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Supporting Information

Isoindole-BODIPY Dyes as Red to Near-Infrared Fluorophores

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Contents:

1. General Methods

Reagents were purchased as reagent-grade and used without further purification unless otherwise stated. Solvents were used as received from commercial suppliers unless noted otherwise. Toluene was distilled from CaH_2. All reactions were performed in oven-dried or flame-dried glassware unless otherwise stated, and were monitored by TLC using 0.25 mm silica gel plates with UV indicator (60F-254). ^{1}H- and ^{13}C-NMR were obtained on a 300 spectrometer at 298 K. Chemical shifts (δ) are given in ppm relative to $CDCl_3$ 7.26 (^{1}H) and 77.16 ppm (^{13}C). Coupling constants J are given in [Hz] and the multiplicities are expressed as follows: s = singlet, d = doublet, t = triplet, m = multiplet. High-resolution mass spectras were obtained by using ESI-TOF with positive mode. The isotope peaks were matched with the calculated pattens; only the most abundant peaks for all the compounds are listed.

UV-visible absorption spectra were recorded on a Hitachi U-3010 Spectrophotometer (190-1100 nm scan range). Fluorescence emission spectra were recorded on a Hitachi F-4600 FL Spectrophotometer. Relative quantum efficiencies of fluorescence of BODIPY derivatives were obtained by comparing the areas under the corrected emission spectrum of the test sample in various solvent with that of methylene blue[1a] or Rhodamin B (0.49 in EtOH)[1b]. Non-degassed, spectroscopic grade solvents and a 10 mm quartz cuvette were used. Dilute solutions ($0.01<A<0.05$) were used to minimize the reabsorption effects. Quantum yields were determined using the following equation[2]:

$$\Phi_X = \Phi_S (I_X/I_S) (A_S/A_X) (\eta_X/\eta_S)^2$$

Where Φ_S stands for the reported quantum yield of the standard, I stands for the integrated emission spectra, A stands for the absorbance at the excitation wavelength and η stands for the refractive index of the solvent being

used (η = 1 when the same solvent was used for both the test sample and the standard). X subscript stands for the test sample, and S subscript stands for the standard.

2. Crystal Data of Compounds

2.1 Methods and crystal data

Crystals of BODIPYs **3ac**, **3ba**, **5** and **6c** suitable for X-ray analysis were obtained by slow evaporation of their dichloromethane solutions. The vial containing this solution was placed, loosely capped, to promote the crystallization.

Crystal data for BODIPYs **3ac**, **3ba**, **5** and **6c** were collected using a Bruker SMART APEXIIdiffractometer with CCD area detector and multi-layer mirror monochromated Mo-Kα radiation (λ = 0.71073 Å) at 293 K.

The structures were solved by the direct method using the SHELXS-974 program and refined by the least-squares method on F^2, SHELXL-97,[3] incorporated in SHELXTL V5.10.[4] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealized positions and were included in structure factors calculations.

CCDC-859405 (**3ac**), 859406 (**3ba**), 859407 (**5**), and 859408 (**6c**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data for **3ac**: $C_{21}H_{20}BF_2N_3$, M_w = 363.21, purple, monoclinic, space group P2(1)/n, a = 11.177(1), b = 7.630(1), c = 21.521(4) Å, α = 90, β = 97.98 (0), γ = 90°, V = 1817.6(5) Å^3, Z = 4, D_{calcd} = 1.327 gcm^{-3}, T = 293(2) K, μ = 0.093 mm^{-1}, *F(000)* = 760, *GooF*(F^2) = 1.007, R_1 = 0.0408, wR^2 = 0.0940 for I>2σ(I), R_1 = 0.0653, wR^2 = 0.1074 for all data, 12536 independent reflections [2θ ≤ 50.0°].

Crystal data for **3ba**: $C_{18}H_{14}BF_2N_3$, M_w = 321.13, purple, monoclinic, space group C2/c, a = 27.768(2), b = 7.7158(6), c = 16.7367(1) Å, α = 90, β = 119.6960 (1), γ = 90°, V = 2993.8(4) Å^3, Z = 8, D_{calcd} = 1.425 gcm^{-3}, T = 293(2) K, μ = 0.103 mm^{-1}, *F(000)* = 1328, *GooF*(F^2) = 1.054, R_1 = 0.0411, wR^2 = 0.0985 for I>2σ(I), R_1 = 0.0647, wR^2 = 0.1107 for all data, 12512 independent reflections [2θ ≤ 55.18°].

Crystal data for **5**: $C_{19}H_{16}BF_2N_3$, M_w = 335.16, purple, monoclinic, space group P2(1)/n, a = 10.1992(1), b = 7.0097(8), c = 22.155(3) Å, α = 90, β = 94.6710 (1), γ = 90°, V = 1578.7(3) Å^3, Z = 4, D_{calcd} = 1.410 gcm^{-3}, T = 293(2) K, μ = 0.101 mm^{-1}, *F(000)* = 696, *GooF*(F^2) = 1.069, R_1 = 0.0704, wR^2 = 0.1998 for I>2σ(I), R_1 = 0.0937, wR^2 = 0.2194 for all data, 12128 independent reflections [2θ ≤ 55.12°].

Crystal data for **6c**: $C_{33}H_{32}BF_2N_3O_3$, M_w = 567.43, purple, triclinic, space group P1, a = 10.248(6), b = 11.011(7), c = 13.670(9) Å, α = 73.817(8), β = 79.085 (9), γ = 86.538(9)°, V = 1454.5(1) Å^3, Z = 2, D_{calcd} = 1.296 gcm^{-3}, T = 293(2) K, μ = 0.091 mm^{-1}, *F(000)* = 596, *GooF*(F^2) = 1.090, R_1 = 0.0867, wR^2 = 0.2169 for I>2σ(I), R_1 = 0.1820, wR^2 = 0.2633 for all data, 12222 independent reflections [2θ ≤ 55.3°].

2.2 The packing of BODIPYs 3ac, 3ba, 5 and 6c

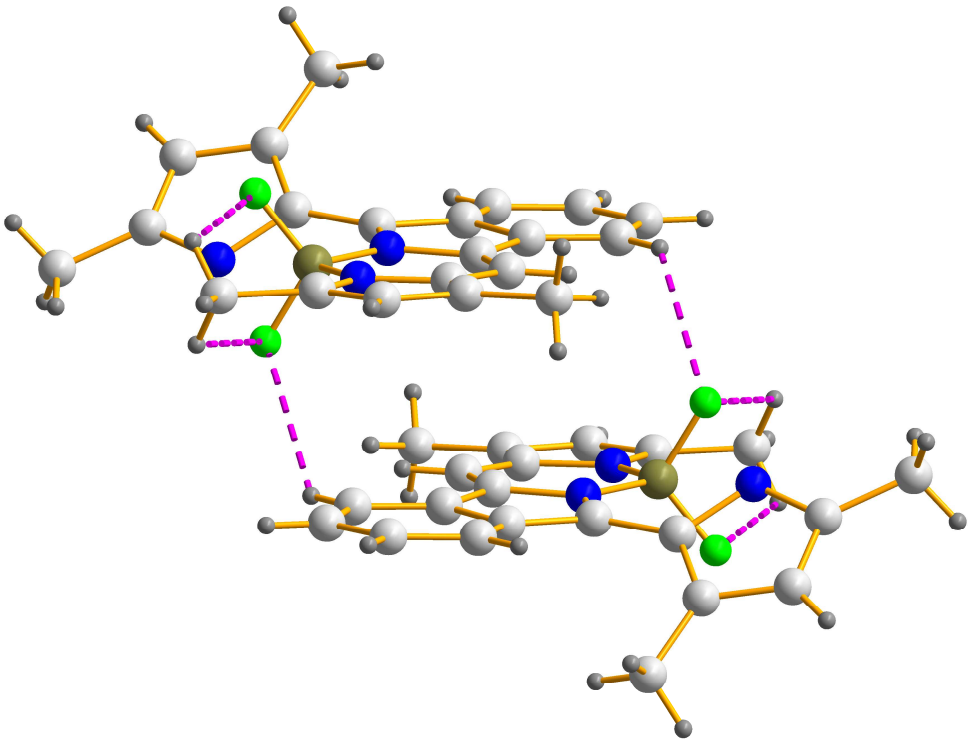
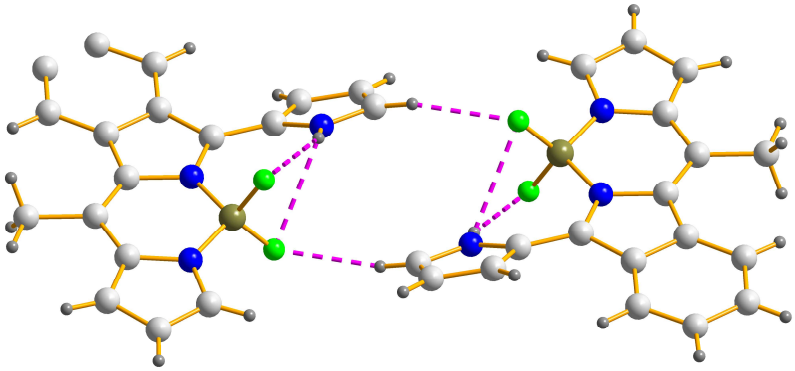


Figure S1. Crystal structure of the dimer of BODIPY **3ac** through intermolecular H-bonding. Dashed line was used to show H-bonding.



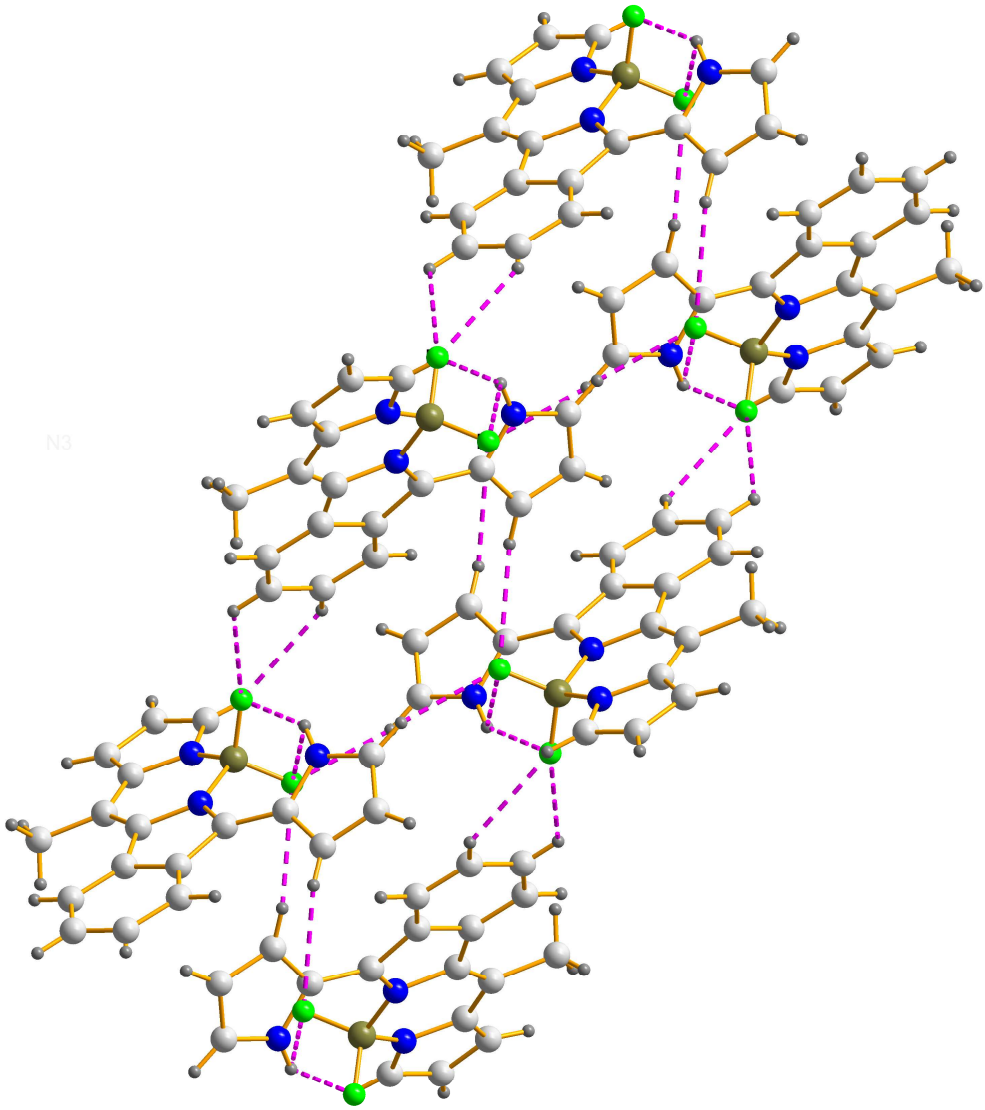


Figure S2. Intermolecular H-bonding of Crystal structure of **3ba** (top) and its crystal packing structure (bottom). Dashed line was used to show intermolecular H-bonding.

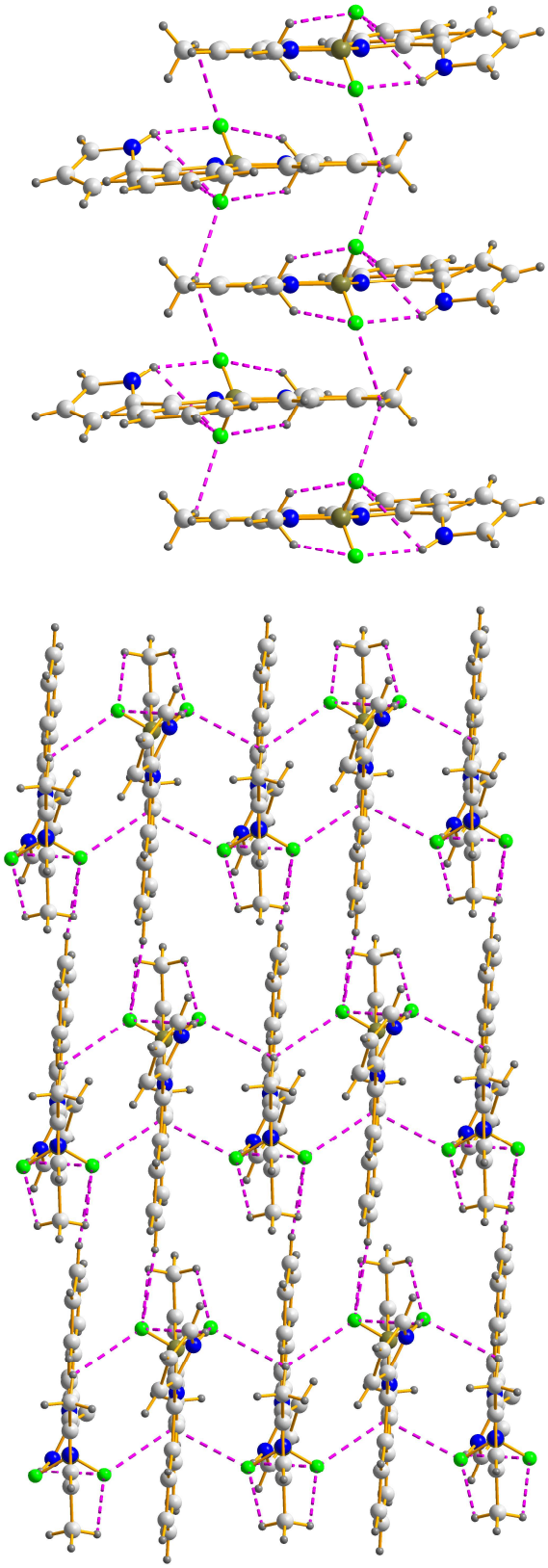


Figure S3. Intermolecular H-bonding of Crystal structure of **5** (top) and its crystal packing structure (bottom). Dashed line was used to show intermolecular H-bonding.

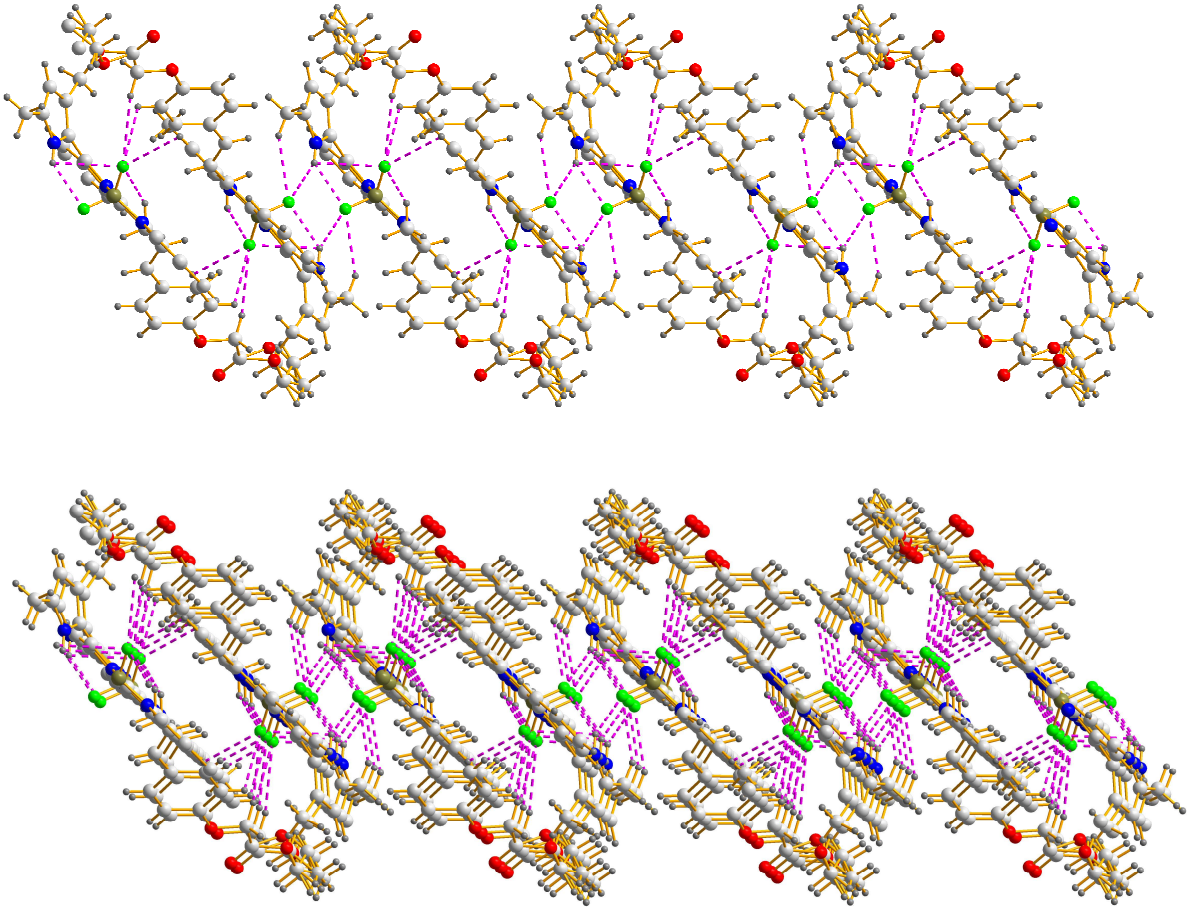


Figure S4. Intermolecular H-bonding of Crystal structure of **6c** (top) and its crystal packing structure (bottom). Dashed line was used to show intermolecular H-bonding.

3. Syntheses and Characterizations of Compounds

Compounds **1** and **2** were synthesized from literature[5] or purchased from commercial sources.

General procedure for the preparation of BODIPYs 3: To the mixture of compound **1** (0.5 mmol) and pyrrole (5 mmol) were added 20 ml CH_2Cl_2 and $POCl_3$ (470 □l, 5 mmol) in 1 ml CH_2Cl_2 almost at the same time and quickly at ice-cold condition under argon. The reaction mixture was stirred at room temperature and was monitored by TLC. When compound **1** had been consumed, to the reaction mixture was added Et_3N (1 ml) under ice-cold condition, and the mixture was stirred for 10 min before addition of $BF_3{\cdot}OEt_2$ (1.2 ml) under ice-cold condition through syringe. The reaction mixture was left stirring for overnight, poured into water and extracted with CH_2Cl_2. Organic layers were combined, and solvent was removed under vacuum. The crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), affording the desired compound as greenish (or bluish, or reddish) powder.

BODIPY 3aa: To compound **1a** (90 mg, 0.5 mmol) in pyrrole (0.69 ml, 10 mmol) were added 20 ml CH_2Cl_2 and $POCl_3$ (470 μl, 5 mmol) in 1 ml CH_2Cl_2 almost at the same time and quickly at ice-cold condition under argon. The reaction mixture was stirred at room temperature (35 ℃) for 16 h. Reaction was monitored by TLC. When compound **1** had been consumed, to the reaction mixture was added Et_3N (1 ml) under ice-cold condition, and

the mixture was stirred for 10 min before addition of $BF_3{\cdot}OEt_2$ (1.2 ml) under ice-cold condition through syringe. The reaction mixture was left stirring for overnight, poured into water and extracted with CH_2Cl_2. Organic layers were combined, and solvent was removed under vacuum. The crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), affording the desired compound **3aa** as reddish powder in 35% yield (54 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.10(s, 1H), 7.95(d, J = 7.2 Hz, 1H), 7.75(d, J = 7.2 Hz, 1H), 7.41-7.31(m, 2H), 7.14(s, 1H), 7.02(s, 1H), 6.90(s, 1H), 6.80(s, 1H), 6.50(s, 1H), 6.32(s, 1H), 6.14(s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 150.2, 136.9, 133.4, 132.7, 131.6, 131.4, 131.3, 127.7, 127.5, 125.1, 122.2, 120.6, 120.0, 119.7, 115.8, 114.5, 112.5. HRMS (EI) Calcd. for $C_{17}H_{12}N_3BF_2$ $[M]^+$: 307.1092, found 307.1087.

BODIPY 3ab: To compound **1a** (90 mg, 0.5 mmol) in 2-methylpyrrole (0.42 ml, 5 mmol) were added 20 ml CH_2Cl_2 and $POCl_3$ (470 μl, 5 mmol) in 1 ml CH_2Cl_2 almost at the same time and quickly at ice-cold condition under argon. The reaction mixture was stirred at room temperature (35 ℃) for 2 h. Reaction was monitored by TLC. When compound **1** had been consumed, to the reaction mixture was added Et_3N (1 ml) under ice-cold condition, and the mixture was stirred for 10 min before addition of $BF_3{\cdot}OEt_2$ (1.2 ml) under ice-cold condition through syringe. The reaction mixture was left stirring for overnight, poured into water and extracted with CH_2Cl_2. Organic layers were combined, and solvent was removed under vacuum. The crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), affording the desired compound **3ab** as bluish powder in 41% yield (69 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.59(s, 1H), 8.12(d, J = 7.8 Hz, 1H), 7.78(d, J = 7.5 Hz, 1H), 7.54(t, J = 7.5 Hz, 1H), 7.40(t, J = 7.8, 1H), 7.19(s, 1H), 6.64 (s, 1H), 6.24(s, 1H), 6.13(s, 1H), 2.59 (s, 3H), 2.50(s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 146.8, 138.5, 136.6, 132.1, 131.7, 131.4, 130.6, 127.0, 125.0, 121.5, 121.2, 120.6, 119.5, 114.8, 114.4, 111.6, 14.5, 14.0. HRMS(EI) calcd. for $C_{19}H_{17}N_3BF_2$ $[M+H]^+$: 336.1478, found 336.1473.

BODIPY 3ac: Prepared using the procedure above by reacting compound **1a**[3] (90 mg, 0.5 mmol) with 2, 4-dimethylpyrrole (0.5 ml, 5 mmol) under $POCl_3$ (470 μl, 5 mmol) using the same procedure described above (35 ℃) for 2 h, and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), the desired compound **3ac** was obtained as bluish powder in 43% yield (78 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.70(s, 1H), 7.82-7.77(m, 2H), 7.49(d, J = 7.2 Hz, 1H), 7.34-7.26(m, 2H), 6.03-5.98 (m, 2H), 2.50 (s, 3H), 2.40(s, 3H), 2.30(s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.4, 147.8, 136.2, 134.7, 134.6, 131.2, 131.0, 130.5, 130.1, 127.2, 125.8, 125.7, 119.1, 118.5, 116.7, 113.6, 112.3, 14.5, 13.7, 11.4. HRMS (EI) Calcd. for $C_{21}H_{20}N_3BF_2$ $[M]^+$: 363.1718, found 363.1714.

BODIPY 3ad: Prepared using the procedure above by reacting compound **1a**[3] (90 mg, 0.5 mmol) with 2, 4-dimethyl-3-ethylpyrrole (0.65 ml, 5 mmol) under $POCl_3$ (470 μl, 5 mmol) using the same procedure described above (35 ℃) for 2 h, and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 4/1, v/v), the desired compound **3ad** was obtained as greenish powder in 38% yield (79 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.64(s, 1H), 7.81-7.74(m, 2H), 7.46(d, J = 7.2 Hz, 1H), 7.31-7.22(m, 2H), 2.52-2.35(m, 10H), 2.45-2.22(m, 6H), 1.16(d, J = 7.5 Hz, 3H), 1.09(d, J= 7.5 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.5, 146.9, 136.0, 132.0, 131.0, 130.3,

130.1, 129.7, 129.6, 125.9, 125.2, 125.2, 124.9, 119.0, 117.8, 112.9, 17.9, 17.5, 15.3, 15.0, 13.0, 12.0, 9.6. HRMS (EI) Calcd. for $C_{25}H_{28}N_3BF_2$ $[M]^+$: 419.2344, found 419.2347.

BODIPY 3ae: Prepared using the procedure above by reacting compound **1a**[3] (165 mg, 0.92 mmol) with 3-methylindole (1.2 g, 9.2 mmol) under $POCl_3$ (0.86 ml, 9.2 mmol) using the same procedure described above (35 ℃) for 8.5 h, and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), the desired compound **3ad** was obtained as brown powder in 22% yield (95 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.06(s, 1H), 8.00(d, J = 4.2 Hz, 1H), 7.89(d, J = 7.2 Hz, 1H), 7.72-7.66(m, 4H), 7.54-7.53(m, 2H), 7.42-7.37(t, J = 6.6 Hz, 1H), 7.29-7.21(m, 3H), 7.06(s, 1H), 2.61-2.59(m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.8, 132.0, 131.4, 131.4, 127.7, 127.5, 127.4, 127.2, 127.0, 126.7, 126.1, 125.6, 125.1, 122.9, 122.5, 120.7, 120.5, 120.1, 120.0, 119.5, 115.8, 114.1, 113.1, 111.9, 109.7, 12.0, 9.3. HRMS (EI) Calcd. for $C_{27}H_{21}N_3BF_2$ $[M]^+$: 436.1791, found 436.1782.

BODIPY 3ba: Prepared using the procedure above by reacting compound **1b** (97 mg, 0.5 mmol) with pyrrole (0.69 ml, 10 mmol) under $POCl_3$ (470 μl, 5 mmol) using the same procedure described above for 16h, the crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), affording the desired compound **3ba** as reddish powder in 42% yield (67 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.79(s, 1H), 8.19(d, J = 7.8 Hz, 1H), 8.00(d, J = 7.2, 1H), 7.59(t, J = 7.5 Hz, 1H), 7.48-1.30(m, 4H), 6.90(s, 1H), 6.51-6.43(m, 2H), 2.76(s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.1, 136.4, 133.6, 132.4, 132.4, 132.0, 131.3, 130.8, 126.7, 126.2, 125.7, 122.9, 121.6, 119.7, 118.3, 114.1, 111.9, 16.5. HRMS (EI) Calcd. for $C_{18}H_{14}N_3BF_2$[M]$^+$: 321.1249, found 321.1242.

BODIPY 3bc: Prepared using the procedure above by reacting compound **1b** (97 mg, 0.5 mmol) with 2, 4-dimethylpyrrole (0.5 ml, 5 mmol) under $POCl_3$ (470 μl, 5 mmol) using the same procedure described above (35 ℃) for 2 h, the crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), affording the desired compound **3bc** as blue powder in 43% yield (81 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.52(s, 1H), 8.00(d, J = 8.1 Hz, 1H), 7.78(d, J = 8.1 Hz, 1H), 7.49(t, J = 7.5 Hz, 1H), 7.30(t, J = 7.5 Hz, 1H), 6.01-5.98(m, 2H), 2.85(s, 3H), 2.53(s, 3H), 2.48-2.38(m, 9H), 2.23(s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.7, 135.5, 134.9, 133.3, 131.0, 130.1, 126.7, 126.2, 125.7, 124.8, 122.4, 119.4, 117.8, 112.6, 111.9, 16.9, 16.7, 14.3, 14.1, 13.6. HRMS (EI) Calcd. for $C_{22}H_{22}N_3BF_2$ $[M]^+$: 377.1875, found 377.1882.

BODIPY 3bd: Prepared using the procedure above by reacting compound **1b** (97 mg, 0.5 mmol) with 2, 4-dimethy-3-ethyllpyrrole (0.65 ml, 5 mmol) under $POCl_3$ (470 μl, 5 mmol) using the same procedure described above (35 ℃) for 2 h, and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), the desired compound **3bd** was obtained as greenish powder in 40% yield (87 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.46(s, 1H), 8.00(d, J = 8.4 Hz, 1H), 7.76(d, J = 8.1 Hz, 1H), 7.46(t, J = 7.8 Hz, 1H), 7.29(d, J = 7.8 Hz, 1H), 2.88(s, 3H), 2.50-2.34(m, 13H), 2.18(s, 3H), 1.16(t, J = 7.5 Hz, 3H), 1.06(t, J = 7.5 Hz, 3H). ^{13}C NMR (75 MHz,

$CDCl_3$): δ 146.0, 145.3, 135.3, 133.9, 132.3, 131.4, 129.7, 129.6, 128.7, 126.3, 124.3, 123.6, 122.3, 117.0, 17.9, 17.2, 16.9, 15.2, 13.9, 12.5, 12.1, 11.8. HRMS (EI) Calcd. for $C_{26}H_{30}N_3BF_2$ $[M]^+$: 433.2501, found 433.2506.

Dipyrromethene 4: To compound **1a** (179 mg, 1 mmol) in 20 ml CH_2Cl_2 were added 2,4-dimethylpyrrole (103 μl, 1 mmol) in 1 ml CH_2Cl_2, and $POCl_3$ (94 μl, 1 mmol) in 1 ml CH_2Cl_2 at ice-cold condition under argon. The reaction mixture was stirred in ice-cold condition for 30 min. The starting material disappeared according to TLC. After that, the mixture was quenched by Et_3N (1.2 ml), poured into water and extracted with CH_2Cl_2. Organic layers were combined, dried and was removed under vacuum. The crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), affording the desired compound **4** as reddish powder in 90% yield (230 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.81(s, 1H), 7.76(d, J = 7.5 Hz, 1H), 7.62(d, J = 7.5 Hz, 1H), 7.44(t, J = 7.2 Hz, 1H), 7.34(t, J = 7.2 Hz, 1H), 7.10(s, 1H), 5.88(s, 1H), 2.38(s, 3H), 2.28(s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.8, 140.3, 138.4, 137.6, 133.0, 130.8, 128.4, 127.1, 125.8, 120.5, 118.7, 114.8, 111.6, 13.8, 11.4. HRMS (EI) calcd for $C_{15}H_{13}N_2Cl$ $[M]^+$: 256.0767, found 256.0774.

BODIPY 5: To compound **4** (128 mg, 0.5 mmol) in 20 ml CH_2Cl_2 were added pyrrole (0.69 ml, 10mmol), and $POCl_3$ (470 μl, 5 mmol) in 1 ml CH_2Cl_2 at ice-cold condition under argon. The reaction mixture was stirred at room temperature for 12 h. To the reaction mixture was added Et_3N (1 ml), and the mixture was stirred for 10 min before addition of $BF_3{\cdot}OEt_2$ (1.2 ml) through syringe. The reaction mixture was left stirring for overnight, poured into water and extracted with CH_2Cl_2. Organic layers were combined, and solvent was removed under vacuum. The crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), affording the desired compound **5** as greenish powder in 48% yield (80 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.73(s, 1H), 8.12(d, J = 8.1 Hz, 1H), 7.81(d, J = 7.8 Hz, 1H), 7.51(t, 7.5 Hz, 1H), 7.40-7.33(m, 2H), 6.49(s, 1H), 5.99(s, 1H), 2.54(s, 3H), 2.27(s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.1, 146.4, 136.2, 134.6, 131.0, 130.8, 130.4, 130.2, 126.6, 125.5, 124.8, 122.7, 119.3, 118.3, 116.8, 113.6, 111.7, 14.5, 11.3. HRMS (EI) Calcd. for $C_{19}H_{16}N_3BF_2$ $[M]^+$: 335.1405, found 335.1408.

Monostyryl-BODIPY 6a: To compound **3ac** (40 mg, 0.11 mmol) and ethyl-2-(4-formyphenoxy)acetate (46mg, 0.22 mmol) in 20 ml toluene were added piperidine (1 ml) through syringe, and a crystal of p-TsOH. The solution was refluxed over its boiling point up to 140□ for 14 h in a round-bottomed flask and any water formed during the reaction was removed by using a Soxhlet extractor containing anhydrous $CaCl_2$. Reaction was monitored by TLC. When **3ac** had been consumed, the resulting mixture was cooled to room temperature, poured into water and extracted with CH_2Cl_2. Organic layers were combined, and solvent was removed under vacuum. The crude product was purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v) and then recrystallized from CH_3OH, affording the desired compound **6a** (52 mg) in 87% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.71(s, 1H), 7.85-7.77(m, 2H), 7.50-7.47(m, 3H), 7.41(s, 1H), 7.33(t, J = 7.5 Hz, 1H), 7.11(d, J = 12.9 Hz, 1H), 6.91-6.89(m, 2H), 6.62(s, 1H), 6.07(s, 1H), 4.65(s, 2H), 4.29(q, J = 6.9 Hz, 2H), 2.45(s, 3H), 2.32(s, 6H), 1.31(t, J = 6.9 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.9, 158.1, 148.6, 147.5, 135.8, 134.9, 134.8, 132.9, 132.0, 131.1, 130.0, 128.5, 127.3, 125.8, 119.3, 118.7, 118.3, 115.1, 113.9, 112.9, 112.2, 65.7, 61.6, 14.5, 14.3, 13.8, 11.4. UPLC MS (EI) Calcd. for $C_{32}H_{31}N_3O_3BF_2$ $[M + H]^+$: 554.2421, found 554.2419.

Monostyryl-BODIPY 6b : Prepared using the procedure above from compound **3ad** (40 mg, 92 μmol), ethyl-2-(4-formyphenoxy)acetate (38 mg, 184 μmol), piperidine (1 ml), and a crystal of p-TsOH in toluene (20 ml), and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), the desired compound **6b** was recrystallized from CH_3OH and obtained as greenish power(17 mg) in 30% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.56(s, 1H), 8.03(d, J = 8.4, 1H), 7.79 (d, J = 8.1Hz, 1H), 7.55-7.47(m, 4H), 7.32(t, J = 7.5 Hz, 1H), 7.03-6.89(m, 2H), 4.65(s, 2H), 4.29(q, J = 7.2 Hz, 2H), 2.91(s, 3H), 2.70(q, J = 7.5 Hz, 2H), 2.50(q, J = 7.5 Hz, 2H), 2.43(s, 3H), 2.35(s, 3H), 2.20(s, 3H), 1.33-1.15(m, 9H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.0, 157.8, 143.5, 135.5, 132.2, 132.0, 131.7, 131.6, 130.7, 130.3, 130.1, 128.3, 126.7, 124.9, 124.5, 122.8, 119.1, 117.2, 115.0, 65.7, 61.6, 18.5, 18.1, 17.3, 15.4, 14.9, 14.3, 13.7, 12.8, 12.1. UPLC MS (EI) Calcd. for $C_{37}H_{41}N_3O_3BF_2$ [M + H]$^+$: 624.3204, found 624.3200.

Monostyryl-BODIPY 6c: Prepared using the procedure above from compound **3ac** (40 mg, 106 μmol), ethyl-2-(4-formyphenoxy)acetate (44 mg, 212μmol), piperidine (1 ml), and a crystal of p-TsOH in toluene (20 ml), and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), the desired compound **6c** was recrystallized from CH_3OH and obtained as reddish power (20 mg) in 33% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.60(s, 1H), 7.96(d, J = 8.1 Hz, 1H), 7.76(d, J = 7.8 Hz, 1H), 7.55-7.52(m, 2H), 7.35-7.18(m, 4H), 7.01-6.98(m, 2H), 6.88(d, J = 16.5 Hz, 1H), 6.03-5.98(m, 2H), 4.69(s, 2H), 4.31(q, J = 7.2 Hz, 2H), 2.50(s, 3H), 2.40(s, 3H), 2.28-2.26(m, 6H), 1.33(t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.9, 158.6, 148.2, 147.1, 137.6, 135.8, 134.3, 133.8, 131.8, 129.9, 129.4, 128.4, 126.3, 125.9, 125.1, 122.8, 120.7, 118.9, 118.2, 115.4, 112.2, 65.5, 61.7, 16.6, 14.4, 14.3, 13.7. UPLC MS (EI) Calcd. for $C_{33}H_{33}N_3O_3BF_2$ [M + H]$^+$: 568.2578, found 568.2573.

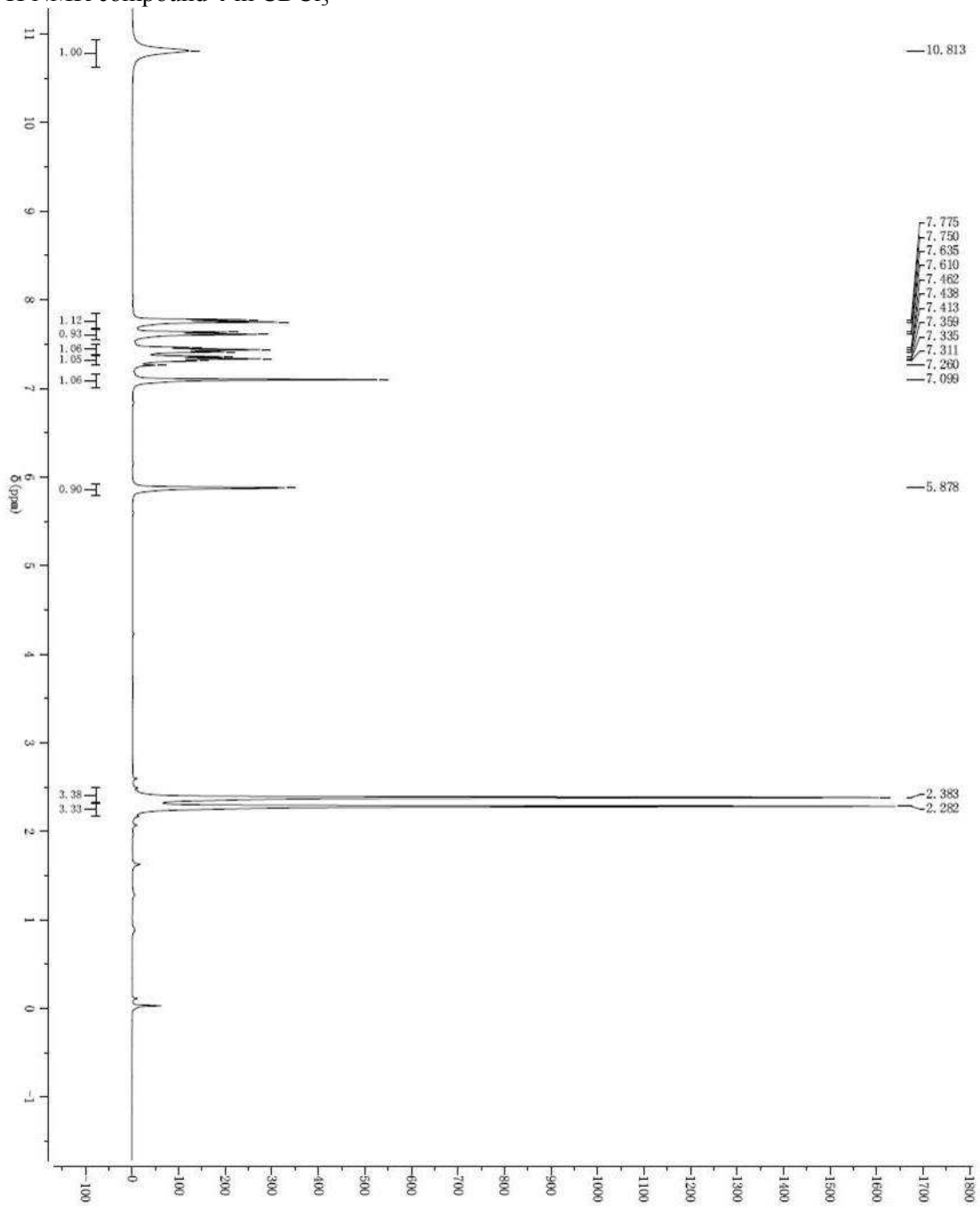
Distyryl-BODIPY 6d: Prepared using the procedure above from compound **3bc** (40 mg, 106 μmol), ethyl-2-(4-formyphenoxy)acetate (88 mg, 424 μmol), piperidine (1 ml), and a crystal of p-TsOH in toluene (20 ml), and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 1/1, v/v), the desired compound **6d** was recrystallized from CH_3OH and obtained as greenish (33 mg) in 41% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.60(s, 1H), 7.98(d, J = 7.8 Hz, 1H), 7.76(d, J = 7.5 Hz, 1H), 7.55-7.47(m, 5H), 7.35-7.19(m, 4H), 7.12-6.98(m, 3H), 6.91-6.86(m, 2H), 6.61(s, 1H), 6.07(s, 1H), 4.69(s, 2H), 4.64(s, 2H), 4.35-4.25(m, 4H), 2.45(s, 3H), 2.32(s, 3H), 2.27(s, 3H), 1.36-1.26(m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.9, 168.8, 158.7, 158.0, 147.5, 146.7, 137.7, 136.1, 135.9, 134.0, 133.0, 131.9, 131.8, 131.4, 131.2, 130.1, 129.9, 128.7, 128.5, 128.4, 126.3, 125.9, 125.2, 123.0, 120.7, 118.3, 116.0, 115.4, 115.0, 112.4, 110.1, 65.7, 65.5, 61.7, 61.6, 16.9, 14.3, 14.2, 13.8. UPLC MS (EI) Calcd. for $C_{44}H_{43}N_3O_6BF_2$ [M + H]$^+$: 758.3208, found 758.3212.

Monostyryl-BODIPY 6e: Prepared using the procedure above from compound **3ba** (40 mg, 0.12 mmol), ethyl-2-(4-formyphenoxy)acetate (50 mg, 0.24 mmol), piperidine (1 ml), and a crystal of p-TsOH in toluene (20 ml), and purified from chromatograph (silica gel, petroleum/CH_2Cl_2 = 2/1, v/v), the desired compound **6e** was recrystallized from CH_3OH and obtained as reddish power (46 mg) in 75% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.85(s, 1H), 8.20(d, J = 7.8 Hz, 1H), 7.95(d, J = 7.8 Hz, 1H), 7.60-7.22(m, 9H), 7.02-6.99(m, 2H), 6.89(s, 1H), 6.53(s, 1H), 6.43(s, 1H), 4.70(s, 2H), 4.31(q, J = 6.9 Hz, 2H), 1.34(d, J = 6.9 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.9, 138.8, 136.4, 132.8, 132.7, 132.1, 130.1, 128.8, 127.2, 127.0, 126.5, 125.7, 123.5, 122.1, 120.4,

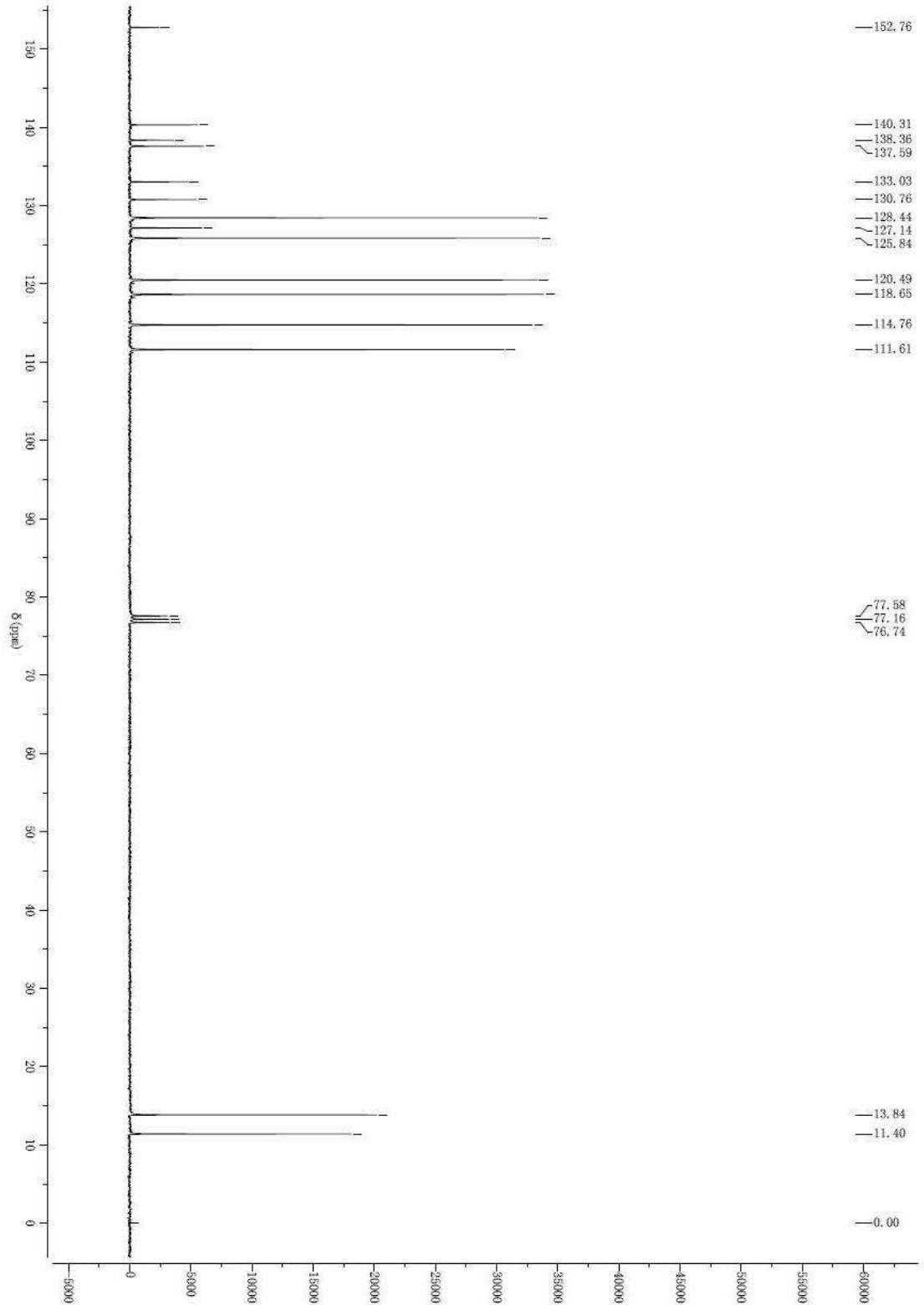
120.1, 119.8, 115.4, 114.2, 112.1, 65.5, 61.7, 14.3. UPLC MS (EI) Calcd. for $C_{29}H_{25}N_3O_3BF_2$ $[M + H]^+$: 512.1952, found 512.1954.

3. Copies of ^{1}H NMR and ^{13}C NMR spectra for all new compounds

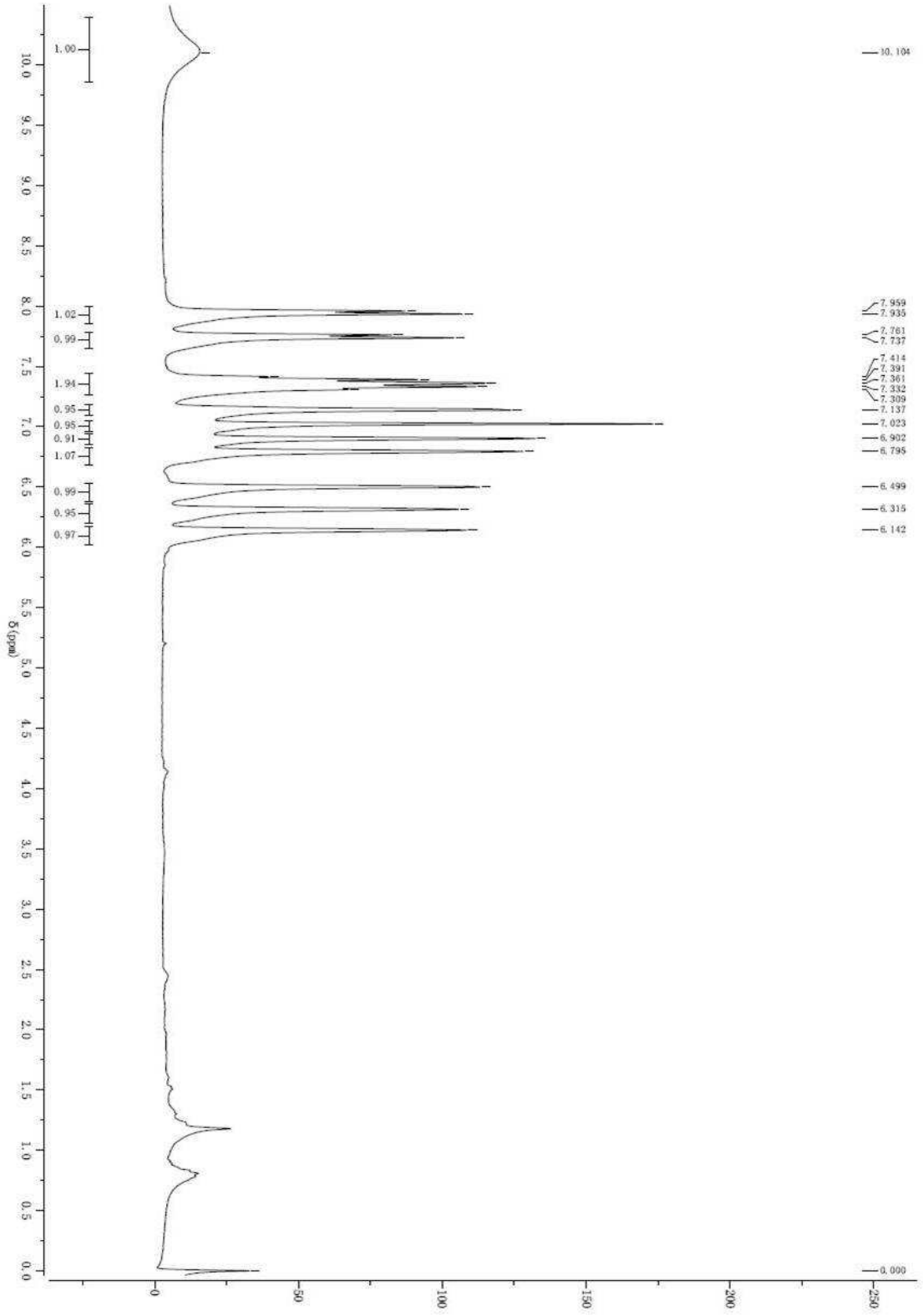
^{1}H NMR compound **4** in $CDCl_3$



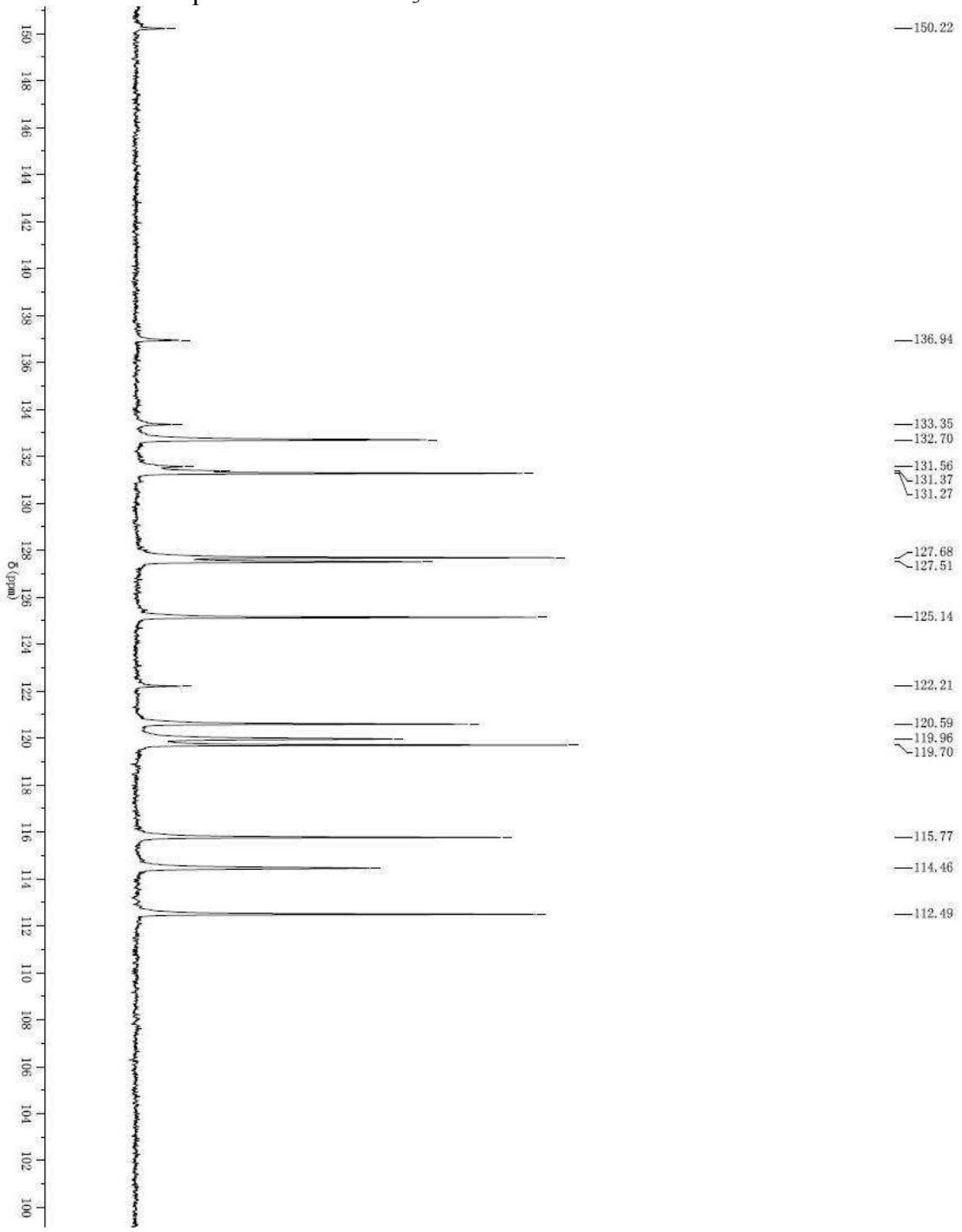
^{13}C NMR of compound **4** in $CDCl_3$

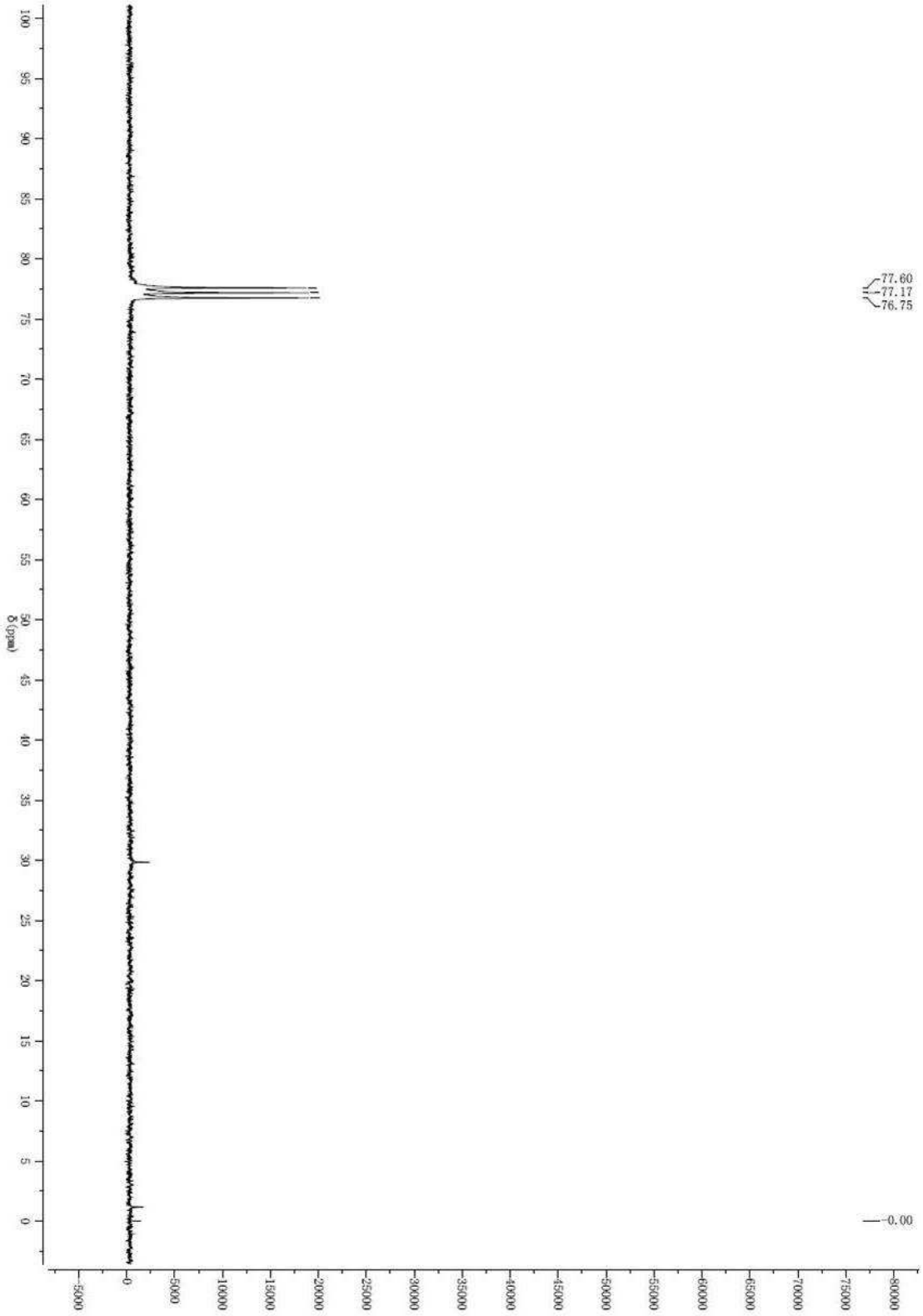


^{1}H NMR compound **3aa** in $CDCl_3$

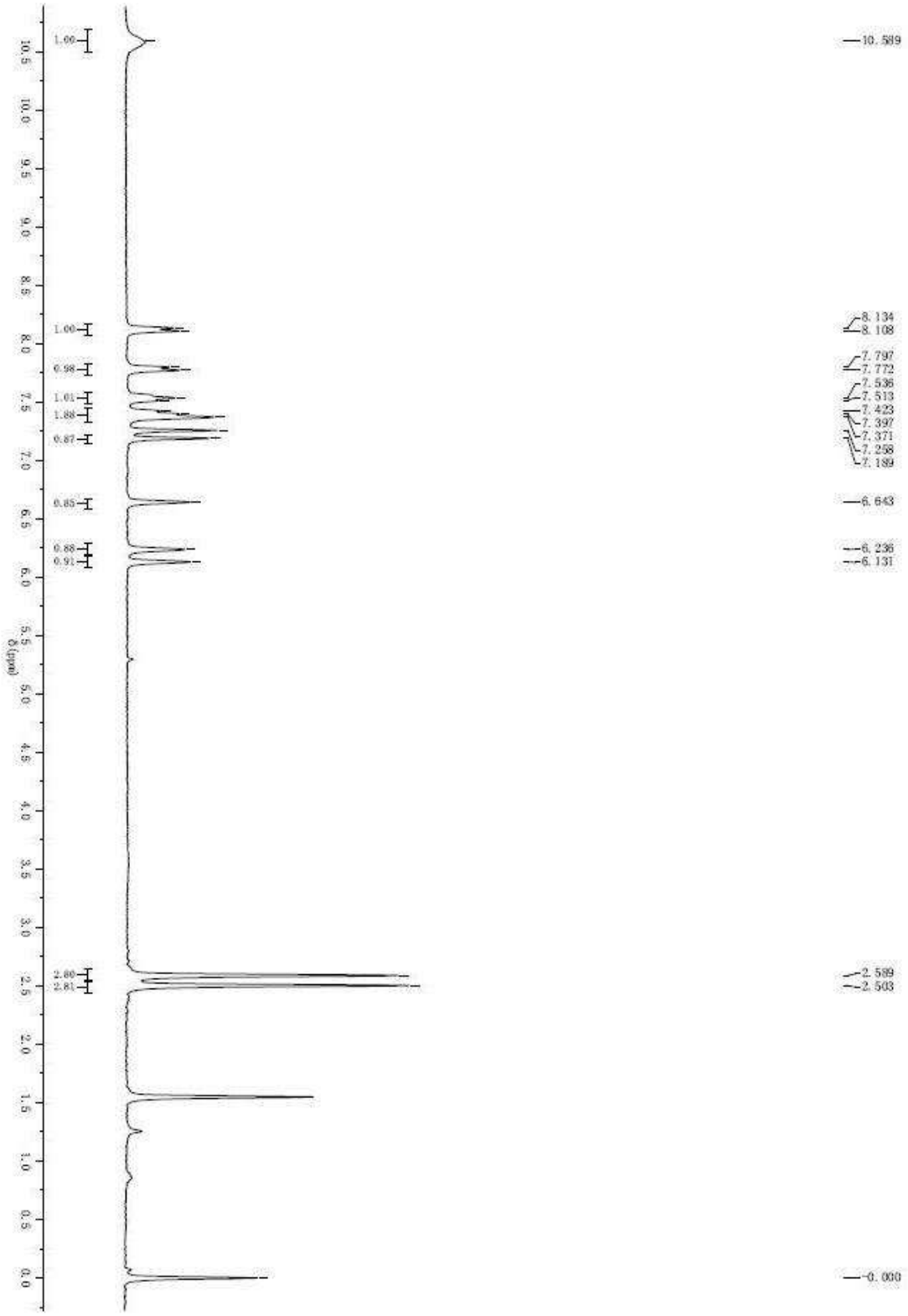


^{13}C NMR of compound **3aa** in $CDCl_3$

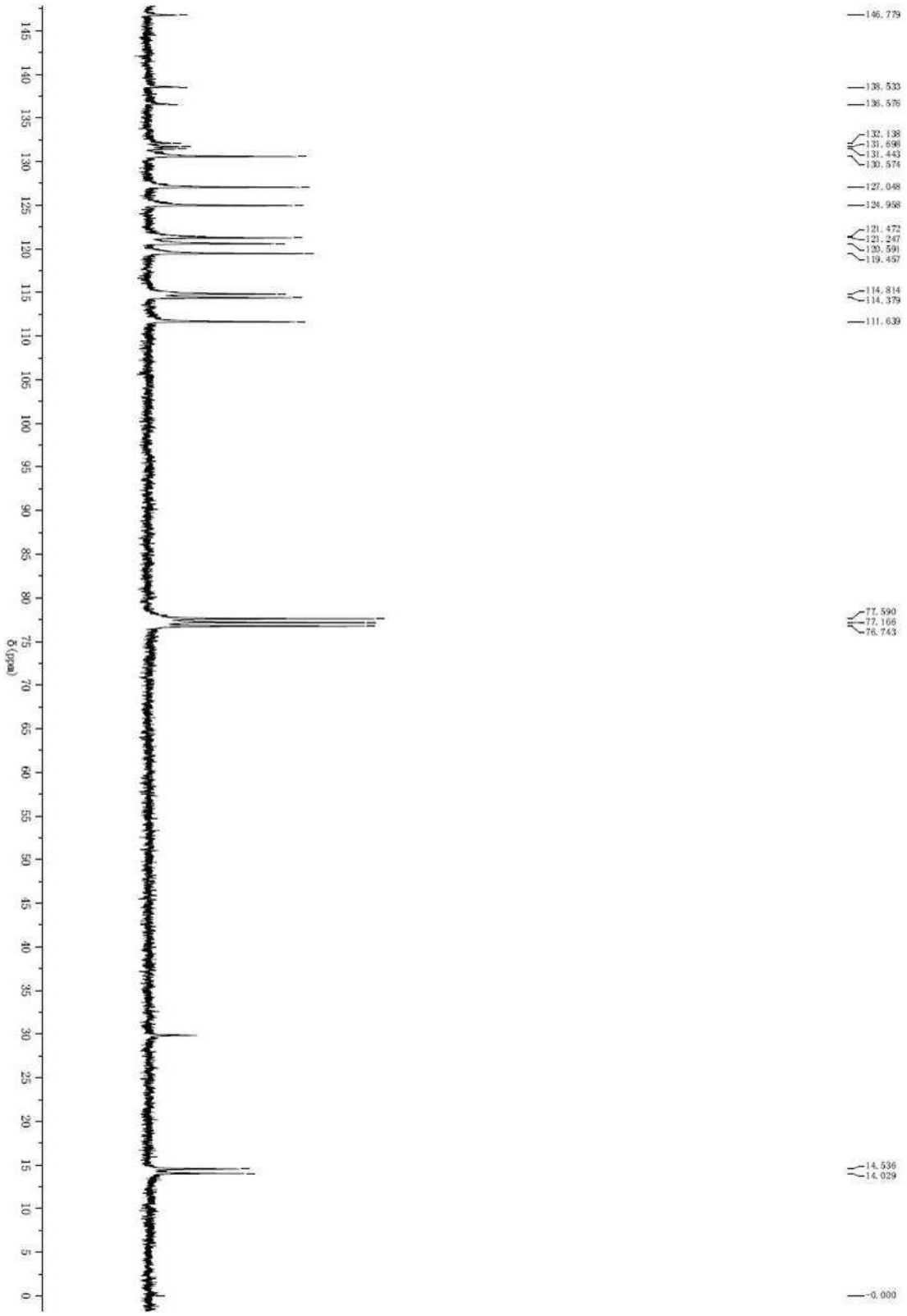



77.60
77.17
76.75
0.00
δ (ppm)

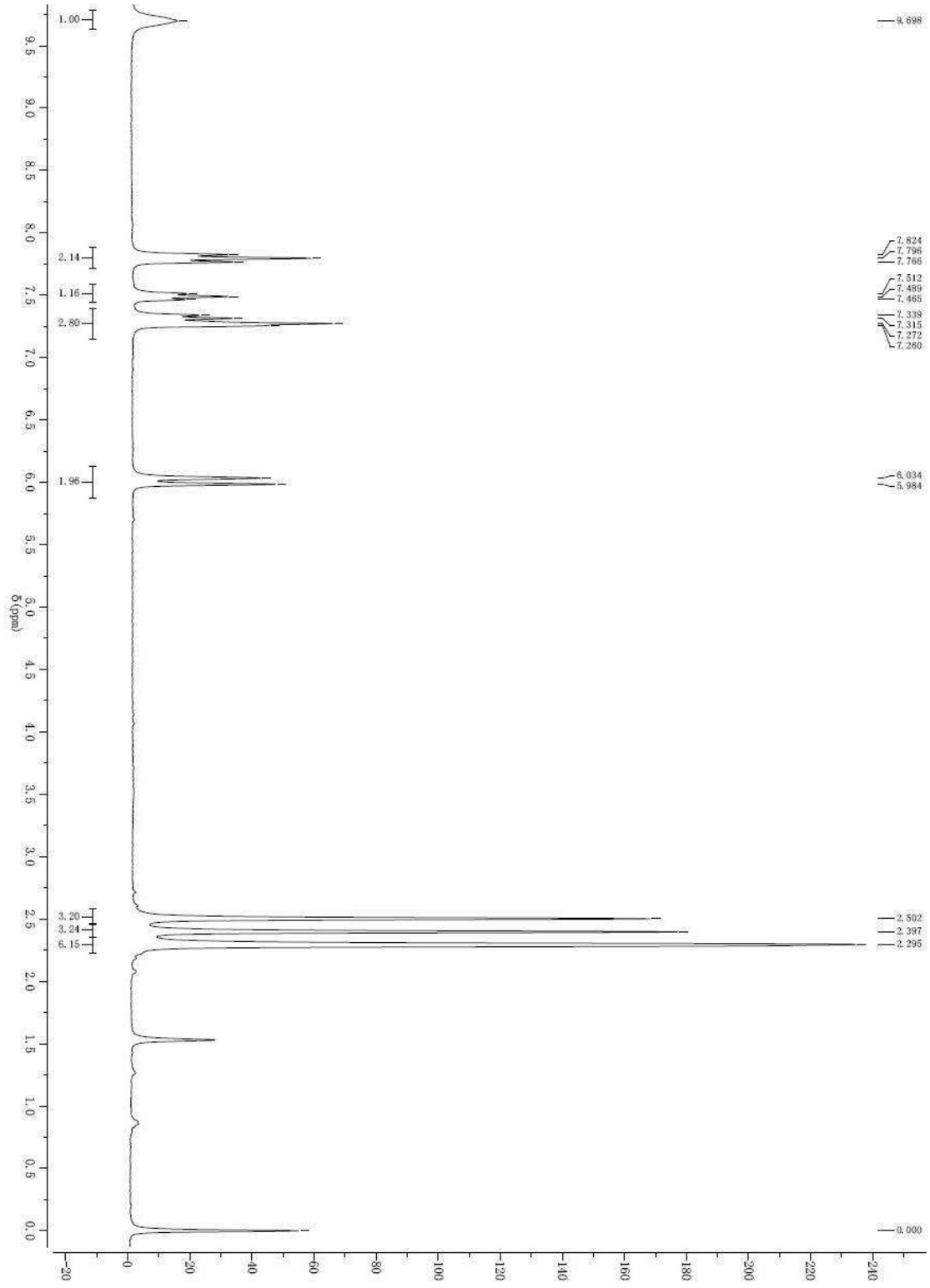
^{1}H NMR compound **3ab** in $CDCl_3$



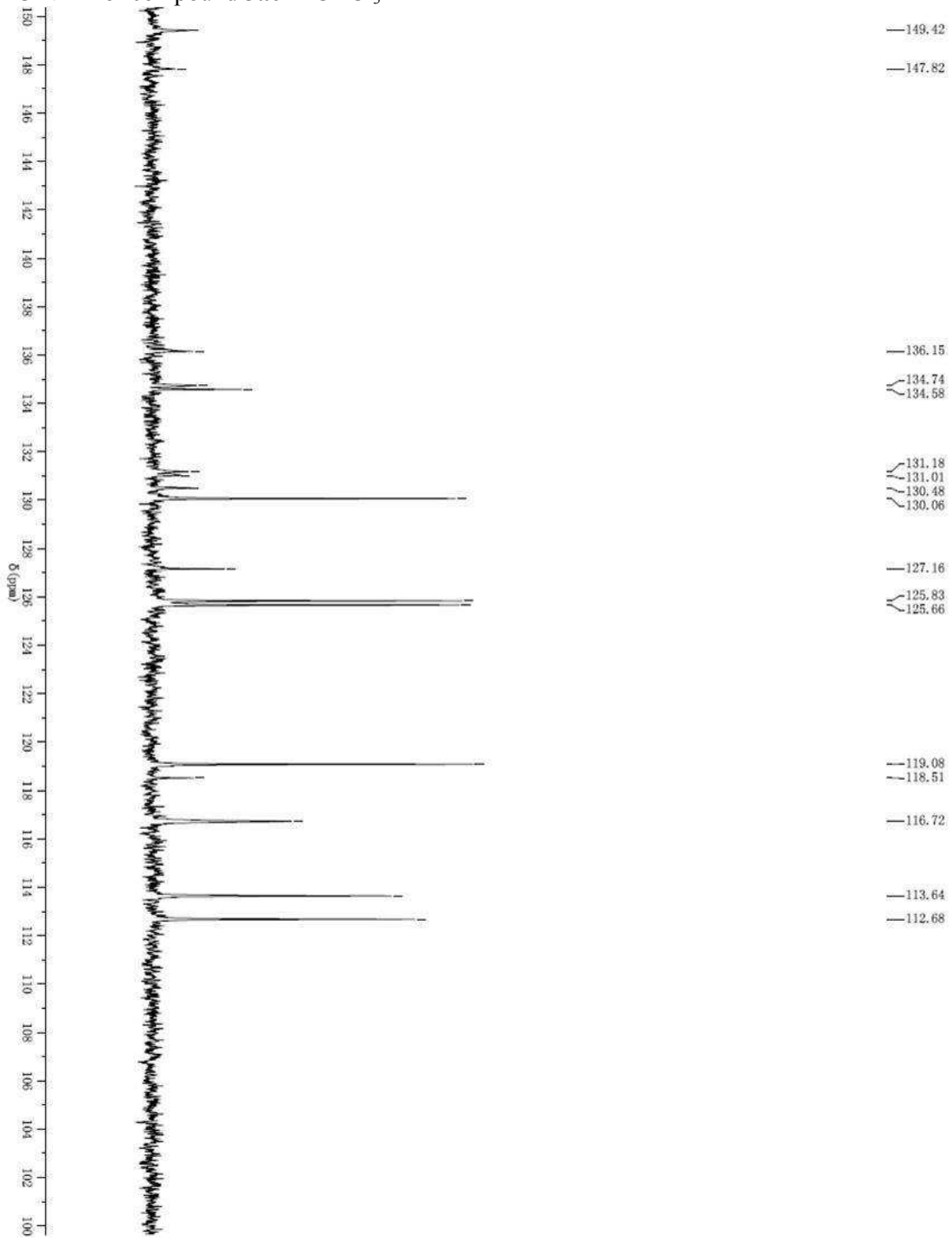
^{13}C NMR of compound **3ab** in $CDCl_3$

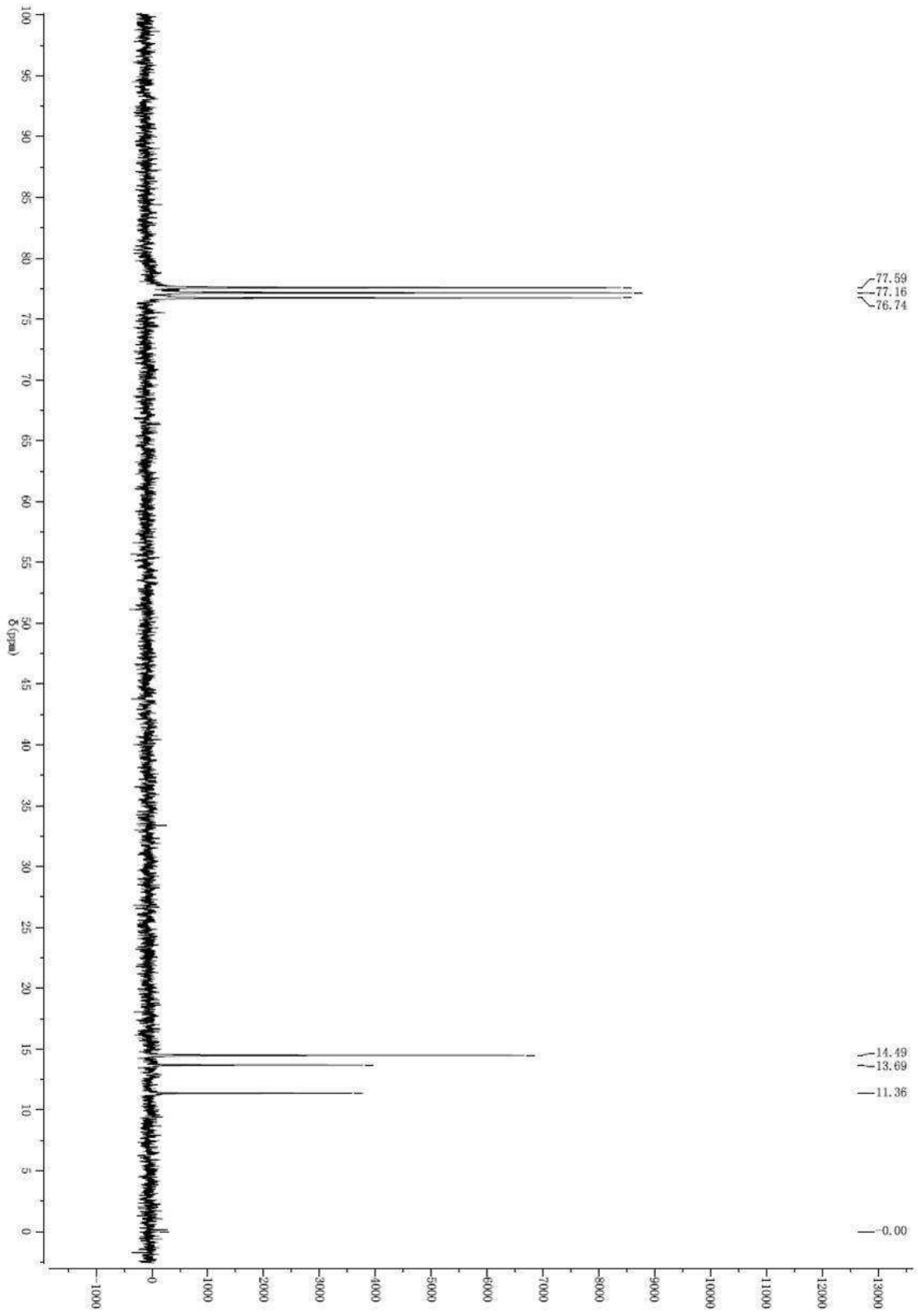


^{1}H NMR compound **3ac** in $CDCl_3$

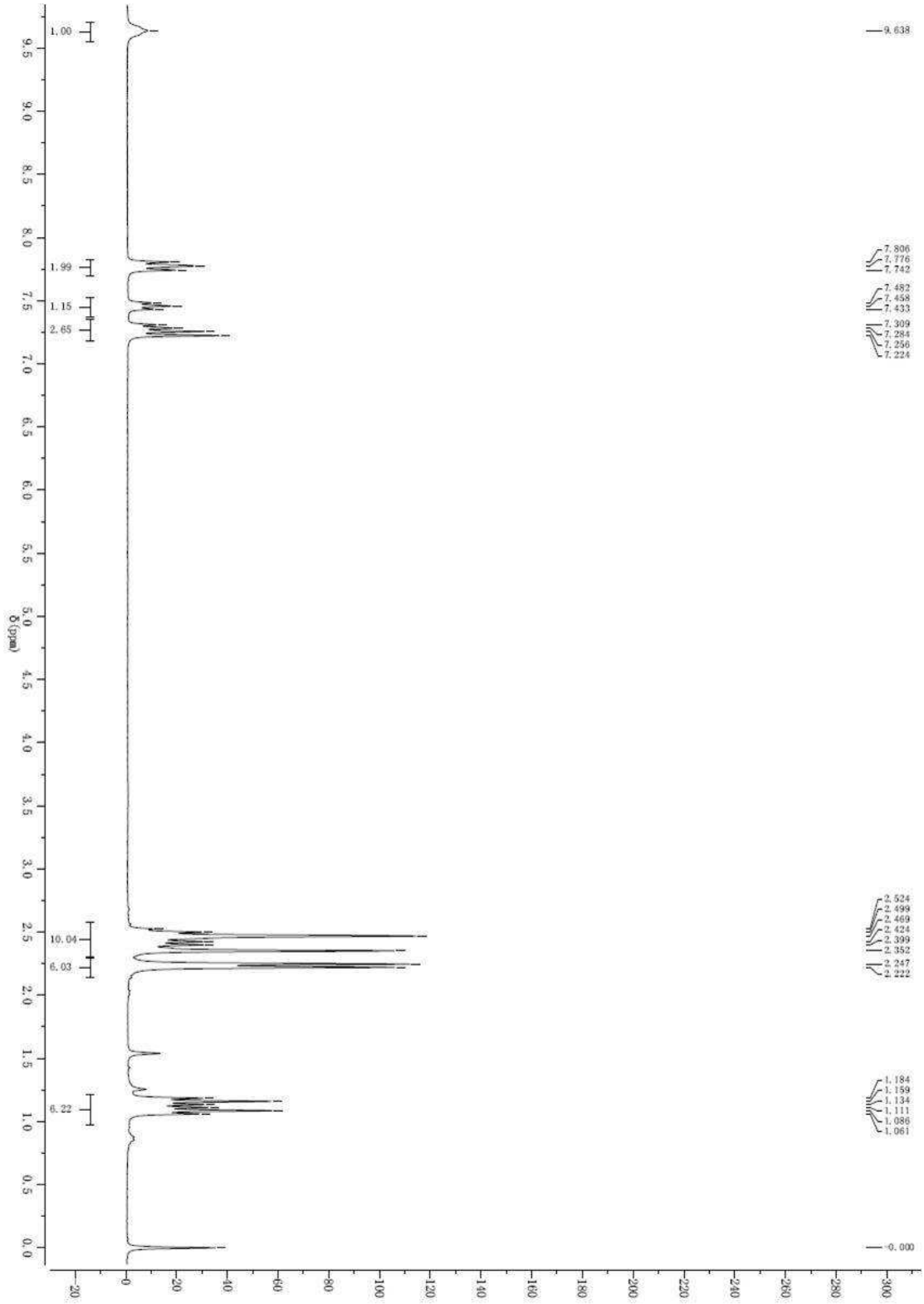


^{13}C NMR of compound **3ac** in $CDCl_3$

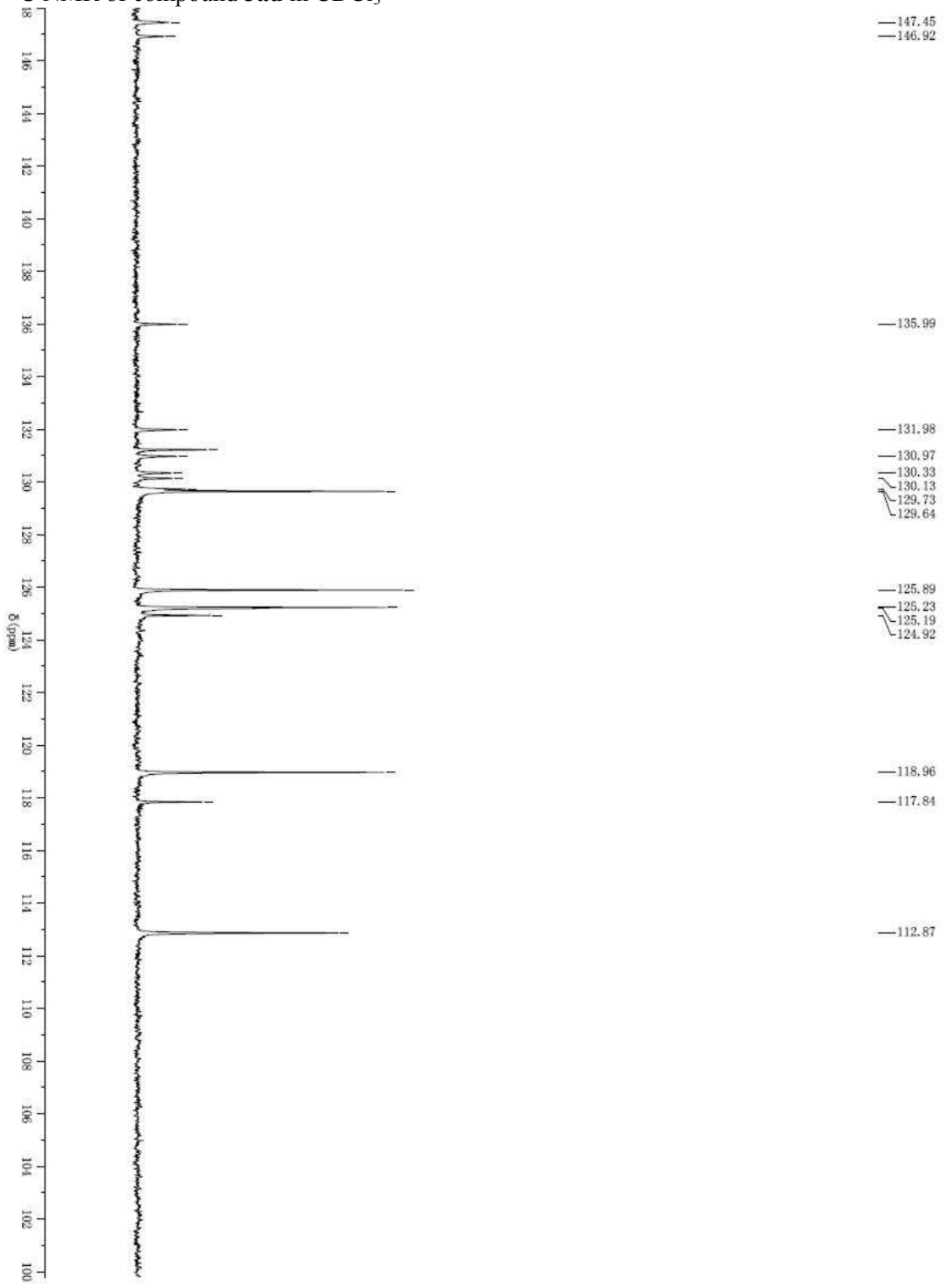


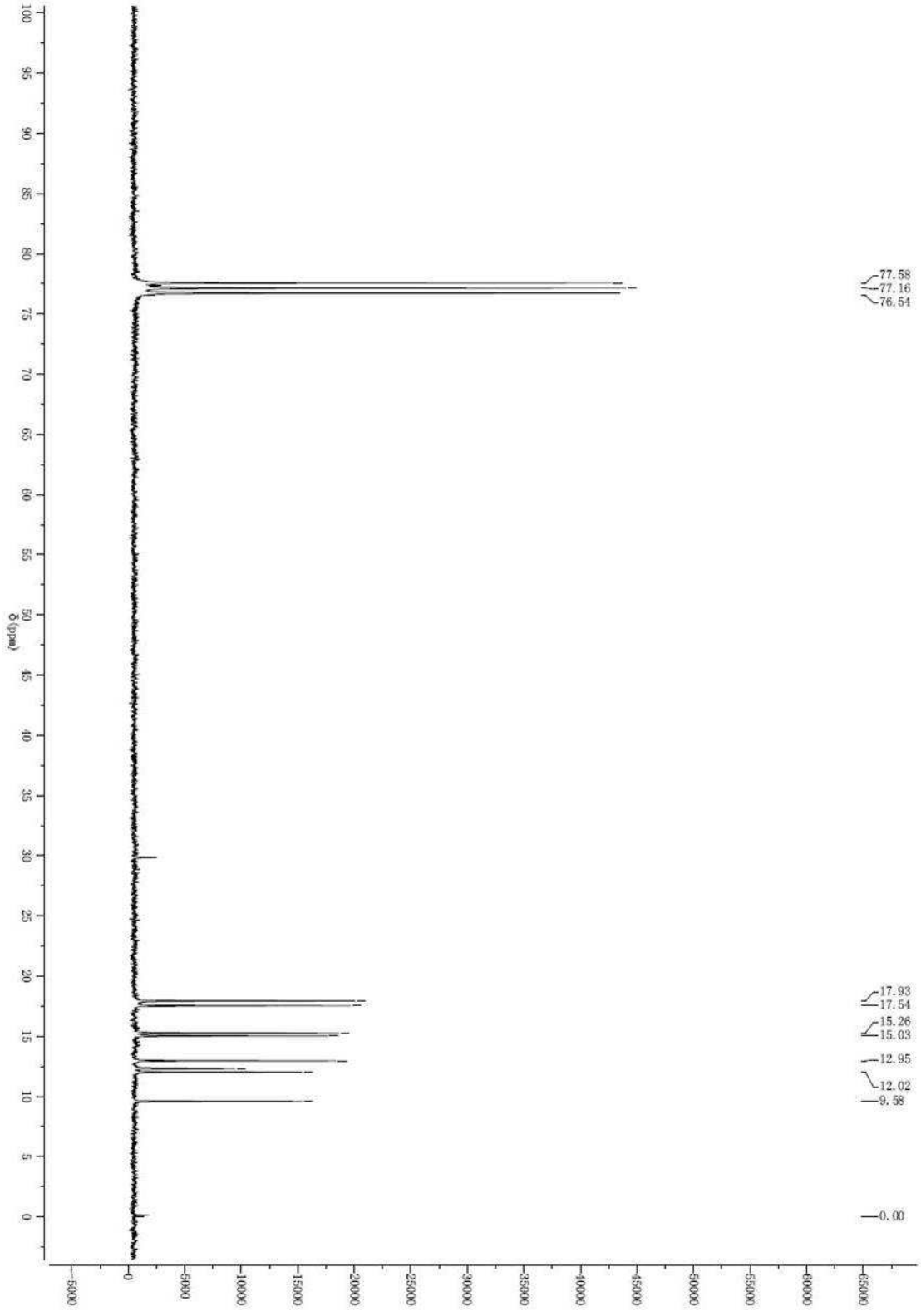

77.59
77.16
76.74
14.49
13.69
11.36
0.00
δ (ppm)

^{1}H NMR compound **3ad** in $CDCl_3$

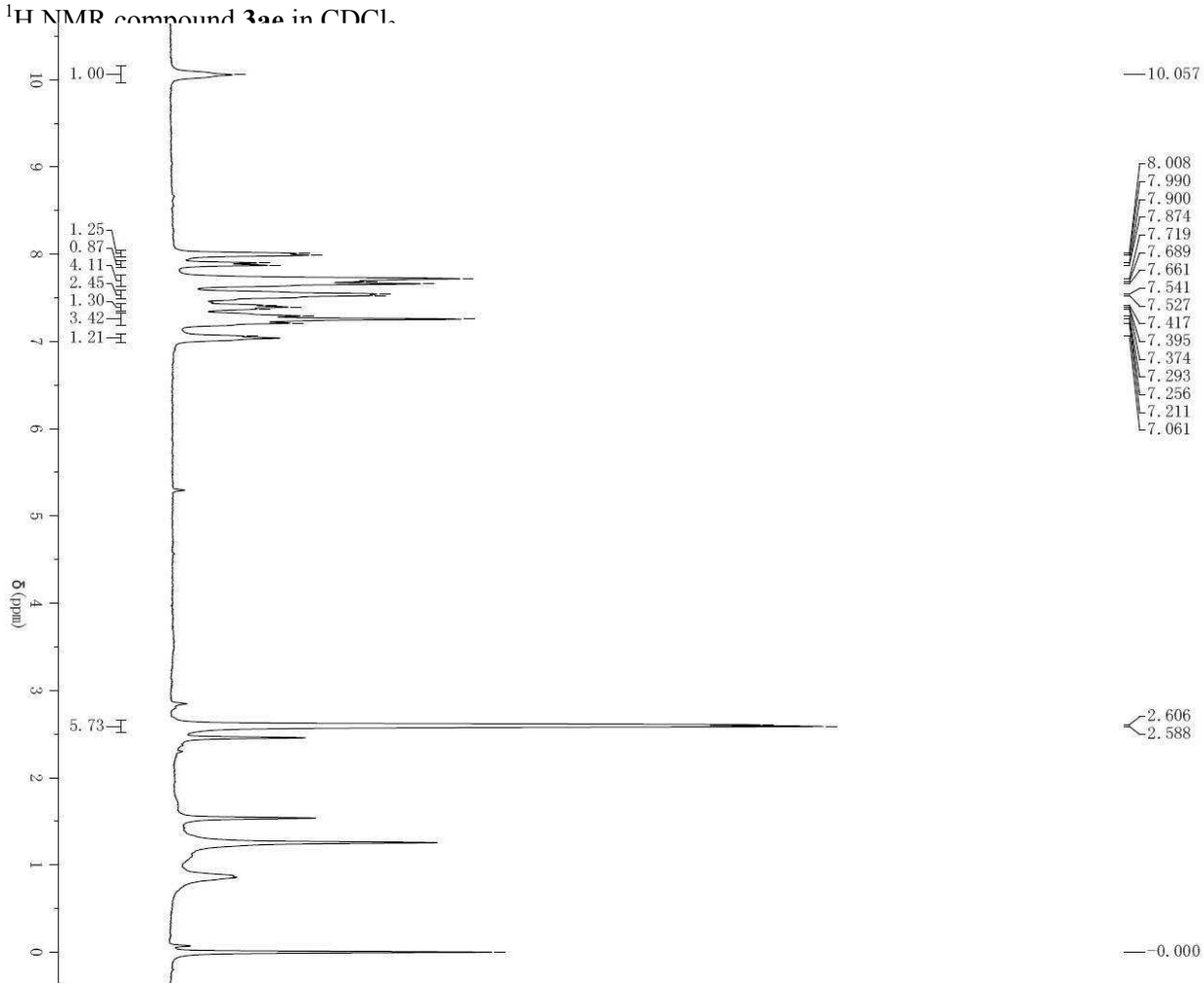


^{13}C NMR of compound **3ad** in $CDCl_3$

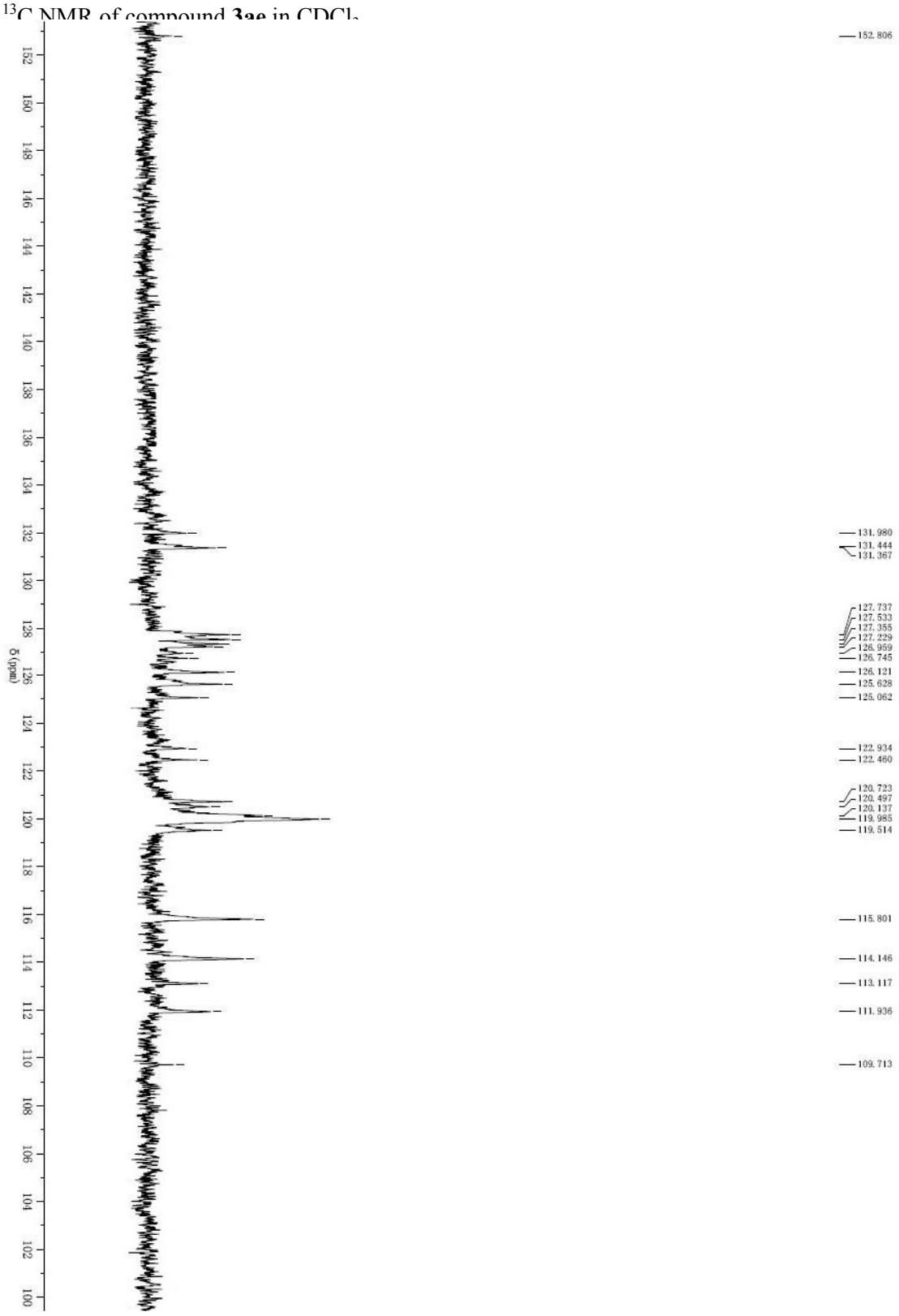


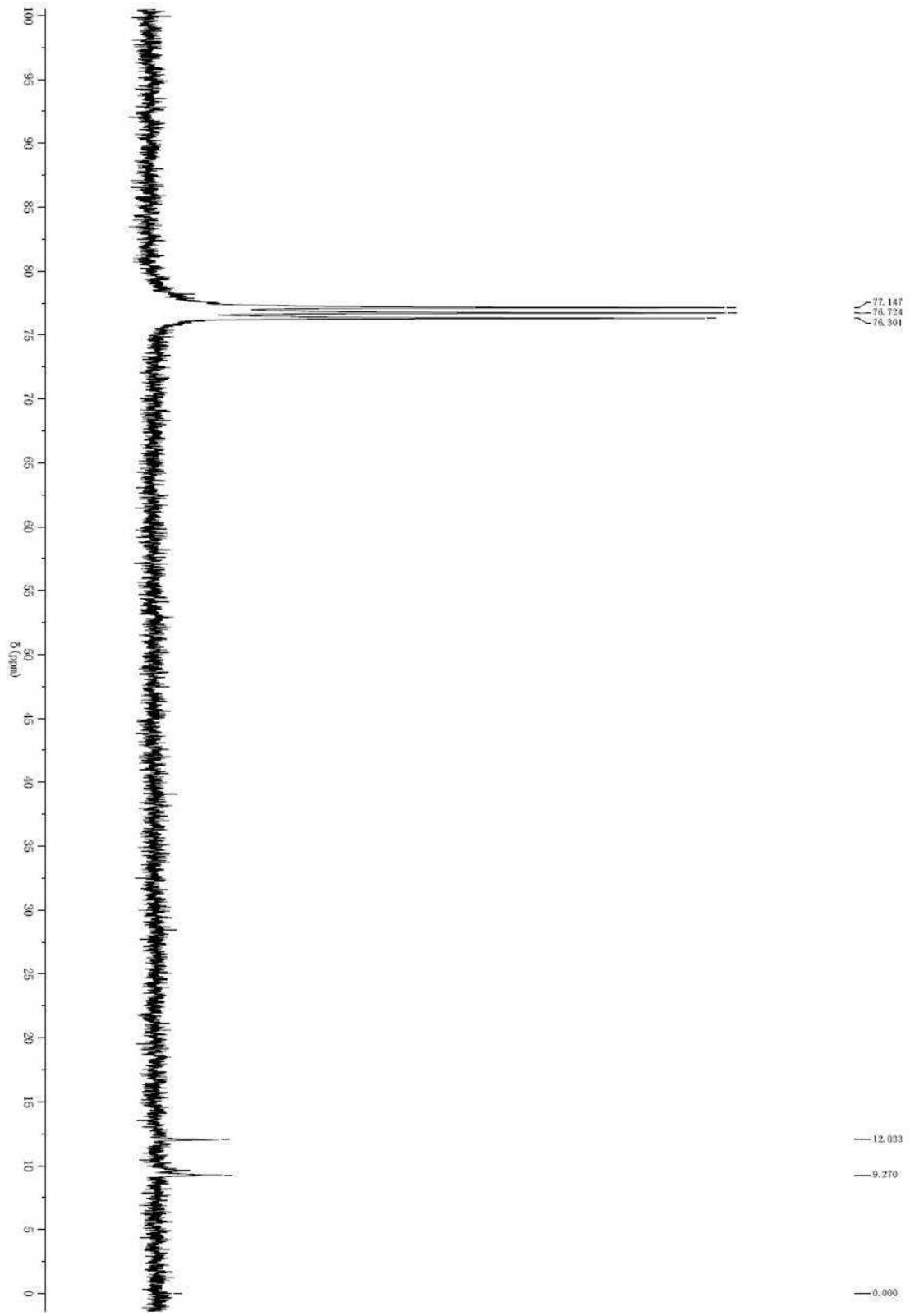

77.58
77.16
76.54
17.93
17.54
15.26
15.03
12.95
12.02
9.58
0.00
δ(ppm)

^{1}H NMR compound **3ae** in $CDCl_3$

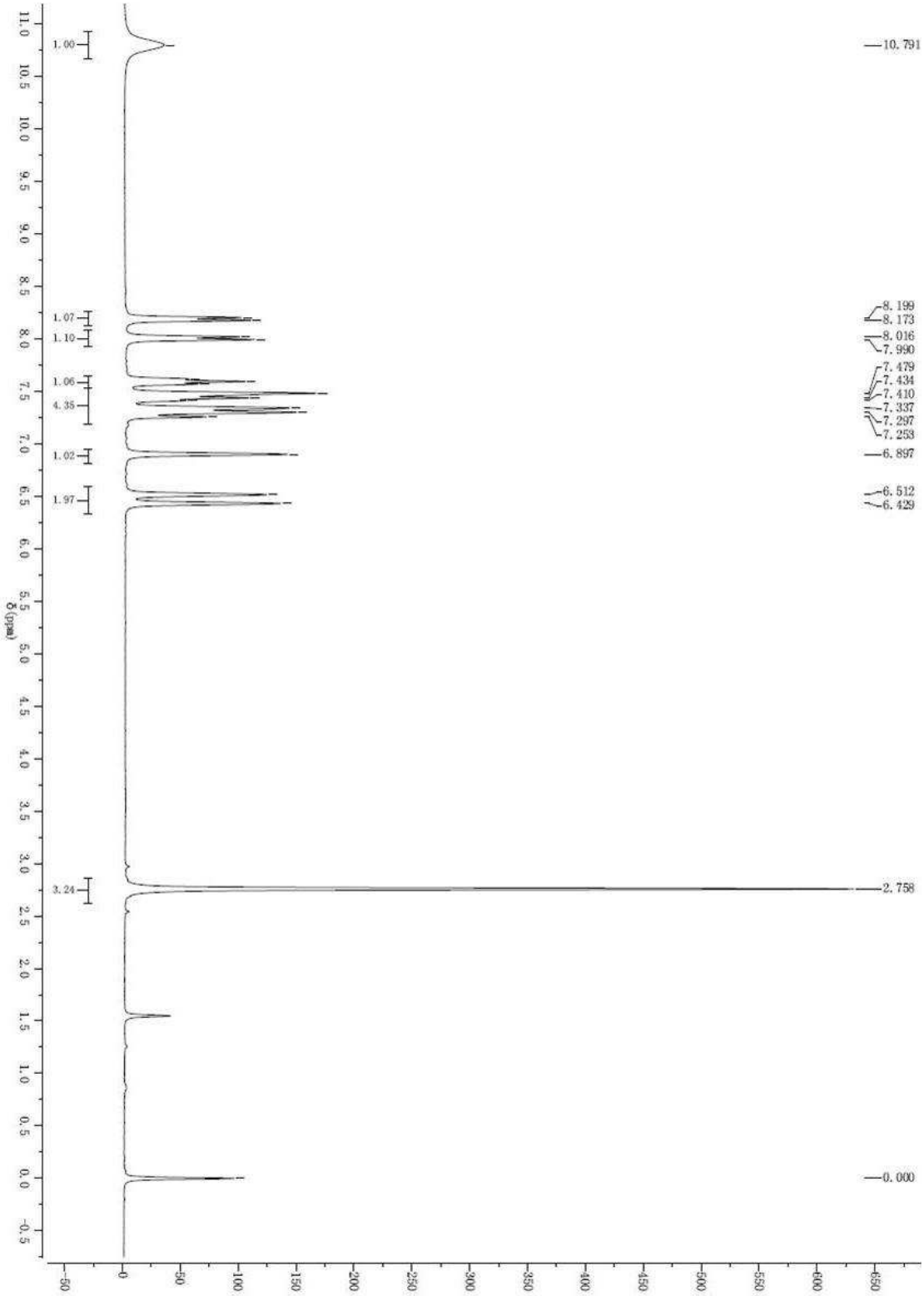


^{13}C NMR of compound **3ae** in $CDCl_3$

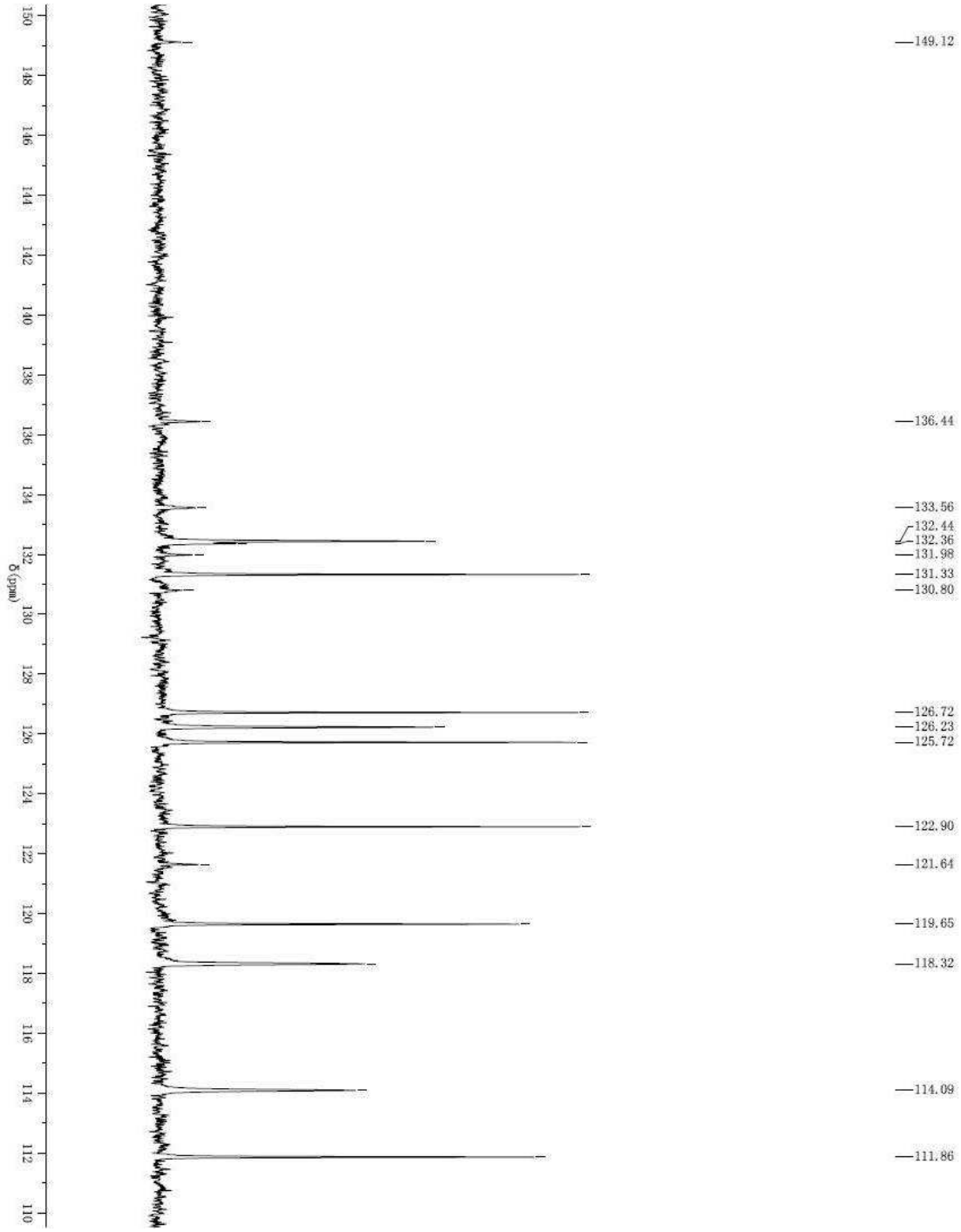


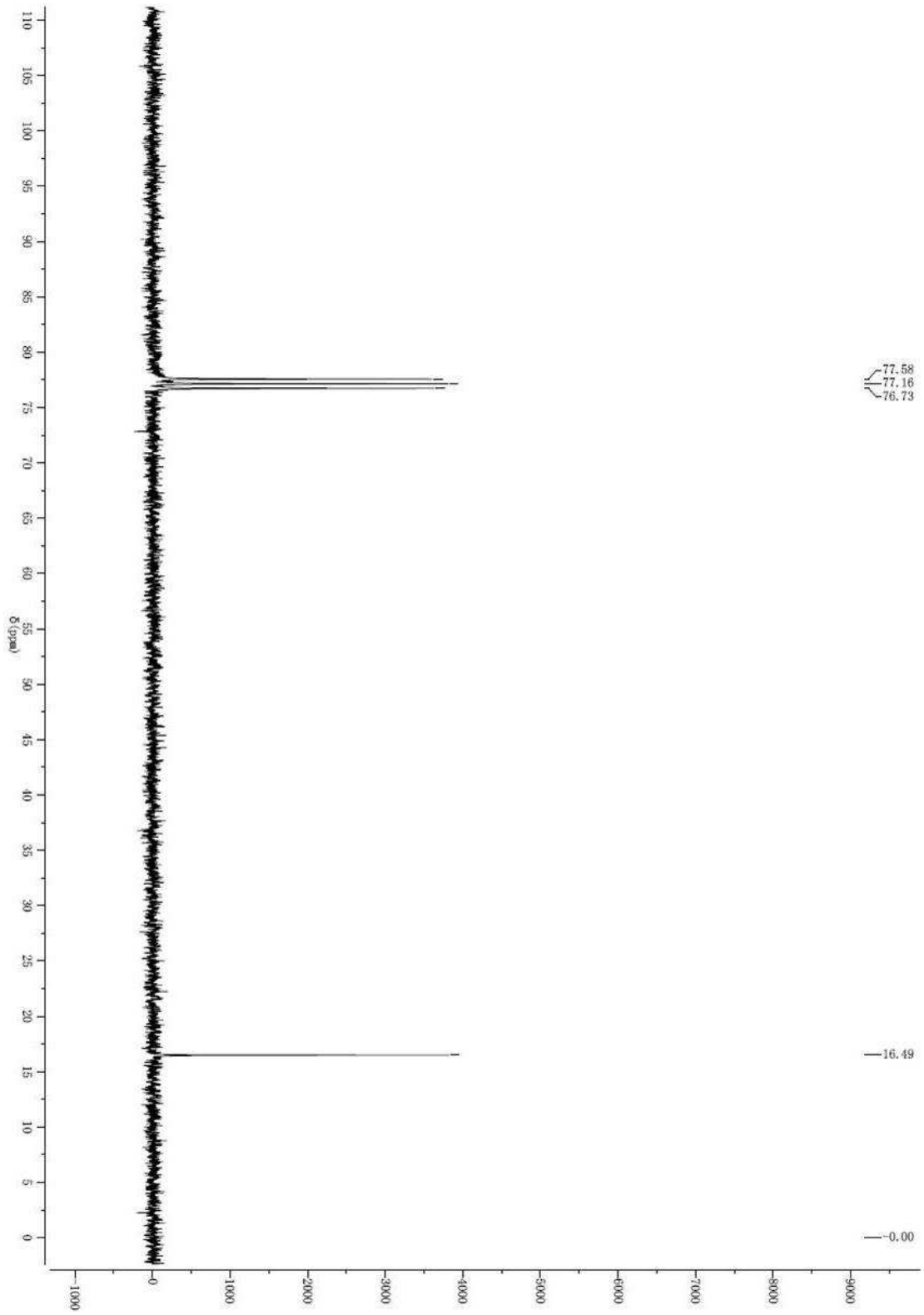

100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
δ(ppm)
77.147
76.724
76.301
12.033
9.270
0.000

^{1}H NMR compound **3ba** in $CDCl_3$

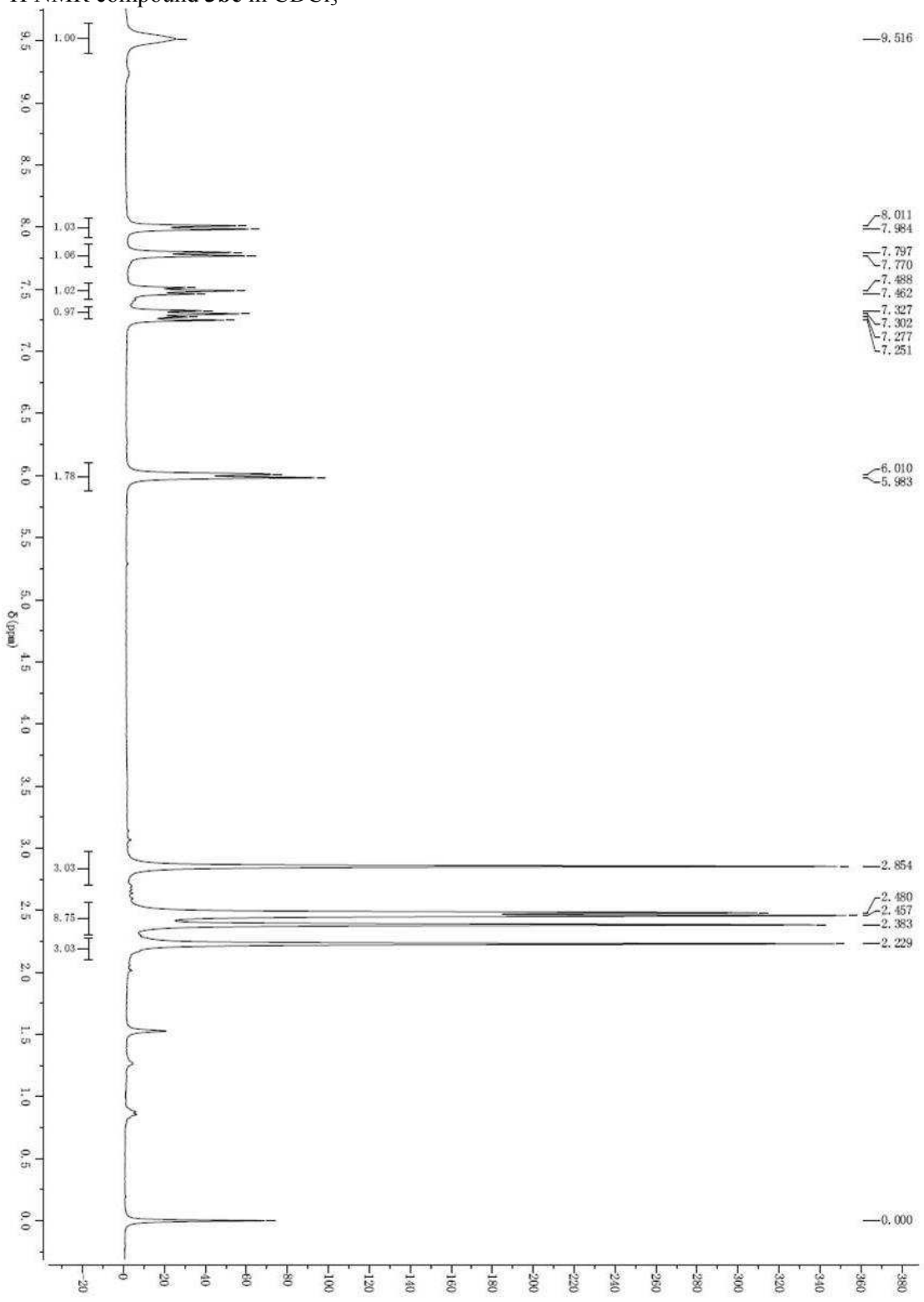


^{13}C NMR of compound **3ba** in $CDCl_3$

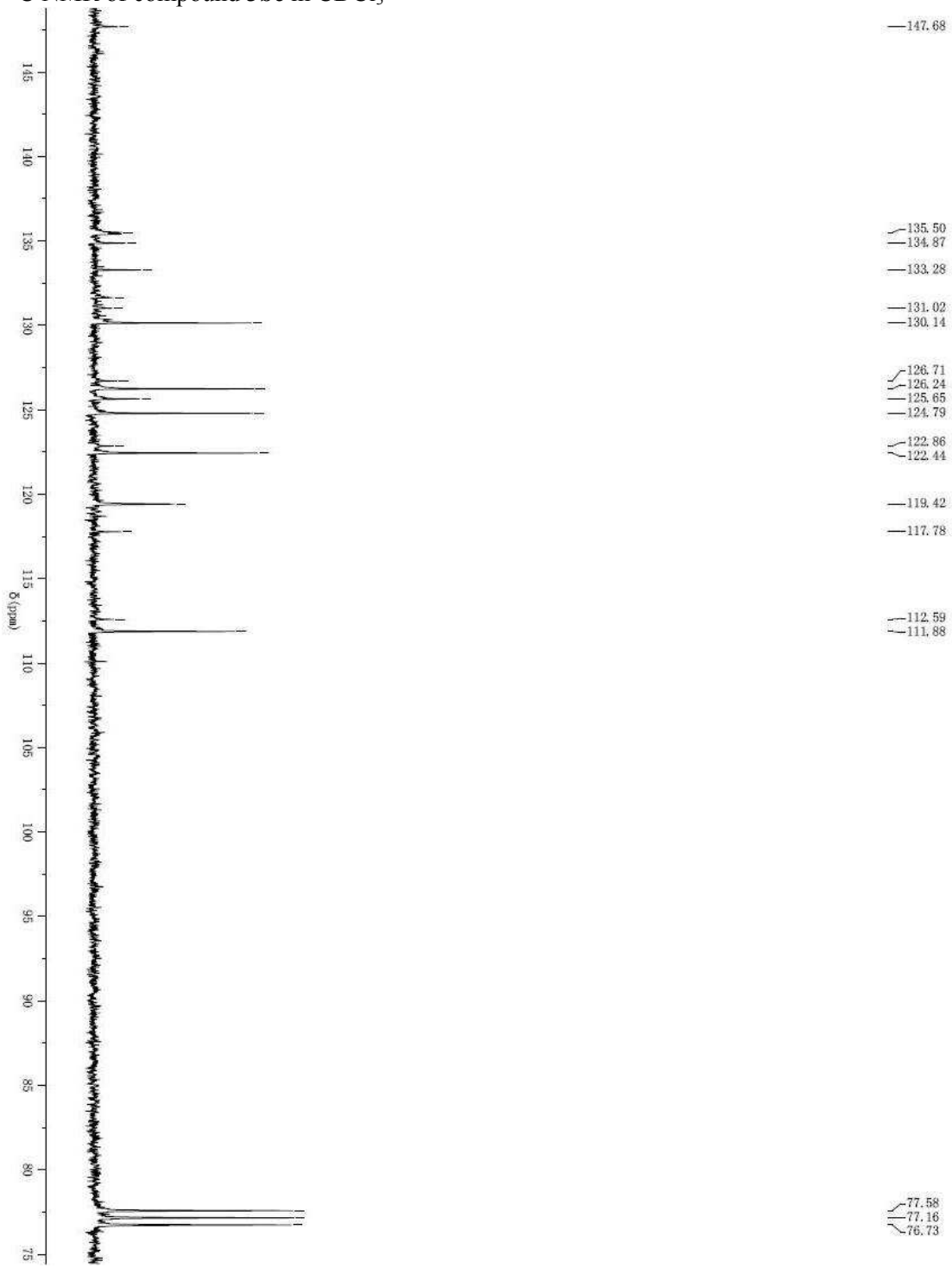


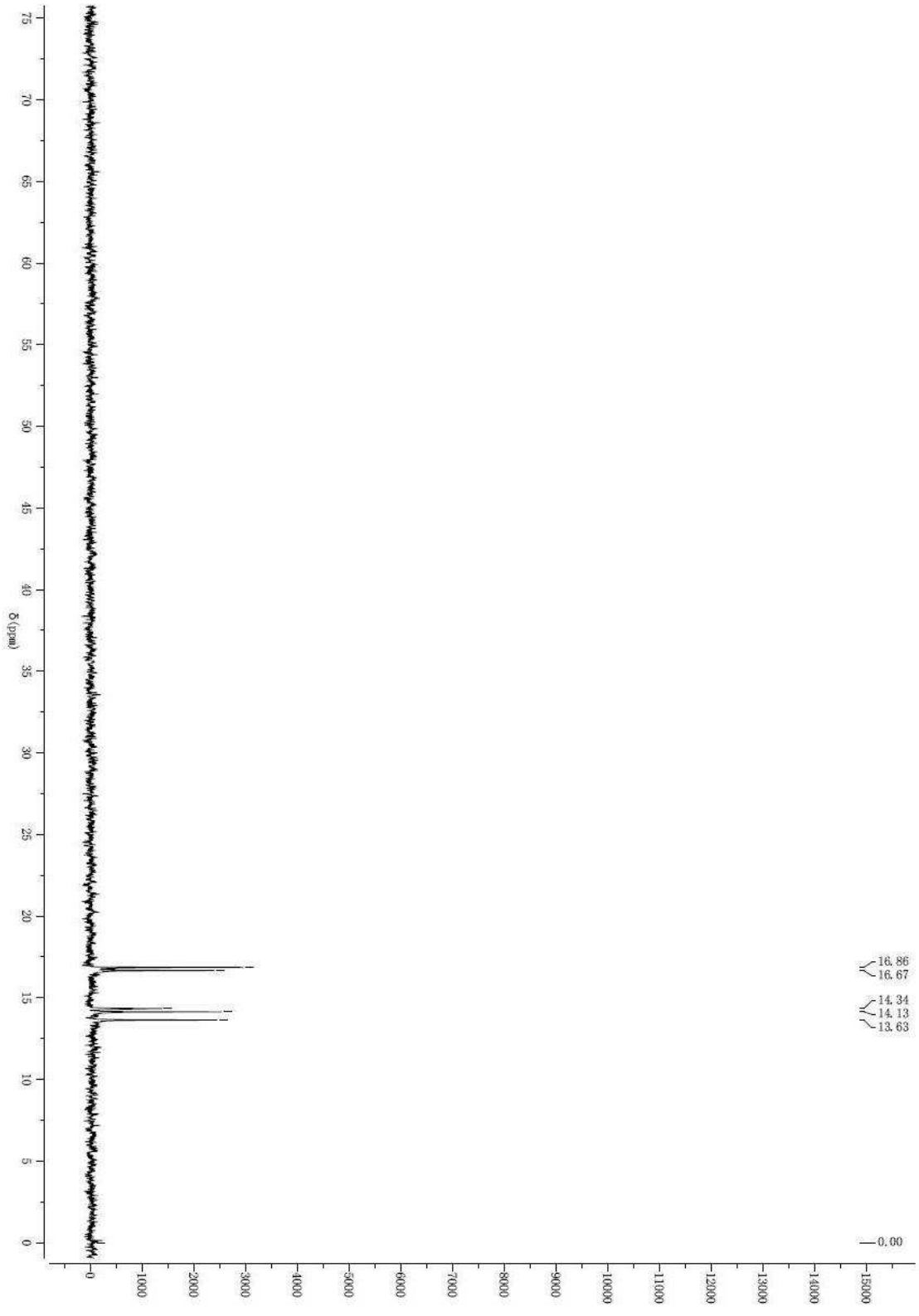

77.58
77.16
76.73
16.49
0.00
δ (ppm)

^{1}H NMR compound **3bc** in $CDCl_3$

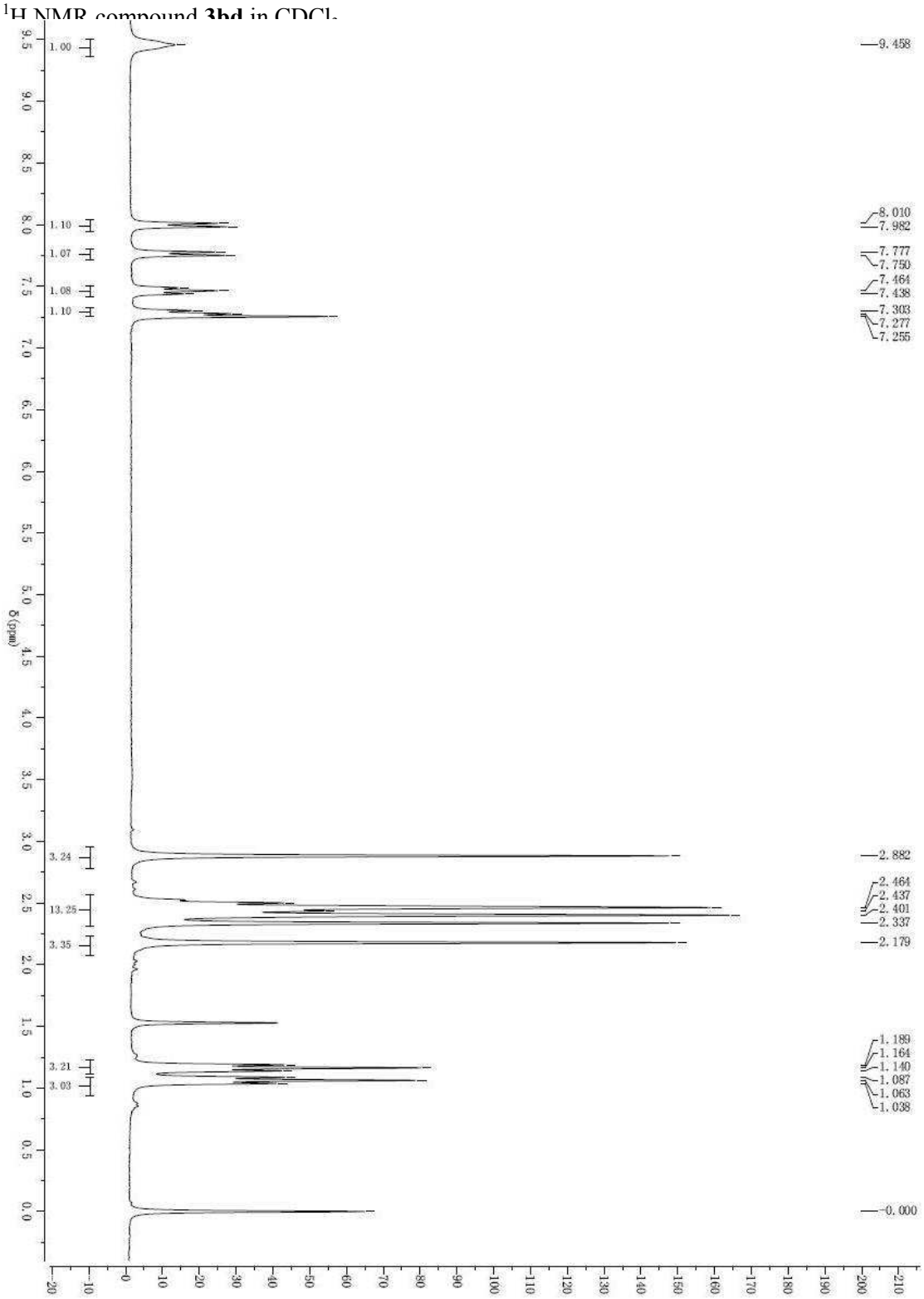


^{13}C NMR of compound **3bc** in $CDCl_3$

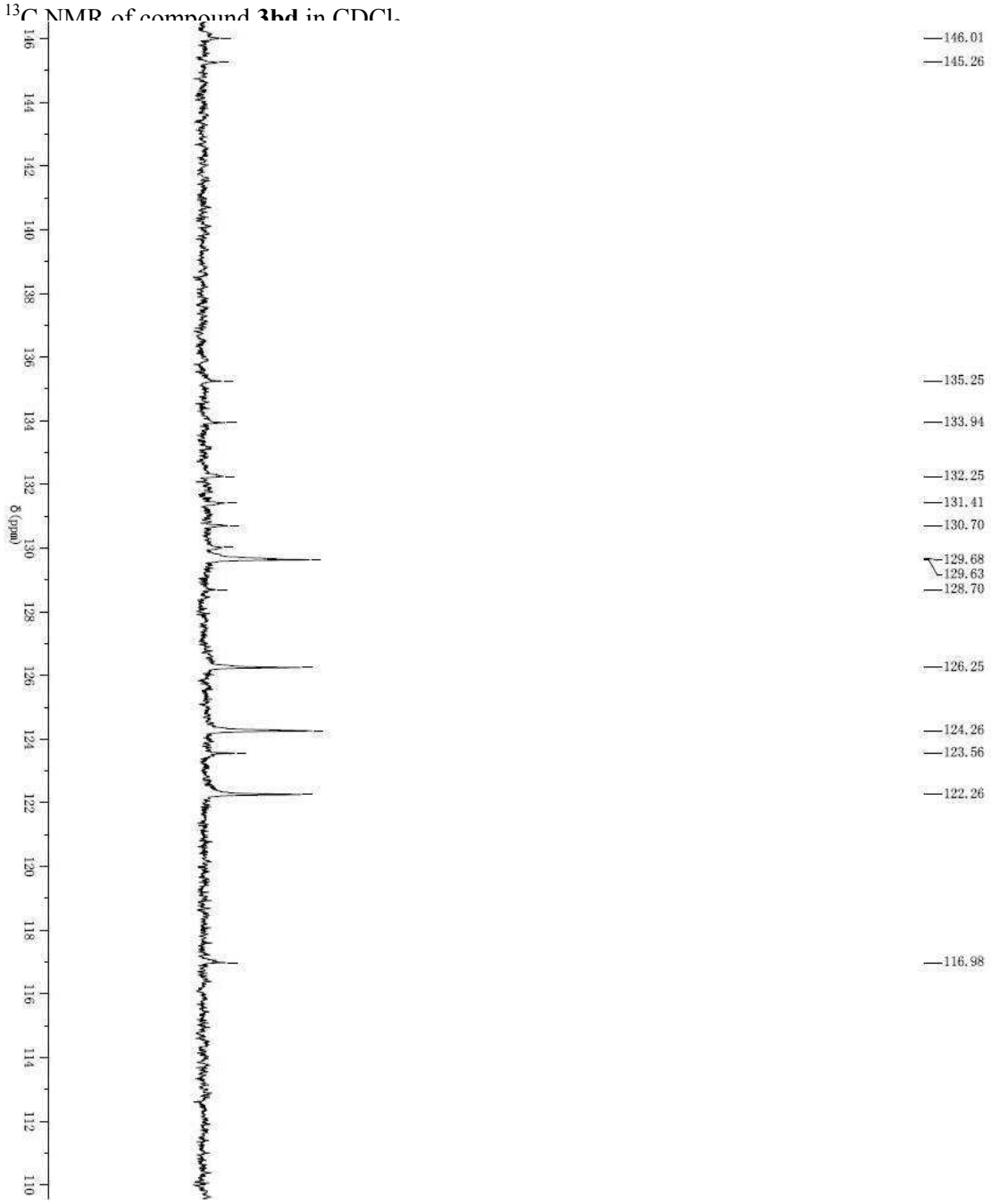


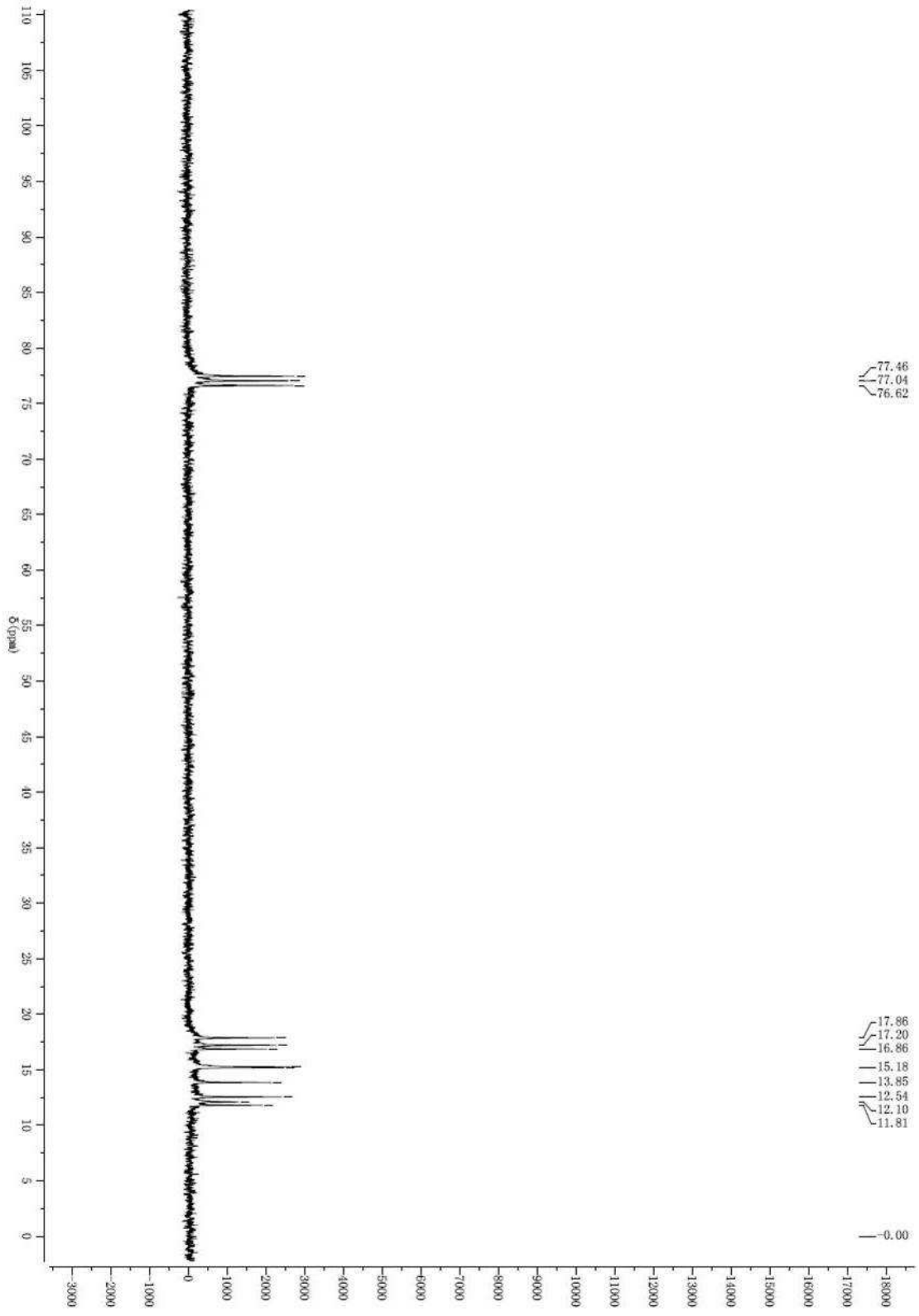

δ (ppm)
16.86
16.67
14.34
14.13
13.63
0.00

^{1}H NMR compound **3bd** in $CDCl_3$

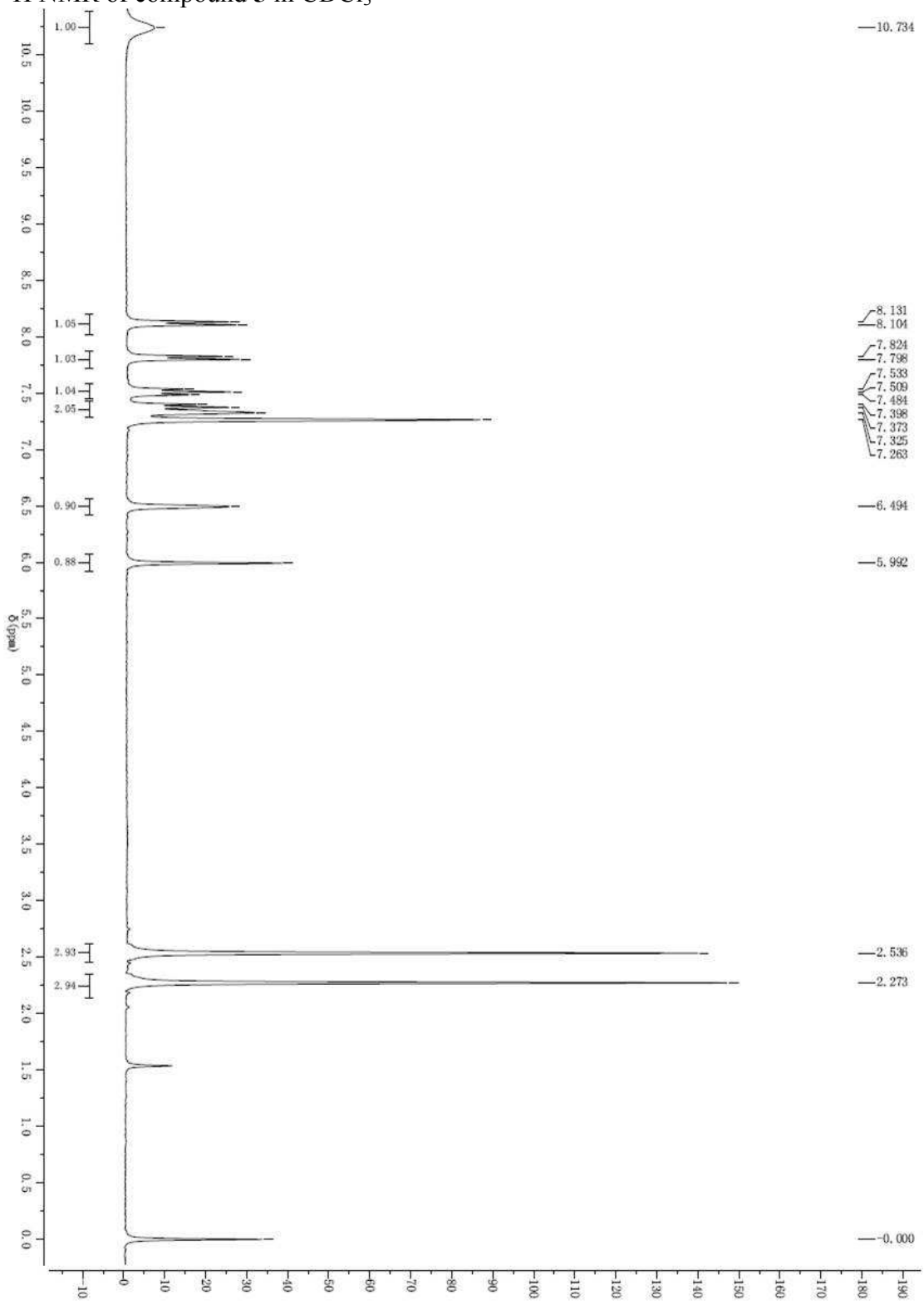


^{13}C NMR of compound **3bd** in $CDCl_3$

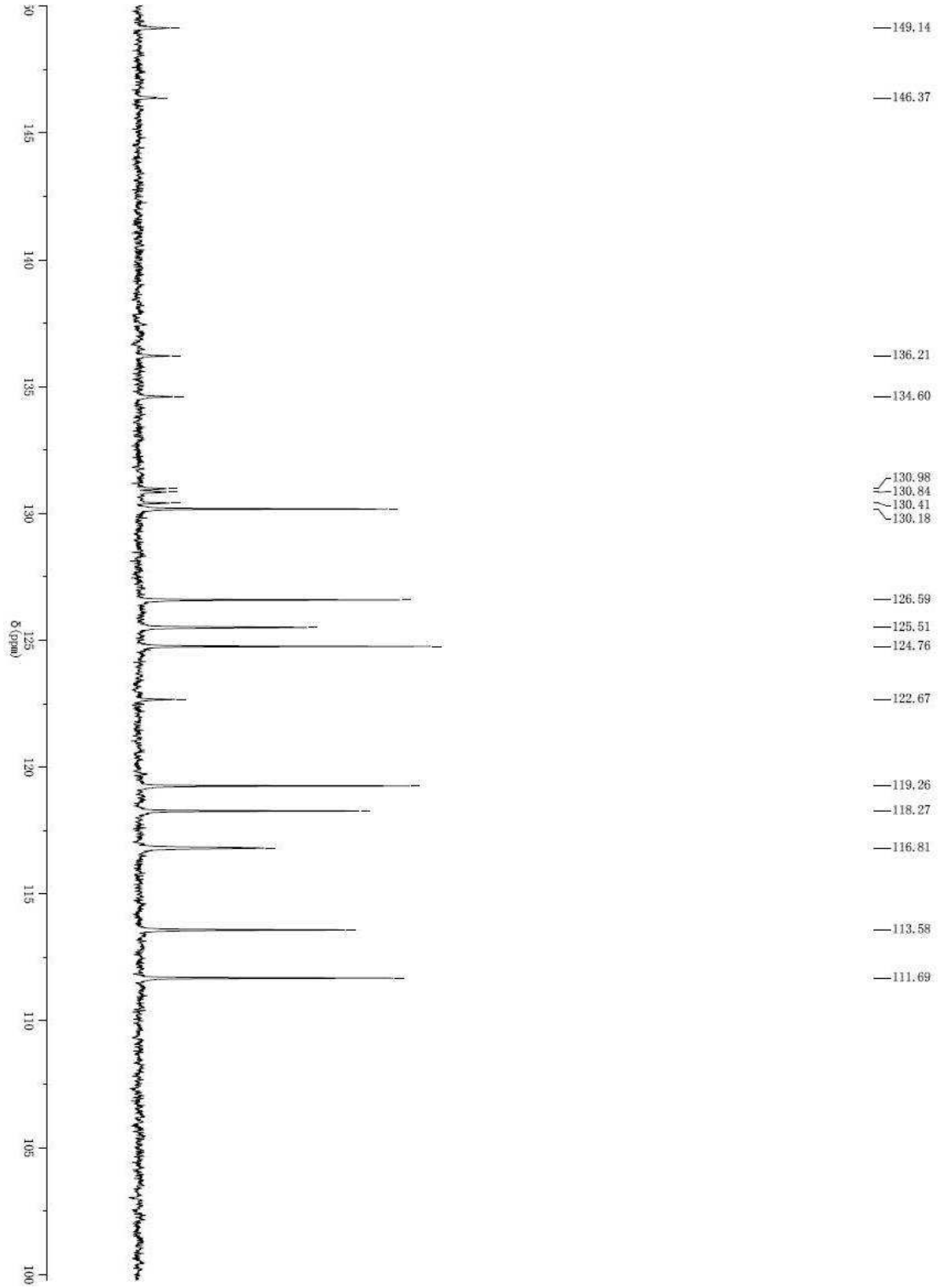


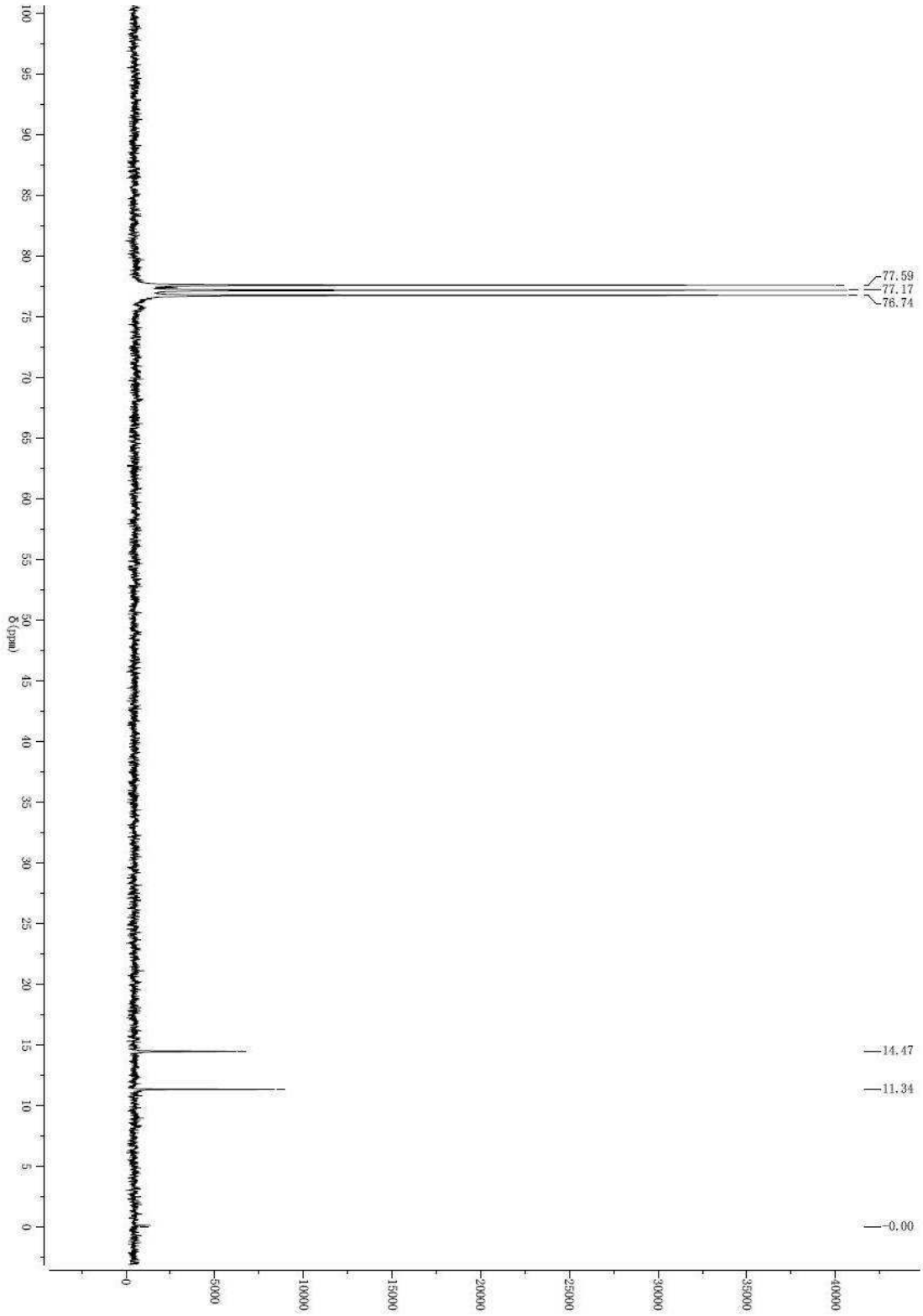

77.46
77.04
76.62
17.86
17.20
16.86
15.18
13.85
12.54
12.10
11.81
0.00
δ (ppm)

^{1}H NMR of compound **5** in $CDCl_3$

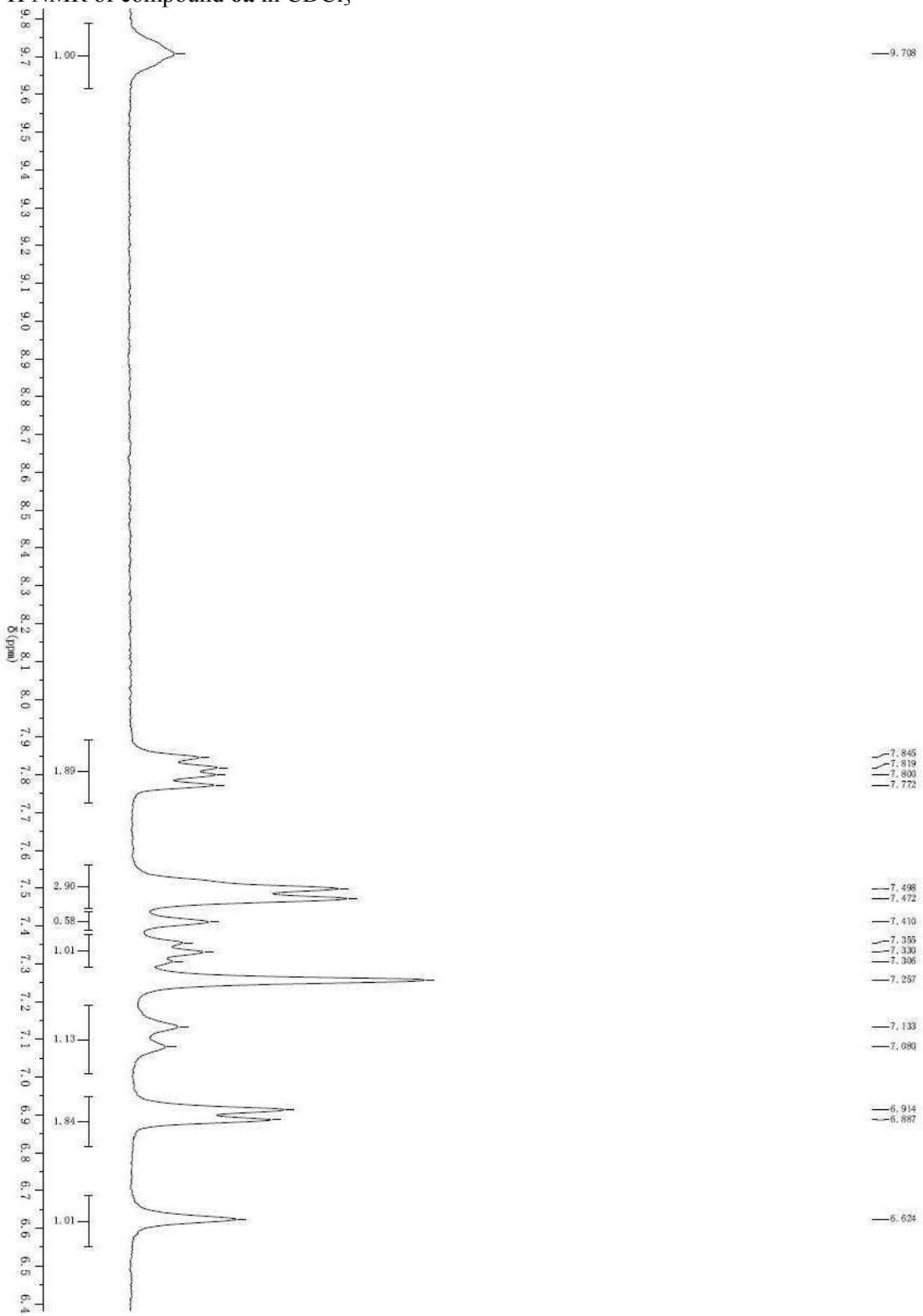


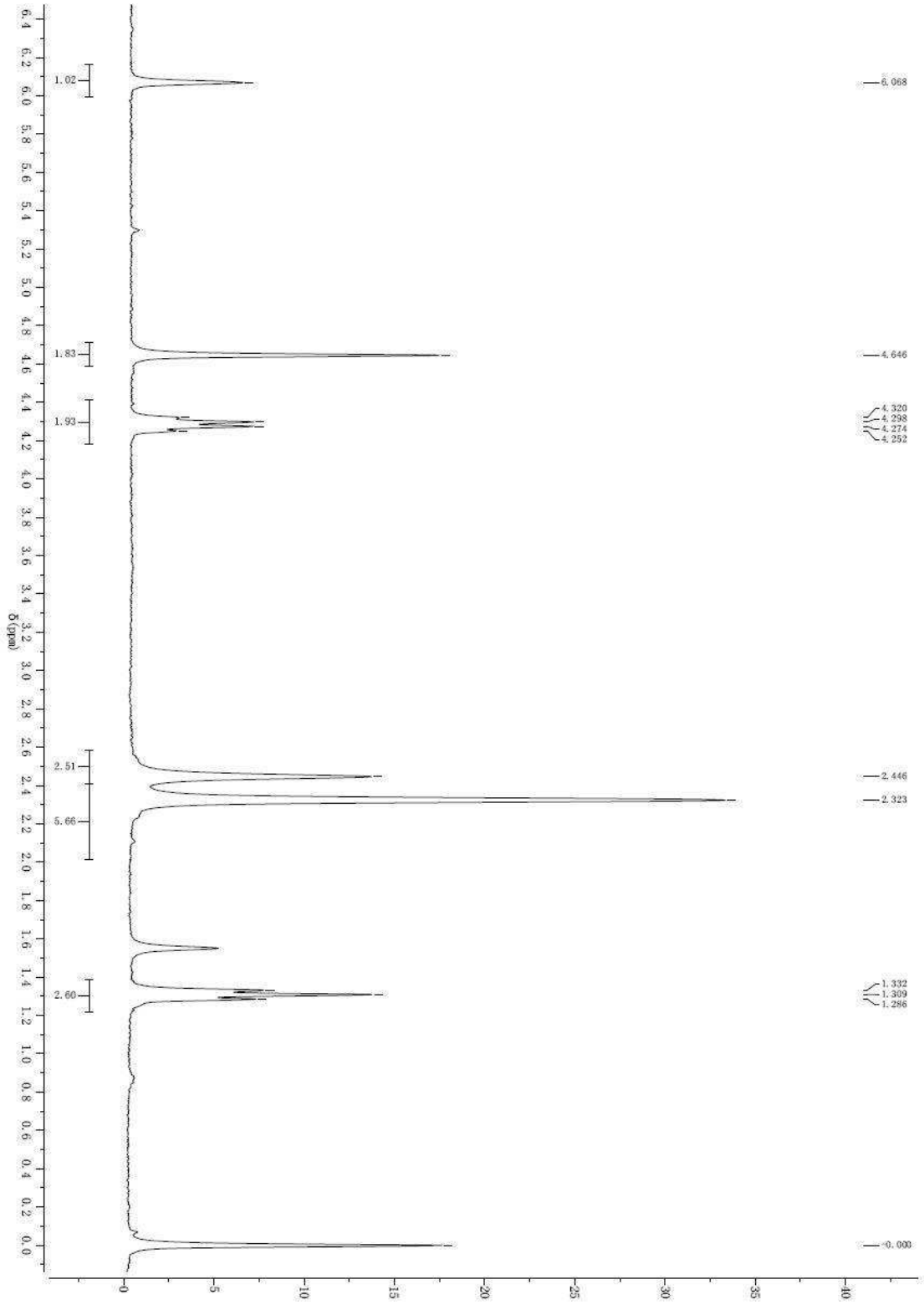
^{13}C NMR of compound **5** in $CDCl_3$



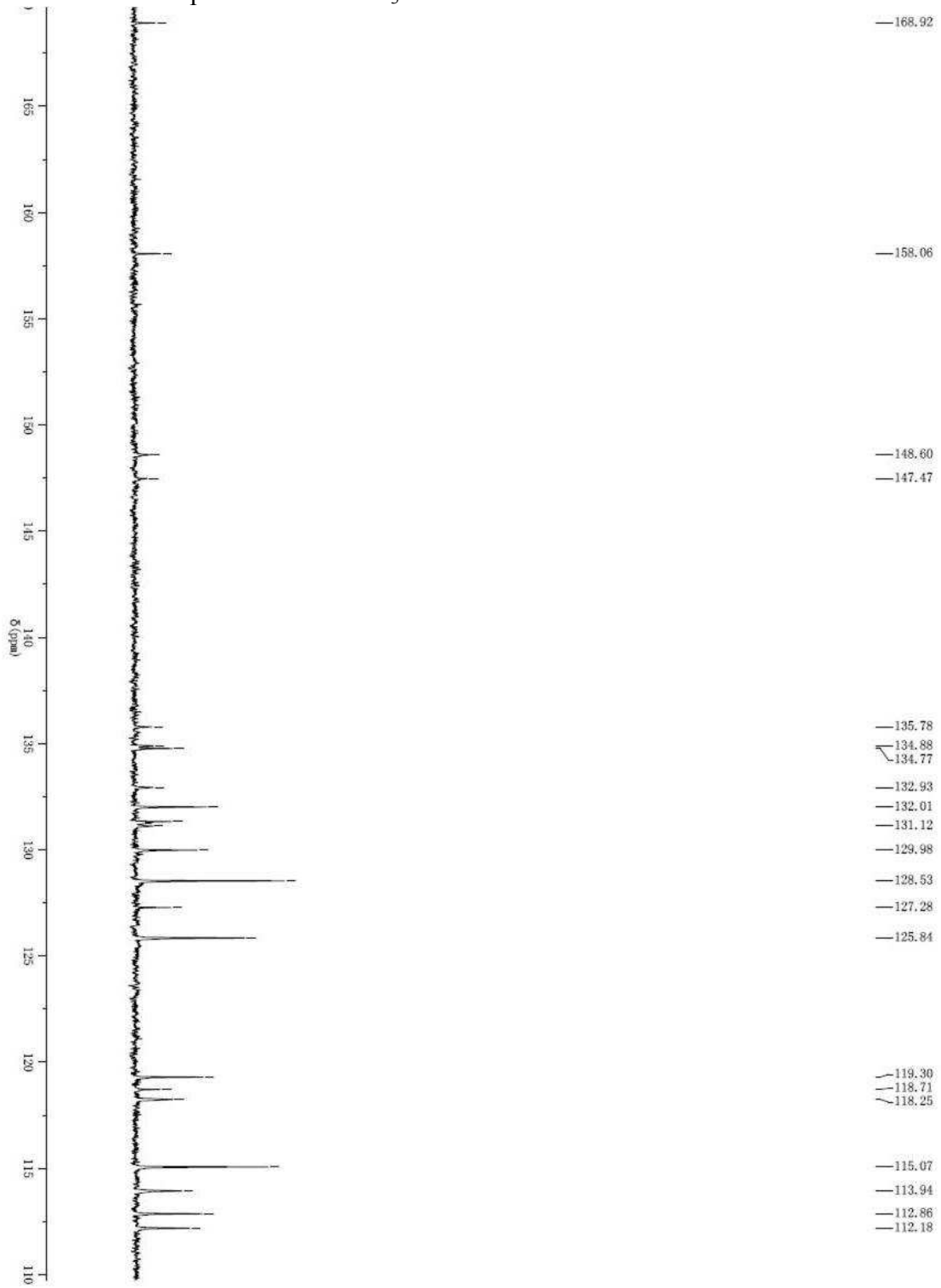

77.59
77.17
76.74
14.47
11.34
0.00
δ(ppm)

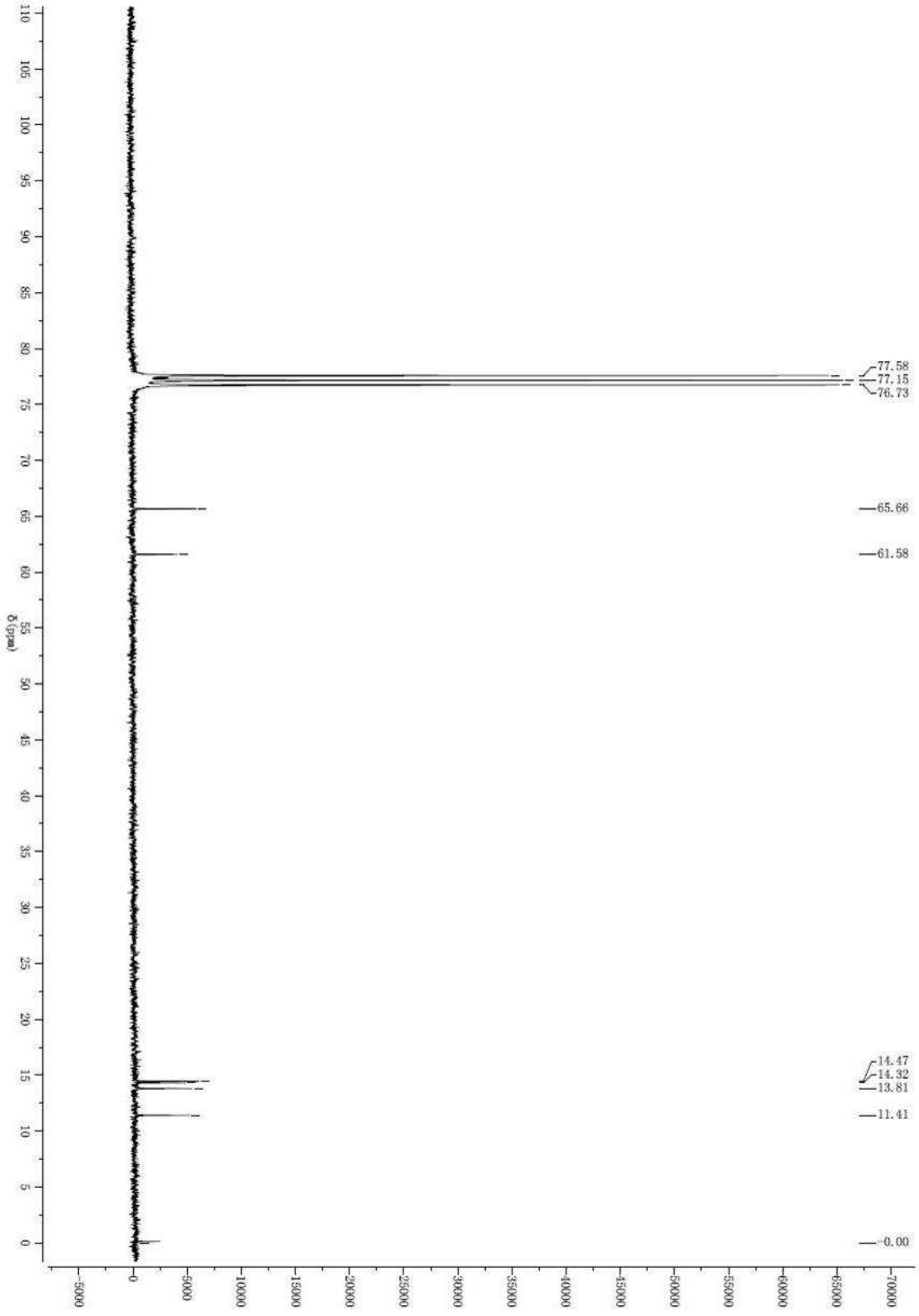
^{1}H NMR of compound **6a** in $CDCl_3$



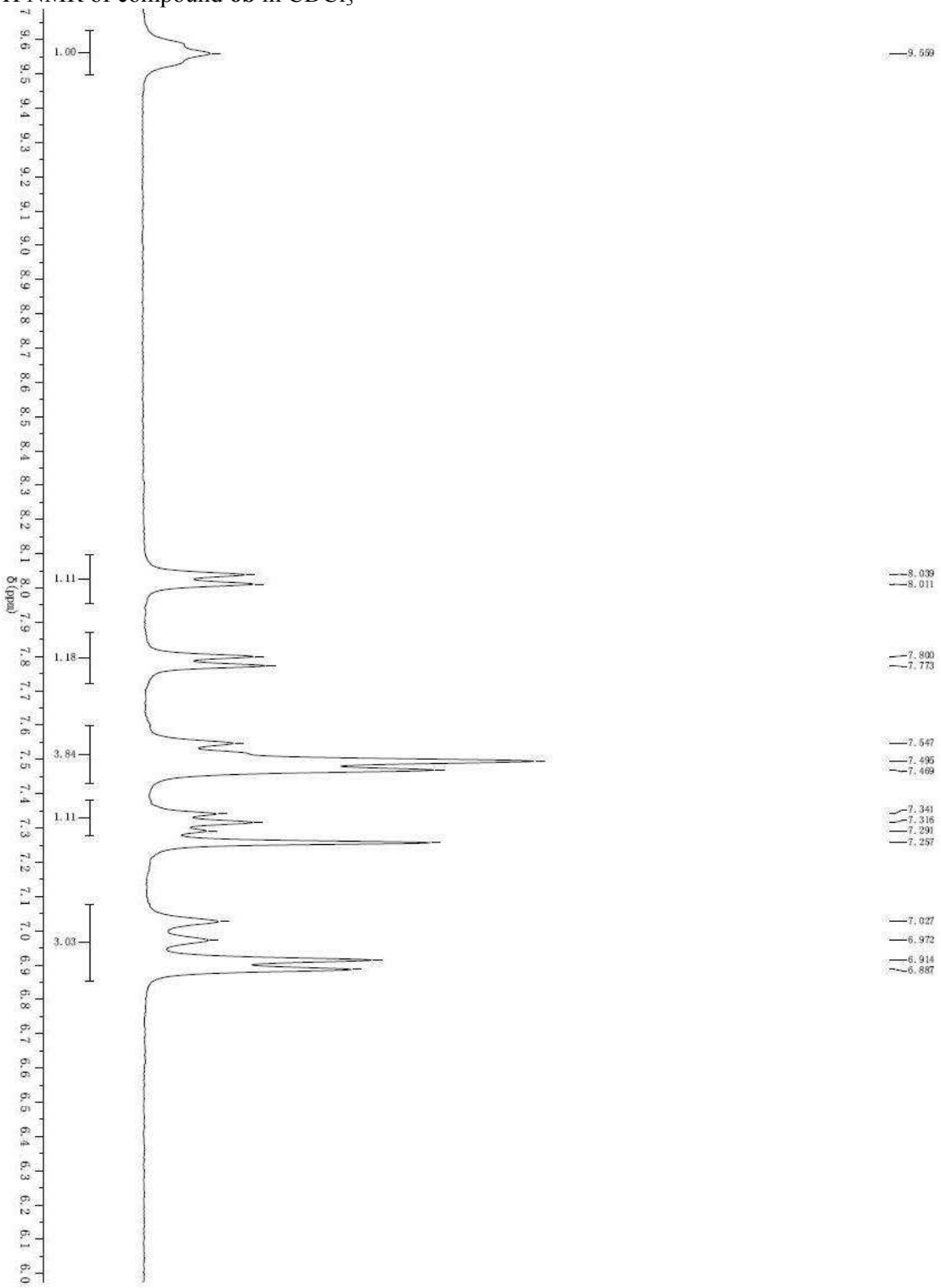

δ (ppm)
1.02
1.83
1.93
2.51
5.66
2.60
6.068
4.646
4.320
4.298
4.274
4.252
2.446
2.323
1.332
1.309
1.286
0.000

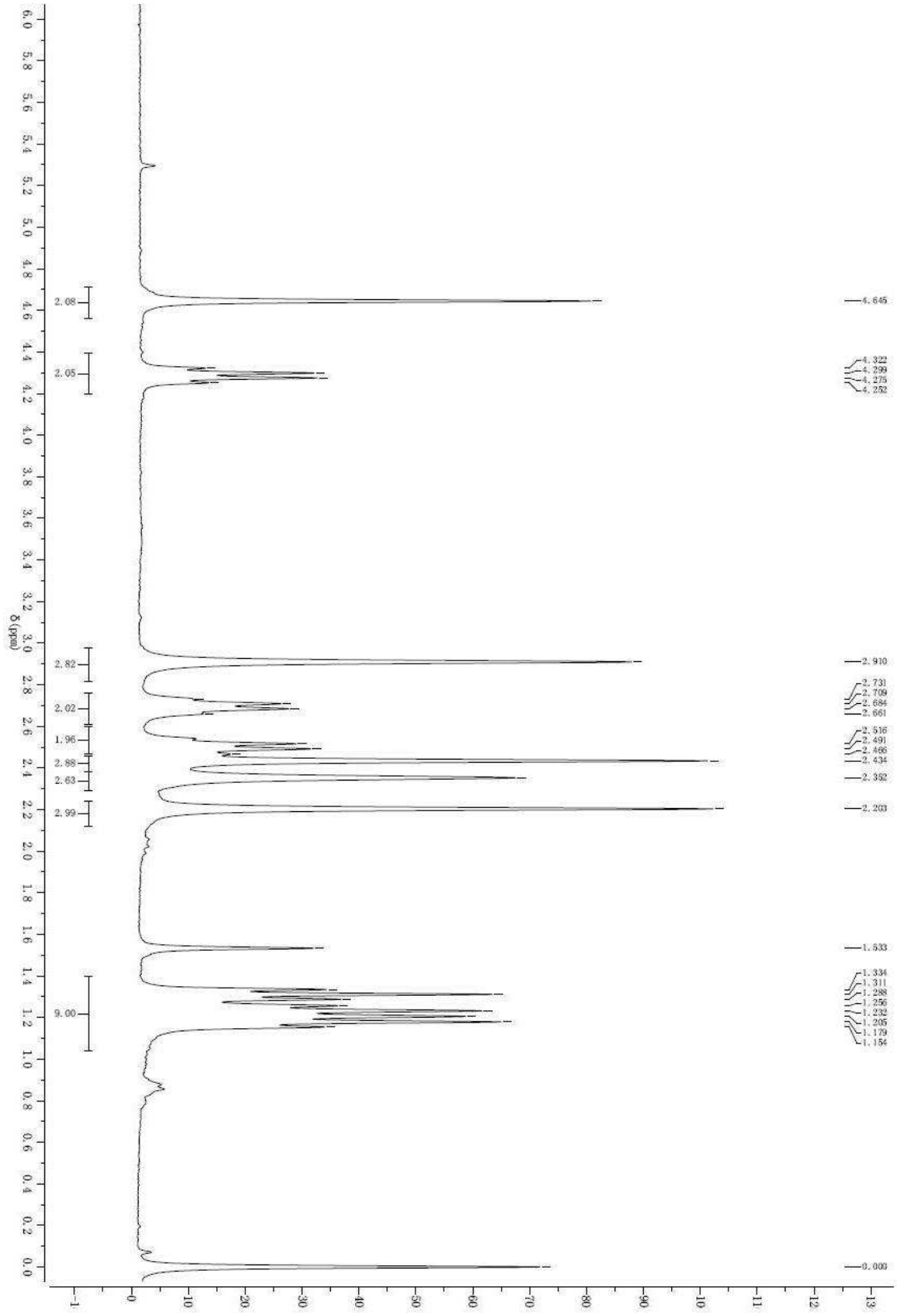
^{13}C NMR of compound **6a** in $CDCl_3$



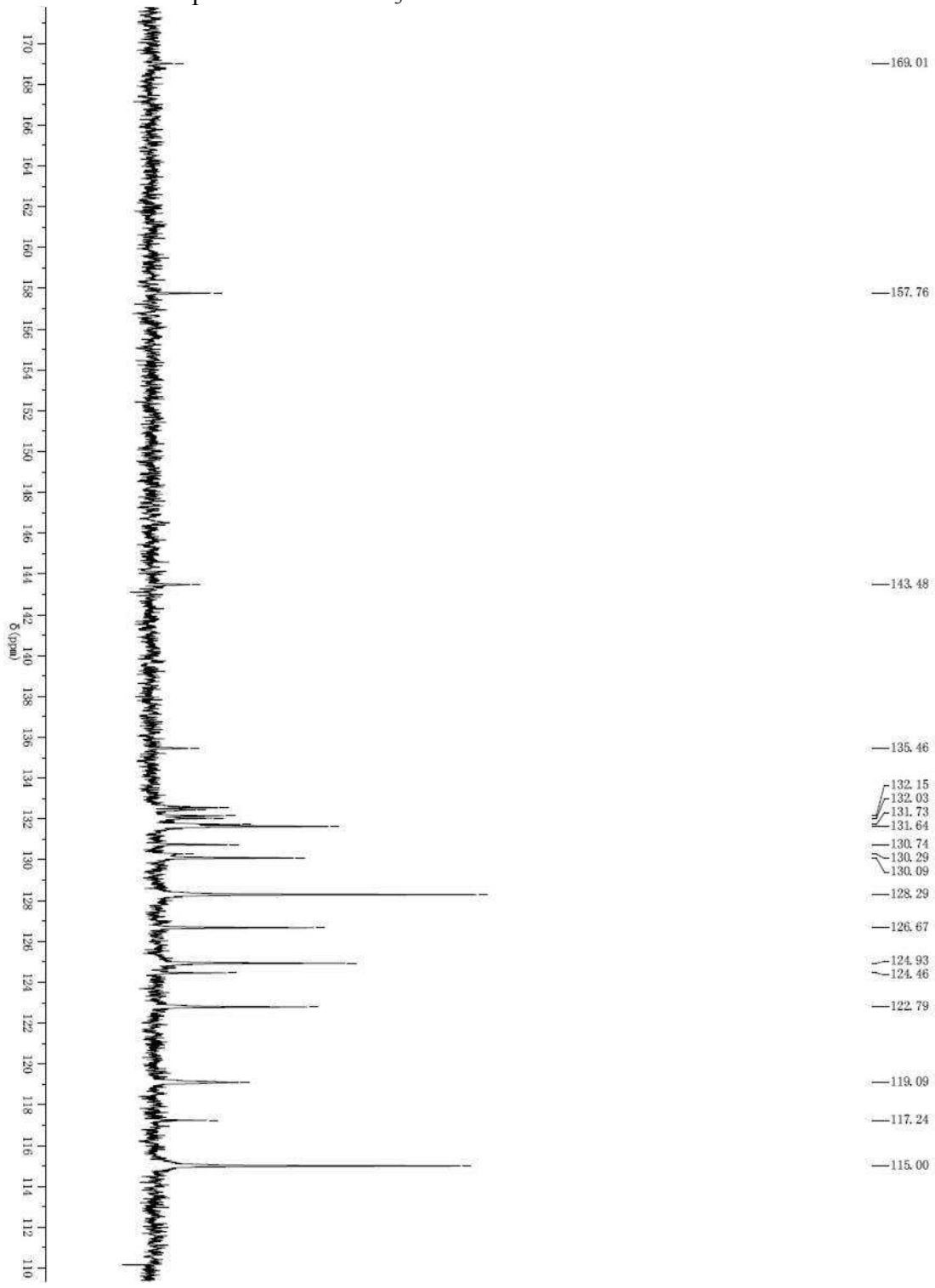

77.58
77.15
76.73
65.66
61.58
14.47
14.32
13.81
11.41
0.00
δ (ppm)

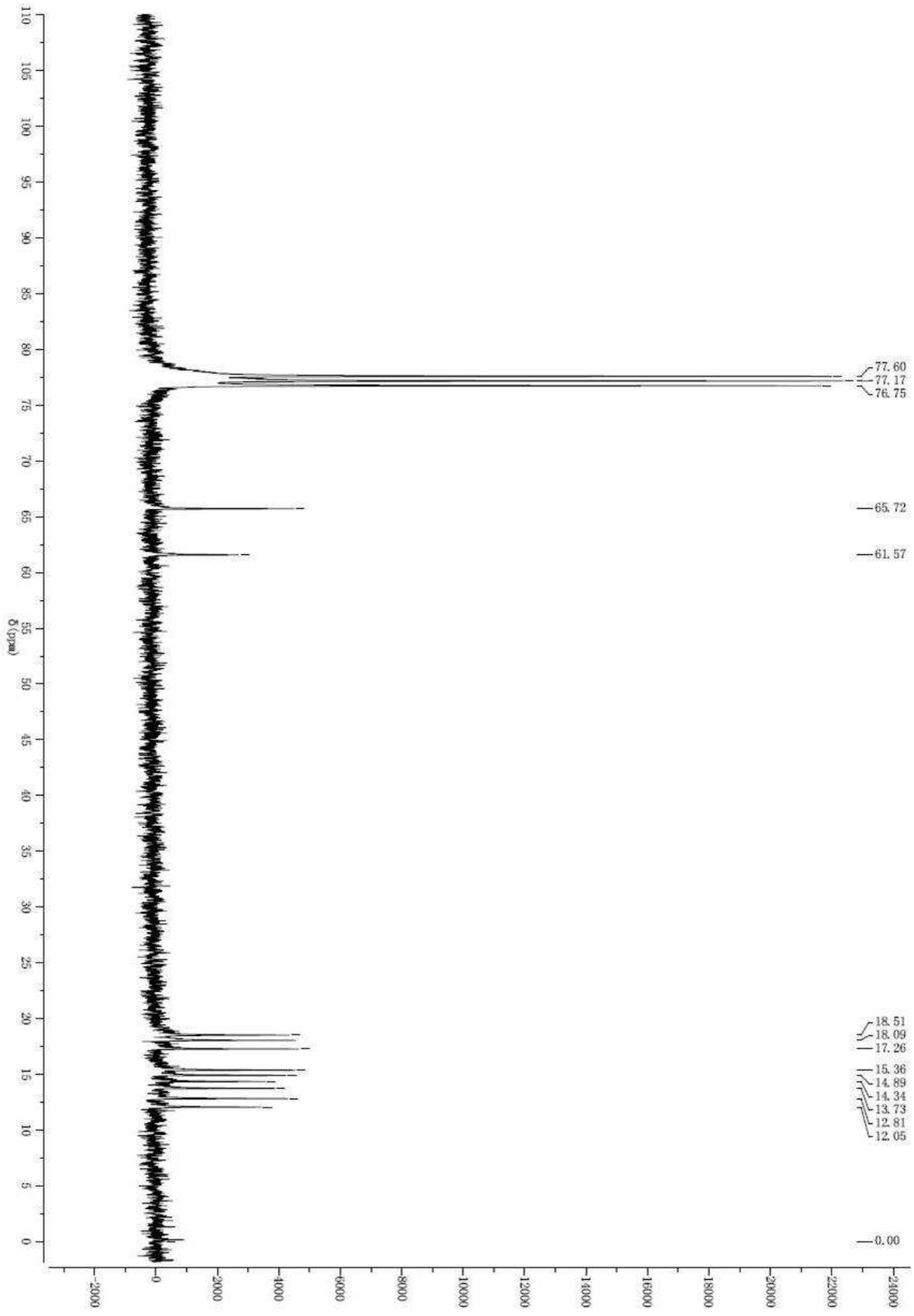
H NMR of compound **6b** in $CDCl_3$



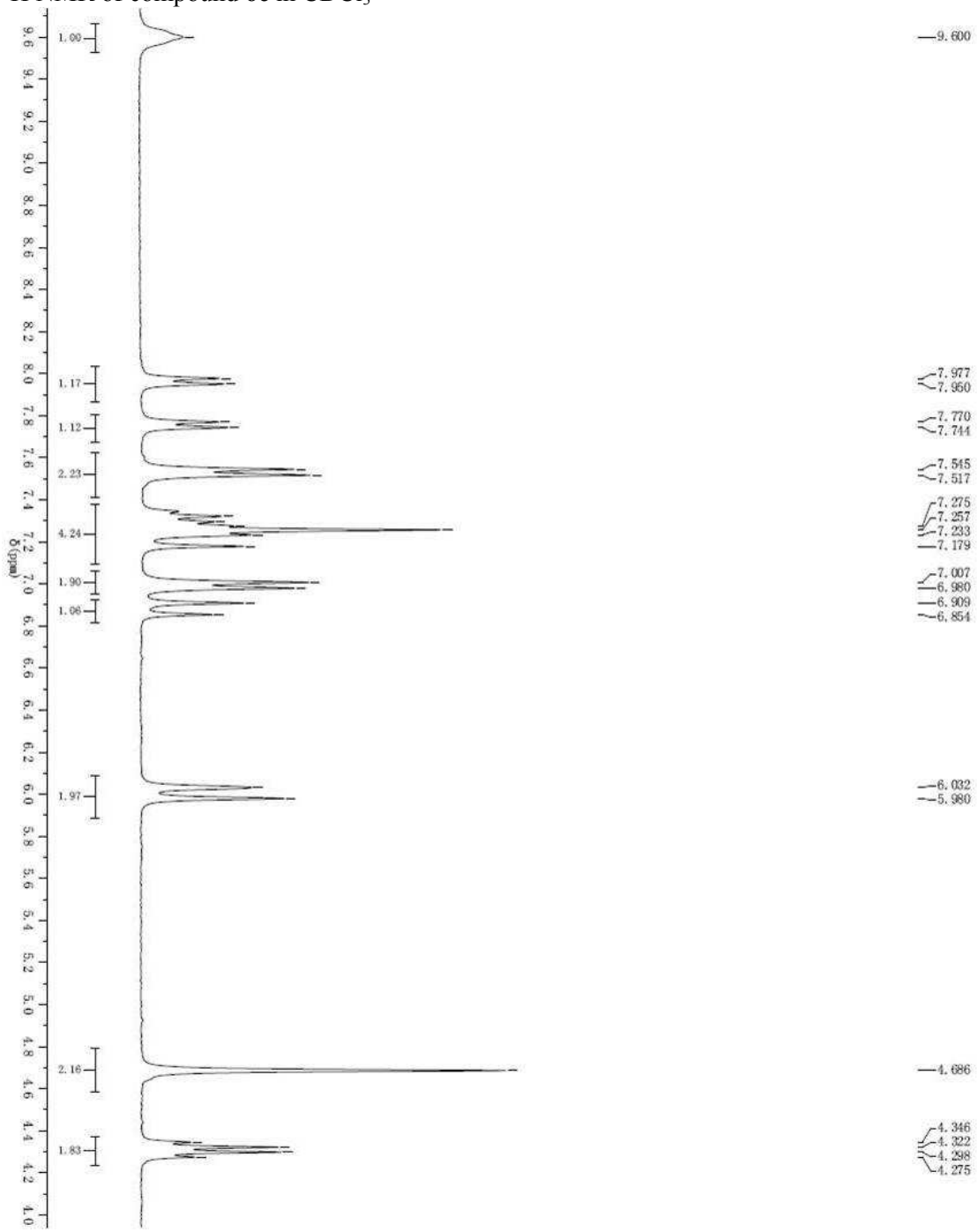

δ (ppm)
2.08
2.05
2.82
2.02
1.96
2.88
2.63
2.99
9.00
4.645
4.322
4.299
4.275
4.252
2.910
2.731
2.709
2.684
2.661
2.516
2.491
2.466
2.434
2.352
2.203
1.533
1.334
1.311
1.288
1.256
1.232
1.205
1.179
1.154
0.000

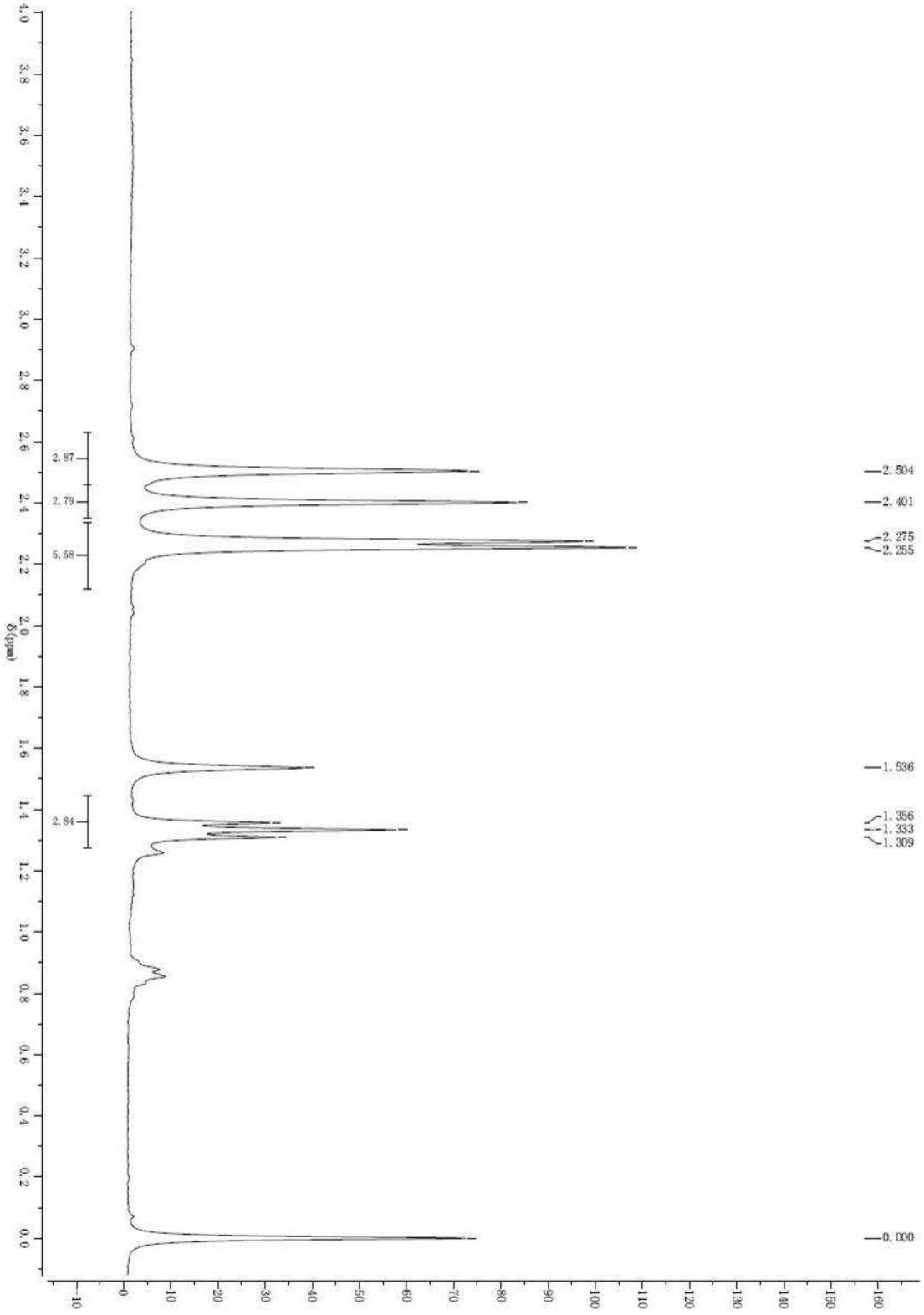
^{13}C NMR of compound **6b** in $CDCl_3$



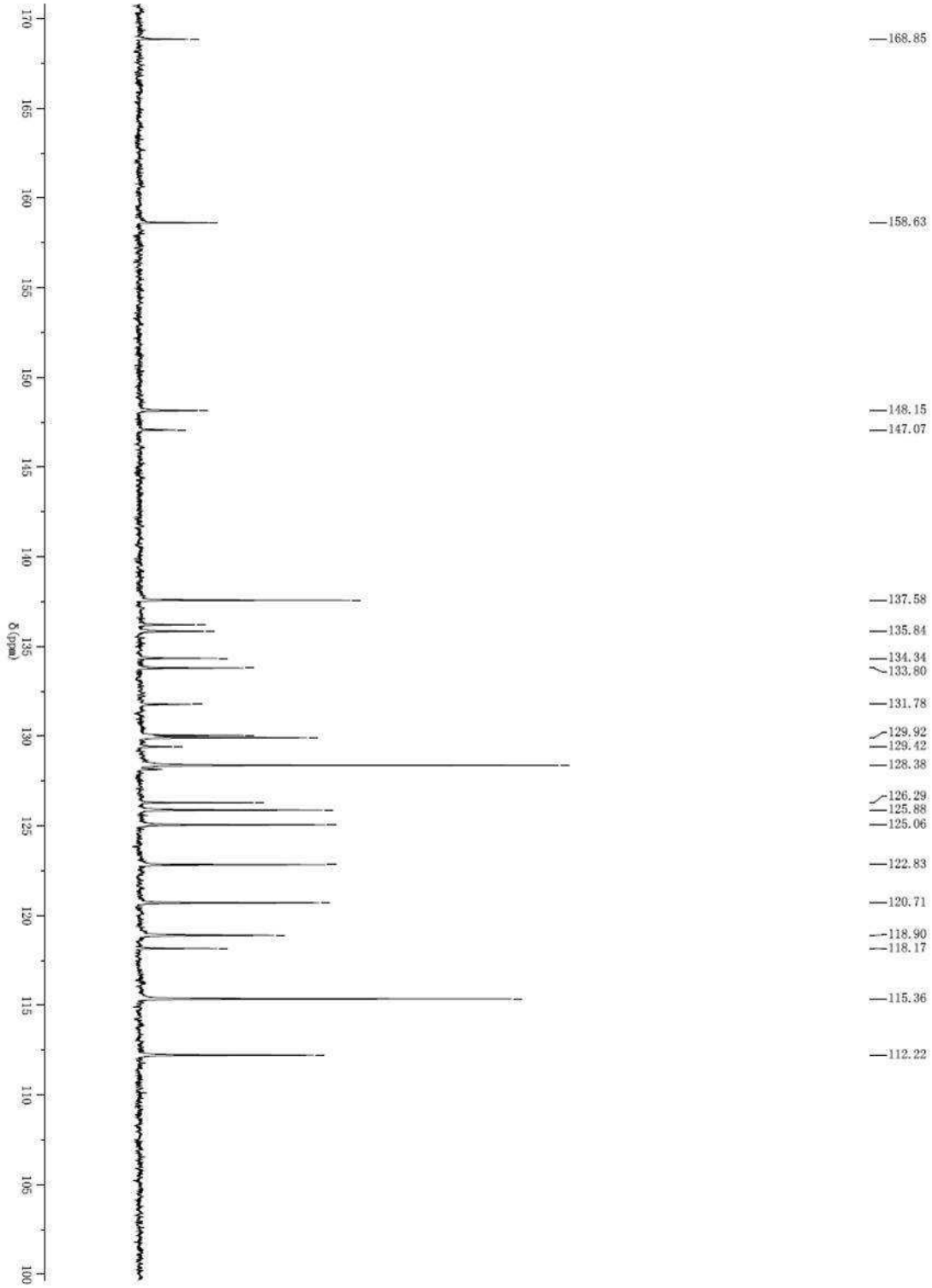

77.60
77.17
76.75
65.72
61.57
18.51
18.09
17.26
15.36
14.89
14.34
13.73
12.81
12.05
0.00
δ (ppm)

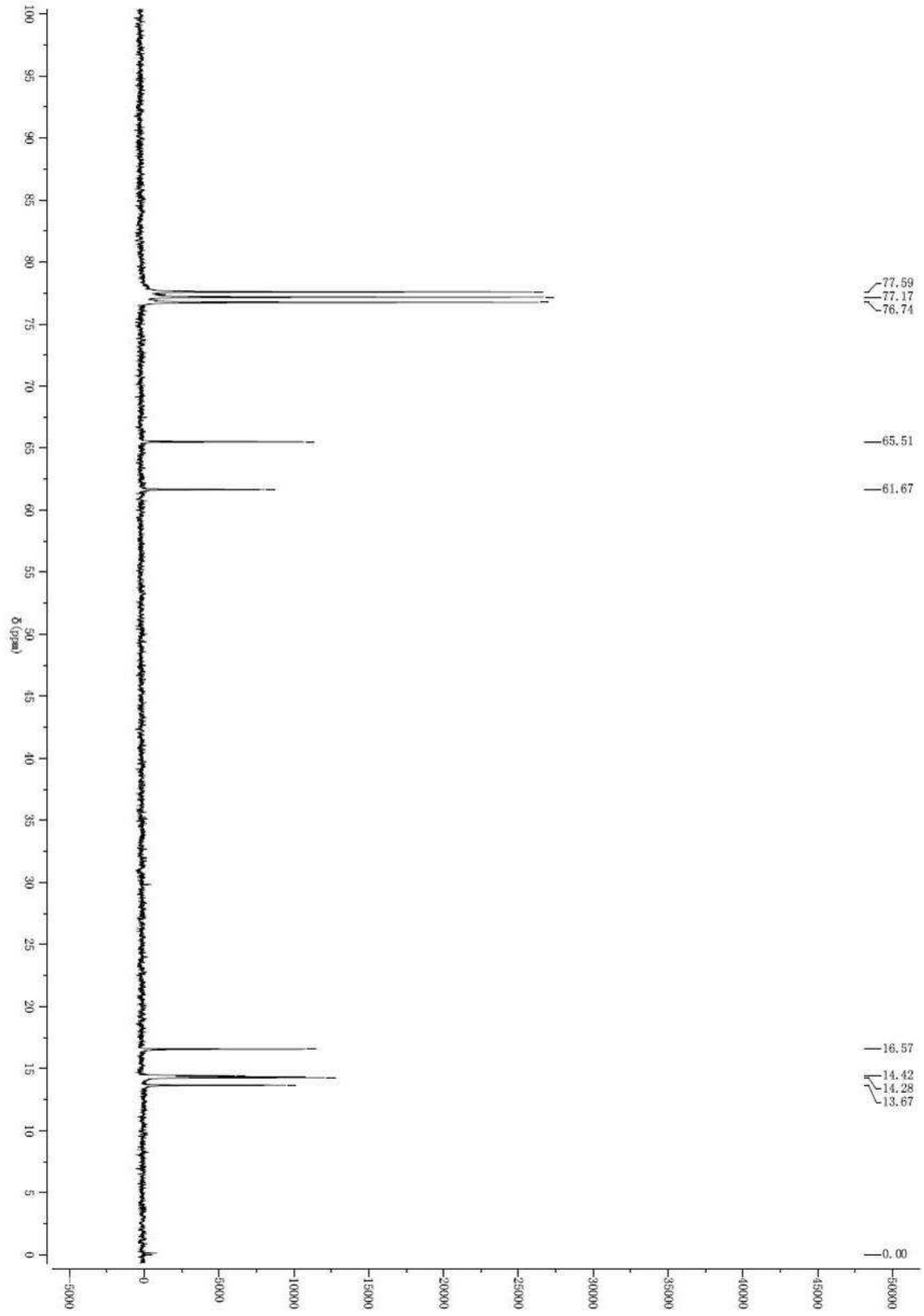
^{1}H NMR of compound **6c** in $CDCl_3$



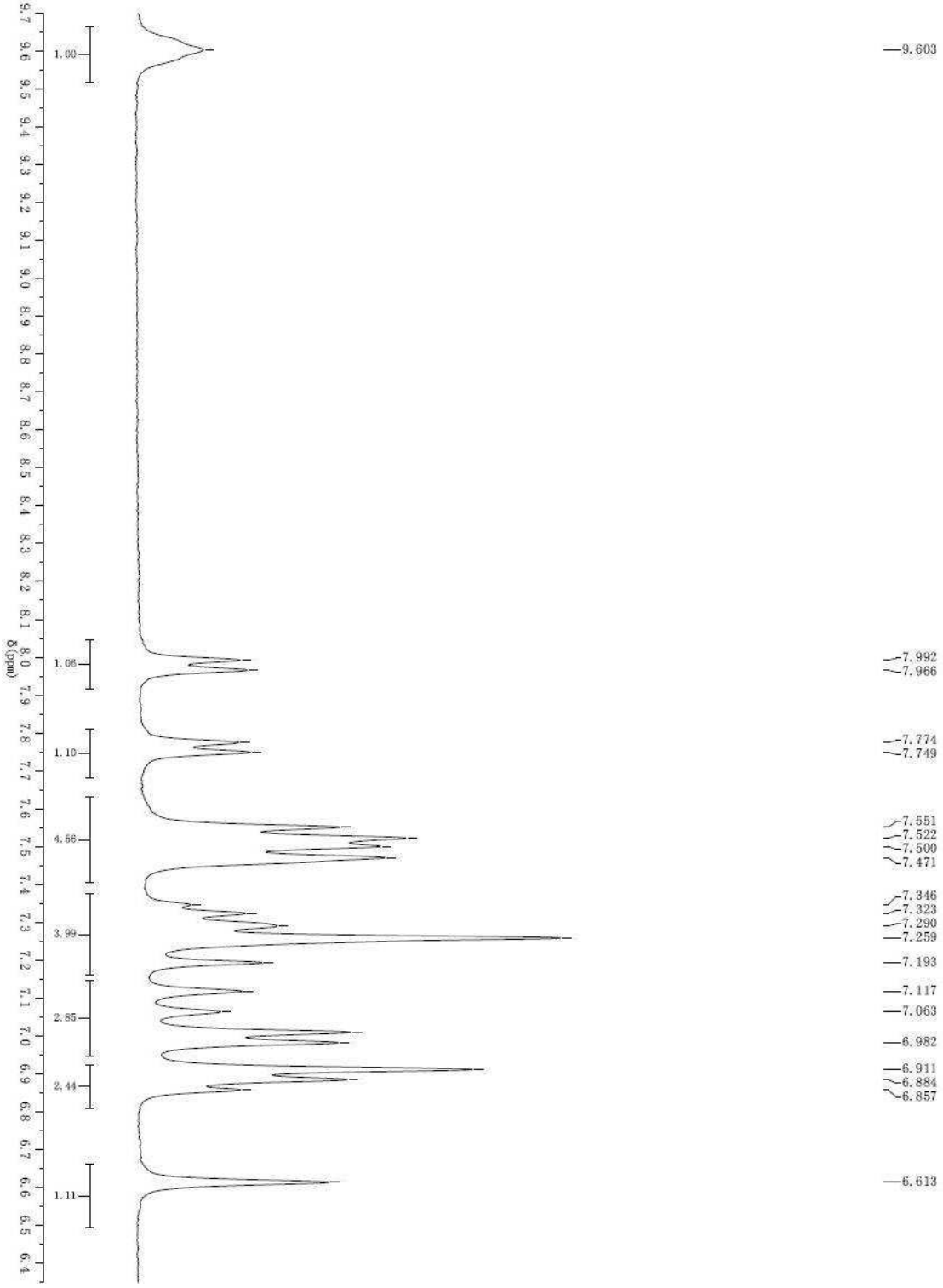

2.87
2.79
5.58
2.84
δ(ppm)
2.504
2.401
2.275
2.255
1.536
1.356
1.333
1.309
0.000

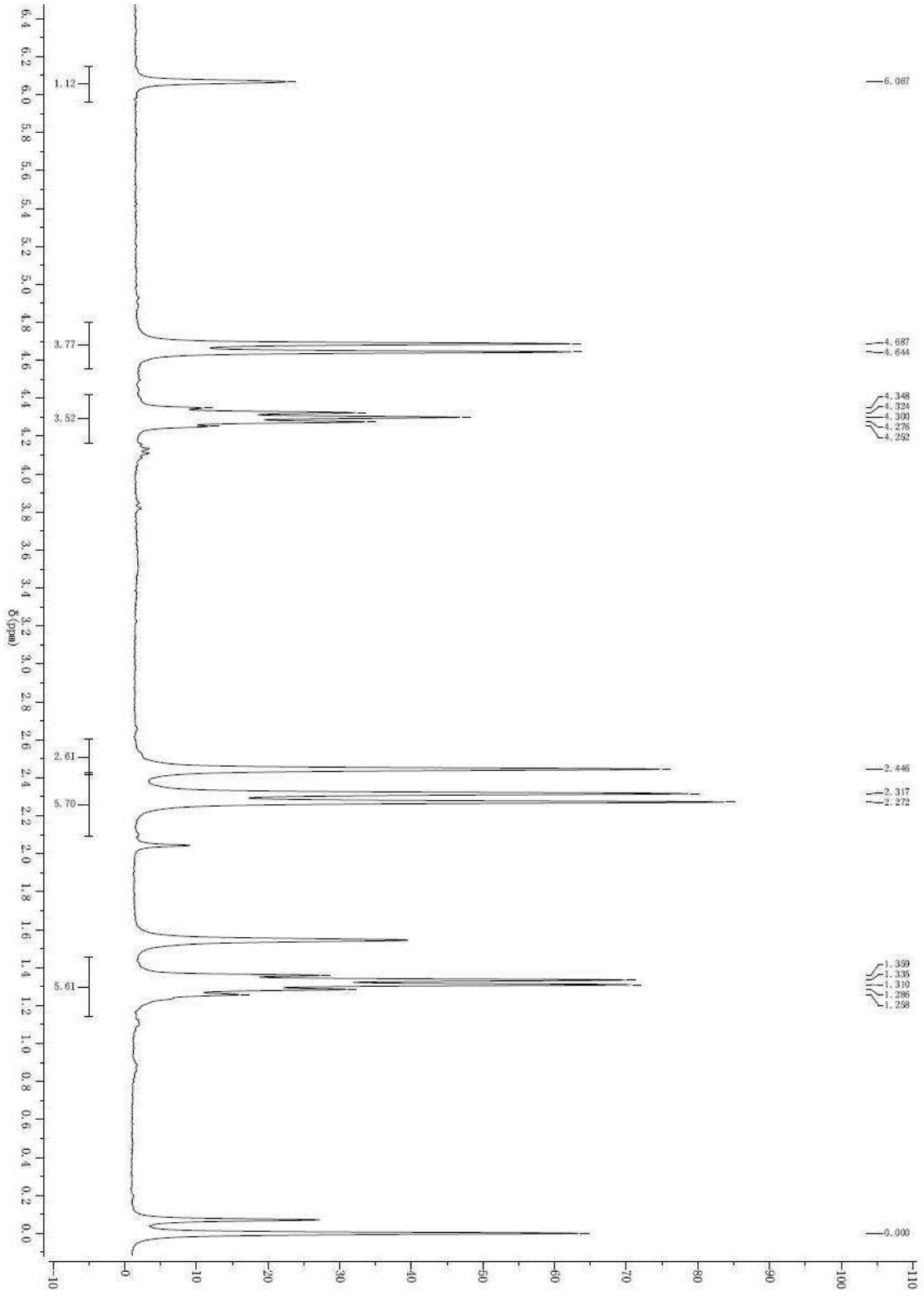
^{13}C NMR of compound **6c** in $CDCl_3$



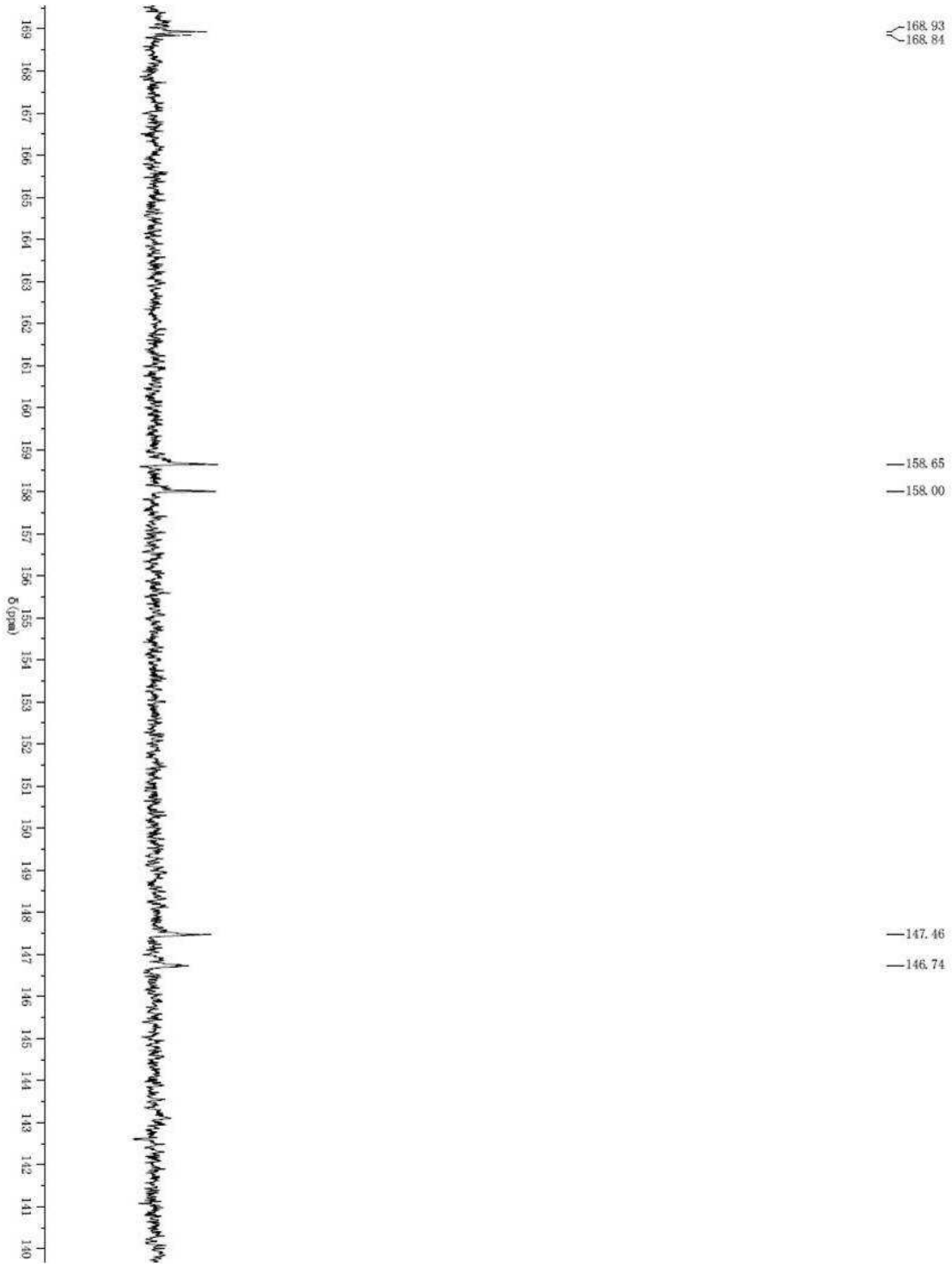

77.59
77.17
76.74
65.51
61.67
16.57
14.42
14.28
13.67
0.00
δ (ppm)

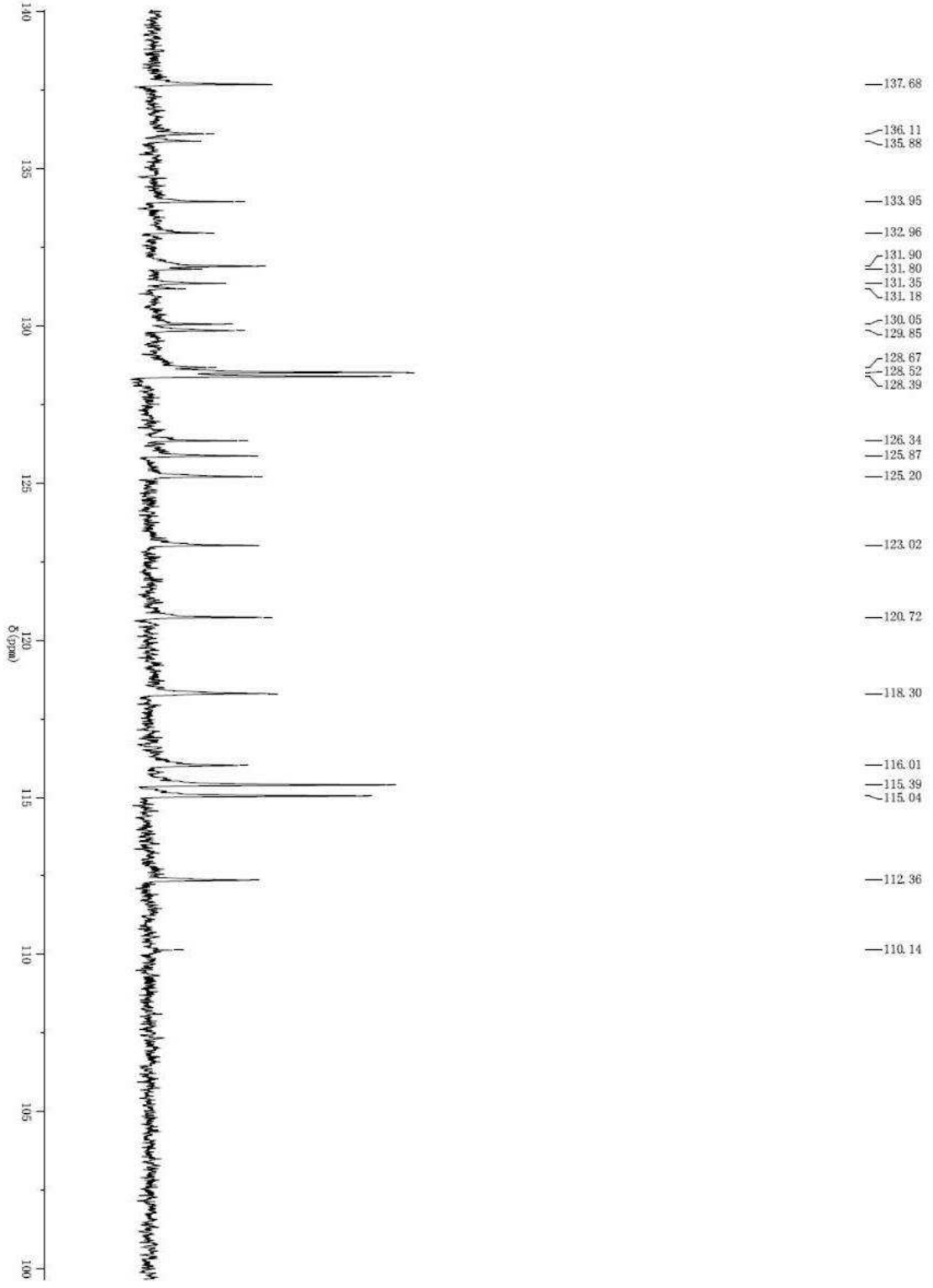
^{1}H NMR of compound **6d** in $CDCl_3$

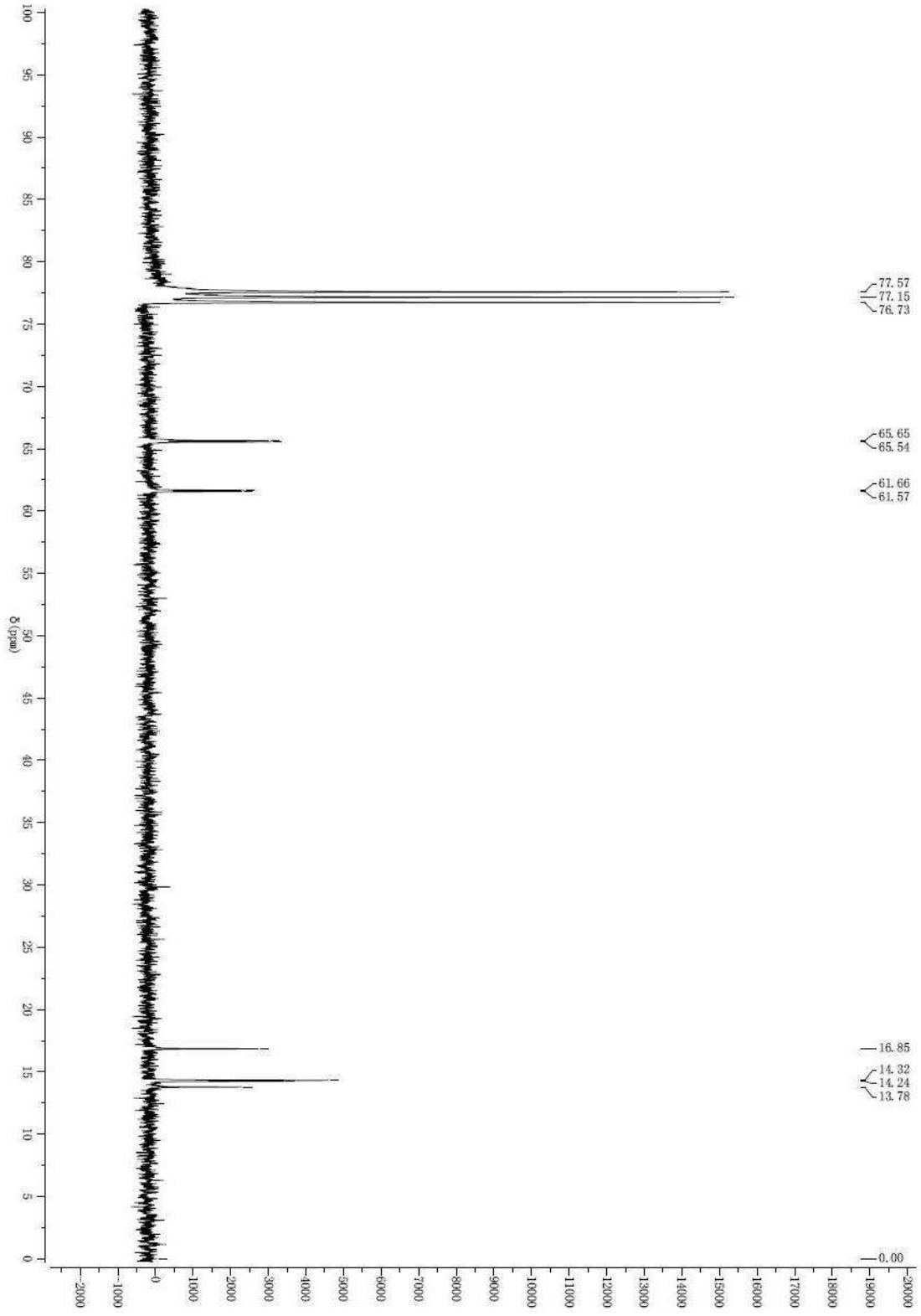



1.12
3.77
3.52
2.61
5.70
5.61
6.067
4.687
4.644
4.348
4.324
4.300
4.276
4.252
2.446
2.317
2.272
1.359
1.335
1.310
1.286
1.258
0.000
δ (ppm)

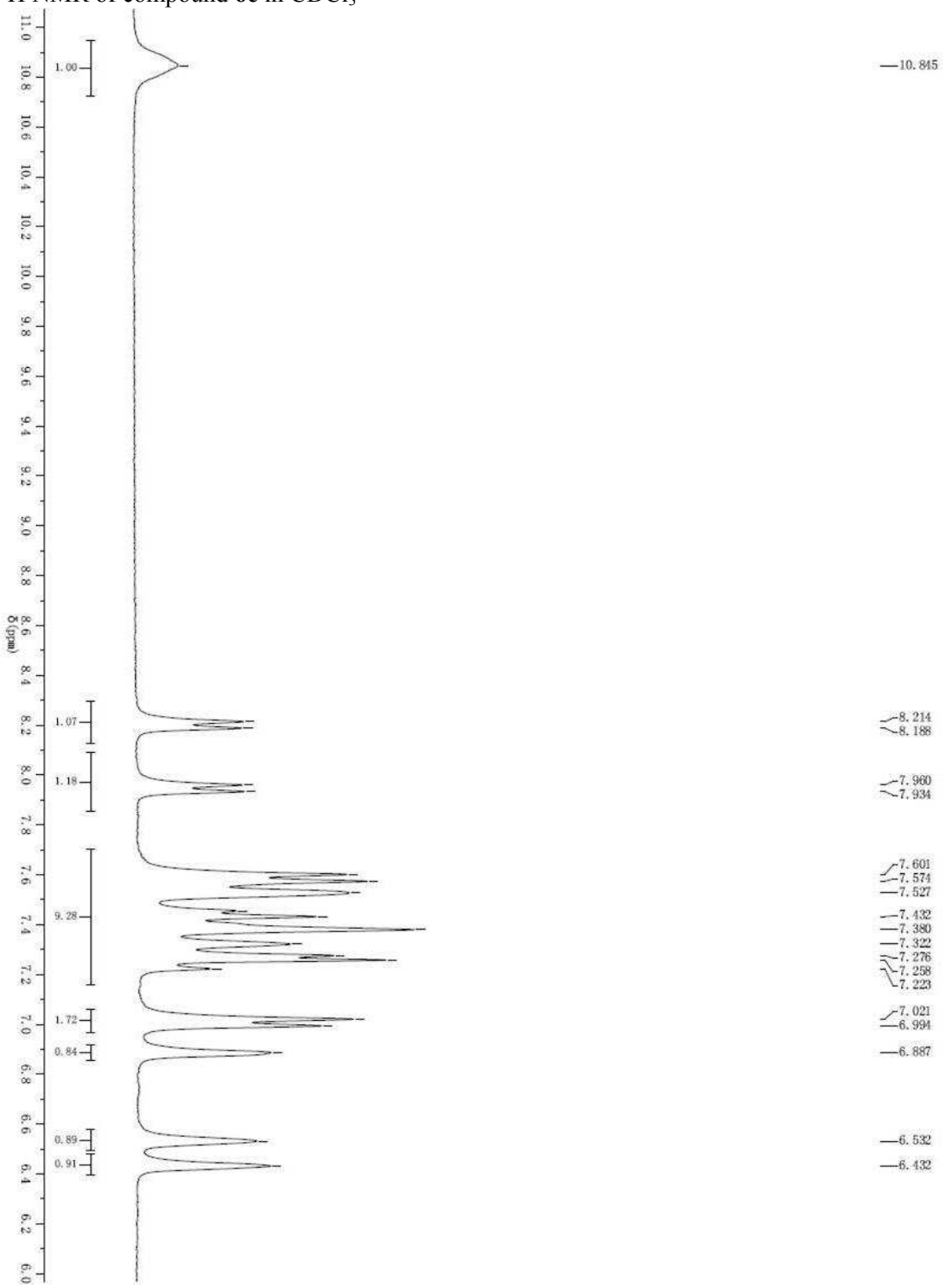
^{13}C NMR of compound **6d** in $CDCl_3$

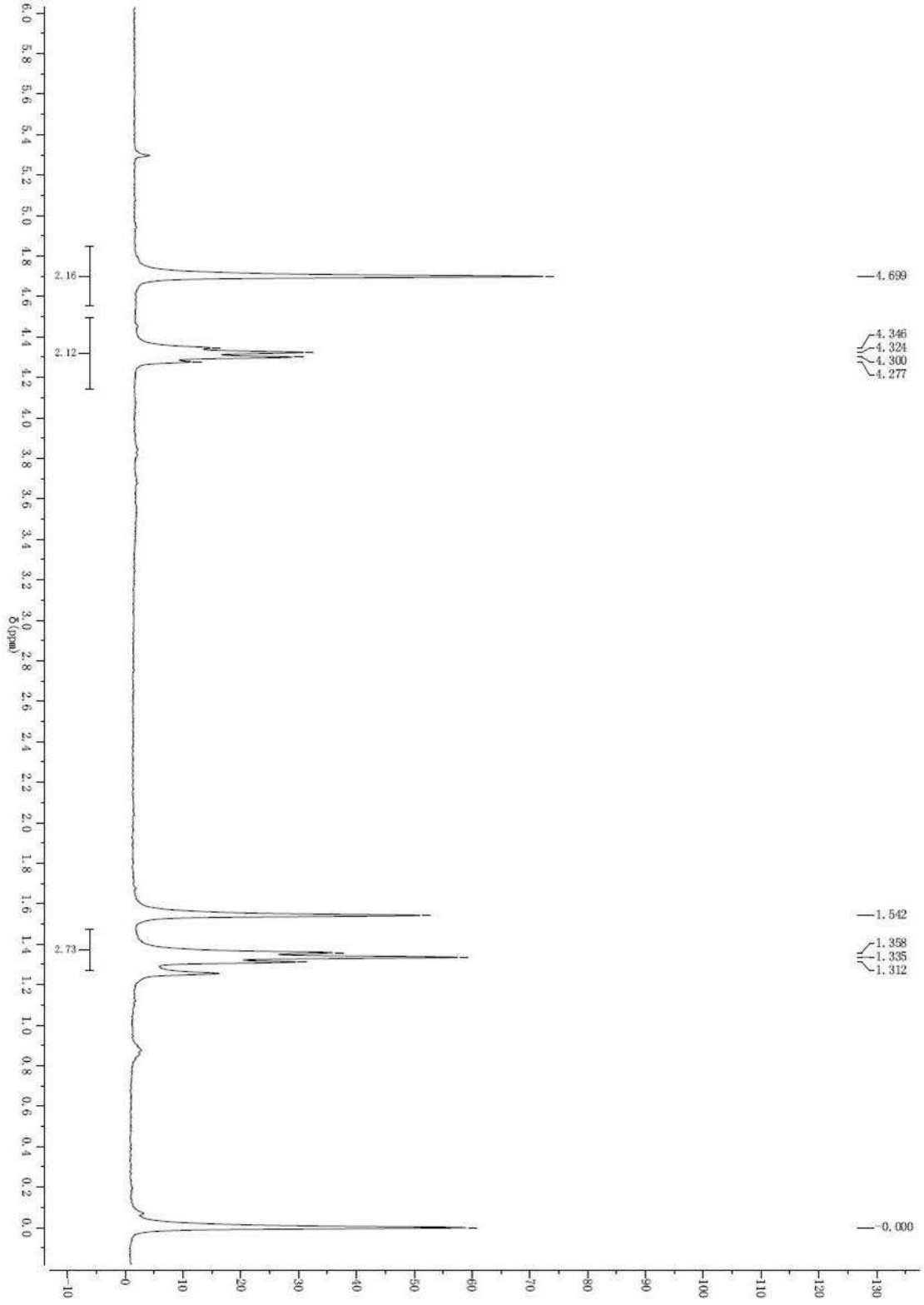



140
135
130
125
120
115
110
105
100
δ(ppm)
137.68
136.11
135.88
133.95
132.96
131.90
131.80
131.35
131.18
130.05
129.85
128.67
128.52
128.39
126.34
125.87
125.20
123.02
120.72
118.30
116.01
115.39
115.04
112.36
110.14

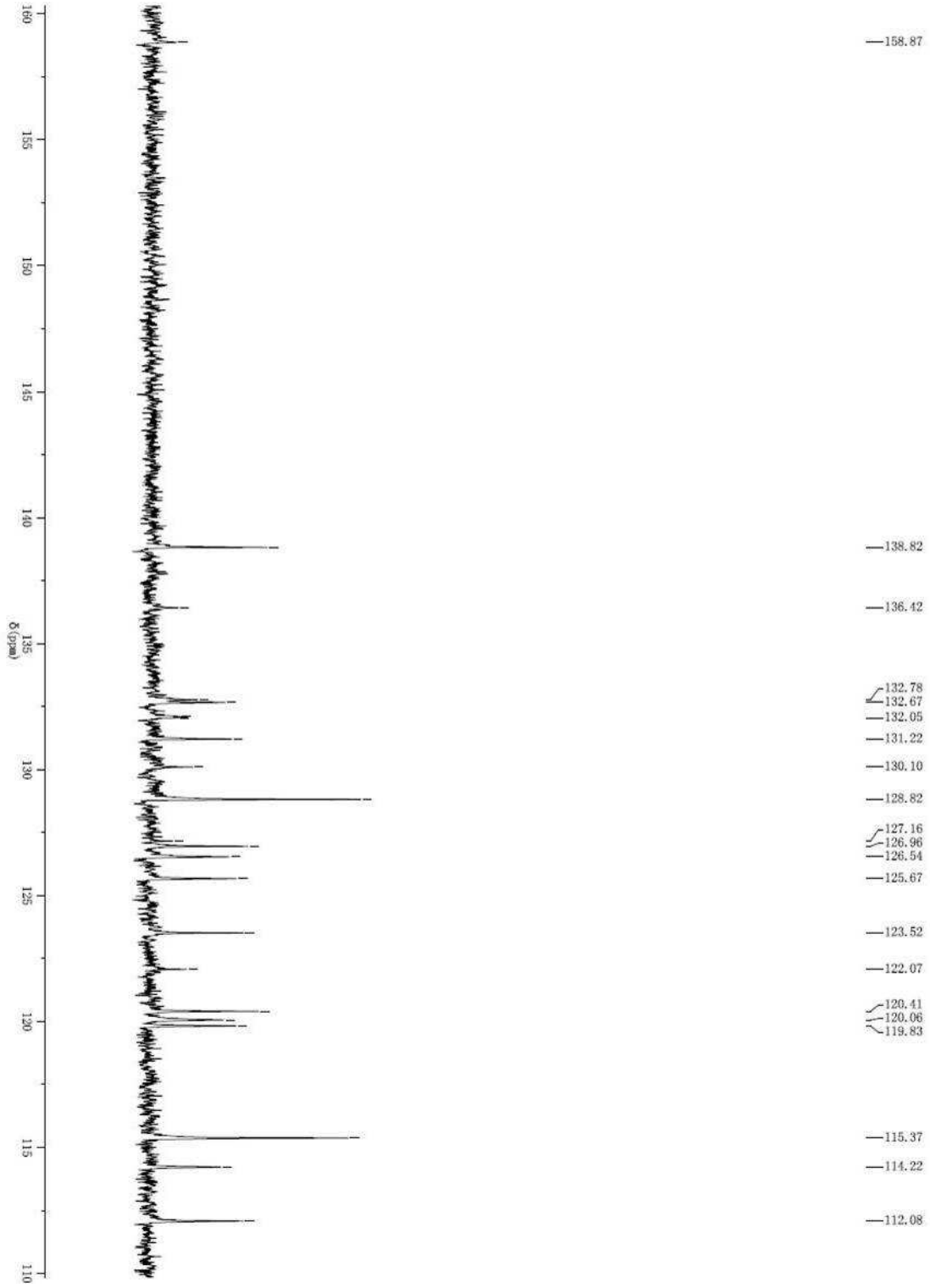

77.57
77.15
76.73
65.65
65.54
61.66
61.57
16.85
14.32
14.24
13.78
0.00
δ (ppm)

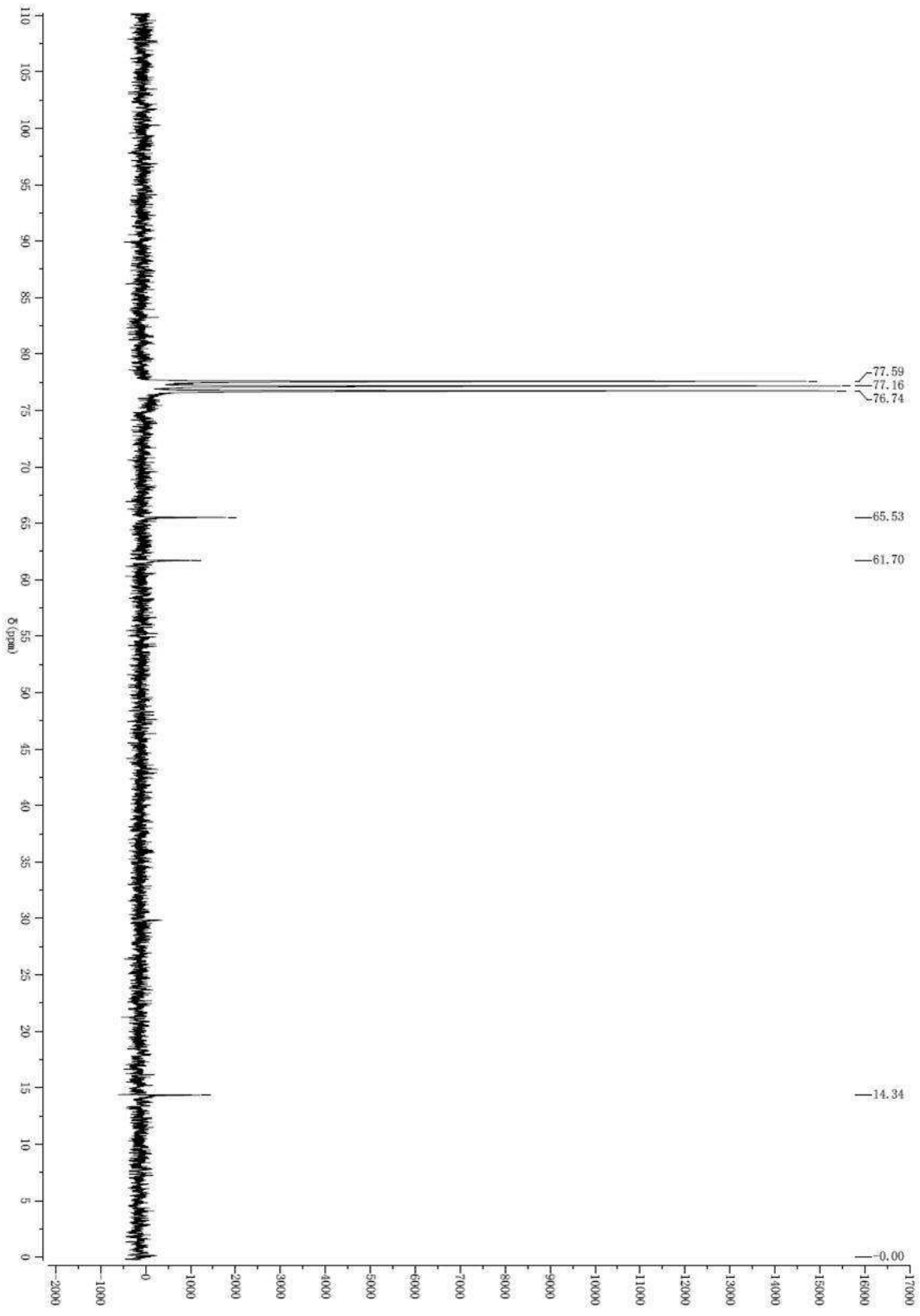
^{1}H NMR of compound **6e** in $CDCl_3$




2.16
2.12
2.73
4.699
4.346
4.324
4.300
4.277
1.542
1.358
1.335
1.312
0.000
δ(ppm)

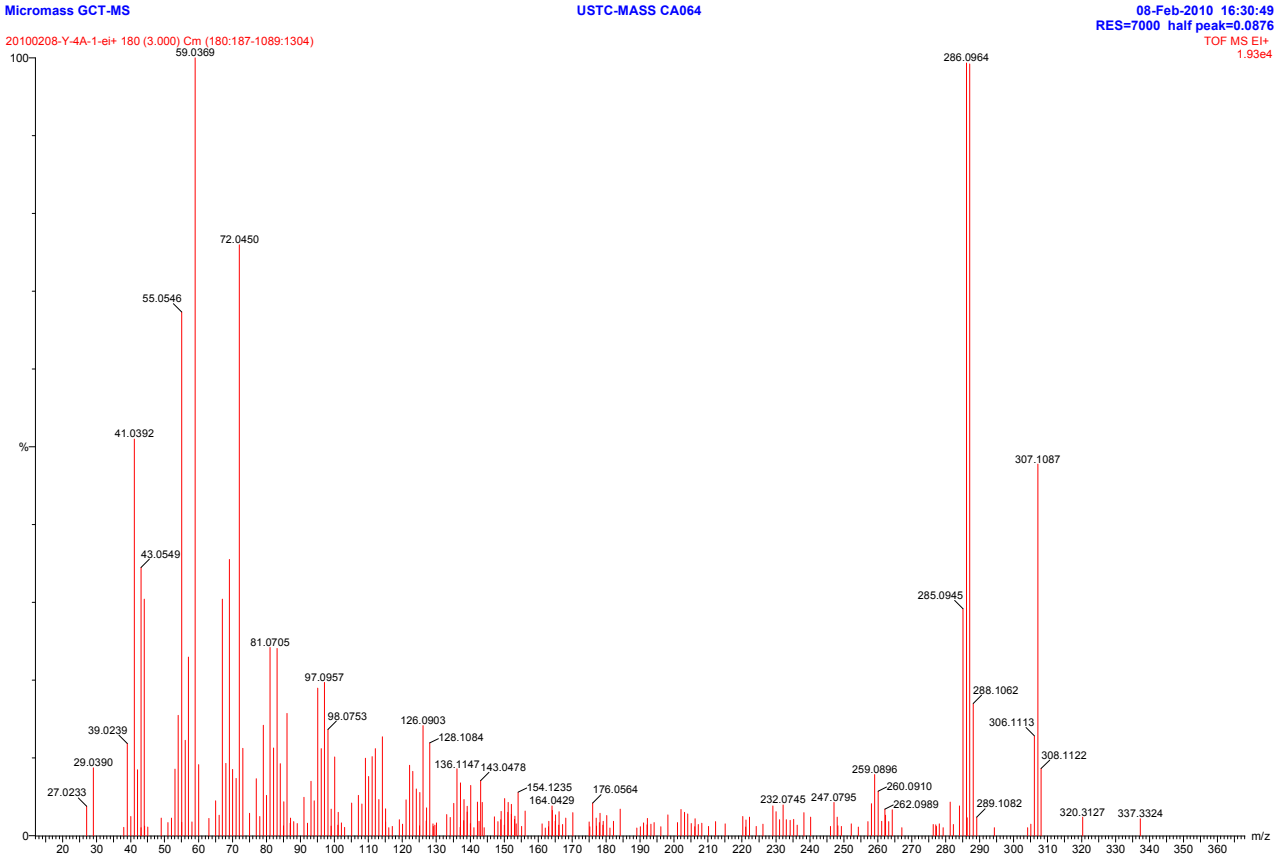
^{13}C NMR of compound **6e** in $CDCl_3$



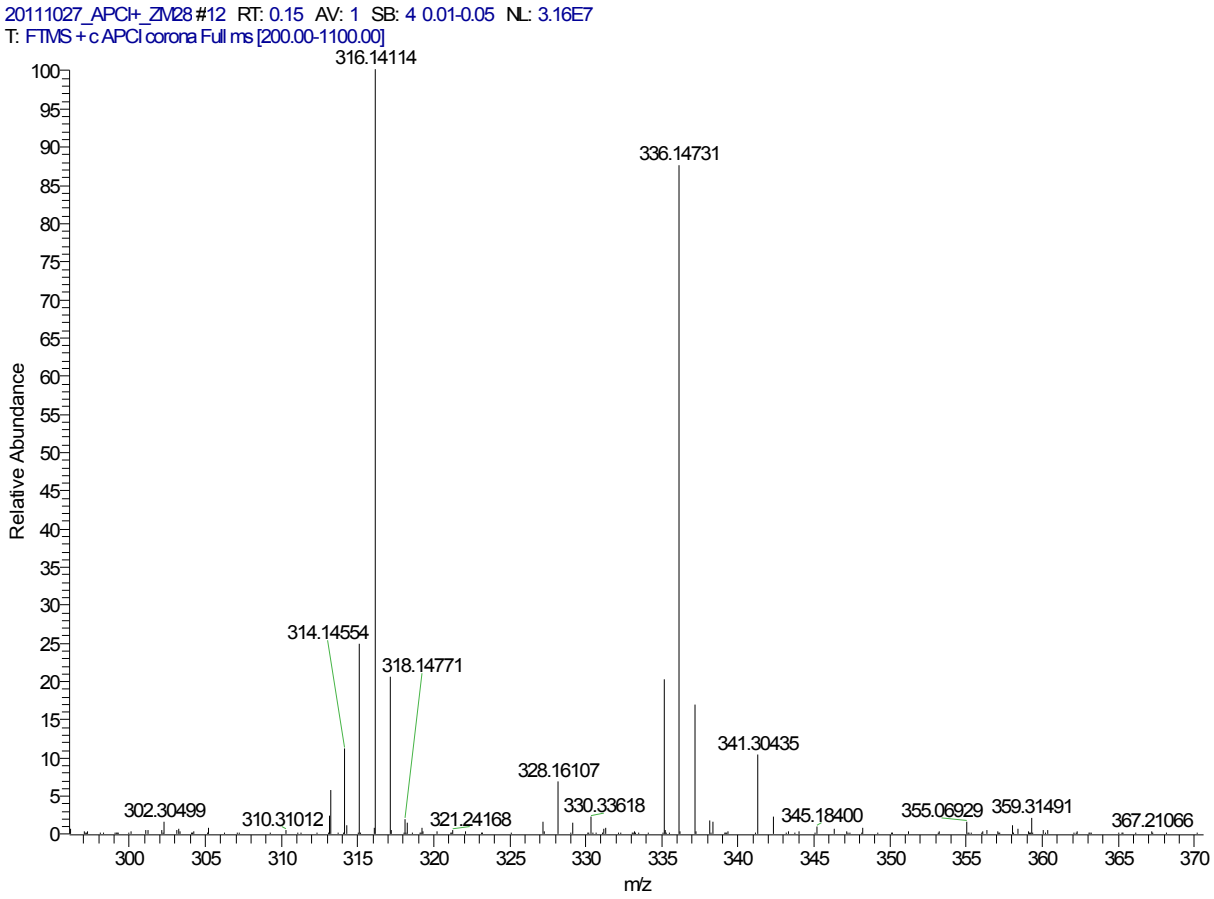

77.59
77.16
76.74
65.53
61.70
14.34
0.00
δ (ppm)

4. HRMS for all the compounds:

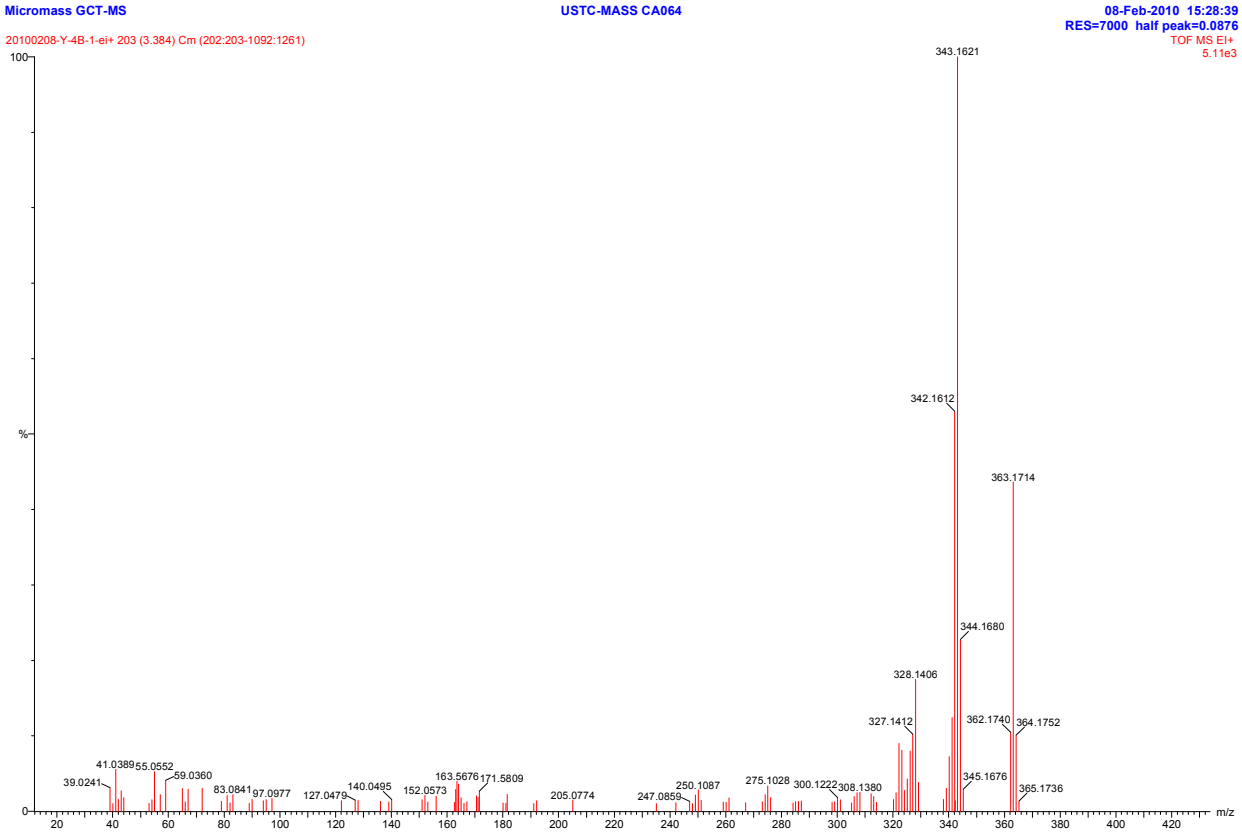
MS for 3aa



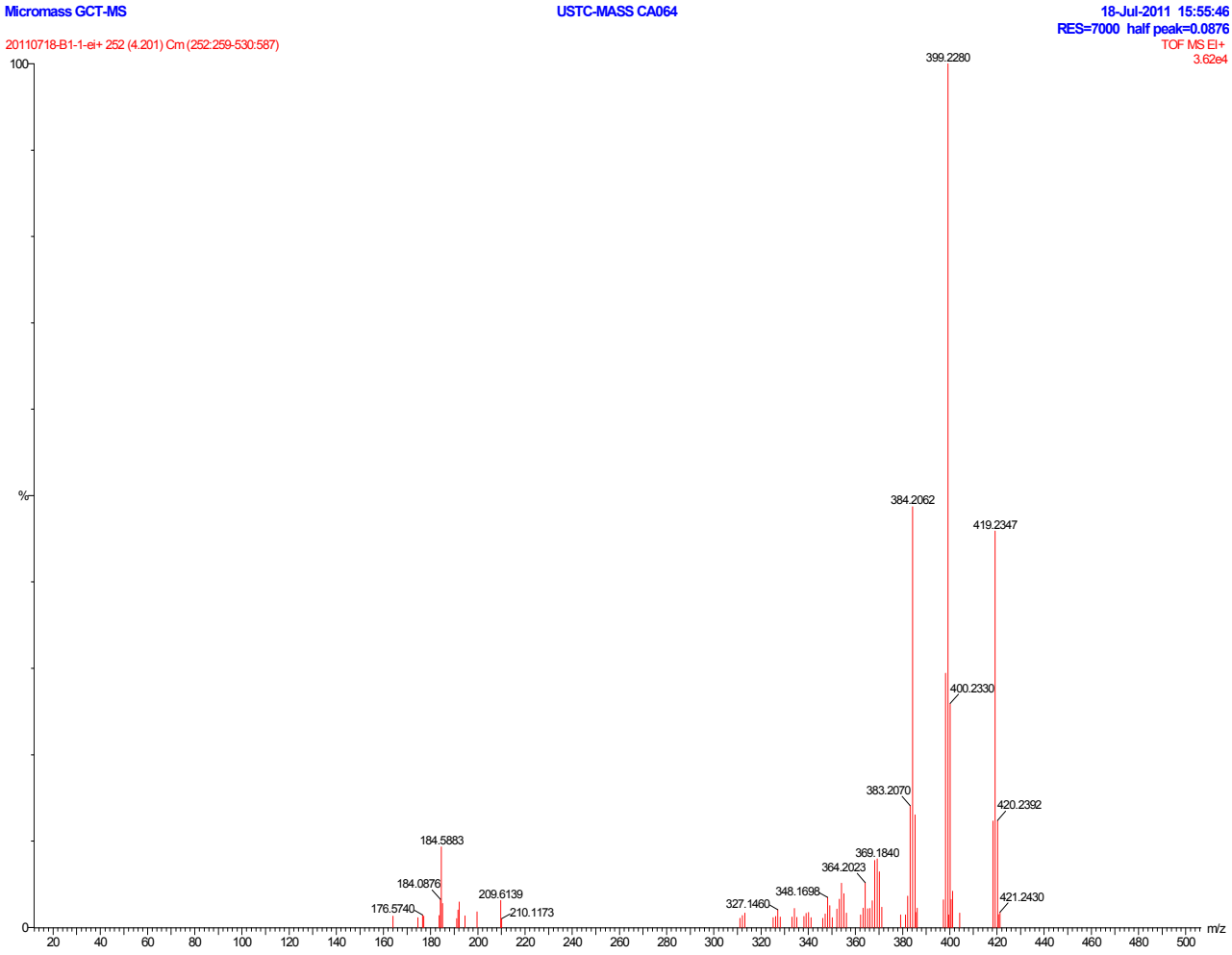
MS for 3ab


20111027_APCI+_ZM28 #12 RT: 0.15 AV: 1 SB: 4 0.01-0.05 NL: 3.16E7
T: FTMS + c APCI corona Full ms [200.00-1100.00]
316.14114
336.14731
314.14554
318.14771
341.30435
328.16107
330.33618
302.30499
310.31012
321.24168
345.18400
355.06929
359.31491
367.21066
Relative Abundance
m/z

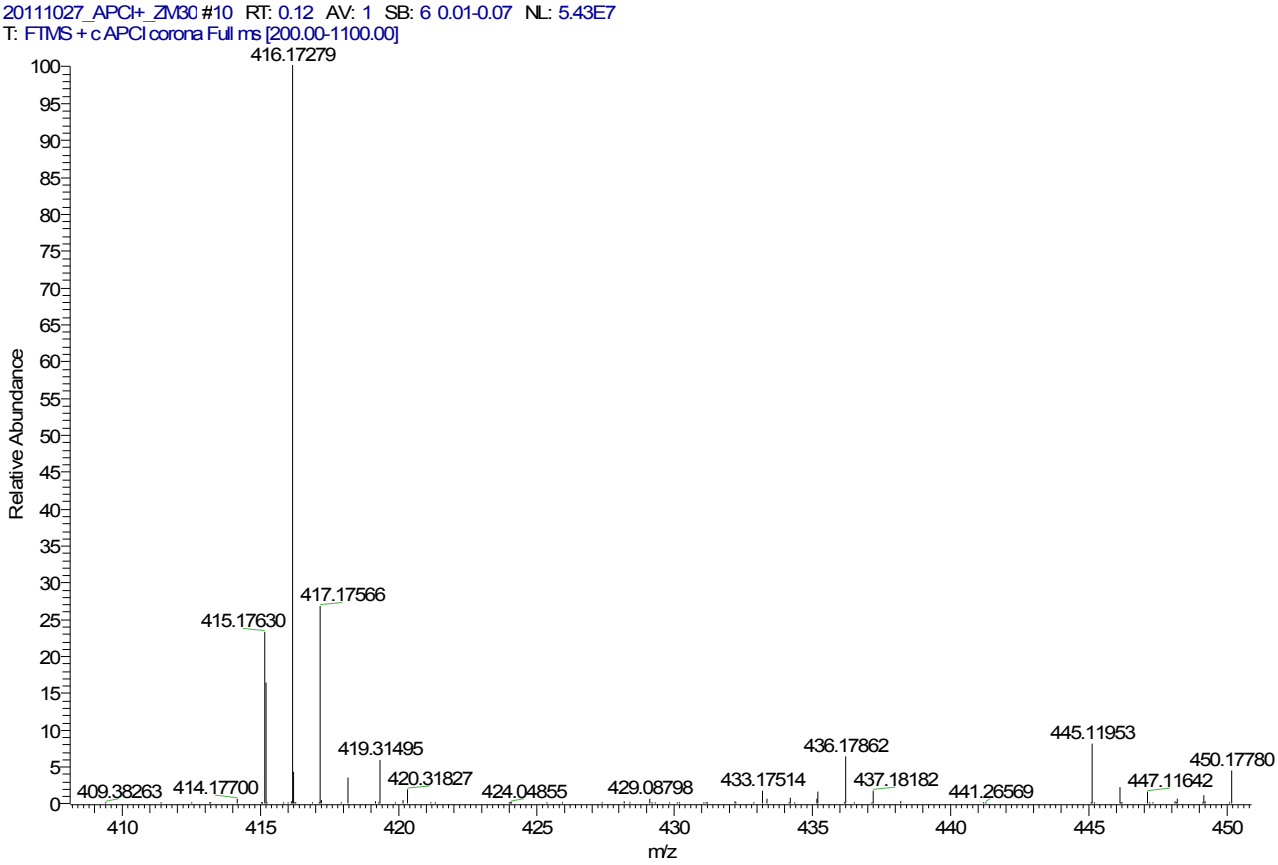
MS for 3ac


Micromass GCT-MS
USTC-MASS CA064
08-Feb-2010 15:28:39
RES=7000 half peak=0.0876
20100208-Y-4B-1-ei+ 203 (3.384) Cm (202:203-1092:1261)
TOF MS EI+
5.11e3
100
%
0
343.1621
342.1612
363.1714
344.1680
328.1406
327.1412
362.1740
364.1752
345.1676
365.1736
41.0389
55.0552
59.0360
39.0241
83.0841
97.0977
127.0479
140.0495
152.0573
163.5676
171.5809
205.0774
247.0859
250.1087
275.1028
300.1222
308.1380
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
m/z

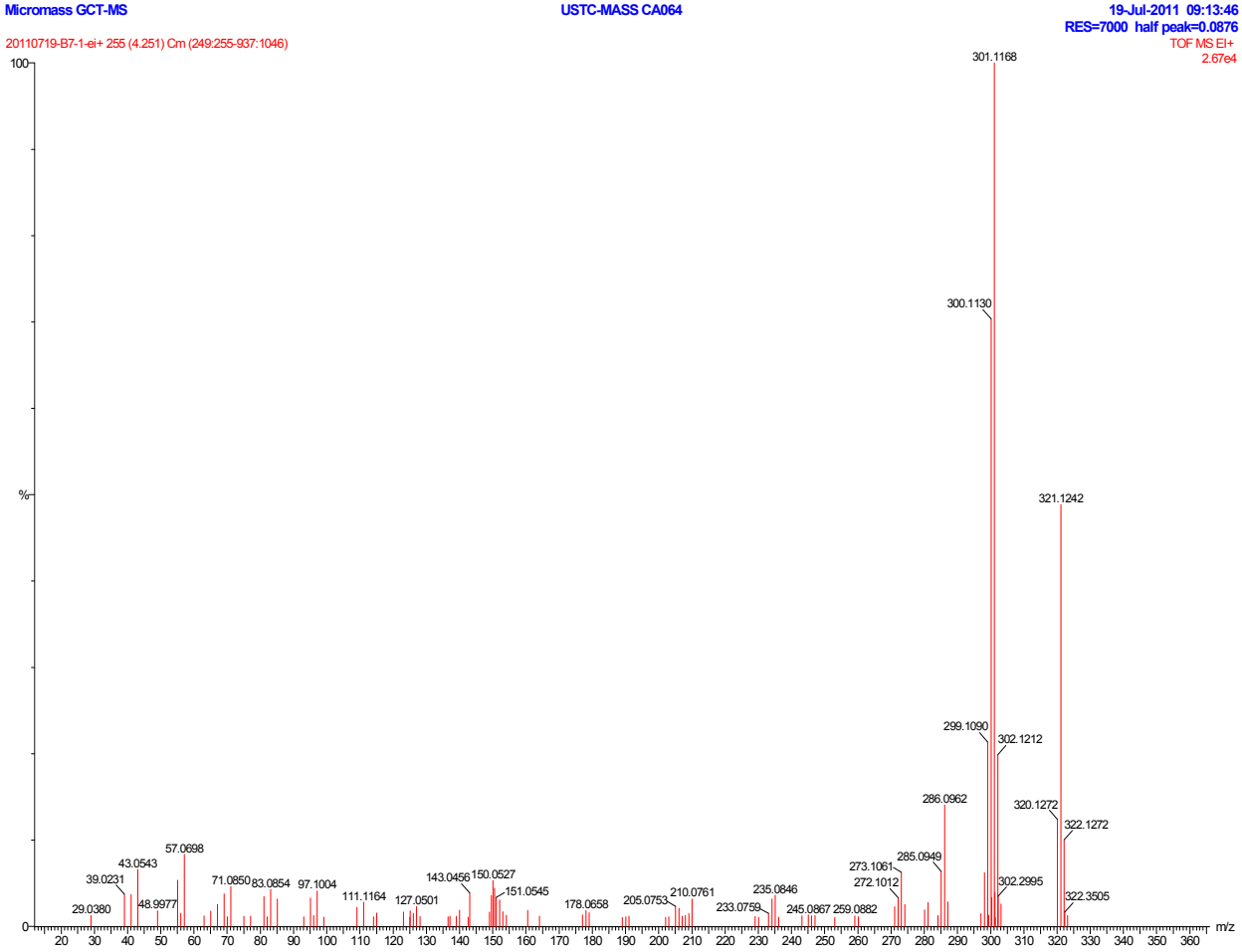
MS for 3ad


Micromass GCT-MS
USTC-MASS CA064
18-Jul-2011 15:55:46
RES=7000 half peak=0.0876
20110718-B1-1-ei+ 252 (4.201) Cm (252:259-530:587)
TOF MS EI+
3.62e4
100
%
0
399.2280
384.2062
419.2347
400.2330
383.2070
420.2392
184.5883
369.1840
364.2023
184.0876
209.6139
348.1698
176.5740
210.1173
327.1460
421.2430
m/z
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500

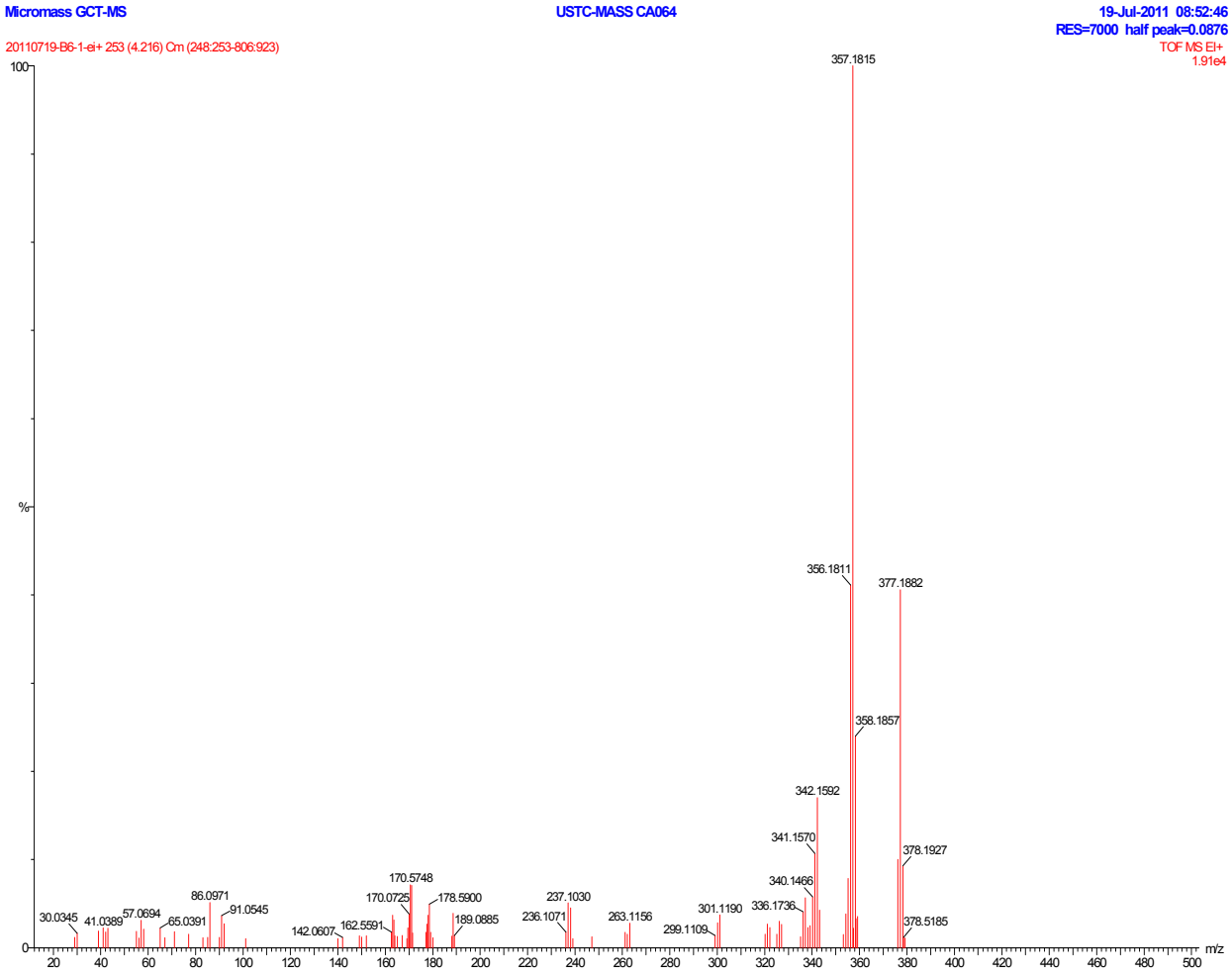
MS for 3ae


20111027_APCI+_ZM30 #10 RT: 0.12 AV: 1 SB: 6 0.01-0.07 NL: 5.43E7
T: FTMS + c APCI corona Full ms [200.00-1100.00]
Relative Abundance
m/z
416.17279
417.17566
415.17630
419.31495
420.31827
409.38263
414.17700
424.04855
429.08798
433.17514
436.17862
437.18182
441.26569
445.11953
447.11642
450.17780

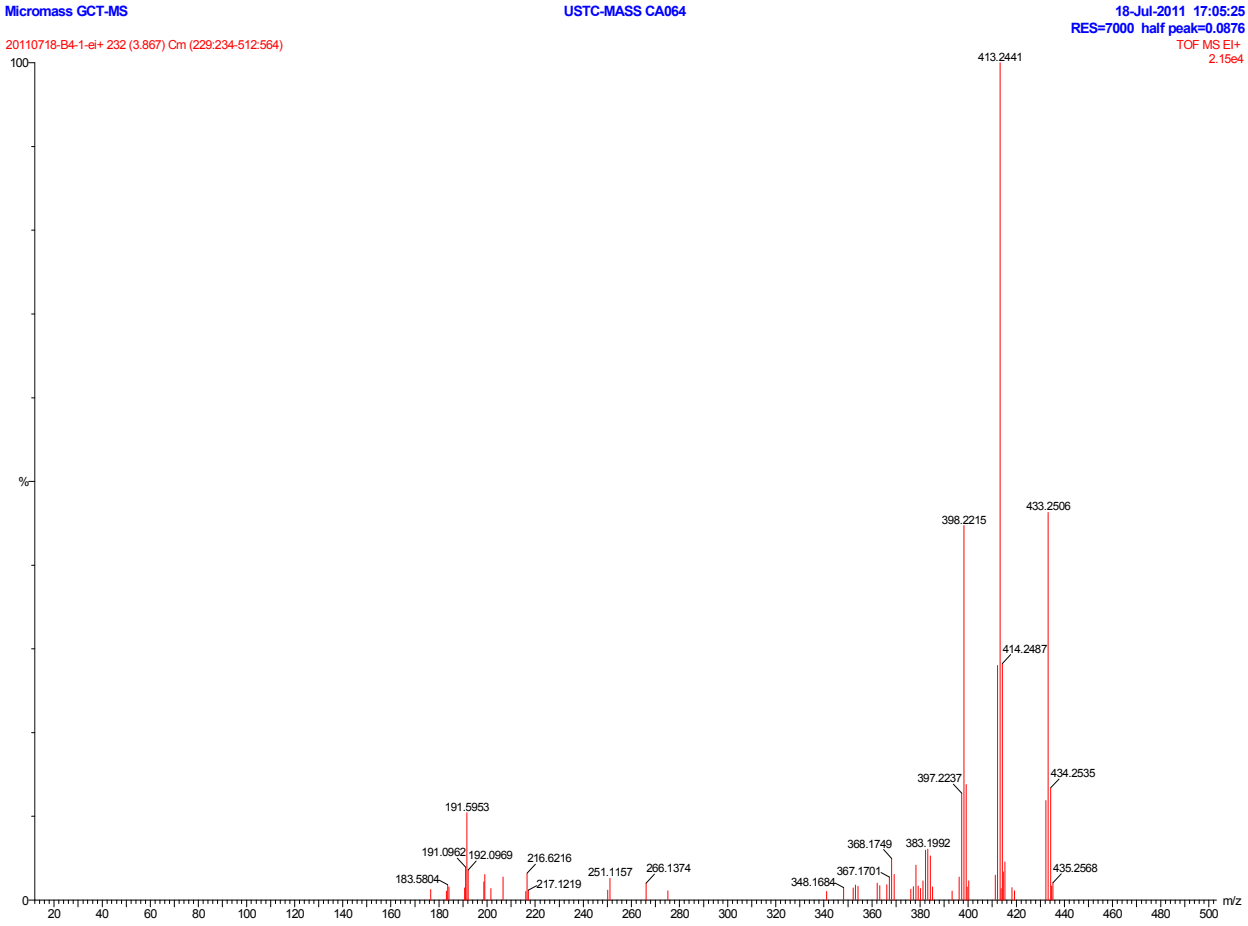
MS for 3ba


Micromass GCT-MS
USTC-MASS CA064
19-Jul-2011 09:13:46
RES=7000 half peak=0.0876
20110719-B7-1-ei+ 255 (4.251) Cm (249:255-937:1046)
TOF MS EI+
2.67e4
100
%
0
301.1168
300.1130
321.1242
299.1090
302.1212
286.0962
320.1272
322.1272
285.0949
273.1061
272.1012
302.2995
322.3505
57.0698
43.0543
39.0231
48.9977
29.0380
71.0850
83.0854
97.1004
111.1164
127.0501
143.0456
150.0527
151.0545
178.0658
205.0753
210.0761
233.0759
235.0846
245.0867
259.0882
m/z

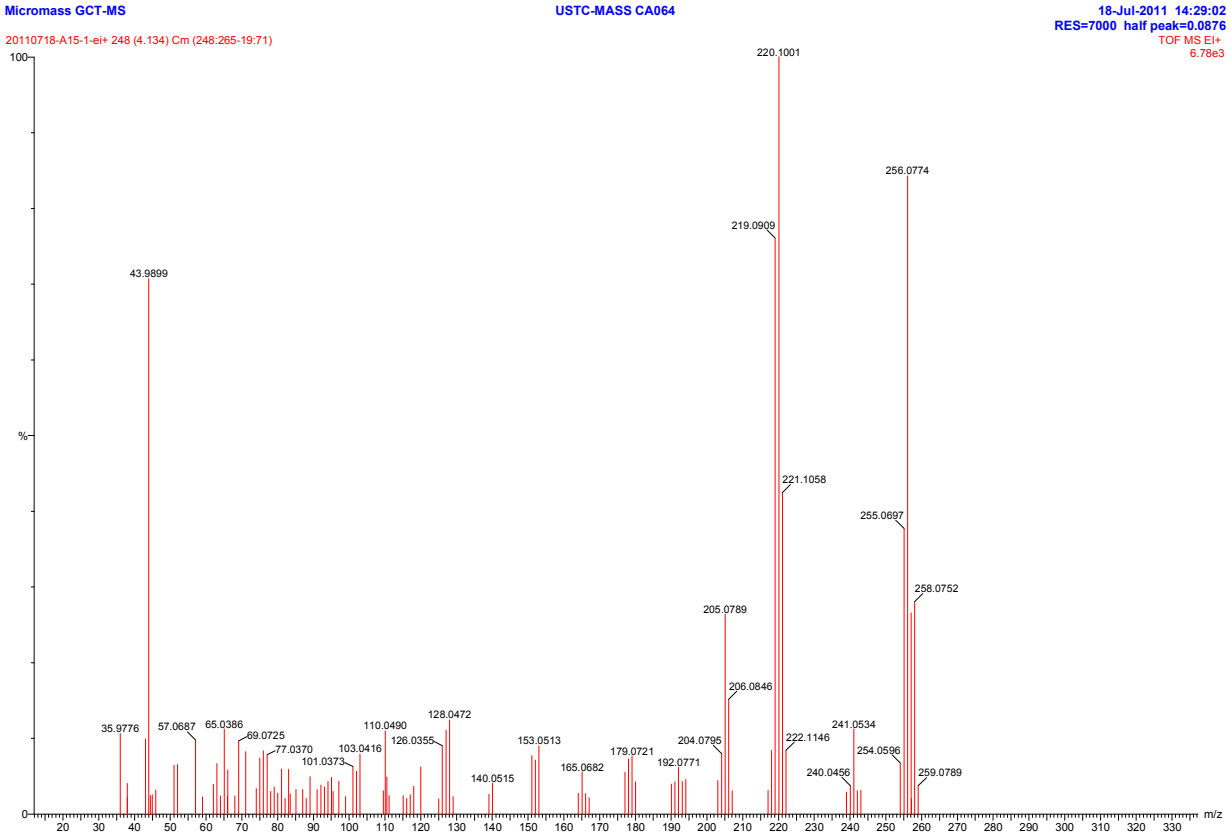
MS for 3bc


Micromass GCT-MS
USTC-MASS CA064
19-Jul-2011 08:52:46
RES=7000 half peak=0.0876
20110719-B6-1-ei+ 253 (4.216) Cm (248:253-806:923)
TOF MS EI+
1.91e4
100
%
0
m/z
357.1815
356.1811
377.1882
358.1857
342.1592
341.1570
378.1927
340.1466
336.1736
378.5185
170.5748
170.0725
178.5900
189.0885
86.0971
91.0545
30.0345
41.0389
57.0694
65.0391
142.0607
162.5591
237.1030
236.1071
263.1156
301.1190
299.1109
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500

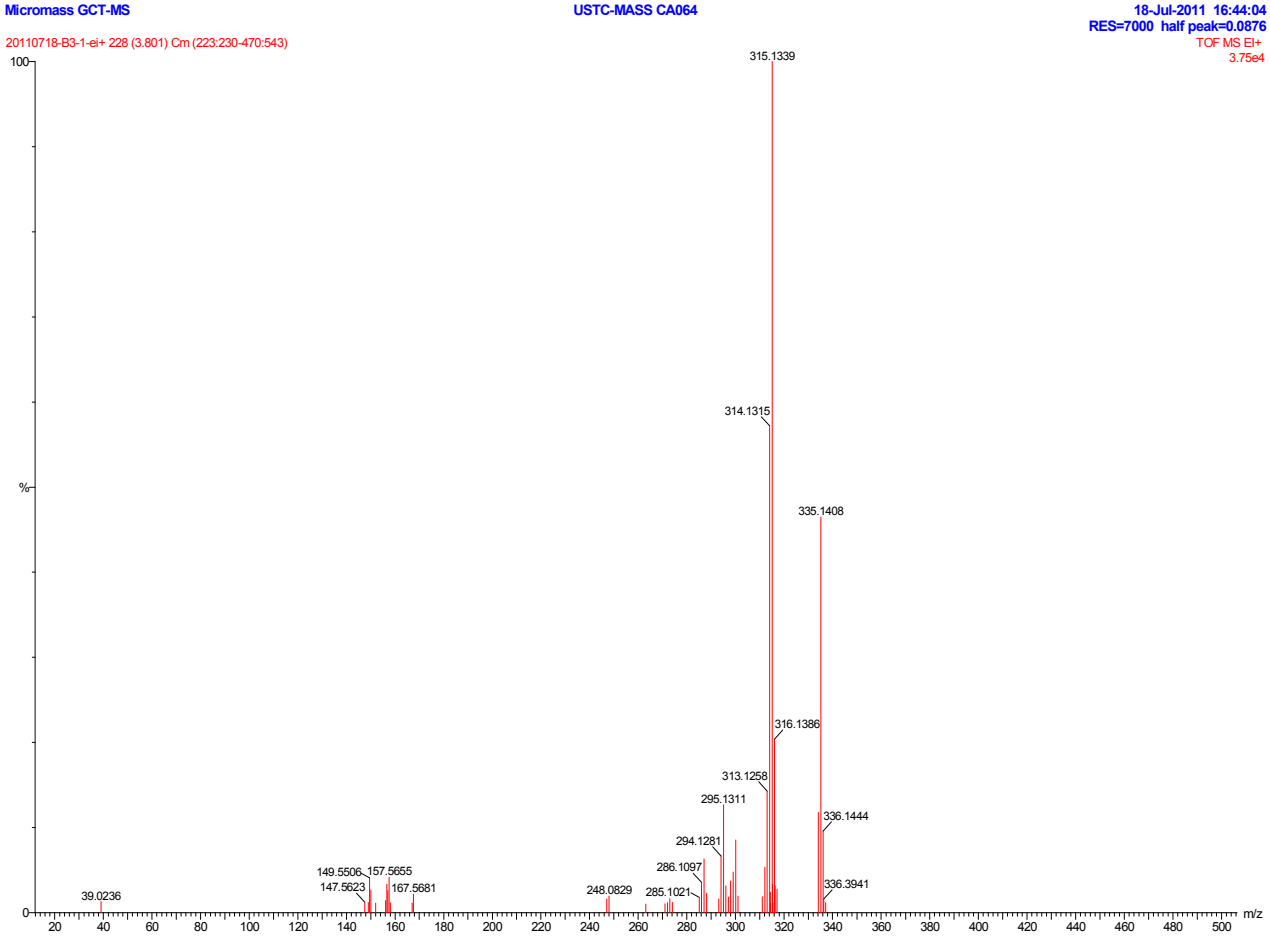
MS for 3bd


Micromass GCT-MS
USTC-MASS CA064
18-Jul-2011 17:05:25
RES=7000 half peak=0.0876
20110718-B4-1-ei+ 232 (3.867) Cm (229:234-512:564)
TOF MS EI+
2.15e4
100
%
0
413.2441
433.2506
398.2215
414.2487
434.2535
397.2237
435.2568
191.5953
191.0962
192.0969
216.6216
183.5804
217.1219
251.1157
266.1374
368.1749
383.1992
367.1701
348.1684
m/z
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500

MS for 4


Micromass GCT-MS
USTC-MASS CA064
18-Jul-2011 14:29:02
RES=7000 half peak=0.0876
20110718-A15-1-ei+ 248 (4.134) Cm (248:265-19:71)
TOF MS EI+
6.78e3
100
%
0
m/z
220.1001
256.0774
219.0909
43.9899
221.1058
255.0697
258.0752
205.0789
206.0846
128.0472
110.0490
126.0355
35.9776
57.0687
65.0386
69.0725
77.0370
103.0416
101.0373
153.0513
165.0682
140.0515
179.0721
204.0795
192.0771
222.1146
241.0534
254.0596
240.0456
259.0789

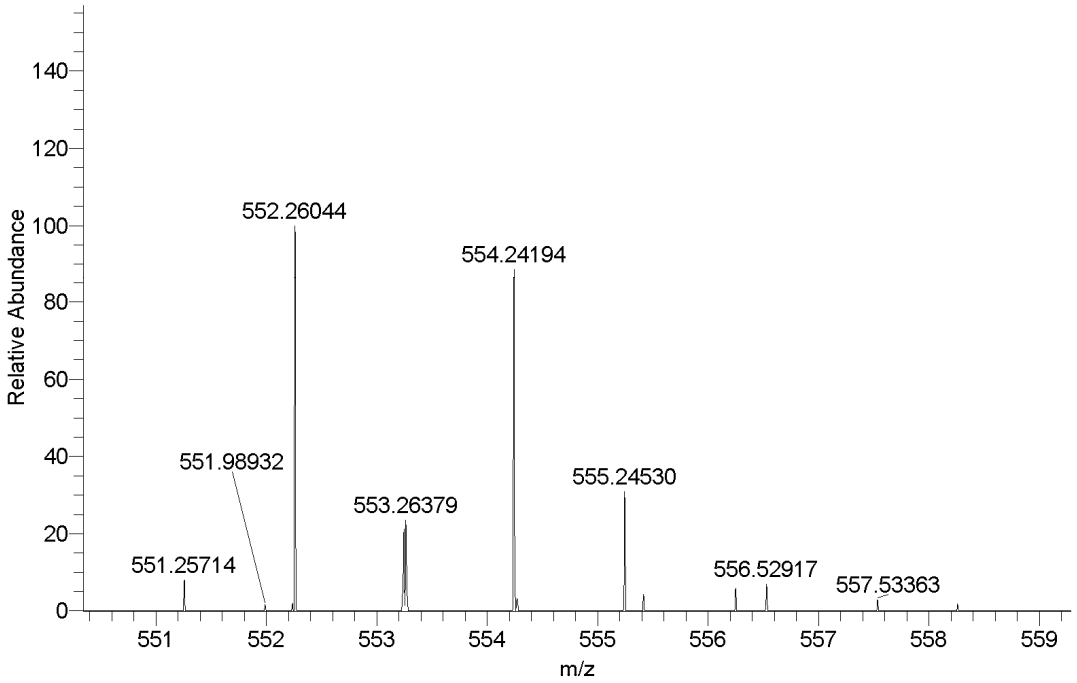
MS for 5


Micromass GCT-MS
USTC-MASS CA064
18-Jul-2011 16:44:04
RES=7000 half peak=0.0876
20110718-B3-1-ei+ 228 (3.801) Cm (223:230-470:543)
TOF MS EI+
3.75e4
100
%
0
315.1339
314.1315
335.1408
316.1386
313.1258
295.1311
336.1444
294.1281
286.1097
336.3941
149.5506
157.5655
147.5623
167.5681
248.0829
285.1021
39.0236
20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500
m/z

MS for 6a

E:\data\20110715\20110715_HESI+_B15 2011-7-15 15:47:03

20110715_HESI+_B15 #13 RT: 0.17 AV: 1 NL: 5.67E6
T: FTMS + p ESI Full ms [300.00-1000.00]



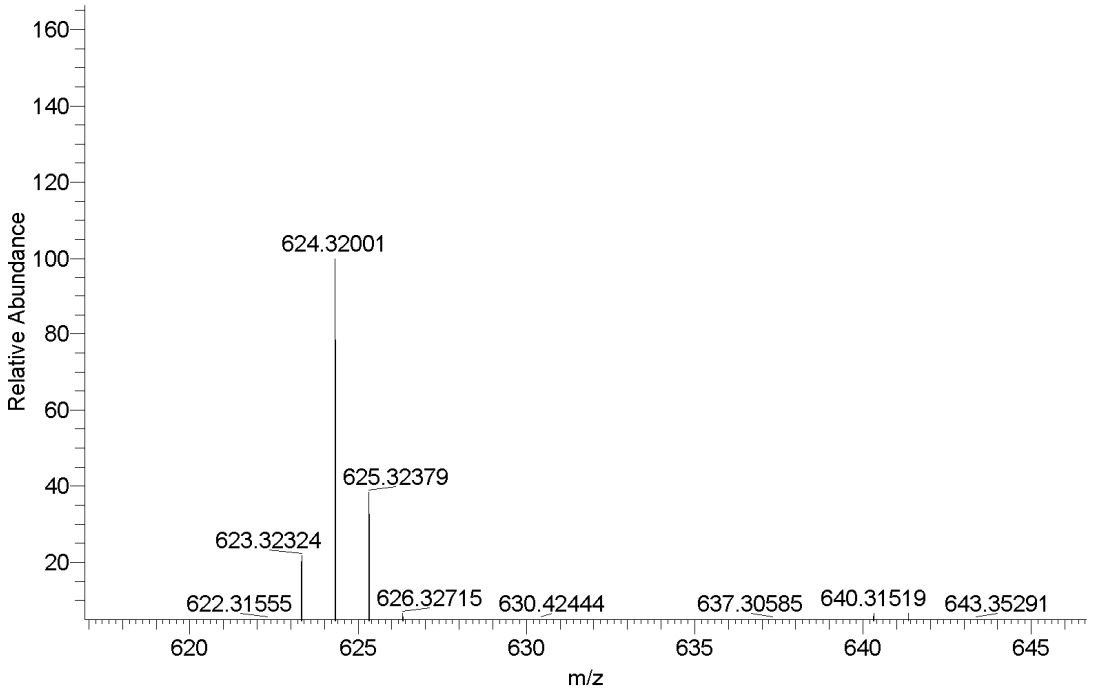
20110715_HESI+_B15#13 RT: 0.17
T: FTMS + p ESI Full ms [300.00-1000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
537.53522	19139094.0	26.80	537.49994	35.28	$C_{32}H_{62}N_3BF_2$
538.53876	6786591.5	9.50	538.49063	48.13	$C_{33}H_{62}N_3F_2$
539.55078	16240074.0	22.74	539.47920	71.58	$C_{31}H_{60}ON_3BF_2$
540.53479	5540454.5	7.76	540.48703	47.76	$C_{31}H_{61}ON_3BF_2$
540.55414	5946008.0	8.33	540.48703	67.11	$C_{31}H_{61}ON_3BF_2$
546.55670	5382773.5	7.54	546.48046	76.24	$C_{31}H_{62}O_2N_3F_2$
552.26044	5815521.5	8.14	552.26284	-2.40	$C_{33}H_{33}O_2N_3BF_2$
554.24194	5127363.0	7.18	554.24211	-0.16	$C_{32}H_{31}O_3N_3BF_2$
563.55090	8034143.5	11.25	563.47920	71.70	$C_{33}H_{60}ON_3BF_2$
565.56659	9026583.0	12.64	565.49485	71.74	$C_{33}H_{62}ON_3BF_2$
824.38110	14831320.0	20.77			
825.38458	8876065.0	12.43			

MS for 6b

E:\data\20110715\20110715_HESI+_B16 2011-7-15 15:50:49

20110715_HESI+_B16 #11 RT: 0.14 AV: 1 NL: 3.65E7
T: FTMS + p ESI Full ms [300.00-1000.00]



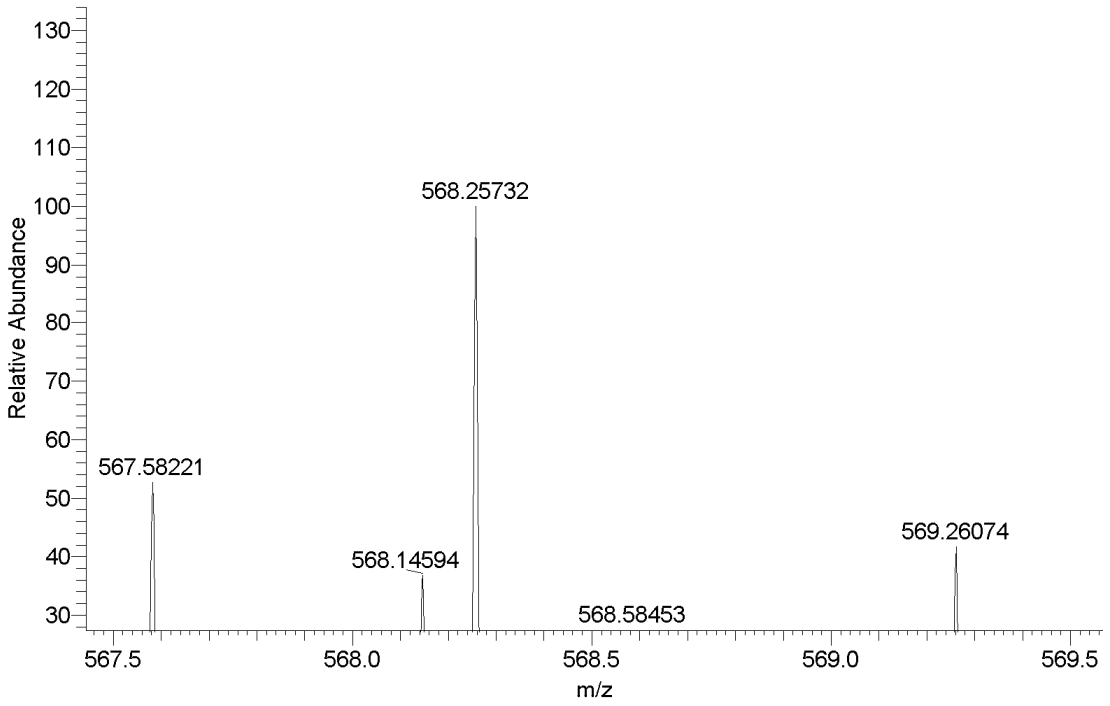
20110715_HESI+_B16#11 RT: 0.14
T: FTMS + p ESI Full ms [300.00-1000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
432.23840	15588299.0	17.80	432.24171	-3.31	$C_{26}H_{29}N_3BF_2$
511.51996	8516383.0	9.73	511.48429	35.67	$C_{30}H_{60}N_3BF_2$
529.56683	87557128.0	100.00	529.49485	71.98	$C_{30}H_{62}ON_3BF_2$
530.57019	31987086.0	36.53	530.48555	84.64	$C_{31}H_{62}ON_3F_2$
537.53534	9320441.0	10.64	537.49994	35.40	$C_{32}H_{62}N_3BF_2$
539.55090	7673450.5	8.76	539.47920	71.70	$C_{31}H_{60}ON_3BF_2$
623.32324	8191740.5	9.36	623.32779	-4.54	$C_{41}H_{40}N_3BF_2$
624.32001	36844704.0	42.08	624.32036	-0.35	$C_{37}H_{41}O_3N_3BF_2$
625.32379	14483908.0	16.54	625.32631	-2.51	$C_{42}H_{41}N_3F_2$
865.59814	8620575.0	9.85			

MS for 6c

E:\data\20110715\20110715_HESI+_B13_2 2011-7-15 16:12:09

20110715_HESI+_B13_2 #27 RT: 0.37 AV: 1 NL: 1.65E6
T: FTMS + p ESI Full ms [300.00-1000.00]



20110715_HESI+_B13_2#27 RT: 0.37
T: FTMS + p ESI Full ms [300.00-1000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
529.56653	124533768.0	34.44	529.49485	71.68	$C_{30}H_{62}ON_3BF_2$
530.56989	44569376.0	12.33	530.48555	84.34	$C_{31}H_{62}ON_3F_2$
531.57312	7801877.5	2.16	531.47412	99.00	$C_{29}H_{60}O_2N_3BF_2$
539.55072	1894403.6	0.52	539.47920	71.52	$C_{31}H_{60}ON_3BF_2$
566.13947	19571828.0	5.41	566.14633	-6.87	$C_{39}H_{18}N_3F_2$
567.14288	4945627.5	1.37	567.13890	3.98	$C_{35}H_{19}O_3N_3F_2$
568.25732	1661030.9	0.46	568.25776	-0.43	$C_{33}H_{33}O_3N_3BF_2$
597.55383	1970983.1	0.55	597.49994	53.90	$C_{37}H_{62}N_3BF_2$
739.22388	2806393.8	0.78	739.28123	-57.35	$C_{47}H_{36}O_3N_3BF_2$
799.31812	1708005.6	0.47			
799.35858	361595264.0	100.00			
799.38135	1955425.0	0.54			
799.39331	2077300.3	0.57			
800.36176	193412880.0	53.49			
801.36481	52463520.0	14.51			
802.36774	9265345.0	2.56			
813.37402	2208199.3	0.61			
821.34045	4454998.5	1.23			
822.34387	1916674.8	0.53			
958.46375	10092923.0	2.79			
959.46722	6473624.5	1.79			
960.46997	2232604.8	0.62			

MS for 6d

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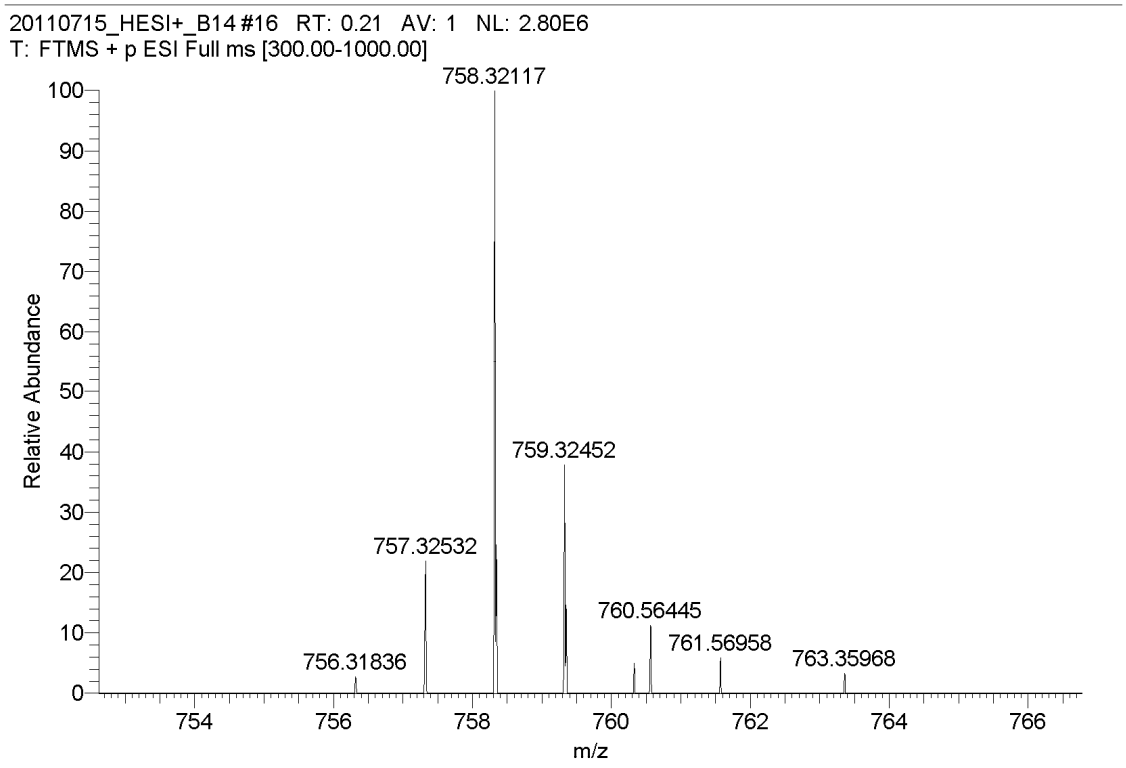

20110715_HESI+_B14#16 RT: 0.21
T: FTMS + p ESI Full ms [300.00-1000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
521.53546	9780831.0	18.91	521.47264	62.83	$C_{29}H_{61}O_2N_3F_2$
522.53864	3579722.8	6.92	522.48046	58.17	$C_{29}H_{62}O_2N_3F_2$
529.56702	51735232.0	100.00	529.49485	72.16	$C_{30}H_{62}ON_3BF_2$
530.57043	19048200.0	36.82	530.48555	84.89	$C_{31}H_{62}ON_3F_2$
537.53558	6037601.5	11.67	537.49994	35.65	$C_{32}H_{62}N_3BF_2$
539.55115	15400833.0	29.77	539.47920	71.95	$C_{31}H_{60}ON_3BF_2$
540.53522	3555506.3	6.87	540.48703	48.19	$C_{31}H_{61}ON_3BF_2$
540.55450	5496313.0	10.62	540.48703	67.48	$C_{31}H_{61}ON_3BF_2$
567.58258	5072007.5	9.80	567.47412	108.46	$C_{32}H_{60}O_2N_3BF_2$
597.55457	3965864.5	7.67	597.49994	54.63	$C_{37}H_{62}N_3BF_2$
758.32117	2805055.5	5.42	758.32075	0.42	$C_{44}H_{43}O_6N_3BF_2$
887.39679	3239703.0	6.26			

MS for 6e

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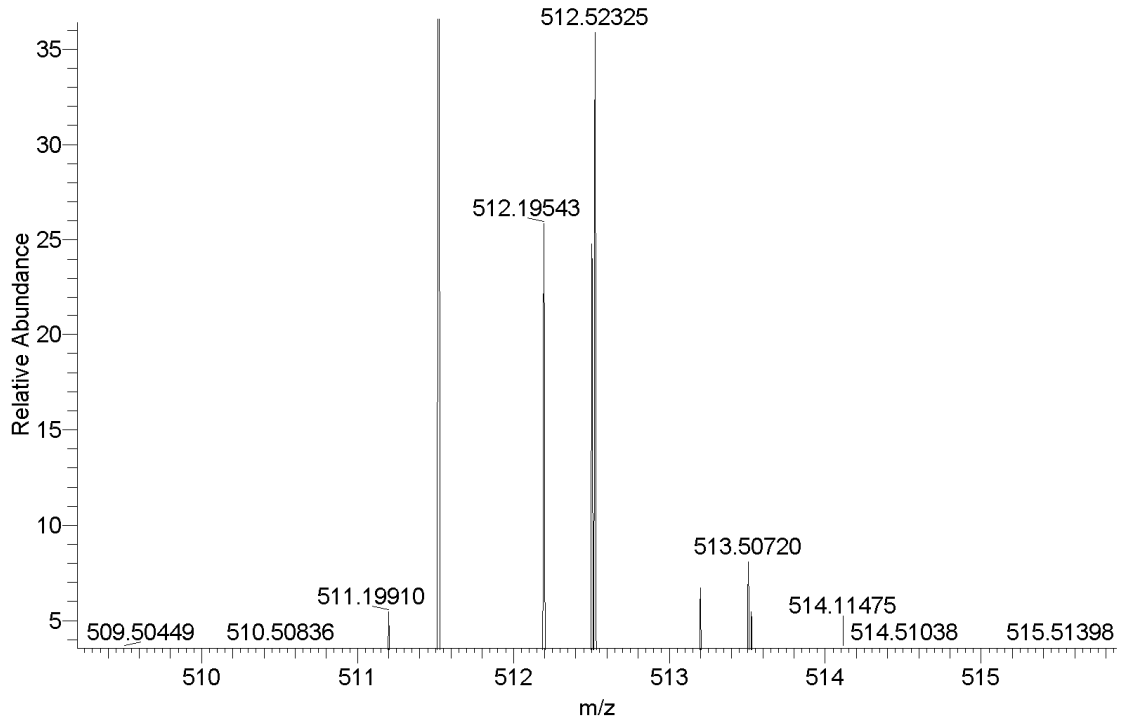

20110715_HESI+_B12#20 RT: 0.28
T: FTMS + p ESI Full ms [300.00-1000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
318.30063	750033.7	27.74	318.28866	11.97	$C_{16}H_{35}N_3BF_2$
432.23849	1145575.5	42.36	432.24171	-3.22	$C_{26}H_{29}N_3BF_2$
511.52002	2704256.0	100.00	511.48429	35.73	$C_{30}H_{60}N_3BF_2$
512.19543	707165.6	26.15	512.19516	0.28	$C_{29}H_{25}O_3N_3BF_2$
512.50397	667674.3	24.69	512.49211	11.85	$C_{30}H_{61}N_3BF_2$
512.52325	954484.6	35.30	512.49211	31.14	$C_{30}H_{61}N_3BF_2$
529.56696	2064903.9	76.36	529.49485	72.10	$C_{30}H_{62}ON_3BF_2$
530.57031	766265.7	28.34	530.48555	84.77	$C_{31}H_{62}ON_3F_2$
539.55115	2433335.5	89.98	539.47920	71.95	$C_{31}H_{60}ON_3BF_2$
540.55457	859908.3	31.80	540.48703	67.54	$C_{31}H_{61}ON_3BF_2$

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