Assembly of Isoquinolines via CuI-catalyzed Coupling of β-Keto Esters and 2-Halobenzylamines

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Supporting information

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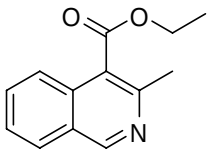
Experimental Section

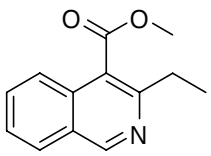
General methods. ^{1}H NMR or ^{13}C NMR spectra were recorded on Varian EM360A, EM-390, Bruker AMX-300. Proton chemical shifts were given in relative to tetramethylsilane (δ 0.00 ppm) in $CDCl_3$. Carbon chemical shifts were internally referenced to the deuterated solvent signals in $CDCl_3$ (δ 77.00 ppm). Mass spectra were recorded on a Shimadzu LCMS-2010EV mass spectrometer (ESI). High resolution mass spectra were recorded on IonSpec 4.7 Tesla FTMS mass spectrometer (ESI) or Waters Micromass GCT mass spectrometer (EI).

General Procedure for synthesis of isoquinolines. An oven-dried Schlenk tube was charged with CuI (10 mg, 0.05 mmol), and potassium carbonate (207 mg, 1.5 mmol), and 2-bromobenzylamine (0.5 mmol). The tube was evacuated and backfilled with argon (3 times), and then 2-bromobenzylamine, ethyl acetoacetate (130 μL, 1 mmol) and *i*-PrOH (1.5 mL) were added. The reaction mixture was stirred at 90 ^{o}C for 24-28 h. The cooled mixture was stirred at room temperature under the air atmosphere for 12-24 h before it was partitioned between ethyl acetate (40 mL) and saturated brine (10 mL). The organic layer was dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by silica gel chromatography to give the desired product.



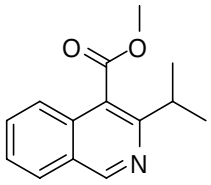
6a

Ethyl 3-methylisoquinoline-4-carboxylate (6a). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 8.7 Hz, 1H), 7.74(t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 4.57 (q, *J* = 7.5 Hz, 2H), 2.75 (s, 3H), 1.48(t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 153.3, 149.5, 133.2, 131.4, 127.9, 126.8, 126.5, 123.6, 123.2, 61.7, 23.0, 14.3; ESI-MS *m/z* 216.0 $(M + H)^+$; HRMS (EI) calcd for $C_{13}H_{13}NO_2$ 215.0948 $(M)^+$, found 215.0946.



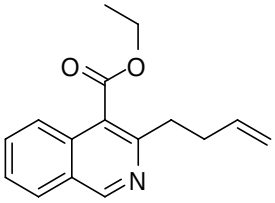
6b

Methyl 3-ethylisoquinoline-4-carboxylate (6b). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.26 (s, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.72(t, *J* = 6.9 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 4.06 (s, 3H), 2.97 (q, *J* = 7.5 Hz, 2H), 1.39 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 154.6, 153.7, 133.2, 131.3, 127.9, 126.9, 126.5, 123.8, 122.5, 52.5, 29.9, 14.4; ESI-MS *m/z* 216.0 $(M + H)^+$; HRMS (ESI) calcd for $C_{13}H_{14}NO_2$ 216.1028 $(M + H)^+$, found 216.1019.



6c

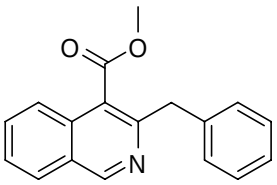
Methyl 3-isopropylisoquinoline-4-carboxylate (6c).^{1}H NMR (300 MHz, $CDCl_3$) δ 9.29 (s, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.74-7.58 (m, 3H), 4.06(s, 3H), 3.26-3.18 (m, 1H), 1.38 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 157.4, 153.7, 133.0, 131.2, 127.8, 126.8, 126.5, 123.8, 122.1, 52.5, 33.8, 22.4 (2C); ESI-MS *m/z* 230.1 $(M + H)^+$; HRMS (ESI) calcd for $C_{14}H_{16}NO_2$ 230.1184 $(M + H)^+$, found 230.1176.



6d

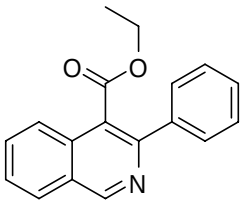
Ethyl 3-(but-3-enyl)isoquinoline-4-carboxylate (6d). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.25 (s, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 8.7 Hz, 1H), 7.72 (t, *J* = 7.2 Hz, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 5.98-5.84 (m, 1H), 5.11-4.97 (m, 2H), 4.55 (q, *J* = 7.2 Hz, 2H), 3.05 (t, *J* = 7.8 Hz, 2H), 2.63-2.56 (m, 2H), 1.47 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 153.5, 152.4, 137.9, 133.2, 131.3, 127.9, 126.9, 126.5, 123.8, 123.3, 115.0, 61.7, 35.9, 34.1, 14.3; ESI-MS *m/z* 256.1 $(M + H)^+$;

HRMS (ESI) calcd for $C_{16}H_{18}NO_2$ 256.1339 $(M + H)^+$, found 256.1332.



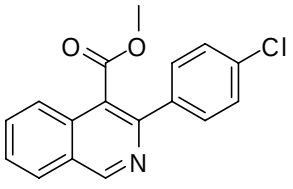
6e

Methyl 3-benzylisoquinoline-4-carboxylate (6e). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.25 (s, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.7 Hz, 1H), 7.73 (t, *J* = 7.2 Hz, 1H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.29-7.18 (m, 5H), 4.37 (s, 2H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.9, 153.9, 151.8, 139.5, 133.3, 131.4, 129.1 (2C), 128.4 (2C), 127.9, 127.2, 126.6, 126.3, 124.0, 123.5, 52.5, 42.4; ESI-MS *m/z* 278.1 $(M + H)^+$; HRMS (ESI) calcd for $C_{18}H_{16}NO_2$ 278.1182 $(M + H)^+$, found 278.1176.



6f

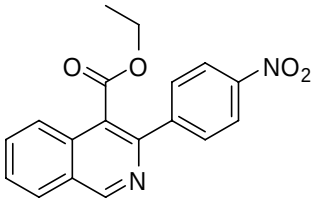
Ethyl 3-phenylisoquinoline-4-carboxylate (6f). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.05 (d, *J* = 8.7 Hz, 2H), 7.81-7.63 (m, 3H), 7.49-7.42 (m, 3H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 153.5, 151.1, 140.3, 133.4, 131.7, 128.8 (2C), 128.5, 128.4 (2C), 127.9, 127.6, 126.9, 124.2, 123.4, 61.7, 13.7; ESI-MS *m/z* 278.0 $(M + H)^+$; HRMS (ESI) calcd for $C_{18}H_{16}NO_2$ 278.1182 $(M + H)^+$, found 278.1176.



6g

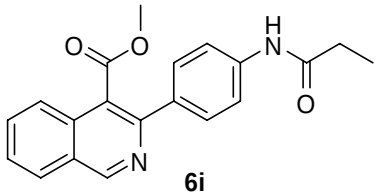
Methyl 3-(4-chlorophenyl)isoquinoline-4-carboxylate (6g). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.37 (s, 1H), 8.07 (d, *J* = 8.1 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.81 (t, *J* = 7.2 Hz, 3H), 7.71-7.65 (m, 3H), 7.46 (d, *J* = 8.4 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 153.6, 149.5, 138.5, 134.9, 133.4, 131.9, 130.1 (2C), 128.7 (2C), 128.0, 127.9, 126.9, 124.2, 123.2, 52.7; IR (CH_2Cl_2): *v* 2947, 1727, 1618,

1577, 1498, 1221, 1092, 1026, 1011, 843, 798, 759 cm^{-1}; ESI-MS *m/z* 298.0 $(M + H)^+$; HRMS (ESI) calcd for $C_{17}H_{13}NO_2Cl$ 298.0635 $(M + H)^+$, found 298.0629.



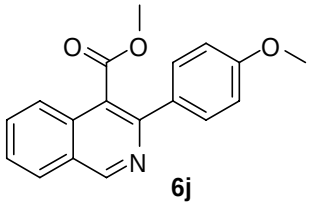
6h

Ethyl 3-(4-nitrophenyl)isoquinoline-4-carboxylate (6h). ^1H NMR (300 MHz, $CDCl_3$) δ 9.40 (s, 1H), 8.35 (d, *J* = 8.7 Hz, 2H), 8.09 (t, *J* = 6.9 Hz, 1H), 7.92-7.74 (m, 4H), 4.30 (q, *J* = 7.2 Hz, 2H), 1.12 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 153.7, 148.3, 147.8, 146.5, 133.1, 132.1, 129.8 (2C), 128.4, 128.0, 127.3, 124.3, 124.2, 123.4 (2C), 62.0, 13.7; IR (CH_2Cl_2): *v* 2987, 1718, 1604, 1517, 1497, 1348, 1230, 1033, 862, 850, 763, 706 cm^{-1}; ESI-MS *m/z* 323.1 $(M + H)^+$; HRMS (ESI) calcd for $C_{18}H_{15}N_2O_4$ 323.1034 $(M + H)^+$, found 323.1026.



6i

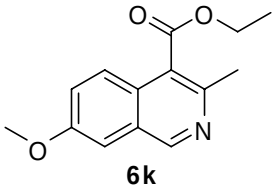
Methyl 3-(4-propionamidophenyl)isoquinoline-4-carboxylate (6i). ^1H NMR (300 MHz, $CDCl_3$) δ 9.36 (s, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.79 (t, *J* = 6.9 Hz, 1H), 7.73-7.64 (m, 4H), 7.30 (s, 1H), 3.81 (s, 3H), 2.43 (q, *J* = 6.9 Hz, 2H), 1.27 (t, *J* = 6.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 169.4, 153.5, 150.1, 138.7, 135.5, 133.5, 131.7, 129.4 (3C), 127.9, 127.6, 126.7, 124.1, 122.8, 119.4, 52.6, 30.7, 9.6; IR (CH_2Cl_2): *v* 3295, 3253, 2976, 1732, 1661, 1597, 1570, 1525, 1421, 1223, 1078, 1032, 842, 762 cm^{-1}; ESI-MS *m/z* 335.2 $(M + H)^+$; HRMS (ESI) calcd for $C_{20}H_{19}N_2O_3$ 335.1397 $(M + H)^+$, found 335.1390.



6j

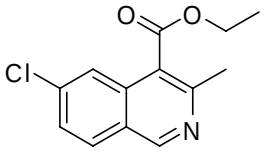
Methyl 3-(4-methoxyphenyl)isoquinoline-4-carboxylate (6j). ^1H NMR (300

MHz, $CDCl_3$) δ 9.35 (s, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.77-7.63 (m, 3H), 7.01 (d, *J* = 8.7Hz, 2H), 3.87 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.5, 160.1, 153.4, 150.4, 133.5, 132.6, 131.6, 130.0 (2C), 127.9, 127.3, 126.5, 124.0, 122.3, 114.0 (2C), 55.3, 52.5; IR (CH_2Cl_2): *v* 3014, 2950, 2844, 1712, 1609, 1515, 1436, 1299, 1259, 1228, 1177, 1033, 840, 801, 752 cm^{-1}; ESI-MS *m/z* 294.1 $(M + H)^+$; HRMS (ESI) calcd for $C_{18}H_{16}NO_3$ 294.1120 $(M + H)^+$, found 294.1125.



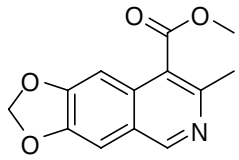
6k

Ethyl 7-methoxy-3-methylisoquinoline-4-carboxylate (6k). ^1H NMR (300 MHz, $CDCl_3$) δ 9.12 (s, 1H), 7.81 (d, *J* = 9.3 Hz, 1H), 7.38 (dd, *J* = 2.7, 9.3 Hz, 1H), 7.21(d, *J* = 2.7 Hz, 1H), 4.54 (q, *J* = 7.2 Hz, 2H), 3.95 (s, 3H), 2.72 (s, 3H), 1.47(t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 158.0, 151.8, 147.5, 128.8, 127.8, 125.3, 124.5, 123.1, 105.0, 61.6, 55.5, 22.7, 14.3; IR (CH_2Cl_2): *v* 2985, 2935, 2922, 2836, 1722, 1625, 1579, 1500, 1255, 1222, 1167, 1129, 1019, 925, 823 cm^{-1}; ESI-MS *m/z* 246.0 $(M + H)^+$; HRMS (ESI) calcd for $C_{14}H_{16}NO_3$ 246.1127 $(M + H)^+$, found 246.1125.



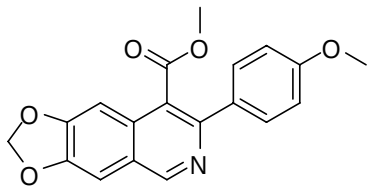
6l

Ethyl 6-chloro-3-methylisoquinoline-4-carboxylate (6l). ^1H NMR (300 MHz, $CDCl_3$) δ 9.19 (s, 1H), 7.92-7.89 (m, 2H), 7.53 (dd, *J* = 2.1, 8.7 Hz, 1H), 4.56 (q, *J* = 7.2 Hz, 2H), 2.76 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0, 153.0, 151.1, 137.9, 134.0, 129.4, 128.0, 124.7 123.0, 122.3, 61.9, 23.2, 14.3; ESI-MS *m/z* 249.9 $(M + H)^+$; HRMS (ESI) calcd for $C_{13}H_{13}NO_2Cl$ 250.0631 $(M + H)^+$, found 250.0629.



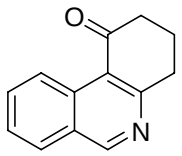
6m

Methyl 7-methyl-[1,3]dioxolo[4,5-g]isoquinoline-8-carboxylate (6m). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.93 (s, 1H), 7.18 (s, 1H), 7.17 (s, 1H), 6.11 (s, 2H), 4.03 (s, 3H), 2.67(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 152.0, 150.9, 148.9, 147.9, 131.9, 123.8, 103.2, 101.8, 100.3, 52.4, 22.0; ESI-MS *m/z* 246.0 $(M + H)^+$; HRMS (ESI) calcd for $C_{13}H_{11}NO_4$ 246.0690 $(M + H)^+$, found 246.0688.



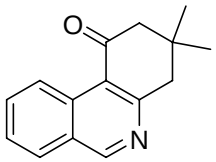
6n

Methyl7-(4-methoxyphenyl)-[1,3]dioxolo[4,5-g]isoquinoline-8-carboxylate (6n). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.07 (s, 1H), 7.63 (d, *J* = 9.0 Hz, 2H), 7.28 (s, 1H), 7.24 (s, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 6.14 (s, 2H), 3.87(s, 3H), 3.76(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 159.9, 152.2, 151.0, 150.0, 148.4, 132.8, 132.1, 129.8 (2C), 124.1, 122.2, 113.9 (2C), 103.3, 102.0, 100.6, 55.3, 52.5; IR (CH_2Cl_2): *v* 3011, 2957, 2919, 2839, 1716, 1605, 1583, 1462, 1247, 1220, 1179, 1104, 1033, 935, 844 cm^{-1}; ESI-MS *m/z* 338.2 $(M + H)^+$; HRMS (ESI) calcd for $C_{19}H_{16}NO_5$ 338.1014 $(M + H)^+$, found 338.1023.



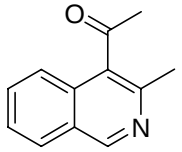
6o

3,4-Dihydrophenanthridin-1-(2H)-one (6o). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.39 (d, *J* = 8.4 Hz, 1H), 9.28 (s, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.84 (t, *J* = 7.2 Hz, 1H), 7.62 (t, *J* = 8.1 Hz, 1H), 3.35 (t, *J* = 6.6 Hz, 2H), 2.81 (t, *J* = 6.3 Hz, 2H), 2.30-2.24 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 161.2, 157.0, 133.8, 133.2, 128.3, 127.9, 127.1, 125.9, 120.7, 40.6, 33.9, 21.9; ESI-MS *m/z* 198.1 $(M + H)^+$; HRMS (ESI) calcd for $C_{13}H_{12}NO$ 198.0923 $(M + H)^+$, found 198.0913.



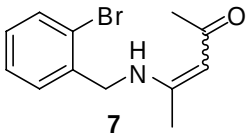
6p

3,3-dimethyl-3,4-dihydrophenanthridin-1(2H)-one (6p). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.41 (d, *J* = 9.0 Hz, 1H), 9.30 (s, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.85 (t, *J* = 6.9 Hz, 1H), 7.63 (t, *J* = 6.9 Hz, 1H), 3.24 (s, 2H), 2.67 (s, 2H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.0, 159.6, 157.3, 133.5, 133.2, 128.3, 127.8, 127.1, 125.8, 119.7, 54.2, 47.7, 32.8, 28.1 (2C); ESI-MS *m/z* 226.1 $(M + H)^+$; HRMS (ESI) calcd for $C_{15}H_{16}NO$ 226.1236 $(M + H)^+$, found 226.1226.



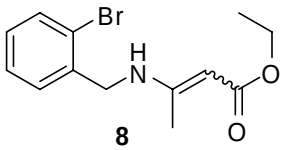
6q

1-(3-methylisoquinolin-4-yl)ethanone (6q). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.13 (s, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.66-7.48 (m, 3H), 2.59(s, 3H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 152.7, 145.9, 132.1, 131.3, 128.8, 128.1, 126.8, 126.5, 122.9, 32.7, 22.3; ESI-MS *m/z* 186.0 $(M + H)^+$; HRMS (ESI) calcd for $C_{12}H_{12}NO$ 186.0922 $(M + H)^+$, found 186,0913.



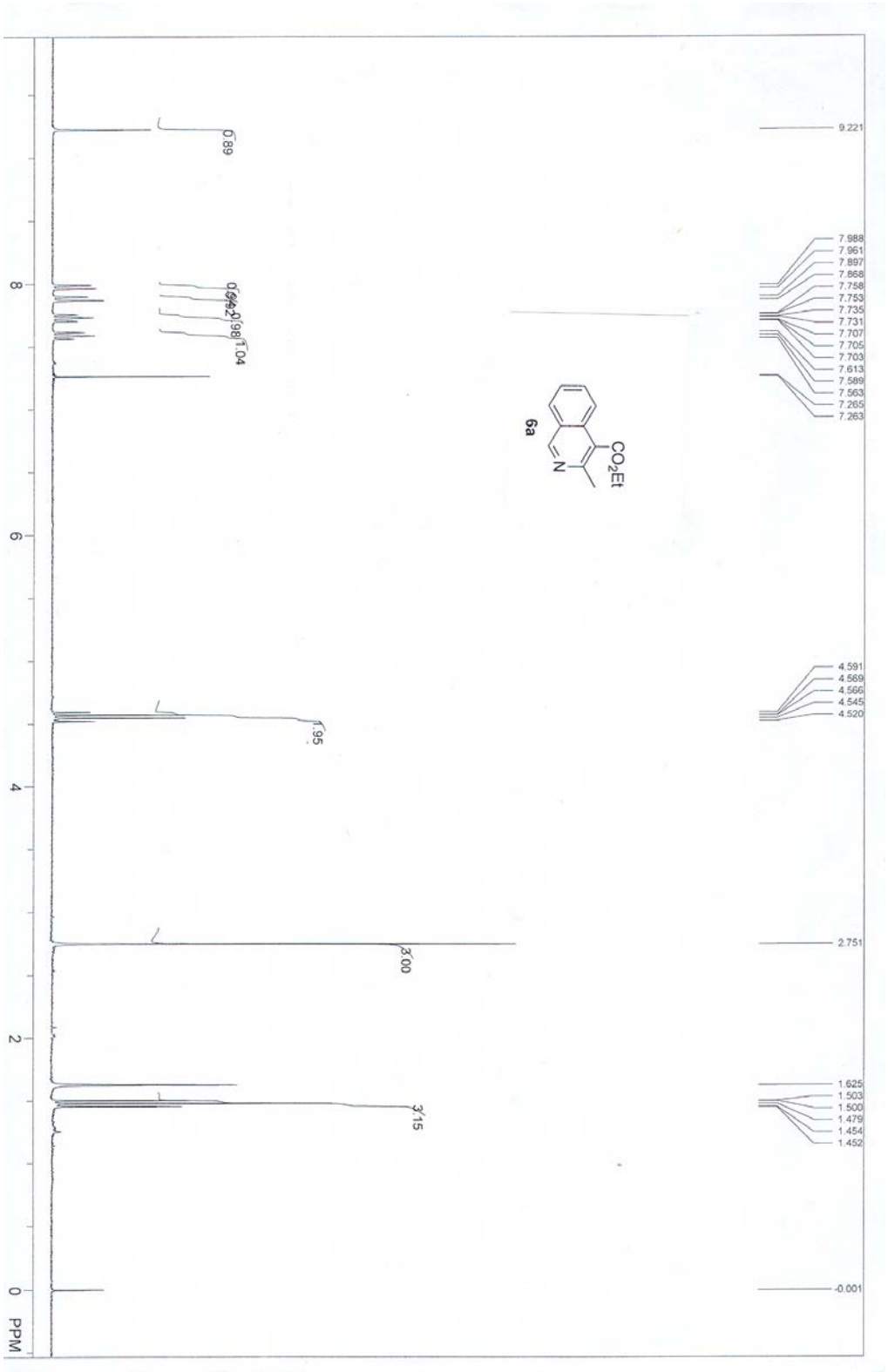
7

4-(2-bromobenzylamino)pent-3-en-2-one (7). ^{1}H NMR (300 MHz, $CDCl_3$) δ 11.2 (br s, 1H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.34-7.28 (m, 2H), 7.18-7.12 (m, 1H), 5.08 (s, 1H), 4.50 (d, *J* = 6.9 Hz, 2H), 2.05 (s, 3H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.7, 162.9, 137.3, 132.9, 129.0, 128.2, 127.9, 122.7, 96.3, 47.0, 29.0, 18.8; ESI-MS *m/z* 268.0 $(M + H)^+$; HRMS (EI) calcd for $C_{12}H_{14}NOBr$ 267.0259 $(M)^+$, found 267.0270.



8

Ethyl 3-(2-bromobenzylamino)but-2-enoate (8). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.97 (br s, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.31-7.29 (m, 2H), 7.17-7.13 (m, 1H), 4.56 (s, 1H), 4.46 (d, *J* = 6.6 Hz, 2H), 4.10 (q, *J* = 6.9 Hz, 2H), 1.90 (s, 3H), 1.26 (t, *J* = 6.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 161.5, 137.8, 132.8, 128.8, 128.2, 127.8, 122.6, 83.7, 58.4, 47.0, 19.1, 14.6; ESI-MS *m/z* 298.0 $(M + H)^+$; HRMS (EI) calcd for $C_{13}H_{16}NO_2Br$ 297.0364 $(M)^+$, found 297.0377.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7.263
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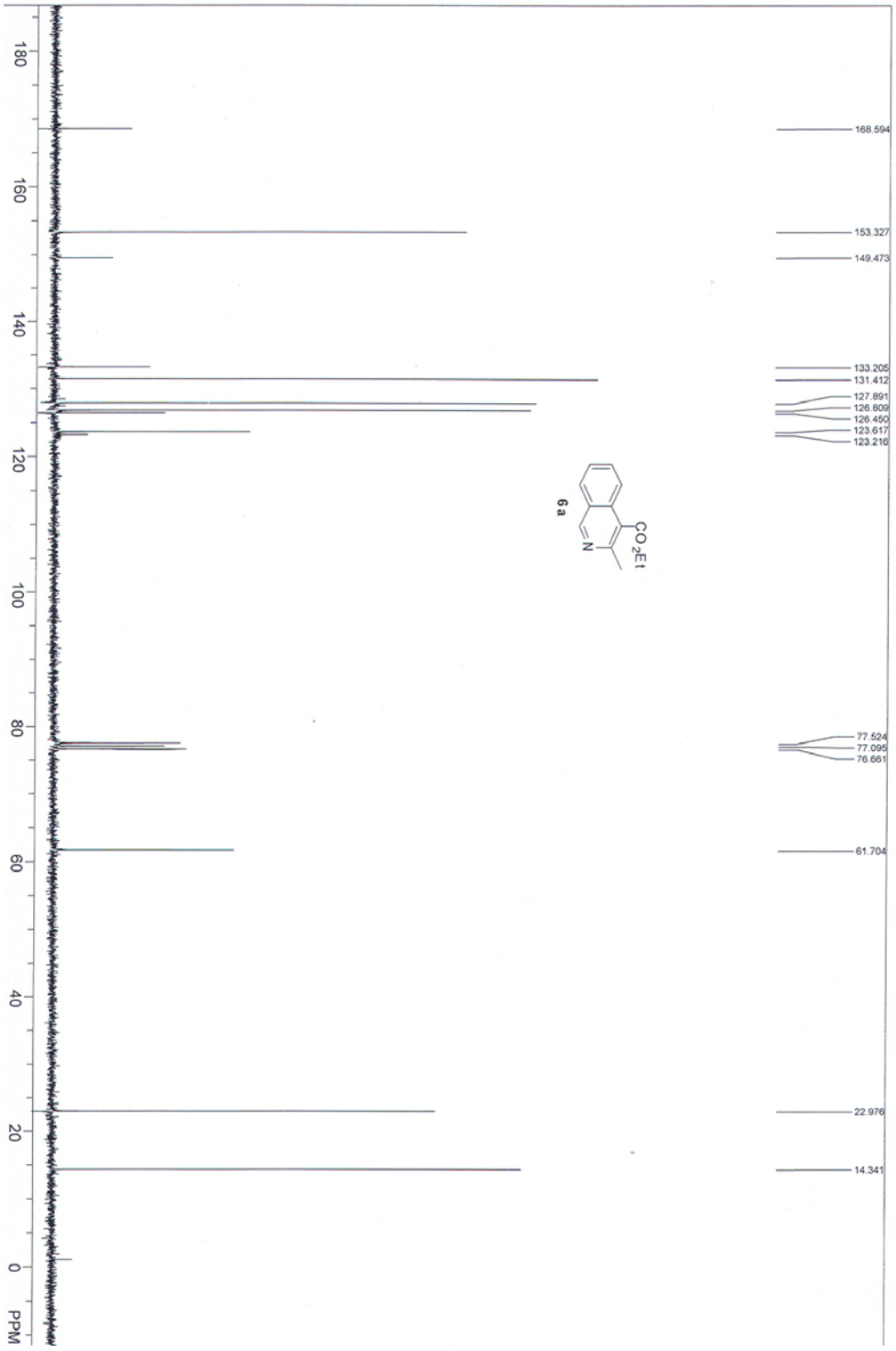
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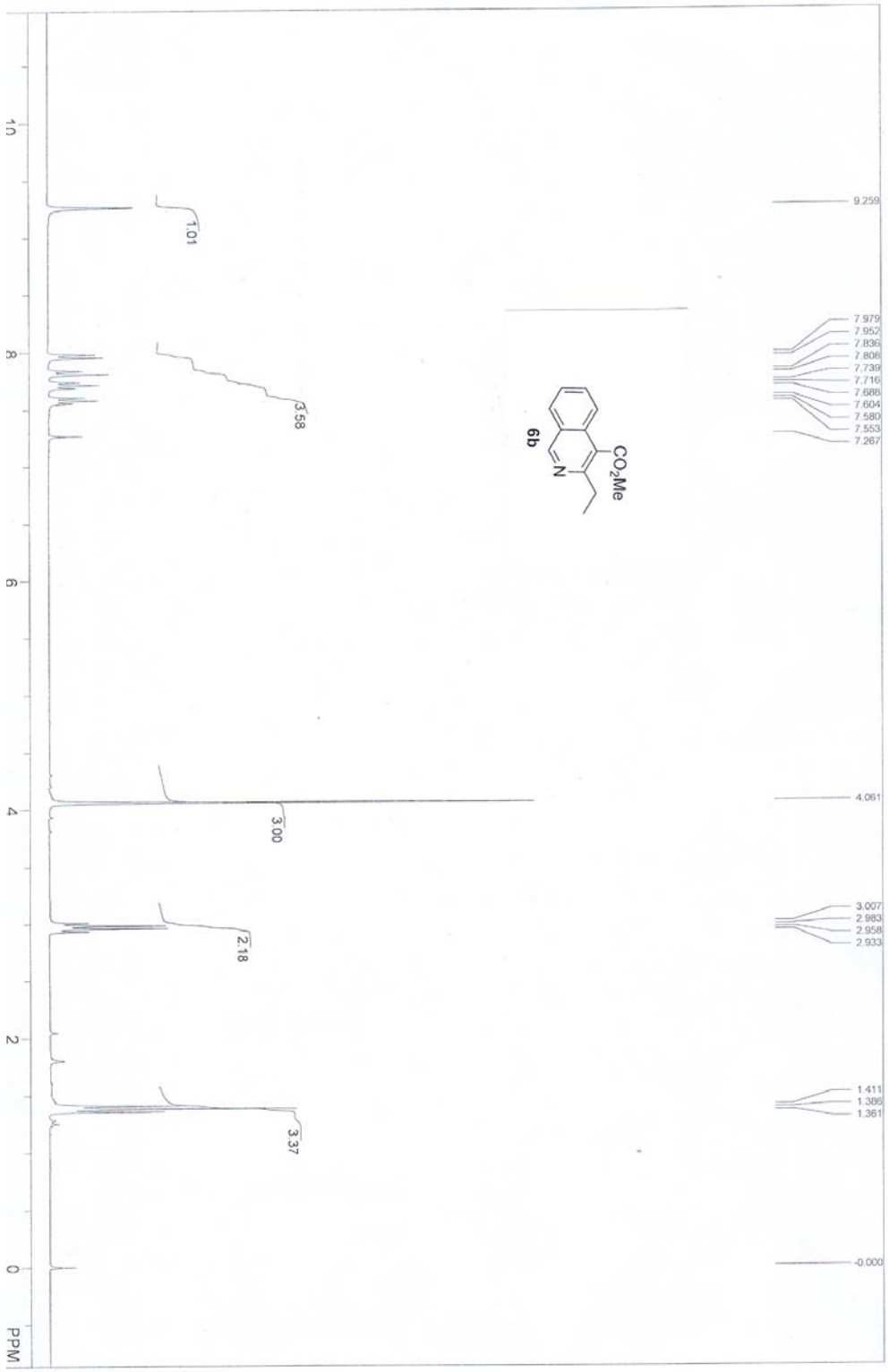
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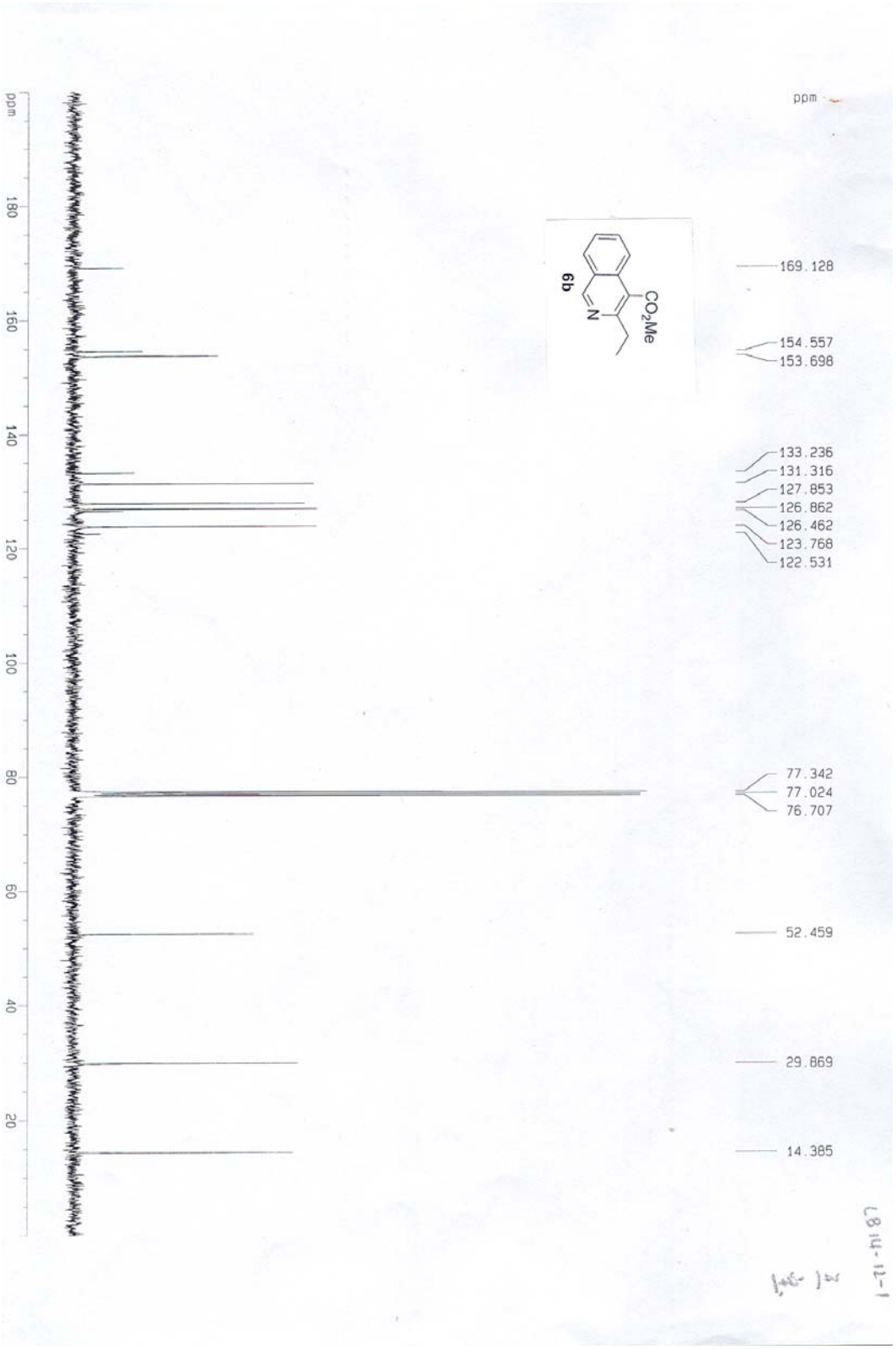
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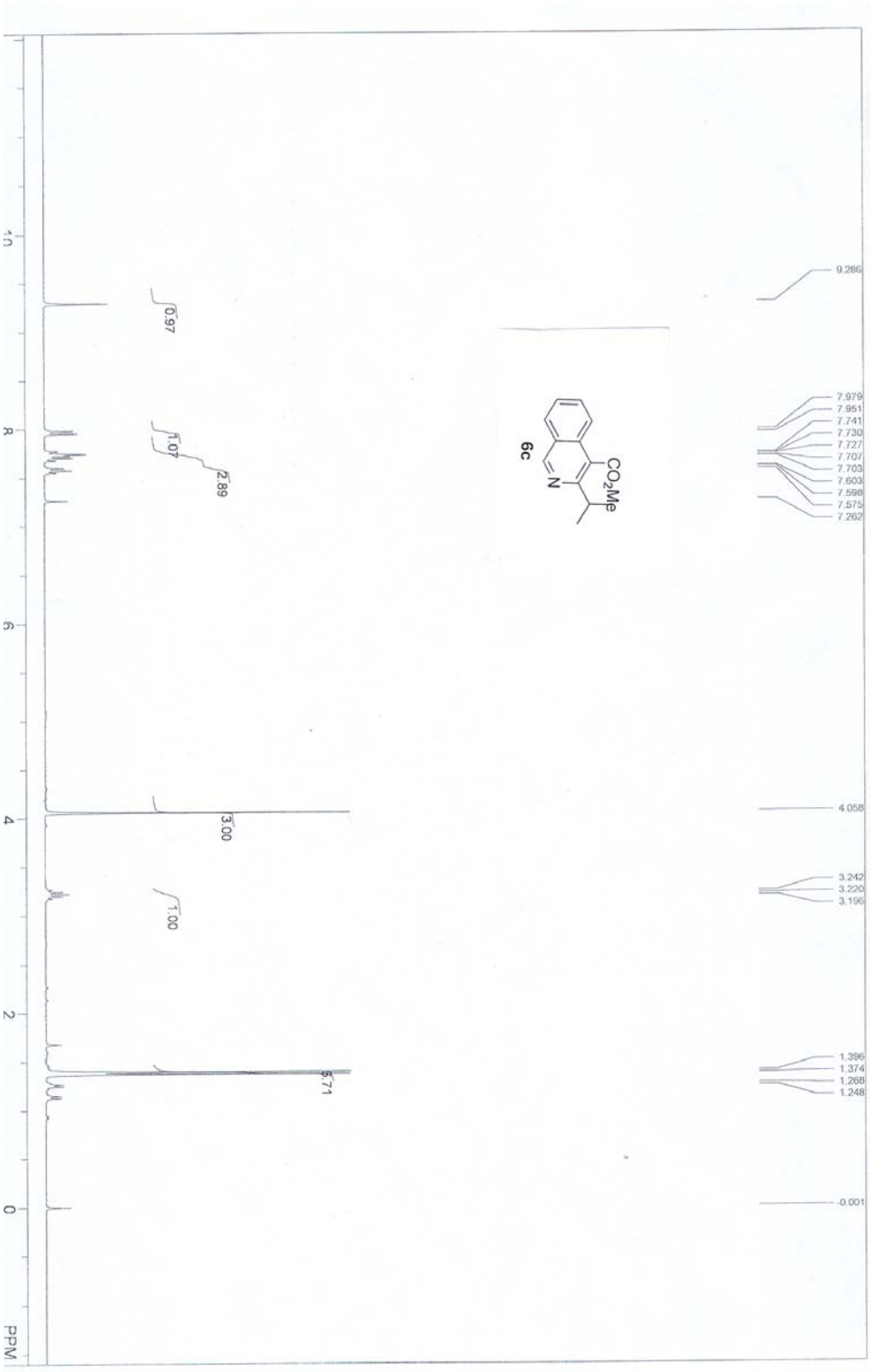
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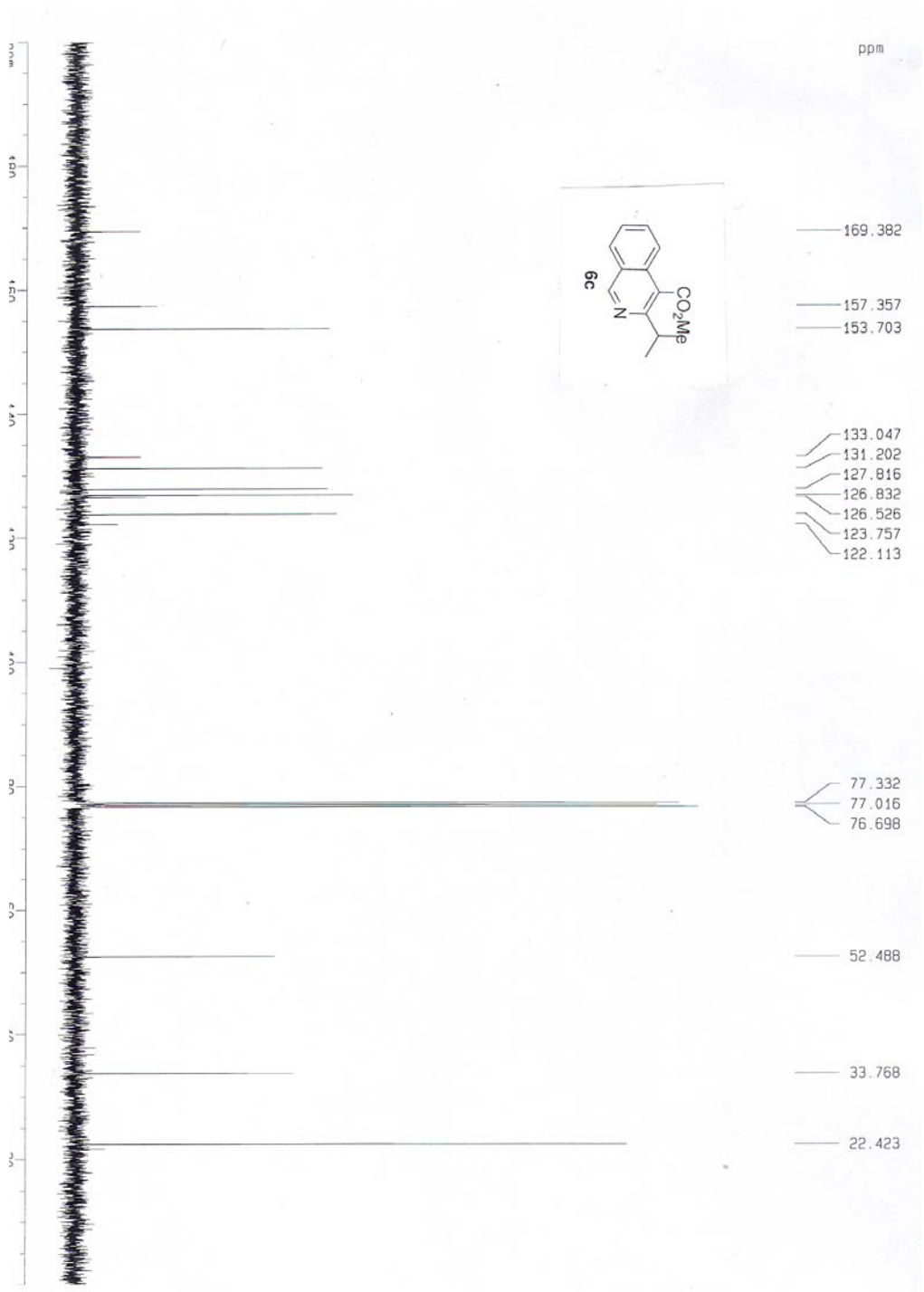
PPM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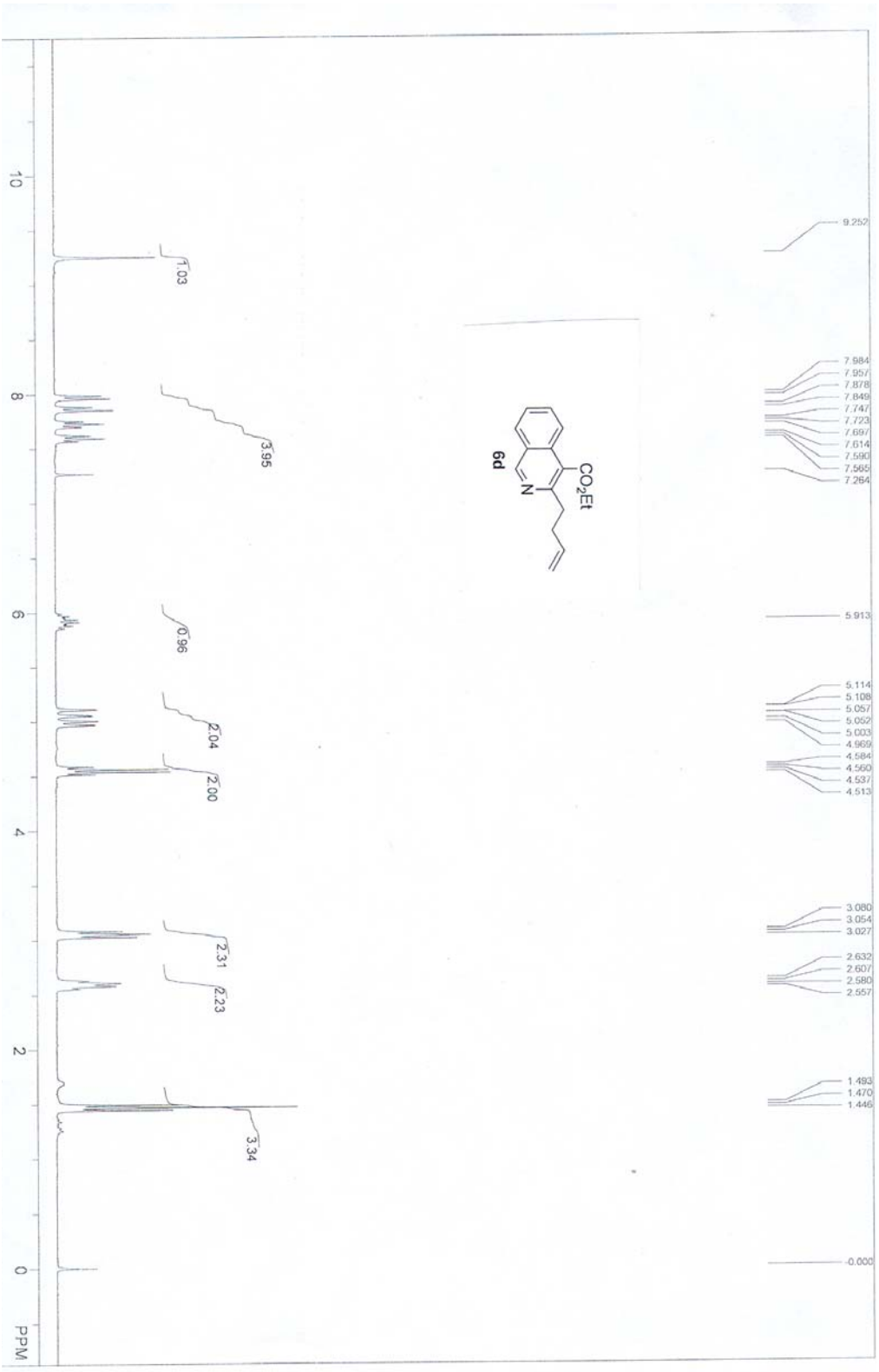
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7.565
7.264
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5.108
5.057
5.052
5.003
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4.560
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4.513
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3.054
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2.580
2.557
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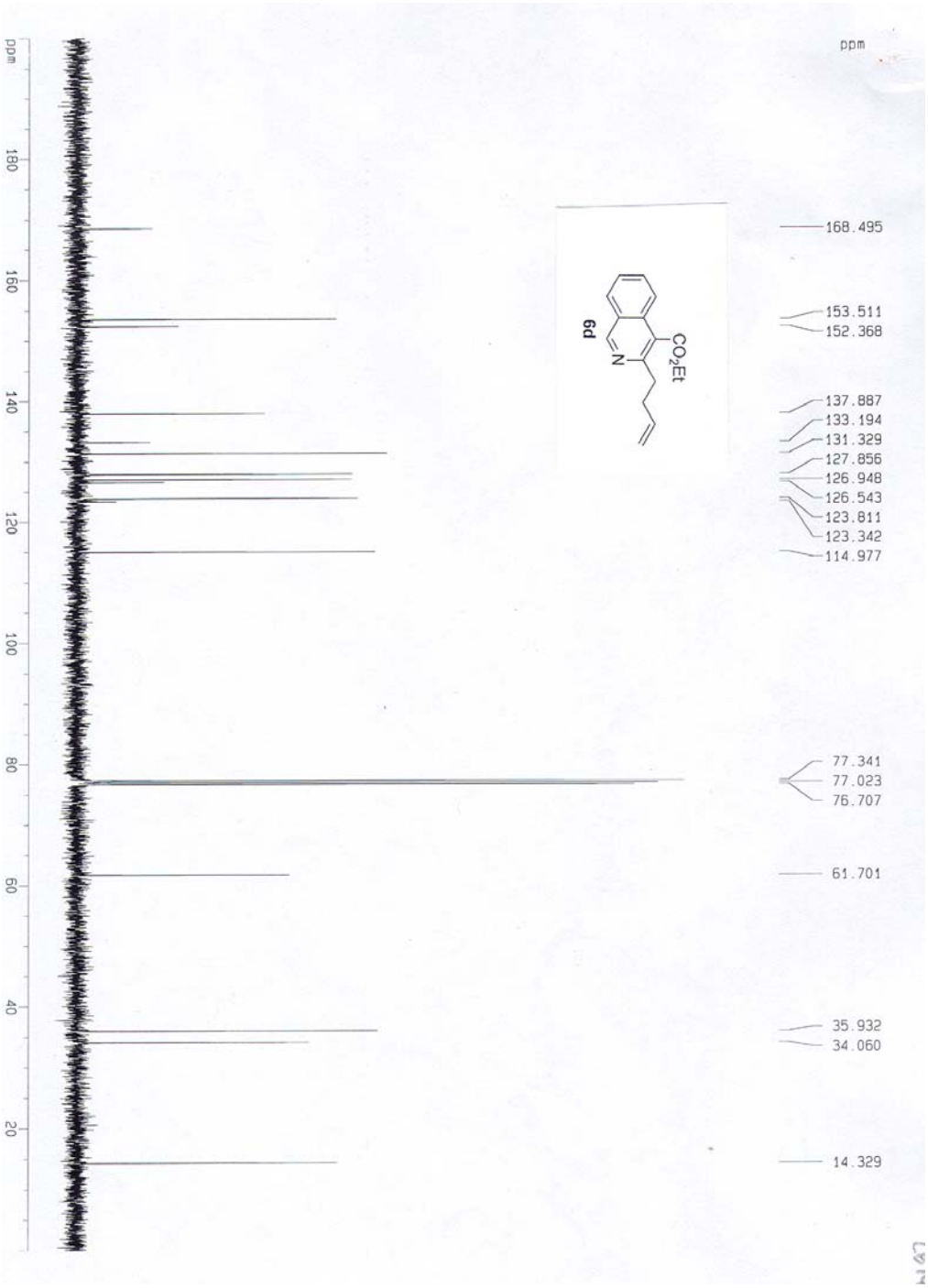
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34.060
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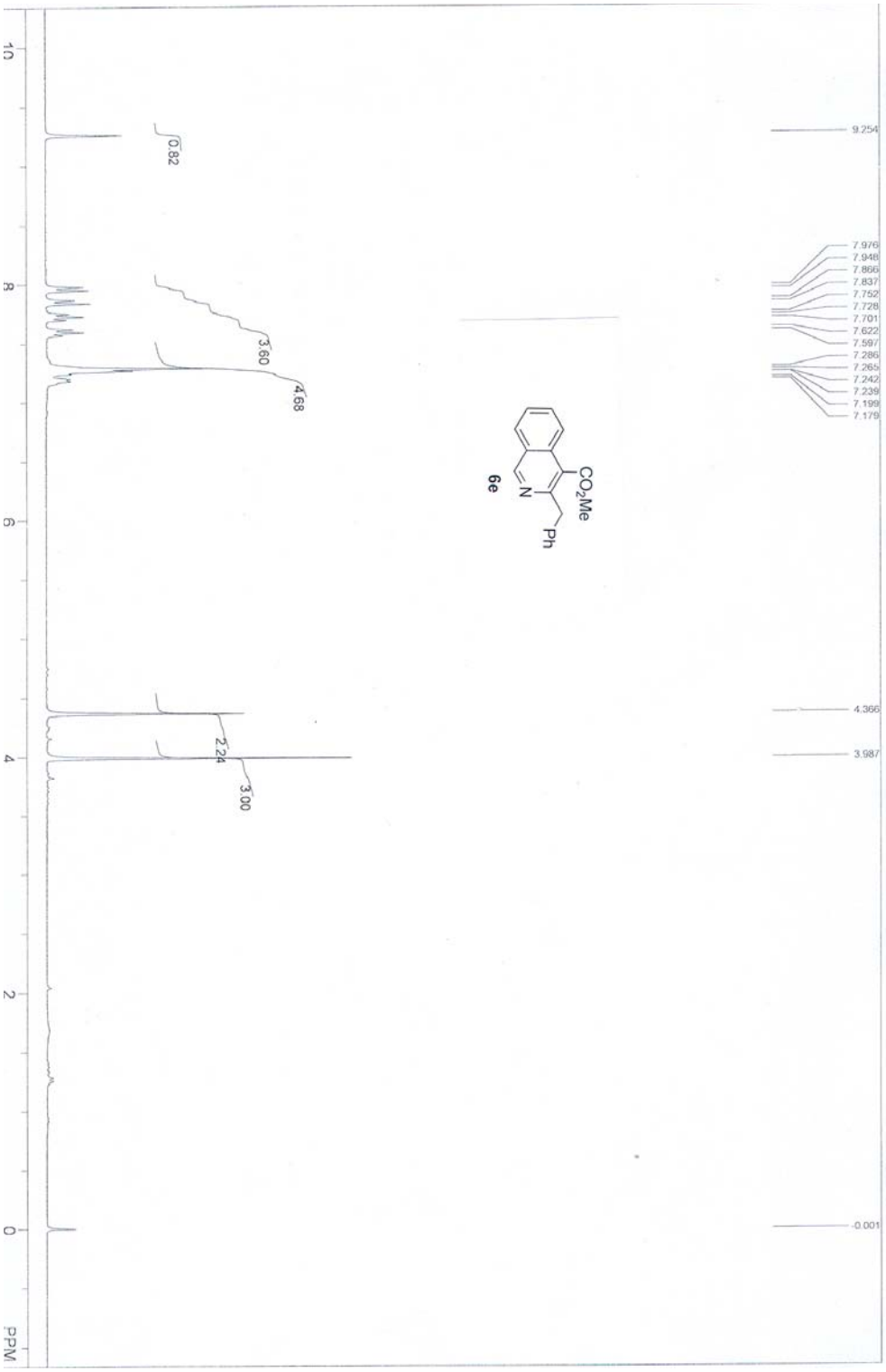
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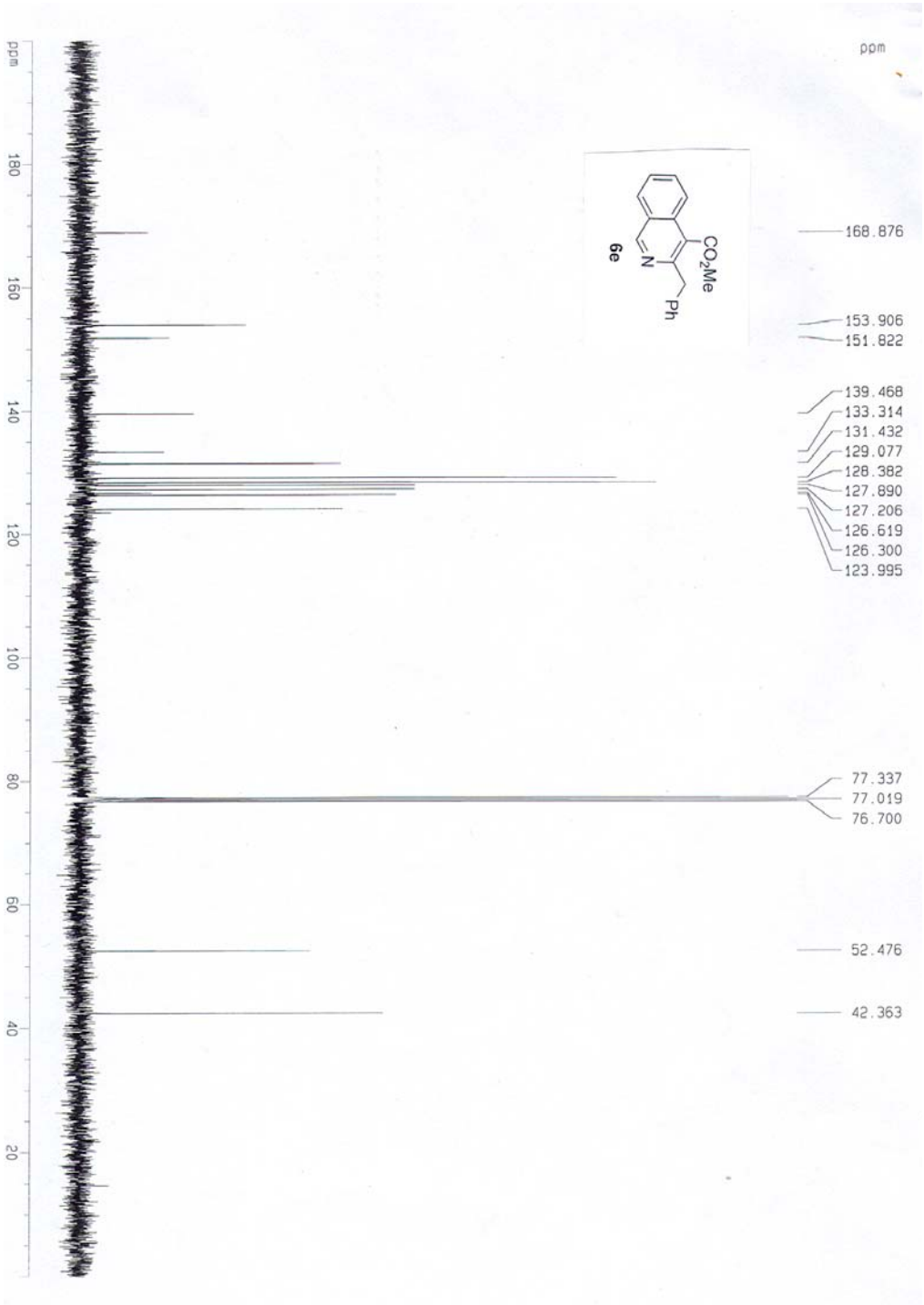
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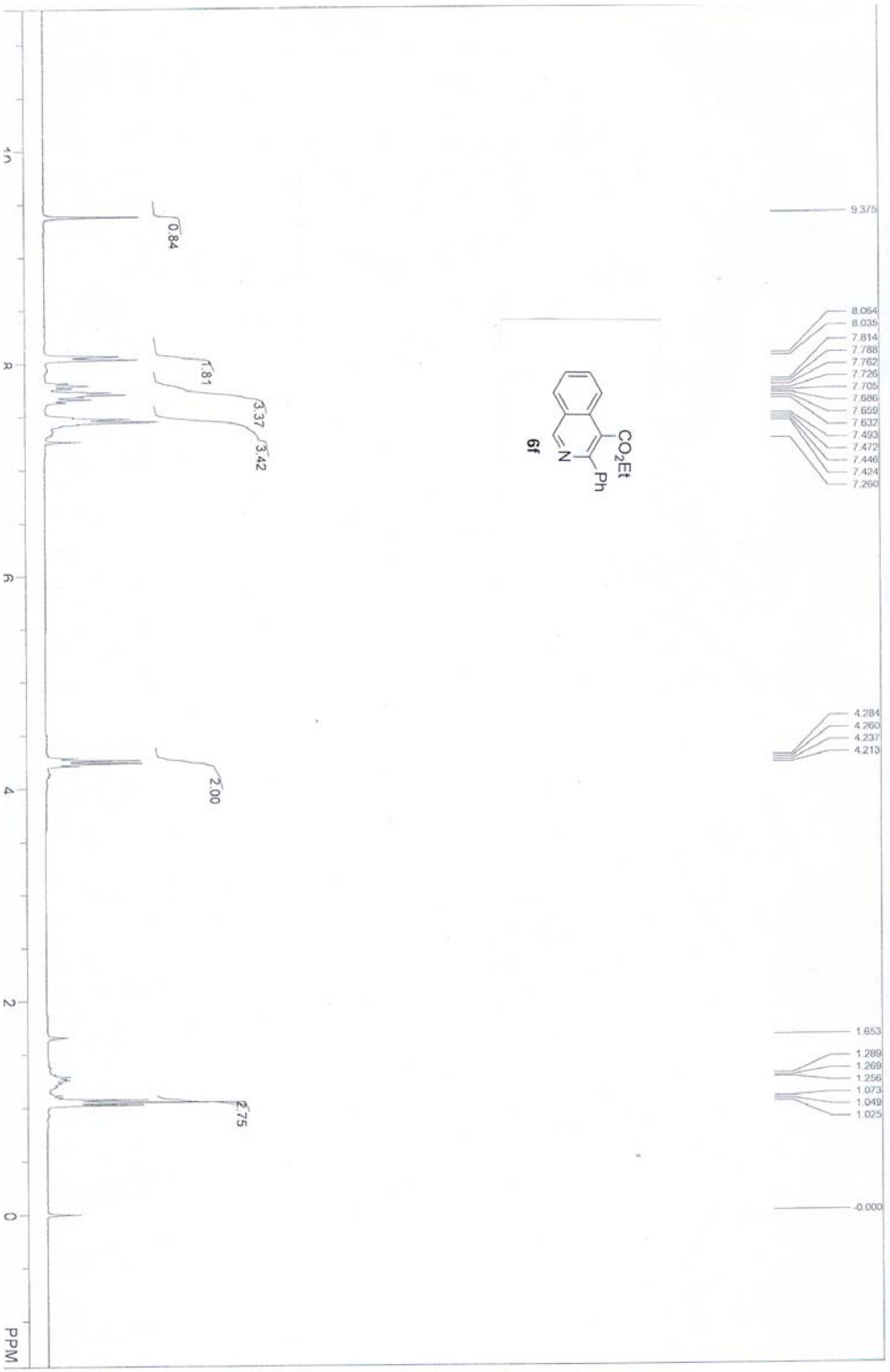
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Ph
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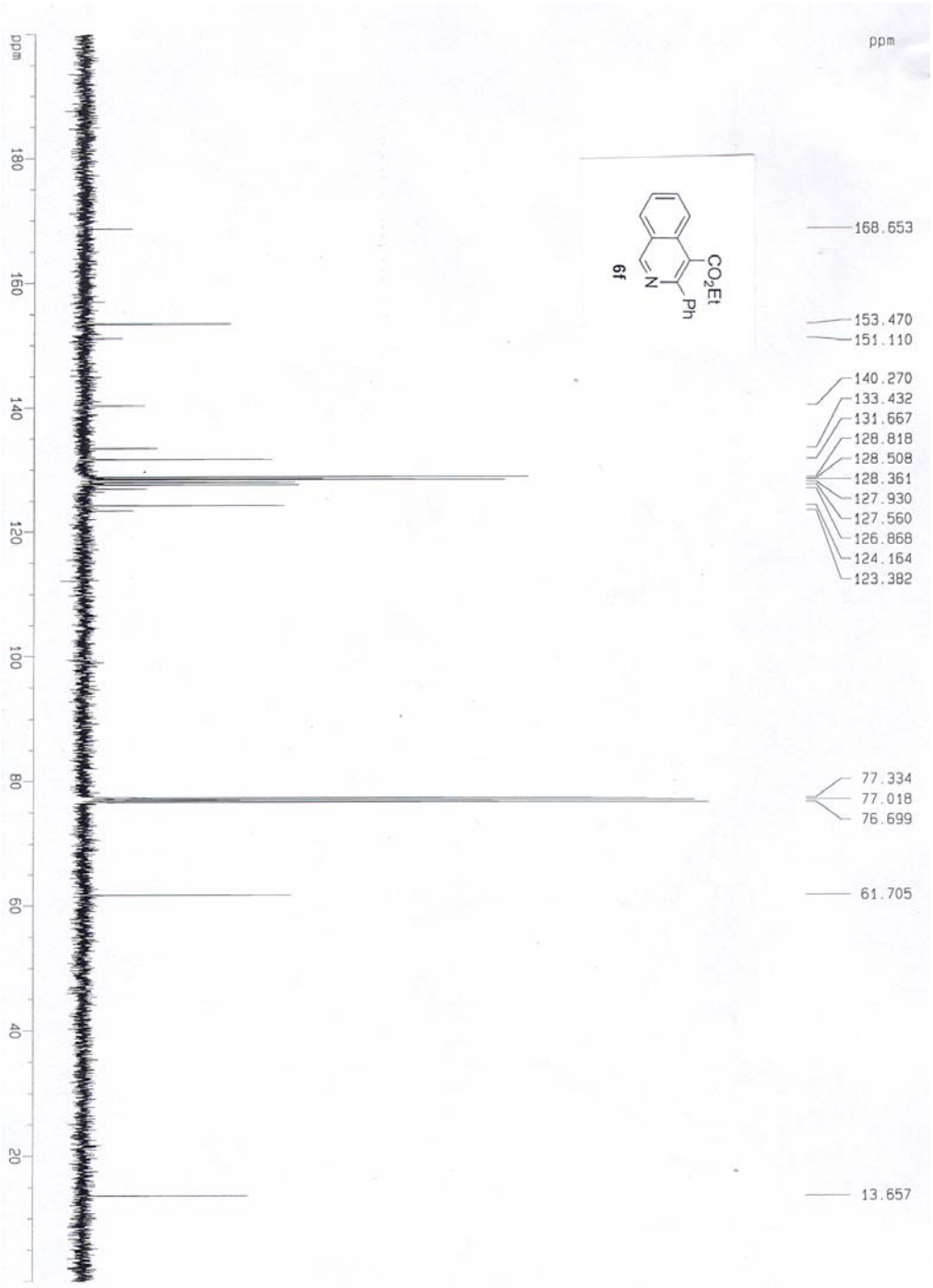
PPM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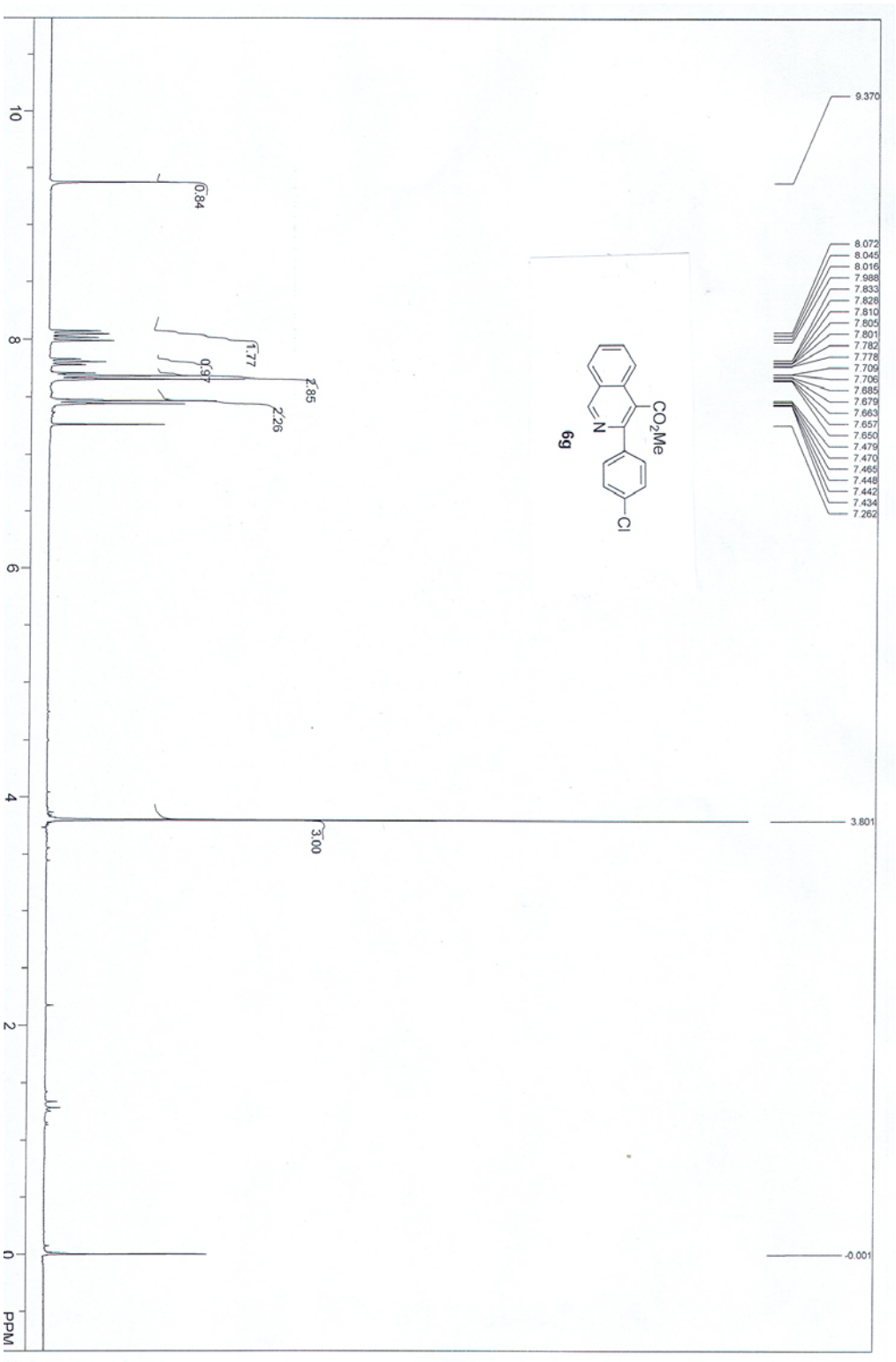
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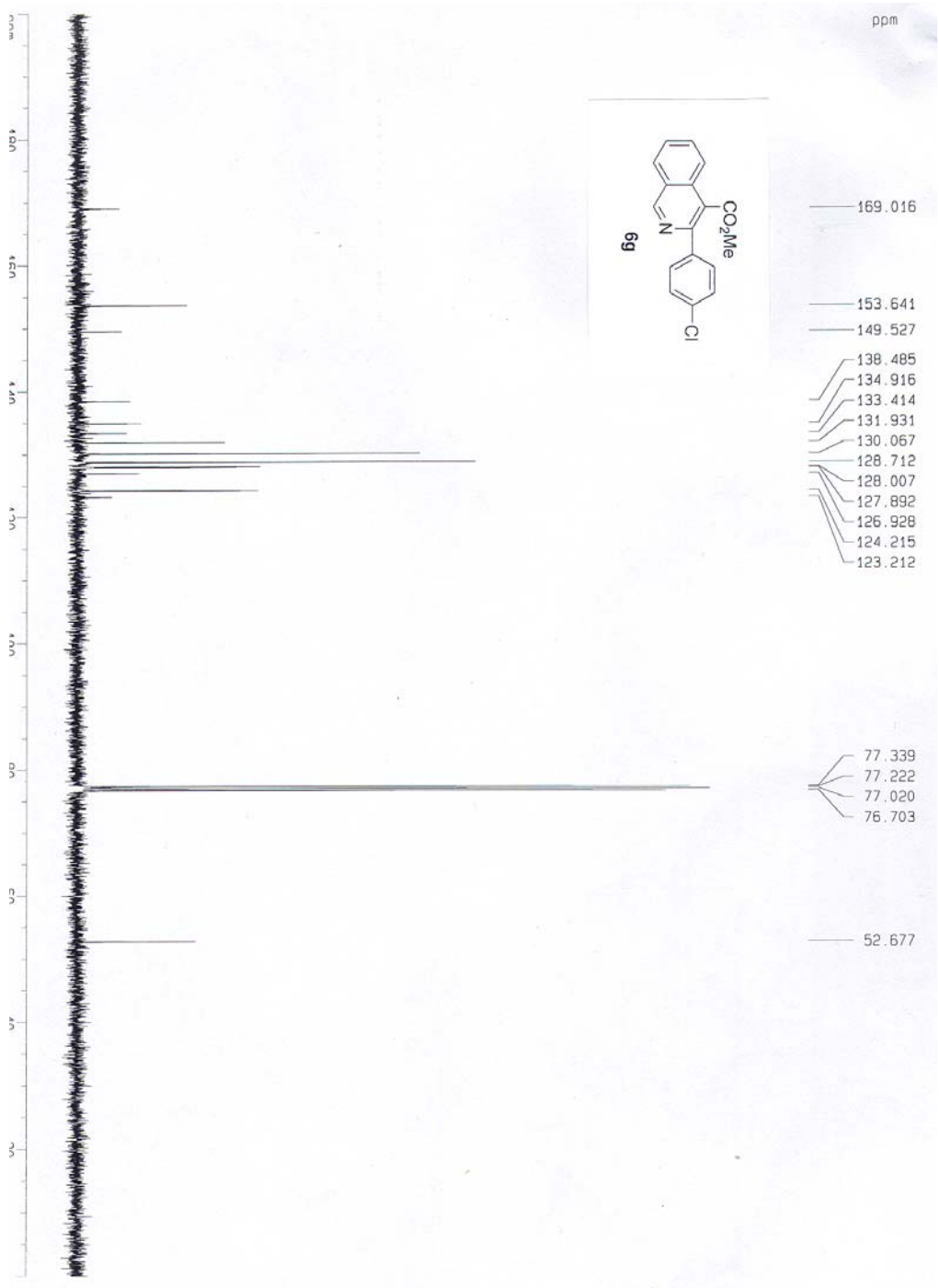
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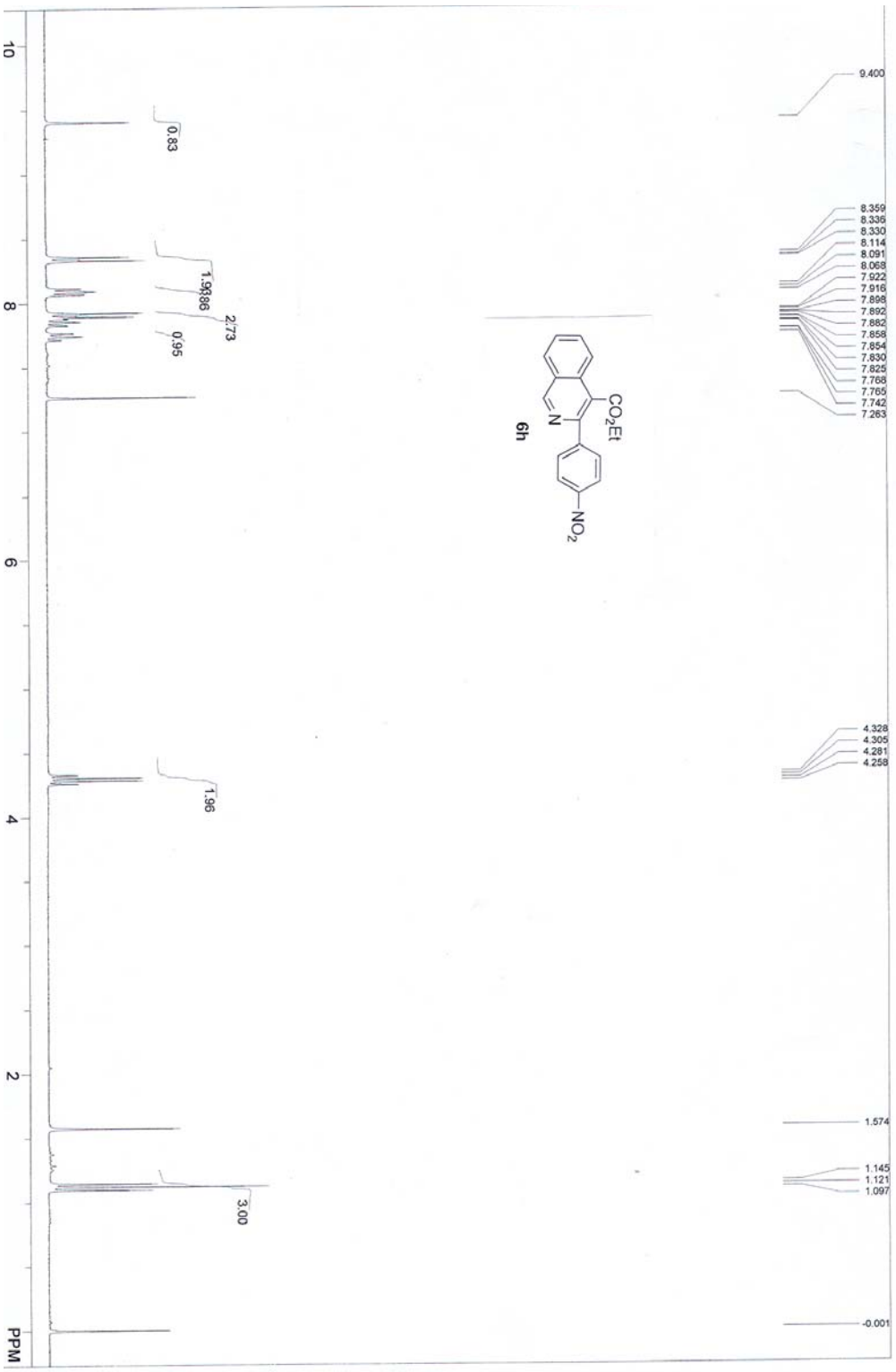
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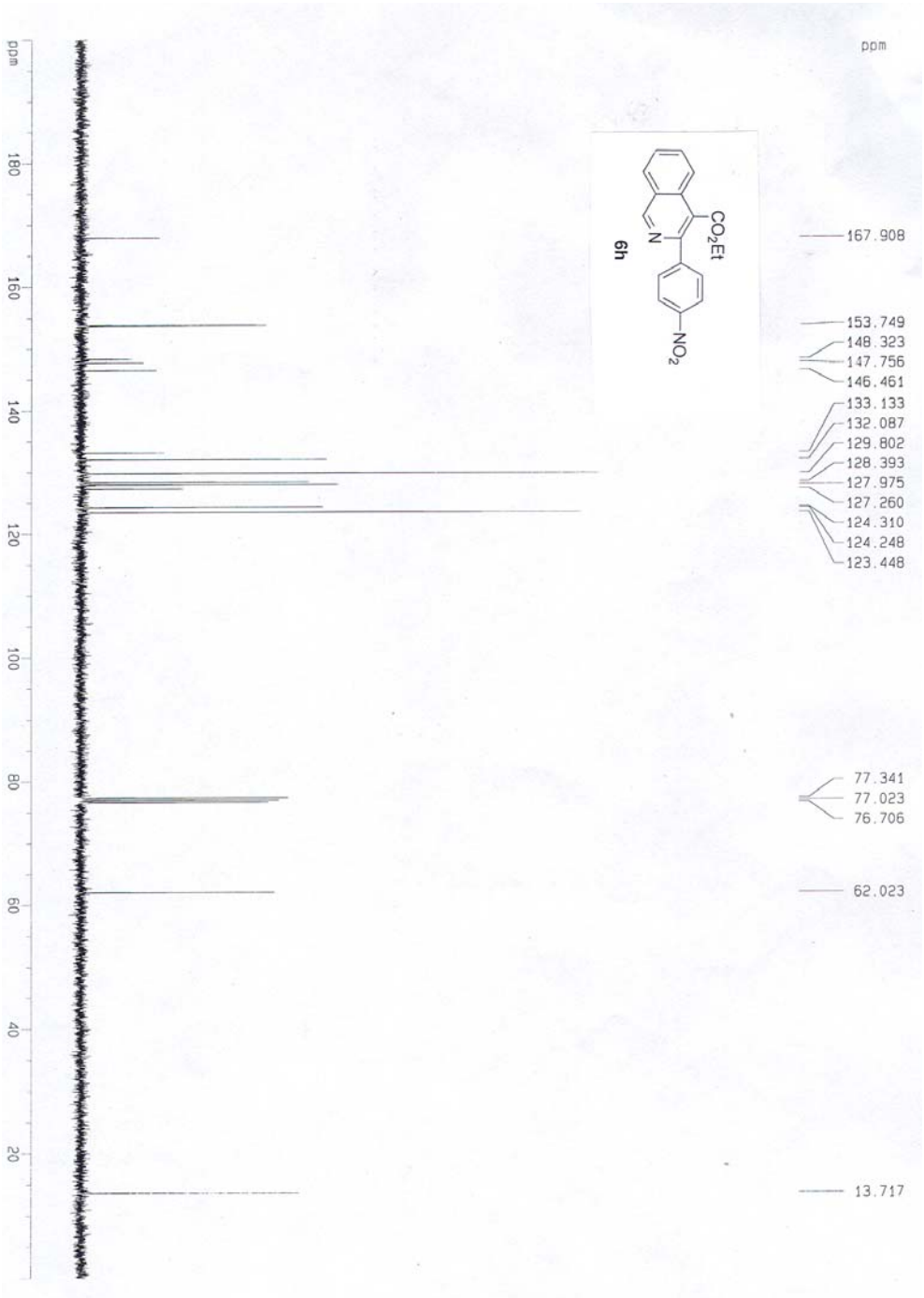
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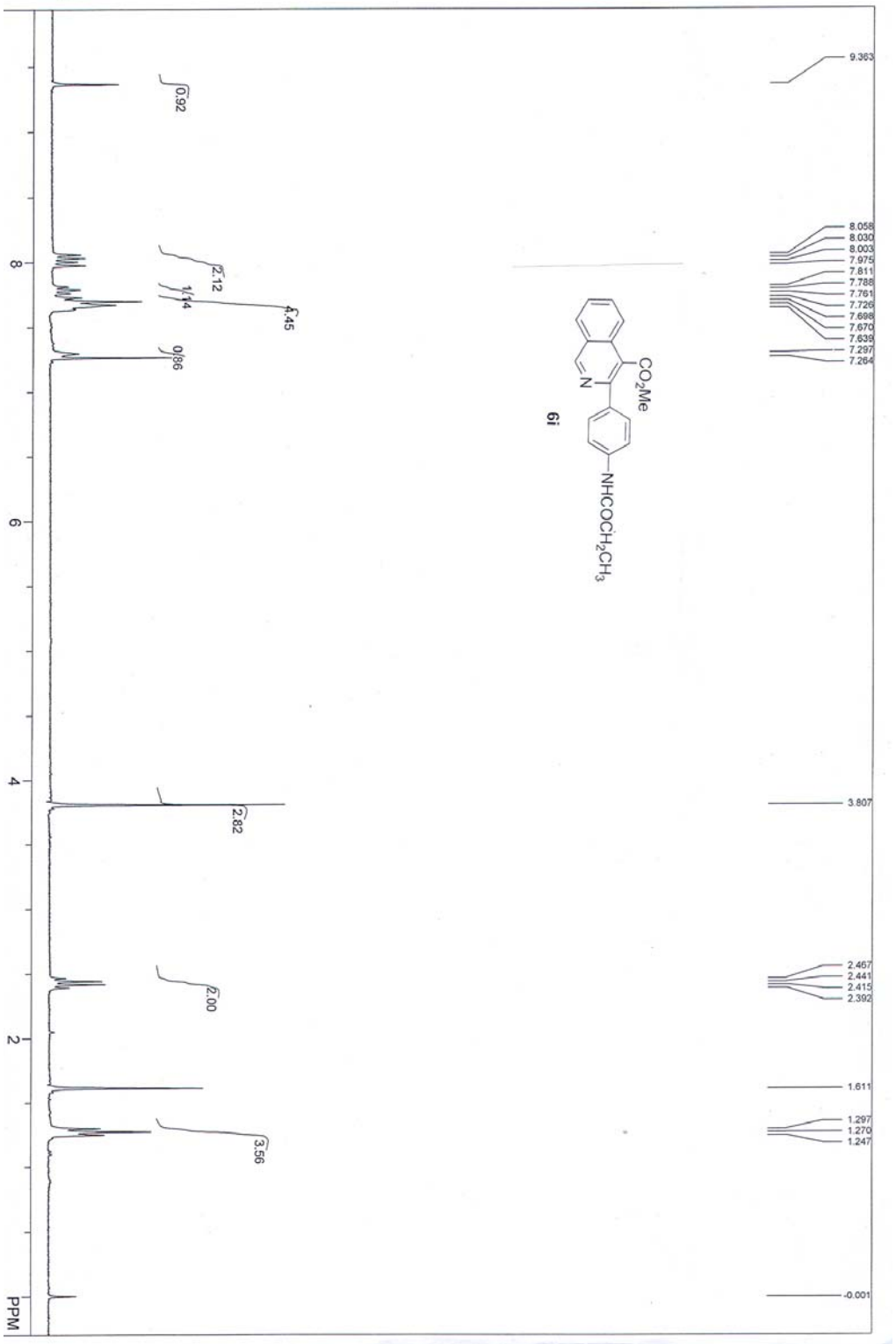
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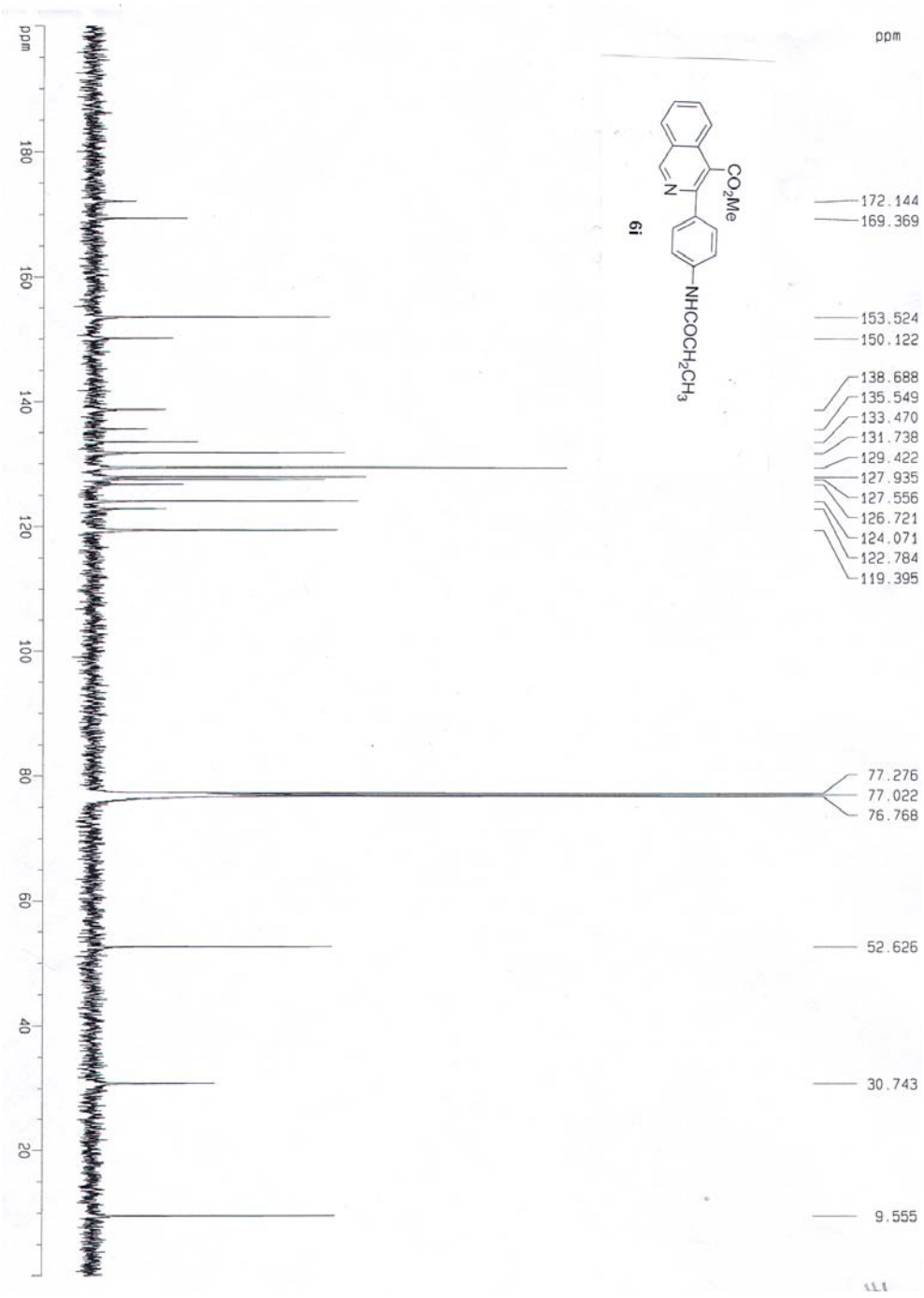
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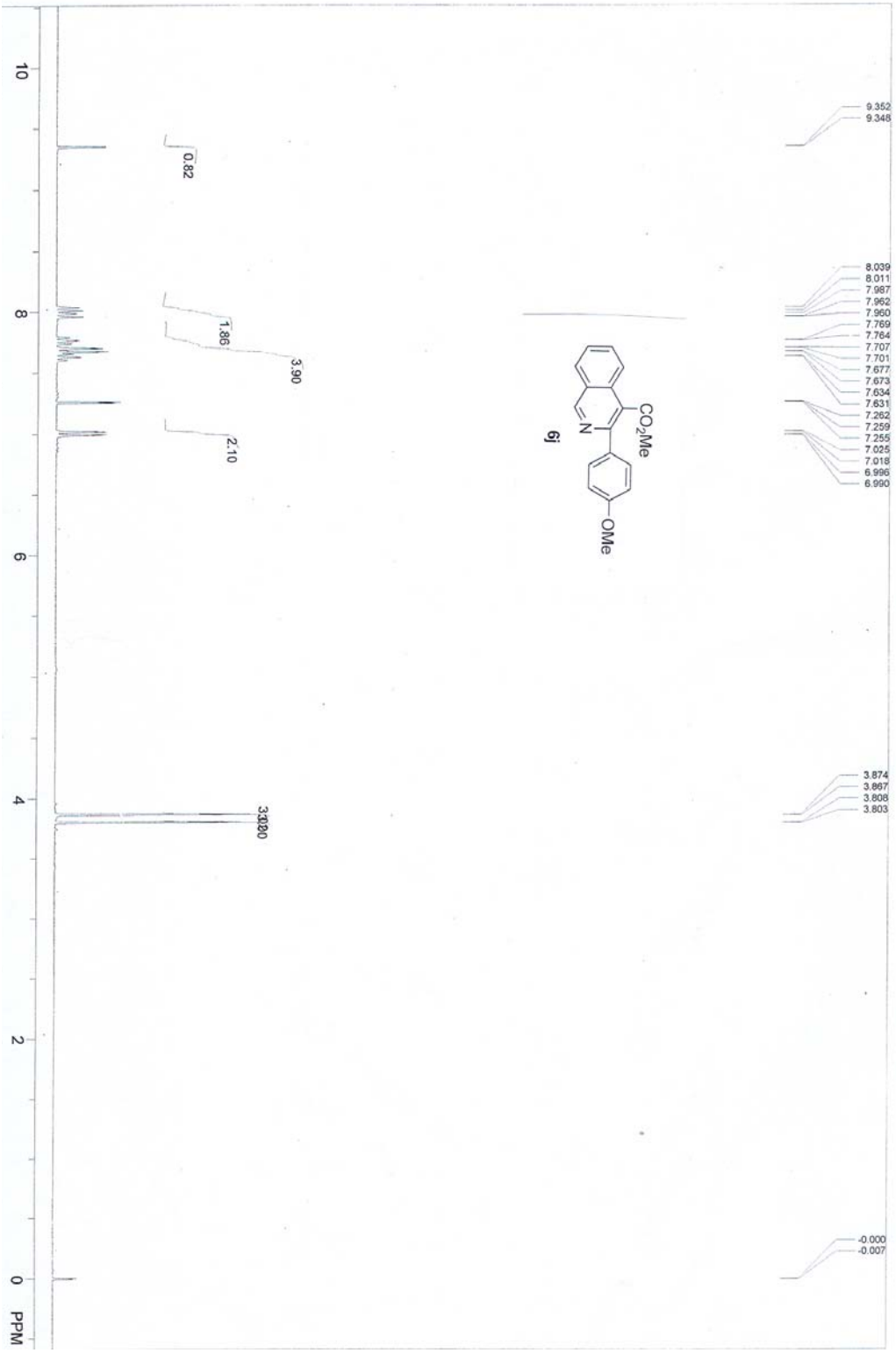
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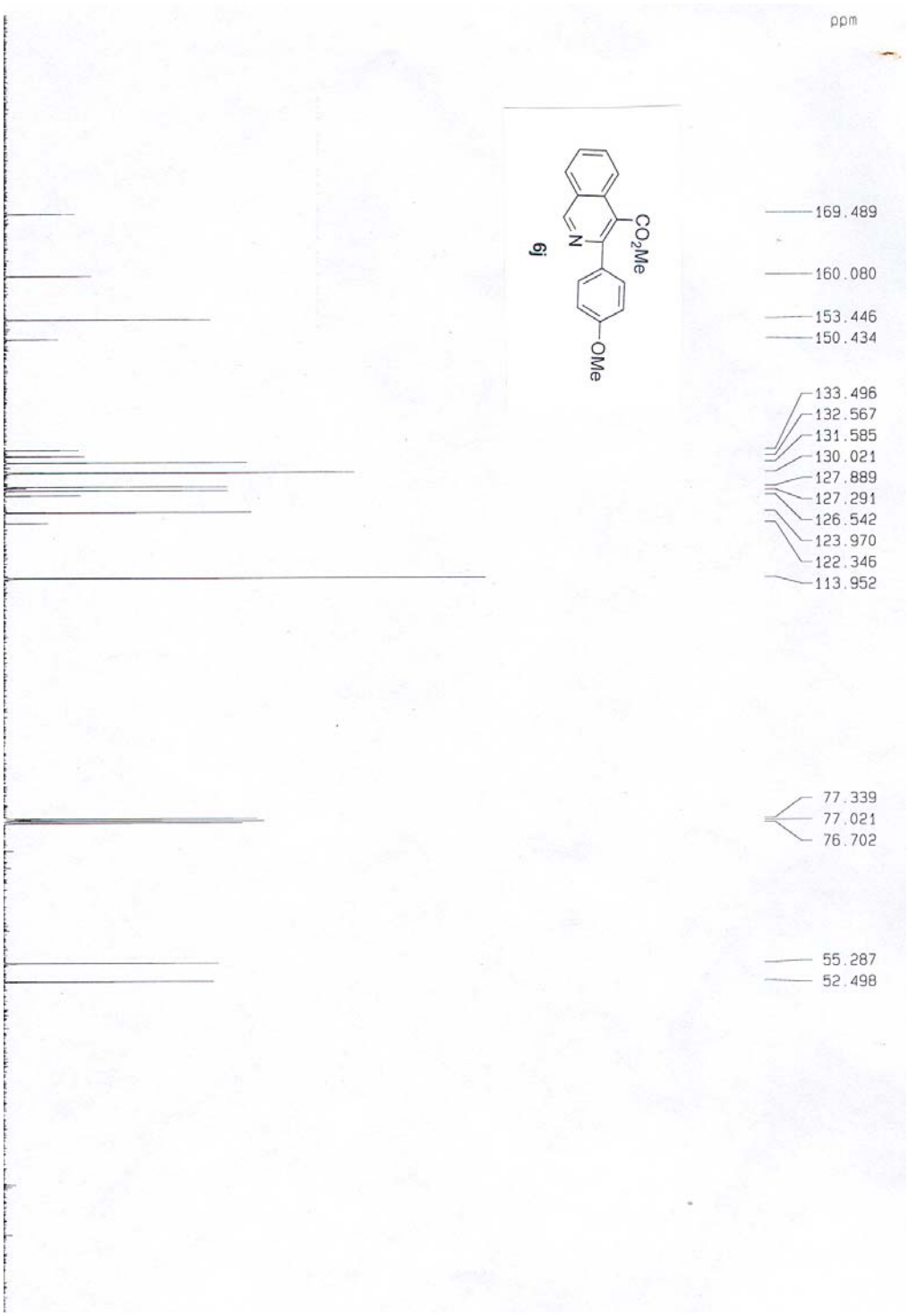
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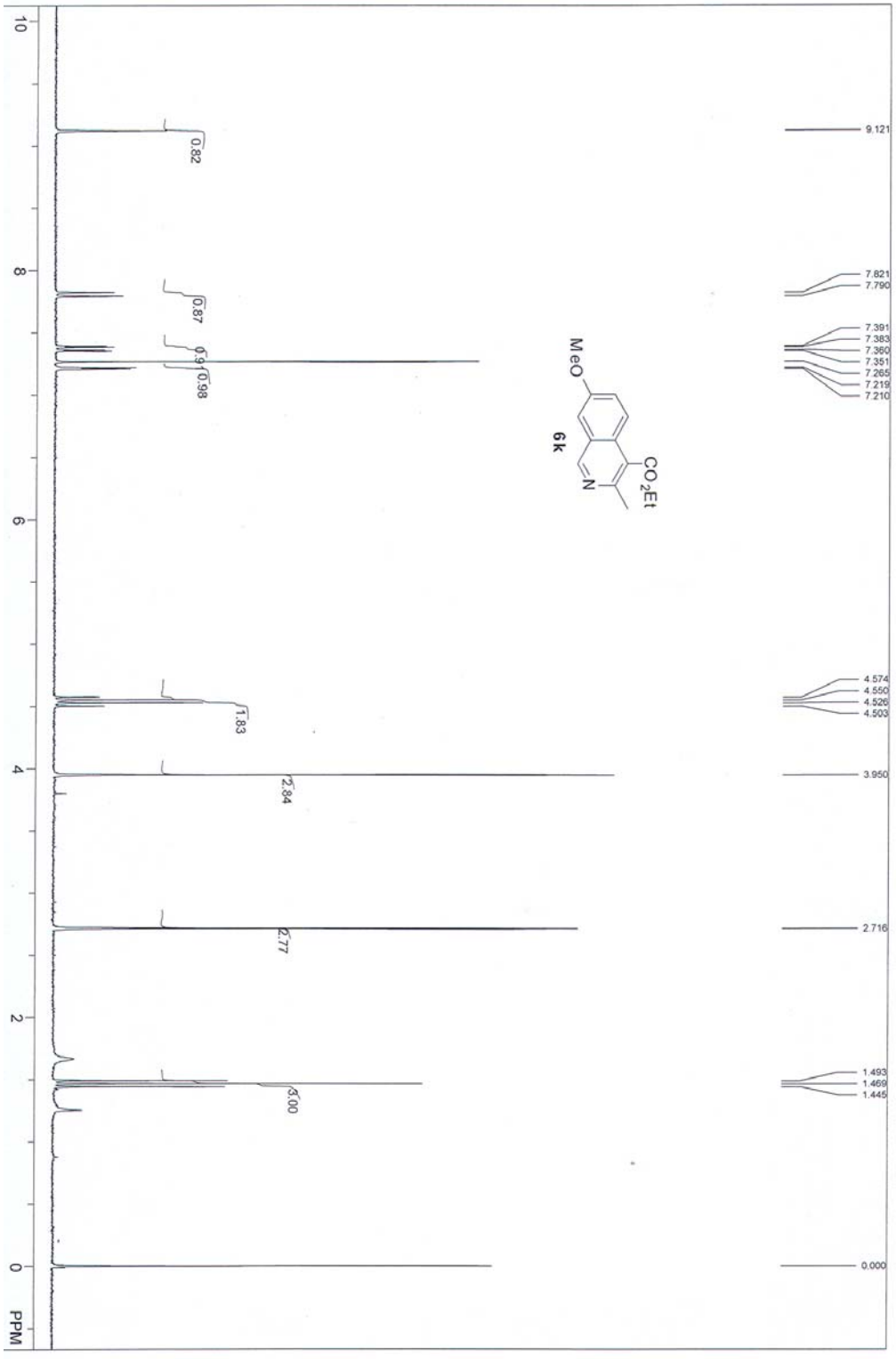
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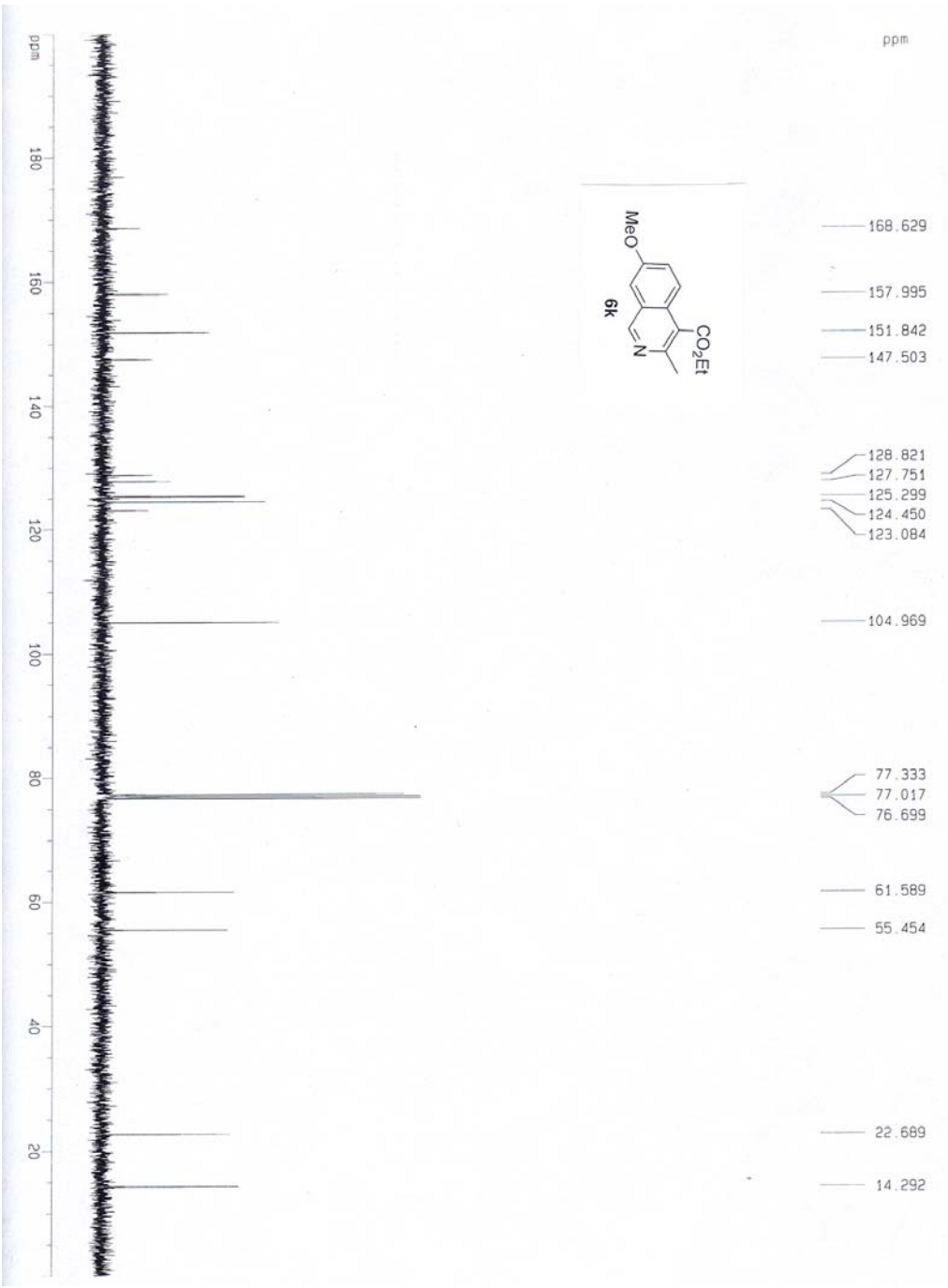
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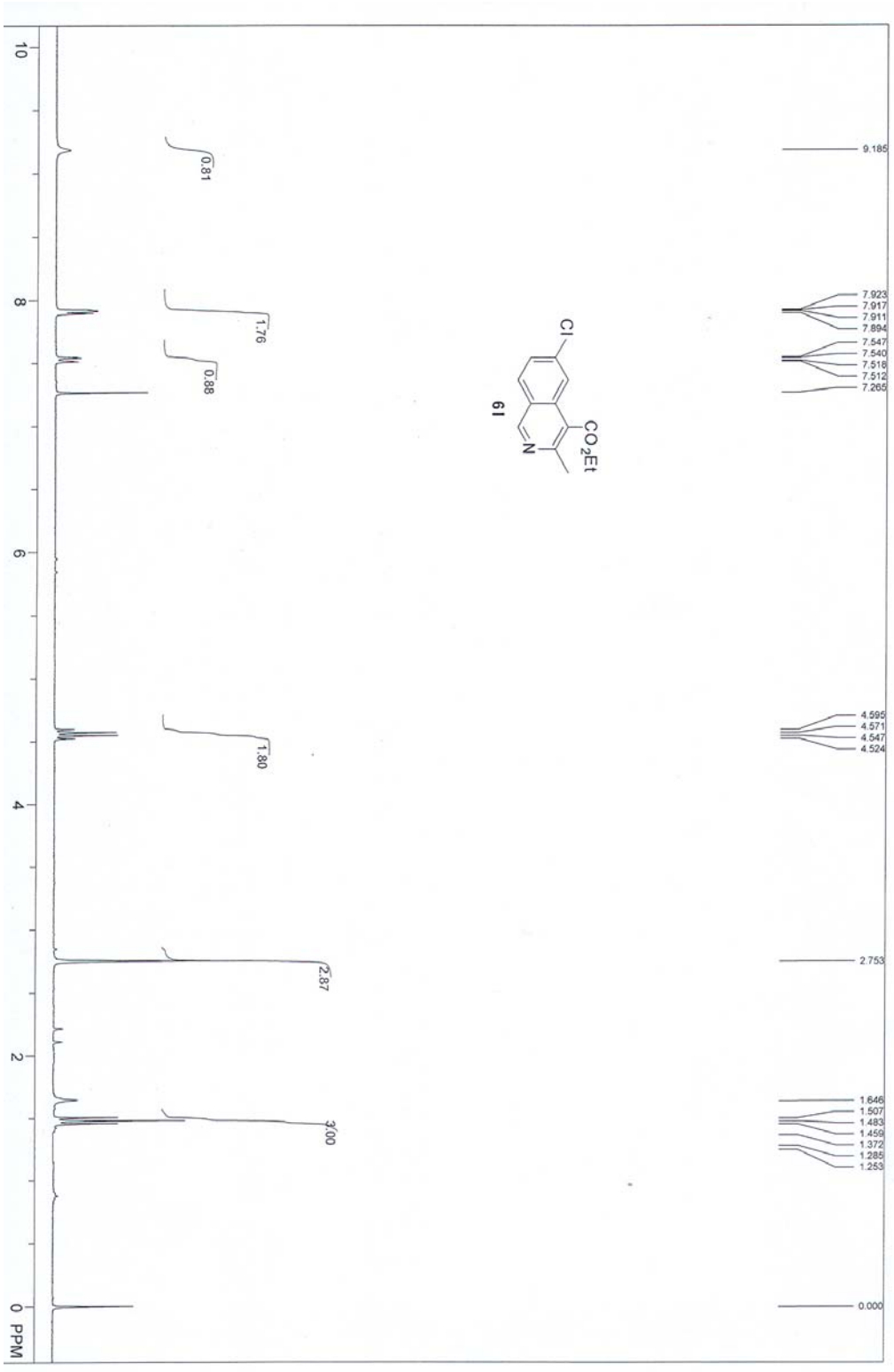
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6l
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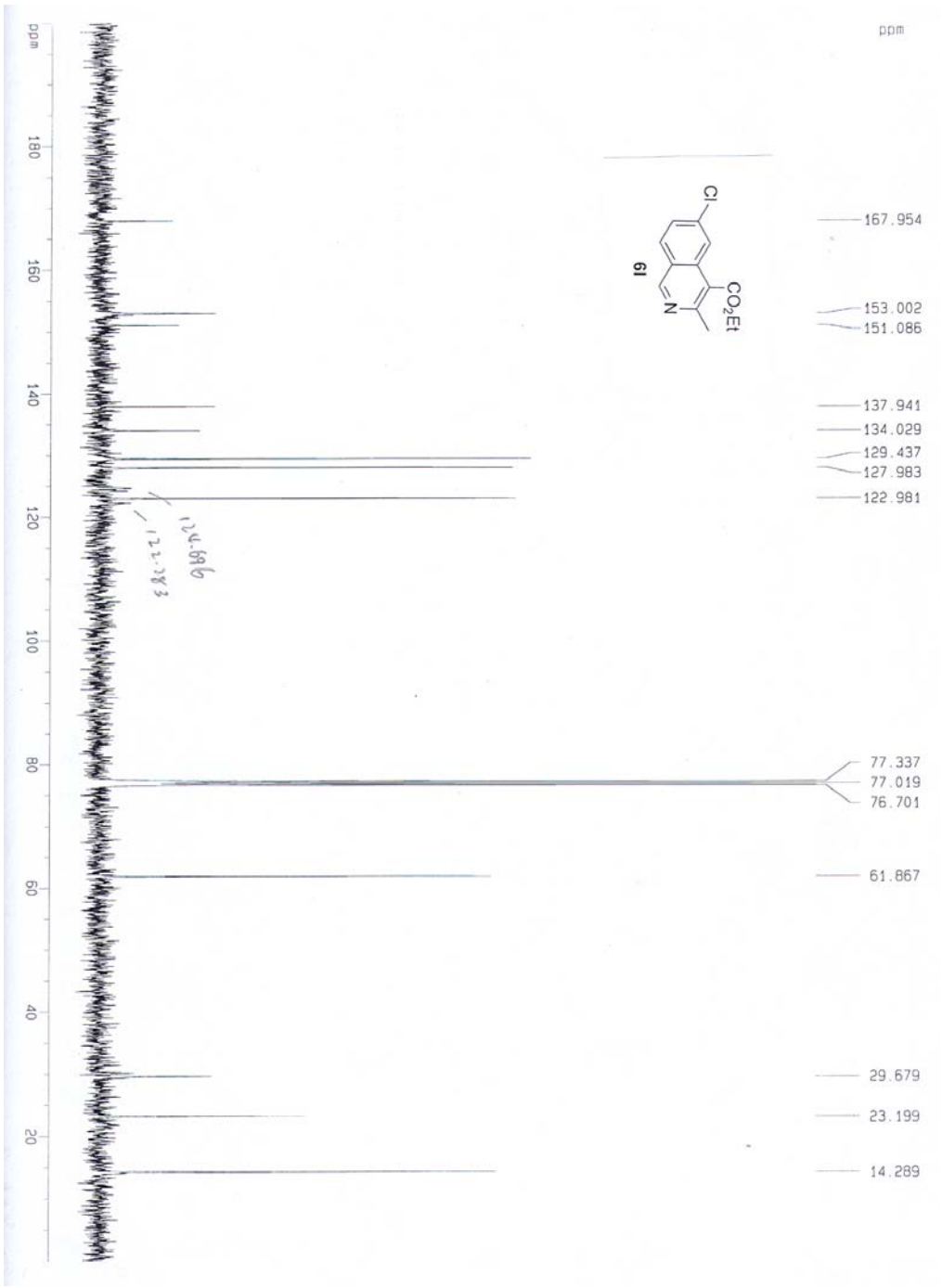
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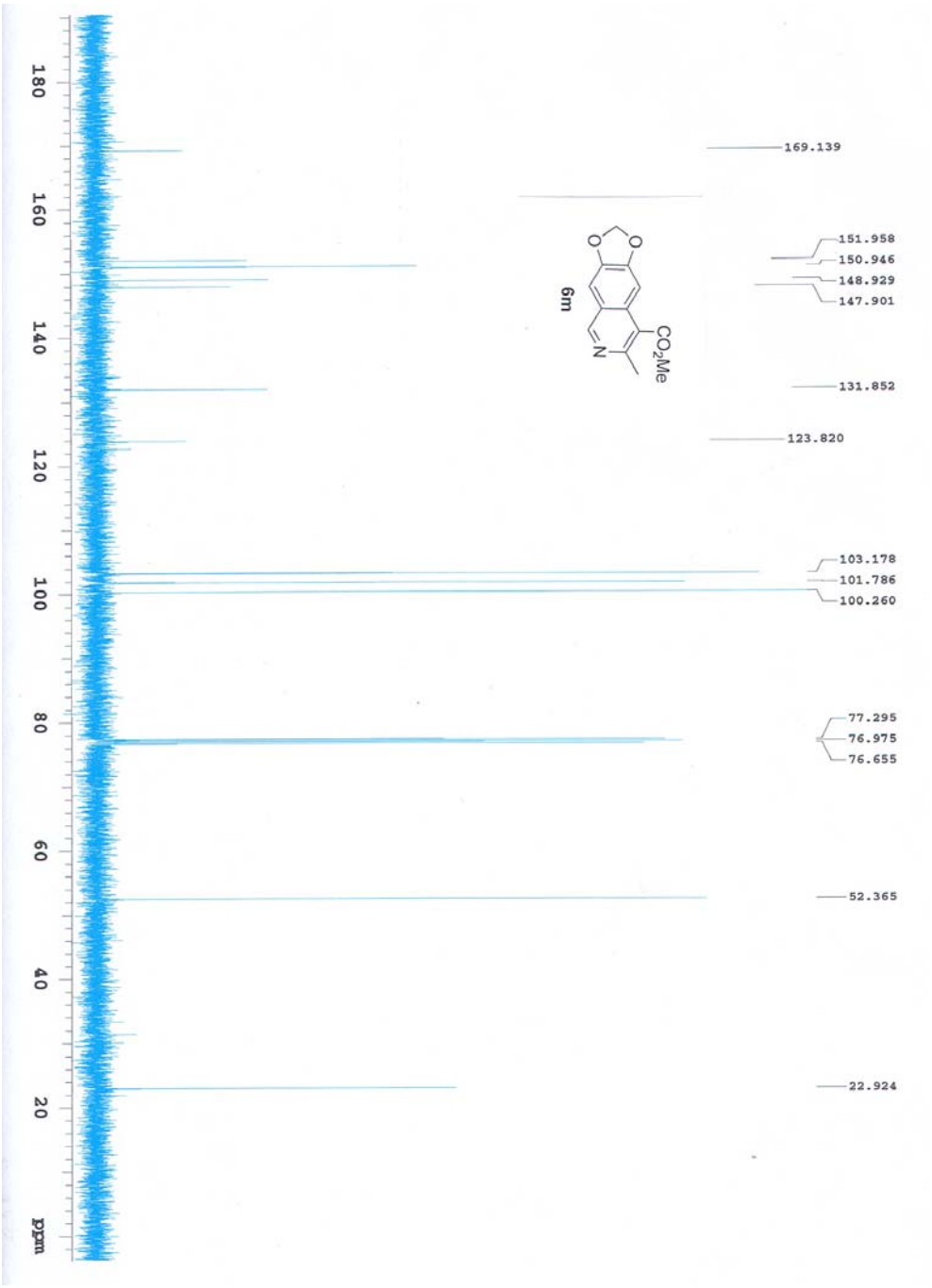
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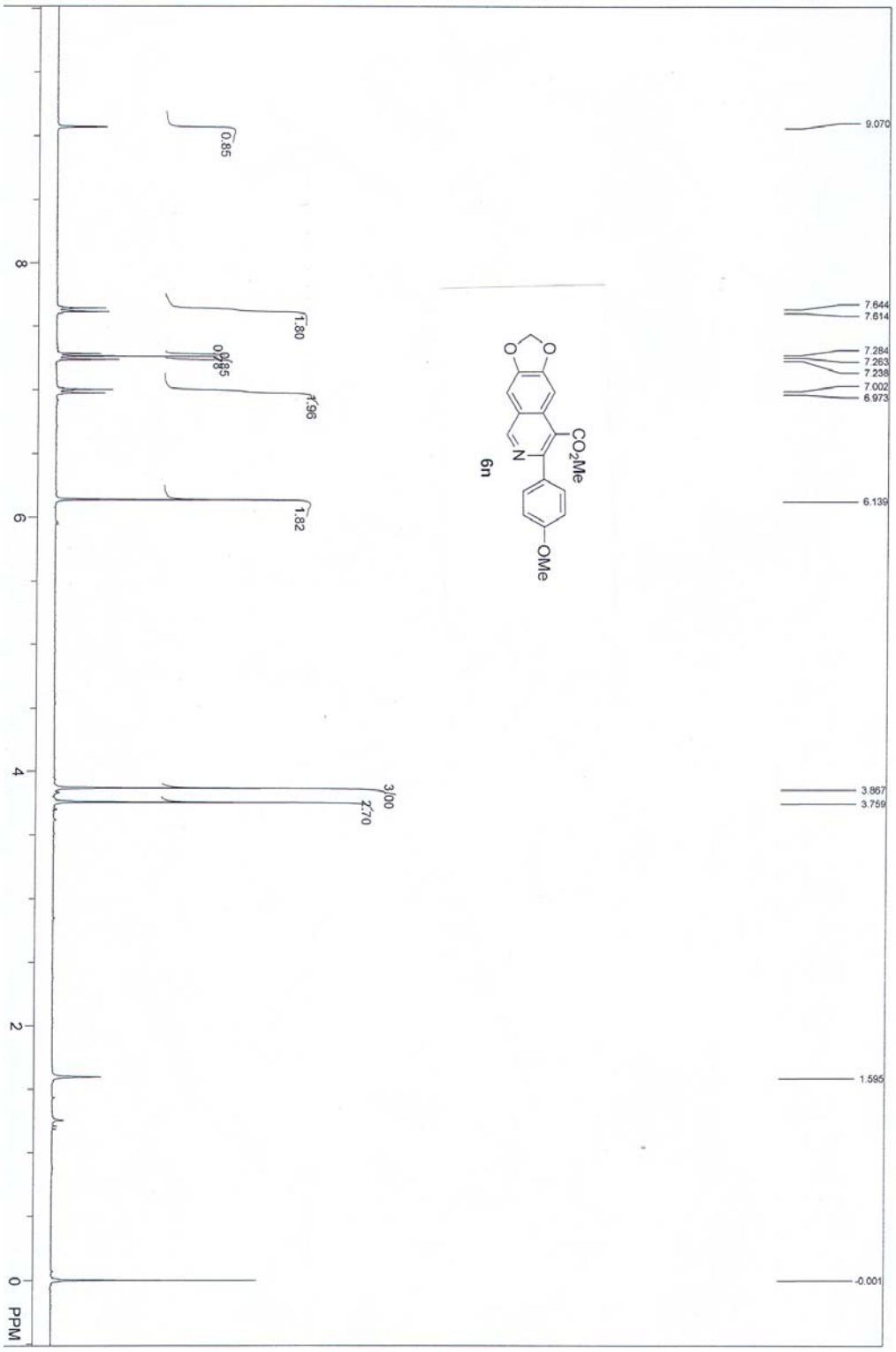
76.655
52.365
22.924
6m
CO2Me
N
O
O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7.644
7.614
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7.238
7.002
6.973
6.139
3.867
3.759
1.595
-0.001
0.85
1.80
0.85
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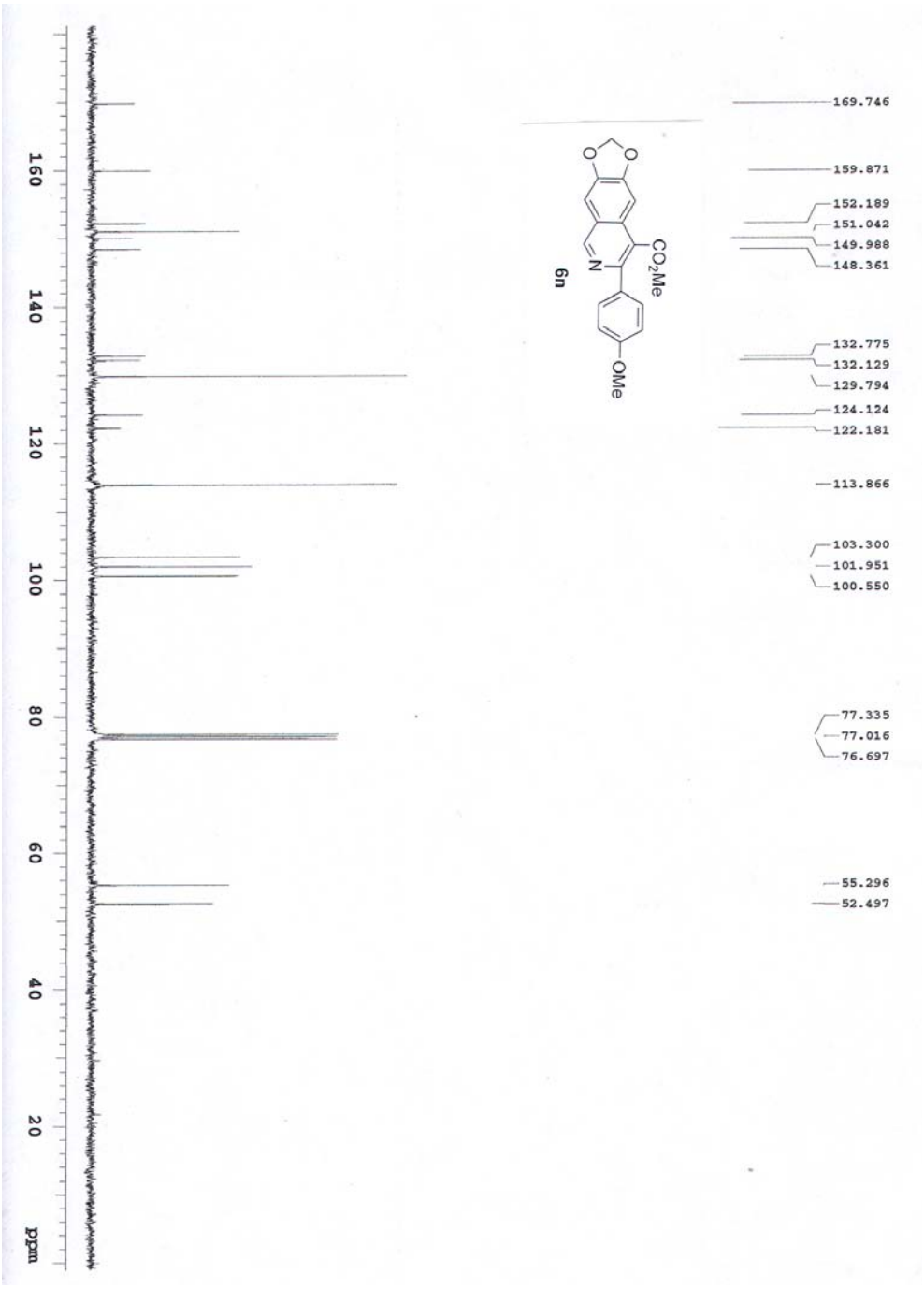
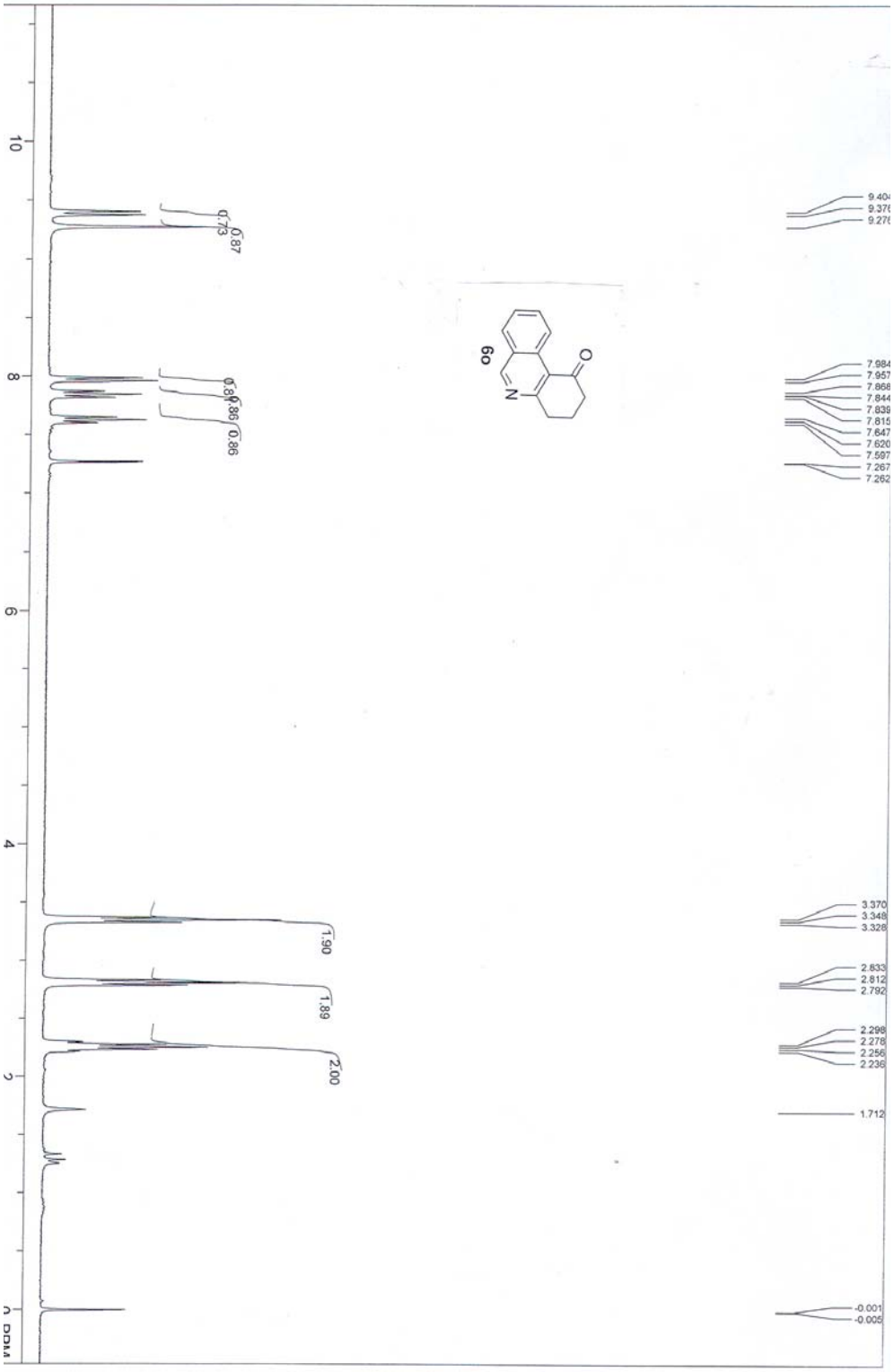
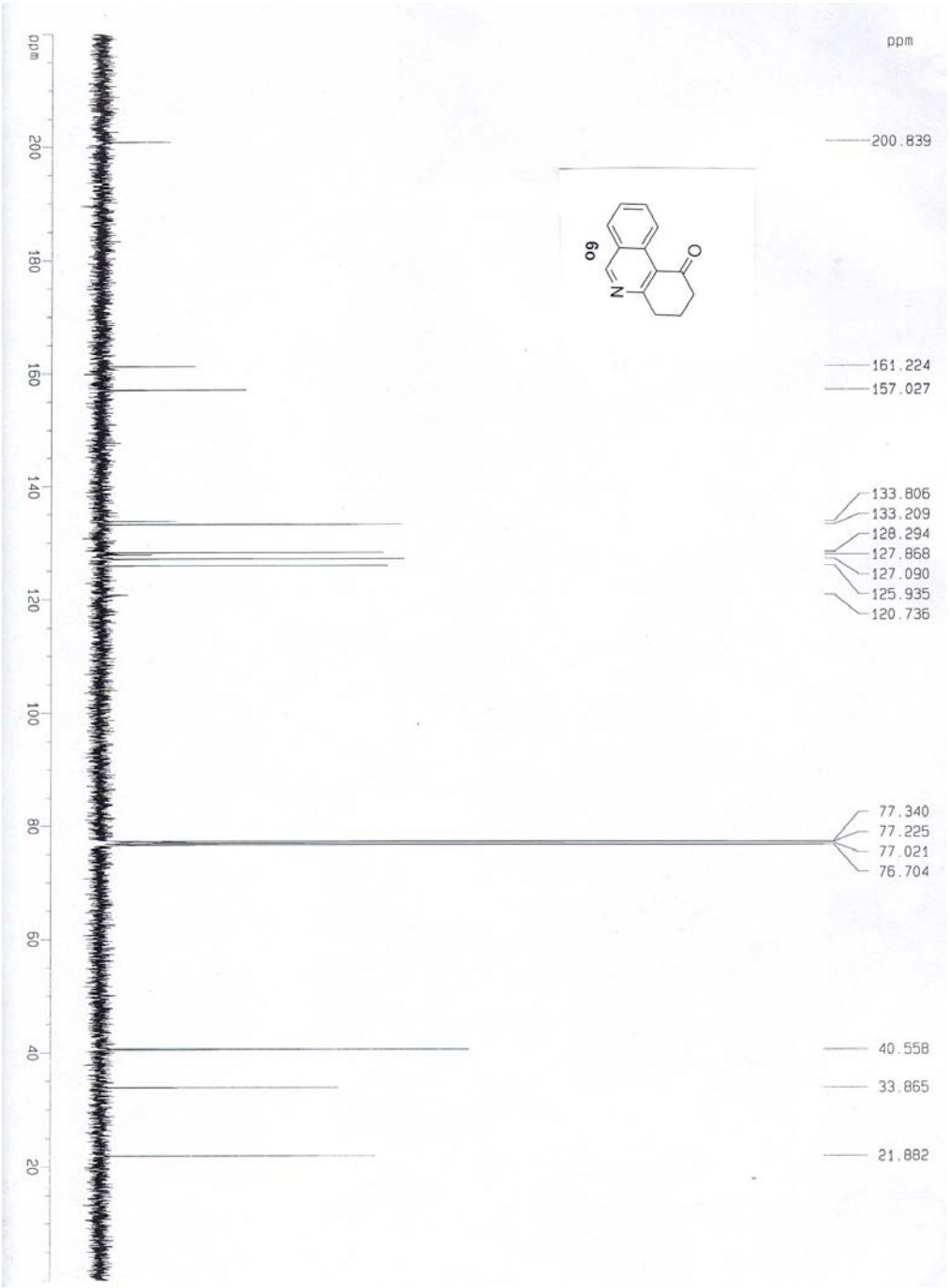
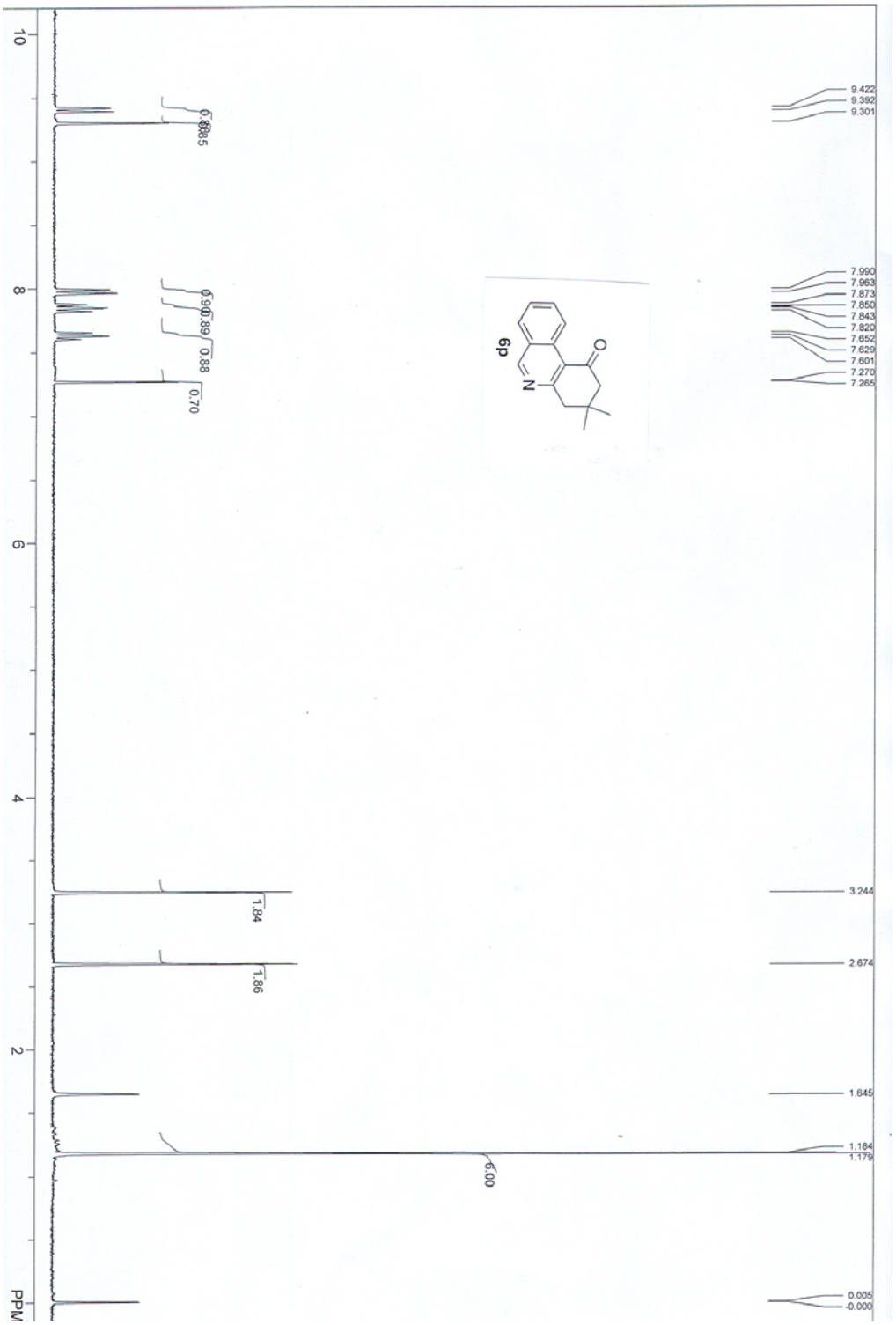
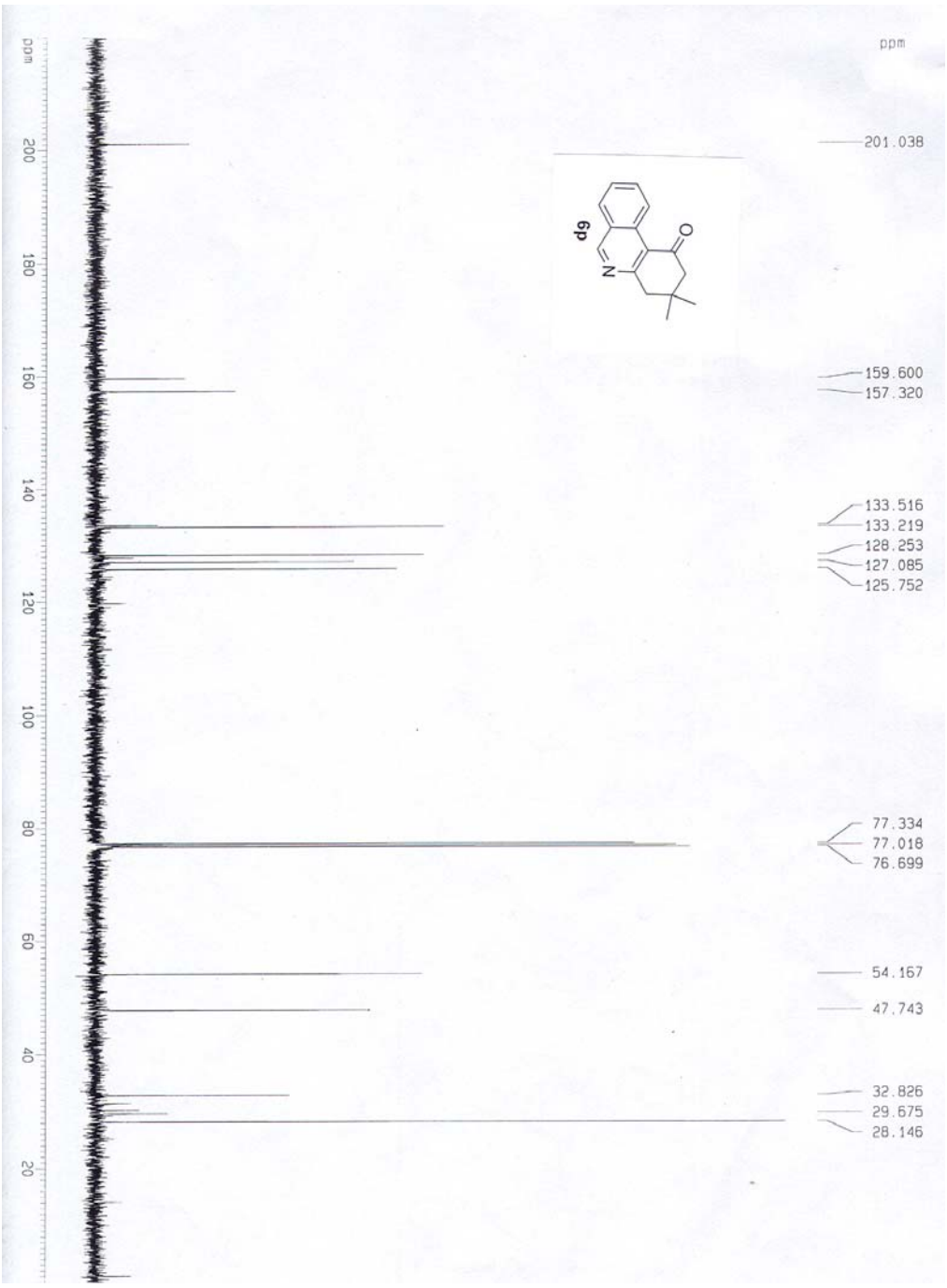
1.82
3.00
2.70
CO2Me
OMe
N
6n
8
6
4
2
0
PPM


169.746
159.871
152.189
151.042
149.988
148.361
132.775
132.129
129.794
124.124
122.181
113.866
103.300
101.951
100.550
77.335
77.016
76.697
55.296
52.497
CO2Me
OMe
N
6n
160
140
120
100
80
60
40
20
ppm


6o
O
N
9.404
9.378
9.278
7.984
7.957
7.868
7.844
7.839
7.815
7.647
7.620
7.597
7.267
7.262
3.370
3.348
3.328
2.833
2.812
2.792
2.298
2.278
2.256
2.236
1.712
-0.001
-0.005
0.87
0.73
0.89
0.86
0.86
1.90
1.89
2.00
10
8
6
4
2
0 PPM


ppm
200.839
161.224
157.027
133.806
133.209
128.294
127.868
127.090
125.935
120.736
77.340
77.225
77.021
76.704
40.558
33.865
21.882
O
N
6a


9.422
9.392
9.301
7.990
7.963
7.873
7.850
7.843
7.820
7.652
7.629
7.601
7.270
7.265
3.244
2.674
1.645
1.184
1.179
0.005
-0.000
6p
O
N
PPM


ppm
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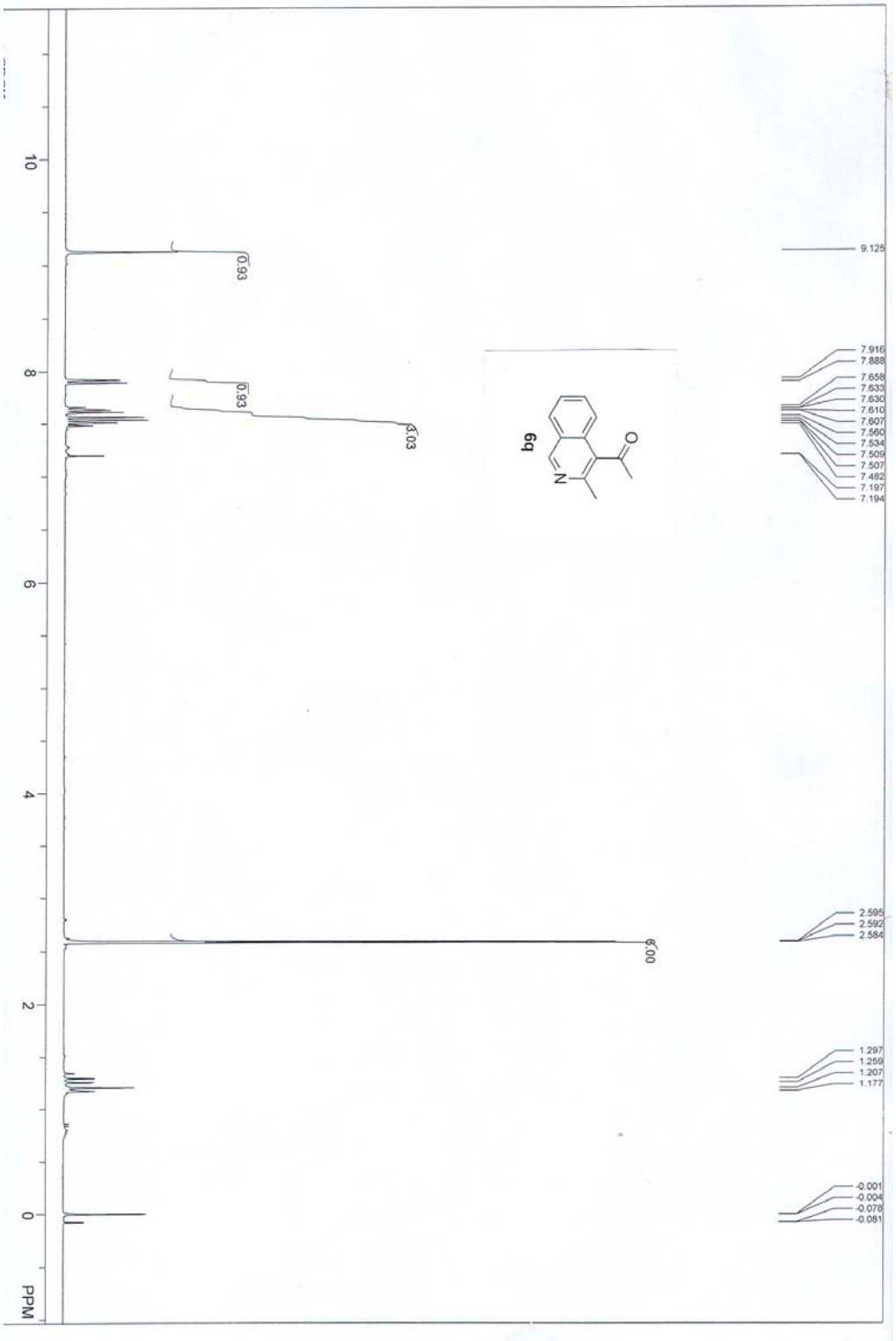
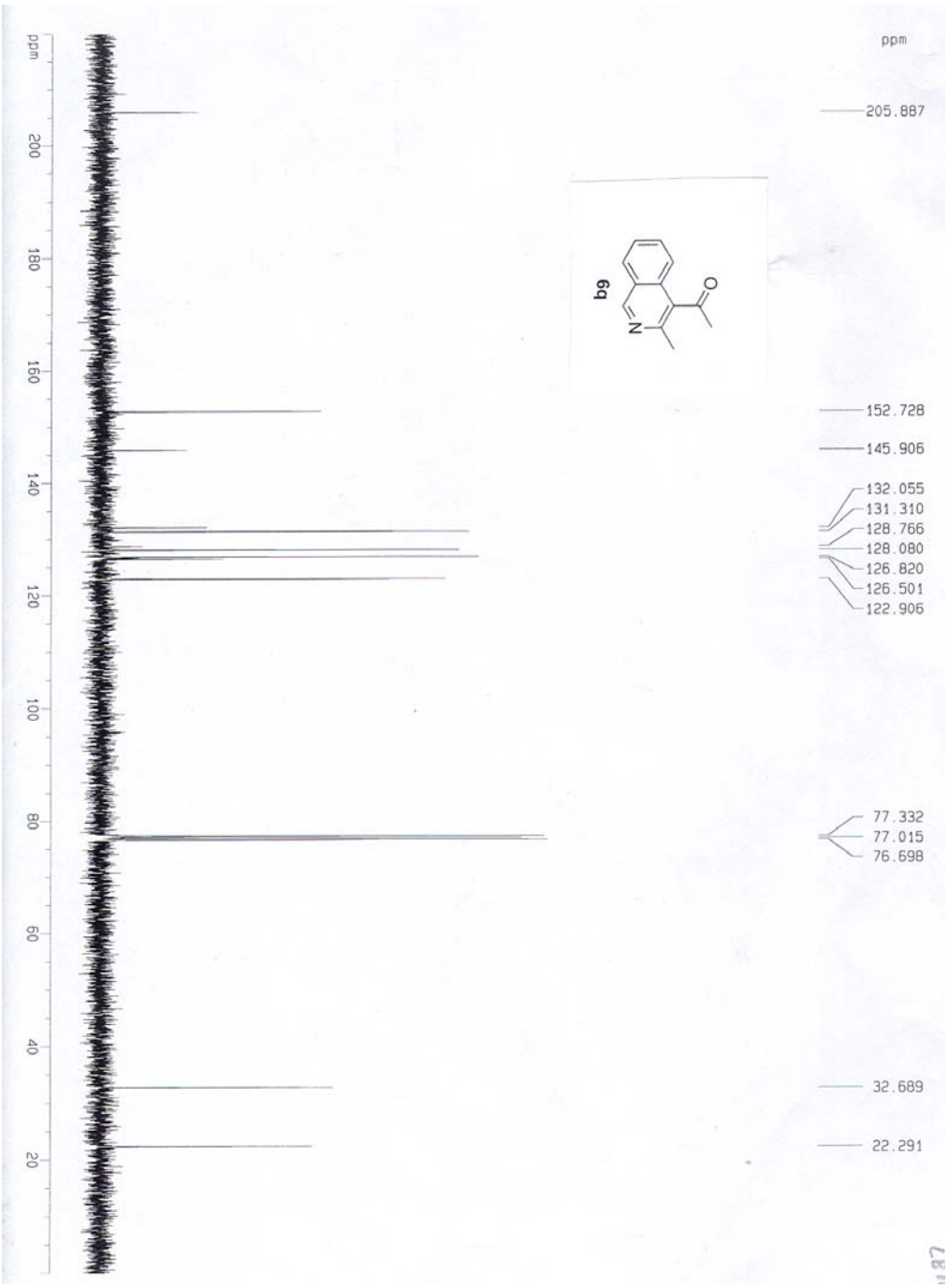
157.320
133.516
133.219
128.253
127.085
125.752
77.334
77.018
76.699
54.167
47.743
32.826
29.675
28.146
d9
O
N


6g
9.125
7.916
7.888
7.658
7.633
7.630
7.610
7.607
7.560
7.534
7.509
7.507
7.482
7.197
7.194
2.595
2.592
2.584
1.297
1.259
1.207
1.177
-0.001
-0.004
-0.078
-0.081
0.93
0.93
3.03
6.00
PPM


ppm
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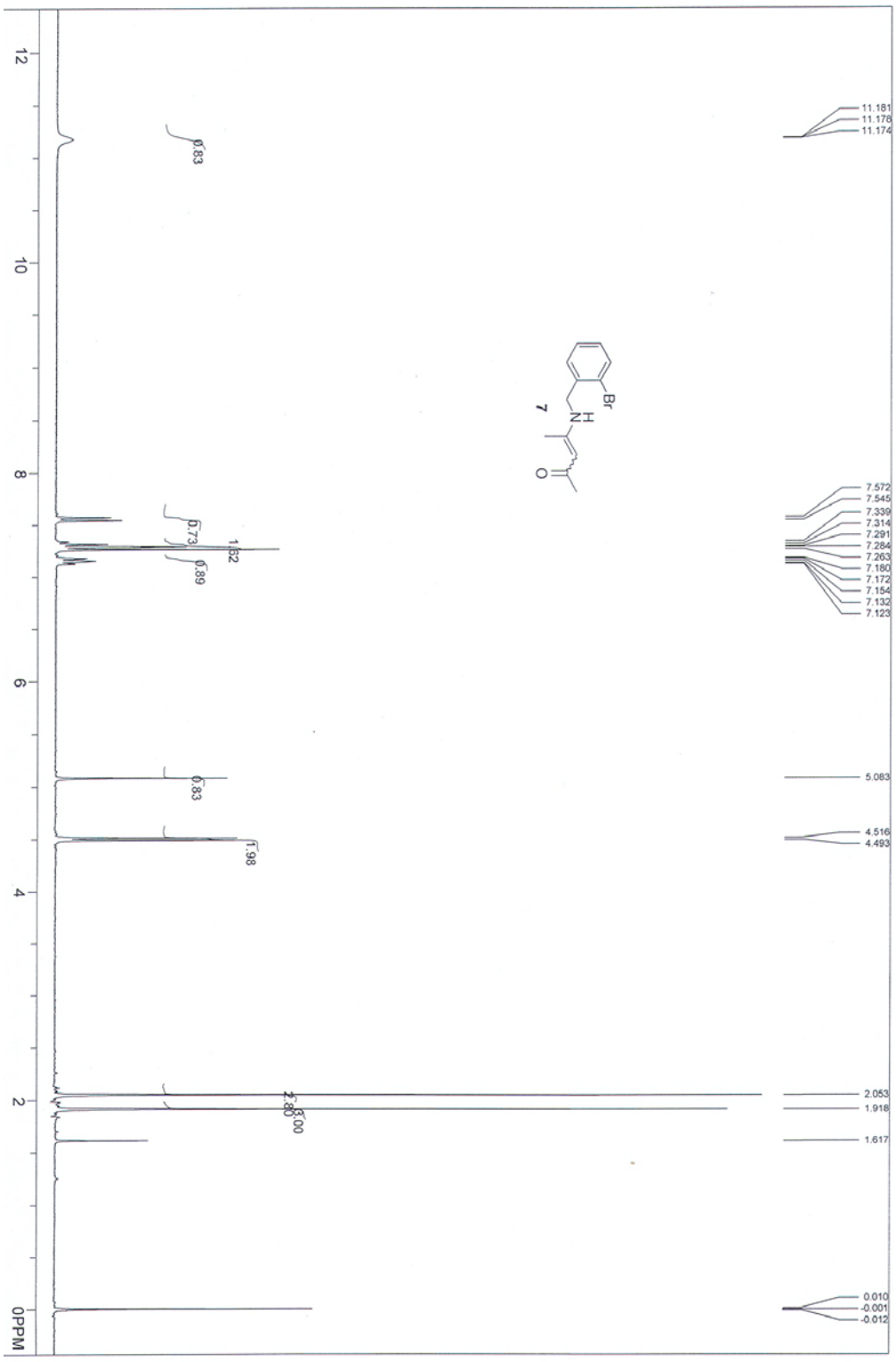
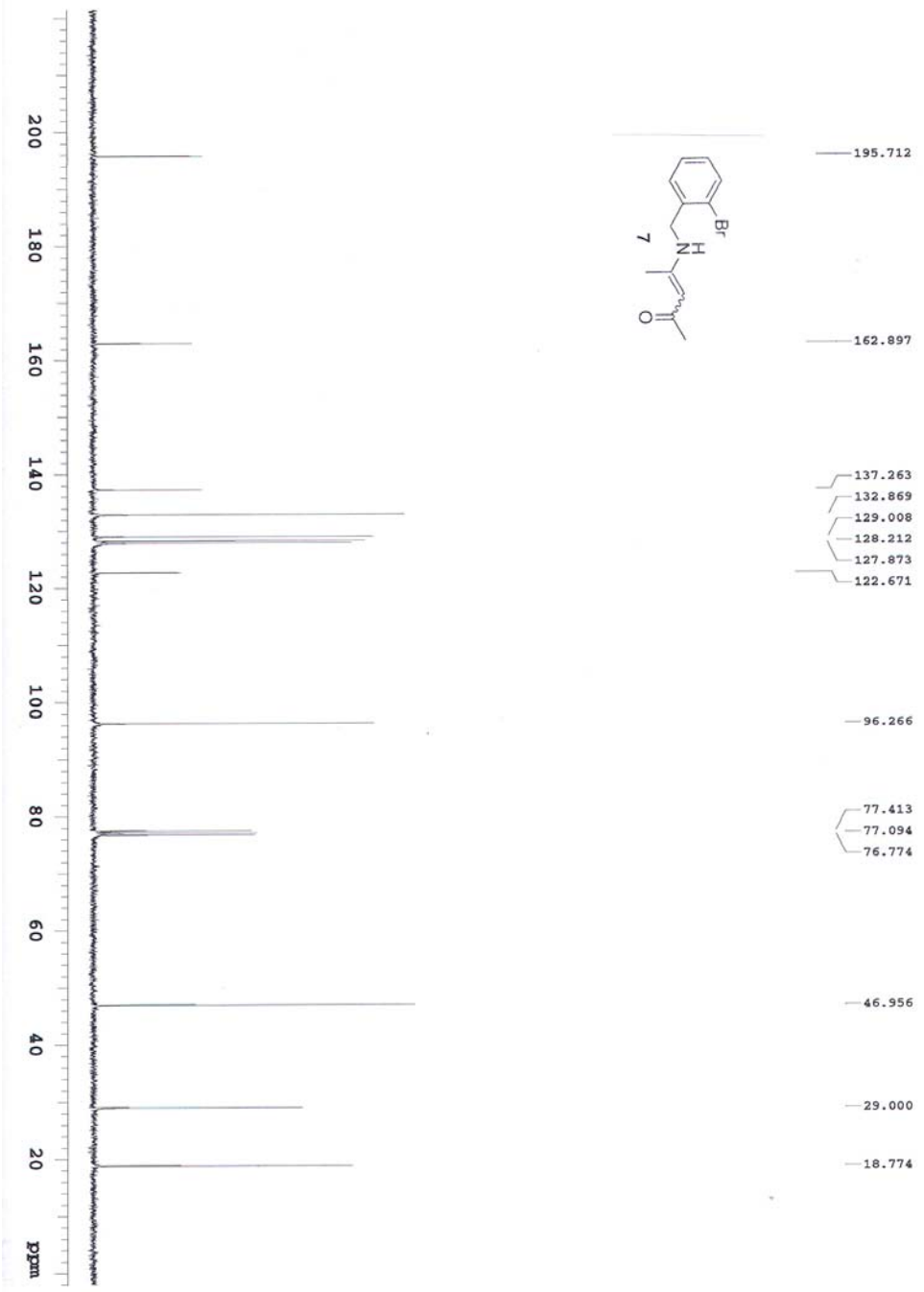
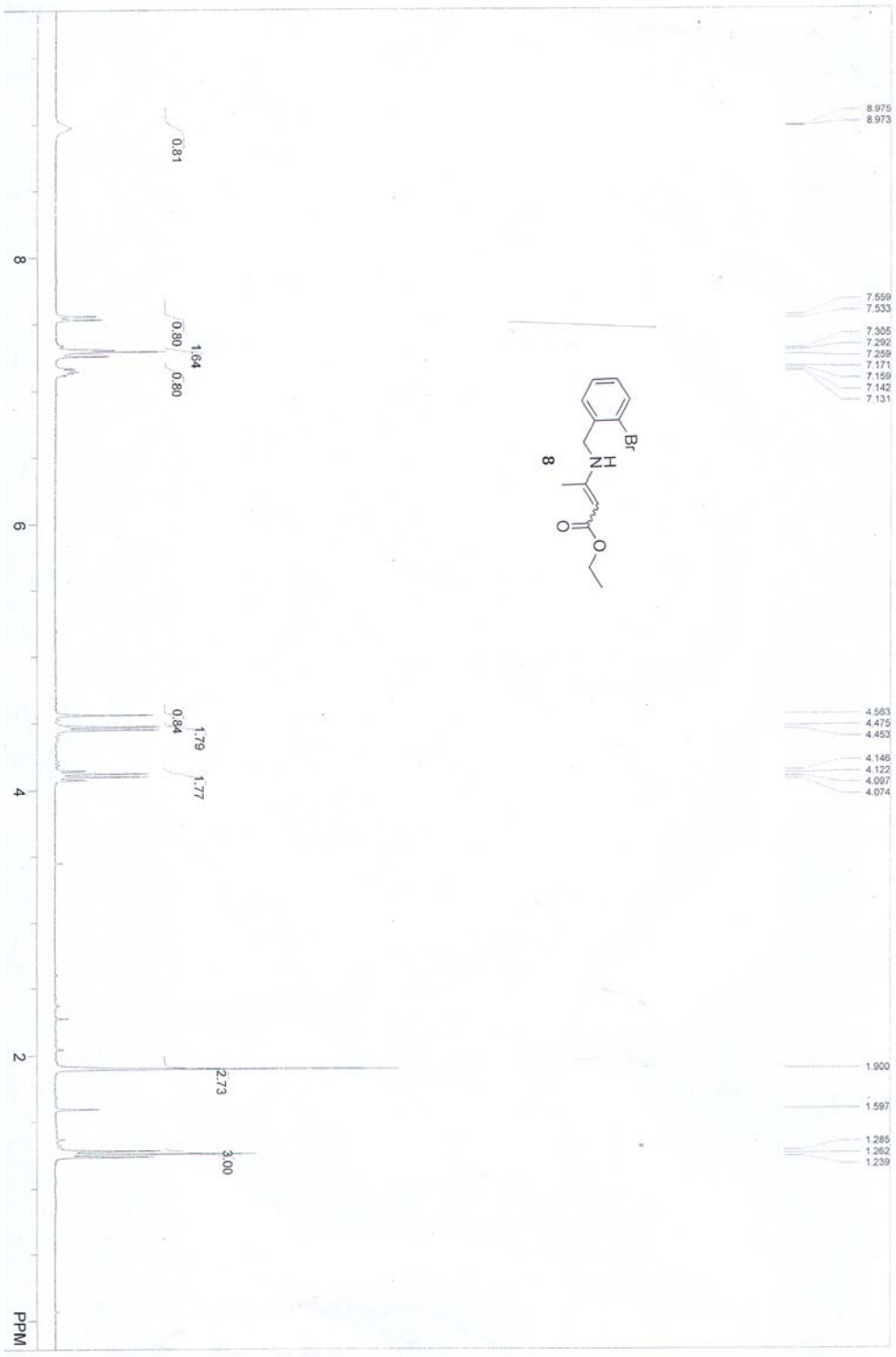
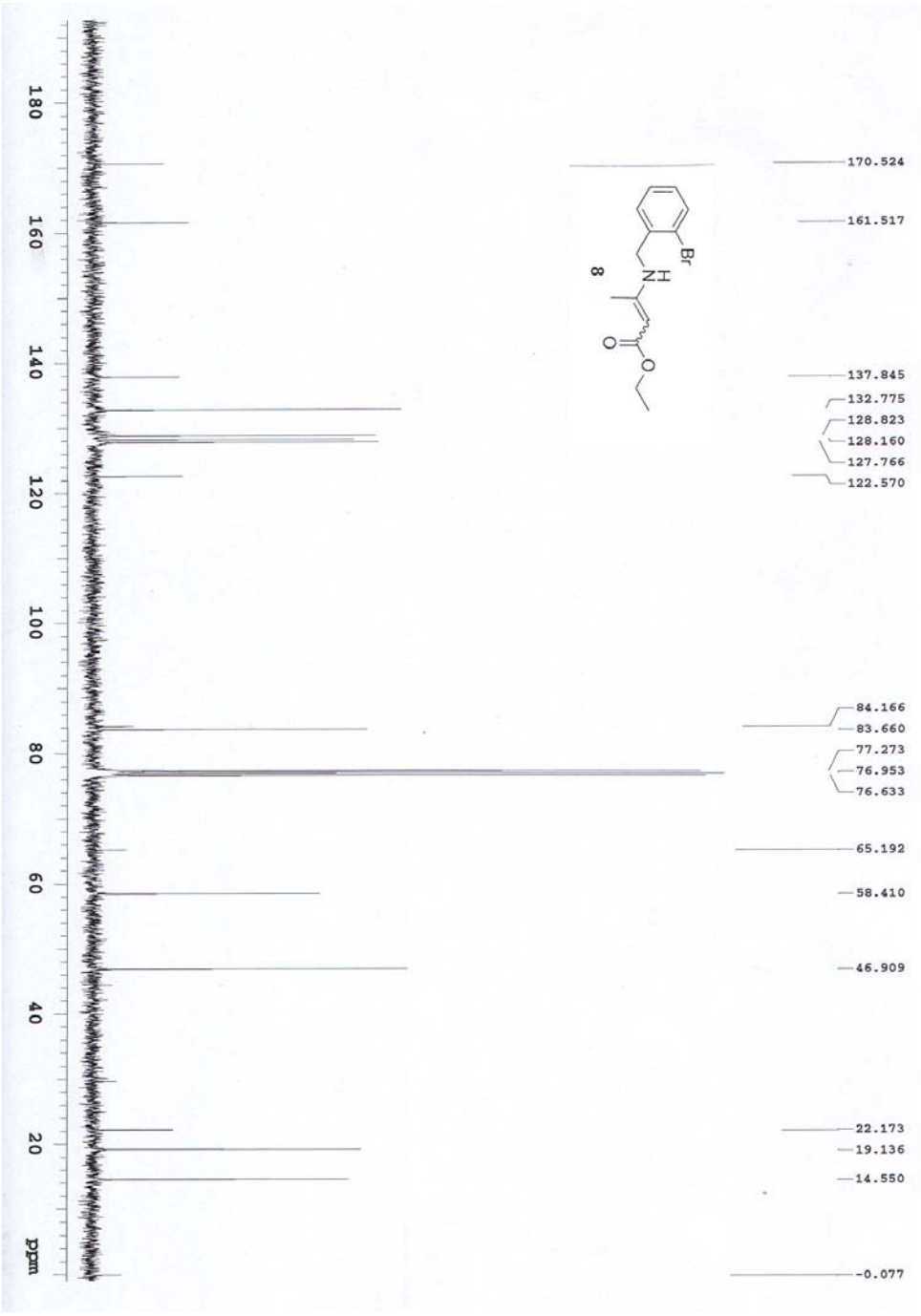
145.906
132.055
131.310
128.766
128.080
126.820
126.501
122.906
77.332
77.015
76.698
32.689
22.291
6g
O
N


12
10
8
6
4
2
0PPM
11.181
11.178
11.174
7.572
7.545
7.339
7.314
7.291
7.284
7.263
7.180
7.172
7.154
7.132
7.123
5.083
4.516
4.493
2.053
1.918
1.617
0.010
-0.001
-0.012
0.83
0.73
1.62
0.89
0.83
1.98
2.80
3.00
Br
H
N
O
7


195.712
162.897
137.263
132.869
129.008
128.212
127.873
122.671
96.266
77.413
77.094
76.774
46.956
29.000
18.774
Br
H
N
O
7
200
180
160
140
120
100
80
60
40
20
ppm


8.975
8.973
7.559
7.533
7.305
7.292
7.259
7.171
7.159
7.142
7.131
4.583
4.475
4.453
4.146
4.122
4.097
4.074
1.900
1.597
1.285
1.262
1.239
0.81
0.80
1.64
0.80
0.84
1.79
1.77
2.73
3.00
Br
N
H
O
O
8
PPM


170.524
161.517
137.845
132.775
128.823
128.160
127.766
122.570
84.166
83.660
77.273
76.953
76.633
65.192
58.410
46.909
22.173
19.136
14.550
-0.077
Br
N
H
O
O
8
180
160
140
120
100
80
60
40
20
ppm