

Supporting information

Nickel-PNN catalysed sustainable synthesis of polysubstituted quinolines under microwave irradiation

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Crystal structure determination of complexes.

Single crystals of all complexes were mounted on a Cryoloop with a drop of paratone oil and positioned in the cold nitrogen stream on a Bruker D8 Venture diffractometer. The data collections were performed at 100 K to 150 K using Bruker D8 Venture diffractometer with a graphite monochromated Mo K α radiation source ($\lambda = 0.71073 \text{ \AA}$) with the ω -scan technique. The data were reduced using CrysAlisPro Red 171.41_64.93a software.¹ The structures were solved using Olex2 1.5² with the ShelXT³ structure solution program using intrinsic phasing and refined with SHELXL³ refinement package using least-squares minimization. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions and included as riding contributions with isotropic displacement parameters tied to those of the attached non-hydrogen atoms. The given chemical formula and other crystal data do not take into account the unknown solvent molecule(s). The reflections with error/esd more than 10 were excluded in order to avoid problems related to better refinement of the data. The data completeness is more than 99.8% in most of the cases, which is enough to guarantee a very good refinement of data. The details of X-ray structural determinations are given in Tables S1. In complex **Ni1** the disordered solvent molecules could not be recognized or modelled to a known solvent; hence, it was *SQUEEZED* using PLATON. The results indicated 1461 electrons

and a volume of 2905 Å³ for **Ni1**. The given chemical formula and other crystal data do not take into account the unknown solvent molecule(s). Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC: 2362530(Comp. L2), 2362531(Comp. Ni1), 2362532(Comp. Ni2), 2362533(Comp. Ni3), 2362534(Comp. Ni4), -2362535(Comp. Ni5).

Table S1 Crystallographic information of **compounds L2 and Ni1-Ni5**

	L2	Ni1	Ni2	Ni3	Ni4	Ni5
Formula	C ₂₆ H ₂₂ N ₅ P	C ₅₂ H ₄₀ Cl ₂ F ₆ N ₁₀ Ni ₂ O ₆ P ₂ S ₂	C ₂₇ H ₂₂ ClF ₃ N ₅ NiO ₃ PS	C ₂₂ H ₂₈ ClF ₃ N ₅ NiO ₃ PS	C ₂₅ H ₁₉ ClN ₅ NiP	C ₄₈ H ₆₂ Cl ₂ N ₁₀ Ni ₂ OP ₂
Formula weight	435.45	1329.32	678.68	624.68	514.58	1045.33
Temperature/K	150.00(10)	293.15	273.15(10)	150.0	150.00(10)	113.00
Crystal system	monoclinic	trigonal	triclinic	Orthorhombic	monoclinic	triclinic
Space group	P21/n	R-3	P-1	Pna2 ₁	I2/a	P-1
a/Å	9.7622(2)	42.930(3)	8.5305(4)	17.3501(8)	21.2519(14)	7.8912(7)
b/Å	11.3546(2)	42.930(3)	9.4375(4)	10.6515(5)	10.0002(5)	8.8336(10)
c/Å	20.4691(3)	16.9889(15)	17.6861(6)	14.9182(6)	24.7491(15)	18.4362(19)
α/°	90	90	90.703(3)	90	90	85.707(4)
β/°	90.507(2)	90	98.984(3)	90	114.089(7)	85.978(4)
γ/°	90	120	99.254(4)	90	90	74.077(4)
Volume/Å ³	2268.83(7)	27115(4)	1387.05(10)	2757.0(2)	4801.7(5)	1230.7(2)
Z	4	18	2	4	8	1
ρ _{calc} /cm ³	1.275	1.465	1.625	1.505	1.424	1.410
μ/mm ⁻¹	0.145	0.910	0.990	0.988	1.009	0.986
F(000)	912.0	12168.0	692.0	1288.0	2112.0	548.0
Crystal size/mm ³	0.095 × 0.068 × 0.056	0.125 × 0.098 × 0.078	0.098 × 0.075 × 0.052	0.093 × 0.075 × 0.052	0.085 × 0.072 × 0.056	0.286 × 0.156 × 0.125
2θ range, deg	5.504 to 50	3.762 to 50.106	4.376 to 63.658	5.254 to 49.996	4.198 to 50	4.438 to 57.068
Total no of reflection	23165	72220	42950	15439	13298	61201
Independent reflections	3974 [R _{int} = 0.08343]	10665 [R _{int} = 0.1396]	8927 [R _{int} = 0.1133]	4632 [R _{int} = 0.0794]	4213 [R _{int} = 0.1000]	6249 [R _{int} = 0.0550]
Goodness-of-fit on F ²	1.037	1.025	1.025	1.005	0.986	1.028
R ₁ (all data)	0.0381	0.0596	0.0576	0.0389	0.0546	0.0264
wR ₂ (I > 2σ(I))	0.0817	0.1636	0.1262	0.0876	0.1331	0.0647

NMR and HRMS spectra

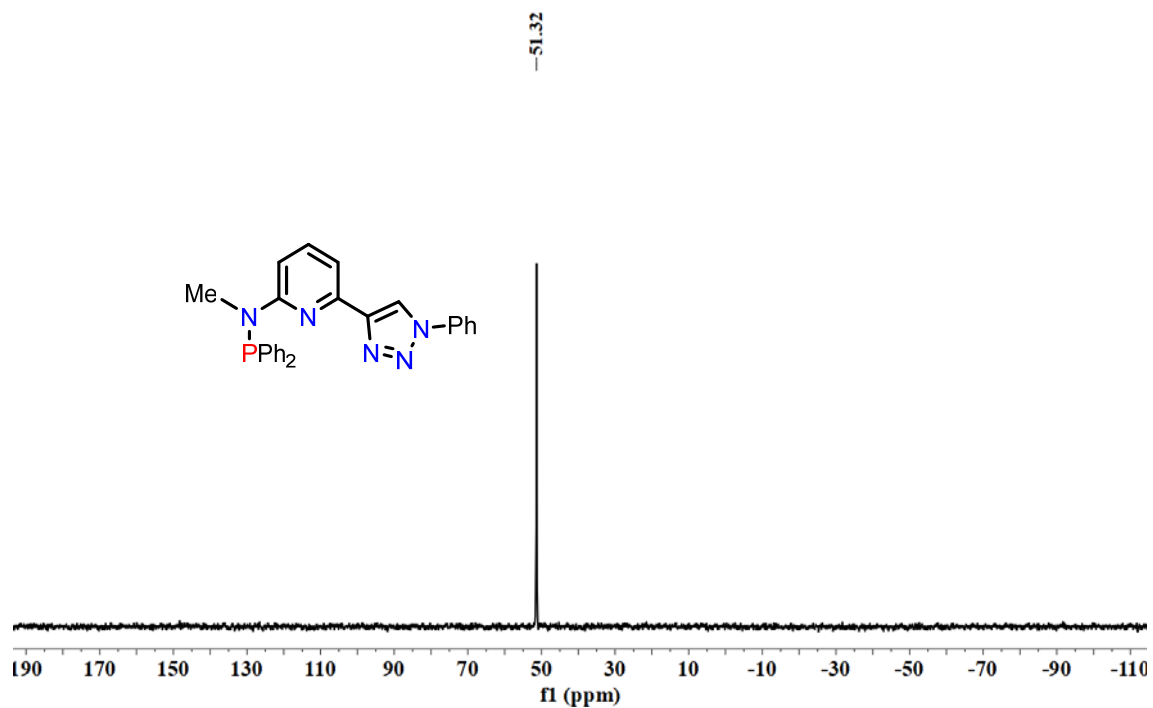


Fig. S1 ^{31}P NMR spectrum of L2 in CDCl_3 (162 MHz).

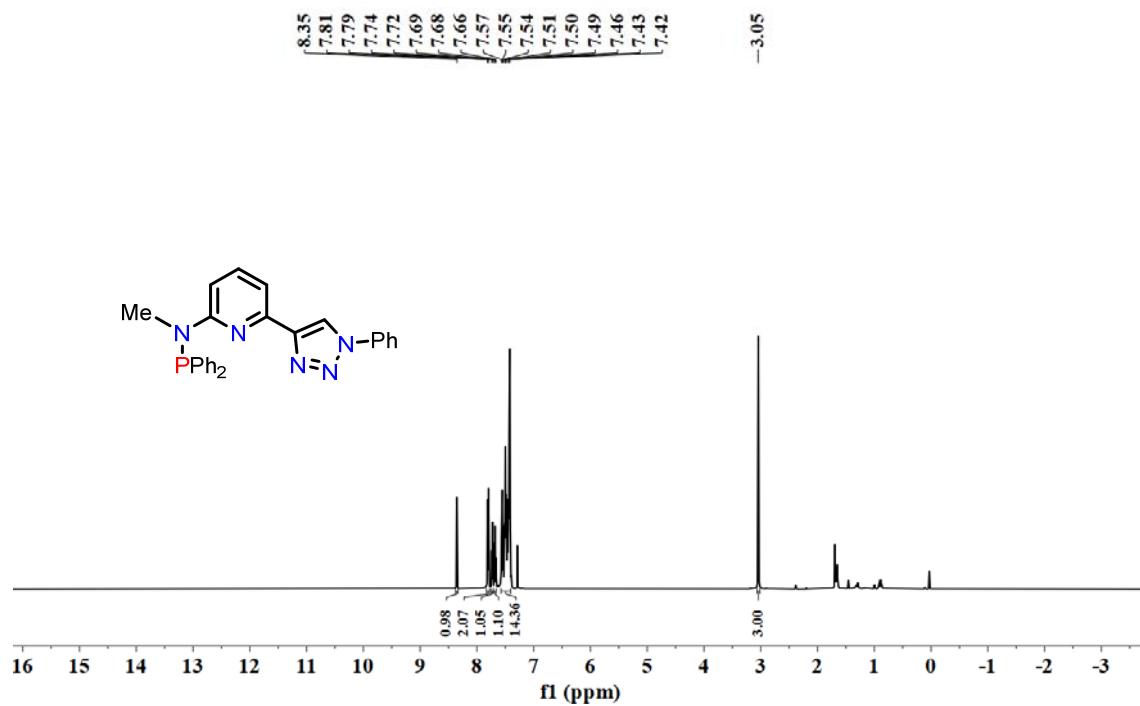


Fig. S2 ^1H NMR spectrum of L2 in CDCl_3 (400 MHz).

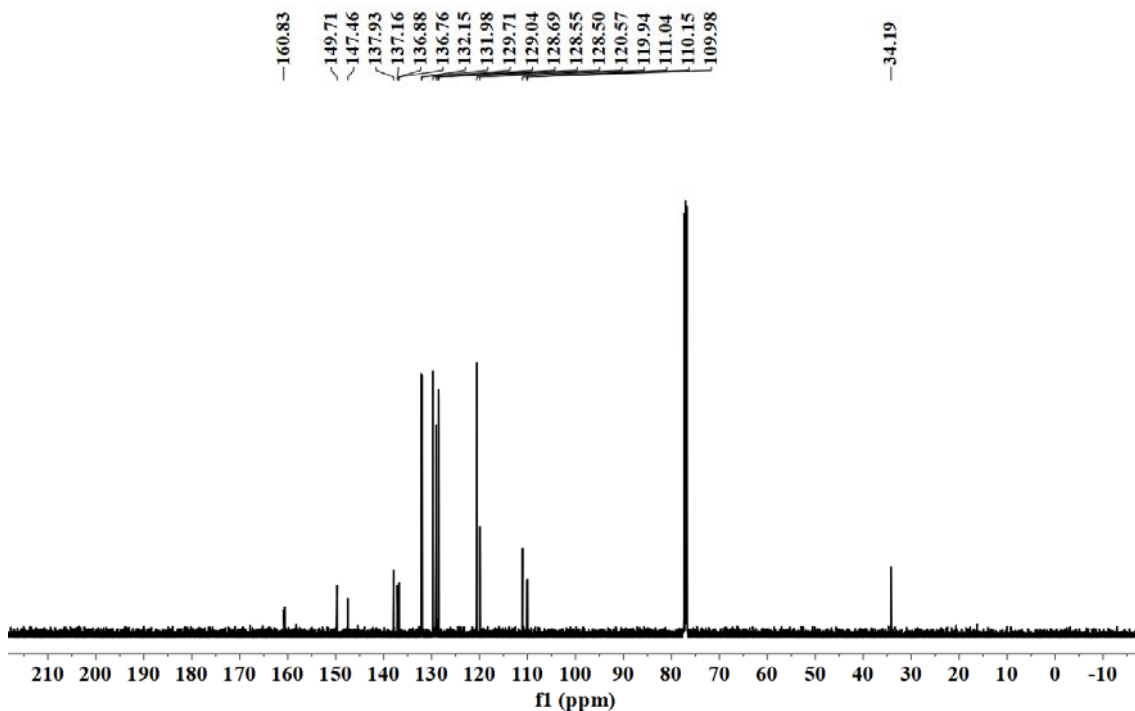


Fig.S3 ^{13}C NMR spectrum of L2 in CDCl_3 (101 MHz).

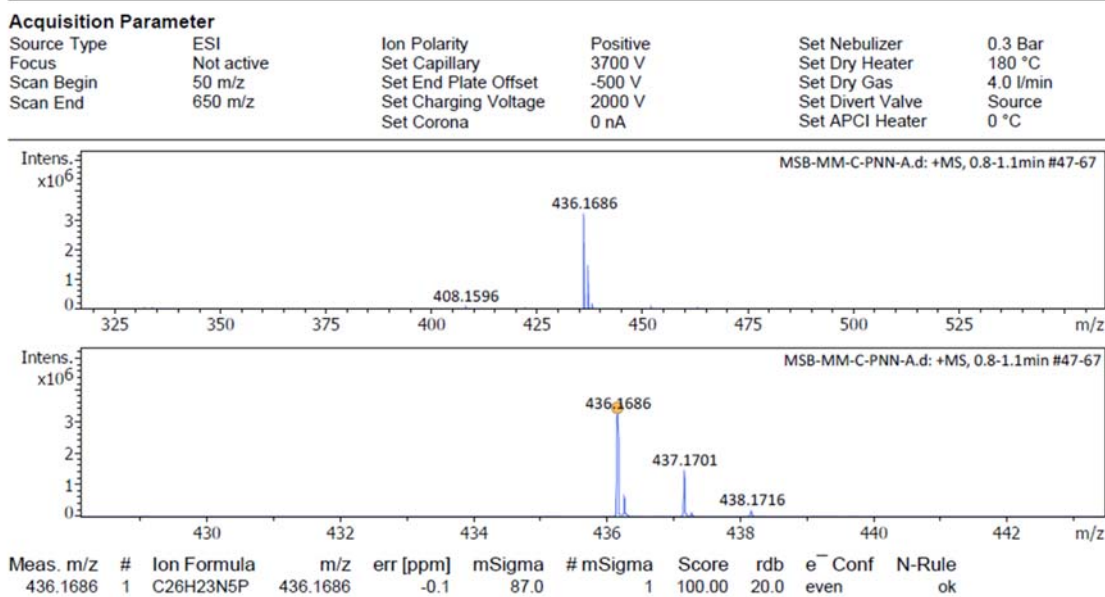


Fig. S4 HRMS spectrum of L2.

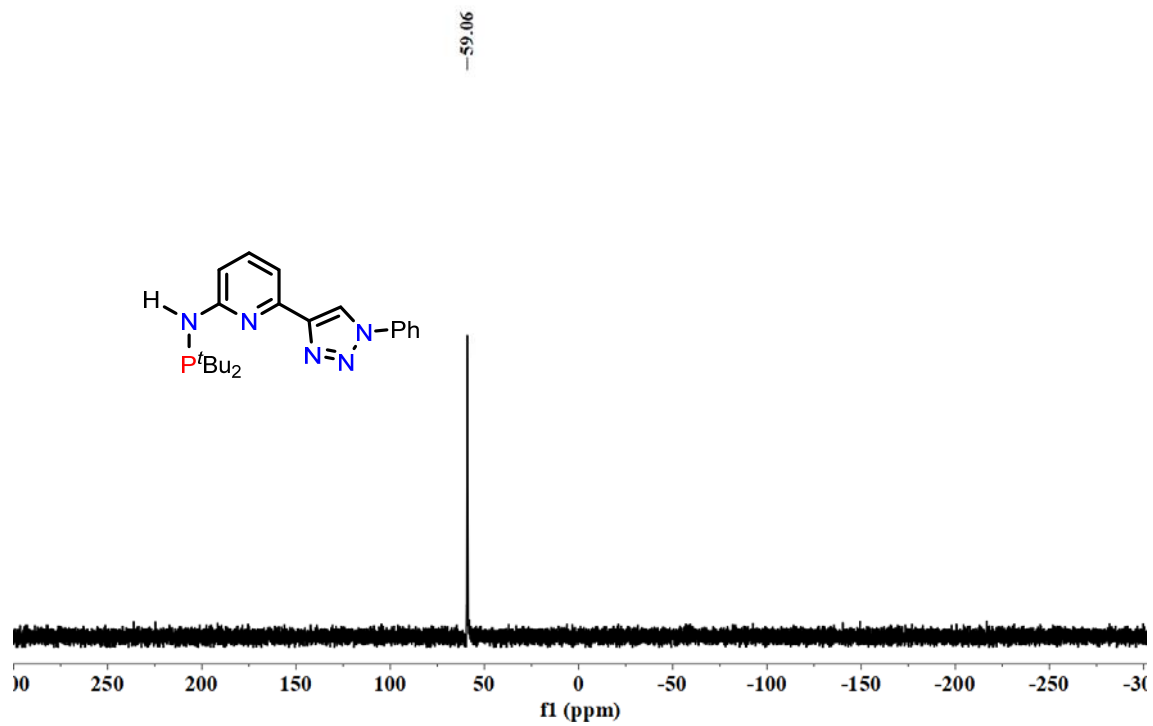


Fig. S5 ^{31}P NMR spectrum of L3 in CDCl_3 (162 MHz).

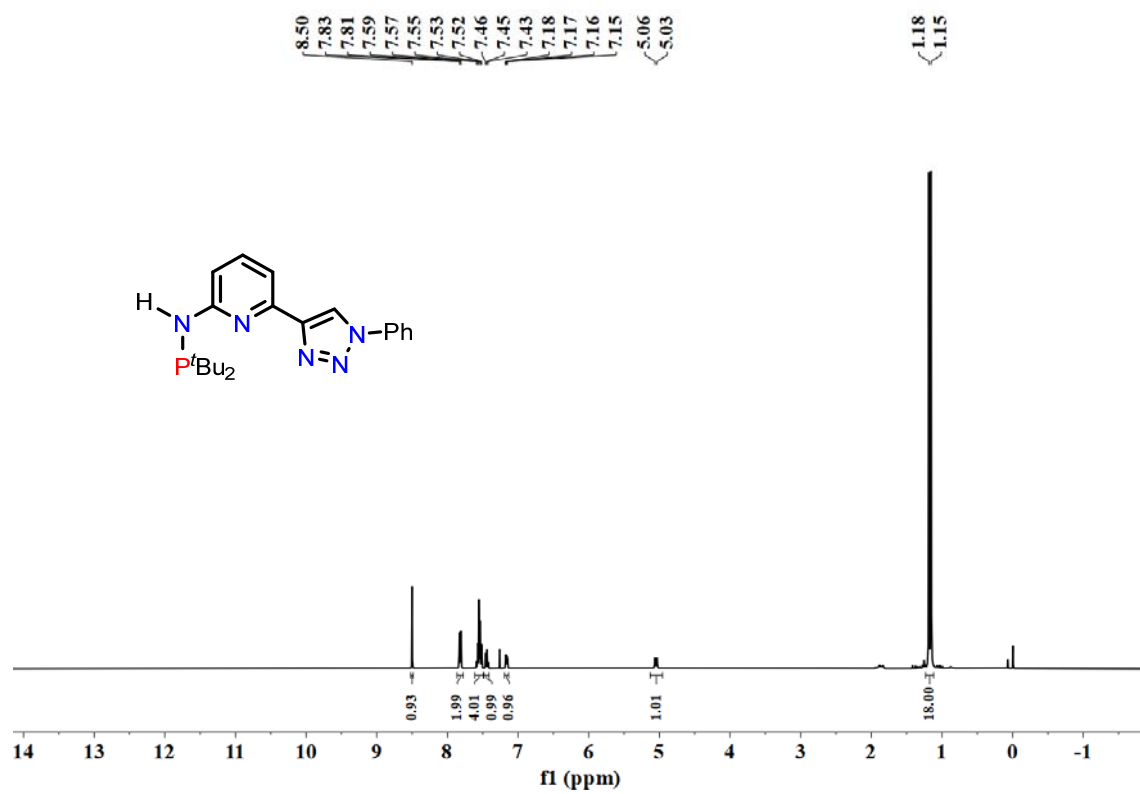


Fig. S6 ^1H NMR spectrum of L3 in CDCl_3 (400 MHz).

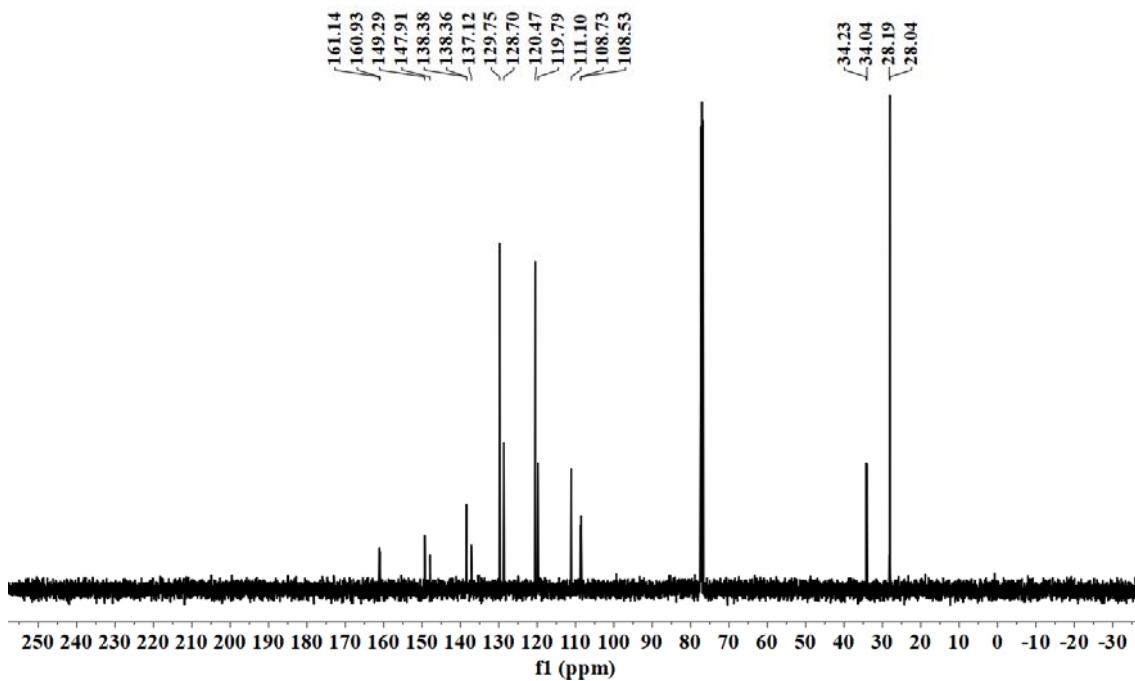


Fig.S7 ^{13}C NMR spectrum of L3 in CDCl_3 (101 MHz).

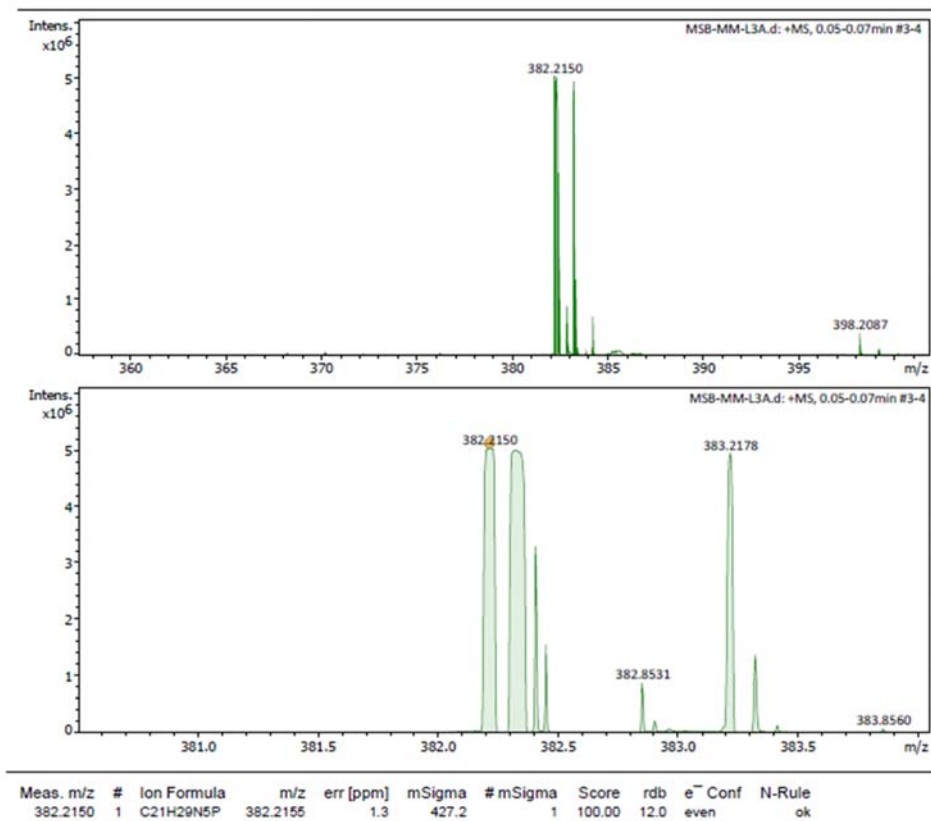


Fig. S8 HRMS spectrum of L3.

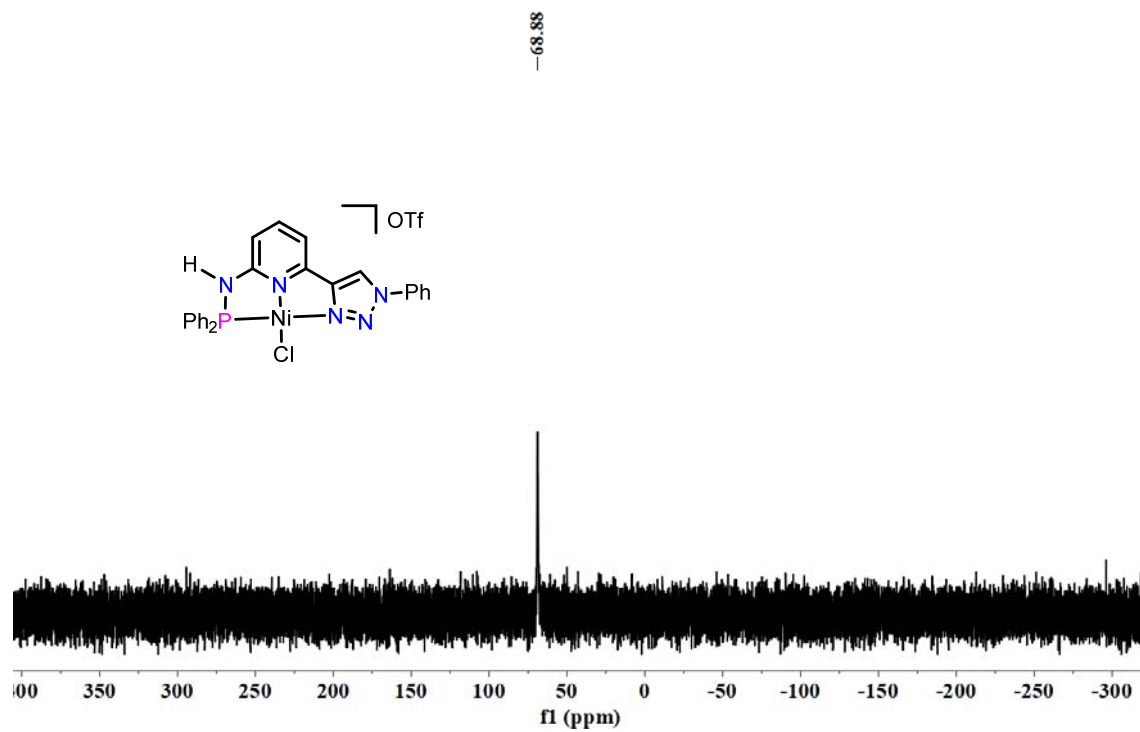


Fig. S9 ³¹P NMR spectrum of Ni1 in CDCl₃ (162 MHz).

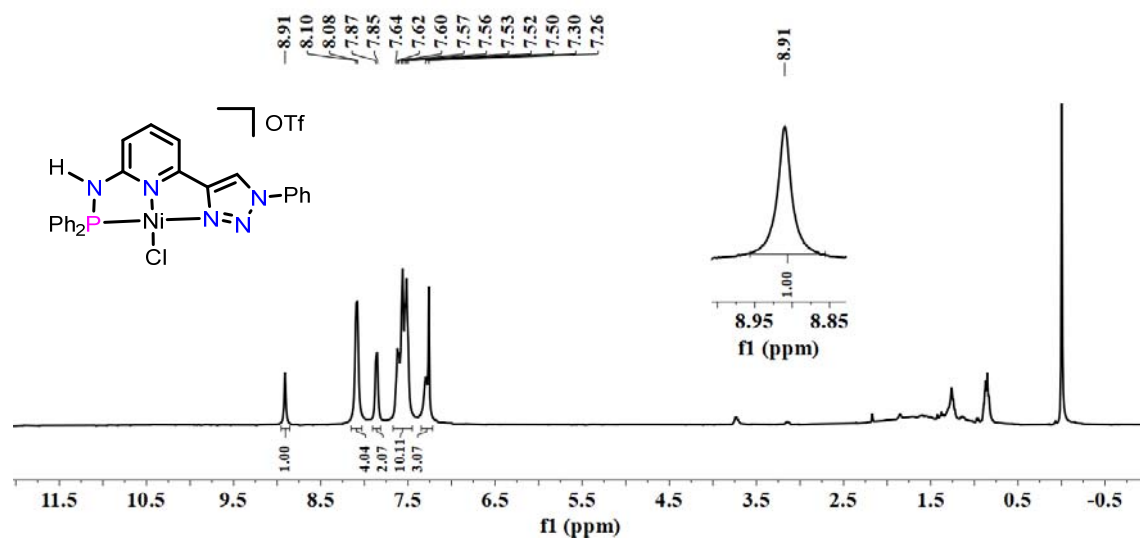


Fig.S10 ¹H NMR spectrum of Ni1 in CDCl₃ (400 MHz).

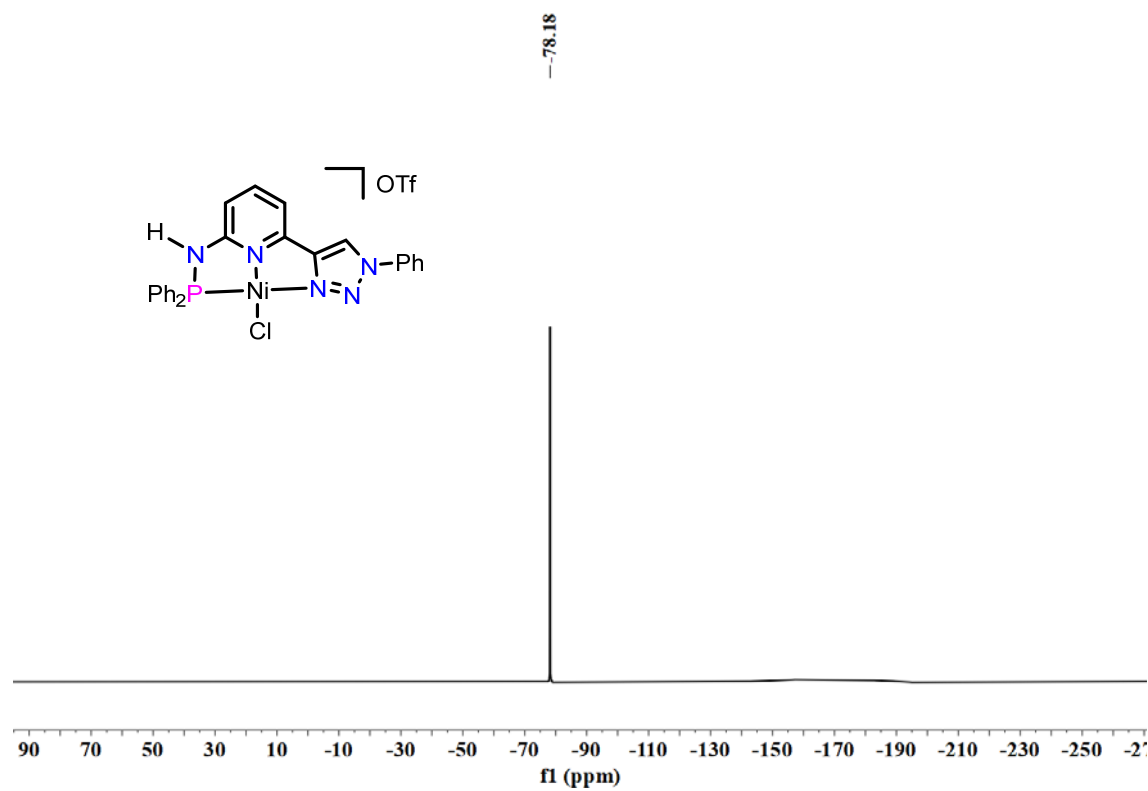


Fig. S11 ^{19}F NMR spectrum of Ni1 in CDCl_3 (377 MHz).

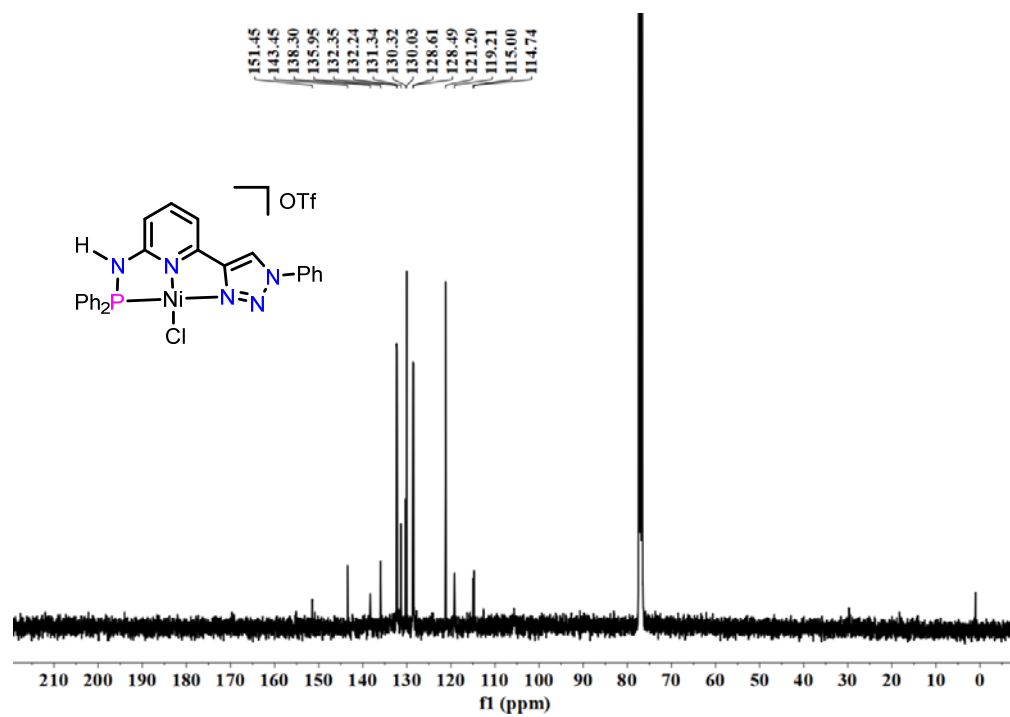


Fig.S12 ^{13}C NMR spectrum of Ni1 in CDCl_3 (101 MHz).

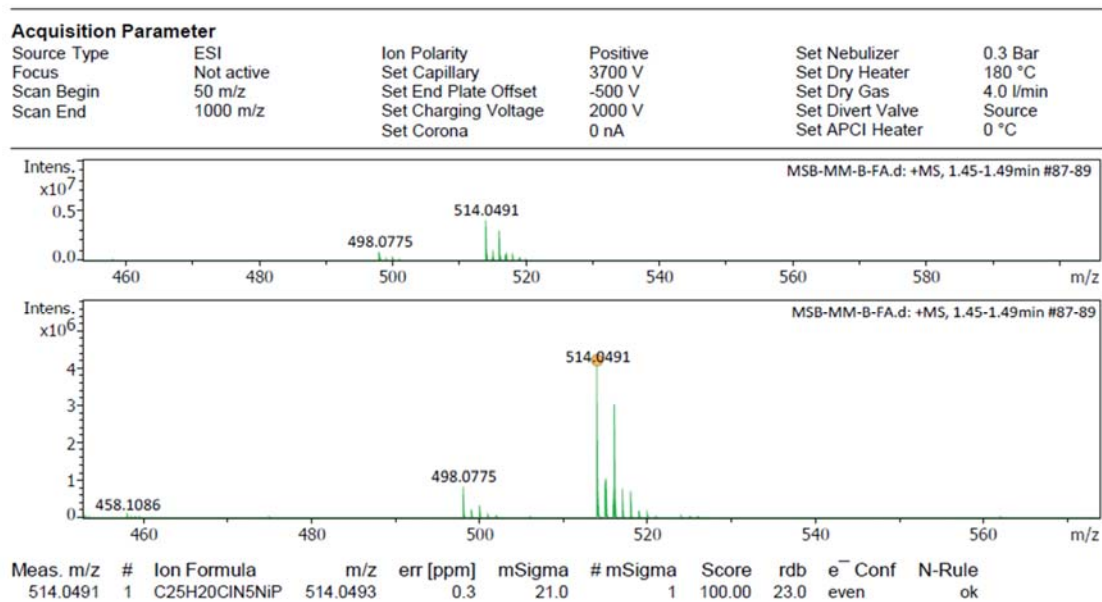


Fig. S13 HRMS spectrum of Ni1.

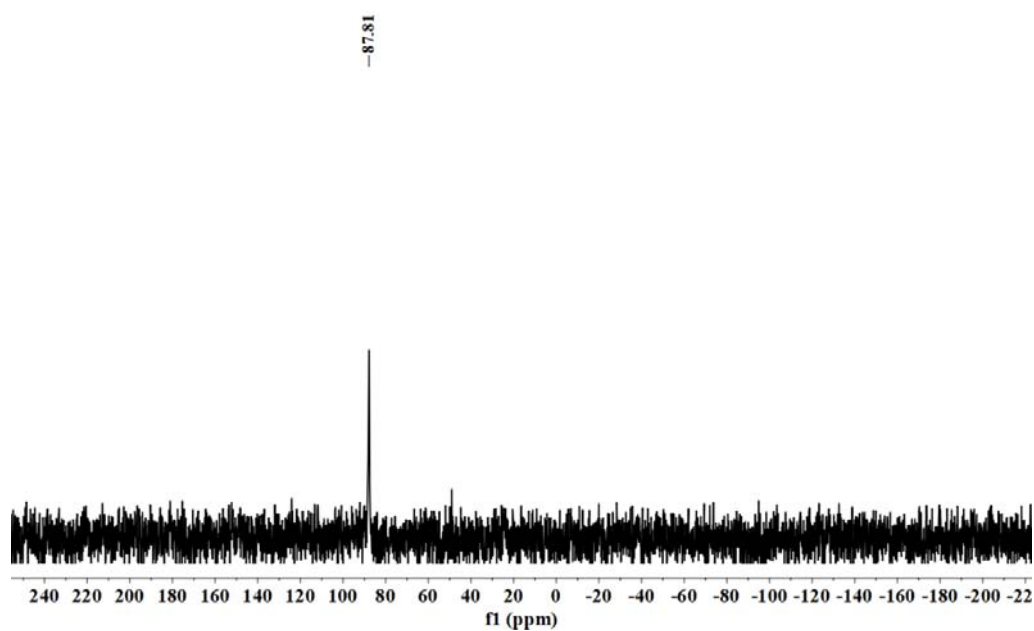


Fig. S14 ³¹P NMR spectrum of Ni2 in CDCl₃ (162 MHz).

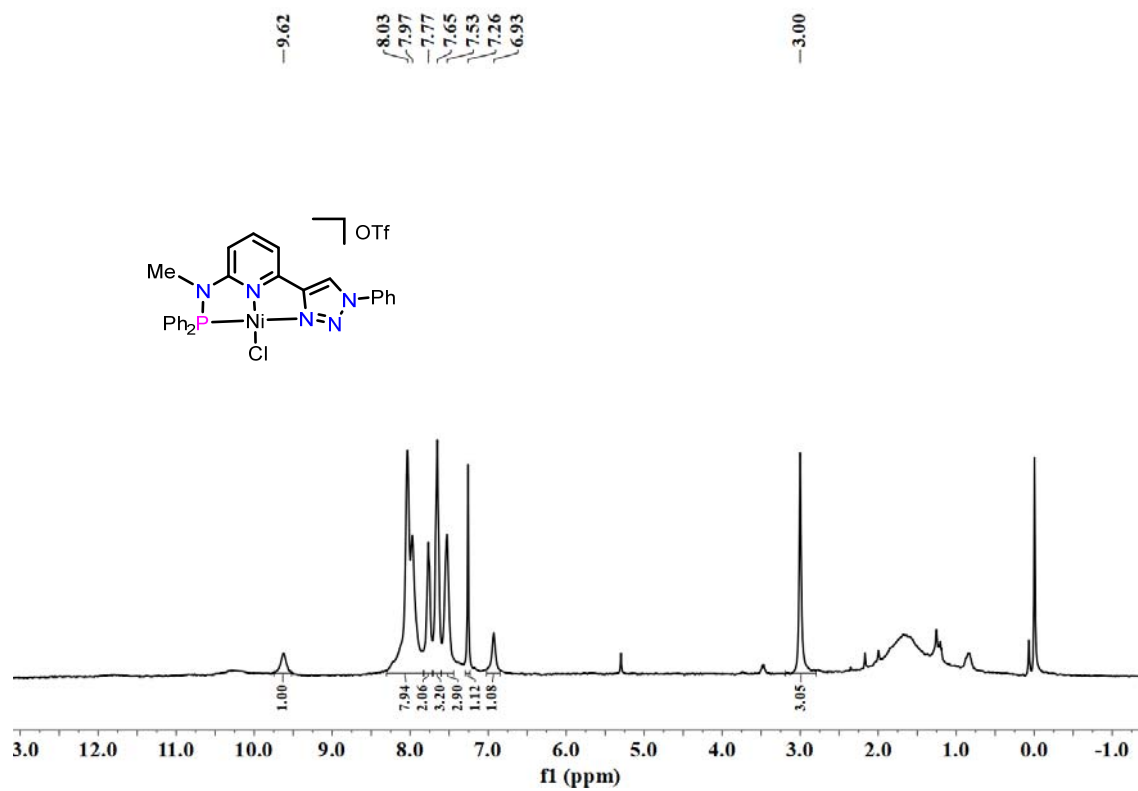


Fig.S15 ¹H NMR spectrum of Ni2 in CDCl₃ (400 MHz).

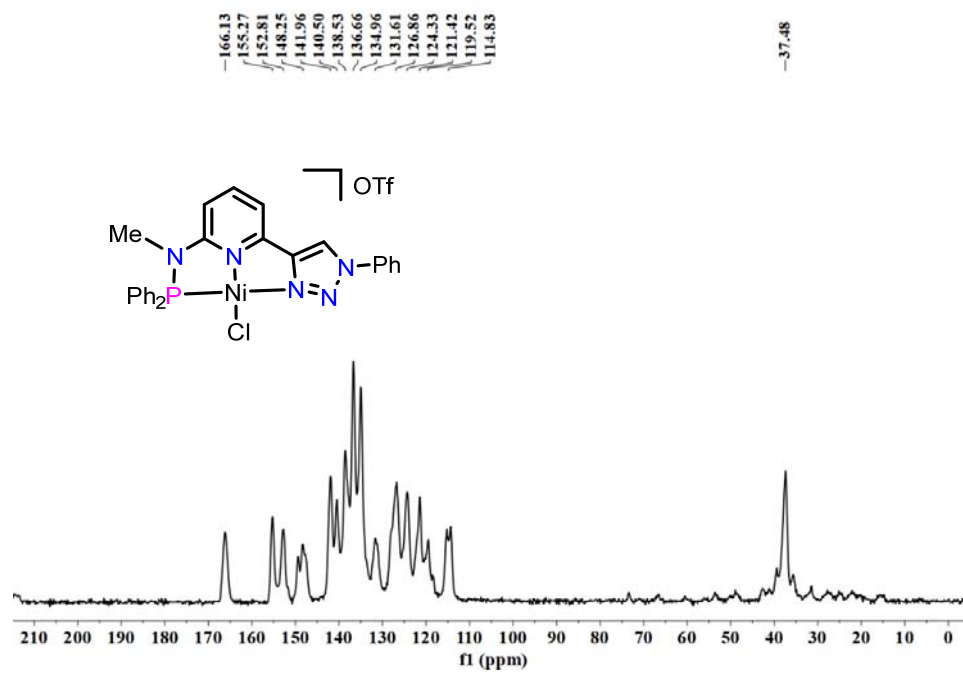


Fig. S16 Solid state ¹³C NMR spectrum of Ni2 (101 MHz, Solid State).

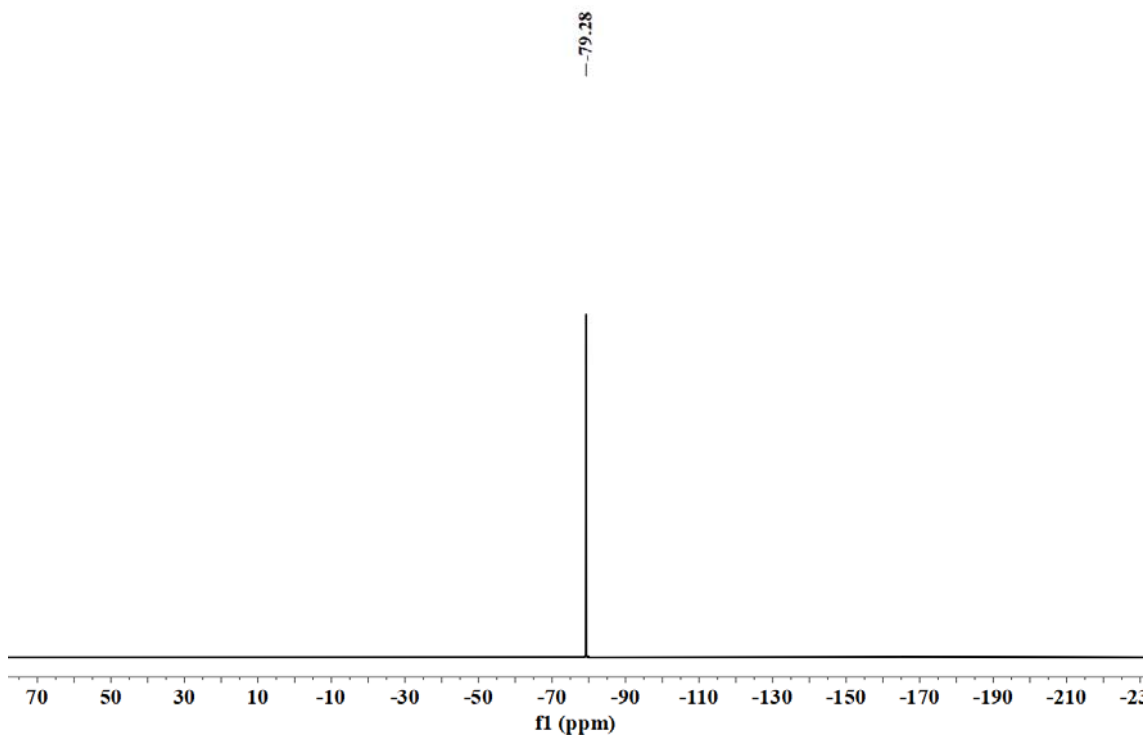
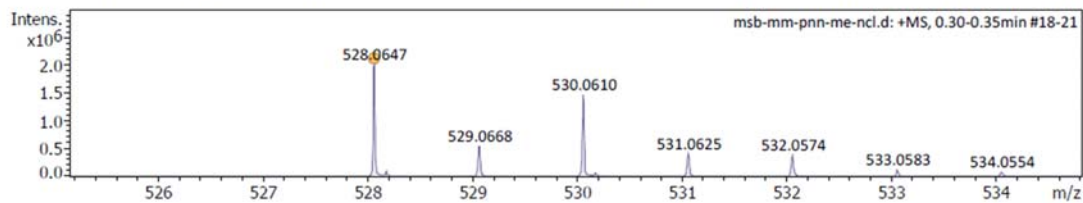
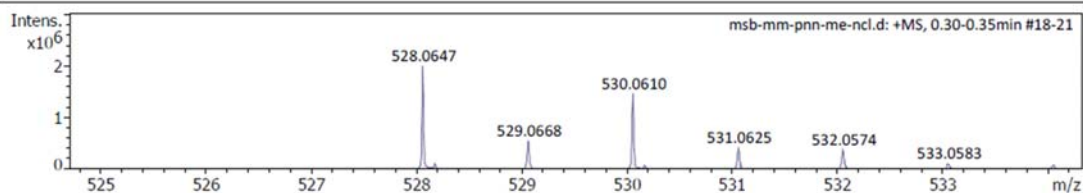


Fig. S17 ^{19}F NMR spectrum of **Ni2** in CDCl_3 (377MHz).

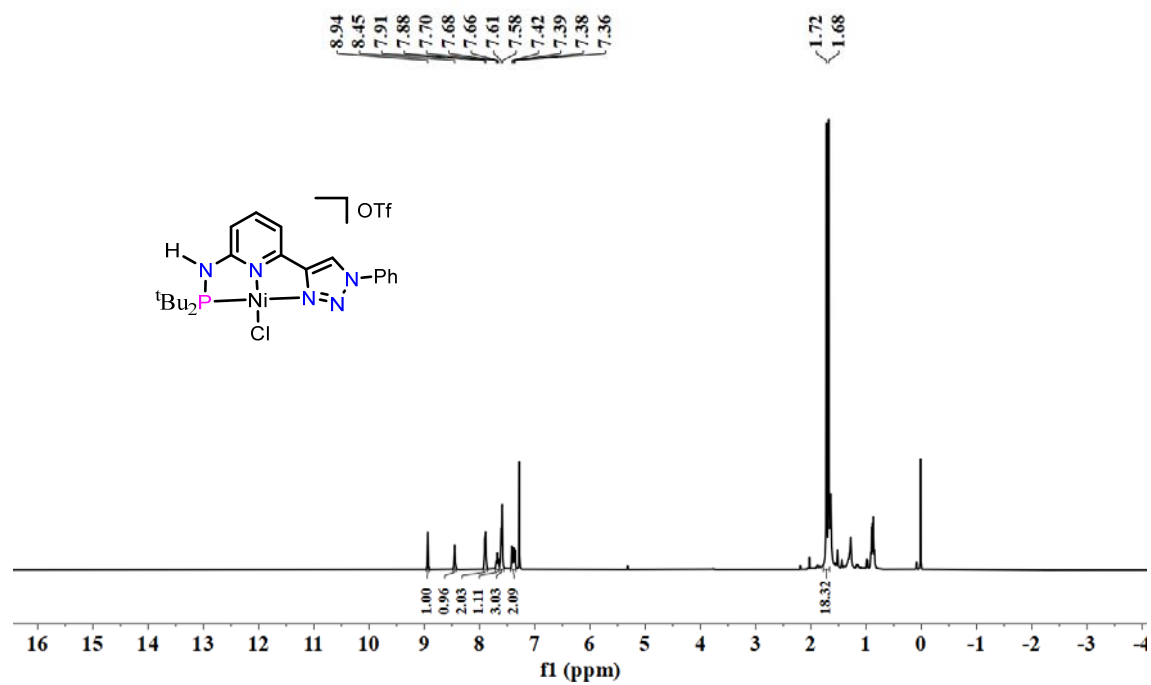
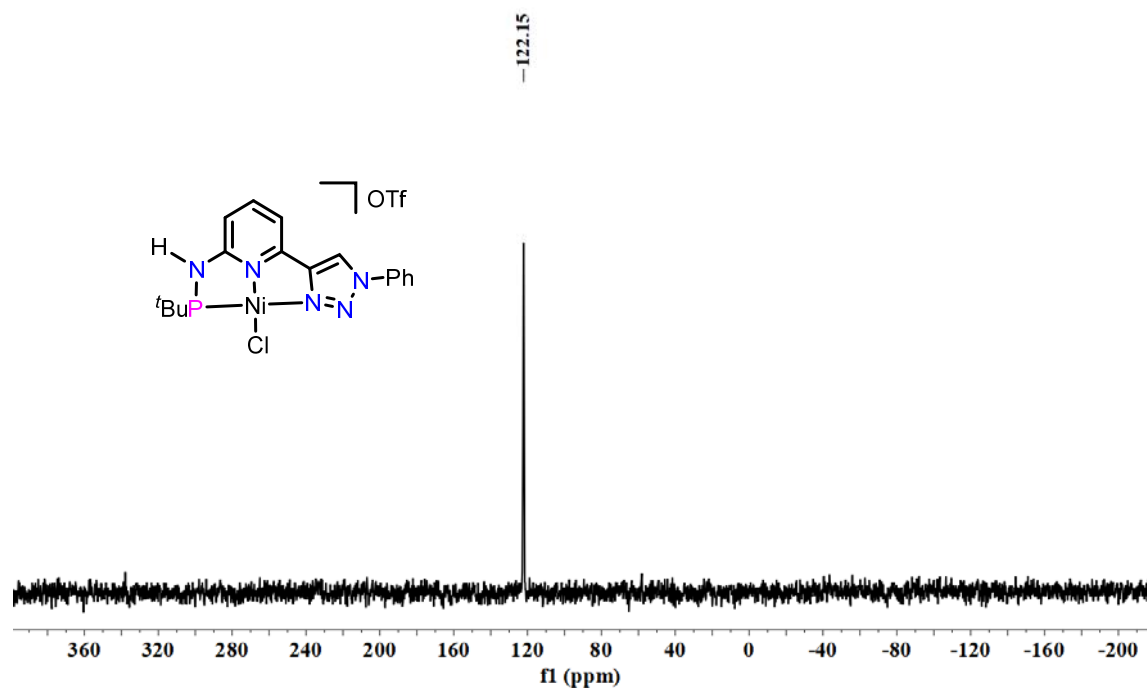
Acquisition Parameter

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Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.5 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
528.0647	1	C ₂₆ H ₂₂ CIN ₅ NIP	528.0649	0.4	19.3	1	100.00	23.0	even	ok

Fig. S18 HRMS spectrum of **Ni2**



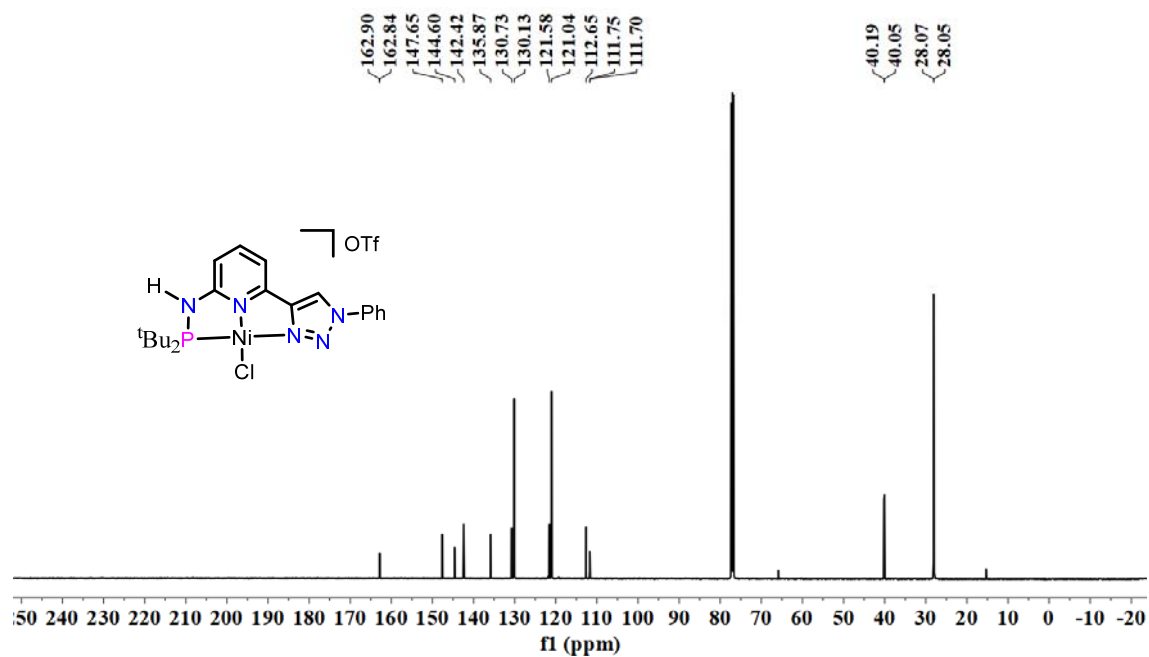


Fig.S21 ¹³C NMR spectrum of Ni3 in CDCl₃ (101 MHz).

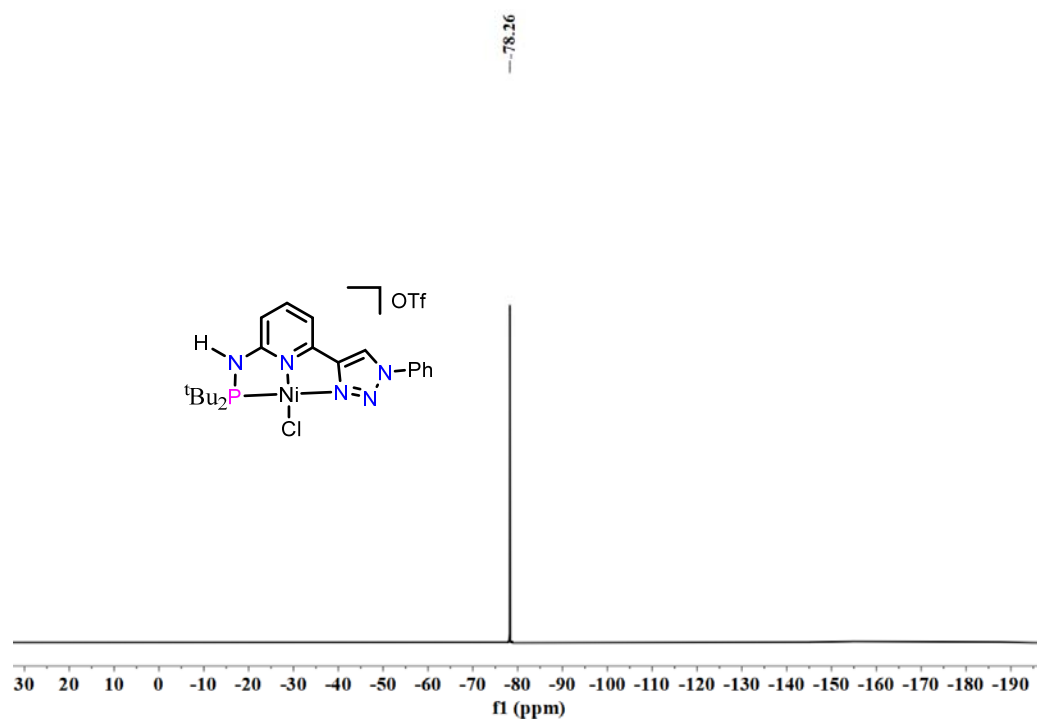


Fig. S22 ¹⁹F NMR spectrum of Ni3 in CDCl₃ (377 MHz).

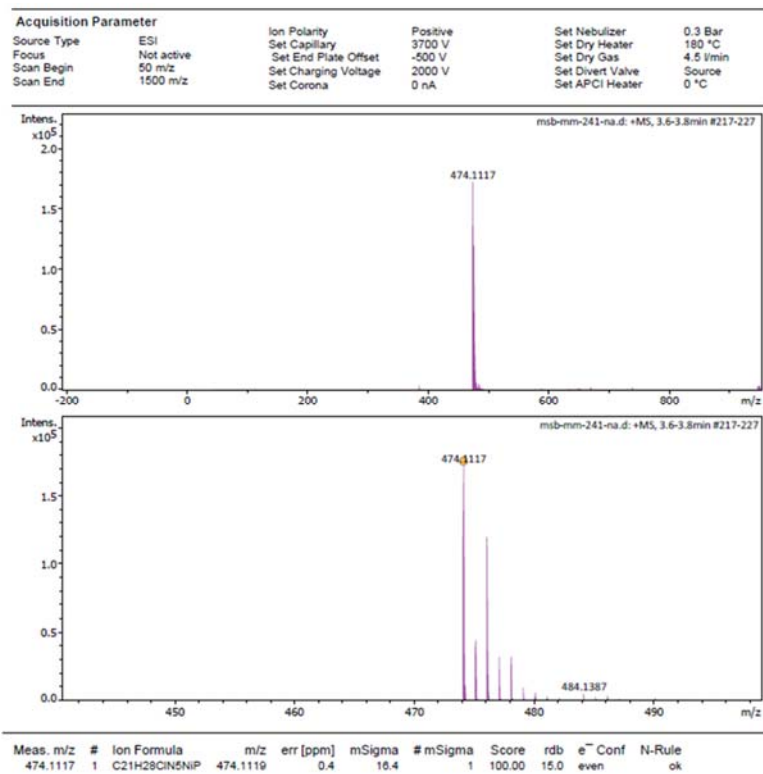


Fig. S23 HRMS spectrum of Ni3

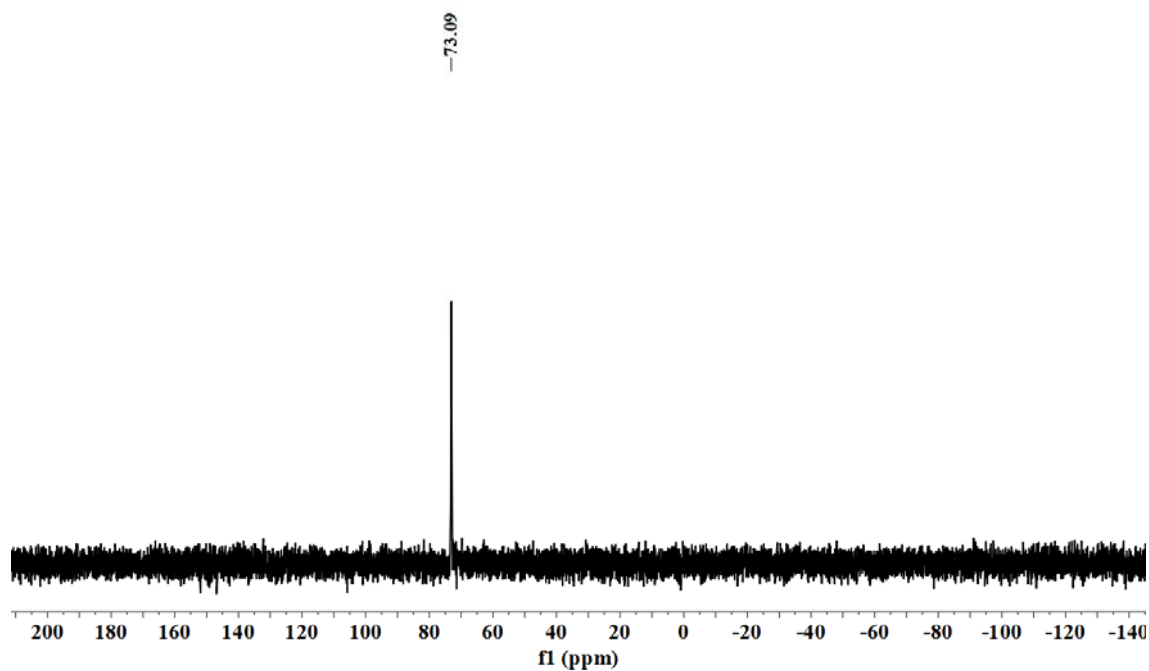


Fig. S24 ³¹P NMR spectrum of Ni4 in CDCl₃ (162 MHz).

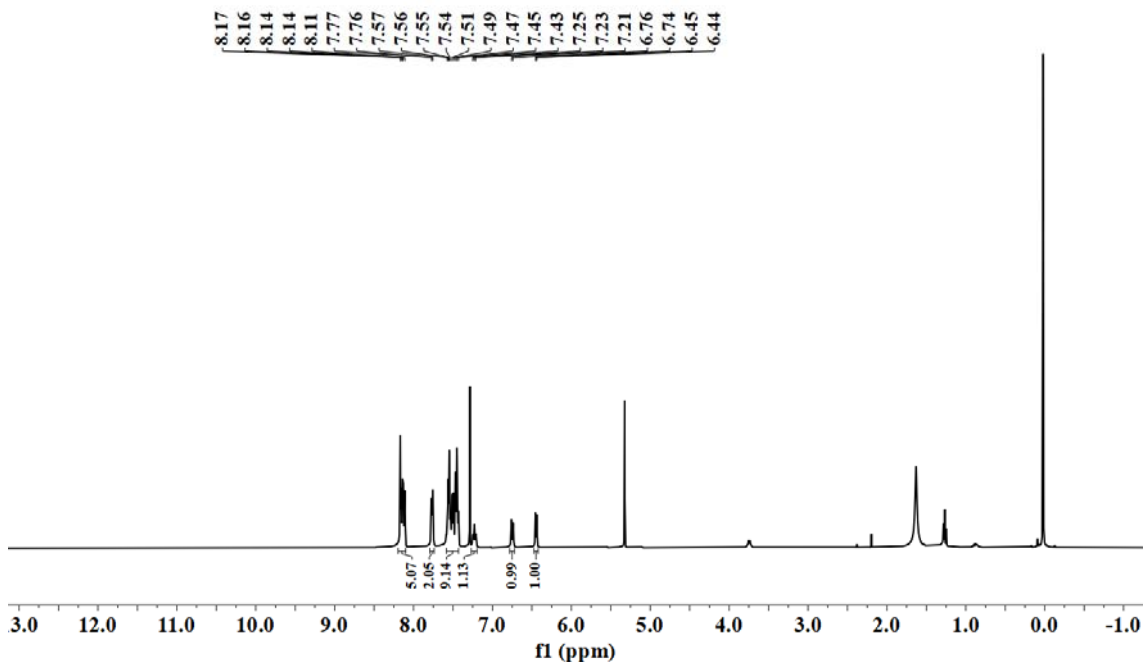


Fig. S25 ^1H NMR spectrum of Ni4 in CDCl_3 (400 MHz).

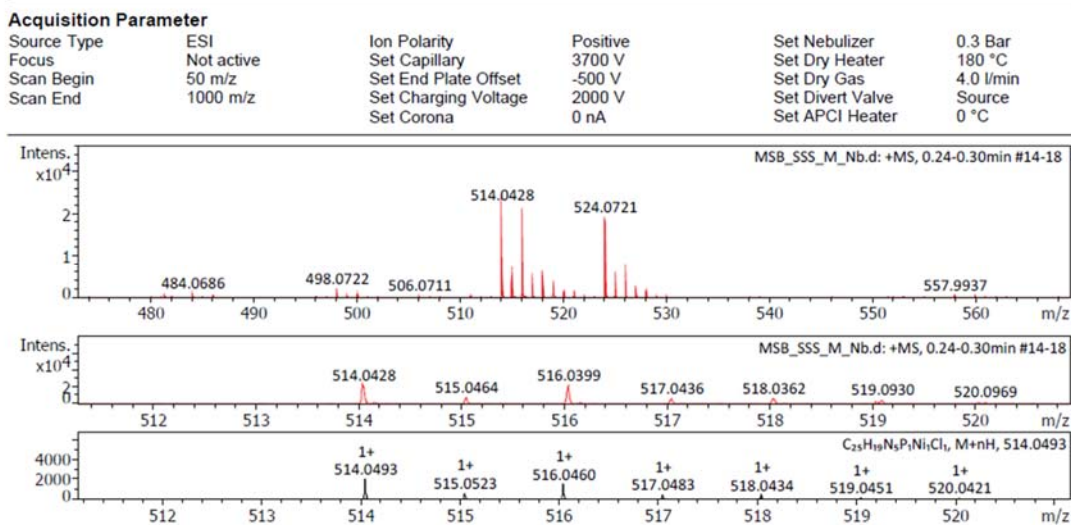


Fig. S26 HRMS spectrum of Ni4

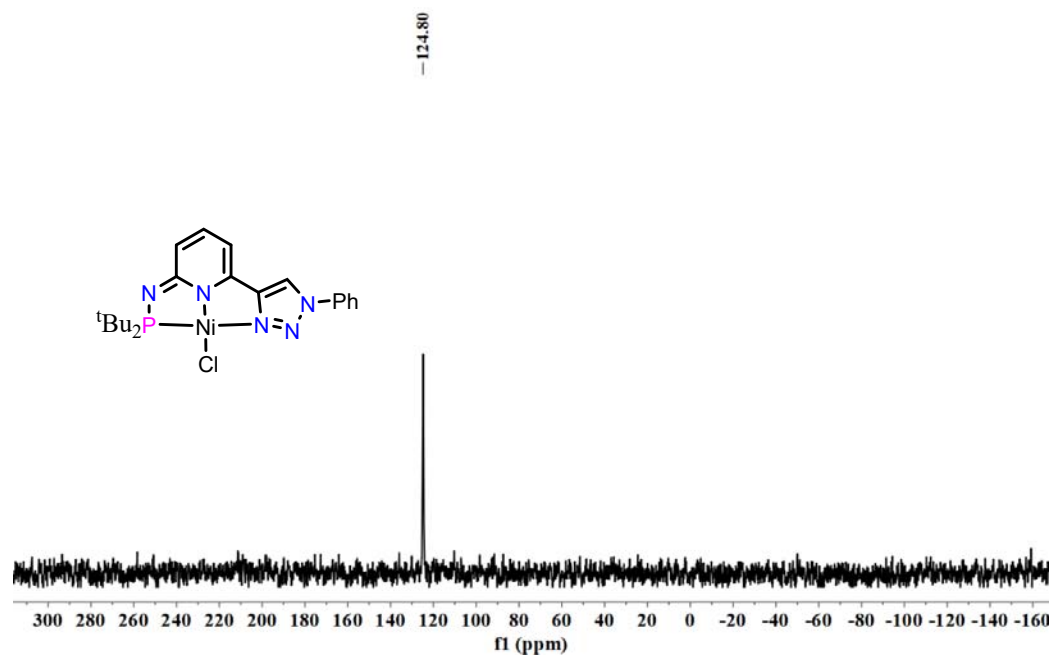


Fig. S27 ^{31}P NMR spectrum of Ni5 in CDCl_3 (162 MHz).

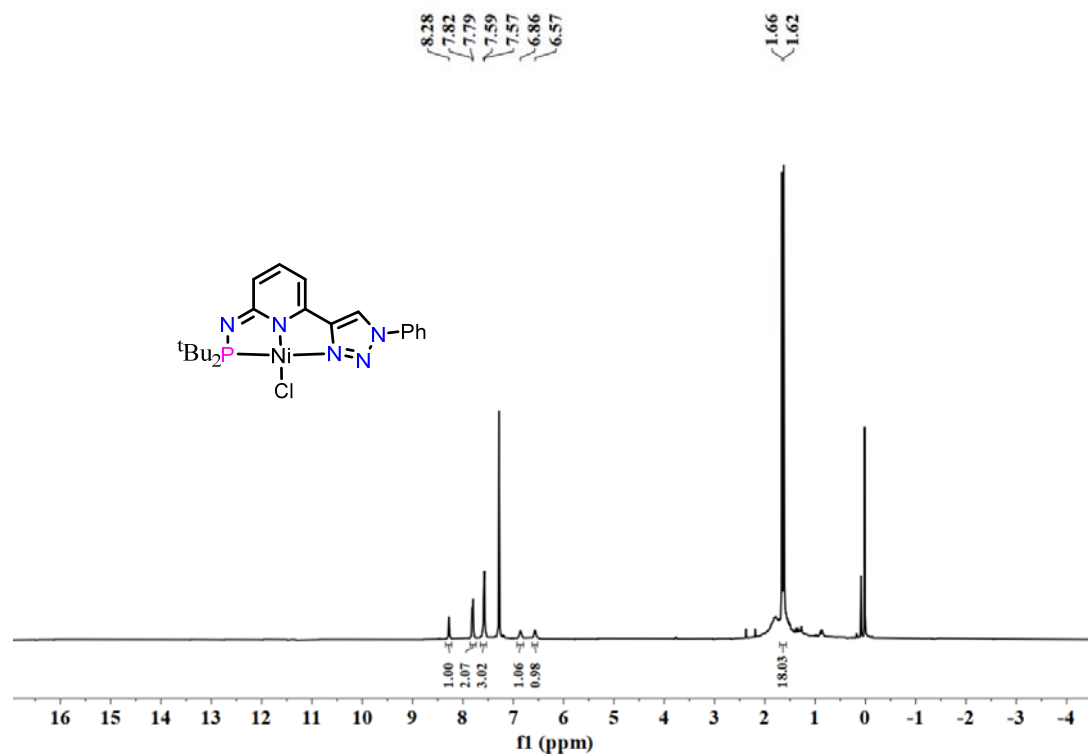


Fig. S28 ^1H NMR spectrum of Ni5 in CDCl_3 (400 MHz).

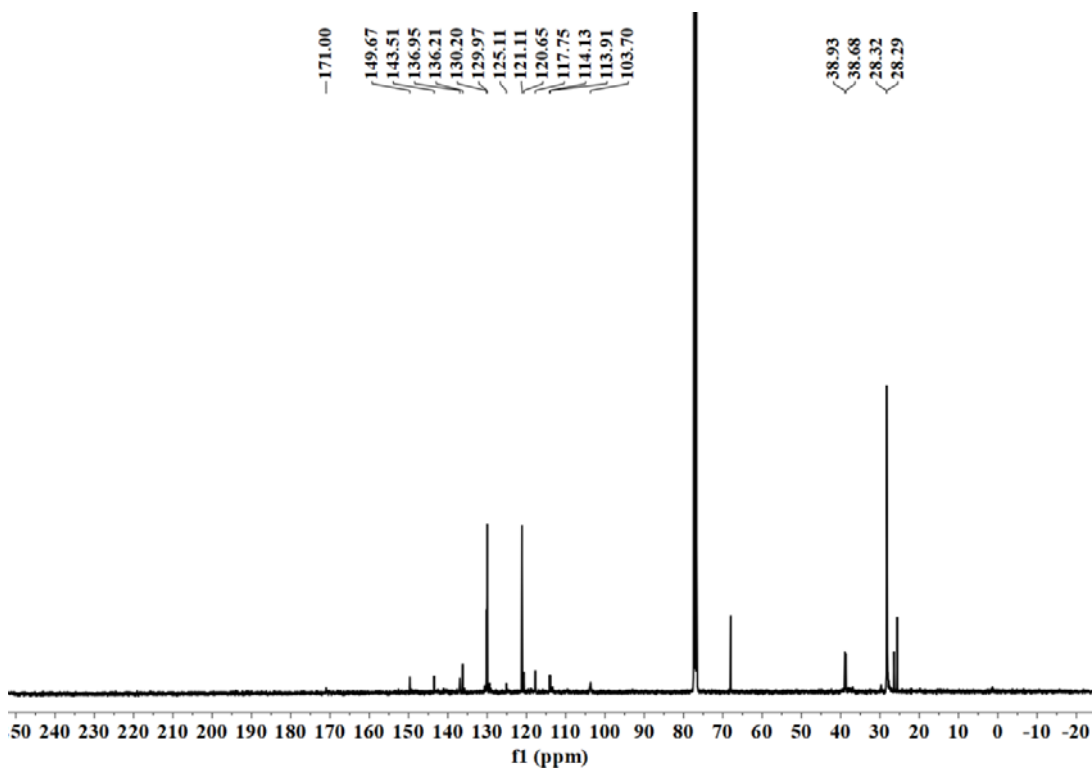


Fig.S29 ^{13}C NMR spectrum of Ni5 in CDCl_3 (101 MHz).

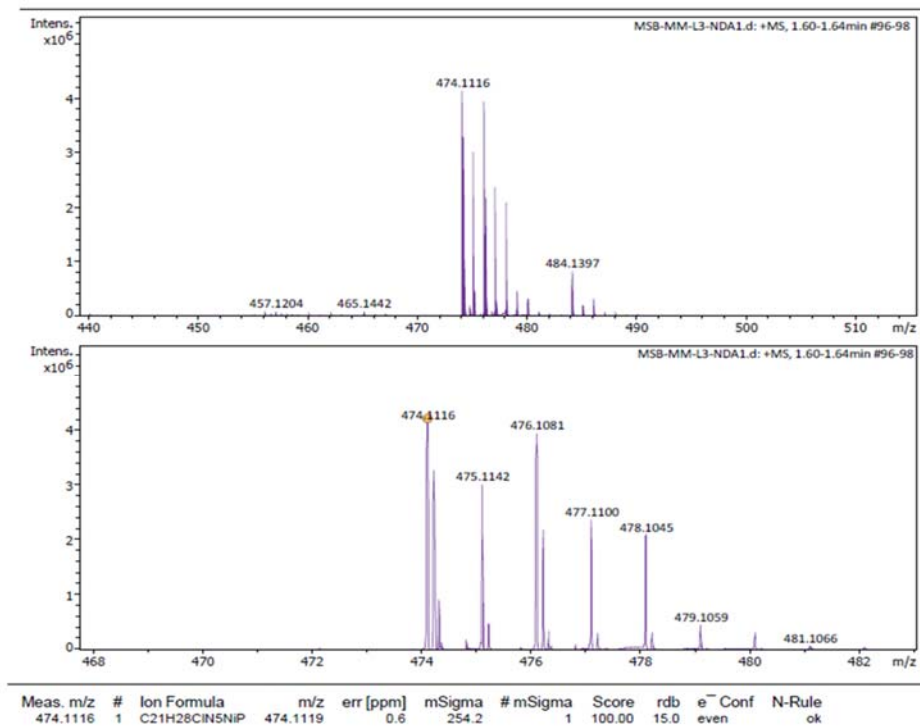


Fig. S30 HRMS spectrum of Ni5

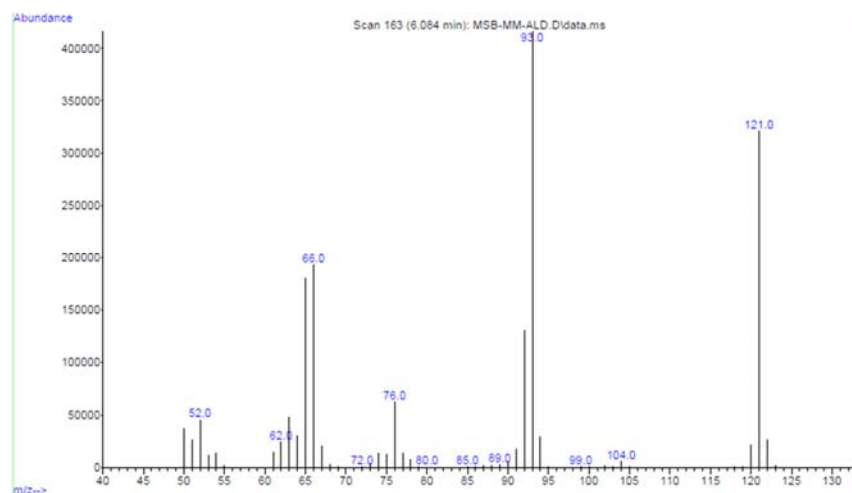
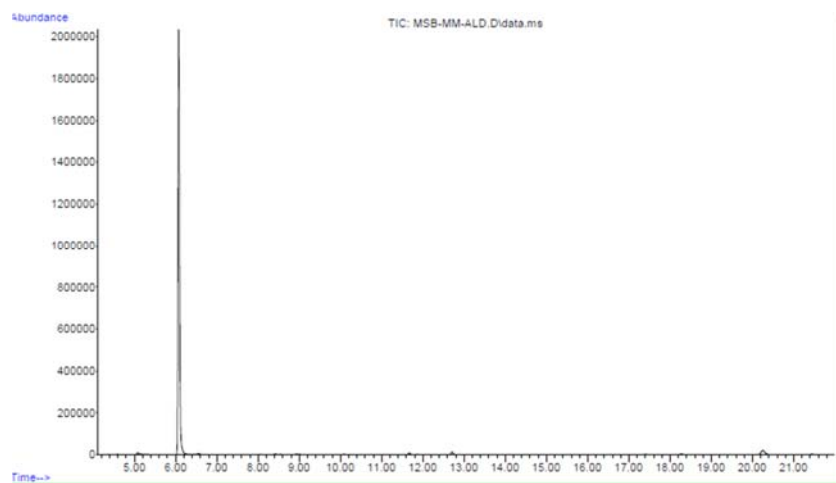


Fig. S31 Formation of aldehyde from the independent reaction.

Detection of Ni-H Intermediate:

In a microwave tube mixture 2-aminobenzyl alcohol (0.5 mmol) Acetophenone (0.55 mmol), **Ni3** (0.5 mol%) and KOH (20 mol%) was taken in toluene. The reaction mixture was degassed and purged with nitrogen gas and then subjected to microwave irradiation at 110 °C for 10 min. After that aliquot was taken and HRMS analysis was carried out, which showed peak at 440.1506 corresponds to Nickel hydride $[P^HNNNiH-Cl]^+$ species.

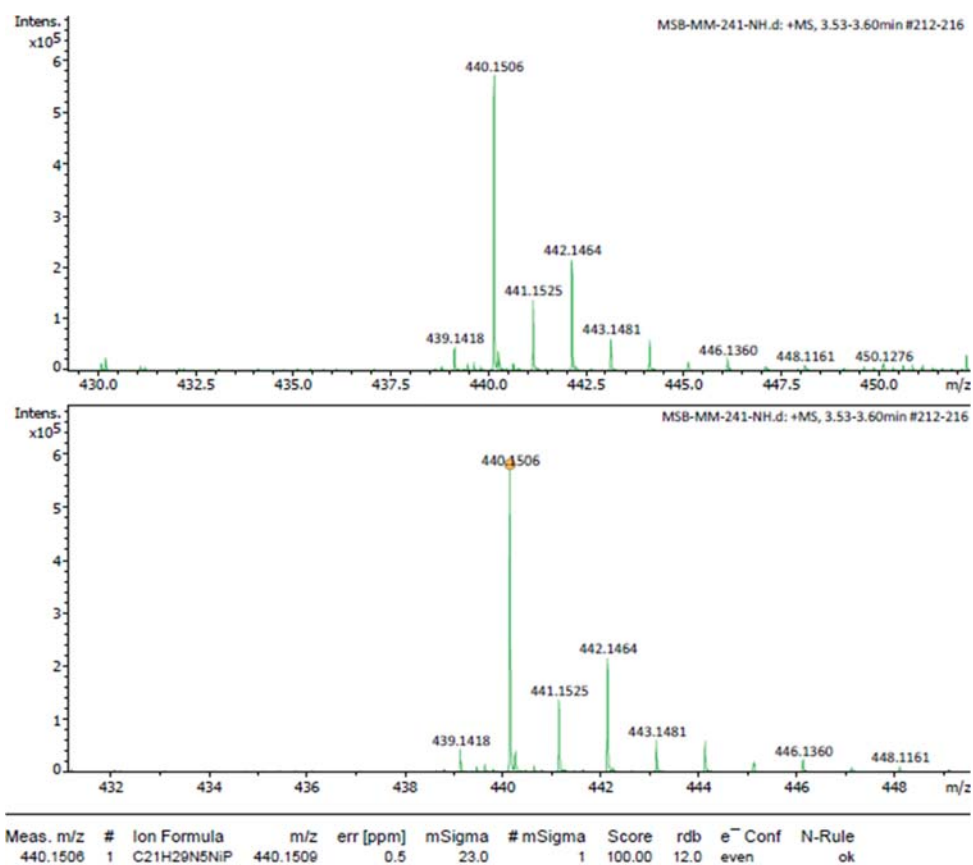


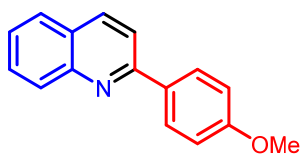
Fig. S32 HRMS spectrum of Nickel hydride intermediate II.

NMR Spectral data of catalytic products

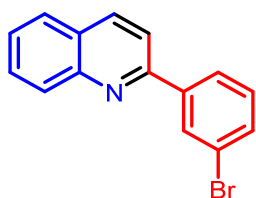
2-phenylquinoline (**1**) 98% (50 mg) ¹H NMR (400 MHz, CDCl₃): δ 8.21 (d, *J* = 7.3 Hz, 4H), 7.93 – 7.82 (m, 2H), 7.80 – 7.73 (m, 1H), 7.62 – 7.48 (m, 4H). ¹³C NMR (101 MHz, CDCl₃): δ 157.4, 148.3, 139.7, 136.8, 129.8, 129.7, 129.4, 128.9, 127.6, 127.5, 127.2, 126.3, 119.0.

2-(p-tolyl)quinoline (**2**) 88% (96 mg). ¹H NMR (500 MHz, CDCl₃): δ 8.26 – 8.18 (m, 2H), 8.13 (d, *J* = 8.2 Hz, 2H), 7.91 – 7.82 (m, 2H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.38 (d, *J* =

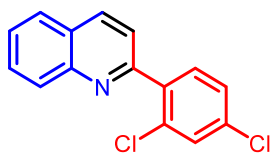
7.9 Hz, 2H), 2.50 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 157.4, 148.3, 139.4, 136.9, 136.7, 129.7, 129.6, 127.5, 127.1, 126.1, 118.9, 21.4.



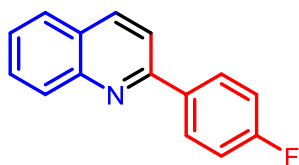
2-(4-methoxyphenyl)quinoline (**3**) 84% (98 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.16 (dd, $J = 8.6, 6.3$ Hz, 4H), 7.80 (t, $J = 8.5$ Hz, 2H), 7.71 (t, $J = 8.5$ Hz, 1H), 7.54 – 7.46 (m, 1H), 7.05 (d, $J = 8.9$ Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 160.8, 156.9, 148.3, 136.7, 132.3, 129.6, 129.5, 128.9, 127.5, 126.9, 125.3, 118.6, 114.3, 55.4.



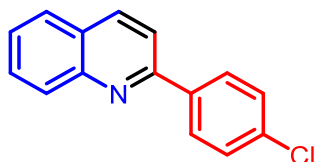
2-(3-bromophenyl)quinoline (**4**) 81% (114 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.39 (t, $J = 1.9$ Hz, 1H), 8.27 – 8.18 (m, 2H), 8.10 (d, $J = 9.5$ Hz, 1H), 7.88 – 7.82 (m, 2H), 7.77 (t, $J = 7.6$ Hz, 1H), 7.64 – 7.55 (m, 2H), 7.41 (t, $J = 7.9$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3): δ 155.6, 148.2, 141.7, 137.1, 132.2, 130.7, 130.3, 129.9, 129.8, 127.5, 126.7, 126.1, 123.2, 118.7.



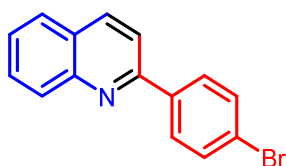
2-(2,4-dichlorophenyl)quinoline (**5**) 94% (129 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.25 (d, $J = 8.4$ Hz, 1H), 8.19 (d, $J = 8.5$ Hz, 1H), 7.90 (d, $J = 8.2$ Hz, 1H), 7.81 – 7.74 (m, 2H), 7.69 (d, $J = 8.2$ Hz, 1H), 7.62 (t, $J = 7.6$ Hz, 1H), 7.56 (d, $J = 2.0$ Hz, 1H), 7.43 (dd, $J = 8.2, 2.1$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3): δ 156.3, 148.1, 138.2, 135.9, 135.2, 133.1, 132.7, 129.9, 129.7, 127.6, 127.6, 127.2, 127.0, 122.5.



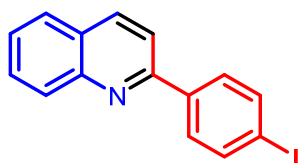
2-(4-fluorophenyl)quinoline (**6**) 87% (97 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.27 – 8.14 (m, 4H), 7.83 (d, $J = 10.1$ Hz, 2H), 7.74 (t, $J = 8.5$ Hz, 1H), 7.57 – 7.51 (m, 1H), 7.21 (t, $J = 8.7$ Hz, 2H). ^{13}C NMR (126 MHz, CDCl_3): δ 164.8, 162.9, 156.2, 148.1, 137.0, 129.9, 129.6, 129.5, 129.4, 127.5, 127.1, 126.4, 118.7, 115.9, 115.7.



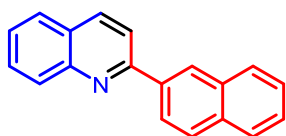
2-(4-chlorophenyl)quinoline (**7**) 83% (99 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.21 (dd, $J = 14.4, 8.5$ Hz, 2H), 8.14 (d, $J = 6.6$ Hz, 2H), 7.88 – 7.81 (m, 2H), 7.80 – 7.74 (m, 1H), 7.60 – 7.49 (m, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 156.0, 148.2, 138.0, 137.0, 135.6, 129.9, 129.7, 129.0, 128.8, 127.5, 127.2, 126.5, 118.6.



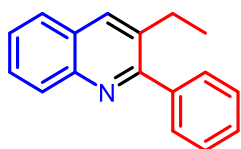
2-(4-bromophenyl)quinoline (**8**) 80% (113 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.25 – 8.00 (m, 4H), 7.88 – 7.69 (m, 3H), 7.64 (d, $J = 8.6$ Hz, 2H), 7.58 – 7.49 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 156.0, 148.3, 138.5, 137.0, 132.0, 129.9, 129.7, 129.1, 127.5, 127.3, 126.5, 124.0, 118.5.



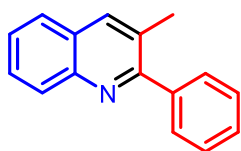
2-(4-iodophenyl)quinoline (**9**) 79% (112 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.22 (dd, $J = 8.6, 2.2$ Hz, 1H), 8.16 (d, $J = 8.4$ Hz, 1H), 7.92 (d, $J = 7.5$ Hz, 2H), 7.84 (dd, $J = 13.7, 8.7$ Hz, 4H), 7.77 – 7.71 (m, 1H), 7.54 (t, $J = 7.0$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.2, 148.2, 139.1, 138.0, 137.0, 129.9, 129.7, 129.3, 127.5, 127.3, 126.6, 118.5, 95.9.



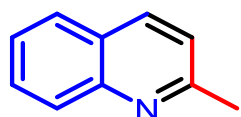
2-(naphthalen-2-yl)quinoline (10) 83% (106 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.34 – 8.25 (m, 2H), 8.19 – 8.13 (m, 1H), 8.03 – 7.92 (m, 3H), 7.85 – 7.79 (m, 1H), 7.79 – 7.73 (m, 2H), 7.68 – 7.61 (m, 2H), 7.59 – 7.48 (m, 2H). ^{13}C NMR (126 MHz, CDCl_3): δ 159.5, 148.1, 138.8, 136.3, 134.0, 131.3, 129.8, 129.7, 129.2, 128.4, 127.8, 127.6, 127.0, 126.6, 126.0, 125.7, 125.4, 123.3.



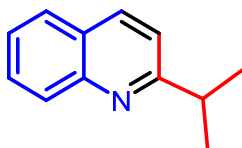
3-ethyl-2-phenylquinoline (11) 89% (104 mg). ^1H (400 MHz, CDCl_3): δ 8.17 (d, $J = 8.4$ Hz, 1H), 8.07 (s, 1H), 7.82 (d, $J = 8.0$ Hz, 1H), 7.71 – 7.65 (m, 1H), 7.60 – 7.42 (m, 6H), 2.81 (q, $J = 7.5$ Hz, 2H), 1.21 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 160.6, 146.2, 140.8, 135.4, 135.1, 129.2, 128.9, 128.8, 128.3, 128.2, 127.8, 127.0, 126.5, 125.9, 26.0, 14.8.



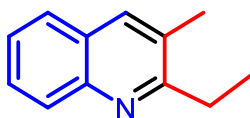
3-methyl-2-phenylquinoline (12) 88% (96 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.19 (d, $J = 8.5$ Hz, 1H), 8.03 (s, 1H), 7.81 (d, $J = 8.1$ Hz, 1H), 7.70 (t, $J = 7.7$ Hz, 1H), 7.63 (d, $J = 6.9$ Hz, 2H), 7.58 – 7.45 (m, 4H), 2.51 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 160.6, 146.6, 140.8, 136.8, 129.3, 128.9, 128.8, 128.4, 128.3, 127.6, 126.8, 126.5, 20.7.



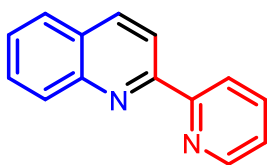
2-methylquinoline (13) 83% (59 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.04 (d, $J = 4.7$ Hz, 2H), 7.76 (d, $J = 8.0$ Hz, 1H), 7.73 – 7.65 (m, 1H), 7.48 (d, $J = 5.8$ Hz, 1H), 7.26 (d, $J = 8.4$ Hz, 1H), 2.76 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 158.9, 147.9, 136.2, 129.4, 128.6, 127.5, 126.5, 125.7, 122.0, 25.4.



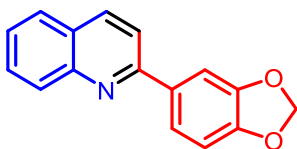
2-isopropylquinoline (14) 89% (76 mg). ^1H (500 MHz, CDCl_3): δ 8.11 (t, $J = 7.6$ Hz, 2H), 7.80 (d, $J = 8.1$ Hz, 1H), 7.74 – 7.68 (m, 1H), 7.53 – 7.48 (m, 1H), 7.37 (d, $J = 8.5$ Hz, 1H), 3.31 (p, $J = 6.9$ Hz, 1H), 1.43 (d, $J = 7.0$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3): δ 167.7, 147.6, 136.5, 129.3, 128.9, 127.5, 127.0, 125.7, 119.2, 37.2, 22.6.



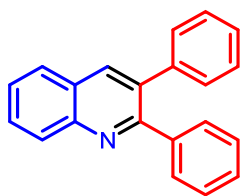
2-ethyl-3-methylquinoline (15) 93% (76 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.05 (d, $J = 8.4$ Hz, 1H), 7.84 (s, 1H), 7.71 (d, $J = 8.1$ Hz, 1H), 7.66 – 7.61 (m, 1H), 7.49 – 7.44 (m, 1H), 3.02 (q, $J = 7.6$ Hz, 2H), 2.50 (s, 3H), 1.40 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 163.4, 146.7, 135.8, 129.4, 128.5, 128.3, 127.3, 126.7, 125.6, 29.5, 19.1, 12.9.



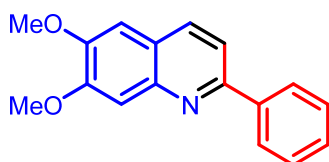
2-(pyridin-4-yl)quinoline (16) 75% (77 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.77 (d, $J = 4.9$ Hz, 1H), 8.68 (d, $J = 8.1$ Hz, 1H), 8.59 (d, $J = 8.7$ Hz, 1H), 8.31 (d, $J = 8.7$ Hz, 1H), 8.21 (d, $J = 8.4$ Hz, 1H), 7.94 – 7.85 (m, 2H), 7.80 – 7.73 (m, 1H), 7.58 (t, $J = 7.5$ Hz, 1H), 7.43 – 7.34 (m, 1H). ^{13}C NMR (126 MHz, CDCl_3): δ 156.4, 156.2, 149.2, 147.94, 1, 136.9, 129.8, 129.6, 128.3, 127.7, 126.8, 124.1, 121.9, 119.0.



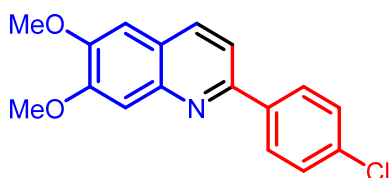
2-(benzo[d][1,3]dioxol-5-yl)quinoline (17) 85% (105mg). ^1H NMR (400 MHz, CDCl_3): δ 8.15 (dd, $J = 12.4, 8.5$ Hz, 2H), 7.84 – 7.64 (m, 5H), 7.56 – 7.47 (m, 1H), 6.94 (s, 1H), 6.04 (s, 2H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.7, 148.9, 148.4, 148.2, 136.7, 134.1, 129.7, 129.6, 127.4, 127.0, 126.1, 121.8, 118.6, 108.5, 107.9, 101.4.



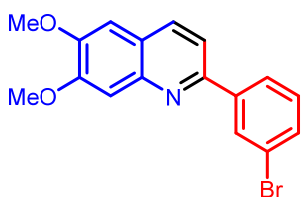
2,3-diphenylquinoline (**18**) 87% (122 mg) ^1H NMR (500 MHz, CDCl_3): δ 8.27 (d, $J = 8.4$ Hz, 1H), 8.22 (s, 1H), 7.90 (d, $J = 8.2$ Hz, 1H), 7.80 – 7.75 (m, 1H), 7.63 – 7.58 (m, 1H), 7.51 – 7.47 (m, 2H), 7.34 – 7.27 (m, 8H). ^{13}C NMR (126 MHz, CDCl_3): δ 158.4, 139.9, 137.7, 134.6, 130.1, 129.8, 129.7, 129.4, 128.3, 128.1, 127.9, 127.5, 127.3, 127.2, 126.8.



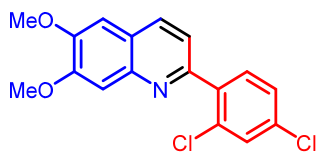
6,7-dimethoxy-2-phenylquinoline(**19**) 90% (119 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.16 – 8.10 (m, 2H), 8.04 (d, $J = 8.6$ Hz, 1H), 7.73 (d, $J = 8.4$ Hz, 1H), 7.56 – 7.50 (m, 3H), 7.48 – 7.42 (m, 1H), 7.05 (s, 1H), 4.07 (s, 3H), 4.02 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.4, 152.6, 149.7, 145.3, 140.0, 134.9, 128.9, 128.8, 127.3, 122.7, 117.3, 108.4, 104.9, 56.2, 56.1.



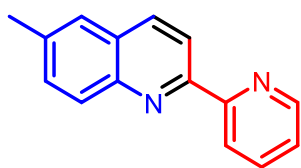
2-(4-chlorophenyl)-6,7-dimethoxyquinoline(**20**) 93% (139 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.07 – 7.98 (m, 3H), 7.66 (d, $J = 8.4$ Hz, 1H), 7.46 (s, 3H), 7.03 (s, 1H), 4.05 (s, 3H), 4.01 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 153.9, 152.7, 149.8, 145.3, 138.4, 135.1, 134.9, 128.9, 128.5, 122.8, 116.9, 108.3, 104.9, 56.2, 56.1.



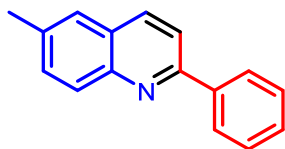
2-(3-bromophenyl)-6,7-dimethoxyquinoline (**21**) 92% (158 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.32 (s, 1H), 8.03 (dd, $J = 13.3$, 8.1 Hz, 2H), 7.68 (d, $J = 8.4$ Hz, 1H), 7.56 (d, $J = 8.1$ Hz, 1H), 7.49 (s, 1H), 7.37 (t, $J = 7.9$ Hz, 1H), 7.05 (s, 1H), 4.07 (s, 3H), 4.03 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 153.5, 152.7, 149.9, 145.2, 141.9, 135.1, 131.7, 130.3, 130.3, 125.7, 123.1, 123.0, 116.9, 108.3, 104.9, 56.2, 56.1.



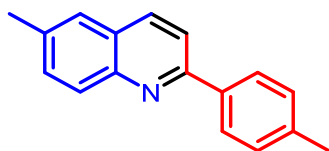
2-(2,4-dichlorophenyl)-6,7-dimethoxyquinoline (22) 85% (142 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.07 (d, $J = 8.4$ Hz, 1H), 7.67 – 7.56 (m, 2H), 7.54 (s, 1H), 7.50 (s, 1H), 7.40 (d, $J = 8.2$ Hz, 1H), 7.11 (s, 1H), 4.05 (s, 6H). ^{13}C NMR (126 MHz, CDCl_3): δ 153.9, 152., 150.2, 145.1, 138.4, 134.8, 134.0, 133., 132.5, 129.8, 127.4, 122., 120.8, 108.2, 104.9, 56.2, 56.1.



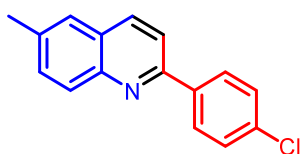
6-methyl-2-(pyridin-2-yl)quinoline (23) 82% (92 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.75 (d, $J = 6.7$ Hz, 1H), 8.64 (d, $J = 7.9$ Hz, 1H), 8.53 (d, $J = 8.5$ Hz, 1H), 8.18 (d, $J = 8.7$ Hz, 1H), 8.09 (d, $J = 8.5$ Hz, 1H), 7.85 (t, $J = 7.7$ Hz, 1H), 7.63 – 7.54 (m, 2H), 7.38 – 7.30 (m, 1H), 2.54 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 156.5, 155.3, 149.2, 146.5, 136.9, 136.7, 136.1, 131.9, 129.5, 128.3, 126.5, 123., 121.7, 118.9, 21.7.



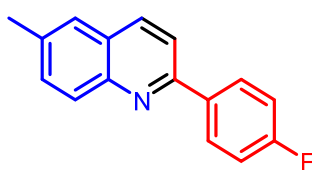
6-methyl-2-phenylquinoline (24) 91% (100 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.20 (d, $J = 8.5$ Hz, 2H), 8.13 (dd, $J = 8.8, 2.2$ Hz, 2H), 7.86 (s, 1H), 7.62 – 7.54 (m, 4H), 7.50 (d, $J = 7.5$ Hz, 1H), 2.57 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 156.5, 146.9, 139.8, 136.1, 131.9, 129.4, 129.2, 128.7, 127.5, 127.3, 126.4, 119.0, 21.7.



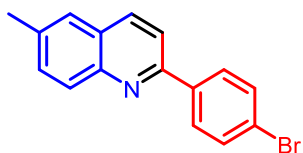
6-methyl-2-(p-tolyl)quinoline (25) 90% (105 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.11 (dd, $J = 18.0, 8.4$ Hz, 4H), 7.84 (d, $J = 8.6$ Hz, 1H), 7.62 – 7.56 (m, 2H), 7.36 (d, $J = 7.9$ Hz, 2H), 2.57 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 156.5, 146.9, 139.2, 137.0, 136.0, 135.9, 131.9, 129.6, 129.3, 127.4, 127.1, 126.4, 118.9, 21.6, 21.4



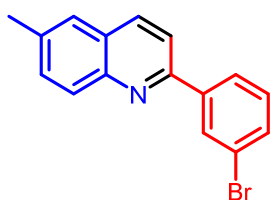
2-(4-chlorophenyl)-6-methylquinoline (**26**) 86% (109 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.09 (dd, $J = 16.8, 8.9$ Hz, 4H), 7.78 (d, $J = 8.6$ Hz, 1H), 7.58 (d, $J = 7.1$ Hz, 2H), 7.50 (d, $J = 8.7$ Hz, 2H), 2.57 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.1, 146.8, 138.2, 136.4, 136.3, 135.3, 132.2, 129.4, 128.9, 128.7, 127.3, 126.4, 118.5, 21.7.



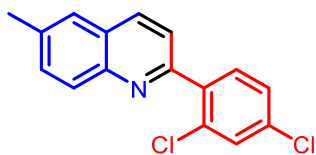
2-(4-Fluorophenyl)-6-methylquinoline (**27**) 88% (104 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.22 – 8.03 (m, 4H), 7.79 (d, $J = 8.6$ Hz, 1H), 7.58 (d, $J = 7.4$ Hz, 2H), 7.22 (t, $J = 8.8$ Hz, 2H), 2.59 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 164.9, 162.5, 155.4, 146.8, 136.2, 135.9, 132.1, 129.3, 129.3, 127.1, 126.4, 118.6, 115.8, 115.6, 21.6.



2-(4-Bromophenyl)-6-methylquinoline (**28**) 85% (127 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.16 – 8.01 (m, 4H), 7.78 (d, $J = 8.7$ Hz, 1H), 7.70 – 7.56 (m, 4H), 2.56 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.2, 146.8, 138.6, 136.5, 136.3, 132.2, 131.9, 129.4, 129.0, 127.3, 126.4, 123.7, 118.5, 21.7.



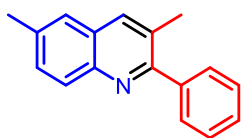
2-(3-Bromophenyl)-6-methylquinoline (**29**) 81% (121 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.37 (s, 1H), 8.13 – 8.04 (m, 3H), 7.77 (d, $J = 8.5$ Hz, 1H), 7.59 (d, $J = 10.8$ Hz, 3H), 7.39 (t, $J = 7.9$ Hz, 1H), 2.56 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 154.7, 146.8, 141.8, 136.6, 136.3, 132.2, 132.0, 130.5, 130.3, 129.5, 127.4, 126.4, 125.9, 123.2, 118.6, 21.7.



2-(2,4-dichlorophenyl)-6-methylquinoline (**30**) 84% (120 mg).

^1H NMR (400 MHz, CDCl_3): δ 8.17 – 8.05 (m, 2H), 7.72 – 7.58 (m, 4H), 7.54 (d, $J = 2.1$ Hz, 1H), 7.40 (dd, $J = 8.3, 2.1$ Hz, 1H),

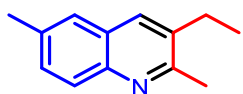
2.58 (d, $J = 0.9$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.3, 146.7, 138.3, 136.9, 135.2, 135.0, 133.2, 132.7, 132.2, 129.8, 129.3, 127.5, 127.2, 126.4, 122.5, 21.7.



3,6-dimethyl-2-phenylquinoline (**31**) 78% (92 mg). ^1H NMR (400

MHz, CDCl_3): δ 8.04 (d, $J = 8.4$ Hz, 1H), 7.90 (s, 1H), 7.63 – 7.57 (m, 2H), 7.54 – 7.40 (m, 5H), 2.54 (s, 3H), 2.44 (s, 3H). ^{13}C NMR

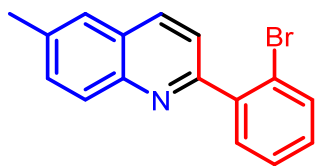
(101 MHz, CDCl_3): δ 159.6, 145.3, 141.0, 136.1, 131.1, 129.1, 129.0, 128.9, 128.30, 128.1, 127.7, 126.0, 125.6, 21.7, 20.7.



3-ethyl-2,6-dimethylquinoline (**32**) 72% (67 mg). ^1H NMR (400

MHz, CDCl_3): δ 7.93 (d, $J = 9.9$ Hz, 1H), 7.73 (s, 1H), 7.45 (d, $J =$

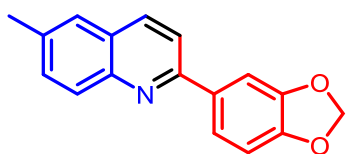
6.7 Hz, 2H), 2.99 (q, $J = 7.5$ Hz, 2H), 2.53 – 2.45 (m, 6H), 1.38 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 162.3, 145.3, 135.3, 135.2, 130.5, 129.3, 128.2, 127.4, 125.6, 29.4, 21.5, 19.1, 12.9.



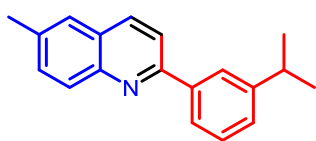
2-(2-bromophenyl)-6-methylquinoline (**33**) 81% (121 mg). ^1H

NMR (400 MHz, CDCl_3): δ 8.12 (dd, $J = 12.1, 8.6$ Hz, 2H), 7.76 – 7.63 (m, 4H), 7.60 (d, $J = 8.6$ Hz, 1H), 7.47 (t, $J = 7.5$

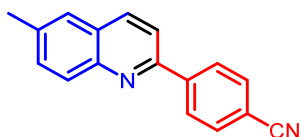
Hz, 1H), 7.35 – 7.28 (m, 1H), 2.58 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 157.9, 146.5, 141.8, 136.7, 135.0, 133.3, 132.0, 131.6, 129.9, 129.4, 127.7, 127.2, 126.4, 122.7, 121.9, 21.7.



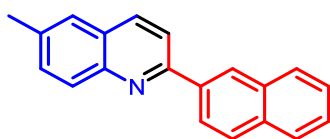
2-(benzo[d][1,3]dioxol-5-yl)-6-methylquinoline (**34**) 80% (105 mg). ^1H NMR (400 MHz, CDCl_3) δ 8.11 – 7.98 (m, 2H), 7.73 (d, $J = 10.5$ Hz, 2H), 7.63 (d, $J = 6.3$ Hz, 1H), 7.54 (d, $J = 8.3$ Hz, 2H), 6.94 (d, $J = 8.2$ Hz, 1H), 6.03 (s, 2H), 2.53 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.9, 148.7, 148.4, 146.8, 136.0, 135.9, 134.3, 131.9, 129.2, 127.0, 126.3, 121.6, 118.6, 108.5, 107.9, 101.3, 21.6.



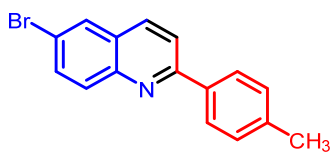
2-(3-isopropylphenyl)-6-methylquinoline (**35**) 77% (100 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.03 – 7.95 (m, 2H), 7.53 (d, $J = 13.0$ Hz, 2H), 7.32 (d, $J = 8.5$ Hz, 1H), 3.28 (dq, $J = 13.9, 7.0$ Hz, 1H), 2.53 (d, $J = 0.9$ Hz, 3H), 1.41 (d, $J = 6.9$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3): δ 166.7, 146.3, 135.8, 135.4, 131.5, 128.7, 126.9, 126.4, 119.1, 37.3, 22.6, 21.5.



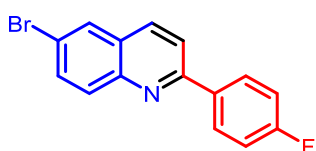
4-(6-methylquinolin-2-yl)benzonitrile (**36**) 87% (106 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.30 (d, $J = 8.5$ Hz, 2H), 8.21 (d, $J = 8.6$ Hz, 1H), 8.09 (d, $J = 8.5$ Hz, 1H), 7.89 – 7.80 (m, 3H), 7.63 (d, $J = 11.7$ Hz, 2H), 2.59 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 154.1, 146.9, 143.9, 137.2, 136.6, 132.6, 132.5, 129.6, 127.9, 127.6, 126.4, 118.9, 118.6, 112.5, 21.7.



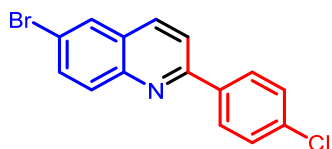
6-methyl-2-(naphthalen-2-yl)quinoline (**37**) 92% (124 mg). ^1H NMR (500 MHz, CDCl_3): δ 8.24 – 8.15 (m, 3H), 7.98 (t, $J = 6.7$ Hz, 2H), 7.76 (d, $J = 8.4$ Hz, 1H), 7.72 – 7.67 (m, 2H), 7.67 – 7.61 (m, 2H), 7.58 – 7.48 (m, 2H), 2.62 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3): δ 158.5, 146.7, 138.9, 136.5, 135.6, 134.1, 132.1, 131.4, 129.4, 129.0, 128.4, 127.7, 127.1, 126.6, 126.5, 125.9, 125.8, 125.4, 123.3, 21.7.



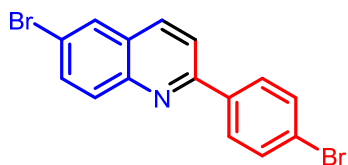
6-bromo-2-(p-tolyl)quinoline (38) 92% (137 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.10 – 7.99 (m, 4H), 7.95 (s, 1H), 7.86 (d, $J = 8.7$ Hz, 1H), 7.77 (d, $J = 8.9$ Hz, 1H), 7.33 (d, $J = 8.2$ Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 157.6, 146.9, 139.8, 136.4, 135.6, 133.0, 131.4, 129.7, 129.5, 128.2, 127.4, 119.8, 119.6, 21.4



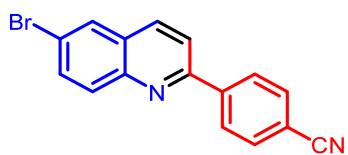
6-bromo-2-(4-fluorophenyl)quinoline (39) 88% (133 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.21 – 8.06 (m, 3H), 8.04 – 7.93 (m, 2H), 7.87 – 7.75 (m, 2H), 7.26 – 7.16 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3): δ 165.2, 162.7, 156.5, 146.8, 135.9, 135.3, 133.2, 131.4, 129.5, 129., 129.4, 128.1, 120.1, 119.4, 115.9, 115.8.



6-bromo-2-(4-Chlorophenyl)quinoline (40) 87% (137 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.10 (dd, $J = 8.3, 3.9$ Hz, 3H), 8.03 – 7.95 (m, 2H), 7.87 – 7.76 (m, 2H), 7.49 (d, $J = 8.5$ Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.3, 146.8, 137.6, 135.9, 135.9, 133.3, 131.4, 129.5, 129.1, 128.8, 128.3, 120.3, 119.3.

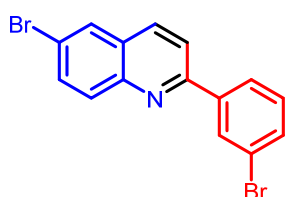


6-bromo-2-(4-Bromophenyl)quinoline (41) 83% (151 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.11 (d, $J = 8.8$ Hz, 1H), 8.07 – 7.96 (m, 4H), 7.84 (d, $J = 8.7$ Hz, 1H), 7.79 (dd, $J = 8.9, 2.3$ Hz, 1H), 7.68 – 7.62 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.5, 146.8, 135.9, 133.2, 131.5, 129.5, 129.4, 129.4, 128.1, 120.1, 119.4, 115.9, 115.8.



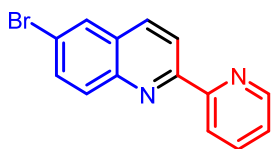
4-(6-bromoquinolin-2-yl)benzonitrile (**42**) 82% (127 mg).

^1H NMR (400 MHz, CDCl_3): δ 8.73 (d, $J = 2.9$ Hz, 1H), 8.66 – 8.53 (m, 2H), 8.15 (d, $J = 8.7$ Hz, 1H), 8.06 – 7.95 (m, 2H), 7.86 (td, $J = 7.7$, 1.9 Hz, 1H), 7.77 (dd, $J = 9.0$, 2.2 Hz, 1H), 7.41 – 7.31 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.5, 155.9, 149.2, 146.5, 137.0, 135.8, 133.1, 131.5, 129.7, 129.3, 124.3, 121.3, 120., 119.8.



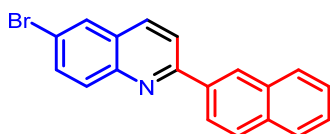
6-bromo-2-(3-bromophenyl)quinoline (**43**) 84% (152 mg). ^1H

NMR (400 MHz, CDCl_3): δ 8.35 (d, $J = 3.7$ Hz, 1H), 8.13 – 7.95 (m, 4H), 7.85 – 7.78 (m, 2H), 7.61 (d, $J = 7.9$ Hz, 1H), 7.39 (t, $J = 7.9$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.9, 146.8, 141.1, 135.9, 133.4, 132.5, 131.5, 130.6, 130.4, 129.5, 128.4, 125.9, 123.2, 120.5, 119.4.



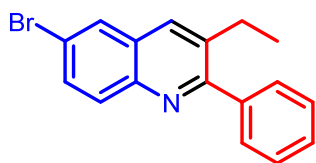
6-bromo-2-(pyridin-2-yl)quinoline (**44**) 80% (114 mg). ^1H NMR

(400 MHz, CDCl_3): δ 8.28 (d, $J = 8.7$ Hz, 2H), 8.19 (d, $J = 8.9$ Hz, 1H), 8.03 (d, $J = 8.7$ Hz, 2H), 7.90 (d, $J = 8.5$ Hz, 1H), 7.82 (dd, $J = 8.8$, 4.3 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.2, 146.8, 143.2, 136.3, 133.7, 132.7, 131.6, 129.6, 128.56, 128.0, 121.1, 119.4, 118.8, 113.0.



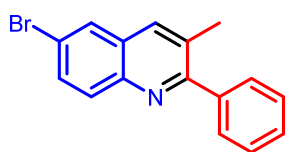
6-bromo-2-(naphthalen-2-yl)quinoline (**45**) 83% (139 mg).

^1H NMR (400 MHz, CDCl_3): δ 8.21 – 8.07 (m, 4H), 7.98 (t, $J = 8.9$ Hz, 2H), 7.86 (dd, $J = 8.9$, 2.2 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.65 – 7.60 (m, 1H), 7.58 – 7.49 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3): δ 159.9, 146.7, 138.3, 135.3, 134.0, 133.3, 131.5, 131.1, 129.6, 129.4, 128.5, 128.1, 127.9, 126.8, 126.1, 125.5, 125.4, 124.1, 120.5.



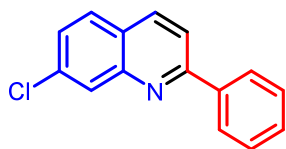
6-bromo-3-ethyl-2-phenylquinoline (**46**) 76% (118 mg). ^1H NMR (400 MHz, CDCl_3): δ 7.97 (dd, $J = 13.8, 9.8$ Hz, 3H), 7.72 (dd, $J = 8.9, 2.3$ Hz, 1H), 7.54 (d, $J = 6.4$ Hz, 2H), 7.52 – 7.42 (m, 3H), 2.79 (q, $J = 7.5$ Hz, 2H), 1.19 (t, $J = 7.5$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3): δ 161.1, 144.9, 140.5, 136.4, 133.9, 132.2, 131.1, 128.9, 128.9, 128.7, 128.4, 128.3, 120.2, 26.1, 14.6



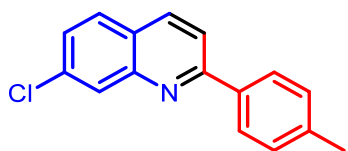
6-bromo-3-methyl-2-phenylquinoline (**47**) 78% (116 mg). ^1H NMR (400 MHz, CDCl_3): δ 7.98 (d, $J = 9.0$ Hz, 1H), 7.93 – 7.85 (m, 2H), 7.70 (dd, $J = 8.9, 2.3$ Hz, 1H), 7.58 (d, $J = 6.5$ Hz, 2H),

7.53 – 7.41 (m, 3H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 160.9, 145.2, 140.5, 135.7, 132.2, 131.1, 130.4, 128.8, 128.7, 128.7, 128.4, 128.4, 120.2, 20.7.



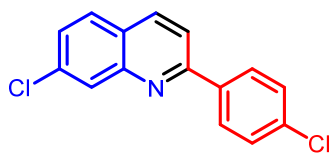
7-chloro-2-phenylquinoline (**48**) 84% (100 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.22 – 8.10 (m, 4H), 7.84 (d, $J = 8.6$ Hz, 1H), 7.72 (d, $J = 8.6$ Hz, 1H), 7.60 – 7.43 (m, 4H). ^{13}C NMR (101 MHz,

CDCl_3): δ 158.2, 148.7, 139.2, 136.6, 135.5, 129.7, 128.9, 128.7, 127.6, 127.3, 125.5, 119.1.

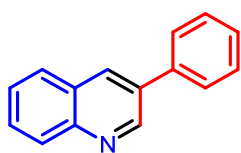


7-chloro-2-(p-tolyl)quinoline (**49**) 77% (98 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.19 – 8.12 (m, 2H), 8.07 (d, $J = 8.4$ Hz, 2H), 7.84 (d, $J = 8.5$ Hz, 1H), 7.72 (d, $J = 8.7$ Hz, 1H),

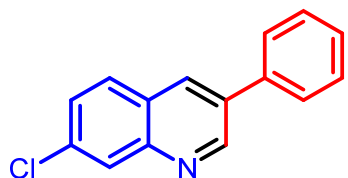
7.45 (dd, $J = 8.6, 2.0$ Hz, 1H), 7.34 (d, $J = 7.9$ Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 158.21, 148.7, 139.9, 136.5, 136.4, 135.4, 129.7, 128.7, 128.6, 127.5, 127.1, 125.4, 118.9, 21.4.



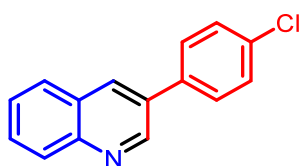
7-chloro-2-(4-chlorophenyl)quinoline (50) ^1H NMR (400 MHz, CDCl_3): δ 8.21 – 8.09 (m, 4H), 7.82 (d, $J = 8.6$ Hz, 1H), 7.75 (d, $J = 8.6$ Hz, 1H), 7.54 – 7.46 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.85, 148.58, 137.51, 136.75, 135.93, 135.67, 129.08, 128.82, 128.69, 128.66, 127.5, 125.5, 118.6.



3-phenylquinoline (51) 86% (44 mg). ^1H NMR (400 MHz, CDCl_3): δ 9.19 (d, $J = 2.4$ Hz, 1H), 8.29 (d, $J = 2.5$ Hz, 1H), 8.15 (d, $J = 8.4$ Hz, 1H), 7.87 (d, $J = 9.8$ Hz, 1H), 7.71 (d, $J = 8.2$ Hz, 3H), 7.61 – 7.49 (m, 3H), 7.44 (t, $J = 8.0$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3): δ 149.9, 147.4, 137.8, 133.9, 133.3, 129.4, 129.3, 129.1, 128.1, 128.0, 127.4, 127.0.

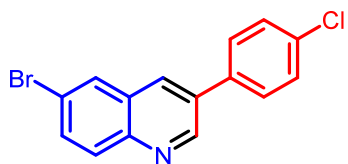


7-chloro-3-phenylquinoline (52) 81% (97 mg). ^1H NMR (400 MHz, CDCl_3): δ 9.18 (s, 1H), 8.27 (d, $J = 2.5$ Hz, 1H), 8.13 (d, $J = 2.4$ Hz, 1H), 7.81 (d, $J = 8.7$ Hz, 1H), 7.70 (d, $J = 8.7$ Hz, 2H), 7.58 – 7.49 (m, 3H), 7.49 – 7.42 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3): δ 150.9, 147.6, 137.5, 135.2, 134.1, 132.9, 129.3, 129.2, 128.4, 128.3, 128., 127.4, 126.4.



3-(4-chlorophenyl)quinoline (53) 79% (93 mg). ^1H NMR (400 MHz, CDCl_3): δ 9.14 (d, $J = 2.4$ Hz, 1H), 8.25 (d, $J = 1.6$ Hz, 1H), 8.19 – 8.13 (m, 1H), 7.89 – 7.84 (m, 1H), 7.73 (ddd, $J = 8.4, 6.9, 1.5$ Hz, 1H), 7.64 – 7.56 (m, 3H), 7.50 – 7.46 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3):

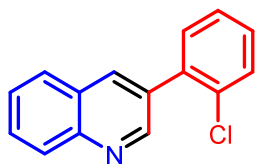
δ 152.2, 147.5, 136.6, 135.9, 135.6, 132.9, 132.6, 131.5, 130.3, 129.7, 129.3, 128.3, 128.1, 127.3, 125.9.



6-bromo-3-(4-chlorophenyl)quinoline (54) 75% (119 mg).

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.16 (d, $J = 2.3$ Hz, 1H), 8.20 (d, $J = 2.1$ Hz, 1H), 8.09 – 8.02 (m, 2H), 7.82 (d, $J = 11.0$

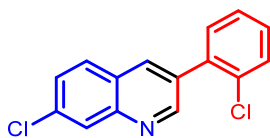
Hz, 1H), 7.65 (d, $J = 6.6$ Hz, 2H), 7.53 (d, $J = 8.7$ Hz, 2H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3): δ 149.8, 145.8, 135.8, 134.8, 133.6, 133.2, 132.2, 131.0, 130.0, 129.5, 129.1, 128.7, 121.2.



3-(2-chlorophenyl)quinoline (55) 78% (93 mg). $^1\text{H NMR}$ (400 MHz,

CDCl_3): δ 9.01 (d, $J = 2.3$ Hz, 1H), 8.24 – 8.12 (m, 2H), 7.85 (d, $J = 8.2$ Hz, 1H), 7.74 (t, $J = 6.9$ Hz, 1H), 7.60 – 7.51 (m, 2H), 7.45 –

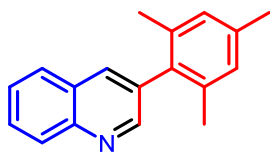
7.34 (m, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3): δ 151.2, 147.2, 137.0, 136.1, 133.0, 132.4, 131.6, 130.2, 129.8, 129.5, 129.2, 128.1, 127.6, 127.3, 127.0



7-chloro-3-(2-chlorophenyl)quinoline (56) 75% (102 mg). ^1H

NMR (400 MHz, CDCl_3): δ 9.04 (s, 1H), 8.23 (s, 1H), 8.18 (s, 1H), 7.83 (d, $J = 8.7$ Hz, 1H), 7.60 – 7.55 (m, 2H), 7.47 – 7.40 (m,

3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3): δ 152.2, 147.5, 136.6, 135.9, 135.6, 132.9, 132.6, 131.5, 130.3, 129.7, 129.3, 128.3, 128.1, 127.3, 125.9.

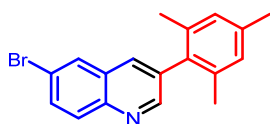


3-mesitylquinoline (57) 83% (102 mg). $^1\text{H NMR}$ (400 MHz,

CDCl_3): δ 8.77 (d, $J = 2.2$ Hz, 1H), 8.20 (d, $J = 8.4$ Hz, 1H), 8.00 (d, $J = 3.2$ Hz, 1H), 7.87 (d, $J = 9.9$ Hz, 1H), 7.78 (t, $J = 7.7$ Hz,

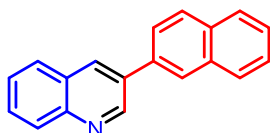
1H), 7.65 – 7.59 (m, 1H), 7.04 (s, 1H), 2.40 (s, 3H), 2.07 (s, 6H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3):

δ 151.8, 146.9, 137.7, 136.5, 136.0, 135.8, 135.2, 134.9, 134.1, 129.4, 129.2, 128.5, 127.8, 126.9, 21.1, 20.9.



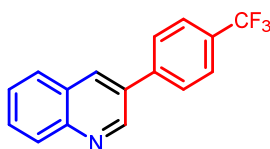
6-bromo-3-mesitylquinoline (58) 81% (132 mg). ^1H NMR (400 MHz, CDCl_3): δ 8.74 (s, 1H), 8.07 – 7.99 (m, 2H), 7.88 (d, $J = 2.4$ Hz, 1H), 7.81 (d, $J = 11.2$ Hz, 1H), 7.01 (s, 2H), 2.37 (s, 3H), 2.02

(s, 6H). ^{13}C NMR (101 MHz, CDCl_3): δ 152.2, 145.5, 137.9, 136.4, 135.0, 134.9, 134.4, 132.8, 131.0, 129.8, 129.2, 128.5, 120.8, 21.1, 20.9.



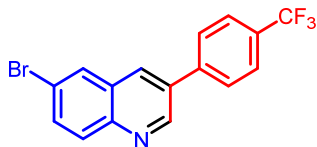
3-(naphthalen-2-yl)quinoline (59) 80% (102 mg). ^1H NMR (400 MHz, CDCl_3): δ 9.10 (s, 1H), 8.32 – 8.22 (m, 2H), 7.95 (dd, $J = 8.2, 3.4$ Hz, 2H), 7.88 (t, $J = 7.2$ Hz, 2H), 7.84 – 7.76 (m, 1H), 7.66

– 7.51 (m, 4H), 7.49 – 7.44 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3): δ 151.9, 147.3, 136.4, 136.3, 135.7, 135.2, 133.9, 133.8, 131.7, 129.8, 129.3, 128.7, 128.6, 128.0, 127.9, 127.1, 126.7, 126.2, 125.5, 125.4.



3-(4-(trifluoromethyl)phenyl)quinoline (60) 79% (107 mg). ^1H NMR (400 MHz, CDCl_3): δ 9.15 (s, 1H), 8.24 (d, $J = 2.6$ Hz, 1H), 8.16 (d, $J = 8.2$ Hz, 1H), 7.87 (d, $J = 9.8$ Hz, 1H), 7.74 (t, $J = 7.6$

Hz, 1H), 7.67 (dd, $J = 8.9, 5.2$ Hz, 2H), 7.59 (t, $J = 6.9$ Hz, 1H), 7.26 – 7.20 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3): δ 163.9, 161.9, 149.7, 147.3, 134.0, 133.9, 133.1, 132.9, 129.5, 129.3, 129.1, 129.1, 128.0, 127.9, 127.1.



6-bromo-3-(4-(trifluoromethyl)phenyl)quinoline (61) 74% (130mg). ^1H NMR (400 MHz, CDCl_3): δ 9.14 (s, 1H), 8.15 (d, $J = 2.6$ Hz, 1H), 8.06 – 7.98 (m, 2H), 7.79 (d, $J = 6.7$ Hz, 1H),

7.67 (dd, $J = 8.9, 5.2$ Hz, 2H), 7.28 – 7.21 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3): δ 164.1, 162.1, 150.0, 145.8, 133.7, 133.5, 133.5, 132.9, 131.9, 130.9, 129.9, 129.2, 129.1, 129.1, 121.1, 116.4, 116.2.

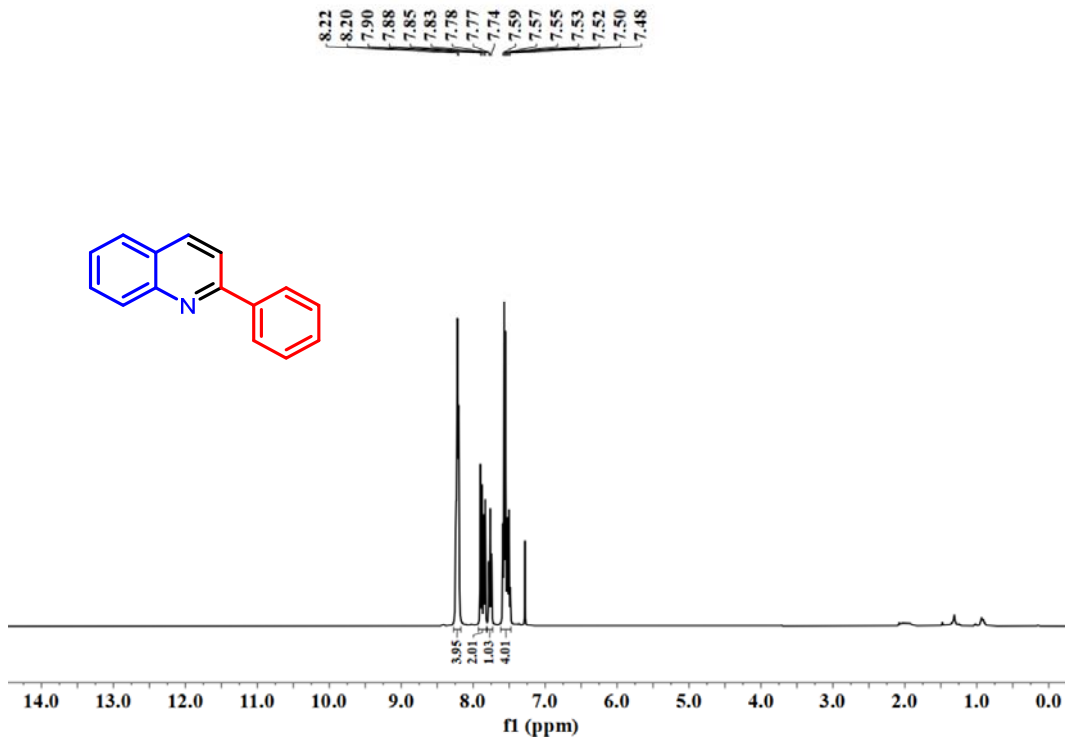


Fig. S33. ^1H NMR spectrum of **1** in CDCl_3 (500 MHz).

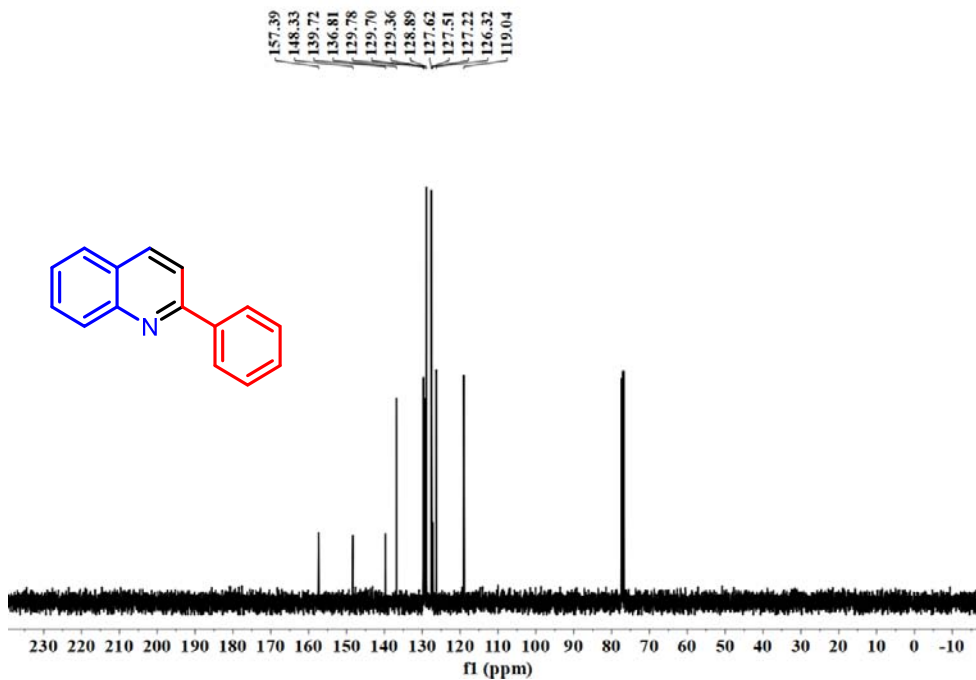


Fig. S34 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** in CDCl_3 (126 MHz).

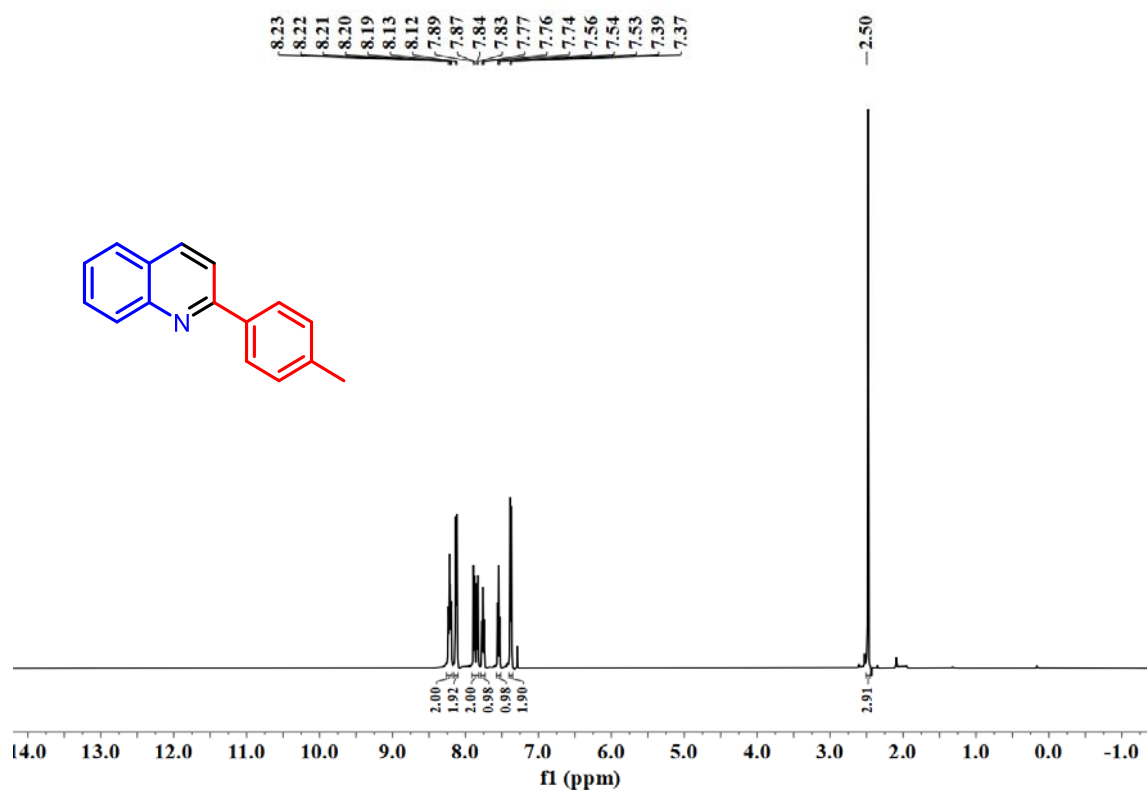


Fig. S35 ^1H NMR spectrum of **2** in CDCl_3 (500 MHz).

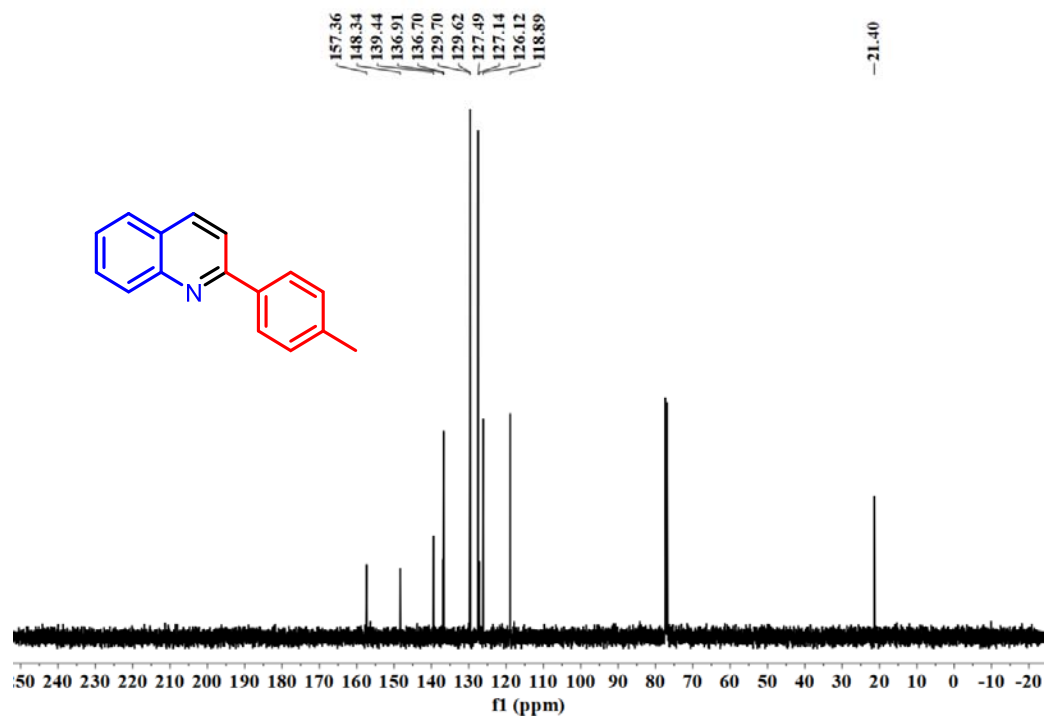


Fig. S36 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in CDCl_3 (101 MHz).

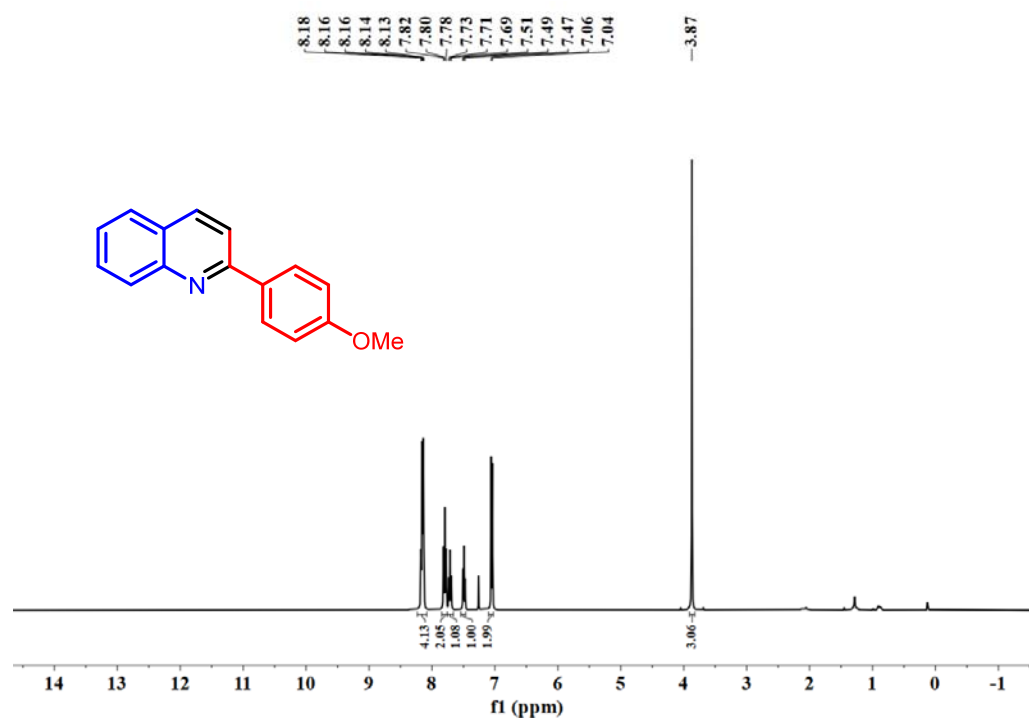


Fig. S37 ^1H NMR spectrum of **3** in CDCl_3 (400 MHz).

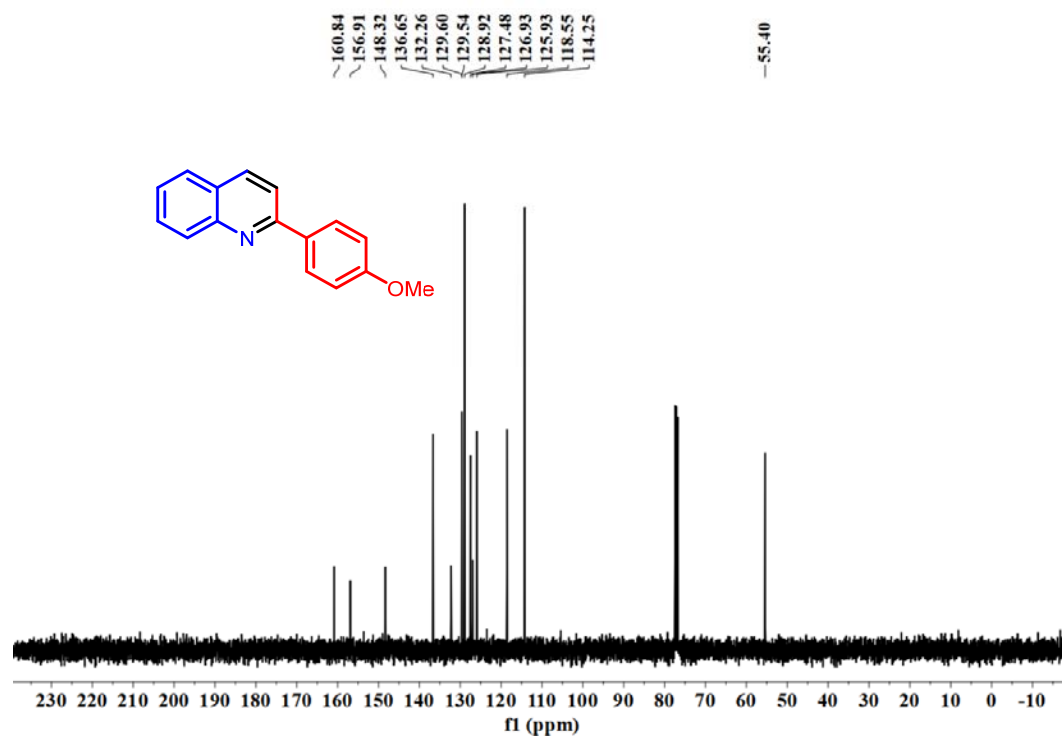


Fig. S38 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** in CDCl_3 (101MHz).

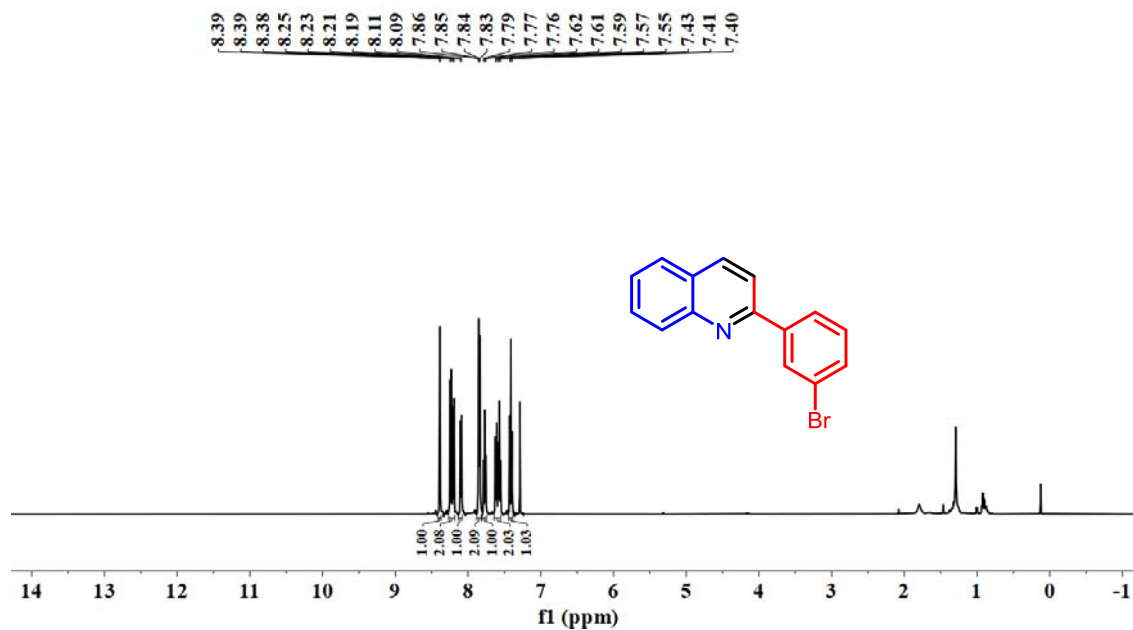


Fig. S39 ^1H NMR spectrum of **4** in CDCl_3 (500 MHz).

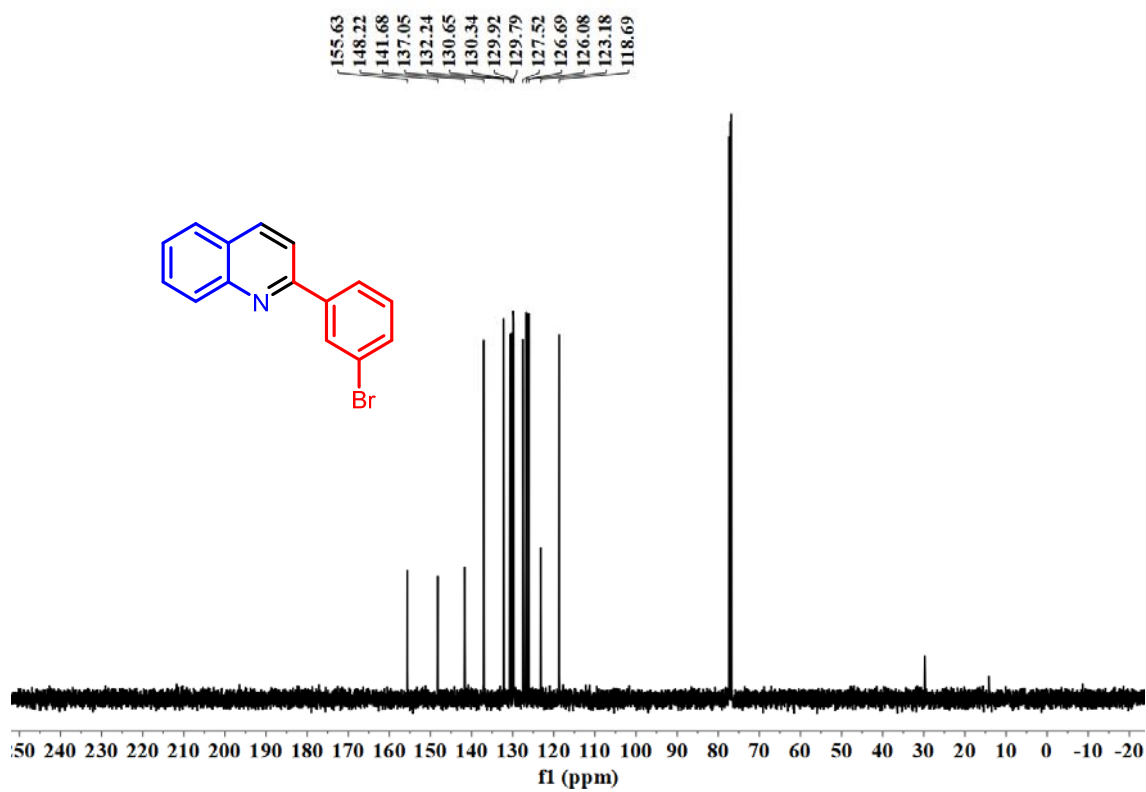


Fig. S40 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** in CDCl_3 (126 MHz).

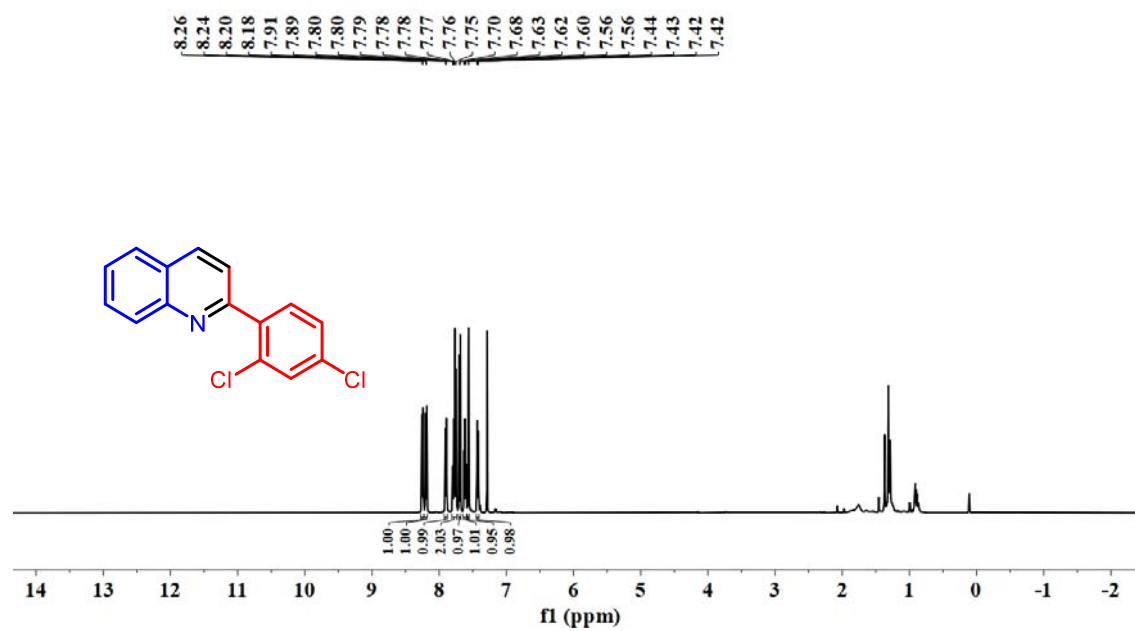


Fig. S41 ¹H NMR spectrum of **5** in CDCl₃ (500 MHz).

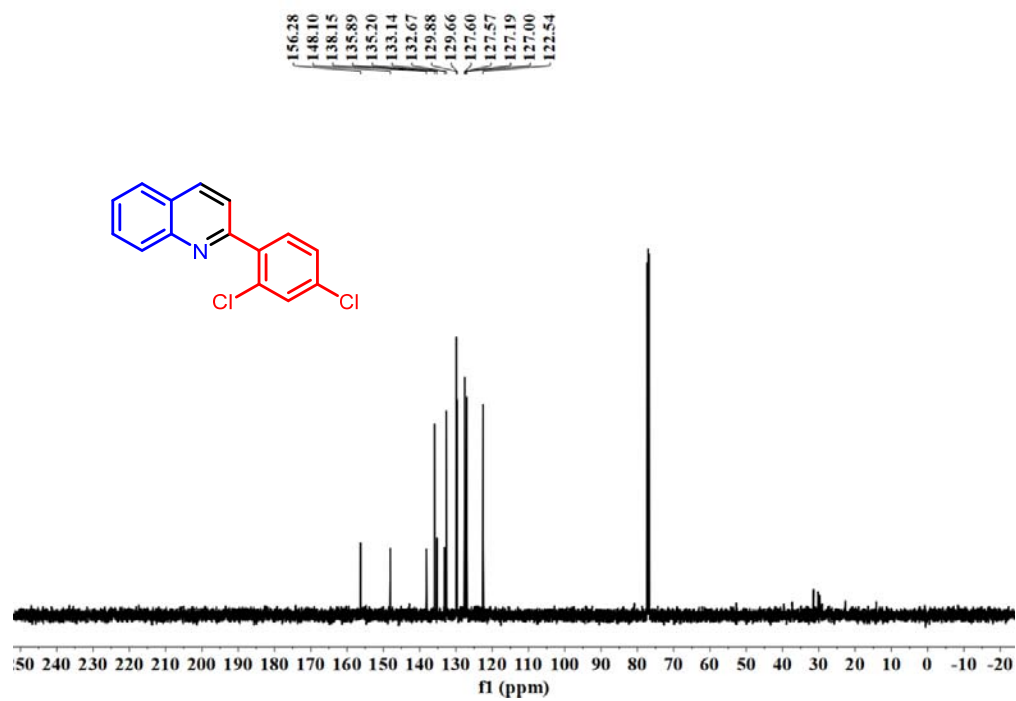


Fig. S42 ¹³C {¹H} NMR spectrum of **5** in CDCl₃ (126 MHz).

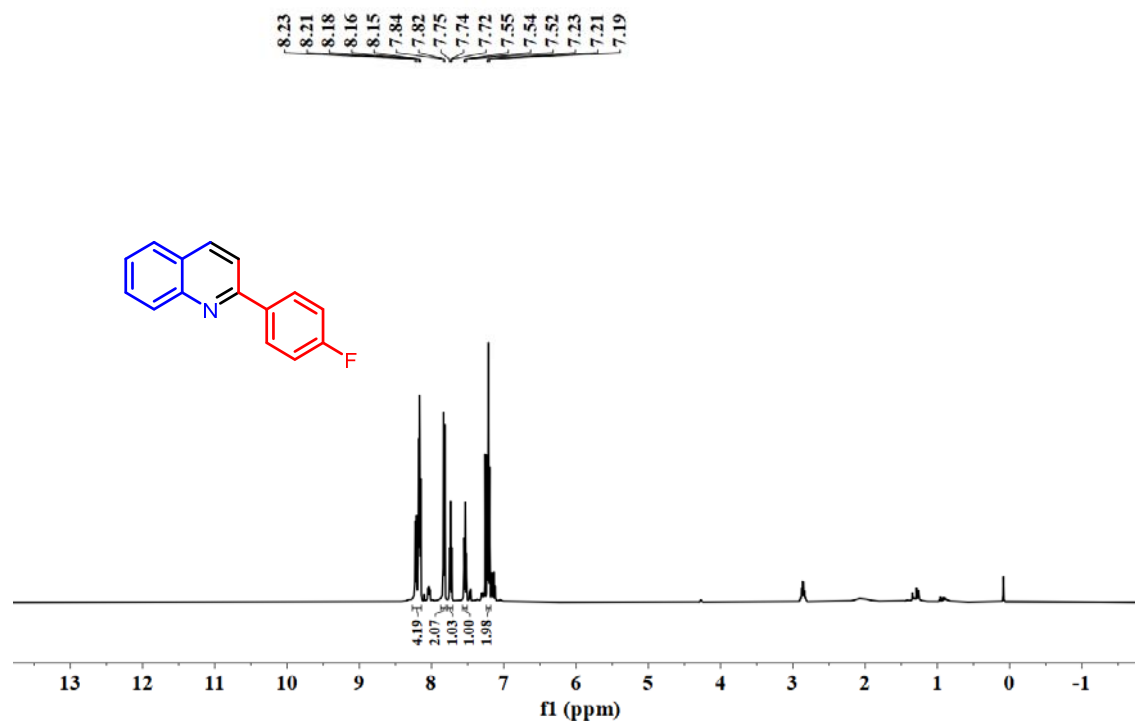


Fig. S43 ^1H NMR spectrum of **6** in CDCl_3 (500 MHz).

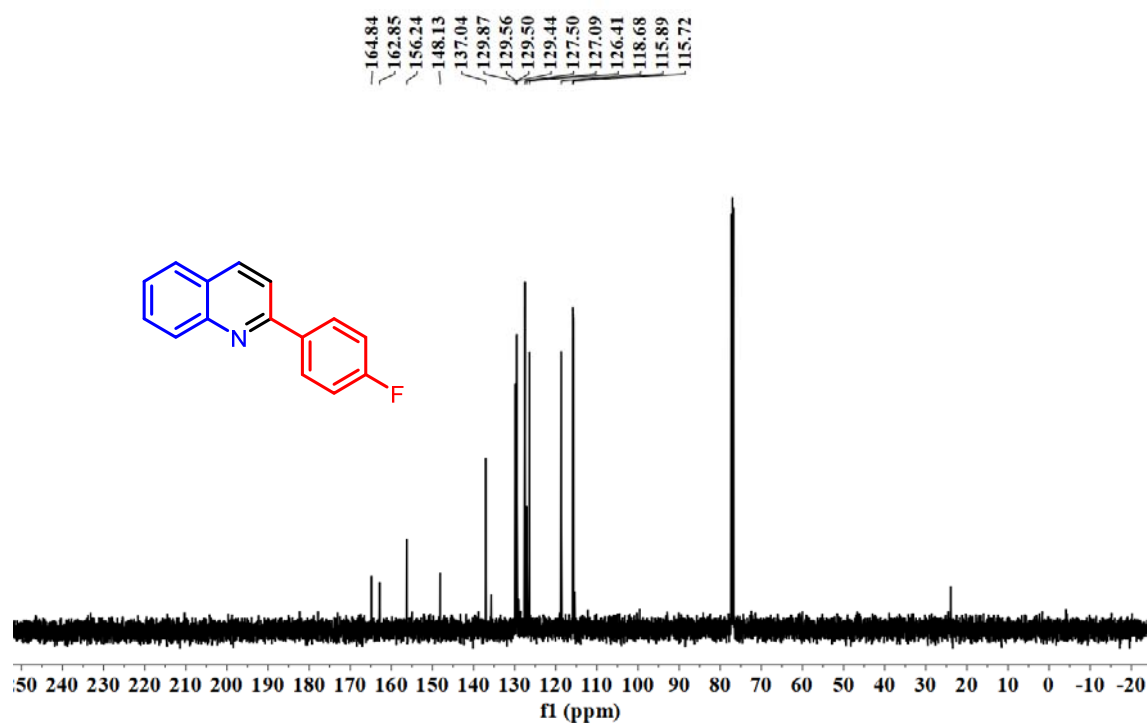


Fig. S44 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** in CDCl_3 (126 MHz).

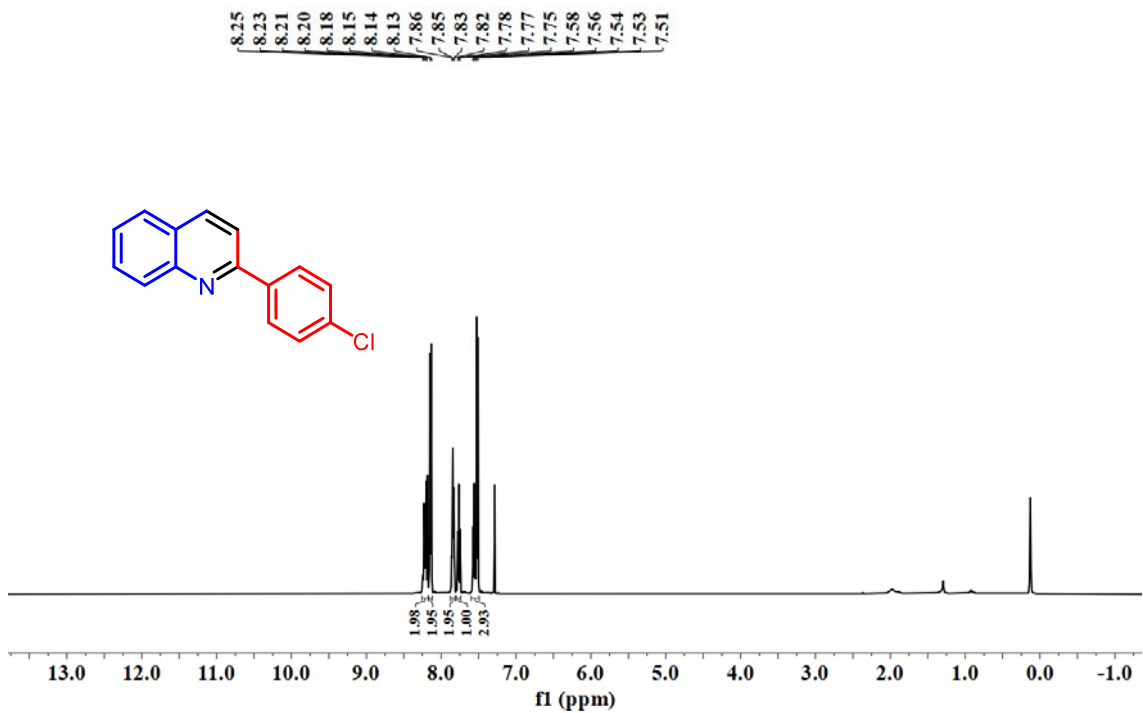


Fig. S45 ¹H NMR spectrum of 7 in CDCl₃ (500 MHz).

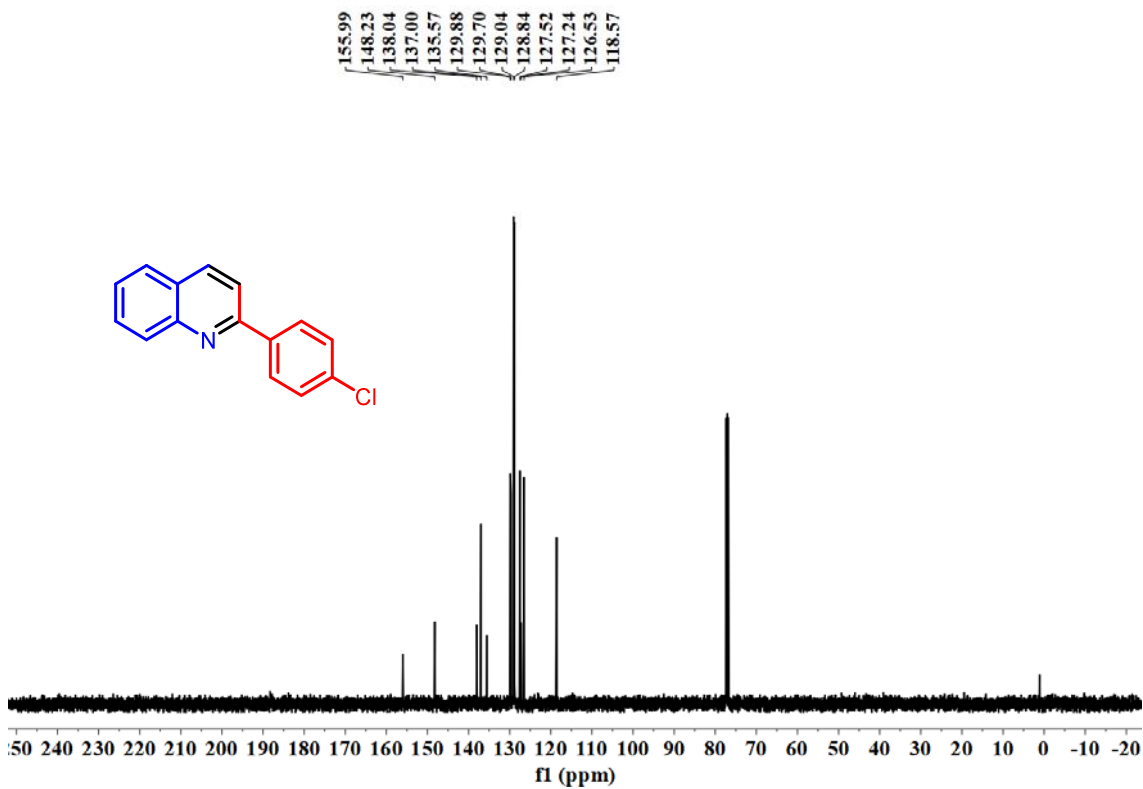


Fig. S46 ¹³C{¹H} NMR spectrum of 7 in CDCl₃ (126 MHz).

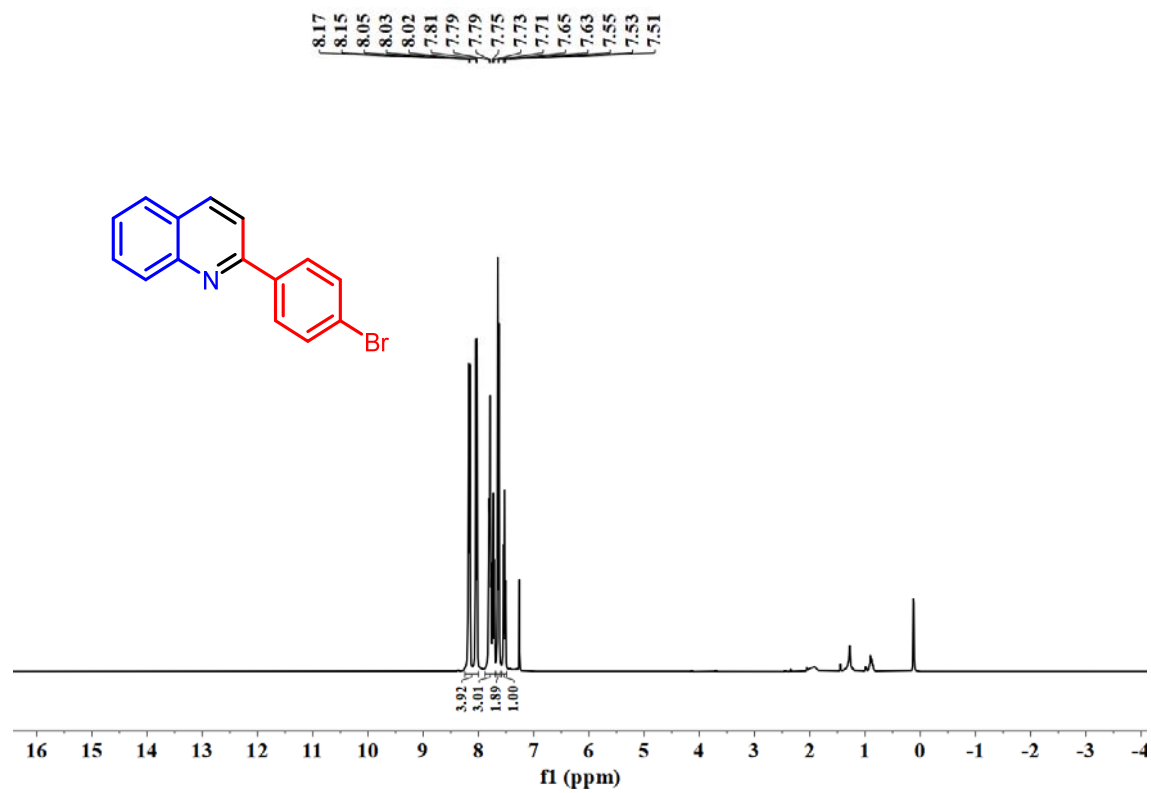


Fig. S47 ¹H NMR spectrum of **8** in CDCl₃ (400MHz).

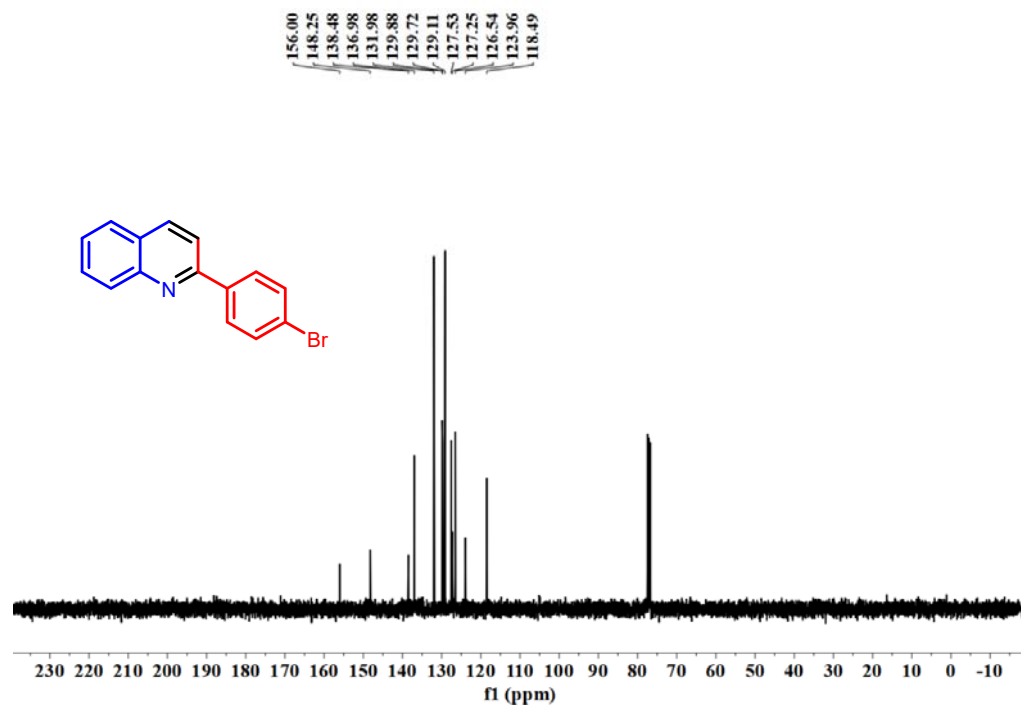


Fig. S48 ¹³C {¹H} NMR spectrum of **8** in CDCl₃ (101 MHz).

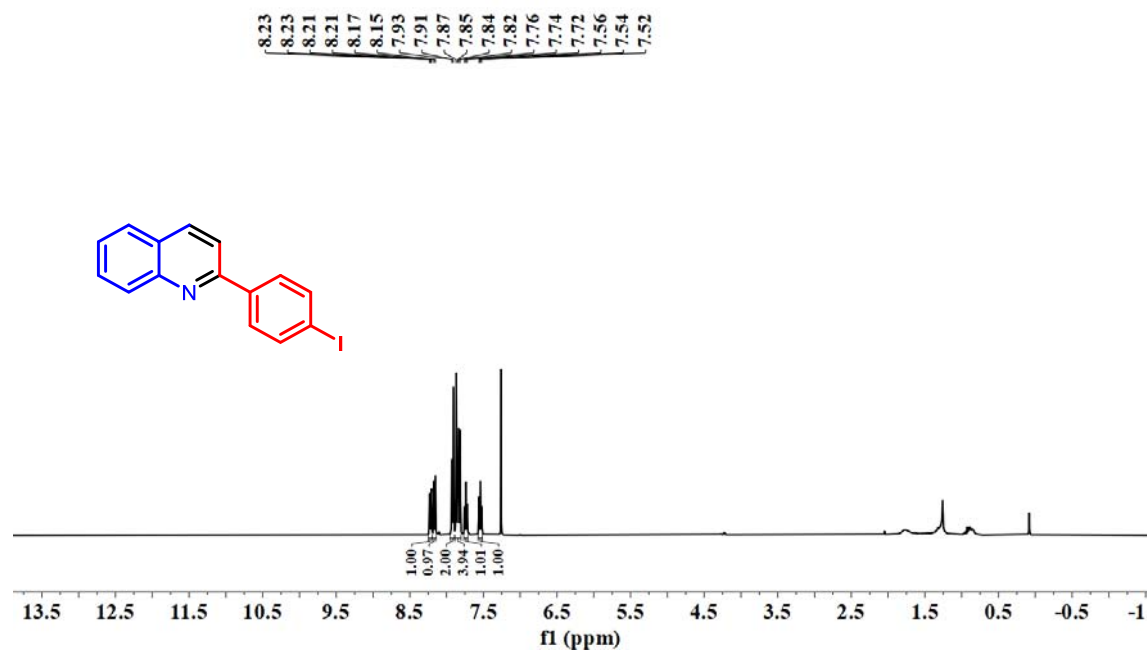


Fig. S49 ^1H NMR spectrum of **9** in CDCl_3 (400 MHz).

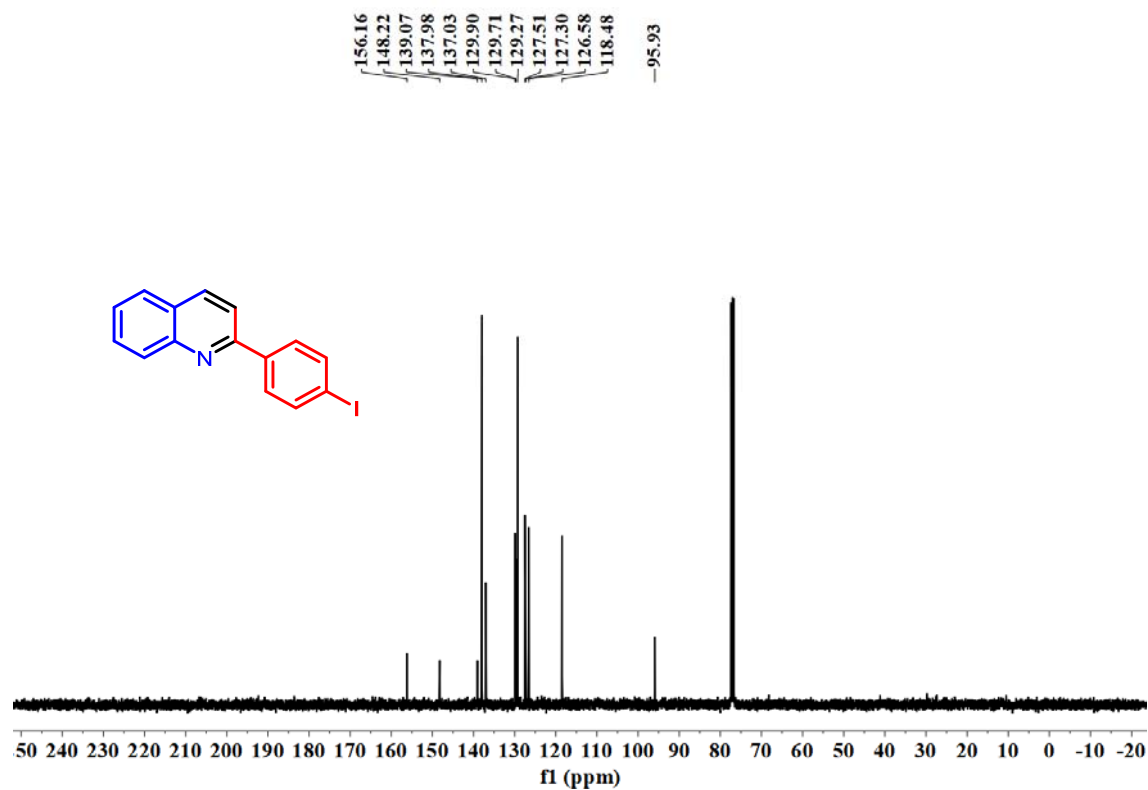


Fig. S50 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** in CDCl_3 (101 MHz).

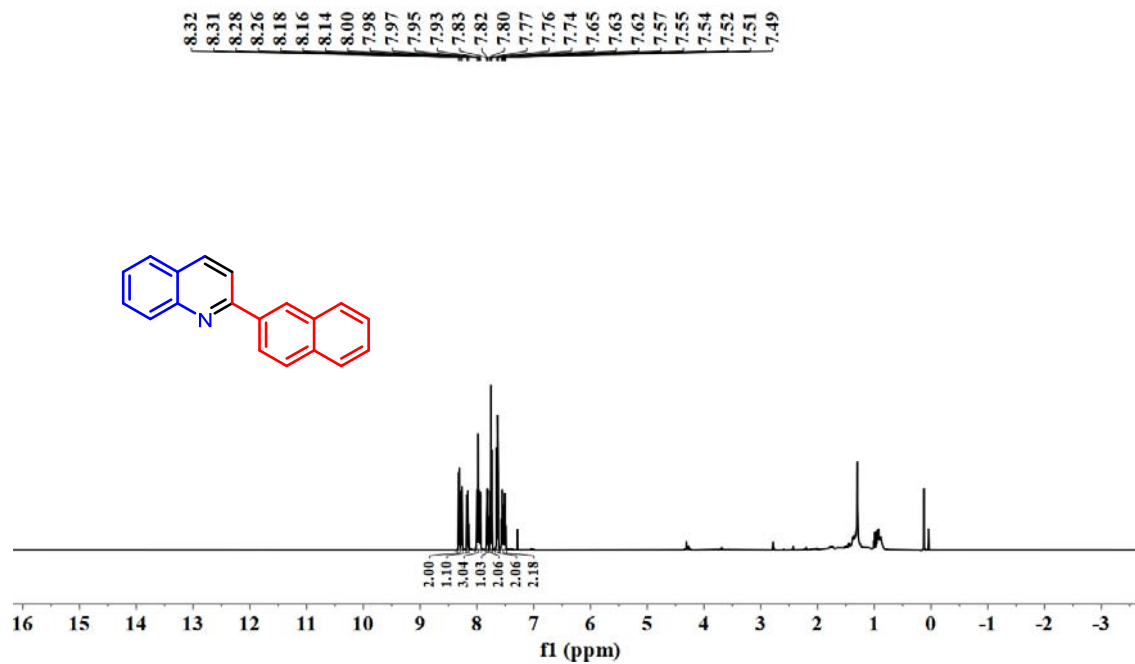


Fig. S51 ^1H NMR spectrum of **10** in CDCl_3 (500 MHz).

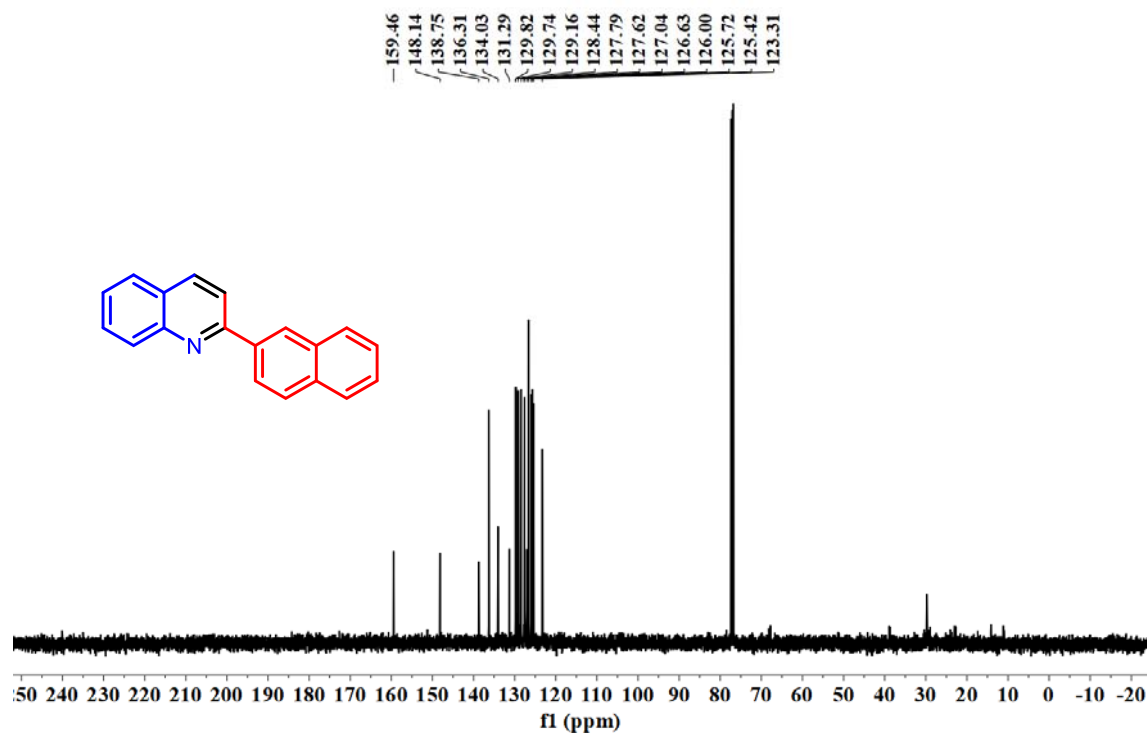


Fig. S52 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10** in CDCl_3 (126MHz).

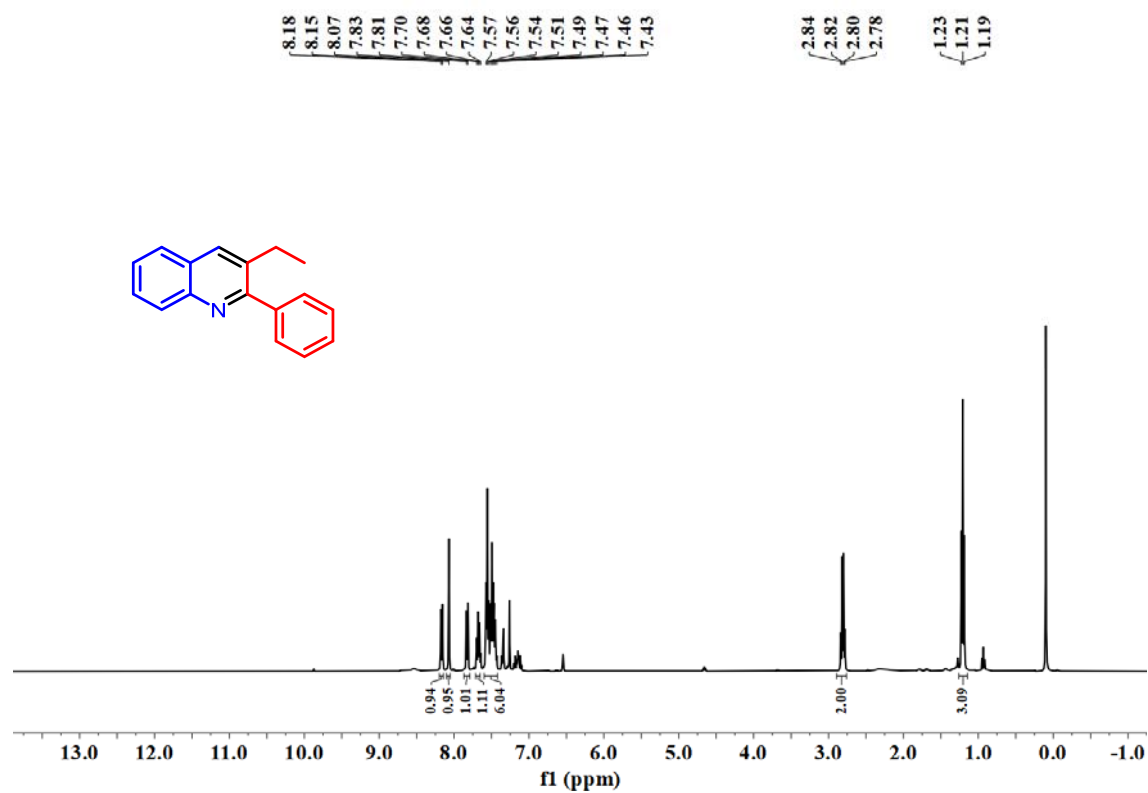


Fig. S53 ¹H NMR spectrum of **11** in CDCl₃ (400 MHz).

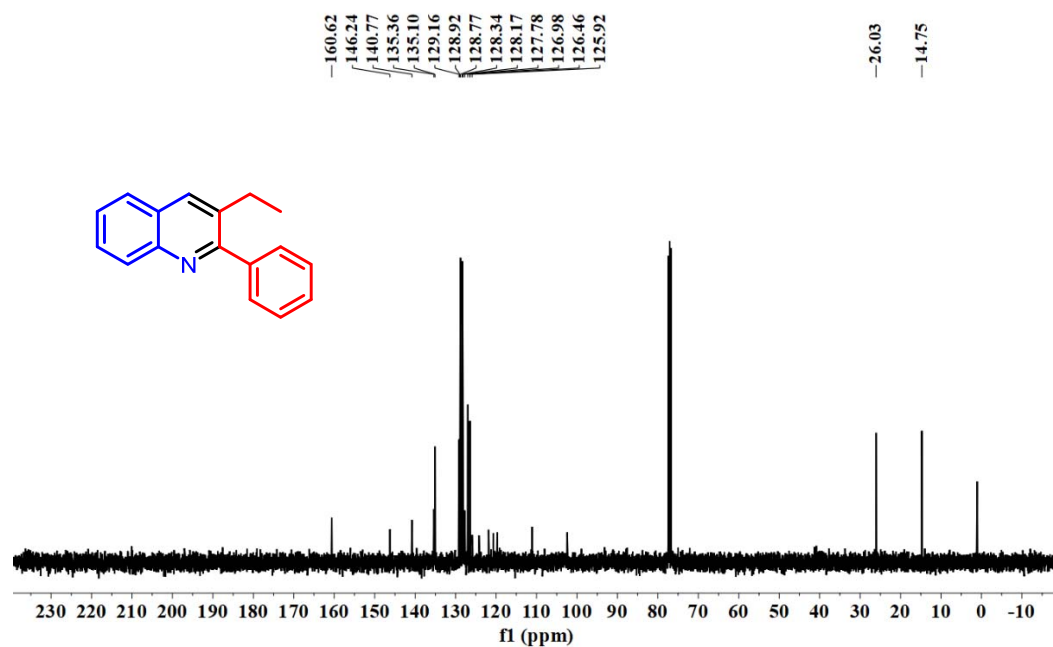


Fig. S54 ¹³C{¹H} NMR spectrum of **11** in CDCl₃ (101 MHz).

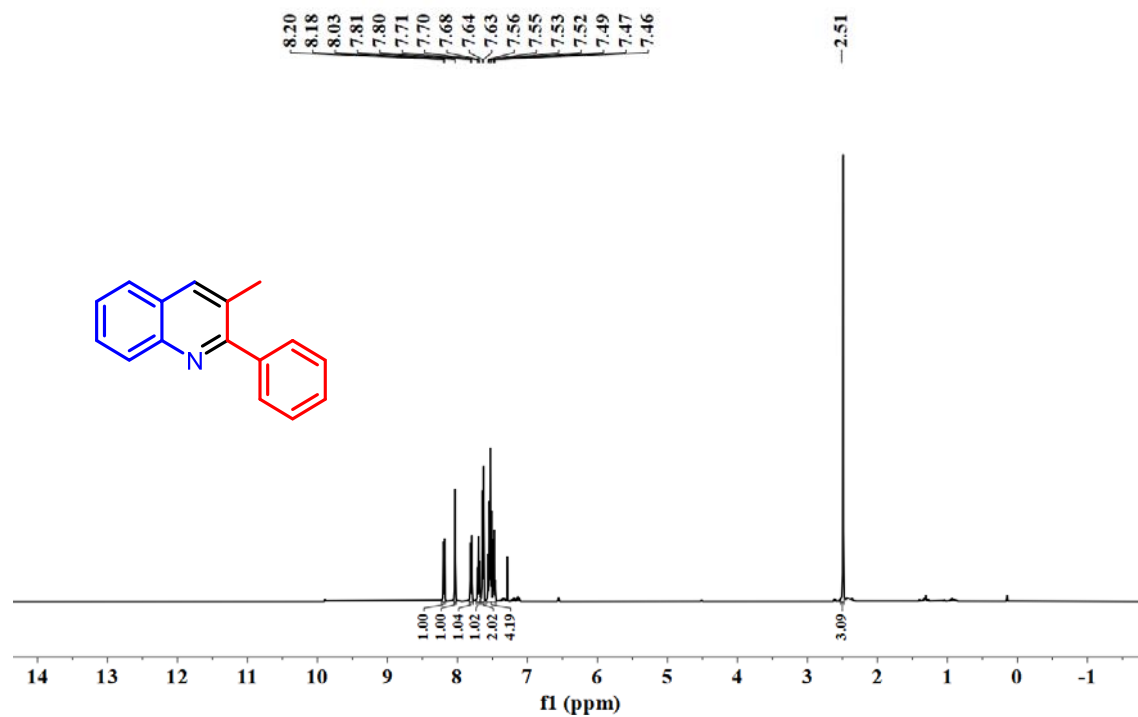


Fig. S55 ¹H NMR spectrum of **12** in CDCl₃ (500 MHz).

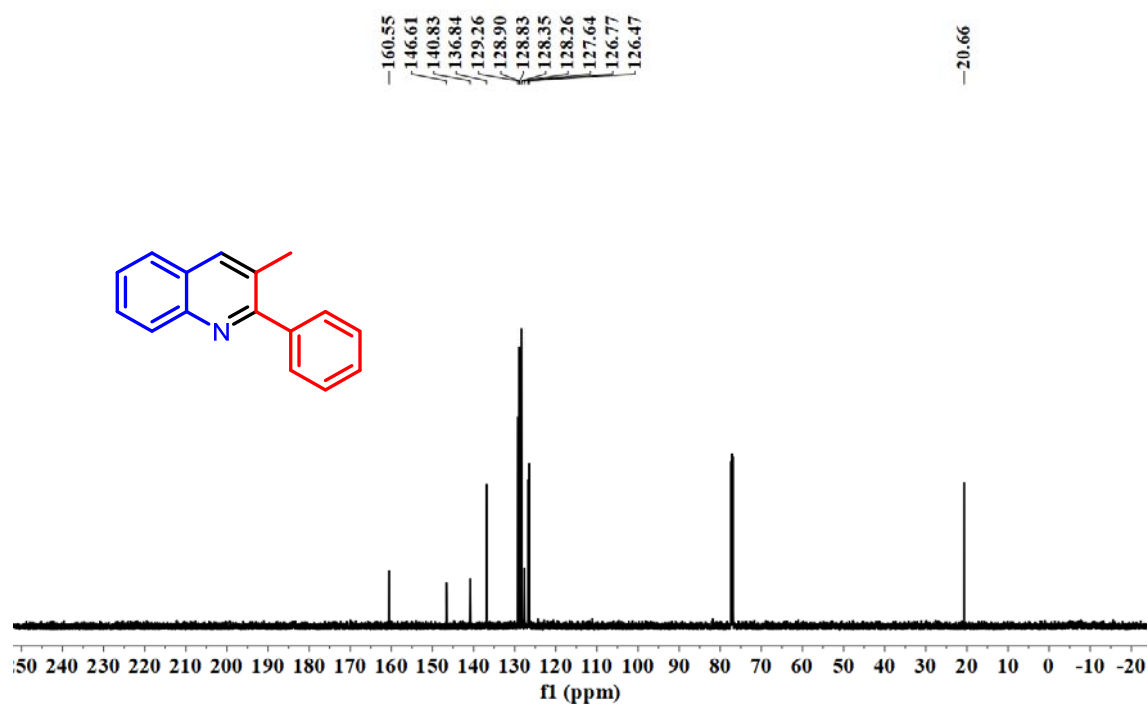


Fig. S56 ¹³C{¹H} NMR spectrum of **12** in CDCl₃ (126 MHz).

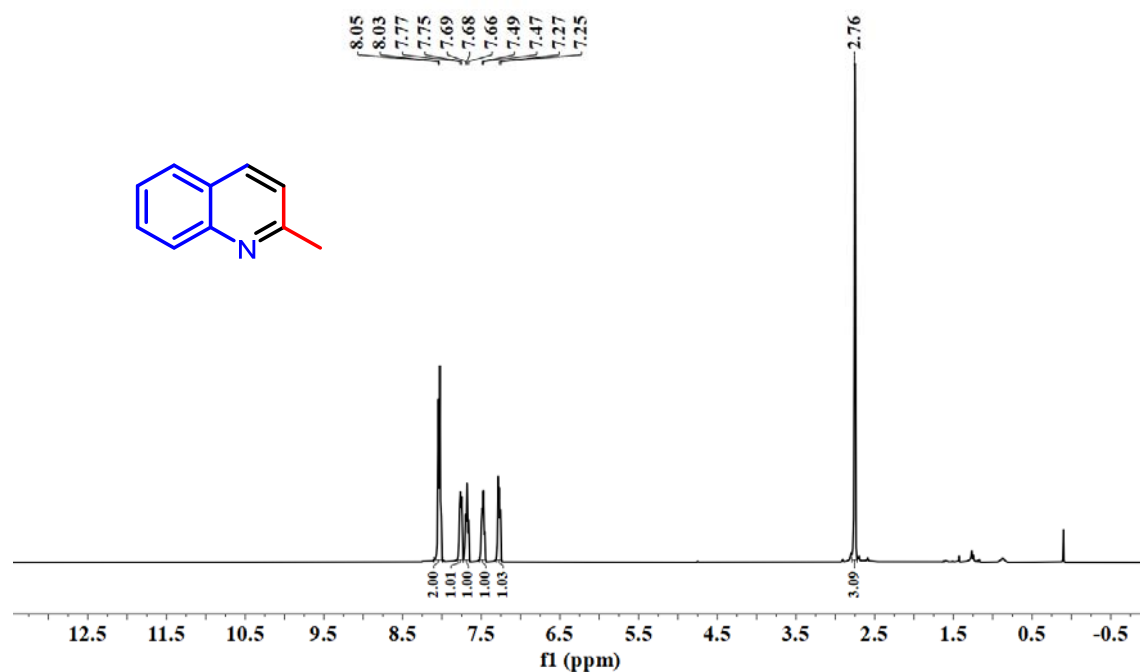


Fig. S57 ^1H NMR spectrum of **13** in CDCl_3 (400 MHz).

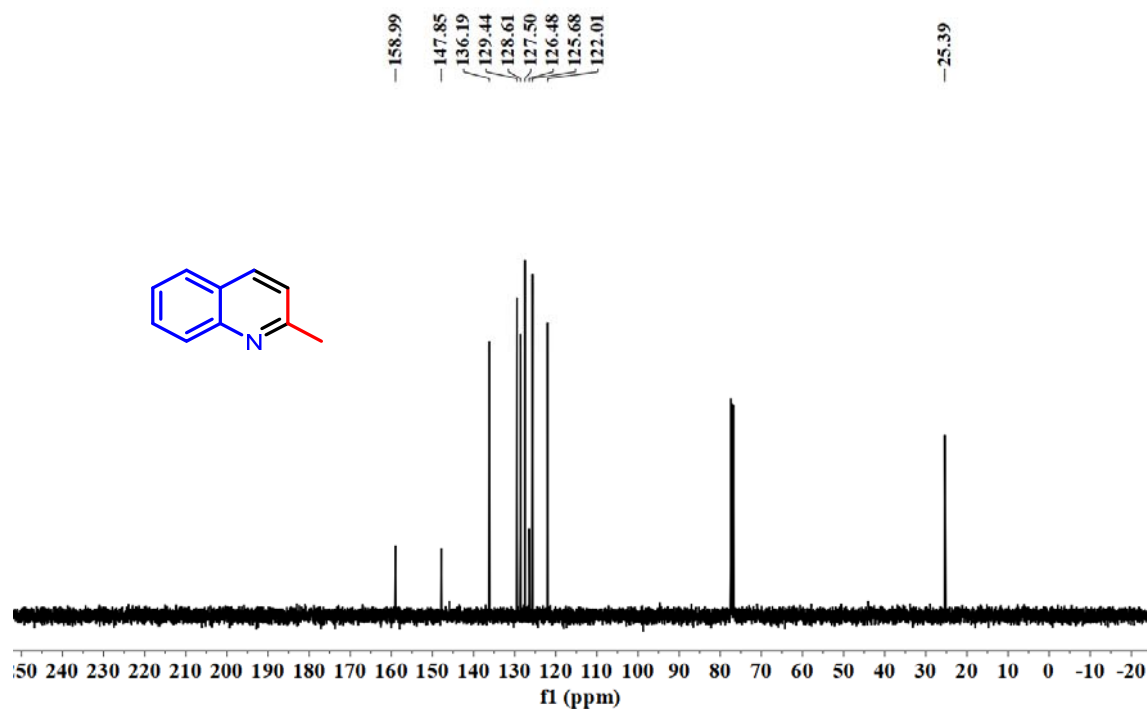


Fig. S58 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **13** in CDCl_3 (101 MHz).

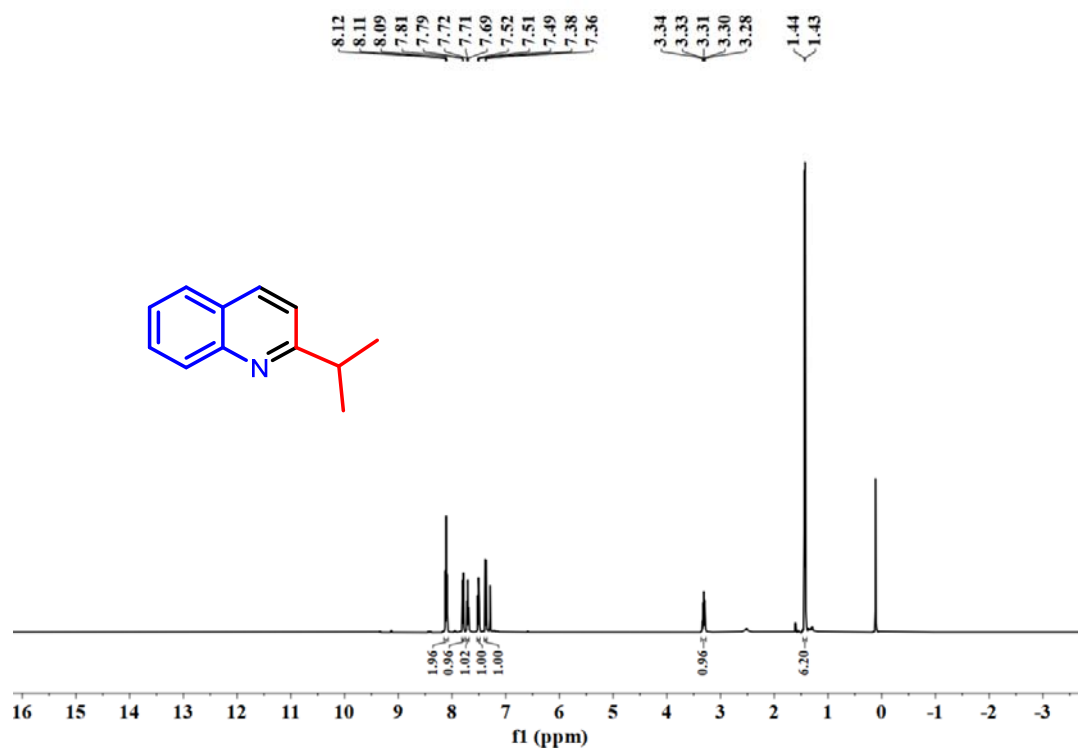


Fig. S59 ¹H NMR spectrum of **14** in CDCl₃ (500 MHz).

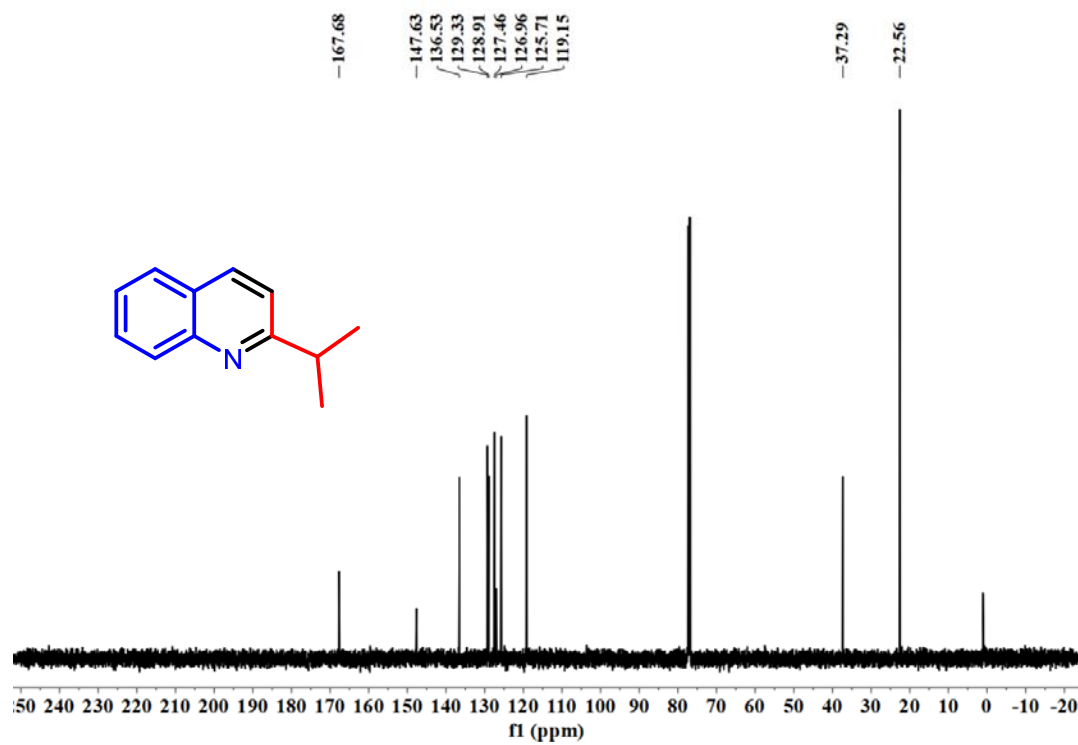


Fig. S60 ¹³C{¹H} NMR spectrum of **14** in CDCl₃ (126 MHz).

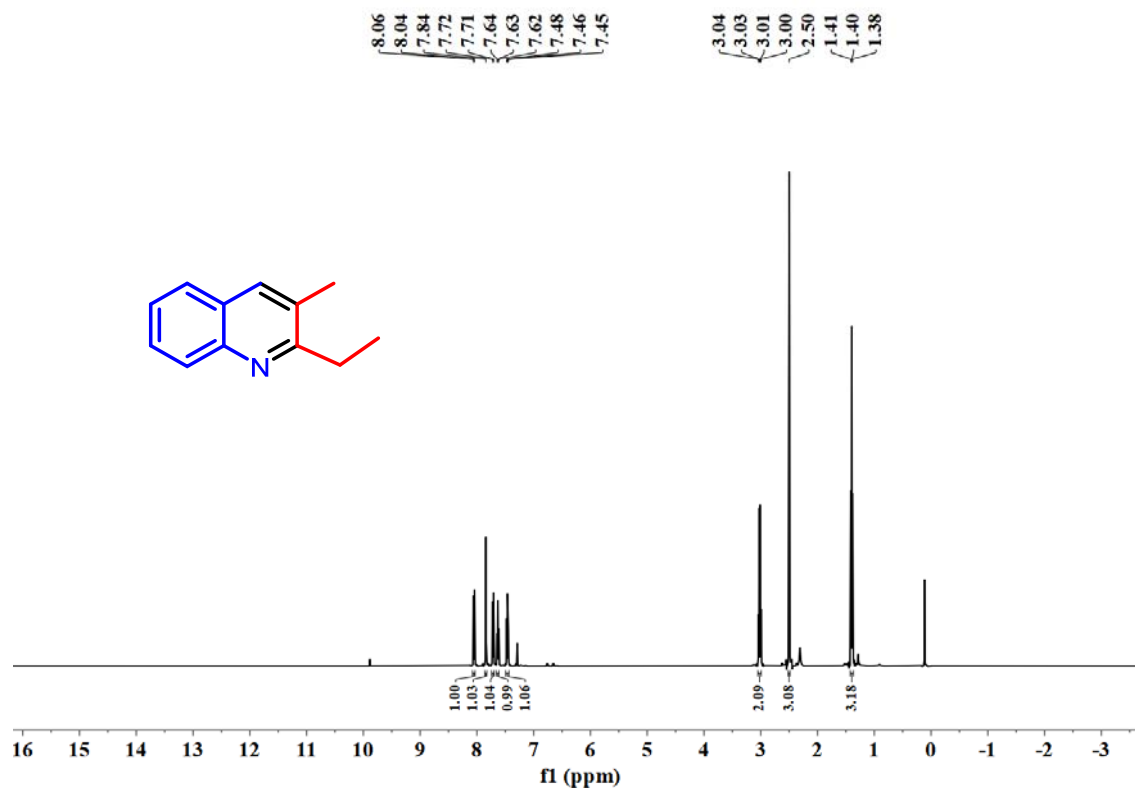


Fig. S61 ^1H NMR spectrum of **15** in CDCl_3 (500 MHz).

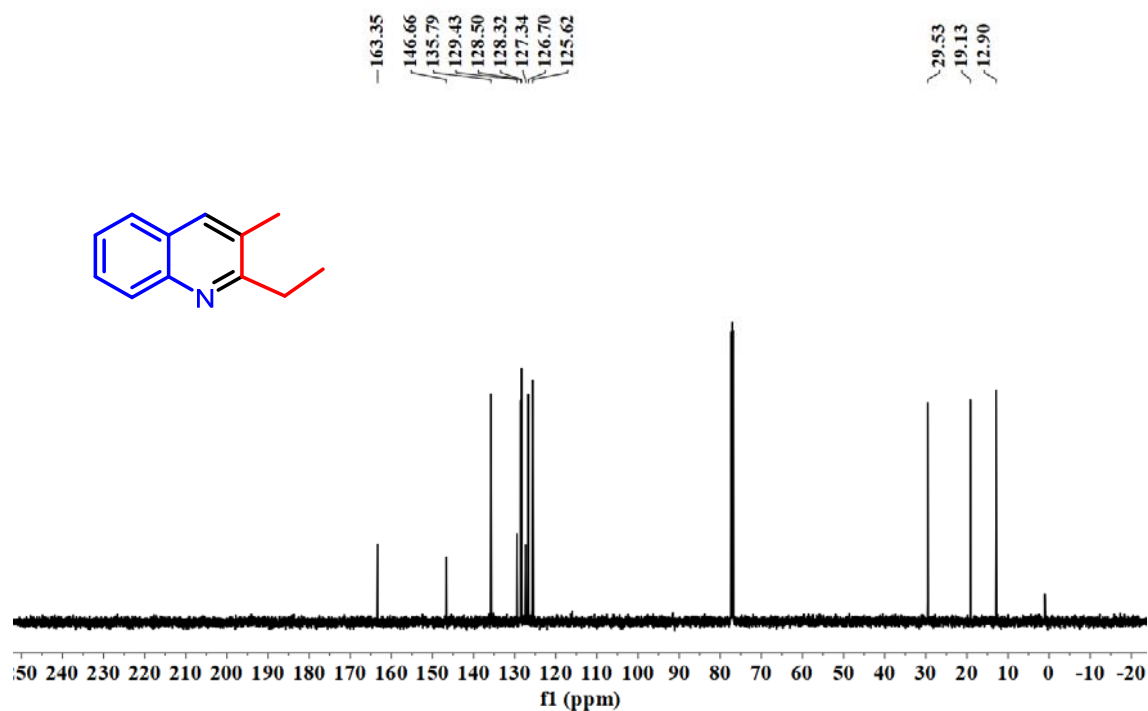


Fig. S62 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **15** in CDCl_3 (126 MHz).

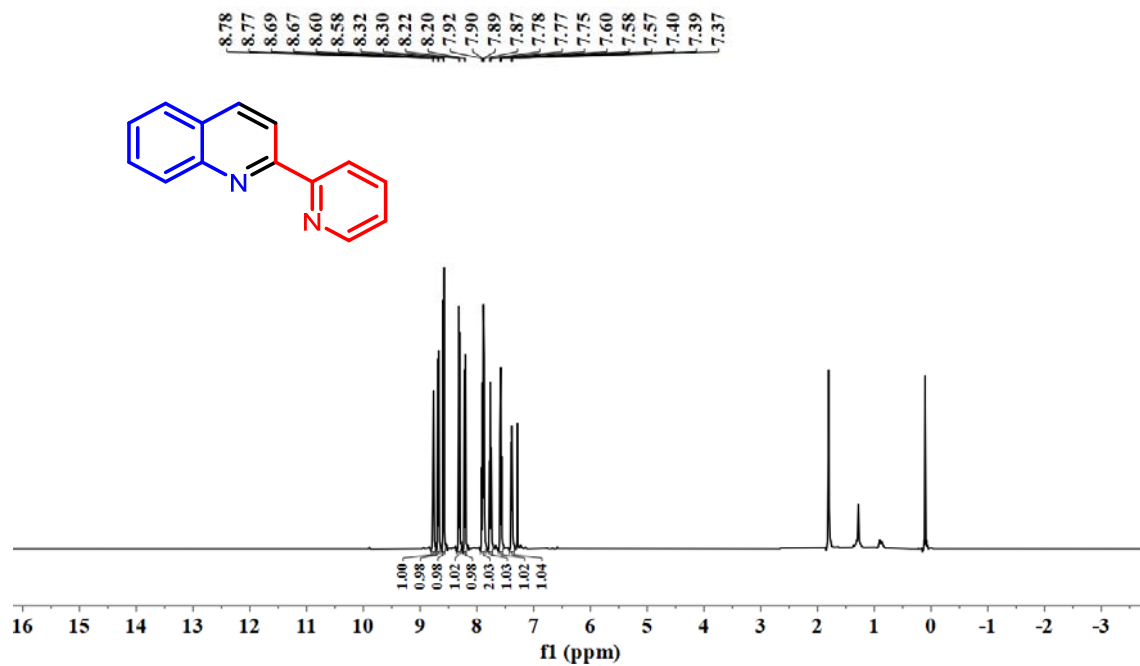


Fig. S63 ^1H NMR spectrum of **16** in CDCl_3 (500 MHz).

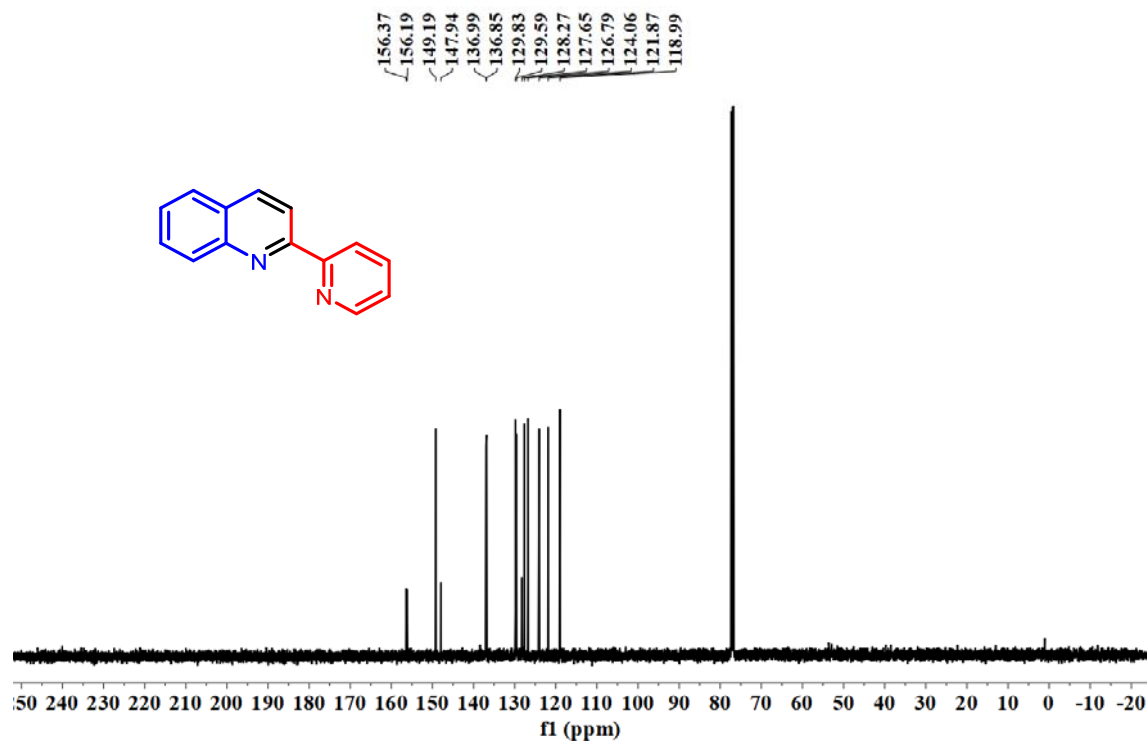


Fig. S64 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **16** in CDCl_3 (126 MHz).

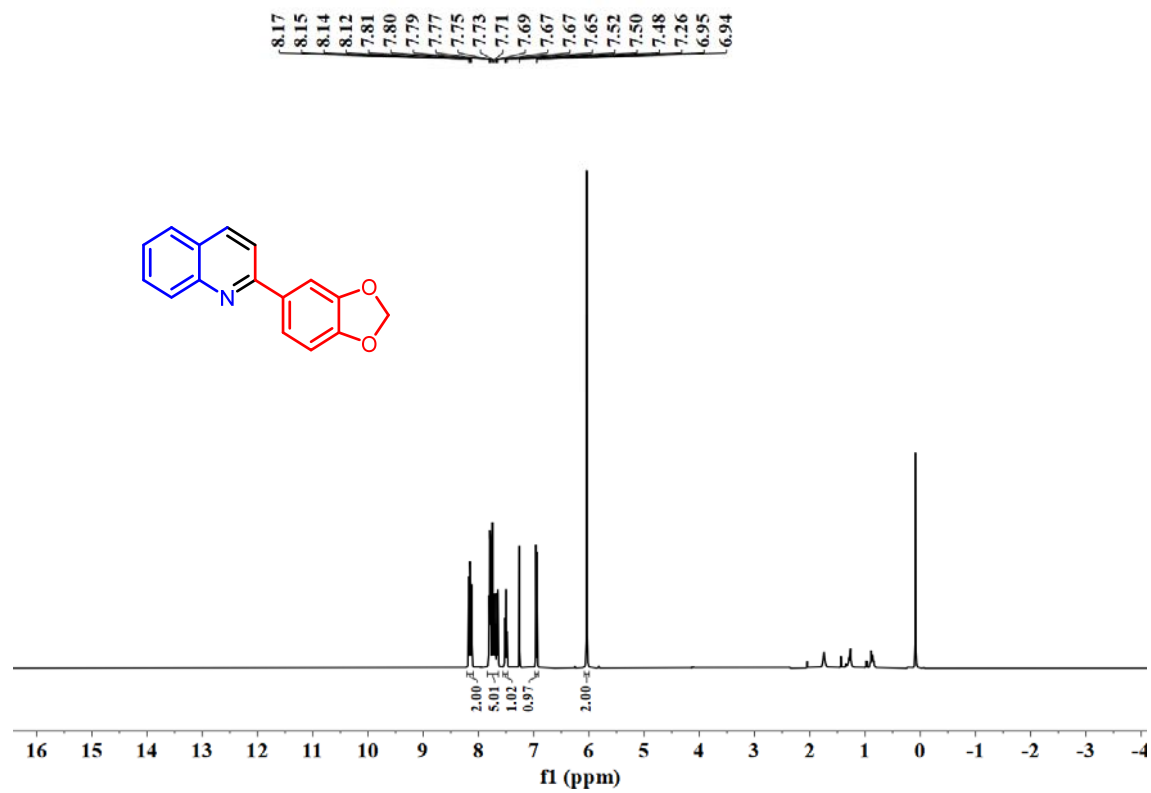


Fig. S65 ¹H NMR spectrum of 17 in CDCl₃ (400 MHz).

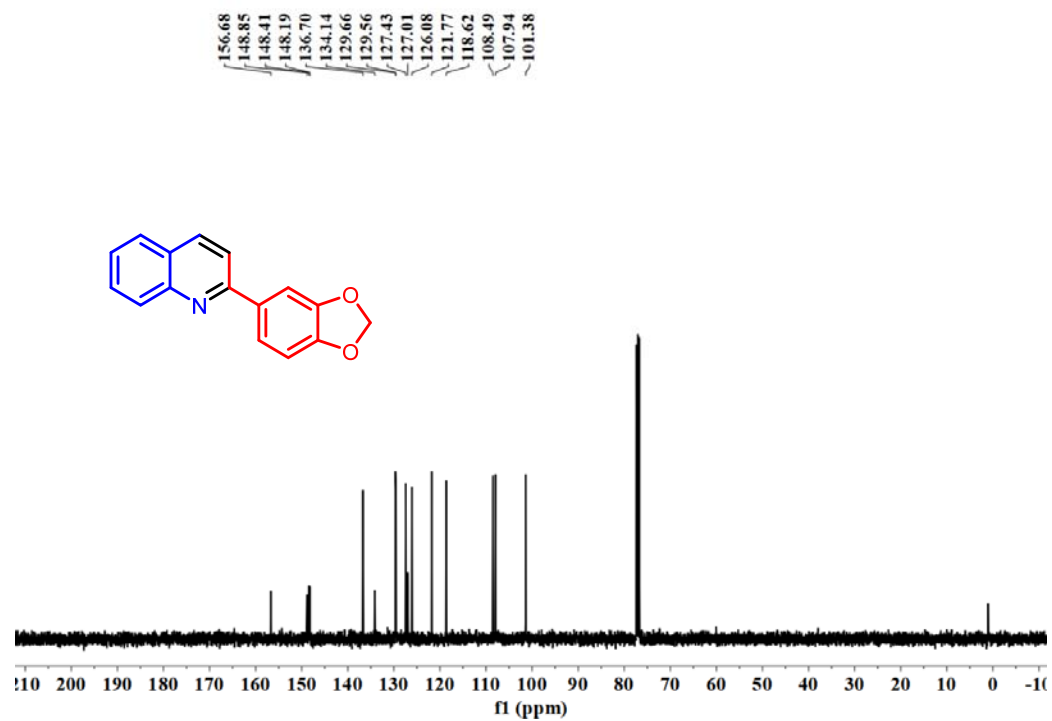


Fig. S66 ¹³C {¹H} NMR spectrum of 17 in CDCl₃ (101 MHz).

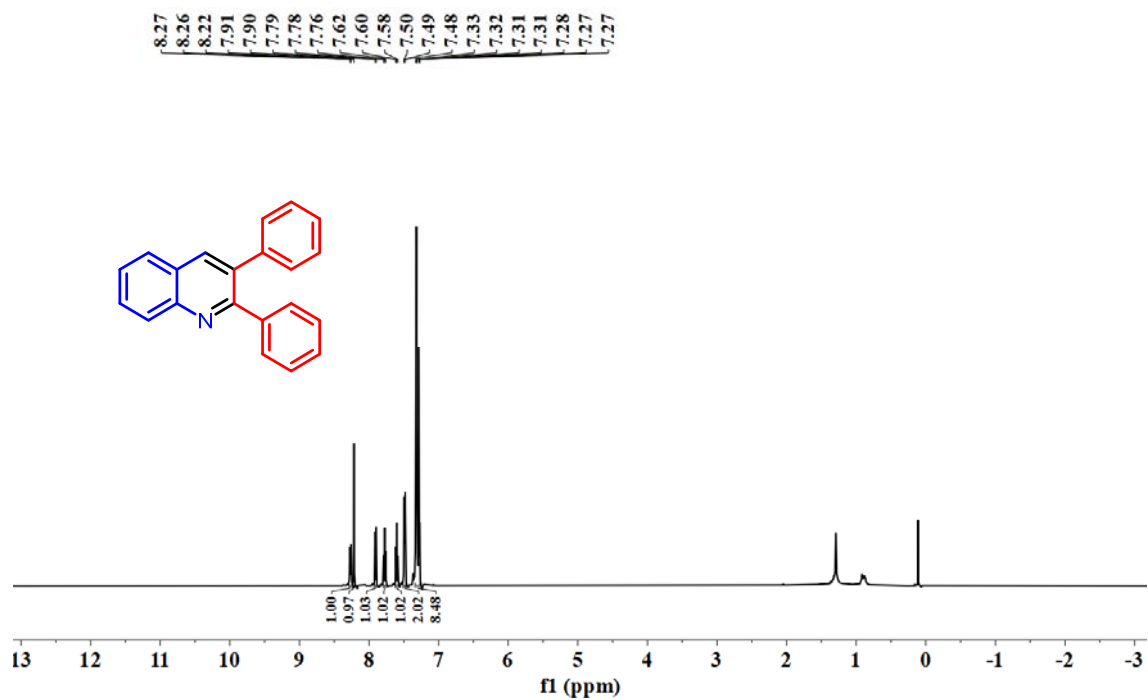


Fig. S67 ¹H NMR spectrum of **18** in CDCl₃ (500 MHz).

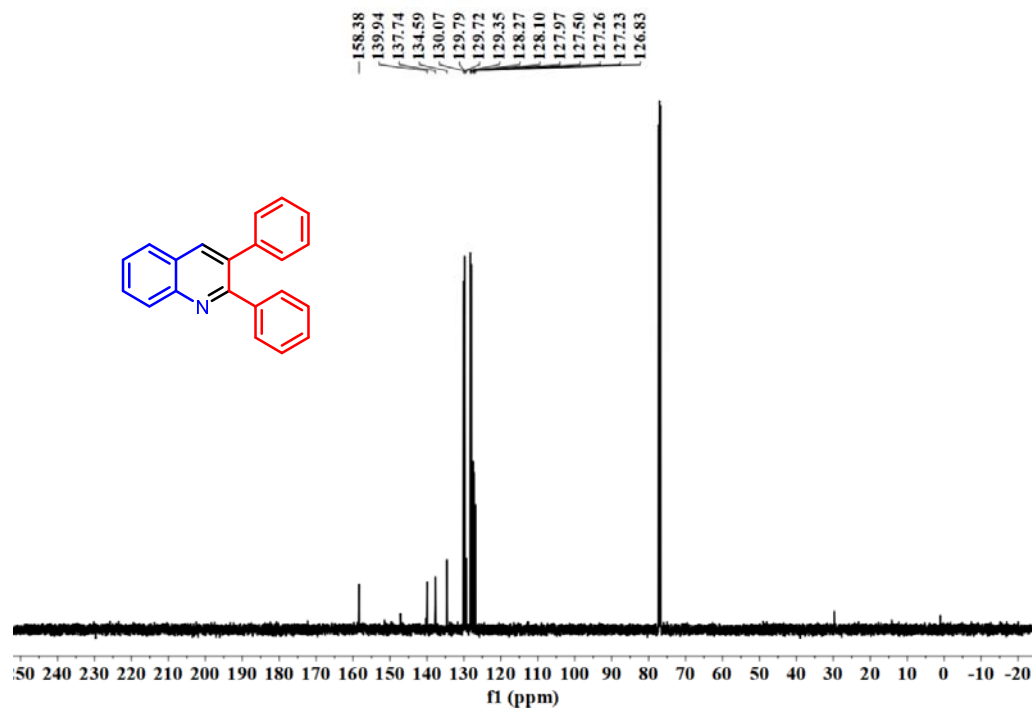


Fig. S68 ¹³C {¹H} NMR spectrum of **18** in CDCl₃ (126 MHz).

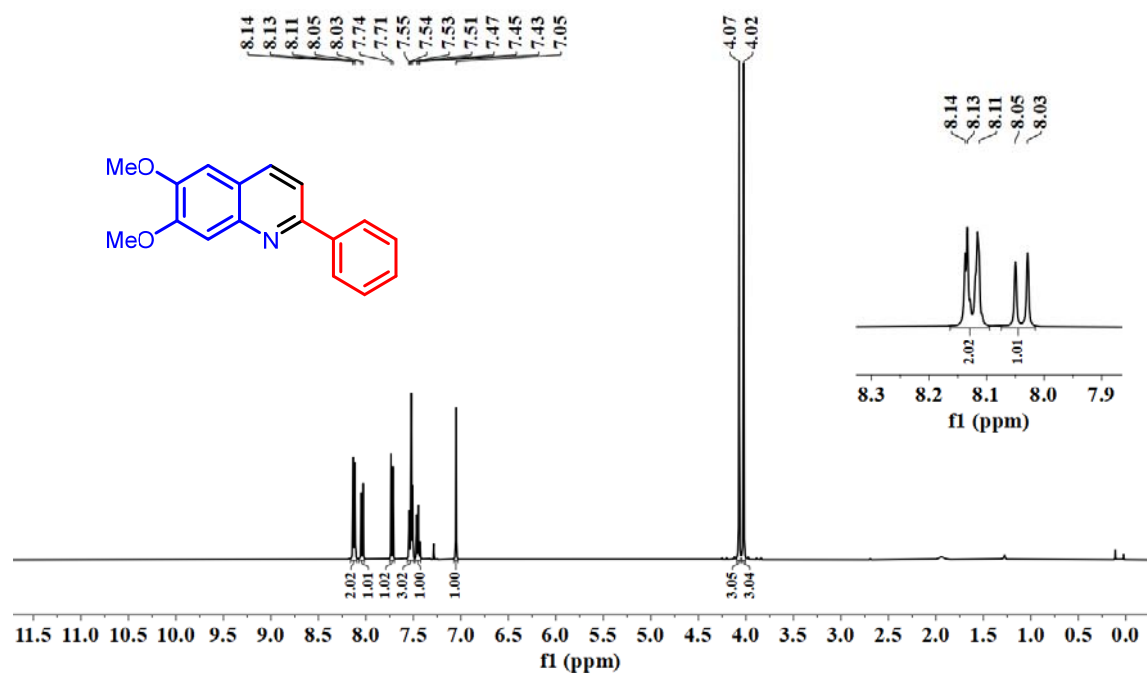


Fig. S69 ¹H NMR spectrum of **19** in CDCl₃ (400 MHz).

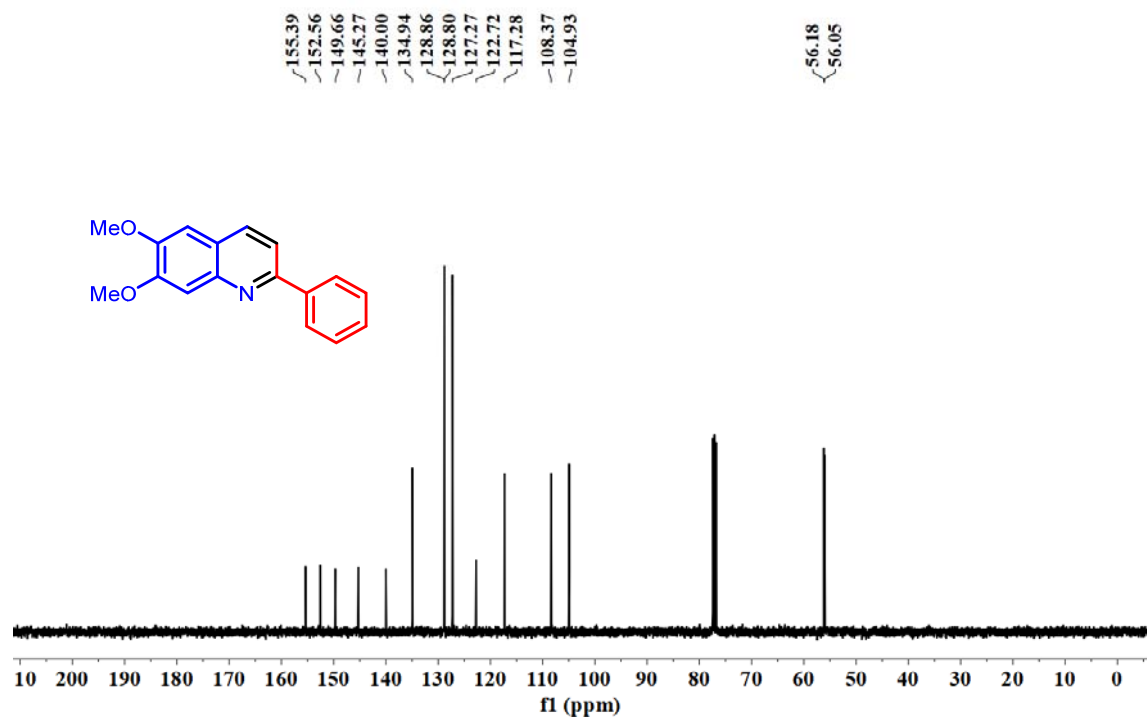


Fig. S70 ¹³C{¹H} NMR spectrum of **19** in CDCl₃ (101 MHz).

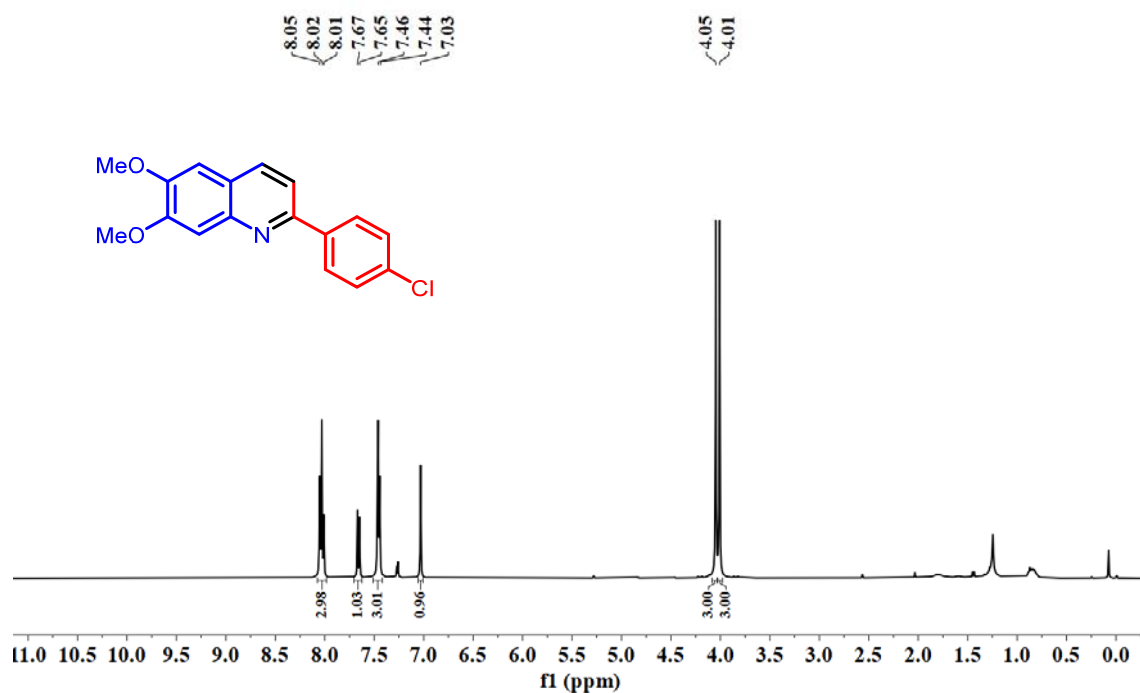


Fig. S71 ¹H NMR spectrum of **20** in CDCl₃ (400 MHz).

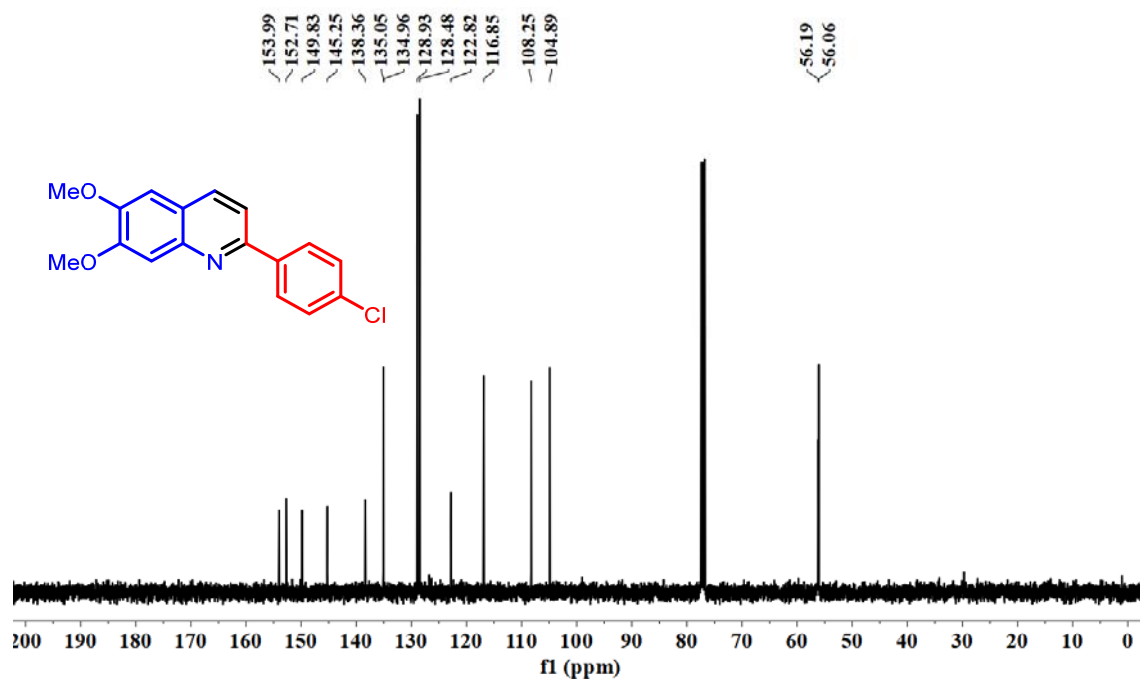


Fig. S72 ¹³C {¹H} NMR spectrum of **20** in CDCl₃ (101 MHz).

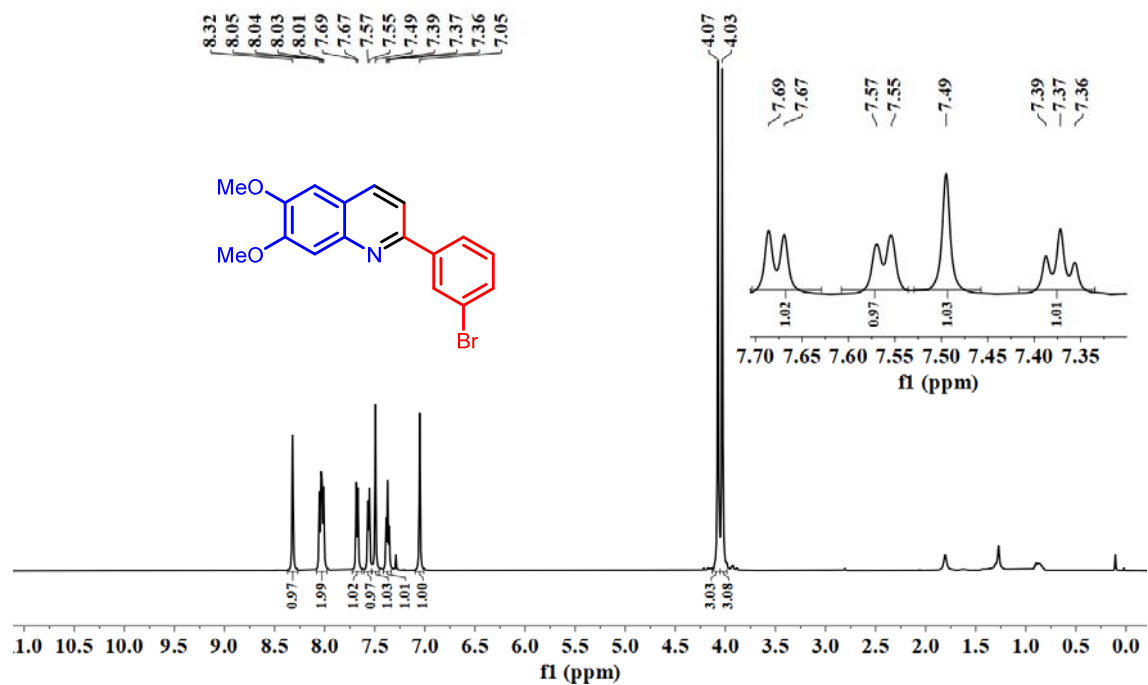


Fig. S73 ¹H NMR spectrum of **21** in CDCl₃ (500 MHz).

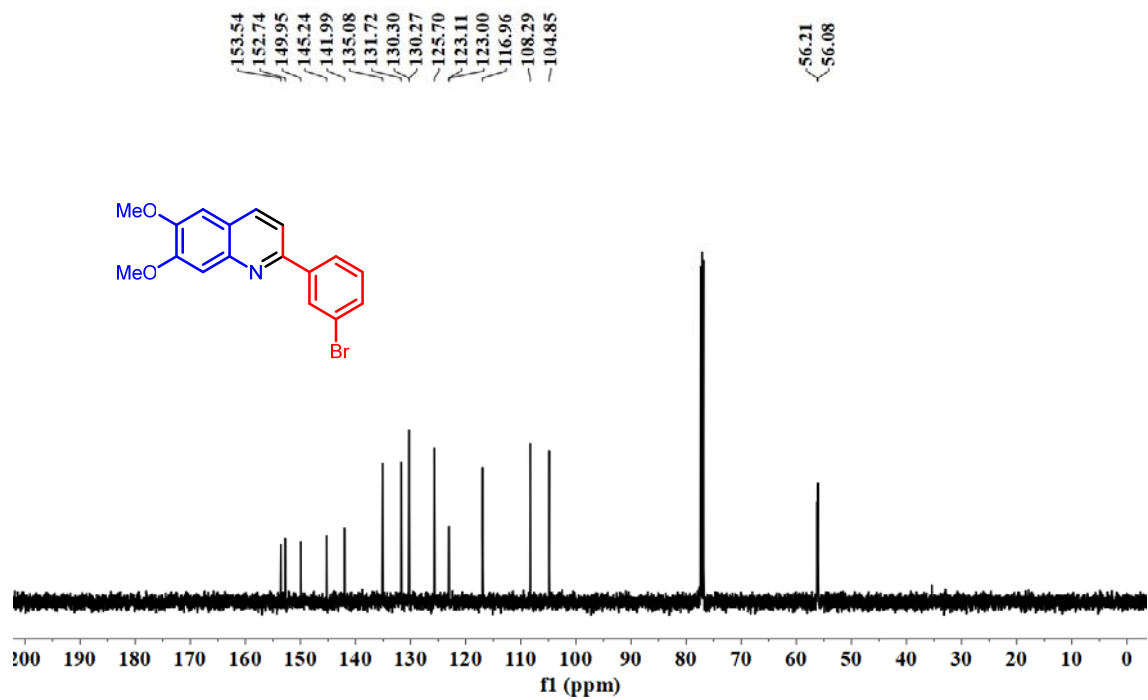


Fig. S74 ¹³C{¹H} NMR spectrum of **21** in CDCl₃ (126 MHz).

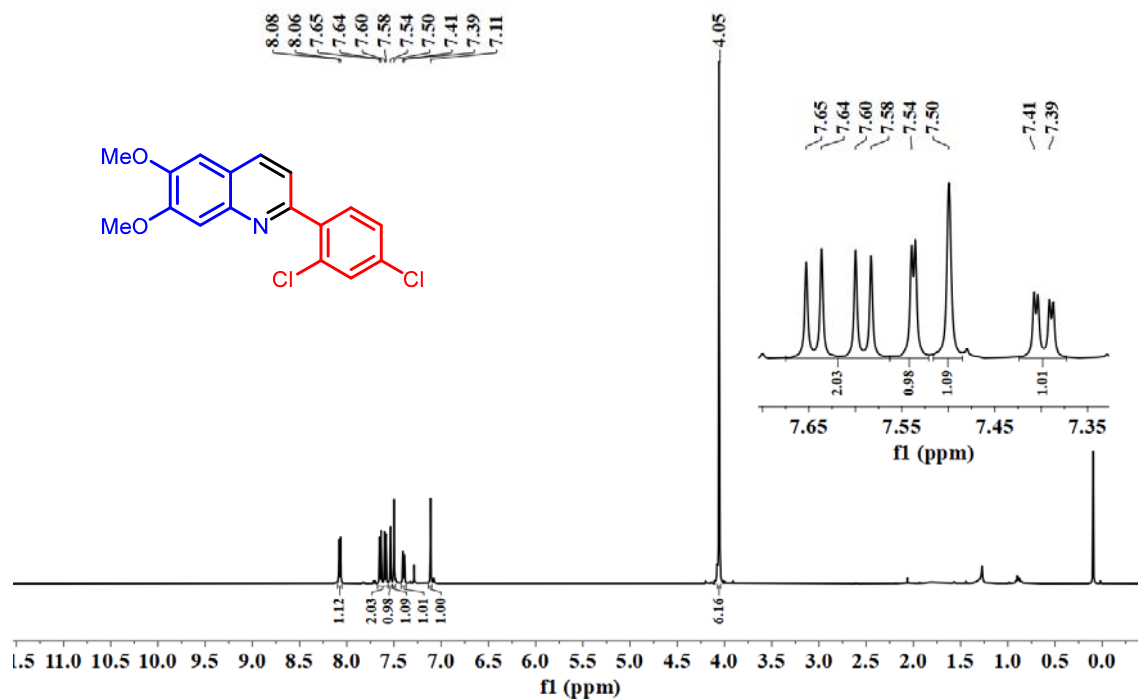


Fig. S75 ¹H NMR spectrum of **22** in CDCl₃ (500 MHz).

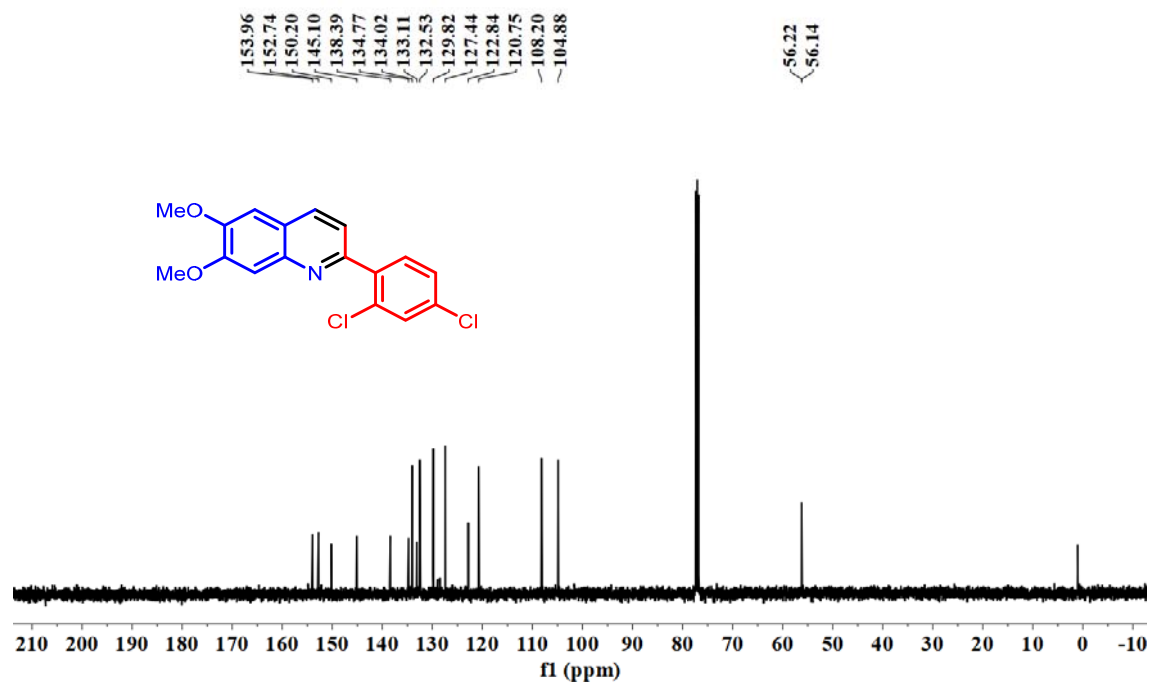


Fig. S76 ¹³C{¹H} NMR spectrum of **22** in CDCl₃ (126 MHz).

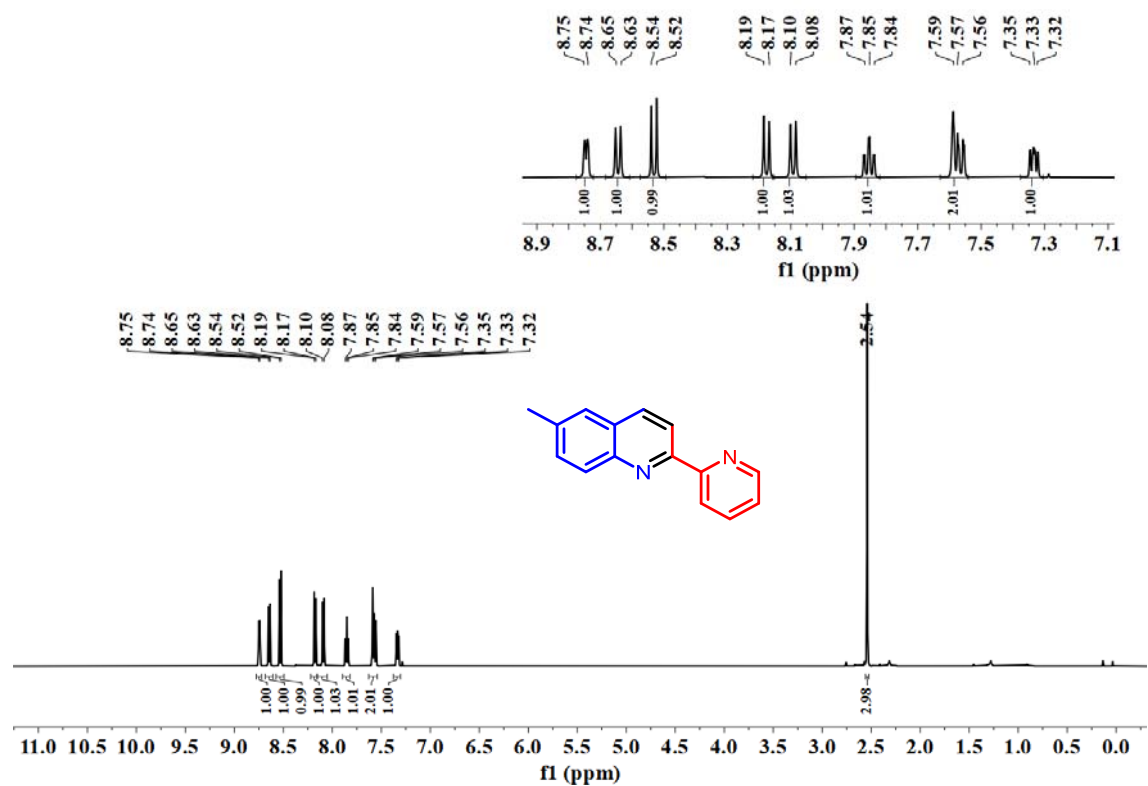


Fig. S77 ¹H NMR spectrum of **23** in CDCl₃ (500 MHz).

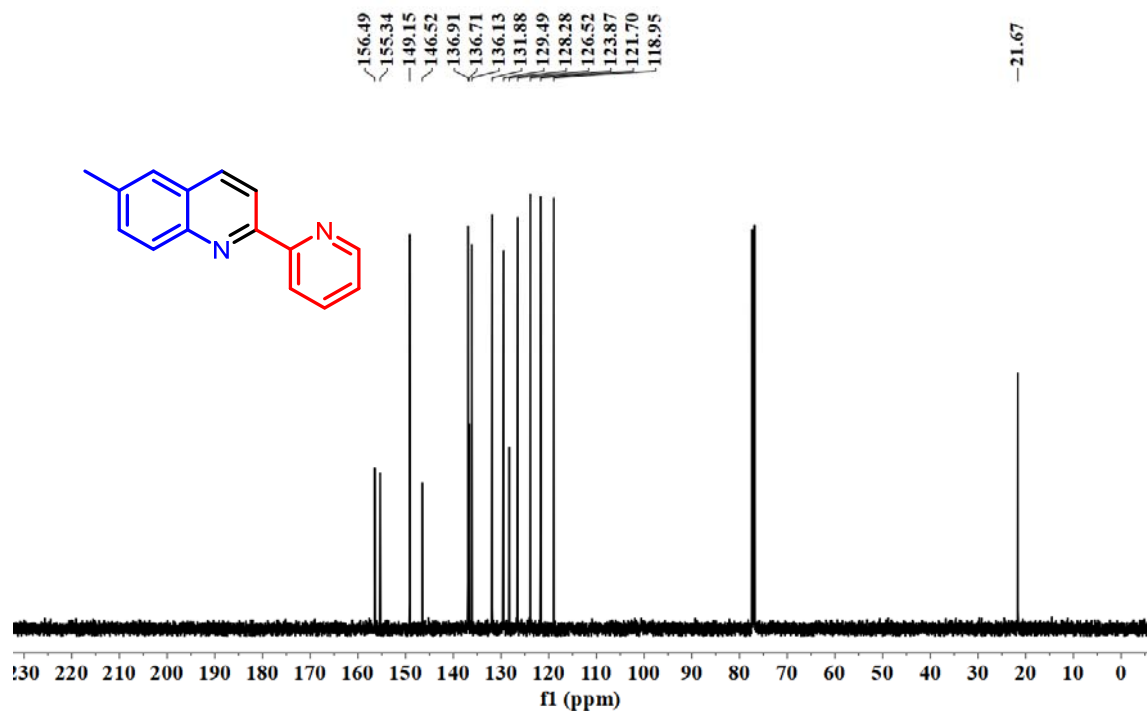


Fig. S78 ¹³C{¹H} NMR spectrum of **23** in CDCl₃ (126 MHz).

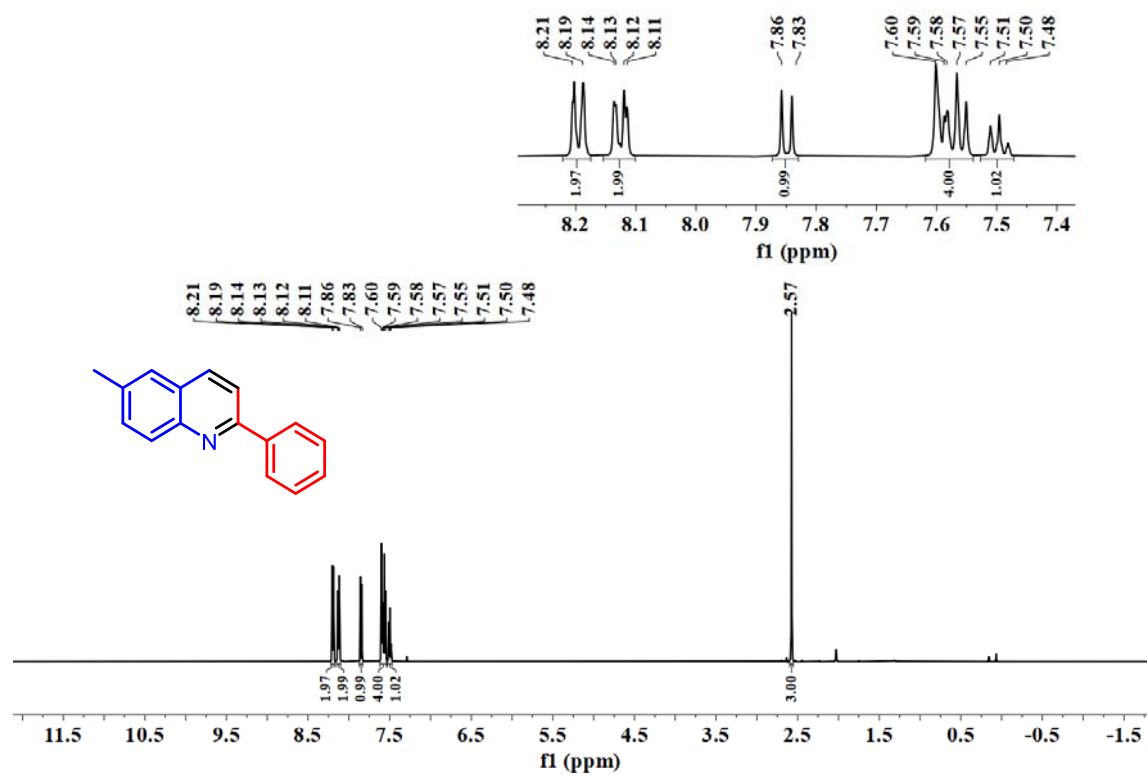


Fig. S79 ¹H NMR spectrum of **24** in CDCl₃ (500 MHz).

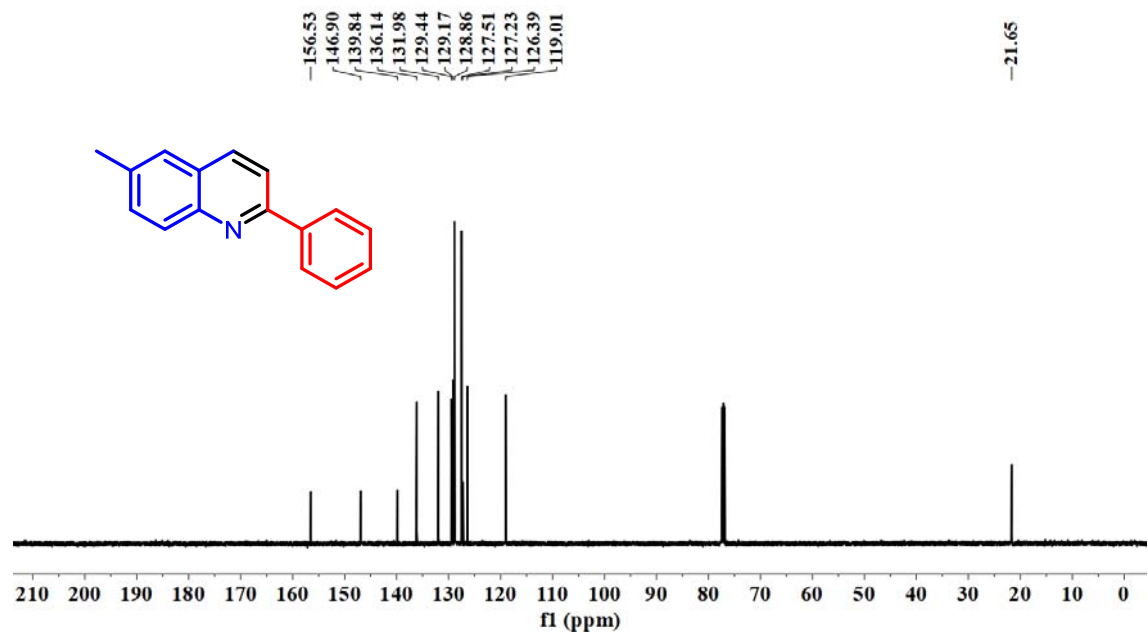


Fig. S80 ¹³C {¹H} NMR spectrum of **24** in CDCl₃ (126 MHz).

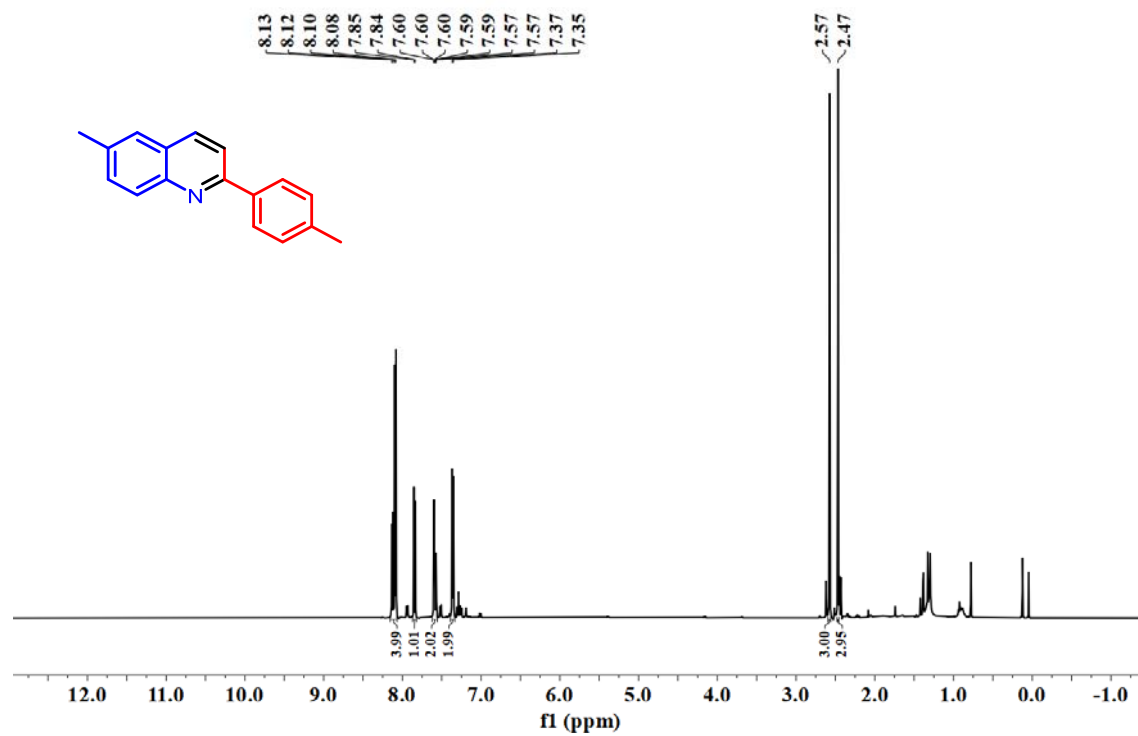


Fig. S81 ¹H NMR spectrum of **25** in CDCl₃ (400 MHz).

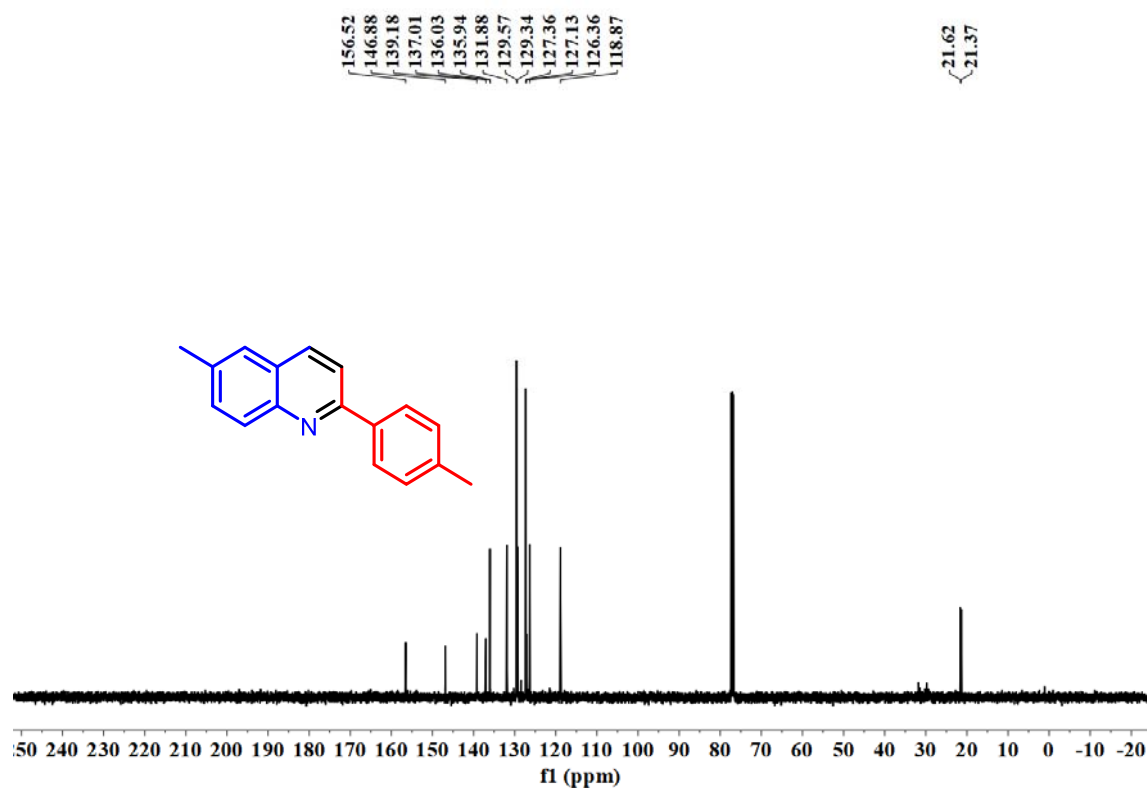


Fig. S82 ¹³C {¹H} NMR spectrum of **25** in CDCl₃ (101 MHz).

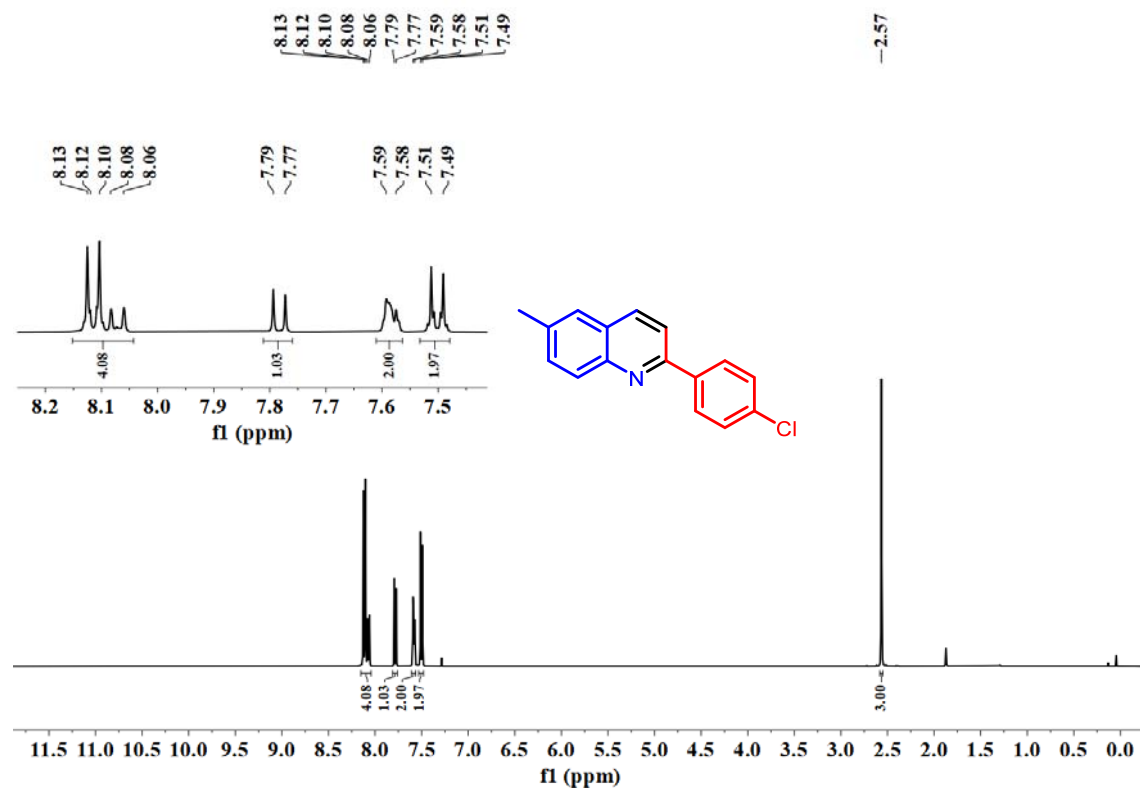


Fig. S83 ¹H NMR spectrum of **26** in CDCl₃ (400 MHz).

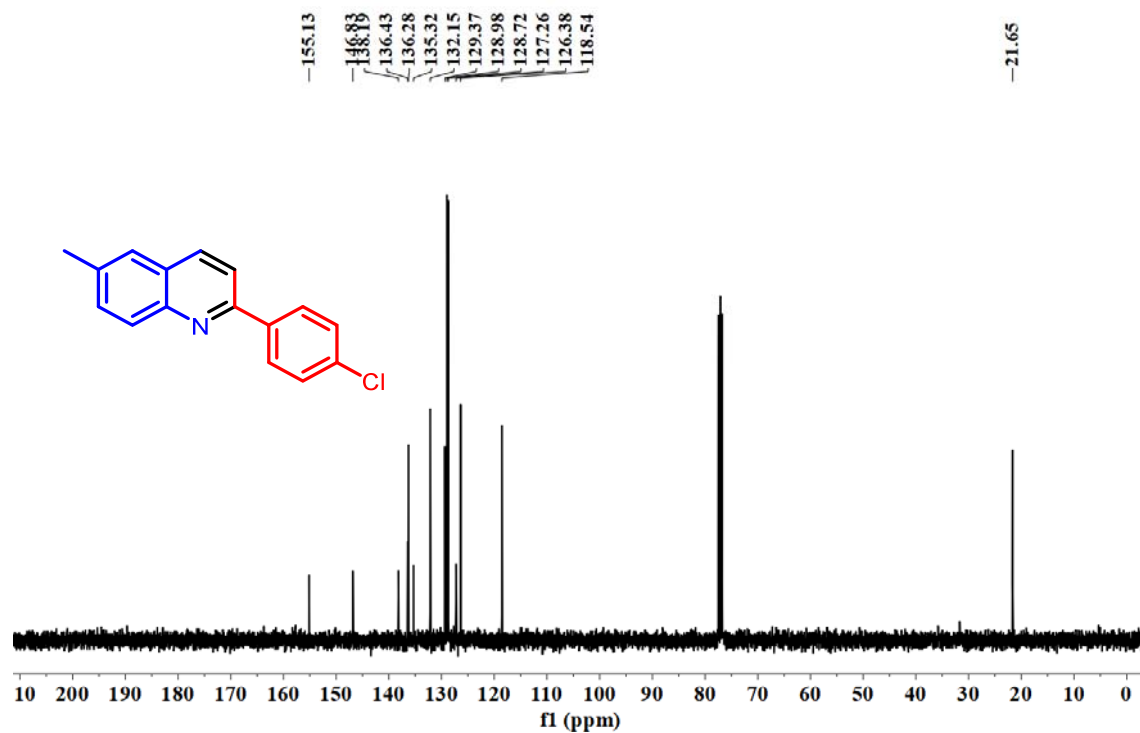


Fig. S84 ¹³C {¹H} NMR spectrum of **26** in CDCl₃ (101 MHz).

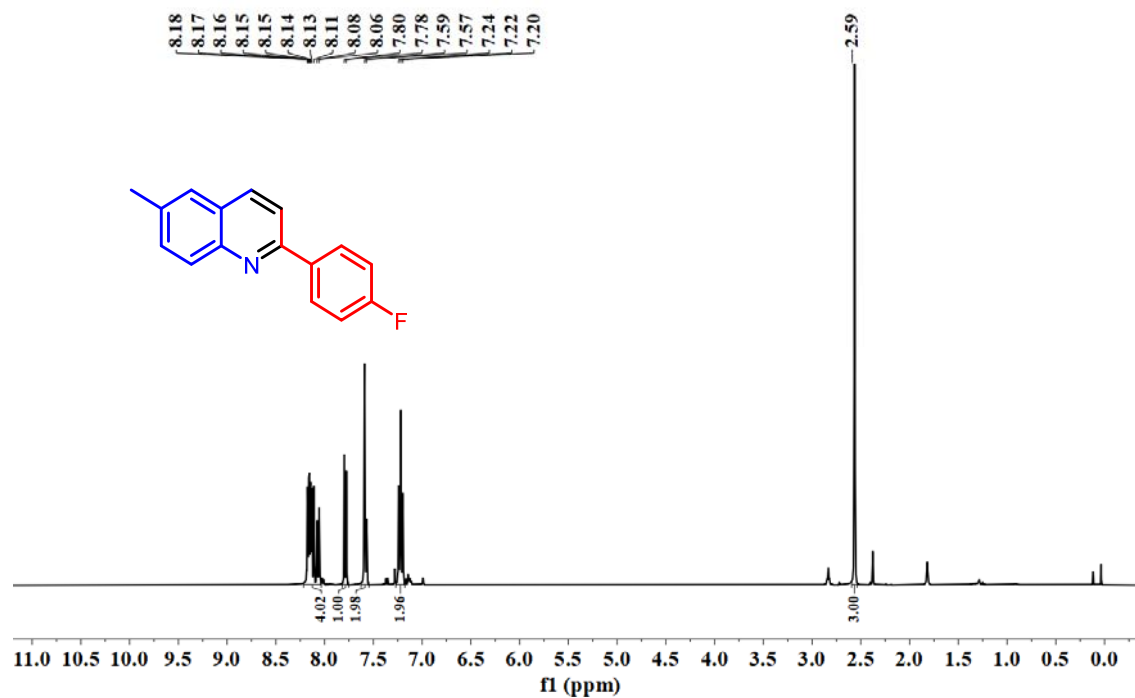


Fig. S85 ¹H NMR spectrum of **27** in CDCl₃ (400 MHz).

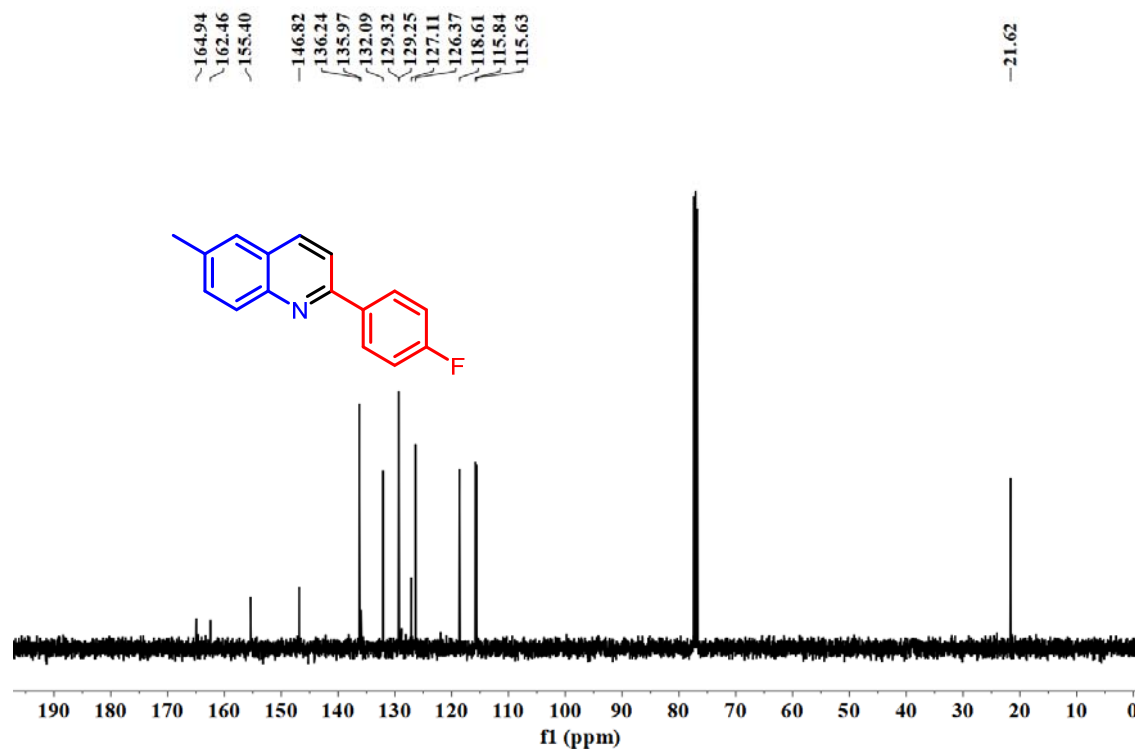


Fig. S86 ¹³C{¹H} NMR spectrum of **27** in CDCl₃ (101 MHz).

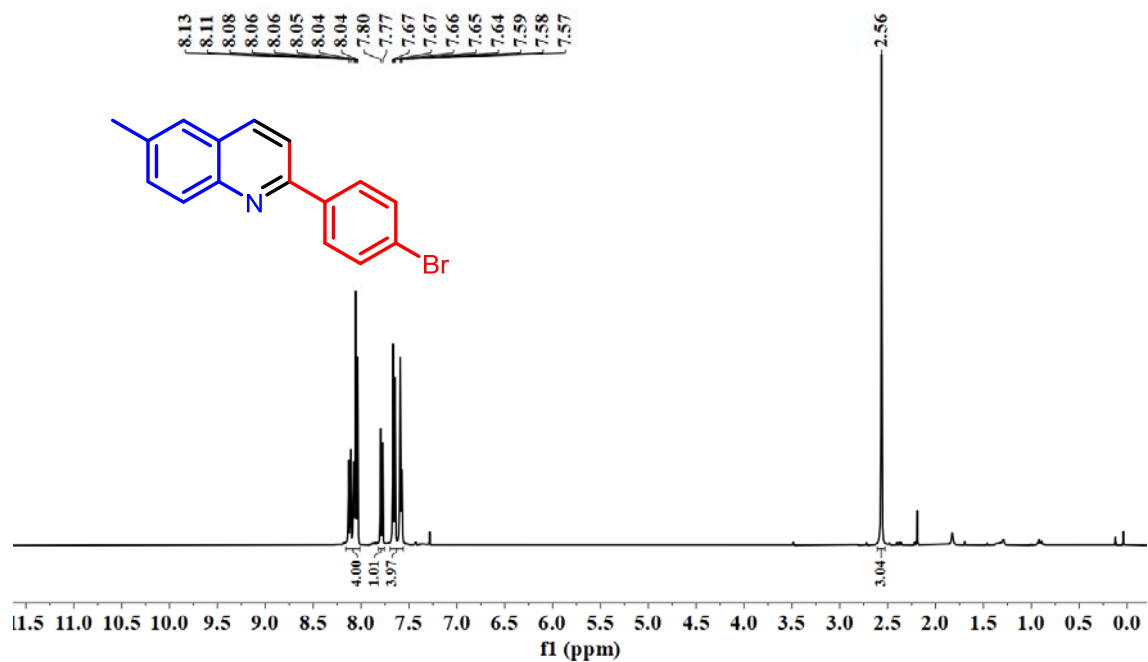


Fig. S87 ¹H NMR spectrum of **28** in CDCl₃ (500 MHz).

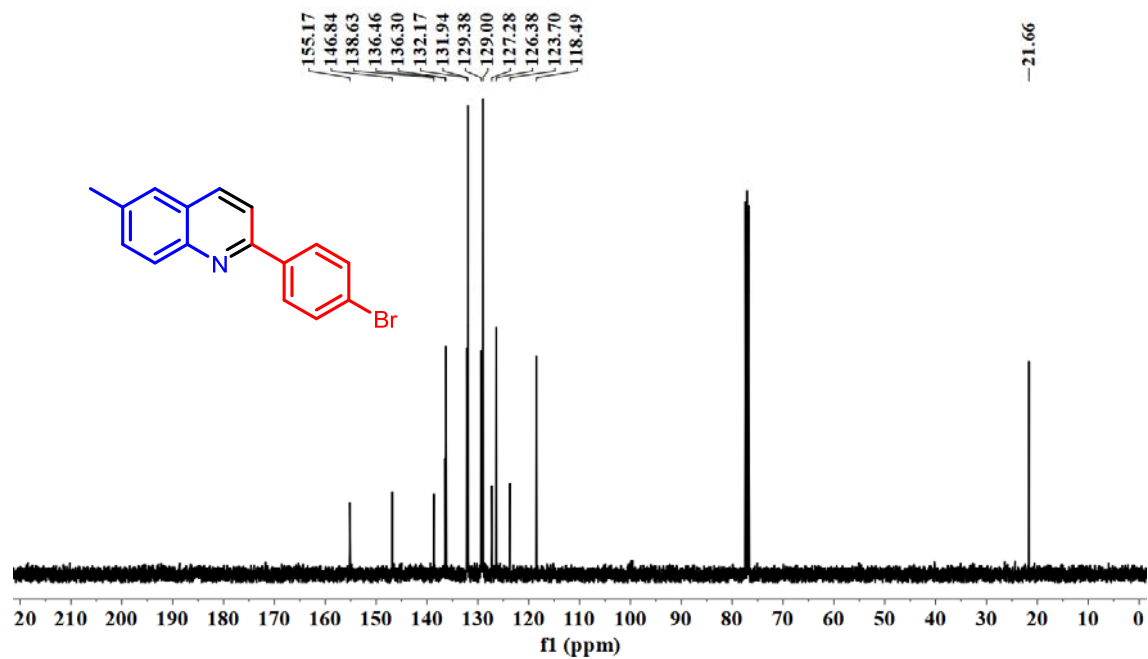


Fig. S88 ¹³C {¹H} NMR spectrum of **28** in CDCl₃ (126 MHz).

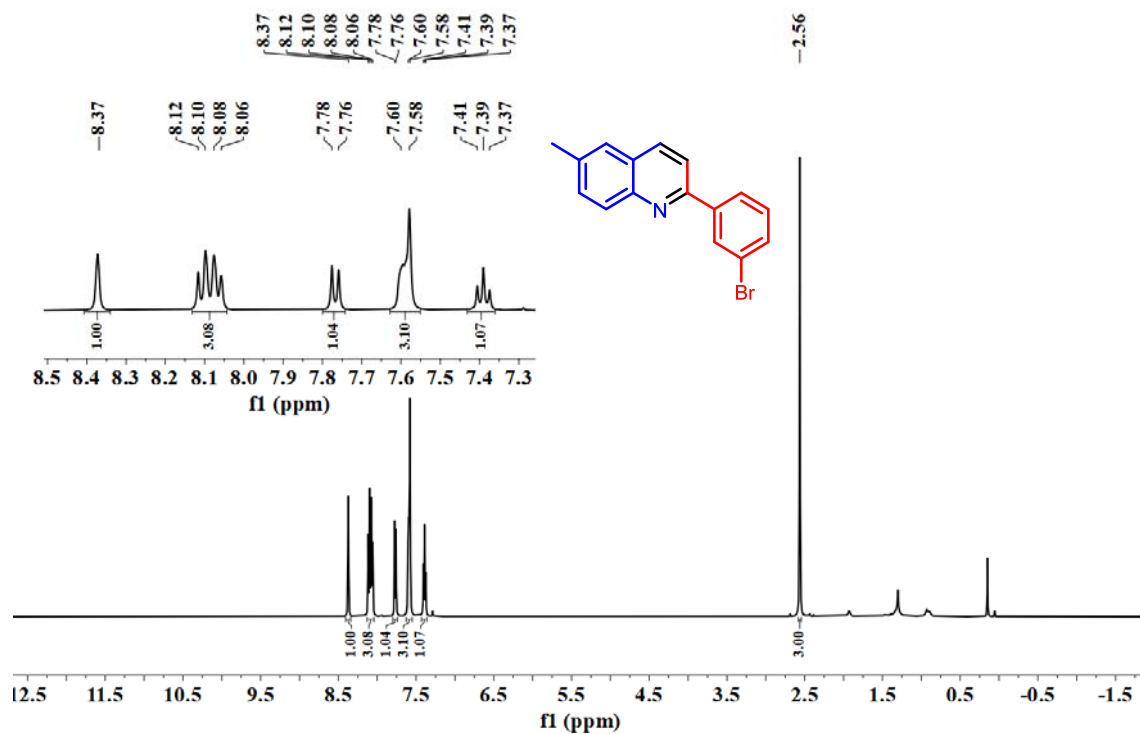


Fig. S89 ¹H NMR spectrum of **29** in CDCl₃ (400 MHz).

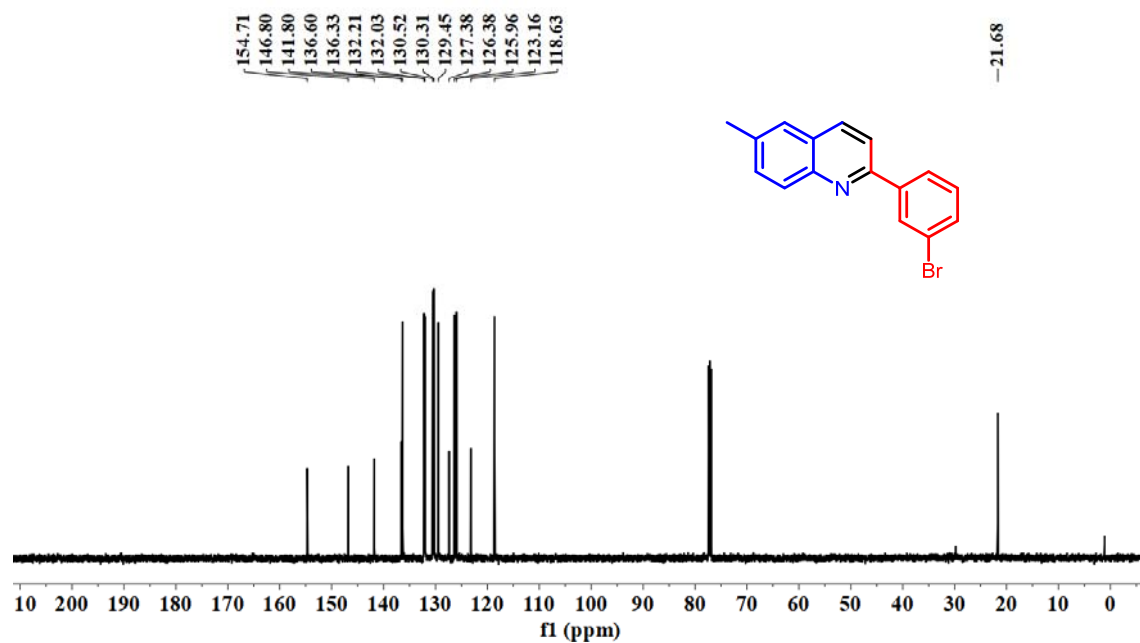


Fig. S90 ¹³C{¹H} NMR spectrum of **29** in CDCl₃ (101 MHz).

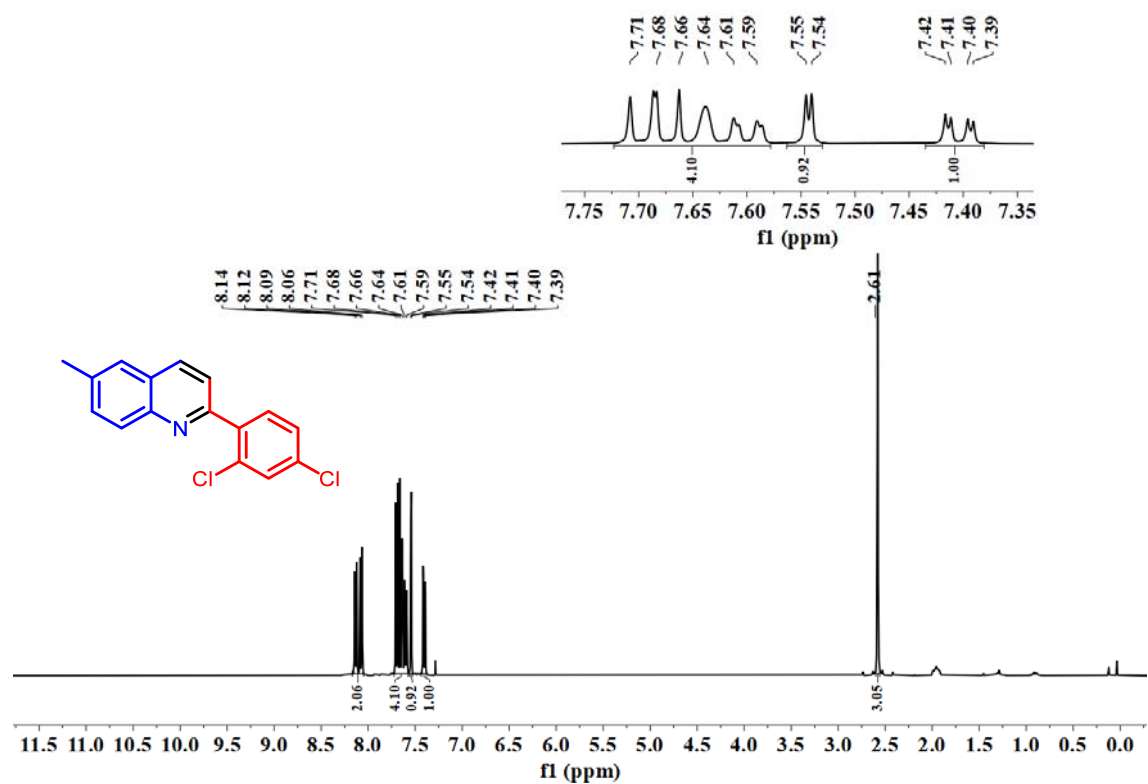


Fig. S91 ¹H NMR spectrum of **30** in CDCl₃ (400 MHz).

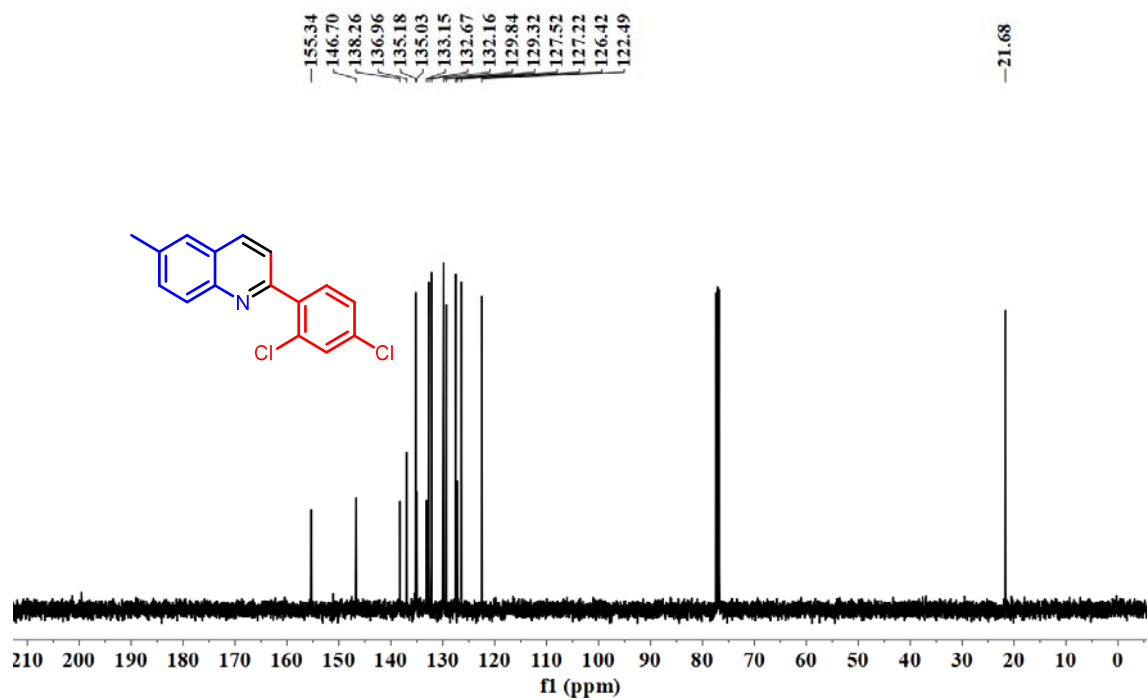


Fig. S92 ¹³C{¹H} NMR spectrum of **30** in CDCl₃ (101 MHz).

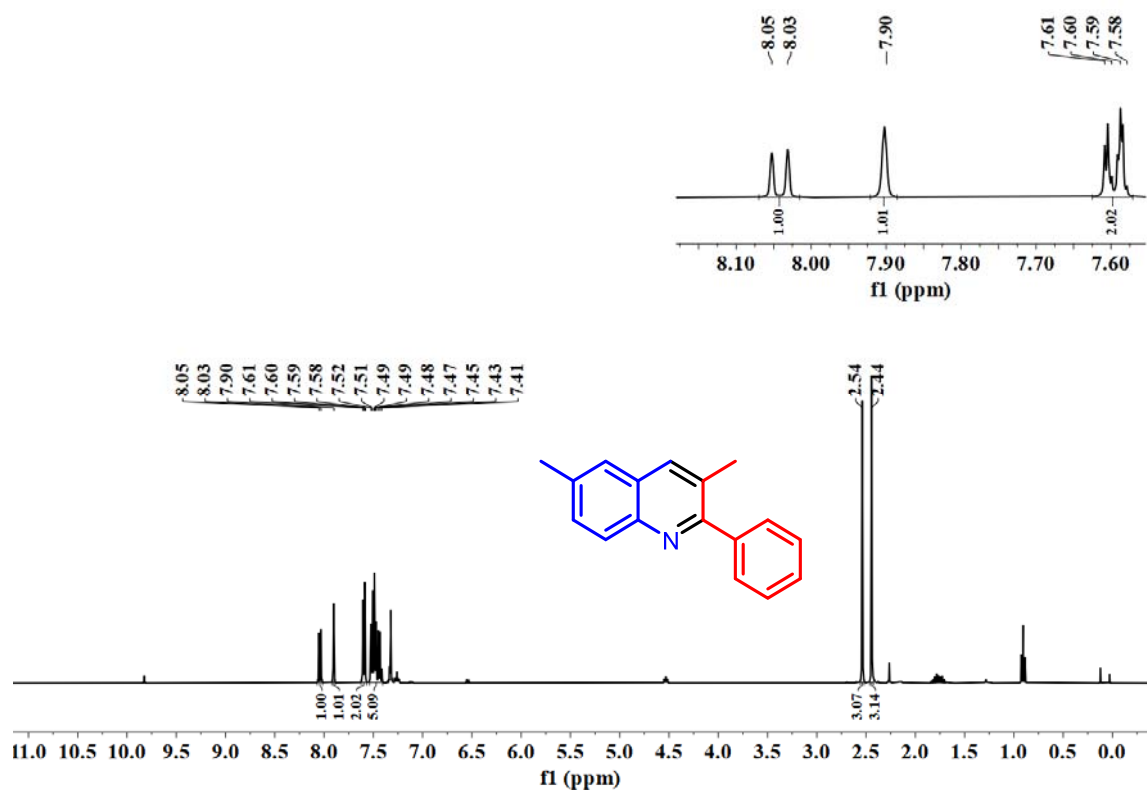


Fig. S93 ^1H NMR spectrum of **31** in CDCl_3 (400 MHz).

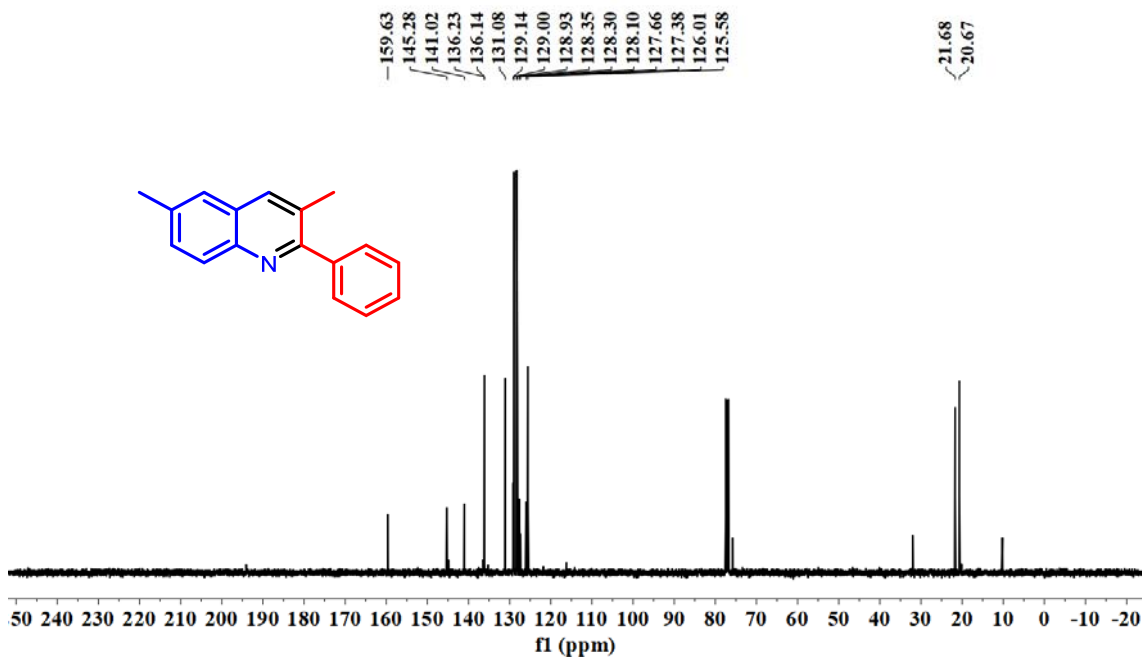


Fig. S94 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **31** in CDCl_3 (101 MHz).

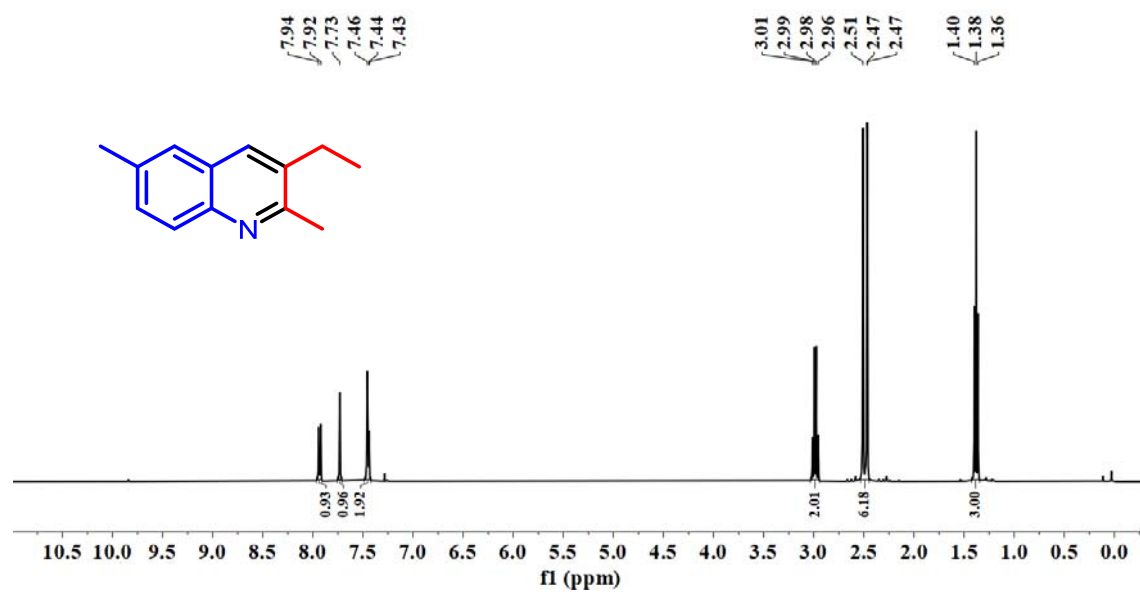


Fig. S95 ¹H NMR spectrum of **32** in CDCl₃ (400 MHz).

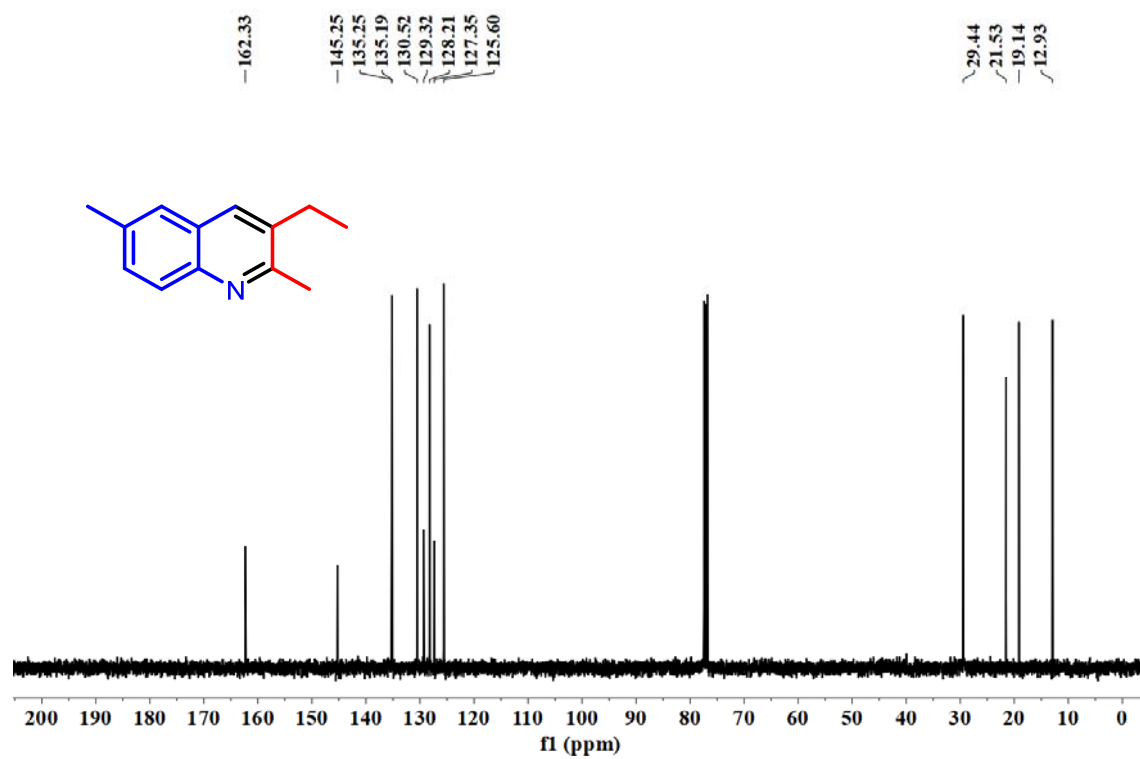


Fig. S96 ¹³C {¹H} NMR spectrum of **32** in CDCl₃ (101 MHz).

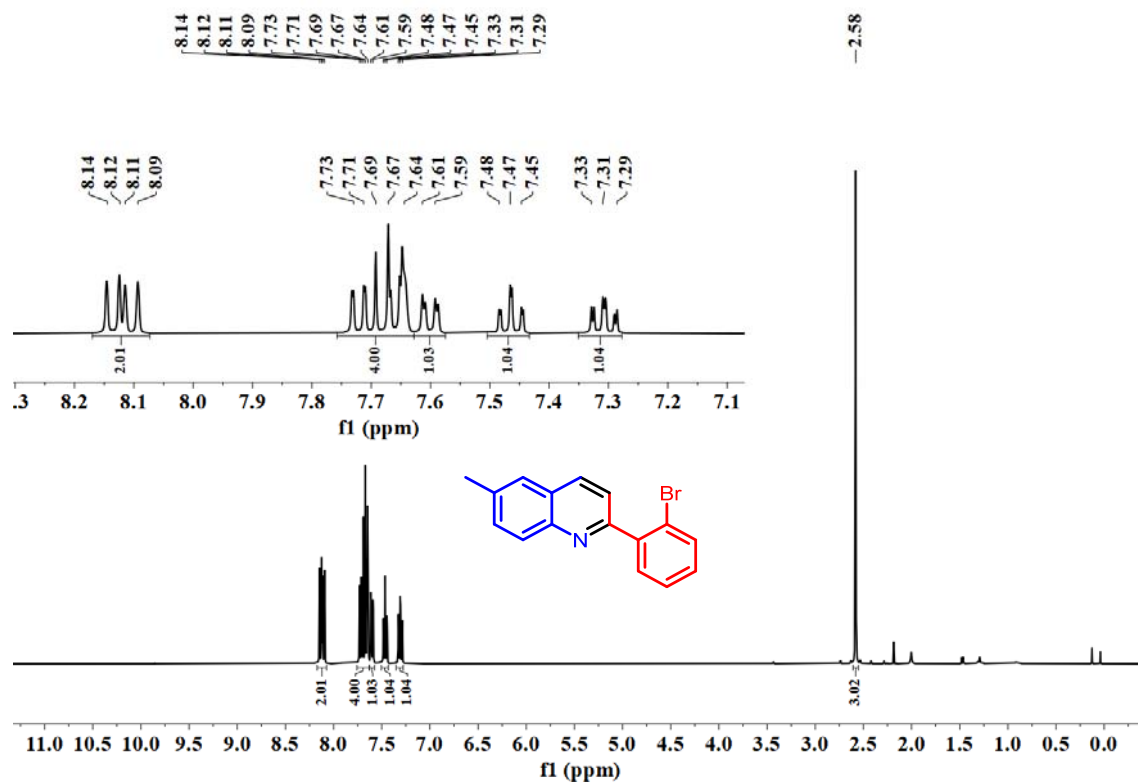


Fig. S97 ¹H NMR spectrum of **33** in CDCl₃ (400 MHz).

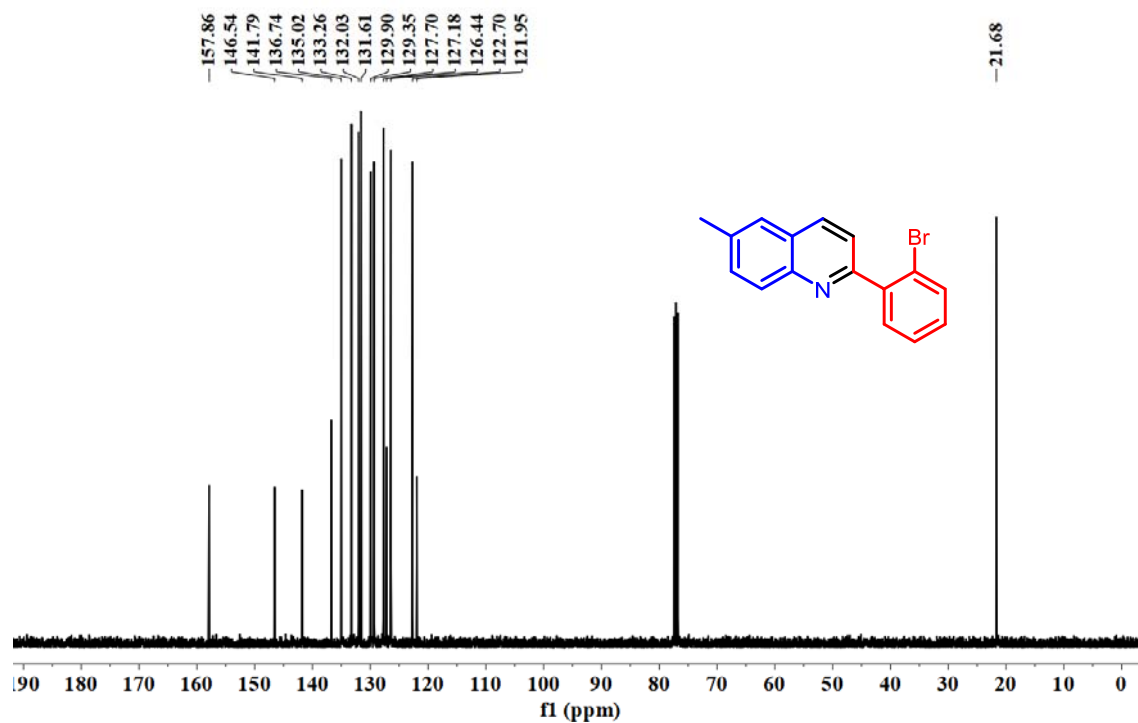


Fig. S98 ¹³C {¹H} NMR spectrum of **33** in CDCl₃ (101 MHz).

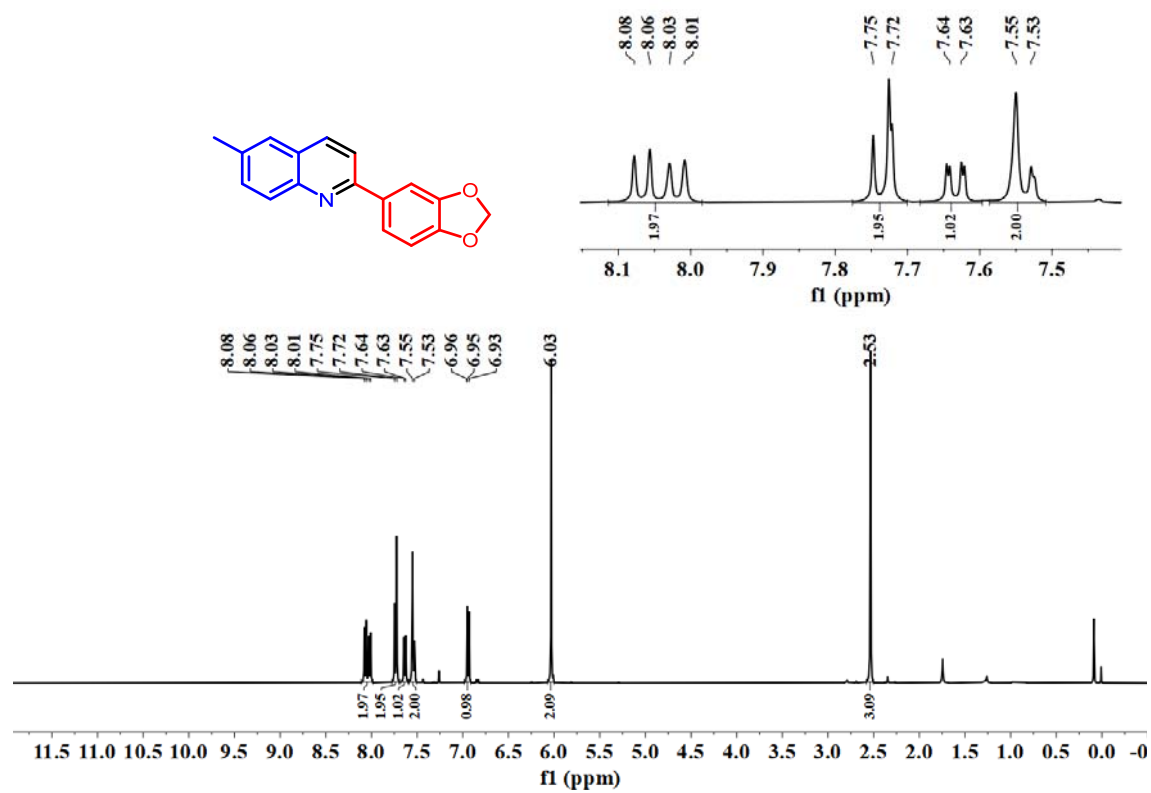


Fig. S99 ^1H NMR spectrum of **34** in CDCl_3 (500 MHz).

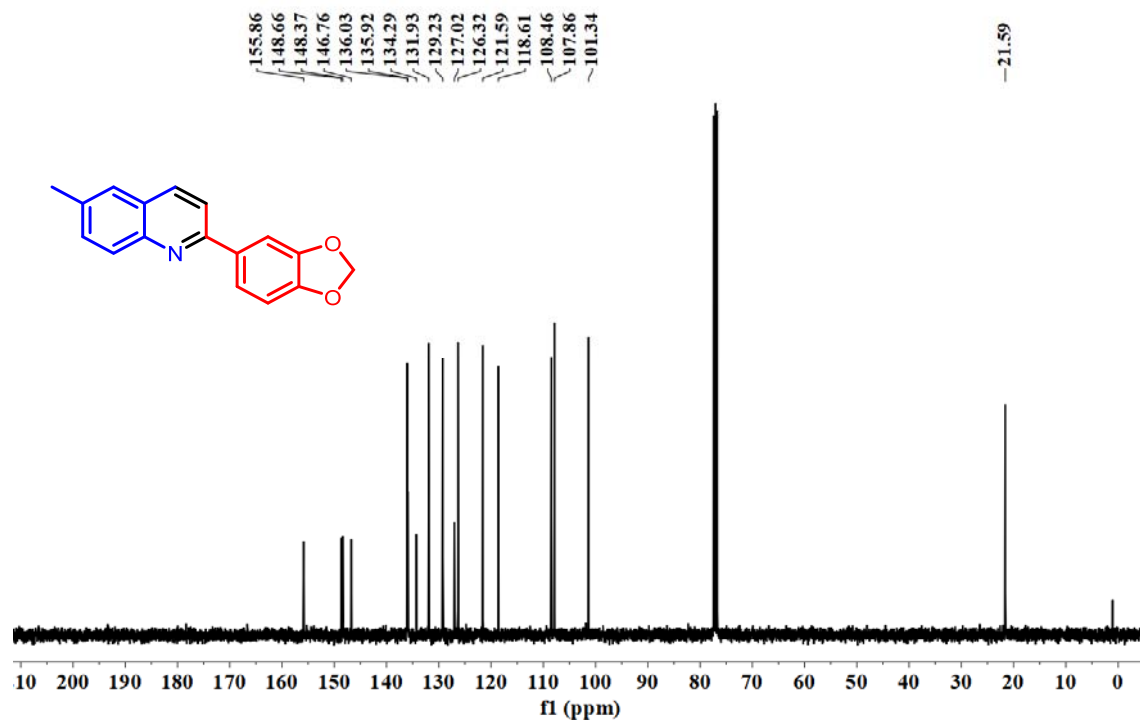


Fig. S100 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **34** in CDCl_3 (126 MHz).

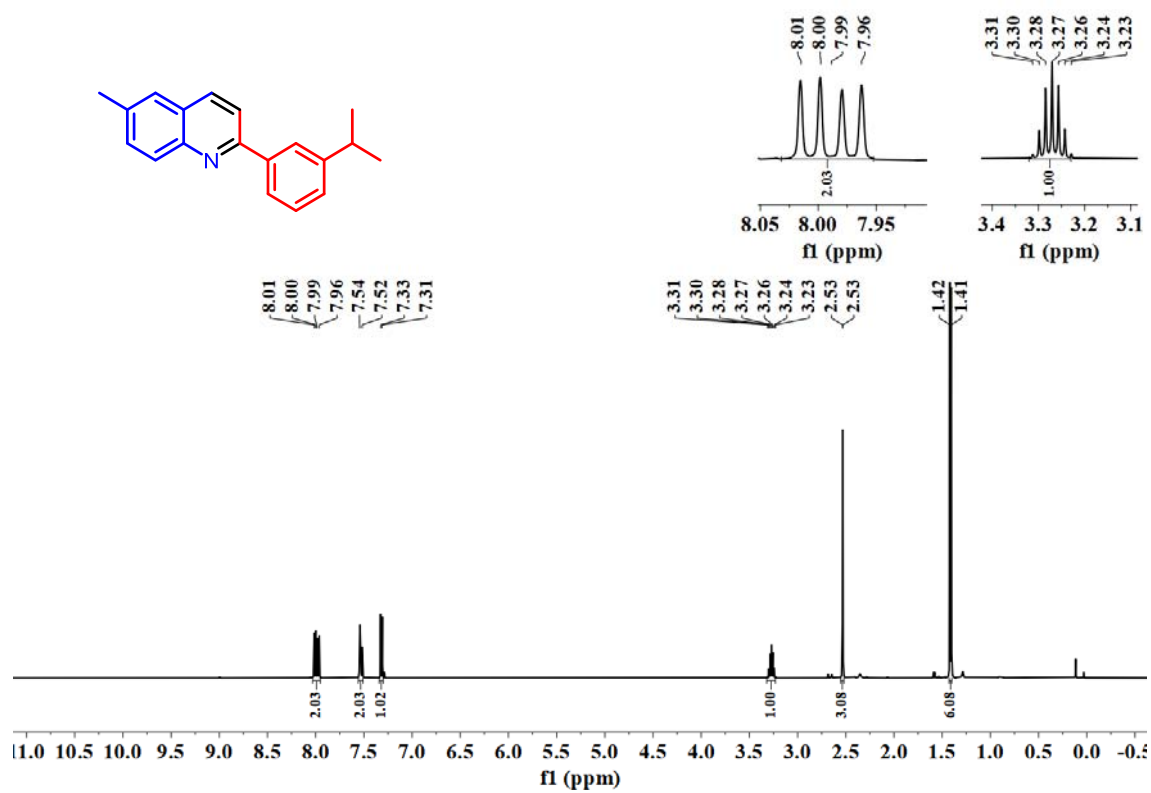


Fig. S101 ^1H NMR spectrum of **35** in CDCl_3 (500 MHz).

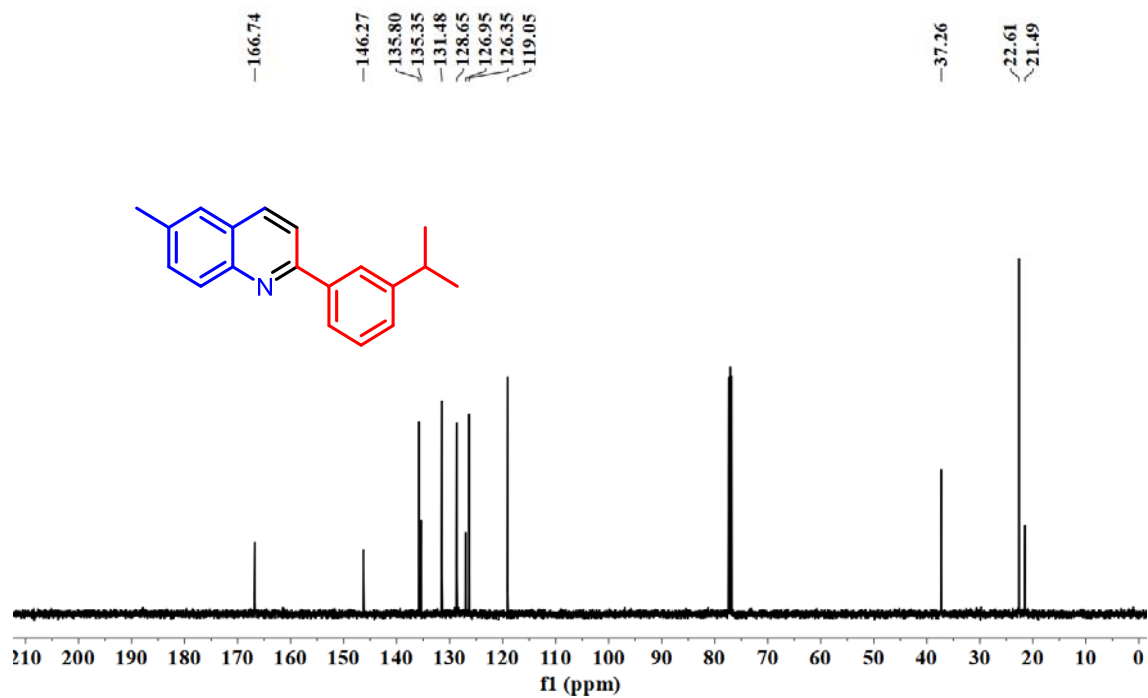


Fig. S102 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **35** in CDCl_3 (126 MHz).

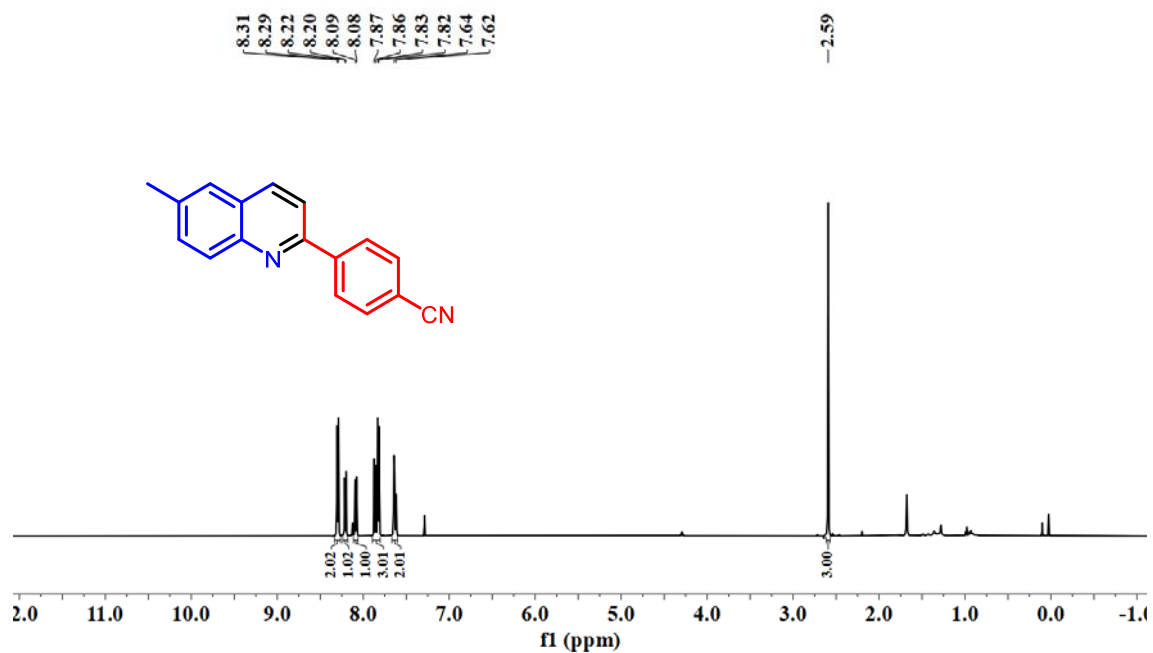


Fig. S103 ^1H NMR spectrum of **36** in CDCl_3 (500 MHz).

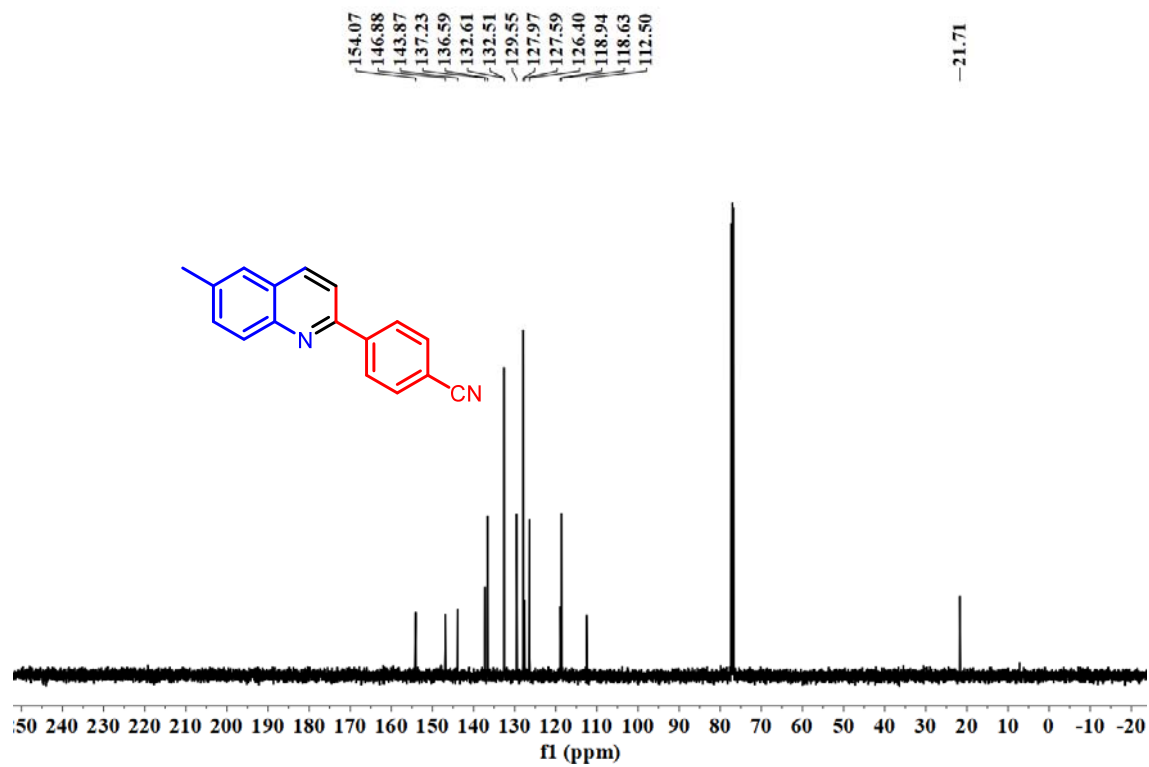


Fig. S104 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **36** in CDCl_3 (126 MHz).

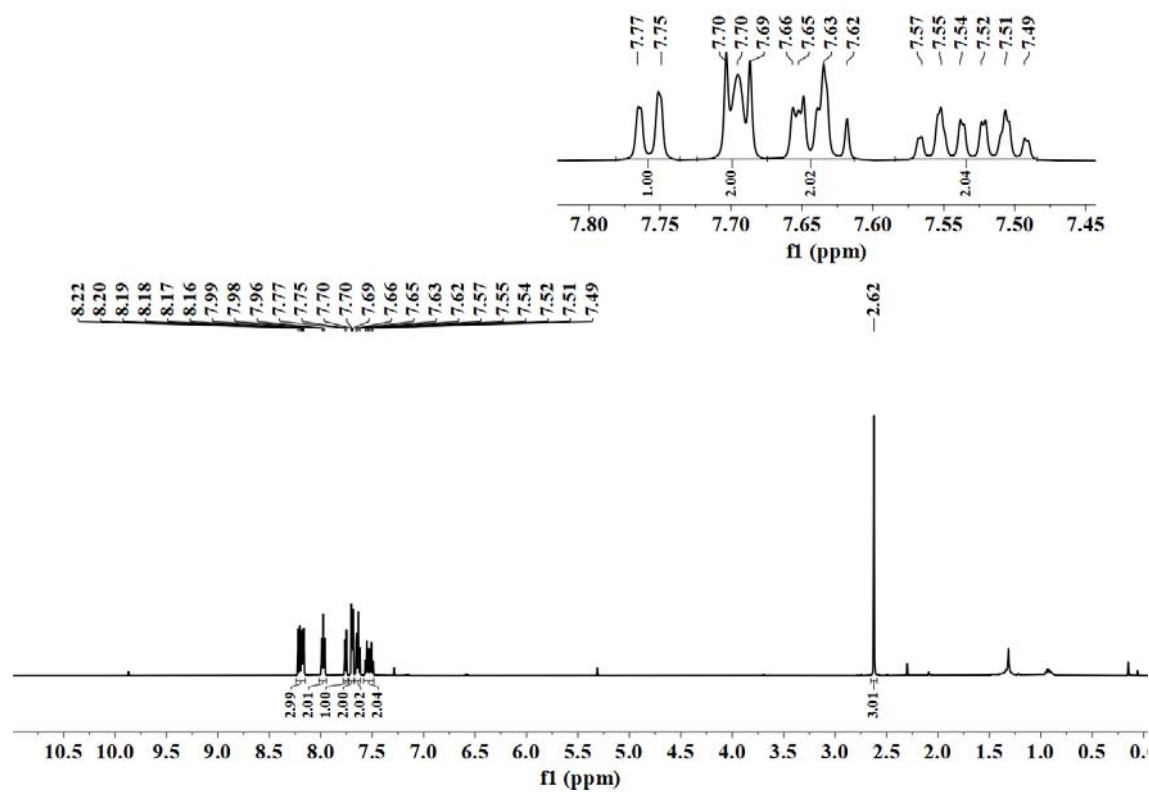


Fig. S105 ^1H NMR spectrum of **37** in CDCl_3 (400 MHz).

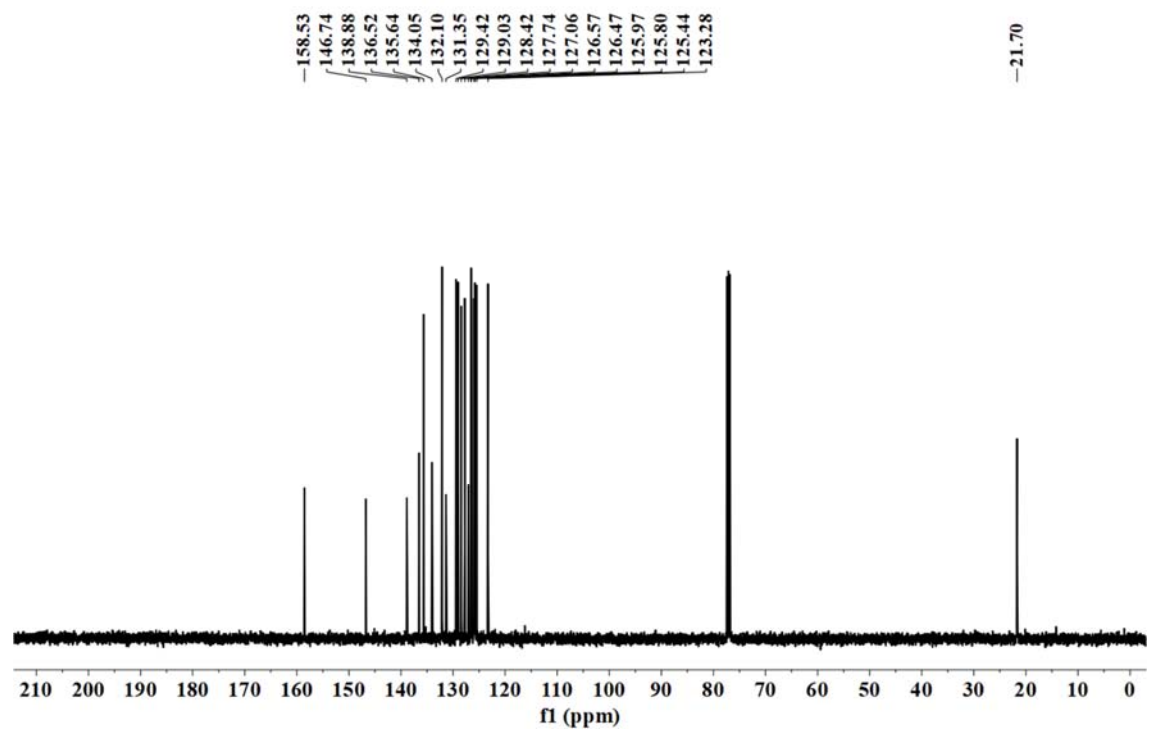


Fig. S106 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **37** in CDCl_3 (1201 MHz).

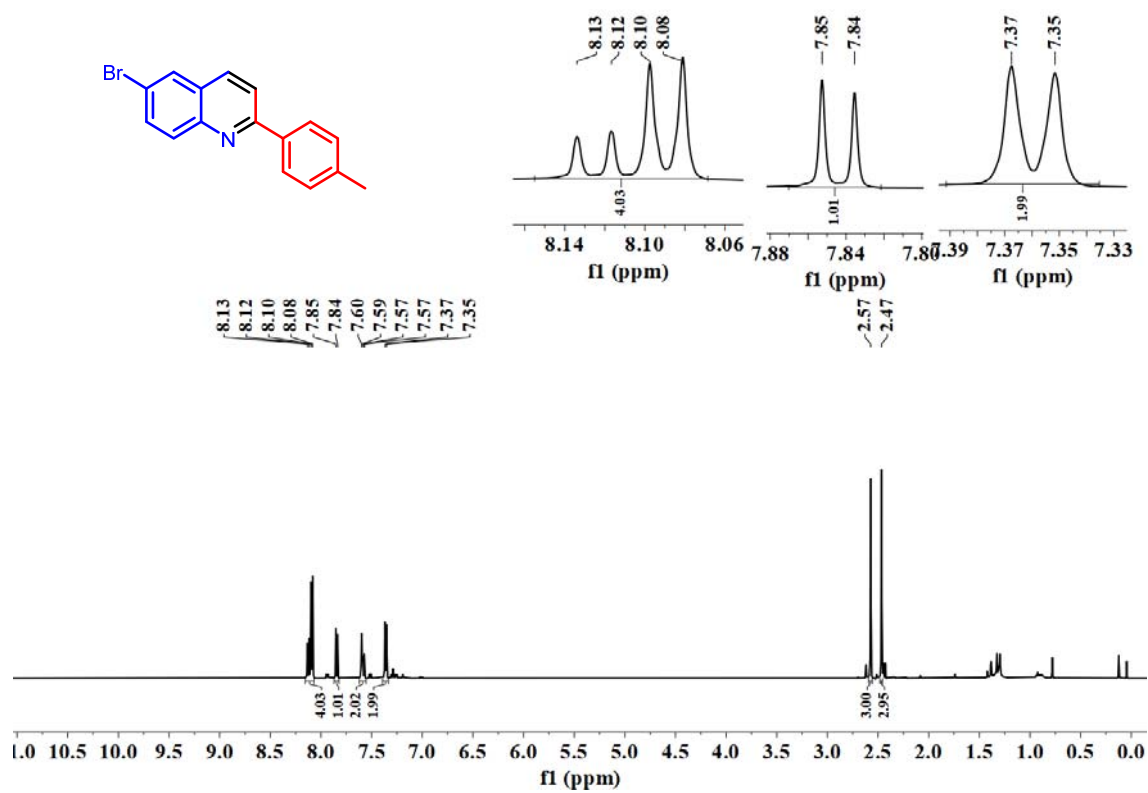


Fig. S107 ^1H NMR spectrum of **38** in CDCl_3 (400 MHz).

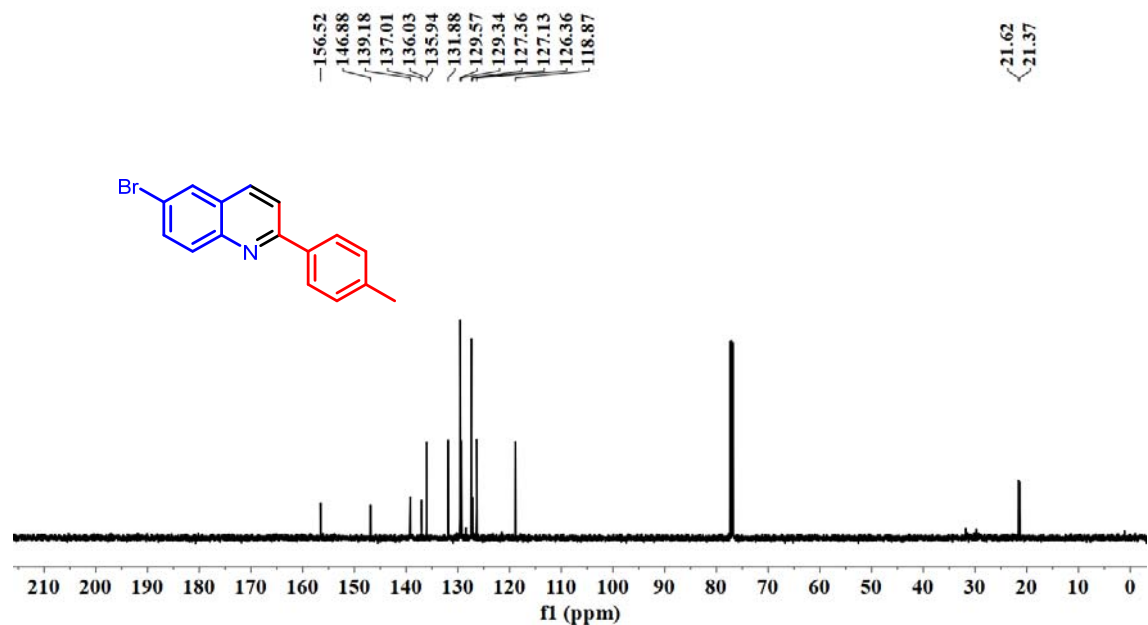


Fig. S108 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **38** in CDCl_3 (101 MHz).

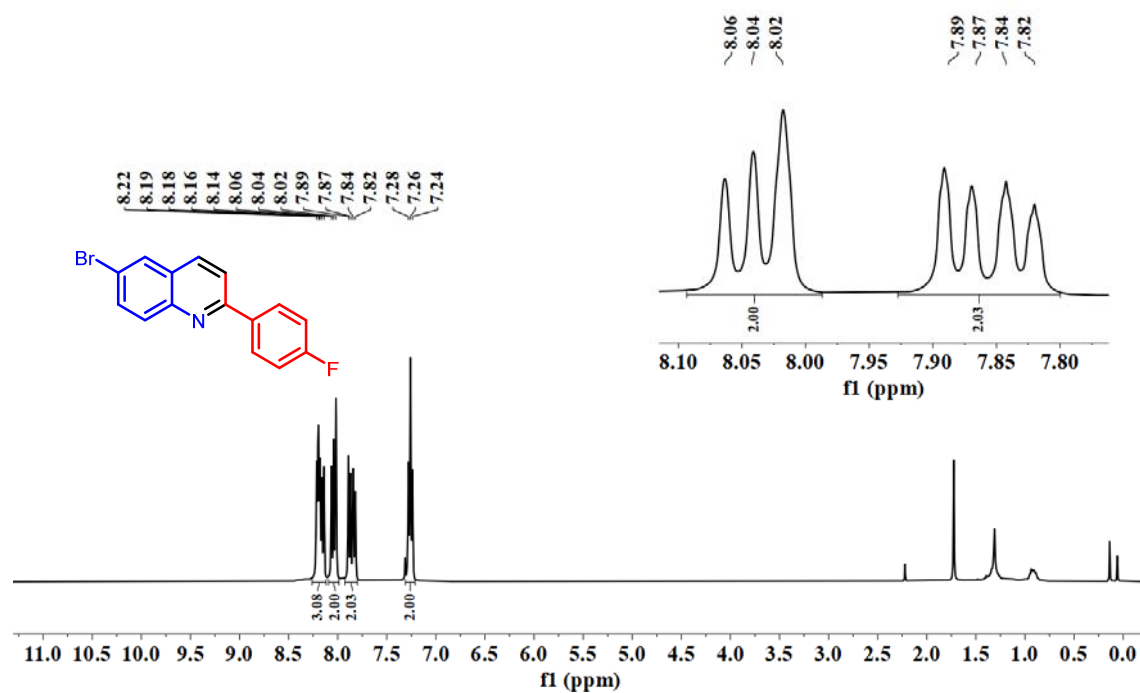


Fig. S109 ¹H NMR spectrum of **39** in CDCl₃ (400 MHz).

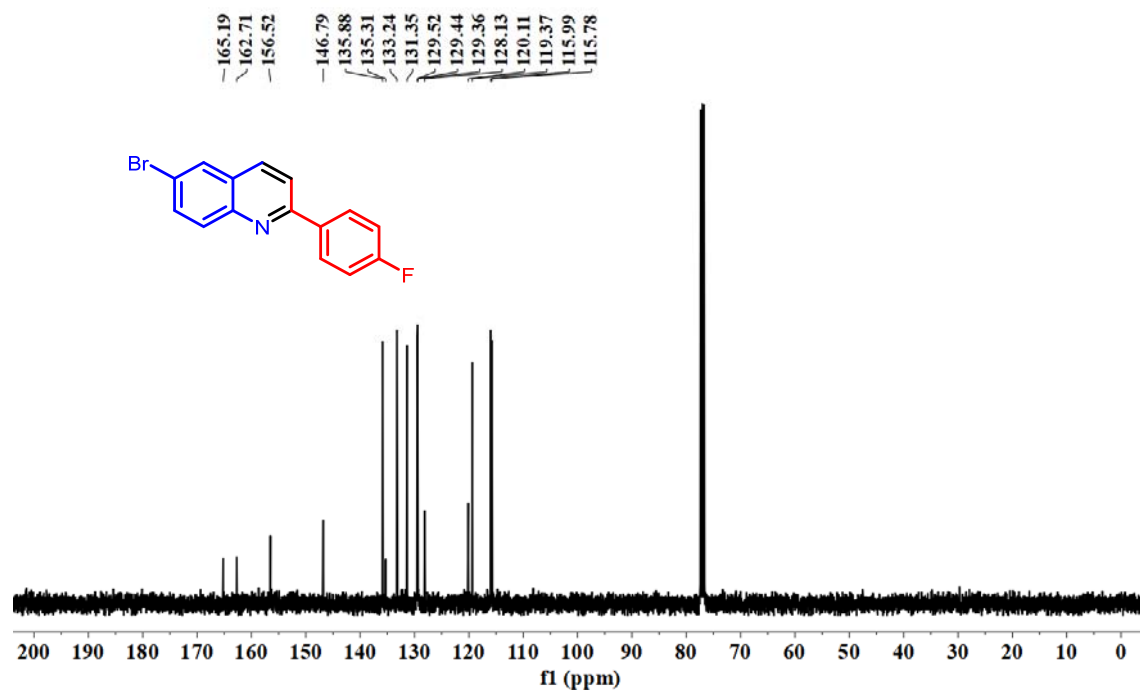


Fig. S110 ¹³C{¹H} NMR spectrum of **39** in CDCl₃ (101 MHz).

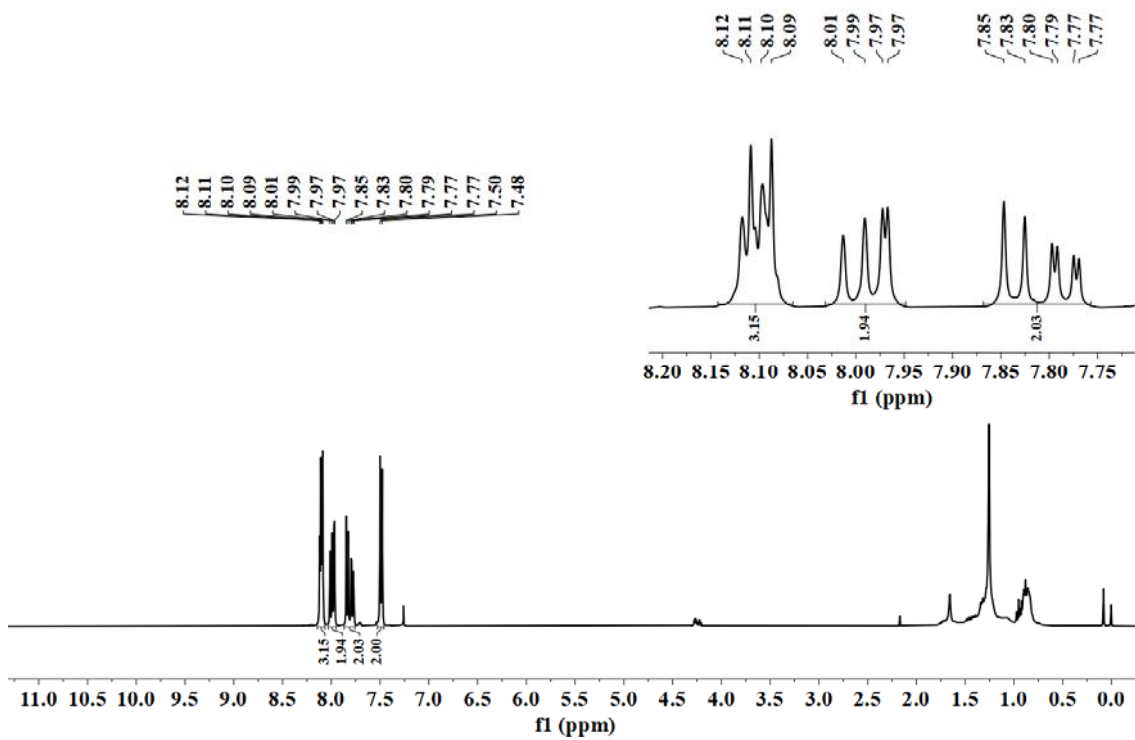


Fig. S111 ^1H NMR spectrum of **40** in CDCl_3 (400 MHz).

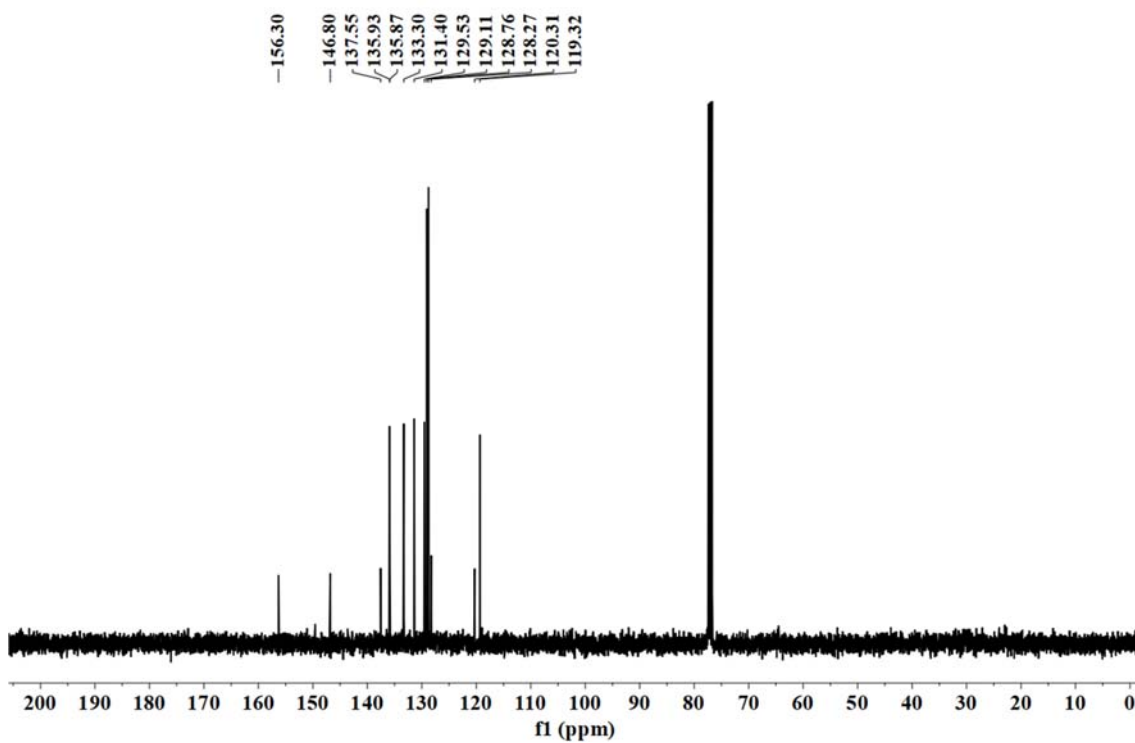


Fig. S112 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **40** in CDCl_3 (101 MHz).

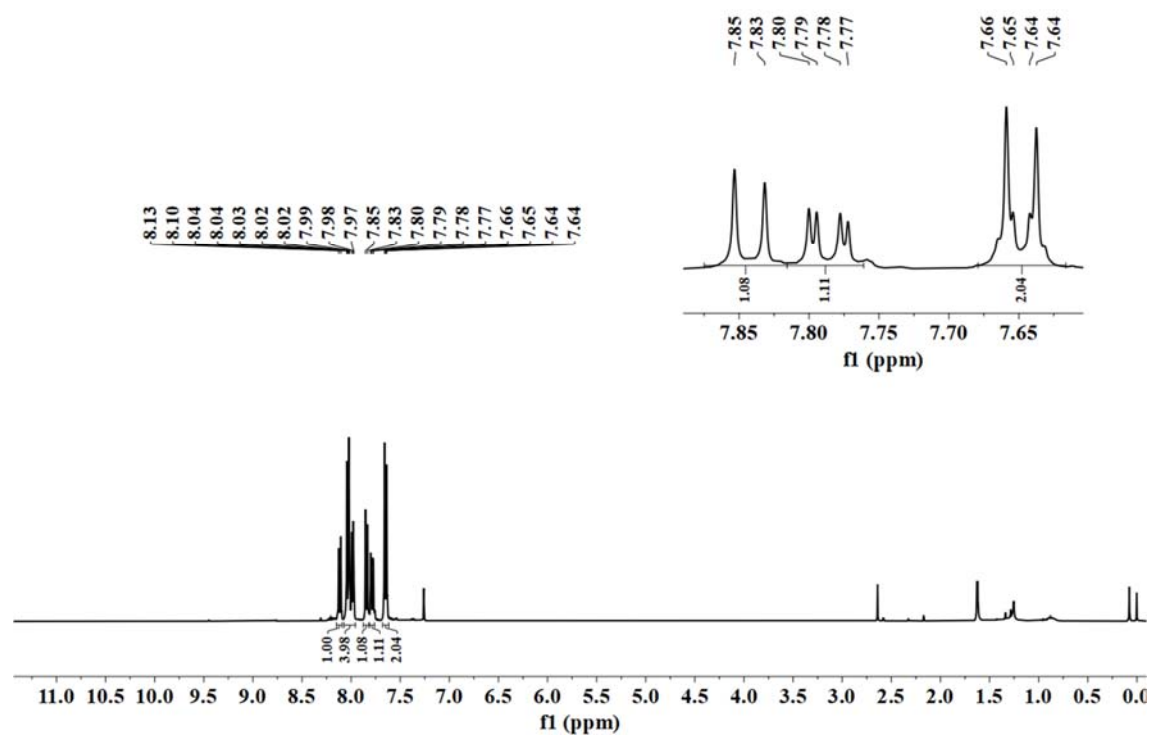


Fig. S113 ^1H NMR spectrum of **41** in CDCl_3 (400 MHz).

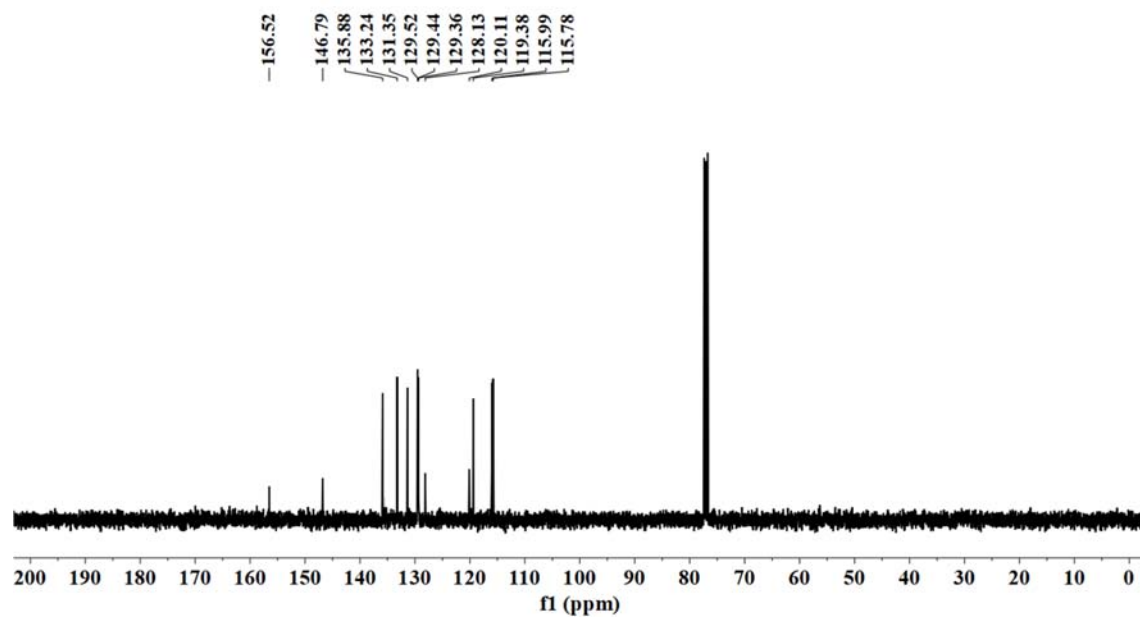


Fig. S114 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **41** in CDCl_3 (101 MHz).

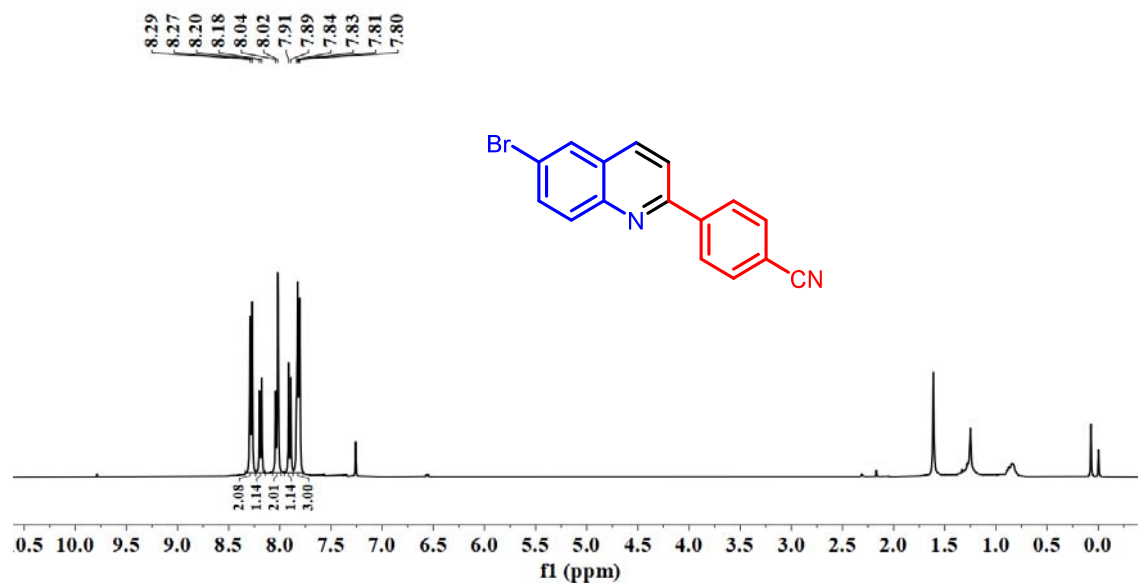


Fig. S115 ¹H NMR spectrum of **42** in CDCl₃ (400 MHz).

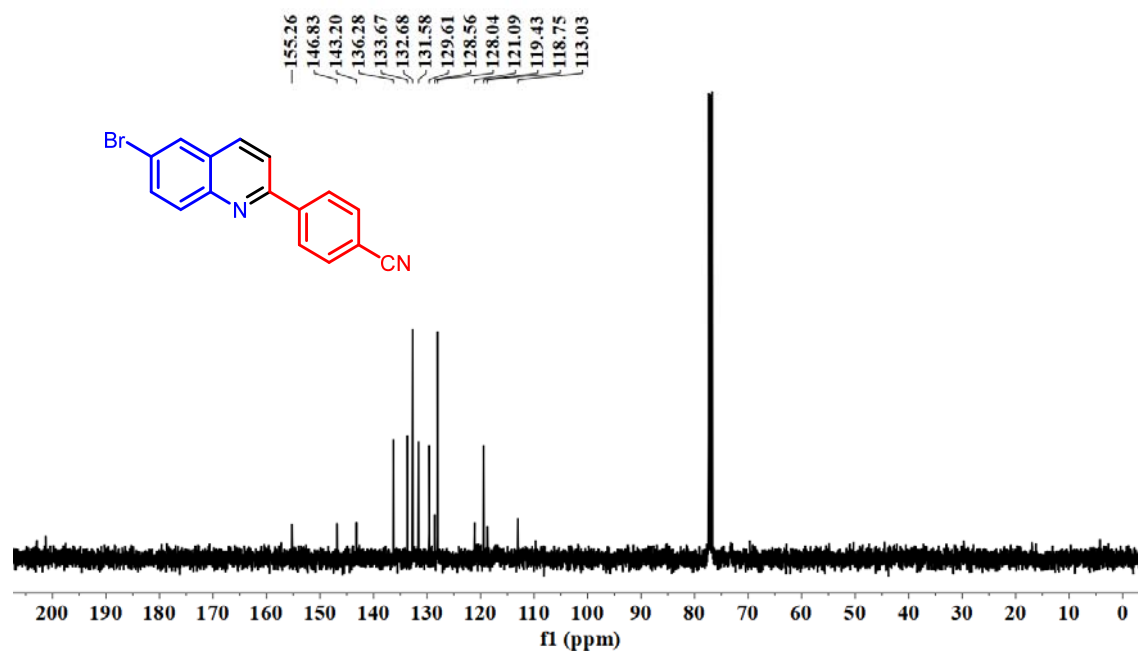


Fig. S116 ¹³C{¹H} NMR spectrum of **42** in CDCl₃ (101MHz).

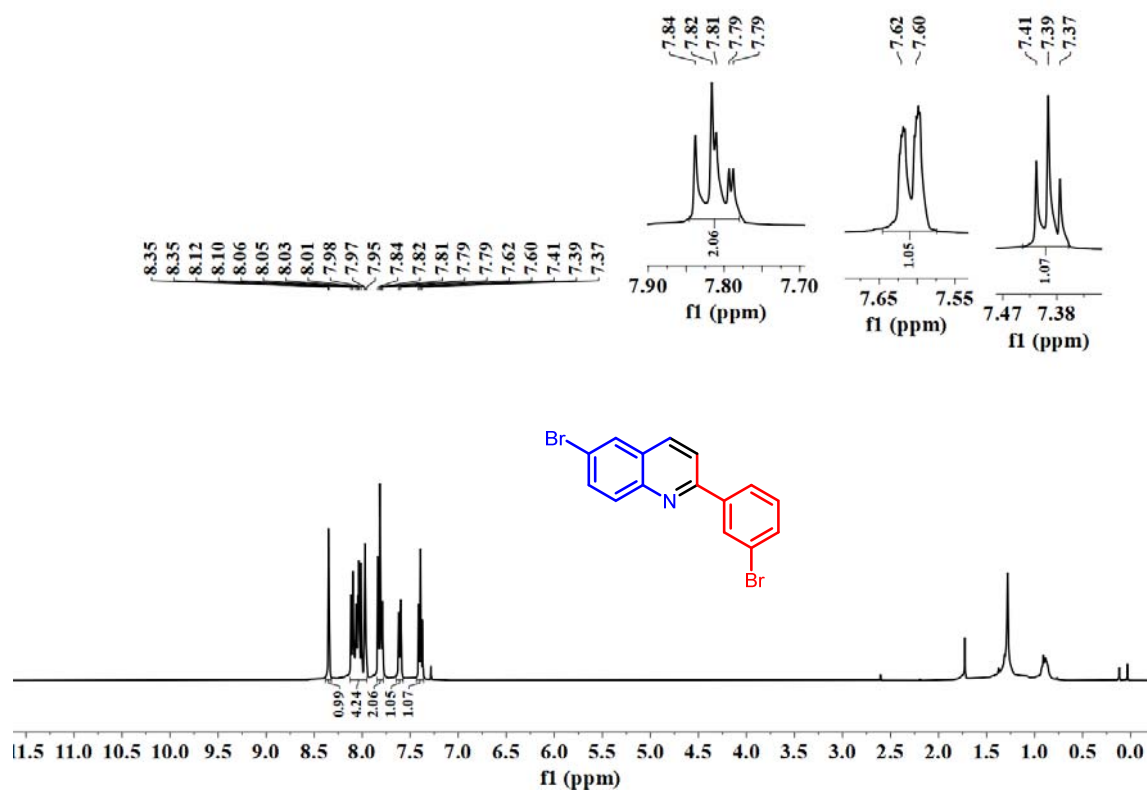


Fig. S117 ¹H NMR spectrum of **43** in CDCl₃ (400 MHz).

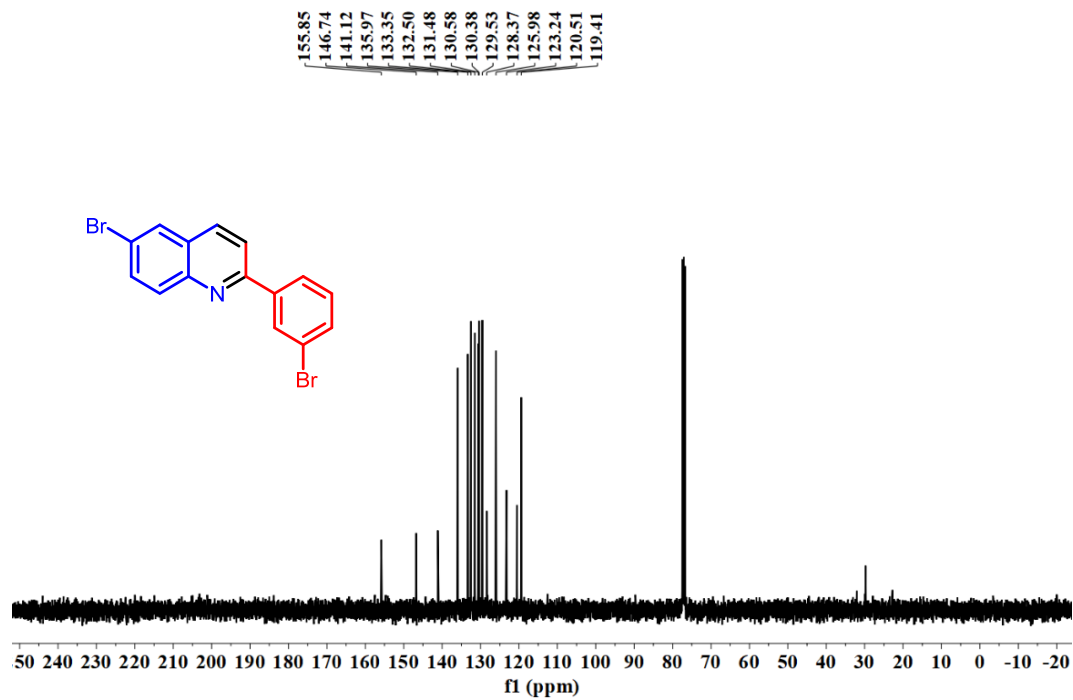


Fig. S118 ¹³C{¹H} NMR spectrum of **43** in CDCl₃ (101 MHz).

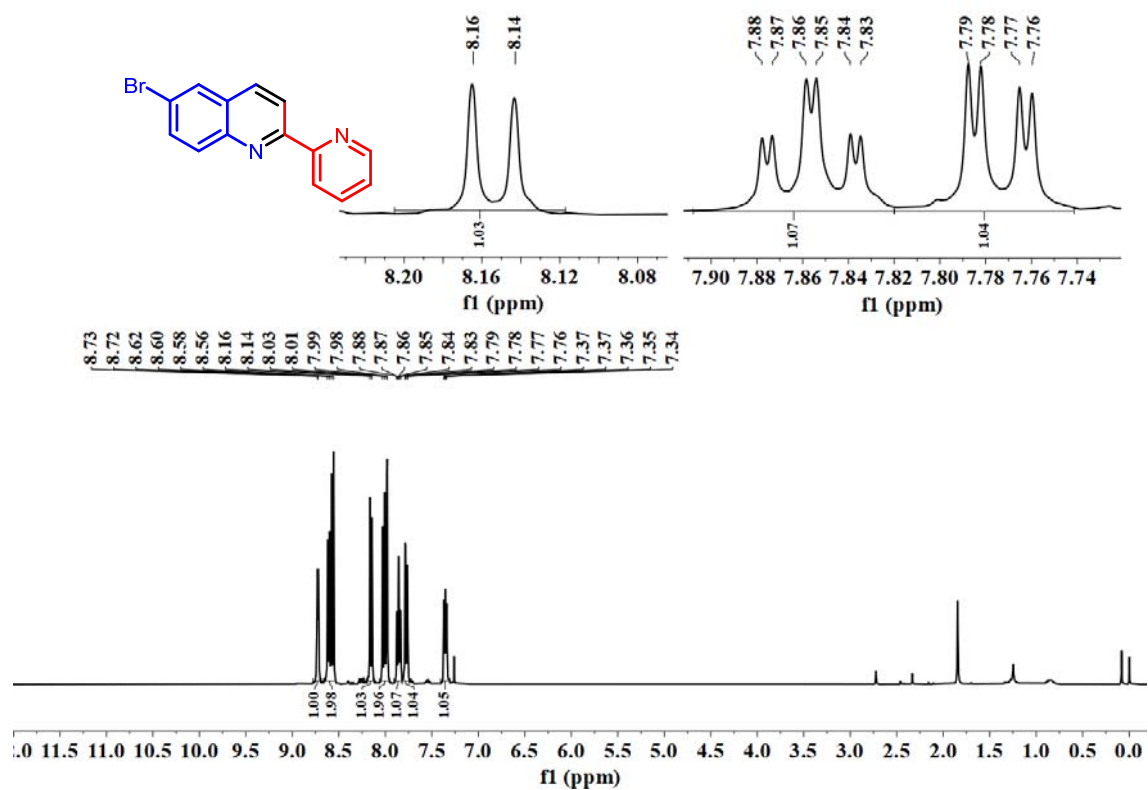


Fig. S119 ^1H NMR spectrum of **44** in CDCl_3 (400 MHz).

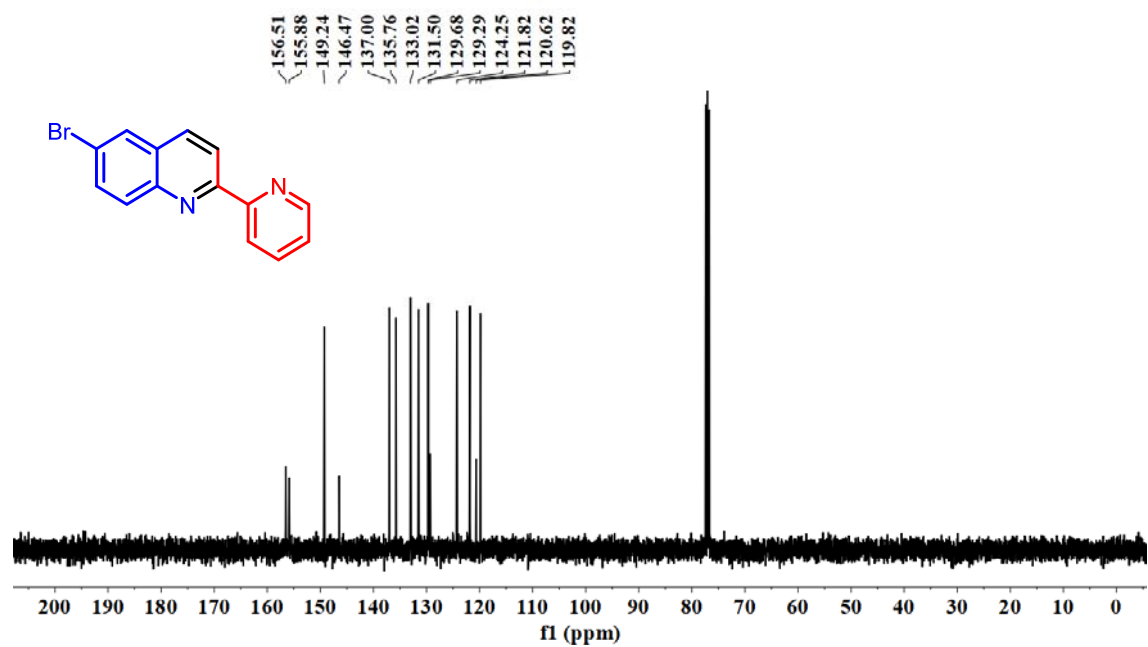


Fig. S120. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **44** in CDCl_3 (1101 MHz).

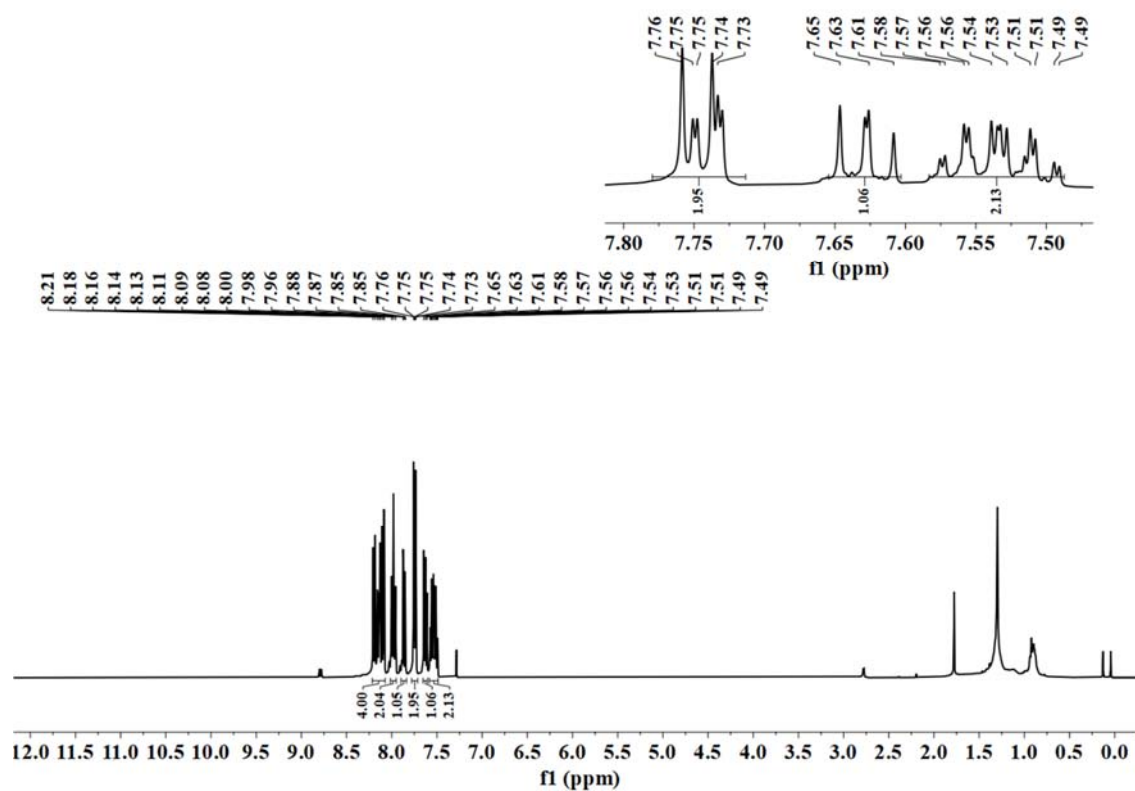


Fig. S121 ^1H NMR spectrum of **45** in CDCl_3 4 MHz).

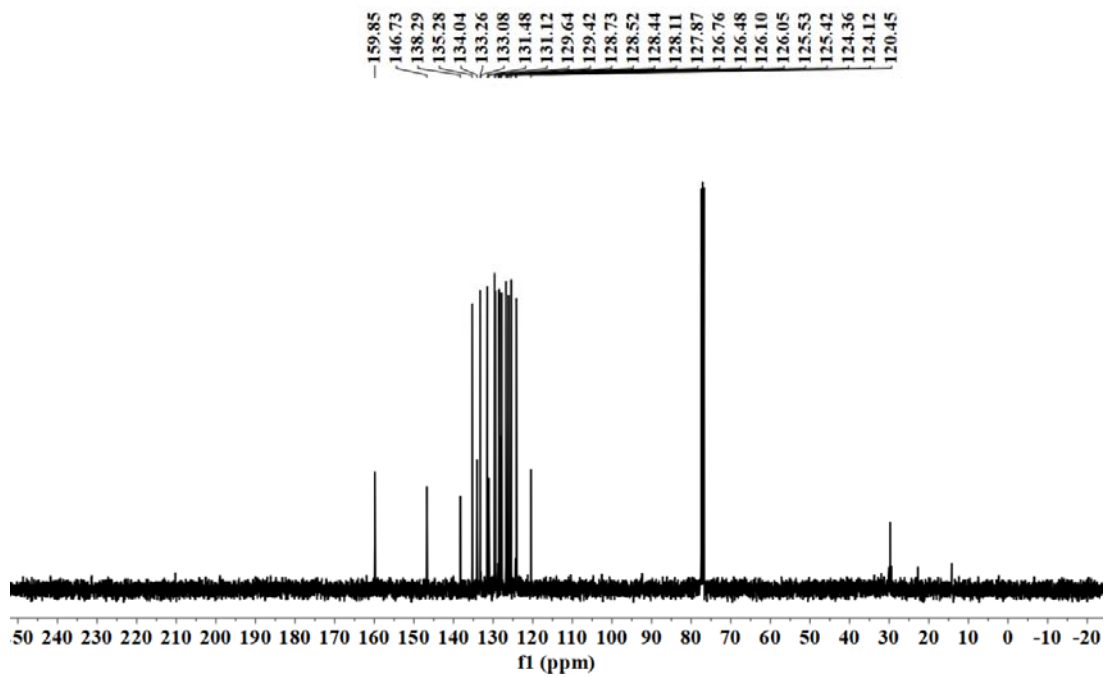


Fig. S122 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **45** in CDCl_3 (101MHz).

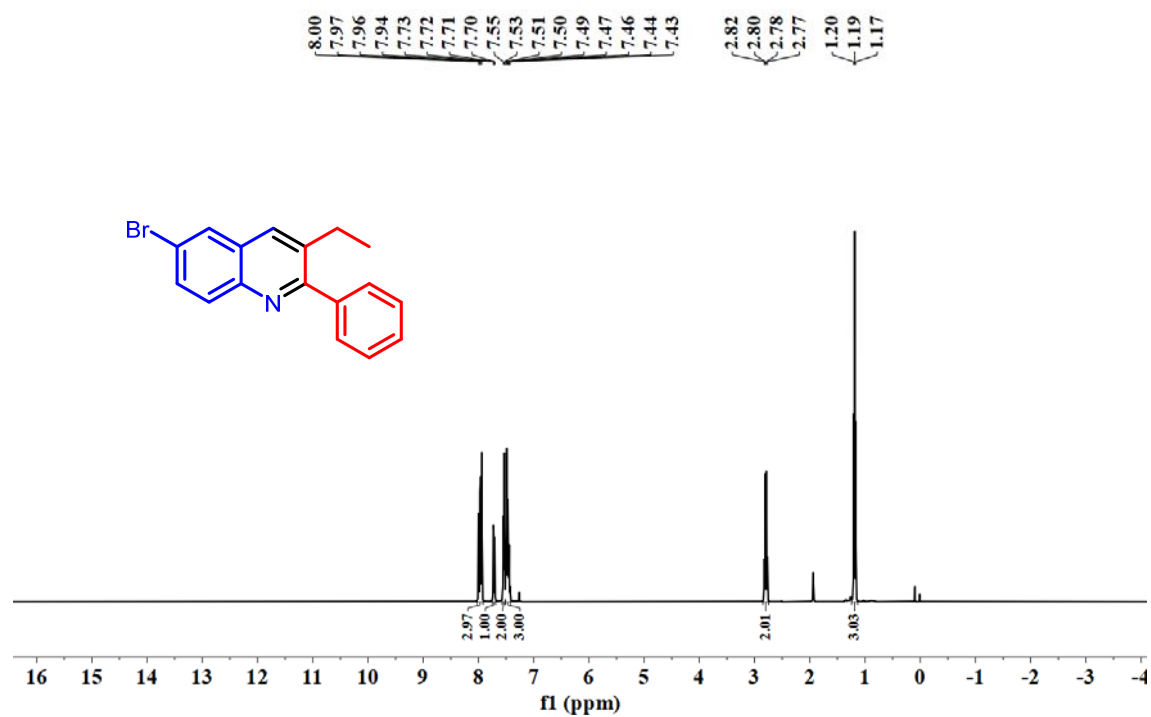


Fig. S123 ¹H NMR spectrum of **46** in CDCl₃ (400 MHz).

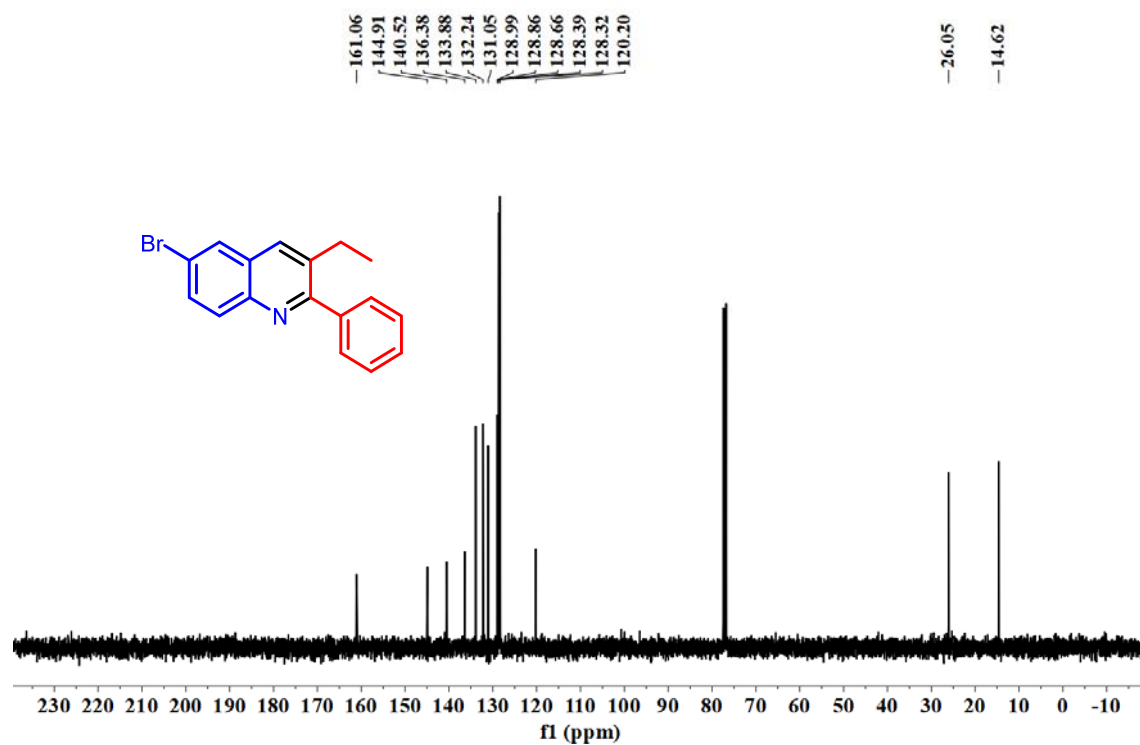


Fig. S124 ¹³C{¹H} NMR spectrum of **46** in CDCl₃ (101 MHz).

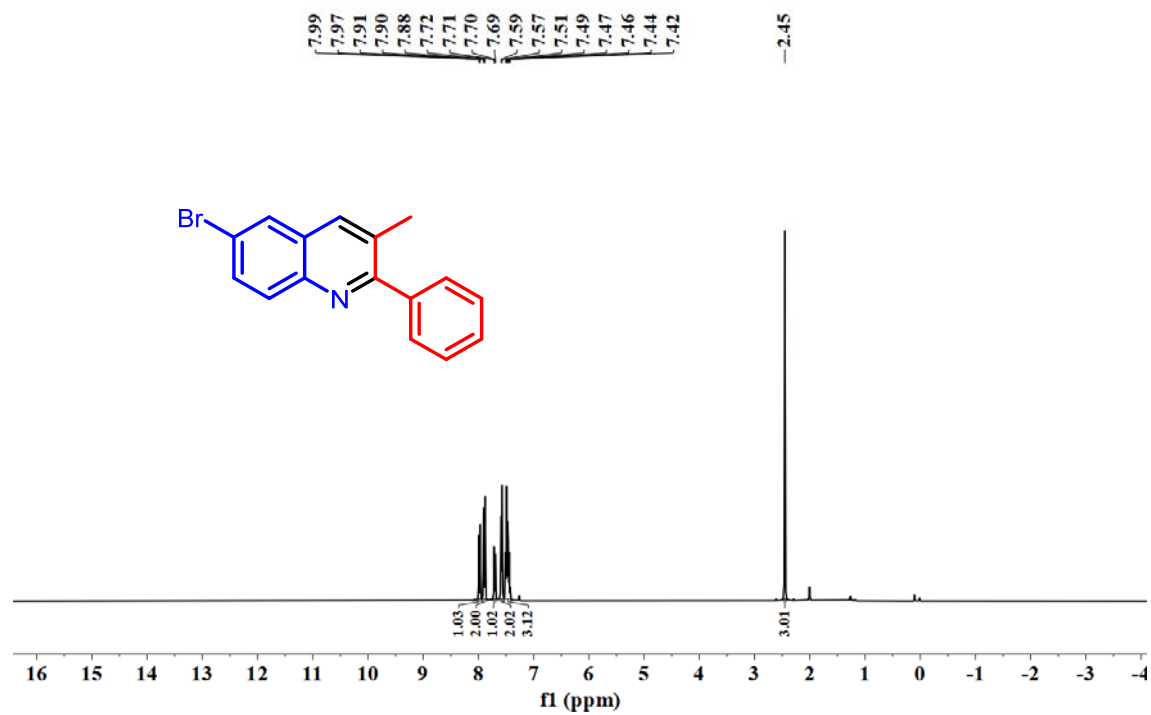


Fig. S125 ¹H NMR spectrum of 47 in CDCl₃ (400 MHz).

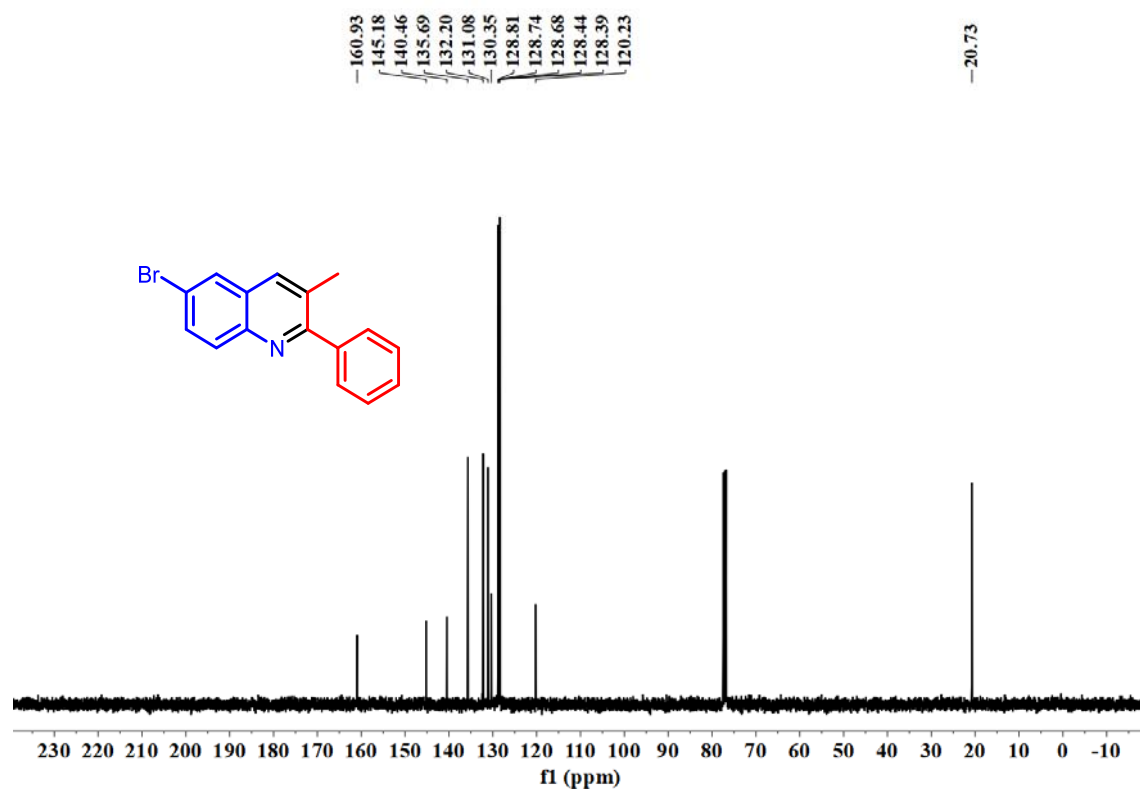


Fig. S126 ¹³C{¹H} NMR spectrum of 47 in CDCl₃ (101 MHz).

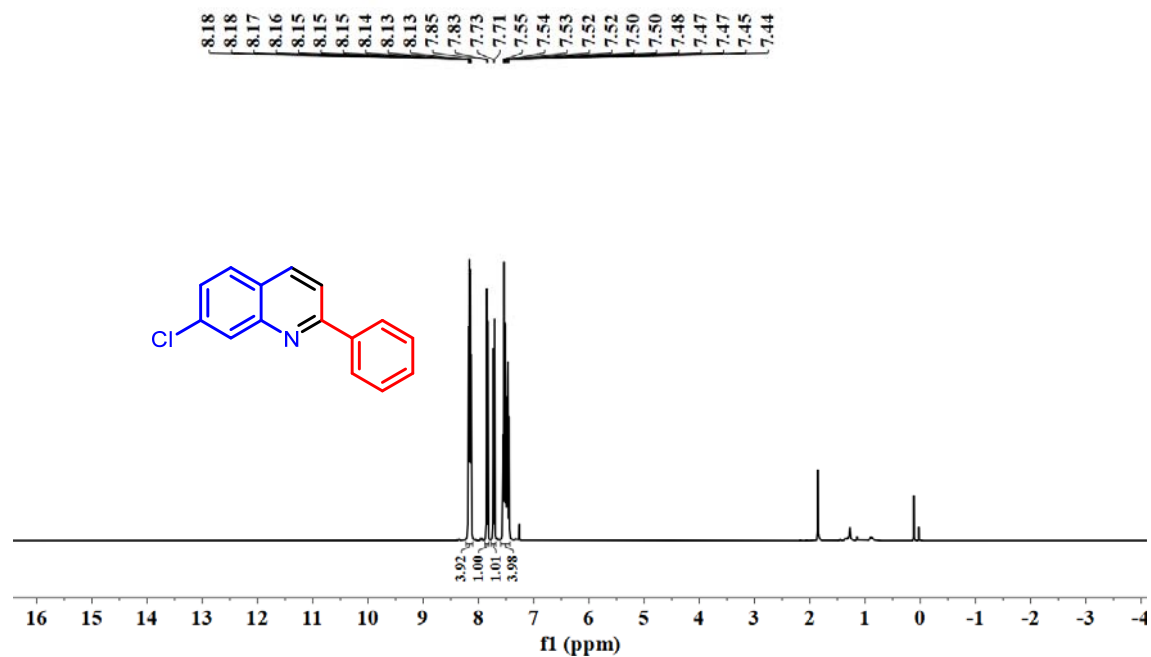


Fig. S127 ¹H NMR spectrum of **48** in CDCl₃ (400 MHz).

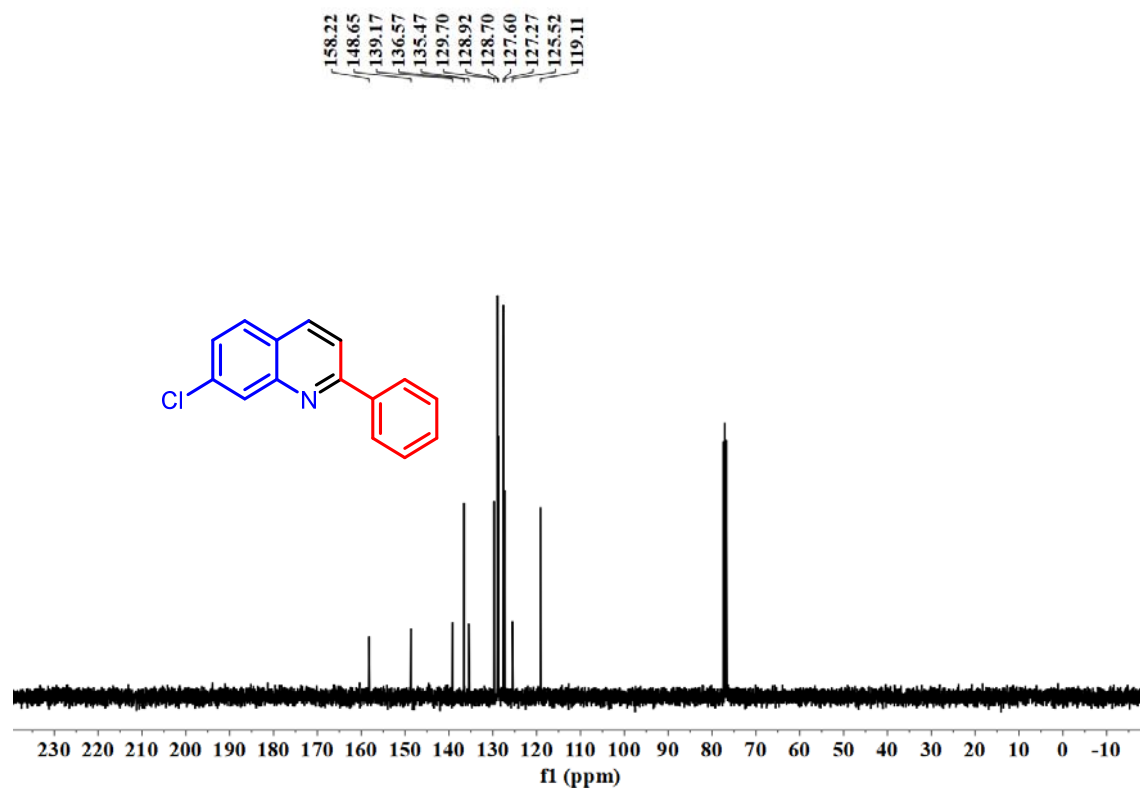


Fig. S128 ¹³C{¹H} NMR spectrum of **48** in CDCl₃ (101 MHz).

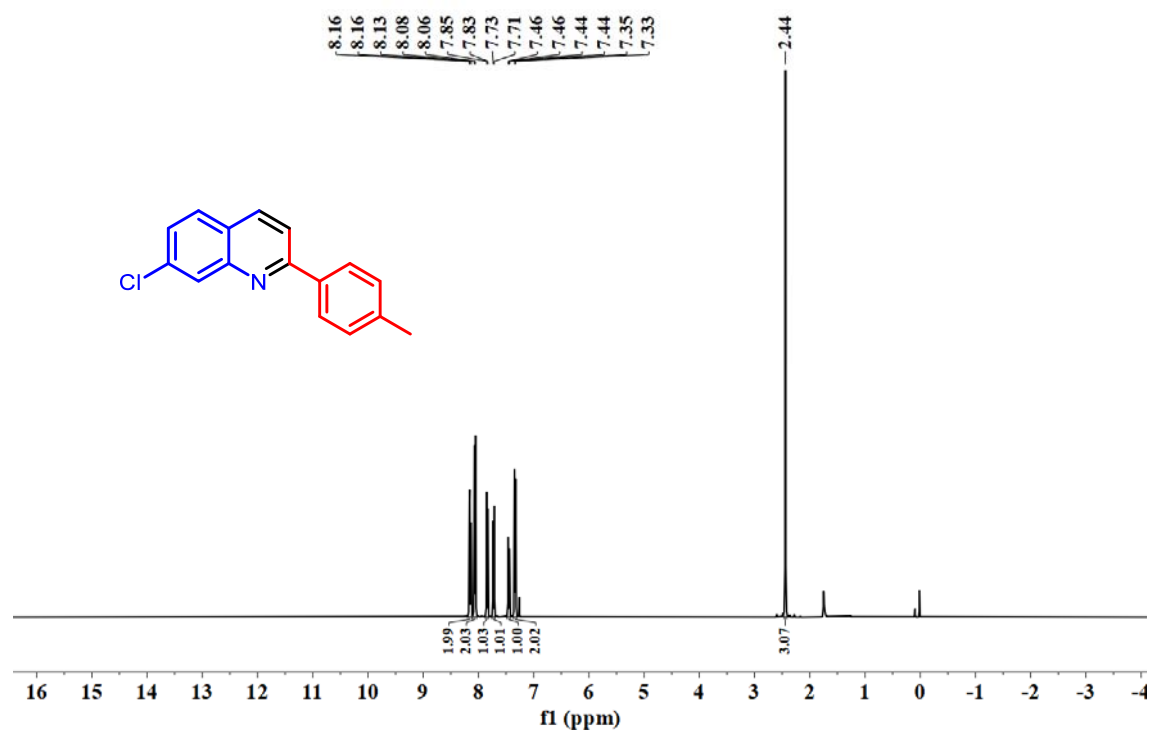


Fig. S129 ¹H NMR spectrum of **49** in CDCl₃ (400 MHz).

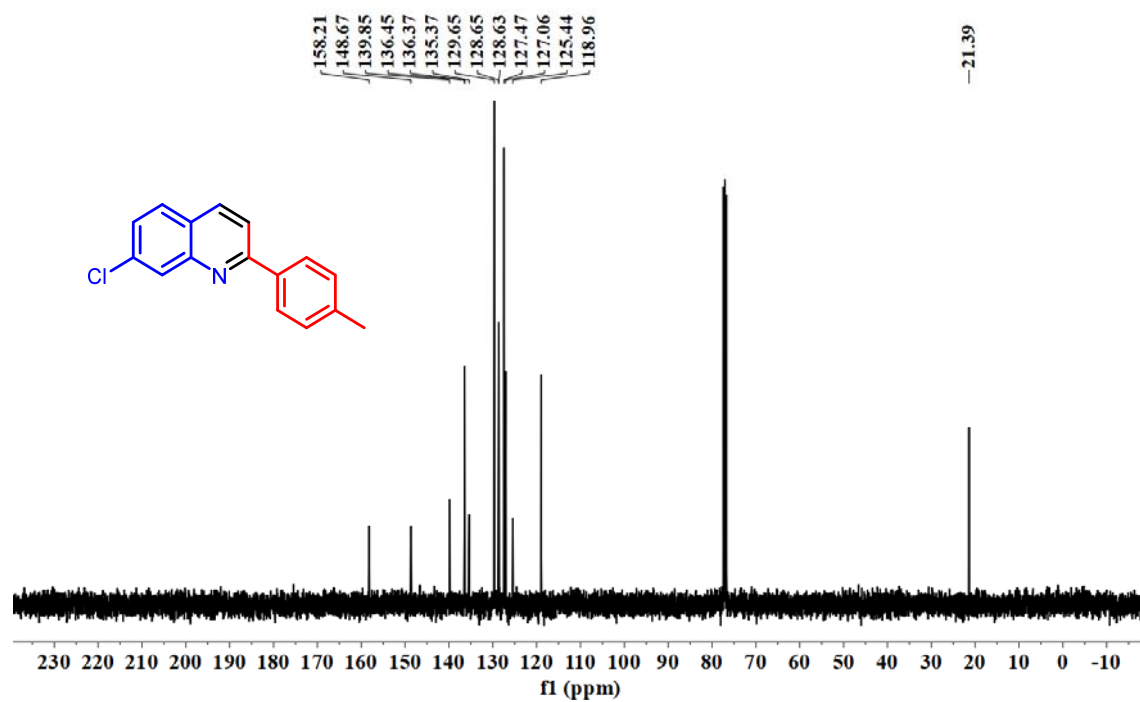


Fig. S130 ¹³C{¹H} NMR spectrum of **49** in CDCl₃ (101 MHz).

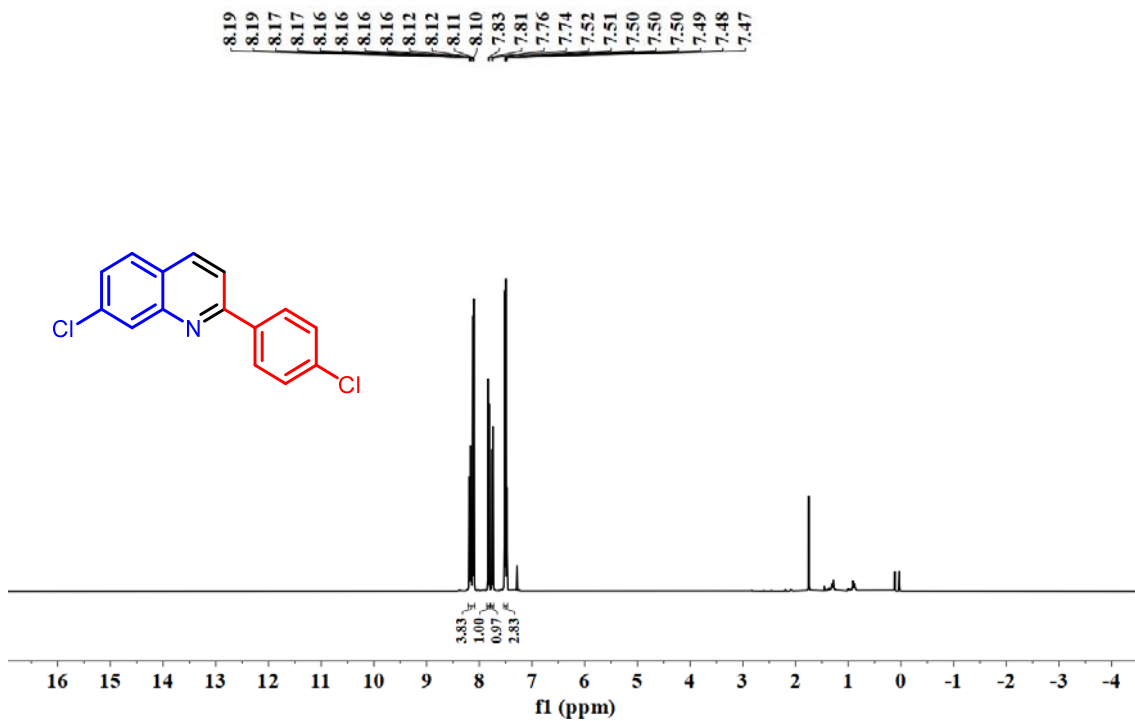


Fig. S131 ¹H NMR spectrum of **50** in CDCl₃ (400 MHz).

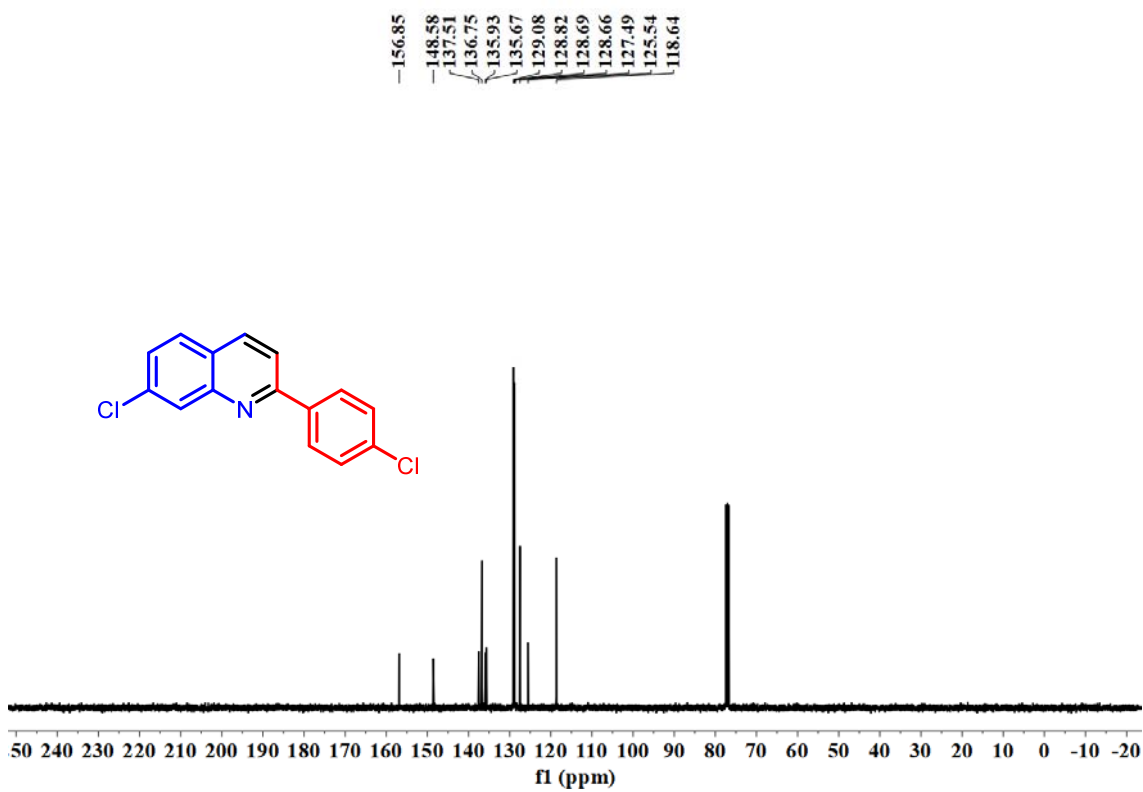


Fig. S132 ¹³C{¹H} NMR spectrum of **50** in CDCl₃ (101 MHz).

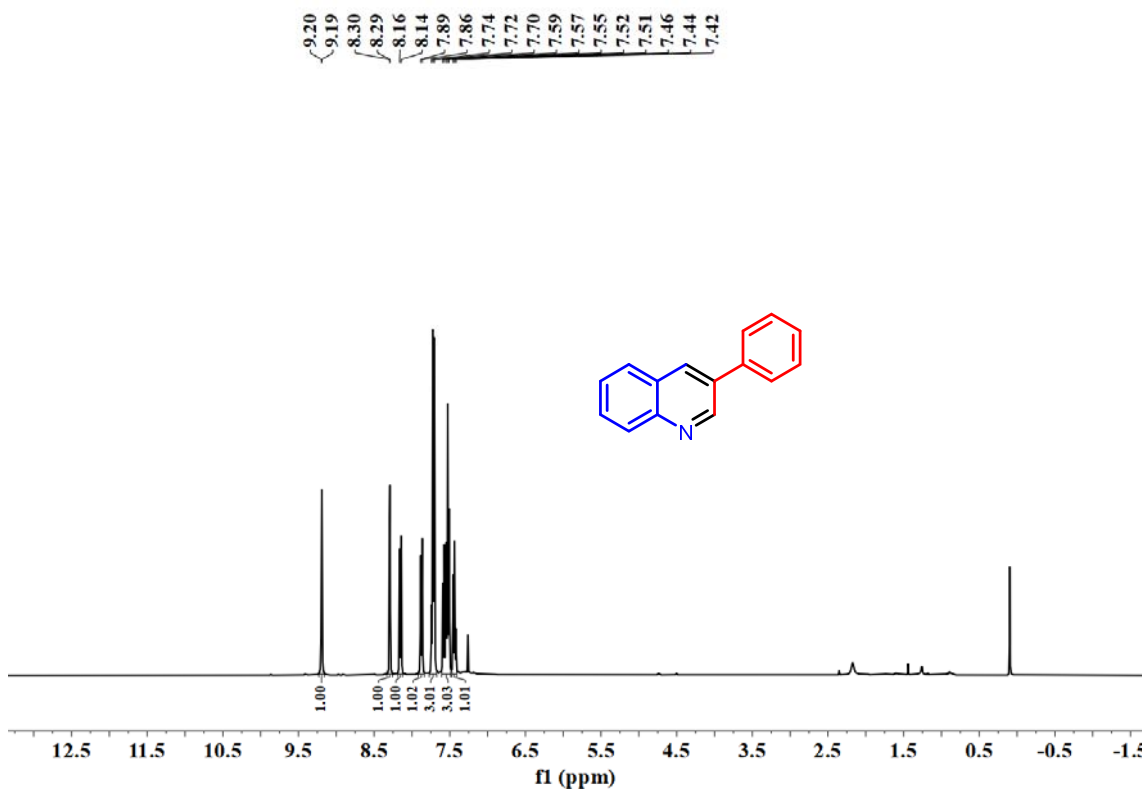


Fig. S133 ^1H NMR spectrum of **51** in CDCl_3 (400 MHz).

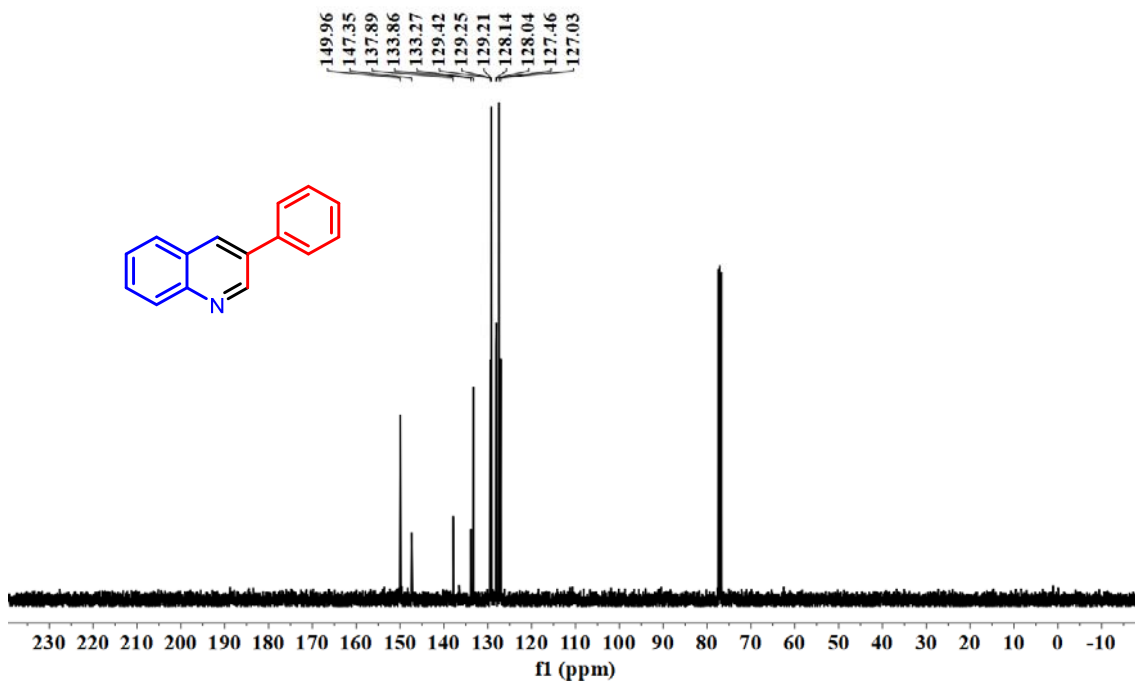


Fig. S134 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **51** in CDCl_3 (101 MHz).

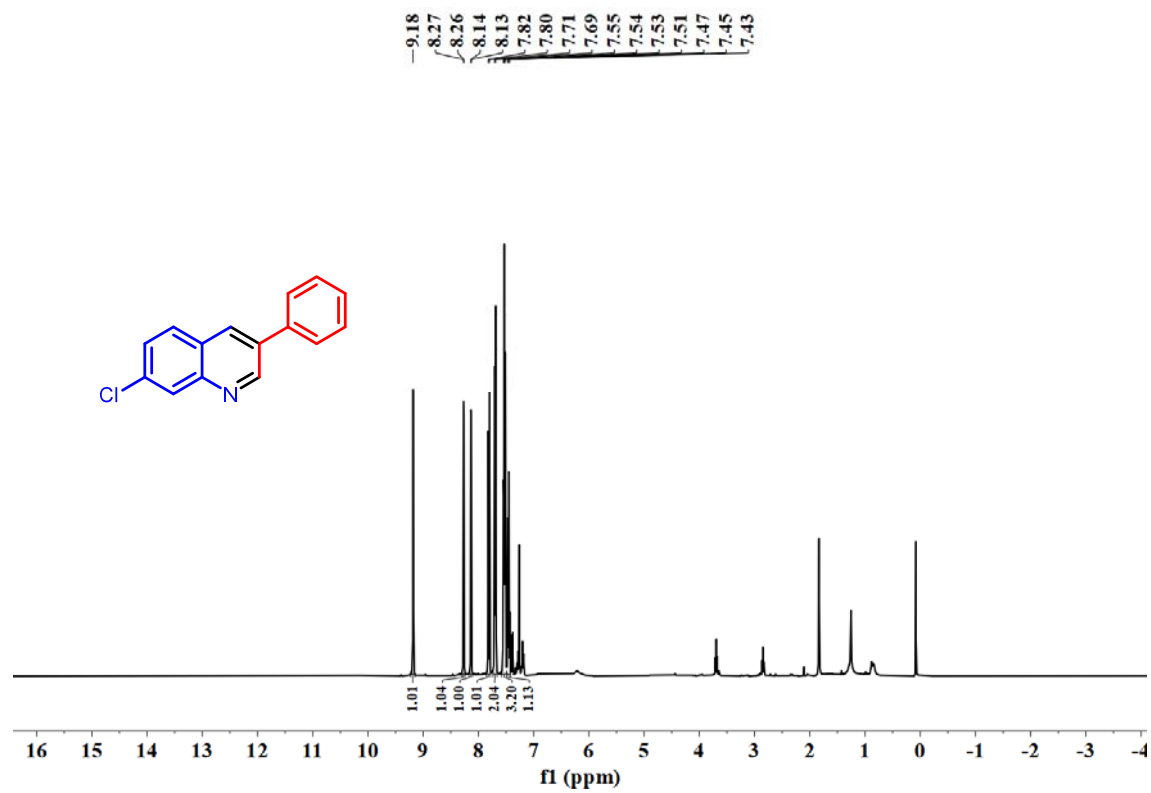


Fig. S135 ^1H NMR spectrum of **52** in CDCl_3 (400 MHz).

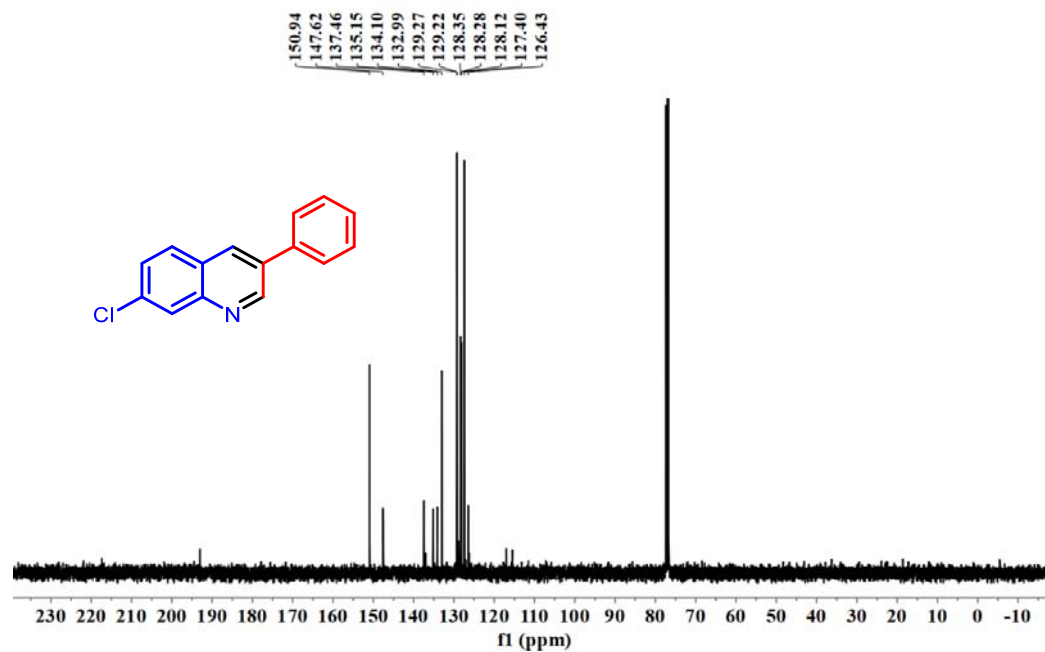


Fig. S136 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **52** in CDCl_3 (101 MHz).

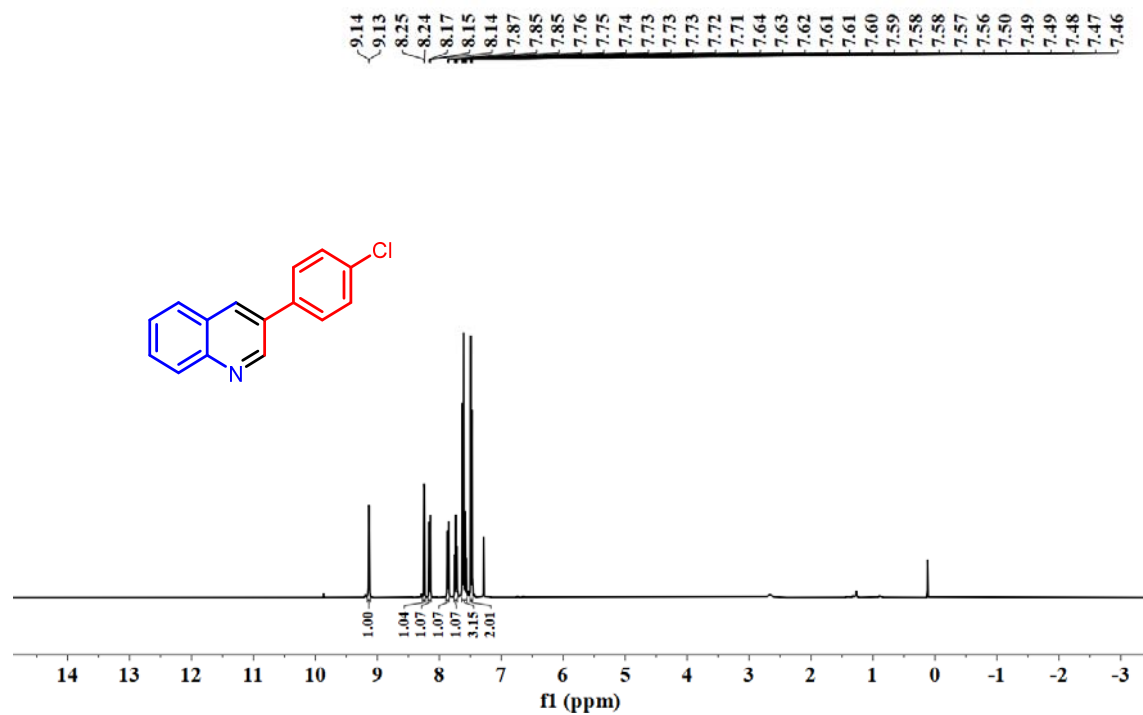


Fig. S137 ¹H NMR spectrum of **53** in CDCl₃ (400 MHz).

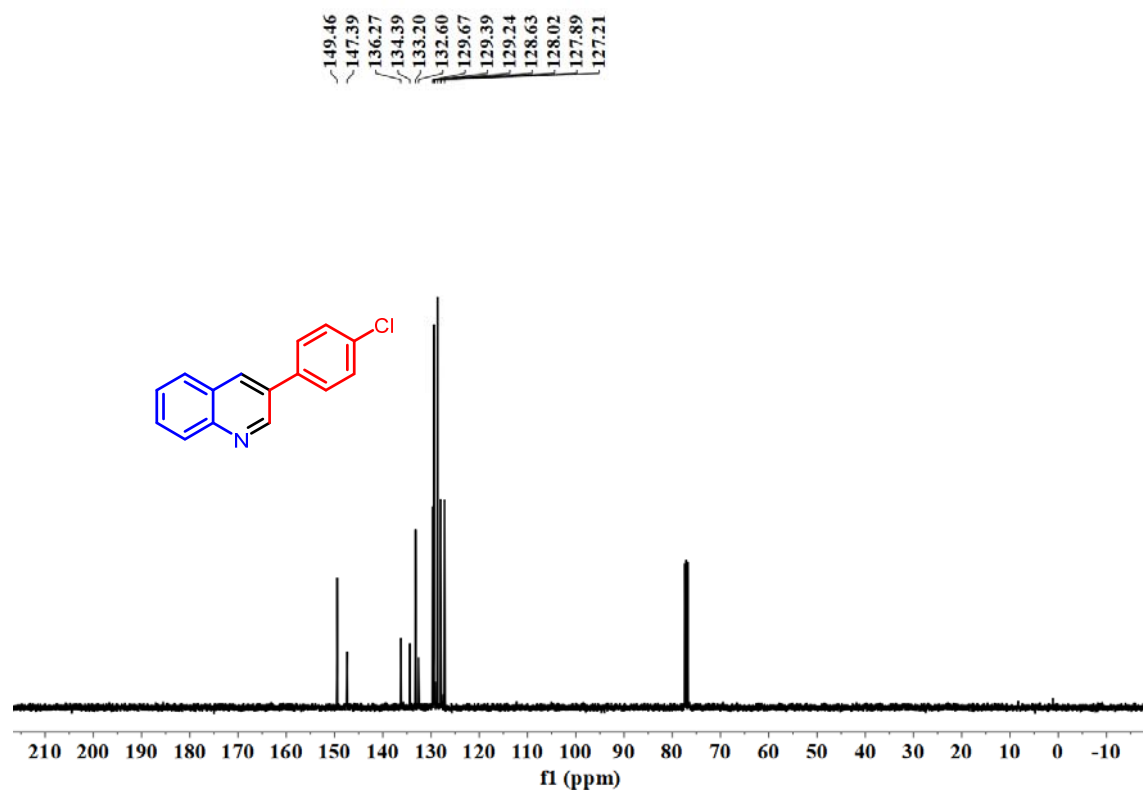


Fig. S138 ¹³C{¹H} NMR spectrum of **53** in CDCl₃ (101 MHz).

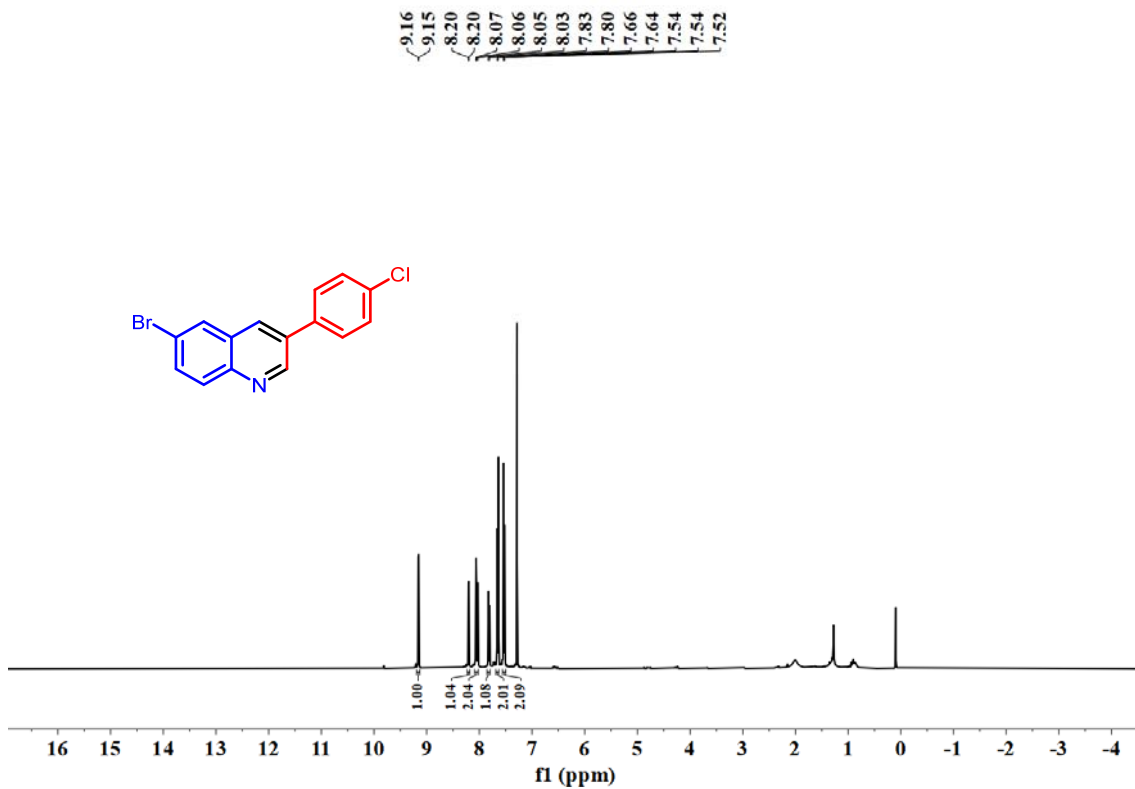


Fig. S139 ¹H NMR spectrum of **54** in CDCl₃ (400 MHz).

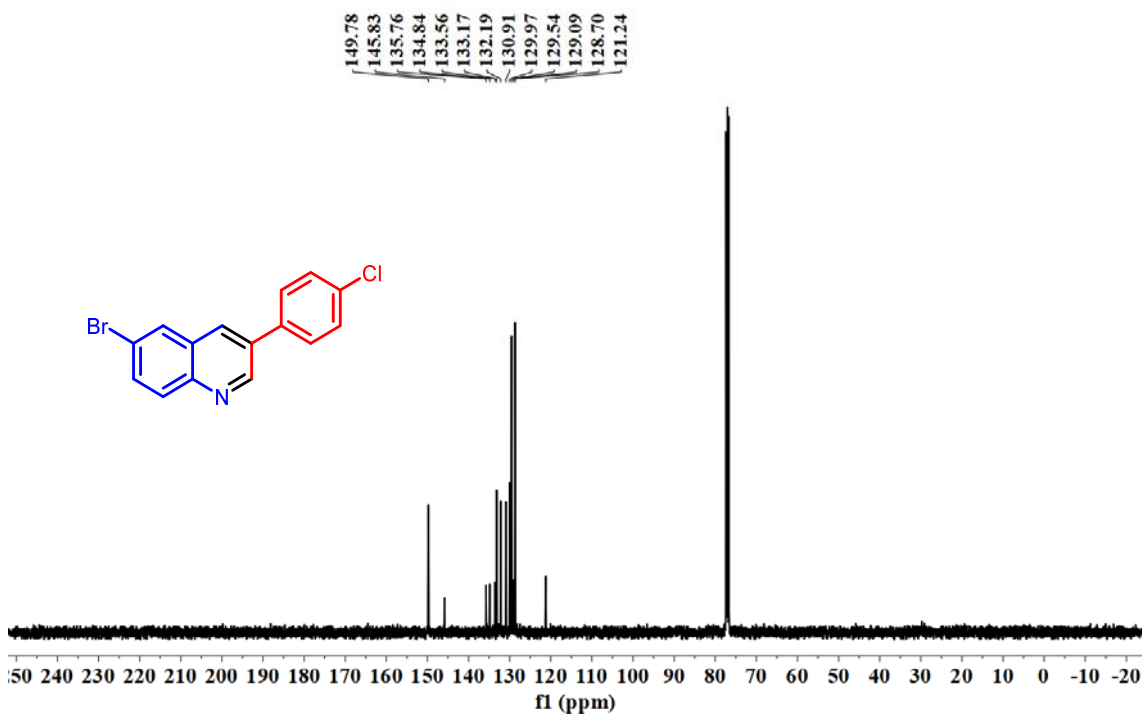


Fig. S140 ¹³C{¹H} NMR spectrum of **54** in CDCl₃ (101 MHz).

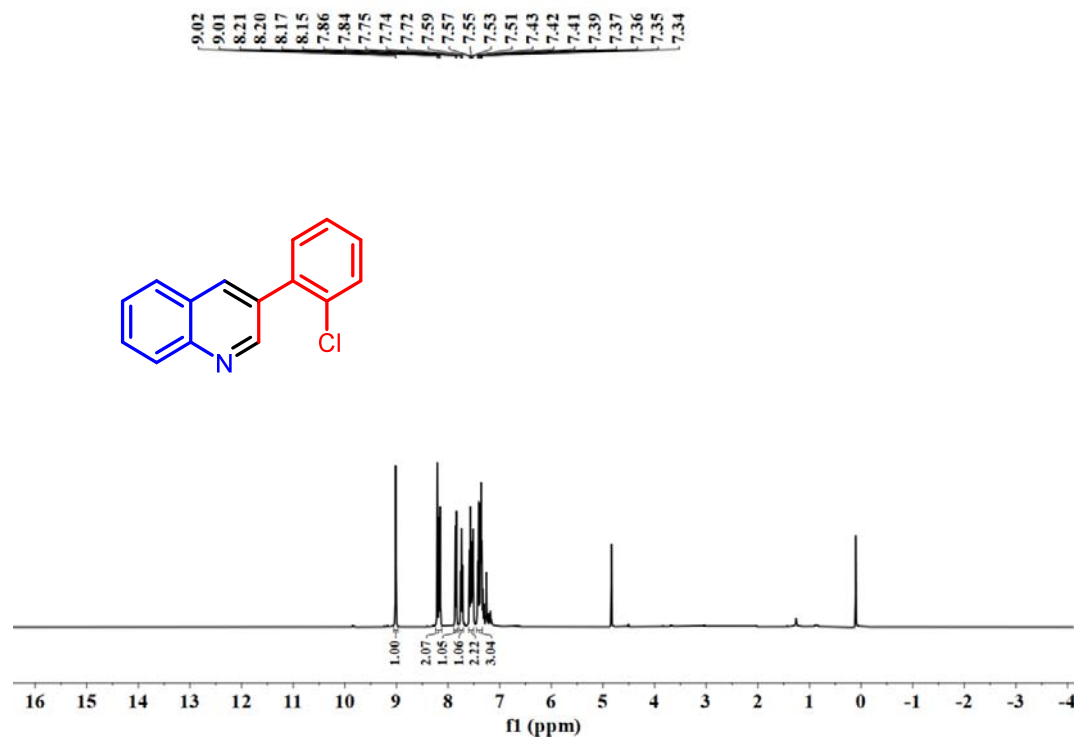


Fig. S141 ¹H NMR spectrum of **55** in CDCl₃ (400 MHz).

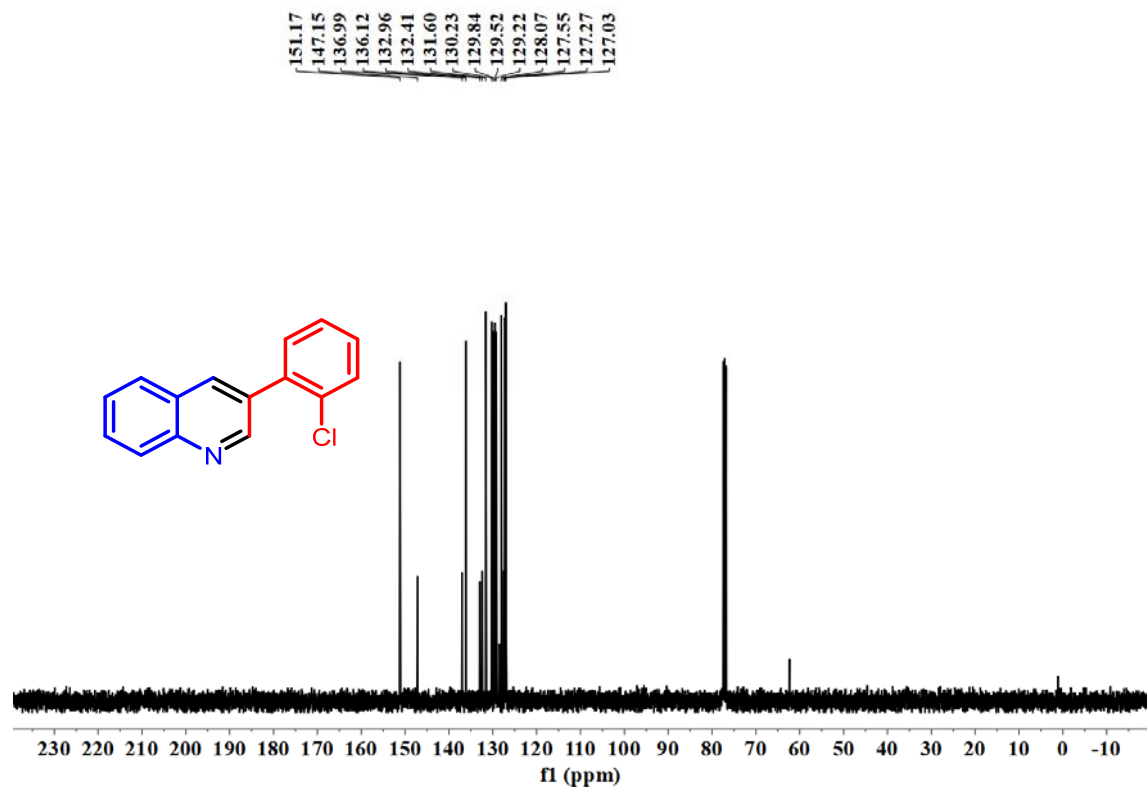


Fig. S142 ¹³C{¹H} NMR spectrum of **55** in CDCl₃ (101 MHz).

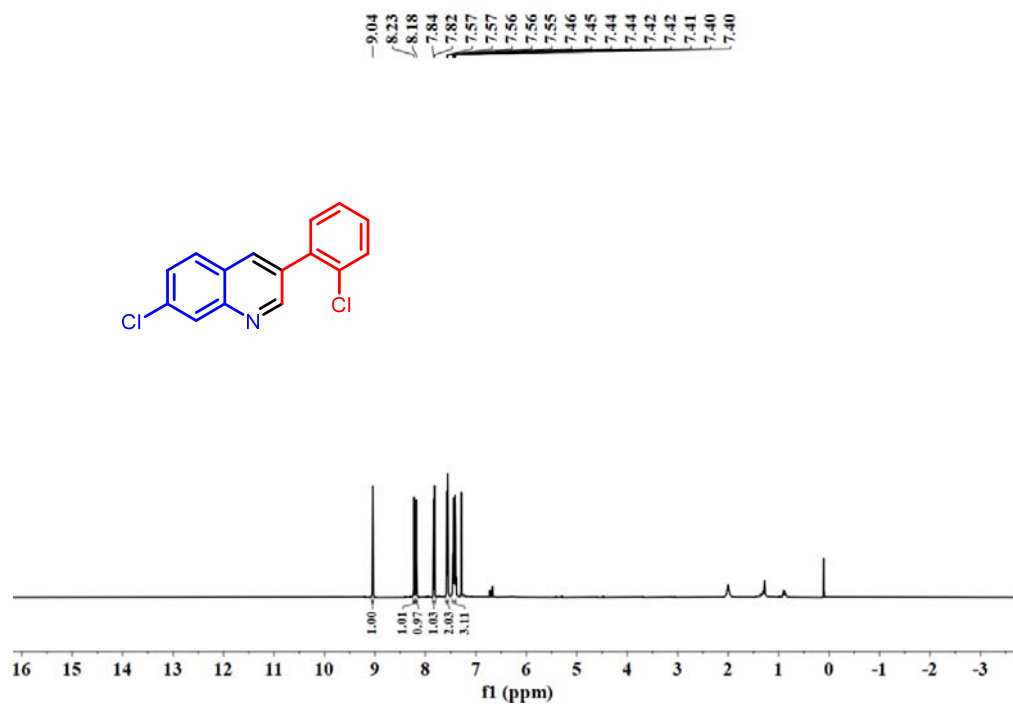


Fig. S143 ¹H NMR spectrum of **56** in CDCl₃ (400 MHz).

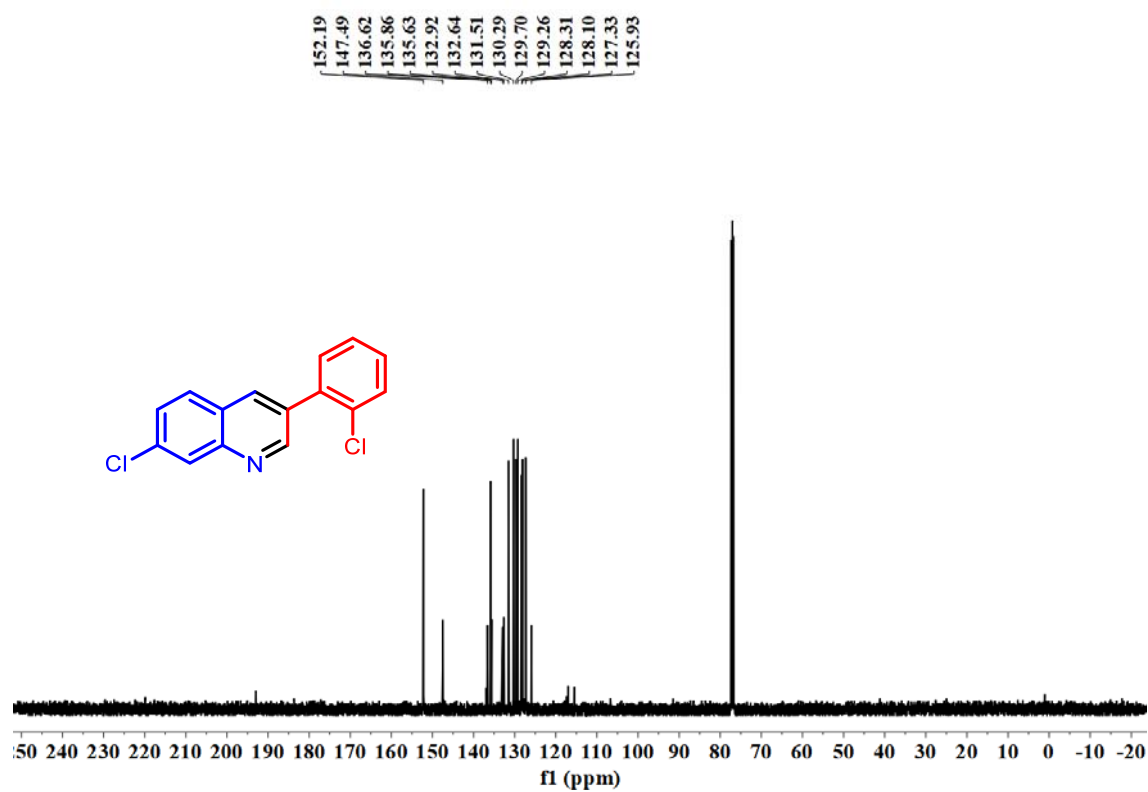


Fig. S144 ¹³C{¹H} NMR spectrum of **56** in CDCl₃ (101 MHz).

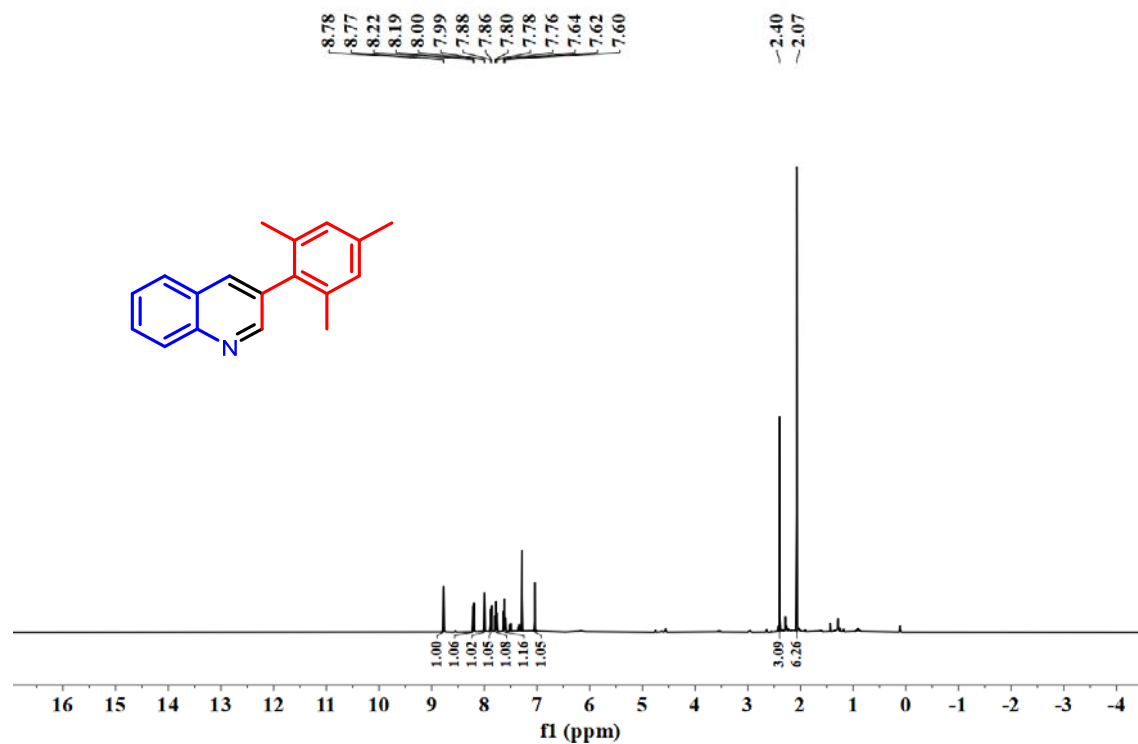


Fig. S145 ^1H NMR spectrum of **57** in CDCl_3 (400 MHz).

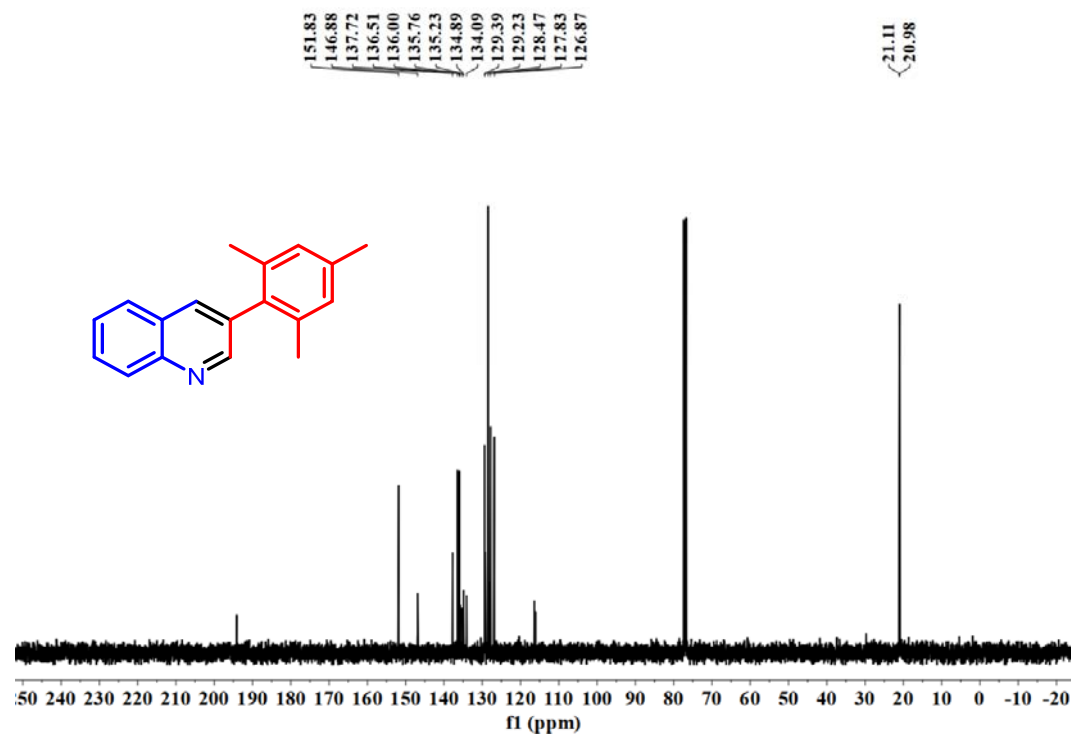
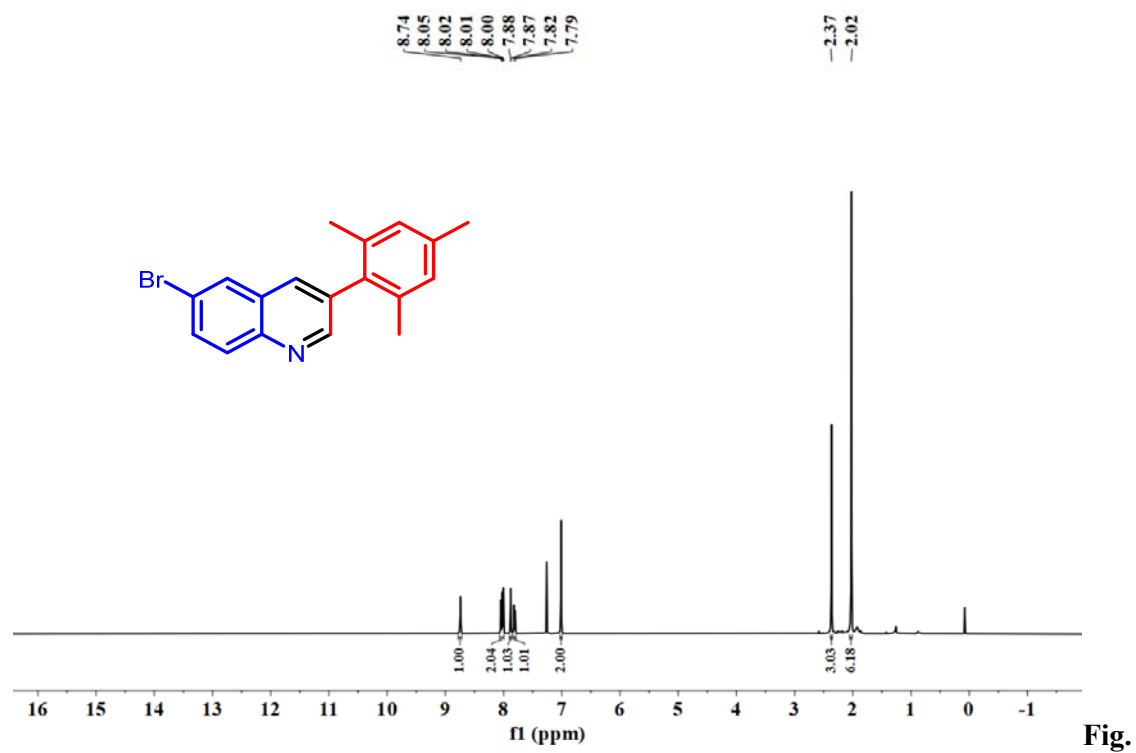


Fig. S146 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **57** in CDCl_3 (101 MHz).



S147 ^1H NMR spectrum of **58** in CDCl_3 (400 MHz).

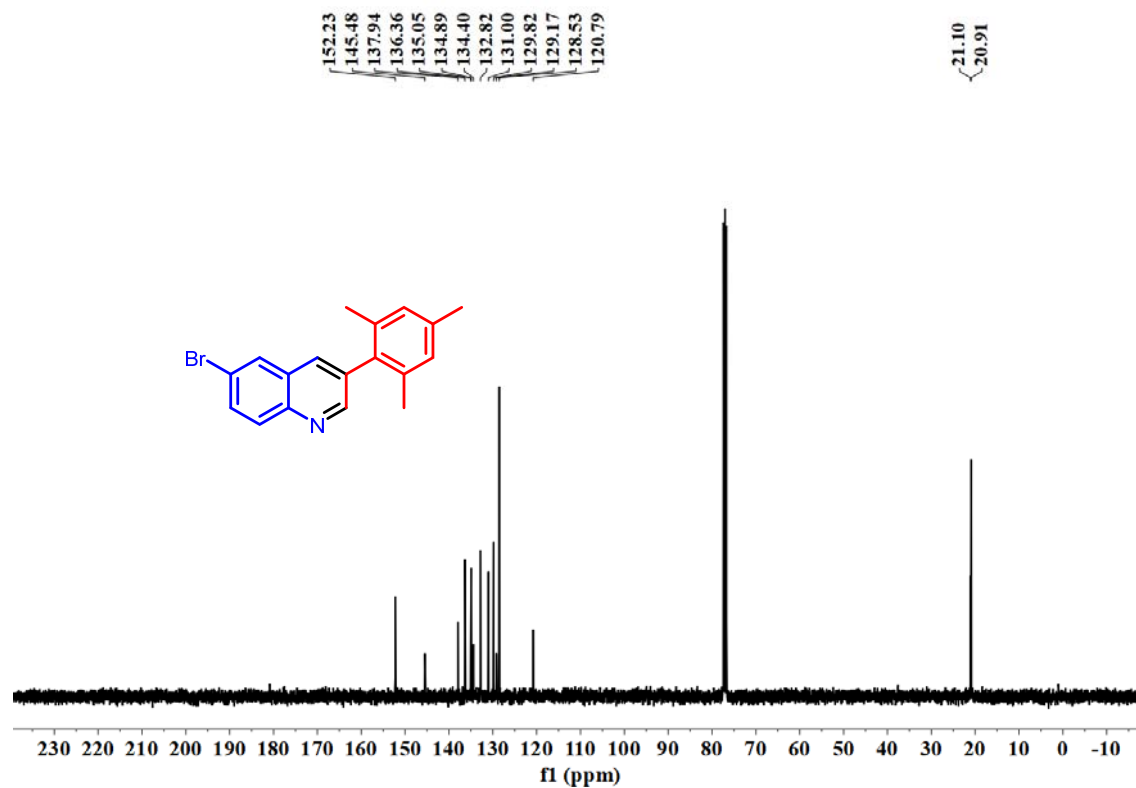


Fig. S148 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **58** in CDCl_3 (101 MHz).

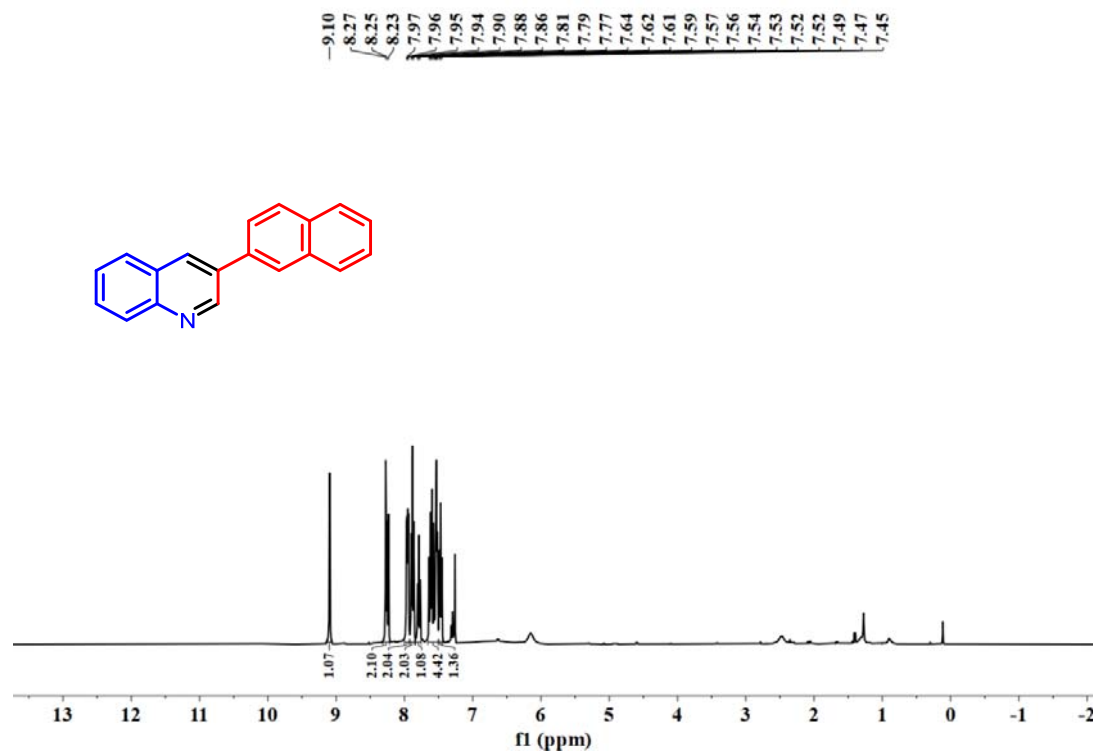


Fig. S149 ¹H NMR spectrum of **59** in CDCl₃ (400 MHz).

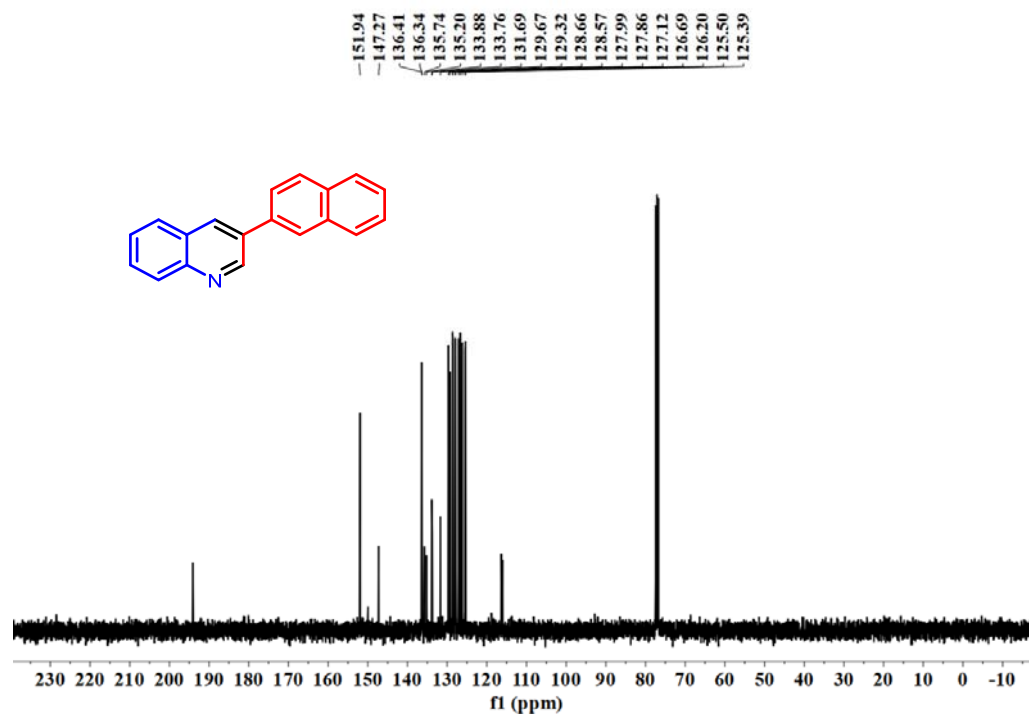


Fig. S150 ¹³C{¹H} NMR spectrum of **59** in CDCl₃ (101 MHz).

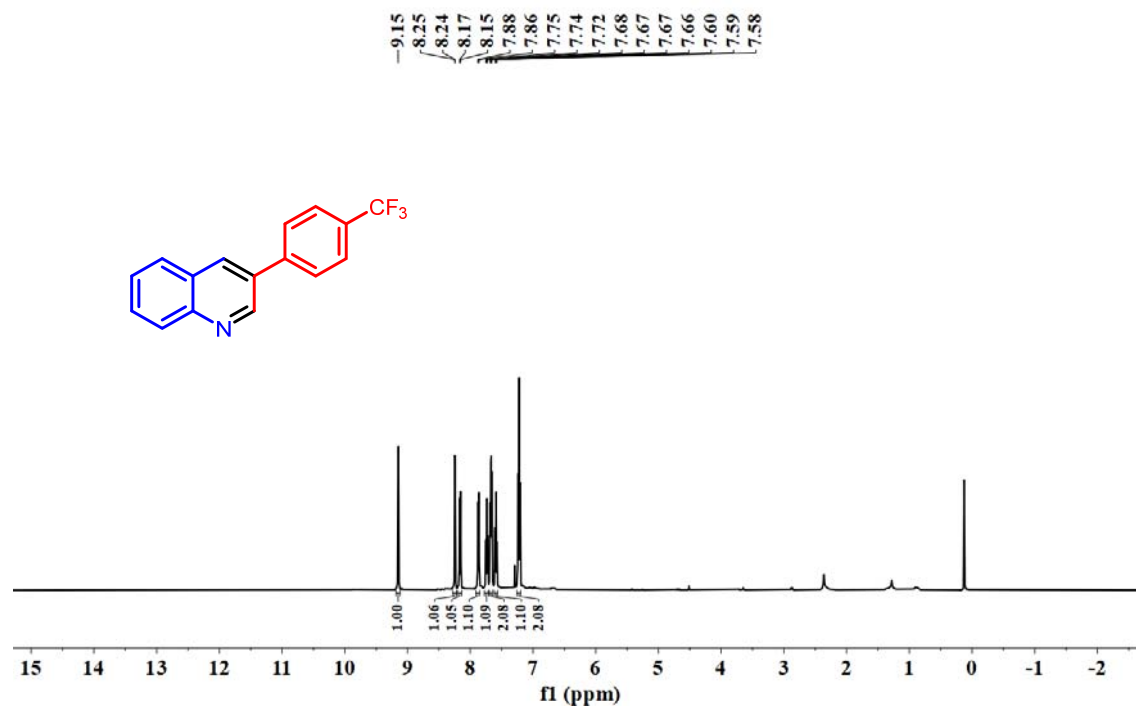


Fig. S151 ¹H NMR spectrum of **60** in CDCl₃ (400 MHz).

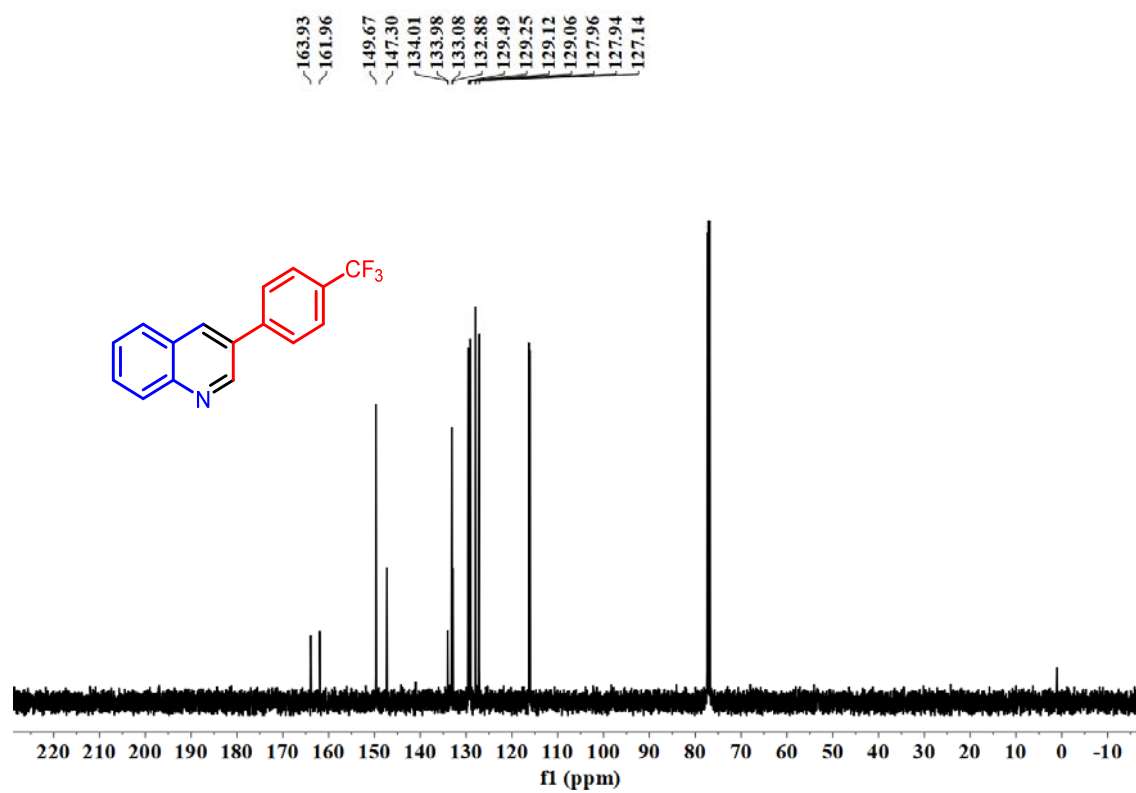


Fig. S152 ¹³C{¹H} NMR spectrum of **60** in CDCl₃ (101 MHz).

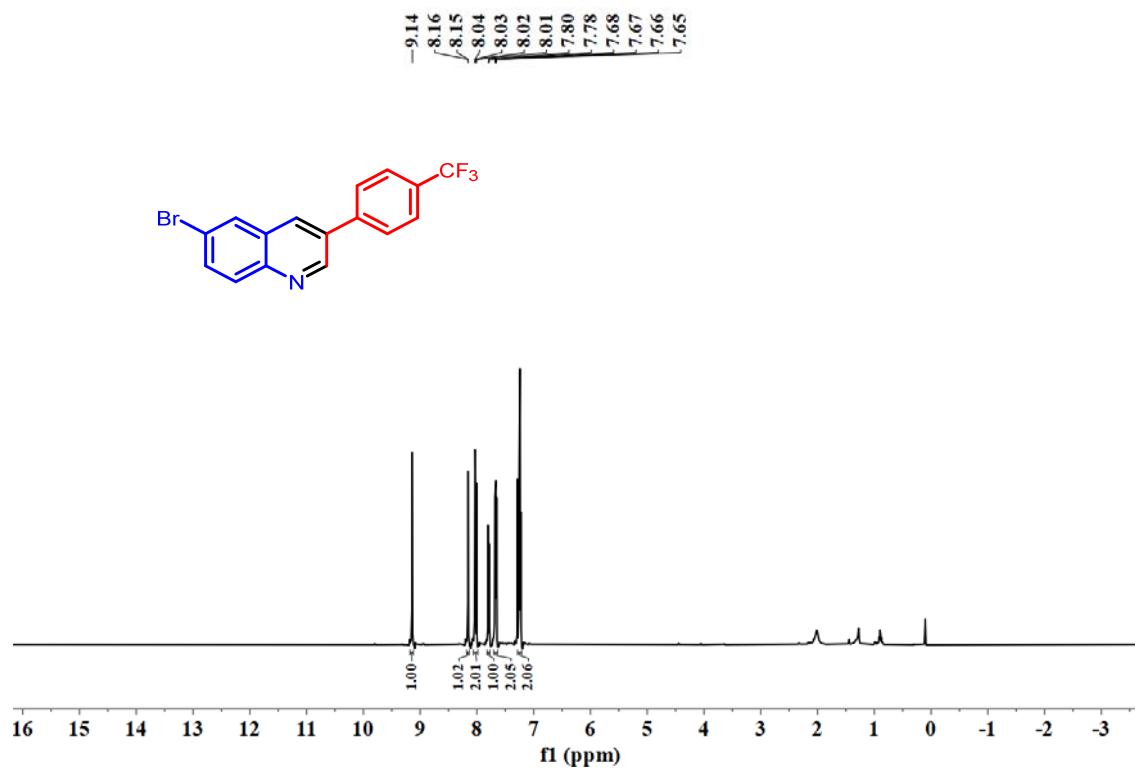


Fig. S153 ¹H NMR spectrum of **61** in CDCl₃ (400 MHz).

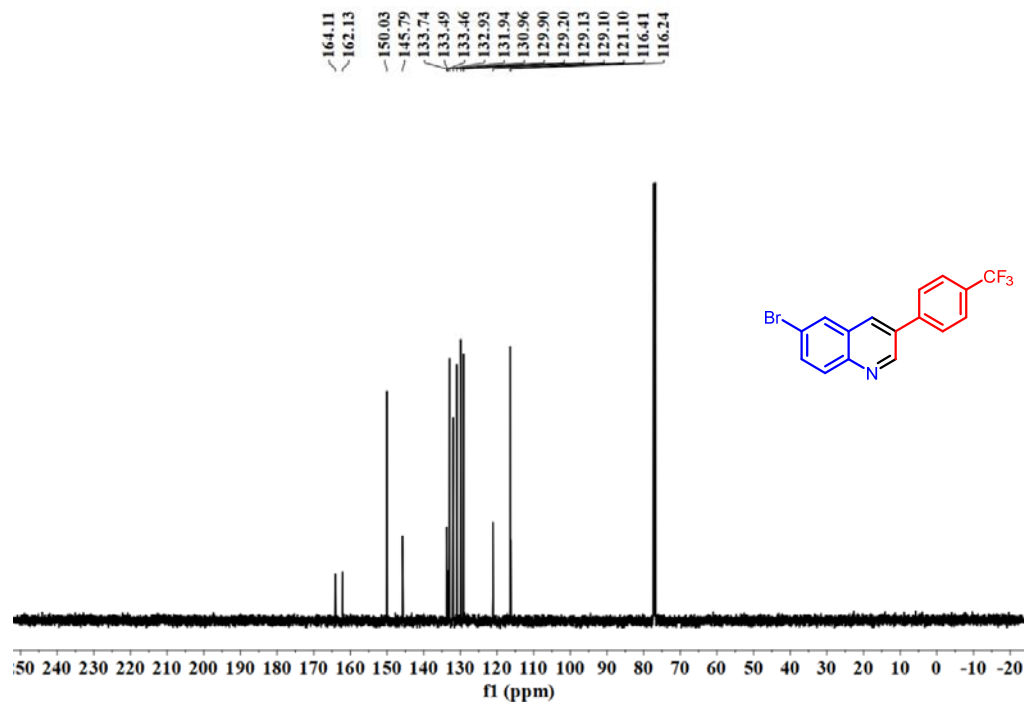
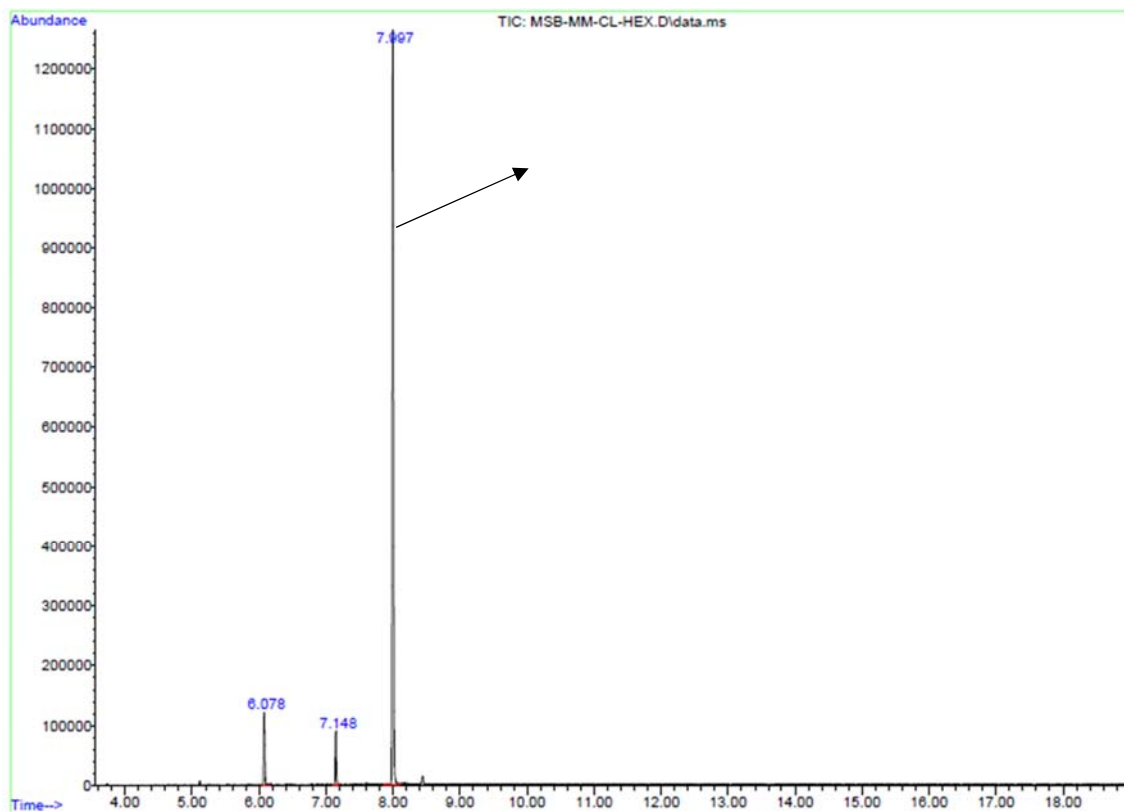


Fig. S154 ¹³C {¹H} NMR spectrum of **61** in CDCl₃ (101 MHz).



Area Percent Report

Data Path : D:\GCMS DATA\2024\MAR2024\
 Data File : MSB-MM-CL-HEX.D
 Acq On : 07 Mar 2024 12:46
 Operator : HA
 Sample : MSB-MM-CL-HEX
 Misc :
 ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
 Integrator: ChemStation

Method : D:\SRK\CF_29SEP2023.M
 Title :

Signal : TIC: MSB-MM-CL-HEX.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.078	439	444	458	BV	119016	1330705	9.39%	8.063%
2	7.148	623	631	639	BV	88994	997655	7.04%	6.045%
3	7.997	756	779	797	BV	1182811	14175591	100.00%	85.892%

Fig. S155 GC-MS spectra of compound 62.

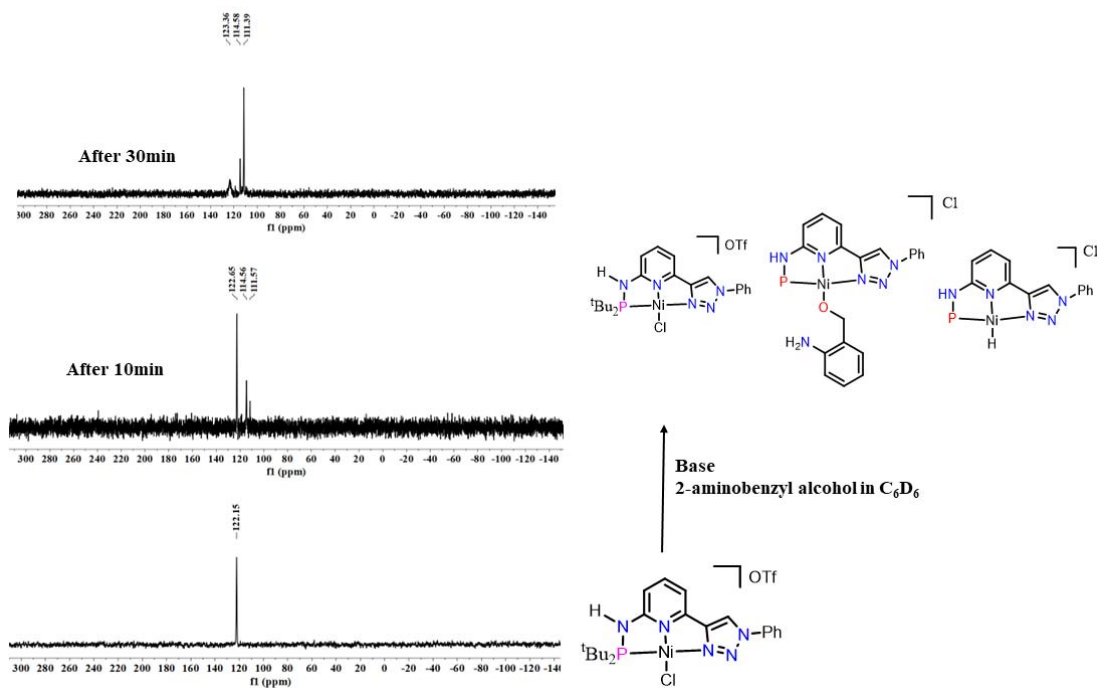


Fig. S156 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of reaction mixture at variable time in C_6D_6 (101 MHz).

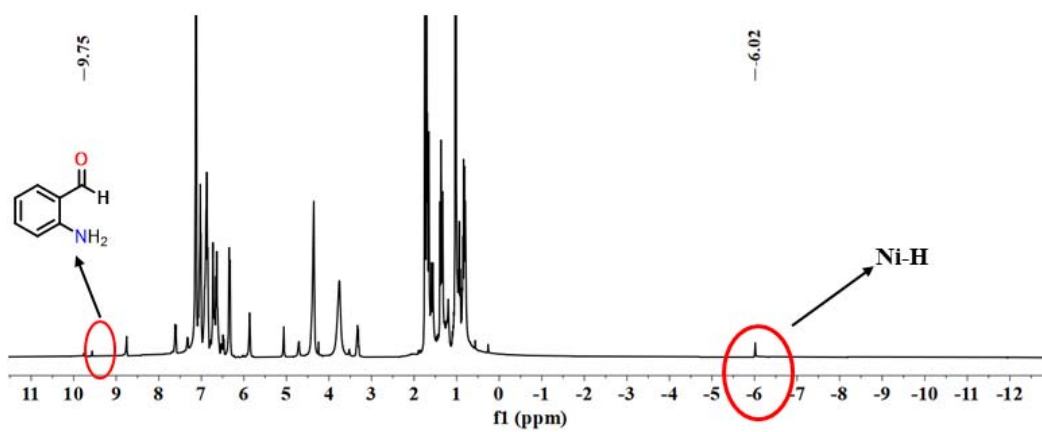


Fig. S157 ^1H NMR spectrum of reaction mixture in C_6D_6 (400 MHz).

References:

1. Z. Li, C. Brouwer and C. He, *Chem. Rev.*, 2008, **108**, 3239-3265.
2. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.
3. G. Sheldrick, *Acta Crystallographica Section A*, 2015, **71**, 3-8.