Supporting Information

Copper Promoted Synthesis of Substituted Quinolines from Benzylic Azides and Alkynes

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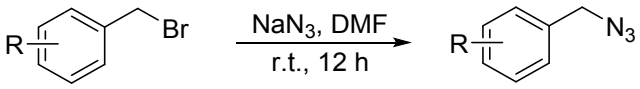
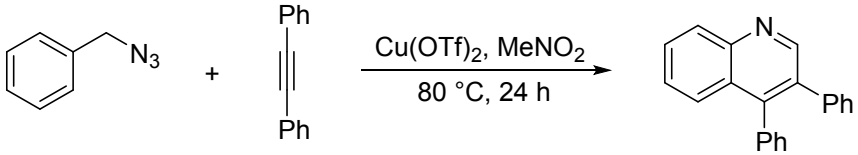
General procedure for the synthesis of benzylic azides[1]



Substituted benzyl bromides (1.0 equiv.) and sodium azide (1.5 equiv.) were dissolved in DMF (2.0 mL/mmol) and stirred at 30 °C for 12 h. At the end of the reaction, the mixture was diluted with water and extracted with diethyl ether. The combined solution was concentrated in vacuo and the mixture was purified by a silica gel column (hexane/EtOAc, 90:10) to afford benzyl azide derivatives.

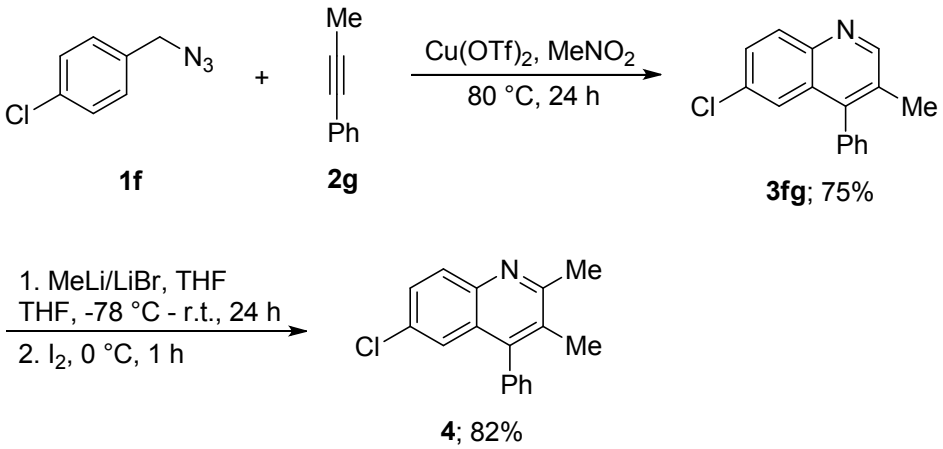
Typical procedure for the synthesis of quinolines



1a **2a** **3aa**

A sealed tube that contained $Cu(OTf)_2$ (254 mg, 0.70 mmol) and diphenylacetylene **2a** (100 mg, 0.56 mmol) was evacuated and purged with nitrogen gas three times. Then, a solution of benzyl azide **1a** (38 mg, 0.28 mmol) in $MeNO_2$ (2.0 mL) was added to the system by syringe under a nitrogen atmosphere and the reaction was stirred at 80 °C for 24 h. At the end of the reaction, the mixture was diluted with CH_2Cl_2 (10 mL), filtered through a Celite pad, and washed three times with CH_2Cl_2 (3 X 20 mL). The combined filtrate was concentrated in vacuo and the mixture was purified by a silica gel column (Hexane/EtOAc, 95:5) to afford the desired pure product **3aa** in 91% (71 mg) yield.

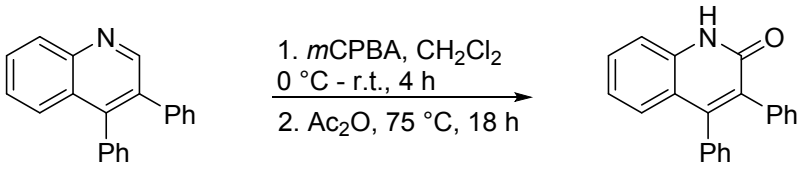
Synthesis of biologically active compound 4[2]



Compound **3fg** was synthesized in 75% yield from 1-(azidomethyl)-4-chlorobenzene (**1f**) and phenylpropyne (**2g**) using a similar procedure for the synthesis of quinoline **3aa**.

Compound **3fg** (110 mg, 0.43 mmol) was dissolved in THF (4.0 mL) and MeLi/LiBr (0.40 mL (2.2 M), 0.87 mmol) was added to the solution at -78 °C. The mixture was allowed to warm to room temperature for 24 h. At the end of the reaction, the mixture was added iodine (328 mg, 1.29 mmol) at 0 °C, stirred for 1 h and then quenched with saturated sodium thiosulfate solution (10 mL). The resulted biphasic solution was extracted with EtOAc (3 X 30 mL). The combined organic solution was concentrated in vacuo and the mixture was purified by a silica gel column (hexane/EtOAc, 95:5) to afford the desired pure product **4** in 82% (94 mg) yield.

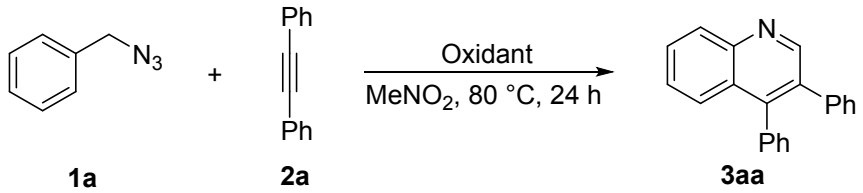
Synthesis of 3,4-diphenylquinolin-2(1*H*)-one 5[3]



3aa **6**, 52%

Compound **3aa** (100 mg, 0.36 mmol) was dissolved in CH_2Cl_2 (4.0 mL) and *meta*-chloroperoxybenzoic acid (*m*CPBA, 134 mg, 0.54 mmol) was added to the solution at 0 °C and stirred for 4 h at the same temperature. After that the reaction was quenched with saturated sodium bicarbonate solution (5 mL). The resulted biphasic solution was extracted by CH_2Cl_2 (3 X 10 mL) and the combined organic layer was dried over $MgSO_4$ and concentrated by rotary evaporation. The crude product was dissolved in Ac_2O (3.0 mL) and heated at 75 °C for 18 h. At the end of the reaction, the mixture was quenched with saturated sodium bicarbonate solution and extracted with CH_2Cl_2 (3 X 10 mL). The combined solution was dried over $MgSO_4$ and concentrated in vacuo and the mixture was purified by a silica gel column (hexane/EtOAc, 75:25) to afford the desired pure product **5** in 52% (55 mg) yield.

Table S1. Effect of oxidant in the synthesis of 3,4-diphenylquinoline[a]

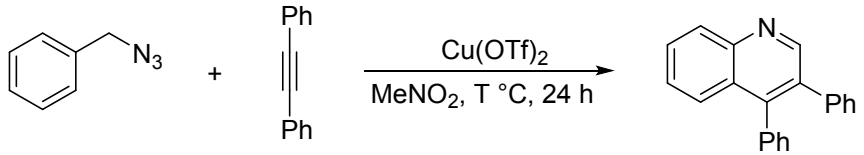


1a **2a** **3aa**

Entry	Oxidant	Yield (%)[b]
1	$Cu(OAc)_2 \cdot H_2O$	--
2	$Cu(OAc)_2$	--
3	$Cu(OTf)_2$	36
4	$Cu(OCOCF_3)_2 \cdot H_2O$	trace
5	$CuSO_4$	--
6	$CuSO_4 \cdot 5H_2O$	--
7	$Cu(BF_4)_2 \cdot 6H_2O$	33
8	CuF_2	--
9	$CuCl_2$	--
10	$CuCl_2 \cdot 2H_2O$	--
11	$CuBr_2$	--
12	$Cu(NO_3)_2 \cdot 3H_2O$	--
13	CuI, O_2	--[c]
14	CuBr, O_2	--[c]
15	CuCl, O_2	--[c]
16	CuOAc, O_2	--[c]
17	$FeCl_3$, O_2	trace[d]
18	$FeCl_2$, O_2	--[d]
19	$FeBr_3$, O_2	trace[d]
20	$FeBr_2$, O_2	--[d]
21	$Fe(acac)_3$, O_2	--[d]
22	$InCl_3$, O_2	trace[d]
23	$In(OTf)_3$, O_2	6[d]

[a]Except otherwise mentioned, all reactions were carried out using benzyl azide **1a** (0.34 mmol), diphenylacetylene **2a** (0.28 mmol), oxidant (0.56 mmol) and $MeNO_2$ (2.0 mL) at 100 °C for 24 h. [b]Isolated yields calculated based on diphenylacetylene. [c]Reaction was carried out with Cu(I) (0.28 mmol) under O_2 (1 atm). [d]Reaction was carried out with oxidant (0.028 mmol) under O_2.

Table S2. Effect of the amount of $Cu(OTf)_2$ in the synthesis of 3,4-diphenylquinoline[a]

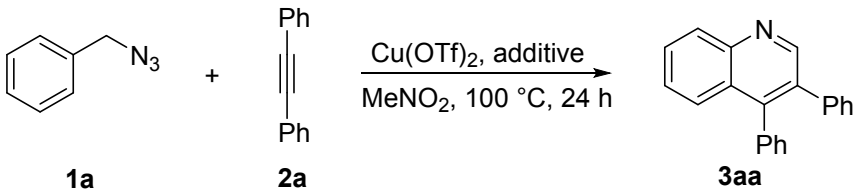


1a **2a** **3aa**

Entry	$Cu(OTf)_2$ (equiv)	T °C	Yield (%)[b]
1	2.0	100	63[c]
2	2.0	100	77
3	3.0	100	92
4	4.0	100	87
5	3.0	80	89
6	3.0	60	80
7	2.5	80	93
8	1.0, O_2	80	45[d]

[a]All reactions were carried out using benzyl azide **1a** (0.28 mmol), diphenylacetylene **2a** (0.56 mmol) and $MeNO_2$ (2.0 mL) for 24 h. [b]Isolated yields were calculated based on benzyl azide. [c]The reaction was carried out using diphenylacetylene **2a** (0.34 mmol). [d]The reaction was carried out with $Cu(OTf)_2$ (0.28 mmol) under O_2.

Table S3. Effect of oxidants in the synthesis of 3,4-diphenylquinoline[a]

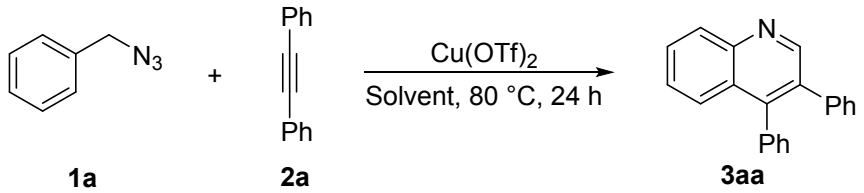


1a **2a** **3aa**

Entry	Additive	Yield (%)[b]
1	$K_2S_2O_8$	49
2	$Na_2S_2O_8$	49
3	$(NH_4)_2S_2O_8$	52
4	*m*CPBA	18
5	DTBP	trace
6	BQ	24
7	$PhI(OAc)_2$	19
8	TBHP	trace
9	H_2O_2	19
10	Oxone	26
11	IBX	17

[a]All reactions were carried out using benzyl azide **1a** (0.28 mmol), diphenylacetylene **2a** (0.56 mmol), $Cu(OTf)_2$ (0.14 mmol), additive (0.34 mmol) and $MeNO_2$ (2.0 mL) at 100 °C for 24 h. [b]Isolated yields were calculated based on benzyl azide.

Table 4. Effect of solvent on the synthesis of 3,4-diphenylquinoline[a]



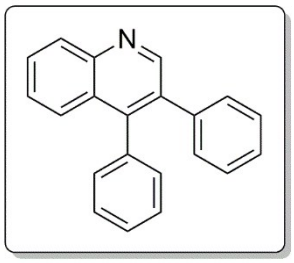
1a **2a** **3aa**

Entry	Additive	Yield(%)[b]
1	EtOH	0
2	Acetone	0
3	$MeNO_2$	93
4	EtOAc	36
5	DCE	22
6	THF	0
7	$PhNO_2$	60
8	TFE	75
9	DMSO	0
10	DMA	0

*a*All reactions were carried out using benzyl azide **1a** (0.28 mmol), diphenylacetylene **2a** (0.56 mmol), $Cu(OTf)_2$ (0.70 mmol) and $MeNO_2$ (2.0 mL) at 80 ^oC for 24 h. *b*Isolated yields were calculated based on benzyl azide.

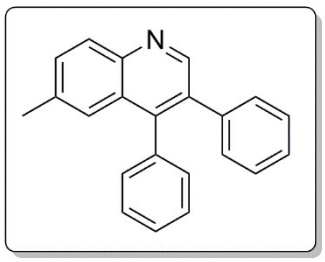
^{1}H, and ^{13}C NMR, HRMS and IR Data

3,4-Diphenylquinoline (3aa)



Yellow solid: m.p. 135-137 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.99 (s, 1 H), 8.18 (d, *J* = 8.4 Hz, 1 H), 7.74-7.64 (m, 2 H), 7.49-7.43 (m, 1 H), 7.37-7.30 (m, 3 H), 7.23-7.14 (m, 7 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.8 (*C*H), 147.5 (C), 145.5 (C), 138.1 (C), 136.3 (C), 133.1 (C), 130.5 (2 *C*H), 130.1 (2 *C*H), 129.5 (*C*H), 129.1 (*C*H), 128.1 (2 *C*H), 128.0 (2 *C*H), 127.7 (*C*H), 127.2 (C), 127.0 (*C*H), 126.8 (*C*H), 126.6 (*C*H); **HRMS** (FAB) cal for $C_{21}H_{15}N$ [M^+] 281.1204, found 281.1204; **IR** (KBr): 2923, 2854, 1727, 1565, 1488, 1442, 1380, 1272, 1072, 1025, 763 and 701 cm^{-1}.

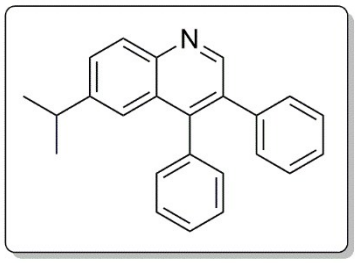
6-Methyl-3,4-diphenylquinoline (3ba)



Yellow solid: m.p. 176-178 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.92 (s, 1 H), 8.07 (d, *J* = 8.8 Hz, 1 H), 7.53 (dd, *J* = 8.8, 2.0 Hz, 1 H), 7.43-7.41 (m, 1 H), 7.35-7.31 (m, 3 H), 7.22-7.16 (m, 5 H), 7.15-7.12 (m, 2 H), 2.42 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.9 (*C*H), 146.1 (C), 144.8 (C), 138.3 (C), 136.8 (C), 136.4 (C), 133.1 (C), 131.3 (*C*H), 130.5 (2 *C*H), 130.1 (2 *C*H), 129.2 (*C*H), 128.1 (2 *C*H), 127.9 (2 *C*H), 127.6 (*C*H), 127.1 (C), 126.9 (*C*H), 125.2 (*C*H), 21.8 (CH_3); **HRMS** (EI) cal for $C_{22}H_{17}N$ [M^+] 295.1361, found 295.1364; **IR** (KBr): 3054, 2923, 2861, 1604, 1496,

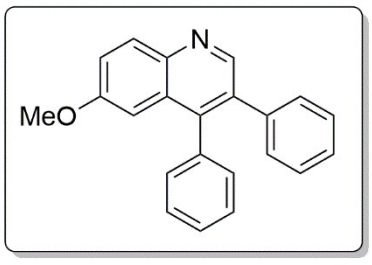
1450, 1373, 1249, 825, 755 and 701 cm^{-1}.

6-Isopropyl-3,4-diphenylquinoline (3ca)



Yellow solid: m.p. 122-124 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.93 (s, 1 H), 8.12 (d, *J* = 8.4 Hz, 1 H), 7.63 (dd, *J* = 8.4, 1.6 Hz, 1 H), 7.46 (d, *J* = 1.6 Hz, 1 H), 7.36-7.31 (m, 3 H), 7.23-7.18 (m, 5 H), 7.16-7.13 (m, 2 H), 3.03-2.92 (m, 1 H), 1.23 (d, *J* = 7.2 Hz, 6 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.9 (*C*H), 147.5 (C), 146.5 (C), 145.0 (C), 138.3 (C), 136.4 (C), 133.1 (C), 130.5 (2 *C*H), 130.1 (2 *C*H), 129.4 (*C*H), 128.5 (*C*H), 128.1 (2 *C*H), 127.9 (2 *C*H), 127.6 (*C*H), 127.1 (C), 126.9 (*C*H), 122.8 (*C*H), 34.3 (*C*H), 23.8 (2 CH_3); **HRMS** (EI) cal for $C_{24}H_{21}N$ [M^+] 323.1674, found 323.1675; **IR** (KBr): 2954, 2923, 2816, 1735, 1604, 1496, 1457, 1373, 1257, 1103, 833, 763 and 701 cm^{-1}.

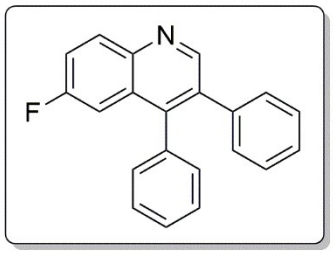
6-Methoxy-3,4-diphenylquinoline (3da)



Yellow solid: m.p. 102-104 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.83 (s, 1 H), 8.07 (d, *J* = 8.8 Hz, 1 H), 7.38-7.31 (m, 4 H), 7.22-7.17 (m, 5 H), 7.16-7.12 (m, 2 H), 6.93 (d, *J* = 2.8 Hz, 1 H), 3.71 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 158.1 (C), 149.4 (*C*H), 144.2 (C), 143.8 (C), 138.4 (C), 136.6 (C), 133.4 (C), 130.9 (*C*H), 130.4 (2 *C*H),

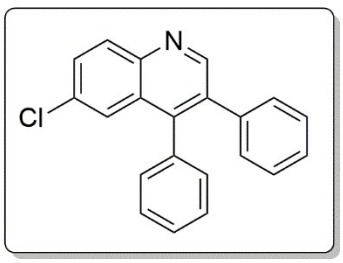
130.1 (2 *C*H), 128.2 (2 *C*H, C), 127.9 (2 *C*H), 127.7 (*C*H), 126.9 (*C*H), 121.4 (*C*H), 104.6 (*C*H), 55.4 (*C*H$_3$); **HRMS** (FAB) [M+H]$^+$ cal for $C_{22}H_{18}ON$ 312.1388, found 312.1387; **IR** (KBr): 2877, 1720, 1619, 1527, 1450, 1349, 1226, 1103, 941, 809 and 732 cm^{-1}.

6-Fluoro-3,4-diphenylquinoline (3ea)



Yellow solid: m.p. 168-170 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.95 (s, 1 H), 8.17 (dd, *J* = 9.2, 5.6 Hz, 1 H), 7.49-7.43 (m, 1 H), 7.36-7.26 (m, 4 H), 7.23-7.20 (m, 3 H), 7.18-7.13 (m, 4 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 160.8 (d, $J_{C\text{-}F}$ = 246.2 Hz, C), 151.1 (d, $J_{C\text{-}F}$ = 2.7 Hz, *C*H), 144.9 (d, $J_{C\text{-}F}$ = 5.5 Hz, C), 144.6 (d, $J_{C\text{-}F}$ = 0.6 Hz, C), 137.8 (C), 135.8 (C), 133.7 (C), 131.9 (d, $J_{C\text{-}F}$ = 9.2 Hz, *C*H), 130.3 (2 *C*H), 130.0 (2 *C*H), 128.3 (2 *C*H), 128.2 (d, $J_{C\text{-}F}$ = 9.5 Hz, C), 128.1 (2 *C*H), 127.9 (*C*H), 127.2 (*C*H), 119.2 (d, $J_{C\text{-}F}$ = 25.8 Hz, *C*H), 109.9 (d, $J_{C\text{-}F}$ = 23.2 Hz, *C*H); **HRMS** (FAB) [M+H]$^+$ cal for $C_{21}H_{15}FN$ 300.1189, found 300.1189; **IR** (KBr): 3062, 2923, 2869, 1720, 1619, 1504, 1450, 1349, 1257, 1203, 1110, 948, 833, 748 and 701 cm^{-1}.

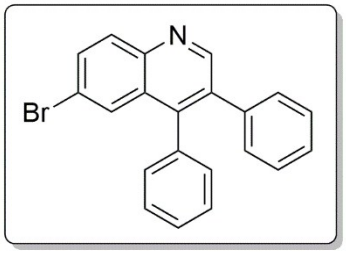
6-Chloro-3,4-diphenylquinoline (3fa)



Yellow solid: m.p. 196-198 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.97 (s, 1 H), 8.11

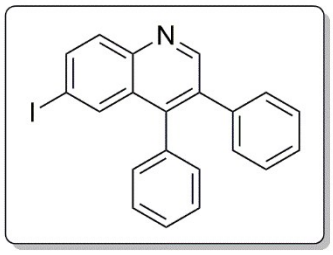
(dd, J = 7.2, 2.4 Hz, 1 H), 7.66-7.61 (m, 2 H), 7.37-7.32 (m, 3 H), 7.23-7.19 (m, 3 H), 7.18-7.12 (m, 4 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.9 (*C*H), 145.9 (C), 144.7 (C), 137.6 (C), 135.5 (C), 133.9 (C), 132.8 (C), 131.1 (*C*H), 130.3 (2 *C*H), 130.0 (2 *C*H), 129.9 (*C*H), 128.3 (2 *C*H), 128.1 (2 *C*H), 128.0 (C), 127.9 (*C*H), 127.2 (*C*H), 125.3 (*C*H); **HRMS** (EI) cal for $C_{21}H_{14}ClN$ [M^+] 315.0815, found 315.0818; **IR** (KBr): 3062, 2923, 2854, 1604, 1481, 1442, 1357, 1265, 1079, 833, 763 and 701 cm^{-1}.

6-Bromo-3,4-diphenylquinoline (3ga)



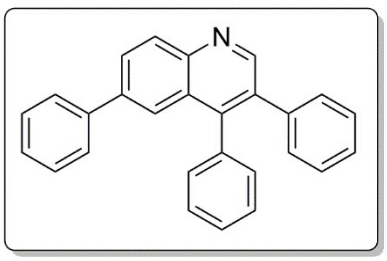
Yellow solid: m.p. 214-216 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.98 (s, 1 H), 8.03 (d, J = 8.8 Hz, 1 H), 7.81 (d, J = 2.0 Hz, 1 H), 7.76 (dd, J = 8.8, 2.0 Hz, 1 H), 7.37-7.33 (m, 3 H), 7.23-7.20 (m, 2 H), 7.18-7.05 (m, 5 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.2 (*C*H), 146.2 (C), 144.6 (C), 137.7 (C), 135.5 (C), 133.9 (C), 132.6 (*C*H), 131.3 (*C*H), 130.4 (2 *C*H), 130.1 (2 *C*H), 128.6 (*C*H), 128.5 (C), 128.4 (2 *C*H), 128.1 (2 *C*H), 128.0 (*C*H), 127.3 (*C*H), 121.1 (C); **HRMS** (EI) cal for $C_{21}H_{14}BrN$ [M^+] 359.0310, found 359.0310; **IR** (KBr): 3062, 2923, 2854, 1666, 1596, 1481, 1442, 1357, 1257, 1064, 971, 902, 833, 763 and 701 cm^{-1}.

6-Iodo-3,4-diphenylquinoline (3ha)



Yellow solid: m.p. 181-183 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.97 (s, 1 H), 8.02 (d, *J* = 1.6 Hz, 1 H), 7.94 (dd, *J* = 8.8, 1.6 Hz, 1 H), 7.88 (d, *J* = 8.8 Hz, 1 H), 7.36-7.33 (m, 3 H), 7.23-7.21 (m, 3 H), 7.17-7.10 (m, 4 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.3 (*C*H), 146.5 (C), 144.4 (C), 137.9 (*C*H), 137.7 (C), 135.5 (C), 135.3 (*C*H), 133.8 (C), 131.2 (*C*H), 130.4 (2 *C*H), 130.0 (2 *C*H), 128.9 (C), 128.3 (2 *C*H), 128.1 (2 *C*H), 128.0 (*C*H), 127.2 (*C*H), 92.9 (C); **HRMS** (FAB) $[M+H]^+$ cal for $C_{21}H_{15}IN$ 408.0249, found 408.0247; **IR** (KBr): 3062, 2923, 1589, 1481, 1357, 1257, 1079, 1025, 971, 894, 833, 763 and 701 cm^{-1}.

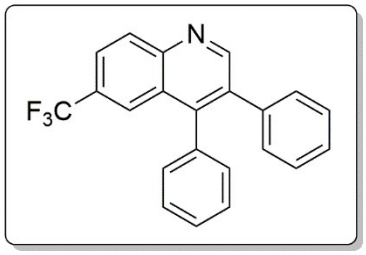
3,4,6-Triphenylquinoline (3ia)



Yellow solid: m.p. 205-207 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.98 (s, 1 H), 8.24 (d, *J* = 8.8 Hz, 1 H), 7.97 (dd, *J* = 8.8, 2.0 Hz, 1 H), 7.86 (d, *J* = 2.0 Hz, 1 H), 7.58-7.52 (m, 2 H), 7.44-7.38 (m, 2 H), 7.36-7.29 (m, 5 H), 7.23-7.20 (m, 4 H), 7.18-7.15 (m, 2 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.8 (*C*H), 146.9 (C), 145.6 (C), 140.6 (C), 139.6 (C), 138.1 (C), 136.2 (C), 133.5 (C), 130.5 (2 *C*H), 130.1 (2 *C*H), 129.9 (*C*H), 128.9 (3 *C*H), 128.2 (2 *C*H), 128.0 (2 *C*H), 127.8 (*C*H), 127.6 (*C*H), 127.4 (2 *C*H), 127.3 (C), 127.0 (*C*H), 124.3 (*C*H); **HRMS** (EI) cal for $C_{27}H_{19}N$ $[M^+]$ 357.1517,

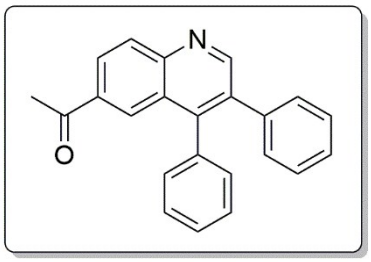
found 357.1515; **IR** (KBr): 3054, 2923, 2854, 1658, 1604, 1481, 1365, 1257, 1079, 1025, 917, 840, 763 and 701 cm^{-1}.

3,4-Diphenyl-6-(trifluoromethyl)quinoline (3ja)



Yellow solid: m.p. 175-177 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.08 (s, 1 H), 8.29 (d, *J* = 8.8 Hz, 1 H), 7.99 (s, 1 H), 7.87 (d, *J* = 8.8 Hz, 1 H), 7.39-7.34 (m, 3 H), 7.26-7.22 (m, 2 H), 7.21-7.12 (m, 5H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 153.9 (*C*H), 148.5 (C), 146.4 (C), 137.4 (C), 135.2 (C), 134.3 (C), 130.8 (*C*H), 130.4 (2 *C*H), 130.0 (2 *C*H), 128.7 (d, $J_{C\text{-}F}$ = 32.4 Hz, C), 128.4 (2 *C*H), 128.3 (*C*H), 128.2 (2 *C*H), 127.4 (*C*H), 126.5 (C), 124.8 (q, $J_{C\text{-}F}$ = 3.0 Hz, *C*H), 124.5 (q, $J_{C\text{-}F}$ = 4.5 Hz, *C*H), 124.0 (d, $J_{C\text{-}F}$ = 271.1 Hz, C); **HRMS** (EI) cal for $C_{22}H_{14}F_3N$ [M^+] 349.1078, found 349.1080; **IR** (KBr): 3062, 2923, 2854, 1581, 1427, 1373, 1311, 1126, 1064, 840, 763 and 701 cm^{-1}.

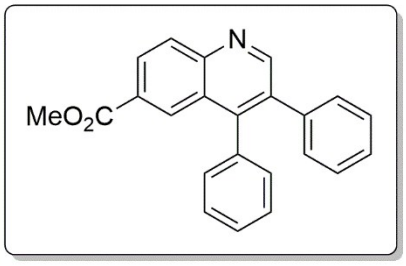
1-(3,4-Diphenylquinolin-6-yl)ethan-1-one (3ka)



Yellow solid: m.p. 169-171 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.06 (s, 1 H), 8.31 (d, *J* = 1.6 Hz, 1 H), 8.25 (dd, *J* = 8.8, 1.6 Hz, 1 H), 8.22 (d, *J* = 8.8 Hz, 1 H), 7.38-7.35 (m, 4 H), 7.25-7.23 (m, 1 H), 7.21-7.18 (m, 3 H), 7.17-7.14 (m, 2 H), 2.54 (s, 3 H);

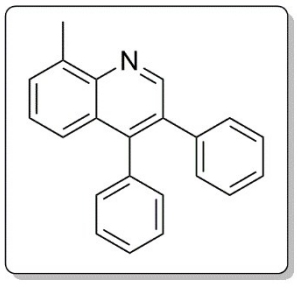
^{13}C NMR (100 MHz, $CDCl_3$): δ 197.6 (C), 154.0 (*C*H), 149.4 (C), 146.9 (C), 137.6 (C), 135.5 (C), 135.2 (C), 134.0 (C), 130.5 (2 *C*H), 130.2 (*C*H), 130.1 (2 *C*H), 128.7 (*C*H), 128.4 (2 *C*H), 128.2 (*C*H), 128.1 (2 *C*H), 127.4 (*C*H), 127.3 (*C*H), 126.6 (C), 26.6 (*C*H_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{23}H_{18}ON$ 324.1388, found 324.1388; **IR** (KBr): 3054, 2923, 1681, 1604, 1488, 1419, 1365, 1249, 840, 763, 701 and 617 cm^{-1}.

Methyl 3,4-diphenylquinoline-6-carboxylate (3la)



Yellow solid: m.p. 168-170 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.05 (s, 1 H), 8.45 (d, *J* = 1.6 Hz, 1 H), 8.28 (dd, *J* = 8.4, 1.6 Hz, 1 H), 8.20 (d, *J* = 8.4 Hz, 1 H), 7.37-7.34 (m, 3 H), 7.23-7.21 (m, 2 H), 7.20-7.12 (m, 5 H), 3.88 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.7 (C), 153.8 (*C*H), 149.3 (C), 146.8 (C), 137.6 (C), 135.4 (C), 133.9 (C), 130.5 (2 *C*H), 130.0 (2 *C*H), 129.9 (*C*H), 129.7 (*C*H), 128.6 (*C*H), 128.4 (C), 128.3 (2 *C*H), 128.1 (2 *C*H), 128.0 (*C*H), 127.3 (*C*H), 126.5 (C), 52.3 (*C*H_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{23}H_{18}O_2N$ 340.1338, found 340.1335; **IR** (KBr): 2923, 2861, 1720, 1596, 1442, 1365, 1249, 1103, 763 and 701 cm^{-1}.

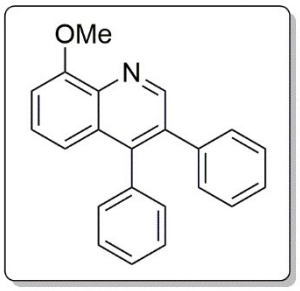
8-Methyl-3,4-diphenylquinoline (3ma)



Yellow solid: m.p. 129-131 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.02 (s, 1 H), 7.58-

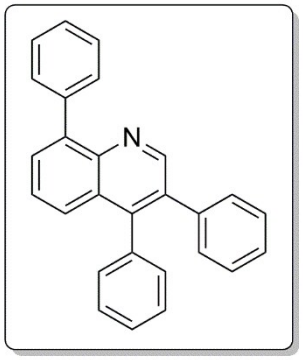
7.49 (m, 2 H), 7.37-7.30 (m, 4 H), 7.23-7.14 (m, 7 H), 2.89 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.5 (*C*H), 146.6 (C), 145.7 (C), 138.3 (C), 137.1 (C), 136.7 (C), 132.8 (C), 130.5 (2 *C*H), 130.1 (2 *C*H), 129.3 (*C*H), 128.0 (2 *C*H), 127.9 (2 *C*H), 127.6 (*C*H), 127.2 (C), 126.9 (*C*H), 126.5 (*C*H), 124.7 (*C*H), 18.4 (CH_3); **HRMS** (EI) cal for $C_{22}H_{17}N$ [M^+] 295.1361, found 295.1359; **IR** (KBr): 2923, 2861, 1820, 1727, 1666, 1596, 1481, 1442, 1380, 1257, 1110, 763, 701 and 593 cm^{-1}.

8-Methoxy-3,4-diphenylquinoline (3na)



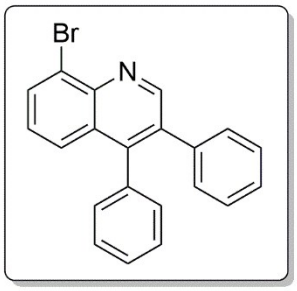
Yellow solid: m.p. 132-134 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.99 (s, 1 H), 7.37 (t, *J* = 8.0 Hz, 1 H), 7.34-7.29 (m, 3 H), 7.23-7.20 (m, 4 H), 7.19-7.13 (m, 4 H), 7.05 (t, *J* = 8.0 Hz, 1 H), 4.12 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 155.6 (C), 150.5 (*C*H), 145.4 (C), 139.6 (C), 138.1 (C), 136.6 (C), 133.7 (C), 130.5 (2 *C*H), 130.1 (2 *C*H), 128.3 (C), 128.1 (2 *C*H), 128.0 (2 *C*H), 127.6 (*C*H), 127.0 (*C*H), 126.8 (*C*H), 118.4 (*C*H), 107.2 (*C*H), 56.1 (CH_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{22}H_{18}ON$ 312.1388, found 312.1386; **IR** (KBr): 2954, 2923, 2869, 1604, 1527, 1457, 1411, 1349, 1257, 1211, 1095, 948, 825 and 732 cm^{-1}.

3,4,8-Triphenylquinoline (3oa)



Yellow solid: m.p. 190-192 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.03 (s, 1 H), 7.76-7.66 (m, 4 H), 7.54-7.49 (m, 3 H), 7.45-7.32 (m, 5 H), 7.23-7.19 (m, 5 H), 7.17-7.14 (m, 1 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.4 (*C*H), 145.5 (C), 145.3 (C), 140.9 (C), 139.8 (C), 138.2 (C), 136.6 (C), 132.8 (C), 130.7 (2 *C*H), 130.5 (2 *C*H), 130.1 (2 *C*H), 129.9 (*C*H), 128.1 (2 *C*H), 128.0 (2 *C*H), 127.9 (2 *C*H), 127.7 (*C*H), 127.6 (C), 127.3 (*C*H), 126.9 (*C*H), 126.4 (*C*H), 126.3 (*C*H); **HRMS** (EI) cal for $C_{27}H_{19}N$ [M^+] 357.1517, found 357.1519; **IR** (KBr): 3054, 2923, 2861, 1951, 1882, 1812, 1727, 1673, 1596, 1481, 1442, 1396, 1265, 1072, 1025, 763 and 701 cm^{-1}.

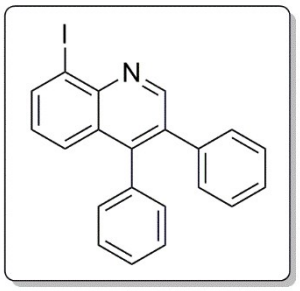
8-Bromo-3,4-diphenylquinoline (3pa)



Yellow solid: m.p. 166-168 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.12 (s, 1 H), 8.04 (dd, *J* = 7.6, 1.2 Hz, 1 H), 7.64 (dd, *J* = 8.4, 1.2 Hz, 1 H), 7.35-7.28 (m, 4 H), 7.26-7.20 (m, 3 H), 7.18-7.12 (m, 4 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.5 (*C*H), 146.1 (C), 144.5 (C), 137.5 (C), 135.9 (C), 133.9 (C), 132.8 (*C*H), 130.4 (2 *C*H), 130.0 (2 *C*H), 128.8 (C), 128.2 (2 *C*H), 128.1 (2 *C*H), 127.9 (*C*H), 127.3 (*C*H), 127.1 (*C*H),

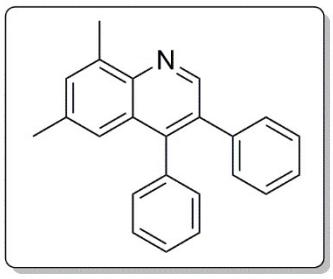
126.6 (*C*H), 124.9 (C); **HRMS** (EI) cal for $C_{21}H_{14}BrN$ [M^+] 359.0310, found 359.0310; **IR** (KBr): 3054, 1727, 1666, 1596, 1473, 1442, 1373, 1257, 1172, 1087, 1025, 987, 763 and 701 cm^{-1}.

8-Iodo-3,4-diphenylquinoline (3qa)



Yellow solid: m.p. 175-177 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.07 (s, 1 H), 8.33 (dd, *J* = 7.2, 0.8 Hz, 1 H), 7.66 (dd, *J* = 8.4, 0.8 Hz, 1 H), 7.35-7.32 (m, 3 H), 7.23-7.21 (m, 3 H), 7.17-7.12 (m, 5 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.7 (*C*H), 146.3 (C), 146.2 (C), 139.7 (*C*H), 137.6 (C), 135.8 (C), 133.9 (C), 130.4 (2 *C*H), 130.0 (2 *C*H), 128.2 (2 *C*H), 128.1 (2 *C*H), 128.0 (C), 127.9 (*C*H), 127.8 (*C*H), 127.6 (*C*H), 127.2 (*C*H), 103.6 (C); **HRMS** (FAB) $[M+H]^+$ cal for $C_{21}H_{15}IN$ 408.0249, found 408.0247; **IR** (KBr): 2923, 2869, 1820, 1589, 1442, 1349, 1257, 1103 and 755 cm^{-1}.

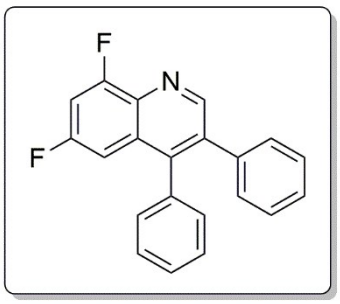
6,8-Dimethyl-3,4-diphenylquinoline (3ra)



Yellow solid: m.p. 102-104 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.95 (s, 1 H), 7.41 (s, 1 H), 7.34-7.31 (m, 3 H), 7.26 (s, 1 H), 7.22-7.13 (m, 7 H), 2.86 (s, 3 H), 2.38 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 149.6 (*C*H), 145.3 (C), 144.9 (C), 138.5 (C), 136.9

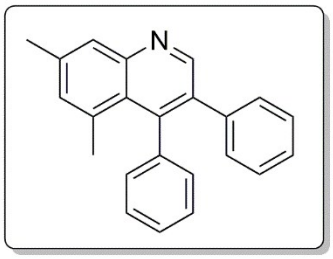
(C), 136.7 (C), 136.3 (C), 132.9 (C), 131.7 (*C*H), 130.5 (2 *C*H), 130.1 (2 *C*H), 128.0 (2 *C*H), 127.9 (2*C*H), 127.4 (*C*H), 127.1 (C), 126.8 (*C*H), 123.3 (*C*H), 21.8 ($C H_3$), 18.3 ($C H_3$); **HRMS** (FAB) $[M+H]^+$ cal for $C_{23}H_{20}N$ 310.1596, found 310.1597; **IR** (KBr): 2954, 2923, 2869, 1720, 1604, 1527, 1457, 1349, 1249, 1095, 948, 825 and 701 cm^{-1}.

6,8-Difluoro-3,4-diphenylquinoline (3sa)



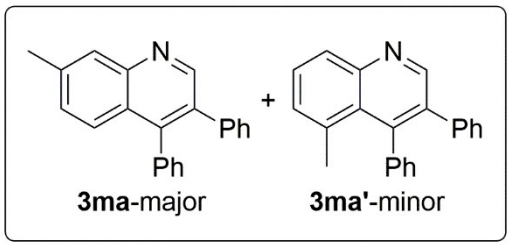
Yellow solid: m.p. 144-146 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.98 (s, 1 H), 7.36-7.32 (m, 3 H), 7.25-7.21 (m, 4 H), 7.17-7.07 (m, 5 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 159.8 (dd, J_{C-F} = 247.0, 11.8 Hz, C), 158.8 (dd, J_{C-F} = 258.6, 11.8 Hz, C), 151.2 (dd, J_{C-F} = 2.6, 1.7 Hz, *C*H), 144.9 (dd, J_{C-F} = 5.7, 3.0 Hz, C), 137.3 (C), 135.4 (C), 135.2 (dd, J_{C-F} = 11.5, 1.7 Hz, C), 134.9 (C), 130.2 (2 *C*H), 129.9 (2 *C*H), 129.1 (dd, J_{C-F} = 10.8, 2.8 Hz, C), 128.4 (2 *C*H), 128.2 (3 *C*H), 127.5 (*C*H), 105.9 (dd, J_{C-F} = 23.0, 4.8 Hz, *C*H), 104.7 (dd, J_{C-F} = 29.5, 22.5 Hz, *C*H); **HRMS** (FAB) $[M+H]^+$ cal for $C_{21}H_{14}F_2N$ 318.1094, found 318.1096; **IR** (KBr): 2923, 1727, 1589, 1481, 1349, 1257, 1110, 748, 678 and 609 cm^{-1}.

5,7-Dimethyl-3,4-diphenylquinoline (3ta)



Yellow solid: m.p. 146-148 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.80 (s, 1 H), 7.84 (s, 1 H), 7.23-7.19 (m, 3 H), 7.17-7.12 (m, 4 H), 7.11-7.08 (m, 2 H), 7.05-7.02 (m, 2 H), 2.50 (s, 3 H), 1.88 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.6 (*C*H), 149.1 (C), 145.6 (C), 139.9 (C), 138.8 (C), 138.6 (C), 135.7 (C), 134.1 (C), 132.9 (*C*H), 130.3 (2 *C*H), 130.2 (2 *C*H), 127.7 (*C*H), 127.6 (2 *C*H), 127.4 (2 *C*H), 127.3 (*C*H), 126.6 (*C*H), 124.0 (C), 24.4 (CH_3), 21.3 (CH_3); **HRMS** (EI) cal for $C_{23}H_{19}N$ [M^+] 309.1517, found 309.1515; **IR** (KBr): 3054, 2923, 2861, 1604, 1573, 1481, 1442, 1357, 1319, 1218, 1072, 1025, 917, 856, 763 and 701 cm^{-1}.

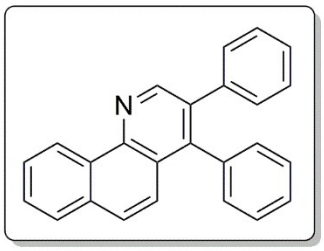
7-Methyl-3,4-diphenylquinoline and 5-Methyl-3,4-diphenylquinoline (3ua and 3ua')



Yellow solid: m.p. 147-149 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.94 (s, 1 H), 8.86 (s, 1 H), 8.06 (d, *J* = 8.4 Hz, 1 H), 7.95 (s, 1 H), 7.60-7.54 (m, 2 H), 7.36-7.25 (m, 7 H), 7.23-7.09 (m, 13 H), 7.07-7.03 (m, 2 H), 2.56 (s, 3 H), 1.92 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.7 (*C*H), 150.6 (*C*H), 148.9 (C), 147.8 (C), 145.8 (C), 145.2 (C), 139.8 (C), 139.4 (C), 138.5 (C), 138.3 (C), 136.5 (C), 136.2 (C), 134.8 (C), 132.4 (C), 130.6 (*C*H), 130.5 (2 *C*H), 130.4 (2 *C*H), 130.2 (2 *C*H), 130.1 (2 *C*H), 129.1 (*C*H),

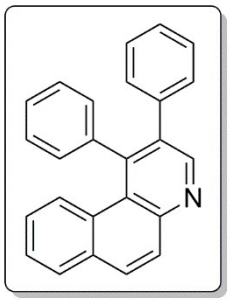
128.8 (*C*H), 128.7 (*C*H), 128.5 (*C*H), 128.1 (2 *C*H), 127.9 (2 *C*H), 127.7 (2 *C*H), 127.6 (*C*H), 127.4 (2 *C*H), 127.3 (*C*H), 126.9 (*C*H), 126.7 (*C*H), 126.2 (*C*H), 126.0 (C), 125.2 (C), 24.5 (*C*H_3), 21.7 (*C*H_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{22}H_{18}N$ 296.1439, found 296.1441; **IR** (KBr): 3054, 2923, 2869, 1573, 1527, 1488, 1442, 1349, 1072, 917, 825, 763 and 701 cm^{-1}.

3,4-Diphenylbenzo[*h*]quinoline (3va)



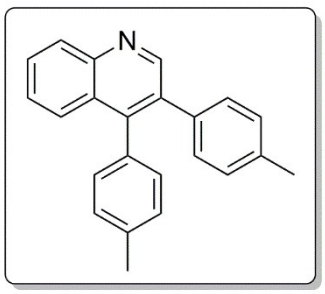
Yellow solid: m.p. 159-161 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.36 (d, *J* = 8.4 Hz, 1 H), 9.06 (s, 1 H), 7.88 (d, *J* = 6.8 Hz, 1 H), 7.78-7.66 (m, 3 H), 7.56 (d, *J* = 9.2 Hz, 1 H), 7.37-7.33 (m, 3 H), 7.23-7.16 (m, 7 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 149.8 (*C*H), 145.8 (C), 145.7 (C), 138.2 (C), 136.7 (C), 134.1 (C), 133.2 (C), 131.5 (C), 130.6 (2 *C*H), 130.2 (2 *C*H), 128.2 (*C*H), 128.1 (2 *C*H), 128.0 (2 *C*H), 127.8 (*C*H), 127.6 (2 *C*H), 127.2 (*C*H), 126.9 (*C*H), 124.8 (C), 124.6 (*C*H), 123.7 (*C*H); **HRMS** (EI) cal for $C_{25}H_{17}N$ $[M^+]$ 331.1361, found 331.1361; **IR** (KBr): 3054, 2923, 2854, 1812, 1727, 1596, 1442, 1257, 1087, 1025, 802, 748 and 701 cm^{-1}.

1,2-Diphenylbenzo[*f*]quinoline (3wa)



Yellow solid: m.p. 218-220 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.92 (s, 1 H), 8.04 (d, *J* = 8.8 Hz, 1 H), 7.97 (d, *J* = 8.8 Hz, 1 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.47-7.41 (m, 2 H), 7.33-7.28 (m, 3 H), 7.23-7.17 (m, 4 H), 7.12-7.10 (m, 2 H), 7.08-7.04 (m, 2 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.2 (*C*H), 148.8 (C), 145.8 (C), 140.1 (C), 138.3 (C), 135.5 (C), 133.4 (C), 131.5 (*C*H), 130.2 (C), 130.1 (2 *C*H), 129.8 (2 *C*H), 128.9 (2 *C*H), 128.7 (*C*H), 128.6 (*C*H), 128.3 (*C*H), 127.7 (2 *C*H), 127.6 (*C*H), 126.8 (*C*H), 126.5 (*C*H), 125.4 (*C*H), 123.7 (C); **HRMS** (EI) cal for $C_{25}H_{17}N$ [M^+] 331.1361, found 331.1361; **IR** (KBr): 3046, 2923, 2861, 1596, 1488, 1442, 1349, 1110, 1072, 833, 755 and 701 cm^{-1}.

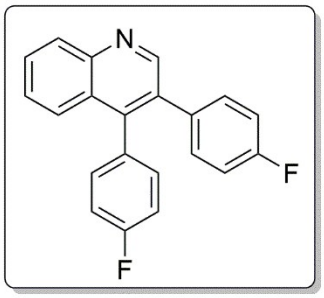
3,4-Di-*p*-tolylquinoline (3ab)



Yellow solid: m.p. 155-157 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.95 (s, 1 H), 8.15 (d, *J* = 8.8 Hz, 1 H), 7.70-7.66 (m, 2 H), 7.44 (t, *J* = 7.6 Hz, 1 H), 7.14 (d, *J* = 8.0 Hz, 2 H), 7.07 (d, *J* = 8.0 Hz, 2 H), 7.05-7.04 (m, 4 H), 2.37 (s, 3 H), 2.29 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.0 (*C*H), 147.4 (C), 145.4 (C), 137.3 (C), 136.7 (C),

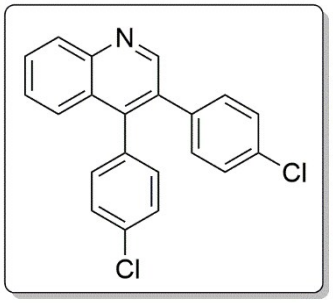
135.3 (C), 133.3 (C), 133.0 (C), 130.4 (2 *C*H), 129.9 (2 *C*H), 129.4 (*C*H), 128.9 (3 *C*H), 128.8 (2 *C*H), 127.5 (C), 126.7 (*C*H), 126.6 (*C*H), 21.3 (*C*H_3), 21.1 (*C*H_3); **HRMS** (EI) cal for $C_{23}H_{19}N$ [M^+] 309.1517, found 309.1516; **IR** (KBr): 3023, 2923, 2854, 1565, 1496, 1450, 1373, 1257, 1180, 1110, 1025, 817 and 763 cm^{-1}.

3,4-Bis(4-fluorophenyl)quinoline (3ac)



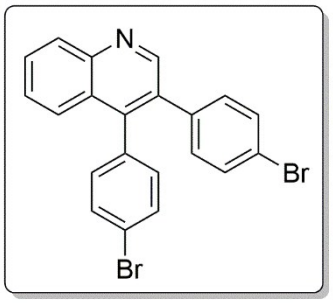
Yellow solid: m.p. 122-124 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.94 (s, 1 H), 8.17 (d, *J* = 8.4 Hz, 1 H), 7.75-7.69 (m, 1 H), 7.63 (dd, *J* = 8.4, 0.8 Hz, 1 H), 7.51-7.46 (m, 1 H), 7.16-7.02 (m, 6 H), 6.98-6.91 (m, 2 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 162.3 (d, J_{C-F} = 246.7 Hz, C), 162.0 (d, J_{C-F} = 246.3 Hz, C), 151.5 (*C*H), 147.6 (C), 144.5 (C), 133.9 (d, J_{C-F} = 3.4 Hz, C), 132.3 (C), 132.1 (d, J_{C-F} = 8.0 Hz, 2 *C*H), 131.9 (d, J_{C-F} = 3.6 Hz, C), 131.7 (d, J_{C-F} = 8.1 Hz, 2 *C*H), 129.6 (*C*H), 129.3 (*C*H), 127.2 (*C*H), 127.1 (C), 126.2 (*C*H), 115.4 (d, J_{C-F} = 19.7 Hz, 2 *C*H), 115.2 (d, J_{C-F} = 19.7 Hz, 2 *C*H); **HRMS** (EI) cal for $C_{21}H_{13}F_2N$ [M^+] 317.1016, found 317.1017; **IR** (KBr): 3062, 2923, 2854, 1604, 1511, 1380, 1226, 1157, 1095, 1018, 833, 763, 586 and 555 cm^{-1}.

3,4-Bis(4-chlorophenyl)quinoline (3ad)



Yellow solid: m.p. 131-133 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.93 (s, 1 H), 8.17 (d, *J* = 8.4 Hz, 1 H), 7.75-7.70 (m, 1 H), 7.61 (dd, *J* = 8.4, 0.8 Hz, 1 H), 7.52-7.46 (m, 1 H), 7.34 (d, *J* = 8.4 Hz, 2 H), 7.23 (d, *J* = 8.4 Hz, 2 H), 7.11 (d, *J* = 8.4 Hz, 2 H), 7.07 (d, *J* = 8.4 Hz, 2 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.3 (*C*H), 147.7 (C), 144.3 (C), 136.2 (C), 134.4 (C), 134.1 (C), 133.6 (C), 131.9 (C), 131.8 (2 *C*H), 131.3 (2 *C*H), 129.7 (*C*H), 129.5 (*C*H), 128.7 (2 *C*H), 128.5 (2 *C*H), 127.3 (*C*H), 126.8 (C), 126.2 (*C*H); **HRMS** (EI) cal for $C_{21}H_{13}Cl_2N$ [M^+] 349.0425, found 349.0428; **IR** (KBr): 2923, 2854, 1727, 1658, 1596, 1488, 1373, 1257, 1095, 1018, 825 and 763 cm^{-1}.

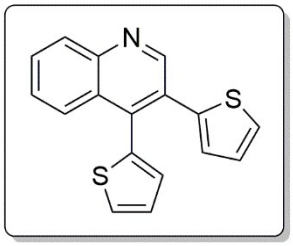
3,4-Bis(4-bromophenyl)quinoline (3ae)



Yellow solid: m.p. 128-130 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.92 (s, 1 H), 8.17 (d, *J* = 8.4 Hz, 1 H), 7.73 (t, *J* = 7.2 Hz, 1 H), 7.61 (d, *J* = 8.4 Hz, 1 H), 7.52-7.49 (m, 3 H), 7.39 (d, *J* = 8.4 Hz, 2 H), 7.05 (d, *J* = 8.4 Hz, 2 H), 7.00 (d, *J* = 8.4 Hz, 2 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.3 (*C*H), 147.7 (C), 144.2 (C), 136.7 (C), 134.9 (C), 132.0 (2 *C*H), 131.9 (C), 131.7 (2 *C*H), 131.6 (2 *C*H), 131.5 (2 *C*H), 129.7 (*C*H),

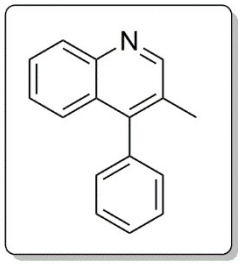
129.5 (*C*H), 127.3 (*C*H), 126.8 (C), 126.2 (*C*H), 122.3 (C), 121.8 (C); **HRMS** (EI) cal for $C_{21}H_{13}Br_2N$ [M^+] 436.9415, found 436.9412; **IR** (KBr): 3062, 2923, 2854, 1727, 1589, 1488, 1373, 1249, 1072, 1010, 825 and 763 cm^{-1}.

3,4-Di(thiophen-2-yl)quinoline (3af)



Yellow solid: m.p. 110-112 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.26 (s, 1 H), 7.96 (d, *J* = 8.0 Hz, 1 H), 7.64-7.52 (m, 4 H), 7.30 (d, *J* = 4.8 Hz, 1 H), 7.26 (dd, *J* = 5.2, 3.6 Hz, 1 H), 7.09 (d, *J* = 3.6 Hz, 1 H), 6.89 (t, *J* = 4.8 Hz, 1 H), 6.69 (d, *J* = 4.0 Hz, 1 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.5 (CH), 145.6 (C), 144.6 (C), 137.7 (C), 137.5 (C), 131.0 (*C*H), 129.1 (*C*H), 127.9 (*C*H), 127.8 (2 *C*H), 127.6 (*C*H), 127.5 (*C*H), 127.4 (*C*H), 126.9 (*C*H), 126.8 (C), 125.4 (*C*H), 120.5 (C); **HRMS** (EI) cal for $C_{17}H_{11}S_2N$ [M^+] 293.0333, found 293.0334; **IR** (KBr): 3071, 2923, 2854, 1727, 1612, 1565, 1442, 1272, 1072, 925, 817, 755 and 701 cm^{-1}.

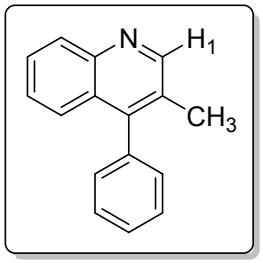
3-Methyl-4-phenylquinoline (3ag)



Yellow solid: m.p. 88-90 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.83 (s, 1 H), 8.09 (d, *J* = 8.4 Hz, 1 H), 7.64-7.58 (m, 1 H), 7.54-7.35 (m, 6 H), 7.27-7.25 (m, 1 H), 2.25 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.6 (*C*H), 146.9 (C), 146.3 (C), 136.9 (C),

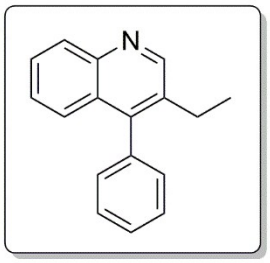
129.3 (*C*H), 129.2 (2 *C*H), 128.6 (2 *C*H), 128.2 (*C*H), 128.0 (C), 127.9 (*C*H), 127.5 (C), 126.4 (*C*H), 125.9 (*C*H), 17.6 (*C*H_3); **HRMS** (EI) cal for $C_{16}H_{13}N$ [M^+] 219.1048, found 219.1048; **IR** (KBr): 3054, 2923, 2861, 1720, 1573, 1450, 1380, 1249, 1126, 925, 763 and 701 cm^{-1}.

NOE data



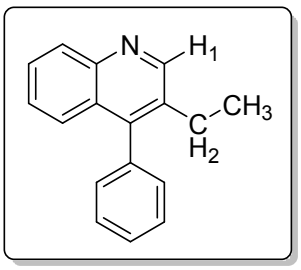
Irradiation	Intensity increase
H_1 (δ 8.83)	CH_3 (δ 2.25, 4.83 %)
CH_3 (δ 2.25)	H_1 (δ 8.83, 2.17 %)

3-Ethyl-4-phenylquinoline (3ah)



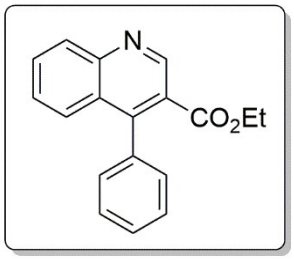
Yellow solid: m.p. 98-100 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.86 (s, 1 H), 8.09 (d, *J* = 8.4 Hz, 1 H), 7.64-7.59 (m, 1 H), 7.53-7.45 (m, 3 H), 7.36 (d, *J* = 3.6 Hz, 2 H), 7.28-7.25 (m, 2 H), 2.59 (q, *J* = 7.6 Hz, 2 H), 1.12 (t, *J* = 7.6 Hz, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.0 (*C*H), 146.7 (C), 145.7 (C), 136.6 (C), 134.1 (C), 129.4 (2 *C*H), 129.2 (*C*H), 128.4 (2 *C*H), 128.2 (*C*H), 127.8 (*C*H), 127.7 (C), 126.4 (*C*H), 126.1 (*C*H), 24.4 (*C*H_2), 15.9 (*C*H_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{17}H_{16}N$ 234.1283, found 234.1284; **IR** (KBr): 2915, 2877, 1527, 1457, 1349, 1095, 941, 887, 802, 763 and 732 cm^{-1}.

NOE data



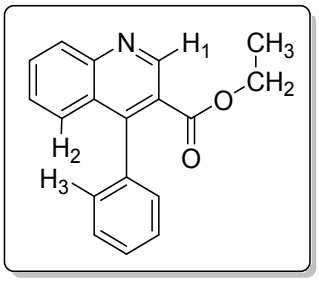
Irradiation	Intensity increase
H_1 (δ 8.86)	CH_2 (δ 2.59, 3.67 %)
	CH_3 (δ 1.12, 1.94 %)
CH_2 (δ 2.59)	H_1 (δ 8.86, 1.49 %)
	CH_3 (δ 1.12, 3.48 %)
CH_3 (δ 1.12)	H_1 (δ 8.86, 0.49 %)
	CH_2 (δ 2.59, 1.61 %)

Ethyl 4-phenylquinoline-3-carboxylate (3ai)



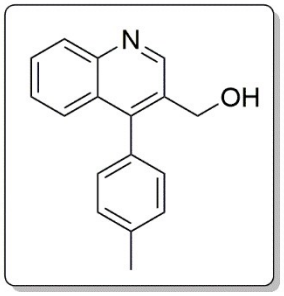
Yellow solid: m.p. 62-64 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.33 (s, 1 H), 8.16 (d, *J* = 8.4 Hz, 1 H), 7.79-7.74 (m, 1 H), 7.58 (d, *J* = 8.4 Hz, 1 H), 7.50-7.46 (m, 4 H), 7.29-7.26 (m, 2 H), 4.09 (q, *J* = 6.8 Hz, 2 H), 0.98 (t, *J* = 6.8 Hz, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.6 (C), 150.1 (*C*H), 149.7 (C), 149.2 (C), 136.5 (C), 130.9 (*C*H), 129.6 (*C*H), 128.8 (2 *C*H), 128.1 (*C*H), 128.0 (2 *C*H), 127.5 (*C*H), 127.2 (*C*H), 127.0 (C), 123.3 (C), 61.2 (CH_2), 13.6 (CH_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{18}H_{16}O_2N$ 278.1181, found 278.1180; **IR** (KBr): 3070, 2923, 2869, 1712, 1573, 1527, 1349, 1319, 1226, 1118, 771 and 701 cm^{-1}.

NOE data



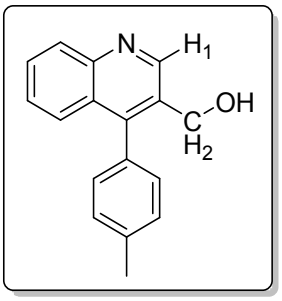
Irradiation	Intensity increase
H_1 (δ 9.33)	CH_2 (δ 4.09, 0.38 %)
H_2 (δ 7.58)	H_3 (δ 7.29-7.26, 3.72 %)
H_3 (δ 7.29-7.26)	H_2 (δ 7.58, 0.82 %)

(4-(*p*-Tolyl)quinolin-3-yl)methanol (3aj)



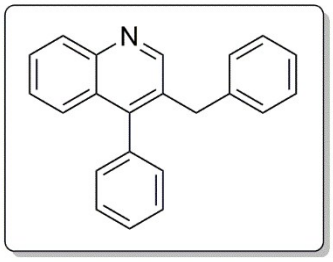
Yellow solid: m.p. 112-114 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.33 (d, *J* = 8.4 Hz, 2 H), 8.12 (s, 1 H), 7.97 (d, *J* = 8.0 Hz, 1 H), 7.40-7.36 (m, 2 H), 7.32-7.26 (m, 3 H), 5.59 (s, 2 H), 2.42 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 185.2 (C), 148.6 (C), 144.2 (C), 133.9 (C), 133.7 (C), 130.7 (2 *C*H), 130.2 (*C*H), 129.3 (*C*H), 129.2 (*C*H), 129.1 (*C*H), 129.0 (2 *C*H), 128.4 (*C*H, C), 54.4 (CH_2), 21.7 (CH_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{17}H_{16}ON$ 250.1232, found 250.1228; **IR** (KBr): 2923, 2861, 1820, 1658, 1604, 1442, 1349, 1241, 902 and 755 cm^{-1}.

NOE data



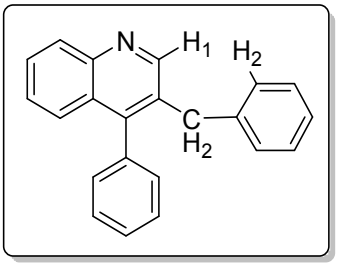
Irradiation	Intensity increase
H_1 (δ 8.12)	CH_2 (δ 5.59, 2.14 %)
CH_2 (δ 5.59)	H_1 (δ 8.12, 1.25 %)

3-Benzyl-4-phenylquinoline (3ak)



Yellow solid: m.p. 87-89 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.85 (s, 1 H), 8.11 (d, *J* = 8.4 Hz, 1 H), 7.67-7.62 (m, 1 H), 7.48-7.37 (m, 5 H), 7.21-7.12 (m, 5 H), 6.94 (d, *J* = 7.6 Hz, 2 H), 3.97 (s, 2 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.7 (*C*H), 146.9 (C), 146.7 (C), 140.2 (C), 136.2 (C), 130.9 (C), 129.4 (2 *C*H), 129.3 (*C*H), 128.6 (2 *C*H), 128.5 (*C*H), 128.4 (2 *C*H), 128.3 (2 *C*H), 127.9 (*C*H), 127.7 (C), 126.5 (*C*H), 126.3 (*C*H), 126.1 (*C*H), 36.9 (CH_2); **HRMS** (FAB) $[M+H]^+$ cal for $C_{22}H_{18}N$ 296.1439, found 296.1440; **IR** (KBr): 3062, 3031, 2923, 2869, 1658, 1573, 1488, 1450, 1380, 1265, 1126, 1072, 1025, 763 and 701 cm^{-1}.

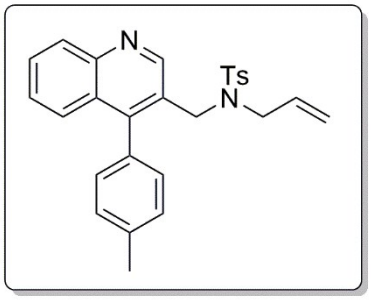
NOE data



Irradiation	Intensity increase
H_1 (δ 8.85)	CH_2 (δ 3.97, 3.79 %)
	H_2 (δ 6.94, 1.58 %)
CH_2 (δ 3.97)	H_1 (δ 8.85, 3.19 %)
	H_2 (δ 6.94, 2.11 %)
H_2 (δ 6.94)	H_1 (δ 8.85, 0.63 %)
	CH_2 (δ 3.97, 1.14 %)

***N*-Allyl-4-methyl-*N*-((4-(*p*-tolyl)quinolin-3-yl)methyl)**

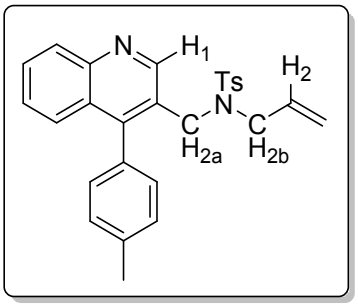
benzenesulfonamide (3al)



Yellow liquid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.01 (s, 1 H), 8.11 (d, *J* = 8.4 Hz, 1 H), 7.68-7.60 (m, 3 H), 7.41-7.38 (m, 2 H), 7.29 (d, *J* = 8.0 Hz, 2 H), 7.23 (d, *J* = 8.0 Hz, 2 H), 7.06 (d, *J* = 8.0 Hz, 2 H), 5.46-5.35 (m, 1 H), 4.91-4.80 (m, 2 H), 4.32 (s, 2 H), 3.61 (d, *J* = 6.4 Hz, 2 H), 2.45 (s, 3 H), 2.39 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.2 (*C*H), 147.4 (C), 146.7 (C), 143.5 (C), 138.2 (C), 136.8 (C), 132.3 (*C*H), 132.1 (C), 129.7 (2 *C*H), 129.4 (*C*H), 129.3 (2 *C*H), 129.2 (2 *C*H), 129.1 (*C*H), 127.3 (2 *C*H), 127.2 (C), 126.6 (*C*H), 126.5 (C), 126.3 (*C*H), 119.2 (CH_2), 50.7 (CH_2), 46.4 (CH_2), 21.5 (CH_3), 21.3 (CH_3); **HRMS** (FAB) $[M+H]^+$ cal for $C_{27}H_{27}O_2SN_2$ 443.1793, found 443.1790; **IR** (KBr): 2923, 2861, 1704, 1604, 1457, 1349, 1249, 1126, 1072,

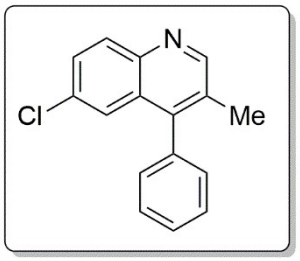
817, 755 and 701 cm^{-1}.

NOE data



Irradiation	Intensity increase
H_1 (δ 9.01)	CH_{2a} (δ 4.32, 2.68 %)
	CH_{2b} (δ 3.61, 1.34 %)
H_2 (δ 5.46-5.35)	H_1 (δ 9.01, 0.67 %)
	CH_{2b} (δ 3.61, 2.42 %)
CH_{2a} (δ 4.32)	H_1 (δ 9.01, 3.05 %)
	H_2 (δ 5.46-5.35, 1.26 %)
	CH_{2b} (δ 3.61, 1.23 %)
CH_{2b} (δ 3.61)	H_1 (δ 9.01, 1.35 %)
	H_2 (δ 5.46-5.35, 3.04 %)
	CH_{2a} (δ 4.32, 1.53 %)

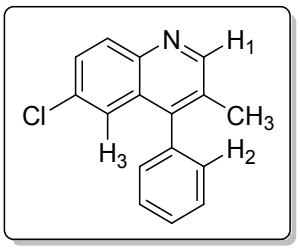
6-Chloro-3-methyl-4-phenylquinoline (3fg)



Yellow solid: m.p. 110-112 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.80 (s, 1 H), 8.01 (d, *J* = 8.8 Hz, 1 H), 7.55-7.44 (m, 4 H), 7.38 (d, *J* = 2.4 Hz, 1 H), 7.23-7.20 (m, 2 H), 2.23 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.8 (*C*H), 145.5 (C), 145.2 (C), 136.1 (C), 132.3 (C), 130.9 (*C*H), 129.1 (3 *C*H), 129.0 (C), 128.8 (2 *C*H), 128.3 (C), 128.2 (*C*H), 124.6 (*C*H), 17.6 (CH_3); **HRMS** (ESI) $[M+H]^+$ cal for $C_{16}H_{13}ClN$ 254.0737, found 254.0728; **IR** (KBr): 3054, 1604, 1488, 1442, 1349, 1257, 1164,

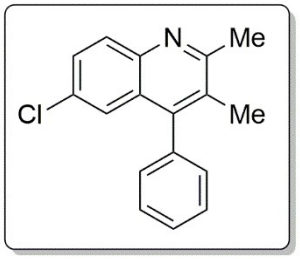
1079, 941, 833, 748 and 701 cm^{-1}.

NOE data



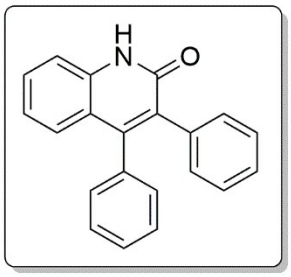
Irradiation	Intensity increase
H_1 (δ 8.80)	CH_3 (δ 2.23, 5.87 %)
CH_3 (δ 2.23)	H_1 (δ 8.80, 3.74 %)
	H_2 (δ 7.23-7.20, 1.89 %)
H_2 (δ 7.23-7.20)	CH_3 (δ 2.23, 2.61 %)
	H_3 (δ 7.38, 1.78 %)

6-Chloro-2,3-dimethyl-4-phenylquinoline (4)



Yellow solid: m.p. 125-127 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8.8 Hz, 1 H), 7.54-7.44 (m, 4 H), 7.25 (d, *J* = 2.4 Hz, 1 H), 7.21-7.18 (m, 2 H), 2.72 (s, 3 H), 2.15 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 159.3 (C), 145.5 (C), 144.4 (C), 136.9 (C), 131.2 (C), 130.1 (*C*H), 129.3 (2 *C*H), 128.9 (*C*H), 128.7 (2 *C*H), 128.5 (C), 128.0 (*C*H), 127.6 (C), 124.8 (*C*H), 24.5 (CH_3), 17.0 (CH_3); **HRMS** (ESI) $[M+H]^+$ cal for $C_{17}H_{15}ClN$ 268.0893, found 268.0885; **IR** (KBr): 3062, 2923, 2854, 1727, 1666, 1589, 1481, 1373, 1172, 1072, 948, 825 and 701 cm^{-1}.

3,4-Diphenylquinolin-2(1*H*)-one (5)



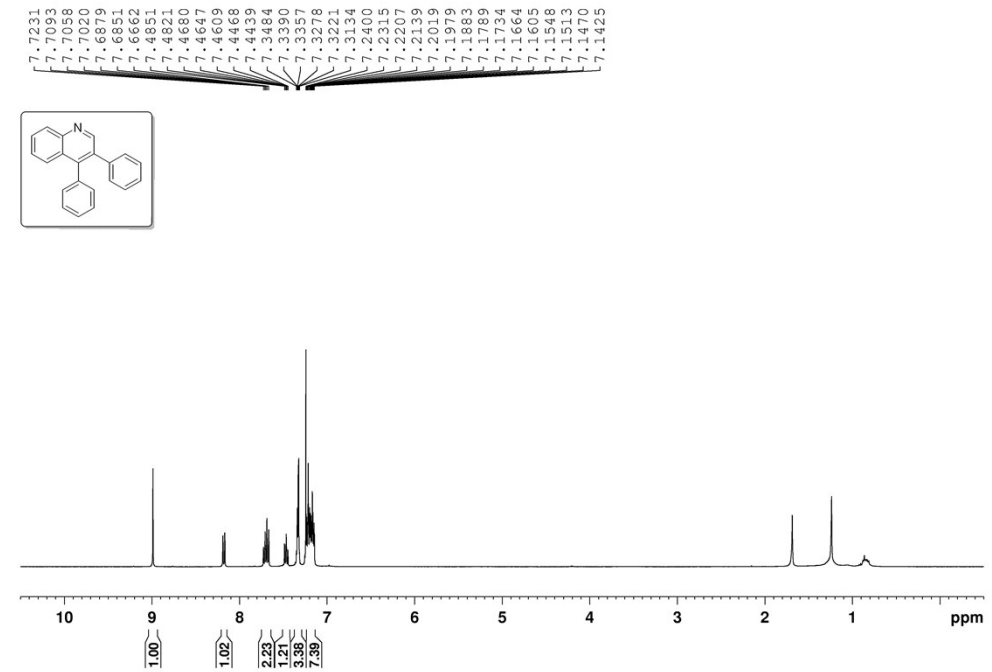
Yellow solid: m.p. 173-175 °C; **^{1}H NMR** (400 MHz, d_6-DMSO): δ 12.0 (bs, 1 H), 7.49 (t, J = 7.6 Hz, 1 H), 7.39 (d, J = 8.0 Hz, 1 H), 7.32-7.22 (m, 3 H), 7.18-7.04 (m, 8 H), 6.99 (d, J = 8.0 Hz, 1 H); **^{13}C NMR** (100 MHz, d_6-DMSO): δ 161.2 (C), 148.1 (C), 138.2 (C), 136.1 (C), 135.7 (C), 131.9 (C), 130.6 (2 *C*H), 130.1 (*C*H), 129.5 (2 *C*H), 127.9 (2 *C*H), 127.5 (*C*H), 127.1 (2 *C*H), 126.8 (*C*H), 126.5 (*C*H), 121.7 (*C*H), 119.9 (C), 115.1 (*C*H); **HRMS** (ESI) $[M+H]^+$ cal for $C_{21}H_{16}ON$ 298.1232, found 298.1225; **IR** (KBr): 3162, 1727, 1643, 1596, 1481, 1442, 1288, 705 and 701 cm^{-1}.

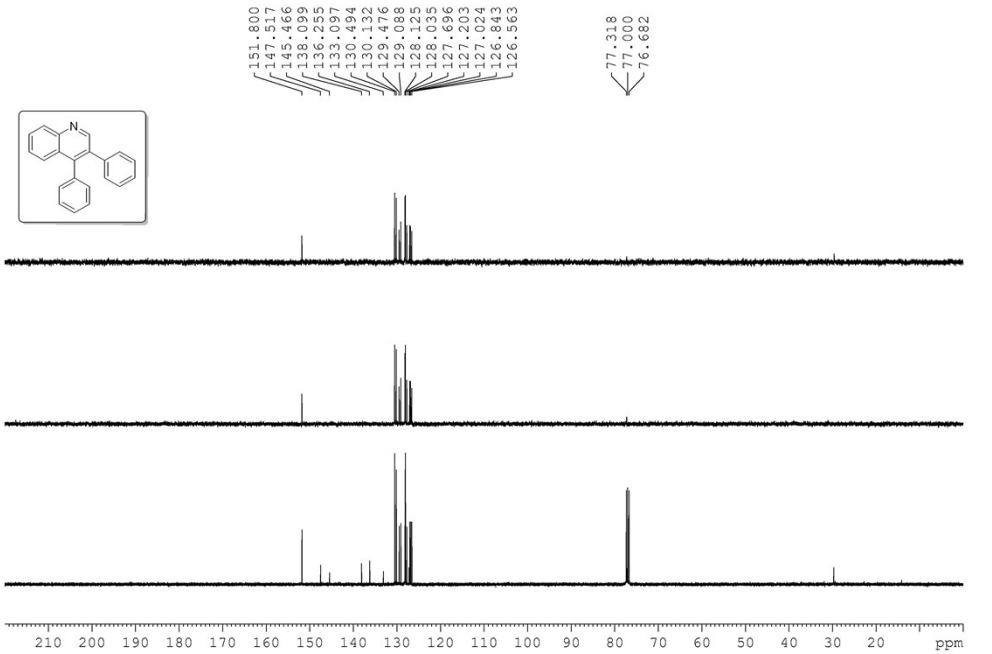
References

1. Berger, O.; Kaniti, A.; van Ba, C.; Vial, H.; Ward, S.; Biagini, G.; Bray, P.; O'Neill, P. *ChemMedChem* **2011**, *6*, 2094.
2. Johansson, C. C. C.; Bremeyer, N.; Ley, S. V.; Owen, D. R.; Smith, S. C.; Gaunt, M. J. *Angew. Chem., Int. Ed.* **2006**, *45*, 6024.
3. DeRuiter, J.; Swearingen, B. E.; Wandrekar, V.; Mayfield, C. A. *J. Med. Chem.* **1989**, *32*, 1033.

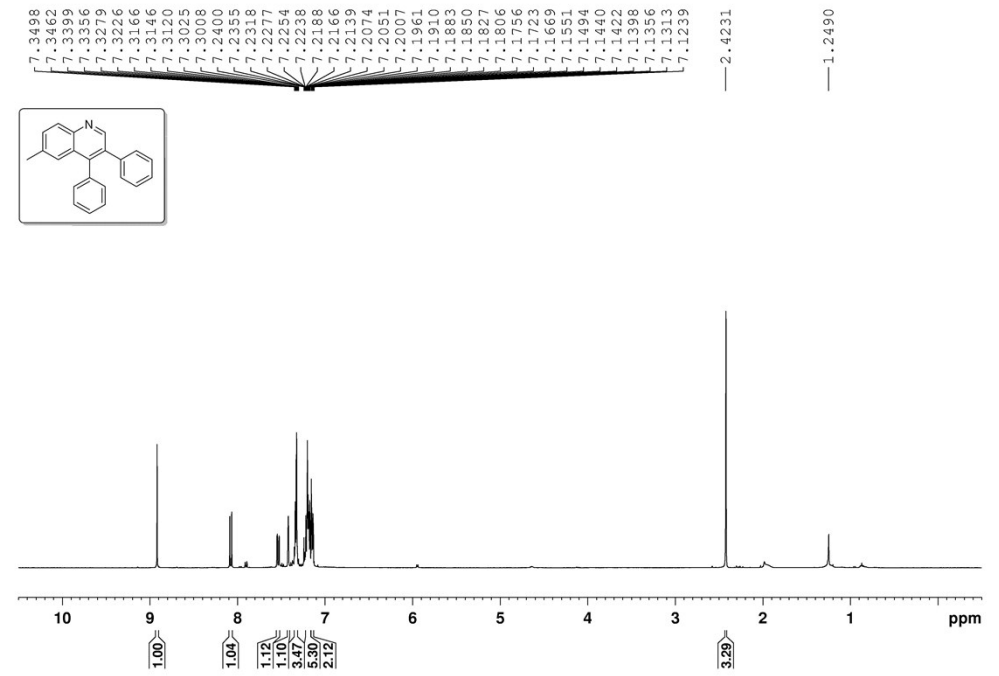
Copies of ^{1}H and ^{13}C NMR spectra

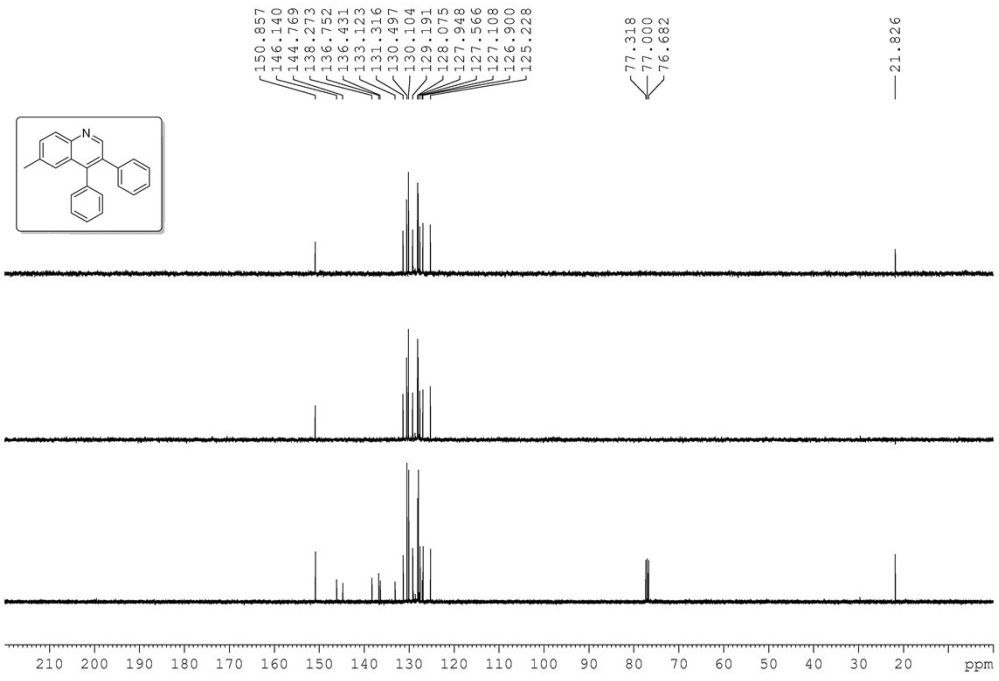
^{1}H and ^{13}C NMR spectra of compound **3aa**.



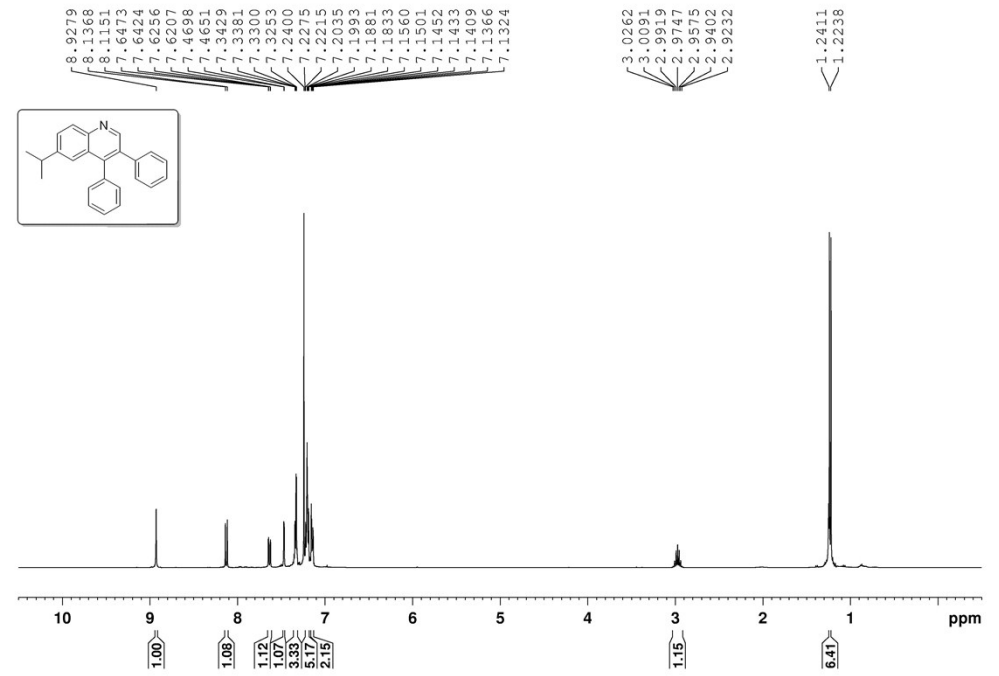


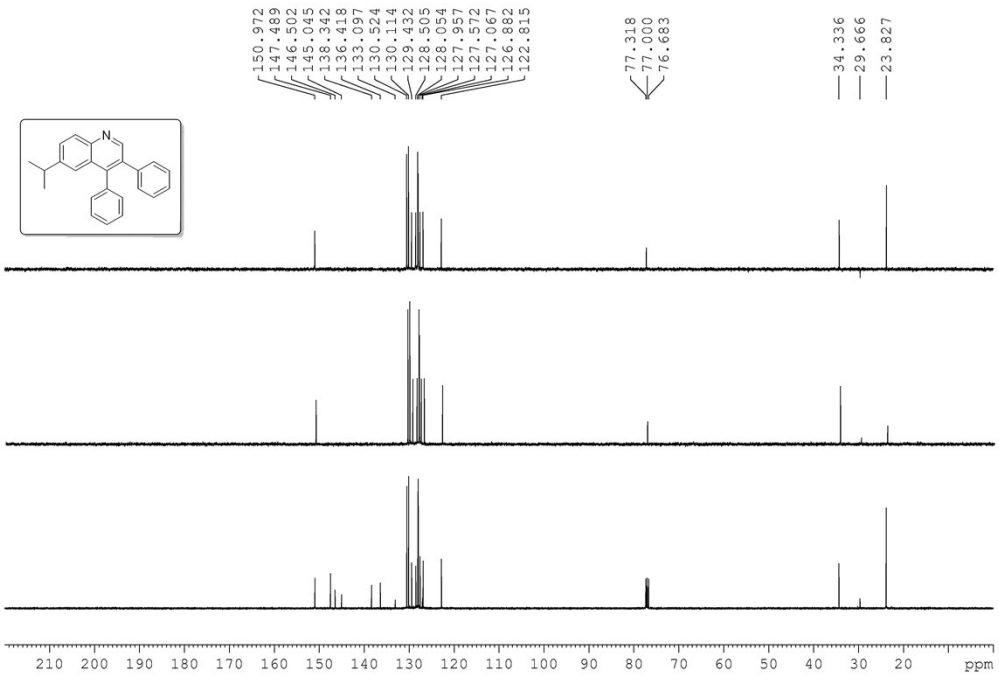
^{1}H and ^{13}C NMR spectra of compound **3ba**.



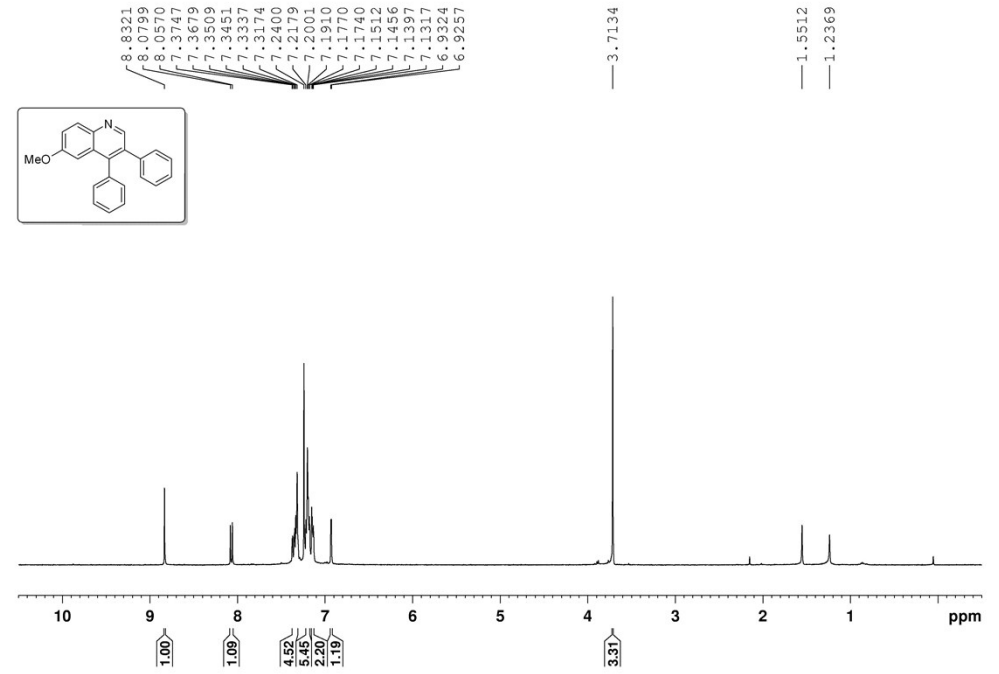


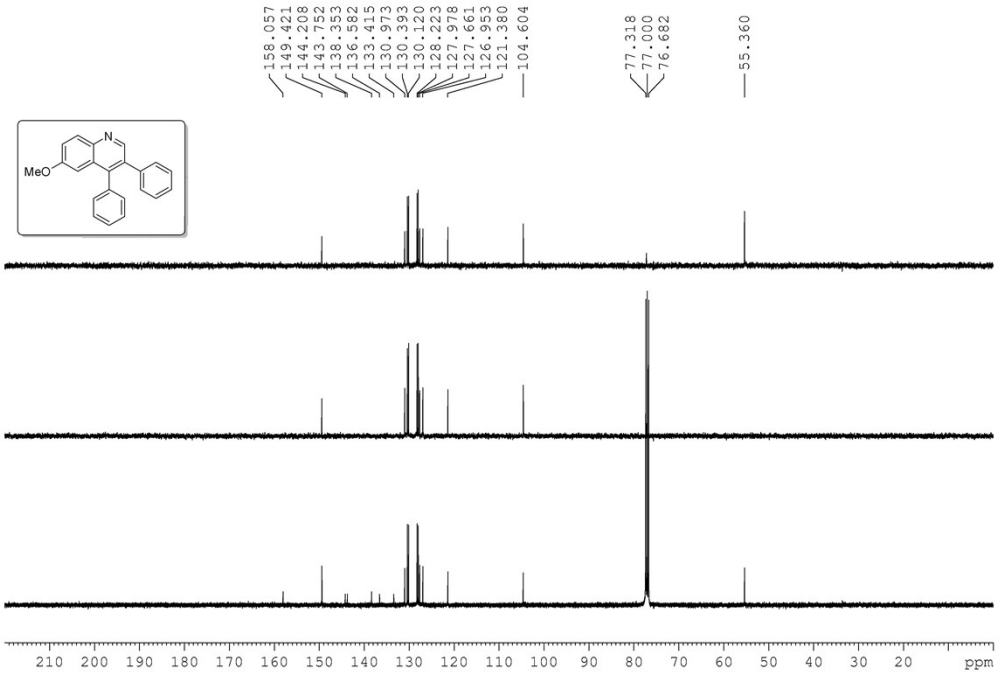
^{1}H and ^{13}C NMR spectra of compound **3ca**.



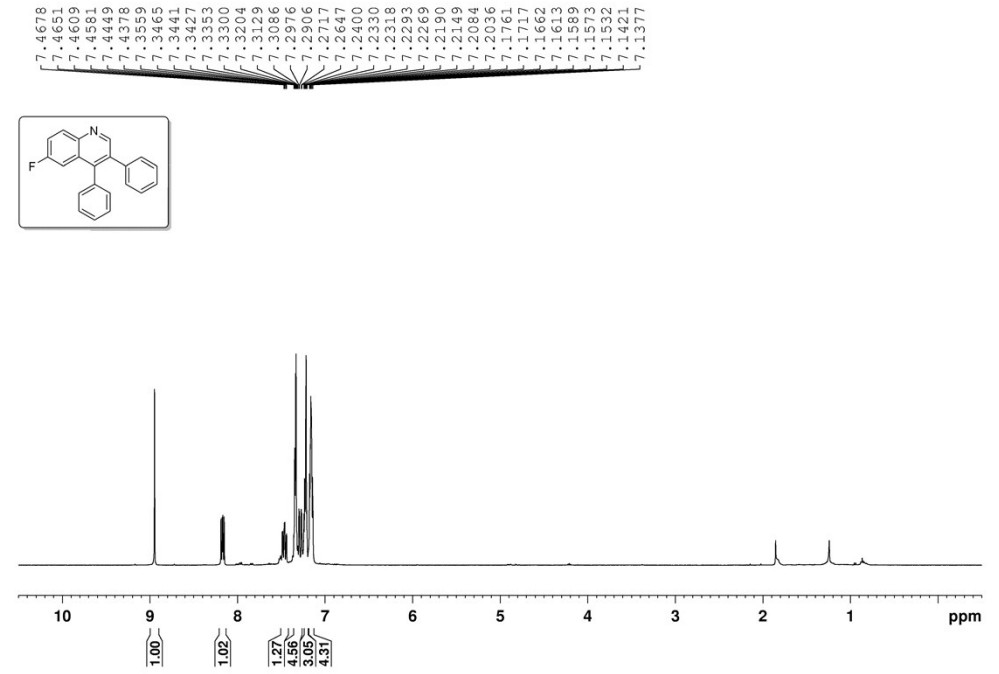


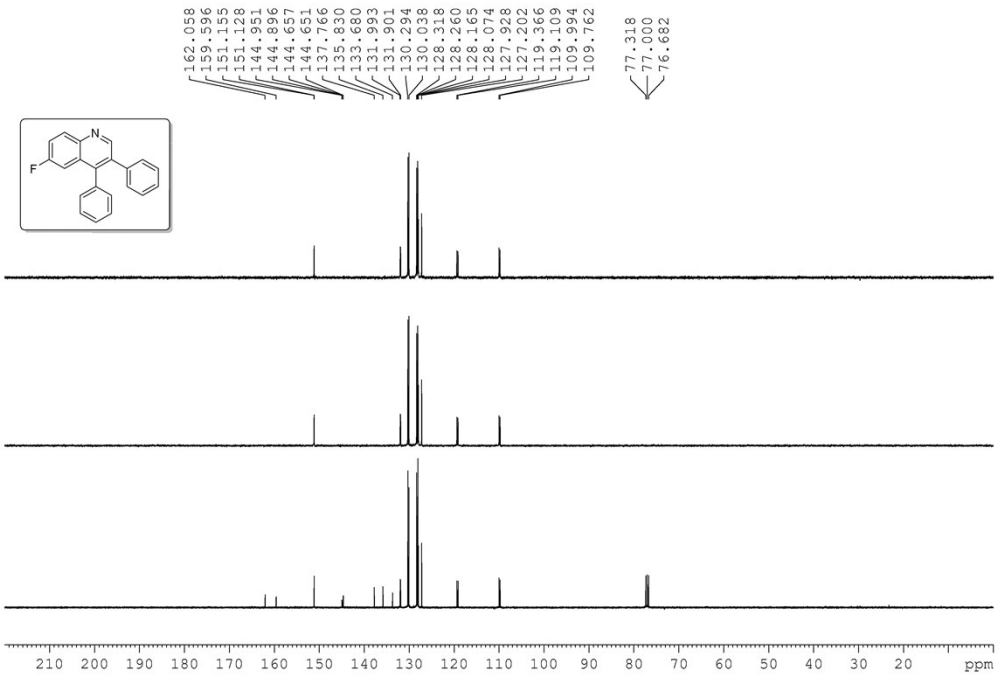
^{1}H and ^{13}C NMR spectra of compound **3da**.



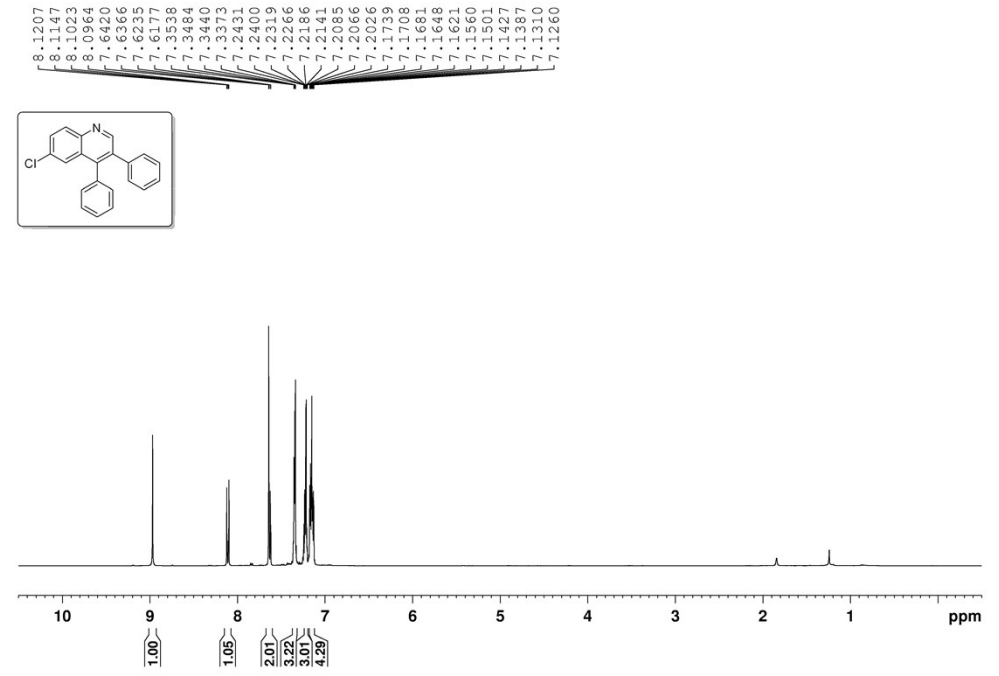


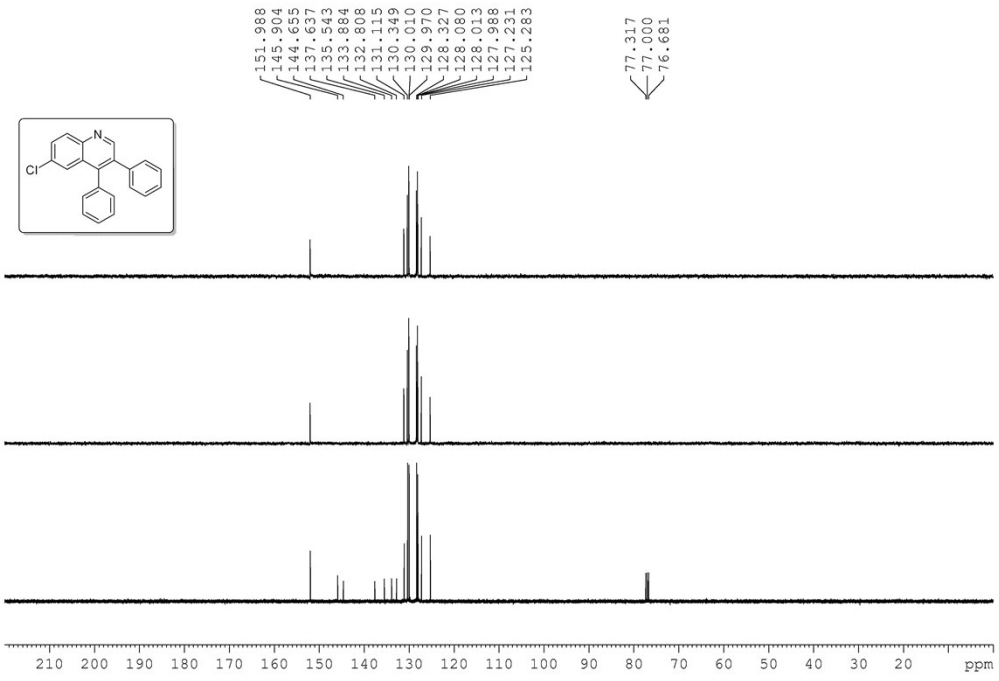
^{1}H and ^{13}C NMR spectra of compound **3ea**.



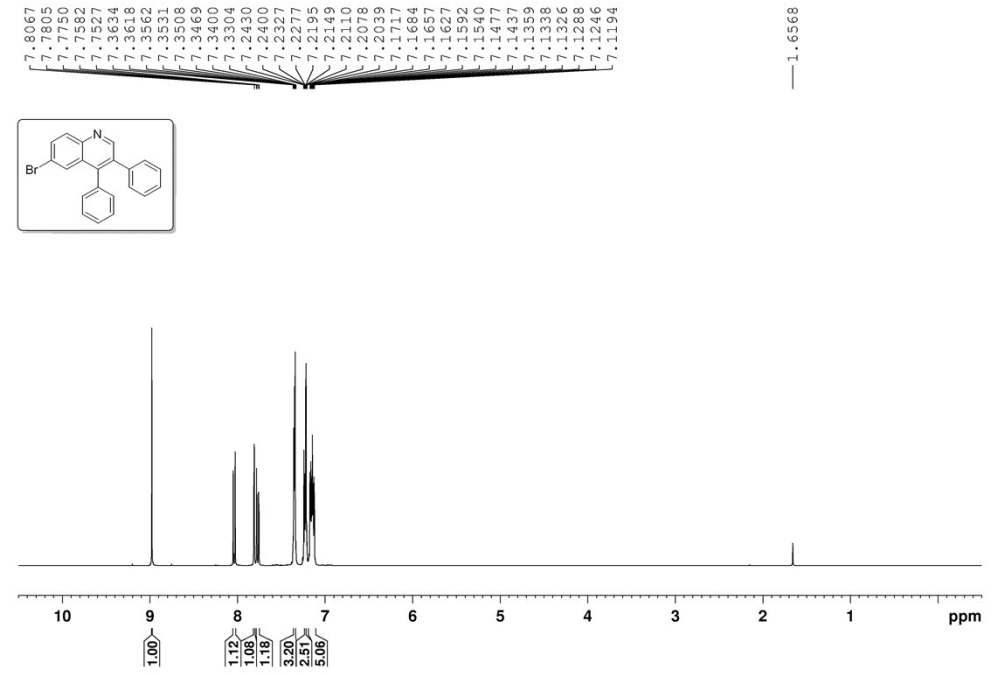


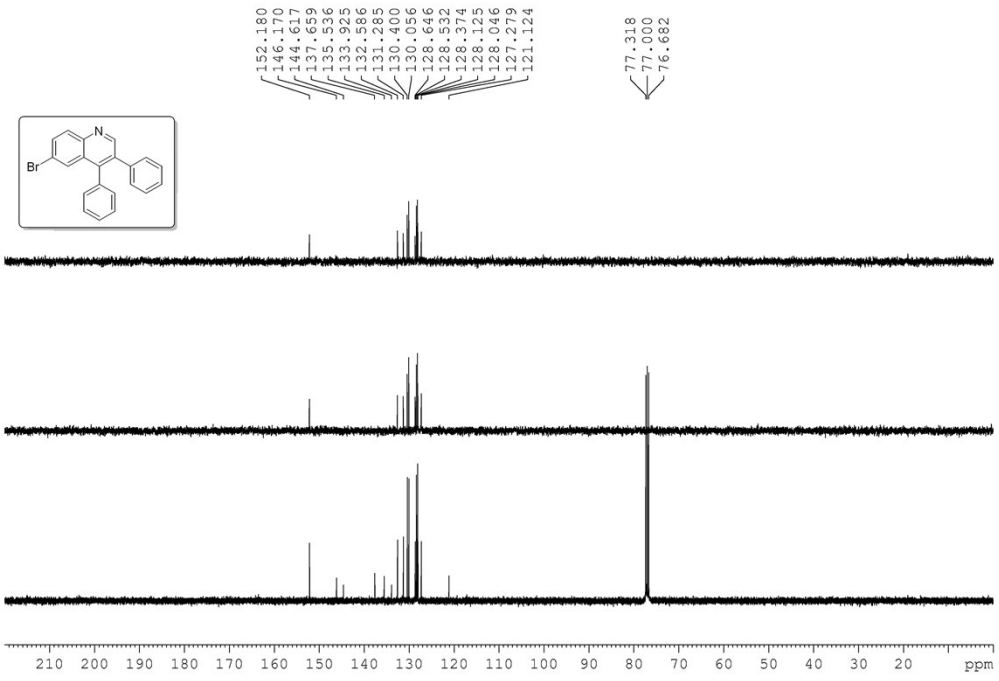
^{1}H and ^{13}C NMR spectra of compound **3fa**.



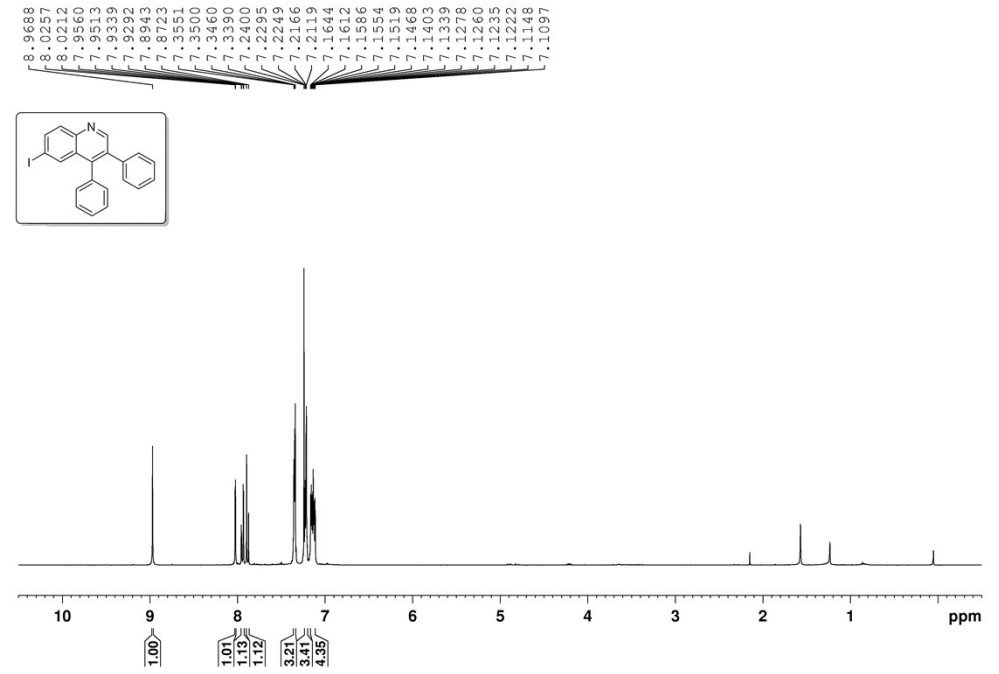


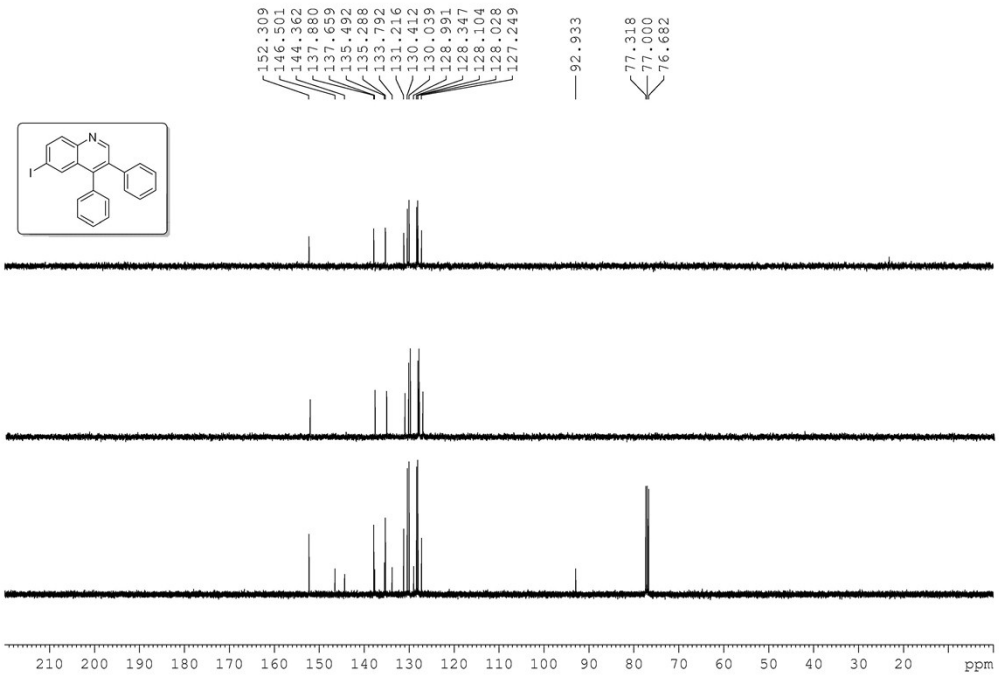
^{1}H and ^{13}C NMR spectra of compound **3ga**.



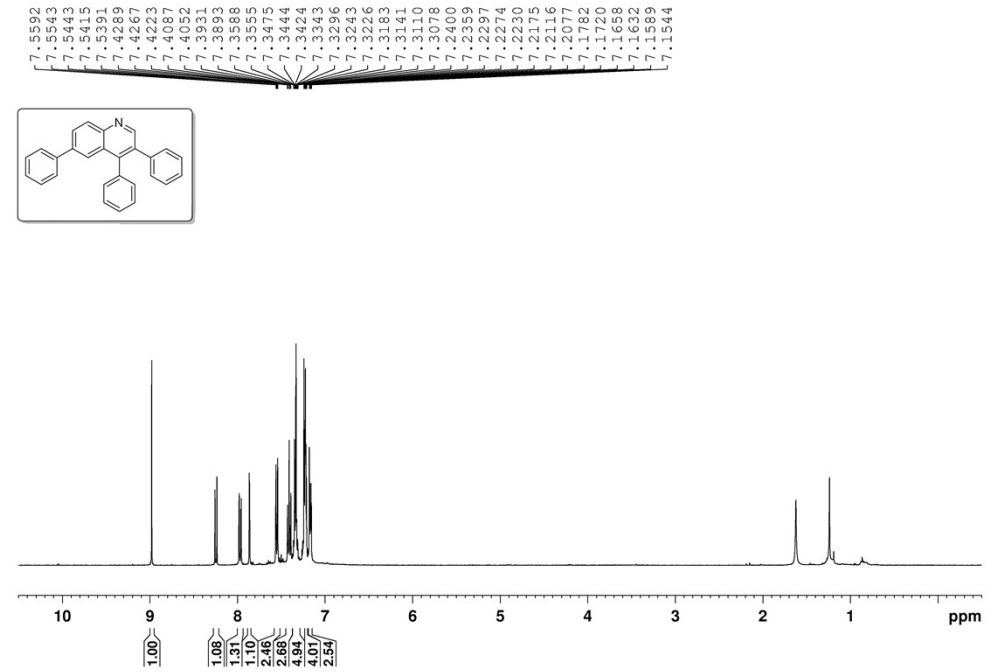


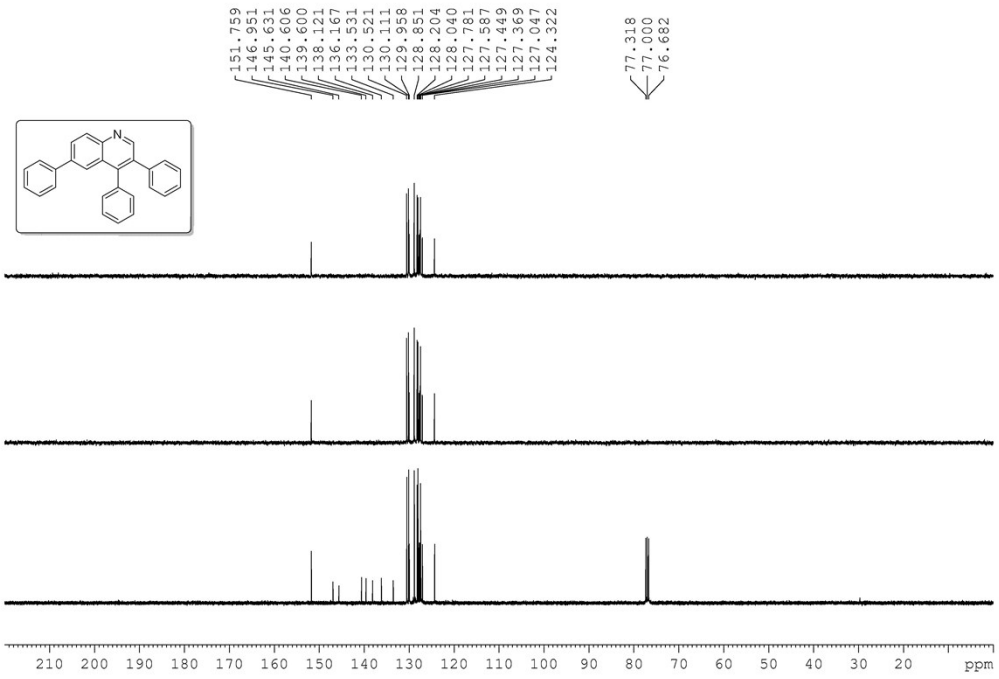
^{1}H and ^{13}C NMR spectra of compound **3ha**.



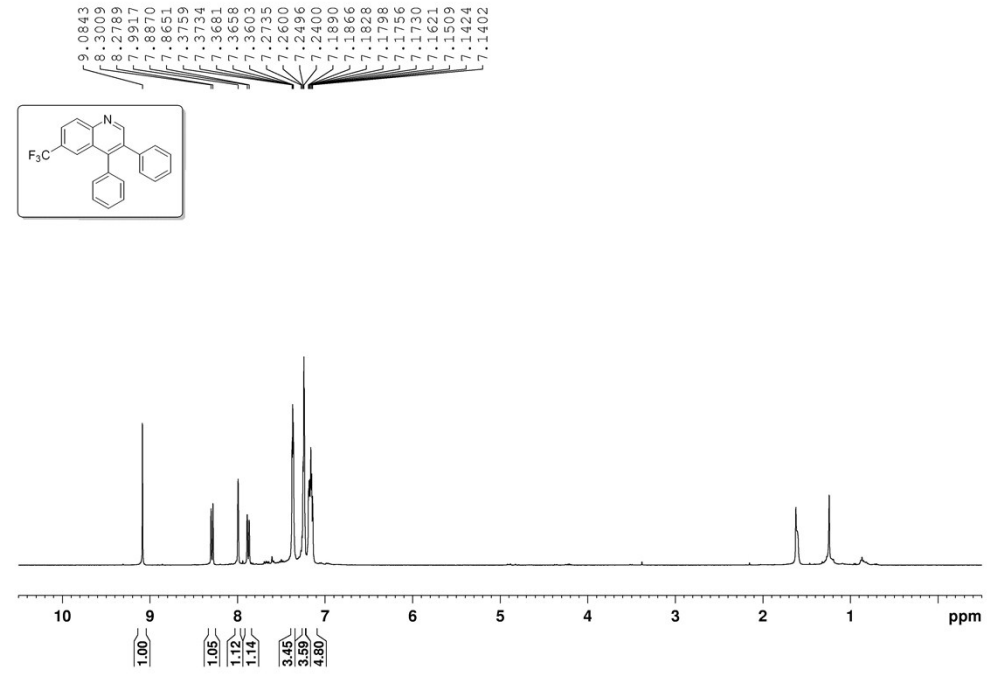


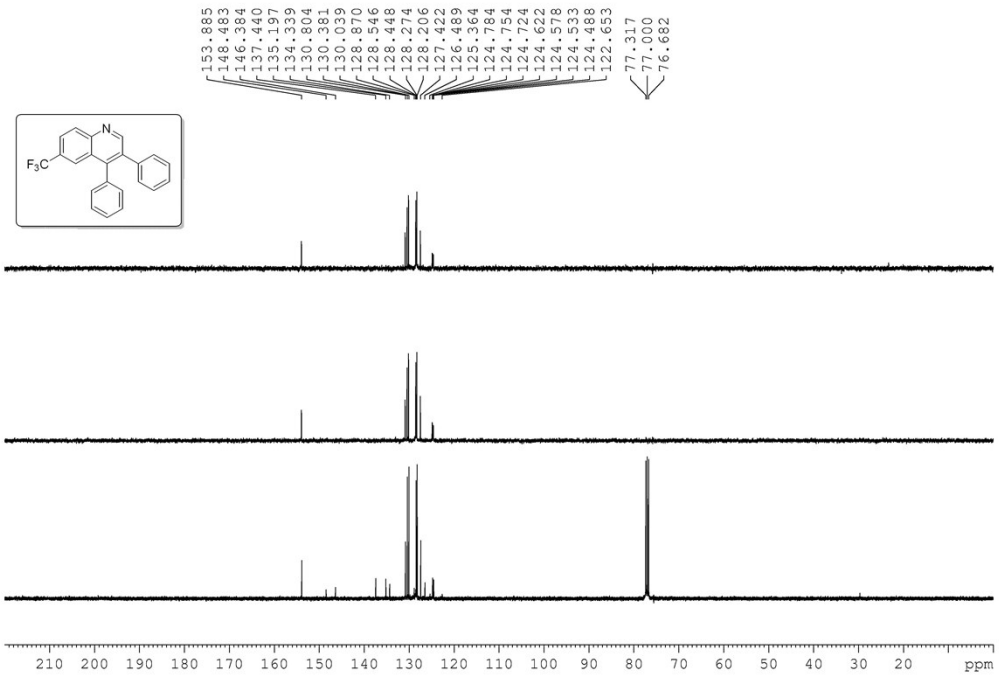
^{1}H and ^{13}C NMR spectra of compound **3ia**.



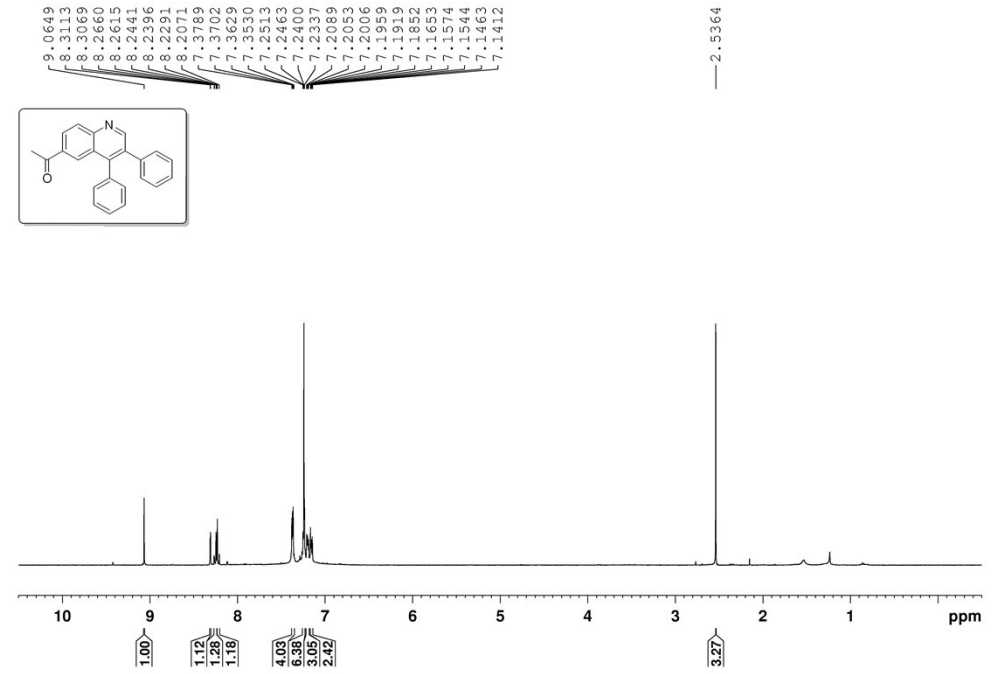


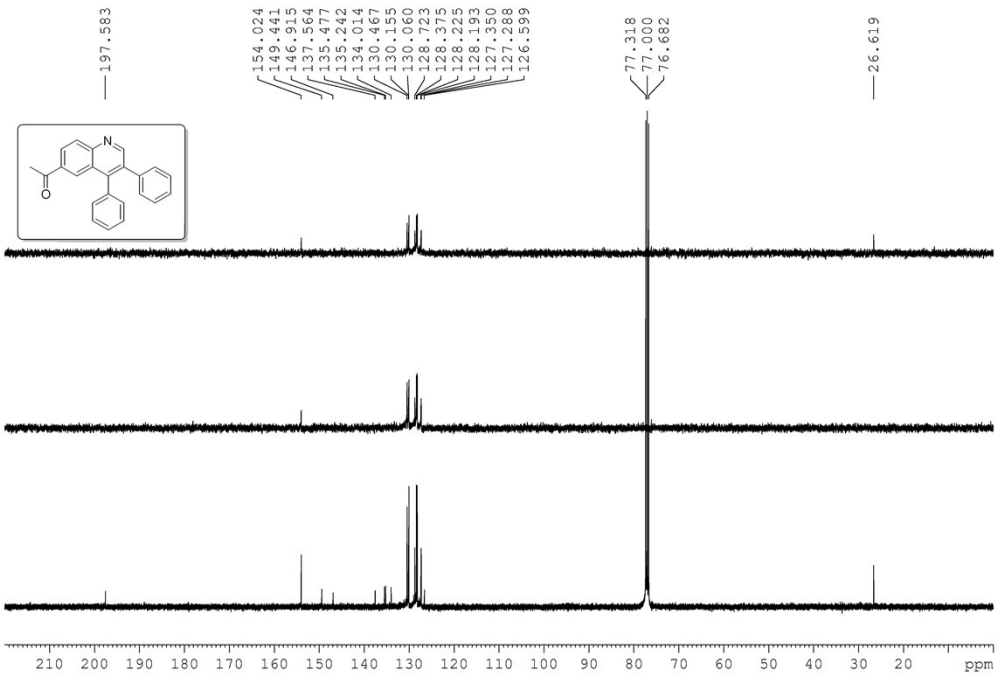
^{1}H and ^{13}C NMR spectra of compound **3ja**.



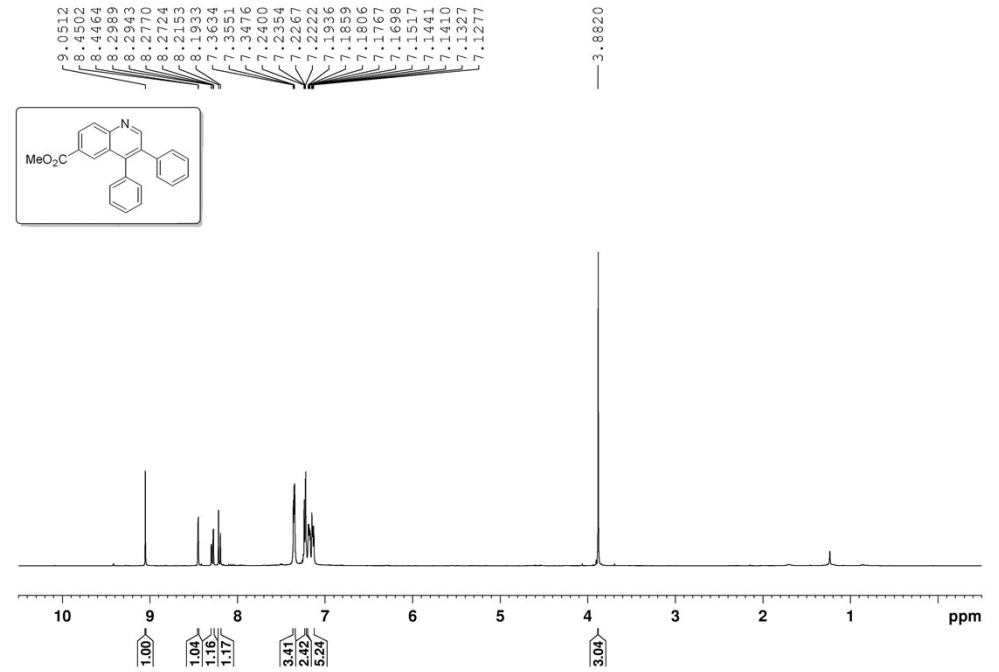


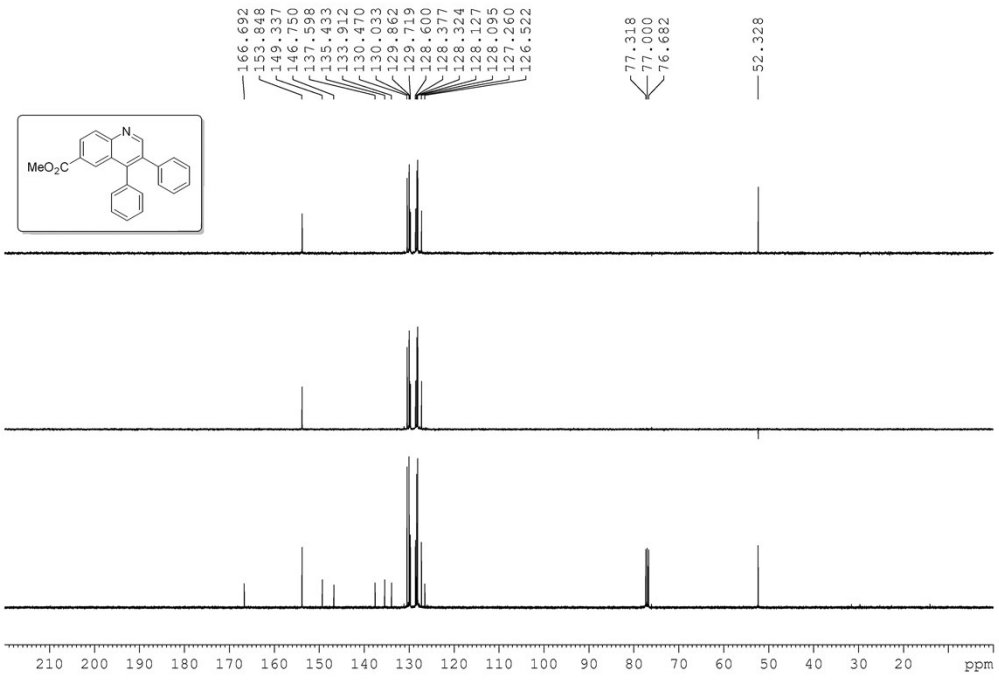
^{1}H and ^{13}C NMR spectra of compound **3ka**.



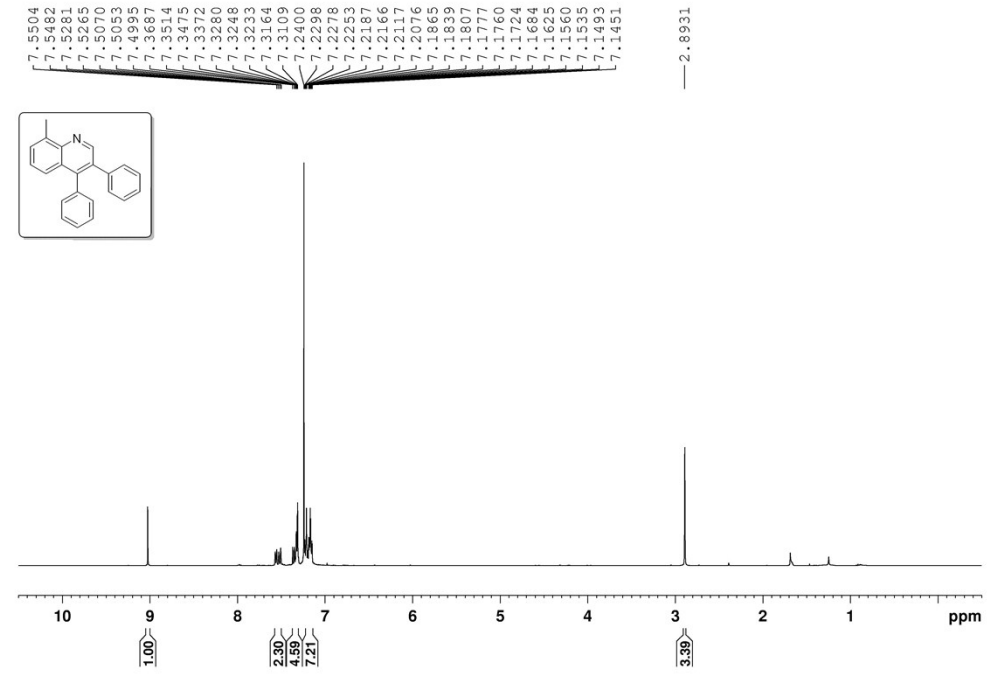


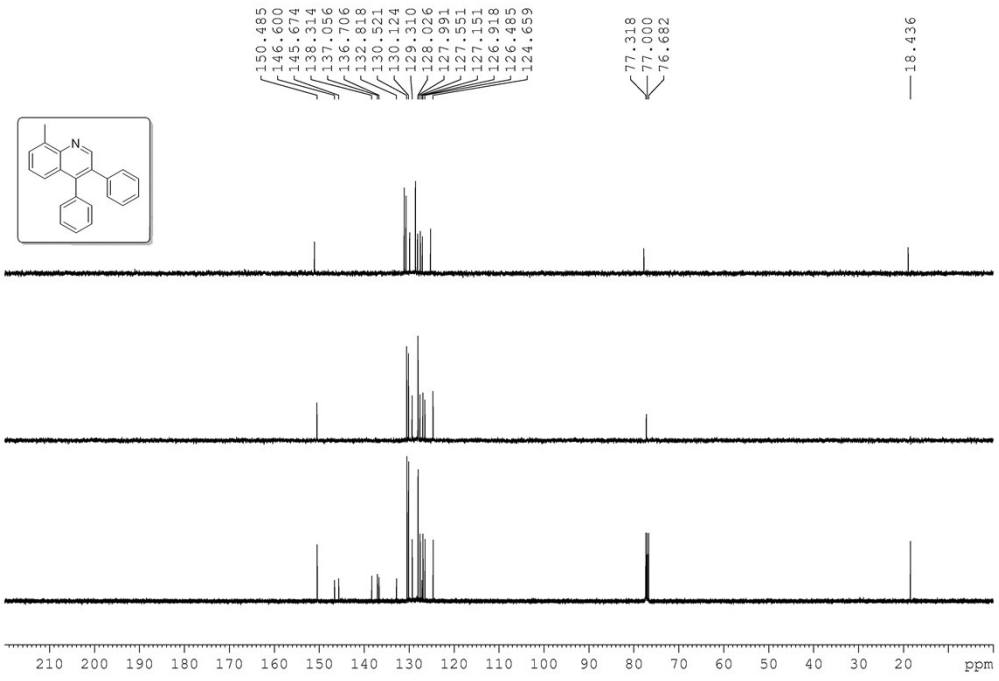
^{1}H and ^{13}C NMR spectra of compound **3la**.



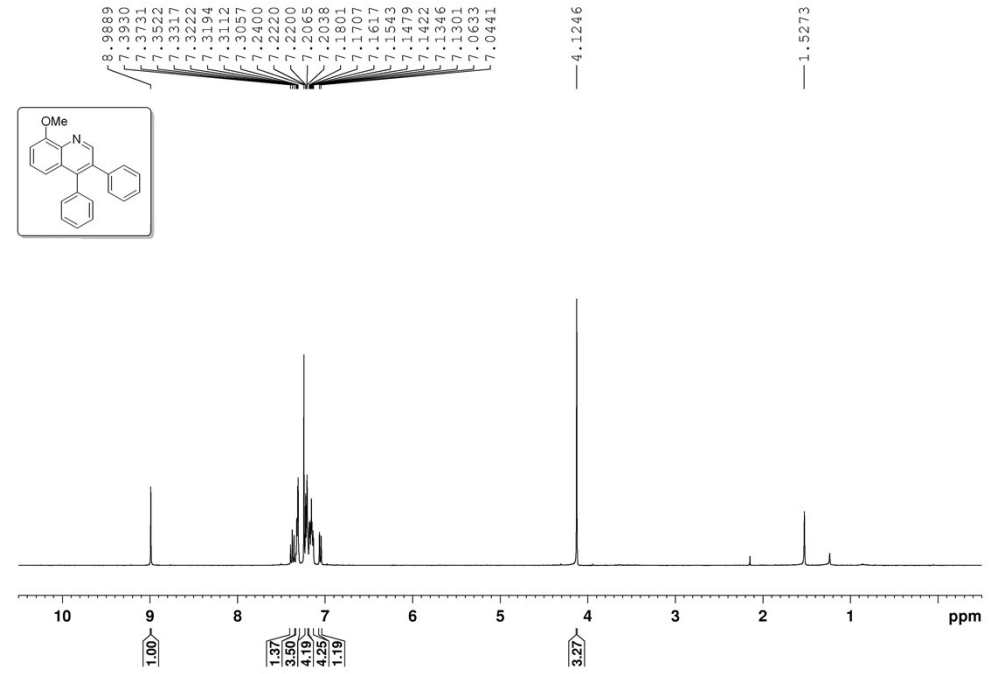


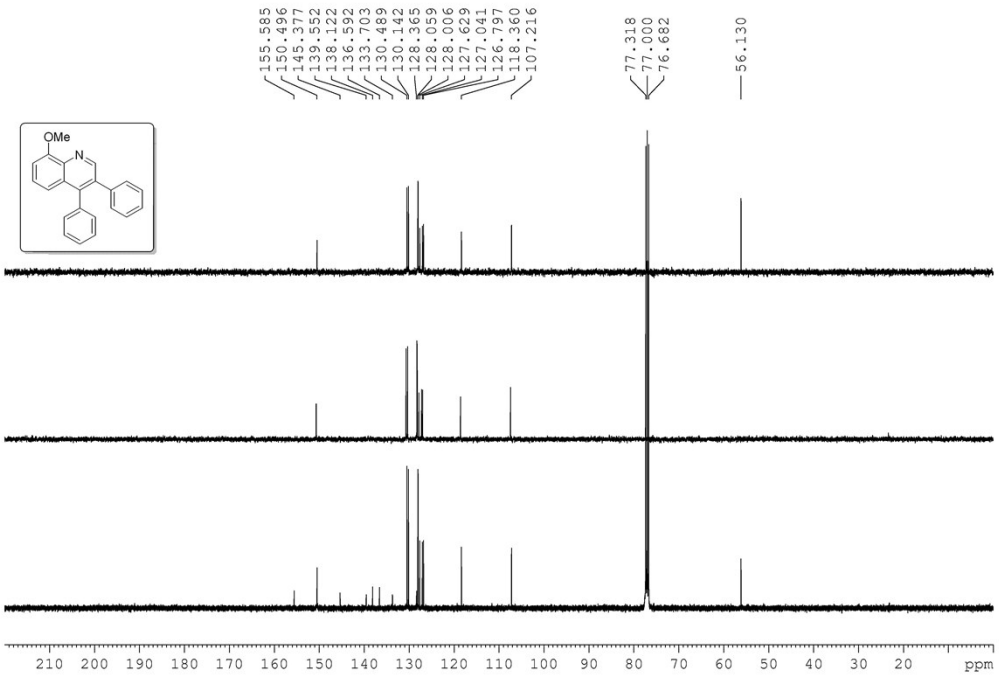
^{1}H and ^{13}C NMR spectra of compound **3ma**.



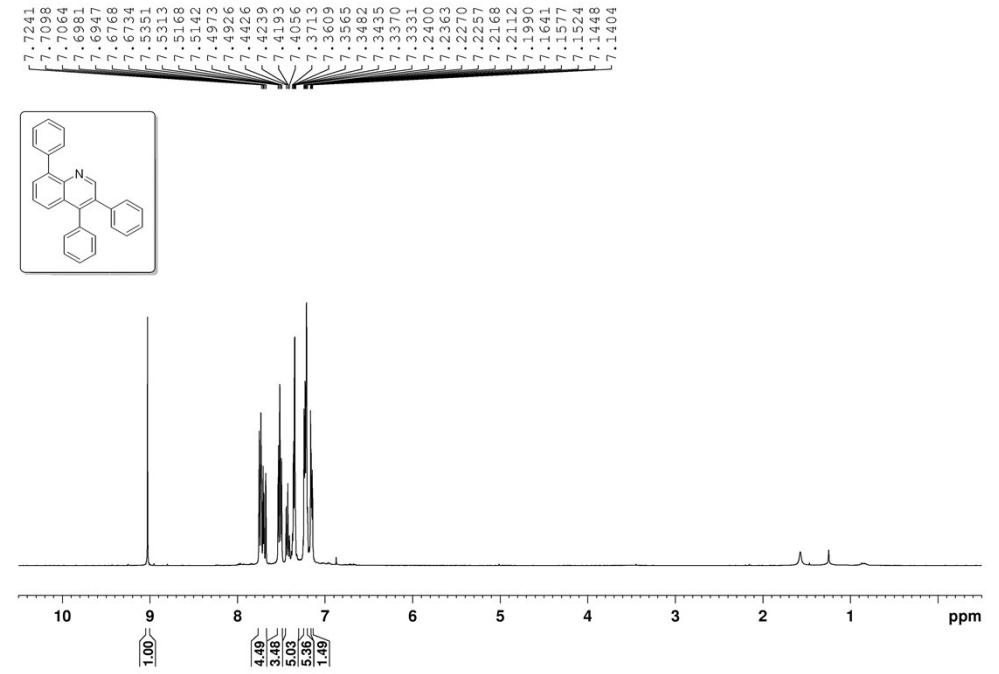


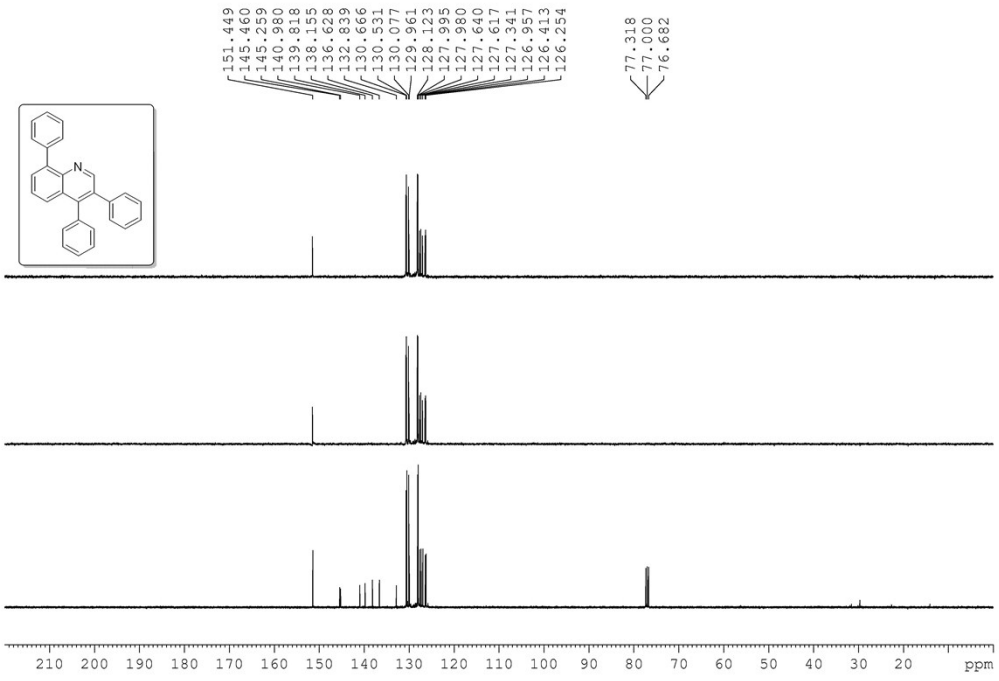
^{1}H and ^{13}C NMR spectra of compound **3na**.



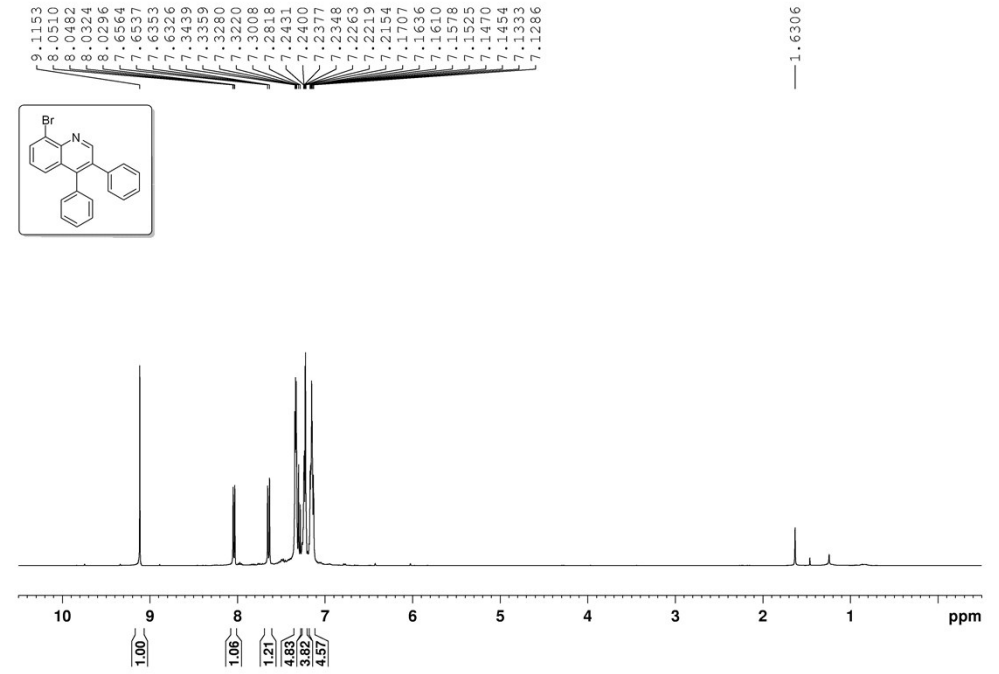


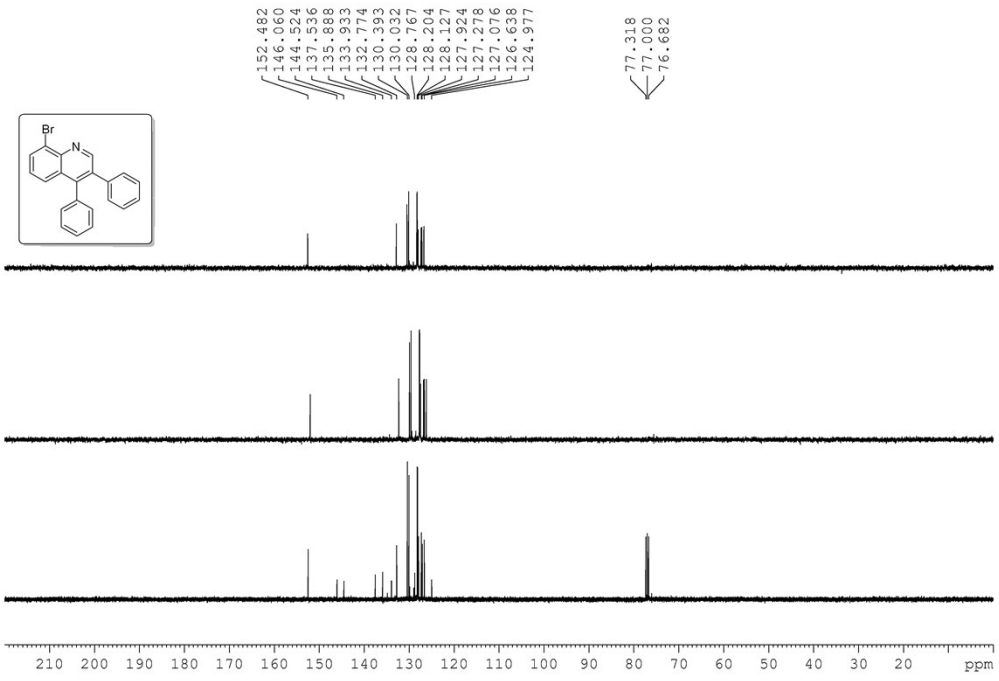
^{1}H and ^{13}C NMR spectra of compound **3oa**.



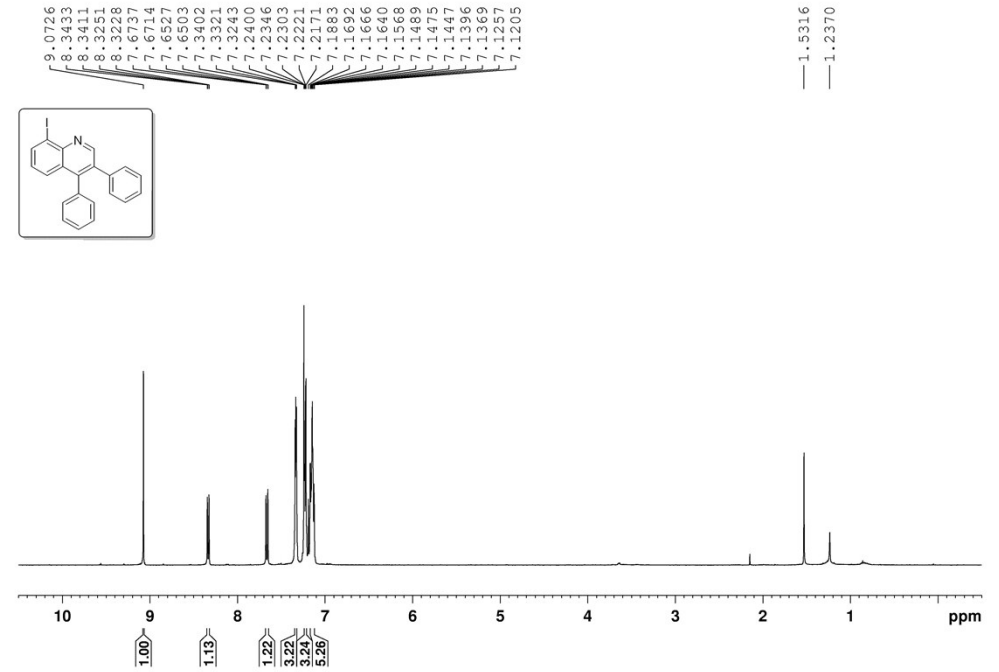


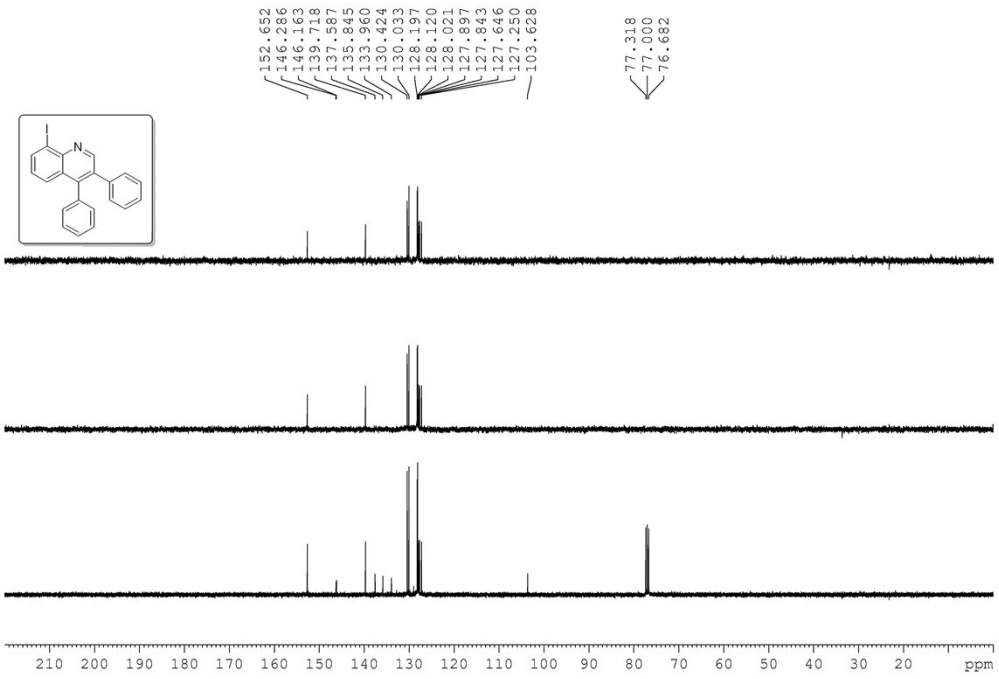
^{1}H and ^{13}C NMR spectra of compound **3pa**.



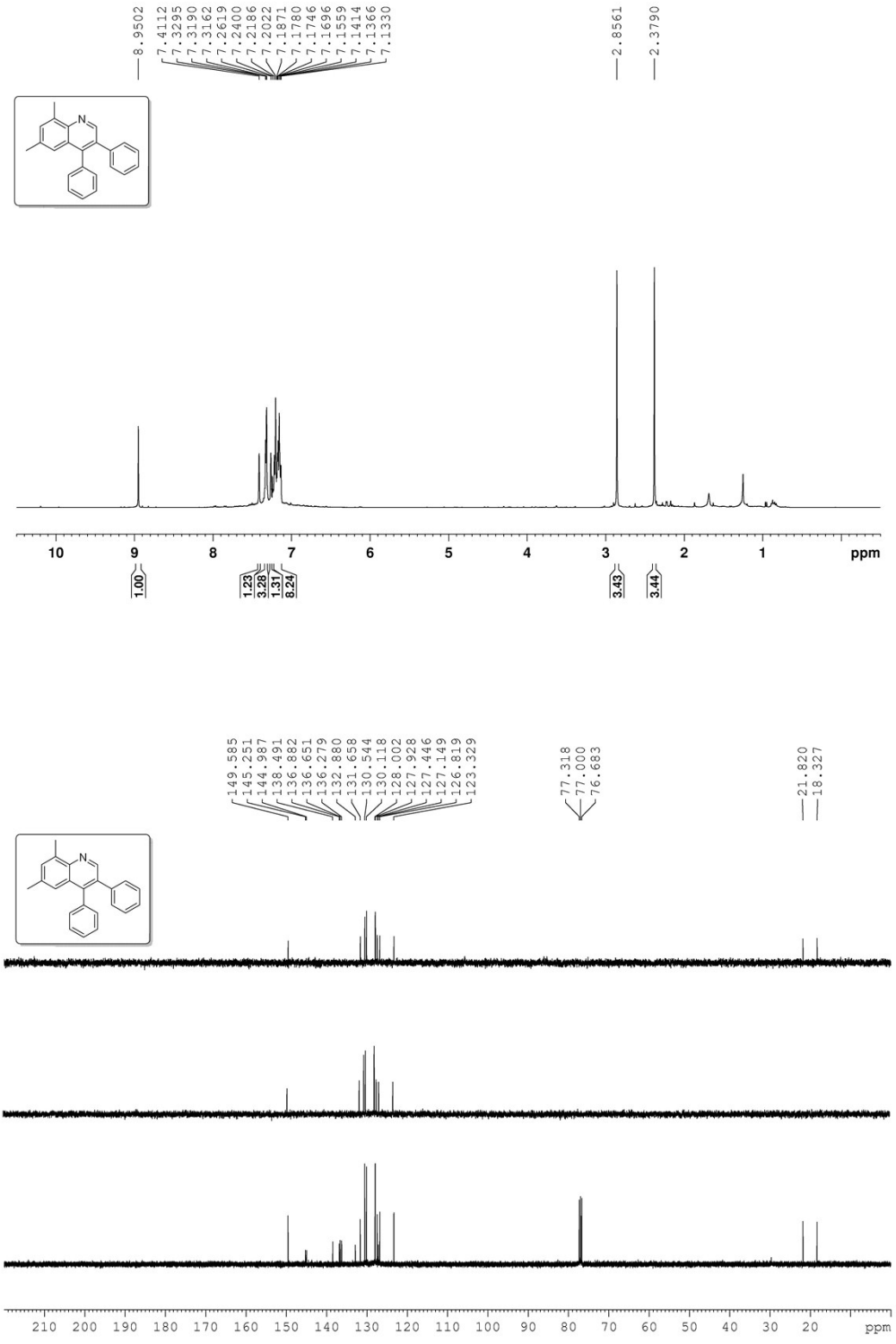


^{1}H and ^{13}C NMR spectra of compound **3qa**.

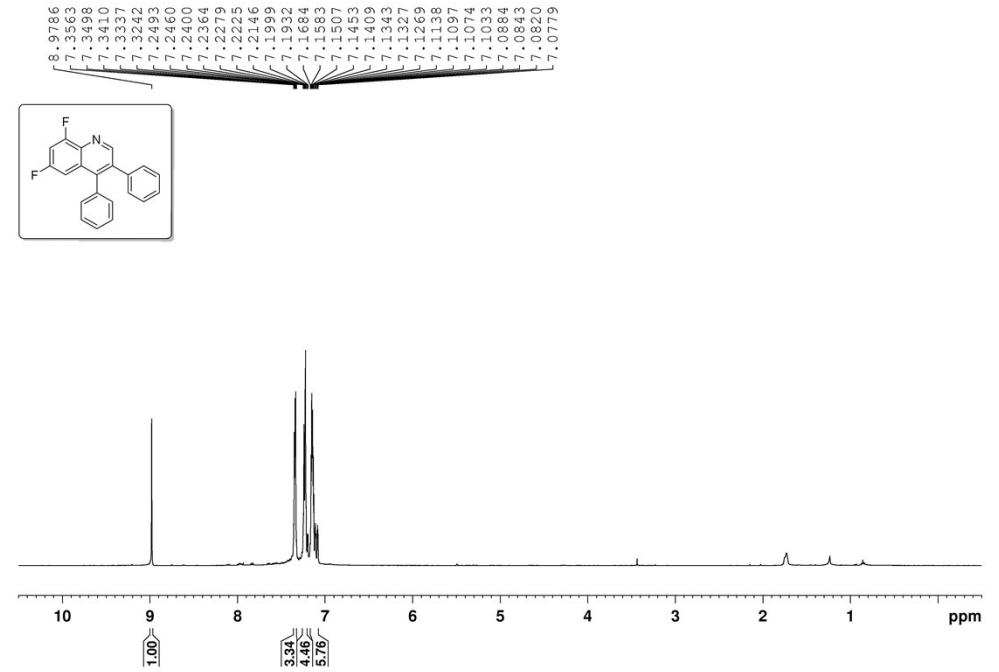


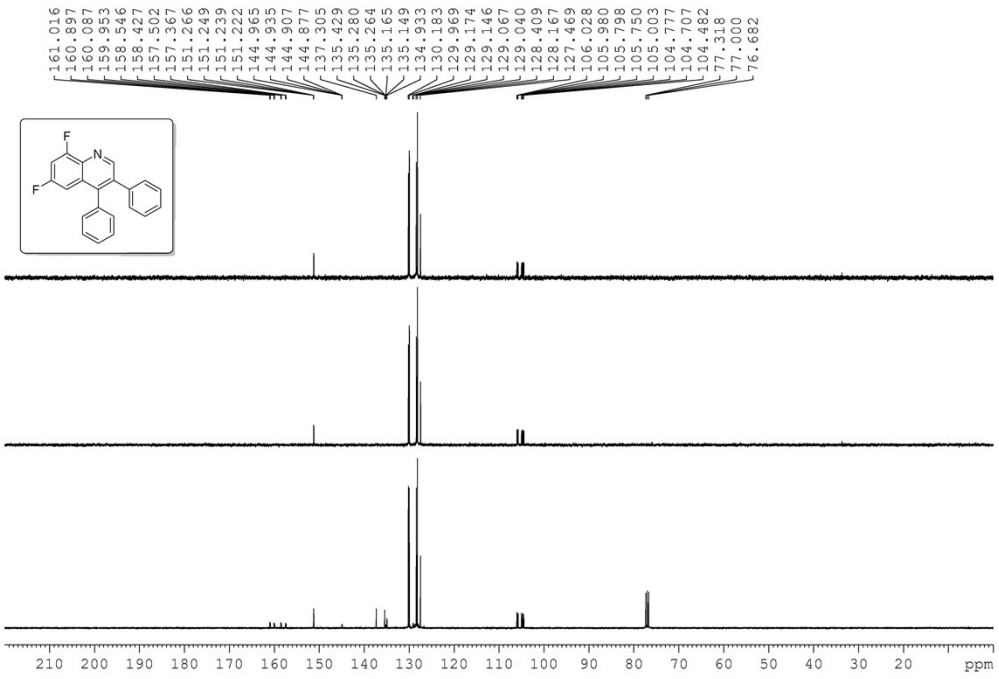


^{1}H and ^{13}C NMR spectra of compound **3ra**.

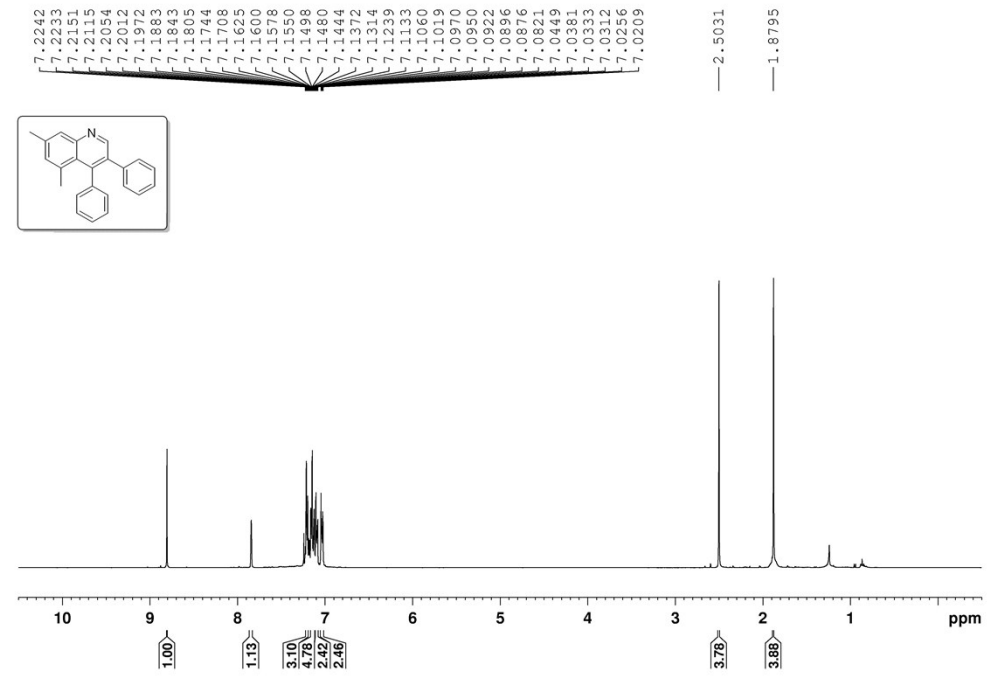


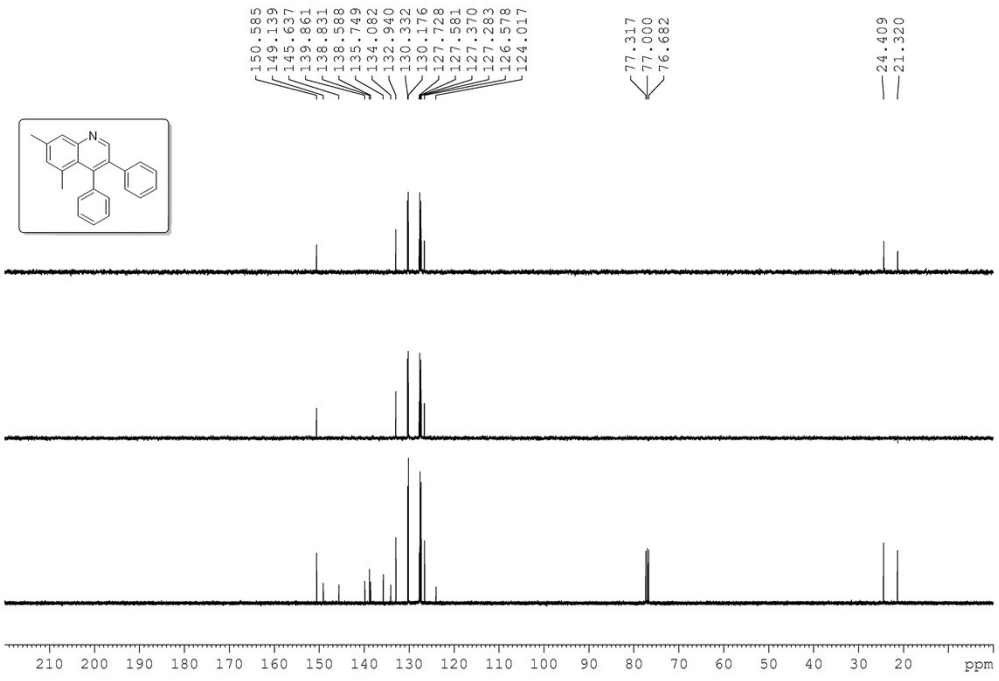
^{1}H and ^{13}C NMR spectra of compound **3sa**.



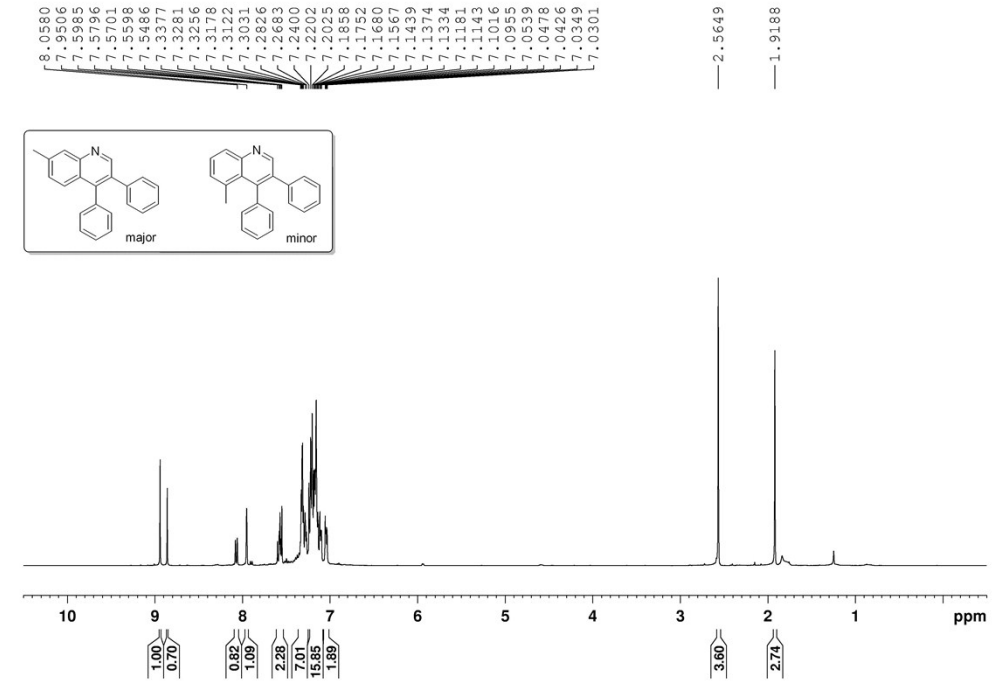


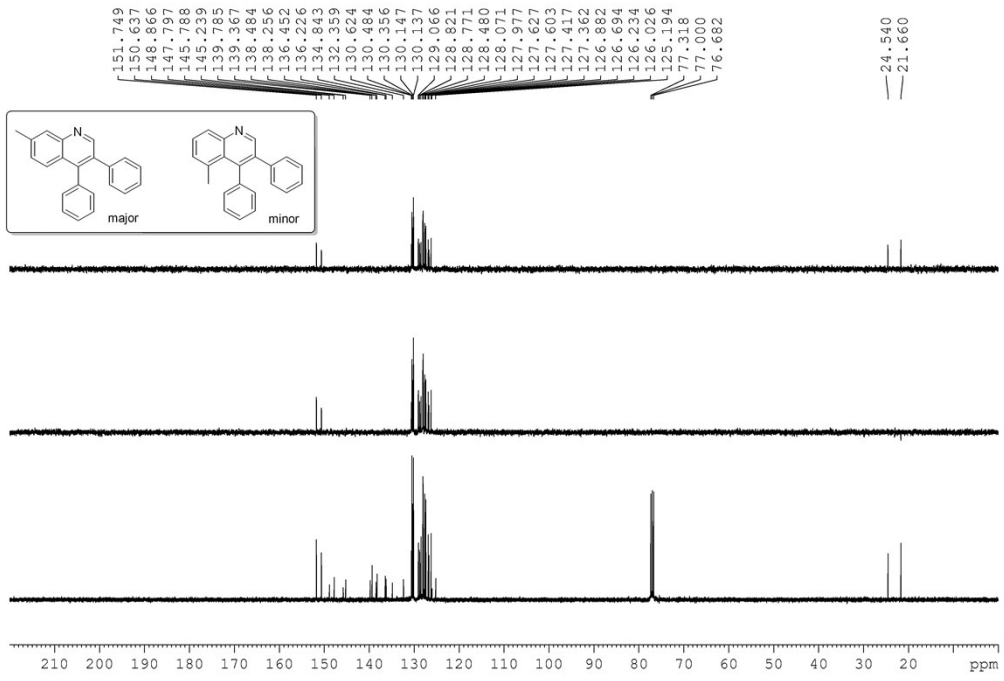
^{1}H and ^{13}C NMR spectra of compound **3ta**.



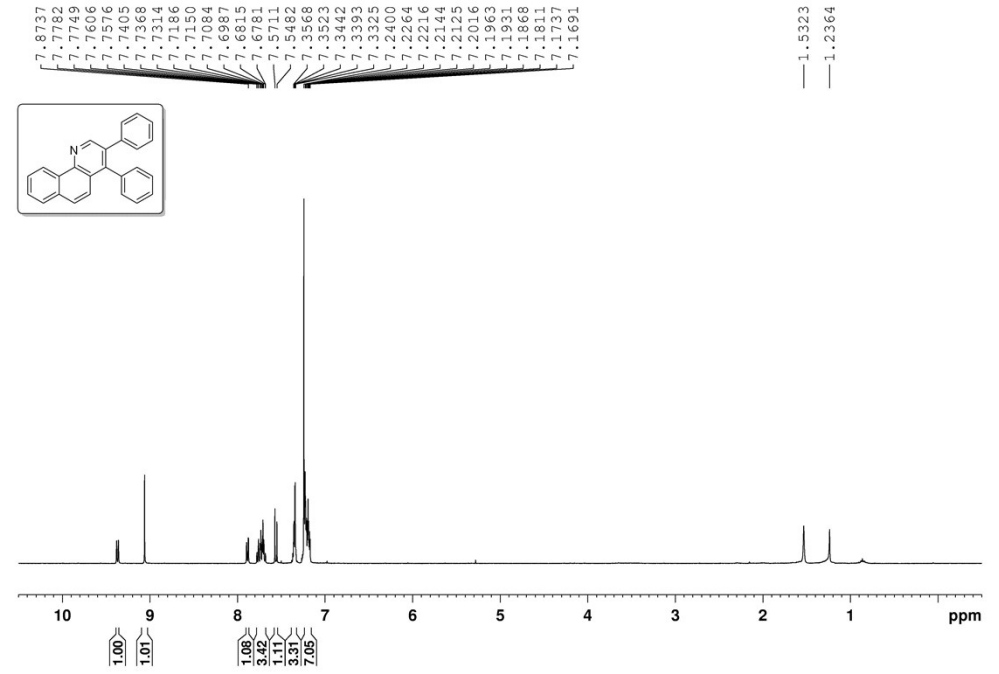


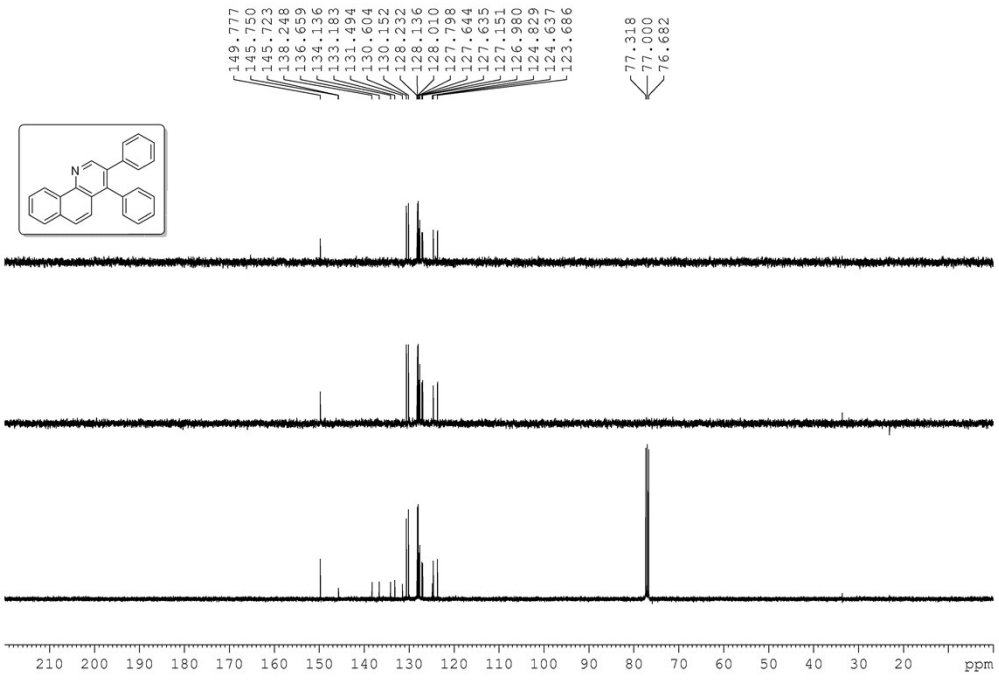
^{1}H and ^{13}C NMR spectra of compound **3ua** and **3ua'**.



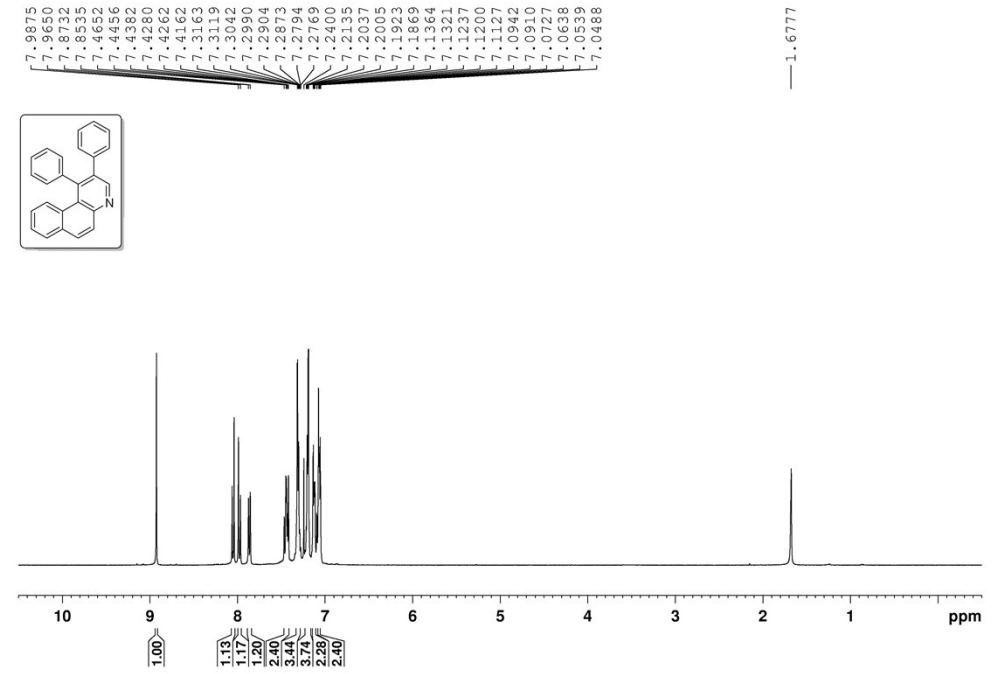


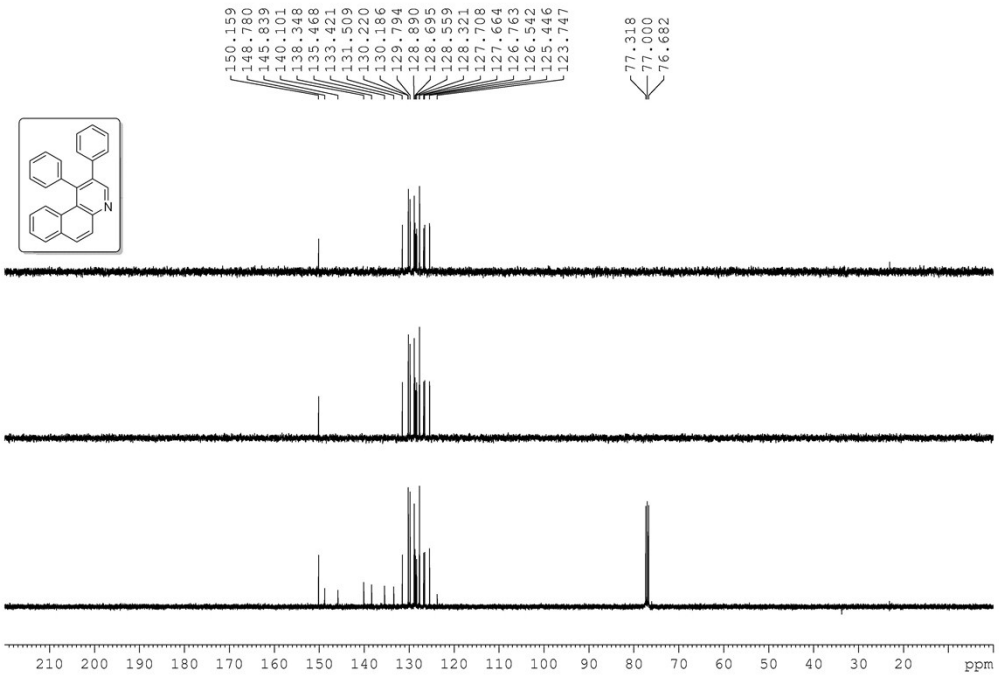
^{1}H and ^{13}C NMR spectra of compound **3va**.



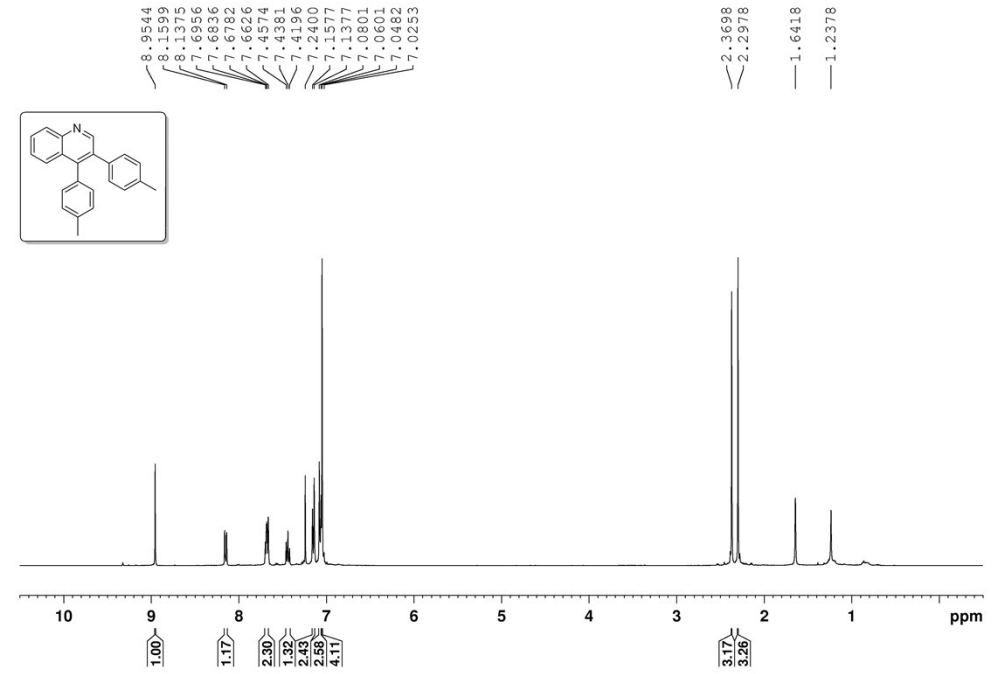


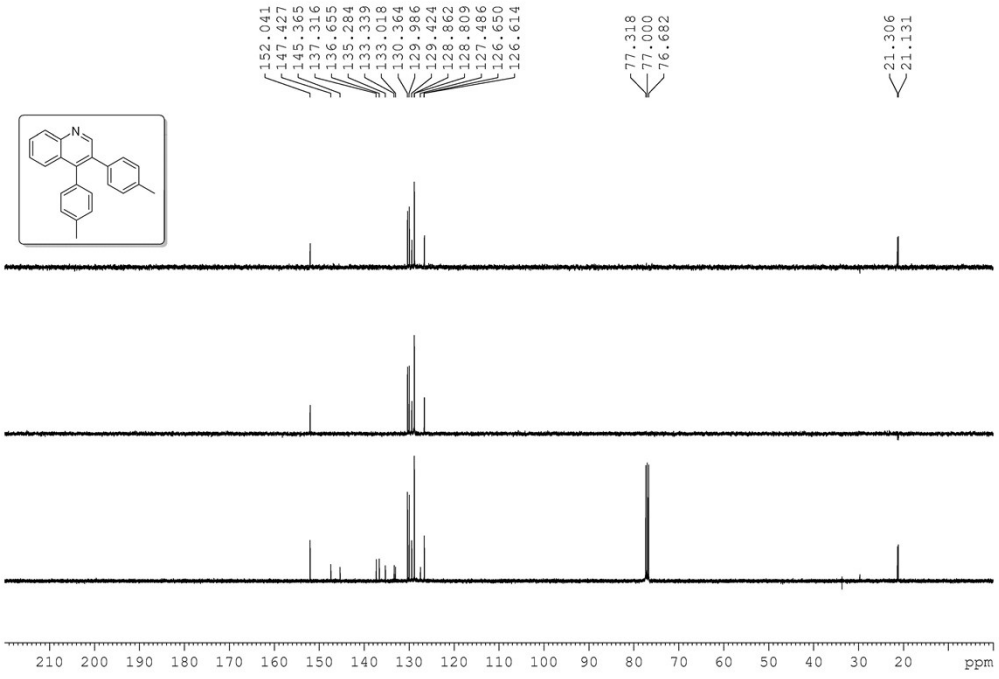
^{1}H and ^{13}C NMR spectra of compound **3wa**.



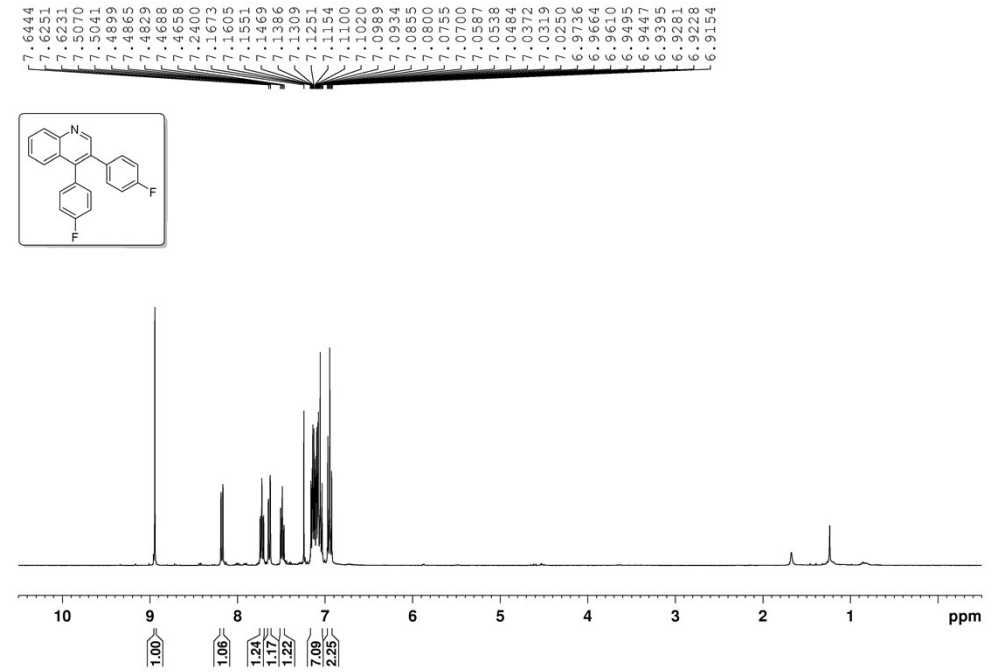


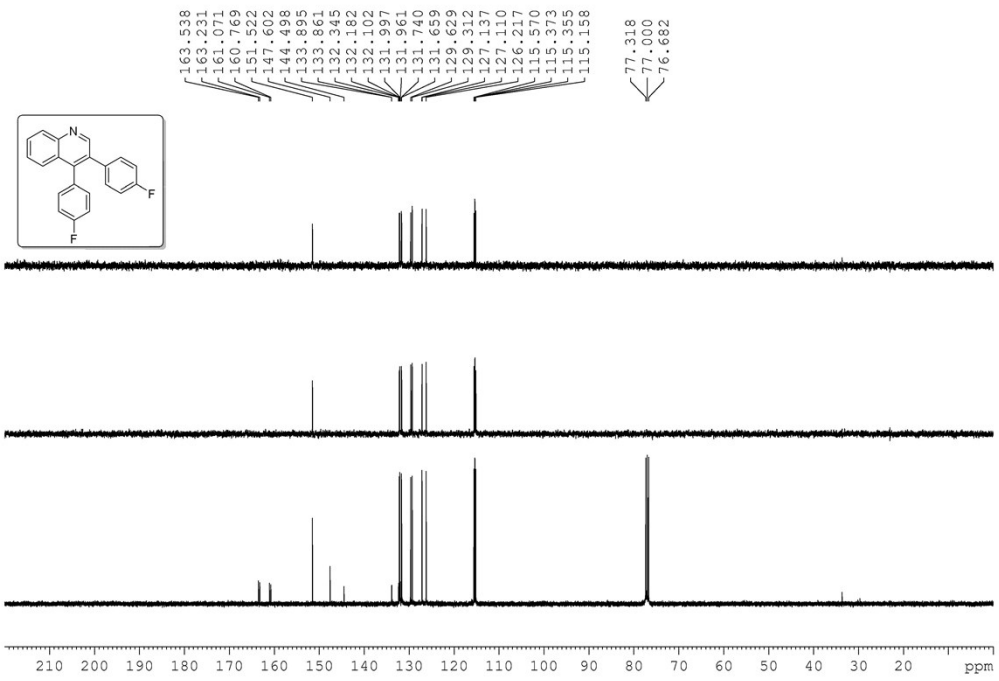
^{1}H and ^{13}C NMR spectra of compound **3ab**.



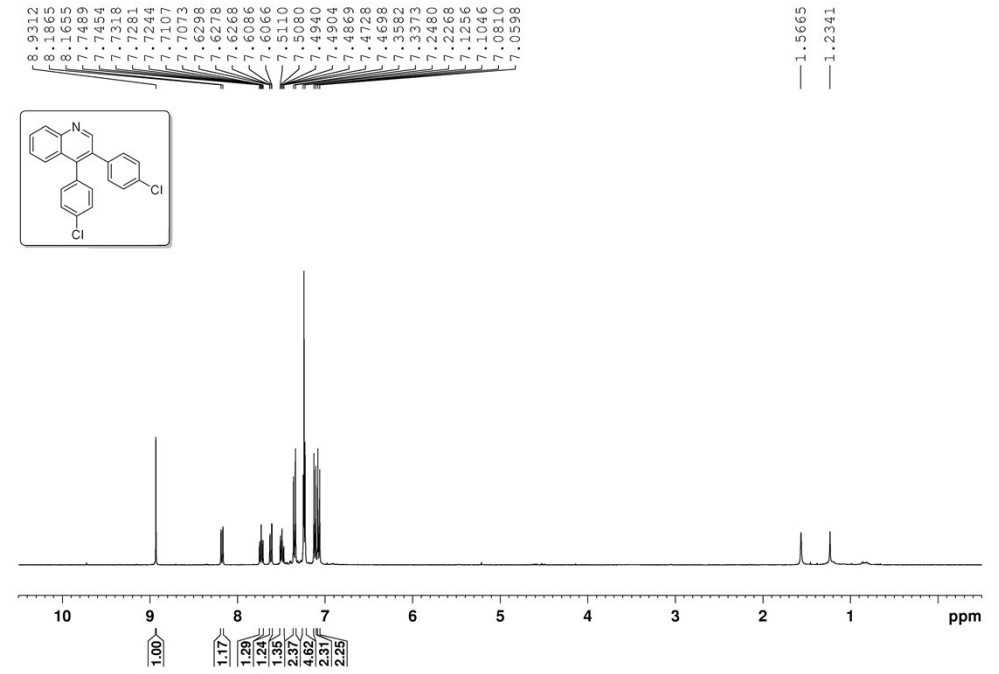


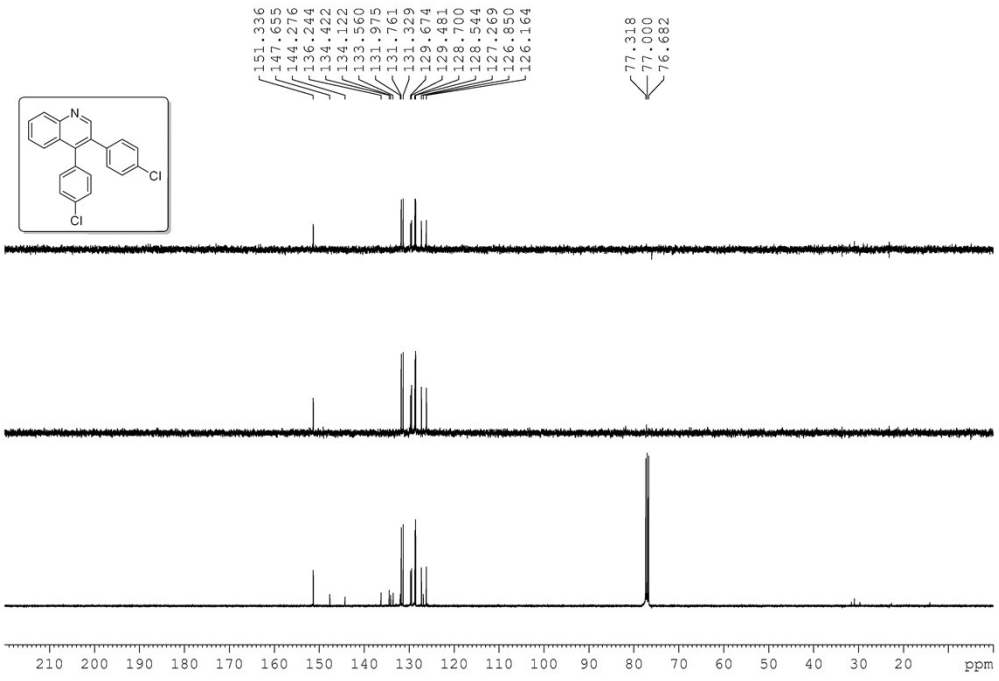
^{1}H and ^{13}C NMR spectra of compound **3ac**.



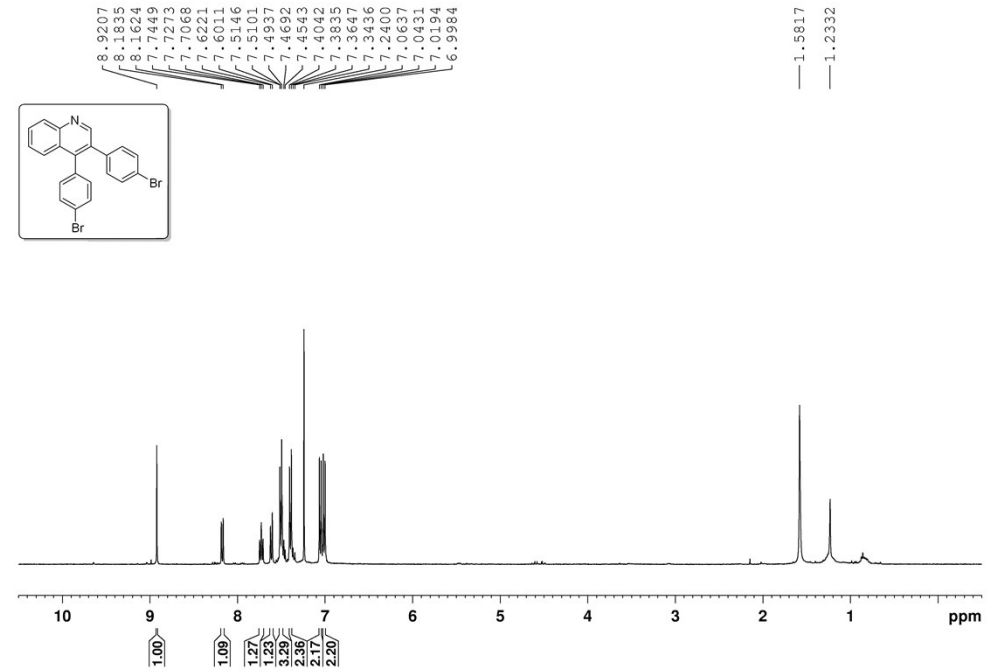


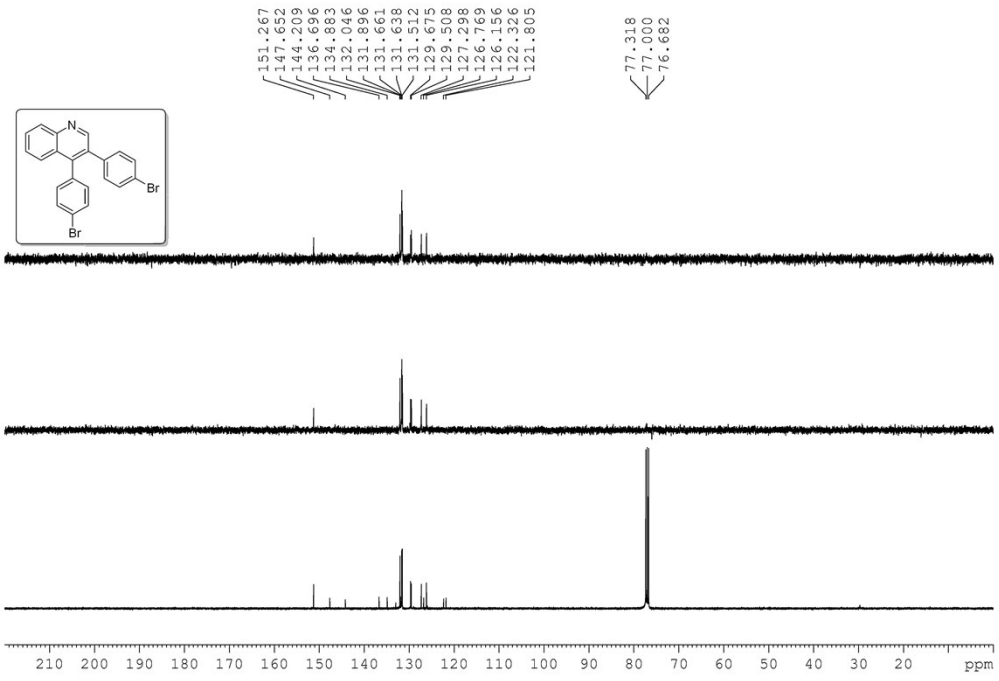
^{1}H and ^{13}C NMR spectra of compound **3ad**.



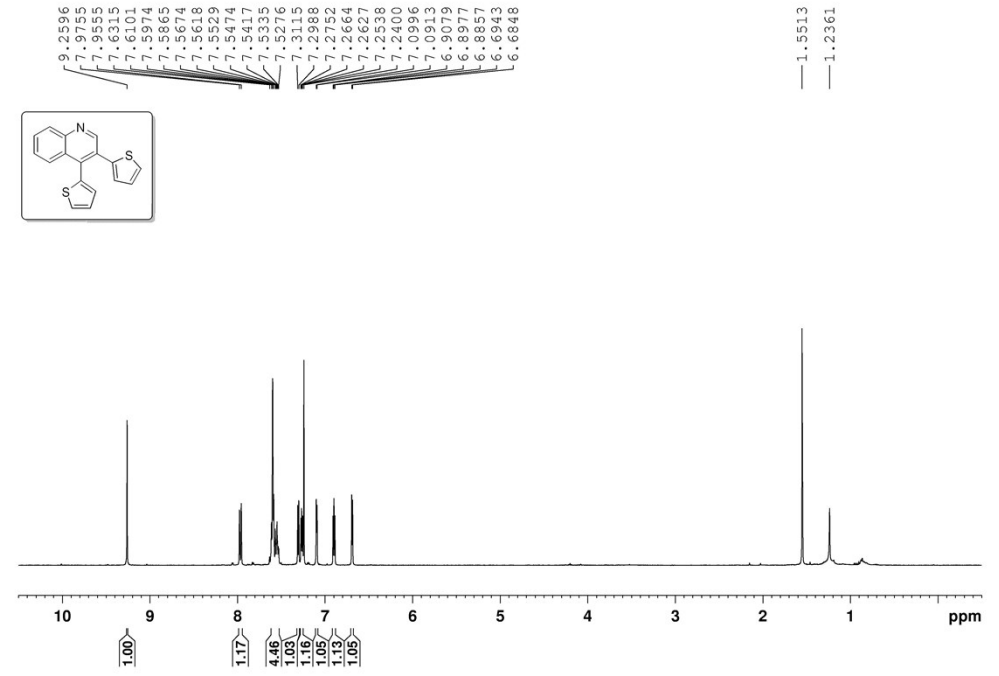


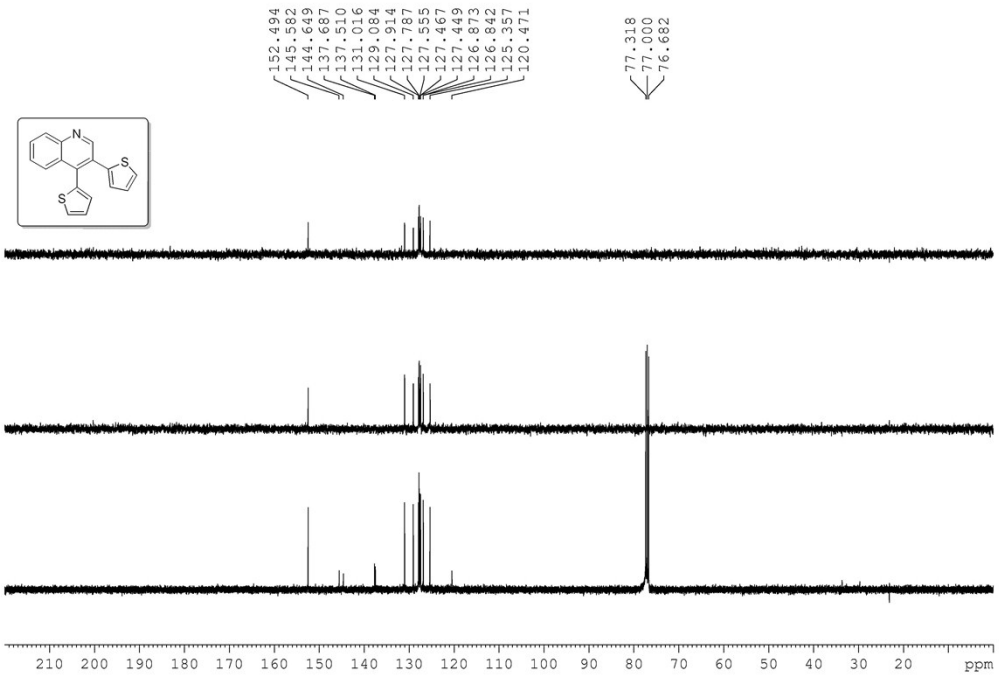
^{1}H and ^{13}C NMR spectra of compound **3ae**.



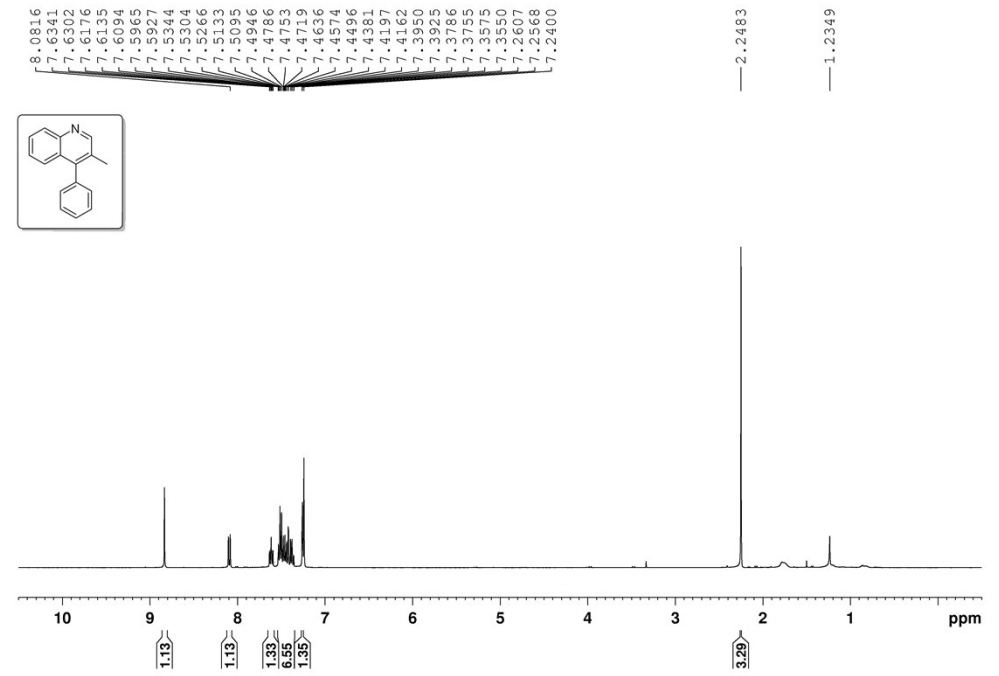


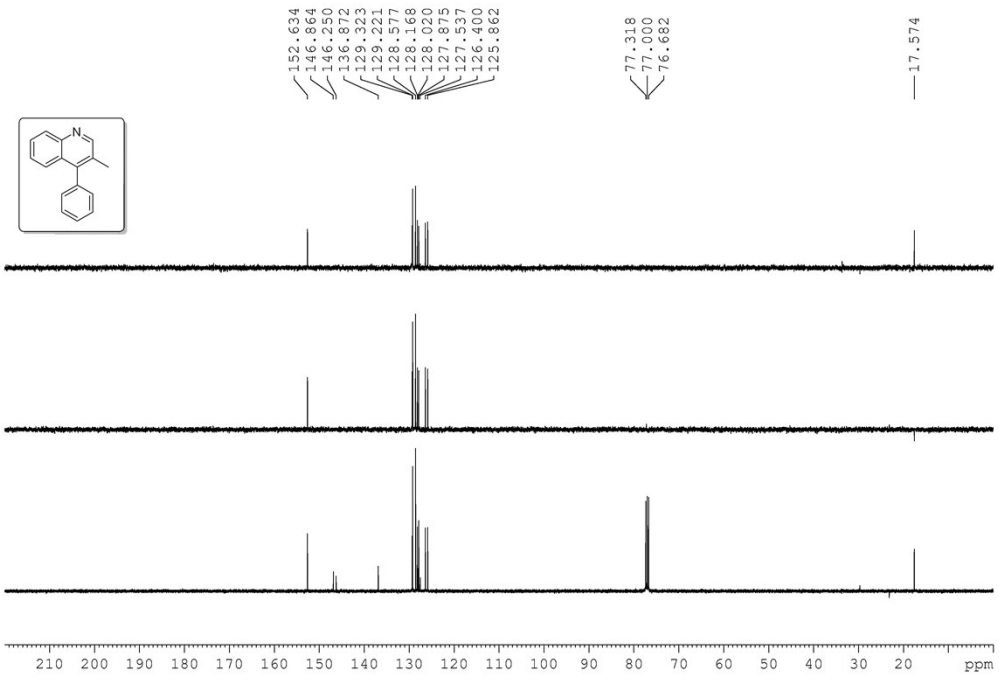
^{1}H and ^{13}C NMR spectra of compound **3af**.



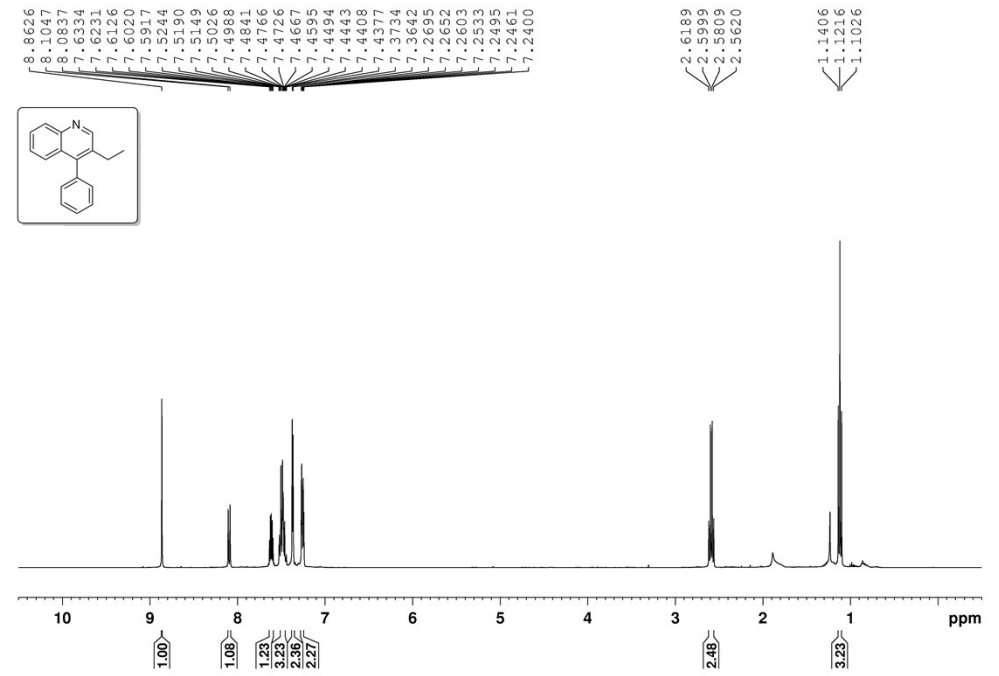


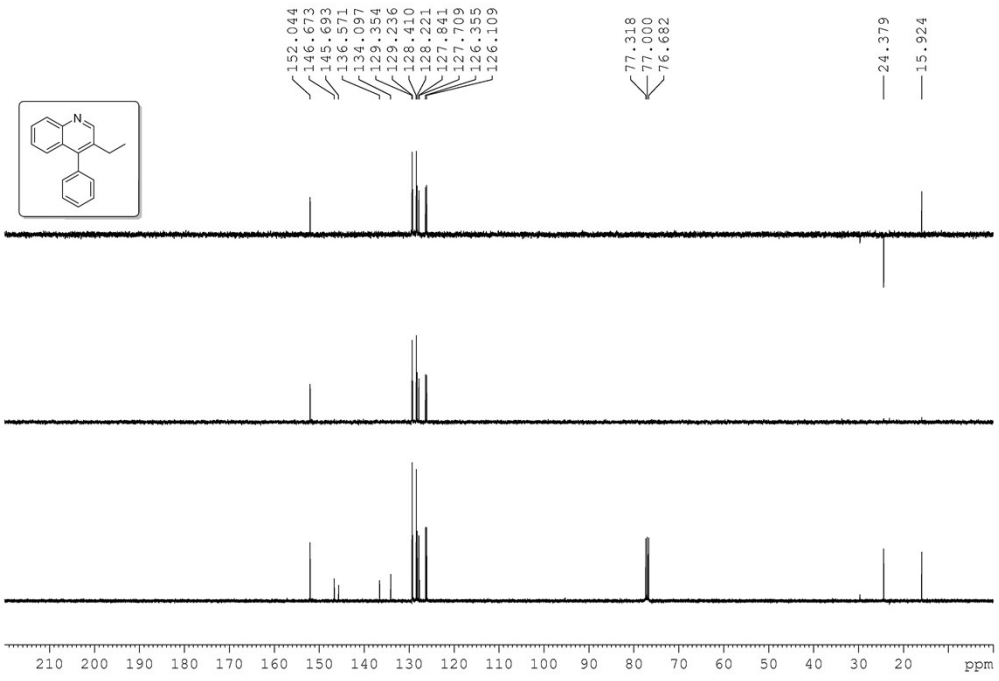
^{1}H and ^{13}C NMR spectra of compound **3ag**.



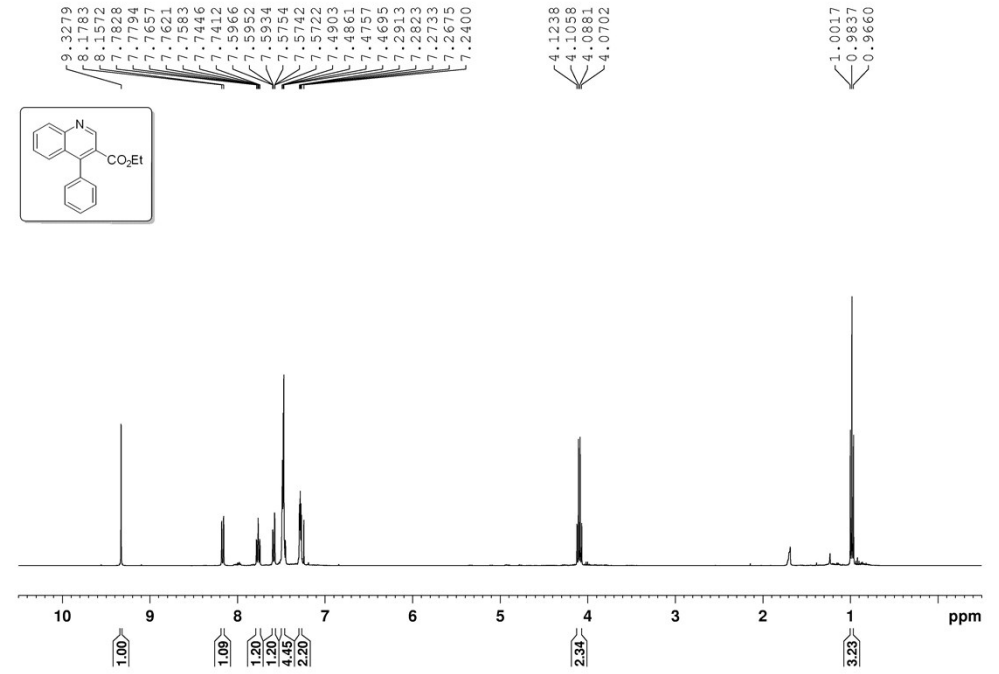


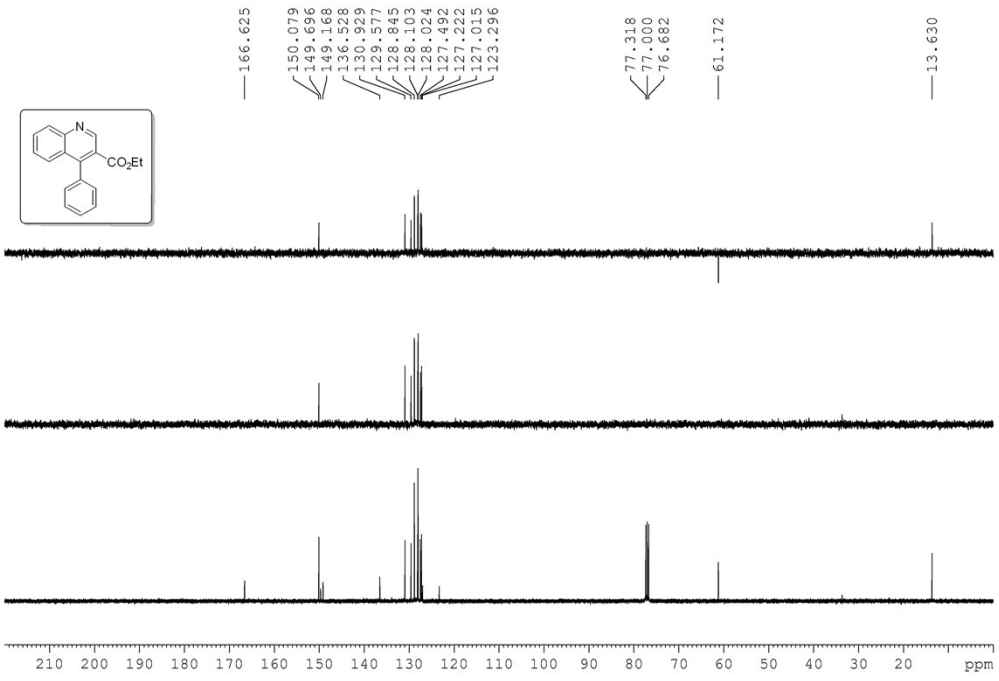
^{1}H and ^{13}C NMR spectra of compound **3ah**.



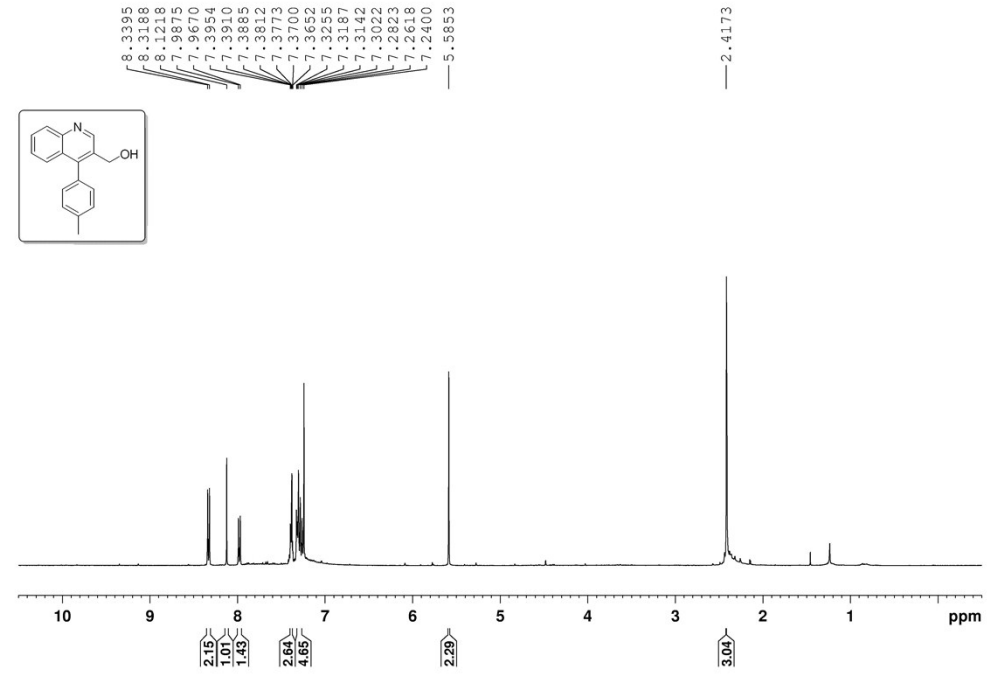


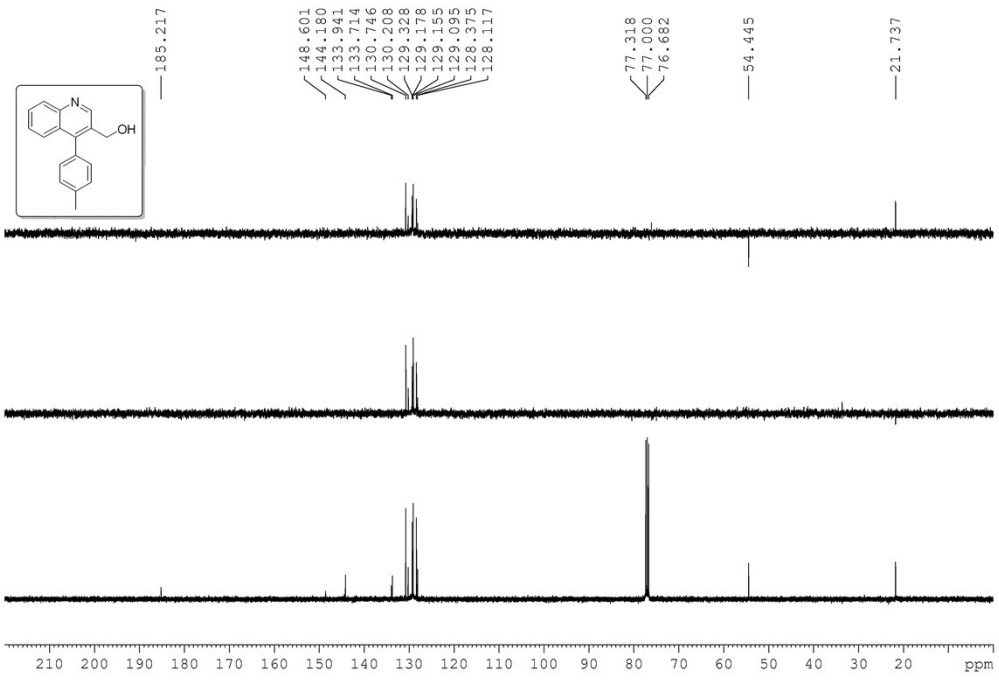
^{1}H and ^{13}C NMR spectra of compound **3ai**.



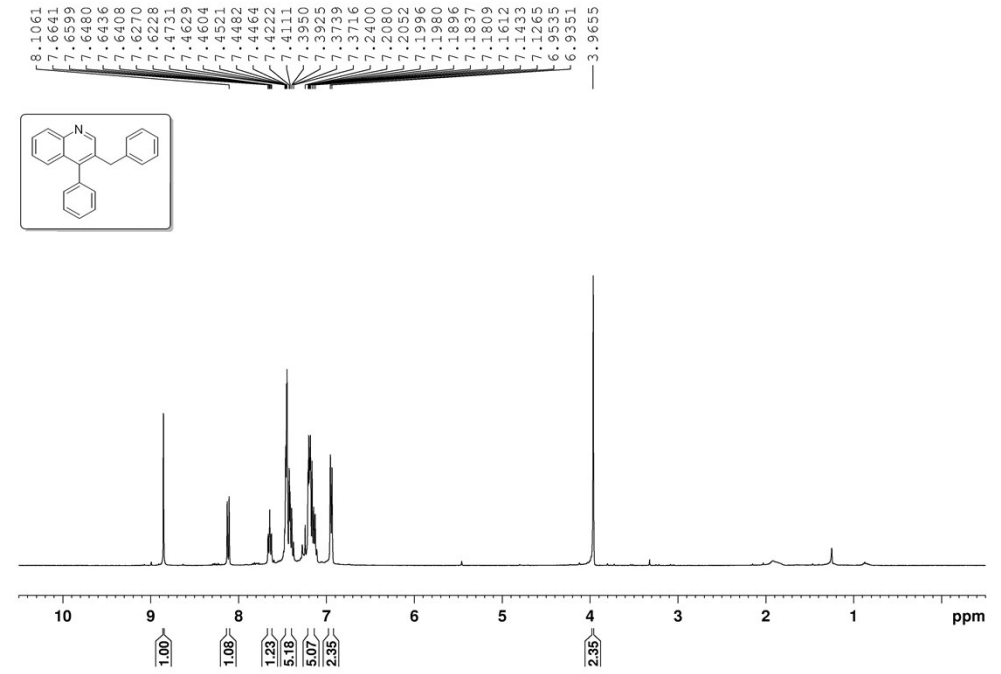


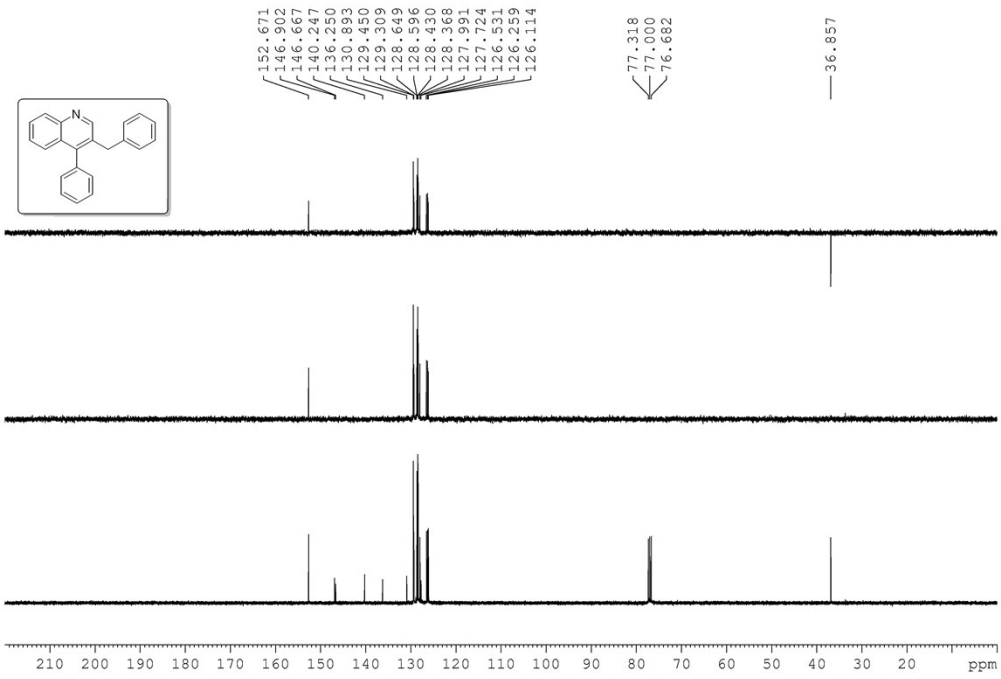
^{1}H and ^{13}C NMR spectra of compound **3aj**.



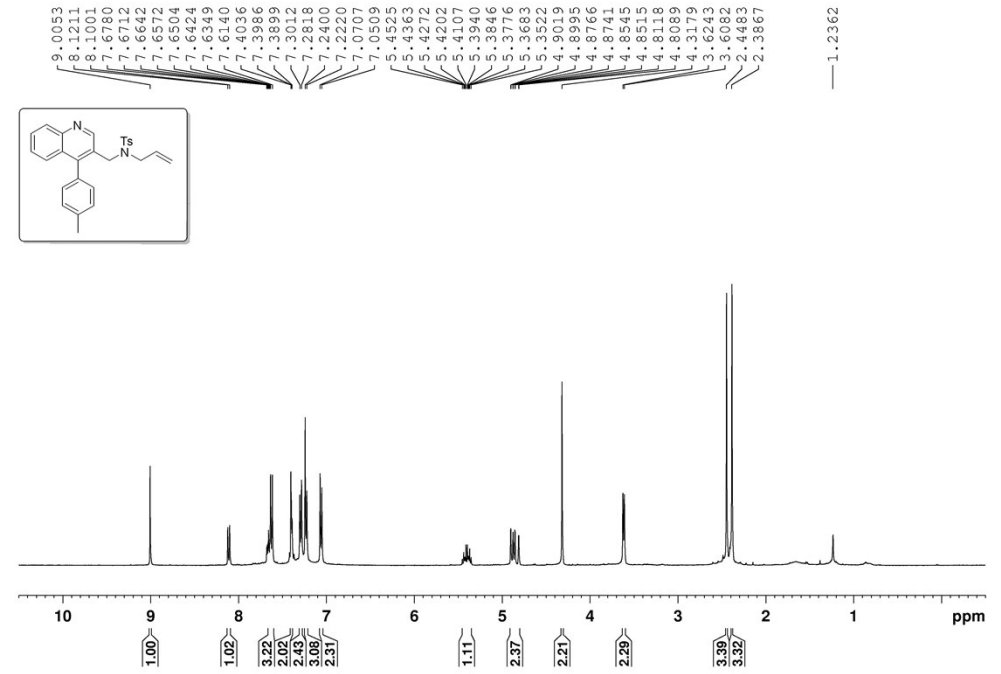


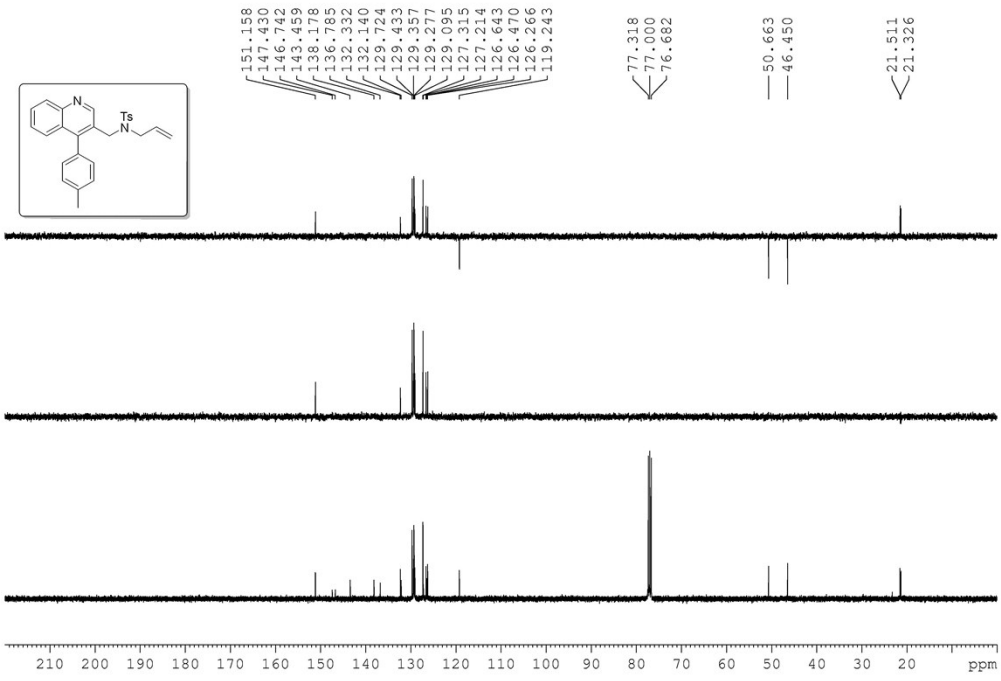
^{1}H and ^{13}C NMR spectra of compound **3ak**.



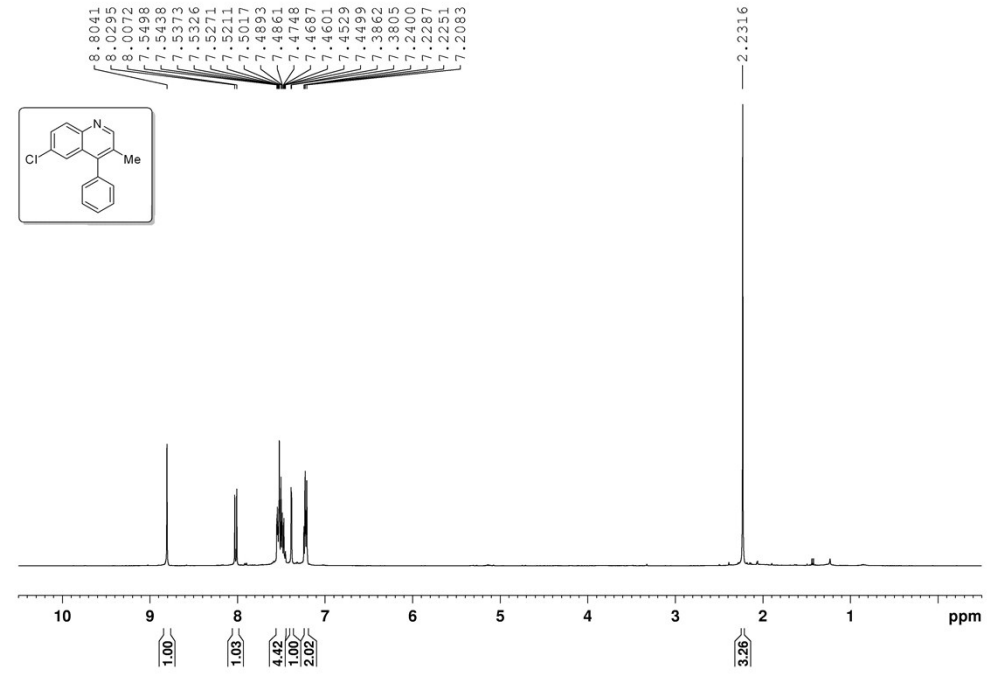


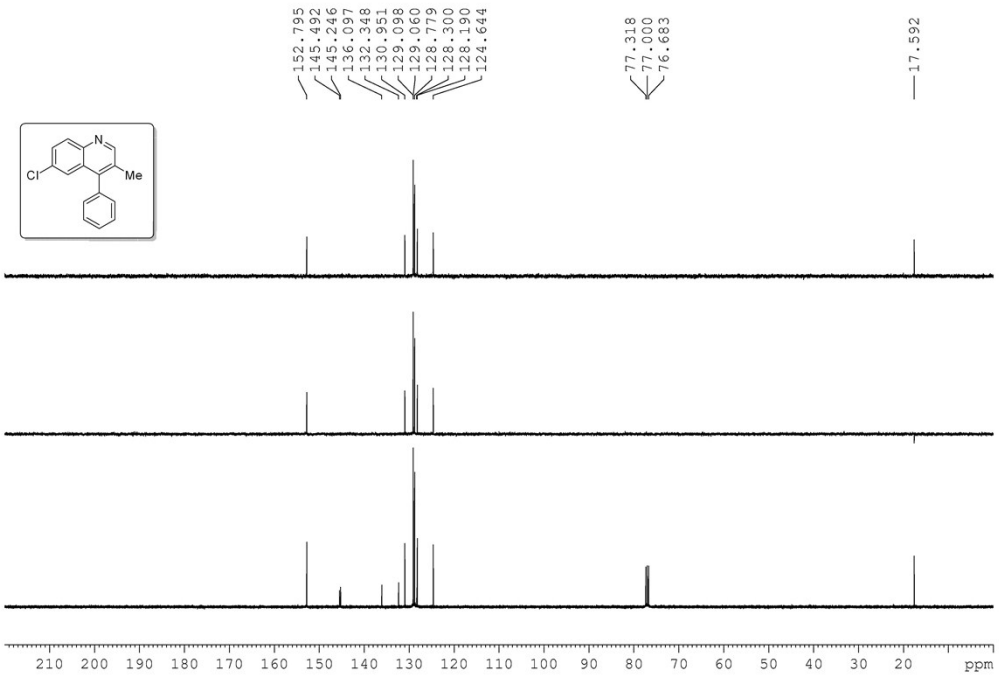
^{1}H and ^{13}C NMR spectra of compound **3al**.



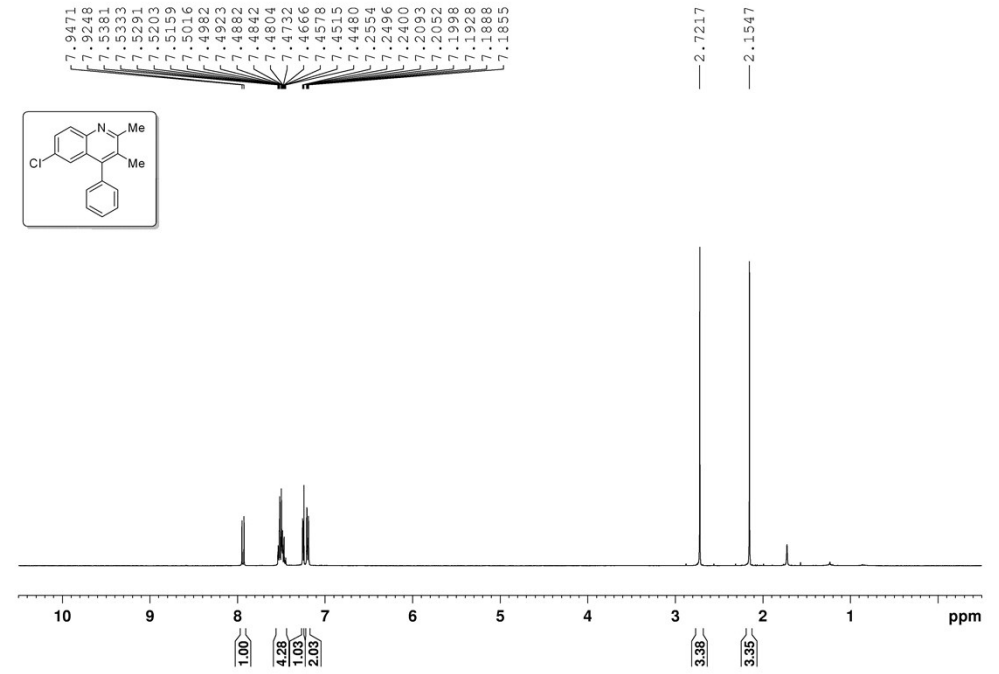


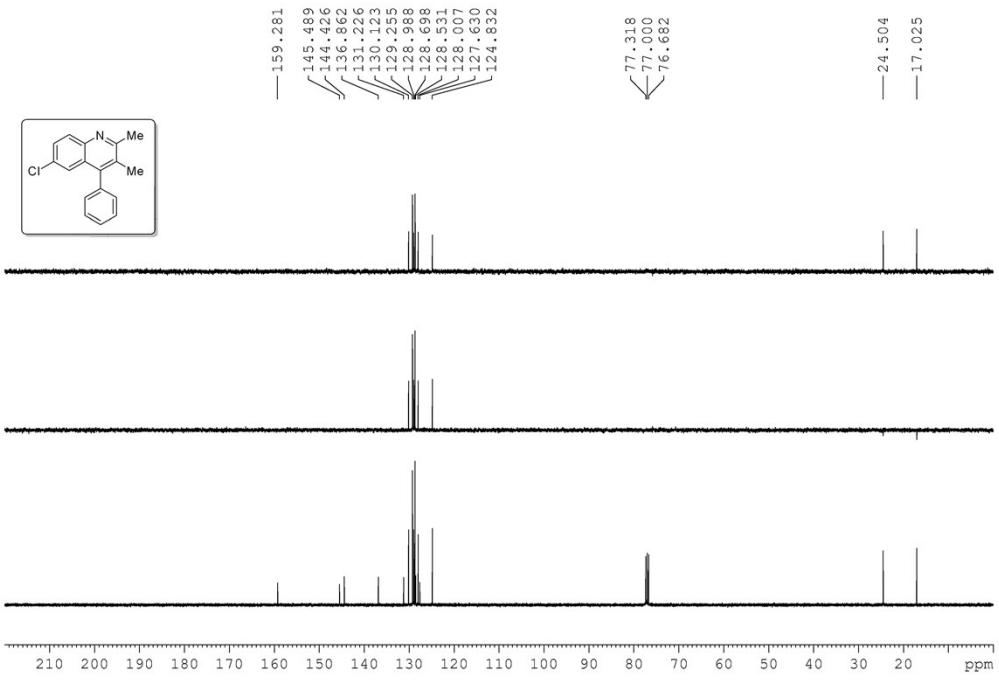
^{1}H and ^{13}C NMR spectra of compound **3fg**.



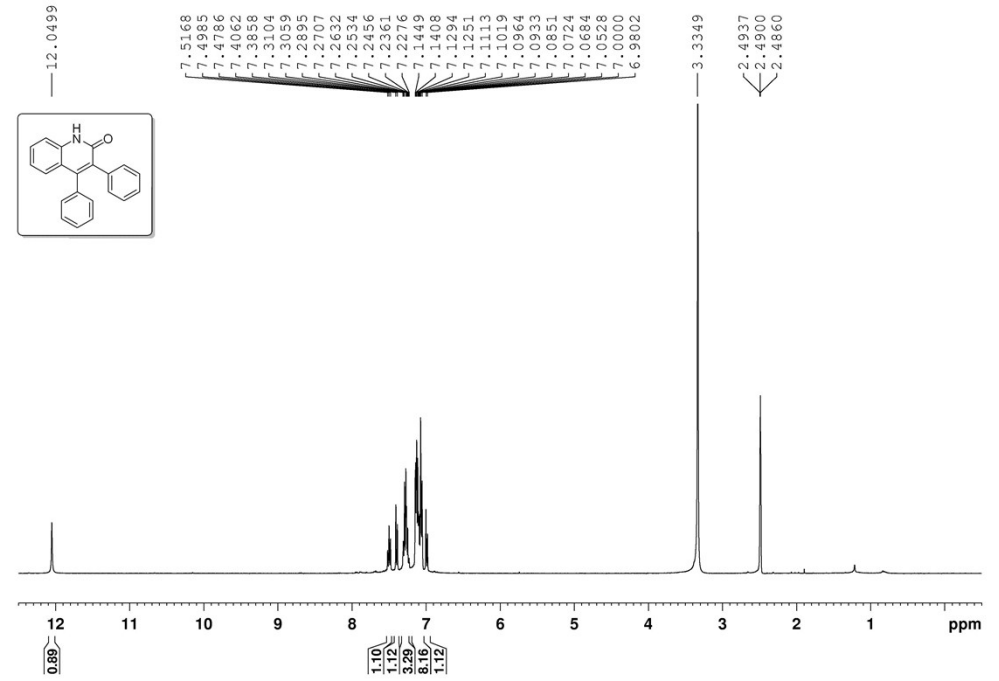


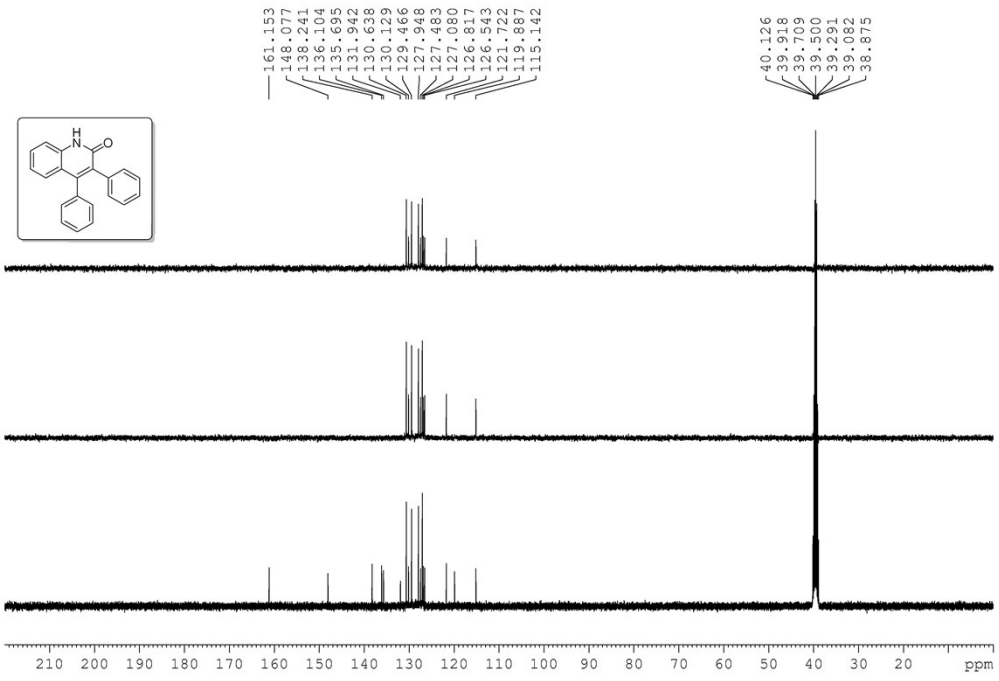
^{1}H and ^{13}C NMR spectra of compound **4**.





^{1}H and ^{13}C NMR spectra of compound **5**.





X-ray Crystallographic Analysis:

ORTEP diagram of compound **3aa**.

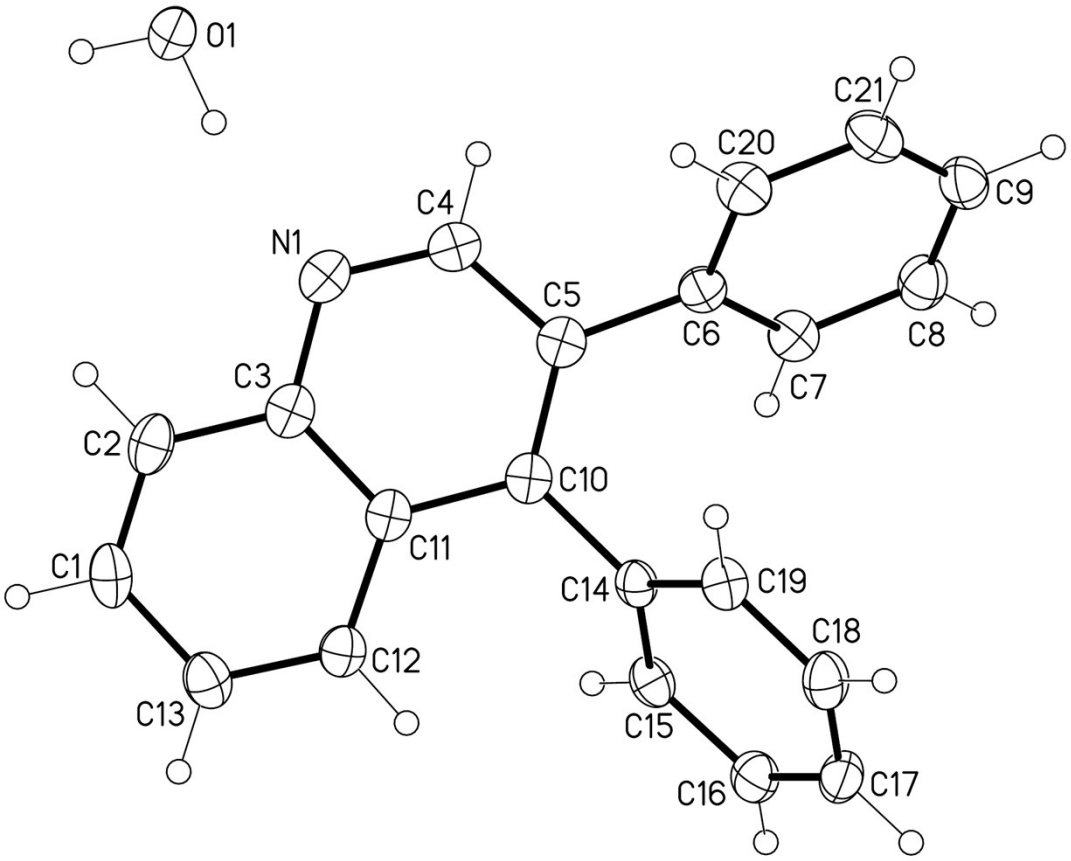


Table S5. Crystal data and structure refinement for mo_130938lt_0m.

Identification code	mo_130938lt_0m	
Empirical formula	C21 H16 N O0.50	
Formula weight	290.35	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 15.8693(8) Å	α= 90°.
	b = 9.9218(5) Å	β= 102.4240(10)°.
	c = 20.1836(10) Å	γ = 90°.
Volume	3103.5(3) $Å^3$	
Z	8	
Density (calculated)	1.243 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	1224	
Crystal size	0.25 x 0.12 x 0.12 mm^3	
Theta range for data collection	2.07 to 26.50°.	
Index ranges	-19<=h<=19, -8<=k<=12, -25<=l<=25	
Reflections collected	12498	
Independent reflections	3210 [R(int) = 0.0398]	
Completeness to theta = 26.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8850	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3210 / 0 / 204	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.0845	
R indices (all data)	R1 = 0.0656, wR2 = 0.0947	
Largest diff. peak and hole	0.186 and -0.189 $e.Å^{-3}$	

ORTEP diagram of compound **3va**.

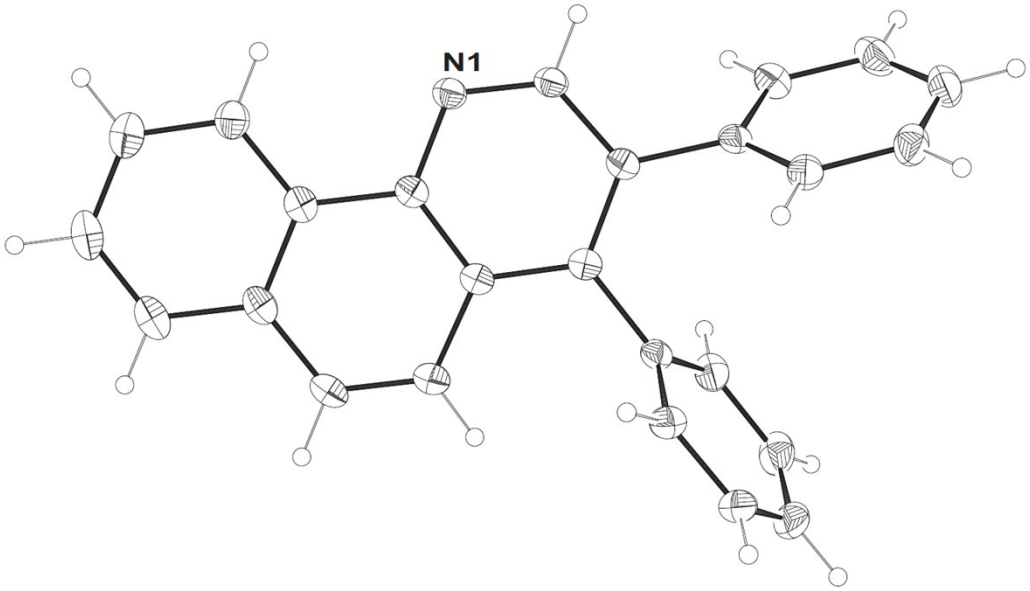


Table S6. Crystal data and structure refinement for ch16647.

Identification code	ch16647	
Empirical formula	C25 H17 N	
Formula weight	331.40	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.6366(11) Å	α= 101.660(2)°.
	b = 9.9502(13) Å	β= 94.005(2)°.
	c = 11.2433(15) Å	γ = 111.536(2)°.
Volume	869.1(2) $Å^3$	
Z	2	
Density (calculated)	1.266 Mg/m^3	
Absorption coefficient	0.073 mm^{-1}	
F(000)	348	
Crystal size	0.79 x 0.47 x 0.41 mm^3	
Theta range for data collection	1.87 to 25.09°.	
Index ranges	-10<=h<=8, -11<=k<=10, -13<=l<=12	
Reflections collected	7792	
Independent reflections	3089 [R(int) = 0.0266]	
Completeness to theta = 25.09°	99.7 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9706 and 0.9445	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3089 / 0 / 235	
Goodness-of-fit on F^2	1.080	
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.1135	
R indices (all data)	R1 = 0.0533, wR2 = 0.1314	
Largest diff. peak and hole	0.245 and -0.330 $e.Å^{-3}$	

ORTEP diagram of compound **3ag**.

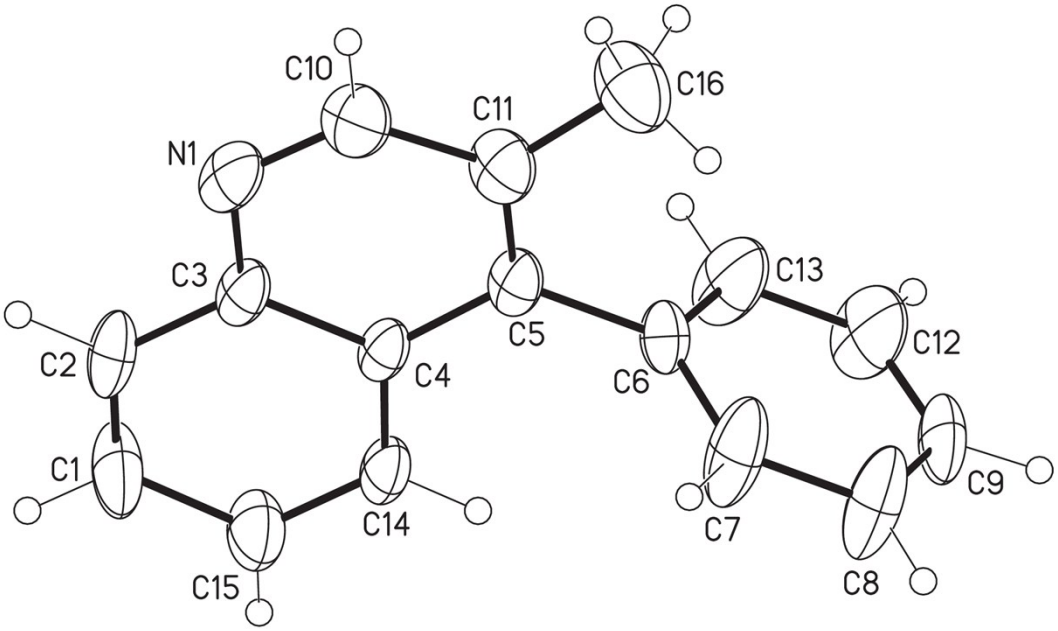


Table S7. Crystal data and structure refinement for 141206LT.

Identification code	141206LT	
Empirical formula	C16 H13 N	
Formula weight	219.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.8347(5) Å	α= 82.727(3)°.
	b = 8.6813(5) Å	β= 73.371(3)°.
	c = 9.1755(8) Å	γ = 78.005(2)°.
Volume	583.42(7) $Å^3$	
Z	2	
Density (calculated)	1.248 Mg/m^3	
Absorption coefficient	0.073 mm^{-1}	
F(000)	232	
Crystal size	0.12 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.323 to 26.429°.	
Index ranges	-9<=h<=9, -10<=k<=10, -11<=l<=11	
Reflections collected	8929	
Independent reflections	2381 [R(int) = 0.0267]	
Completeness to theta = 25.242°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8564	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2381 / 0 / 155	
Goodness-of-fit on F^2	1.104	
Final R indices [I>2sigma(I)]	R1 = 0.0682, wR2 = 0.1961	
R indices (all data)	R1 = 0.0949, wR2 = 0.2345	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.542 and -0.417 $e.Å^{-3}$	

ORTEP diagram of compound **3ah**.

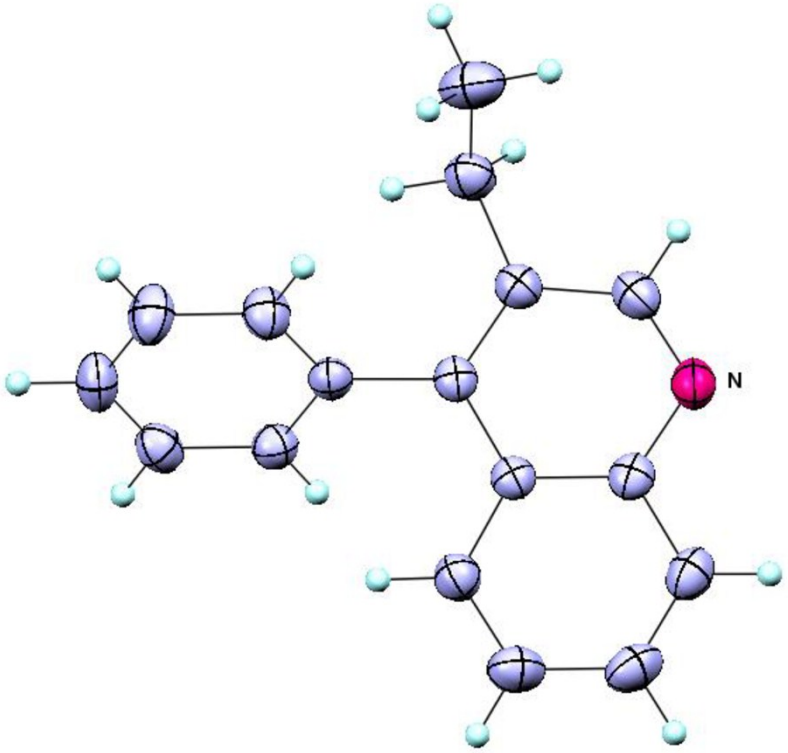


Table S8. Crystal data and structure refinement for a16797.

Identification code	a16797	
Empirical formula	C17 H15 N	
Formula weight	233.30	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.1521(7) Å	α= 90°.
	b = 25.648(2) Å	β= 97.064(4)°.
	c = 18.4479(13) Å	γ = 90°.
Volume	3827.8(6) $Å^3$	
Z	12	
Density (calculated)	1.214 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	1488	
Crystal size	0.62 x 0.35 x 0.10 mm^3	
Theta range for data collection	2.22 to 25.02°.	
Index ranges	-9<=h<=9, -30<=k<=28, -21<=l<=17	
Reflections collected	21787	
Independent reflections	6688 [R(int) = 0.0436]	
Completeness to theta = 25.02°	99.0 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9930 and 0.9577	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6688 / 0 / 487	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.0944	
R indices (all data)	R1 = 0.0707, wR2 = 0.1080	
Largest diff. peak and hole	0.130 and -0.176 $e.Å^{-3}$	