

Supporting Information for

Design and Synthesis of New α -Naphthoflavones as Cytochrome P450 (CYP) 1B1 Inhibitors to Overcome Docetaxel-resistance Associated with CYP1B1 Overexpression

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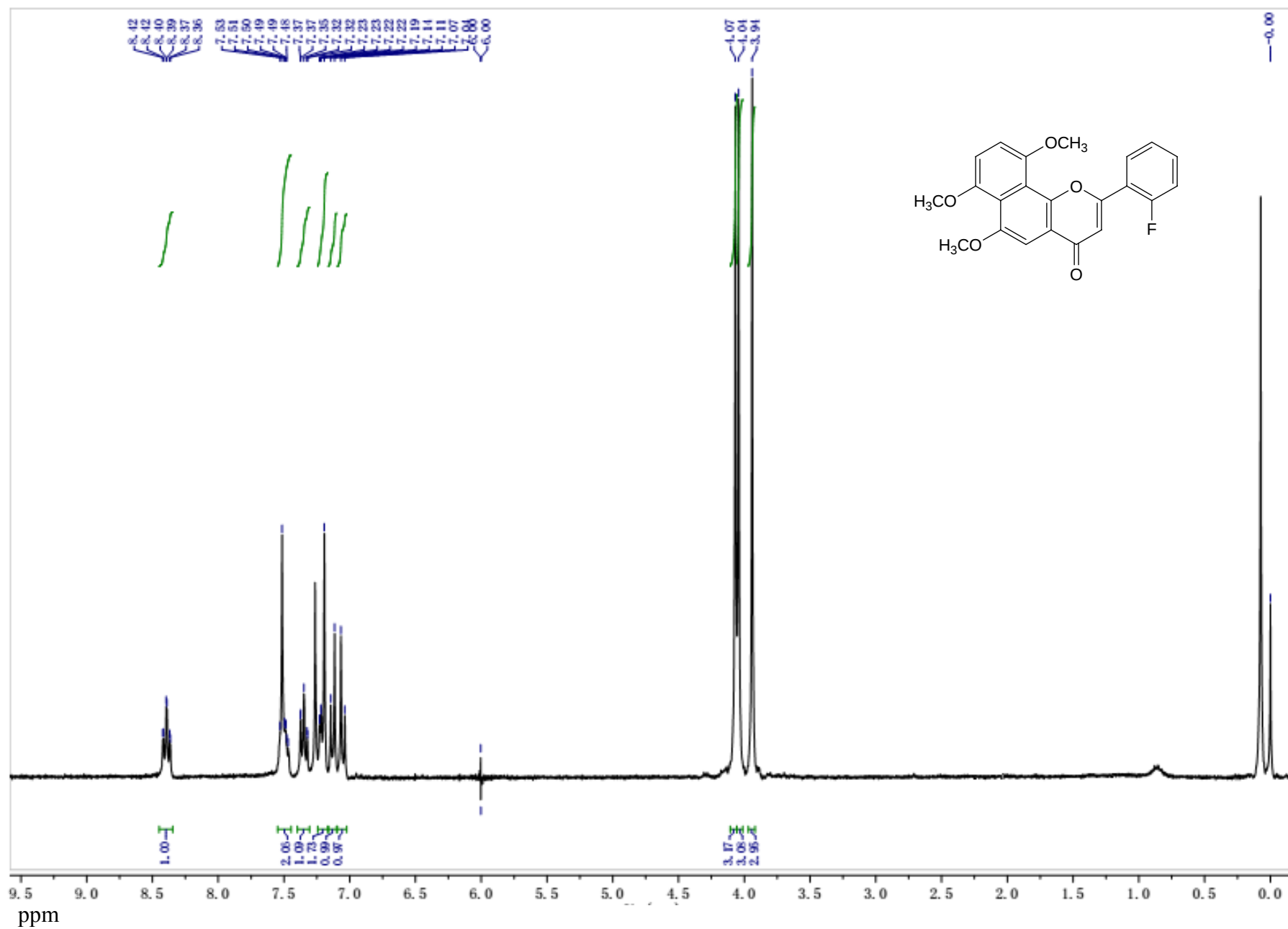
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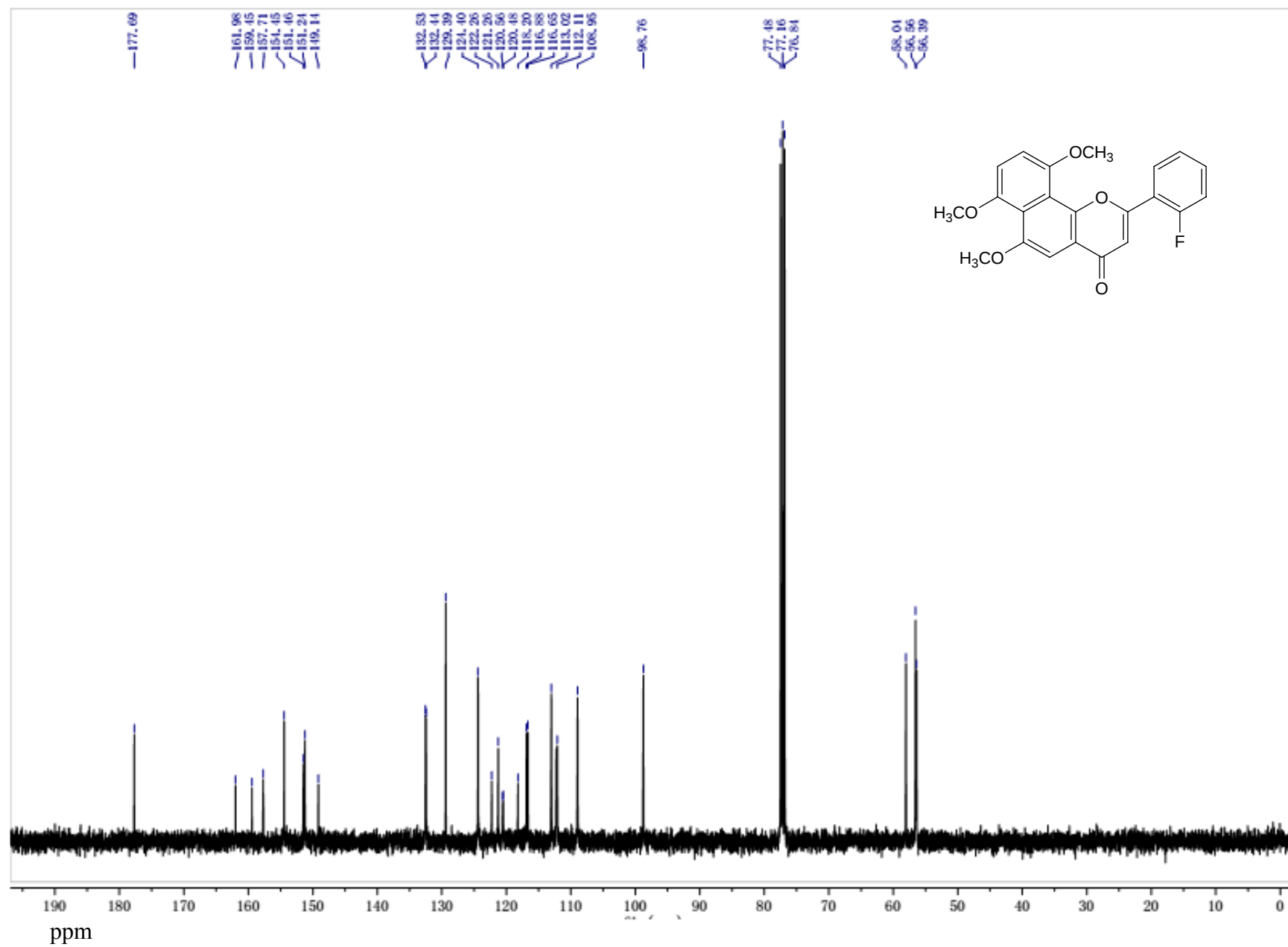
1. General Information

^1H NMR spectra were recorded on a Varian Mercury 300 spectrometer (300 MHz) or a Bruker Avance 400 spectrometer (400 MHz). Chemical shifts were reported in δ units with TMS as the internal standard. ^{13}C NMR spectra were recorded on a Bruker Avance 400 spectrometer (101 MHz). Chemical shifts in ^{13}C spectra were recorded with solvent signals as the internal standard (δ_{C} of CDCl_3 at 77.16 ppm [central line of the triplet], δ_{C} of d^6 -DMSO at 39.52 ppm [central line of the septet], δ_{C} of d^6 -Pyridine at 135.91 ppm [central line of the middle triplet]). HRMS spectra were measured on a Waters Q-TOF Premier mass spectrometer.

2. NMR and HRMS spectra of fluoro atom-contained compounds



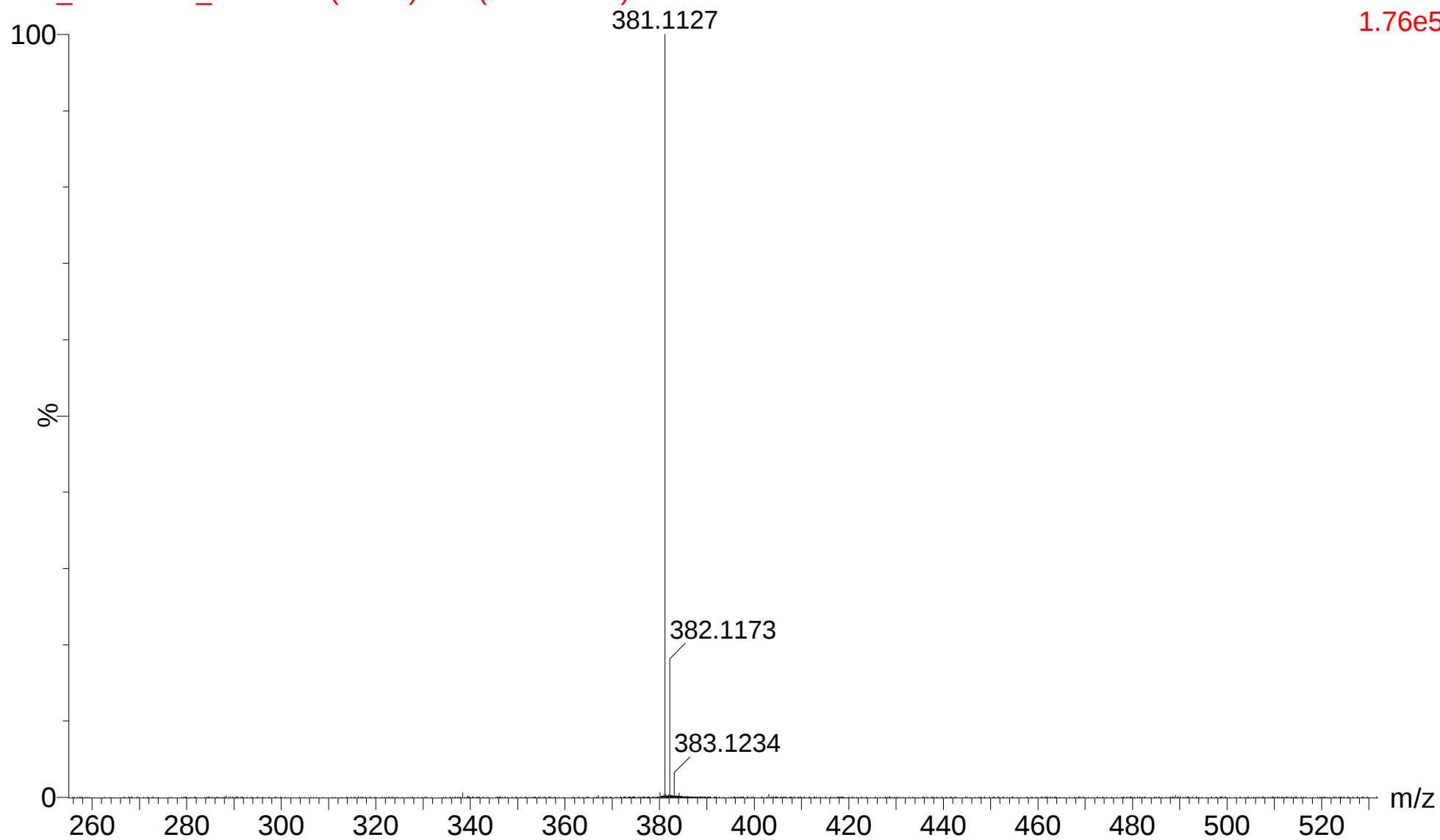
¹H NMR spectrum of compound **4b** (300 MHz, CDCl₃)



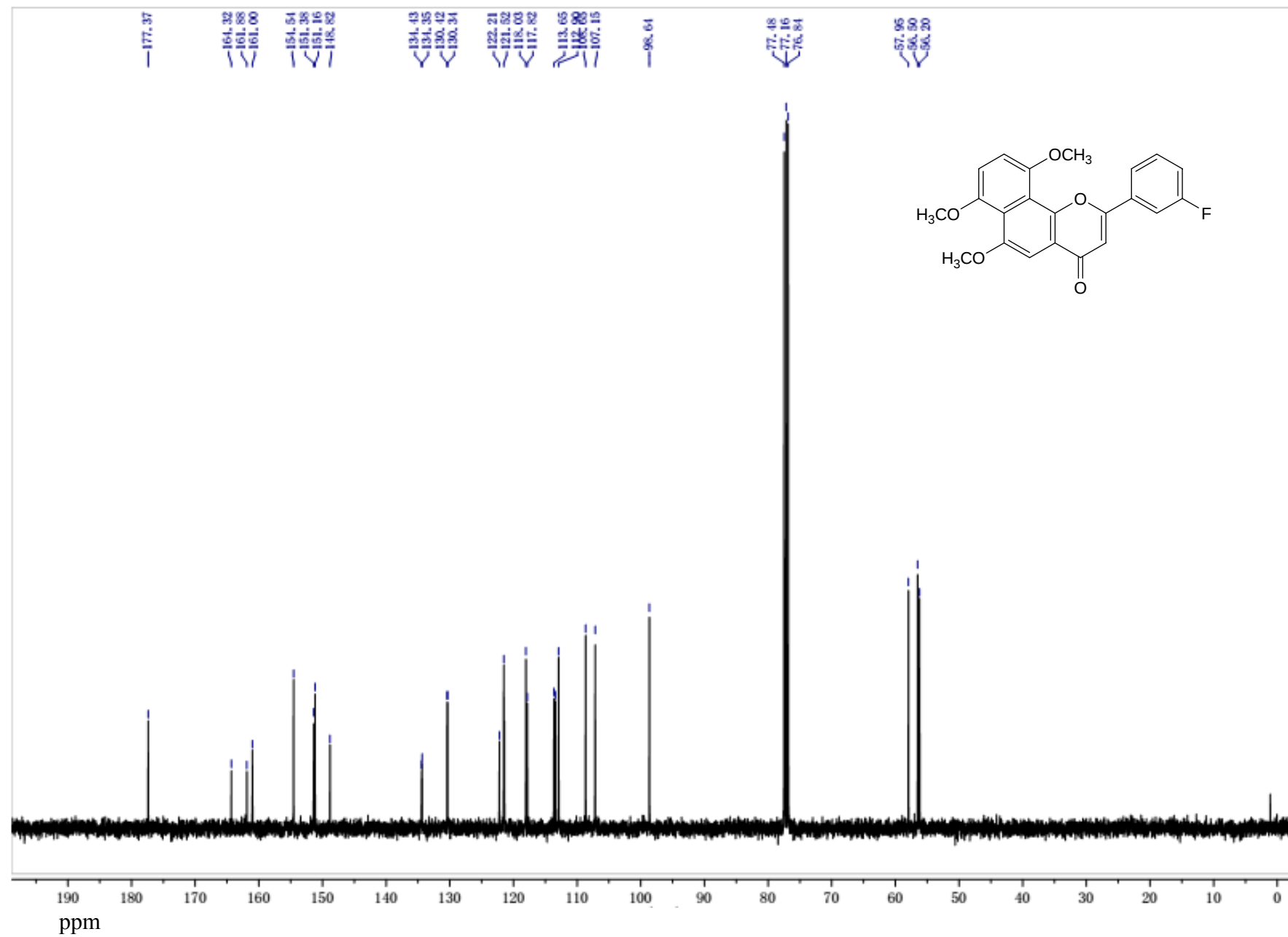
¹³C NMR spectrum of compound **4b** (101 MHz, CDCl₃)

LSS_20140416_01-02 28 (0.519) Cm (26:32-1:18)

1: TOF MS ES+
1.76e5



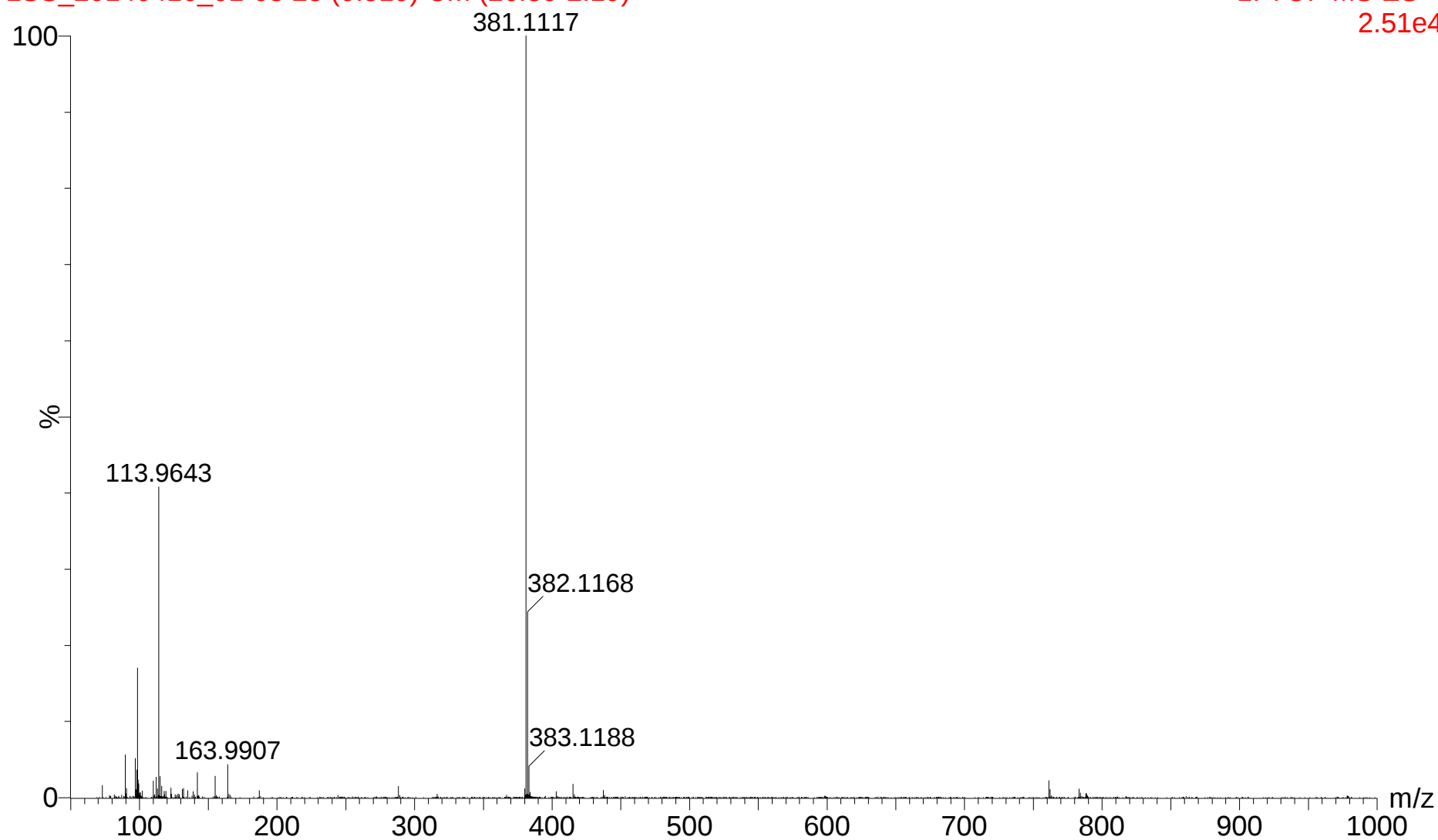
HRMS spectrum of compound **4b** (Calcd. for C₂₂H₁₈FO₅ 381.1138)



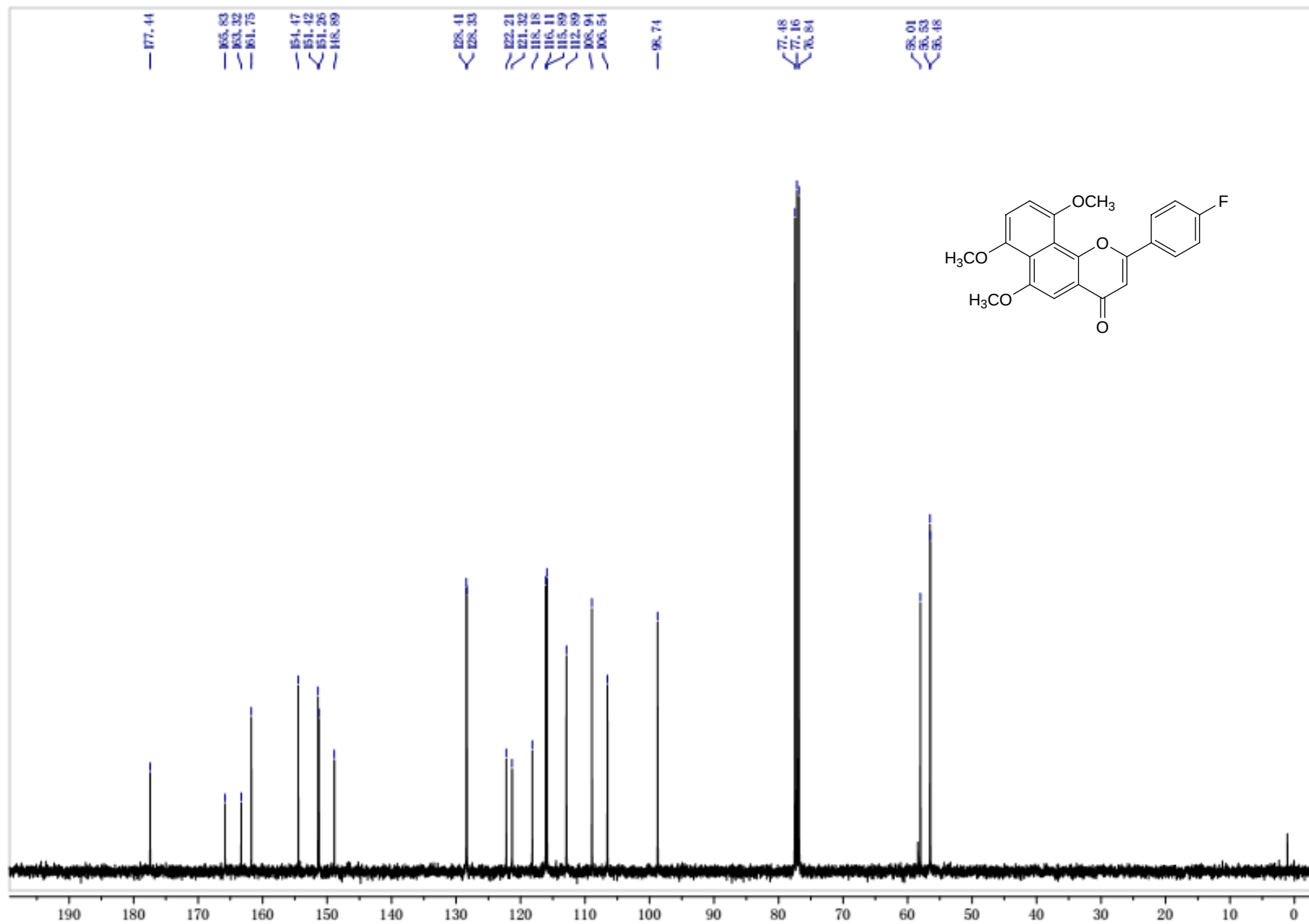
^{13}C NMR spectrum of compound **4c** (101 MHz, CDCl_3)

LSS_20140416_01-03 28 (0.519) Cm (26:30-2:19)

1: TOF MS ES+
2.51e4



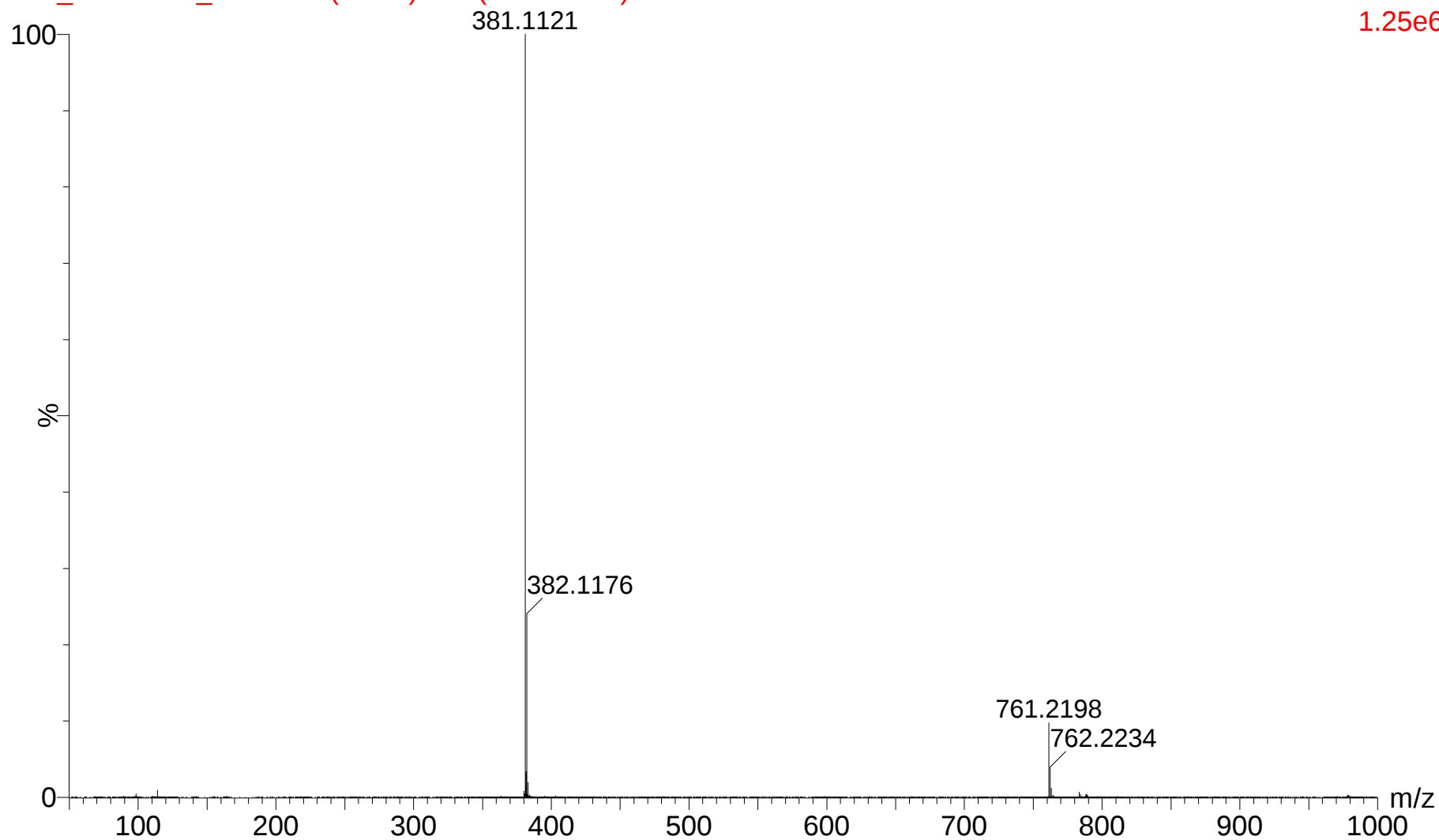
HRMS spectrum of compound **4c** (Calcd. for C₂₂H₁₈FO₅ 381.1138)



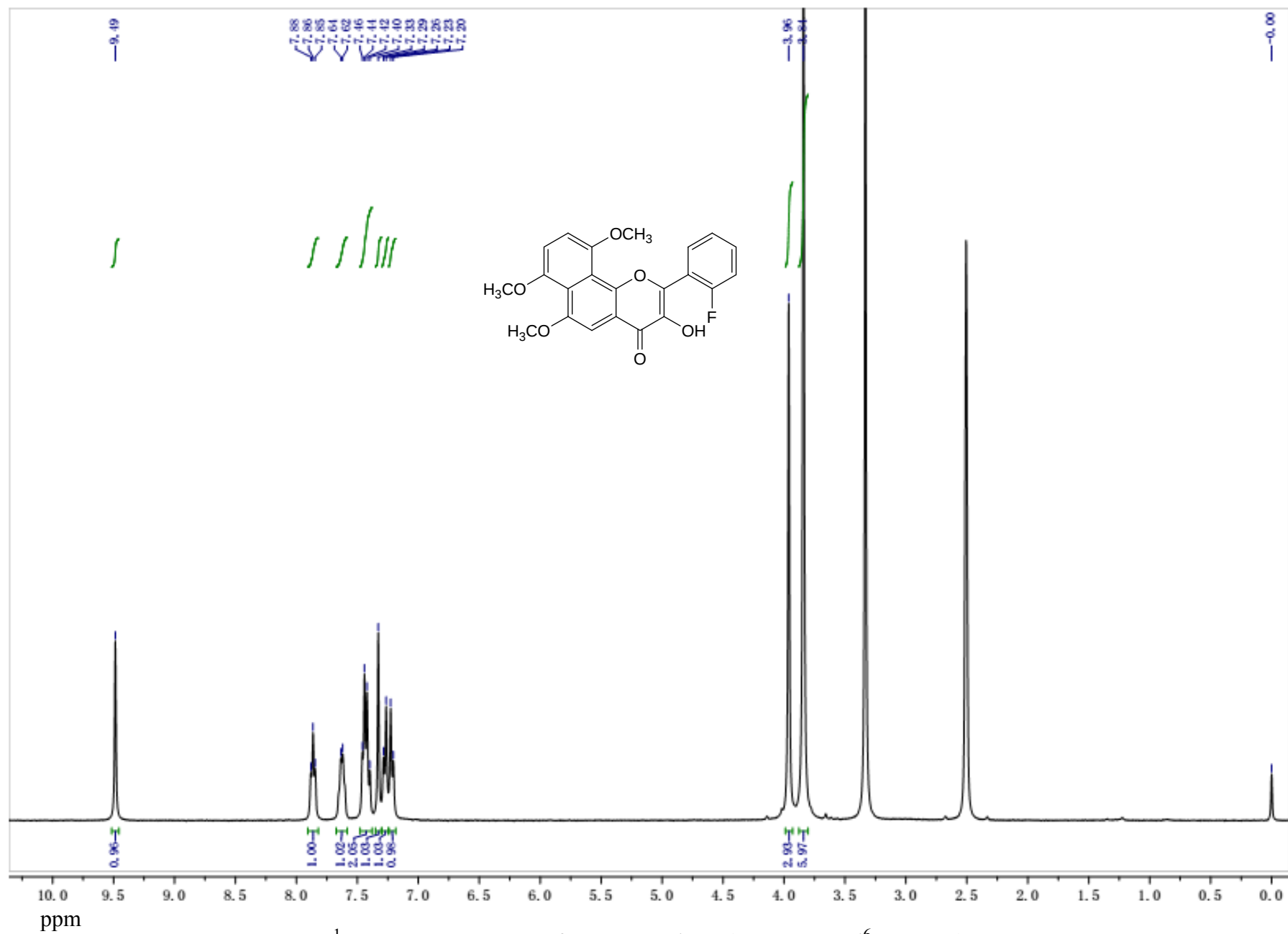
^{13}C NMR spectrum of compound **4d** (101 MHz, CDCl_3)

LSS_20140416_01-04 28 (0.519) Cm (25:32-2:19)

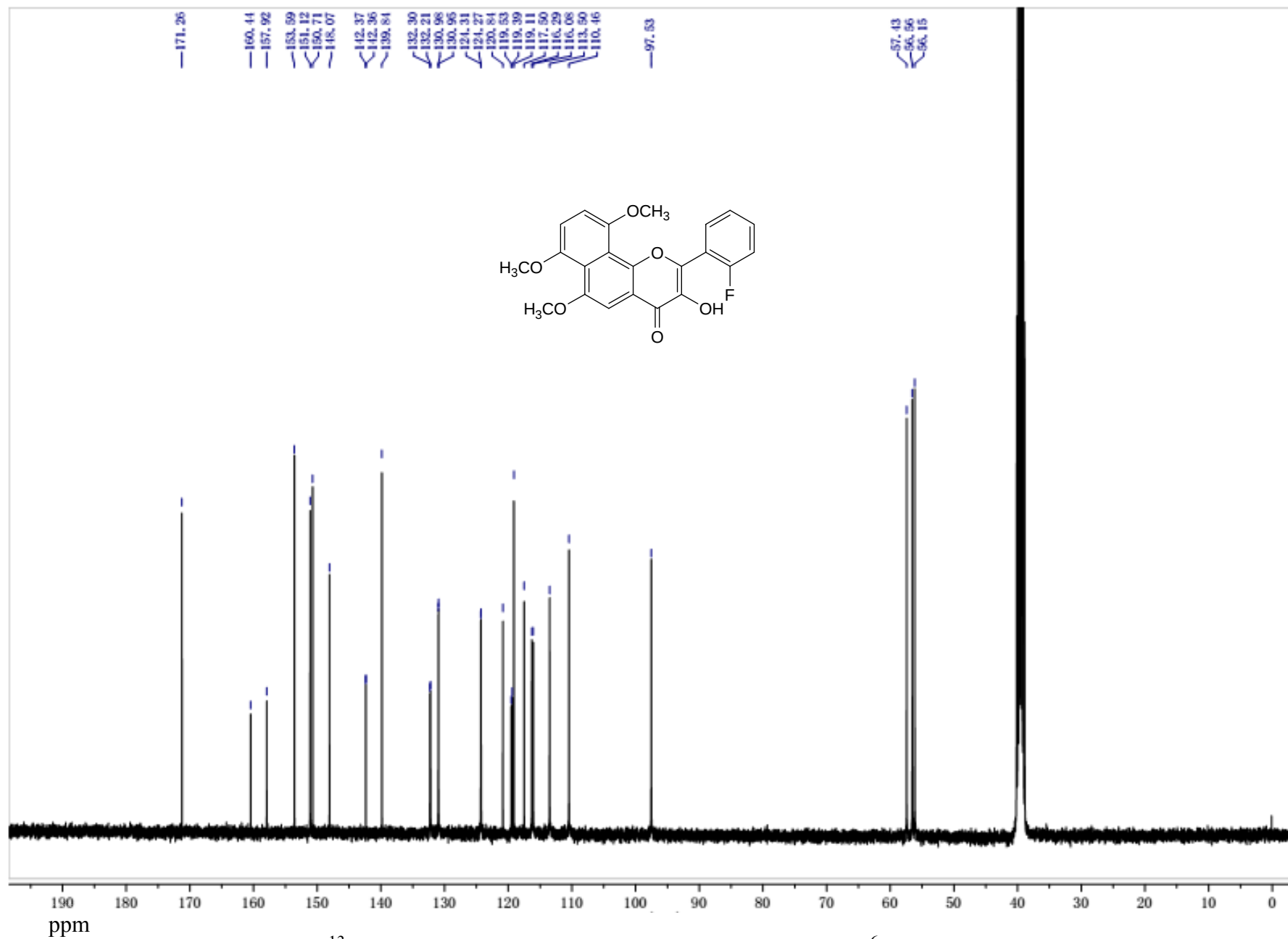
1: TOF MS ES+
1.25e6



HRMS spectrum of compound **4d** (Calcd. for C₂₂H₁₈FO₅ 381.1138)



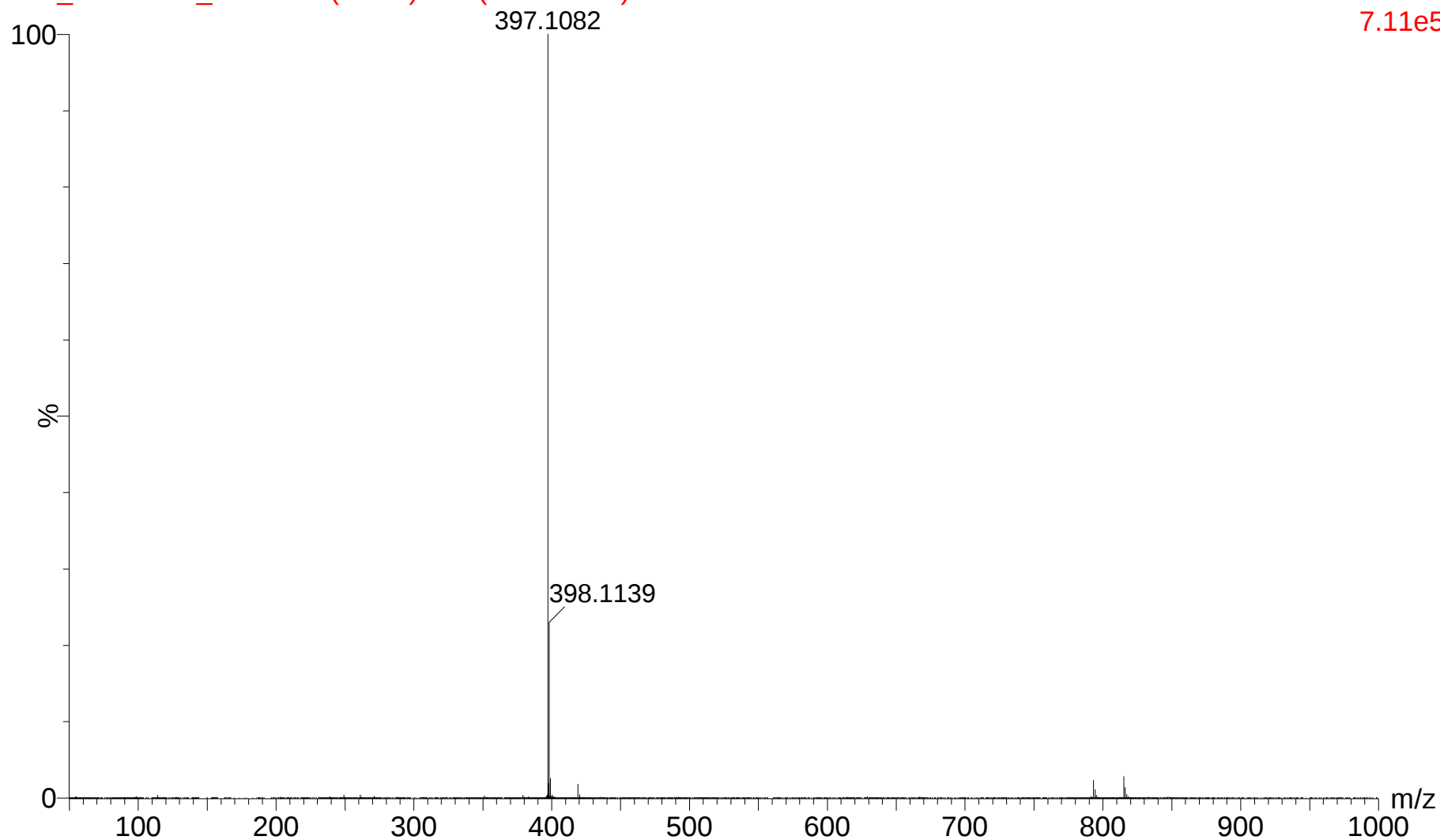
¹H NMR spectrum of compound **8b** (400 MHz, d⁶-DMSO)



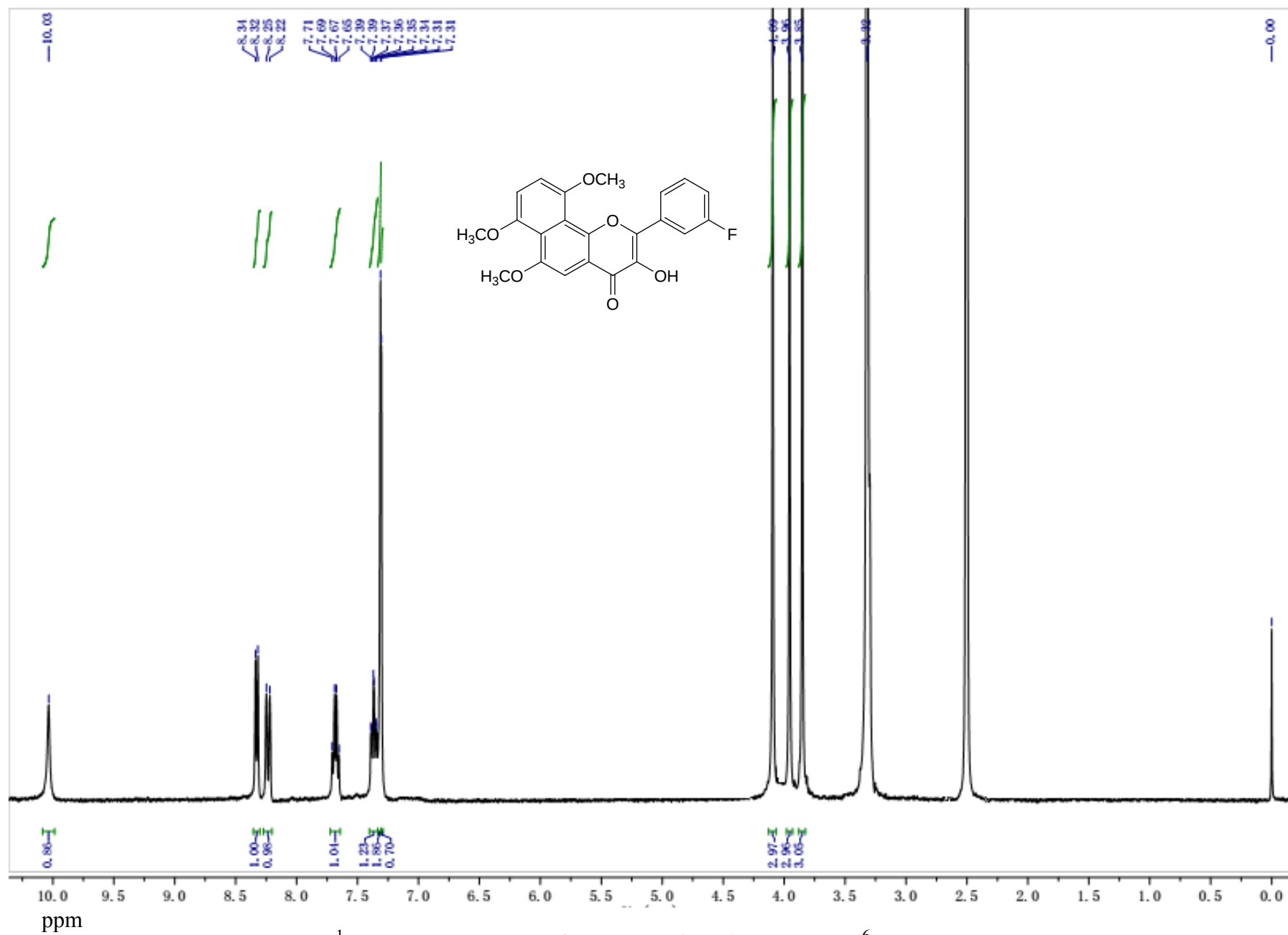
¹³C NMR spectrum of compound **8b** (101 MHz, d⁶-DMSO)

LSS_20140416_06-02 28 (0.519) Cm (24:33-1:19)

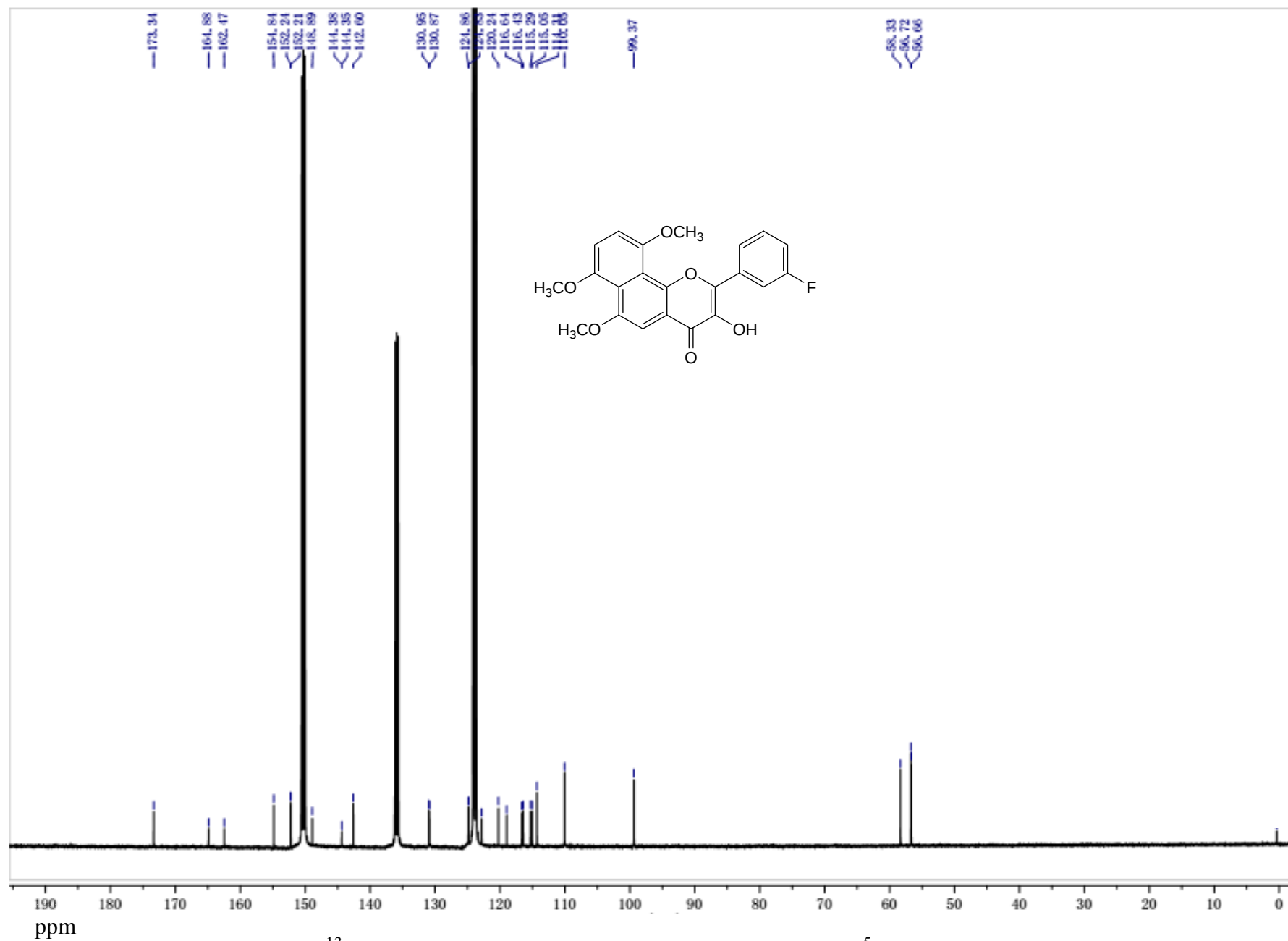
1: TOF MS ES+
7.11e5



HRMS spectrum of compound **8b** (Calcd. for $C_{22}H_{18}FO_6$ 397.1087)



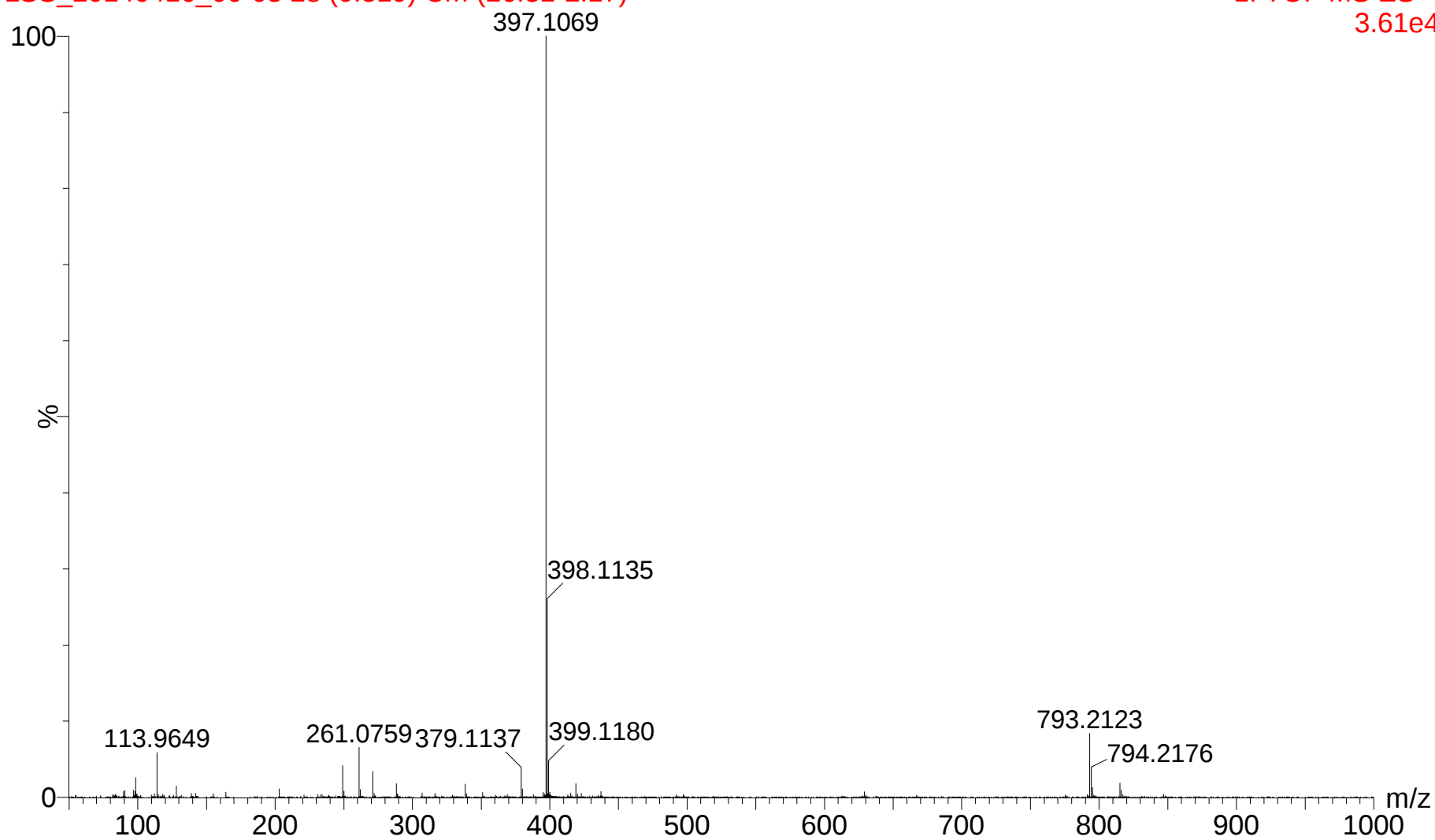
¹H NMR spectrum of compound **8c** (400 MHz, d⁶-DMSO)

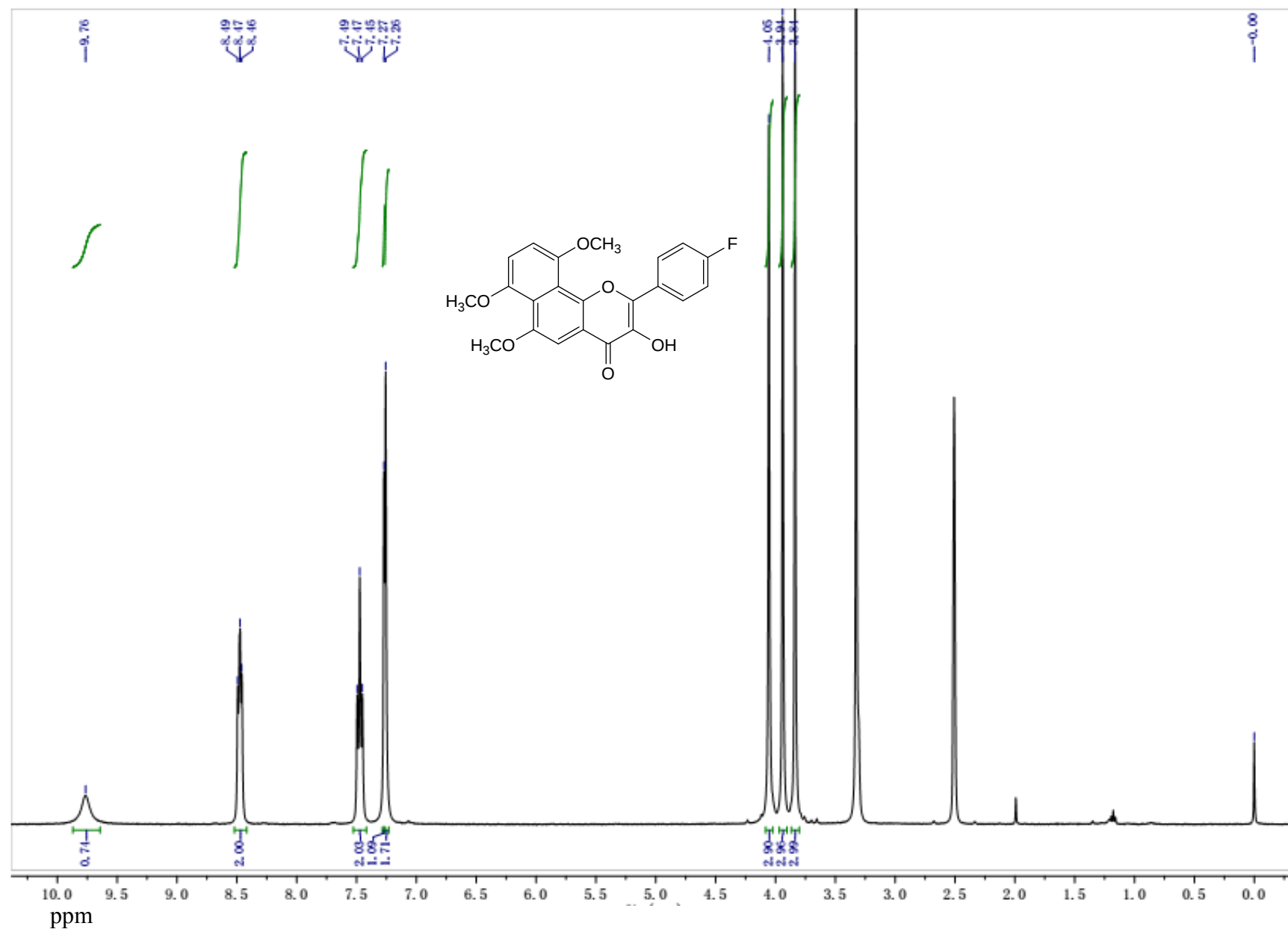


¹³C NMR spectrum of compound **8c** (101 MHz, d⁵-pyridine)

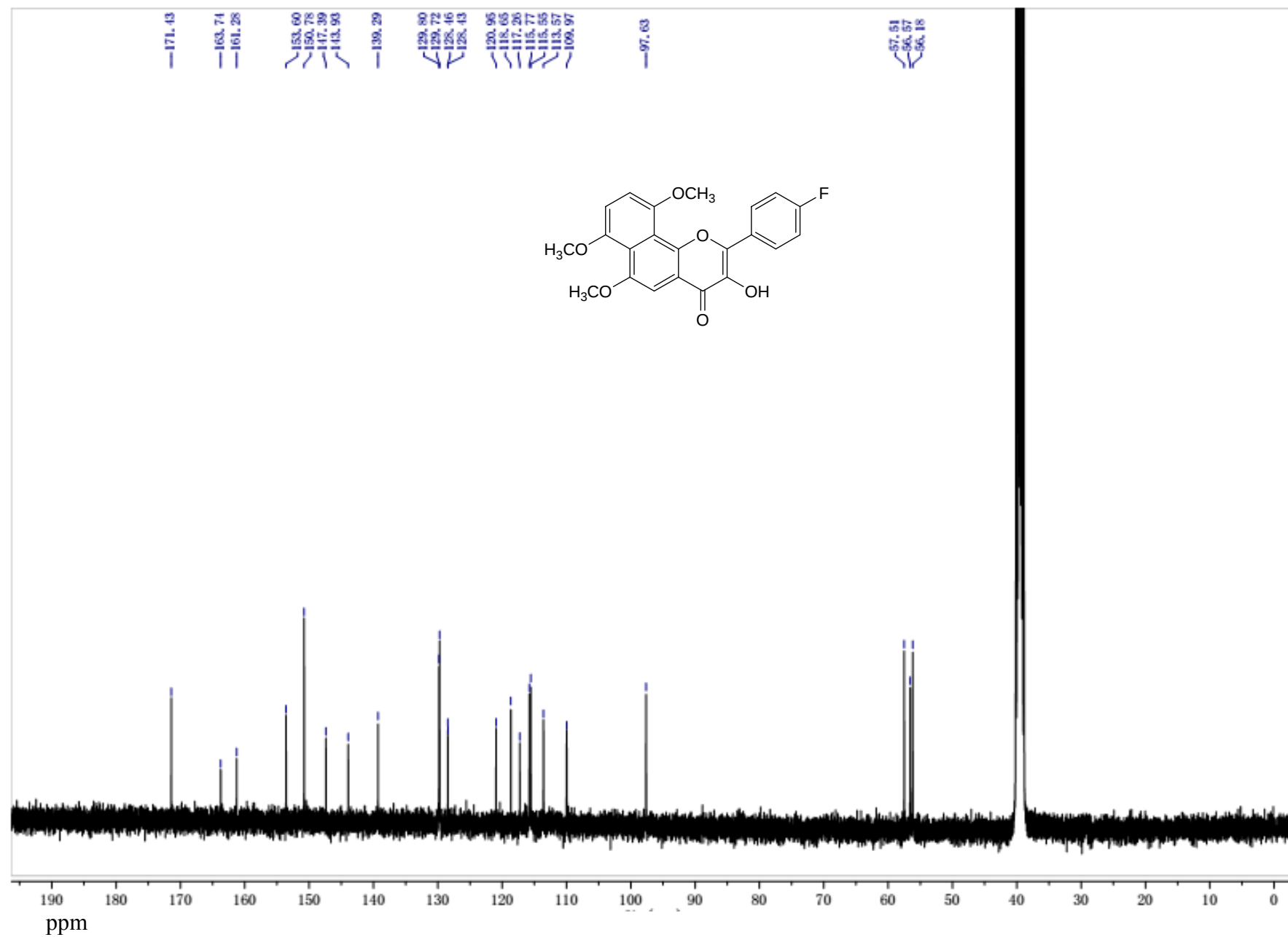
LSS_20140416_06-03 28 (0.519) Cm (26:31-2:17)

1: TOF MS ES+
3.61e4





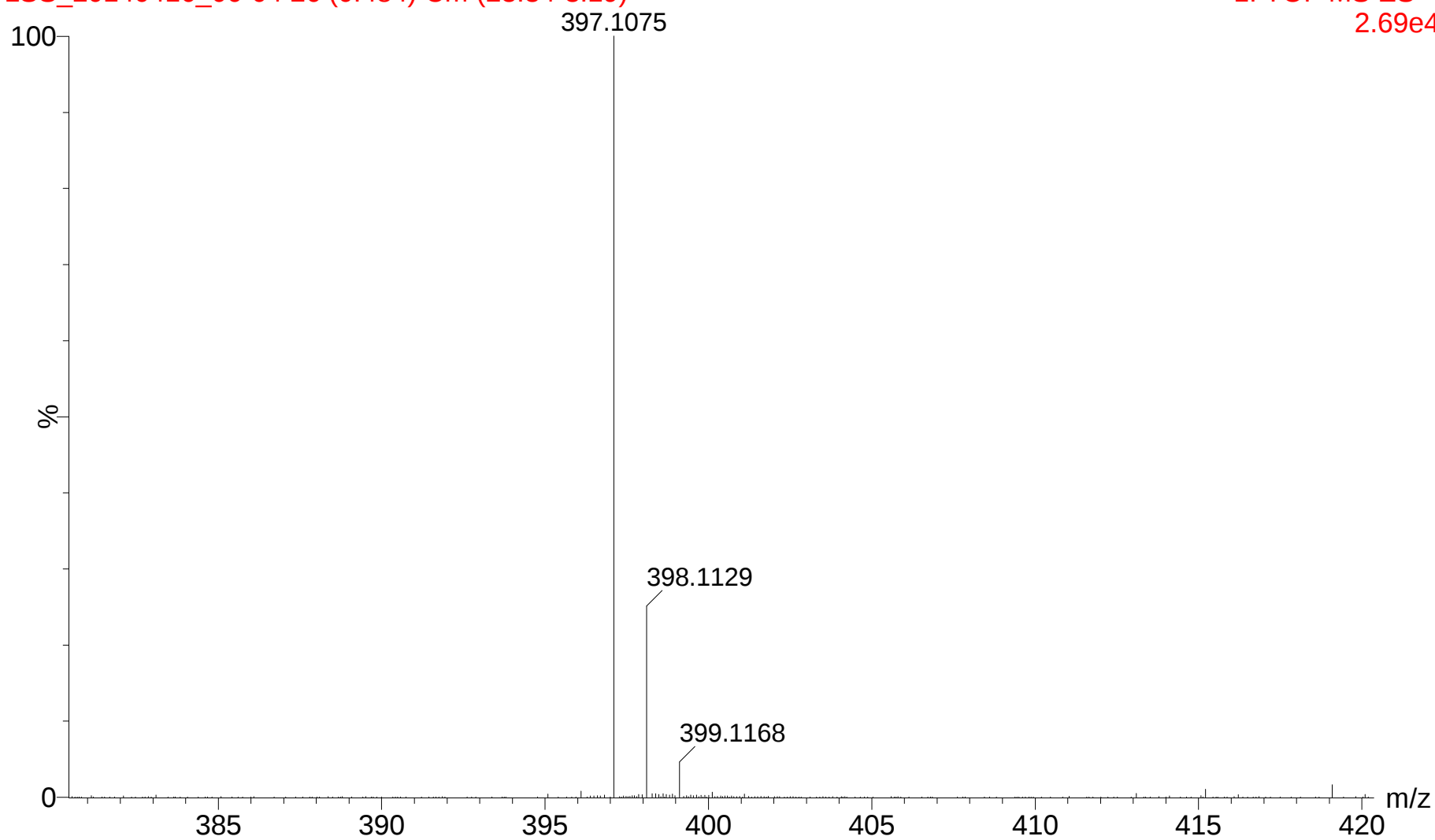
¹H NMR spectrum of compound **8d** (400 MHz, d⁶-DMSO)



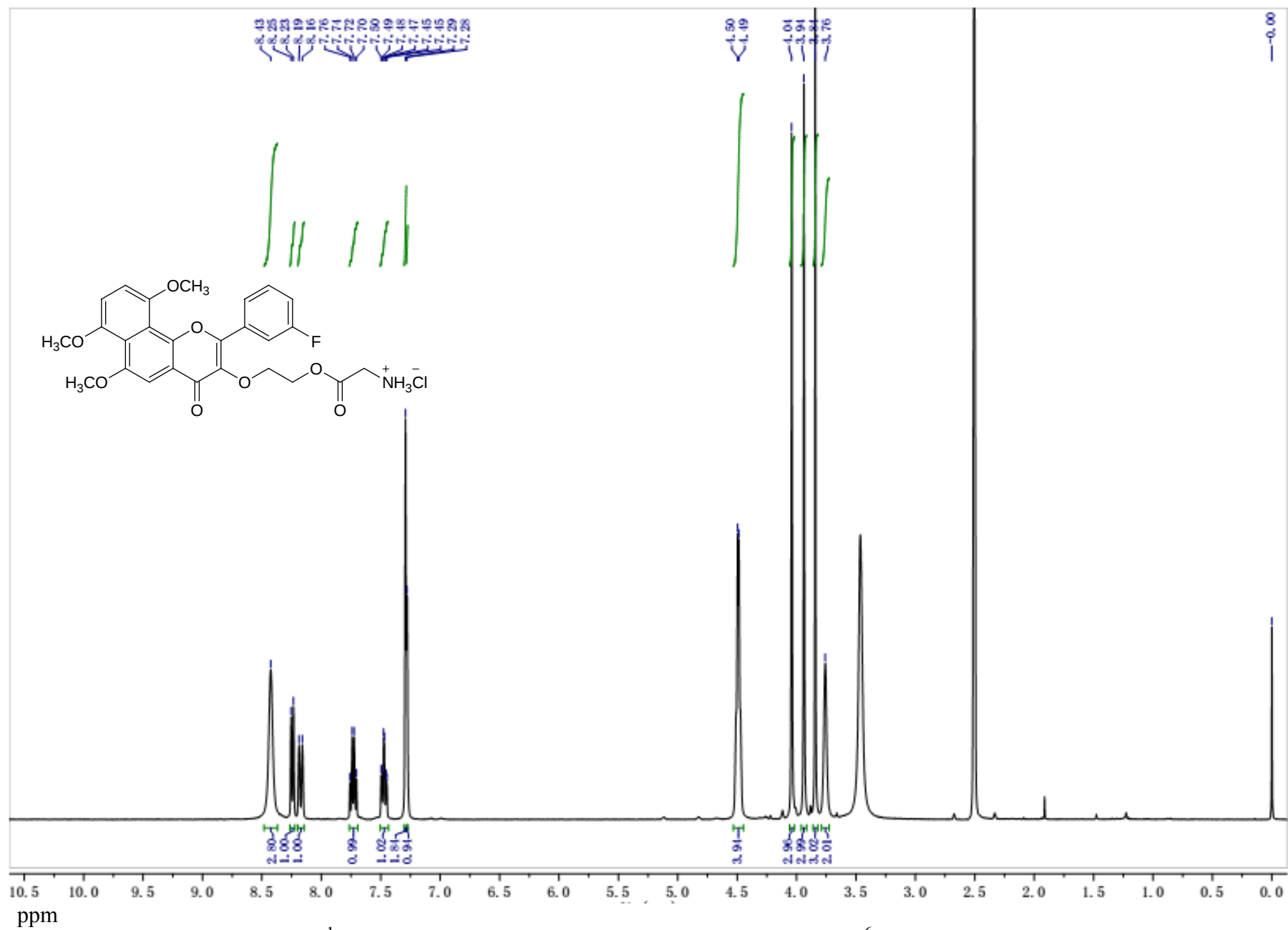
¹³C NMR spectrum of compound **8d** (101 MHz, d⁶-DMSO)

LSS_20140416_06-04 26 (0.484) Cm (23:34-3:19)

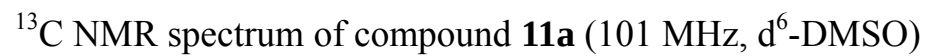
1: TOF MS ES+
2.69e4



HRMS spectrum of compound **8d** (Calcd. for C₂₂H₁₈FO₆ 397.1087)

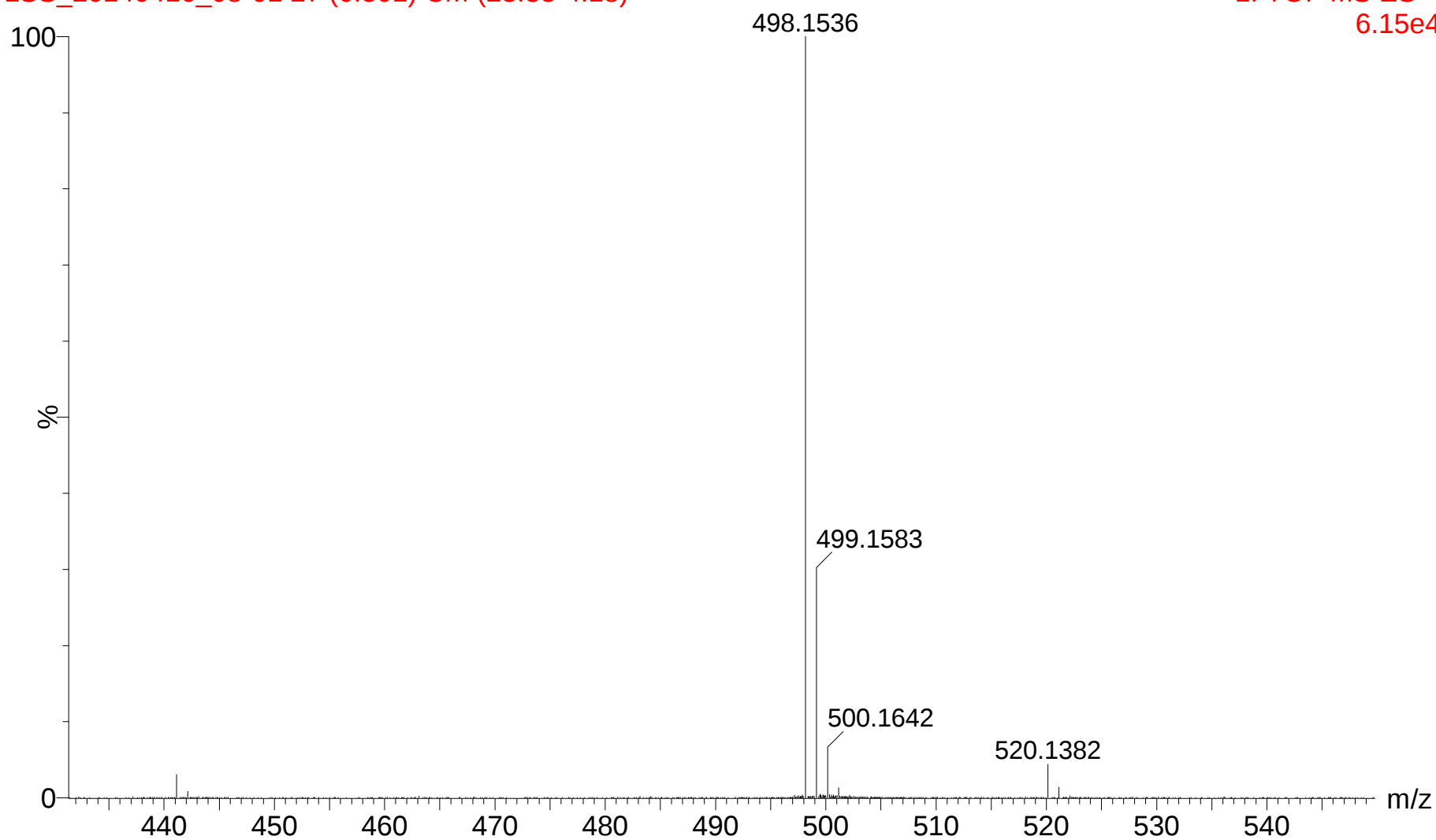


^1H NMR spectrum of compound **11a** (400 MHz, $\text{d}^6\text{-DMSO}$)

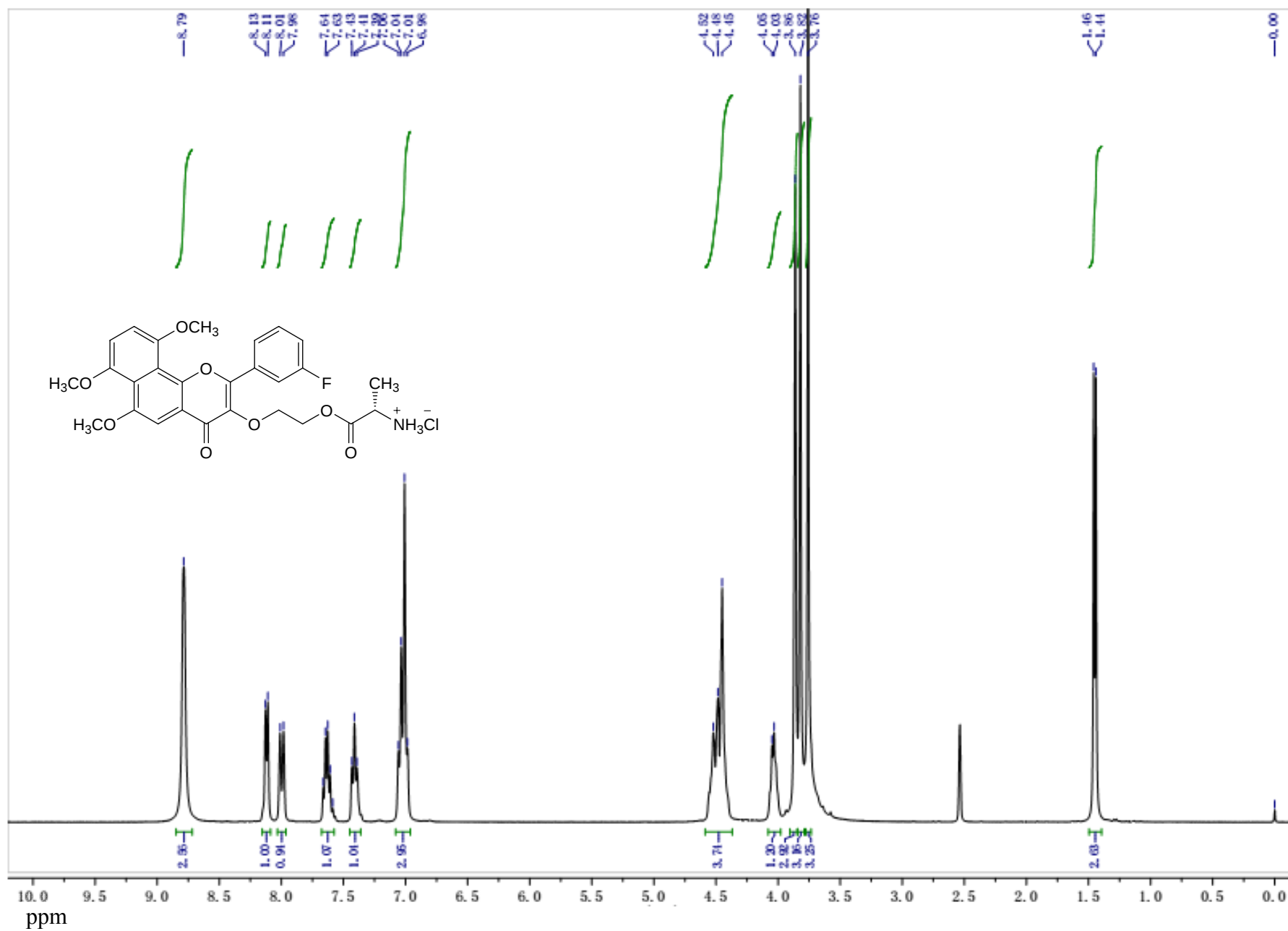


LSS_20140416_08-01 27 (0.501) Cm (23:33-4:18)

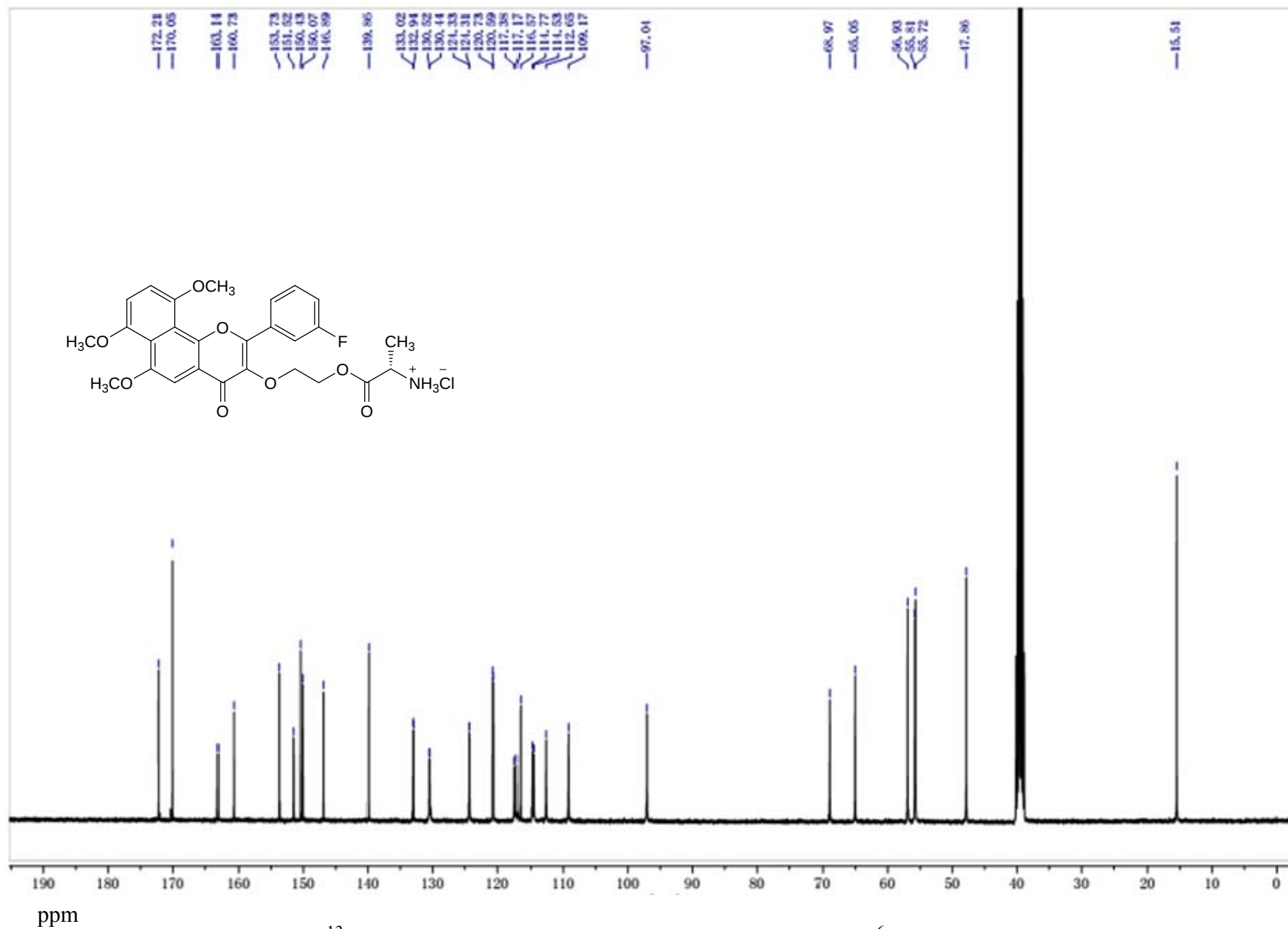
1: TOF MS ES+
6.15e4



HRMS spectrum of compound **11a** (Calcd. for $C_{26}H_{25}FNO_8$ 498.1564)



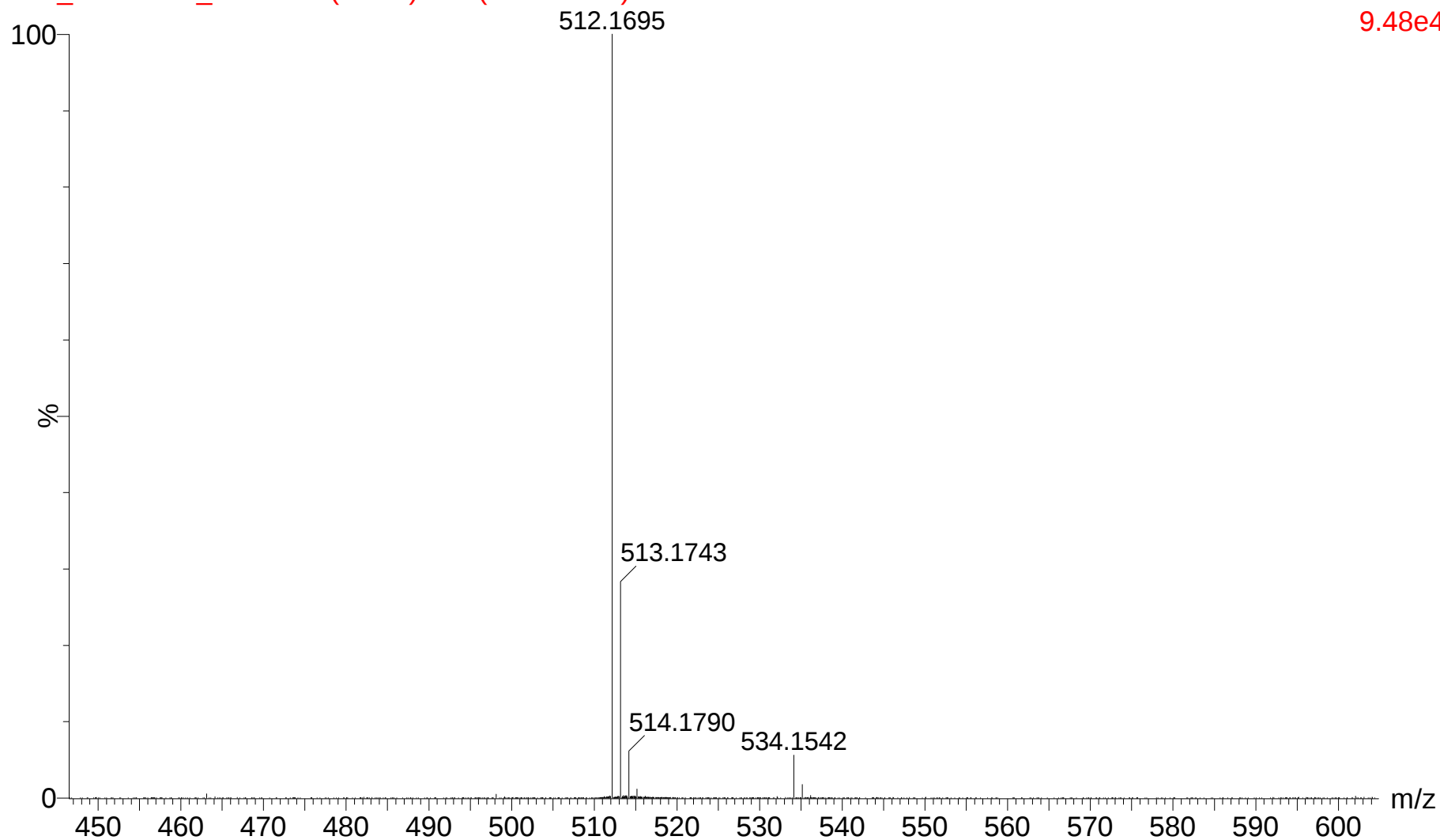
^1H NMR spectrum of compound **11b** (400 MHz, $\text{d}^6\text{-DMSO}$)



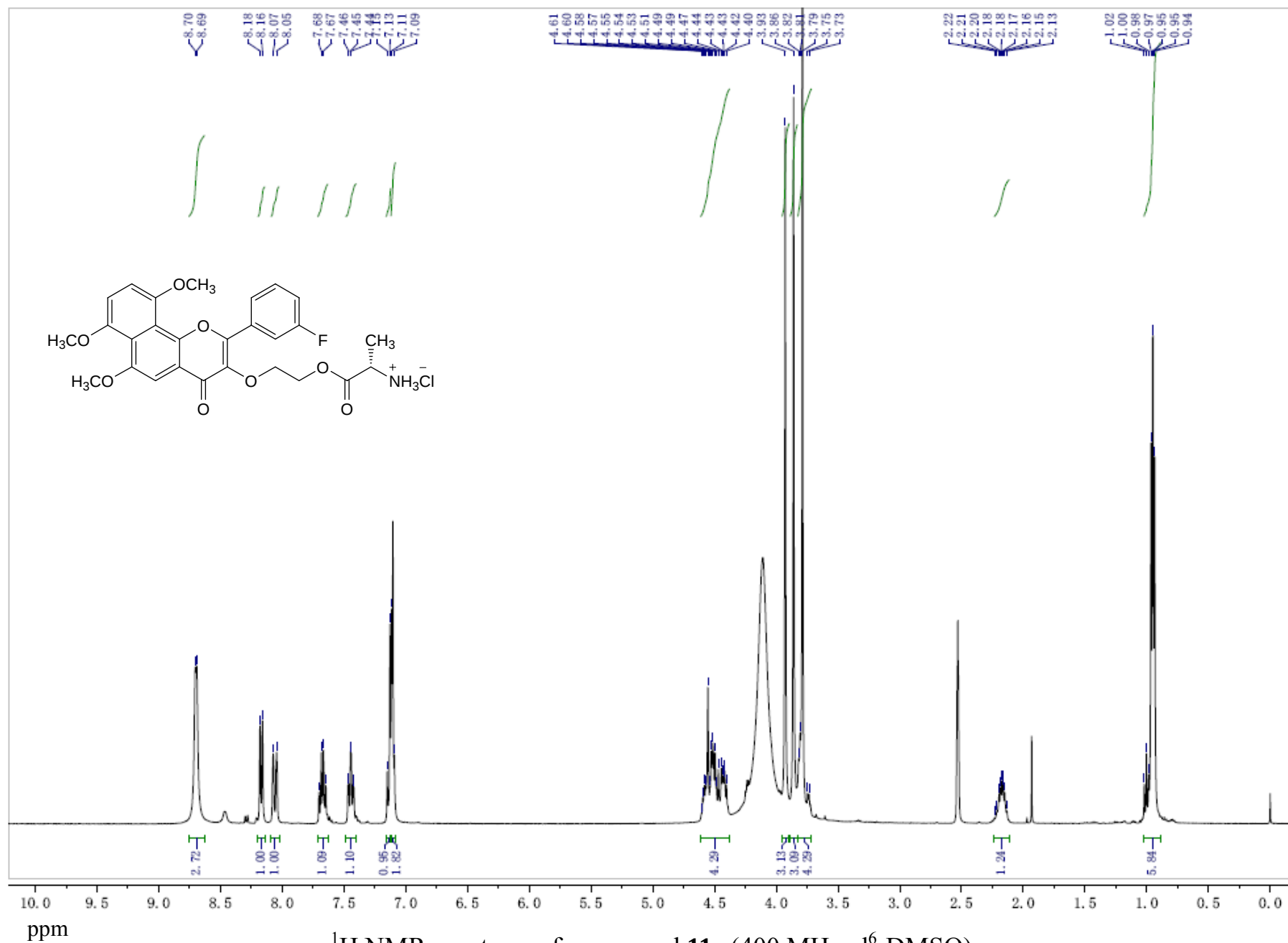
¹³C NMR spectrum of compound **11b** (101 MHz, d⁶-DMSO)

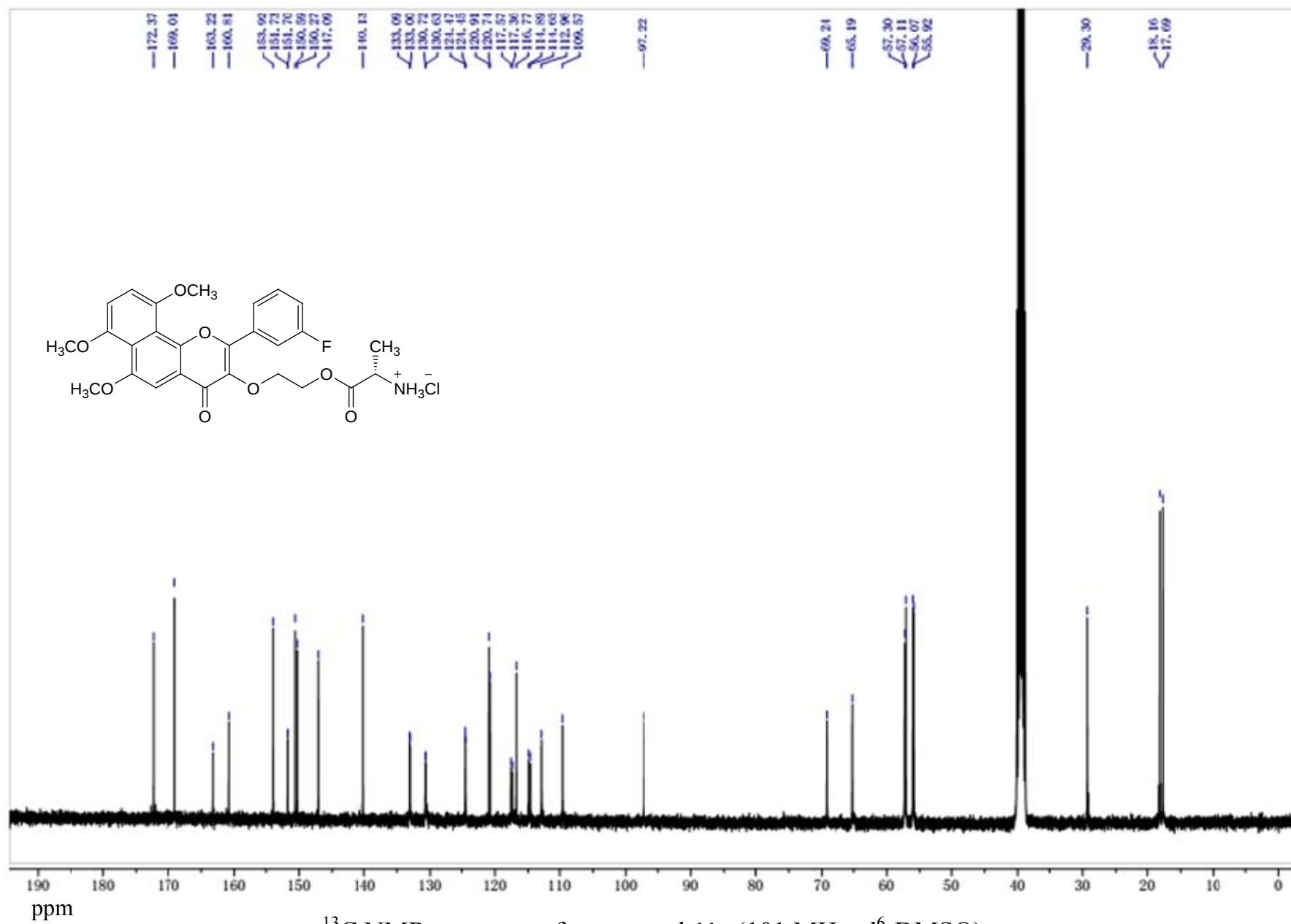
LSS_20140416_08-02 28 (0.519) Cm (23:34-3:20)

1: TOF MS ES+
9.48e4



HRMS spectrum of compound **11b** (Calcd. for C₂₇H₂₇FNO₈ 512.1721)

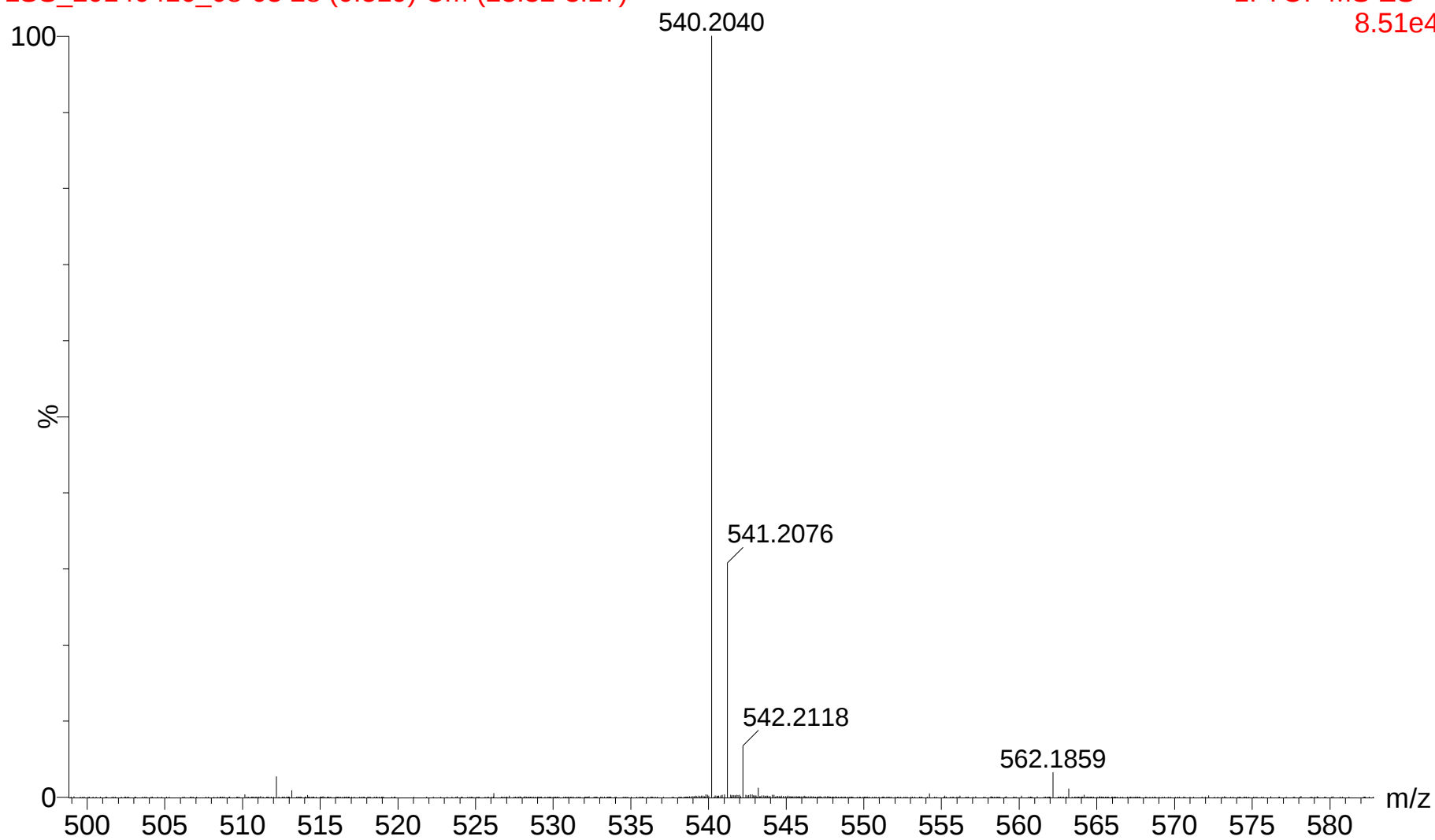




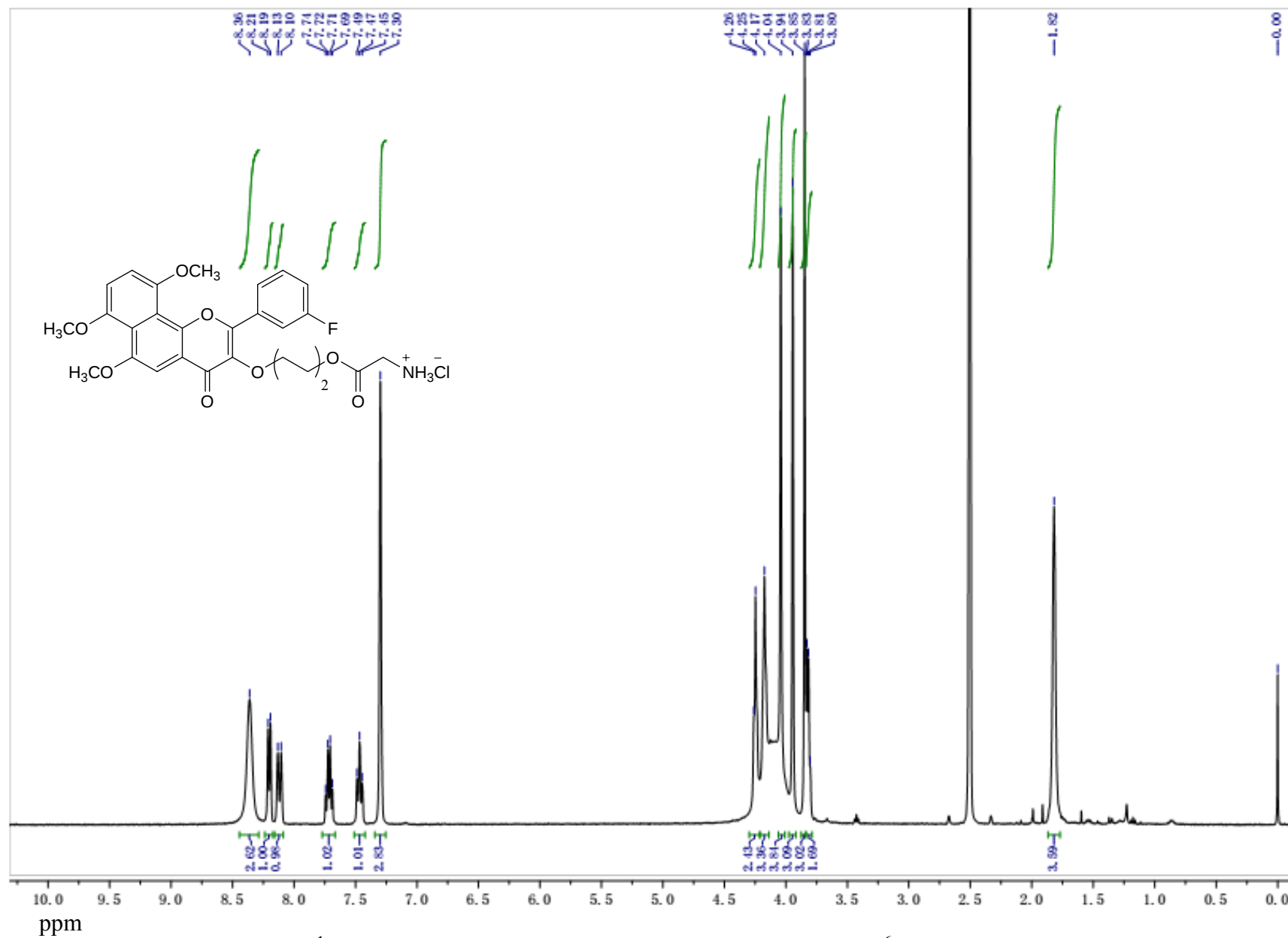
¹³C NMR spectrum of compound **11c** (101 MHz, d⁶-DMSO)

LSS_20140416_08-03 28 (0.519) Cm (23:32-3:17)

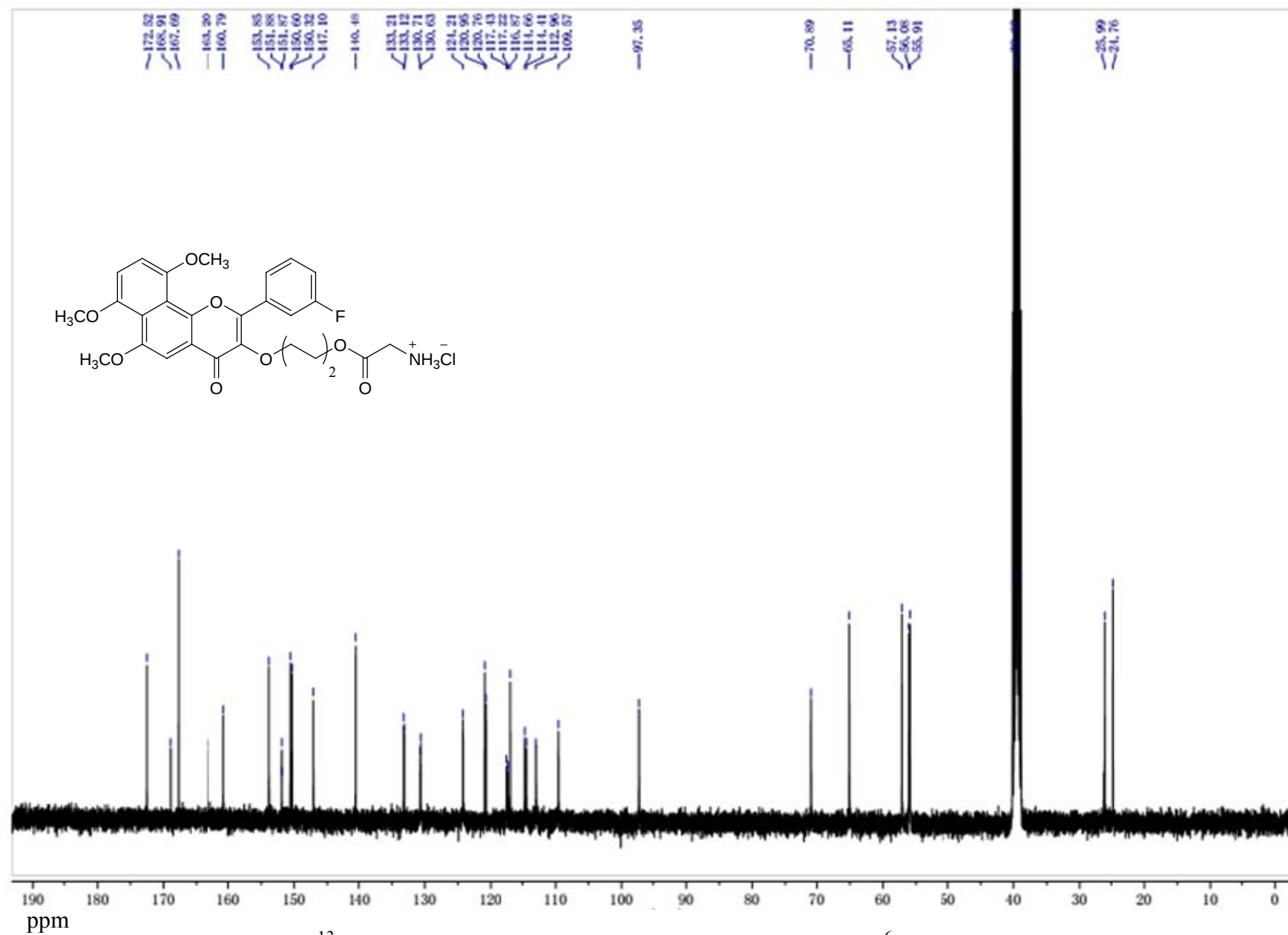
1: TOF MS ES+
8.51e4



HRMS spectrum of compound **11c** (Calcd. for C₂₉H₃₁FNO₈ 540.2034)



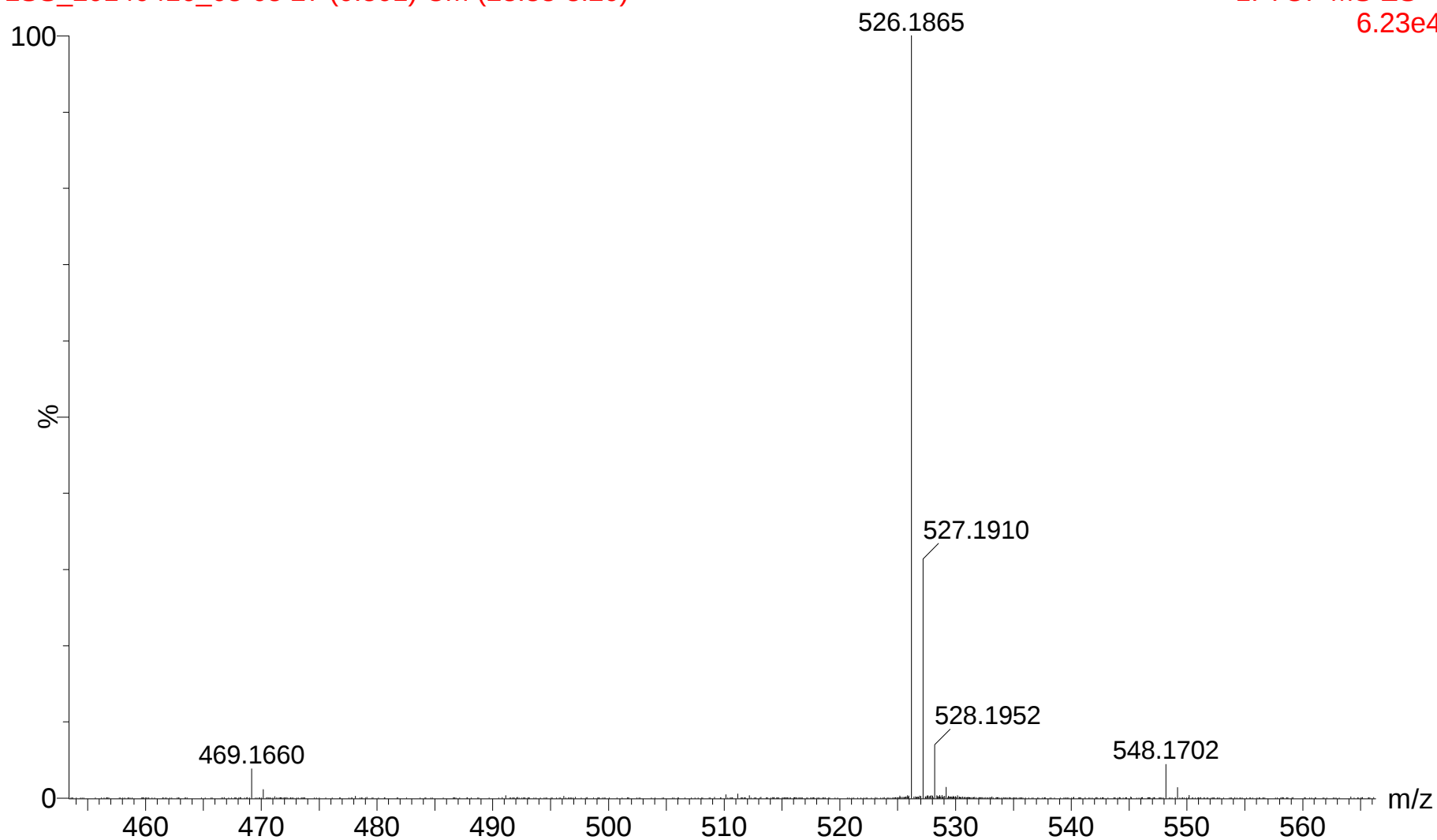
^1H NMR spectrum of compound **11d** (400 MHz, $\text{d}^6\text{-DMSO}$)



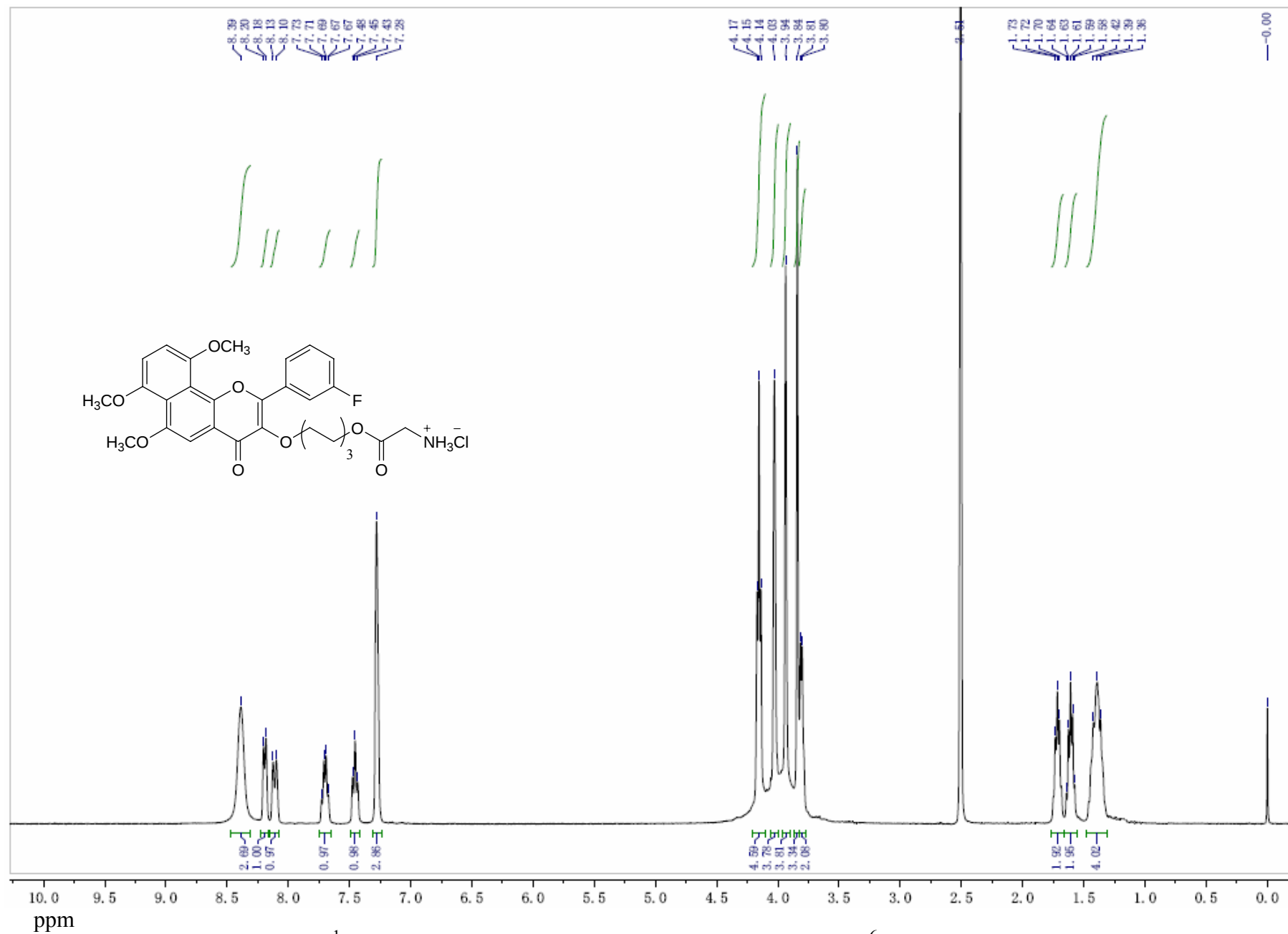
¹³C NMR spectrum of compound **11d** (101 MHz, d⁶-DMSO)

LSS_20140416_08-05 27 (0.501) Cm (23:33-3:20)

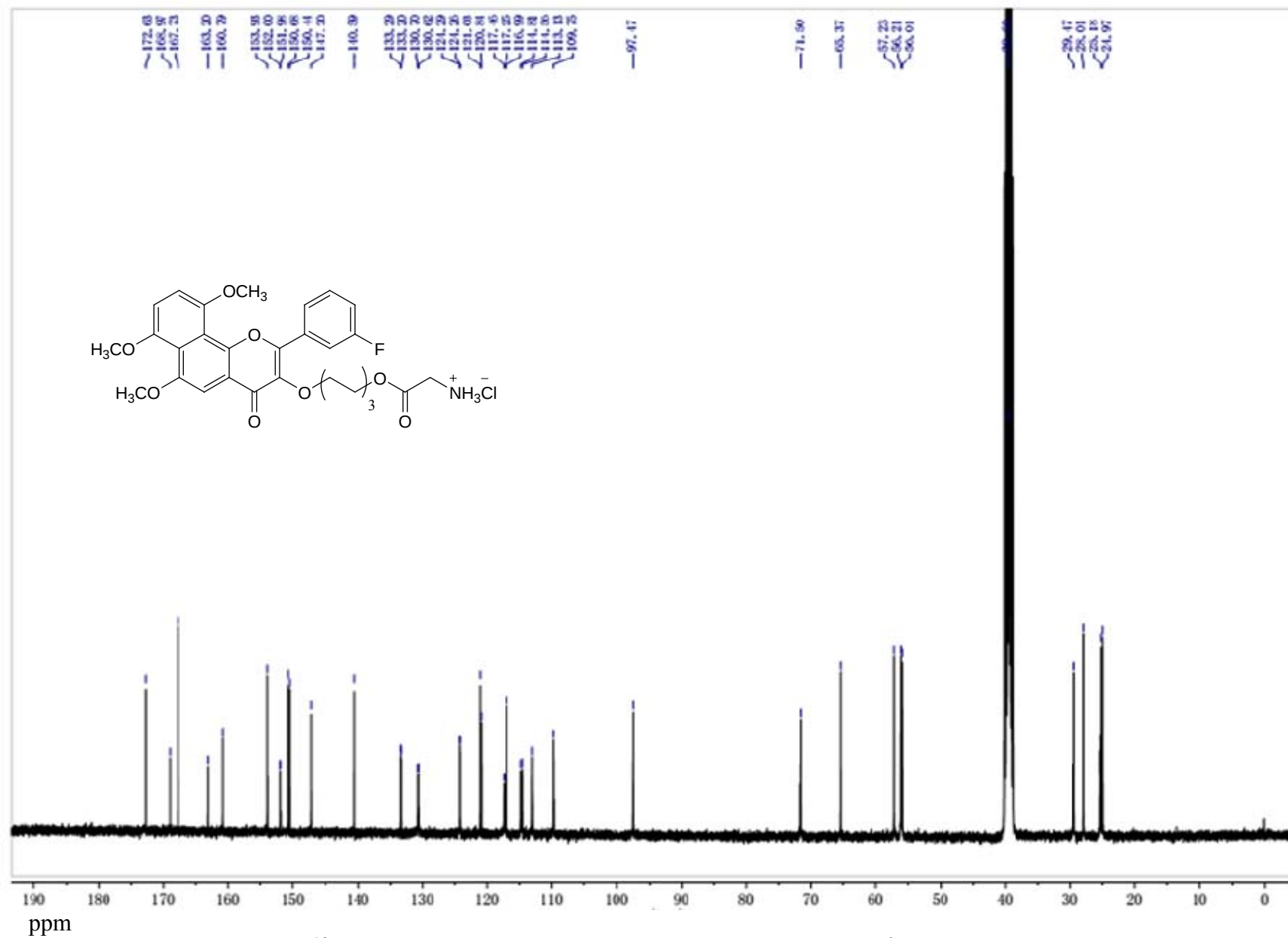
1: TOF MS ES+
6.23e4



HRMS spectrum of compound **11d** (Calcd. for C₂₈H₂₉FNO₈ 526.1877)



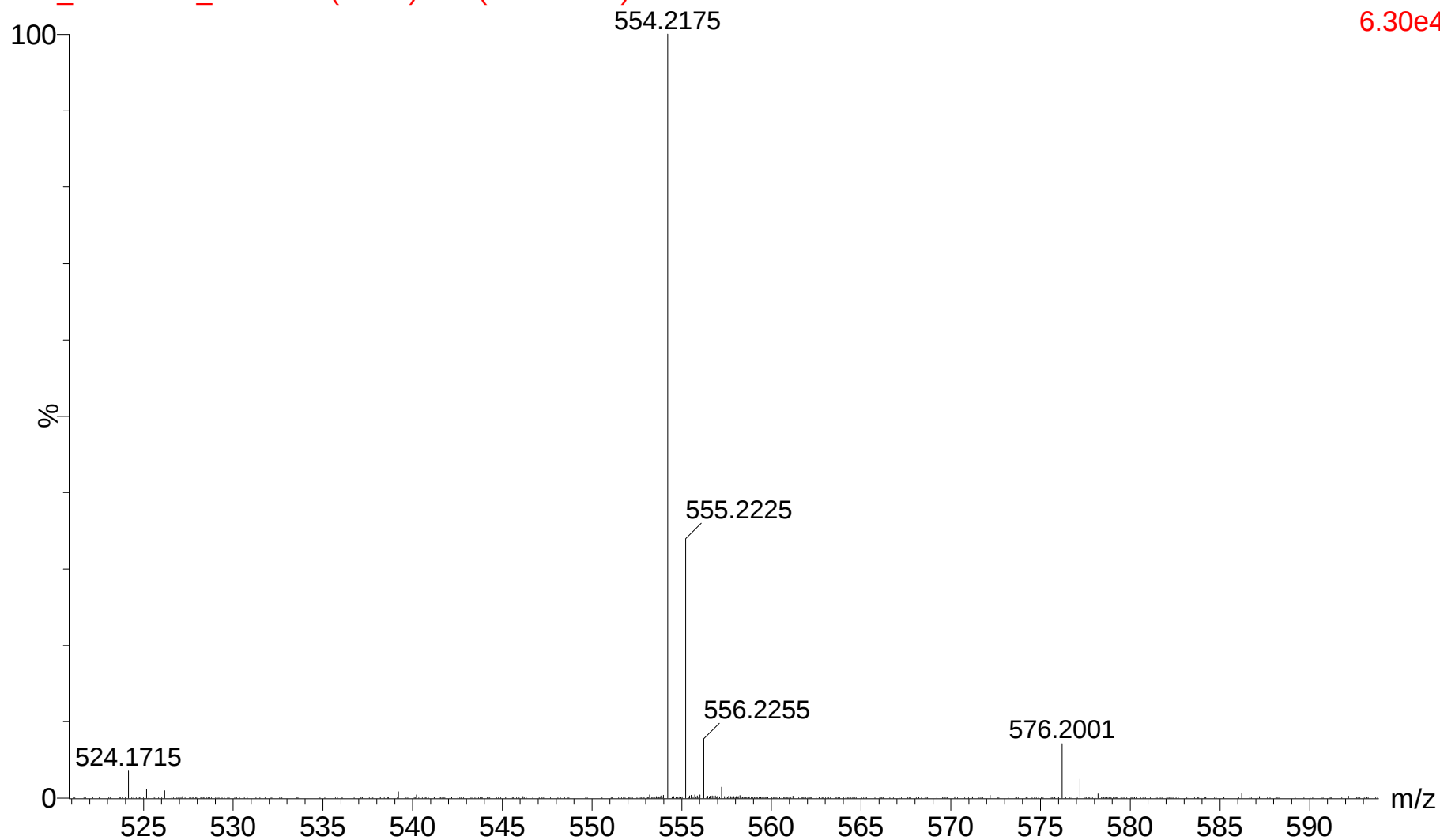
¹H NMR spectrum of compound **11e** (400 MHz, d⁶-DMSO)



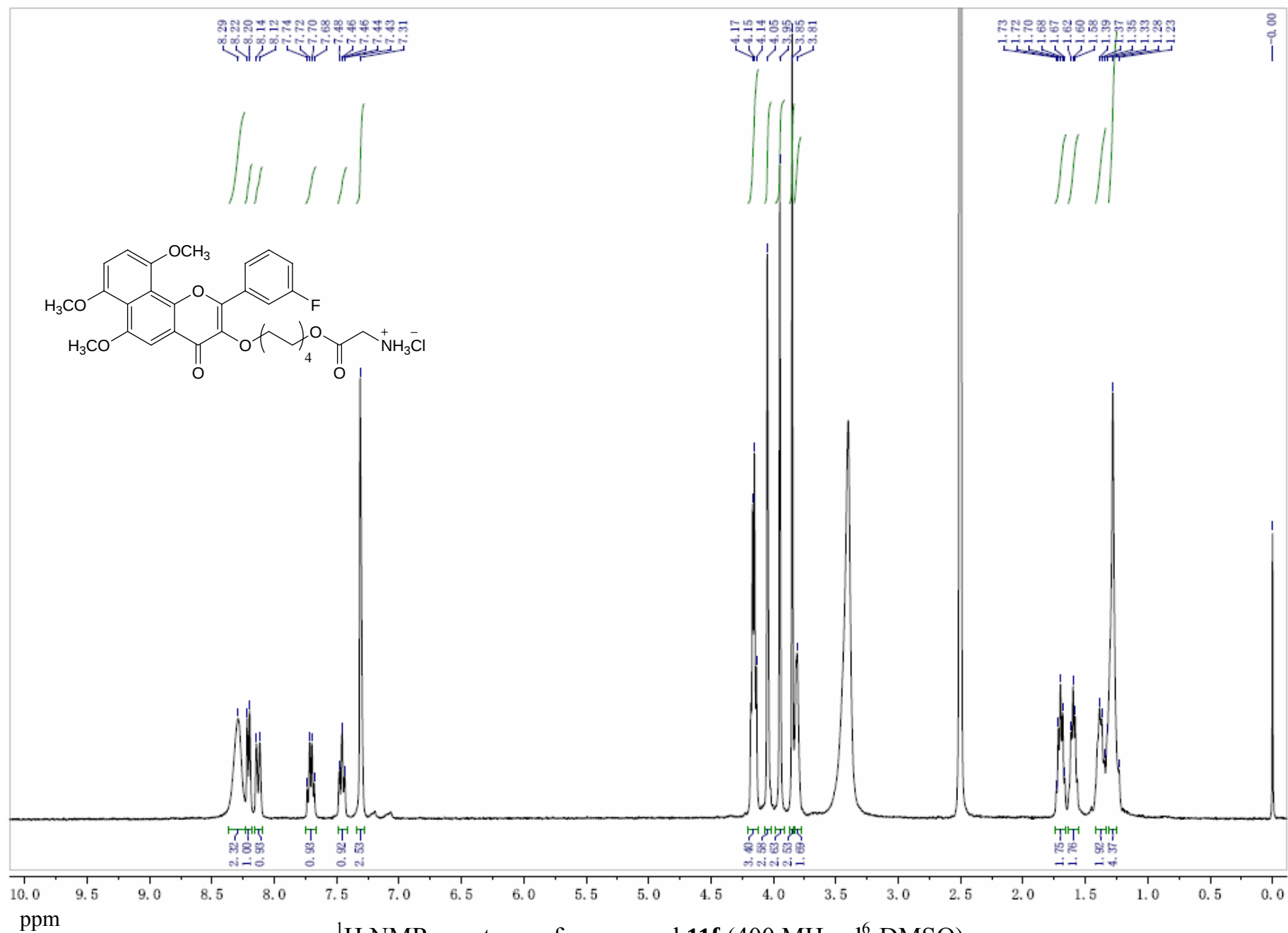
¹³C NMR spectrum of compound **11e** (101 MHz, d⁶-DMSO)

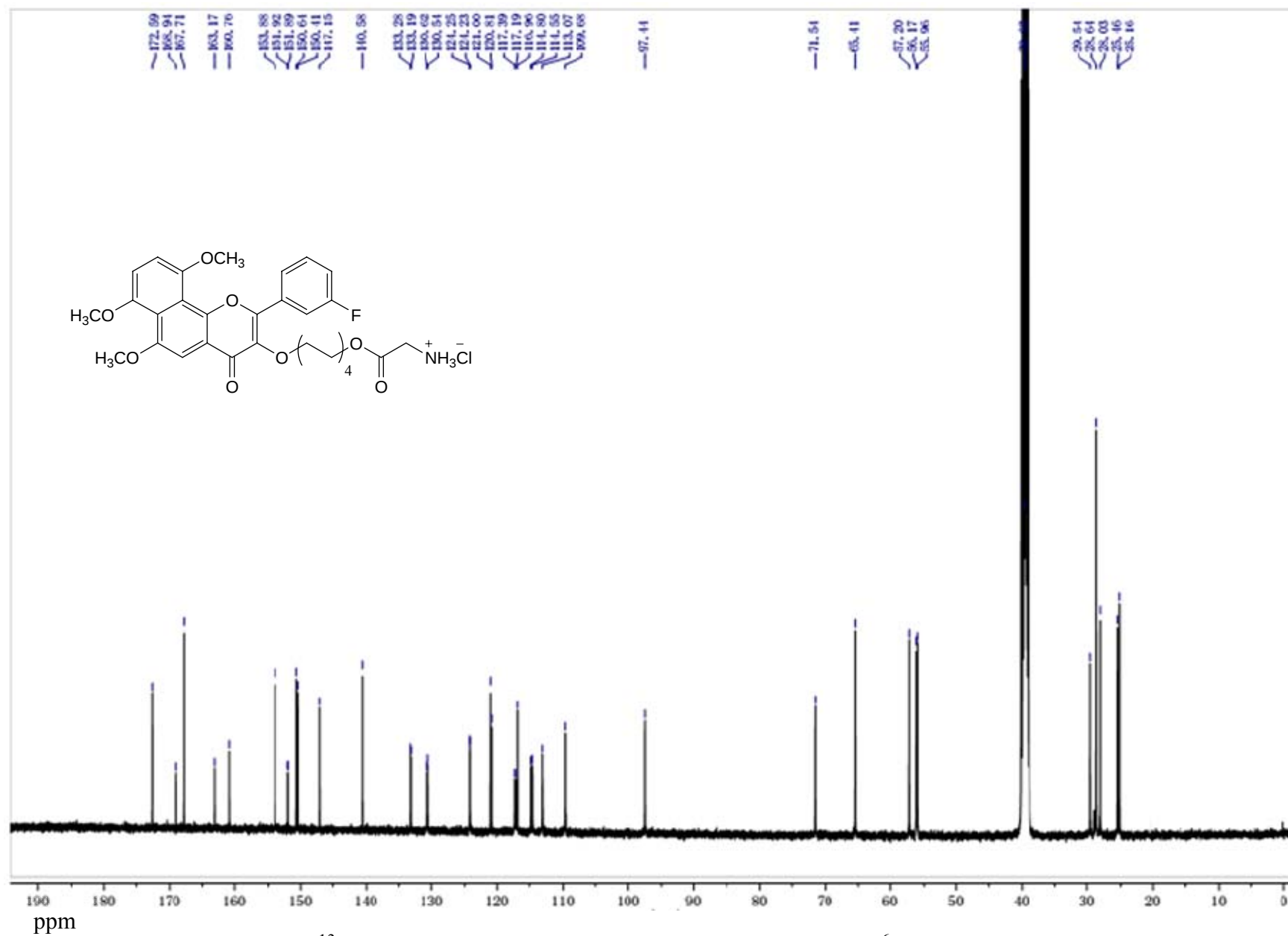
LSS_20140416_08-06 27 (0.501) Cm (23:34-2:20)

1: TOF MS ES+
6.30e4



HRMS spectrum of compound **11e** (Calcd. for $C_{30}H_{33}FNO_8$ 554.2190)





¹³C NMR spectrum of compound **11f** (101 MHz, d⁶-DMSO)

LSS_20140416_08-07 28 (0.519) Cm (23:35-4:18)

1: TOF MS ES+
6.12e4

