Electronic Supporting Information

Copper-catalyzed Borylamidation of Vinyl Arenes with Isocyanates

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Contents

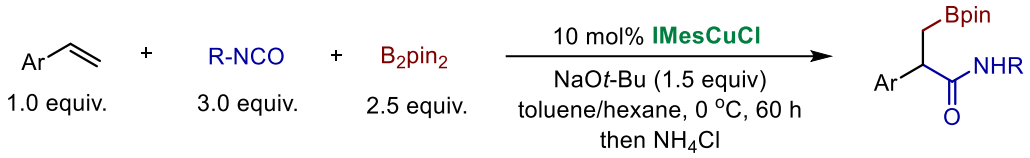
1. General Considerations

Unless otherwise noted, all reactions were performed under an argon atmosphere (purity ≥ 99.999%) using standard Schlenk-type tubes on a dual-manifold Schlenk line. Various reagents were purchased from commercial sources and used without further purification. All the solvents were refluxed with CaH_2 for 12 h, then distilled, further degassed by bubbling with argon for 20 min at room temperature, and stored with activated 4 Å molecular sieves. Isolated yields were determined after purification of the crude product by column chromatography with

10 ~ 40 μm silica gel. Literature methods[1-5] were used to synthesize IMesCuCl, SIMesCuCl, IPrCuCl, SIPrCuCl and ICyCuCl.

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on Bruker Advance III HD 400, Bruker Advance III HD 500 or Bruker Advance III HD 600 spectrometer with complete proton decoupling. All NMR data were obtained in $CDCl_3$ at ambient temperature. High-resolution mass spectrometric (HRMS) were recorded on a solariX-70FT-MS. Melting points were acquired on a Shenguang SGW X-4 melting point apparatus without correction. X-ray crystallographic analysis was carried out by Bruker APEII CCD. Infrared spectra were obtained on a Thermo Scientific Nicolet iS10 FT-IR spectrometer.

2. General Procedure for Borylamidation of Vinyl Arenes

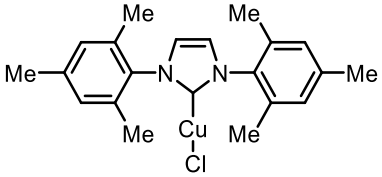


To an oven-dried Schlenk tube were added IMesCuCl (0.04 mmol, 18.0 mg), B_2pin_2(1.0 mmol, 254.0 mg), NaO*t*-Bu (0.6 mmol, 58.0 mg) and vinyl arene (0.4 mmol, if the vinyl arene is solid). The tube was evacuated and backfilled with argon for three times. The mixture was cooled to 0 °C (ice bath) and treated with toluene (1.0 mL, anhydrous and degassed). The reaction mixture was stirred at 0 °C for 20 mins, and alkene (0.4 mmol, if the alkene is liquid.) was injected. After further stirring for 5 mins, hexane (1.0 mL, anhydrous and degassed) was added with continuing stirring. Then, isocyanate (1.2 mmol, dissolved in toluene if the isocyanate is solid) was added dropwise over 5 mins. The resultant mixture was stirred at 0 °C for 60 h. The reaction mixture was allowed to warm to room temperature, then a saturated solution of NH_4Cl (0.1 mL) and EtOAc (5.0 mL) were added and stirred for 30 mins. The combined organic layers were concentrated in vacuo and purified by chromatography on silica gel.

3. Characterization Data

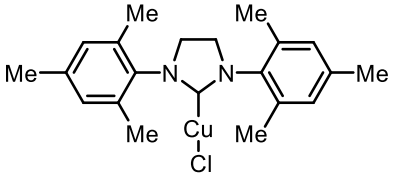
3.1 Characterization of the Catalysts

[1,3-Bismesitylimidazol-2-ylidene]copper(I) chloride [2]**:**



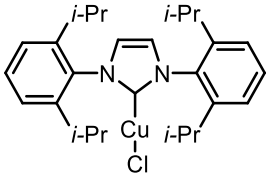
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (s, 2H), 7.00 (s, 4H), 2.35 (s, 6H), 2.10 (s, 12H).

[1,3-Bis(2,4,6-trimethylphenyl)imidazolidin-2-ylidene]copper(I) chloride [2]**:**



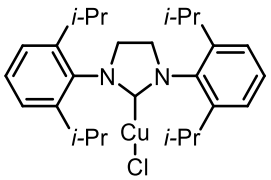
^{1}H NMR (600 MHz, $CDCl_3$) δ 6.96 (s, 4H), 3.96 (s, 4H), 2.32 (s, 12H), 2.30 (s, 6H).

[1,3-Bis[2,6-diisopropylphenyl)]imidazol-2-ylidene]copper(I) chloride [2]**:**



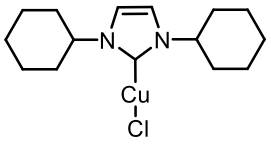
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 (t, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 4H), 7.13 (s, 2H), 2.56 (dt, *J* = 13.8, 6.9 Hz, 4H), 1.31 (s, 6H), 1.30 (s, 6H), 1.24 (s, 6H), 1.22 (s, 6H).

[1,3-Bis[2,6-(diisopropylphenyl)]imidazolidin-2-ylidene]copper(I) chloride [2]**:**



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (t, *J* = 7.7 Hz, 2H), 7.31 – 7.13 (m, 4H), 4.02 (s, 2H), 3.06 (hept, *J* = 6.9 Hz, 2H), 1.38 (s, 6H), 1.36 (s, 6H), 1.35 (s, 6H), 1.34 (s, 6H).

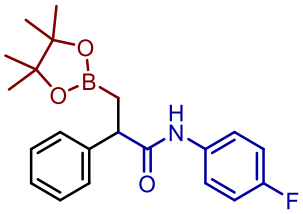
[1,3-Dicyclohexylimidazol-2-ylidene]copper(I) chloride [5]**:**



^{1}H NMR (500 MHz, $CDCl_3$) δ 6.93 (s, 2H), 4.30 (tt, *J* = 12.0, 3.6 Hz, 2H), 2.08 (d, *J* = 11.7 Hz, 4H), 1.89 (d, *J* = 13.7 Hz, 4H), 1.76 (d, *J* = 13.2 Hz, 2H), 1.65 (qd, *J* = 12.5, 3.2 Hz, 4H), 1.50 – 1.41 (m, 4H), 1.23 (ddd, *J* = 13.0, 10.1, 3.4 Hz, 2H).

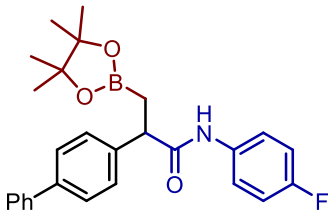
3.2 Characterization of the Borylamidation Products

N-(4-fluorophenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3aa):



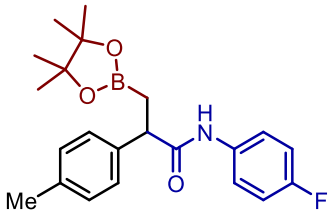
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 74% yield (109.3 mg). M.p. 156.6 – 158.6 °C. IR(KBr): *v*(cm^{-1}) = 3340, 2979, 1683, 1614, 1539, 1509, 1404, 1373, 1320, 1215, 1143, 967, 836, 761, 695. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (dd, *J* = 10.3, 4.3 Hz, 6H), 7.29 (dd, *J* = 8.7, 4.9 Hz, 1H), 7.06 (s, 1H), 6.95 (t, *J* = 8.7 Hz, 2H), 3.86 (dd, J = 9.7, 6.4 Hz, 1H), 1.66 (dd, *J* = 15.8, 9.7 Hz, 1H), 1.29 (dd, *J* = 15.7, 6.4 Hz, 1H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.57, 159.30 (d, *J* = 243.1 Hz), 141.53, 134.14, 129.20, 128.10, 127.61, 121.42 (d, *J* = 8.0 Hz), 115.59 (d, *J* = 22.2 Hz), 83.49, 49.91, 24.93, 24.80, 16.93. ^{19}F NMR (565 MHz, $CDCl_3$) δ – 118.48. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.56. HRMS (ESI) m/z: calculated for $[C_{21}H_{25}BFNO_3 + H]^+$ 370.1988, found 370.1987.

2-(Biphenyl-4-yl)-N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3ba):



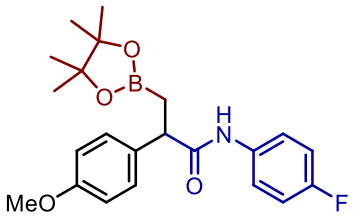
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 70% yield (124.6 mg). M.p. 182.9 – 186.7 °C. IR(KBr): *v*(cm^{-1}) = 3445, 2918, 1682, 1622, 1539, 1509, 1373, 1318, 1217, 1140, 847, 769, 697. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 – 7.56 (m, 4H), 7.44 (dd, *J* = 14.8, 7.7 Hz, 4H), 7.41 – 7.37 (m, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.14 (s, 1H), 6.96 (t, *J* = 8.7 Hz, 2H), 3.91 (dd, *J* = 9.6, 6.4 Hz, 1H), 1.69 (dd, *J* = 15.8, 9.8 Hz, 1H), 1.33 (dd, *J* = 15.8, 6.4 Hz, 1H), 1.22 (s, 6H), 1.20 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.51, 158.54, 140.69, 140.57, 140.49, 134.18, 128.97, 128.53, 127.87, 127.55, 127.16, 121.47 (d, *J* = 7.7 Hz), 115.62 (d, *J* = 22.6 Hz), 83.55, 49.59. 24.96, 24.83, 16.89. ^{19}F NMR (565 MHz, $CDCl_3$) δ -118.40. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.50. HRMS (ESI) m/z: calculated for $[C_{27}H_{29}BFNO_3 + H]^+$ 446.2302, found 446.2304.

N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2-p-tolylpropanamide (3ca):



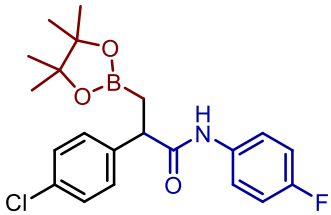
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 64% yield (98.1 mg). M.p. 154.1 – 155.3 °C. IR(KBr): ν(cm^{-1}) = 3432, 2976, 1684, 1615, 1541, 1508, 1403, 1384, 1320, 1213, 1140, 1076, 967, 845, 680. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 2H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 7.04 (s, 1H), 6.94 (t, *J* = 8.7 Hz, 2H), 3.83 (dd, *J* = 9.9, 6.2 Hz, 1H), 2.34 (s, 3H), 1.63 (dd, *J* = 15.7, 9.9 Hz, 1H), 1.27 - 1.24 (m, 1H), 1.22 (s, 6H), 1.20 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.80, 159.27 (d, *J* = 242.9 Hz), 138.52, 137.27, 134.21, 129.88, 127.97, 121.38 (d, *J* = 7.7 Hz), 115.55 (d, *J* = 22.2 Hz), 83.44, 49.55, 24.95, 24.82, 21.22, 16.91. ^{19}F NMR (565 MHz, $CDCl_3$) δ -118.61. ^{11}B NMR (128 MHz, $CDCl_3$) δ 34.01. HRMS (ESI) m/z: calculated for $[C_{22}H_{27}BFNO_3 + H]^+$ 384.2145, found 384.2144.

N-(4-fluorophenyl)-2-(4-methoxyphenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3da):



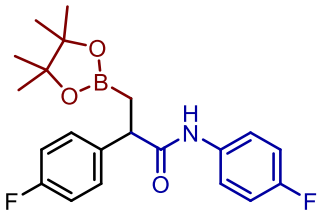
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 55% yield (87.8 mg). M.p. 161.2 – 163.3 °C. IR(KBr): ν(cm^{-1}) = 3442, 2988, 1682, 1615, 1541, 1511, 1405, 1373, 1322, 1217, 1139, 1037, 834. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (ddd, *J* = 9.0, 4.7, 2.9 Hz, 2H), 7.27 (s, 1H), 7.19 (t, *J* = 8.5 Hz, 1H), 7.05 (s, 1H), 6.95 (t, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 8.6 Hz, 2H), 3.84 – 3.81 (m, 1H), 3.81 (s, 3H), 1.63 (dd, *J* = 15.7, 9.6 Hz, 1H), 1.25 (dd, *J* = 15.7, 6.6 Hz, 1H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.96, 161.08 (d, *J* = 302.1 Hz), 159.01, 134.19, 130.35, 129.19, 121.37 (d, *J* = 8.0 Hz), 115.57 (d, *J* = 22.2 Hz), 114.54, 83.45, 55.44, 49.09, 24.89 (d, *J* = 14.2 Hz), 16.94. ^{19}F NMR (565 MHz, $CDCl_3$) δ -118.57. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.65. HRMS (ESI) m/z: calculated for $[C_{22}H_{27}BFNO_4 + H]^+$ 400.2094, found 400.2097.

2-(4-Chlorophenyl)-N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3ea):



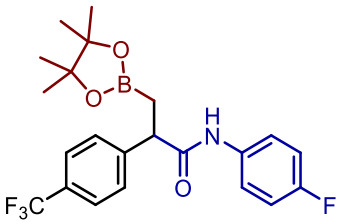
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 71% yield (114.5 mg). M.p. 152.8 – 154.4 °C. IR(KBr): ν(cm^{-1}) = 3339, 2978, 1685, 1615, 1542, 1509, 1405, 1374, 1329, 1217, 1140, 966, 846, 830, 782. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 – 7.35 (m, 2H), 7.31 (q, J = 8.6 Hz, 4H), 7.14 (s, 1H), 6.96 (t, J = 8.7 Hz, 2H), 3.82 (dd, J = 9.5, 6.4 Hz, 1H), 1.63 (dd, J = 15.9, 9.6 Hz, 1H), 1.28 (dd, J = 16.0, 6.4 Hz, 1H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.08, 159.41 (d, J = 243.3 Hz), 140.04, 134.02, 133.40, 129.42, 129.25, 121.50 (d, J = 8.0 Hz), 115.67 (d, J = 22.2 Hz), 83.65, 49.21, 24.93, 24.83, 17.06. ^{19}F NMR (565 MHz, $CDCl_3$) δ -118.17. ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.93. HRMS (ESI) m/z: calculated for $[C_{21}H_{24}BClFNO_3 + H]^+$ 404.1598, found 404.1594.

N,2-bis(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3fa):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 76% yield (117.7 mg). M.p. 157.4 – 158.5 °C. IR(KBr): ν(cm^{-1}) = 3442, 2978, 1655, 1606, 1547, 1509, 1409, 1381, 1325, 1228, 1143, 969, 847, 830. ^{1}H NMR (600 MHz, CDCl3) δ 7.41 – 7.36 (m, 2H), 7.33 (dd, J = 8.5, 5.4 Hz, 2H), 7.10 (s, 1H), 7.04 (t, J = 8.6 Hz, 2H), 6.96 (t, J = 8.7 Hz, 2H), 3.83 (dd, J = 9.4, 6.6 Hz, 1H), 1.63 (dd, J = 15.9, 9.5 Hz, 1H), 1.29 (dd, J = 15.8, 6.5 Hz, 1H), 1.20 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.38, 162.20 (d, J = 246.1 Hz), 159.37 (d, J = 243.0 Hz), 137.27, 134.03, 129.64 (d, J = 7.8 Hz), 121.45 (d, J = 8.0 Hz), 115.98 (d, J = 21.3 Hz), 115.66 (d, J = 22.5 Hz), 83.60, 49.07, 24.92, 24.82, 17.12. ^{19}F NMR (565 MHz, $CDCl_3$) δ -115.02, -118.25. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.71. HRMS (ESI) m/z: calculated for $[C_{21}H_{24}BF_2NO_3 + H]^+$ 388.1894, found 388.1891.

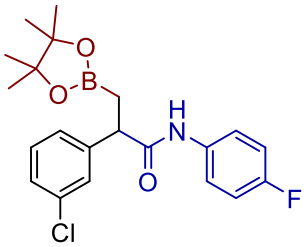
N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2-(4-(trifluoromethyl)phenyl)-propanamide (3ga):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 75% yield (130.4 mg). M.p. 138.8 – 139.8 °C. IR(KBr): ν(cm^{-1}) = 3445, 2981, 1682, 1658, 1615, 1544, 1510, 1406, 1374, 1326,1213, 1166, 1141, 1070, 843. ^{1}H NMR (501 MHz, $CDCl_3$) δ 7.59 (d, J = 8.1 Hz, 2H), 7.48 (d, J = 8.1 Hz, 2H), 7.39 (dd, J = 8.9, 4.7 Hz, 3H), 6.95 (t, J = 8.7 Hz, 2H), 3.89 (dd, J = 9.6, 6.3 Hz, 1H), 1.67 (dd, J = 16.0, 9.6 Hz, 1H), 1.32 (dd, J = 16.0, 6.3 Hz, 1H), 1.20 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz,

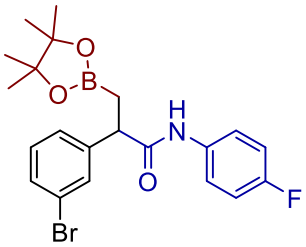
$CDCl_3$) δ 171.77 (s), 159.47 (d, *J* = 243.4 Hz), 145.62, 133.99, 129.74 (q, *J* = 32.4 Hz), 128.38, 125.91 (d, *J* = 3.6 Hz), 124.20 (d, *J* = 272.2 Hz), 121.65 (d, *J* = 7.9 Hz), 115.66 (d, *J* = 22.5 Hz), 83.75, 49.50, 24.90, 24.77. 17.00. ^{19}F NMR (565 MHz, $CDCl_3$) δ -62.54 (s), -117.99. ^{11}B NMR (128 MHz, $CDCl_3$) δ 34.11. HRMS (ESI) m/z: calculated for $[C_{22}H_{24}BF_4NO_3 + H]^+$ 438.1862, found 438.1869.

2-(3-Chlorophenyl)-N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3ia):



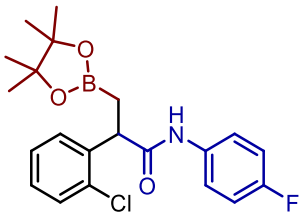
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 58% yield (93.5 mg). M.p. 103.5 – 104.9 °C. IR(KBr): *v*(cm^{-1}): 3433, 2977, 2857, 1659, 1617, 1545, 1511, 1470, 1374, 1323, 1215, 1141, 1079, 883, 840, 778. ^1H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.37 (m, 2H), 7.35 (s, 1H), 7.32 (s, 1H), 7.26 – 7.21 (m, 3H), 6.95 (t, *J* = 8.7 Hz, 2H), 3.81 (dd, *J* = 9.2, 6.7 Hz, 1H), 1.63 (dd, *J* = 16.0, 9.3 Hz, 1H), 1.30 (dd, *J* = 16.0, 6.7 Hz, 1H), 1.20 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.90, 159.38 (d, *J* = 243.4 Hz), 143.53, 134.67, 134.04, 130.28, 128.32, 127.62, 126.08, 121.61 (d, *J* = 7.8 Hz), 115.59 (d, *J* = 22.4 Hz), 83.63, 49.37, 24.89, 24.79, 16.86. ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.16 (s). ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.59. HRMS (ESI) m/z: calculated for $[C_{21}H_{24}BClFNO_3 + Na]^+$ 426.1414, found 426.1452.

2-(3-bromophenyl)-N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3ja):



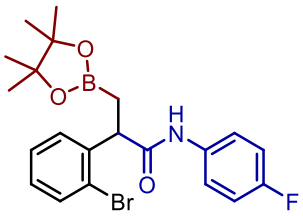
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 64% yield (114.4 mg). M.p. 142.9 – 144.8 °C. IR(KBr): *v*(cm^{-1}): 3305, 2980, 1661, 1615, 1545, 1510, 1470, 1370, 1327, 1216, 1143, 1100, 838, 775, 689. ^1H NMR (500 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.43 – 7.34 (m, 4H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 6.95 (t, *J* = 8.7 Hz, 2H), 3.80 (dd, *J* = 9.1, 6.8 Hz, 1H), 1.63 (dd, *J* = 16.0, 9.2 Hz, 1H), 1.31 (dd, *J* = 16.0, 6.7 Hz, 1H), 1.19 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.91, 159.36 (d, *J* = 243.4 Hz), 143.81, 134.02, 131.21, 130.55, 126.51, 122.86, 121.64 (d, *J* = 7.8 Hz), 115.58 (d, *J* = 22.5 Hz), 83.62, 49.29, 24.88, 24.79, 16.94. ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.12. ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.91. HRMS (ESI) m/z: calculated for $[C_{21}H_{24}BBrFNO_3 + Na]^+$ 470.0909, found 470.0955.

2-(2-Chlorophenyl)-N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3ka):



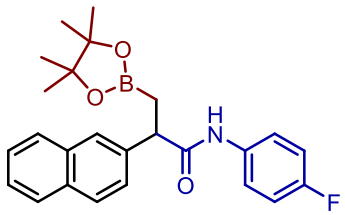
Purified by column chromatograph (20:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 24% yield (38.7 mg). M.p. 115.3 – 119.3 °C. IR(KBr): ν(cm^{-1}) = 3329, 2987, 1682, 1541, 1514, 1395, 1364, 1220, 1063, 1025, 845, 717. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.44 – 7.37 (m, 3H), 7.34 (s, 1H), 7.29 – 7.25 (m, 1H), 7.20 (td, *J* = 7.7, 1.5 Hz, 1H), 6.95 (t, *J* = 8.7 Hz, 2H), 4.36 (dd, *J* = 9.8, 6.3 Hz, 1H), 1.66 (dd, *J* = 15.9, 9.8 Hz, 1H), 1.34 (dd, *J* = 15.9, 6.3 Hz, 1H), 1.19 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.64, 159.32 (d, *J* = 243.1 Hz), 138.98, 134.19, 133.60, 129.74, 129.24, 128.61, 127.73, 121.57 (d, *J* = 7.8 Hz), 115.58 (d, *J* = 22.5 Hz), 83.58, 45.60, 24.88, 24.74, 15.30. ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.41. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.41. HRMS (ESI) m/z: calculated for $[C_{21}H_{24}BClFNO_3 + H]^+$ 404.1598, found 404.1598.

2-(2-Bromophenyl)-N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3la):



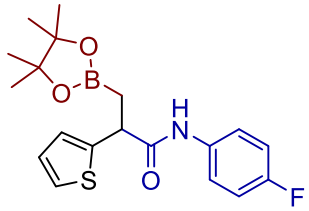
Purified by column chromatograph (20:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white oily liquid in 18% yield (33.1 mg). IR(KBr): ν(cm^{-1}) = 3425, 1662, 1614, 1509, 1469, 1404, 1372, 1319, 1212, 1140, 833, 753, 513. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 1H), 7.47 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.41 (dd, *J* = 8.9, 4.8 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.13 (dd, *J* = 10.9, 4.4 Hz, 1H), 6.96 (t, *J* = 8.7 Hz, 2H), 4.35 (dd, *J* = 9.6, 6.4 Hz, 1H), 1.67 – 1.62 (m, 1H), 1.36 (dd, *J* = 14.2, 4.6 Hz, 1H), 1.18 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.58, 161.93 (d, *J* = 397.3 Hz), 140.77, 133.09, 129.37, 128.95, 128.43, 124.56, 121.59 (d, *J* = 7.9 Hz), 120.90, 115.64 (d, *J* = 22.6 Hz), 83.61, 48.21, 24.90, 24.79, 15.35. ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.42. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.82. HRMS (ESI) m/z: calculated for $[C_{21}H_{24}BBrFNO_3 + H]^+$ 450.1071, found 450.1074.

N-(4-fluorophenyl)-2-(naphthalen-2-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3ma):



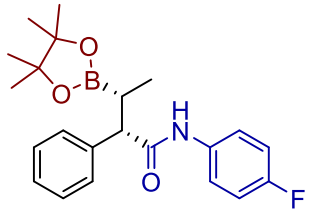
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 78% yield (130.4 mg). M.p. 166.3 – 170.5 °C. IR(KBr): ν(cm^{-1}) = 3428, 2980, 1683, 1614, 1538, 1509, 1468, 1404, 1384, 1326, 1214, 1139, 1075, 845, 781. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (dd, J = 16.7, 9.4 Hz, 4H), 7.49 (dt, J = 14.3, 7.7 Hz, 3H), 7.35 (dd, J = 8.9, 4.8 Hz, 2H), 7.09 (s, 1H), 6.93 (t, J = 8.7 Hz, 2H), 4.05 (dd, J = 9.6, 6.4 Hz, 1H), 1.75 (dd, J = 15.8, 9.7 Hz, 1H), 1.35 (dd, J = 15.8, 6.4 Hz, 1H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.54, 159.26 (d, J = 242.9 Hz), 138.99, 134.11 (d, J = 2.6 Hz), 133.57, 132.74, 129.04, 127.84, 127.81, 126.92, 126.48, 126.12, 125.83, 121.48 (d, J = 7.7 Hz), 115.50 (d, J = 22.2 Hz), 83.49, 49.94, 24.89, 24.78, 16.85. ^{19}F NMR (565 MHz, $CDCl_3$) δ -118.46. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.58. HRMS (ESI) m/z: calculated for $[C_{25}H_{27}BFNO_3 + H]^+$ 420.2145, found 420.2149.

N-(4-fluorophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2-(thiophen-2-yl)propenamide (3na):



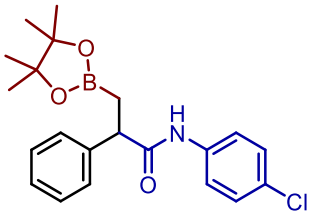
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 41% yield (61.5 mg). M.p. 126.4 – 127.8 °C. IR(KBr): ν(cm^{-1}): 3434, 3305, 2976, 2856, 1660, 1618,1552, 1509, 1464, 1326, 1214, 1139, 840, 700. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.37 (m, 3H), 7.24 (dd, J = 5.1, 0.7 Hz, 1H), 7.03 (d, J = 3.1 Hz, 1H), 7.00 – 6.93 (m, 3H), 4.18 (dd, J = 9.2, 6.7 Hz, 1H), 1.70 (dd, J = 15.8, 9.2 Hz, 1H), 1.43 (dd, J = 15.8, 6.7 Hz, 1H), 1.21 (d, J = 3.3 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.53, 159.43 (d, J = 243.3 Hz), 144.33, 134.00 (d, J = 2.7 Hz), 127.16, 125.66, 125.17, 121.60 (d, J = 7.9 Hz), 115.61 (d, J = 22.5 Hz), 83.63, 45.00, 24.90, 24.83, 19.73. ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.23. ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.33. HRMS (ESI) m/z: calculated for $[C_{19}H_{23}BFNO_3S + H]^+$ 376.1552, found 376.1558.

N-(4-fluorophenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butanamide (3pa):



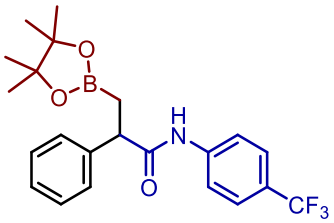
Purified by column chromatograph (25:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 21% yield (32.2 mg). M.p. 178.8 – 180.2 °C. IR(KBr): ν(cm^{-1}): 3431, 2926, 2856, 1681, 1622, 1544, 1508, 1456, 1404, 1318, 1074, 839, 782, 738, 669. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (t, J = 7.3 Hz, 2H), 7.35 – 7.32 (m, 2H), 7.29 (dd, J = 6.4, 5.2 Hz, 2H), 6.96 – 6.89 (m, 3H), 3.57 (d, J = 11.7 Hz, 1H), 1.66 (dq, J = 11.8, 7.4 Hz, 1H), 1.30 (s, 6H), 1.25 (s, 6H), 0.79 (d, J = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.74, 159.31 (d, J = 243.3 Hz), 139.50, 134.10, 129.28, 128.83, 127.74, 121.37 (d, J = 7.8 Hz), 115.54 (d, J = 22.4 Hz), 83.14, 57.71, 24.96, 24.70, 21.67, 13.31. ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.52. ^{11}B NMR (128 MHz, $CDCl_3$) δ 34.23. HRMS (ESI) m/z: calculated for $[C_{22}H_{27}BFNO_3 + Na]^+$ 406.1960, found 406.1999.

N-(4-chlorophenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3ab):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 74% yield (113.4 mg). M.p. 195.1 – 198.9 °C. IR(KBr): ν(cm^{-1}) = 3446, 2983, 1681, 1595, 1525, 1493, 1396, 1372, 1333, 1255, 1141, 973, 830, 700. ^{1}H NMR (501 MHz, $CDCl_3$) δ 7.37 (s, 1H), 7.37 – 7.33 (m, 5H), 7.31 – 7.27 (m, 1H), 7.22 (s, 1H), 7.20 (s, 1H), 7.18 (s, 1H), 3.86 (dd, J = 9.7, 6.4 Hz, 1H), 1.65 (dd, J = 15.8, 9.7 Hz, 1H), 1.31 – 1.27 (m, 1H), 1.21 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.67, 141.43, 136.76, 129.85, 129.18, 128.96, 128.06, 127.61, 120.90, 83.52, 49.98, 24.92, 24.78, 16.84. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.62. HRMS (ESI) m/z: calculated for $[C_{21}H_{25}BClNO_3 + H]^+$ 386.1693, found 386.1693.

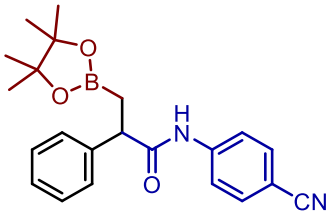
2-Phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-(4-(trifluoromethyl)phenyl)propanamide (3ac):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 76% yield (127.4 mg). M.p. 172.7 – 178.6 °C. IR(KBr): ν(cm^{-1}) = 3446, 2981, 1690, 1603, 1530, 1434, 1407, 1373, 1326, 1254, 1166, 1122, 1067, 1024, 846, 758. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (dd, J = 19.0, 9.8 Hz, 5H), 7.35 (d, J = 6.1 Hz, 4H), 7.29 (s, 1H), 3.89 (dd, J = 9.7, 6.3 Hz, 1H), 1.67 (dd, J = 15.9, 9.8 Hz, 1H), 1.34 – 1.30 (m, 1H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.92, 141.26, 129.28, 128.06, 127.74, 126.27 (q, J = 3.7 Hz), 126.04, 125.31, 123.15, 119.20, 83.60, 50.15, 24.95, 24.80, 16.75. ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.12. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.86. HRMS (ESI) m/z: calculated for $[C_{22}H_{25}BF_3NO_3$

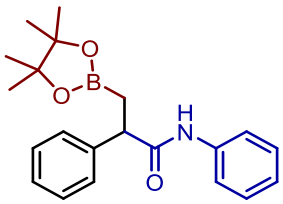
+ H]$^+$ 420.1956, found 420.1951.

N-(4-cyanophenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3ad):



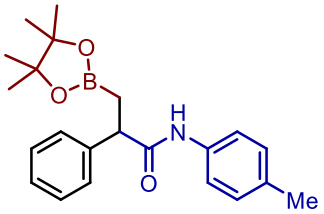
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 53% yield (79.8 mg). M.p. 177.1 – 184.1 °C. IR(KBr): ν(cm^{-1}) = 3445, 2925, 2228, 1682, 1595, 1516, 1405, 1143, 845, 700. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (s, 4H), 7.39 – 7.32 (m, 5H), 7.32 – 7.27 (m, 1H), 3.89 (dd, J = 9.7, 6.2 Hz, 1H), 1.66 (dd, J = 15.9, 9.8 Hz, 1H), 1.34 – 1.30 (m, 1H), 1.21 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.04, 142.17, 140.99, 133.30, 129.33, 128.04, 127.84, 119.41, 118.97, 107.04, 83.65, 50.20, 24.95, 24.80, 16.77. ^{11}B NMR (128 MHz, $CDCl_3$) δ 30.85. HRMS (ESI) m/z: calculated for [$C_{22}H_{25}BN_2O_3$ + H]$^+$ 377.2035, found 377.2039.

N,2-diphenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3ae):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 62% yield (87.1 mg). M.p. 138.3 – 140.2 °C. IR(KBr): ν(cm^{-1}) = 3446, 1687, 1601, 1536, 1498, 1438, 1373, 1319, 1139, 1105, 968, 802, 755, 700. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (d, J = 8.0 Hz, 2H), 7.34 (q, J = 7.7 Hz, 4H), 7.29 – 7.22 (m, 3H), 7.16 (s, 1H), 7.04 (t, J = 7.4 Hz, 1H), 3.88 (dd, J = 9.6, 6.6 Hz, 1H), 1.66 (dd, J = 15.8, 9.6 Hz, 1H), 1.32 – 1.23 (m, 2H), 1.20 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.56, 141.60, 138.15, 129.08, 128.92, 128.05, 127.46, 124.06, 119.59, 83.42, 49.97, 24.88, 24.75, 16.82. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.86. HRMS (ESI) m/z: calculated for [$C_{21}H_{26}BNO_3$ + H]$^+$ 352.2082, found 352.2081.

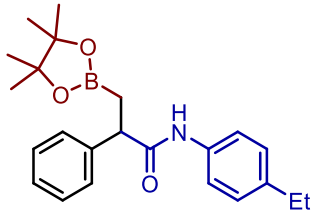
2-Phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-p-tolylpropanamide (3af):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 69% yield (100.8 mg). M.p. 167.1 – 169.9 °C. IR(KBr): ν(cm^{-1}) = 3362, 2979, 1682, 1600, 1522, 1454, 1373, 1325, 1250, 1142, 970, 822, 697. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 4H), 7.29 (d, J = 8.3 Hz,

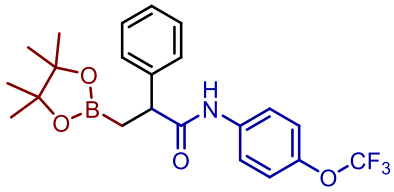
2H), 7.25 (t, *J* = 6.9 Hz, 1H), 7.14 (s, 1H), 7.04 (d, *J* = 8.2 Hz, 2H), 3.86 (dd, *J* = 9.5, 6.6 Hz, 1H), 2.26 (s, 3H), 1.65 (dd, *J* = 15.8, 9.6 Hz, 1H), 1.32 – 1.25 (m, 2H), 1.20 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.42, 141.69, 135.60, 133.57, 129.35, 129.00, 128.03, 127.37, 119.66, 83.36, 49.86, 24.86, 24.72, 20.88, 16.83. ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.97. HRMS (ESI) m/z: calculated for $[C_{22}H_{28}BNO_3 + H]^+$ 366.2238, found 366.2235.

N-(4-ethylphenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3ag):



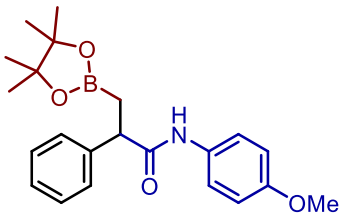
Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 63% yield (95.6 mg). M.p. 150.2 – 152.6 °C. IR(KBr): *v*(cm^{-1}) = 3446, 2979, 1650, 1607, 1515, 1411, 1379, 1318, 1144, 845, 782, 701. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (dt, *J* = 8.5, 5.6 Hz, 6H), 7.28 – 7.23 (m, 1H), 7.08 (t, *J* = 7.6 Hz, 3H), 3.86 (dd, *J* = 9.5, 6.6 Hz, 1H), 2.56 (q, *J* = 7.6 Hz, 2H), 1.66 (dd, *J* = 15.8, 9.5 Hz, 1H), 1.29 (dd, *J* = 15.8, 6.7 Hz, 1H), 1.23 – 1.14 (m, 15H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.41, 141.77, 140.13, 135.84, 129.05, 128.24, 128.08, 127.41, 119.78, 83.41, 49.96, 28.37, 24.91, 24.78, 16.89, 15.76. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.55. HRMS (ESI) m/z: calculated for $[C_{23}H_{30}BNO_3 + H]^+$ 380.2396, found 380.2398.

2-Phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-(4-(trifluoromethoxy)phenyl)propanamide (3ah):



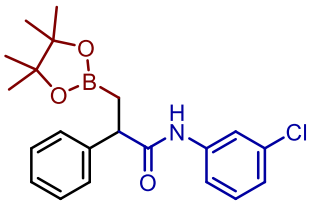
Purified by column chromatograph (25:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 81% yield (141.7 mg). M.p. 129.1 – 134.0 °C. IR(KBr): *v*(cm^{-1}) = 3446, 2927, 1667, 1612, 1510, 1468, 1404, 1382, 1324, 1264, 1201, 1168, 1143, 847, 804, 741, 612. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 9.0 Hz, 2H), 7.38 – 7.33 (m, 4H), 7.30 – 7.27 (m, 1H), 7.15 (s, 1H), 7.11 (d, *J* = 8.7 Hz, 2H), 3.87 (dd, *J* = 9.7, 6.4 Hz, 1H), 1.66 (dd, *J* = 15.8, 9.7 Hz, 1H), 1.34 – 1.29 (m, 1H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.57, 145.06, 141.28, 136.71, 129.08, 127.93, 127.52, 121.60, 120.62, 119.44, 83.41, 49.86, 24.79, 24.66, 16.78. ^{19}F NMR (471 MHz, $CDCl_3$) δ -58.18. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.46. HRMS (ESI) m/z: calculated for $[C_{22}H_{25}BF_3NO_4 + H]^+$ 436.1905, found 436.1908.

N-(4-methoxyphenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3ai):



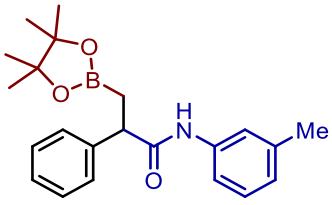
Purified by column chromatograph (20:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 26% yield (39.6 mg). M.p. 146.3 – 151.5 °C. IR(KBr): ν(cm^{-1}) = 3422, 1962, 1650, 1607, 1510, 1379, 1329, 1246, 1145, 809, 700. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.53 (s, 1H), 7.46 (d, J = 9.0 Hz, 2H), 7.21 – 7.17 (m, 3H), 6.87 (dd, J = 6.5, 2.8 Hz, 2H), 6.83 (d, J = 9.0 Hz, 2H), 3.88 – 3.82 (m, 4H), 1.63 – 1.58 (m, 1H), 1.26 (s, 6H), 1.22 (s, 6H), 1.07 (dd, J = 16.2, 5.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 179.38, 156.27, 140.66, 131.26, 130.35, 128.66, 127.19, 121.67, 114.25, 83.68, 55.60, 48.68, 25.20, 24.63, 19.25. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.36. HRMS (MALDI) m/z: calculated for $[C_{22}H_{28}BNO_4 + H]^+$ 382.2188, found 382.2180.

N-(3-chlorophenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3aj):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 67% yield (103.2 mg). M.p. 154.2 – 156.3 °C. IR(KBr): ν(cm^{-1}) = 3446, 2982, 1685, 1599, 1530, 1421, 1369, 1318, 1248, 1140, 968, 843, 782, 698. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.38 – 7.32 (m, 4H), 7.30 – 7.27 (m, 1H), 7.26 – 7.22 (m, 1H), 7.19 – 7.12 (m, 2H), 7.02 (dd, J = 7.9, 0.9 Hz, 1H), 3.86 (dd, J = 9.6, 6.4 Hz, 1H), 1.66 (dd, J = 15.7, 9.5 Hz, 1H), 1.29 (dd, J = 15.8, 6.4 Hz, 1H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.71, 141.34, 139.32, 134.66, 129.94, 129.22, 128.07, 127.66, 124.16, 119.74, 117.58, 83.56, 50.04, 24.94, 24.81, 16.76. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.75. HRMS (ESI) m/z: calculated for $[C_{21}H_{25}BClNO_3 + H]^+$ 386.1693, found 386.1693.

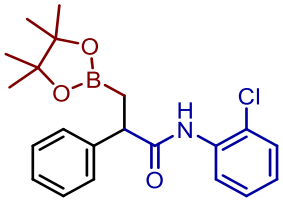
2-Phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-m-tolylpropanamide (3ak):



Purified by column chromatograph (15:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 73% yield (106.5 mg). M.p. 140.0 – 143.3 °C. IR(KBr): ν(cm^{-1}) = 3366, 2982, 1684, 1594, 1542, 1492, 1454, 1369, 1141, 970, 783, 698. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (dd, J = 8.9, 5.1 Hz, 4H), 7.28 (dd, J = 8.4, 6.0 Hz, 2H), 7.19 (d, J = 8.2 Hz, 1H), 7.13 (t, J = 7.8 Hz, 1H), 7.07 (s, 1H), 6.86 (d, J = 7.4 Hz, 1H), 3.86 (dd, J

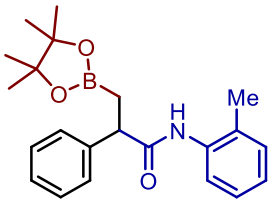
= 9.4, 6.7 Hz, 1H), 2.28 (s, 3H), 1.66 (dd, *J* = 15.8, 9.4 Hz, 1H), 1.30 (dd, *J* = 15.8, 6.7 Hz, 1H), 1.20 (s, 6H), 1.18 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.51, 141.69, 138.86, 138.12, 129.10, 128.78, 128.10, 127.47, 124.91, 120.29, 116.71, 83.45, 50.05, 24.92, 24.80, 21.54, 16.78. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.83. HRMS (ESI) m/z: calculated for $[C_{22}H_{28}BNO_3 + H]^+$ 366.2239, found 366.2238.

N-(2-chlorophenyl)-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3al):



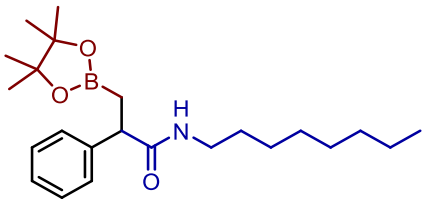
Purified by column chromatograph (40:1 to 10:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 43% yield (66.3 mg). M.p. 110.7 – 118.3 °C. IR(KBr): *ν*(cm^{-1}) = 3367, 2981, 1694, 1591, 1526, 1492, 1470, 1439, 1373, 1317, 1248, 1212, 1178, 1139, 842, 754, 702. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.1 Hz, 1H), 7.63 (s, 1H), 7.41 – 7.33 (m, 4H), 7.29 (d, *J* = 6.7 Hz, 1H), 7.26 – 7.19 (m, 2H), 6.95 (td, *J* = 7.8, 1.4 Hz, 1H), 3.95 (dd, *J* = 9.4, 7.0 Hz, 1H), 1.70 (dd, *J* = 15.6, 9.4 Hz, 1H), 1.33 (dd, *J* = 15.7, 7.0 Hz, 1H), 1.20 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.73, 141.04, 134.87, 129.21, 128.91, 128.21, 127.71, 127.68, 124.35, 122.65, 121.21, 83.42, 50.35, 24.85, 24.75, 16.18. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.90. HRMS (ESI) m/z: calculated for $[C_{21}H_{25}BClNO_3 + H]^+$ 386.1693, found 386.1694.

2-Phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-(o-tolyl)propanamide (3am):



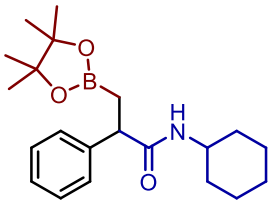
Purified by column chromatograph (20:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 34% yield (50.3 mg). M.p. 116.6 – 119.0 °C. IR(KBr): *ν*(cm^{-1}) = 3301, 2975, 1661, 1585, 1525, 1492, 1457, 1405, 1377, 1317, 1260, 1214, 1180, 1143, 1108, 966, 845, 750, 697. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.37 (q, *J* = 7.9 Hz, 4H), 7.28 (t, *J* = 6.7 Hz, 1H), 7.14 (t, *J* = 7.7 Hz, 1H), 7.05 (d, *J* = 7.3 Hz, 1H), 6.97 (t, *J* = 7.3 Hz, 1H), 6.89 (s, 1H), 3.94 (dd, *J* = 9.1, 7.1 Hz, 1H), 1.87 (s, 3H), 1.70 (dd, *J* = 15.6, 9.5 Hz, 1H), 1.31 (dd, *J* = 15.5, 6.8 Hz, 1H), 1.20 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.34, 141.56, 135.80, 130.11, 128.98, 127.98, 127.42, 126.55, 124.49, 121.97, 83.15, 49.80, 24.66, 24.60, 17.02, 16.23. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.47. HRMS (ESI) m/z: calculated for $[C_{22}H_{28}BNO_3 + H]^+$ 366.2239, found 366.2235.

N-octyl-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propenamide (3an):



Purified by column chromatograph (10:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 35% yield (54.2 mg). M.p. 40.4 – 44.3 °C. IR(KBr): ν(cm^{-1}) = 3307, 2960, 1643, 1551, 1467, 1371, 1323, 1263, 1145, 969, 846, 735, 698. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.27 (m, 4H), 7.25 – 7.21 (m, 1H), 3.69 (dd, J = 9.4, 7.0 Hz, 1H), 3.15 (ddd, J = 13.1, 7.1, 2.4 Hz, 2H), 1.56 (dd, J = 15.5, 9.5 Hz, 1H), 1.36 (dt, J = 14.1, 7.1 Hz, 2H), 1.28 – 1.20 (m, 10H), 1.19 (s, 6H), 1.18 (s, 6H), 0.87 (t, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.37, 142.30, 128.88, 128.12, 127.17, 83.20, 49.11, 39.89, 31.87, 29.58, 29.29, 29.27, 26.87, 24.88, 24.83, 22.74, 16.90, 14.19. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.56. HRMS (ESI) m/z: calculated for $[C_{23}H_{38}BNO_3 + H]^+$ 388.3022, found 388.3030.

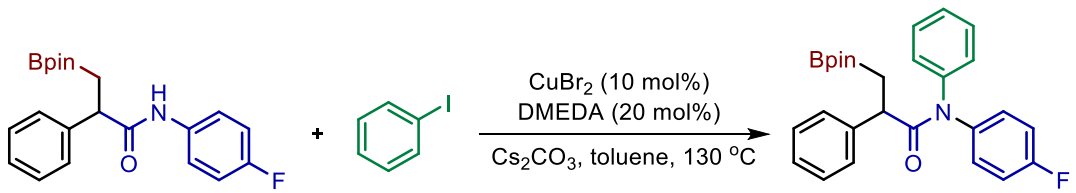
N-cyclohexyl-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (3ao):



Purified by column chromatograph (12:1 to 7:1 petroleum ether/ethyl acetate) to afford the product as a white solid in 15% yield (21.4 mg). M.p. 99.4 – 101.2 °C. IR(KBr): ν(cm^{-1}) = 3421, 2925, 2854, 1654, 1615, 1544, 1510, 1457, 1373, 1326, 1143, 967, 795, 699. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (d, J = 7.5 Hz, 1H), 7.29 (s, 1H), 7.28 (s, 1H), 7.25 – 7.21 (m, 1H), 3.72 (ddd, J = 14.1, 7.1, 3.0 Hz, 1H), 3.66 (dd, J = 9.5, 6.7 Hz, 1H), 2.01 (dd, J = 12.2, 6.6 Hz, 1H), 1.84 (d, J = 13.5 Hz, 1H), 1.74 (d, J = 10.7 Hz, 1H), 1.65 – 1.57 (m, 2H), 1.52 (s, 2H), 1.36 – 1.28 (m, 4H), 1.20 (s, 6H), 1.19 (s, 6H), 1.08 – 1.05 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.49, 142.49, 128.87, 128.06, 127.12, 83.22, 49.17, 48.31, 32.96, 25.66, 24.92, 24.88, 24.77, 17.87. ^{11}B NMR (128 MHz, $CDCl_3$) δ 33.52. HRMS (ESI) m/z: calculated for $[C_{21}H_{32}BNO_3 + H]^+$ 358.2552, found 358.2553.

4. Further Functionalization Reactions

N-(4-fluorophenyl)-N,2-diphenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanamide (4):

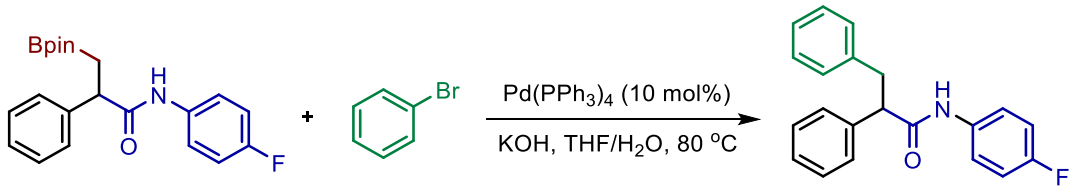


3aa **4**, 54%

The following procedure was in the light of a previously-reported method.[6] A oven-dried 25 mL Schlenk tube

were charged with **3aa** (0.1 mmol, 37 mg), $CuBr_2$ (0.01 mmol, 2.3 mg) and Cs_2CO_3 (0.20 mmol, 66 mg). The tube was evacuated and backfilled with argon for three times. Iodobenzene (0.2 mmol, 23.0 μL), 1,2-bis(methylamino)ethane (DMEDA, 0.02 mmol, 2.2 μL) and toluene (2.0 mL, degassed) were injected into the tube under an argon atmosphere. The mixture was allowed to stir at 130 °C (pre-heated oil bath) for 24 h. After cooling to room temperature, 2 mL H_2O was added and the mixture was extracted with ethyl acetate (3 x 5.0 mL). The combined organic layers were concentrated in vacuo, and the residue was purified by flash column chromatography (PE/EA) to give **4** (24 mg, 54%) as a yellow oily liquid. IR(KBr): ν(cm^{-1}) = 3439, 2927, 1670, 1622, 1555, 1507, 1455, 1373, 1318, 1219, 1141, 1074, 844, 738, 696. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (br, 2H), 7.22 – 7.15 (m, 4H), 7.09 (br, 4H), 6.96 (dd, J = 13.1, 7.2 Hz, 4H), 3.93 (d, J = 5.2 Hz, 1H), 1.67 (dd, J = 16.2, 10.8 Hz, 1H), 1.22 (d, J = 10.5 Hz, 12H), 1.12 (dd, J = 16.2, 5.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.37, 142.95 (d, br, J = 67.0 Hz), 142.17, 139.47(br), 131.37(br), 129.35(br), 129.00(br), 128.52, 128.04(br), 127.76, 126.72, 126.18 (d, br, J = 21.9 Hz), 115.88 (d, br, J = 19.0 Hz), 83.37, 46.23, 25.11, 24.97, 18.66. ^{19}F NMR (471 MHz, $CDCl_3$) δ -113.72, -116.54 (major). ^{11}B NMR (128 MHz, $CDCl_3$) δ 32.92. HRMS (ESI) m/z: calculated for $[C_{27}H_{29}BFNO_3 + H]^+$ 446.2302, found 446.2300.

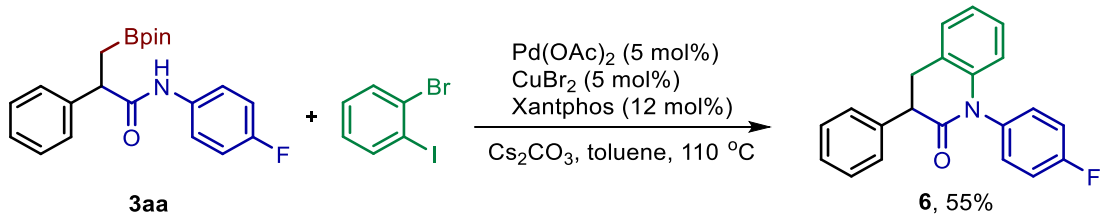
N-(4-fluorophenyl)-2,3-diphenylpropanamide (5):



3aa **5**, 73%

The following procedure was adapted from a previously-published method.[7] A oven-dried 25 mL Schlenk tube were charged with **3aa** (0.1 mmol, 37 mg), KOH (0.3 mmol, 17.0 mg) and $Pd(PPh_3)_4$ (0.01 mmol, 12.0 mg). The tube was evacuated and backfilled with argon for three times. THF (1.0 mL, degassed), bromobenzene (0.3 mmol, 31.4 μL) and H_2O (1.0 mL) were added under an argon atmosphere. The reaction tube was sealed and stirred at 80 °C (pre-heated oil bath) for 20 h. After cooling to room temperature, the reaction mixture was extracted with ethyl acetate (3 x 5.0 mL). The combined organic layers were concentrated in vacuo, and the residue was purified by flash column chromatography (PE/EA) to give **5** (23.4 mg, 73%) as a white solid. M.p. 166.2 – 168.3 °C. IR(KBr): ν(cm^{-1}) = 3420, 1651, 1617, 1553, 1508, 1455, 1362, 1295, 1217, 1179, 1079, 836, 745, 702. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, J = 4.3 Hz, 4H), 7.30 (ddd, J = 13.3, 7.0, 4.0 Hz, 3H), 7.22 (t, J = 7.2 Hz, 2H), 7.17 (t, J = 7.3 Hz, 1H), 7.14 – 7.10 (m, 2H), 6.94 (dd, J = 14.8, 6.2 Hz, 3H), 3.71 (t, J = 7.4 Hz, 1H), 3.65 – 3.57 (m, 1H), 3.05 (dd, J = 13.6, 6.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.01, 159.53 (d, J = 243.5 Hz), 139.57, 139.22, 133.74, 129.16, 129.12, 128.53, 128.24, 127.82, 126.51, 121.93 (d, J = 7.9 Hz), 115.65 (d, J = 22.5 Hz), 56.63, 39.90. ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.90. HRMS (ESI) m/z: calculated for $[C_{21}H_{18}FNO + H]^+$ 320.1445, found 320.1449.

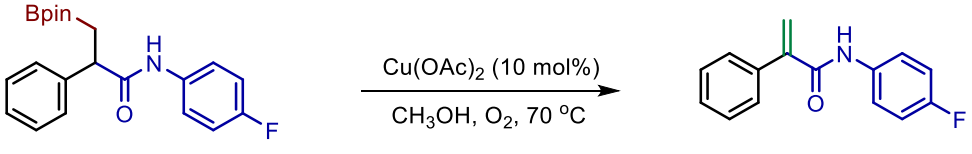
1-(4-Fluorophenyl)-3-phenyl-3,4-dihydroquinolin-2(1H)-one (6):



3aa **6**, 55%

A oven-dried 25 mL Schlenk tube was charged with **3aa** (0.1 mmol, 37 mg), $Pd(OAc)_2$ (5 mol%, 1.2 mg), $CuBr_2$ (5 mol%, 1.2 mg), Xantphos (12 mol%, 7 mg) and Cs_2CO_3 (0.28 mmol, 91 mg). The tube was evacuated and backfilled with argon for three times. Toluene (2.0 mL, anhydrous and degassed) and 1-bromo-2-iodobenzene (0.2 mmol, 20.0 μL) was added under an argon atmosphere. The mixture was allowed to stir at 110 °C (pre-heated oil bath) for 24 h. After cooling to room temperature, 2 mL H_2O was added and the mixture was extracted to ethyl acetate (3 x 5.0 mL). The combined organic layers were concentrated in vacuo, and the residue was purified by flash column chromatography (PE/EA) to give **6** (17.4 mg, 55%) as a yellow solid. M.p. 121.2 – 127.4 °C. IR(KBr): ν(cm^{-1}) = 3029, 2925, 1658, 1615, 1550, 1508, 1471, 835, 753, 693. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 7.0 Hz, 2H), 7.35 – 7.32 (m, 3H), 7.31 – 7.26 (m, 1H), 7.10 (d, J = 4.2 Hz, 2H), 7.07 – 7.02 (m, 1H), 6.99 – 6.91 (m, 3H), 3.90 (dd, J = 8.0, 6.7 Hz, 1H), 3.68 (dd, J = 13.6, 8.2 Hz, 1H), 3.17 (dd, J = 13.6, 6.5 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.61, 159.54 (d, J = 243.6 Hz), 139.09, 138.63, 133.74, 132.88, 132.18, 129.11, 128.39, 128.11, 127.84, 127.51, 124.66, 121.93(d, J = 7.9 Hz), 115.67 (d, J = 22.5 Hz), 53.82, 40.42. ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.89. HRMS (ESI) m/z: calculated for $[C_{21}H_{16}FNO + H]^+$ 318.1289, found 318.1289.

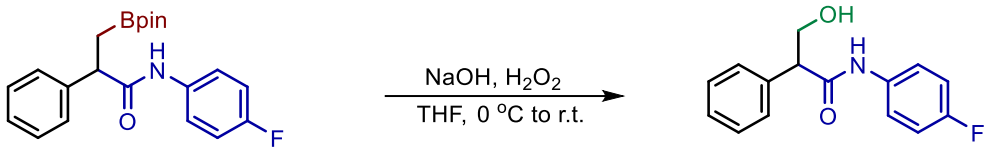
N-(4-fluorophenyl)-2-phenylacrylamide (7):



3aa **7**, 88%

To a round-bottom flask (50 mL), **3aa** (0.1 mmol, 37 mg), $Cu(OAc)_2$ (0.01 mmol, 2.0 mg) and CH_3OH (2.0 mL) were added. The flask was flushed with O_2 for 2 mins and sealed. After stirring at 70 °C for 24 h, the reaction mixture was cooled to room temperature. The mixture was concentrated in vacuo and purified by flash column chromatography (PE/EA) to give pure 7 (21.1 mg, 88%) as a white solid. M.p. 137.0 – 140.4 °C. IR(KBr): ν(cm^{-1}) = 3446, 3241, 3062, 1649, 1608, 1547, 1515, 1102, 836, 780. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.46 – 7.40 (m, 5H), 7.36 (s, 1H), 7.06 – 6.97 (m, 2H), 6.30 (s, 1H), 5.73 (d, J = 1.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.24, 159.67 (d, J = 244.0 Hz), 144.99, 136.73, 133.77 (d, J = 2.8 Hz), 129.14, 129.06, 128.42, 123.74, 121.89 (d, J = 7.9 Hz), 115.79 (d, J = 22.5 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.53. HRMS (ESI) m/z: calculated for $[C_{15}H_{12}FNO + H]^+$ 242.0975, found 242.0978.

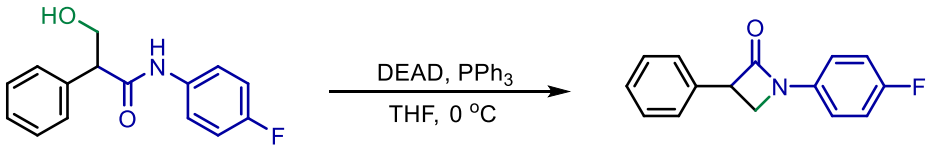
N-(4-fluorophenyl)-2-hydroxy-2-phenylacetamide (8):



3aa **8**, 93%

The following procedure was adapted from a previously-published method.[8] Compound **3aa** (0.2 mmol, 73.8 mg) was dissolved in THF (1.5 mL). While stirring at 0 °C, NaOH (3 M, 0.8 mL) was added dropwise followed by H_2O_2 solution (30 % in water, 0.4 mL). This mixture was stirred at ambient temperature for 0.5 h. The product was extracted to ethyl acetate (3 x 5 mL) and concentrated in vacuo. The crude product was then purified by flash column chromatography (PE/EA) to give pure **8** (48.3 mg, 93%) as a white solid. M.p. 146.3 – 148.9 °C. IR(KBr): ν(cm^{-1}) = 3420, 3239, 3058, 1654, 1615, 1556, 1509, 1454, 1409, 1067, 1021, 833, 765, 702. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.31 (m, 6H), 7.21 (s, 1H), 7.06 – 6.92 (m, 2H), 4.31 – 4.16 (m, 1H), 3.95 – 3.75 (m, 2H), 3.12 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.76, 159.74 (d, J = 244.2 Hz), 136.27, 133.39, 129.54, 128.64, 128.40, 122.09 (d, J = 8.0 Hz), 115.82 (d, J = 22.5 Hz), 65.08, 55.46. ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.35. HRMS (ESI) m/z: calculated for $[C_{15}H_{14}FNO_2 + H]^+$ 260.1081, found 260.1088.

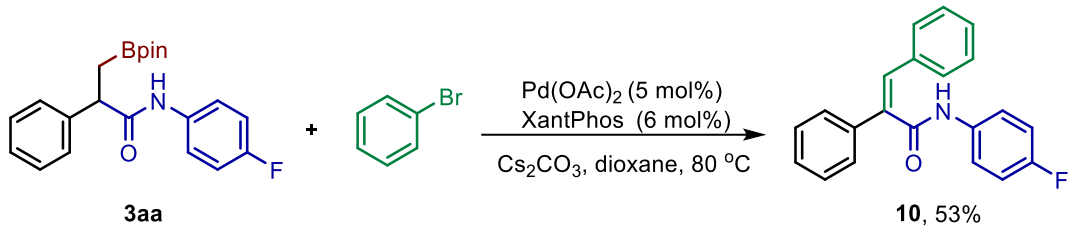
1-(4-fluorophenyl)-3-phenylazetidin-2-one (9):



8 **9**, 88%

The following procedure was in the light of a previously-reported method.[9] Compound **8** (0.2 mmol, 52 mg) and PPh_3 (0.28 mmol, 74 mg) was dissolved in THF (1.0 mL). Diethyl azodicarboxylate (DEAD, 0.24 mmol, 38.0 μL) was added dropwise to the mixture which was cooled to 0 °C. The reaction was stirred at room temperature for 36 h. The mixture was concentrated in vacuo and purified by flash column chromatography (DCE/EA) to give pure **9** (42.3 mg, 88%) as a white solid. M.p. 107.1 – 109.6 °C. IR(KBr): ν(cm^{-1}) = 3459, 3077, 2982, 1632, 1601, 1508, 1497, 1473, 1457, 1387, 1229, 1212, 1180, 1147, 1102, 1078, 779, 725. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.33 (m, 6H), 7.33 – 7.28 (m, 1H), 7.10 – 7.02 (m, 2H), 4.53 (dd, J = 5.9, 2.8 Hz, 1H), 4.06 (t, J = 5.8 Hz, 1H), 3.67 (dd, J = 5.7, 2.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.18, 159.30 (d, J = 243.3 Hz), 135.25, 134.68 (d, J = 2.7 Hz), 129.10, 127.91, 127.50, 117.94 (d, J = 7.9 Hz), 116.12 (d, J = 22.7 Hz), 53.91, 47.03. ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.86. HRMS (ESI) m/z: calculated for $[C_{15}H_{12}FNO + H]^+$ 242.0975, found 242.0979.

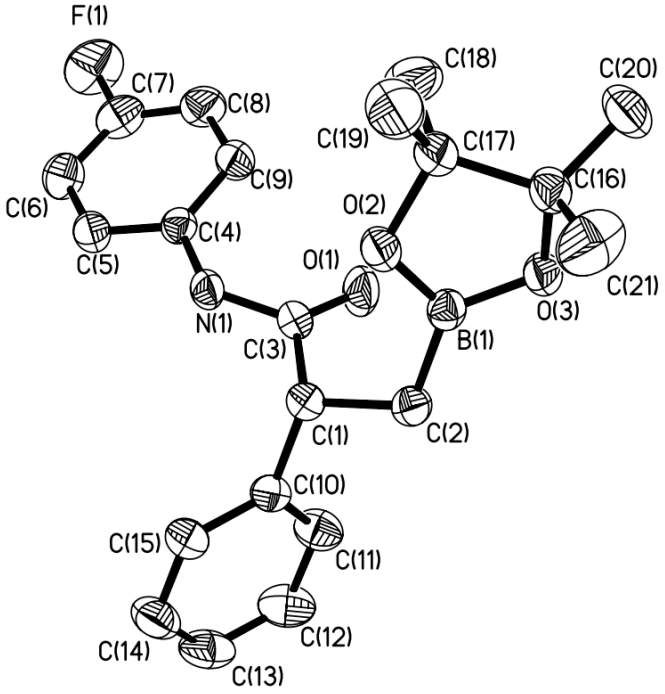
(*Z*)-N-(4-fluorophenyl)-2,3-diphenylacrylamide (10):



3aa **10**, 53%

A oven-dried 25 mL Schlenk tube was charged with **3aa** (0.1 mmol, 36.9 mg), $Pd(OAc)_2$ (5 mol%, 1.2 mg), XantPhos (6 mol%, 3.5 mg), Cs_2CO_3 (0.14 mmol, 45.6 mg). The tube was evacuated and backfilled with argon for three times. Dioxane (2.0 mL, anhydrous and degassed) and bromobenzene (0.15 mmol, 19.0 µL) was added under an argon atmosphere. The mixture was allowed to stir at 80 °C (pre-heated oil bath) for 48 h. After cooling to room temperature, 2 mL H_2O was added and the mixture was extracted with ethyl acetate (3 x 5.0 mL). The combined organic layers were concentrated in vacuo, and the residue was purified by flash column chromatography (PE/EA) to give **10** (17 mg, 53%) as a white solid. M.p. 179.8 – 182.7 ℃. IR(KBr): ν(cm^{-1}) = 3447, 1644, 1612, 1537, 1508, 1446, 1157, 1076, 925, 808, 757, 724, 701, 690. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.55 – 7.47 (m, 3H), 7.45 – 7.39 (m, 2H), 7.35 (dd, *J* = 7.5, 1.6 Hz, 2H), 7.20 (dd, *J* = 8.3, 6.1 Hz, 1H), 7.16 (t, *J* = 7.3 Hz, 3H), 7.05 – 6.95 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.11, 159.59 (d, *J* = 243.9 Hz), 138.55, 135.88, 134.85, 134.44, 134.01 (d, *J* = 2.8 Hz), 130.62, 130.12, 130.11, 129.15, 129.04, 128.39, 121.84 (d, *J* = 7.9 Hz), 115.71 (d, *J* = 22.5 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.78. HRMS (ESI) m/z: calculated for $[C_{21}H_{16}FNO + H]^+$ 318.1289, found 318.1289.

5. X-Ray Data of 3aa



CCDC 1971971 (**3aa**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

6. References

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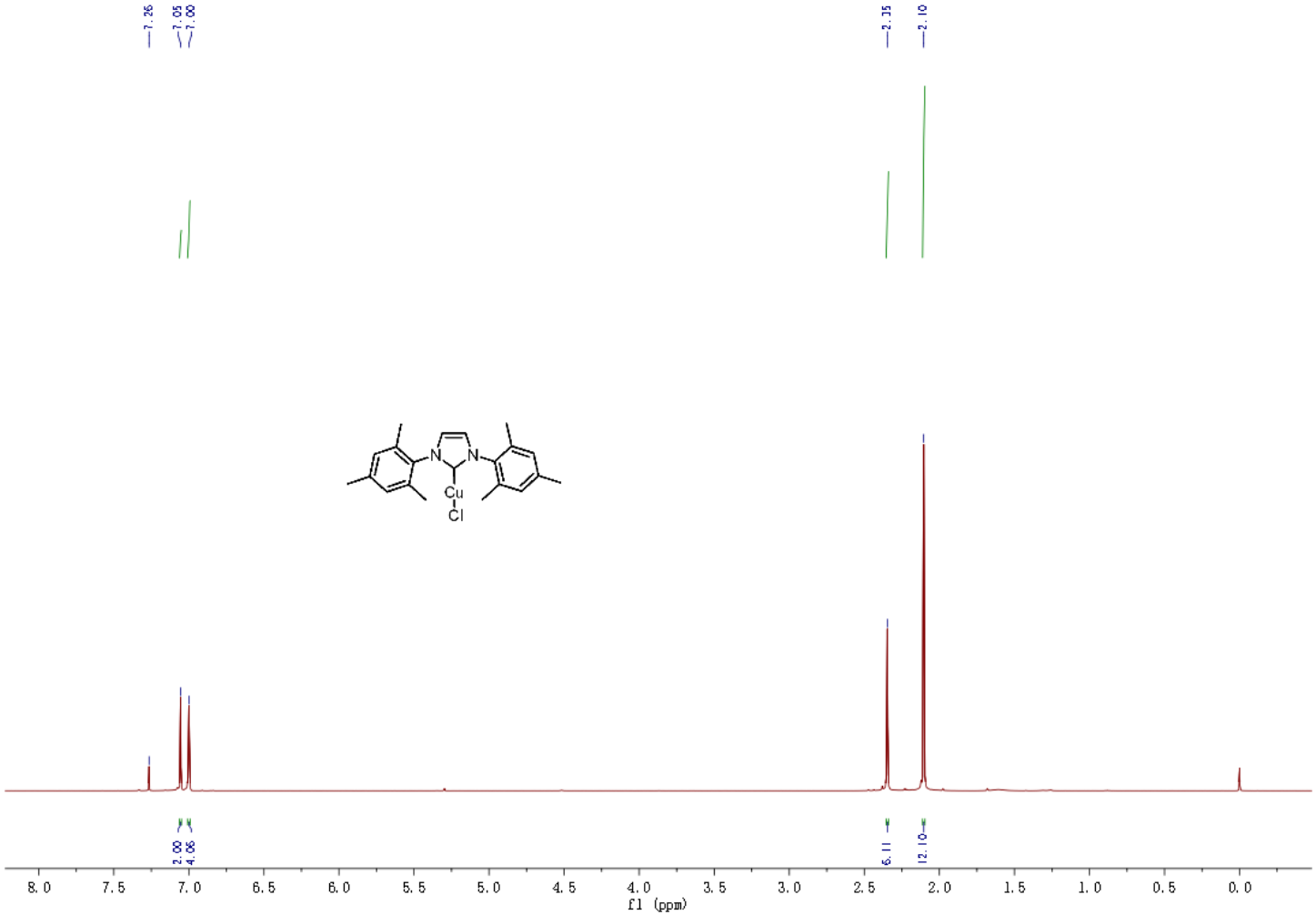
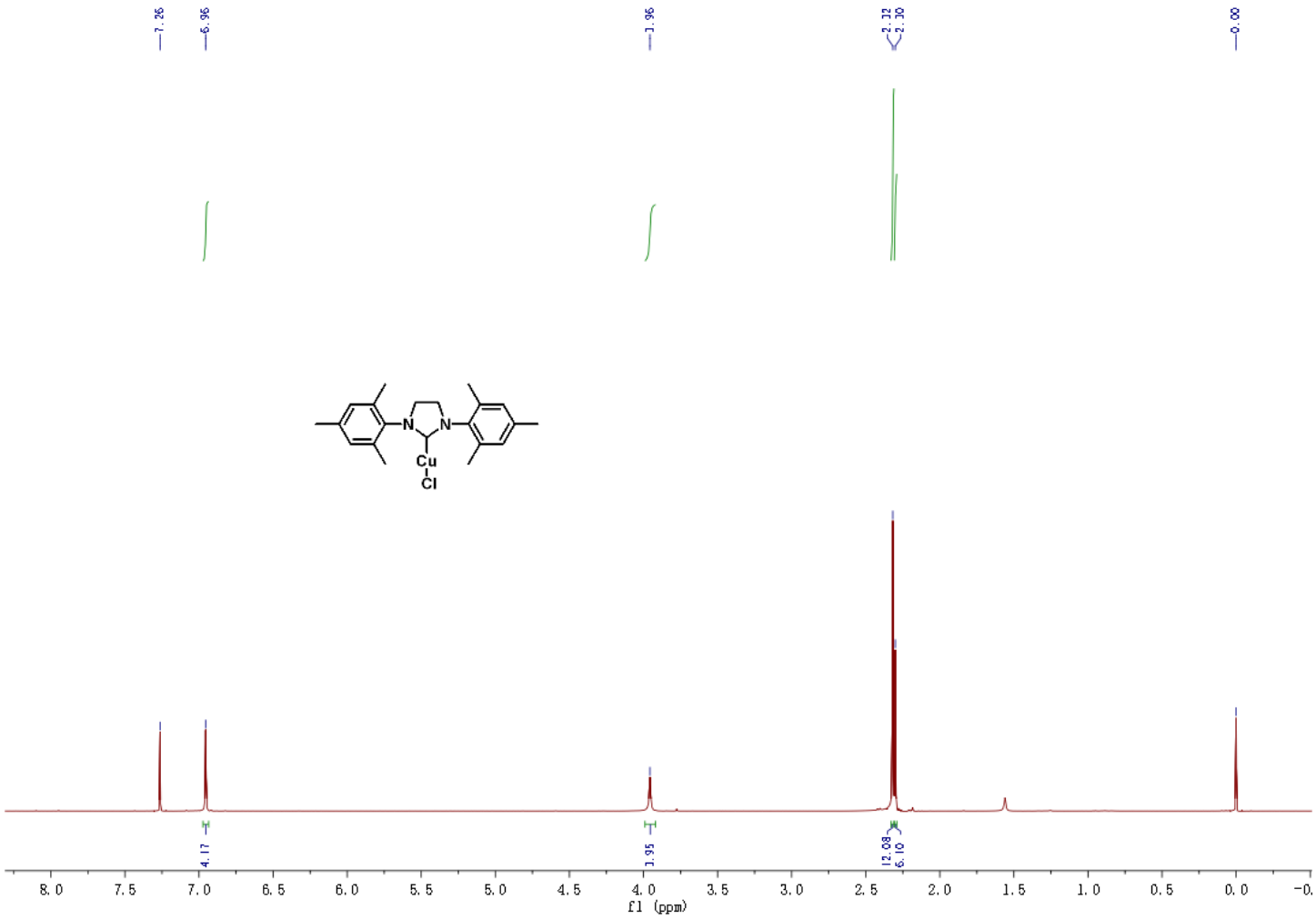
9. J. M. Keith, L. Gomez, *J. Org. Chem.*, 2006, **71**, 7113.

7. Spectroscopic Data (NMR Spectrum)

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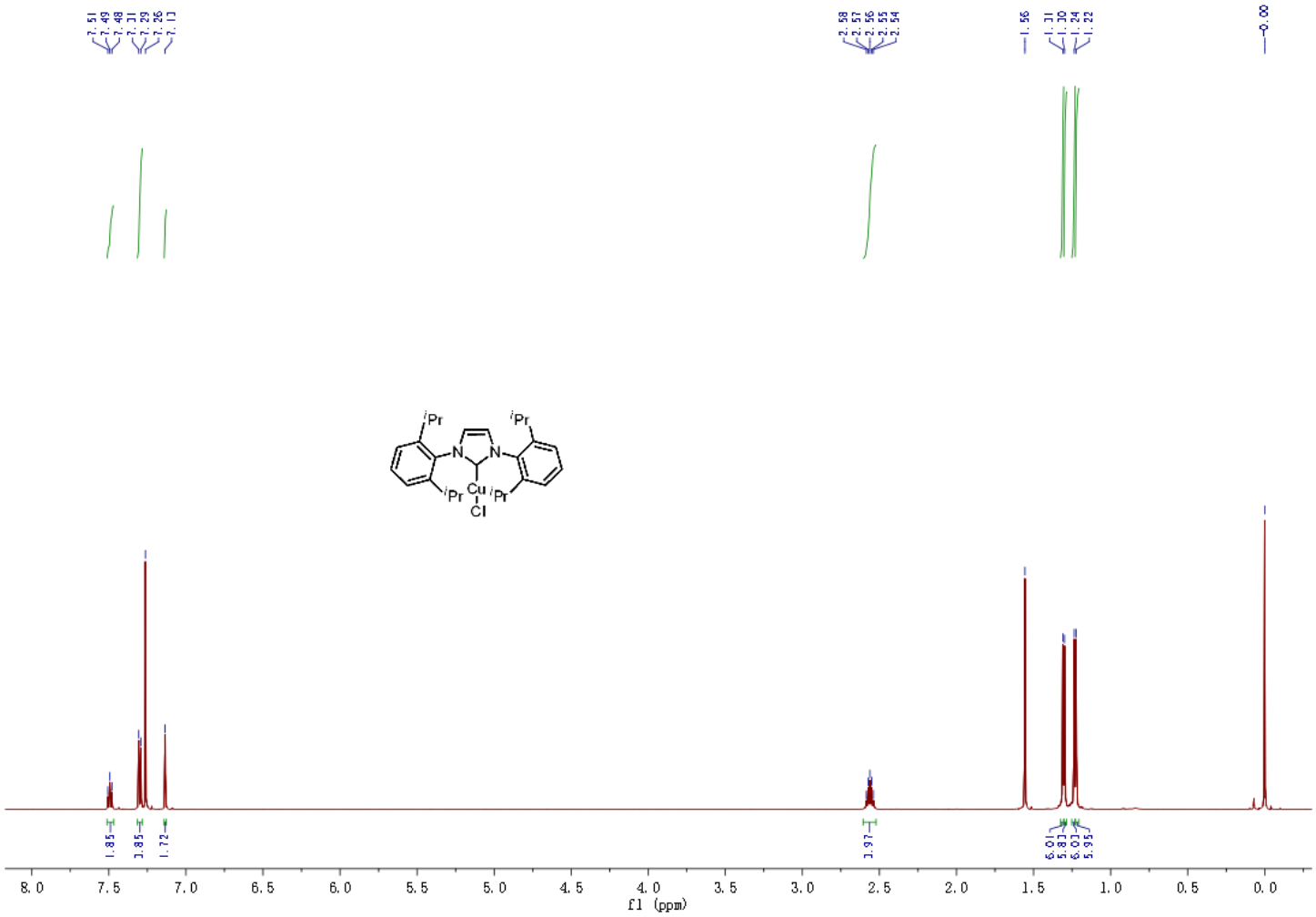
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iPr
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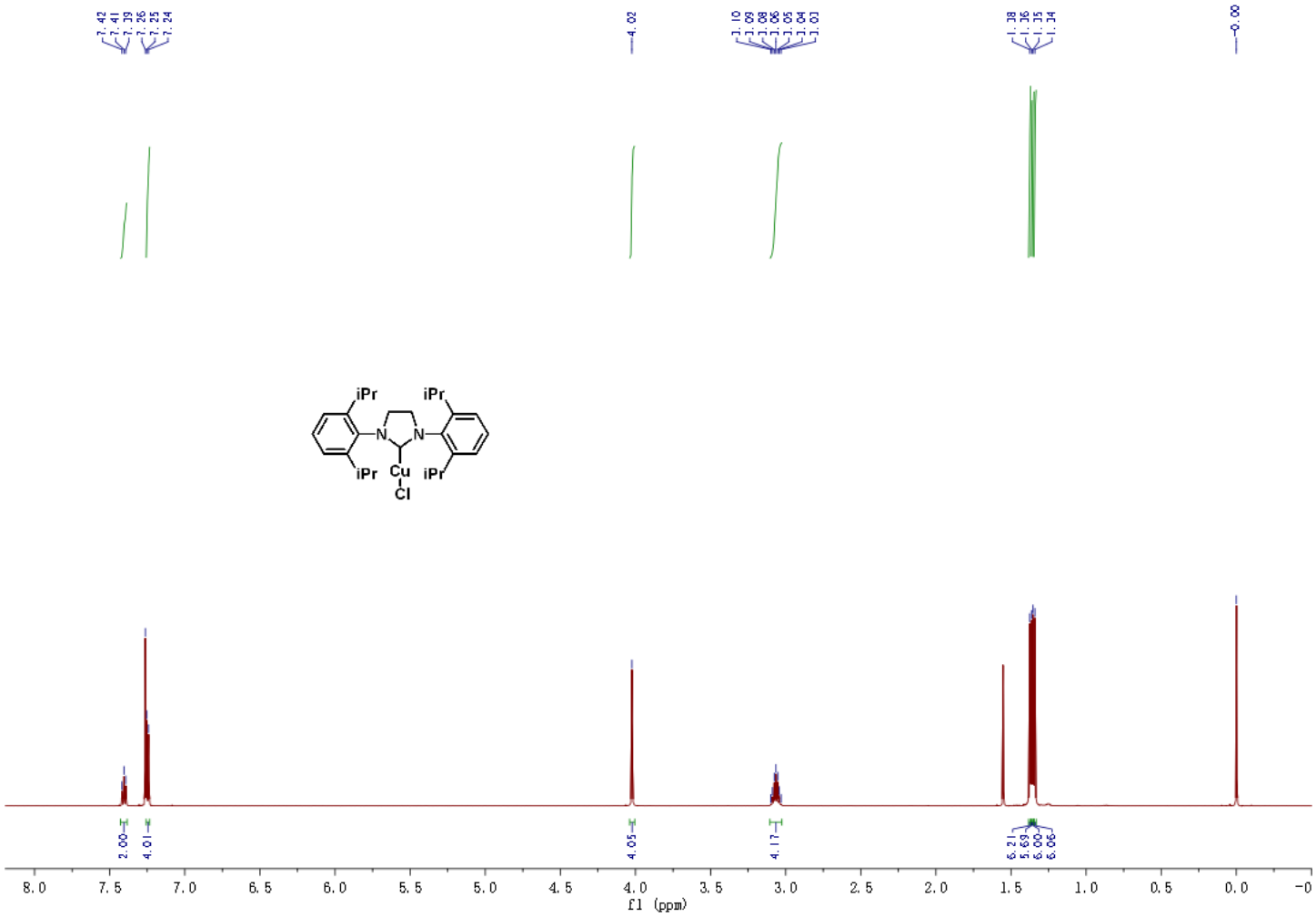
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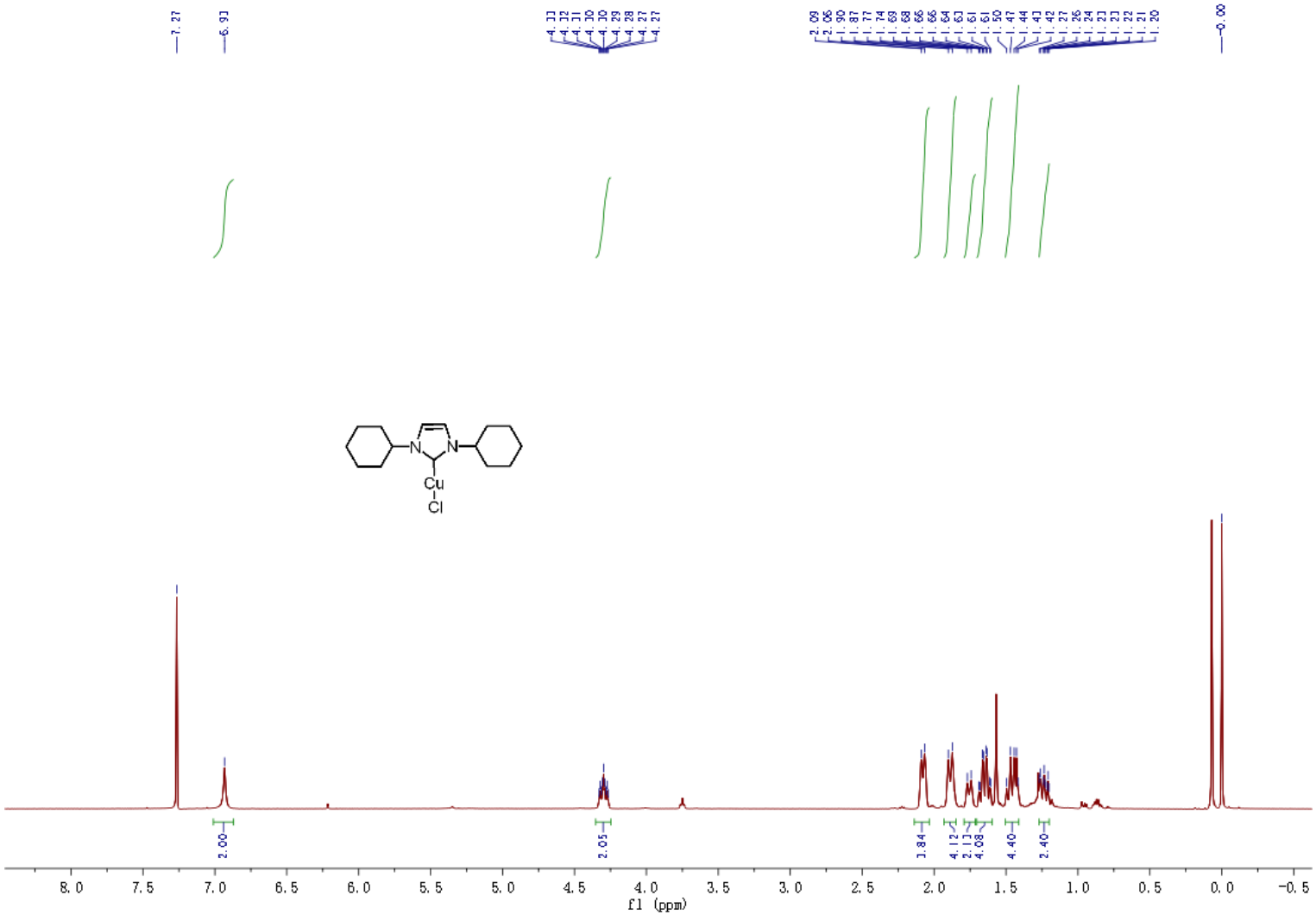
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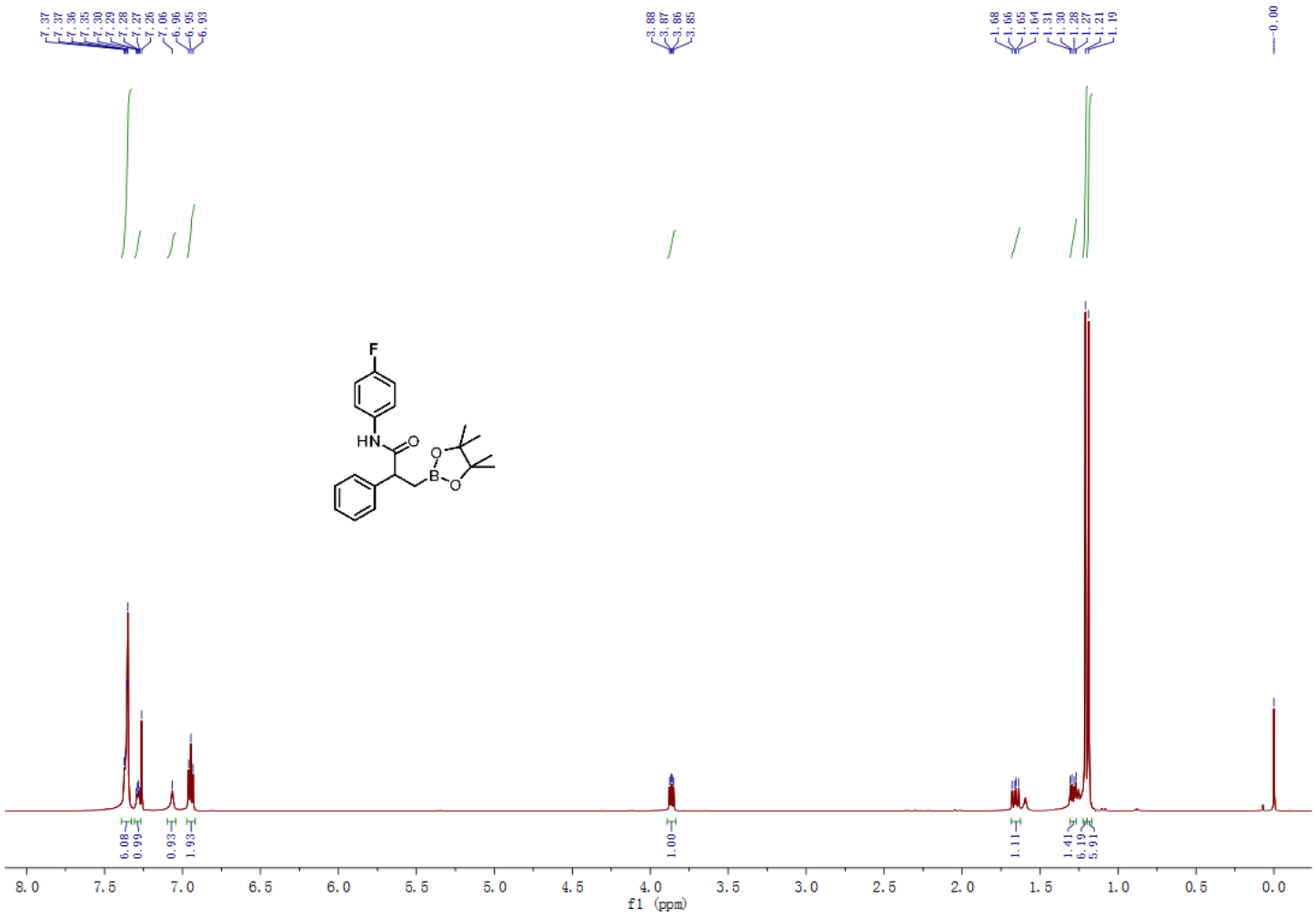
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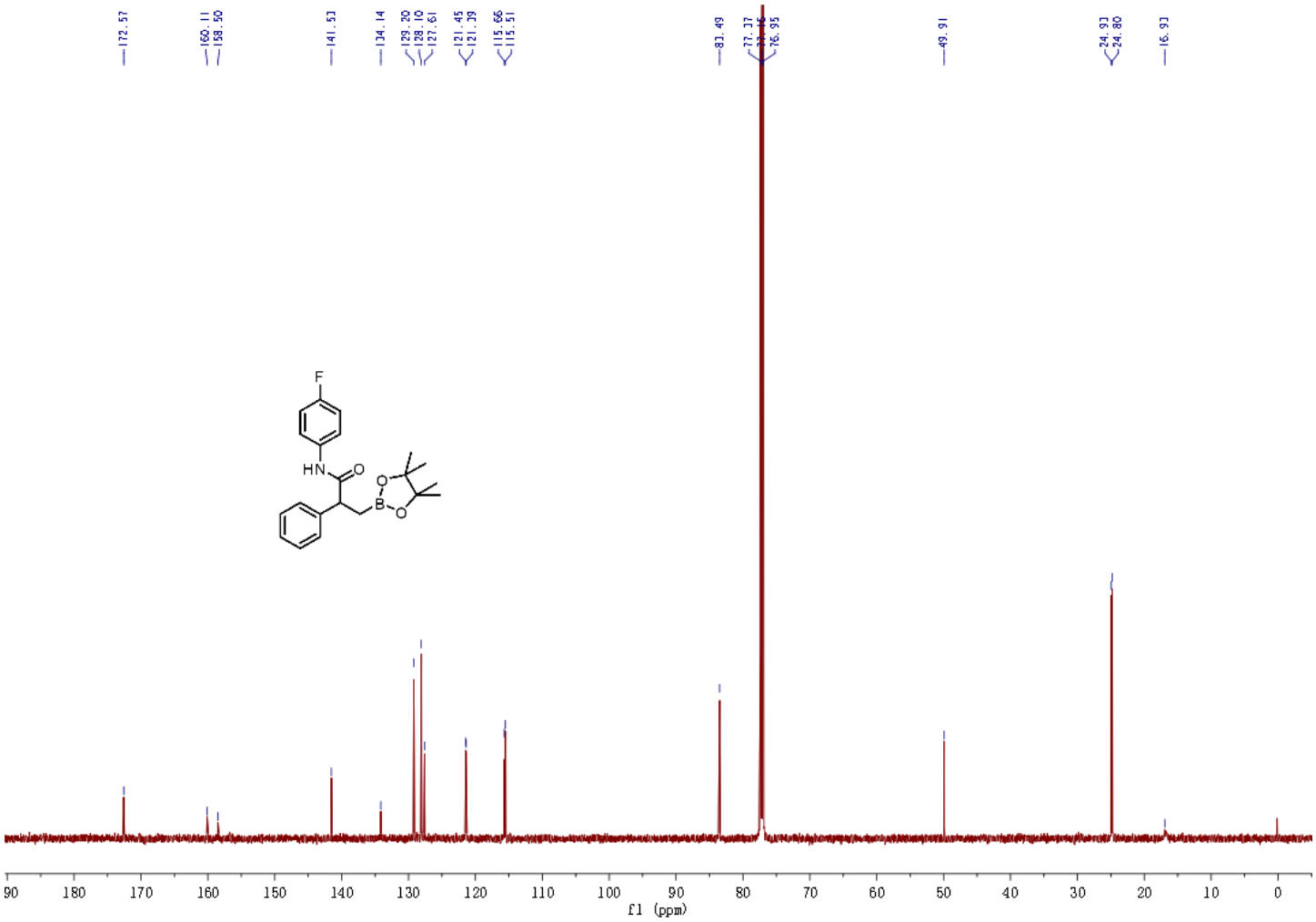
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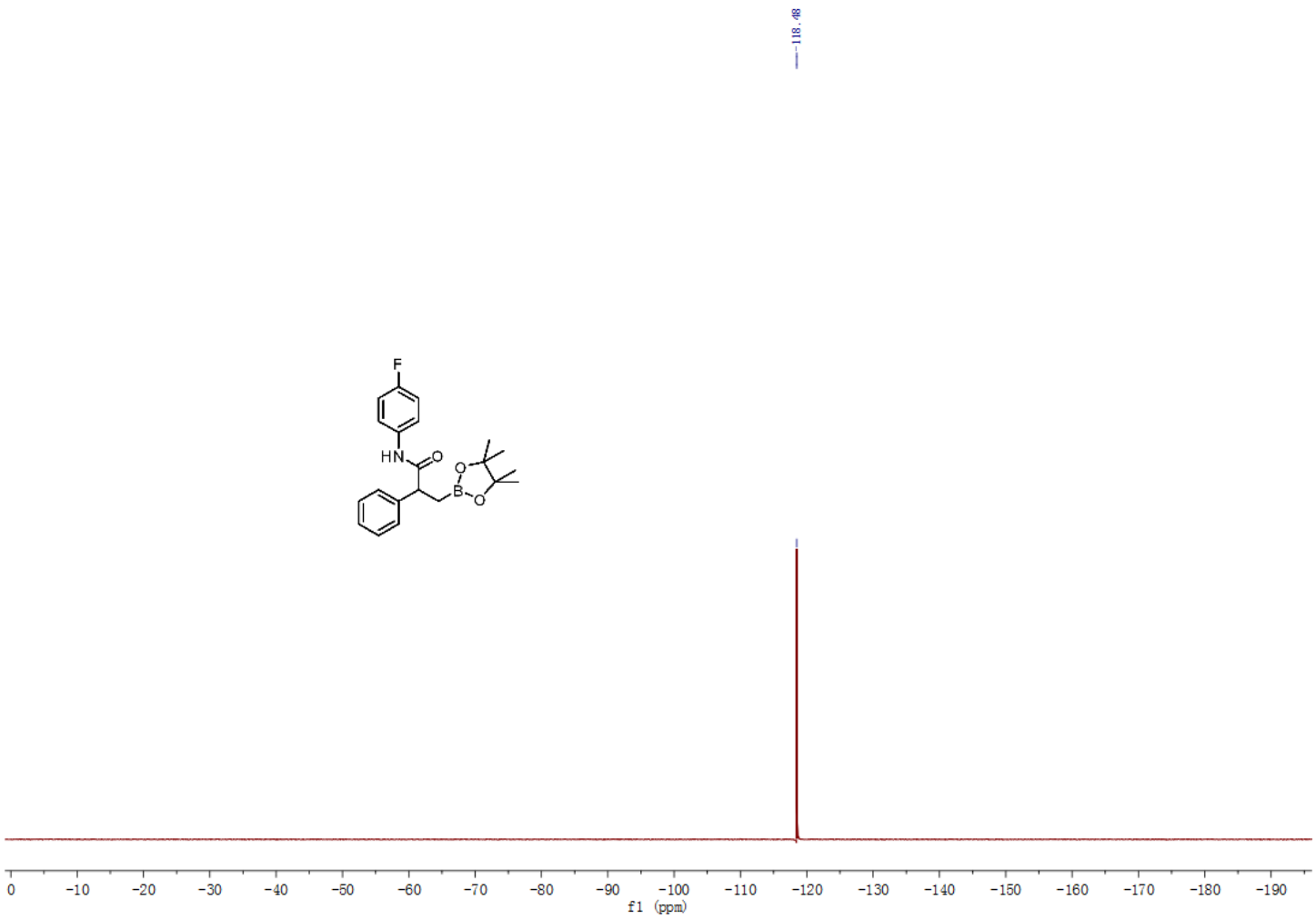
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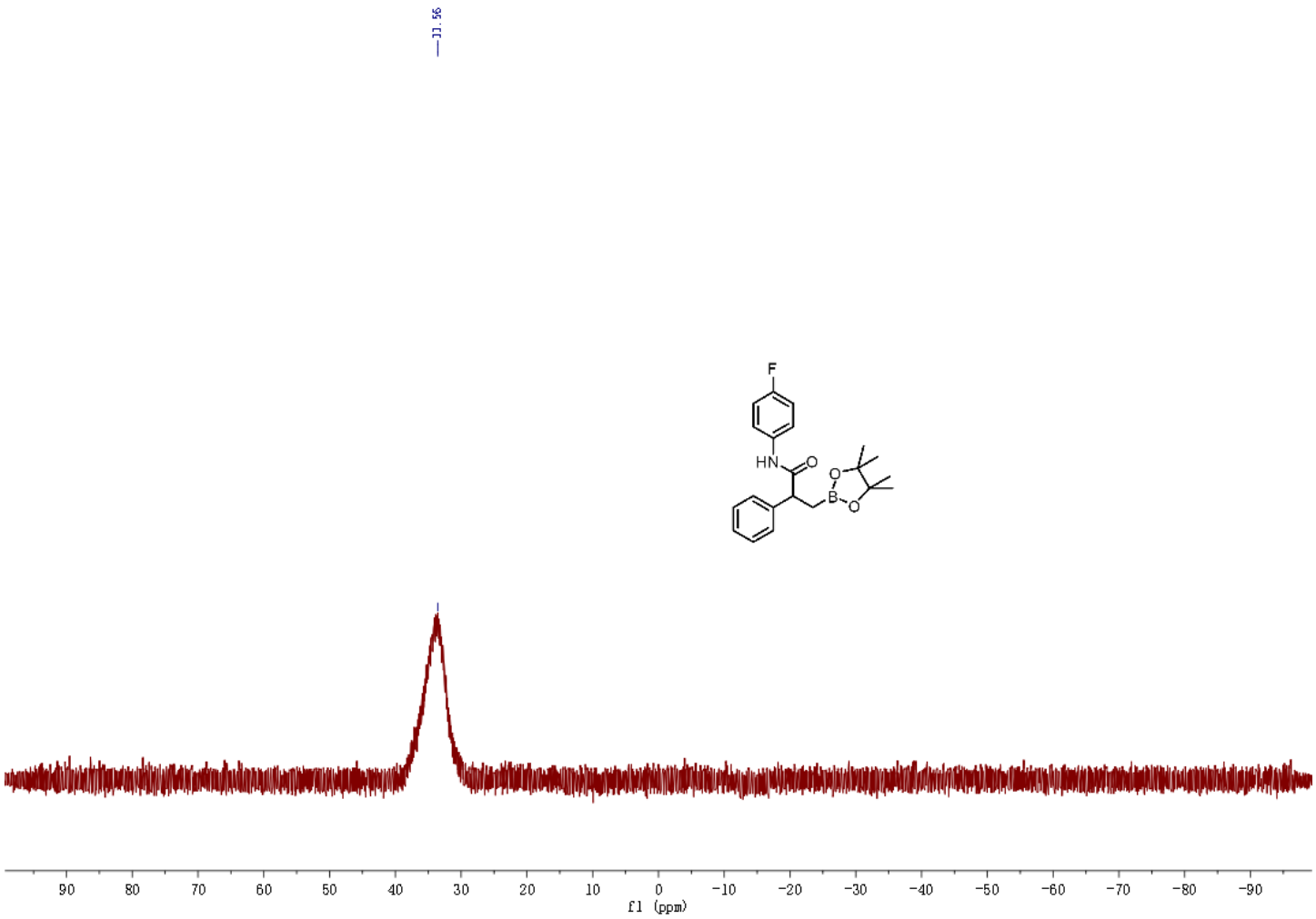
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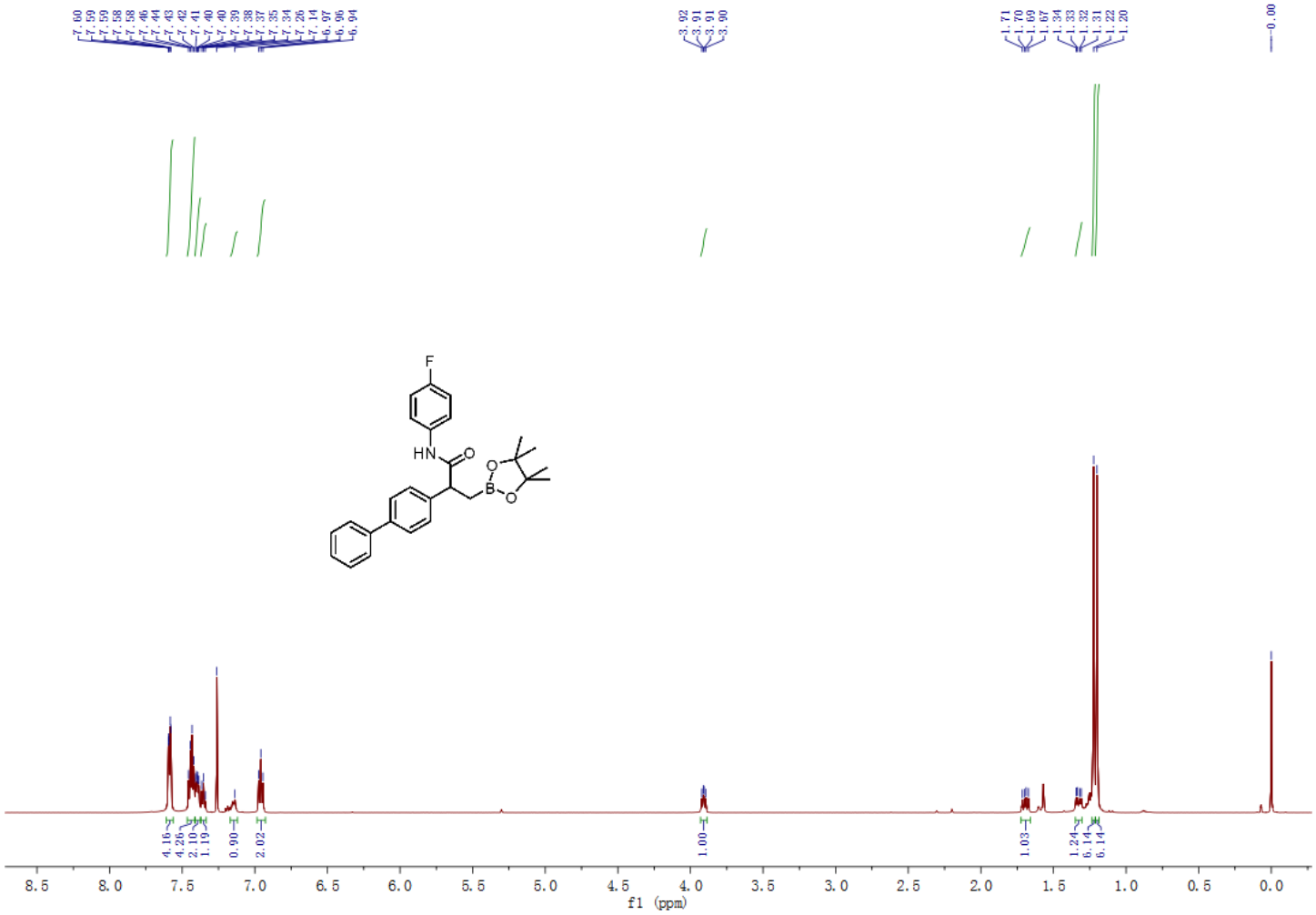
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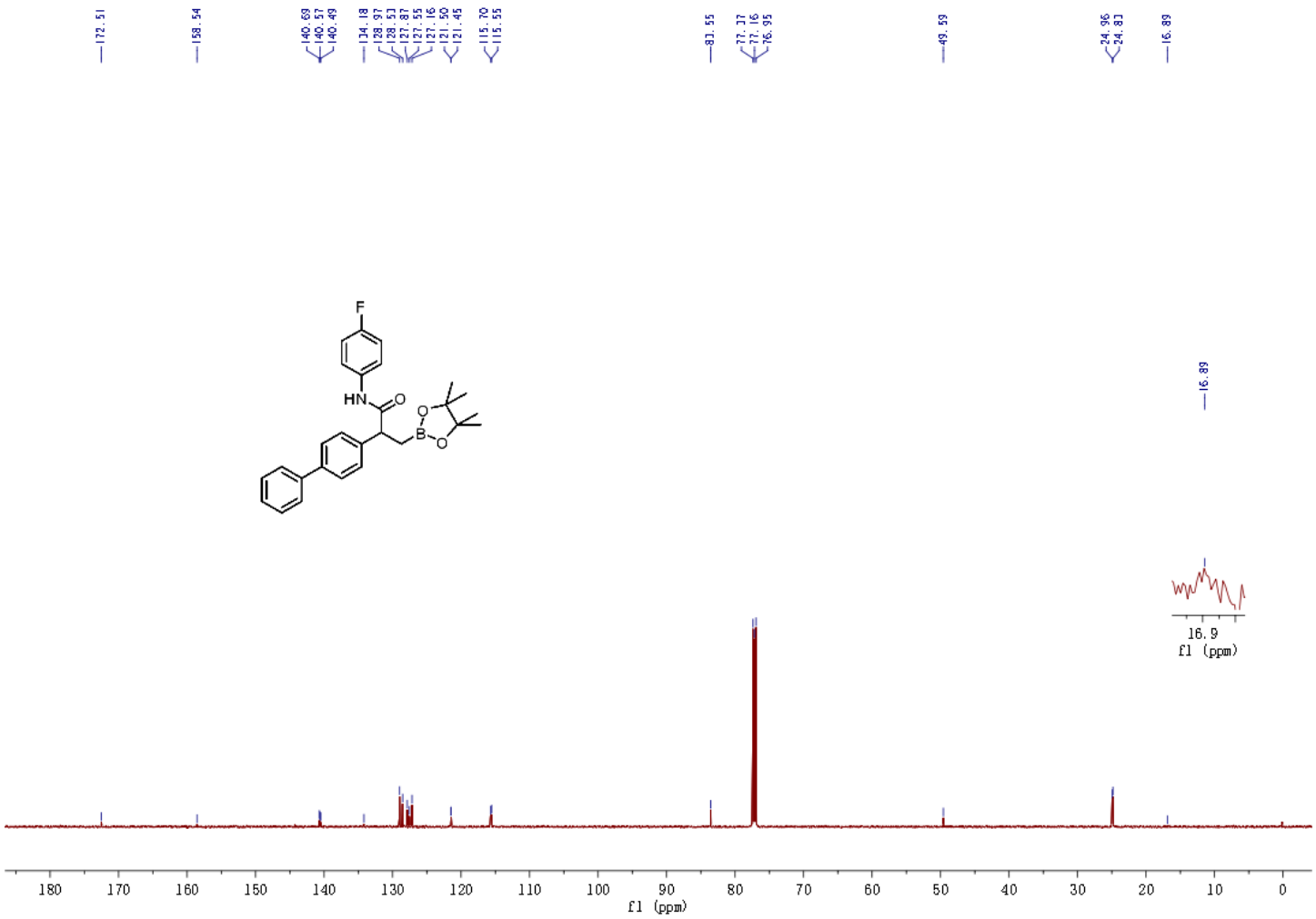
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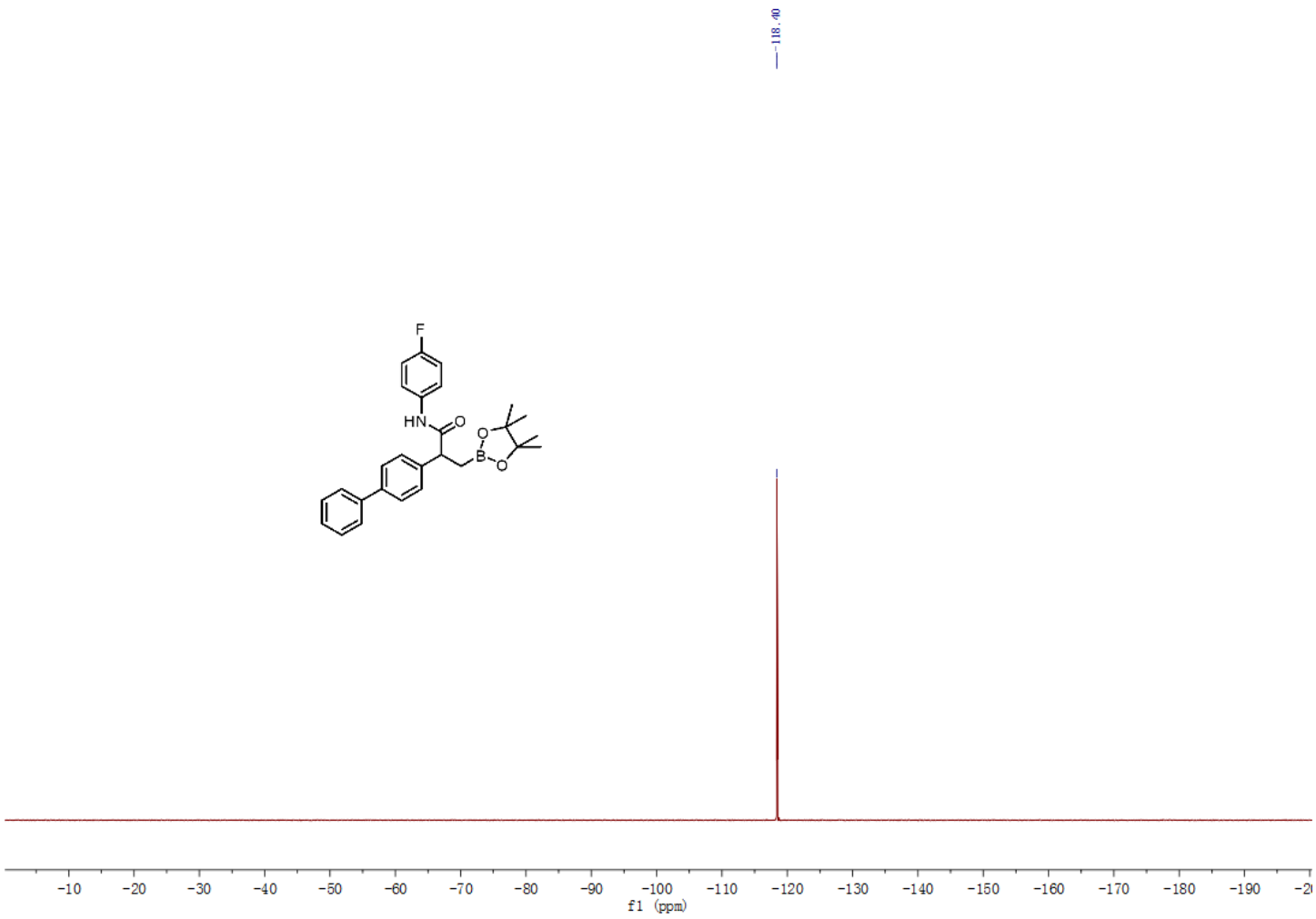
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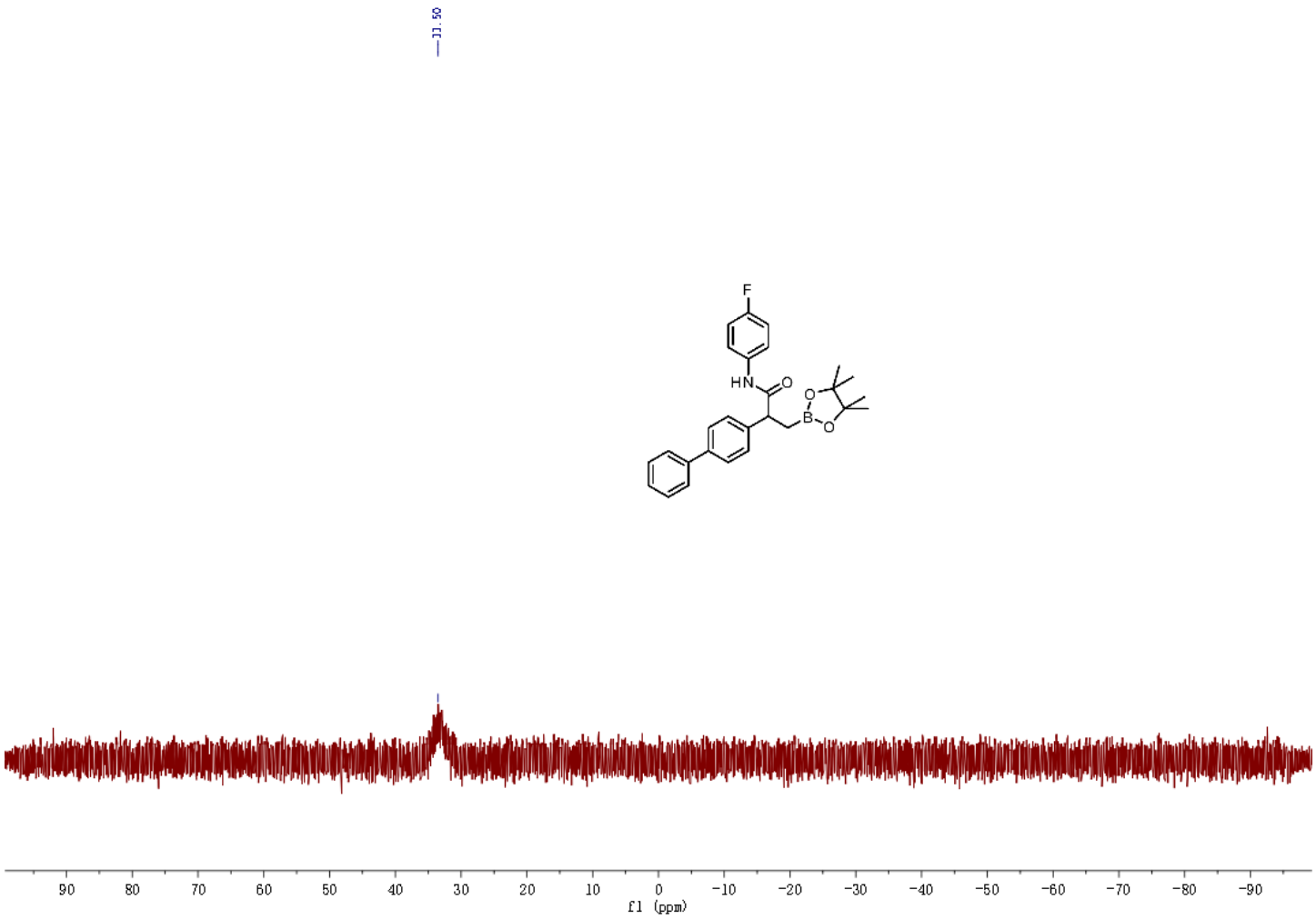
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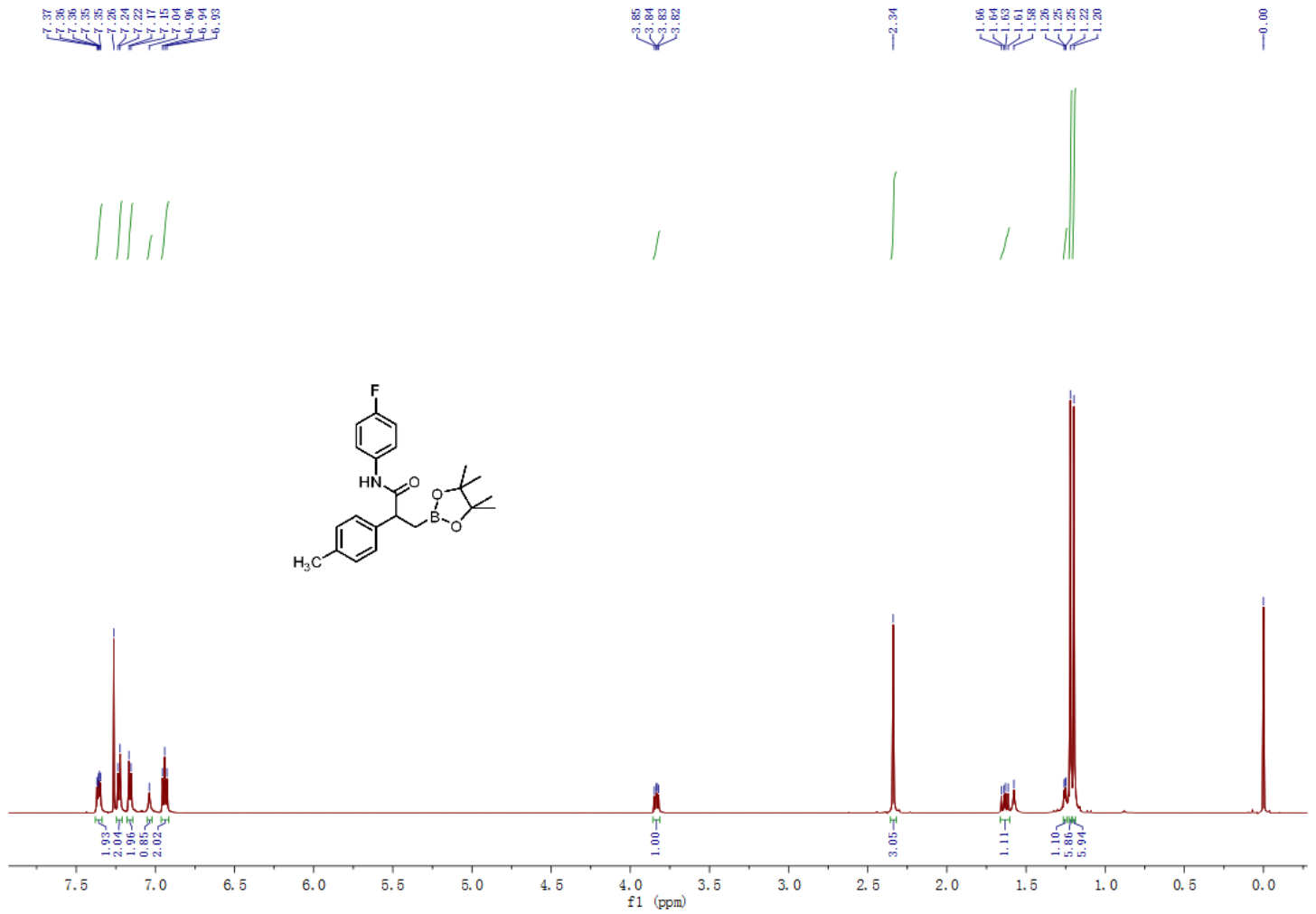
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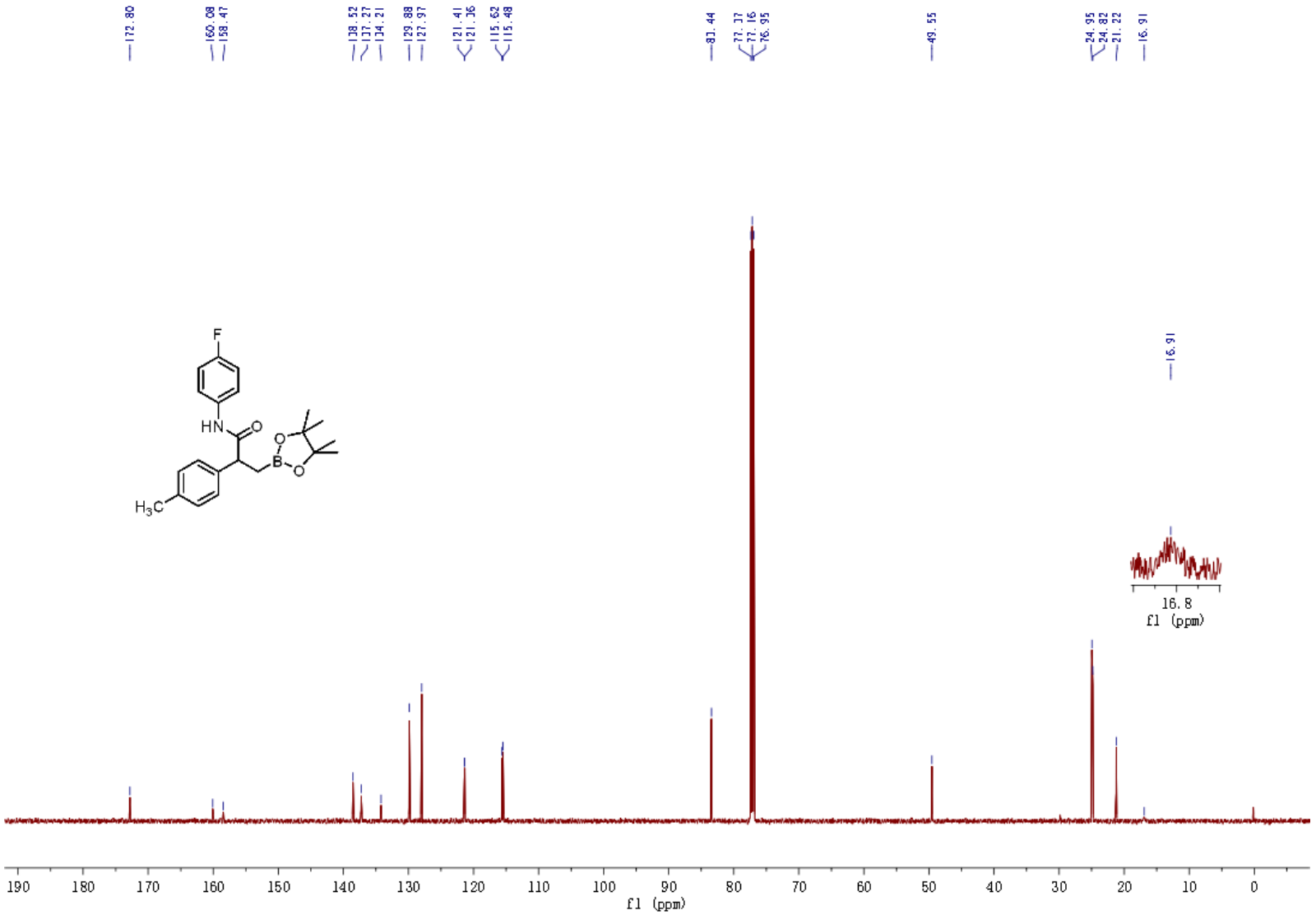
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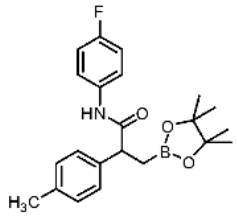
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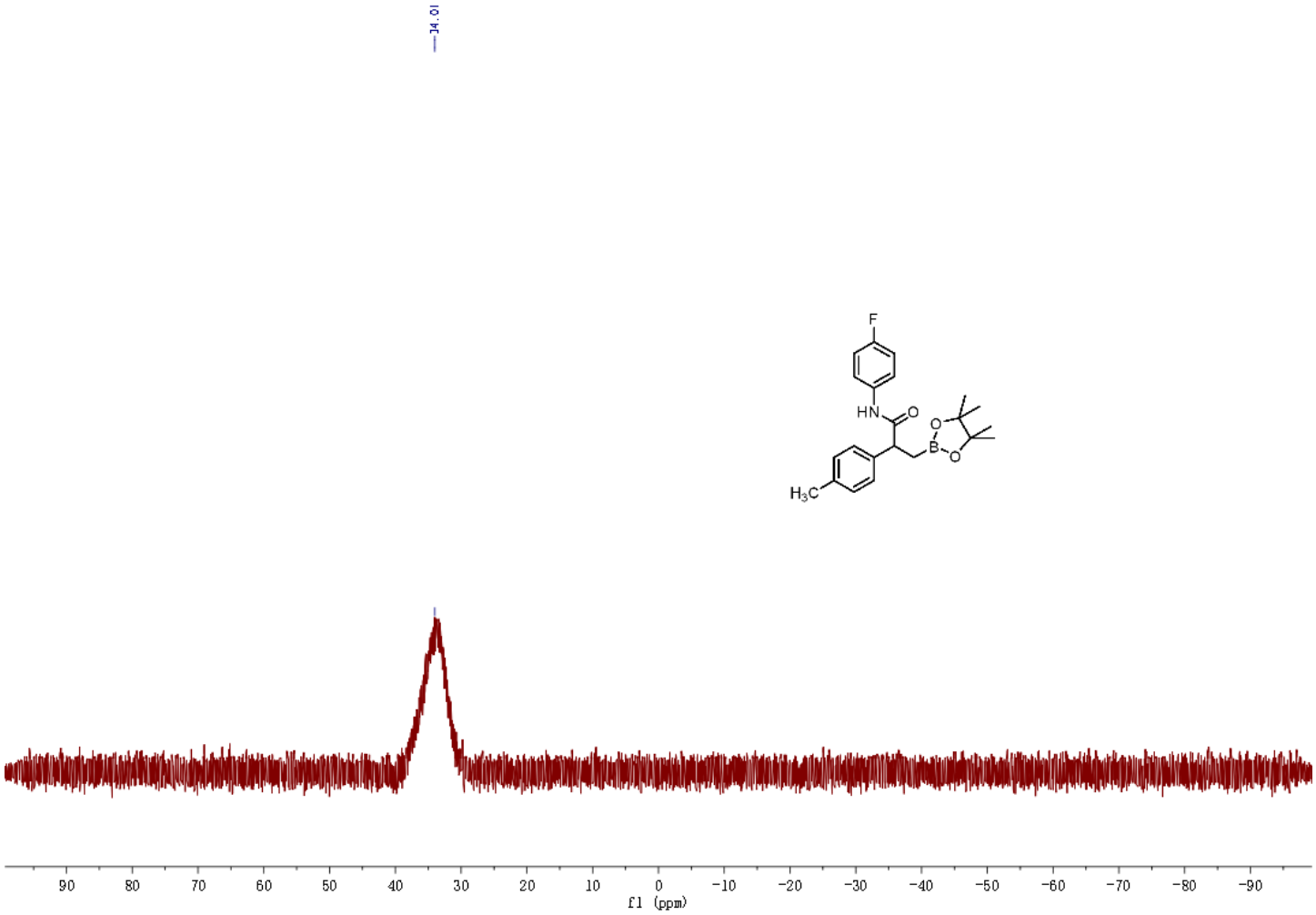
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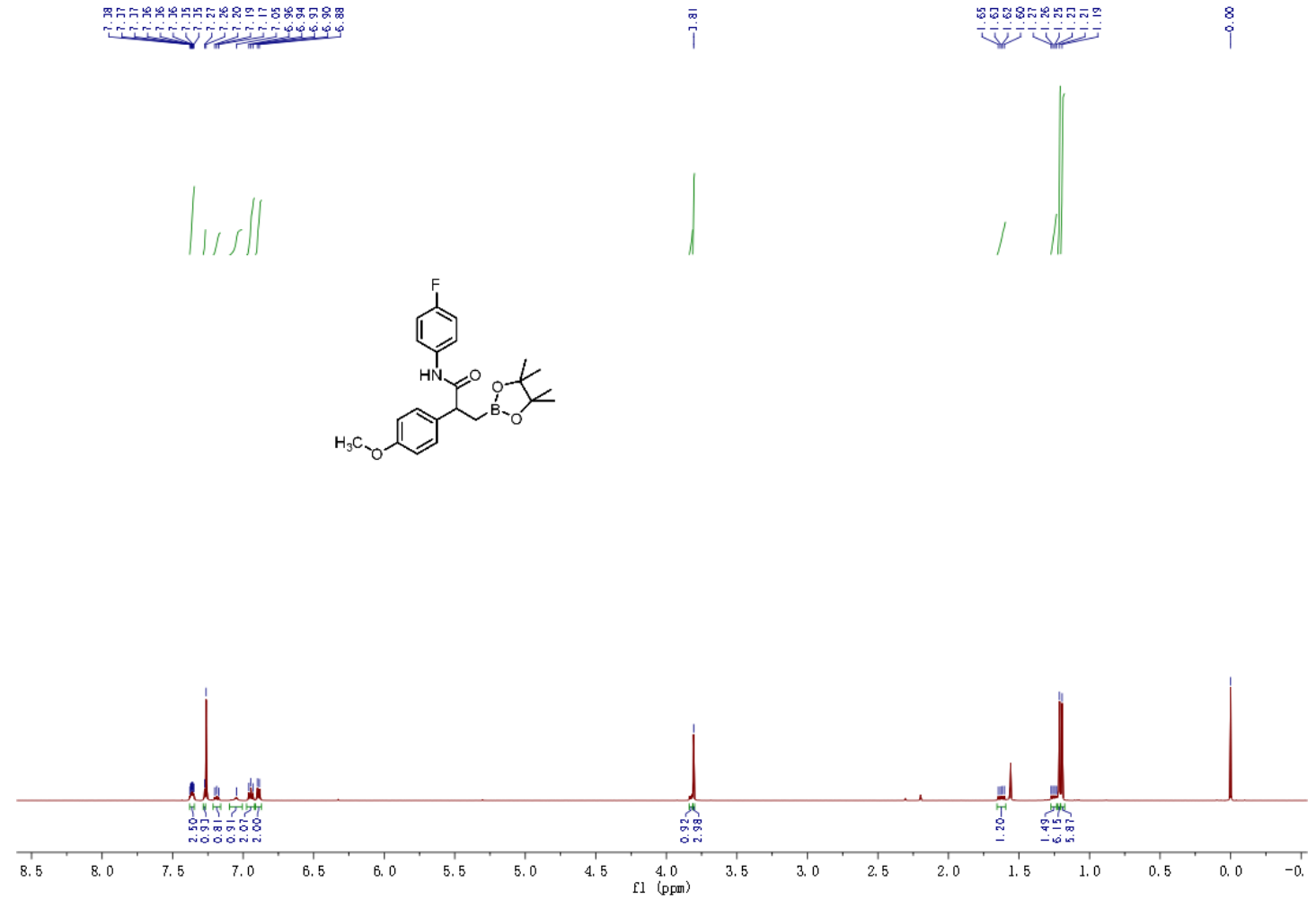
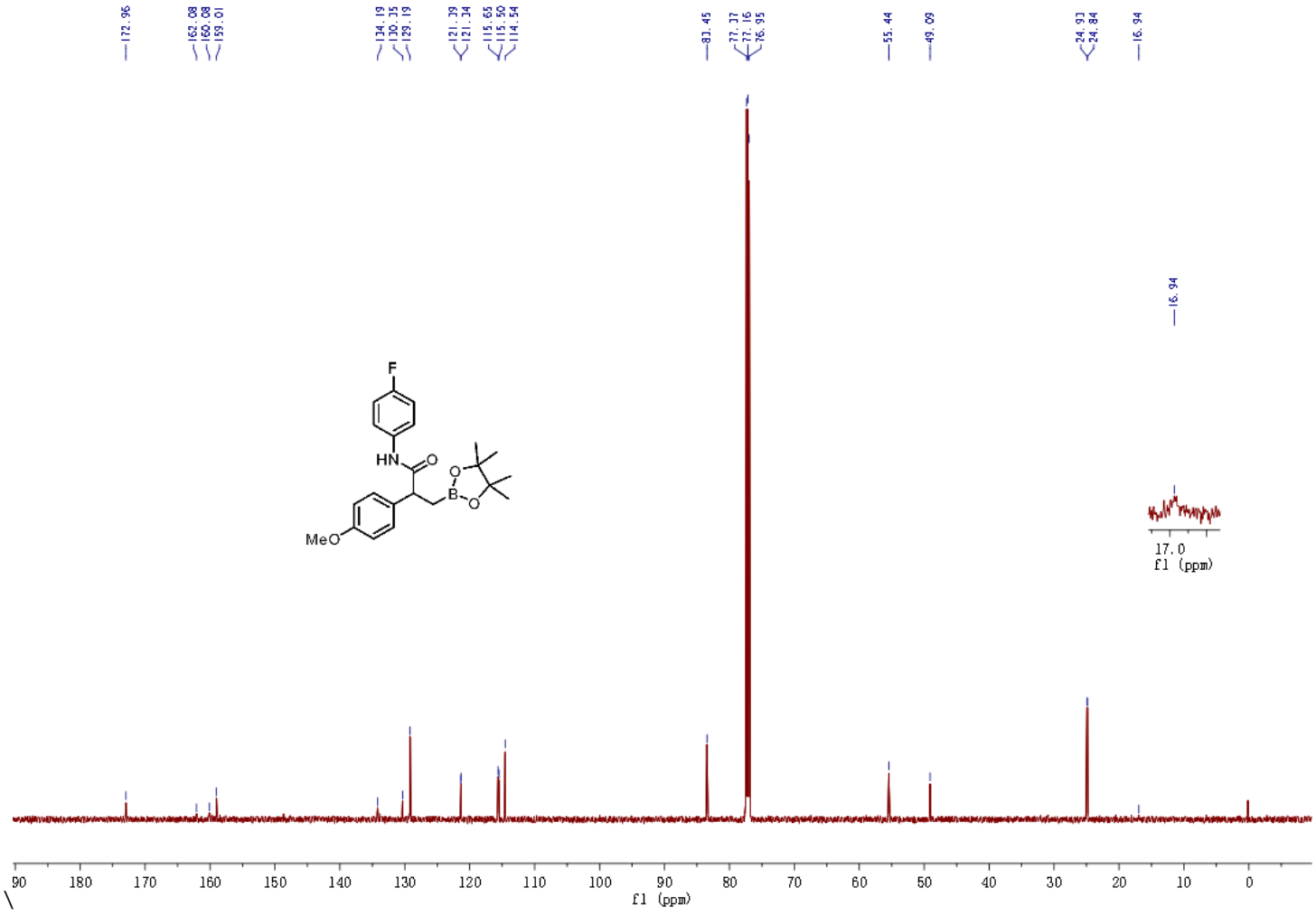
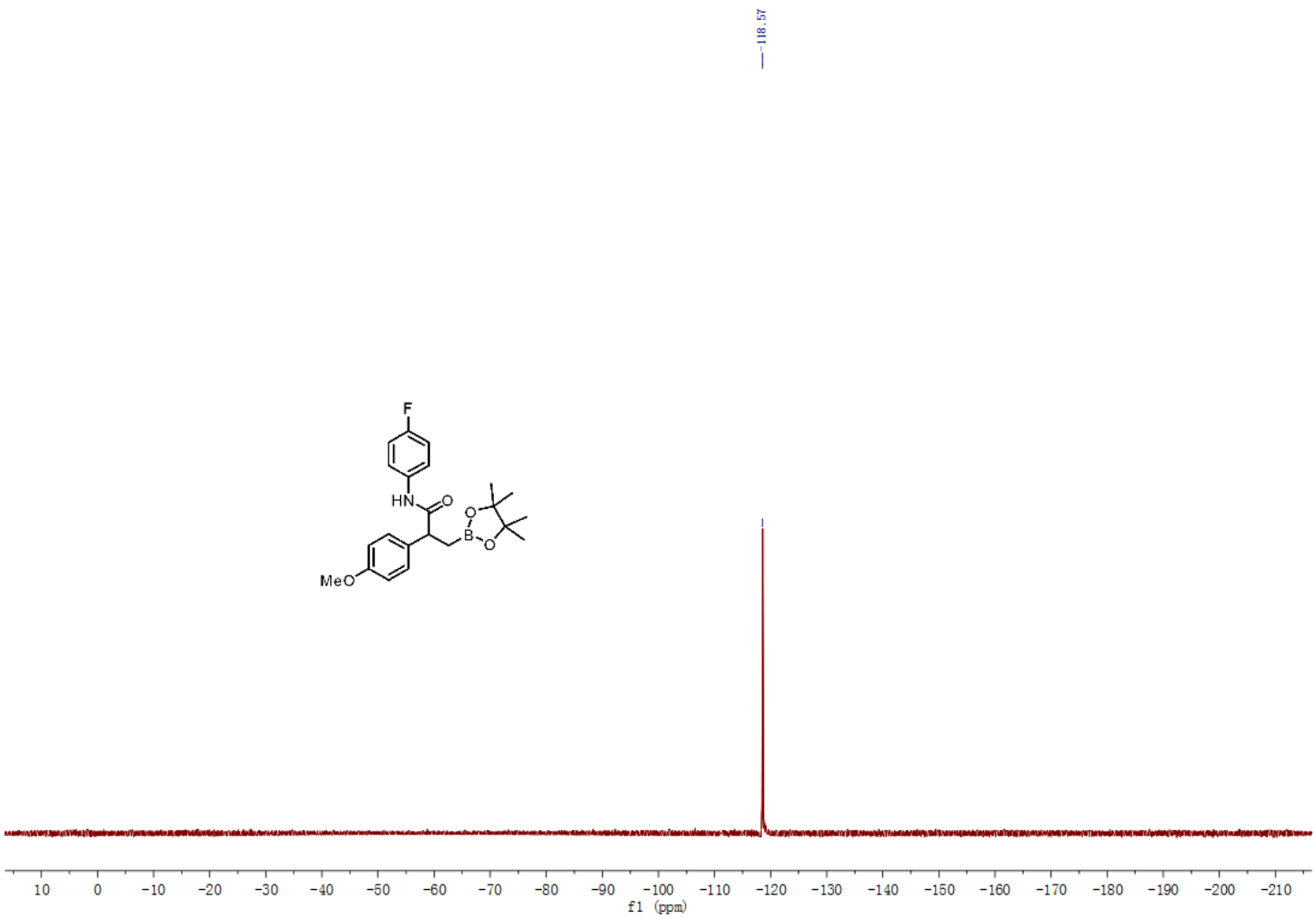
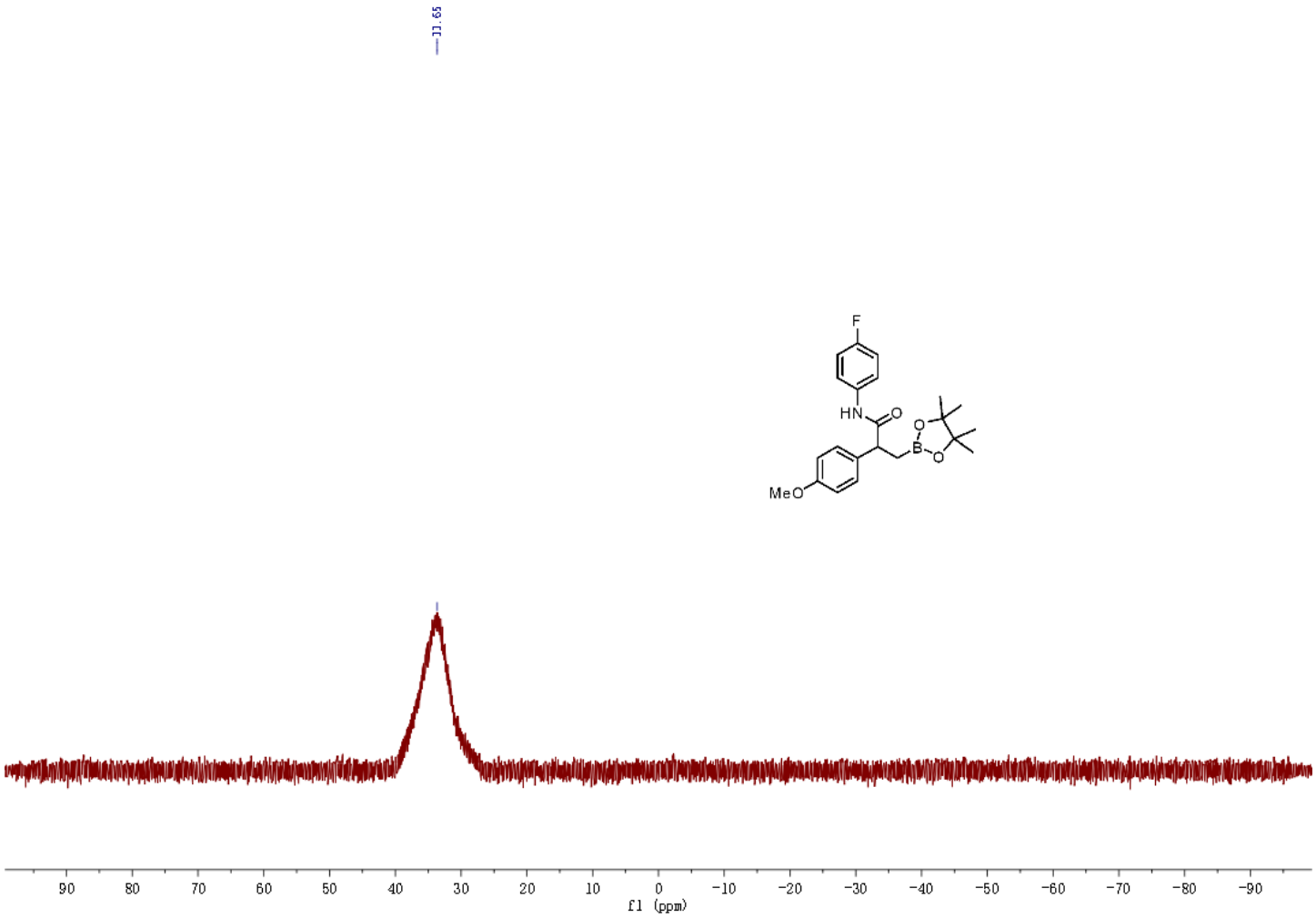
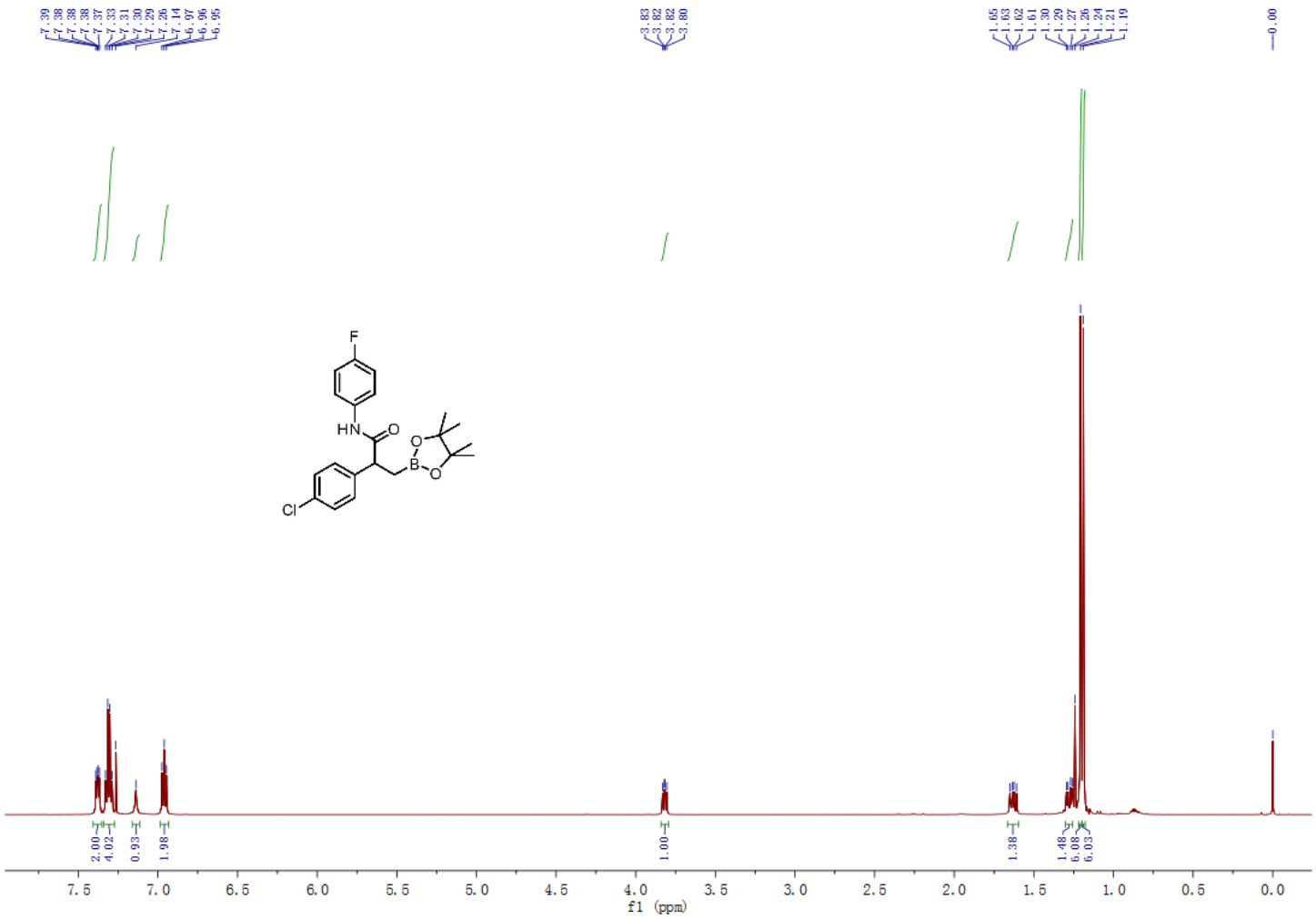
-90
f1 (ppm)

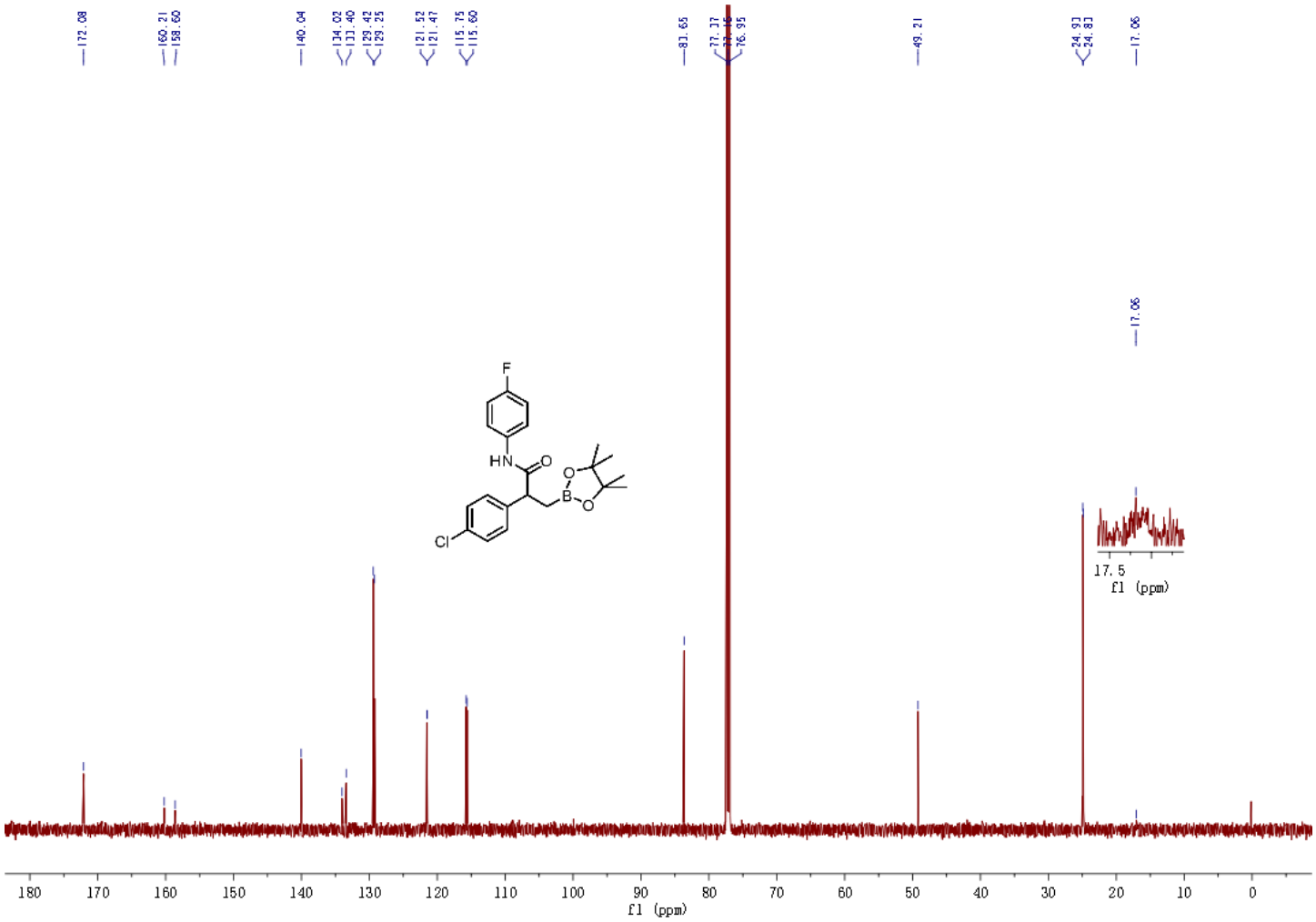

7.38
7.37
7.37
7.36
7.36
7.36
7.35
7.27
7.26
7.20
7.19
7.17
7.05
6.96
6.94
6.93
6.90
6.88
3.81
1.65
1.63
1.62
1.60
1.27
1.26
1.25
1.23
1.21
1.19
0.00
F
HN
O
O
B
O
H3C
O
2.50
0.93
0.81
0.91
2.07
2.00
0.92
2.98
1.20
1.49
6.15
5.87
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

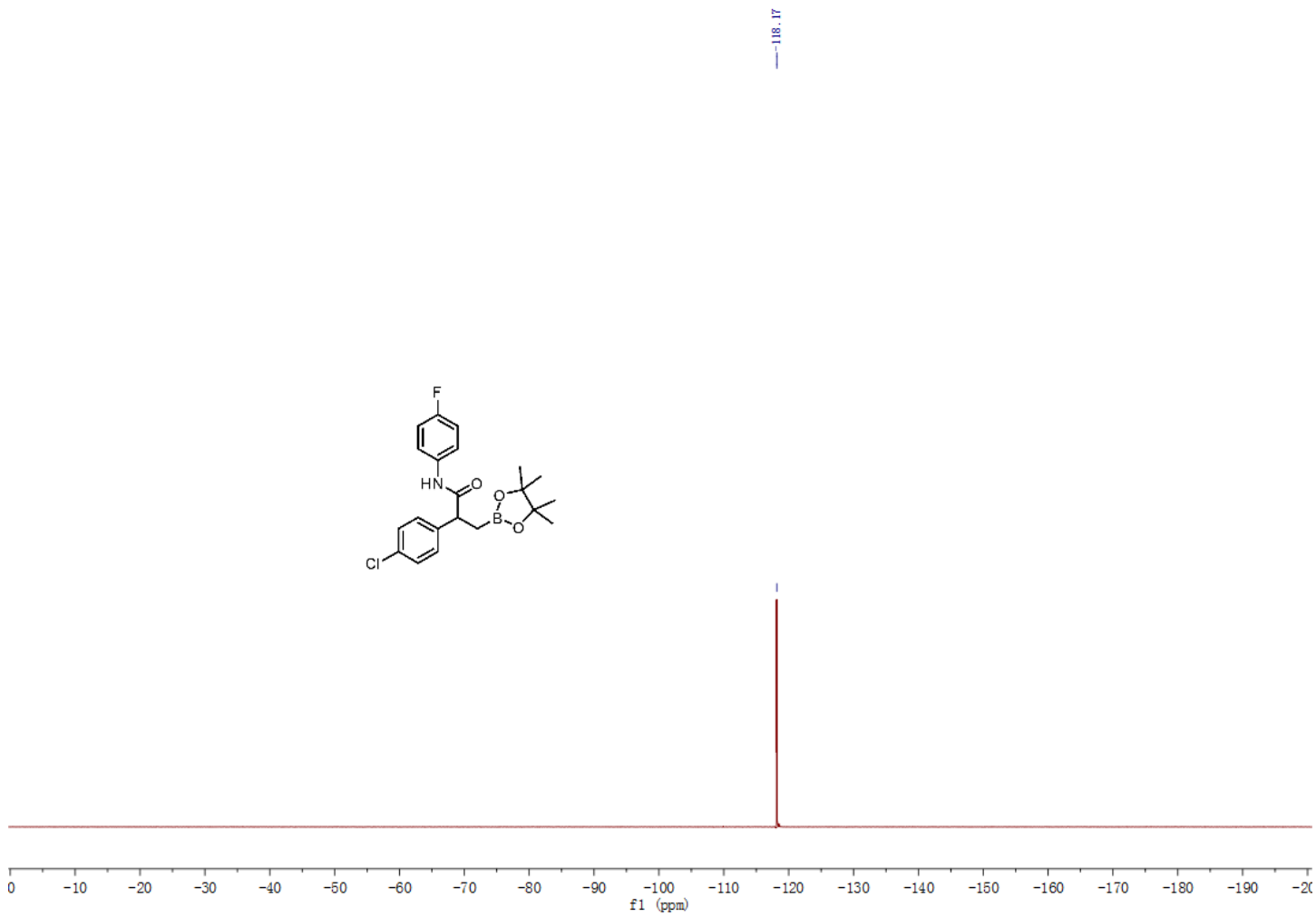

172.96
162.08
160.08
159.01
134.19
130.35
129.19
121.39
121.34
115.65
115.50
114.54
83.45
77.37
77.16
76.95
55.44
49.09
24.93
24.84
16.94
F
HN
O
O
O
B
MeO
16.94
17.0
f1 (ppm)
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

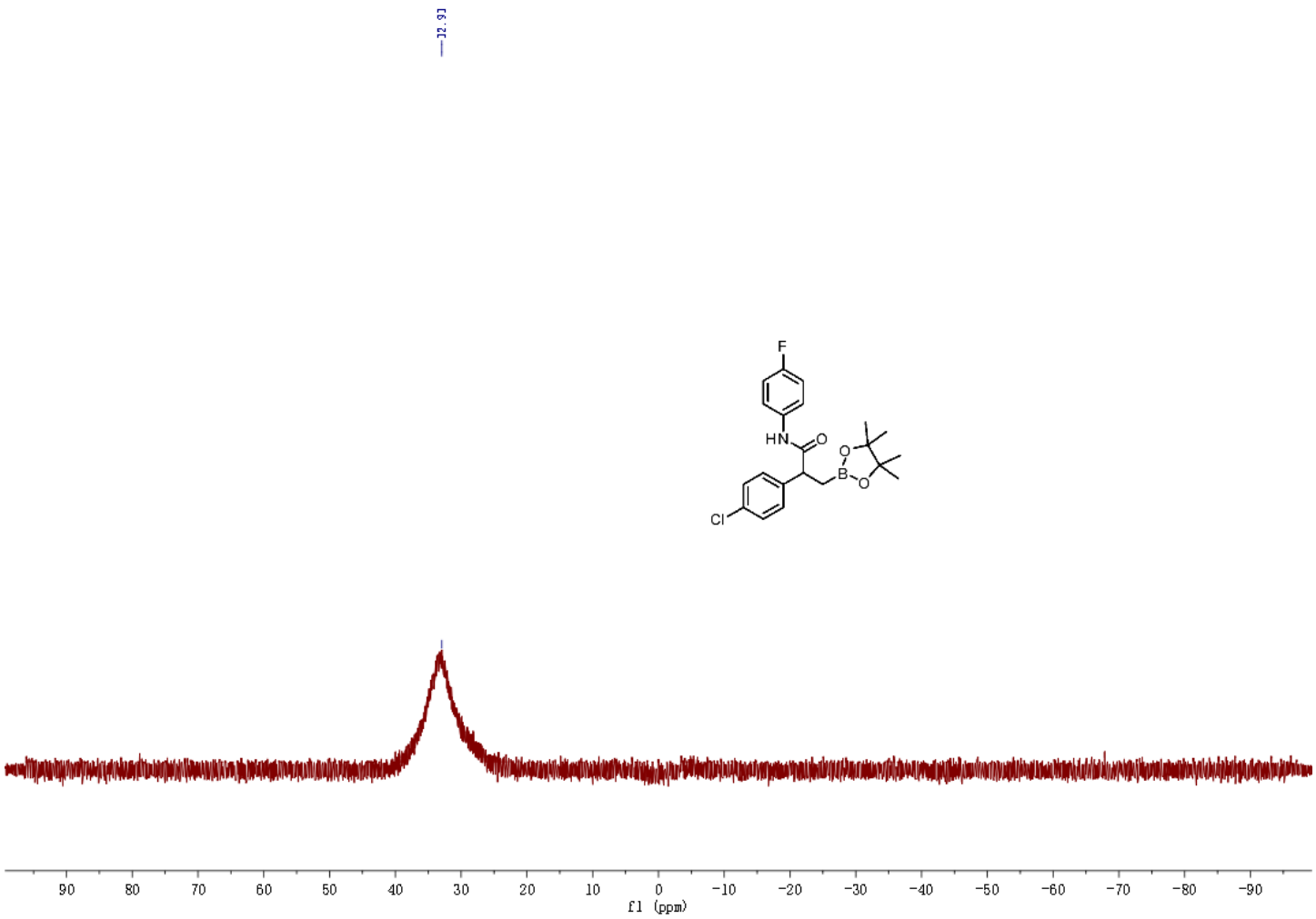

-118.57
F
HN
O
O
B
O
MeO
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

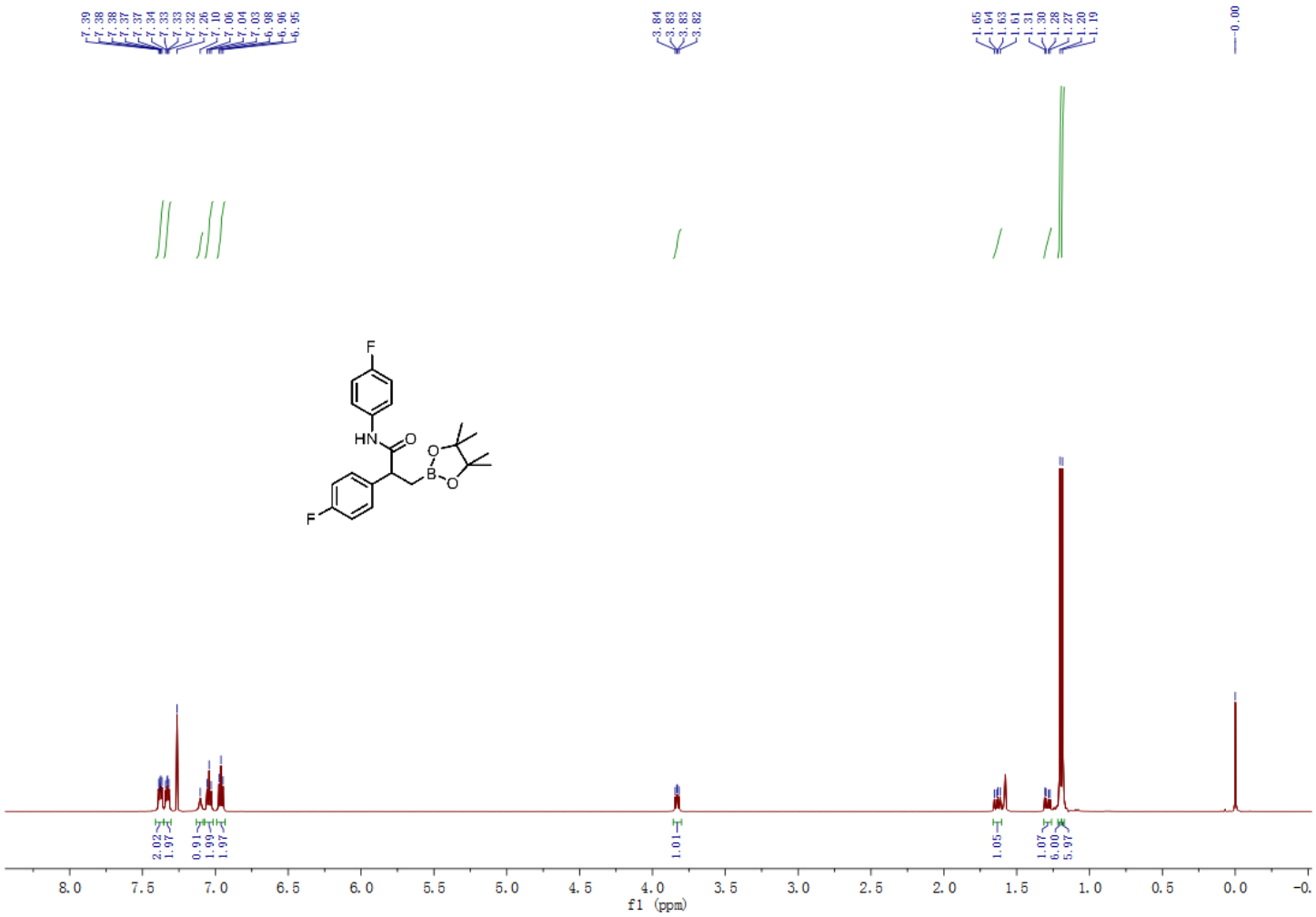

11.65
F
HN
O
O
B
O
MeO
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

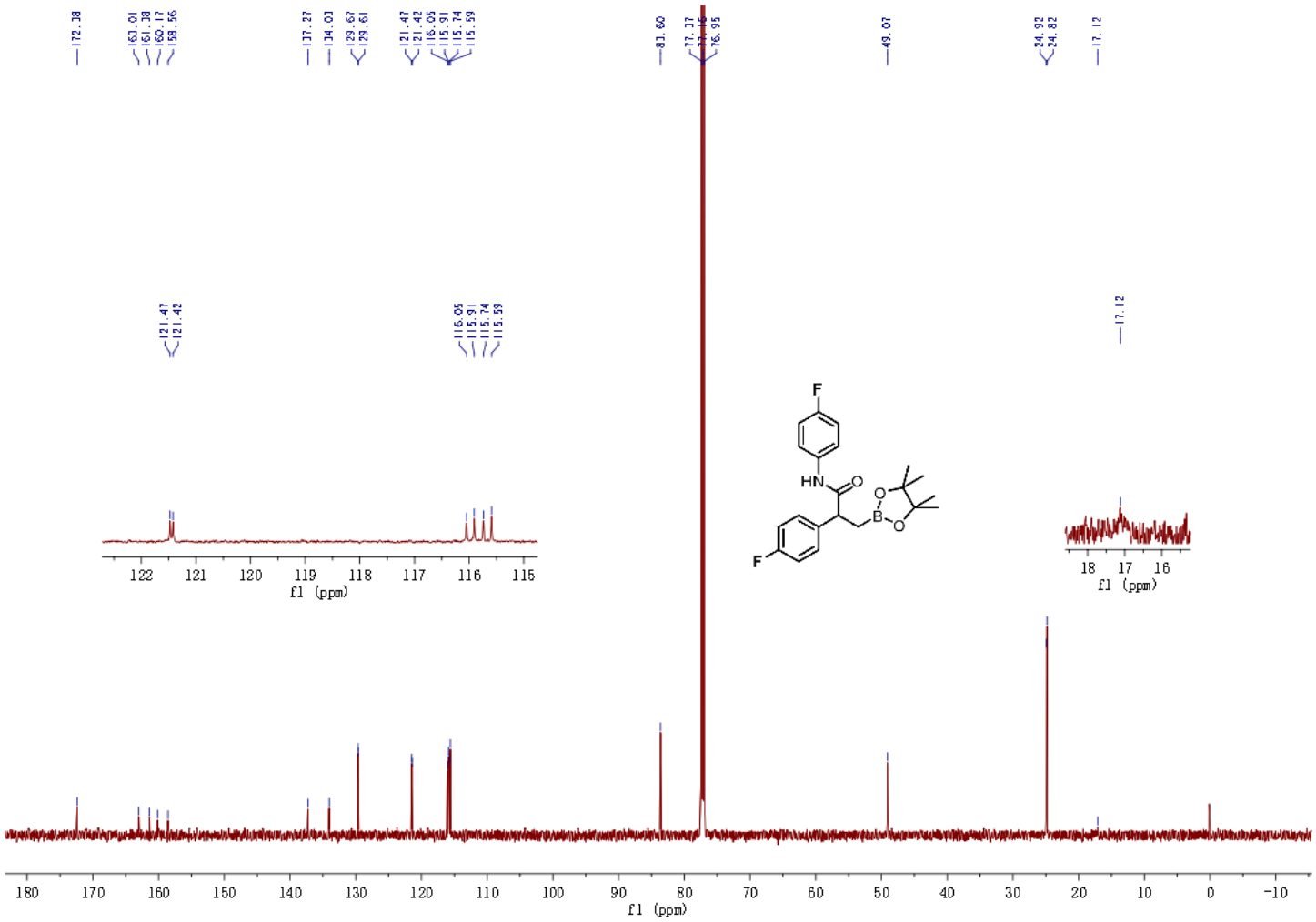

7.39
7.38
7.38
7.38
7.37
7.33
7.31
7.30
7.29
7.26
7.14
6.97
6.96
6.95
3.83
3.82
3.82
3.80
1.65
1.63
1.62
1.61
1.30
1.29
1.27
1.26
1.24
1.21
1.19
0.00
F
HN
O
O
B
O
Cl
2.00
4.02
0.93
1.98
1.00
1.38
1.48
6.08
6.03
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

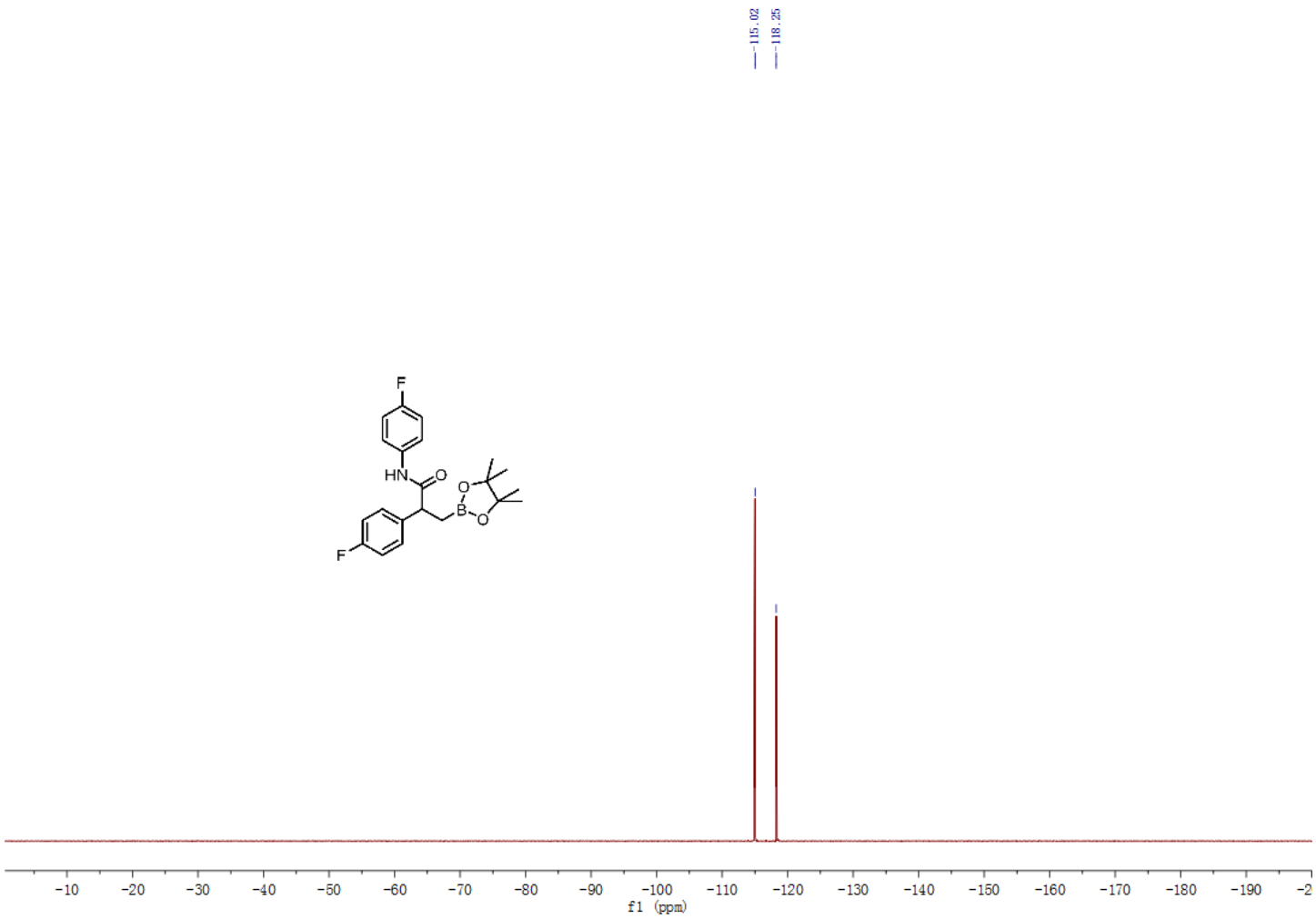

172.08
160.21
158.60
140.04
134.02
133.40
129.42
129.25
121.52
121.47
115.75
115.60
83.65
77.37
77.16
76.95
49.21
24.93
24.83
17.06
17.06
F
HN
O
O
B
O
Cl
17.5
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

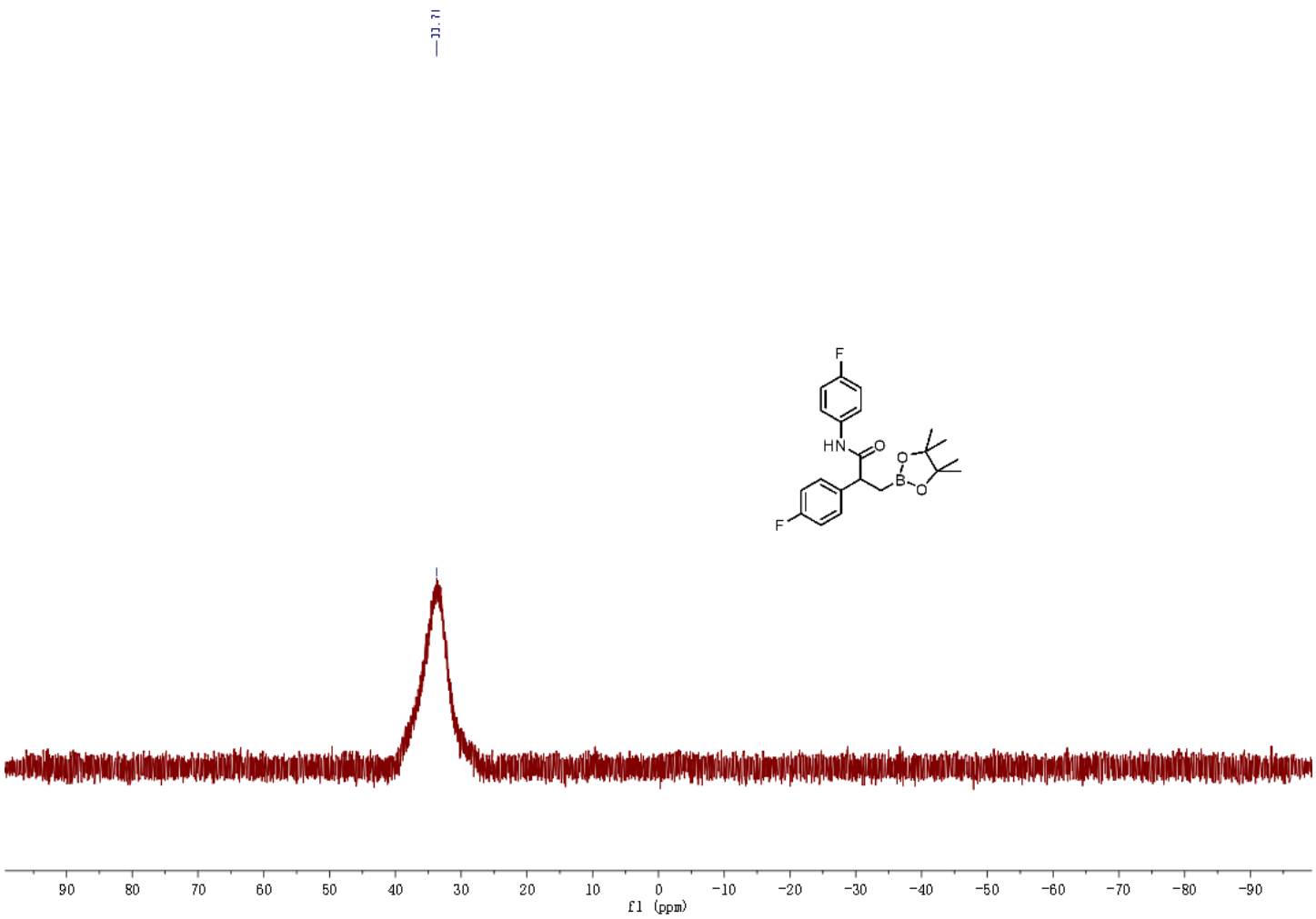

-118.17
F
HN
O
O
B
O
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

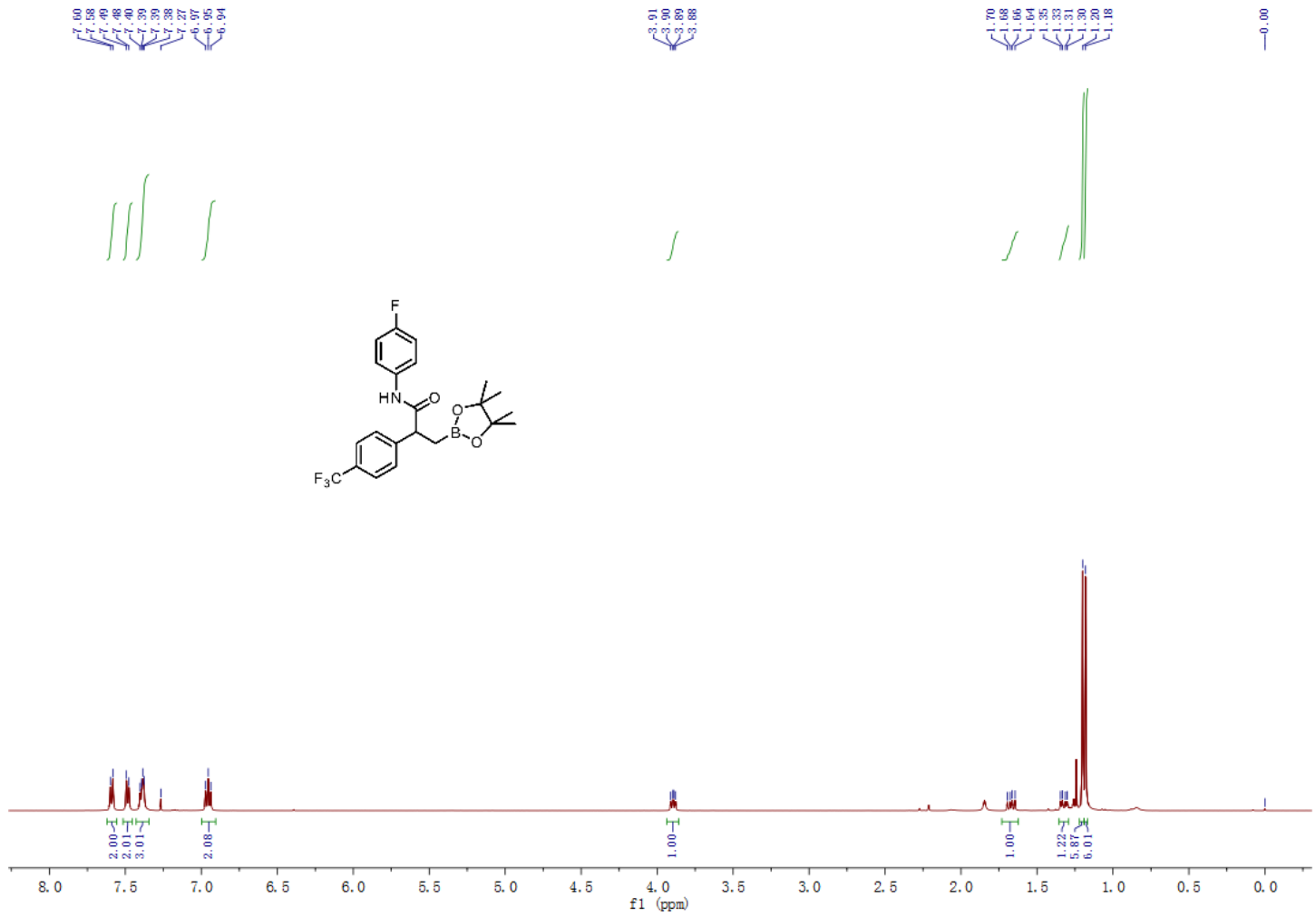

32.93
F
HN
O
O
O
B
O
Cl
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

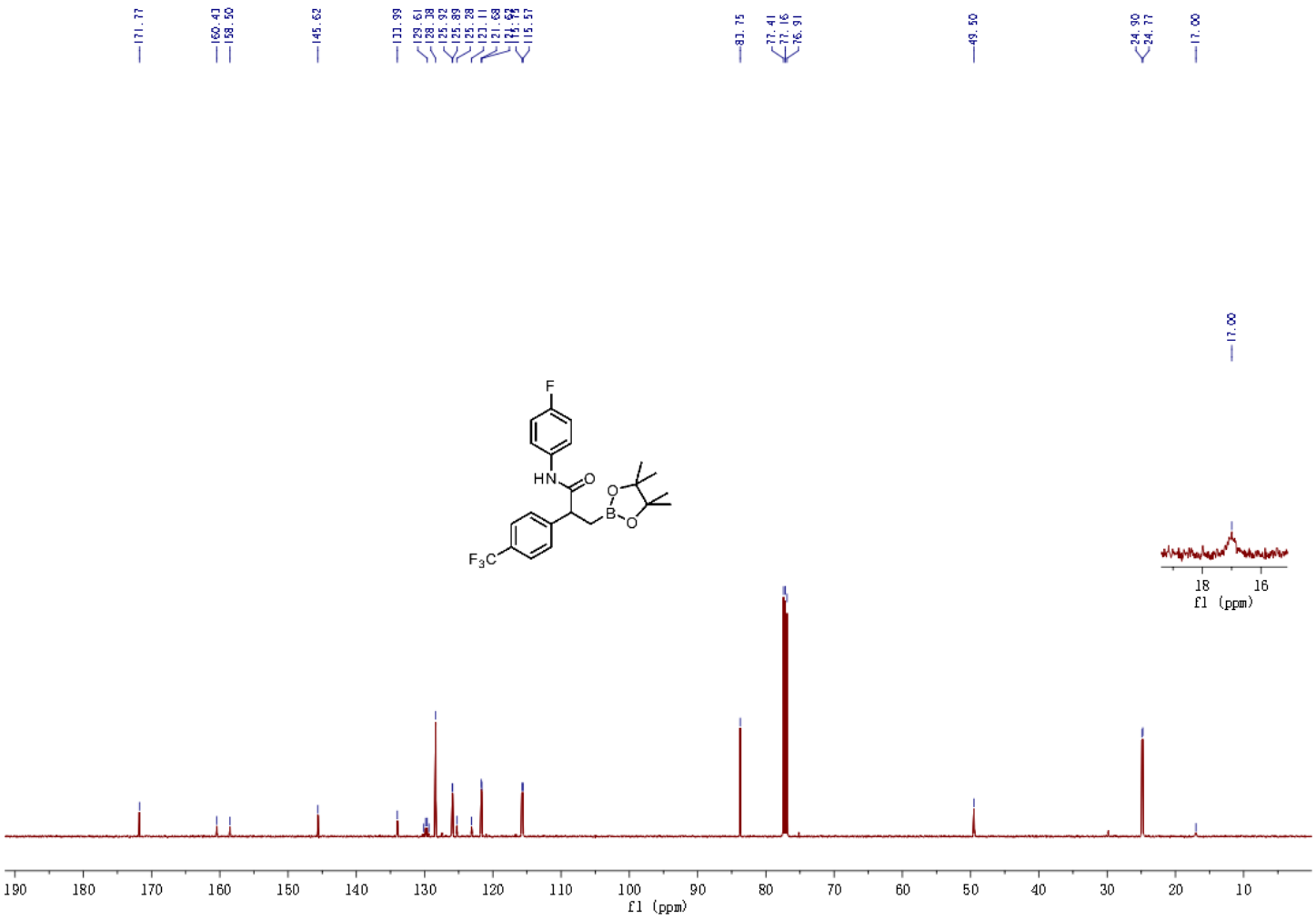

7.39
7.38
7.38
7.37
7.37
7.34
7.33
7.32
7.26
7.10
7.06
7.04
7.03
6.98
6.96
6.95
3.84
3.83
3.83
3.82
1.65
1.64
1.63
1.61
1.31
1.30
1.28
1.27
1.20
1.19
0.00
F
HN
O
O
O
B
F
2.02
1.97
0.91
1.99
1.97
1.01
1.05
1.07
6.00
5.97
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

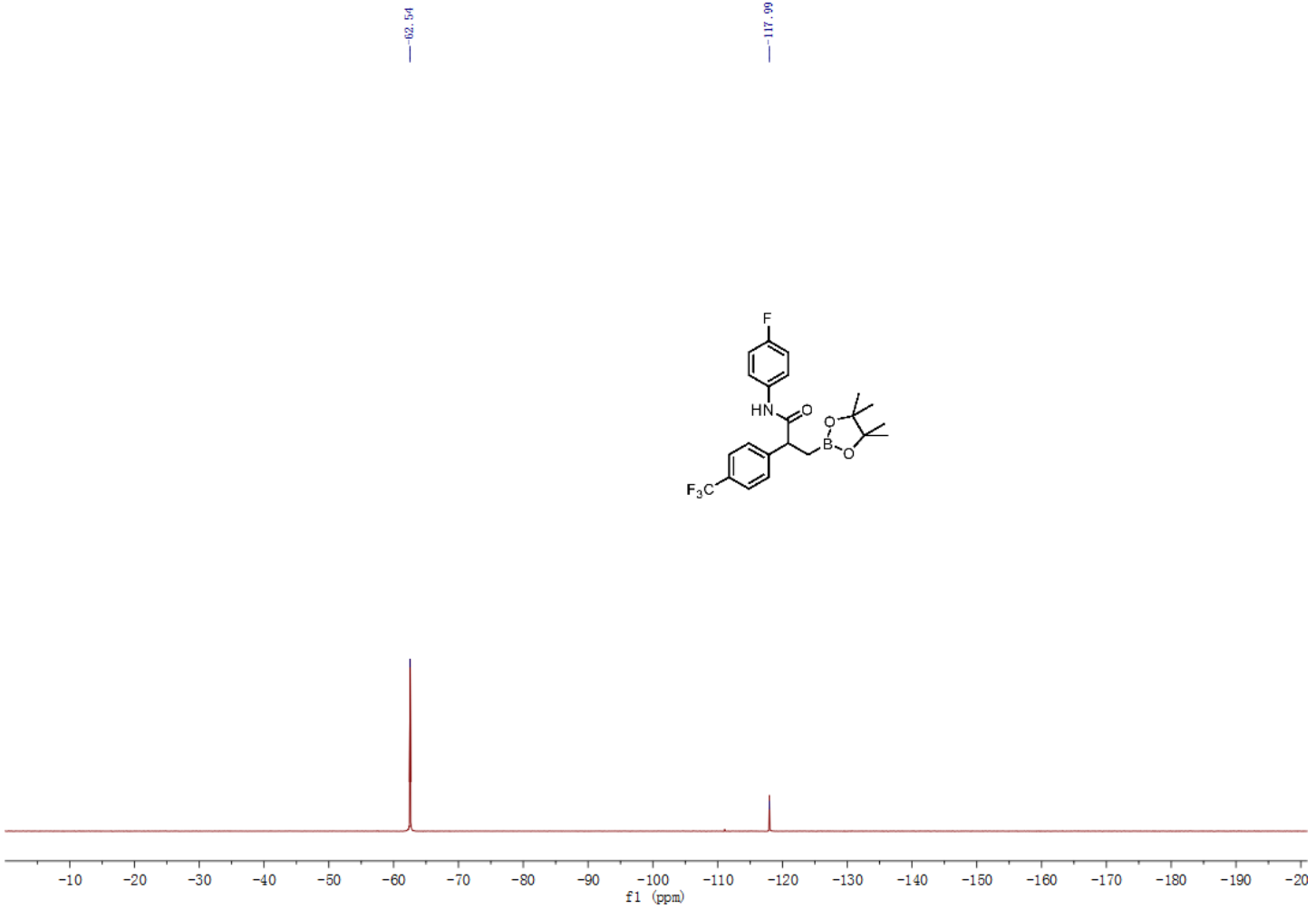

172.38
163.01
161.38
160.17
158.56
137.27
134.03
129.63
129.61
121.47
121.42
116.05
115.91
115.74
115.59
83.60
77.37
77.16
76.95
49.07
24.92
24.82
17.12
F
HN
O
O
O
B
F
122 121 120 119 118 117 116 115
f1 (ppm)
18 17 16
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

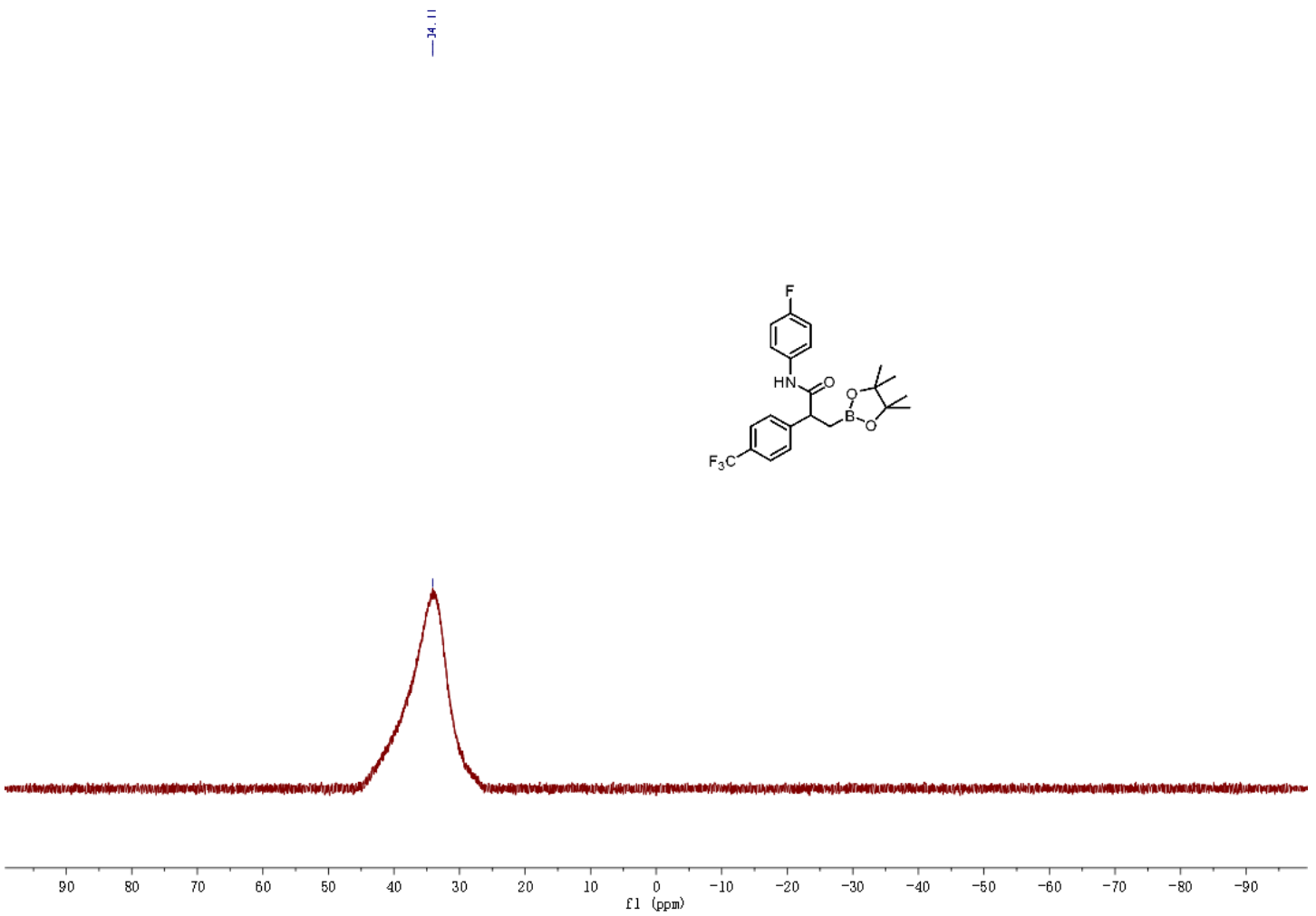

-115.02
-118.25
F
HN
O
O
O
B
F
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-2
f1 (ppm)

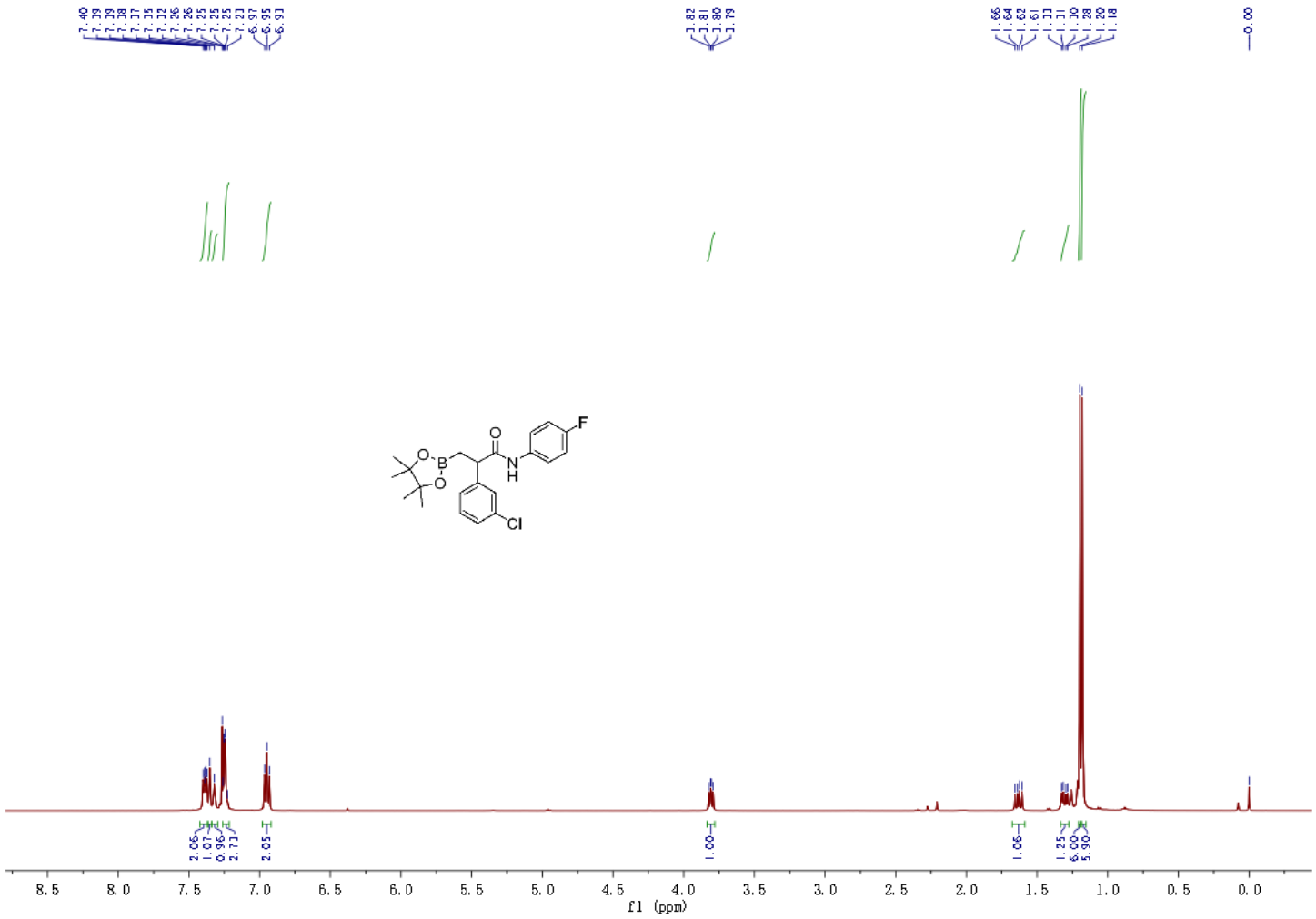

33.71
F
HN
O
O
B
O
F
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

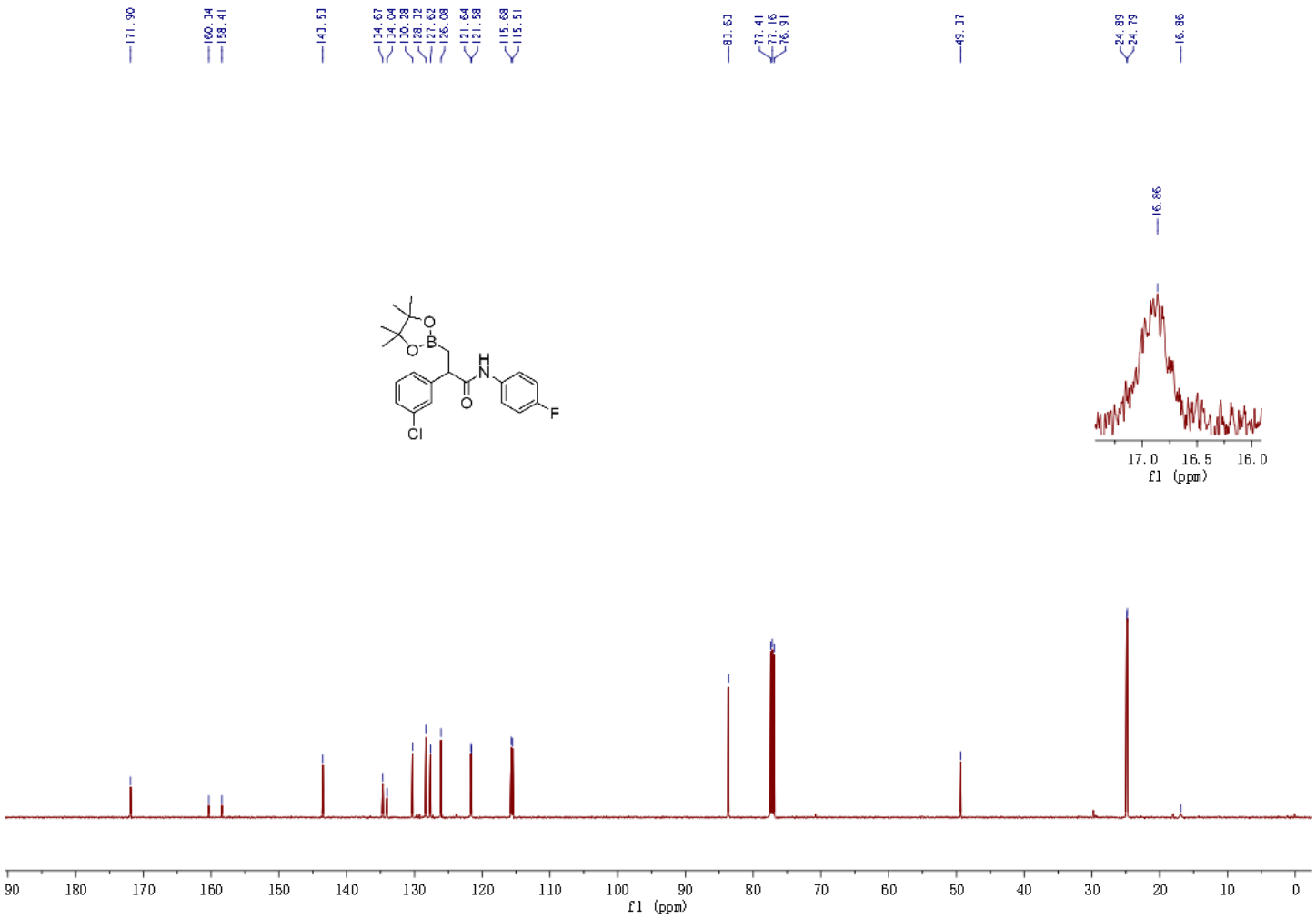

7.60
7.58
7.49
7.48
7.40
7.39
7.39
7.38
7.27
6.97
6.95
6.94
3.91
3.90
3.89
3.88
1.70
1.68
1.66
1.64
1.35
1.33
1.31
1.30
1.20
1.18
0.00
F
HN
O
O
B
O
F3C
2.00
2.01
3.01
2.08
1.00
1.00
1.22
5.87
6.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

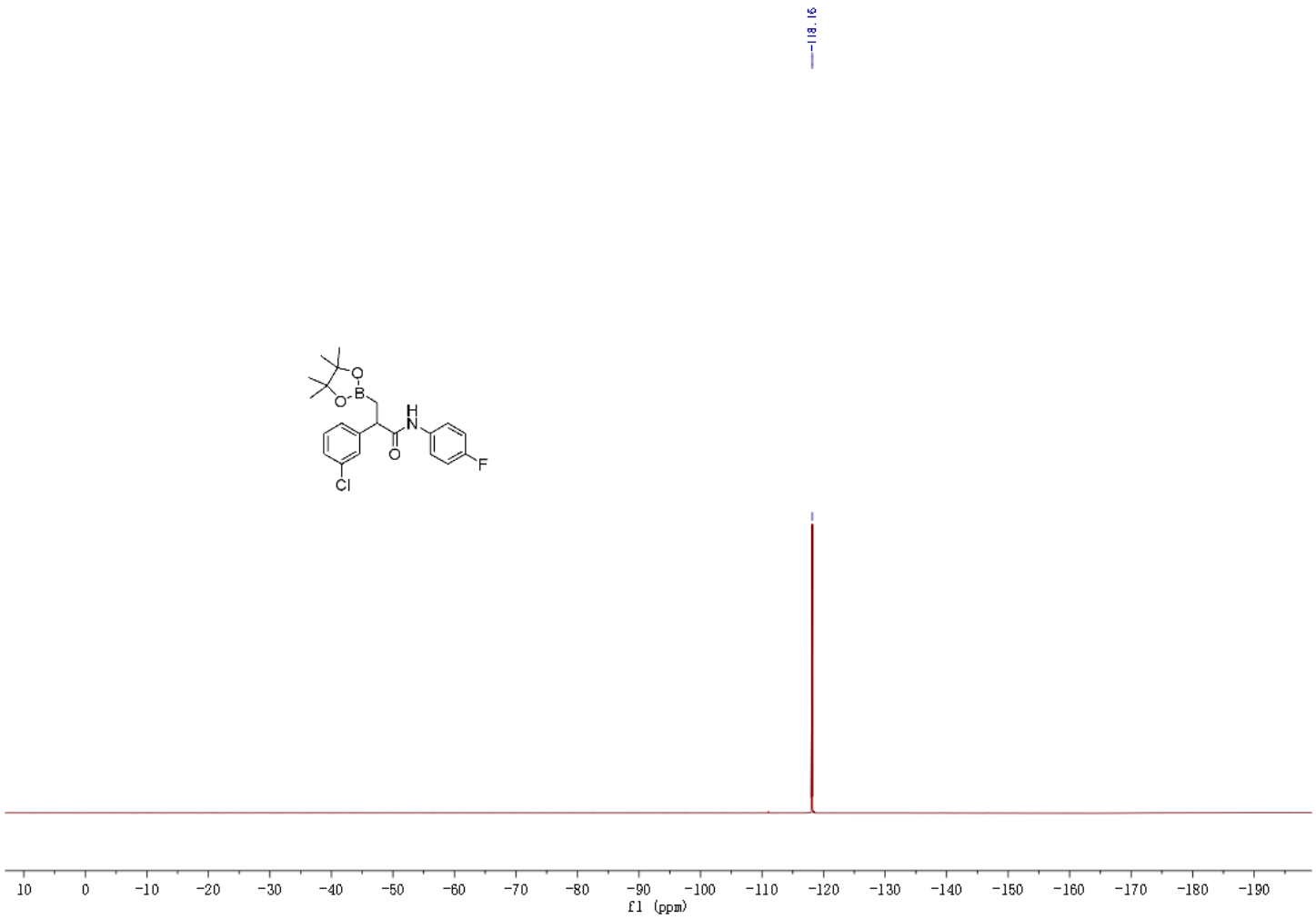

171.77
160.43
158.50
145.62
133.99
129.61
128.38
125.92
125.89
125.28
123.11
121.68
83.75
77.41
77.16
76.91
49.50
24.90
24.77
17.00
F
HN
O
O
B
O
F3C
17.00
18
16
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

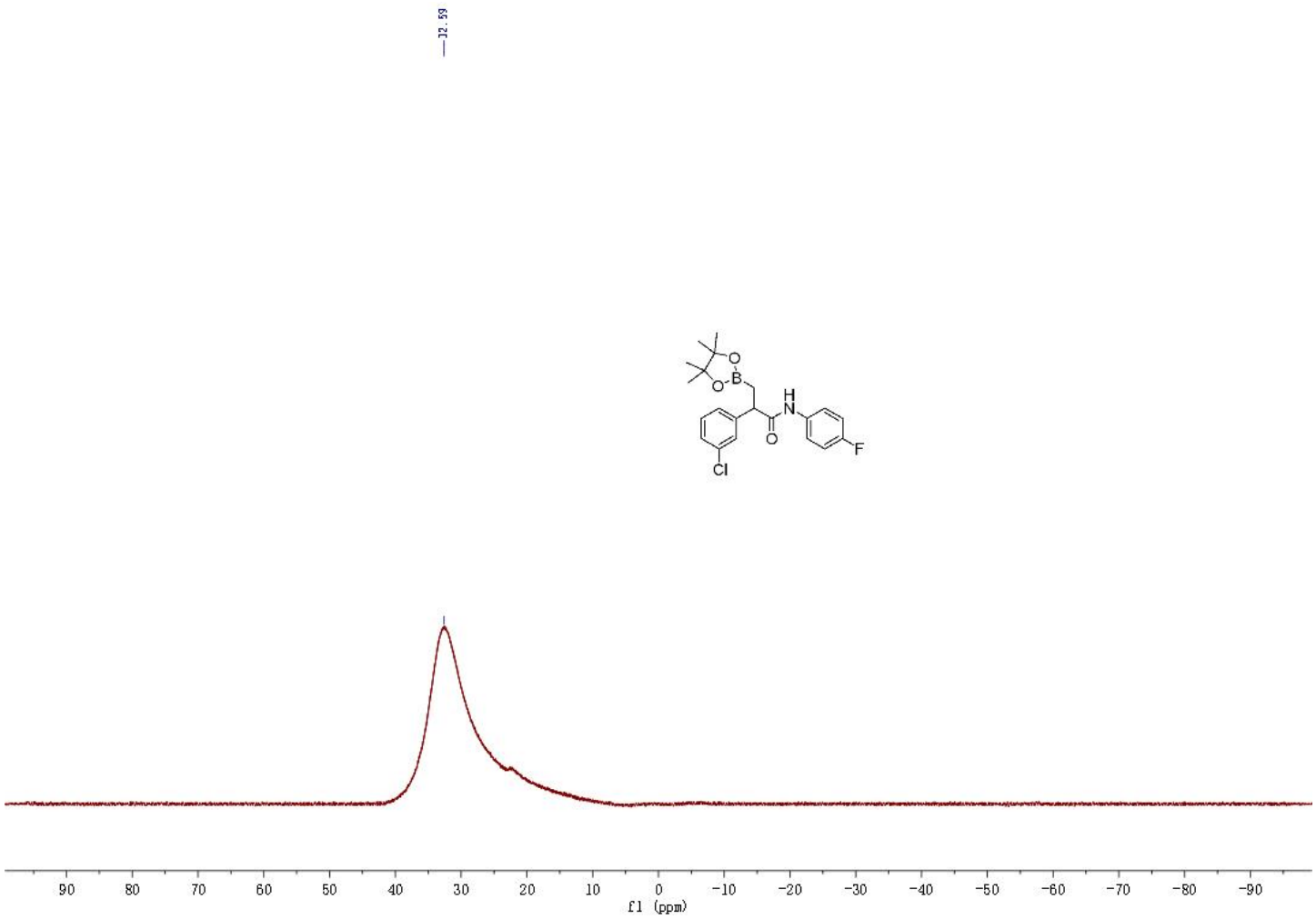

-62.54
-117.99
F
HN
O
O
B
O
F3C
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-20
f1 (ppm)

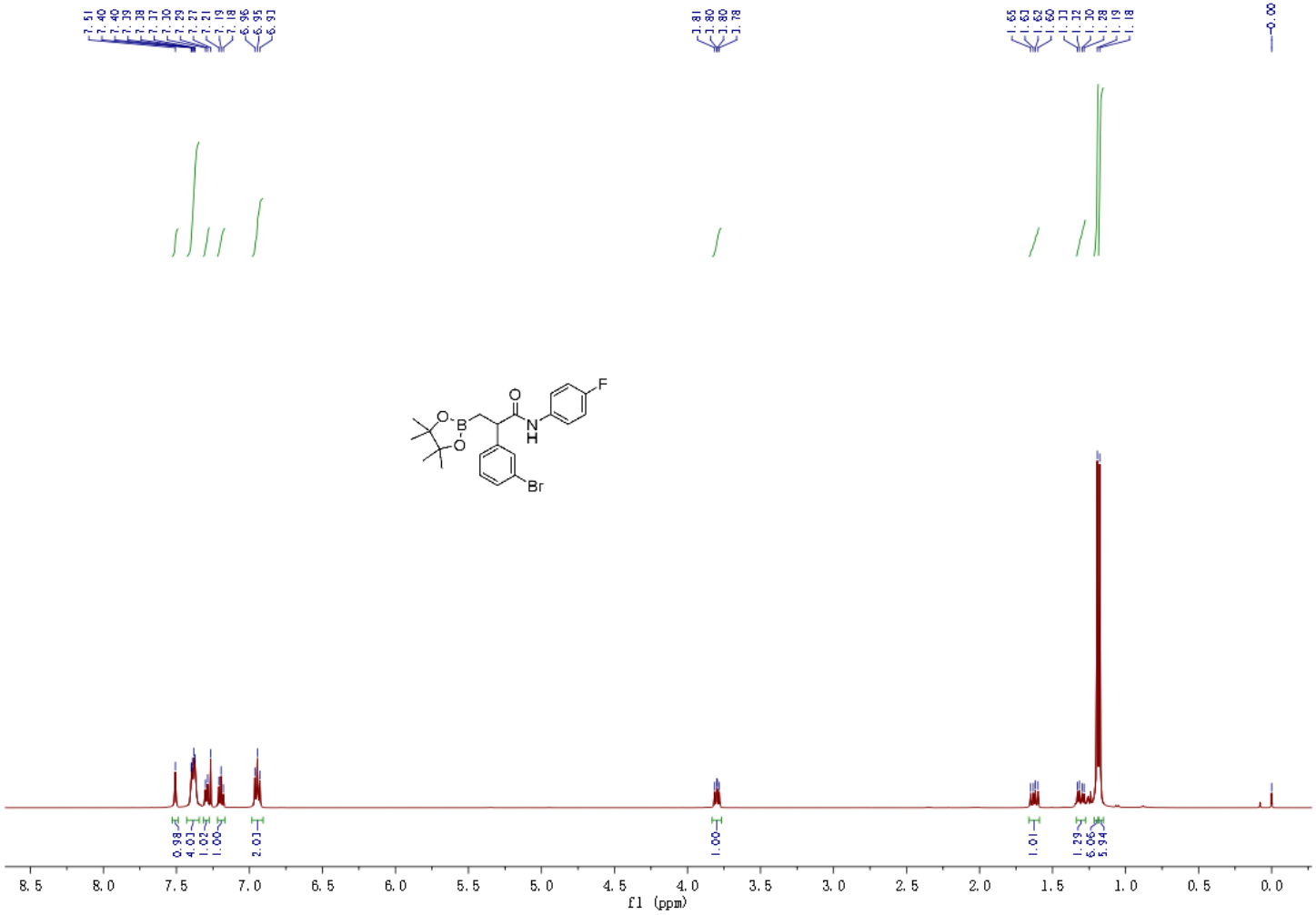

34.11
F
HN
O
O
B
O
F3C
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

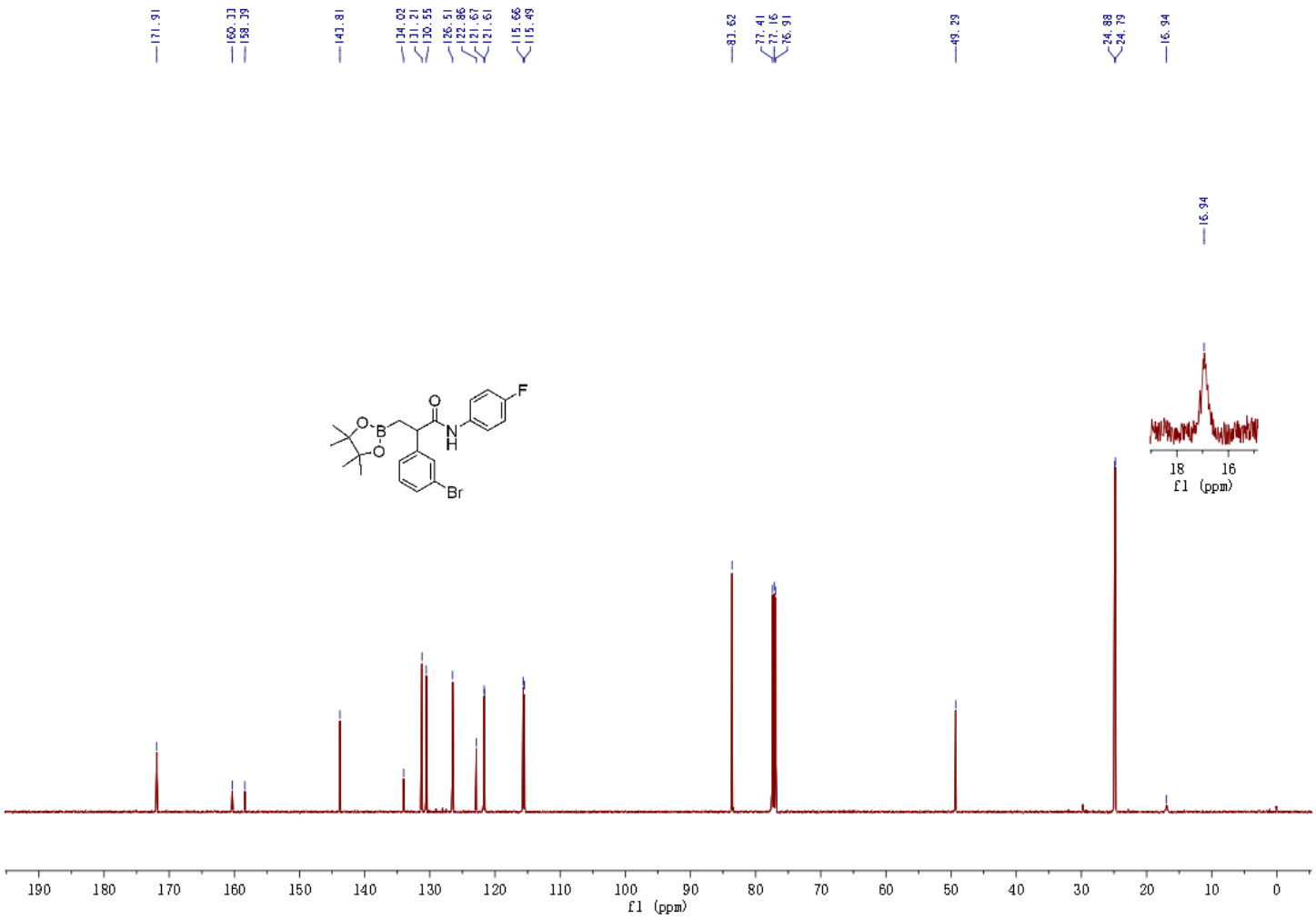

7.40
7.39
7.39
7.38
7.37
7.35
7.32
7.26
7.26
7.25
7.25
7.25
7.23
6.97
6.95
6.93
1.82
1.81
1.80
1.79
1.66
1.64
1.62
1.61
1.31
1.30
1.28
1.20
1.18
0.00
F
O
N
H
O
B
O
Cl
2.06
1.07
0.96
2.73
2.05
1.00
1.06
1.25
6.00
5.90
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

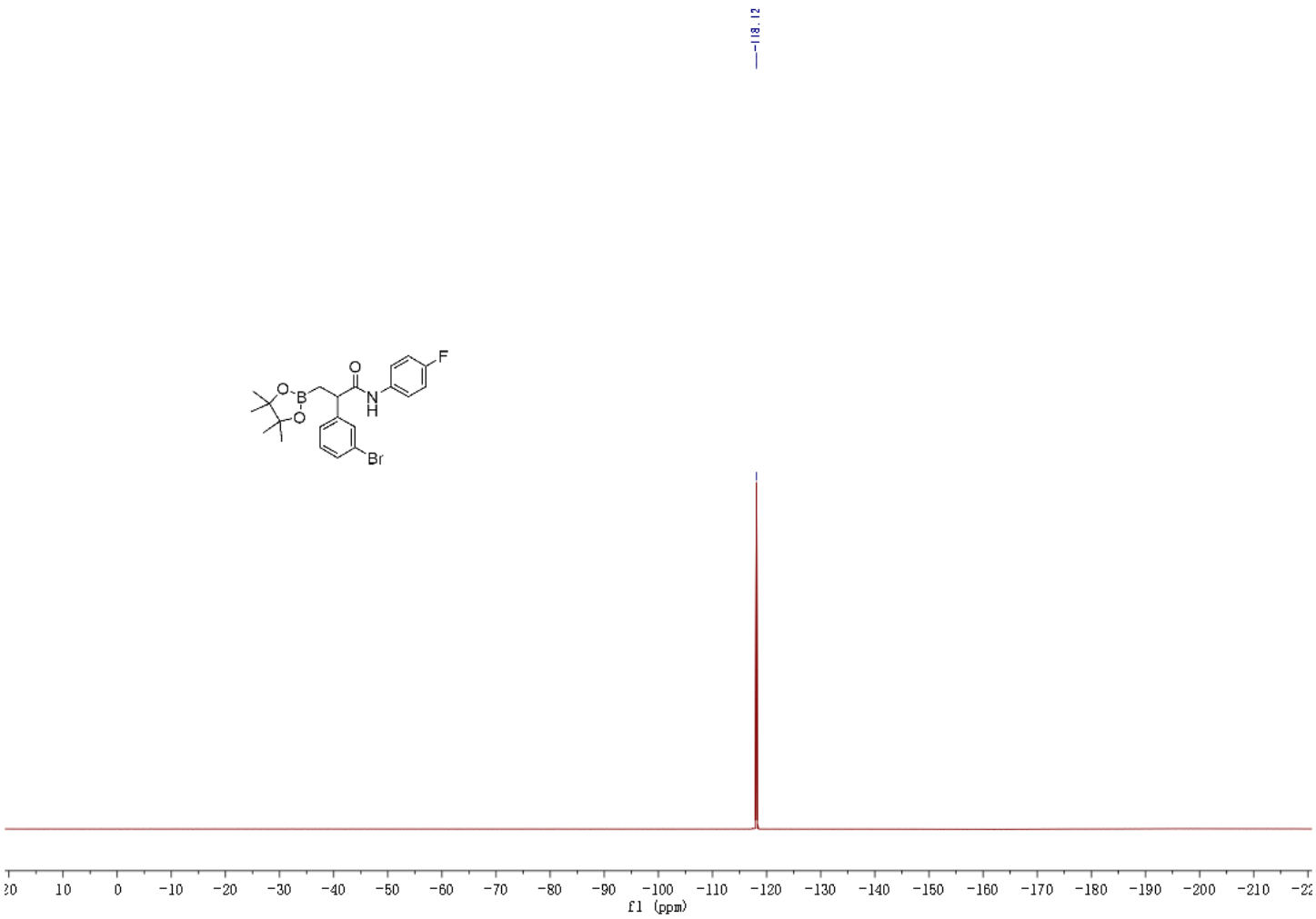

171.90
160.34
158.41
143.53
134.67
134.04
130.28
128.12
127.62
126.08
121.64
121.58
115.68
115.51
83.63
77.41
77.16
76.91
49.37
24.89
24.79
16.86
O
B
O
H
N
O
Cl
F
16.86
17.0
16.5
16.0
f1 (ppm)
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

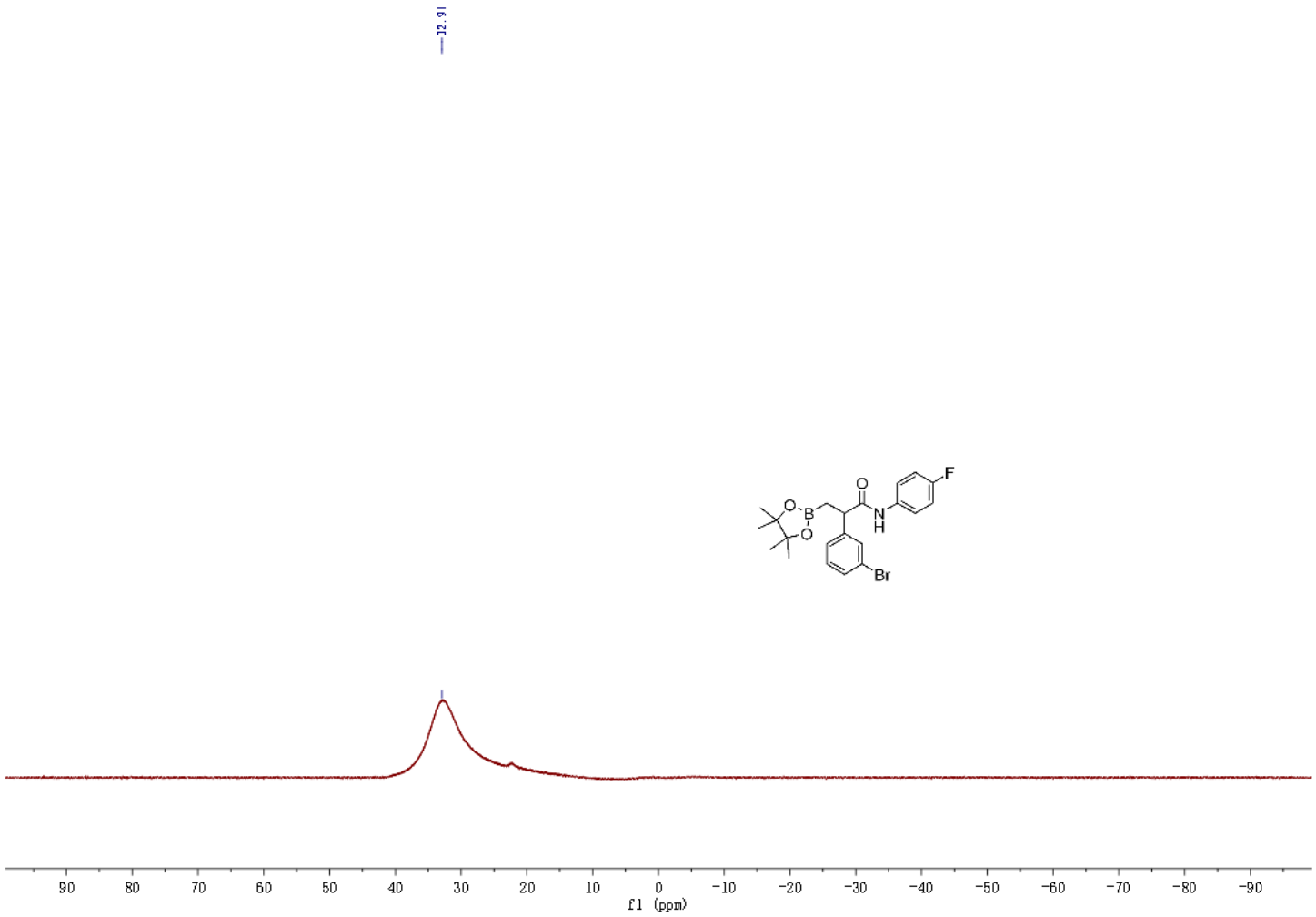

-118.16
O
B
O
H
N
O
F
Cl
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

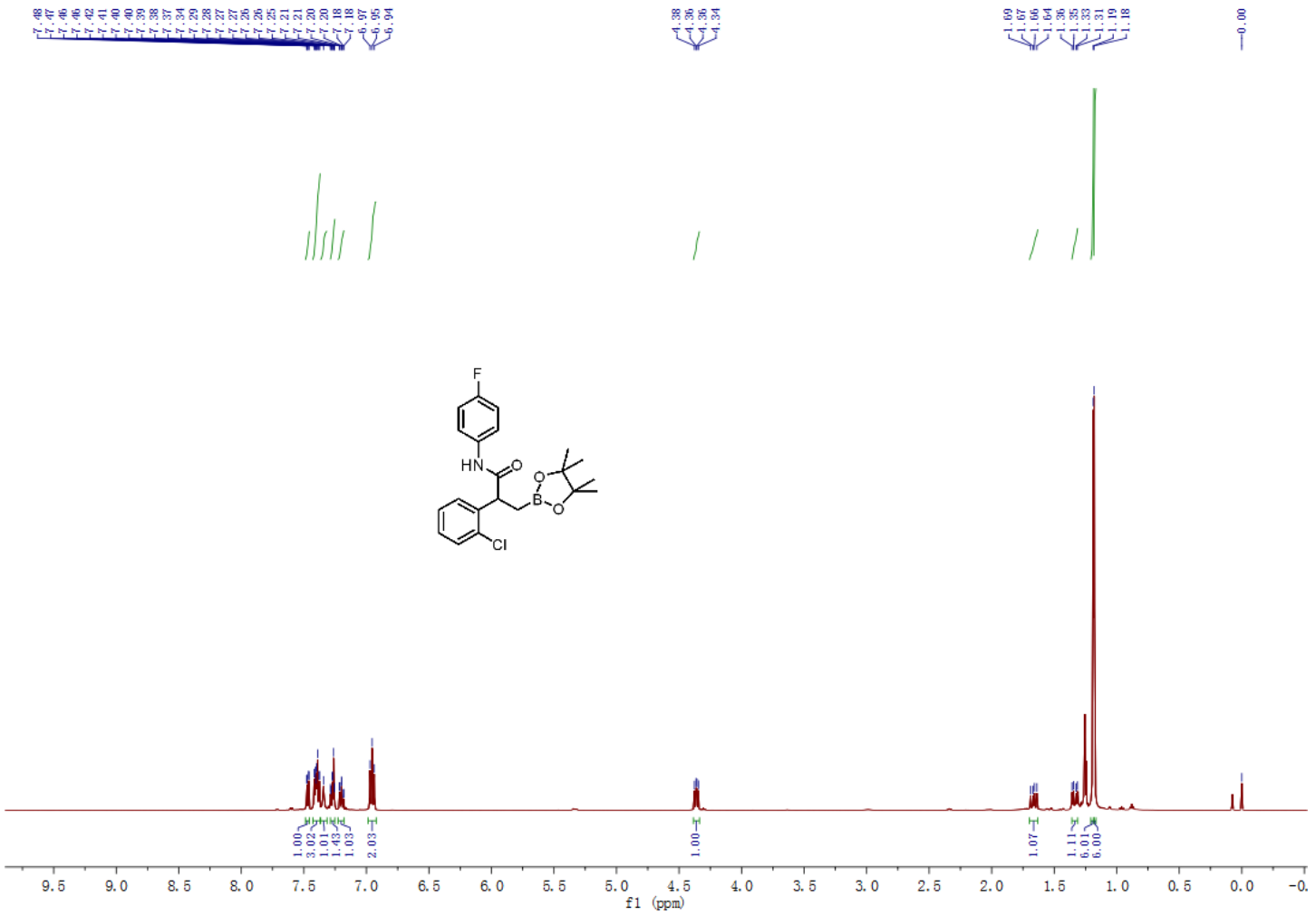

32.59
O
B
O
H
N
O
Cl
F
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

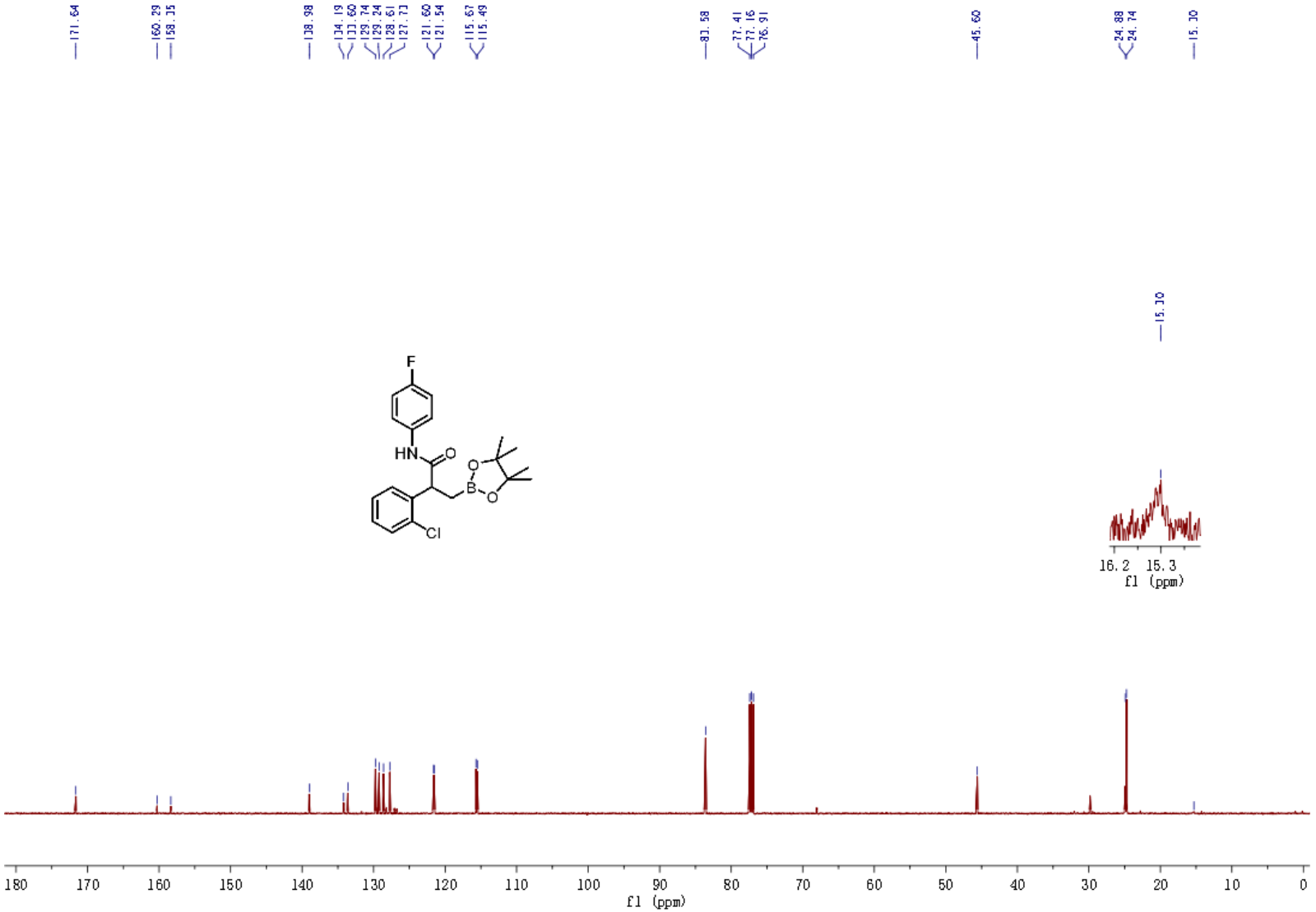

7.51
7.40
7.40
7.39
7.38
7.37
7.30
7.29
7.27
7.21
7.19
7.18
6.96
6.95
6.93
1.81
1.80
1.80
1.78
1.65
1.63
1.62
1.60
1.33
1.32
1.30
1.28
1.19
1.18
0.00
O
O
B
O
N
H
F
Br
0.98
4.03
1.02
1.00
2.03
1.00
1.01
1.29
6.06
5.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

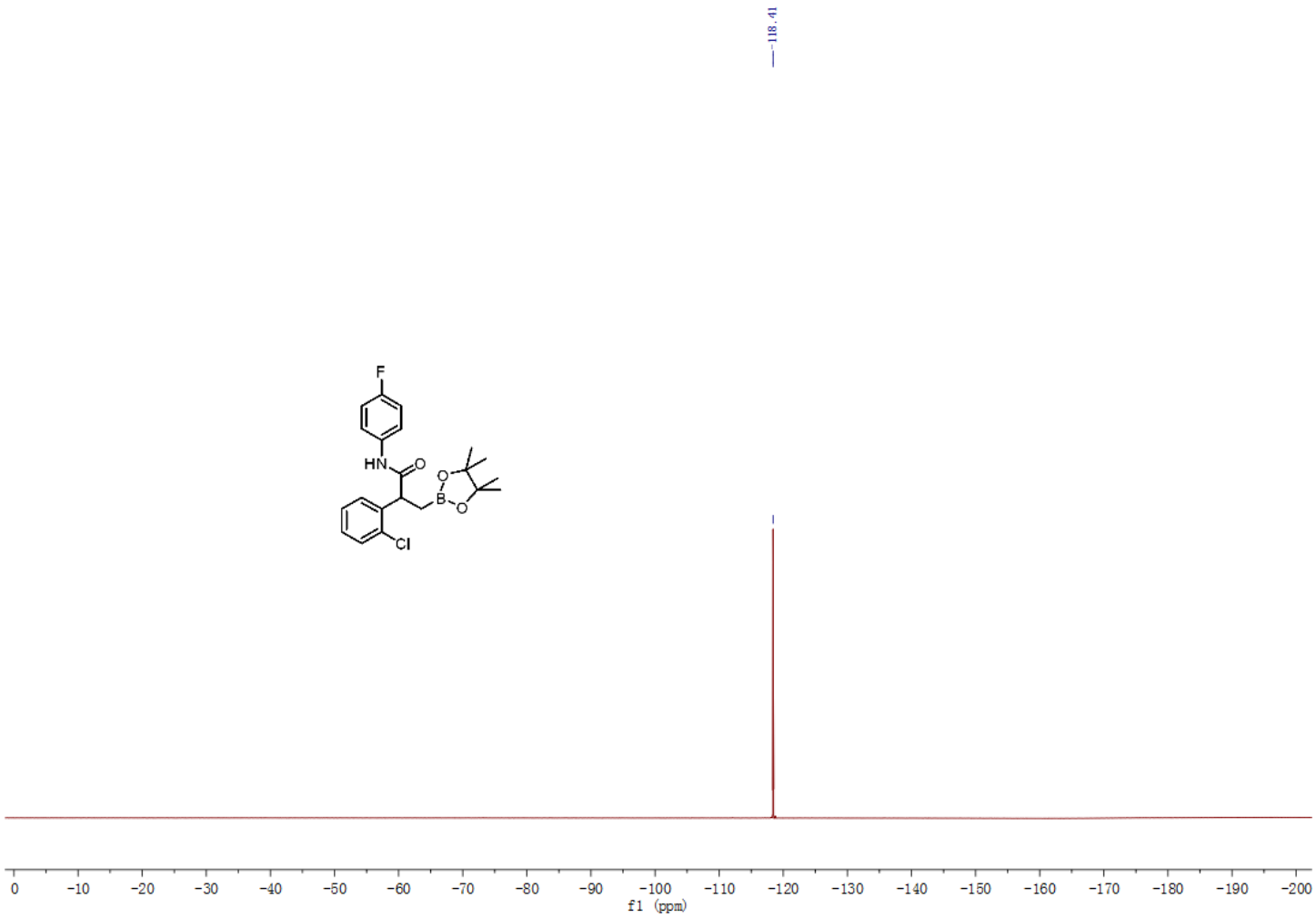

171.91
160.13
158.39
143.81
134.02
131.21
130.55
126.51
122.86
121.67
121.61
115.66
115.49
83.62
77.41
77.16
76.91
49.29
24.88
24.79
16.94
F
O
B
O
O
N
H
Br
16.94
18
16
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

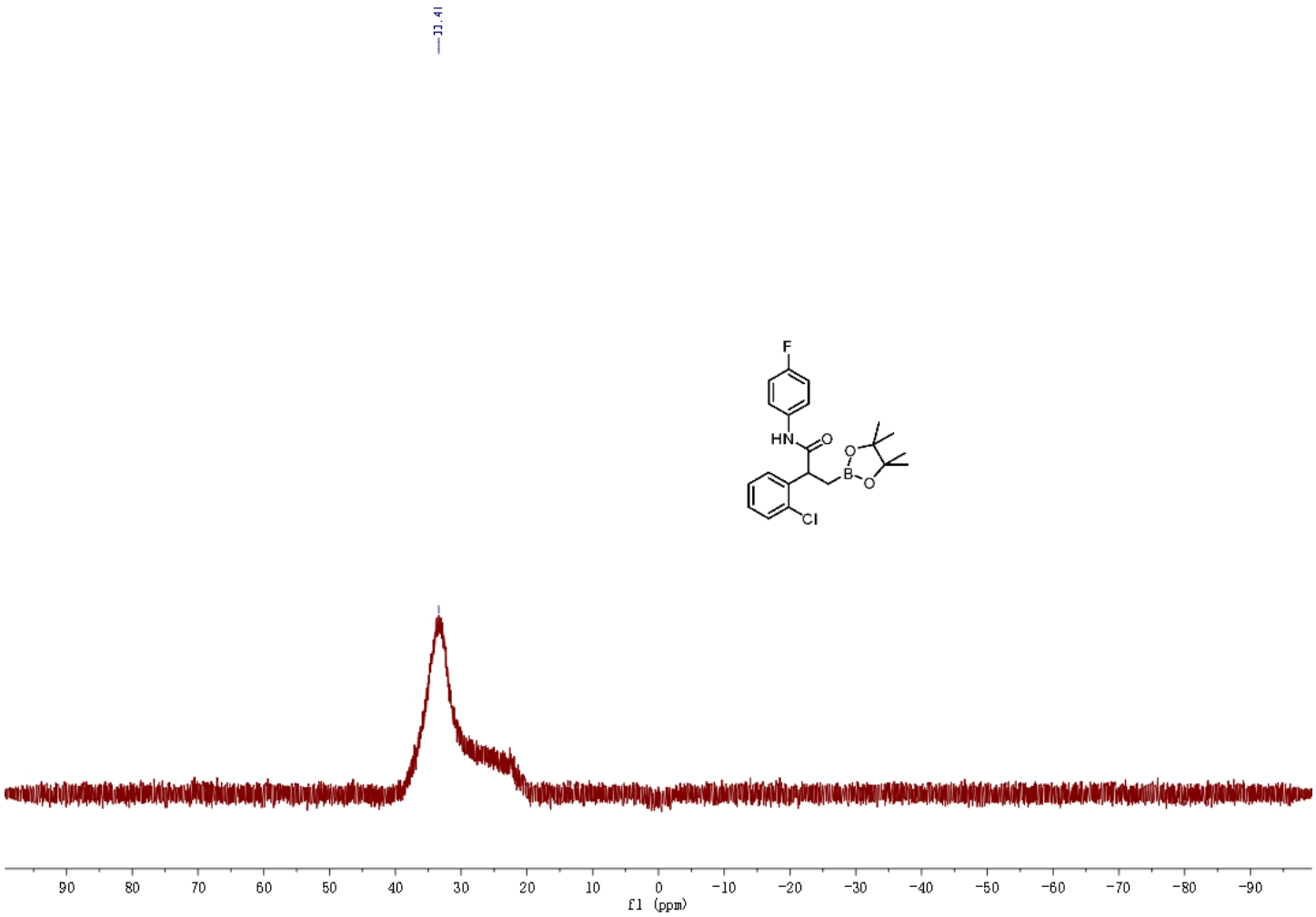

-118.12
F
O
N
H
B
O
O
Br
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

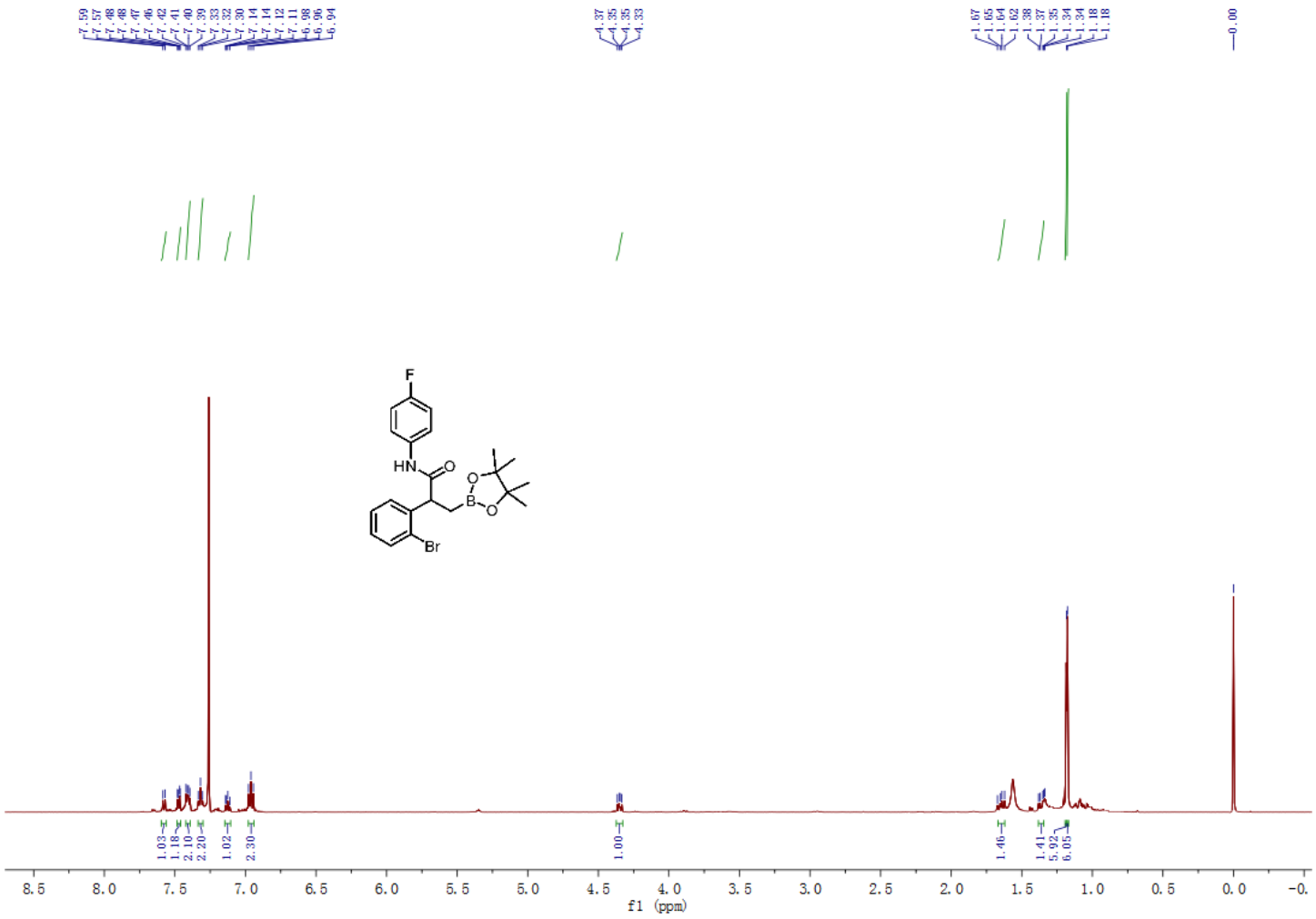

32.91
O
B
O
O
N
H
F
Br
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

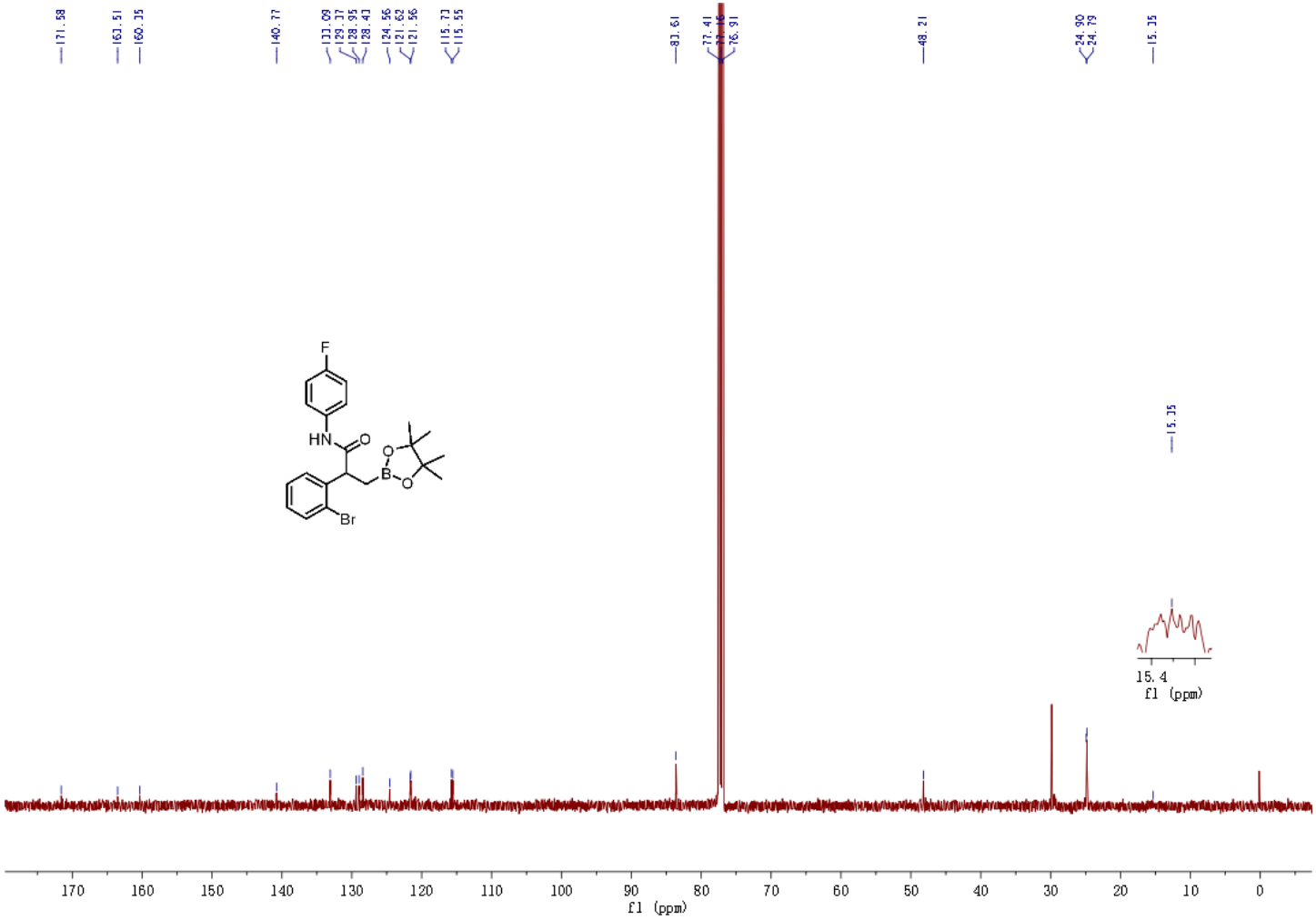

7.48
7.47
7.46
7.46
7.42
7.41
7.40
7.40
7.39
7.38
7.37
7.34
7.29
7.28
7.27
7.27
7.26
7.25
7.21
7.20
7.20
7.18
7.18
6.97
6.95
6.94
4.38
4.36
4.36
4.34
1.69
1.67
1.66
1.64
1.36
1.35
1.33
1.31
1.19
1.18
0.00
F
HN
O
O
O
B
Cl
1.00
3.02
1.01
1.43
1.03
2.03
1.00
1.07
1.11
6.01
6.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

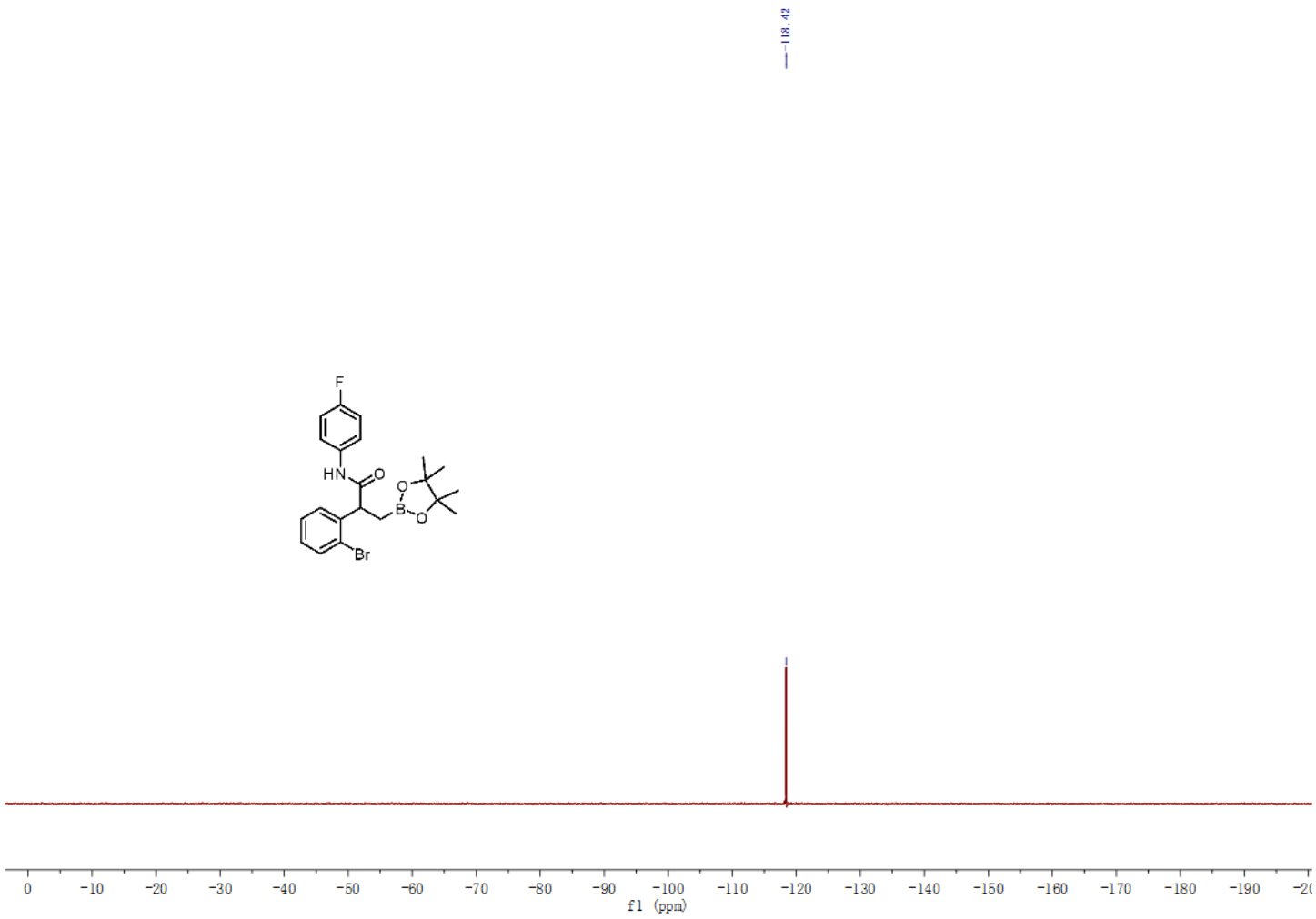

171.64
160.29
158.35
138.98
134.19
133.60
129.74
129.24
128.61
127.73
121.60
121.54
115.67
115.49
83.58
77.41
77.16
76.91
45.60
24.88
24.74
15.30
F
HN
O
O
B
O
Cl
15.30
16.2
15.3
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-118.41
F
HN
O
O
B
O
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


33.41
F
HN
O
O
B
O
Cl
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.59
7.57
7.48
7.48
7.47
7.46
7.42
7.41
7.40
7.39
7.33
7.32
7.30
7.14
7.14
7.12
7.11
6.98
6.96
6.94
4.37
4.35
4.35
4.33
1.67
1.65
1.64
1.62
1.38
1.37
1.35
1.34
1.34
1.18
1.18
0.00
F
HN
O
O
O
B
Br
1.03
1.18
2.10
2.20
1.02
2.30
1.00
1.46
1.41
5.92
6.05
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
0.0
-0.
f1 (ppm)


171.58
163.51
160.35
140.77
133.09
129.37
128.95
128.43
124.56
121.62
121.56
115.73
115.55
83.61
77.41
77.16
76.91
48.21
24.90
24.79
15.35
F
HN
O
O
O
B
Br
15.4
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-118.42
F
HN
O
O
B
O
Br
0
-10
-20
-30
-40
-50
-60
-70
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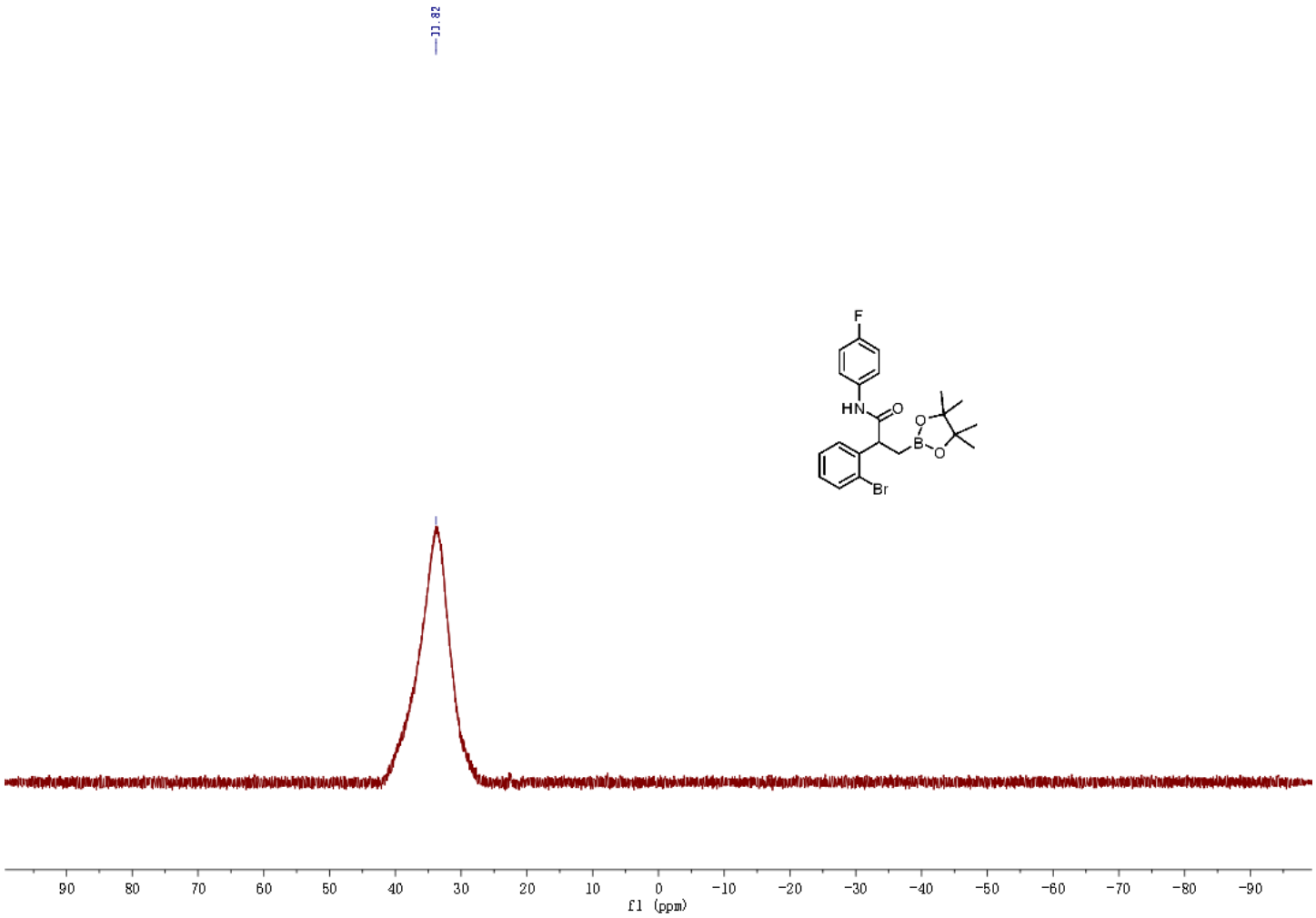
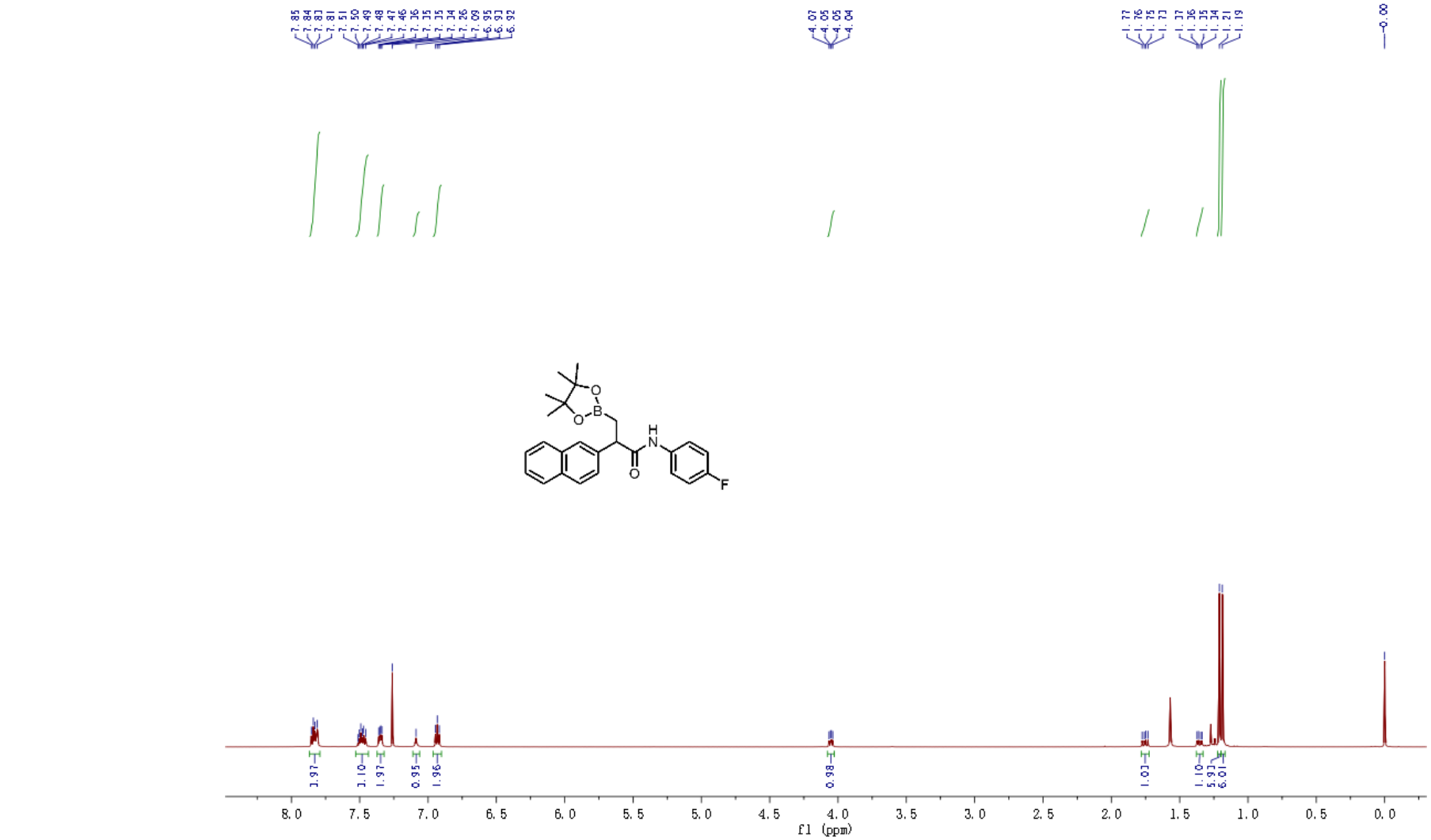
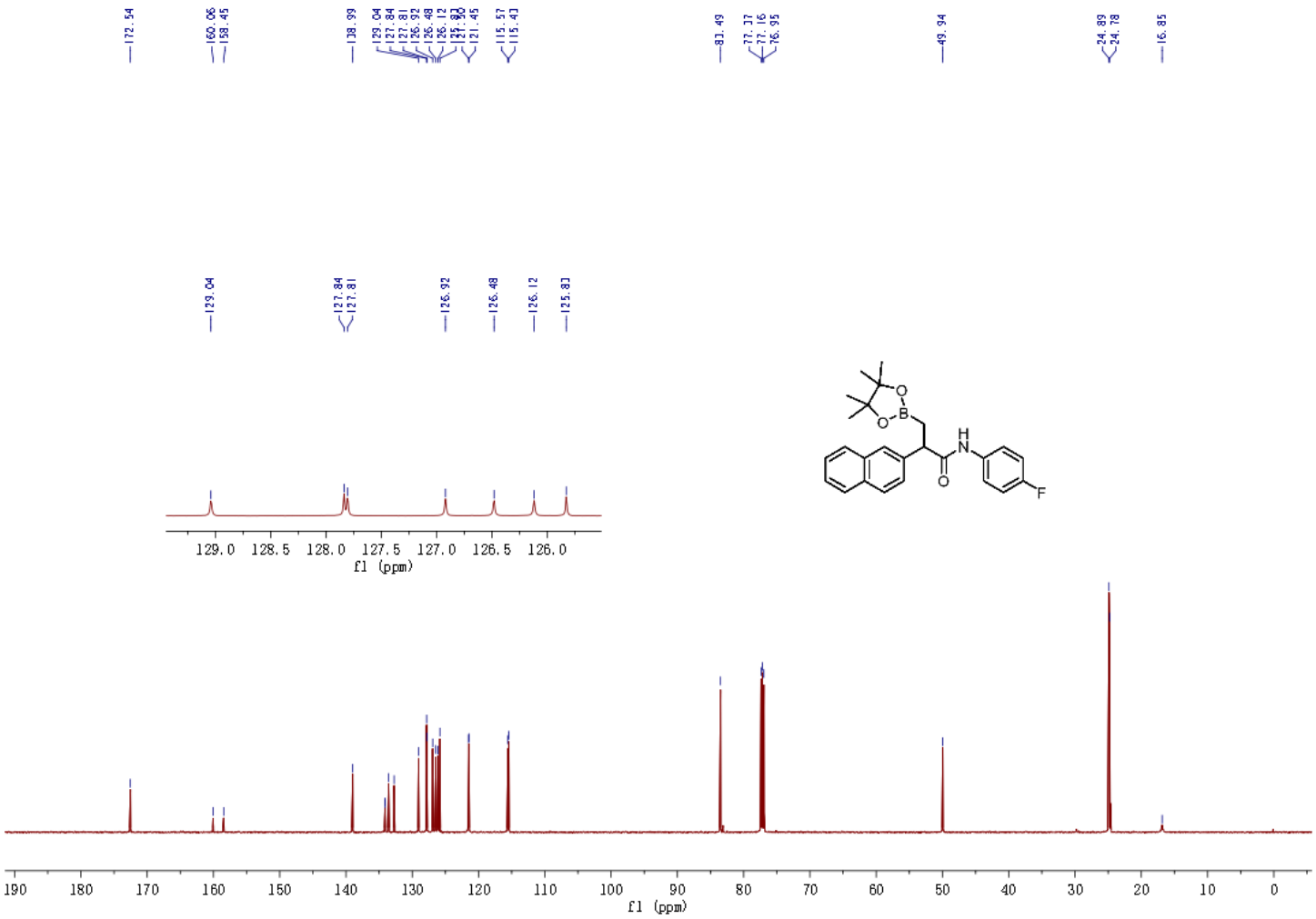
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


11.82
F
HN
O
O
B
O
Br
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.85
7.84
7.83
7.81
7.51
7.50
7.49
7.48
7.47
7.46
7.36
7.35
7.35
7.34
7.26
7.09
6.95
6.93
6.92
4.07
4.05
4.05
4.04
1.77
1.76
1.75
1.73
1.37
1.36
1.35
1.34
1.21
1.19
0.00
O
O
B
H
N
O
F
3.97
3.10
1.97
0.95
1.96
0.98
1.03
1.10
5.93
6.01
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
0.0
f1 (ppm)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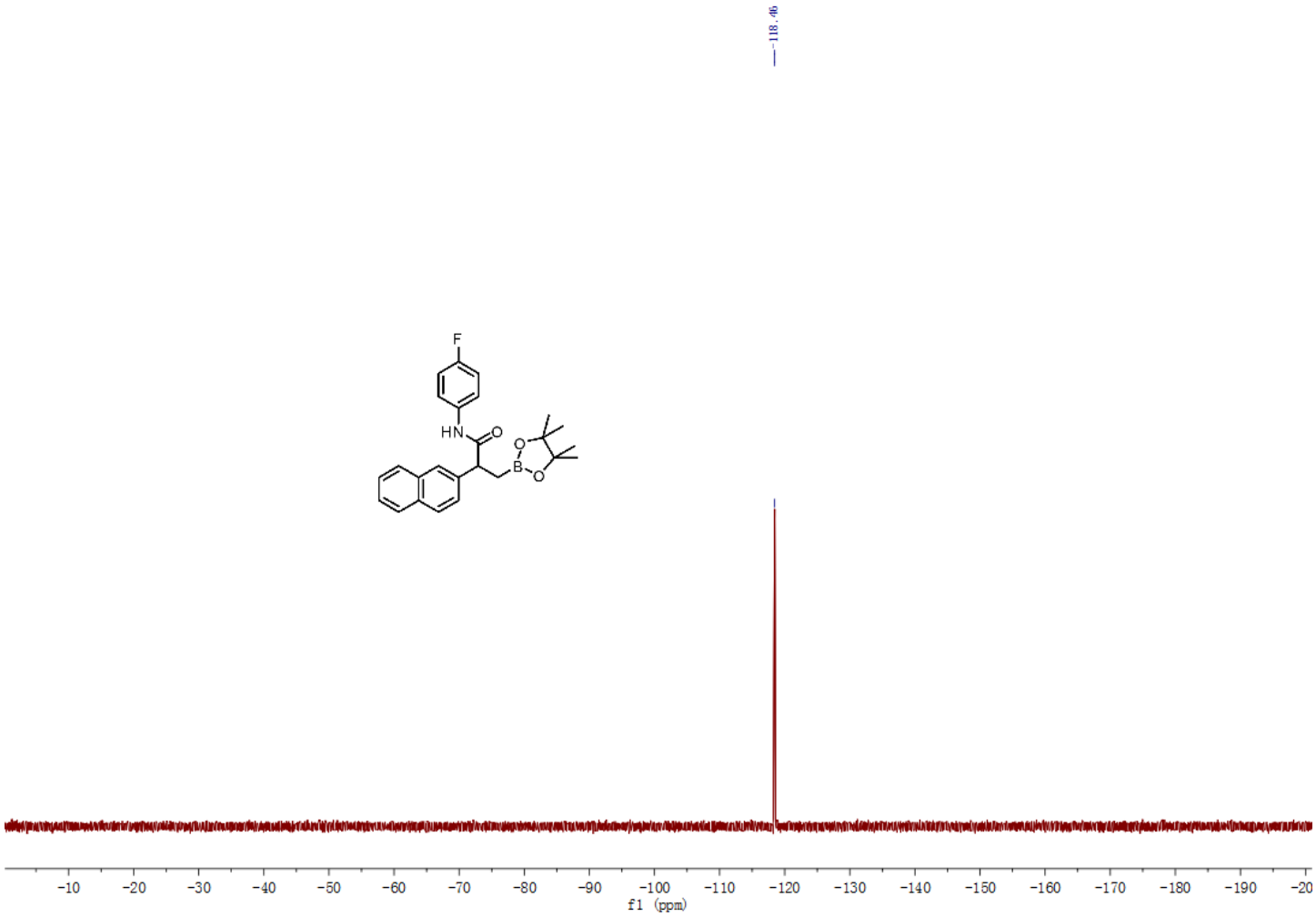
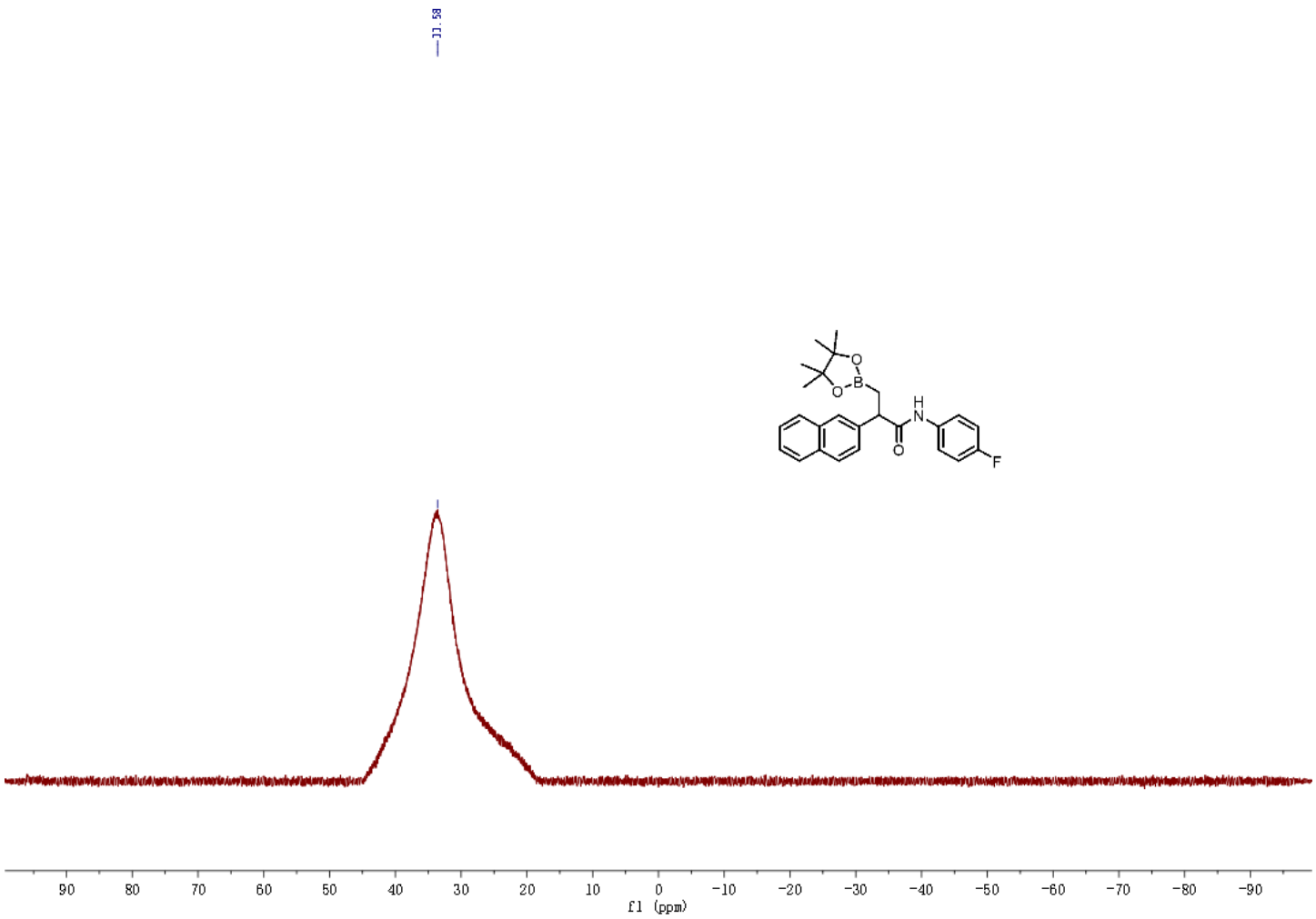
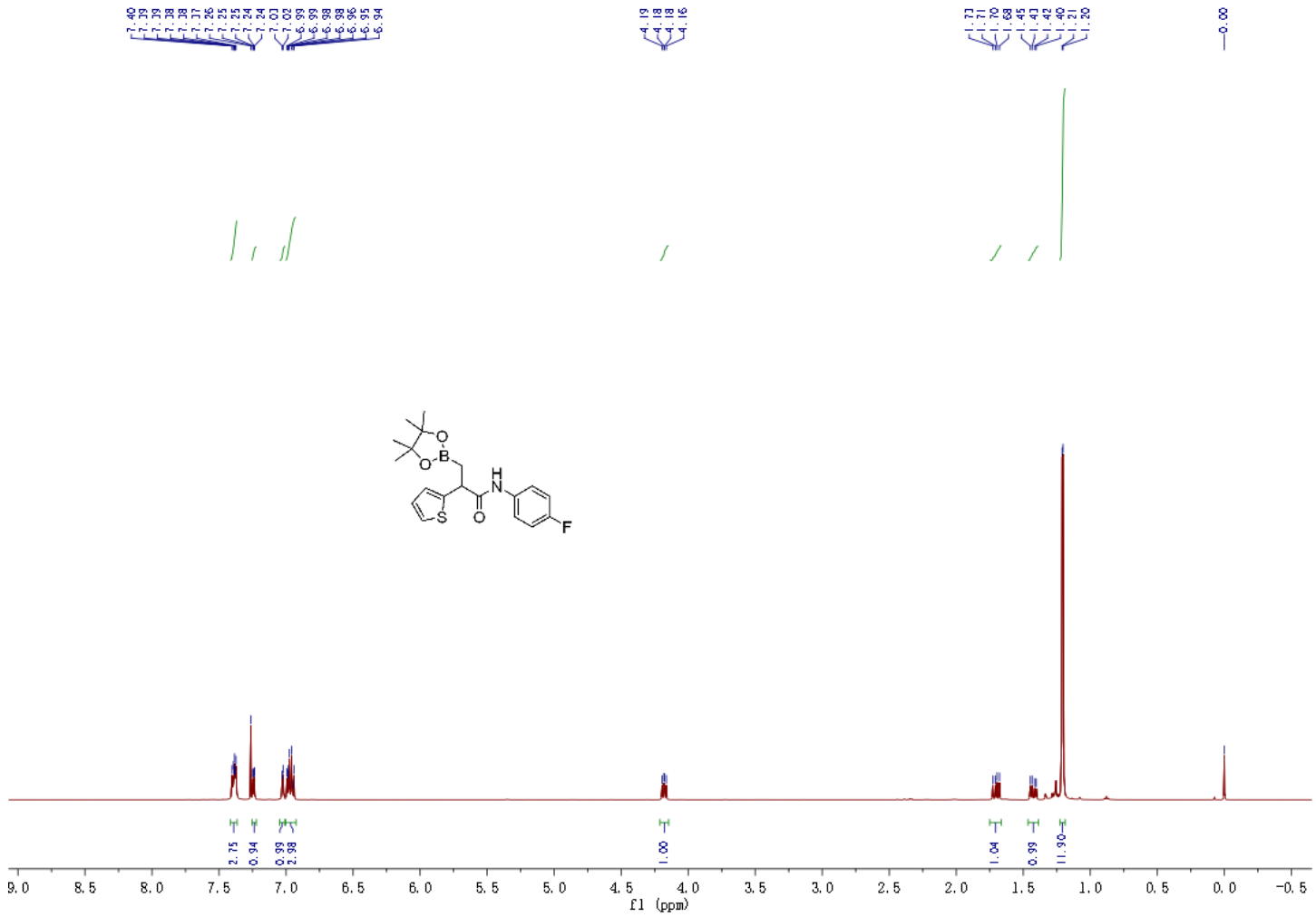
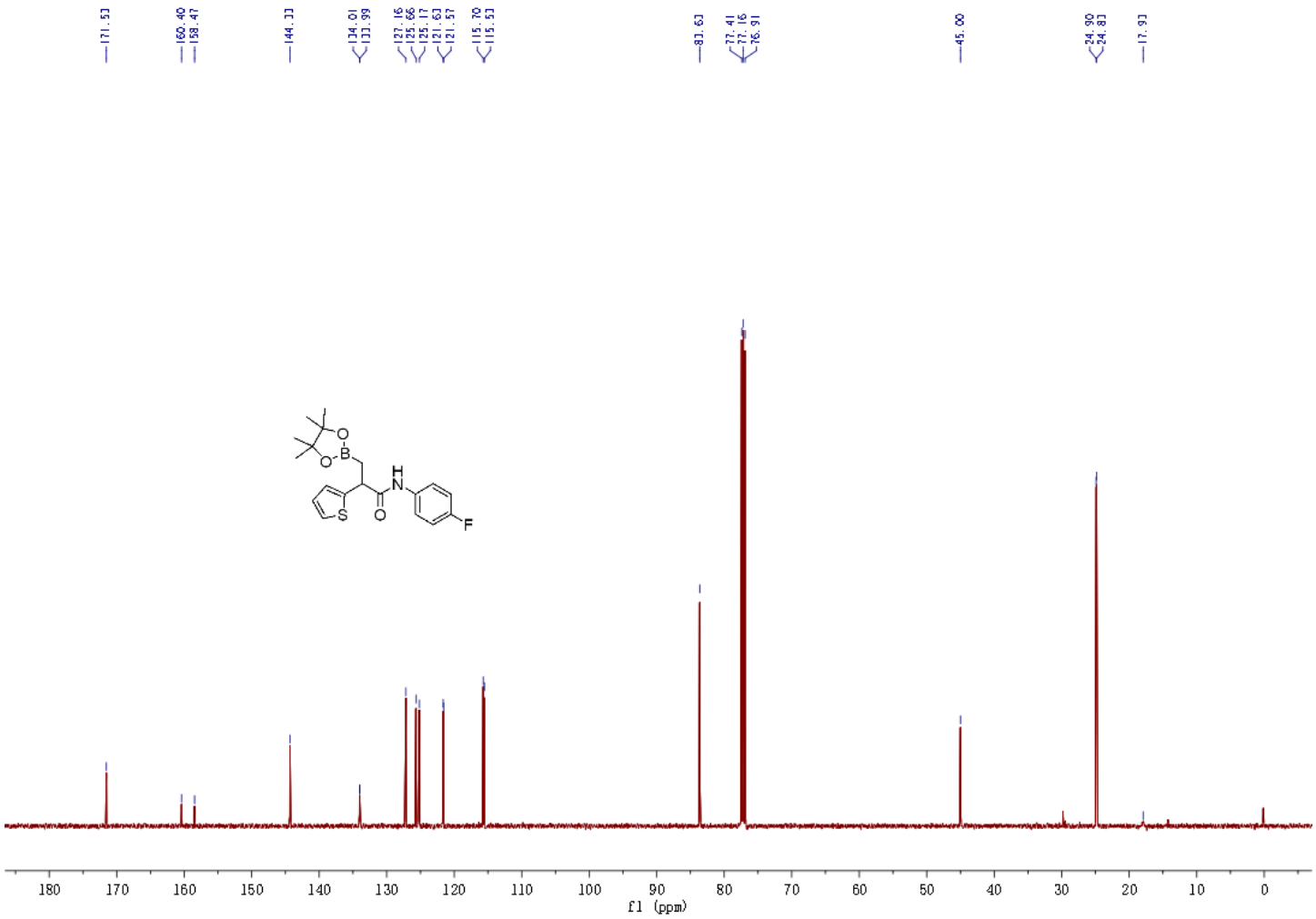
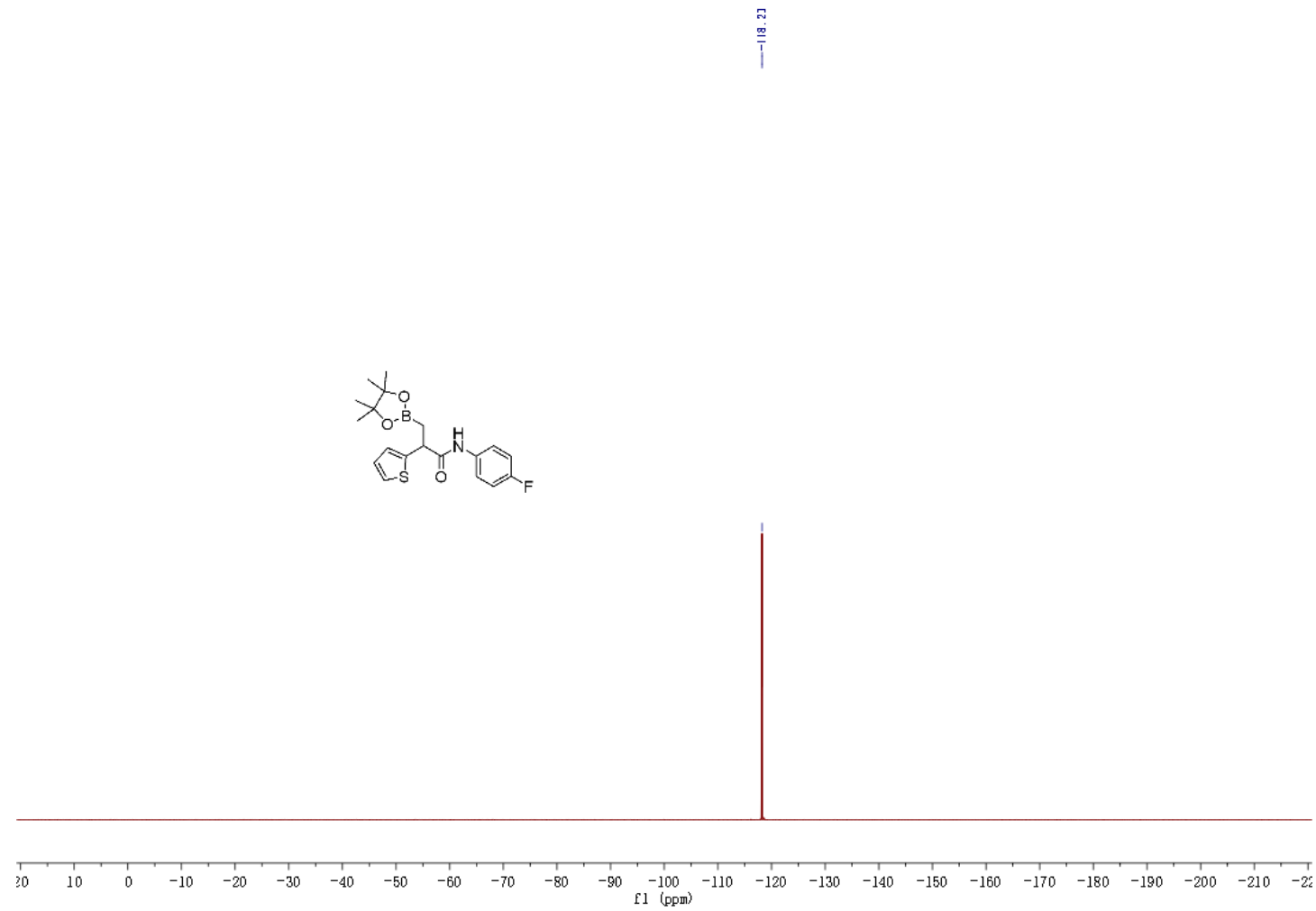
160.06
158.45
138.99
129.04
127.84
127.81
126.92
126.48
126.12
125.83
121.45
115.57
115.43
83.49
77.37
77.16
76.95
49.94
24.89
24.78
16.85
129.04
127.84
127.81
126.92
126.48
126.12
125.83
129.0 128.5 128.0 127.5 127.0 126.5 126.0
f1 (ppm)
O
B
O
H
N
O
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

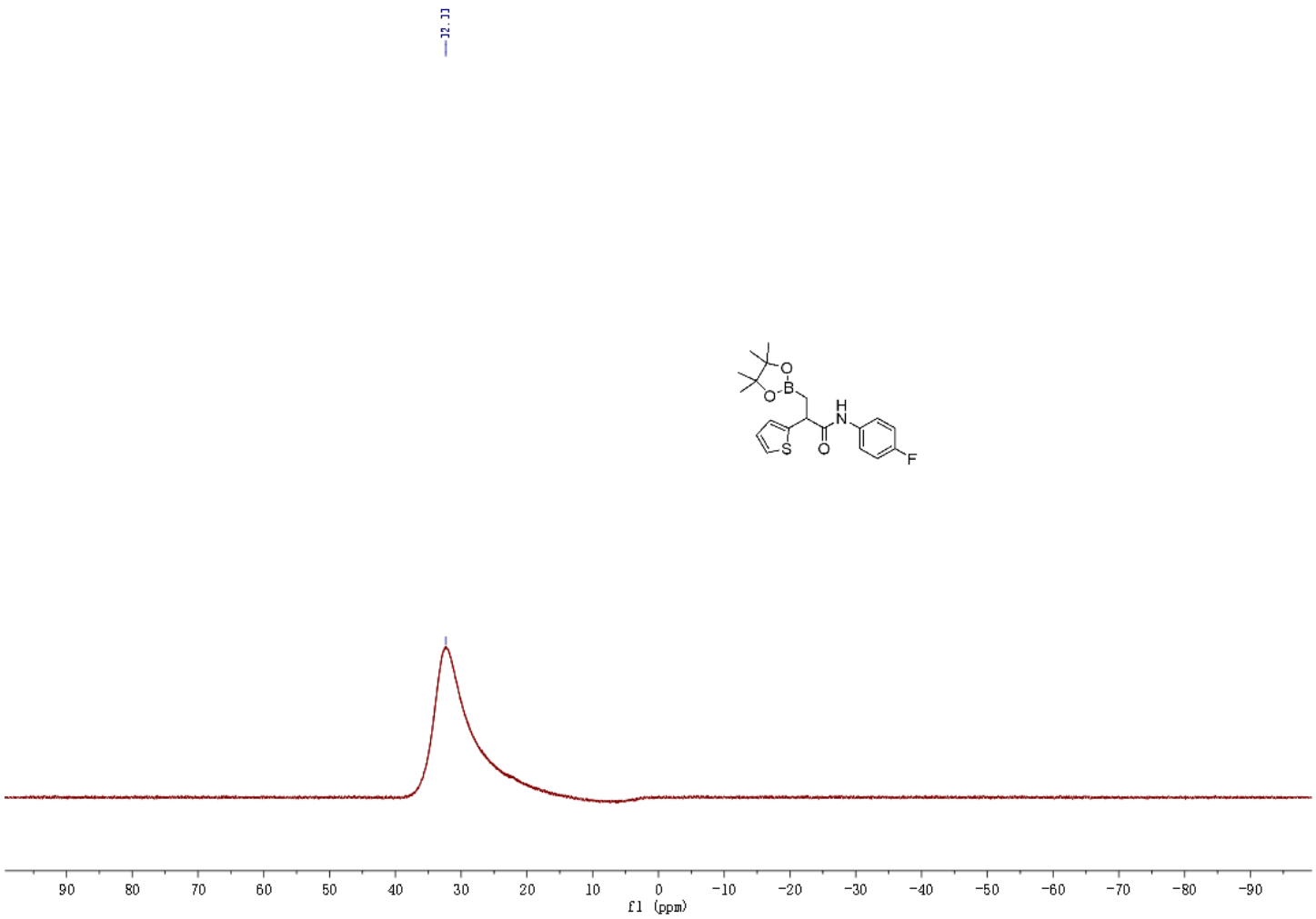

-118.46
F
HN
O
O
B
O
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-20
f1 (ppm)

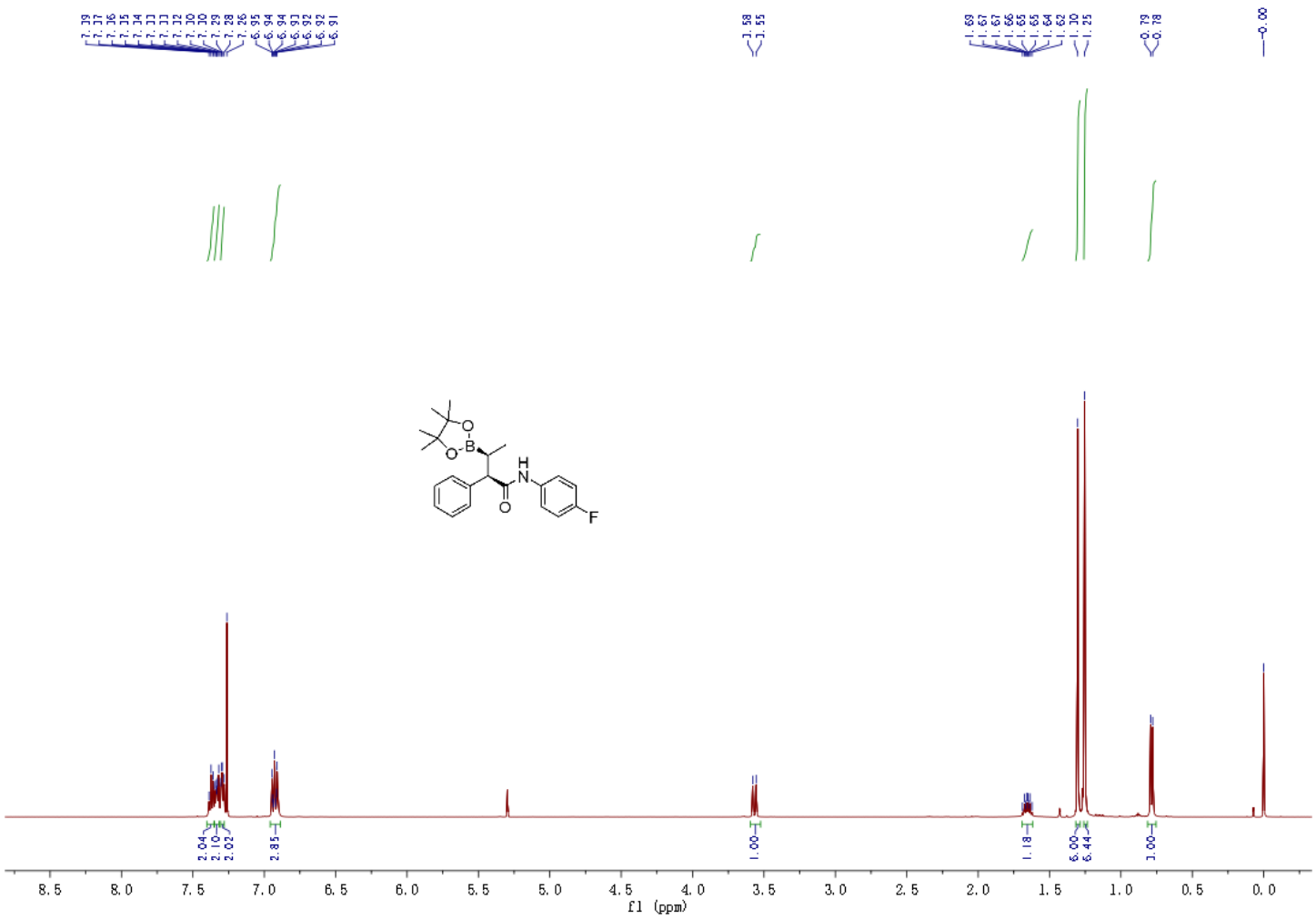

11.58
O
O
B
H
N
O
F
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

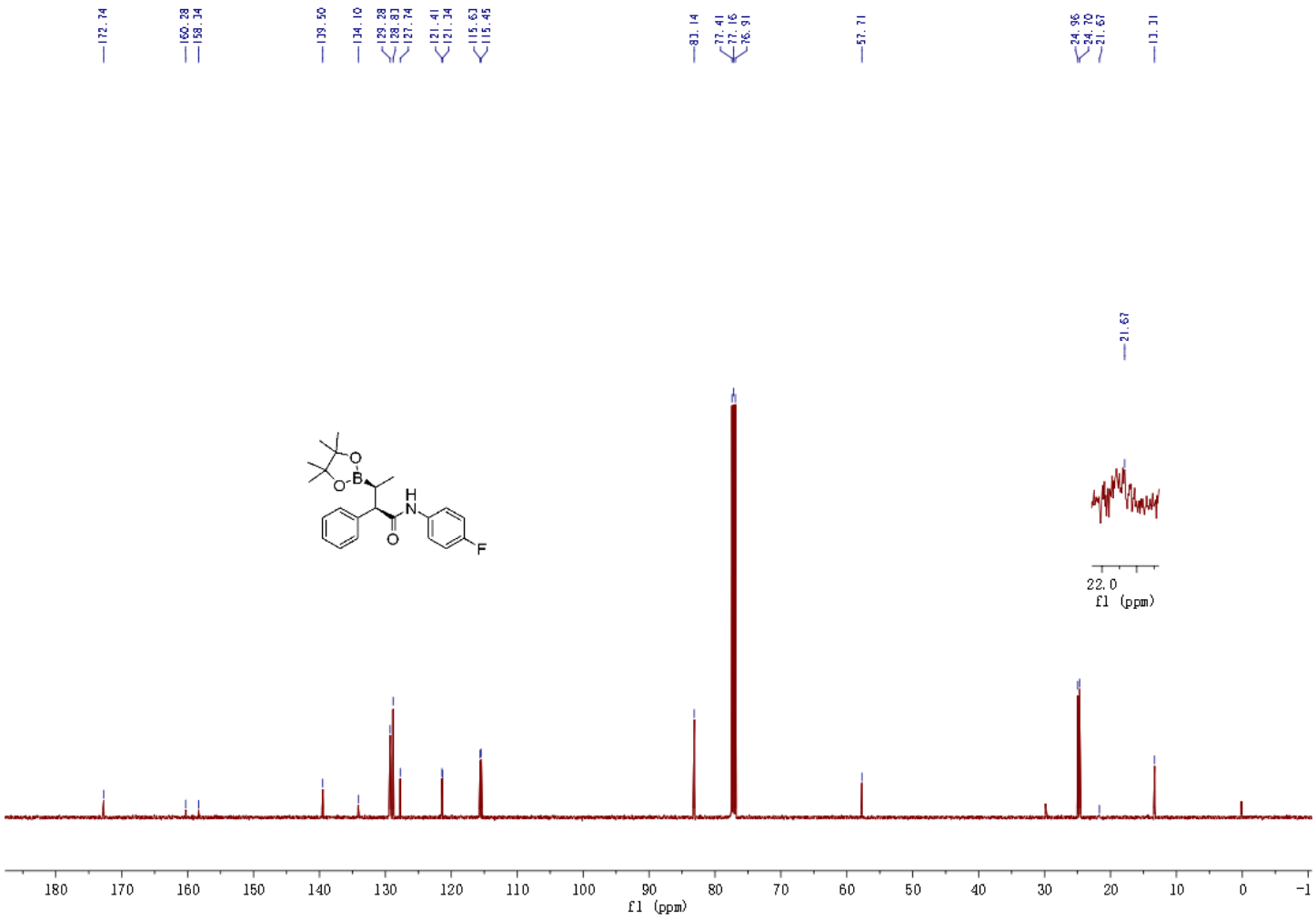

7.40
7.39
7.39
7.38
7.38
7.37
7.26
7.25
7.25
7.24
7.24
7.01
7.02
6.99
6.98
6.98
6.96
6.95
6.94
4.19
4.18
4.18
4.16
1.73
1.71
1.70
1.68
1.45
1.43
1.42
1.40
1.21
1.20
0.00
O
O
B
H
N
S
O
F
2.75
0.94
0.99
2.98
1.00
1.04
0.99
11.90
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


171.53
160.40
158.47
144.33
134.01
133.99
127.16
125.66
125.17
121.63
121.57
115.70
115.53
83.63
77.41
77.16
76.91
45.00
24.90
24.83
17.93
O
B
O
H
N
S
O
F
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-118.23
O
B
O
H
N
S
O
F
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


32.33
O
O
B
H
N
S
O
F
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.39
7.37
7.36
7.35
7.34
7.33
7.33
7.32
7.30
7.30
7.29
7.28
7.26
6.95
6.94
6.94
6.93
6.92
6.92
6.91
3.58
3.55
1.69
1.67
1.67
1.66
1.65
1.65
1.64
1.62
1.30
1.25
0.79
0.78
0.00
O
O
B
H
N
O
F
2.04
2.10
2.02
2.85
1.00
1.18
6.00
6.44
3.00
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
0.0
f1 (ppm)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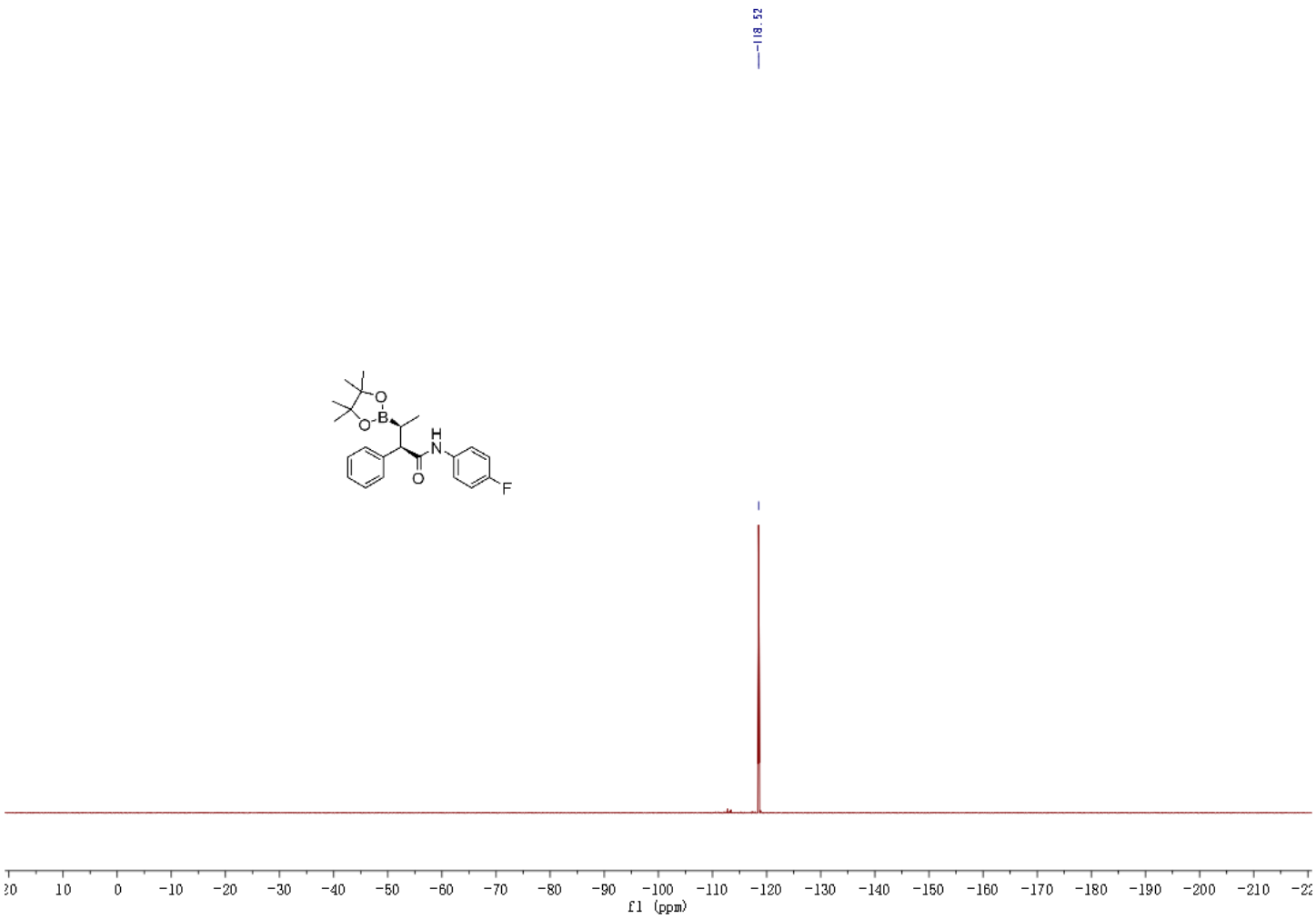
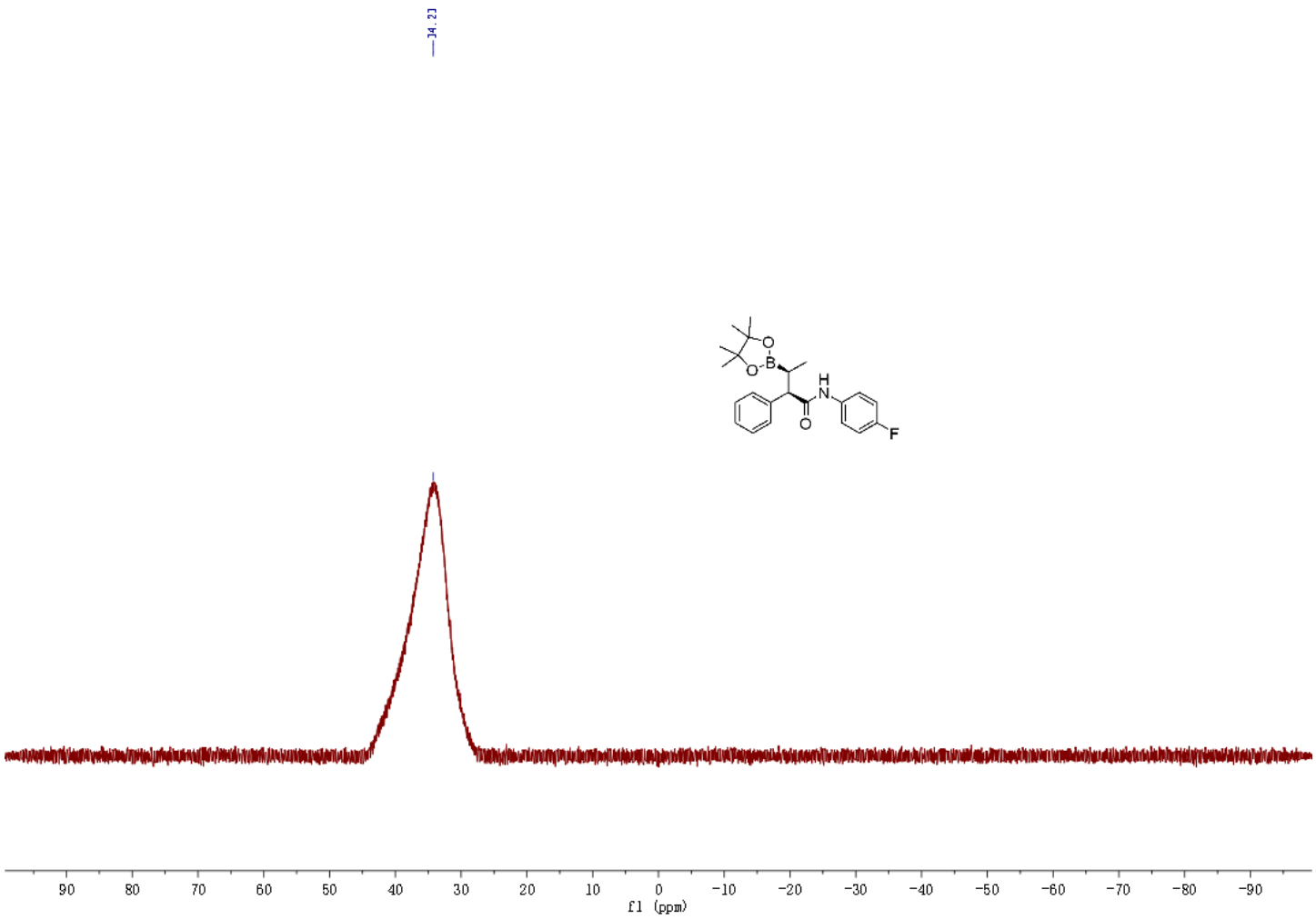
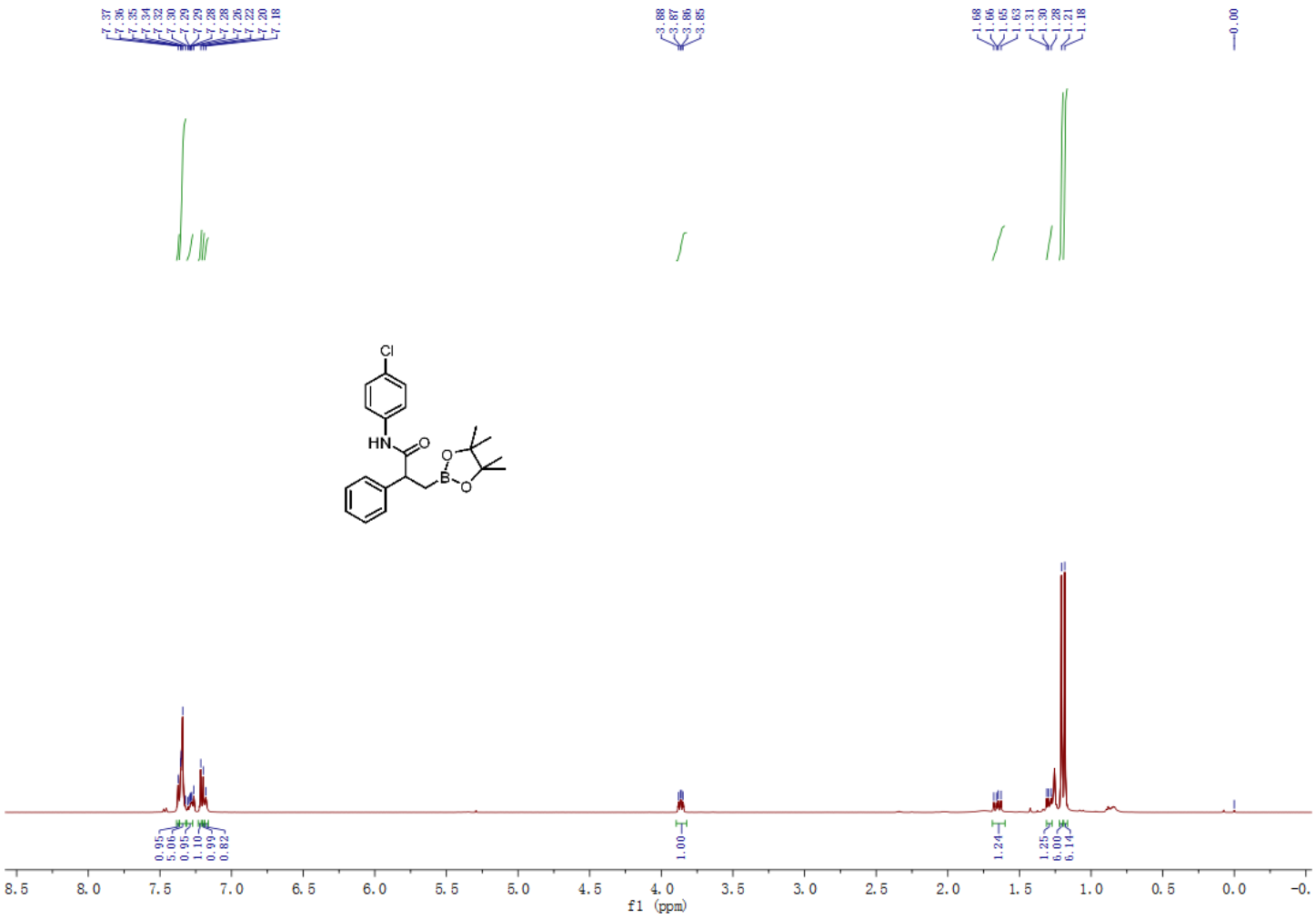
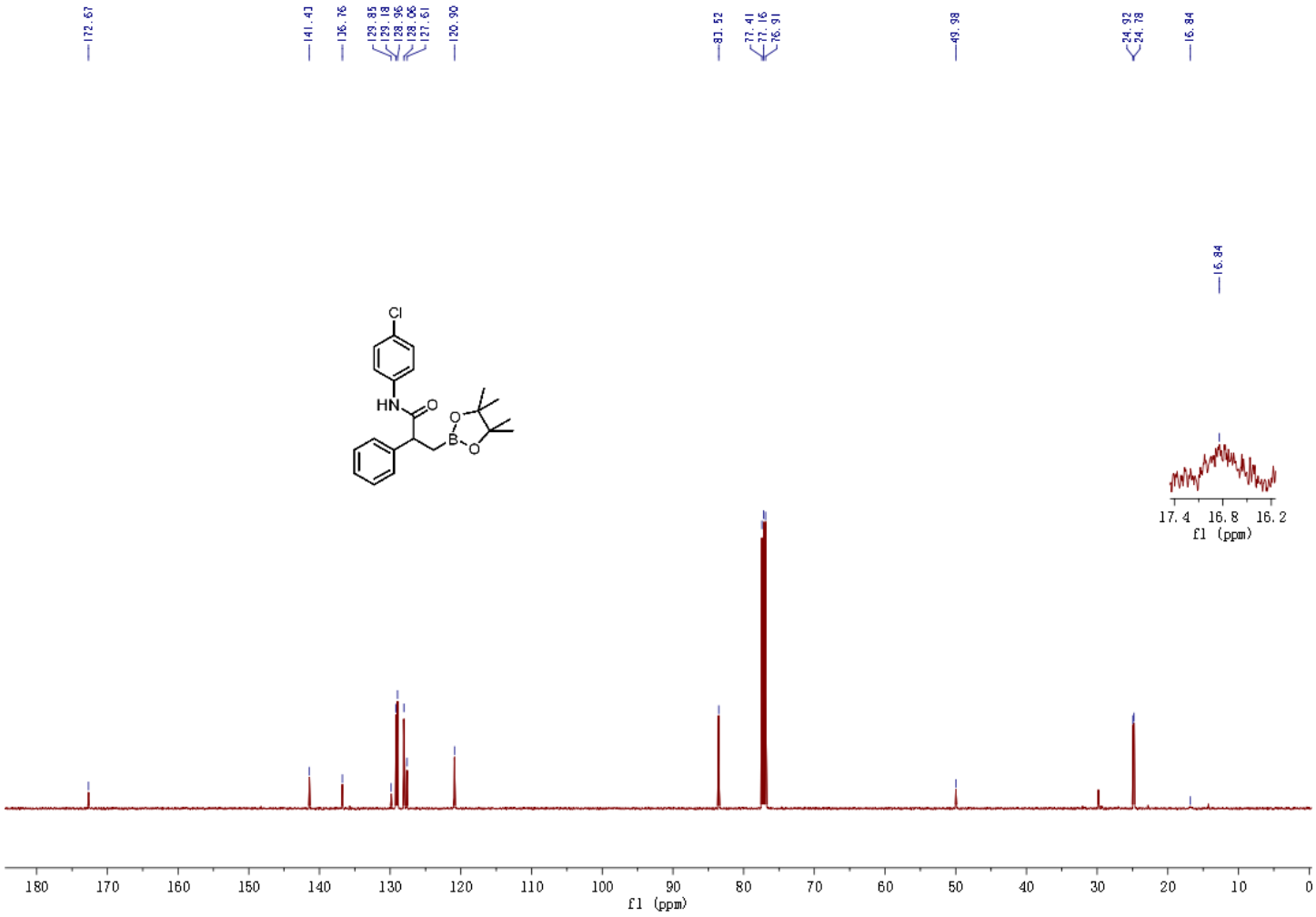
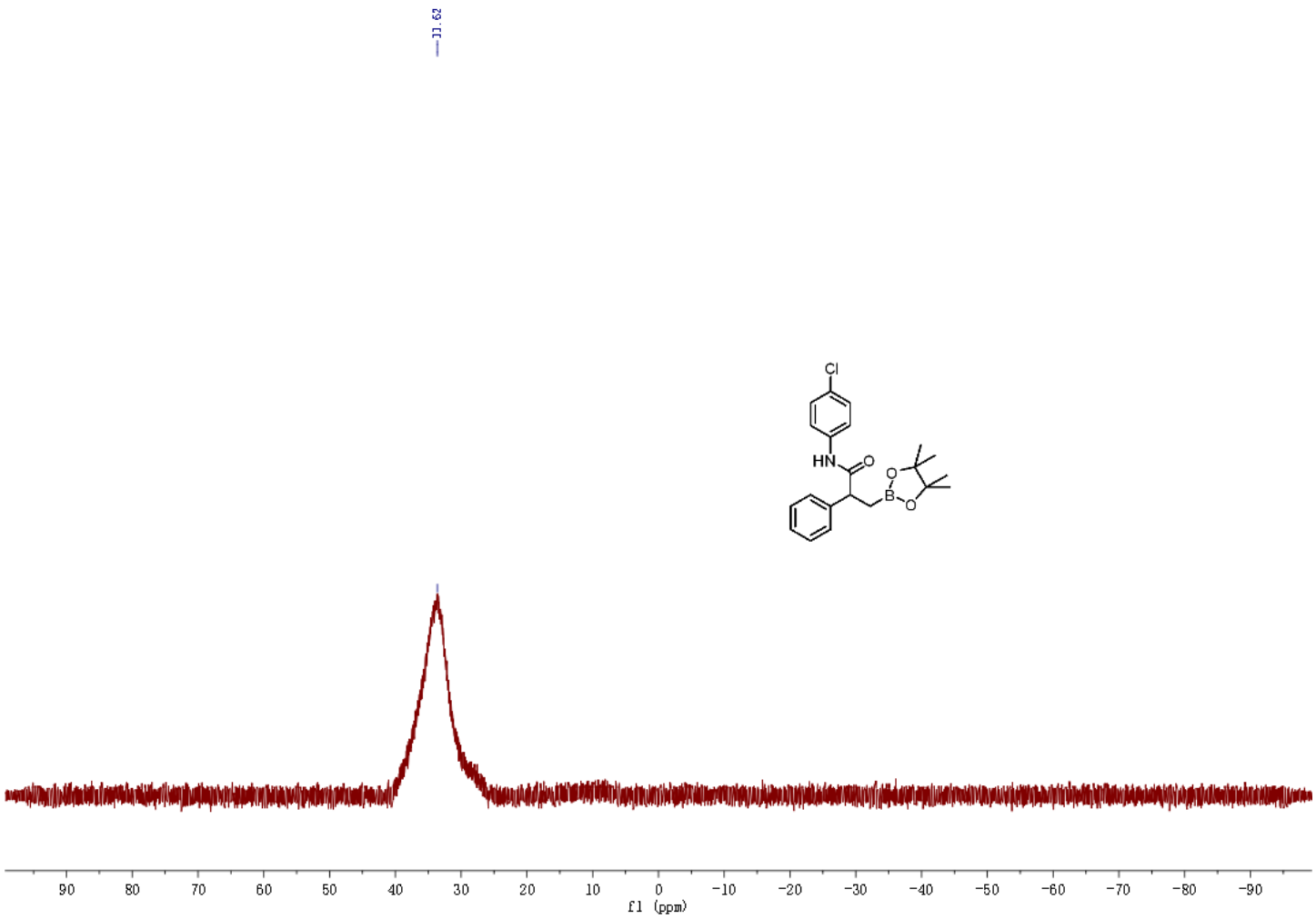
160.28
158.34
139.50
134.10
129.28
128.83
127.74
121.41
121.34
115.63
115.45
83.14
77.41
77.16
76.91
57.71
24.96
24.70
21.67
13.31
21.67
22.0
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

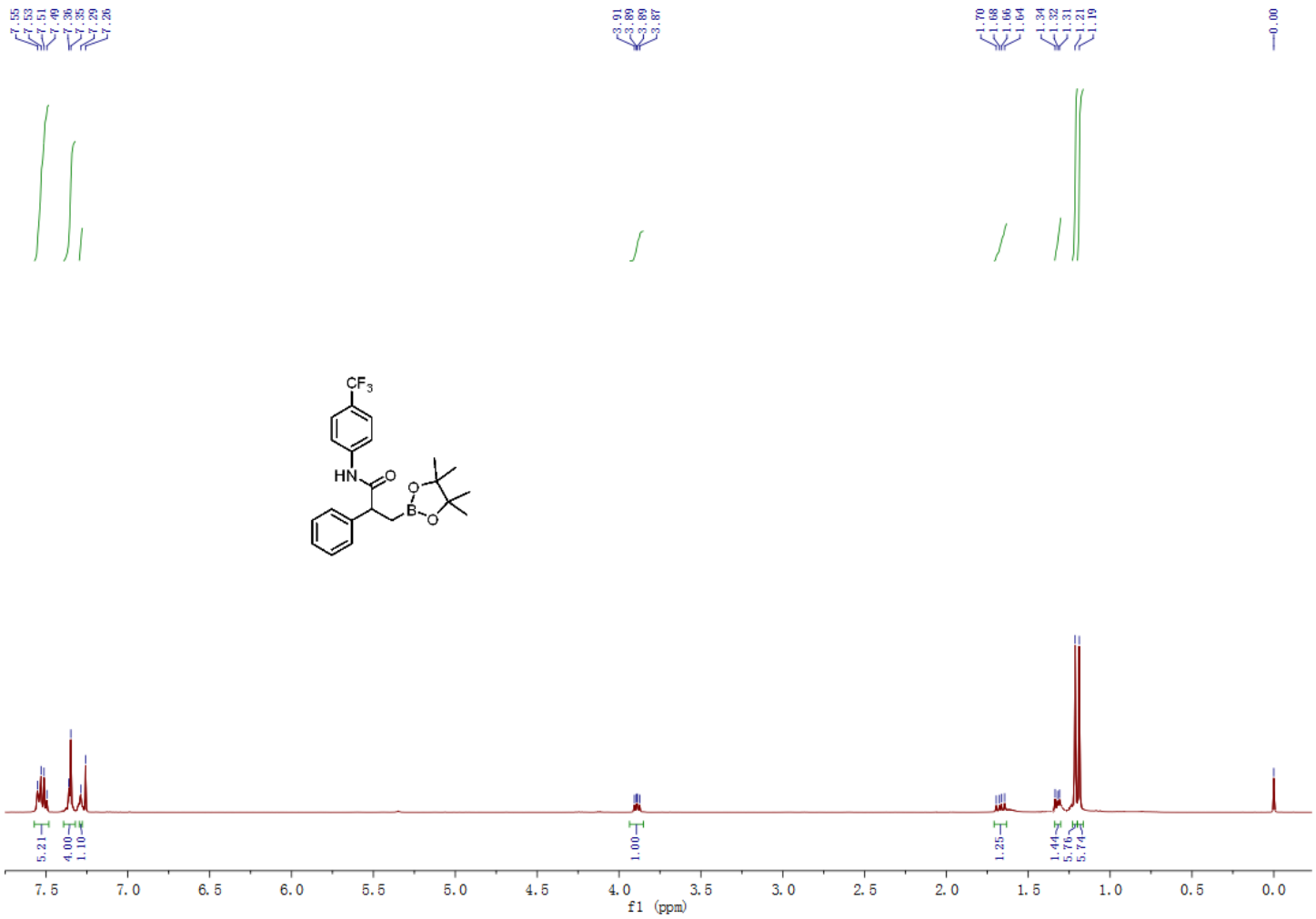

-118.52
O
B
O
H
N
O
F
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)

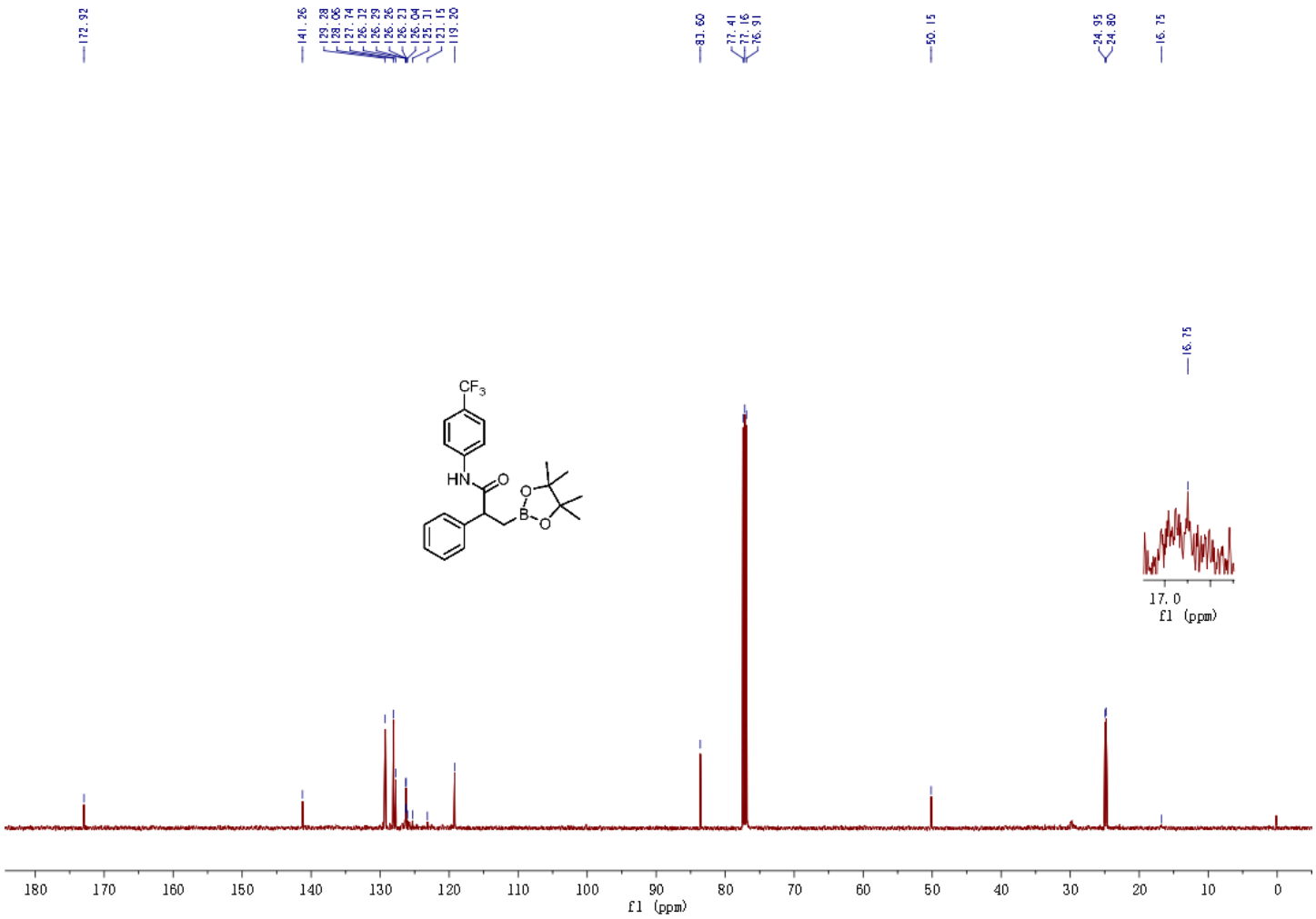

34.23
O
O
B
H
N
O
F
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

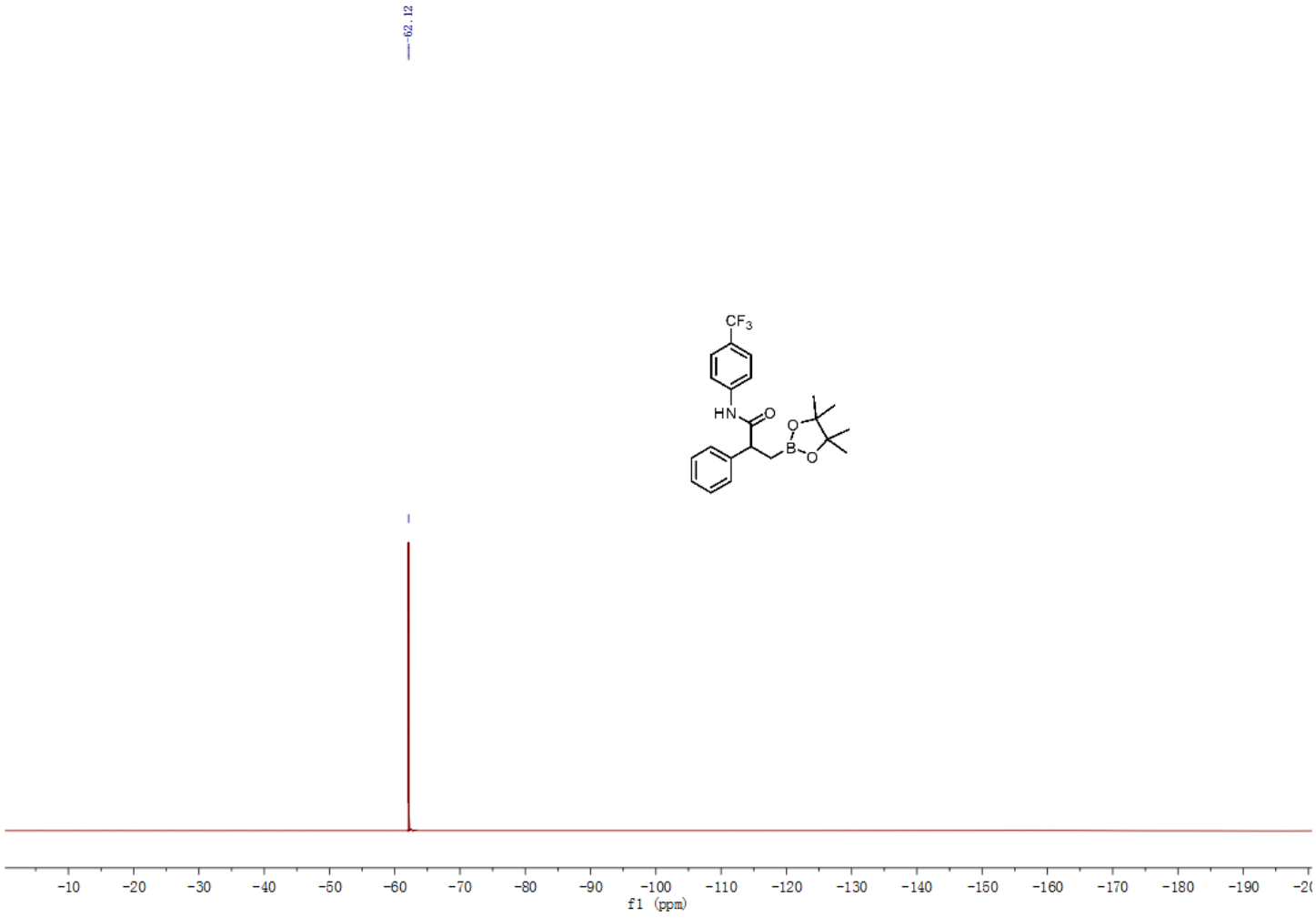

7.37
7.36
7.35
7.34
7.32
7.30
7.29
7.29
7.28
7.28
7.26
7.22
7.20
7.18
3.88
3.87
3.86
3.85
1.68
1.66
1.65
1.63
1.31
1.30
1.28
1.21
1.18
0.00
Cl
HN
O
O
O
B
0.95
5.05
0.95
1.10
0.99
0.82
1.00
1.24
1.25
6.00
6.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

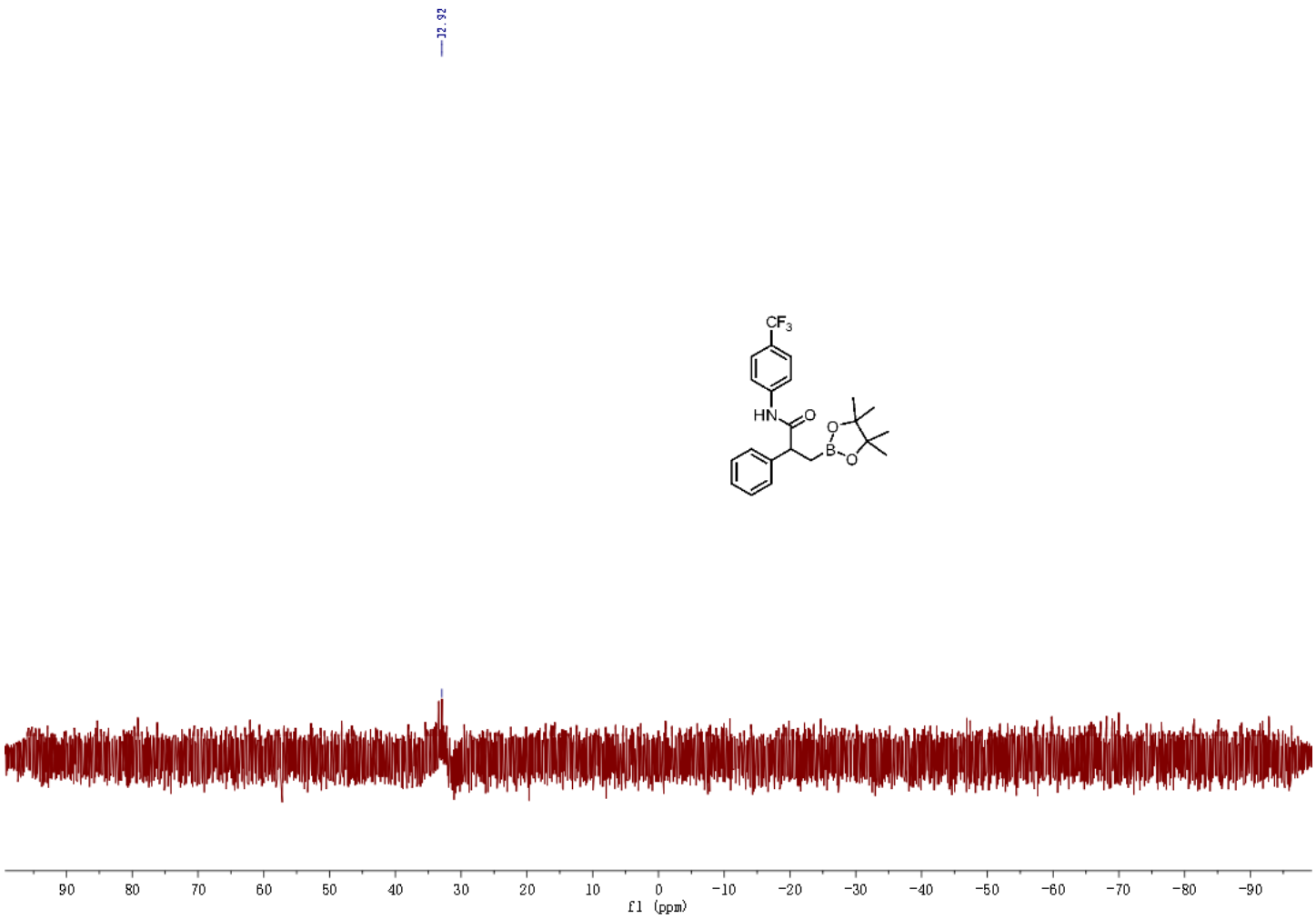

172.67
141.43
136.76
129.85
129.18
128.96
128.06
127.61
120.90
83.52
77.41
77.16
76.91
49.98
24.92
24.78
16.84
Cl
HN
O
O
B
O
16.84
17.4
16.8
16.2
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

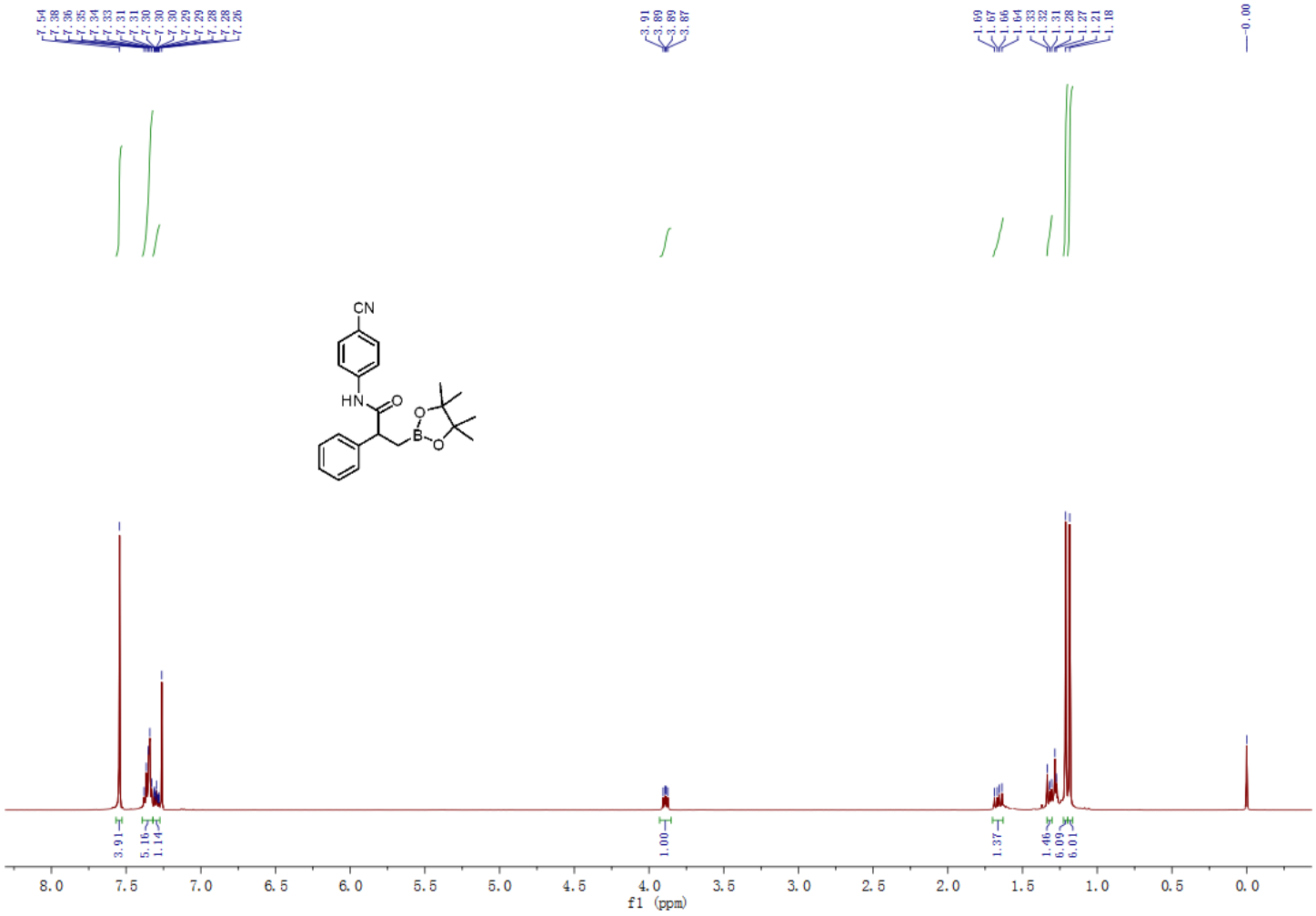

11.62
Cl
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.55
7.53
7.51
7.49
7.36
7.35
7.29
7.26
3.91
3.89
3.89
3.87
1.70
1.68
1.66
1.64
1.34
1.32
1.31
1.21
1.19
0.00
CF3
HN
O
O
O
B
5.21
4.00
1.10
1.00
1.25
1.44
5.76
5.74
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
0.0
f1 (ppm)


172.92
141.26
129.28
128.06
127.74
126.12
126.29
126.26
126.23
126.04
125.31
123.15
119.20
83.60
77.41
77.16
76.91
50.15
24.95
24.80
16.75
CF3
HN
O
O
O
B
16.75
17.0
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.12
CF3
HN
O
O
B
O
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


32.92
CF3
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)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7.36
7.35
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7.31
7.31
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7.30
7.30
7.29
7.29
7.28
7.28
7.26
3.91
3.89
3.89
3.87
1.69
1.67
1.66
1.64
1.33
1.32
1.31
1.28
1.27
1.21
1.18
0.00
CN
HN
O
O
B
O
3.91
5.16
1.14
1.00
1.37
1.46
6.09
6.01
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
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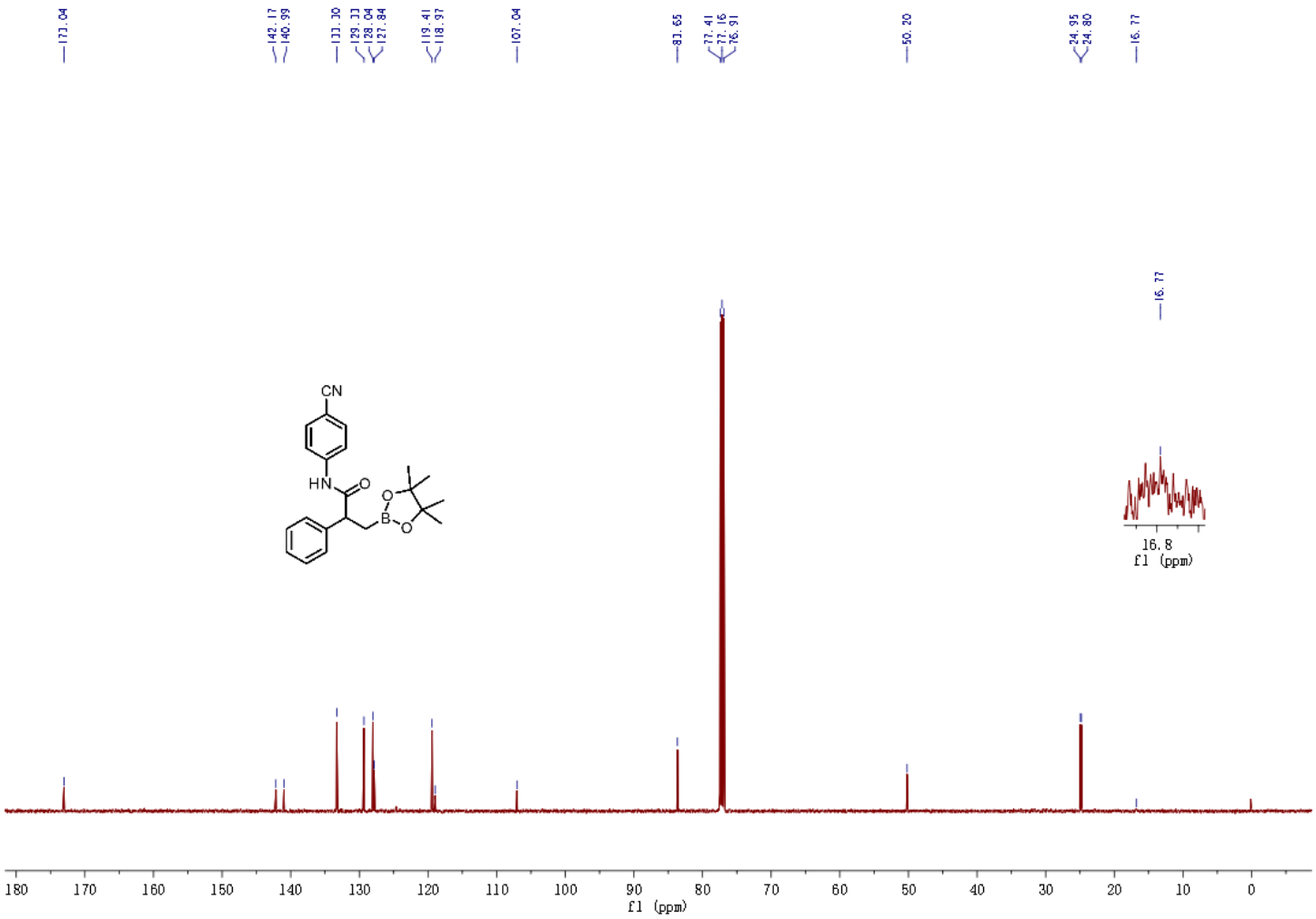
0.0
f1 (ppm)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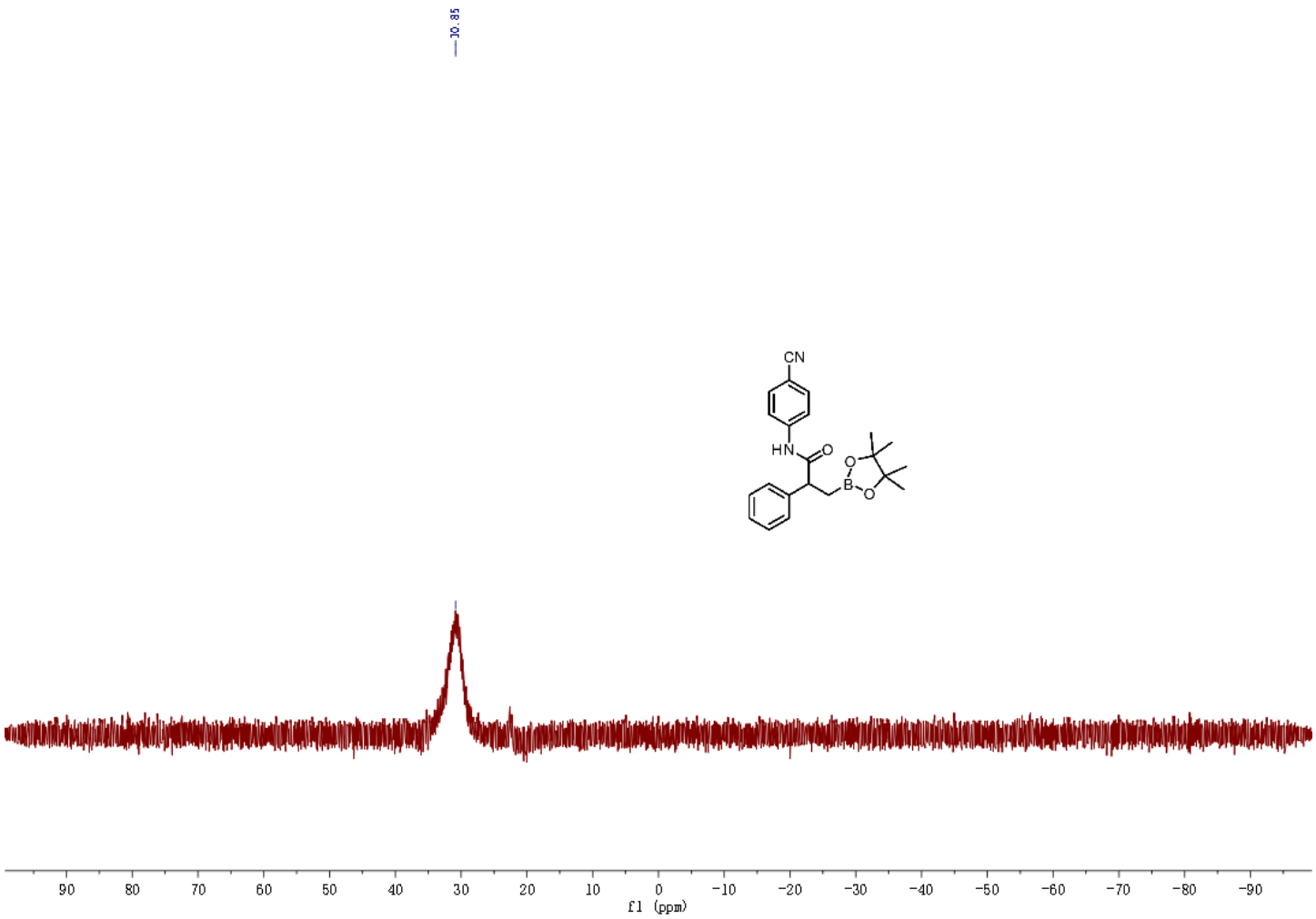
142.17
140.99
133.30
129.33
128.04
127.84
119.41
118.97
107.04
83.65
77.41
77.16
76.91
50.20
24.95
24.80
16.77
CN
HN
O
O
B
O
16.77
16.8
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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60
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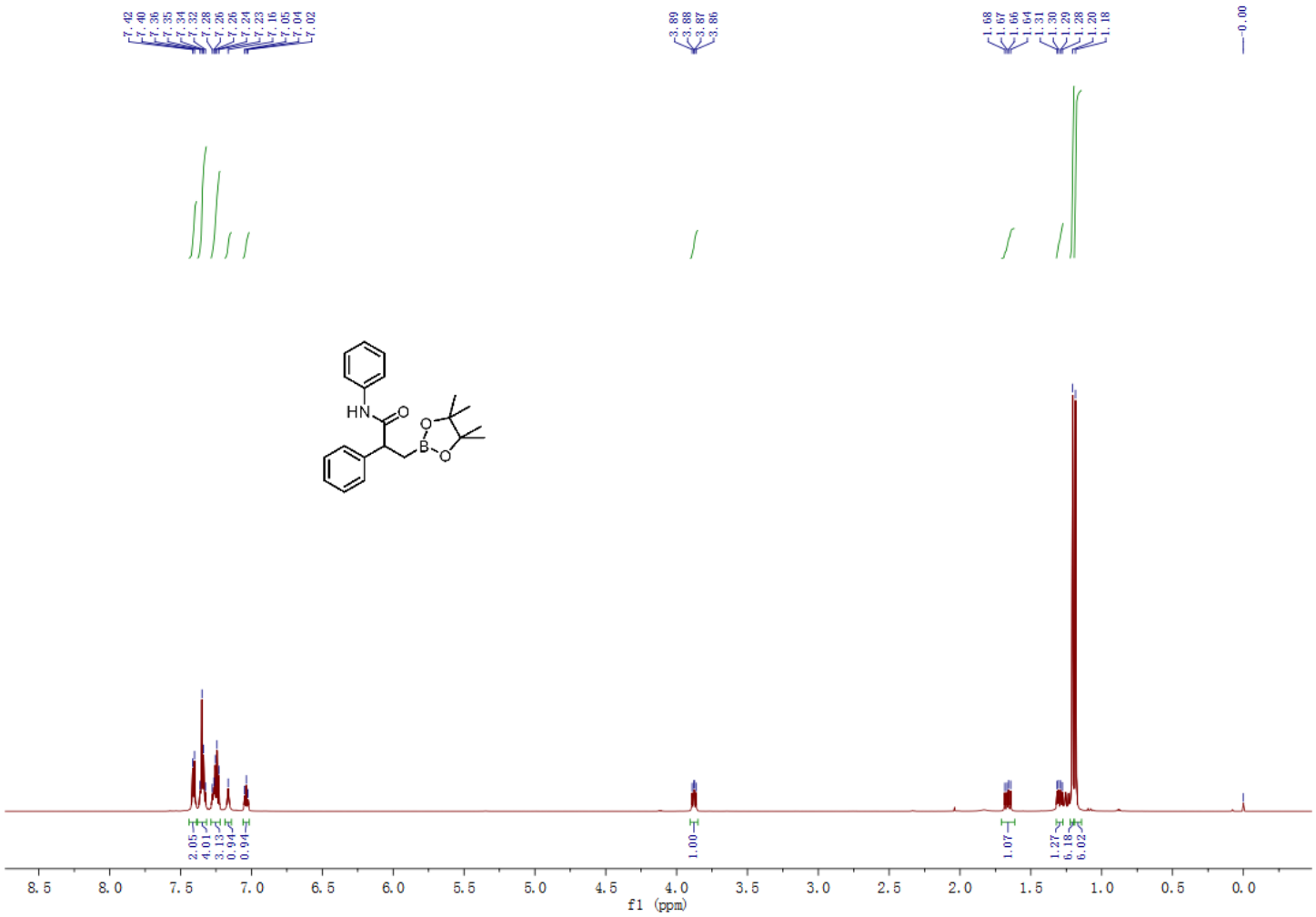
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.42
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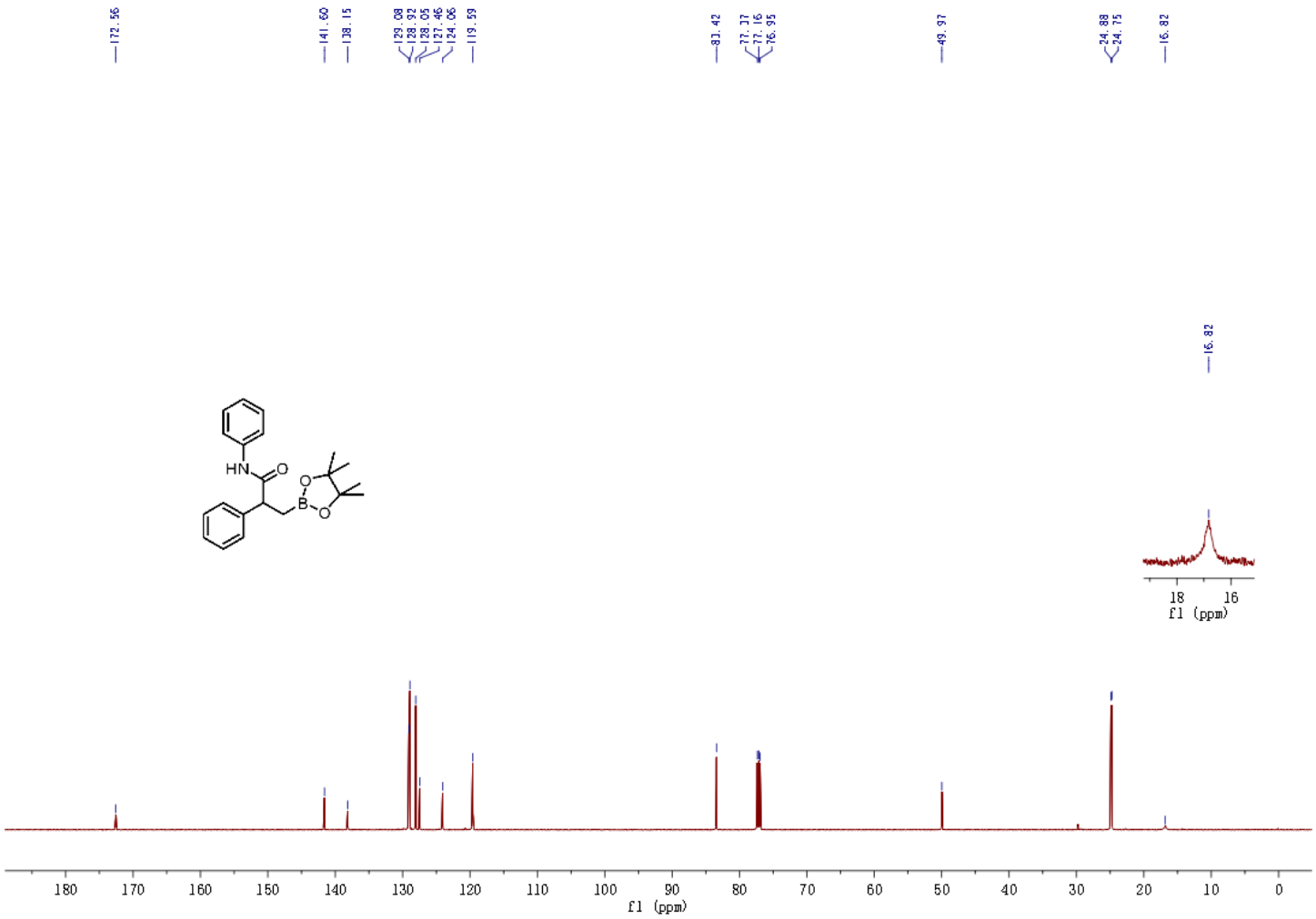
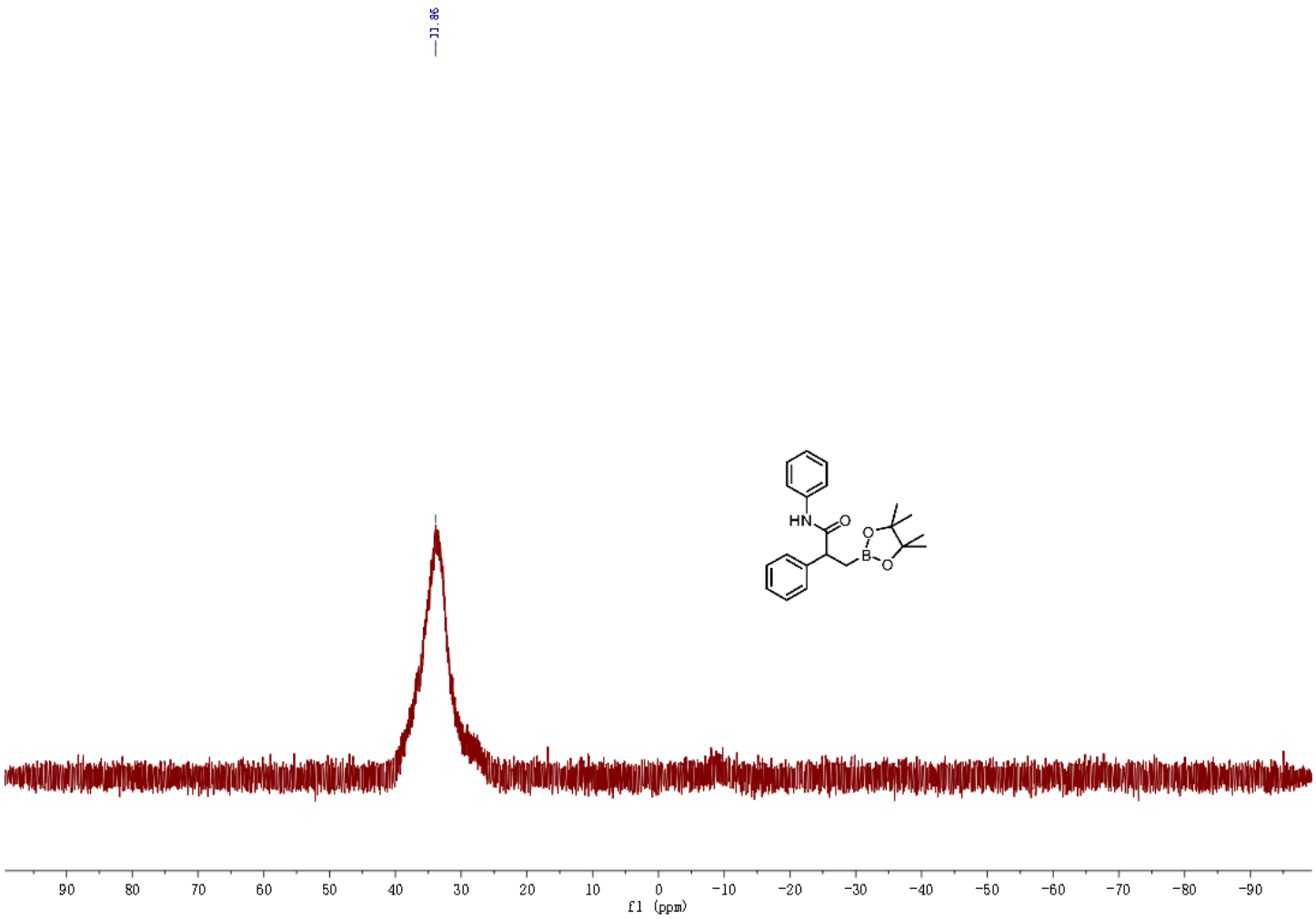
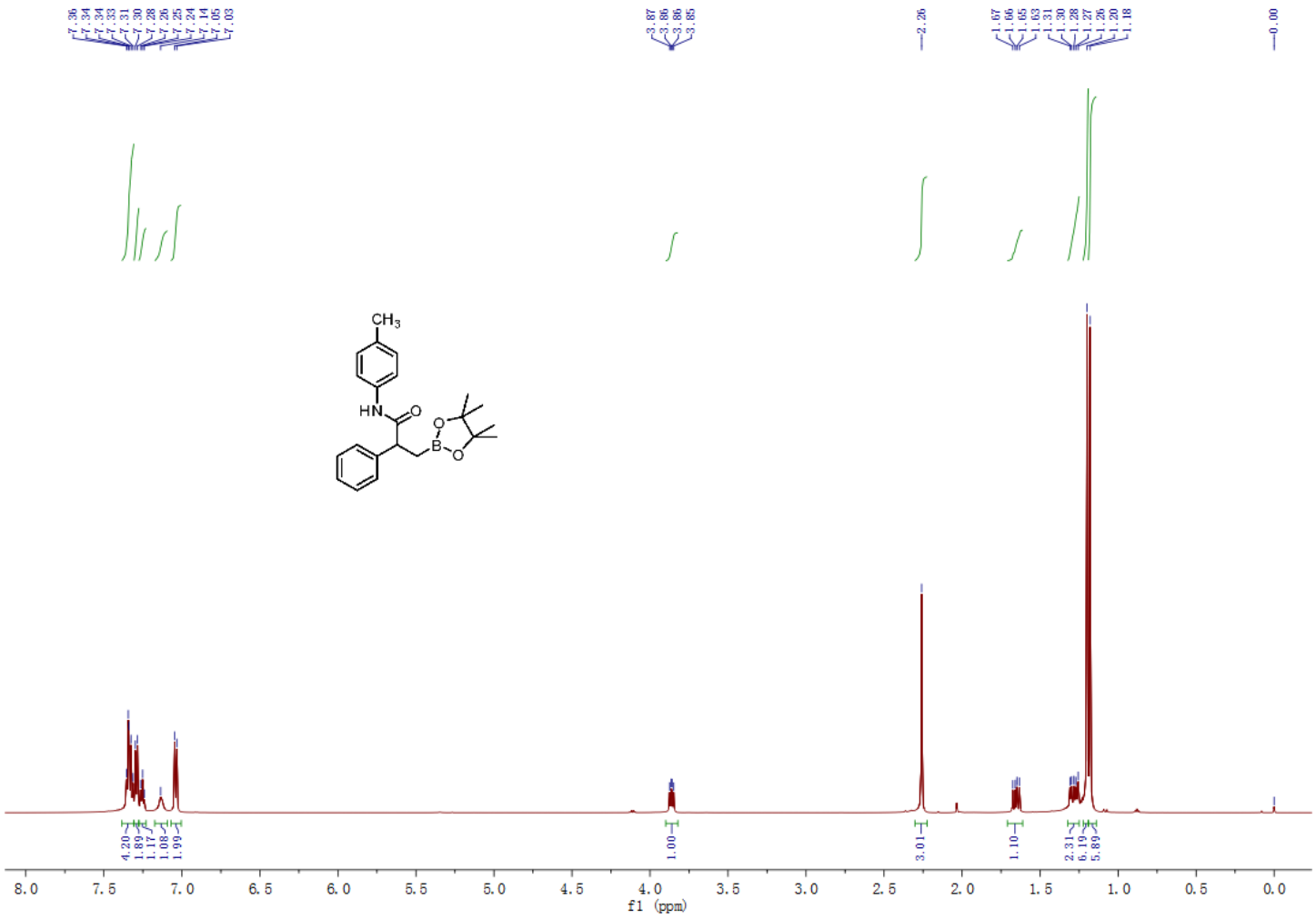
7.28
7.26
7.26
7.24
7.23
7.16
7.05
7.04
7.02
3.89
3.88
3.87
3.86
1.68
1.67
1.66
1.64
1.31
1.30
1.29
1.28
1.20
1.18
0.00
HN
O
O
O
B
2.05
4.01
3.13
0.94
0.94
1.00
1.07
1.27
6.18
6.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


172.56
141.60
138.15
129.08
128.92
128.05
127.46
124.06
119.59
83.42
77.37
77.16
76.95
49.97
24.88
24.75
16.82
HN
O
O
O
B
16.82
18
16
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.86
HN
O
O
O
B
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)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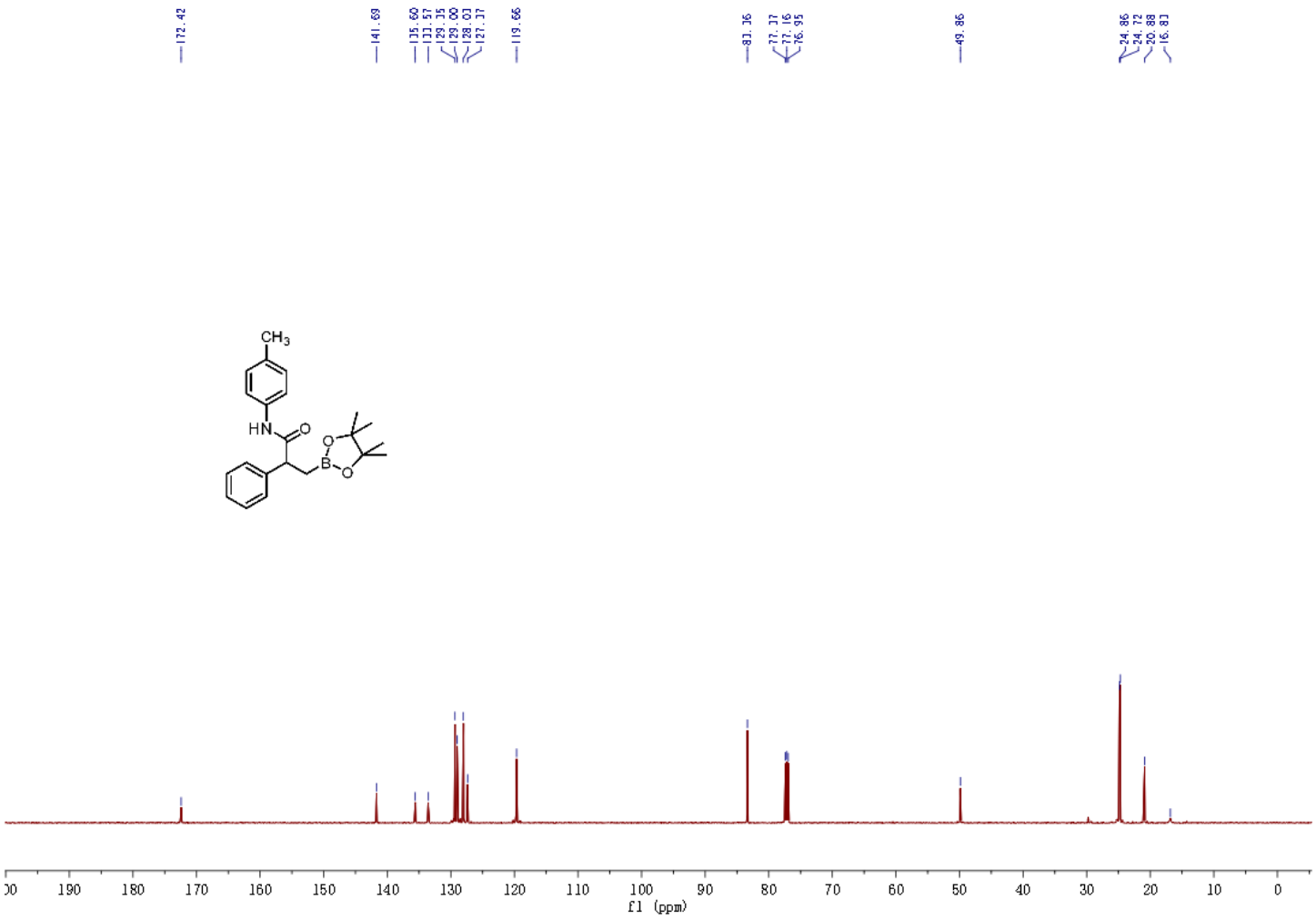
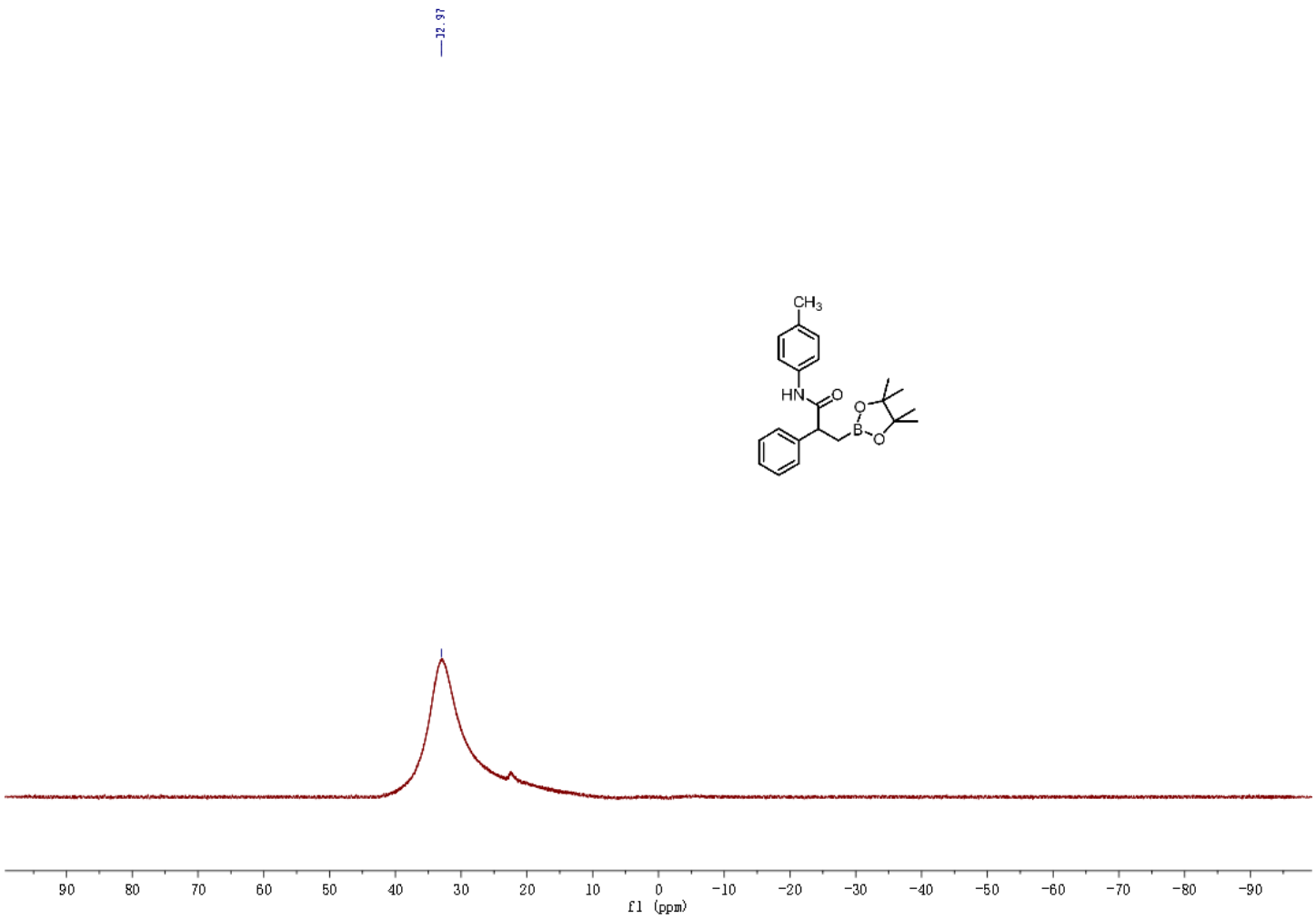
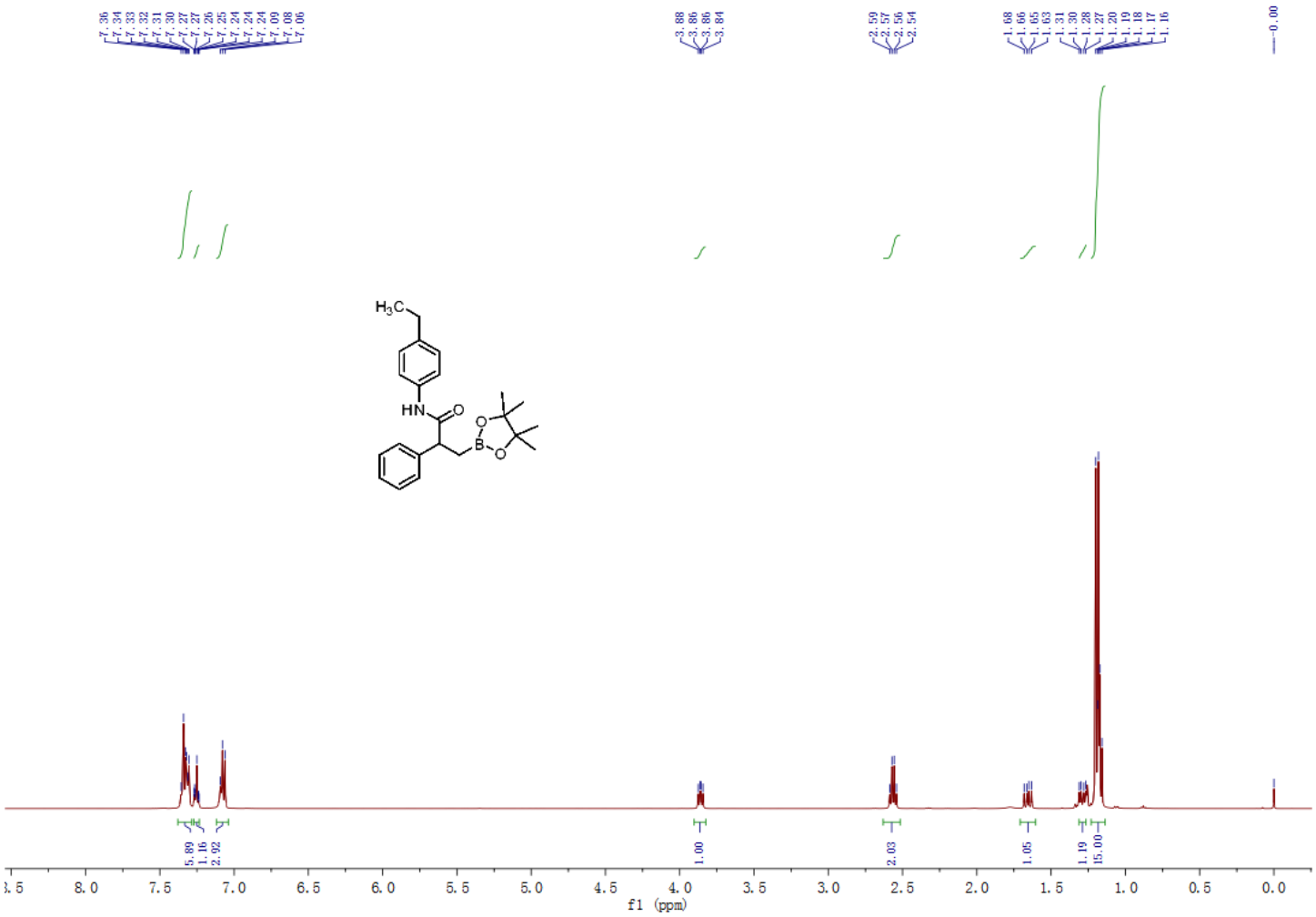
7.34
7.34
7.33
7.31
7.30
7.28
7.26
7.25
7.24
7.14
7.05
7.03
3.87
3.86
3.86
3.85
2.26
1.67
1.66
1.65
1.63
1.31
1.30
1.28
1.27
1.26
1.20
1.18
0.00
CH3
HN
O
O
O
B
4.20
1.89
1.17
1.08
1.99
1.00
3.01
1.10
2.31
6.19
5.89
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


172.42
141.69
135.60
133.57
129.35
129.00
128.03
127.37
119.66
83.36
77.37
77.16
76.95
49.86
24.86
24.72
20.88
16.83
CH3
HN
O
O
O
B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


32.97
CH3
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)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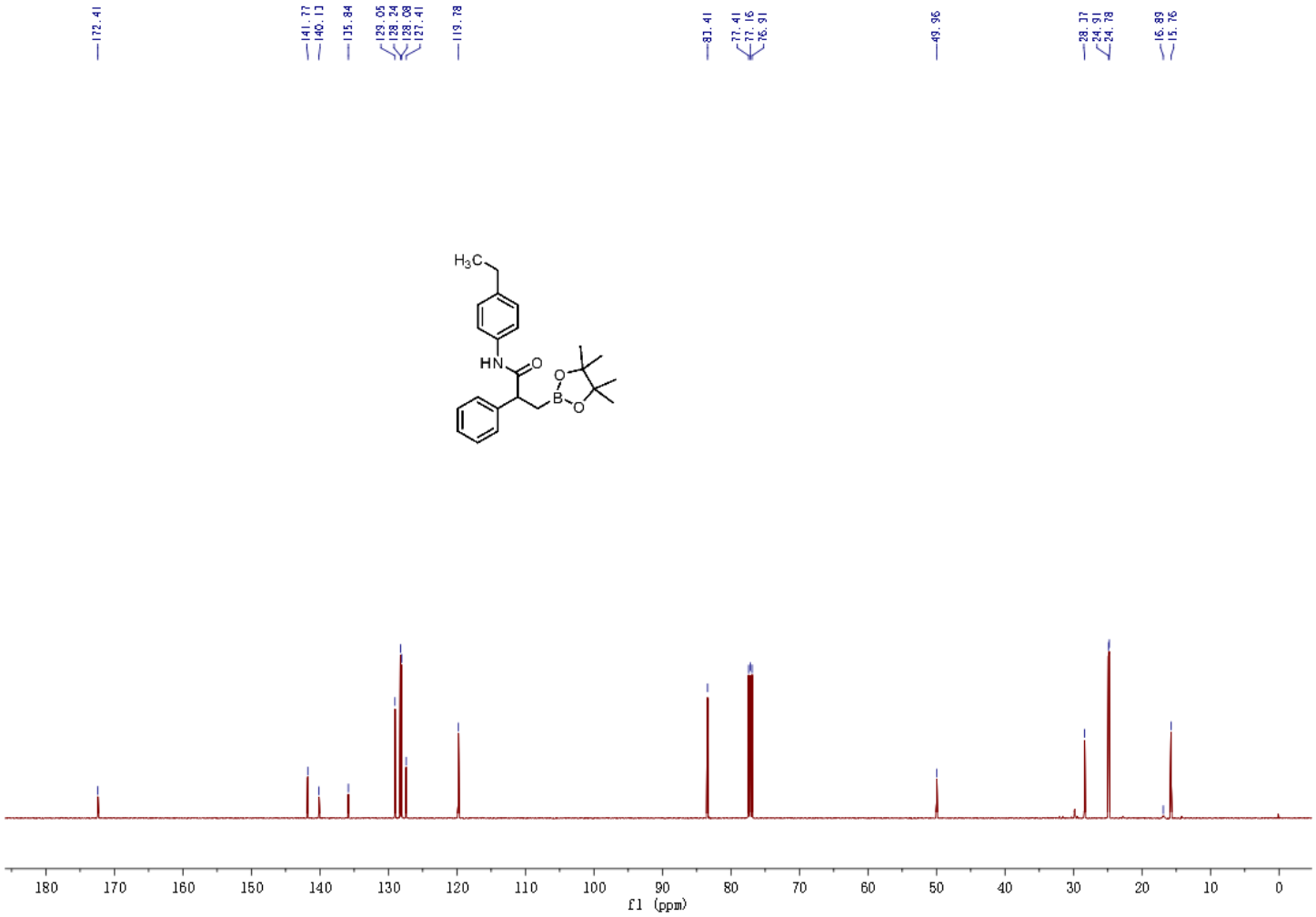
7.34
7.33
7.32
7.31
7.30
7.27
7.27
7.26
7.25
7.24
7.24
7.24
7.09
7.08
7.06
3.88
3.86
3.86
3.84
2.59
2.57
2.56
2.54
1.68
1.66
1.65
1.63
1.31
1.30
1.28
1.27
1.20
1.19
1.18
1.17
1.16
0.00
H3C
HN
O
O
O
B
5.89
1.16
2.92
1.00
2.03
1.05
1.19
15.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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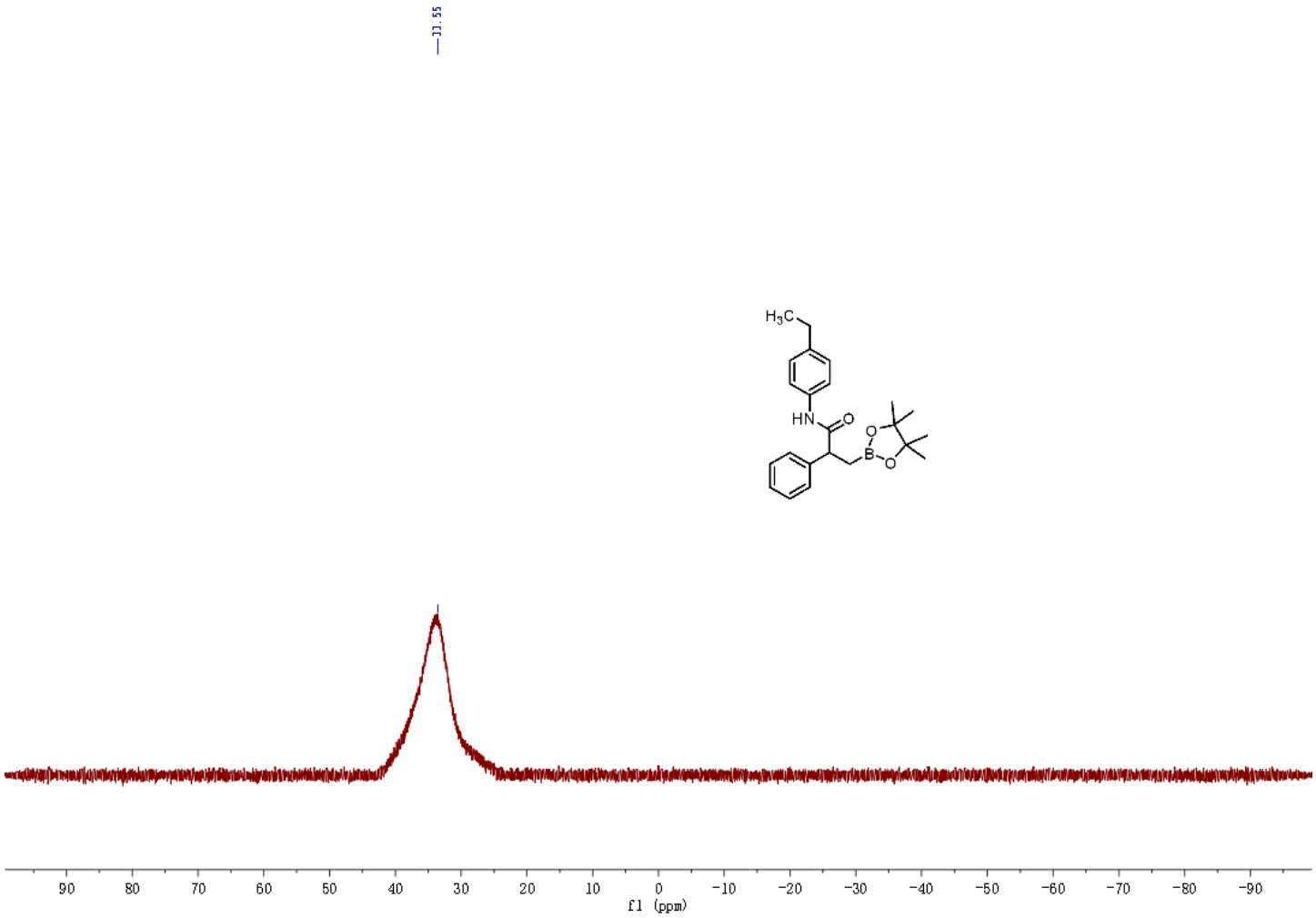
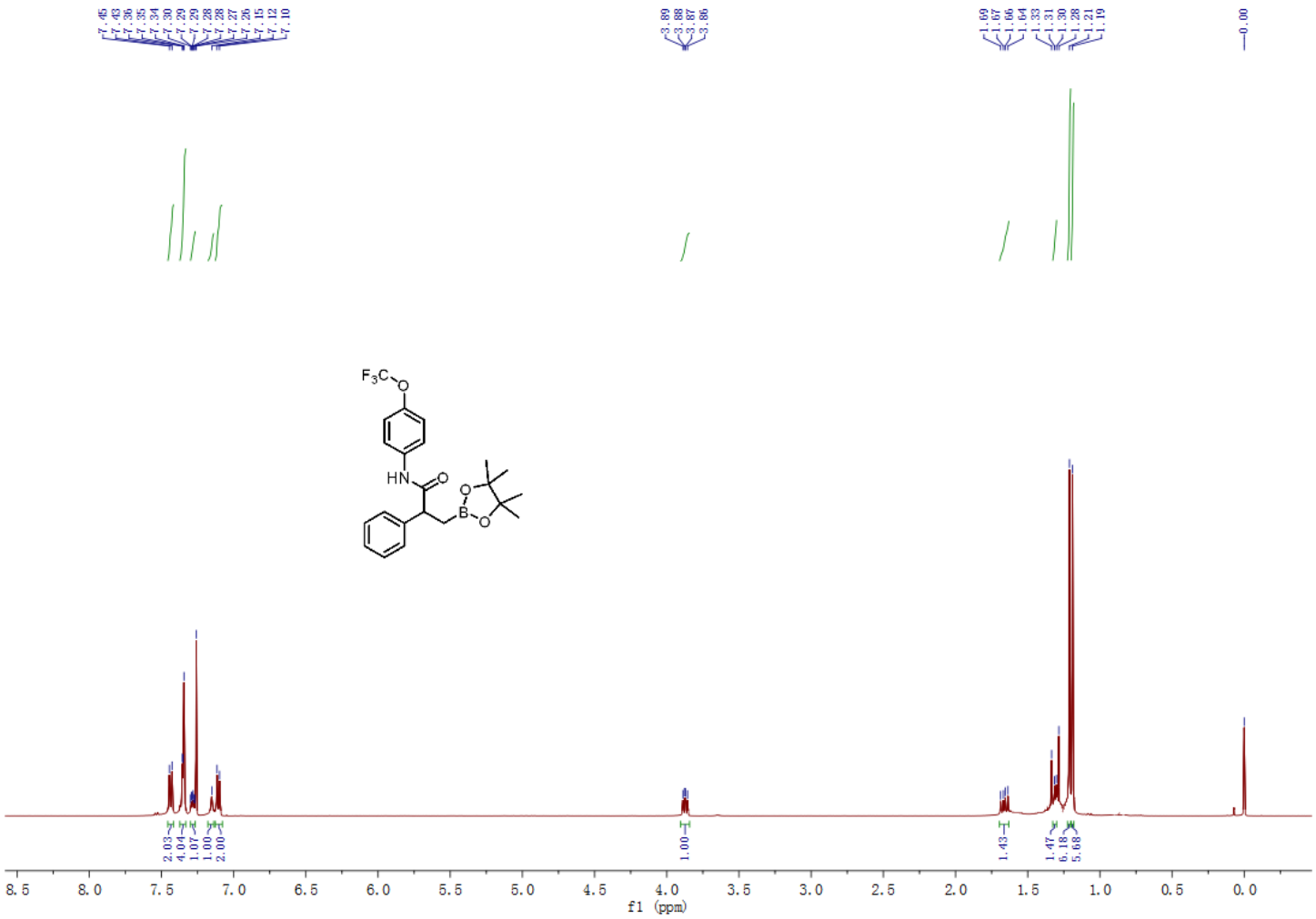
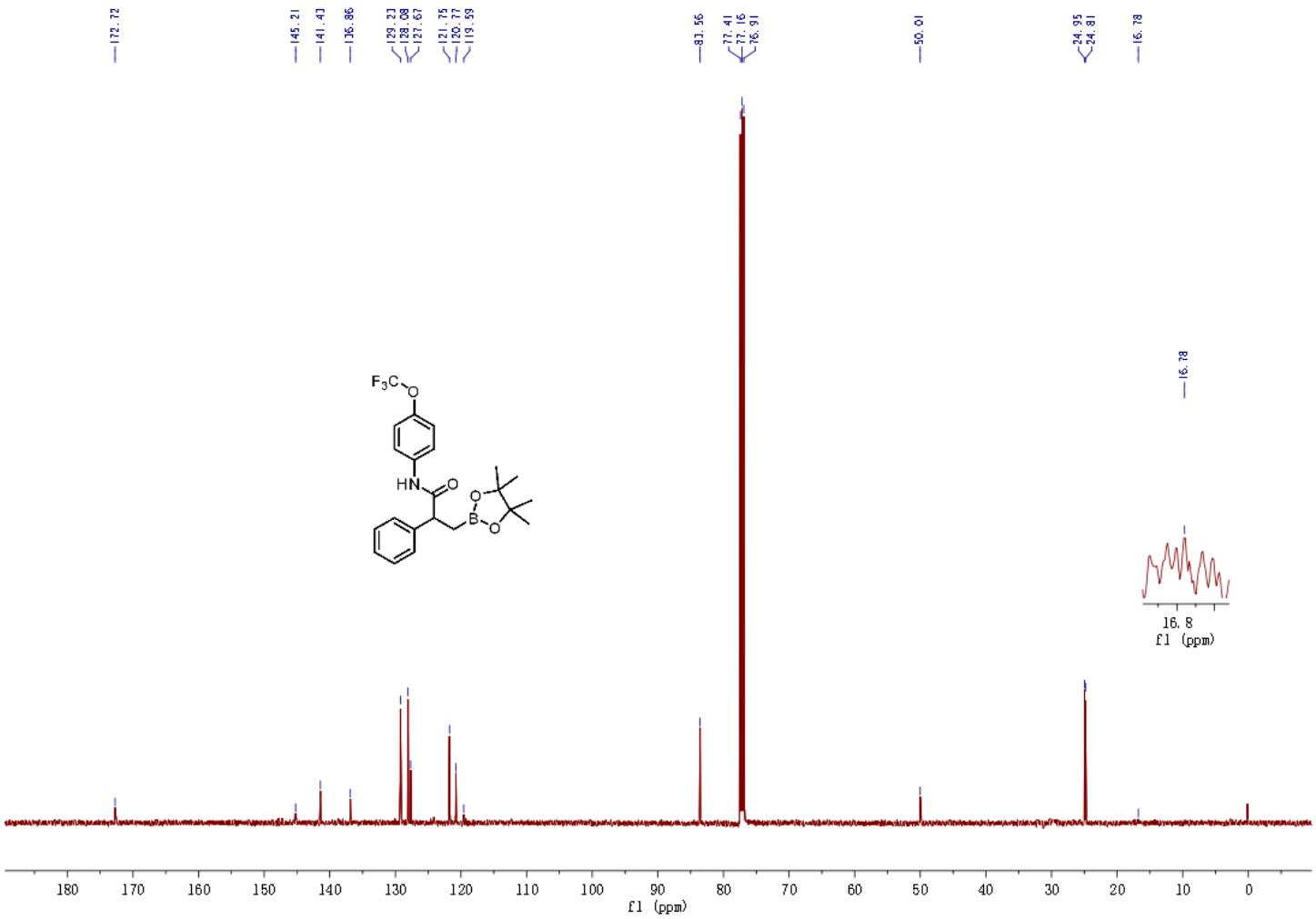
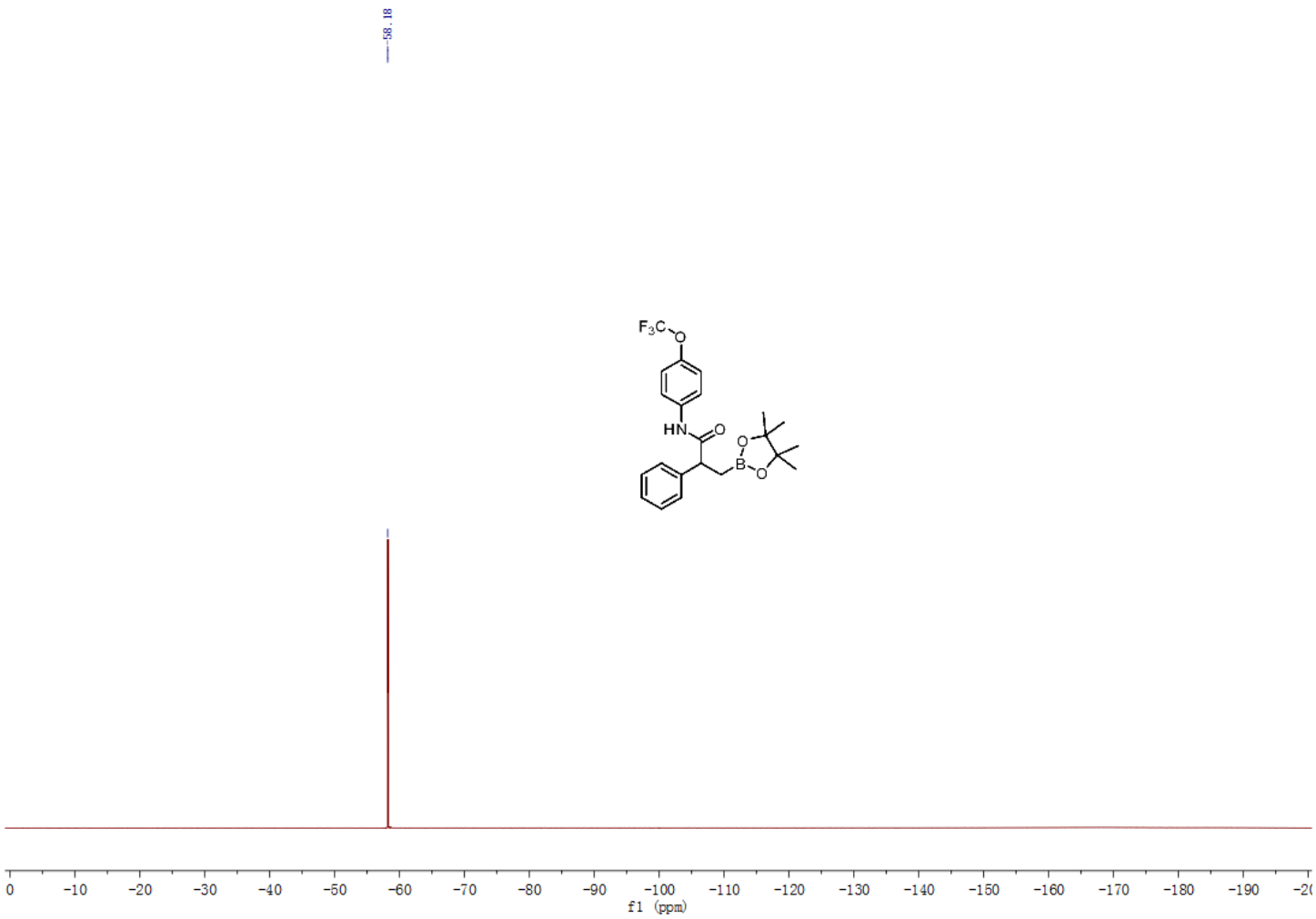
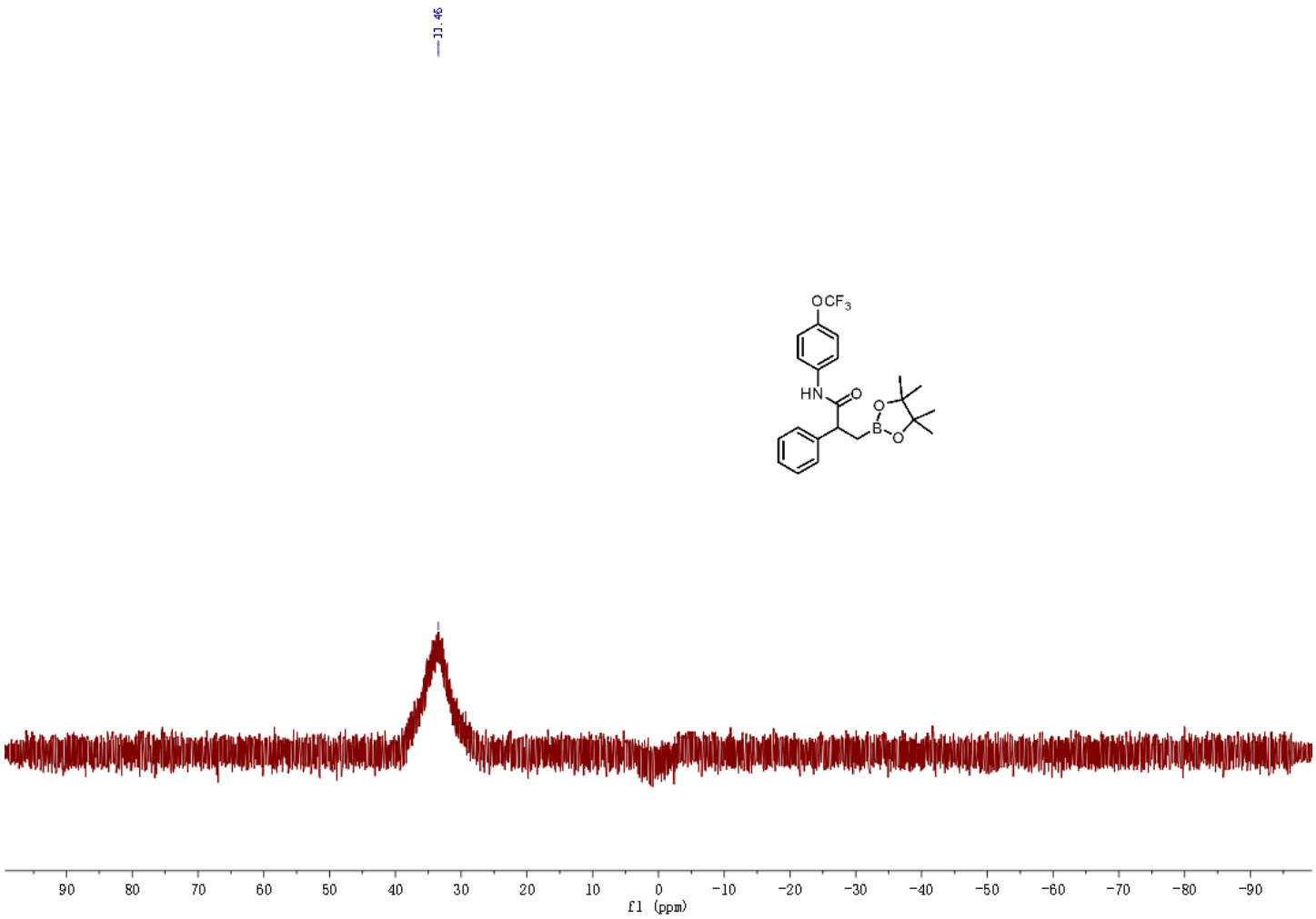
141.77
140.13
135.84
129.05
128.24
128.08
127.41
119.78
83.41
77.41
77.16
76.91
49.96
28.37
24.91
24.78
16.89
15.76
H3C
HN
O
O
B
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

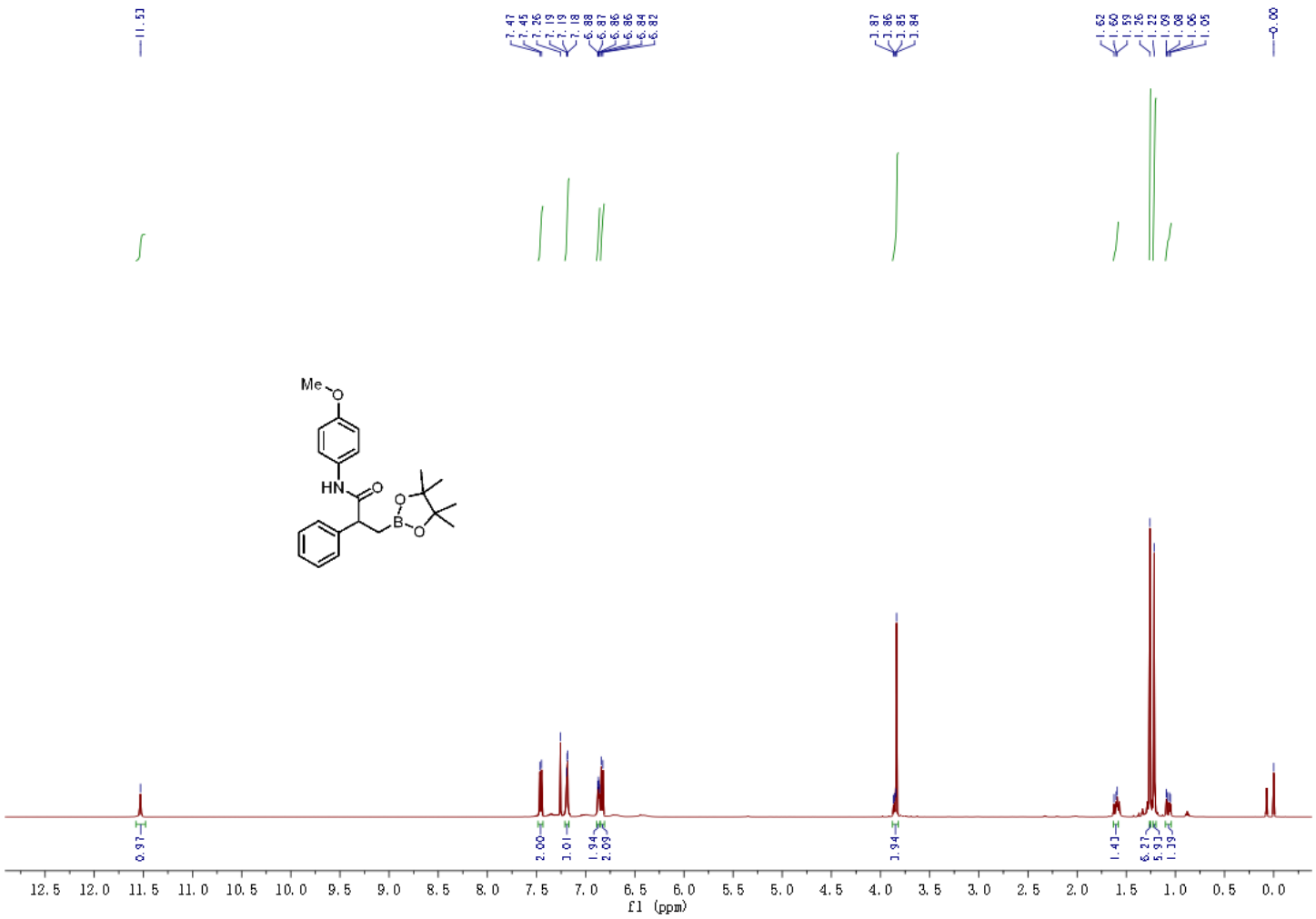

11.55
H3C
HN
O
O
O
B
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.45
7.43
7.36
7.35
7.34
7.30
7.29
7.29
7.28
7.28
7.27
7.26
7.15
7.12
7.10
3.89
3.88
3.87
3.86
1.69
1.67
1.66
1.64
1.33
1.31
1.30
1.28
1.21
1.19
0.00
F3C
O
HN
O
O
B
O
2.03
4.04
1.07
1.00
2.00
1.00
1.43
1.47
6.18
5.68
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
0.0
f1 (ppm)


172.72
145.21
141.43
136.86
129.23
128.08
127.67
121.75
120.77
119.59
83.56
77.41
77.16
76.91
50.01
24.95
24.81
16.78
F3C
O
HN
O
O
O
B
16.78
16.8
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-58.18
F3C
O
HN
O
O
B
O
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


-11.46
OCF3
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


11.53
7.47
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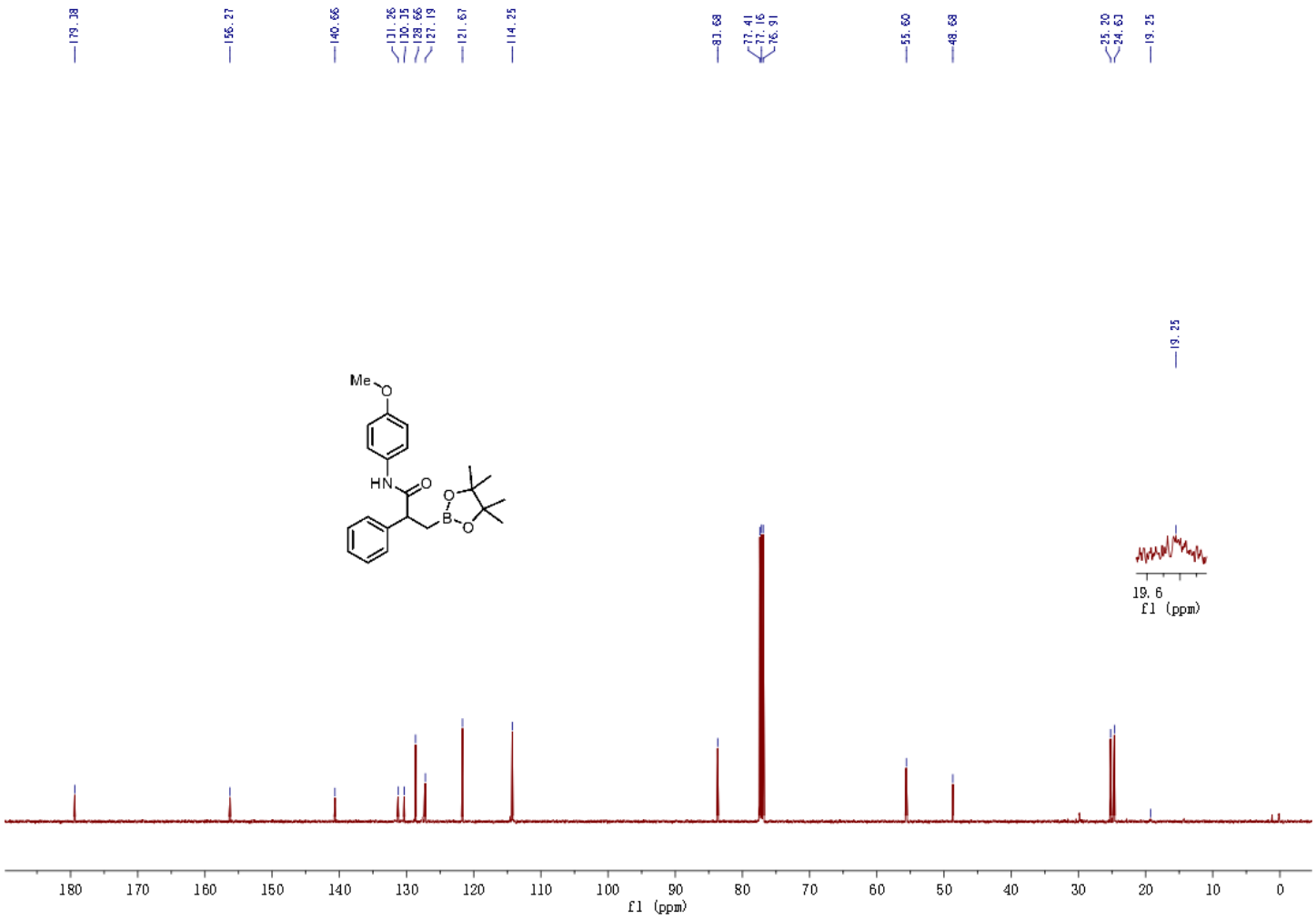
7.19
7.18
6.88
6.87
6.86
6.86
6.84
6.82
3.87
3.86
3.85
3.84
1.62
1.60
1.59
1.26
1.22
1.09
1.08
1.06
1.05
0.00
Me
O
HN
O
O
B
O
0.97
2.00
3.01
1.94
2.09
3.94
1.41
6.27
5.93
1.39
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


179.38
156.27
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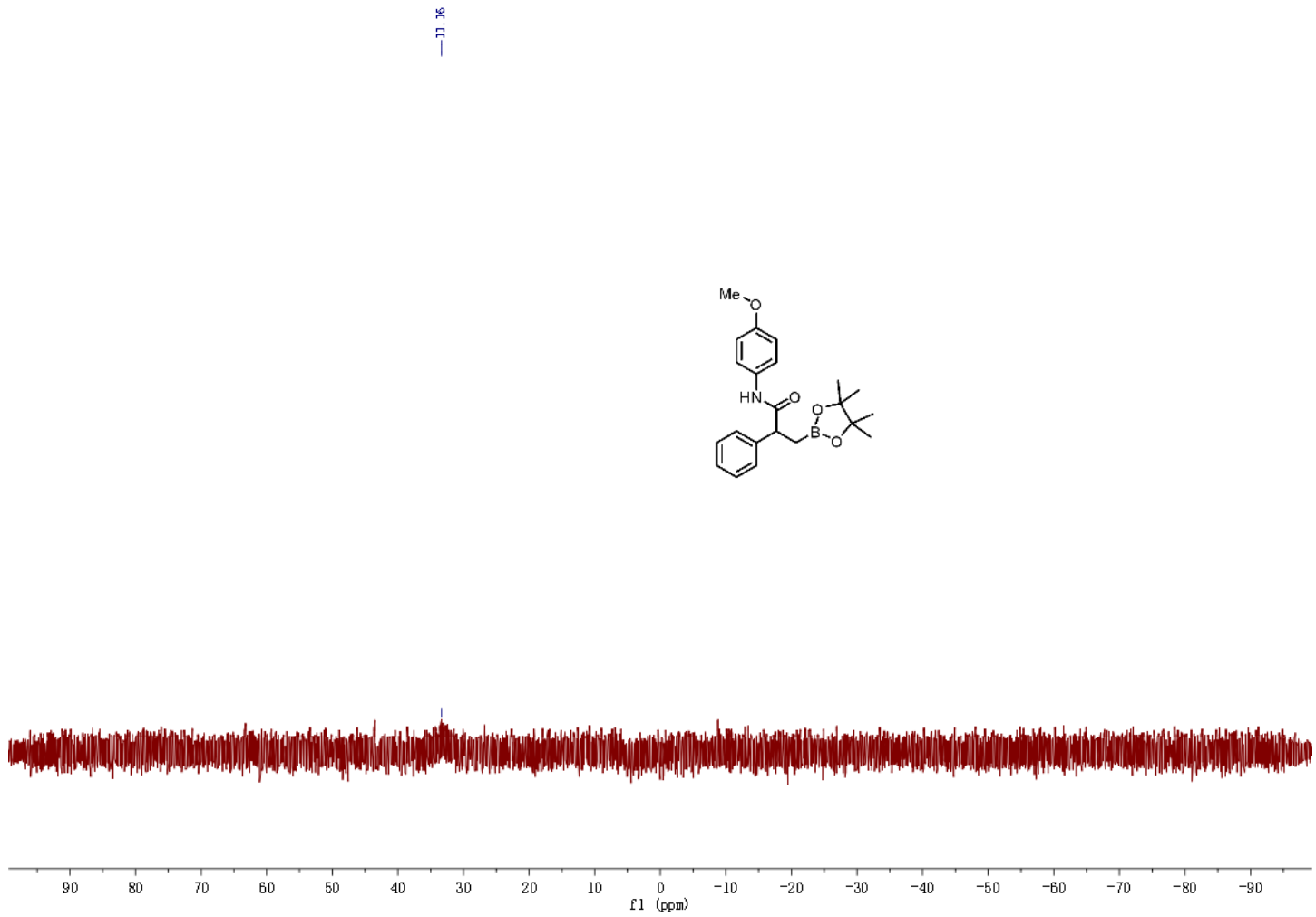
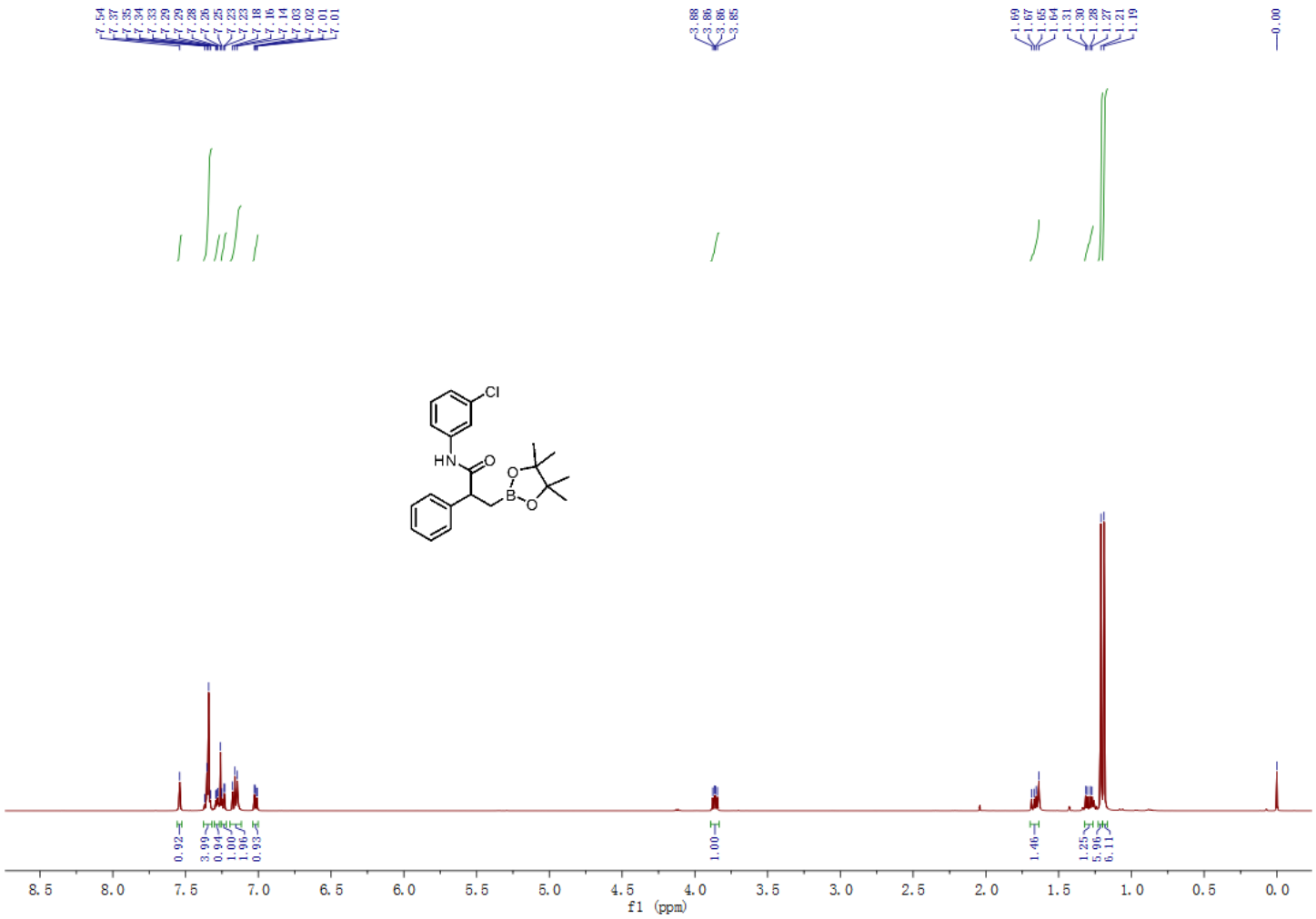
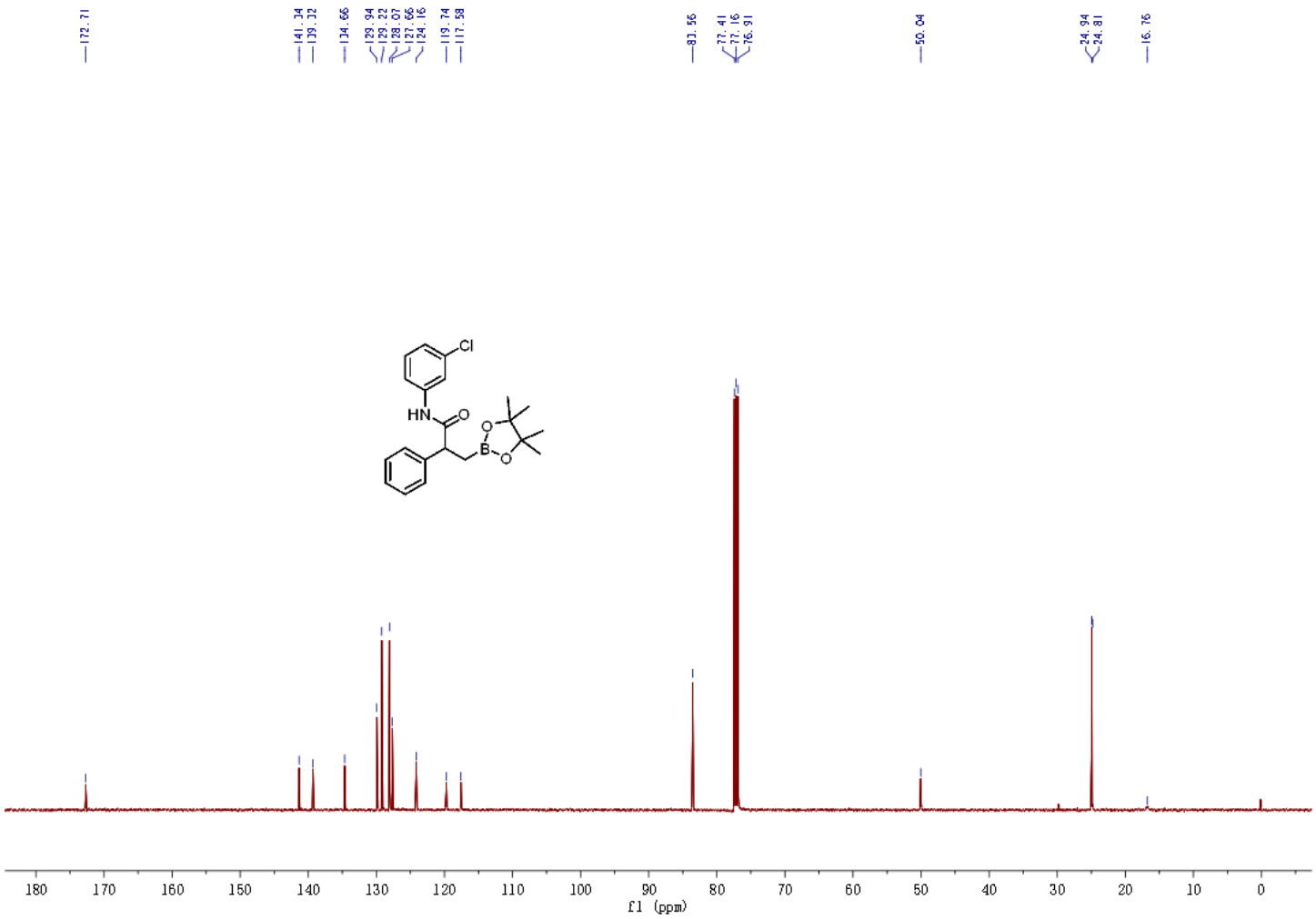
131.26
130.35
128.66
127.19
121.67
114.25
83.68
77.41
77.16
76.91
55.60
48.68
25.20
24.63
19.25
Me
O
HN
O
O
B
O
19.25
19.6
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.36
Me
O
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.54
7.37
7.35
7.34
7.33
7.29
7.29
7.28
7.26
7.25
7.23
7.23
7.18
7.16
7.14
7.03
7.02
7.01
7.01
3.88
3.86
3.86
3.85
1.69
1.67
1.65
1.64
1.31
1.30
1.28
1.27
1.21
1.19
0.00
Cl
HN
O
O
O
B
0.92
3.99
0.94
1.00
1.96
0.93
1.00
1.46
1.25
5.96
6.11
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
0.0
f1 (ppm)


172.71
141.34
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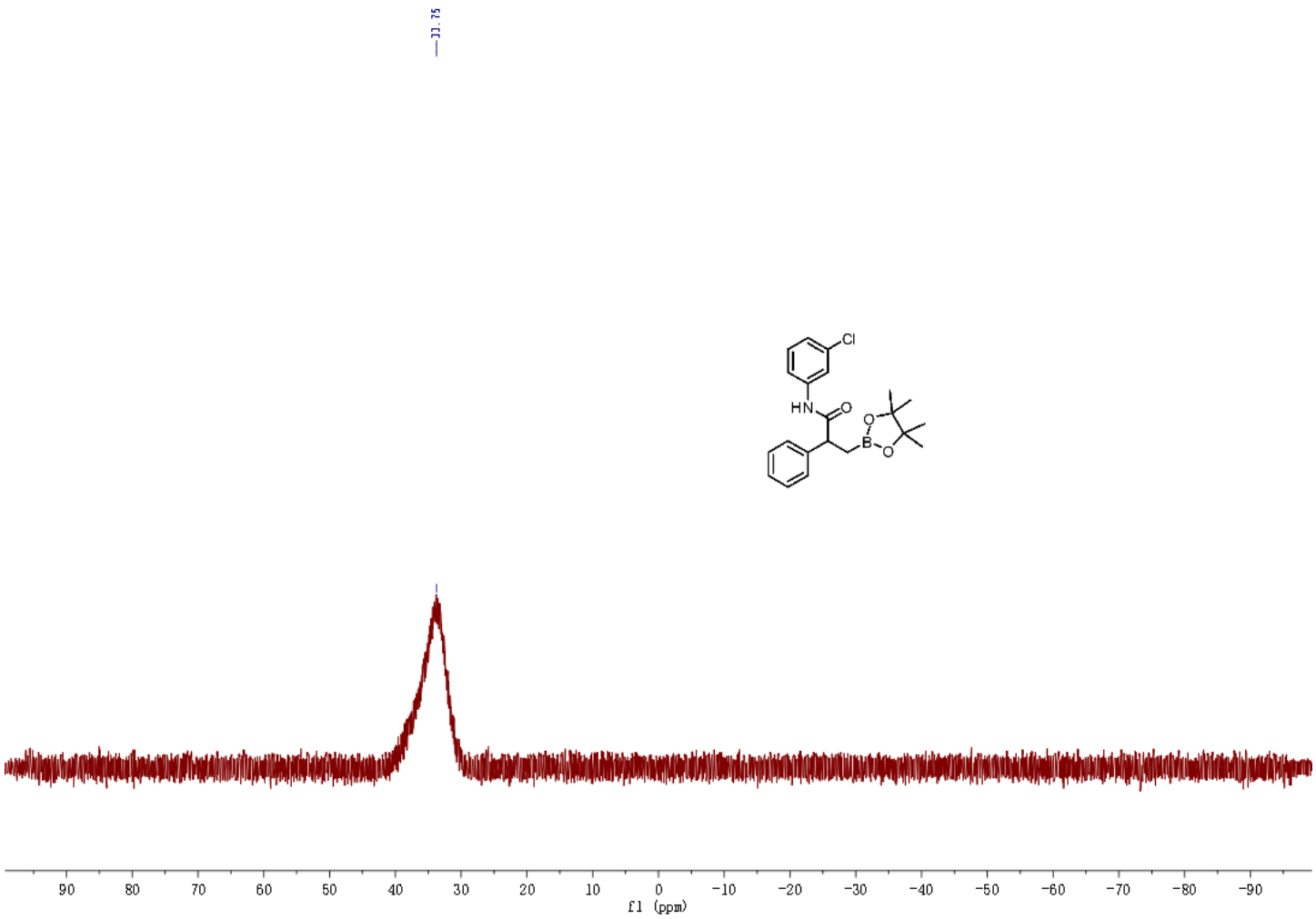
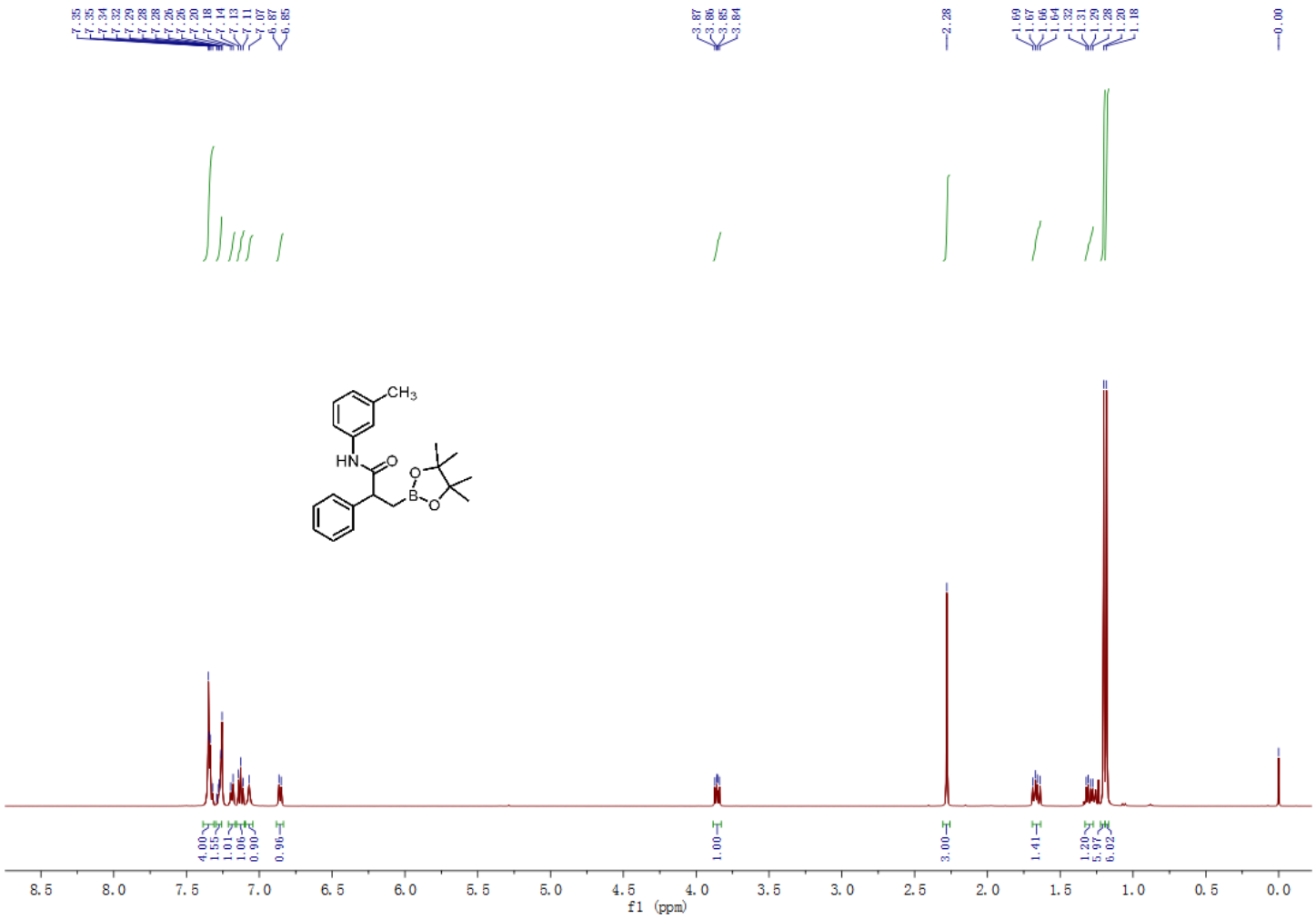
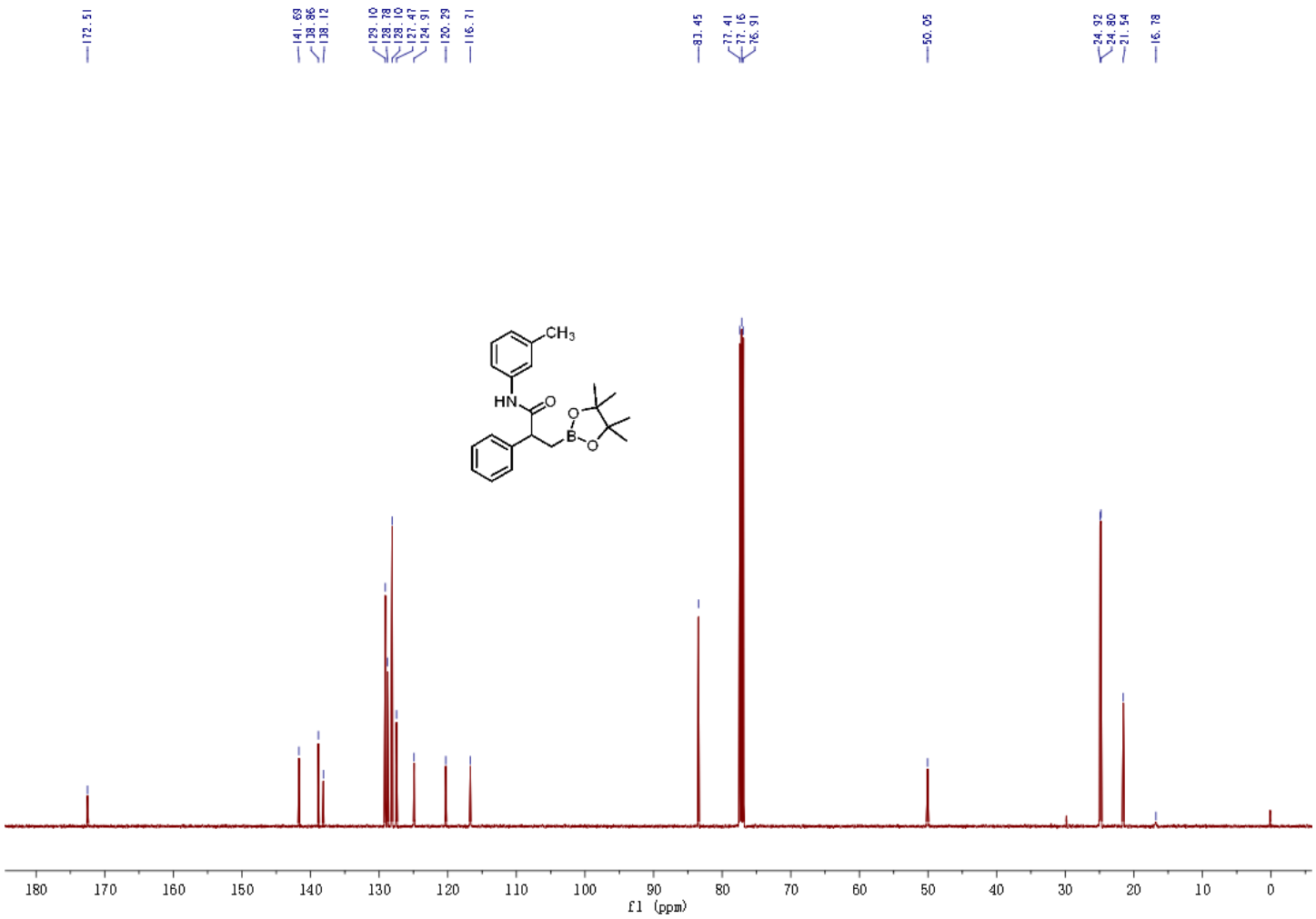
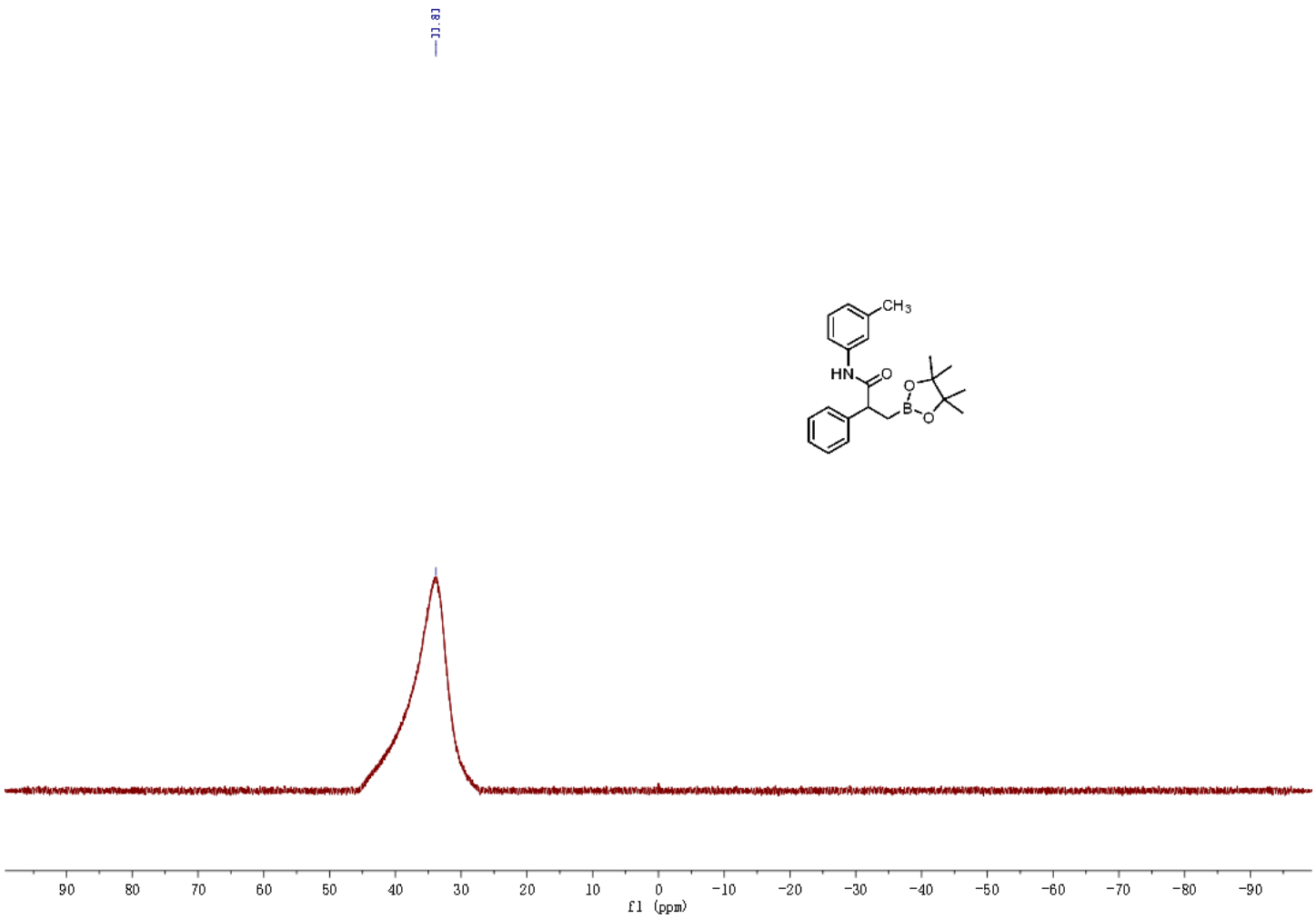
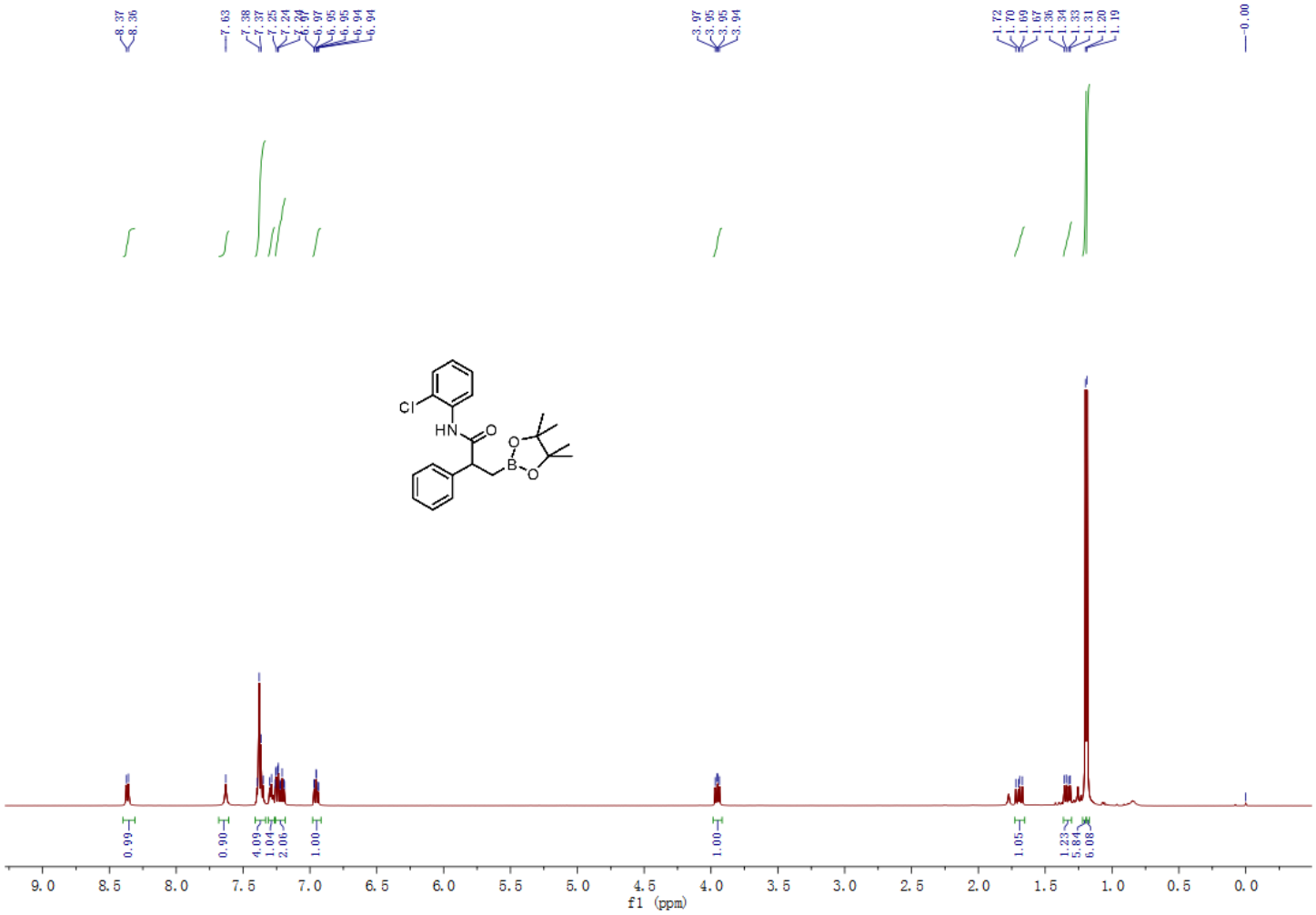
134.66
129.94
129.22
128.07
127.66
124.16
119.74
117.58
83.56
77.41
77.16
76.91
50.04
24.94
24.81
16.76
Cl
HN
O
O
O
B
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

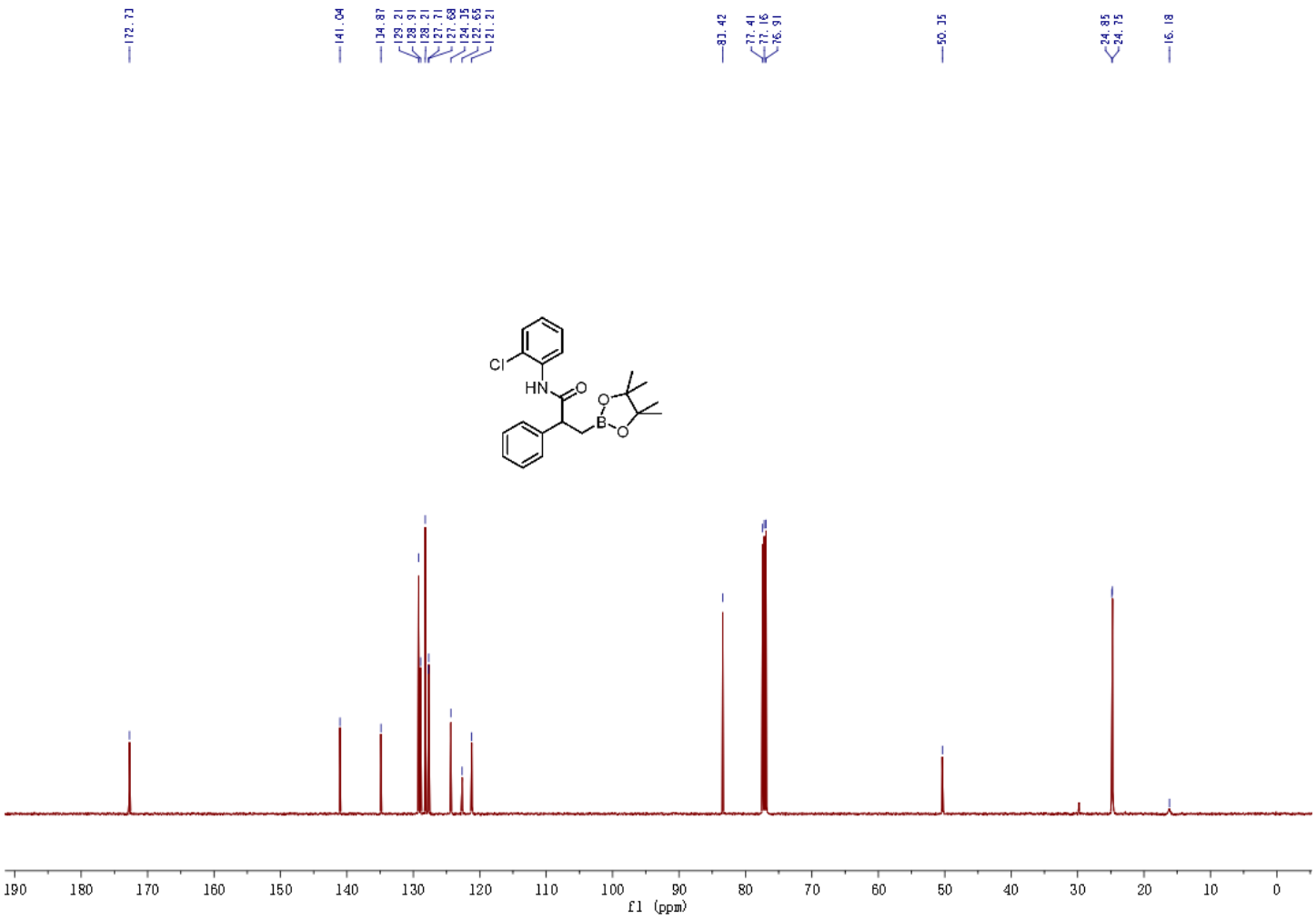

33.75
Cl
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

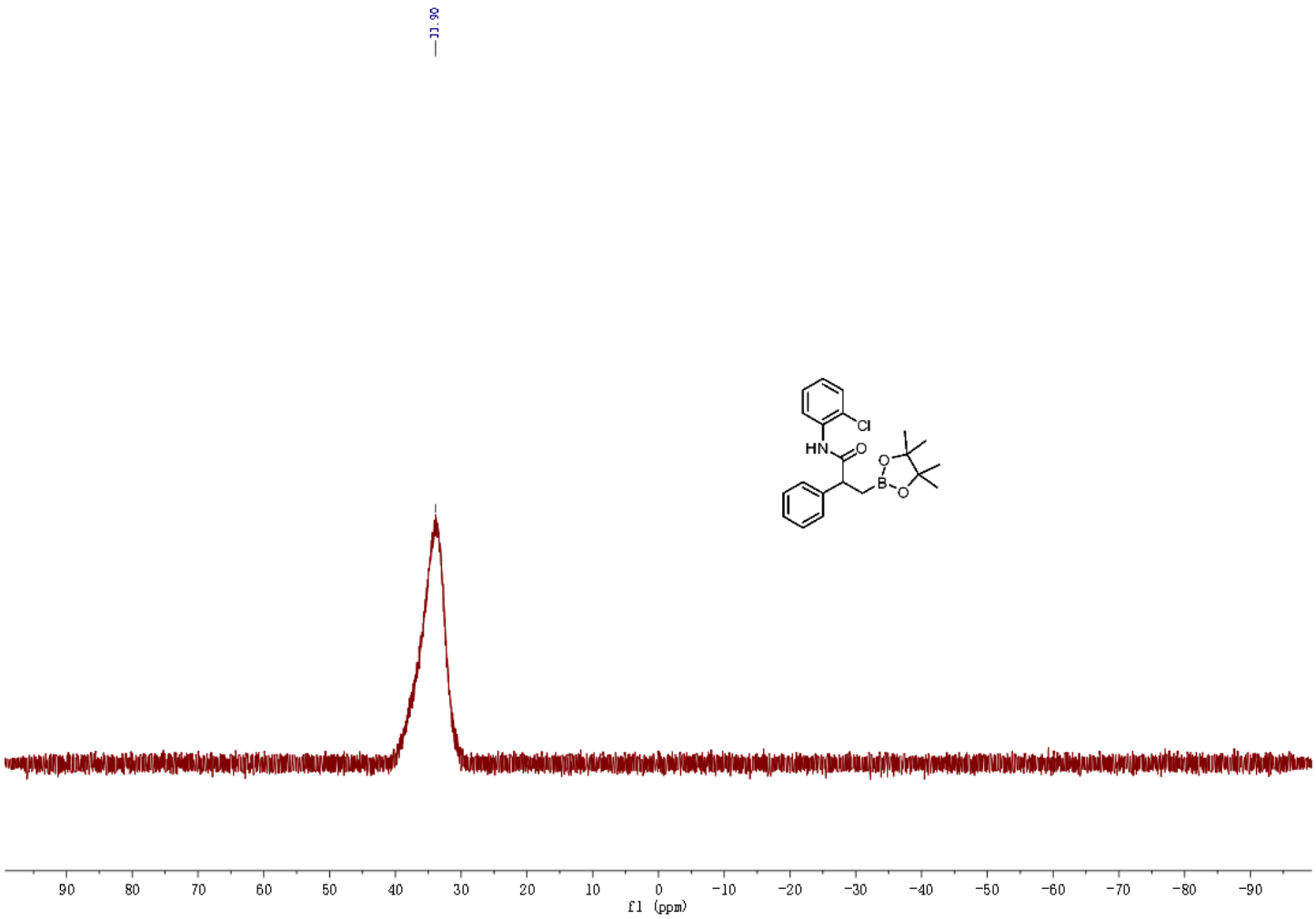

7.35
7.35
7.34
7.32
7.29
7.28
7.28
7.26
7.26
7.20
7.18
7.14
7.13
7.11
7.07
6.87
6.85
3.87
3.86
3.85
3.84
2.28
1.69
1.67
1.66
1.64
1.32
1.31
1.29
1.28
1.20
1.18
0.00
CH3
HN
O
O
O
B
4.00
1.55
1.01
1.06
0.90
0.96
1.00
3.00
1.41
1.20
5.97
6.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

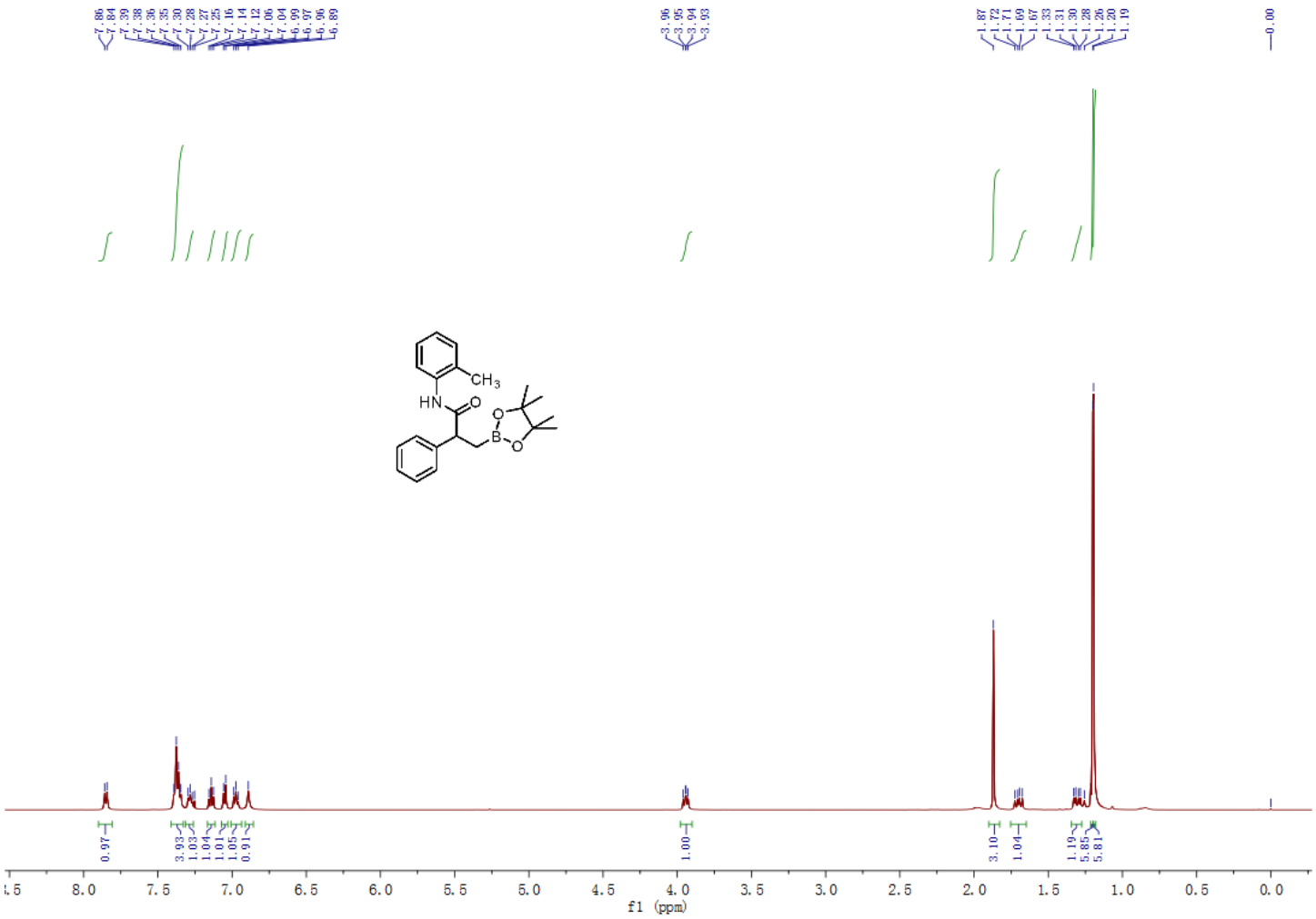

172.51
141.69
138.86
138.12
129.10
128.78
128.10
127.47
124.91
120.29
116.71
83.45
77.41
77.16
76.91
50.05
24.92
24.80
21.54
16.78
CH3
HN
O
O
B
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

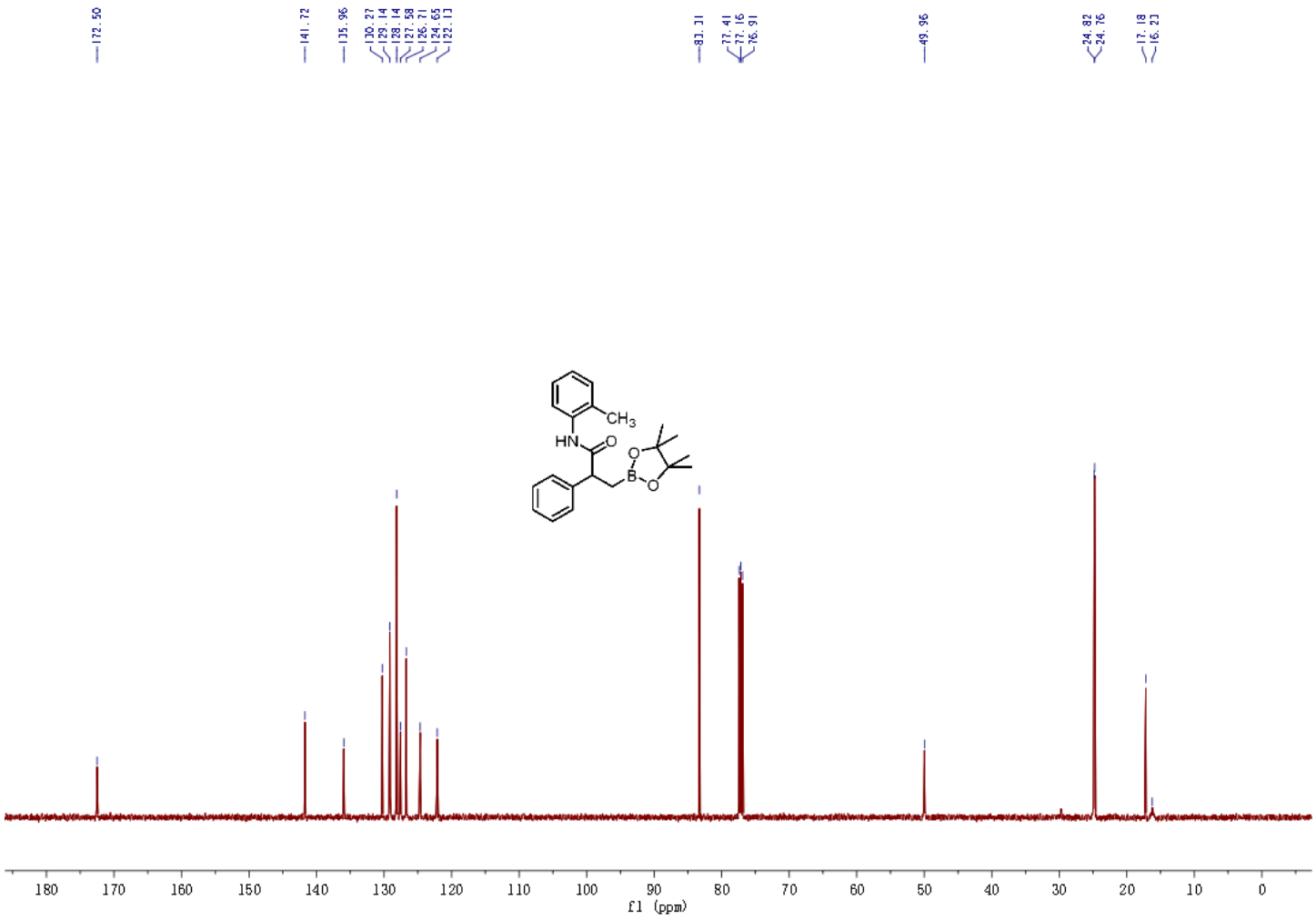

33.83
CH3
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

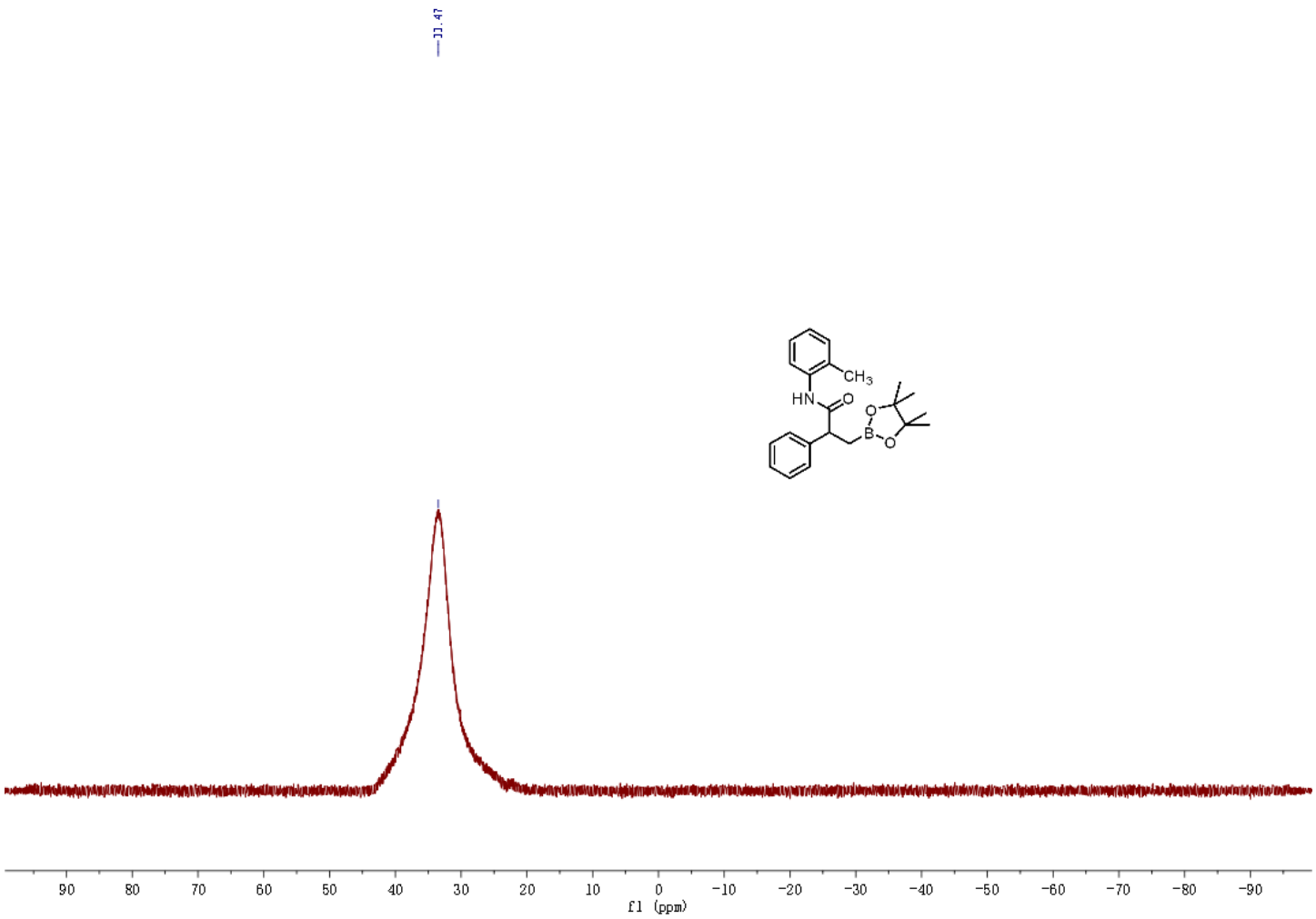

8.37
8.36
7.63
7.38
7.37
7.25
7.24
6.97
6.95
6.95
6.94
6.94
3.97
3.95
3.95
3.94
1.72
1.70
1.69
1.67
1.36
1.34
1.33
1.31
1.20
1.19
0.00
Cl
HN
O
O
O
B
0.99
0.90
4.09
1.04
2.06
1.00
1.00
1.05
1.23
5.84
6.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

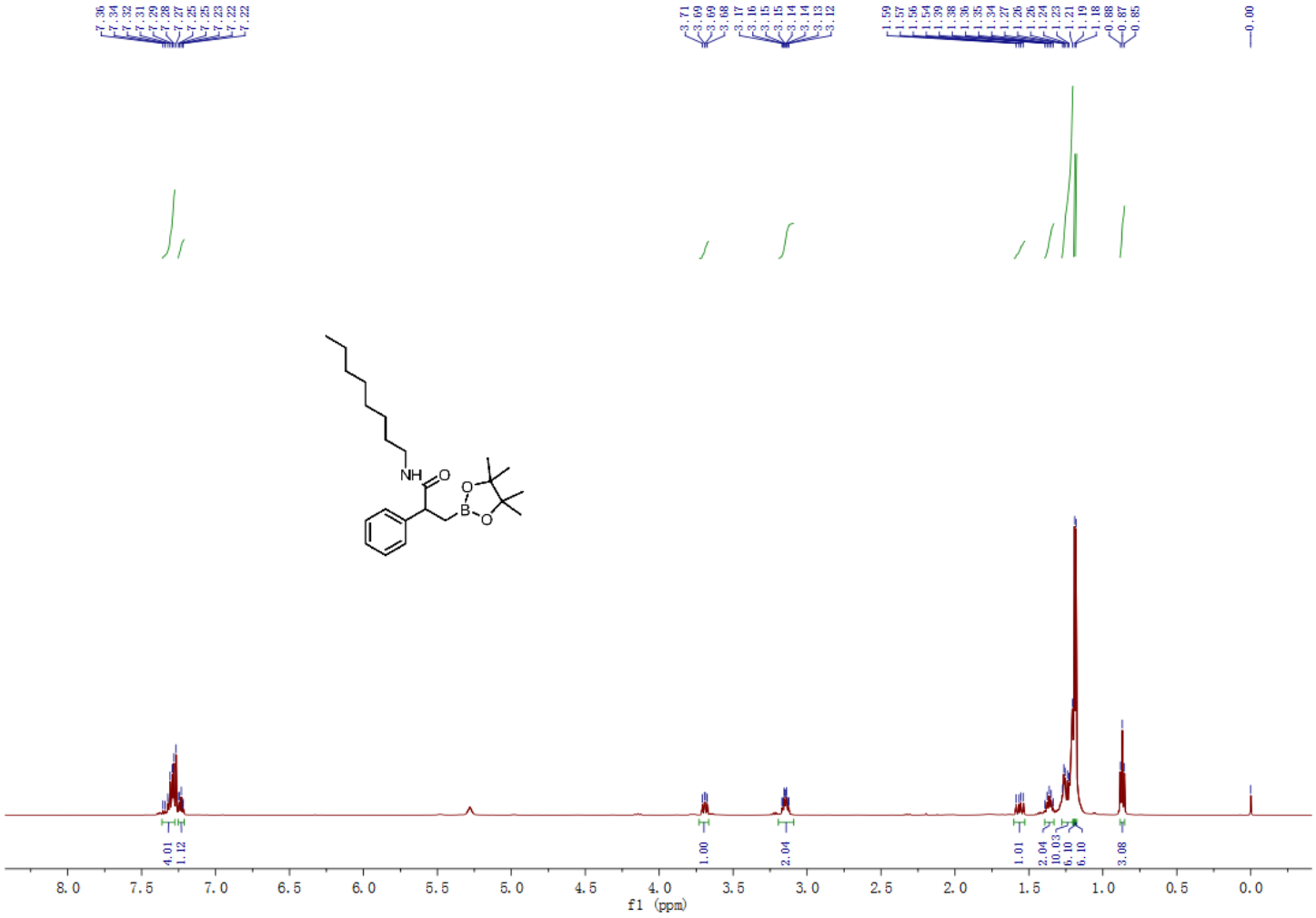

172.73
141.04
134.87
129.21
128.91
128.21
127.71
127.68
124.35
122.65
121.21
83.42
77.41
77.16
76.91
50.35
24.85
24.75
16.18
Cl
HN
O
O
O
B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

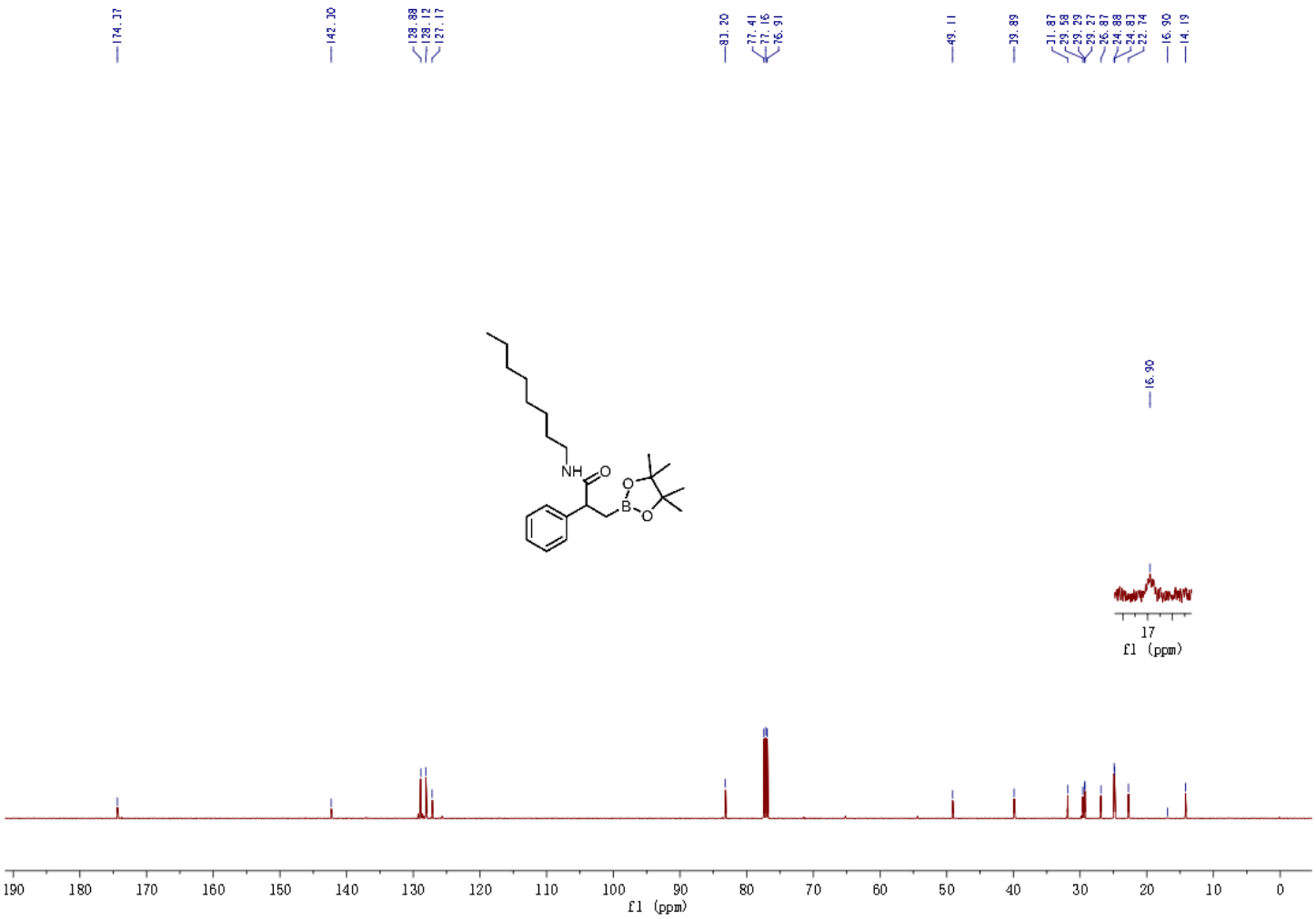

11.99
Cl
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

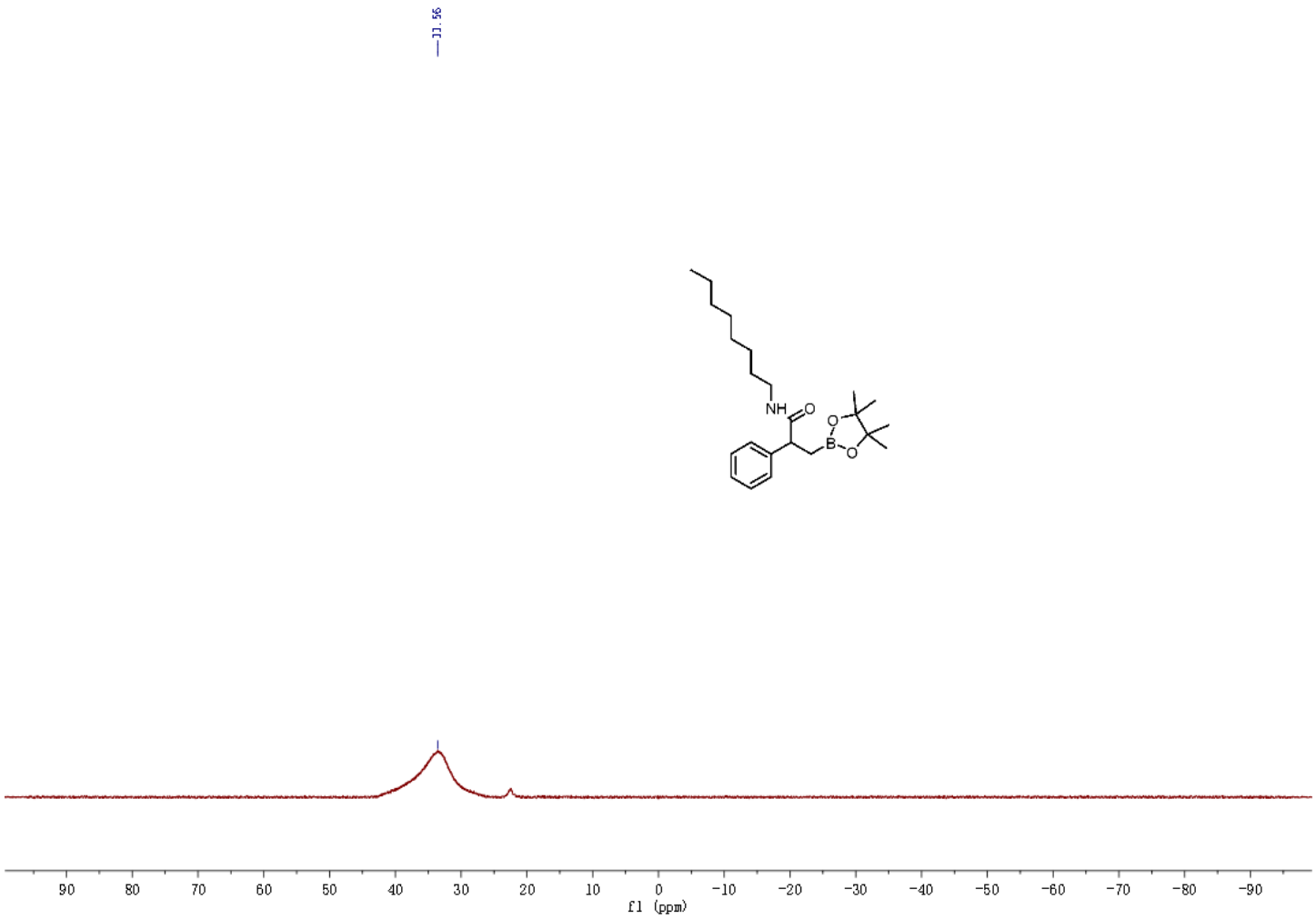

7.86
7.84
7.39
7.38
7.36
7.35
7.30
7.28
7.27
7.25
7.16
7.14
7.12
7.06
7.04
6.99
6.97
6.96
6.89
3.96
3.95
3.94
3.93
1.87
1.72
1.71
1.69
1.67
1.33
1.31
1.30
1.28
1.26
1.20
1.19
0.00
HN
O
O
B
O
CH3
0.97
3.93
1.03
1.04
1.01
1.05
0.91
1.00
3.10
1.04
1.19
5.85
5.81
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

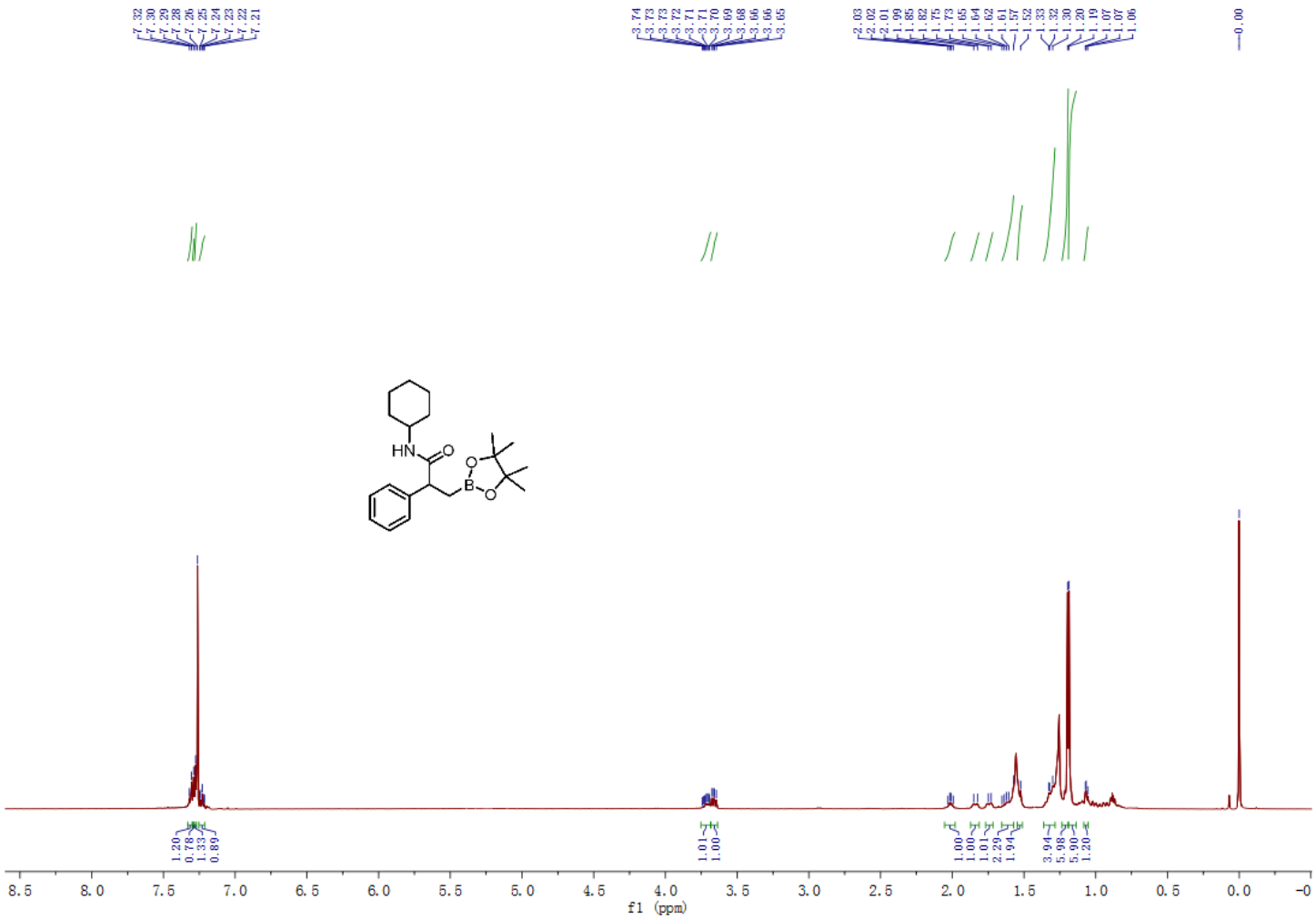

172.50
141.72
135.96
130.27
129.14
128.14
127.58
126.71
124.65
122.13
83.31
77.41
77.16
76.91
49.96
24.82
24.76
17.18
16.23
CH3
HN
O
O
O
B
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

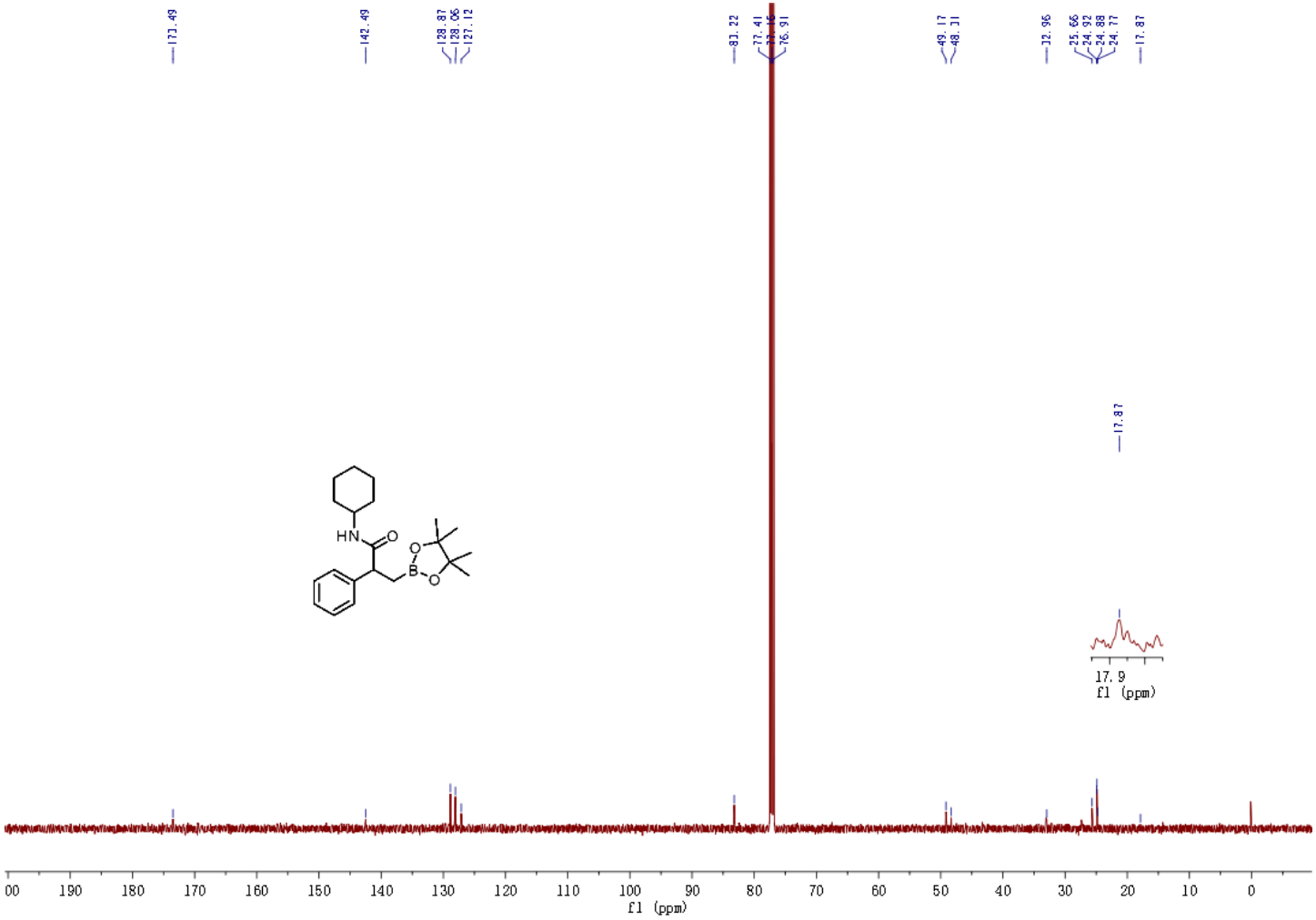

33.47
CH3
HN
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

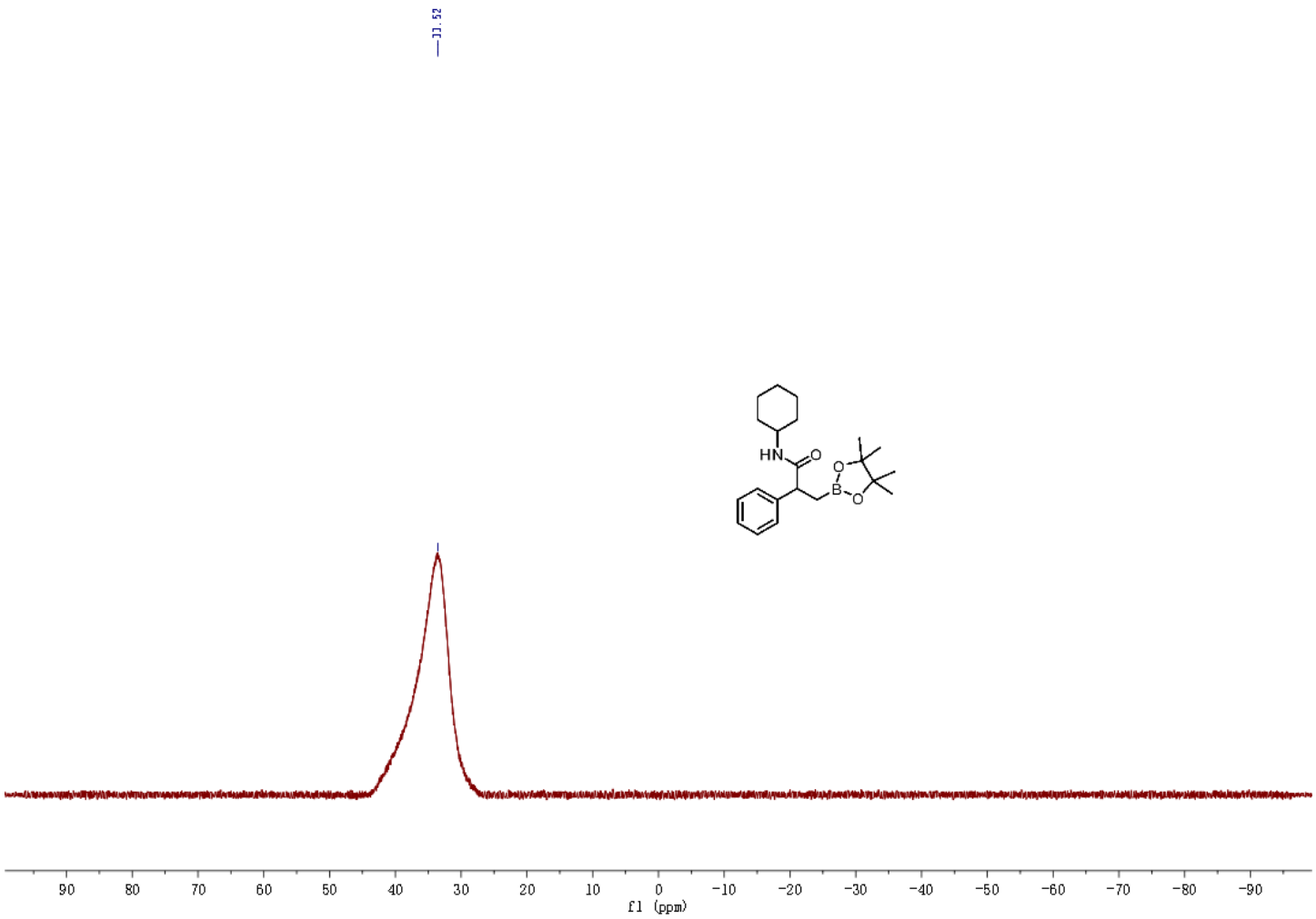

7.36
7.34
7.32
7.31
7.29
7.28
7.27
7.25
7.23
7.22
7.22
3.71
3.69
3.69
3.68
3.17
3.16
3.15
3.15
3.14
3.14
3.13
3.12
1.59
1.57
1.56
1.54
1.39
1.38
1.36
1.35
1.34
1.27
1.26
1.26
1.24
1.23
1.21
1.19
1.18
0.88
0.87
0.85
0.00
NH
O
O
B
O
4.01
1.12
1.00
2.04
1.01
2.04
10.03
6.10
6.10
3.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

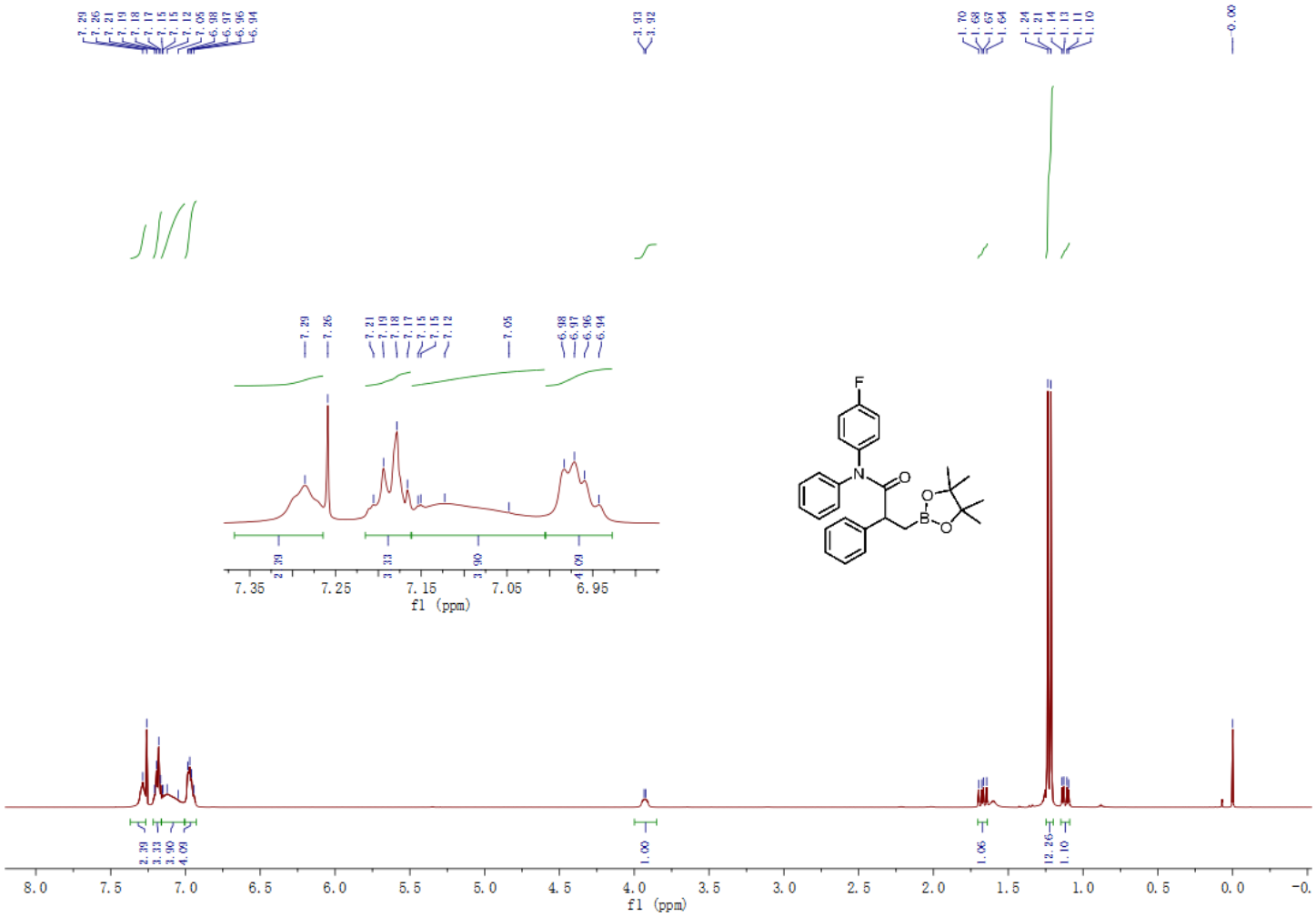

174.37
142.30
138.88
138.12
137.17
83.20
77.41
77.16
76.91
49.11
39.89
31.87
29.58
29.29
29.27
26.87
24.88
24.83
22.74
16.90
14.19
NH
O
O
B
O
16.90
17
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

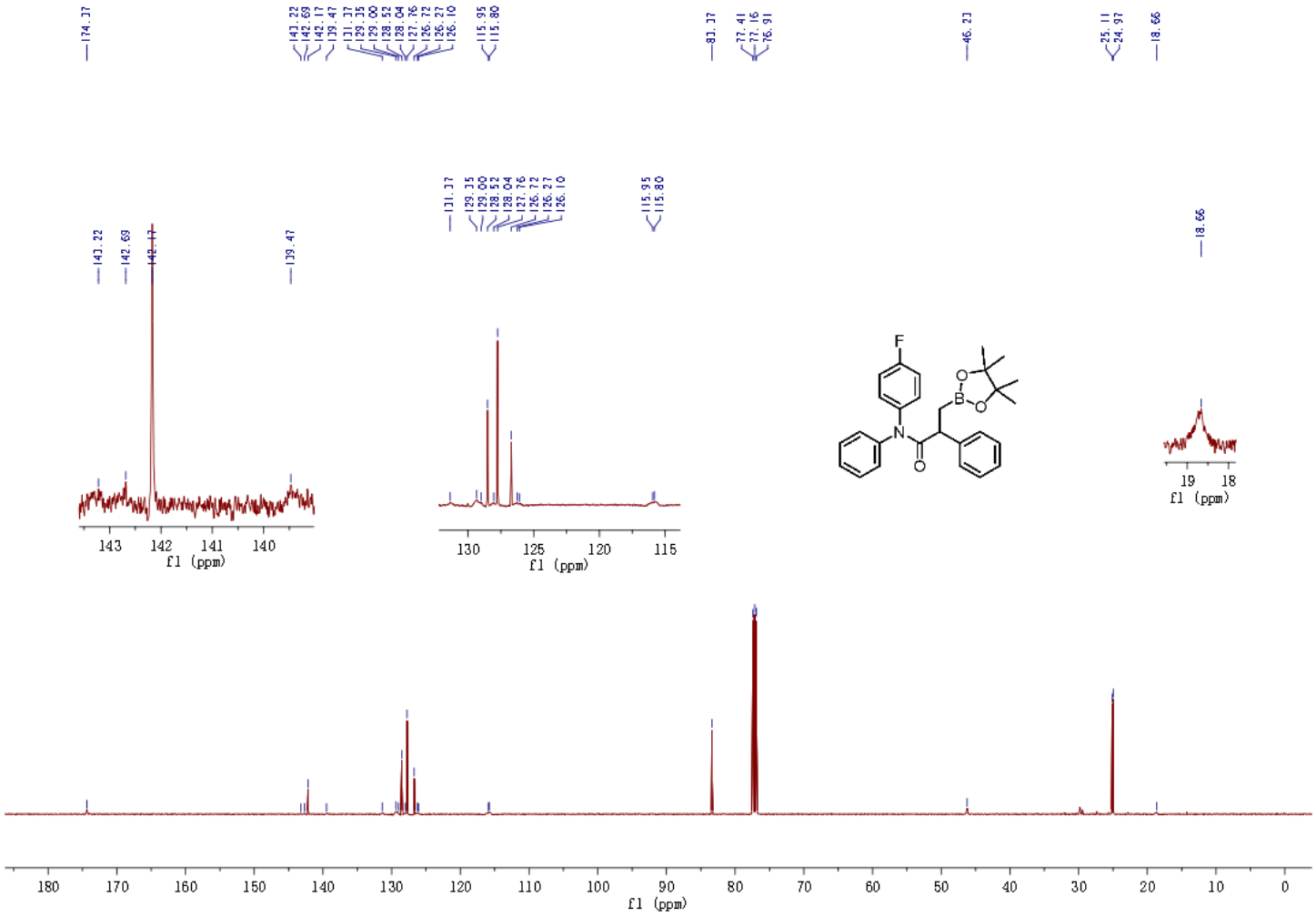

11.56
NH
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

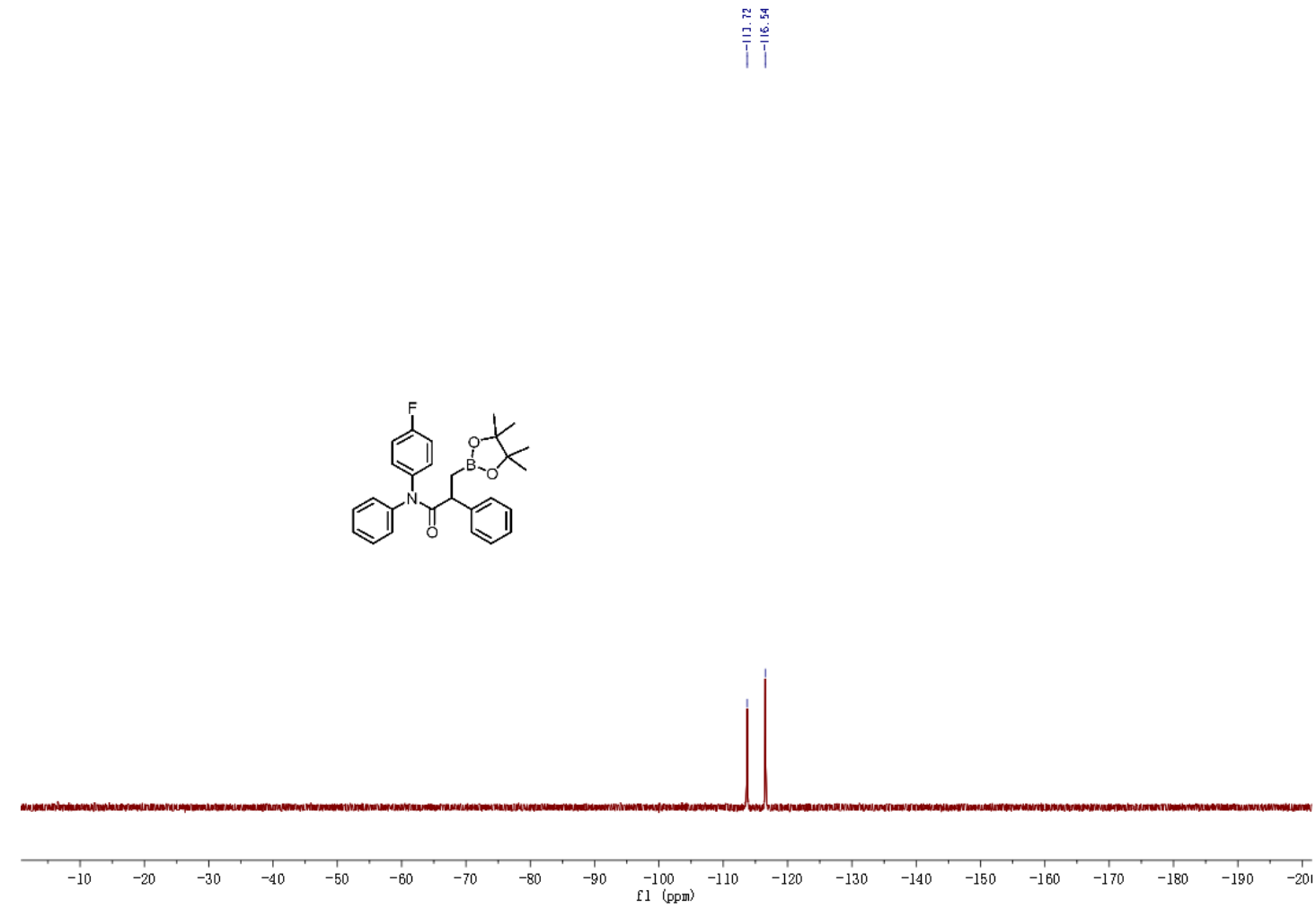

7.32
7.30
7.29
7.28
7.26
7.25
7.24
7.23
7.22
7.21
3.74
3.73
3.73
3.72
3.71
3.71
3.70
3.69
3.68
3.66
3.66
3.65
2.03
2.02
2.01
1.99
1.85
1.82
1.75
1.73
1.65
1.64
1.62
1.61
1.57
1.52
1.33
1.32
1.30
1.20
1.19
1.07
1.07
1.06
0.00
HN
O
O
O
B
1.20
0.78
1.33
0.89
1.01
1.00
1.00
1.00
1.01
2.29
1.94
3.94
5.98
5.90
1.20
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
0.0
-0
f1 (ppm)

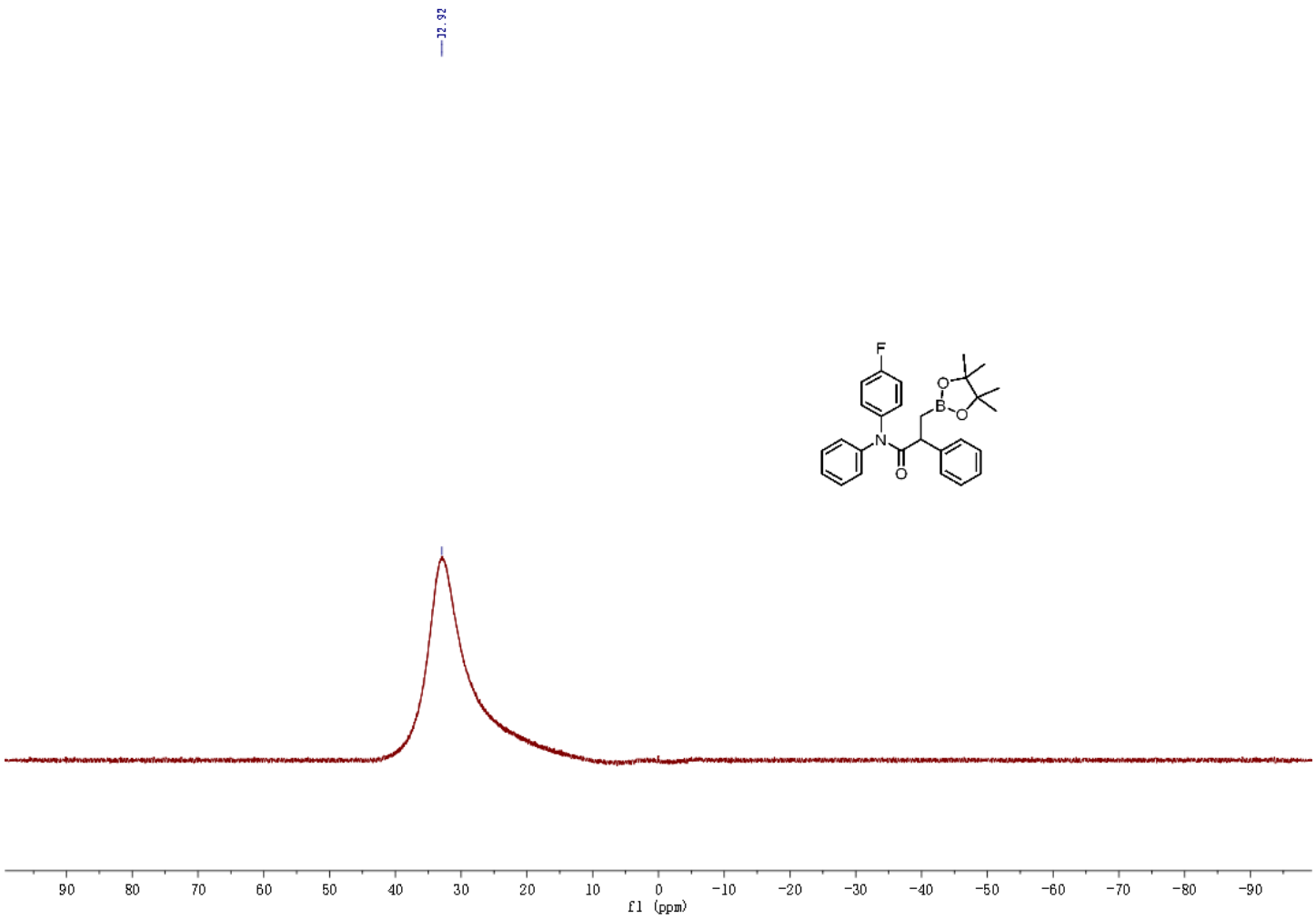

172.49
142.49
128.87
128.06
127.12
83.22
77.41
76.91
49.17
48.31
32.96
25.66
24.92
24.88
24.77
17.87
HN
O
O
B
O
17.87
17.9
f1 (ppm)
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

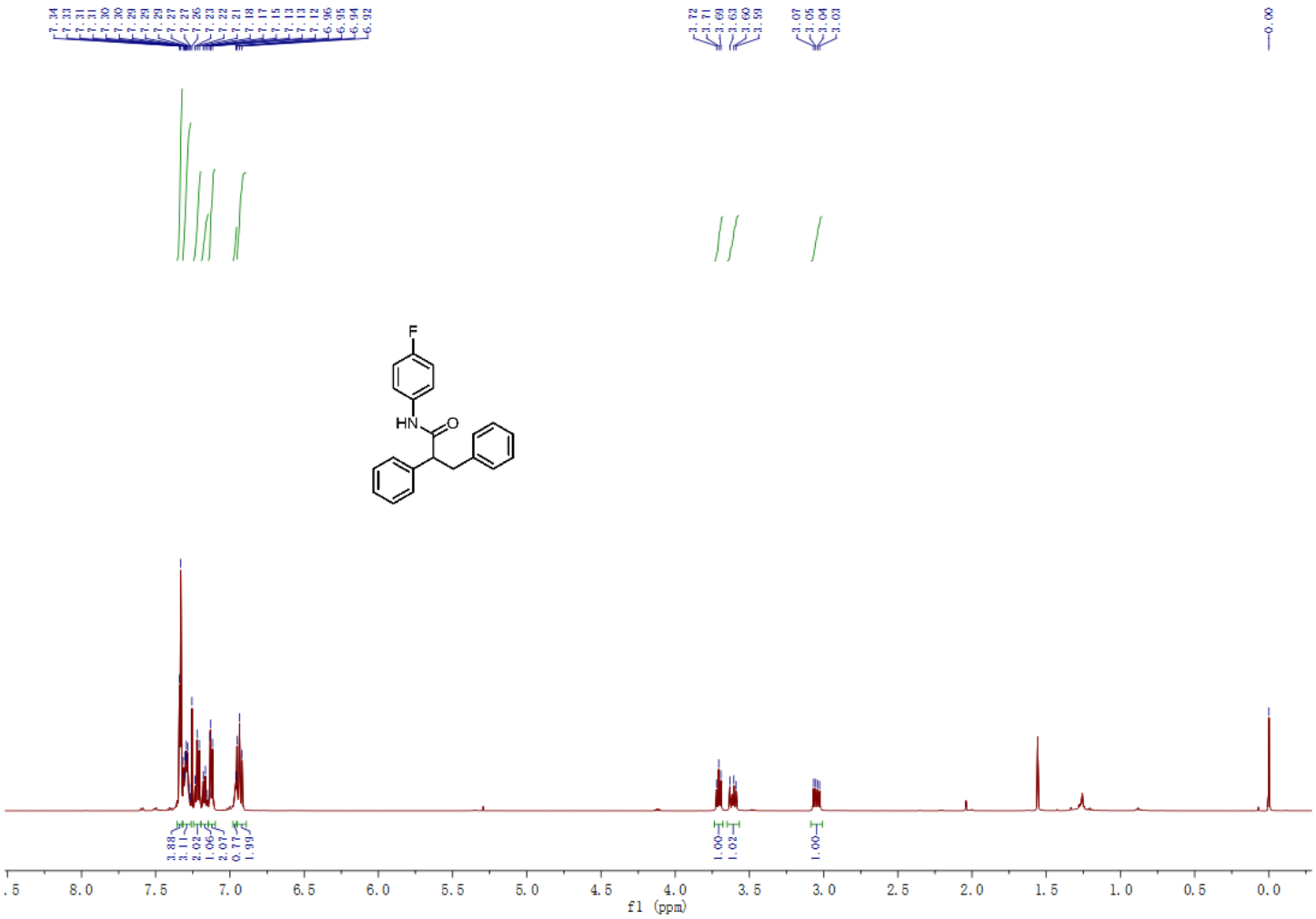

33.52
HN
O
O
O
B
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

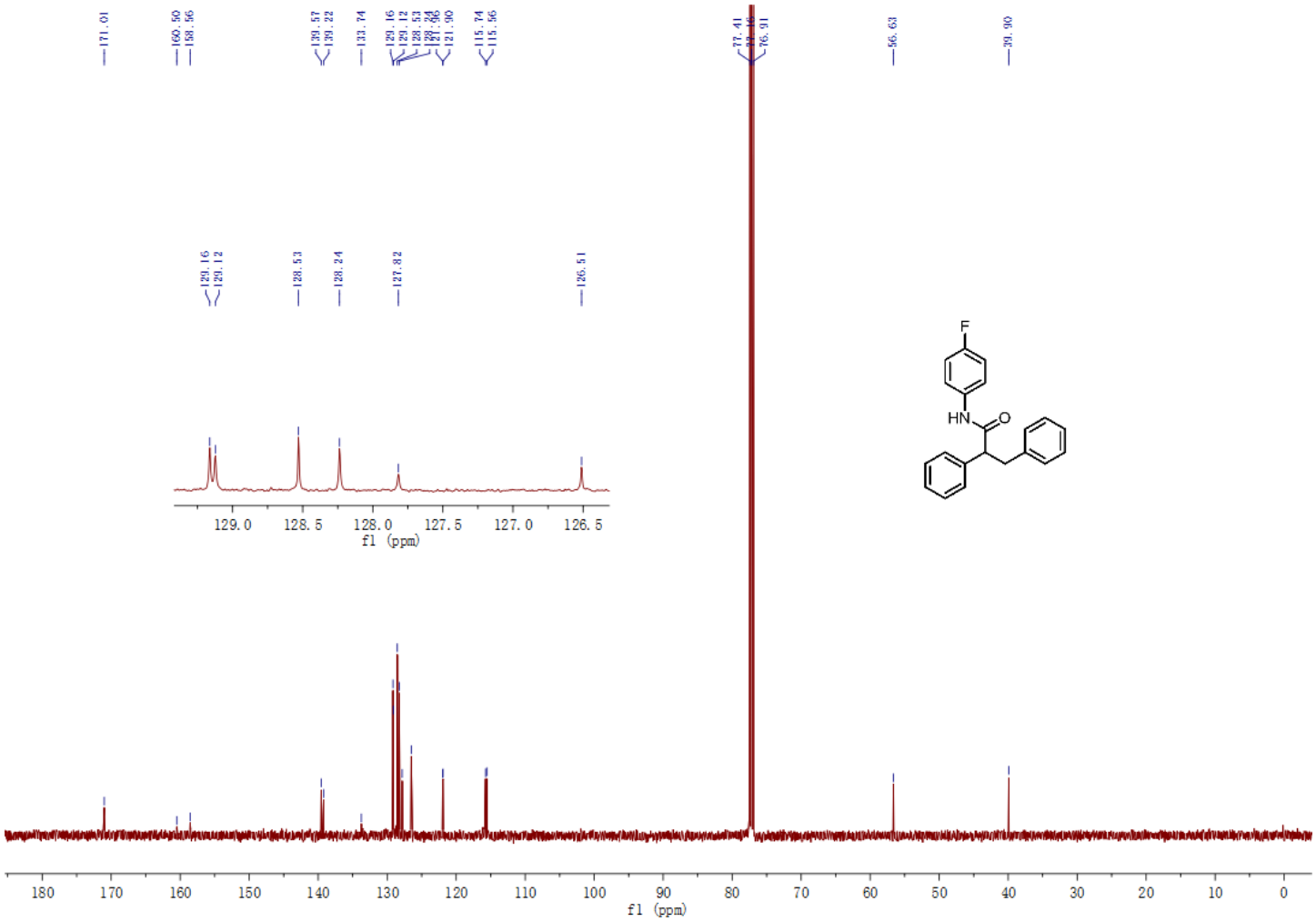

7.29
7.26
7.21
7.19
7.18
7.17
7.15
7.12
7.05
6.98
6.97
6.96
6.94
3.93
3.92
1.70
1.68
1.67
1.64
1.24
1.21
1.14
1.13
1.11
1.10
0.00
F
N
O
O
O
B
O
2.39
3.33
3.90
4.09
1.00
1.06
12.26
1.10
f1 (ppm)

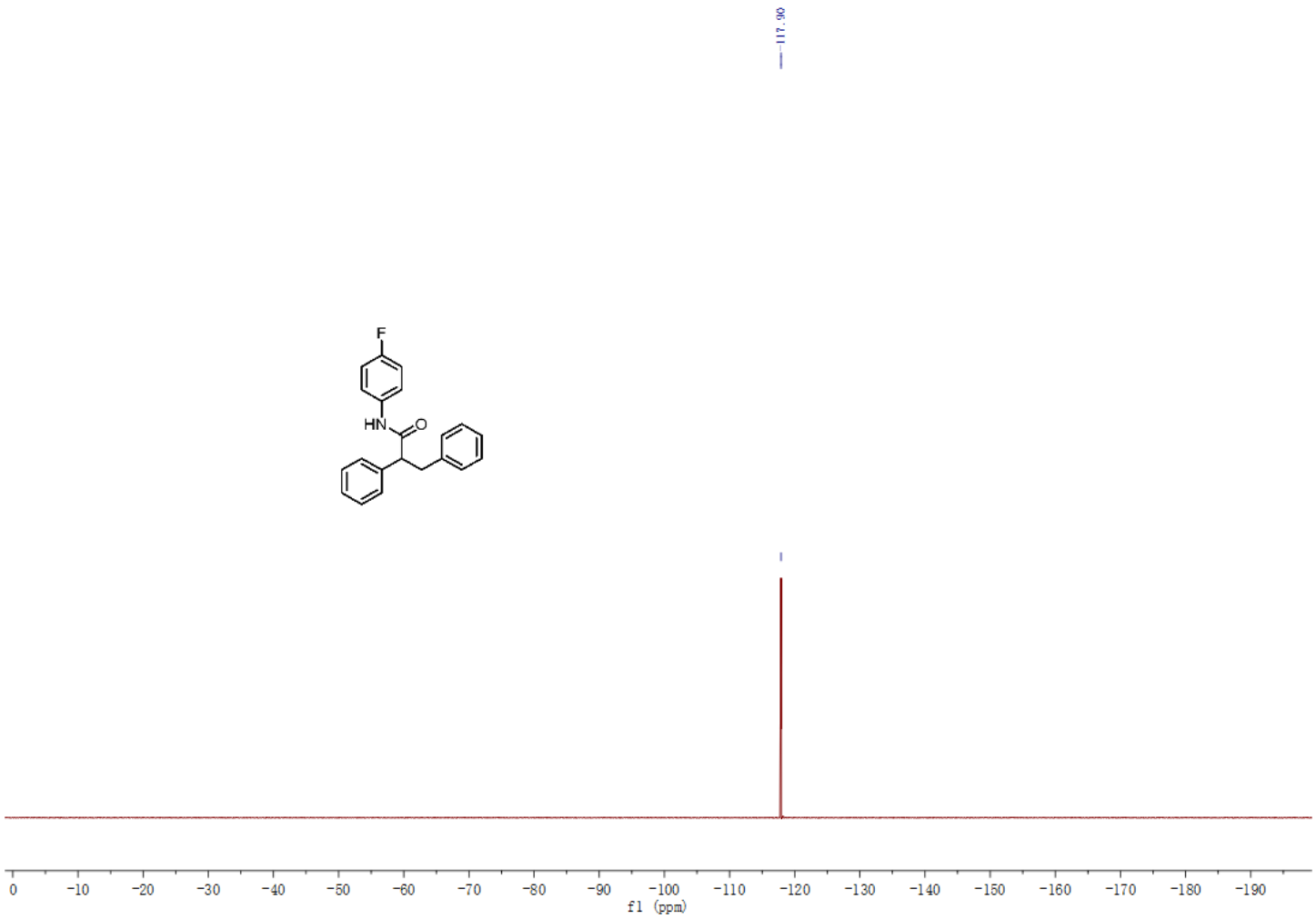

174.37
143.22
142.69
142.17
139.47
131.37
129.35
129.00
128.52
128.04
127.76
126.72
126.27
126.10
115.95
115.80
83.37
77.41
77.16
76.91
46.23
25.11
24.97
18.66
F
O
B
O
N
O
143
142
141
140
f1 (ppm)
130
125
120
115
f1 (ppm)
19
18
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

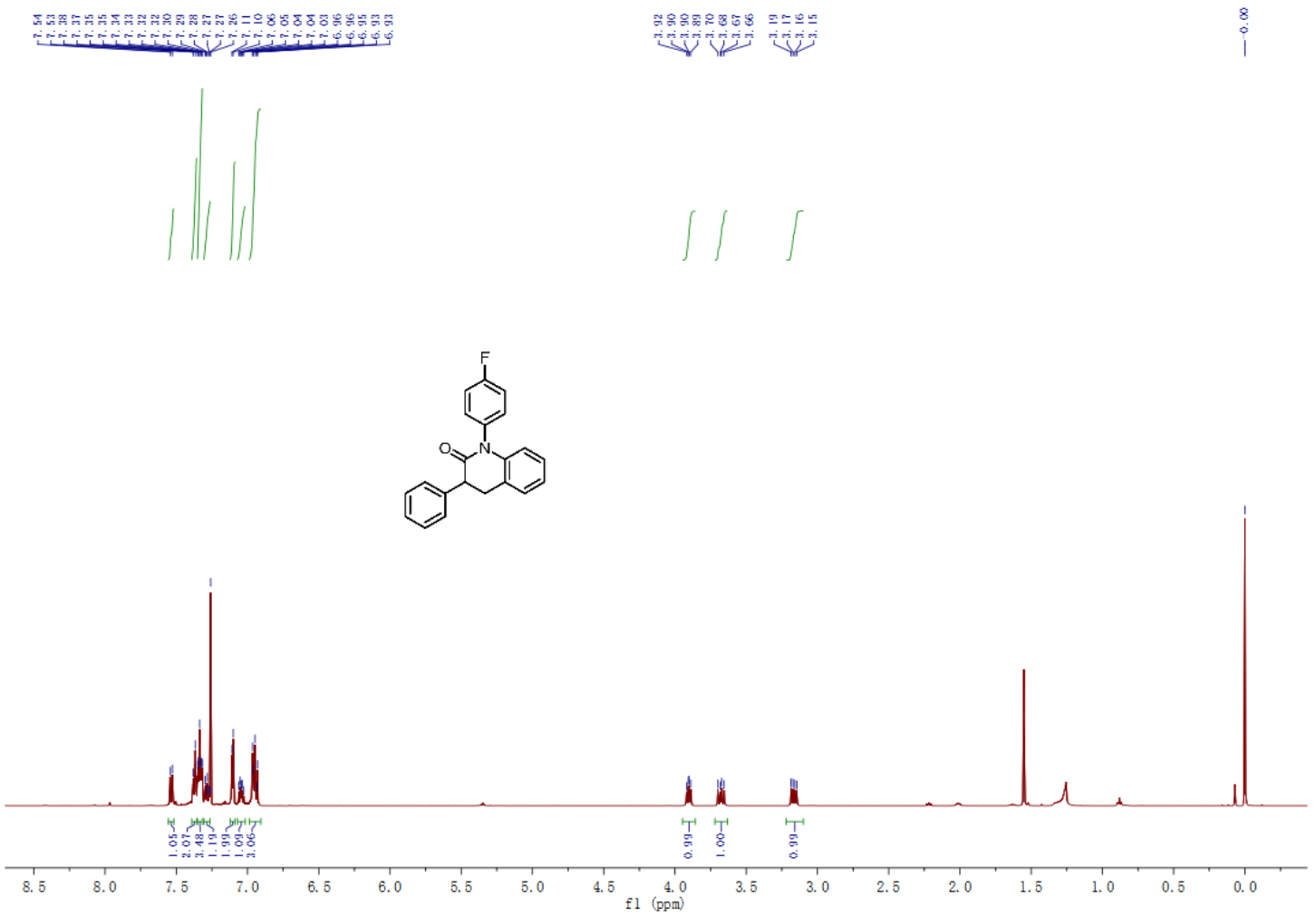

-113.72
-116.54
F
N
O
O
B
O
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

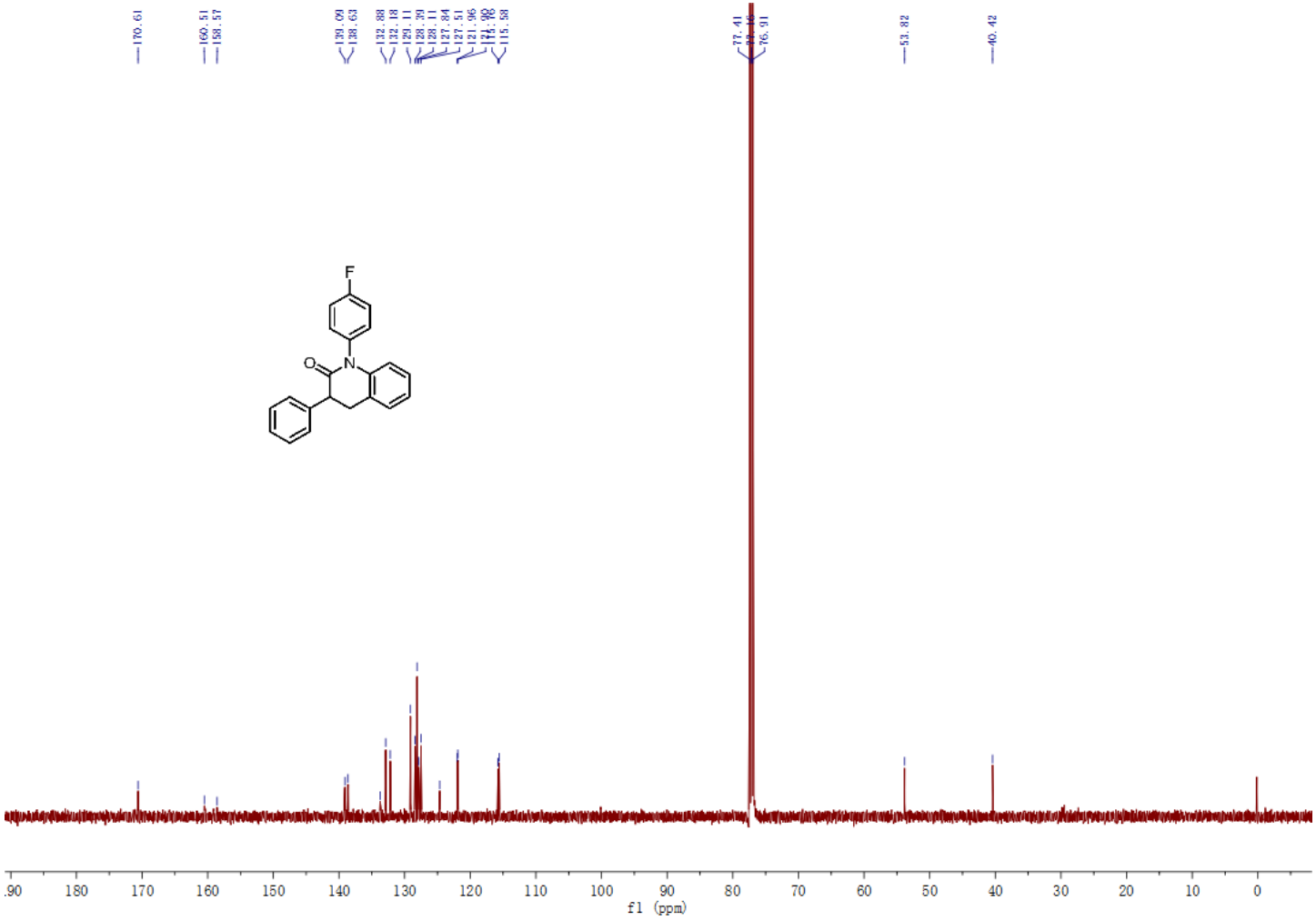

32.92
F
O
B
O
N
O
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

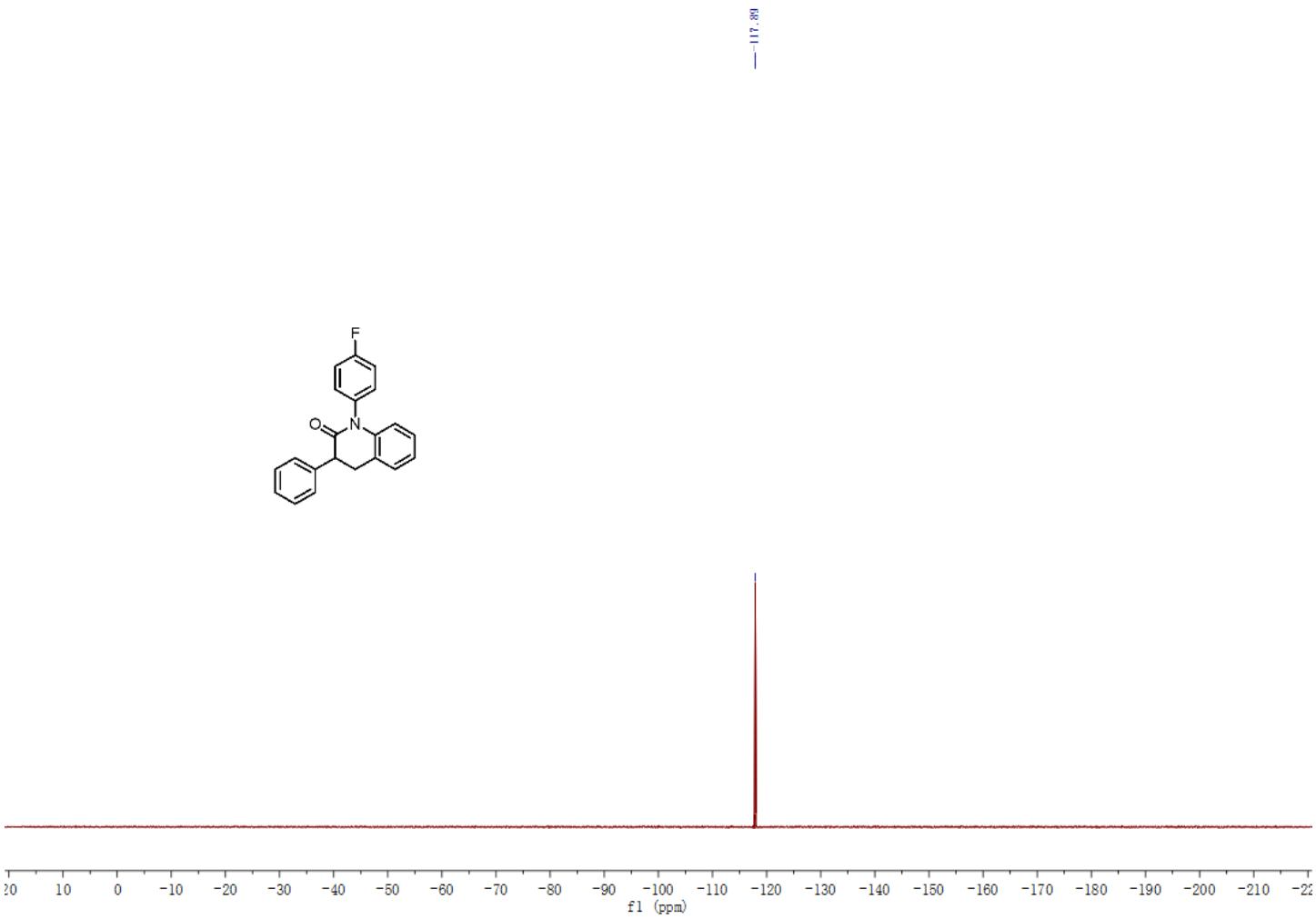

7.34
7.33
7.31
7.31
7.30
7.30
7.29
7.29
7.29
7.27
7.27
7.26
7.23
7.22
7.21
7.18
7.17
7.15
7.13
7.12
6.96
6.95
6.94
6.92
3.72
3.71
3.69
3.63
3.60
3.59
3.07
3.06
3.04
3.03
0.00
F
HN
O
3.88
3.11
2.02
1.06
2.07
0.71
1.99
1.00
1.02
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

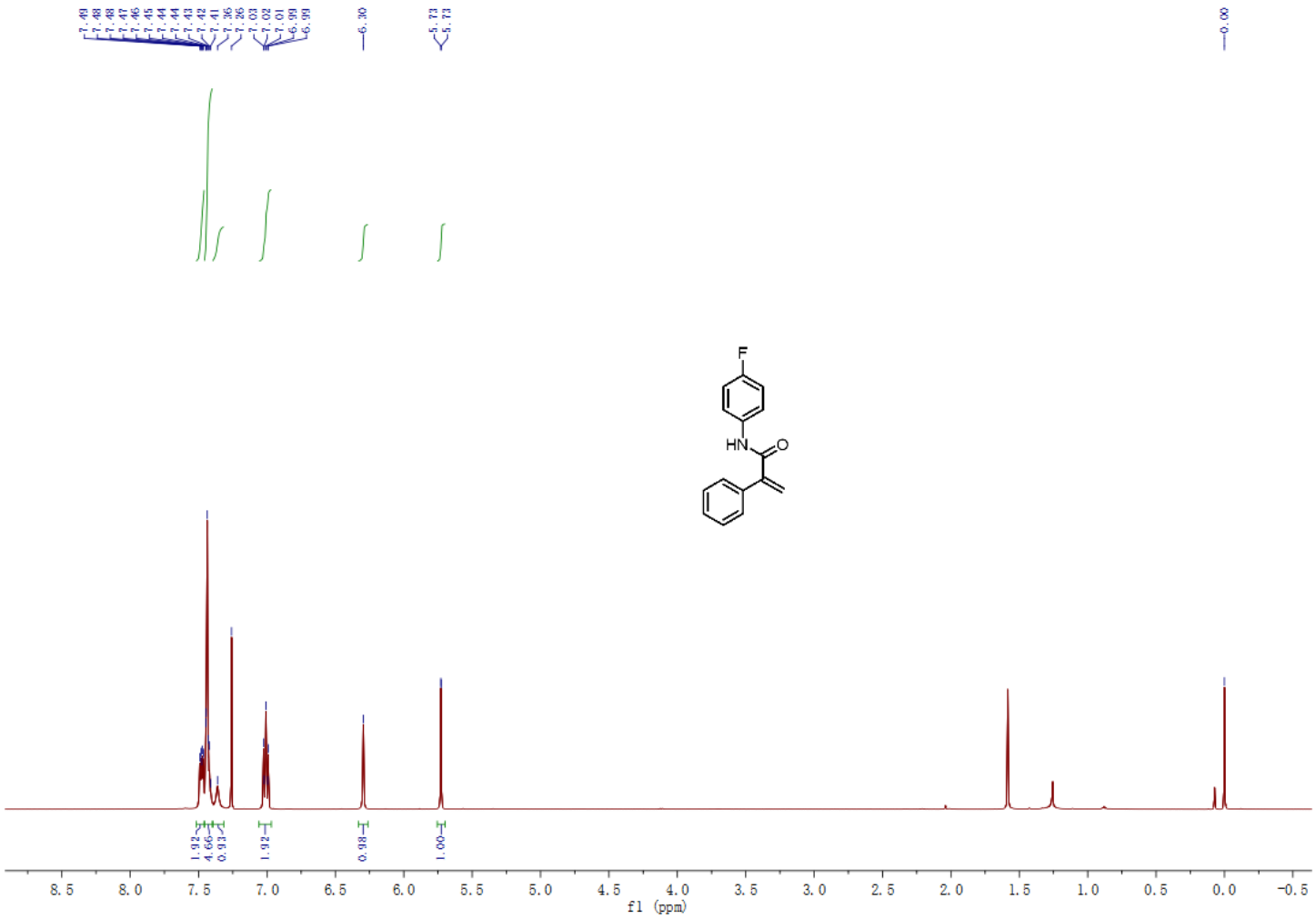

171.01
160.50
158.56
139.57
139.22
133.74
129.16
129.12
128.53
128.24
127.82
121.90
115.74
115.56
77.41
76.91
56.63
39.90
129.16
129.12
128.53
128.24
127.82
126.51
129.0
128.5
128.0
127.5
127.0
126.5
f1 (ppm)
F
HN
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

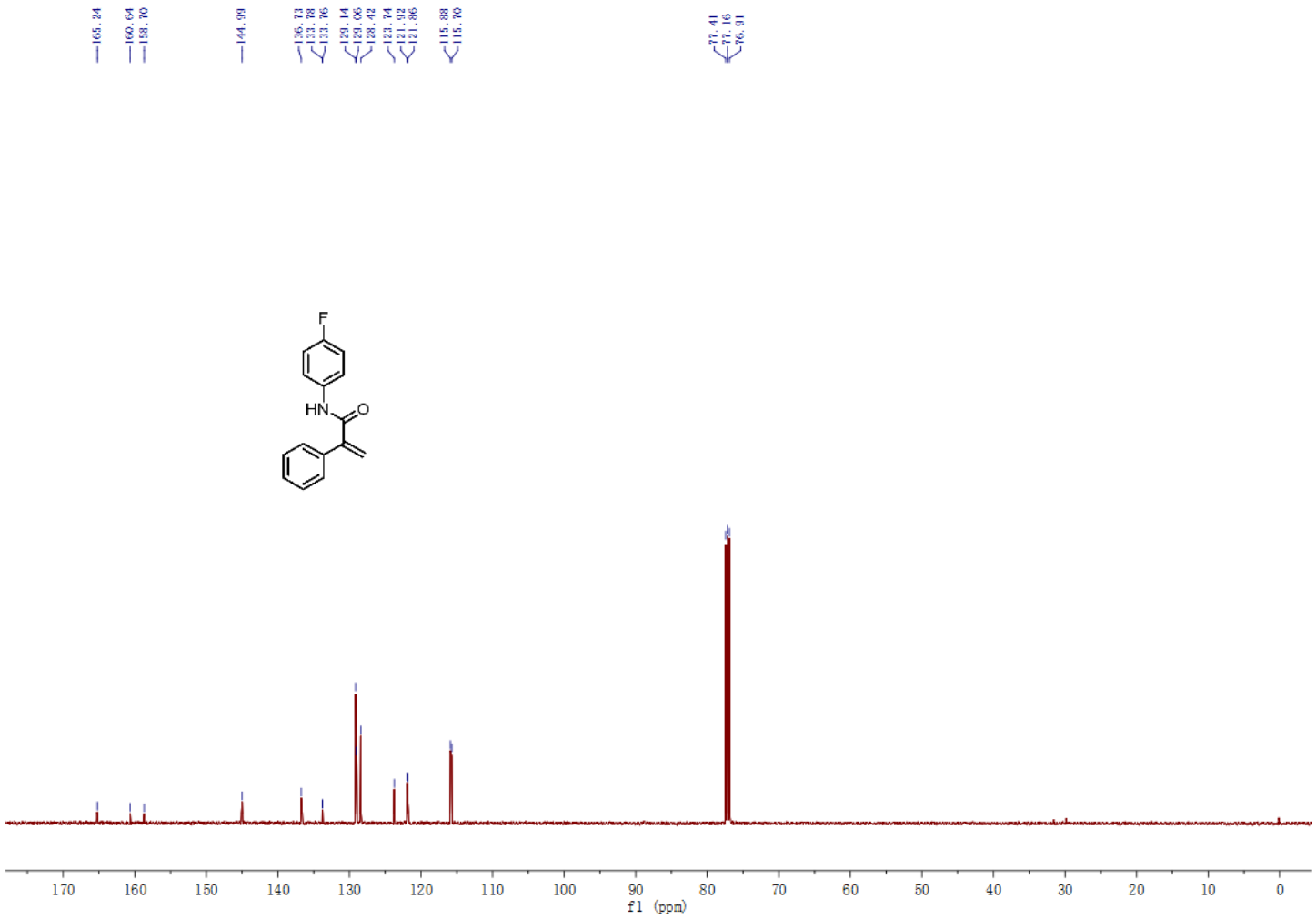

-117.90
F
HN
O
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

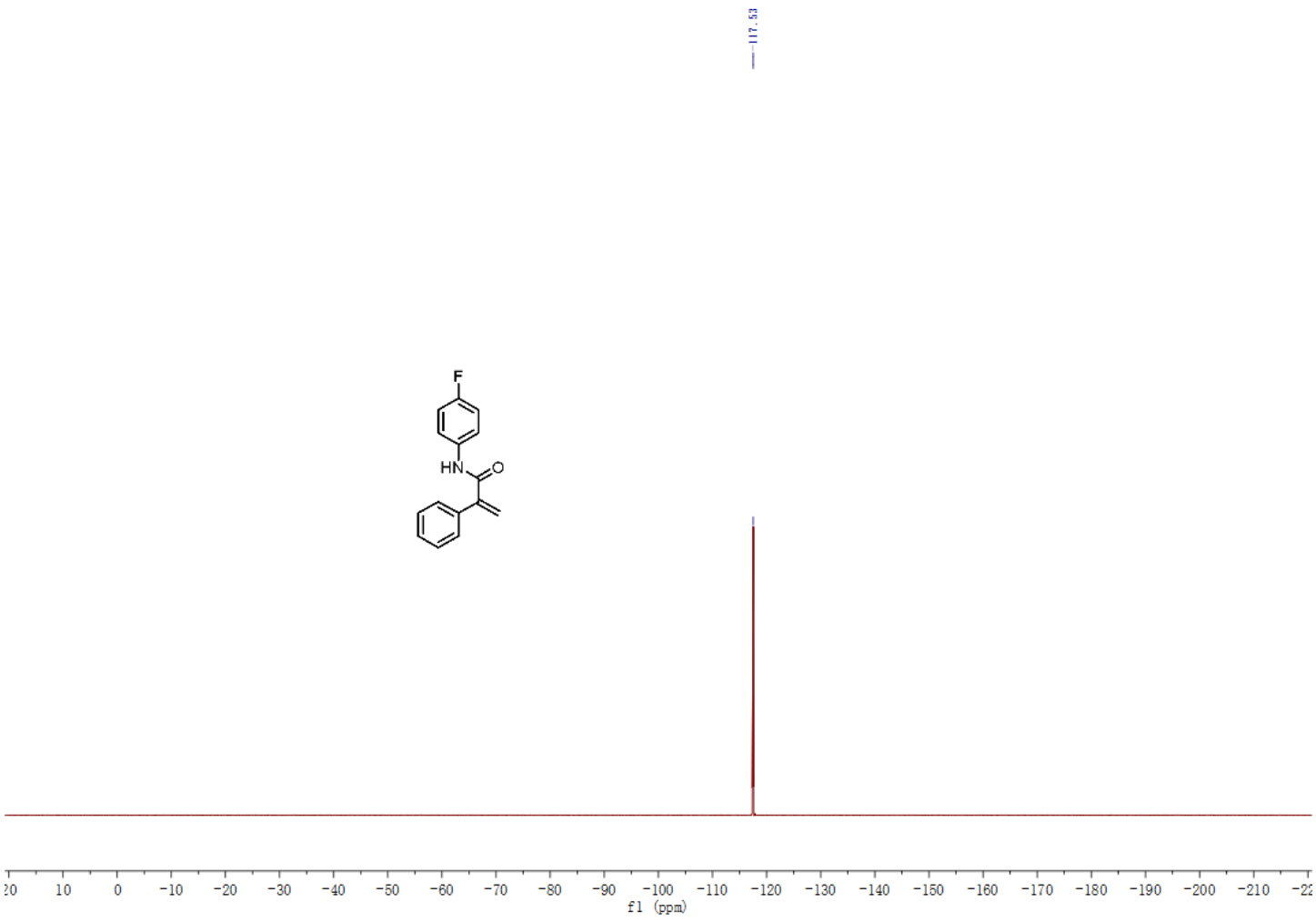

7.54
7.53
7.38
7.37
7.35
7.35
7.34
7.33
7.32
7.32
7.30
7.29
7.28
7.27
7.27
7.26
7.11
7.10
7.06
7.05
7.04
7.04
7.03
6.96
6.95
6.93
6.93
3.92
3.90
3.90
3.89
3.70
3.68
3.67
3.66
3.19
3.17
3.16
3.15
0.00
F
O
N
1.05
2.07
3.48
1.19
1.99
1.69
3.06
0.99
1.00
0.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

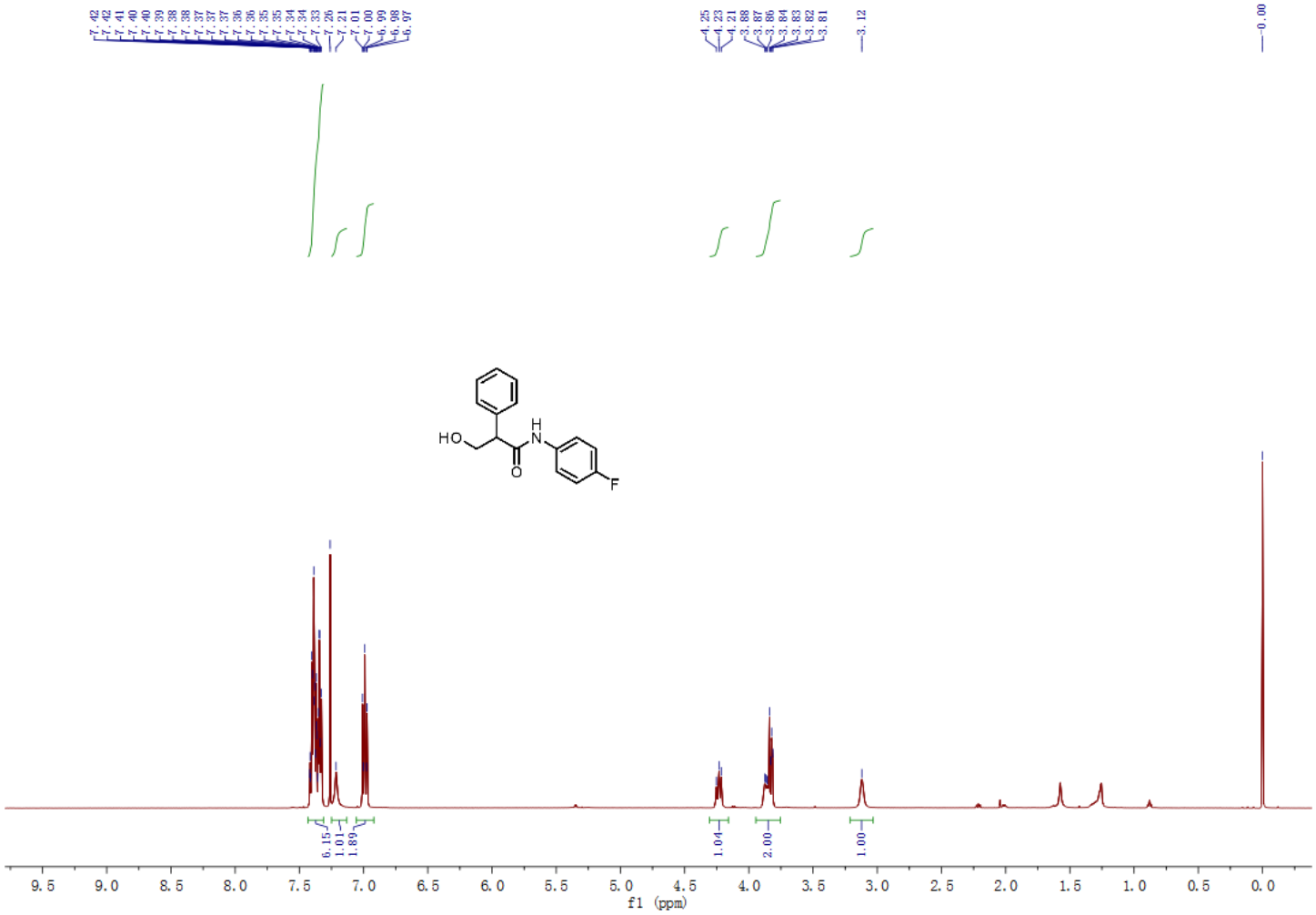

170.61
160.51
158.57
139.09
138.63
132.88
132.18
129.11
128.39
128.11
127.84
127.51
121.96
77.41
76.91
53.82
40.42
F
O
N
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

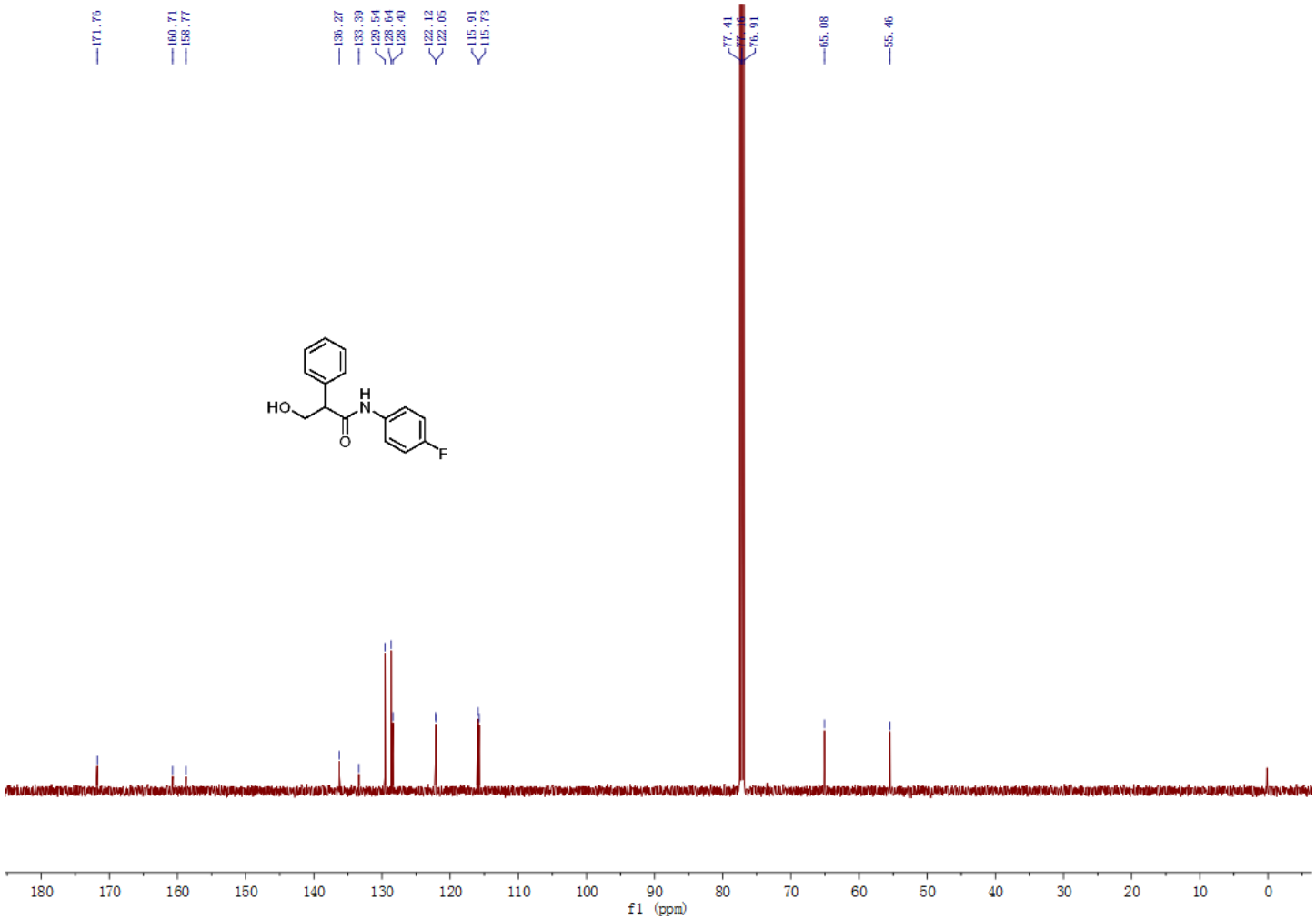

-117.89
F
O
N
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

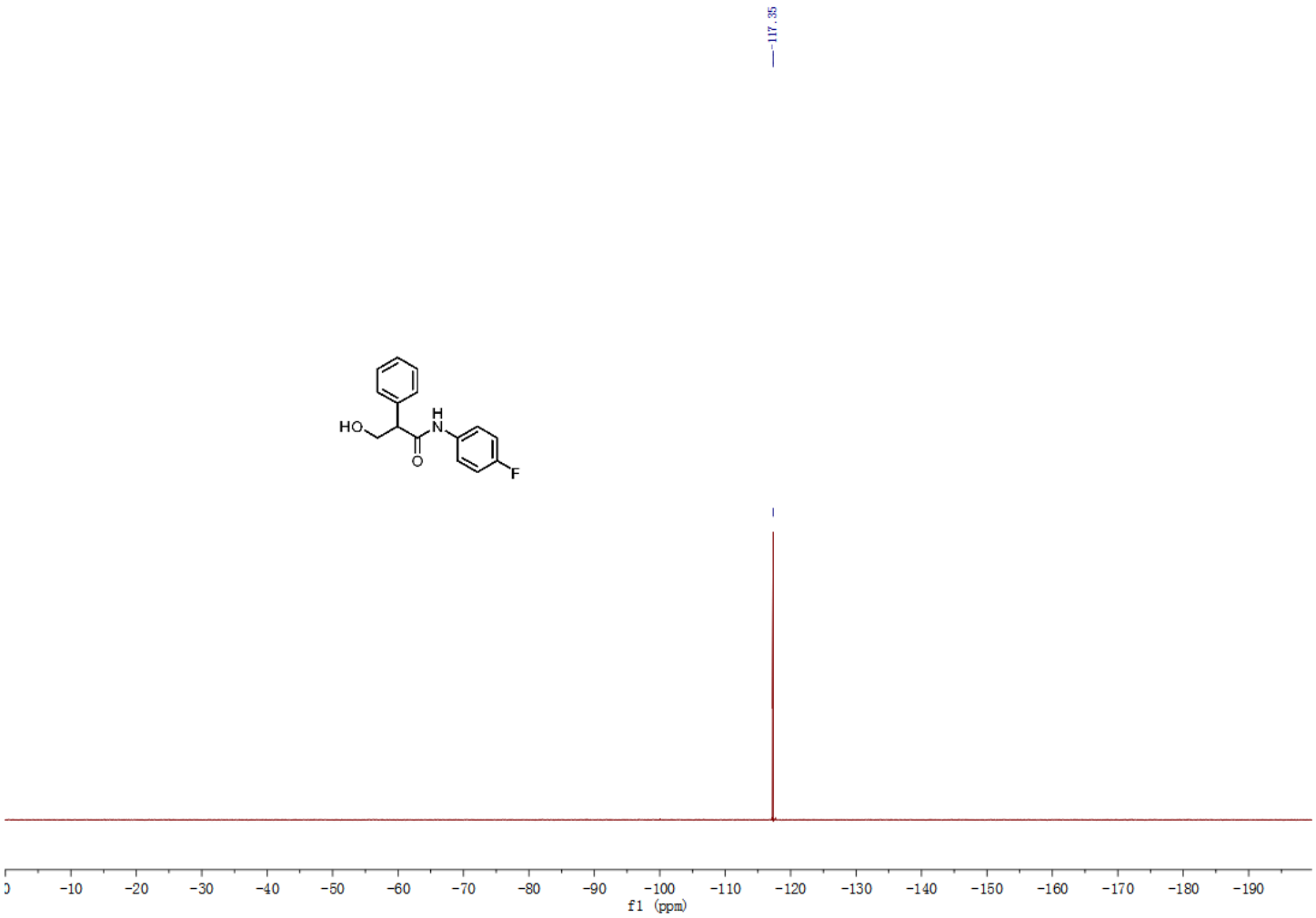

7.49
7.48
7.48
7.47
7.46
7.45
7.44
7.44
7.43
7.42
7.41
7.36
7.26
7.03
7.02
7.01
6.99
6.99
6.30
5.73
5.73
0.00
F
HN
O
1.92
4.66
0.93
1.92
0.98
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


165.24
160.64
158.70
144.99
136.73
133.78
133.76
129.14
129.06
128.42
123.74
121.92
121.385
115.88
115.70
77.41
77.16
76.91
F
HN
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-117.53
F
HN
O
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.42
7.42
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.26
7.21
7.01
7.00
6.99
6.98
6.97
4.25
4.23
4.21
3.88
3.87
3.86
3.84
3.83
3.82
3.81
3.12
0.00
HO
N
H
O
F
6.15
1.01
1.89
1.04
2.00
1.00
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
0.0
f1 (ppm)


171.76
160.71
158.77
136.27
133.39
129.54
128.64
128.40
122.12
122.05
115.91
115.73
77.41
77.16
76.91
65.08
55.46
HO
H
N
O
F
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-117.35
HO
H
N
O
F
0
-10
-20
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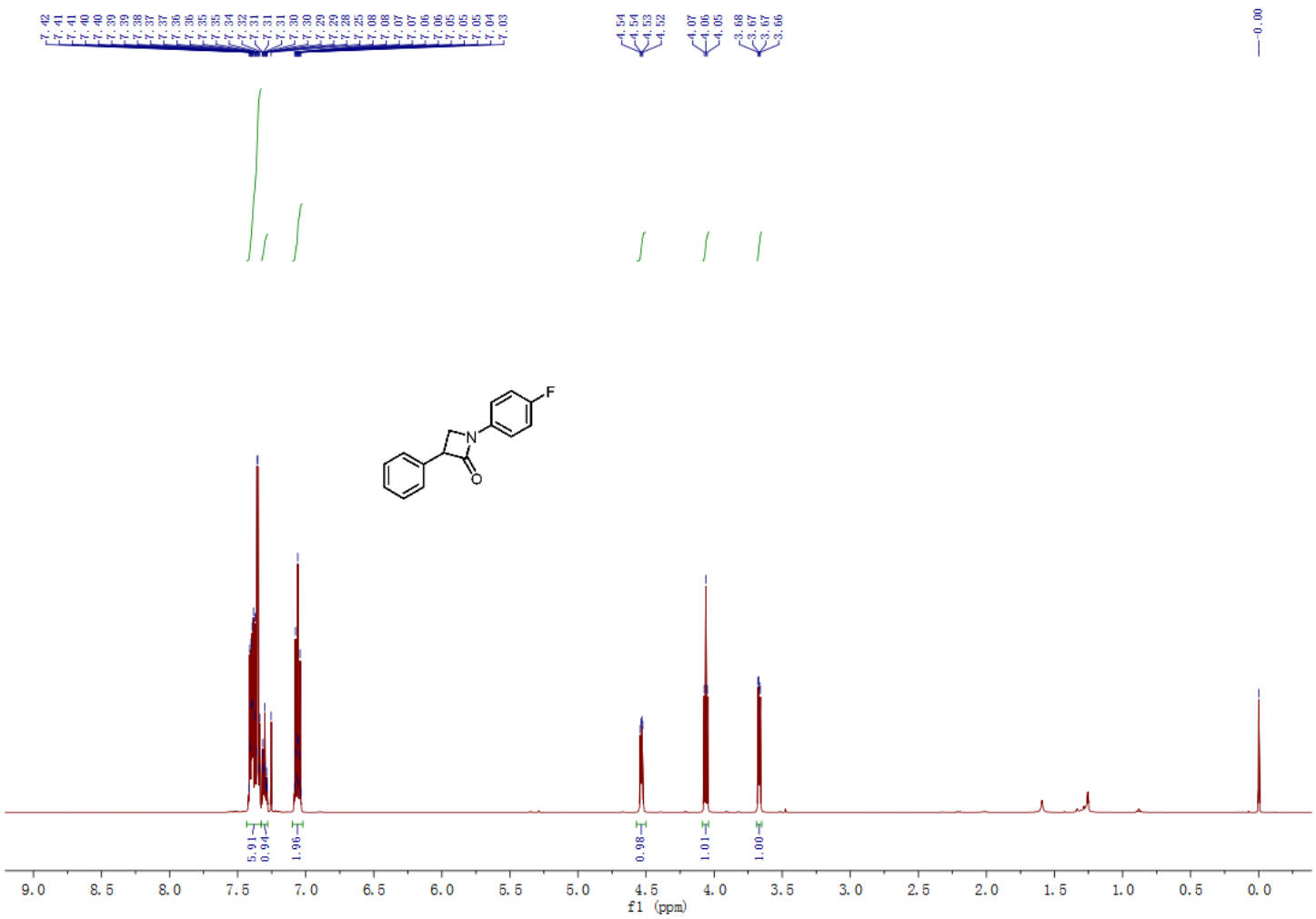
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)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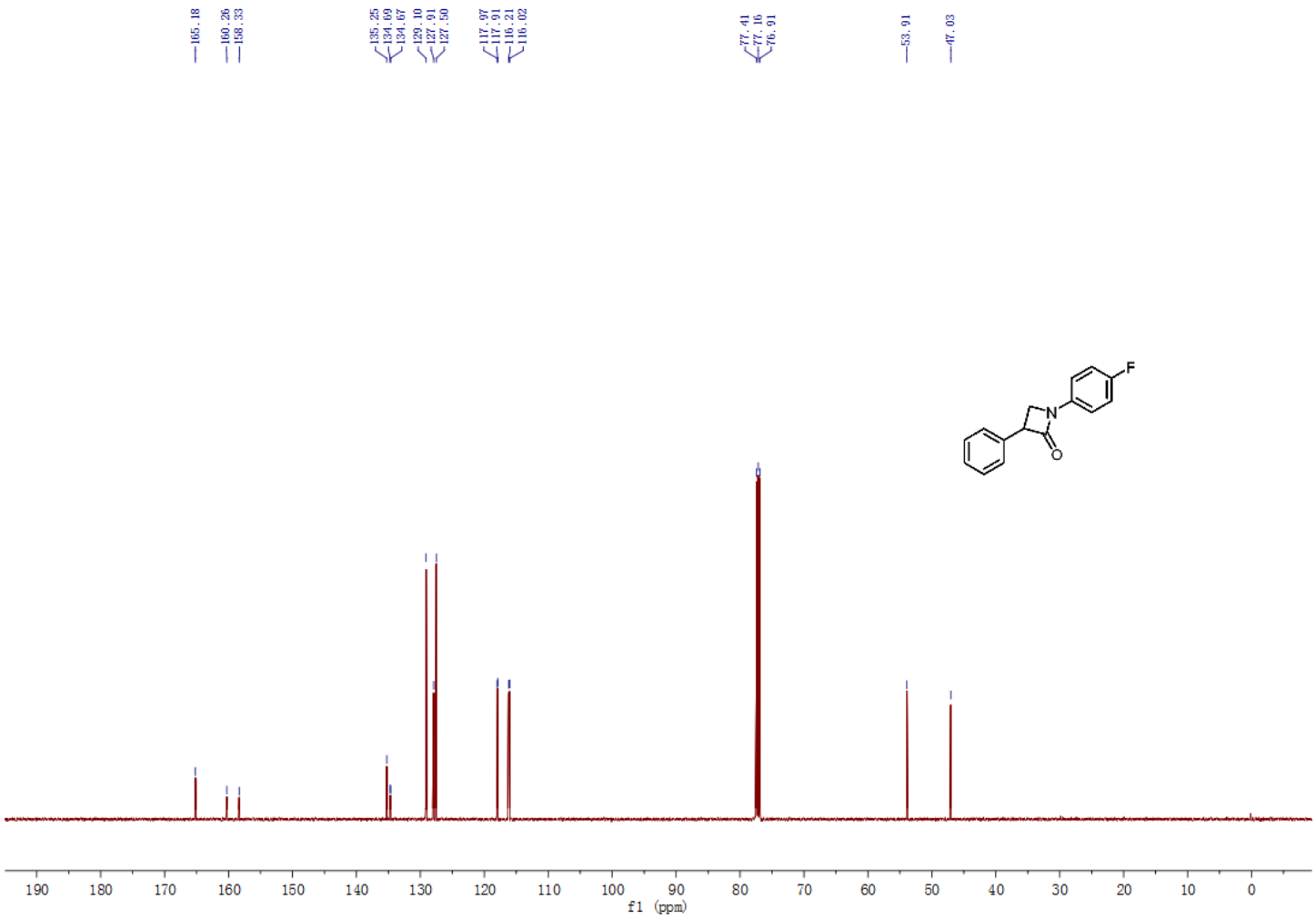
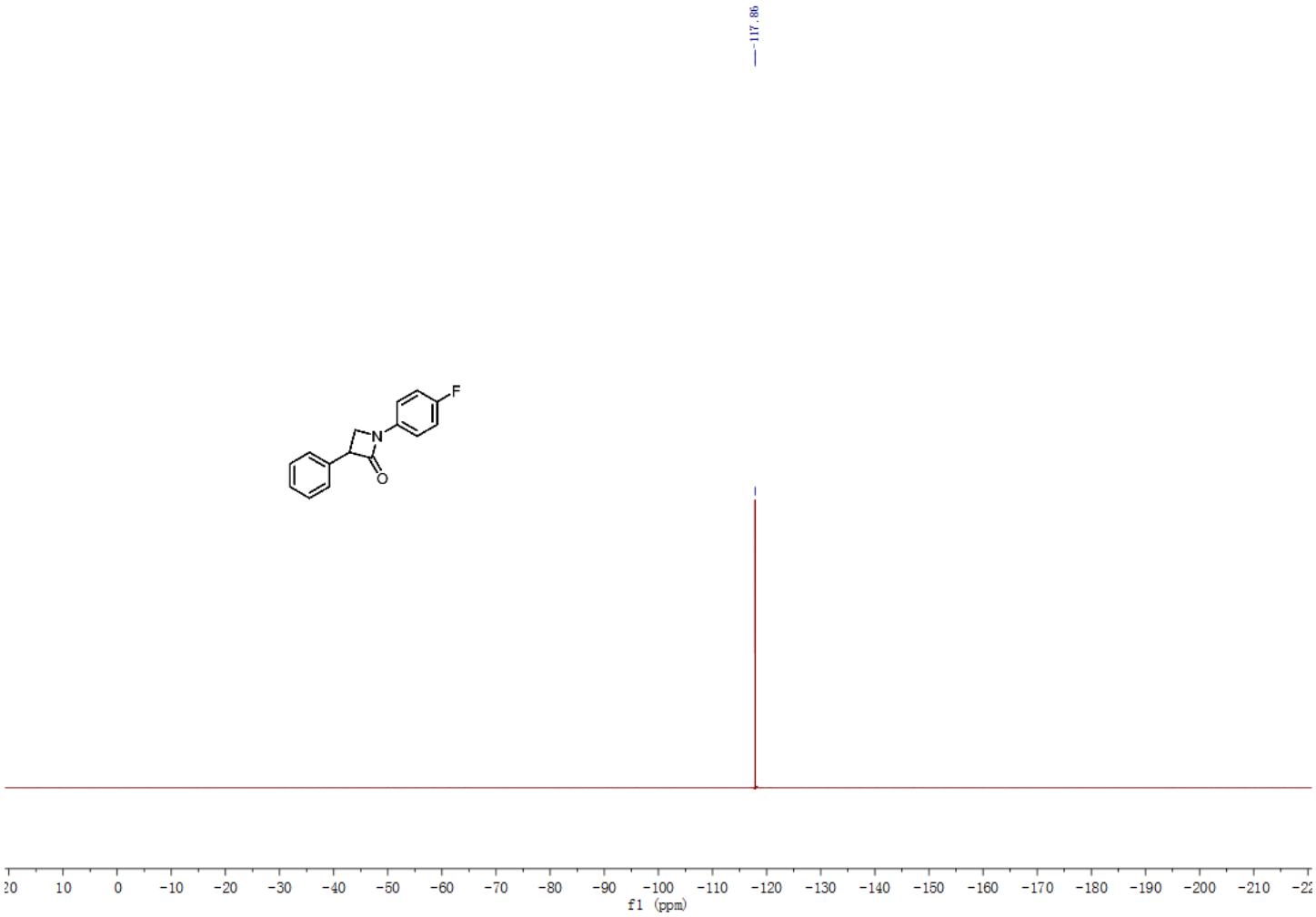
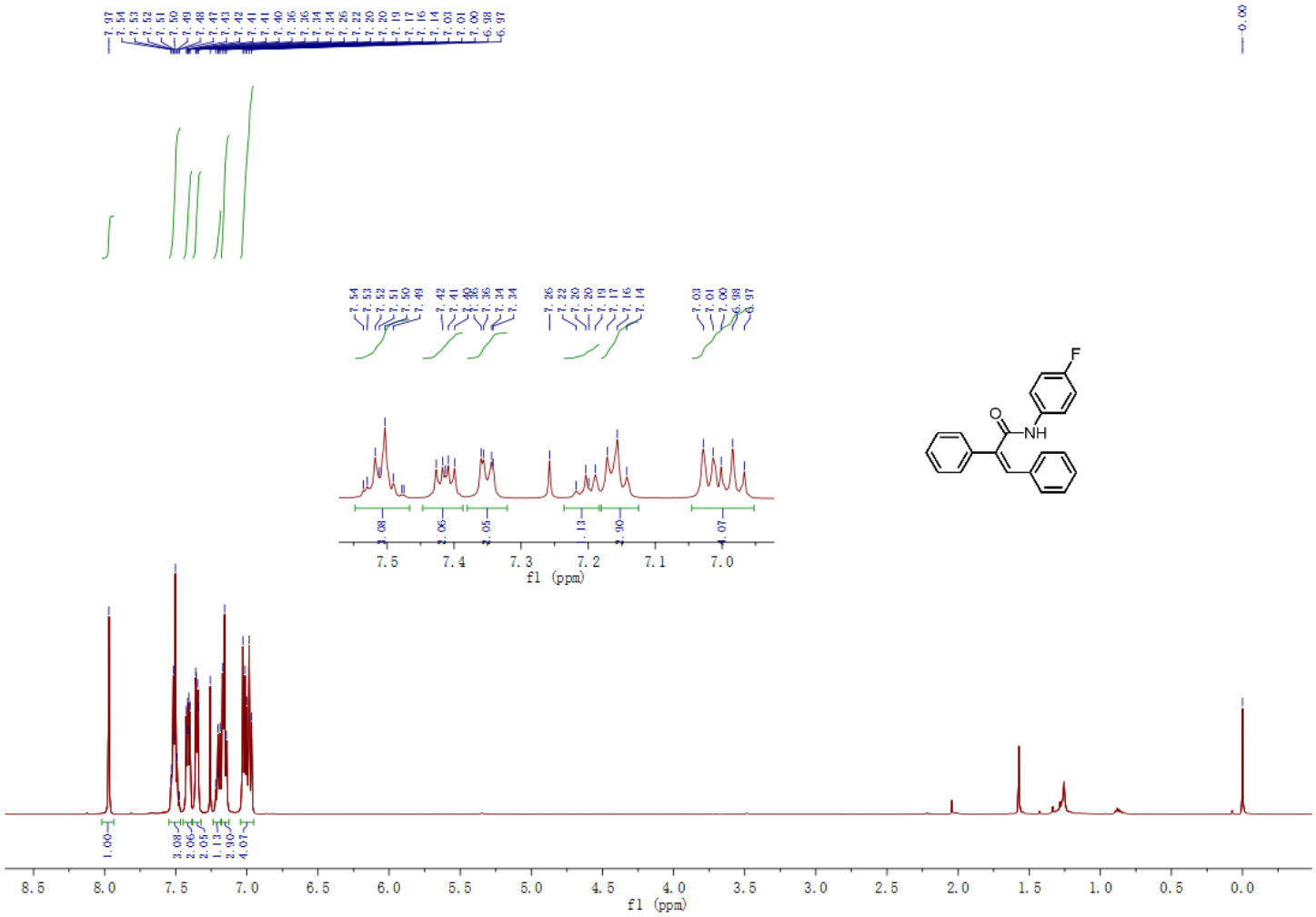
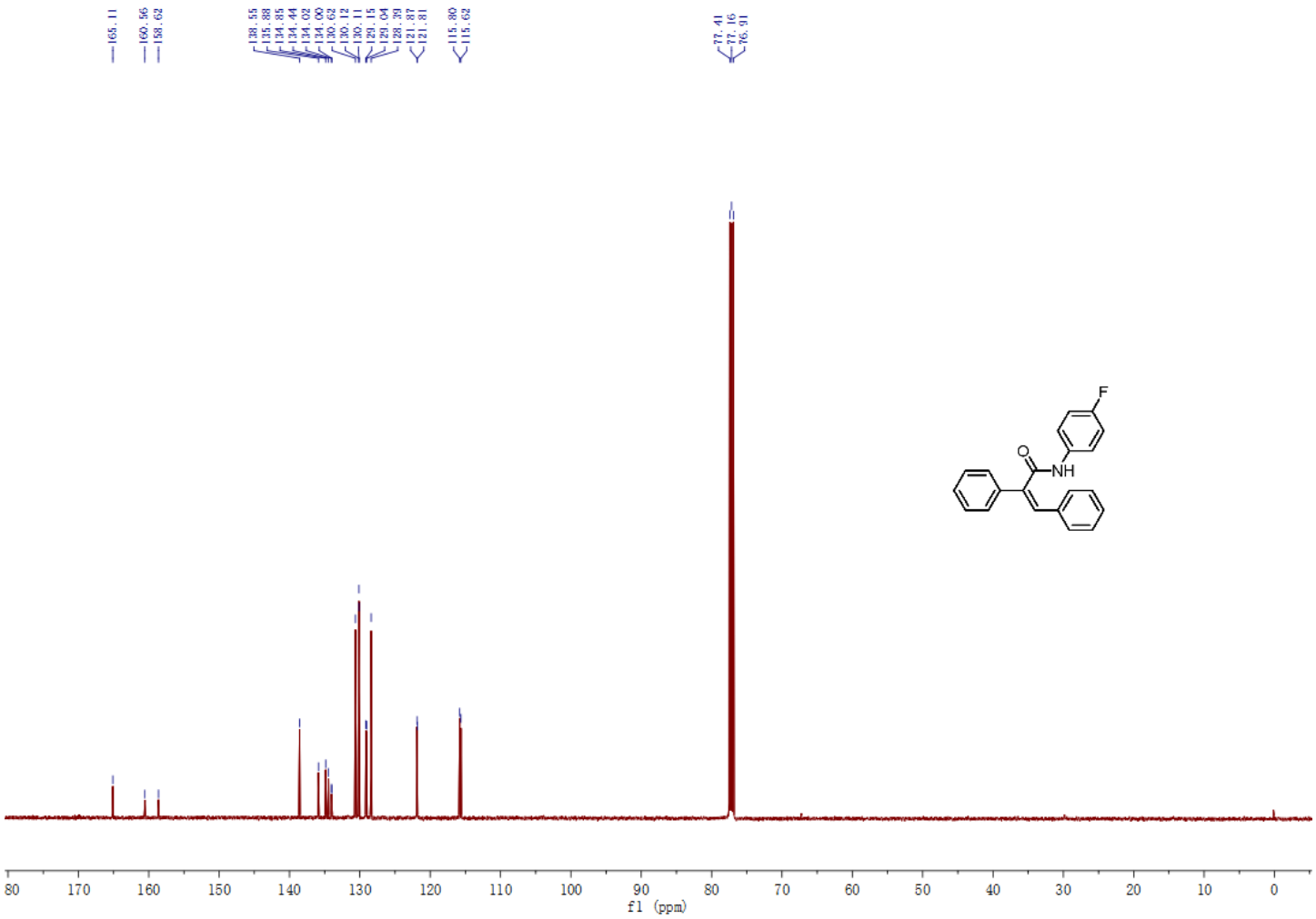
4.54 4.54 4.53 4.52
4.07 4.06 4.05
3.68 3.67 3.67 3.66
0.00
F
N
O
5.91
0.94
1.96
0.98
1.01
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


165.18
160.26
158.33
135.25
134.69
134.67
129.10
127.91
127.50
117.97
117.91
116.21
116.02
77.41
77.16
76.91
53.91
47.03
F
N
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-117.86
F
N
O
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.97
7.54
7.53
7.52
7.51
7.50
7.49
7.48
7.47
7.43
7.42
7.41
7.41
7.40
7.36
7.36
7.34
7.34
7.26
7.22
7.20
7.20
7.19
7.17
7.16
7.14
7.03
7.01
7.00
6.98
6.97
0.00
F
O
NH
1.00
3.08
2.06
2.05
1.13
2.90
4.07
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
0.0
f1 (ppm)
1.08
2.05
2.05
1.13
2.90
4.07
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)


165.11
160.56
158.62
138.55
135.88
134.85
134.44
134.02
134.00
130.62
130.12
130.11
129.15
129.04
128.39
121.87
121.81
115.80
115.62
77.41
77.16
76.91
F
O
NH
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-117.78
F
O
NH
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)