

Electronic Supplementary Information (ESI) for

Recyclable covalent triazine framework-supported iridium(III) terpyridine complex for the acceptorless dehydrogenative couplings of *o*-aminobenzyl alcohols with ketones to quinolines

Xiaozhong Chen, Yao Ai, Deyun Liu, Peng Liu, Xiangchao Xu, Jiazhi Yang* and Feng Li*

School of Chemistry and Chemical Engineering, Nanjing University of Science & Technology, Nanjing 210094, P.
R. China

Contents

General Experimental Details.

Synthesis of CTF.

Synthesis of Ir(tpy)@CTF

Experimental procedures and characterization data of products

Fig. S1. FT-IR spectra of 2,6-pyridinedicarbonitrile, CTF, Ir(tpy)@CTF and recovered Ir(tpy)@CTF.

Fig. S2. XRD of CTF and Ir(tpy)@CTF

Fig. S3. TGA of CTF and Ir(tpy)@CTF

Fig. S4. SEM image of CTF.

Fig. S5. SEM image of Ir(tpy)@CTF and recovered Ir(tpy)@CTF.

Fig. S6. SEM image of Ir(tpy)@CTF and EDS mapping in Ir(tpy)@CTF.

Fig. S7. SEM image of recovered Ir(tpy)@CTF and EDS mapping.

Fig. S8. XPS of Ir(tpy)@CTF.

Fig. S9. The structure of [Ir(tpy)(bpy)Cl][Cl₂]

Table S1. Atomic composition by EDS.

Table S2. BET analysis of CTF and Ir(tpy)@CTF

¹H NMR and ¹³C NMR spectra of products.

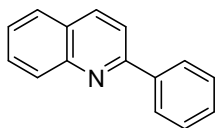
General Experimental Details. All reagents and materials used in this study were obtained from commercial sources and used as received unless mentioned otherwise. ATR-IR measurements were recorded on a Thermo Fisher Scientific Nicolet iS 10 instrument. XRD patterns were collected on a Bruker D8 Advanced Diffractometer using Cu K α irradiation ($\lambda=0.15406$ Å). TGA was performed on a Mettler 851e instrument with a heating rate of 10 °C min⁻¹ in oxygen atmosphere. Quant 250 FEG operated at an accelerating voltage of 20.0 kV was used for the Scanning Electron Microscopy (SEM) and Energy-Dispersive X-ray Spectroscopy (EDS) measurements. X-ray Photoelectron Spectroscopy (XPS) analysis was performed on a PHI QUANTERA II using Mg K α as the excitation source. All binding energy values were calibrated using the adventitious carbon C1s peak at 284.5 eV. Metal contents in Ir(tpy)@CTF was determined by inductively coupled plasma optical emission spectrometry (ICP-MS) (iCAP-Q, Thermo Fisher Scientific) using microwave assisted acid digestion system (MARS6, CEM/U.S.A). BET surface area and N₂ adsorption-desorption measurements were conducted at 77 K using an automated gas sorption system (ASAP 2020). Melting points were measured on a X-6 micro-melting apparatus. Proton nuclear magnetic resonance (¹H NMR) spectra were recorded at 500 MHz using a 500 spectrometer. Chemical shifts are reported in delta (δ) units, parts per million (ppm) downfield from tetramethylsilane or ppm relative to the center of the singlet at 7.26 ppm for CDCl₃ and 2.50 ppm for DMSO-d₆. Coupling constants *J* values are reported in Hertz (Hz), and the splitting patterns were designated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; b, broad. Carbon-13 nuclear magnetic resonance (¹³C NMR) spectra were recorded at 125 MHz using a 500 spectrometer. Chemical shifts are reported in delta (δ) units, ppm relative to the center of the triplet at 77.0 ppm for CDCl₃ and 39.5 ppm for DMSO-d₆. ¹³C NMR spectra were routinely run with broadband decoupling. Analytical thin-layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates. [Ir(tpy)Cl₃]¹ was synthesized according to the previously reported methods.

Synthesis of CTF. 2,6-Pyridinedicarbonitrile (0.30 g) and zinc chloride (1.61 g) were charged to a 20 mL ampoule under N₂ atmosphere and closed with septum. The ampoule was then sealed under vacuum by flame and the contents were heated to 400 °C in a furnace for a period of 48 h. The heating rate was maintained to be 60 °C/h. The furnace was cooled to 20 °C after 48 h. The crude product was collected, ground well and stirred with 500 mL of water for 3 h. The black solid was filtered and washed with water and acetone. The resulting solid was refluxed with 1M HCl solution (500 mL) for 16 h, filtered and washed with 1M HCl (3 × 100 ml), H₂O (3 × 100 ml), THF (3 × 100 ml), and acetone (3 × 100 ml). The black solid was dried under vacuum at 90 °C for 6 h.

Synthesis of Ir(tpy)@CTF. To a suspension of CTF (0.5 g) in 30 mL of ethylene glycol was added [Ir(tpy)Cl₃] (0.2 g) under N₂ atm. The resulting suspension was refluxed under N₂ atm for 18 h. After 18 h, the black solid was filtered and washed with an excess of ethylene glycol (10 x 25 mL) to remove the unreacted metal precursor. The as-synthesized catalyst was dried under vacuum at 60 °C for 36 h.

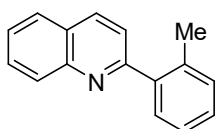
General procedure for the acceptorless dehydrogenative coupling of *o*-aminobenzyl alcohols with ketones to quinolines catalyzed by Ir(tpy)@CTF. In a round-bottomed flask with a condenser tube were added *o*-aminobenzyl alcohols (0.5 mmol), ketones (0.6 mmol, 1.2 equiv), Ir(tpy)@CTF (22 mg, 1 mol % Ir), KOH (8.4 mg, 0.3 equiv) and *t*-amyl alcohol (1 mL) under air atmosphere. The mixture of reaction was heated at reflux in an oil bath for 12 h. The reaction mixture was cooled to ambient temperature, concentrated in *vacuo* and purified by flash column chromatography with hexanes/ethyl acetate to afford the corresponding product.

2-phenylquinoline (3aa).²



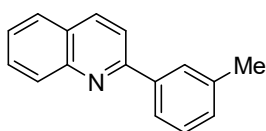
White solid; 87% yield (89 mg); mp 84–85 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.18–8.12 (m, 4H), 7.81 (d, J = 8.5 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.71–7.68 (m, 1H), 7.52–7.42 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ 157.2, 148.2, 139.6, 136.6, 129.7, 129.2, 129.1, 128.8, 127.5, 127.4, 127.1, 126.1, 118.9.

2-o-tolylquinoline (3ab).³



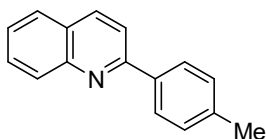
White solid; 84% yield (92 mg); mp 73–74 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.21 (d, J = 8.4 Hz, 2H), 7.86 (d, J = 8.2 Hz, 1H), 7.74 (t, J = 7.0 Hz, 1H), 7.77–7.73 (m, 1H), 7.58–7.52 (m, 3H), 7.35–7.30 (m, 3H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 160.2, 147.8, 140.7, 135.9, 130.8, 129.6, 129.6, 129.5, 128.4, 127.4, 126.6, 126.3, 125.9, 122.3, 20.3.

2-(m-tolyl)quinoline (3ac).⁴



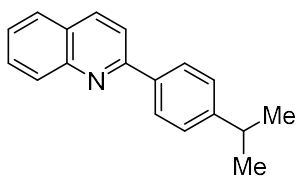
White solid; 82% yield (90mg); mp 278–279 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.19–8.17 (m, 2H), 8.00 (s, 1H), 7.91 (d, J = 7.7 Hz, 1H), 7.86–7.79 (m, 2H), 7.73–7.70 (m, 1H), 7.51 (t, J = 7.1 Hz, 1H), 7.40 (t, J = 7.7 Hz, 1H), 7.27 (d, J = 7.5 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 157.4, 148.2, 139.5, 138.4, 136.6, 129.6, 130.0, 129.5 (d, J = 10.1 Hz), 128.6, 128.2, 127.4, 127.1, 126.1, 124.6, 119.0, 21.5.

2-p-tolylquinoline (3ad).²



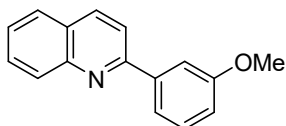
White solid; 91% yield (100 mg); mp 74–75 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.18 (t, $J = 8.7$ Hz, 2H), 8.09 (d, $J = 8.1$ Hz, 2H), 7.86 (d, $J = 8.6$ Hz, 1H), 7.81 (d, $J = 8.1$ Hz, 1H), 7.72 (t, $J = 7.2$ Hz, 1H), 7.51 (t, $J = 7.7$ Hz, 1H), 7.34 (d, $J = 7.95$ Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 157.3, 148.3, 139.3, 136.8, 136.6, 129.5, 129.4, 127.4, 127.1, 126.0, 118.8, 21.3.

2-(4-isopropylphenyl)quinoline (3ae).⁵



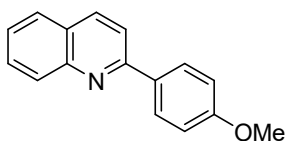
White solid; 81% yield (100 mg); mp 85–86 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.21–8.16 (m, 2H), 8.09 (d, $J = 8.2$ Hz, 2H), 7.86 (d, $J = 8.6$ Hz, 1H), 7.82 (d, $J = 8.1$ Hz, 1H), 7.72 (t, $J = 7.2$ Hz, 1H), 7.51 (t, $J = 7.8$ Hz, 1H), 7.39 (d, $J = 8.2$ Hz, 2H), 3.02–2.96 (m, 1H), 1.31 (d, $J = 6.9$ Hz, 6H); ^{13}C NMR (125 MHz, CDCl_3) δ 157.3, 150.2, 148.2, 137.2, 136.5, 129.5, 129.4, 127.4, 127.0, 126.8, 125.9, 118.8, 33.9, 23.8.

2-(3-methoxyphenyl)quinoline (3af).⁶



White solid; 88% yield (104 mg); mp 106–107 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.17 (d, $J = 8.5$ Hz, 2H), 7.84–7.77 (m, 3H), 7.73–7.69 (m, 2H), 7.50 (t, $J = 7.6$ Hz, 1H), 7.42 (t, $J = 7.9$ Hz, 1H), 7.02–7.00 (m, 1H), 3.91 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 160.0, 156.9, 148.1, 141.1, 136.6, 129.7, 129.6, 129.5, 127.3, 127.1, 126.2, 119.9, 118.9, 115.2, 112.6, 55.3

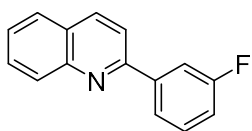
2-(4-methoxyphenyl)quinoline (3ag).²



White solid; 84% yield (99 mg); mp 123–124 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.14–8.12 (m, 4H), 7.81–7.77

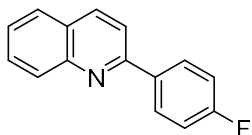
(m, 2H), 7.69 (t, $J = 7.8$ Hz, 1H), 7.48 (t, $J = 7.4$ Hz, 1H), 7.03 (d, $J = 8.2$ Hz, 2H), 3.86 (s, 3H); ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 160.7, 156.8, 148.2, 136.5, 132.1, 129.4, 129.4, 128.8, 127.3, 126.8, 125.8, 118.4, 114.1, 55.3.

2-(3-fluorophenyl)quinoline (3ah).⁷



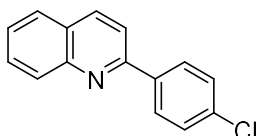
Pale-yellow solid; 82% yield (91 mg); mp 46–47 °C; ^1H NMR (500 MHz, CDCl_3) 8.24 (d, $J = 8.6$ Hz, 1H), 8.18 (d, $J = 8.5$ Hz, 1H), 7.93 (d, $J = 7.6$ Hz, 2H), 7.84 (t, $J = 5.75$ Hz, 2H), 7.76–7.73 (m, 1H), 7.55 (t, $J = 7.2$ Hz, 1H), 7.49 (q, $J = 6.3$ Hz, 1H), 7.18–7.14 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 164.3, 162.3, 155.7, 148.1, 141.8, 136.9, 130.2 (d, $J = 7.0$ Hz), 129.7 (d, $J_{\text{C-F}} = 7.8$ Hz), 127.4, 127.3, 126.5, 123.0, 118.6, 116.1 (d, $J_{\text{C-F}} = 21.1$ Hz), 114.4 (d, $J_{\text{C-F}} = 22.6$ Hz).

2-(4-fluorophenyl)quinoline (3ai).⁸



White solid; 85% yield (95 mg); mp 90–91 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.18–8.13 (m, 4H), 7.79–7.78 (m, 2H), 7.71 (t, $J = 7.7$ Hz, 1H), 7.50 (t, $J = 7.6$ Hz, 1H), 7.19 (t, $J = 8.6$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 163.7 (d, $J_{\text{C-F}} = 322.7$ Hz), 156.1, 148.2, 136.8, 135.7, 129.6 (d, $J_{\text{C-F}} = 15.5$ Hz), 129.3, 127.4, 127.0, 126.3, 118.5, 115.7 (d, $J_{\text{C-F}} = 21.4$ Hz).

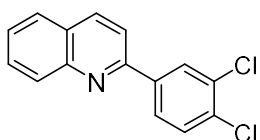
2-(4-chlorophenyl)quinoline (3aj).⁷



White solid; 87% yield (104 mg); mp 110–111 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.22 (d, $J = 8.5$ Hz, 1H),

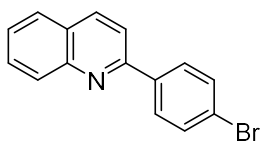
8.16-8.11 (m, 3H), 7.84-7.82 (m, 2H), 7.73 (t, $J = 7.6$ Hz, 1H), 7.54 (t, $J = 7.4$ Hz, 1H), 7.49 (d, $J = 8.4$ Hz, 2H); ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 155.9, 148.1, 137.9, 136.8, 135.4, 129.7, 129.6, 128.9, 128.7, 127.3, 127.1, 126.4, 118.4.

2-(3,4-dichlorophenyl)quinoline (3ak).³



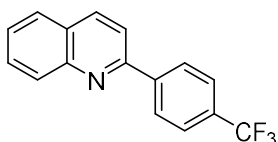
White solid; 79% yield (108 mg); mp 105–106 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.24 (d, $J = 8.5$ Hz, 1H), 8.17 (d, $J = 8.5$ Hz, 1H), 7.89 (d, $J = 8.1$ Hz, 1H), 7.77-7.72 (m, 2H), 7.68 (d, $J = 8.3$ Hz, 1H), 7.59 (t, $J = 7.5$ Hz, 1H), 7.54 (d, $J = 1.9$ Hz, 1H), 7.41 (dd, $J = 8.3$ and 1.9 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 154.4, 148.0, 139.3, 137.0, 133.4, 133.0, 130.6, 129.9, 129.6, 129.3, 127.4, 127.2, 126.7, 126.4, 118.1.

2-(4-bromophenyl)quinoline (3al).³



White solid; 84% yield (119 mg); mp 113–114 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.21-8.15 (m, 2H), 7.82 (d, $J = 8.6$ Hz, 2H), 7.75-7.72 (m, 1H), 7.65 (d, $J = 8.5$ Hz, 2H), 7.54 (t, $J = 7.1$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 155.9, 148.2, 138.4, 136.9, 131.9, 129.8, 129.6, 129.0, 127.4, 127.2, 126.5, 123.9, 118.4

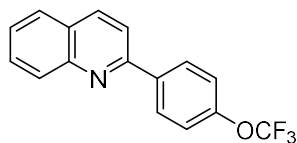
2-(4-(trifluoromethyl)phenyl)quinoline (3am).⁷



White solid; 87% yield (119 mg); mp 124-125 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.29-8.25 (m, 3H), 8.19 (d, $J = 8.5$ Hz, 1H), 7.90-7.85 (m, 2H), 7.79-7.75 (m, 3H), 7.57 (t, $J = 7.7$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 155.6, 148.3, 142.9, 137.1, 131.2 (q, $J_{\text{C-F}} = 32.0$ Hz), 123.0, 129.9, 127.8, 127.5, 126.8, 125.7, 125.3, 123.1,

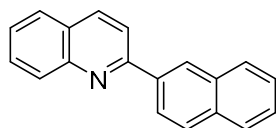
118.7.

2-(4-(trifluoromethoxy)phenyl)quinoline (3an).⁹



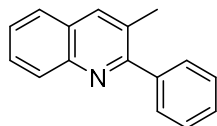
Light yellow oil; 85% yield (123 mg); ¹H NMR (500 MHz, DMSO-d₆) δ 8.43 (d, *J* = 8.6 Hz, 1H), 8.36 (d, *J* = 8.6 Hz, 2H), 8.12-8.06 (m, 2H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.77 (t, *J* = 7.7 Hz, 1H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 2H); ¹³C {¹H} NMR (125 MHz, DMSO-d₆) δ 154.9, 149.6, 147.8, 138.1, 137.7, 130.3, 129.5, 129.4, 128.1, 127.3, 127.0, 121.4, 119.4, 118.9.

2-(naphthalen-2-yl)quinoline (3ao).¹⁰



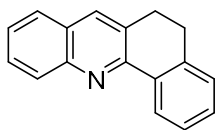
White solid; 84% yield (107 mg); mp 162-163 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.63 (s, 1H), 8.39 (dd, *J* = 8.6 and 1.7 Hz, 1H), 8.2-8.23 (m, 2H), 8.04-8.00 (m, 3H), 7.92-7.90 (m, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.78-7.45 (m, 1H), 7.57-7.53 (m, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 157.1, 148.3, 136.9, 136.8, 133.8, 133.5, 129.7, 128.8, 128.5, 127.7, 127.5, 127.2, 127.1, 126.7, 126.3, 125.0, 119.1.

3-methyl-2-phenylquinoline (3ap).³



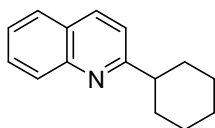
Pale-yellow oil; 82% yield (90 mg); ¹H NMR (500 MHz, CDCl₃) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.99 (s, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.65 (t, *J* = 8.1 Hz, 1H), 7.59-7.57 (m, 2H), 7.51-7.41 (m, 4H), 2.44 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 160.4, 146.5, 140.8, 136.6, 129.2, 129.1, 128.7, 128.6, 128.2, 128.1, 127.5, 126.6, 126.3, 20.5.

5,6-dihydrobenzo[c]acridine (3aq).⁸



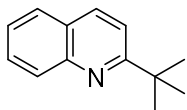
White solid; 80% yield (93 mg); mp 63-64 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.66-8.64 (m, 1H), 8.21-8.18 (m, 1H), 7.86 (s, 1H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.49-7.45 (m, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.28 (d, *J* = 7.4 Hz, 1H), 3.10-3.09 (m, 2H), 3.01-2.98 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 153.3, 147.5, 139.3, 134.6, 133.6, 130.5, 129.6, 129.3, 128.6, 127.9, 127.8, 127.2, 126.9, 126.0, 28.7, 28.3

2-cyclohexylquinoline (3ar).¹¹



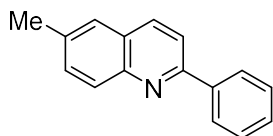
Yellow oil; 79% yield (83 mg); ¹H NMR (500 MHz, CDCl₃) δ 8.07-8.04 (m, 2H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.68-7.64 (m, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 1H), 2.95-2.89 (m, 1H), 2.03-2.01 (m, 2H), 1.90-1.87 (m, 2H), 1.80-1.77 (m, 1H), 1.67-1.59 (m, 2H), 1.52-1.42 (m, 2H), 1.37-1.31 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 166.7, 147.7, 136.2, 129.1, 128.8, 128.7, 127.3, 126.8, 125.5, 119.4, 47.5, 32.7, 26.4, 26.0.

2-(Tert-butyl)quinoline (3as).¹²



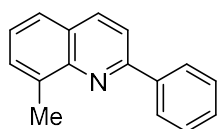
Light yellow oil; 81% yield (75 mg); ¹H NMR (500 MHz, CDCl₃) δ 8.07 (d, *J* = 8.5 Hz, 1H), 8.01 (d, *J* = 9.7 Hz, 1H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 8.7 Hz, 1H), 7.43 (t, *J* = 7.4 Hz, 1H), 1.46 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 169.1, 147.4, 135.8, 129.4, 128.9, 127.1, 126.4, 125.5, 118.1, 38.0, 30.1.

6-methyl-2-phenylquinoline (3ba).¹³



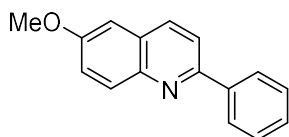
White solid; 90% yield (99 mg); mp 60-61 °C; ^1H NMR (500 MHz, CDCl_3) δ 9.03 (s, 1H), 7.93-7.88 (m, 4H), 7.63-7.60 (m, 1H), 7.49 (t, J = 7.8 Hz, 2H), 7.35 (d, J = 8.2 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 156.4, 146.7, 139.7, 136.0, 136.0, 131.8, 129.3, 129.0, 128.7, 127.4, 127.1, 126.2, 118.9, 21.5.

8-methyl-2-phenylquinoline (3ca).¹⁴



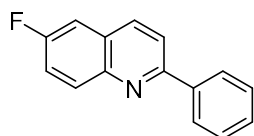
Pale-yellow oil; 87% yield (95 mg); mp 55-56 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.27 (d, J = 7.4 Hz, 2H), 8.19 (d, J = 8.6 Hz, 1H), 7.91 (d, J = 8.6 Hz, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.58 (d, J = 6.9 Hz, 1H), 7.54 (t, J = 7.4 Hz, 2H), 7.47 (t, J = 7.3 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 2.92 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 155.5, 147.1, 139.8, 137.6, 136.9, 129.6, 129.2, 128.7, 127.4, 127.0, 126.0, 125.3, 118.1, 17.9.

6-methoxy-2-phenylquinoline (3da).¹⁵



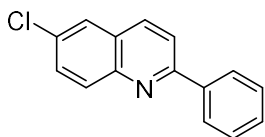
White solid; 85% yield (100 mg); mp 128-129 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.13-8.06 (m, 4H), 7.80 (d, J = 8.6 Hz, 1H), 7.50 (t, J = 7.5 Hz, 2H), 7.44-7.36 (m, 2H), 7.06 (d, J = 2.2 Hz, 1H), 3.92 (s, 3H); ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 157.5, 154.9, 144.2, 139.7, 135.4, 131.0, 128.8, 128.7, 128.0, 127.2, 122.2, 119.1, 104.9, 55.4.

6-fluoro-2-phenylquinoline (3ea).¹⁶



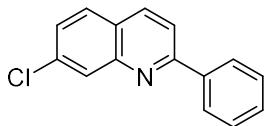
White solid; 82% yield (91 mg); mp 90-91 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.18-8.14 (m, 4H), 7.89 (d, J = 8.7 Hz, 1H), 7.55-7.42 (m, 5H); ^{13}C NMR (125 MHz, CDCl_3) δ 161.3, 159.4, 156.7, 145.4, 139.4, 136.1, 132.2 (d, $J_{\text{C-F}}$ = 8.3 Hz), 129.4, 128.9, 127.4, 119.9, 119.7, 110.5 (d, $J_{\text{C-F}}$ = 21.7 Hz).

6-chloro-2-phenylquinoline (3fa).¹⁶



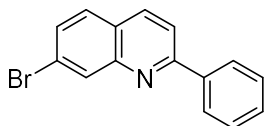
White solid; 83% yield (99 mg); mp 109-110 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.13 (d, J = 7.6 Hz, 2H), 8.07 (t, J = 8.0 Hz, 2H), 7.84 (d, J = 8.7 Hz, 1H), 7.75 (d, J = 1.8 Hz, 1H), 7.63 (dd, J = 9.0 and 2.0 Hz, 1H), 7.53-7.44 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 157.5, 146.6, 139.2, 135.8, 131.9, 131.3, 130.5, 129.5, 128.9, 127.7, 127.5, 126.1, 119.7.

7-chloro-2-phenylquinoline (3ga).¹⁴



White solid; 85% yield (102 mg); mp 112-113 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.20-8.15 (m, 4H), 7.88 (d, J = 4.9 Hz, 1H), 7.56 (d, J = 8.7 Hz, 1H), 7.55-7.47 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ 158.2, 148.6, 139.2, 136.5, 135.4, 129.6, 128.9, 128.7, 127.6, 127.2, 125.5, 119.1.

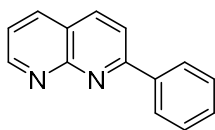
7-bromo-2-phenylquinoline (3ha).¹⁷



White solid; 88% yield (125 mg); mp 114-115 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.40 (s, 1H), 8.16-8.14 (m, 3H), 7.87 (d, J = 8.6 Hz, 1H), 7.67 (d, J = 8.7 Hz, 1H), 7.60-7.58 (m, 1H), 7.55-7.52 (m, 2H), 7.50-7.48 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 158.1, 148.8, 139.1, 136.6, 132.0, 129.7, 129.6, 128.9, 128.7, 127.5,

125.7, 123.7, 119.2.

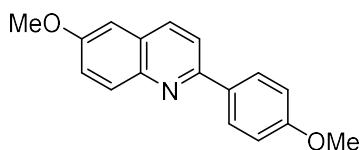
2-phenyl-1,8-naphthyridine (3ia).¹⁸



White solid; 86% yield (89 mg); mp 96-97 °C; ¹H NMR (500 MHz, CDCl₃) δ 9.10 (m, 1H), 8.28 (d, *J* = 7.5 Hz, 2H), 8.18 (d, *J* = 8.5 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.51-7.44 (m, 3H), 7.42-39 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 160.1, 155.9, 153.7, 138.3, 137.7, 136.6, 130.0, 128.7, 127.8, 121.6, 121.5, 119.5.

Procedure for acceptorless dehydrogenative cyclization of 1d with 2g catalyzed by Ir(tpy)@CTF. In a round-bottomed flask with a condenser tube were added **1d** (1.53 g, 10 mmol), **2g** (1.8 g, 12 mmol, 1.2 equiv), Ir(tpy)@CTF (440 mg, 0.1 mmol Ir, 1 mol % Ir), KOH (168 mg, 0.3 equiv) and *t*-amyl alcohol (10 mL) under air atmosphere. The mixture of reaction was heated at reflux for 12 h. The reaction mixture was cooled to ambient temperature, concentrated in *vacuo* and purified by flash column chromatography with hexanes/ethyl acetate to afford the corresponding product.

6-methoxy-2-(4-methoxyphenyl)quinoline (3dg).¹⁹

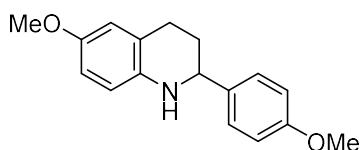


White solid; 80% yield (2.12 g); mp 89-90°C; ¹H NMR (500 MHz, CDCl₃) δ 8.09 (d, *J* = 8.6 Hz, 2H), 8.05-8.02 (m, 2H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.35 (dd, *J* = 9.1 and 2.6 Hz, 1H), 7.05-7.01 (m, 3H), 3.91 (s, 3H), 3.86 (s, 3H); ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 160.4, 157.3, 154.5, 144.2, 135.3, 132.3, 130.8, 128.4, 127.7, 122.0, 118.7, 114.1, 105.0, 55.4, 55.2.

Procedure for the transfer hydrogenation of 3dg. In a round-bottomed flask with a condenser tube were

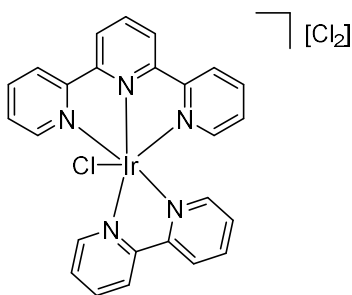
added **3dg** (1.33 g, 5 mmol), [Cp*RhCl₂]₂ (15 mg, 0.025 mmol, 0.5 mol %), and HCOOH/Et₃N (v/v = 5:2) (15 mL). The mixture of reaction was heated at 80 °C in an oil bath for 12 h. The reaction mixture was cooled to ambient temperature, concentrated in *vacuo* and purified by flash column chromatography with hexanes/ethyl acetate to afford the corresponding product.

6-methoxy-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoline (4).¹⁹



White solid; 81% yield (1.09 g); mp 99-100 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.30 (d, *J* = 8.6 Hz, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.62-6.60 (m, 2H), 4.30 (dd, *J* = 9.8, 2.9 Hz, 1H), 3.78 (s, 3H), 3.72 (s, 3H), 2.95-2.88 (m, 1H), 2.74-2.68 (m, 1H), 2.07-2.02 (m, 1H), 1.98-1.90 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 158.8, 151.8, 138.9, 136.9, 127.6, 122.1, 115.1, 114.6, 113.8, 112.9, 56.0, 55.7, 55.2, 31.1, 26.9.

Procedure for the synthesis of [Ir(tpy)(bpy)Cl][Cl₂].²⁰ To an oven-dried Schlenk tube were added [Ir(tpy)Cl₃] (106.2 mg, 0.2 mmol), 2,2'-bipyridine (31.2 mg, 0.2 mmol, 1 equiv) and ethylene glycol (10.0 mL), and the mixture was heated at 180 °C for 15 h. The reaction mixture was allowed to cool to ambient temperature. Then, the mixture was concentrated in *vacuo* to afford the resulting product.



Yellow solid; 70% yield (96 mg); ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.64 (d, *J* = 5.5 Hz, 2H), 9.07-8.90 (m, 5H), 8.59-8.47 (m, 3H), 8.22-8.07 (m, 5H), 7.84 (d, *J* = 5.6 Hz, 2H), 7.52 (t, *J* = 6.6 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 157.8, 157.6, 151.3, 151.2, 141.6, 141.0, 129.0, 128.9, 125.5, 125.4.

Procedure for the hydrogen evolution experiment. **1a** (1 mmol, 123 mg), **2a** (145 mg, 1.2 mmol, 1.2 equiv), Ir(tpy)@CTF (44 mg, 0.01 mmol Ir, 1 mol % Ir), KOH (16.8 mg, 0.3 mmol, 0.3 equiv) and tert-amyl alcohol (1 mL) were added to a 5 mL thick walled glass vessel with a condenser tube, which was previously degassed three times and placed under a N₂ atmosphere. The vessel was connected to the gas collection apparatus (standard water displacement apparatus, using a graduated cylinder to determine volume), and the entire system was flushed with N₂ for 5 min and allowed to equilibrate for 5 min. The reaction was stirred vigorously at reflux for 12 h. The presence of hydrogen in the collected gas was confirmed by GC analysis. The GC analysis was performed on a gas chromatograph with TCD detector. Injector temperature = 180 °C, column temperature = 160 °C, detector temperature (TCD) = 280 °C, carrier gas = N₂, t = 0.423 min.

The volume of 1 mol of H₂ at 298.15 K, 100900 Pa was calculated according to the van der Waals equation as shown below

$$(p + \frac{n^2 a}{V^2}) (V - nb) = nRT$$

where R = 8.3145 m³·Pa·mol⁻¹·K⁻¹; T = 298.15 K; p = 100900 Pa; a = 0.02476 Pa·m⁶·mol⁻²; b = 0.02661 × 10⁻³ m³·mol⁻¹; thus, V (H₂, 298.15 K, 100900 Pa) = 24.6 L·mol⁻¹.

The collected volume of gas in this experiment above was 21.2 mL, which corresponds to 0.86 mmol of H₂.

References

- (1) S. Takizawa, S. Katoh, A. Okazawa, N. Ikuta, S. Matsushima, F. Zeng and S. Murata, Triplet Excited States Modulated by Push–Pull Substituents in Monocyclometalated Iridium(III) Photosensitizers, *Inorg. Chem.*, 2021, **60**, 4891-4903.
- (2) M. J. Iglesias, A. Prieto and M. C. Nicasio, Kumada-Tamao-Corriu Coupling of Heteroaromatic Chlorides and Aryl Ethers Catalyzed by (IPr)Ni(allyl)Cl, *Org. Lett.*, 2012, **14**, 4318-4321.
- (3) L. Xi, R. Zhang, L. Zhang, S. Chen and X. Yu, An Efficient Synthesis of Quinolines via Copper-Catalyzed C-N Cleavage, *Org. Biomol. Chem.*, 2015, **13**, 3924-3930.
- (4) L. Cao, H. Zhao, R. Guan, H. Jiang, P. H. Dixneuf and M. Zhang, Practical Iridium-Catalyzed Direct α -Arylation of N-Heteroarenes with (Hetero)arylboronic Acids by H₂O-Mediated H₂ Evolution, *Nat. Commun.*, 2021, **12**, 4206.
- (5) C. Li, J. Li, Y. An, J. Peng, W. Wu and H. Jiang, Palladium-Catalyzed Allylic C-H Oxidative Annulation for Assembly of Functionalized 2-Substituted Quinoline Derivatives, *J. Org. Chem.*, 2016, **81**, 12189-12196.
- (6) R. Wang, H. Fan, W. Zhao and F. Li, Acceptorless Dehydrogenative Cyclization of o-Aminobenzyl Alcohols with Ketones to Quinolines in Water Catalyzed by Water-Soluble Metal-Ligand Bifunctional Catalyst [Cp*(6,6'-(OH)₂bpy)(H₂O)][OTf]₂, *Org. Lett.*, 2016, **18**, 3558-3561.
- (7) J. Zhou, G. Wu, M. Zhang, X. Jie and W. Su, Pd-Catalyzed Cross-Coupling of Aryl Carboxylic Acids with Propiophenones through a Combination of Decarboxylation and Dehydrogenation, *Chem. Eur. J.*, 2012, **18**, 8032-8036.
- (8) K. Wu, Z. Huang, C. Liu, H. Zhang and A. Lei, Aerobic C-N Bond Activation: a Simple Strategy to Construct Pyridines and Quinolines, *Chem. Commun.*, 2015, **51**, 2286-2289.

- (9) X. Xu, Y. Ai, R. Wang, L. Liu, J. Yang and F. Li, Ruthenium-Catalyzed Acceptorless Dehydrogenative Coupling of o-Aminobenzyl Alcohols with Ketones to Quinolines in the Presence of Carbonate Salt, *J. Catal.*, 2021, **395**, 340-349.
- (10) Y. Gao, S. Yang, Y. Huo, Q. Chen, X. Li and X. Hu, NiH-Catalyzed Hydroamination/Cyclization Cascade: Rapid Access to Quinolines, *ACS Catal.*, 2021, **11**, 7772-7779.
- (11) G. A. Molander and P. E. Gormisky, Cross-Coupling of Cyclopropyl- and Cyclobutyltrifluoroborates with Aryl and Heteroaryl Chlorides, *J. Org. Chem.*, 2008, **73**, 7481-7485.
- (12) M. Movassaghi and M. D. Hill, Synthesis of Substituted Pyridine Derivatives via the Ruthenium-Catalyzed Cycloisomerization of 3-Azadienynes, *J. Am. Chem. Soc.*, 2006, **128**, 4592-4593.
- (13) X. Yi and C. Xi, Copper-Promoted Tandem Reaction of Azobenzenes with Allyl Bromides via N=N Bond Cleavage for the Regioselective Synthesis of Quinolines, *Org. Lett.*, 2015, **17**, 5836-5839.
- (14) X. Ji, H. Huang, Y. Li, H. Chen and H. Jiang, Palladium-Catalyzed Sequential Formation of C-C Bonds: Efficient Assembly of 2-Substituted and 2,3-Disubstituted Quinolines, *Angew. Chem. Int. Ed.*, 2012, **51**, 7292-7296.
- (15) S. Mahato, A. Mukherjee, S. Santra, G. V. Zyryanov and A. Majee, Facile Synthesis of Substituted Quinolines by Iron(III)-Catalyzed Cascade Reaction between Anilines, Aldehydes and Nitroalkanes, *Org. Biomol. Chem.*, 2019, **17**, 7907-7917.
- (16) H. Li, C. Wang, S. Zhu, C. Dai and Y. Wu, Ruthenium(II)-Catalyzed Hydrogen Transfer/Annulation Cascade Processes between Alcohols and 2-Nitrobenzaldehydes, *Adv. Synth. Catal.*, 2015, **357**, 583-588.
- (17) A. H. Li, D. J. Beard, H. Coate, A. Honda, M. Kadalbajoo, A. Kleinberg, R. Laufer, K. M. Mulvihill, A. Nigro, P. Rastogi, D. Sherman, K. W. Siu, A. G. Steinig, T. Wang, D. Werner, A. P. Crew and M. J. Mulvihill, One-Pot Friedländer Quinoline Synthesis: Scope and Limitations, *Synthesis*, 2010, **10**, 1678-1686.

- (18) S. K. Das, S. Roy, H. Khatua and B. Chattopadhyay, Iron-Catalyzed Amination of Strong Aliphatic C(sp³)–H Bonds, *J. Am. Chem. Soc.*, 2020, **142**, 16211-16217.
- (19) O. B. Wallace, K. S. Lauwers, S. A. Jones and J. A. Dodge, Tetrahydroquinoline-Based Selective Estrogen Receptor Modulators (SERMs), *Bioorg. Med. Chem. Lett.*, 2003, **13**, 1907-1910.
- (20) N. Yoshikawa, S. Yamabe, N. Kanehisa, Y. Kai, H. Takashima, K. Tsukahara, Structures of Polypyridine Mononuclear IrIII Complexes in the Ground state and the Lowest Triplet state, *Inorganica Chim. Acta*, 2009, **362**, 361-371.

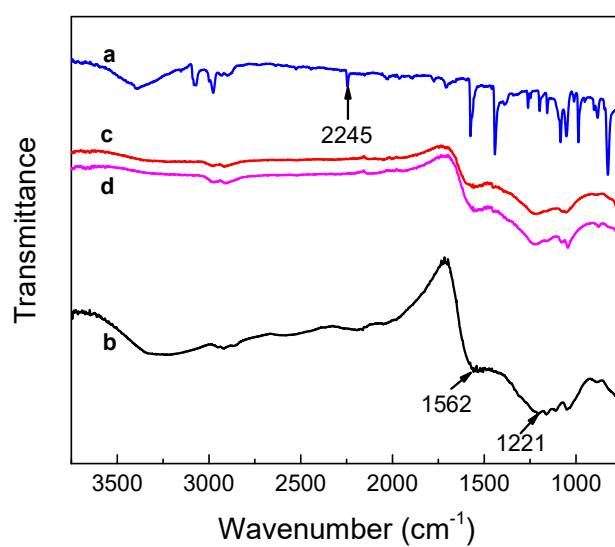


Fig. S1. FT-IR spectra of (a) 2,6-pyridinedicarbonitrile; (b) CTF; (c) Ir(tpy)@CTF; (d) recovered Ir(tpy)@CTF.

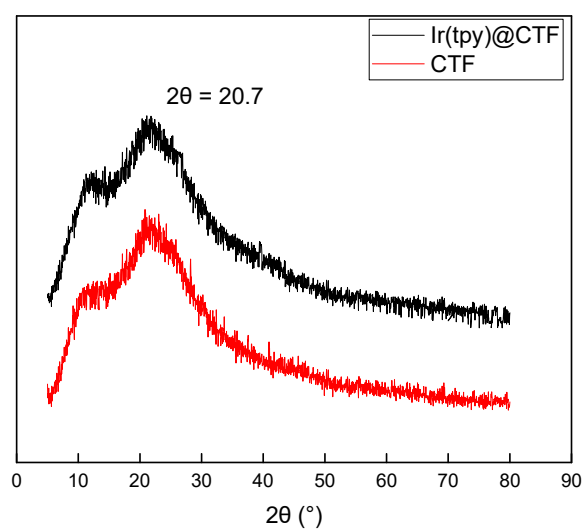


Fig. S2. XRD of CTF and Ir(tpy)@CTF

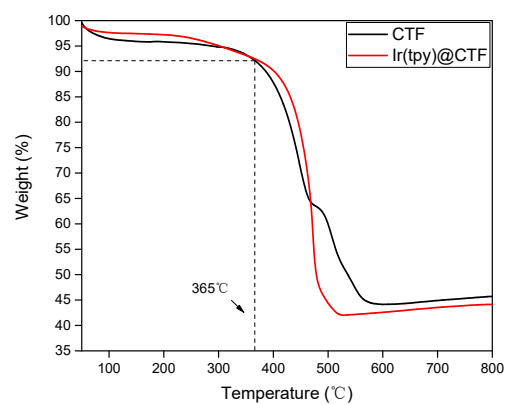


Fig. S3. TGA of CTF and Ir(tpy)@CTF

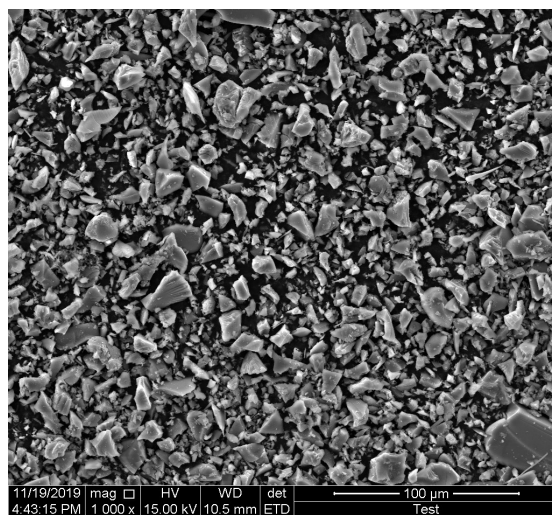


Fig. S4. SEM image of CTF.

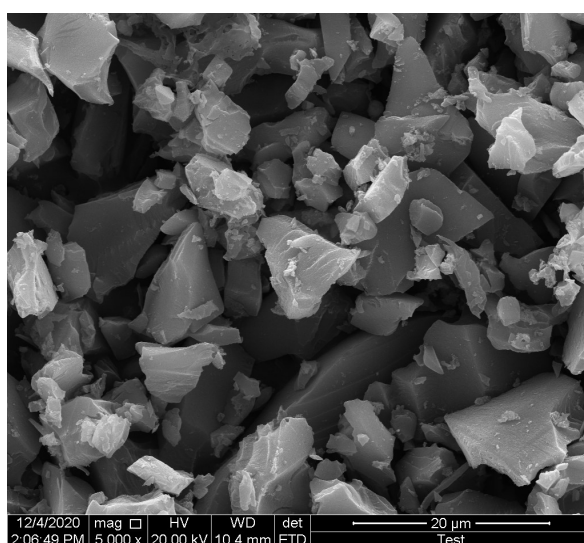
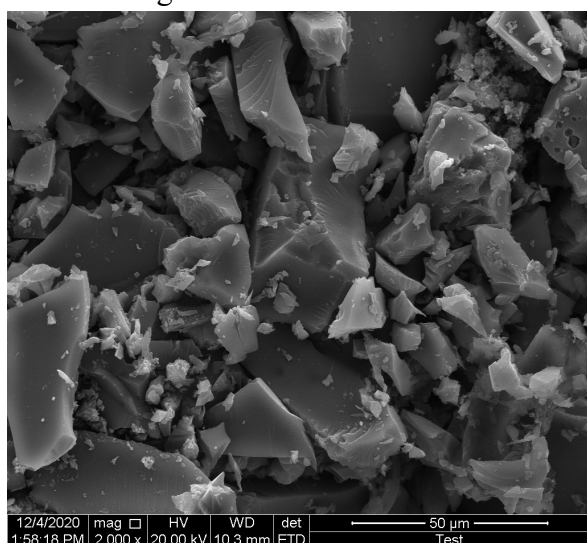


Fig. S5. SEM image of Ir(tpy)@CTF (left) and recovered Ir(tpy)@CTF (right).

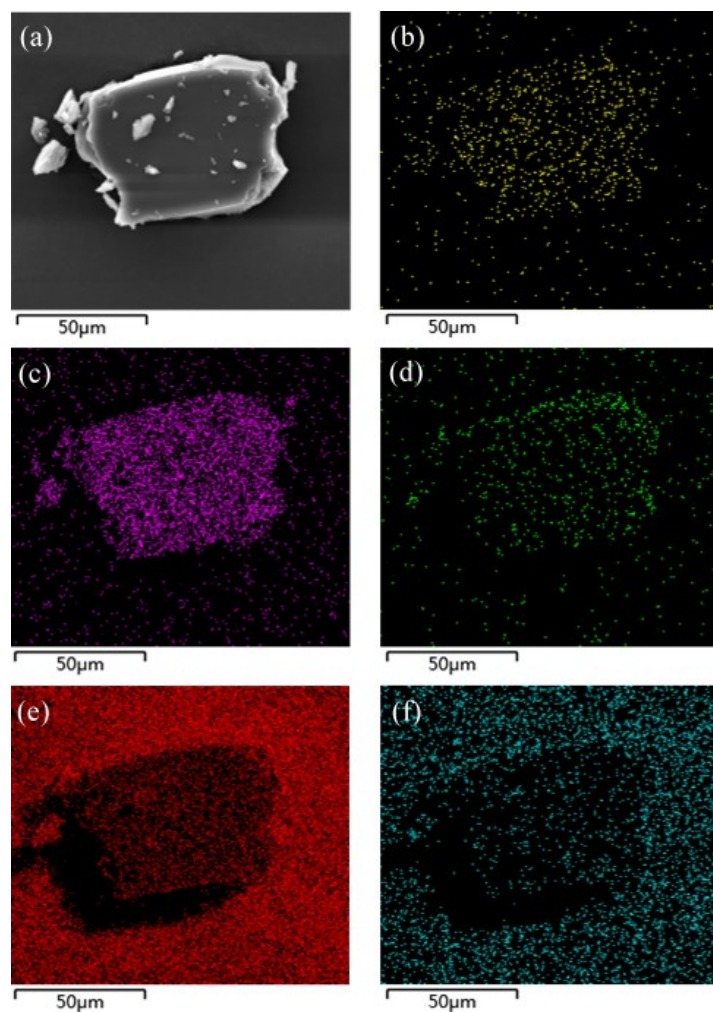


Fig. S6. SEM image of Ir(tpy)@CTF (a). EDS mapping of (b) Ir; (c) Cl; (d) N; (e) C and (f) O atoms in Ir(tpy)@CTF.

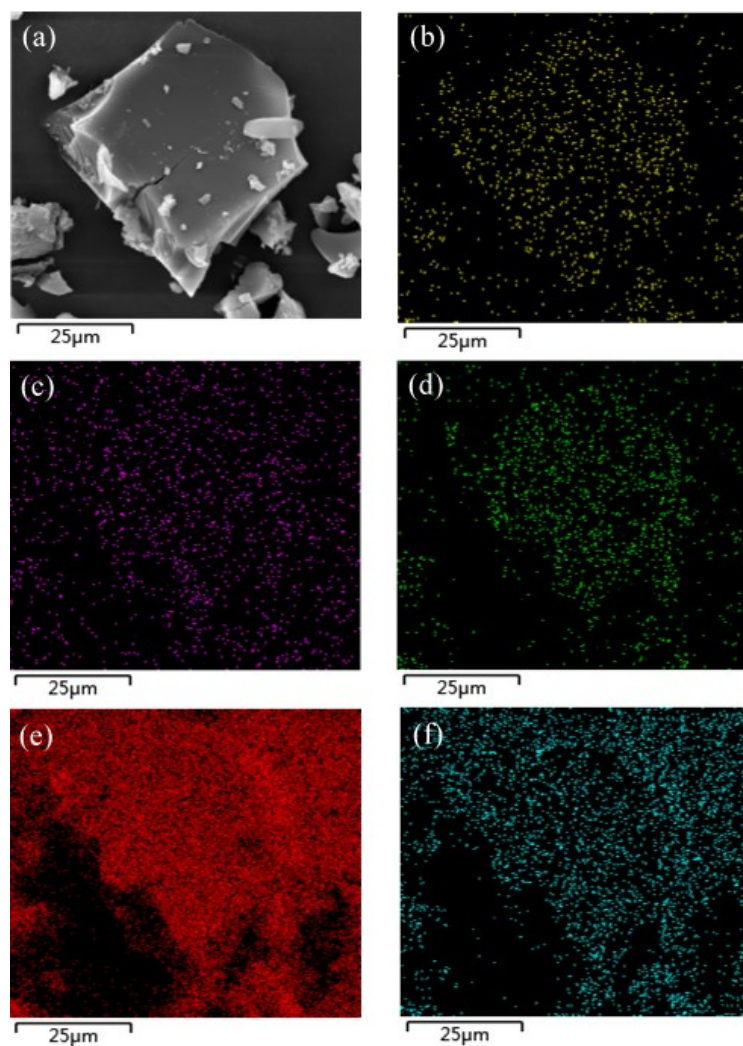


Fig. S7. SEM image of recovered Ir(tpy)@CTF (a). EDS mapping of (b) Ir; (c) Cl; (d) N; (e) C and (f) O atoms in recovered Ir(tpy)@CTF.

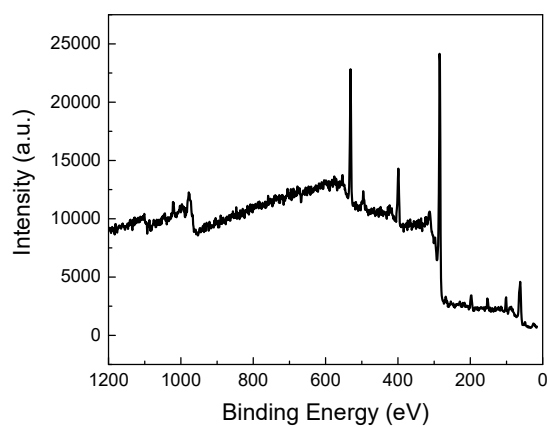


Fig. S8. XPS of Ir(tpy)@CTF.

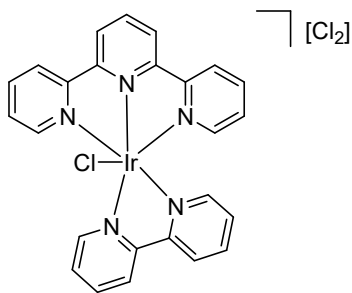


Figure S9. The structure of $[\text{Ir}(\text{tpy})(\text{bpy})\text{Cl}][\text{Cl}_2]$

Table S1. Atomic composition by SEM-EDS.

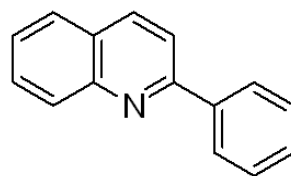
Element	Before catalysis (Wt%)	After VI cycles (Wt%)
C	70.83	62.99
N	7.49	13.76
O	16.85	19.73
Cl	0.91	0.04
Ir	3.92	3.49
Total	100.00	100.00

Table S2. BET analysis of CTF and $\text{Ir}(\text{tpy})@\text{CTF}$, and ICP-MS data.

Material	S_{BET} (m^2/g)	Pore volume (cm^3/g)	Pore size (nm)	wt% of Ir content
CTF	693	0.23	2.37	—
$\text{Ir}(\text{tpy})@\text{CTF}$	342	0.12	2.31	4.36

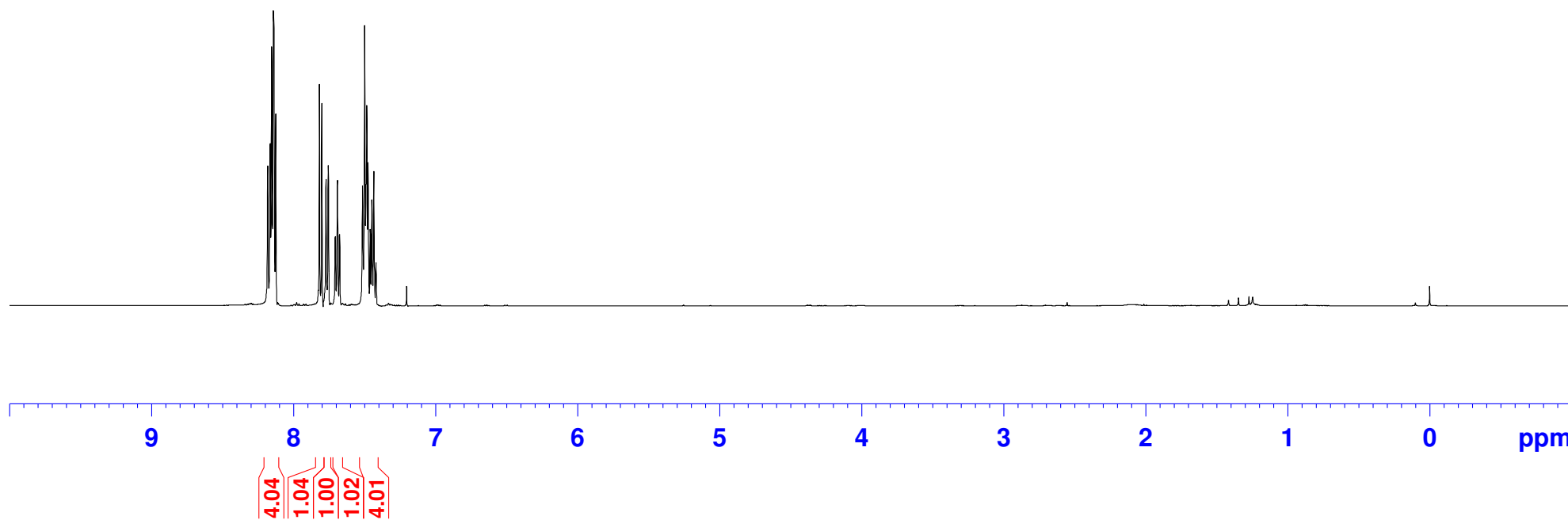
2-phenylquinoline
Proton CDCl₃

8.180
8.163
8.152
8.140
8.138
8.124
8.124
7.816
7.799
7.770
7.754
7.708
7.707
7.693
7.678
7.516
7.501
7.486
7.477
7.462
7.450
7.436
7.421
7.205



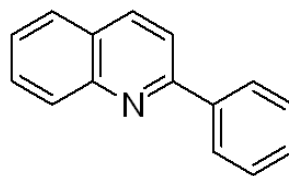
3aa

¹H NMR (500 MHz, CDCl₃)



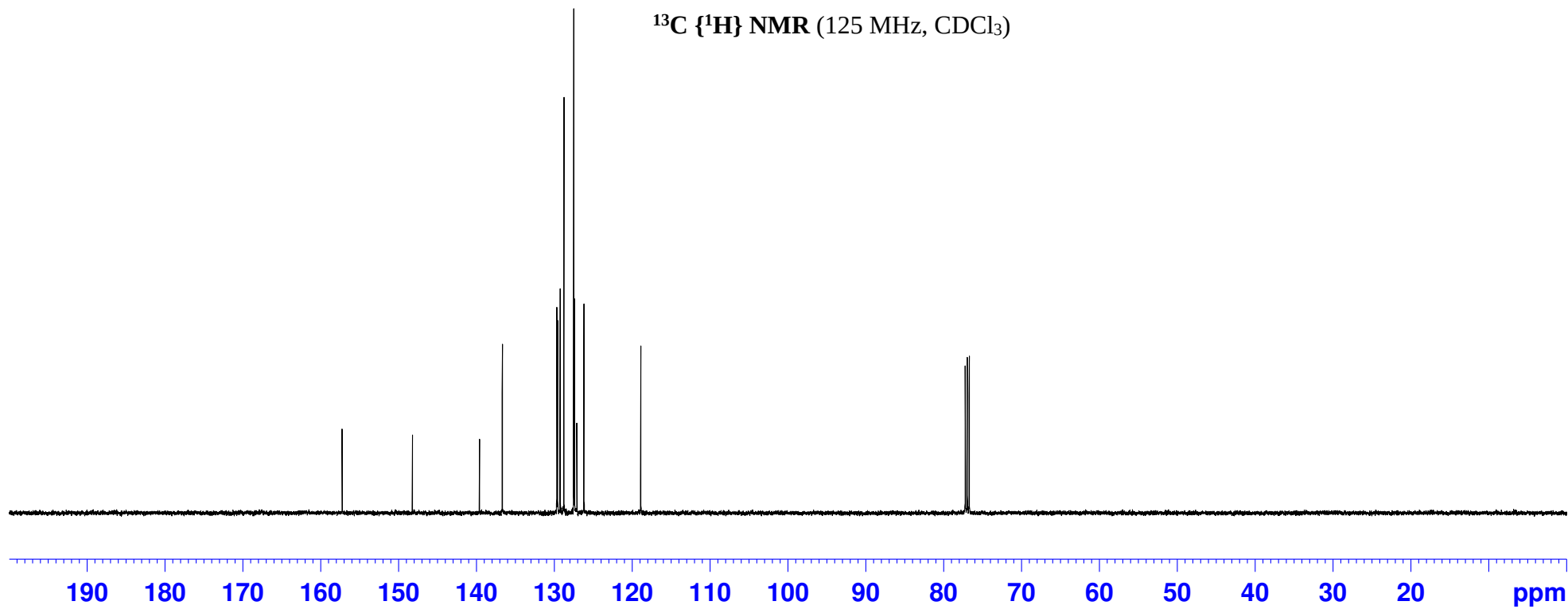
2-phenylquinoline
C13CPD CDC13

157.227
148.198
139.585
136.654
129.653
129.552
129.228
128.750
127.481
127.374
127.082
126.171
118.875
77.257
77.002
76.748



3aa

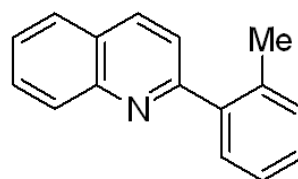
^{13}C { ^1H } NMR (125 MHz, CDCl_3)



2-o-tolylquinoline
Proton CDCl₃

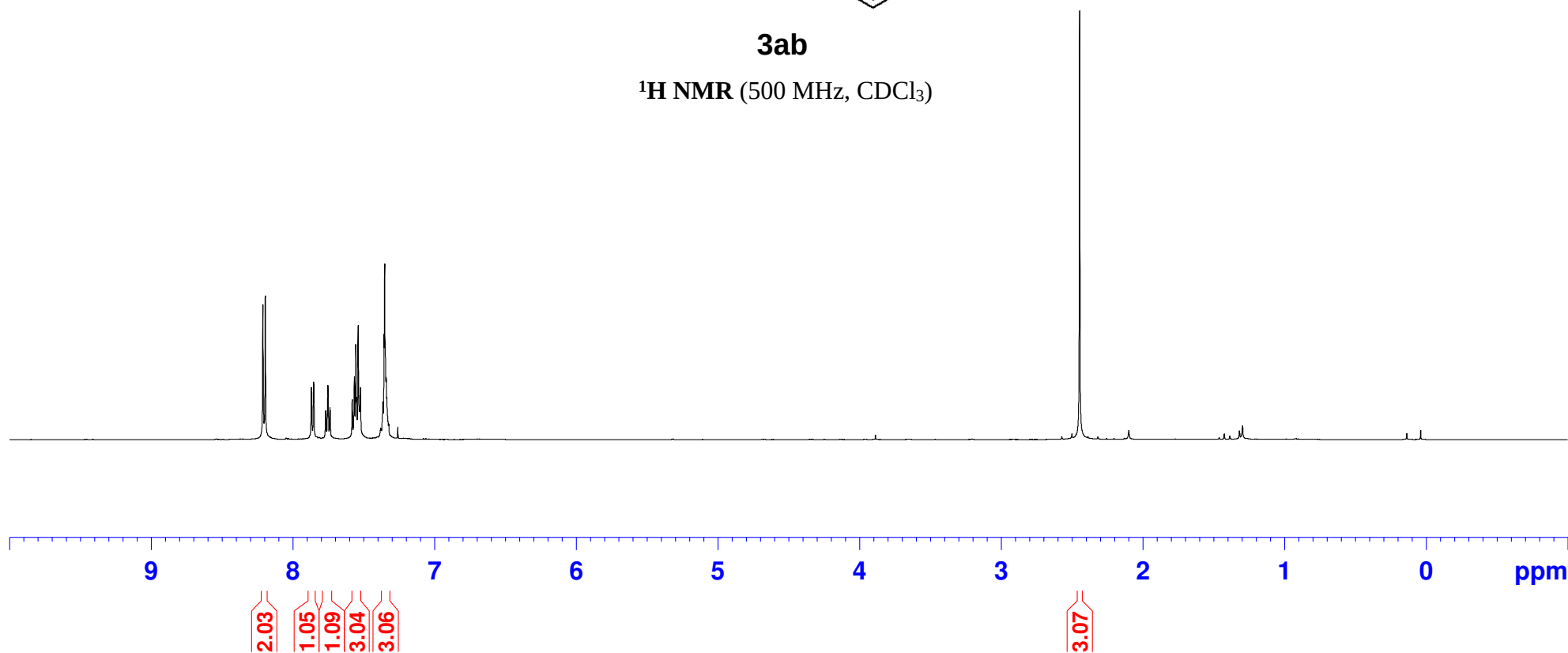
8.213
8.196
7.871
7.855
7.770
7.768
7.753
7.740
7.737
7.582
7.566
7.557
7.553
7.540
7.532
7.526
7.523
7.357
7.353
7.260

— 2.447

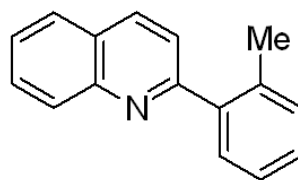
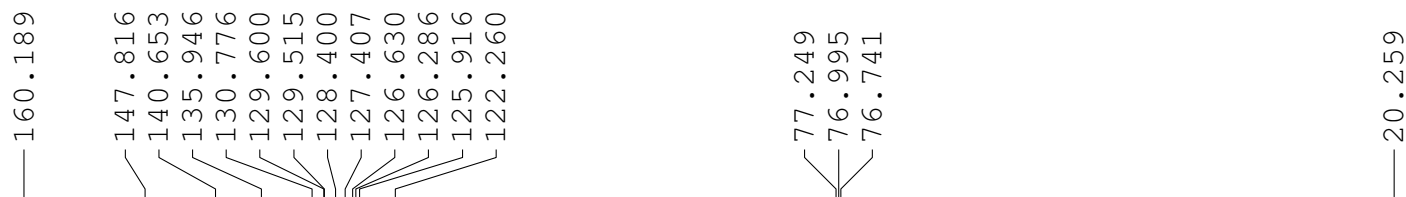


3ab

¹H NMR (500 MHz, CDCl₃)

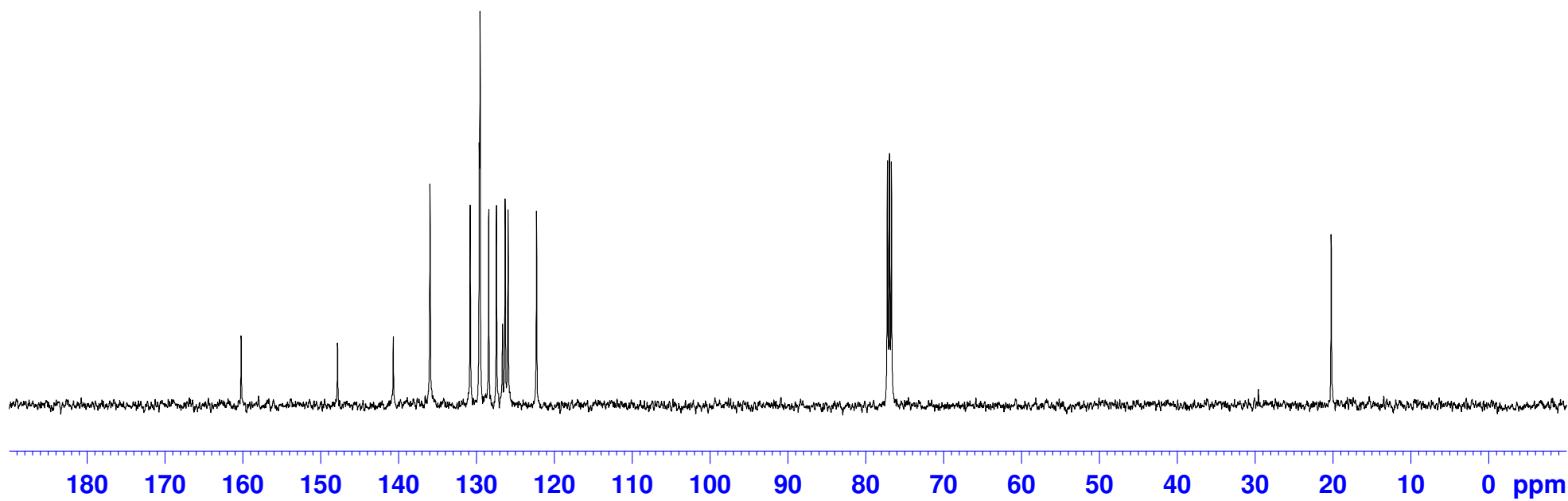


2-o-tolylquinoline
C13CPD CDC13



3ab

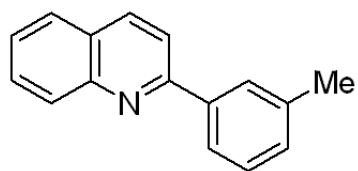
^{13}C { ^1H } NMR (125 MHz, CDCl_3)



2-(m-tolyl)quinoline
Proton CDCl₃

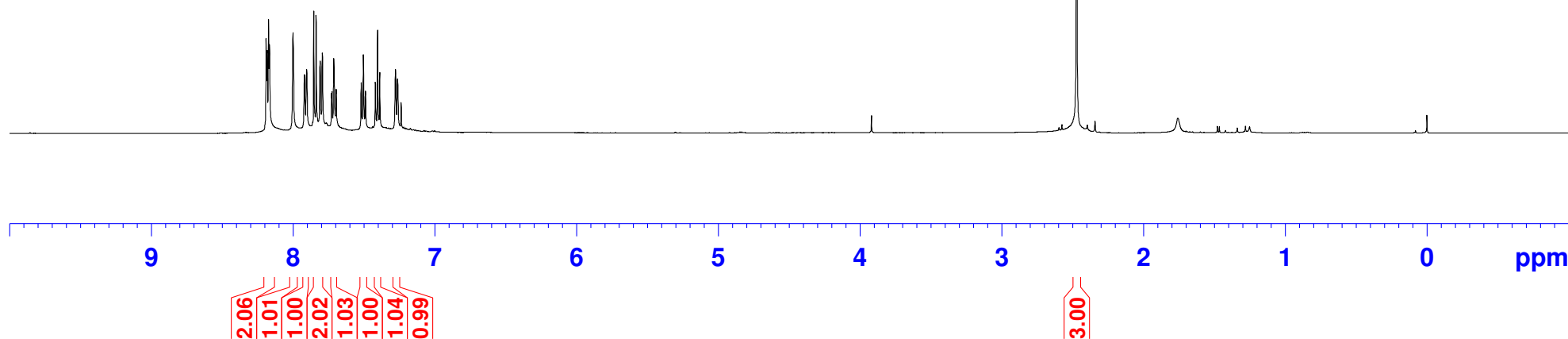
8.184
8.174
8.168
8.001
7.921
7.905
7.855
7.838
7.810
7.794
7.729
7.727
7.715
7.713
7.699
7.696
7.520
7.506
7.491
7.420
7.405
7.390
7.279
7.263

— 2.471



3ac

¹H NMR (500 MHz, CDCl₃)

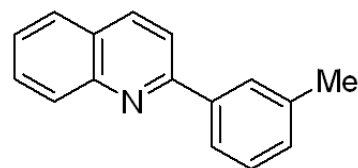


2-(m-tolyl)quinoline
C13CPD CDC13

157.449
148.168
139.541
138.381
136.578
130.010
129.586
129.505
128.619
128.165
127.350
127.064
126.093
124.613
119.025

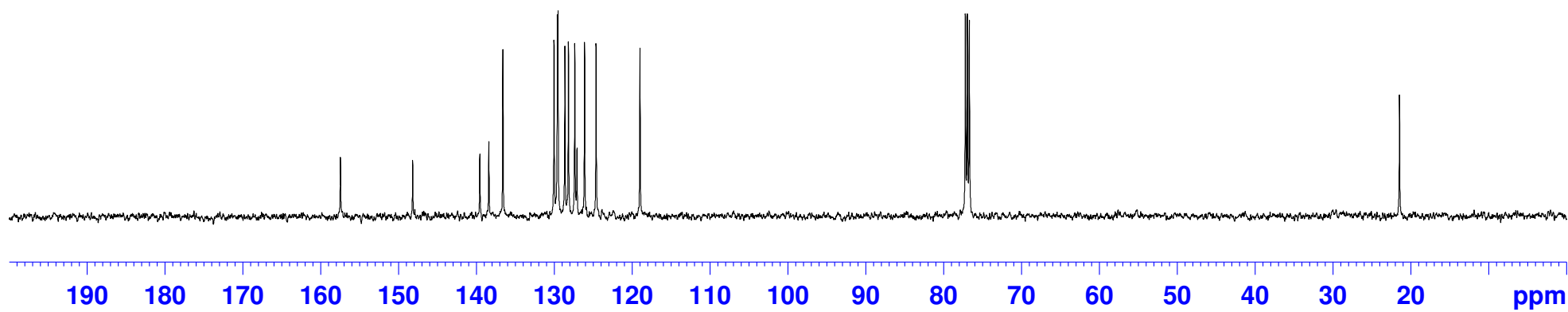
77.239
76.985
76.730

21.486



3ac

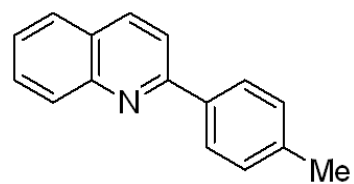
^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



2-p-tolylquinoline
Proton CDCl₃

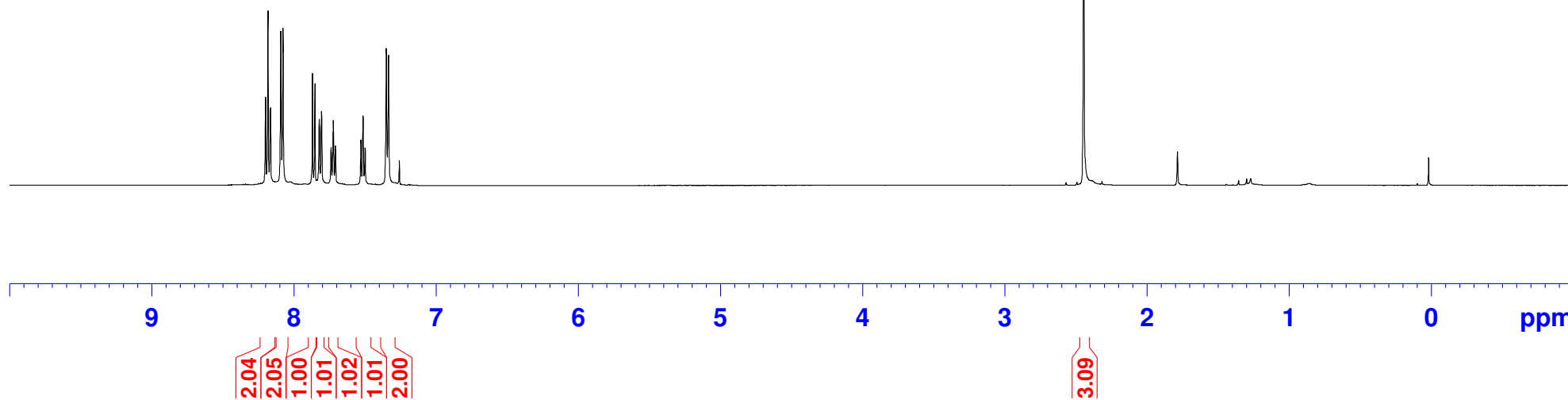
8.200
8.183
8.166
8.093
8.077
7.870
7.853
7.823
7.807
7.740
7.724
7.709
7.530
7.515
7.500
7.351
7.335
7.259

— 2.444

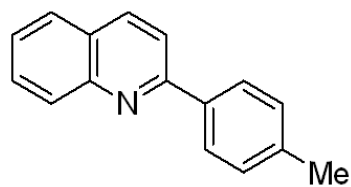


3ad

¹H NMR (500 MHz, CDCl₃)

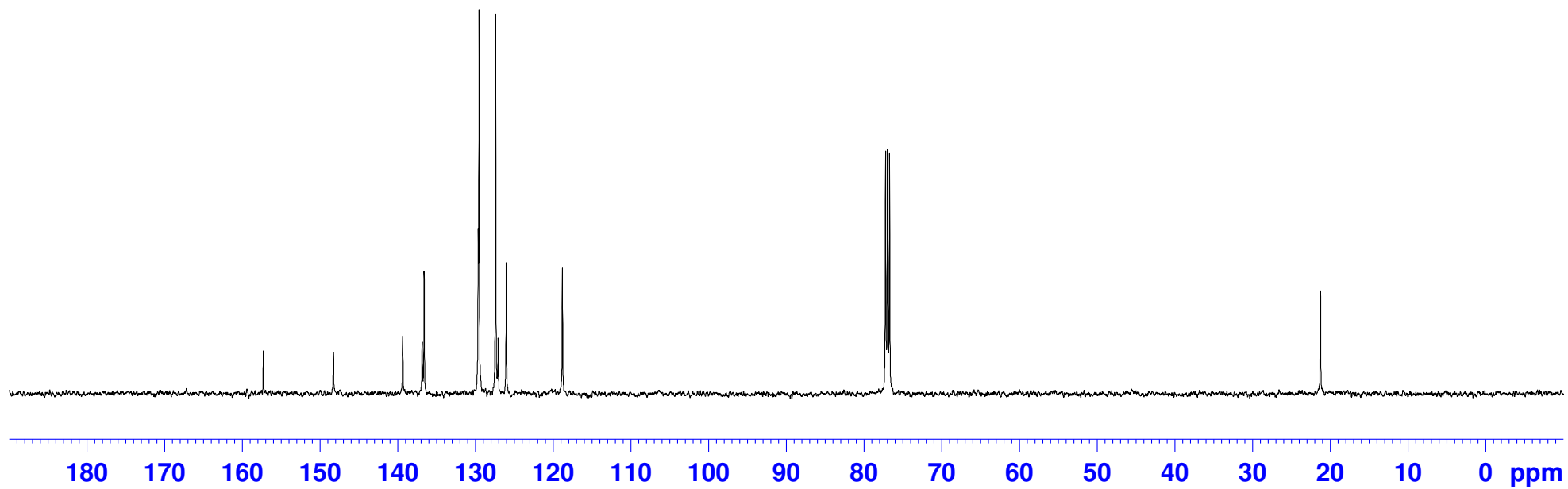


2-p-tolylquinoline
C13CPD CDC13



3ad

^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

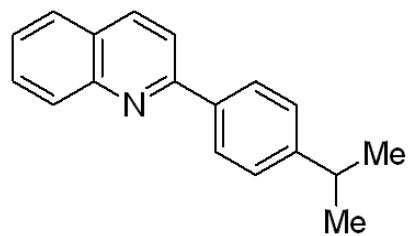


2-(4-isopropylphenyl)quinoline
Proton CDCl₃

8.210
8.193
8.174
8.157
8.100
8.084
7.873
7.856
7.827
7.811
7.733
7.719
7.702
7.529
7.514
7.499
7.401
7.385

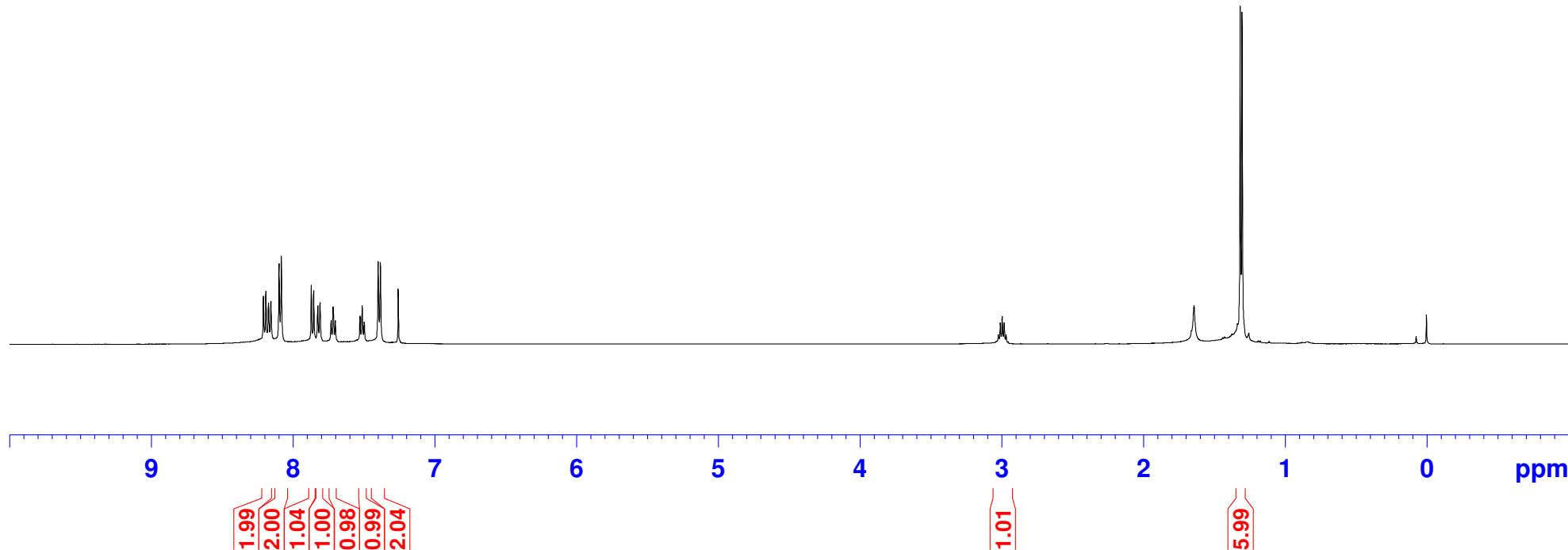
3.025
3.011
2.997
2.983
2.970
2.956

1.319
1.305

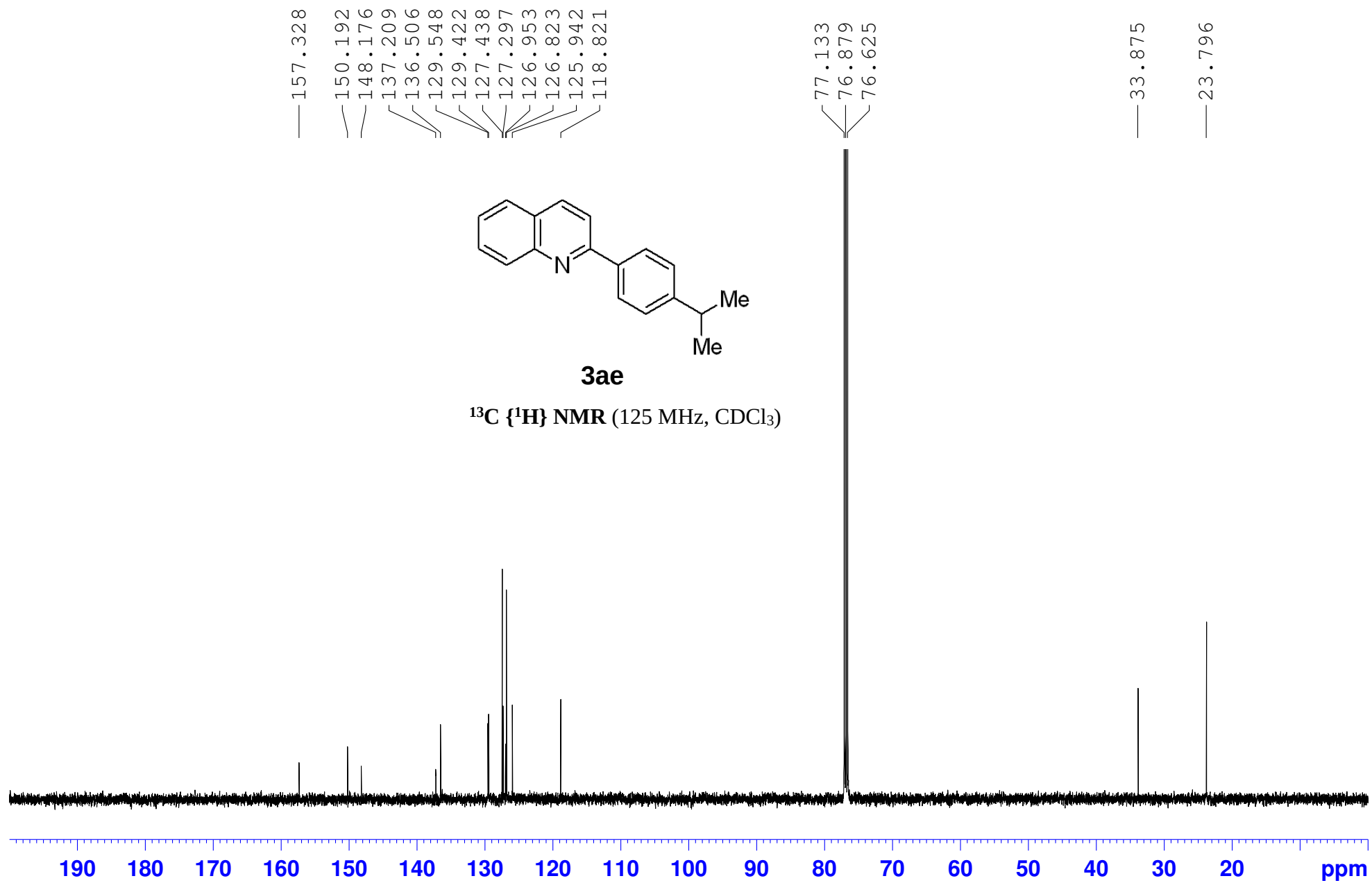


3ae

¹H NMR (500 MHz, CDCl₃)



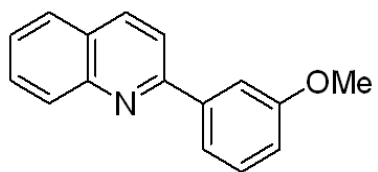
2-(4-isopropylphenyl)quinoline
C13CPD CDCl3



2-(3-methoxyphenyl)quinoline
Proton CDCl₃

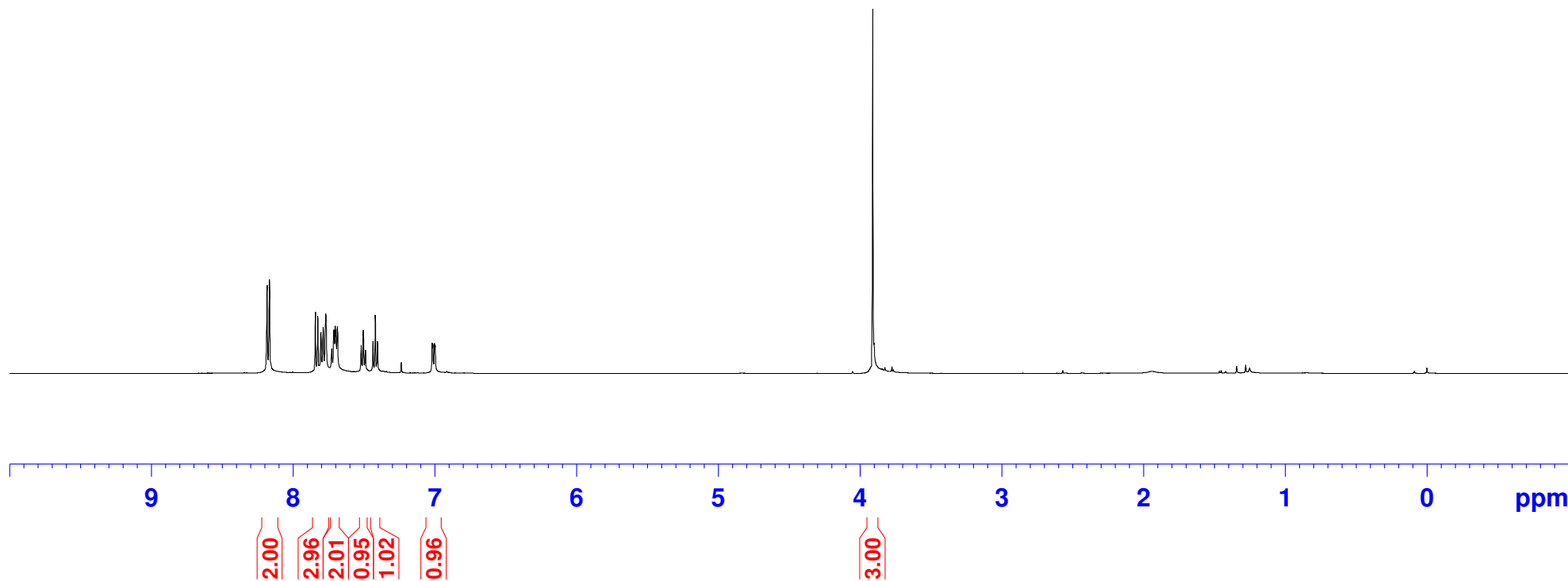
8.182
8.165
7.841
7.824
7.802
7.785
7.768
7.726
7.710
7.701
7.686
7.517
7.503
7.488
7.434
7.418
7.402
7.017
7.012
7.001
6.996

— 3.911

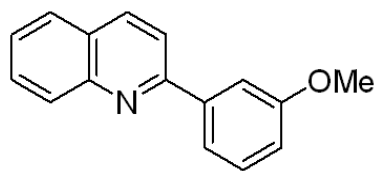
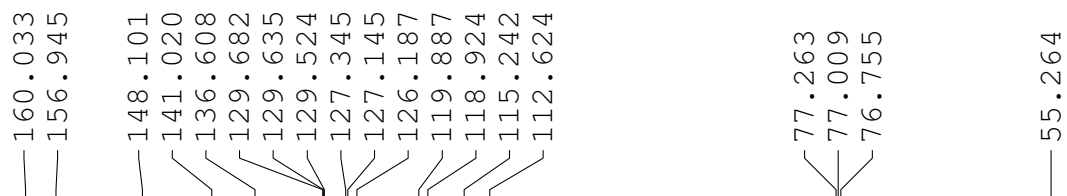


3af

¹H NMR (500 MHz, CDCl₃)

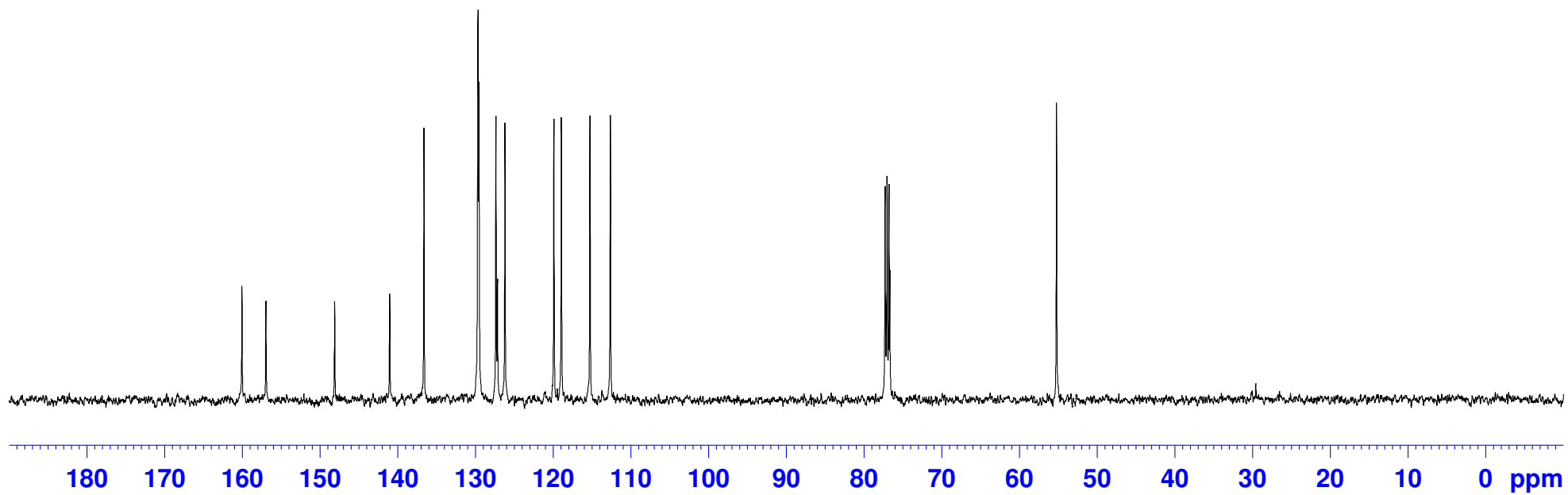


2-(3-methoxyphenyl)quinoline
C13CPD CDCl3



3af

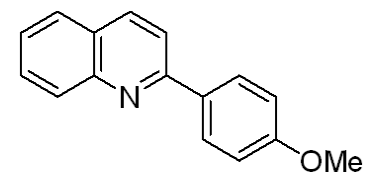
^{13}C { ^1H } NMR (125 MHz, CDCl_3)



2-(4-methoxyphenyl)quinoline
Proton CDCl₃

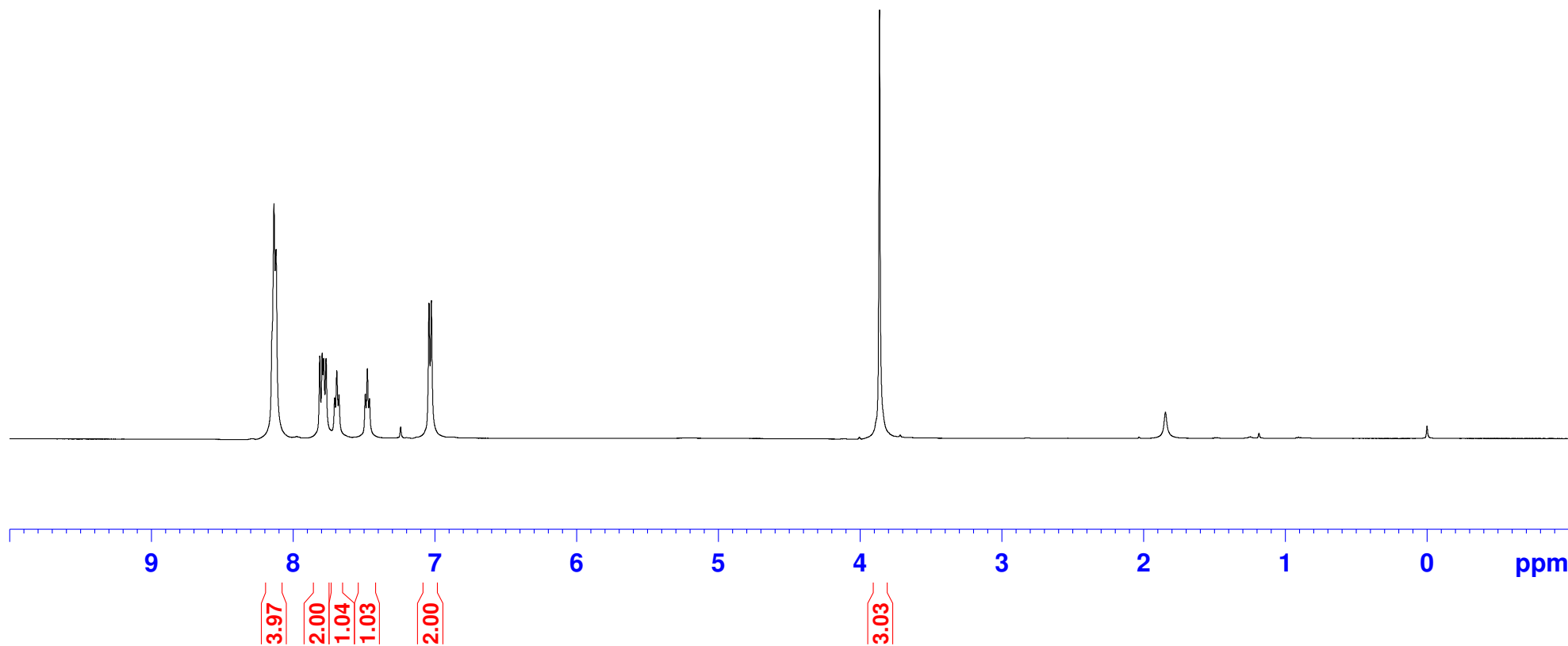
8.135
8.121
7.813
7.795
7.785
7.768
7.707
7.693
7.677
7.492
7.477
7.462
7.042
7.026

3.863



3ag

¹H NMR (500 MHz, CDCl₃)



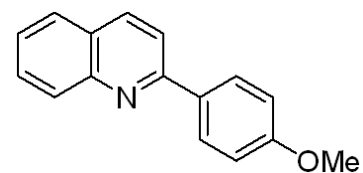
2-(4-methoxyphenyl)quinoline
C13CPD CDCl3

—160.695
—156.780

—148.172
136.484
132.137
129.432
129.393
128.759
127.302
126.784
125.774
118.413
114.101

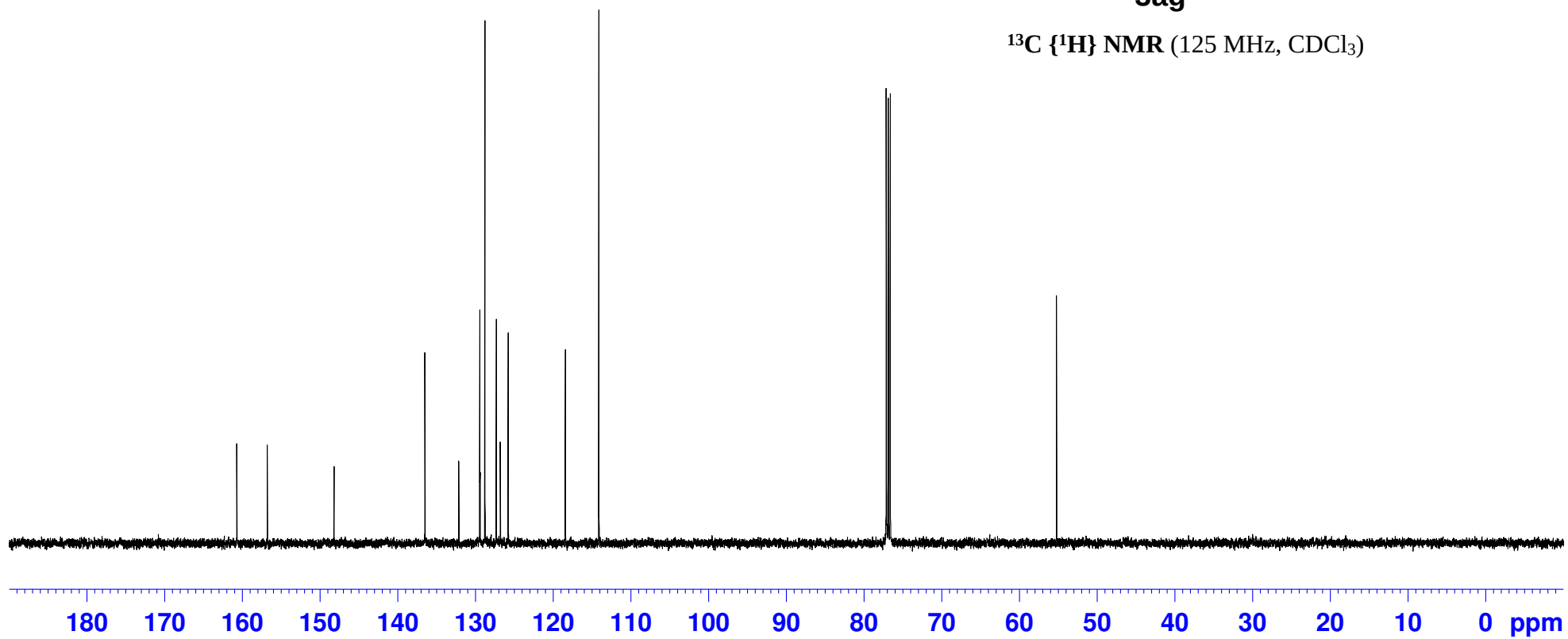
77.172
76.918
76.663

—55.256



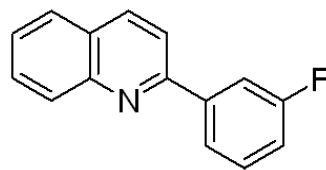
3ag

^{13}C { ^1H } NMR (125 MHz, CDCl_3)



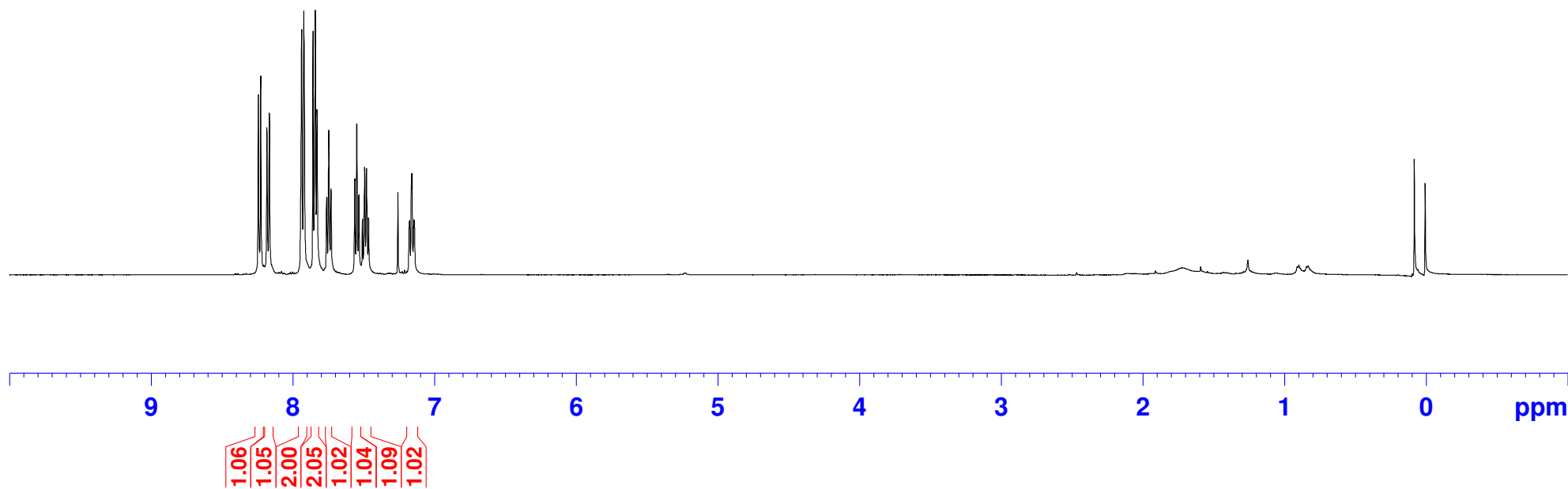
2-(3-fluorophenyl)quinoline
Proton CDCl₃

8.167
7.939
7.924
7.859
7.842
7.831
7.764
7.762
7.747
7.733
7.731
7.564
7.550
7.536
7.535
7.510
7.494
7.482
7.467
7.260
7.180
7.177
7.176
7.164
7.160
7.149
7.146
7.142



3ah

¹H NMR (500 MHz, CDCl₃)

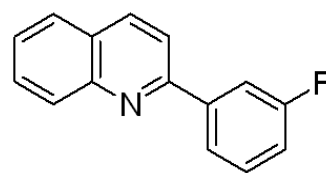


2-(3-fluorophenyl)quinoline
C13CPD CDCl3

157.449
148.168
139.541
138.381
136.578
130.010
129.586
129.505
128.619
128.165
127.350
127.064
126.093
124.613
119.025

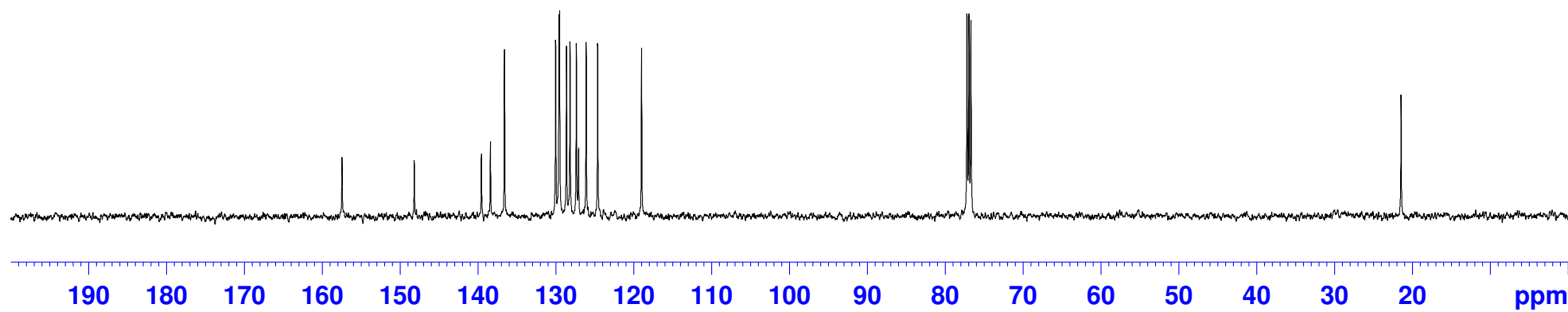
77.239
76.985
76.730

21.486



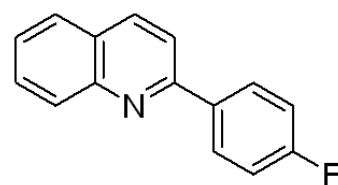
3ah

^{13}C { ^1H } NMR (125 MHz, CDCl₃)



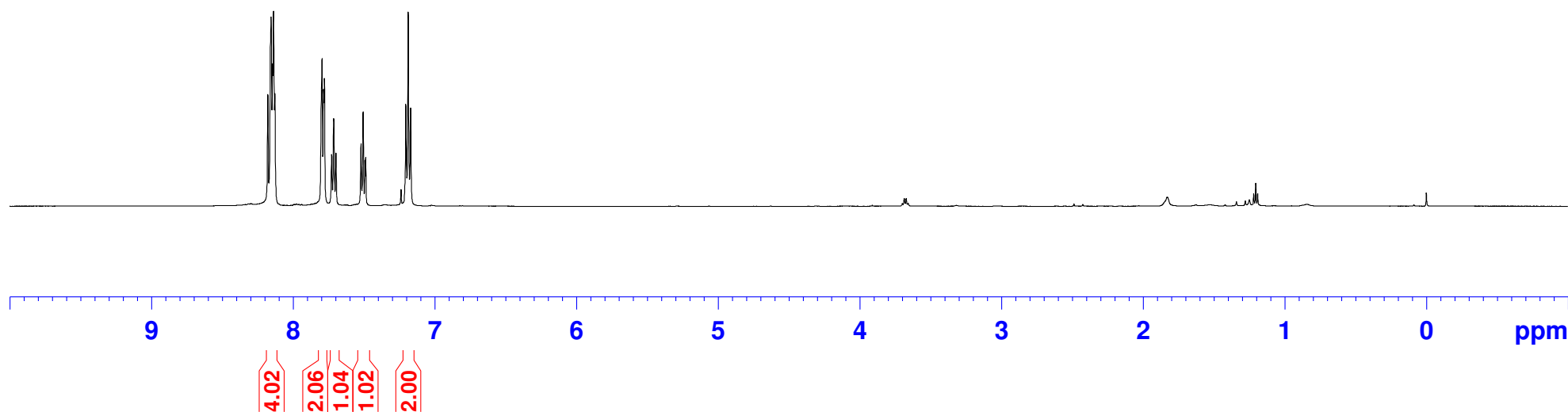
2-(4-fluorophenyl)quinoline
Proton CDCl₃

8.176
8.153
8.143
8.136
8.126
7.793
7.783
7.776
7.726
7.710
7.696
7.519
7.504
7.489
7.205
7.188
7.171



3ai

¹H NMR (500 MHz, CDCl₃)

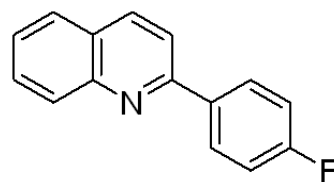


2-(4-fluorophenyl)quinoline
C13CPD CDCl₃

157.449
148.168
139.541
138.381
136.578
130.010
129.586
129.505
128.619
128.165
127.350
127.064
126.093
124.613
119.025

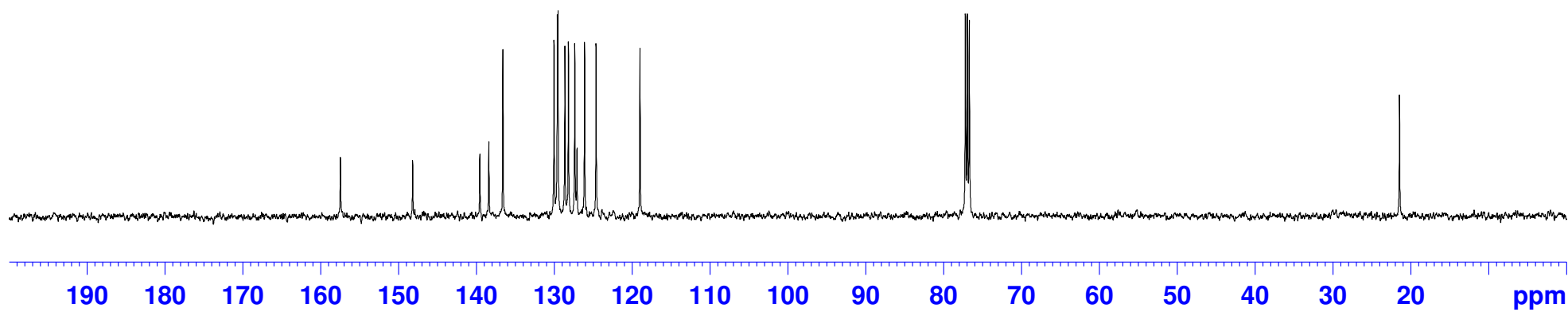
77.239
76.985
76.730

21.486



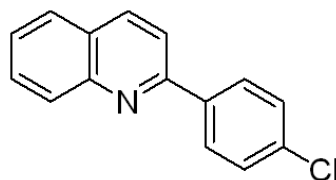
3ai

¹³C {¹H} NMR (125 MHz, CDCl₃)



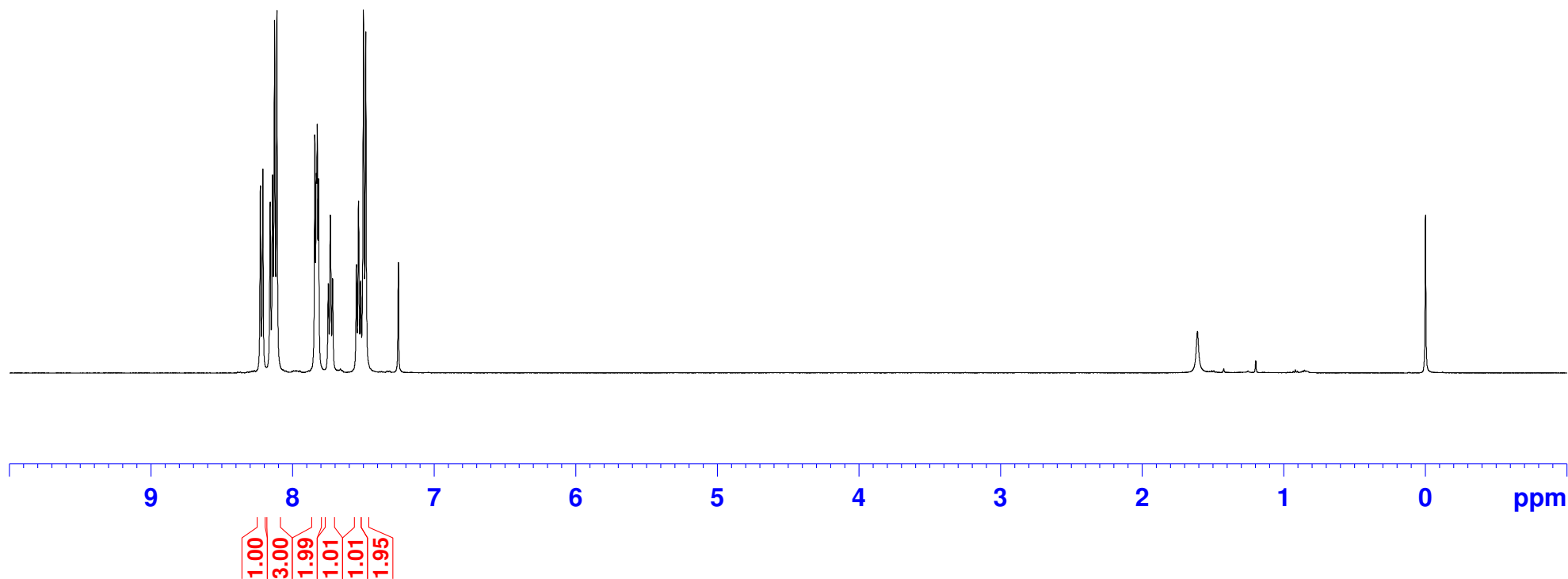
2-(4-chlorophenyl)quinoline
Proton CDCl₃

8.229
8.212
8.160
8.143
8.129
8.112
7.845
7.834
7.828
7.819
7.749
7.734
7.719
7.551
7.536
7.521
7.501
7.485

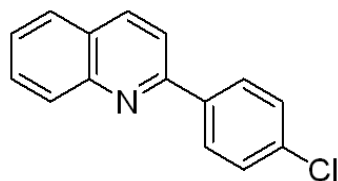


3aj

¹H NMR (500 MHz, CDCl₃)

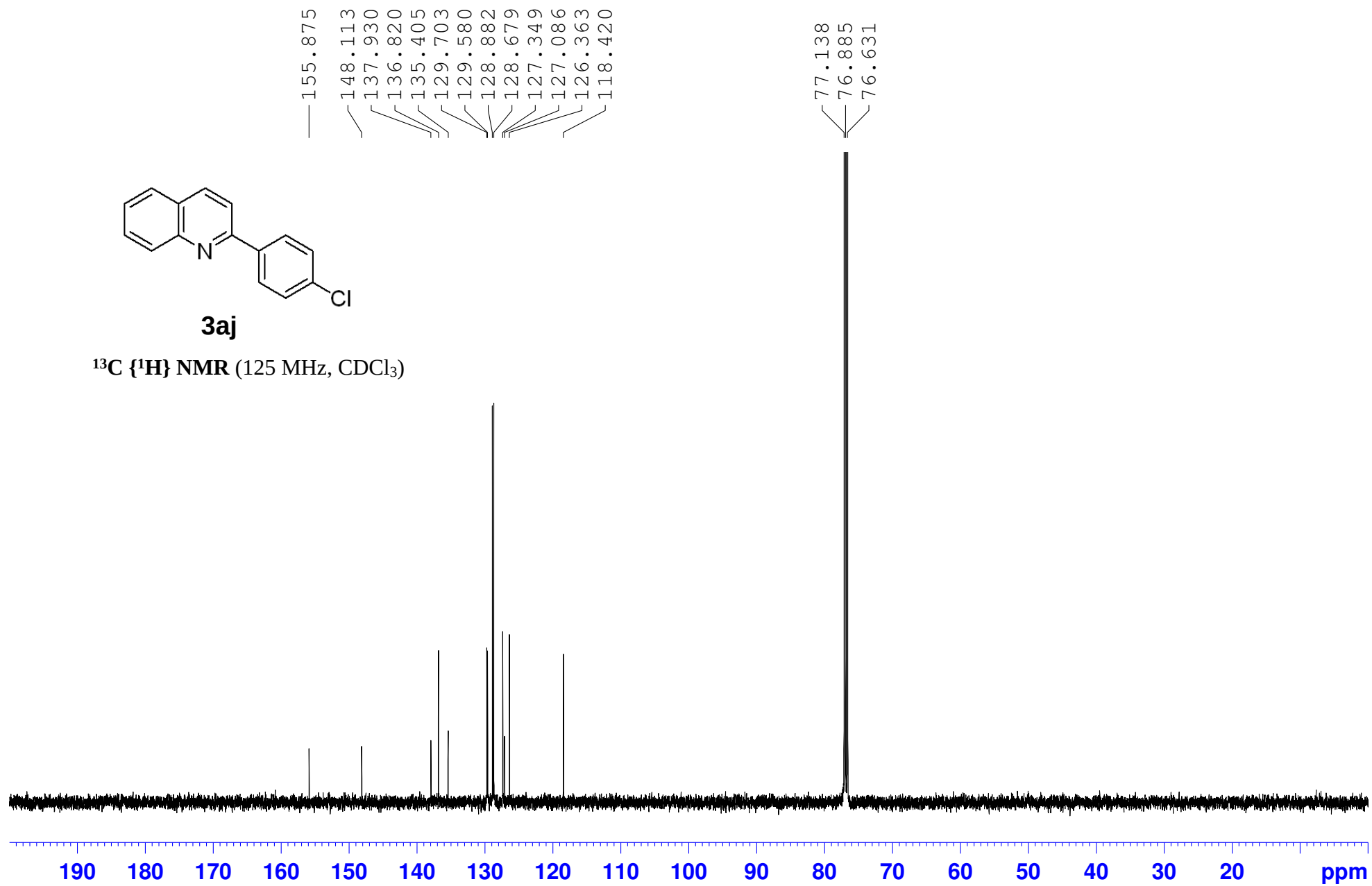


2-(4-chlorophenyl)quinoline
C13CPD CDCl3



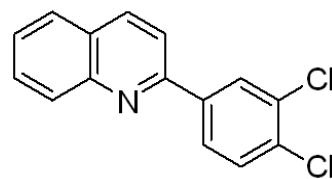
3aj

^{13}C { ^1H } NMR (125 MHz, CDCl_3)



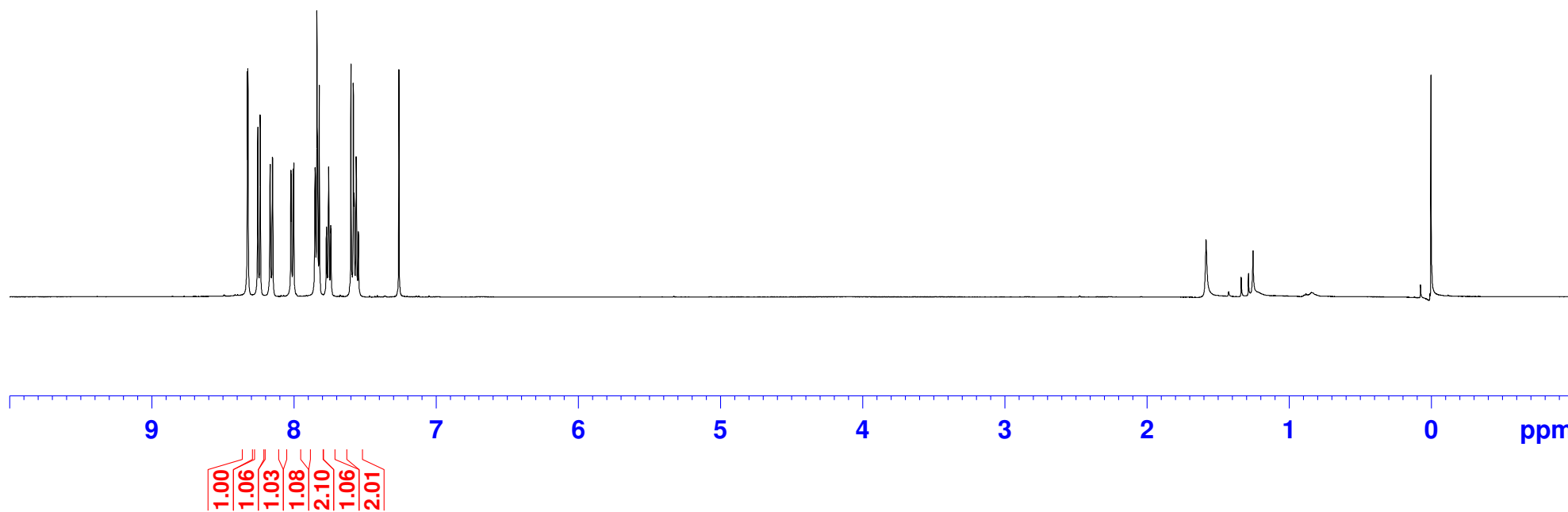
2-(3,4-dichlorophenyl)quinoline
Proton CDCl₃

8.253
8.236
8.166
8.149
8.020
8.016
8.004
8.000
7.849
7.837
7.820
7.771
7.768
7.754
7.740
7.738
7.597
7.580
7.576
7.575
7.560
7.545
7.260

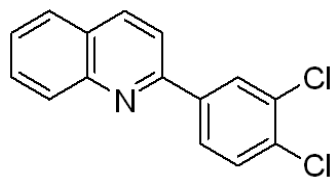


3ak

¹H NMR (500 MHz, CDCl₃)

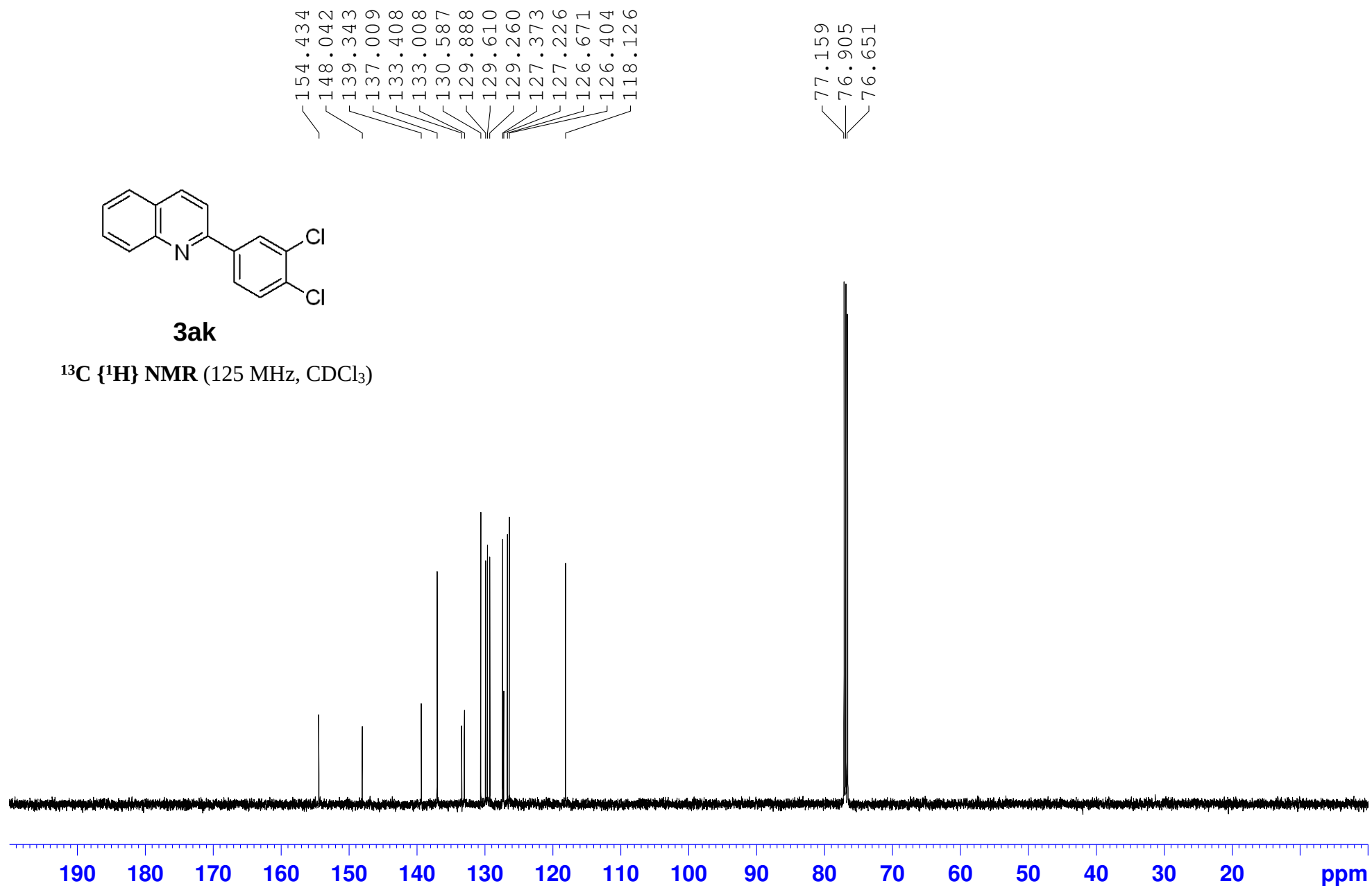


2-(3,4-dichlorophenyl)quinoline
C13CPD CDCl₃



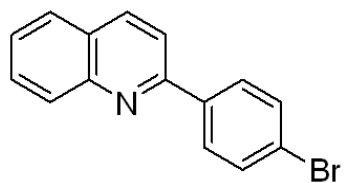
3ak

¹³C {¹H} NMR (125 MHz, CDCl₃)



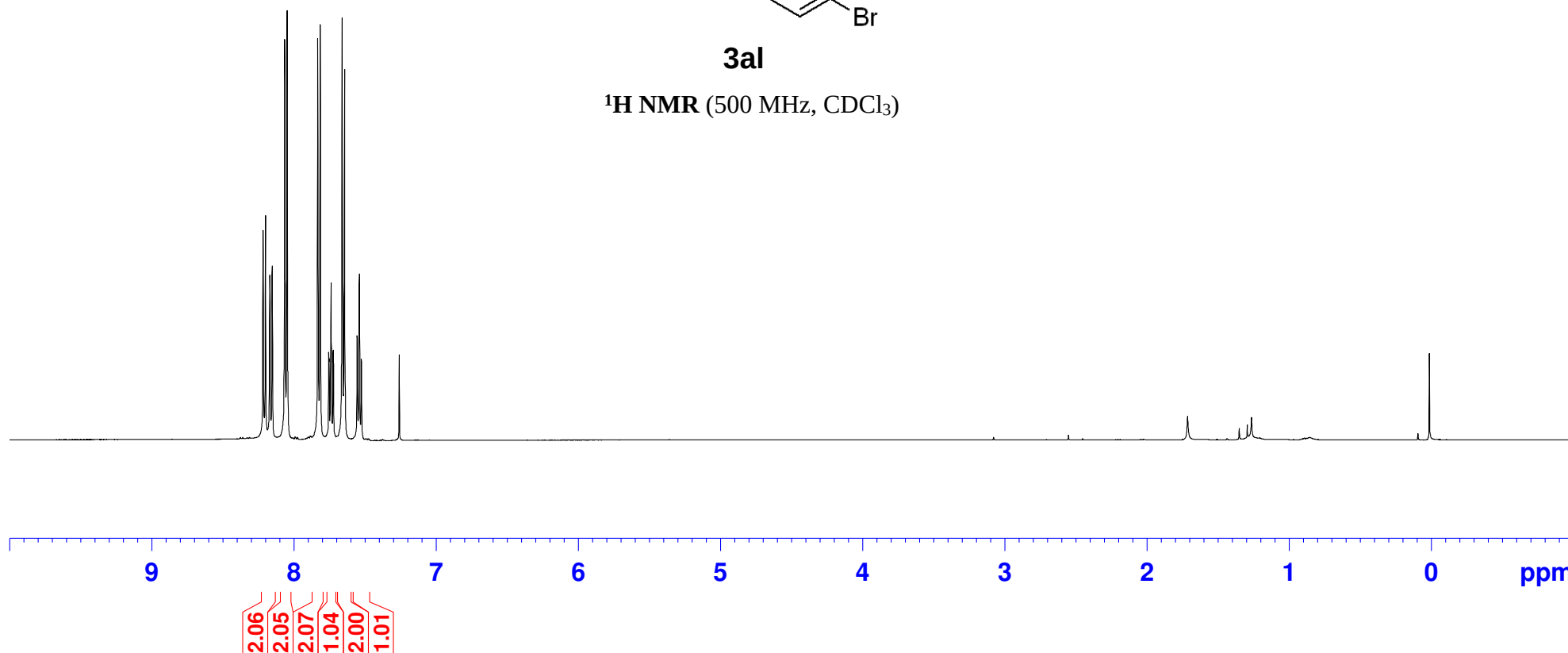
2-(4-bromophenyl)quinoline
Proton CDCl₃

8.216
8.198
8.168
8.151
8.063
8.046
7.831
7.814
7.753
7.751
7.737
7.723
7.721
7.659
7.642
7.554
7.538
7.524
7.260



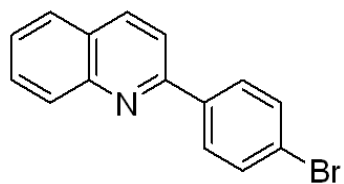
3al

¹H NMR (500 MHz, CDCl₃)



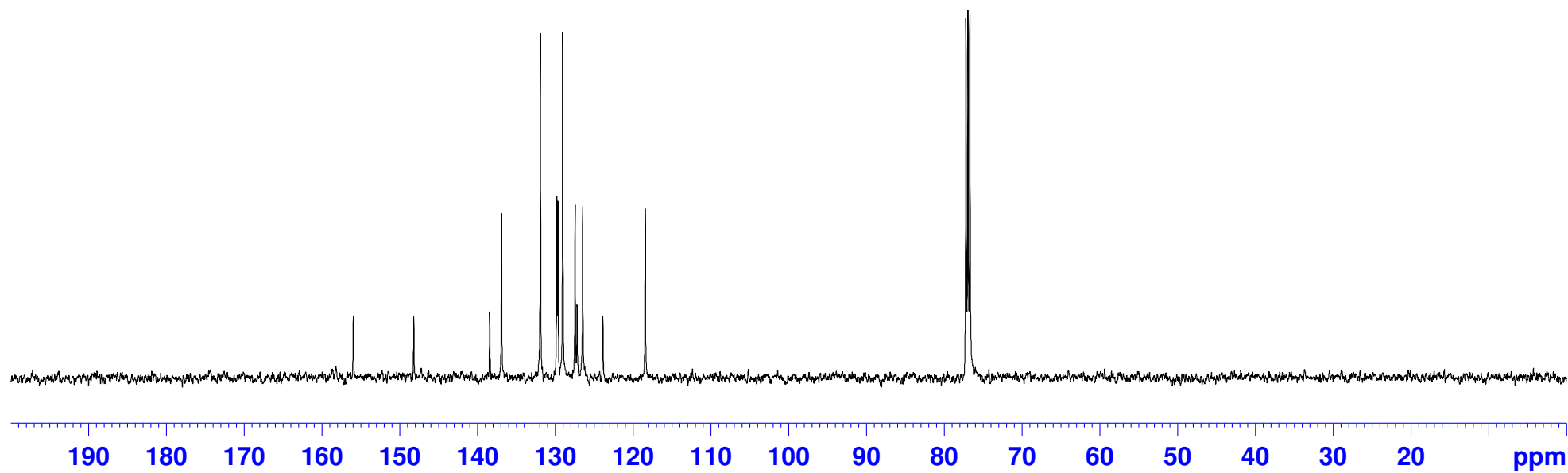
2-(4-bromophenyl)quinoline
C13CPD CDCl₃

155.946
148.177
138.421
136.900
131.901
129.791
129.641
129.028
127.436
127.179
126.458
123.868
118.420
77.249
76.995
76.741



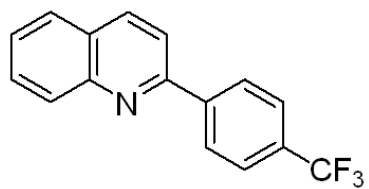
3al

¹³C {¹H} NMR (125 MHz, CDCl₃)



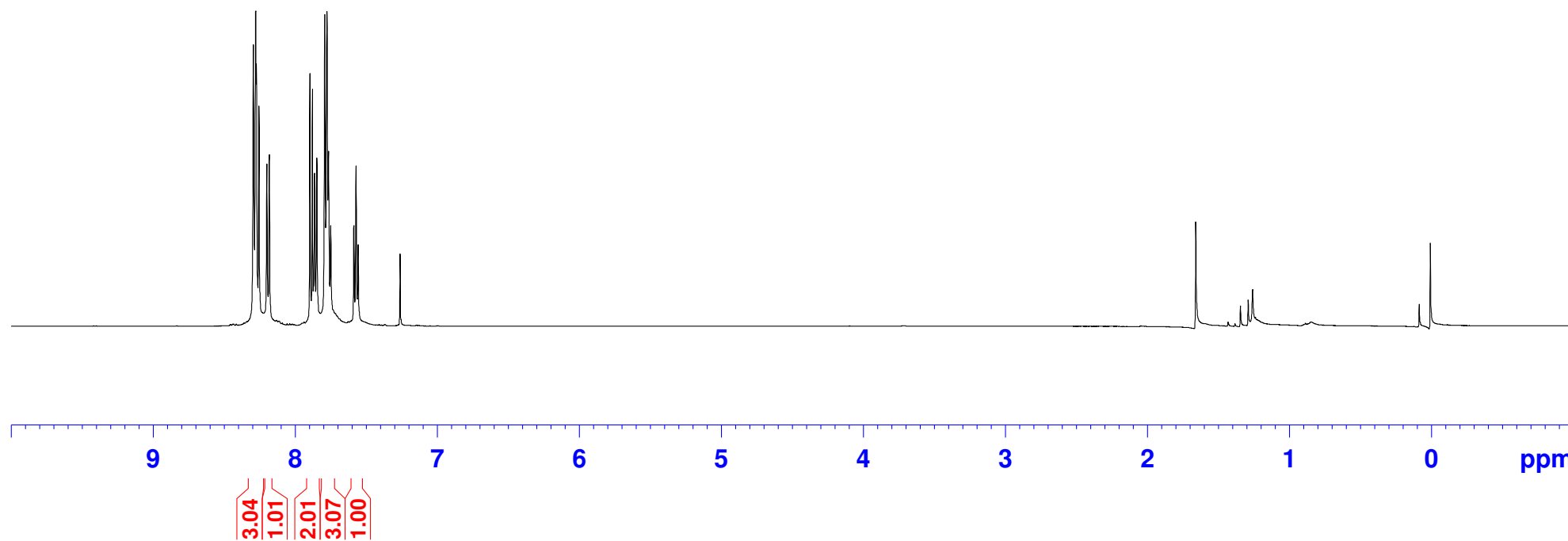
2-(4-(trifluoromethyl)phenyl)quinoline
Proton CDCl₃

8.294
8.277
8.272
8.254
8.198
8.181
7.895
7.878
7.863
7.847
7.791
7.775
7.766
7.764
7.749
7.585
7.570
7.556
7.260



3am

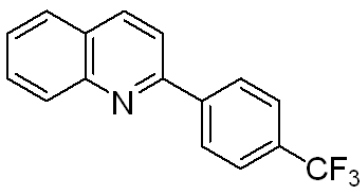
¹H NMR (500 MHz, CDCl₃)



2-(4-(trifluoromethyl)phenyl)quinoline
C13CPD CDCl3

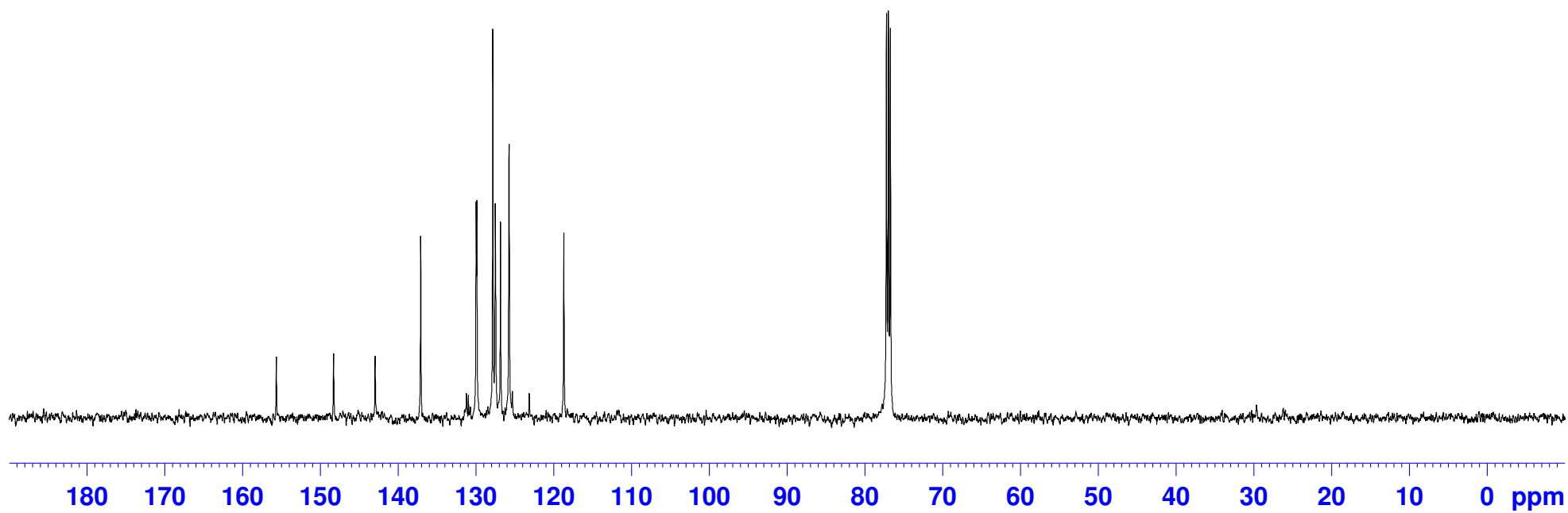
155.635
148.273
142.938
137.084
131.197
130.941
129.955
129.863
127.813
127.500
126.826
125.721
125.293
123.124
118.730

77.261
77.007
76.753

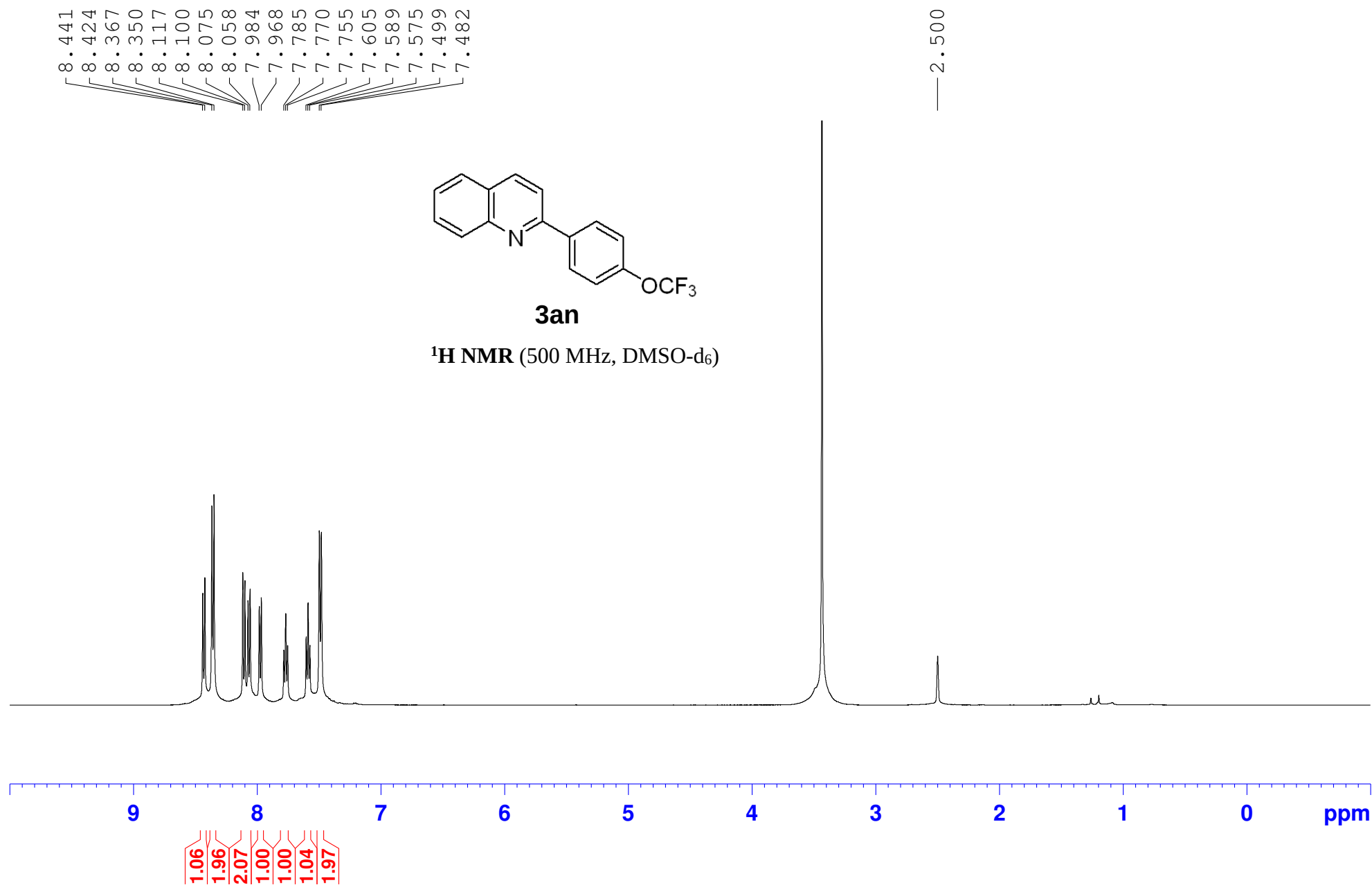


3am

^{13}C { ^1H } NMR (125 MHz, CDCl_3)



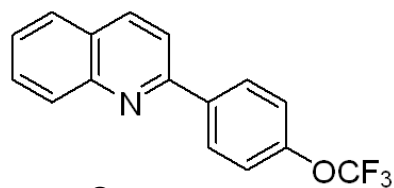
2-(4-(trifluoromethoxy)phenyl)quinoline
Proton DMSO-d₆



2-(4-(trifluoromethoxy)phenyl)quinoline
C13CPD DMSO-d6

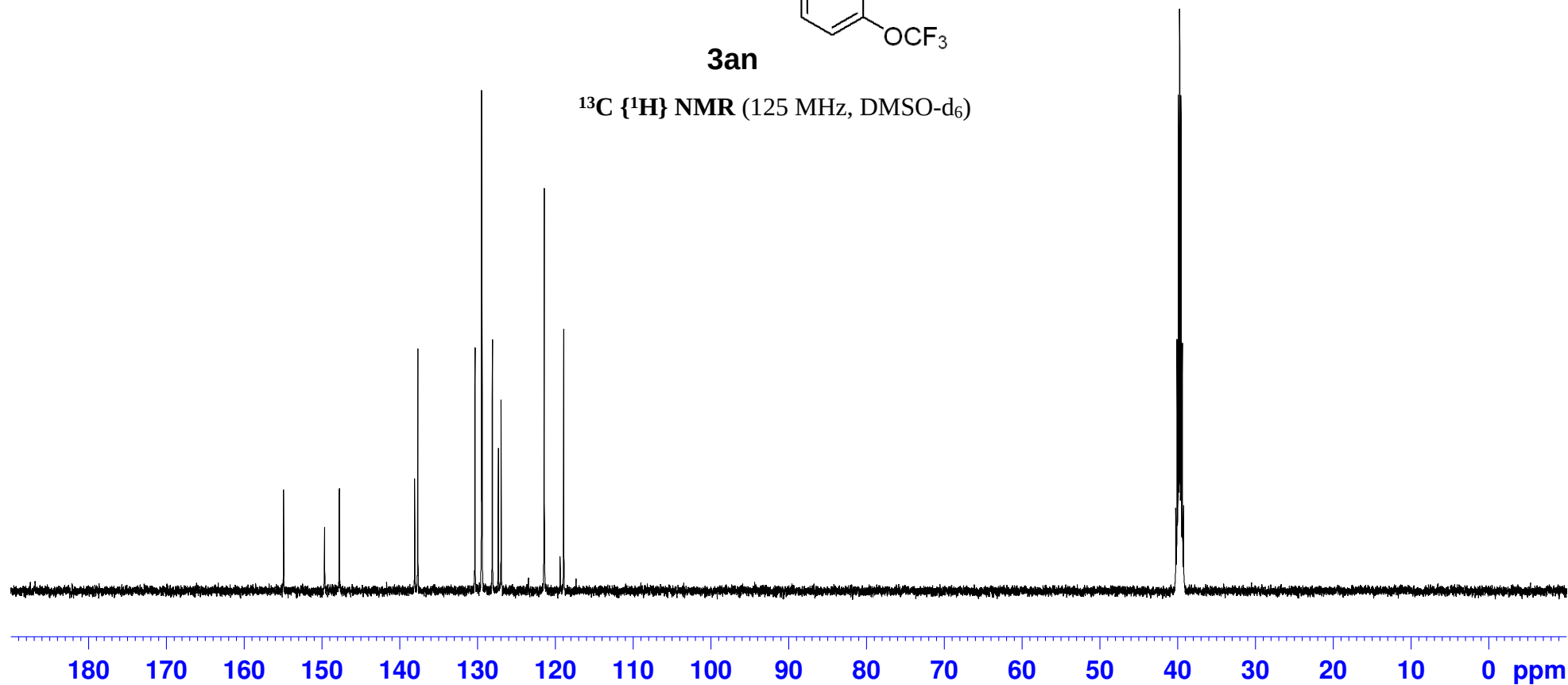
154.926
149.648
147.753
138.057
137.657
130.314
129.451
129.387
128.074
127.314
126.950
121.403
119.361
118.899

40.269
40.102
39.935
39.768
39.602
39.434
39.268



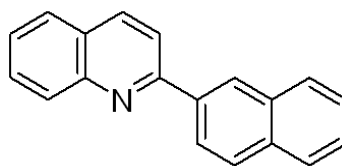
3an

^{13}C { ^1H } NMR (125 MHz, DMSO- d_6)



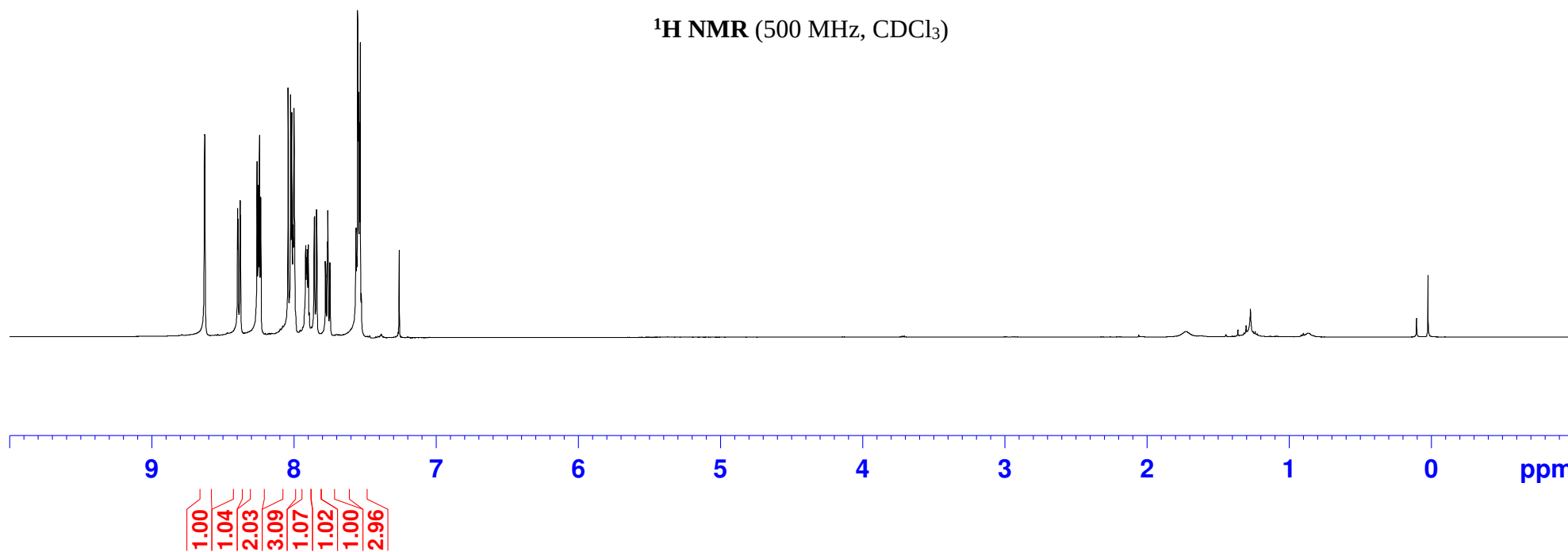
2-(naphthalen-2-yl)quinoline
Proton CDCl₃

8.251
8.243
8.235
8.042
8.024
8.017
8.001
7.919
7.912
7.907
7.900
7.857
7.841
7.779
7.777
7.765
7.763
7.748
7.746
7.566
7.564
7.553
7.547
7.540
7.534
7.260



3ao

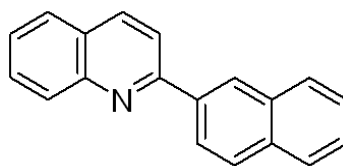
¹H NMR (500 MHz, CDCl₃)



2-(naphthalen-2-yl)quinoline
C13CPD CDCl3

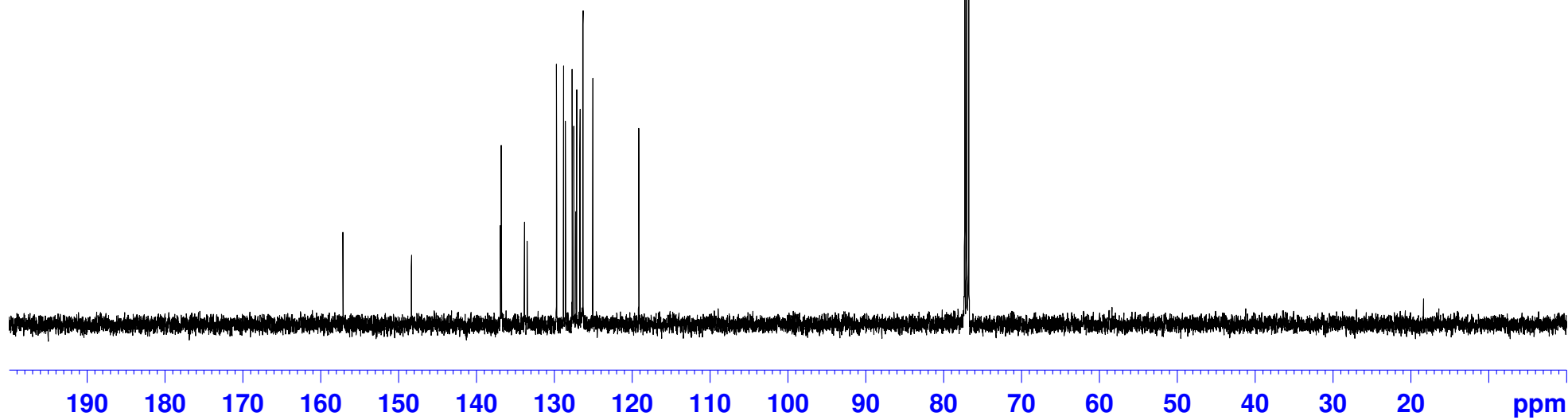
157.128
148.324
136.914
136.785
133.817
133.458
129.695
128.795
128.547
127.690
127.470
127.186
127.119
126.681
126.306
125.031
119.131

77.259
77.004
76.750



3ao

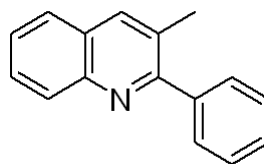
^{13}C { ^1H } NMR (125 MHz, CDCl_3)



3-methyl-2-phenylquinoline
Proton CDCl3

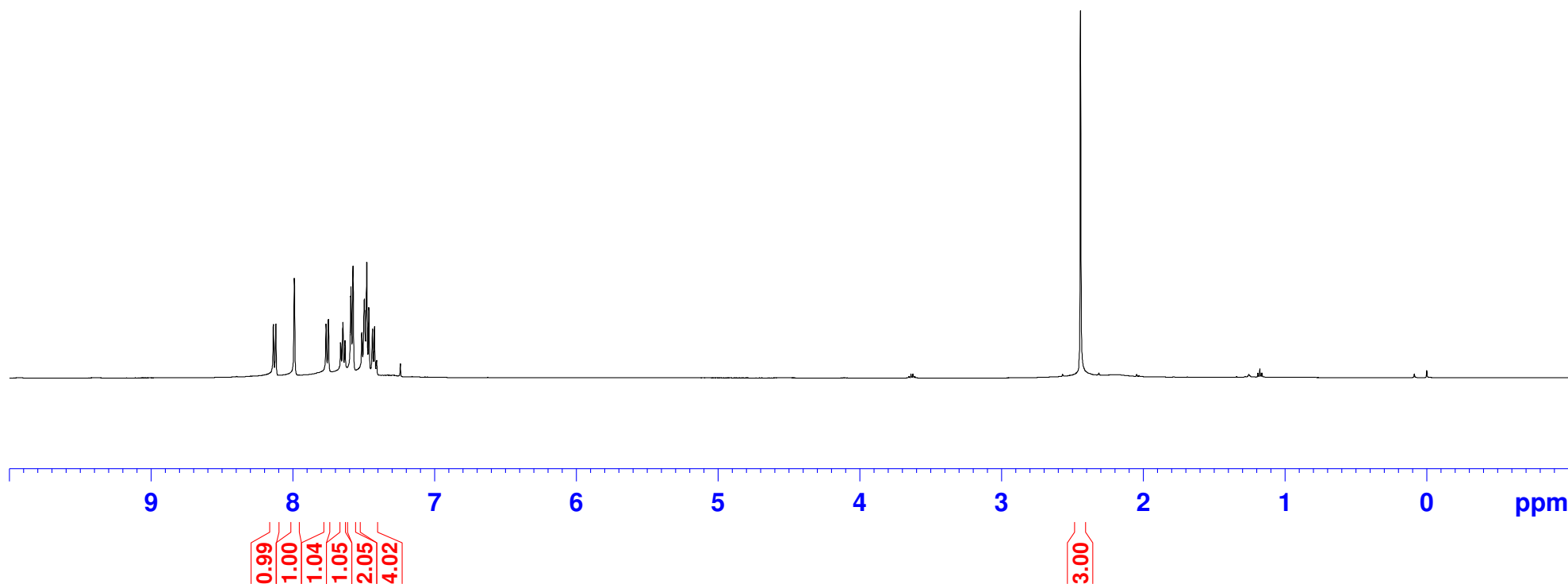
8.136
8.120
7.989
7.765
7.749
7.662
7.646
7.632
7.591
7.589
7.575
7.513
7.496
7.495
7.492
7.478
7.463
7.437
7.423
7.408

2.444



3ap

¹H NMR (500 MHz, CDCl₃)



3-methyl-2-phenylquinoline
C13CPD CDCl3

— 160.420

146.528

140.777

136.605

129.194

129.085

128.740

128.621

128.188

128.063

127.481

126.593

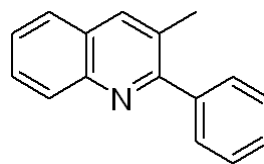
126.283

77.216

76.961

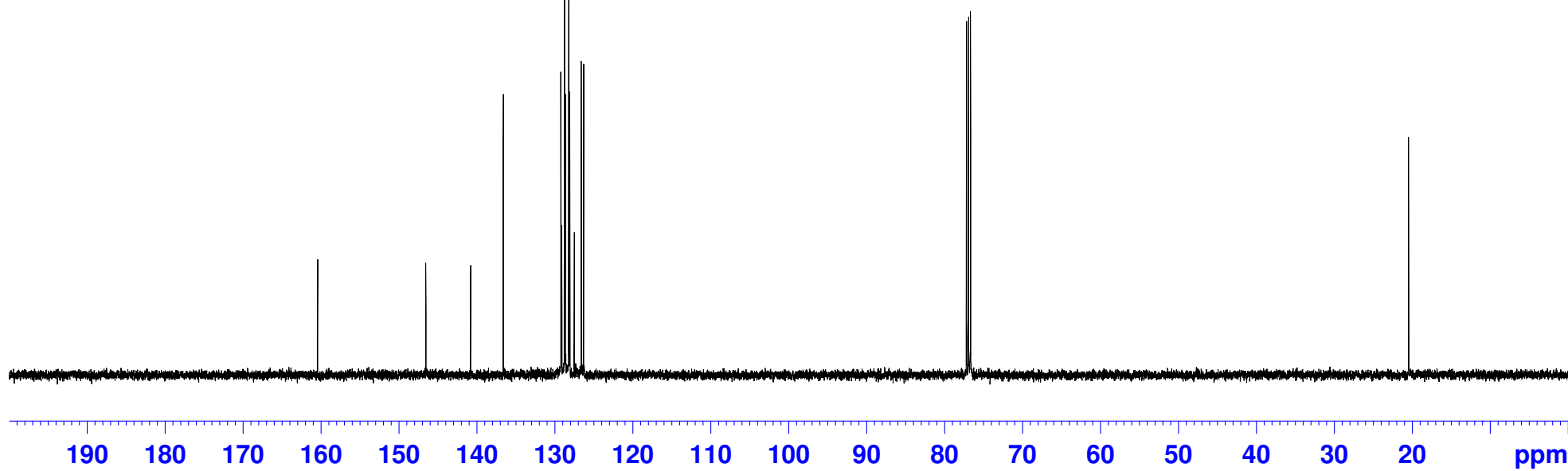
76.707

— 20.510



3ap

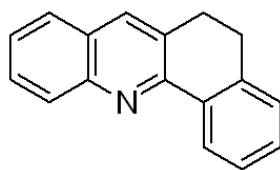
^{13}C { ^1H } NMR (125 MHz, CDCl_3)



5,6-dihydrobenzo[c]acridine
Proton CDCl₃

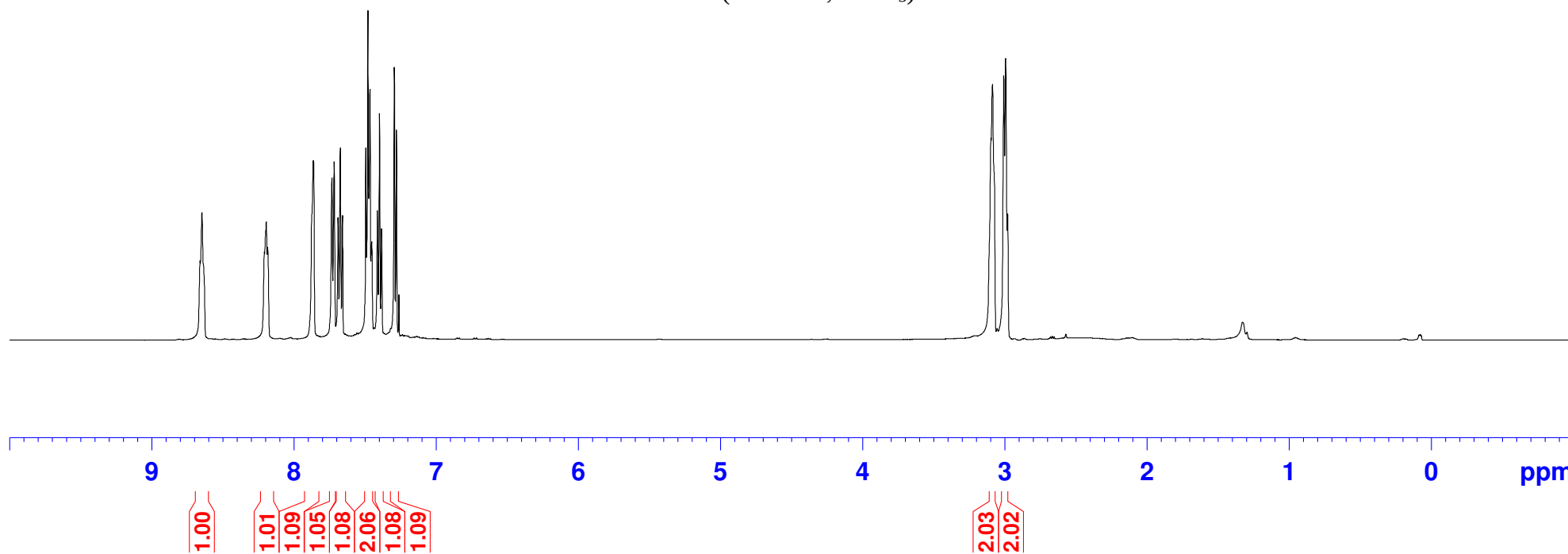
8.659
8.645
8.636
8.207
8.193
8.183
7.862
7.731
7.715
7.688
7.674
7.672
7.657
7.493
7.492
7.478
7.464
7.452
7.411
7.396
7.382
7.292
7.277

3.098
3.087
3.007
2.981



3aq

¹H NMR (500 MHz, CDCl₃)

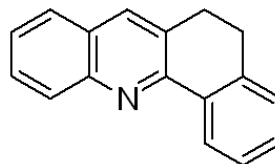


5,6-dihydrobenzo[c]acridine
C13CPD CDC13

153.278
147.508
139.329
134.598
133.621
130.485
129.593
129.288
128.561
127.868
127.762
127.235
126.851
125.963

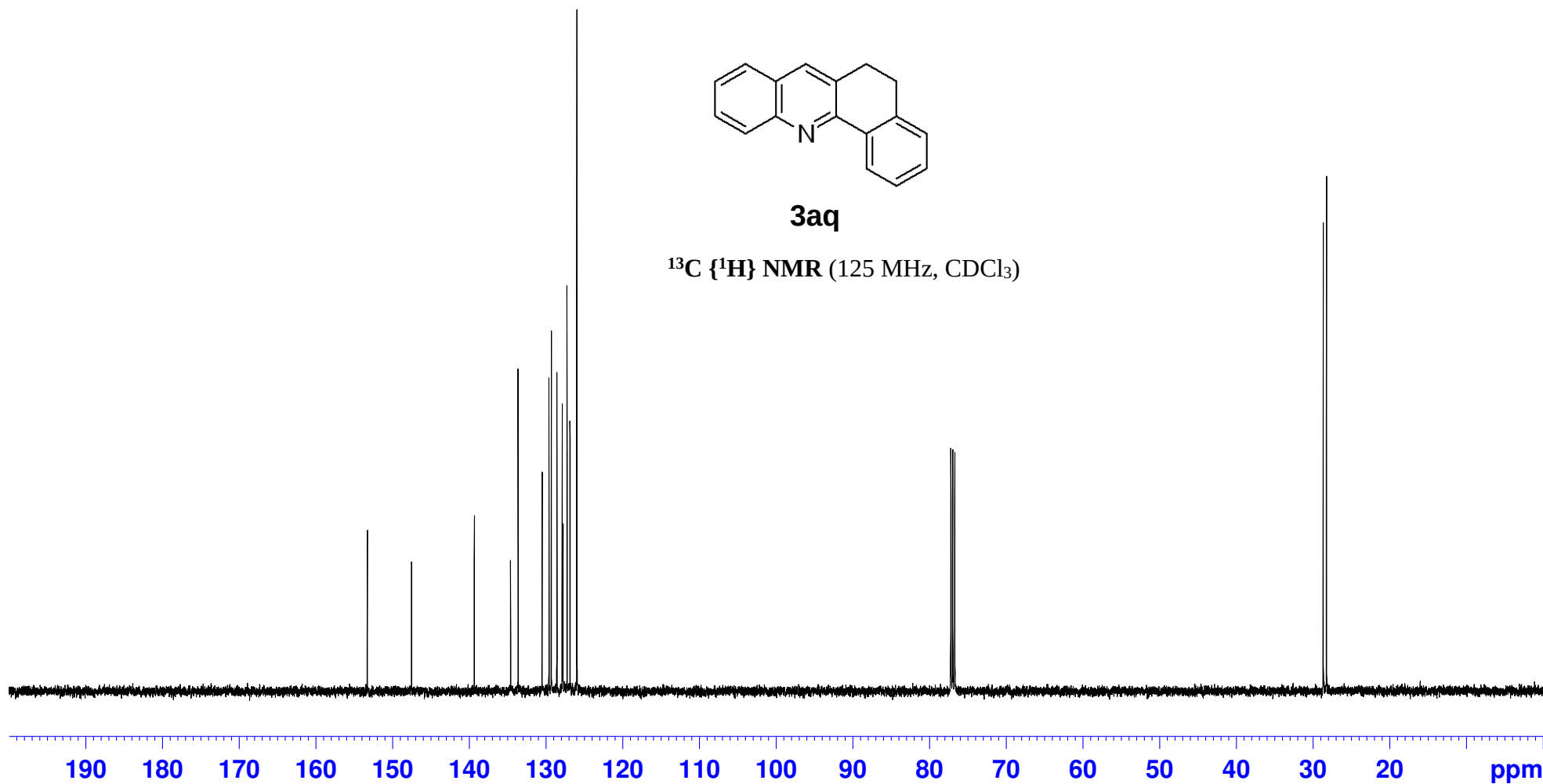
77.248
76.994
76.741

28.704
28.284



3aq

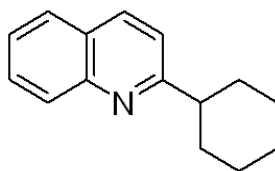
$^{13}\text{C} \{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



2-cyclohexylquinoline
Proton CDCl₃

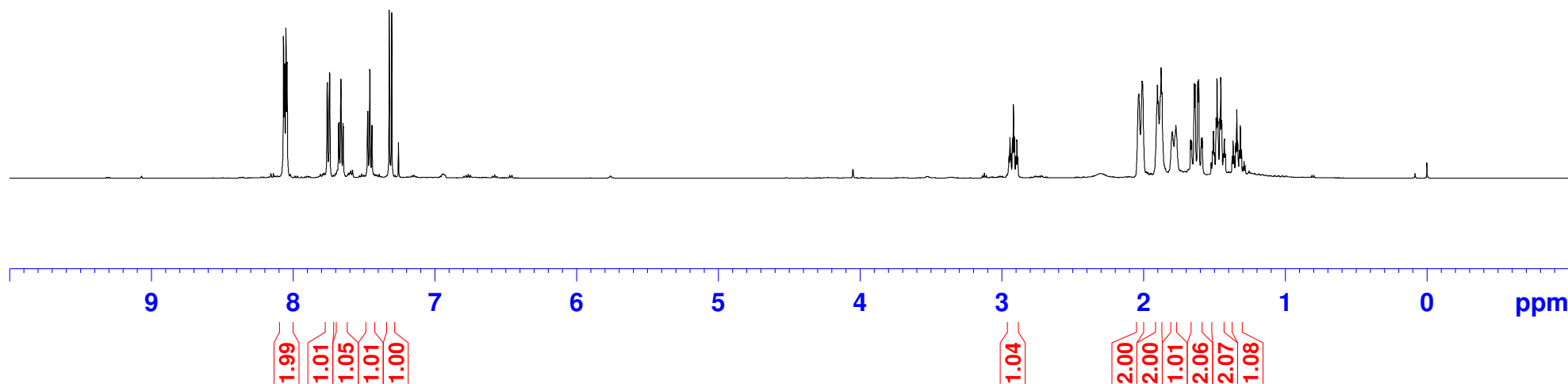
8.066
8.058
8.049
8.042
7.757
7.741
7.677
7.663
7.646
7.644
7.472
7.457
7.441
7.320
7.303

2.949
2.918
2.901
2.888
2.034
2.007
1.902
1.896
1.870
1.798
1.778
1.772
1.668
1.643
1.617
1.586
1.513
1.488
1.436
1.423
1.375
1.342
1.324
1.310



3ar

¹H NMR (500 MHz, CDCl₃)



2-cyclohexylquinoline
C13CPD CDCl₃

— 166.699

— 147.685

— 136.160

— 129.082

— 128.846

— 127.300

— 126.837

— 125.457

— 119.445

— 77.185

— 76.931

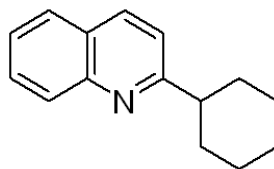
— 76.677

— 47.513

— 32.712

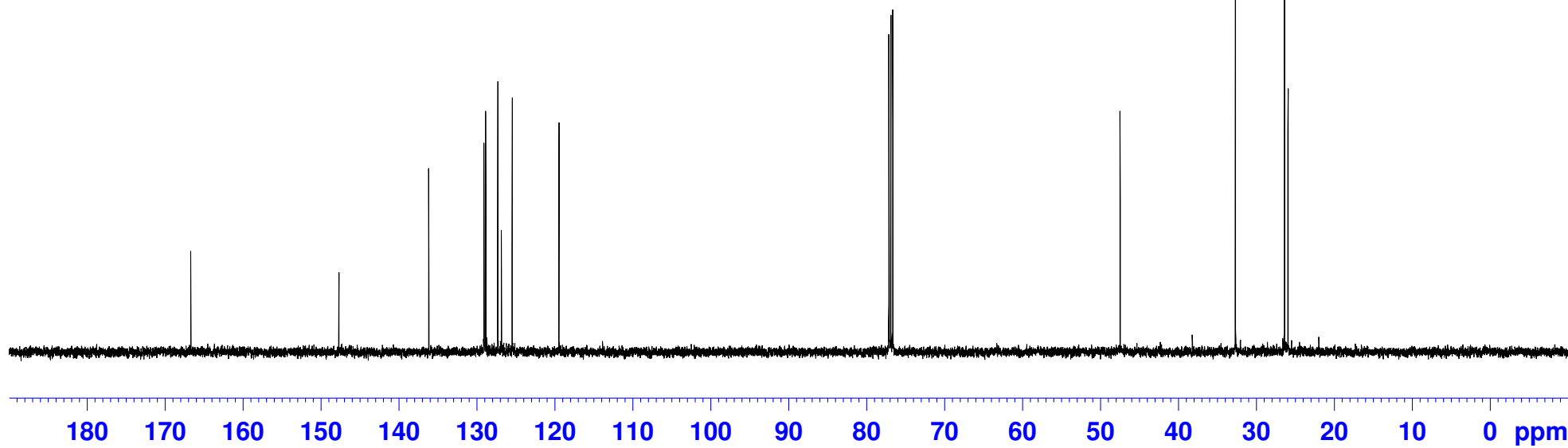
— 26.420

— 25.974



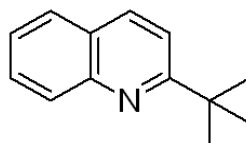
3ar

¹³C {¹H} NMR (125 MHz, CDCl₃)



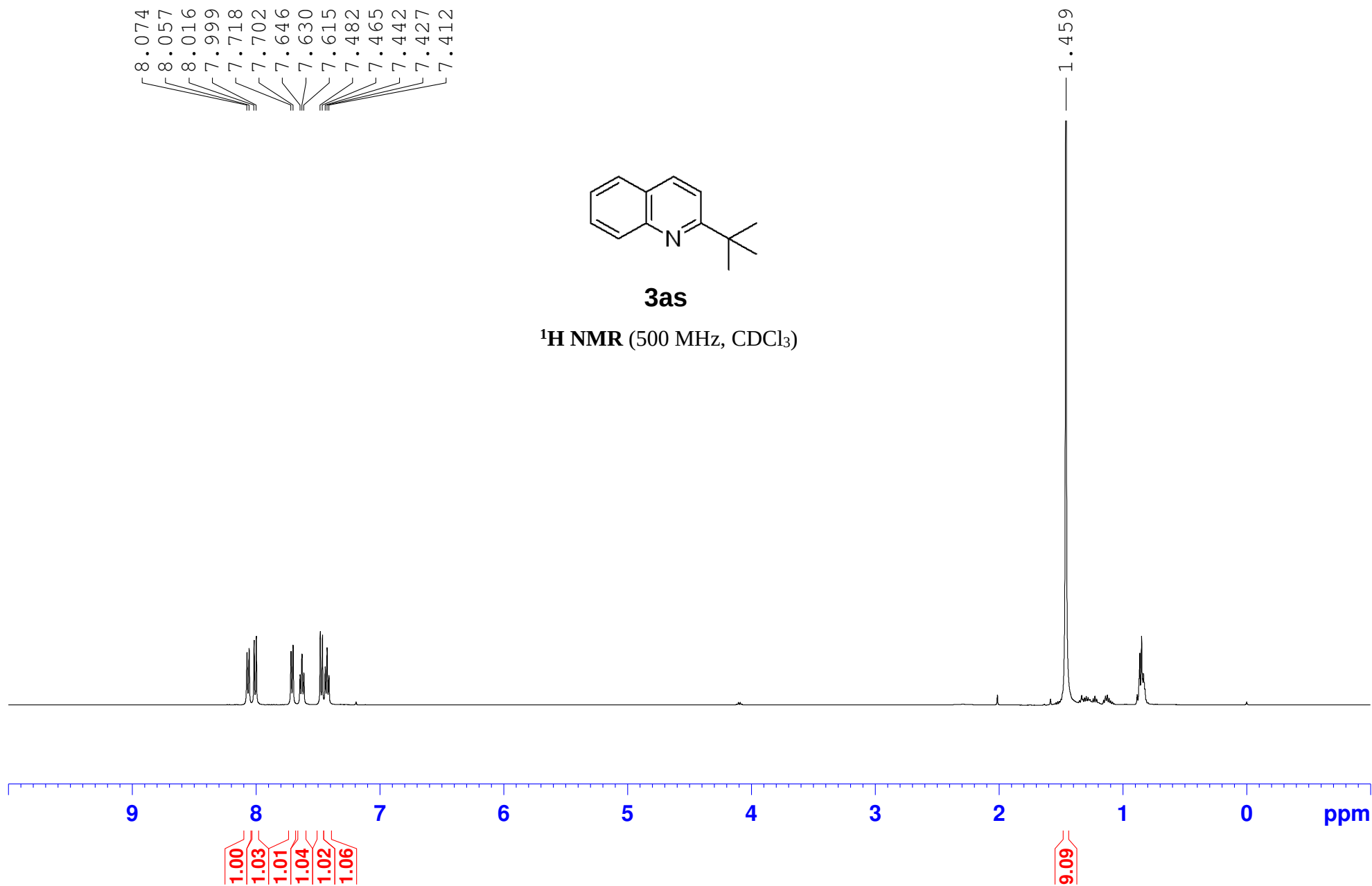
2-(Tert-butyl)quinoline
Proton CDCl₃

8.074
8.057
8.016
7.999
7.718
7.702
7.646
7.630
7.615
7.482
7.465
7.442
7.427
7.412



3as

¹H NMR (500 MHz, CDCl₃)



2-(Tert-butyl)quinoline
C13CPD CDCl₃

— 169.124

— 147.374

135.751

129.353

128.875

127.125

126.365

125.517

118.095

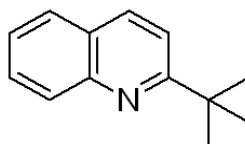
77.225

76.971

76.716

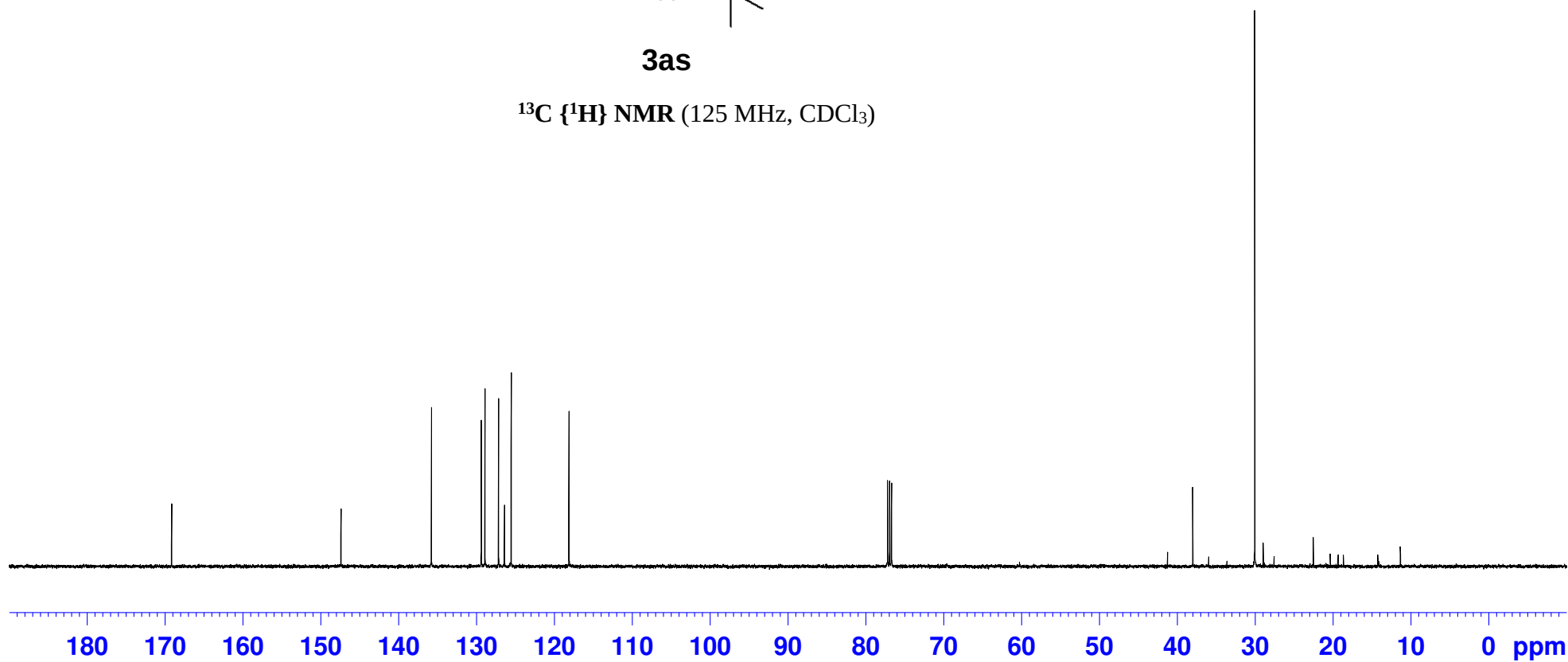
— 38.037

— 30.074



3as

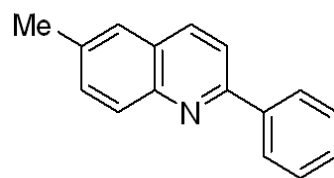
¹³C {¹H} NMR (125 MHz, CDCl₃)



6-methyl-2-phenylquinoline
Proton CDCl₃

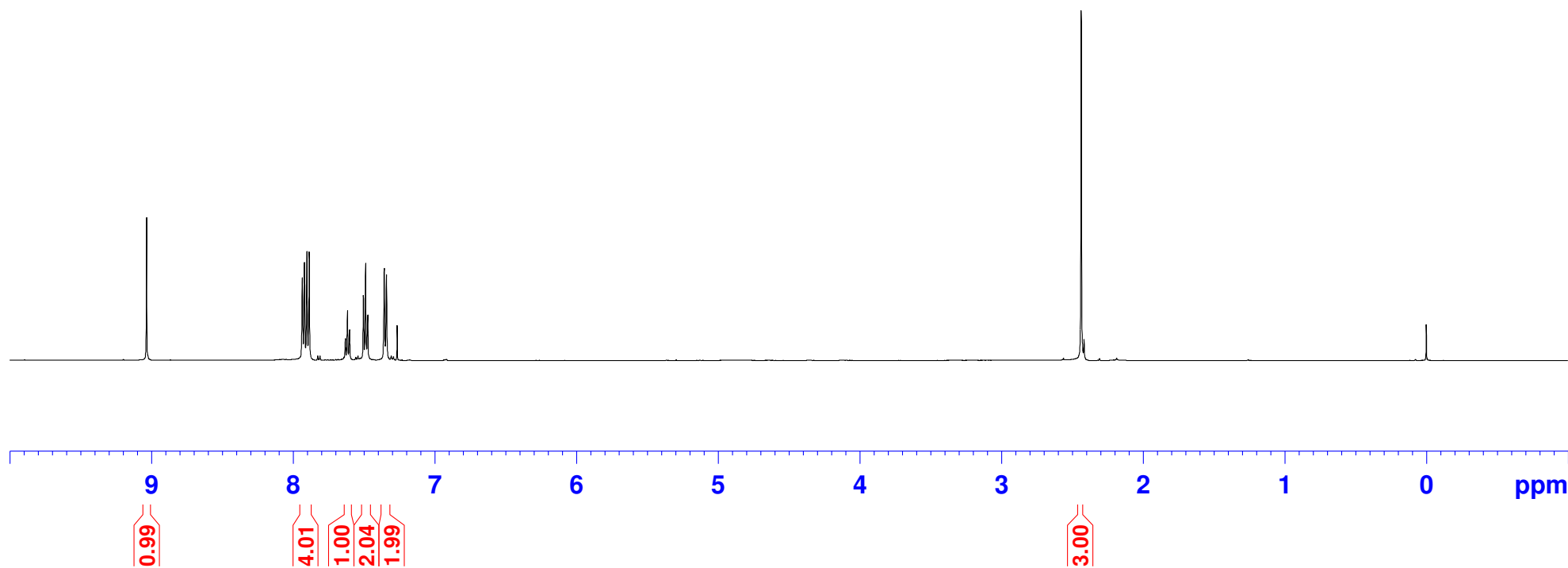
9.032
7.934
7.932
7.918
7.915
7.900
7.884
7.629
7.614
7.601
7.599
7.501
7.486
7.470
7.355
7.338

2.436



3ba

¹H NMR (500 MHz, CDCl₃)

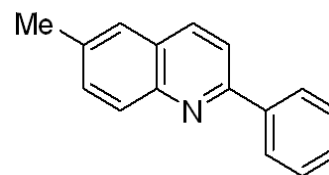


6-methyl-2-phenylquinoline
C13CPD CDCl3

156.381
146.772
139.704
136.020
135.990
131.834
129.303
129.035
128.713
127.379
127.101
126.247
118.853

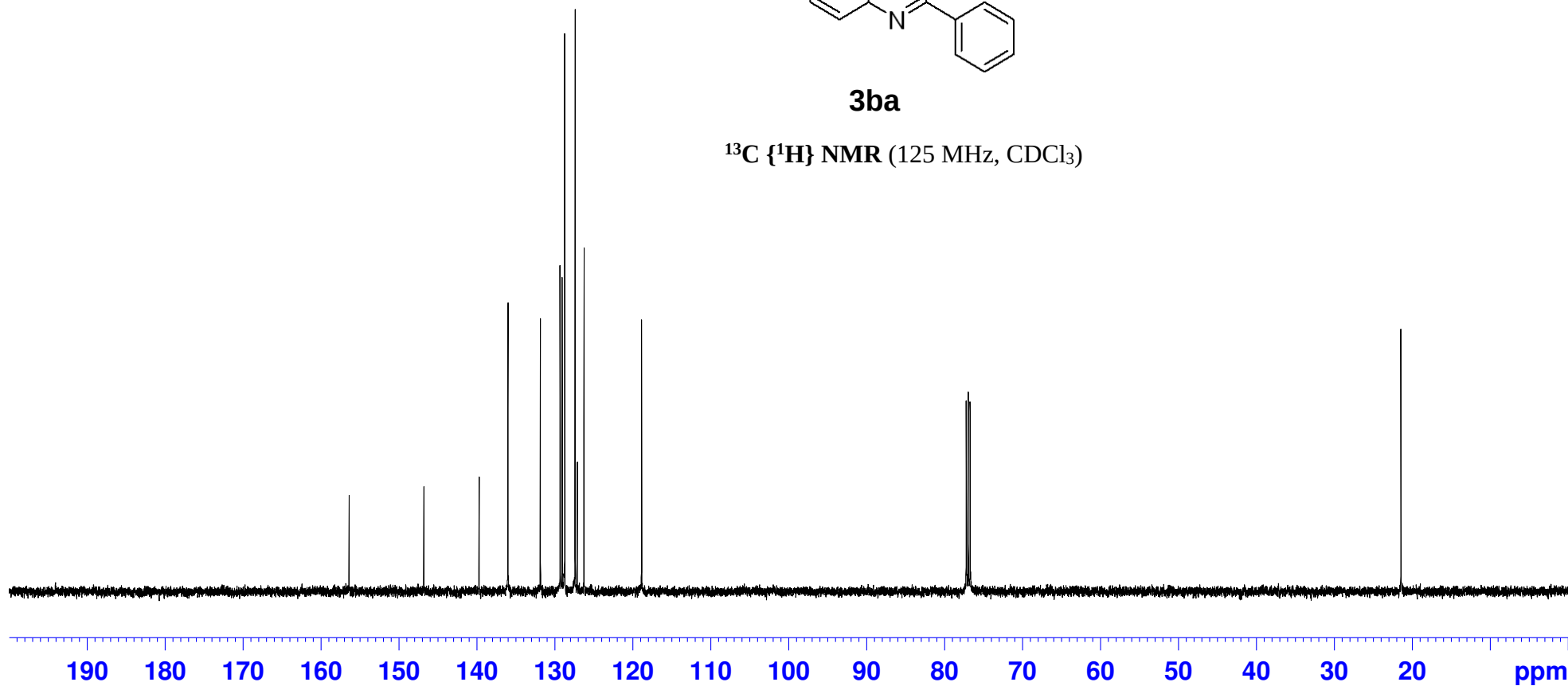
77.256
77.002
76.748

21.490



3ba

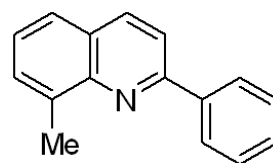
^{13}C { ^1H } NMR (125 MHz, CDCl_3)



8-methyl-2-phenylquinoline
Proton CDCl₃

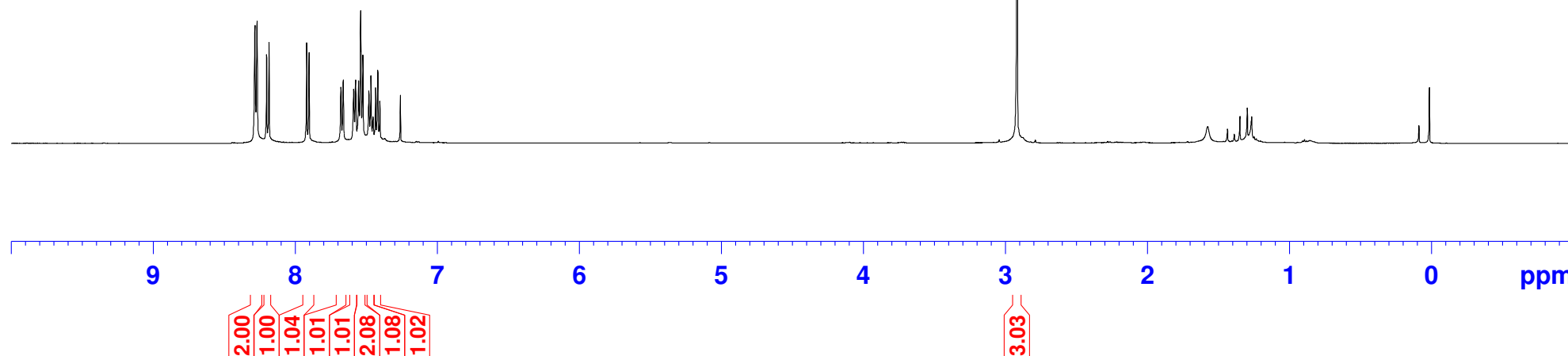
8.282
8.267
8.200
8.182
7.921
7.904
7.679
7.663
7.590
7.576
7.555
7.540
7.525
7.482
7.468
7.453
7.435
7.420
7.405

— 2.917



3ca

¹H NMR (500 MHz, CDCl₃)

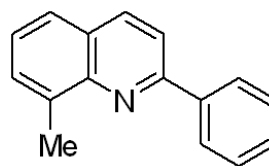


8-methyl-2-phenylquinoline
C13CPD CDCl₃

155.453
147.118
139.802
137.609
136.860
129.621
129.166
128.711
127.414
127.034
125.961
125.331
118.119

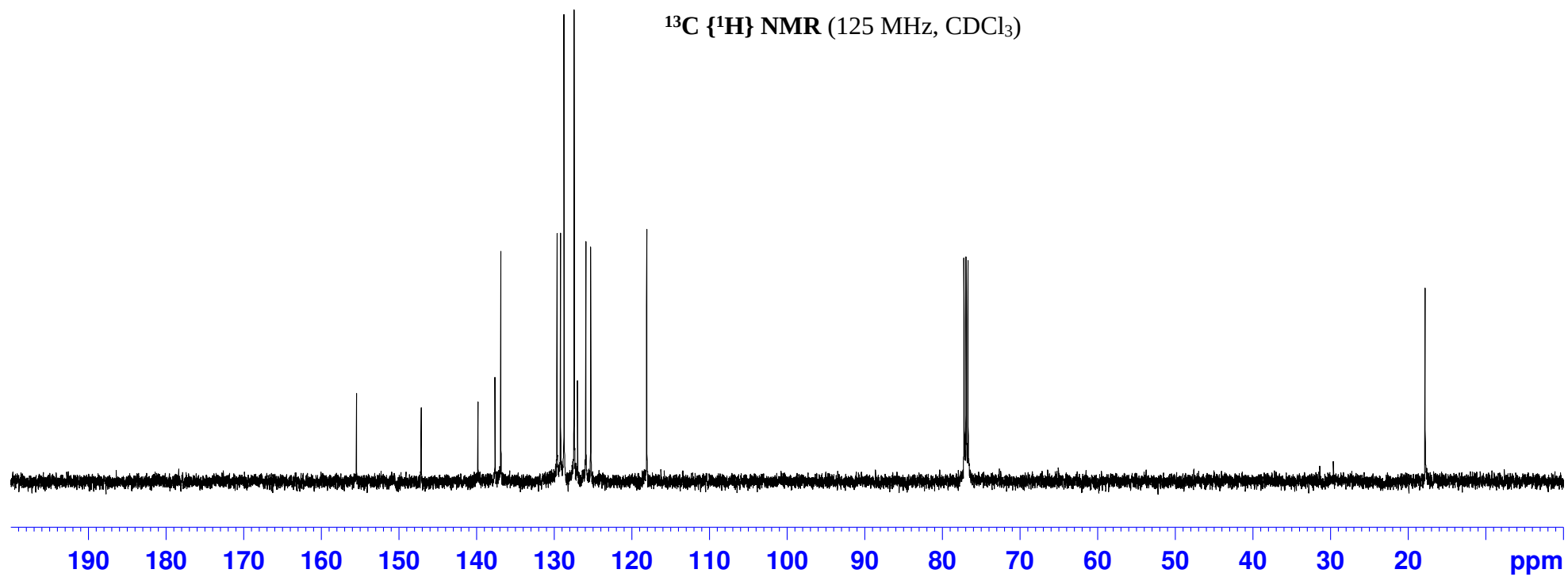
77.246
76.992
76.737

17.854



3ca

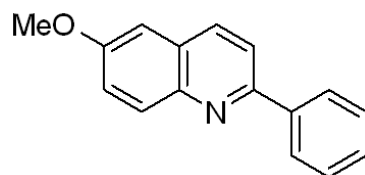
¹³C {¹H} NMR (125 MHz, CDCl₃)



6-methoxy-2-phenylquinoline
Proton CDCl₃

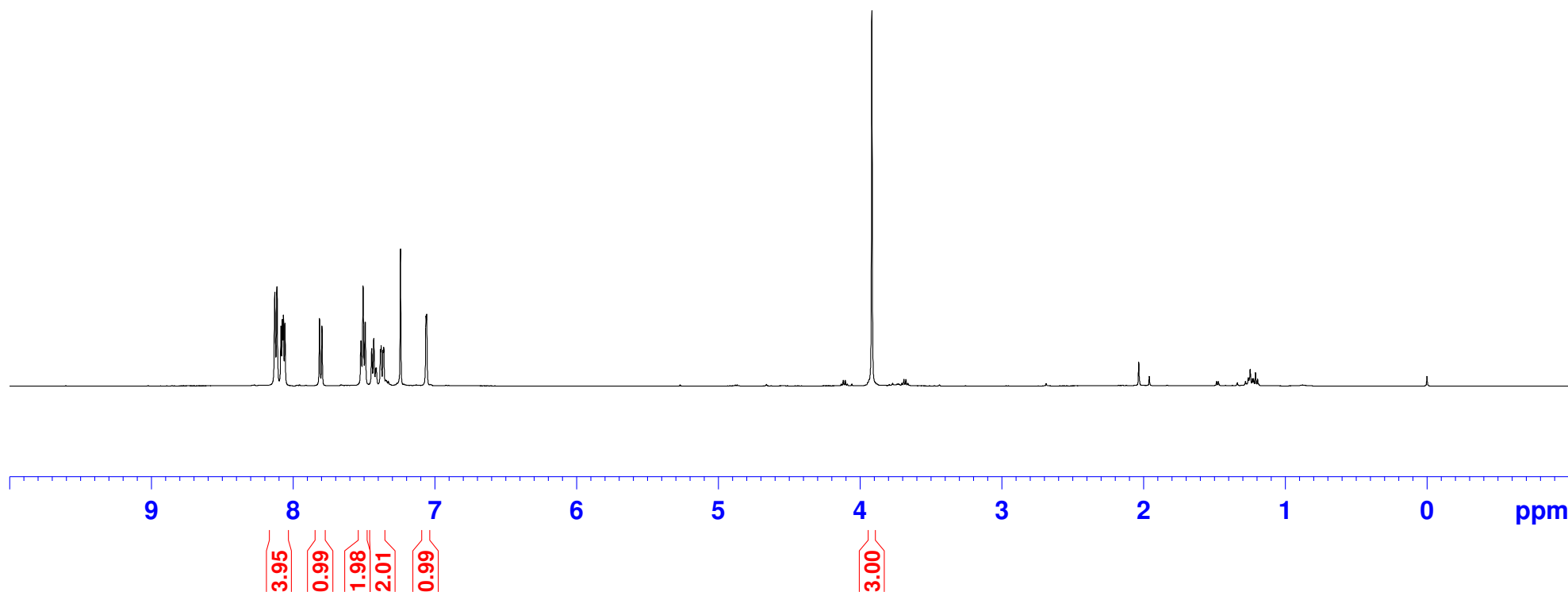
8.127
8.112
8.084
8.074
8.067
8.056
7.812
7.795
7.519
7.504
7.489
7.443
7.429
7.414
7.385
7.380
7.367
7.362
7.063
7.059

— 3.917



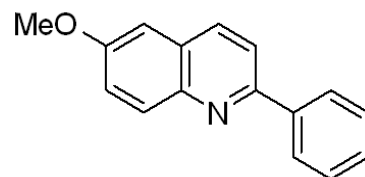
3da

¹H NMR (500 MHz, CDCl₃)



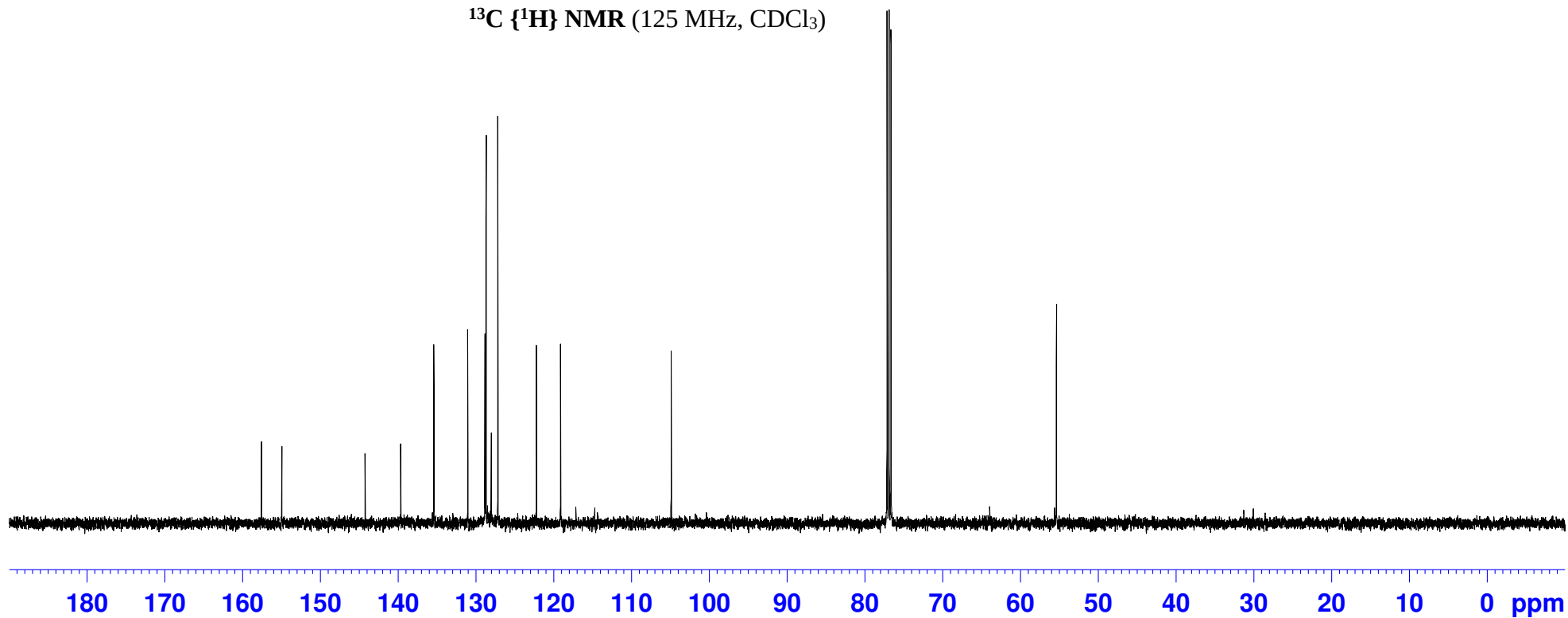
6-methoxy-2-phenylquinoline
C13CPD CDCl3

157.544
154.923
144.235
139.658
135.384
131.033
128.815
128.674
128.005
127.162
122.202
119.109
104.878
77.182
76.928
76.674
55.410



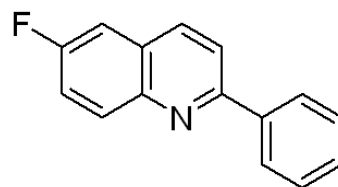
3da

^{13}C { ^1H } NMR (125 MHz, CDCl_3)



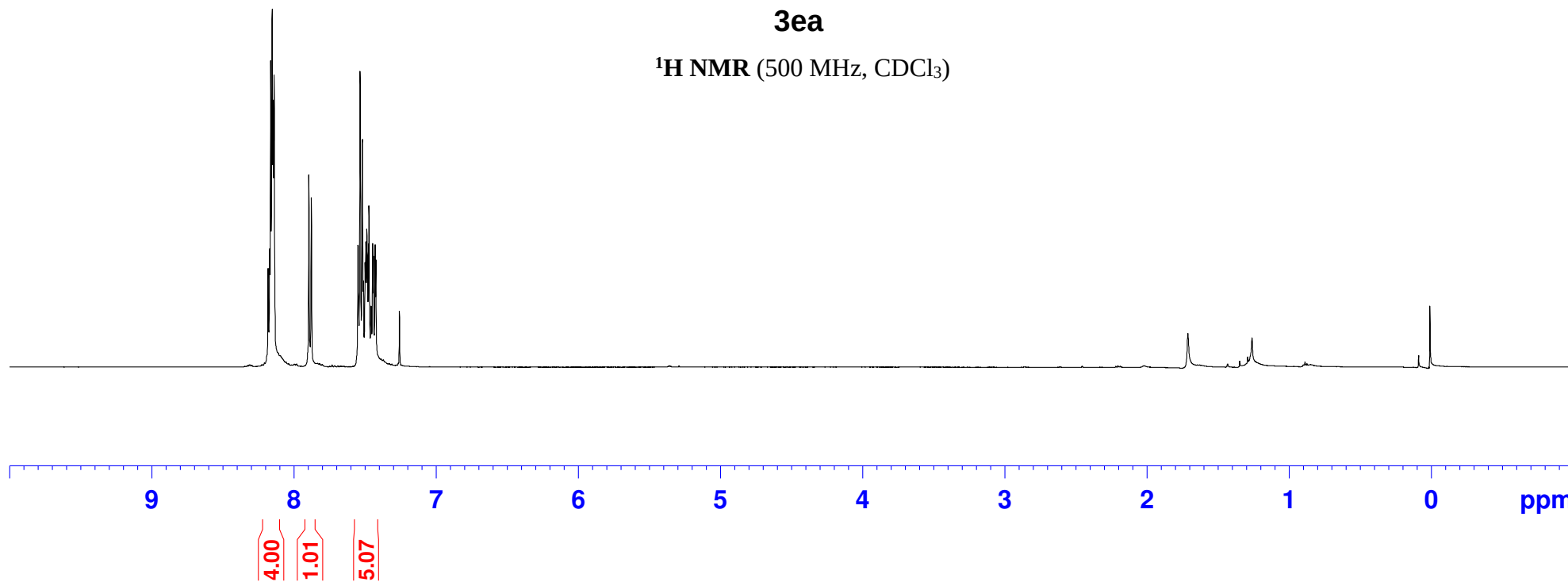
6-fluoro-2-phenylquinoline
Proton CDCl₃

8.182
8.172
8.165
8.155
8.148
8.140
7.896
7.878
7.550
7.535
7.520
7.513
7.500
7.495
7.487
7.477
7.473
7.458
7.447
7.442
7.430
7.424
7.258



3ea

¹H NMR (500 MHz, CDCl₃)

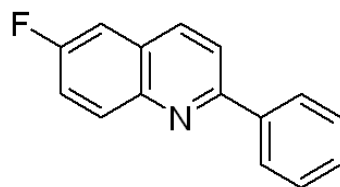


6-fluoro-2-phenylquinoline
C13CPD CDCl₃

161.322
159.354
156.743

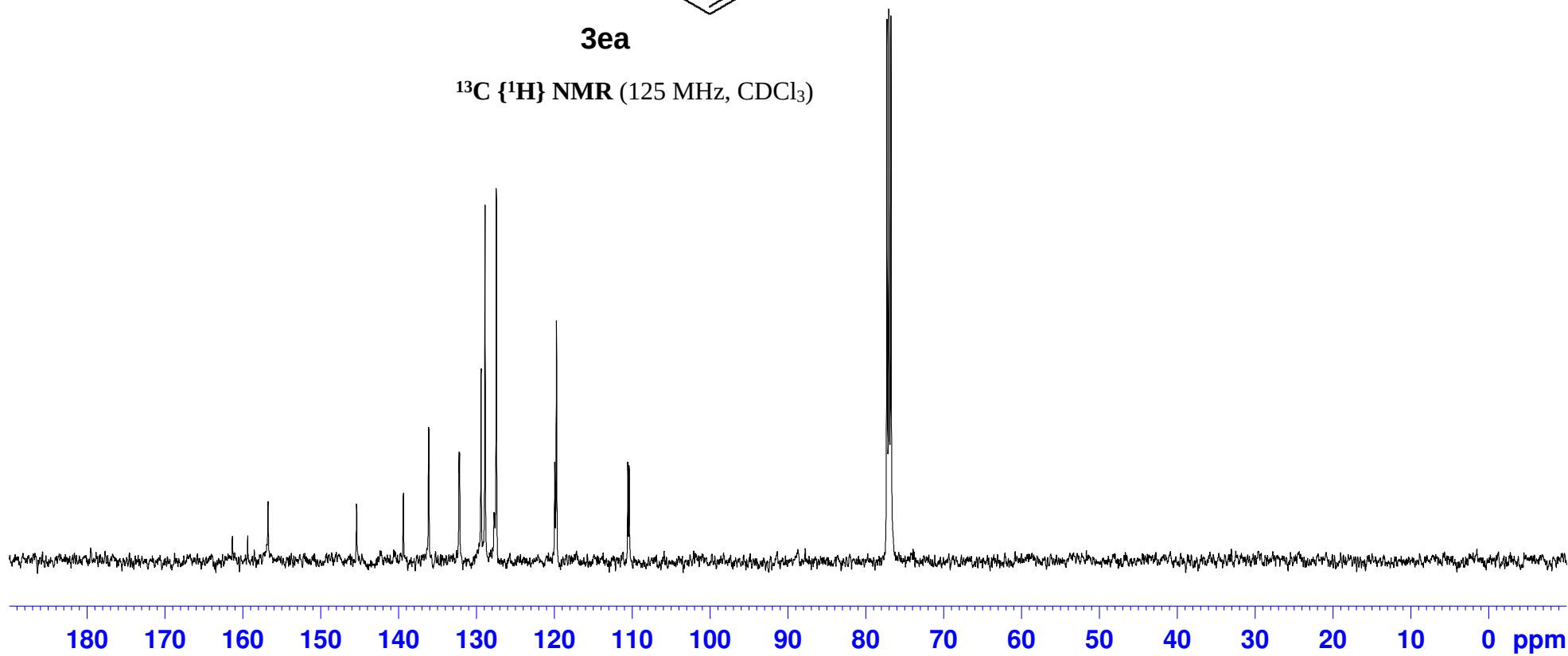
145.373
139.360
136.108
132.207
132.140
129.386
128.871
127.427
119.924
119.697
110.539
110.366

77.264
77.010
76.756



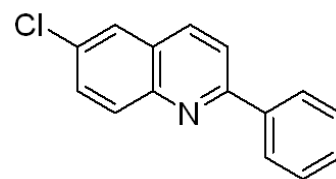
3ea

¹³C {¹H} NMR (125 MHz, CDCl₃)



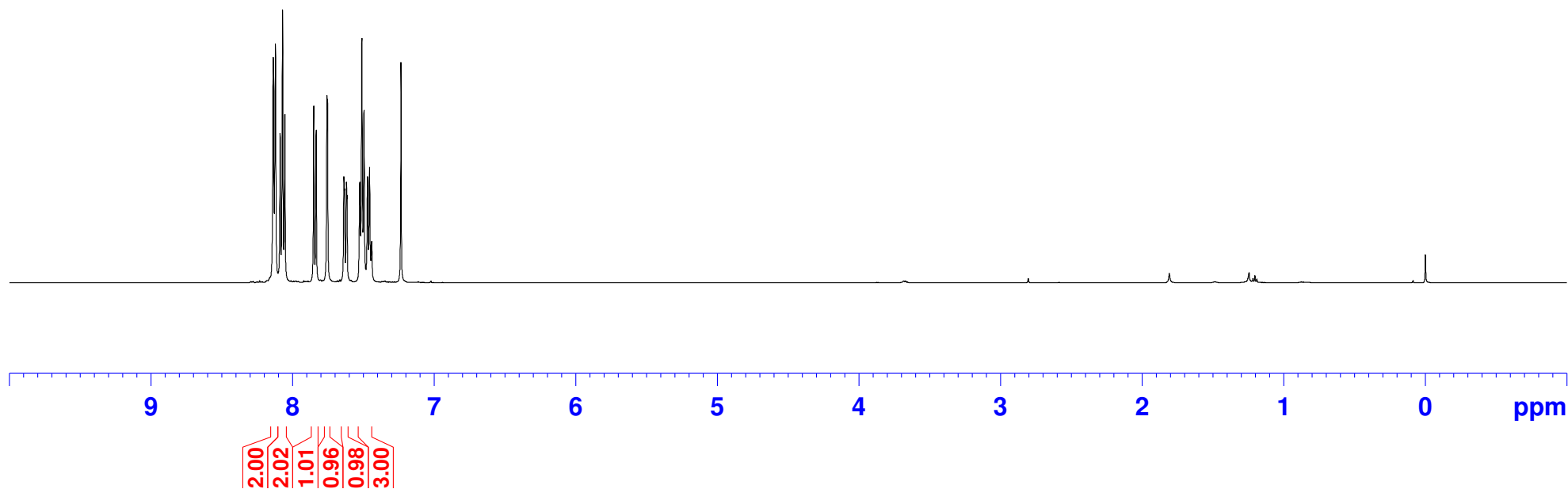
6-chloro-2-phenylquinoline
Proton CDCl₃

8.135
8.120
8.086
8.070
8.054
7.849
7.832
7.756
7.752
7.640
7.636
7.622
7.618
7.527
7.513
7.497
7.473
7.458
7.444



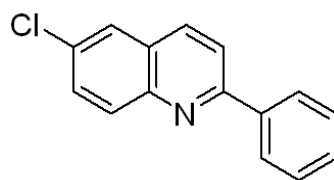
3fa

¹H NMR (500 MHz, CDCl₃)



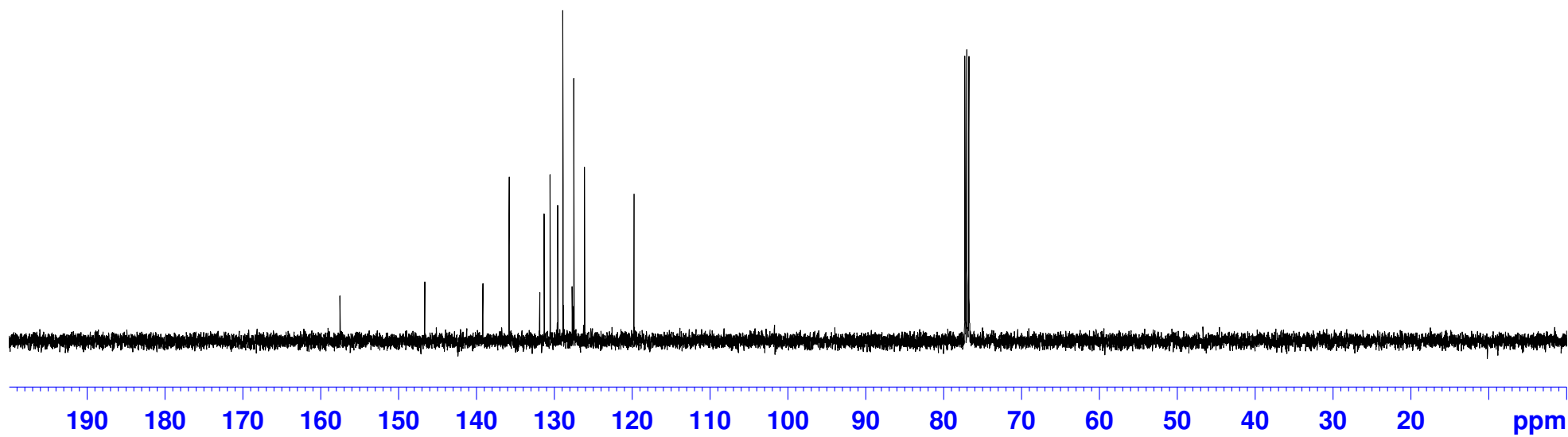
6-chloro-2-phenylquinoline
C13CPD CDCl₃

157.508
146.610
139.162
135.789
131.854
131.285
130.522
129.538
128.868
127.672
127.469
126.094
119.744
77.254
77.000
76.746



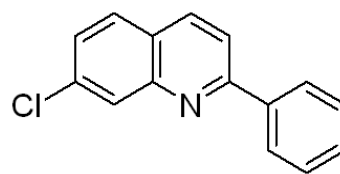
3fa

¹³C {¹H} NMR (125 MHz, CDCl₃)



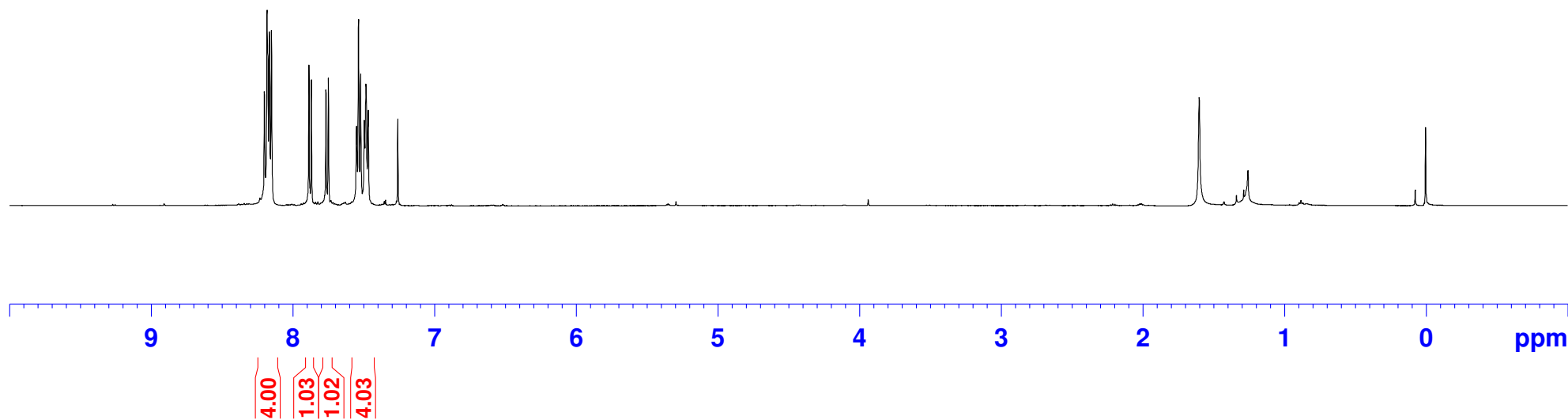
7-chloro-2-phenylquinoline
Proton CDCl₃

8.202
8.183
8.167
8.152
7.888
7.871
7.768
7.751
7.552
7.538
7.522
7.497
7.489
7.485
7.483
7.472
7.468
7.260



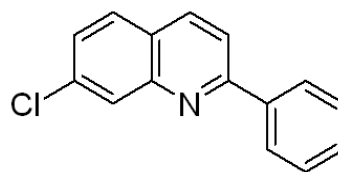
3ga

¹H NMR (500 MHz, CDCl₃)



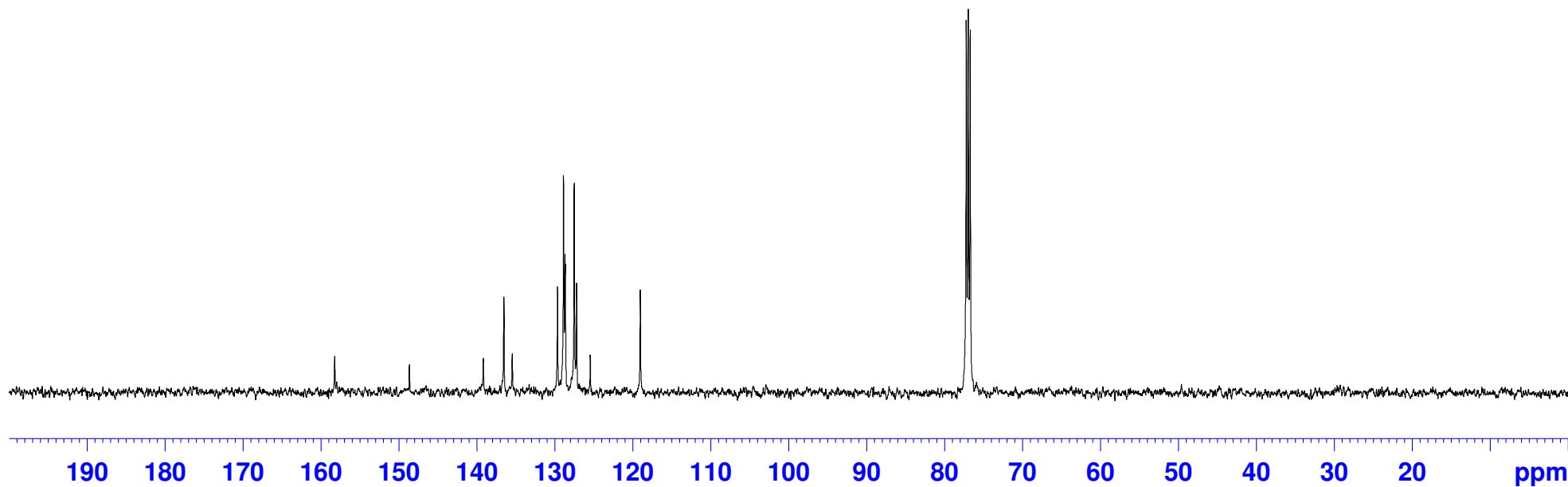
7-chloro-2-phenylquinoline
C13CPD CDCl3

158.219
148.637
139.153
136.517
135.441
129.636
128.867
128.686
127.551
127.245
125.492
119.072
77.253
76.999
76.746



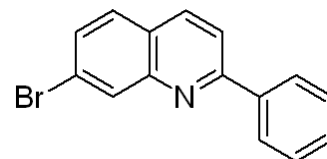
3ga

^{13}C { ^1H } NMR (125 MHz, CDCl_3)



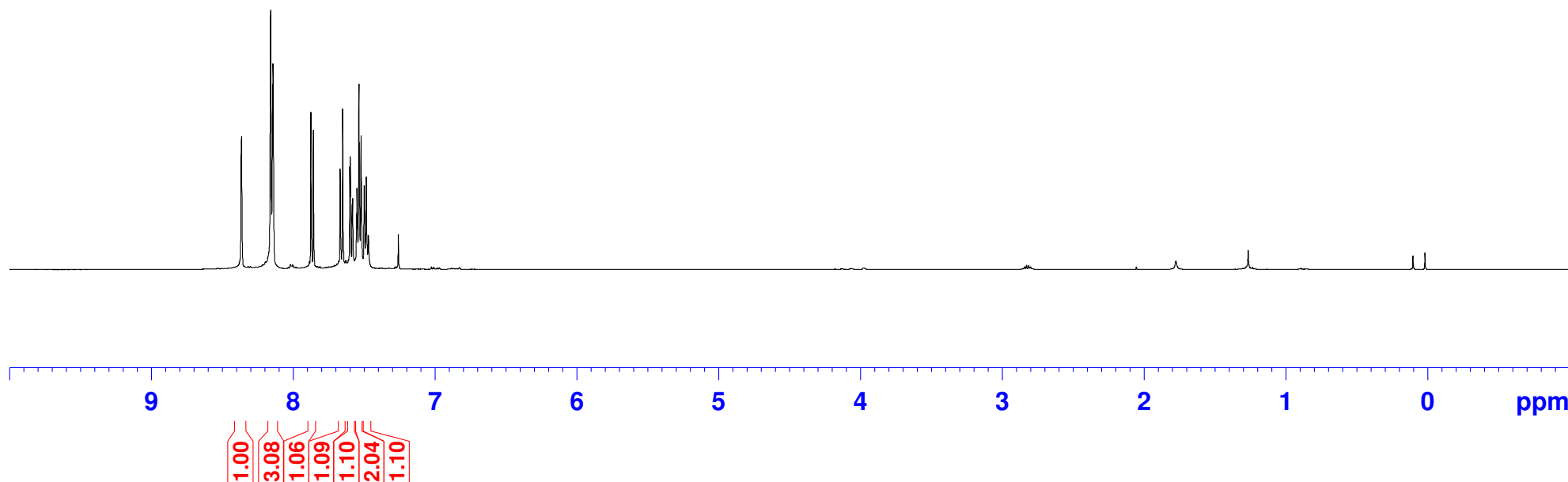
7-bromo-2-phenylquinoline
Proton CDCl₃

8.365
8.163
8.160
8.144
7.876
7.859
7.670
7.652
7.602
7.598
7.585
7.581
7.551
7.537
7.535
7.522
7.499
7.497
7.489
7.485
7.480
7.470
7.260



3ha

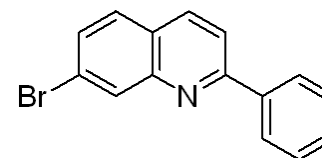
¹H NMR (500 MHz, CDCl₃)



7-bromo-2-phenylquinoline
C13CPD CDC13

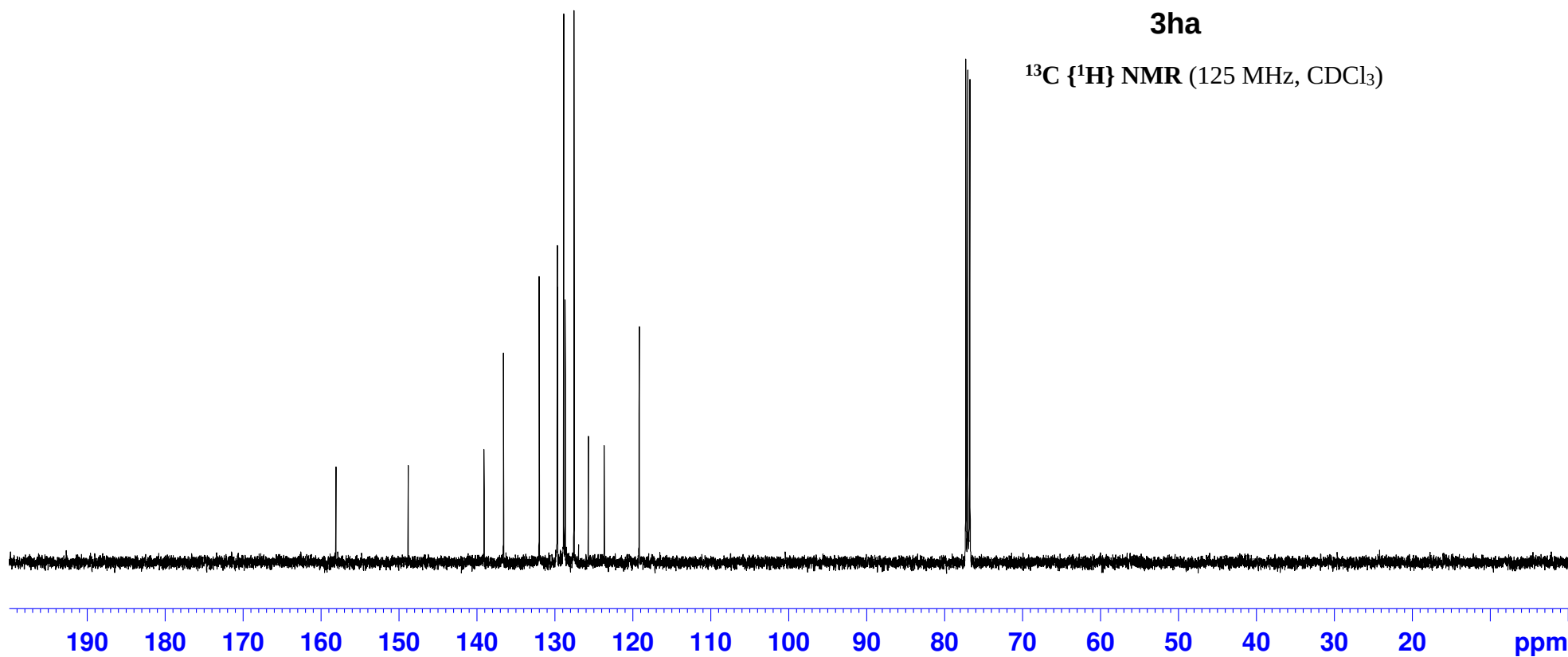
158.068
148.807
139.060
136.565
131.981
129.676
129.629
128.845
128.650
127.512
125.683
123.651
119.157

77.253
76.999
76.744



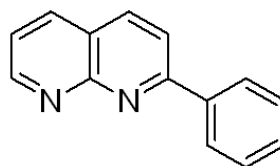
3ha

^{13}C { ^1H } NMR (125 MHz, CDCl_3)



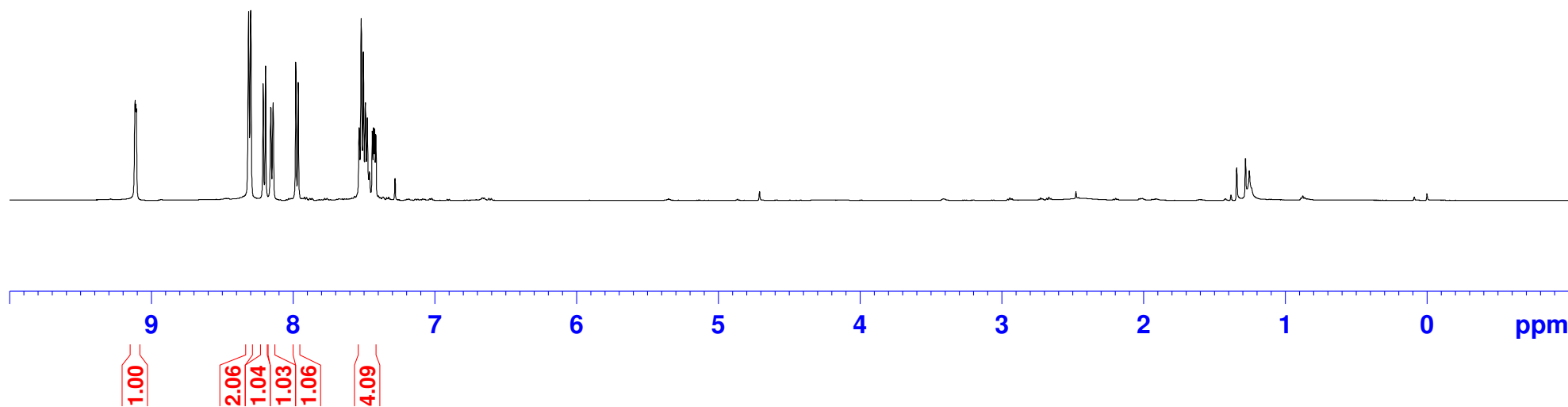
2-phenyl-1,8-naphthyridine
Proton CDCl₃

9.113
9.108
9.105
8.315
8.300
8.212
8.195
8.158
8.142
7.982
7.965
7.535
7.520
7.505
7.491
7.477
7.463
7.442
7.433
7.426
7.417



3ia

¹H NMR (500 MHz, CDCl₃)

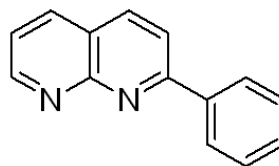


2-phenyl-1,8-naphthyridine
C13CPD CDC13

160.082
155.944
153.678

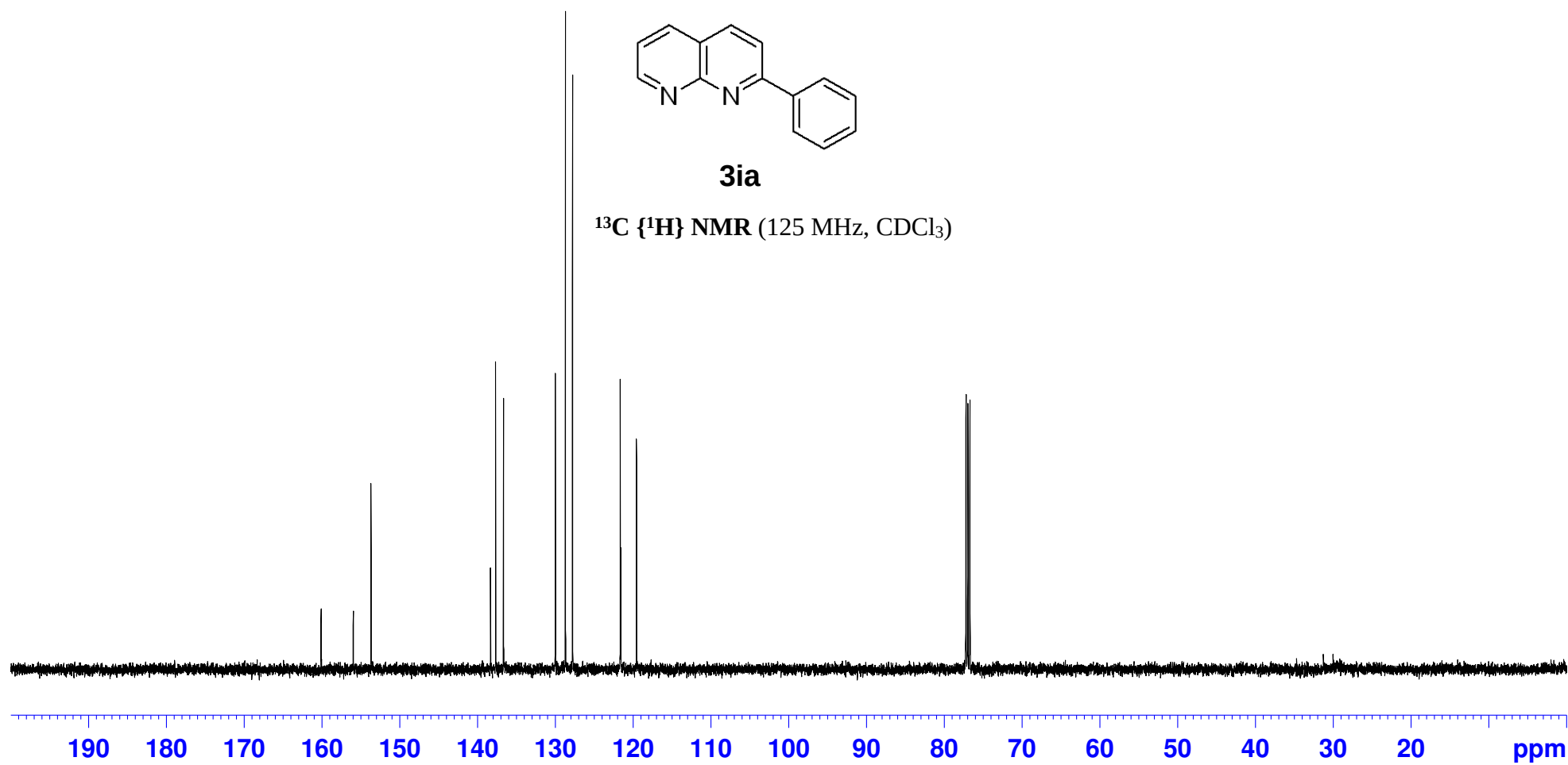
138.314
137.653
136.638
129.983
128.679
127.769
121.637
121.544
119.548

77.239
76.984
76.730



3ia

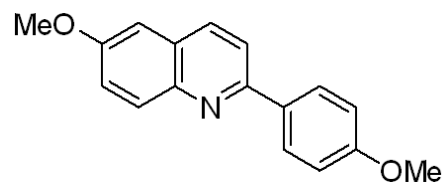
^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



6-methoxy-2-(4-methoxyphenyl)quinoline
Proton CDCl₃

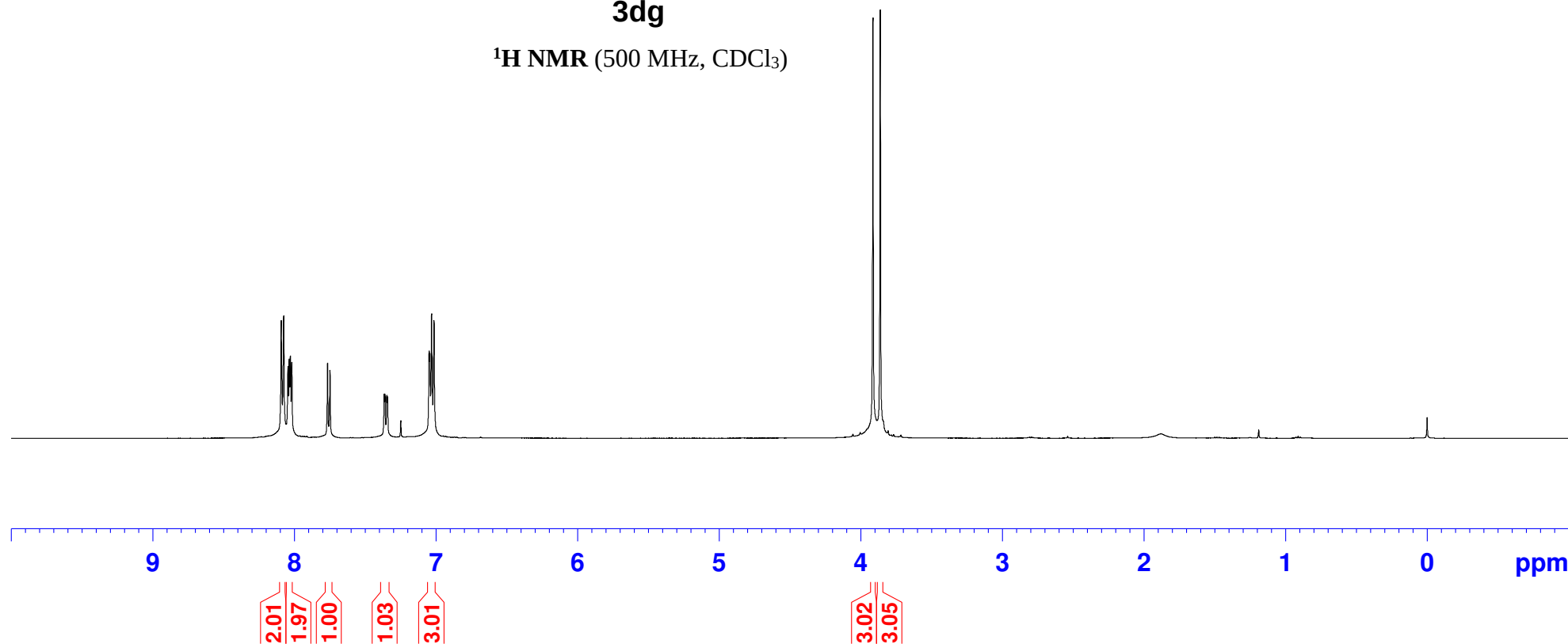
8.094
8.076
8.046
8.037
8.029
8.019
7.767
7.749
7.366
7.361
7.348
7.343
7.049
7.044
7.032
7.015

3.914
3.863



3dg

¹H NMR (500 MHz, CDCl₃)



6-methoxy-2-(4-methoxyphenyl)quinoline
C13CPD CDCl3

160.376
157.281
154.547

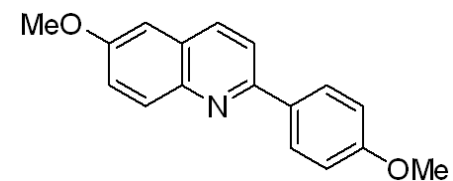
144.209

135.266
132.284
130.824
128.411
127.652
122.003
118.654
114.051

104.957

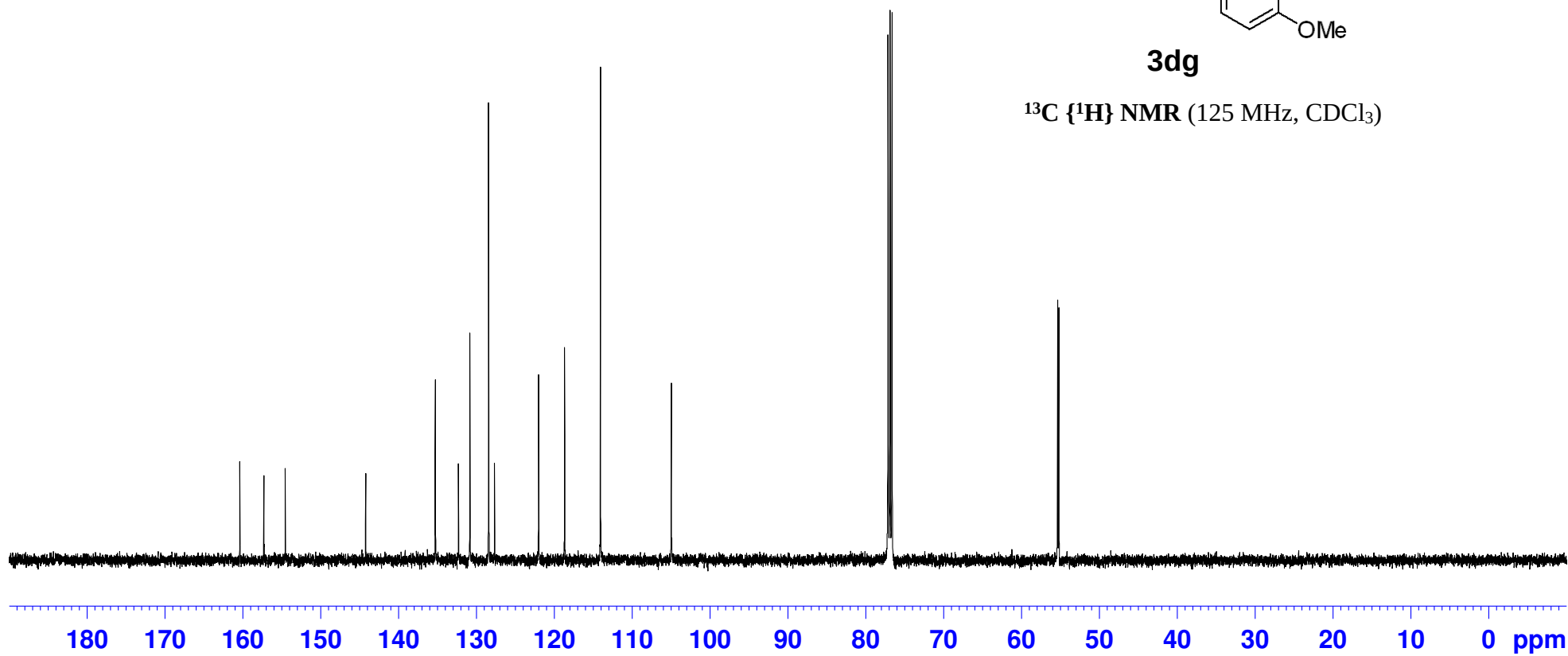
77.170
76.916
76.662

55.388
55.243

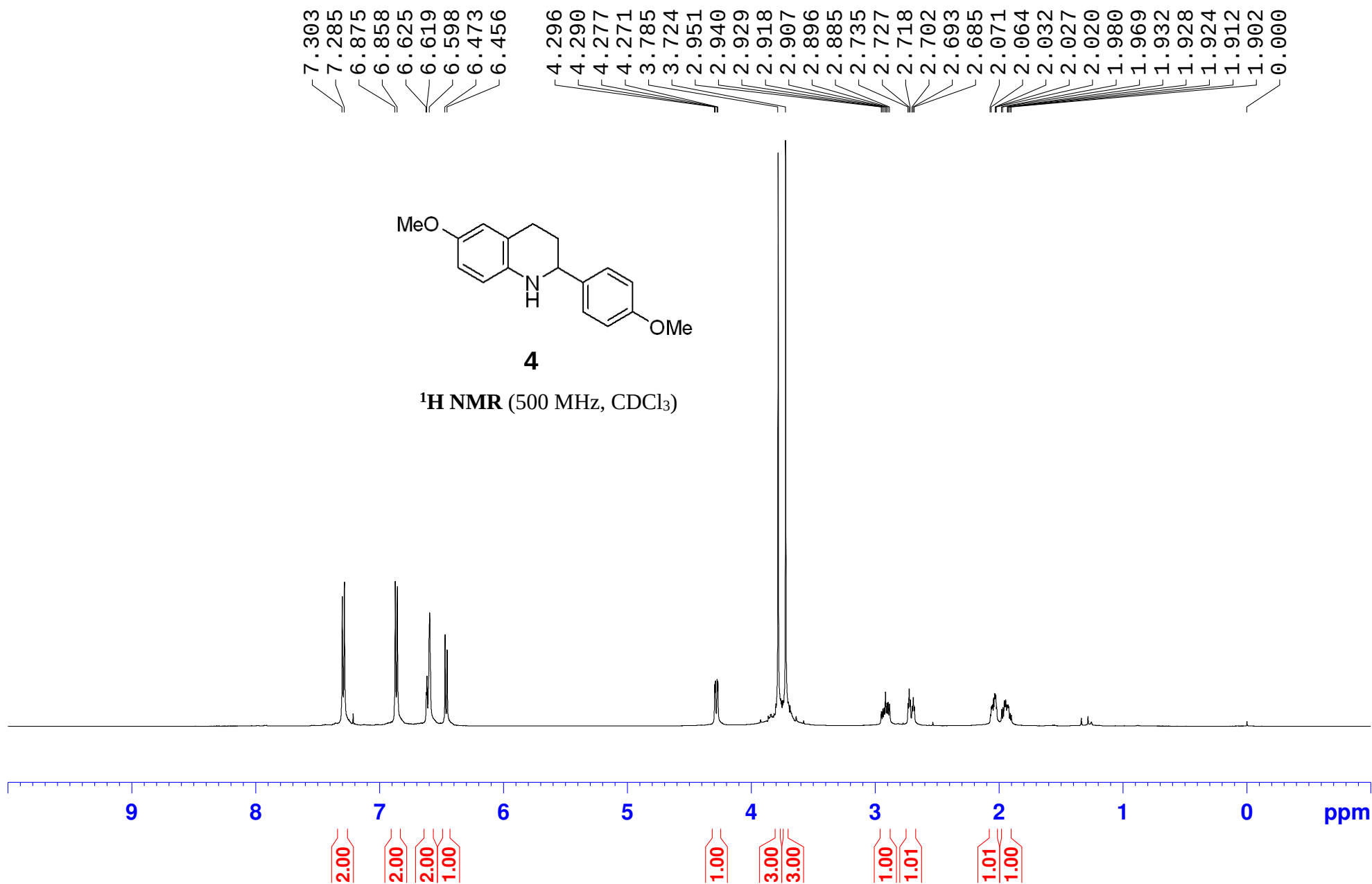


3dg

^{13}C { ^1H } NMR (125 MHz, CDCl_3)

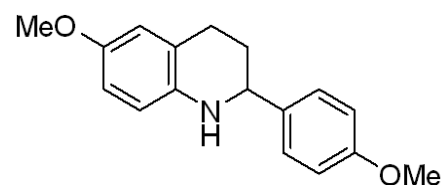


6-methoxy-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoline
Proton CDCl₃

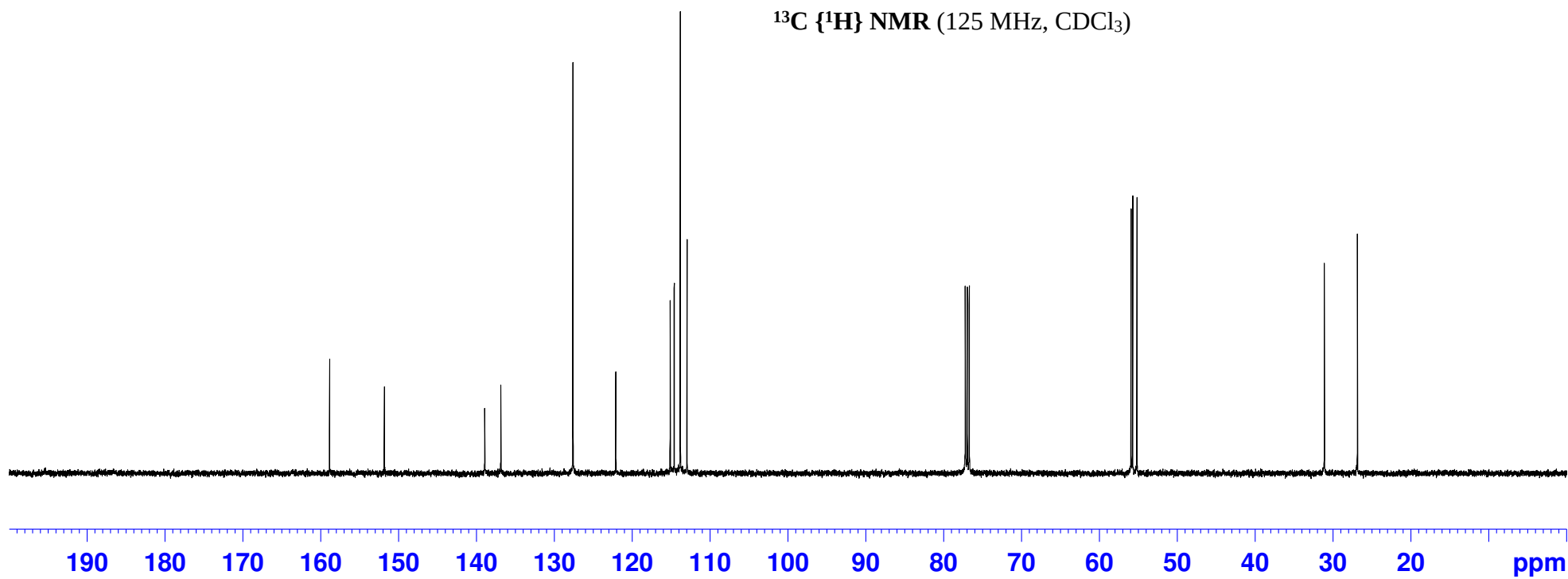


6-methoxy-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoline
C13CPD CDCl3

— 158.841
— 151.807
— 138.916
— 136.851
— 127.589
— 122.086
— 115.102
— 114.585
— 113.800
— 112.934
— 77.000
— 55.961
— 55.745
— 55.209
— 31.139
— 26.893

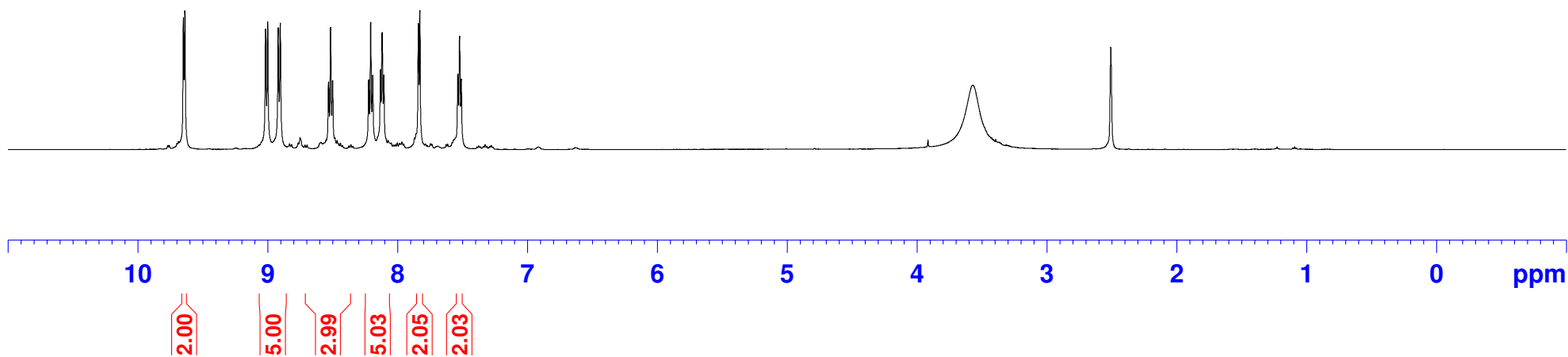
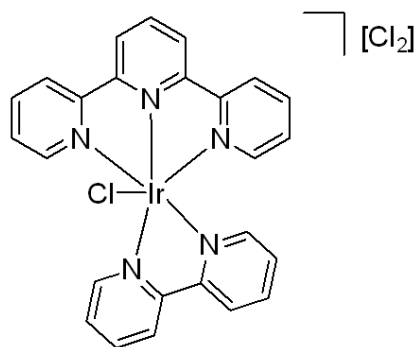


^{13}C { ^1H } NMR (125 MHz, CDCl_3)



[Ir(tpy)(bpy)Cl] [Cl₂]
Proton DMSO-d₆

9.647
9.636
9.066
9.015
8.999
8.917
8.901
8.588
8.533
8.517
8.502
8.484
8.467
8.224
8.208
8.193
8.133
8.120
8.107
8.074
7.841
7.830
7.537
7.524
7.511



[Ir(tpy)(bpy)Cl][Cl₂]
C13CPD DMSO-d₆

157.788
157.636
151.276
151.205
141.568
141.012
128.982
128.881
125.514
125.383

40.311
40.144
39.977
39.810
39.643
39.476
39.308

