Supporting Information

Pd-Catalyzed N-H Bond Insertion of Vinyldiazoacetates and Intramolecular Cyclization Cascade: The Divergent Synthesis of Heterocyclics

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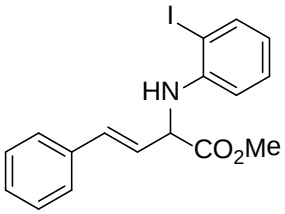
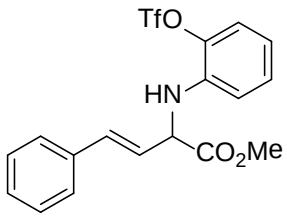
General All experiments were conducted under a nitrogen atmosphere. Flasks were flame dried and cooled under nitrogen before use. All solvents were dried appropriately. Dichloromethane and N,N-Dimethylformamide (DMF) were distilled over calcium hydride under nitrogen. For column chromatography, 200-300 mesh silica gel was employed. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR were recorded on 300 MHz, 400MHz or 500 MHz spectrometers. IR spectra were recorded on a FTIR-8400S FTIR spectrometer and only major peaks were recorded in cm^{-1}. HRMS were performed using electrospray ionization (ESI) with a ion-trap analyzer or electron impact mode (EI) with a TOF mass analyzer. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. All the diazo compounds[1], 2-substituted anilines[2]were prepared according to the reference.

Typical procedure for Pd(II)-catalyzed N-H insertion between vinyldiazoacetates and anilines

To a solution of anilines (0.52 mmol) and $PdCl_2$ (5 mol%) in CH_2Cl_2 (2 mL), was added vinyldiazoacetates (0.5 mmol). Then the mixture was stirred at room temperature under nitrogen atmosphere. After the reaction mixture was stirred for 3h, the mixture was filtered and filtrate was concentrated under vacuum. The residue was purified by column chromatography to give the desired product.



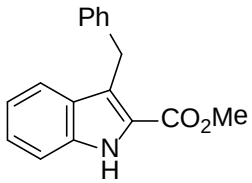
*(E)-methyl 2-((2-iodophenyl)amino)-4-phenylbut-3-enoate (**4a**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **4a** as a white solid (yield 84%, 165.2 mg). Mp = 62-64 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 7.3 Hz, 2H), 7.34-7.22 (m, 3H), 7.15 (t, *J* = 7.8 Hz, 1H), 6.76 (d, *J* = 15.8 Hz, 1H), 6.48 (t, *J* = 8.0 Hz, 2H), 6.30 (dd, *J* = 15.9, 5.8 Hz, 1H), 5.31 (d, *J* = 5.7 Hz, 1H), 4.75 (t, *J* = 5.8 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.48, 145.59, 139.22, 135.95, 133.27, 129.41, 128.62, 128.16, 126.74, 124.24, 119.56, 111.60, 85.72, 59.09, 52.96. HRMS (MALDI-FT) m/z: calcd for $C_{17}H_{16}{}^{127}INO_2$: $M+Na^{+}$= 416.0123; found: 416.0118.



*(E)-methyl 2-(2-trifluoromethanesulfonyloxy-phenylamino)-4-phenylbut-3-enoate (**9a**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **9a** as colorless oil (yield 83%, 172.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.36 (m, 2H), 7.32-7.29 (m, 2H), 7.27-7.21 (m, 2H), 7.17-7.13 (t, *J* = 8.0 Hz, 1H), 6.78-6.71 (m, 2H), 6.69-6.67 (m, 1H), 6.29-6.23 (dd, *J* = 16.0 & 6.0 Hz, 1H), 5.16-5.15 (d, *J* = 4.0 Hz, 1H), 4.78-4.75 (m, 1H), 3.82 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.1, 138.4, 137.2, 135.8, 133.5, 129.2, 128.7, 128.3, 126.8, 123.6, 121.8, 117.9, 113.8, 58.0, 53.0; ^{19}F NMR (470 MHz, $CDCl_3$) δ: -73.8; HRMS (ESI-FT) exact mass calcd for $C_{18}H_{16}F_3NO_5S$: m/z 438.0591 ($[M + Na]^+$), found: m/z 438.0593 ($[M + Na]^+$).

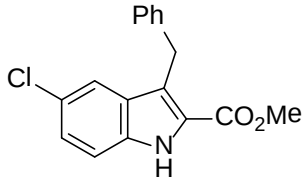
Typical procedure for one pot reaction of Pd(II)-catalyzed N-H insertions and Pd(0)-catalyzed Heck cyclization

To a solution of anilines (0.52 mmol) and $PdCl_2$ (5 mol%) in CH_2Cl_2 (2 mL), was added vinyldiazoacetates (0.5 mmol). Then the mixture was stirred at room temperature under nitrogen atmosphere. After the reaction mixture was stirred for 3 hours, then PPh_3 (0.05 mmol, 10 mol%), $NaHCO_3$ (0.75 mmol) and DMF (2 mL) were added and the reaction mixture was continued to be stirred at 80^{o}C for another 2 hours. Then the resulting mixture was cooled and diluted with ether (20 mL); then washed with brine (10 mL×3); the organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated; the residue was purified by column chromatography to give the desired product.

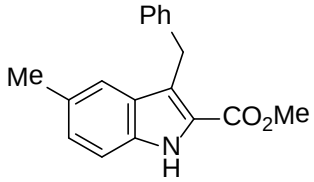


*methyl 3-benzyl-1H-indole-2-carboxylate (**5a**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5a** as a white solid (yield 74%, 98.2 mg); Mp = 145-147 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.38 (d, *J* = 8.3 Hz, 1H), 7.35-7.19 (m, 5H), 7.19-7.06 (m, 2H), 4.51 (s, 2H), 3.93 (s, 3H); ^{13}C NMR (125 MHz,

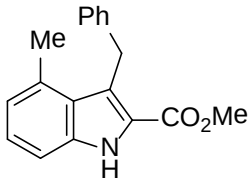
$CDCl_3$) δ 162.72, 140.91, 135.99, 128.42, 128.29, 128.05, 125.85, 125.71, 123.38, 122.89, 121.31, 120.35, 111.74, 51.80, 30.58. HRMS (MALDI-FT) m/z: calcd for $C_{17}H_{15}NO_2$: $M+H^+$= 266.1181; found: 266.1176. IR (KBr, cm^{-1}): 3330, 1685, 1458, 1337, 1257, 1205, 741.



*methyl 3-benzyl-5-chloro-1H-indole-2-carboxylate (**5b**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5b** as a white solid (yield 72%, 107.9 mg); Mp: 172-174 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (s, 1H), 7.56 (s, 1H), 7.30 (d, *J* = 8.7 Hz, 1H), 7.25 (dd, *J* = 6.1, 3.5 Hz, 5H), 7.17 (dd, *J* = 8.7, 4.4 Hz, 1H), 4.45 (s, 2H), 3.94 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.42, 140.42, 134.24, 129.02, 128.42, 128.35, 126.25, 126.12, 126.07, 124.64, 122.23, 120.55, 112.93, 51.98, 30.47. HRMS (MALDI-FT) m/z: calcd for $C_{17}H_{14}{}^{35}ClNO_2$: $M+Na^+$= 322.0611; found: 322.0605. IR (KBr, cm^{-1}): 3320, 1684, 1451, 1310, 1214, 910, 785.

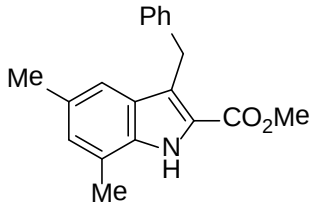


*methyl 3-benzyl-5-methyl-1H-indole-2-carboxylate (**5c**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5c** as a white solid (yield 63%, 88.0 mg); Mp = 154-156 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (s, 1H), 7.39 (s, 1H), 7.30-7.25 (m, 3H), 7.23 (t, *J* = 7.6 Hz, 2H), 7.15 (dd, *J* = 7.6, 5.5 Hz, 2H), 4.47 (s, 2H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.72, 141.02, 134.41, 129.70, 128.38, 128.30, 128.27, 127.71, 125.79, 123.47, 122.32, 120.46, 111.43, 51.71, 30.50, 21.53. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{17}NO_2$: $M+H^+$= 280.1338; found: 280.1332. IR (KBr, cm^{-1}): 3327, 1682, 1470, 1259, 1227, 802, 775, 692.

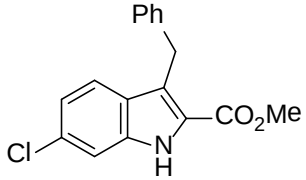


*methyl 3-benzyl-4-methyl-1H-indole-2-carboxylate (**5d**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5d** as a white solid (yield 70%, 97.8 mg); Mp = 168-170 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.86 (s, 1H), 7.27-7.18 (m, 4H), 7.12 (dd,

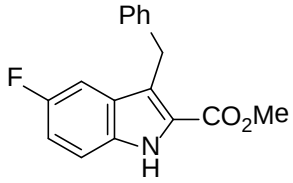
J = 16.7, 7.7 Hz, 3H), 6.82 (d, *J* = 6.7 Hz, 1H), 4.72 (s, 2H), 3.88 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.73, 141.54, 136.64, 133.50, 128.36, 128.09, 126.96, 125.82, 125.70, 124.02, 122.87, 122.14, 109.75, 51.84, 31.38, 20.32. HRMS (EI-TOF) m/z: calcd for $C_{18}H_{17}NO_2$: M = 279.1259; found: 279.1255. IR (KBr, cm^{-1}): 3329, 1674, 1464, 1450, 1215, 7634, 729.



*methyl 3-benzyl-5,7-dimethyl-1H-indole-2-carboxylate (**5e**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5e** as a white solid (yield 48%, 70.4 mg); Mp: 157-159 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 7.147.26 (m, 5H), 7.14 (d, *J* = 6.7 Hz, 1H), 6.95 (s, 1H), 4.46 (s, 2H), 3.92 (s, 3H), 2.46 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.88, 141.10, 134.27, 130.00, 128.38, 128.25, 128.06, 127.96, 125.75, 123.28, 122.80, 120.71, 118.03, 51.70, 30.67, 21.48, 16.50. HRMS (EI-TOF) m/z: calcd for $C_{19}H_{19}NO_2$: M= 293.1416; found: 293.1421. IR (KBr, cm^{-1}): 3350, 1684, 1242, 1259, 852, 779, 727.

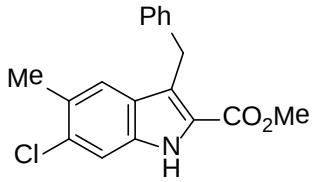


*methyl 3-benzyl-6-chloro-1H-indole-2-carboxylate (**5f**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5f** as a white solid (yield 71%, 106.4mg); Mp = 164-166 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (s, 1H), 7.48 (d, *J* = 8.6 Hz, 1H), 7.36 (d, *J* = 1.6 Hz, 1H), 7.23 (d, *J* = 4.4 Hz, 4H), 7.16 (m, 1H), 7.05 (dd, *J* = 8.6, 1.8 Hz, 1H), 4.47 (s, 2H), 3.94 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.45, 140.53, 136.21, 131.74, 128.37, 126.63, 126.02, 124.05, 122.95, 122.35, 121.43, 111.55, 51.92, 30.54. HRMS (EI-TOF) m/z: calcd for $C_{17}H_{14}{}^{35}ClNO_2$: M = 299.0713; found: 299.0716. IR (KBr, cm^{-1}): 3313, 1688, 1452, 1317, 1223, 916, 789, 698.

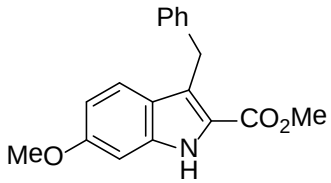


*methyl 3-benzyl-5-fluoro-1H-indole-2-carboxylate (**5g**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5g** as a white solid (yield

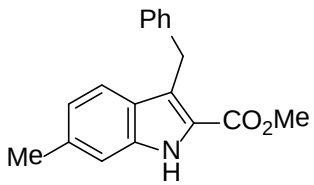
68%, 96.3 mg); Mp = 155-157 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (s, 1H), 7.30 (dd, *J* = 8.9, 4.3 Hz, 1H), 7.27-7.12 (m, 6H), 7.06 (td, *J* = 9.0, 2.4 Hz, 1H), 4.45 (s, 2H), 3.94 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.52, 158.83, 156.95, 140.53, 132.59, 128.39, 126.03, 124.95, 122.69, 114.94, 114.73, 112.79, 112.72, 105.74, 105.56, 51.91, 30.64. HRMS (EI-TOF) m/z: calcd for $C_{17}H_{14}FNO_2$: M = 283.1009; found: 283.1011. IR (KBr, cm^{-1}): 3304, 1690, 1468, 1261, 1070, 849, 806.



*methyl 3-benzyl-6-chloro-5-methyl-1H-indole-2-carboxylate (**5h**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5h** as a white solid (yield 74%, 116.1 mg); Mp: 174-176 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.39 (d, *J* = 10.3 Hz, 2H), 7.33-7.18 (m, 4H), 7.16 (dd, *J* = 8.7, 4.4 Hz, 1H), 4.45 (s, 2H), 3.92 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.51, 140.67, 134.91, 132.86, 128.35, 128.33, 128.18, 127.09, 125.95, 124.00, 122.32, 122.11, 111.83, 51.84, 30.48, 20.51. HRMS (EI-TOF) m/z: calcd for $C_{18}H_{16}{}^{35}ClNO_2$: M= 313.0870; found: 313.0871. IR (KBr, cm^{-1}): 3317, 1693, 1464, 1236, 1001, 847, 777, 698.

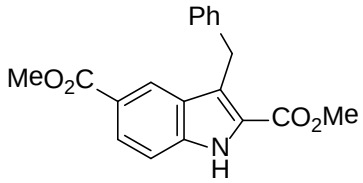


*methyl 3-benzyl-6-methoxy-1H-indole-2-carboxylate (**5i**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5i** as a white solid (yield 78%, 115.2 mg); Mp = 176-178 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (s, 1H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.39-7.02 (m, 5H), 6.76 (d, *J* = 9.6 Hz, 2H), 4.46 (s, 2H), 3.91 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.78, 159.27, 141.03, 137.18, 128.50, 128.37, 125.93, 123.49, 122.59, 122.40, 122.26, 111.85, 93.67, 55.57, 51.69, 30.78. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{17}NO_3$: M+Na^+= 318.1106; found: 318.1101. IR (KBr, cm^{-1}): 3342, 1682, 1628, 1448, 1256, 1202, 1097, 710.

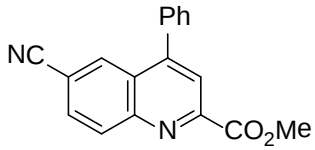


*methyl 3-benzyl-6-methyl-1H-indole-2-carboxylate (**5j**)*. The title compound was purified by column

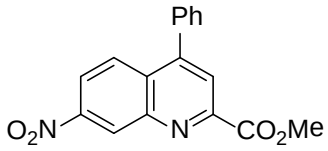
chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5j** as a white solid (yield 62%, 86.6 mg); Mp = 158-160 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (s, 1H), 7.47 (d, *J* = 8.3 Hz, 1H), 7.30-7.18 (m, 4H), 7.14 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 8.3 Hz, 1H), 4.48 (s, 2H), 3.92 (s, 3H) , 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.80, 141.01, 136.45, 136.01, 128.42, 128.27, 126.04, 125.81, 123.00, 122.83, 122.48, 120.96, 111.38, 51.68, 30.66, 21.95. HRMS (EI-TOF) m/z: calcd for $C_{18}H_{17}NO_2$: M= 279.1259; found: 279.1262. IR (KBr, cm^{-1}): 3321, 1690, 1458, 1254, 1221, 797, 781, 714.



*dimethyl 3-benzyl-1H-indole-2,5-dicarboxylate (**5k**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **5k** as a white solid (yield 68%, 109.9 mg); Mp: 164-166 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.96 (brs, 1H), 8.43 (s, 1H), 8.01 (dd, *J* = 8.7, 1.5 Hz, 1H), 7.40 (d, *J* = 8.7 Hz, 1H), 7.31-7.11 (m, 5H), 4.52 (s, 2H), 3.95 (s, 3H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.56, 162.28, 140.44, 138.24, 128.40, 128.38, 127.75, 126.69, 126.05, 124.77, 124.47, 124.27, 122.71, 111.53, 51.99, 30.41. HRMS (MALDI-FT) m/z: calcd for $C_{19}H_{17}NO_4$: M+Na^+= 346.1055; found: 346.1050. IR (KBr, cm^{-1}): 3346, 1720, 1699, 1433, 1331, 1317, 1234, 1113, 764, 746.

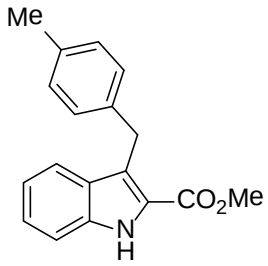


*methyl 6-cyano-4-phenylquinoline-2-carboxylate (**6l**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **6l** as a white solid (yield 62%, 89.4 mg); Mp = 212-214 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.8 Hz, 1H), 8.39 (s, 1H), 8.27 (s, 1H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.61 (s, 3H), 7.57-7.43 (m, 2H), 4.12 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.39, 150.98, 150.08, 149.12, 136.06, 132.60, 132.50, 130.70, 129.69, 129.56, 129.26, 127.40, 122.69, 118.40, 112.39, 53.61. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{12}N_2O_2$: M+H^+= 289.0977; found: 289.0972. IR (KBr, cm^{-1}): 3421, 2231, 1718, 1435, 1263, 849, 706.

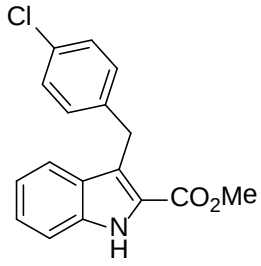


*methyl 7-nitro-4-phenylquinoline-2-carboxylate (**6m**)*. The title compound was purified by column

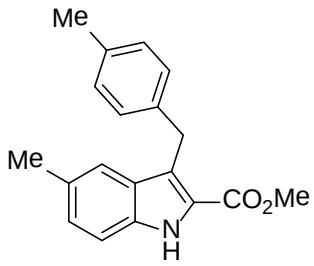
chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **6m** as a white solid (yield 83%, 127.9 mg); Mp = 237-239 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.30 (d, *J* = 2.3 Hz, 1H), 8.36 (dd, *J* = 9.3, 2.3 Hz, 1H), 8.31 (s, 1H), 8.16 (d, *J* = 9.3 Hz, 1H), 7.60 (dd, *J* = 8.9, 3.3 Hz, 3H), 7.56-7.50 (m, 2H), 4.13 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.25, 150.51, 149.81, 148.51, 147.31, 136.27, 130.87, 129.51, 129.50, 129.10, 127.85, 127.12, 123.78, 121.76, 53.57. HRMS (MALDI-FT) m/z: calcd for $C_{17}H_{12}N_2O_4$: $M+H^+$= 309.0875; found: 309.0870. IR (KBr, cm^{-1}): 3061, 1718, 1533, 1366, 1344, 1259, 1126, 827,766.



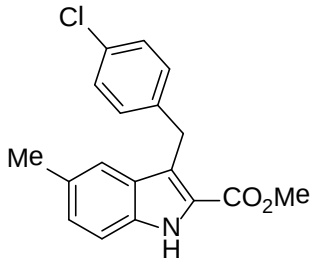
*methyl 3-(4-methylbenzyl)-1H-indole-2-carboxylate (**7a**)*[12]. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7a** as a white solid (yield 80%, 111.7 mg); Mp = 151-153 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.62 (d, *J* = 8.1 Hz, 1H), 7.32 (m, 2H), 7.21-6.90 (m, 5H), 4.46 (s, 2H), 3.94 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.78, 137.87, 136.00, 135.32, 129.00, 128.30, 128.05, 125.69, 123.28, 123.20, 121.35, 120.32, 111.74, 76.62, 51.83, 30.15, 21.02. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{17}NO_2$: $M+H^+$= 280.1338; found: 280.1332. IR (KBr, cm^{-1}): 3323, 1688, 1462, 1263, 1223, 1099, 742.



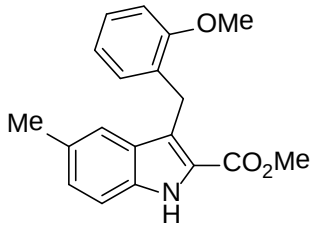
*methyl 3-(4-chlorobenzyl)-1H-indole-2-carboxylate (**7b**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7b** as a white solid (yield 71%, 106.4 mg); Mp: 148-150 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.19 (s, 4H), 7.11 (t, *J* = 7.4 Hz, 1H), 4.46 (s, 1H), 3.93 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.50, 139.39, 135.98, 131.58, 129.74, 128.38, 127.85, 125.86, 123.41, 122.36, 121.06, 120.52, 111.85, 51.84, 29.93. HRMS (EI-TOF) m/z: calcd for $C_{17}H_{14}{}^{35}ClNO_2$: M= 299.0713; found: 299.0710. IR (KBr, cm^{-1}): 3315, 1681, 1443, 1304, 1212, 907, 783.



*methyl 5-methyl-3-(4-methylbenzyl)-1H-indole-2-carboxylate (**7c**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7c** as a white solid (yield 64%, 93.9 mg); Mp: 158-160 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (s, 1H), 7.40 (s, 1H), 7.27 (d, *J* = 7.3 Hz, 2H), 7.15 (t, *J* = 7.4 Hz, 3H), 7.04 (d, *J* = 7.9 Hz, 2H), 4.43 (s, 2H), 3.92 (s, 3H), 2.41 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.78, 137.98, 135.21, 134.45, 129.64, 128.97, 128.32, 128.24, 127.68, 123.39, 122.62, 120.49, 111.41, 51.69, 30.05, 21.53, 20.98. HRMS (EI-TOF) m/z: calcd for $C_{19}H_{19}NO_2$: M= 293.1416; found: 293.1420. IR (KBr, cm^{-1}): 3342, 1693, 1470, 1256, 1219, 1088, 797, 766.

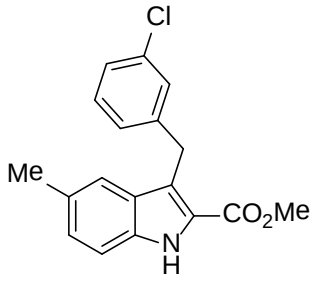


*methyl 3-(4-chlorobenzyl)-5-methyl-1H-indole-2-carboxylate (**7d**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7d** as a white solid (yield 80%, 125.5 mg); Mp = 154-156 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.39 (s, 1H), 7.35-7.25 (m, 1H), 7.27-7.15 (m, 5H), 4.43 (s, 1H), 3.91 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.53, 139.51, 134.41, 131.50, 129.90, 129.70, 128.35, 128.10, 127.85, 123.48, 121.77, 120.18, 111.55, 51.76, 29.84, 21.54. HRMS (EI-TOF) m/z: calcd for $C_{18}H_{16}{}^{35}ClNO_2$: M= 313.0870; found: 313.0874. IR (KBr, cm^{-1}): 3320, 1691, 1459, 1232, 1004, 850, 767, 692.

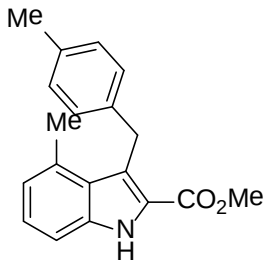


*methyl 3-(2-methoxybenzyl)-5-methyl-1H-indole-2-carboxylate (**7e**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7e** as a white solid

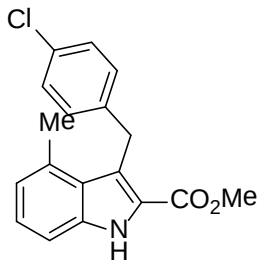
(yield 67%, 103.6 mg); Mp: 151-153 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (s, 1H), 7.35 (s, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.14 (t, *J* = 8.1 Hz, 2H), 6.88 (t, *J* = 6.1 Hz, 2H), 6.75 (t, *J* = 7.4 Hz, 1H), 4.46 (s, 2H), 3.92 (s, 3H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.98, 157.15, 134.51, 129.46, 129.33, 129.24, 128.71, 127.67, 126.89, 124.05, 122.06, 120.96, 120.44, 111.36, 110.00, 55.40, 51.77, 24.04, 21.57. HRMS (MALDI-FT) m/z: calcd for $C_{19}H_{19}NO_3$: $M+Na^+$= 332.1263; found: 332.1257. IR (KBr, cm^{-1}): 3358, 1680, 1464, 1339, 1252, 1242, 1108, 804, 773, 756.



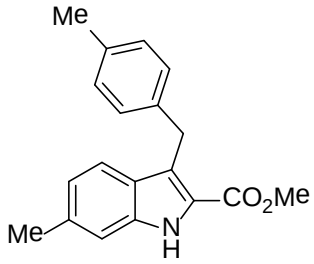
*methyl 3-(3-chlorobenzyl)-5-methyl-1H-indole-2-carboxylate (**7f**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7f** as a white solid (yield 82%, 128.6 mg); Mp = 148-150 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.73 (brs, 1H), 7.417.01 (m, 7H), 4.44 (s, 2H), 3.92 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.56, 143.06, 134.37, 134.02, 129.95, 129.50, 128.45, 128.10, 127.88, 126.59, 126.06, 123.58, 121.29, 120.17, 111.56, 51.83, 30.16, 21.58. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{16}{}^{35}ClNO_2$: $M+Na^+$= 336.0767; found: 336.0762. IR (KBr, cm^{-1}): 3342, 1672, 1464, 1254, 1213, 1086, 862, 804.



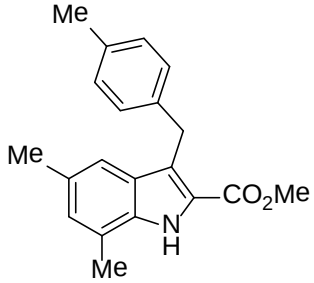
*methyl 4-methyl-3-(4-methylbenzyl)-1H-indole-2-carboxylate (**7g**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7g** as a white solid (yield 67%, 103.6 mg); Mp: 178-180 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.86 (brs, 1H), 7.44-7.11 (m, 2H), 7.01 (q, *J* = 8.1 Hz, 4H), 6.81 (d, *J* = 6.7 Hz, 1H), 4.67 (s, 2H), 3.88 (s, 3H), 2.52 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.69, 138.38, 136.56, 135.01, 133.45, 128.98, 127.87, 126.90, 125.69, 123.86, 123.07, 122.01, 109.64, 51.75, 30.87, 20.95, 20.25. HRMS (EI-TOF) m/z: calcd for $C_{19}H_{19}NO_2$: M= 293.1416; found: 293.1418. IR (KBr, cm^{-1}): 3321, 1686, 1263, 1248, 1107, 858, 787, 754.



*methyl 3-(4-chlorobenzyl)-4-methyl-1H-indole-2-carboxylate (**7h**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7h** as a white solid (yield 72%, 113.0 mg); Mp = 176-178 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (brs, 1H), 7.25-7.14 (m, 4H), 7.02 (d, *J* = 8.3 Hz, 2H), 6.83 (d, *J* = 6.9 Hz, 1H), 4.68 (s, 2H), 3.88 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.43, 139.96, 136.52, 133.15, 131.38, 129.32, 128.39, 126.69, 125.87, 123.89, 122.24, 122.21, 109.76, 51.80, 30.71, 20.19. HRMS (EI-TOF) m/z: calcd for $C_{18}H_{16}{}^{35}ClNO_2$: M= 313.0870; found: 313.0866. IR (KBr, cm^{-1}): 3321, 1682, 1464, 1267, 1248, 1095, 796, 760.

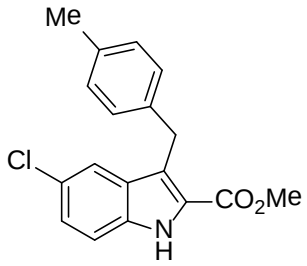


*methyl 5-methyl-3-(4-methylbenzyl)-1H-indole-2-carboxylate (**7i**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7i** as a white solid (yield 76%, 111.5 mg); Mp: 162-164 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (brs, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 3H), 7.03 (d, *J* = 7.8 Hz, 2H), 6.92 (d, *J* = 8.2 Hz, 1H), 4.43 (s, 2H), 3.92 (s, 3H), 2.44 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.82, 137.96, 136.51, 135.95, 135.23, 128.96, 128.28, 126.05, 123.29, 122.74, 122.43, 120.98, 111.36, 51.67, 30.22, 21.95, 20.98. HRMS (EI-TOF) m/z: calcd for $C_{19}H_{19}NO_2$: M= 293.1416; found: 293.1414. IR (KBr, cm^{-1}): 3340, 1693, 1470, 1256, 1219, 1088, 797, 766.

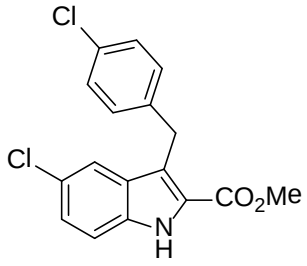


*methyl 5,7-dimethyl-3-(4-methylbenzyl)-1H-indole-2-carboxylate (**7j**)*. The title compound was purified by

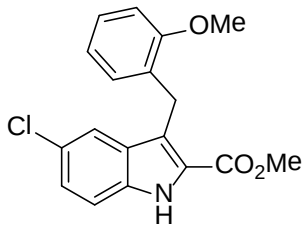
column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7j** as a white solid (yield 46%, 70.7 mg); Mp: 158-160 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.59 (brs, 1H), 7.25 (s, 1H), 7.15 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 7.7 Hz, 2H), 6.95 (s, 1H), 4.41 (s, 2H), 3.92 (s, 3H), 2.45 (s, 3H), 2.38 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.98, 138.04, 135.19, 134.27, 129.96, 128.97, 128.23, 128.04, 127.93, 123.18, 123.07, 120.73, 118.04, 51.76, 30.22, 21.53, 21.03, 16.56. HRMS (MALDI-FT) m/z: calcd for $C_{20}H_{21}NO_2$: M+Na^+= 330.1470; found: 330.1464. IR (KBr, cm^{-1}): 3348, 1684, 1247, 1261, 852, 795, 758.



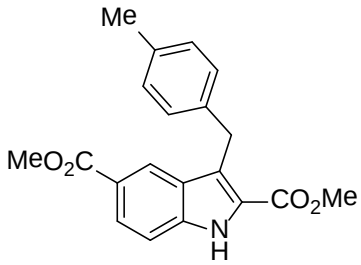
*methyl 5-chloro-3-(4-methylbenzyl)-1H-indole-2-carboxylate (**7k**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7k** as a white solid (yield 73%, 114.5 mg); Mp = 184-186 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.85 (brs, 1H), 7.61m7.53 (m, 1H), 7.36-7.19 (m, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 7.9 Hz, 2H), 4.40 (s, 2H), 3.94 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.51, 137.37, 135.55, 134.25, 129.12, 128.99, 128.21, 126.20, 126.04, 124.52, 122.52, 120.56, 112.93, 52.00, 30.03, 21.02. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{16}{}^{35}ClNO_2$: M+$Na^+$= 336.0767; found: 336.0762. IR (KBr, cm^{-1}): 3334, 1691, 1460, 1258, 1217, 1109, 763.8.



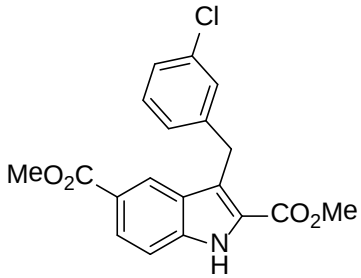
*methyl 5-chloro-3-(4-chlorobenzyl)-1H-indole-2-carboxylate (**7l**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7l** as a white solid (yield 74%, 123.7 mg); Mp: 160-162 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.85 (brs, 1H), 7.54 (s, 1H), 7.36-7.05 (m, 6H), 4.41 (s, 1H), 3.94 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.18, 138.89, 134.20, 131.83, 129.64, 128.82, 128.50, 126.39, 126.31, 124.67, 121.67, 120.27, 113.04, 52.01, 29.78. HRMS (EI-TOF) m/z: calcd for $C_{17}H_{13}{}^{35}Cl_2NO_2$: M= 333.0323; found: 333.0324. IR (KBr, cm^{-1}): 3379, 1734, 1583, 1500, 1490, 1435, 1244, 1159, 1091, 814, 798.



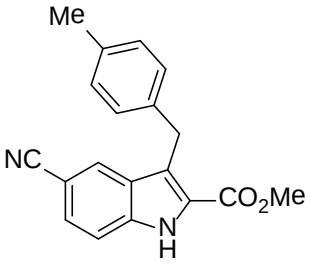
*methyl 5-chloro-3-(2-methoxybenzyl)-1H-indole-2-carboxylate (**7m**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7m** as a white solid (yield 72%, 118.7 mg); Mp: 186-188 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (brs, 1H), 7.60 (s, 1H), 7.36-7.20 (m, 2H), 7.16 (t, *J* = 7.7 Hz, 1H), 6.96 (d, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 8.1 Hz, 1H), 6.78 (t, *J* = 7.4 Hz, 1H), 4.44 (s, 2H), 3.92 (s, 3H), 3.91 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.63, 157.07, 134.28, 129.47, 129.38, 128.78, 127.24, 126.15, 125.90, 125.04, 122.35, 121.22, 120.50, 112.78, 110.17, 55.34, 52.00, 24.06. HRMS (EI-TOF) m/z: calcd for $C_{18}H_{16}{}^{35}ClNO_3$: M= 329.0819; found: 329.0823. IR (KBr, cm^{-1}): 3348, 1684, 1454, 1254, 1244, 1113, 1024, 811, 756.



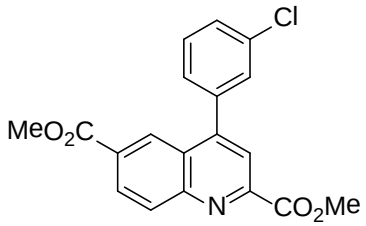
*dimethyl 3-(4-methylbenzyl)-1H-indole-2,5-dicarboxylate (**7n**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7n** as a white solid (yield 66%, 111.3 mg); Mp: 185-187 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.44 (s, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.38 (d, *J* = 8.7 Hz, 1H), 7.16 (d, *J* = 7.7 Hz, 2H), 7.05 (d, *J* = 7.6 Hz, 2H), 4.48 (s, 2H), 3.95 (s, 3H), 3.92 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.68, 162.42, 138.33, 137.47, 135.60, 129.18, 128.32, 127.81, 126.73, 124.72, 124.65, 124.58, 122.71, 111.59, 52.07, 30.04, 29.78, 21.06. HRMS (MALDI-FT) m/z: calcd for $C_{20}H_{19}NO_4$: M+Na^+= 360.1212; found: 360.1206. IR (KBr, cm^{-1}): 3315, 1718, 1690, 1435, 1256, 1209, 1115, 754.



*dimethyl 3-(3-chlorobenzyl)-1H-indole-2,5-dicarboxylate (**7o**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7o** as a white solid (yield 33%, 59.0 mg); Mp: 177-179 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.03 (brs, 1H), 8.42-8.35 (m, 1H), 8.02 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.42 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.24-7.08 (m, 4H), 4.49 (s, 2H), 3.95 (s, 3H), 3.93 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.51, 162.11, 142.44, 138.22, 134.17, 129.60, 128.43, 127.56, 126.80, 126.55, 126.29, 124.95, 124.15, 123.17, 122.87, 111.67, 52.07, 52.05, 30.03. HRMS (MALDI-FT) m/z: calcd for $C_{19}H_{16}{}^{35}ClNO_4$: $M+Na^+$= 380.0666; found: 380.0660. IR (KBr, cm^{-1}): 3317, 1713, 1695, 1433, 1261, 1250, 1117, 1076, 756.

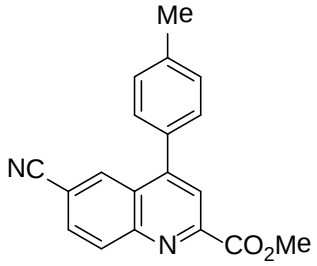


*methyl 5-cyano-3-(4-methylbenzyl)-1H-indole-2-carboxylate (**7p**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **7p** as a white solid (yield 32%, 48.7 mg); Mp: 201-204 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.09 (s, 1H), 7.94 (s, 1H), 7.48 (dt, *J* = 20.3, 4.8 Hz, 2H), 7.10 (dd, *J* = 18.8, 8.1 Hz, 4H), 4.45 (s, 2H), 3.98 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.16, 137.25, 136.79, 135.90, 129.28, 128.20, 127.89, 127.77, 127.50, 125.38, 123.67, 120.07, 112.80, 103.77, 52.23, 30.05, 20.99. HRMS (MALDI-FT) m/z: calcd for $C_{19}H_{16}N_2O_2$: $M+Na^+$= 327.1110; found: 327.1104. IR (KBr, cm^{-1}): 3363, 3311, 2220, 1690, 1678, 1463, 1350, 1259, 1080, 810, 768.

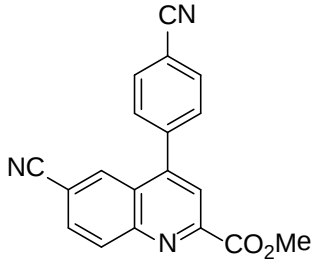


*dimethyl 4-(3-chlorophenyl)quinoline-2,6-dicarboxylate (**8a**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **8a** as a white solid (yield 31%, 55.1 mg); Mp: 175-178 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 1.0 Hz, 1H), 8.48-8.31 (m, 2H), 8.19 (s, 1H), 7.54 (dd, *J* = 5.4, 1.8 Hz, 3H), 7.47-7.35 (m, 1H), 4.12 (s, 3H), 3.96 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.26, 165.52, 155.85, 149.90, 149.25, 138.53, 135.09, 131.54, 130.29, 130.21, 129.79,

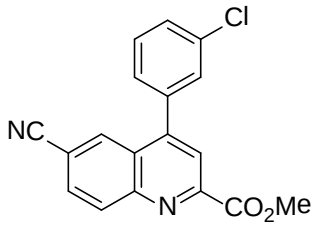
129.52, 129.38, 128.35, 127.79, 126.81, 121.92, 53.47, 52.29. HRMS (MALDI-FT) m/z: calcd for $C_{19}H_{14}{}^{35}ClNO_4$: M+H$^+$= 356.0690; found: 356.0684. IR (KBr, cm^{-1}): 3429, 2922, 1730, 1437, 1364, 1271, 1142, 781.



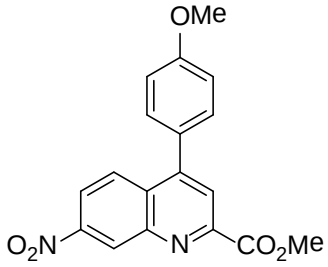
*methyl 6-cyano-4-(p-tolyl)quinoline-2-carboxylate (**8b**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **8b** as a white solid (yield 33%, 49.9 mg); Mp: 190-192 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 10, 5.2 Hz, 2H), 8.25 (s, 1H), 7.92 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.41 (s, 4H), 4.12 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.40, 151.04, 149.97, 149.09, 139.85, 133.07, 132.56, 132.49, 130.55, 129.89, 129.44, 127.44, 122.54, 118.39, 112.18, 53.53, 21.37. HRMS (MALDI-FT) m/z: calcd for $C_{19}H_{14}N_2O_2$: M+H$^+$= 303.1134; found: 303.1129. IR (KBr, cm^{-1}): 3312, 2220, 1691, 1263, 1219, 812, 768.



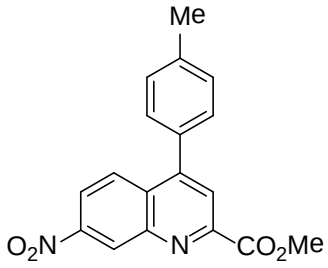
*methyl 6-cyano-4-(4-cyanophenyl)quinoline-2-carboxylate (**8c**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **8c** as a white solid (yield 70%, 109.7 mg); Mp: 270-272 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (d, *J* = 1.4 Hz, 1H), 8.43 (dt, *J* = 8.9, 5.3 Hz, 2H), 8.19 (s, 1H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.68 (d, *J* = 8.3 Hz, 2H), 4.12 (s, 3H), 3.96 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.10, 165.39, 149.89, 149.17, 141.39, 132.78, 131.74, 130.60, 130.35, 129.99, 127.84, 126.37, 121.82, 118.22, 113.35, 111.93, 53.55, 52.73. HRMS (MALDI-FT) m/z: calcd for $C_{20}H_{14}N_2O_4$: M+H$^+$= 347.1032; found: 347.1026. IR (KBr, cm^{-1}): 3439, 2920, 2231, 1733, 1265, 1122, 835.



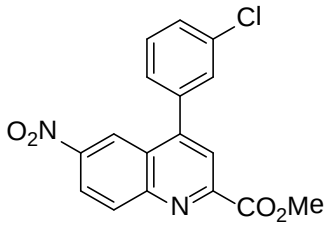
*methyl 4-(3-chlorophenyl)-6-cyanoquinoline-2-carboxylate (**8d**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30/1) to afford pure **8d** as a white solid (yield 73%, 117.8 mg); Mp: 200-203 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.8 Hz, 1H), 8.32 (d, *J* = 1.2 Hz, 1H), 8.25 (s, 1H), 7.96 (dd, *J* = 8.8, 1.5 Hz, 1H), 7.65-7.43 (m, 3H), 7.40 (d, *J* = 6.6 Hz, 1H), 4.13 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.12, 150.05, 149.26, 148.97, 137.68, 135.36, 132.64, 131.92, 130.88, 130.45, 129.79, 129.43, 127.64, 127.03, 122.61, 118.17, 112.70, 53.60. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{11}{}^{35}ClN_2O_2$: M+H$^+$= 323.0587; found: 323.0582. IR (KBr, cm^{-1}): 3067, 2947, 2231, 1724, 1435, 1362, 1259, 1115, 849.



*methyl 4-(4-methoxyphenyl)-7-nitroquinoline-2-carboxylate (**8e**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford pure **8e** as a white solid (yield 81%, 137.0 mg); Mp: 190-193 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.35 (d, *J* = 9.3 Hz, 1H), 8.28 (s, 1H), 8.21 (d, *J* = 9.3 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 4.13 (s, 3H), 3.93 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.36, 160.73, 150.27, 149.78, 148.46, 147.41, 131.04, 130.93, 128.49, 127.91, 127.11, 123.62, 121.57, 114.61, 55.52, 53.53. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{14}N_2O_5$: M+H$^+$= 339.0981; found: 339.0976. IR (KBr, cm^{-1}): 3427, 2949, 1724, 1512, 1445, 1344, 1259, 1248, 1128, 845.



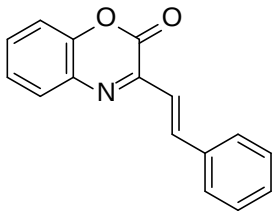
methyl 7-nitro-4-(p-tolyl)quinoline-2-carboxylate ***(8f)***. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 25/1) to afford pure **8f** as a white solid (yield 78%, 125.7 mg); Mp: 200-202 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.29 (d, *J* = 2.1 Hz, 1H), 8.35 (dd, *J* = 9.3, 2.2 Hz, 1H), 8.29 (s, 1H), 8.19 (d, *J* = 9.3 Hz, 1H), 7.42 (q, *J* = 8.2 Hz, 4H), 4.13 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.33, 150.62, 149.82, 148.50, 147.35, 139.71, 133.39, 131.00, 129.79, 129.44, 127.92, 127.11, 123.69, 121.61, 53.52, 21.36. HRMS (MALDI-FT) m/z: calcd for $C_{18}H_{14}N_2O_4$: $M+H^+$= 323.1032; found: 323.1026. IR (KBr, cm^{-1}): 3109, 2957, 1722, 1527, 1514, 1440, 1365, 1344, 1258, 1124, 829, 743.



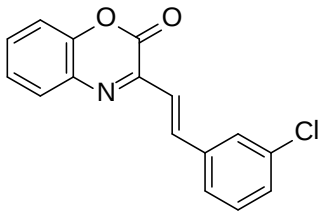
methyl 4-(3-chlorophenyl)-6-nitroquinoline-2-carboxylate ***(8g)***. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 15/1) to afford pure **8g** as a white solid (yield 73%, 125.1 mg); Mp: 204-207 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.86 (d, *J* = 2.0 Hz, 1H), 8.65-8.42 (m, 2H), 8.28 (s, 1H), 7.66-7.49 (m, 3H), 7.47-7.30 (m, 1H), 4.14 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 165.07, 150.79, 150.52, 150.07, 147.14, 137.66, 135.46, 133.13, 130.52, 129.93, 129.46, 127.65, 126.70, 123.78, 122.69, 122.33, 53.66. HRMS (MALDI-FT) m/z: calcd for $C_{17}H_{11}{}^{35}ClN_2O_4$: $M+H^+$= 343.0486; found: 343.0480. IR (KBr, cm^{-1}): 3435, 1722, 1622, 1499,1364, 1342, 1256, 1143, 1117, 800.

Typical procedure for one-pot reaction of 2-triflate anilines and arylvinyldiazoacetates

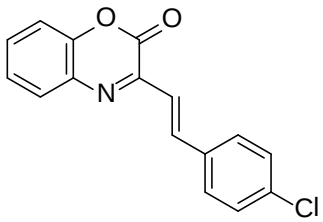
To a solution of 2-triflate anilines (0.52 mmol) and $PdCl_2$ (5 mol%) in CH_2Cl_2 (2 mL), was added vinyldiazoacetates (0.5 mmol). Then the mixture was stirred at room temperature under nitrogen atmosphere. After the reaction mixture was stirred for 3 hours, then $NaHCO_3$ (0.75 mmol) and DMF (2 mL) were added and the reaction mixture was continue to be stirred at 80^{o}C for another 2 hours. Then the resulting mixture was cooled and diluted with ether (20 mL); then washed with brine (10 mL×3); the organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated; the residue was purified by column chromatography to give the desired product.



(E)-3-styryl-2H-benzo[b][1,4]oxazin-2-one ***(10a)***[15]. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10a** as a yellow solid (yield 71%, 88.5 mg); Mp: 144-146 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.16 (d, *J* = 15.0 Hz, 1H), 7.78 (d, *J* = 6.0 Hz, 1H), 7.67 (d, *J* = 6.0 Hz, 2H), 7.56 (s, 1H), 7.48-7.30 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.1, 149.6, 146.1, 140.4, 135.8, 132.0, 130.6, 130.0, 129.0, 128.9, 128.1, 125.7, 121.2, 116.3; HRMS (MALDI-FT) m/z: calcd for $C_{16}H_{12}NO_2$: $M+H^+$ = 250.0868; found : 250.0863. IR (KBr, cm^{-1}): 3012, 2996, 1742, 1623, 1600, 1503, 1488, 1265, 1069, 979, 756.

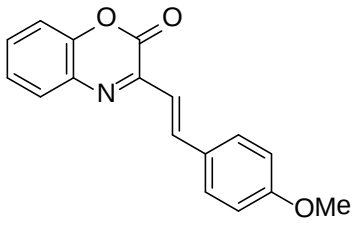


(E)-3-(3-chlorostyryl)-2H-benzo[b][1,4]oxazin-2-one ***(10b)***. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10b** as a yellow solid (yield 82%, 116.3 mg); Mp: 140-143 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (d, *J* = 16.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.65 (s, 1H), 7.54-7.47 (m, 3H), 7.41-7.30 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.0, 149.2, 146.1, 138.7, 137.6, 135.0, 131.9, 130.9, 130.1, 129.7, 129.1, 127.8, 126.2, 125.7, 122.6, 116.4; HRMS (EI-TOF) m/z: calcd for $C_{16}H_{10}NO_2{}^{35}Cl$: 283.0400; found: 283.0402. IR (KBr, cm^{-1}): 3078, 2924, 1734, 1628, 1601, 1524, 1462, 1421, 1287, 1072, 988, 764, 681.

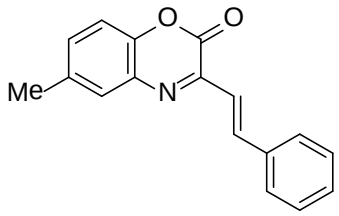


(E)-6-chloro-3-styryl-2H-benzo[b][1,4]oxazin-2-one ***(10c)***. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10c** as a yellow solid (yield 80%, 113.5 mg); Mp: 146-148 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 16.0 Hz, 1H), 7.78 (d, *J* = 4.0 Hz, 1H), 7.69-7.67 (m, 2H), 7.52 (d, *J* = 16.0 Hz, 1H), 7.44-7.41 (m, 4H), 7.27-7.24 (m, 1H); ^{13}C NMR

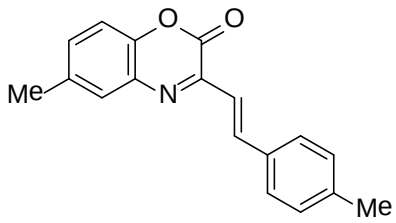
(125 MHz, $CDCl_3$) δ 152.6, 150.6, 144.6, 141.5, 135.6, 132.6, 130.8, 130.3, 130.3, 129.0, 128.4, 128.3, 120.7, 117.4; HRMS (EI-TOF) m/z: calcd for $C_{16}H_{10}NO_2{}^{35}Cl$: 283.0400; found: 283.0405. IR (KBr, cm^{-1}): 3082, 3051, 1738, 1622, 1603, 1464, 1286, 1074, 976, 824, 752, 615.



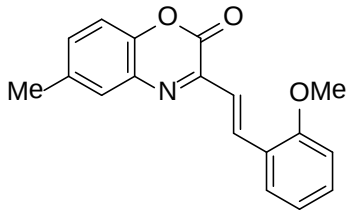
*(E)-3-(4-methoxystyryl)-2H-benzo[b][1,4]oxazin-2-one (**10d**)*[15]. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1) to afford pure **10d** as a yellow solid (yield 75%, 104.7 mg); Mp: 161-164 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ 8.12 (d, *J* = 15.0 Hz, 1H), 7.77-7.74 (m, 1H), 7.63 (d, *J* = 9.0 Hz, 2H), 7.45-7.36 (m, 3H), 7.31-7.28 (m, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 153.3, 149.8, 146.0, 140.2, 132.5, 130.1, 129.8, 128.8, 125.6, 118.9, 116.3, 114.5, 113.3, 55.4; HRMS (MALDI-FT) m/z: calcd for $C_{17}H_{14}NO_3$: $M+H^+$ = 280.0977; found: 280.0974. IR (KBr, cm^{-1}): 2956, 2905, 1732, 1626, 1601, 1524, 1511, 1464, 1261, 1081, 978, 756.



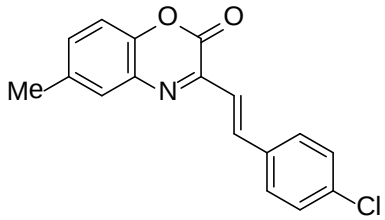
*(E)-6-methyl-3-styryl-2H-benzo[b][1,4]oxazin-2-one (**10e**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10e** as a yellow solid (yield 72%, 94.8 mg); Mp: 147-149 ^oC; ^1H NMR (500 MHz, $CDCl_3$): δ 8.13 (d, *J* = 20.0 Hz, 1H), 7.67 (d, *J* = 5.0 Hz, 2H), 7.57 (s, 1H), 7.52 (d, *J* = 20.0 Hz, 1H), 7.43-7.36 (m, 3H), 7.28-7.26 (m, 1H), 7.19 (d, *J* = 10.0 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.5, 149.6, 144.1, 140.2, 136.0, 135.7, 131.8, 131.7, 130.0, 129.0, 128.9, 128.2, 121.4, 116.0, 20.9; HRMS (EI-TOF) m/z: calcd for $C_{17}H_{13}NO_2$: 263.0946; found: 263.0947. IR (KBr, cm^{-1}): 3016, 2965, 1736, 1602, 1588, 1509, 1468, 1420, 1326, 1285, 1032, 962, 785.



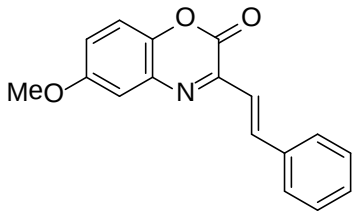
*(E)-6-methyl-3-(4-methylstyryl)-2H-benzo[b][1,4]oxazin-2-one (**10f**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10f** as a yellow solid (yield 62%, 86.0 mg); Mp: 182-184 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.11 (d, *J* = 15.0 Hz, 1H), 7.58-7.55 (m, 3H), 7.48 (d, *J* = 18.0 Hz, 1H), 7.28-7.14 (m, 5H), 2.45 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.5, 149.6, 144.0, 140.2, 135.5, 133.2, 131.8, 131.4, 130.3, 129.7, 128.7, 128.1, 120.3, 115.8, 21.5, 20.9; HRMS (EI-TOF) m/z: calcd for $C_{18}H_{15}NO_2$: 277.1103; found: 277.1105. IR (KBr, cm^{-1}): 3026, 2920, 1730, 1622, 1587, 1520, 1489, 1281, 1078, 978, 777.



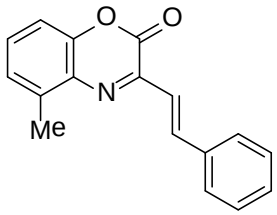
*(E)-3-(2-methoxystyryl)-6-methyl-2H-benzo[b][1,4]oxazin-2-one (**10g**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10g** as a yellow solid (yield 66%, 96.8 mg); Mp: 121-122 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.44 (d, *J* = 18.0 Hz, 1H), 7.71-7.68 (m, 1H), 7.62-7.56 (m, 2H), 7.34-7.32 (m, 1H), 7.25-7.16 (m, 2H), 7.01-6.92 (m, 1H), 3.93 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.4, 153.6, 150.0, 144.1, 135.4, 135.2, 131.9, 131.2, 131.1, 128.8, 128.3, 124.9, 121.5, 120.8, 115.8, 111.1, 55.6, 20.9; HRMS (EI-TOF) m/z: calcd for $C_{18}H_{15}NO_3$: 293.1052; found: 293.1051. IR (KBr, cm^{-1}): 3072, 2999, 1741, 1614, 1587, 1518, 1491, 1300, 1248, 1074, 983, 746.



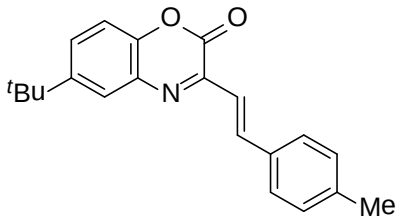
*(E)-3-(4-chlorostyryl)-6-methyl-2H-benzo[b][1,4]oxazin-2-one (**10h**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1) to afford pure **10h** as a yellow solid (yield 76%, 113.1 mg); Mp: 161-164 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.07 (d, *J* = 15.0 Hz, 1H), 7.60-7.56 (m, 3H), 7.47 (d, *J* = 18.0 Hz, 1H), 7.38 (d, *J* = 6.0 Hz, 2H), 7.30-7.27 (m, 1H), 7.19 (d, *J* = 6.0 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.3, 149.2, 144.1, 138.6, 135.7, 134.4, 131.8, 131.7, 129.2, 128.9, 121.9, 115.9, 20.9; HRMS (EI-TOF) m/z: calcd for $C_{17}H_{12}NO_2{}^{35}Cl$: 297.0557; found: 297.0559. IR (KBr, cm^{-1}): 2950, 2921, 1747, 1626, 1585, 1510, 1491, 1132, 1086, 976, 820, 781, 588.



*(E)-6-methoxy-3-styryl-2H-benzo[b][1,4]oxazin-2-one (**10i**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10i** as a yellow solid (yield 67%, 93.6 mg); Mp: 154-156 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, *J* = 16.0 Hz, 1H), 7.67 (d, *J* = 4.0 Hz, 1H), 7.52 (d, *J* = 16.0 Hz, 1H), 7.43-7.38 (m, 3H), 7.26-7.21 (m, 2H), 7.06 (dd, *J* = 8.0, 4.0 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 153.4, 149.9, 140.4, 140.4, 135.9, 132.4, 130.0, 128.9, 128.2, 121.3, 118.8, 116.9, 110.8, 55.9; HRMS (EI-TOF) m/z: calcd for $C_{17}H_{13}NO_3$: 279.0895; found: 279.0900. IR (KBr, cm^{-1}): 3058, 3011, 1745, 1602, 1577, 1499, 1450, 1321, 1256, 1052, 952, 739.

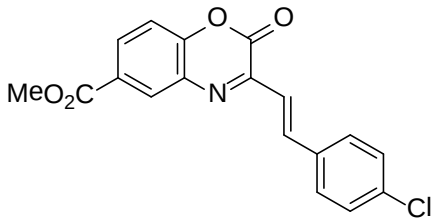


*(E)-5-methyl-3-styryl-2H-benzo[b][1,4]oxazin-2-one (**10j**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10j** as a yellow solid (yield 69%, 90.8 mg); Mp: 123-125 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.13 (d, *J* = 15.0 Hz, 1H), 7.68-7.65 (m, 2H), 7.53 (d, *J* = 15.0 Hz, 1H), 7.41-7.31 (m, 4H), 7.20 (d, *J* = 6.0 Hz, 1H), 7.12 (d, *J* = 9.0 Hz, 1H), 2.68 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.3, 147.9, 146.4, 139.8, 138.4, 136.0, 130.6, 130.3, 129.8, 128.9, 128.1, 126.7, 121.7, 113.9, 17.0; HRMS (EI-TOF) m/z: calcd for $C_{17}H_{13}NO_2$: 263.0946; found: 263.0944. IR (KBr, cm^{-1}): 3024, 2920, 1726, 1622, 1605, 1522, 1479, 1450, 1375, 1265, 1076, 978, 777.

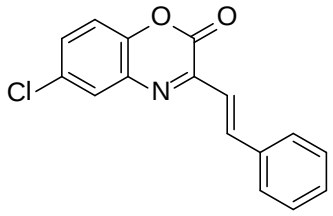


*(E)-6-(tert-butyl)-3-(4-methylstyryl)-2H-benzo[b][1,4]oxazin-2-one (**10k**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1) to afford pure **10k** as a yellow solid (yield 74%, 118.2 mg); Mp: 164-166 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.12 (d, *J* = 15.0 Hz, 1H), 7.77 (d, 1H), 7.58-7.46 (m, 4H), 7.26-7.22 (m, 3H), 2.39 (s, 3H), 1.39 (s, 9H); ^{13}C NMR (125 MHz,

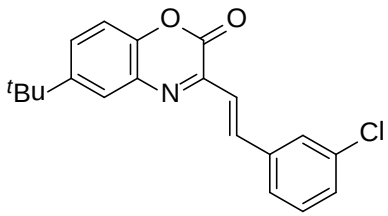
$CDCl_3$):δ 153.5, 149.6, 149.1, 143.8, 140.1, 133.2, 131.6, 130.2, 129.7, 128.1, 128.0, 125.4, 120.3, 115.7, 34.7, 31.3, 21.5; HRMS (EI-TOF) m/z: calcd for $C_{21}H_{21}NO_2$: 319.1572; found: 319.1574. IR (KBr, cm^{-1}): 3029, 2959, 1732, 1620, 1583, 1520, 1489, 1267, 1072, 974, 780.



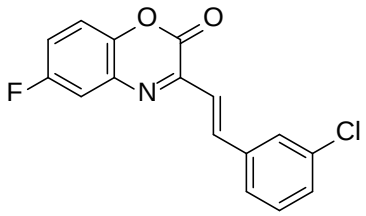
*(E)-methyl 3-(4-chlorostyryl)-2-oxo-2H-benzo[b][1,4]oxazine-6-carboxylate (**10l**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1) to afford pure **10l** as a yellow solid (yield 80%, 136.7 mg); Mp: 189-191 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.47 (d, *J* = 4.0 Hz, 1H), 8.16-8.10 (m, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 16.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.7, 152.4, 150.2, 149.1, 139.9, 136.2, 134.2, 131.7, 131.6, 130.9, 129.5, 129.4, 128.1, 121.3, 116.6, 52.6; HRMS (EI-TOF) m/z: calcd for $C_{18}H_{12}NO_4{}^{35}Cl$: 341.0455; found: 341.0450. IR (KBr, cm^{-1}): 3030, 2953, 1746, 1722, 1624, 1599, 1492, 1431, 1302, 1213, 1072, 984, 762.



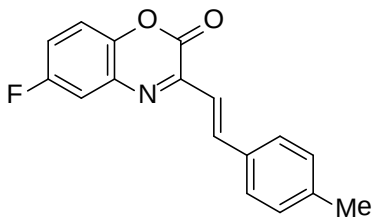
*(E)-6-chloro-3-styryl-2H-benzo[b][1,4]oxazin-2-one (**10m**).* The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10m** as a yellow solid (yield 80%, 113.5 mg); Mp: 146-148 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 16.0 Hz, 1H), 7.78 (d, *J* = 4.0 Hz, 1H), 7.69-7.67 (m, 2H), 7.52 (d, *J* = 16.0 Hz, 1H), 7.44-7.41 (m, 4H), 7.27-7.24 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.6, 150.6, 144.6, 141.5, 135.6, 132.6, 130.8, 130.3, 130.3, 129.0, 128.4, 128.3, 120.7, 117.4; HRMS (EI-TOF) m/z: calcd for $C_{16}H_{10}NO_2{}^{35}Cl$: 283.0400; found: 283.0405. IR (KBr, cm^{-1}): 3042, 2982, 1729, 1615, 1589, 1534, 1482, 1453, 1321, 1292, 1070, 979, 772, 672.



*(E)-6-(tert-butyl)-3-(3-chlorostyryl)-2H-benzo[b][1,4]oxazin-2-one (**10n**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1) to afford pure **10n** as a yellow solid (yield 72%, 122.3 mg); Mp: 136-138 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, *J* = 16.0 Hz, 1H), 7.78 (d, 1H), 7.65 (s, 1H), 7.55-7.49 (m, 3H), 7.35-7.34 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 1H), 1.39 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.3, 149.3, 149.0, 143.9, 138.4, 137.7, 135.0, 131.4, 130.1, 129.7, 128.6, 127.8, 126.2, 125.6, 122.7, 115.7, 34.7, 31.3; HRMS (EI-TOF) m/z: calcd for $C_{20}H_{18}NO_2{}^{35}Cl$: 339.1026; found: 339.1023. IR (KBr, cm^{-1}): 3068, 2962, 1732, 1626, 1587, 1487, 1471, 1425, 1261, 1198, 1068, 962, 770.



*(E)-3-(3-chlorostyryl)-6-fluoro-2H-benzo[b][1,4]oxazin-2-one (**10o**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1) to afford pure **10o** as a yellow solid (yield 84%, 126.7 mg); Mp: 174-176 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 16.0 Hz, 1H), 7.65 (s, 1H), 7.55-7.46 (m, 3H), 7.37-7.35 (m, 2H), 7.30-7.27 (m, 1H), 7.23-7.19 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.5, 158.6, 152.7, 150.2, 139.7, 137.4, 135.0, 130.2, 130.0, 128.0, 126.4, 122.2, 118.3, 118.1, 117.4, 117.3, 114.8, 114.6; HRMS (EI-TOF) m/z: calcd for $C_{16}H_9NO_2F^{35}Cl$: 301.0306; found: 301.0312. IR (KBr, cm^{-1}): 3038, 2996, 1734, 1624, 1593, 1510, 1479, 1437, 1274, 1250, 1092, 989, 773, 681, 558.



*(E)-6-fluoro-3-(4-methylstyryl)-2H-benzo[b][1,4]oxazin-2-one (**10p**)*. The title compound was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1) to afford pure **10p** as a yellow solid (yield 76%, 106.9 mg); Mp: 172-174 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.14 (d, *J* = 18.0 Hz, 1H), 7.57 (d, *J* = 6.0 Hz, 2H), 7.50-7.43 (m, 2H), 7.29-7.17 (m, 5H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.5, 158.6, 152.9, 150.7, 141.4, 140.8, 132.9, 130.4, 129.8, 128.7, 128.3, 119.8, 117.6, 117.4, 117.2, 114.5, 114.4, 21.5; HRMS (EI-TOF) m/z: calcd for $C_{17}H_{12}NO_2F$: 281.0852; found: 281.0851. IR (KBr, cm^{-1}): 3047,

2920, 1734, 1624, 1595, 1514, 1485, 1261, 1076, 968, 602.

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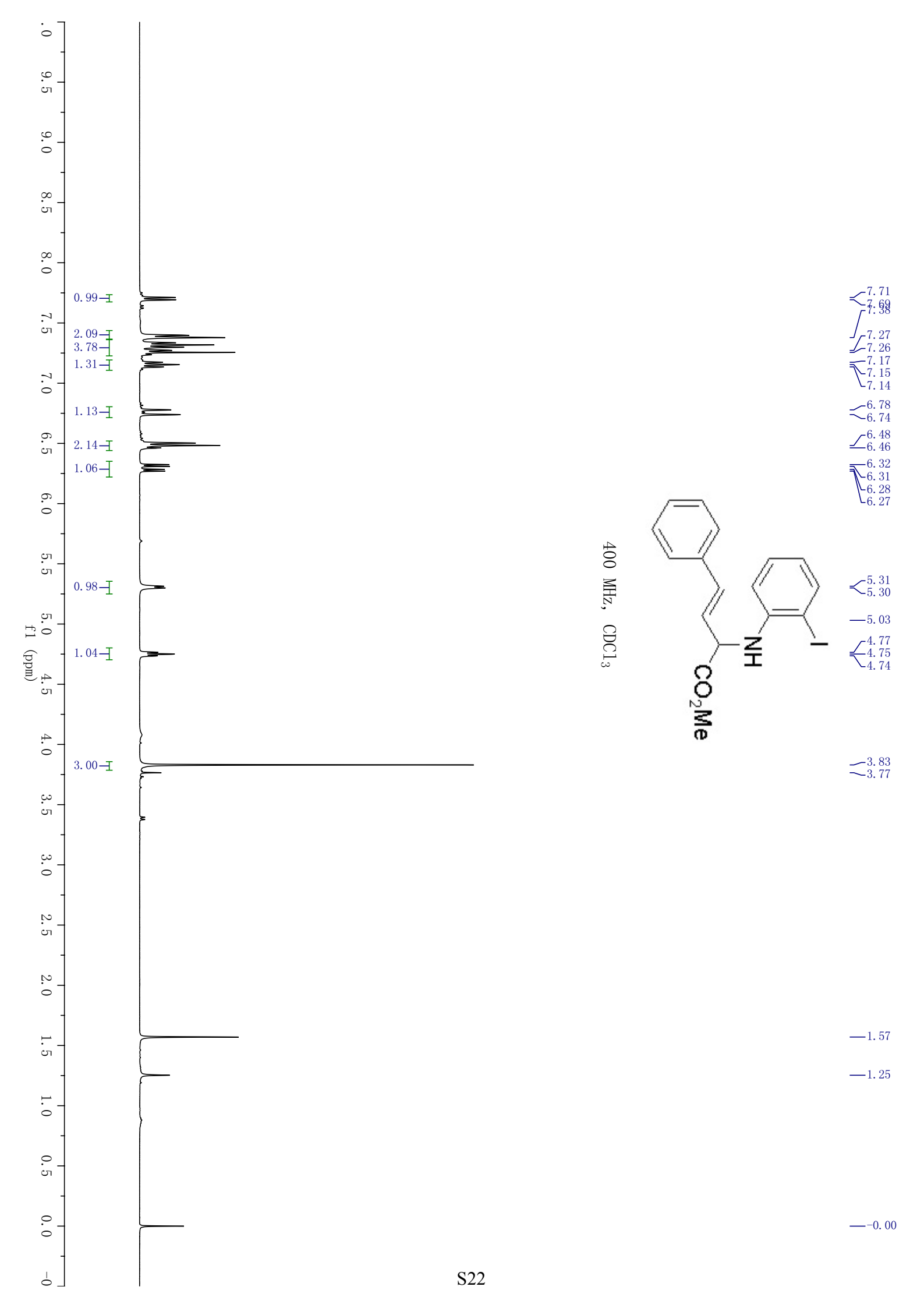
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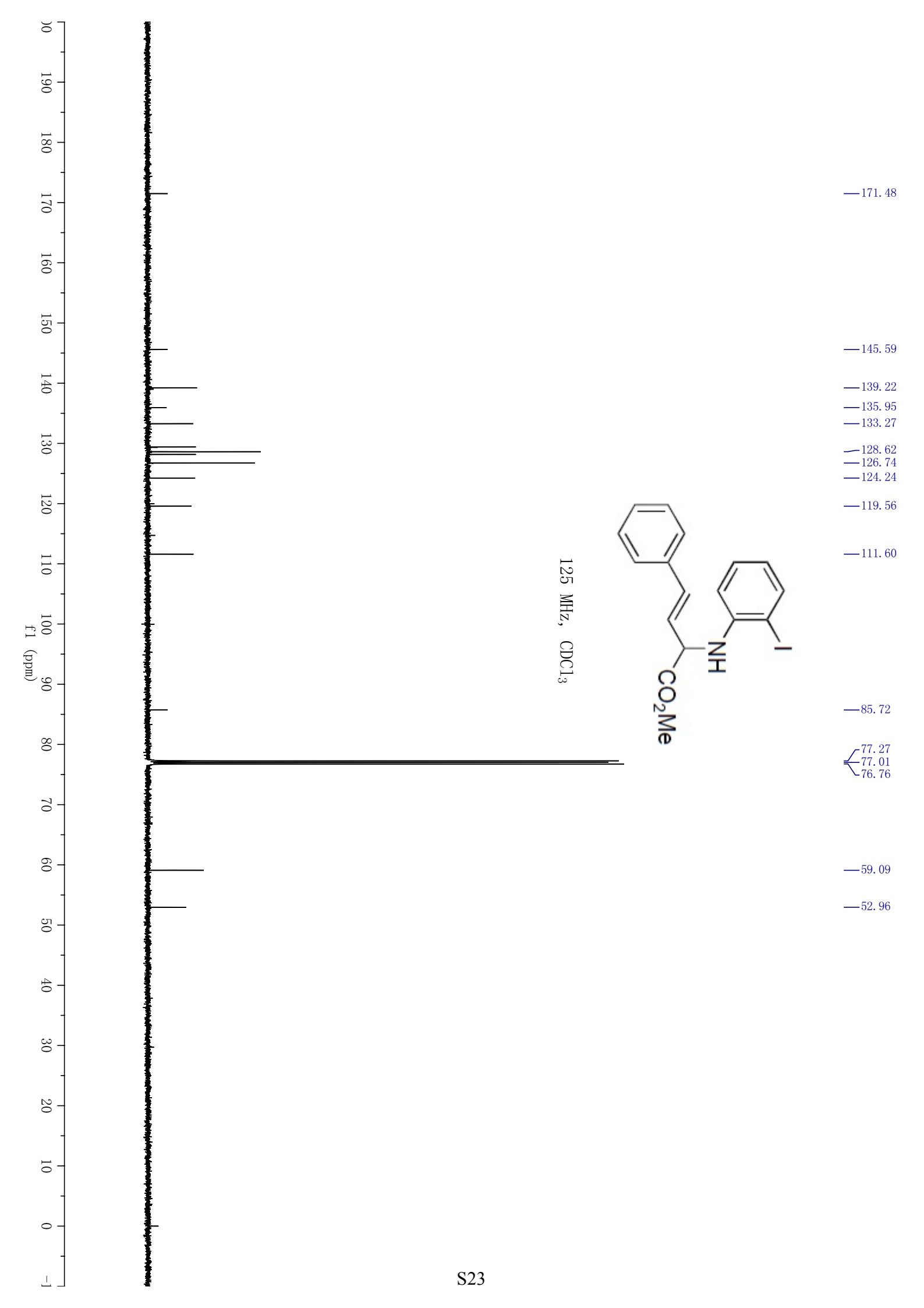
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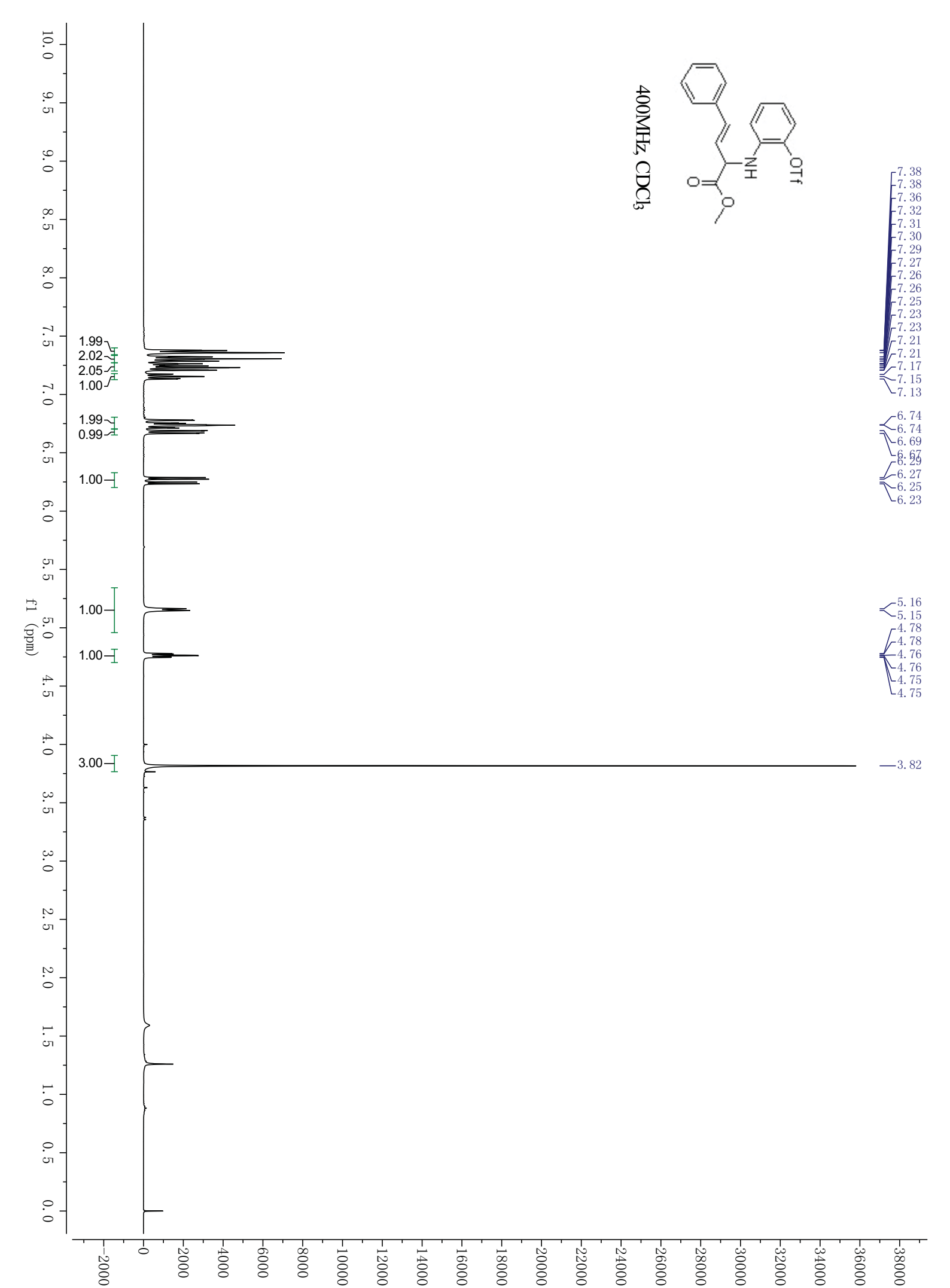
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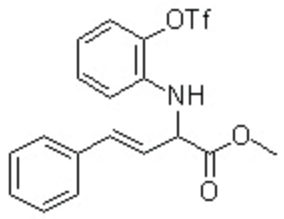

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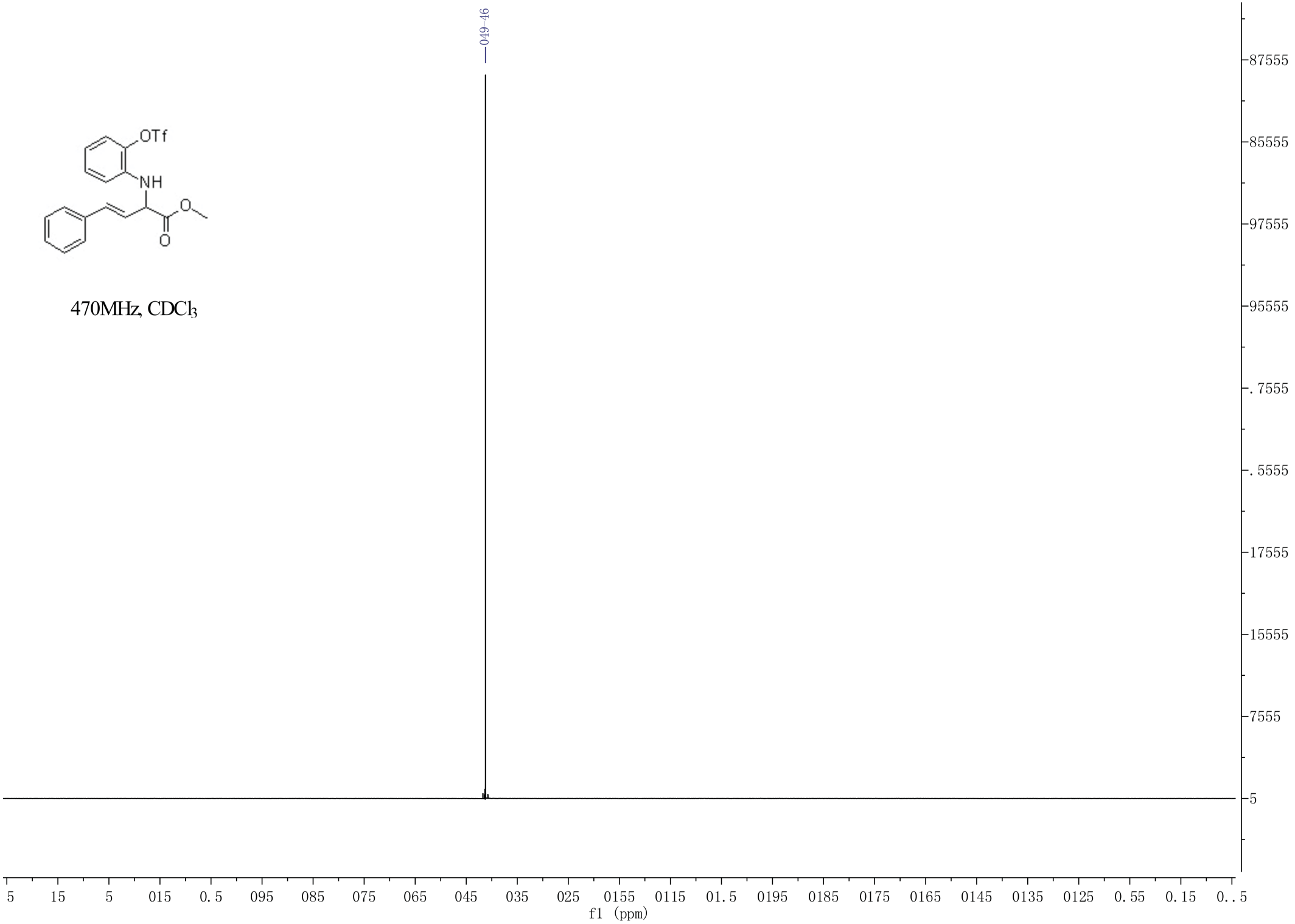

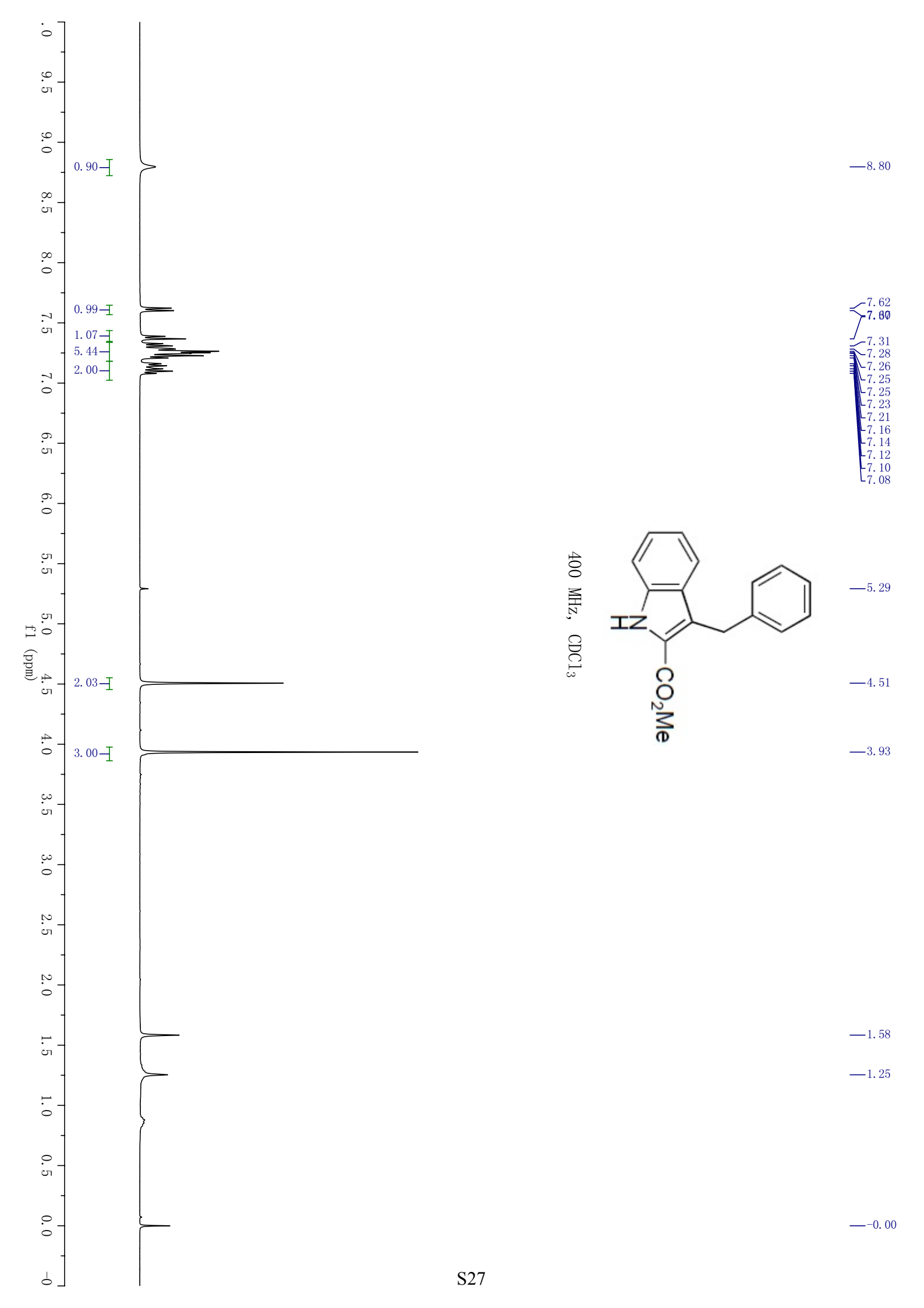
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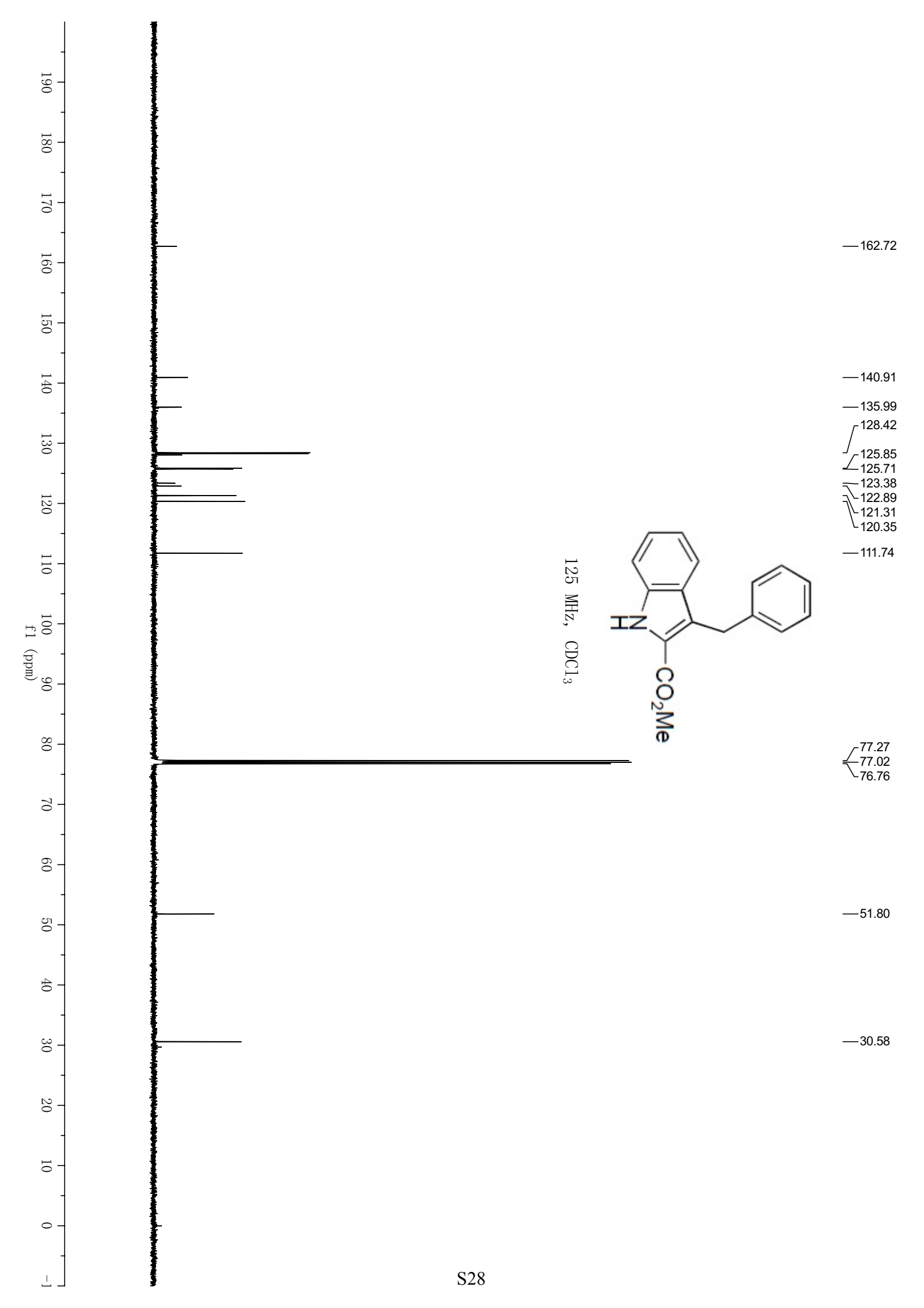
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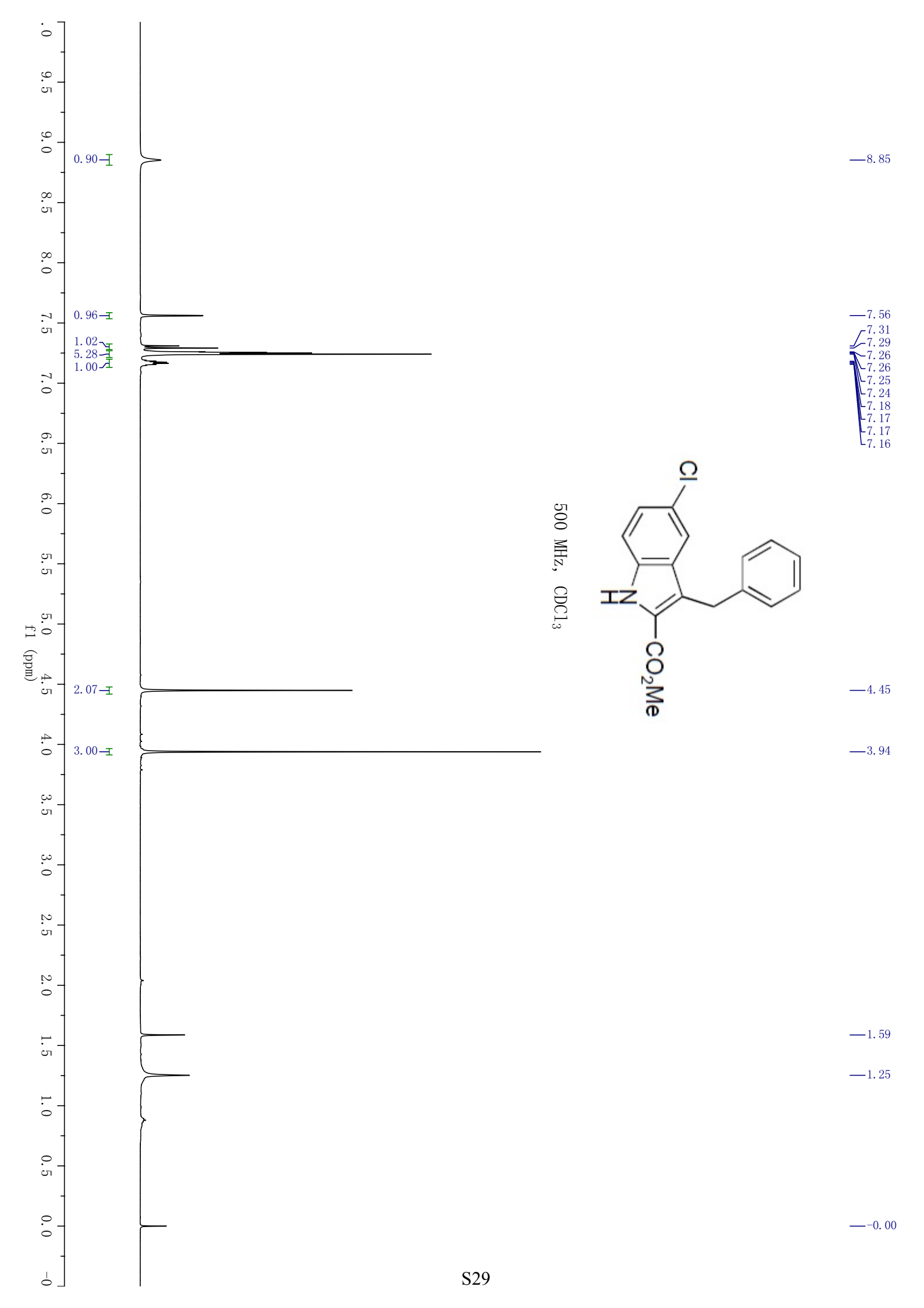
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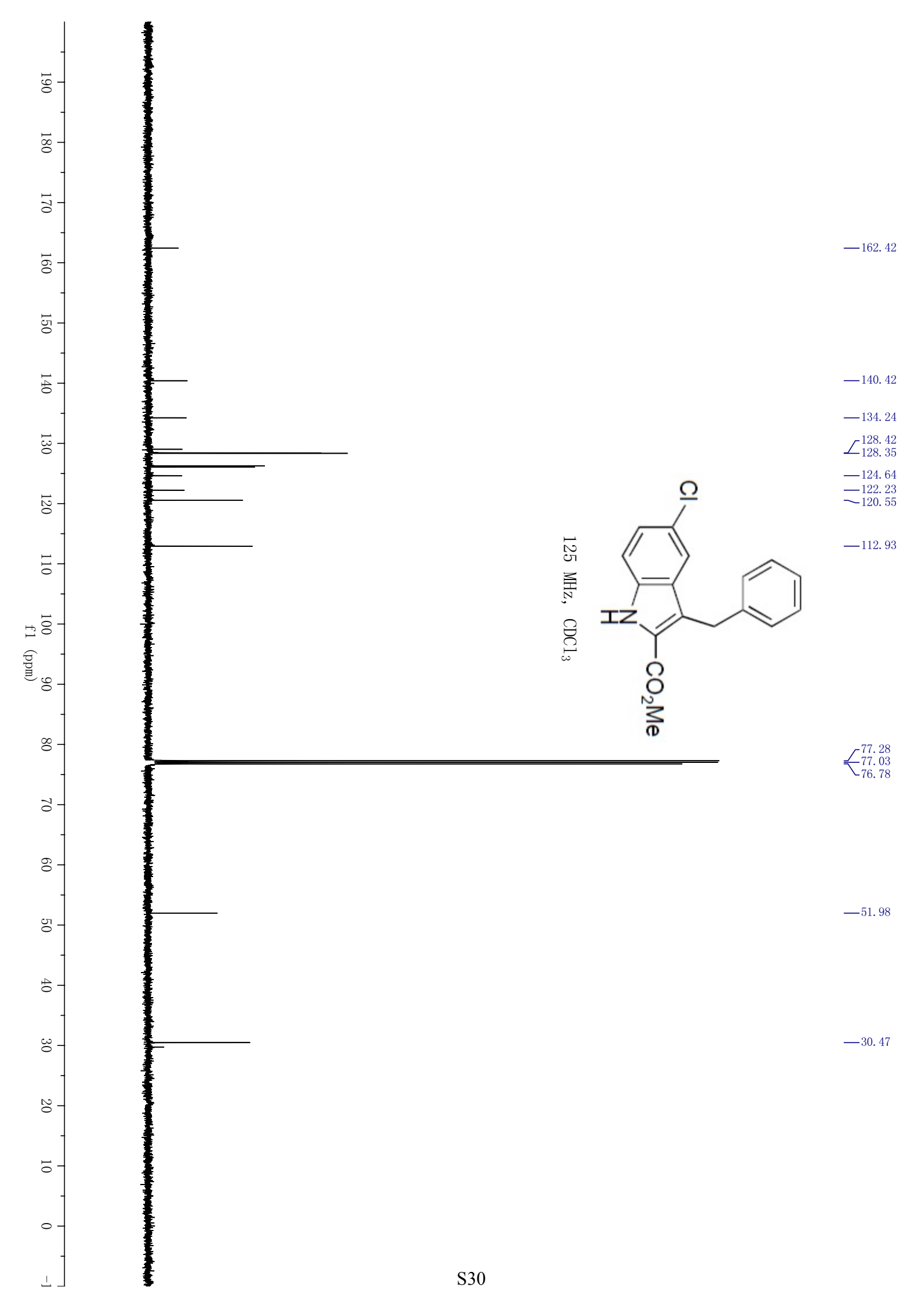
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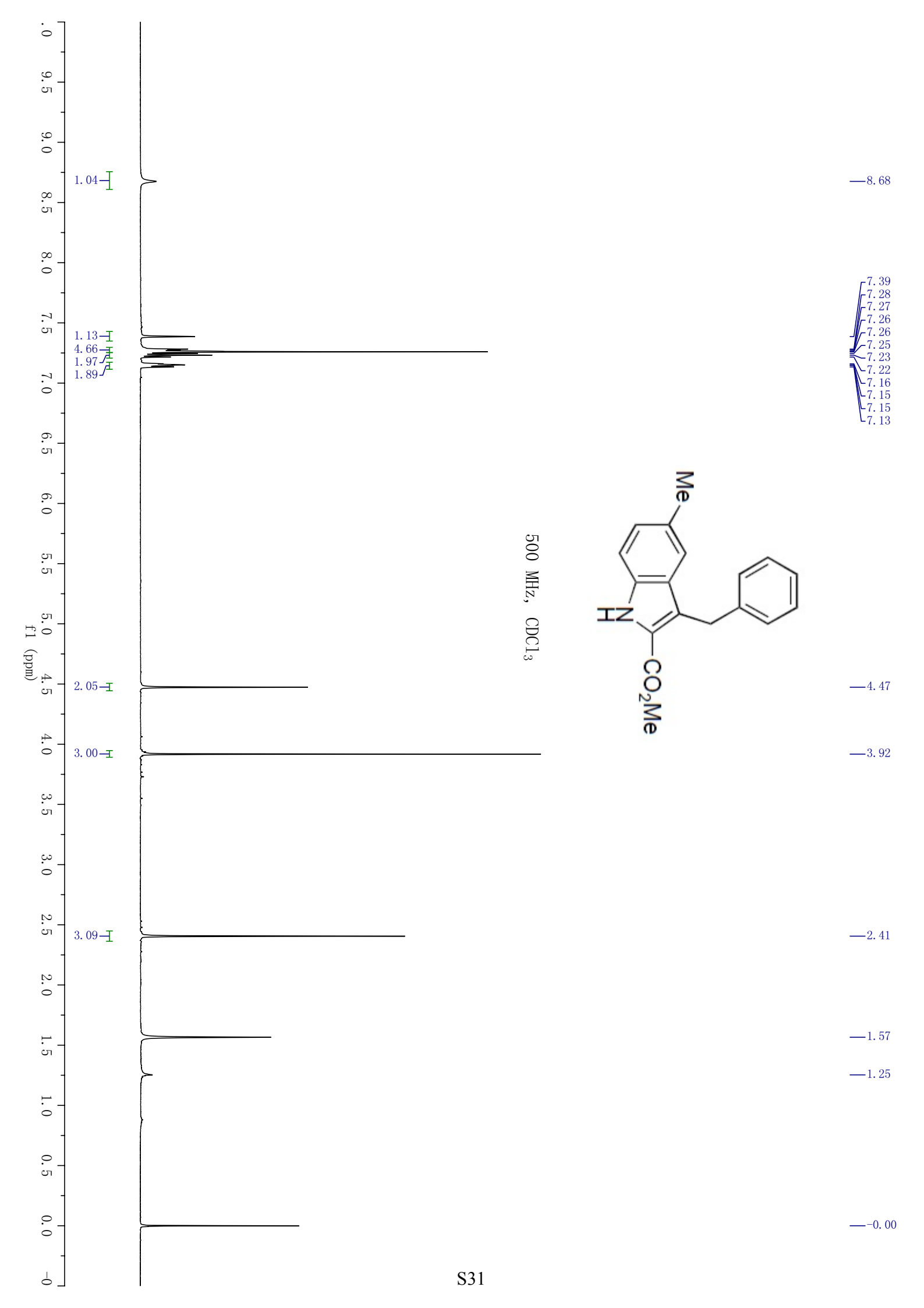
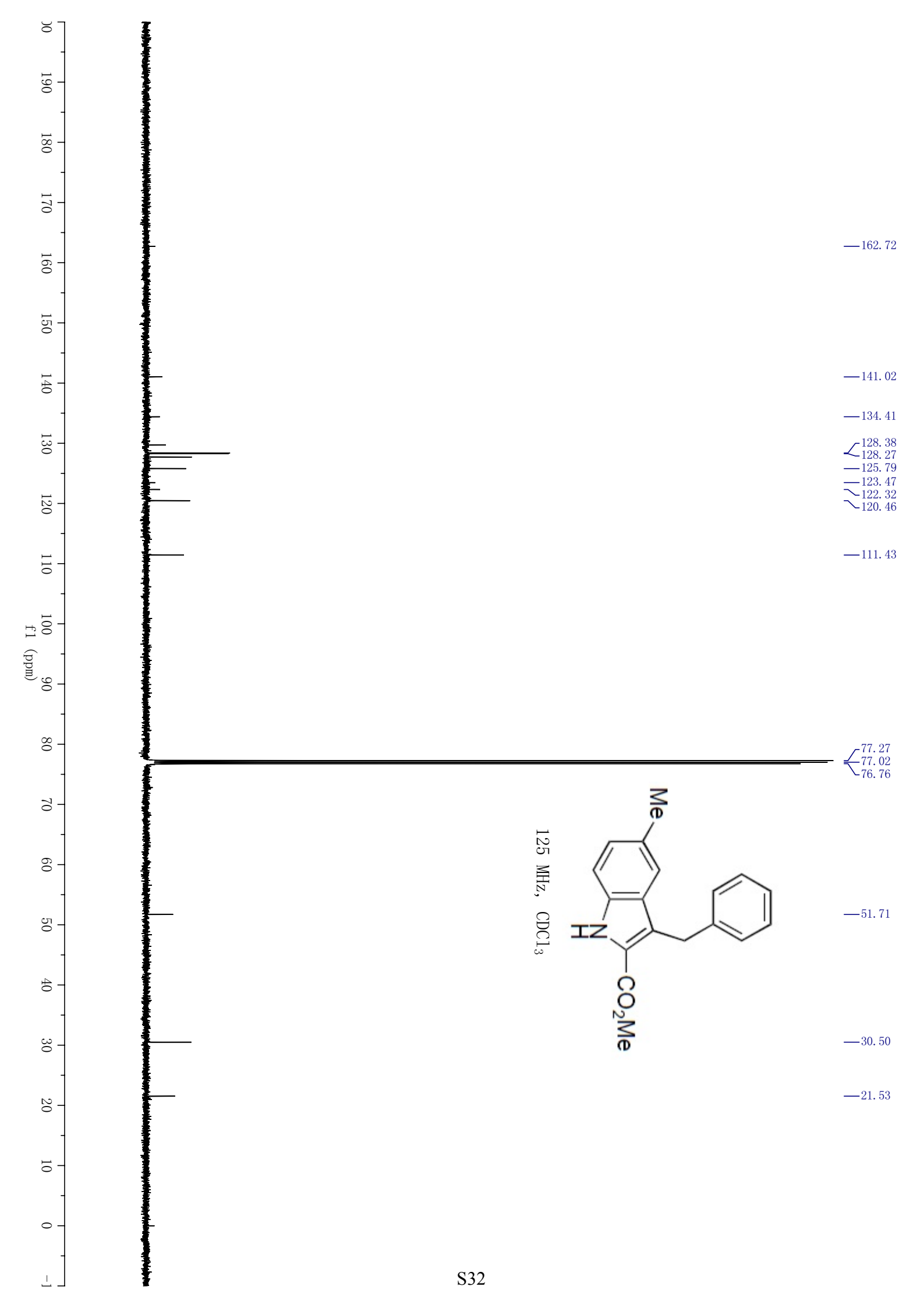
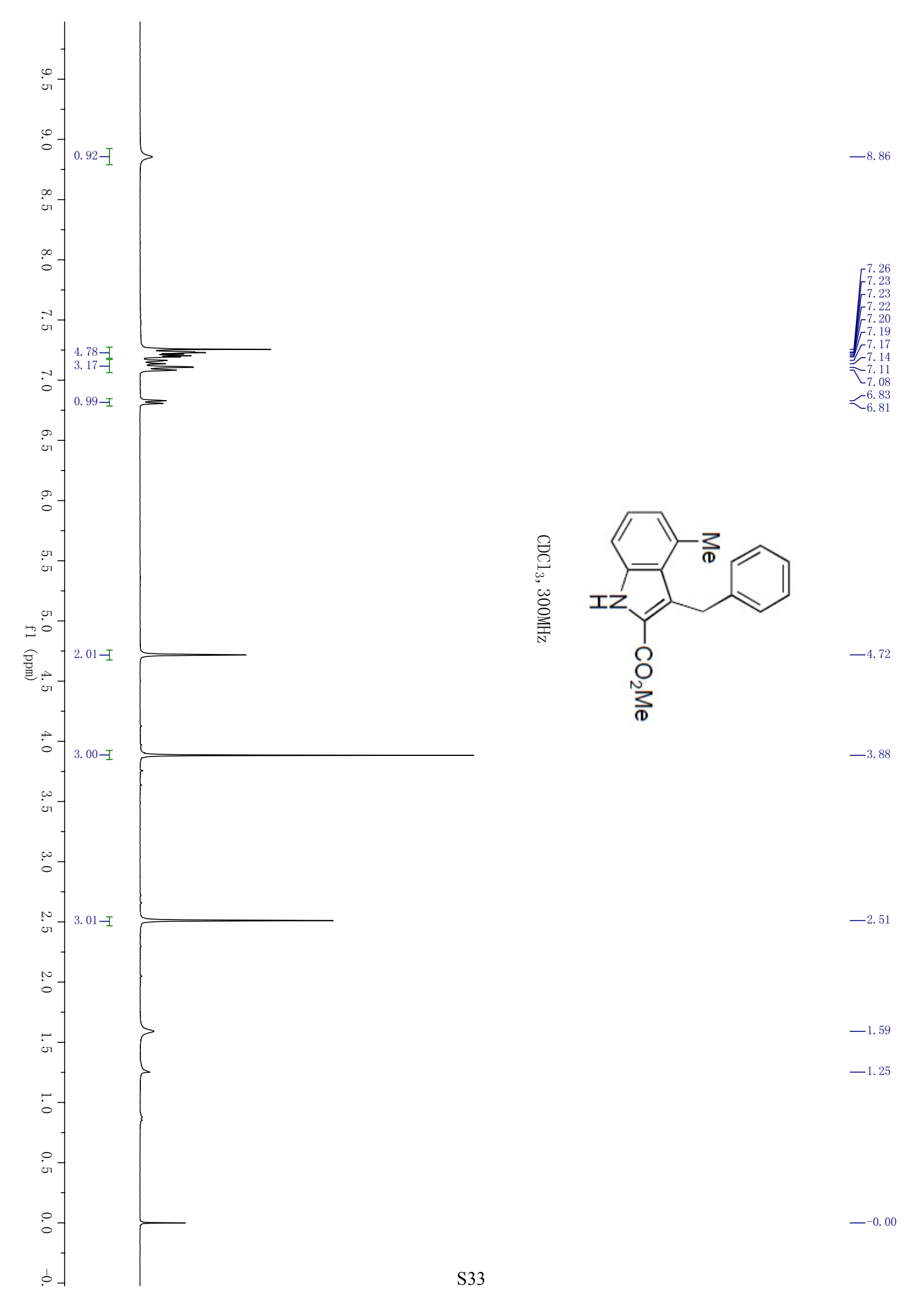
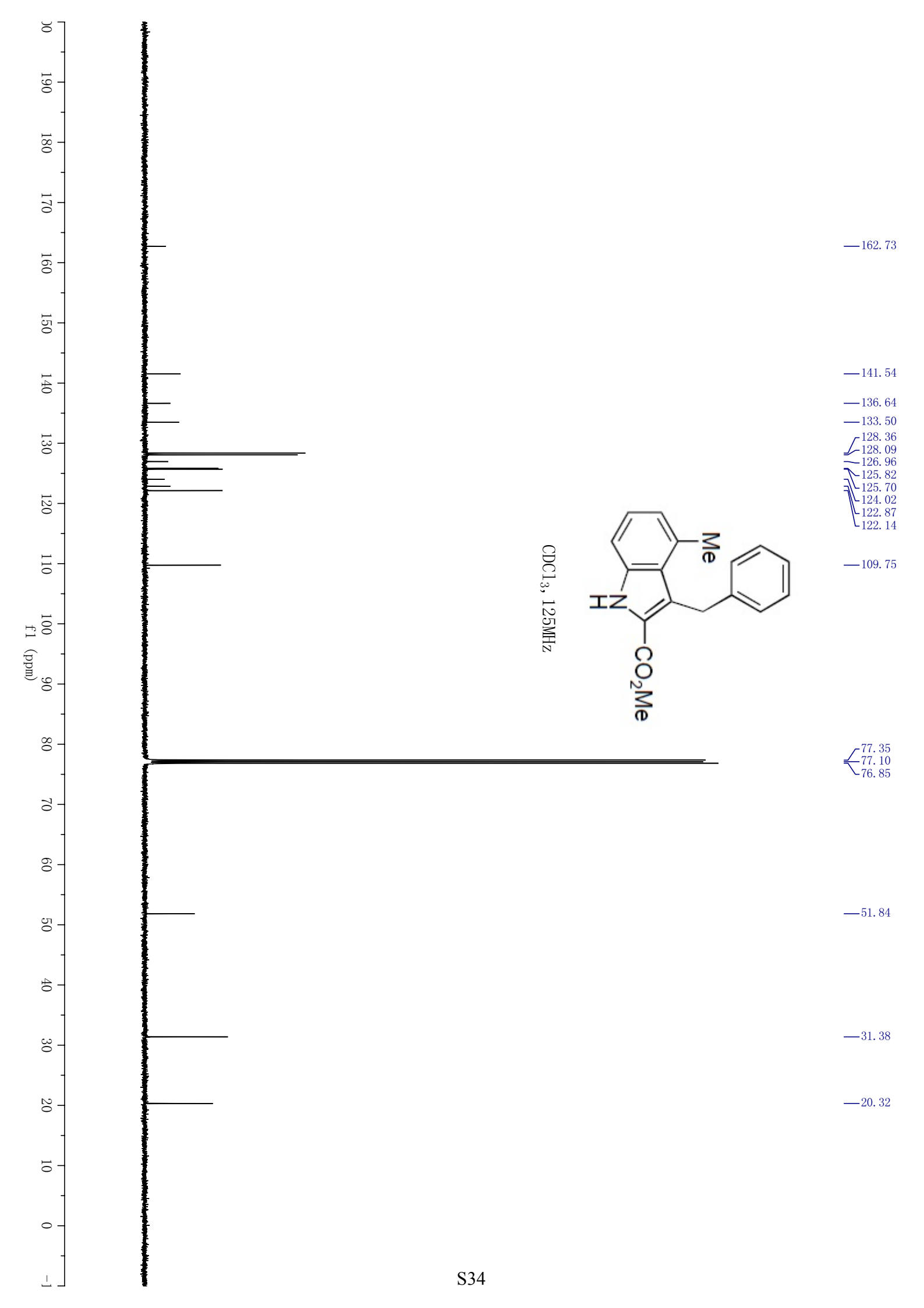
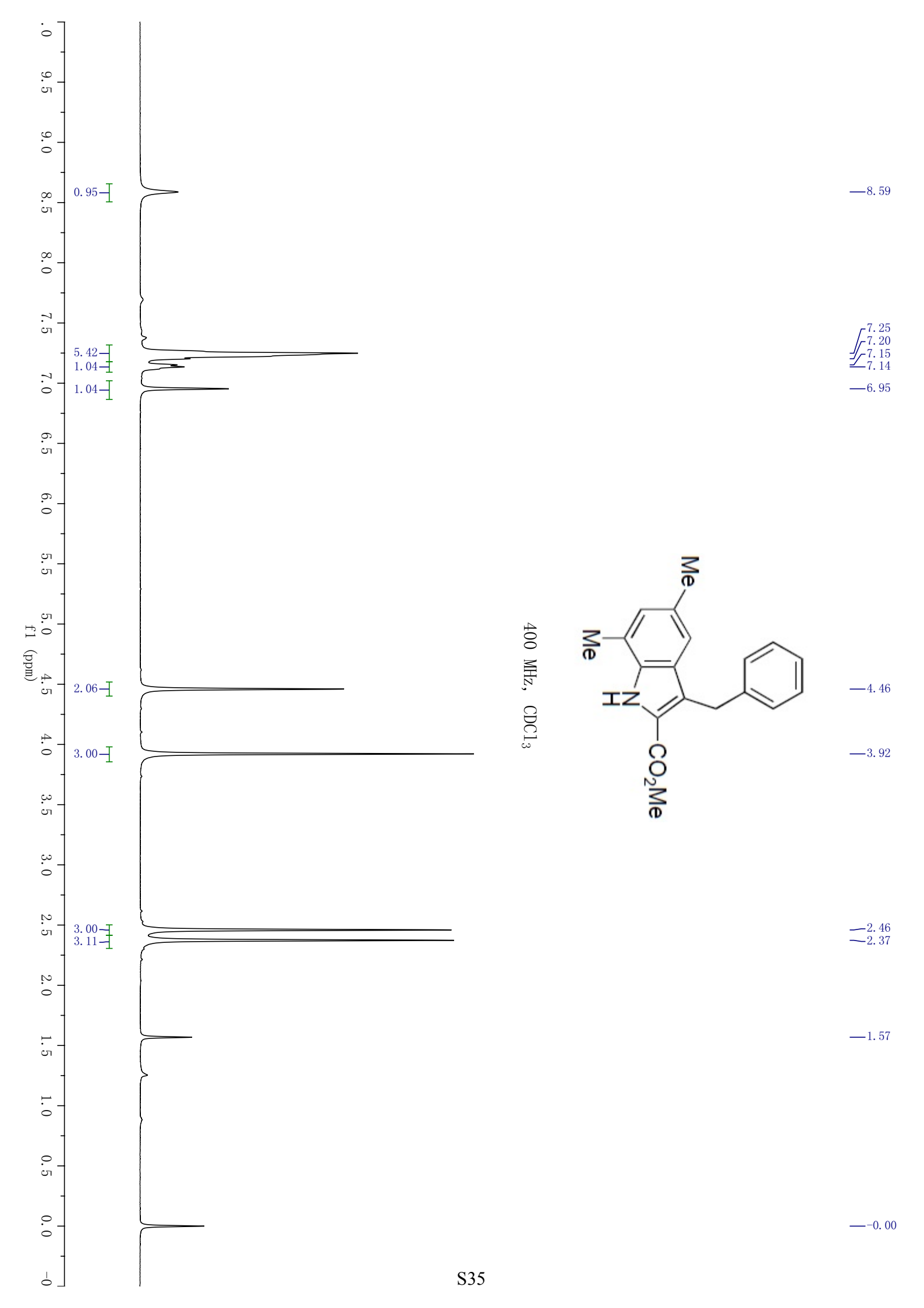
CO2Me
f1 (ppm)

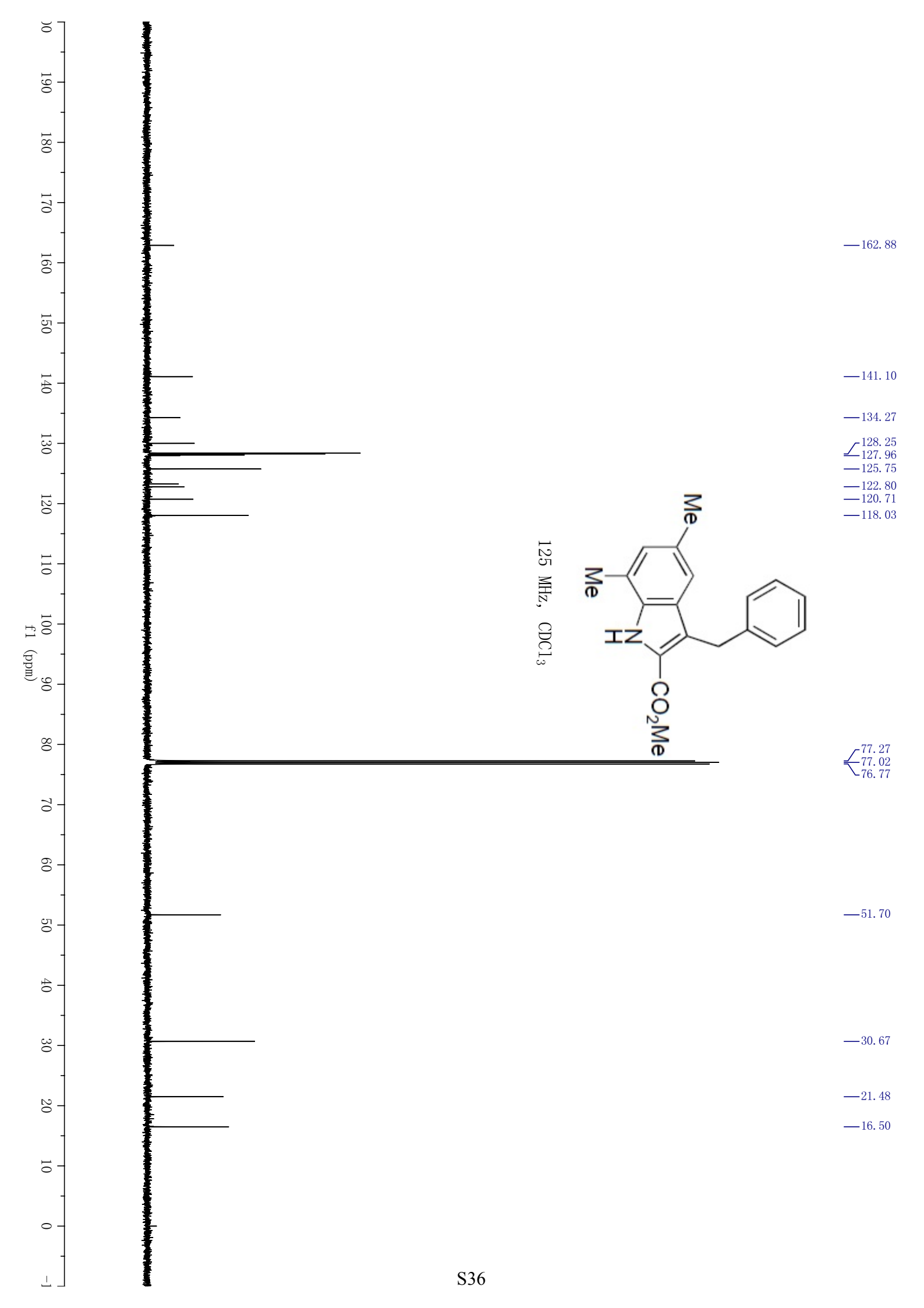

500 MHz, CDCl3
f1 (ppm)
1.04
1.13
4.66
1.97
1.89
2.05
3.00
3.09
8.68
7.39
7.28
7.27
7.26
7.26
7.25
7.23
7.22
7.16
7.15
7.15
7.13
4.47
3.92
2.41
1.57
1.25
0.00
Me
N
H
CO2Me

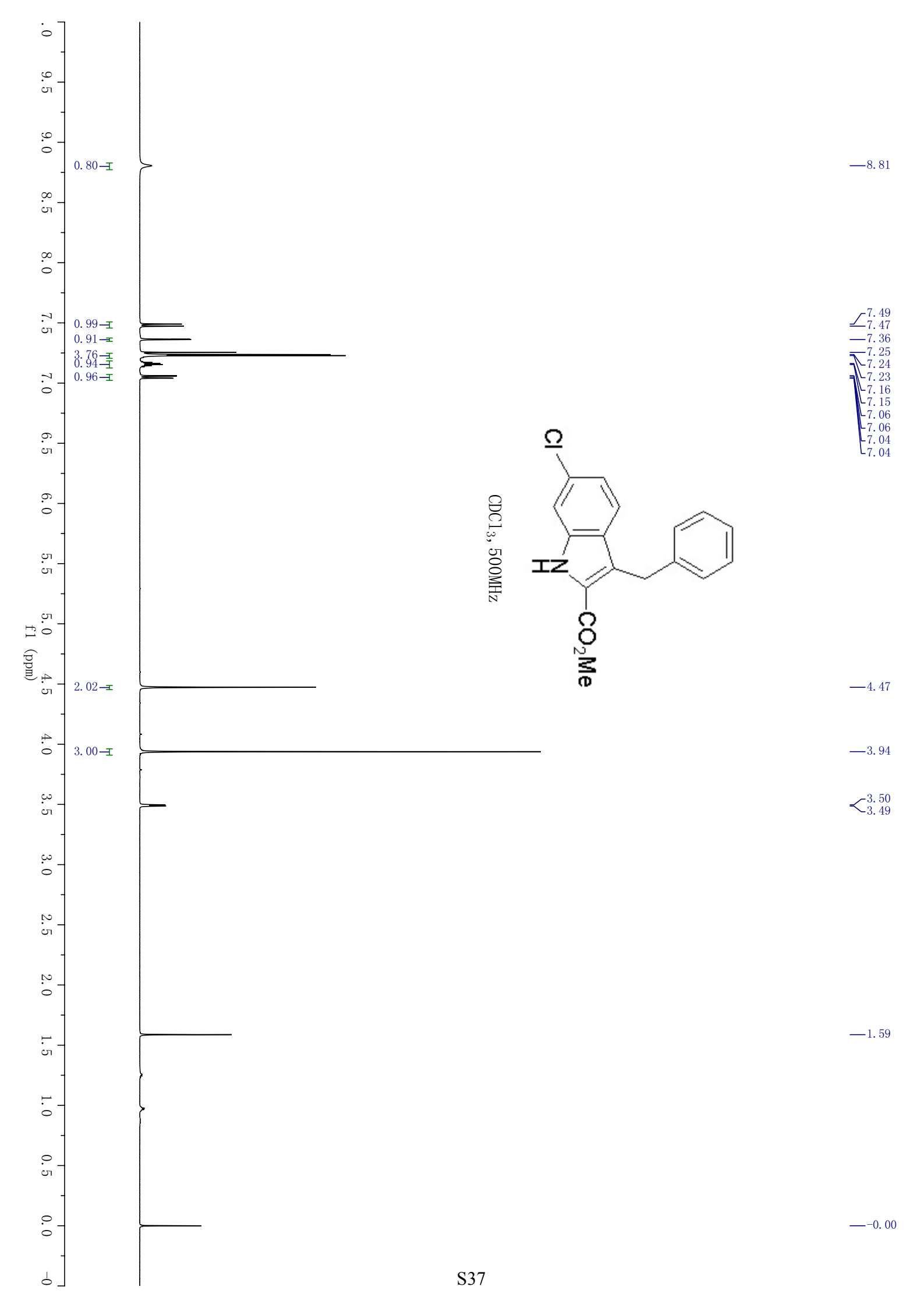

162.72
141.02
134.41
128.38
128.27
125.79
123.47
122.32
120.46
111.43
77.27
77.02
76.76
51.71
30.50
21.53
f1 (ppm)
125 MHz, CDCl3
Me
N
H
CO2Me

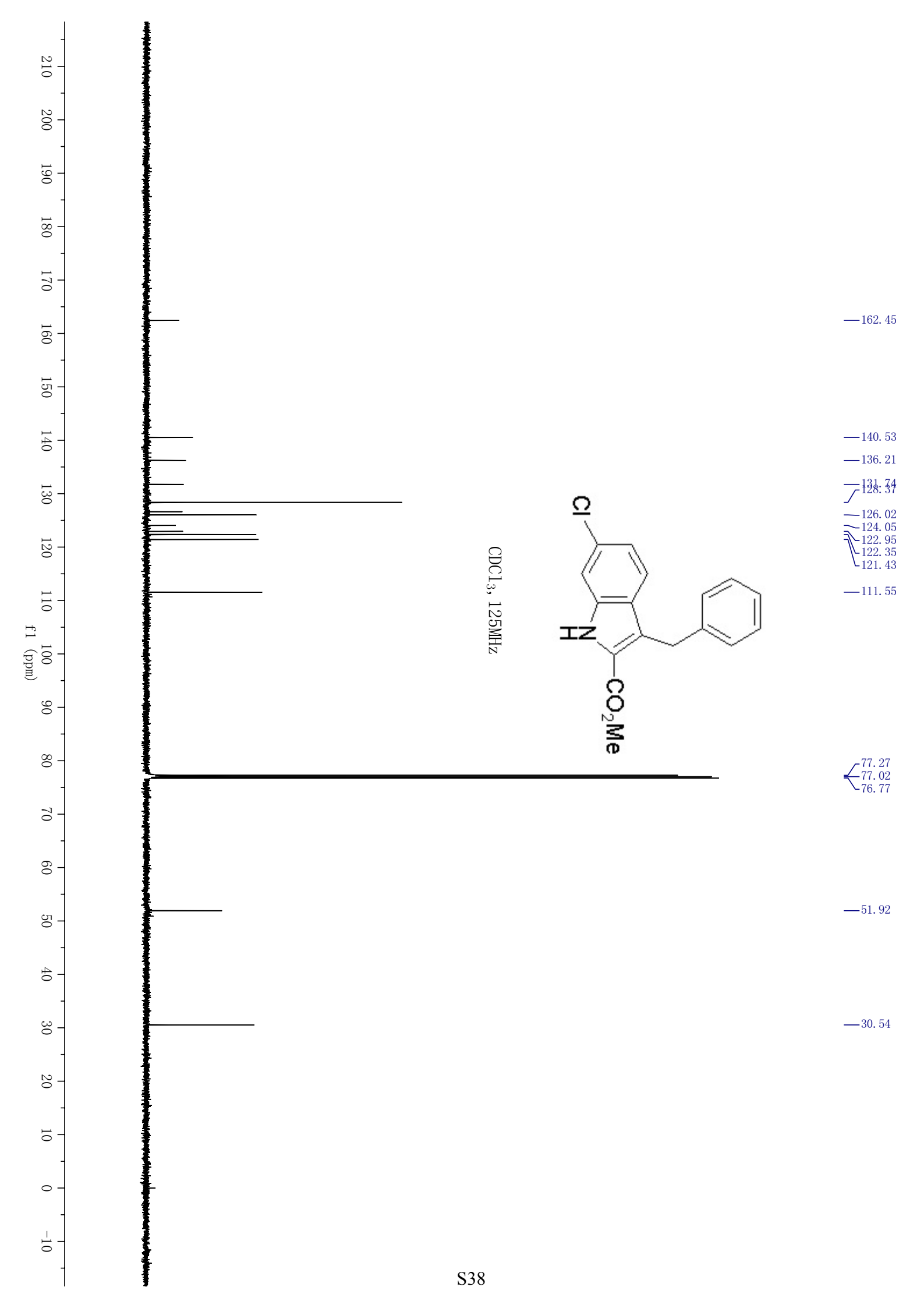

0.92
4.78
3.17
0.99
2.01
3.00
3.01
f1 (ppm)
CDCl3, 300MHz
Me
N
H
CO2Me
8.86
7.26
7.23
7.23
7.22
7.20
7.19
7.17
7.14
7.11
7.08
6.83
6.81
4.72
3.88
2.51
1.59
1.25
0.00

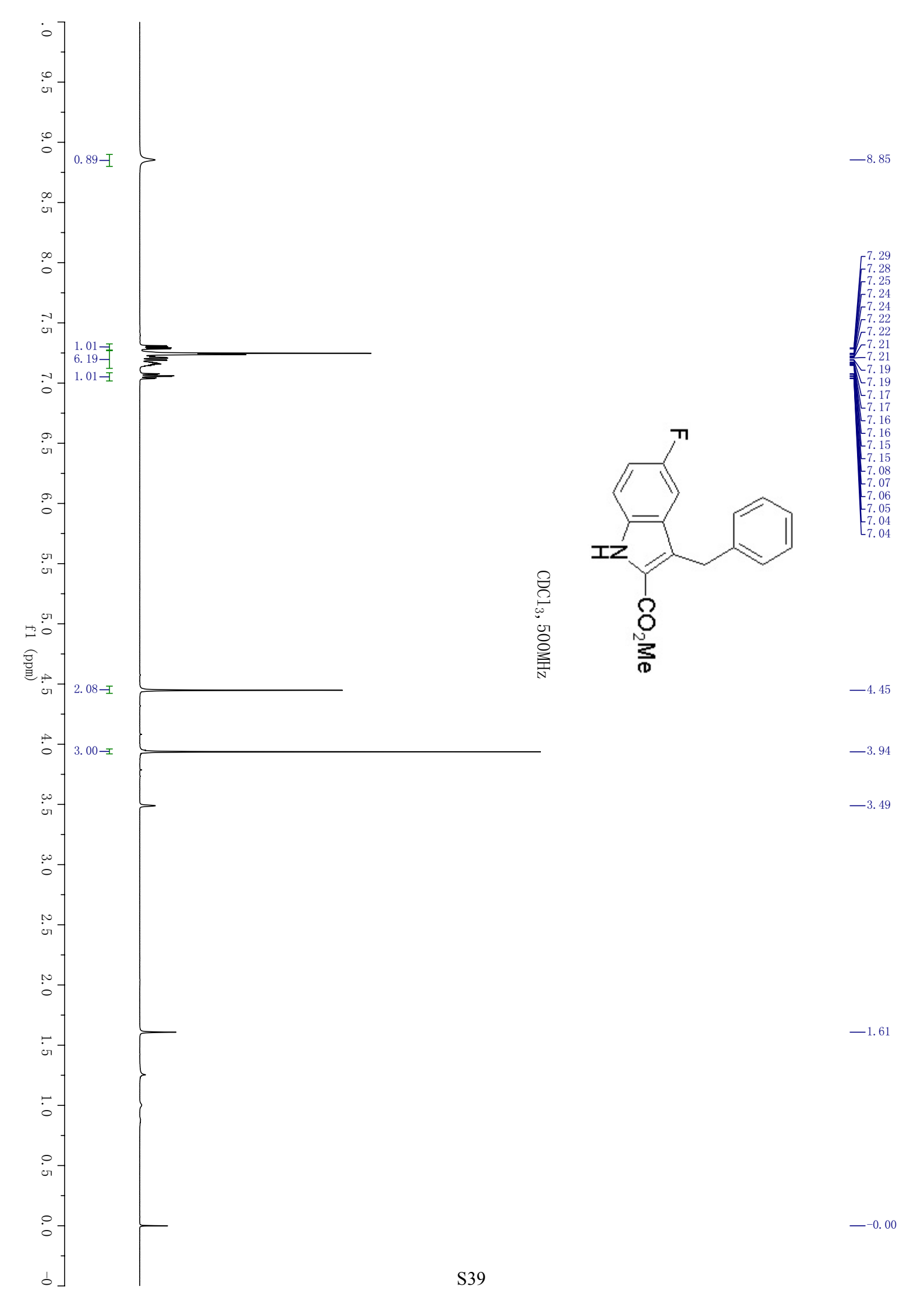

CDCl3, 125MHz
Me
N
H
CO2Me
162.73
141.54
136.64
133.50
128.36
128.09
126.96
125.82
125.70
124.02
122.87
122.14
109.75
77.35
77.10
76.85
51.84
31.38
20.32
f1 (ppm)

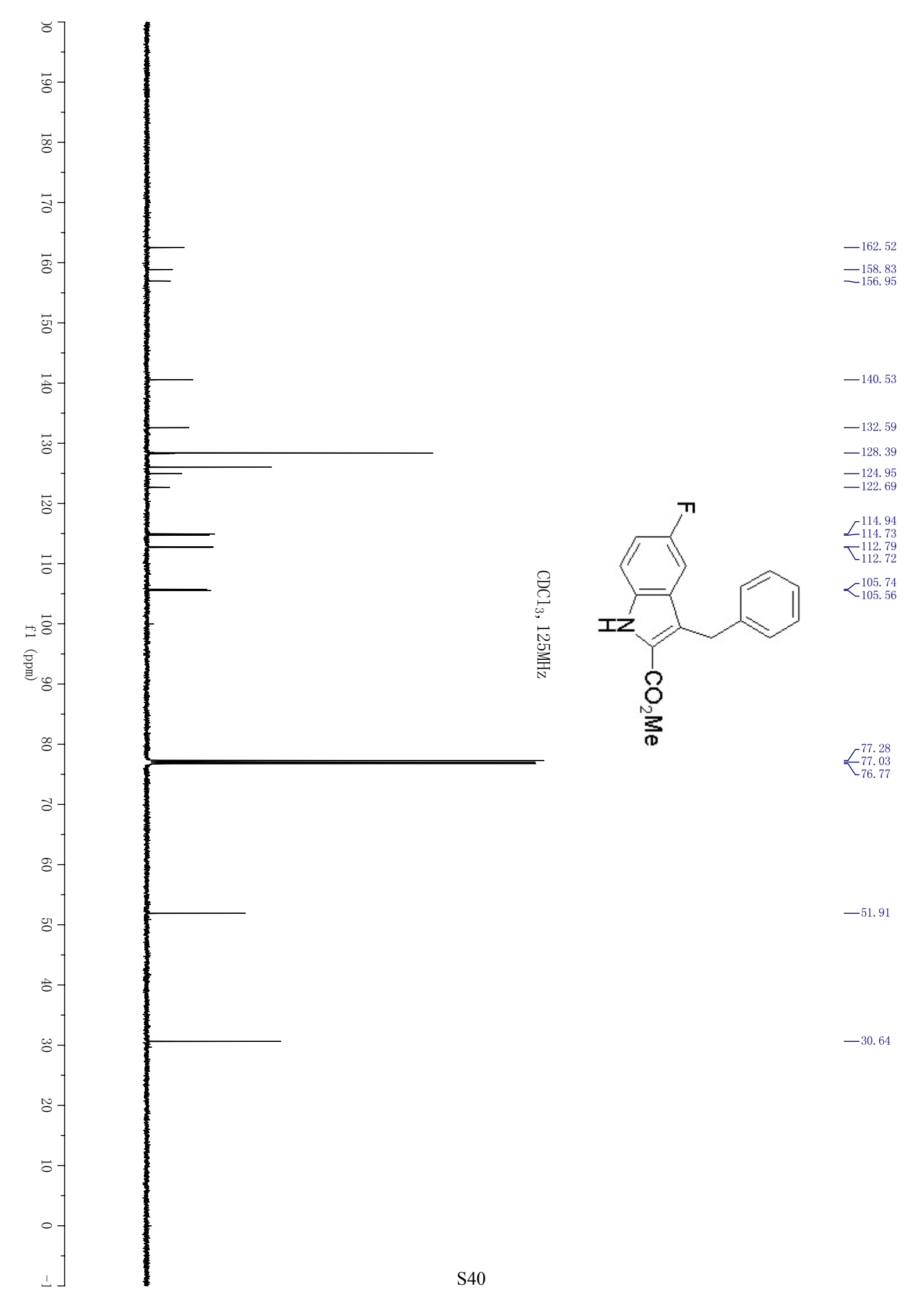

0.95
5.42
1.04
1.04
2.06
3.00
3.00
3.11
8.59
7.25
7.20
7.15
7.14
6.95
4.46
3.92
2.46
2.37
1.57
0.00
400 MHz, CDCl3
Me
Me
N
H
CO2Me
f1 (ppm)

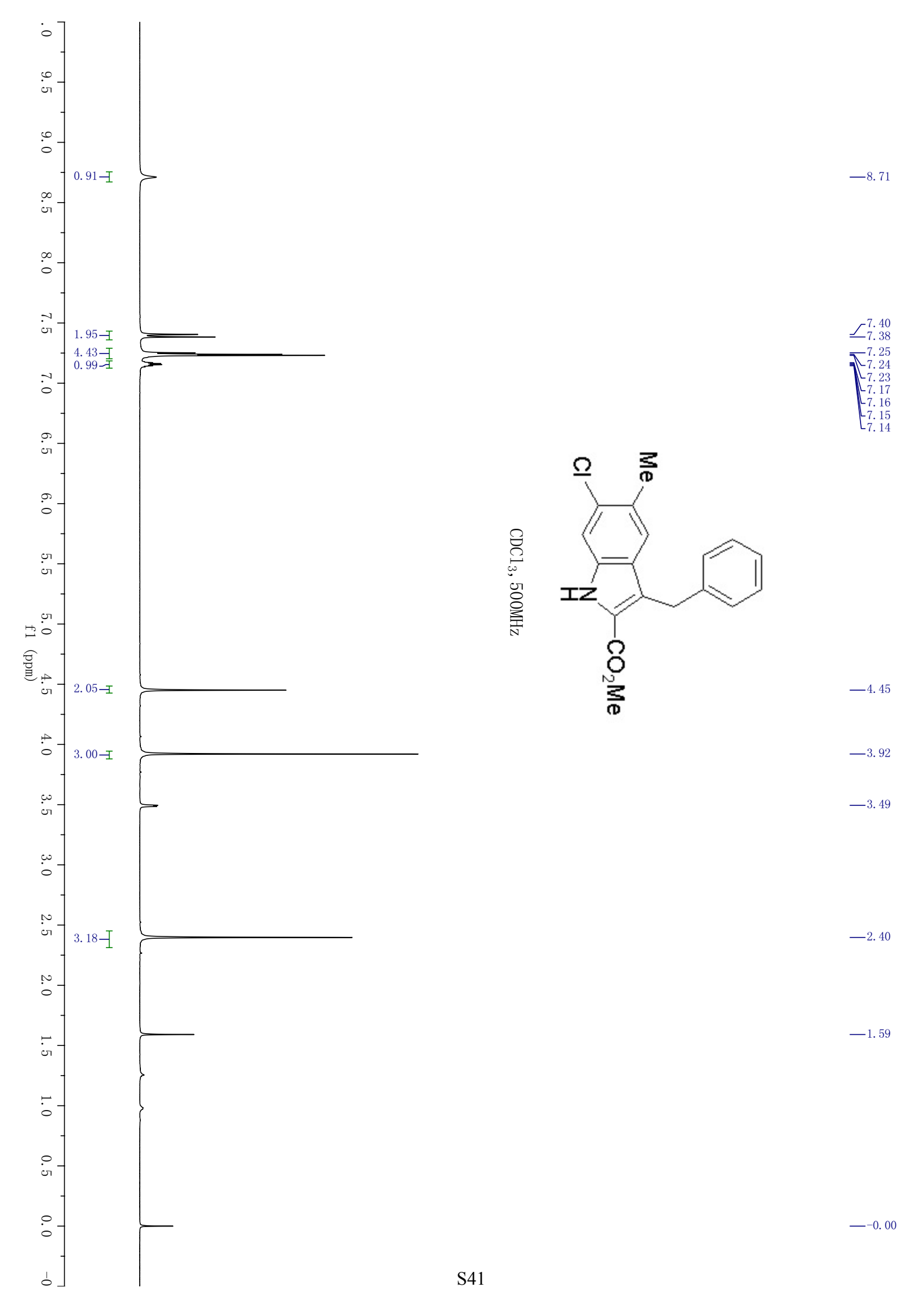

162.88
141.10
134.27
128.25
127.96
125.75
122.80
120.71
118.03
77.27
77.02
76.77
51.70
30.67
21.48
16.50
125 MHz, CDCl3
Me
Me
N
H
CO2Me
f1 (ppm)

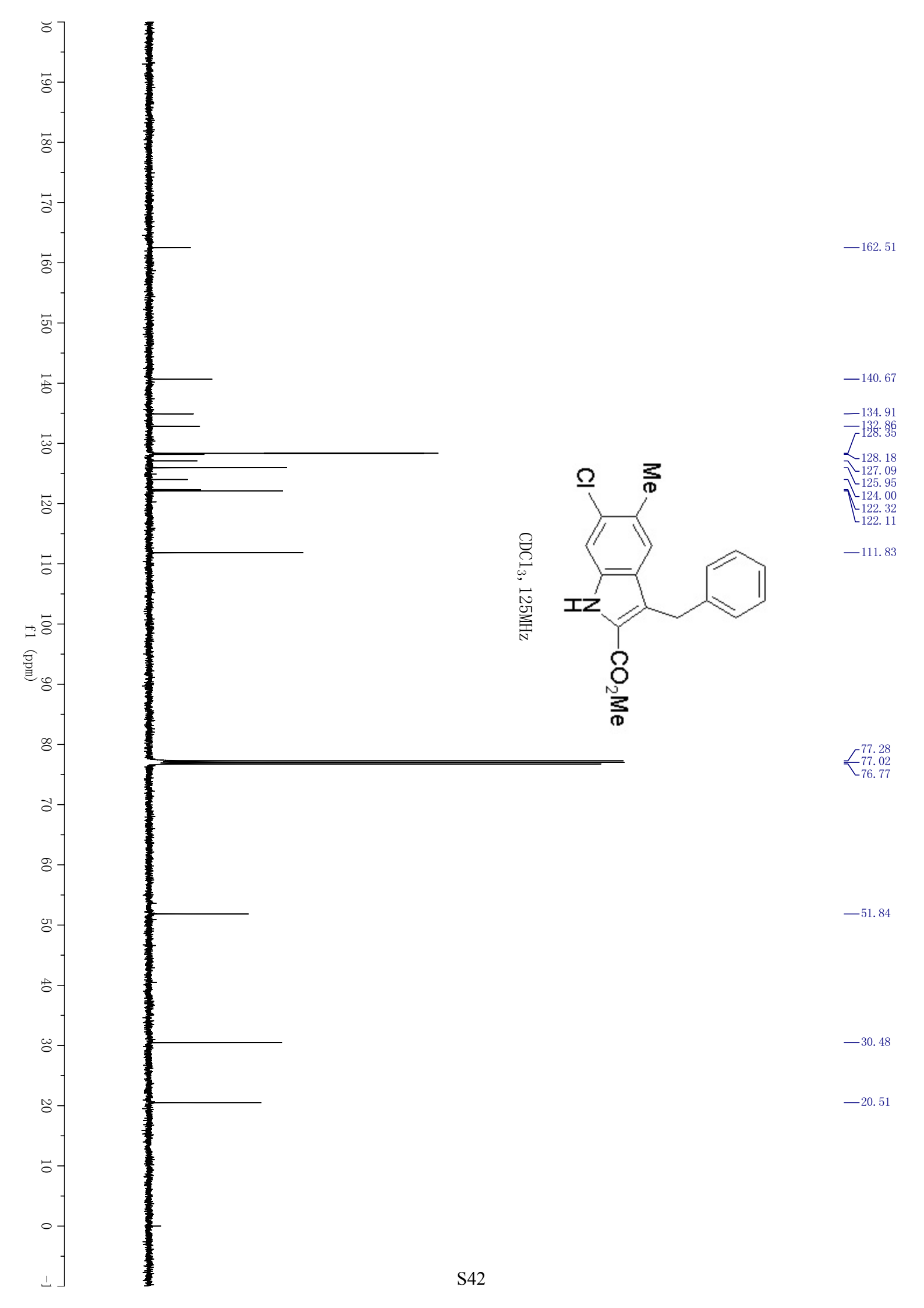

0.80
0.99
0.91
3.76
0.94
0.96
2.02
3.00
8.81
7.49
7.47
7.36
7.25
7.24
7.23
7.16
7.15
7.06
7.06
7.04
7.04
4.47
3.94
3.50
3.49
1.59
0.00
f1 (ppm)
CDCl3, 500MHz
Cl
HN
CO2Me

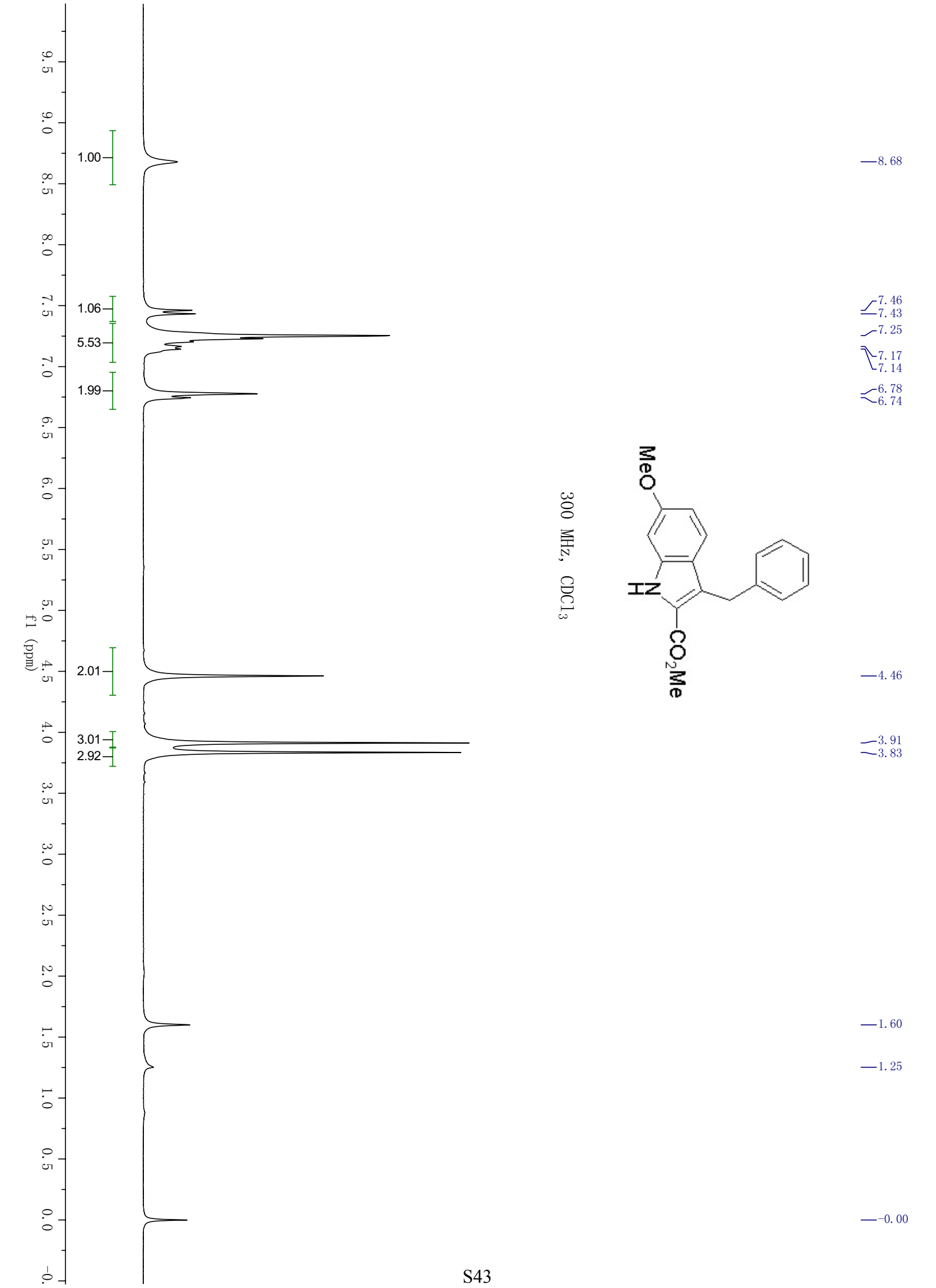

f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
CDCl3, 125MHz
Cl
HN
CO2Me
162.45
140.53
136.21
131.74
128.37
126.02
124.05
122.95
122.35
121.43
111.55
77.27
77.02
76.77
51.92
30.54

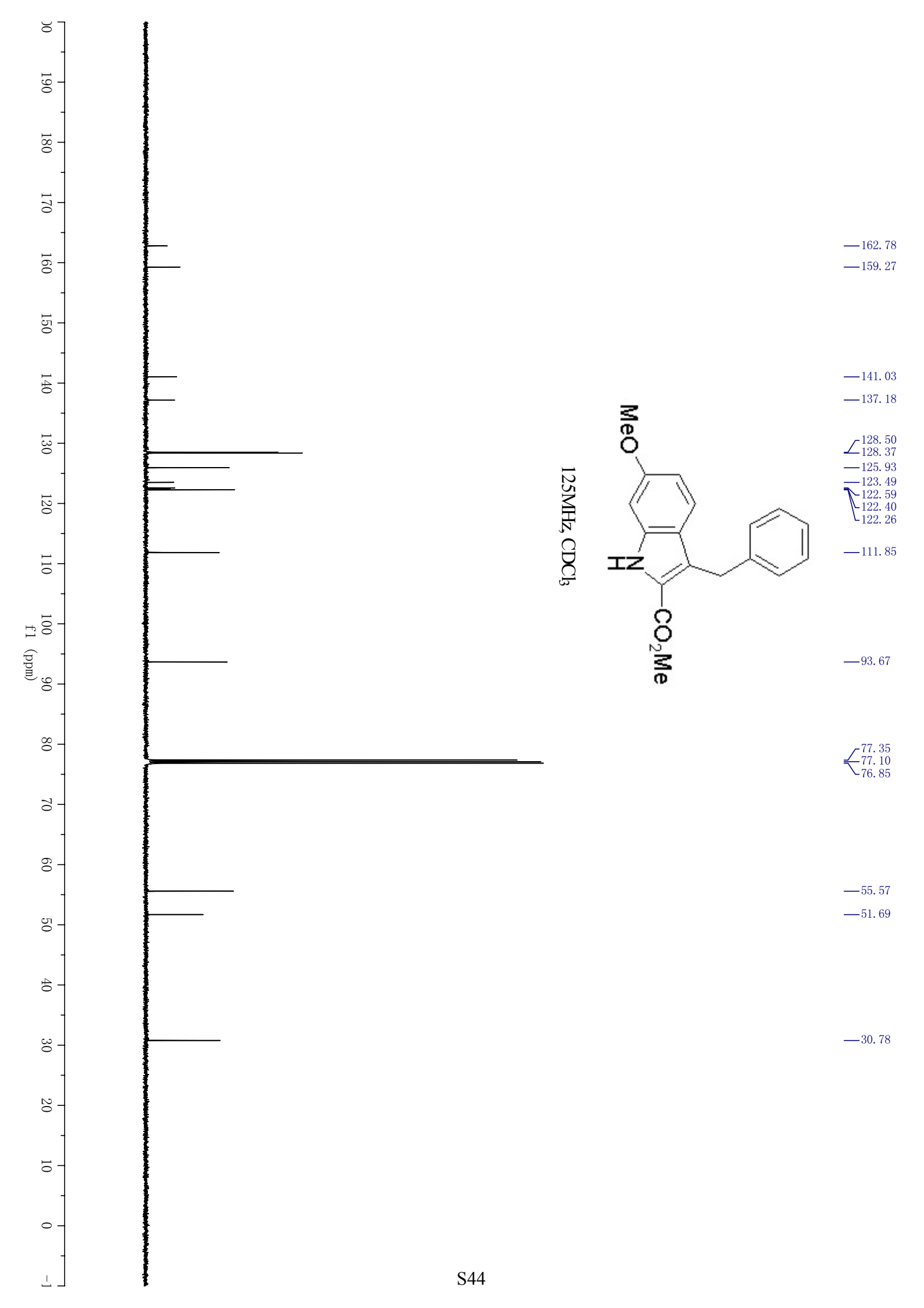

0.89
1.01
6.19
1.01
2.08
3.00
8.85
7.29
7.28
7.25
7.24
7.24
7.22
7.22
7.21
7.21
7.19
7.19
7.17
7.17
7.16
7.16
7.15
7.15
7.08
7.07
7.06
7.05
7.04
7.04
4.45
3.94
3.49
1.61
0.00
CDCl3, 500MHz
F
HN
CO2Me
f1 (ppm)

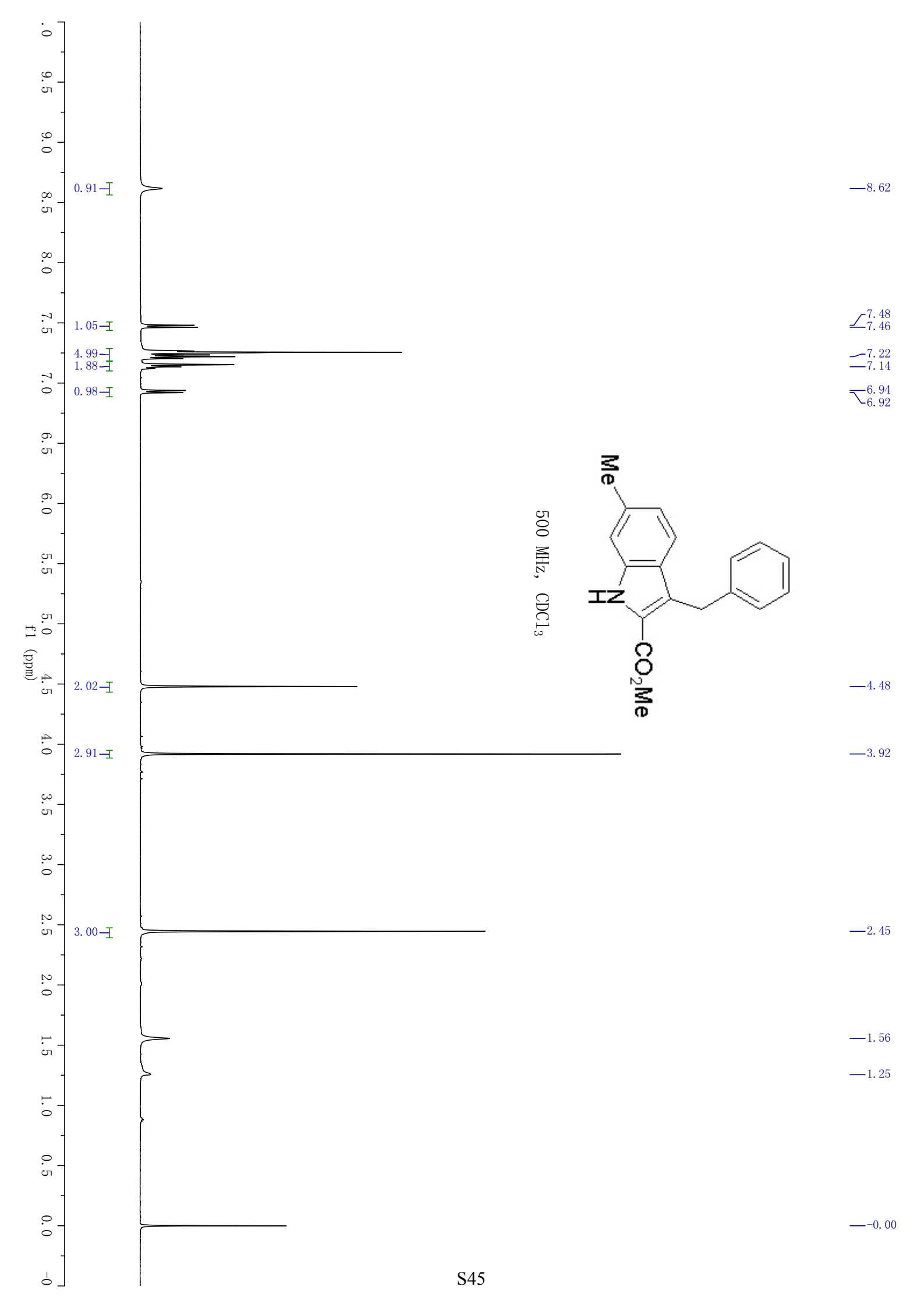

162.52
158.83
156.95
140.53
132.59
128.39
124.95
122.69
114.94
114.73
112.79
112.72
105.74
105.56
77.28
77.03
76.77
51.91
30.64
CDCl3, 125MHz
F
HN
CO2Me
f1 (ppm)

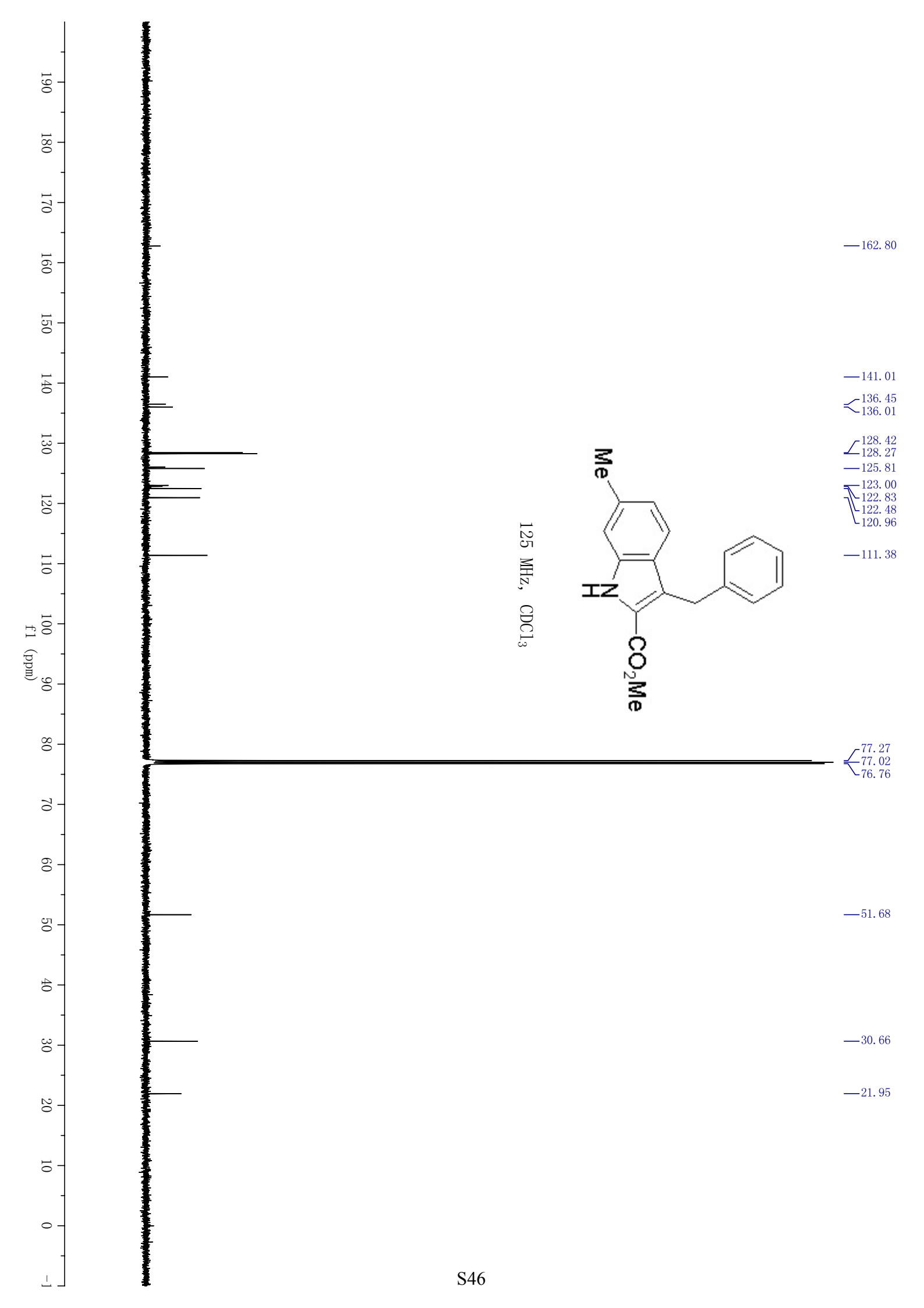

0.91
1.95
4.43
0.99
2.05
3.00
3.18
8.71
7.40
7.38
7.25
7.24
7.23
7.17
7.16
7.15
7.14
4.45
3.92
3.49
2.40
1.59
0.00
f1 (ppm)
CDCl3, 500MHz
Cl
Me
N
H
CO2Me

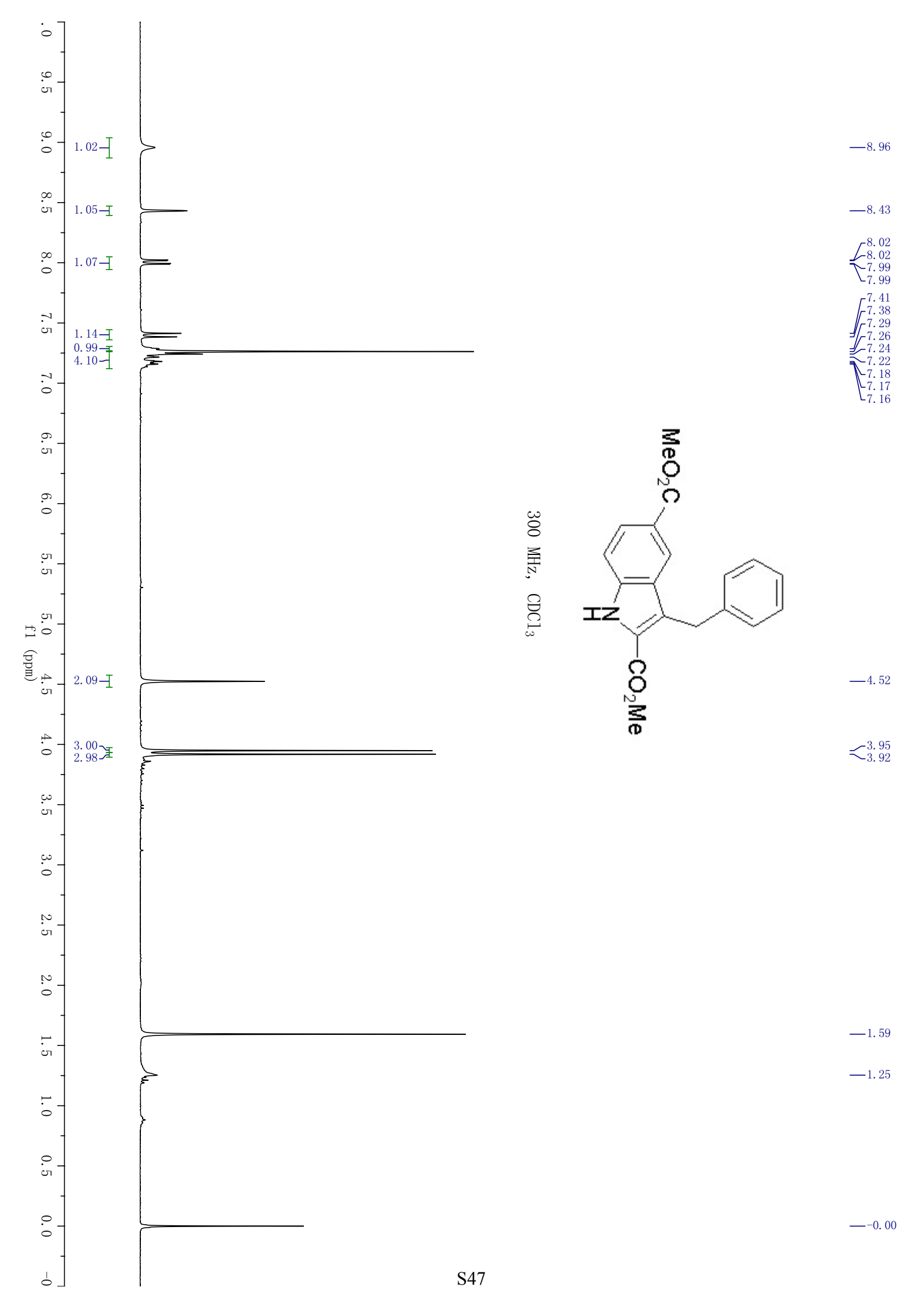

162.51
140.67
134.91
132.86
128.35
128.18
127.09
125.95
124.00
122.32
122.11
111.83
77.28
77.02
76.77
51.84
30.48
20.51
CDCl3, 125MHz
Cl
Me
N
H
CO2Me
f1 (ppm)

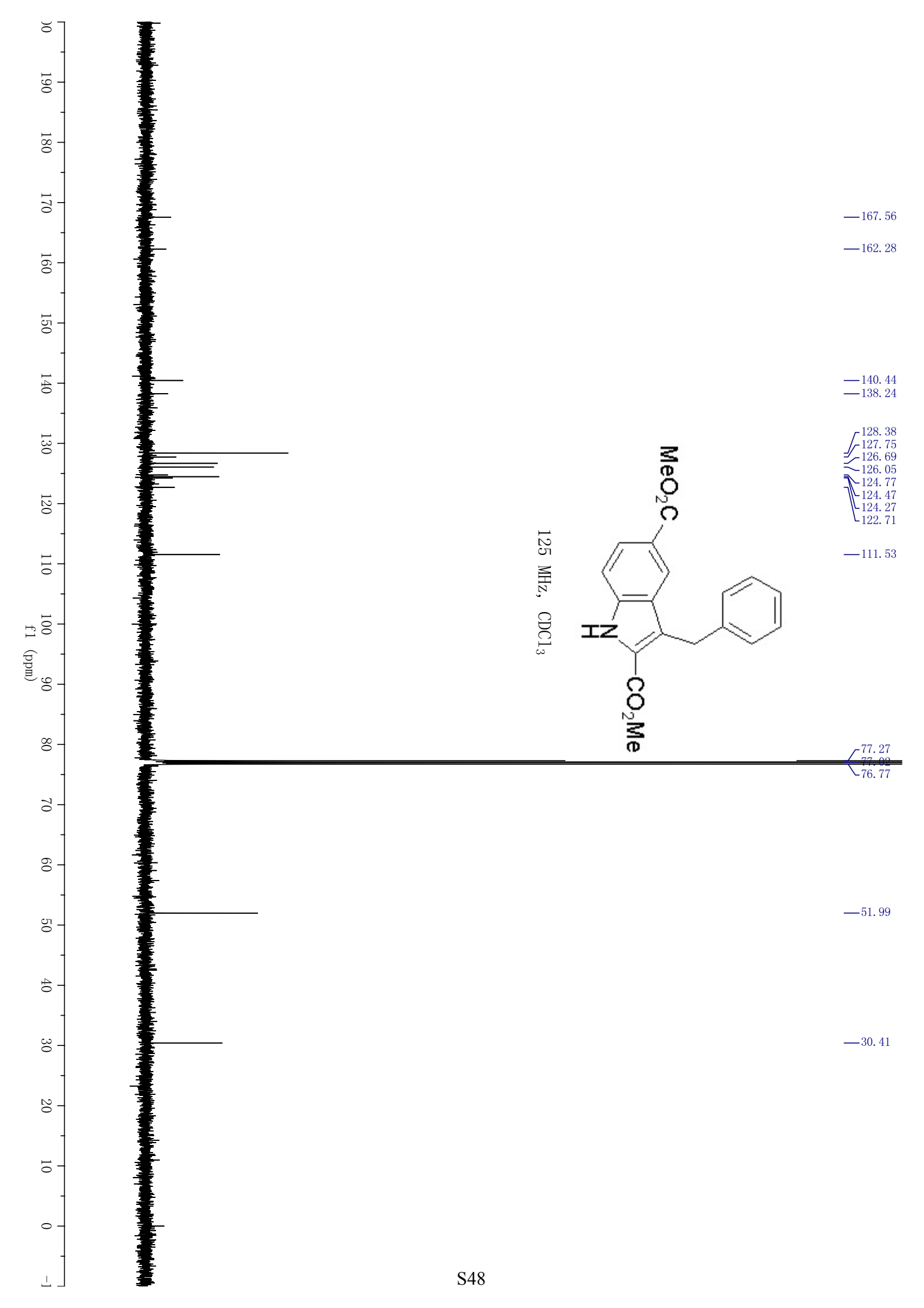

1.00
1.06
5.53
1.99
2.01
3.01
2.92
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)
300 MHz, CDCl3
MeO
N
H
CO2Me
8.68
7.46
7.43
7.25
7.17
7.14
6.78
6.74
4.46
3.91
3.83
1.60
1.25
0.00

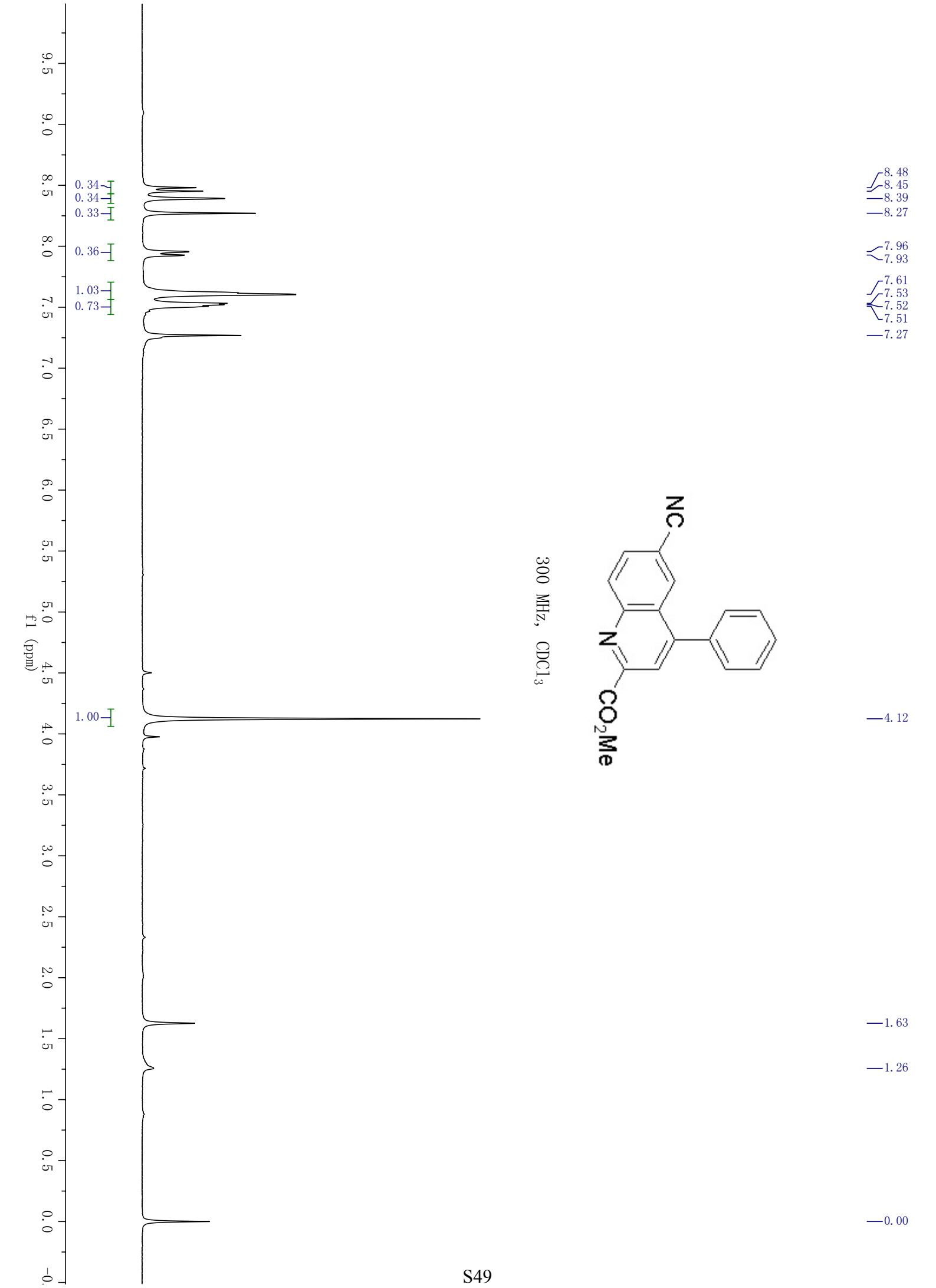

125MHz, CDCl3
MeO
N
H
CO2Me
162.78
159.27
141.03
137.18
128.50
128.37
125.93
123.49
122.59
122.40
122.26
111.85
93.67
77.35
77.10
76.85
55.57
51.69
30.78
f1 (ppm)

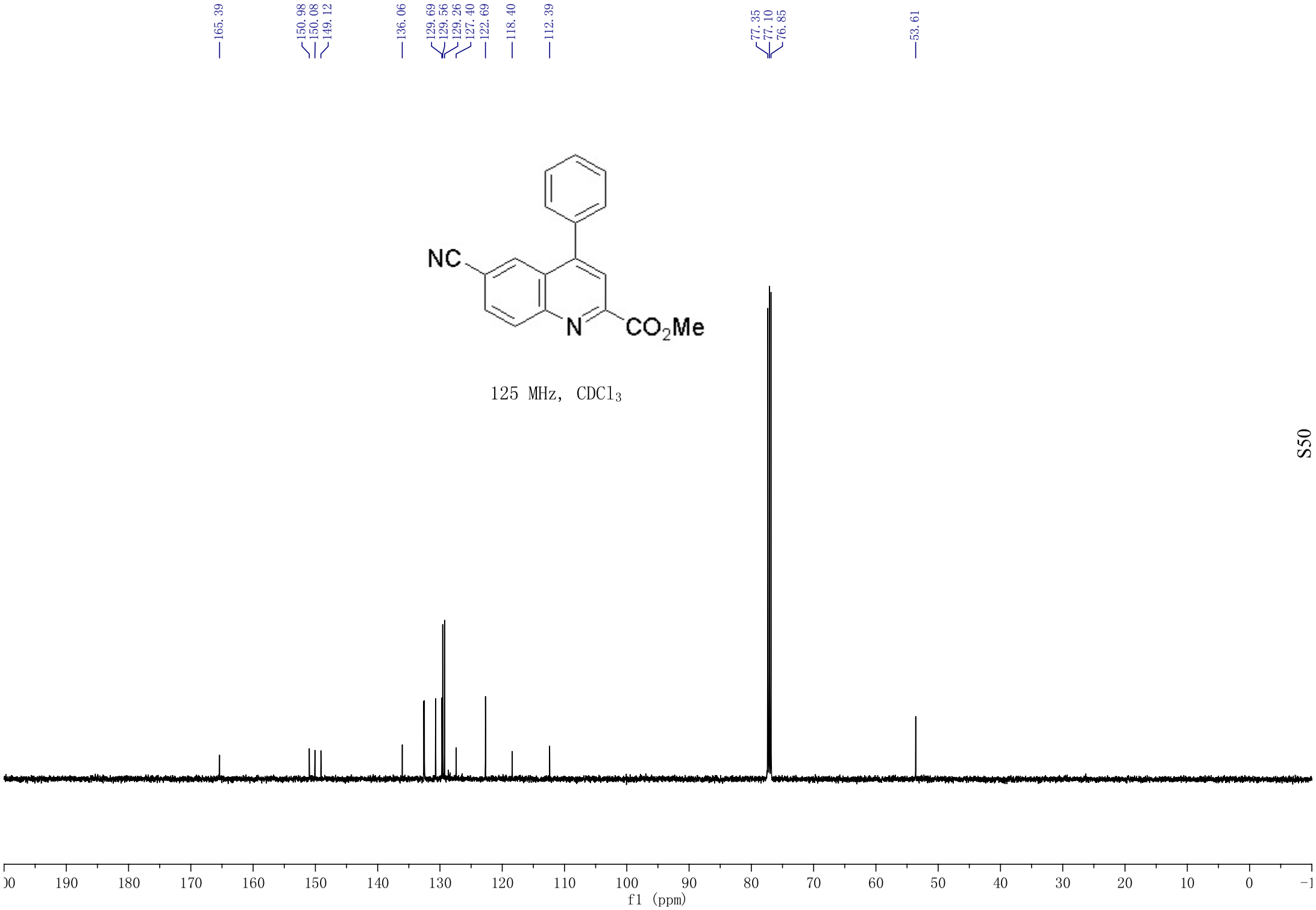

500 MHz, CDCl3
f1 (ppm)
0.91
1.05
4.99
1.88
0.98
2.02
2.91
3.00
8.62
7.48
7.46
7.22
7.14
6.94
6.92
4.48
3.92
2.45
1.56
1.25
0.00
Me
N
H
CO2Me

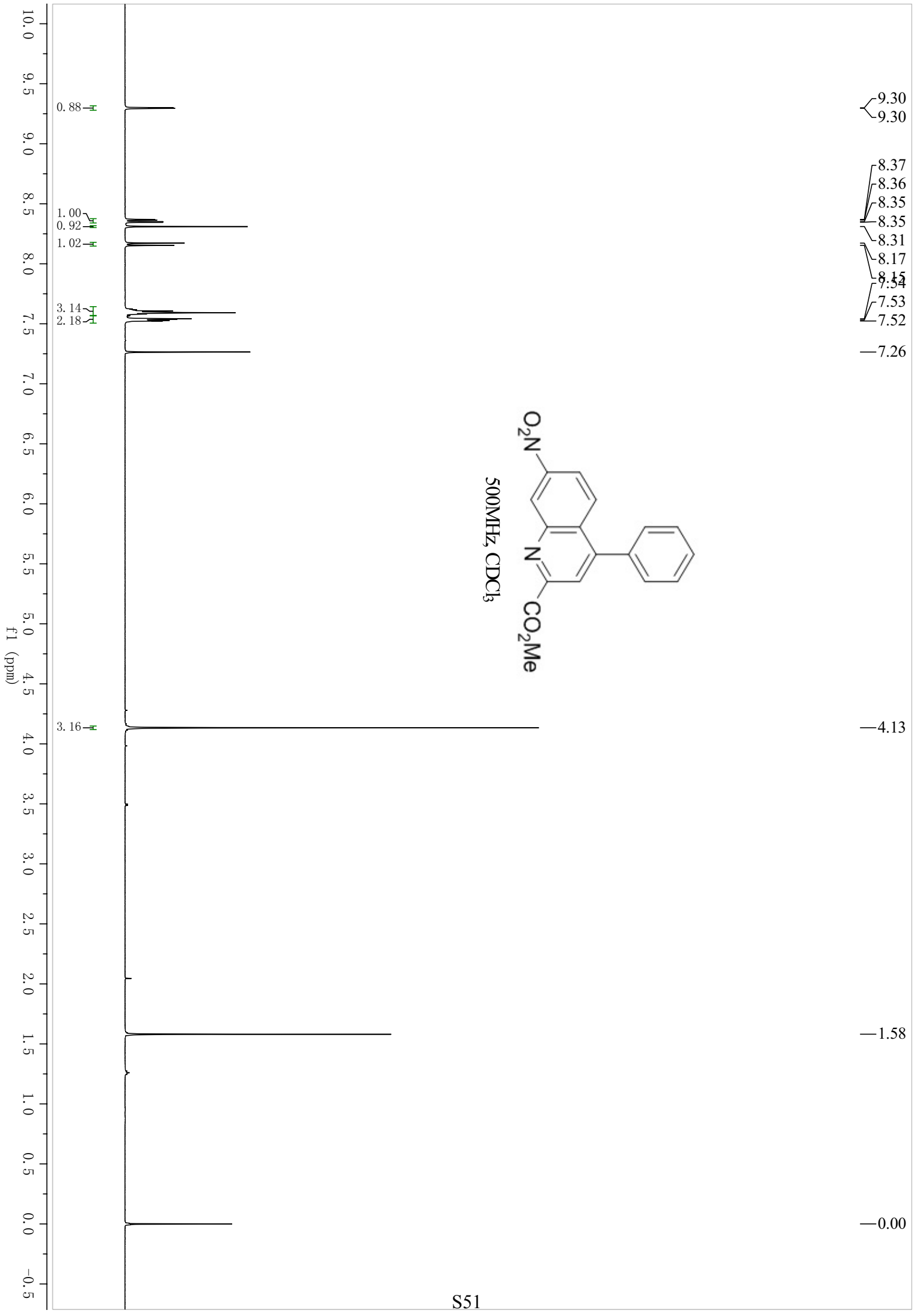

162.80
141.01
136.45
136.01
128.42
128.27
125.81
123.00
122.83
122.48
120.96
111.38
77.27
77.02
76.76
51.68
30.66
21.95
125 MHz, CDCl3
Me
N
H
CO2Me
f1 (ppm)

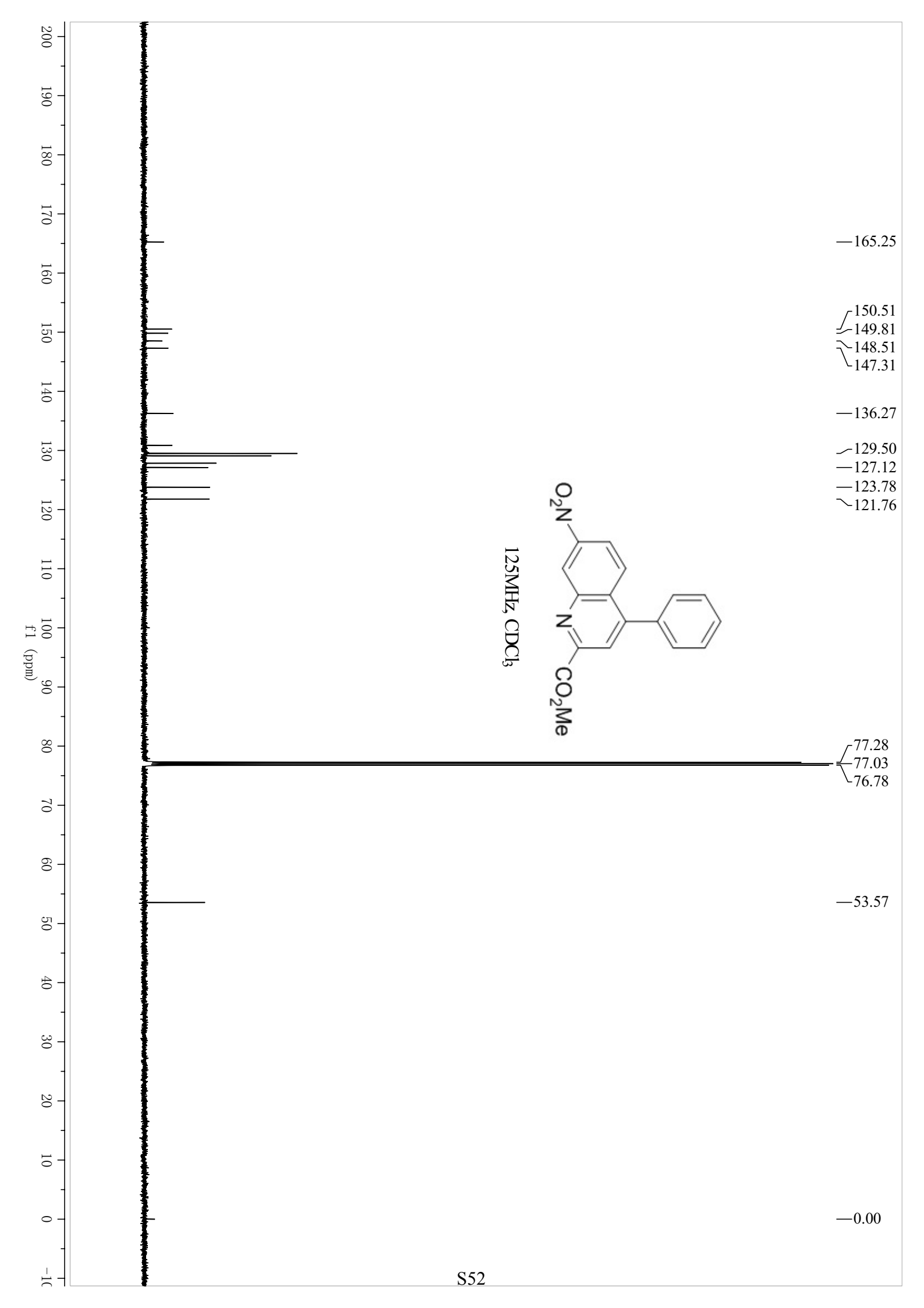

1.02
1.05
1.07
1.14
0.99
4.10
2.09
3.00
2.98
8.96
8.43
8.02
8.02
7.99
7.99
7.41
7.38
7.29
7.26
7.24
7.22
7.18
7.17
7.16
4.52
3.95
3.92
1.59
1.25
0.00
f1 (ppm)
300 MHz, CDCl3
MeO2C
CO2Me
N
H

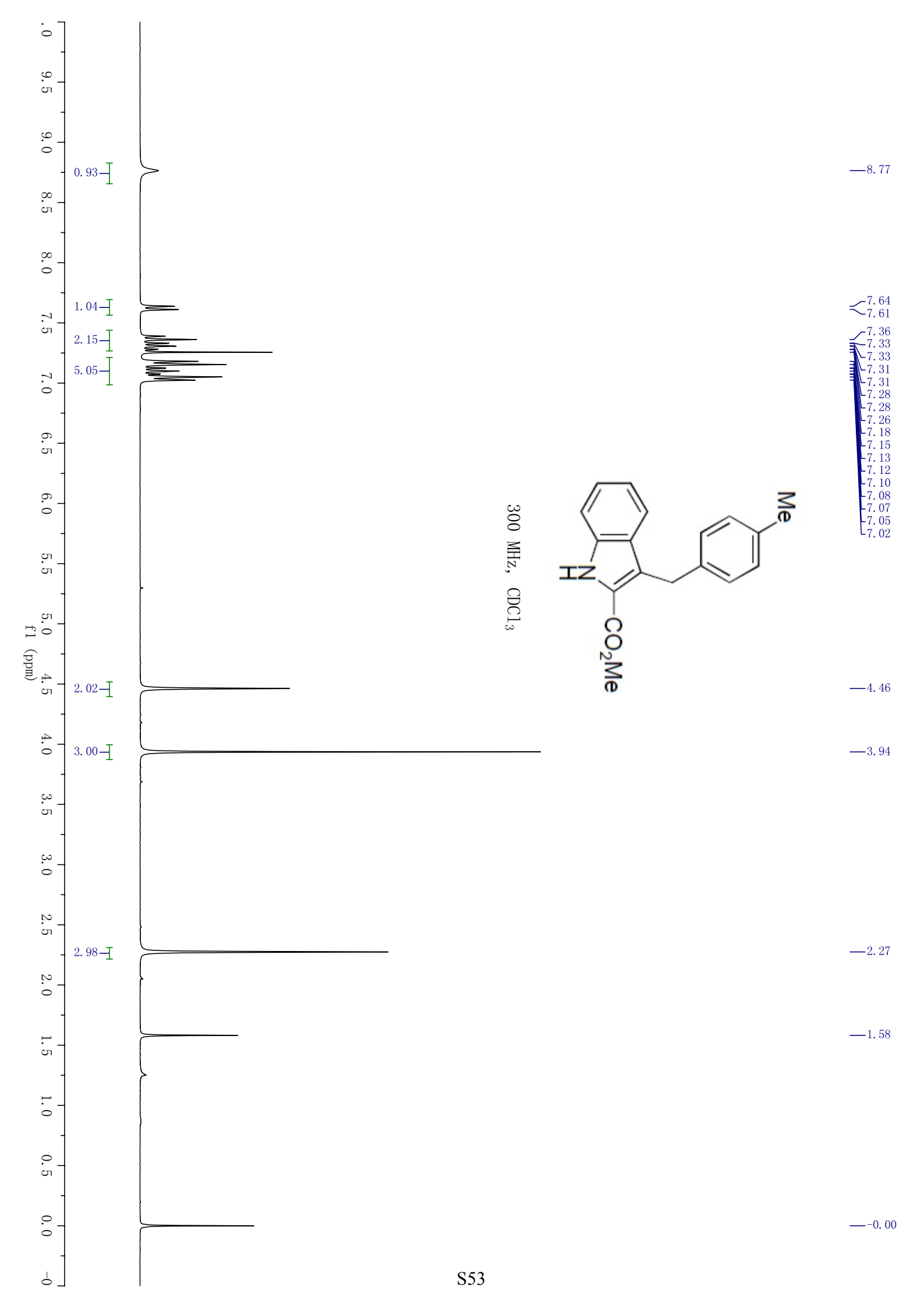

167.56
162.28
140.44
138.24
128.38
127.75
126.69
126.05
124.77
124.47
124.27
122.71
111.53
77.27
76.77
51.99
30.41
125 MHz, CDCl3
MeO2C
CO2Me
N
H
f1 (ppm)

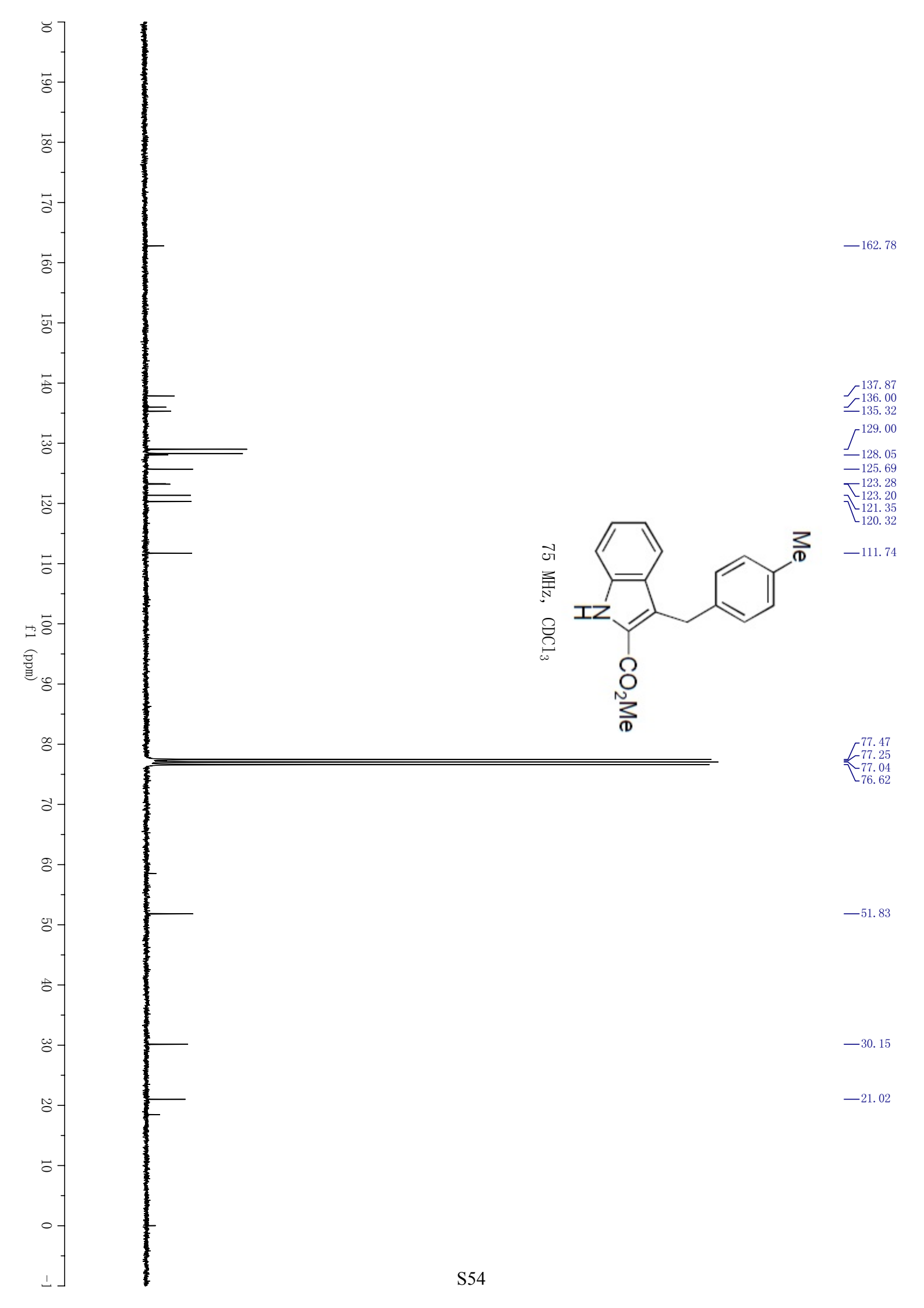

300 MHz, CDCl3
NC
N
CO2Me
8.48
8.45
8.39
8.27
7.96
7.93
7.61
7.53
7.52
7.51
7.27
4.12
1.63
1.26
0.00
0.34
0.34
0.33
0.36
1.03
0.73
1.00
f1 (ppm)

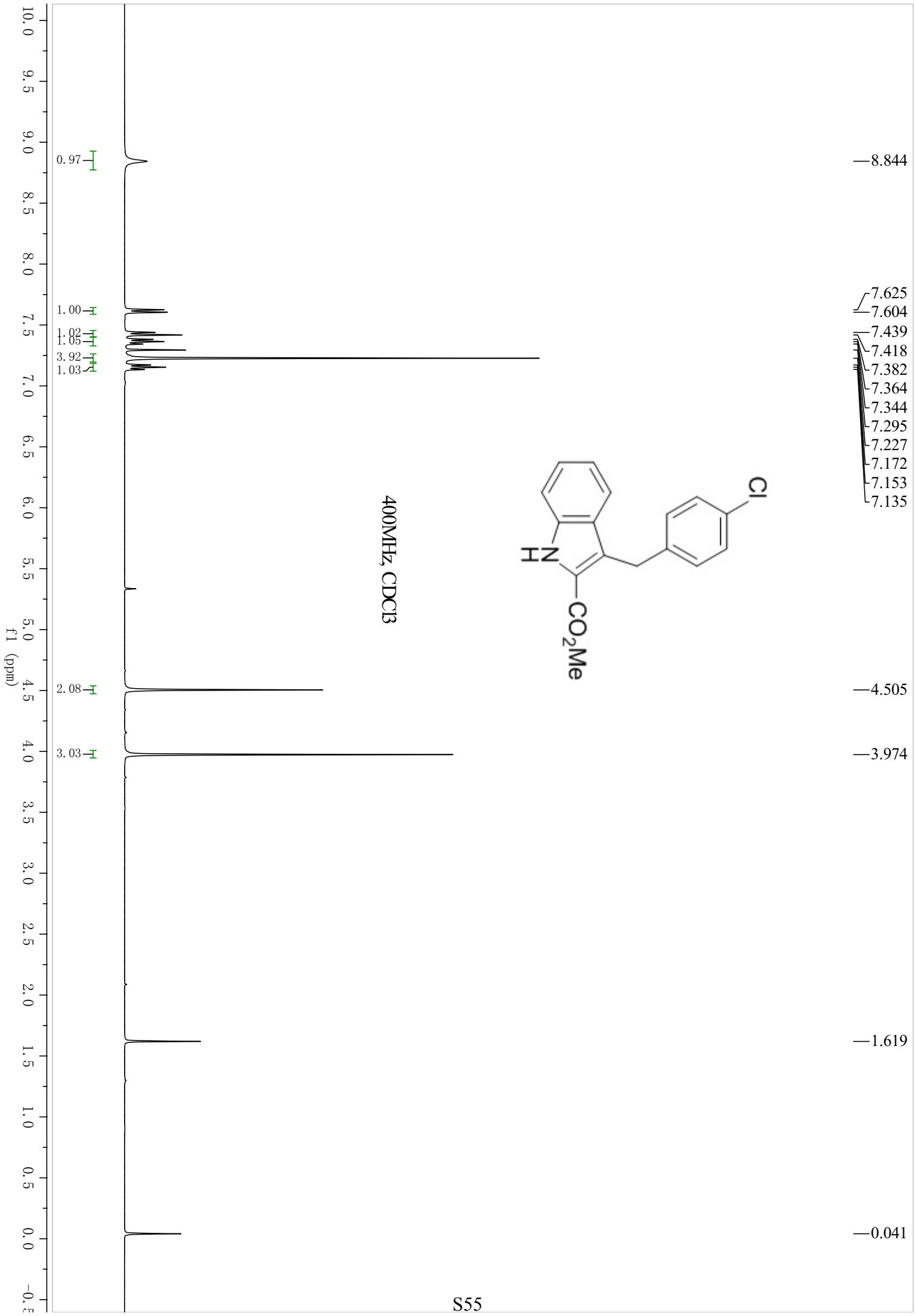

165.39
150.98
150.08
149.12
136.06
129.69
129.56
129.26
127.40
122.69
118.40
112.39
77.35
77.10
76.85
53.61
NC
N
CO2Me
125 MHz, CDCl3
f1 (ppm)

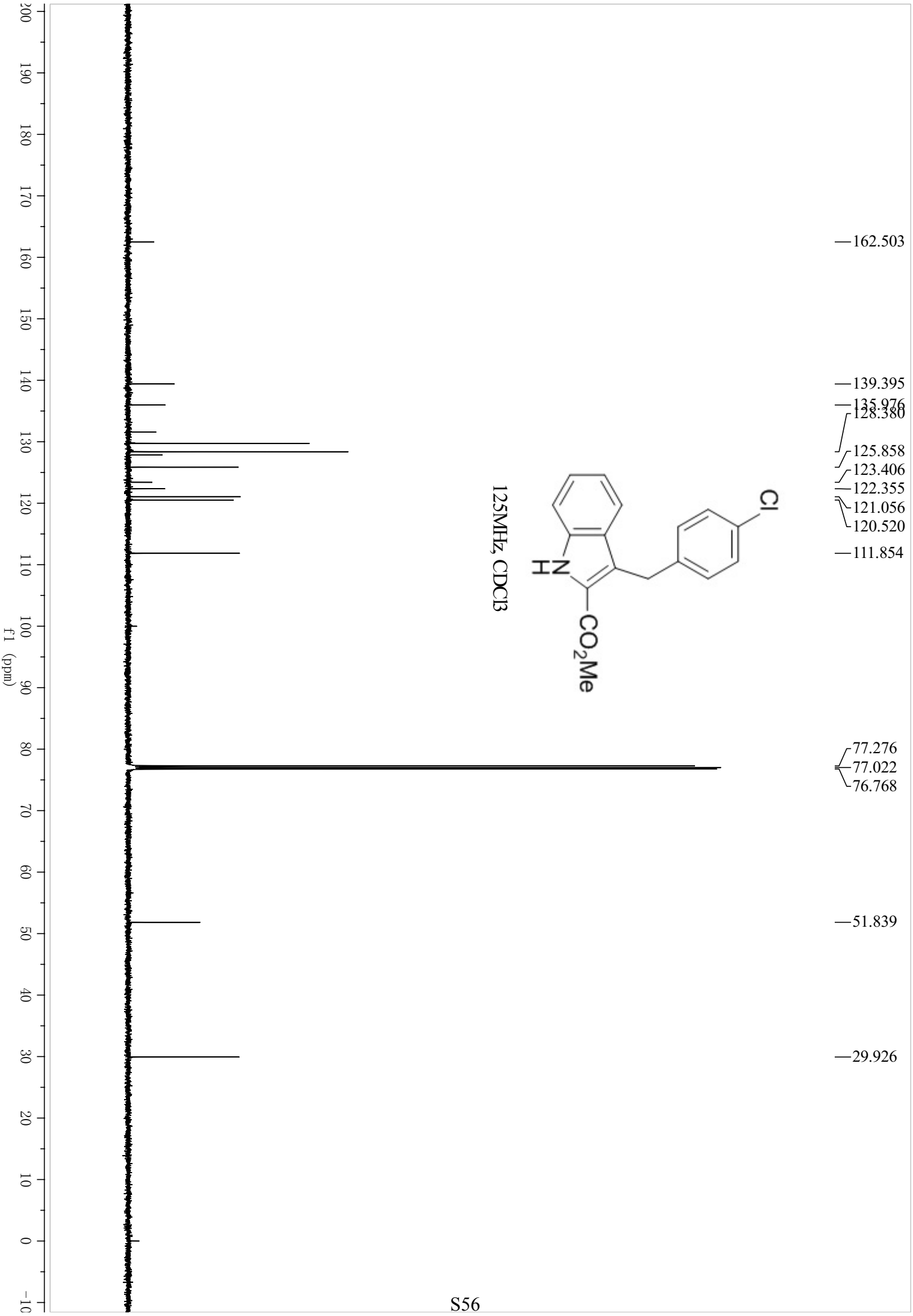

0.88
1.00
0.92
1.02
3.14
2.18
3.16
9.30
9.30
8.37
8.36
8.35
8.35
8.31
8.17
8.15
7.54
7.53
7.52
7.26
4.13
1.58
0.00
f1 (ppm)
500MHz, CDCl3
O2N
N
CO2Me

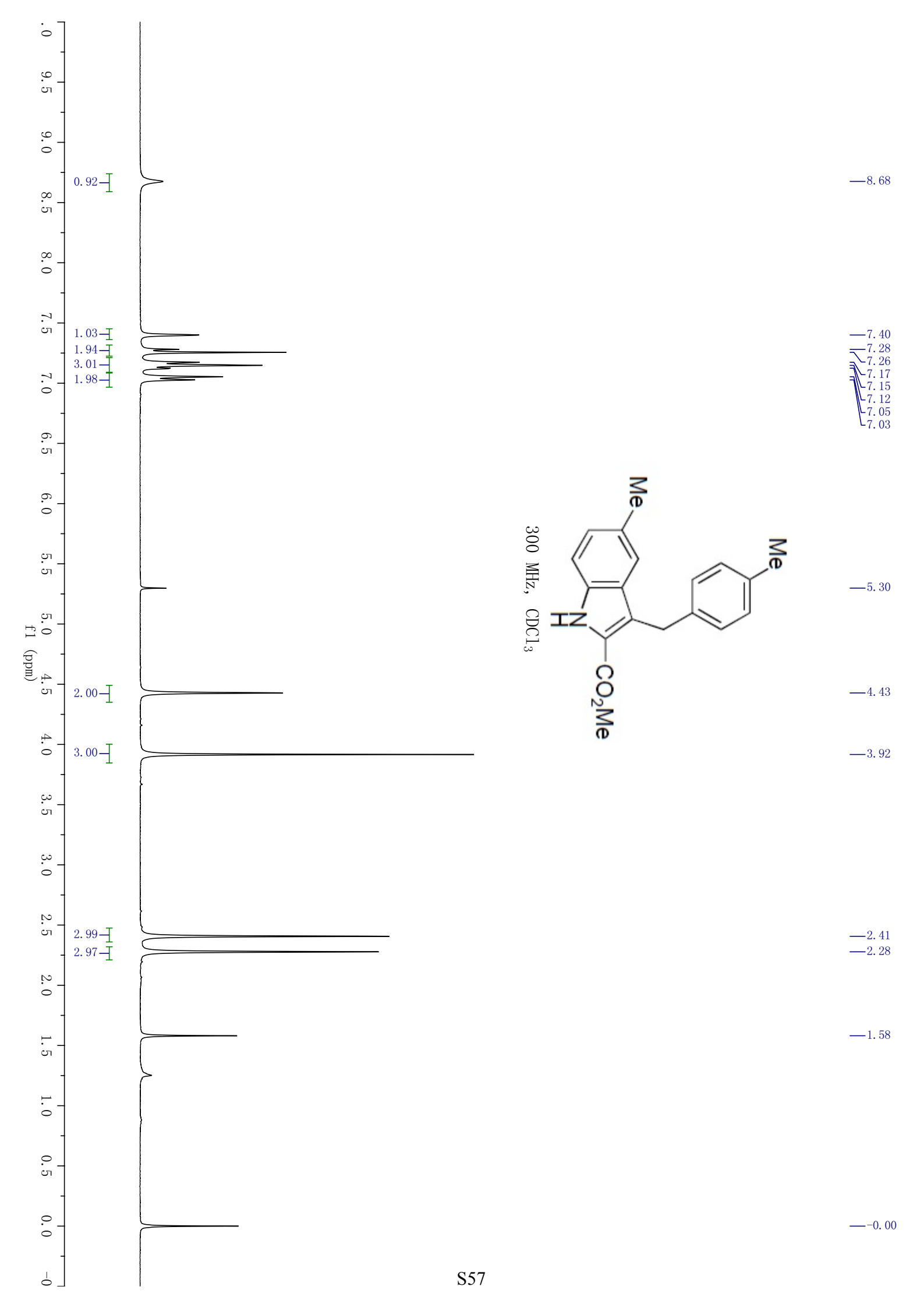

165.25
150.51
149.81
148.51
147.31
136.27
129.50
127.12
123.78
121.76
77.28
77.03
76.78
53.57
0.00
125MHz, CDCl3
O2N
N
CO2Me
f1 (ppm)

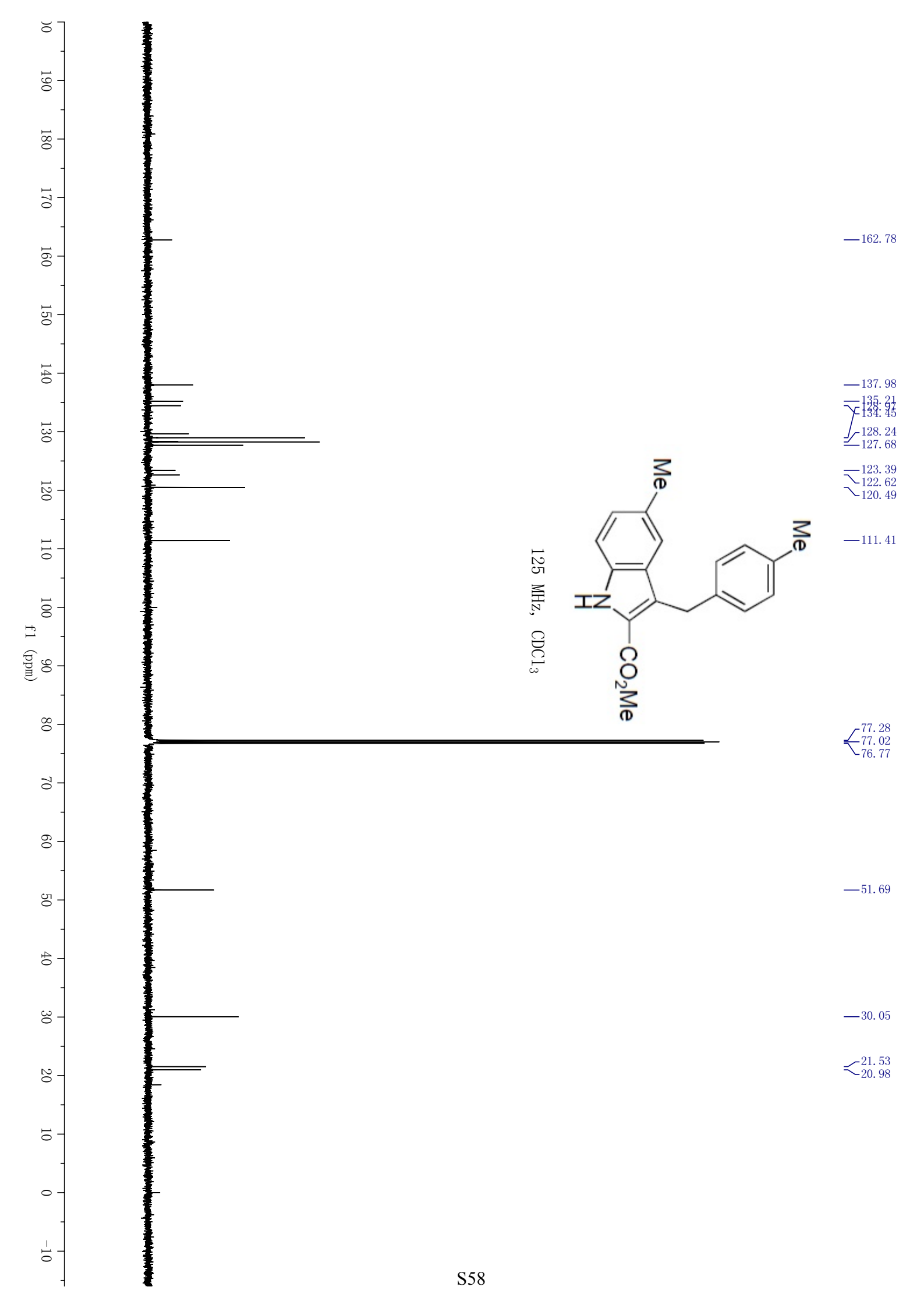

0.93
1.04
2.15
5.05
2.02
3.00
2.98
8.77
7.64
7.61
7.36
7.33
7.33
7.31
7.31
7.28
7.28
7.26
7.18
7.15
7.13
7.12
7.10
7.08
7.07
7.05
7.02
4.46
3.94
2.27
1.58
0.00
300 MHz, CDCl3
Me
HN
CO2Me
f1 (ppm)

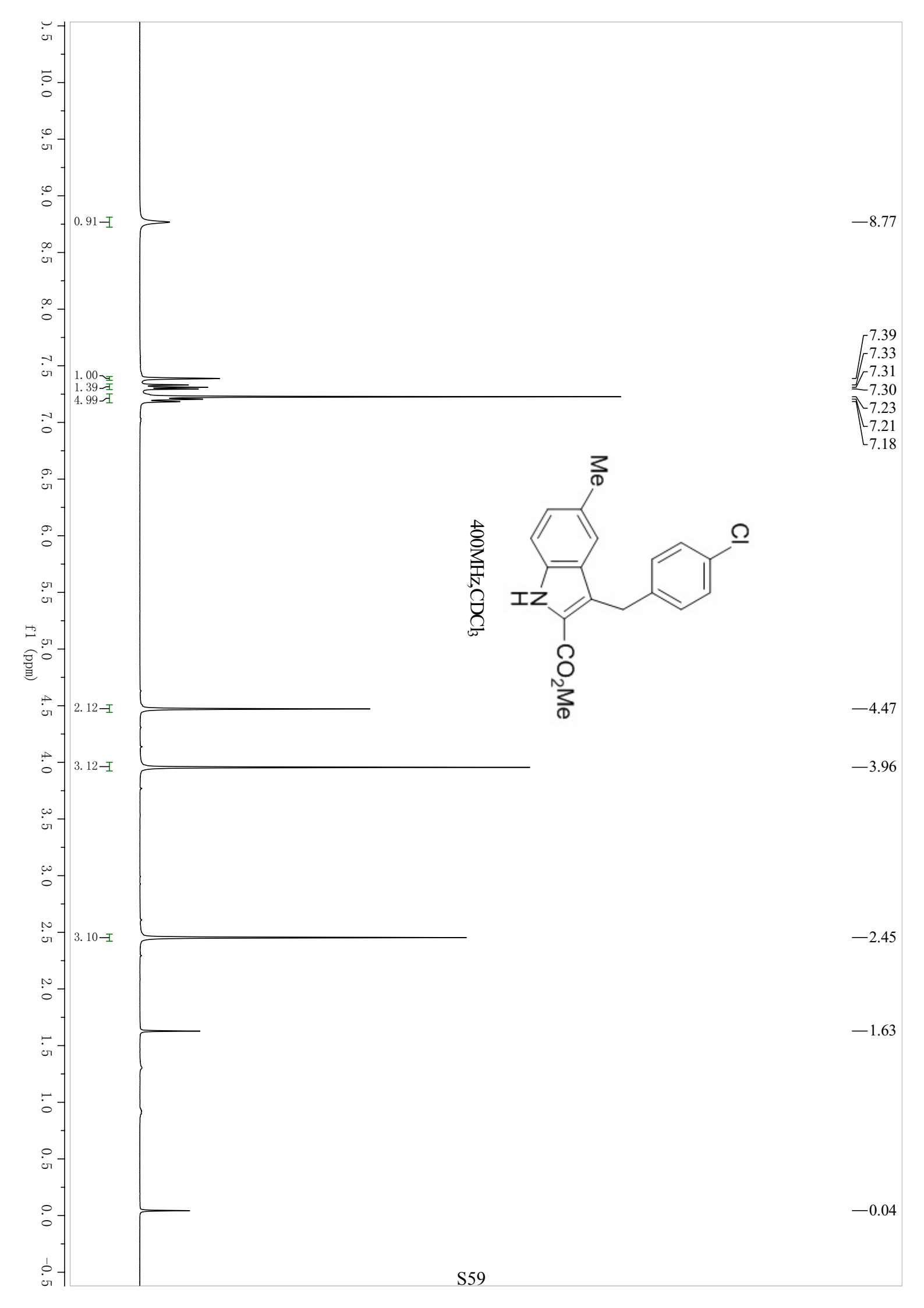

75 MHz, CDCl3
Me
N
H
CO2Me
162.78
137.87
136.00
135.32
129.00
128.05
125.69
123.28
123.20
121.35
120.32
111.74
77.47
77.25
77.04
76.62
51.83
30.15
21.02
f1 (ppm)

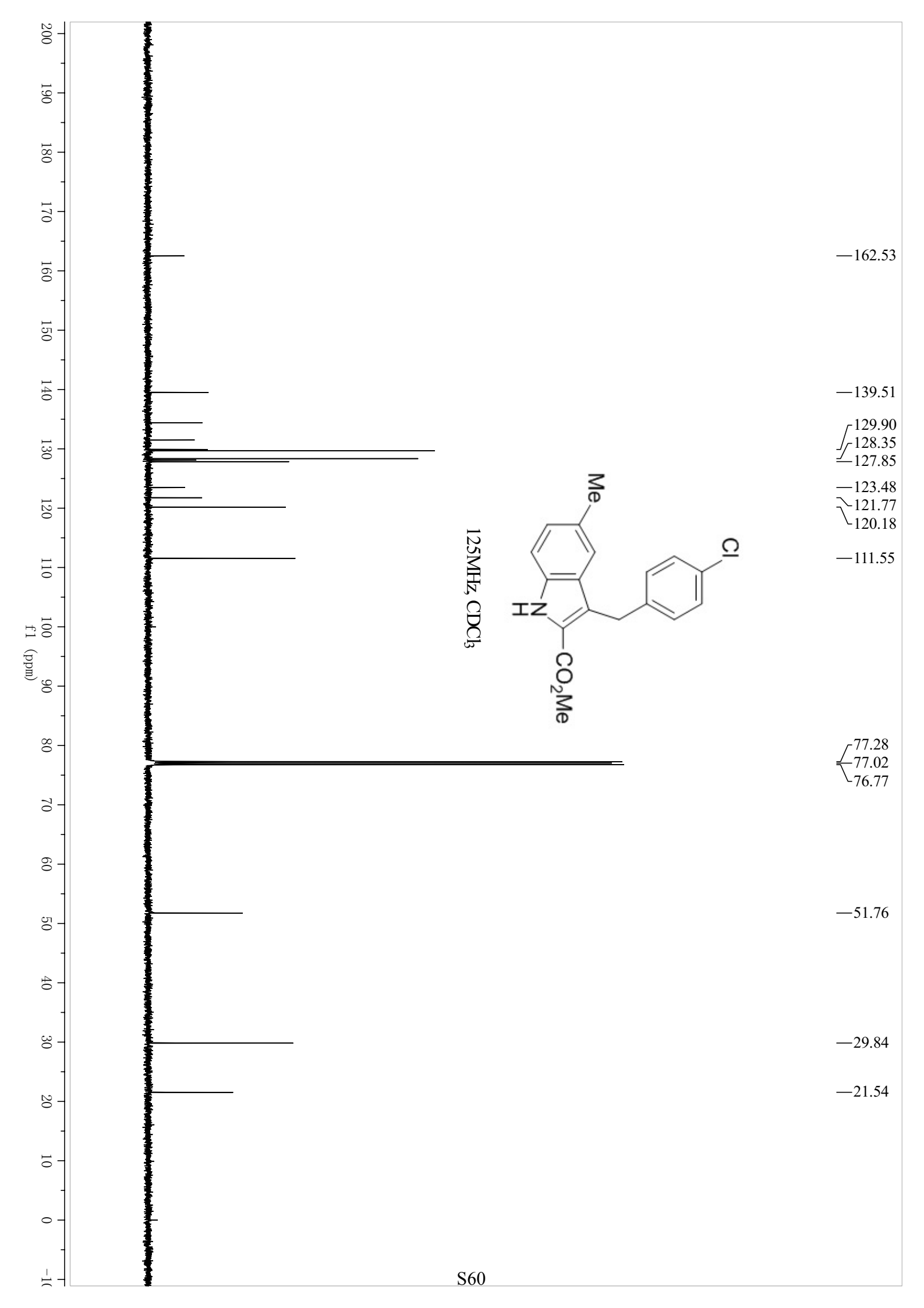

400MHz, CDCl3
Cl
HN
CO2Me
0.97
1.00
1.02
1.05
3.92
1.03
2.08
3.03
8.844
7.625
7.604
7.439
7.418
7.382
7.364
7.344
7.295
7.227
7.172
7.153
7.135
4.505
3.974
1.619
0.041
f1 (ppm)

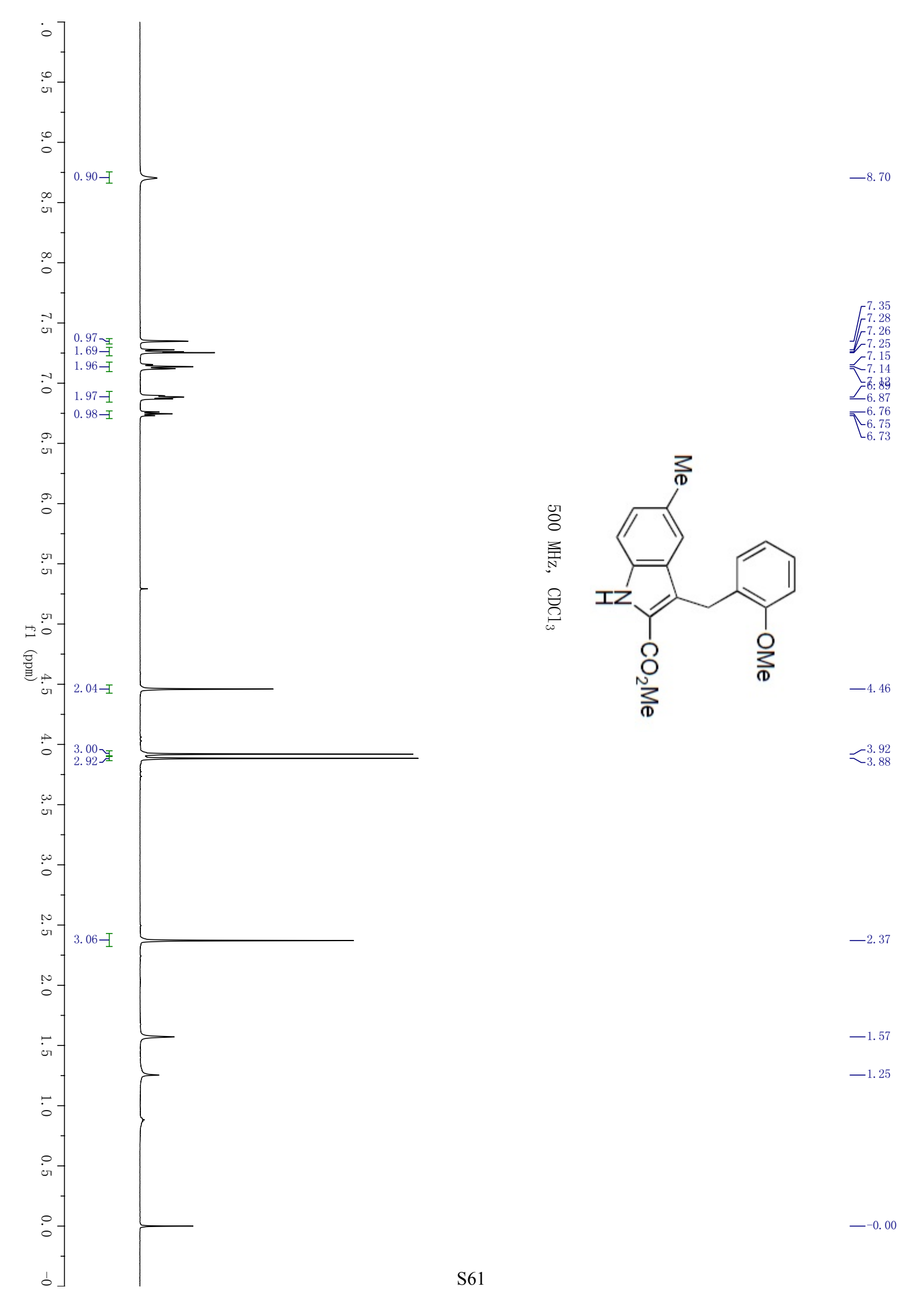

125MHz, CDCl3
Cl
N
H
CO2Me
162.503
139.395
135.976
128.380
125.858
123.406
122.355
121.056
120.520
111.854
77.276
77.022
76.768
51.839
29.926
f1 (ppm)

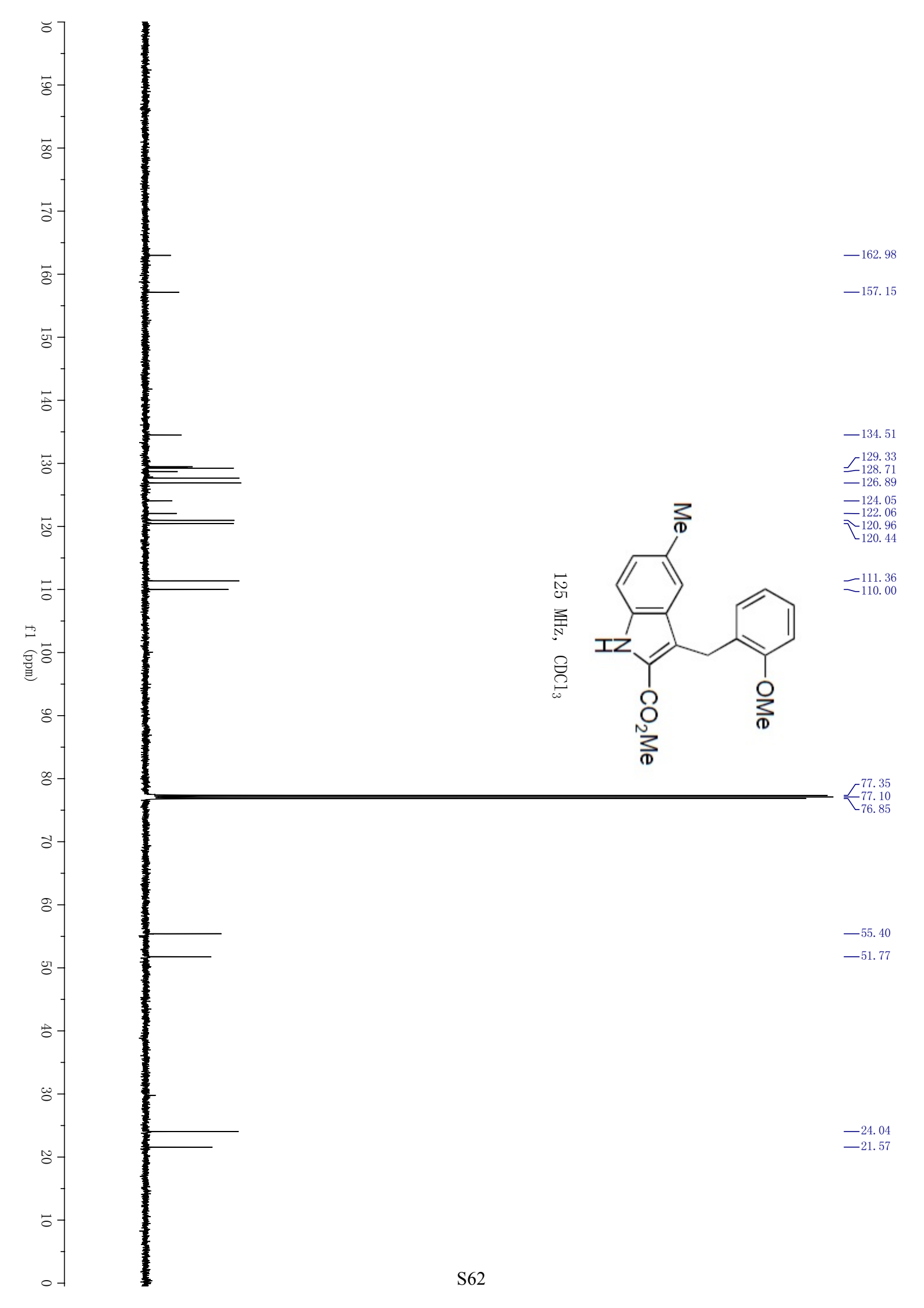

0.92
1.03
1.94
3.01
1.98
2.00
3.00
2.99
2.97
8.68
7.40
7.28
7.26
7.17
7.15
7.12
7.05
7.03
5.30
4.43
3.92
2.41
2.28
1.58
0.00
f1 (ppm)
300 MHz, CDCl3
Me
Me
N
H
CO2Me

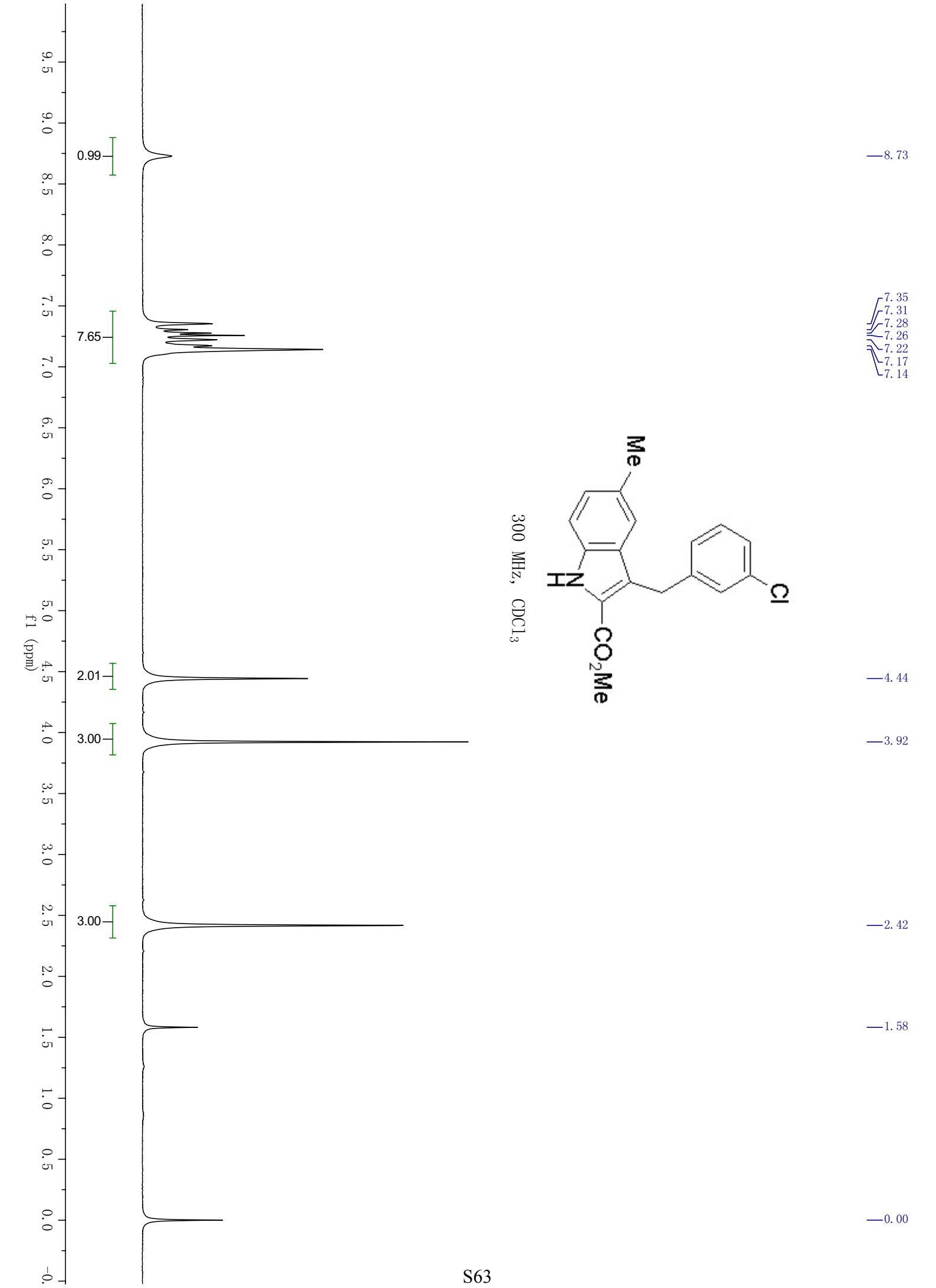

162.78
137.98
135.21
134.45
128.24
127.68
123.39
122.62
120.49
111.41
77.28
77.02
76.77
51.69
30.05
21.53
20.98
125 MHz, CDCl3
Me
Me
N
H
CO2Me
f1 (ppm)

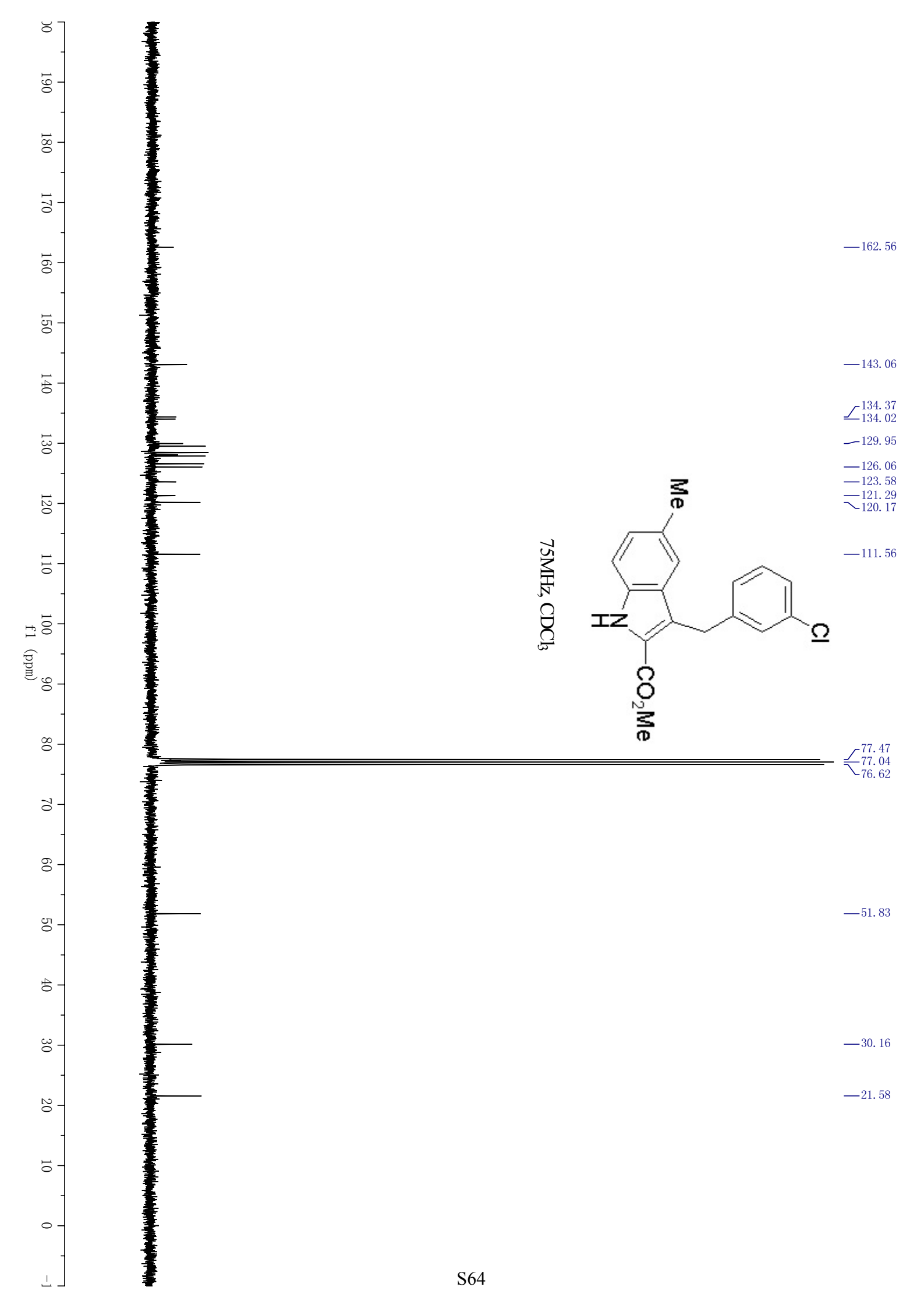

0.91
1.00
1.39
4.99
2.12
3.12
3.10
8.77
7.39
7.33
7.31
7.30
7.23
7.21
7.18
4.47
3.96
2.45
1.63
0.04
400MHz,CDCl3
Me
Cl
N
H
CO2Me
f1 (ppm)


162.53
139.51
129.90
128.35
127.85
123.48
121.77
120.18
111.55
77.28
77.02
76.77
51.76
29.84
21.54
125MHz, CDCl3
Me
Cl
N
H
CO2Me
f1 (ppm)

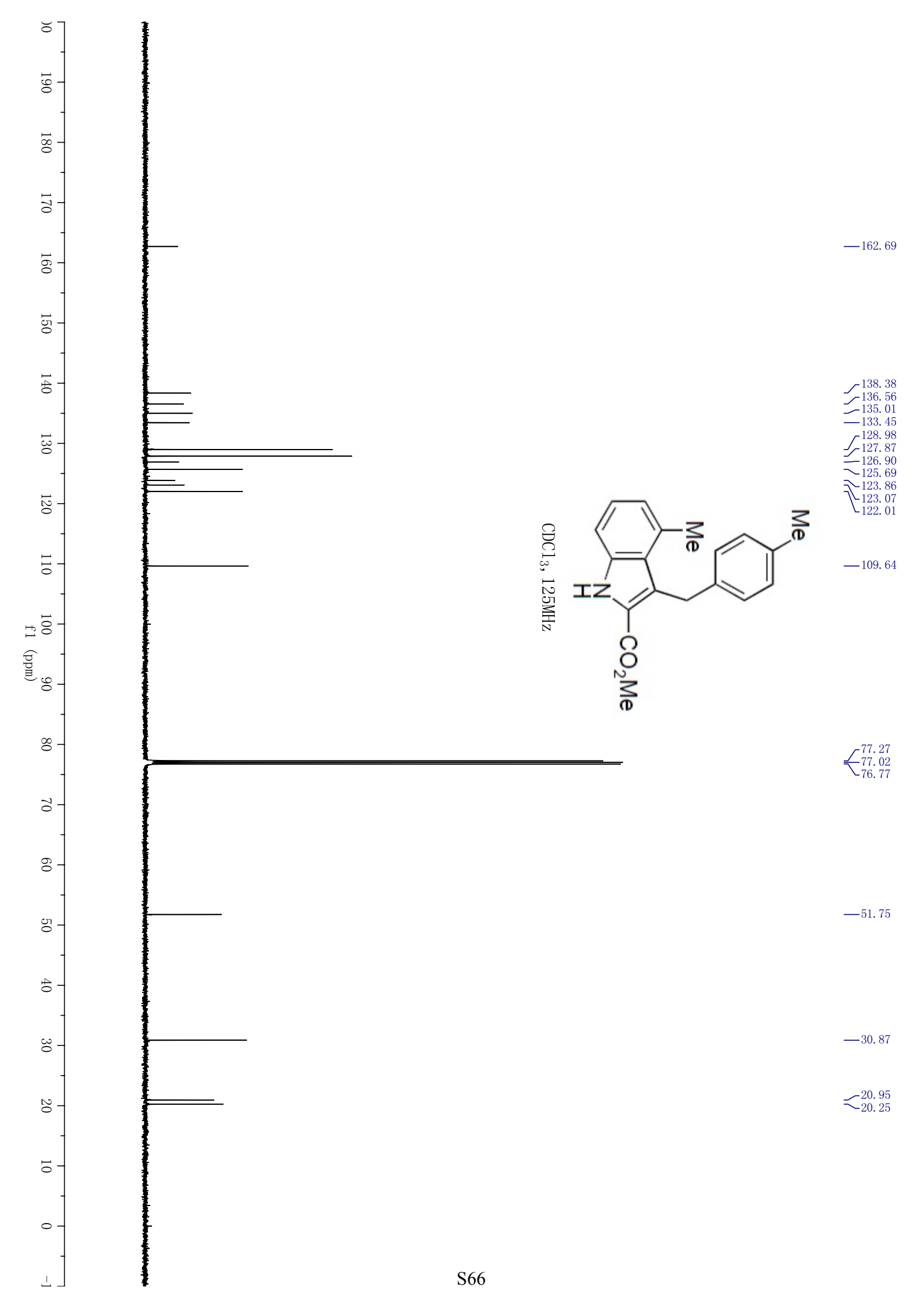

500 MHz, CDCl3
f1 (ppm)
0.90
0.97
1.69
1.96
1.97
0.98
2.04
3.00
2.92
3.06
8.70
7.35
7.28
7.26
7.25
7.15
7.14
7.12
6.89
6.87
6.76
6.75
6.73
4.46
3.92
3.88
2.37
1.57
1.25
0.00
Me
OMe
CO2Me
N
H

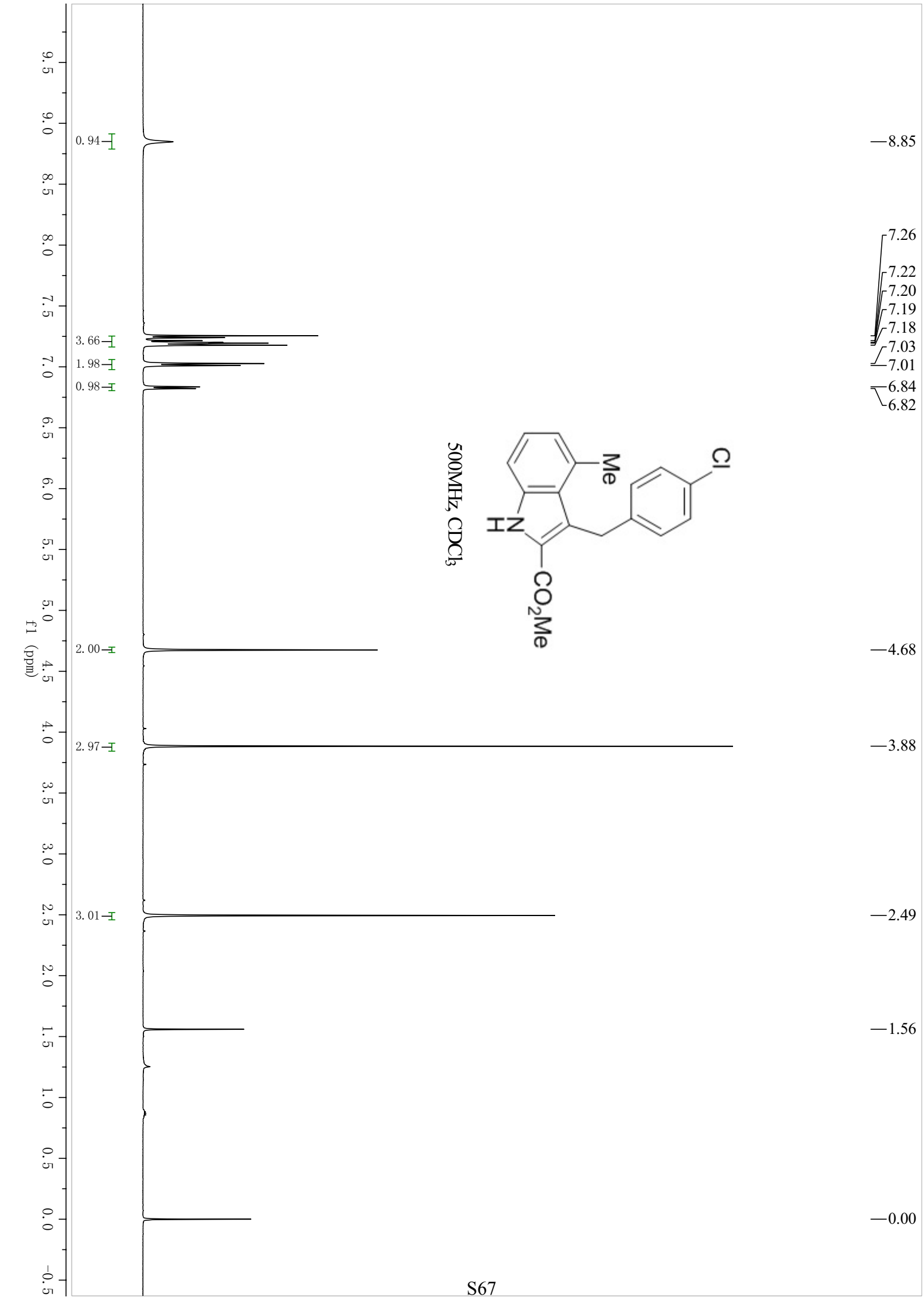

162.98
157.15
134.51
129.33
128.71
126.89
124.05
122.06
120.96
120.44
111.36
110.00
77.35
77.10
76.85
55.40
51.77
24.04
21.57
125 MHz, CDCl3
Me
N
H
CO2Me
OMe
f1 (ppm)

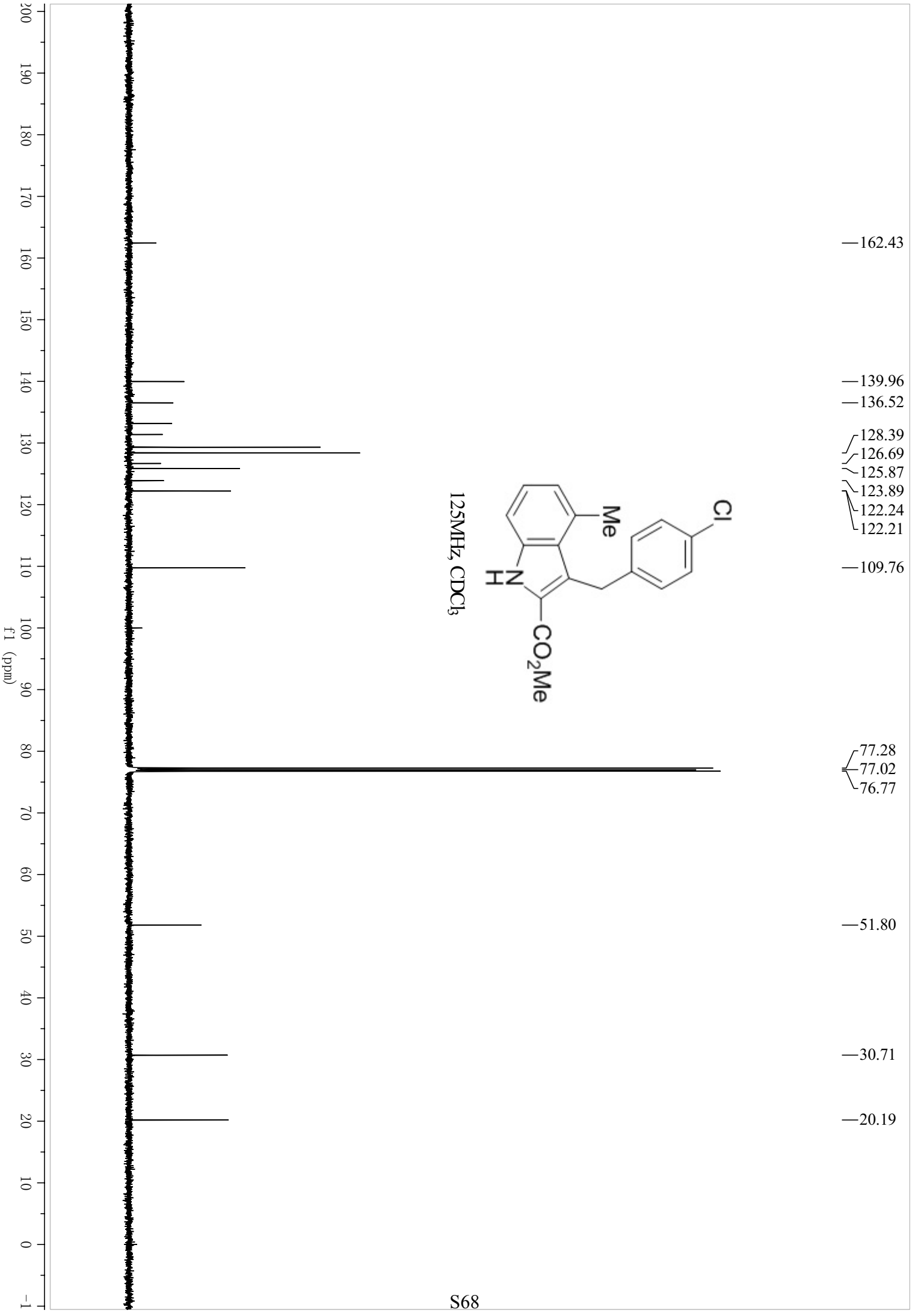

0.99
7.65
2.01
3.00
3.00
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.
8.73
7.35
7.31
7.28
7.26
7.22
7.17
7.14
4.44
3.92
2.42
1.58
0.00
300 MHz, CDCl3
Me
N
H
Cl
CO2Me

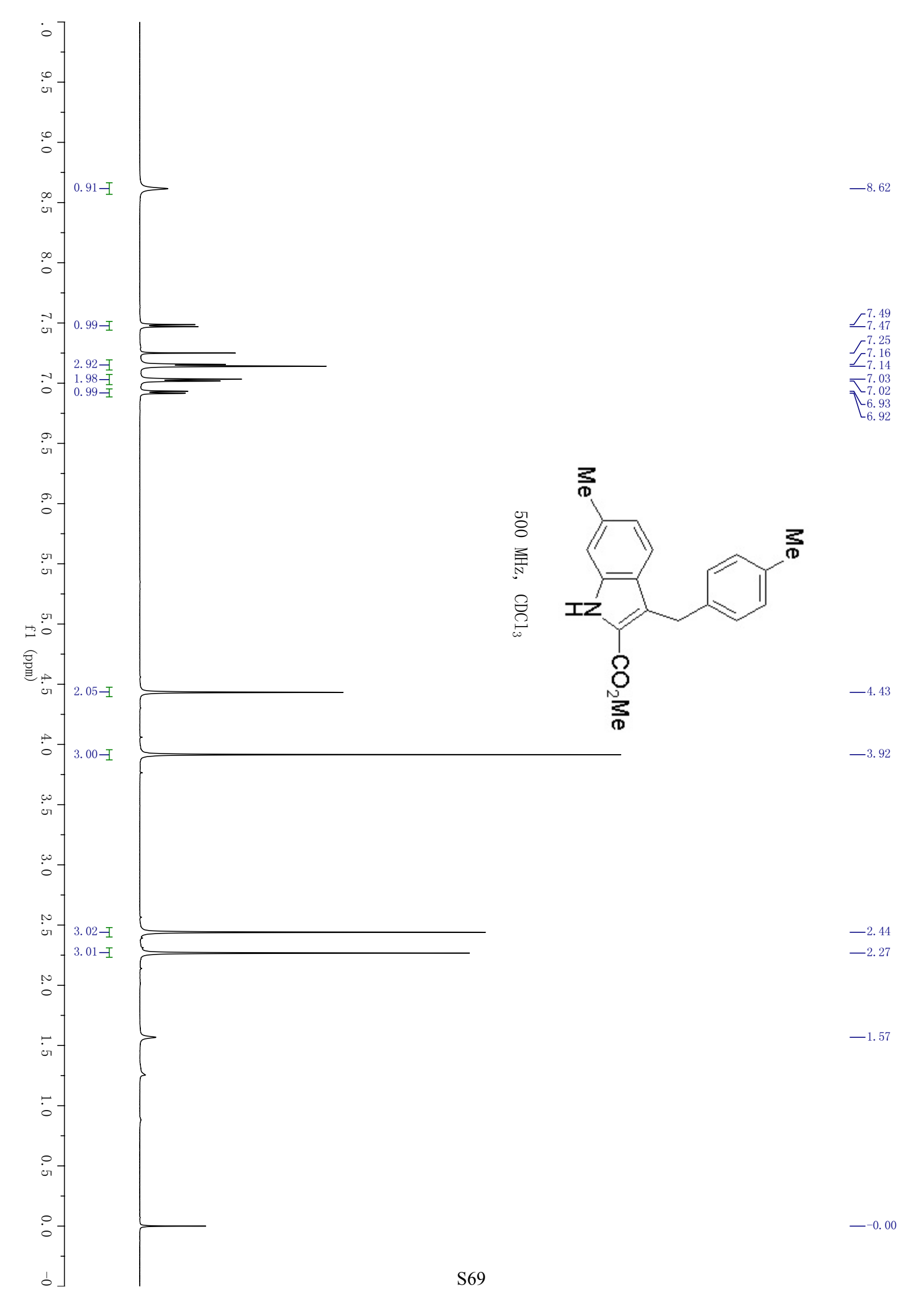

75MHz, CDCl3
Me
N
H
Cl
CO2Me
162.56
143.06
134.37
134.02
129.95
126.06
123.58
121.29
120.17
111.56
77.47
77.04
76.62
51.83
30.16
21.58
f1 (ppm)

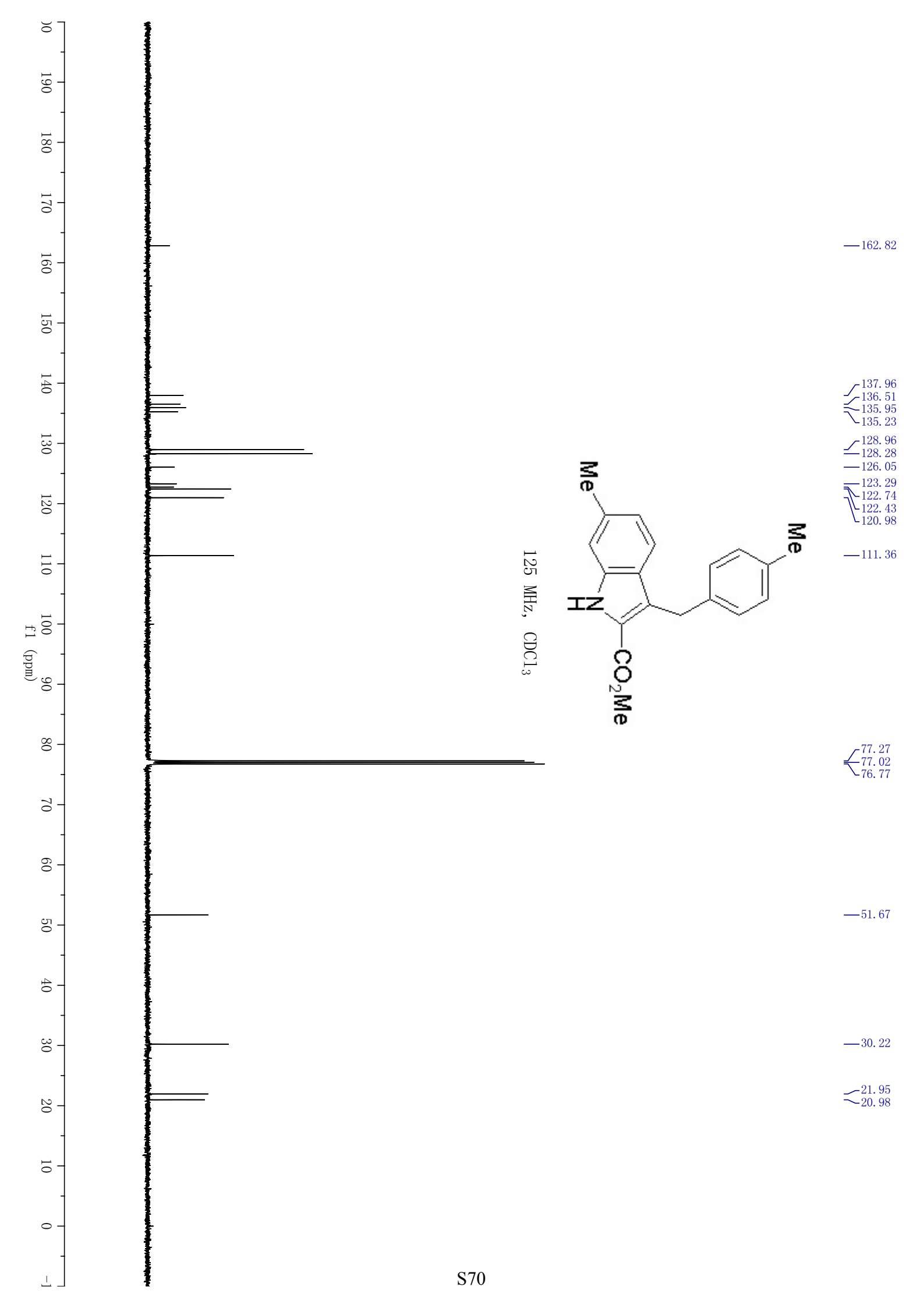

0.90
2.58
4.04
1.00
1.94
2.99
3.00
2.94
8.86
7.25
7.23
7.21
7.19
7.16
6.97
6.82
6.80
4.67
3.88
2.52
2.28
1.60
1.25
0.00
f1 (ppm)
CDCl3, 300MHz
Me
Me
N
H
CO2Me

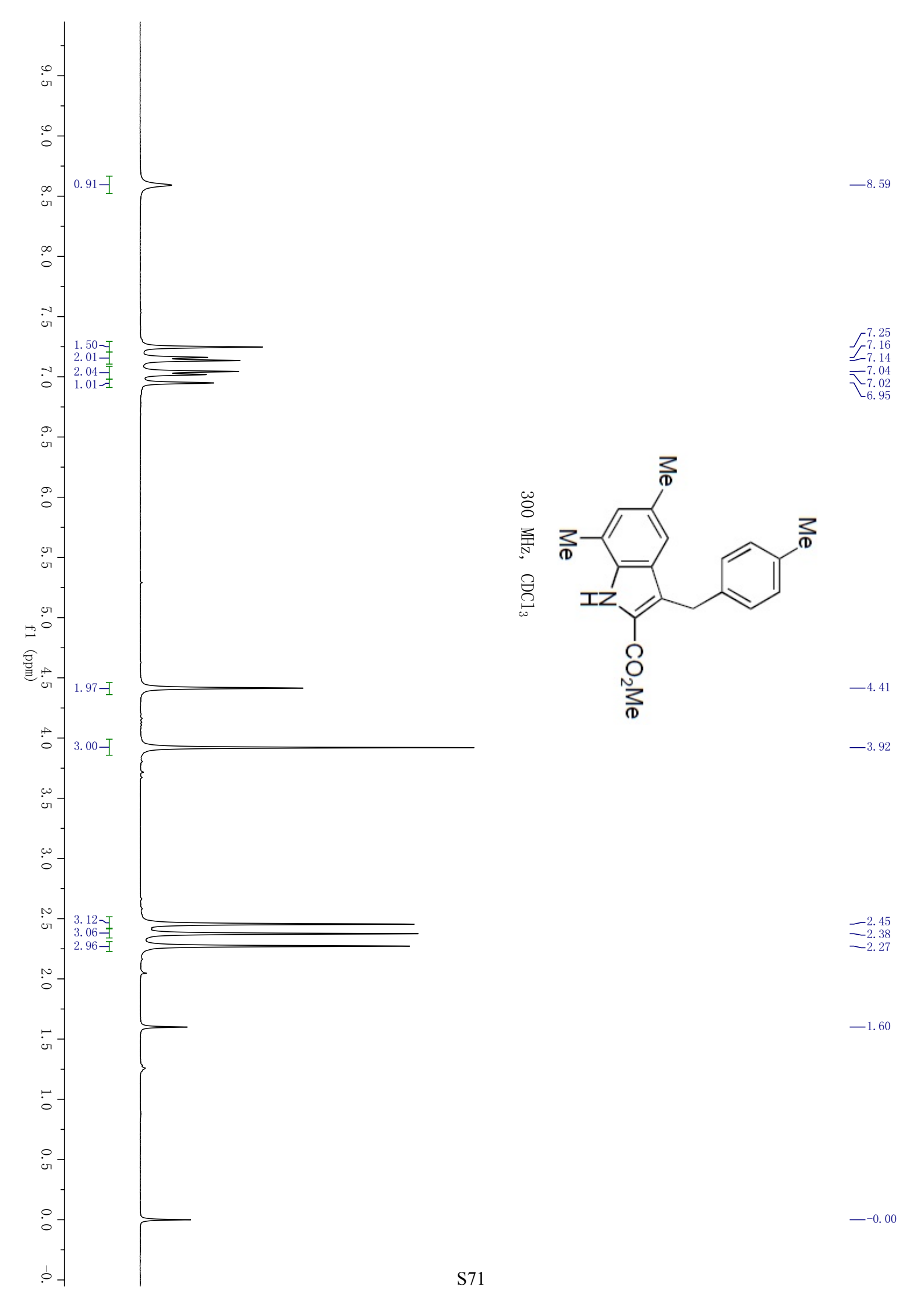

162.69
138.38
136.56
135.01
133.45
128.98
127.87
126.90
125.69
123.86
123.07
122.01
109.64
77.27
77.02
76.77
51.75
30.87
20.95
20.25
CDCl3, 125MHz
Me
Me
N
H
CO2Me
f1 (ppm)

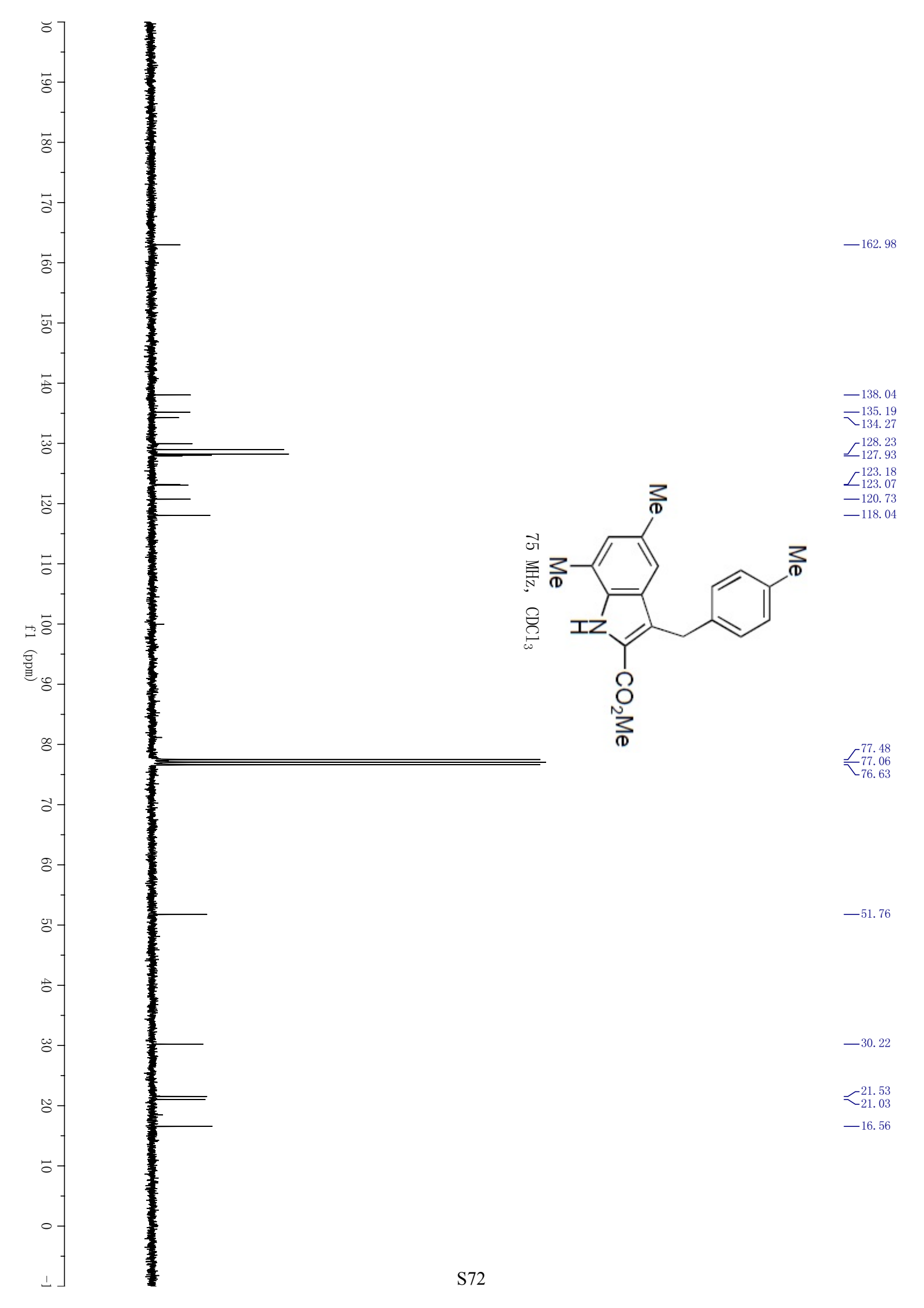

0.94
3.66
1.98
0.98
2.00
2.97
3.01
8.85
7.26
7.22
7.20
7.19
7.18
7.03
7.01
6.84
6.82
4.68
3.88
2.49
1.56
0.00
f1 (ppm)
500MHz, CDCl3
Me
Cl
N
H
CO2Me

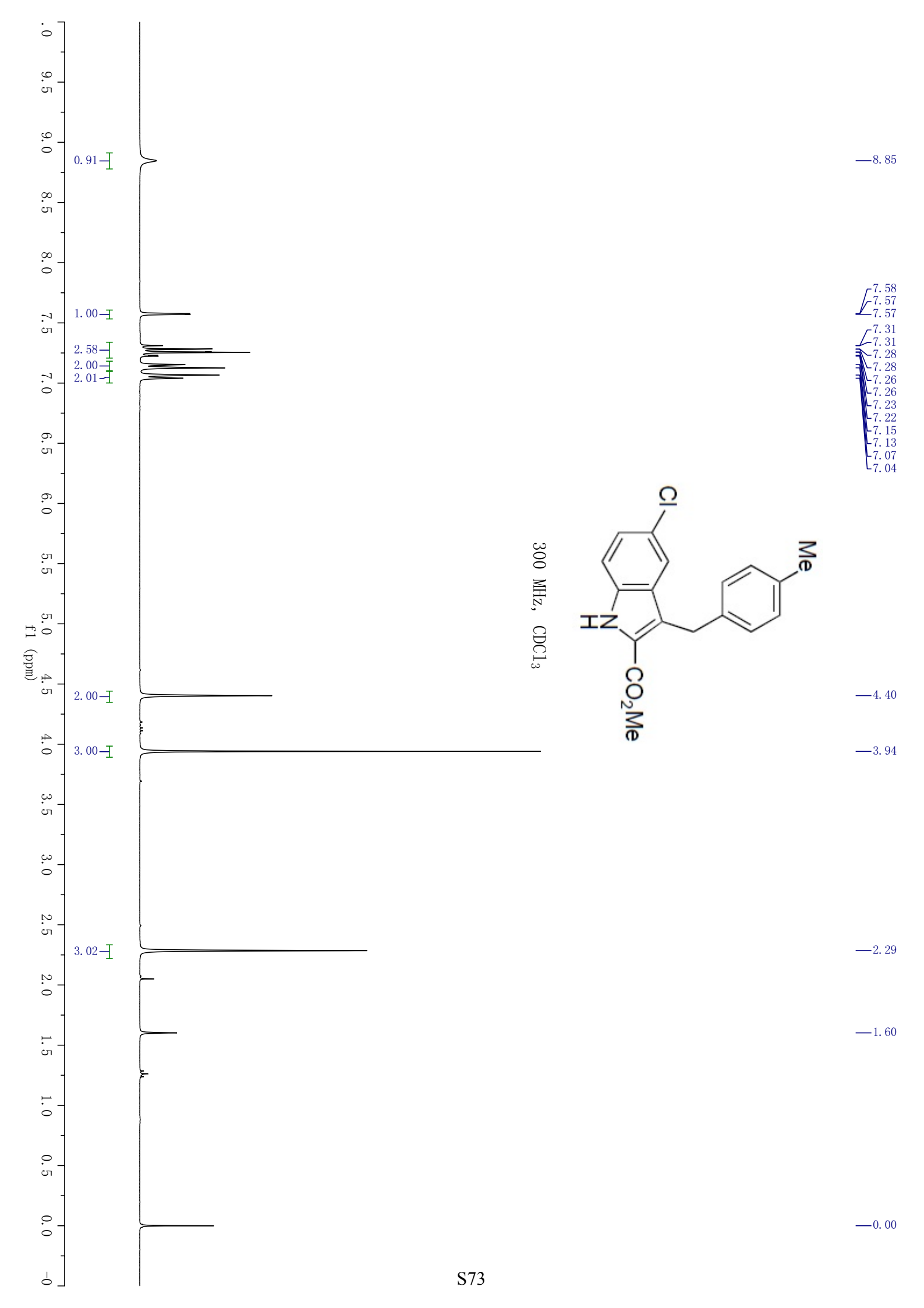

125MHz, CDCl3
Me
Cl
N
H
CO2Me
162.43
139.96
136.52
128.39
126.69
125.87
123.89
122.24
122.21
109.76
77.28
77.02
76.77
51.80
30.71
20.19
f1 (ppm)

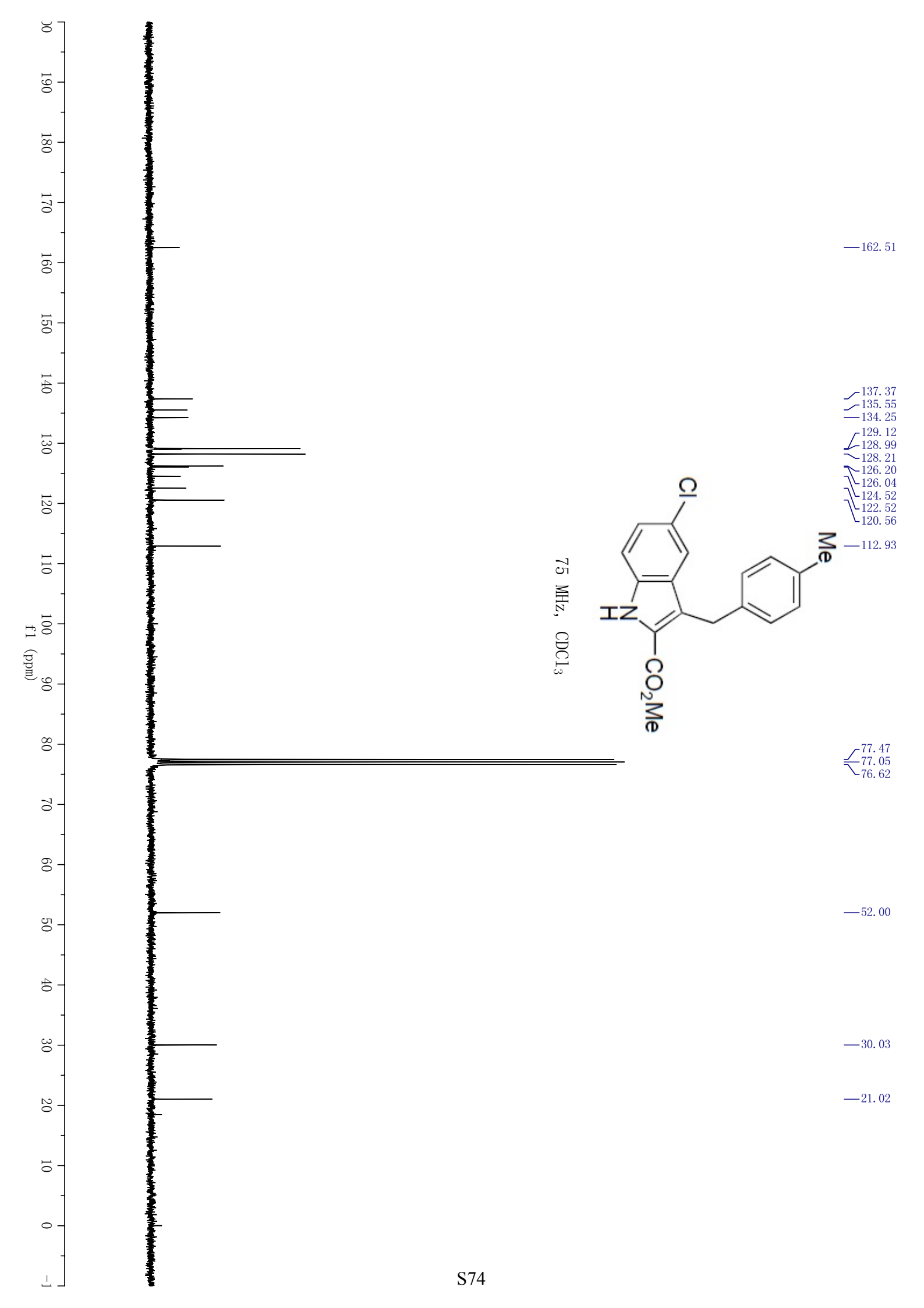

0.91
0.99
2.92
1.98
0.99
2.05
3.00
3.02
3.01
8.62
7.49
7.47
7.25
7.16
7.14
7.03
7.02
6.93
6.92
4.43
3.92
2.44
2.27
1.57
0.00
500 MHz, CDCl3
Me
Me
HN
CO2Me
f1 (ppm)

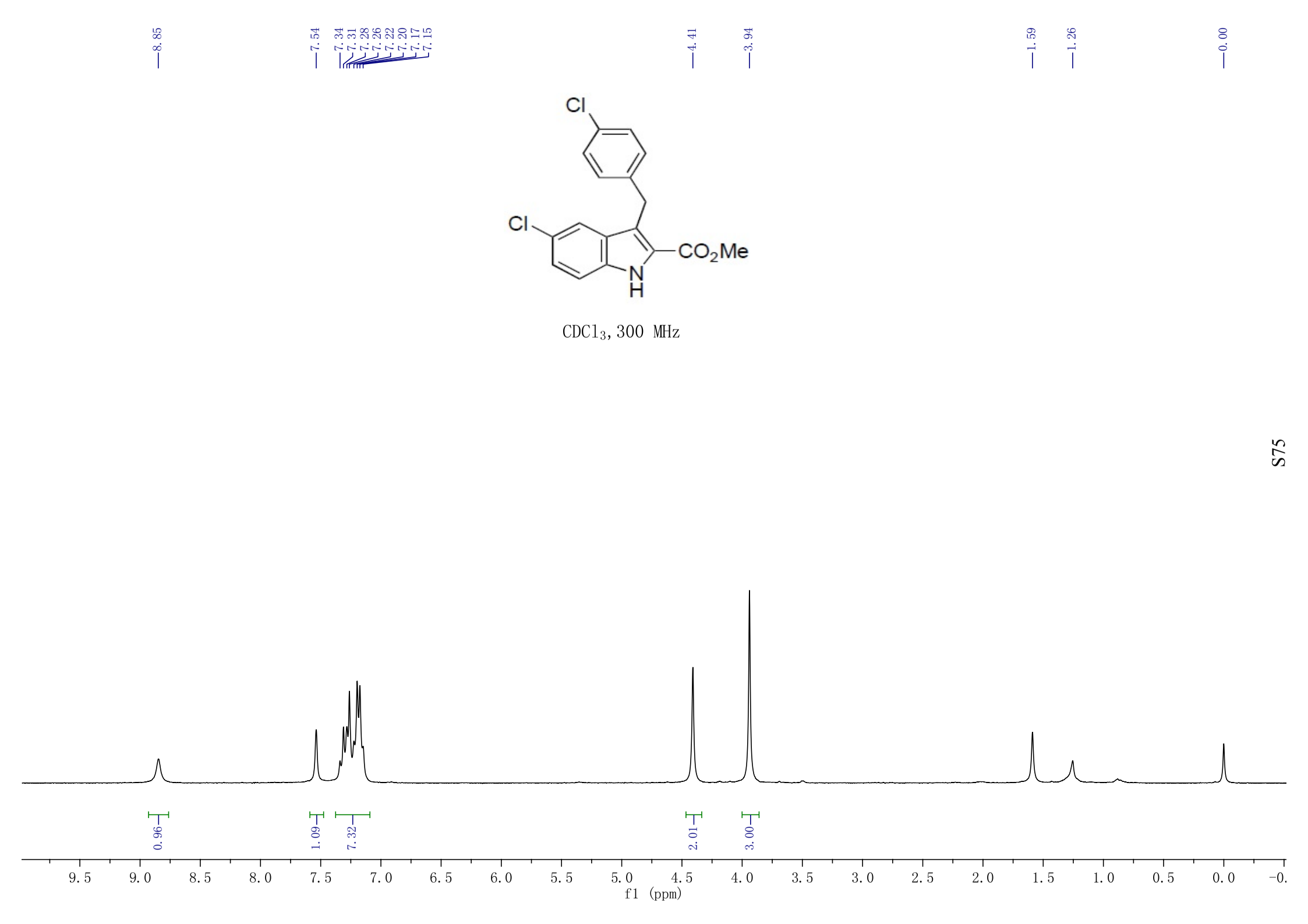

125 MHz, CDCl3
Me
N
H
CO2Me
Me
162.82
137.96
136.51
135.95
135.23
128.96
128.28
126.05
123.29
122.74
122.43
120.98
111.36
77.27
77.02
76.77
51.67
30.22
21.95
20.98
f1 (ppm)

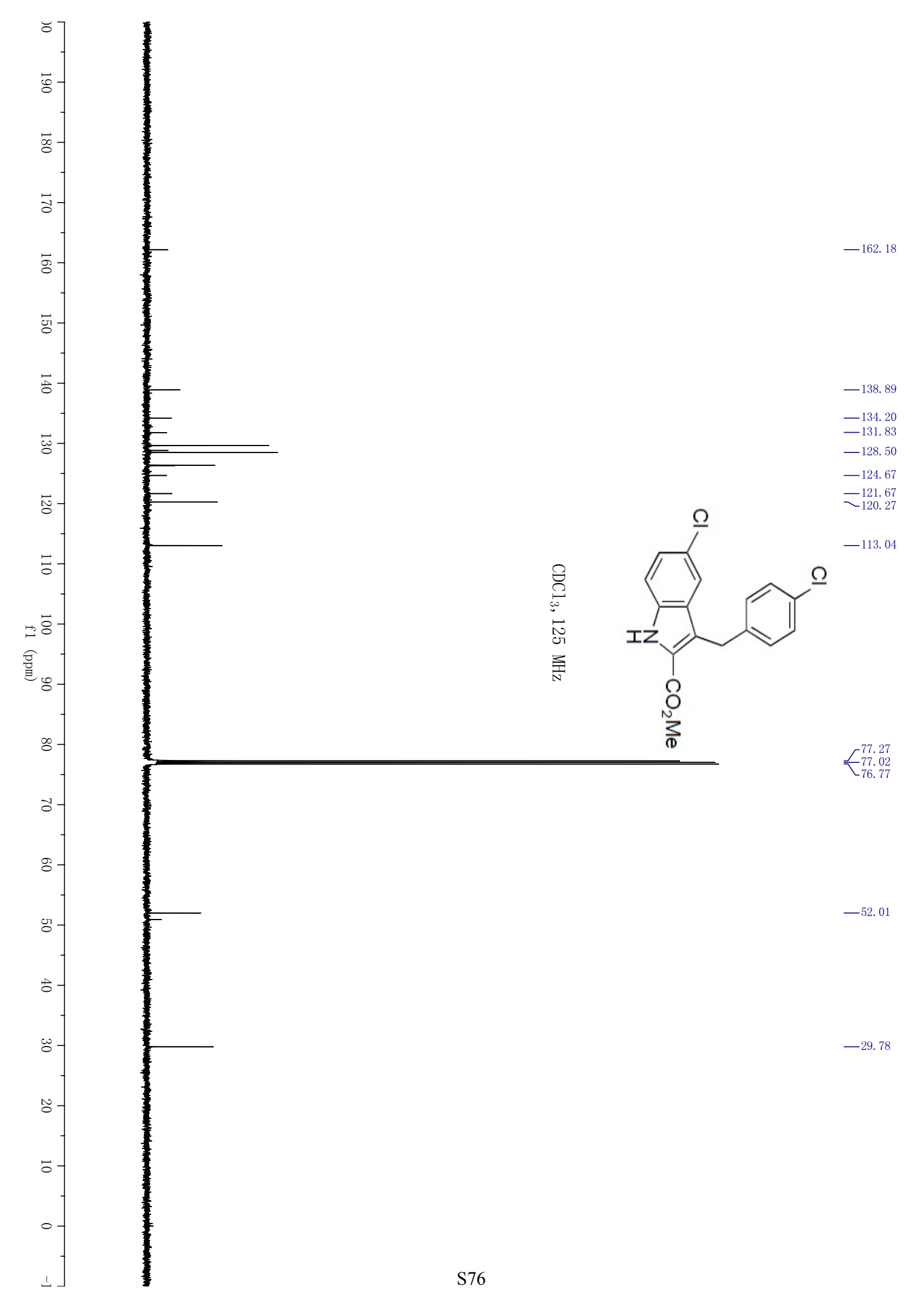

0.91
1.50
2.01
2.04
1.01
1.97
3.00
3.12
3.06
2.96
8.59
7.25
7.16
7.14
7.04
7.02
6.95
4.41
3.92
2.45
2.38
2.27
1.60
0.00
f1 (ppm)
300 MHz, CDCl3
Me
Me
Me
N
H
CO2Me

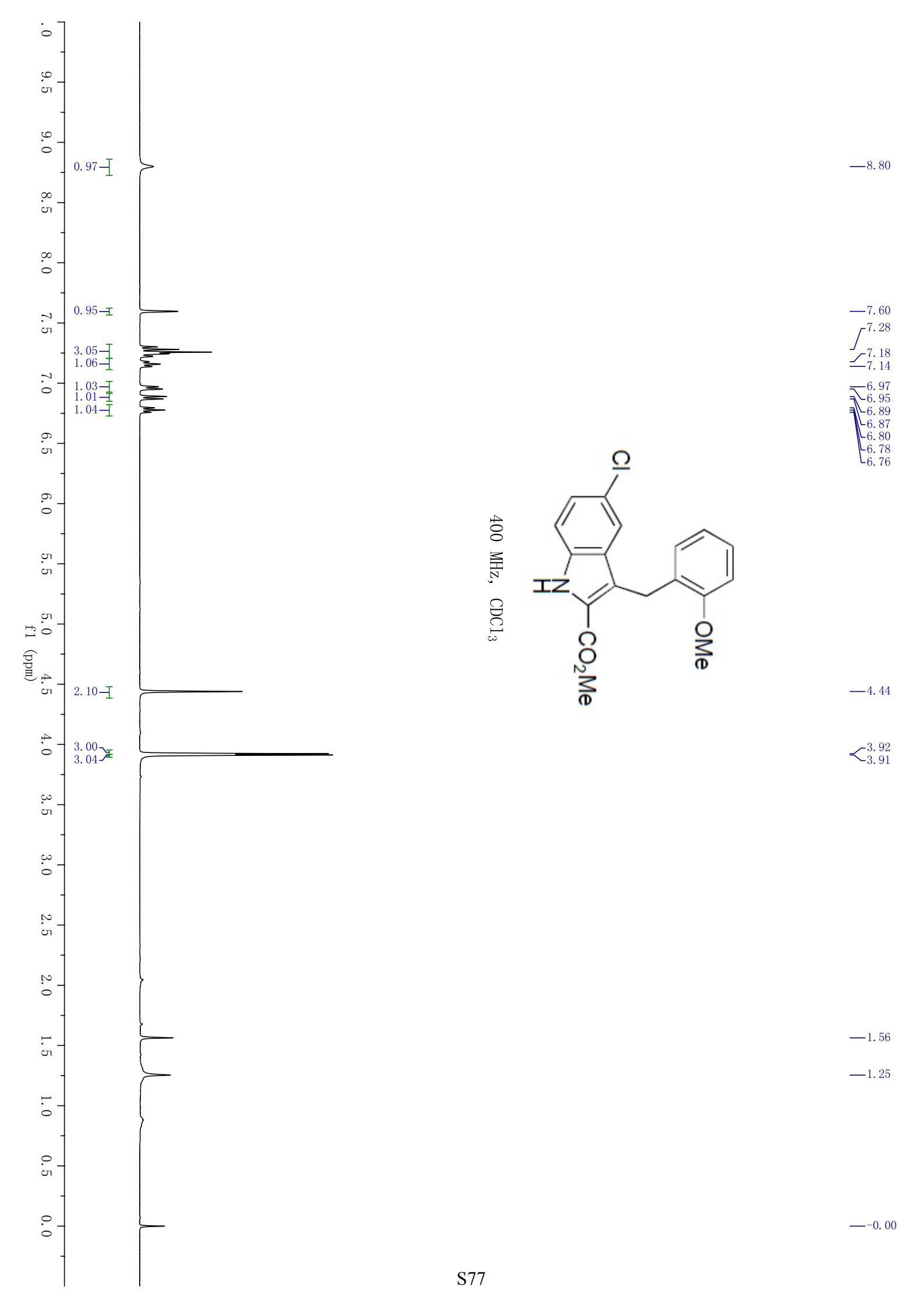

75 MHz, CDCl3
f1 (ppm)
Me
Me
Me
N
H
CO2Me
162.98
138.04
135.19
134.27
128.23
127.93
123.18
123.07
120.73
118.04
77.48
77.06
76.63
51.76
30.22
21.53
21.03
16.56

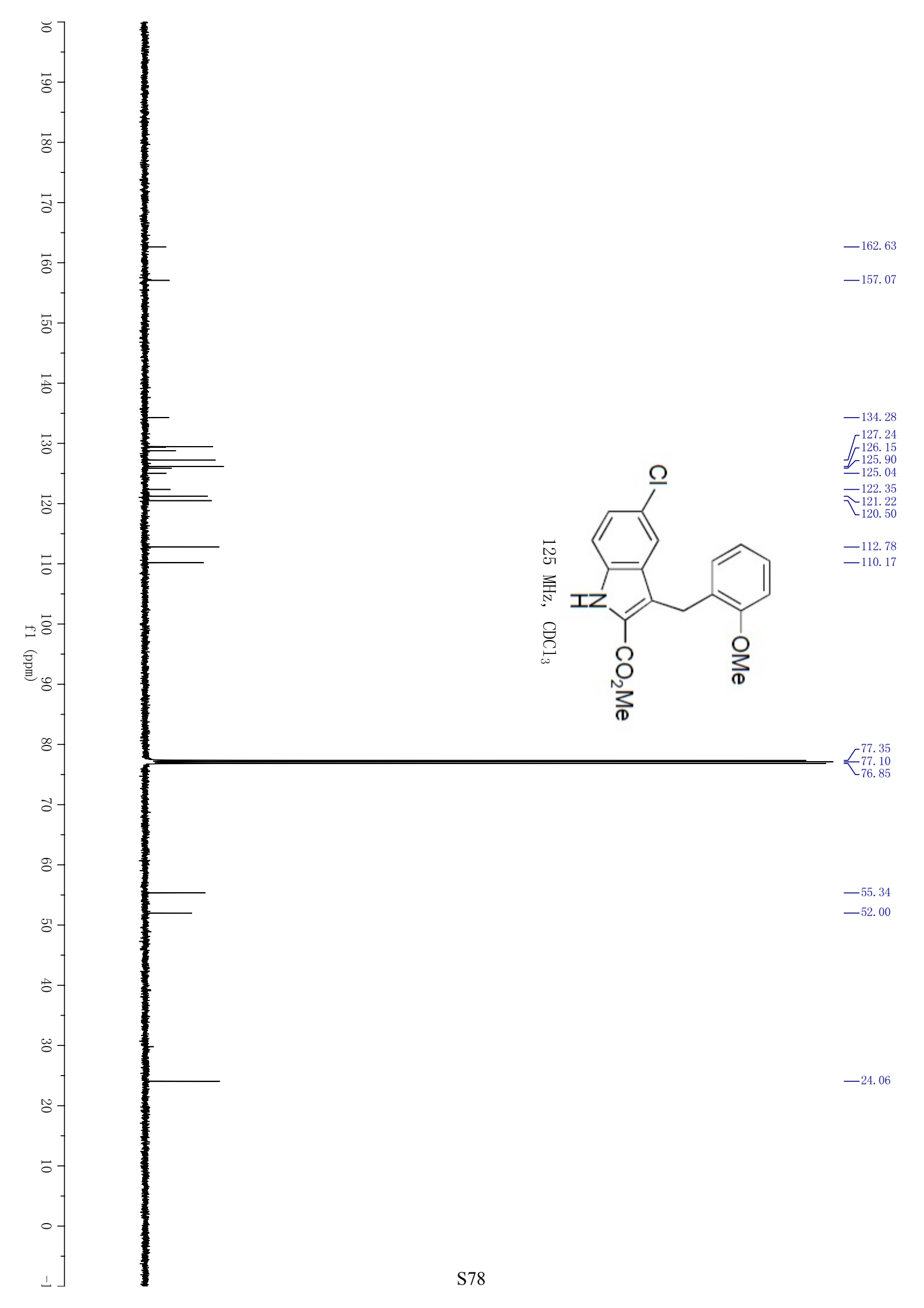

0.91
1.00
2.58
2.00
2.01
2.00
3.00
3.02
8.85
7.58
7.57
7.57
7.31
7.31
7.28
7.28
7.26
7.26
7.23
7.22
7.15
7.13
7.07
7.04
4.40
3.94
2.29
1.60
0.00
300 MHz, CDCl3
f1 (ppm)
Cl
Me
N
H
CO2Me

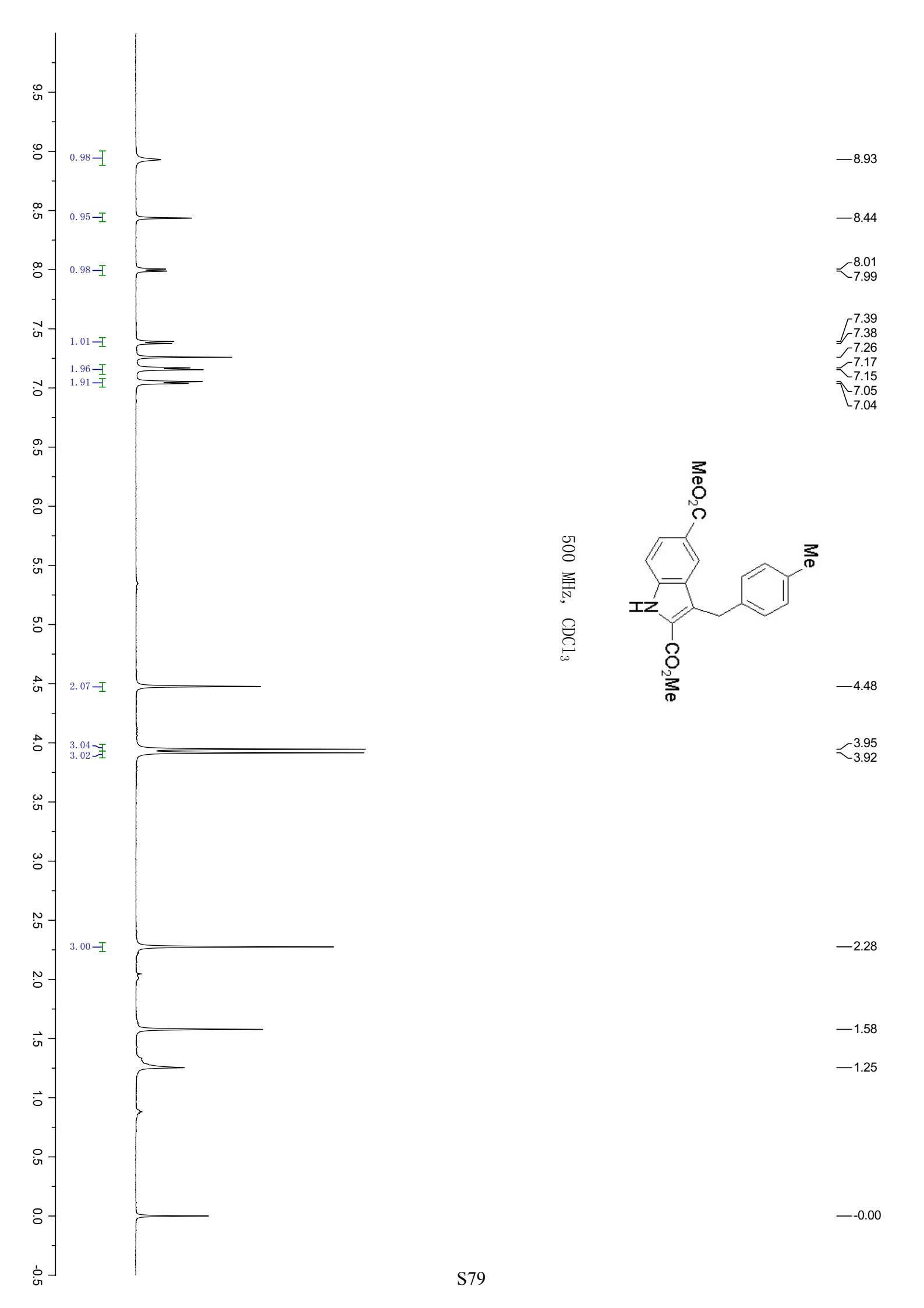

162.51
137.37
135.55
134.25
129.12
128.99
128.21
126.20
126.04
124.52
122.52
120.56
112.93
77.47
77.05
76.62
52.00
30.03
21.02
75 MHz, CDCl3
Cl
Me
N
H
CO2Me
f1 (ppm)

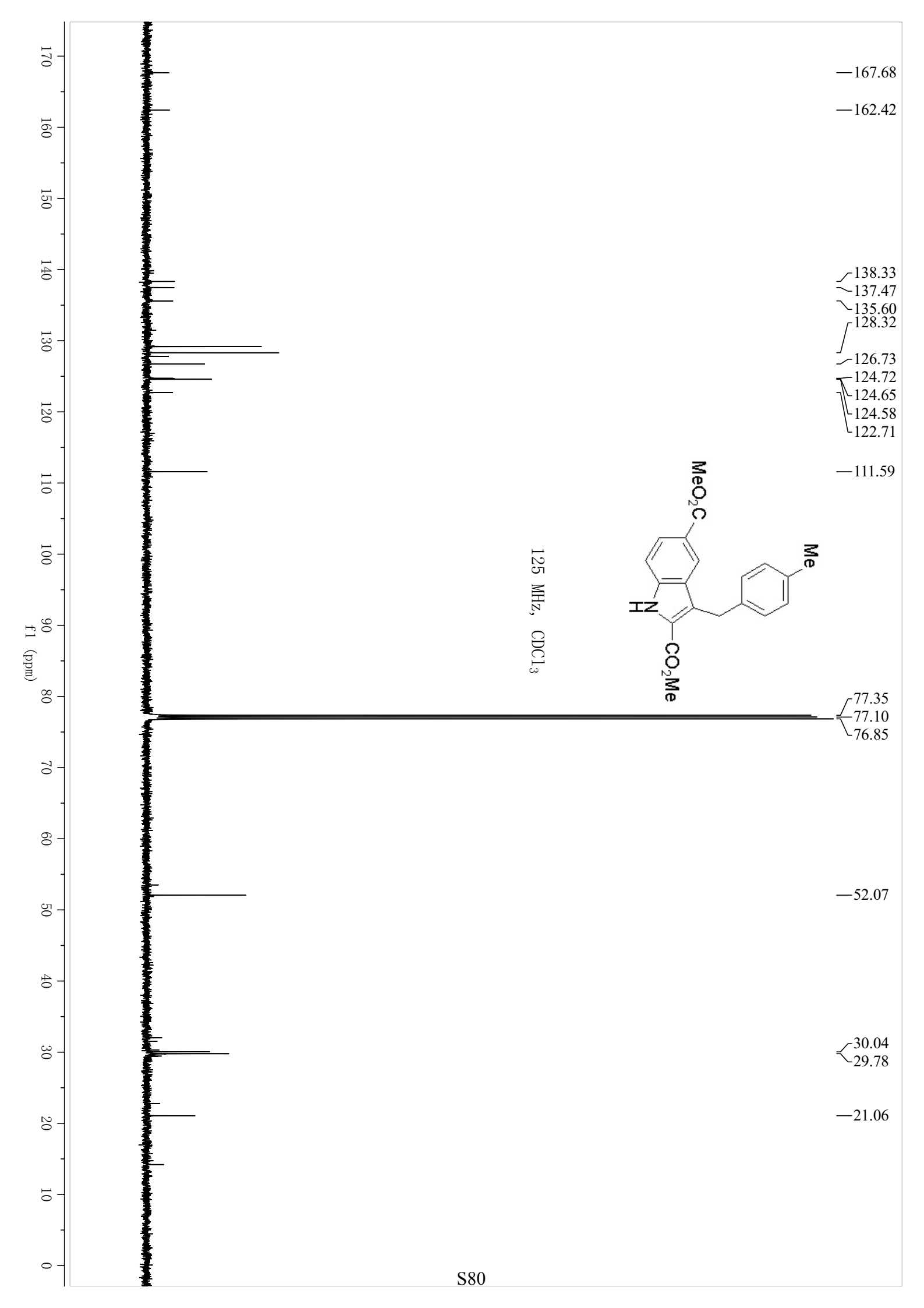

8.85
7.54
7.34
7.31
7.28
7.26
7.22
7.20
7.17
7.15
4.41
3.94
1.59
1.26
0.00
Cl
Cl
CO2Me
N
H
CDCl3, 300 MHz
0.96
1.09
7.32
2.01
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

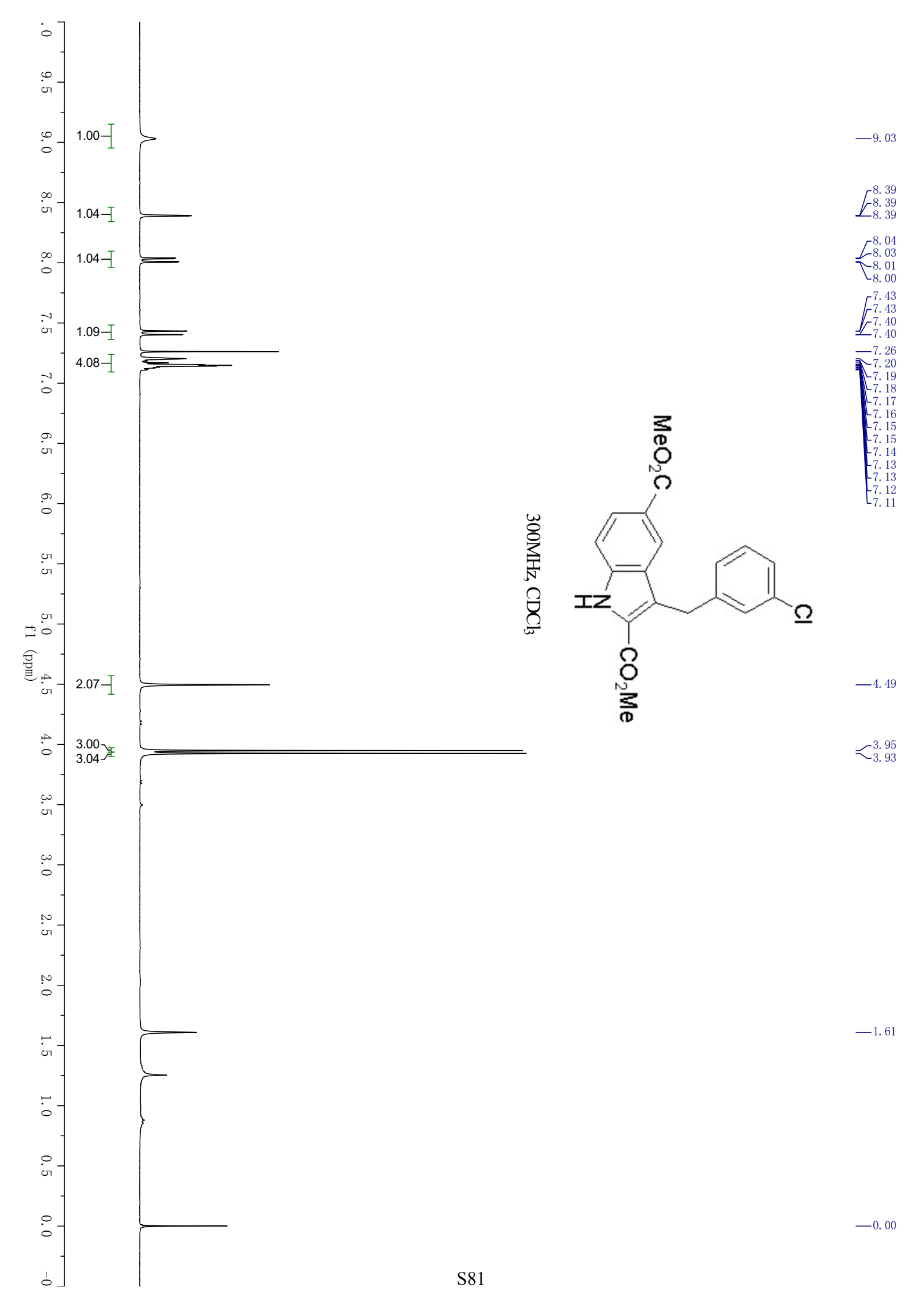

162.18
138.89
134.20
131.83
128.50
124.67
121.67
120.27
113.04
77.27
77.02
76.77
52.01
29.78
CDCl3, 125 MHz
f1 (ppm)
Cl
Cl
N
H
CO2Me

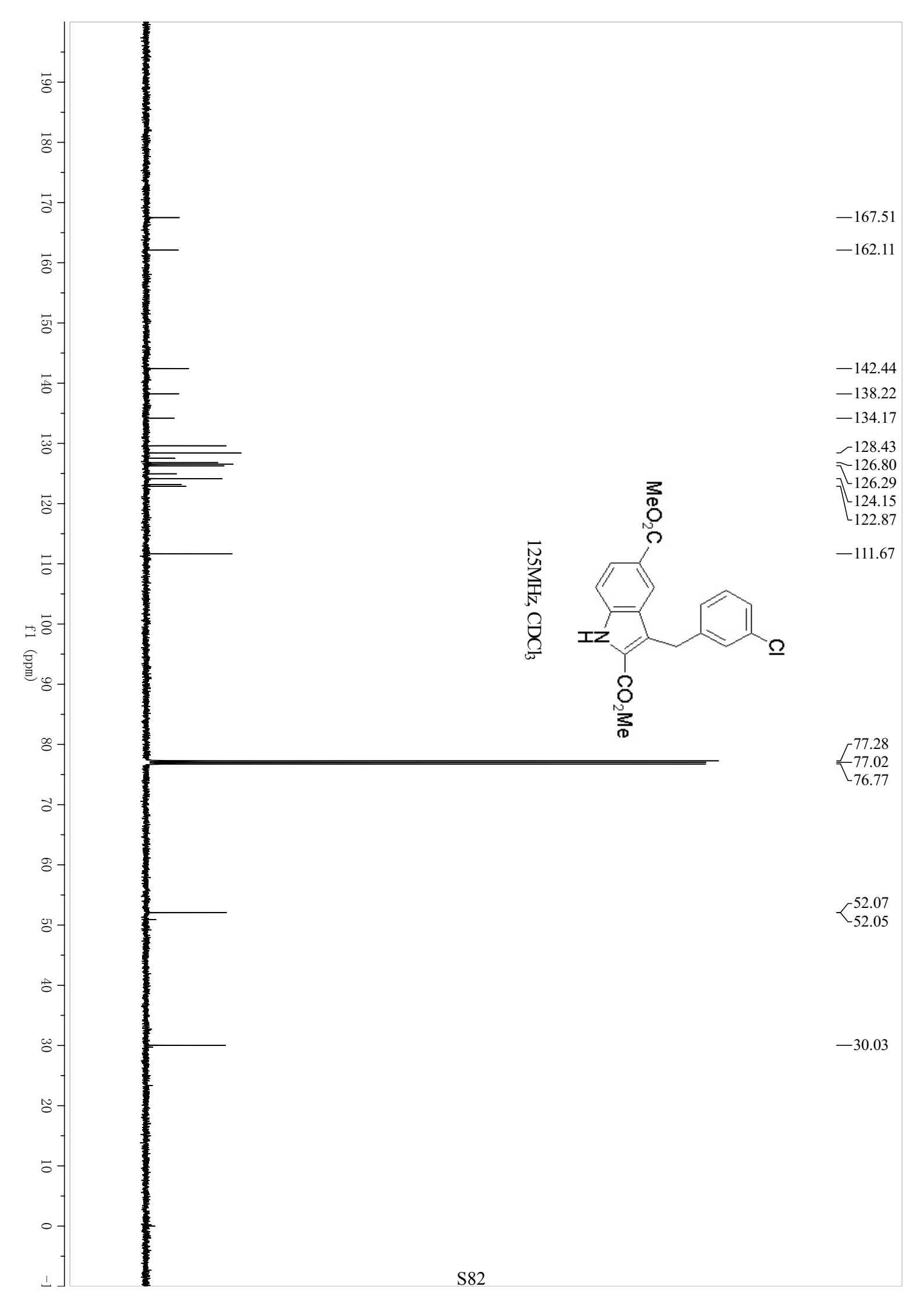

0.97
0.95
3.05
1.06
1.03
1.01
1.04
2.10
3.00
3.04
8.80
7.60
7.28
7.18
7.14
6.97
6.95
6.89
6.87
6.80
6.78
6.76
4.44
3.92
3.91
1.56
1.25
0.00
f1 (ppm)
400 MHz, CDCl3
Cl
N
H
CO2Me
OMe

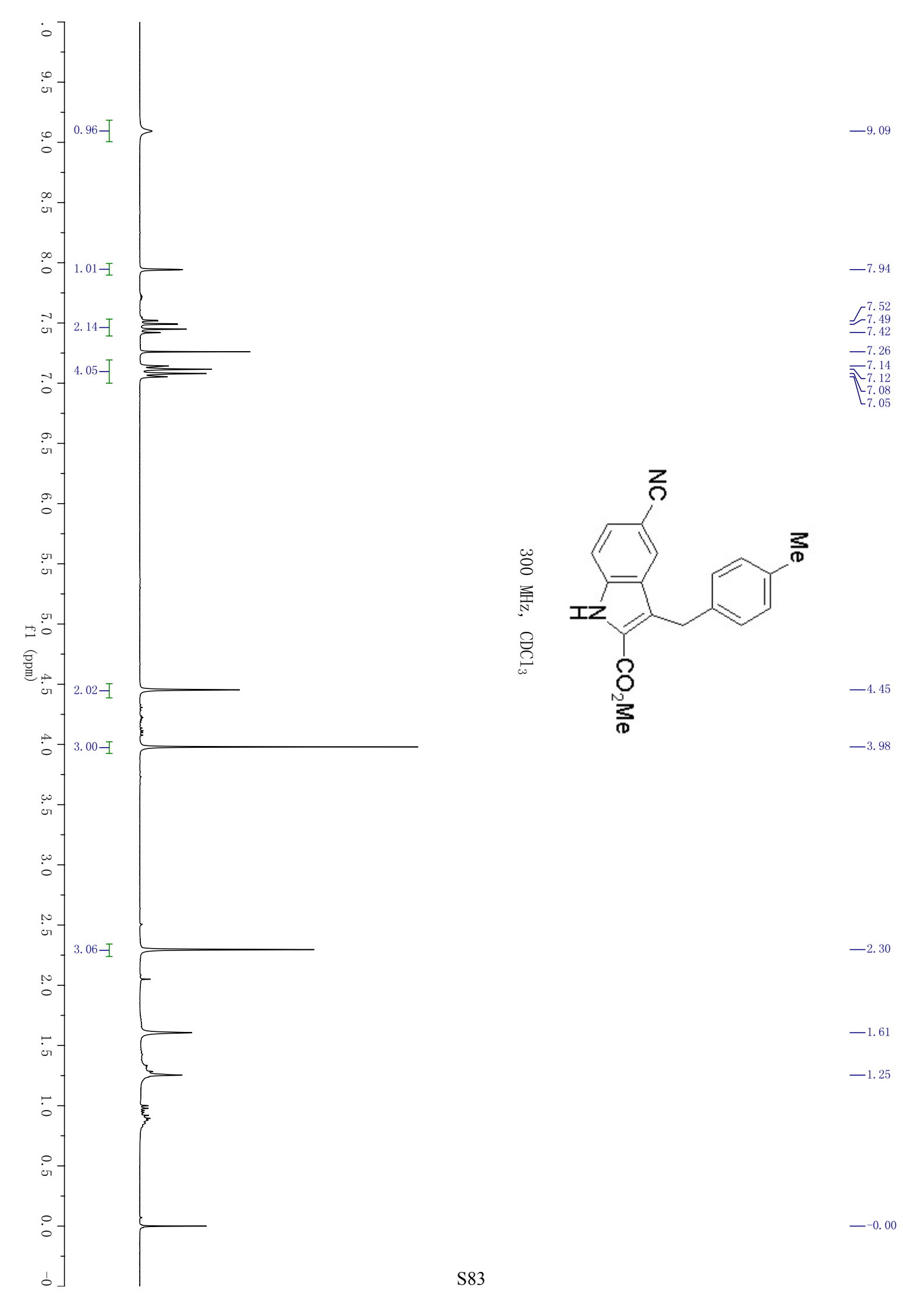

162.63
157.07
134.28
127.24
126.15
125.90
125.04
122.35
121.22
120.50
112.78
110.17
77.35
77.10
76.85
55.34
52.00
24.06
125 MHz, CDCl3
Cl
N
H
CO2Me
OMe
f1 (ppm)

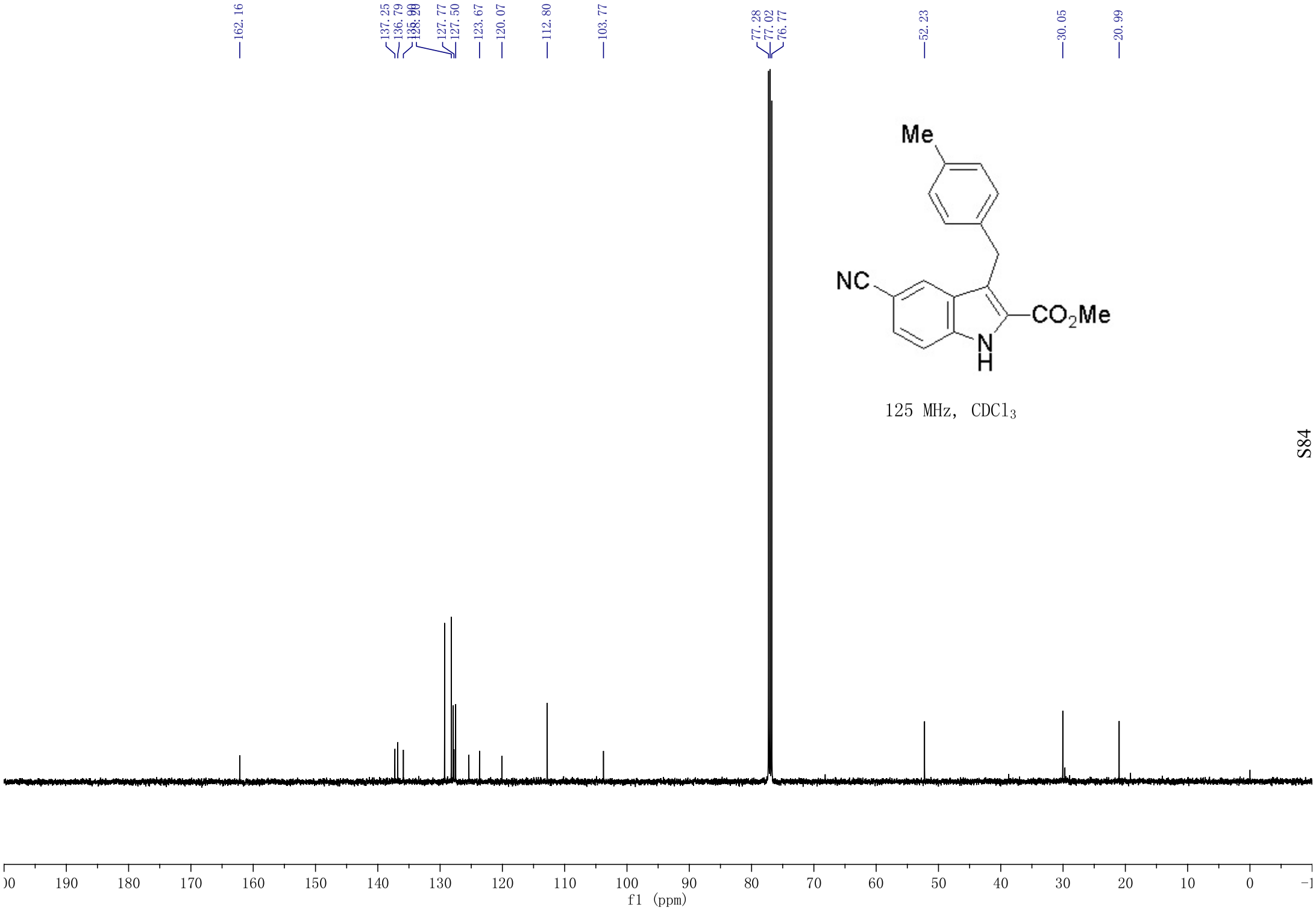

500 MHz, CDCl3
MeO2C
Me
N
H
CO2Me
0.98
0.95
0.98
1.01
1.96
1.91
2.07
3.04
3.02
3.00
8.93
8.44
8.01
7.99
7.39
7.38
7.26
7.17
7.15
7.05
7.04
4.48
3.95
3.92
2.28
1.58
1.25
-0.00

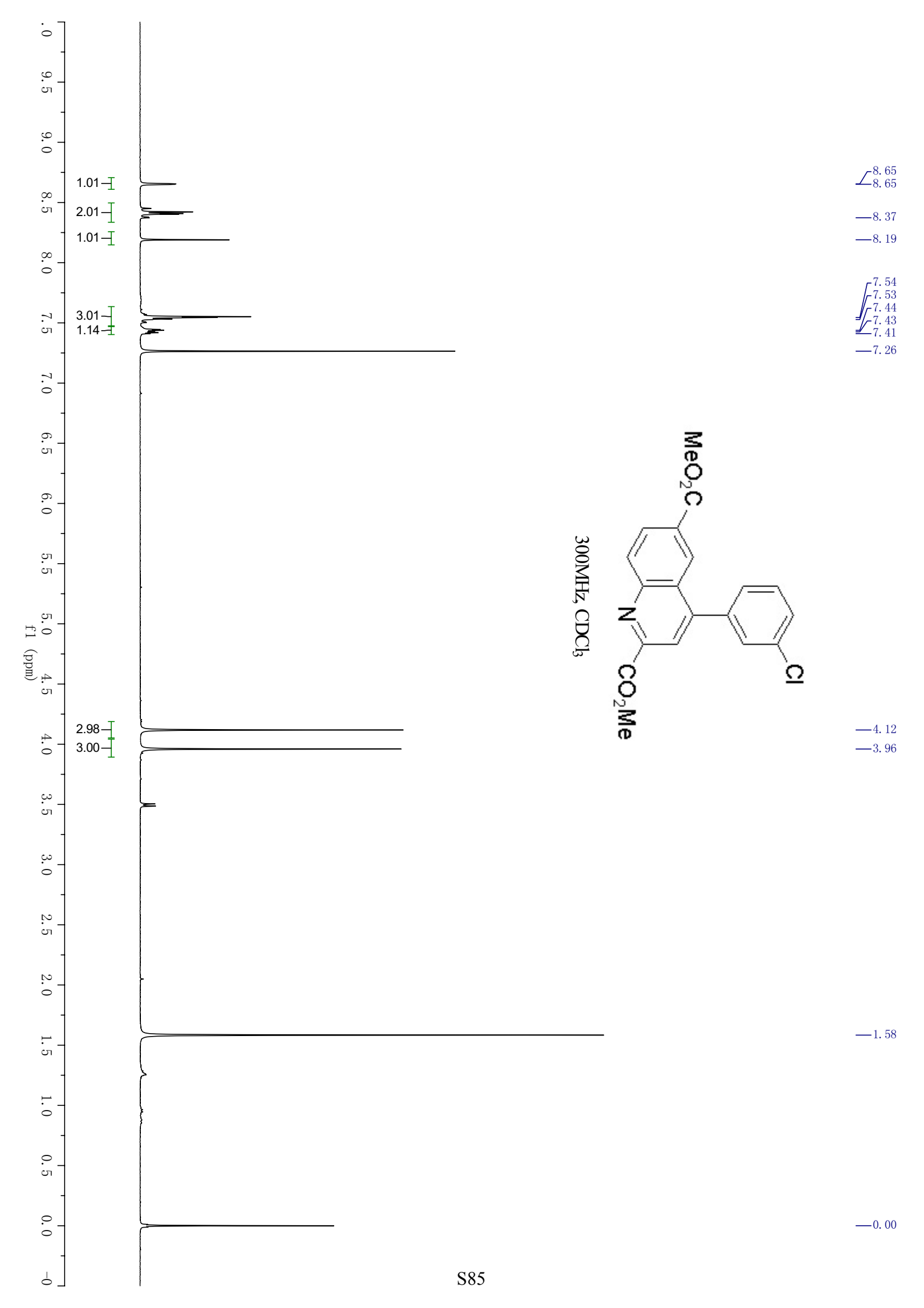

167.68
162.42
138.33
137.47
135.60
128.32
126.73
124.72
124.65
124.58
122.71
111.59
77.35
77.10
76.85
52.07
30.04
29.78
21.06
125 MHz, CDCl3
MeO2C
Me
N
H
CO2Me
f1 (ppm)

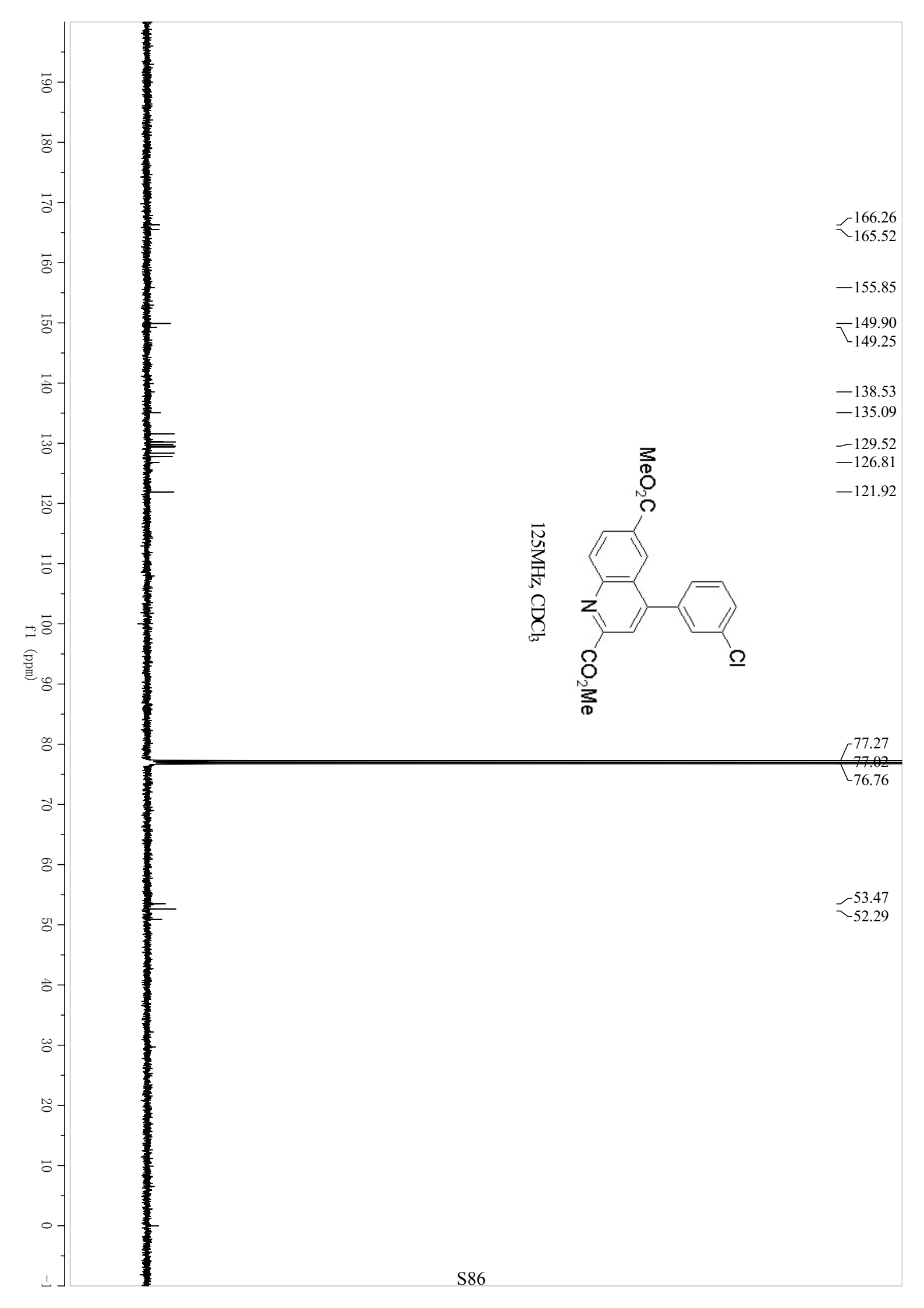

1.00
1.04
1.04
1.09
4.08
2.07
3.00
3.04
9.03
8.39
8.39
8.39
8.04
8.03
8.01
8.00
7.43
7.43
7.40
7.40
7.26
7.20
7.19
7.19
7.18
7.17
7.16
7.15
7.15
7.14
7.13
7.13
7.12
7.11
4.49
3.95
3.93
1.61
0.00
f1 (ppm)
300MHz, CDCl3
MeO2C
CO2Me
Cl
N
H

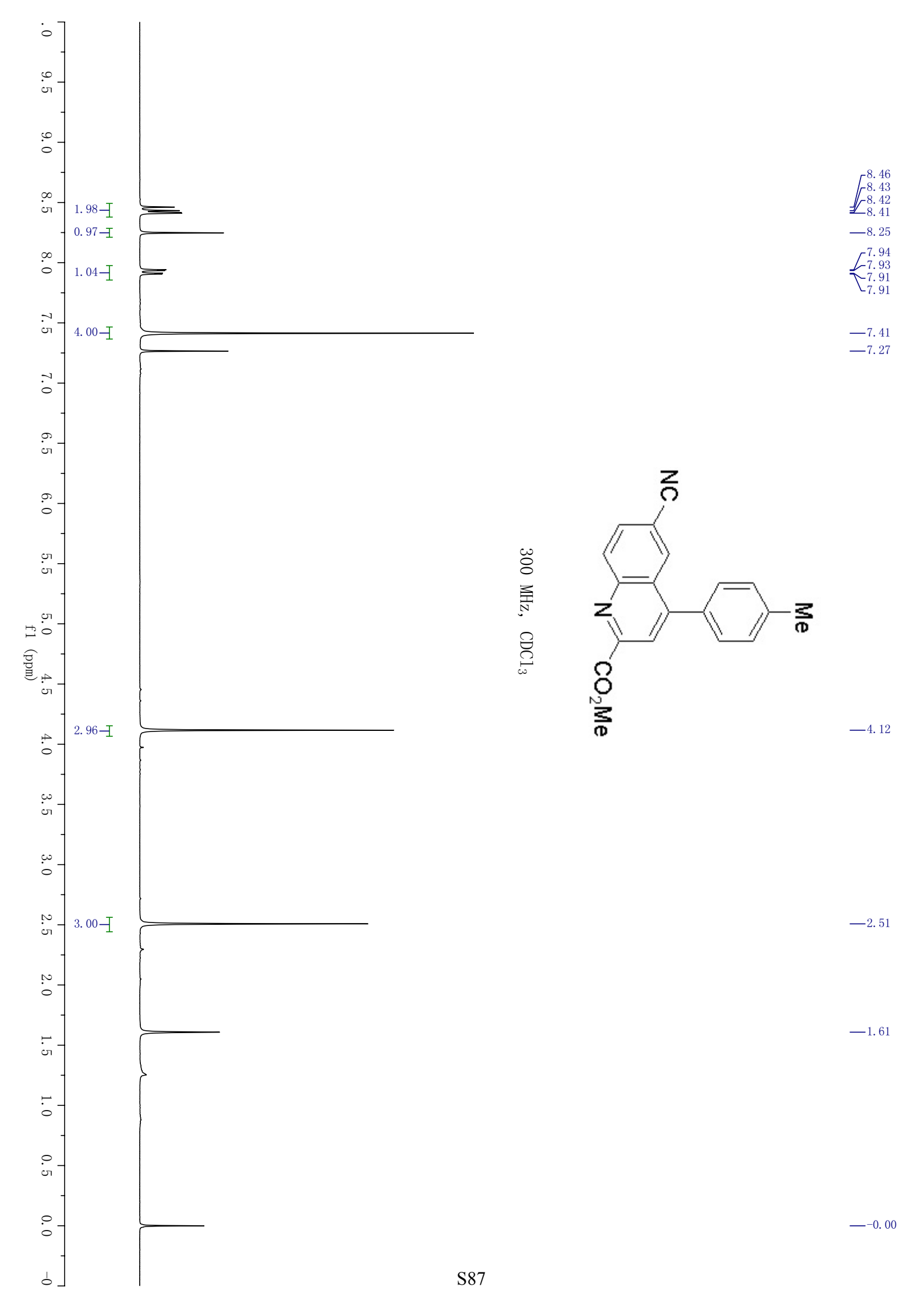

167.51
162.11
142.44
138.22
134.17
128.43
126.80
126.29
124.15
122.87
111.67
77.28
77.02
76.77
52.07
52.05
30.03
125MHz, CDCl3
MeO2C
N
H
CO2Me
Cl
f1 (ppm)

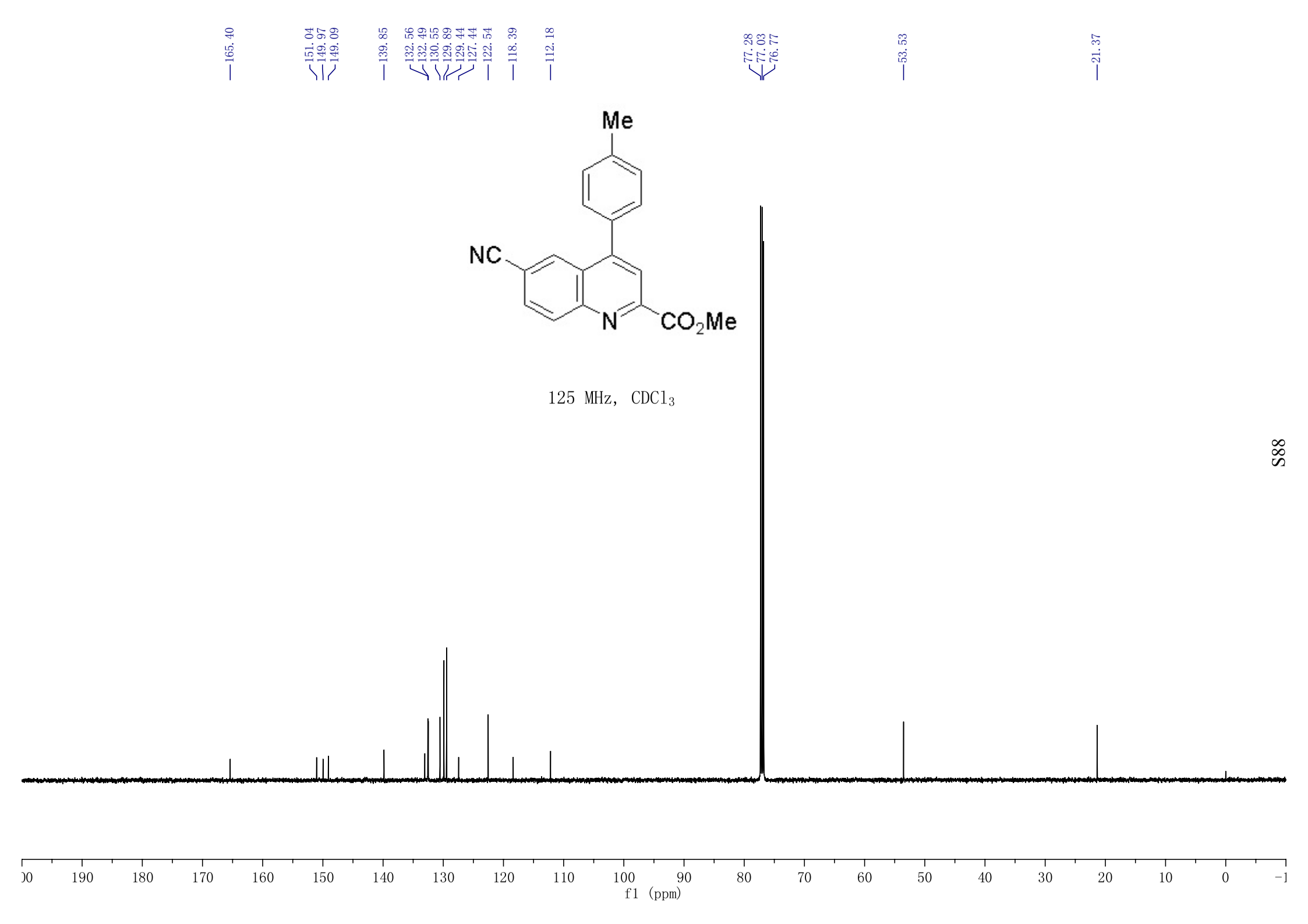

0.96
1.01
2.14
4.05
2.02
3.00
3.06
9.09
7.94
7.52
7.49
7.42
7.26
7.14
7.12
7.08
7.05
4.45
3.98
2.30
1.61
1.25
0.00
f1 (ppm)
300 MHz, CDCl3
NC
Me
H
N
CO2Me

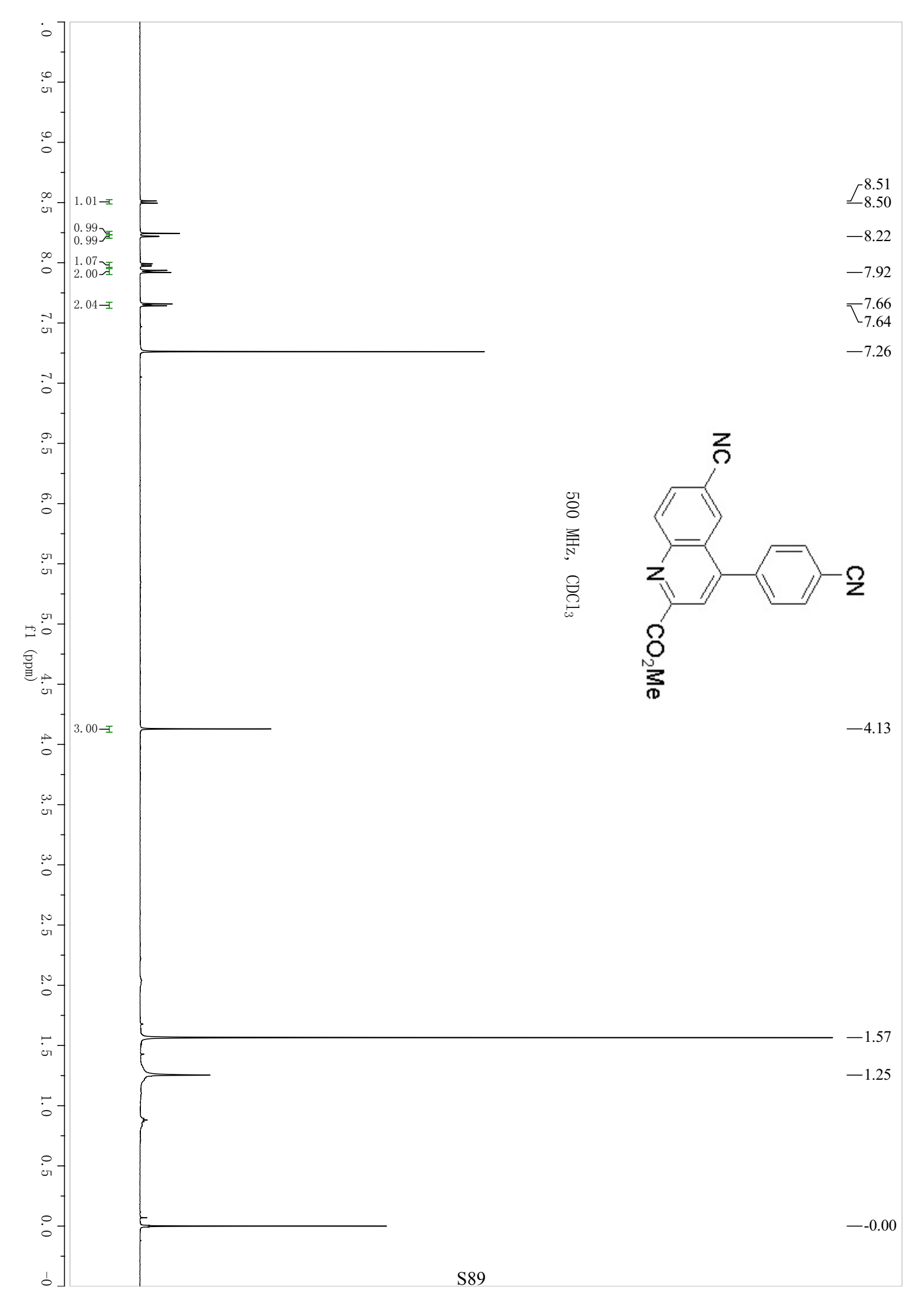

162.16
137.25
136.79
135.90
128.20
127.77
127.50
123.67
120.07
112.80
103.77
77.28
77.02
76.77
52.23
30.05
20.99
Me
NC
CO2Me
N
H
125 MHz, CDCl3
f1 (ppm)

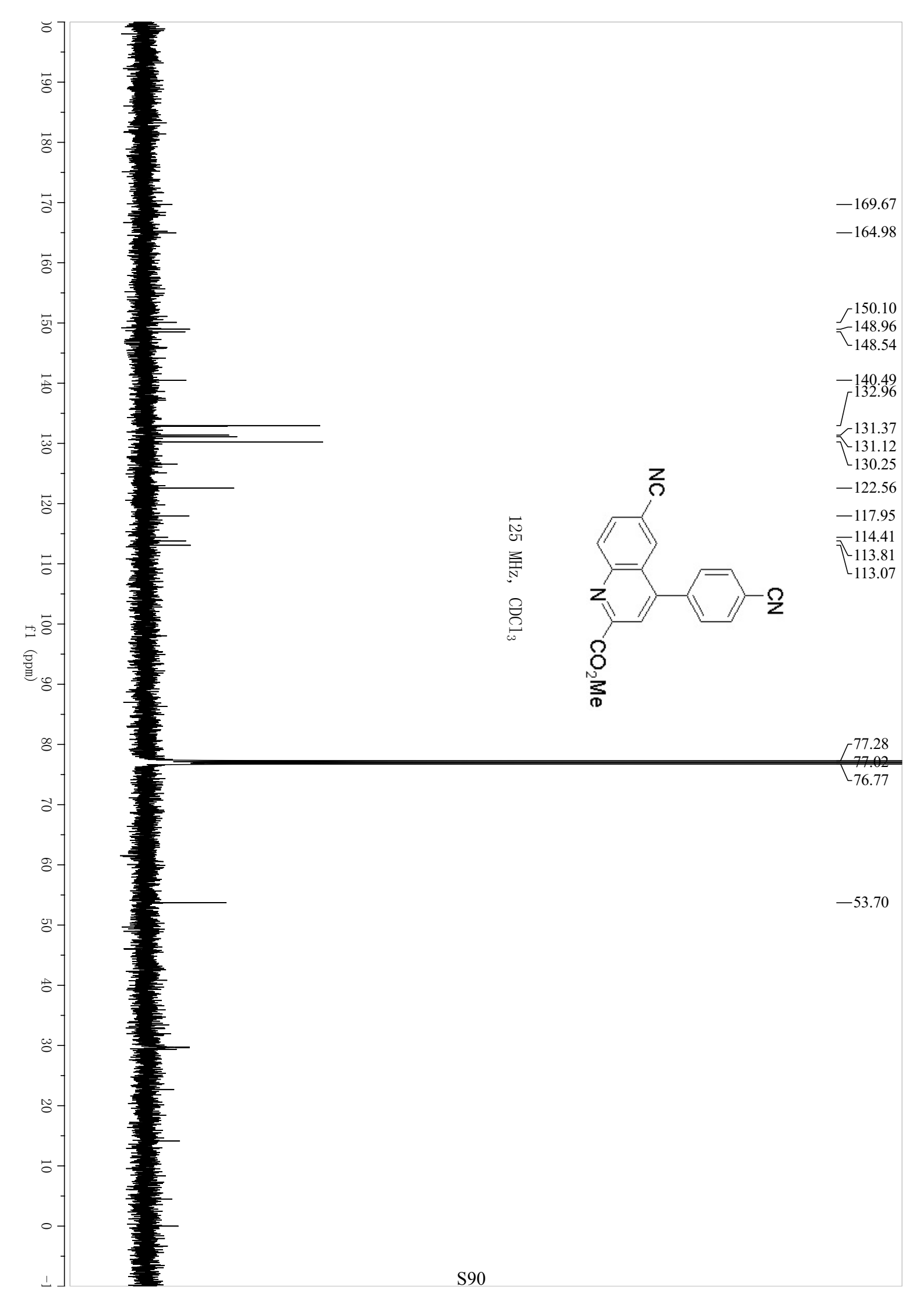

8.65
8.65
8.37
8.19
7.54
7.53
7.44
7.43
7.41
7.26
4.12
3.96
1.58
0.00
1.01
2.01
1.01
3.01
1.14
2.98
3.00
f1 (ppm)
300MHz, CDCl3
MeO2C
N
CO2Me
Cl


166.26
165.52
155.85
149.90
149.25
138.53
135.09
129.52
126.81
121.92
77.27
77.02
76.76
53.47
52.29
125MHz, CDCl3
MeO2C
CO2Me
N
Cl
f1 (ppm)

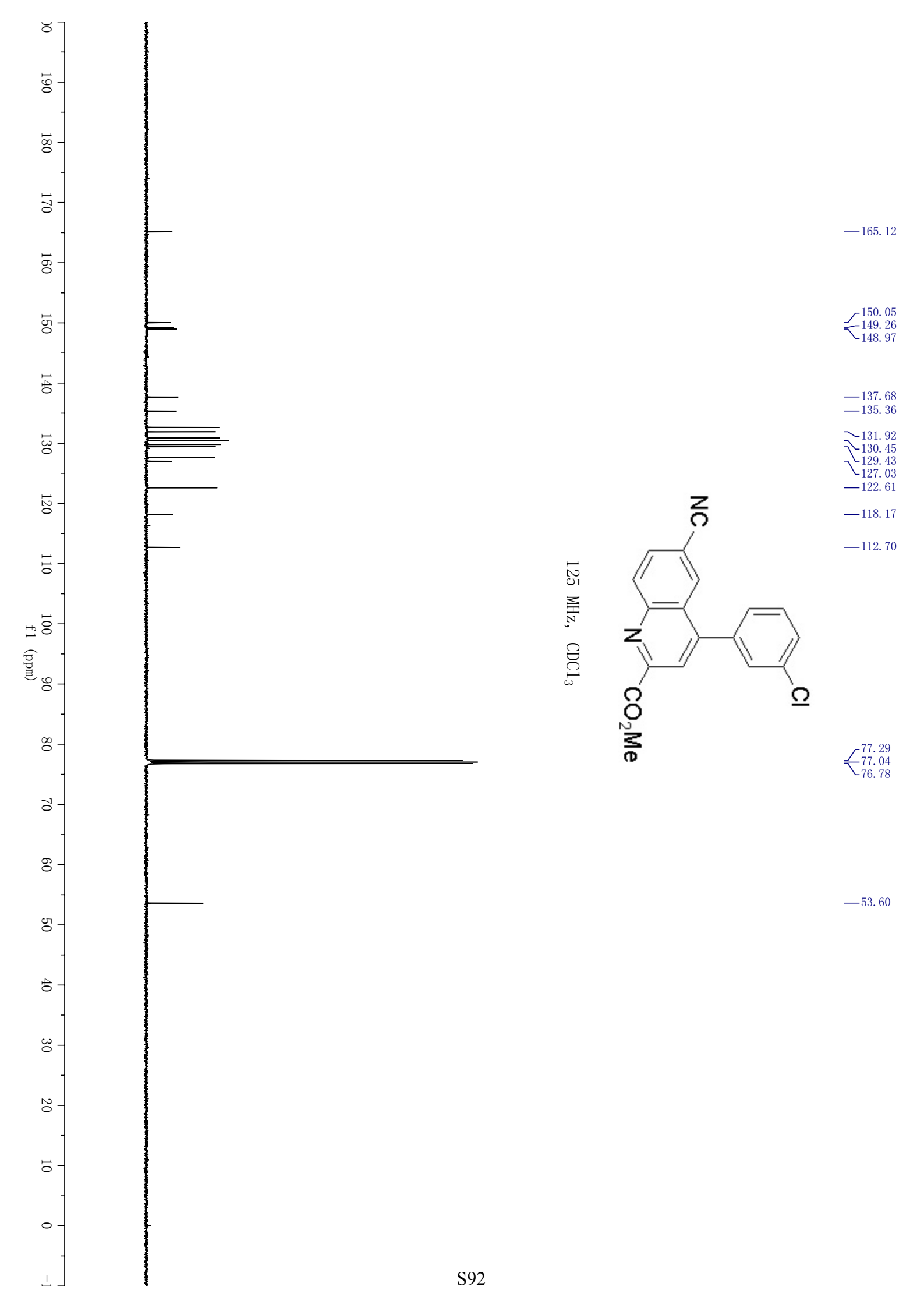

8.46
8.43
8.42
8.41
8.25
7.94
7.93
7.91
7.91
7.41
7.27
4.12
2.51
1.61
0.00
1.98
0.97
1.04
4.00
2.96
3.00
f1 (ppm)
300 MHz, CDCl3
NC
N
CO2Me
Me

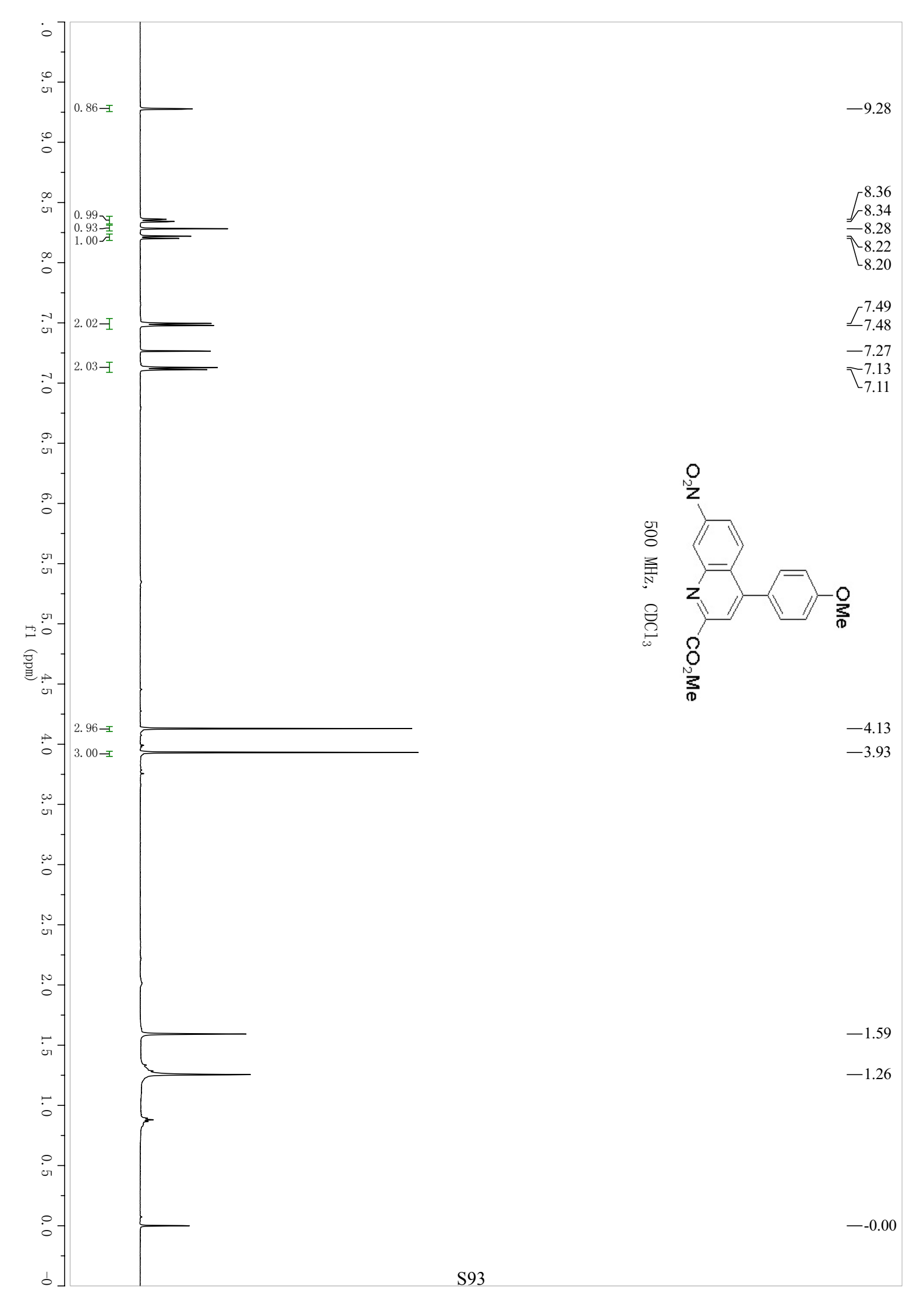

165.40
151.04
149.97
149.09
139.85
132.56
132.49
130.55
129.89
129.44
127.44
122.54
118.39
112.18
77.28
77.03
76.77
53.53
21.37
Me
NC
N
CO2Me
125 MHz, CDCl3
f1 (ppm)

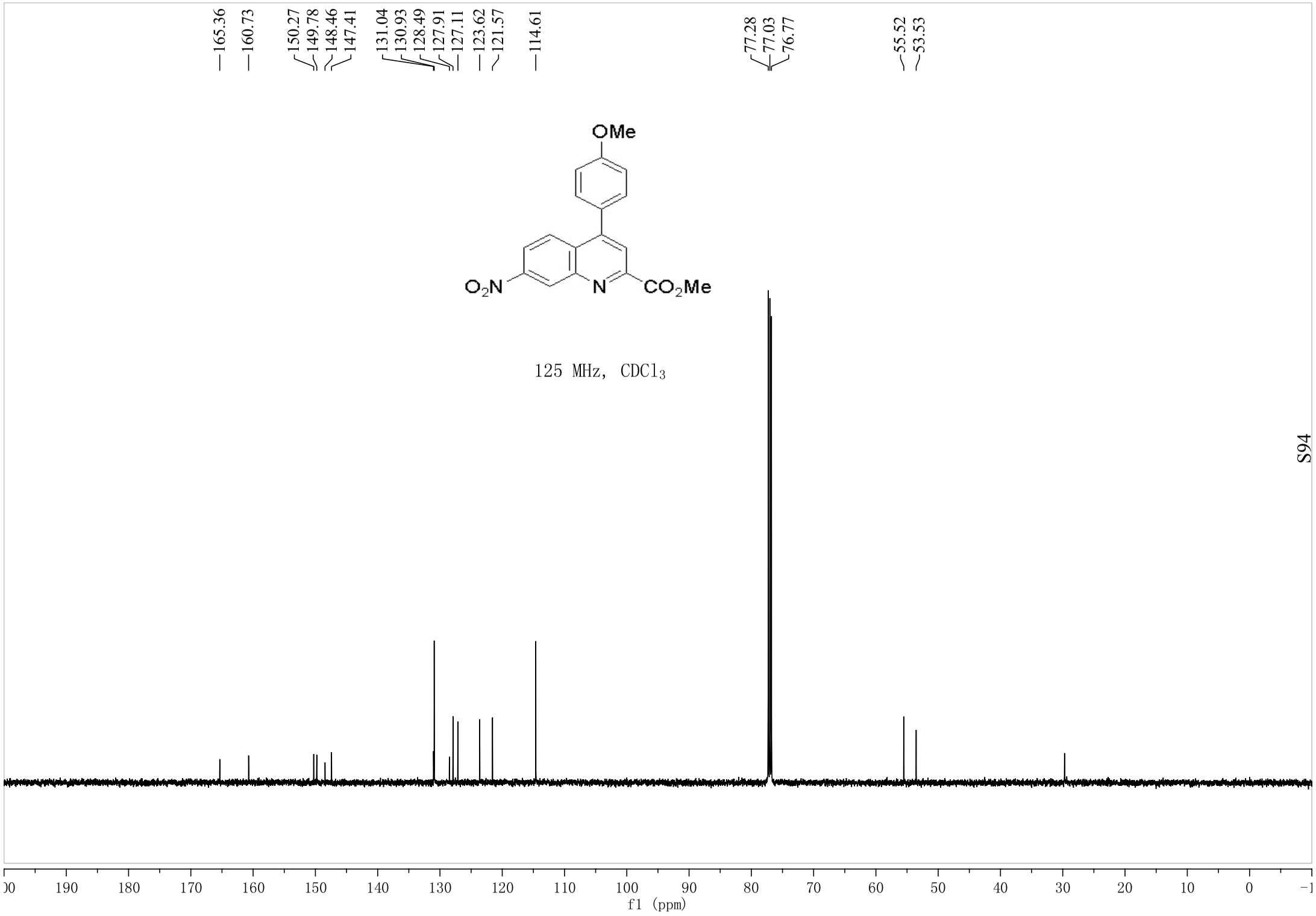

8.51
8.50
8.22
7.92
7.66
7.64
7.26
4.13
1.57
1.25
-0.00
1.01
0.99
0.99
1.07
2.00
2.04
3.00
500 MHz, CDCl3
NC
CN
N
CO2Me
f1 (ppm)

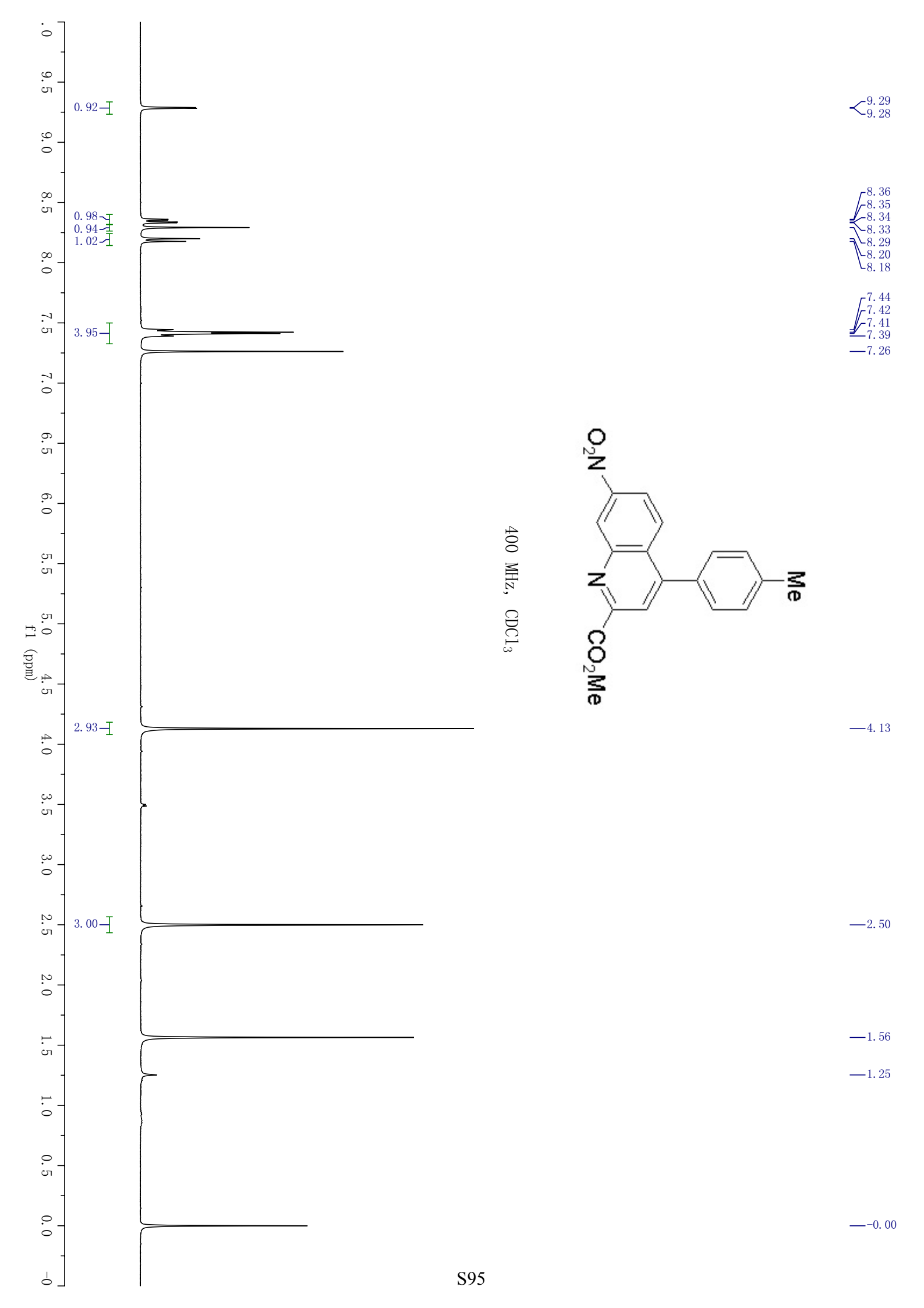

169.67
164.98
150.10
148.96
148.54
140.49
132.96
131.37
131.12
130.25
122.56
117.95
114.41
113.81
113.07
77.28
77.02
76.77
53.70
125 MHz, CDCl3
NC
CN
N
CO2Me
f1 (ppm)

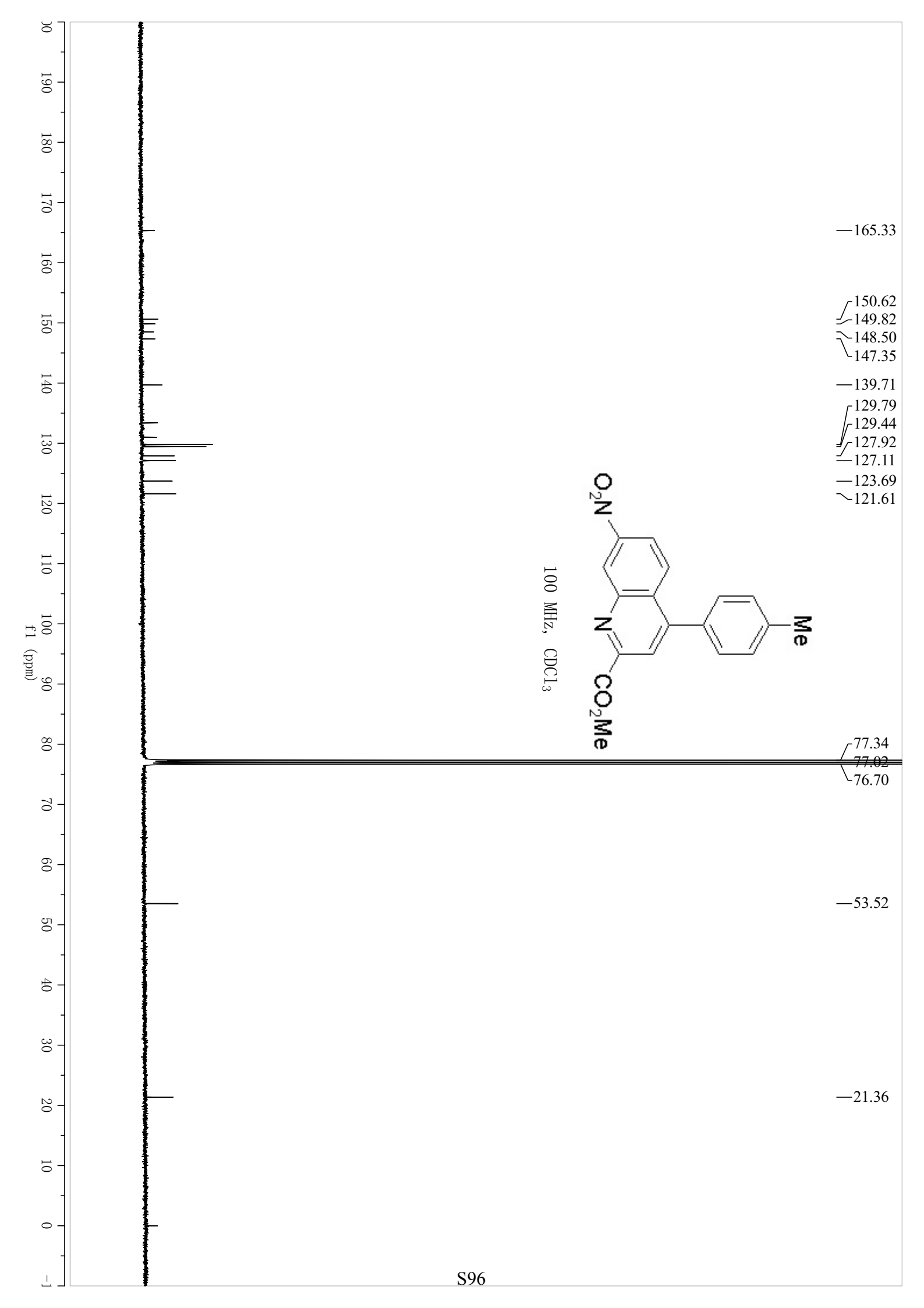
8.49
8.46
8.25
7.98
7.95
7.95
7.58
7.56
7.52
7.39
7.27
4.13
1.88
0.00
1.04
1.01
0.99
1.02
3.02
1.03
3.00
300 MHz, CDCl3
NC
N
CO2Me
Cl
f1 (ppm)

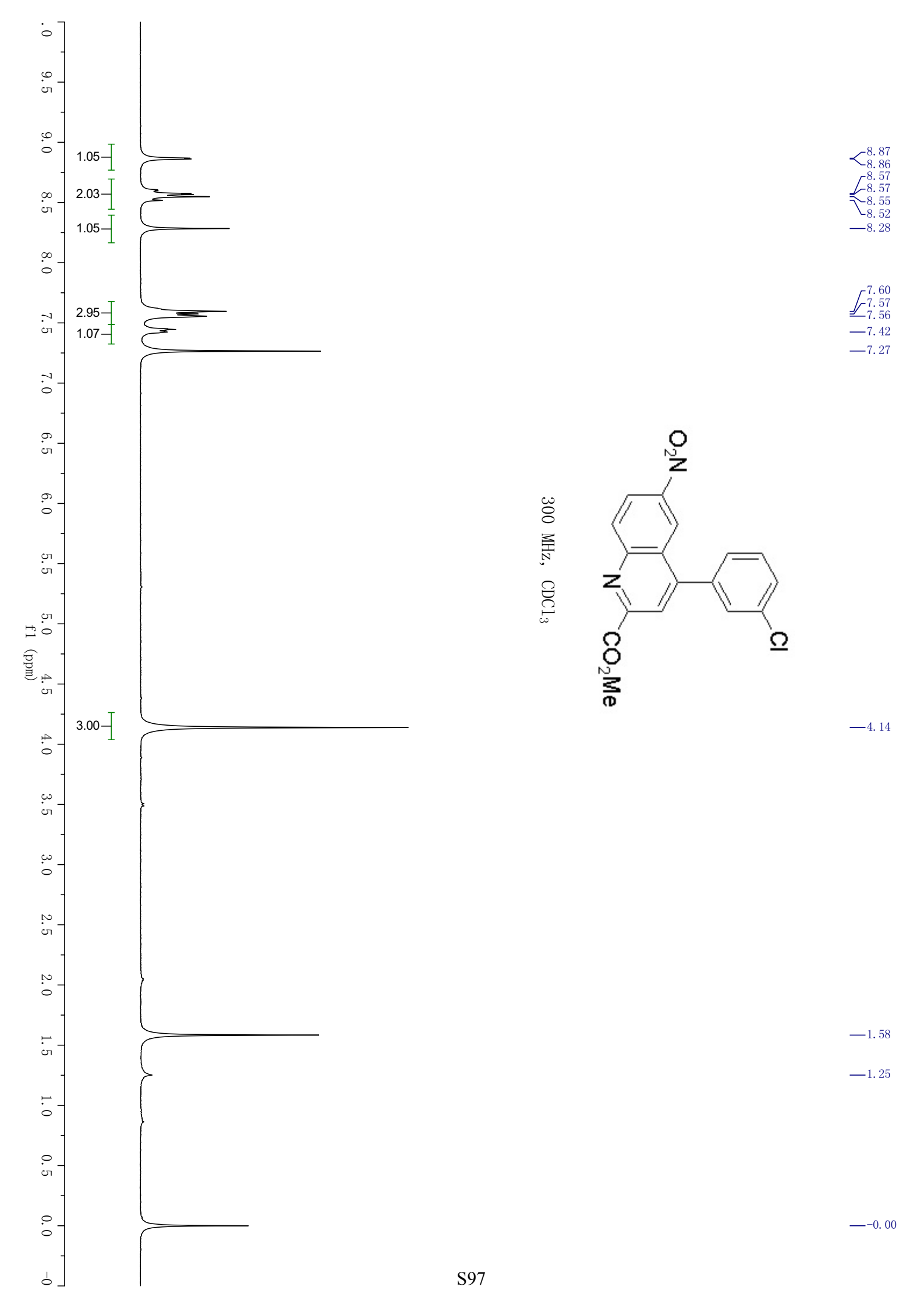

165.12
150.05
149.26
148.97
137.68
135.36
131.92
130.45
129.43
127.03
122.61
118.17
112.70
77.29
77.04
76.78
53.60
125 MHz, CDCl3
NC
N
CO2Me
Cl
f1 (ppm)

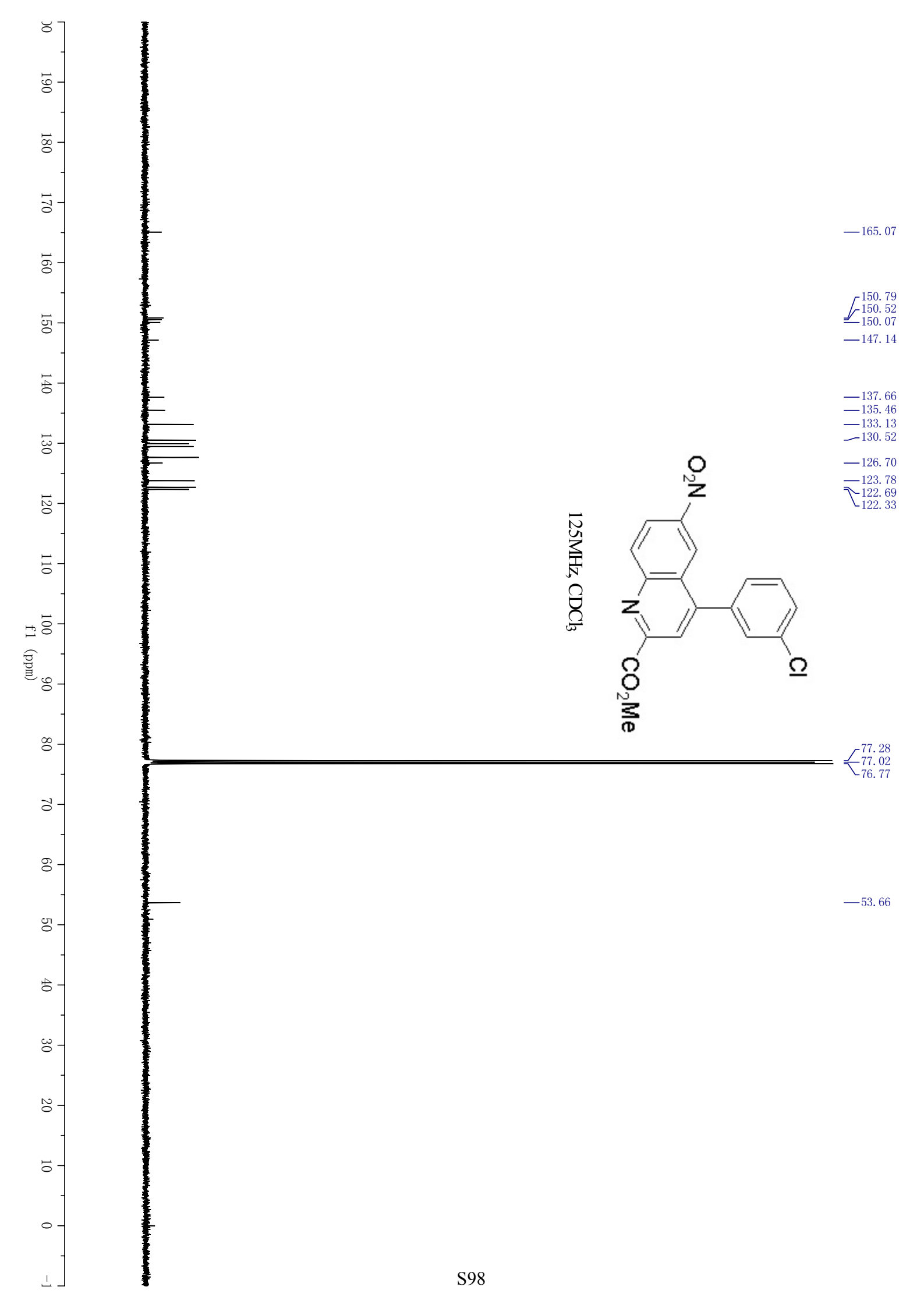

9.28
8.36
8.34
8.28
8.22
8.20
7.49
7.48
7.27
7.13
7.11
4.13
3.93
1.59
1.26
-0.00
0.86
0.99
0.93
1.00
2.02
2.03
2.96
3.00
500 MHz, CDCl3
O2N
N
CO2Me
OMe
f1 (ppm)


165.36
160.73
150.27
149.78
148.46
147.41
131.04
130.93
128.49
127.91
127.11
123.62
121.57
114.61
77.28
77.03
76.77
55.52
53.53
OMe
O2N
N
CO2Me
125 MHz, CDCl3
f1 (ppm)

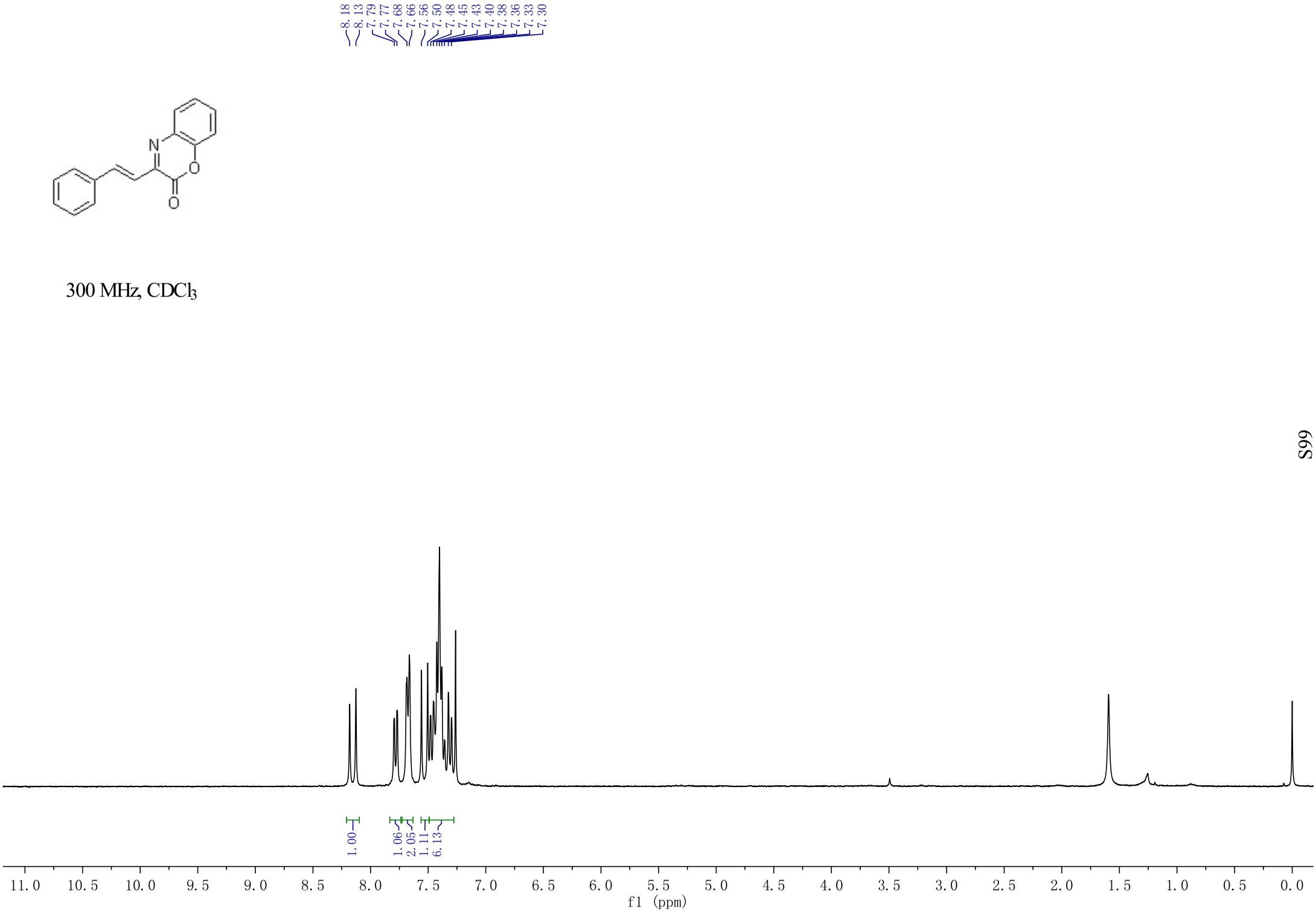

9.29
9.28
8.36
8.35
8.34
8.33
8.29
8.20
8.18
7.44
7.42
7.41
7.39
7.26
4.13
2.50
1.56
1.25
0.00
0.92
0.98
0.94
1.02
3.95
2.93
3.00
400 MHz, CDCl3
f1 (ppm)
O2N
N
CO2Me
Me

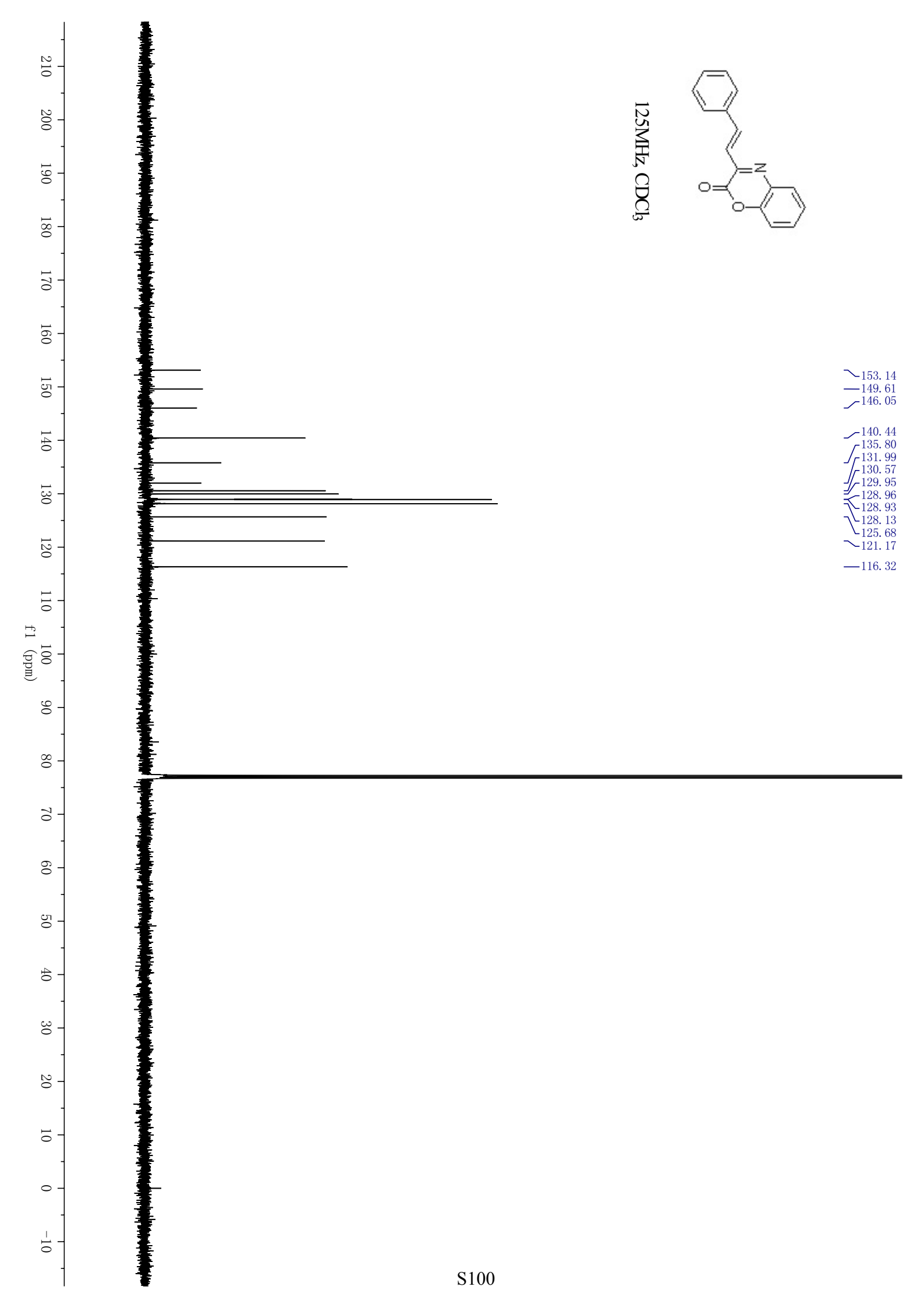

165.33
150.62
149.82
148.50
147.35
139.71
129.79
129.44
127.92
127.11
123.69
121.61
77.34
77.02
76.70
53.52
21.36
100 MHz, CDCl3
O2N
N
CO2Me
Me
f1 (ppm)

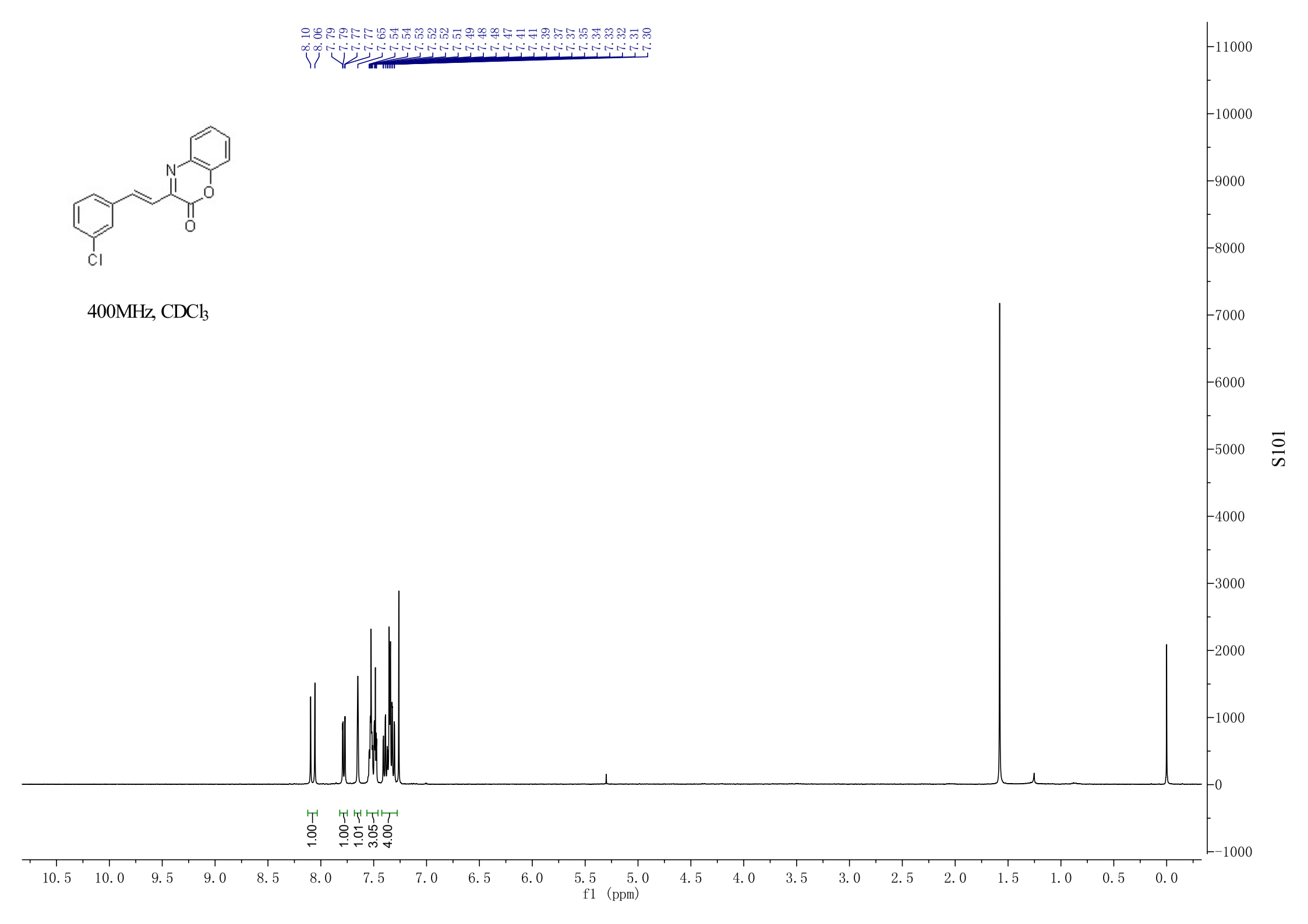

1.05
2.03
1.05
2.95
1.07
3.00
8.87
8.86
8.57
8.57
8.55
8.52
8.28
7.60
7.57
7.56
7.42
7.27
4.14
1.58
1.25
0.00
300 MHz, CDCl3
O2N
N
CO2Me
Cl
f1 (ppm)

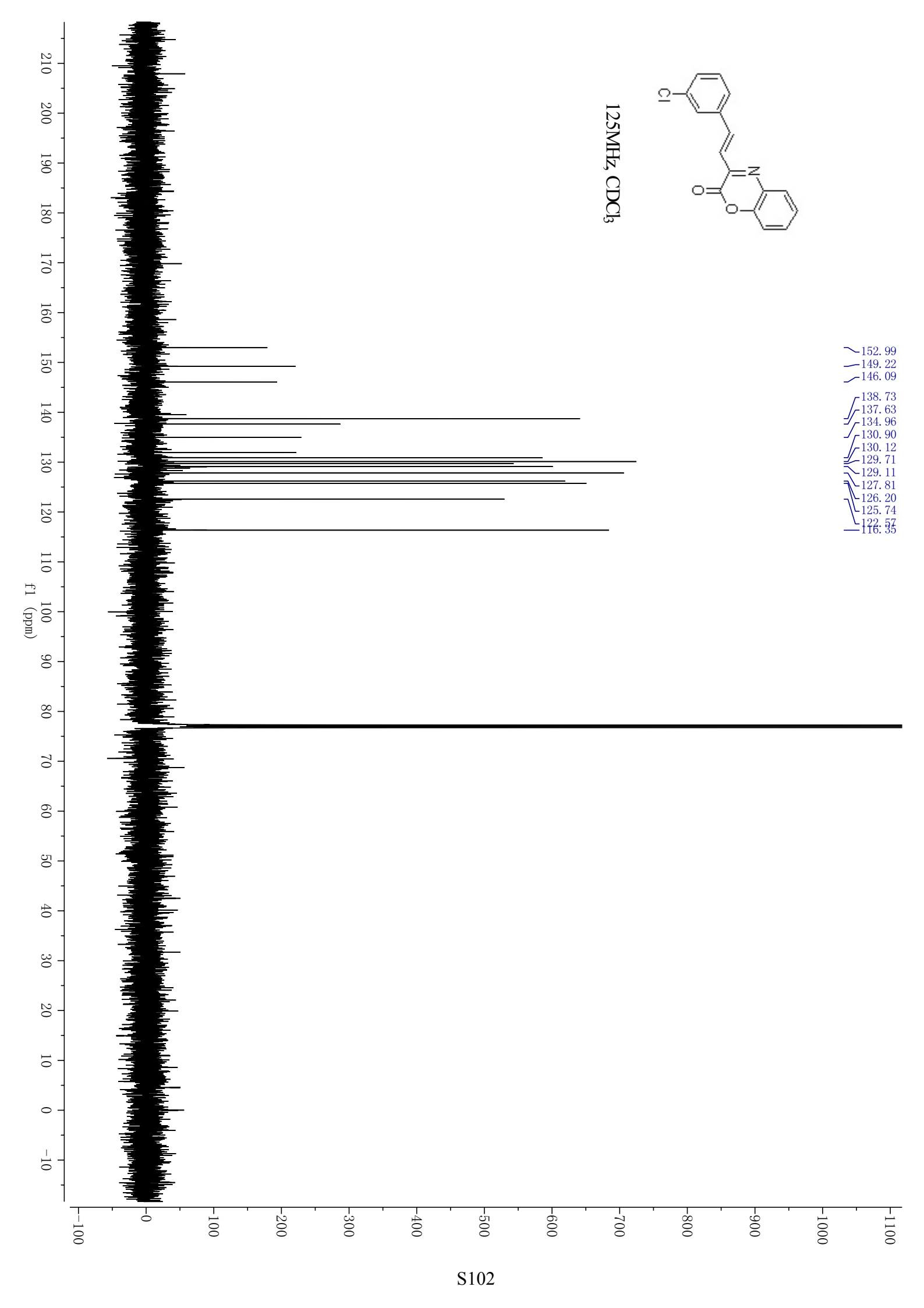

165.07
150.79
150.52
150.07
147.14
137.66
135.46
133.13
130.52
126.70
123.78
122.69
122.33
77.28
77.02
76.77
53.66
125MHz, CDCl3
O2N
N
CO2Me
Cl
f1 (ppm)

300 MHz, $CDCl_3$

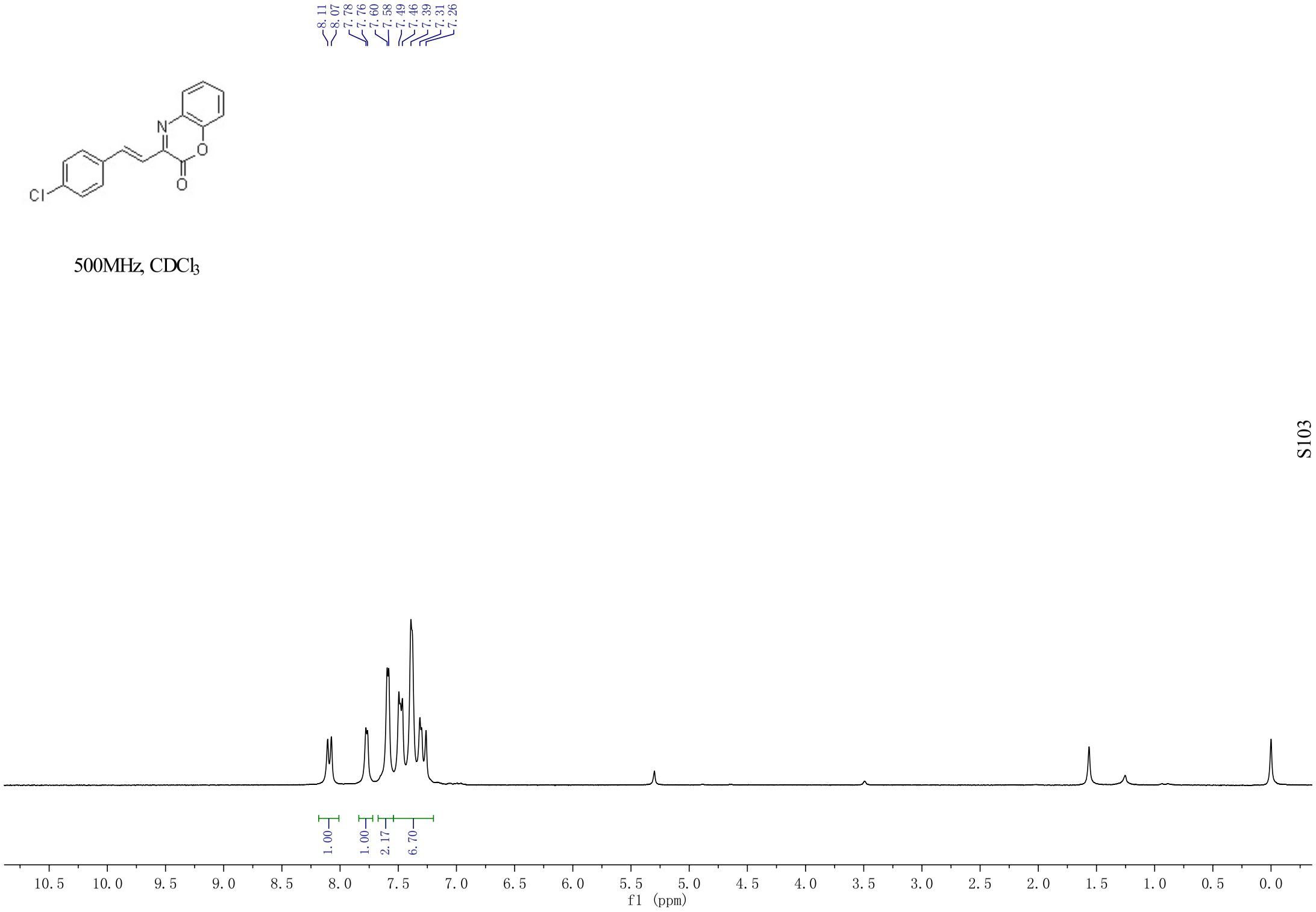


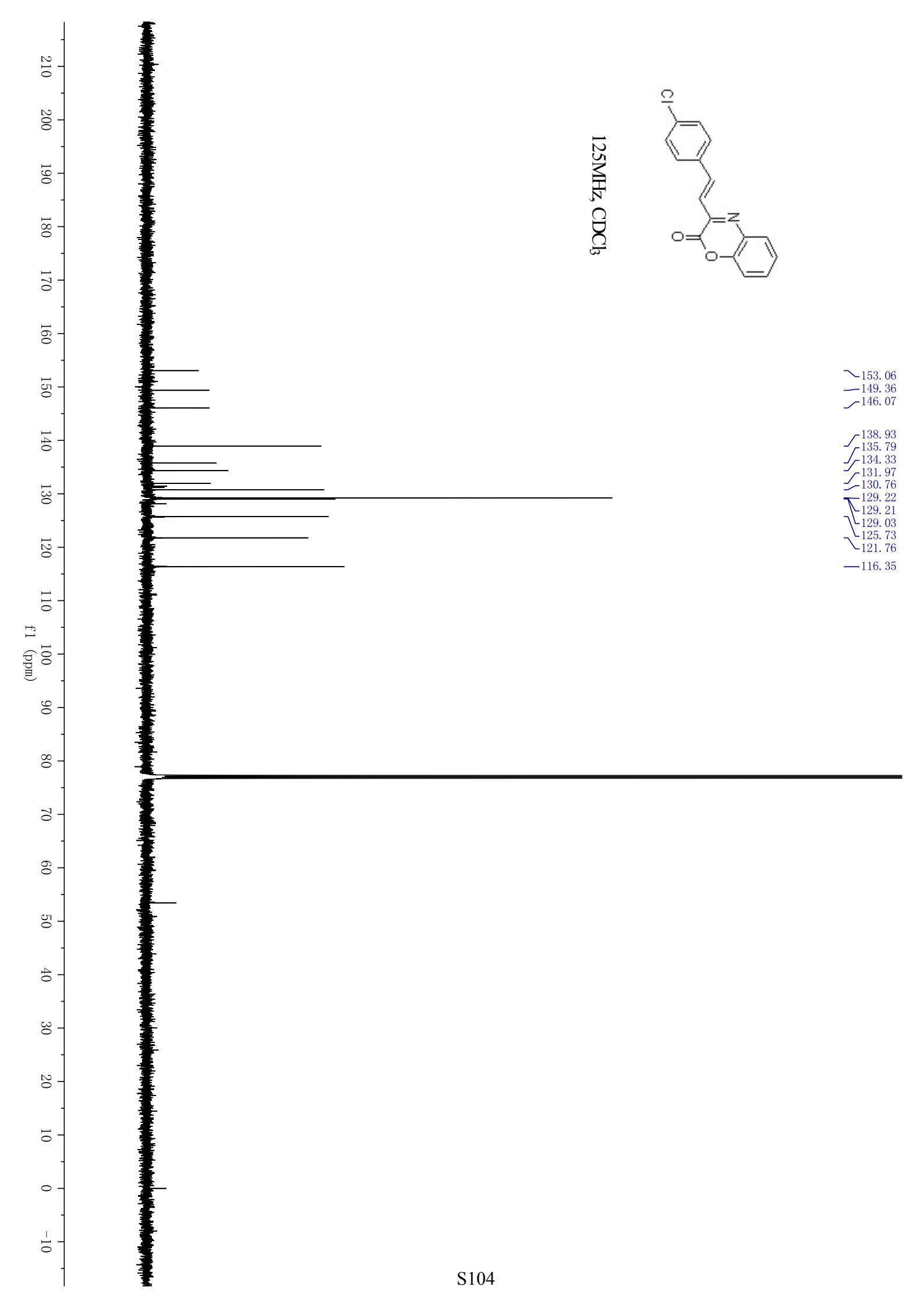

125MHz, CDCl3
153.14
149.61
146.05
140.44
135.80
131.99
130.57
129.95
128.96
128.93
128.13
125.68
121.17
116.32
f1 (ppm)

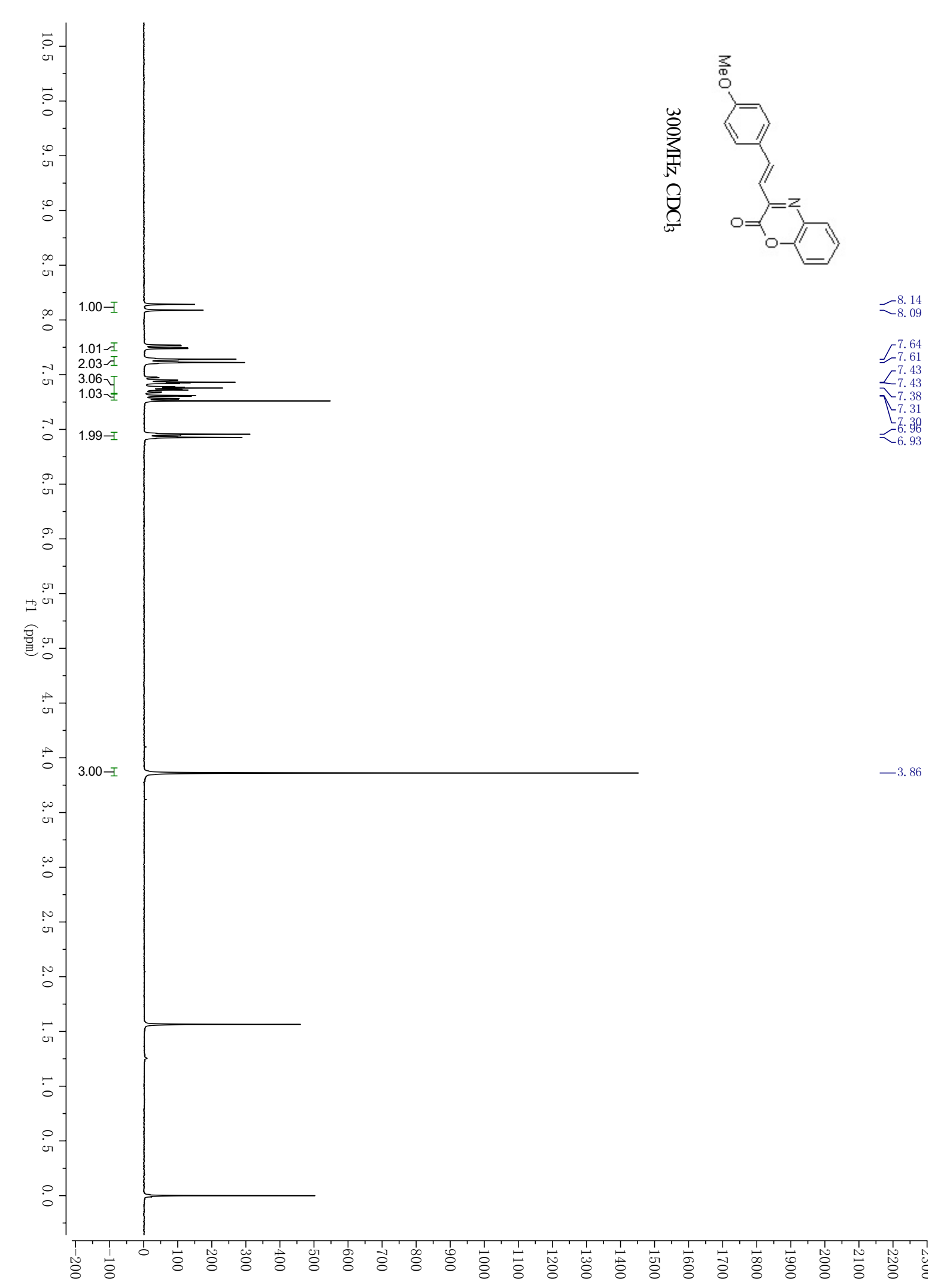

8.10
8.06
7.79
7.79
7.77
7.77
7.65
7.54
7.54
7.53
7.52
7.52
7.51
7.49
7.48
7.48
7.47
7.41
7.41
7.39
7.37
7.37
7.35
7.34
7.33
7.32
7.31
7.30
N
O
O
Cl
400MHz, CDCl3
1.00
1.00
1.01
3.05
4.00
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

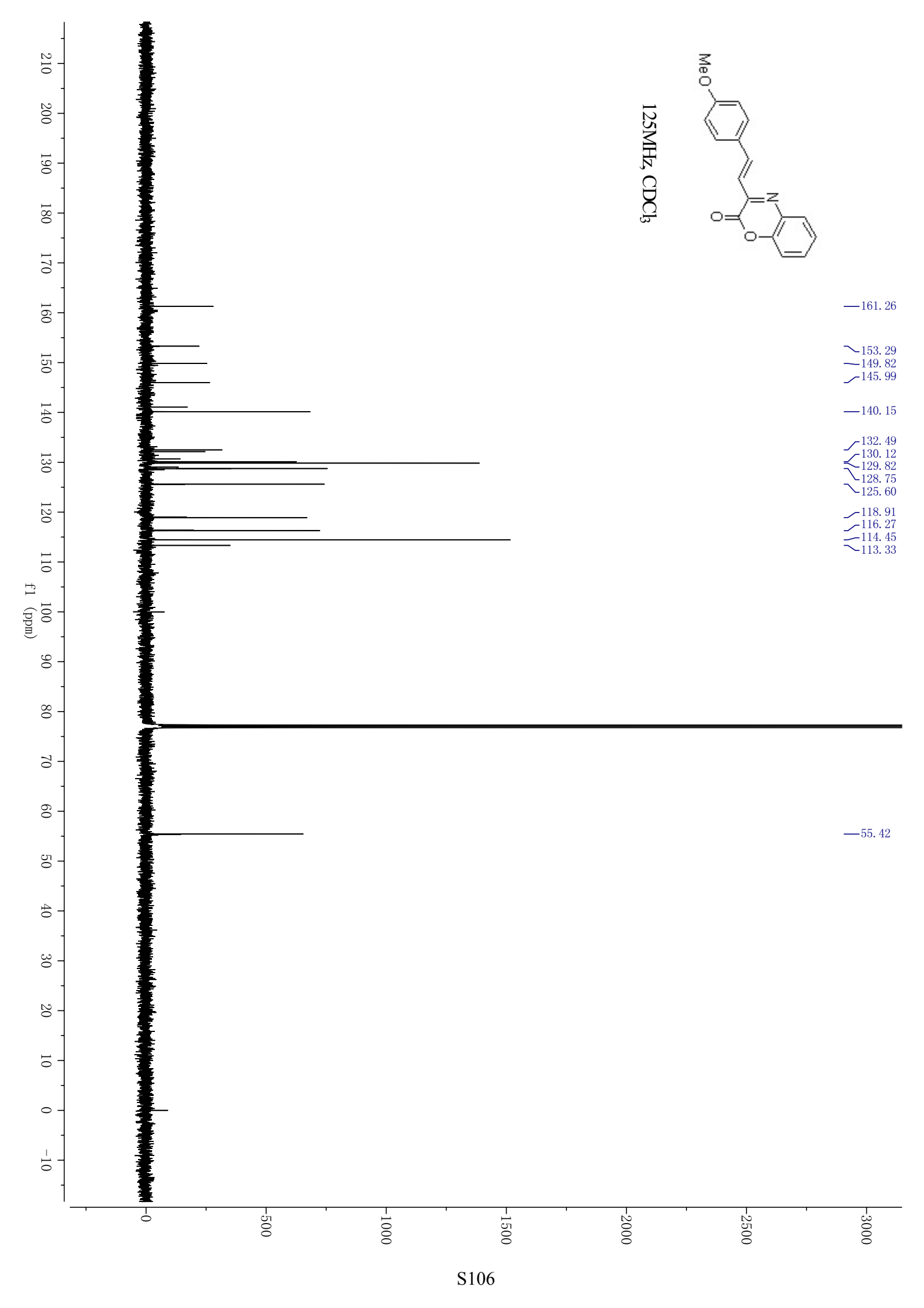

125MHz, CDCl3
Cl
N
O
O
152.99
149.22
146.09
138.73
137.63
134.96
130.90
130.12
129.71
129.11
127.81
126.20
125.74
122.57
116.35
f1 (ppm)

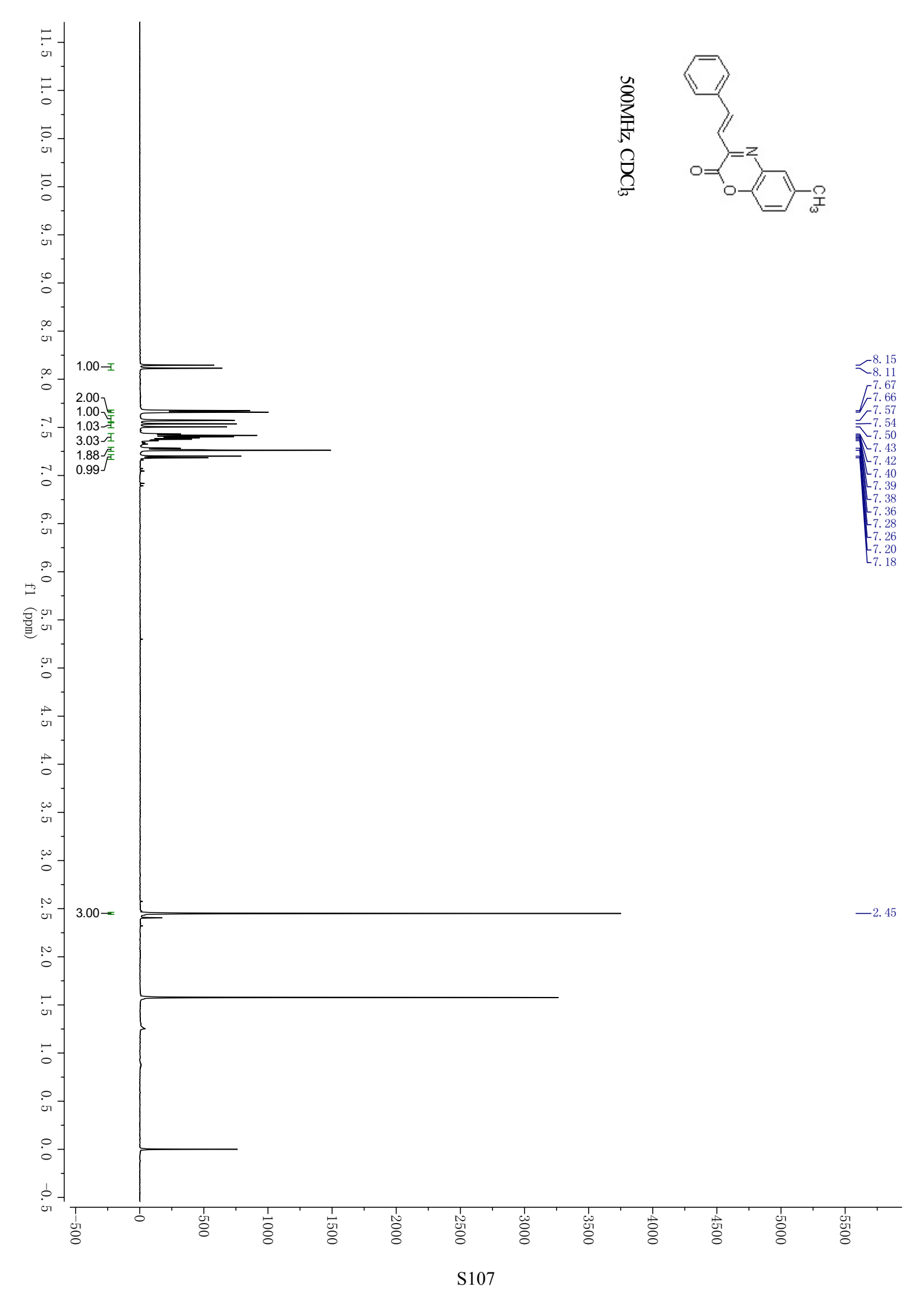
500MHz, $CDCl_3$

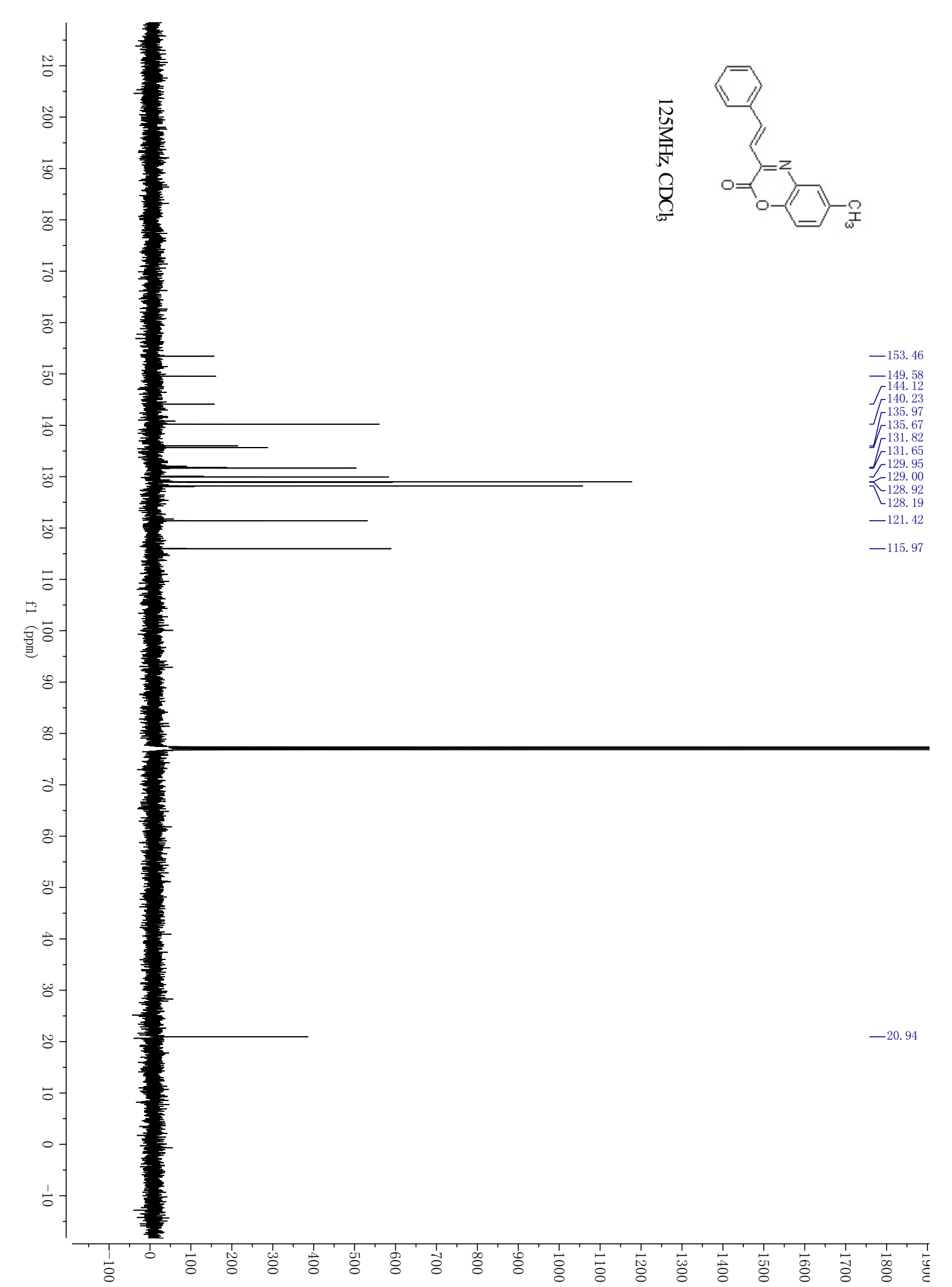



125MHz, CDCl3
Cl
N
O
O
153.06
149.36
146.07
138.93
135.79
134.33
131.97
130.76
129.22
129.21
129.03
125.73
121.76
116.35
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

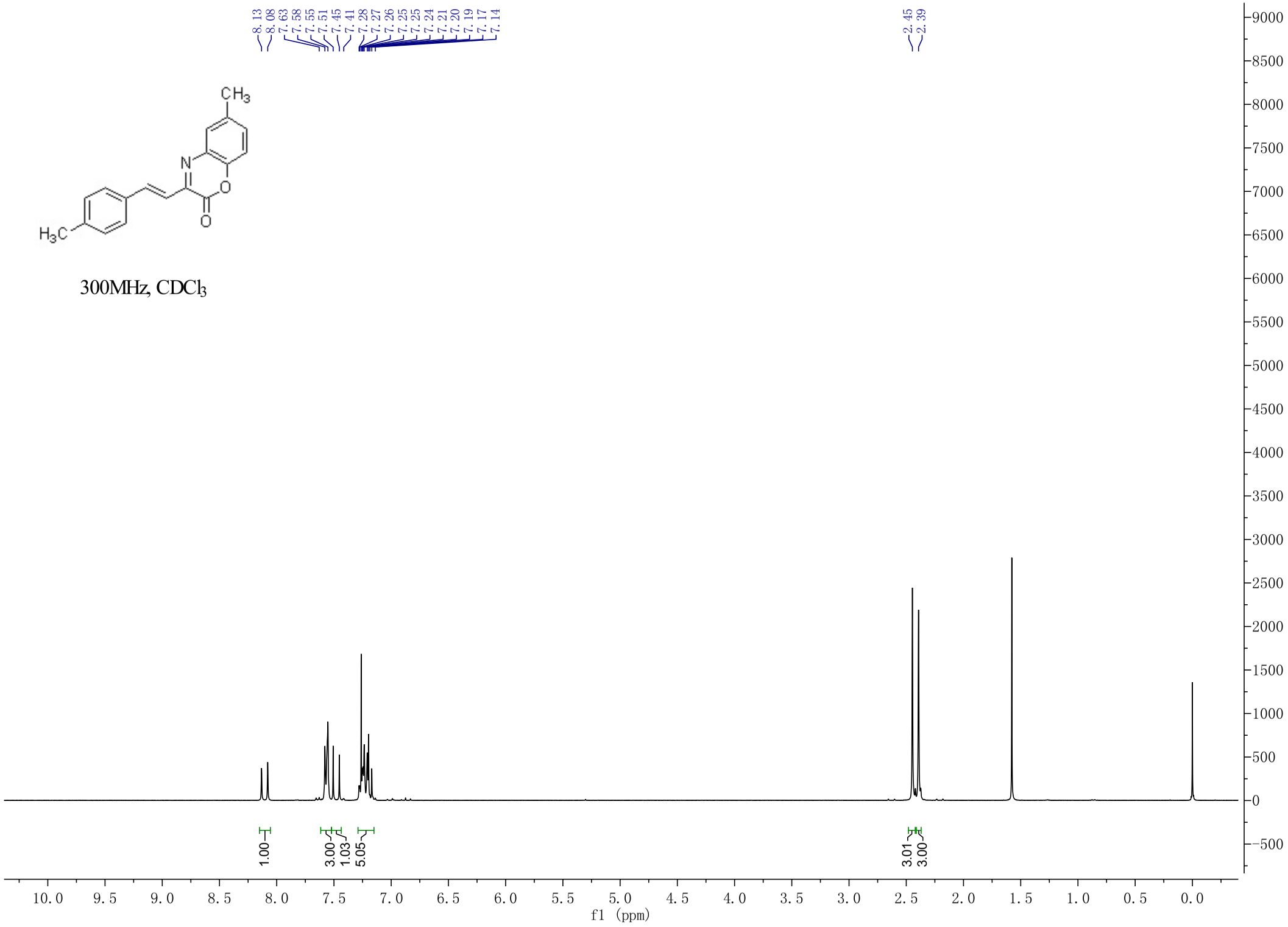

300MHz, CDCl3
MeO
N
O
O
8.14
8.09
7.64
7.61
7.43
7.43
7.38
7.31
7.30
6.96
6.93
3.86
1.00
1.01
2.03
3.06
1.03
1.99
3.00
f1 (ppm)

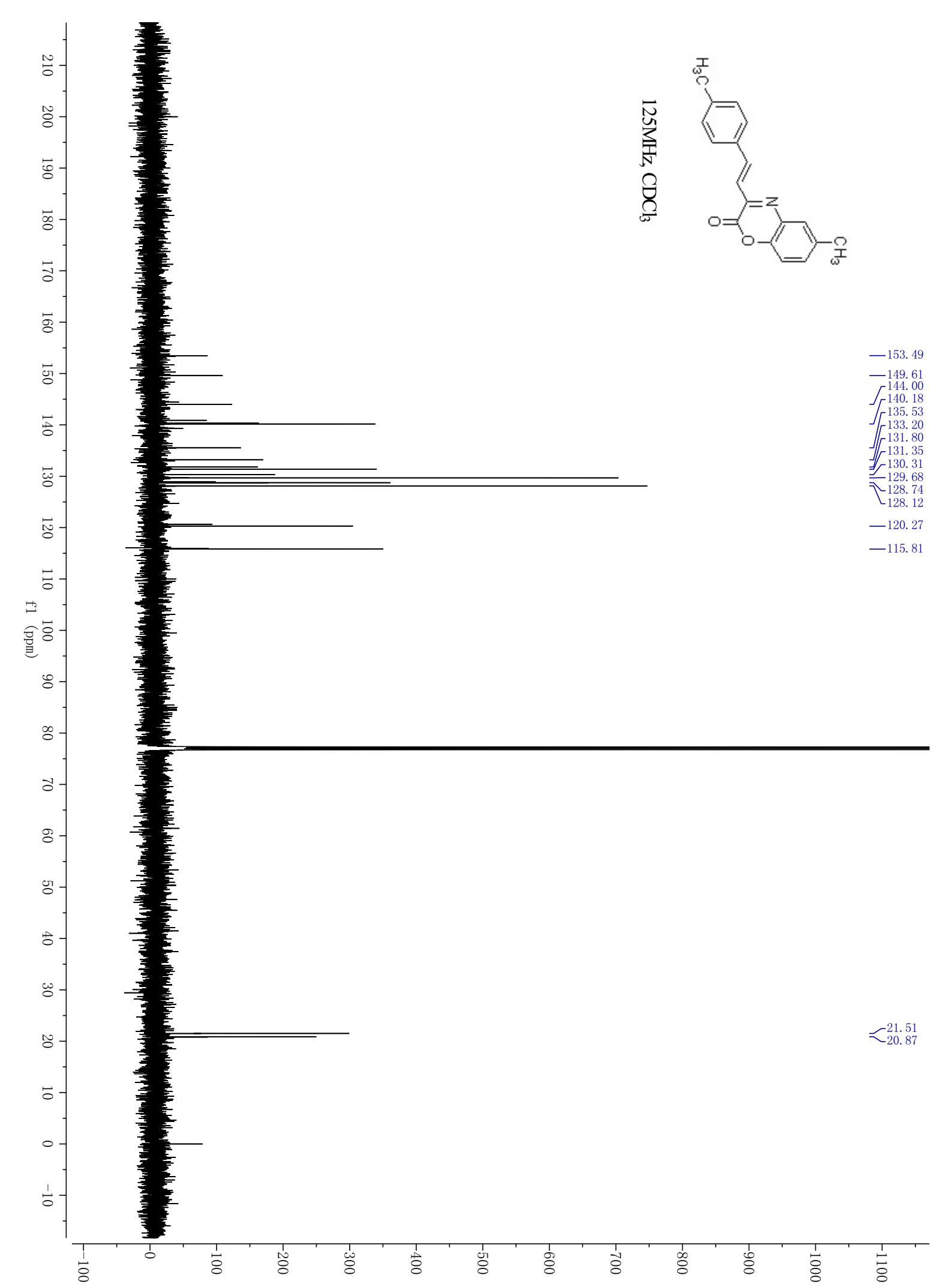

125MHz, CDCl3
MeO
N
O
O
161.26
153.29
149.82
145.99
140.15
132.49
130.12
129.82
128.75
125.60
118.91
116.27
114.45
113.33
55.42
f1 (ppm)

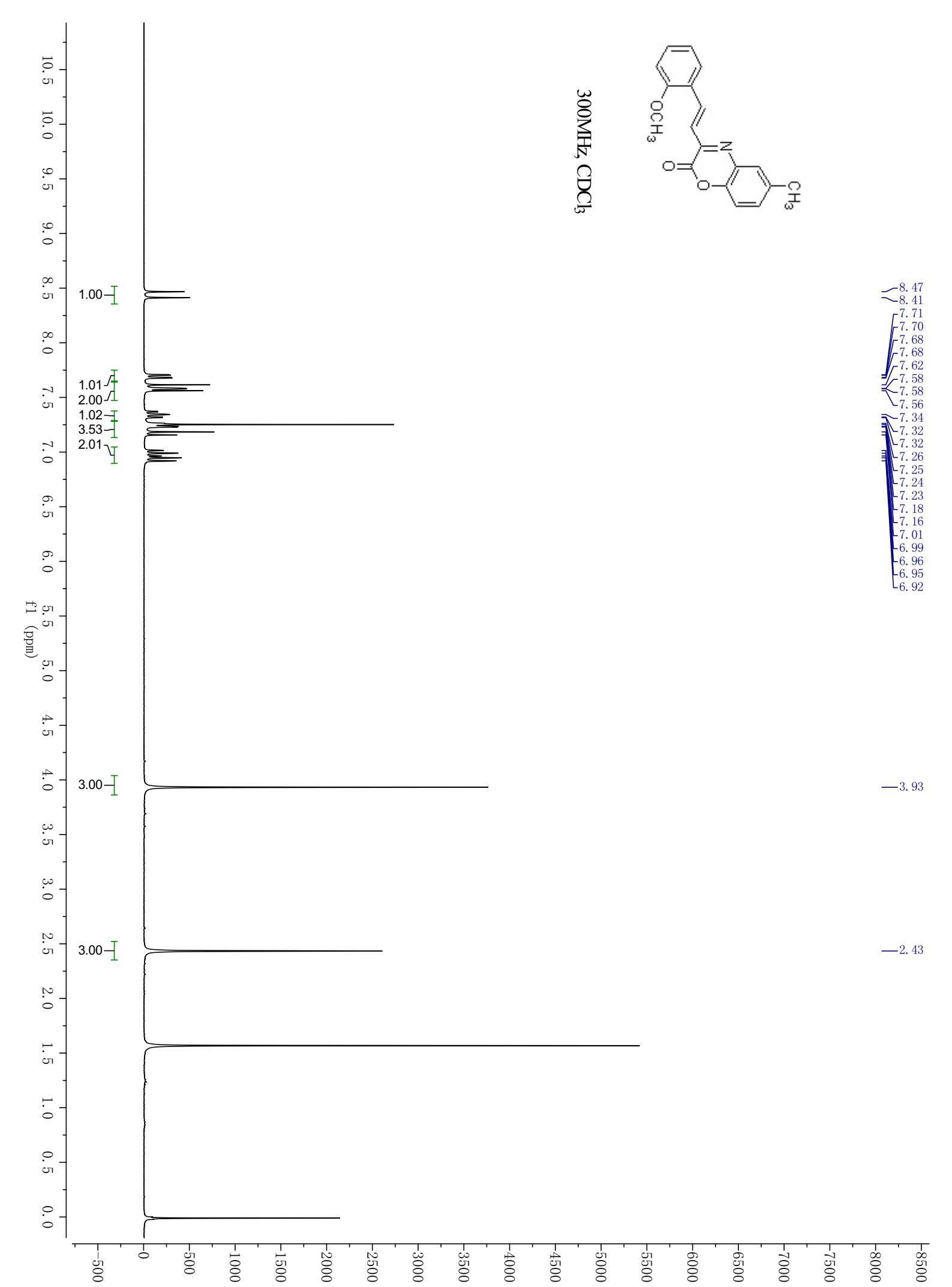

500MHz, CDCl3
1.00
2.00
1.00
1.03
3.03
1.88
0.99
3.00
8.15
8.11
7.67
7.66
7.57
7.54
7.50
7.43
7.42
7.40
7.39
7.38
7.36
7.28
7.26
7.20
7.18
2.45
f1 (ppm)

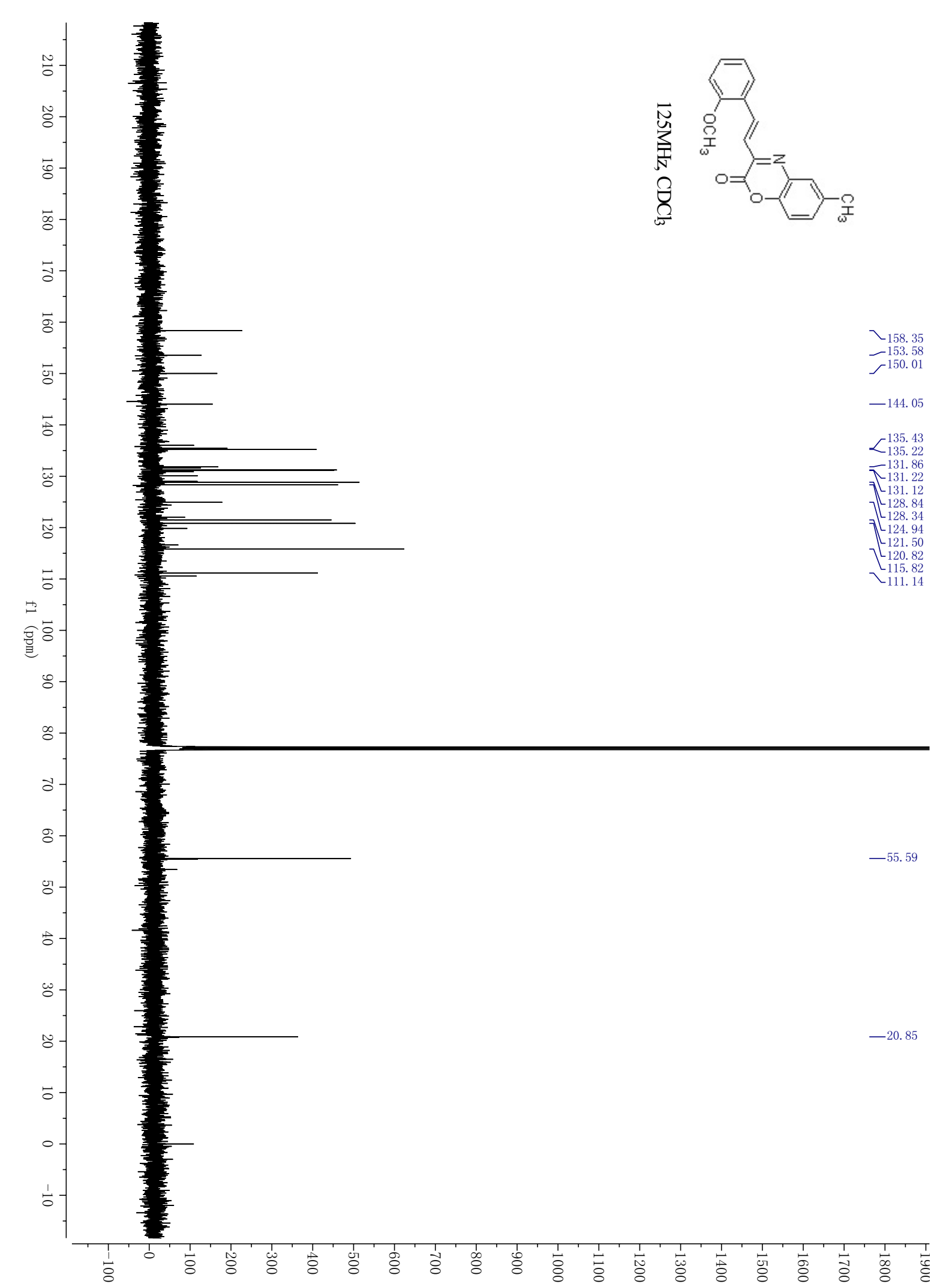

125MHz, CDCl3
153.46
149.58
144.12
140.23
135.97
135.67
131.82
131.65
129.95
129.00
128.92
128.19
121.42
115.97
20.94
f1 (ppm)

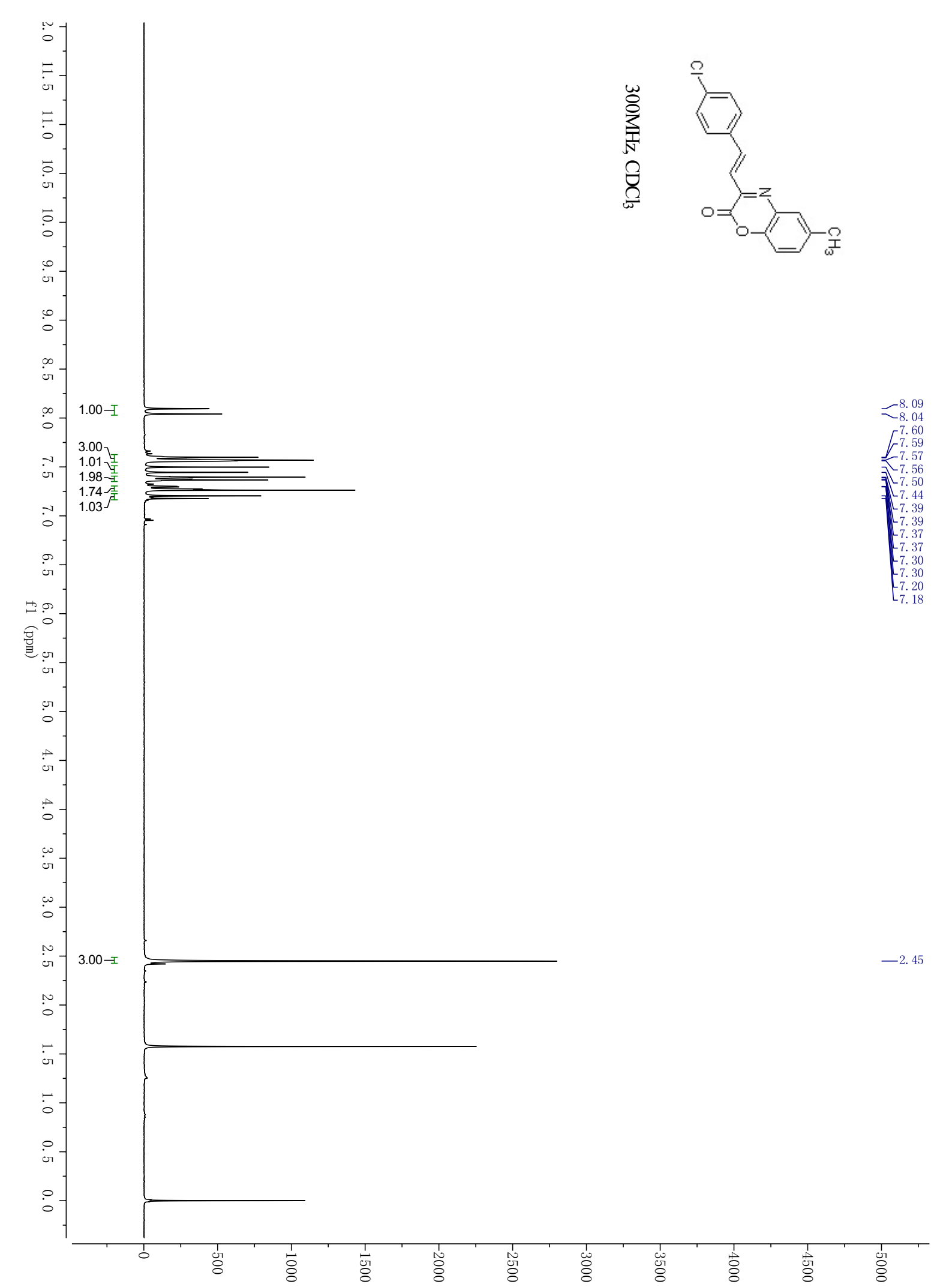
300MHz, $CDCl_3$

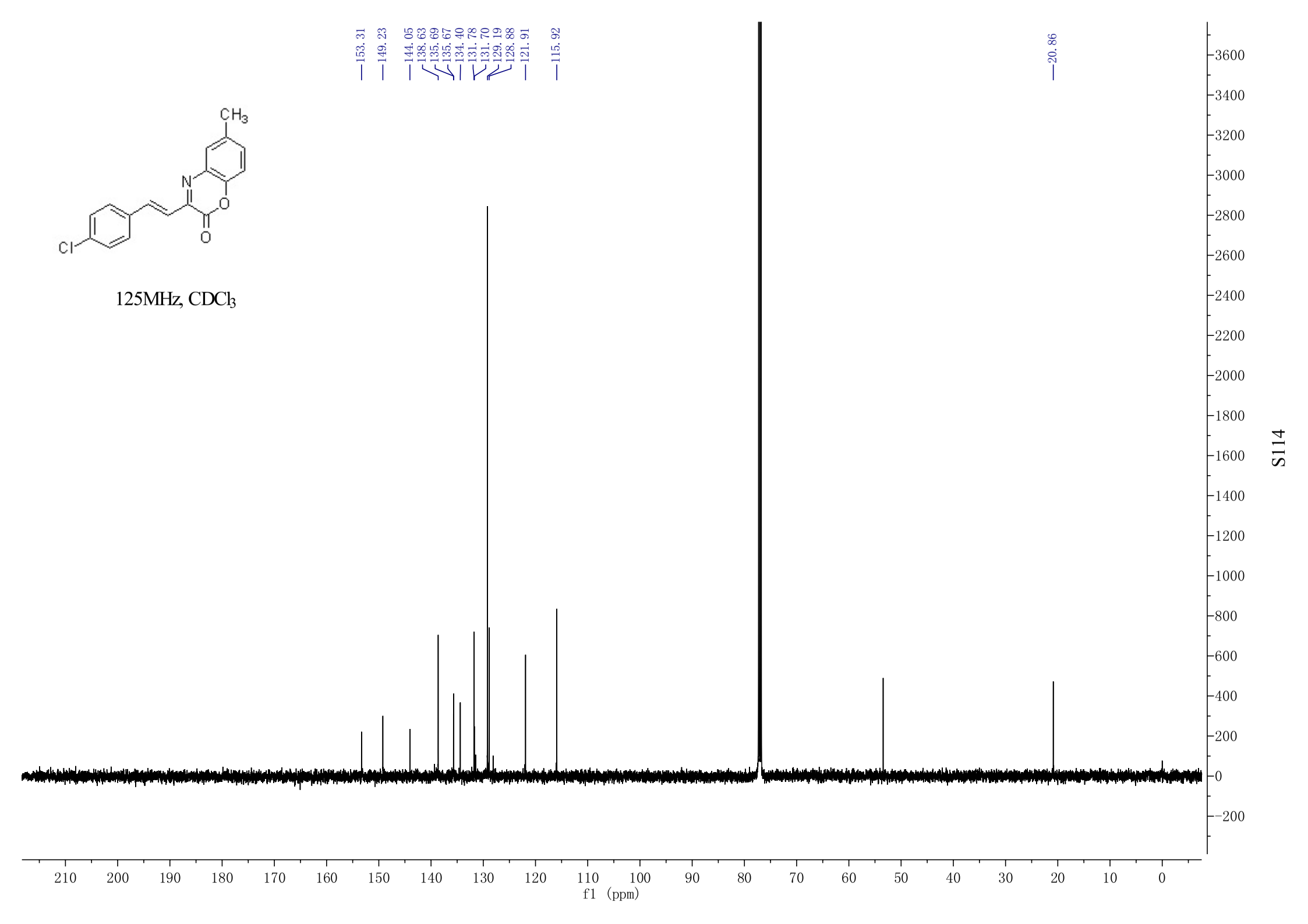


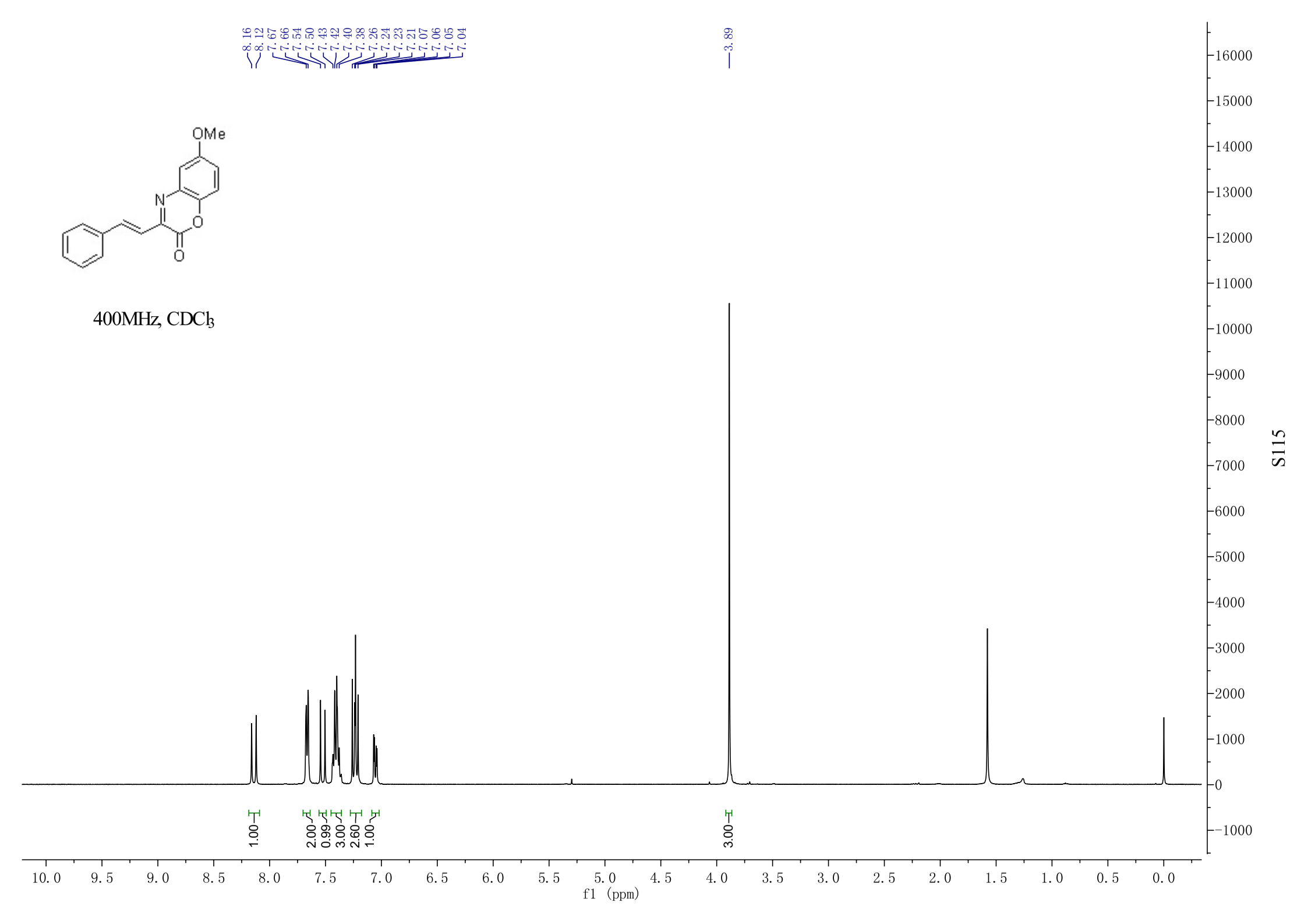

125MHz, CDCl3
H3C
CH3
O
O
N
153.49
149.61
144.00
140.18
135.53
133.20
131.80
131.35
130.31
129.68
128.74
128.12
120.27
115.81
21.51
20.87
f1 (ppm)

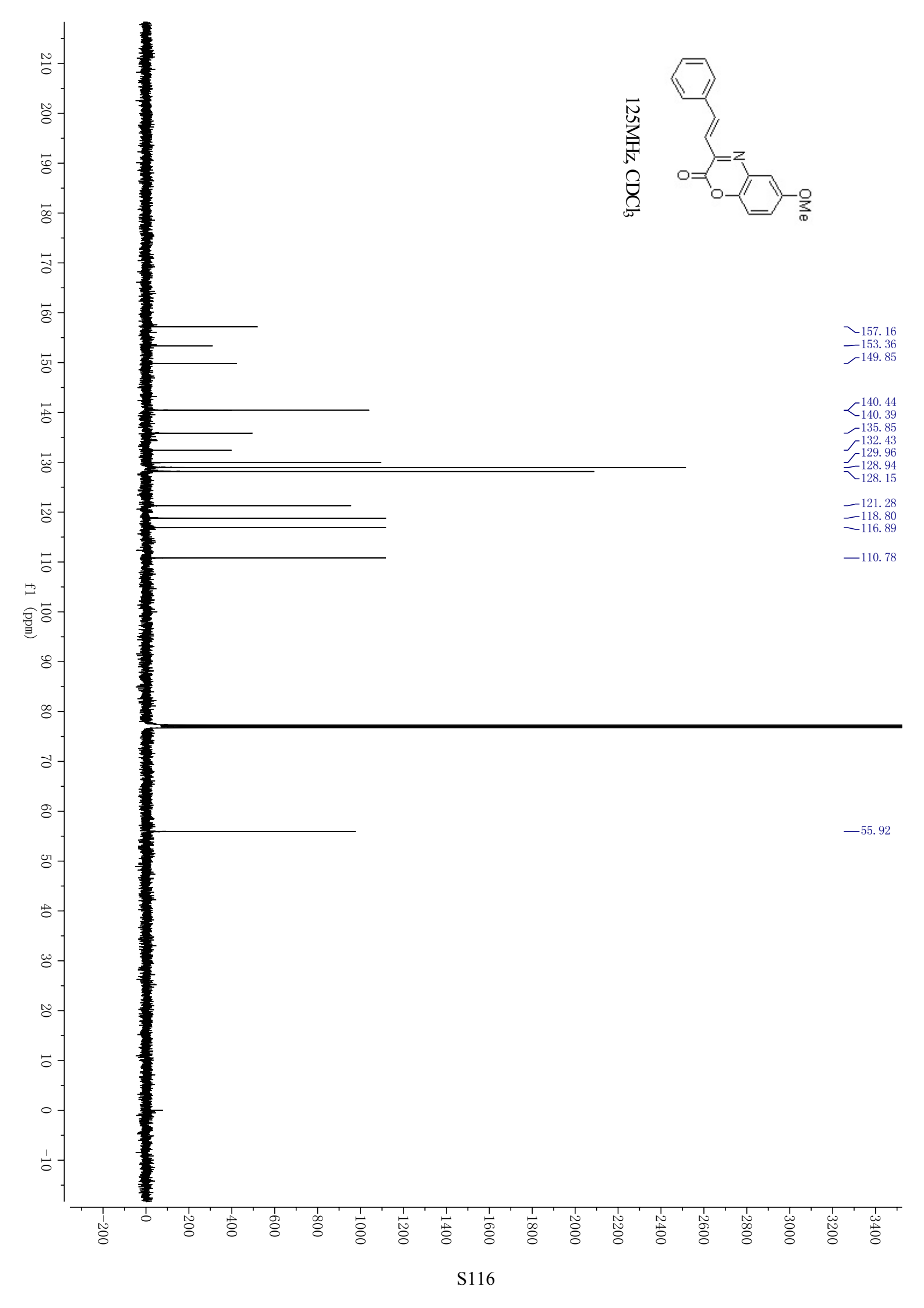

300MHz, CDCl3
OCH3
N
O
O
CH3
8.47
8.41
7.71
7.70
7.68
7.68
7.62
7.58
7.58
7.56
7.34
7.32
7.32
7.26
7.25
7.24
7.23
7.18
7.16
7.01
6.99
6.96
6.95
6.92
3.93
2.43
1.00
1.01
2.00
1.02
3.53
2.01
3.00
3.00
f1 (ppm)

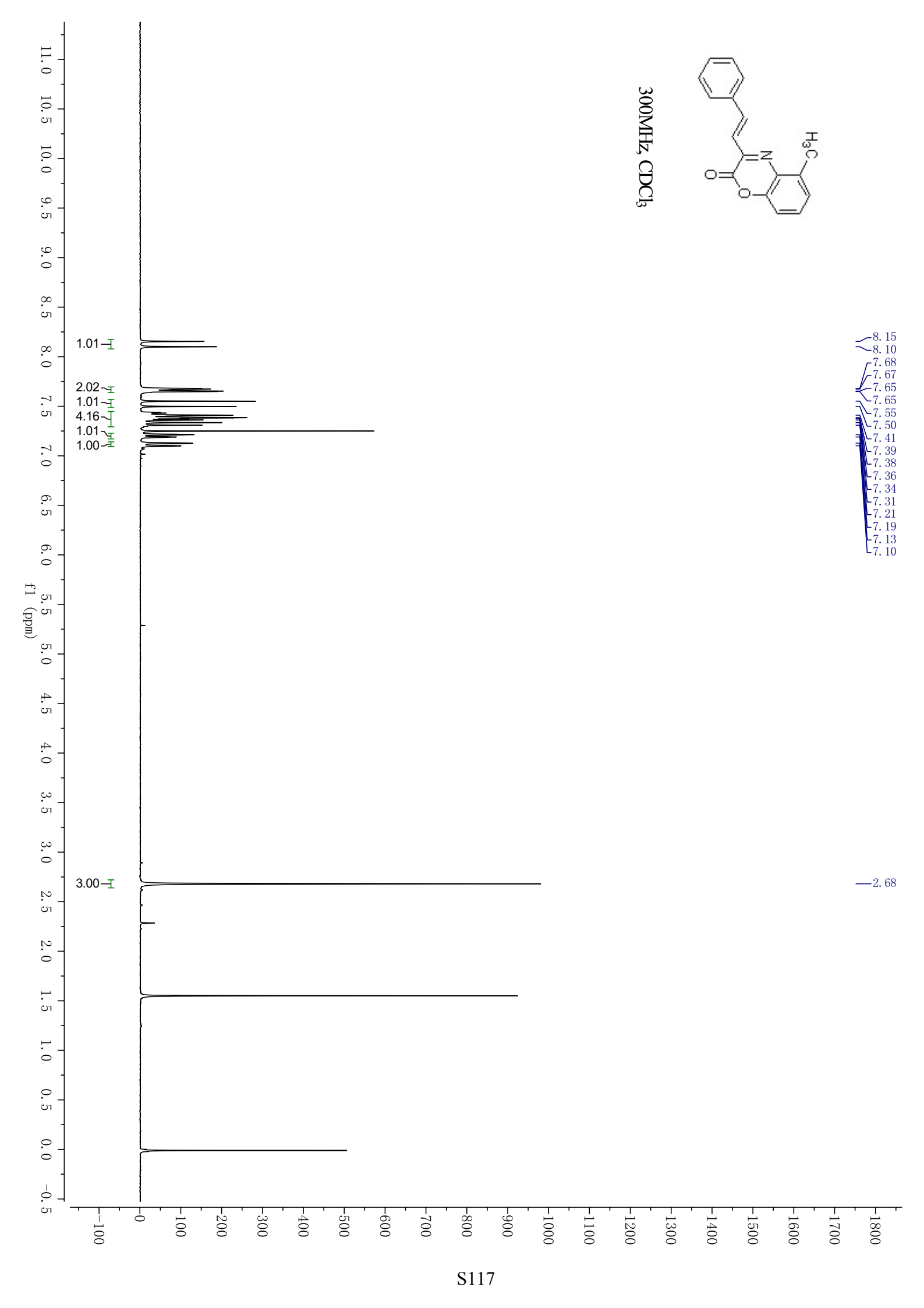

125MHz, CDCl3
OCH3
N
O
O
CH3
158.35
153.58
150.01
144.05
135.43
135.22
131.86
131.22
131.12
128.84
128.34
124.94
121.50
120.82
115.82
111.14
55.59
20.85
f1 (ppm)

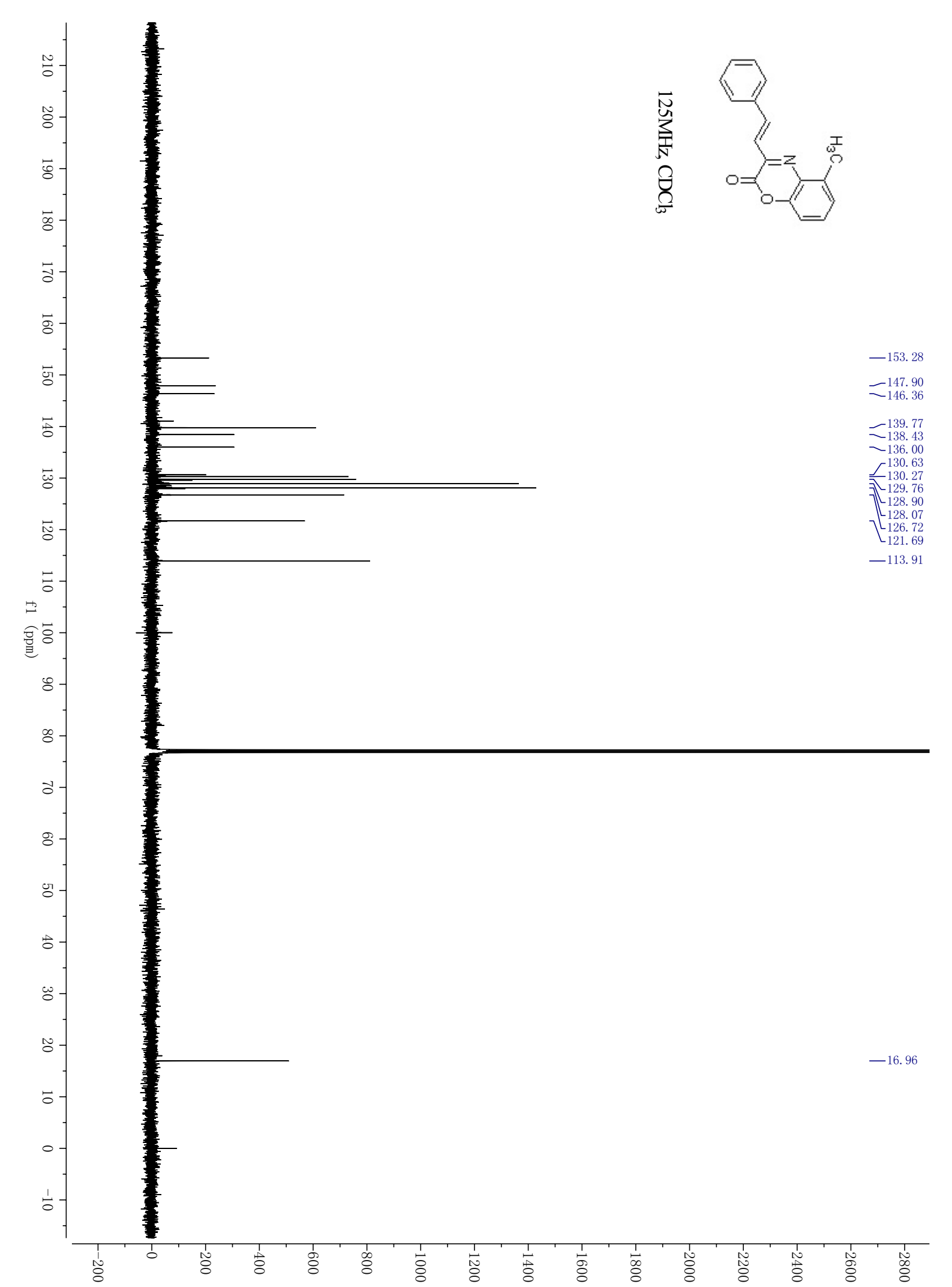

300MHz, CDCl3
Cl
N
O
O
CH3
1.00
3.00
1.01
1.98
1.74
1.03
3.00
8.09
8.04
7.60
7.59
7.57
7.56
7.50
7.44
7.39
7.39
7.37
7.37
7.30
7.30
7.20
7.18
2.45
f1 (ppm)

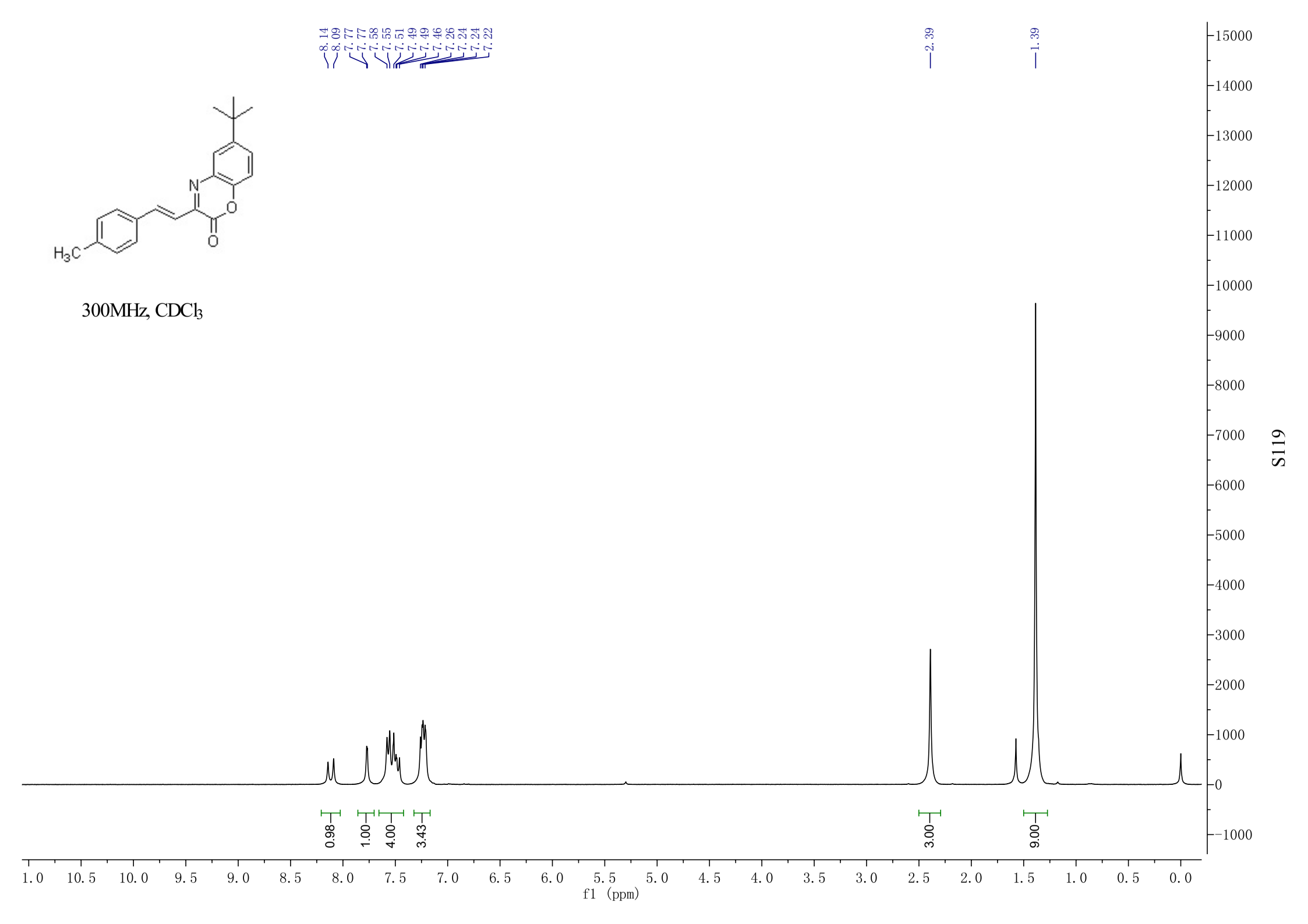

153.31
149.23
144.05
138.63
135.69
135.67
134.40
131.78
131.70
129.19
128.88
121.91
115.92
20.86
CH3
N
O
O
Cl
125MHz, CDCl3
f1 (ppm)

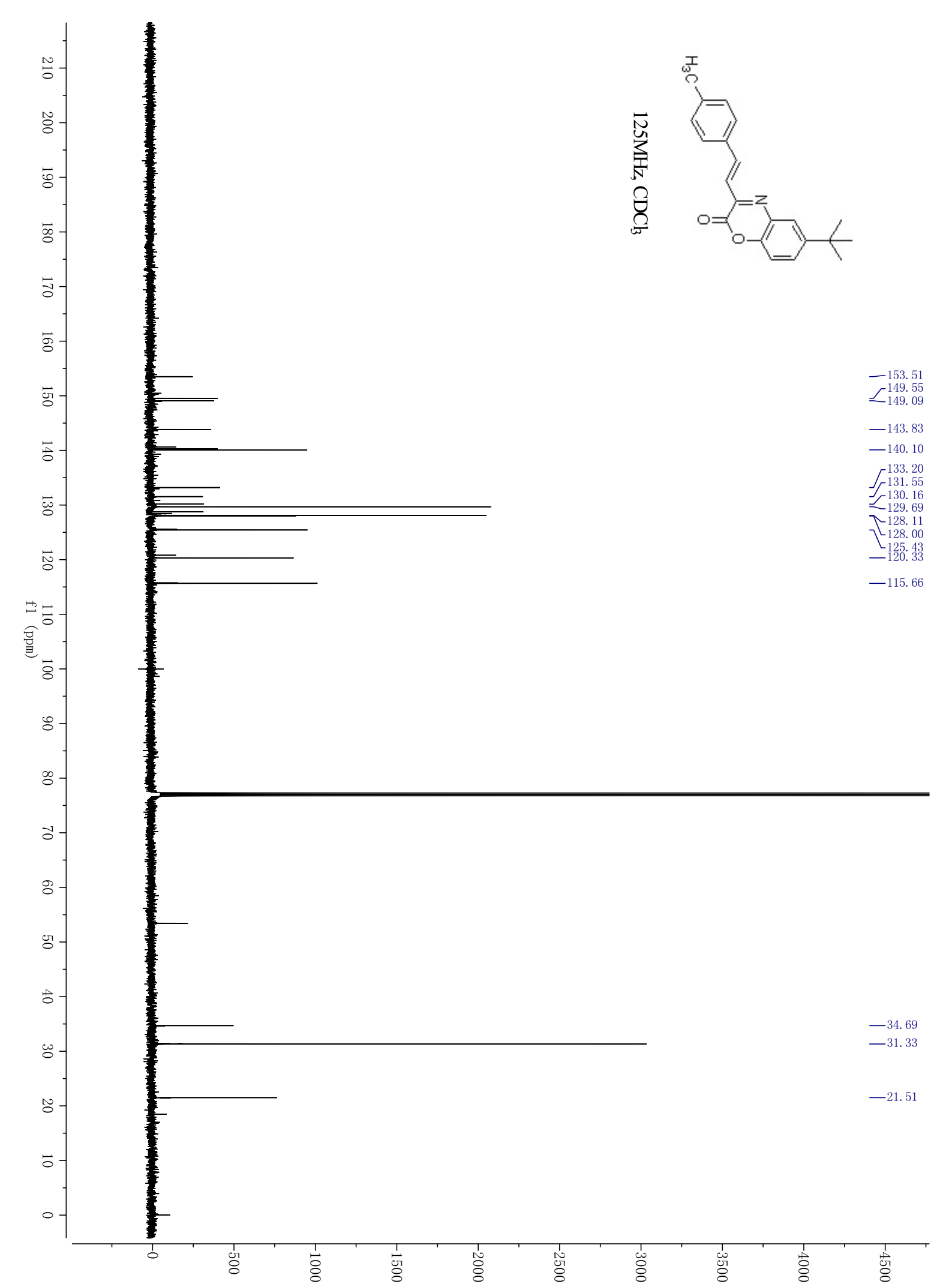

8.16
8.12
7.67
7.66
7.54
7.50
7.43
7.42
7.40
7.38
7.26
7.24
7.23
7.21
7.07
7.06
7.05
7.04
3.89
OMe
N
O
O
400MHz, CDCl3
1.00
2.00
0.99
3.00
2.60
1.00
3.00
f1 (ppm)

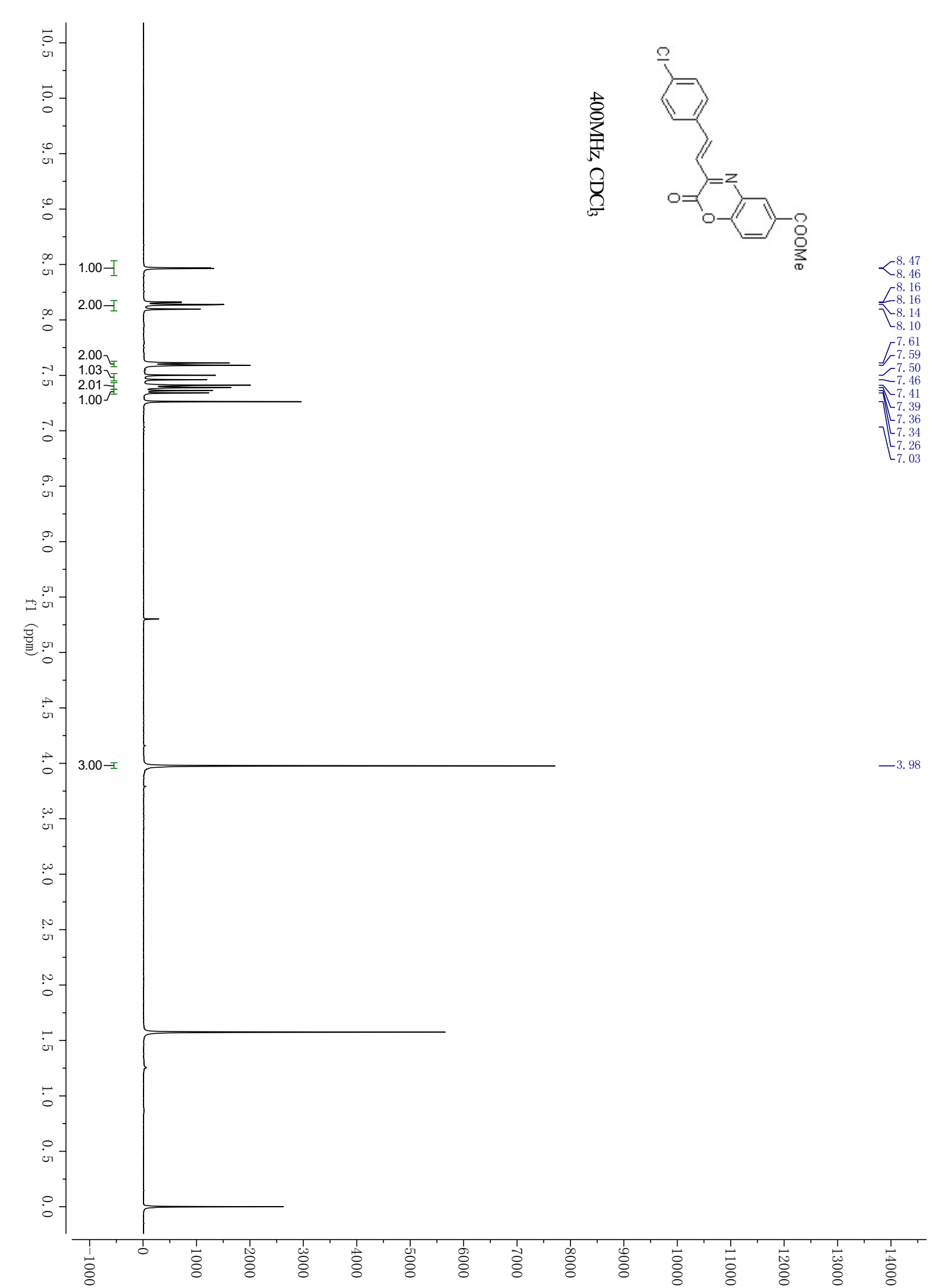

125MHz, CDCl3
OMe
157.16
153.36
149.85
140.44
140.39
135.85
132.43
129.96
128.94
128.15
121.28
118.80
116.89
110.78
55.92
f1 (ppm)

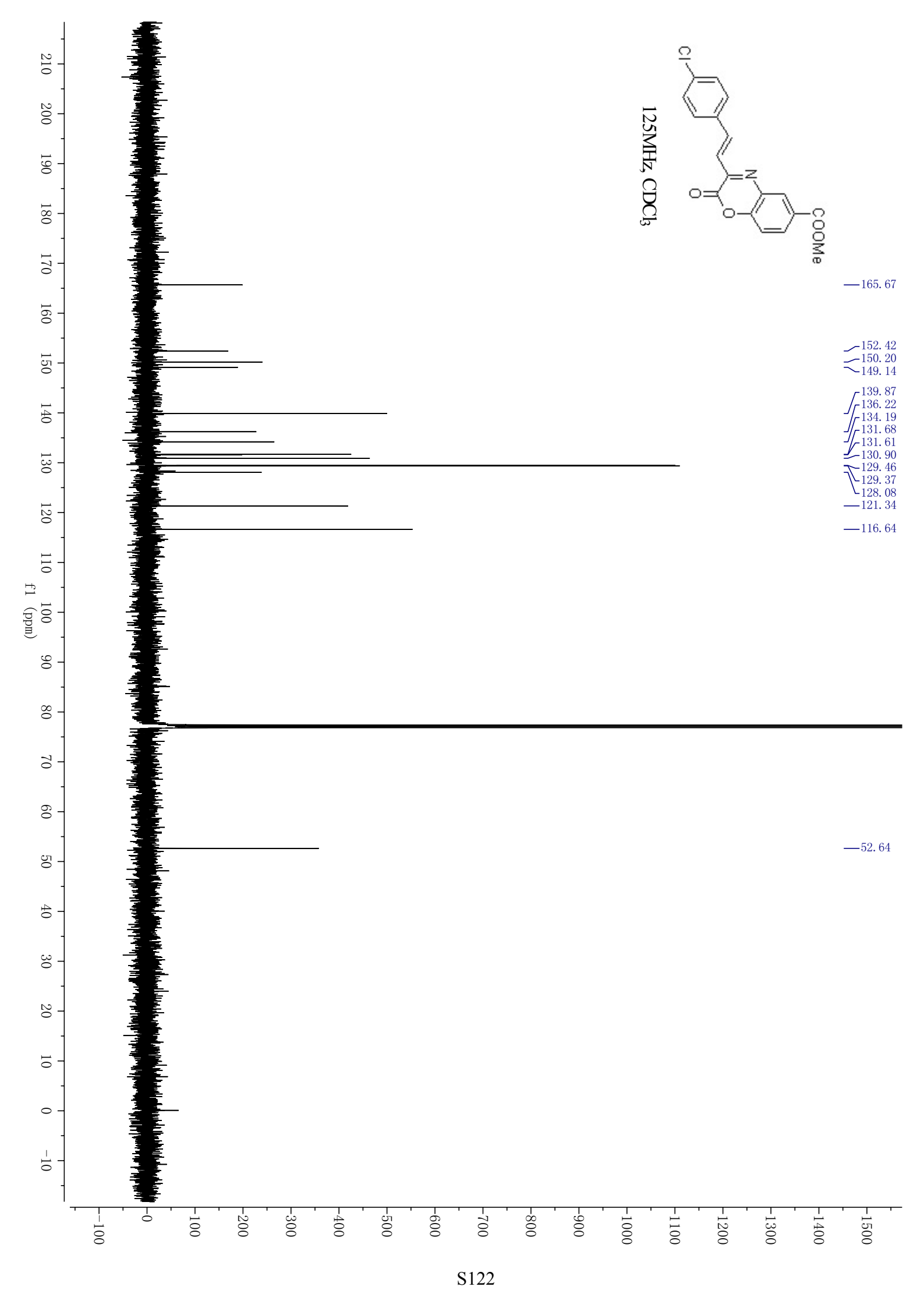

300MHz, CDCl3
H3C
N
O
O
1.01
2.02
1.01
4.16
1.01
1.00
3.00
8.15
8.10
7.68
7.67
7.65
7.65
7.55
7.50
7.41
7.39
7.38
7.36
7.34
7.31
7.21
7.19
7.13
7.10
2.68
f1 (ppm)


125MHz, CDCl3
H3C
N
O
O
153.28
147.90
146.36
139.77
138.43
136.00
130.63
130.27
129.76
128.90
128.07
126.72
121.69
113.91
16.96
f1 (ppm)

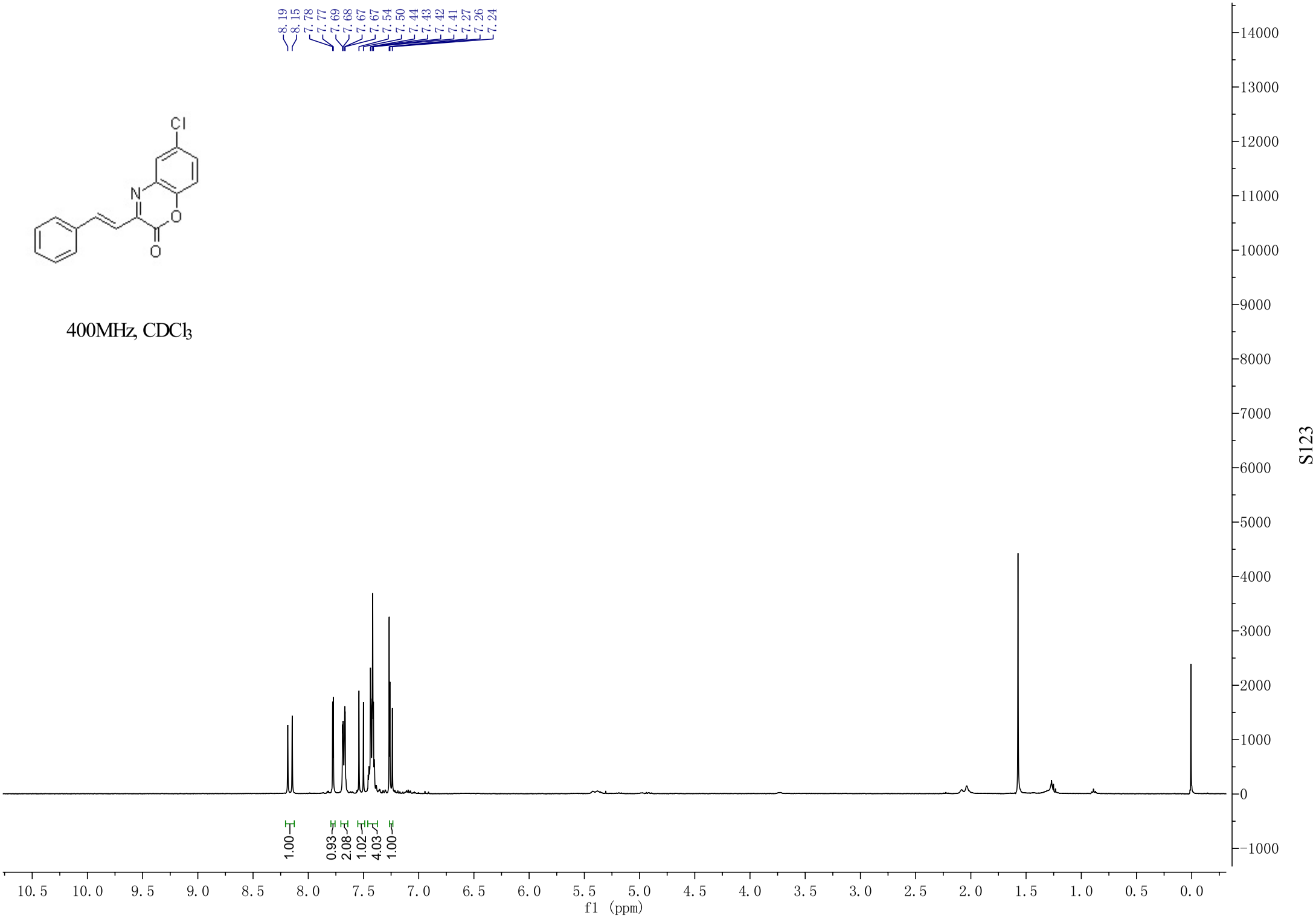

8.14
8.09
7.77
7.77
7.58
7.55
7.51
7.49
7.49
7.46
7.26
7.24
7.24
7.22
2.39
1.39
N
O
O
H3C
300MHz, CDCl3
0.98
1.00
4.00
3.43
3.00
9.00
f1 (ppm)

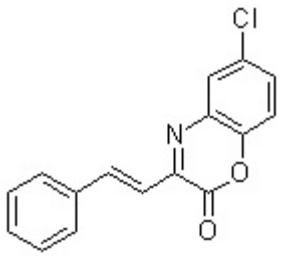

125MHz, CDCl3
H3C
O
N
O
153.51
149.55
149.09
143.83
140.10
133.20
131.55
130.16
129.69
128.11
128.00
125.43
120.33
115.66
34.69
31.33
21.51
f1 (ppm)


400MHz, CDCl3
Cl
N
O
O
COOMe
8.47
8.46
8.16
8.16
8.14
8.10
7.61
7.59
7.50
7.46
7.41
7.39
7.36
7.34
7.26
7.03
3.98
1.00
2.00
2.00
1.03
2.01
1.00
3.00
f1 (ppm)


125MHz, CDCl3
Cl
N
O
O
COOMe
165.67
152.42
150.20
149.14
139.87
136.22
134.19
131.68
131.61
130.90
129.46
129.37
128.08
121.34
116.64
52.64
f1 (ppm)

400MHz, $CDCl_3$

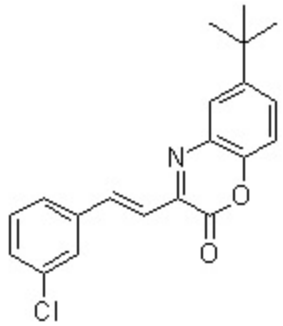




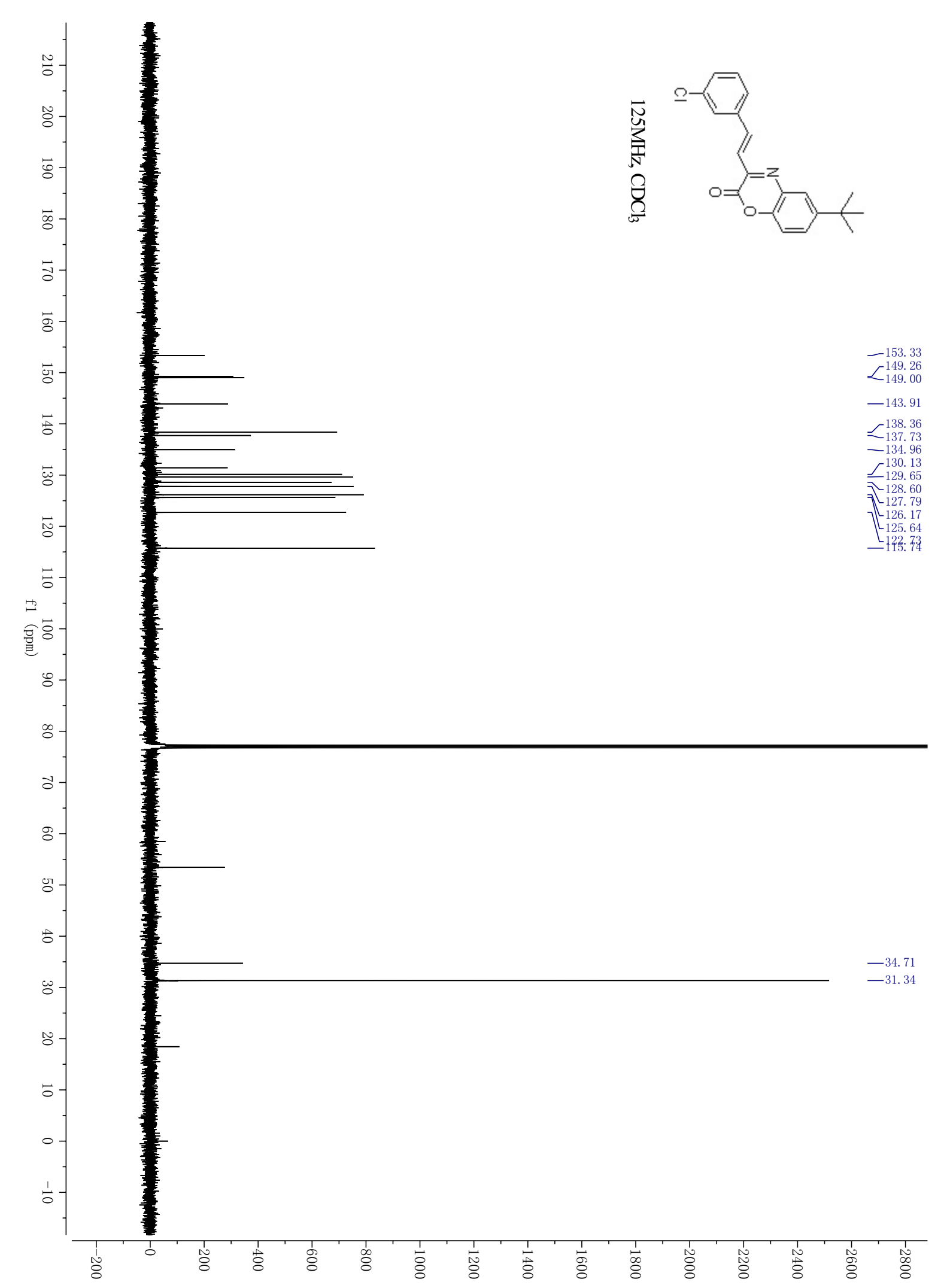
125MHz, $CDCl_3$

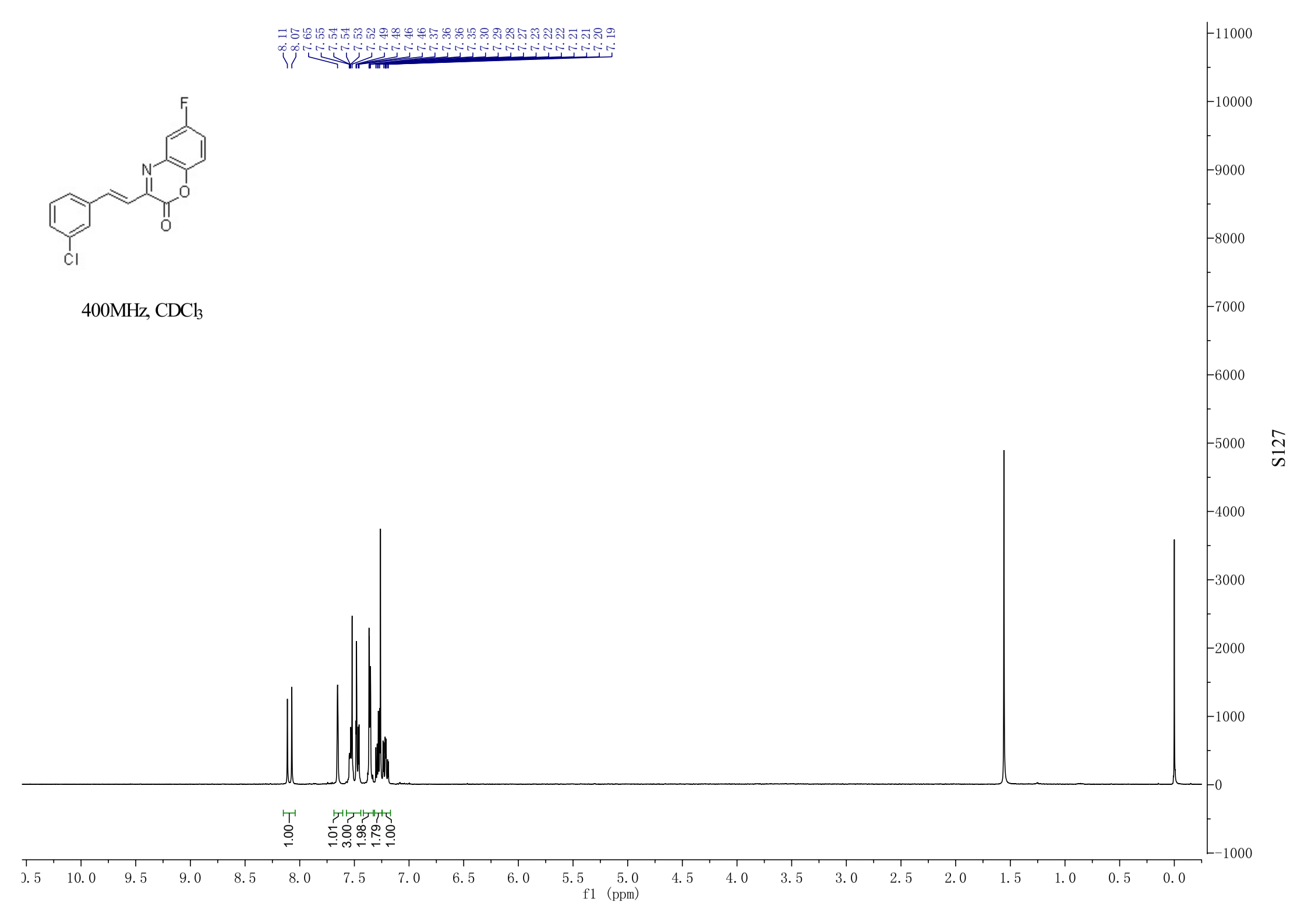
152.61
150.57
144.62
141.45
135.59
130.76
130.31
130.27
128.99
128.36
117.39

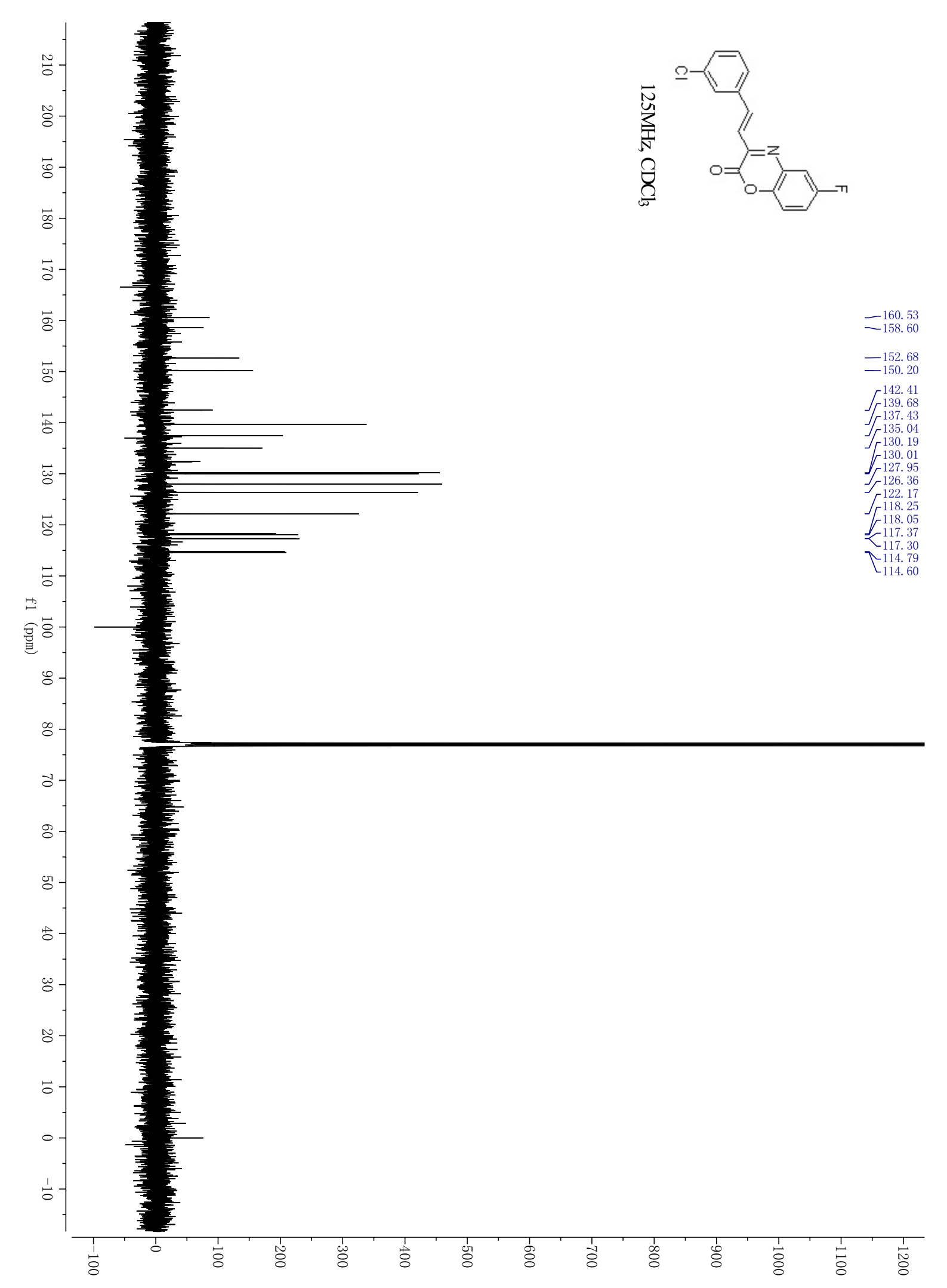
f1 (ppm)

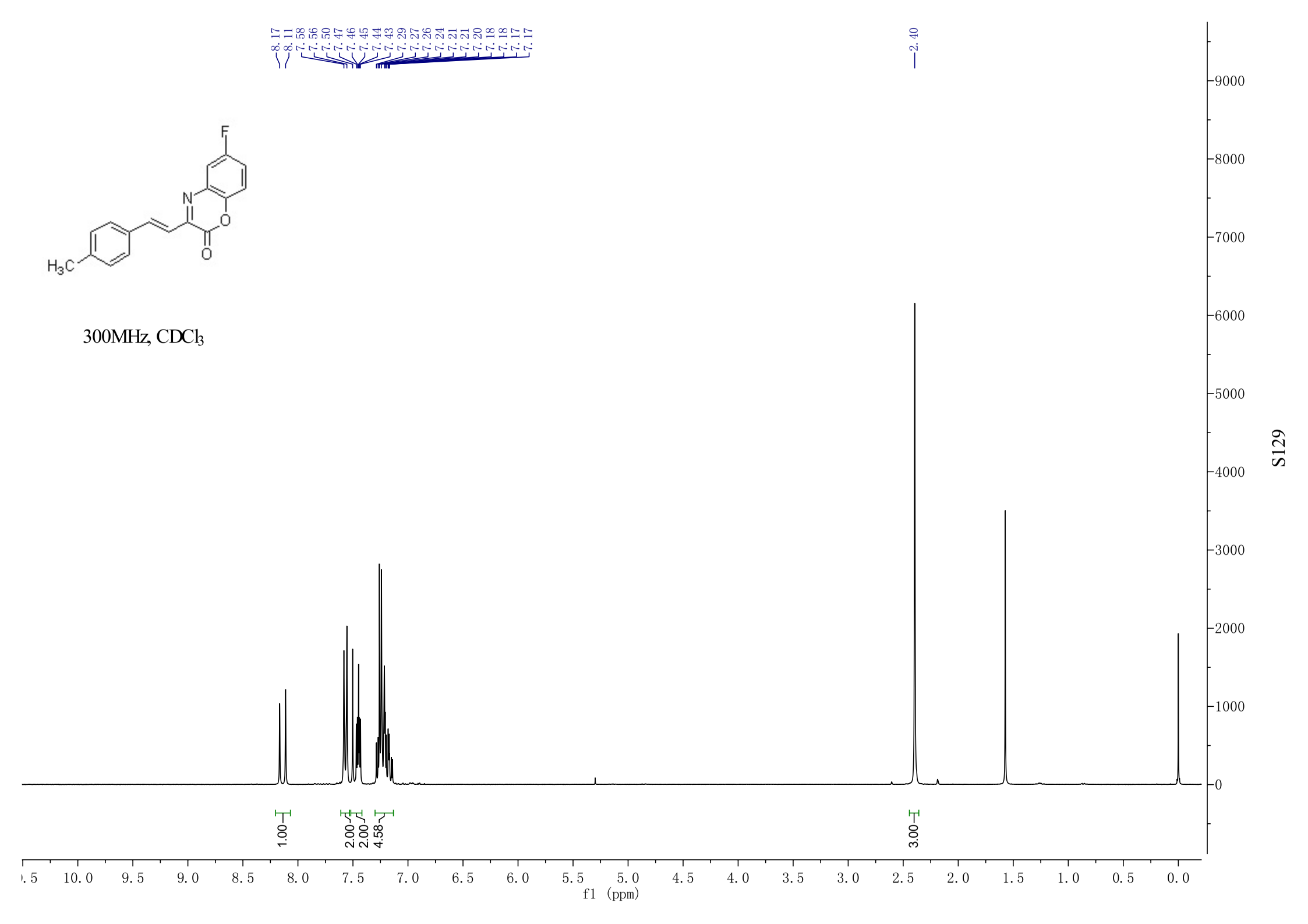


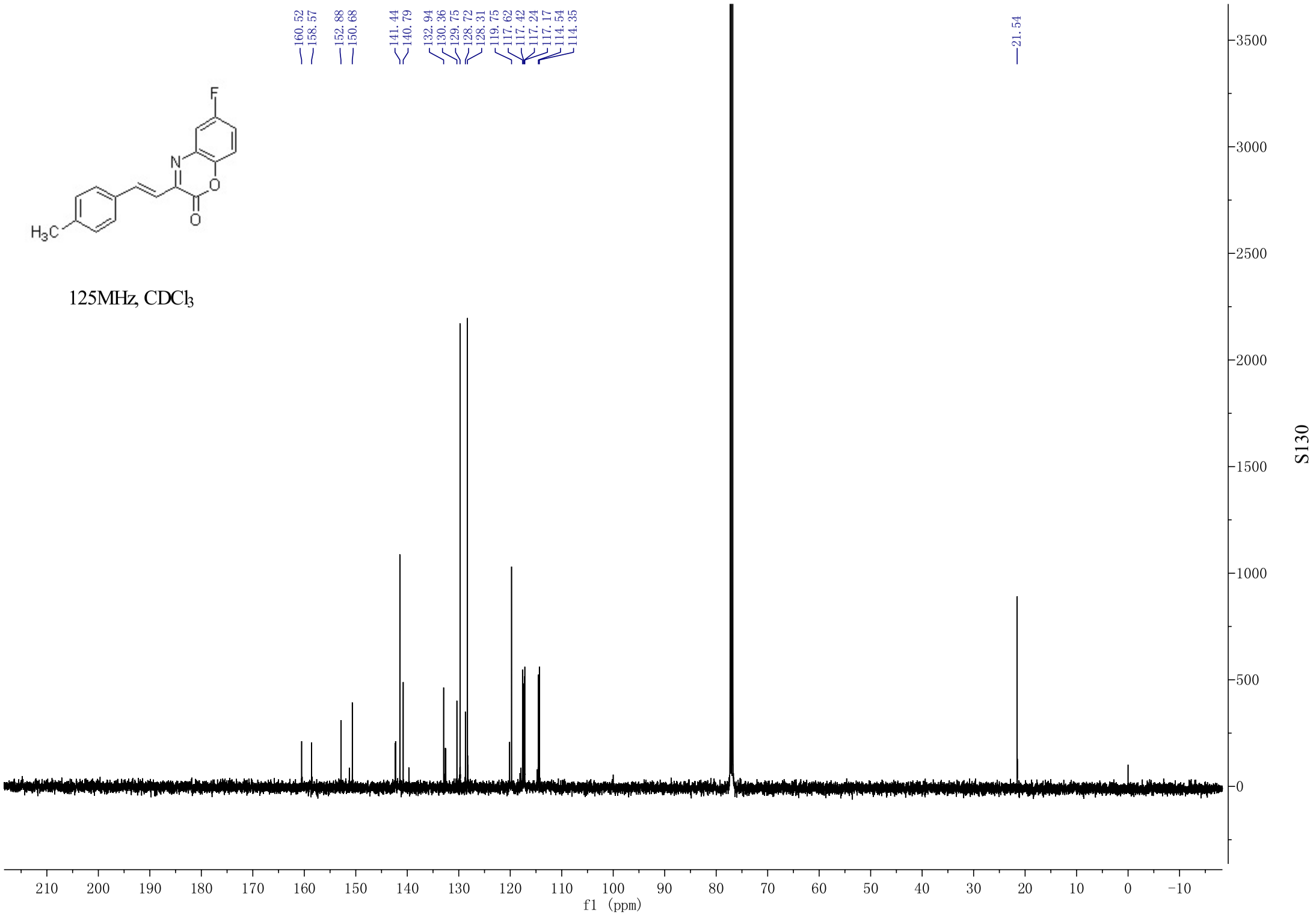
400MHz, $CDCl_3$


125MHz, CDCl3
Cl
N
O
O
153.33
149.26
149.00
143.91
138.36
137.73
134.96
130.13
129.65
128.60
127.79
126.17
125.64
122.73
115.74
34.71
31.34
f1 (ppm)

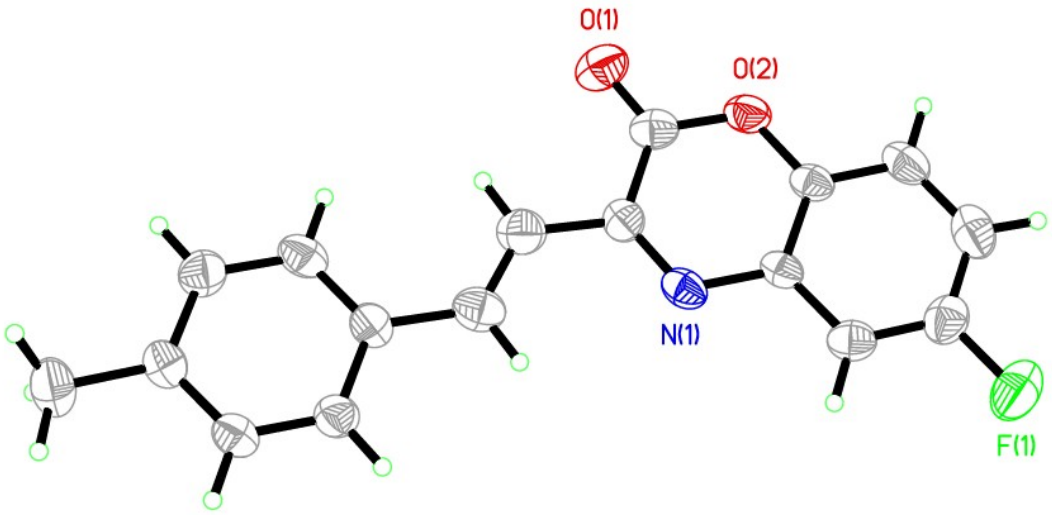

8.11
8.07
7.65
7.55
7.54
7.54
7.53
7.52
7.49
7.48
7.46
7.46
7.37
7.36
7.36
7.35
7.30
7.29
7.28
7.27
7.23
7.22
7.22
7.21
7.21
7.20
7.19
F
N
O
O
Cl
400MHz, CDCl3
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
1.00
1.01
3.00
1.98
1.79
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

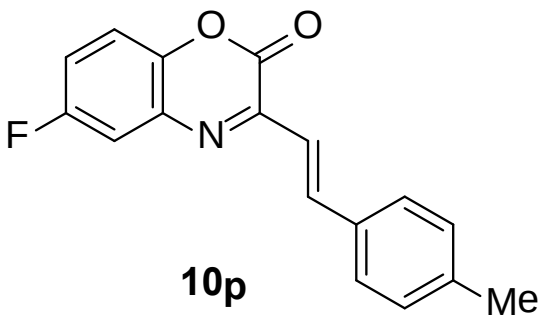

125MHz, CDCl3
Cl
N
O
O
F
160.53
158.60
152.68
150.20
142.41
139.68
137.43
135.04
130.19
130.01
127.95
126.36
122.17
118.25
118.05
117.37
117.30
114.79
114.60
f1 (ppm)


8.17
8.11
7.58
7.56
7.50
7.47
7.46
7.45
7.44
7.43
7.29
7.27
7.26
7.24
7.21
7.21
7.20
7.18
7.18
7.17
7.17
2.40
F
N
O
O
H3C
300MHz, CDCl3
1.00
2.00
2.00
4.58
3.00
f1 (ppm)


160.52
158.57
152.88
150.68
141.44
140.79
132.94
130.36
129.75
128.72
128.31
119.75
117.62
117.42
117.24
117.17
114.54
114.35
21.54
F
N
O
O
H3C
125MHz, CDCl3
3500
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 944907). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/conts/retrieving.html.





10p