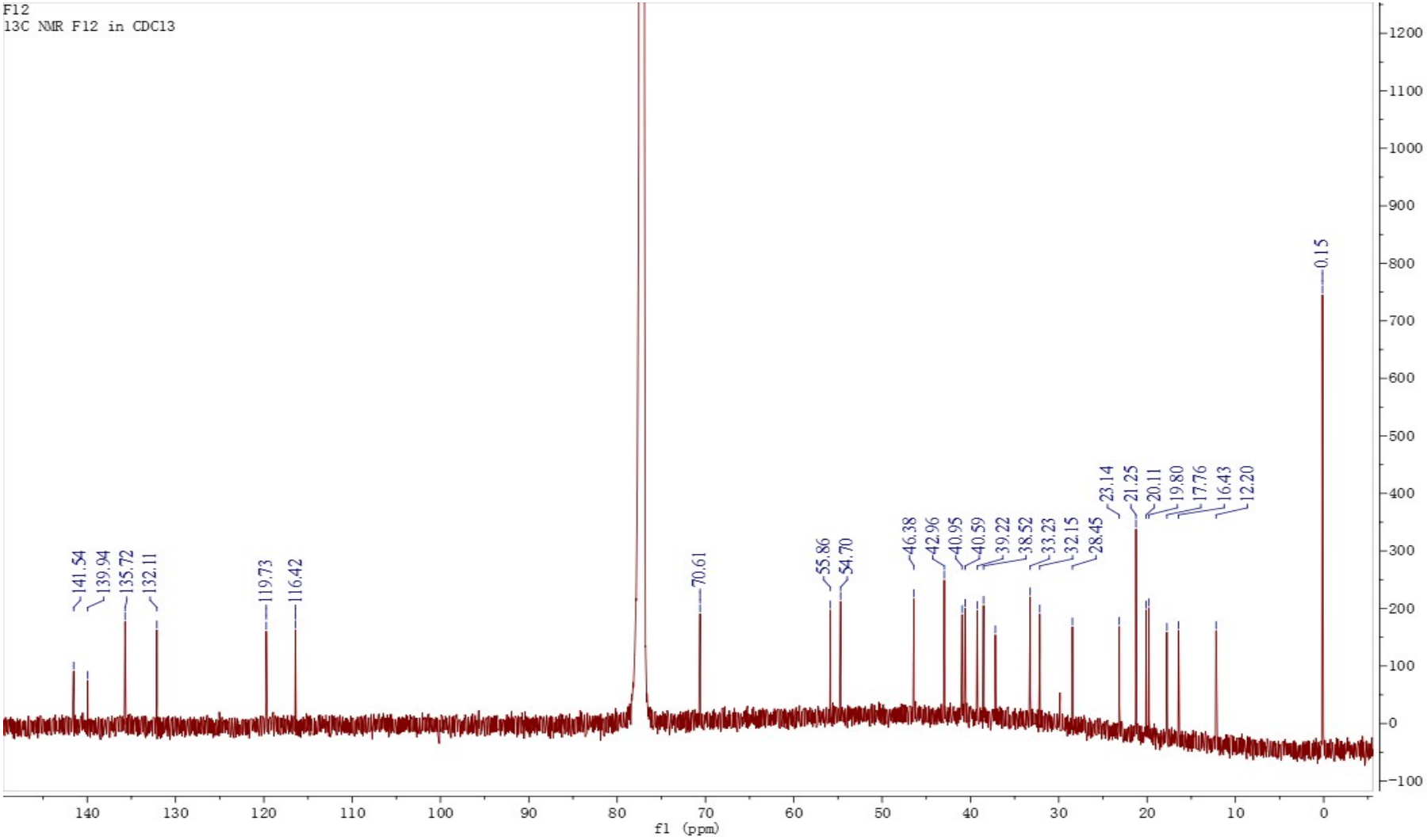

F12
13C NMR F12 in CDCl3
141.54
139.94
135.72
132.11
119.73
116.42
70.61
55.86
54.70
46.38
42.96
40.95
40.59
39.22
38.52
33.23
32.15
28.45
23.14
21.25
20.11
19.80
17.76
16.43
12.20
0.15
f1 (ppm)

**Figure S43**

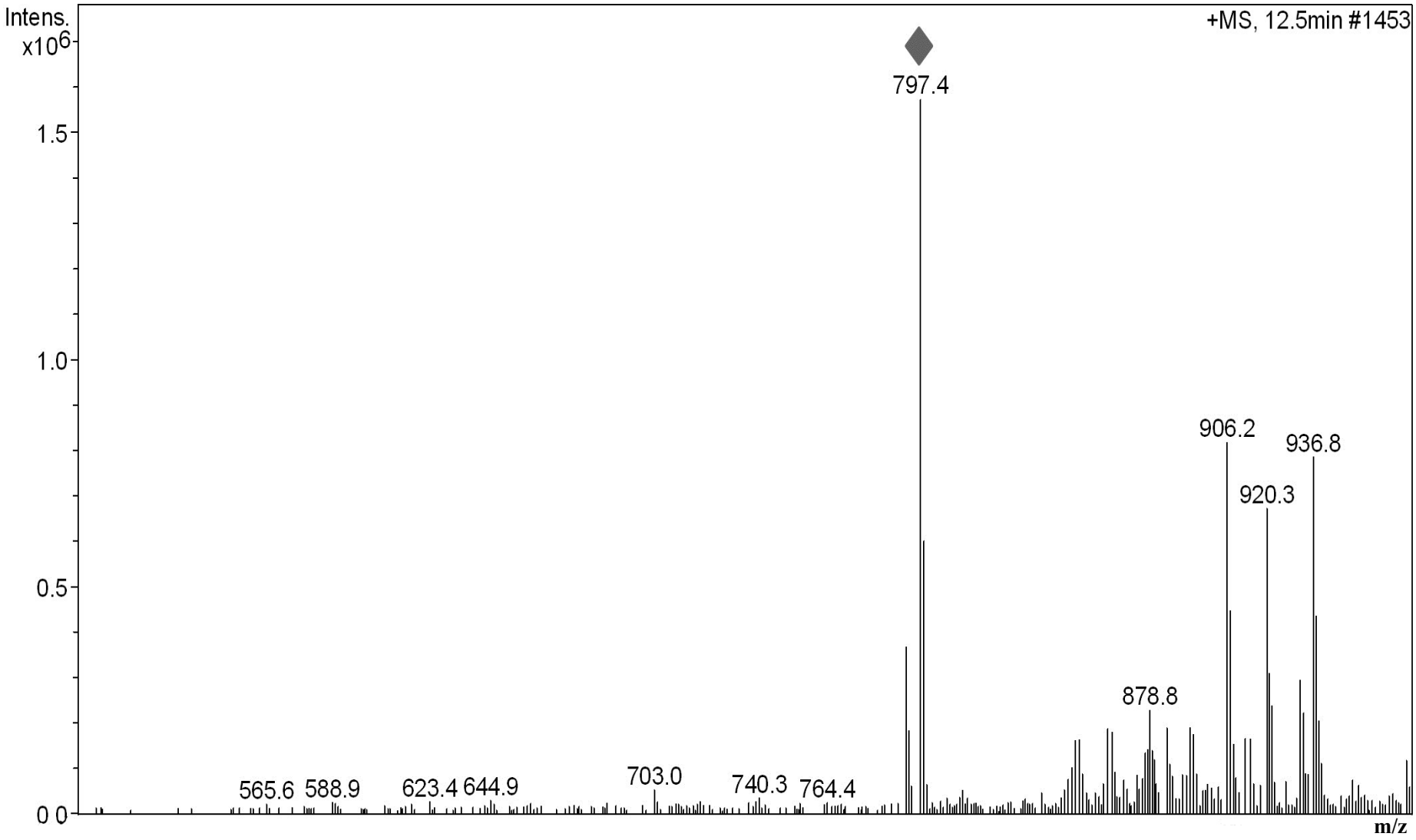

Intens.
x10^6
1.5
1.0
0.5
0 0
+MS, 12.5min #1453
797.4
906.2
936.8
920.3
878.8
565.6
588.9
623.4
644.9
703.0
740.3
764.4
m/z

**Figure S44**

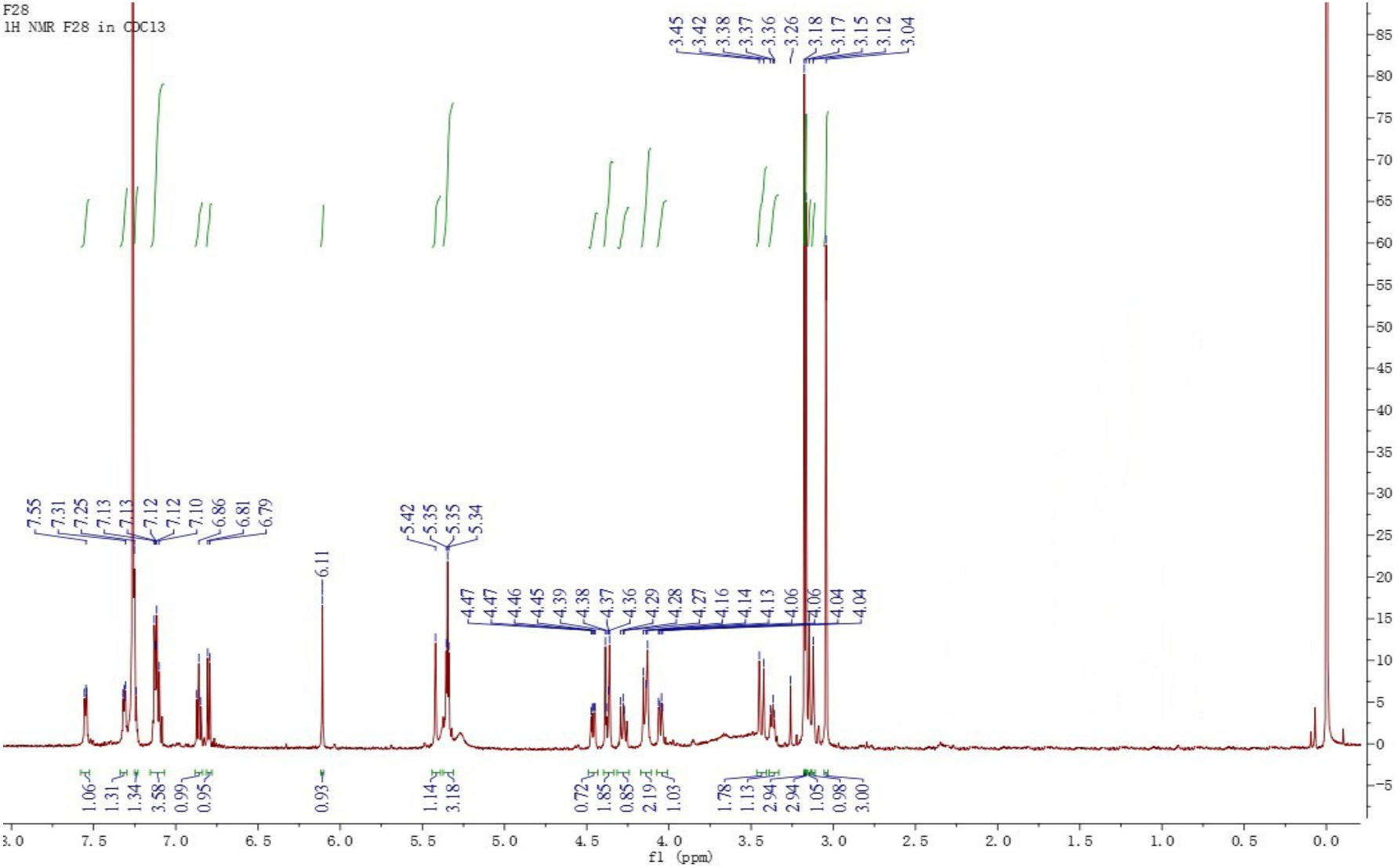


**Figure S45**

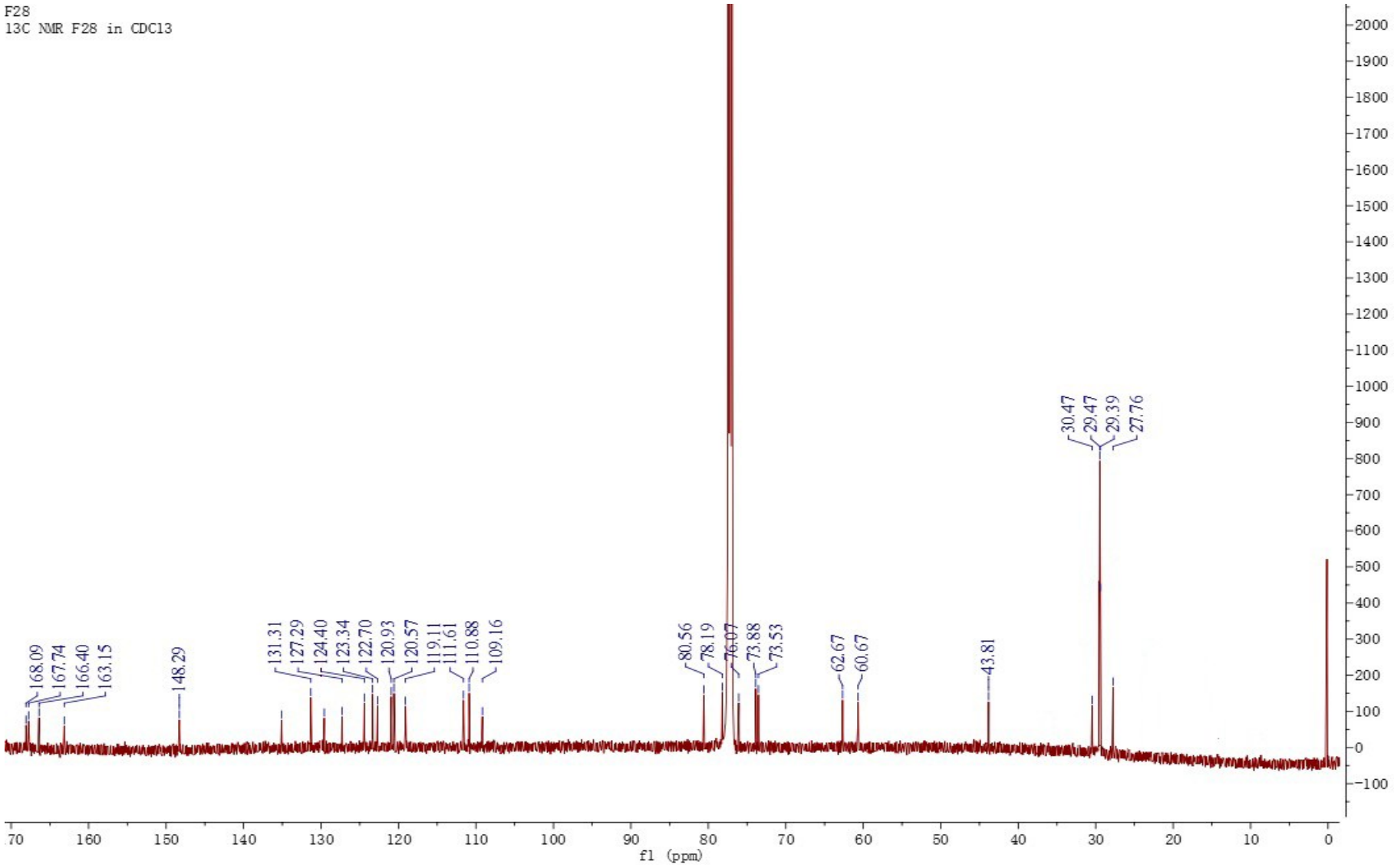

F28
13C NMR F28 in CDCl3
168.09
167.74
166.40
163.15
148.29
131.31
127.29
124.40
123.34
122.70
120.93
120.57
119.11
111.61
110.88
109.16
80.56
78.19
76.07
73.88
73.53
62.67
60.67
43.81
30.47
29.47
29.39
27.76
f1 (ppm)

**Figure S46**

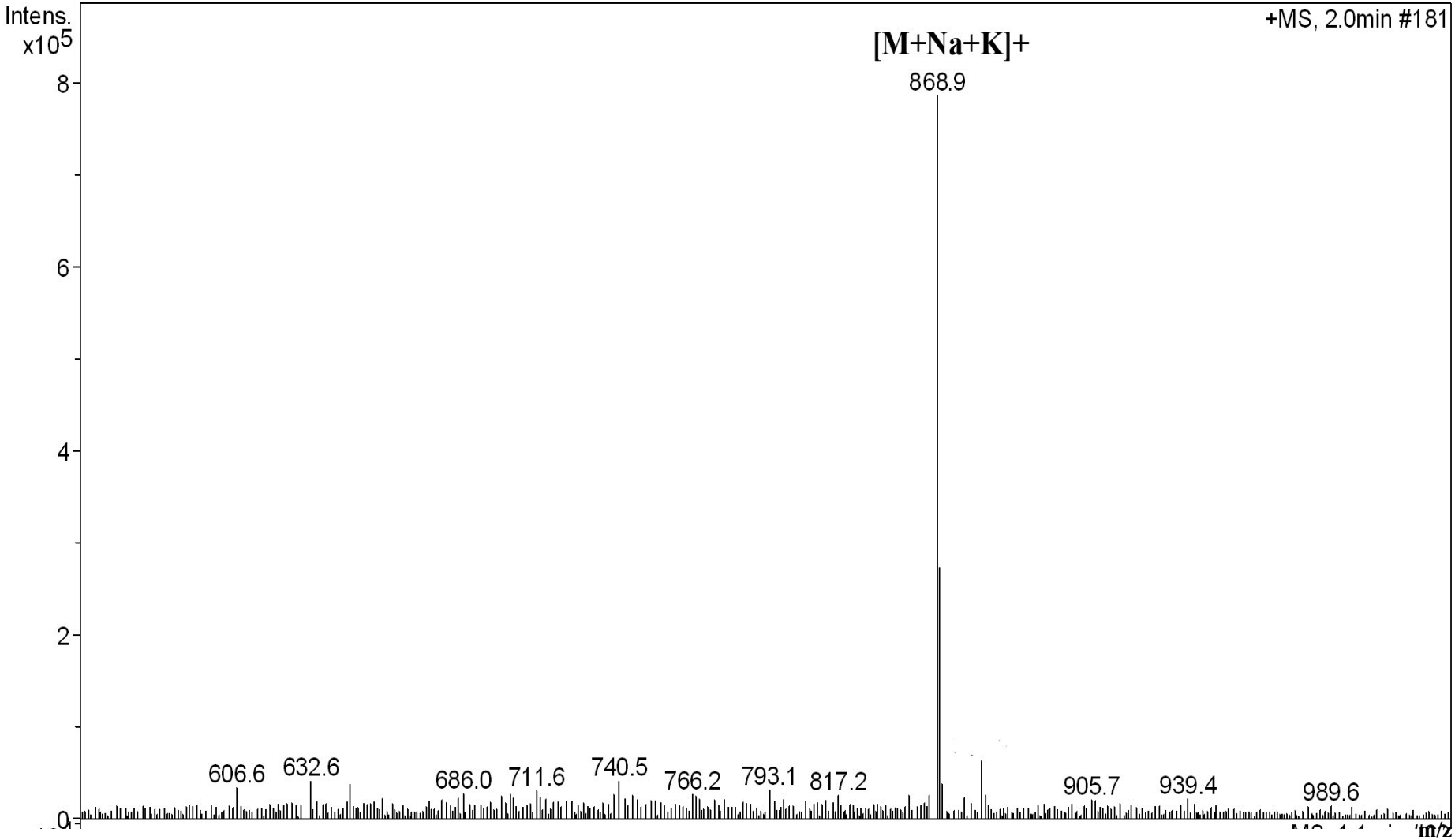

Intens.
x10^5
8
6
4
2
0
+MS, 2.0min #181
[M+Na+K]+
868.9
606.6
632.6
686.0
711.6
740.5
766.2
793.1
817.2
905.7
939.4
989.6
m/z

**Figure S47**

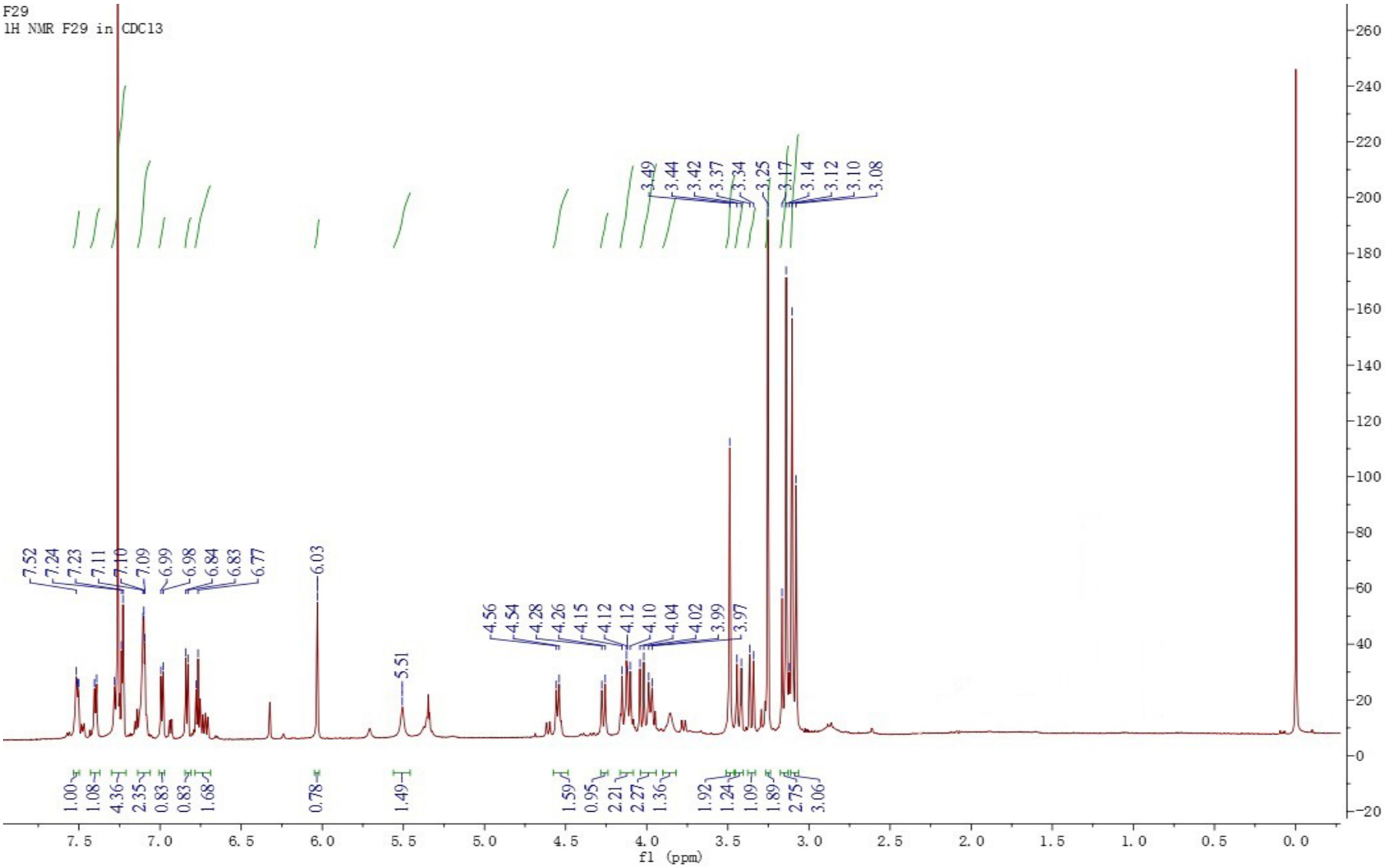

F29
1H NMR F29 in CDCl3
7.52
7.24
7.23
7.11
7.10
7.09
6.99
6.98
6.84
6.83
6.77
6.03
5.51
4.56
4.54
4.28
4.26
4.15
4.12
4.12
4.10
4.04
4.02
3.99
3.97
3.49
3.44
3.42
3.37
3.34
3.25
3.17
3.14
3.12
3.10
3.08
1.00
1.08
4.36
2.35
0.83
0.83
1.68
0.78
1.49
1.59
0.95
2.21
2.27
1.36
1.92
1.24
1.09
1.89
2.75
3.06
f1 (ppm)

**Figure S48**

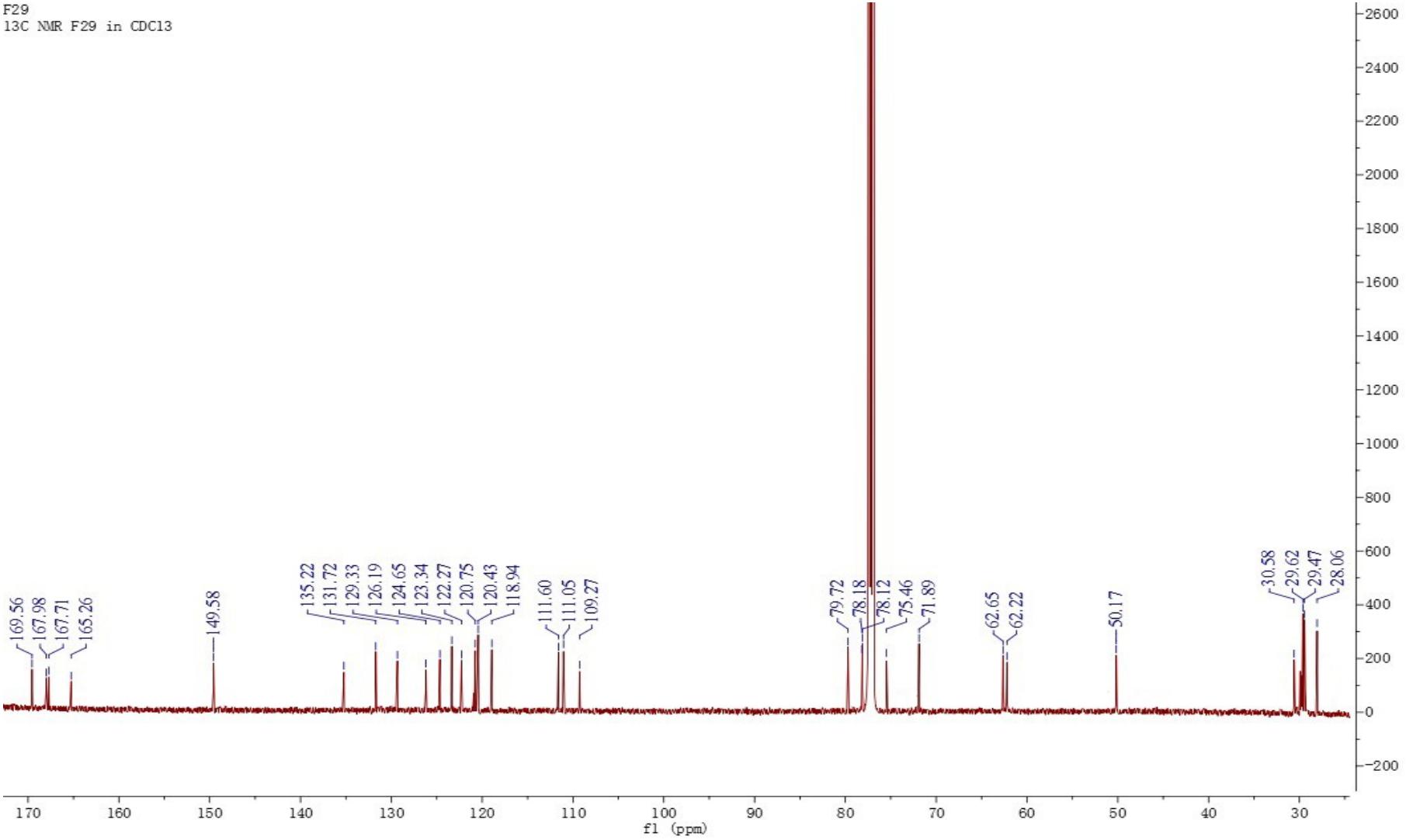

F29
13C NMR F29 in CDCl3
169.56
167.98
167.71
165.26
149.58
135.22
131.72
129.33
126.19
124.65
123.34
122.27
120.75
120.43
118.94
111.60
111.05
109.27
79.72
78.18
78.12
75.46
71.89
62.65
62.22
50.17
30.58
29.62
29.47
28.06
f1 (ppm)

**Figure S49**

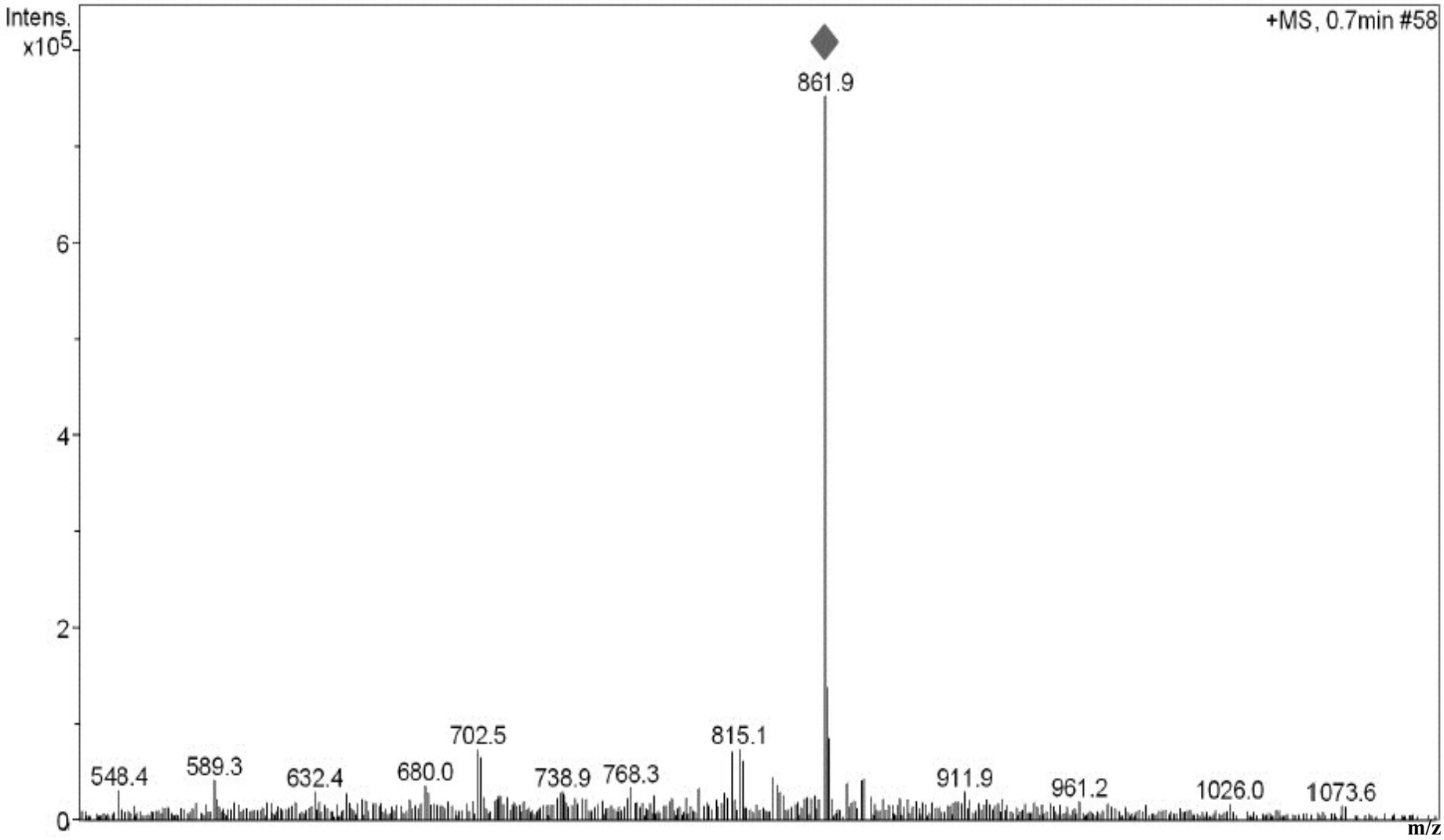

Intens.
x10^5
+MS, 0.7min #58
861.9
6
4
2
0
548.4
589.3
632.4
680.0
702.5
738.9
768.3
815.1
911.9
961.2
1026.0
1073.6
m/z

**Figure S50**

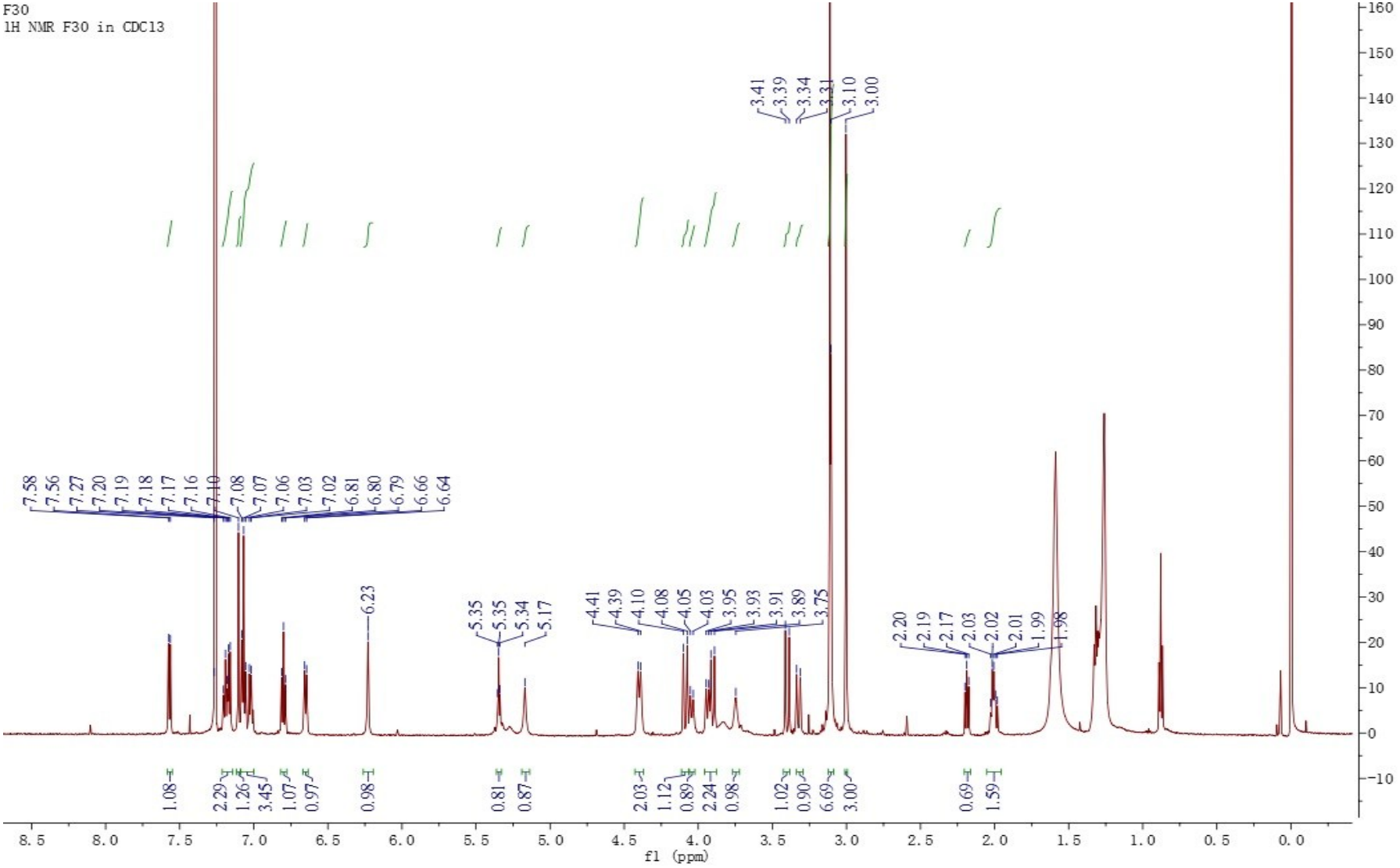


**Figure S51**

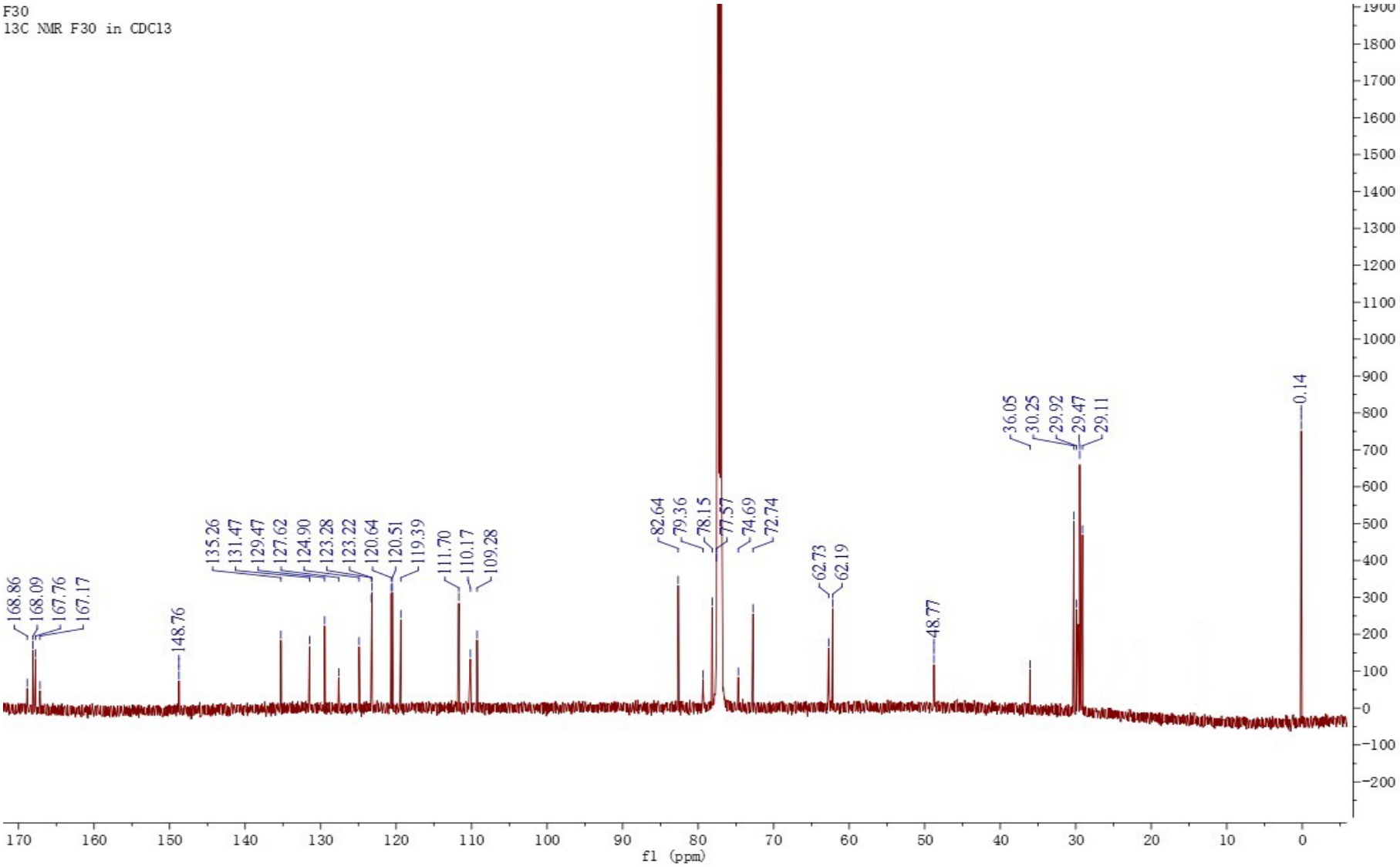

F30
13C NMR F30 in CDCl3
168.86
168.09
167.76
167.17
148.76
135.26
131.47
129.47
127.62
124.90
123.28
123.22
120.64
120.51
119.39
111.70
110.17
109.28
82.64
79.36
78.15
77.57
74.69
72.74
62.73
62.19
48.77
36.05
30.25
29.92
29.47
29.11
0.14
f1 (ppm)

**Figure S52**

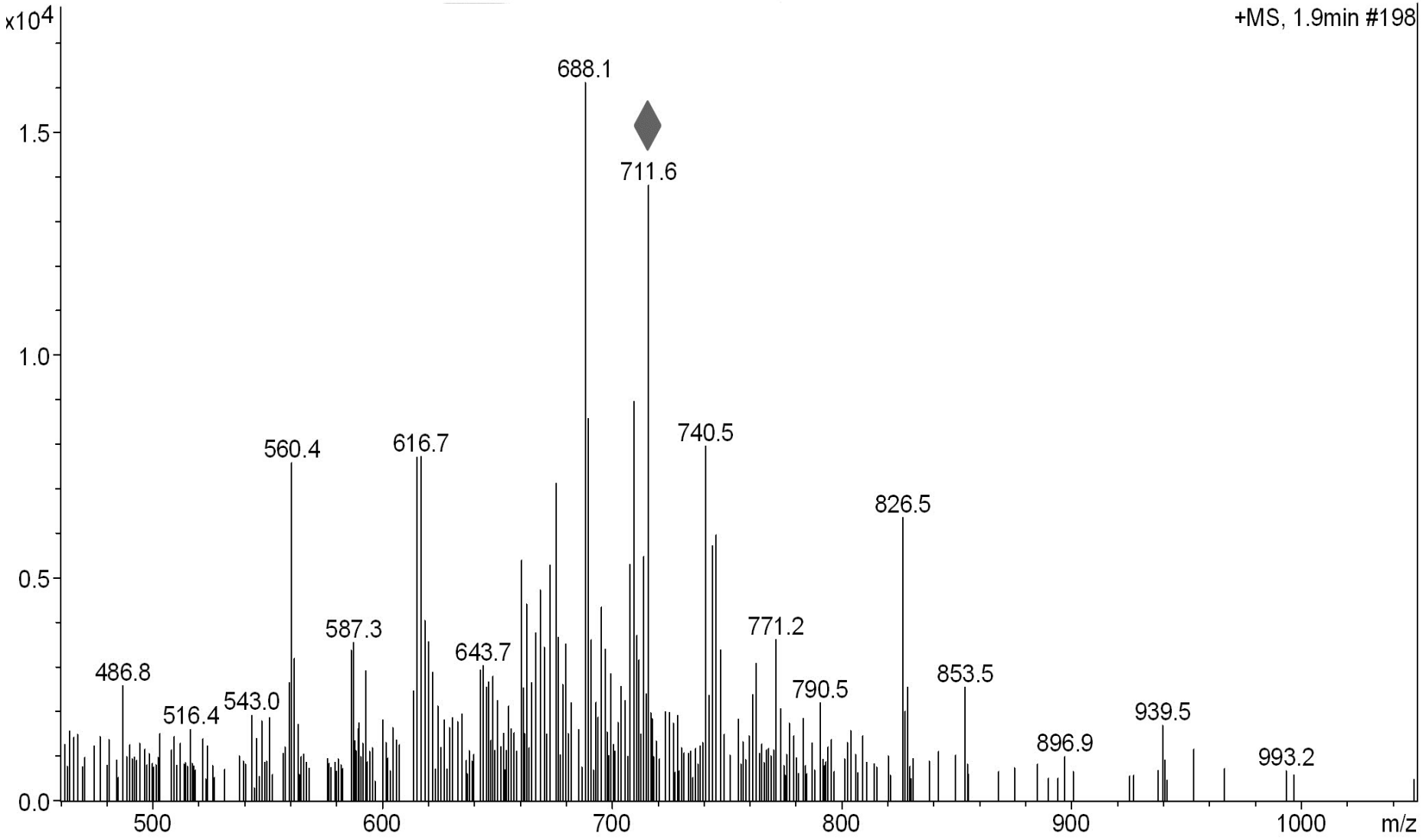

x10^4
+MS, 1.9min #198
1.5
1.0
0.5
0.0
688.1
711.6
560.4
616.7
740.5
826.5
587.3
643.7
771.2
486.8
516.4
543.0
790.5
853.5
939.5
896.9
993.2
500
600
700
800
900
1000
m/z

**Figure S53**

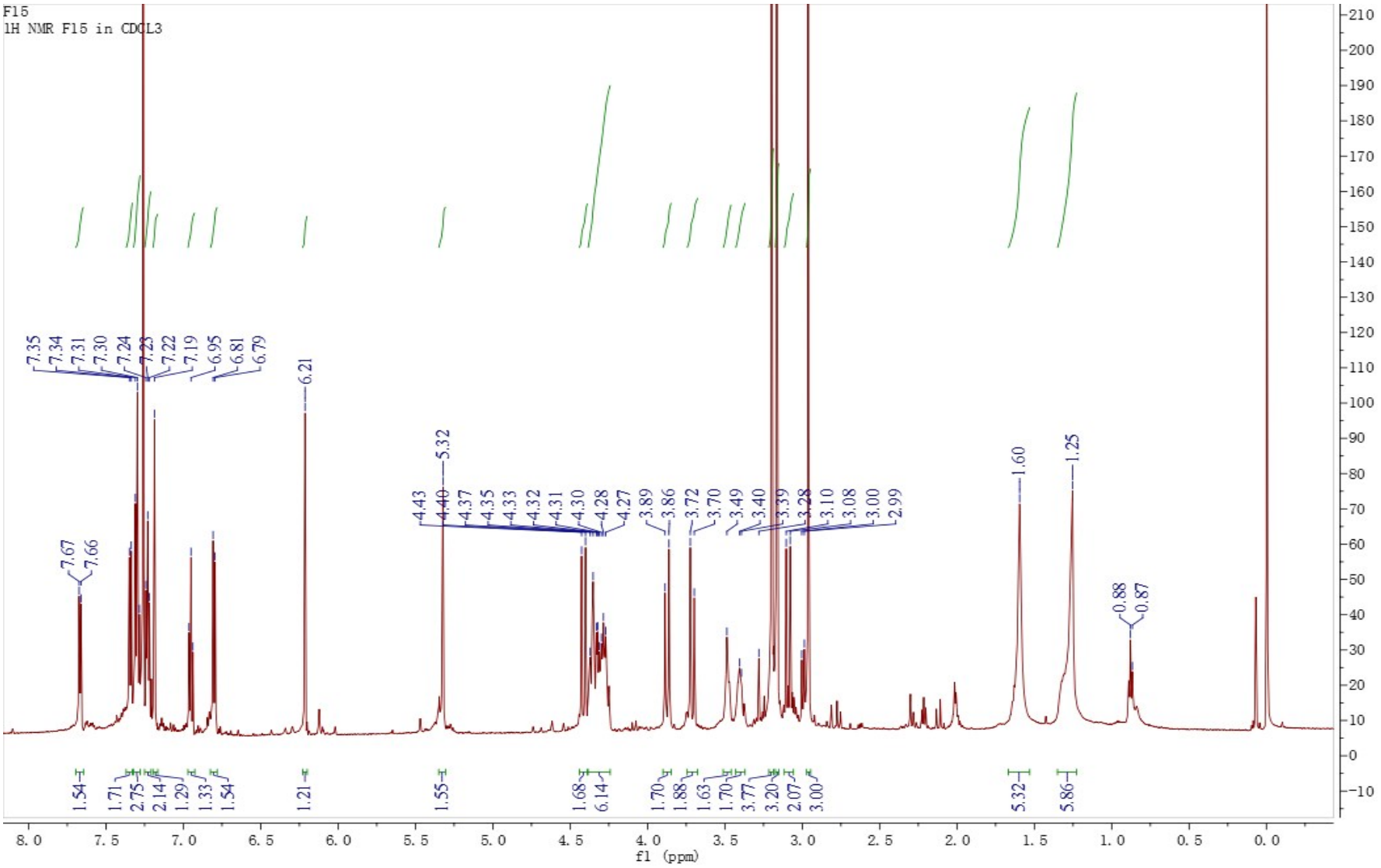

F15
1H NMR F15 in CDCL3
7.35
7.34
7.31
7.30
7.24
7.23
7.22
7.19
6.95
6.81
6.79
6.21
5.32
4.43
4.40
4.37
4.35
4.33
4.32
4.31
4.30
4.28
4.27
3.89
3.86
3.72
3.70
3.49
3.40
3.39
3.28
3.10
3.08
3.00
2.99
1.60
1.25
0.88
0.87
7.67
7.66
1.54
1.71
2.75
2.14
1.29
1.33
1.54
1.21
1.55
1.68
6.14
1.70
1.88
1.63
1.70
3.77
3.20
2.07
3.00
5.32
5.86
f1 (ppm)

**Figure S54**

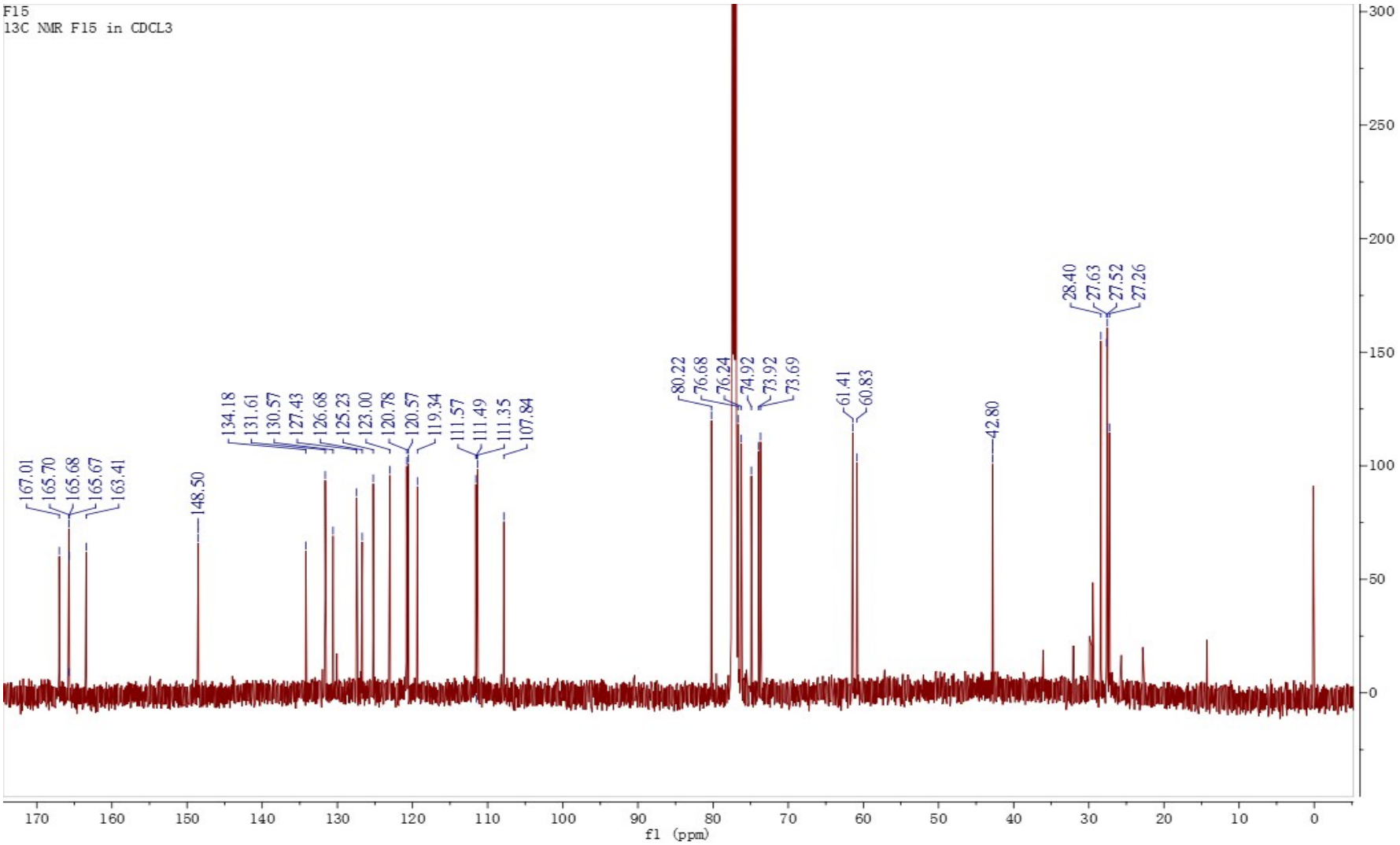

F15
13C NMR F15 in CDCL3
167.01
165.70
165.68
165.67
163.41
148.50
134.18
131.61
130.57
127.43
126.68
125.23
123.00
120.78
120.57
119.34
111.57
111.49
111.35
107.84
80.22
76.68
76.24
74.92
73.92
73.69
61.41
60.83
42.80
28.40
27.63
27.52
27.26
f1 (ppm)

**Figure S55**

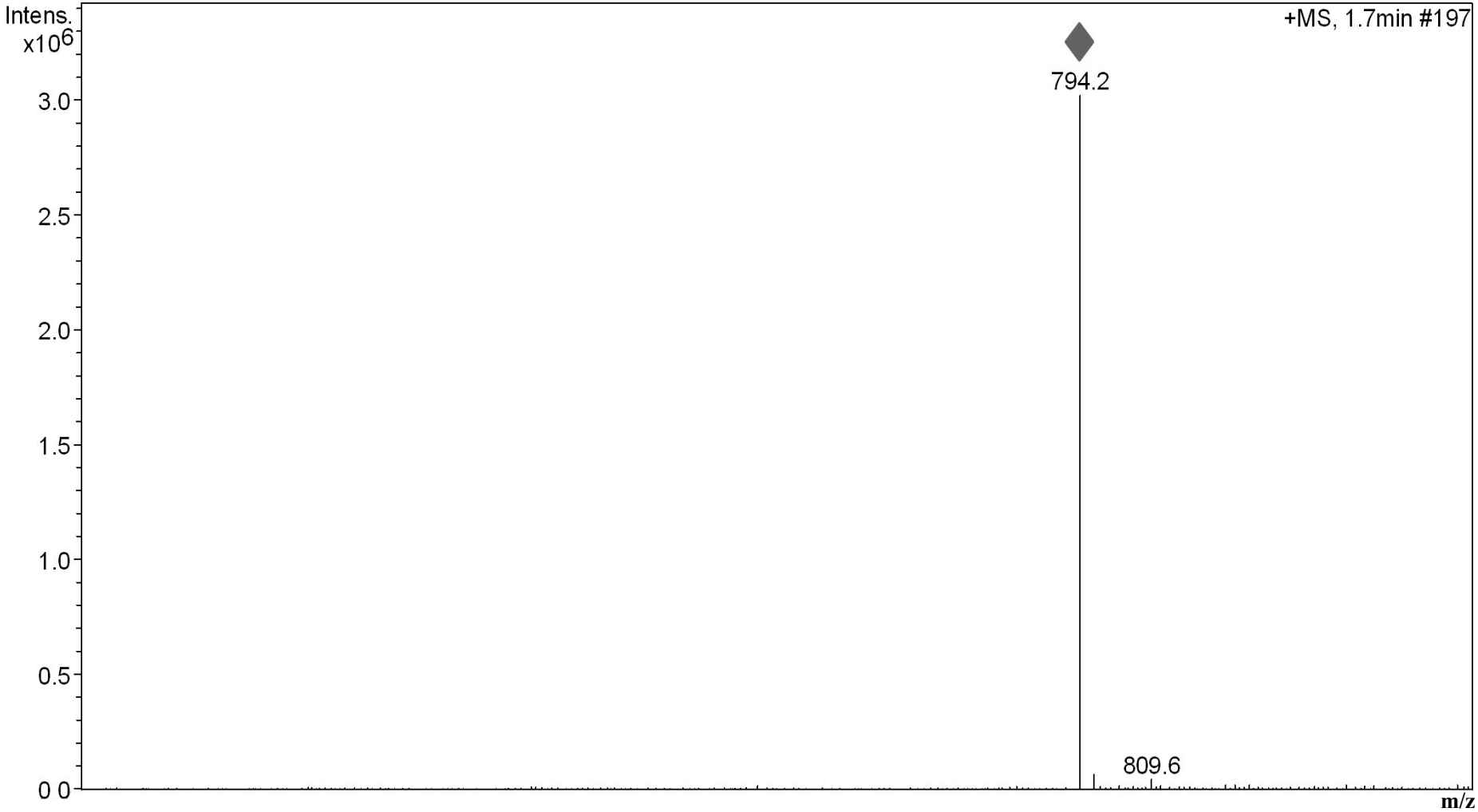


**Figure S56**

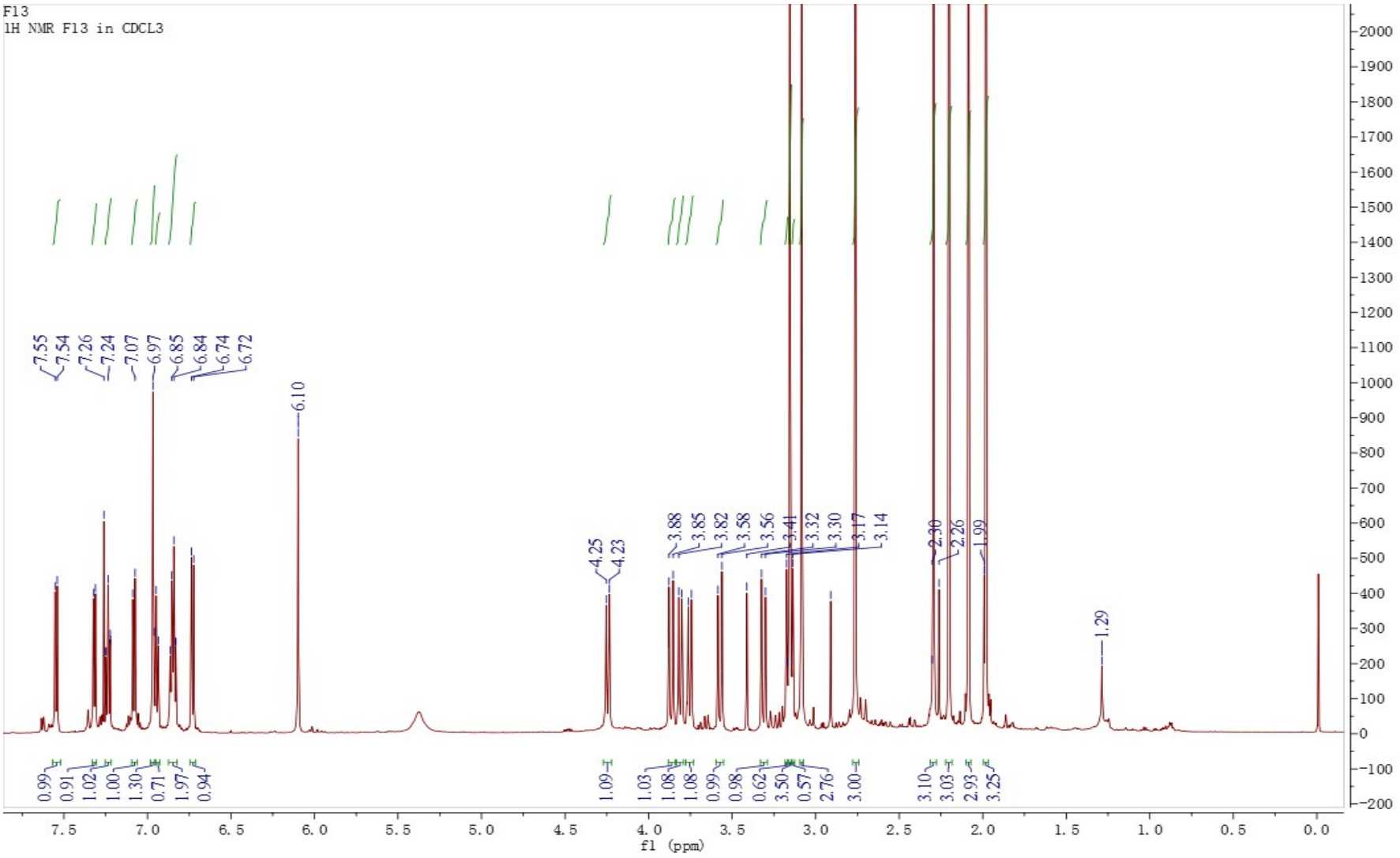
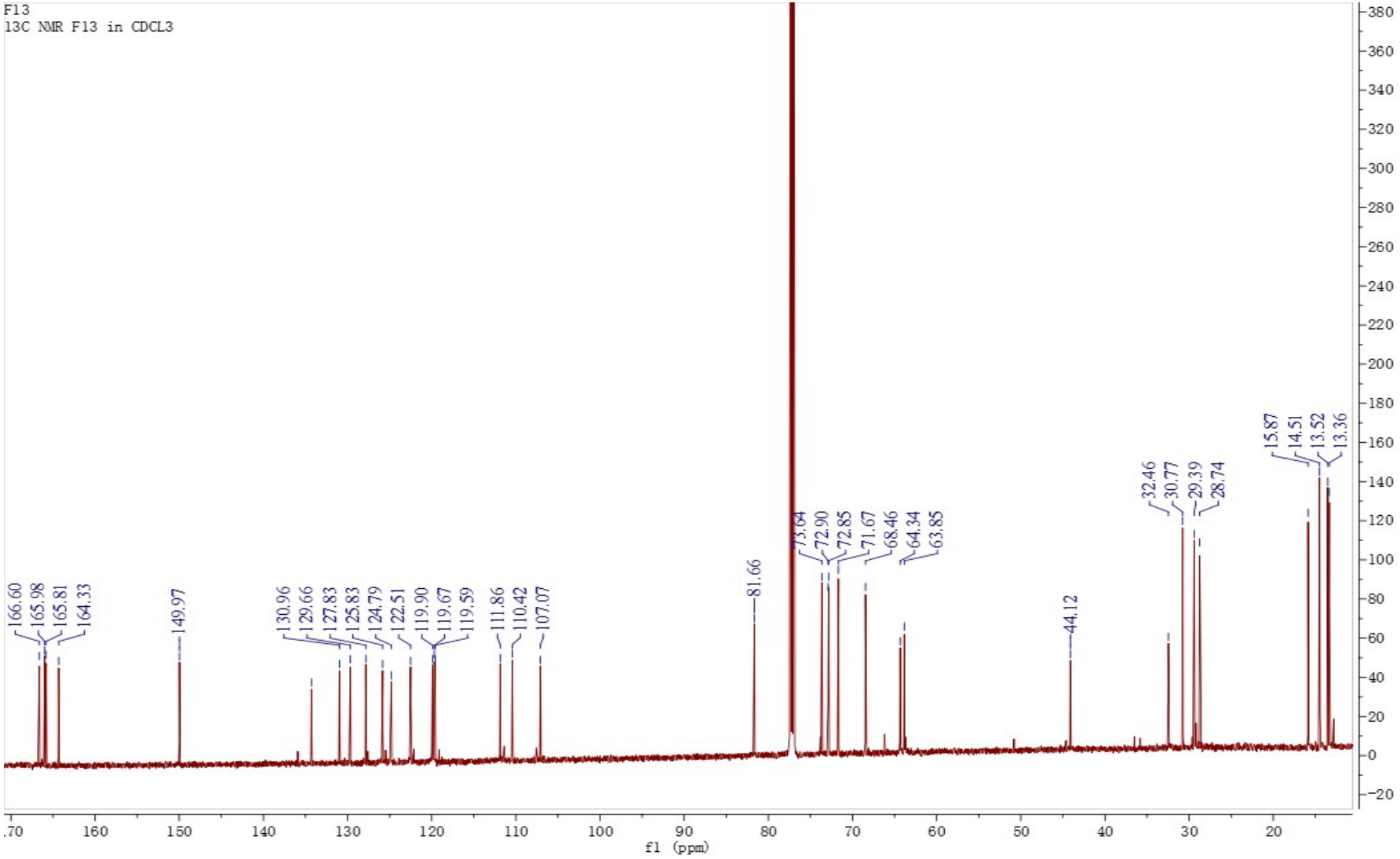

F13
1H NMR F13 in CDCL3
7.55
7.54
7.26
7.24
7.07
6.97
6.85
6.84
6.74
6.72
6.10
4.25
4.23
3.88
3.85
3.82
3.58
3.56
3.41
3.32
3.30
3.17
3.14
2.30
2.26
1.99
1.29
0.99
0.91
1.02
1.00
1.30
0.71
1.97
0.94
1.09
1.03
1.08
1.08
0.99
0.98
0.62
3.50
0.57
2.76
3.00
3.10
3.03
2.93
3.25
f1 (ppm)

**Figure S57**


F13
13C NMR F13 in CDCL3
166.60
165.98
165.81
164.33
149.97
130.96
129.66
127.83
125.83
124.79
122.51
119.90
119.67
119.59
111.86
110.42
107.07
81.66
73.64
72.90
72.85
71.67
68.46
64.34
63.85
44.12
32.46
30.77
29.39
28.74
15.87
14.51
13.52
13.36
f1 (ppm)