Amine-Mediated Transimination and Aromatization-Triggered Domino Reaction in the Synthesis of Polyfunctionalized 4-Aminoquinolines

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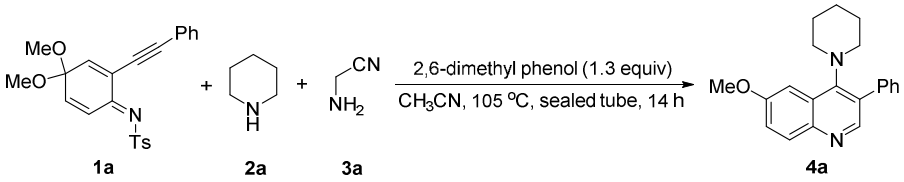
Supporting Information

1. General Information

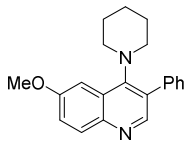
All reactions were performed in Schlenk tubes under nitrogen atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr (house vacuum) at 35–40 °C. Commercial reagents and solvents were used as received. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale.

2. Representative Procedure and Spectral Data of Products

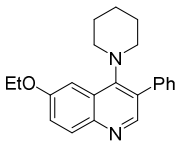


1a 2a 3a 4a

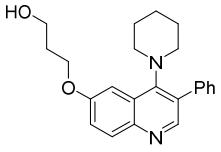
In a sealed tube, a solution of *N*-Ts 2-phenyl-ethynyl quinone imine ketal **1a** (0.1 mmol) in acetonitrile (2.0 mL) was mixed with piperidine (0.11 mmol), 2-aminoacetonitrile (0.13 mmol), and 2,6-dimethylphenol (0.13 mmol) in a nitrogen atmosphere. The resulting mixture in the sealed tube was stirred at 105 °C for 14 h., then the mixture was concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (eluent: *n*-hexane/ethyl acetate = 12/1) to furnish the desired compound **4a**



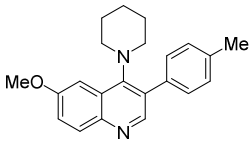
6-methoxy-3-phenyl-4-(piperidin-1-yl)quinoline **4a** (27 mg, yield 88%): yellow solid; m.p. 116-119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1 H), 8.02 (d, J = 9.1 Hz, 1 H), 7.48-7.31 (m, 7 H), 3.97 (s, 3 H), 2.98-2.80 (m, 4 H), 1.68-1.60 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.7, 151.0, 139.2, 130.6, 129.9, 128.8, 128.2, 127.3, 127.2, 121.2, 102.6, 55.4, 53.6, 26.8, 24.3; HRMS m/z calcd for $C_{21}H_{22}N_2O$ ([M+H]$^+$): 319.1805, found 319.1807.



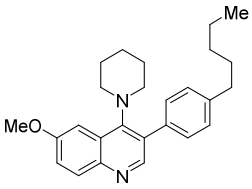
6-ethoxy-3-phenyl-4-(piperidin-1-yl)quinoline **4b** (27 mg, yield 83%): yellow solid; m.p. 150-152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1 H), 7.98 (d, J = 9.1 Hz, 1 H), 7.48-7.31 (m, 7 H), 4.20 (q, J = 7.0 Hz, 2 H), 3.03-2.70 (m, 4 H), 1.66-1.64 (m, 6 H), 1.52 (t, J = 7.0 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.0, 152.7, 151.4, 144.6, 139.5, 131.1, 130.0, 128.8, 128.2, 127.3, 127.2, 121.4, 103.2, 63.7, 53.6, 26.9, 24.4, 14.8; HRMS m/z calcd for $C_{22}H_{24}N_2O$ ([M+H]$^+$): 333.1961, found 333.1955.



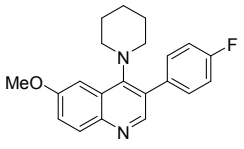
3-((3-phenyl-4-(piperidin-1-yl)quinolin-6-yl)oxy)propan-1-ol **4c** (23 mg, yield 64%): yellow solid; m.p. 145-147 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1 H), 7.97 (d, J = 9.1 Hz, 1 H), 7.48-7.40 (m, 4 H), 7.31-7.26 (m, 3 H), 4.28 (t, J = 5.9 Hz, 2 H), 3.94 (t, J = 5.9 Hz, 2 H), 2.95-2.75 (m, 4 H), 2.16 (m, 2 H), 1.65-1.57 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 156.8, 152.8, 151.3, 144.4, 139.3, 130.9, 129.9, 128.8, 128.2, 127.3, 127.2, 121.3, 103.3, 65.5, 60.0, 53.6, 32.0, 26.8, 24.3; HRMS m/z calcd for $C_{23}H_{26}N_2O_2$ ($[M+H]^+$): 363.2067, found 363.2072.



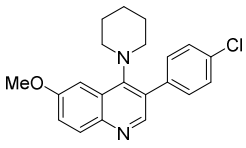
6-methoxy-4-(piperidin-1-yl)-3-(*p*-tolyl)quinoline **4d** (21 mg, yield 72%): yellow solid; m.p. 155-157 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1 H), 7.98 (d, J = 9.1 Hz, 1 H), 7.48 (d, J = 2.8 Hz, 1 H), 7.32 (dd, J = 9.1 Hz, 2.8 Hz, 1 H), 7.26 (d, J =7.9 Hz, 2 H), 7.20 (d, J = 8.0, 2 H), 3.96 (s, 3 H), 3.16-2.60 (m, 4 H), 2.44 (s, 3 H), 1.80-1.47 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.6, 152.6, 151.8, 144.7, 137.0,136.5, 131.2, 129.9, 128.9, 128.9, 127.3, 120.9, 102.5, 55.5, 53.6, 26.9, 24.4, 21.3; HRMS m/z calcd for $C_{22}H_{24}N_2O$ ($[M+H]^+$): 333.1961, found 333.1954.



6-methoxy-3-(4-pentylphenyl)-4-(piperidin-1-yl)quinoline **4e** (30 mg, yield 76%): yellow solid; m.p. 101-103 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1 H), 7.98 (d, J = 9.1 Hz, 1 H), 7.48 (d, J = 2.8 Hz, 1 H), 7.32 (dd, J = 9.1 Hz, 2.8 Hz, 1 H), 7.26 (d, J = 8.0 Hz, 2 H), 7.21 (d, J = 8.0 Hz, 2 H), 3.96 (s, 3 H), 2.94-2.78 (m, 4 H), 2.68 (t, J = 7.8 Hz, 2 H), 1.69-1.66 (m, 8 H), 1.39-1.35 (m, 4 H), 0.92 (t, J = 6.7 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.6, 152.6, 151.8, 144.7, 142.1, 136.6, 131.2, 129.8, 129.0, 128.2, 127.3, 120.9, 102.5, 55.5, 53.5, 35.7, 31.6, 31.1, 26.9, 24.4, 22.6, 14.1; HRMS m/z calcd for $C_{26}H_{32}N_2O$ ($[M+H]^+$): 389.2587, found 389.2609.

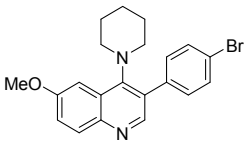


3-(4-fluorophenyl)-6-methoxy-4-(piperidin-1-yl)quinoline **4f** (26 mg, yield 78%): yellow solid; m.p. 149-151 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1 H), 8.00 (d, J = 9.1 Hz, 1 H), 7.46 (d, J = 2.7 Hz, 1 H), 7.34 (dd, J = 9.1, 2.8 Hz, 1 H), 7.30-7.26 (m, 2 H), 7.16 (t, J = 8.6 Hz, 2 H), 3.97 (s, 3 H), 2.86 (m, 4 H), 1.69-1.59 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 162.3 (d, J (C,F) = 246.7 Hz), 157.8, 153.0, 151.1, 144.5, 135.2, 131.5 (d, J (C,F) = 8.0 Hz), 130.9, 127.8, 127.2, 121.3, 115.3 (d, J (C,F) = 21.4 Hz), 102.6, 55.5, 53.6, 26.8, 24.3; HRMS m/z calcd for $C_{21}H_{21}FN_2O$ ($[M+H]^+$): 337.1711, found 337.1701.

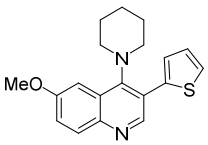


3-(4-chlorophenyl)-6-methoxy-4-(piperidin-1-yl)quinoline **4g** (21 mg, yield 60%): yellow solid; m.p. 148-150 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1 H), 7.98 (d, J = 9.1 Hz, 1 H), 7.45-7.43 (m, 3 H), 7.34 (d, J = 9.1 Hz, 1 H), 7.25 (d, J = 8.4 Hz, 2 H), 3.97 (s, 3 H), 3.20-2.50 (m, 4 H), 1.68-1.61 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.7, 152.7, 151.1, 144.9, 137.9, 133.5, 131.2, 128.5, 127.6,

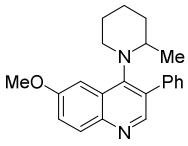
127.1, 121.3, 102.5, 55.5, 53.7, 26.8, 24.3; HRMS m/z calcd for $C_{21}H_{21}ClN_2O$ ($[M+H]^+$): 353.1415, found 353.1410.



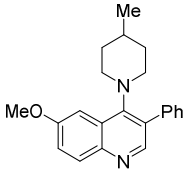
3-(4-bromophenyl)-6-methoxy-4-(piperidin-1-yl)quinoline **4h** (22 mg, yield 57%): yellow solid; m.p. 148-150 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1 H), 7.98 (d, J = 9.1 Hz, 1 H), 7.58 (d, J = 8.3 Hz, 2H), 7.45 (d, J = 2.8 Hz, 1 H), 7.33 (dd, J = 9.1 Hz, 2.8 Hz, 1 H), 7.18 (d, J = 8.3 Hz, 2 H), 3.96 (s, 3 H), 3.15-2.59 (m, 4 H), 1.68-1.60 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.6, 152.6, 150.8, 144.7, 138.3, 131.5, 131.3, 131.0, 127.4, 127.0, 121.5, 121.2, 102.4, 55.4, 53.6, 26.7, 24.2; HRMS m/z calcd for $C_{21}H_{21}BrN_2O$ ($[M+H]^+$): 397.0910, found 397.0916.



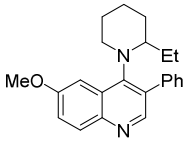
6-methoxy-4-(piperidin-1-yl)-3-(thiophen-2-yl)quinoline **4i** (18 mg, yield 54%): yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 1 H), 8.02 (d, J = 9.1 Hz, 1 H), 7.47 (d, J = 2.8 Hz, 1 H), 7.42 (dd, J = 5.1 Hz, 1.0 Hz, 1 H), 7.33 (dd, J = 9.1 Hz, 2.8 Hz, 1 H), 7.13 (dd, J = 5.1 Hz, 3.5 Hz, 1 H), 7.07 (d, J = 3.4 Hz, 1 H), 3.97 (s, 3 H), 3.20-2.83 (m, 4 H), 1.74-1.62 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.8, 153.8, 151.2, 144.7, 139.8, 131.0, 127.8, 127.3, 127.1, 126.4, 121.9, 121.3, 102.7, 55.5, 52.8, 26.7, 24.3; HRMS m/z calcd for $C_{19}H_{20}N_2OS$ ($[M+H]^+$): 325.1369, found 325.1369.



6-methoxy-4-(2-methylpiperidin-1-yl)-3-phenylquinoline **4j** (27 mg, yield 82%): yellow solid; m.p. 137-139 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1 H), 8.01 (d, J = 9.1 Hz, 1 H), 7.80-7.60 (m, 1 H), 7.44-7.33 (m, 6 H), 3.95 (s, 3 H), 3.37-3.21 (m, 1 H), 2.95-2.93 (m, 1 H), 2.55-2.35 (m, 1 H), 1.76-1.64 (m, 4 H), 1.29-1.26 (m, 2 H), 0.71 (m, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.9, 151.0, 145.1, 139.0, 132.7, 130.9, 130.0, 129.7, 128.0, 127.5, 121.1, 102.8, 55.3, 54.8, 52.7, 35.3, 27.0, 24.5, 20.7; HRMS m/z calcd for $C_{22}H_{24}N_2O$ ($[M+H]^+$): 333.1961, found 333.1957.

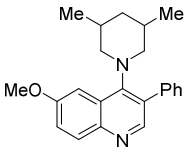


6-methoxy-4-(4-methylpiperidin-1-yl)-3-phenylquinoline **4k** (28 mg, yield 86%): yellow solid; m.p. 120-122 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1 H), 7.99 (d, J =9.1 Hz, 1 H), 7.47-7.30 (m, 7 H), 3.96 (s, 3 H), 3.17-3.14 (m, 2 H), 2.63-2.57 (m, 2 H), 1.64-1.62 (m, 2 H), 1.38-1.34 (m, 3 H), 0.97 (d, J = 6.1 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.6, 152.5, 151.4, 144.6, 139.4, 131.1, 129.9, 129.0, 128.2, 127.3, 127.1, 120.9, 102.6, 55.4, 52.8, 35.2, 30.8, 22.2; HRMS m/z calcd for $C_{22}H_{24}N_2O$ ($[M+H]^+$): 333.1961, found 333.1949.

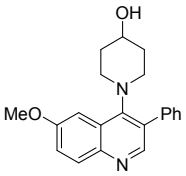


4-(2-ethylpiperidin-1-yl)-6-methoxy-3-phenylquinoline **4l** (27 mg, yield 86%): yellow solid; m.p. 109-111 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1 H), 8.00 (d, J = 9.1 Hz, 1 H), 7.67 (s, 1 H), 7.47-7.33 (m, 6 H), 3.95 (s, 3 H), 3.40-3.20 (m,

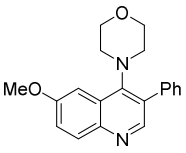
1 H), 3.00-2.94 (m, 1 H), 2.28 (m, 1 H), 1.78-1.65 (m, 4 H), 1.26-1.03 (m, 4 H), 0.49 (m, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.8, 151.1, 151.0, 145.2, 139.0, 132.6, 131.0, 130.1, 129.2, 128.0, 127.5, 121.1, 102.8, 58.2, 55.4, 54.8, 30.7, 27.0, 26.0, 24.1, 9.5; HRMS m/z calcd for $C_{23}H_{26}N_2O$ ($[M+H]^+$): 347.2118, found 347.2122.



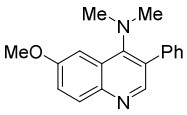
4-(3,5-dimethylpiperidin-1-yl)-6-methoxy-3-phenylquinoline **4m** (31 mg, yield 90%): yellow solid; m.p. 132-134 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1 H), 7.98 (d, J = 9.1 Hz, 1 H), 7.47-7.30 (m, 7 H), 3.93 (s, 3 H), 3.12 (d, J = 11.5 Hz, 2 H), 2.13-2.08 (m, 2 H), 1.87-1.80 (m, 3 H), 0.77 (d, J = 6.4 Hz, 6 H), 0.67-0.59 (m, 1 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.6, 152.1, 151.5, 144.9, 139.3, 131.2, 129.9, 129.0, 128.2, 127.3, 127.2, 121.0, 102.4, 60.1, 55.4, 42.3, 32.3, 19.0; HRMS m/z calcd for $C_{23}H_{26}N_2O$ ($[M+H]^+$): 347.2118, found 347.2129.



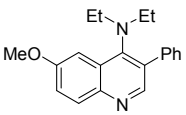
1-(6-methoxy-3-phenylquinolin-4-yl)piperidin-4-ol **4n** (28 mg, yield 85%): yellow solid; m.p. 206-208 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1 H), 7.99 (d, J = 9.1 Hz, 1 H), 7.47-7.29 (m, 7 H), 3.93 (m, 3 H), 3.79-3.75 (m, 1 H), 3.16 (m, 2 H), 2.70-2.66 (m, 2 H), 1.97-1.94 (m, 2 H), 1.73-1.71 (m, 2 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.8, 152.0, 151.2, 144.6, 139.1, 131.1, 129.8, 129.3, 128.3, 127.5, 127.0, 121.2, 102.2, 55.4, 50.2, 35.5, 29.6; HRMS m/z calcd for $C_{21}H_{22}N_2O_2$ ($[M+H]^+$): 335.1754, found 335.1764.



4-(6-methoxy-3-phenylquinolin-4-yl)morpholine **4o** (21 mg, yield 70%): yellow solid; m.p. 164-166 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1 H), 8.02 (d, J = 9.1 Hz, 1 H), 7.50-7.33 (m, 7 H), 3.96 (s, 3 H), 3.80 (t, J = 4.4 Hz, 4 H), 2.94 (t, J = 4.1 Hz, 4 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.9, 151.4, 150.9, 144.9, 138.7, 131.4, 129.9, 129.5, 128.5, 127.7, 121.1, 102.4, 67.6, 55.5, 52.4; HRMS m/z calcd for $C_{20}H_{20}N_2O_2$ ($[M+H]^+$): 321.1598, found 321.1595.

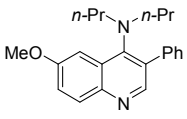


6-methoxy-*N*,*N*-dimethyl-3-phenylquinolin-4-amine **4p** (14 mg, yield 52%): yellow solid; m.p. 47-50 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1 H), 8.01 (d, J = 9.1 Hz, 1 H), 7.49-7.32 (m, 7 H), 3.97 (s, 3 H), 2.77 (s, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.5, 153.1, 151.1, 144.6, 139.1, 130.9, 129.6, 128.8, 128.7, 128.4, 127.3, 121.0, 103.2, 55.5, 44.3; HRMS m/z calcd for $C_{18}H_{18}N_2O$ ($[M+H]^+$): 279.1492, found 279.1488.

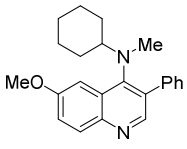


N,*N*-diethyl-6-methoxy-3-phenylquinolin-4-amine **4q** (15 mg, yield 49%): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1 H), 8.00 (d, J = 9.1 Hz, 1 H), 7.51-7.33 (m, 7 H), 3.96 (s, 3 H), 3.01 (q, J = 7.1 Hz, 4 H), 1.04 (t, J = 7.1 Hz, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.6, 151.5, 151.0, 139.1, 130.9, 129.8,

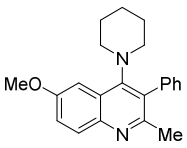
129.6, 128.9, 128.3, 127.4, 121.1, 103.4, 55.5, 47.1, 14.2; HRMS m/z calcd for $C_{20}H_{22}N_2O$ ($[M+H]^+$): 307.1805, found 307.1797.



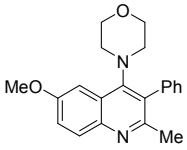
6-methoxy-3-phenyl-*N,N*-dipropylquinolin-4-amine **4r** (15 mg, yield 48%): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1 H), 8.00 (dd, J = 9.0 Hz, 3.9 Hz, 1 H), 7.55-7.32 (m, 7 H), 3.95 (s, 3 H), 2.89 (t, J = 7.6 Hz, 4 H), 1.49-1.46 (m, 4 H), 0.78 (t, J = 7.4 Hz, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.5, 151.7, 151.1, 145.1, 139.3, 131.0, 130.6, 129.6, 128.6, 128.3, 127.4, 121.1, 103.4, 55.5, 55.5, 22.1, 11.6; HRMS m/z calcd for $C_{22}H_{26}N_2O$ ($[M+H]^+$): 335.2118, found 335.2121.



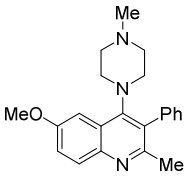
N-cyclohexyl-6-methoxy-*N*-methyl-3-phenylquinolin-4-amine **4s** (18 mg, yield 52%): yellow solid; m.p. 113-115 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1 H), 8.01 (d, J = 9.0 Hz, 1 H), 7.47-7.32 (m, 7 H), 3.94 (s, 3 H), 3.65-3.58 (m, 1 H), 2.80 (s, 3 H), 1.66-1.60 (m, 5 H), 1.52-1.42 (m, 1 H), 1.05-1.04 (m, 4 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.5, 152.2, 150.6, 144.9, 139.2, 131.2, 130.7, 129.7, 129.0, 128.2, 127.3, 121.1, 103.4, 60.5 55.4, 38.2, 31.0, 25.7, 25.1; HRMS m/z calcd for $C_{23}H_{26}N_2O$ ($[M+H]^+$): 347.2118, found 347.2115.



6-methoxy-2-methyl-3-phenyl-4-(piperidin-1-yl)quinoline **4t** (16 mg, yield 58%): yellow solid; m.p. 128-131 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 9.1 Hz, 1 H), 7.48–7.40 (m, 4 H), 7.32–7.21 (m, 3 H), 3.95 (s, 3 H), 3.04–2.81 (m, 1 H), 2.50-2.02 (m, 3 H), 2.35 (s, 3 H), 1.80–1.39 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.1, 156.7, 153.3, 144.1, 139.3, 130.5, 130.2, 130.0, 128.2, 127.2, 126.3, 120.8, 102.7, 55.4, 53.3, 26.9, 24.8, 24.2; HRMS m/z calcd for $C_{22}H_{24}N_2O$ ($[M+H]^+$): 333.1961, found 333.1958.

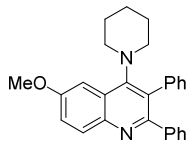


4-(6-methoxy-2-methyl-3-phenylquinolin-4-yl)morpholine **4u** (15 mg, yield 49%): yellow solid; m.p. 145-147 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.7 Hz, 1 H), 7.50–7.43 (m, 4 H), 7.35 (dd, J = 9.1 Hz, 2.7 Hz, 1 H), 7.26–7.22 (m, 2 H), 3.95 (s, 3 H), 3.72–3.66 (m, 4 H), 2.87-2.77 (m, 4 H), 2.37 (s, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.4, 156.7, 138.5, 131.1, 130.9, 130.5, 130.2, 128.8, 128.5, 127.7, 125.9, 121.1, 102.5, 67.6, 65.5, 55.4, 52.2; HRMS m/z calcd for $C_{21}H_{22}N_2O_2$ ($[M+H]^+$): 335.1754, found 335.1760.

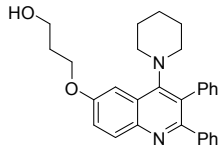


6-methoxy-2-methyl-4-(4-methylpiperazin-1-yl)-3-phenylquinoline **4v** (14 mg, yield 41%): yellow solid; m.p. 138-141 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 9.1 Hz, 1 H), 7.47–7.20 (m, 7 H), 3.94 (s, 3 H), 2.99-2.90 (m, 4 H), 2.69-2.48 (m, 4 H), 2.34 (s, 3 H), 2.28 (s, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.2, 156.8, 152.0, 144.2, 138.8, 130.4, 130.2, 129.5, 128.5, 127.4, 127.2, 120.8, 102.7, 55.9,

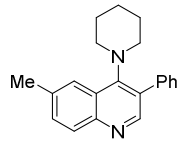
55.4, 51.6, 46.3, 24.8; HRMS m/z calcd for $C_{22}H_{25}N_3O$ ([M+H]$^+$): 348.2070, found 348.2070.



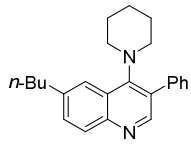
6-methoxy-2,3-diphenyl-4-(piperidin-1-yl)quinoline **4w** (17 mg, yield 44%): yellow solid; m.p. 160-162 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 9.1 Hz, 1 H), 7.54 (d, J = 2.7 Hz, 1 H), 7.37-7.34 (m, 1 H), 7.25–7.03 (m, 10 H), 3.99 (s, 3 H), 3.20-3.12 (m, 2 H), 2.50–2.26 (m, 2 H), 1.72-1.60 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 158.6, 157.6, 153.9, 144.4, 141.5, 138.7, 131.5, 131.4, 129.5, 129.3, 127.6, 127.3, 126.9, 126.7, 121.2, 102.4, 55.5, 53.2, 26.9, 24.2; HRMS m/z calcd for $C_{27}H_{26}N_2O$ ([M+H]$^+$): 395.2118, found 395.2123.



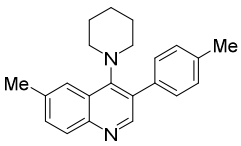
3-((2,3-diphenyl-4-(piperidin-1-yl)quinolin-6-yl)oxy)propan-1-ol **4x** (16 mg, yield 41%): yellow solid; m.p. 190-192 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 9.1 Hz, 1 H), 7.54 (d, J = 2.8 Hz, 1 H), 7.34 (dd, J = 9.1 Hz, 2.8 Hz, 1 H), 7.26–7.04 (m, 10 H), 4.30 (t, J = 5.8 Hz, 2 H), 3.94 (t, J = 5.9 Hz, 2 H), 3.39–2.85 (m, 2 H), 2.43–2.39 (m, 2 H), 2.19–2.13 (m, 2 H), 1.74–1.48 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 158.6, 156.8, 154.0, 144.3, 141.3, 138.6, 131.5, 131.3, 129.6, 129.5, 127.6, 127.3, 127.0, 126.8, 126.4, 121.5, 103.2, 65.7, 60.2, 53.2, 32.0, 26.9, 24.2; HRMS m/z calcd for $C_{29}H_{30}N_2O_2$ ([M+H]$^+$): 439.2380, found 439.2378.



6-methyl-3-phenyl-4-(piperidin-1-yl)quinoline **8a** (23 mg, yield 74%): yellow solid; m.p. 163-165 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1 H), 7.97 (d, J = 8.5 Hz, 1 H), 7.95 (s, 1 H), 7.51-7.31 (m, 6 H), 3.05-2.75 (m, 4 H), 2.58 (s 3 H), 1.67-1.57 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 153.3, 153.0, 147.4, 139.5, 135.5, 130.9, 130.0, 129.5, 128.4, 128.2, 127.2, 126.2, 123.2, 53.9, 26.6, 24.3, 22.1; HRMS m/z calcd for $C_{21}H_{22}N_2$ ([M+H]$^+$): 303.1856, found 303.1855.

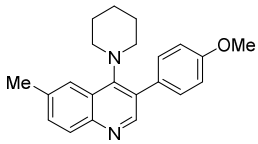


6-butyl-3-phenyl-4-(piperidin-1-yl)quinoline **8b** (15 mg, yield 44%): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1 H), 7.99 (d, J = 8.5 Hz, 1 H), 7.95 (d, J = 1.3 Hz, 1 H), 7.53-7.30 (m, 6 H), 2.94-2.82 (m, 4 H), 2.84 (t, J = 7.66 Hz, 2 H), 1.76-1.59 (m, 8 H), 1.46-1.38 (m, 2 H), 0.98 (t, J = 7.3 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 153.5, 152.8, 147.2, 145.6, 140.4, 139.5, 130.4, 130.0, 129.2, 128.2, 127.2, 126.0, 122.6, 53.9, 35.9, 33.3, 26.6, 24.3, 22.2, 13.9; HRMS m/z calcd for $C_{24}H_{28}N_2$ ([M+H]$^+$): 345.2325, found 345.2331.

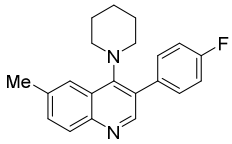


6-methyl-4-(piperidin-1-yl)-3-(*p*-tolyl)quinoline **8c** (17 mg, yield 54%): yellow solid; m.p. 128-130 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1 H), 7.96 (d, J = 8.7 Hz, 1 H), 7.94 (s, 1 H), 7.49 (dd, J = 8.4Hz, 1.4 Hz, 1 H), 7.26 (d, J = 7.7 Hz, 2 H), 7.20 (d, J = 7.9 Hz, 2 H), 3.03-2.80 (m, 4 H), 2.58 (s, 3 H), 2.44 (s, 3 H), 1.67-1.58 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 153.2, 147.3, 136.9, 136.5,

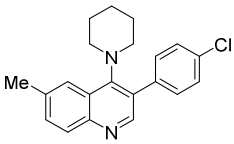
135.5, 130.8, 129.8, 129.4, 129.2, 128.9, 128.4, 126.2, 123.2, 53.8, 26.6, 24.3, 22.1, 21.2; HRMS m/z calcd for $C_{22}H_{24}N_2$ ($[M+H]^+$): 317.2012, found 317.2010.



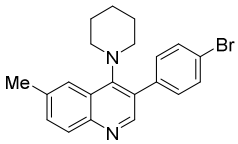
3-(4-methoxyphenyl)-6-methyl-4-(piperidin-1-yl)quinoline **8d** (24 mg, yield 72%): yellow solid; m.p. 149-153°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1 H), 7.98–7.94 (m, 2 H), 7.49 (d, J = 8.2 Hz, 1 H), 7.23 (d, J = 8.5 Hz, 2 H), 7.00 (d, J = 8.5 Hz, 2 H), 3.89 (s, 3 H), 2.89-2.88 (m, J = 5.8 Hz, 4H), 2.58 (s, 3H), 1.68–1.59 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 158.9, 153.2, 147.2, 135.5, 131.7, 131.0, 130.8, 130.0, 129.4, 128.2, 126.2, 123.2, 113.6, 55.3, 53.8, 26.6, 24.3, 22.1; HRMS m/z calcd for $C_{22}H_{24}N_2O$ ($[M+H]^+$): 332.1889, found 332.1893.



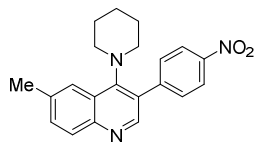
3-(4-fluorophenyl)-6-methyl-4-(piperidin-1-yl)quinoline **8e** (21 mg, yield 68%): yellow solid; m.p. 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1 H), 7.97 (d, J = 8.5 Hz, 1 H), 7.93 (s, 1 H), 7.51 (dd, J = 8.5 Hz, 1.5 Hz, 1 H), 7.27 (td, J = 8.5 Hz, 2.2 Hz, 2 H), 7.15 (t, J = 8.6 Hz, 2 H), 3.03-2.73 (m, 4 H), 2.58 (s, 3 H), 1.68-1.59 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 162.2 (d, J (C,F) = 246.5 Hz), 153.5, 152.7, 147.3, 135.7, 135.4, 131.5(d, J(C,F) = 7.9 Hz), 131.1, 129.4, 127.4, 126.1, 123.2, 115.2 (d, J (C,F) = 21.4 Hz), 53.9, 26.5, 24.3, 22.1; HRMS m/z calcd for $C_{21}H_{21}FN_2$ ($[M+H]^+$): 321.1762, found 321.1754.



3-(4-chlorophenyl)-6-methyl-4-(piperidin-1-yl)quinoline **8f** (23 mg, yield 70%): yellow solid; m.p. 103-105 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1 H), 7.96 (d, J = 8.5 Hz, 1 H), 7.93 (s, 1 H), 7.50 (dd, J = 8.5 Hz, 1.8 Hz, 1 H), 7.43 (d, J = 8.3 Hz, 2 H), 7.24 (d, J = 8.3 Hz, 2 H), 3.10-2.68 (m, 4 H), 2.58 (s, 3 H), 1.70-1.60 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 153.4, 152.5, 147.5, 138.0, 135.7, 133.4, 131.2, 129.5, 128.4, 127.1, 126.0, 123.2, 54.0, 26.5, 24.3, 22.1; HRMS m/z calcd for $C_{21}H_{21}ClN_2$ ($[M+H]^+$): 337.1466, found 337.1465.

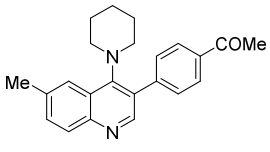


3-(4-bromophenyl)-6-methyl-4-(piperidin-1-yl)quinoline **8g** (26 mg, yield 69%): yellow solid; m.p. 148-149 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1 H), 7.96 (d, J = 8.5 Hz, 1 H), 7.93 (s, 1 H), 7.59 (d, J = 8.3 Hz, 2 H), 7.50 (dd, J = 8.5 Hz, 1.2 Hz, 1 H), 7.19 (d, J = 8.3 Hz, 2 H), 2.94-2.74 (m, 4 H), 2.58 (s, 3 H), 1.68-1.60 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 153.4, 152.5, 147.5, 138.5, 135.8, 131.6, 131.4, 131.2, 129.5, 127.1, 126.1, 123.2, 121.5, 54.0, 26.6, 24.3, 22.2; HRMS m/z calcd for $C_{21}H_{21}BrN_2$ ($[M+H]^+$): 381.0961, found 381.0963.

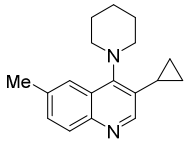


6-methyl-3-(4-nitrophenyl)-4-(piperidin-1-yl)quinoline **8h** (15 mg, yield 44%): yellow solid; m.p. 185-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1 H), 8.34 (d, J = 8.8 Hz, 2 H), 7.99-7.94 (m, 2 H), 7.56-7.48 (m, 3 H), 3.01-2.82 (m, 4 H), 2.59 (s, 3 H), 1.71-1.62 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 153.7, 151.8,

148.0, 147.1, 146.7, 136.1, 131.7, 130.7, 130.2, 129.7, 125.9, 123.6, 123.2, 54.3, 26.5, 24.2, 22.2; HRMS m/z calcd for $C_{21}H_{21}N_3O_2$ ($[M+H]^+$): 348.1707, found 348.1727.

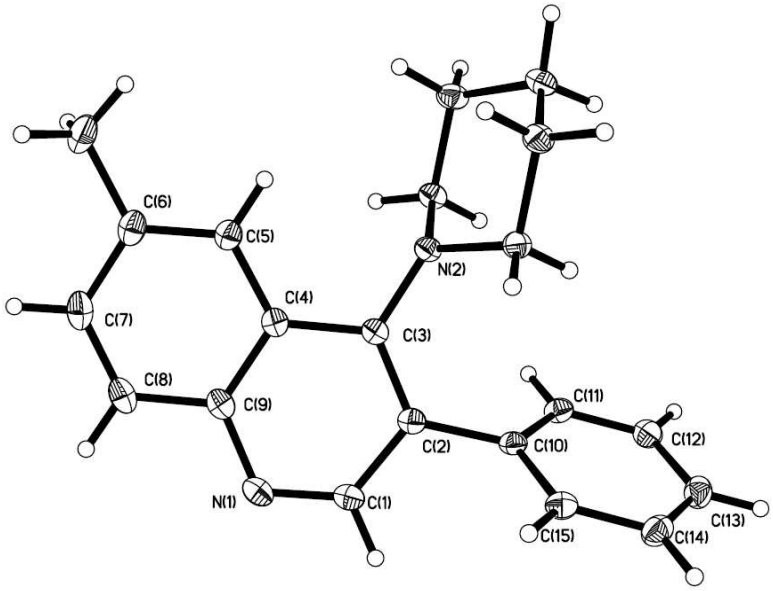


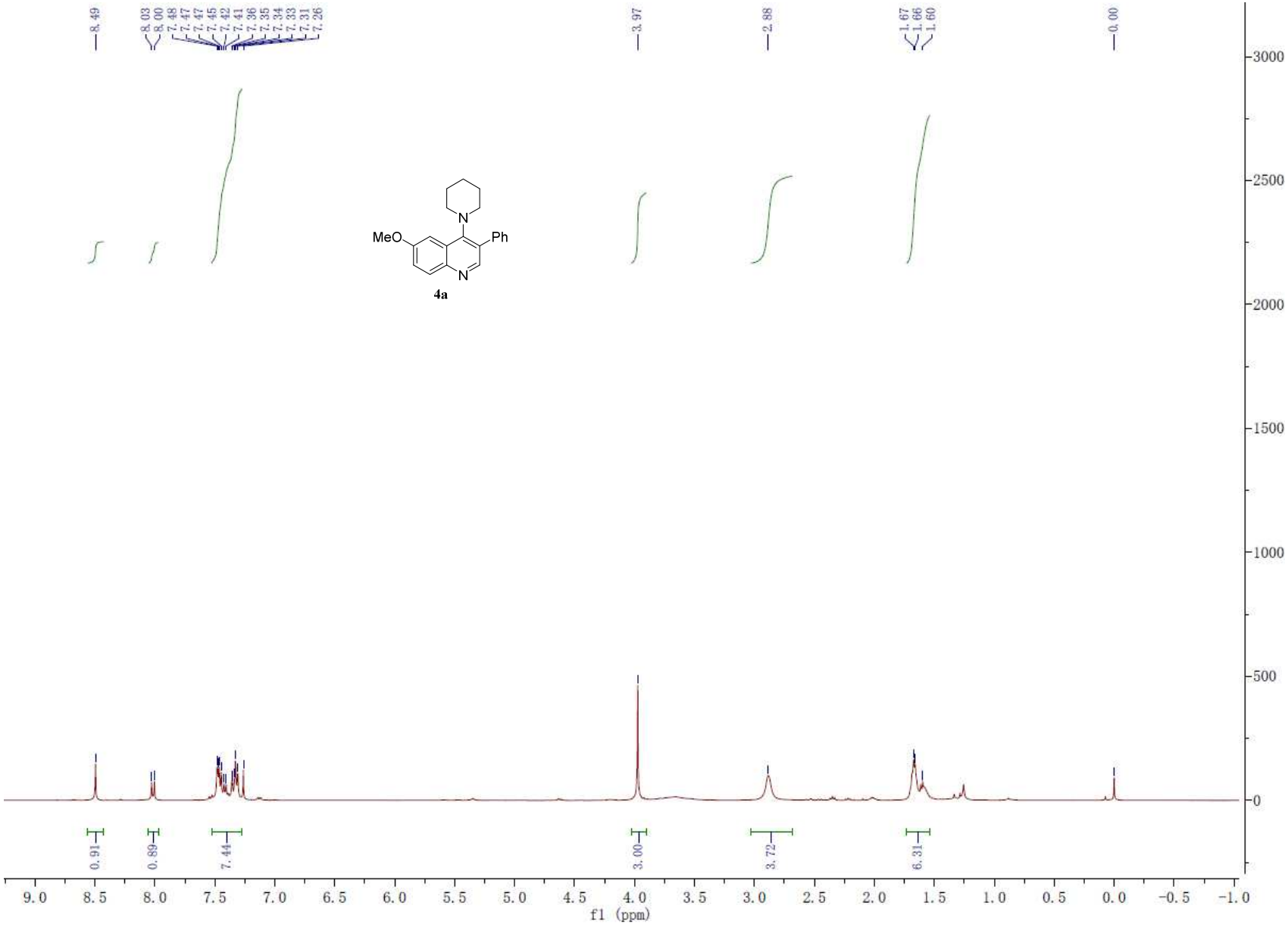
1-(4-(6-methyl-4-(piperidin-1-yl)quinolin-3-yl)phenyl)ethan-1-one **8i** (25 mg, yield 72%): light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1 H), 8.06 (d, J = 8.3 Hz, 2 H), 7.98 (d, J = 8.5 Hz, 1 H), 7.93 (s, 1 H), 7.52 (dd, J = 8.5 Hz, 1.8 Hz, 3 H), 7.42 (d, J = 8.3 Hz, 2 H), 2.94-2.88 (m, 4 H), 2.68 (s, 3 H), 2.59 (s, 3 H), 1.70-1.60 (m, 6 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 197.8, 160.9, 153.8, 152.0, 147.3, 144.6, 136.0, 131.5, 130.2, 129.3, 128.4, 127.0, 126.0, 123.3, 54.1, 29.7, 26.5, 24.3, 22.2; HRMS m/z calcd for $C_{23}H_{24}N_2O$ ($[M+H]^+$): 345.1961, found 345.1959.

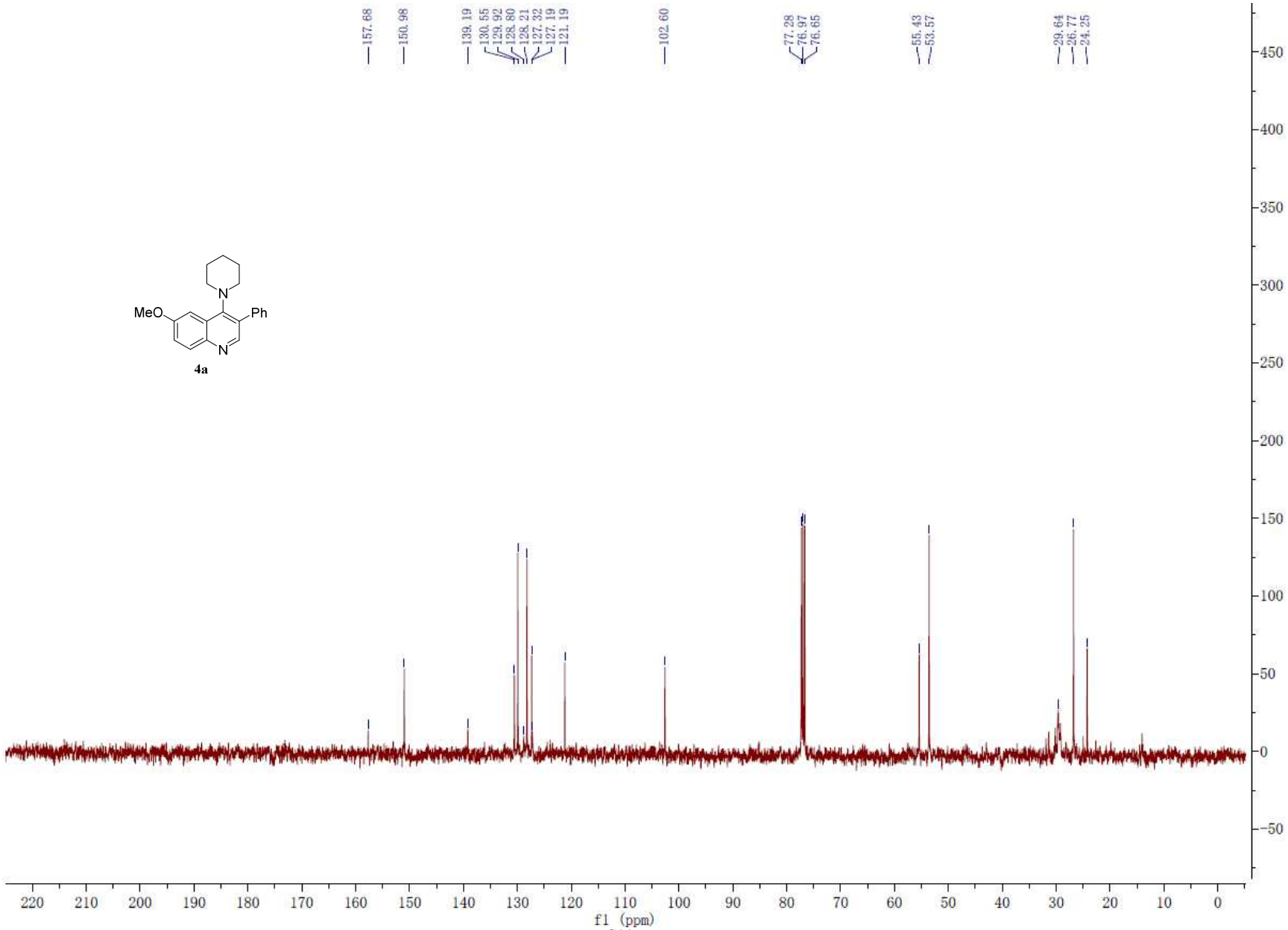


3-cyclopropyl-6-methyl-4-(piperidin-1-yl)quinoline **8j** (18 mg, yield 68%): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1 H), 7.92 (s, 1 H), 7.90 (d, J = 8.9 Hz, 1 H), 7.42 (dd, J = 8.5 Hz, 1.3 Hz, 1 H), 3.42-3.40 (m, 4 H), 2.55 (s, 3 H), 2.16-2.12 (m, 1 H), 1.81-1.75 (m, 6 H), 1.03 (d, J = 7.4 Hz, 2 H), 0.78 (d, J = 5.1 Hz, 2 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 155.9, 151.3, 146.8, 135.4, 130. 5, 129.2, 129.0, 126.5, 123.0, 52.6, 27.0, 24.6, 22.1, 12.4, 8.1; HRMS m/z calcd for $C_{18}H_{22}N_2$ ($[M+H]^+$): 267.1856, found 267.1846.

3. X-Ray Diffraction Structure of Compound 8a




8.49
8.03
8.00
7.48
7.47
7.47
7.45
7.42
7.41
7.36
7.35
7.34
7.33
7.31
7.26
3.97
2.88
1.67
1.66
1.60
0.00
MeO
Ph
N
N
4a
3000
2500
2000
1500
1000
500
0
0.91
0.89
7.44
3.00
3.72
6.31
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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127.32
127.19
121.19
102.60
77.28
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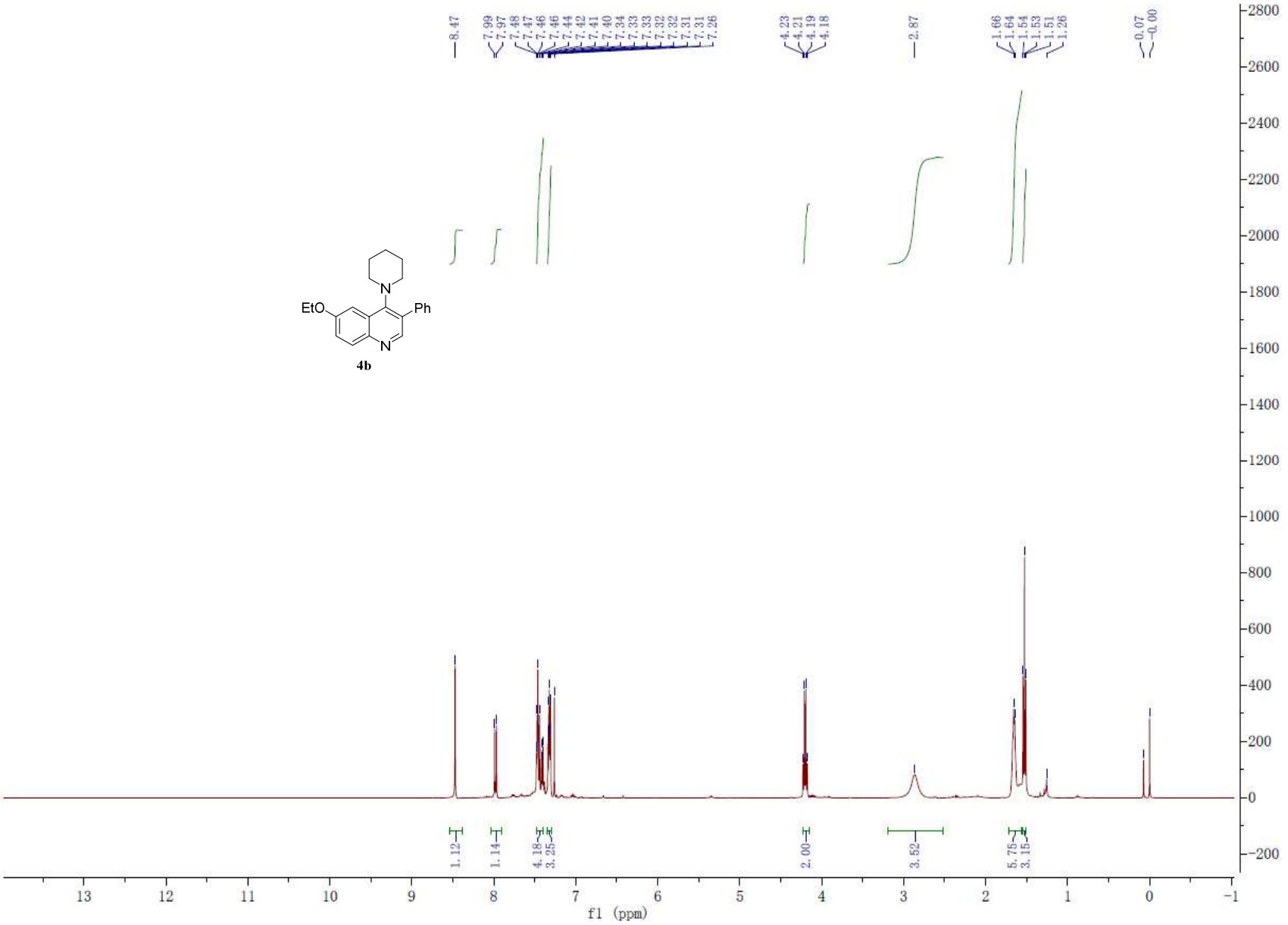
55.43
53.57
29.64
26.77
24.25
MeO
Ph
N
N
4a
f1 (ppm)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7.41
7.40
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.26
4.23
4.21
4.19
4.18
2.87
1.66
1.64
1.54
1.53
1.51
1.26
0.07
0.00
EtO
Ph
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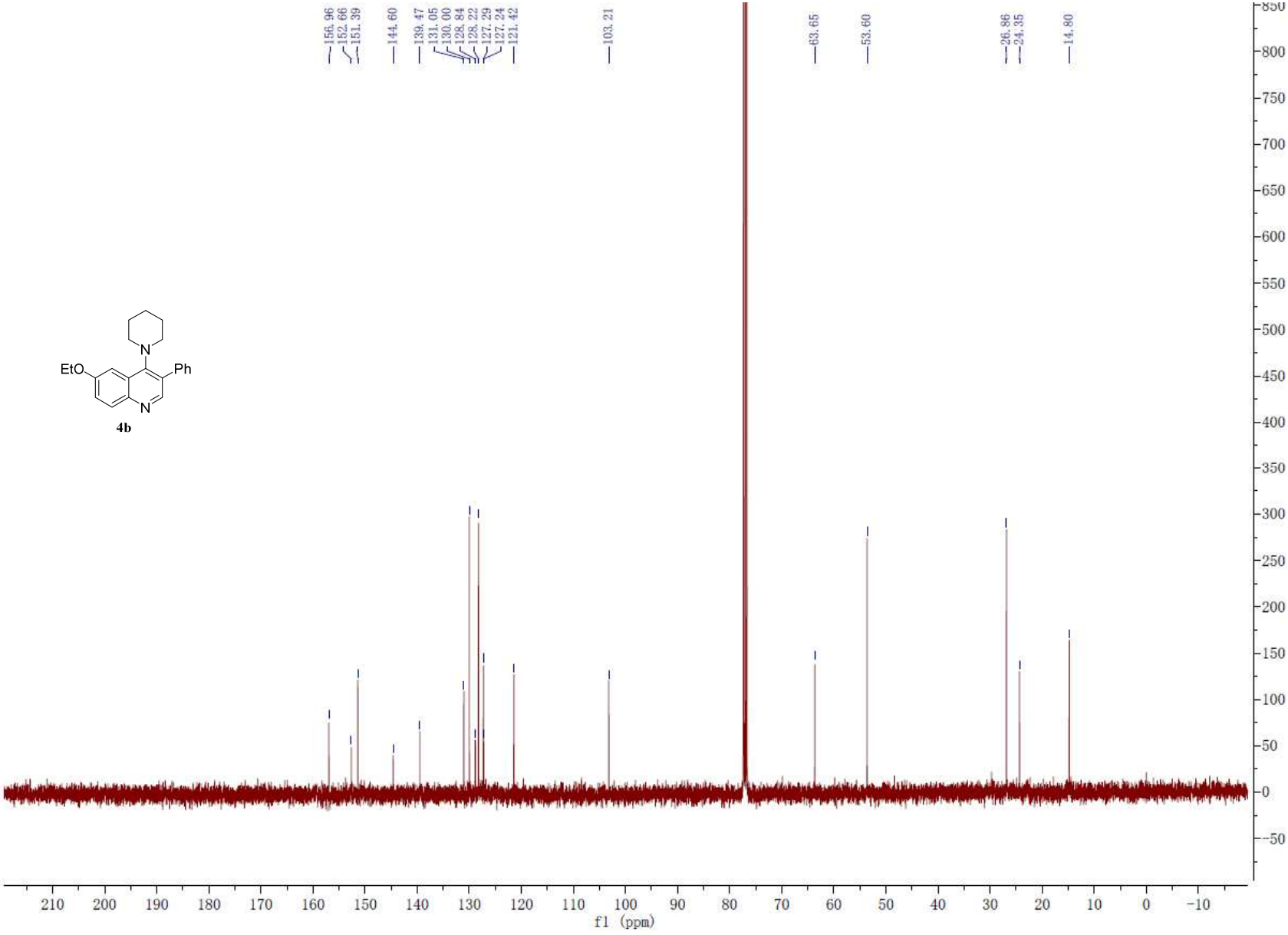
1.14
4.18
3.25
2.00
3.52
5.75
3.15
f1 (ppm)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127.29
127.24
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53.60
26.86
24.35
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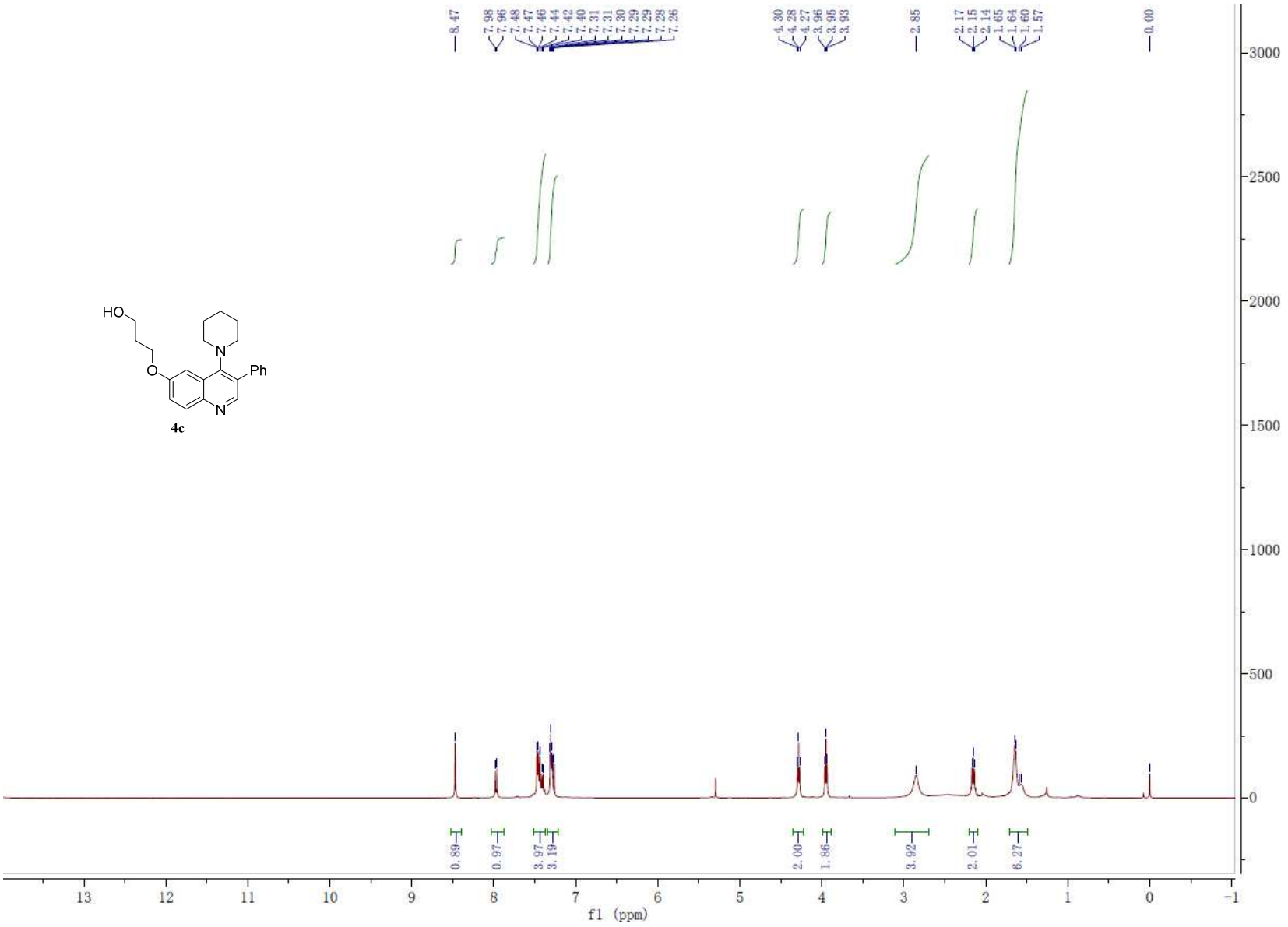
EtO
Ph
N
N
4b
f1 (ppm)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7.31
7.30
7.29
7.29
7.28
7.26
4.30
4.28
4.27
3.96
3.95
3.93
2.85
2.17
2.15
2.14
1.65
1.64
1.60
1.57
0.00
HO
O
N
N
Ph
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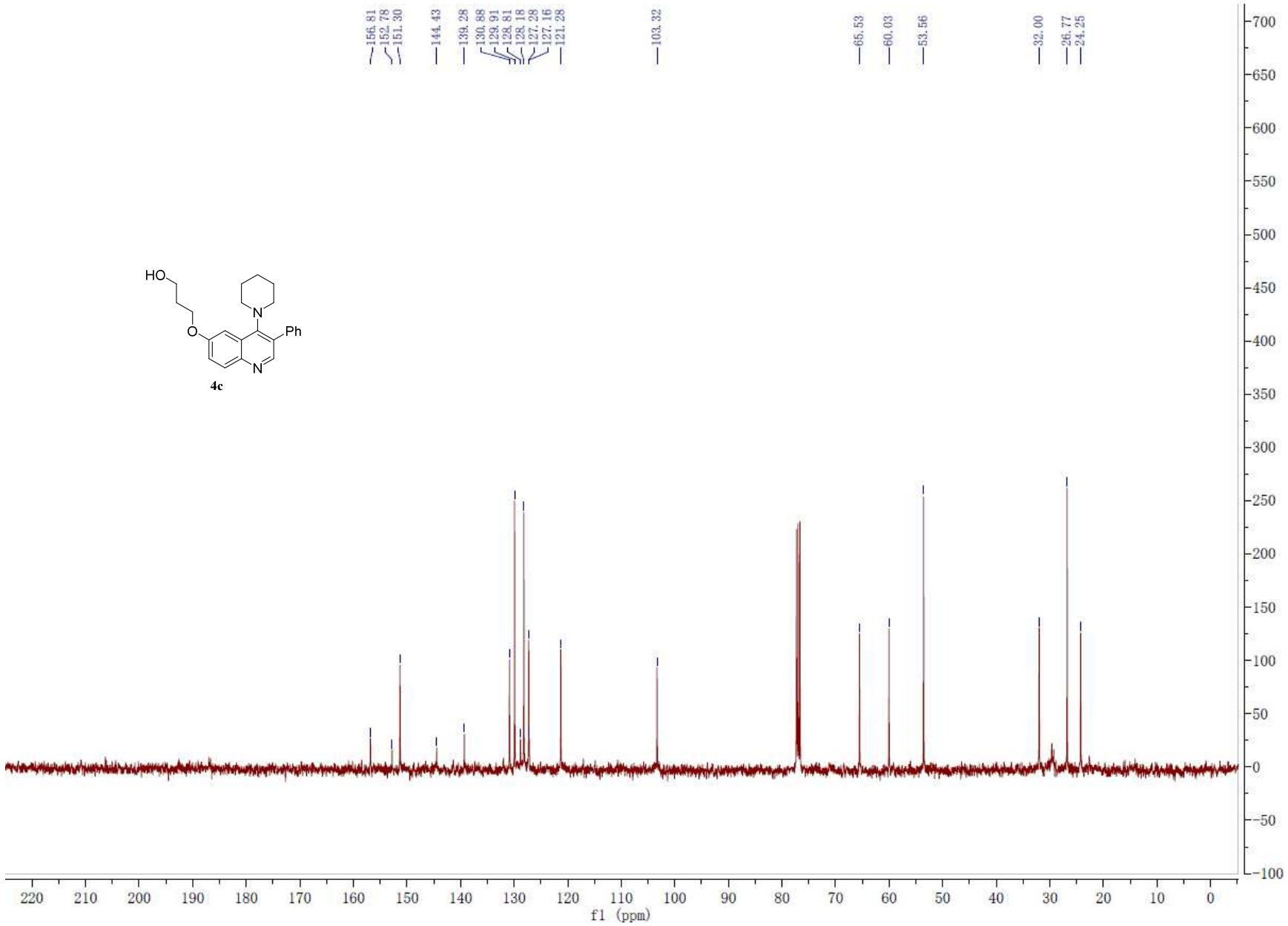
0.97
3.97
3.19
2.00
1.86
3.92
2.01
6.27
f1 (ppm)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127.16
121.28
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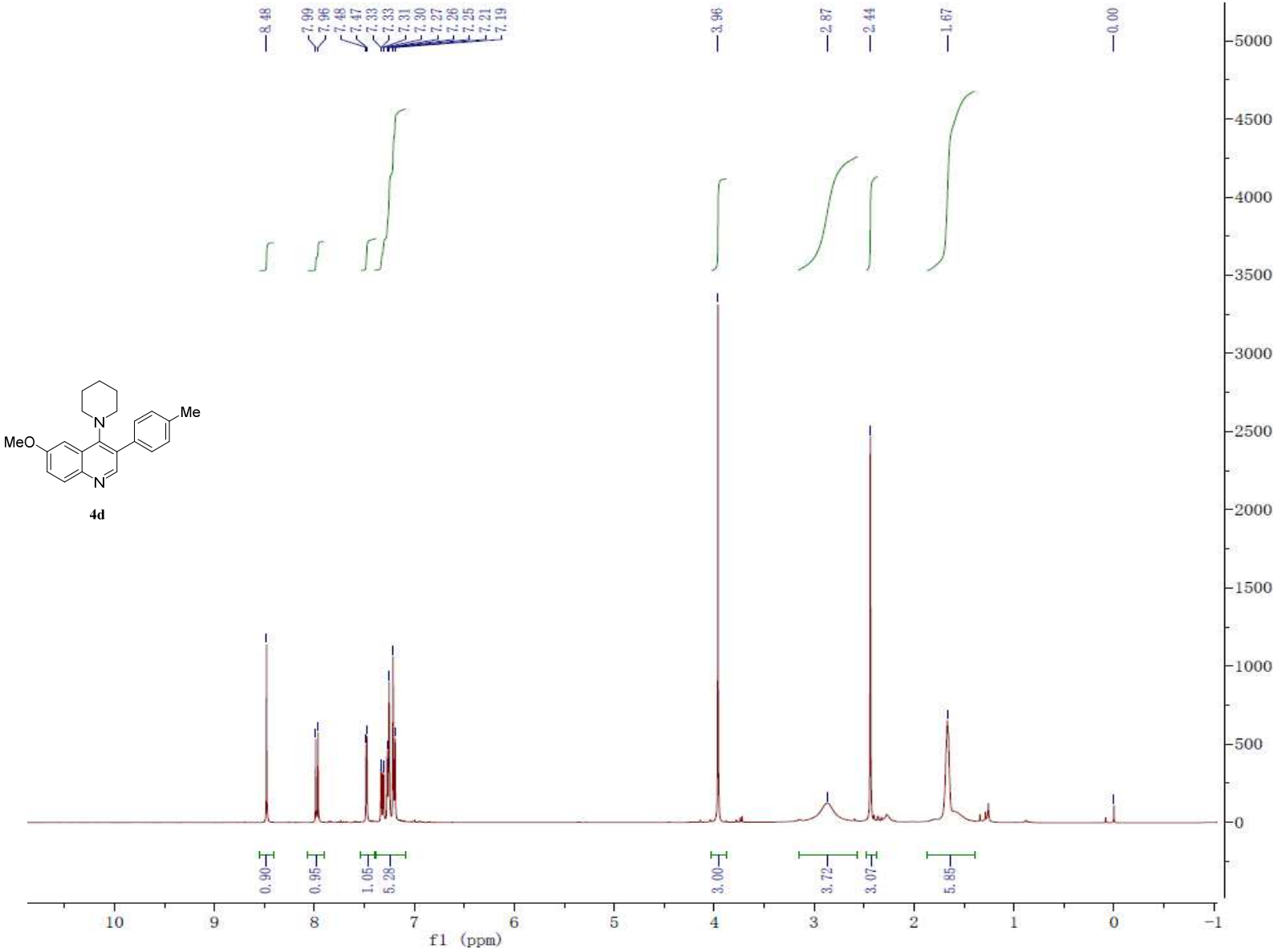
26.77
24.25
HO
O
N
N
Ph
4c
f1 (ppm)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7.27
7.26
7.25
7.21
7.19
3.96
2.87
2.44
1.67
0.00
MeO
Me
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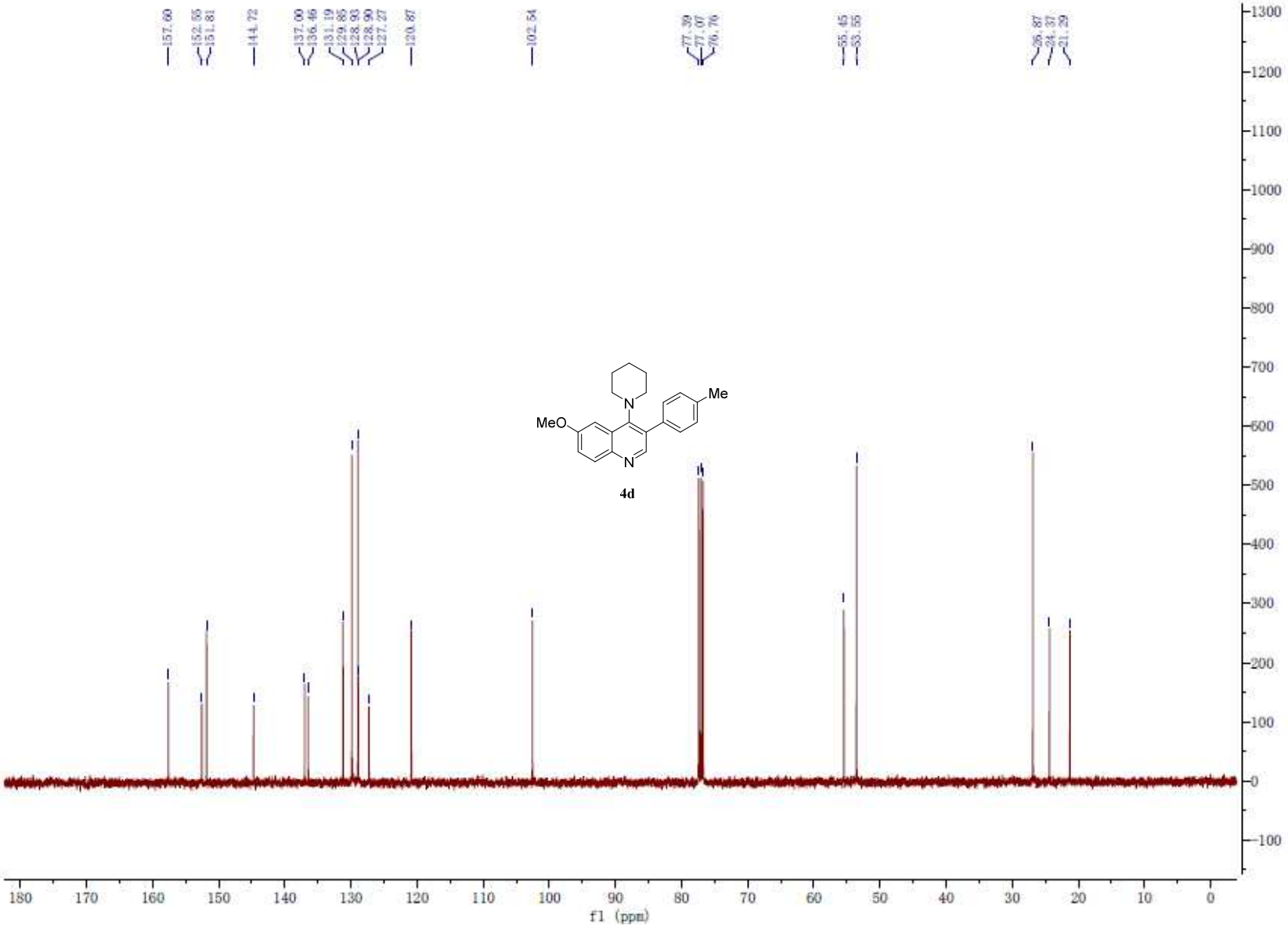
0.95
1.05
5.28
3.00
3.72
3.07
5.85
f1 (ppm)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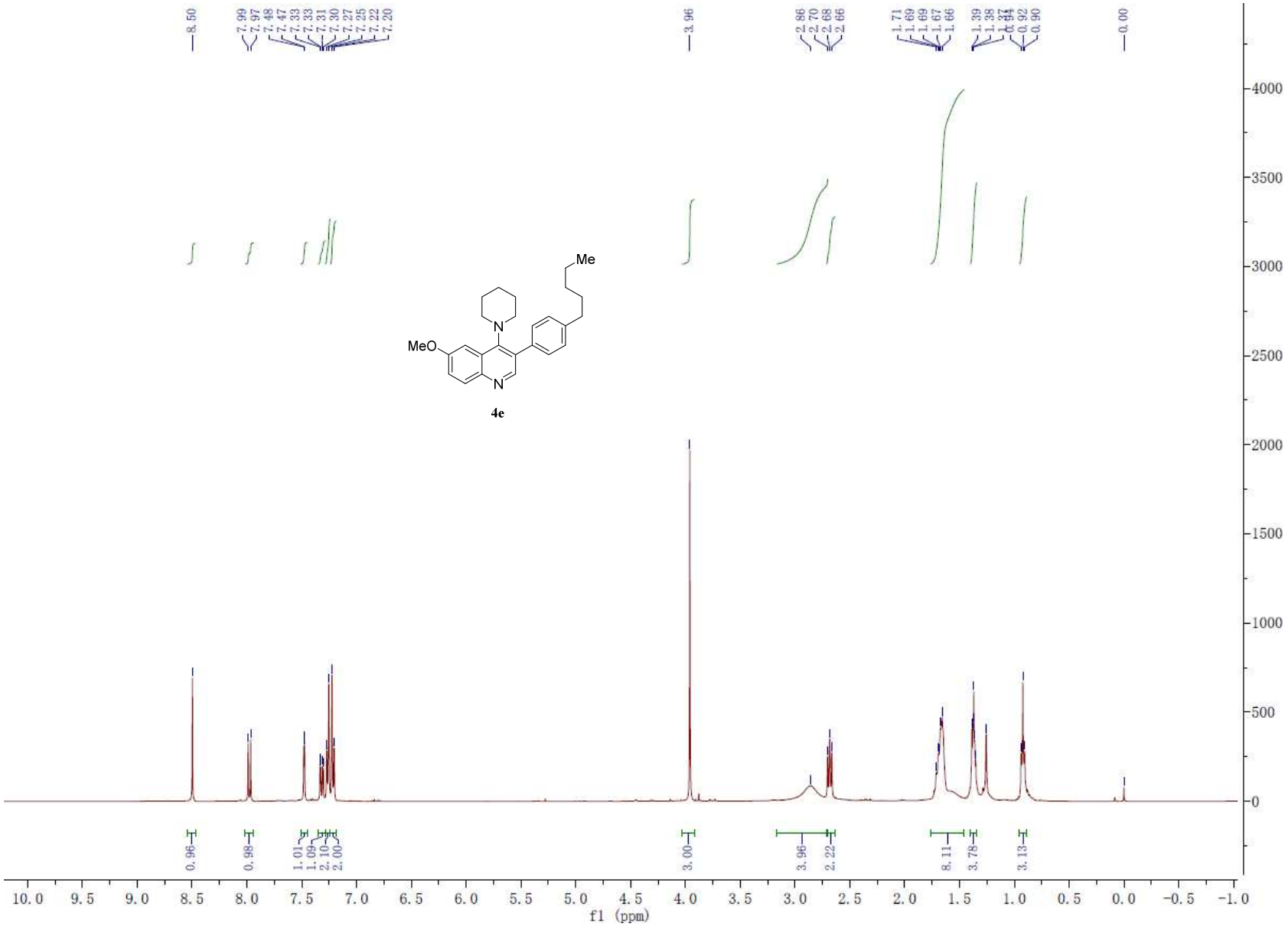
129.85
128.93
128.90
127.27
120.87
102.54
77.39
77.07
76.76
55.45
53.55
26.87
24.37
21.29
MeO
Me
N
N
4d
f1 (ppm)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7.31
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7.25
7.22
7.20
3.96
2.86
2.70
2.68
2.66
1.71
1.69
1.69
1.67
1.66
1.39
1.38
0.92
0.90
0.00
Me
MeO
N
N
4e
4000
3500
3000
2500
2000
1500
1000
500
0
0.96
0.98
1.01
1.09
2.10
2.00
3.00
3.96
2.22
8.11
3.78
3.13
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
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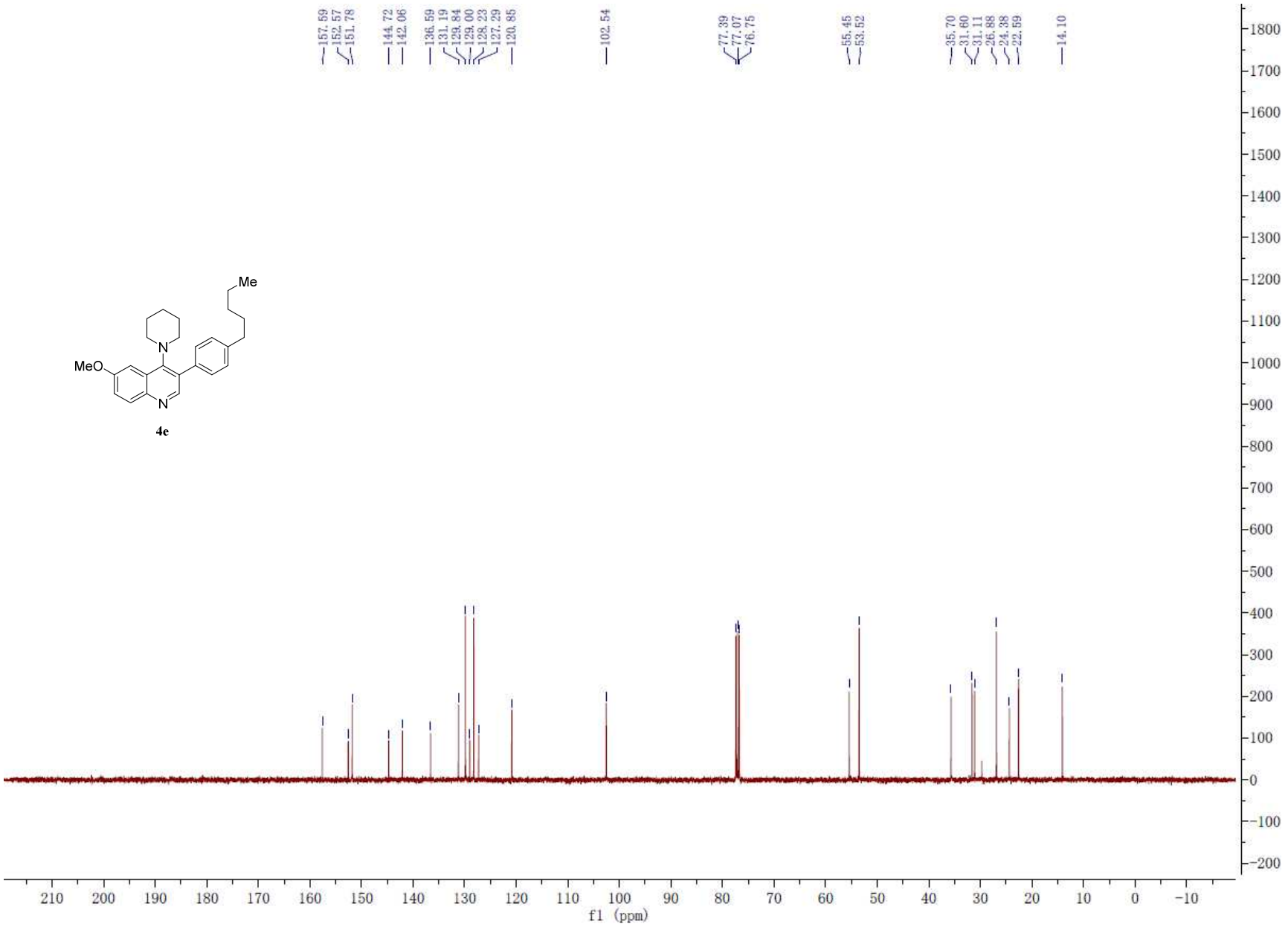
-1.0
f1 (ppm)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136.59
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129.84
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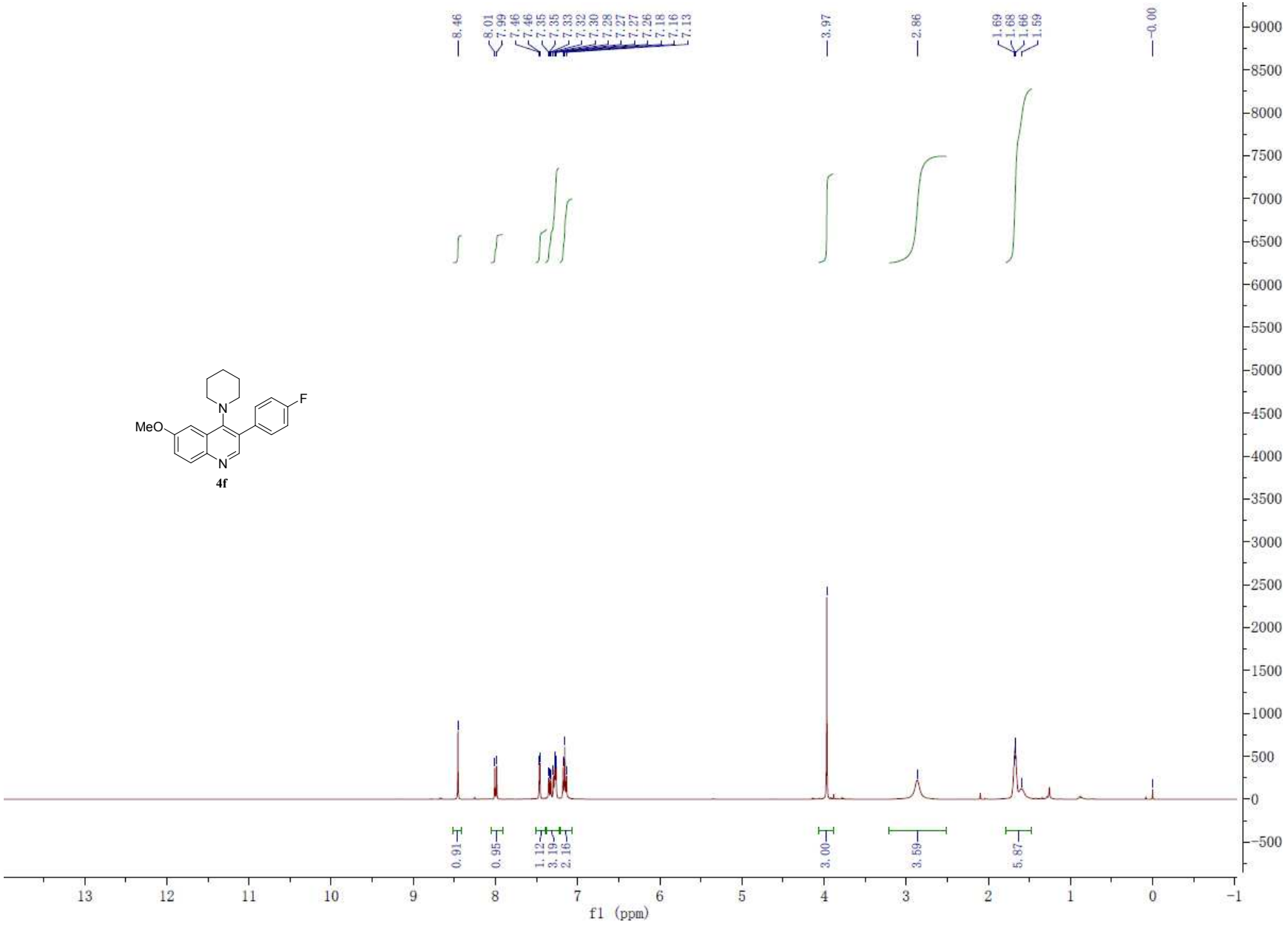
128.23
127.29
120.85
102.54
77.39
77.07
76.75
55.45
53.52
35.70
31.60
31.11
26.88
24.38
22.59
14.10
Me
MeO
N
N
f1 (ppm)

4e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7.28
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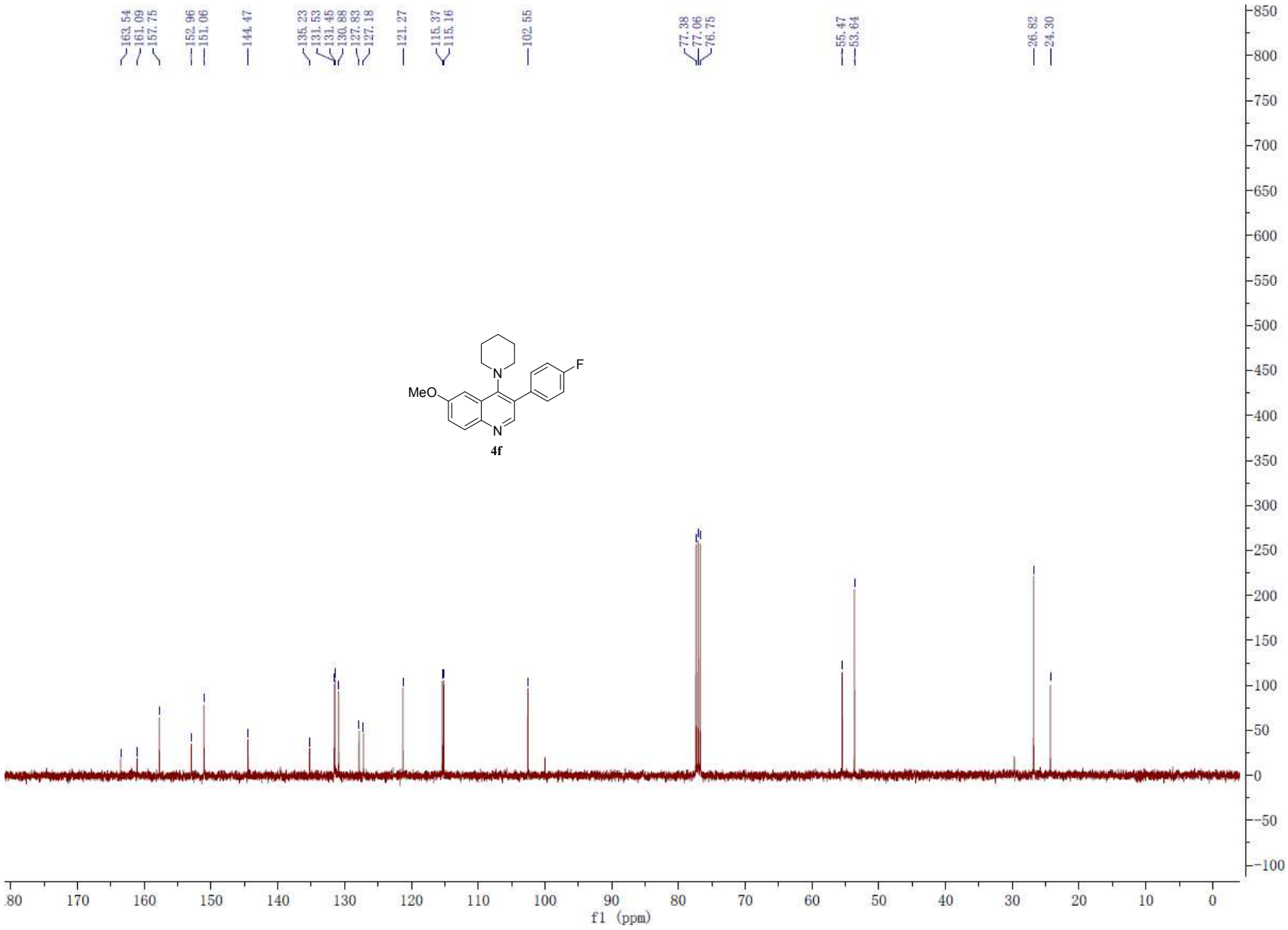
7.27
7.26
7.18
7.16
7.13
3.97
2.86
1.69
1.68
1.66
1.59
0.00
MeO
F
N
N
4f
0.91
0.95
1.12
3.19
2.16
3.00
3.59
5.87
f1 (ppm)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127.83
127.18
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115.37
115.16
102.55
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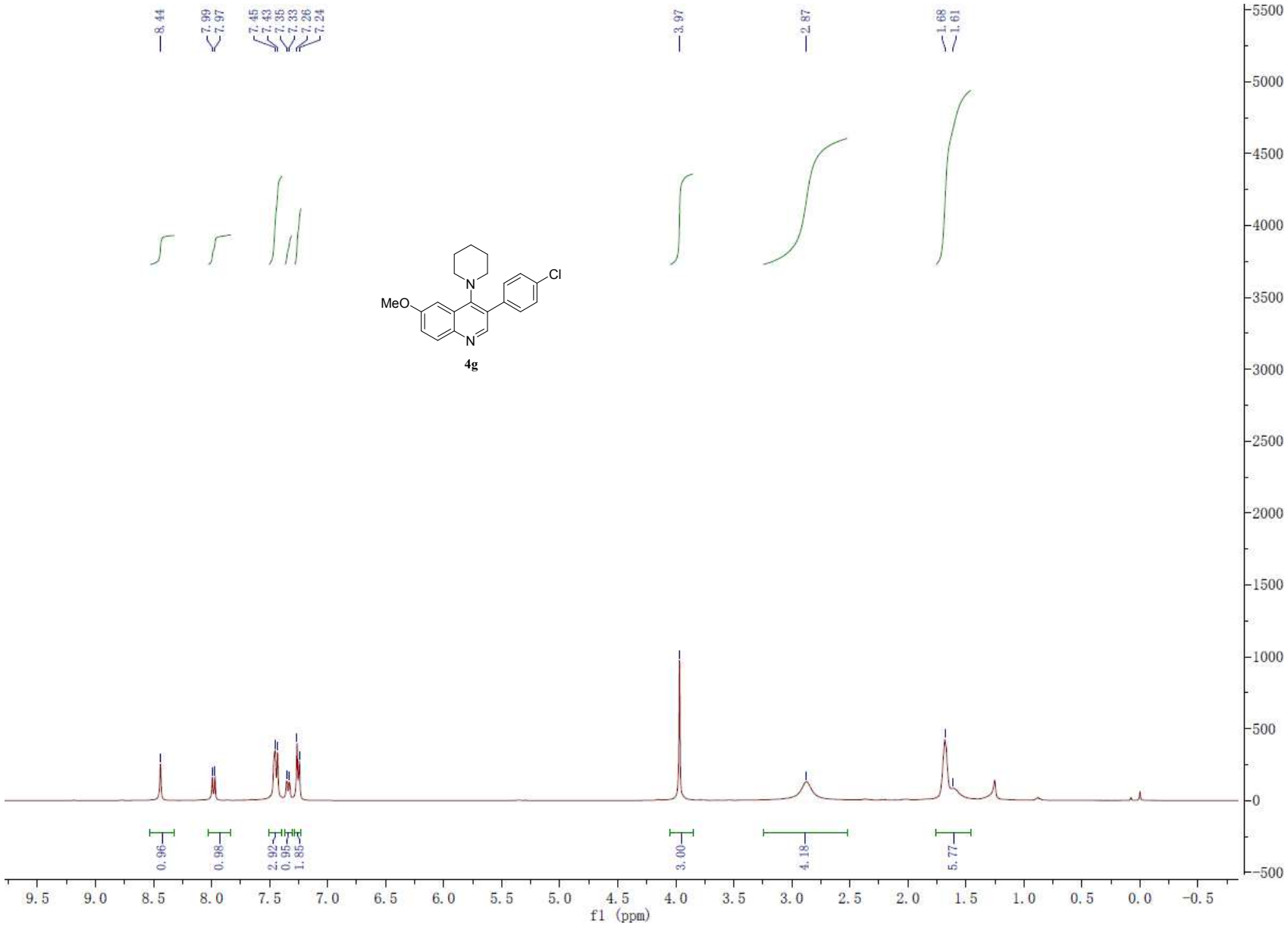
76.75
55.47
53.64
26.82
24.30
MeO
N
N
F
4f
f1 (ppm)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7.33
7.26
7.24
3.97
2.87
1.68
1.61
MeO
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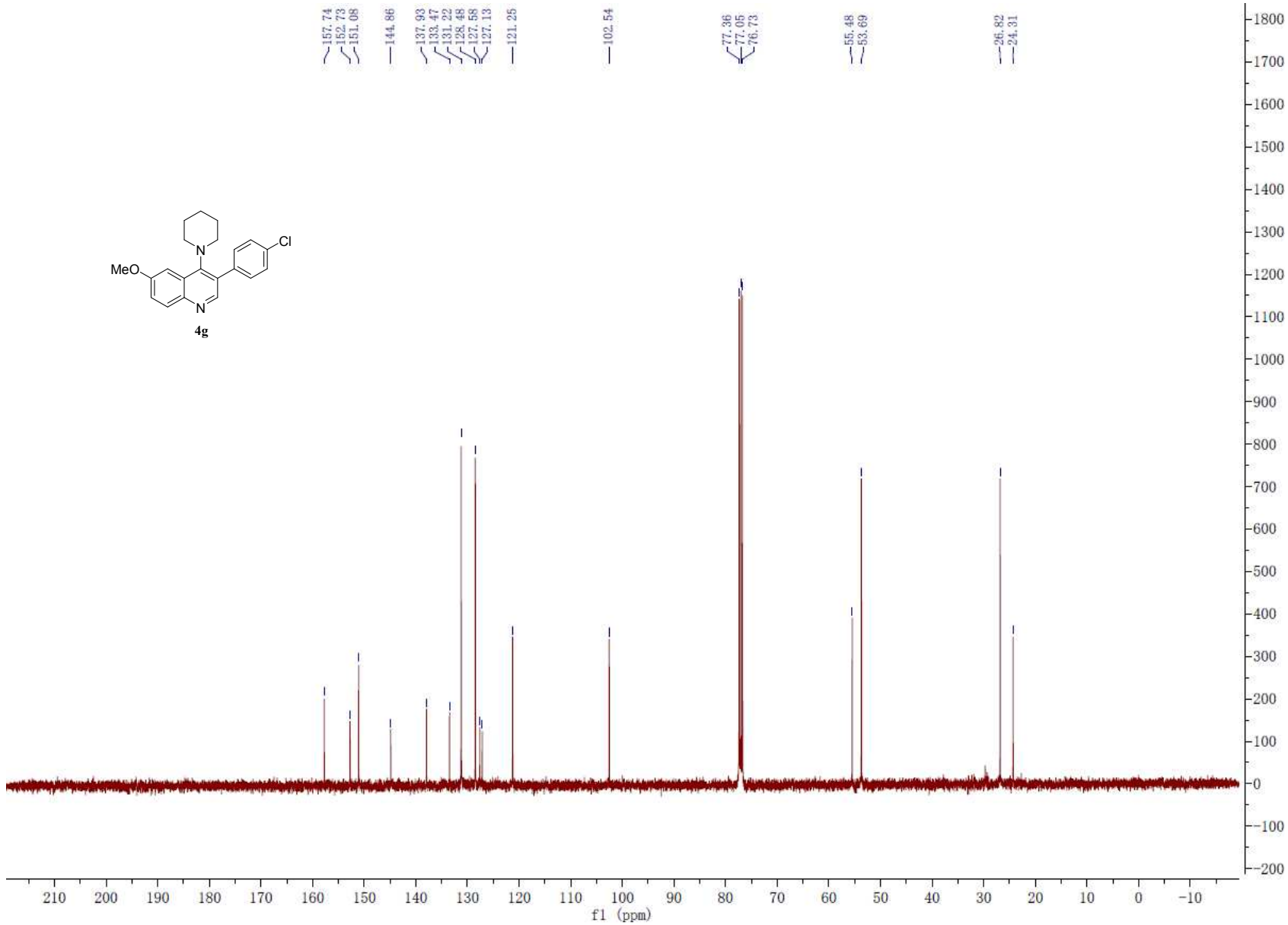
N
Cl
4g
0.96
0.98
2.92
0.95
1.85
3.00
4.18
5.77
f1 (ppm)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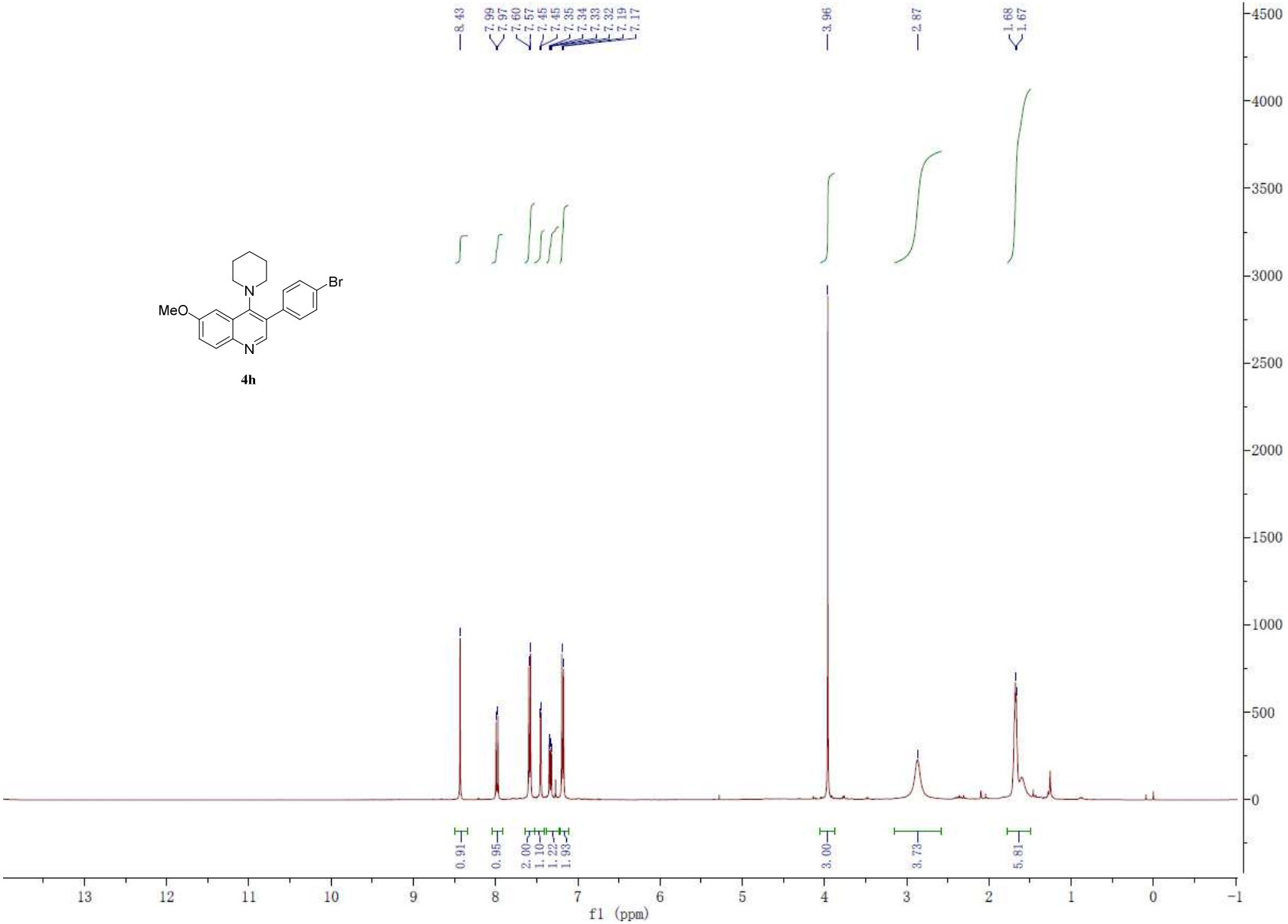
131.22
128.48
127.58
127.13
121.25
102.54
77.36
77.05
76.73
55.48
53.69
26.82
24.31
MeO
Cl
N
N
4g
f1 (ppm)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7.33
7.32
7.19
7.17
3.96
2.87
1.68
1.67
MeO
Br
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0.95
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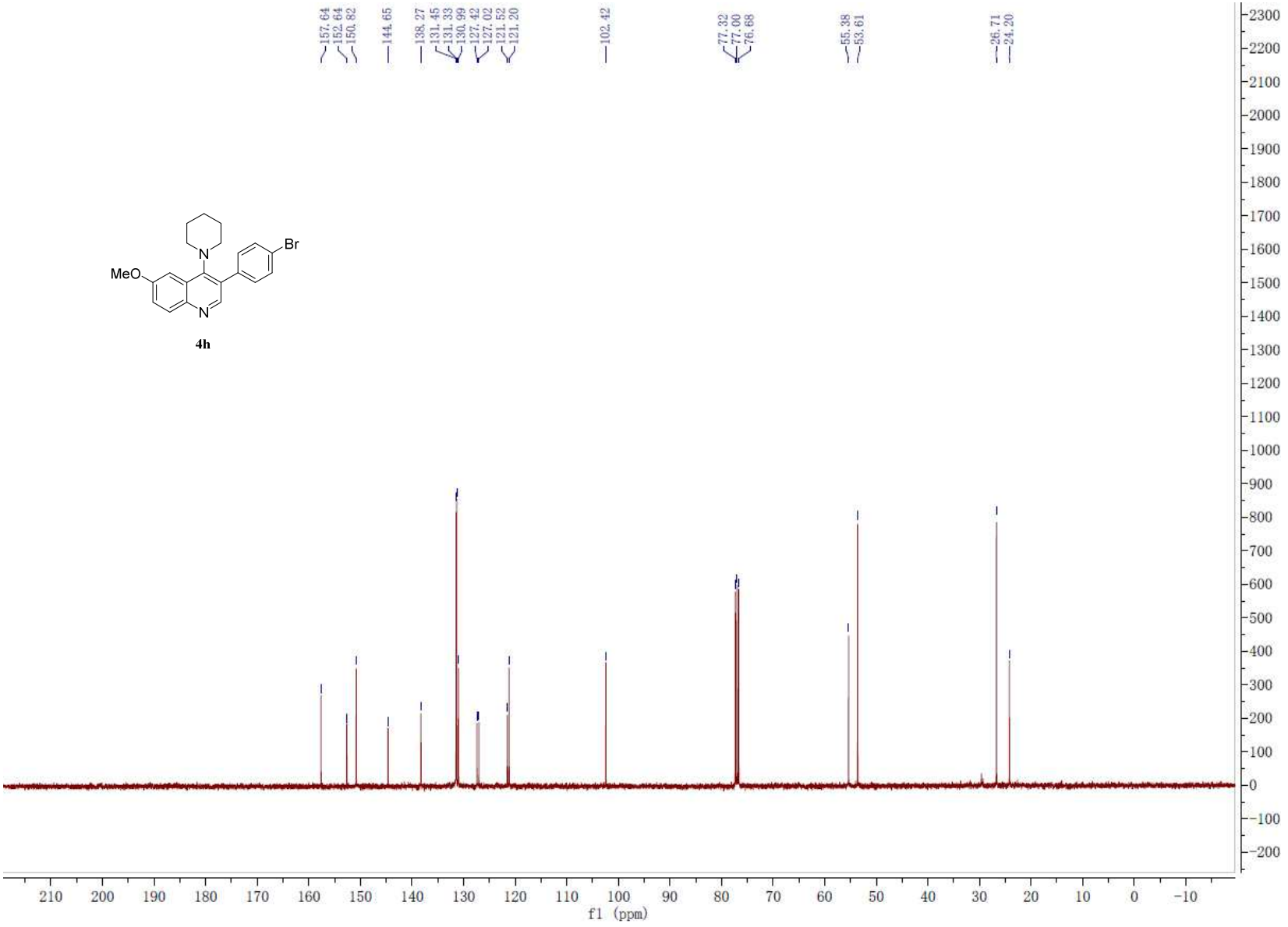
1.10
1.22
1.93
3.00
3.73
5.81
f1 (ppm)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127.02
121.52
121.20
102.42
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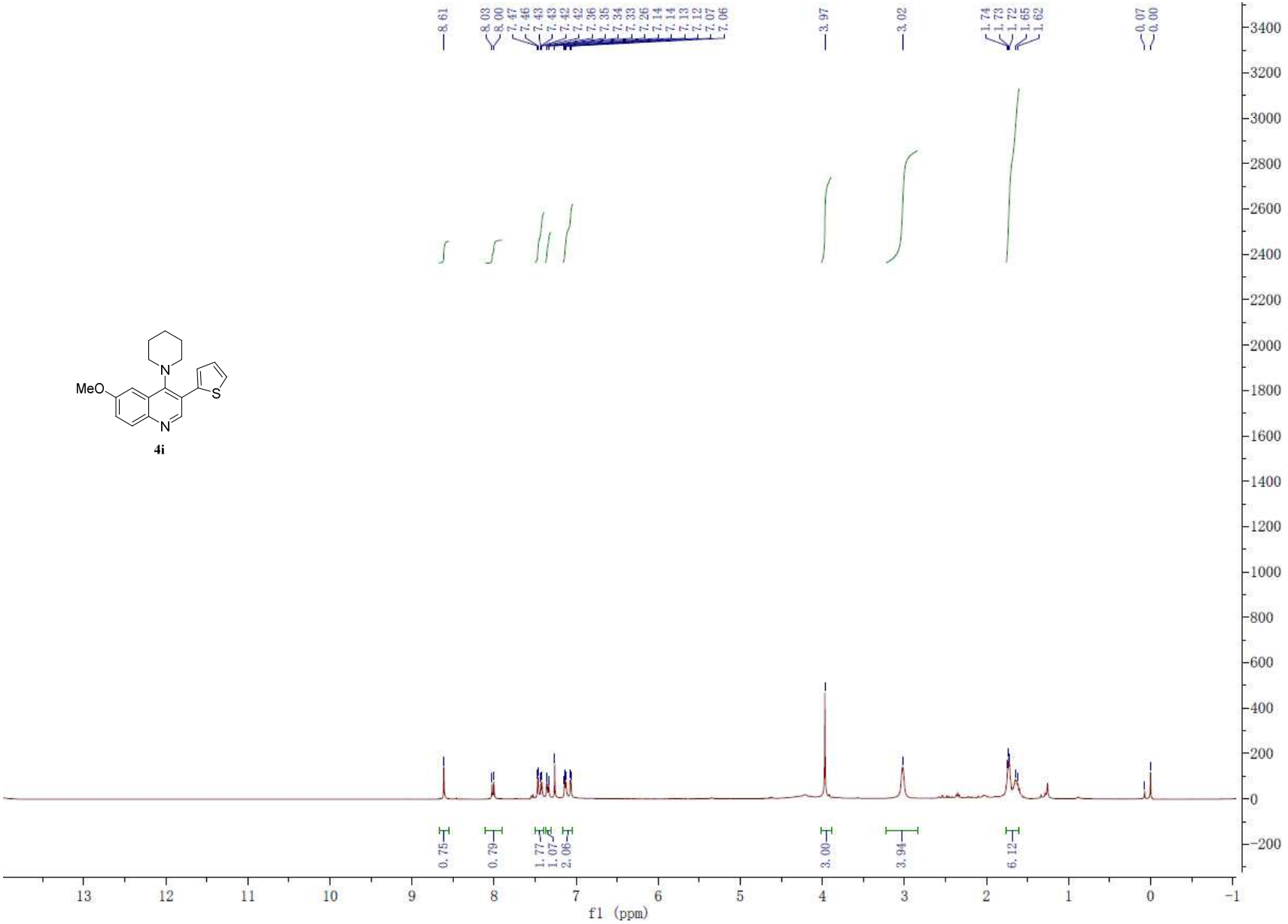
76.68
55.38
53.61
26.71
24.20
MeO
Br
N
N
4h
f1 (ppm)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7.42
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7.36
7.35
7.34
7.33
7.26
7.14
7.14
7.13
7.12
7.07
7.06
3.97
3.02
1.74
1.73
1.72
1.65
1.62
0.07
0.00
MeO
N
S
N
4i
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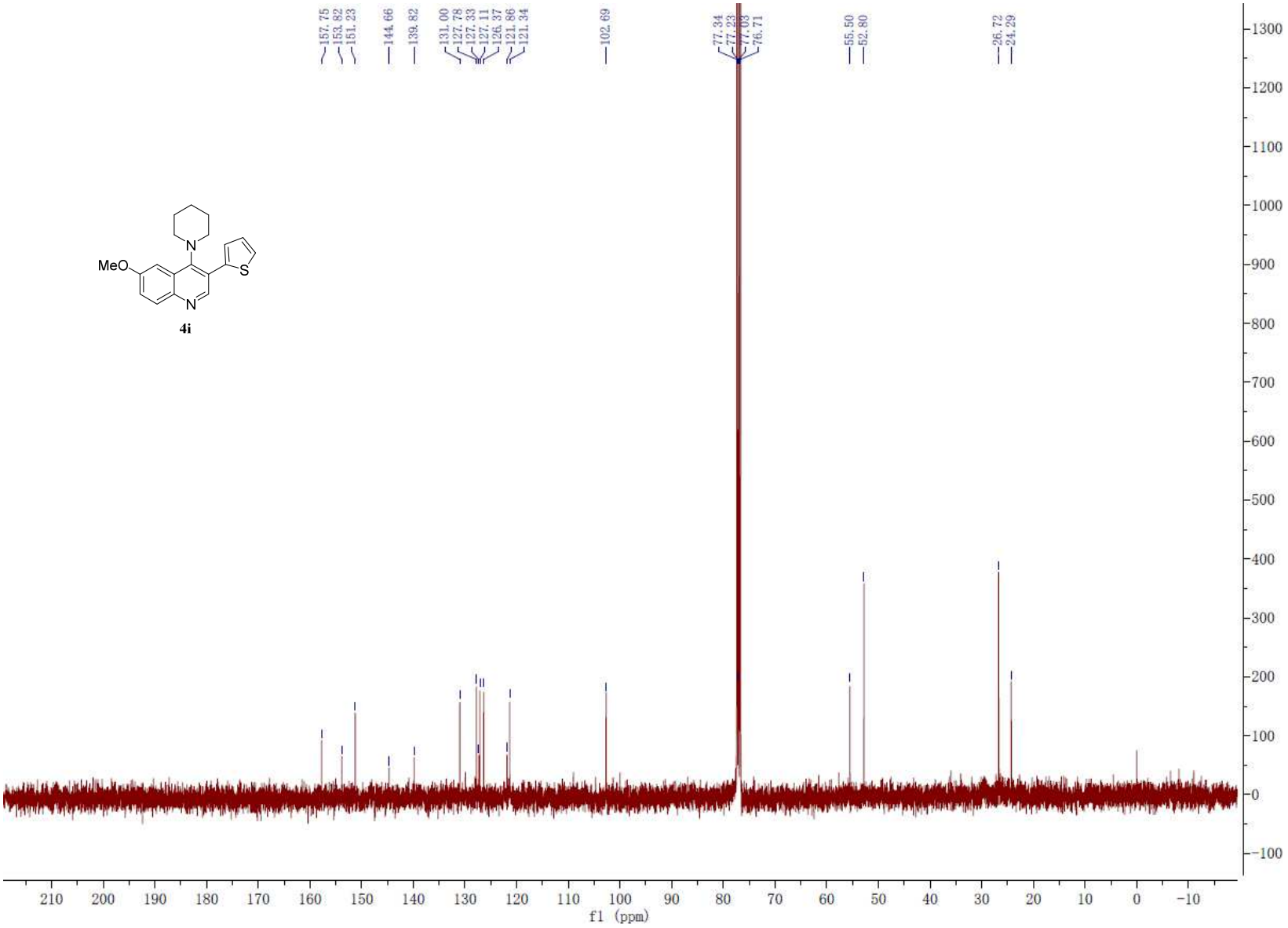
0.79
1.77
1.07
2.06
3.00
3.94
6.12
f1 (ppm)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121.34
102.69
77.34
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55.50
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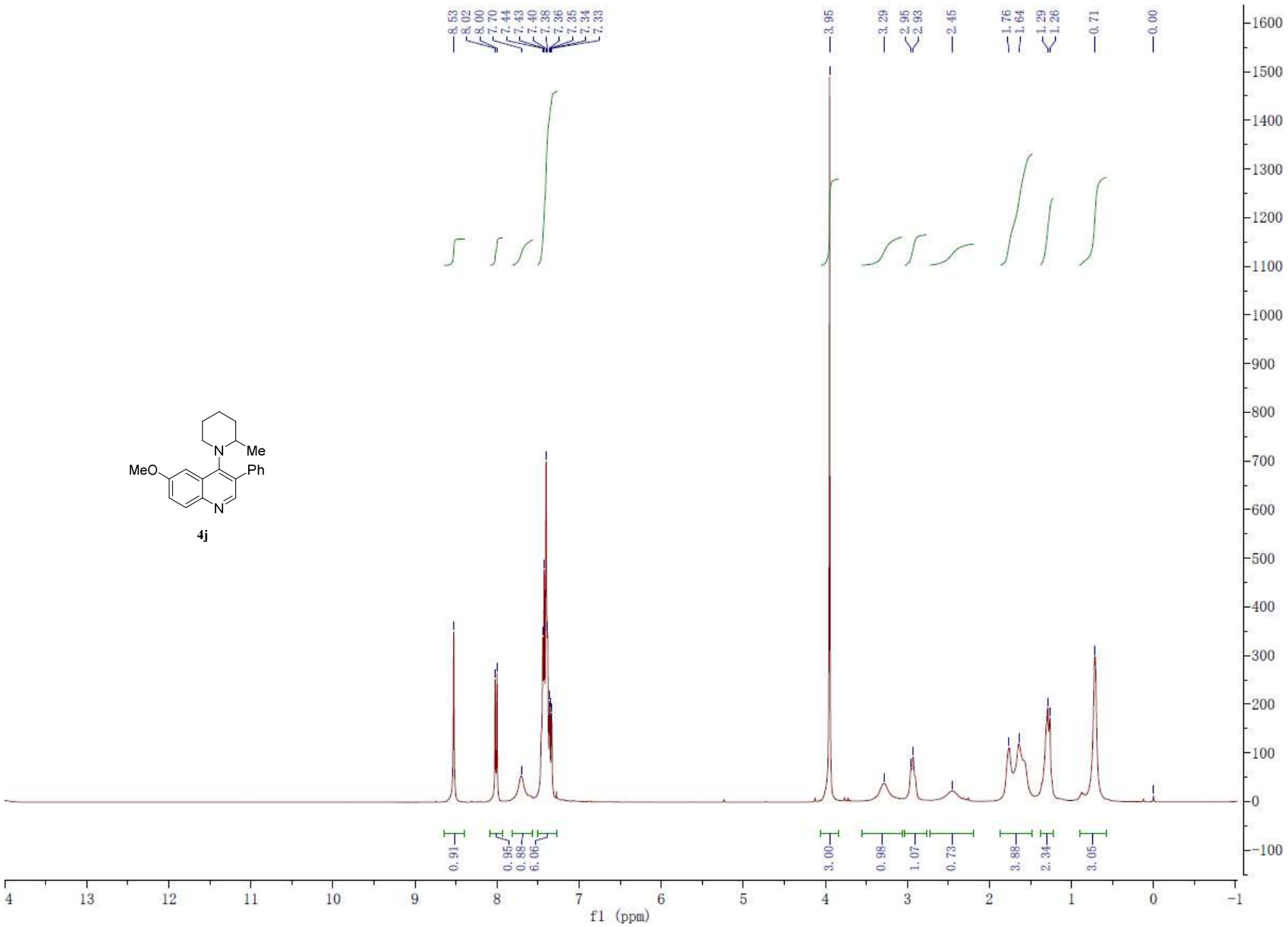
26.72
24.29
MeO
N
S
N
4i
f1 (ppm)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7.34
7.33
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3.29
2.95
2.93
2.45
1.76
1.64
1.29
1.26
0.71
0.00
MeO
N
Me
Ph
N
4j
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0.95
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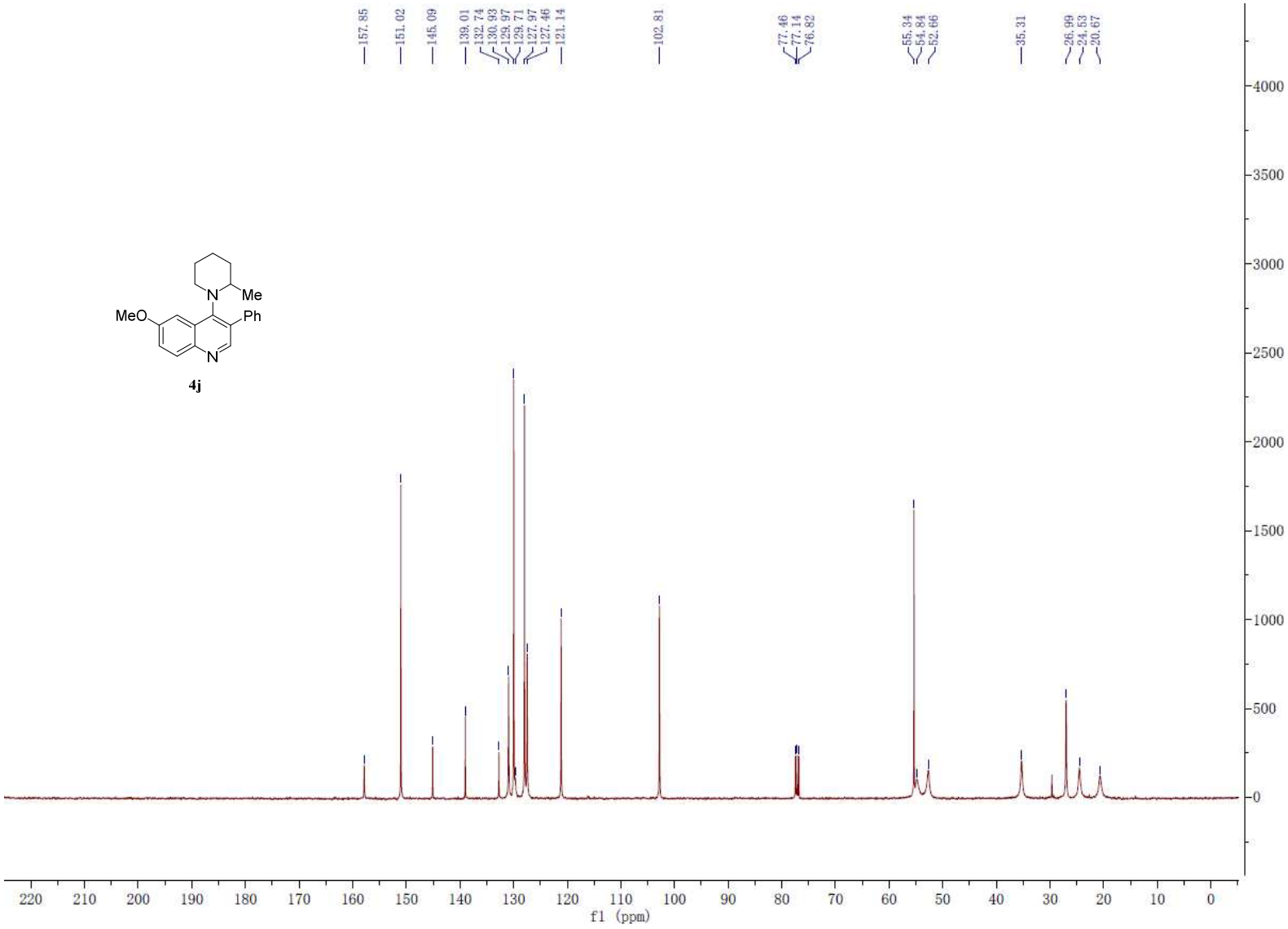
6.06
3.00
0.98
1.07
0.73
3.88
2.34
3.05
f1 (ppm)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77.46
77.14
76.82
55.34
54.84
52.66
35.31
26.99
24.53
20.67
MeO
N
Me
Ph
N
4j
4000
3500
3000
2500
2000
1500
1000
500
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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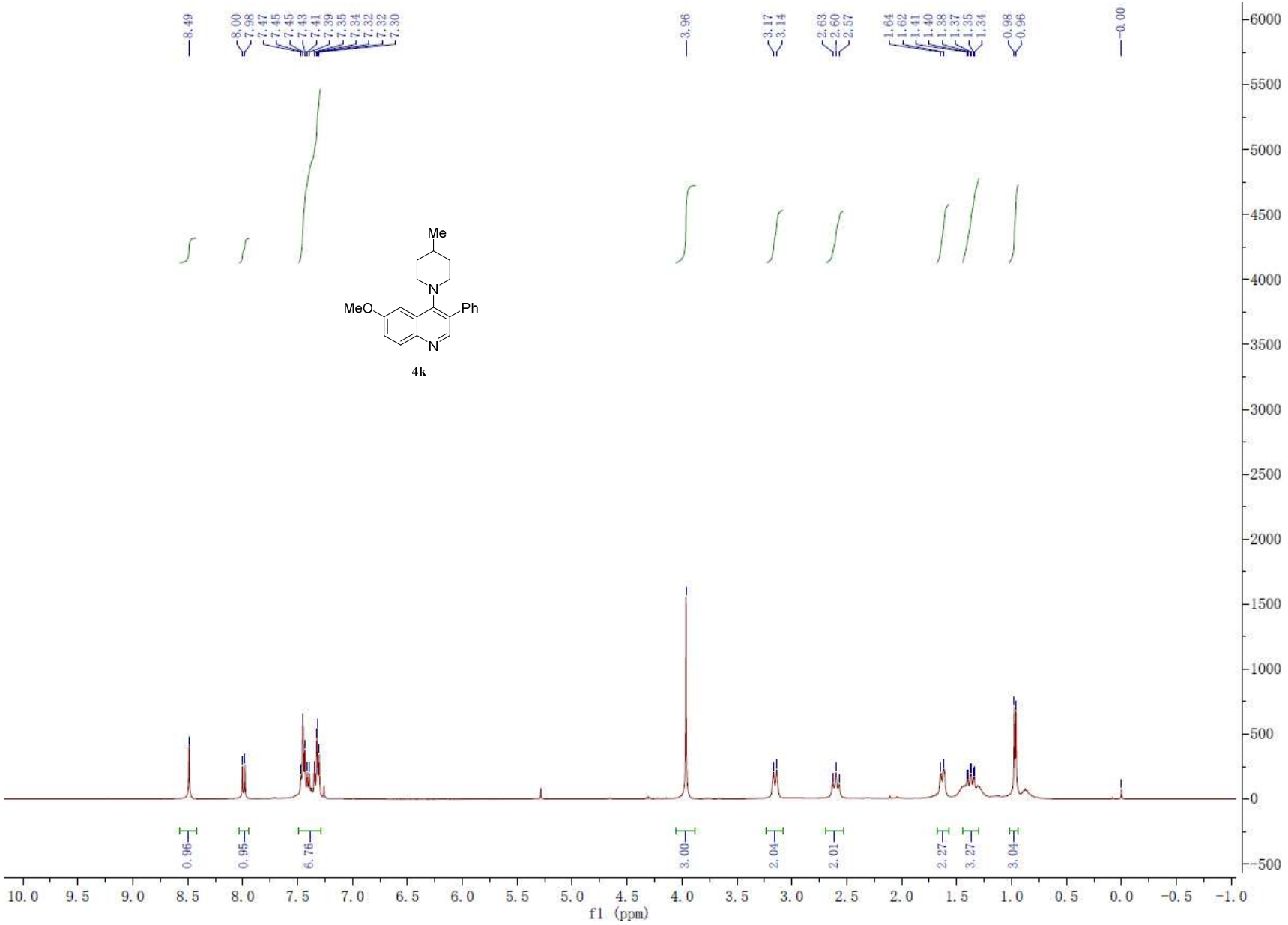
50
40
30
20
10
0
f1 (ppm)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7.34
7.32
7.32
7.30
3.96
3.17
3.14
2.63
2.60
2.57
1.64
1.62
1.41
1.40
1.38
1.37
1.35
1.34
0.98
0.96
0.00
Me
N
MeO
Ph
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4k
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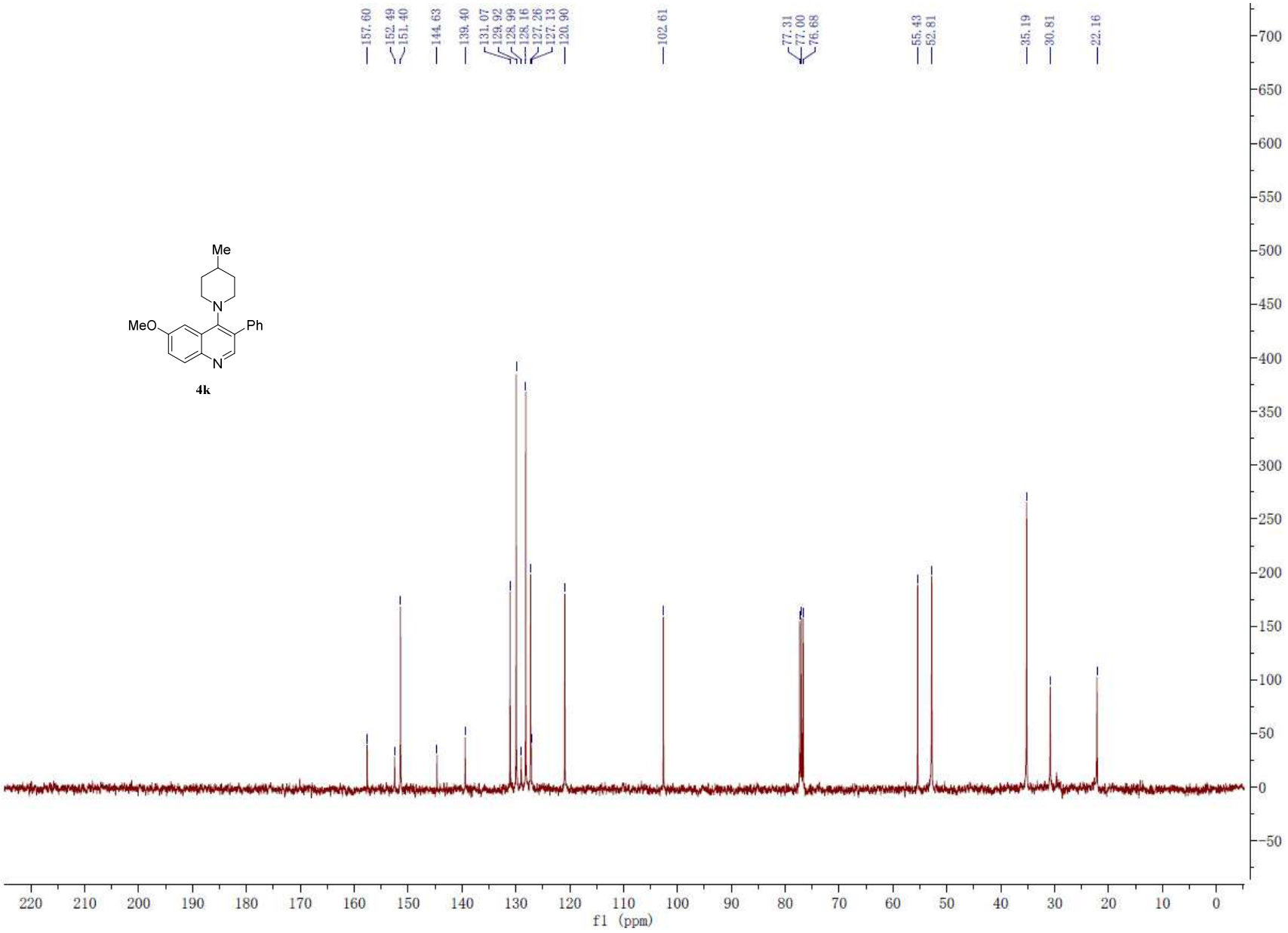
0.95
6.76
3.00
2.04
2.01
2.27
3.27
3.04
f1 (ppm)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127.26
127.13
120.90
102.61
77.31
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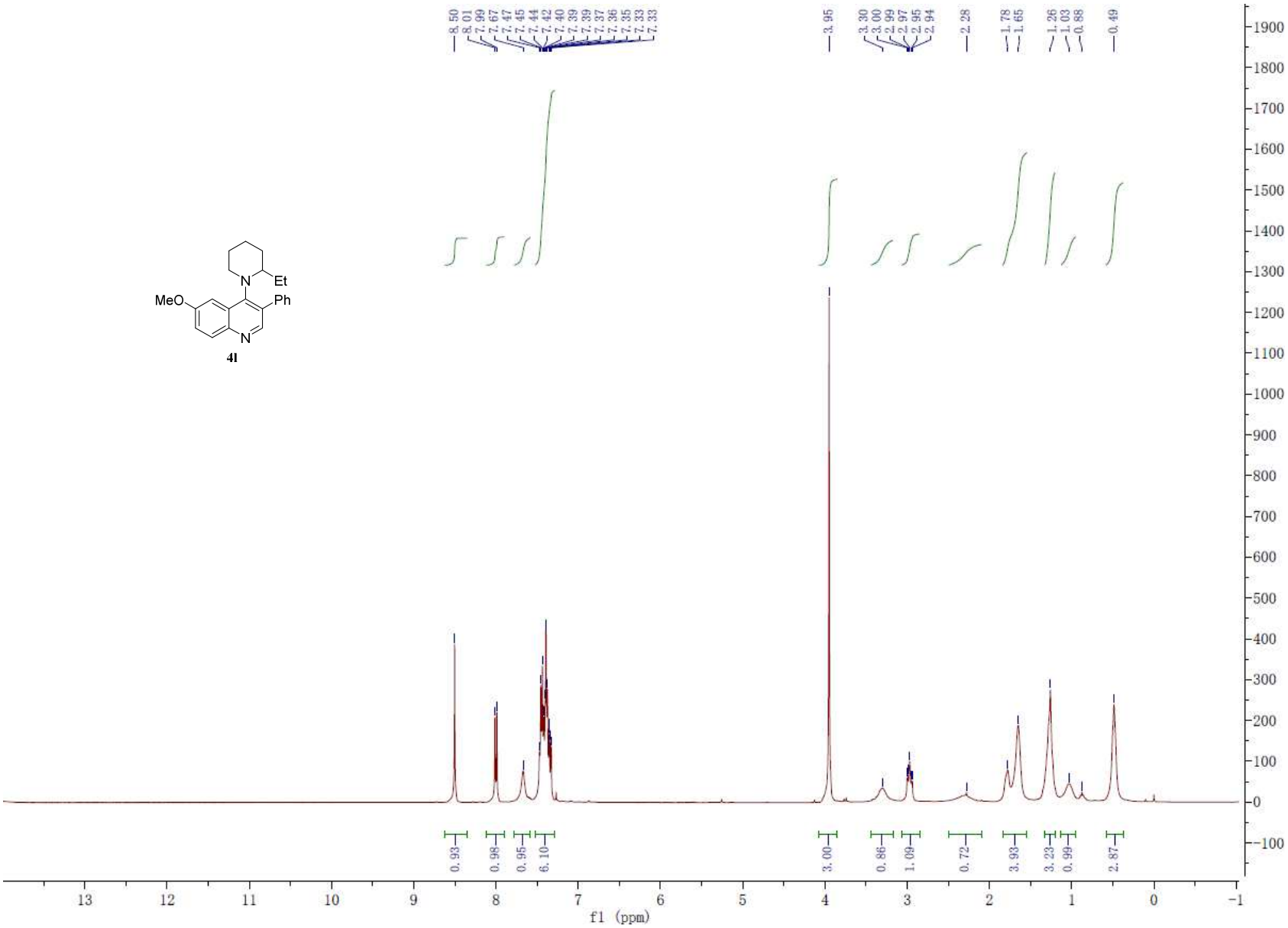
52.81
35.19
30.81
22.16
Me
N
MeO
Ph
N
4k
f1 (ppm)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7.42
7.40
7.39
7.39
7.37
7.36
7.35
7.33
7.33
3.95
3.30
3.00
2.99
2.97
2.95
2.94
2.28
1.78
1.65
1.26
1.03
0.88
0.49
MeO
N
Et
Ph
N
4l
0.93
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0.95
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3.00
0.86
1.09
0.72
3.93
3.23
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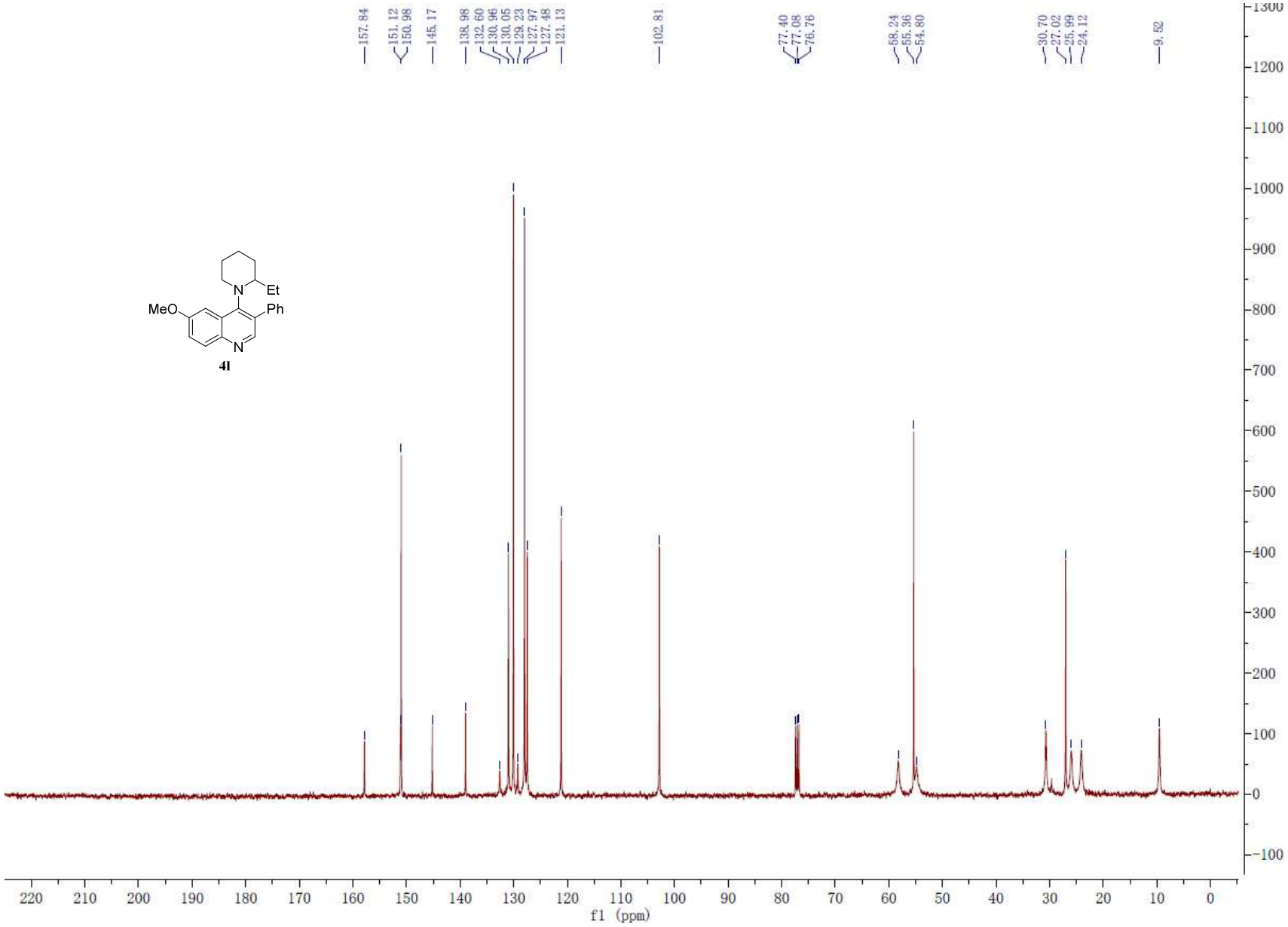
2.87
f1 (ppm)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127.48
121.13
102.81
77.40
77.08
76.76
58.24
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54.80
30.70
27.02
25.99
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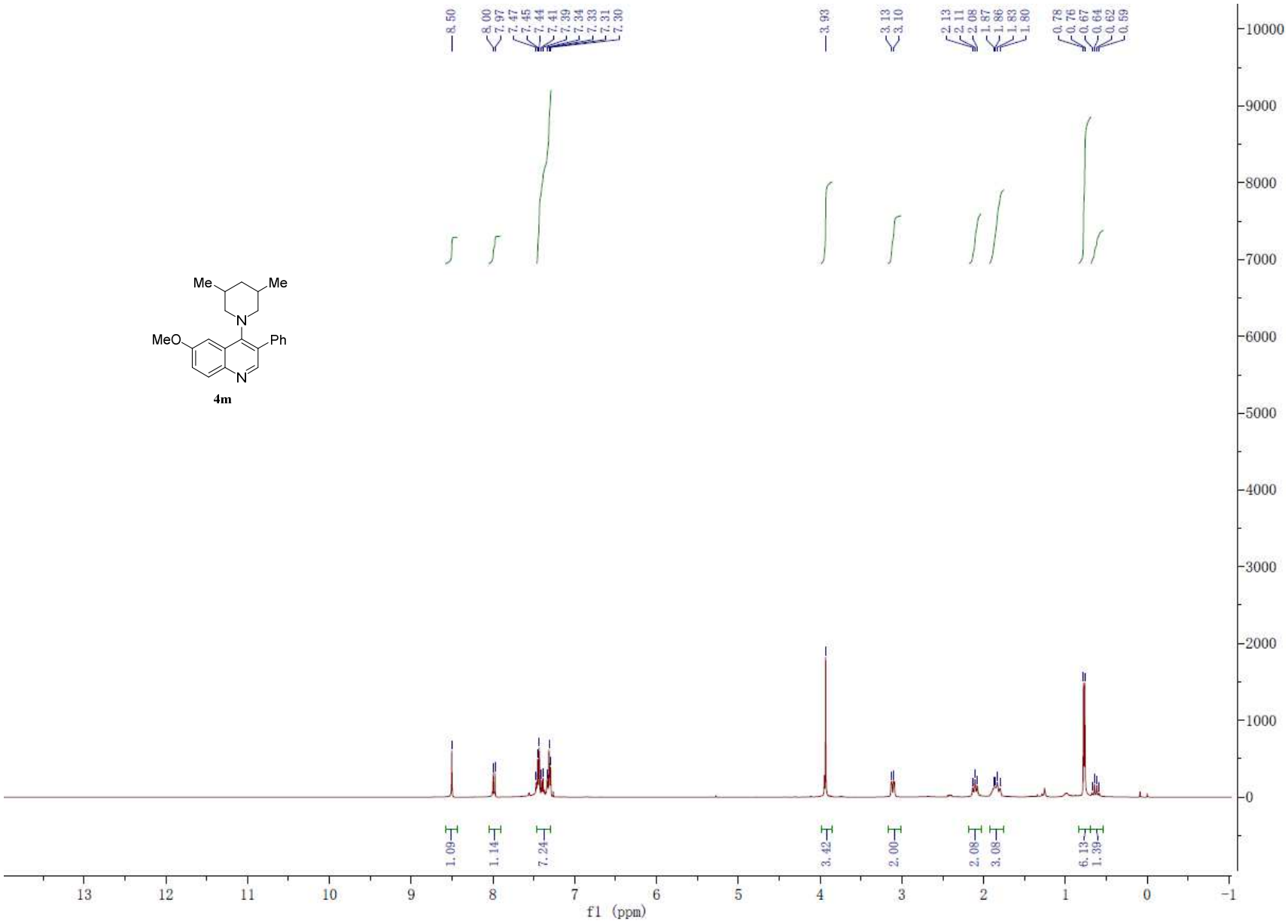
MeO
N
Et
Ph
N
4l
f1 (ppm)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8.00
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7.47
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7.44
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7.31
7.30
3.93
3.13
3.10
2.13
2.11
2.08
1.87
1.86
1.83
1.80
0.78
0.76
0.67
0.64
0.62
0.59
Me
Me
N
MeO
Ph
N
4m
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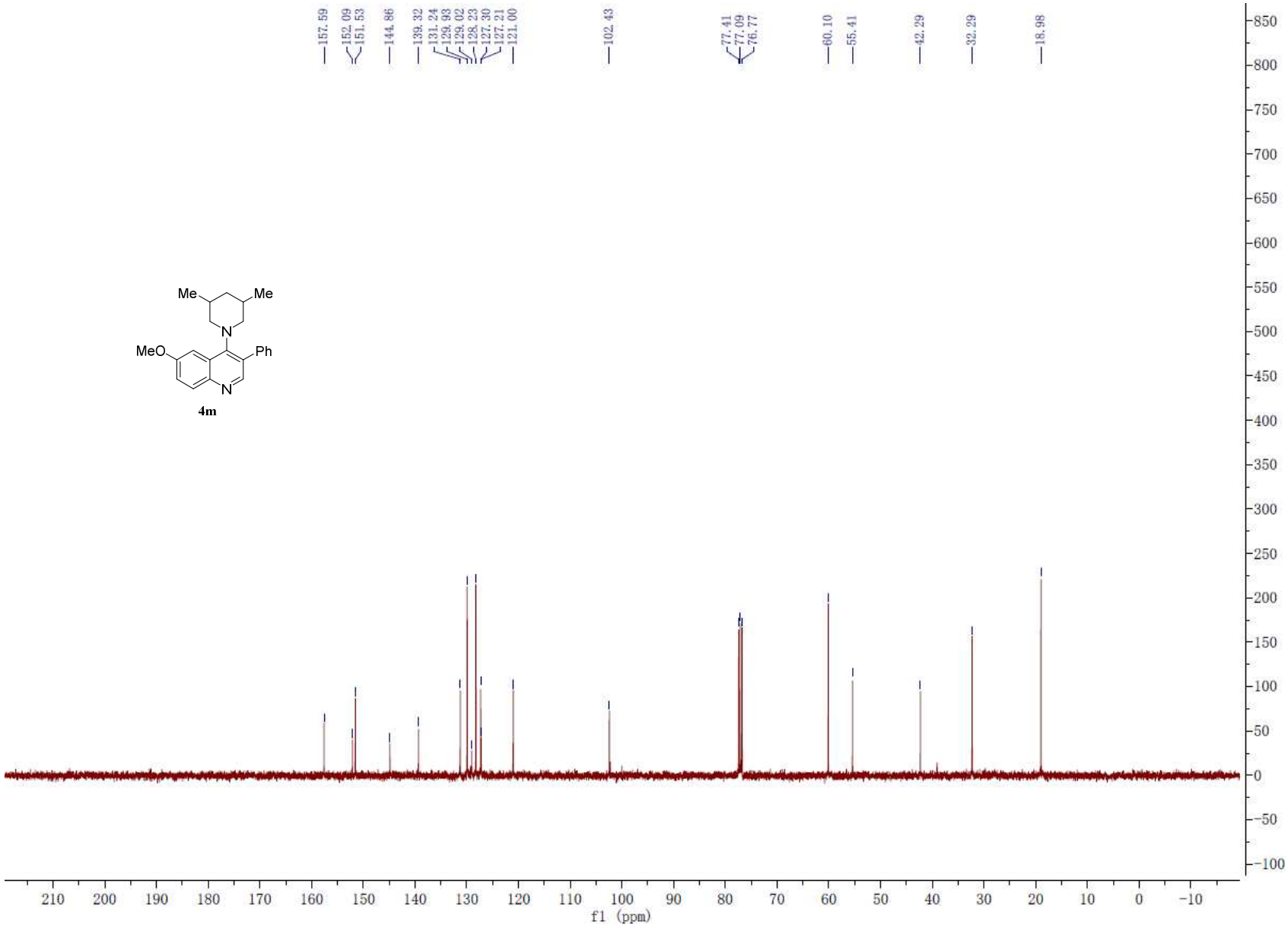
1.14
7.24
3.42
2.00
2.08
3.08
6.13
1.39
f1 (ppm)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129.02
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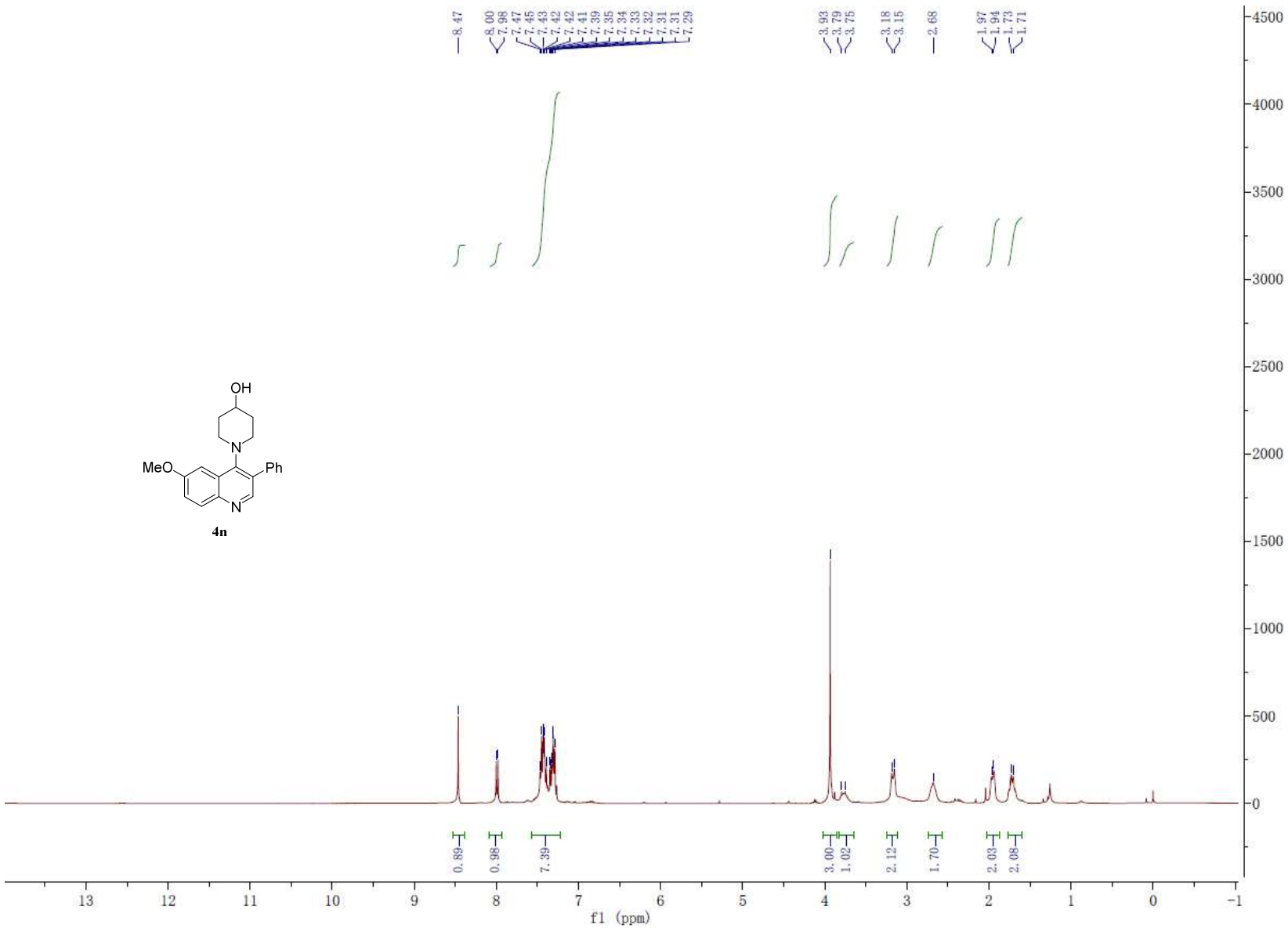
127.30
127.21
121.00
102.43
77.41
77.09
76.77
60.10
55.41
42.29
32.29
18.98
Me
Me
N
MeO
Ph
N
4m
f1 (ppm)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7.42
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7.34
7.33
7.32
7.31
7.31
7.29
3.93
3.79
3.75
3.18
3.15
2.68
1.97
1.94
1.73
1.71
OH
N
MeO
Ph
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4n
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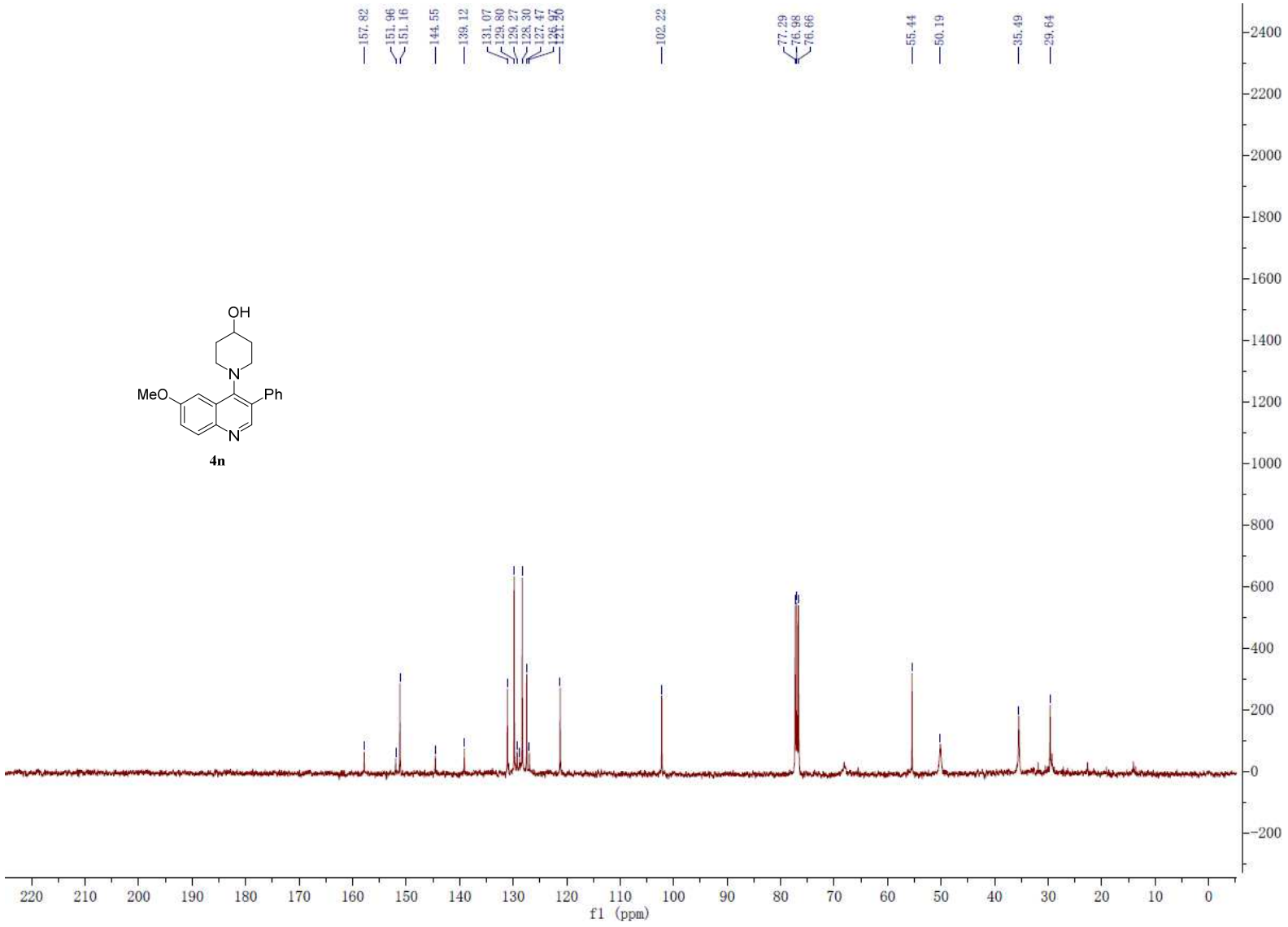
0.98
7.39
3.00
1.02
2.12
1.70
2.03
2.08
f1 (ppm)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127.47
121.20
102.22
77.29
76.98
76.66
55.44
50.19
35.49
29.64
OH
N
MeO
Ph
N
4n
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
220
210
200
190
180
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90
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50
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20
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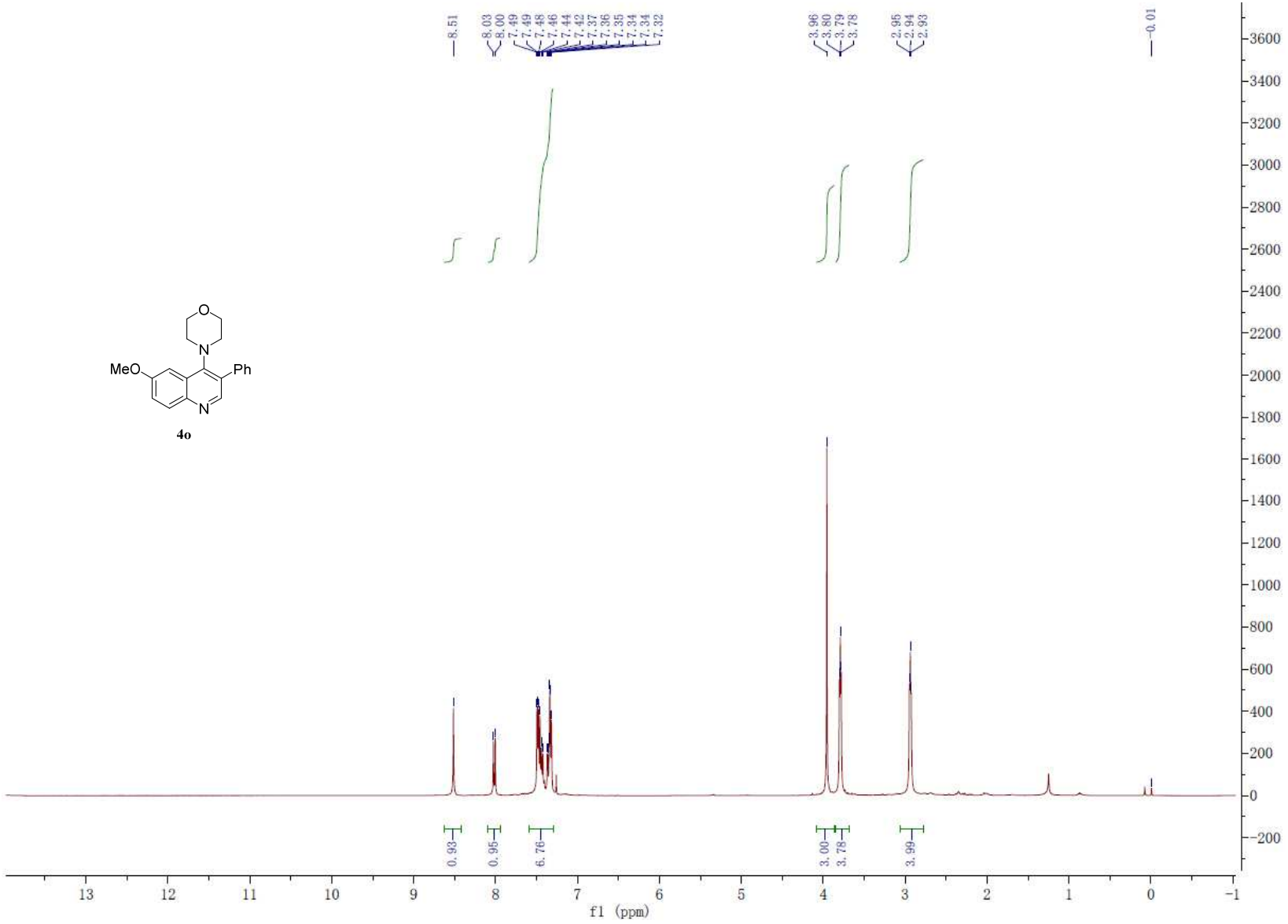
f1 (ppm)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7.36
7.35
7.34
7.34
7.32
3.96
3.80
3.79
3.78
2.95
2.94
2.93
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Ph
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N
N
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0.95
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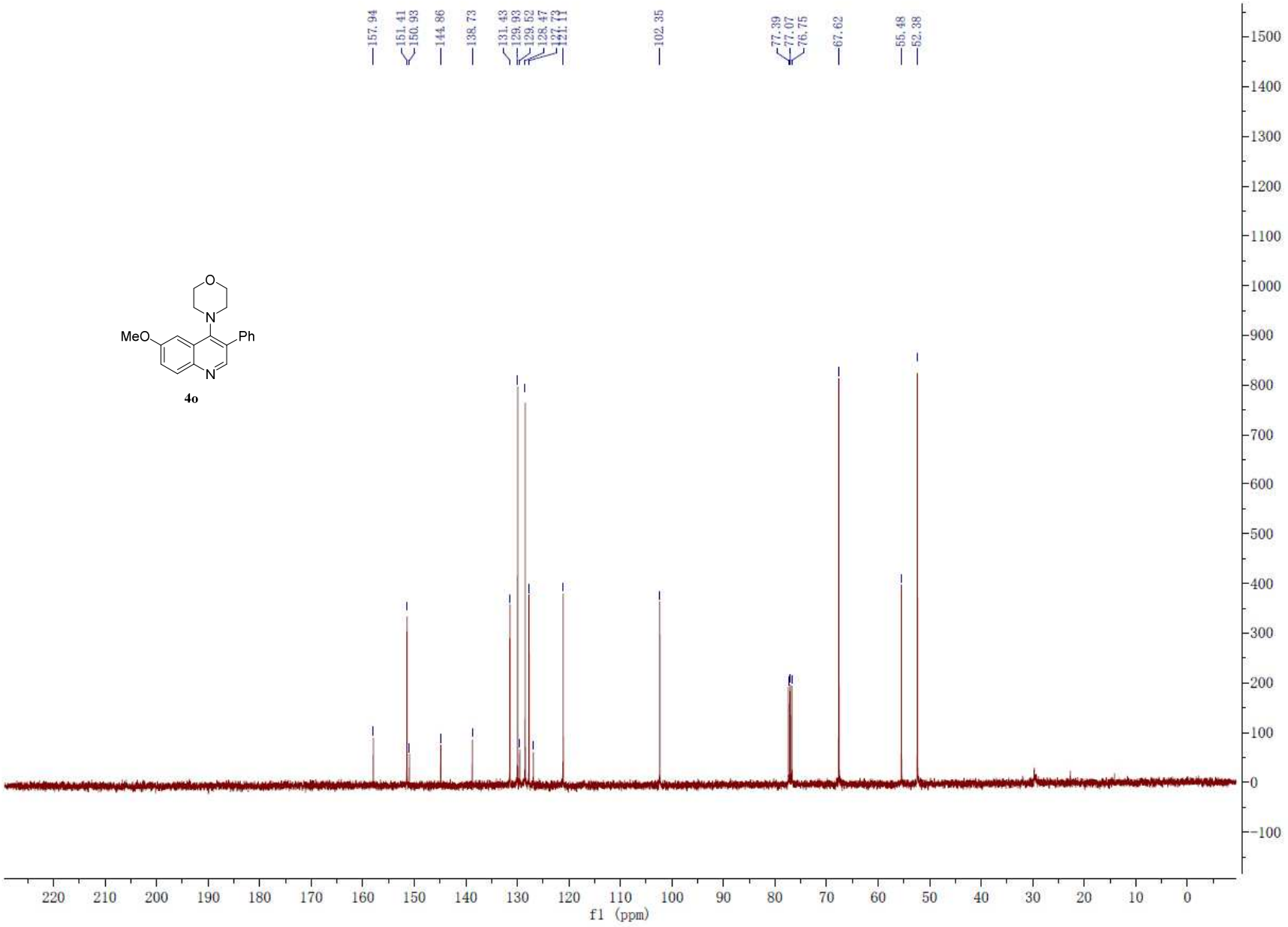
3.00
3.78
3.99
f1 (ppm)

4o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129.52
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127.73
121.11
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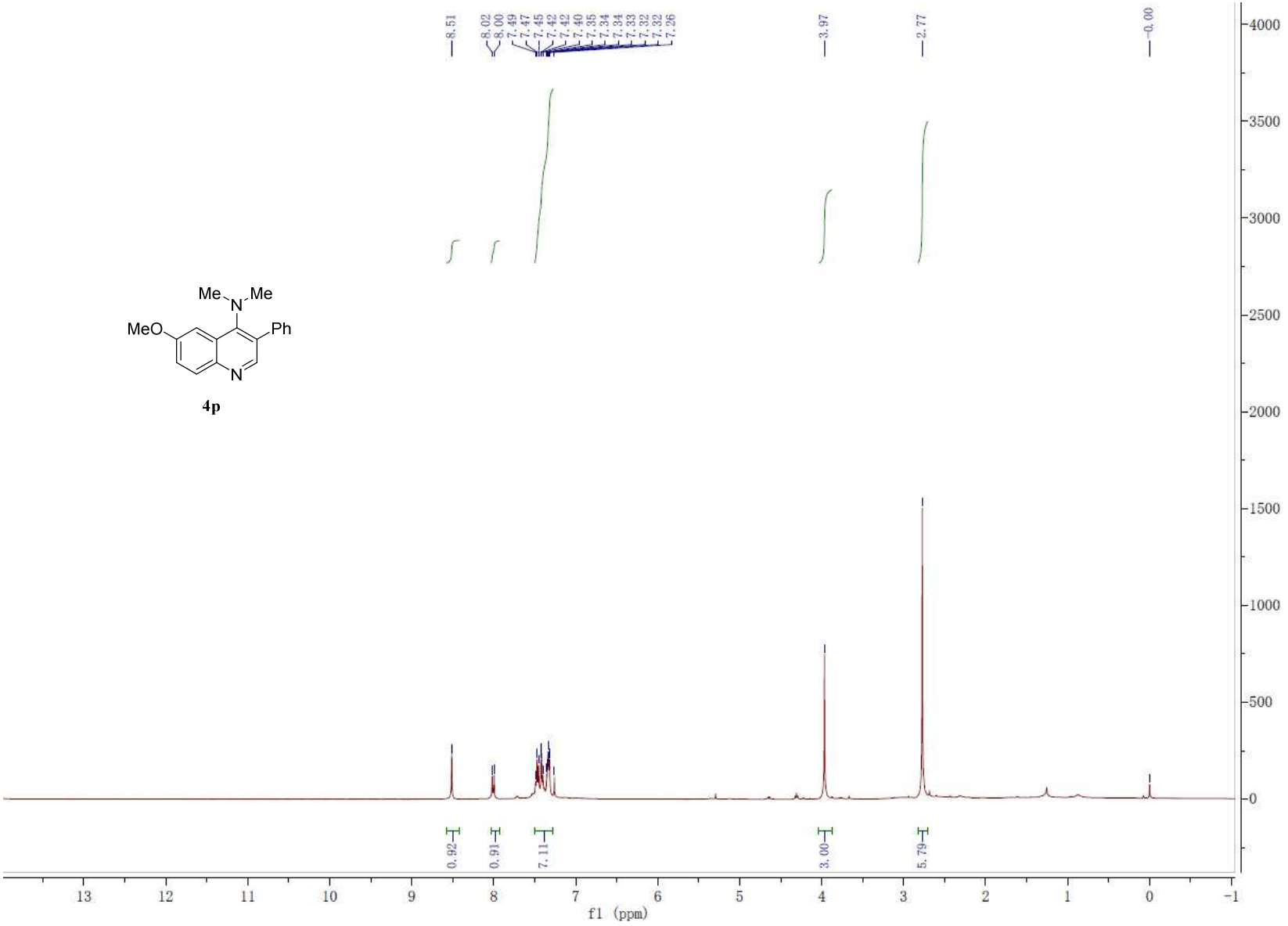
76.75
67.62
55.48
52.38
MeO
Ph
O
N
N
4o
f1 (ppm)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7.42
7.40
7.35
7.34
7.34
7.33
7.32
7.32
7.26
3.97
2.77
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Me
MeO
Ph
N
4p
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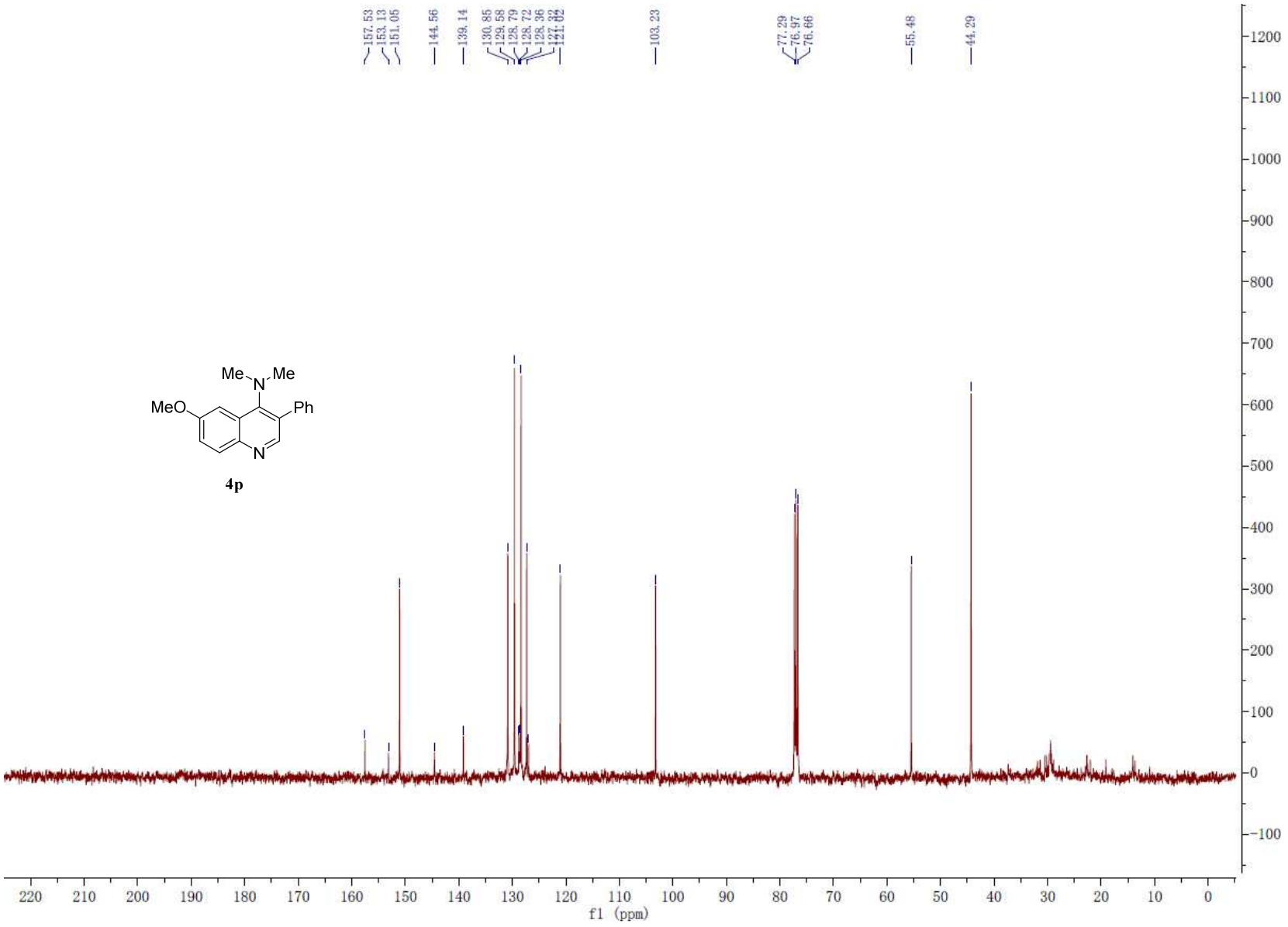
0.91
7.11
3.00
5.79
f1 (ppm)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128.36
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121.02
103.23
77.29
76.97
76.66
55.48
44.29
Me
N
Me
MeO
Ph
N
4p
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
220
210
200
190
180
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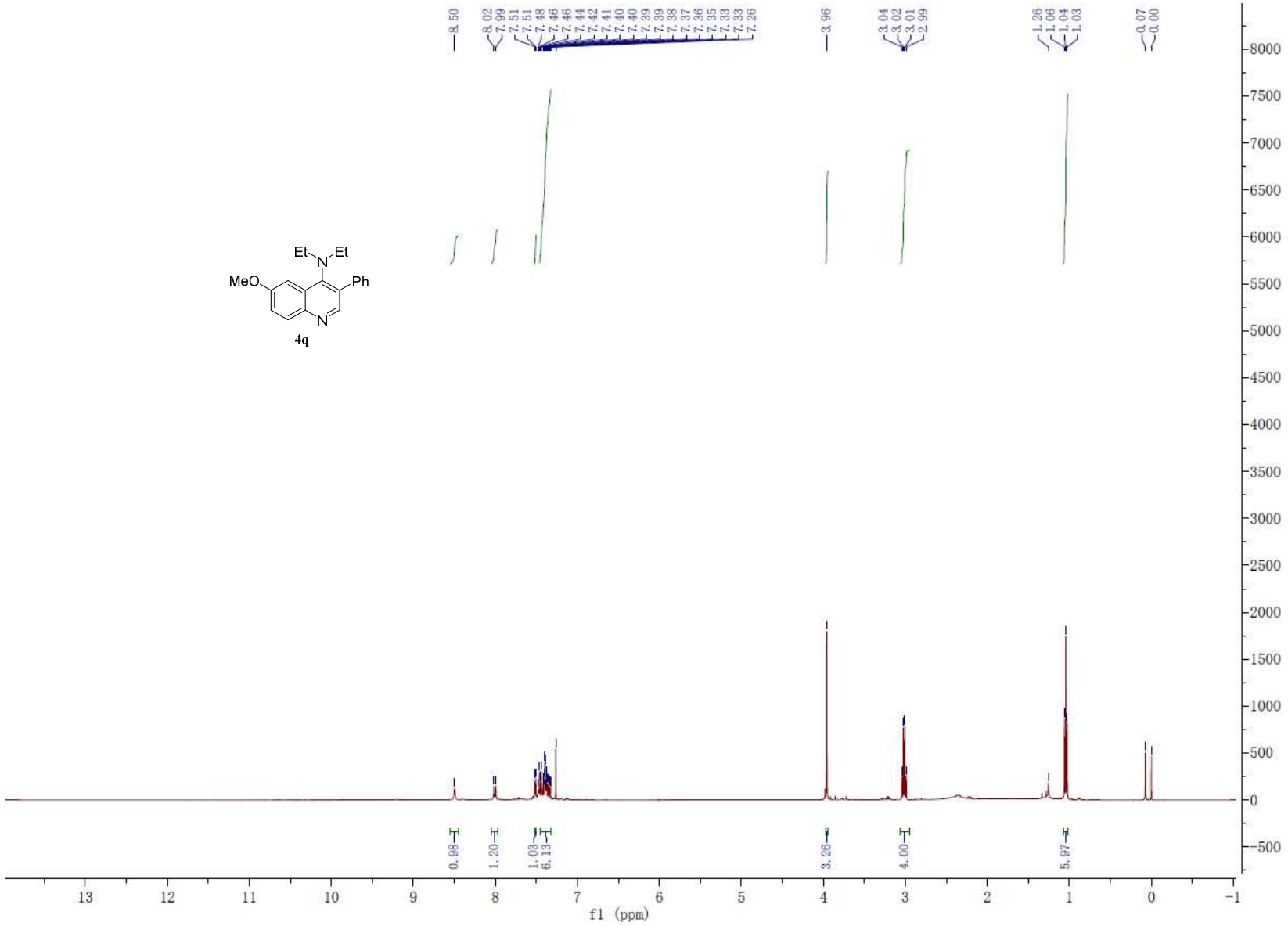
f1 (ppm)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7.42
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7.40
7.40
7.39
7.39
7.38
7.37
7.36
7.35
7.33
7.33
7.26
3.96
3.04
3.02
3.01
2.99
1.26
1.06
1.04
1.03
0.07
0.00
Et
N
Et
MeO
Ph
N
4q
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1.03
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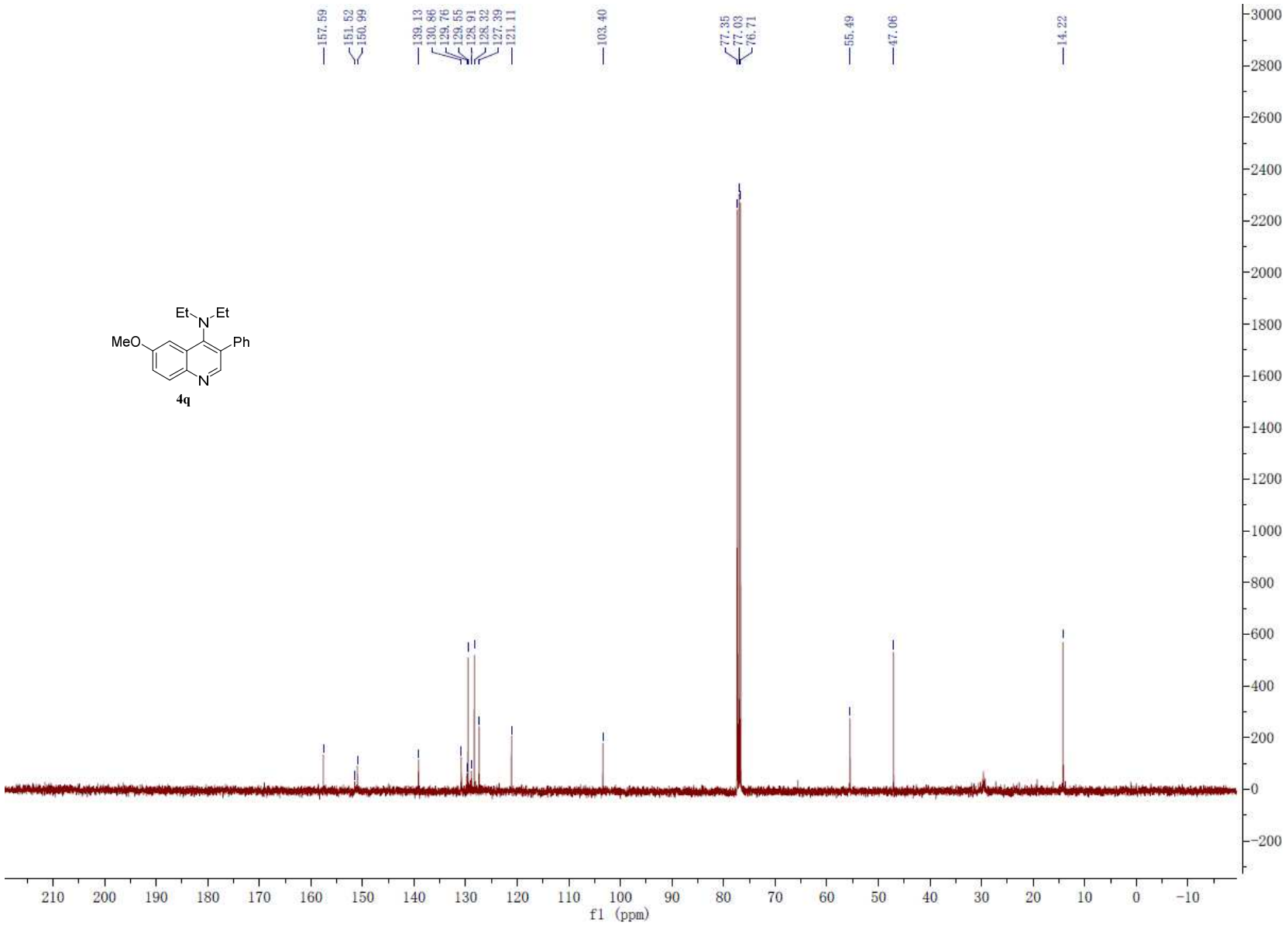
3.26
4.00
5.97
f1 (ppm)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127.39
121.11
103.40
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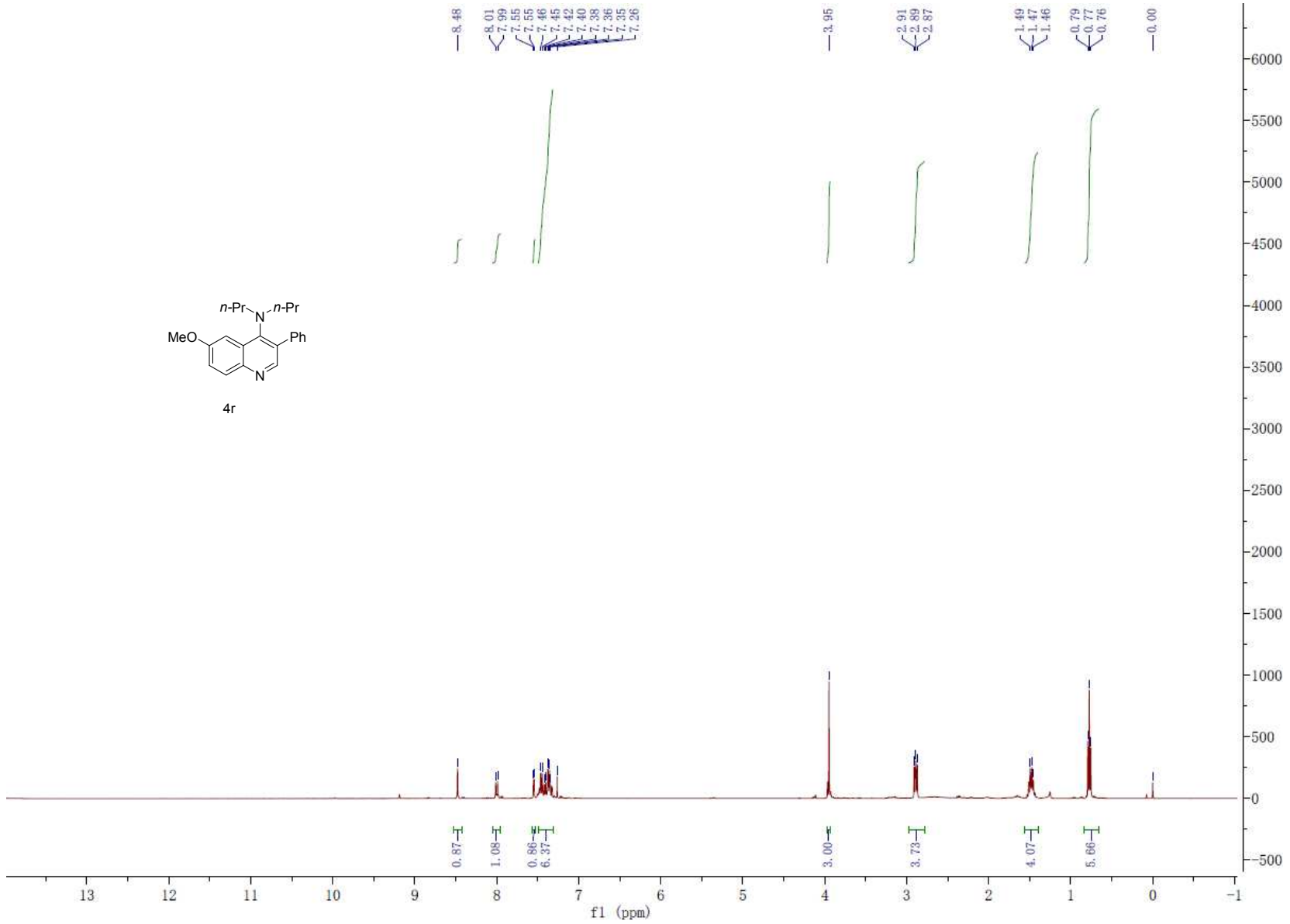
55.49
47.06
14.22
Et
N
Et
MeO
Ph
N
4q
f1 (ppm)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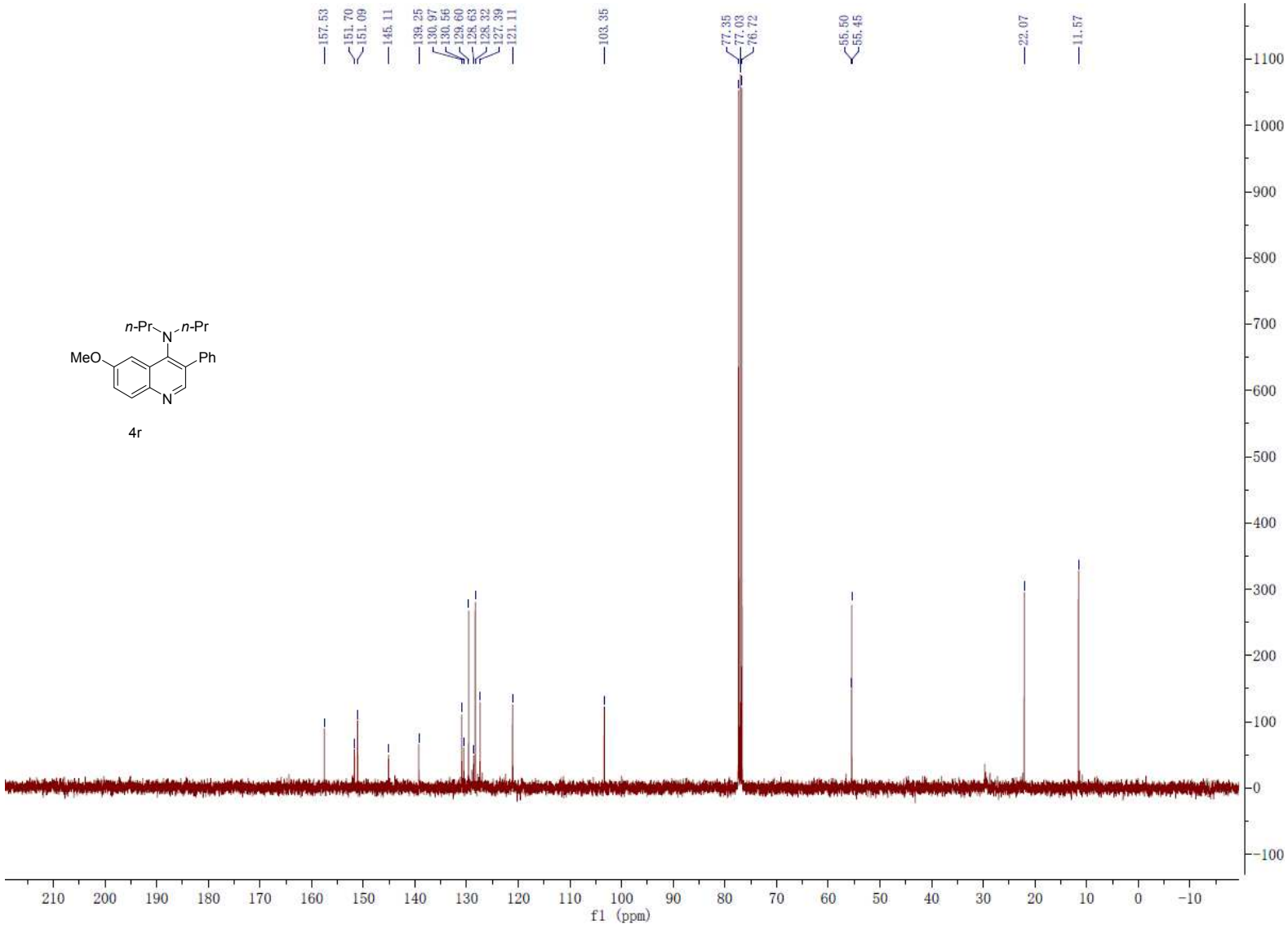
7.46
7.45
7.42
7.40
7.38
7.36
7.35
7.26
3.95
2.91
2.89
2.87
1.49
1.47
1.46
0.79
0.77
0.76
0.00
n-Pr
N
n-Pr
MeO
Ph
N
4r
0.87
1.08
0.86
6.37
3.00
3.73
4.07
5.66
f1 (ppm)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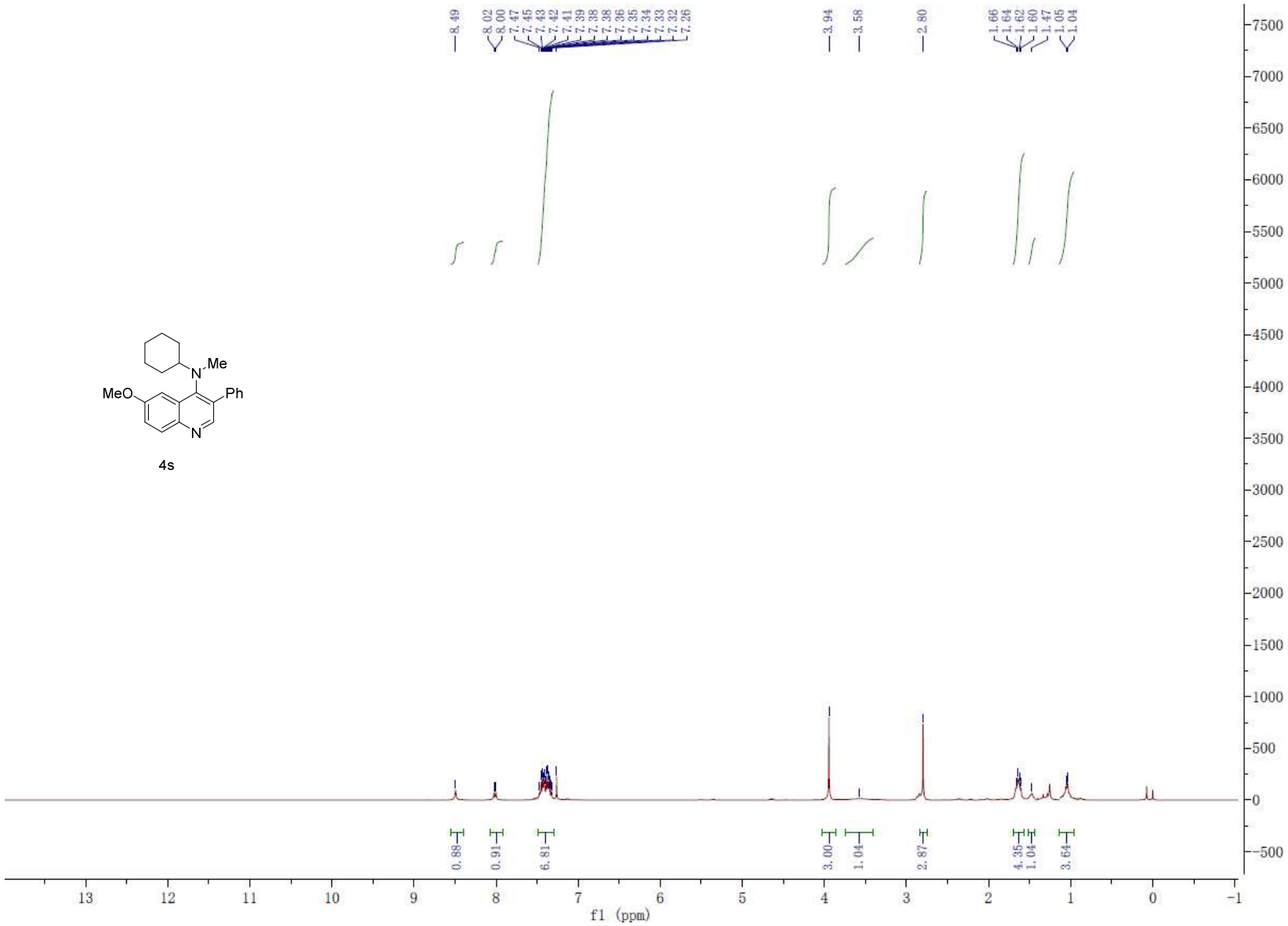
130.56
129.60
128.63
128.32
127.39
121.11
103.35
77.35
77.03
76.72
55.50
55.45
22.07
11.57
n-Pr
N
n-Pr
MeO
Ph
N
4r
f1 (ppm)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8.00
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7.41
7.39
7.38
7.38
7.36
7.35
7.34
7.33
7.32
7.26
3.94
3.58
2.80
1.66
1.64
1.62
1.60
1.47
1.05
1.04
N
Me
MeO
Ph
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0.91
6.81
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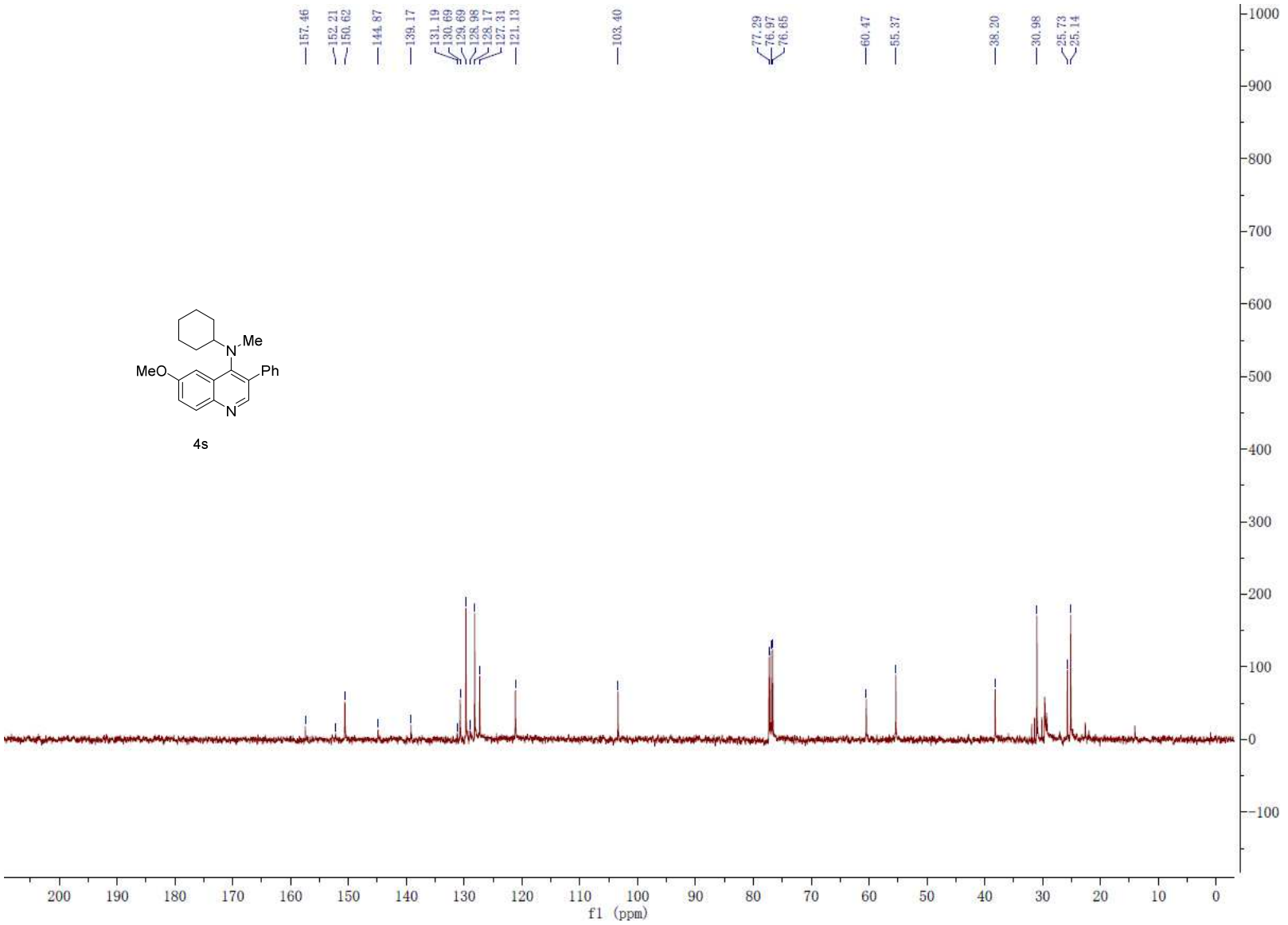
1.04
2.87
4.35
1.04
3.64
f1 (ppm)

4s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128.98
128.17
127.31
121.13
103.40
77.29
76.97
76.65
60.47
55.37
38.20
30.98
25.73
25.14
N
Me
MeO
Ph
N
4s
1000
900
800
700
600
500
400
300
200
100
0
-100
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
20
10
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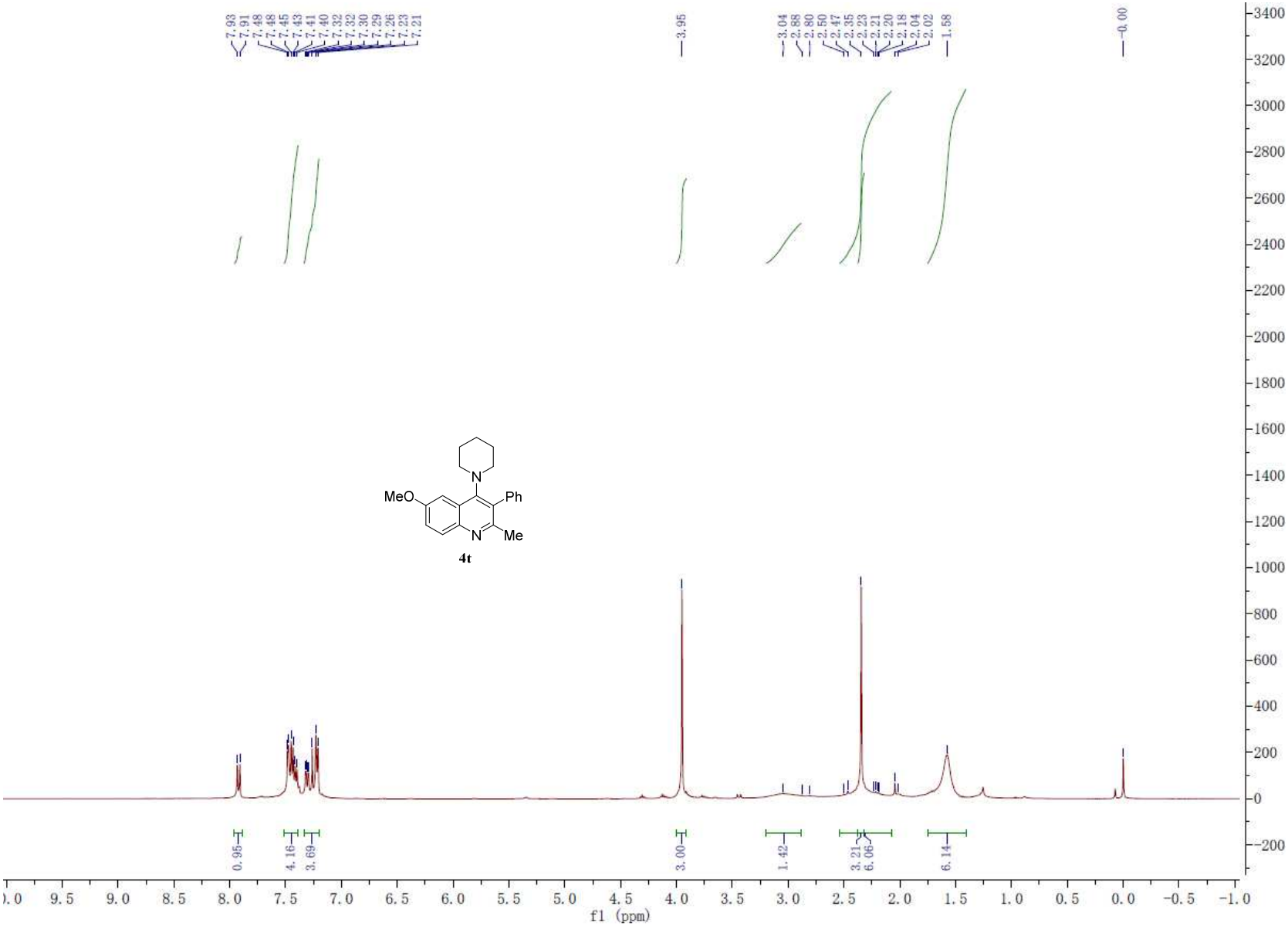
f1 (ppm)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7.91
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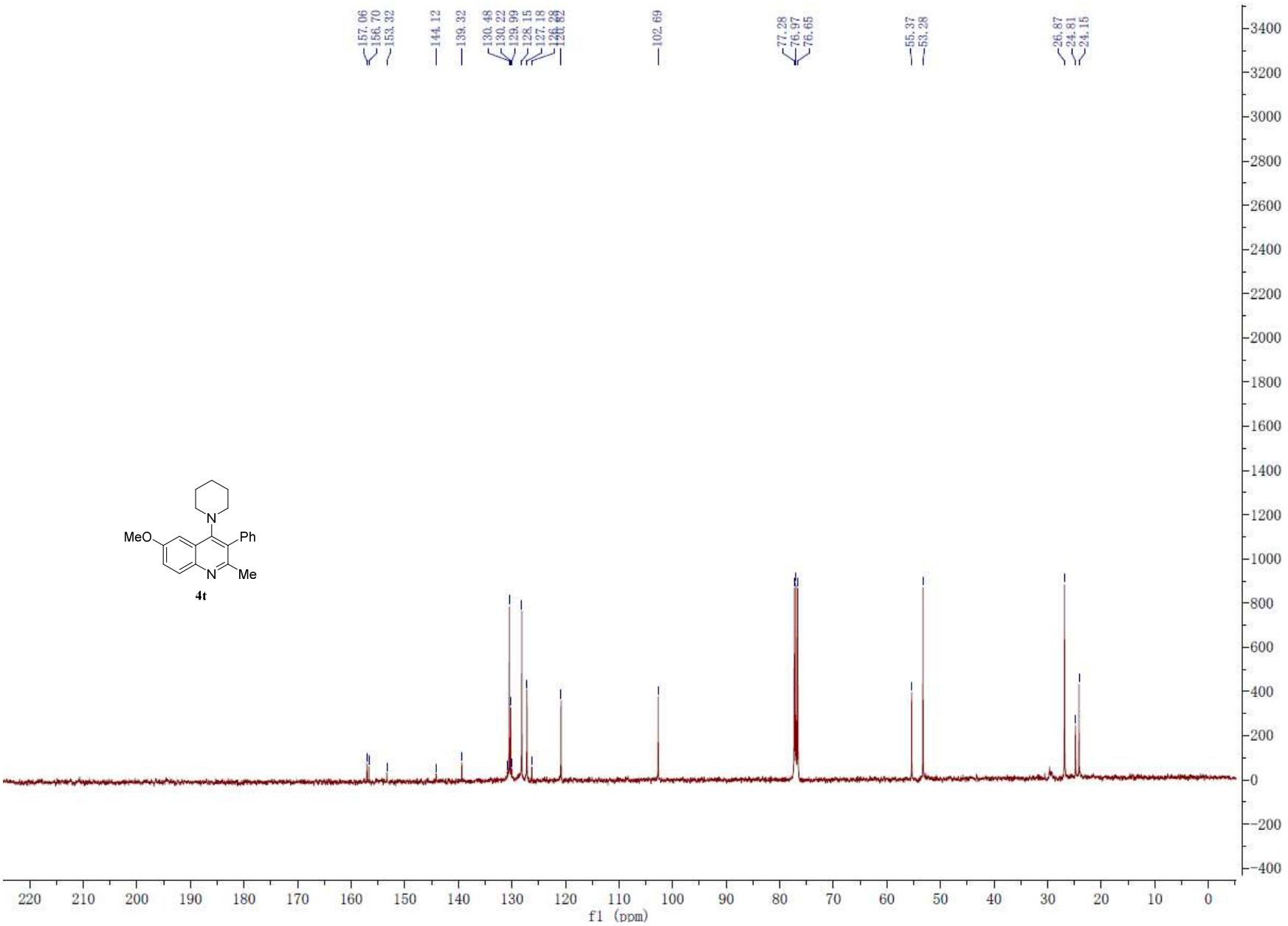
7.48
7.45
7.43
7.41
7.40
7.32
7.32
7.30
7.29
7.26
7.23
7.21
3.95
3.04
2.88
2.80
2.50
2.47
2.35
2.23
2.21
2.20
2.18
2.04
2.02
1.58
0.00
MeO
Ph
N
Me
4t
0.95
4.16
3.69
3.00
1.42
3.21
6.06
6.14
f1 (ppm)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139.32
130.48
130.22
129.99
128.15
127.18
102.69
77.28
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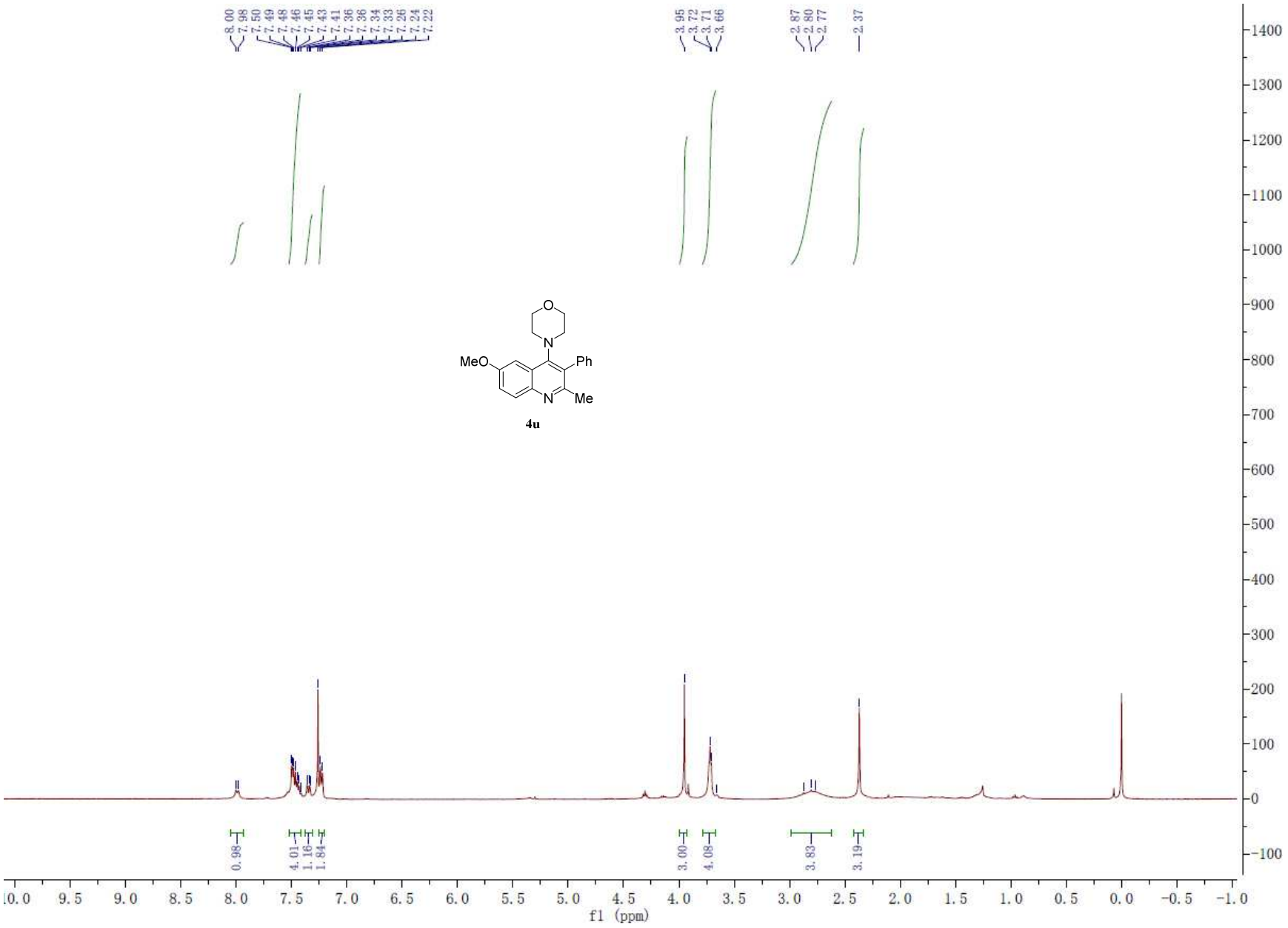
76.65
55.37
53.28
26.87
24.81
24.15
MeO
Ph
N
Me
4t
f1 (ppm)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7.49
7.48
7.46
7.45
7.43
7.41
7.36
7.36
7.34
7.33
7.26
7.24
7.22
3.95
3.72
3.71
3.66
2.87
2.80
2.77
2.37
MeO
Ph
Me
N
O
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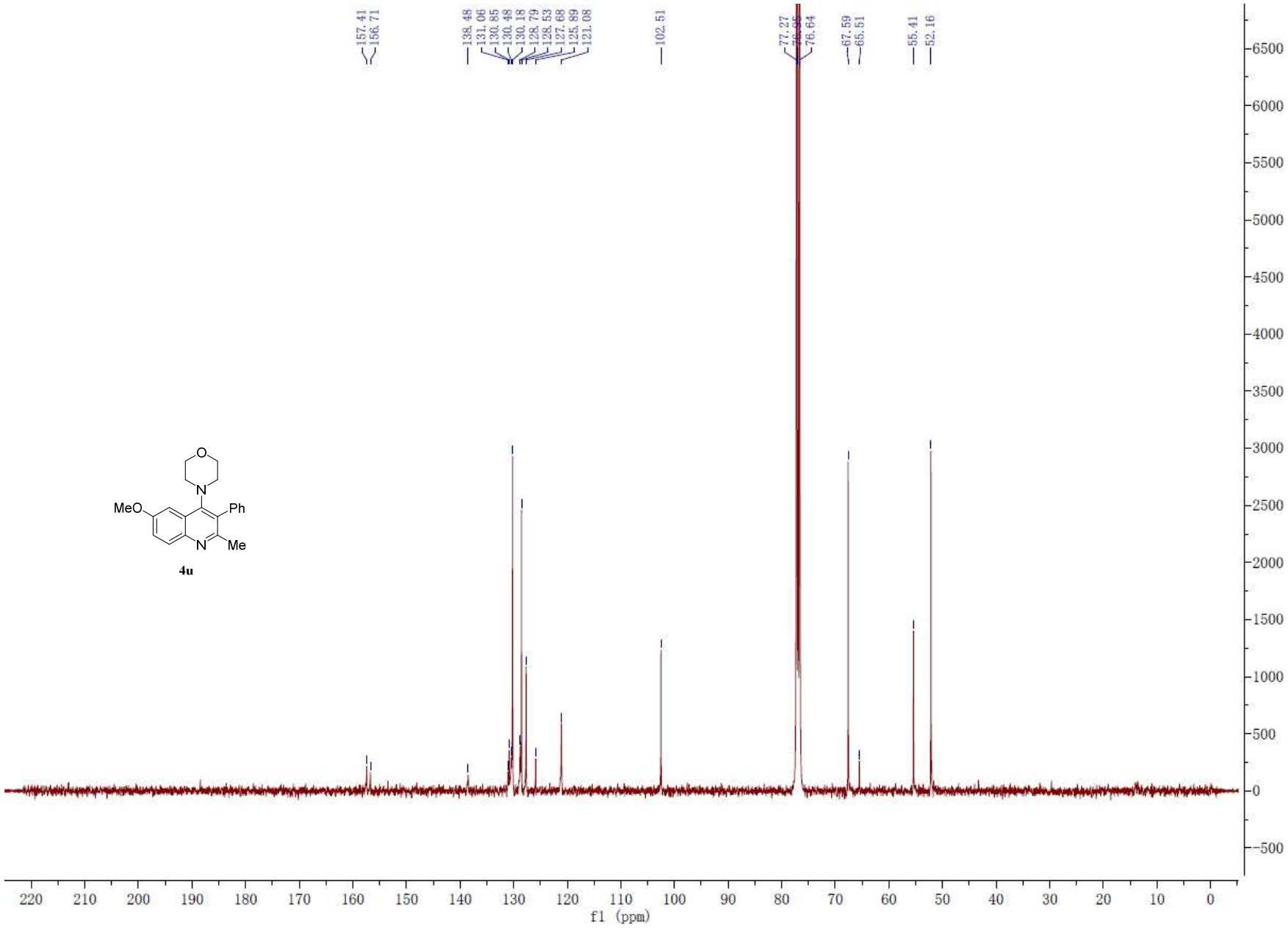
4.01
1.16
1.84
3.00
4.08
3.83
3.19
f1 (ppm)

4u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130.48
130.18
128.79
128.53
127.68
125.89
121.08
102.51
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67.59
65.51
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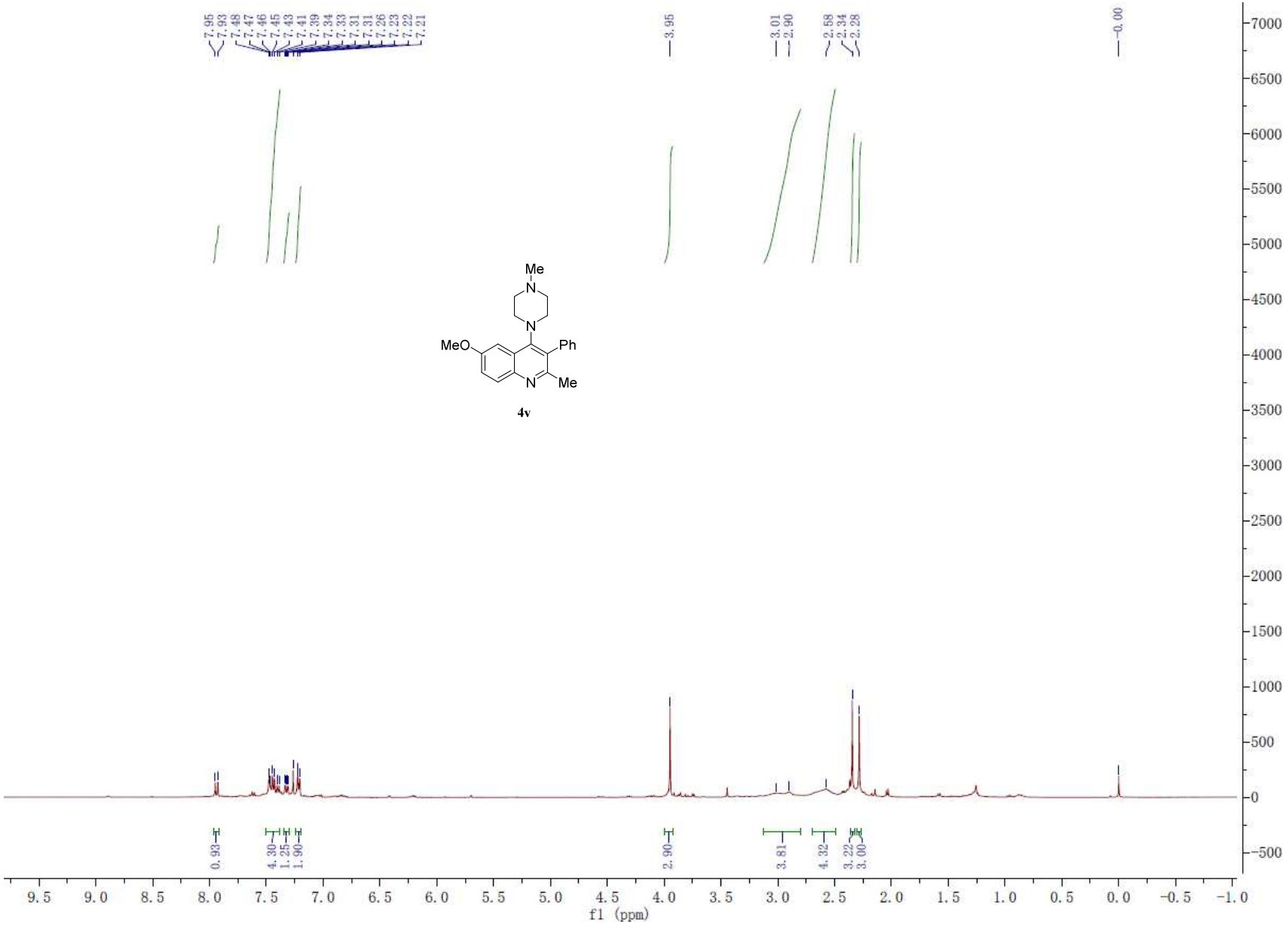
52.16
MeO
Ph
Me
N
O
4u
f1 (ppm)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7.43
7.41
7.39
7.34
7.33
7.31
7.31
7.26
7.23
7.22
7.21
3.95
3.01
2.90
2.58
2.34
2.28
0.00
Me
N
N
MeO
Ph
N
Me
4v
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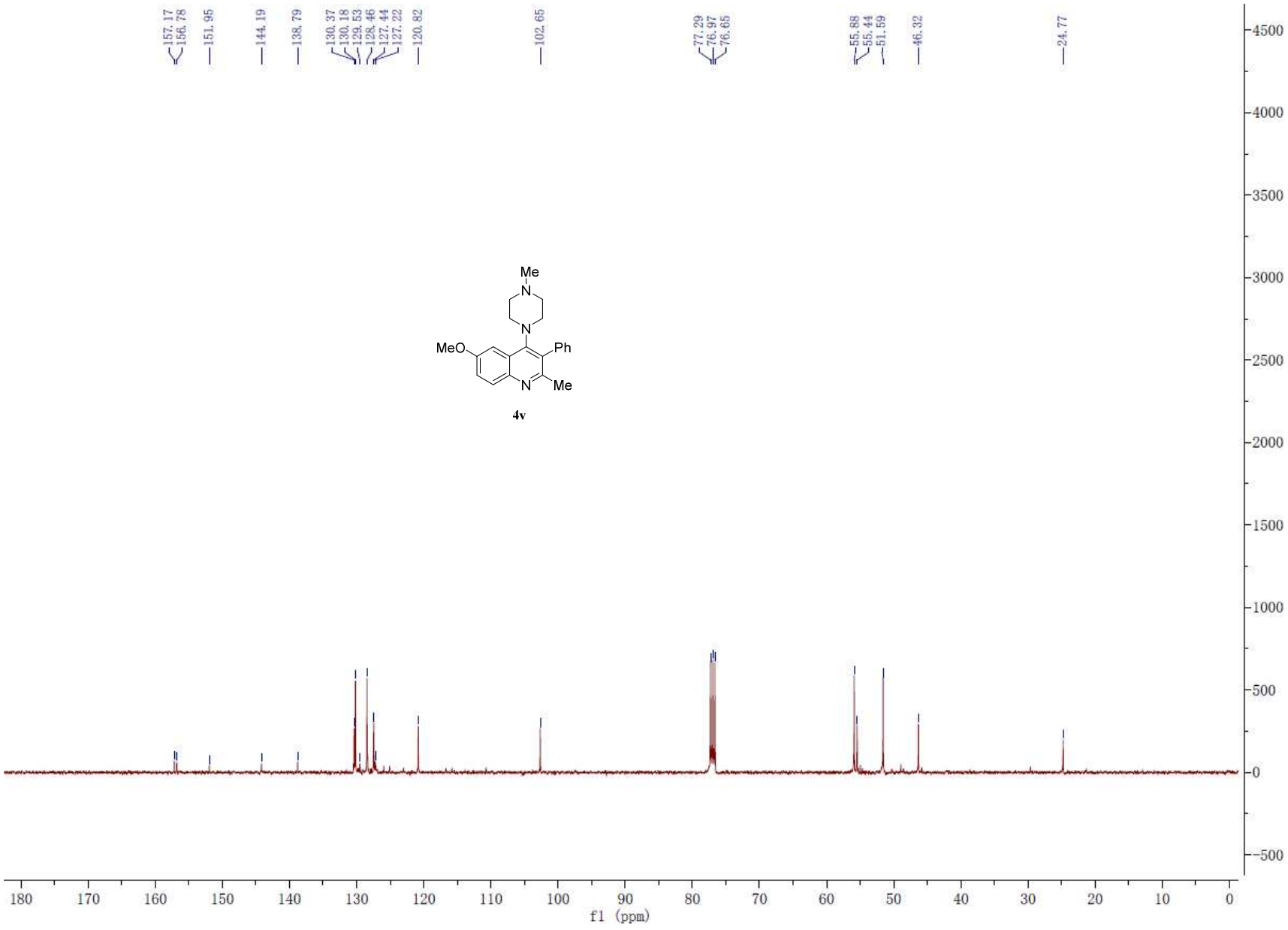
4.30
1.25
1.90
2.90
3.81
4.32
3.22
3.00
f1 (ppm)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127.44
127.22
120.82
102.65
77.29
76.97
76.65
55.88
55.44
51.59
46.32
24.77
Me
N
N
MeO
Ph
N
Me
4v
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
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130
120
110
100
90
80
70
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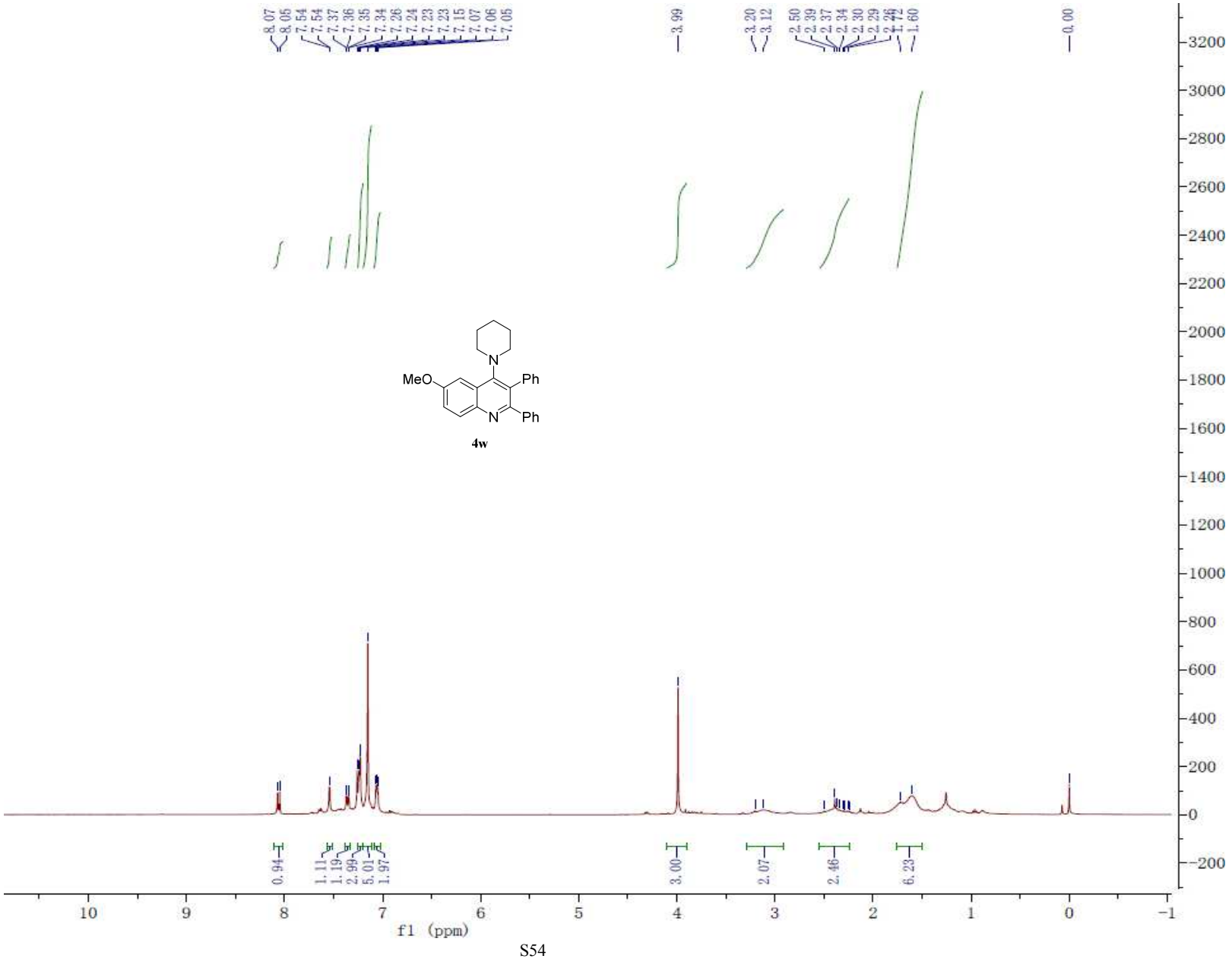
50
40
30
20
10
0
f1 (ppm)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7.34
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7.24
7.23
7.23
7.15
7.07
7.06
7.05
3.99
3.20
3.12
2.50
2.39
2.37
2.34
2.30
2.29
1.60
0.00
MeO
Ph
Ph
N
N
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3.00
2.07
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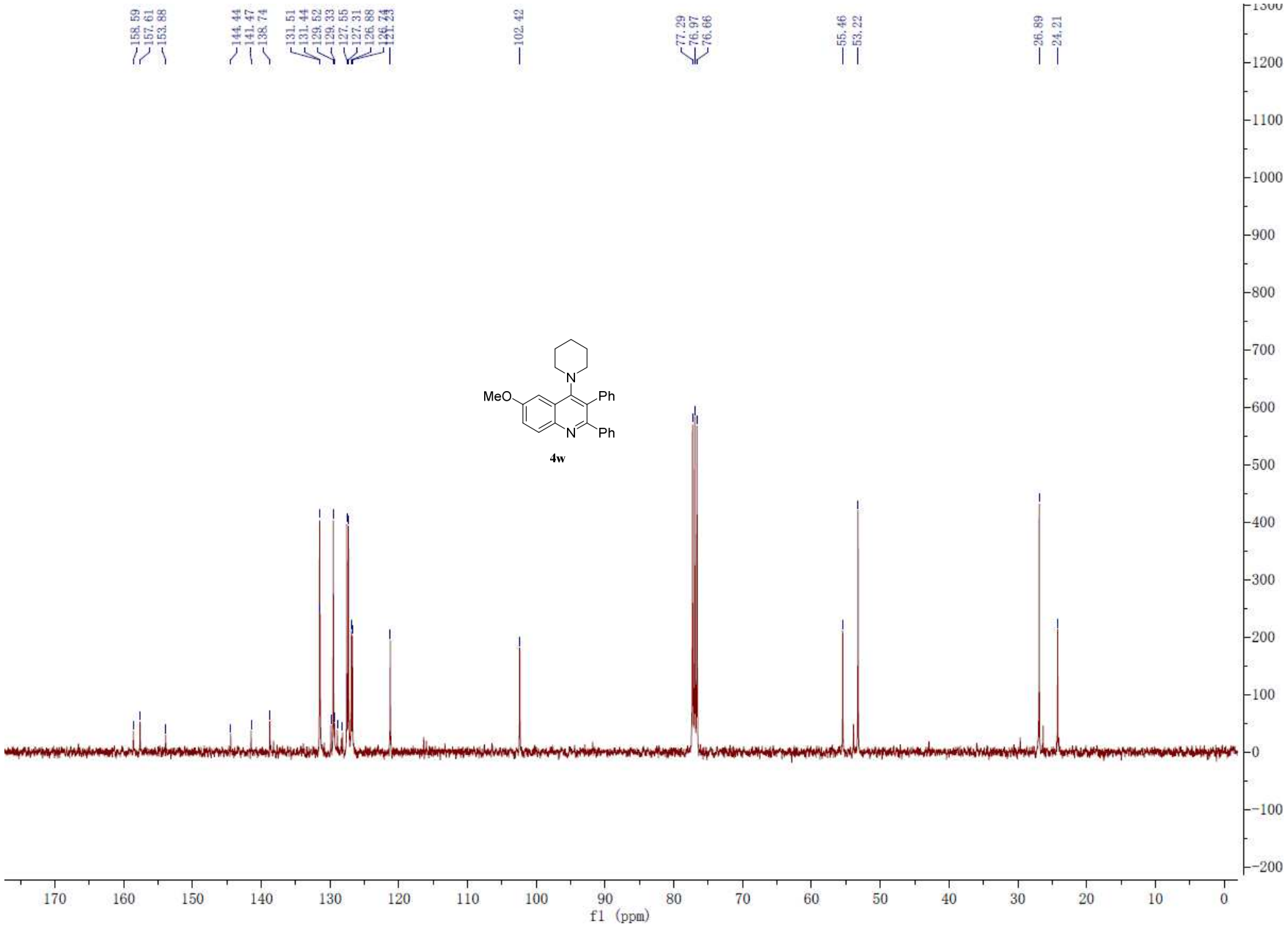
6.23
f1 (ppm)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127.55
127.31
126.88
121.23
102.42
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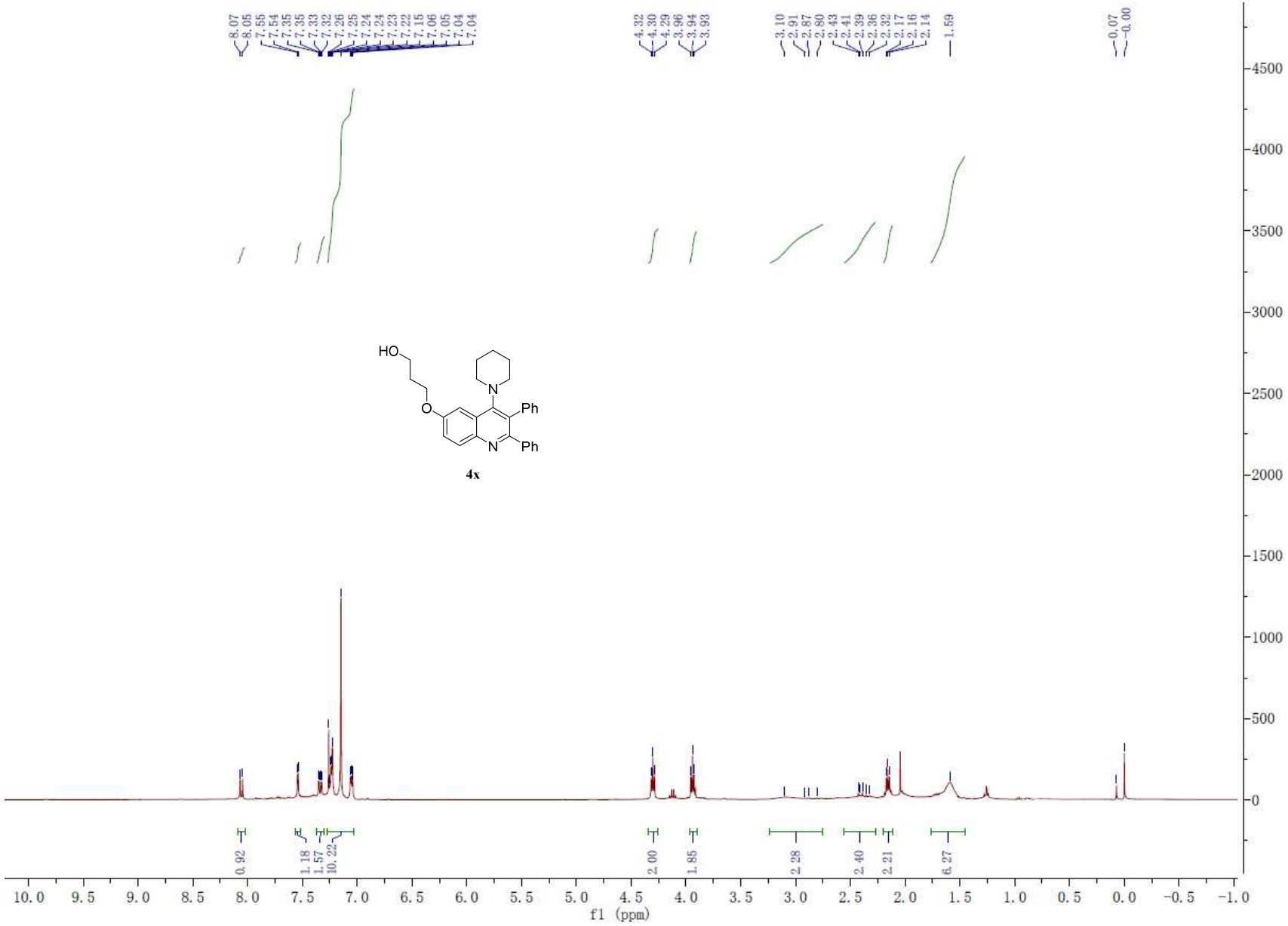
55.46
53.22
26.89
24.21
MeO
Ph
Ph
N
N
4w
f1 (ppm)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7.54
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7.32
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7.25
7.24
7.24
7.23
7.22
7.15
7.06
7.05
7.04
7.04
4.32
4.30
4.29
3.96
3.94
3.93
3.10
2.91
2.87
2.80
2.43
2.41
2.39
2.36
2.32
2.17
2.16
2.14
1.59
0.07
0.00
HO
O
N
Ph
N
Ph
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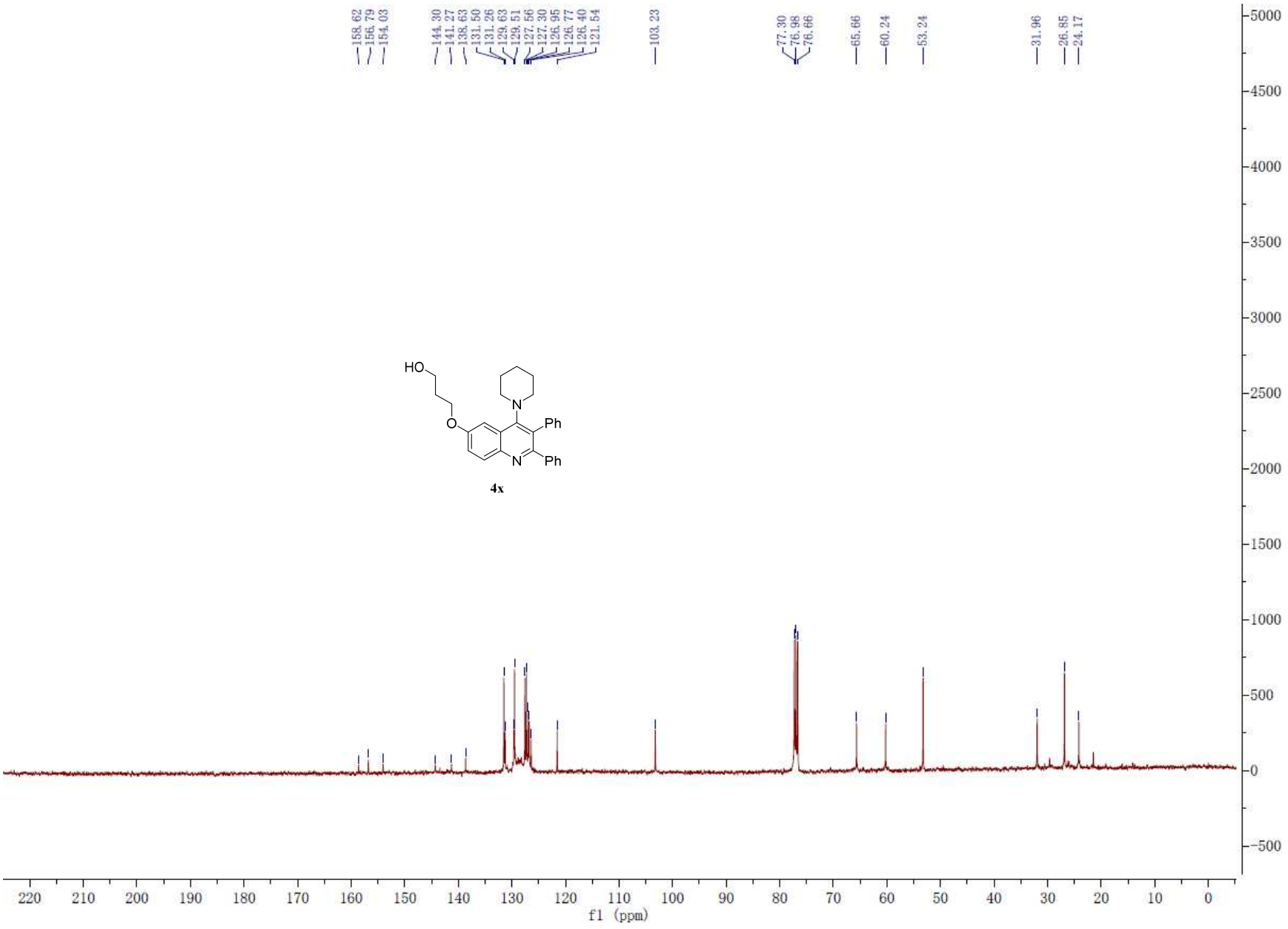
6.27
f1 (ppm)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126.95
126.77
126.40
121.54
103.23
77.30
76.98
76.66
65.66
60.24
53.24
31.96
26.85
24.17
HO
O
N
Ph
N
Ph
4x
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
220
210
200
190
180
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120
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70
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50
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10
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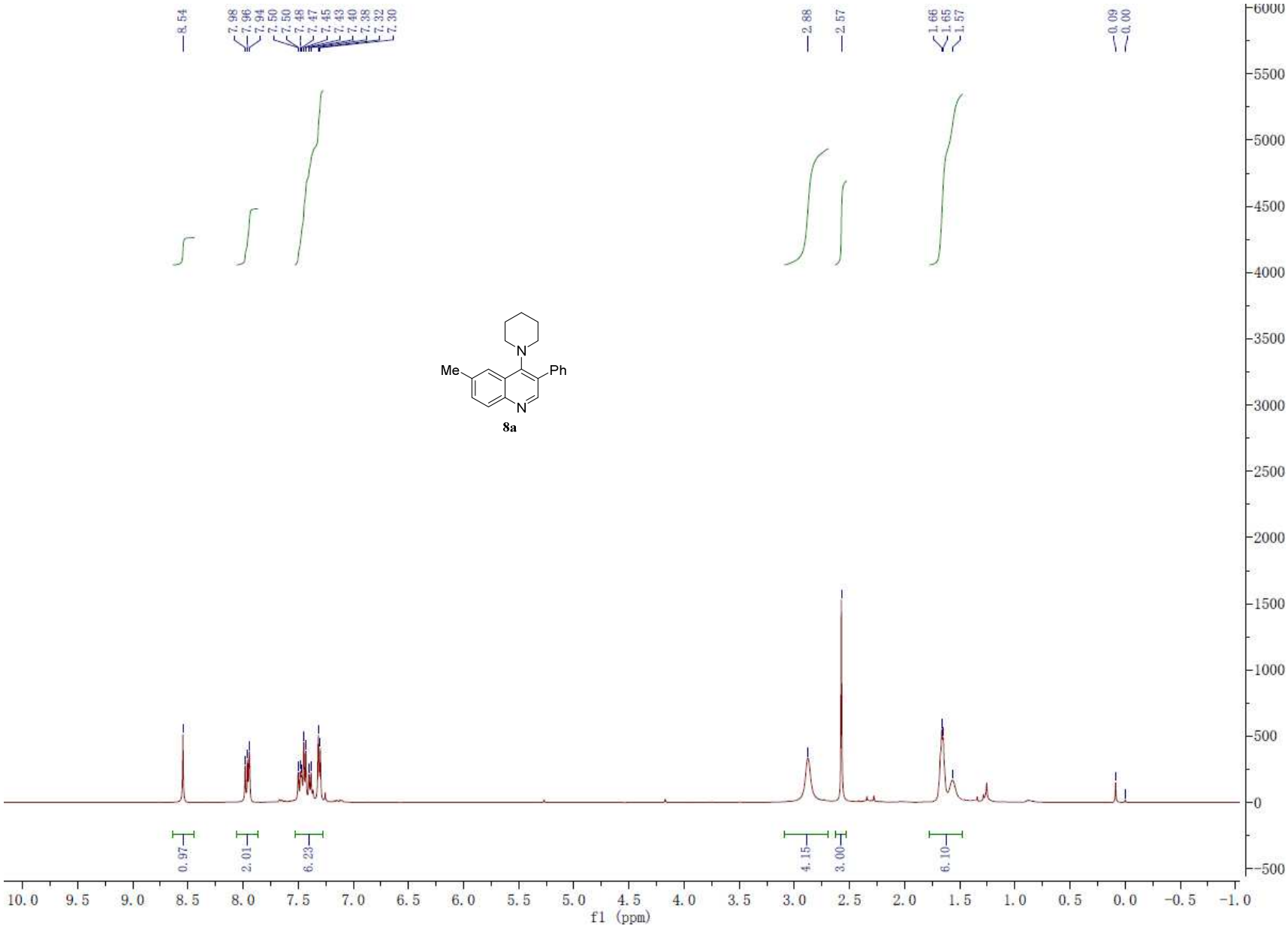
f1 (ppm)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7.38
7.32
7.30
2.88
2.57
1.66
1.65
1.57
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Ph
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N
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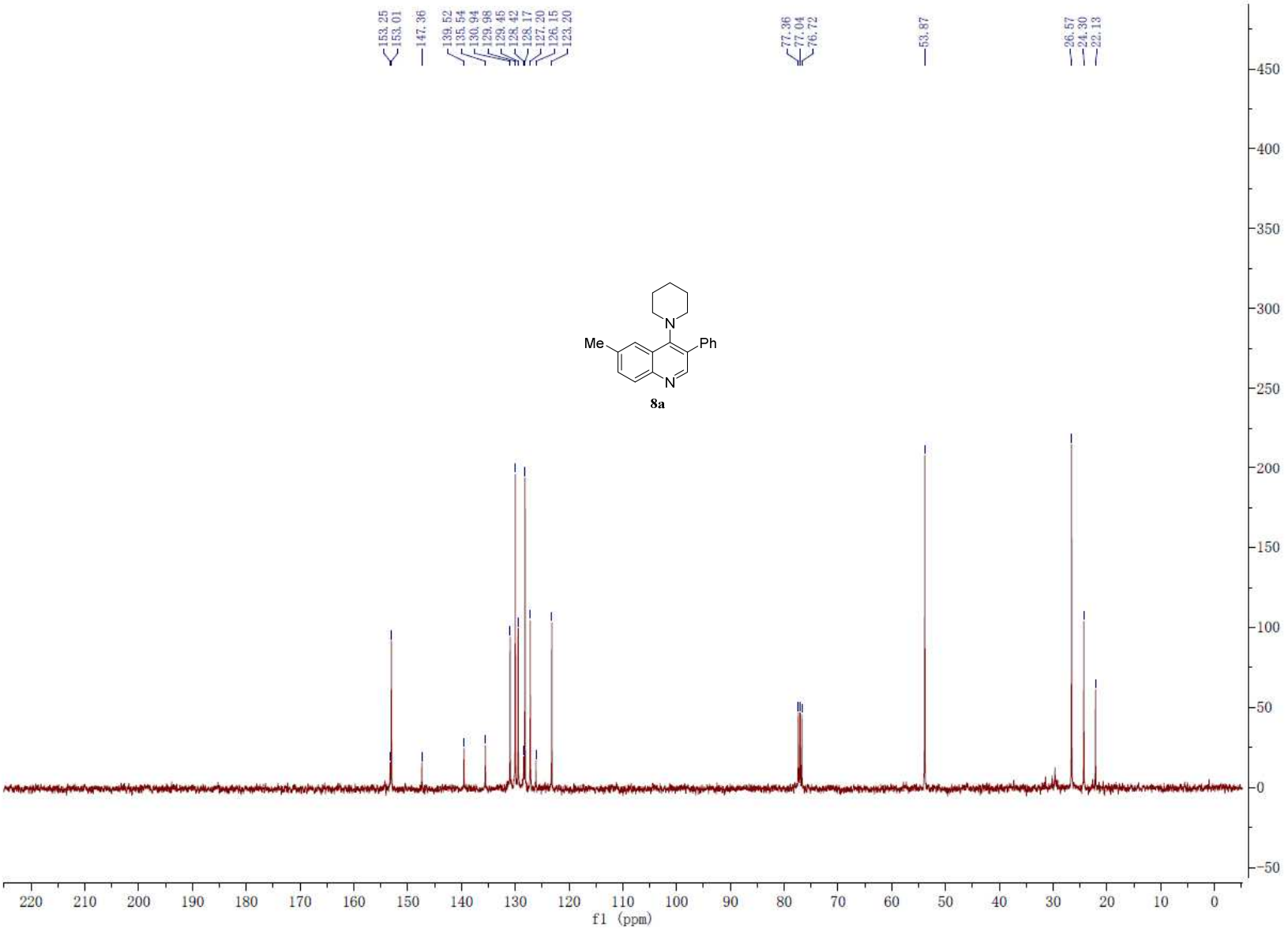
0.97
2.01
6.23
4.15
3.00
6.10
f1 (ppm)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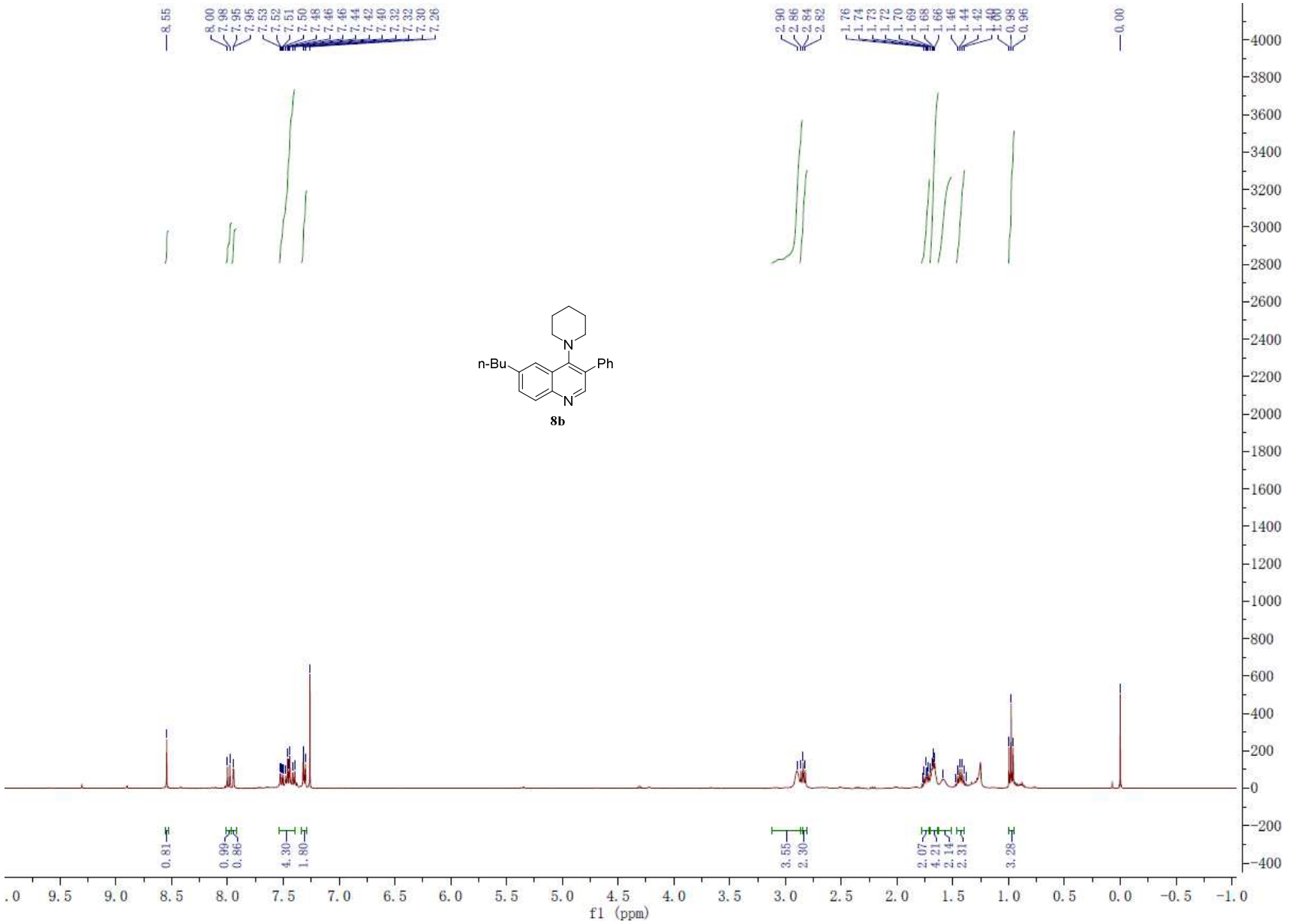
26.57
24.30
22.13
Me
Ph
N
N
8a
f1 (ppm)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7.44
7.42
7.40
7.32
7.32
7.30
7.26
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2.84
2.82
1.76
1.74
1.73
1.72
1.70
1.69
1.68
1.66
1.46
1.44
1.42
0.98
0.96
0.00
n-Bu
Ph
N
N
8b
0.81
0.99
0.86
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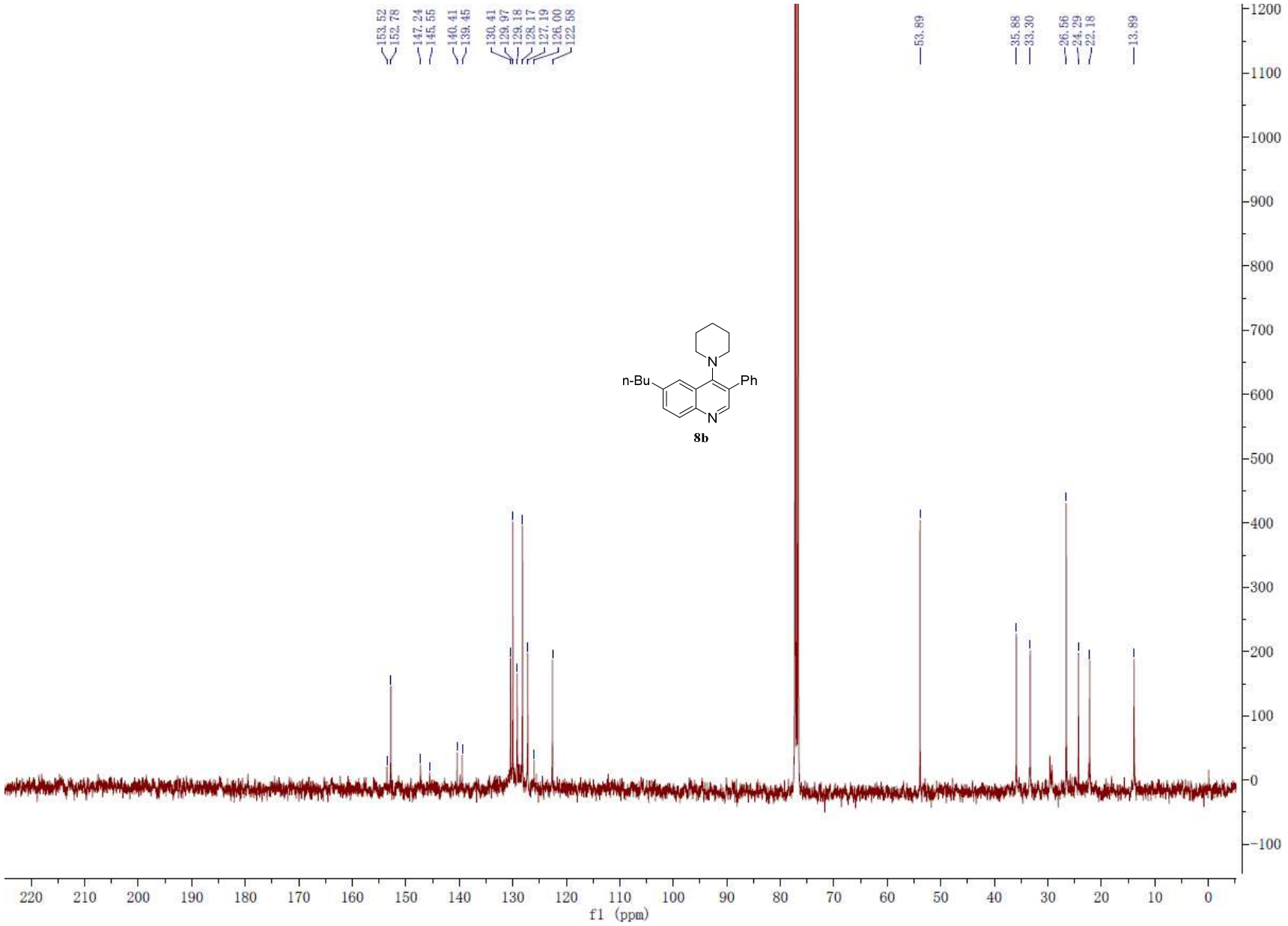
1.80
3.55
2.30
2.07
4.21
2.14
2.31
3.28
f1 (ppm)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128.17
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126.00
122.58
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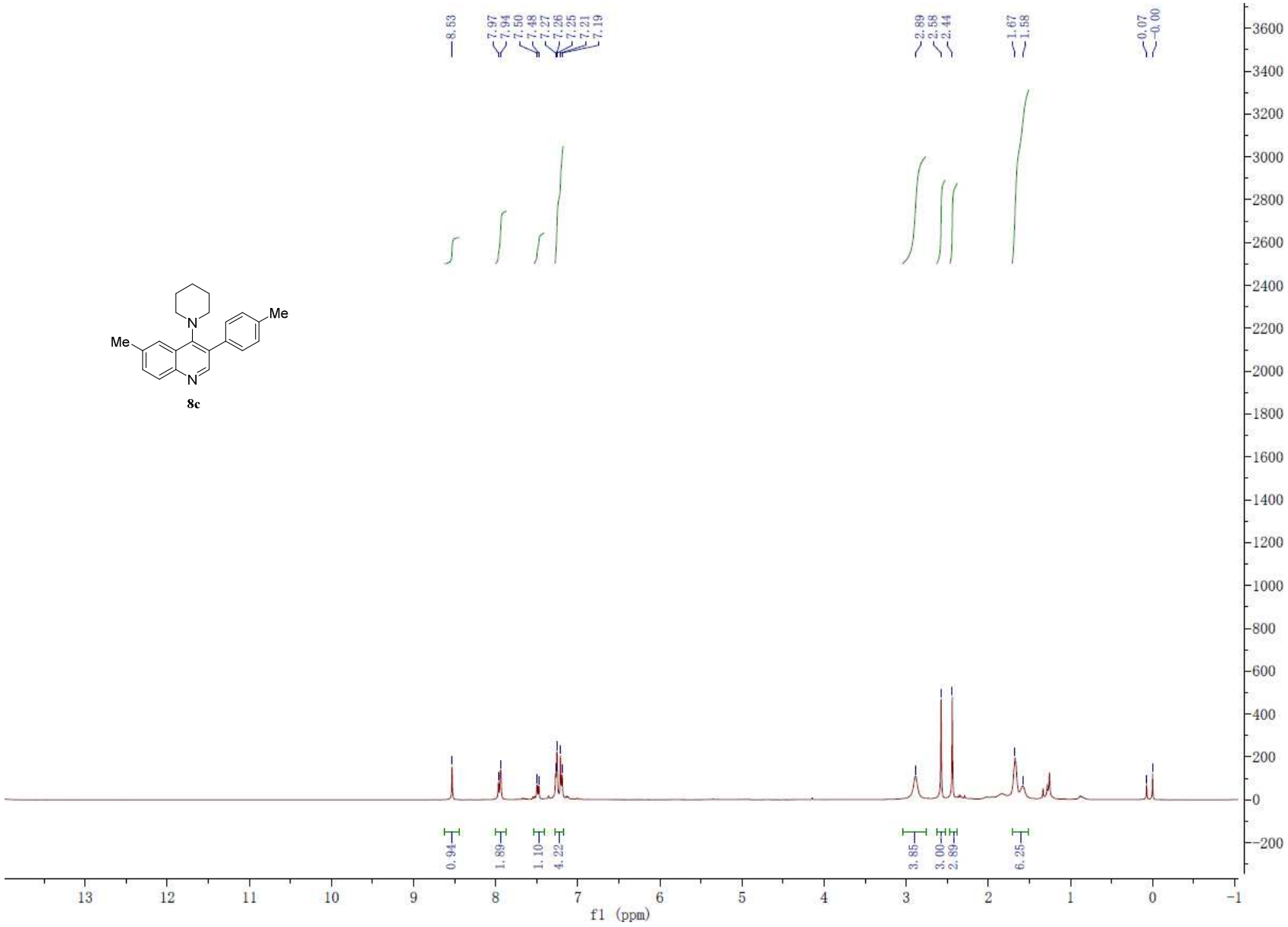
26.56
24.29
22.18
13.89
n-Bu
Ph
N
N
8b
f1 (ppm)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7.26
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7.19
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2.58
2.44
1.67
1.58
0.07
0.00
Me
Me
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N
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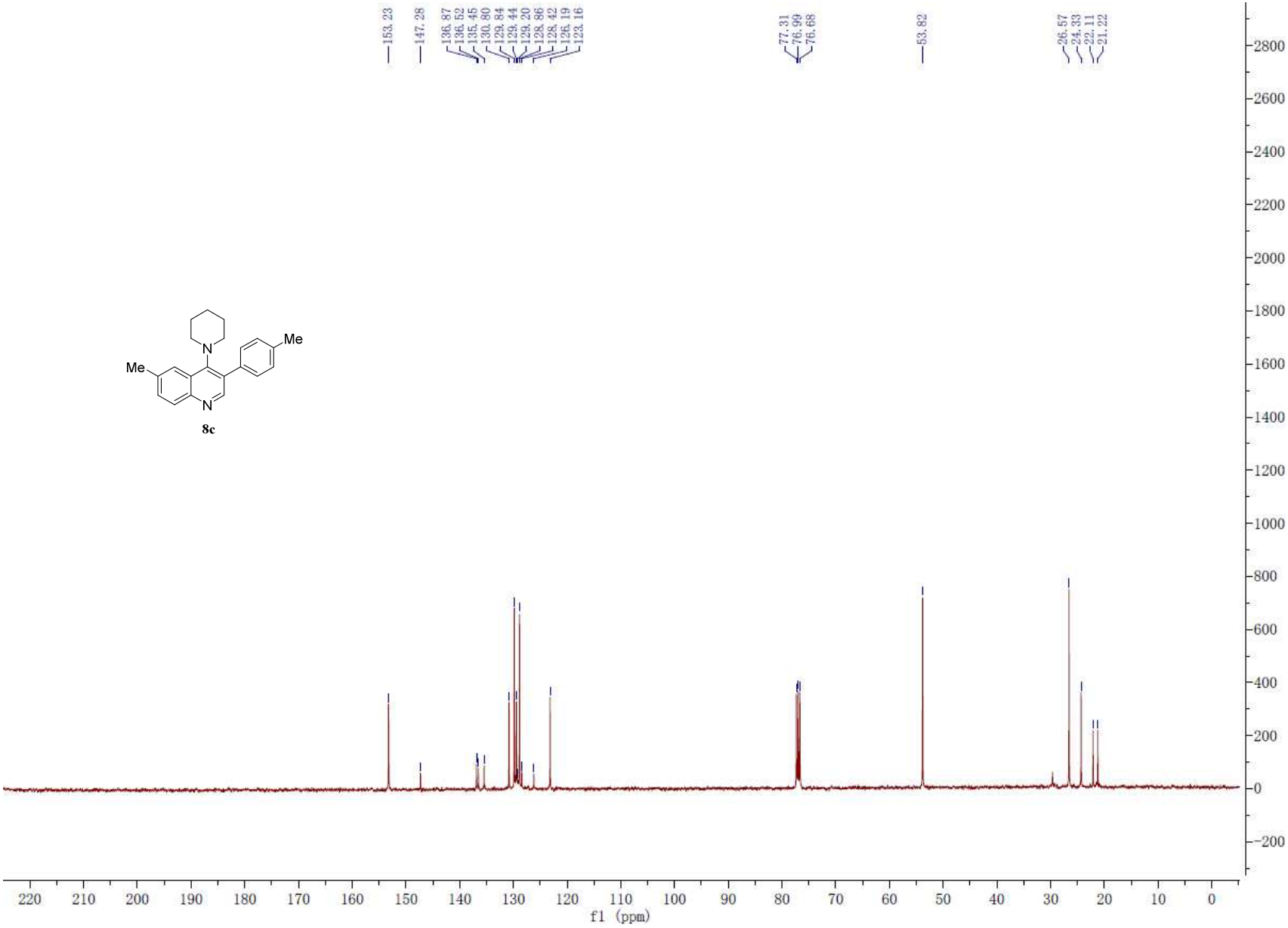
1.89
1.10
4.22
3.85
3.00
2.89
6.25
f1 (ppm)

8c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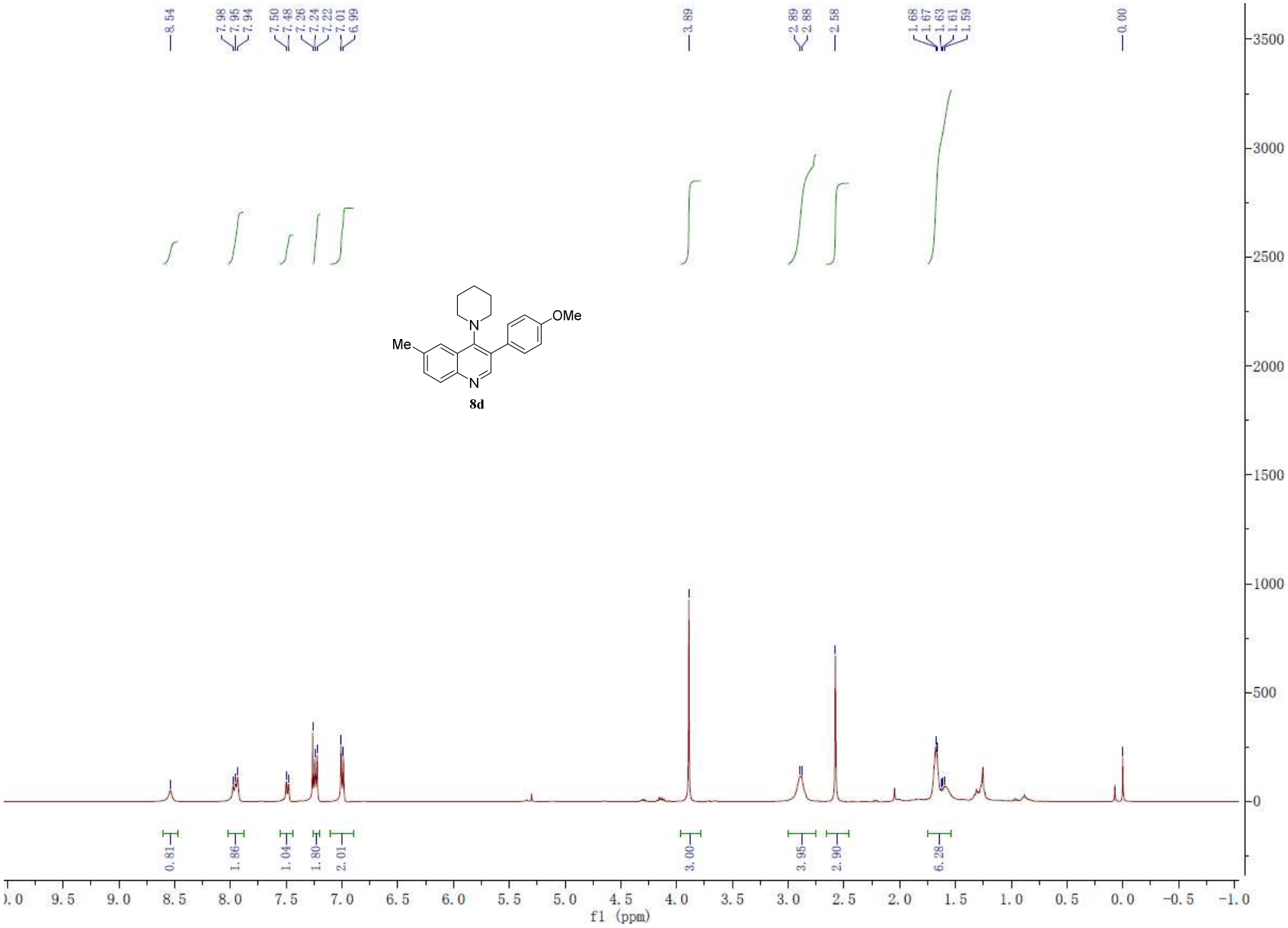
129.44
129.20
128.86
128.42
126.19
123.16
77.31
76.99
76.68
53.82
26.57
24.33
22.11
21.22
Me
Me
N
N
8c
f1 (ppm)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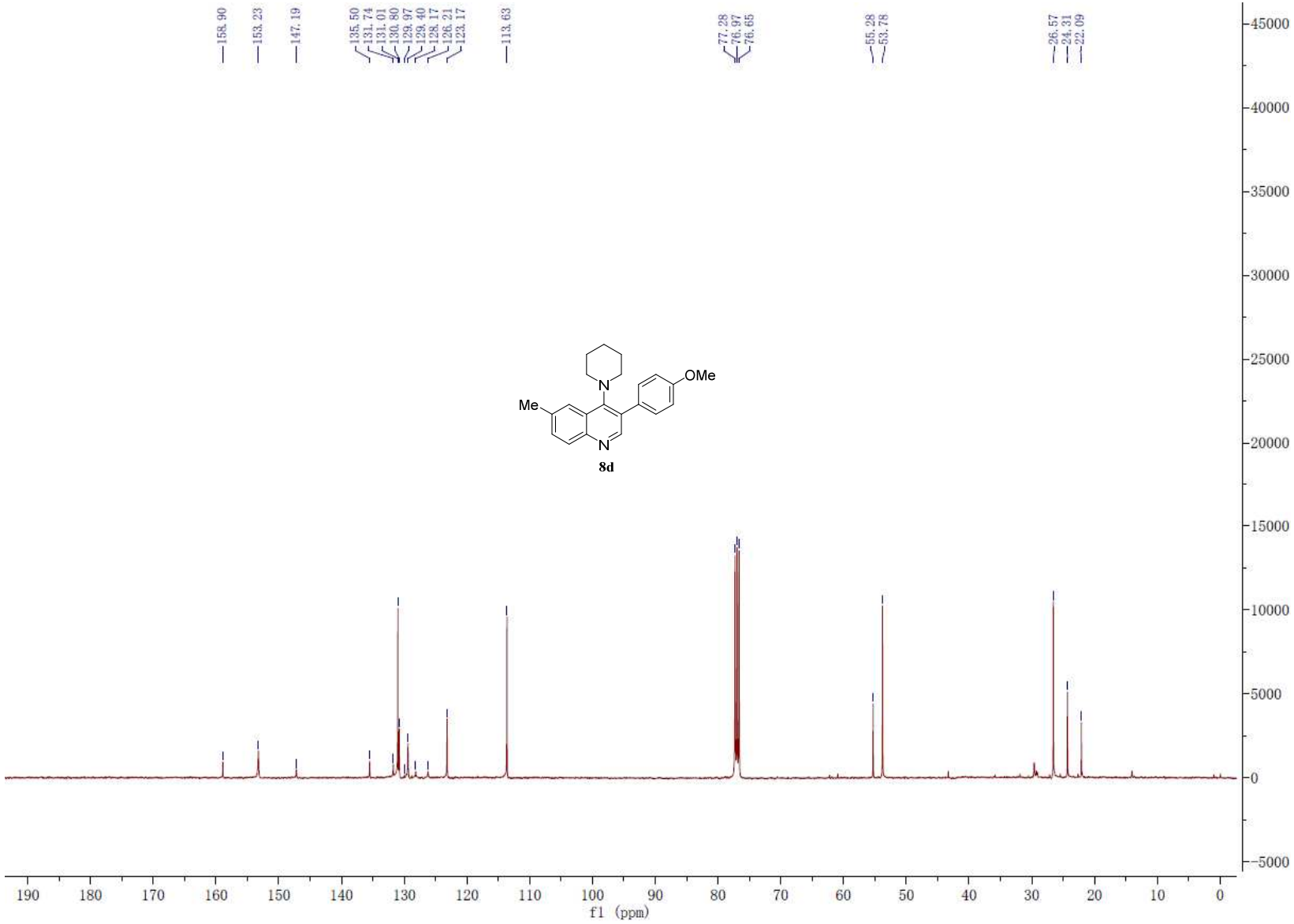
7.98
7.95
7.94
7.50
7.48
7.26
7.24
7.22
7.01
6.99
3.89
2.89
2.88
2.58
1.68
1.67
1.63
1.61
1.59
0.00
Me
OMe
N
N
8d
0.81
1.86
1.04
1.80
2.01
3.00
3.95
2.90
6.29
f1 (ppm)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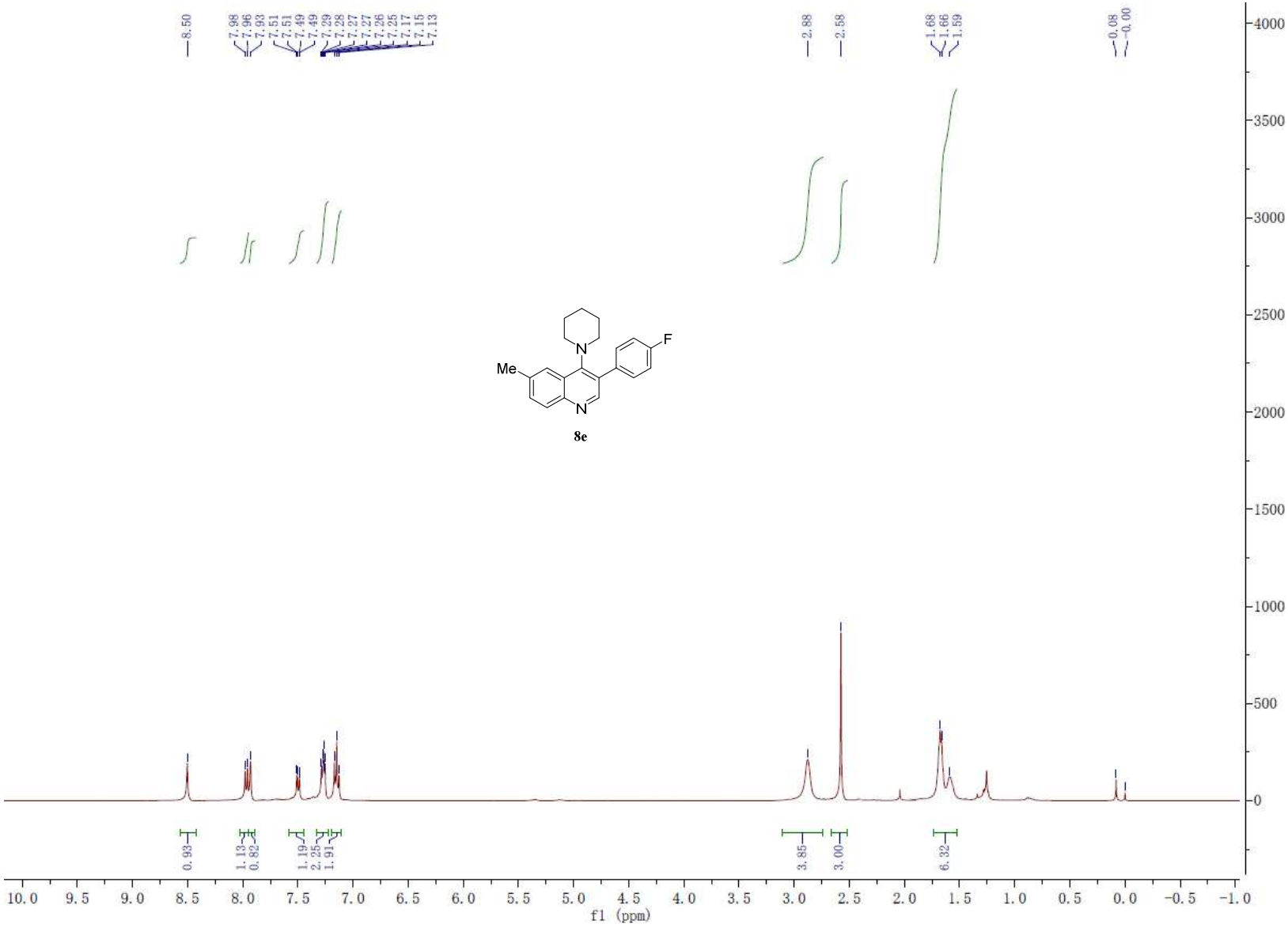
153.23
147.19
135.50
131.74
131.01
130.80
129.97
129.40
128.17
126.21
123.17
113.63
77.28
76.97
76.65
55.28
53.78
26.57
24.31
22.09
Me
OMe
N
N
8d
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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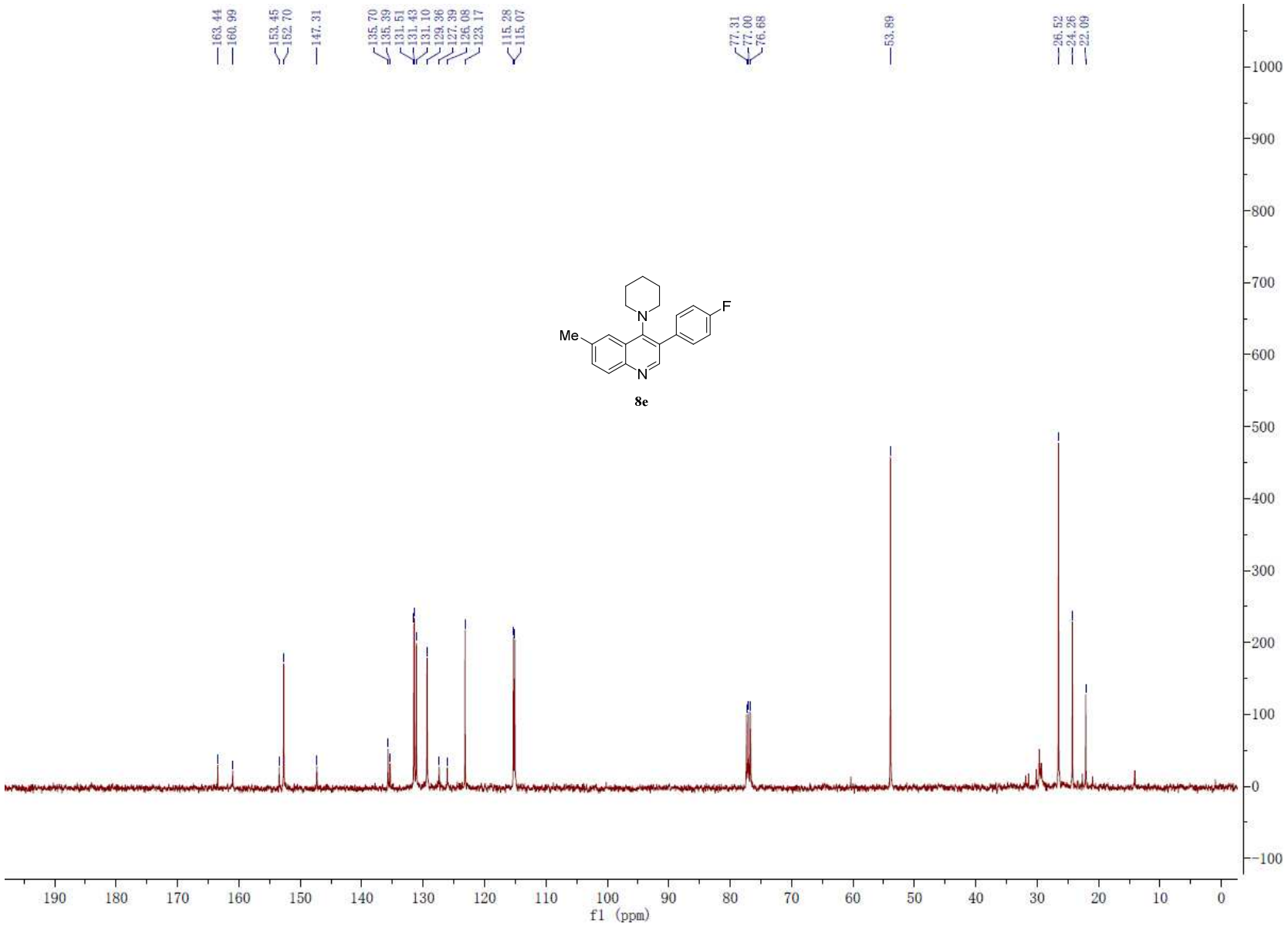
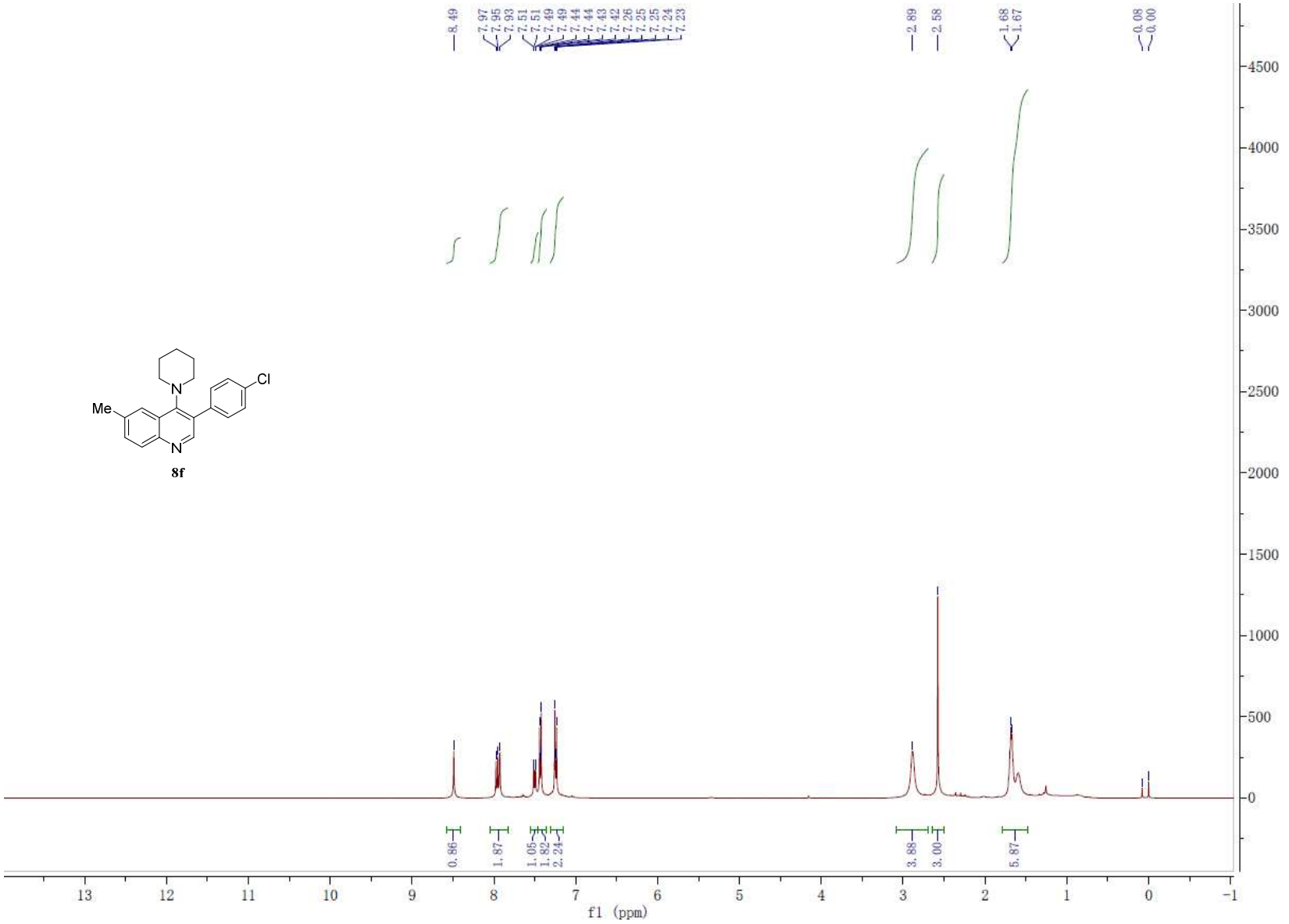
7.98
7.96
7.93
7.51
7.51
7.49
7.49
7.29
7.28
7.27
7.27
7.26
7.25
7.17
7.15
7.13
2.88
2.58
1.68
1.66
1.59
0.08
0.00
Me
N
N
F
0.93
1.13
0.82
1.19
2.25
1.91
3.85
3.00
6.32
f1 (ppm)

8e


163.44
160.99
153.45
152.70
147.31
135.70
135.39
131.51
131.43
131.10
129.36
127.39
126.08
123.17
115.28
115.07
77.31
77.00
76.68
53.89
26.52
24.26
22.09
Me
F
N
N
8e
f1 (ppm)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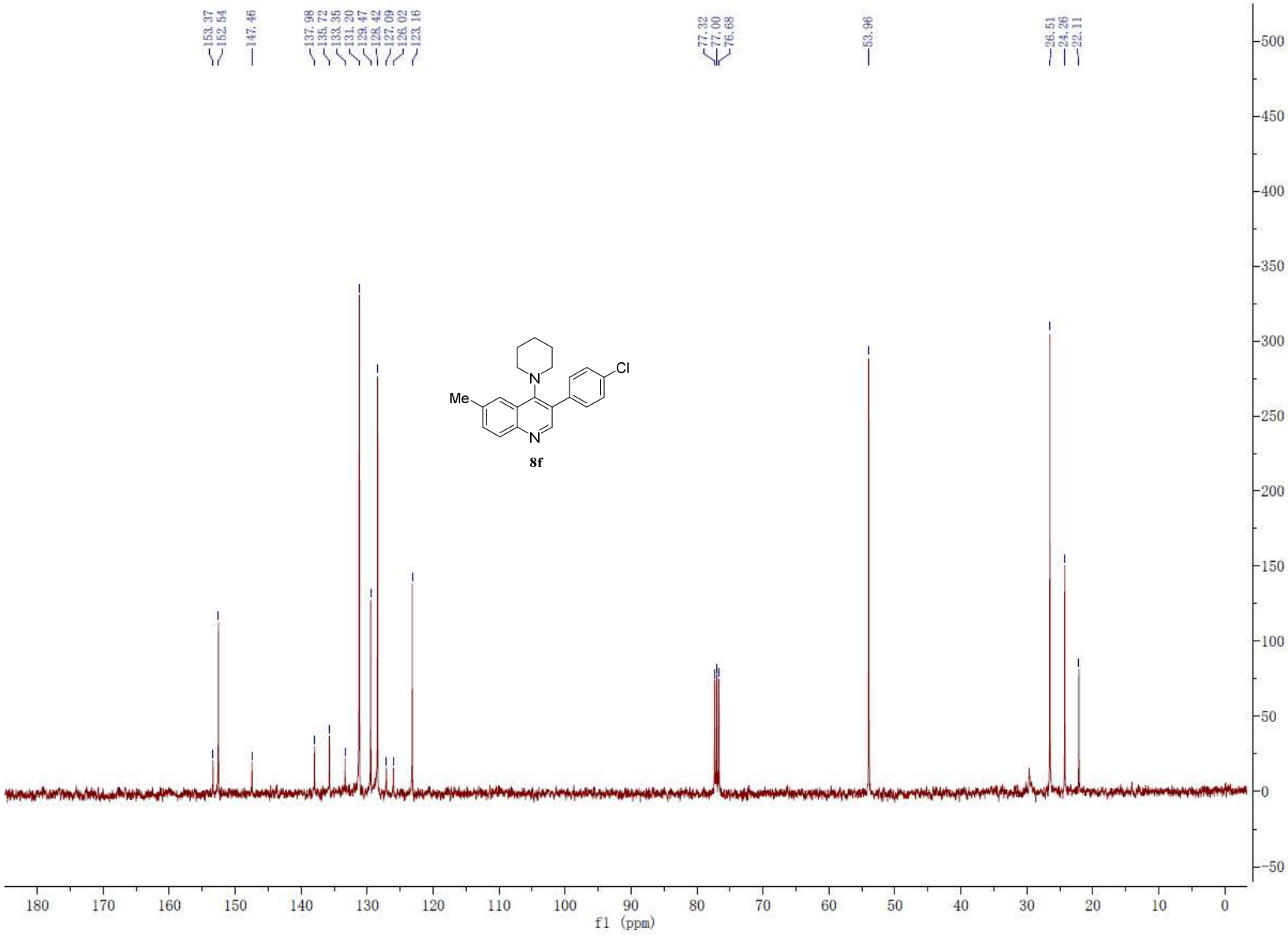
7.95
7.93
7.51
7.51
7.49
7.49
7.44
7.44
7.43
7.42
7.26
7.25
7.25
7.24
7.23
2.89
2.58
1.68
1.67
0.08
0.00
Me
N
N
Cl
8f
0.86
1.87
1.05
1.82
2.24
3.88
3.00
5.87
f1 (ppm)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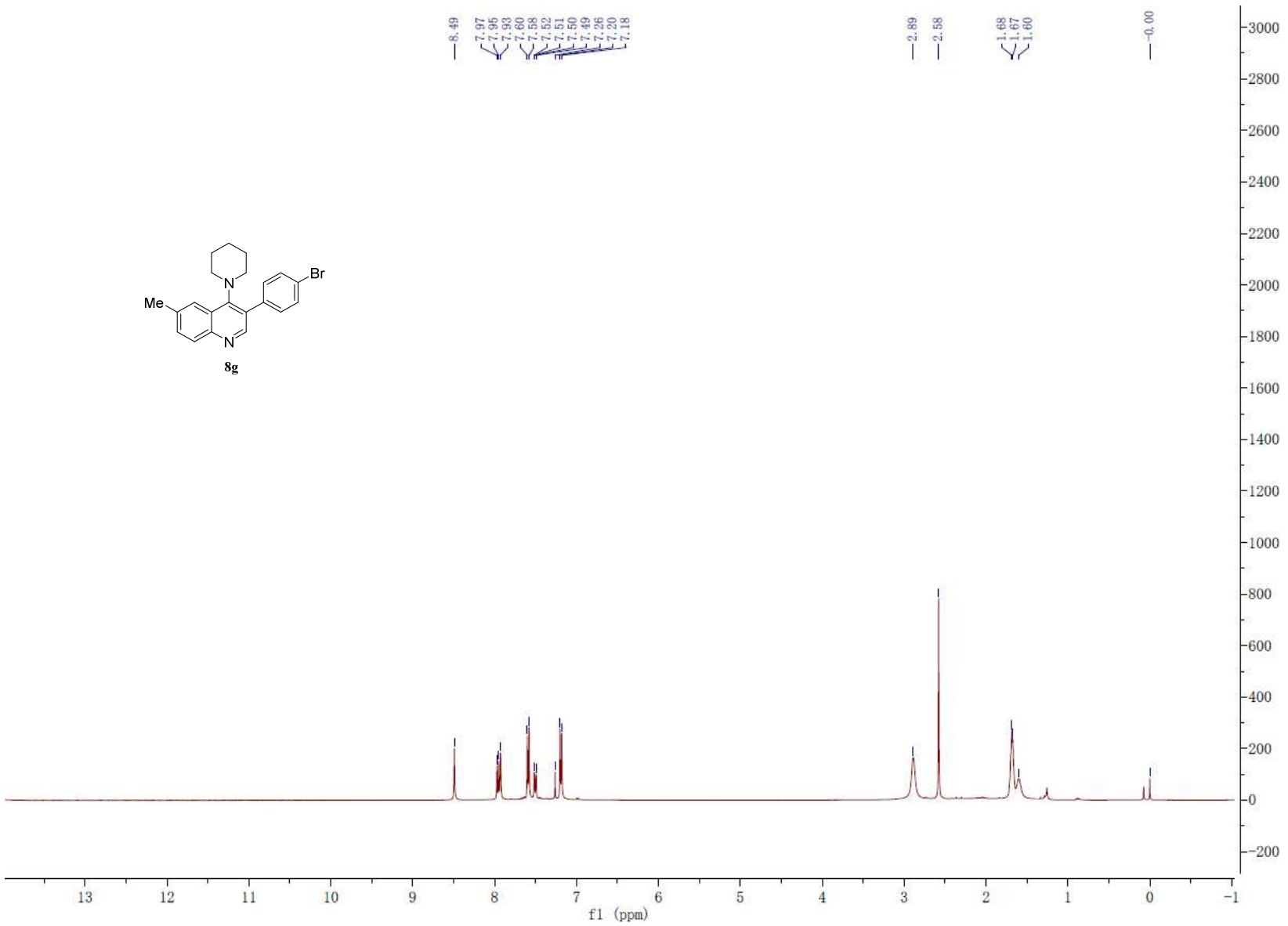
152.54
147.46
137.98
135.72
133.35
131.20
129.47
128.42
127.09
126.02
123.16
77.32
77.00
76.68
53.96
26.51
24.26
22.11
Me
Cl
N
N
8f
fl (ppm)


8.49
7.97
7.95
7.93
7.60
7.58
7.52
7.51
7.50
7.49
7.26
7.20
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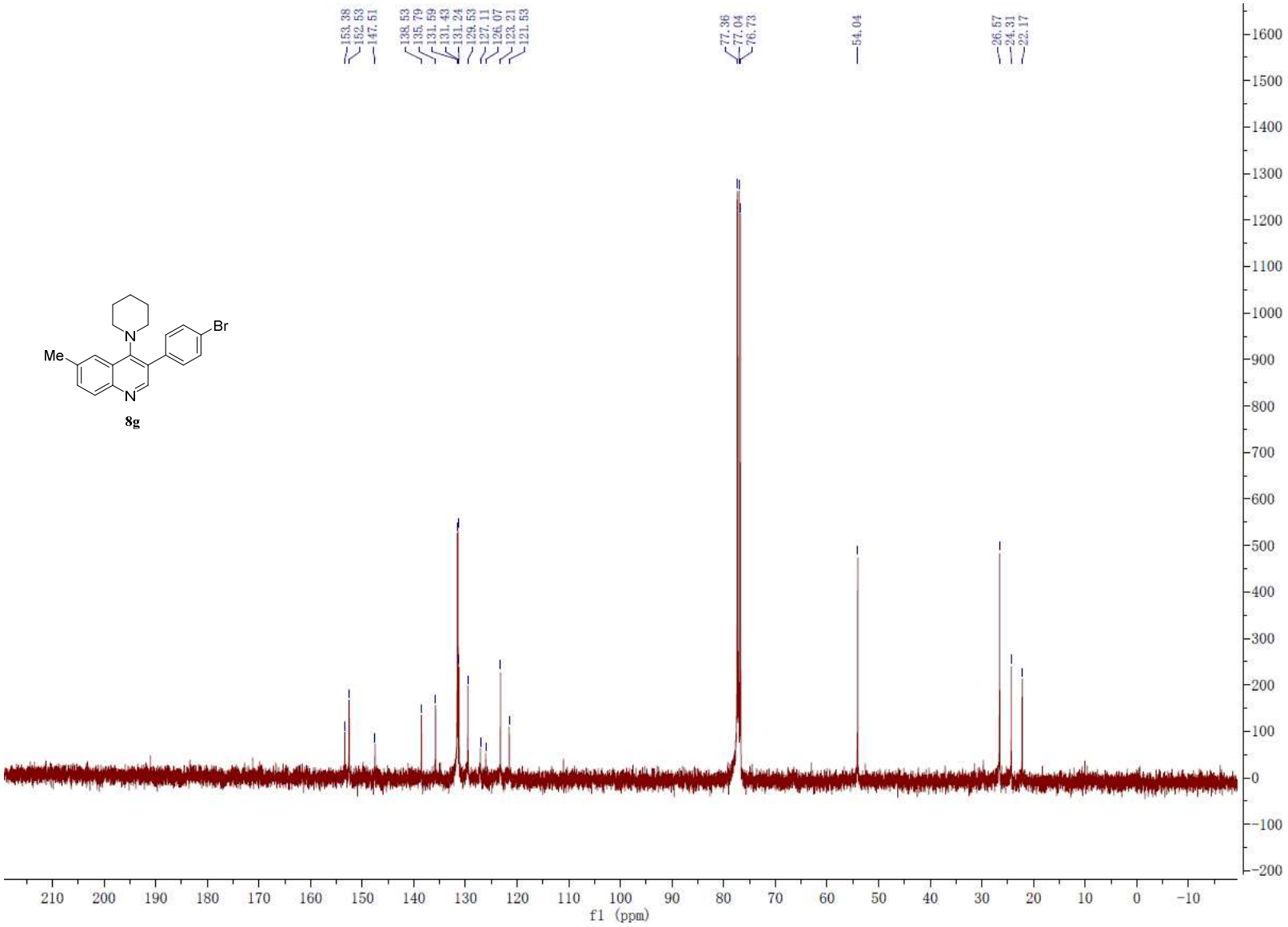
0.00
Me
Br
N
N
8g
f1 (ppm)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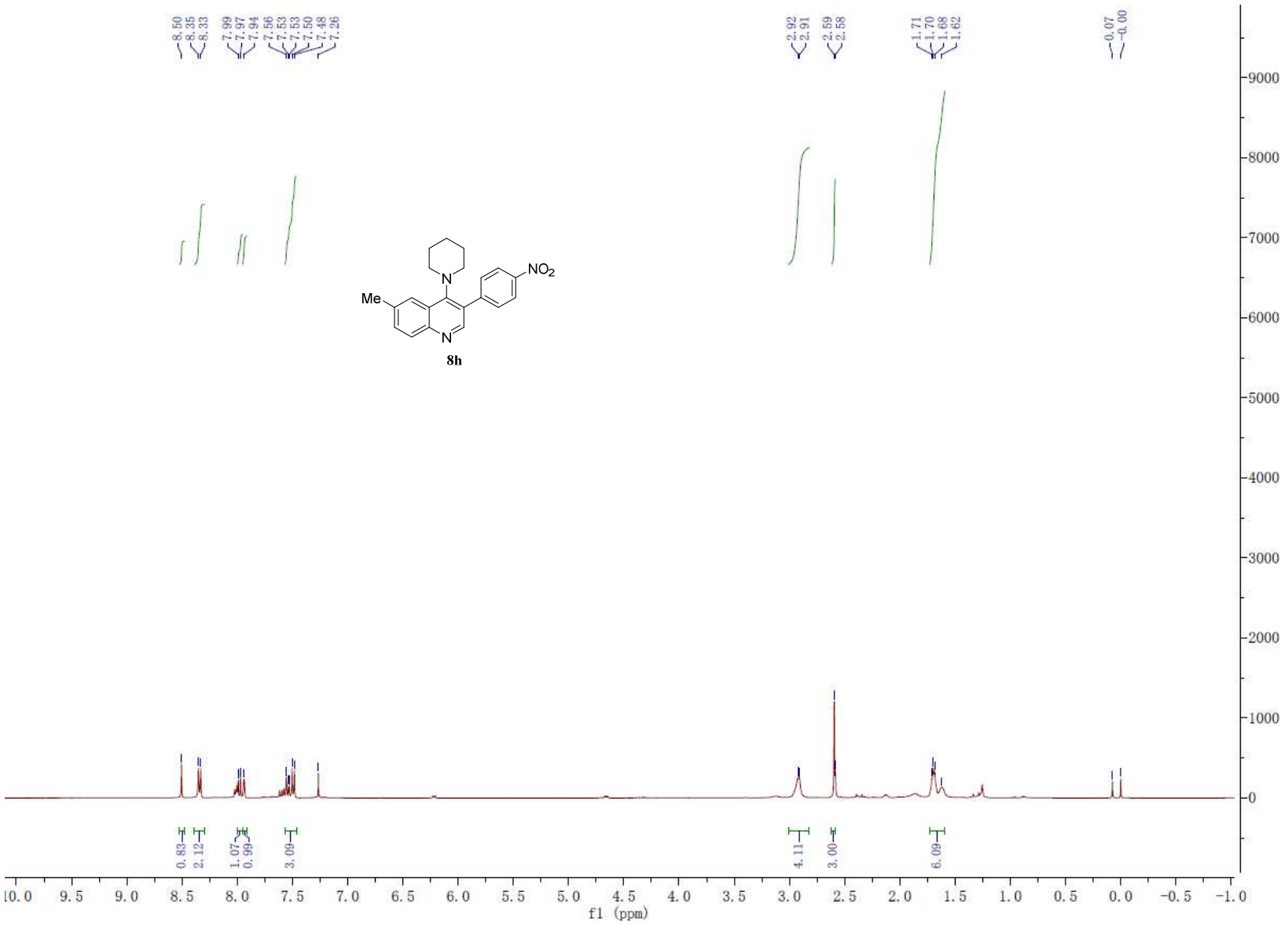
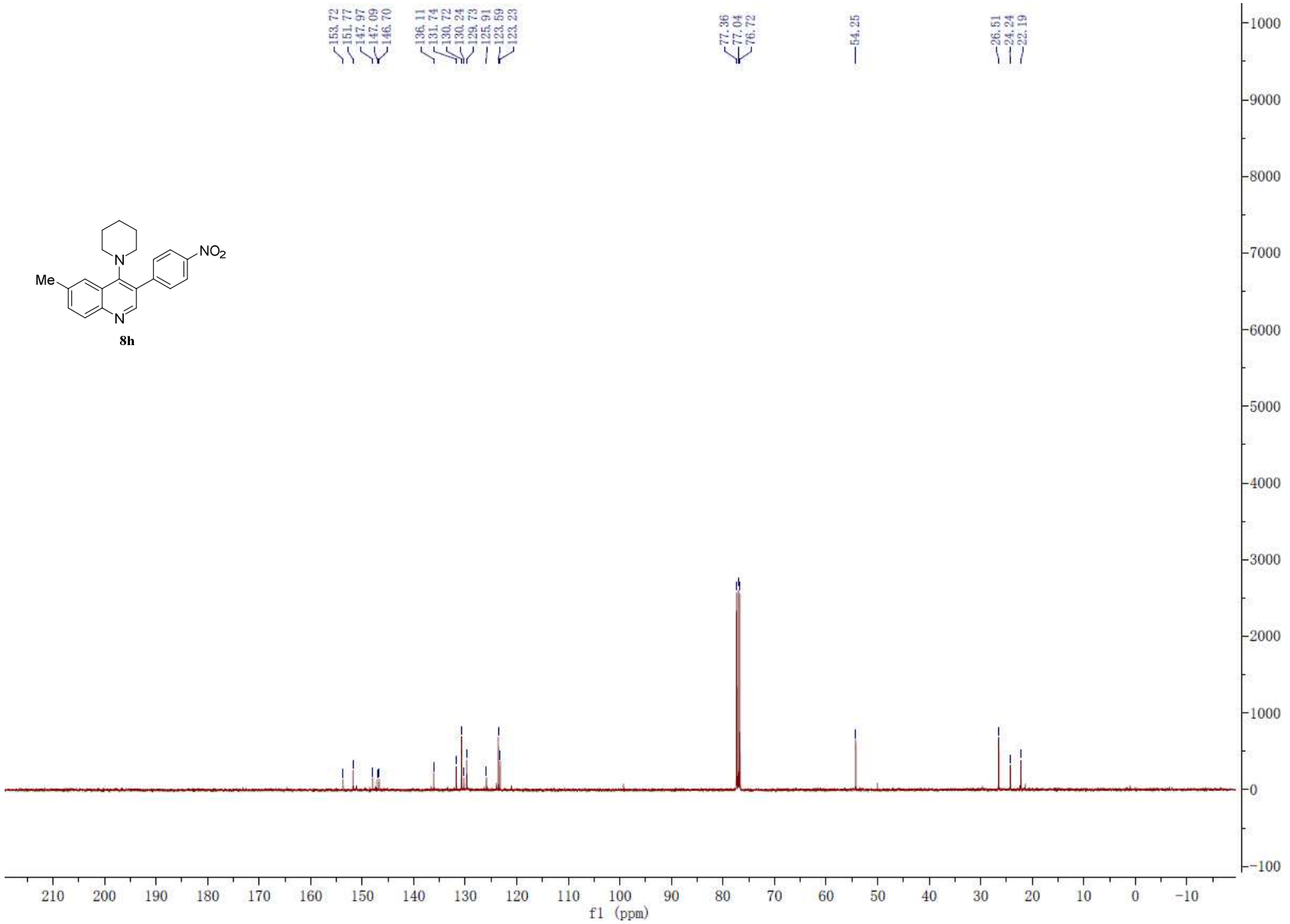
152.53
147.51
138.53
135.79
131.59
131.43
131.24
129.53
127.11
126.07
123.21
121.53
77.36
77.04
76.73
54.04
26.57
24.31
22.17
Me
Br
N
N
8g
f1 (ppm)


8.50
8.35
8.33
7.99
7.97
7.94
7.56
7.53
7.53
7.50
7.48
7.26
2.92
2.91
2.59
2.58
1.71
1.70
1.68
1.62
0.07
0.00
Me
N
N
NO2
8h
0.83
2.12
1.07
0.99
3.09
4.11
3.00
6.09
f1 (ppm)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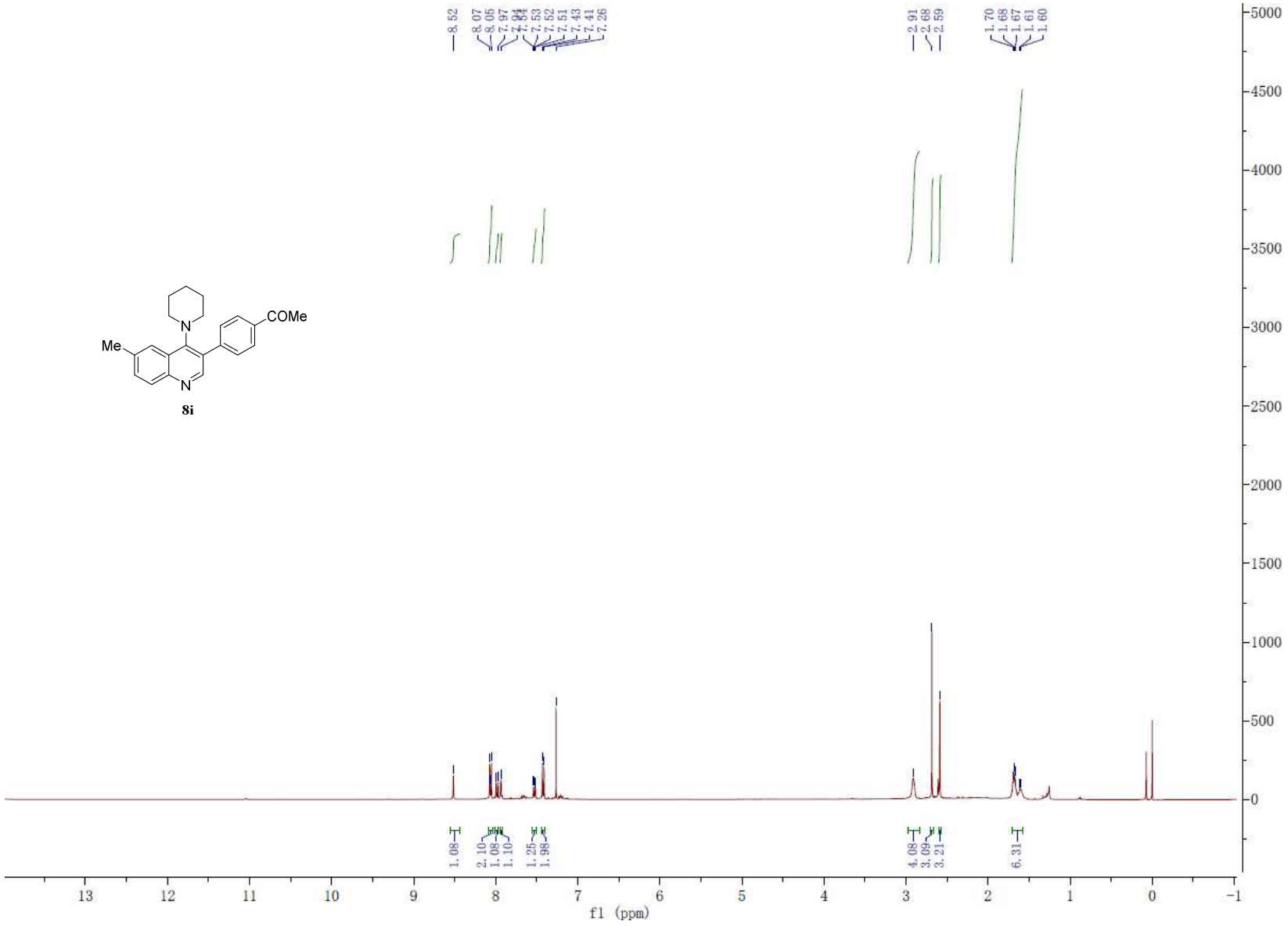
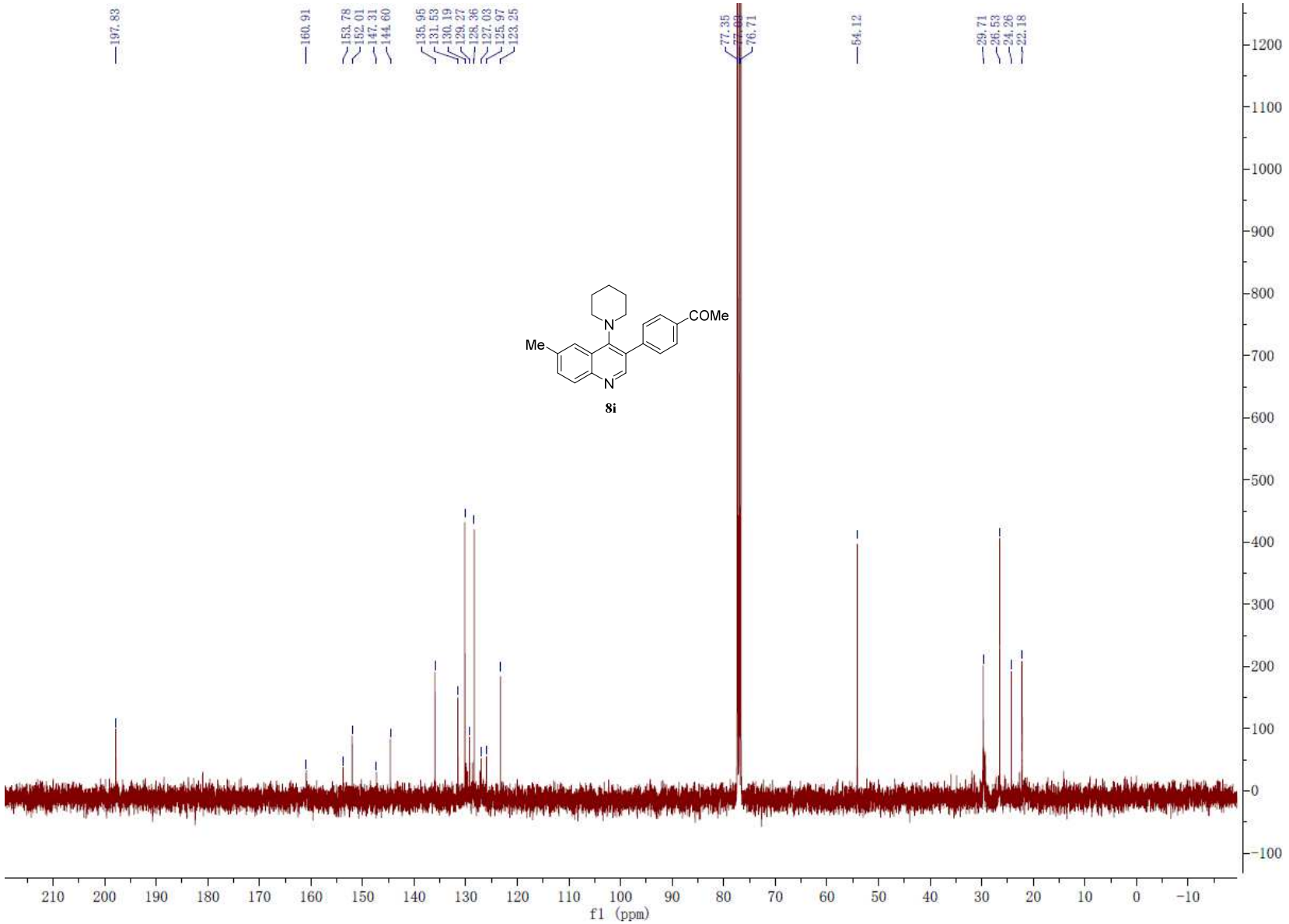
151.77
147.97
147.09
146.70
136.11
131.74
130.72
130.24
129.73
125.91
123.59
123.23
77.36
77.04
76.72
54.25
26.51
24.24
22.19
Me
NO2
N
N
8h
f1 (ppm)


8.52
8.07
8.05
7.97
7.84
7.53
7.52
7.51
7.43
7.41
7.26
2.91
2.68
2.59
1.70
1.68
1.67
1.61
1.60
COMe
Me
N
N
1.08
2.10
1.08
1.10
1.25
1.98
4.08
3.09
3.21
6.31
f1 (ppm)

8i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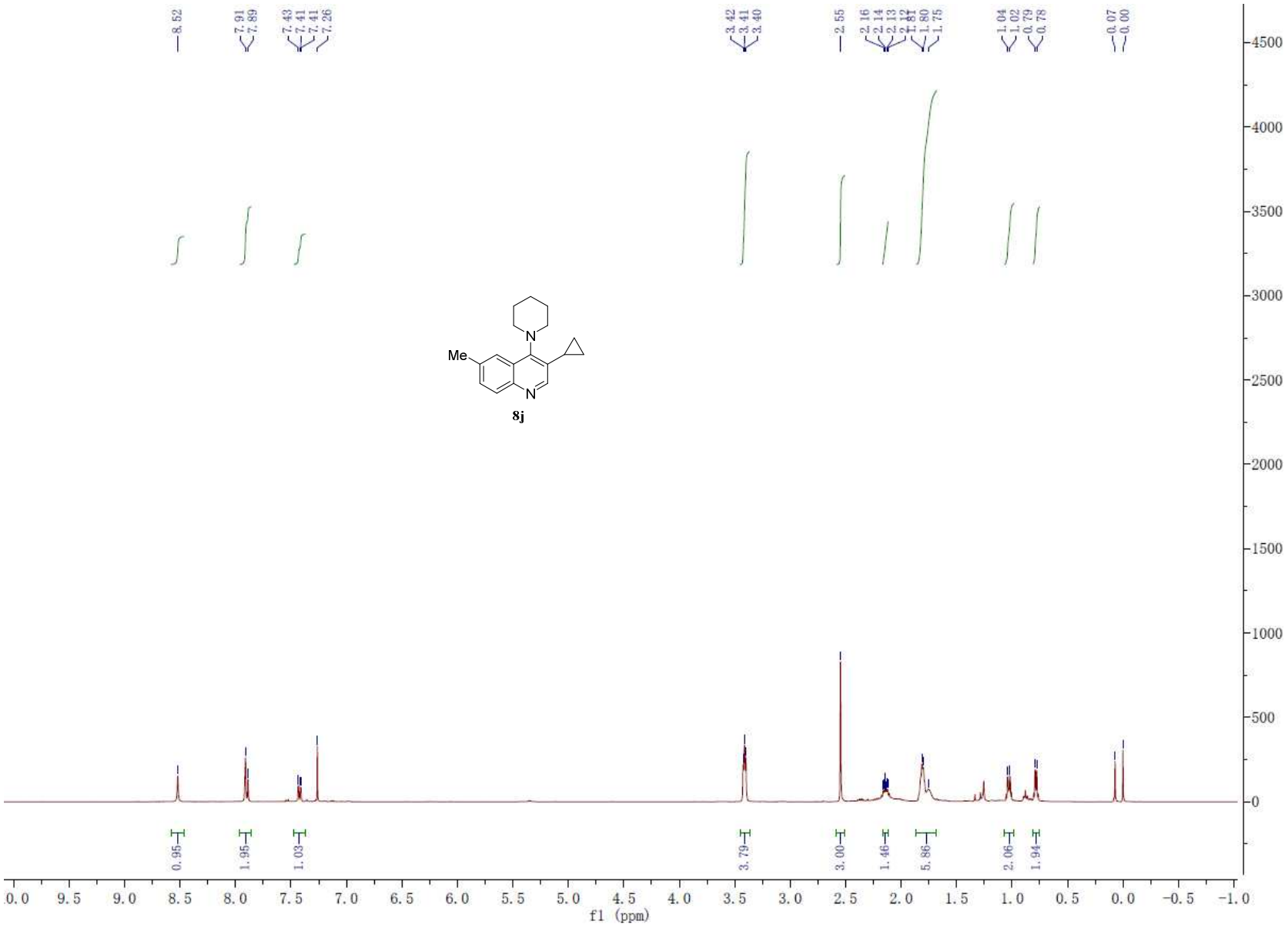
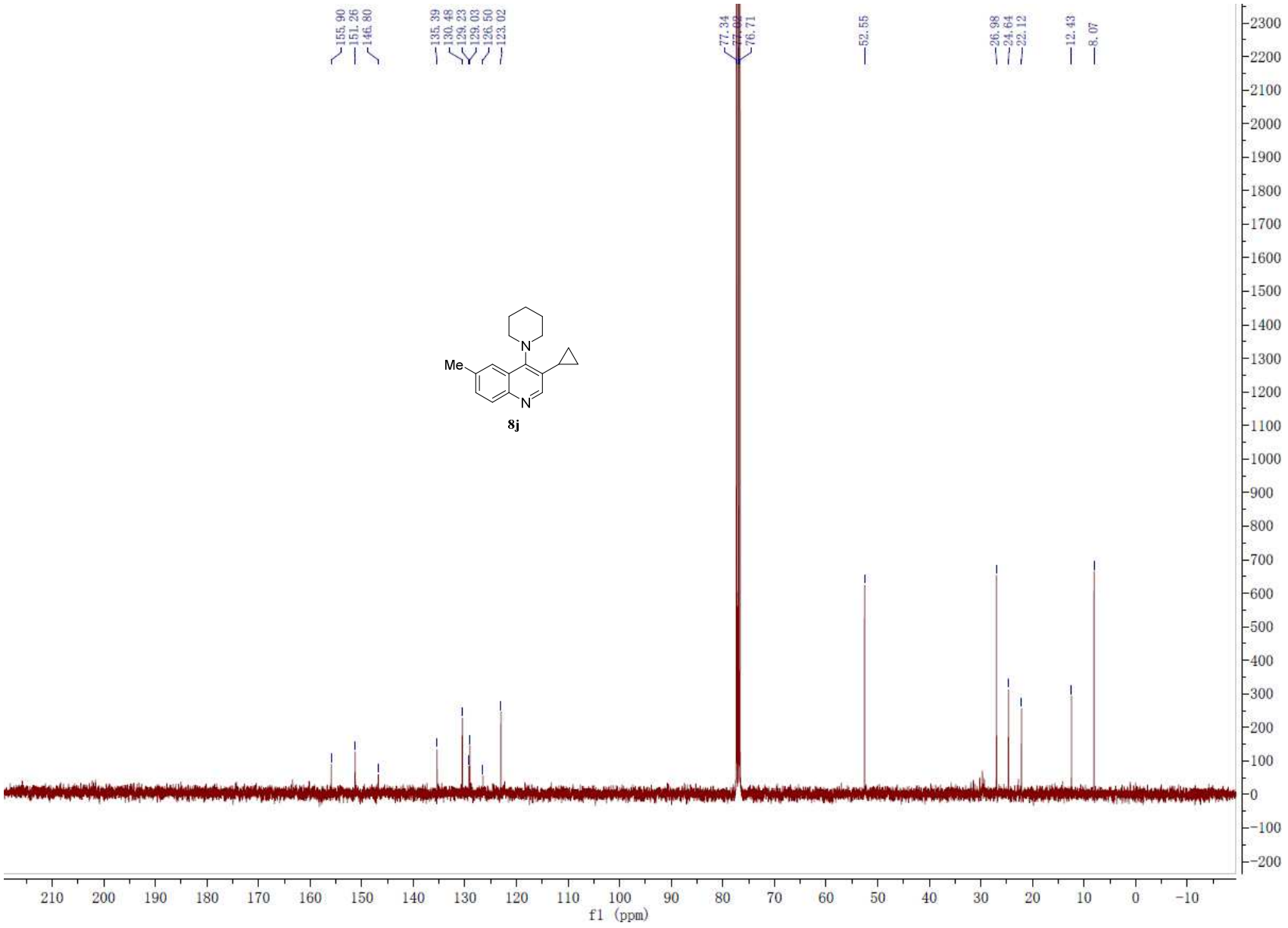
160.91
153.78
152.01
147.31
144.60
135.95
131.53
130.19
129.27
128.36
127.03
125.97
123.25
77.35
77.03
76.71
54.12
29.71
26.53
24.26
22.18
COMe
Me
N
N
8i
f1 (ppm)


8.52
7.91
7.89
7.43
7.41
7.41
7.26
3.42
3.41
3.40
2.55
2.16
2.14
2.13
2.12
1.81
1.80
1.75
1.04
1.02
0.79
0.78
0.07
0.00
Me
N
N
8j
0.95
1.95
1.03
3.79
3.00
1.46
5.86
2.06
1.94
f1 (ppm)


155.90
151.26
146.80
135.39
130.48
129.23
129.03
126.50
123.02
77.34
77.09
76.71
52.55
26.98
24.64
22.12
12.43
8.07
Me
N
N
8j
f1 (ppm)