A General and Practical Bifunctional Cobalt Catalytic System for *N*-Heterocycle Assembly via Acceptorless Dehydrogenation

(Supporting Information)

Haitao Tian,[a] Wenxuan Xue,[a] Jingtao Wu,[a] Ziguang Yang,[b] Hongcheng Lu,[a] and Conghui Tang*[,a,c]

[a] Key Laboratory of Material Chemistry for Energy Conversion and Storage, Ministry of Education, Hubei Key Laboratory of Material Chemistry and Service Failure, School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, 1037 Luoyu Road, Wuhan 430074, China.

[b] Department of Chemistry and Biochemistry, University of California, Santa Barbara, California 93106, USA.

[c] State Key Laboratory of Natural and Biomimetic Drugs, Peking University, Beijing 100191, China.

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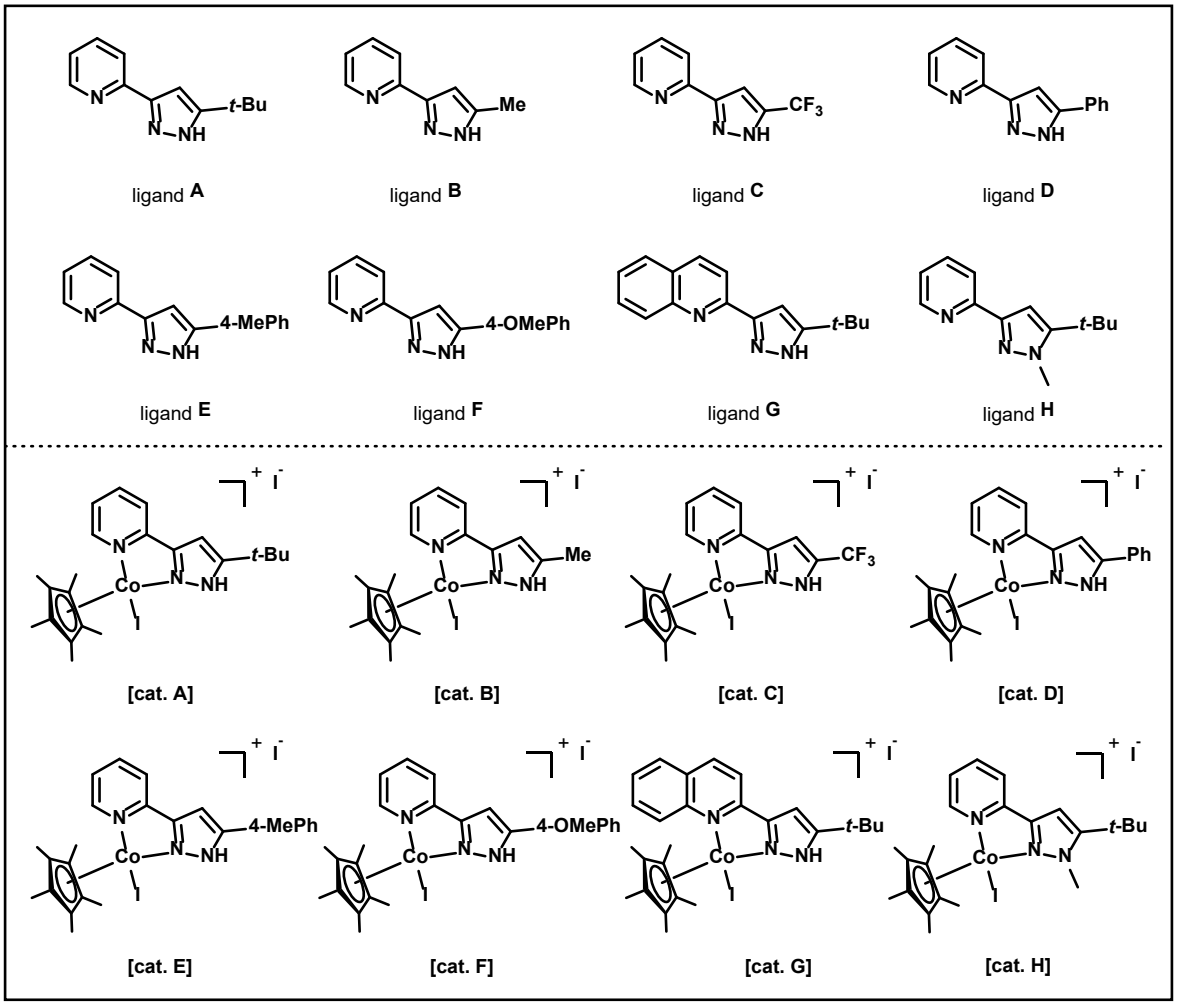
1. General Information

Unless otherwise noted, all reagents were obtained from commercial suppliers (Sigma-Aldrich, Alfa Aesar, TCI, Adamas-beta, Energy Chemical, and Bidepharm) and used as received. All manipulations were conducted with a standard Schlenk technique under argon atmosphere (1 atm). Dry toluene and xylene were distilled over calcium hydride. The reactions were monitored by thin-layer chromatography (TLC) and visualized using a UV lamp (365 or 254 nm). Upon completion, the products were isolated by flash column chromatography on a silica gel (236–400 mesh) column using petroleum ether (PE) and ethyl acetate (EA). ^{1}H-NMR spectra were recorded with a Bruker AVIII-400 spectrometer, chemical shifts (in ppm) were referenced to residual $CDCl_3$ solvent peak (δ (ppm) = 7.26 ppm). ^{13}C-NMR spectra were obtained by the same NMR spectrometer and were calibrated with $CDCl_3$ (δ (ppm) = 77.16 ppm). All NMR spectra were recorded at ambient temperature (293 K) unless otherwise noted. Mass spectra were recorded by PE SCLEX QSTAR spectrometer. Infrared spectra were measured with potassium bromide as background on a Perkin-Elmer spectrum BX FT-IR spectrometer. Peaks are reported in cm^{-1} with indicated relative intensities: s (strong, 0–33% T); m (medium, 34–66% T), w (weak, 67–100% T). Melting points were measured on a X-4 micro melting point apparatus.

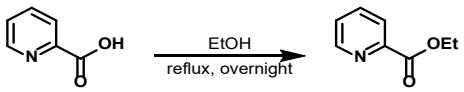
2. General Procedures for the Synthesis of Catalysts

2.1 Structures of Ligands and Cobalt Catalysts



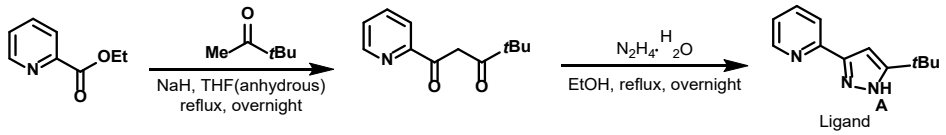
Scheme S1. Structures of ligands and cobalt catalysts.

2.2 General Procedures for the Synthesis of Ligand A



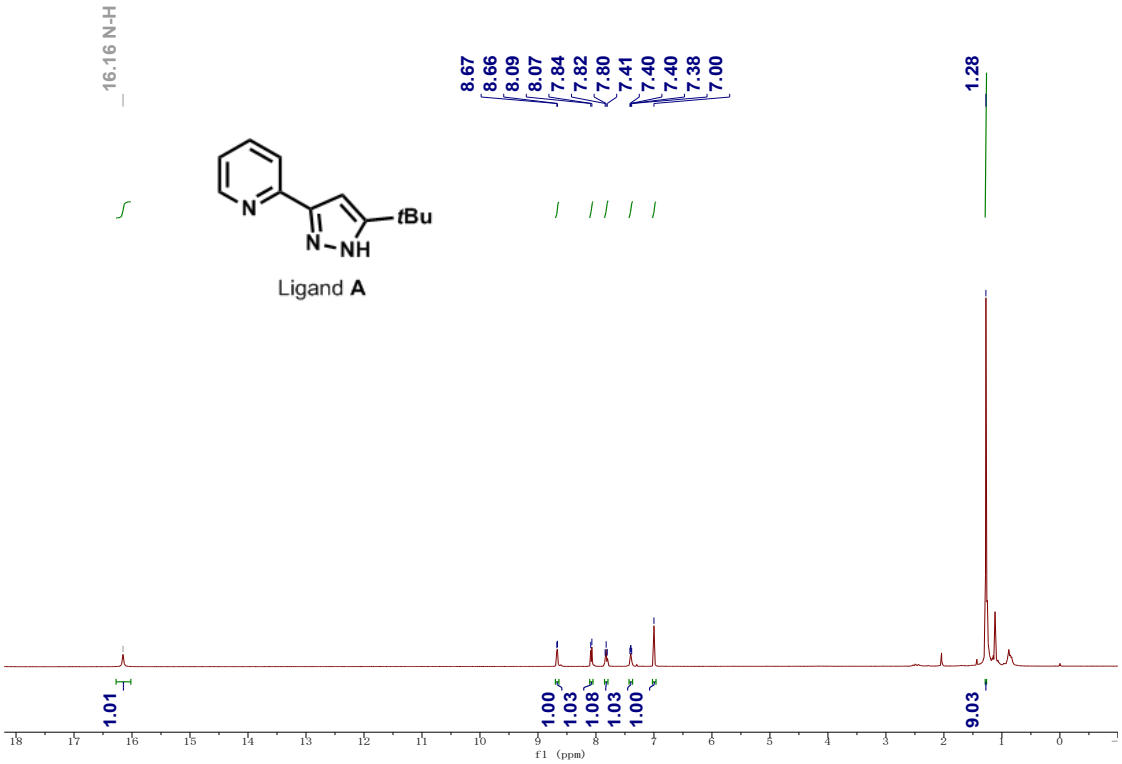
Synthesis of ethyl 2-picolinate: To a 250 mL round bottom flask was added with picolinic acid (1.23 g, 1.0 equiv., 10.0 mmol), and dissolved by 80.0 mL anhydrous ethanol. Sulfuric acid (1.0 mL) was added to the reaction mixture and the whole solution was heated to reflux overnight. The reaction was then cooled to room temperature and the solvent was removed in vacuo. Then the residue was diluted with DCM and washed with saturated sodium carbonate (2 × 30.0 mL) until pH > 8.0, the aqueous phase was washed with DCM (3 × 30.0 mL) and the organic phases were combined and washed with brine (1 ×

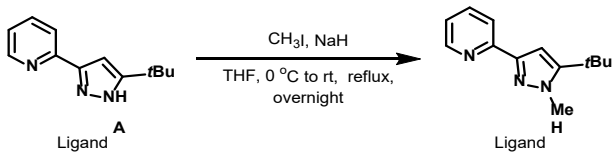
50.0 mL), the organic phase was then dried over magnesium sulfate and the solvent was removed in vacuo. The crude product was further purified with flash column chromatography (PE:EA = 2:1) to obtain the product ethyl 2-picolinate as a colorless oil with 86% yield.



Synthesis of ligand A: Pinacolone (0.841 g, 1.2 equiv., 8.4 mmol) was dissolved in anhydrous THF (20.0 mL) in a 100 mL round bottom flask under ice bath (0 °C). Then 60% NaH in mineral oil (420 mg, 1.5 equiv., 10.5 mmol) was gradually added into the reaction mixture. The reaction mixture was stirred at 0 °C for 30 minutes, then ethyl 2-picolinate (1.06 g, 1.0 equiv., 7.0 mmol) was added dropwise. The reaction was heated to reflux for 24 hours and then cooled down to room temperature and washed with saturated citric acid (1 × 30.0 mL) and brine (1 × 30.0 mL), the organic phase was then dried over magnesium sulfate and the solvent was removed in vacuo. Then the crude product was used for the next step without purification. In a 100 mL round bottom flask, 4,4-dimethyl-1-(pyridin-2-yl)pentane-1,3-dione (1.03 g, 1.0 equiv., 5 mmol) was dissolved in 20.0 mL ethanol. Then hydrazine monohydrate (85 wt%) (0.44 g, 1.5 equiv., 7.5 mmol) was dissolved in 5.0 mL ethanol and added into the reaction mixture dropwise. The reaction mixture was heated to reflux and maintained for 12 hours. Then the reaction mixture was cooled down to room temperature and the solvent was removed in vacuo. The crude product was further purified with flash column chromatography (PE:EA = 1:1) to obtain the final product 2-(5-tert-butyl-1H-pyrazol-3-yl)pyridine (ligand **A**) as a pale yellow viscous liquid with 64% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 16.16 (s, 1H), 8.67 (d, *J* = 4.0 Hz, 1H), 8.08 (d, *J* = 7.9 Hz, 1H), 7.82 (t, *J* = 7.3 Hz, 1H), 7.43 – 7.37 (m, 1H), 7.00 (s, 1H), 1.28 (s, 9H). Ligands **B**-**G** were synthesized using the same procedure with corresponding 1,3-dione compounds as the starting materials.

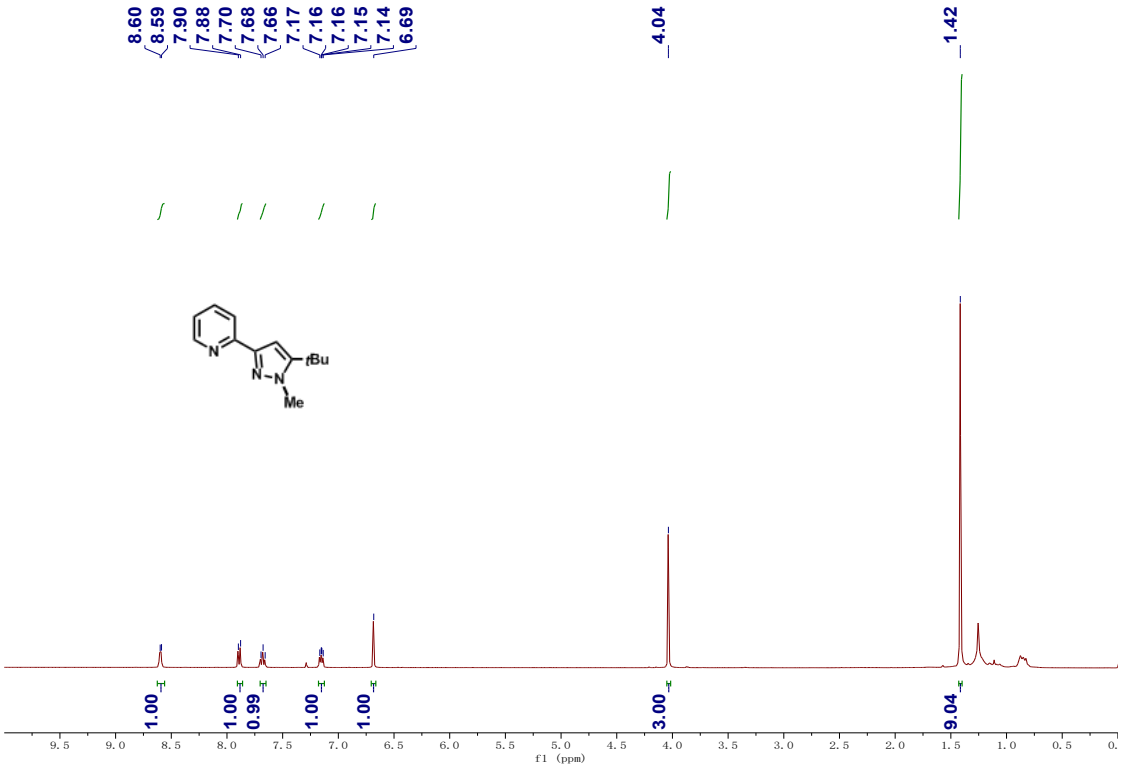
^{1}H NMR spectra of ligand **A** (400 MHz, $CDCl_3$):



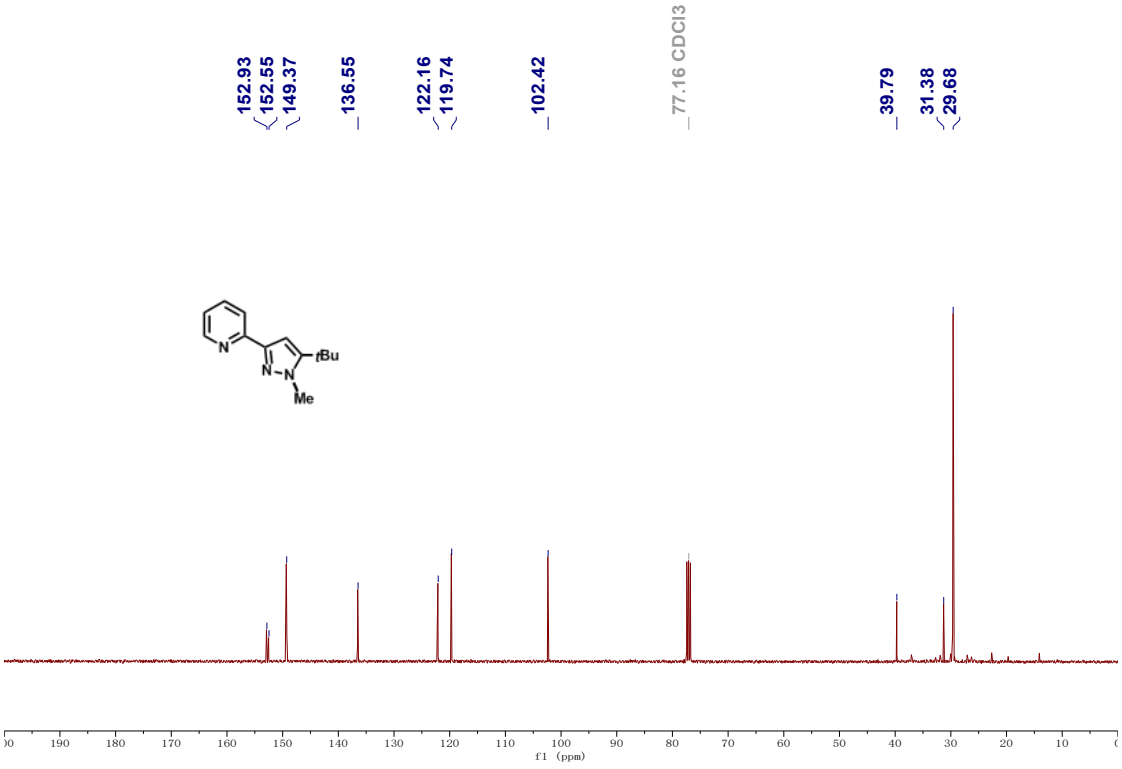


Synthesis of ligand H: To the suspension of NaH (60% wt% in mineral oil, 0.17 g, 0.004 mol) in 15 mL dry THF, ligand **A** (0.41 g, 0.002 mol) was added. To this mixture a THF (10 mL) solution of methyl iodide (156 µL, 0.002 mmol) was added dropwise at 0 °C, and the mixture was warmed slowly to room temperature with stirring. The solution was then refluxed for 6 h and on completion of the reaction, the mixture was cooled to room temperature and was evaporated to dryness. The residue was then purified by alumina column chromatography using 40% ethyl acetate/petroleum ether as eluent to obtain desired compound as light yellow oil. Yield: 0.405 g (92%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.60 (d, J = 4.8 Hz, 1H), 7.89 (d, J = 7.9 Hz, 1H), 7.68 (t, J = 7.4 Hz, 1H), 7.18 – 7.13 (m, 1H), 6.69 (s, 1H), 4.04 (s, 3H), 1.42 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.9, 152.6, 149.4, 136.6, 122.2, 119.7, 102.4, 39.8, 31.4, 29.7.

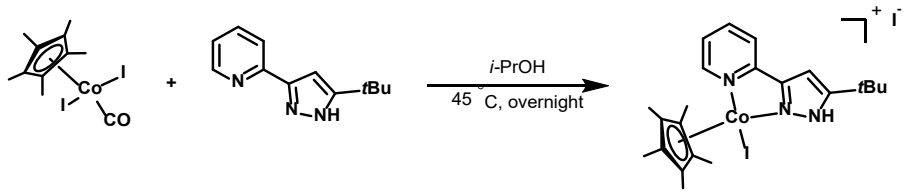
^{1}H NMR spectra of ligand **H** (400 MHz, $CDCl_3$):



^{13}C NMR spectra of ligand **H** (400 MHz, $CDCl_3$):

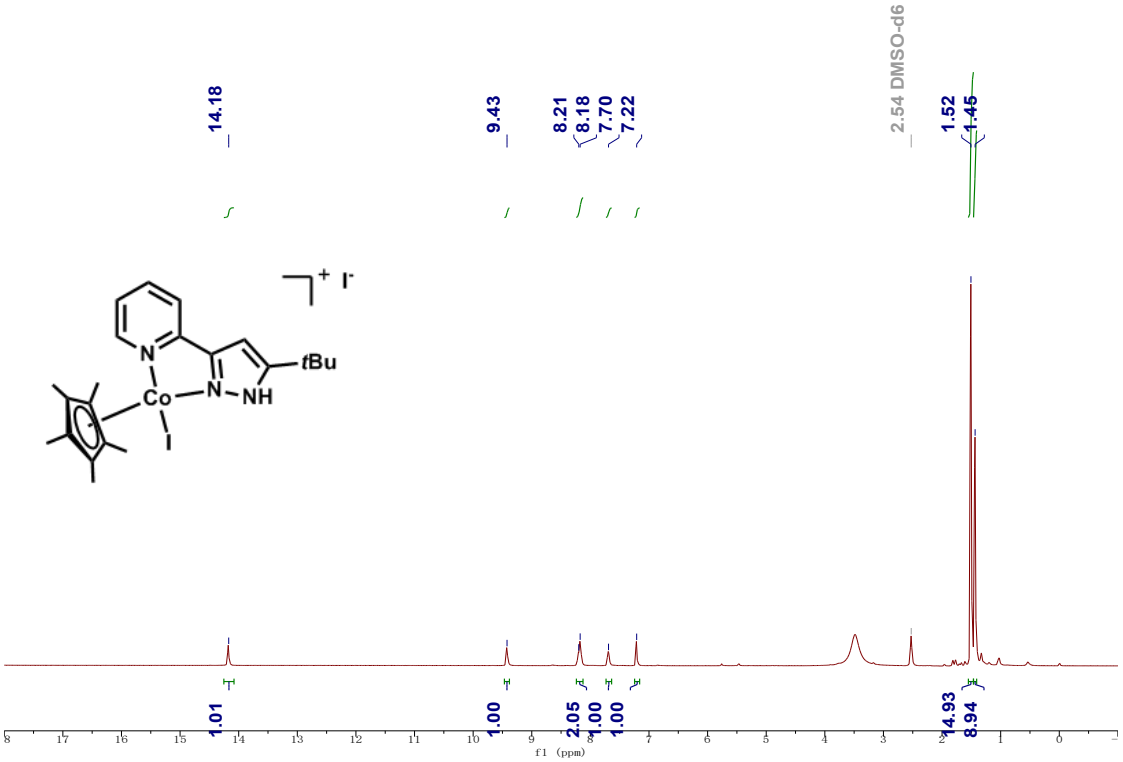


2.3 General Procedures for the Synthesis of Catalyst A

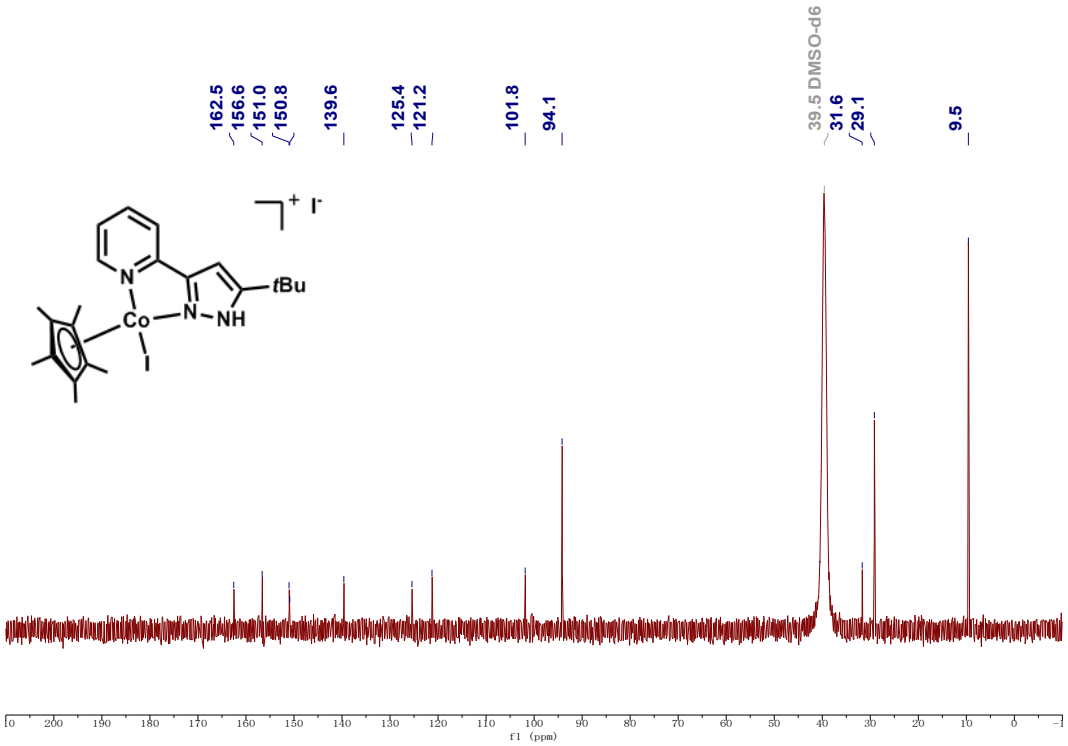


To a 100 mL Schlenk flask was added [$Cp^*Co(CO)I_2$] (1.02 g, 1.0 equiv., 2.22 mmol), and 2-(5-tert-butyl-1H-pyrazol-3-yl)pyridine (492 mg, 1.1 equiv., 2.44 mmol). The system was evacuated and refilled with argon for three times, the solvent isopropanol (20.0 mL) was added via syringe and the reaction was heated under 45 °C for 24 hours. The solvent was removed in vacuo and diethyl ether (30.0 mL) was added to the residue, the catalyst precipitated out as dark green solid and was separated with vacuum filtration. Recrystallization of the crude solid afforded the catalyst **A** as a dark green crystal (85% yield). **^{1}H NMR** (400 MHz, DMSO-d_6) δ (ppm) 14.18 (brs, 1H), 9.43 (s, 1H), 8.25 – 8.13 (m, 2H), 7.70 (s, 1H), 7.22 (s, 1H), 1.52 (s, 15H), 1.45 (s, 9H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ (ppm) 162.5, 156.6, 151.0, 150.8, 139.6, 125.4, 121.2, 101.8, 94.1, 31.6, 29.1, 9.5. Catalysts **B**-**H** were synthesized using the same procedure as above.

^{1}H NMR spectra for cat. **A** (400 MHz, DMSO-d_6):

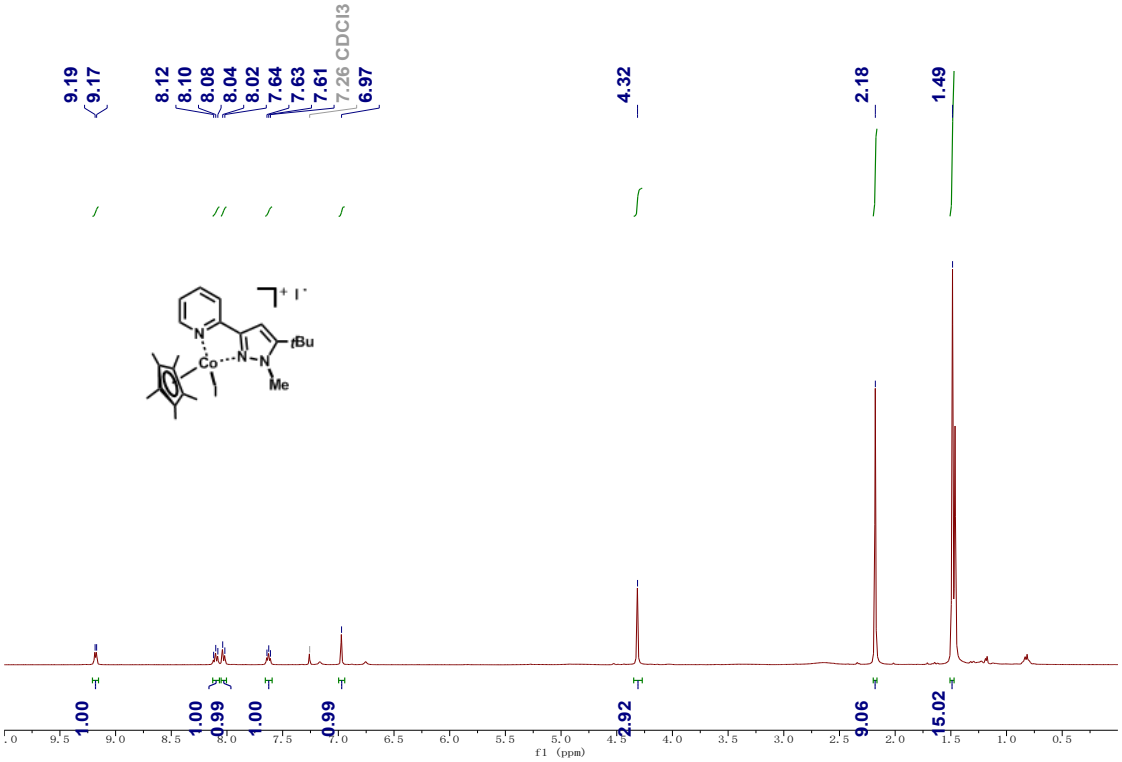


^{13}C NMR spectra for cat. **A** (100 MHz, DMSO-d_6):



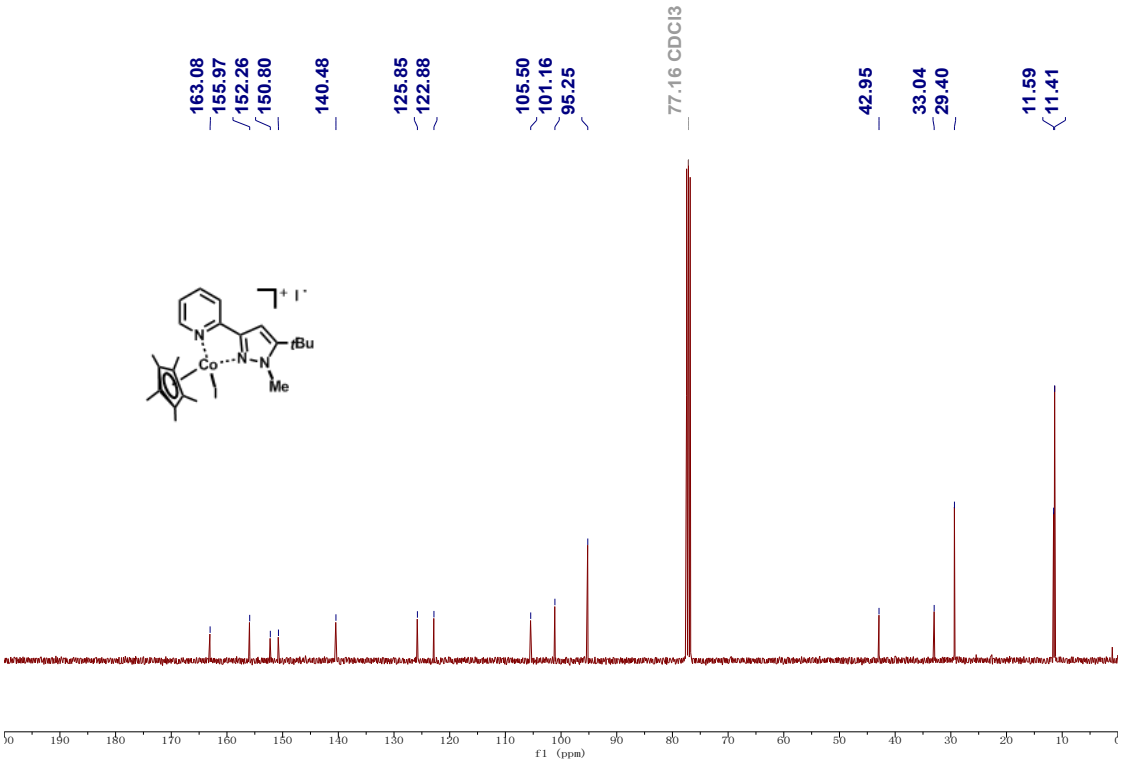
^{1}H NMR spectra for cat. **H** (400 MHz, $CDCl_3$):

^{1}H NMR (400 MHz, CDCl3) δ 9.18 (d, *J* = 5.5 Hz, 1H), 8.10 (t, *J* = 7.6 Hz, 1H), 8.03 (d, *J* = 7.7 Hz, 1H), 7.63 (t, *J* = 6.3 Hz, 1H), 6.97 (s, 1H), 4.32 (s, 3H), 2.18 (s, 9H), 1.49 (s, 15H).



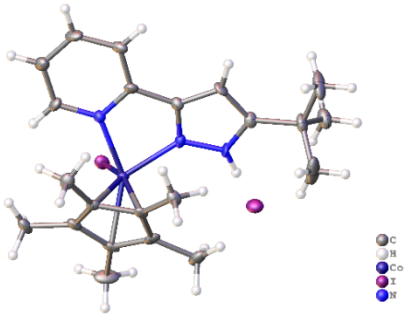
^{13}C NMR spectra for cat. **H** (100 MHz, $CDCl_3$):

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 156.0, 152.3, 150.8, 140.5, 125.9, 122.9, 105.5, 101.2, 95.3, 43.0, 33.0, 29.4, 11.6.



2.4 X–Ray Data Collection and Refinements

Crystallographic data for cat. A



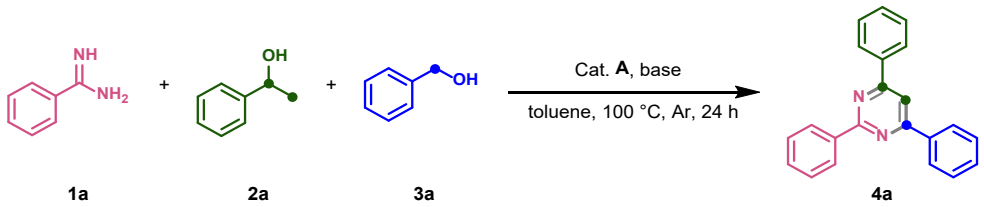
Single crystals of compound **cat. A** were obtained by slow recrystallization from dichloromethane/petroleum ether (4:1) mixtures. A suitable crystal was selected and diffraction data were collected on a Bruker D8 Venture/Photon 100 diffractometer. The crystal was kept at 100.04 K during data collection. The structures were solved and refined with the SHELX suite of programs. All non-hydrogen atoms were refined with anisotropic thermal parameters. The hydrogen atoms of ligands were included into geometrically calcd. positions in the final stages of the refinement and were refined according to 'riding model'. Olex2-1.5 software was used to produce the diagrams.

Identification code	CCDC2124226
Empirical formula	$C_{22}H_{30}CoI_2N_3$
Formula weight	649.22
Temperature/K	100.00
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	13.46140(10)
b/Å	20.18930(2)
c/Å	8.81820(10)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	2396.58(4)
Z	4
ρ_{calc}g/cm^3	1.799
μ/mm^{-1}	25.923
F(000)	1264.0
Crystal size/mm^3	0.2 × 0.12 × 0.05
Radiation	CuKα (λ = 1.54184)

2Θ range for data collection/°	7.894 to 147.756
Index ranges	$-15 \leq h \leq 16$, $-21 \leq k \leq 25$, $-10 \leq l \leq 10$
Reflections collected	24321
Independent reflections	4563 [R_{int} = 0.0641, R_{sigma} = 0.0381]
Data/restraints/parameters	4563/1/262
Goodness-of-fit on F^2	1.081
Final R indexes [I>=2σ (I)]	R_1 = 0.0312, wR_2 = 0.0814
Final R indexes [all data]	R_1 = 0.0318, wR_2 = 0.0816
Largest diff. peak/hole / e $Å^{-3}$	0.82/-1.08
Flack parameter	0.193(9)

3. Additional Optimization of the Reaction Conditions

Table S1. Screening of base[a]

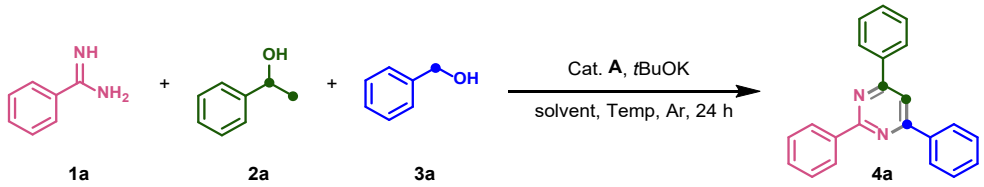


1a **2a** **3a** **4a**

Entry	Base	Yield (%)[b]
1	*t*-BuOK	75
2[c]	*t*-BuOK	26
3[d]	-	trace
4	NaH	13
5	K_2CO_3	9
6	KOH	19
7	Cs_2CO_3	11

[a] Reaction conditions: **1a** (0.2 mmol, 1 equiv), **2a** (1.2 equiv), **3a** (1.2 equiv), cat. **A** (10 mol %), base (0.9 equiv) in toluene (1.5 mL) under Ar, 24 h. [b] Isolated yield. [c] 0.5 equiv *t*BuOK was added. [d] No base was added.

Table S2. Screening of solvent, temperature and time[a]



1a **2a** **3a** **4a**

Entry	Solvent	Yield (%)[b]
1	toluene	75
2	CH_3CN	3
3	1,4-dioxane	16
4	DMSO	15
5	*p*-xylene	49
6[c]	toluene	trace
7[d]	toluene	23
8[e]	toluene	56
9[f]	toluene	trace
10[g]	toluene	45
11[h]	toluene	27
12[i]	toluene	50

[a] Reaction conditions: **1a** (0.1 mmol, 1 equiv), **2a** (1.2 equiv), **3a** (1.2 equiv), cat. **A** (10 mol %), solvent (1.5 mL) under Ar for 24 h. [b] Isolated products. [c] 60 °C. [d] 80 °C. [e] 130 °C. [f] 0.1 mL water was added. [g] Under air. [h] 8 h. [i] 16 h.

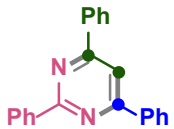
4. General Procedures for the Synthesis of *N*-Heterocycle Compounds

4.1 General procedure A for the synthesis of pyrimidines: Amidine or guanidine (0.2 mmol, 1.0 equiv.), cat. **A** (10 mol%), *t*-BuOK (0.9 equiv.) were placed in a 25 mL Schlenk tube containing a stirring bar, the system was evacuated and refilled with argon for three times. The primary alcohol (1.2 equiv.), secondary alcohol (1.2 equiv.) and anhydrous toluene (1.5 mL) were added. The reaction mixture was stirred at 100 ºC for 24 h. After completion, the reaction was cooled to room temperature and the reaction mixture was diluted with ethyl acetate and passed through celite to give crude product. Then the solvent was removed in vacuo and the crude product was further purified with flash column chromatography to obtain the final product.

4.2 General procedure B for the synthesis of quinoline and indole: 2-Aminobenzyl alcohol (0.2 mmol, 1.0 equiv.), cat. **A** (2.5 mol% from ketone, 10 mol% for secondary alcohol), *t*-BuOK (0.5 equiv. from ketone, 0.9 equiv. for secondary alcohol) were placed in a 25 mL Schlenk tube containing a stirring bar, the system was evacuated and refilled with argon for three times. The ketone (1.2 equiv.) or secondary alcohol (1.2 equiv.) was added along with anhydrous toluene (2.0 mL), the reaction mixture was stirred at 100 ºC for 24 h. After completion, the reaction was cooled to room temperature and the reaction mixture was diluted with ethyl acetate and passed through celite to give crude product. Then the solvent was removed in vacuo and the crude product was further purified with flash column chromatography to obtain the final product. The synthesis of indole from 2-aminophenethanol was carried out using similar conditions to quinoline, with 2-aminophenethanol (1.0 equiv.), cat. **A** (10 mol%), and *t*-BuOK (0.9 equiv.), anhydrous toluene (1.5 mL).

4.3 General procedure C for the synthesis of imidazole and quinoxaline: *o*-Phenylenediamine (0.2 mmol, 1.0 equiv.), cat. **A** (10 mol%), *t*-BuOK (1.0 equiv.) were placed in a 25 mL Schlenk tube containing a stirring bar, the system was evacuated and refilled with argon for three times. The primary alcohol (2.5 equiv., for imidazole) or phenylethylene glycol (2.5 equiv., for quinoxaline) and anhydrous toluene (0.5 mL) were added under argon. The reaction mixture was stirred at 140 ºC for 24 h. After completion, the reaction was cooled to room temperature and the reaction mixture was diluted with ethyl acetate and passed through celite to give crude product. Then the solvent was removed in vacuo and the crude product was further purified with flash column chromatography to obtain the final product.

5. Characterization Data of the Compounds



4a

Synthesis of 2,4,6-triphenylpyrimidine (4a): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (44.3 mg, 75%).

R_f = 0.49 (*n*-hexane:EtOAc = 20:1, UV).

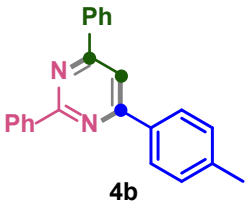
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.80 – 8.73 (m, 2H), 8.37 – 8.25 (m, 4H), 8.02 (s, 1H), 7.58 (m, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.7, 164.5, 138.2, 137.5, 130.8, 130.6, 128.9, 128.5, 128.4, 127.3, 110.3.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{17}N_2$, 309.1; found, 309.1. Spectra data are consistent with the reported literature.[1]

IR: (KBr, cm^{-1}) 1586 (m), 1569 (s), 1526 (s), 1495 (m), 1430 (w), 1365 (s), 1237 (s), 1074 (w), 1028 (w), 859 (m), 834 (w), 775 (m), 748 (s), 708 (m), 688 (s), 632 (m).

m.p.: 187-188 ºC.



4b

Synthesis of 2,4-diphenyl-6-(p-tolyl)pyrimidine (4b): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (55.5 mg, 90%).

R_f = 0.42 (*n*-hexane:EtOAc = 20:1, UV).

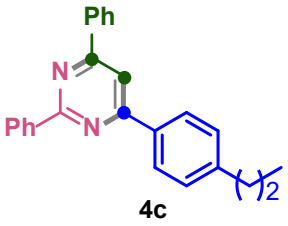
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.80 – 8.68 (m, 2H), 8.34 – 8.26 (m, 2H), 8.21 (d, *J* = 8.0 Hz, 2H), 7.99 (s, 1H), 7.55 (q, *J* = 6.2 Hz, 6H), 7.37 (d, *J* = 7.9 Hz, 2H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.7, 164.6, 164.5, 141.2, 138.3, 137.7, 134.7, 130.7, 130.6, 129.7, 128.9, 128.5, 128.4, 127.3, 127.2, 110.0, 21.5.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{19}N_2$, 323.2; found, 323.2. Spectra data are consistent with the reported literature.[2]

IR: (KBr, cm^{-1}) 1640 (s), 1589 (m), 1570 (m), 1527 (m), 1511 (w), 1495 (w), 1360 (m), 1236 (w), 1112 (w), 1027 (w), 822 (m), 773 (m), 747 (s), 686 (s), 629 (m), 473 (m).

m.p.: 140-142 ºC.



4c

Synthesis of 2,4-diphenyl-6-(4-propylphenyl)pyrimidine (4c): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (41.1 mg, 61%).

R_f = 0.52 (*n*-hexane:EtOAc = 20:1, UV).

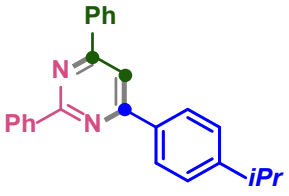
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.77 – 8.68 (m, 2H), 8.32 – 8.24 (m, 2H), 8.21 (d, *J* = 8.1 Hz,21H), 7.99 (s, 1H), 7.54 m, 6H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.69 (t, *J* = 7.6 Hz, 2H), 1.71 (h, *J* = 7.4 Hz, 2H), 0.98 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.8, 164.6, 164.5, 145.9, 138.3, 137.7, 135.0, 130.7, 130.6, 129.1, 128.9, 128.5, 128.4, 127.3, 127.2, 110.0, 38.0, 24.5, 13.8.

HRMS ESI: (m/z) [M+H]+ calcd. for $C_{25}H_{23}N_2$, 351.1856; found, 351.1861.

IR: (KBr, cm^{-1}) 1644 (m), 1608 (m), 1592 (m), 1572 (s), 1529 (s), 1506 (m), 1363 (m), 1296 (s), 1199 (m), 1160 (m), 1073 (w), 1018 (w), 850 (w), 774 (w), 752 (m), 734 (m), 686 (m), 633 (w), 501 (w).

m.p.: 72-74 ºC.



4d

Synthesis of 4-(4-isopropylphenyl)-2,6-diphenylpyrimidine (4d): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane : EtOAc = 20:1) as a white solid (40.1 mg, 68%).

R_f = 0.66 (*n*-hexane:EtOAc = 20:1, UV).

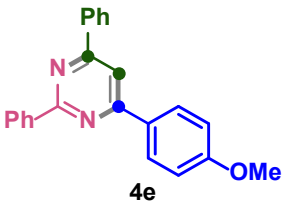
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.78 – 8.73 (m, 2H), 8.33 – 8.29 (m, 2H), 8.24 (d, *J* = 8.1 Hz, 2H), 8.00 (s, 1H), 7.56 (t, *J* = 6.7 Hz, 7H), 7.44 (d, *J* = 8.1 Hz, 2H), 3.0 (dq, *J* = 13.5, 6.7 Hz, 1H), 1.34 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.9, 164.7, 164.6, 152.1, 138.4, 137.8, 135.3, 130.9, 130.8, 130.7, 129.0, 128.6 , 127.5, 127.4, 127.2, 110.2, 34.3, 24.0.

HRMS ESI: (m/z) [M+H]+ calcd. for $C_{25}H_{23}N_2$, 351.1856; found, 351.1864.

IR: (KBr, cm^{-1}) 1637 (w), 1613 (w), 1589 (m), 1569 (s), 1527 (s), 1496 (m), 1446 (w), 1380 (w), 1360 (s), 1261 (w), 1098 (m), 1056 (m), 1026 (m), 840 (m), 830 (m), 804 (m), 775 (m), 754 (m), 739 (s), 686 (s), 630 (w), 535 (m).

m.p.: 123-124 ºC.



4e

Synthesis of 4-(4-methoxyphenyl)-2,6-diphenylpyrimidine (4e): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 30:1) as a white solid (48.0 mg, 74%).

R_f = 0.63 (*n*-hexane:EtOAc = 30:1, UV).

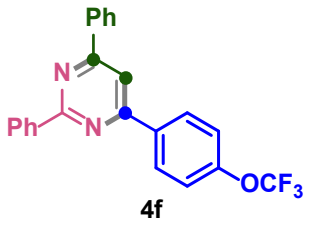
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.76 – 8.66 (m, 2H), 8.25 (m, 4H), 7.91 (s, 1H), 7.52 (m, 6H), 7.04 (d, *J* = 8.6 Hz, 2H), 3.87 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.5, 164.4, 164.2, 161.9, 138.3, 137.7, 130.7, 130.6, 130.0, 128.9, 128.8, 128.5, 128.4, 127.3, 114.3, 109.4, 55.5.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{19}N_2O$, 339.1; found, 339.1. Spectra data are consistent with the reported literature.[1]

IR: (KBr, cm^{-1}) 1610 (w), 1588 (s), 1560 (s), 1528 (s), 1510 (s), 1495 (m), 1458 (w), 1366 (s), 1294 (w), 1255 (s), 1214 (s), 1172 (s), 1075 (w), 1025 (m), 832 (s), 775 (m), 752 (s), 730 (m), 691 (s), 636 (w), 585 (m), 514 (m).

m.p.: 72-74 ºC.



4f

Synthesis of 2,4-diphenyl-6-(4-(trifluoromethoxy)phenyl)pyrimidine (4f): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (48.0 mg, 64%).

R_f = 0.43 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.75 – 8.68 (m, 2H), 8.36 – 8.26 (m, 4H), 7.99 (s, 1H), 7.60 – 7.51 (m, 6H), 7.41 (d, *J* = 8.2 Hz, 2H).

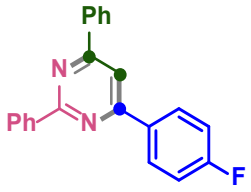
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.2, 164.8, 163.5, 160.2, 151.3, 138.1, 137.5, 136.3, 131.1, 131.0, 129.1, 129.1, 128.7, 128.6, 127.4, 121.3, 110.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -57.63.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{16}F_3N_2O$, 393.1; found, 393.1.

IR: (KBr, cm^{-1}) 1622 (w), 1570 (s), 1533 (s), 1492 (m), 1441 (w), 1359 (m), 1287 (s), 1214 (s), 1155 (s), 1076 (w), 1025 (w), 864 (m), 807 (w), 778 (w), 751 (s), 712 (m), 687 (s), 636 (m), 473 (w).

m.p.: 99-100 ºC.



4g

Synthesis of 4-(4-fluorophenyl)-2,6-diphenylpyrimidine (4g): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (35.7 mg, 57%).

R_f = 0.77 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.76 – 8.66 (m, 2H), 8.34 – 8.21 (m, 4H), 7.95 (s, 1H), 7.55 (m, 6H), 7.27 – 7.19 (m, 2H).

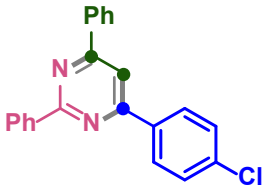
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)165.0, 164.8 (d, J_{CF} = 250.0 Hz) 164.6, 163.7, 163.5, 138.2, 137.6, 133.8 (d, J_{CF} = 3.0 Hz), 131.0, 130.8, 129.5 (d, J_{CF} = 8.2 Hz), 129.1, 128.6, 127.4, 116.1 (d, J_{CF} = 21.6 Hz), 110.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -109.86.

LRMS ESI: (m/z) [M+H]+ calcd. for $C_{22}H_{16}FN_2$, 327.1; found, 327.1. Spectra data are consistent with the reported literature.[1]

IR: (KBr, cm^{-1}) 1644 (w), 1604 (s), 1589 (m), 1572 (s), 1530 (s), 1497 (s), 1361 (s), 1229 (s), 1154 (w), 1103 (w), 1025 (w), 831 (s), 773 (w), 747 (s), 720 (m), 685 (s), 632 (m), 586 (w), 565 (m), 501 (m).

m.p.: 156-158 ºC.



4h

Synthesis of 4-(4-chlorophenyl)-2,6-diphenylpyrimidine (4h): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a white solid (46.2 mg, 70%).

R_f = 0.49 (*n*-hexane:EtOAc = 50:1, UV).

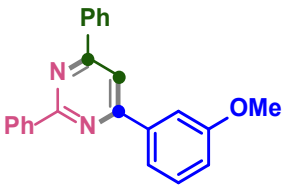
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.73 – 8.62 (m, 2H), 8.28 – 8.15 (m, 4H), 7.90 (s, 1H), 7.50 (dd, *J* = 12.2, 7.1 Hz, 8H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.9, 164.6, 163.5, 138.0, 137.4, 137.0, 135.9, 130.9, 130.8, 129.1, 129.0, 128.6, 128.5, 127.3, 109.9.

LRMS ESI: (m/z) [M+H]+ calcd. for $C_{22}H_{16}ClN_2$, 343.1; found, 343.1. Spectra data are consistent with the reported literature.[1]

IR: (KBr, cm^{-1}) 1641 (w), 1590 (s), 1570 (s), 1526 (s), 1491 (s), 1360 (s), 1238 (w), 1172 (w), 1091 (m), 1010 (m), 836 (s), 775 (m), 750 (s), 717 (w), 689 (s), 636 (m).

m.p.: 160-162 ºC.



4i

Synthesis of 4-(3-methoxyphenyl)-2,6-diphenylpyrimidine (4i): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 100:1) as a white solid (26.8 mg, 41%).

R_f = 0.38 (*n*-hexane:EtOAc = 100:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.78 – 8.66 (m, 2H), 8.32 – 8.21 (m, 2H), 7.96 (s, 1H),

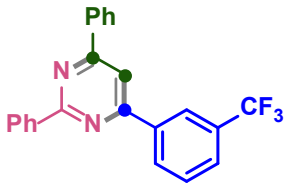
7.87 (s, 1H), 7.80 (d, J = 7.7 Hz, 1H), 7.59 – 7.48 (m, 6H), 7.45 (t, J = 7.9 Hz, 1H), 7.10 – 7.02 (m, 1H), 3.92 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.8, 164.5, 164.5, 160.2, 139.0, 138.2, 137.5, 130.8, 130.7, 129.9, 128.9, 128.5, 128.5, 127.3, 119.7, 116.4, 112.8, 110.5, 55.5.

LRMS ESI: (m/z) [M+H]+ calcd. for $C_{23}H_{19}N_2O$, 339.1; found, 339.1. Spectra data are consistent with the reported literature.[5]

IR: (KBr, cm^{-1}) 1569 (s), 1527 (s), 1491 (m), 1452 (m), 1359 (s), 1285 (m), 1254 (m), 1215 (w), 1042 (m), 859 (m), 834 (w), 772 (m), 747 (s), 684 (s), 632 (m), 473 (w).

m.p.: 118-119 ºC.



4j

Synthesis of 2,4-diphenyl-6-(3-(trifluoromethyl)phenyl)pyrimidine (4j): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 100:1) as a white solid (38.3 mg, 53%).

R_f = 0.67 (*n*-hexane:EtOAc = 100:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.76 – 8.69 (m, 2H), 8.53 (s, 1 H), 8.47 (d, J = 7.7 Hz, 1H), 8.34 – 8.27 (m, 1H), 8.02 (s, 1H), 7.80 (d, J = 7.7 Hz, 1H), 7.69 (t, J = 7.8 Hz, 1H), 7.61 – 7.52 (m, 6H).

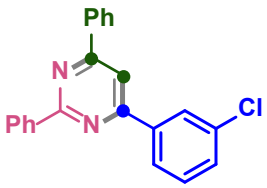
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.2, 164.7, 163.2, 138.4, 137.8, 137.2, 131.6, 131.3, 131.1, 130.9, 130.7, 130.5, 130.2, 129.5, 129.0, 128.6, 128.5, 127.4, 127.31, 127.27, 125.4, 124.2, 124.13, 124.09, 124.05, 122.7, 110.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.54.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{16}F_3N_2$, 377.1260; found, 377.1263.

IR: (KBr, cm^{-1}) 1616 (w), 1589 (s), 1571 (s), 1528 (s), 1494 (m), 1442 (m), 1379 (m), 1357 (s), 1326 (s), 1282 (w), 1232 (m), 1165 (s), 1120 (s), 1074 (s), 1052(m), 1025 (m), 923 (w), 863 (m), 811 (m), 776 (m), 751 (s), 688 (s), 657 (m), 635 (m).

m.p.: 157-158 ºC.



4k

Synthesis of 4-(3-chlorophenyl)-2,6-diphenylpyrimidine (4k): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 100:1) as a white solid (33.6 mg, 51%).

R_f = 0.51 (*n*-hexane:EtOAc = 100:1, UV).

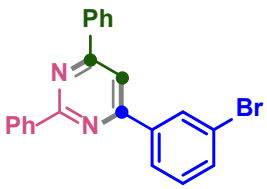
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.76 – 8.68 (m, 2H), 8.35 – 8.24 (m, 3H), 8.18 – 8.12 (m, 1H), 7.98 (s, 1H), 7.60 – 7.47 (m, 8H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.1, 164.7, 163.4, 139.4, 137.9, 137.3, 135.1, 131.0, 130.8, 130.7, 130.2, 129.0, 128.5, 127.5, 127.3, 125.4, 110.3.

LRMS ESI: (m/z) [M+H]+ calcd. for $C_{22}H_{16}ClN_2$, 343.1; found, 343.1. Spectra data are consistent with the reported literature.[6]

IR: (KBr, cm^{-1}) 1642 (w), 1588 (m), 1568 (s), 1525 (s), 1495 (w), 1356 (m), 1237 (w), 1074 (w), 1024 (w), 861 (w), 773 (w), 748 (s), 719 (w), 686 (s), 632 (w).

m.p.: 139-140 ºC.



4l

Synthesis of 4-(3-bromophenyl)-2,6-diphenylpyrimidine (4l): Following the general

procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (47.7 mg, 64%).

R_f = 0.56 (*n*-hexane:EtOAc = 20:1, UV).

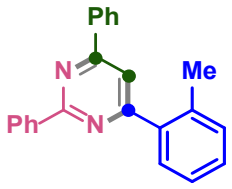
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.77 – 8.64 (m, 2H), 8.32 – 8.23 (m, 2H), 8.17 (d, *J* = 8.5 Hz, 2H), 7.97 (s, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.61 – 7.48 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.2, 164.8, 163.4, 139.8, 138.0, 137.4, 133.8, 131.1, 131.0, 130.6, 130.5, 129.1, 128.7, 127.5, 126.0, 123.4, 110.4.

LRMS ESI: (m/z) [M+H]+ calcd. for $C_{22}H_{16}BrN_2$, 387.0; found, 387.0. Spectra data are consistent with the reported literature.[7]

IR: (KBr, cm^{-1}) 1587 (m), 1568 (s), 1508 (s), 1495 (m), 1356 (m), 1236 (s), 1072 (w), 1025 (w), 860 (m), 775 (m), 748 (s), 686 (s), 660 (w), 633 (m).

m.p.: 128-129 ºC.



4m

Synthesis of 2,4-diphenyl-6-(o-tolyl)pyrimidine (4m): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a light yellow oil (39.9 mg, 65%).

R_f = 0.49 (*n*-hexane:EtOAc = 20:1, UV).

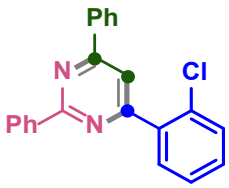
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.74 – 8.59 (m, 2H), 8.32 – 8.21 (m, 2H), 7.74 (s, 1H), 7.62 – 7.48 (m, 7H), 7.42 – 7.32 (m, 3H), 2.57 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.8, 164.7, 163.7, 137.9, 137.3, 137.0, 136.6, 131.4, 131.2, 131.1, 129.8, 129.7, 129.1, 128.7, 128.6, 127.5, 126.3, 114.5, 20.7.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{19}N_2$, 323.2; found, 323.2. Spectra data are consistent

with the reported literature.[8]

IR: (KBr, cm^{-1}) 1622 (m), 1603 (m), 1588 (s), 1568 (s), 1524 (s), 1493 (m), 1449 (m), 1378 (m), 1359 (m), 1283 (m), 1236 (m), 1173 (m), 1074 (w), 1029 (m), 879 (w), 845 (w), 771 (m), 750 (s), 727 (w), 692 (s), 634 (s).



4n

Synthesis of 4-(2-chlorophenyl)-2,6-diphenylpyrimidine (4n): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (37.3 mg, 57%).

R_f = 0.46 (*n*-hexane:EtOAc = 20:1, UV).

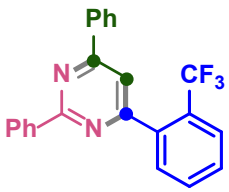
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.68 (m, 2H), 8.33 – 8.24 (m, 2H), 8.03 (s, 1H), 7.86 (dd, *J* = 7.2, 2.1 Hz, 1H), 7.59 – 7.49 (m, 7H), 7.48 – 7.41 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.7, 164.6, 163.9, 138.0, 137.6, 137.3, 132.5, 131.8, 130.9, 130.8, 130.7, 130.5, 129.0, 128.5, 127.4, 127.3, 115.2.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{16}ClN_2$, 343.1; found, 343.1. Spectra data are consistent with the reported literature.[9]

IR: (KBr, cm^{-1}) 1650 (m), 1592 (m), 1570 (s), 1526 (s), 1474 (w), 1362 (s), 1259 (w), 1166 (w), 1067 (m), 1034 (m), 873 (w), 775 (m), 746 (s), 687 (s), 623 (m).

m.p.: 111-112 ºC.



4o

Synthesis of 2,4-diphenyl-6-(2-(trifluoromethyl)phenyl)pyrimidine (4o): Following the

general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (26.0 mg, 36%).

R_f = 0.50 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.65 (dd, *J* = 6.5, 2.8 Hz, 2H), 8.27 (dd, *J* = 6.4, 2.7 Hz, 2H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.76 (s, 1H), 7.65 (dt, *J* = 22.0, 8.9 Hz, 3H), 7.58 – 7.47 (m, 6H).

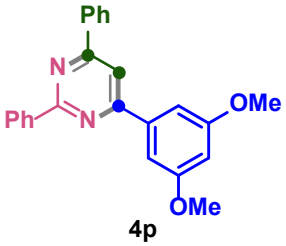
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.4, 164.4, 164.3, 138.6, 137.9, 137.2, 132.0, 131.5, 131.2, 130.9, 129.4, 129.1, 128.9, 128.7, 128.6, 128.5, 127.5, 127.1, 127.0, 126.94, 126.89, 125.5, 122.8, 114.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -56.28.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{16}F_3N_2$, 377.1260; found, 377.1258.

IR: (KBr, cm^{-1}) 1640 (w), 1622 (w), 1590 (m), 1565 (s), 1528 (s), 1494 (m), 1378 (w), 1360 (s), 1311 (s), 1269 (w), 1171 (m), 1148 (w), 1126 (s), 1109 (s), 1067 (w), 1036 (m), 872 (w), 765 (m), 745 (s), 693 (s), 632 (m), 596 (w).

m.p.: 97-98 °C.



4p

Synthesis of 4-(3,5-dimethoxyphenyl)-2,6-diphenylpyrimidine (4p): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (58.1 mg, 82%).

R_f = 0.37 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.78 – 8.63 (m, 2H), 8.33 – 8.22 (m, 2H), 7.95 (s, 1H), 7.61 – 7.48 (m, 6H), 7.43 (d, *J* = 2.0 Hz, 2H), 6.64 (s, 1H), 3.92 (s, 6H).

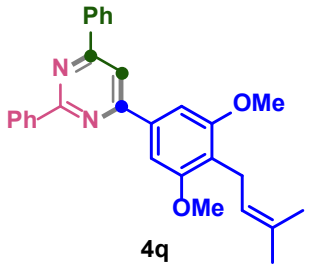
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.8, 164.5, 164.4, 161.3, 139.7, 138.1, 137.5, 130.8,

130.7, 128.9, 128.5, 128.4, 127.3, 110.5, 105.5, 102.6, 55.6.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{24}H_{21}N_2O_2$, 369.1598; found, 369.1598.

IR: (KBr, cm^{-1}) 1591 (m), 1569 (s), 1532 (s), 1496 (w), 1453 (m), 1358 (s), 1333 (w), 1286 (w), 1202(m), 1153 (m), 1068 (w), 1040 (w), 928 (w), 839 (m), 773 (m), 748 (m), 686 (w), 656 (w).

m.p.: 135-136 ºC.



4q

Synthesis of 4-(3,5-dimethoxy-4-(3-methylbut-2-en-1-yl)phenyl)-2,6-diphenylpyrimidine (4q): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc =50:1) as a yellow solid (54.3 mg, 62%).

$\mathbf{R_f}$ = 0.57 (*n*-hexane:EtOAc = 50:1, UV).

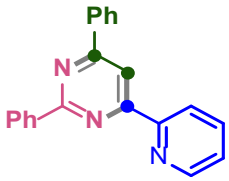
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) δ 8.78 – 8.69 (m, 2H), 8.35 – 8.25 (m, 2H), 7.94 (s, 1H), 7.57 (t, *J* = 7.8 Hz, 6H), 7.46 (s, 2H), 5.26 (t, *J* = 7.0 Hz, 1H), 4.00 (s, 6H), 3.46 (d, *J* = 7.0 Hz, 2H), 1.83 (s, 3H), 1.72 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.1, 164.8, 164.5, 158.6, 138.3, 137.7, 136.5, 131.8, 130.9, 130.7, 129.0, 128.6, 127.4, 122.4, 121.8, 110.4, 103.1, 56.1, 26.0, 22.7, 17.9.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{29}H_{28}N_2O_2$, 437.2224; found, 437.2222.

IR: (KBr, cm^{-1}) 1638 (s), 1590 (m), 1570 (s), 1529 (s), 1494 (w), 1460 (w), 1361 (s), 1302 (w), 1166 (w), 846 (w), 750 (m), 699 (m), 632 (w).

m.p.: 145-147 ºC.



4r

Synthesis of 2,4-diphenyl-6-(pyridin-2-yl)pyrimidine (4r): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc =5:1) as a yellow solid (34.9 mg, 59%).

R_f = 0.31 (*n*-hexane:EtOAc = 5:1, UV).

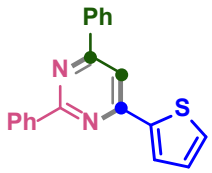
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.97 (d, *J* = 3.9 Hz, 1H), 8.81 (d, *J* = 7.2 Hz, 5H), 8.00 – 7.94 (m, 1H), 7.71 – 7.46 (m, 8H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 172.4, 150.5, 137.0, 135.8, 133.1, 132.8, 132.2, 132.1, 132.0, 131.9, 129.3, 128.7, 128.6, 128.5, 126.1, 124.8, 106.3.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{21}H_{16}N_3$, 310.1; found, 310.1. Spectra data are consistent with the reported literature.[10]

IR: (KBr, cm^{-1}) 1641 (m), 1591 (w), 1525 (s), 1438 (w), 1368 (s), 1179 (w), 1119 (w), 843 (m), 749 (s), 722 (w), 691 (m), 642 (w), 541 (m).

m.p.: 227-228 ºC.



4s

Synthesis of 2,4-diphenyl-6-(thiophen-2-yl)pyrimidine (4s): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a white solid (21.3 mg, 35%).

R_f = 0.29 (*n*-hexane:EtOAc = 5:1, UV).

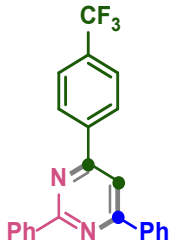
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.69 (d, *J* = 6.2 Hz, 2H), 8.27 (d, *J* = 5.9 Hz, 2H), 7.92 (d, *J* = 3.3 Hz, 1H), 7.86 (s, 1H), 7.54 (d, *J* = 8.9 Hz, 8H), 7.21 (t, *J* = 4.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 175.8, 173.8, 171.7, 167.0, 137.1, 135.9, 133.0, 132.2, 131.9, 130.5, 129.4, 129.3, 128.9, 127.4, 127.4, 114.9.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{20}H_{15}N_2S$, 315.1; found, 315.1. Spectra data are consistent with the reported literature.[2]

IR: (KBr, cm^{-1}) 1641 (s), 1587 (m), 1569 (s), 1526 (s), 1495 (w), 1430 (w), 1365 (s), 1236 (w), 1094 (w), 1074 (w), 1028 (w), 858 (w), 833 (w), 775 (m), 748 (s), 708 (m), 688 (s), 632 (m).

m.p.: 162-163 ºC.



4t

Synthesis of 2,4-diphenyl-6-(4-(trifluoromethyl)phenyl)pyrimidine (4t): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (57.1 mg, 76%).

R_f = 0.56 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.78 – 8.65 (m, 2H), 8.39 (d, *J* = 8.0 Hz, 2H), 8.34 – 8.25 (m, 2H), 8.02 (s, 1H), 7.82 (d, *J* = 8.1 Hz, 2H), 7.62 – 7.50 (m, 6H).

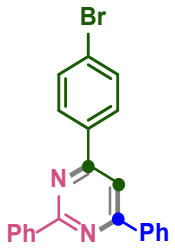
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.4, 164.9, 163.4, 162.2, 141.1, 137.9, 137.3, 131.2, 131.0, 129.1, 128.8, 128.7, 128.63, 128.55, 128.5, 127.8, 127.5, 126.1, 126.0, 126.0, 125.9, 110.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.71.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{16}F_3N_2$, 377.1; found, 377.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1591 (m), 1569 (s), 1528 (s), 1496 (w), 1453 (w), 1358 (s), 1333 (w) 1286 (w), 1202 (m), 1153 (m), 1068 (w), 1040 (w), 928 (w), 839 (m), 773 (w), 748 (m), 725 (w), 686 (s), 656 (w), 633 (w).

m.p.: 137-138 ºC.



4u

Synthesis of 4-(4-bromophenyl)-2,6-diphenylpyrimidine (4u): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (29.6 mg, 40%).

R_f = 0.59 (*n*-hexane:EtOAc = 20:1, UV).

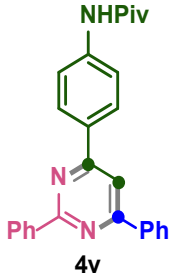
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.77 – 8.64 (m, 2H), 8.32 – 8.23 (m, 2H), 8.17 (d, *J* = 8.5 Hz, 2H), 7.97 (s, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.61 – 7.48 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.0, 164.6, 163.6, 138.0, 137.4, 136.4, 132.1, 130.9, 130.8, 129.0, 128.8, 128.5, 128.4, 127.3, 125.4, 110.0.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{16}BrN_2$, 387.0; found, 387.0. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1588 (s), 1569 (s), 1527 (s), 1488 (m), 1359 (s), 1239 (w), 1172 (w), 1071 (w), 1006 (w), 832 (m), 776 (w), 750 (s), 689 (s), 635 (w), 493 (w).

m.p.: 160-161 ºC.



4v

Synthesis of N-(4-(2,6-diphenylpyrimidin-4-yl)phenyl)pivalamide (4v): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 2:1) as a yellow solid (23.5 mg, 30%).

R_f = 0.51 (*n*-hexane:EtOAc = 2:1, UV).

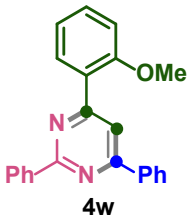
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.72 (d, *J* = 6.5 Hz, 2H), 8.36 – 8.23 (m, 4H), 7.99 (br s, 1H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.60 – 7.46 (m, 7H), 1.37 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 176.8, 164.7, 164.5, 163.9, 140.5, 138.2, 137.6, 133.0, 130.8, 130.6, 128.9, 128.5, 128.1, 127.3, 119.8, 109.7, 39.8, 27.7.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{27}H_{26}N_3O$, 408.2070; found, 408.2075.

IR: (KBr, cm^{-1}) 1658 (s), 1593 (s), 1572 (m), 1520 (s), 1363 (m), 1318 (w), 1237 (w), 1183 (w), 1170 (w), 1025 (w), 925 (w), 845 (w), 836 (w), 752 (m), 689 (m), 628 (w), 513 (w).

m.p.: 209-211 ºC.



4w

Synthesis of 4-(2-methoxyphenyl)-2,6-diphenylpyrimidine (4w): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (29.3 mg, 45%).

R_f = 0.32 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.70 (d, *J* = 6.5 Hz, 2H), 8.34 – 8.20 (m, 4H), 7.54 (m, 7H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 8.3 Hz, 1H), 3.97 (s, 3H).

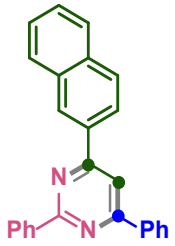
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.4, 163.8, 163.6, 158.2, 138.6, 138.1, 131.7, 131.5, 130.6, 130.5, 129.0, 128.5, 128.5, 127.5, 127.2, 121.4, 115.6, 111.8, 56.0.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{23}H_{19}N_2O$, 339.1; found, 339.1. Spectra data are

consistent with the reported literature.[6]

IR: (KBr, cm^{-1}) 1642 (w), 1589 (m), 1571 (s), 1529 (s), 1494 (m), 1360 (s), 1235 (w), 1171 (w), 1071 (w), 1027 (w), 862 (w), 770 (w), 737 (s), 681 (s), 627 (m), 614 (w), 473 (m).

m.p.: 89-91 ºC.



4x

Synthesis of 4-(naphthalen-2-yl)-2,6-diphenylpyrimidine (4x): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (42.1 mg, 66%).

R_f = 0.53 (*n*-hexane:EtOAc = 20:1, UV).

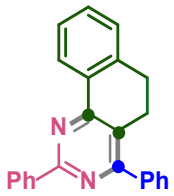
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.79 (m, 3H), 8.41 (d, *J* = 8.6 Hz, 1H), 8.37 – 8.30 (m, 2H), 8.15 (s, 1H), 8.03 (m, 2H), 7.97 – 7.88 (m, 1H), 7.66 – 7.47 (m, 8H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.8, 164.7, 164.6, 138.2, 137.6, 134.9, 134.6, 133.3, 130.8, 130.7, 129.1, 129.0, 128.7, 128.6, 128.5, 127.8, 127.4, 127.4, 127.3, 126.6, 124.3, 110.5.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{26}H_{19}N_2$, 359.2; found, 359.2. Spectra data are consistent with the reported literature.[9]

IR: (KBr, cm^{-1}) 1646 (w), 1589 (s), 1570 (s), 1530 (s), 1495 (m), 1434 (w), 1370 (m), 1332 (w), 1199 (w), 1071 (w), 1023 (w), 852 (m), 810 (m), 772 (m), 755 (s), 691 (s), 663 (m), 634 (m), 561 (w), 473 (m).

m.p.: 153-154 ºC.



4y

Synthesis of 2,4-diphenyl-5,6-dihydrobenzo[h]quinazoline (4y): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a yellow solid (40.4 mg, 63%).

R_f = 0.51 (*n*-hexane:EtOAc = 20:1, UV).

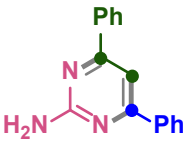
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.71 – 8.55 (m, 3H), 7.74 (d, *J* = 6.4 Hz, 2H), 7.58 – 7.39 (m, 8H), 7.28 (s, 1H), 3.15 – 3.04 (m, 2H), 2.91 (t, *J* = 7.1 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.3, 162.2, 160.1, 139.1, 138.4, 138.3, 133.4, 130.8, 130.2, 129.3, 128.4, 128.3, 128.2, 127.8, 127.3, 126.1, 123.5, 27.9, 24.8.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{19}BrN_2$, 335.2; found, 335.2. Spectra data are consistent with the reported literature.[6]

IR: (KBr, cm^{-1}) 1638 (m), 1538 (s), 1494 (s), 1494 (w), 1446 (w), 1394 (s), 1265 (w), 1101 (w), 1024 (w), 757 (s), 701 (s), 624 (w), 597 (w).

m.p.: 154-156 ºC.



4z

Synthesis of 4,6-diphenylpyrimidin-2-amine (4z): Following the general procedure A, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a light yellow solid (39.8 mg, 84%).

R_f = 0.38 (*n*-hexane:EtOAc = 5:1, UV).

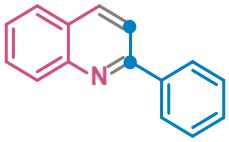
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.05 (m, 4H), 7.55 – 7.43 (m, 7H), 5.29 (brs, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.3, 163.7, 137.8, 130.5, 128.8, 127.2, 104.4.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{16}H_{14}N_3$, 248.1; found, 248.1. Spectra data are consistent with the reported literature.[11]

IR: (KBr, cm^{-1}) 1629 (s), 1587 (m), 1565 (s), 1544 (s), 1495 (m), 1451 (m), 1363 (w), 1232 (w), 1074 (w), 841 (m), 763 (s), 692 (s), 626 (m).

m.p.: 127-129 ºC.



7a

Synthesis of 2-phenylquinoline (7a): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a yellow solid (from ketone, 35.9 mg, 86%; from alcohol, 33.8 mg, 81%).

R_f = 0.38 (*n*-hexane:EtOAc = 20:1, UV).

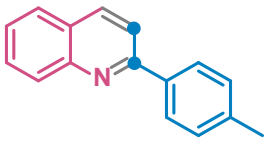
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.28 – 8.11 (m, 4H), 7.86 (dd, *J* = 19.3, 8.3 Hz, 2H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.51 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 157.4, 148.3, 139.7, 136.8, 129.8, 129.7, 129.3, 128.9, 127.6, 127.5, 127.2, 126.3, 119.1.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{12}N$, 206.1; found, 206.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1638 (m), 1597 (m), 1554 (w), 1488 (w), 1445 (w), 1318 (w), 1123 (w), 1075 (w), 1022 (w), 829 (s), 792 (w), 766 (s), 690 (s), 674 (m), 611 (w), 554 (w).

m.p.: 80-81 ºC.



7b

Synthesis of 2-(p-tolyl)quinoline (7b): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a yellow solid (from ketone, 37.7 mg, 84%; from alcohol, 25.2 mg, 56%).

R_f = 0.39 (*n*-hexane:EtOAc = 50:1, UV).

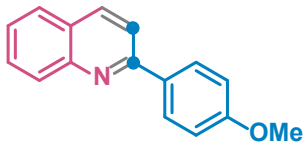
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.08 (dd, *J* = 8.5, 3.8 Hz, 2H), 8.04 – 7.95 (m, 2H), 7.79 – 7.67 (m, 2H), 7.62 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.41 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.24 (d, *J* = 7.9 Hz, 2H), 2.34 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 157.4, 148.3, 139.4, 136.9, 136.7, 129.7, 129.6, 127.5, 127.2, 126.1, 118.9, 21.4.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{16}H_{14}N$, 220.1; found, 220.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1636 (m), 1595 (m), 1574 (w), 1551 (w), 1496 (m), 1430 (w), 1319 (w), 1286 (w), 1125 (w), 1110 (w), 1015 (w), 947 (w), 814 (s), 787 (s), 746 (s), 715 (m), 690 (s), 675 (w), 615 (w), 554 (w).

m.p.: 81-83 ºC.



7c

Synthesis of 2-(4-methoxyphenyl)quinoline (7c): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a dark red solid (from ketone, 39.9 mg, 83%; from alcohol, 26.5 mg, 55%).

R_f = 0.45 (*n*-hexane:EtOAc = 50:1, UV).

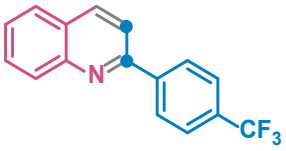
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.11 – 8.02 (m, 4H), 7.77 – 7.67 (m, 2H), 7.62 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 8.7 Hz, 2H), 3.79 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.8, 156.9, 148.3, 136.6, 132.3, 129.6, 129.6, 128.9, 127.5, 126.9, 125.9, 118.6, 114.3, 55.4.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{16}H_{14}NO$, 236.1; found, 236.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1641 (s), 1606 (s), 1498 (m), 1430 (w), 1288 (w), 1250 (m), 1176 (w), 1114 (w), 1028 (w), 818 (s), 789 (m), 750 (s), 724 (w), 677 (m), 557 (m).

m.p.: 114-116 ºC.



7d

Synthesis of 2-(4-(trifluoromethyl)phenyl)quinoline (7d): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a light yellow solid (from ketone, 39.6 mg, 71%; from alcohol, 35.3 mg, 63%).

$\mathbf{R_f}$ = 0.35 (*n*-hexane:EtOAc = 50:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.26 (t, *J* = 9.0 Hz, 3H), 8.18 (d, *J* = 8.5 Hz, 1H), 7.85 (dd, *J* = 11.5, 8.6 Hz, 2H), 7.81 – 7.71 (m, 3H), 7.60 – 7.52 (m, 1H).

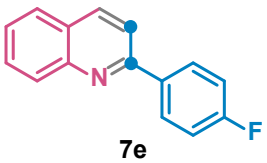
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.8, 148.4, 143.1, 137.2, 131.7, 131.3, 131.0, 130.7, 130.1, 130.0, 128.4, 128.0, 127.7, 127.6, 127.0, 125.9, 125.9, 125.84, 125.80, 125.7, 123.0, 120.3, 118.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -112.48.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{16}H_{11}F_3N$, 274.1; found, 274.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1638 (s), 1595 (w), 1556 (w), 1498 (w), 1433 (w), 1338 (s), 1169 (m), 1124 (s), 1105 (s), 1072 (m), 1010 (w), 818 (s), 789 (w), 759 (m), 676 (w), 597 (w).

m.p.: 119-120 ºC.



7e

Synthesis of 2-(4-fluorophenyl)quinoline (7e): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a white solid (19.4 mg, 43%).

R_f = 0.43 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.18 – 8.00 (m, 4H), 7.79 – 7.72 (m, 2H), 7.66 (ddd, *J* = 8.5, 6.8, 1.5 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.13 (t, *J* = 8.7 Hz, 2H).

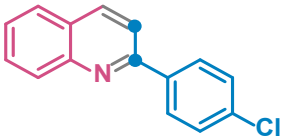
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.9 (d, J_{CF} = 249.0 Hz), 156.3, 148.3, 137.0, 135.9 (d, J_{CF} = 21.6 Hz), 129.9, 129.7, 129.5 (d, J_{CF} = 8.5 Hz), 127.6, 127.2, 126.4, 118.7, 115.9 (d, J_{CF} = 3.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.52.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{11}FN$, 224.1; found, 224.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1651 (w), 1602 (w), 1587 (m), 1566 (s), 1525 (s), 1493 (w), 1454 (w), 1378 (w), 1360 (m), 1260 (w), 1172 (w), 1072 (w), 1029 (m), 833 (w), 751 (s), 694 (s), 635 (m).

m.p.: 102-104 ºC.



7f

Synthesis of 2-(4-chlorophenyl)quinoline (7f): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a light yellow solid (from ketone, 39.5 mg, 81%; from alcohol, 31.3 mg, 64%).

R_f = 0.38 (*n*-hexane:EtOAc = 50:1, UV).

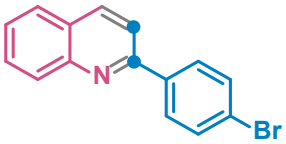
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 8.6 Hz, 1H), 8.19 – 8.07 (m, 3H), 7.83 (dd, *J* = 8.6, 2.6 Hz, 2H), 7.73 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.58 – 7.46 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 156.1, 148.3, 138.2, 137.1, 135.7, 130.0, 129.8, 129.1, 128.9, 127.6, 127.3, 126.6, 118.7.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{11}ClN$, 240.1; found, 240.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1636 (m), 1593 (m), 1553 (w), 1485 (m), 1430 (m), 1317 (w), 1127 (w), 1090 (m), 1007 (w), 817 (s), 787 (m), 751 (m), 714 (w), 671 (w), 620 (w), 550 (w).

m.p.: 107-108 ºC.



7g

Synthesis of 2-(4-bromophenyl)quinoline (7g): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a white solid (from ketone, 48.0 mg, 83%; from alcohol, 38.0 mg, 66%).

R_f = 0.38 (*n*-hexane:EtOAc = 50:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.10 (dd, *J* = 23.4, 8.5 Hz, 2H), 8.00 – 7.93 (m, 2H), 7.74 (dd, *J* = 8.4, 1.8 Hz, 2H), 7.65 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.50 – 7.41 (m, 1H).

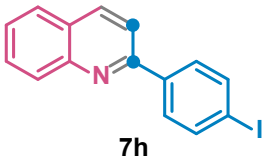
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 156.0, 148.3, 138.5, 137.0, 132.0, 129.9, 129.7, 129.1, 127.5, 127.3, 126.5, 124.0, 118.5.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{11}BrN$, 284.0; found, 284.0. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1637 (m), 1594 (m), 1576 (m), 1550 (w), 1484 (m), 1429 (m), 1316 (w), 1126 (w), 1103 (w), 1069 (m), 1003 (m), 815 (s), 786 (s), 751 (s), 712 (m),690 (s), 670 (w), 618 (w),

550 (w).

m.p.: 109-110 ºC.



7h

Synthesis of 2-(4-iodophenyl)quinoline (7h): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a yellow solid (36.4 mg, 54%).

R_f = 0.46 (*n*-hexane:EtOAc = 20:1, UV).

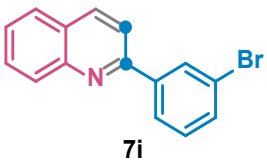
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 8.6 Hz, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.95 – 7.88 (m, 2H), 7.89 – 7.79 (m, 4H), 7.73 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.54 (ddd, *J* = 8.2, 6.8, 1.2 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 156.1, 148.3, 139.1, 138.0, 137.0, 129.9, 129.7, 129.3, 127.5, 127.3, 126.6, 118.5, 95.9.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{11}IN$, 332.0; found, 332.0. Spectra data are consistent with the reported literature.[12]

IR: (KBr, cm^{-1}) 1641 (w), 1594 (m), 1556 (m), 1498 (m), 1474 (w), 1438 (w), 1424 (m), 1310 (w), 1238 (w), 1074 (w), 1027 (w), 830 (s), 761 (s), 742 (s), 709 (s), 641 (m).

m.p.: 82-84 ºC.



7i

Synthesis of 2-(3-bromophenyl)quinoline (7i): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a white solid (34.9 mg, 65%).

R_f = 0.38 (*n*-hexane:EtOAc = 50:1, UV).

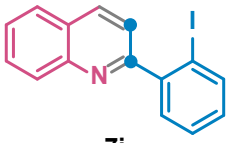
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.35 (t, *J* = 1.8 Hz, 1H), 8.19 (dd, *J* = 20.7, 8.5 Hz, 2H), 8.06 (dt, *J* = 7.9, 1.4 Hz, 1H), 7.82 (dd, *J* = 8.5, 2.2 Hz, 2H), 7.74 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.62 – 7.49 (m, 2H), 7.38 (t, *J* = 7.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 148.2, 141.7, 137.0, 132.2, 130.6, 130.3, 129.9, 129.8, 127.5, 127.4, 126.7, 126.1, 123.2, 118.7.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{11}BrN$, 284.0; found, 284.0. Spectra data are consistent with the reported literature.[13]

IR: (KBr, cm^{-1}) 1643 (w), 1596 (m), 1553 (m), 1498 (s), 1472 (w), 1451 (w), 1424 (s), 1292 (w), 1235 (w), 1119 (w), 1071 (w), 1023 (w), 829 (s), 759 (s), 741 (s), 712 (s), 641 (m), 618 (w).

m.p.: 103-105 ºC.



7j

Synthesis of 2-(2-iodophenyl)quinoline (7j): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a brown solid (27.2 mg, 43%).

R_f = 0.47 (*n*-hexane:EtOAc = 20:1, UV).

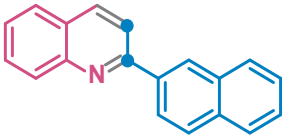
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.21 (dd, *J* = 18.7, 8.5 Hz, 2H), 8.00 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.88 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.76 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.66 – 7.53 (m, 3H), 7.48 (td, *J* = 7.5, 1.2 Hz, 1H), 7.18 – 7.09 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.9, 147.7, 145.4, 139.8, 135.9, 130.5, 130.0, 129.8, 129.7, 128.4, 127.6, 127.2, 126.8, 122.5, 96.6.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{11}IN$, 331.9931; found, 331.9921.

IR: (KBr, cm^{-1}) 1639 (w), 1616 (w), 1592 (m), 1551 (m), 1500 (m), 1474 (w), 1451 (w), 1424 (m), 1310 (w), 1288 (w), 1238 (w), 1120 (w), 1074 (w), 1027 (w), 831 (s), 759 (s), 741 (s), 712 (s), 641 (m), 616 (w).

m.p.: 79-81 ºC.



7k

Synthesis of 2-(naphthalen-2-yl)quinoline (7k): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 10:1) as a yellow solid (from ketone, 54.1 mg, 97%; from alcohol, 33.7 mg, 60%).

R_f = 0.71 (*n*-hexane:EtOAc = 10:1, UV).

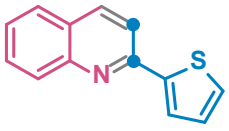
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.61 (s, 1H), 8.37 (d, *J* = 8.5 Hz, 1H), 8.24 (t, *J* = 9.2 Hz, 2H), 8.01 (m, 3H), 7.92 – 7.82 (m, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.57 – 7.49 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 157.2, 148.4, 137.0, 136.8, 133.9, 133.5, 129.8, 128.9, 128.6, 127.8, 127.5, 127.3, 127.2, 126.8, 126.7, 126.4, 125.1, 123.9, 119.2.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{19}H_{14}N$, 256.1; found, 256.1. Spectra data are consistent with the reported literature.[12]

IR: (KBr, cm^{-1}) 1677 (m), 1632 (w), 1596 (m), 1494 (w), 1422 (w), 1360 (w), 1324 (w), 1285 (w), 1195 (w), 1128 (m), 951 (w), 866 (w), 822 (s), 789 (w), 740 (s), 623 (w).

m.p.: 155-156 ºC.



7l

Synthesis of 2-(thiophen-2-yl)quinoline (7l): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a light

yellow solid (38.5 mg, 89%).

R_f = 0.32 (*n*-hexane:EtOAc = 5:1, UV).

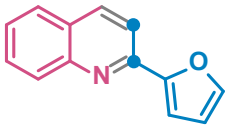
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.17 – 8.10 (m, 2H), 7.84 – 7.76 (m, 2H), 7.78 – 7.69 (m, 2H), 7.54 – 7.47 (m, 2H), 7.19 (dd, *J* = 5.0, 3.7 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 152.4, 148.2, 145.5, 136.7, 129.9, 129.3, 128.7, 128.2, 127.6, 127.3, 126.2, 125.9, 117.7.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{13}H_{10}NS$, 212.1; found, 212.1. Spectra data are consistent with the reported literature.[8]

IR: (KBr, cm^{-1}) 1638 (m), 1589 (w), 1524 (s), 1447 (w), 1367 (s), 1312 (s), 1275 (w), 1177 (m), 1154 (s), 1139 (s), 1117 (m), 1074 (w), 1038 (w), 846 (w), 776 (w), 750 (m), 700 (m), 684 (m), 639 (w).

m.p.: 112-114 ºC.



7m

Synthesis of 2-(furan-2-yl)quinoline (7m): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a brown solid (29.6 mg, 76%).

R_f = 0.36 (*n*-hexane:EtOAc = 5:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.14 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.84 – 7.74 (m, 2H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.62 (s, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.22 (d, *J* = 3.5 Hz, 1H), 6.58 (dd, *J* = 3.5, 1.9 Hz, 1H).

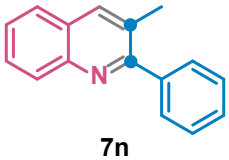
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.8, 149.1, 148.2, 144.2, 136.8, 130.0, 129.4, 127.7, 127.3, 126.3, 117.6, 112.3, 110.2.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{13}H_{10}NS$, 196.1; found, 196.1. Spectra data are

consistent with the reported literature.[14]

IR: (KBr, cm^{-1}) 1638 (s), 1587 (m), 1571 (s), 1527 (s), 1426 (w), 1364 (m), 1314 (w), 1285 (w), 1170 (w), 1154 (w), 1098 (w), 1073 (w), 1028 (w), 855 (w), 823 (m), 771 (m), 747 (s), 686 (s).

m.p.: 107-109 ºC.



7n

Synthesis of 3-methyl-2-phenylquinoline (7n): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a yellow oil (26.2 mg, 63%).

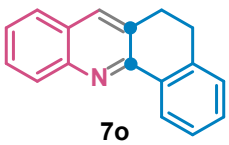
$\mathbf{R_f}$ = 0.41 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.05 (d, *J* = 8.5 Hz, 1H), 7.93 (s, 1H), 7.70 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.58 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.57 – 7.37 (m, 5H), 7.40 – 7.31 (m, 1H), 2.38 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.6, 146.7, 140.9, 136.7, 129.3, 129.2, 128.9, 128.8, 128.3, 128.2, 127.6, 126.7, 126.4, 20.6.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{16}H_{14}N$, 220.1; found, 220.1. Spectra data are consistent with the reported literature.[15]

IR: (KBr, cm^{-1}) 1620 (w), 1598 (m), 1557 (w), 1488 (s), 1447 (m), 1412 (m), 1377 (w), 1331 (w), 1272 (m), 1167 (w), 1120 (w), 1075w), 1010 (s), 904 (m), 860 (w), 767 (s), 753 (s), 702 (s), 618 (w).



7o

Synthesis of 5,6-dihydrobenzo[c]acridine (7o): Following the general procedure B, the title

compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a yellow solid (45.3 mg, 96%).

R_f = 0.42 (*n*-hexane:EtOAc = 20:1, UV).

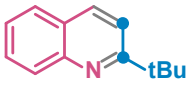
^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.62 (dd, *J* = 7.7, 1.4 Hz, 1H), 8.18 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.94 (d, *J* = 1.2 Hz, 1H), 7.77 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.68 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.41 (td, *J* = 7.4, 1.4 Hz, 1H), 7.33 – 7.27 (m, 1H), 3.15 (ddd, *J* = 8.1, 5.6, 1.1 Hz, 2H), 3.04 (dd, *J* = 8.4, 5.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.4, 147.7, 139.4, 134.8, 133.7, 130.6, 129.7, 129.5, 128.7, 128.0, 127.9, 127.4, 126.9, 126.1, 28.9, 28.4.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{17}H_{14}N$, 232.1; found, 232.1. Spectra data are consistent with the reported literature.[15]

IR: (KBr, cm^{-1}) 1636 (s), 1542 (w), 1493 (w), 1421 (w), 1360 (w), 1127 (m), 950 (w), 866 (w), 821 (s), 761 (w), 740 (m), 622 (m).

m.p.: 161-162 ºC.



7p

Synthesis of 2-(tert-butyl)quinoline (7p): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a colorless oil (17.2 mg, 45%).

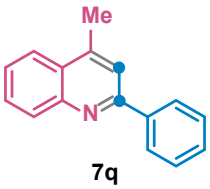
R_f = 0.48 (*n*-hexane:EtOAc = 50:1, UV).

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.12 – 8.07 (m, 2H), 7.79 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.69 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.55 (d, *J* = 8.7 Hz, 1H), 7.50 (ddd, *J* = 8.0, 6.8, 1.2 Hz, 1H), 1.50 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.3, 147.5, 135.9, 129.4, 129.0, 127.2, 126.5, 125.6, 118.2, 38.2, 30.2.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{13}H_{16}N$, 186.1; found, 186.1. Spectra data are consistent with the reported literature.[16]

IR: (KBr, cm^{-1}) 2960 (s), 2928 (m), 2866 (w), 1620 (w), 1601 (m), 1563 (s), 1461 (w), 1427 (w), 1364 (w), 1140 (m), 1103 (m), 1020 (w), 830 (s), 757 (s), 616 (w).



7q

Synthesis of 2-(tert-butyl)quinoline (7q): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a brown oil (32.2 mg, 75%).

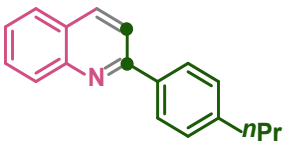
$\mathbf{R_f}$ = 0.31 (*n*-hexane:EtOAc = 50:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) 8.22 – 8.13 (m, 3H), 8.00 (d, J = 8.3 Hz, 1H), 7.73 (m, 2H), 7.54 (q, J = 7.5 Hz, 3H), 7.47 (d, J = 7.0 Hz, 1H), 2.77 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 157.2, 148.3, 144.9, 140.0, 130.4, 129.4, 129.3, 128.9, 127.7, 127.4, 126.1, 123.7, 119.9, 19.1.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{13}H_{13}N$, 220.1; found, 220.1. Spectra data are consistent with the reported literature[12].

IR: (KBr, cm^{-1}) 1644 (s), 1614 (s), 1583 (s), 1549 (s), 1484 (w), 1451 (m), 1361 (m), 1295 (m), 1242 (s), 1162 (m), 955 (w), 751 (s), 613 (m), 520 (w).



7r

Synthesis of 2-(4-propylphenyl)quinoline (7r): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 50:1) as a light yellow solid (34.0 mg, 67%).

R_f = 0.40 (*n*-hexane:EtOAc = 50:1, UV).

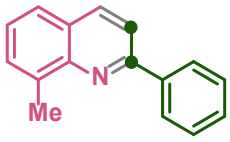
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.18 (dd, *J* = 13.5, 8.6 Hz, 2H), 8.08 (d, *J* = 8.1 Hz, 2H), 7.84 (dd, *J* = 18.3, 8.3 Hz, 2H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 2.67 (t, *J* = 7.6 Hz, 2H), 1.70 (h, *J* = 7.3 Hz, 2H), 0.97 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 157.5, 148.3, 144.2, 137.2, 136.7, 129.8, 129.6, 129.0, 127.5, 127.5, 127.1, 126.1, 119.0, 37.9, 24.5, 13.8.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{18}H_{18}N$, 248.1434; found, 248.1440.

IR: (KBr, cm^{-1}) 1637 (m), 1614 (m), 1595 (s), 1550 (s), 1496 (m), 1461 (w), 1429 (m), 1317 (w), 1284 (w), 1183 (w), 1125 (w), 1014 (w), 822 (s), 801 (s), 784 (m), 756 (s), 679 (w), 616 (w), 562 (w).

m.p.: 73-75 ºC.



7s

Synthesis of 8-methyl-2-phenylquinoline (7s): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a yellow solid (17.9 mg, 43%).

R_f = 0.39 (*n*-hexane:EtOAc = 20:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.27 (d, *J* = 7.2 Hz, 2H), 8.19 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.67 (d, *J* = 8.1 Hz, 1H), 7.60 – 7.51 (m, 3H), 7.44 (m, 2H), 2.91 (s, 3H).

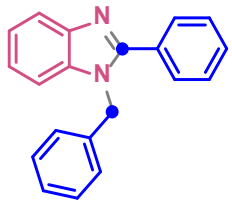
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 147.2, 139.9, 137.7, 137.0, 129.7, 129.2, 128.8, 127.5, 127.1, 126.0, 125.4, 118.2, 17.9.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{16}H_{14}N$, 220.1; found, 220.1. Spectra data are consistent with the reported literature.[17]

IR: (KBr, cm^{-1}) 1636 (m), 1599 (m), 1554 (w), 1492 (m), 1430 (w), 1408 (w), 1290 (w), 1124

(w), 1098 (w), 952 (w), 912 (w), 860 (w), 769 (s), 737 (s), 721 (w), 613 (w).

m.p.: 82-84 ºC.



9a

Synthesis of 1-benzyl-2-phenyl-1H-benzo[d]imidazole (9a): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 2:1) as a white solid (44.6 mg, 77%).

R_f = 0.58 (*n*-hexane:EtOAc = 2:1, UV).

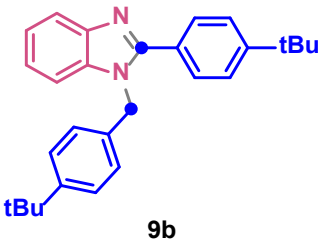
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 6.2 Hz, 2H), 7.46 (q, *J* = 5.8 Hz, 3H), 7.39 – 7.27 (m, 4H), 7.23 (d, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 7.0 Hz, 2H), 5.46 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.6, 143.6, 136.8, 136.5, 130.5, 130.3, 129.7, 129.5, 129.2, 128.2, 126.4, 123.5, 123.1, 120.4, 111.0, 48.8.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{20}H_{17}N_2$, 285.1; found, 285.1. Spectra data are consistent with the reported literature.[18]

IR: (KBr, cm^{-1}) 1639 (w), 1607 (w), 1584 (m), 1493 (m), 1470 (s), 1449 (s), 1390 (s), 1365 (m), 1328 (w), 1277 (w), 1249 (w), 1162 (w), 1074 (w), 1027 (w), 819 (w), 776 (m), 766 (w), 734 (s), 702 (s).

m.p.: 138-139 ºC.



9b

Synthesis of 1-(4-(tert-butyl)benzyl)-2-(4-(tert-butyl)phenyl)-1H-benzo[d]imidazole (9b): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a white solid (48.5 mg, 60%).

R_f = 0.43(*n*-hexane:EtOAc = 5:1, UV).

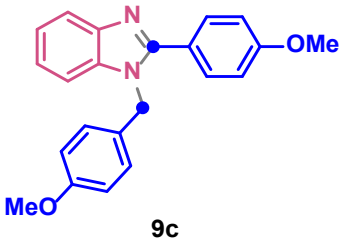
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.32 – 7.27 (m, 1H), 7.23 – 7.18 (m, 2H), 7.05 (d, *J* = 8.1 Hz, 2H), 5.45 (s, 2H), 1.34 (s, 9H), 1.31 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.3, 153.1, 150.7, 143.3, 136.1, 133.5, 129.0, 127.2, 125.9, 125.7, 125.7, 122.8, 122.5, 119.8, 110.6, 48.2, 34.9, 34.6, 31.3, 31.2.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{28}H_{33}N_2$, 397.3; found, 397.3. Spectra data are consistent with the reported literature.[19]

IR: (KBr, cm^{-1}) 1641 (m), 1617 (m), 1584 (m), 1470 (s), 1449 (s), 1394 (m), 1367 (m), 1330 (m), 1277 (m), 1249 (m), 1162 (w), 1072 (w), 1027 (w), 819 (w), 778 (s), 767 (s), 735 (m), 704 (s), 619 (m), 556 (m).

m.p.: 223-225 ºC.



9c

Synthesis of 1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-1H-benzo[d]imidazole (9c): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 4:1) as a brown solid (51.3 mg, 73%).

R_f = 0.39 (*n*-hexane:EtOAc = 4:1, UV).

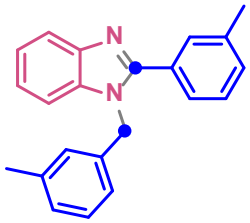
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.7 Hz, 2H), 7.29 (ddd, *J* = 8.1, 5.0, 3.3 Hz, 1H), 7.21 (d, *J* = 4.1 Hz, 2H), 7.03 (d, *J* = 8.3 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.85 (d, *J* = 8.7 Hz, 2H), 5.38 (s, 2H), 3.83 (s, 3H), 3.78 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.9, 159.1, 154.2, 143.1, 136.1, 130.7, 128.5, 127.2, 122.8, 122.6, 122.4, 119.7, 114.4, 114.2, 110.5, 55.4, 55.3, 47.9.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{21}N_2O_2$, 345.2; found, 345.2. Spectra data are consistent with the reported literature.[20]

IR: (KBr, cm^{-1}) 1643 (m), 1610 (s), 1531 (w), 1511 (m), 1480 (m), 1460 (m), 1442 (m), 1417 (w), 1384 (s), 1326 (w), 1295 (m), 1244 (s), 1173 (m), 1108 (w), 984 (w), 834 (m), 812 (m), 782 (w), 764 (w), 736 (s), 544 (w), 517 (w).

m.p.: 119-121 ºC.



9d

Synthesis of 1-(3-methylbenzyl)-2-(m-tolyl)-1H-benzo[d]imidazole (9d): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a yellow oil (50.1 mg, 79%).

R_f = 0.41 (*n*-hexane:EtOAc = 5:1, UV).

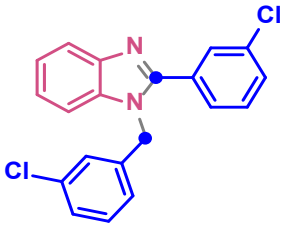
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.88 (d, *J* = 8.0 Hz, 1H), 7.59 (s, 1H), 7.43 (d, *J* = 7.0 Hz, 1H), 7.34 – 7.28 (m, 3H), 7.25 – 7.19 (m, 3H), 7.11 (d, *J* = 7.4 Hz, 1H), 6.96 – 6.88 (m, 2H), 5.41 (s, 2H), 2.38 (s, 3H), 2.30 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.5, 143.2, 138.9, 138.7, 136.6, 136.2, 130.8, 130.3, 130.0, 129.0, 128.6, 128.6, 126.7, 126.1, 123.2, 123.0, 122.7, 120.0, 110.6, 48.5, 21.5, 21.4.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{21}N_2$, 313.2; found, 313.2. Spectra data are consistent with the reported literature.[19]

IR: (KBr, cm^{-1}) 1610 (m), 1591 (w), 1516 (m), 1482 (s), 1454 (s), 1382 (s), 1344 (s), 1330 (s), 1285 (m), 1252 (m), 1201 (w), 1162 (m), 1095 (w), 1040 (w), 1010 (w), 916 (w), 882 (m), 793

(s), 764 (s), 745 (s), 720 (w), 695 (s).



9e

Synthesis of 1-(3-chlorobenzyl)-2-(3-chlorophenyl)-1H-benzo[d]imidazole (9e): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a orange solid (64.9 mg, 90%).

R_f = 0.41 (*n*-hexane:EtOAc = 5:1, UV).

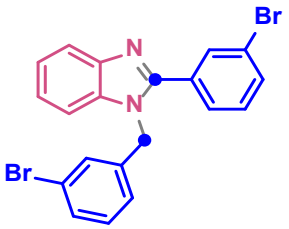
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.88 (d, *J* = 7.9 Hz, 1H), 7.72 (s, 1H), 7.47 (t, *J* = 8.7 Hz, 2H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.28 (t, *J* = 8.5 Hz, 3H), 7.23 (d, *J* = 12.5 Hz, 1H), 7.12 (s, 1H), 6.94 (d, *J* = 6.9 Hz, 1H), 5.41 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 152.5, 143.1, 138.2, 135.9, 135.2, 135.0, 131.6, 130.5, 130.2, 130.1, 129.5, 128.3, 127.1, 126.2, 124.1, 123.7, 123.1, 120.3, 110.4, 47.9.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{20}H_{15}Cl_2N_2$, 353.1; found, 353.1. Spectra data are consistent with the reported literature.[19]

IR: (KBr, cm^{-1}) 1641 (s), 1598 (m), 1572 (m), 1472 (w), 1453 (m), 1440 (m), 1429 (m), 1373 (w), 1340 (w), 1246 (m), 1160 (w), 870 (w), 837 (m), 791 (w), 740 (w), 682 (w).

m.p.: 103-104 ºC.



9f

Synthesis of 1-(3-bromobenzyl)-2-(3-bromophenyl)-1H-benzo[d]imidazole (9f): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-

hexane:EtOAc = 5:1) as a yellow oil (48.6 mg, 54%).

R_f = 0.40 (*n*-hexane:EtOAc = 5:1, UV).

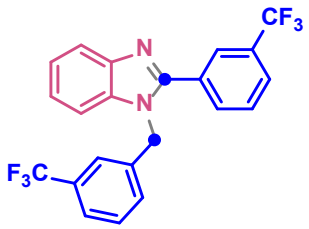
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.88 (d, *J* = 7.4 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.26 (m, 4H), 7.21 (dd, *J* = 15.0, 7.5 Hz, 2H), 6.97 (d, *J* = 7.6 Hz, 1H), 5.40 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 152.4, 143.0, 138.4, 135.9, 133.1, 132.4, 131.8, 131.3, 130.8, 130.3, 129.2, 127.5, 124.6, 123.7, 123.3, 123.2, 123.0, 120.3, 110.3, 47.8.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{20}H_{15}Br_2N_2$, 441.0; found, 441.0. Spectra data are consistent with the reported literature.[21]

IR: (KBr, cm^{-1}) 1638 (s), 1598 (m), 1566 (w), 1513 (w), 1464 (m), 1439 (m), 1398 (m), 1351 (w), 1250 (s), 1162 (w), 1069 (m), 990 (w), 837 (w), 797 (m), 780 (w), 745 (s), 686 (w).

m.p.: 80-81 ºC.



9g

Synthesis of 1-(3-(trifluoromethyl)benzyl)-2-(3-(trifluoromethyl)phenyl)-1H-benzo[d]imidazole (9g): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 2:1) as a brown oil (83.2 mg, 97%).

R_f = 0.55 (*n*-hexane:EtOAc = 2:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90 (m, 2H), 7.76 (dd, *J* = 24.2, 7.7 Hz, 2H), 7.61 – 7.55 (m, 2H), 7.45 (t, *J* = 7.7 Hz, 1H), 7.41 (s, 1H), 7.35 (dd, *J* = 17.3, 7.7 Hz, 2H), 7.29 (s, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 5.49 (s, 2H).

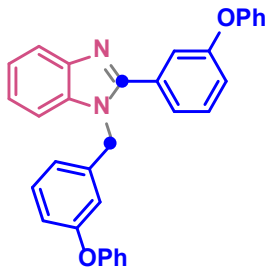
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 152.6, 150.6, 143.1, 137.5, 137.2, 136.1, 132.3, 132.0, 131.8, 131.6, 131.5, 131.3, 131.1, 130.8, 130.0, 130.0, 129.6, 129.5, 129.3, 127.0, 126.93,

126.89, 126.88, 126.85, 126.4, 126.38, 126.36, 126.32, 126.28, 126.2, 125.24, 125.21, 125.17, 125.1, 125.0, 124.1, 123.5, 123.12, 123.08, 123.05, 123.0, 122.5, 122.3, 120.5, 113.9, 110.3, 48.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.82, -62.95.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{15}F_6N_2$, 421.1; found, 421.1. Spectra data are consistent with the reported literature.[21]

IR: (KBr, cm^{-1}) 1616 (w), 1598 (w), 1486 (w), 1457 (s), 1419 (m), 1392 (s), 1329 (s), 1282 (m), 1249 (m), 1168 (s), 1128 (s), 1099 (m), 1073 (s), 910 (w), 848 (w), 808 (m), 746 (s), 700 (s), 662 (w).



9h

Synthesis of 1-(3-phenoxybenzyl)-2-(3-phenoxyphenyl)-1H-benzo[d]imidazole (9h): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 4:1) as a light brown oil (52.6 mg, 55%).

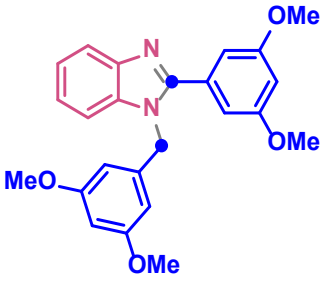
R_f = 0.45 (*n*-hexane:EtOAc = 4:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.83 (d, *J* = 7.9 Hz, 1H), 7.40 (m, 2H), 7.30 (m, 6H), 7.22 (m, 3H), 7.11 (q, *J* = 7.1 Hz, 3H), 7.00 (d, *J* = 7.7 Hz, 2H), 6.95 (d, *J* = 7.8 Hz, 2H), 6.88 (d, *J* = 7.7 Hz, 1H), 6.73 (s, 2H), 5.40 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 158.0, 157.9, 156.5, 153.4, 143.0, 138.2, 135.9, 131.6, 130.5, 130.2, 129.9, 129.9, 123.9, 123.8, 123.7, 123.3, 122.9, 120.5, 120.2, 120.1, 119.3, 119.2, 119.1, 117.8, 116.3, 110.5, 48.1.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{32}H_{25}N_2O_2$, 469.2; found, 469.2. Spectra data are consistent with the reported literature.[22]

IR: (KBr, cm^{-1}) 1584 (s), 1521 (w), 1487 (s), 1447 (s), 1387 (m), 1330 (m), 1251 (s), 1223 (s), 1162 (m), 1072 (w), 945 (w), 919 (m), 787 (m), 747 (s), 693 (s).



9i

Synthesis of 1-(3,5-dimethoxybenzyl)-2-(3,5-dimethoxyphenyl)-1H-benzo[d]imidazole (9i): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 4:1) as a yellow oil (79.5 mg, 96%).

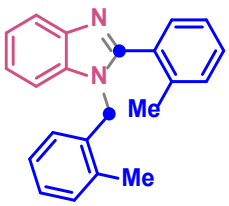
$\mathbf{R}_f$ = 0.36 (*n*-hexane:EtOAc = 4:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.85 (d, *J* = 7.7 Hz, 1H), 7.36 – 7.26 (m, 3H), 6.84 (d, *J* = 1.9 Hz, 2H), 6.54 (s, 1H), 6.36 (s, 1H), 6.26 (s, 2H), 5.39 (s, 2H), 3.69 (d, *J* = 5.0 Hz, 12H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.4, 160.9, 154.0, 142.9, 139.0, 136.2, 131.6 123.3, 122.8, 119.9, 110.5, 107.0, 104.2, 102.9, 99.3, 55.4, 55.3, 48.5.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{24}H_{25}N_2O_4$, 405.2; found, 405.2. Spectra data are consistent with the reported literature.[23]

IR: (KBr, cm^{-1}) 1598 (s), 1517 (m), 1460 (s), 1428 (s), 1389 (m), 1346 (m), 1329 (m), 1253 (w), 1226 (w), 1205 (s), 1158 (s), 1065 (s), 929 (w), 887 (w), 840 (m), 747 (s), 691 (m).



9j

Synthesis of 1-(2-methylbenzyl)-2-(o-tolyl)-1H-benzo[d]imidazole (9j): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-

hexane:EtOAc = 4:1) as a yellow solid (42.3 mg, 66%).

R_f = 0.58 (*n*-hexane:EtOAc = 4:1, UV).

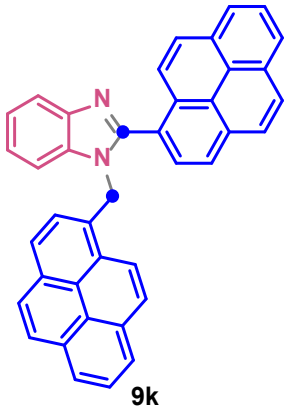
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.26 (m, 4H), 7.24 – 7.09 (m, 5H), 7.02 (t, *J* = 6.1 Hz, 1H), 6.64 (d, *J* = 7.6 Hz, 1H), 5.18 (s, 2H), 2.23 (s, 3H), 2.15 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.9, 143.1, 138.4, 135.0, 134.8, 134.0, 130.6, 130.4, 129.9, 129.8, 127.5, 126.4, 126.0, 125.6, 122.8, 122.4, 120.0, 110.5, 45.8, 19.8, 19.1.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{21}N_2$, 313.2; found, 313.2. Spectra data are consistent with the reported literature.[19]

IR: (KBr, cm^{-1}) 1641 (s), 1481 (m), 1452 (s), 1386 (m), 1358 (w), 1326 (w), 1281 (w), 1251 (w), 1245 (w), 1161 (s), 1103 (w), 1047 (w), 982 (w), 772 (m), 744 (s), 628 (w), 585 (w).

m.p.: 131-132 ºC.



9k

Synthesis of 2-(pyren-1-yl)-1-(pyren-1-ylmethyl)-1H-benzo[d]imidazole (9k): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 2:1) as a light yellow solid (23.0 mg, 21%).

R_f = 0.28 (*n*-hexane:EtOAc = 2:1, UV).

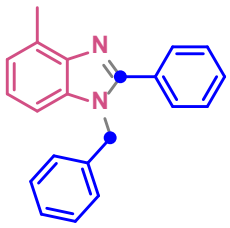
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.20 – 8.12 (m, 4H), 8.06 (d, *J* = 8.3 Hz, 3H), 8.03 – 7.95 (m, 6H), 7.95 – 7.88 (m, 3H), 7.86 – 7.79 (m, 2H), 7.48 – 7.38 (m, 2H), 7.34 – 7.27 (m, 2H), 6.01 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.7, 143.5, 135.7, 132.4, 131.2, 131.1, 130.8, 130.7, 130.4, 128.7, 128.7, 128.6, 128.1, 127.5, 127.4, 127.2, 127.1, 126.3, 126.1, 125.8, 125.7, 125.6, 125.3, 124.8, 124.7, 124.4, 124.3, 124.2, 123.3, 122.8, 121.2, 120.3, 110.8, 46.5.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{40}H_{25}N_2$, 533.2; found, 533.2. Spectra data are consistent with the reported literature.[23]

IR: (KBr, cm^{-1}) 1639 (s), 1601 (m), 1588 (m), 1526 (w), 1483 (w), 1458 (s), 1432 (m), 1397 (s), 1336 (m), 1284 (m), 1255 (w), 1182 (m), 1157 (w), 855 (s), 841 (s), 747 (s), 729 (m), 705 (m), 681 (w).

m.p.: 177-178 ºC.



9l

Synthesis of 1-benzyl-4-methyl-2-phenyl-1H-benzo[d]imidazole (9l): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a yellow solid (39.6 mg, 65%).

R_f = 0.40 (*n*-hexane:EtOAc = 5:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.70 – 7.62 (m, 2H), 7.44 (m, 3H), 7.30 (q, *J* = 8.1, 7.2 Hz, 3H), 7.09 (m, 5H), 5.40 (s, 2H), 2.75 (s, 3H).

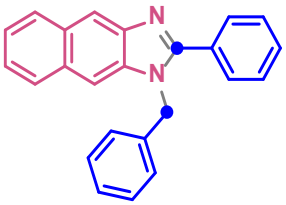
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.5, 142.5, 136.6, 135.6, 130.4, 130.1, 129.8, 129.5, 129.0, 128.7, 127.7, 126.1, 123.0, 122.9, 108.0, 48.4, 16.9.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{21}H_{19}N_2$, 299.2; found, 299.2. Spectra data are consistent with the reported literature.[23]

IR: (KBr, cm^{-1}) 1635 (m), 1601 (m), 1497 (m), 1469 (s), 1451 (s), 1424 (m), 1387 (s), 1358 (s), 1330 (m), 1301 (w), 1260 (m), 1246 (m), 1151 (m), 1111 (w), 1075 (w), 1030 (w), 925 (m),

809 (w), 776 (m), 753 (s), 737 (s), 719 (s), 696 (s), 655 (m), 597 (w), 559 (w).

m.p.: 105-106 ºC.



9m

Synthesis of 1-benzyl-2-phenyl-1H-naphtho[2,3-d]imidazole (9m): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 2:1) as a brown solid (51.8 mg, 76%).

R_f = 0.48 (*n*-hexane:EtOAc = 2:1, UV).

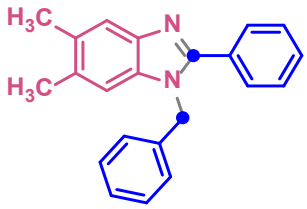
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.26 (s, 1H), 7.99 – 7.91 (m, 1H), 7.81 – 7.72 (m, 1H), 7.69 (d, *J* = 6.7 Hz, 2H), 7.53 (s, 1H), 7.43 (p, *J* = 6.9 Hz, 3H), 7.29 (ddd, *J* = 24.3, 12.5, 6.2 Hz, 5H), 7.18 (s, 1H), 7.10 (d, *J* = 7.1 Hz, 2H), 5.47 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 158.1, 148.6, 143.2, 136.3, 130.7, 130.4, 129.8, 129.4, 129.2, 128.9, 128.6, 127.8, 127.5, 127.0, 126.0, 124.4, 123.6, 116.9, 106.3, 48.7.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{24}H_{19}N_2$, 335.2; found, 335.2. Spectra data are consistent with the reported literature.[24]

IR: (KBr, cm^{-1}) 1634 (s), 1478 (m), 1444 (s), 1396 (m), 1366 (m), 1311 (w), 1262 (m), 1099 (w), 1076 (s), 1026 (s), 855 (w), 802 (m), 775 (m), 738 (m), 702 (s).

m.p.: 88-90 ºC.



9n

Synthesis of 1-benzyl-5,6-dimethyl-2-phenyl-1H-benzo[d]imidazole (9n): Following the

general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 2:1) as a yellow solid (28.8 mg, 45%).

R_f = 0.53 (*n*-hexane:EtOAc = 2:1, UV).

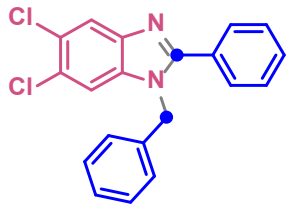
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.69 – 7.64 (m, 2H), 7.62 (s, 1H), 7.43 (m, 3H), 7.33 (q, *J* = 9.6, 8.1 Hz, 3H), 7.10 (d, *J* = 6.9 Hz, 2H), 6.97 (s, 1H), 5.41 (s, 1H), 2.39 (s, 1H), 2.32 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.4, 141.8, 136.7, 134.7, 132.3, 131.6, 130.4, 129.7, 129.2, 129.1, 128.7, 127.7, 125.9, 120.0, 110.6, 48.3, 20.6, 20.3.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{21}N_2$, 313.2; found, 313.2. Spectra data are consistent with the reported literature.[24]

IR: (KBr, cm^{-1}) 1643 (m), 1608 (m), 1495 (m), 1469 (s), 1444 (s), 1415 (m), 1389 (s), 1359 (s), 1303 (m), 1386 (m), 1157 (w), 1108 (w), 1077 (w), 1027 (m), 953 (m), 927 (w), 890 (m), 835 (s), 810 (m), 793 (m), 772 (s), 725 (s), 700 (s), 702 (s), 677 (m), 652 (m), 612 (w), 570 (w).

m.p.: 203-205 ºC.



9o

Synthesis of 1-benzyl-5,6-dichloro-2-phenyl-1H-benzo[d]imidazole (9o): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 4:1) as a white solid (43.1 mg, 60%).

R_f = 0.41 (*n*-hexane:EtOAc = 4:1, UV).

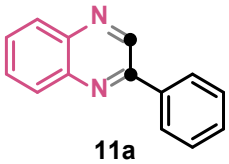
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.93 (s, 1H), 7.66 (d, *J* = 6.6 Hz, 3H), 7.48 (s, 2H), 7.35 (s, 2H), 7.29 (s, 1H), 7.07 (d, *J* = 6.6 Hz, 3H), 5.41 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 156.1, 142.5, 135.5, 130.5, 129.3, 129.2, 129.0, 128.2, 127.0, 126.8, 125.8, 121.2, 111.9, 48.6.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{20}H_{15}Cl_2N_2$, 353.1; found, 353.0. Spectra data are consistent with the reported literature.[24]

IR: (KBr, cm^{-1}) 1644 (m), 1631 (m), 1493 (m), 1477 (s), 1451 (s), 1393 (s), 1366 (s), 1323 (m), 1311 (m), 1282 (w), 1181 (w), 1156 (w), 1075 (w), 1018 (w), 994 (s), 870 (w), 843 (m), 775 (m), 744 (m), 726 (m), 704 (s), 571 (w).

m.p.: 139-141 ºC.



11a

Synthesis of 2-phenylquinoxaline (11a): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a brown solid (41.4 mg, 99%).

R_f = 0.41 (*n*-hexane:EtOAc = 20:1, UV).

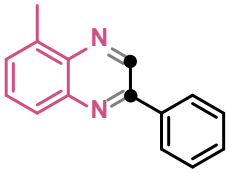
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.34 (s, 1H), 8.17 (m, 4H), 7.84 – 7.73 (m, 2H), 7.57 (dt, *J* = 12.7, 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.9, 143.4, 142.3, 141.6, 136.8, 130.3, 130.2, 129.7, 129.6, 129.2, 129.2, 127.6.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{14}H_{11}N_2$, 207.1; found, 207.1. Spectra data are consistent with the reported literature.[25]

IR: (KBr, cm^{-1}) 1637 (s), 1571 (w), 1542 (m), 1532 (m), 1486 (w), 1444 (w), 1311 (w), 1205 (w), 1121 (w), 1047 (w), 1027 (w), 953 (m), 917 (w), 767 (s), 749 (s), 687 (s), 668 (m), 548 (m).

m.p.: 92-93 ºC.



11b

Synthesis of 5-methyl-2-phenylquinoxaline (11b): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a light orange solid (36.6 mg, 81%).

R_f = 0.27 (*n*-hexane:EtOAc = 20:1, UV).

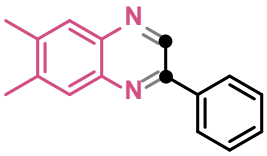
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.34 (s, 1H), 8.26 (d, *J* = 7.2 Hz, 2H), 7.99 – 7.91 (m, 1H), 7.63 (d, *J* = 6.7 Hz, 2H), 7.56 (m, 3H), 2.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 150.2, 142.6, 141.7, 141.4, 138.0, 137.1, 130.2, 130.1, 129.3, 129.1, 127.5, 126.9, 17.1.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{15}H_{13}N_2$, 221.1; found, 221.1. Spectra data are consistent with the reported literature.[25]

IR: (KBr, cm^{-1}) 1643 (m), 1611 (m), 1544 (m), 1485 (m), 1446 (w), 1315 (m), 1205 (w), 1144 (w), 1085 (m), 1021 (w), 972 (w), 918 (w), 822 (m), 768 (s), 685 (s), 540 (m).

m.p.: 95-97 ºC.



11c

Synthesis of 6,7-dimethyl-2-phenylquinoxaline (11c): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 10:1) as an orange solid (35.1 mg, 73%).

R_f = 0.46 (*n*-hexane:EtOAc = 10:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.22 (s, 1H), 8.16 (d, *J* = 7.2 Hz, 2H), 7.87 (d, *J* = 20.7

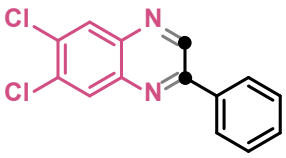
Hz, 1H), 7.53 (m, 3H), 2.51 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.0, 142.4, 141.3, 140.8, 140.6, 140.1, 137.2, 129.9, 129.1, 128.7, 128.2, 127.4, 20.4, 20.4.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{16}H_{15}N_2$, 235.1; found, 235.1. Spectra data are consistent with the reported literature.[25]

IR: (KBr, cm^{-1}) 1634 (s), 1536 (m), 1484 (m), 1449 (m), 1311 (m), 1278 (w), 1210 (m), 1108 (w), 1047 (w), 1022 (m), 1000 (m), 950 (w), 868 (s), 766 (s), 687 (s), 660 (m), 613 (m).

m.p.: 127-129 ºC.



11d

Synthesis of 6,7-dichloro-2-phenylquinoxaline (11d): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 20:1) as a brown solid (**11d**, 38.8 mg, 69%).

R_f = 0.33 (*n*-hexane:EtOAc = 20:1, UV).

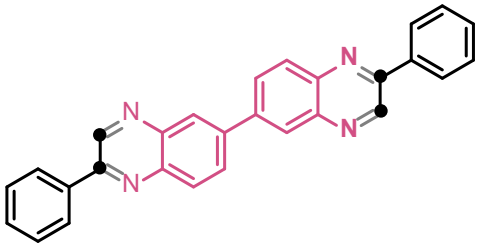
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.32 (s, 1H), 8.34 – 8.09 (m, 4H), 7.58 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 152.7, 144.3, 141.1, 140.3, 136.0, 135.0, 134.0, 130.8, 130.2, 129.8, 129.3, 127.6.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{14}H_9Cl_2N_2$, 275.0; found, 275.0. Spectra data are consistent with the reported literature.[25]

IR: (KBr, cm^{-1}) 1642 (s), 1539 (w), 1464 (s), 1445 (m), 1319 (s), 1280 (w), 1177 (s), 1113 (s), 944 (w), 921 (w), 874 (w), 761 (m), 684 (s), 621 (w), 546 (w).

m.p.: 142-143 ºC.



11e

Synthesis of 2,2'-diphenyl-6,6'-biquinoxaline (11e): Following the general procedure C, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 2:1) as a light yellow solid (22.2 mg, 32%).

R_f = 0.28 (*n*-hexane:EtOAc = 2:1, UV).

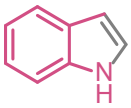
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.39 (d, *J* = 14.6 Hz, 2H), 8.61 – 8.50 (m, 2H), 8.37 – 8.15 (m, 8H), 7.66 – 7.50 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 144.1, 143.7, 142.6, 136.7, 136.1, 130.4, 129.9, 129.2, 129.1, 127.9, 127.6, 127.5.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{28}H_{19}N_4$, 411.1604; found, 411.1600.

IR: (KBr, cm^{-1}) 1638 (s), 1540 (m), 1446 (w), 1400 (w), 1318 (w), 1104 (m), 1051 (w), 1026 (w), 959 (w), 823 (m), 759 (m), 684 (m).

m.p.: 222-224 ºC.



13

Synthesis of indole (13): Following the general procedure B, the title compound was isolated by flash chromatography (SiO_2, *n*-hexane:EtOAc = 5:1) as a white solid (43.1 mg, 91%).

R_f = 0.36 (*n*-hexane:EtOAc = 5:1, UV).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.14 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.17 – 7.11 (m, 1H), 6.58 (s, 1H).

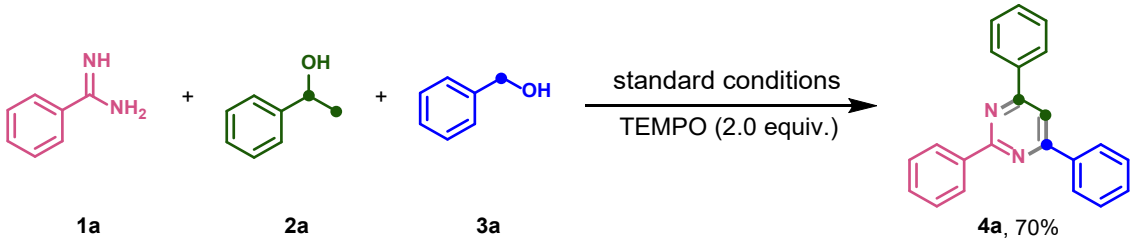
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 135.8, 127.9, 124.2, 122.0, 120.8, 119.9, 111.1, 102.6.

LRMS ESI: (m/z) $[M+H]^+$ calcd. for C_8H_8N, 118.1; found, 118.1. Spectra data are consistent with the reported literature.[26]

IR: (KBr, cm^{-1}) 1619 (s), 1503 (w), 1489 (w), 1455 (s), 1352 (m), 1335 (m), 1277 (w), 1245 (w), 1092 (m), 1008 (w), 932 (w), 767 (s), 745 (s), 725 (s), 609 (m).

m.p.: 52-53 ºC.

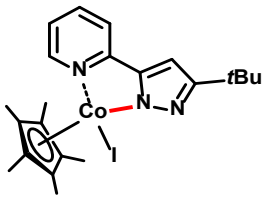
6. Radical Inhibition Experiment



Scheme S2. Radical inhibition experiment for **4a**

Under the standard reaction conditions, 2 equivalents of 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) were added as radical scavenger. The target product **4a** was isolated in 70% yield, which indicates the reaction may not go through a radical pathway.

7. Identification of Catalytic Active Species and Reaction Intermediate



[cat. **A1**]

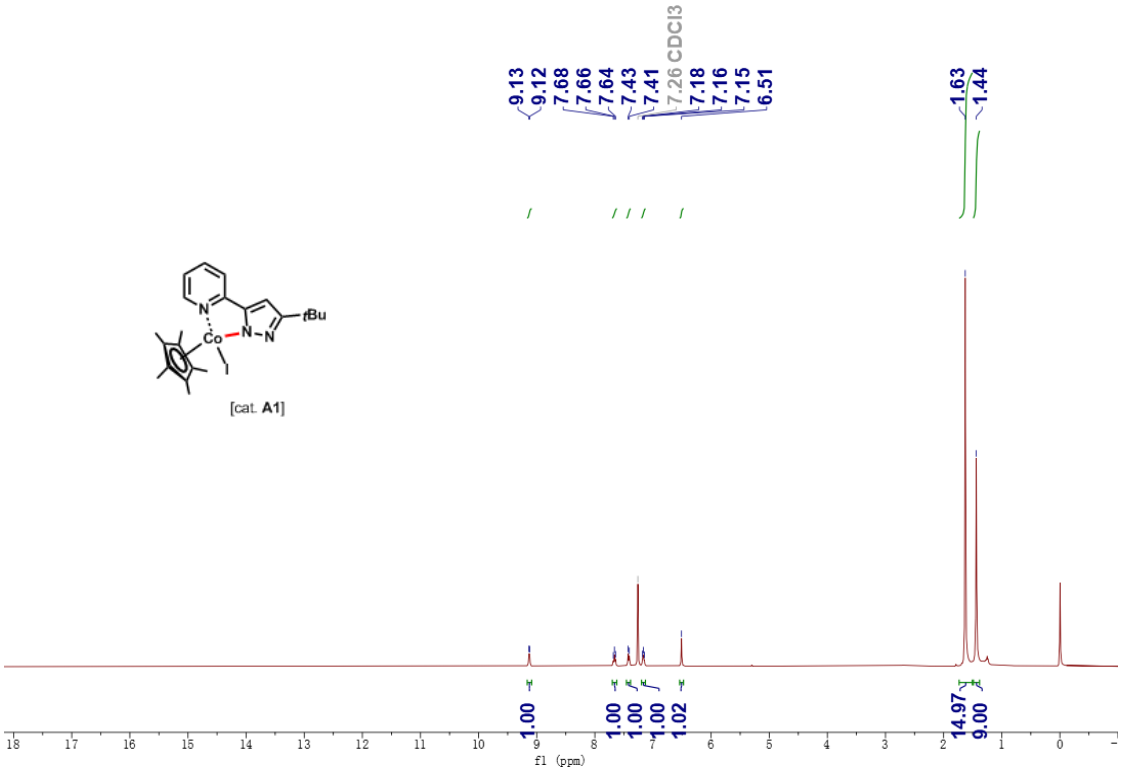
Synthesis of cat. A1: Catalyst **A** (131 mg, 0.2 mmol) was placed in a flame-dried Schlenk flask and was dissolved in 10 mL of dry benzene. Upon addition of potassium tert-butoxide (22.4 mg, 0.2 mmol) at 0 ºC the solution turned dark red and was allowed to stir at room temperature for 3 h. The resulted solution was filtered through a Schlenk frit using a pad of celite under inert atmosphere. The filtrate was evaporated completely under reduced pressure and the residue obtained was redissolved in 0.5 mL of dichloromethane. Hexane was added with stirring to induce precipitation. The solution was discarded by cannula filtration and the precipitate was further washed with hexane (3 × 10 mL). Finally, it was dried under vacuum to afford **A1** as an orange powder. Yield: 83 mg (63%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.13 (d, J = 5.3 Hz, 1H), 7.66 (t, J = 7.7 Hz, 1H), 7.42 (d, J = 7.7 Hz, 1H), 7.16 (t, J = 6.4 Hz, 1H), 6.51 (s, 1H), 1.63 (s, 15H), 1.46 (s, 9H).

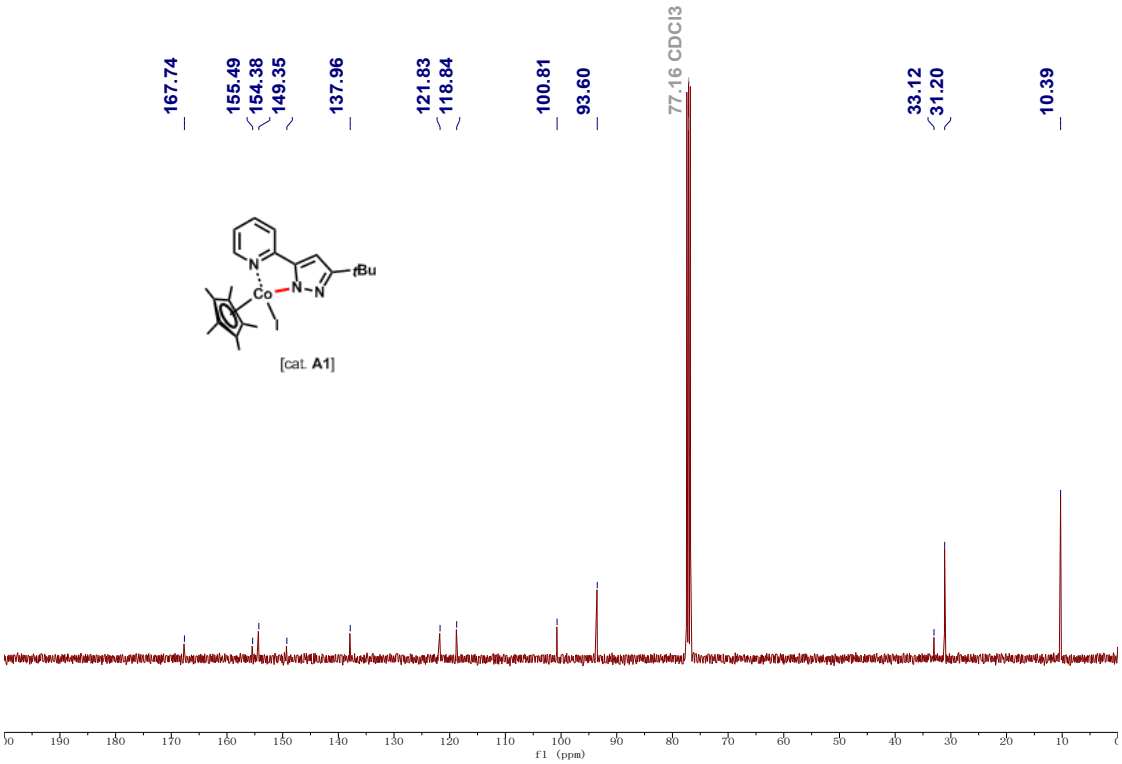
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.7, 155.5, 154.4, 149.4, 138.0, 121.8, 118.8, 100.8, 93.6, 33.1, 31.2, 10.4.

HRMS ESI: (m/z) $[M+H]^+$ calcd. for $C_{22}H_{29}CoIN_3$: 522.0811, found: 522.0820.

^{1}H NMR spectra for cat. **A1** (400 MHz, $CDCl_3$):

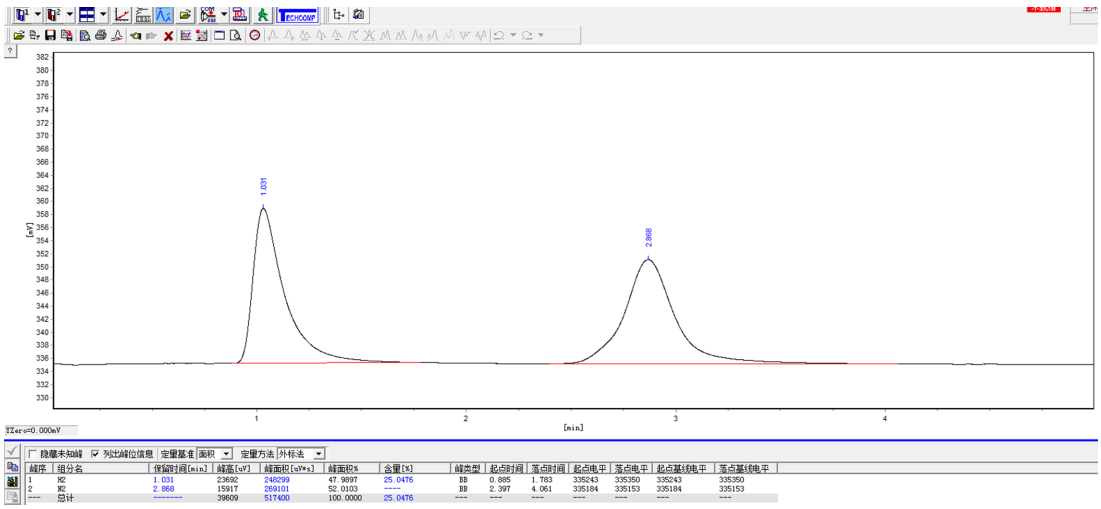


^{13}C NMR spectra for cat. **A1** (100 MHz, $CDCl_3$):



8. Detection of H_2 by GC analysis

The detection of H_2 was carried out using the model reaction, after the completion of the reaction, the content of the gas phase in the reaction vial was determined by gas-phase GC, the retention time of H_2 and N_2 are 1.031 minutes and 2.868 minutes, respectively. The liberation of H_2 was obviously observed.



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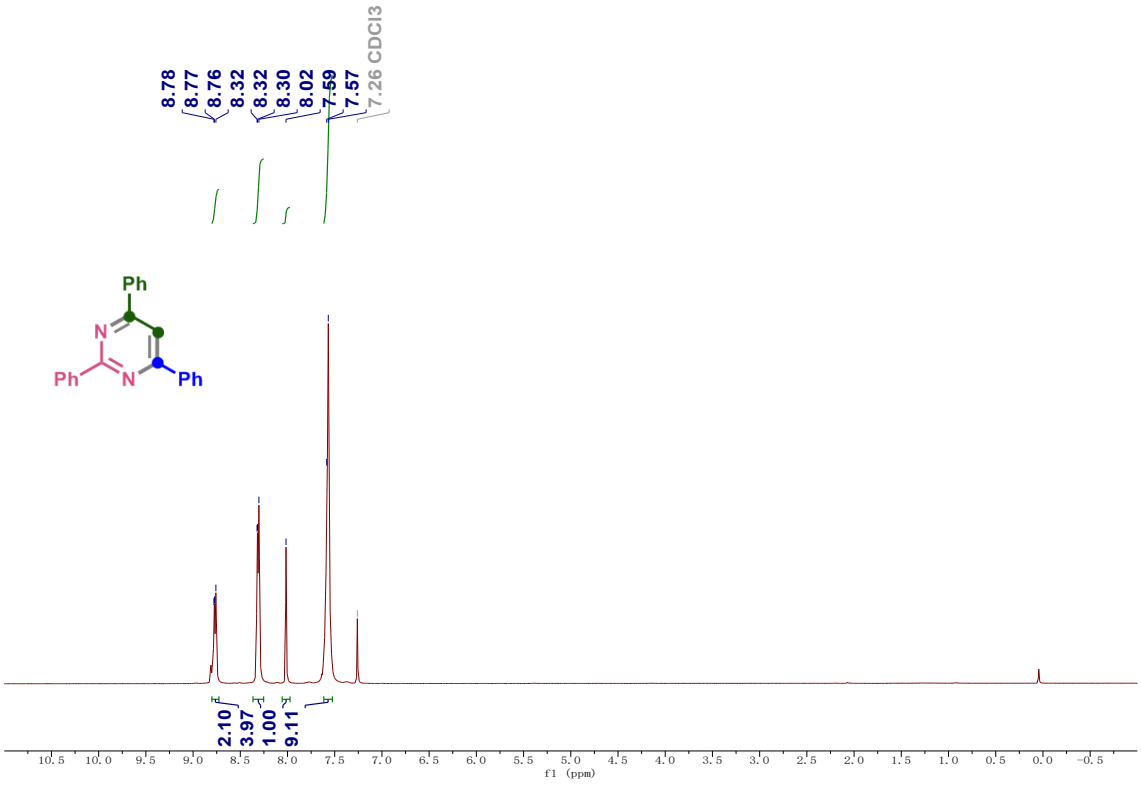
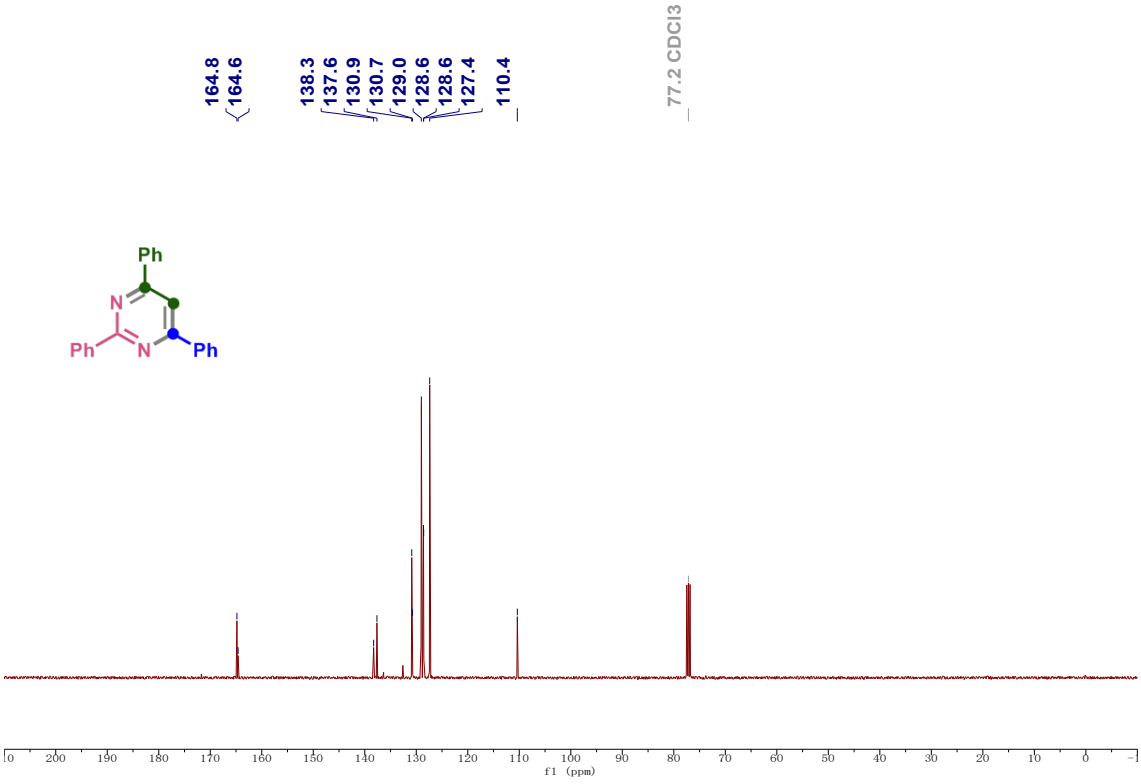
10. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra:

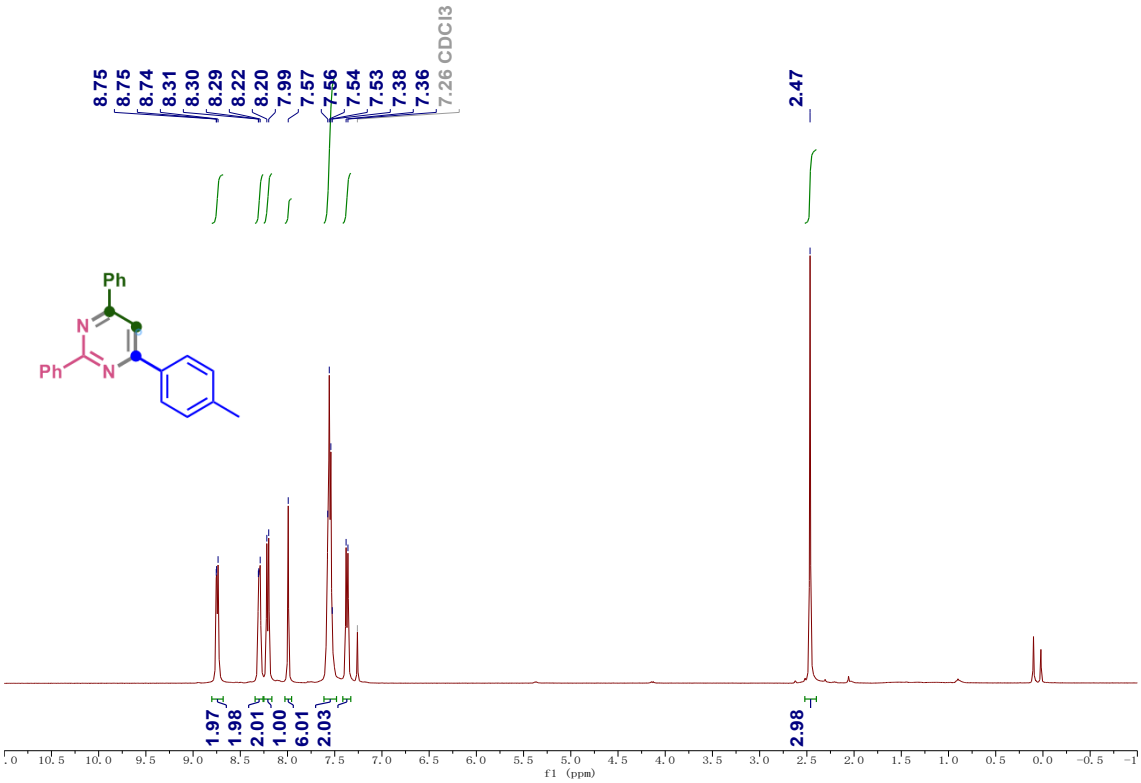
^{1}H NMR spectrum of **4a** (400 MHz, $CDCl_3$)



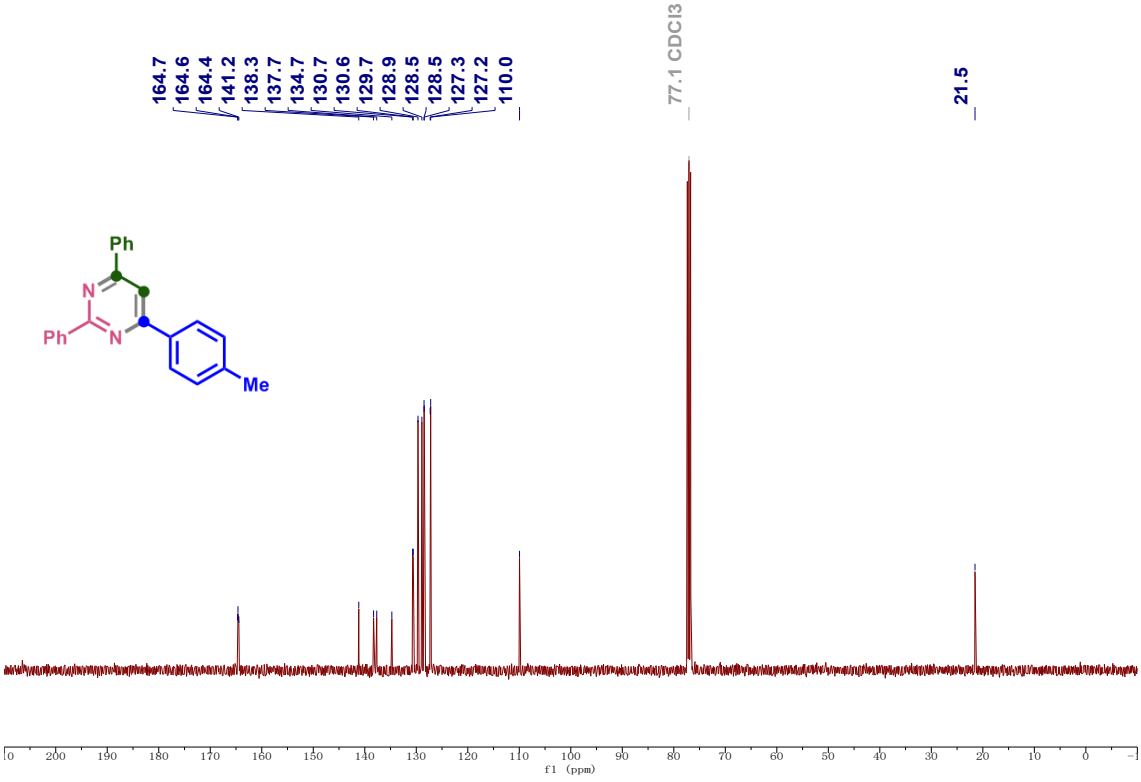
^{13}C NMR spectrum of **4a** (100 MHz, $CDCl_3$)



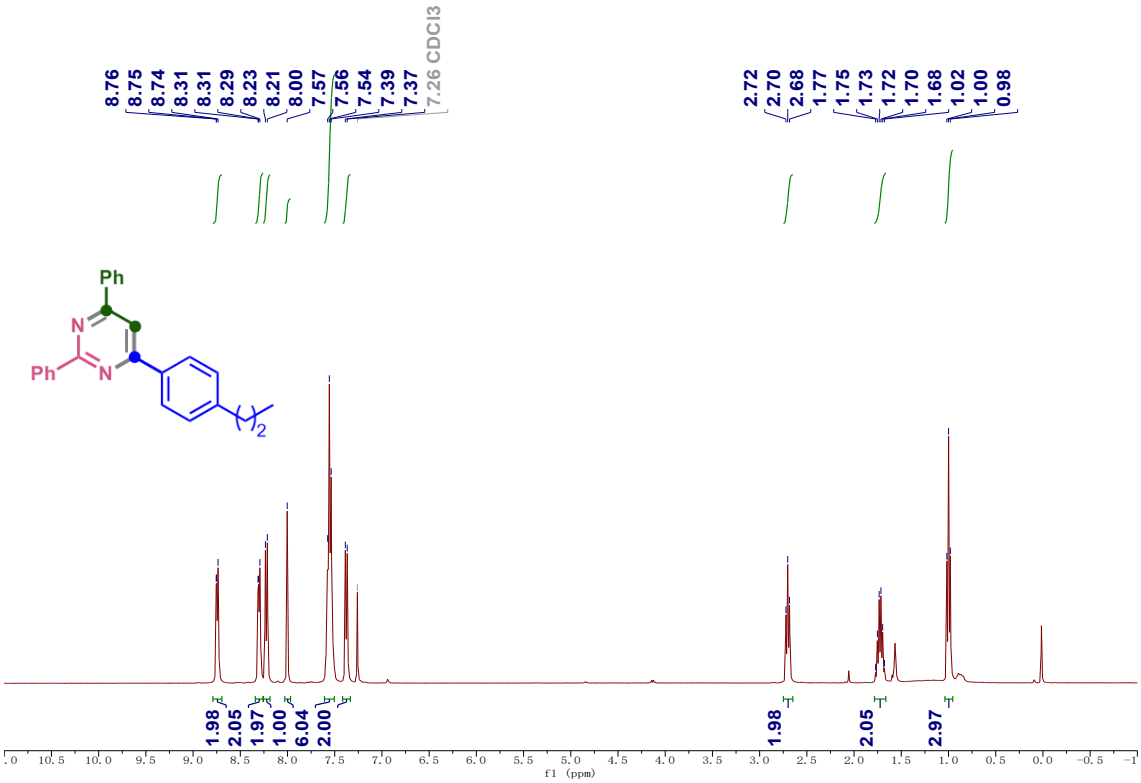
^{1}H NMR spectrum of **4b** (400 MHz, $CDCl_3$)



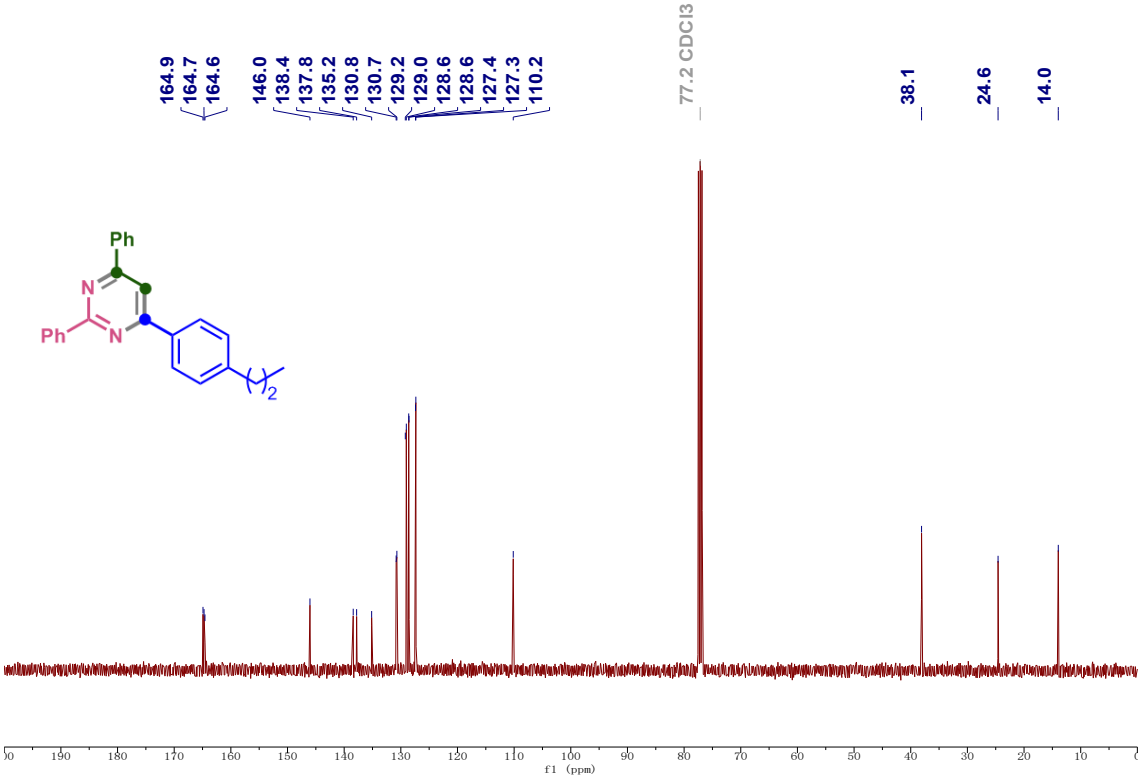
^{13}C NMR spectrum of **4b** (100 MHz, $CDCl_3$)



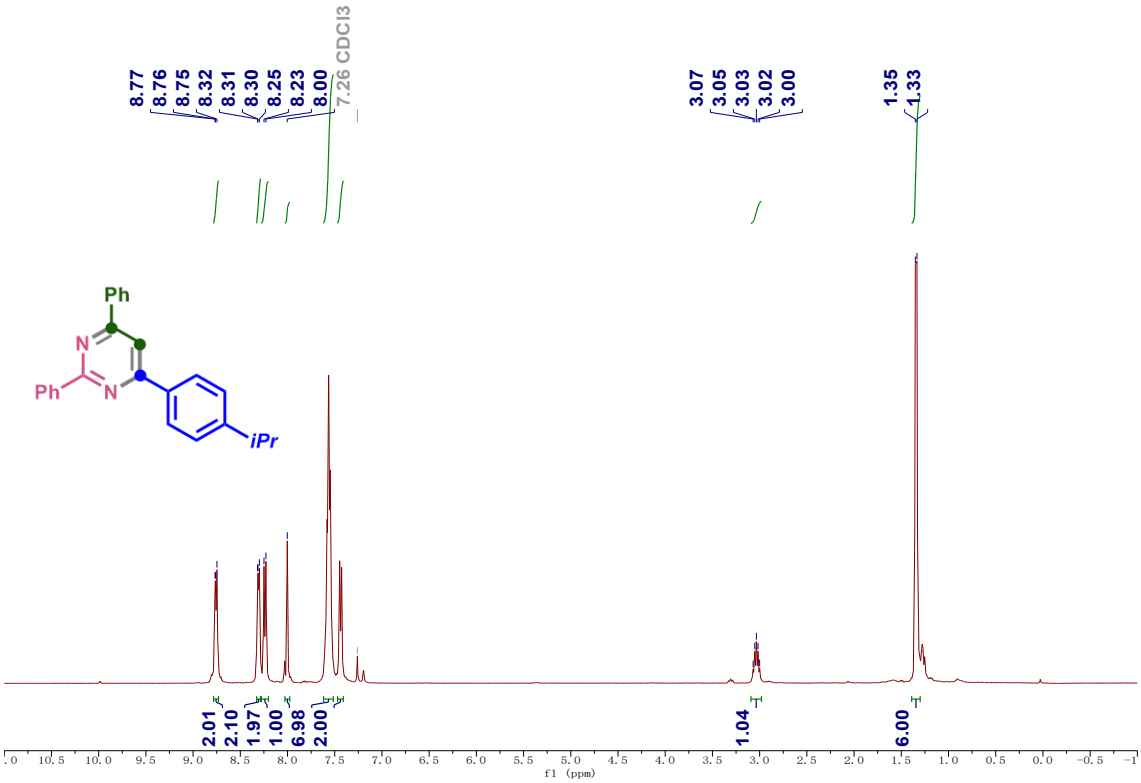
^{1}H NMR spectrum of **4c** (400 MHz, $CDCl_3$)



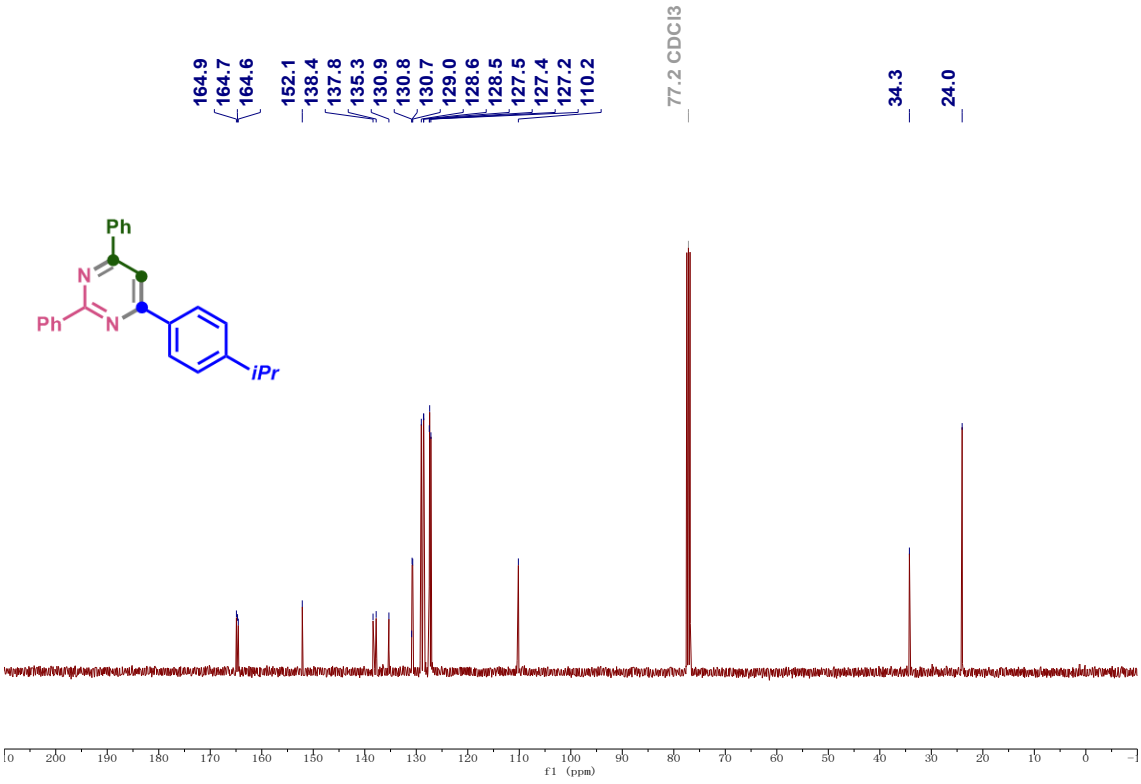
^{13}C NMR spectrum of **4c** (100 MHz, $CDCl_3$)



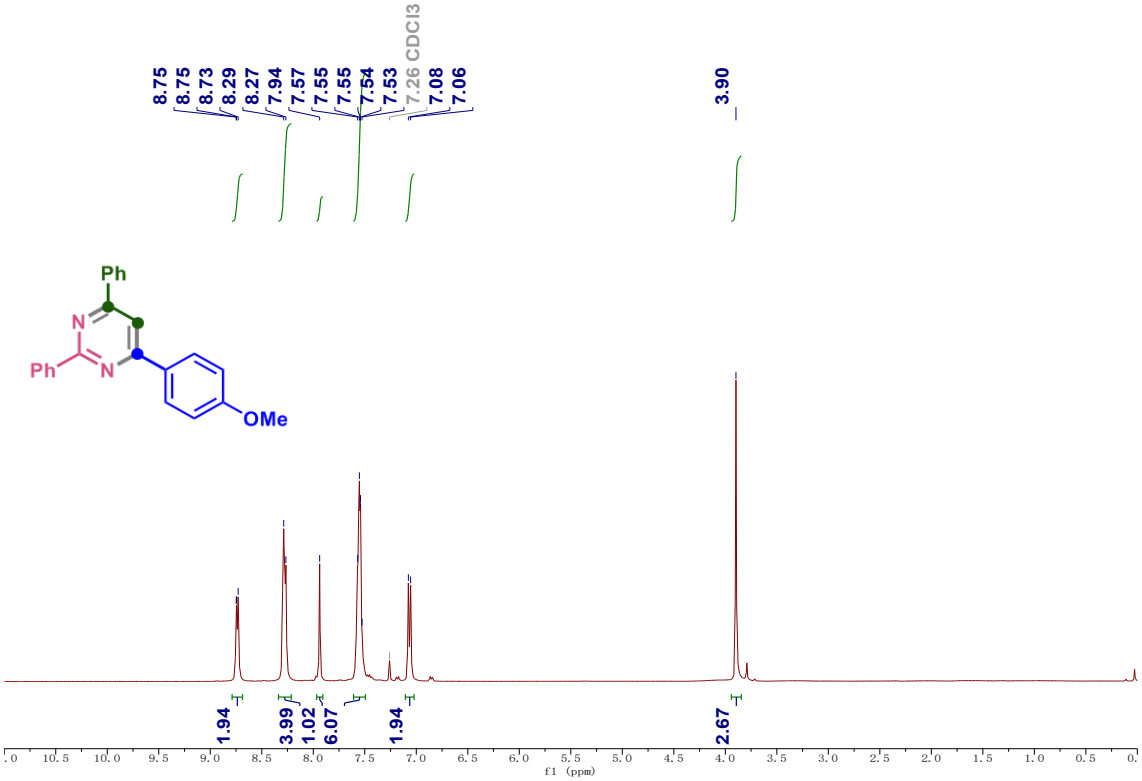
^{1}H NMR spectrum of **4d** (400 MHz, $CDCl_3$)



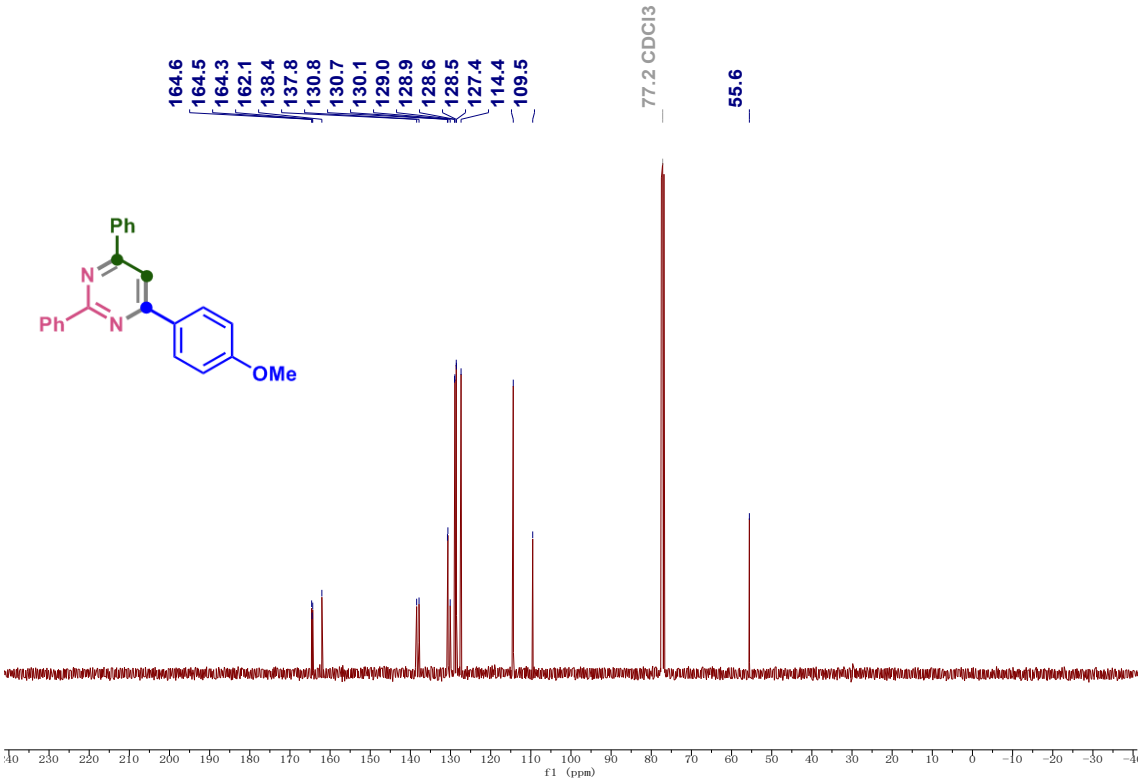
^{13}C NMR spectrum of **4d** (100 MHz, $CDCl_3$)



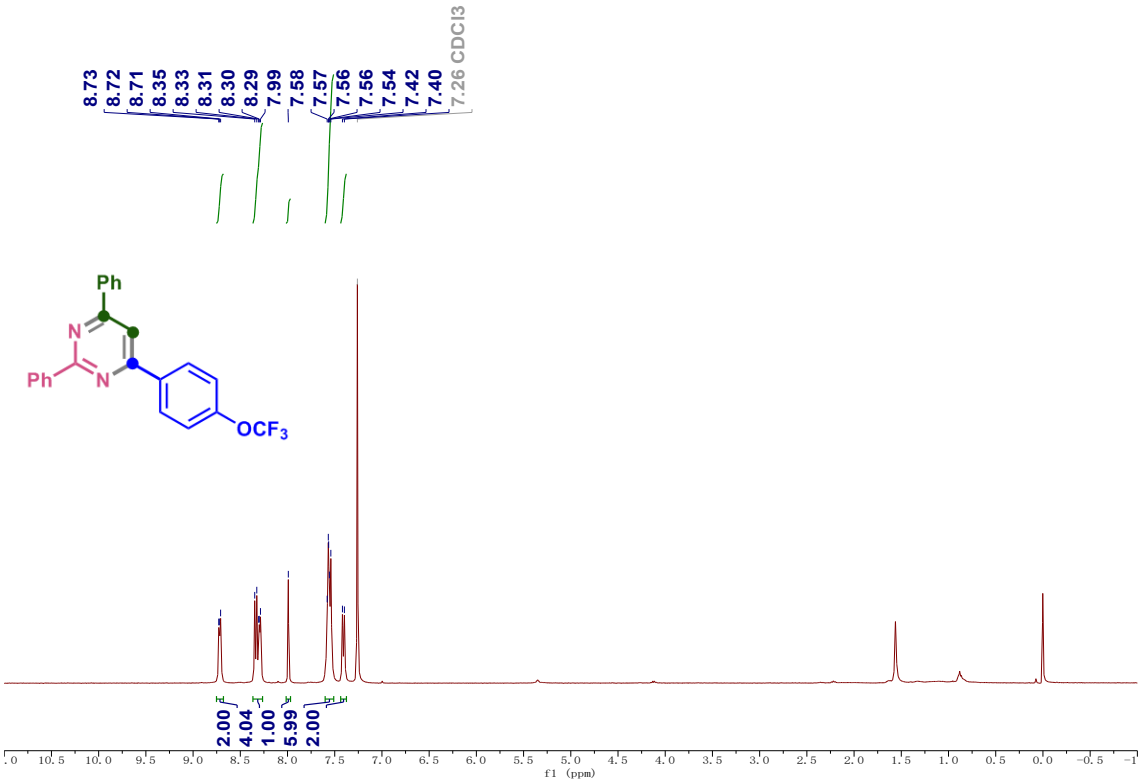
^{1}H NMR spectrum of **4e** (400 MHz, $CDCl_3$)



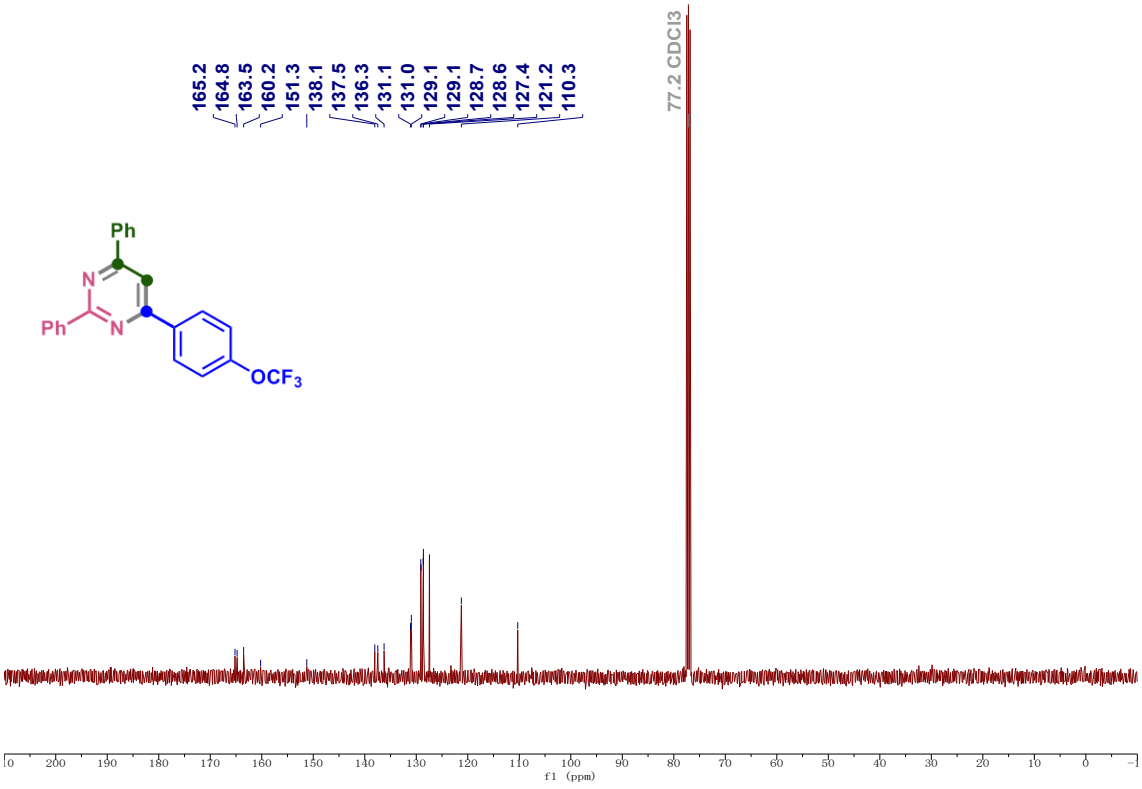
^{13}C NMR spectrum of **4e** (100 MHz, $CDCl_3$)



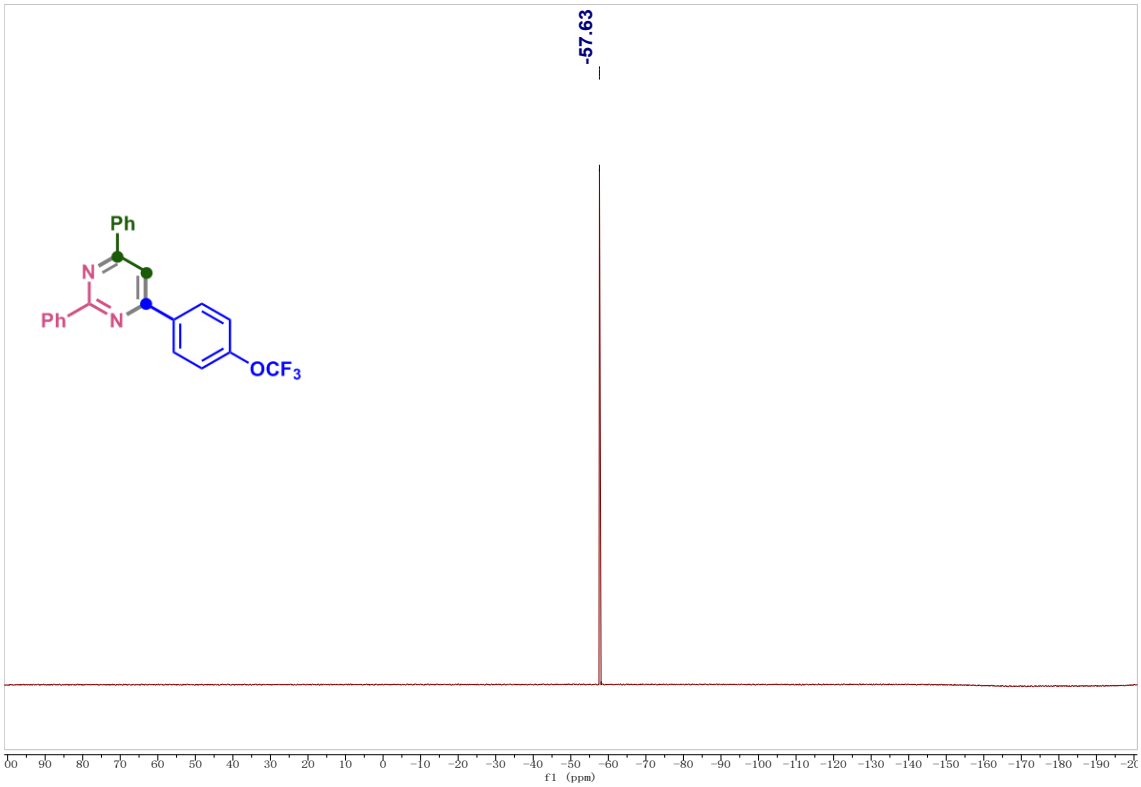
^{1}H NMR spectrum of **4f** (400 MHz, $CDCl_3$)



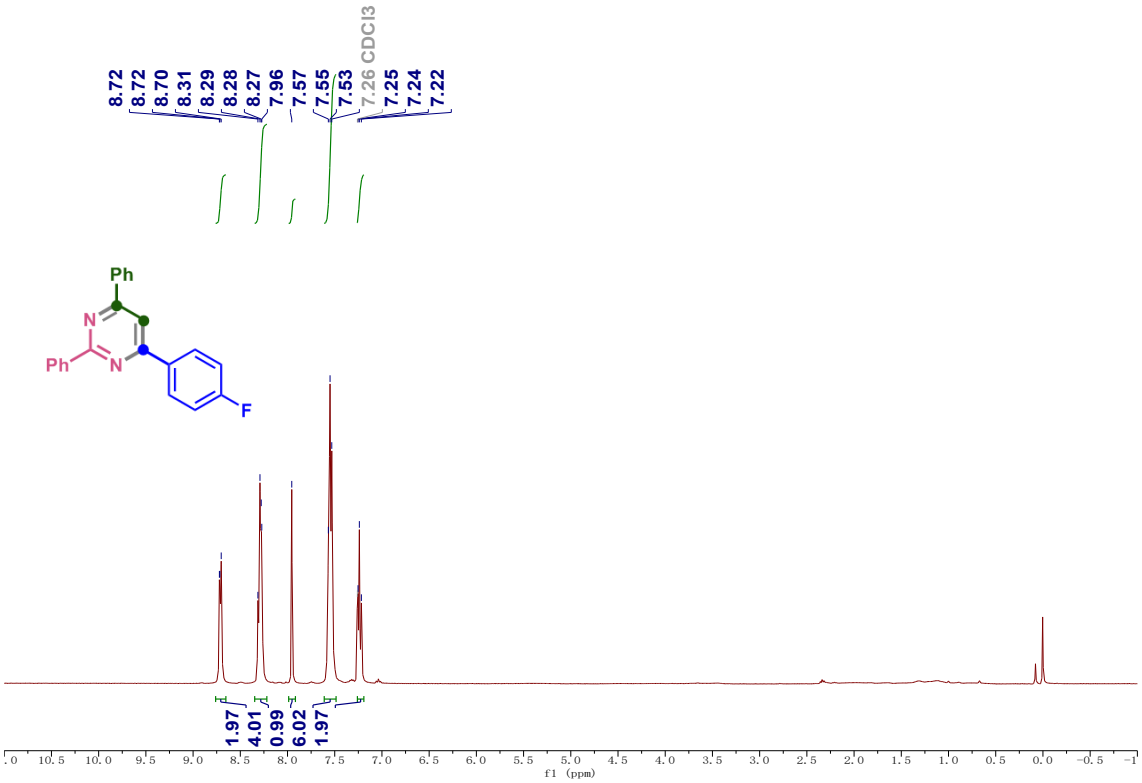
^{13}C NMR spectrum of **4f** (100 MHz, $CDCl_3$)



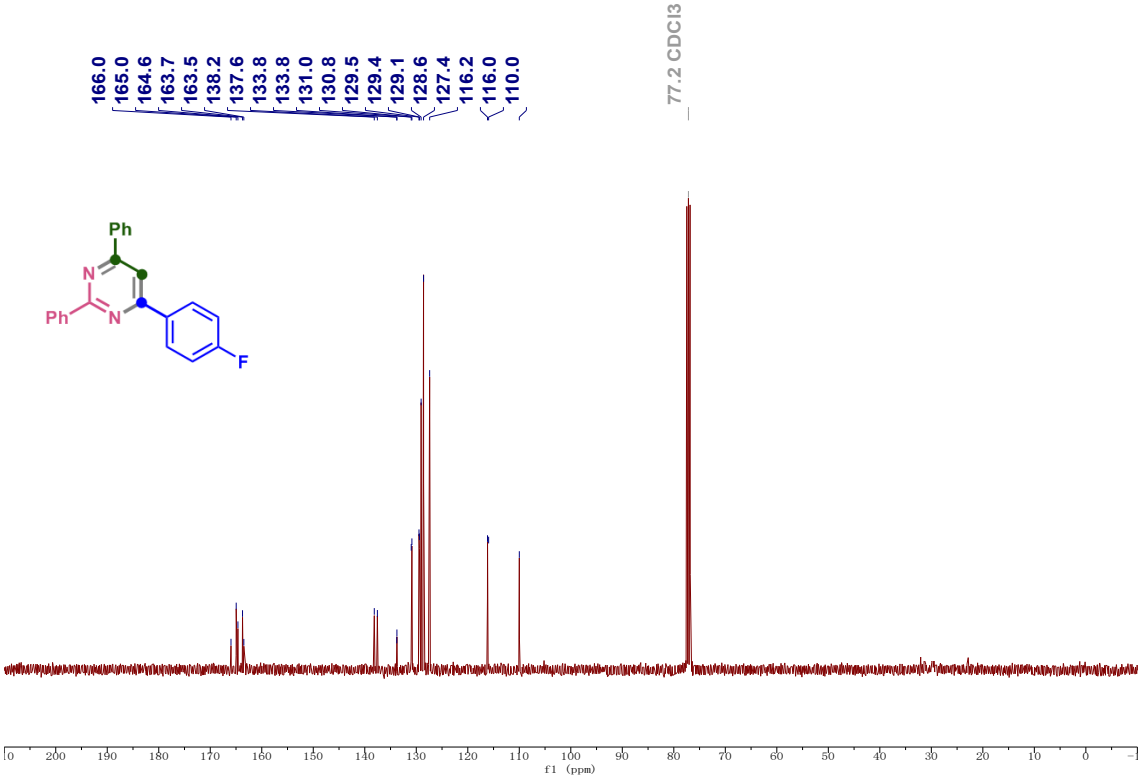
^{19}F NMR spectrum of **4f** (376 MHz, $CDCl_3$)



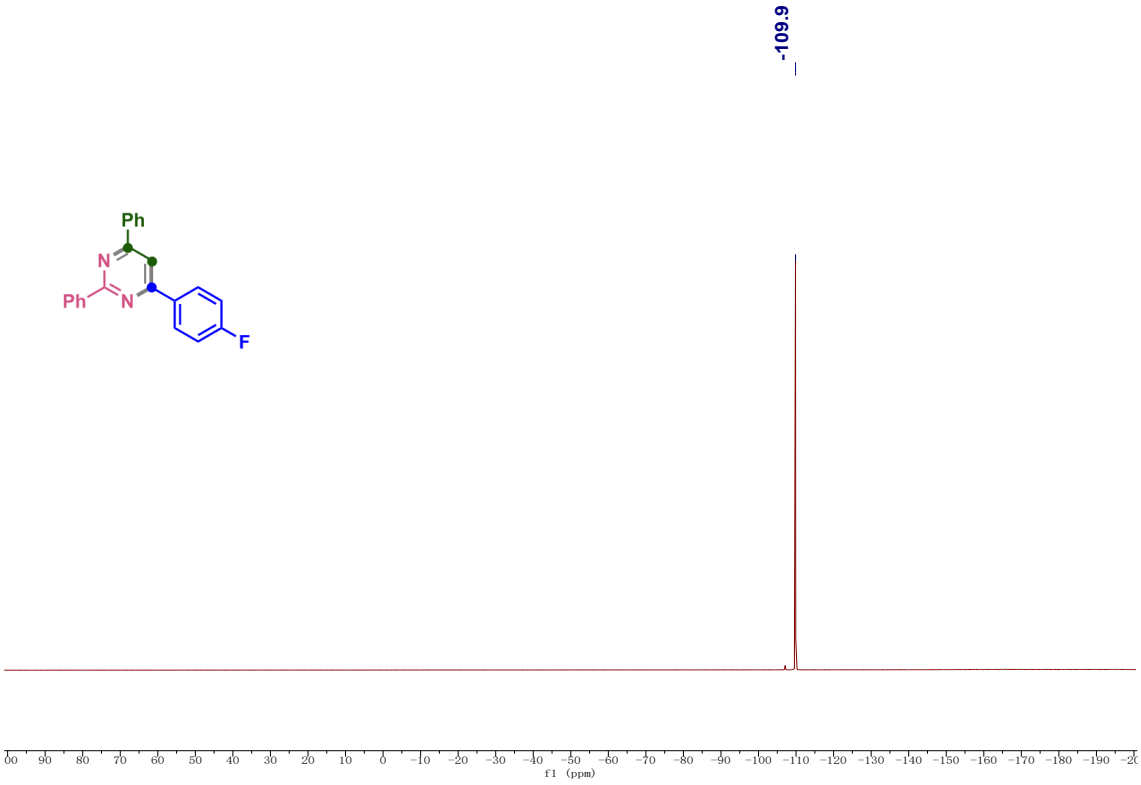
^{1}H NMR spectrum of **4g** (400 MHz, $CDCl_3$)



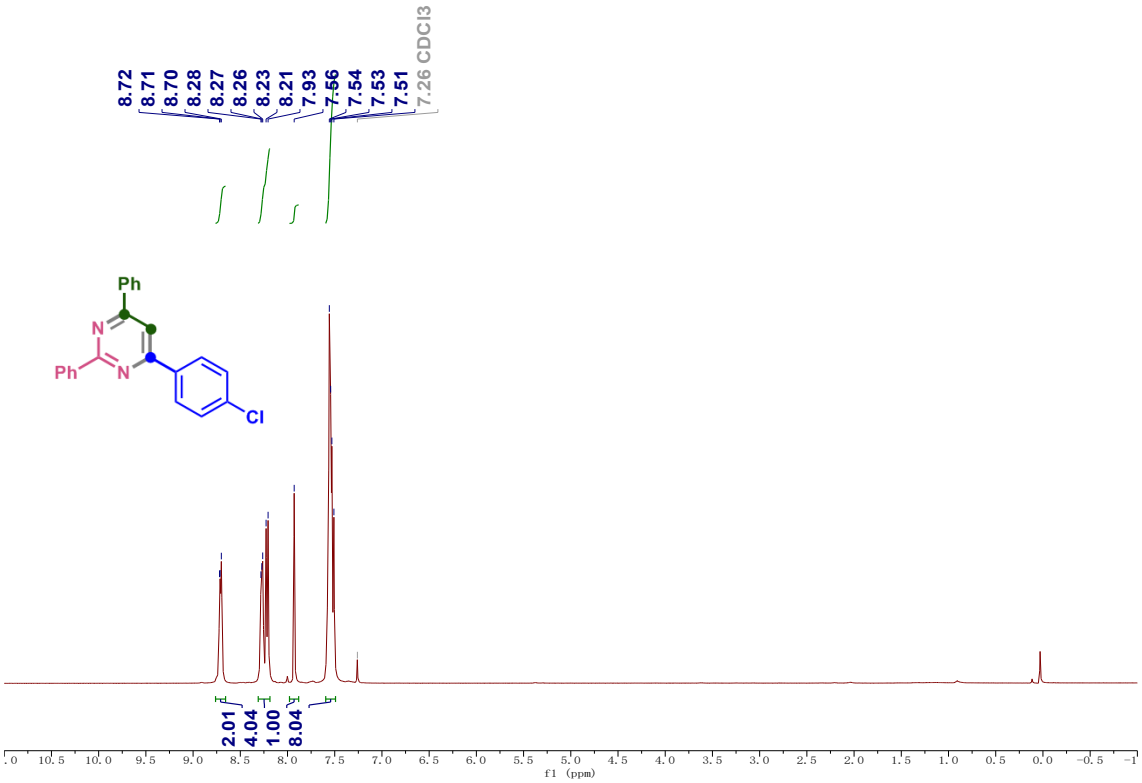
^{13}C NMR spectrum of **4g** (100 MHz, $CDCl_3$)



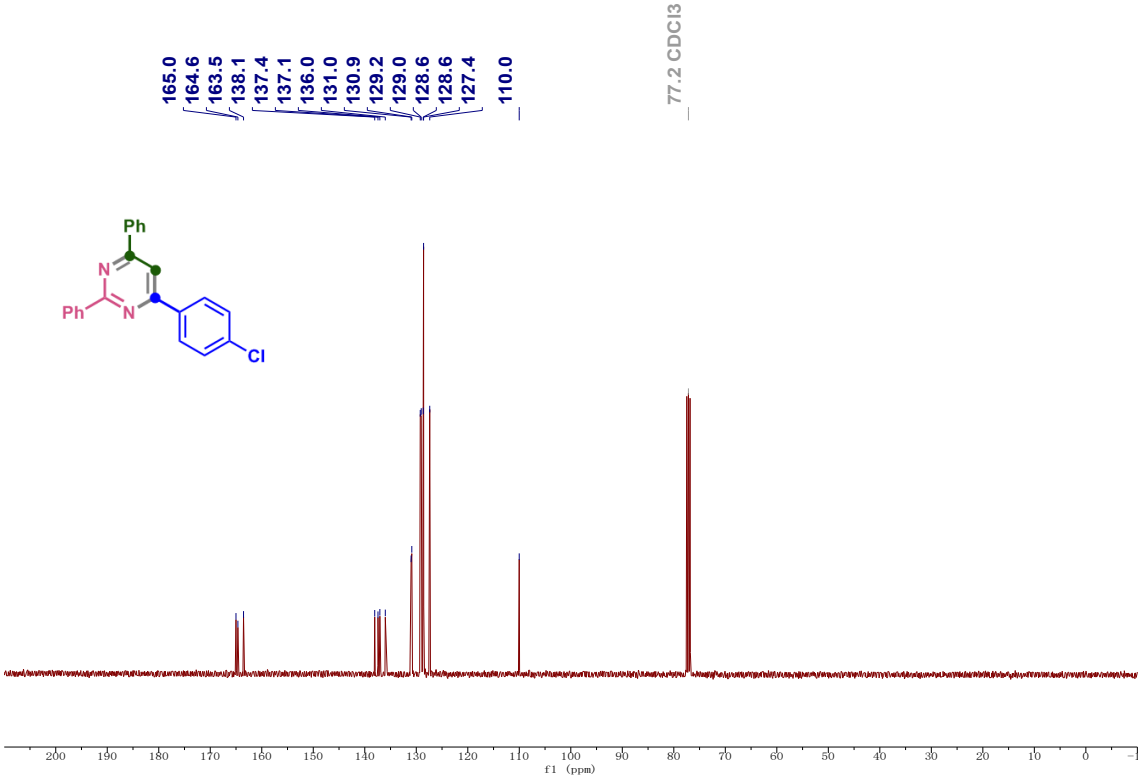
^{19}F NMR spectrum of **4g** (376 MHz, $CDCl_3$)



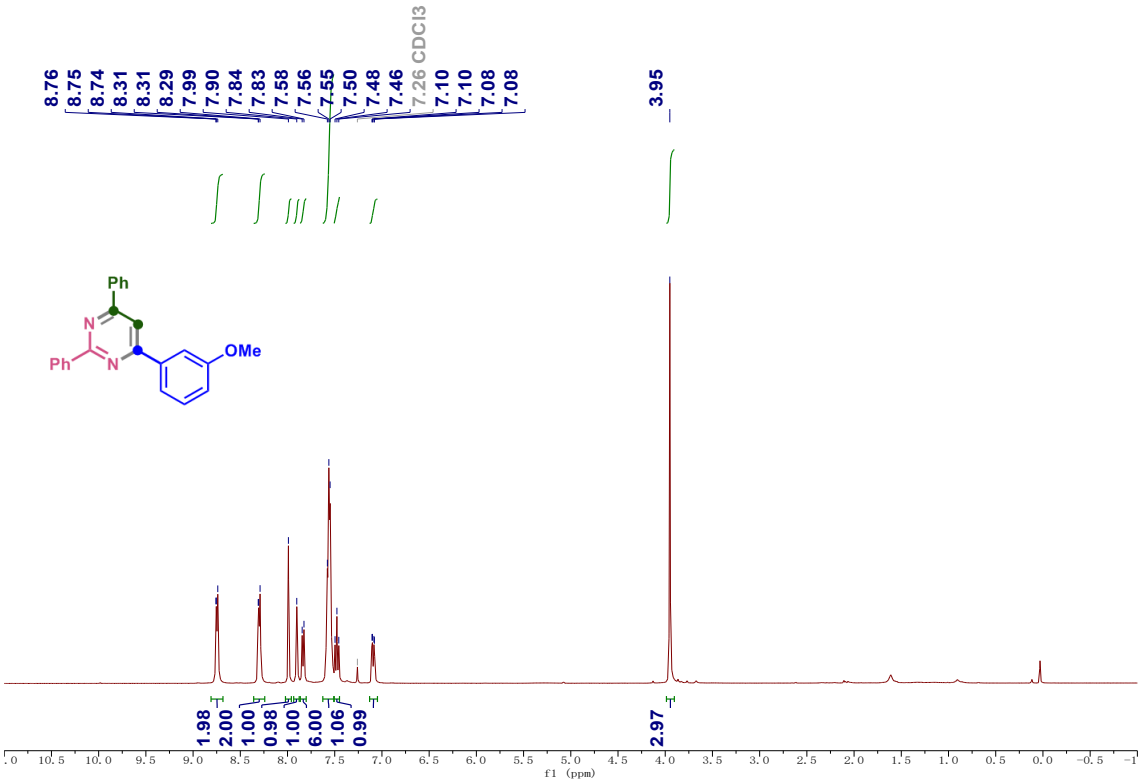
^{1}H NMR spectrum of **4h** (400 MHz, $CDCl_3$)



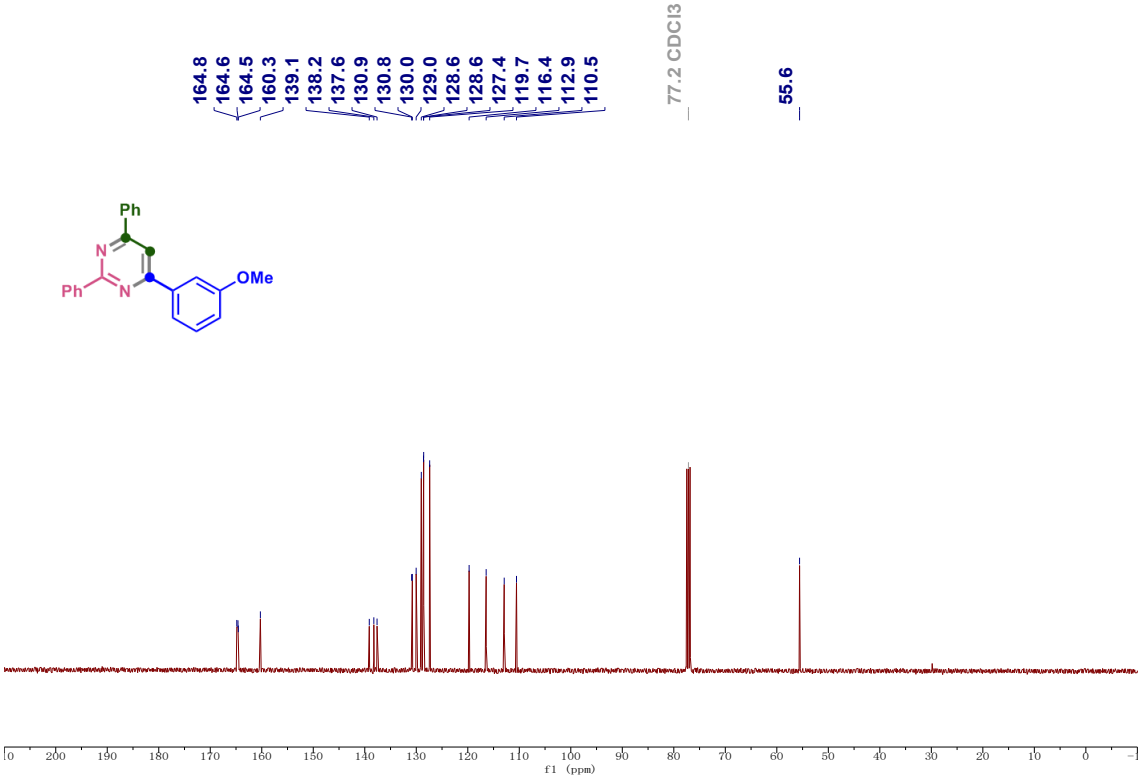
^{13}C NMR spectrum of **4h** (100 MHz, $CDCl_3$)



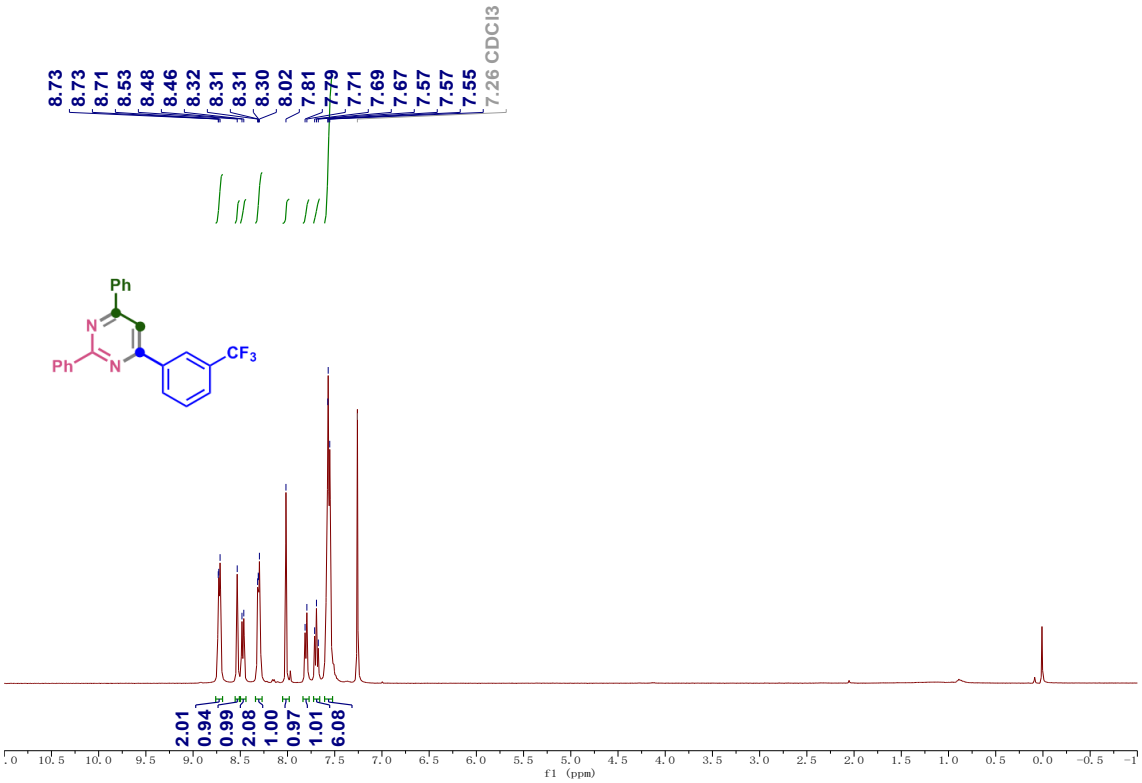
^{1}H NMR spectrum of **4i** (400 MHz, $CDCl_3$)



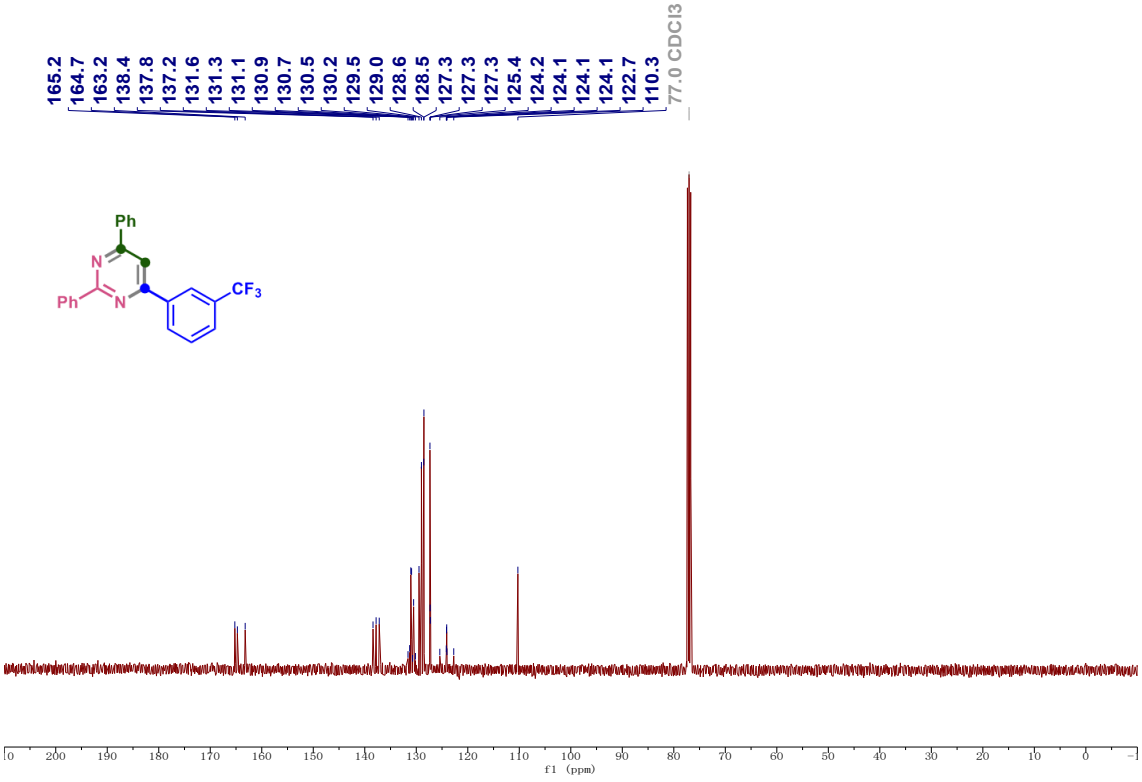
^{13}C NMR spectrum of **4i** (100 MHz, $CDCl_3$)



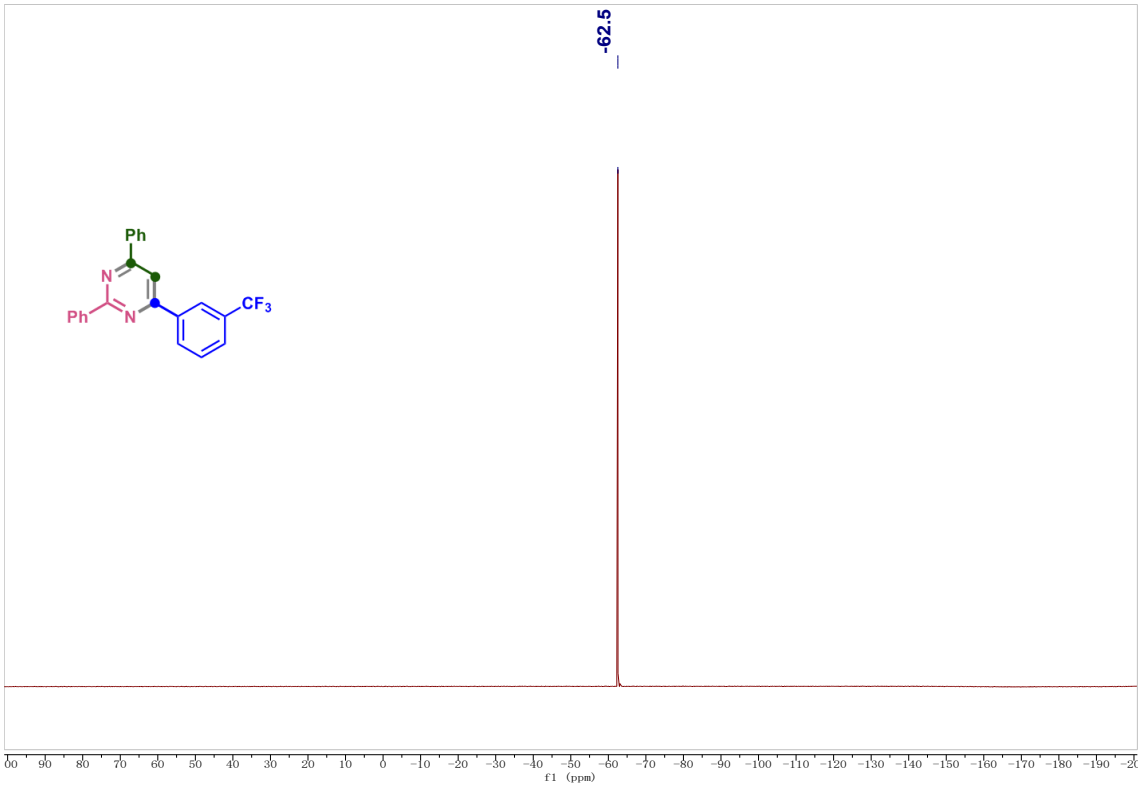
^{1}H NMR spectrum of **4j** (400 MHz, $CDCl_3$)



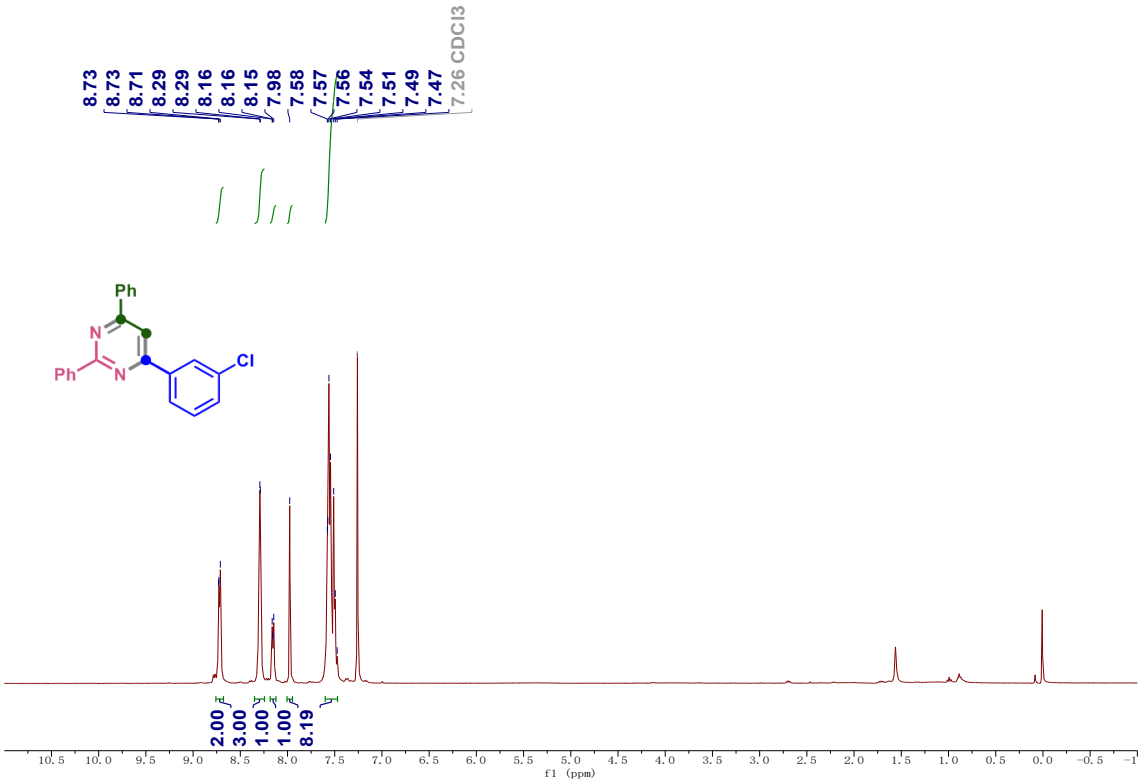
^{13}C NMR spectrum of **4j** (100 MHz, $CDCl_3$)



^{19}F NMR spectrum of **4j** (376 MHz, $CDCl_3$)



^{1}H NMR spectrum of **4k** (400 MHz, $CDCl_3$)



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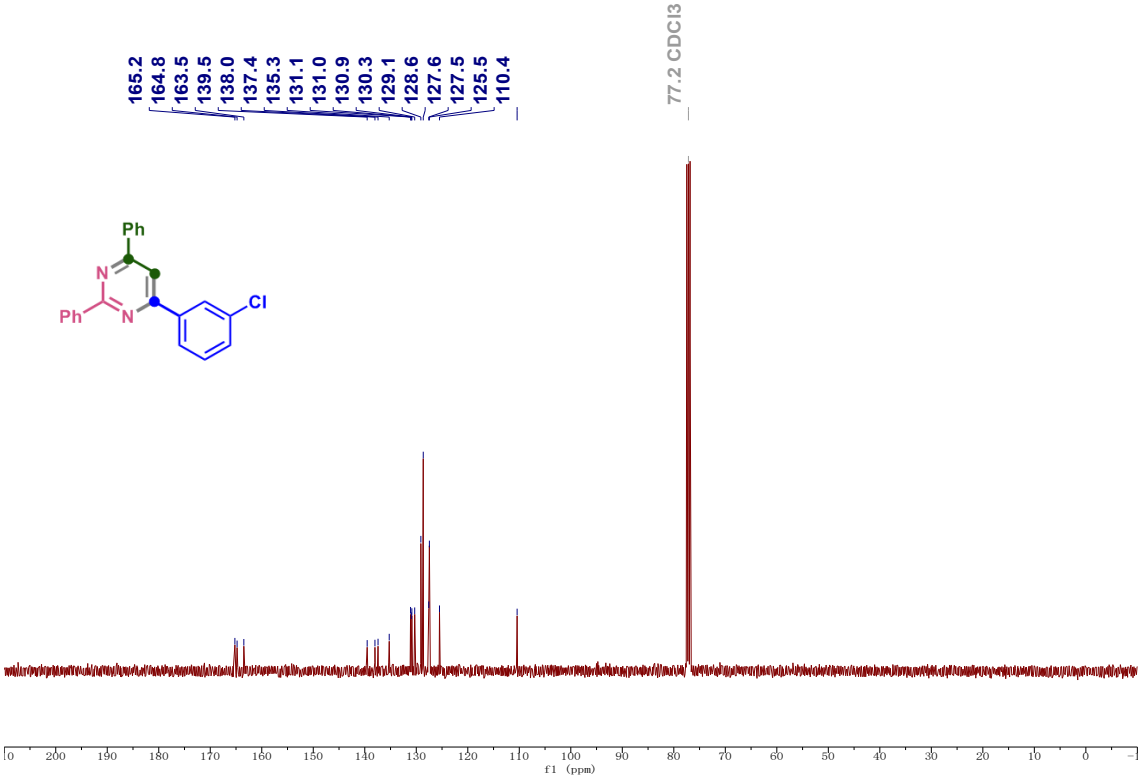
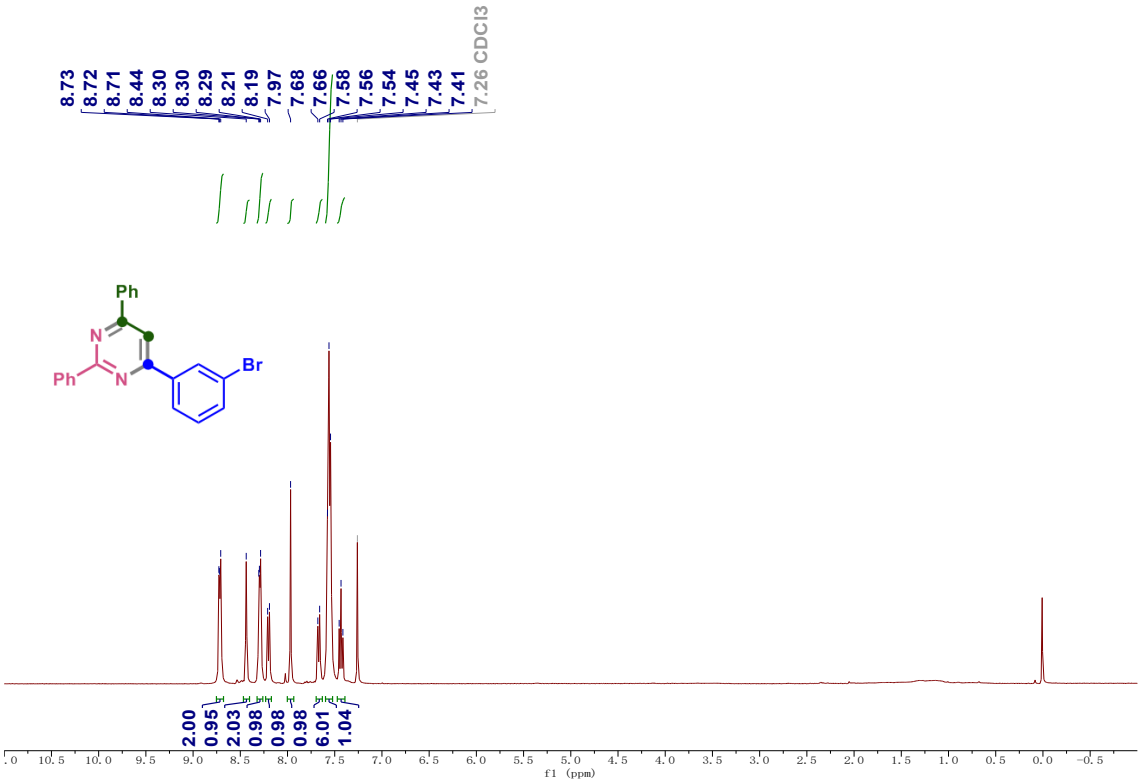
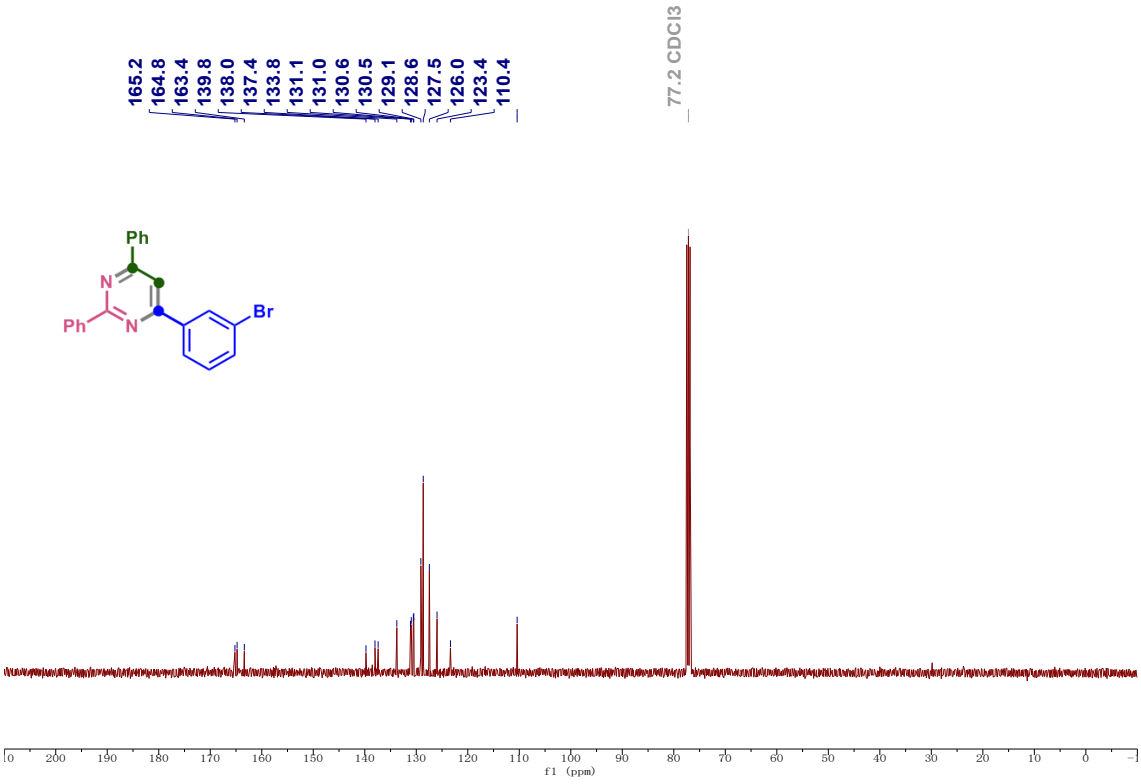


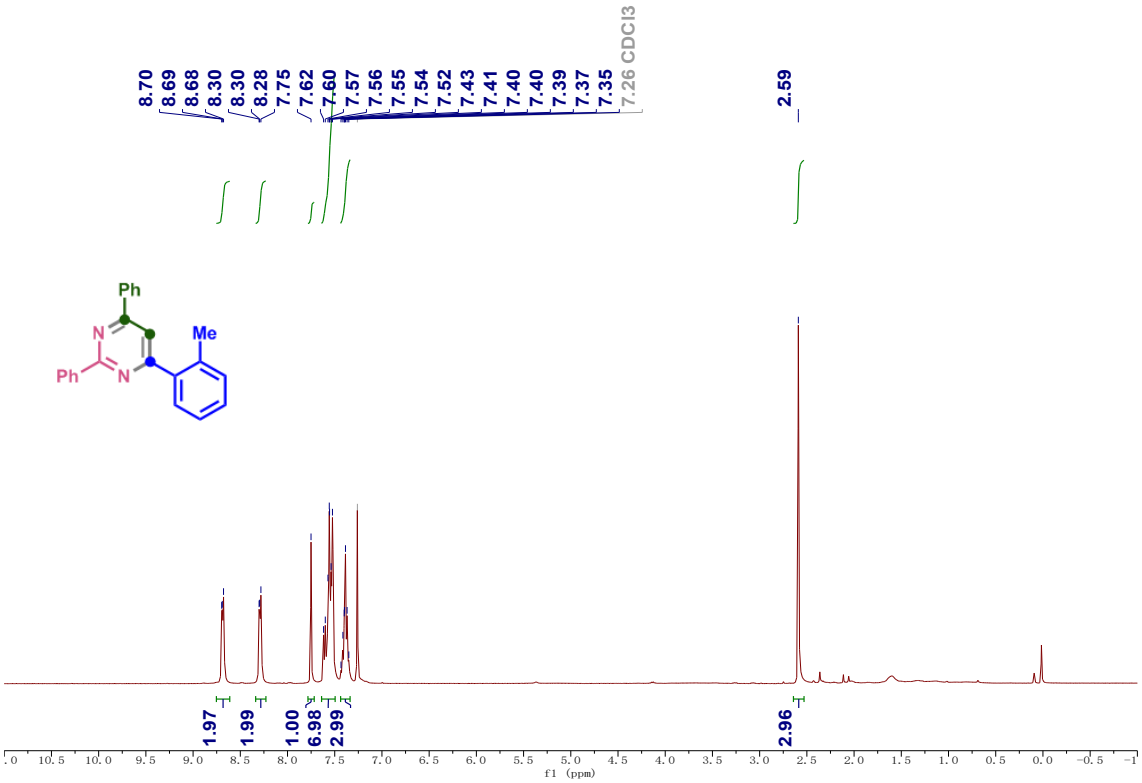
^{1}H NMR spectrum of **4l** (400 MHz, $CDCl_3$)



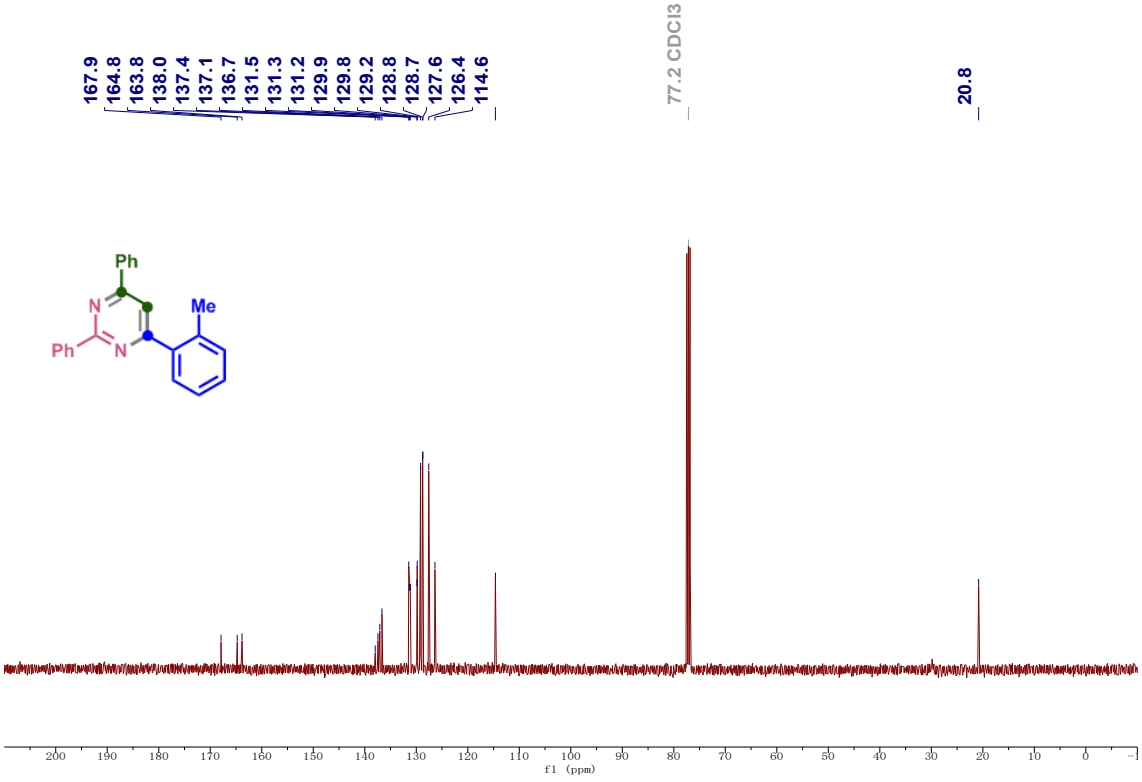
^{13}C NMR spectrum of **4l** (100 MHz, $CDCl_3$)



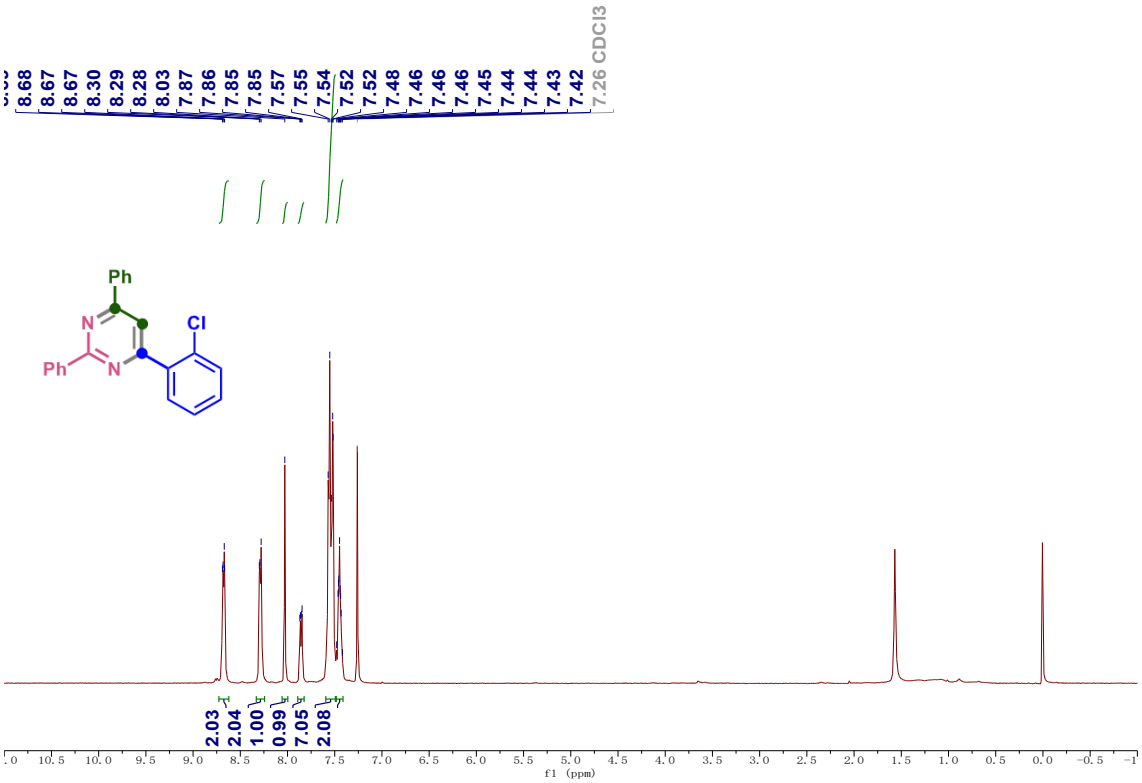
^{1}H NMR spectrum of **4m** (400 MHz, $CDCl_3$)



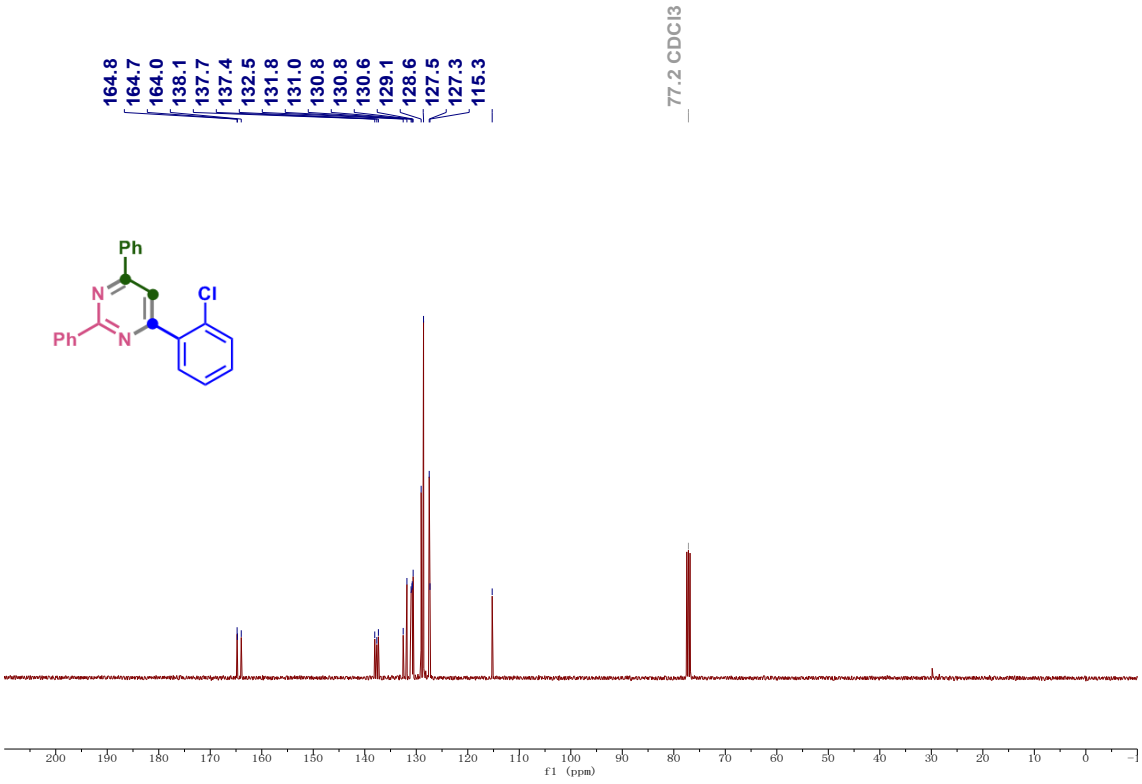
^{13}C NMR spectrum of **4m** (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of **4n** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **4n** (100 MHz, $CDCl_3$)



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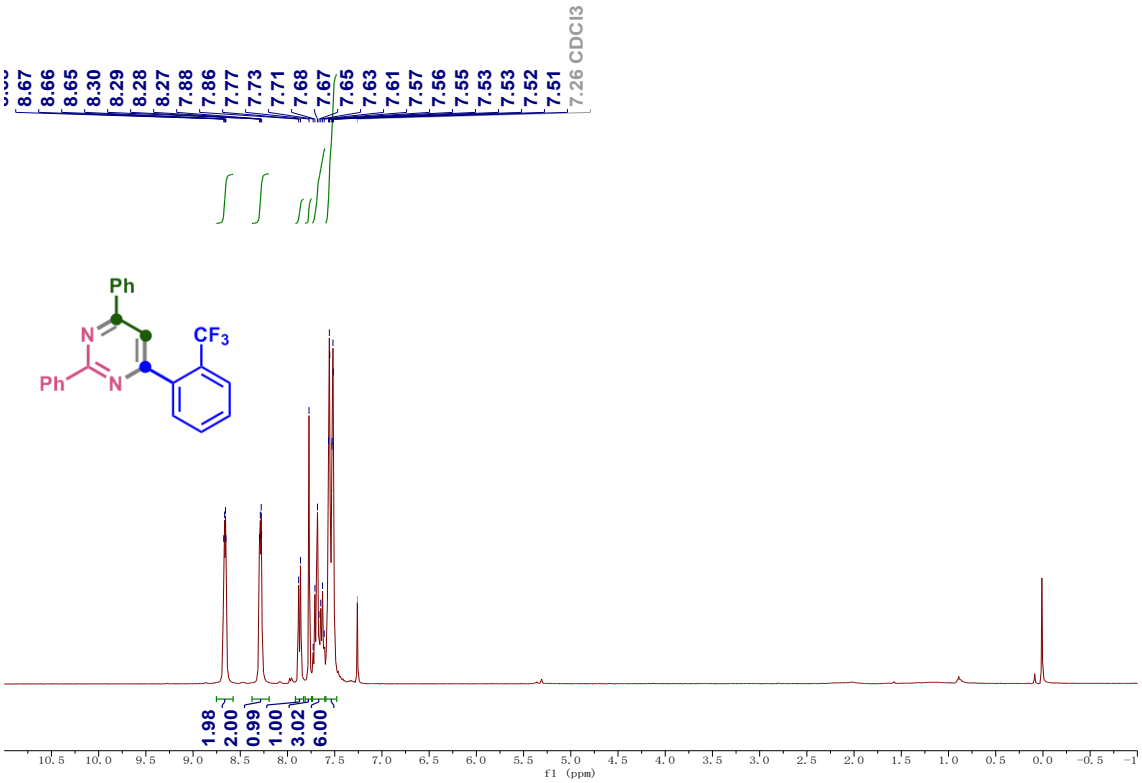

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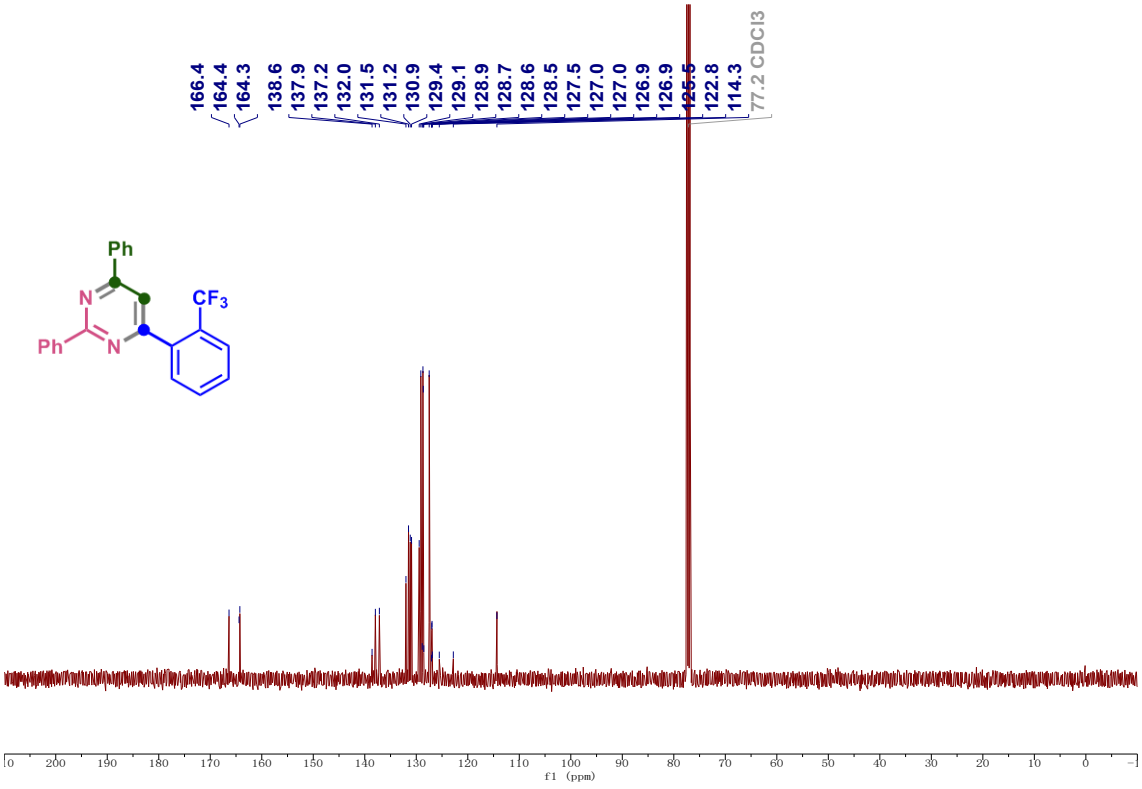
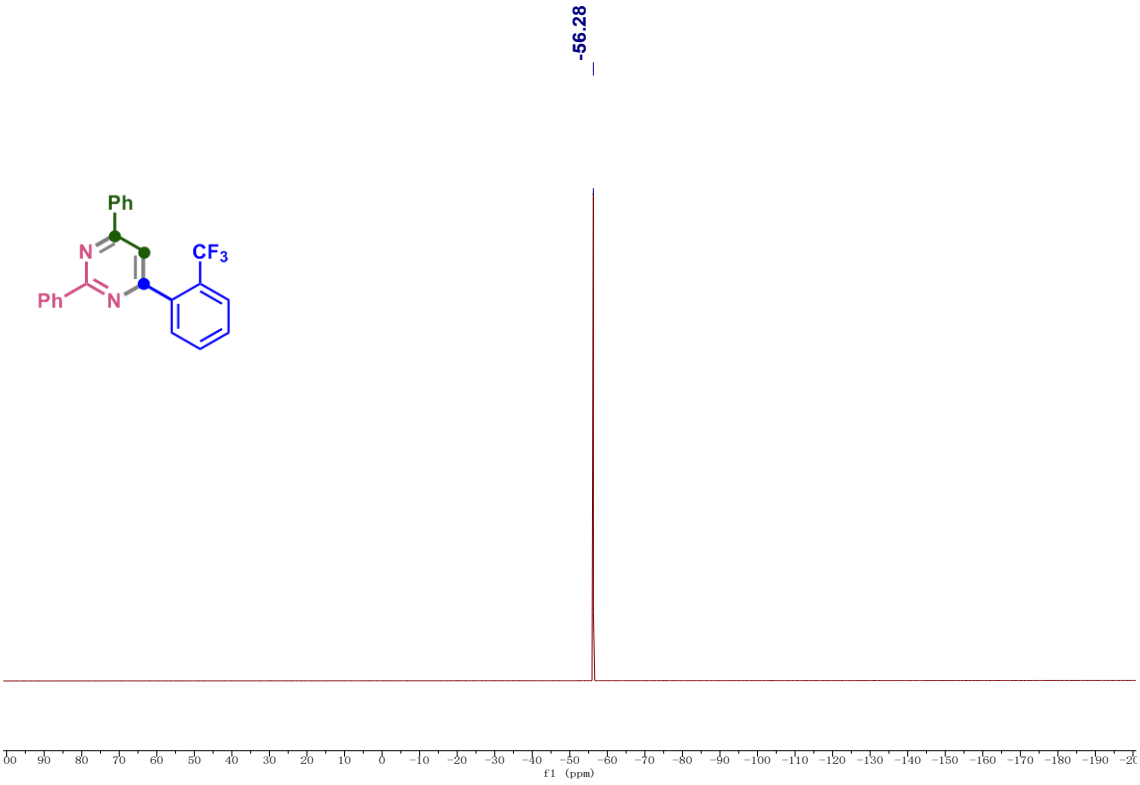


^{19}F NMR spectrum of **4o** (376 MHz, $CDCl_3$)



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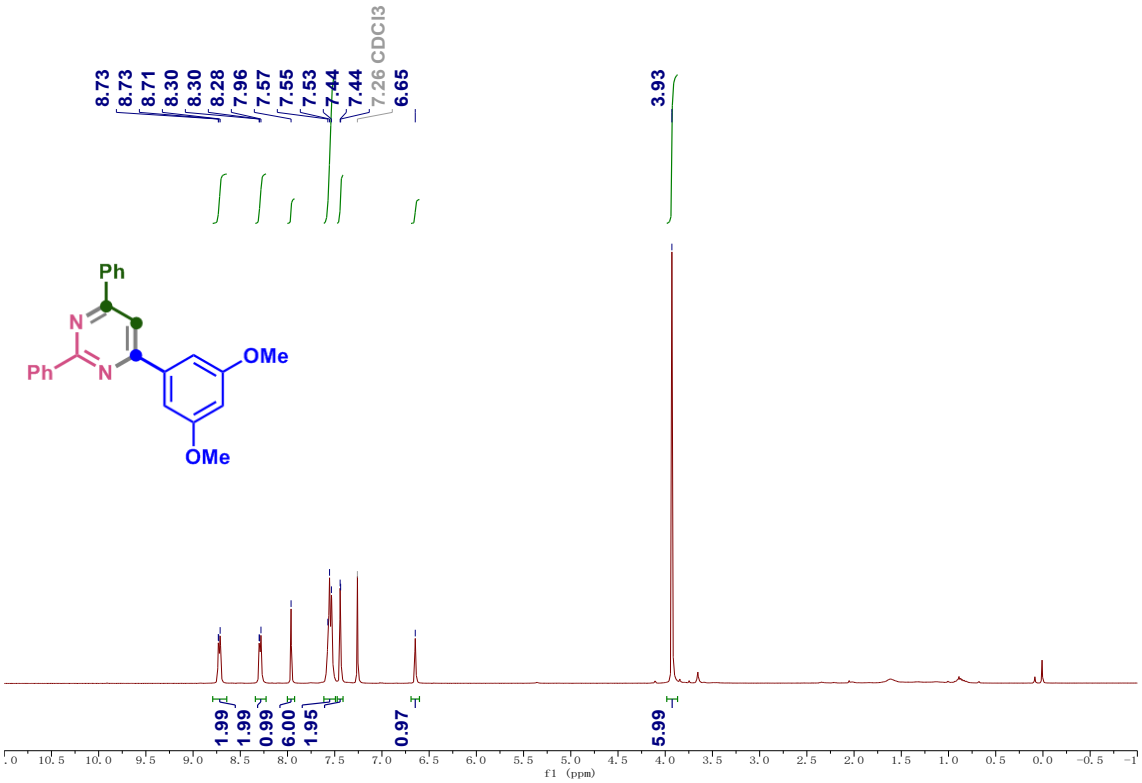

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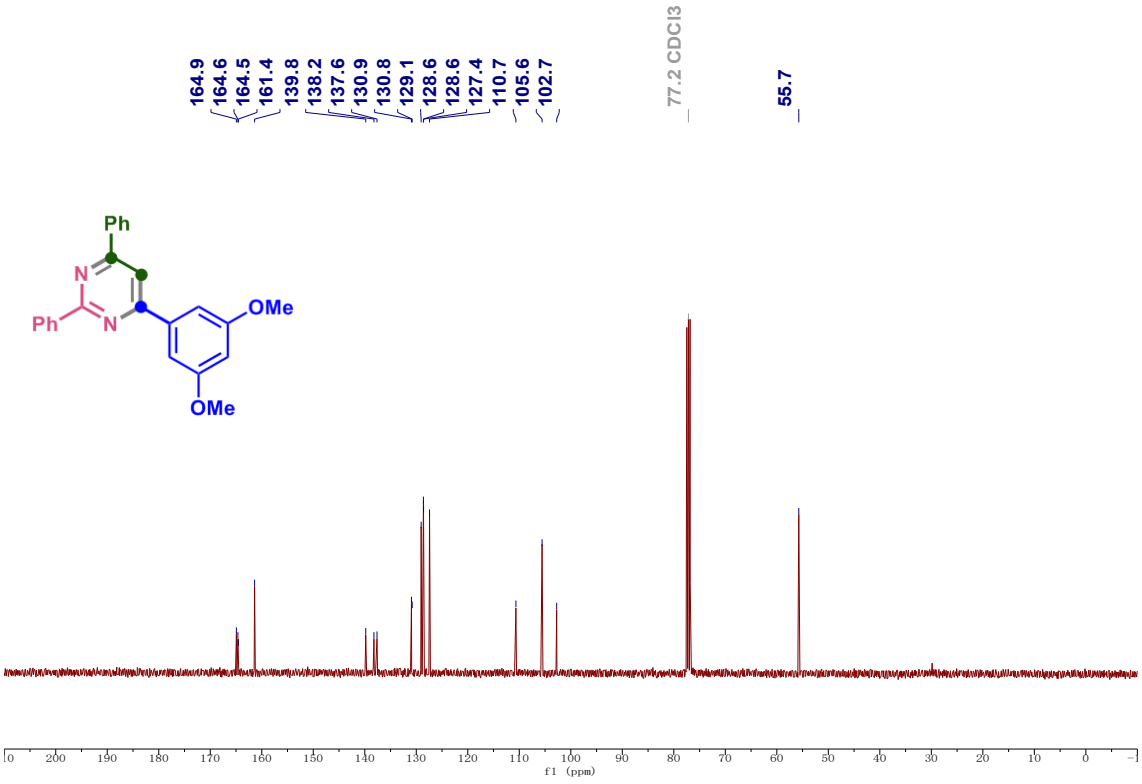

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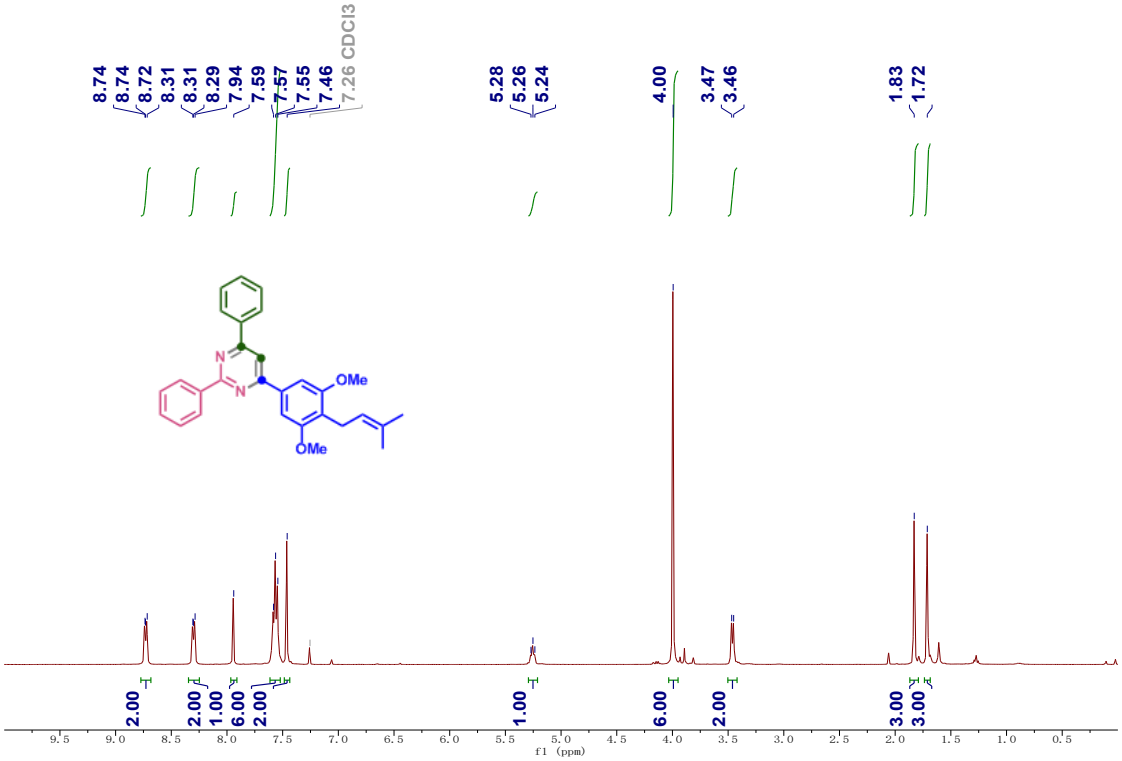
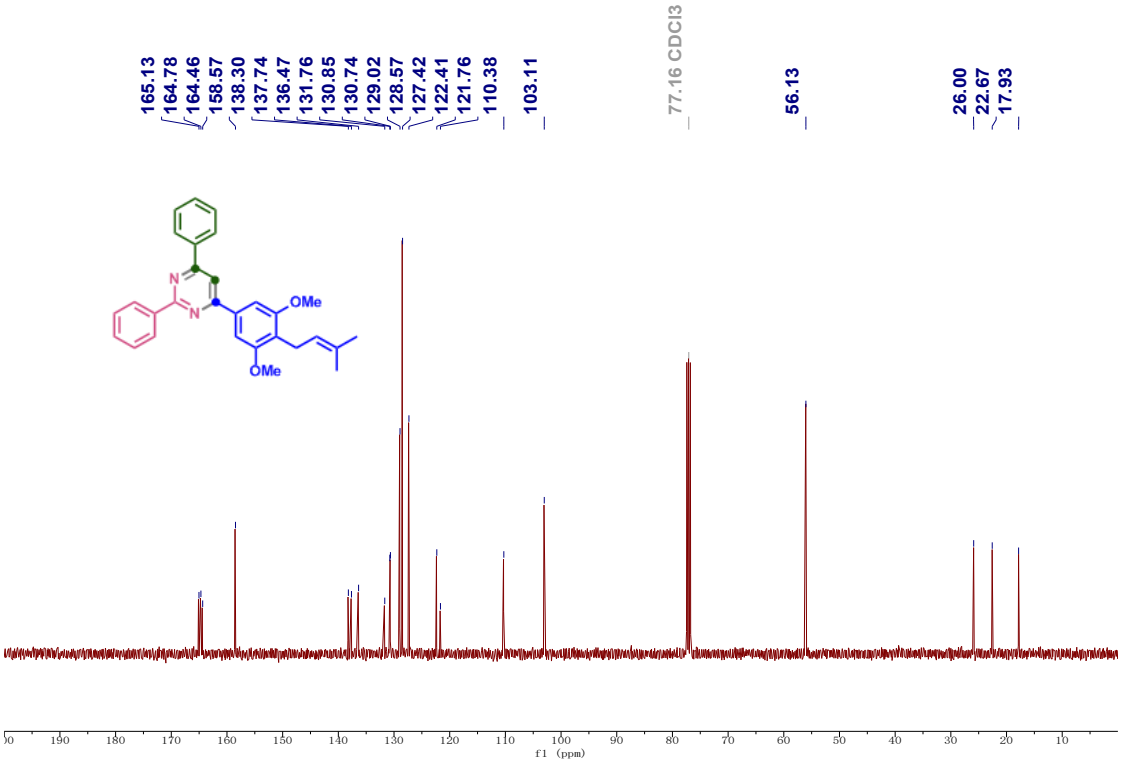
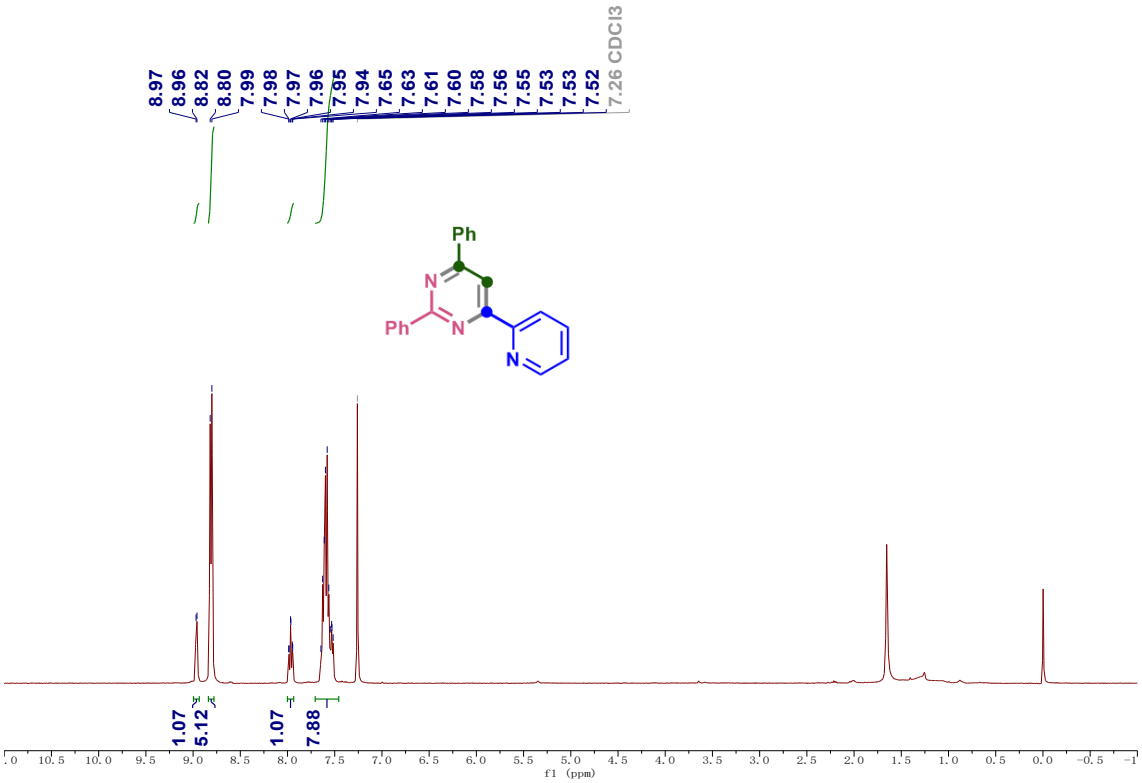


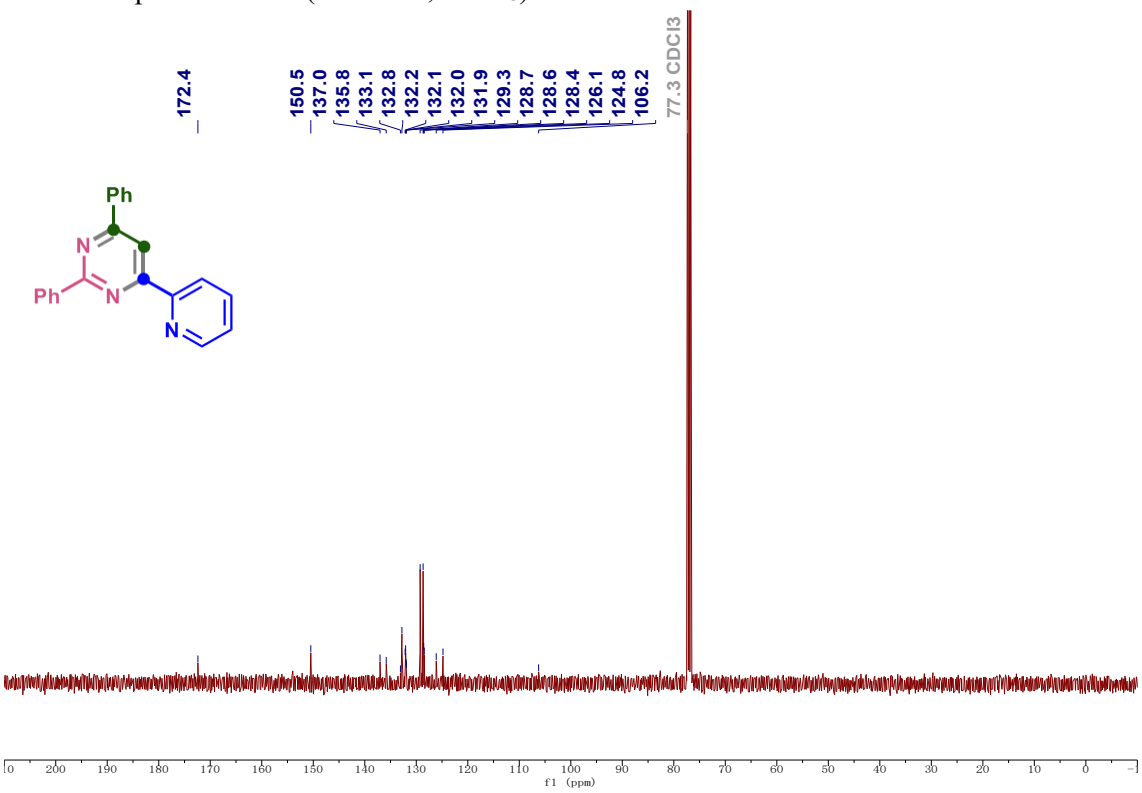
^{13}C NMR spectrum of **4q** (100 MHz, $CDCl_3$)



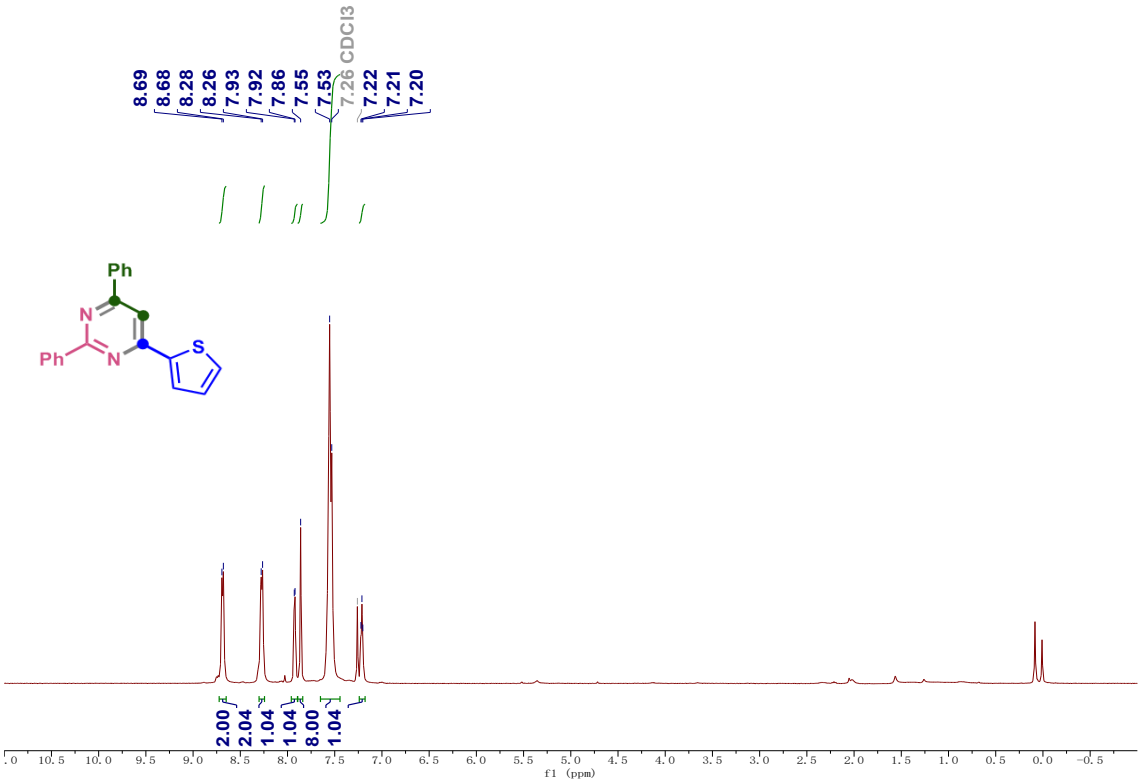
^{1}H NMR spectrum of **4r** (400 MHz, $CDCl_3$)



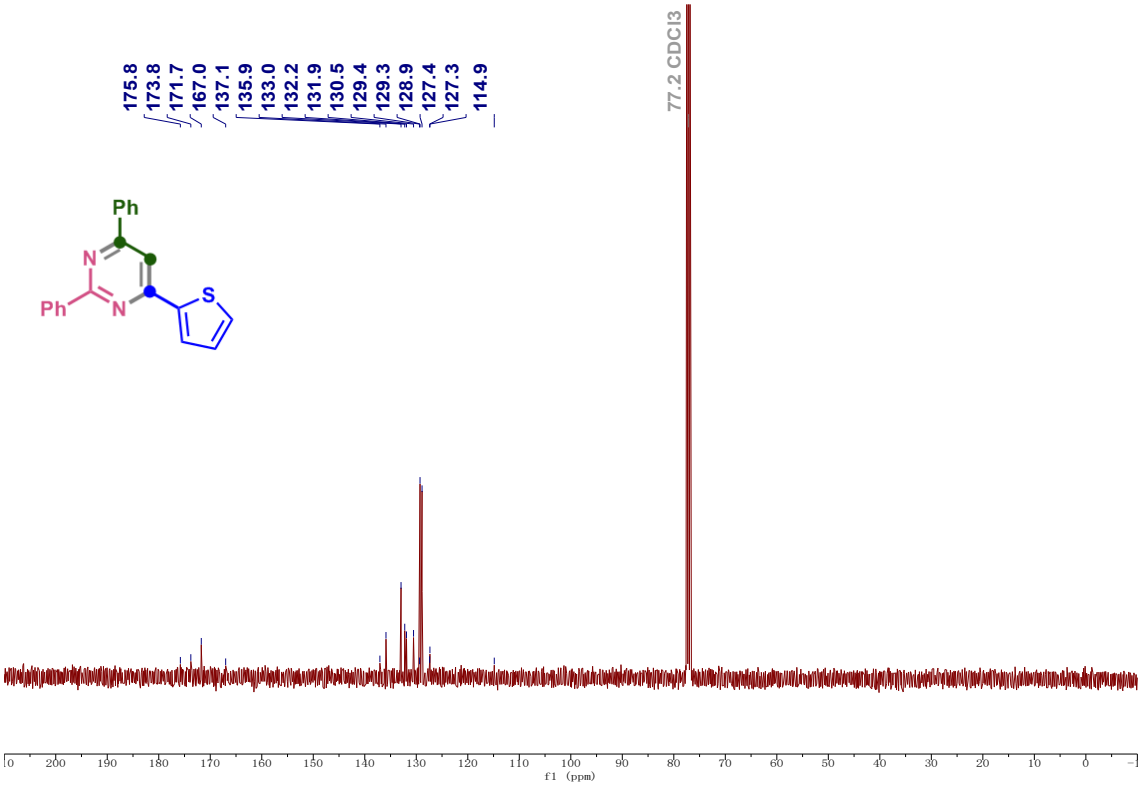
^{13}C NMR spectrum of **4r** (100 MHz, $CDCl_3$)



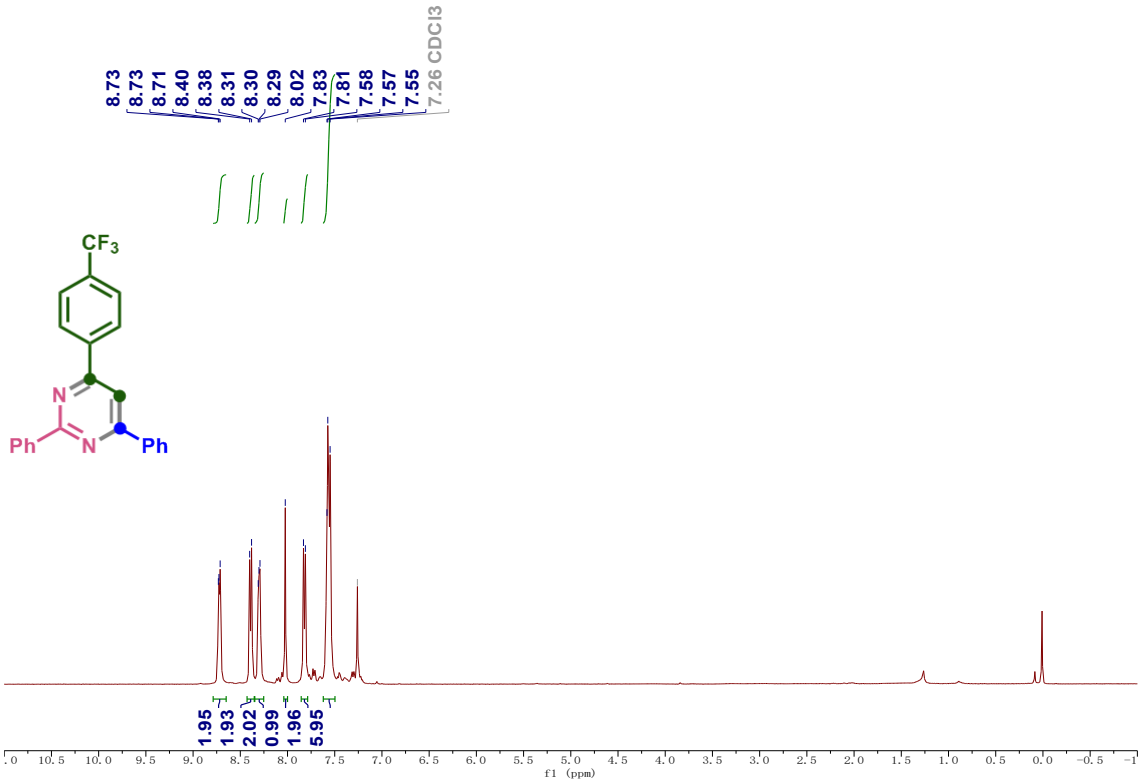
^{1}H NMR spectrum of **4s** (400 MHz, $CDCl_3$)



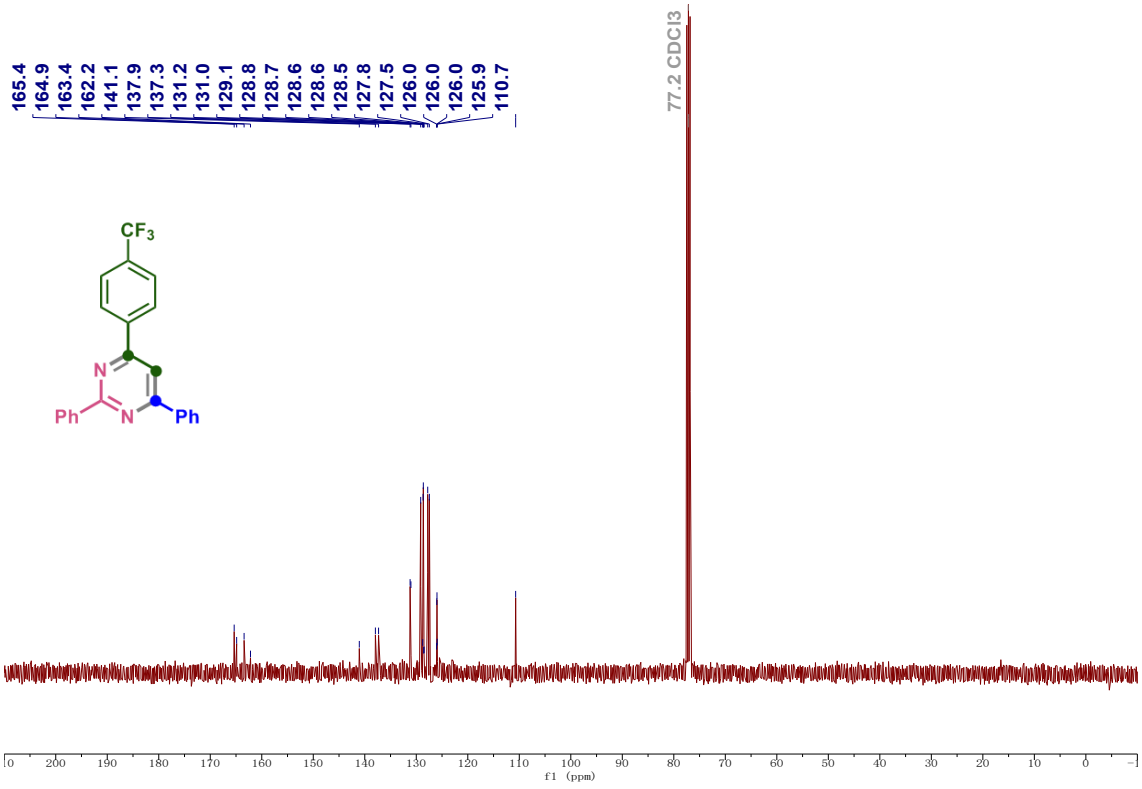
^{13}C NMR spectrum of **4s** (100 MHz, $CDCl_3$)



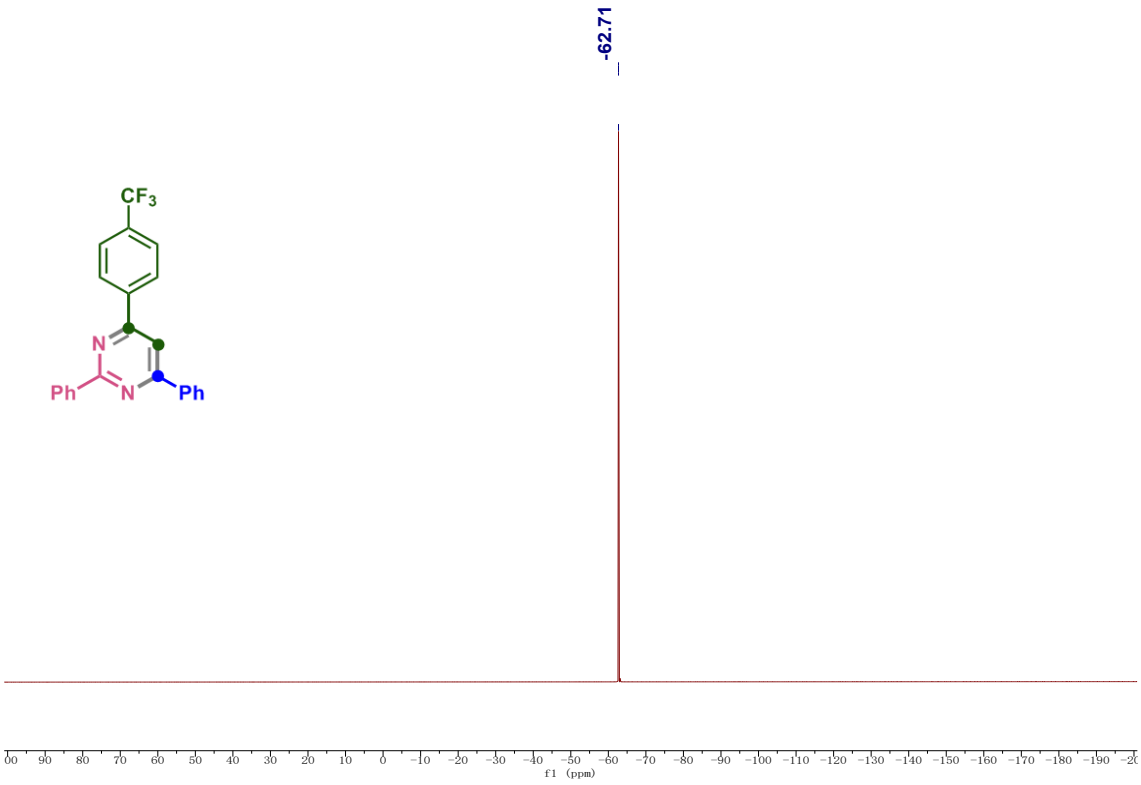
^{1}H NMR spectrum of **4t** (400 MHz, $CDCl_3$)



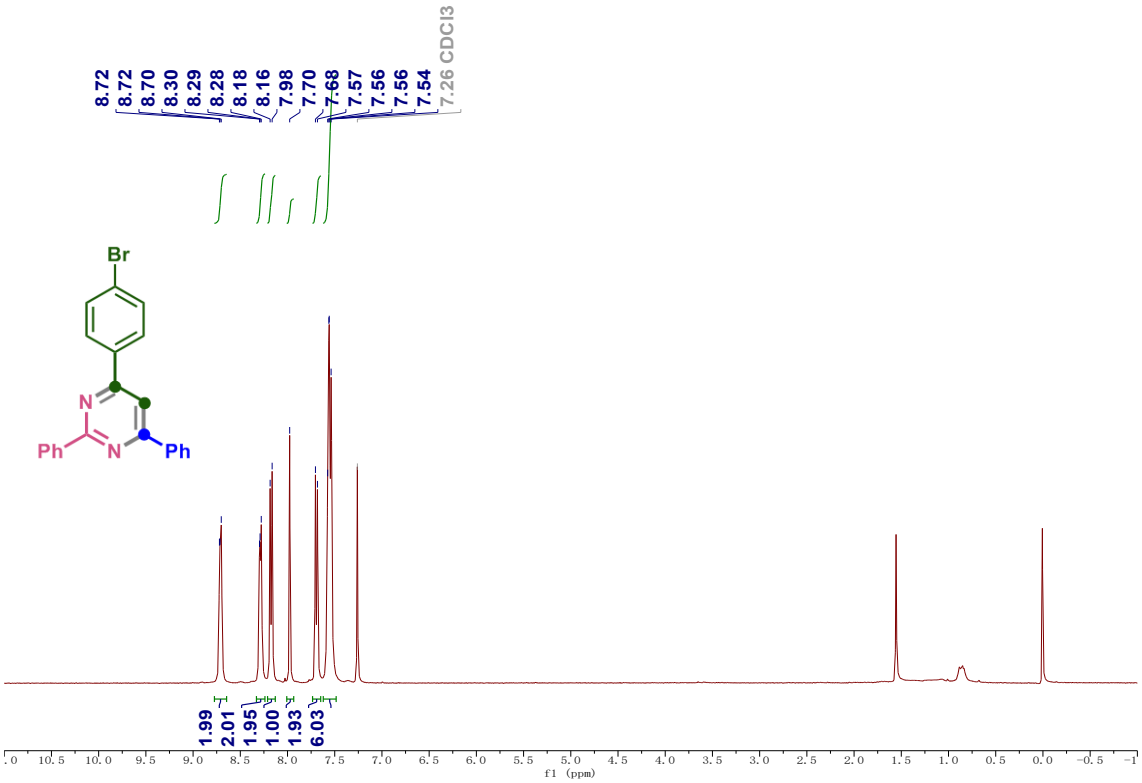
^{13}C NMR spectrum of **4t** (100 MHz, $CDCl_3$)



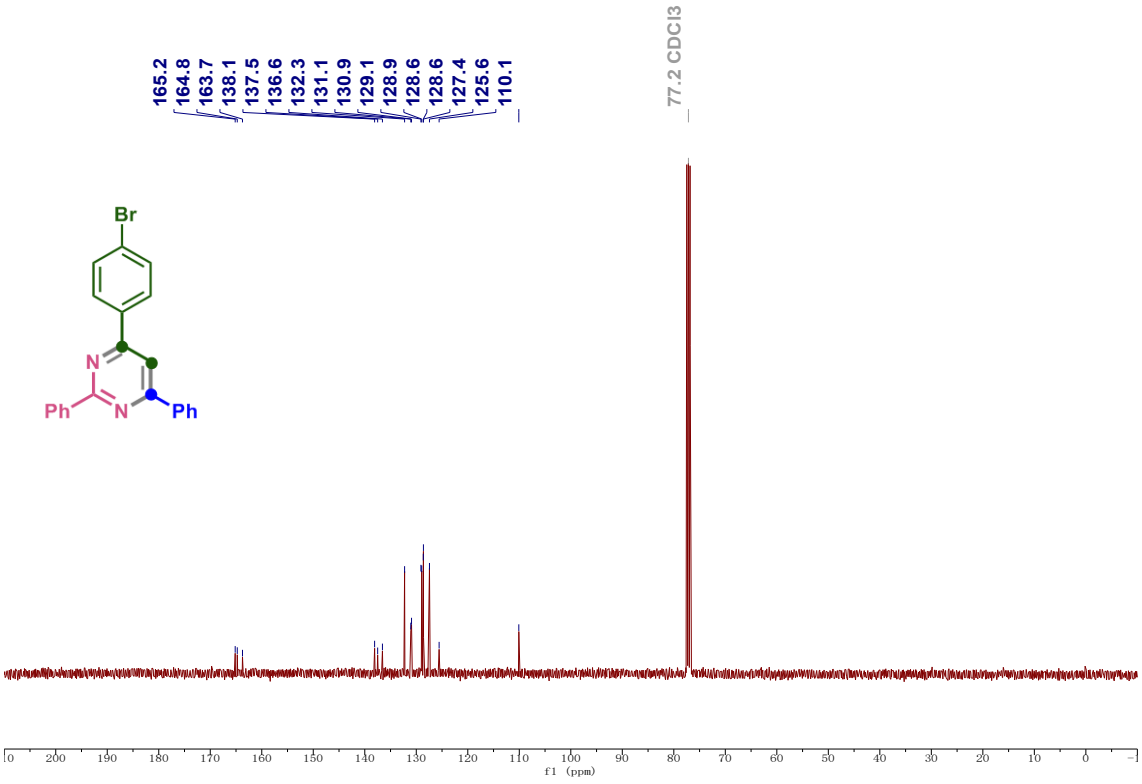
^{19}F NMR spectrum of **4t** (376 MHz, $CDCl_3$)



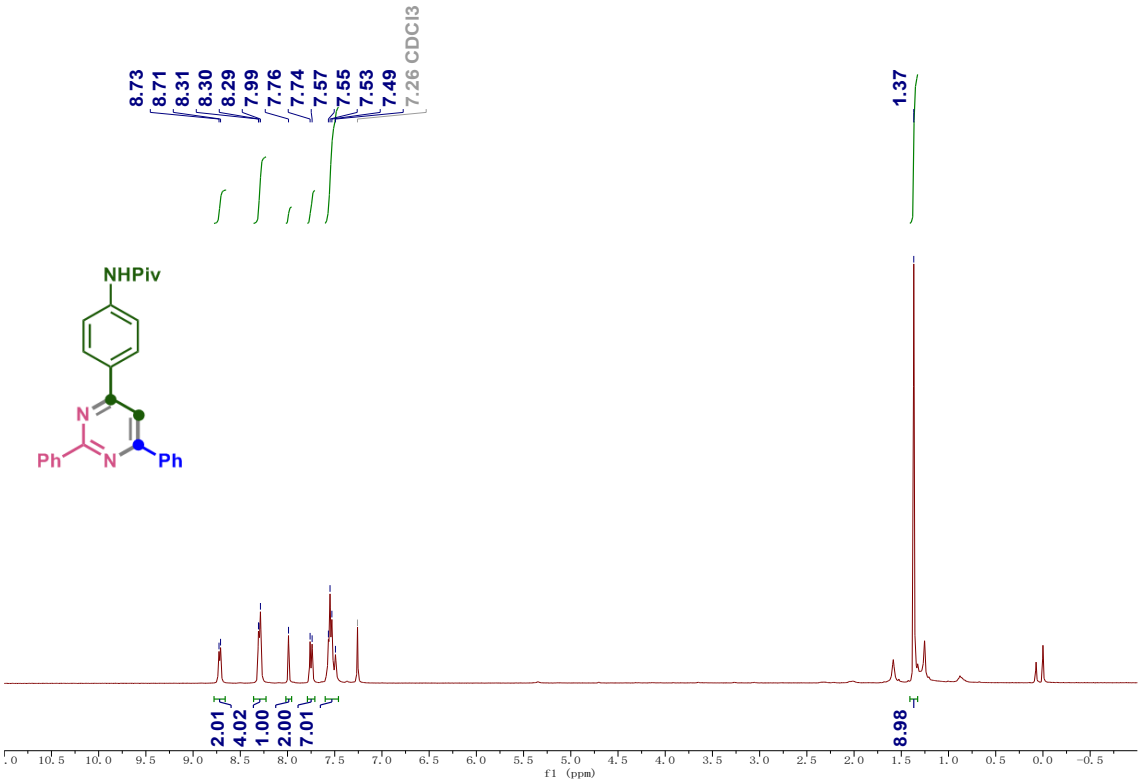
^{1}H NMR spectrum of **4u** (400 MHz, $CDCl_3$)



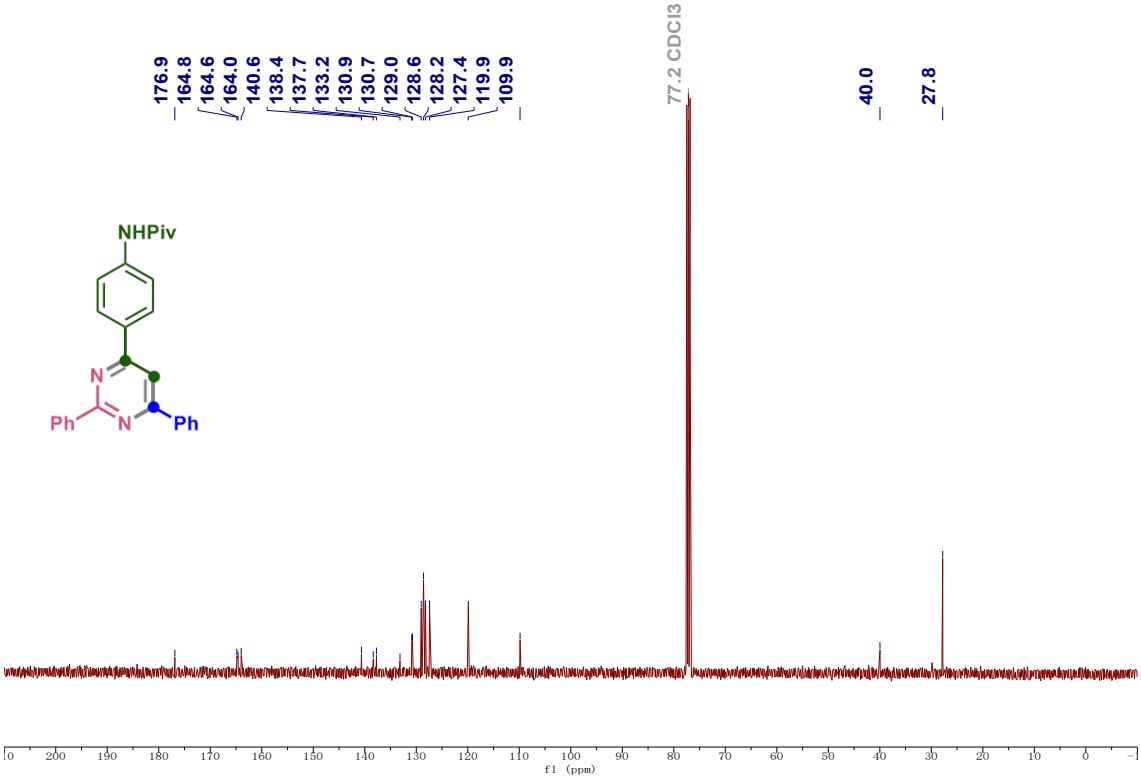
^{13}C NMR spectrum of **4u** (100 MHz, $CDCl_3$)



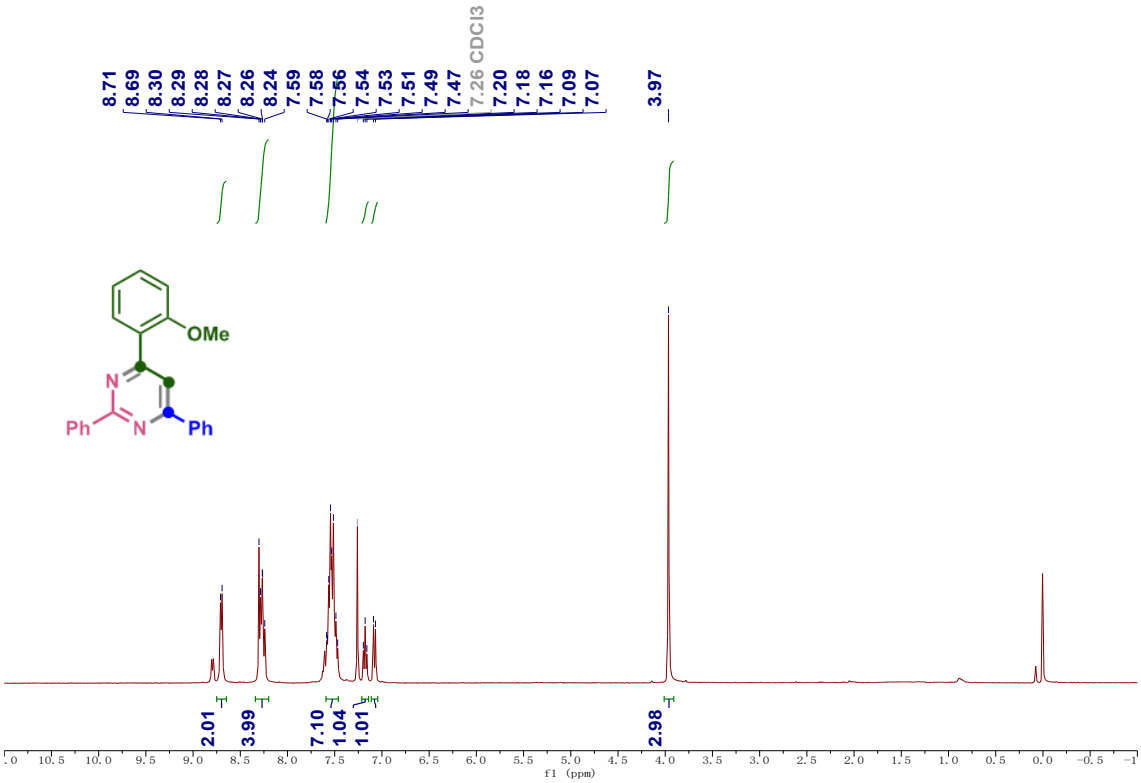
^{1}H NMR spectrum of **4v** (400 MHz, $CDCl_3$)



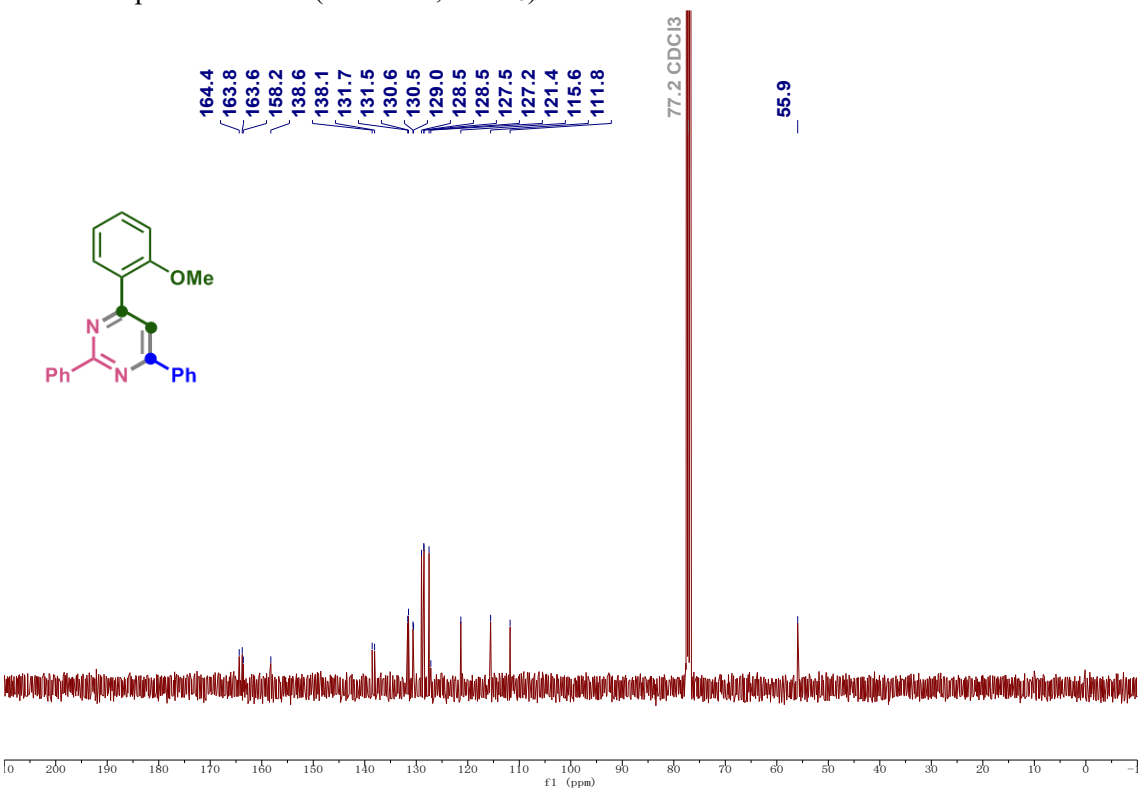
^{13}C NMR spectrum of **4v** (100 MHz, $CDCl_3$)



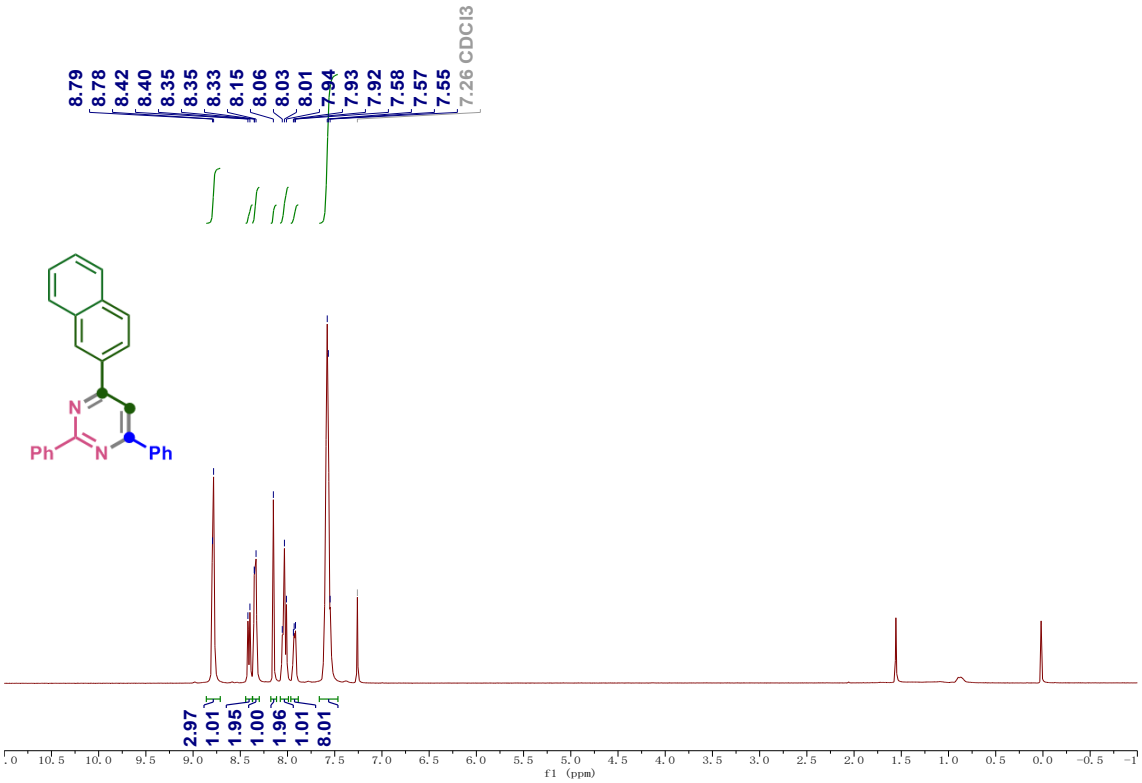
^{1}H NMR spectrum of **4w** (400 MHz, $CDCl_3$)



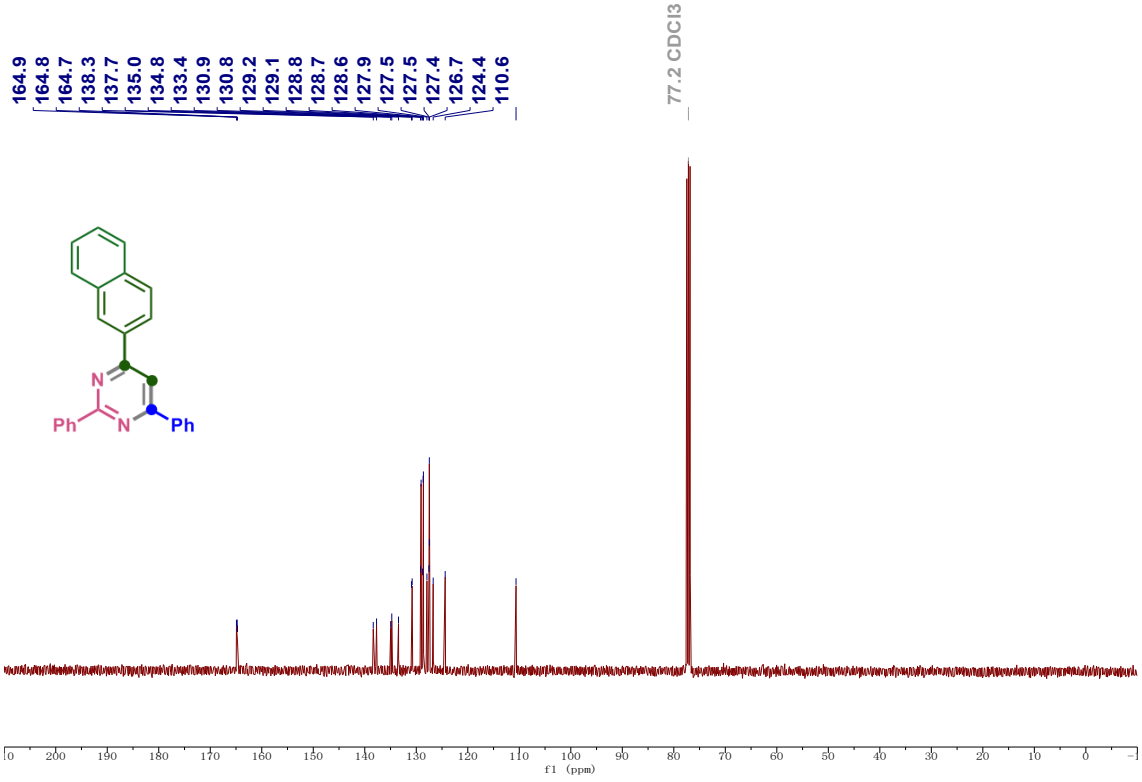
^{13}C NMR spectrum of **4w** (100 MHz, $CDCl_3$)



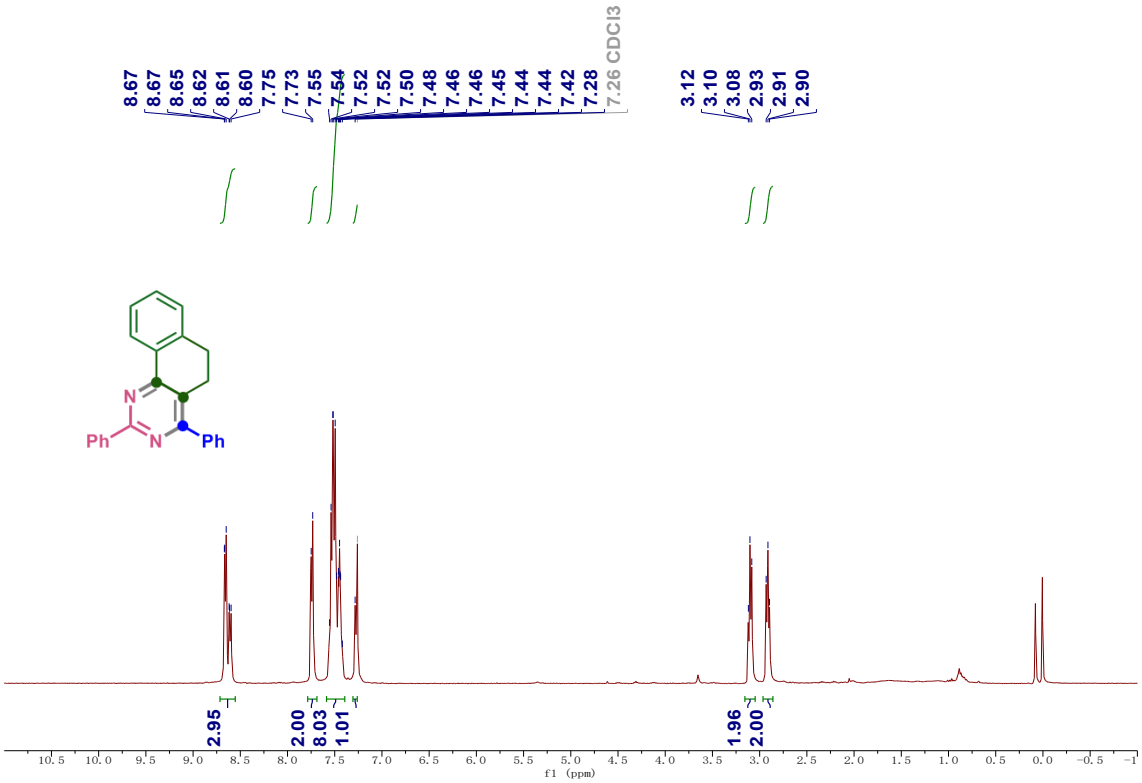
^{1}H NMR spectrum of **4x** (400 MHz, $CDCl_3$)



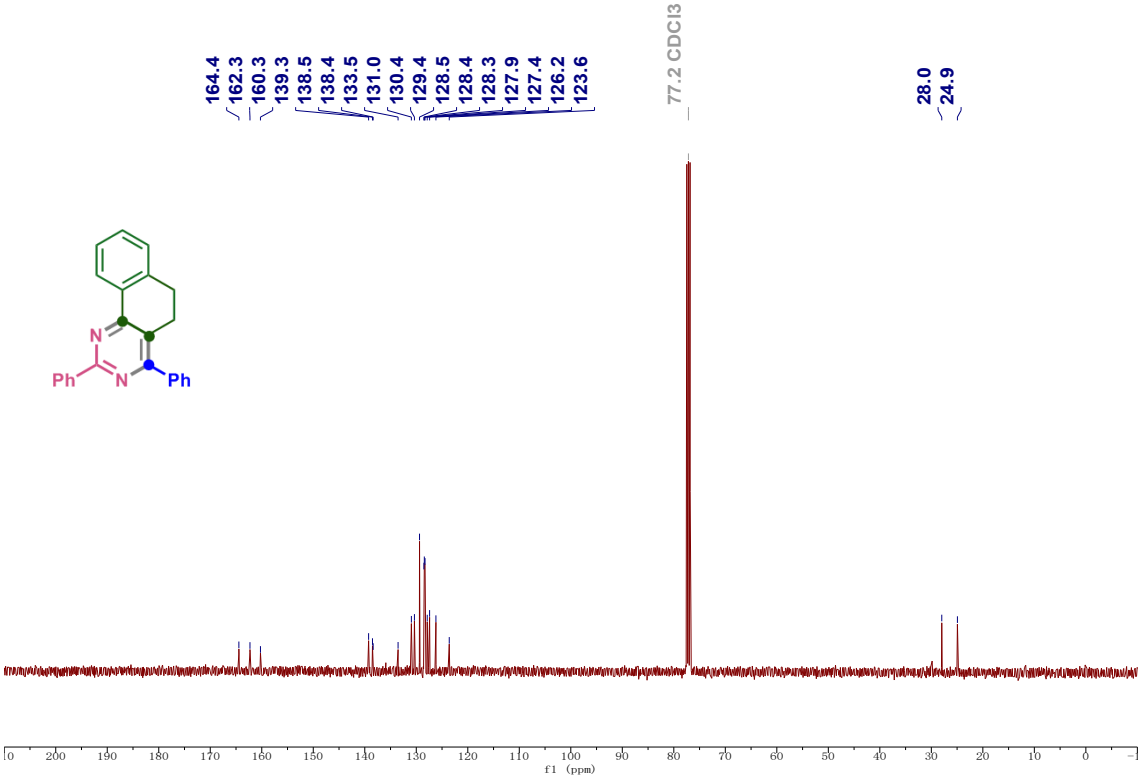
^{13}C NMR spectrum of **4x** (100 MHz, $CDCl_3$)



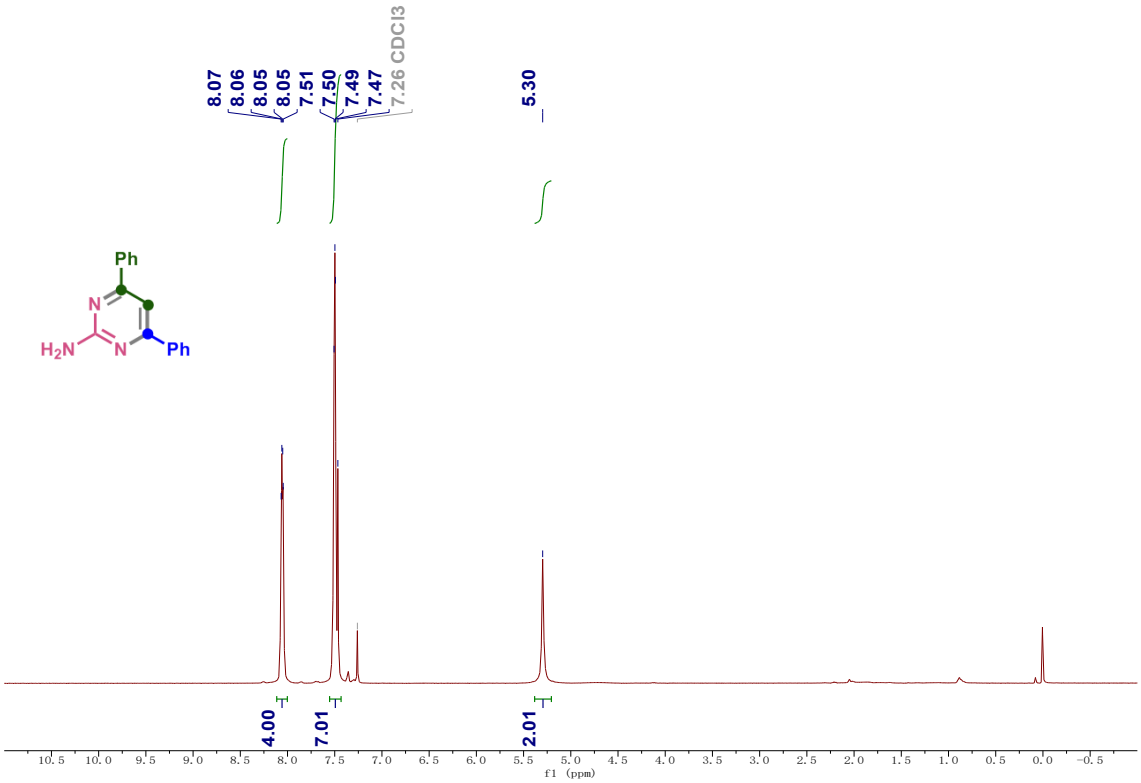
^{1}H NMR spectrum of **4y** (400 MHz, $CDCl_3$)



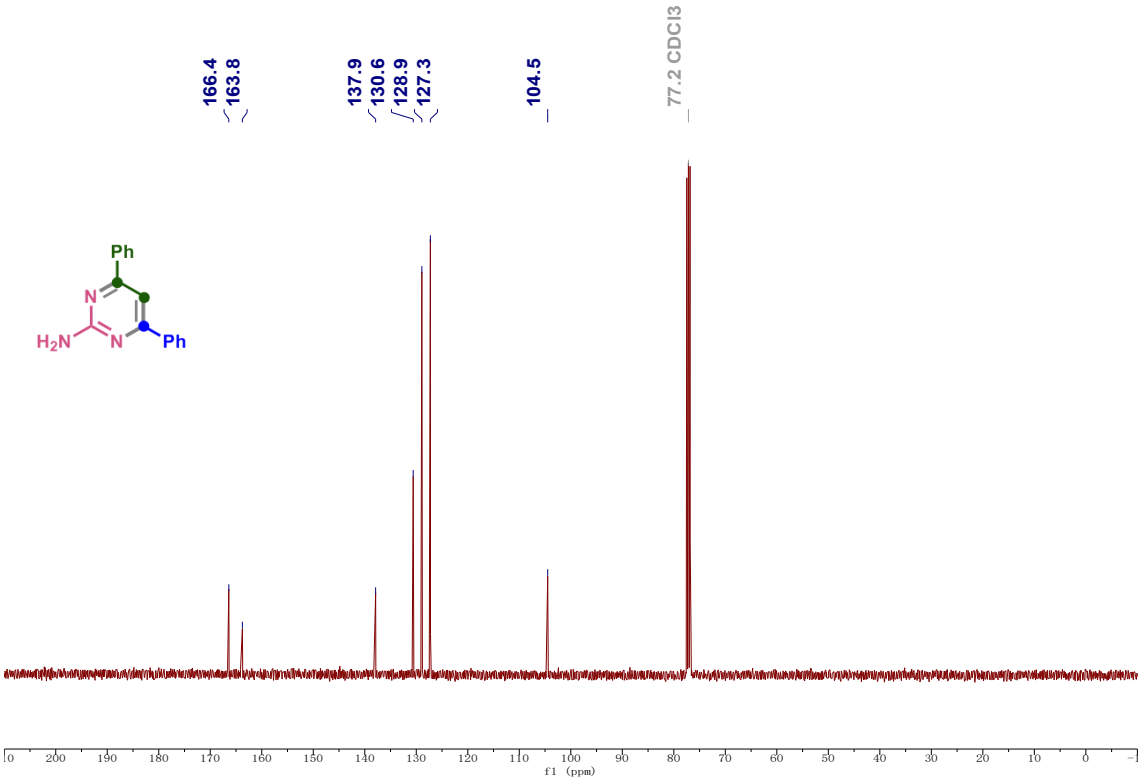
^{13}C NMR spectrum of **4y** (100 MHz, $CDCl_3$)



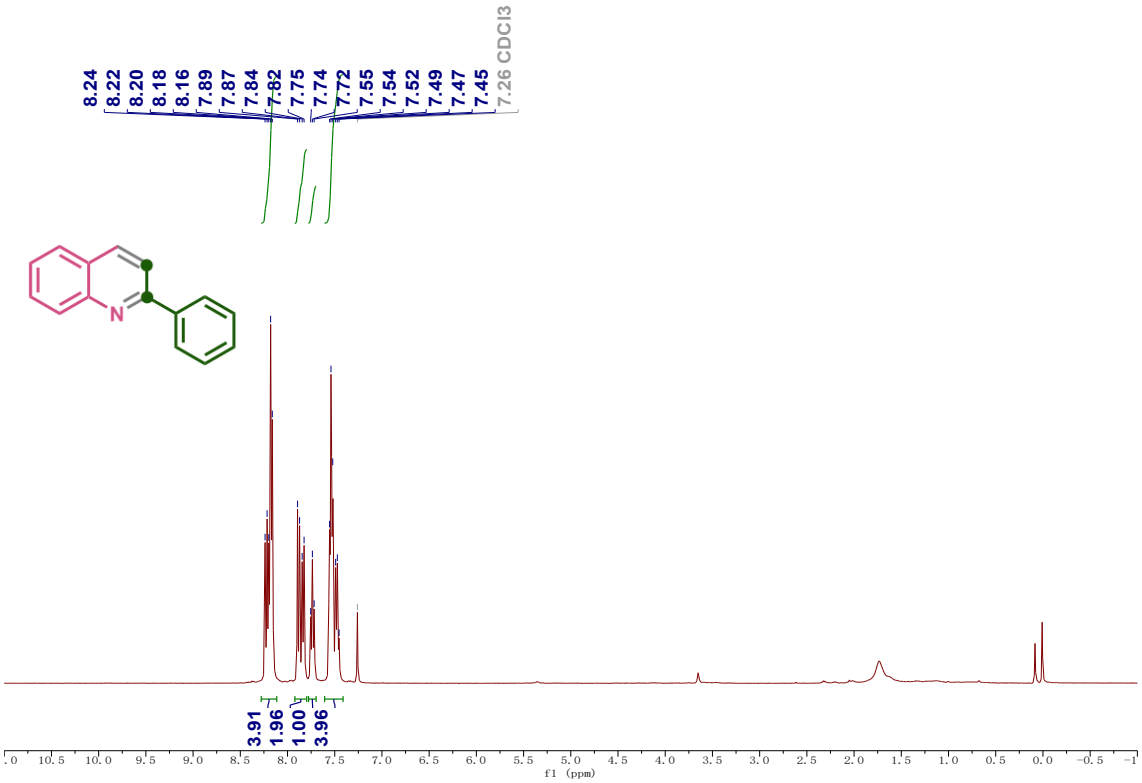
^{1}H NMR spectrum of **4z** (400 MHz, $CDCl_3$)



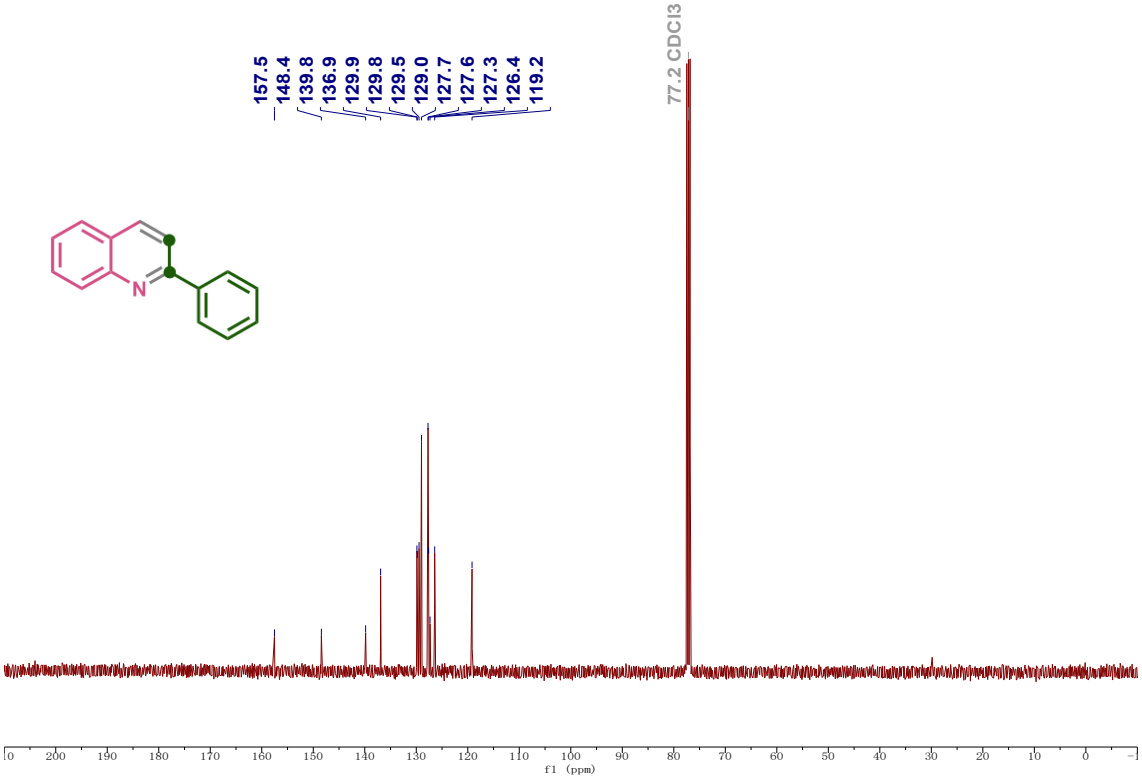
^{13}C NMR spectrum of **4z** (100 MHz, $CDCl_3$)



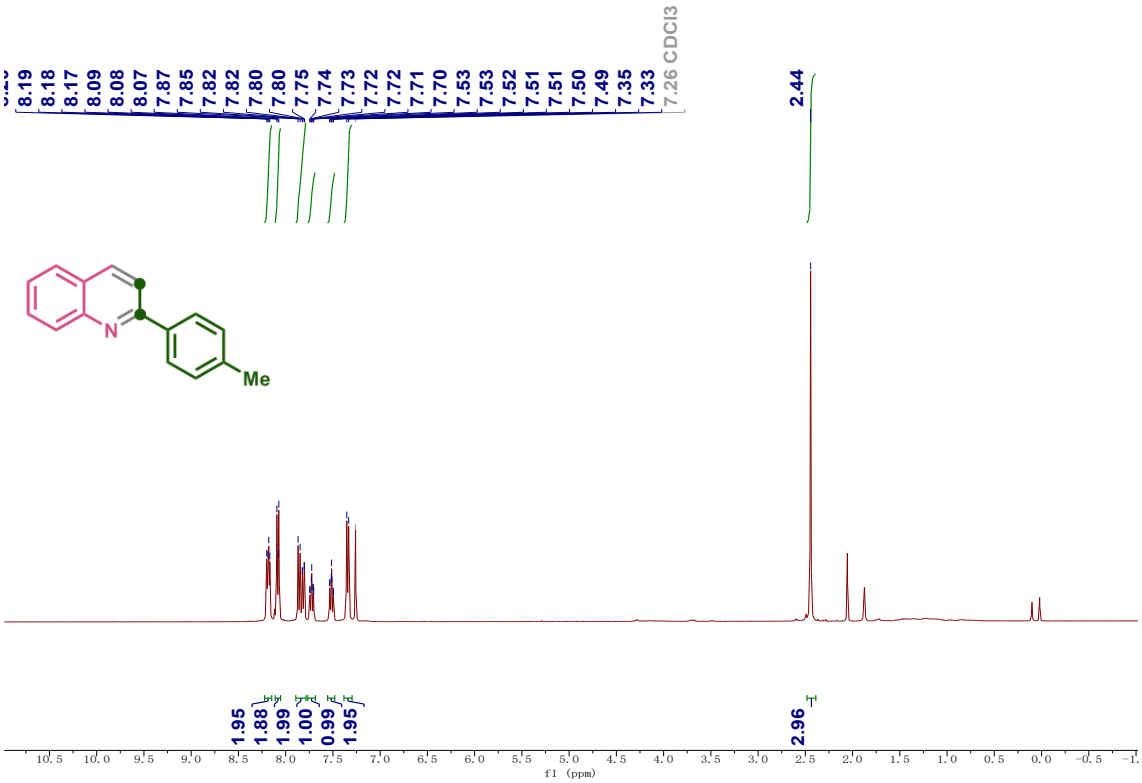
^{1}H NMR spectrum of **7a** (400 MHz, $CDCl_3$)



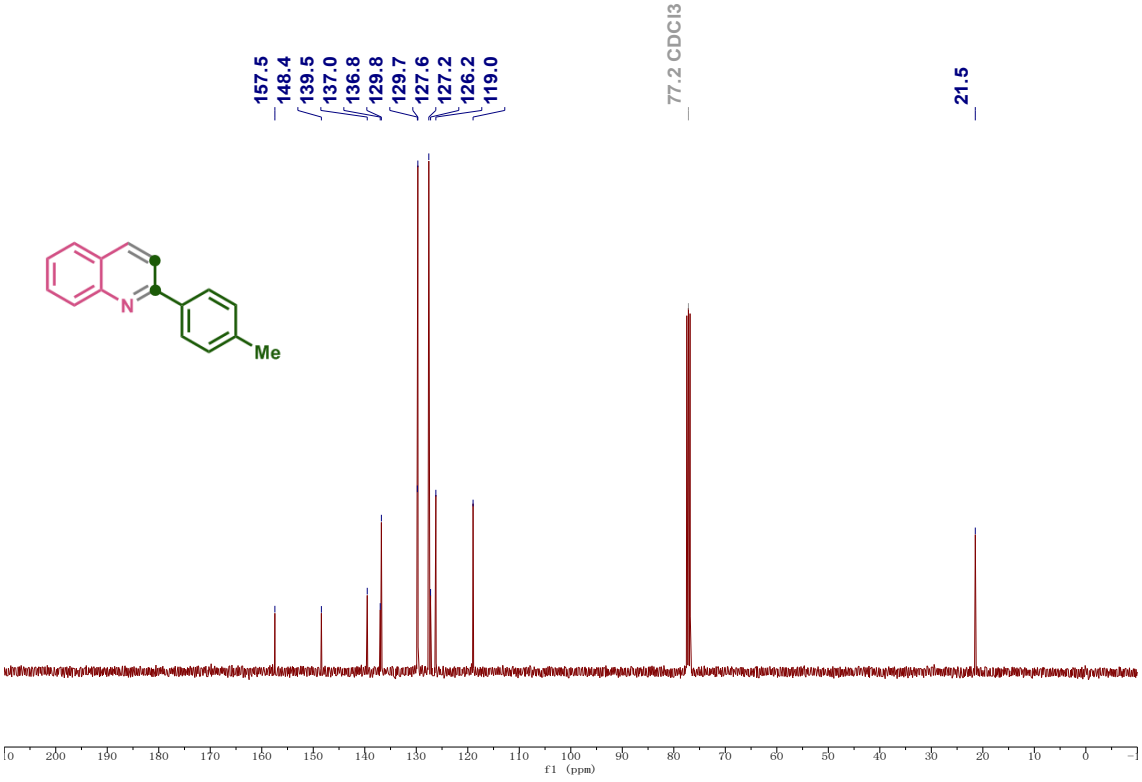
^{13}C NMR spectrum of **7a** (100 MHz, $CDCl_3$)



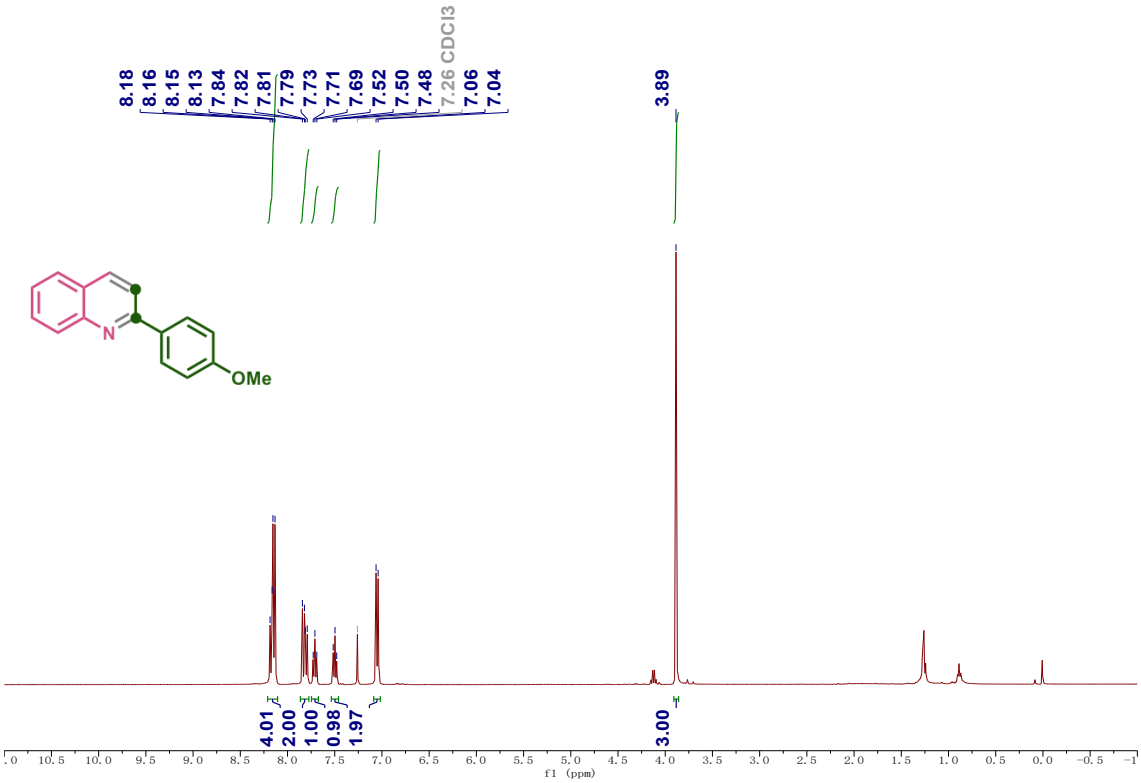
^{1}H NMR spectrum of **7b** (400 MHz, $CDCl_3$)



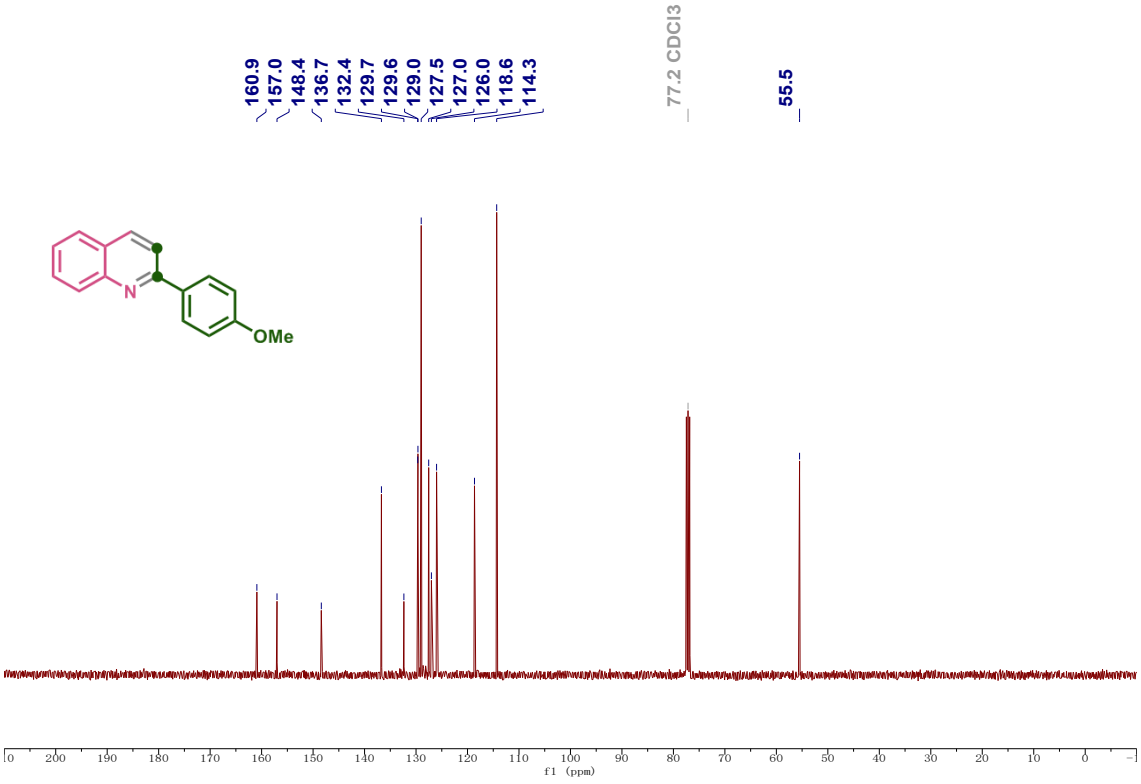
^{13}C NMR spectrum of **7b** (100 MHz, $CDCl_3$)



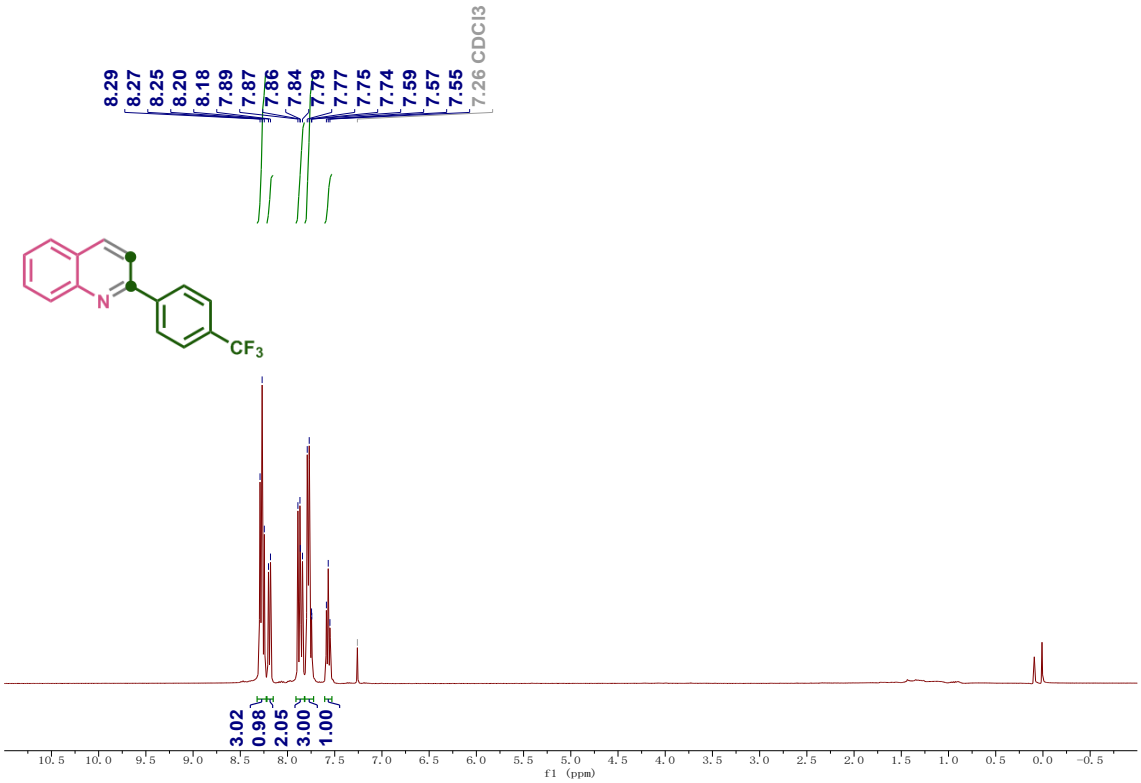
^{1}H NMR spectrum of **7c** (400 MHz, $CDCl_3$)



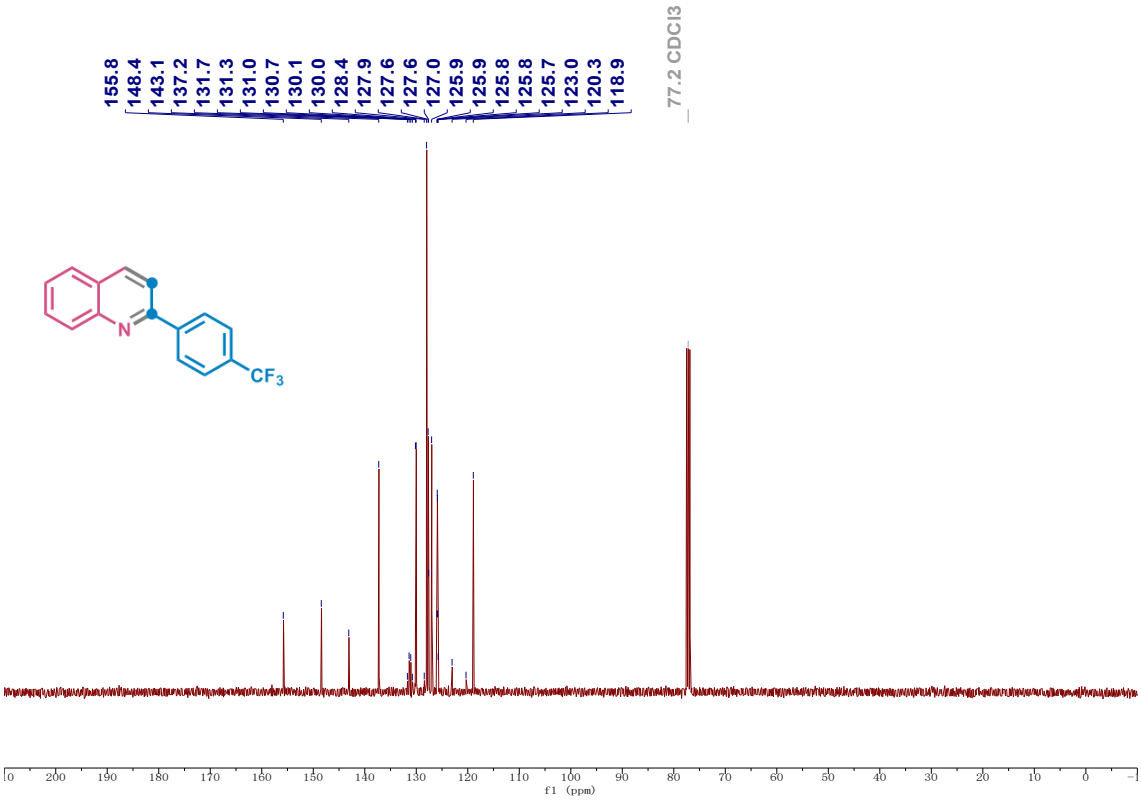
^{13}C NMR spectrum of **7c** (100 MHz, $CDCl_3$)



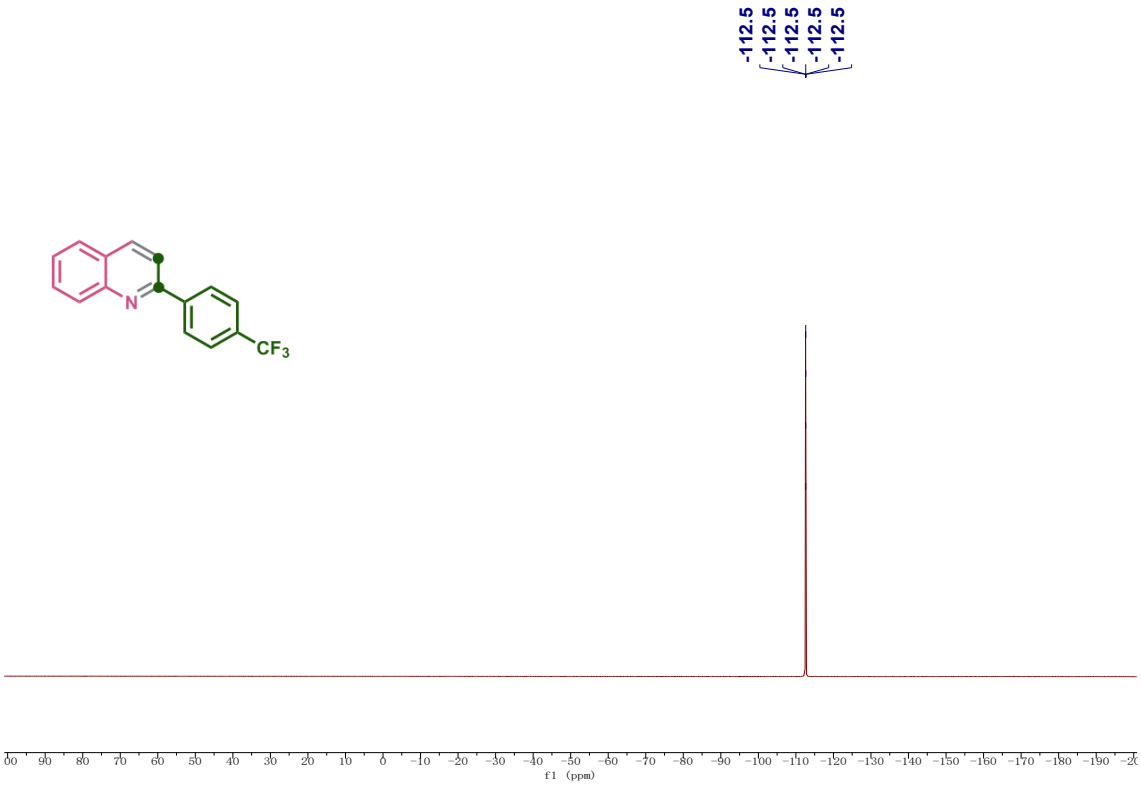
^{1}H NMR spectrum of **7d** (400 MHz, $CDCl_3$)



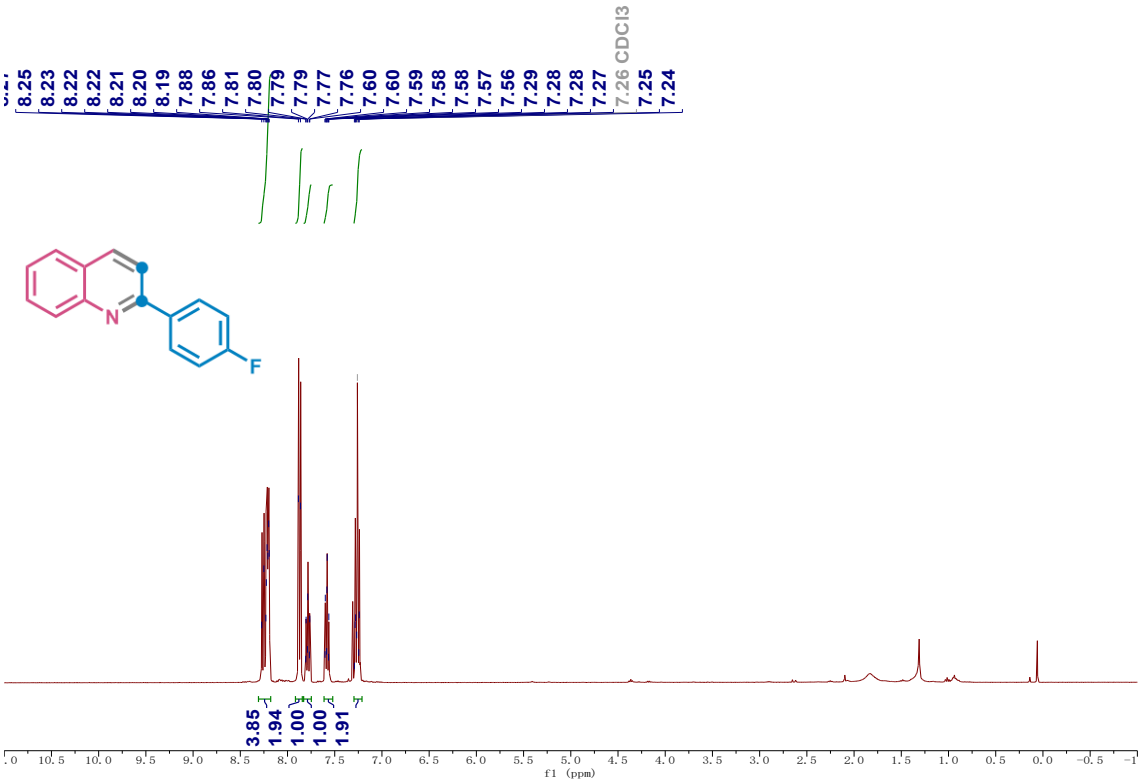
^{13}C NMR spectrum of **7d** (100 MHz, $CDCl_3$)



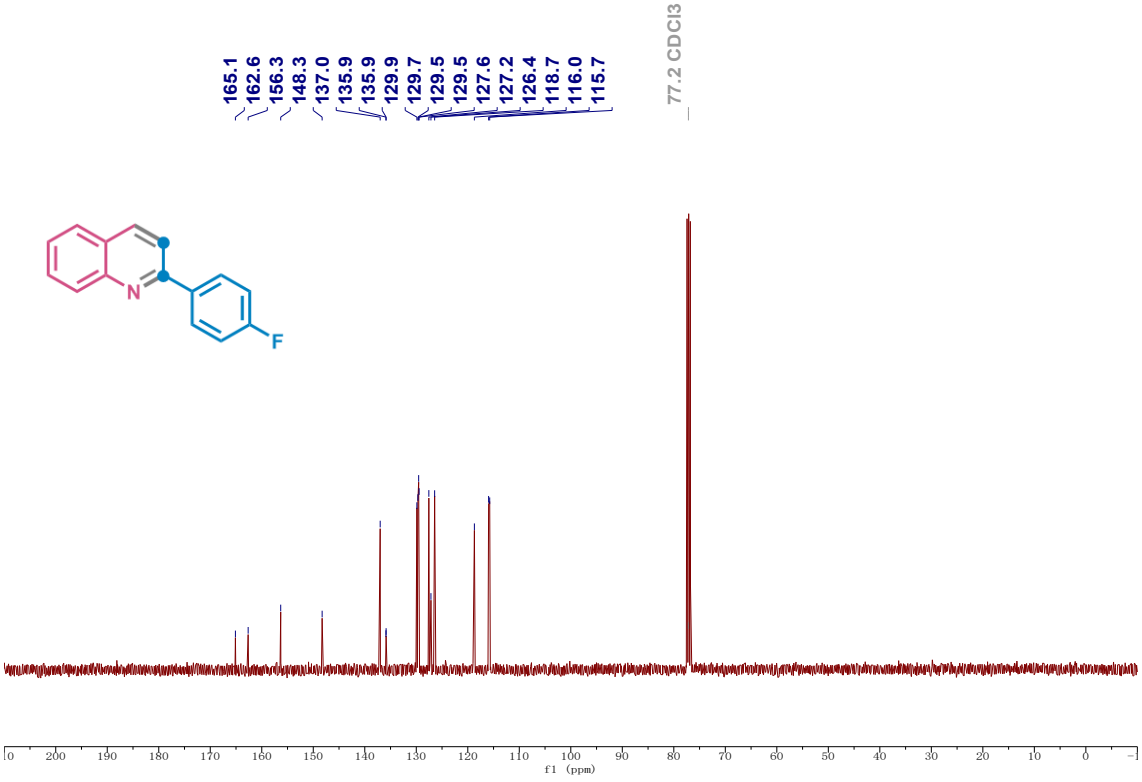
^{19}F NMR spectrum of **7d** (376 MHz, $CDCl_3$)



^{1}H NMR spectrum of **7e** (400 MHz, $CDCl_3$)

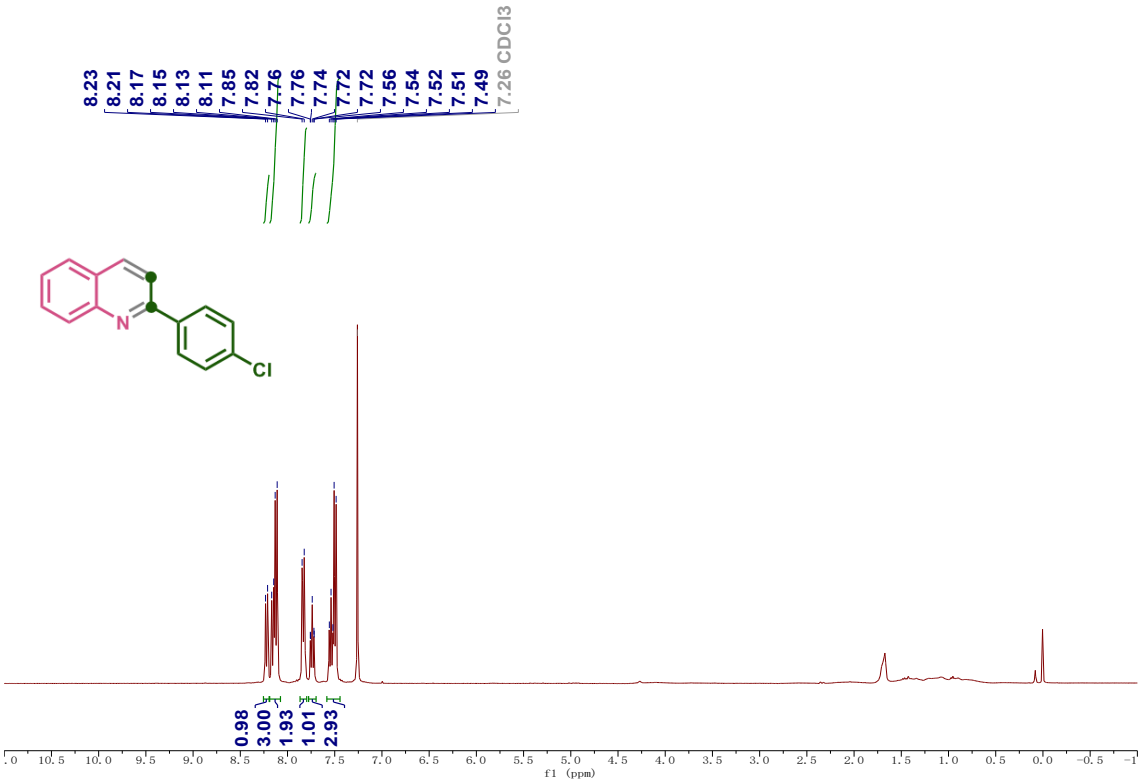


^{13}C NMR spectrum of **7e** (100 MHz, $CDCl_3$)

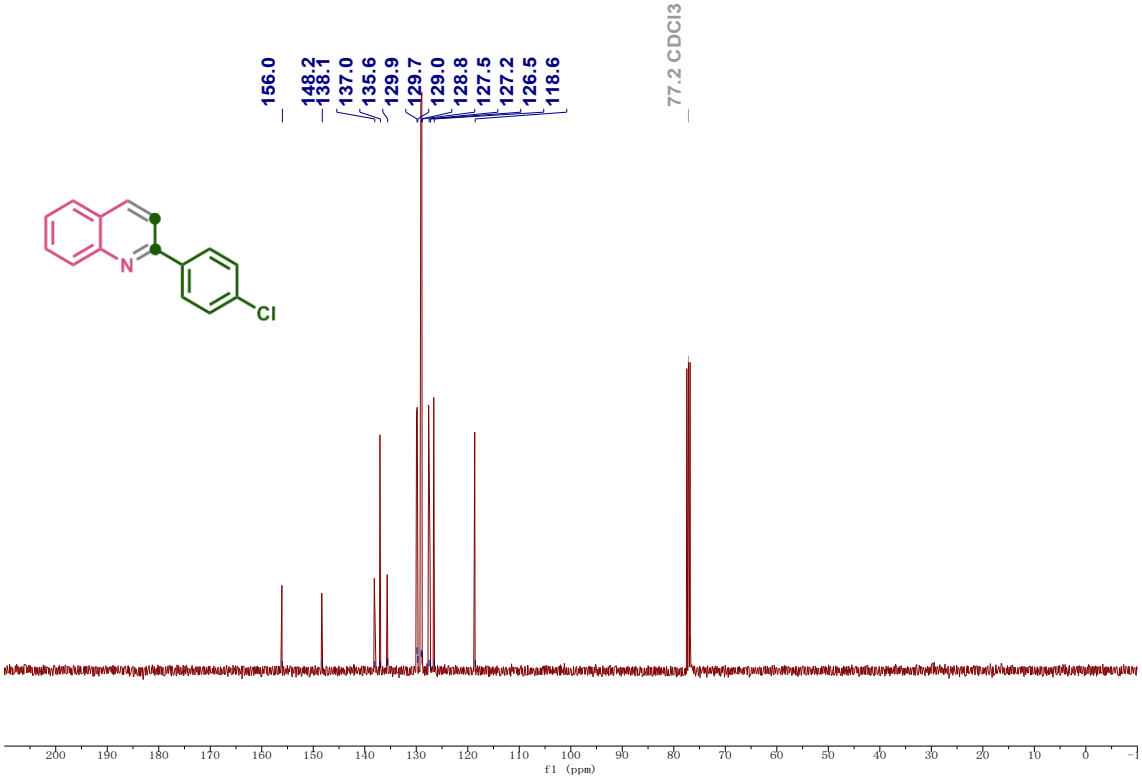


^{19}F NMR spectrum of **7e** (376 MHz, $CDCl_3$)

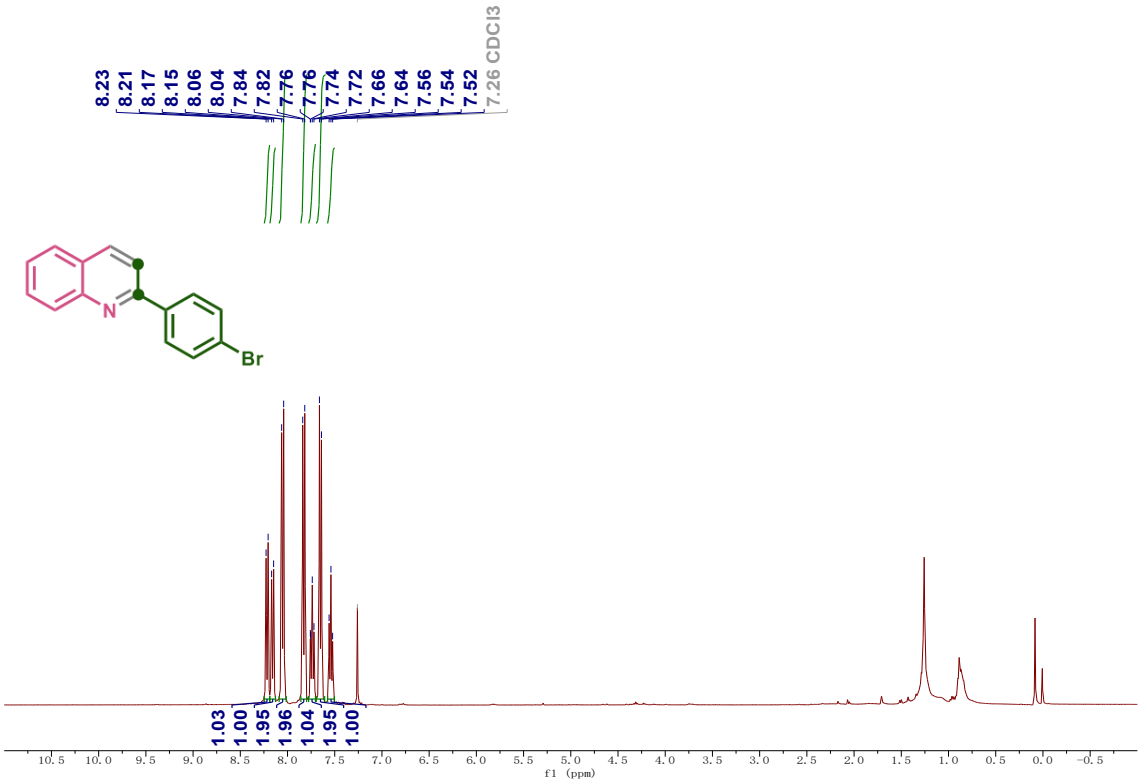
^{1}H NMR spectrum of **7f** (400 MHz, $CDCl_3$)



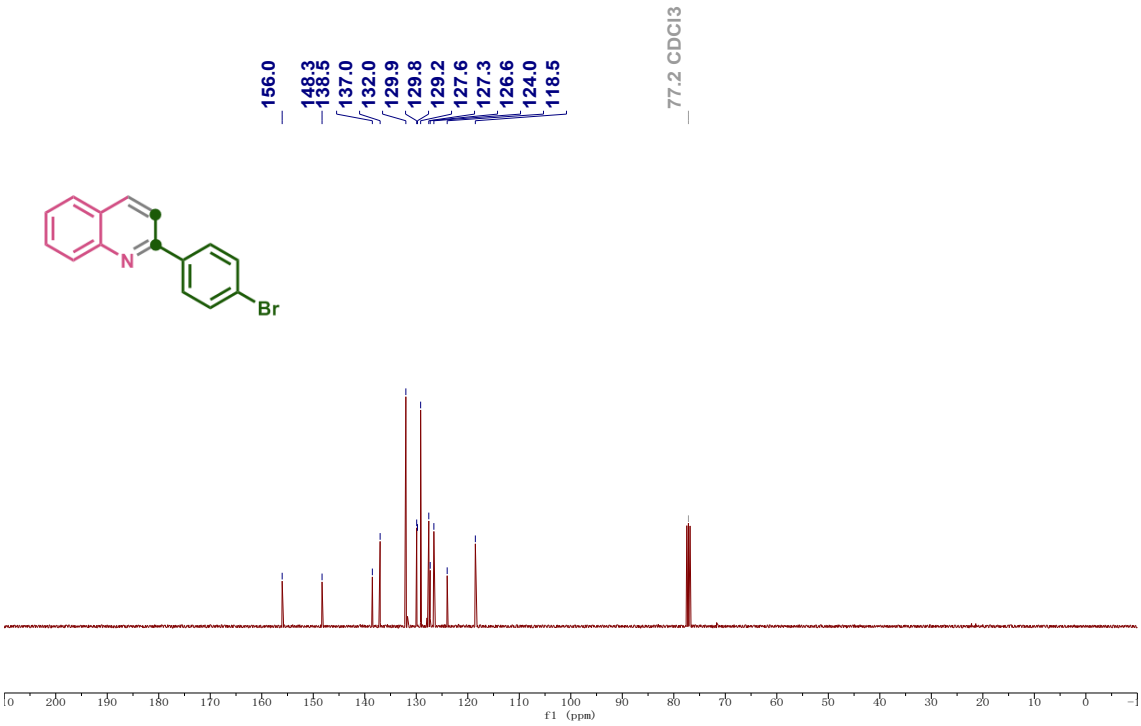
^{13}C NMR spectrum of **7f** (100 MHz, $CDCl_3$)



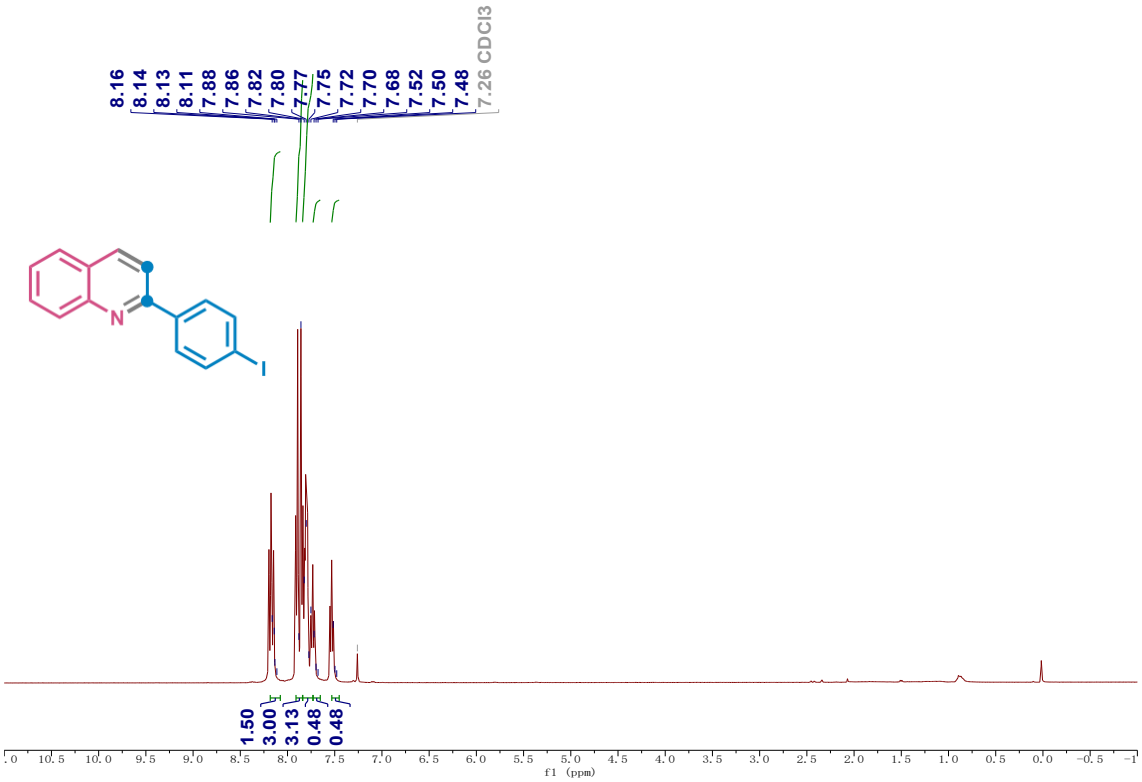
^{1}H NMR spectrum of **7g** (400 MHz, $CDCl_3$)



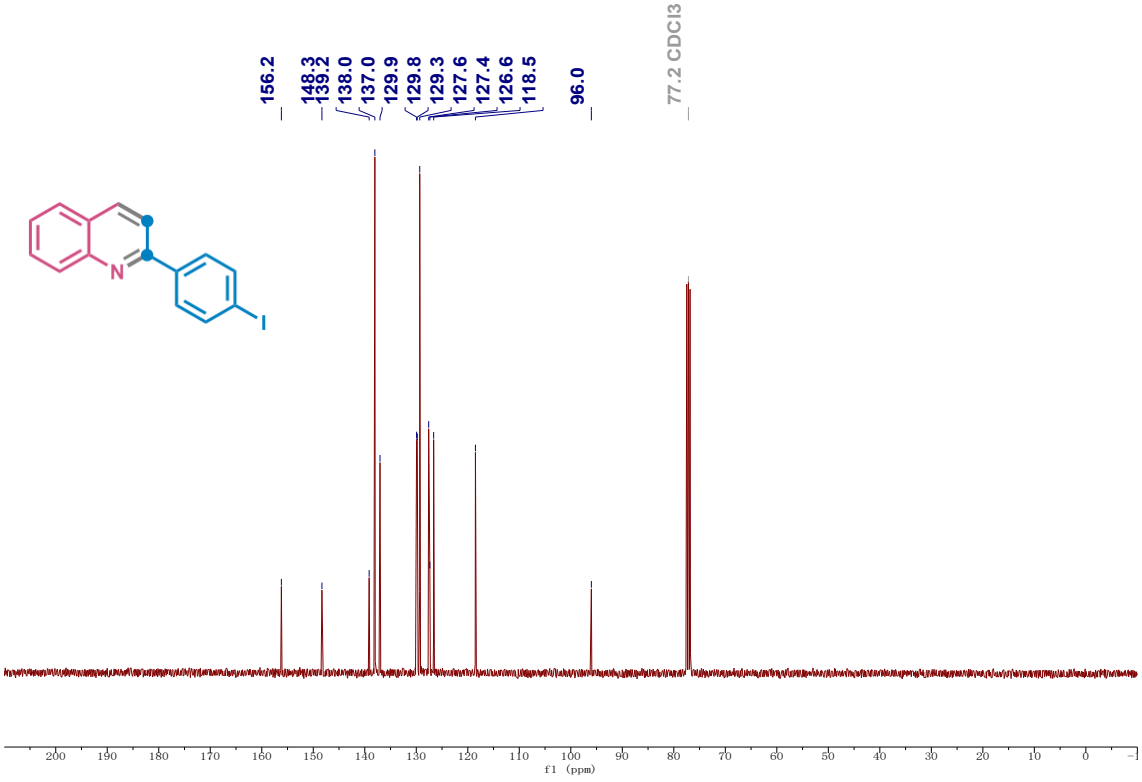
^{13}C NMR spectrum of **7g** (100 MHz, $CDCl_3$)



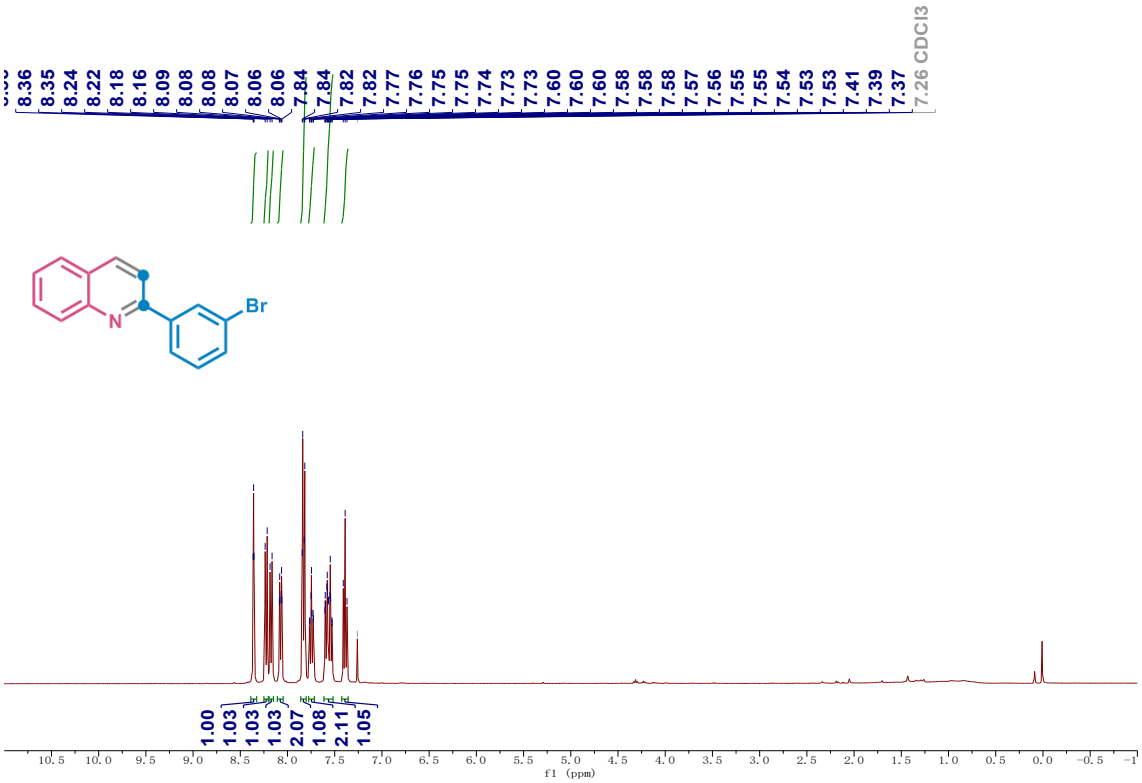
^{1}H NMR spectrum of **7h** (400 MHz, $CDCl_3$)



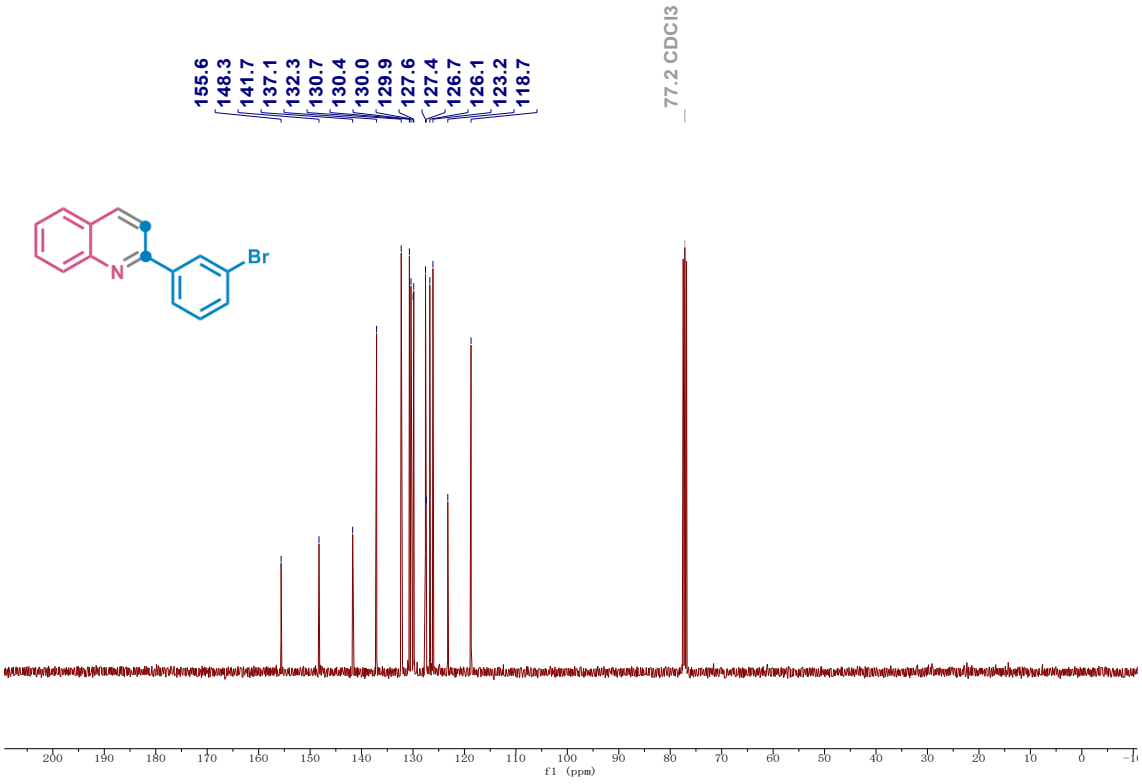
^{13}C NMR spectrum of **7h** (100 MHz, $CDCl_3$)



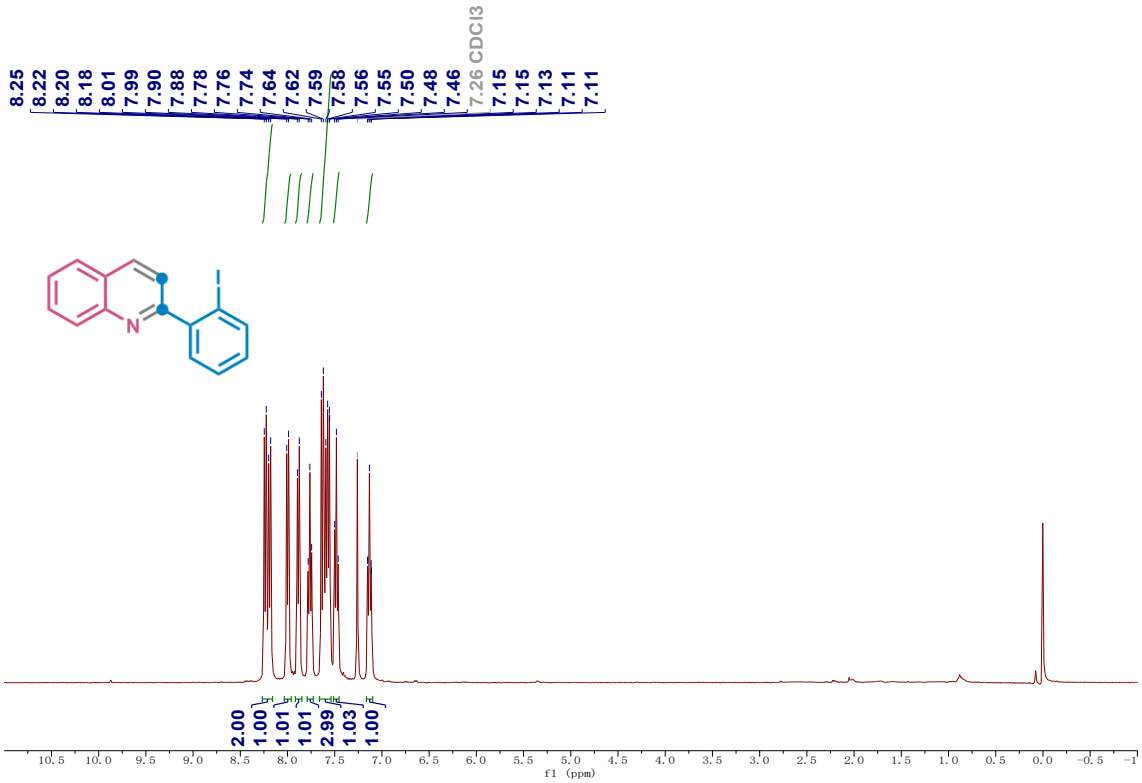
^{1}H NMR spectrum of **7i** (400 MHz, $CDCl_3$)



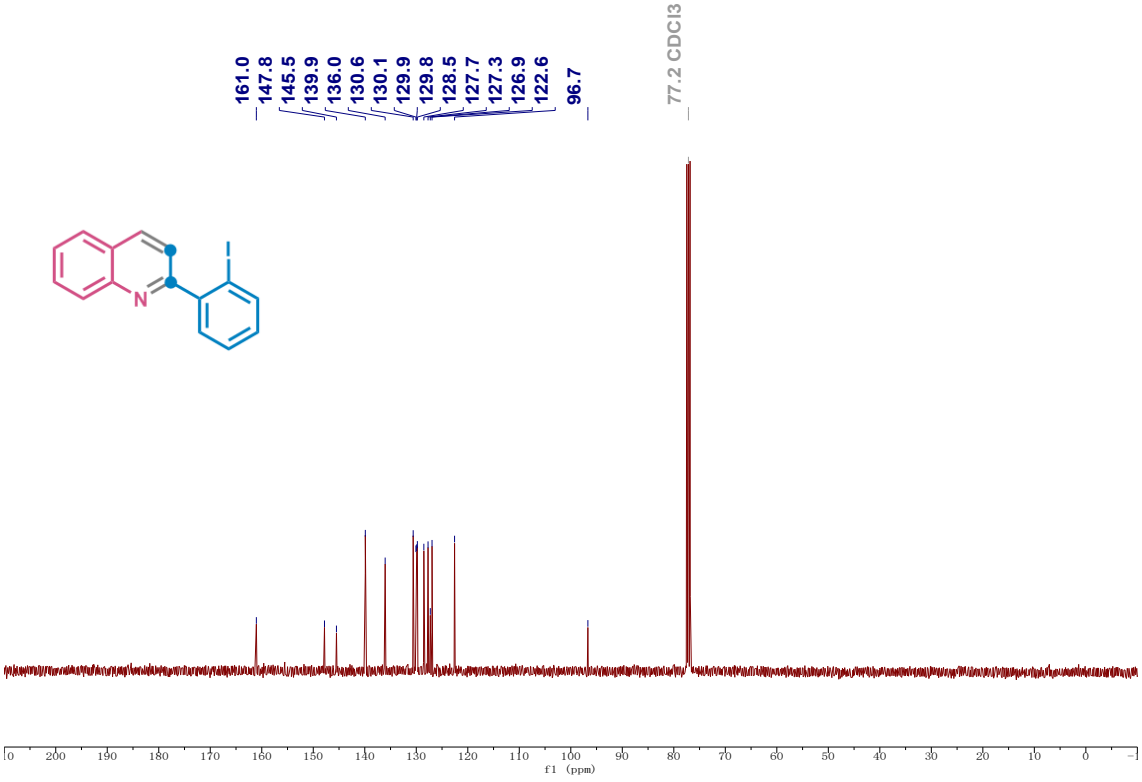
^{13}C NMR spectrum of **7i** (100 MHz, $CDCl_3$)



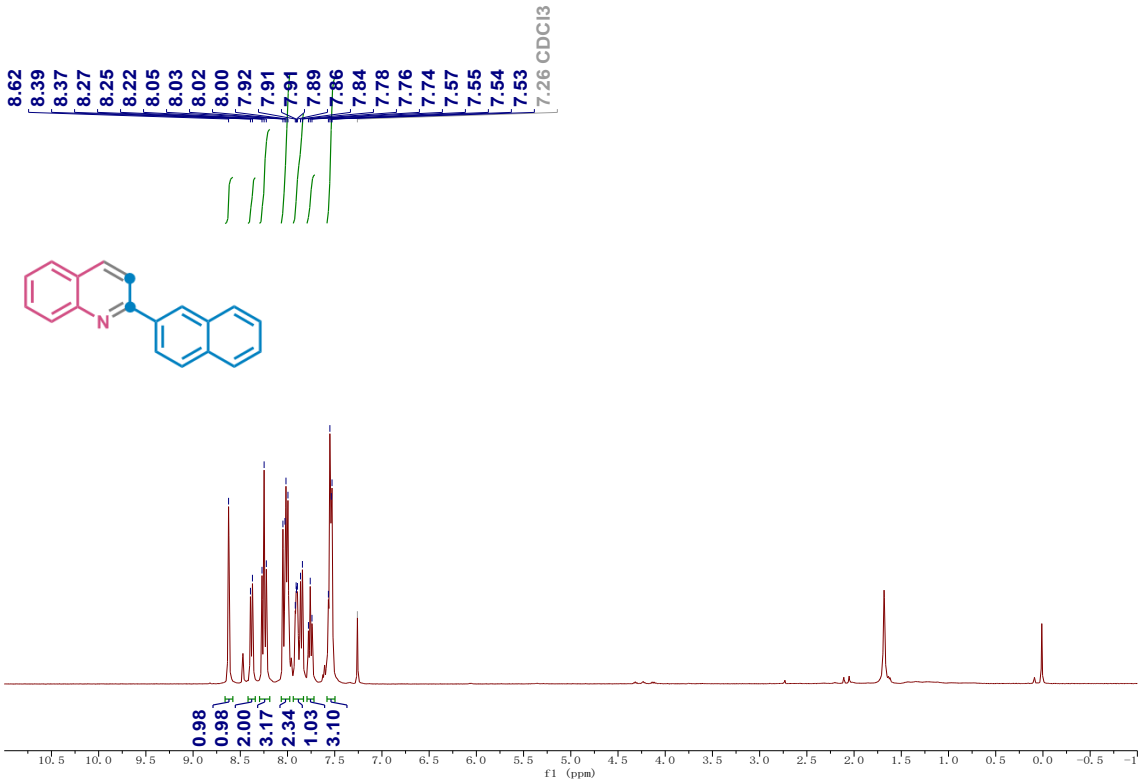
^{1}H NMR spectrum of **7j** (400 MHz, $CDCl_3$)



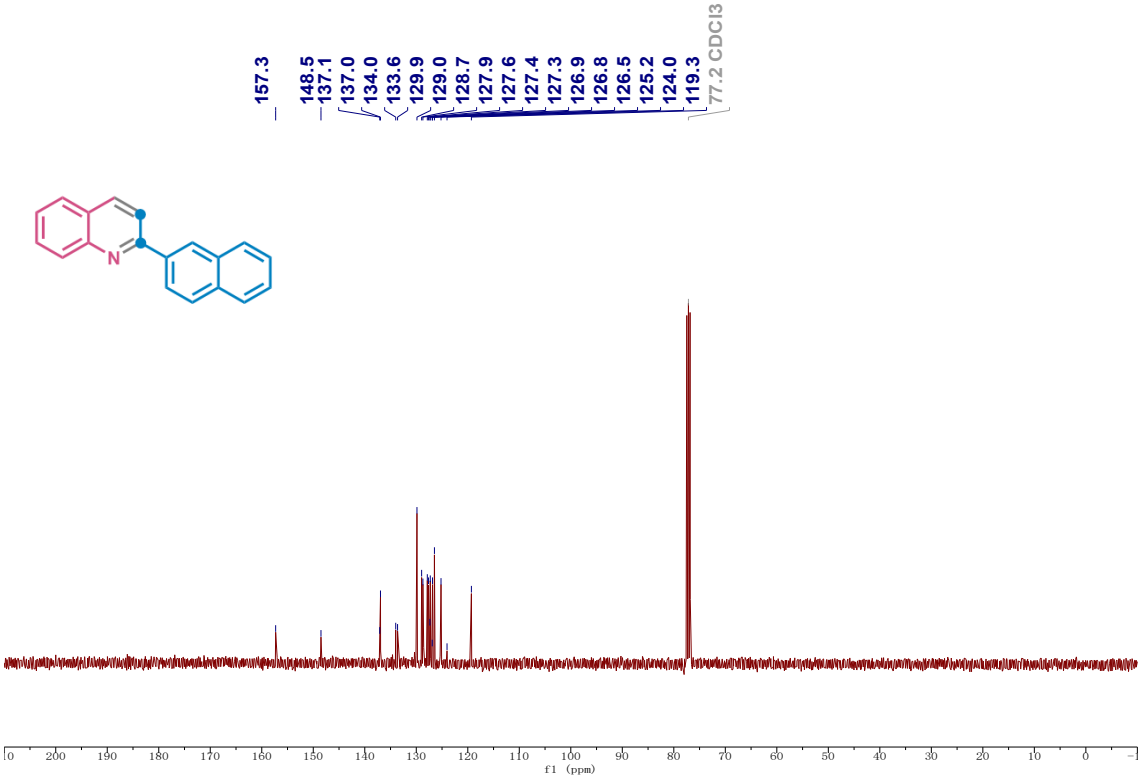
^{13}C NMR spectrum of **7j** (100 MHz, $CDCl_3$)



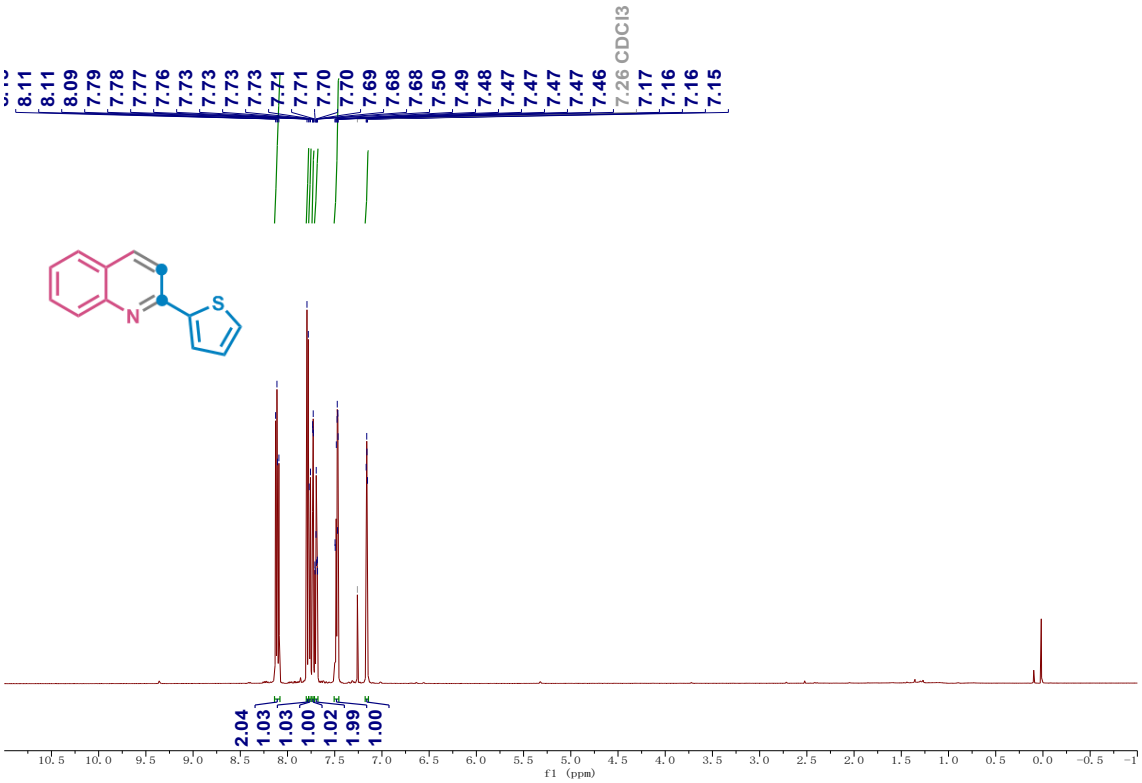
^{1}H NMR spectrum of **7k** (400 MHz, $CDCl_3$)



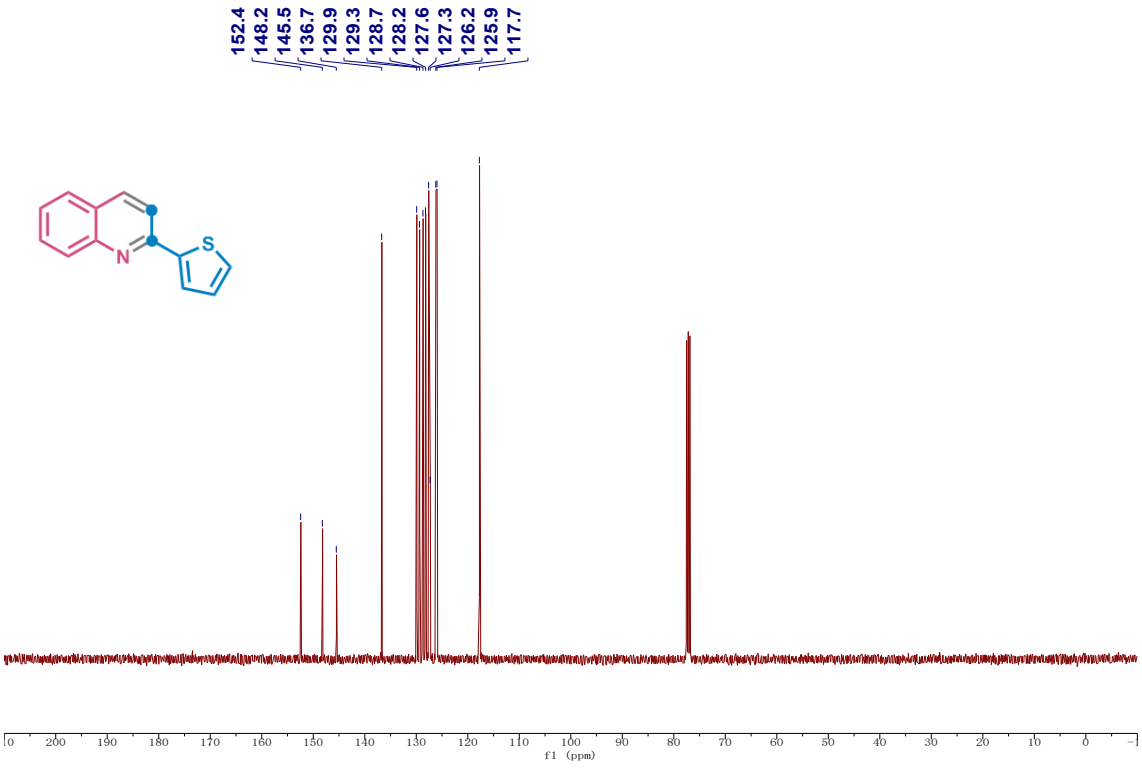
^{13}C NMR spectrum of **7k** (100 MHz, $CDCl_3$)



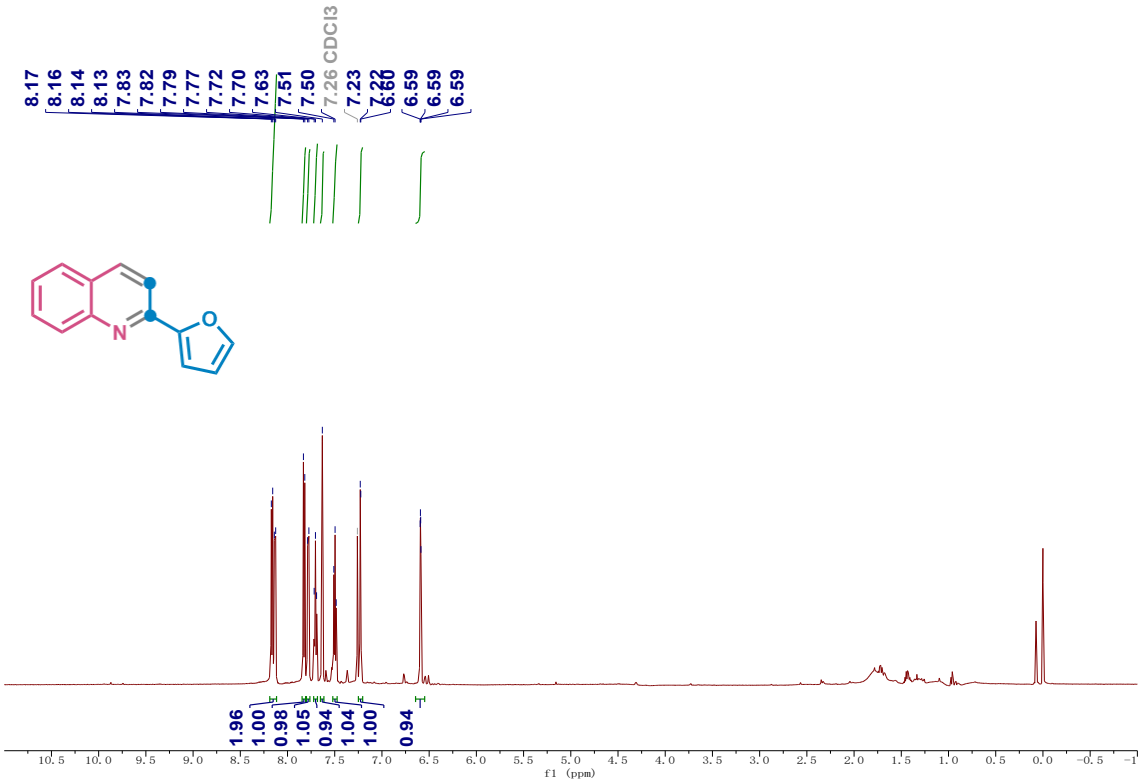
^{1}H NMR spectrum of **7l** (400 MHz, $CDCl_3$)



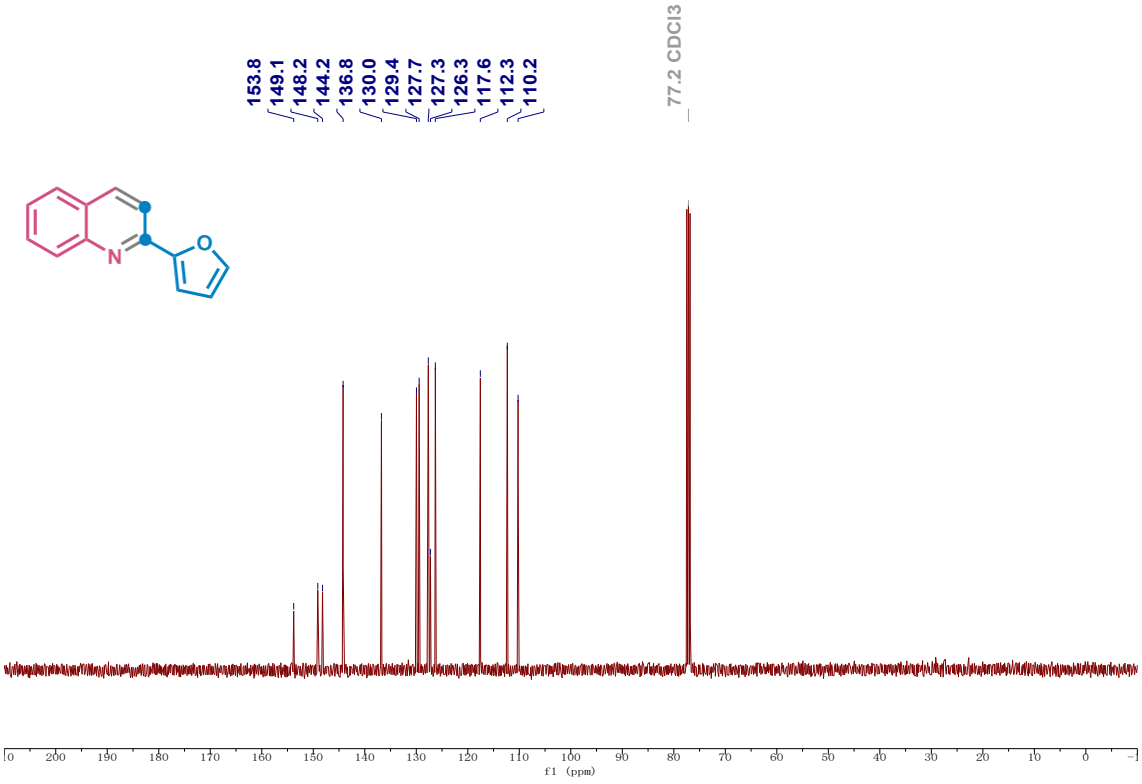
^{13}C NMR spectrum of **7l** (100 MHz, $CDCl_3$)



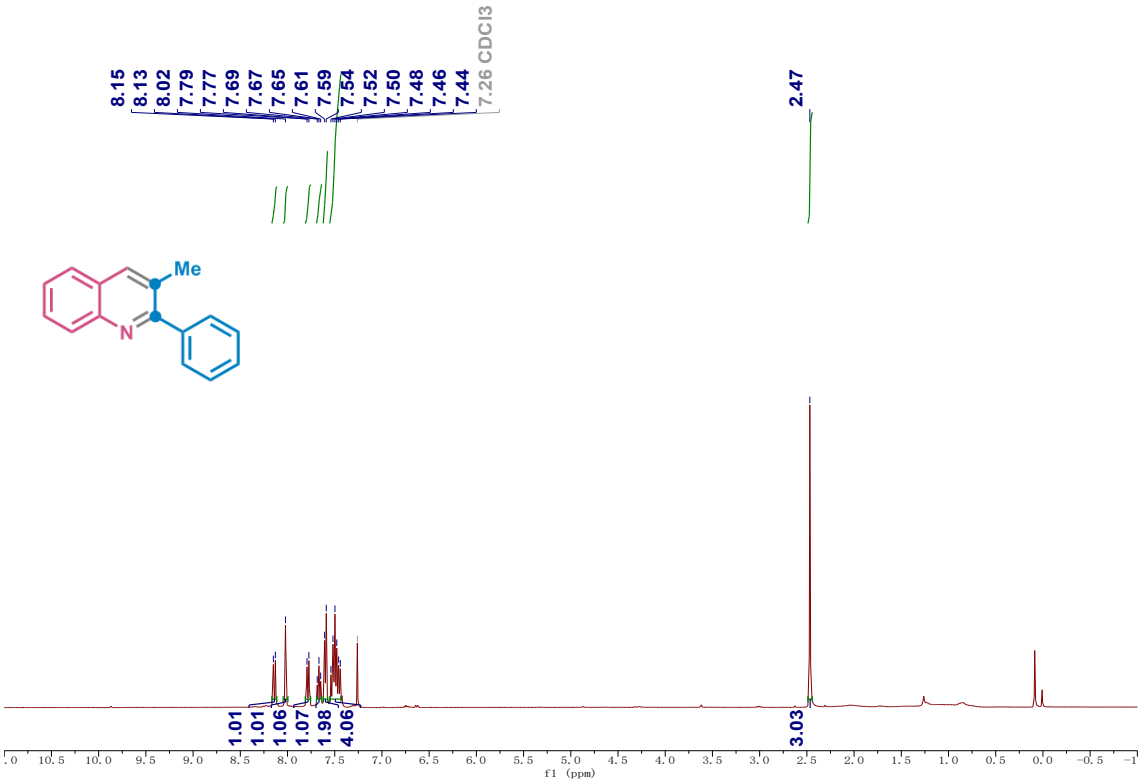
^{1}H NMR spectrum of **7m** (400 MHz, $CDCl_3$)



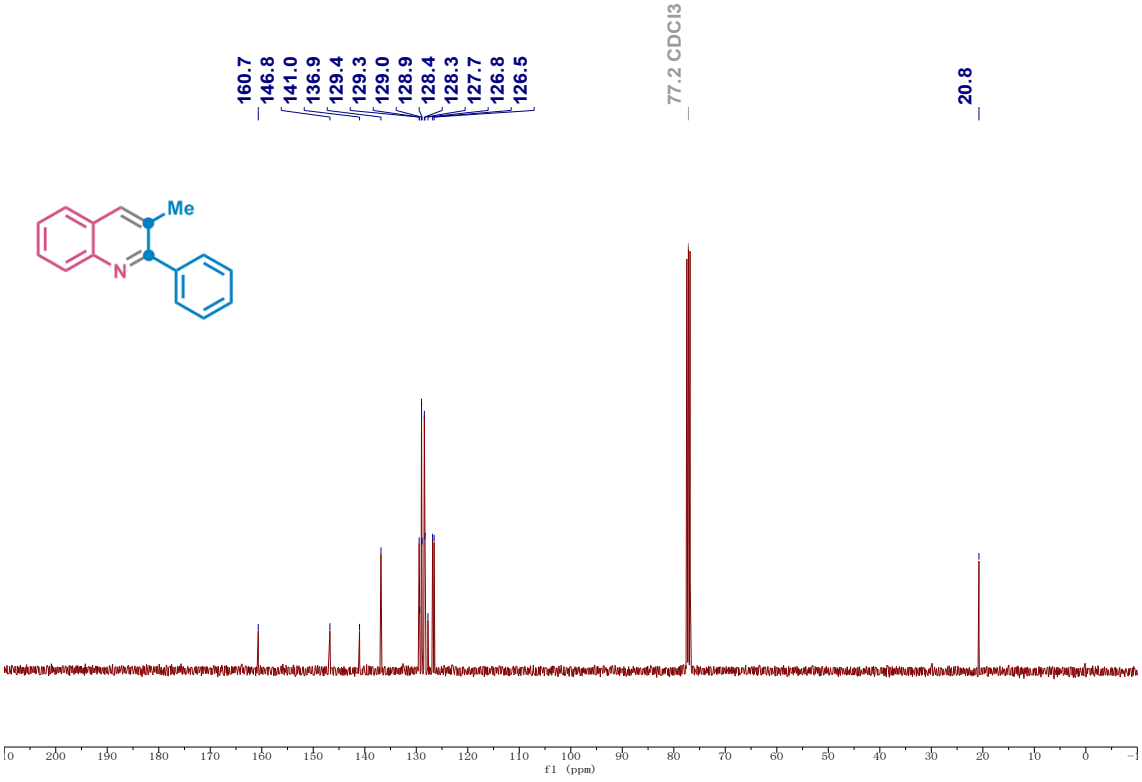
^{13}C NMR spectrum of **7m** (100 MHz, $CDCl_3$)



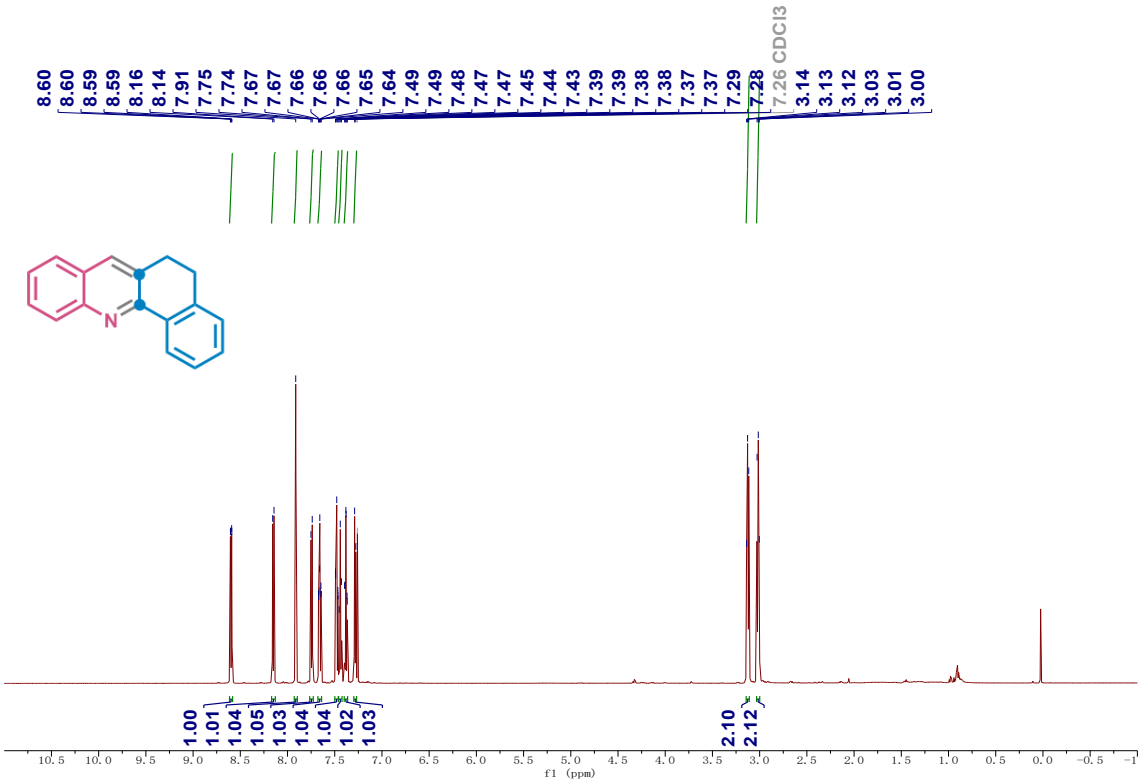
^{1}H NMR spectrum of **7n** (400 MHz, $CDCl_3$)



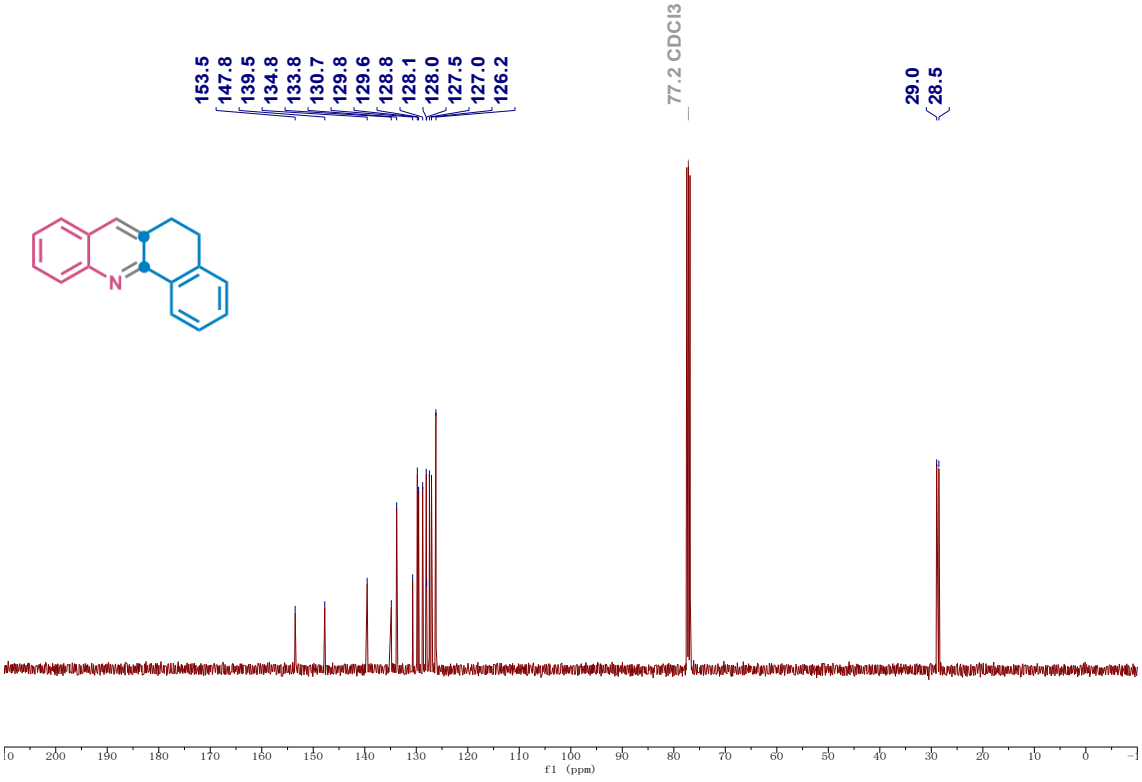
^{13}C NMR spectrum of **7n** (100 MHz, $CDCl_3$)



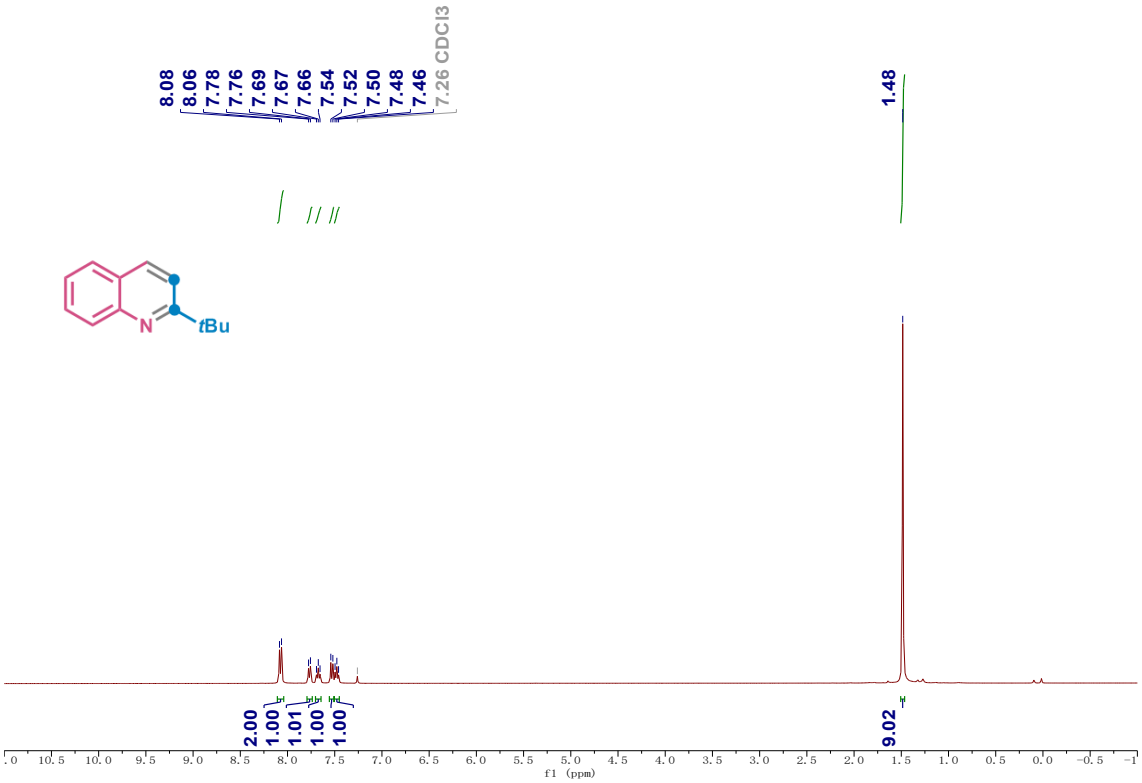
^{1}H NMR spectrum of **7o** (400 MHz, $CDCl_3$)



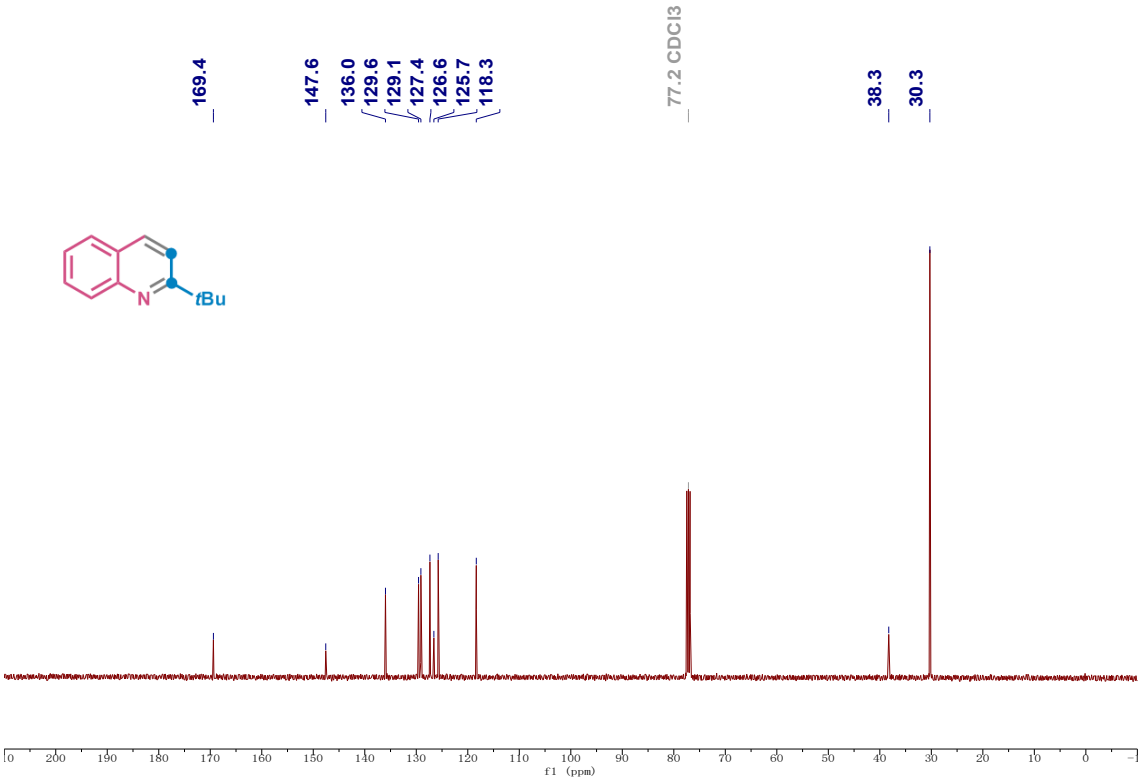
^{13}C NMR spectrum of **7o** (100 MHz, $CDCl_3$)



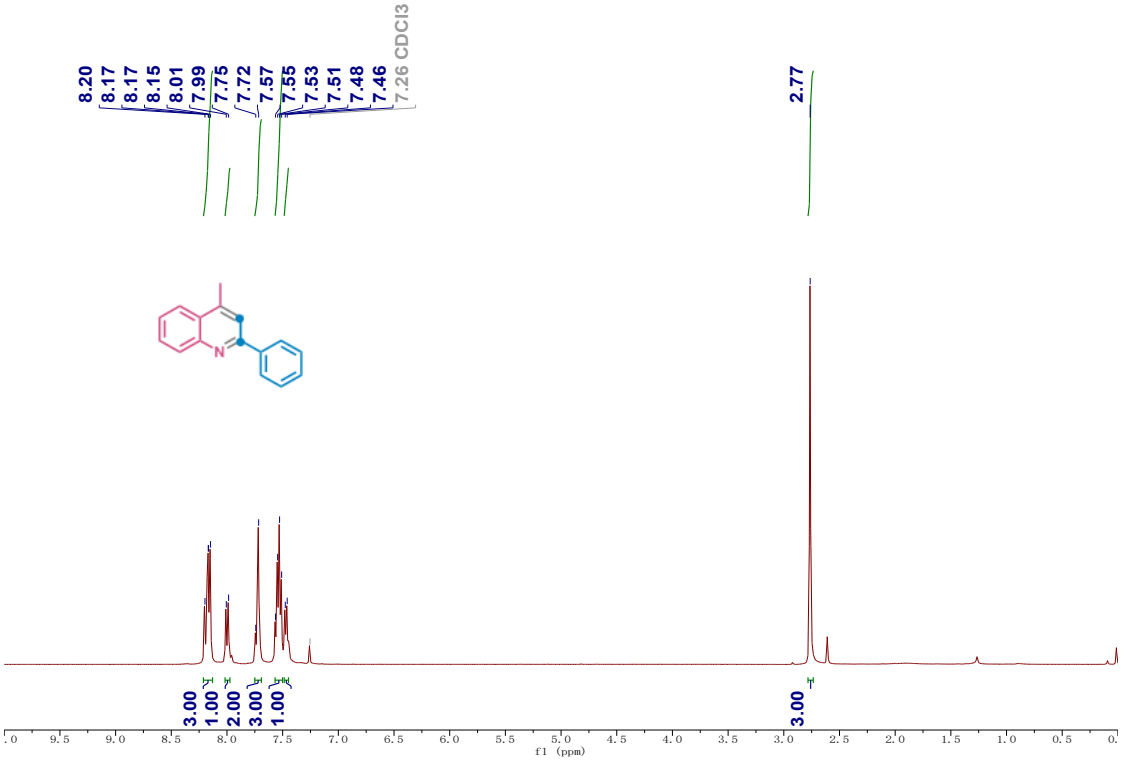
^{1}H NMR spectrum of **7p** (400 MHz, $CDCl_3$)



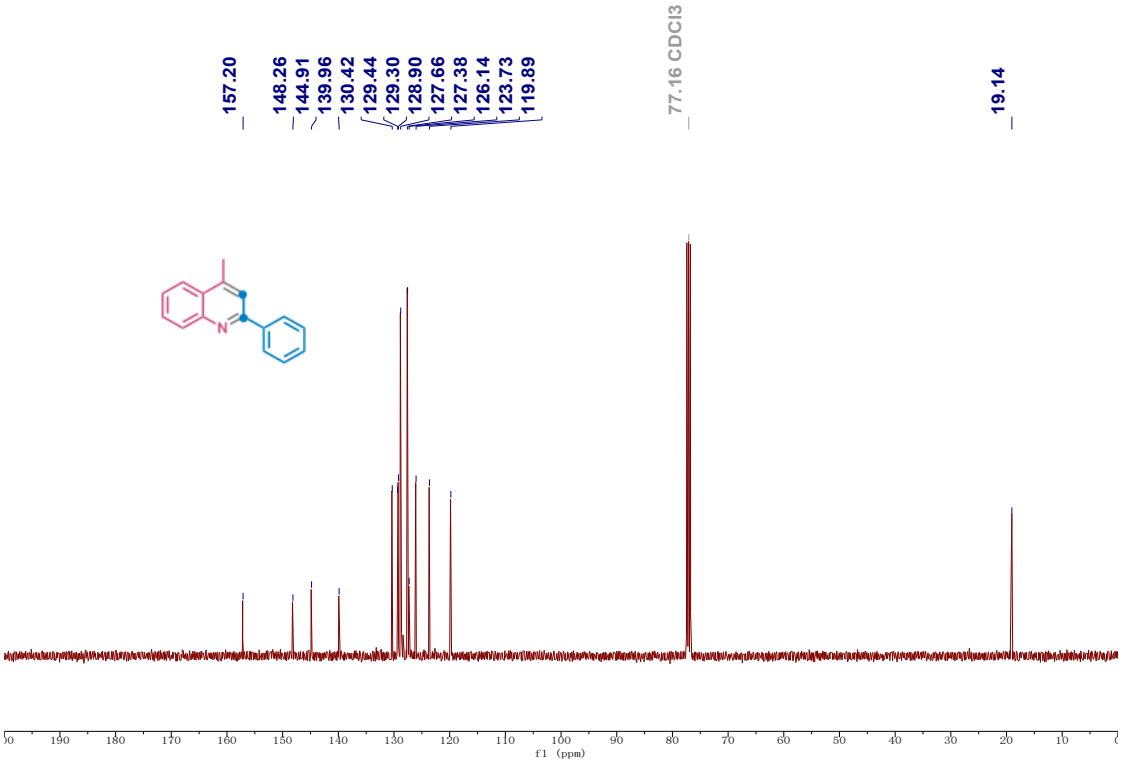
^{13}C NMR spectrum of **7p** (100 MHz, $CDCl_3$)



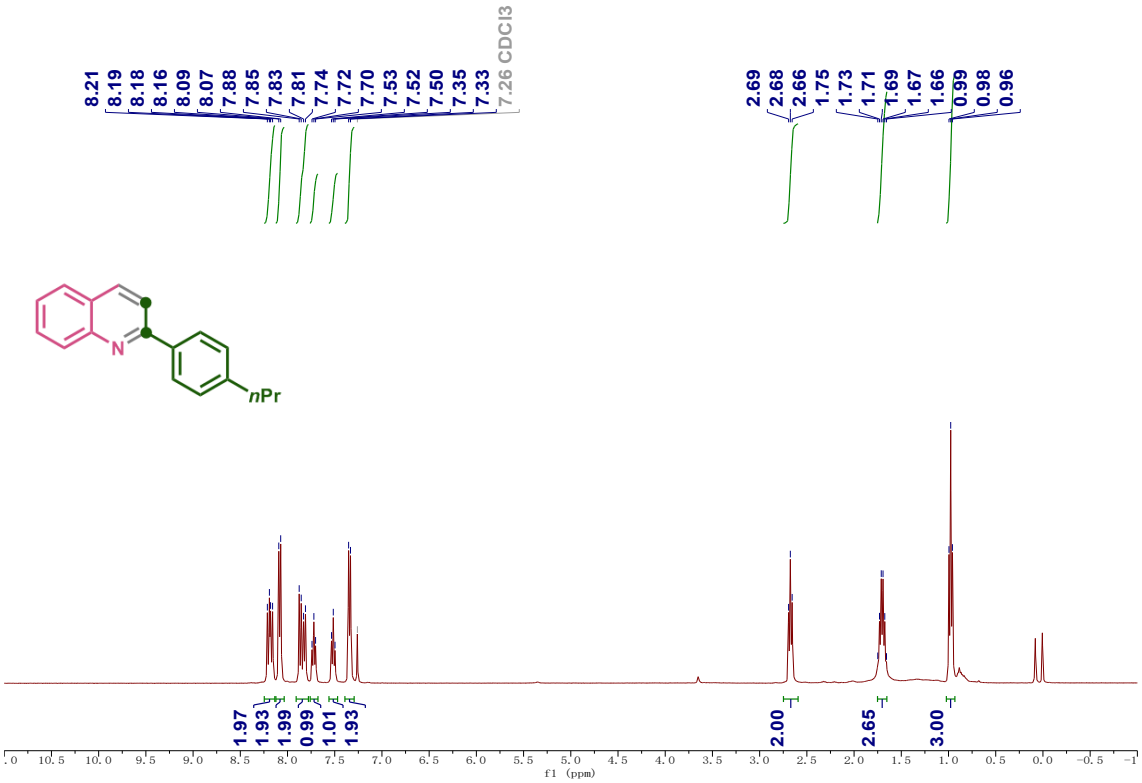
^{1}H NMR spectrum of **7q** (400 MHz, $CDCl_3$)



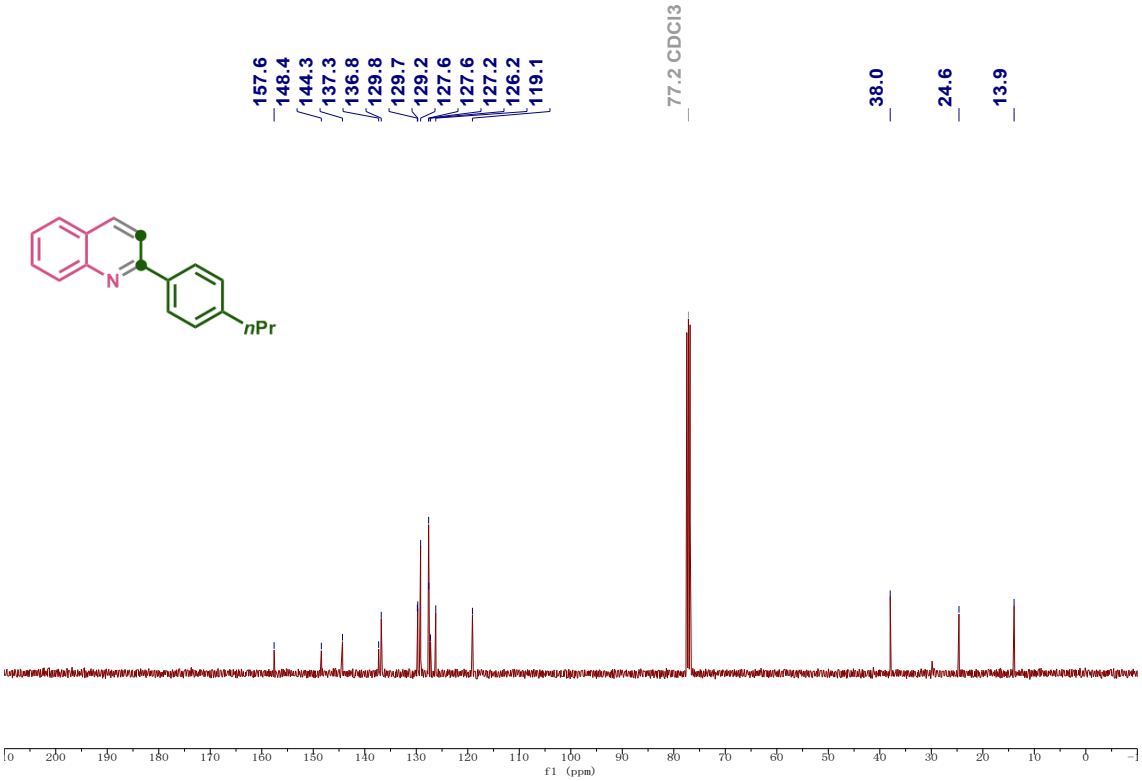
^{13}C NMR spectrum of **7q** (100 MHz, $CDCl_3$)



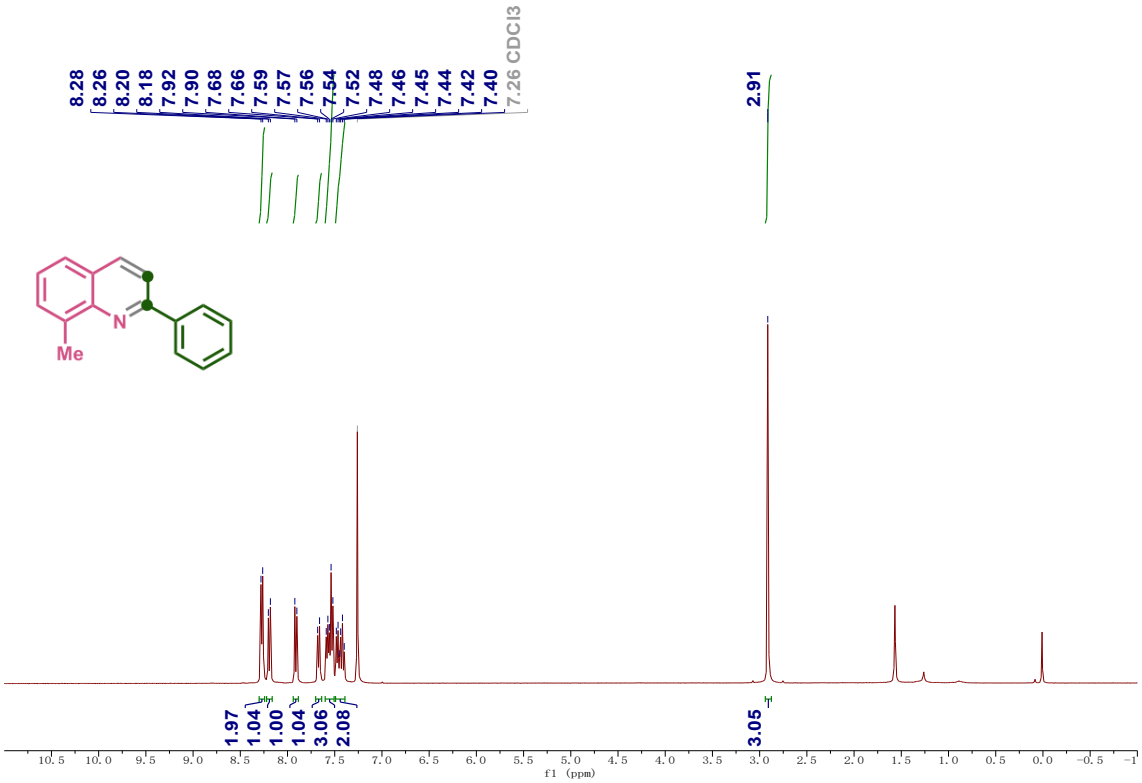
^{1}H NMR spectrum of **7r** (400 MHz, $CDCl_3$)



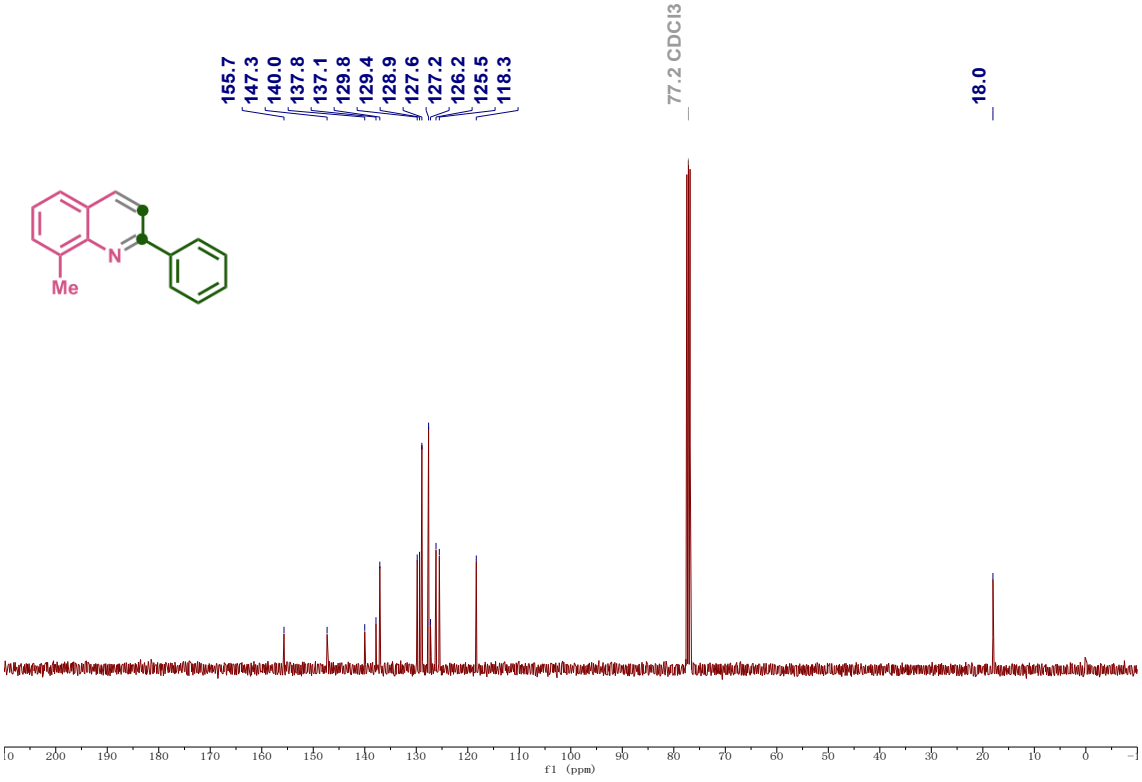
^{13}C NMR spectrum of **7r** (100 MHz, $CDCl_3$)



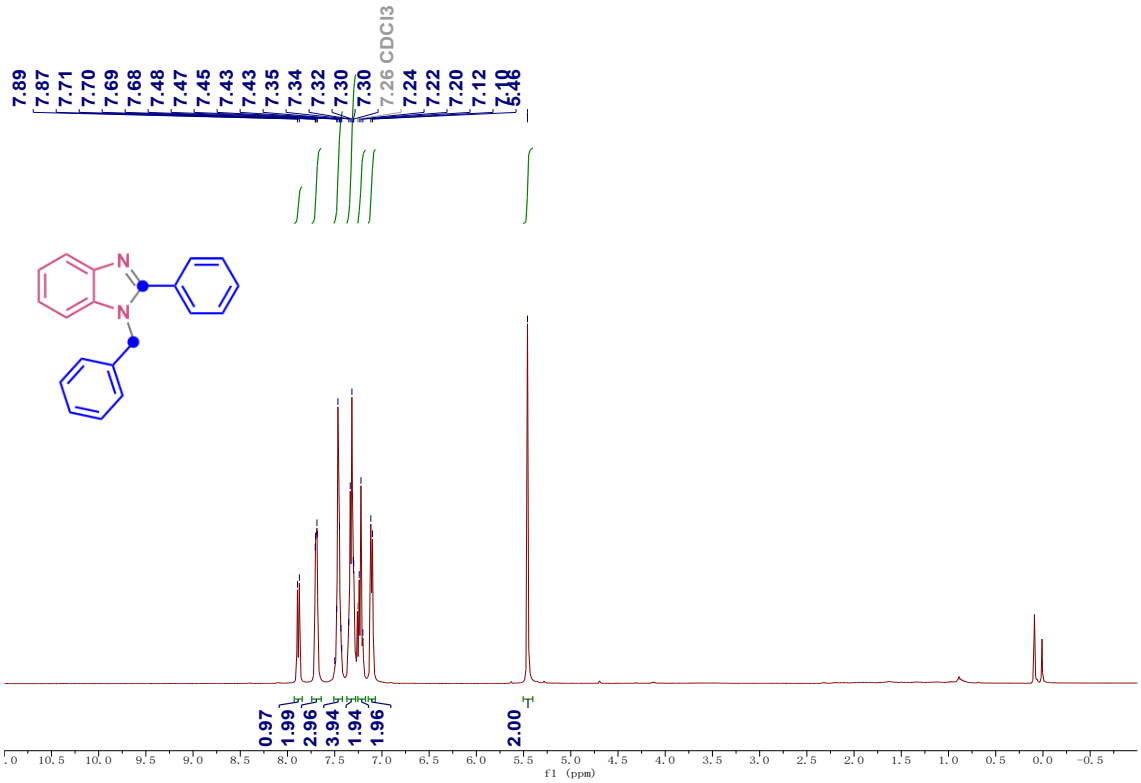
^{1}H NMR spectrum of **7s** (400 MHz, $CDCl_3$)



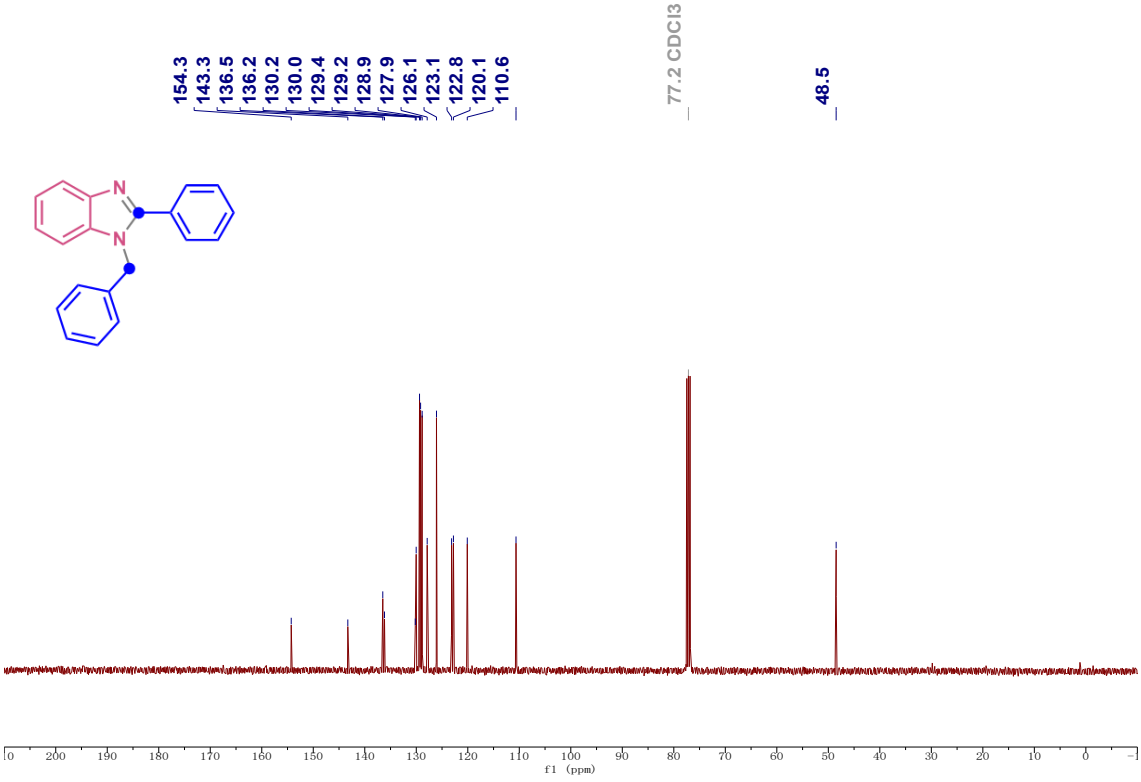
^{13}C NMR spectrum of **7s** (100 MHz, $CDCl_3$)



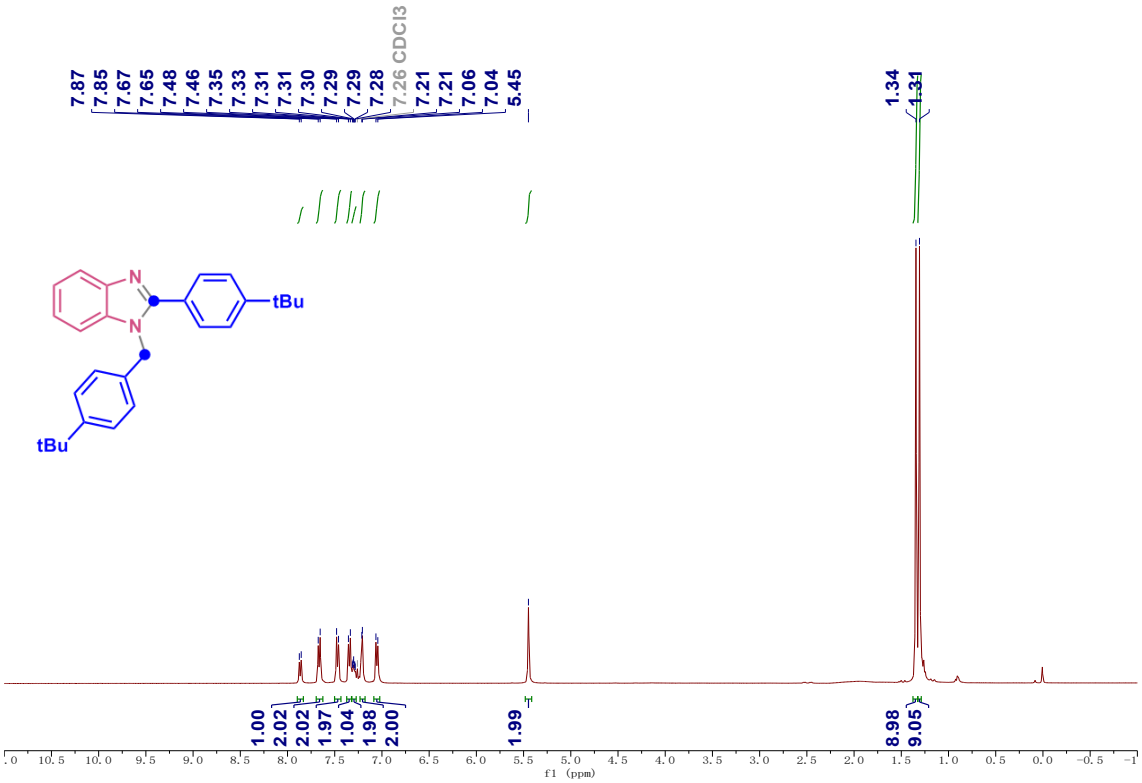
^{1}H NMR spectrum of **9a** (400 MHz, $CDCl_3$)



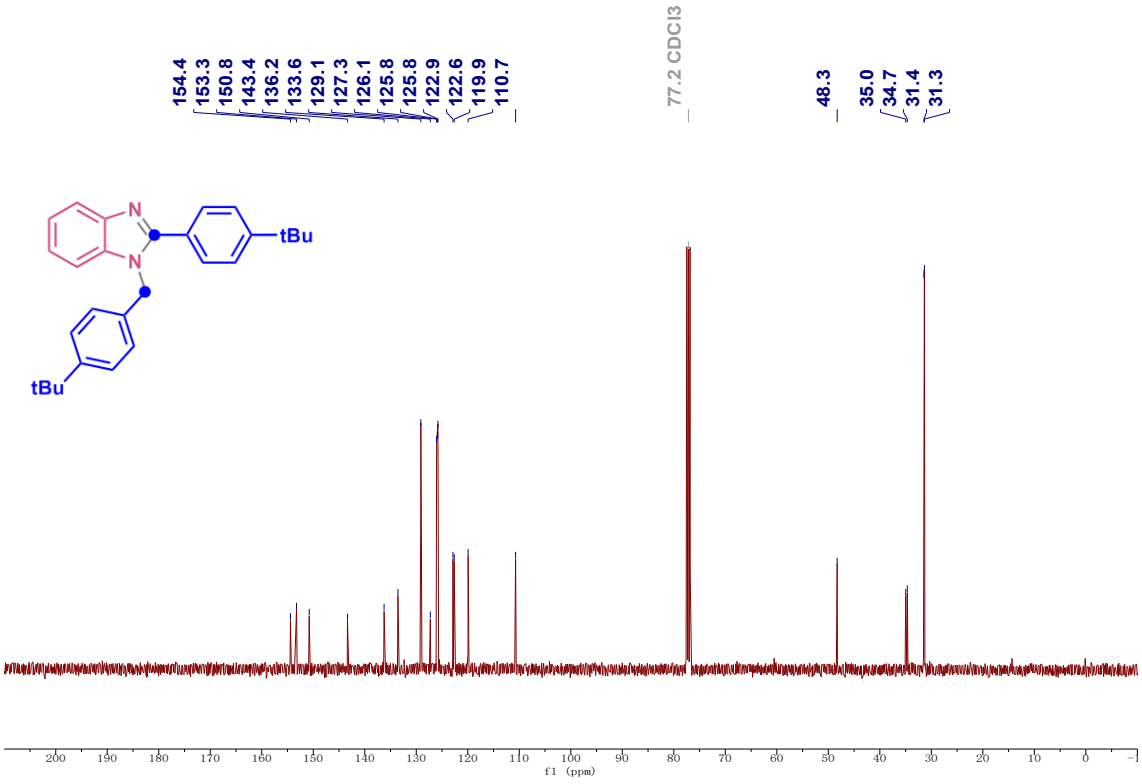
^{13}C NMR spectrum of **9a** (100 MHz, $CDCl_3$)



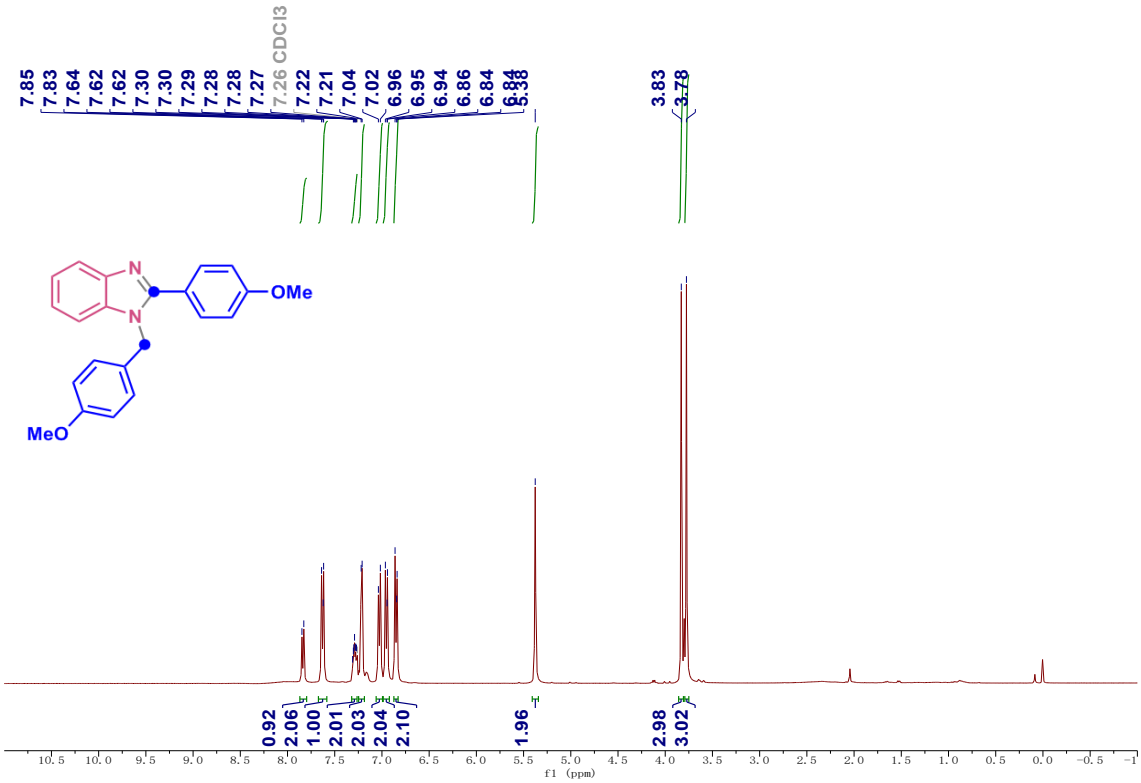
^{1}H NMR spectrum of **9b** (400 MHz, $CDCl_3$)



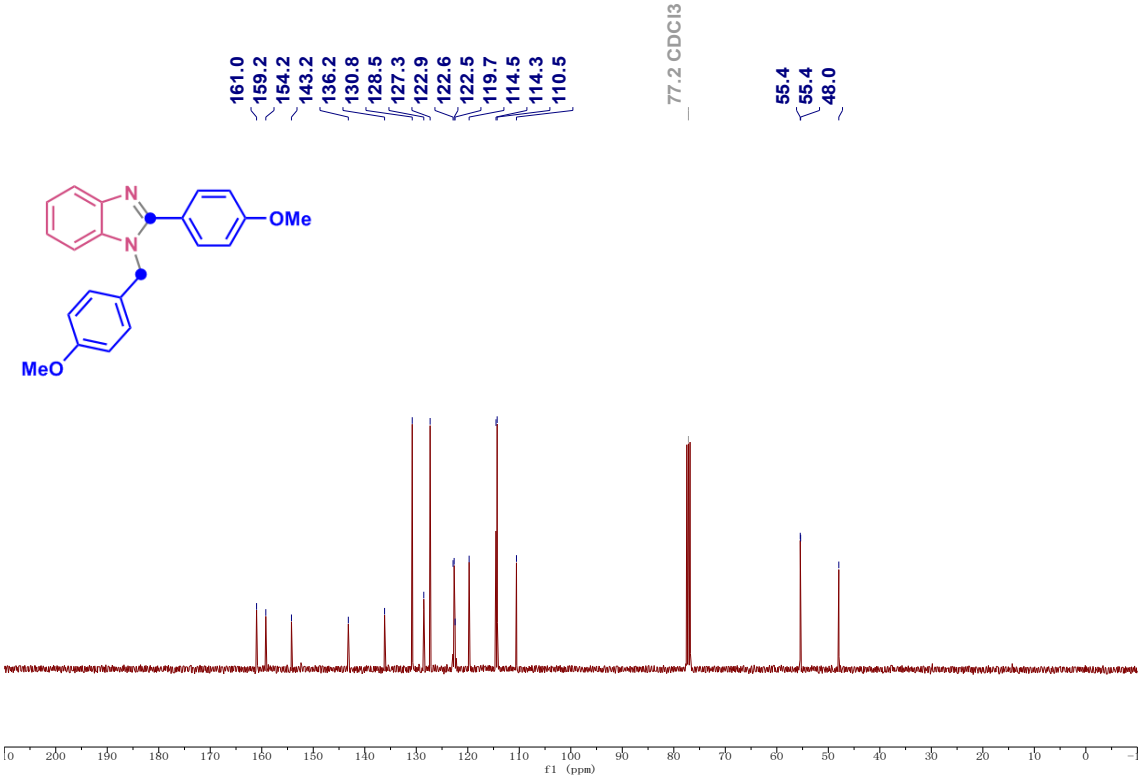
^{13}C NMR spectrum of **9b** (100 MHz, $CDCl_3$)



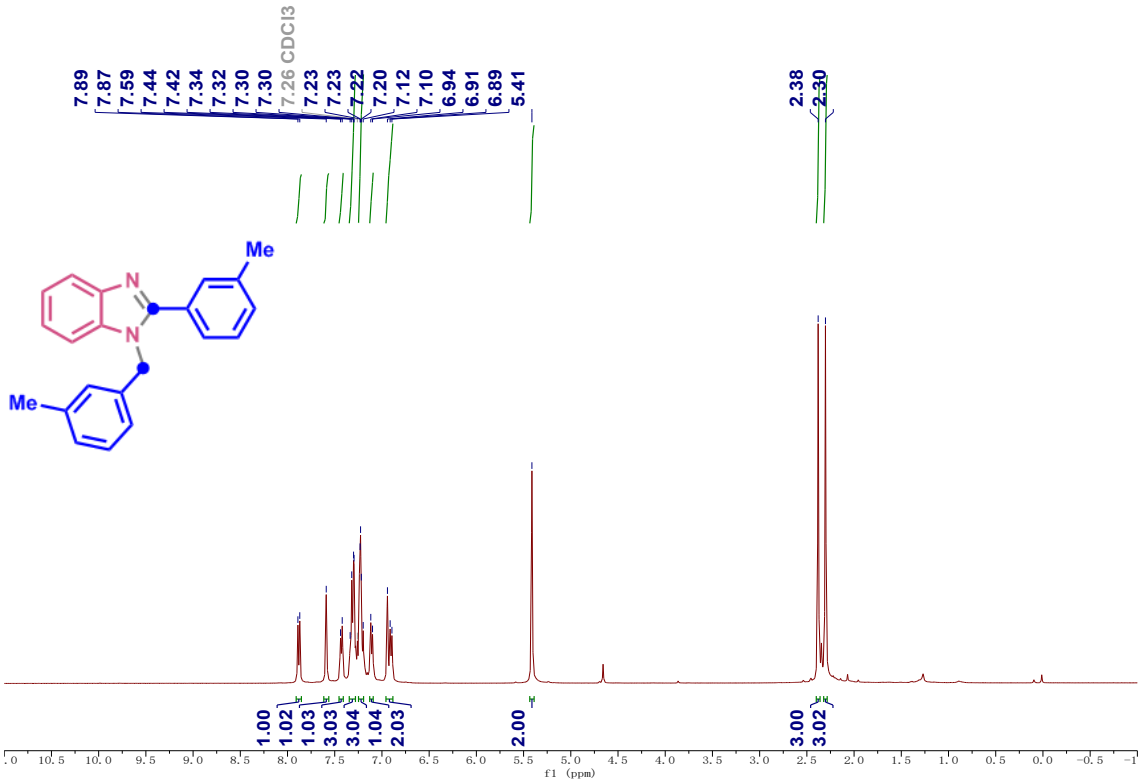
^{1}H NMR spectrum of **9c** (400 MHz, $CDCl_3$)



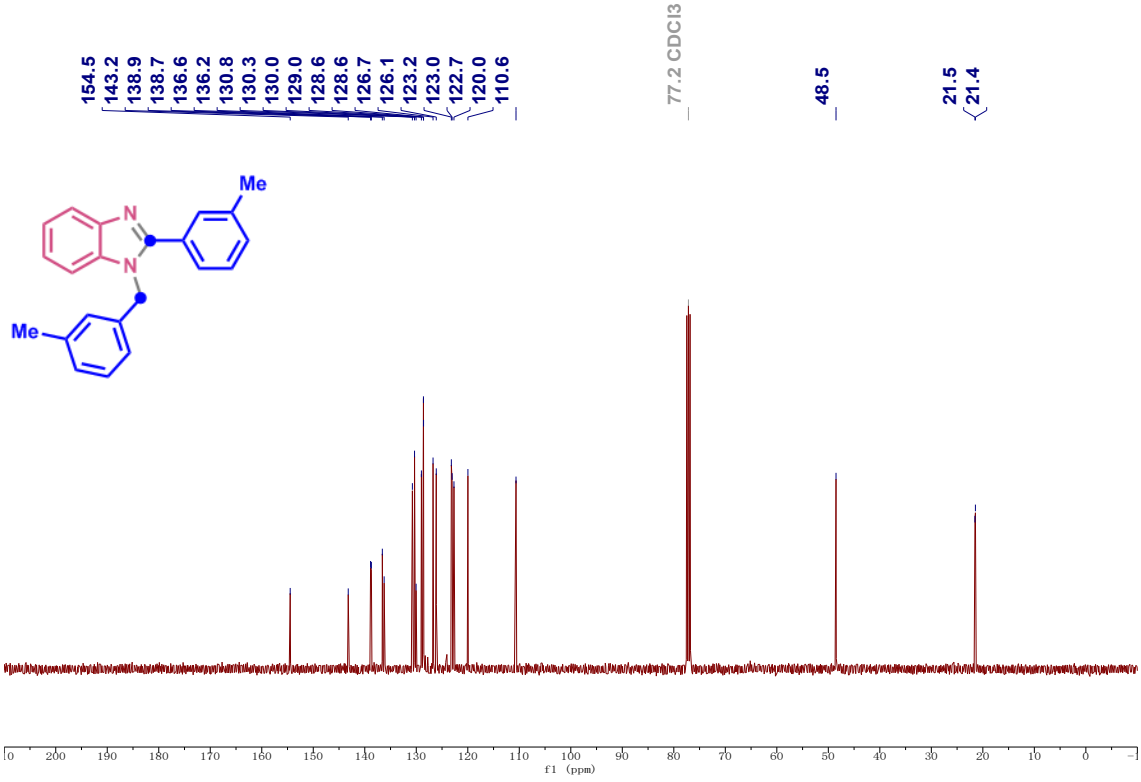
^{13}C NMR spectrum of **9c** (100 MHz, $CDCl_3$)



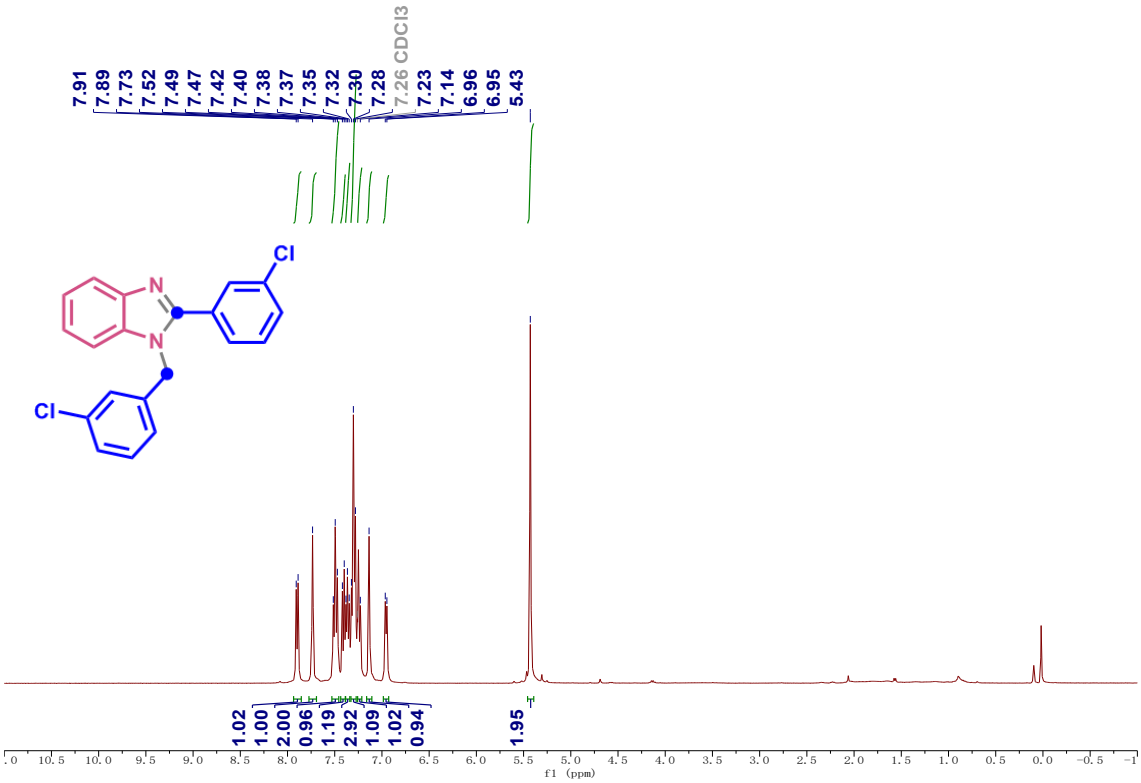
^{1}H NMR spectrum of **9d** (400 MHz, $CDCl_3$)



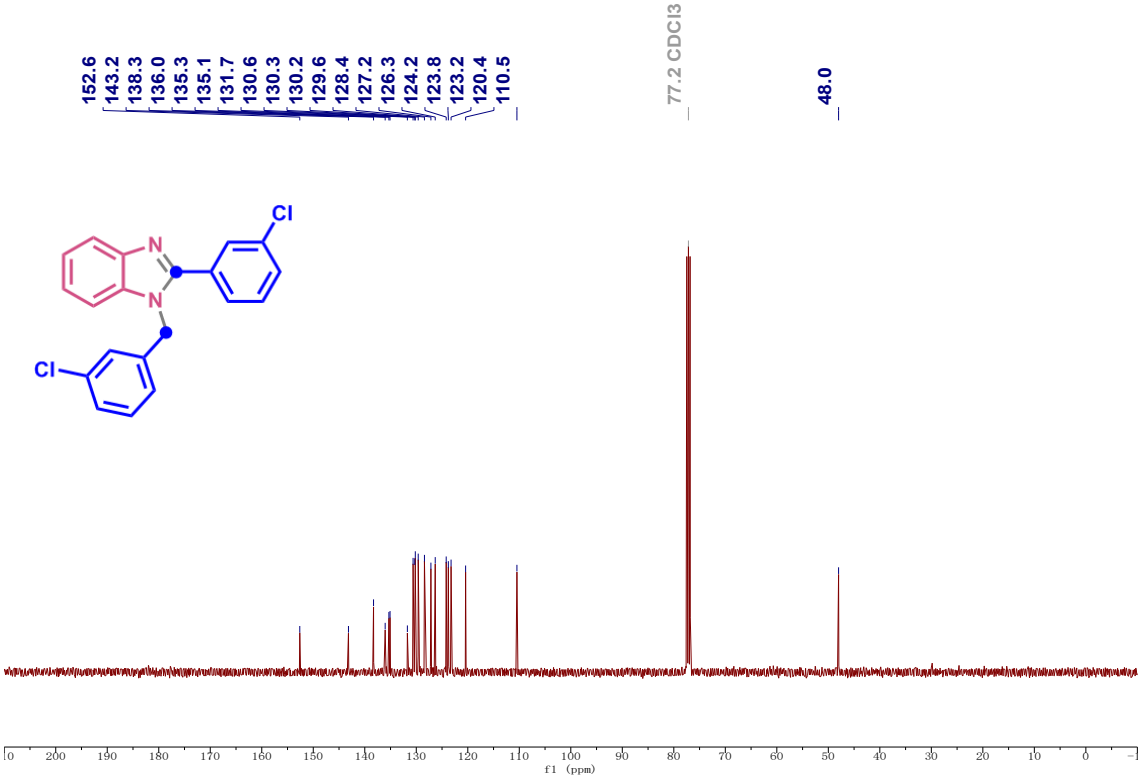
^{13}C NMR spectrum of **9d** (100 MHz, $CDCl_3$)



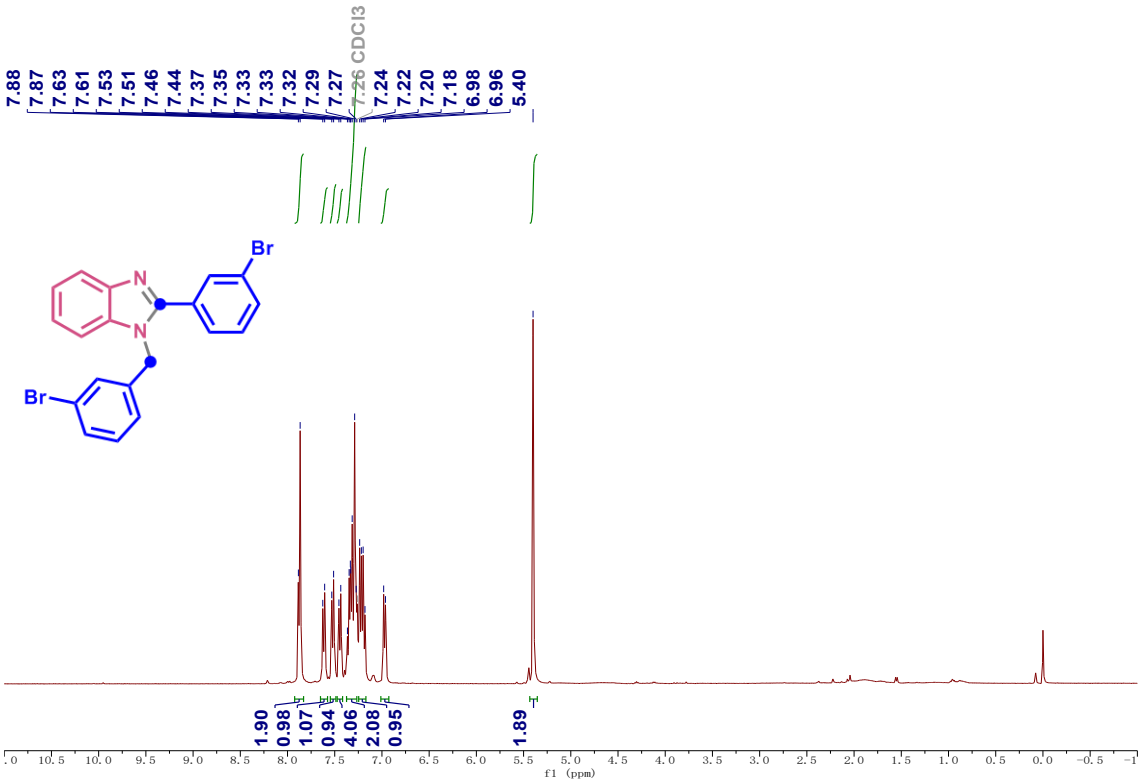
^{1}H NMR spectrum of **9e** (400 MHz, $CDCl_3$)



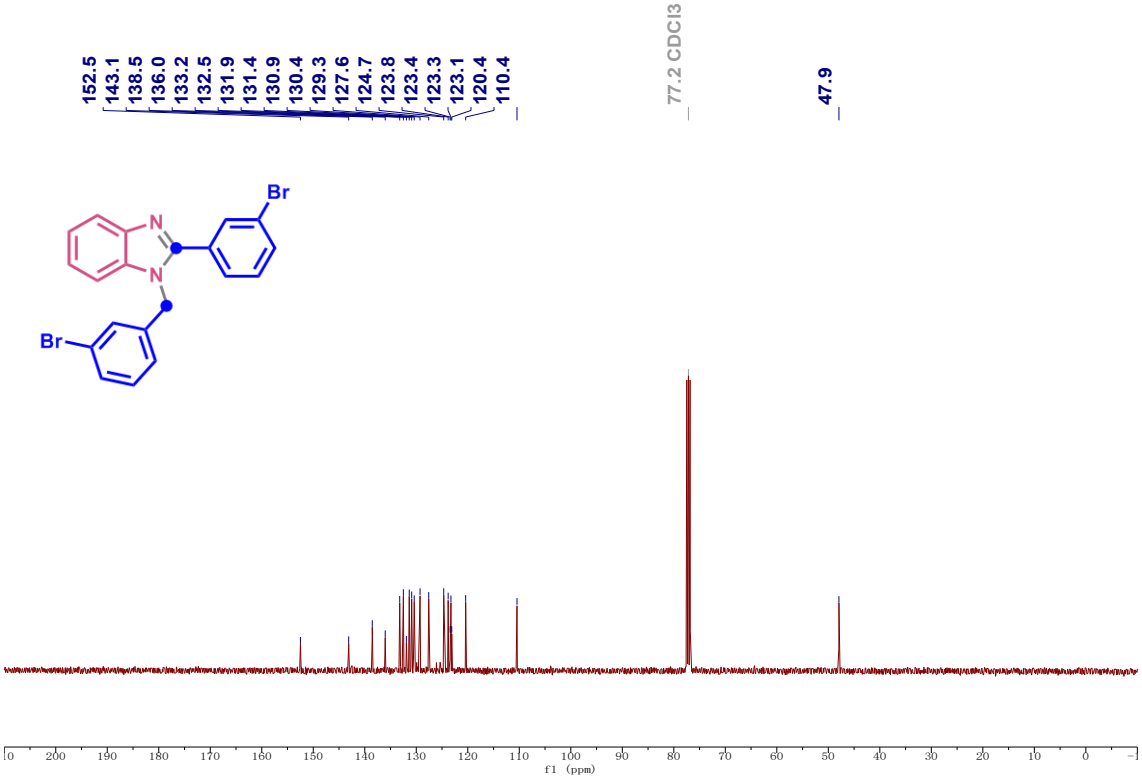
^{13}C NMR spectrum of **9e** (100 MHz, $CDCl_3$)



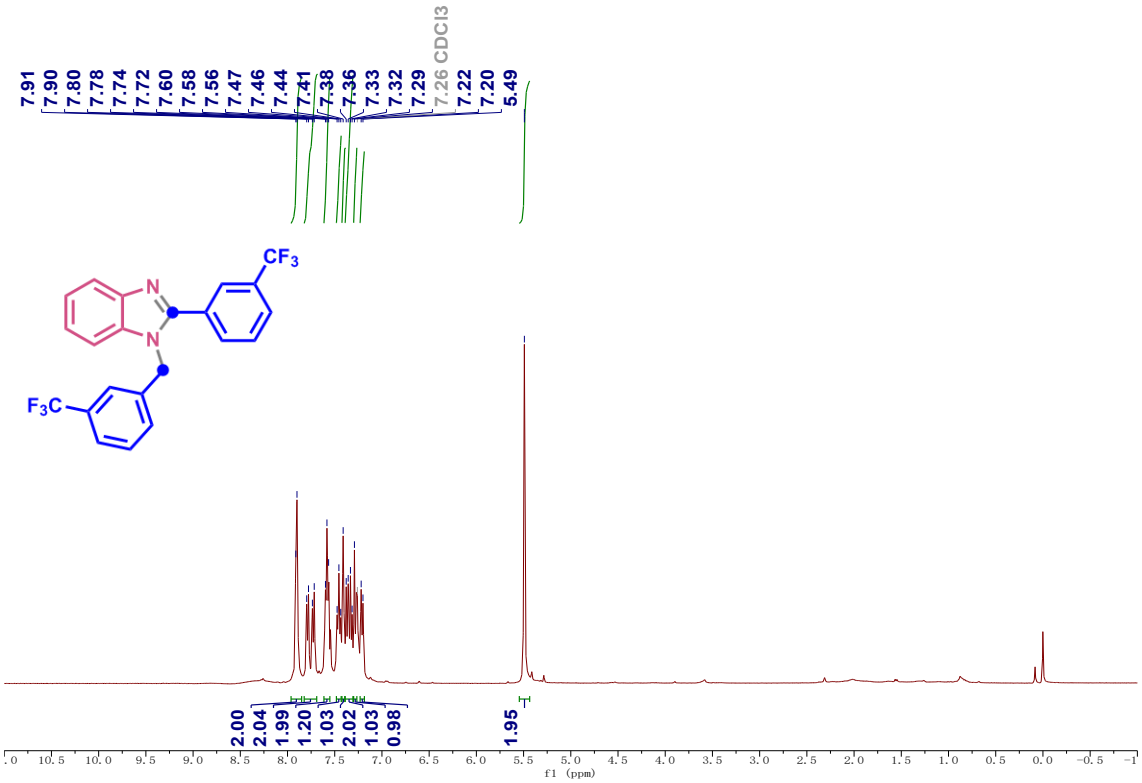
^{1}H NMR spectrum of **9f** (400 MHz, $CDCl_3$)



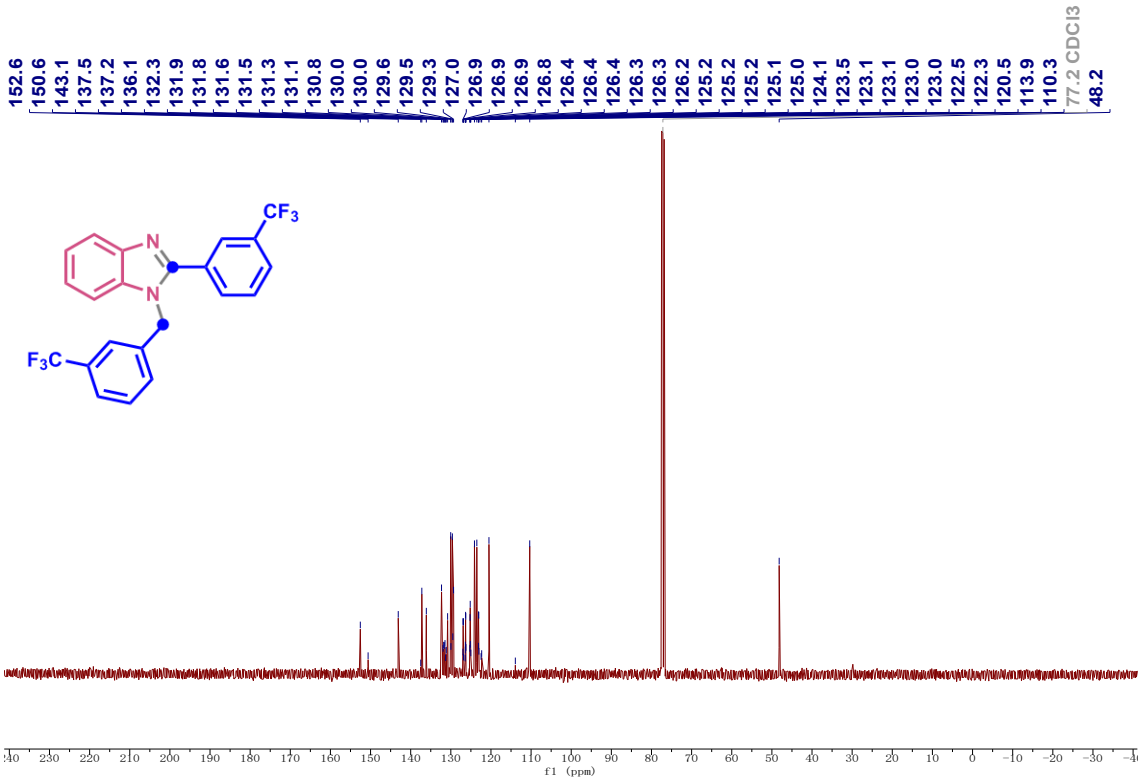
^{13}C NMR spectrum of **9f** (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of **9g** (400 MHz, $CDCl_3$)

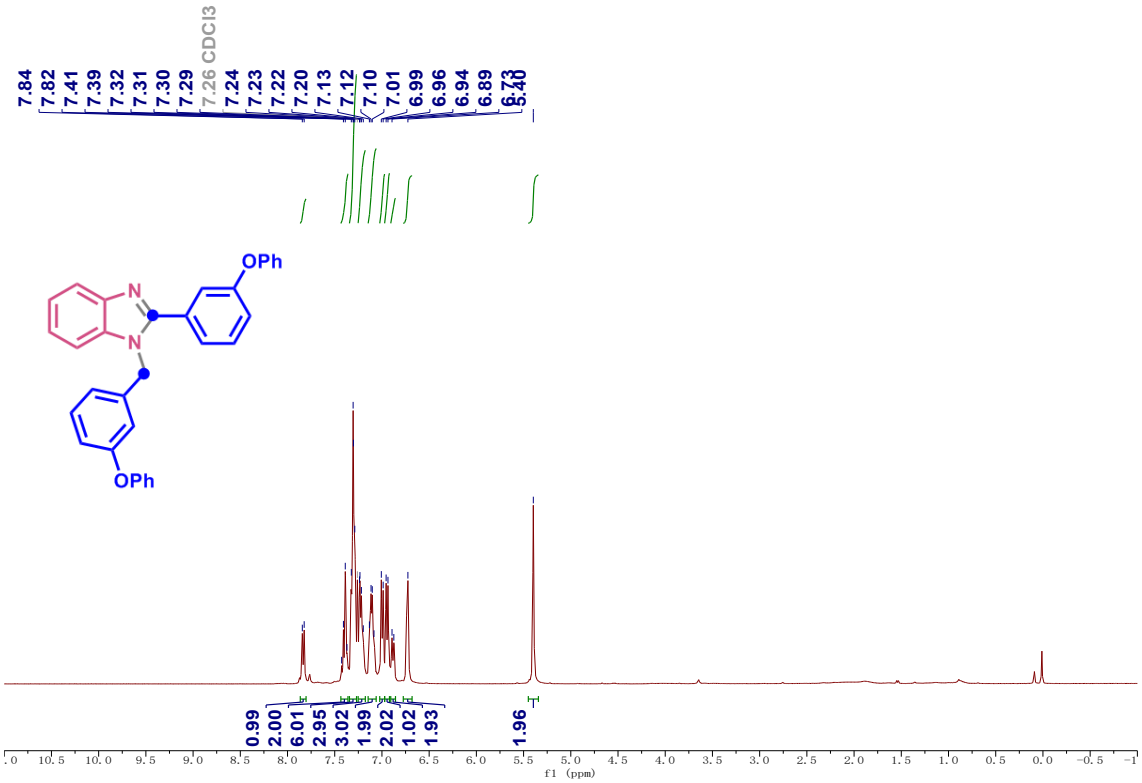


^{13}C NMR spectrum of **9g** (100 MHz, $CDCl_3$)

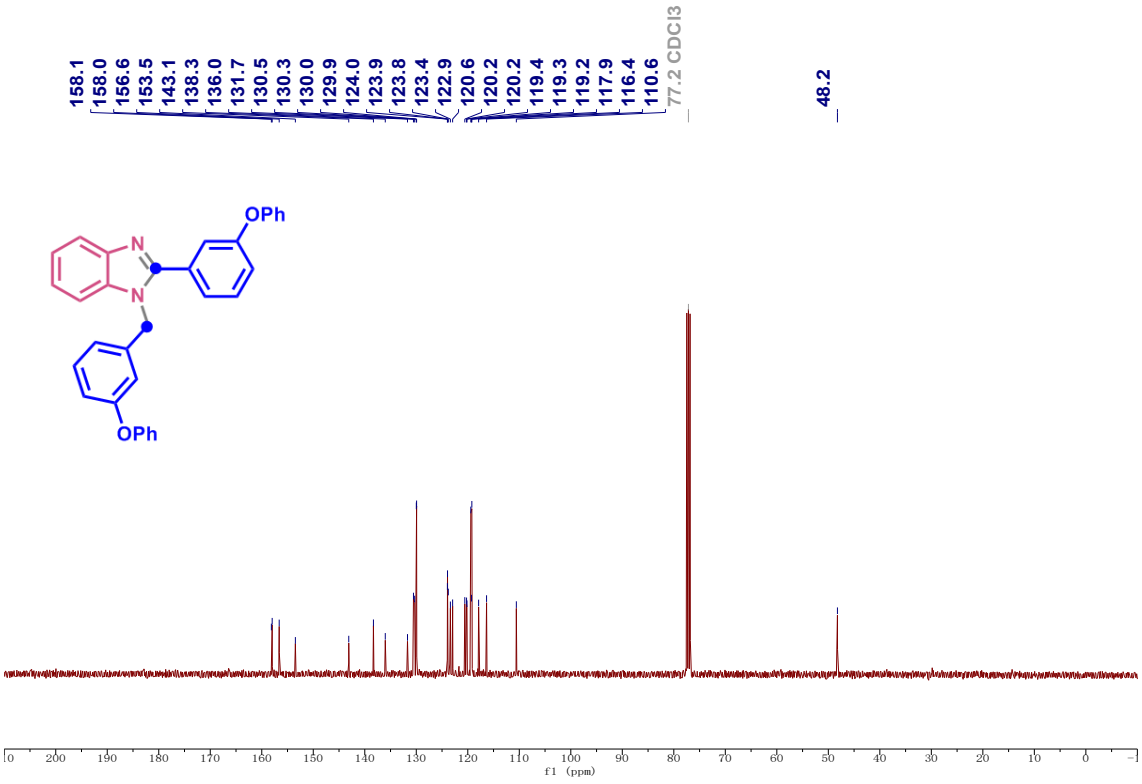


^{19}F NMR spectrum of **9g** (376 MHz, $CDCl_3$)

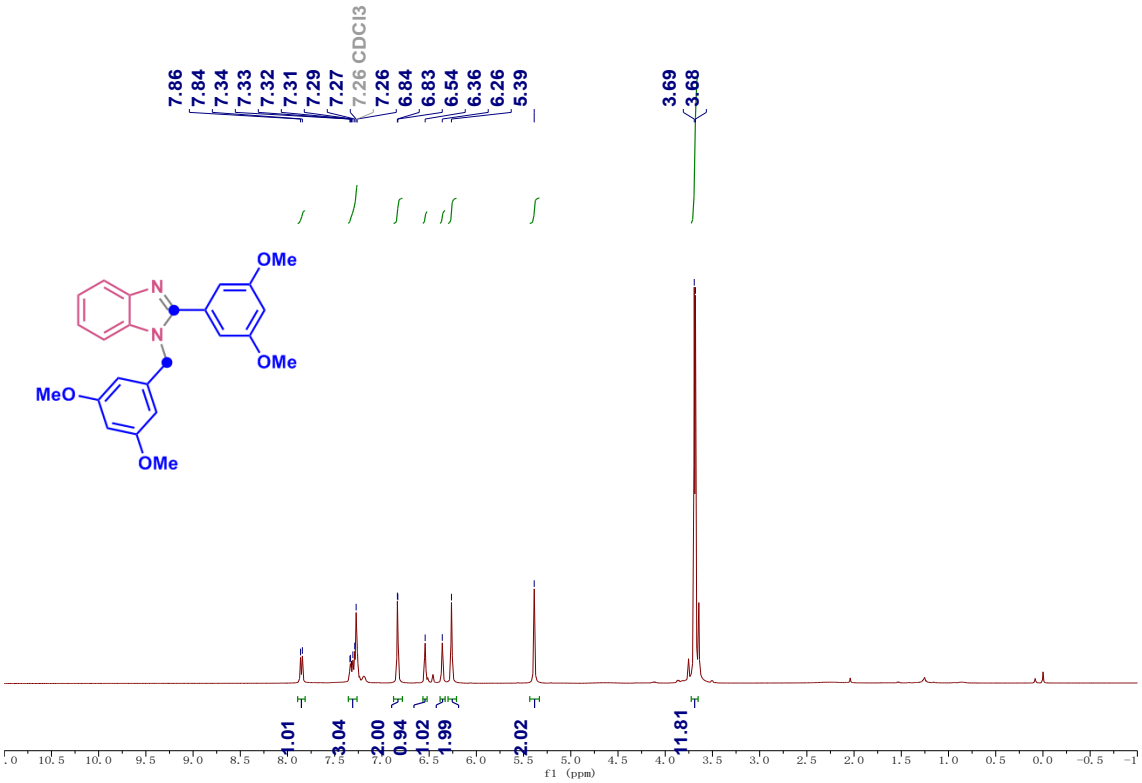
^{1}H NMR spectrum of **9h** (400 MHz, $CDCl_3$)



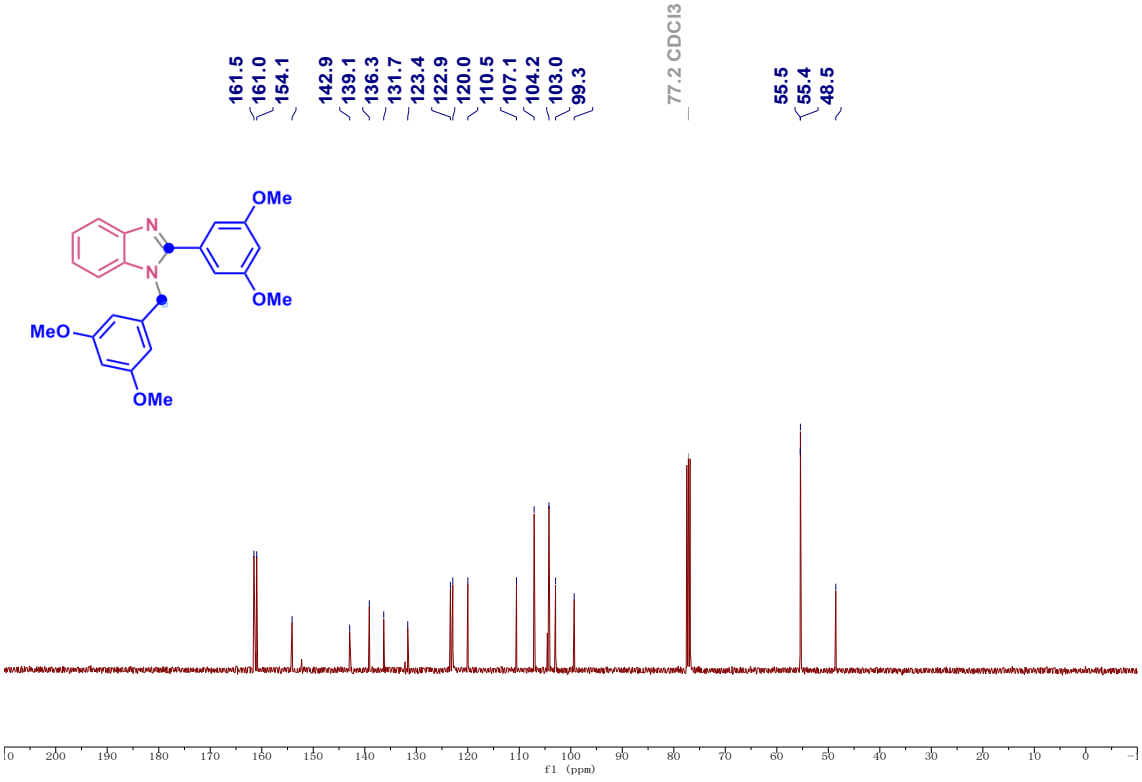
^{13}C NMR spectrum of **9h** (100 MHz, $CDCl_3$)



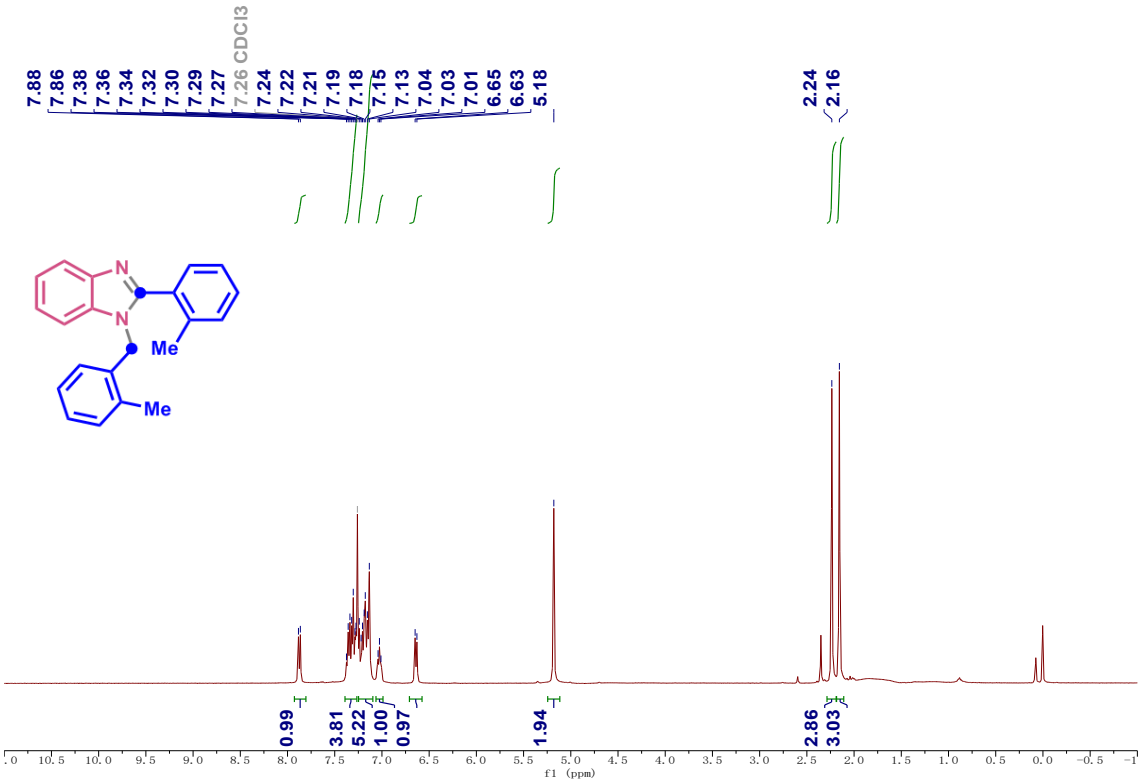
^{1}H NMR spectrum of **9i** (400 MHz, $CDCl_3$)



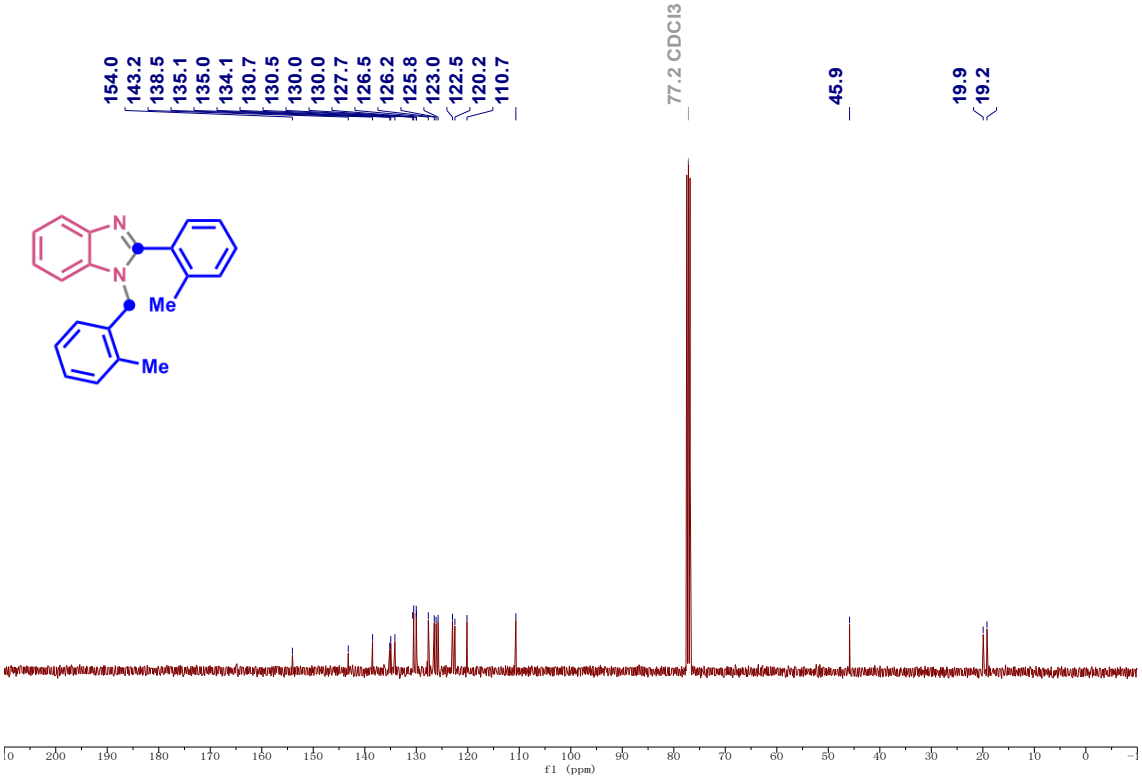
^{13}C NMR spectrum of **9i** (100 MHz, $CDCl_3$)



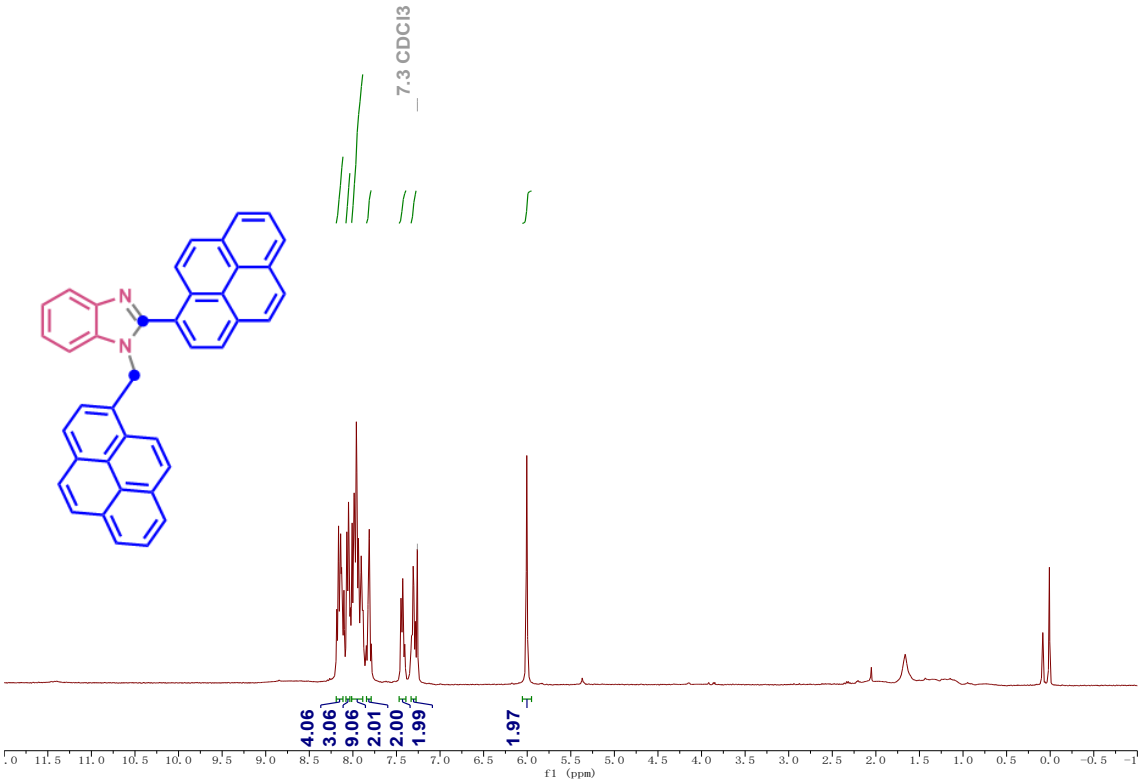
^{1}H NMR spectrum of **9j** (400 MHz, $CDCl_3$)



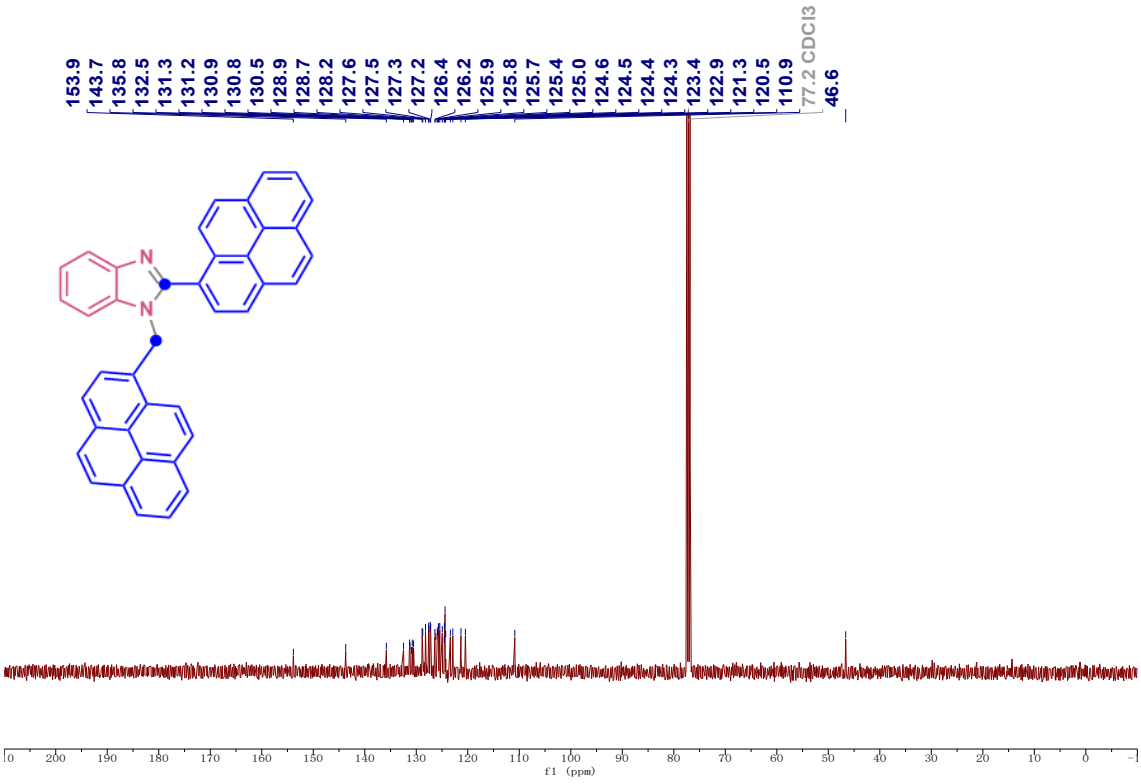
^{13}C NMR spectrum of **9j** (100 MHz, $CDCl_3$)



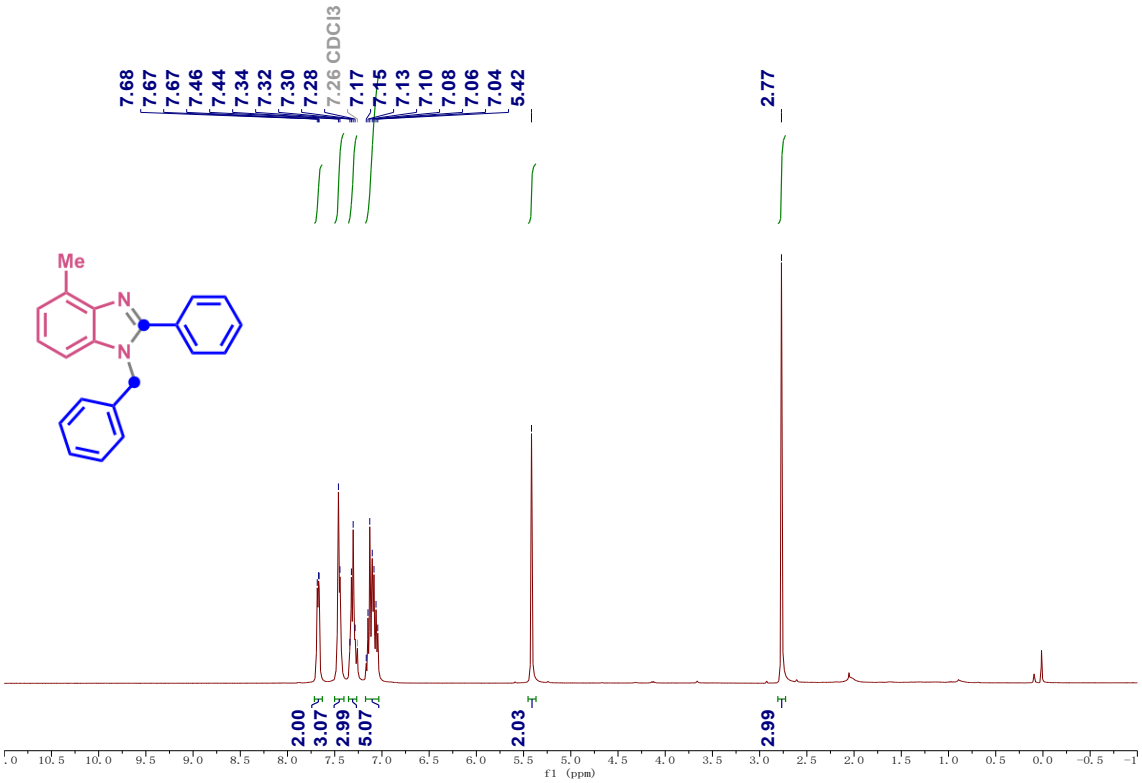
^{1}H NMR spectrum of **9k** (400 MHz, $CDCl_3$)



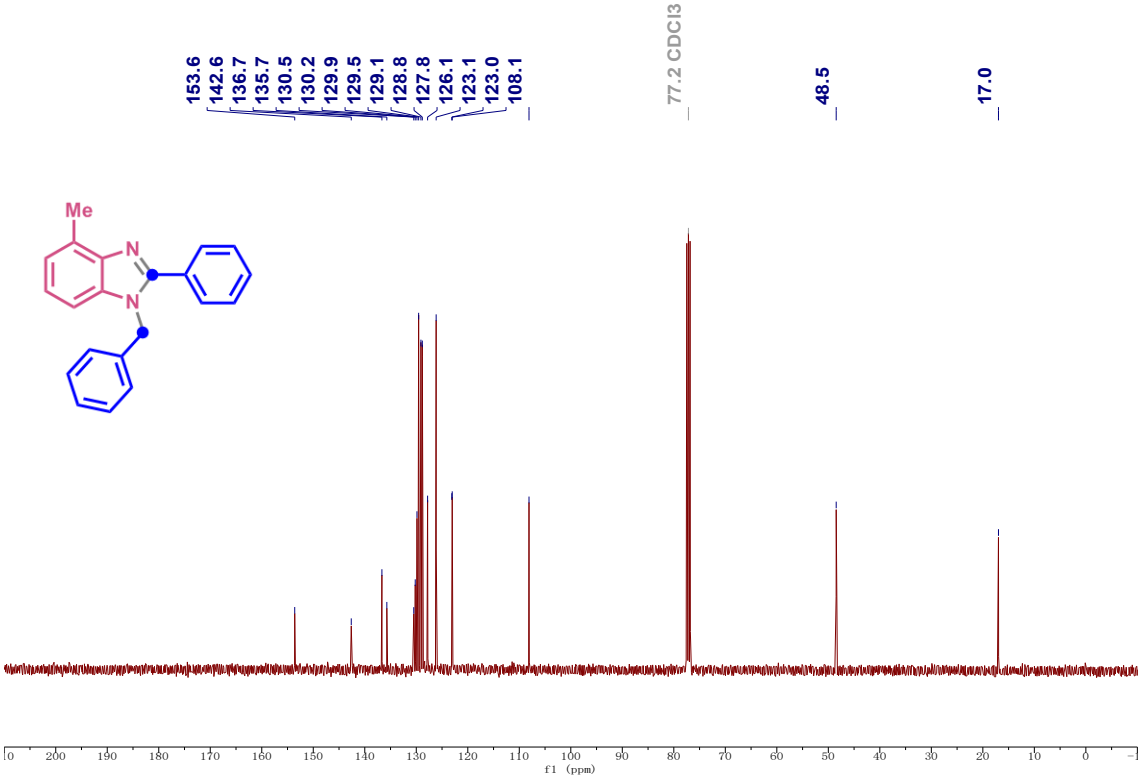
^{13}C NMR spectrum of **9k** (100 MHz, $CDCl_3$)



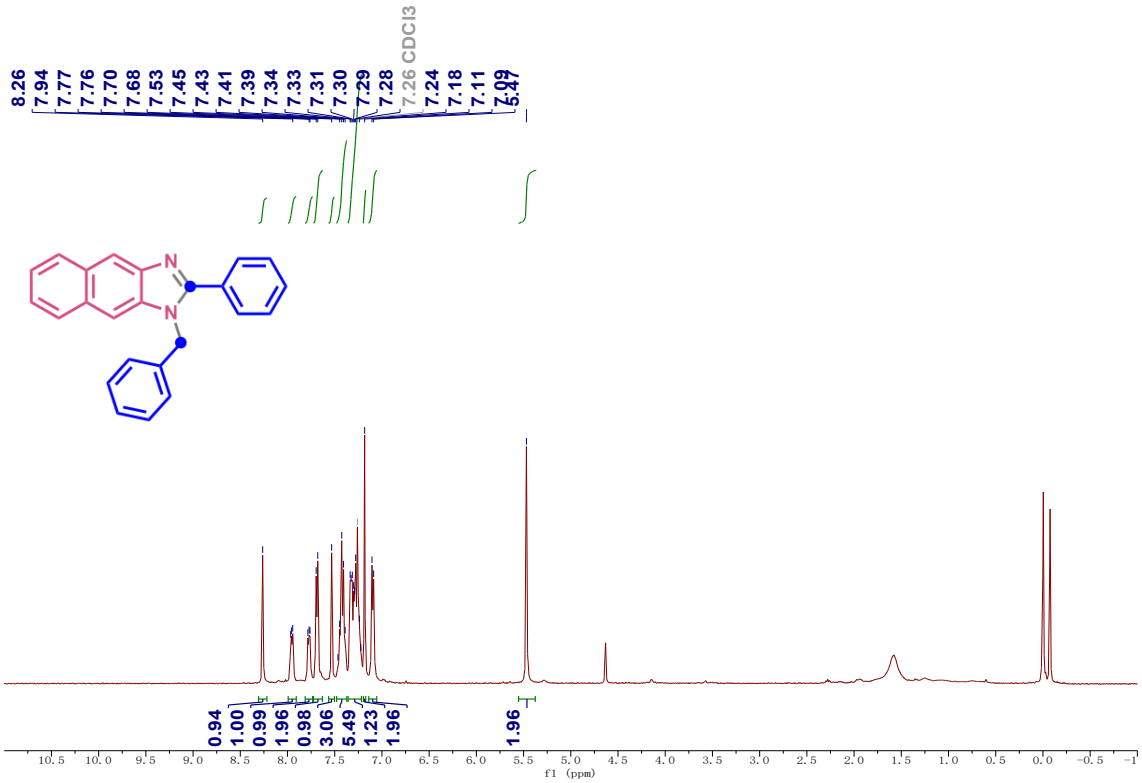
^{1}H NMR spectrum of **9l** (400 MHz, $CDCl_3$)



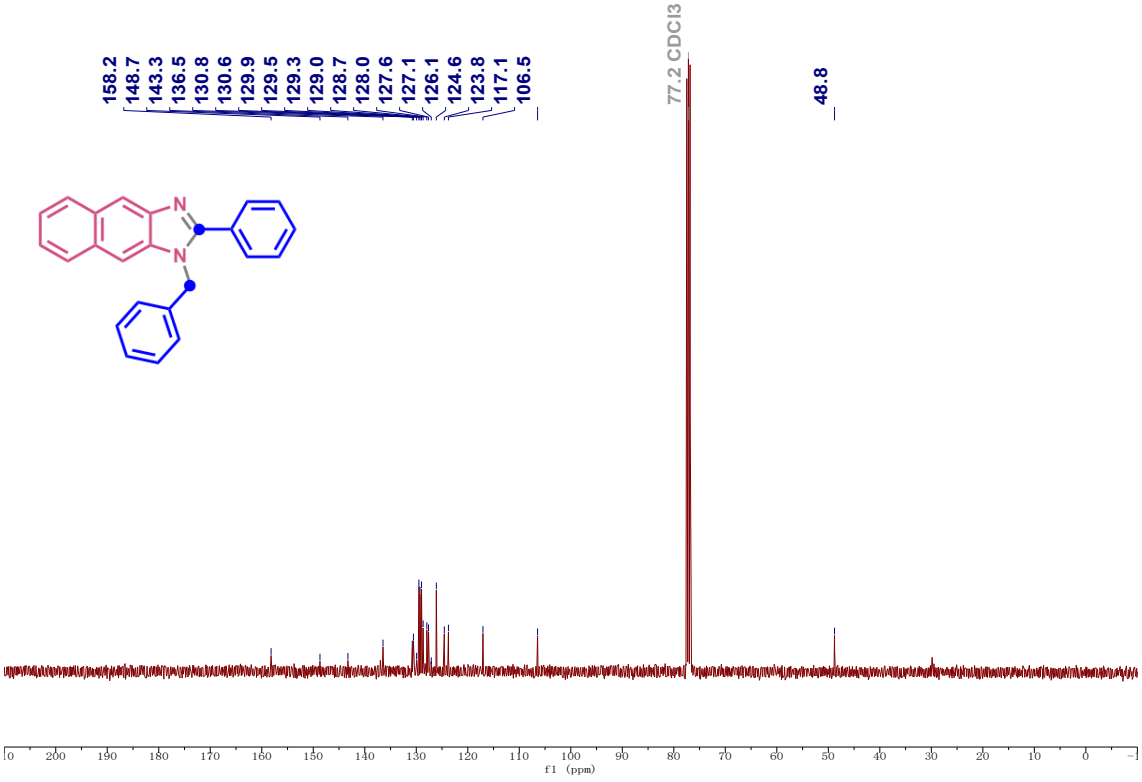
^{13}C NMR spectrum of **9l** (100 MHz, $CDCl_3$)



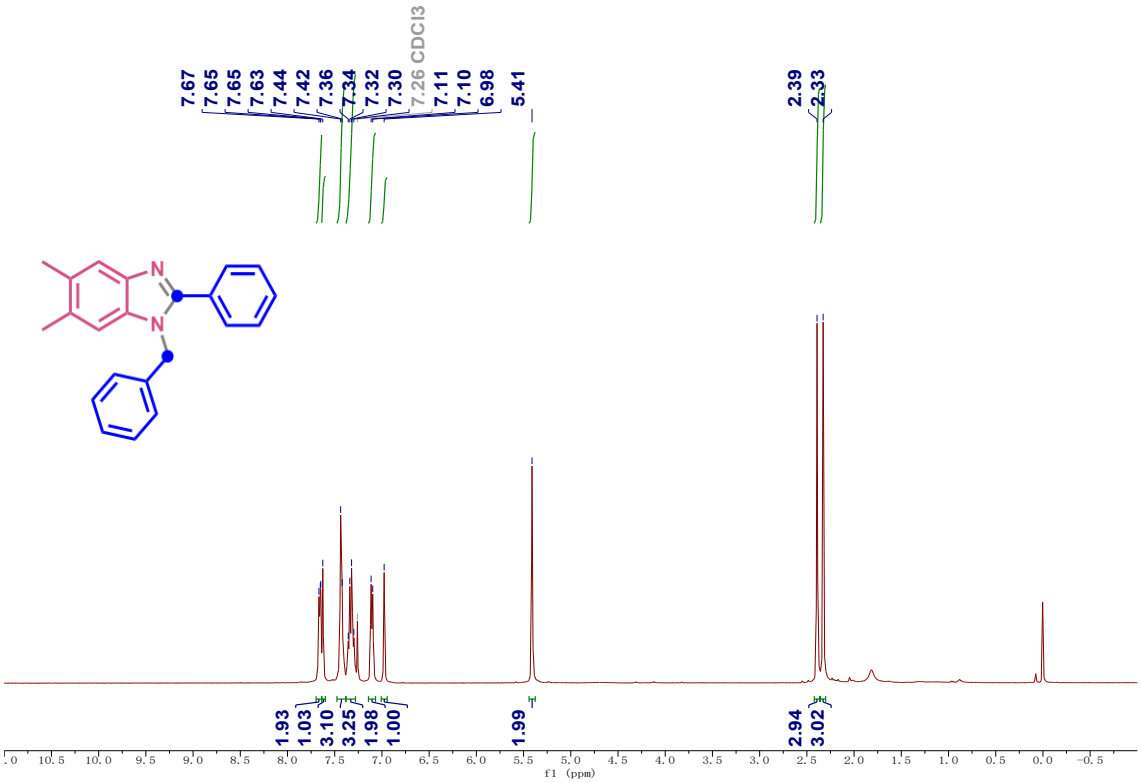
^{1}H NMR spectrum of **9m** (400 MHz, $CDCl_3$)



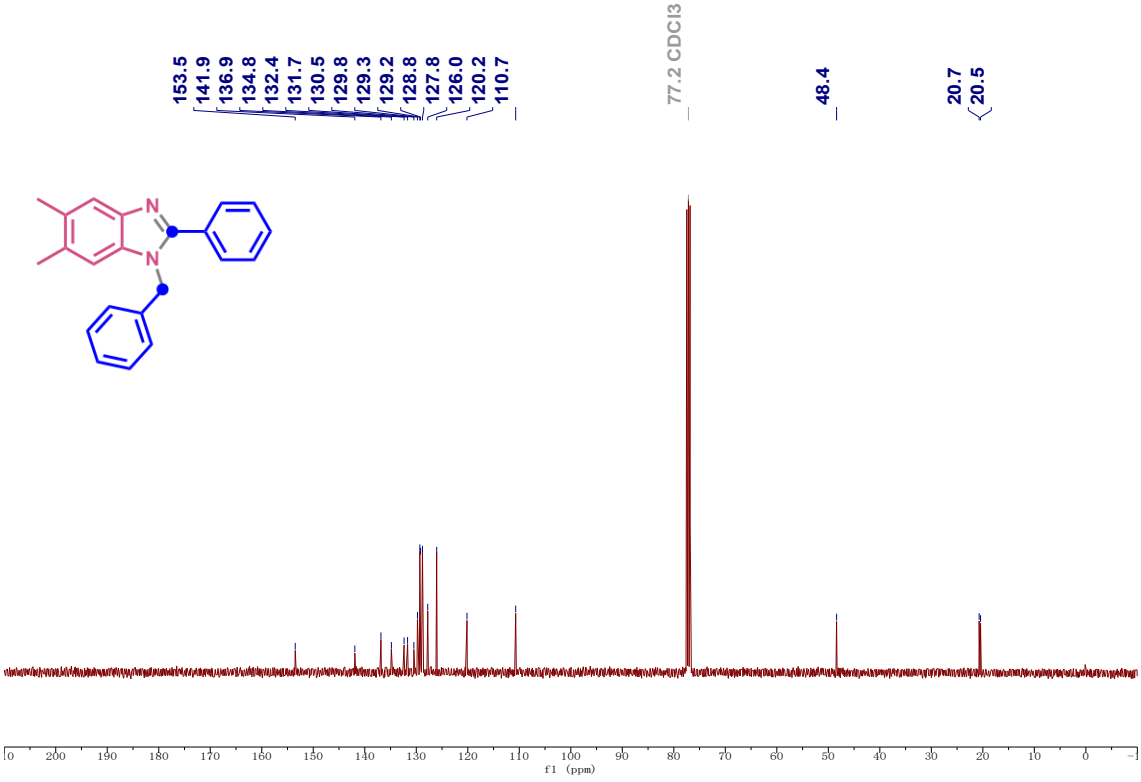
^{13}C NMR spectrum of **9m** (100 MHz, $CDCl_3$)



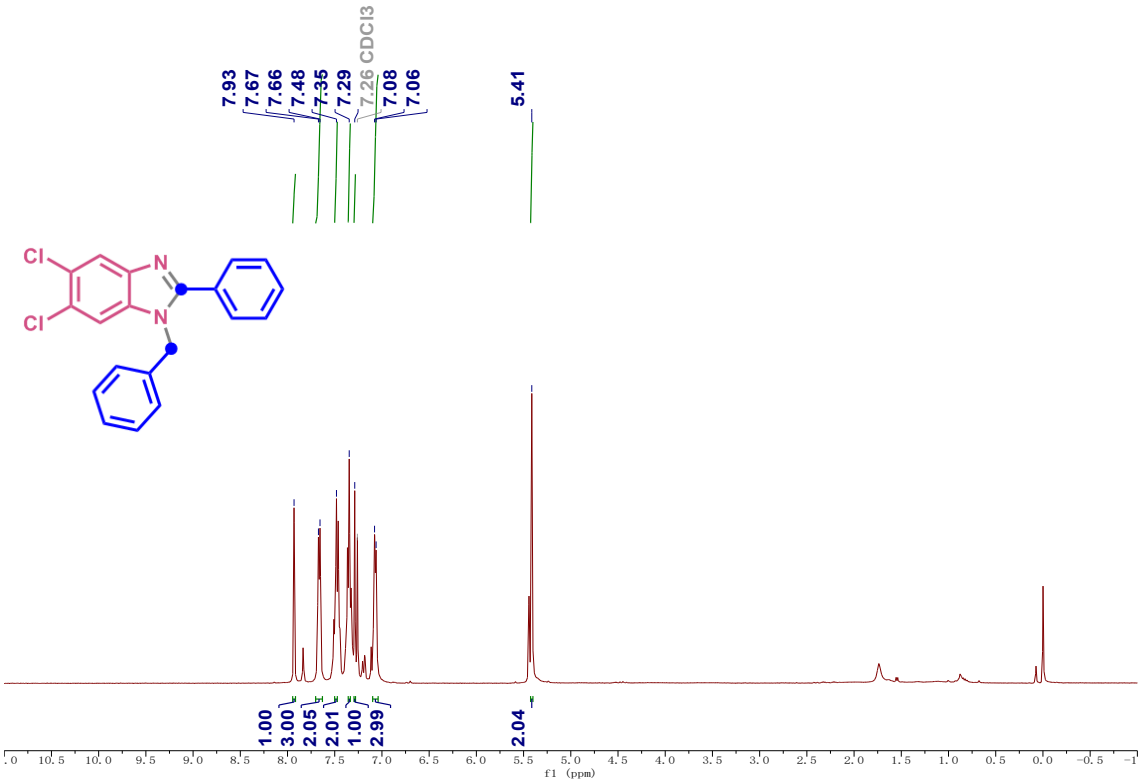
^{1}H NMR spectrum of **9n** (400 MHz, $CDCl_3$)



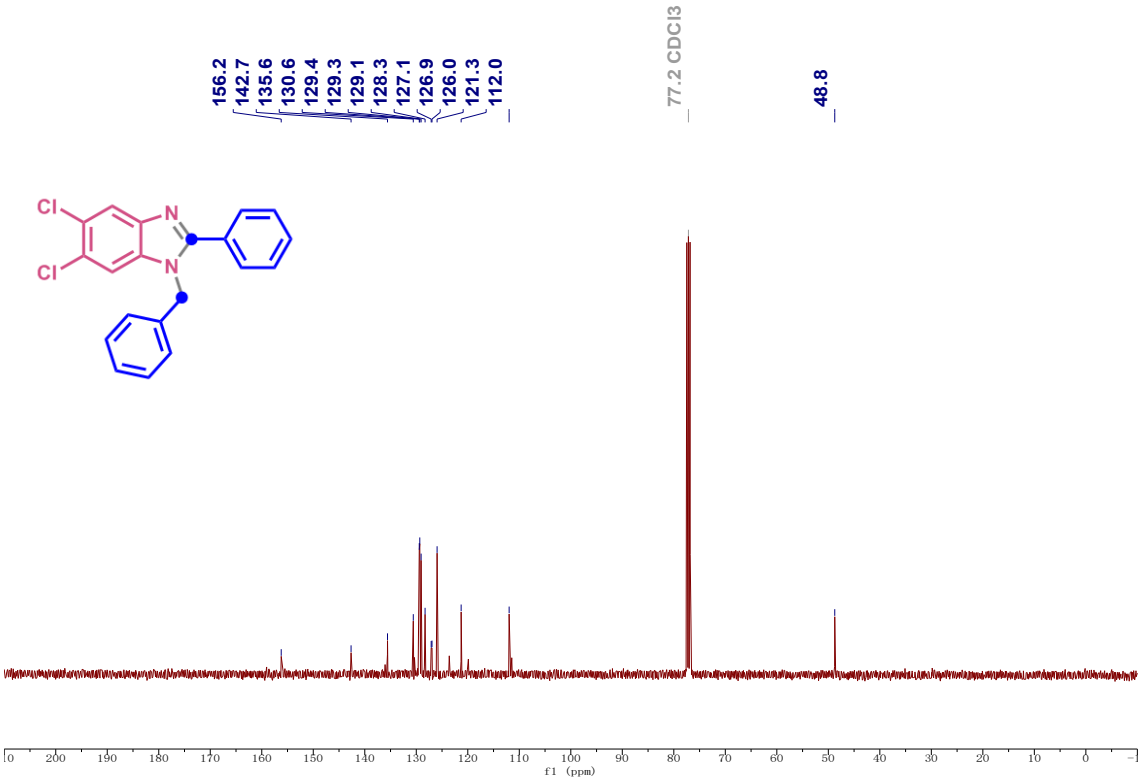
^{13}C NMR spectrum of **9n** (100 MHz, $CDCl_3$)



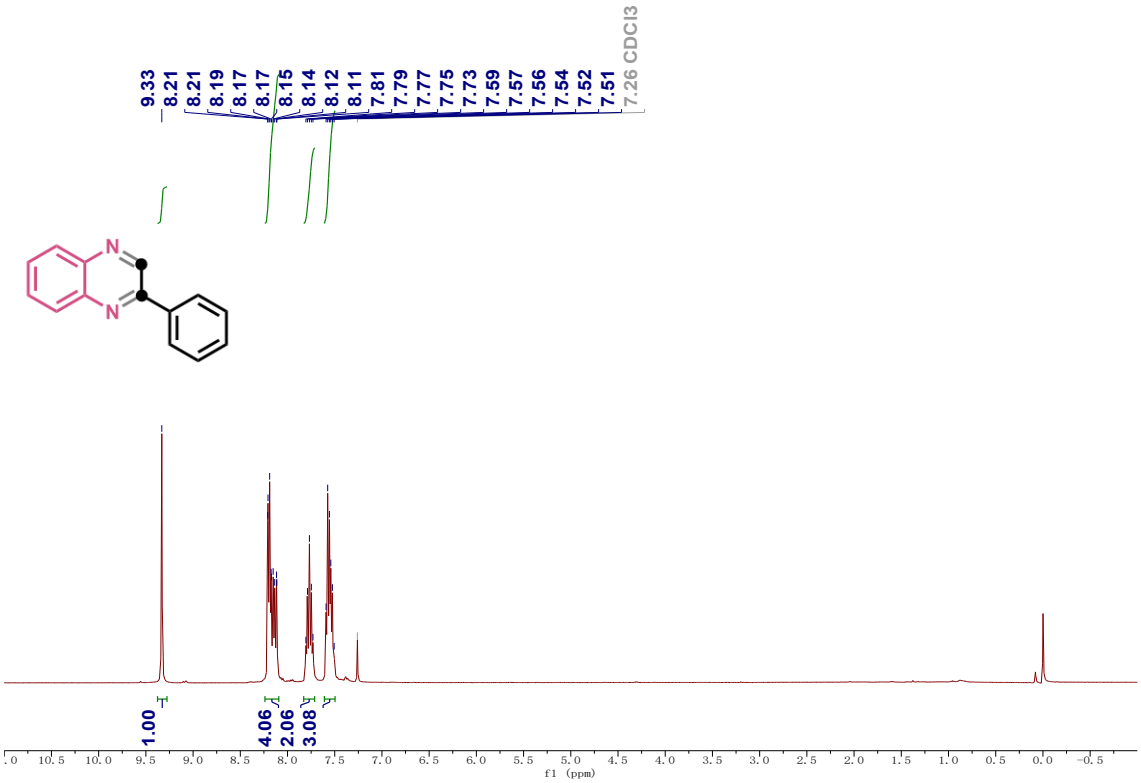
^{1}H NMR spectrum of **9o** (400 MHz, $CDCl_3$)



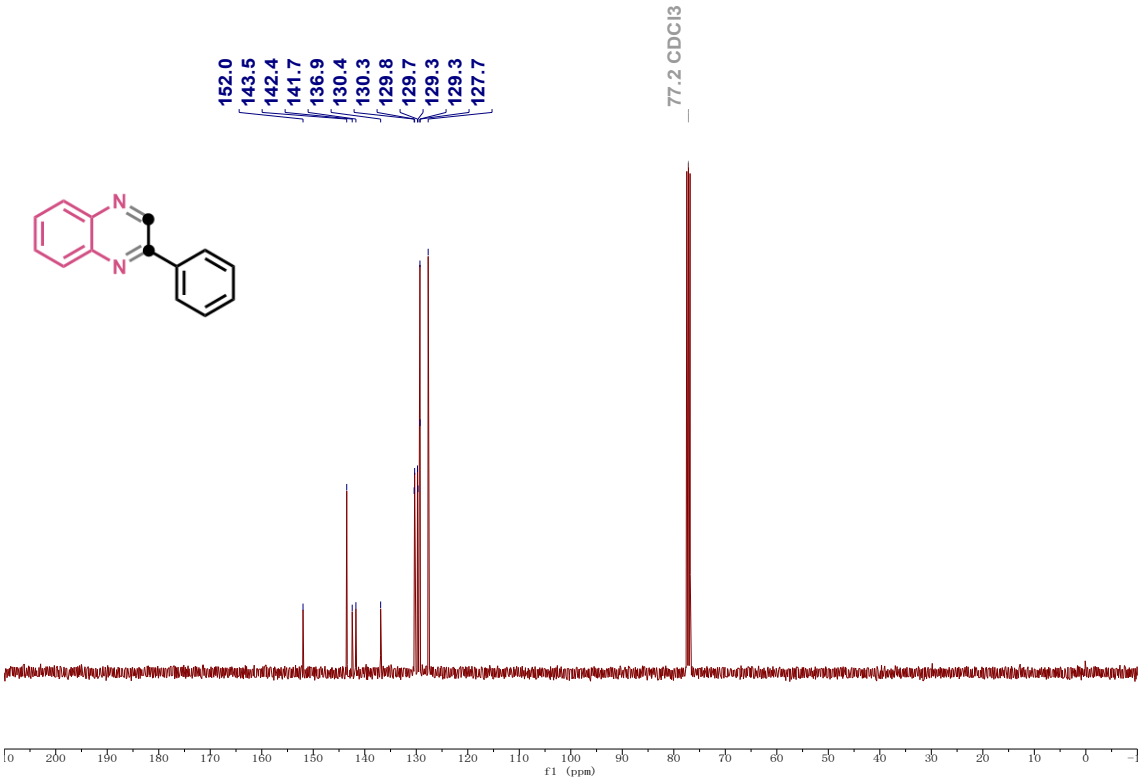
^{13}C NMR spectrum of **9o** (100 MHz, $CDCl_3$)



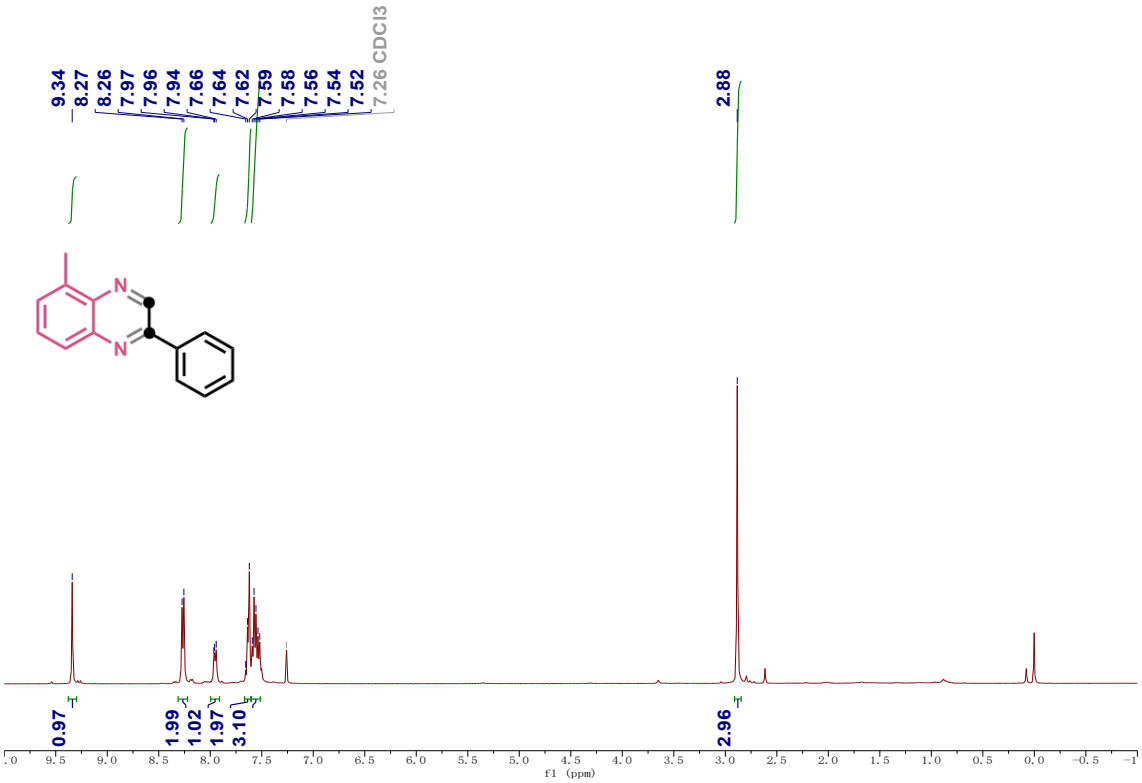
^{1}H NMR spectrum of **11a** (400 MHz, $CDCl_3$)



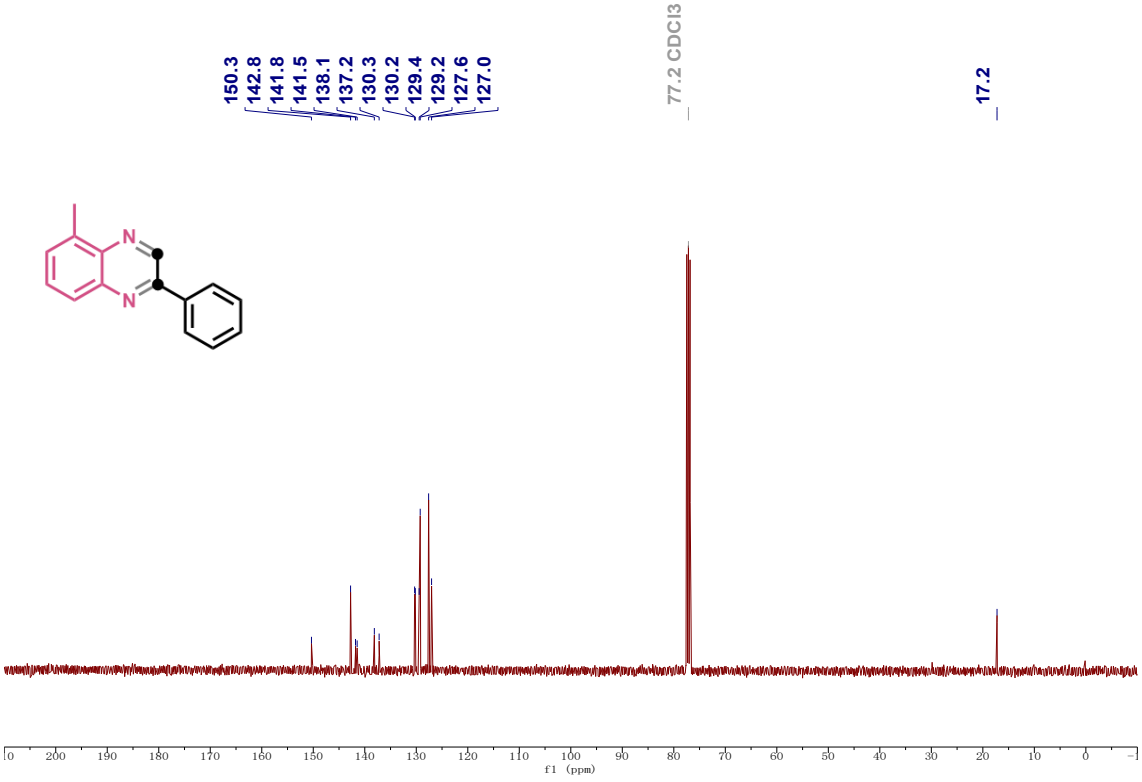
^{13}C NMR spectrum of **11a** (100 MHz, $CDCl_3$)



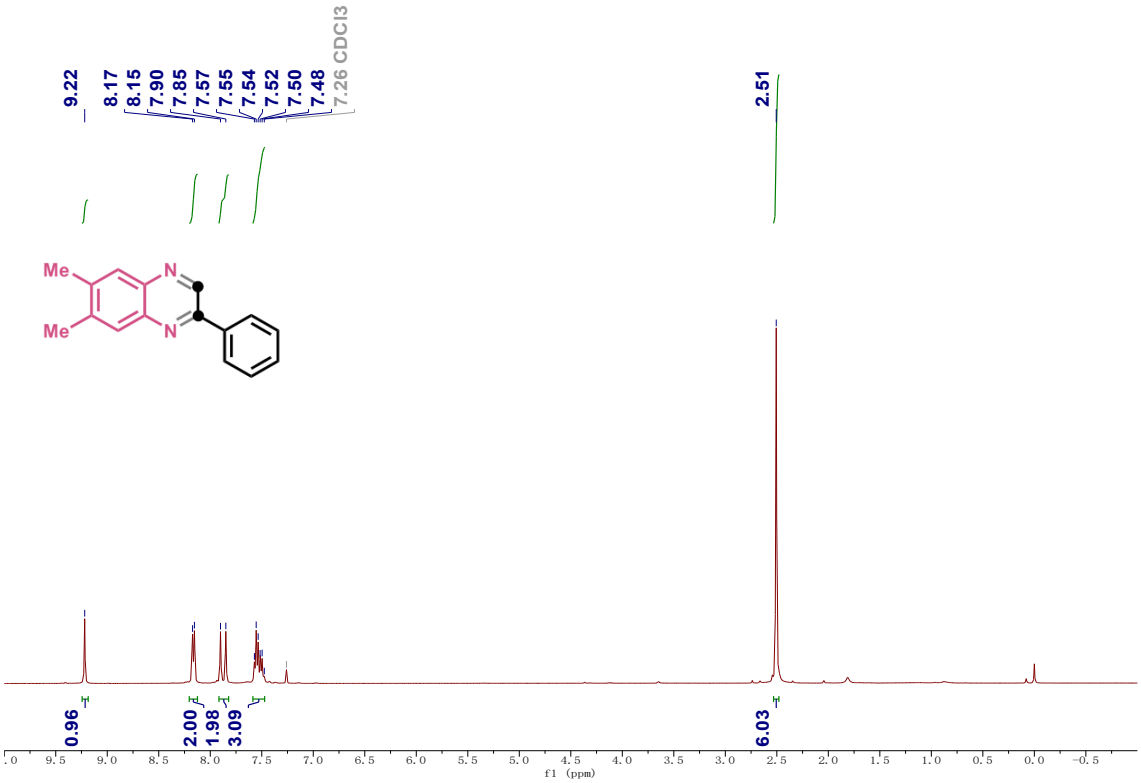
^{1}H NMR spectrum of **11b** (400 MHz, $CDCl_3$)



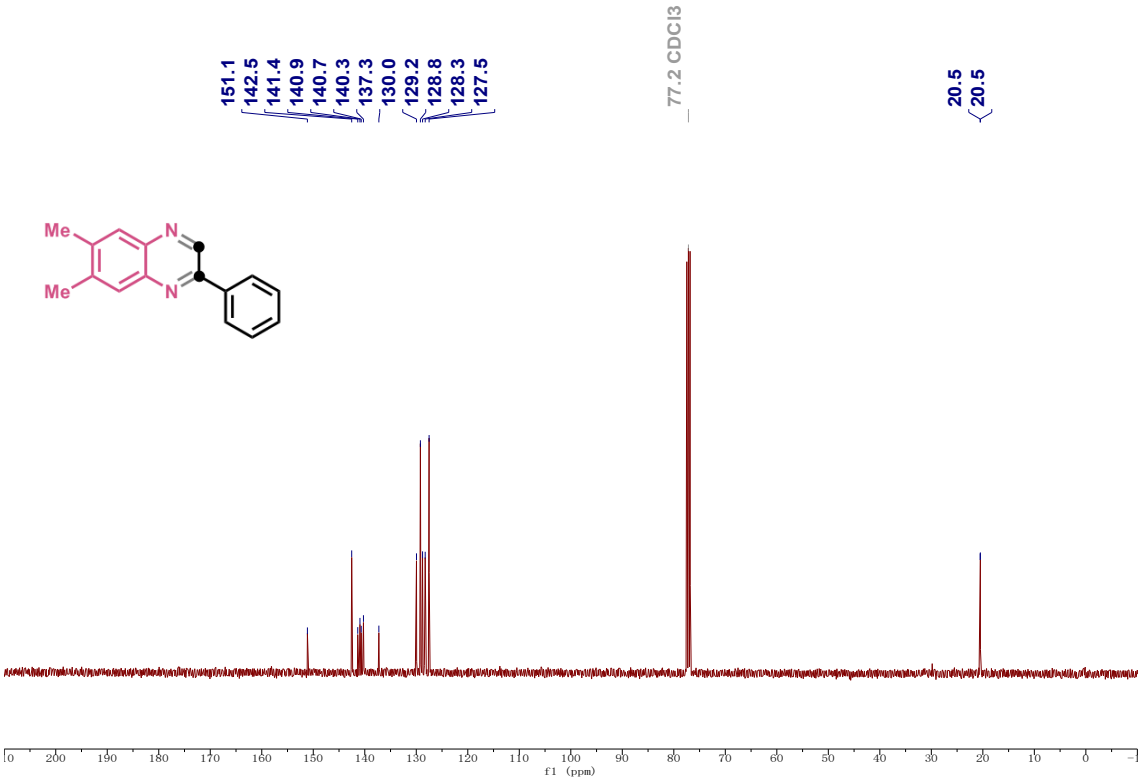
^{13}C NMR spectrum of **11b** (100 MHz, $CDCl_3$)



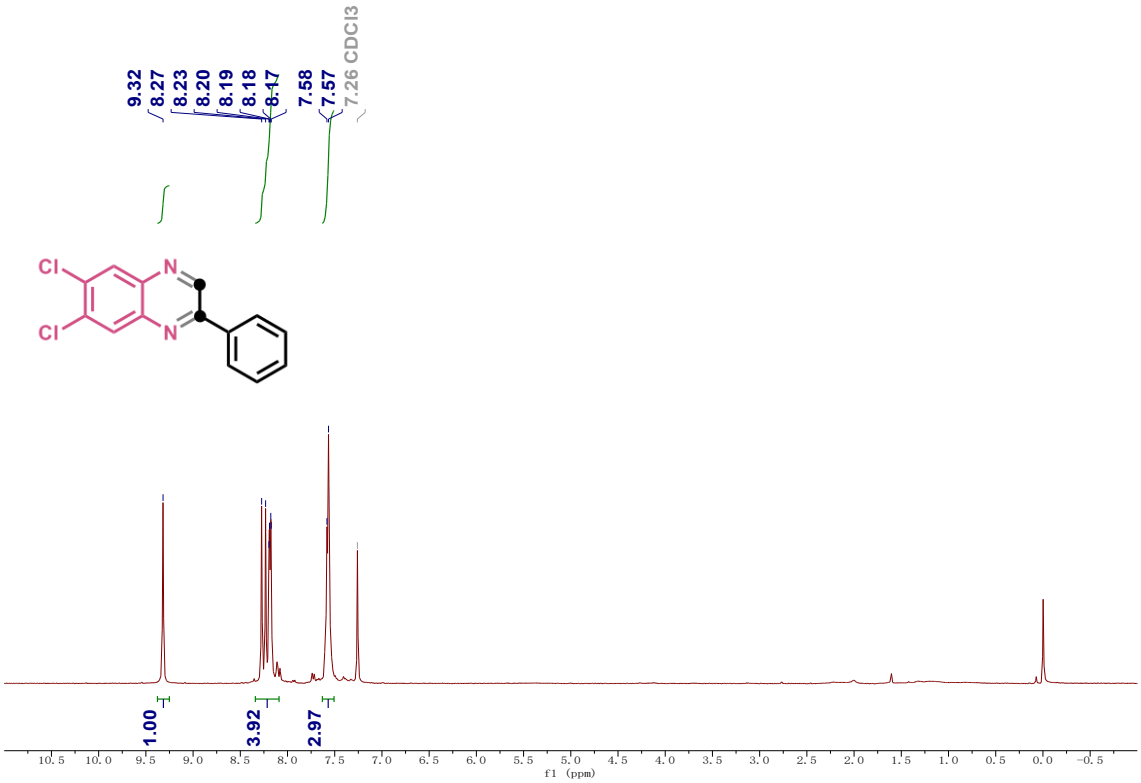
^{1}H NMR spectrum of **11c** (400 MHz, $CDCl_3$)



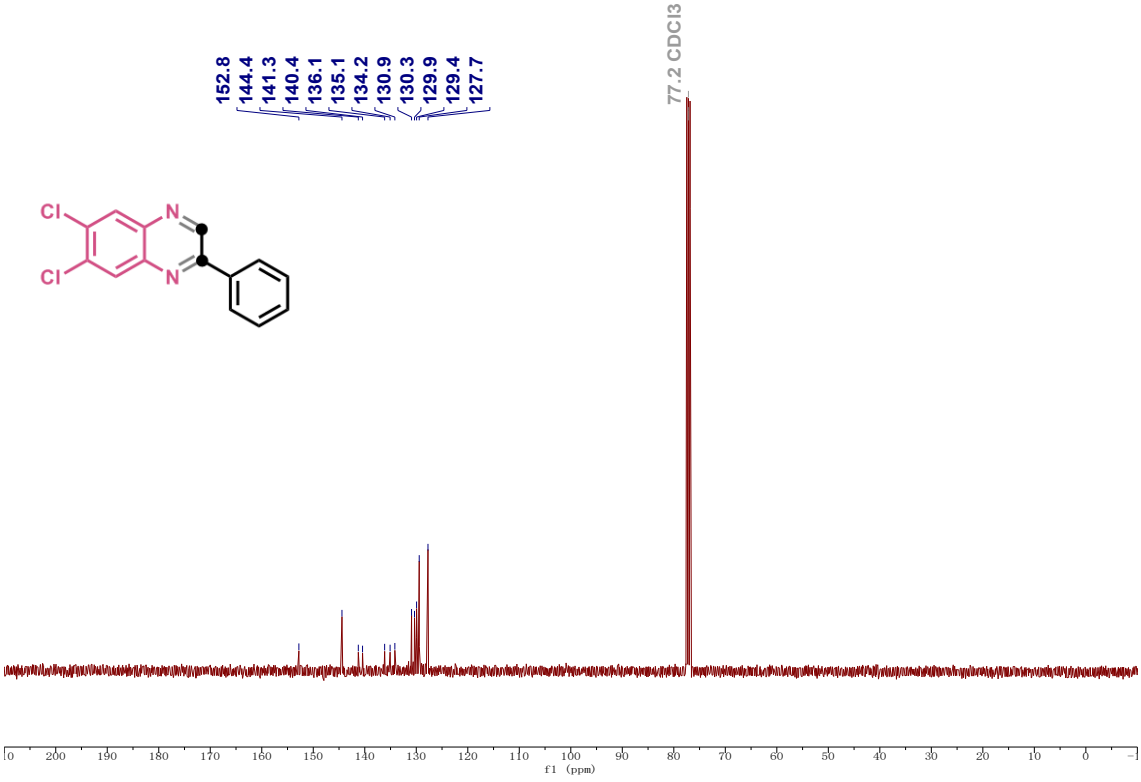
^{13}C NMR spectrum of **11c** (100 MHz, $CDCl_3$)



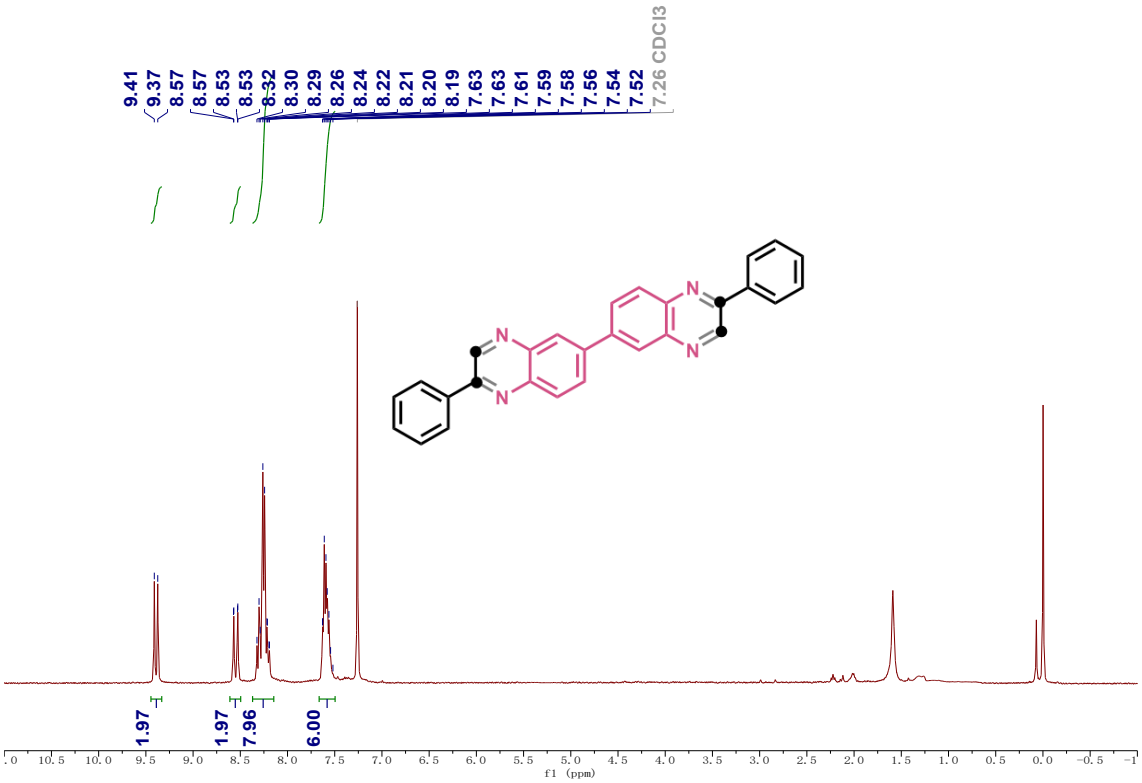
^{1}H NMR spectrum of **11d** (400 MHz, $CDCl_3$)



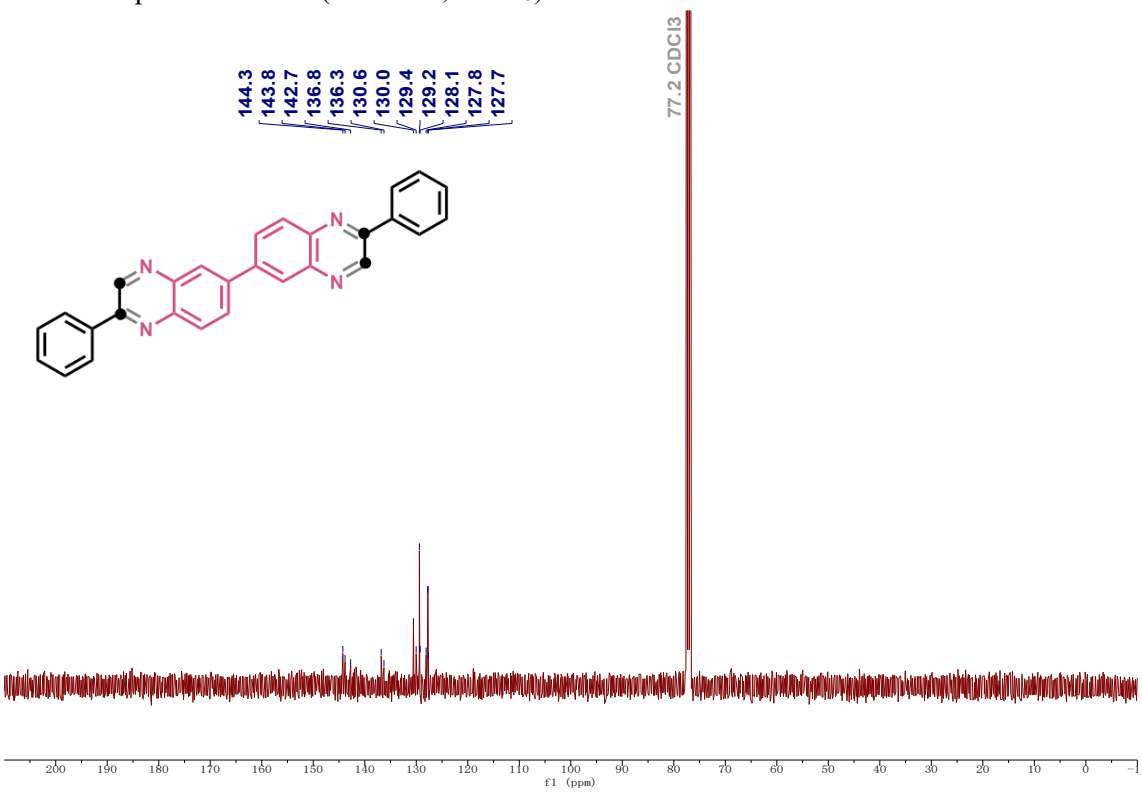
^{13}C NMR spectrum of **11d** (100 MHz, $CDCl_3$)



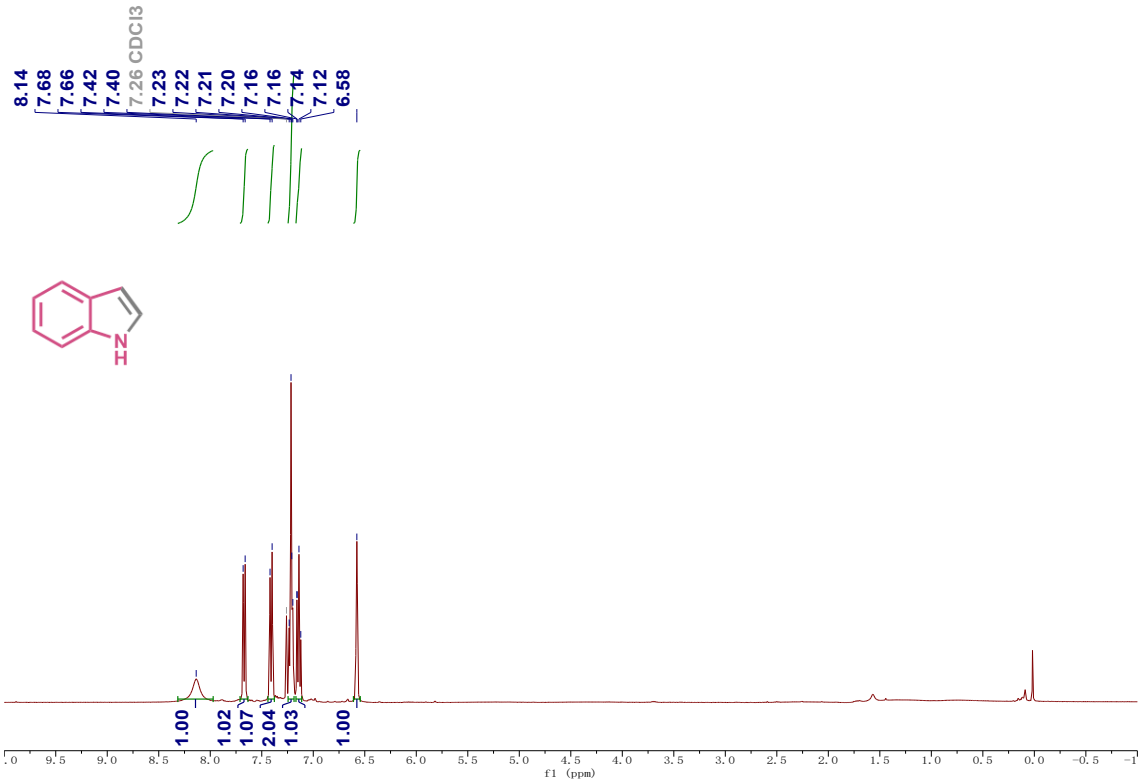
^{1}H NMR spectrum of **11e** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **11e** (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of **13** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **13** (100 MHz, $CDCl_3$)