A well-defined Pd(II)–NHC aqua complex for ambient Buchwald–Hartwig amination in *tert*-butanol

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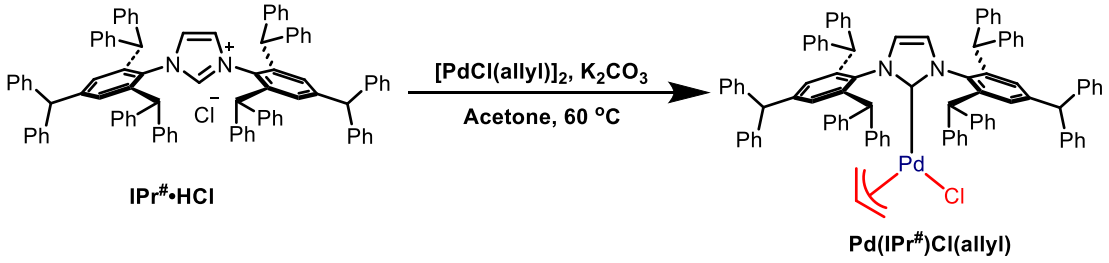
Table of contents

General information

All reactions were performed under inert atmosphere using Glovebox or Schlenk line techniques unless otherwise mentioned. Al the reactions were carried out at 25-30 °C unless otherwise mentioned. All solvents and all other reagents were purchased form commercial suppliers (e.g., Aladdin, Macklin) and used as received without further purification unless otherwise stated. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance-300, 400 or 500 instruments at 298K. Chemical shifts (ppm) in ^{1}H and ^{13}C NMR spectra are referenced to the residual solvent peak ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.23 ppm; DMSO-d_6: δ_H = 2.50 ppm, δ_C = 39.51 ppm). Coupling constants (J) are given in hertz (Hz). Abbreviations used in the designation of the signals: s = singlet, d = doublet, t = triplet, m = multiplet, q = quadruplet. All GC analyses were performed on Agilent 7890A Gas Chromatograph with FID detector using J&W HP-5 column (30 m, 0.32 mm). All reagents and solvents were purchased from commercial suppliers (e.g., Aladdin, Macklin) and used as received without further purification, unless specifically noted.

Preparation of Pd(IPr$^{\#}$)Cl(allyl)

Under aerobic conditions, IPr$^{\#}$·HCl (0.2 mmol, 205.8 mg), $[Pd(allyl)Cl]_2$ (0.1 mmol, 36.6 mg), K_2CO_3 (0.4 mmol, 55.3 mg), and acetone (1.5 mL) were added to a vial. The mixture was stirred at 60 °C for 3 hours. After cooling to room temperature, the mixture was filtered through a short pad of SiO_2, and the solvent was removed under reduced pressure. Recrystallization from DCM/pentane afforded Pd(IPr$^{\#}$)Cl(allyl) as a pale white powder in 96% yield (270 mg).



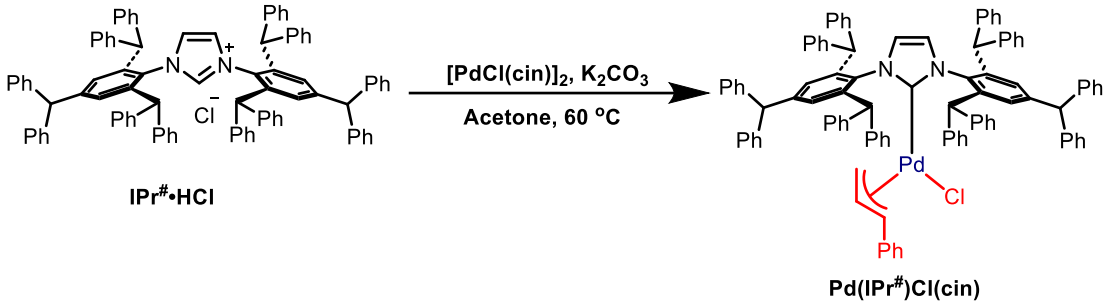
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16-7.077 (m, 44H, CH_{Ar}), 6.92-6.89 (m, 8H, CH_{Ar}), 6.77-6.73 (m, 12H, CH_{Ar}), 5.90 (s, 2H, $\underline{CH}(Ph)_2$), 5.75 (s, 2H, $\underline{CH}(Ph)_2$), 5.35 (s, 2H, $\underline{CH}(Ph)_2$), 5.33 (s, 2H, CH=CH), 4.40 (dq, *J* = 13.4, 6.7 Hz, 1H, CH^{allyl}), 4.08 (dd, *J* = 7.5, 2.1 Hz, 1H, CH^{allyl}), 2.91 (d, *J* = 13.4 Hz, 1H, CH^{allyl}), 2.50 (dd, *J* = 6.3, 2.2 Hz, 1H, CH^{allyl}), 1.04 (d, *J* = 12.0 Hz, 1H, CH^{allyl}).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.25 (C^{Im}-Pd), 144.54 (C_{Ar}), 144.43 (C_{Ar}), 144.25 (C_{Ar}), 143.39 (C_{Ar}), 143.27 (C_{Ar}), 141.40 (C_{Ar}), 141.33 (C_{Ar}), 136.36 (C_{Ar}), 130.87 (CH_{Ar}), 130.70 (CH_{Ar}), 130.30 (CH_{Ar}), 130.26 (CH_{Ar}), 129.30 (CH_{Ar}), 129.24 (CH_{Ar}), 128.41 (CH_{Ar}), 128.34 (CH_{Ar}), 128.07 (CH_{Ar}), 126.37 (CH_{Ar}), 126.34 (CH_{Ar}), 123.36 (CH=CH), 115.03 (CH^{allyl}), 71.78 (CH^{allyl}), 56.34 ($\underline{CH}(Ph)_2$), 51.64 ($\underline{CH}(Ph)_2$), 51.58 ($\underline{CH}(Ph)_2$).

Elemental analysis: Calculated: C 82.33, H 5.54, N 2.00. Found: C 81.98, H 5.25, N 1.69.

Preparation of Pd(IPr$^{\#}$)Cl(cin)

Under aerobic condition, IPr$^{\#}$·HCl (0.2 mmol, 205.8 mg), [Pd(cin)Cl]$_2$ (0.1 mmol, 51.8 mg), K_2CO_3 (0.4 mmol, 55.3 mg), and acetone (1.5 mL) were added to a vial. The mixture was stirring at 60°C for 8 hours. After cooling to room temperature, the mixture was filtered through a short pad of SiO_2, and the solvent was removed under reduced pressure. Recrystallization from DCM/hexane afforded Pd(IPr$^{\#}$)Cl(cin) as a light-yellow powder in 92% yield (272 mg). And the data matched with reported paper.[1]

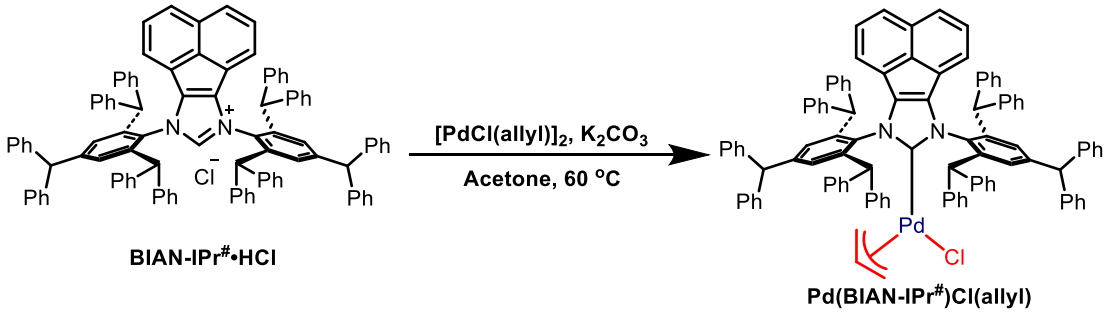


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.34 (m, 5H), 7.19-7.05 (m, 44H), 6.95(t, *J* = 7.1 Hz, 8H), 6.79 (t, *J* = 7.4 Hz, 8H), 6.71 (d, *J* = 8.1 Hz, 4H), 6.09 (s, 2H), 5.62 (s, 2H), 5.36 (d, *J* = 10.6 Hz, 4H), 4.80 (m, 1H), 4.48 (d, *J* = 13.0 Hz, 1H), 2.52 (d, *J* = 6.8 Hz, 1H), 1.19 (d, *J* = 11.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 183.14, 144.70, 144.21, 143.48, 143.45, 143.36, 143.29, 141.70, 140.60, 137.90, 136.29, 130.86, 130.70, 130.62, 130.33, 129.30, 129.18, 129.08, 128.67, 128.44, 128.37, 128.18, 128.15, 127.70, 127.16, 126.36, 123.46, 108.99, 90.79, 56.44, 56.33, 51.68, 47.51.

Elemental analysis: Calculated: C 82.97, H 5.53, N 1.90. Found: C 82.72, H 5.19, N 1.74.

Preparation of Pd(BIAN-IPr$^{\#}$)Cl(allyl)



Under aerobic condition, BIAN-IPr$^{\#}$·HCl (0.29 mmol, 400 mg), [Pd(allyl)Cl]$_2$ (0.145 mmol, 53 mg), K_2CO_3 (0.75 mmol, 103 mg), and acetone (3 mL) were added to a vial. The mixture was stirred at 60°C for 5 hours. After cooling to room temperature, the mixture was filtered through

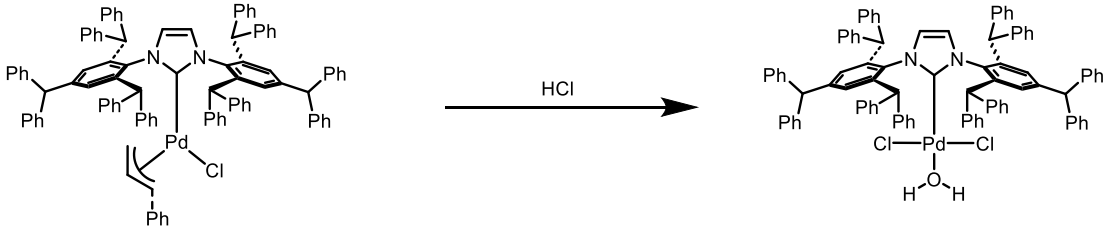
a short pad of SiO_2, and the solvent was removed under reduced pressure. Recrystallization from THF/hexane afforded Pd(BIAN-IPr$^{\#}$)Cl(allyl) as a yellow powder in 93% yield (407 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (t, J = 7.4 Hz, 10H), 7.25-7.21 (m, 6H, CH_{Ar}), 7.16 (s, 10H, CH_{Ar}), 7.11 (d, J = 7.2 Hz, 8H, CH_{Ar}), 7.09-6.99 (m, 12H, CH_{Ar}), 6.75-6.45 (m, 22H, CH_{Ar}), 6.11 (s, 2H, $\underline{CH}(Ph)_2$), 5.96 (s, 2H, $\underline{CH}(Ph)_2$), 5.67 (d, J = 6.9 Hz, 2H, CH_{Ar}), 5.57 (s, 2H, $\underline{CH}(Ph)_2$), 4.45 (dq, J = 13.1, 8.5 Hz, 1H, CH^{allyl}), 4.13 (d, J = 7.4 Hz, 1H, CH^{allyl}), 3.03 (d, J = 13.3 Hz, 1H, CH^{allyl}), 2.38 (s, 1H, CH^{allyl}), 1.26 (d, J = 12.5 Hz, 1H, CH^{allyl}).

^{13}C NMR (126 MHz, $CDCl_3$) δ 190.52 (C^{Im}-Pd), 144.57 (C_{Ar}), 143.49 (C_{Ar}), 141.75 (C_{Ar}), 140.51 (C_{Ar}), 135.97 (C_{Ar}), 131.29 (CH_{Ar}), 130.29 (CH_{Ar}), 129.59 (CH_{Ar}), 129.50 (CH_{Ar}), 129.42 (CH_{Ar}), 129.42 (CH_{Ar}), 128.48 (CH_{Ar}), 128.40 (CH_{Ar}), 127.82 (CH_{Ar}), 127.78 (CH_{Ar}), 127.76 (CH_{Ar}), 126.51 (CH_{Ar}), 126.25 (CH_{Ar}), 126.15 (CH_{Ar}), 126.07 (CH_{Ar}), 125.99 (CH_{Ar}), 125.81 (CH_{Ar}), 125.78 (CH_{Ar}), 124.86 (C=C, backbone), 121.46 (CH_{Ar}), 121.39 (CH_{Ar}), 114.79 (CH^{allyl}), 69.89 (CH^{allyl}), 56.61 ($\underline{CH}(Ph)_2$), 56.53 ($\underline{CH}(Ph)_2$), 51.88 ($\underline{CH}(Ph)_2$).

Elemental analysis: Calculated: C 83.50, H 5.36, N 1.84. Found: C 83.63, H 5.19, N 1.65.

Preparation of Pd(IPr$^{\#}$)Cl$_2$(OH$_2$)



Under a N_2 atmosphere, the Pd(IPr$^{\#}$)Cl(allyl) (0.2 mmol, 280 mg) and excess HCl (2.5 mL, 4M in 1,4-dioxane) were added to a Schlenk flask. The mixture was stirred at 40^{o}C for 24 hours, during which a yellow solution was observed. After cooling to room temperature, the solvent was removed under reduced pressure. A minimal amount of THF was added, followed by the addition of excess hexane to precipitate a yellow solid. The solid was collected, washed with hexane, and dried under vacuum to afford Pd(IPr$^{\#}$)Cl$_2$(OH$_2$) as a fine pale-yellow solid in quantitative yield (267 mg, 94%). In addition, Pd(IPr$^{\#}$)Cl$_2$(OH$_2$) could also be synthesized from Pd(IPr$^{\#}$)Cl(cin) under the same reaction conditions.

^{1}H NMR (500 MHz, DMSO-d_6) δ = 7.24-7.18 (m, 16H, CH_{Ar}), 7.16-7.09 (m, 16H, CH_{Ar}), 7.07 (d, J = 7.3 Hz, 4H, 3,5-CH_{Ar}), 7.02 (t, J = 7.4 Hz, 8H, CH_{Ar}), 6.98 (d, J = 7.1 Hz, 8H, CH_{Ar}), 6.70 (s, 4H, CH_{Ar}), 6.54 (d, J = 7.1 Hz, 8H, CH_{Ar}), 6.11 (s, 4H, $\underline{CH}(Ph)_2$), 5.50 (s, 2H, $\underline{CH}(Ph)_2$), 4.61 (s, 2H, CH=CH).

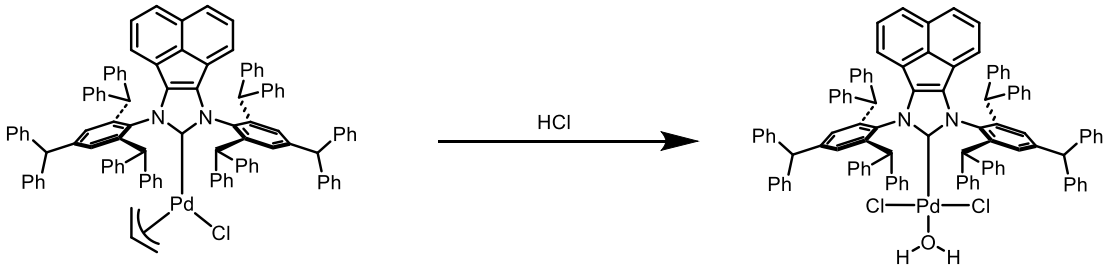
^{13}C NMR (126 MHz, DMSO-d_6) δ 143.76 (C_{Ar}), 143.53 (C_{Ar}), 143.32(C_{Ar}), 143.28 (C_{Ar}), 141.22 (C_{Ar}), 134.73 (C_{Ar}), 132.37 (C_{Ar}), 130.30 (CH_{Ar}), 129.80 (CH_{Ar}), 128.79 (CH_{Ar}), 128.55

(CH_{Ar}), 128.21 (CH_{Ar}), 127.72 (CH_{Ar}), 126.41 (CH_{Ar}), 126.21 (CH_{Ar}), 126.09(CH_{Ar}), 124.14 (CH=CH), 55.02 (<u>CH</u>$(Ph)_2$), 50.28 (<u>CH</u>$(Ph)_2$).

Elemental analysis: Calculated: C 79.06, H 5.28, N 1.98. Found: C 78.93, H 5.17, N 1.58.

Preparation of Pd(BIAN-IPr$^{\#}$)$Cl_2(OH_2)$

Under a N_2 atmosphere, Pd(BIAN-IPr$^{\#}$)Cl(allyl) (0.2 mmol, 306 mg) and excess HCl (2.5 mL, 4 M in 1,4-dioxane) were added to a Schlenk flask. The mixture was stirred at 40 °C for 24 hours, during which a reddish-brown coloration was observed. After cooling to room temperature, the solvent was removed under reduced pressure. A minimal amount of THF was added, followed by the addition of excess hexane to precipitate a yellow solid. The solid was collected, washed with hexane, and dried under vacuum to afford Pd(BIAN-IPr$^{\#}$)$Cl_2(OH_2)$ as a fine yellow solid in quantitative yield (300 mg, 97%).



^{1}H NMR (500 MHz, DMSO-d_6) δ 7.30 (t, *J* = 7.4 Hz, 8H, CH_{Ar}), 7.23 (dt, *J* = 9.2, 5.0 Hz, 6H, CH_{Ar}), 7.12 (d, *J* = 7.8 Hz, 12H, CH_{Ar}), 7.03 (s, 20H, CH_{Ar}), 6.61 (t, *J* = 7.6 Hz, 2H, CH_{Ar}), 6.51 (t, *J* = 7.3 Hz, 4H, CH_{Ar}), 6.29 (t, *J* = 7.5 Hz, 8H, CH_{Ar}), 6.25-6.16 (m, 12H, <u>CH</u>$(Ph)_2$ and CH_{Ar} overlapped), 5.77 (s, 2H, <u>CH</u>$(Ph)_2$), 5.48 (d, *J* = 6.9 Hz, 2H, CH_{Ar}).

^{13}C NMR (126 MHz, DMSO-d_6) δ 144.76 (CH_{Ar}), 144.35 (CH_{Ar}), 143.26 (CH_{Ar}), 141.45 (CH_{Ar}), 140.95 (CH_{Ar}), 140.04 (CH_{Ar}), 134.87 (CH_{Ar}), 131.61 (C_{Ar}), 129.86 (C_{Ar}), 128.87 (C_{Ar}), 128.80 (C_{Ar}), 128.46 (C_{Ar}), 128.36 (C_{Ar}), 127.34 (C_{Ar}), 126.85 (C_{Ar}), 126.37(C_{Ar}), 126.15 (C_{Ar}), 125.84 (C_{Ar}), 125.48 (C_{Ar}), 125.35 (C=C, backbone), 124,21 (C_{Ar}), 120.70 (CH_{Ar}), 55.04 (<u>CH</u>$(Ph)_2$), 50.12 (<u>CH</u>$(Ph)_2$).

Elemental analysis: Calculated: C 80.49, H 5.12, N 1.82. Found: C 80.18, H 5.37, N 1.56.

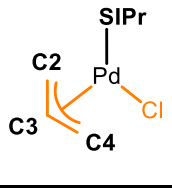
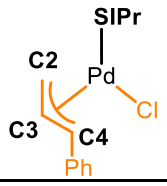
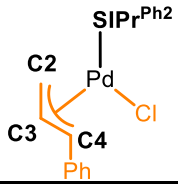
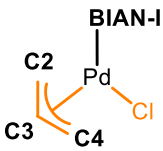
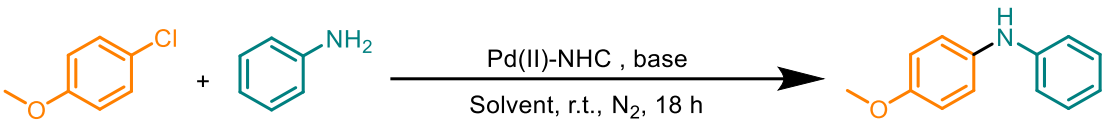
(Å)				
Pd-C2	2.118(6)	2.136(10)	2.155(11)	2.103(5)
Pd-C3	2.132(7)	2.137(8)	2.183(10)	2.143(6)
Pd-C4	2.203(6)	2.136(10)	2.291(10)	2.193(5)

Fig.S1 Selected bond distances in the crystals of Pd(SIPr)Cl(allyl/cin), Pd(SIPr^{Ph2})Cl(allyl) and Pd(BIAN-IPr$^{\#}$)Cl(allyl) complexes.

Procedure of optimization of Buchwald-Hartwig amination reaction

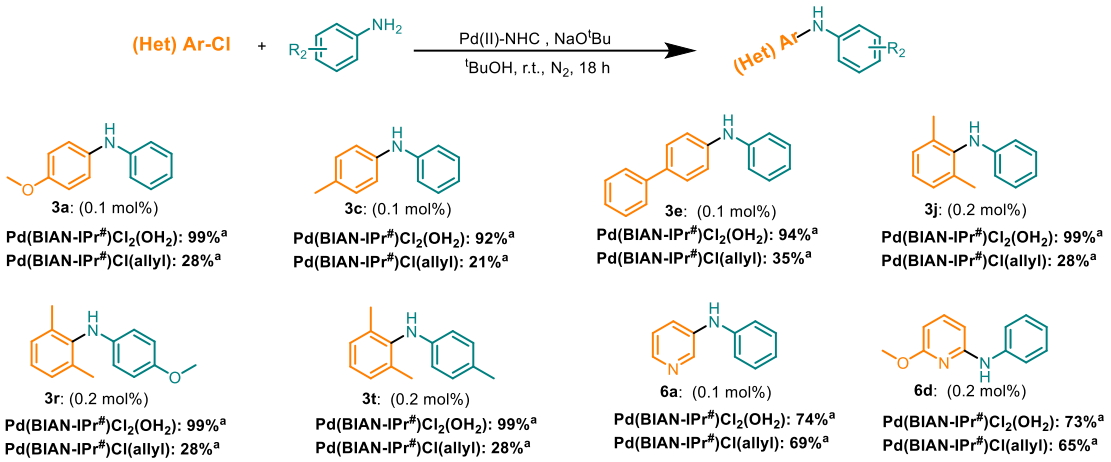
Table S1 The optimization of the model reaction between 4-chloroanisole and aniline[a] [2]



Entry	Pd(II)-NHC	Loading (mol%)	Base	Solvent	Conv.(%)[b]
1	Pd(IPr$^{\#}$)Cl$_2$(OH$_2$)	0.25	KO^{t}Bu	2-MeTHF	< 5
2	Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$)	0.25	KO^{t}Bu	2-MeTHF	16
3	Pd(IPr$^{\#}$)Cl$_2$(OH$_2$)	0.25	NaO^{t}Bu	2-MeTHF	45
4	Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$)	0.25	NaO^{t}Bu	2-MeTHF	>99
5	Pd(IPr$^{\#}$)Cl$_2$(OH$_2$)	0.25	NaO^{t}Bu	^{t}BuOH	42
6	Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$)	0.25	NaO^{t}Bu	^{t}BuOH	>99
7	Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$)	0.1	NaO^{t}Bu	^{t}BuOH	99
8	Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$)	0.05	NaO^{t}Bu	^{t}BuOH	76

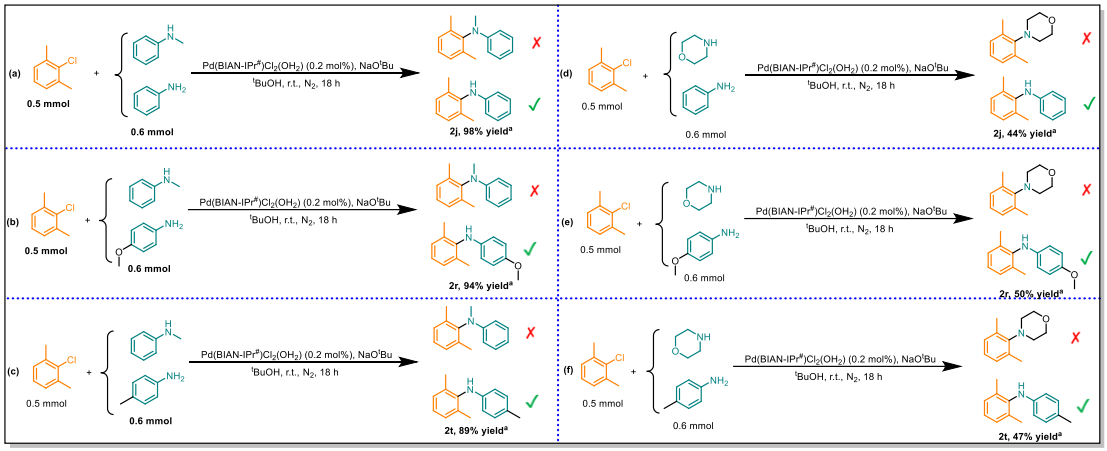
[a] 4-Chloroanisole (1 mmol), aniline (1.2 mmol), KO^{t}Bu or NaO^{t}Bu (1.2 mmol), Pd(II)-NHC (0.05-0.25 mol%), solvent (1.5 mL), room temperature, 18 hours, N_2. [b] The reaction conversions were measured by GC (2 runs).

Comparative of activity of Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$) and Pd(BIAN-IPr$^{\#}$)Cl(allyl)



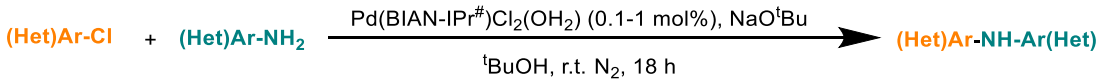
Scheme S1. Comparative of activity of two catalysts in C-N cross-coupling reaction.[3] [a]Reaction yields were determined by GC analysis.

The selectivity of Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$) in C-N cross-coupling reaction



Scheme S2. High chemoselectivity of a Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$) catalyst in Buchwald-Hartwig amination for secondary amine synthesis. [a]Reaction yields were determined by GC analysis.

General procedure of Buchwald-Hartwig amination reaction



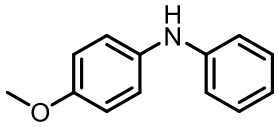
The Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$) (0.1-1 mol%) and a stirring bar were charged in a 4 mL vial. The vial was transferred into a glovebox, where NaO^{t}Bu (1.2 mmol) was added. The cap was then sealed, and the vial was removed from the glovebox. Under a N_2 atmosphere, the aryl chloride (1.0 mmol, liquid), amine (1.2 mmol, liquid), and the degassed ^{t}BuOH (1.5 mL) were added at room temperature. The reaction mixture was stirred at room temperature (25-30^{o}C) for 18 h.

Subsequently, the reaction mixture was filtered through a fritted funnel, and the solvent was removed under reduced pressure. The corresponding product was purified by column chromatography on silica gel (eluent: EtOAc/petroleum ether or DCM/petroleum ether). In addition, the isolated yields were presented in Scheme 3 and 4.

Characterization data of desired product.

4-methoxy-N-phenylaniline (2a)[2b]

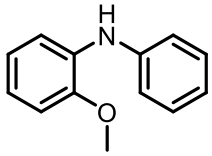
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 (s, 1H), 7.16 (m, 2H), 7.04 (d, J = 8.9 Hz, 2H), 6.91 (d, J = 7.6 Hz, 2H), 6.86 (d, J = 8.9 Hz, 2H), 6.69 (t, J = 7.3 Hz, 1H), 3.71 (s, 3H).

2-methoxy-N-phenylaniline (2b)[4]

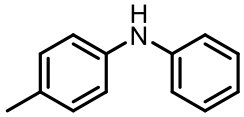
According to the general procedure, the corresponding final product was obtained as yellow oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, J = 8.1 Hz, 2H), 7.24 (d, J = 7.9 Hz, 2H), 2.40 (s, 3H).

4-methyl-N-phenylaniline (2c)[5]

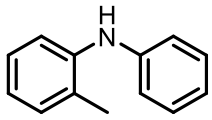
According to the general procedure, the corresponding final product was obtained as a pale white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (t, J = 7.5 Hz, 2H), 7.09 (d, J = 8.0 Hz, 2H), 7.03-7.00 (m, 4H), 6.89 (t, J = 7.3 Hz, 1H), 5.62 (s, 1H), 2.31 (s, 3H).

2-methyl-N-phenylaniline (2d)[4]

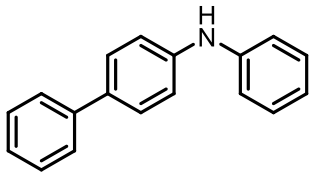
According to the general procedure, the corresponding final product was obtained as yellow oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.22 (m, 3H), 7.19 (dd, J = 7.4, 1.5 Hz, 1H), 7.13 (td, J = 7.7, 1.6 Hz, 1H), 6.98-6.87 (m, 4H), 5.35 (s, 1H), 2.25 (s, 3H).

N-phenyl-[1,1'-biphenyl]-4-amine (2e)[6]

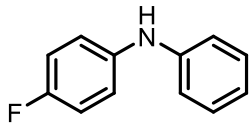
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.36-7.29 (m, 3H), 7.15 (dd, *J* = 8.6, 7.1 Hz, 4H), 6.98 (tt, *J* = 7.3, 1.1 Hz, 1H), 5.40 (s, 1H).

4-fluoro-N-phenylaniline (2f)[2b]

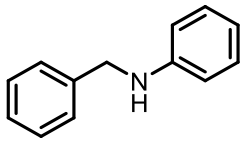
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (m, 2H), 7.08-7.03 (m, 2H), 7.01-6.97 (m, 4H), 6.91 (t, *J* = 7.4 Hz, 1H), 5.61 (s, 1H).

N-benzylaniline (2g)[5]

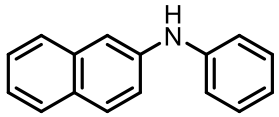
According to the general procedure, the corresponding final product was obtained as yellow oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 4H), 7.30-7.27 (m, 1H), 7.22-7.16 (m, 2H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.66 (d, *J* = 7.6 Hz, 2H), 4.34 (s, 2H), 4.09 (s, 1H).

N-phenylnaphthalen-2-amine (2h)[7]

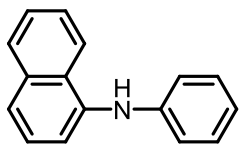
According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.6 Hz, 2H), 7.66 (d, *J* = 9.5 Hz, 1H), 7.46 (d, *J* = 2.3 Hz, 1H), 7.42 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 7.35-7.29 (m, 3H), 7.24 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.18 (d, *J* = 7.5 Hz, 2H), 7.00 (t, *J* = 7.3 Hz, 1H), 5.90 (s, 1H).

N-phenylnaphthalen-1-amine (2i)[8]

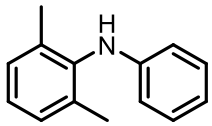
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.85 (dd, *J* = 7.4, 1.9 Hz, 1H), 7.55 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.51-7.43 (m, 2H), 7.40-7.33 (m, 2H), 7.24 (dd, *J* = 6.5, 1.8 Hz, 2H), 6.98 (d, *J* = 7.9 Hz, 2H), 6.90 (t, *J* = 7.3 Hz, 1H), 5.92 (s, 1H).

2,6-dimethyl-N-phenylaniline (2j)[9]

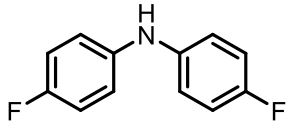
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20-7.08 (m, 5H), 6.77 (t, *J* = 7.3 Hz, 1H), 6.53 (d, *J* = 7.5 Hz, 2H), 5.19 (s, 1H), 2.24 (s, 6H).

bis(4-fluorophenyl)amine (2k)[10]

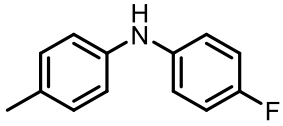
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (d, *J* = 7.0 Hz, 8H), 5.39 (s, 1H).

4-fluoro-N-(p-tolyl)aniline (2l)[5]

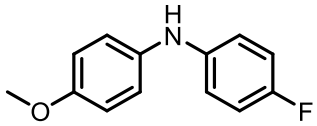
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.2 Hz, 2H), 6.99 (dt, *J* = 10.7, 6.8 Hz, 4H), 6.93 (d, *J* = 8.3 Hz, 2H), 5.40 (s, 1H), 2.31 (s, 3H).

4-fluoro-N-(4-methoxyphenyl)aniline (2m)[11]

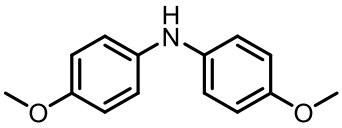
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, *J* = 8.3 Hz, 2H), 6.94-6.84 (m, 6H), 5.35 (s, 1H), 3.80 (s, 3H).

bis(4-methoxyphenyl)amine (2n)[2b]

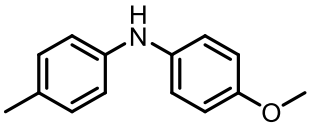
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, DMSO-d_6) δ 7.50 (s, 1H), 6.92 (d, J = 9.0 Hz, 4H), 6.80 (d, J = 9.0 Hz, 4H), 3.68 (s, 6H).

4-methoxy-N-(p-tolyl)aniline (2o)[2b]

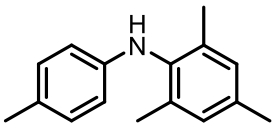
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, DMSO-d_6) δ 7.66 (s, 1H), 6.98 (m, 4H), 6.84 (m, 4H), 3.70 (s, 3H), 2.19 (s, 3H).

2,4,6-trimethyl-N-(p-tolyl)aniline (2p)[2b]

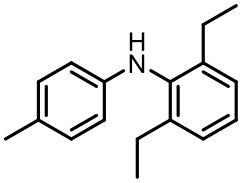
According to the general procedure, the corresponding final product was obtained as yellow oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, J = 8.0 Hz, 2H), 6.94 (s, 2H), 6.43 (d, J = 8.4 Hz, 2H), 5.02 (s, 1H), 2.31 (s, 3H), 2.25 (s, 3H), 2.18 (s, 6H).

2,6-diethyl-N-(p-tolyl)aniline (2q)[2b]

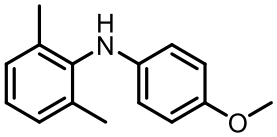
According to the general procedure, the corresponding final product was obtained as yellow oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (m, 3H), 6.96 (d, J = 8.0 Hz, 2H), 6.42 (d, J = 8.4 Hz, 2H), 5.08 (s, 1H), 2.59 (q, J = 7.5 Hz, 4H), 2.24 (s, 3H), 1.15 (t, J = 7.6 Hz, 6H).

N-(4-methoxyphenyl)-2,6-dimethylaniline (2r)[9]

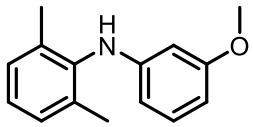
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, J = 7.4 Hz, 2H), 7.05 (dd, J = 8.5, 6.3 Hz, 1H), 6.76 (d, J = 9.0 Hz, 2H), 6.50 (d, J = 8.3 Hz, 2H), 5.06 (s, 1H), 3.75 (s, 3H), 2.21 (s, 6H).

N-(3-methoxyphenyl)-2,6-dimethylaniline (2s)[11]

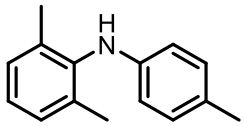
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.05 (m, 4H), 6.32 (ddd, *J* = 8.1, 2.5, 0.8 Hz, 1H), 6.15 (ddd, *J* = 8.0, 2.2, 0.8 Hz, 1H), 6.05 (t, *J* = 2.3 Hz, 1H), 3.74 (s, 3H), 2.23 (s, 6H).

2,6-dimethyl-N-(p-tolyl)aniline (2t)[8]

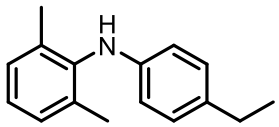
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (d, *J* = 6.3 Hz, 2H), 7.09-7.06 (m, 1H), 6.99 -6.97 (m, 2H), 6.45 (d, *J* = 8.4 Hz, 2H), 5.11 (s, 1H), 2.26 (s, 3H), 2.22 (s, 6H).

N-(4-ethylphenyl)-2,6-dimethylaniline (2u)

According to the general procedure, the corresponding final product was obtained as brown oil.



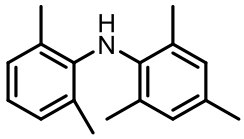
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (d, *J* = 8.3 Hz, 2H, CH_{Ar}), 7.08-7.05 (m, 1H, CH_{Ar}), 7.00 (d, *J* = 8.5 Hz, 2H, CH_{Ar}), 6.46 (d, *J* = 8.4 Hz, 2H, CH_{Ar}), 5.12 (s, 1H, NH), 2.56 (q, *J* = 7.6 Hz, 2H, $\underline{CH_2}CH_3$), 2.22 (s, 6H, CH_3), 1.20 (t, *J* = 7.6 Hz, 3H, $CH_2\underline{CH_3}$).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.17 (C_{Ar}), 138.85 (C_{Ar}), 135.63 (C_{Ar}), 134.19 (C_{Ar}), 128.65 (CH_{Ar}), 128.62 (CH_{Ar}), 125.50 (CH_{Ar}), 113.94 (CH_{Ar}), 28.06 ($\underline{CH_2}CH_3$), 18.54 (CH_3), 15.89 ($CH_2\underline{CH_3}$).

HRMS: Calcd. For $C_{16}H_{20}N$ ($[M+H]^+$): 226.1590, Found: 226.1590

N-(2,6-dimethylphenyl)-2,4,6-trimethylaniline (2v)[13]

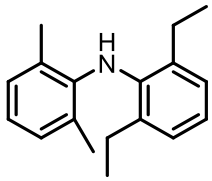
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, *J* = 7.4 Hz, 2H), 6.85-6.79 (m, 3H), 4.73 (s, 1H), 2.27 (s, 3H), 2.02 (s, 6H), 2.01 (s, 6H).

N-(2,6-diethylphenyl)-2,6-dimethylaniline (2w)[8]

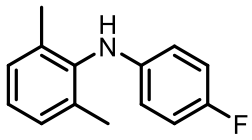
According to the general procedure, the corresponding final product was obtained as colour-less oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08-7.06 (m, 2H), 7.04-7.00 (m, 1H), 6.97 (d, *J* = 7.4 Hz, 2H), 6.79 (t, *J* = 7.4 Hz, 1H), 4.89 (s, 1H), 2.44 (q, *J* = 7.5 Hz, 4H), 2.00 (s, 6H), 1.14 (t, *J* = 7.5 Hz, 6H).

N-(4-fluorophenyl)-2,6-dimethylaniline (2x)[2e]

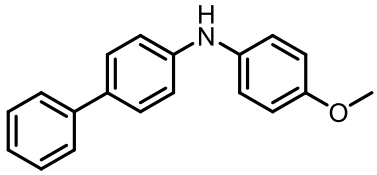
According to the general procedure, the corresponding final product was obtained as a rufous solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.05 (m, 3H), 6.86 (t, *J* = 8.7 Hz, 2H), 6.46- 6.43 (m, 2H), 5.10 (s, 1H), 2.20 (s, 6H).

N-(4-methoxyphenyl)-[1,1'-biphenyl]-4-amine (2y)[14]

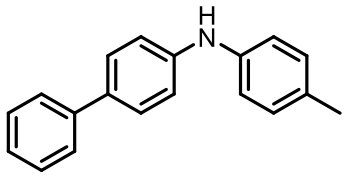
According to the general procedure, the corresponding final product was obtained as a rufous solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.20-7.08 (m, 2H), 7.00 (d, *J* = 8.1 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 5.59 (s, 1H), 3.83 (s, 3H).

N-(p-tolyl)-[1,1'-biphenyl]-4-amine (2z)[8]

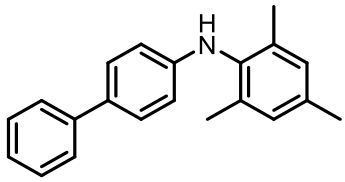
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.0 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.18-7.13 (m, 2H), 7.09 (dd, *J* = 11.7, 8.5 Hz, 4H), 5.70 (s, 1H), 2.36 (s, 3H).

N-mesityl-[1,1'-biphenyl]-4-amine (2aa)[15]

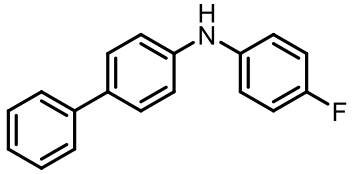
According to the general procedure, the corresponding final product was obtained as pale-yellow oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.3 Hz, 2H), 7.43-7.35 (m, 4H), 7.26 -7.22 (m, 1H), 6.96 (s, 2H), 6.55 (d, *J* = 8.5 Hz, 2H), 5.18 (s, 1H), 2.32 (s, 3H), 2.21 (s, 6H).

N-(4-fluorophenyl)-[1,1'-biphenyl]-4-amine (2ab)[16]

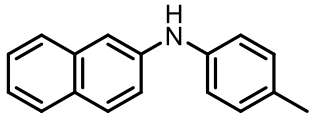
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.0 Hz, 2H), 7.51 (d, *J* = 8.6 Hz, 2H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.16-6.95 (m, 6H), 5.65 (s, 1H).

N-(p-tolyl)naphthalen-2-amine (2ac)[17]

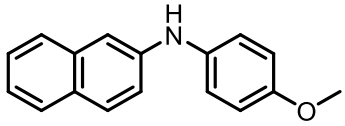
According to the general procedure, the corresponding final product was obtained as a rufous solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.8 Hz, 2H), 7.63 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.42-7.35 (m, 2H), 7.28 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.19 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.13 (q, *J* = 8.5 Hz, 4H), 5.82 (s, 1H), 2.35 (s, 3H).

N-(4-methoxyphenyl)naphthalen-2-amine (2ad)[18]

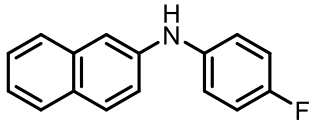
According to the general procedure, the corresponding final product was obtained as a pale-white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.57 (m, 3H), 7.40-7.12 (m, 5H), 7.10-6.89 (m, 2H), 5.71 (s, 1H), 3.8 6 (s, 3H).

N-(4-fluorophenyl)naphthalen-2-amine (2ae)[18]

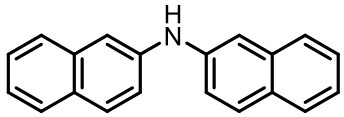
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.43-7.37 (m, 1H), 7.34-7.27 (m, 2H), 7.15 (ddd, *J* = 8.9, 5.2, 3.5 Hz, 3H), 7.03 (t, *J* = 8.7 Hz, 2H), 5.83 (s, 1H).

di(naphthalen-2-yl)amine (2af)[19]

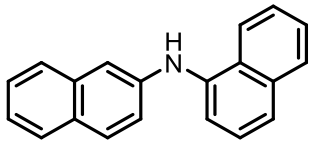
According to the general procedure, the corresponding final product was obtained as a pale-brown solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (t, *J* = 8.1 Hz, 4H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.54 (d, *J* = 2.3 Hz, 2H), 7.44 (ddd, *J* = 8.2, 6.6, 1.3 Hz, 2H), 7.40-7.29 (m, 4H), 6.04 (s, 1H).

N-(naphthalen-2-yl)naphthalen-1-amine (2ag)[20]

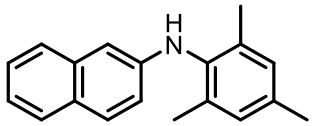
According to the general procedure, the corresponding final product was obtained as a pale-brown solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.3 Hz, 1H), 7.96-7.89 (m, 1H), 7.78 (dd, *J* = 8.4, 3.6 Hz, 2H), 7.65 (dd, *J* = 6.8, 2.6 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.57-7.44 (m, 4H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.34-7.26 (m, 3H), 6.13 (s, 1H).

N-mesitylnaphthalen-2-amine (2ah)[21]

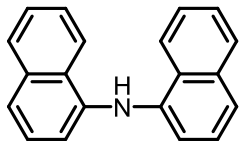
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (t, *J* = 8.1 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.38-7.30 (m, 1H), 7.26-7.19 (m, 1H), 7.01 (s, 2H), 6.96 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.57 (d, *J* = 2.4 Hz, 1H), 5.27 (s, 1H), 2.37 (s, 3H), 2.22 (s, 6H).

di(naphthalen-1-yl)amine (2ai)[22]

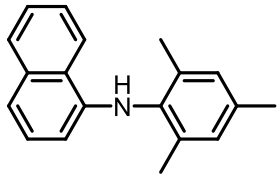
According to the general procedure, the corresponding final product was obtained as a rufous solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.7 Hz, 2H), 7.92 (d, *J* = 8.1 Hz, 2H), 7.63-7.46 (m, 6H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.05 (dd, *J* = 7.4, 1.1 Hz, 2H), 6.36 (s, 1H).

N-mesitylnaphthalen-1-amine (2aj)[8]

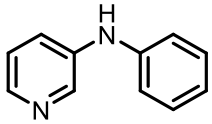
According to the general procedure, the corresponding final product was obtained as rufous oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14-8.06 (m, 1H), 7.92-7.83 (m, 1H), 7.53 (dq, *J* = 6.2, 3.7 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.01 (s, 2H), 6.23 (d, *J* = 7.5 Hz, 1H), 5.68 (s, 1H), 2.36 (s, 3H), 2.19 (s, 6H).

N-phenylpyridin-3-amine (6a)[7]

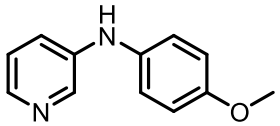
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 2.8 Hz, 1H), 8.16 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.41 (ddd, *J* = 8.3, 2.8, 1.4 Hz, 1H), 7.34-7.27 (m, 2H), 7.20-7.14 (m, 1H), 7.09 (d, *J* = 7.5 Hz, 2H), 7.00 (t, *J* = 7.4 Hz, 1H), 5.85 (s, 1H).

N-(4-methoxyphenyl)pyridin-3-amine (6b)[9]

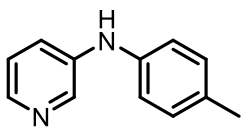
According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 2.8 Hz, 1H), 8.06 (dd, *J* = 4.6, 1.4 Hz, 1H), 7.20 (ddd, *J* = 8.3, 2.8, 1.4 Hz, 1H), 7.13-7.05 (m, 3H), 6.88 (d, *J* = 8.9 Hz, 2H), 5.64 (s, 1H), 3.80 (s, 3H).

N-(p-tolyl)pyridin-3-amine (6c)[8]

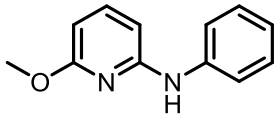
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 2.8 Hz, 1H), 8.11 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.33 (ddd, *J* = 8.3, 2.8, 1.4 Hz, 1H), 7.16-7.08 (m, 3H), 7.01 (d, *J* = 8.4 Hz, 2H), 5.79 (s, 1H), 2.32 (s, 3H).

6-methoxy-N-phenylpyridin-2-amine (6d)[23]

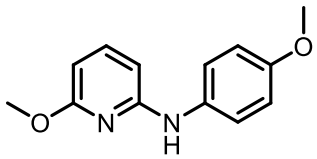
According to the general procedure, the corresponding final product was obtained as yellow oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.37 (m, 3H), 7.35-7.29 (m, 2H), 7.03 (t, *J* = 7.2 Hz, 1H), 6.42 (s, 1H), 6.41 (d, *J* = 3.3 Hz, 1H), 6.20 (dd, *J* = 8.0, 0.6 Hz, 1H), 3.91 (s, 3H).

6-methoxy-N-(4-methoxyphenyl)pyridin-2-amine (6e)

According to the general procedure, the corresponding final product was obtained as brown oil.



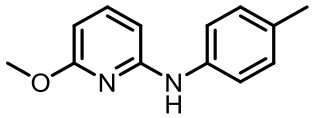
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (t, *J* = 7.9 Hz, 1H, CH_{Ar}), 7.27 (d, *J* = 8.9 Hz, 2H, CH_{Ar}), 6.89 (d, *J* = 8.9 Hz, 2H, CH_{Ar}), 6.25 (s, 1H, NH), 6.22 (d, *J* = 7.9 Hz, 1H, CH_{Ar}), 6.14 (dd, *J* = 7.9, 0.6 Hz, 1H, CH_{Ar}), 3.89 (s, 3H, OCH_3), 3.81 (s, 3H, OCH_3).

^{13}C NMR (126 MHz, $CDCl_3$) δ 163.74 (C_{Ar}), 156.03 (C_{Ar}), 155.79(C_{Ar}), 140.29 (CH_{Ar}), 133.60 (C_{Ar}), 123.57 (CH_{Ar}), 114.57 (CH_{Ar}), 99.33 (CH_{Ar}), 98.71(CH_{Ar}), 55.65 (OCH_3), 53.46 (OCH_3).

HRMS: Calcd. For $C_{13}H_{15}N_2O_2$ ($[M+H]^+$): 231.1128, Found: 231.1127

6-methoxy-N-(p-tolyl)pyridin-2-amine (6f)

According to the general procedure, the corresponding final product was obtained as brown oil.



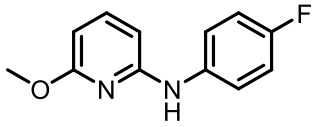
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (t, *J* = 7.9 Hz, 1H, CH_{Ar}), 7.25 (d, *J* = 8.4 Hz, 2H, CH_{Ar}), 7.13 (d, *J* = 8.2 Hz, 2H, CH_{Ar}), 6.34 (d, *J* = 7.8 Hz, 2H, CH_{Ar}), 6.17 (d, *J* = 7.9 Hz, 1H, CH_{Ar}), 3.90 (s, 3H, OCH_3), 2.33 (s, 3H, CH_3).

^{13}C NMR (126 MHz, $CDCl_3$) δ 163.70 (C_{Ar}), 154.97 (C_{Ar}), 140.27 (CH_{Ar}), 138.05 (C_{Ar}), 132.35 (C_{Ar}), 129.81 (CH_{Ar}), 120.75 (CH_{Ar}), 99.77 (CH_{Ar}), 99.32 (CH_{Ar}), 53.49 (OCH_3), 20.91 (CH_3).

HRMS: Calcd. For $C_{13}H_{15}N_2O$ ($[M+H]^+$): 215.1179, Found: 215.1180

N-(4-fluorophenyl)-6-methoxypyridin-2-amine (6g)

According to the general procedure, the corresponding final product was obtained as brown oil.



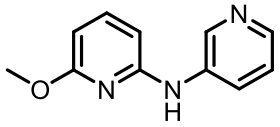
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (t, *J* = 7.9 Hz, 1H, CH_{Ar}), 7.36-7.30 (m, 2H, CH_{Ar}), 7.05-6.99 (m, 2H, CH_{Ar}), 6.31 (s, 1H, NH), 6.27 (dd, *J* = 7.9, 0.6 Hz, 1H, CH_{Ar}), 6.19 (dd, *J* = 7.9, 0.6 Hz, 1H, CH_{Ar}), 3.89 (s, 3H, OCH_3).

^{13}C NMR (126 MHz, $CDCl_3$) δ 163.69 (C_{Ar}), 158.77 (d, *J* = 241.6 Hz, C_{Ar}) 154.84 (C_{Ar}), 140.39 (CH_{Ar}), 136.67 (d, *J* = 2.7 Hz, C_{Ar}), 122.39 (d, *J* = 7.8 Hz, CH_{Ar}), 115.87 (d, *J* = 22.4 Hz, CH_{Ar}), 100.08 (CH_{Ar}), 99.40 (CH_{Ar}), 53.56 (OCH_3).

HRMS: Calcd. For $C_{12}H_{12}FN_2O$ ($[M+H]^+$): 219.0928, Found: 219.0919

6-methoxy-N-(pyridin-3-yl)pyridin-2-amine (6h)

According to the general procedure, the corresponding final product was obtained as a yellow solid.



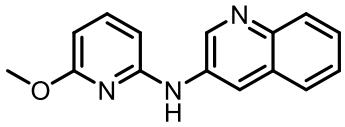
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 2.7 Hz, 1H, CH_{Ar}), 8.23 (dd, *J* = 4.8, 1.4 Hz, 1H, CH_{Ar}), 7.97 (ddd, *J* = 8.3, 2.7, 1.4 Hz, 1H, CH_{Ar}), 7.44 (t, *J* = 7.9 Hz, 1H, CH_{Ar}), 7.24 (dd, *J* = 8.4, 4.8 Hz, 1H, CH_{Ar}), 6.61 (s, 1H, NH), 6.33 (d, *J* = 7.8 Hz, 1H, CH_{Ar}), 6.26 (d, *J* = 8.0 Hz, 1H, CH_{Ar}), 3.91 (s, 3H, OCH_3).

^{13}C NMR (126 MHz, $CDCl_3$) δ 163.64 (C_{Ar}), 153.78 (C_{Ar}), 142.65 (CH_{Ar}), 141.11 (CH_{Ar}), 140.36 (CH_{Ar}), 137.97 (C_{Ar}), 125.81 (CH_{Ar}), 123.74 (CH_{Ar}), 101.06 (CH_{Ar}), 101.01 (CH_{Ar}), 53.73 (OCH_3).

HRMS: Calcd. For $C_{11}H_{12}N_3O$ ($[M+H]^+$): 202.0975, Found: 219.0974

N-(6-methoxypyridin-2-yl)quinolin-3-amine (6i)

According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



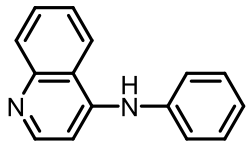
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.90 (d, *J* = 2.7 Hz, 1H, CH_{Ar}), 8.49 (d, *J* = 2.6 Hz, 1H, CH_{Ar}), 8.03 (d, *J* = 8.2 Hz, 1H, CH_{Ar}), 7.71 (dd, *J* = 8.1, 1.5 Hz, 1H, CH_{Ar}), 7.59-7.53 (m, 1H, CH_{Ar}), 7.48 (dt, *J* = 15.6, 7.9 Hz, 2H, CH_{Ar}), 6.92 (s, 1H, NH), 6.40 (d, *J* = 7.7 Hz, 1H, CH_{Ar}), 6.30 (d, *J* = 8.0 Hz, 1H, CH_{Ar}), 3.98 (s, 3H, OCH_3).

^{13}C NMR (126 MHz, $CDCl_3$) δ 163.65 (C_{Ar}), 153.65 (C_{Ar}), 145.34 (C_{Ar}), 144.02 (CH_{Ar}), 140.37 (CH_{Ar}), 134.69 (C_{Ar}), 129.07 (C_{Ar}), 128.82 (CH_{Ar}), 127.19 (CH_{Ar}), 127.17 (CH_{Ar}), 127.12 (CH_{Ar}), 120.77 (CH_{Ar}), 101.39 (CH_{Ar}), 101.11 (CH_{Ar}), 53.74 (OCH_3).

HRMS: Calcd. For $C_{15}H_{14}N_3O$ ($[M+H]^+$): 252.1131, Found: 252.1132

N-phenylquinolin-4-amine (6j)[24]

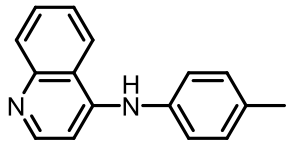
According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 5.3 Hz, 1H,), 8.05 (dd, *J* = 8.5, 1.2 Hz, 1H), 7.97 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.68 (t, *J* = 7.0 Hz, 1H), 7.50 (t, *J* = 7.0 Hz, 1H), 7.46-7.38 (m, 2H), 7.31 (d, *J* = 7.3 Hz, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 5.2 Hz, 1H), 6.89 (s, 1H).

N-(p-tolyl)quinolin-4-amine (6k)[24]

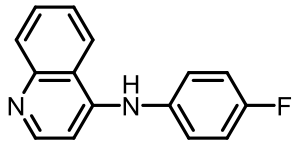
According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 5.3 Hz, 1H), 8.03 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.96 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.66 (t, *J* = 7.9 Hz, 1H), 7.47 (t, *J* = 8.3 Hz, 1H), 7.25-7.16 (m, 4H), 6.90 (d, *J* = 8.3 Hz, 1H), 6.87 (s, 1H), 2.38 (s, 3H).

N-(4-fluorophenyl)quinolin-4-amine (6l)[24]

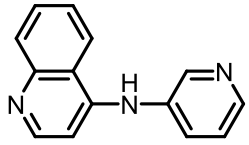
According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 5.3 Hz, 1H), 8.04 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.96 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.70 (ddd, *J* = 8.7, 4.0, 2.4 Hz, 1H), 7.53-7.49 (m, 1H), 7.31-7.26 (m, 2H), 7.12 (t, *J* = 8.6 Hz, 2H), 6.78 (s, 1H), 6.77 (s, 1H).

N-(pyridin-3-yl)quinolin-4-amine (6m)

According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



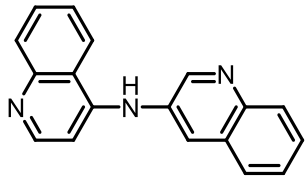
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.67 (d, *J* = 2.6 Hz, 1H, CH_{Ar}), 8.59 (dd, *J* = 8.5, 1.3 Hz, 1H, CH_{Ar}), 8.50 (d, *J* = 5.8 Hz, 1H, CH_{Ar}), 8.42 (d, *J* = 1.5 Hz, 1H, CH_{Ar}), 7.97 (d, *J* = 8.4 Hz, 1H, CH_{Ar}), 7.89-7.79 (m, 2H, CH_{Ar}), 7.67-7.60 (m, 1H, CH_{Ar}), 7.48 (dd, *J* = 8.3, 4.2 Hz, 1H, CH_{Ar}), 6.91 (d, *J* = 5.8 Hz, 1H, CH_{Ar}).

^{13}C NMR (101 MHz, DMSO-d_6) δ 172.50 (CH_{Ar}), 150.25 (C_{Ar}), 148.69 (CH_{Ar}), 145.97 (C_{Ar}), 145.26 (CH_{Ar}), 137.03 (C_{Ar}), 131.32 (CH_{Ar}), 130.77 (CH_{Ar}), 126.83 (CH_{Ar}), 126.10 (CH_{Ar}), 124.67 (CH_{Ar}), 123.26 (CH_{Ar}), 119.61 (C_{Ar}), 101.73 (CH_{Ar}).

HRMS: Calcd. For $C_{14}H_{11}N_3Na$ ($[M+Na]^+$): 244.0845, Found: 244.0854

N-(quinolin-4-yl)quinolin-3-amine (6n)

According to the general procedure, the corresponding final product was obtained as a pale-yellow solid.



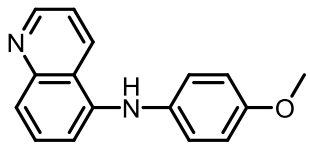
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.90 (d, *J* = 2.6 Hz, 1H, CH_{Ar}), 8.61 (d, *J* = 5.2 Hz, 1H， CH_{Ar}), 8.09 (q, *J* = 8.2 Hz, 3H, CH_{Ar}), 8.00 (d, *J* = 2.6 Hz, 1H, CH_{Ar}), 7.77-7.72 (m, 1H, CH_{Ar}), 7.67 (dt, *J* = 20.2, 7.6 Hz, 2H, CH_{Ar}), 7.52 (dt, *J* = 25.6, 7.6 Hz, 3H, CH_{Ar}), 7.03 (d, *J* = 5.2 Hz, 1H, CH_{Ar}).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.91 (CH_{Ar}), 149.24 (C_{Ar}), 147.32 (C_{Ar}), 147.30 (C_{Ar}), 145.43 (CH_{Ar}), 134.09 (C_{Ar}), 130.16 (C_{Ar}), 129.88 (CH_{Ar}), 129.37 (CH_{Ar}), 128.60 (CH_{Ar}), 128.49 (CH_{Ar}), 127.62 (CH_{Ar}), 127.19 (CH_{Ar}), 125.89 (CH_{Ar}), 125.59 (CH_{Ar}), 120.24 (C_{Ar}), 120.15 (CH_{Ar}), 102.90 (CH_{Ar}).

HRMS: Calcd. For $C_{18}H_{14}N_3$ ($[M+H]^+$): 272.1182, Found: 271.1180

N-(4-methoxyphenyl)quinolin-5-amine (6o)[25]

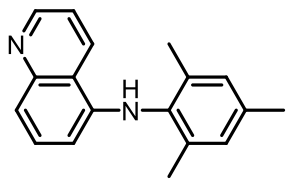
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.90 (dd, *J* = 4.3, 1.6 Hz, 1H), 8.34 (d, *J* = 8.5 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.35 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.8 Hz, 2H), 6.88 (d, *J* = 8.9 Hz, 2H), 5.92 (s, 1H), 3.81 (s, 3H).

N-mesitylquinolin-5-amine (6p)[26]

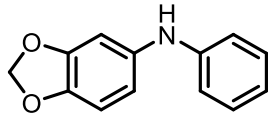
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.43 (d, *J* = 8.5 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.46-7.39 (m, 2H), 6.99 (s, 2H), 6.25 (d, *J* = 8.7 Hz, 1H), 5.68 (s, 1H), 2.34 (s, 3H), 2.16 (s, 6H).

N-phenylbenzo[d][1,3]dioxol-5-amine (6q)[27]

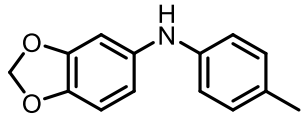
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.20 (m, 2H), 6.94 (d, *J* = 7.5 Hz, 2H), 6.87 (t, *J* = 7.3 Hz, 1H), 6.75 (d, *J* = 8.3 Hz, 1H), 6.70 (d, *J* = 2.2 Hz, 1H), 6.56 (dd, *J* = 8.3, 2.3 Hz, 1H), 5.94 (s, 2H), 5.53 (s, 1H).

N-(p-tolyl)benzo[d][1,3]dioxol-5-amine (6r)[28]

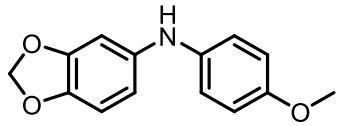
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, *J* = 7.8 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 6.72 (d, *J* = 8.3 Hz, 1H), 6.65 (d, *J* = 2.2 Hz, 1H), 6.50 (dd, *J* = 8.3, 2.3 Hz, 1H), 5.92 (s, 2H), 5.41 (s, 1H), 2.29 (s, 3H).

N-(4-methoxyphenyl)benzo[d][1,3]dioxol-5-amine (6s)[29]

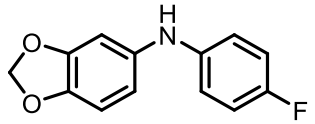
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.9 Hz, 2H), 6.83 (d, *J* = 8.9 Hz, 2H), 6.69 (d, *J* = 8.3 Hz, 1H), 6.56 (d, *J* = 2.3 Hz, 1H), 6.40 (d, *J* = 7.7 Hz, 1H), 5.90 (s, 2H), 3.79 (s, 3H).

N-(4-fluorophenyl)benzo[d][1,3]dioxol-5-amine (6t)[30]

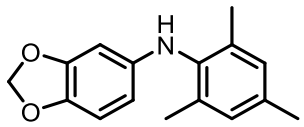
According to the general procedure, the corresponding final product was obtained as brown oil.



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96-6.87 (m, 4H), 6.72 (d, *J* = 8.3 Hz, 1H), 6.61 (d, *J* = 2.2 Hz, 1H), 6.47 (dd, *J* = 8.3, 2.3 Hz, 1H), 5.93 (s, 2H), 5.37 (s, 1H).

N-mesitylbenzo[d][1,3]dioxol-5-amine (6u)[31]

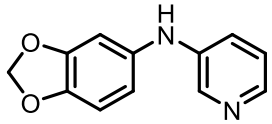
According to the general procedure, the corresponding final product was obtained as a white solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.93 (s, 2H), 6.62 (d, *J* = 8.3 Hz, 1H), 6.12 (d, *J* = 2.3 Hz, 1H), 5.95 (dd, *J* = 8.3, 2.3 Hz, 1H), 5.85 (s, 2H), 4.98 (s, 1H), 2.30 (s, 3H), 2.18 (s, 6H).

N-(benzo[d][1,3]dioxol-5-yl)pyridin-3-amine (6v)

According to the general procedure, the corresponding final product was obtained as a yellow solid.



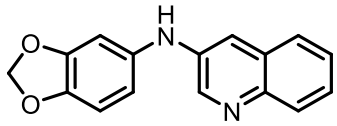
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 2.9 Hz, 1H, CH_{Ar}), 8.07 (dd, *J* = 4.7, 1.4 Hz, 1H, CH_{Ar}), 7.23 (ddd, *J* = 8.3, 2.8, 1.4 Hz, 1H, CH_{Ar}), 7.10 (dd, *J* = 8.3, 4.6 Hz, 1H, CH_{Ar}), 6.74 (d, *J* = 8.2 Hz, 1H, CH_{Ar}), 6.66 (d, *J* = 2.2 Hz, 1H, CH_{Ar}), 6.56 (dd, *J* = 8.2, 2.2 Hz, 1H, CH_{Ar}), 5.94 (s, 3H, NH and O-CH_2-O overlaped).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.48 (O-C_{Ar}), 143.68 (O-C_{Ar}), 141.53 (C_{Ar}), 140.84 (C_{Ar}), 138.74 (CH_{Ar}) , 136.04 (CH_{Ar}), 123.82 (CH_{Ar}), 121.83 (CH_{Ar}), 113.70 (CH_{Ar}), 108.77 (CH_{Ar}), 103.06 (O-CH_2-O), 101.33 (CH_{Ar}).

HRMS: Calcd. For $C_{12}H_{11}N_2O_2$ ($[M+H]^+$): 215.0815, Found: 215.0814

N-(benzo[d][1,3]dioxol-5-yl)quinolin-3-amine (6w)

According to the general procedure, the corresponding final product was obtained as a yellow solid.



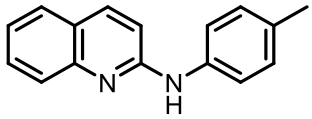
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 2.8 Hz, 1H, CH_{Ar}), 7.97 (d, *J* = 8.1 Hz, 1H, CH_{Ar}), 7.58 (d, *J* = 7.9 Hz, 1H, CH_{Ar}), 7.53-7.41 (m, 3H, CH_{Ar}), 6.83-6.74 (m, 2H, CH_{Ar}), 6.65 (dd, *J* = 8.2, 2.2 Hz, 1H, CH_{Ar}), 6.02 (s, 1H, NH), 5.97 (s, 2H, O-CH_2-O).

^{13}C NMR (126 MHz, $CDCl_3$) δ 148.57 (O-C_{Ar}), 144.33 (O-C_{Ar}), 143.90 (C_{Ar}), 143.26 (C_{Ar}), 138.72 (C_{Ar}), 135.88 (C_{Ar}), 129.10 (CH_{Ar}), 129.05 (CH_{Ar}), 127.20 (CH_{Ar}), 126.39 (CH_{Ar}), 126.16 (CH_{Ar}), 114.94 (CH_{Ar}), 113.91 (CH_{Ar}), 108.90 (CH_{Ar}), 103.17 (O-CH_2-O), 101.42 (CH_{Ar}).

HRMS: Calcd. For $C_{16}H_{13}N_2O_2$ ($[M+H]^+$): 265.0972, Found: 265.0970

N-(p-tolyl)quinolin-2-amine (6x)[32]

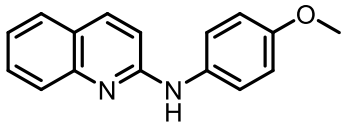
According to the general procedure, the corresponding final product was obtained as a pale-pink solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.9, 0.7 Hz, 1H), 7.77 (d, *J* = 8.3 Hz, 1H), 7.63 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.61-7.55 (m, 1H), 7.42 (d, *J* = 8.3 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.21-7.16 (m, 2H), 6.96 (d, *J* = 8.9 Hz, 1H), 6.90 (s, 1H), 2.36 (s, 3H).

N-(4-methoxyphenyl)quinolin-2-amine (6y)[33]

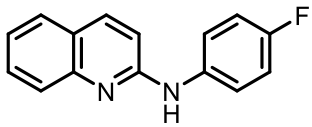
According to the general procedure, the corresponding final product was obtained as a light-yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 9.0, 0.8 Hz, 1H), 7.73 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.60-7.54 (m, 1H), 7.42 (d, *J* = 8.9 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 1H), 6.93 (d, *J* = 8.9 Hz, 2H), 6.87 (d, *J* = 8.9 Hz, 2H).

N-(4-fluorophenyl)quinolin-2-amine (6z)[33]

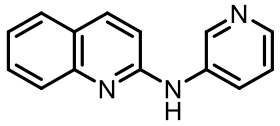
According to the general procedure, the corresponding final product was obtained as a light-yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.9, 0.8 Hz, 1H), 7.77 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.62-7.57 (m, 1H), 7.57-7.52 (m, 2H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.10-7.03 (m, 2H), 6.87 (d, *J* = 8.9 Hz, 2H).

N-(pyridin-3-yl)quinolin-2-amine (6aa)[2e]

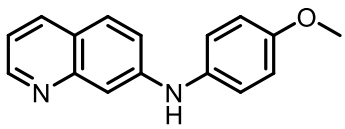
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (s, 1H), 8.43 (d, *J* = 4.3 Hz, 1H), 8.29 (s, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 7.3 Hz, 1H), 7.67 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.65 – 7.59 (m, 1H), 7.34 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 1H).

N-(4-methoxyphenyl)quinolin-7-amine (6ab)[34]

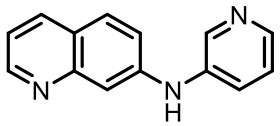
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79-8.70 (m, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.43 (d, *J* = 2.4 Hz, 1H), 7.19 (d, *J* = 8.8 Hz, 2H), 7.16-7.09 (m, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.02 (s, 1H), 3.81 (s, 3H).

N-(pyridin-3-yl)quinolin-7-amine (6ac)

According to the general procedure, the corresponding final product was obtained as a yellow solid.



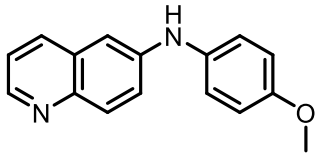
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.2 Hz, 1H, CH_{Ar}), 8.43 (s, 1H, NH), 8.16 (d, *J* = 4.7 Hz, 1H, CH_{Ar}), 7.96 (d, *J* = 8.1 Hz, 1H, CH_{Ar}), 7.69-7.54 (m, 4H, CH_{Ar}), 7.24 (dd, *J* = 8.8, 2.4 Hz, 1H, CH_{Ar}), 7.15 (dd, *J* = 8.1, 4.3 Hz, 1H, CH_{Ar}), 7.09 (dd, *J* = 8.3, 4.6 Hz, 1H, CH_{Ar}).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.77 (CH_{Ar}), 149.66 (C_{Ar}), 144.20 (C_{Ar}), 142.78 (C_{Ar}), 141.41 (CH_{Ar}), 138.86 (C_{Ar}), 135.82 (CH_{Ar}), 129.15 (CH_{Ar}), 125.21 (CH_{Ar}), 123.84 (CH_{Ar}), 123.69 (CH_{Ar}), 119.81 (CH_{Ar}), 118.78 (CH_{Ar}), 110.91 (CH_{Ar}).

HRMS: Calcd. For $C_{14}H_{12}N_3$ ($[M+H]^+$): 222.1026, Found: 265.1024

N-(4-methoxyphenyl)quinolin-6-amine (6ad)[11]

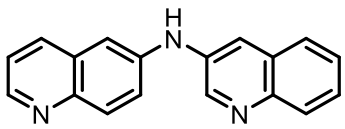
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (dd, *J* = 4.2, 1.6 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.32 (dd, *J* = 9.0, 2.6 Hz, 1H), 7.29-7.26 (m, 1H), 7.20 (d, *J* = 8.6 Hz, 2H), 7.11 (d, *J* = 2.6 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 2H), 5.90 (s, 1H), 3.85 (s, 3H).

N-(quinolin-6-yl)quinolin-3-amine (6ae)

According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (500 MHz, DMSO-d_6) δ 9.11 (s, 1H, NH_{Ar}), 8.84 (d, *J* = 2.8 Hz, 1H, CH_{Ar}), 8.69 (d, *J* = 2.5 Hz, 1H, CH_{Ar}), 8.23 (dd, *J* = 8.3, 1.7 Hz, 1H, CH_{Ar}), 8.11 (d, *J* = 2.8 Hz, 1H, CH_{Ar}),

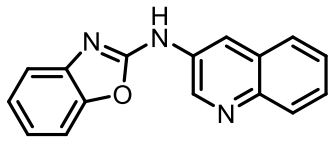
7.97 (d, J = 9.0 Hz, 1H, CH_{Ar}), 7.95-7.90 (m, 1H, CH_{Ar}), 7.90-7.84 (m, 1H, CH_{Ar}), 7.73 (d, J = 2.7 Hz, 1H, CH_{Ar}), 7.64 (d, J = 9.0 Hz, 1H, CH_{Ar}), 7.56-7.50 (m, 2H, CH_{Ar}), 7.43 (dd, J = 8.3, 4.2 Hz, 1H, CH_{Ar}).

^{13}C NMR (126 MHz, DMSO-d_6) δ 147.59 (C_{Ar}), 145.45 (C_{Ar}), 143.86 (C_{Ar}), 142.88 (C_{Ar}), 140.66 (CH_{Ar}), 136.64 (CH_{Ar}), 134.50 (C_{Ar}), 130.20 (CH_{Ar}), 129.27 (CH_{Ar}), 128.64 (CH_{Ar}), 128.50 (CH_{Ar}), 126.90 (CH_{Ar}), 126.25 (C_{Ar}), 123.34 (CH_{Ar}), 121.69 (CH_{Ar}), 115.94 (CH_{Ar}), 109.18 (CH_{Ar}).

HRMS: Calcd. For $C_{18}H_{14}N_3$ ($[M+H]^+$): 272.1182, Found: 272.1178

N-(quinolin-3-yl)benzo[d]oxazol-2-amine (6af)

According to the general procedure, the corresponding final product was obtained as a pale-white solid.



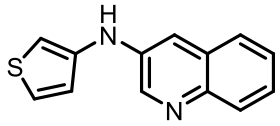
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.19 (s, 1H, NH_{Ar}), 9.02 (d, J = 2.6 Hz, 1H, CH_{Ar}), 8.87 (d, J = 2.7 Hz, 1H, CH_{Ar}), 7.98 (d, J = 9.4 Hz, 2H, CH_{Ar}), 7.68-7.52 (m, 4H, CH_{Ar}), 7.28 (t, J = 7.4 Hz, 1H, CH_{Ar}), 7.22-7.16 (m, 1H, CH_{Ar}).

^{13}C NMR (126 MHz, DMSO-d_6) δ 157.67 (C_{Ar}), 147.18 (C_{Ar}), 143.71 (C_{Ar}), 143.60 (C_{Ar}), 142.10 (CH_{Ar}), 132.70 (C_{Ar}), 128.64 (CH_{Ar}), 128.01 (CH_{Ar}), 127.44 (CH_{Ar}), 127.35 (CH_{Ar}), 127.29 (CH_{Ar}), 124.23 (CH_{Ar}), 122.18 (CH_{Ar}), 119.11(C_{Ar}), 117.03 (CH_{Ar}), 109.23 (CH_{Ar}).

HRMS: Calcd. For $C_{16}H_{12}N_3O$ ($[M+H]^+$): 262.0975, Found: 262.0974

N-(thiophen-3-yl)quinolin-3-amine (6ag)

According to the general procedure, the corresponding final product was obtained as a yellow solid.



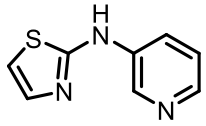
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, J = 2.9 Hz, 1H, CH_{Ar}), 7.99 (d, J = 7.0 Hz, 1H, CH_{Ar}), 7.67-7.56 (m, 2H, CH_{Ar}), 7.52-7.41 (m, 2H, CH_{Ar}), 7.33 (dd, J = 5.1, 3.1 Hz, 1H, CH_{Ar}), 7.00 (d, J = 5.1 Hz, 1H, CH_{Ar}), 6.90 (s, 1H, CH_{Ar}), 6.28 (s, 1H, NH).

^{13}C NMR (126 MHz, $CDCl_3$) δ 143.86 (C_{Ar}), 143.24 (C_{Ar}), 140.23 (C_{Ar}), 138.42 (C_{Ar}), 129.14 (CH_{Ar}), 129.10 (CH_{Ar}), 127.30 (CH_{Ar}), 126.45 (CH_{Ar}), 126.23 (CH_{Ar}), 125.92 (CH_{Ar}), 122.84 (C_{Ar}), 114.55 (CH_{Ar}), 108.27 (CH_{Ar}).

HRMS: Calcd. For $C_{13}H_{11}N_2S$ ($[M+H]^+$): 227.0637, Found: 227.0636

N-(pyridin-3-yl)thiazol-2-amine (6ah)[2e]

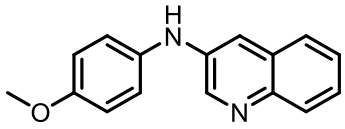
According to the general procedure, the corresponding final product was obtained as a light-yellow solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 2.8 Hz, 1H), 8.36-8.26 (m, 1H), 8.02 (ddd, *J* = 8.4, 2.9, 1.4 Hz, 1H), 7.38-7.28 (m, 2H), 6.71 (d, *J* = 3.6 Hz, 1H).

N-(4-methoxyphenyl)quinolin-3-amine (6ai)[35]

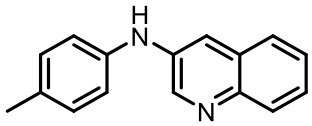
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (d, *J* = 2.8 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 7.5 Hz, 1H), 7.51-7.40 (m, 3H), 7.17 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.9 Hz, 2H), 5.92 (s, 1H), 3.83 (s, 3H).

N-(p-tolyl)quinolin-3-amine (6aj)[35]

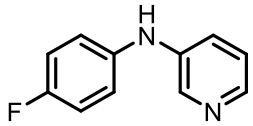
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.66 (d, *J* = 2.9 Hz, 1H), 7.99 (d, *J* = 8.1 Hz, 1H), 7.65-7.58 (m, 2H), 7.51-7.42 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.2 Hz, 2H), 6.03 (s, 1H), 2.35 (s, 3H).

N-(4-fluorophenyl)pyridin-3-amine (6ak)[11]

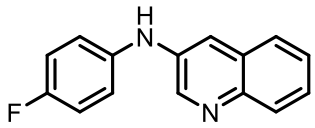
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 2.9 Hz, 1H), 8.12 (dd, *J* = 4.8, 1.4 Hz, 1H), 7.29 (ddd, *J* = 8.3, 2.8, 1.4 Hz, 1H), 7.14 (dd, *J* = 8.3, 4.7 Hz, 1H), 7.06 (dt, *J* = 7.1, 2.6 Hz, 2H), 7.03-6.96 (m, 2H), 5.91 (s, 1H).

N-(4-fluorophenyl)quinolin-3-amine (6al)[36]

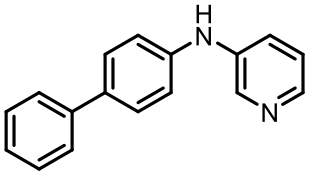
According to the general procedure, the corresponding final product was obtained as a light-brown solid.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (d, *J* = 2.8 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.64-7.55 (m, 2H), 7.48 (dddd, *J* = 21.0, 8.2, 6.9, 1.5 Hz, 2H), 7.16 (dd, *J* = 8.9, 4.6 Hz, 2H), 7.06 (t, *J* = 8.6 Hz, 2H), 6.04 (s, 1H).

N-([1,1'-biphenyl]-4-yl)pyridin-3-amine (6am)

According to the general procedure, the corresponding final product was obtained as a light-yellow solid.



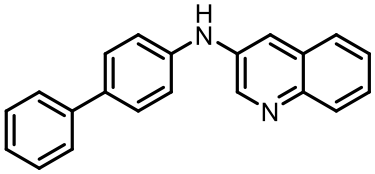
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 2.8 Hz, 1H, CH_{Ar}), 8.18 (dd, *J* = 4.7, 1.4 Hz, 1H, CH_{Ar}), 7.60-7.52 (m, 4H, CH_{Ar}), 7.49 (dd, *J* = 2.8, 1.4 Hz, 1H, CH_{Ar}), 7.43 (t, *J* = 7.6 Hz, 2H, CH_{Ar}), 7.32 (t, *J* = 7.3 Hz, 1H, CH_{Ar}), 7.21 (ddd, *J* = 8.4, 4.7, 0.7 Hz, 1H, CH_{Ar}), 7.16 (d, *J* = 8.6 Hz, 2H, CH_{Ar}), 5.91 (s, 1H, NH).

^{13}C NMR (126 MHz, $CDCl_3$) δ 142.37 (CH_{Ar}), 141.53 (C_{Ar}), 140.80 (C_{Ar}), 140.57 (C_{Ar}), 139.79 (CH_{Ar}), 135.12 (C_{Ar}), 129.00 (CH_{Ar}), 128.40 (CH_{Ar}), 127.06 (CH_{Ar}), 126.83 (CH_{Ar}), 123.97 (CH_{Ar}), 123.95 (CH_{Ar}), 118.58 (CH_{Ar}).

HRMS: Calcd. For $C_{17}H_{14}N_2Na$ ($[M+H]^+$): 269.1049, Found: 269.1057

N-([1,1'-biphenyl]-4-yl)quinolin-3-amine (6an)

According to the general procedure, the corresponding final product was obtained as a light-yellow solid.



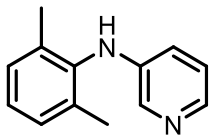
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 2.8 Hz, 1H, CH_{Ar}), 8.04 (d, *J* = 8.2 Hz, 1H, CH_{Ar}), 7.80 (s, 1H, CH_{Ar}), 7.68 (d, *J* = 8.0 Hz, 1H, CH_{Ar}), 7.65-7.57 (m, 4H, CH_{Ar}), 7.57-7.53 (m, 1H, CH_{Ar}), 7.50 (d, *J* = 7.6 Hz, 1H, CH_{Ar}), 7.46 (t, *J* = 7.6 Hz, 2H, CH_{Ar}), 7.34 (t, *J* = 7.4 Hz, 1H, CH_{Ar}), 7.27 (d, *J* = 3.5 Hz, 2H, CH_{Ar}), 6.08 (s, 1H, NH).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.24 (C_{Ar}), 143.87 (C_{Ar}), 141.35 (C_{Ar}), 140.71 (C_{Ar}), 136.94 (C_{Ar}), 135.34 (C_{Ar}), 129.22 (CH_{Ar}), 128.96 (CH_{Ar}), 128.41 (CH_{Ar}), 127.36 (CH_{Ar}), 127.06 (CH_{Ar}), 126.81 (CH_{Ar}), 126.79 (CH_{Ar}), 126.64 (CH_{Ar}), 118.79 (CH_{Ar}), 117.54 (CH_{Ar}).

HRMS: Calcd. For $C_{21}H_{17}N_2$ ($[M+H]^+$): 297.1386, Found: 297.1384

N-(2,6-dimethylphenyl)pyridin-3-amine (6ao)[9]

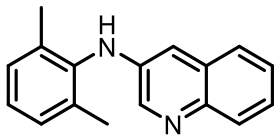
According to the general procedure, the corresponding final product was obtained as a yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 2.9 Hz, 1H), 7.92 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.09-7.01 (m, 3H), 6.96 (dd, *J* = 8.3, 4.7 Hz, 1H), 6.57 (ddd, *J* = 8.3, 2.9, 1.4 Hz, 1H), 5.23 (s, 1H), 2.13 (s, 6H).

N-(2,6-dimethylphenyl)quinolin-3-amine (6ap)

According to the general procedure, the corresponding final product was obtained as a gray solid.



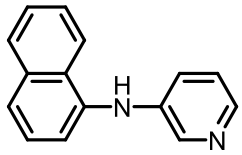
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 2.8 Hz, 1H, CH_{Ar}), 7.98 (d, *J* = 8.1 Hz, 1H, CH_{Ar}), 7.49 (dd, *J* = 7.9, 1.7 Hz, 1H, CH_{Ar}), 7.40 (dddd, *J* = 18.9, 8.1, 6.9, 1.6 Hz, 2H, CH_{Ar}), 7.19 (d, *J* = 2.1 Hz, 3H, CH_{Ar}), 6.70 (d, *J* = 2.8 Hz, 1H, CH_{Ar}), 5.60 (s, 1H, NH), 2.25 (s, 6H, CH_3).

^{13}C NMR (126 MHz, $CDCl_3$) δ 143.10 (C_{Ar}), 142.73 (C_{Ar}), 139.87 (C_{Ar}), 136.93 (C_{Ar}), 136.08 (C_{Ar}), 129.45 (C_{Ar}), 129.11(CH_{Ar}), 128.96 (CH_{Ar}), 127.05 (CH_{Ar}), 126.68 (CH_{Ar}), 126.14 (CH_{Ar}), 125.42 (CH_{Ar}), 111.94 (CH_{Ar}), 18.40 (CH_3).

HRMS: Calcd. For $C_{17}H_{17}N_2$ ($[M+H]^+$): 249.1386, Found: 249.1385

N-(naphthalen-1-yl)pyridin-3-amine (6aq)[8]

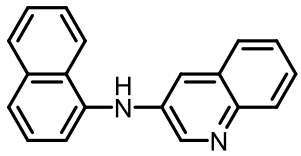
According to the general procedure, the corresponding final product was obtained as a light-brown solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 2.8, 0.8 Hz, 1H), 8.14 (dd, *J* = 4.6, 1.5 Hz, 1H), 8.00 (d, *J* = 9.2 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.54-7.46 (m, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.35 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.20 (ddd, *J* = 8.3, 2.8, 1.4 Hz, 1H), 7.12 (ddd, *J* = 8.3, 4.6, 0.8 Hz, 1H), 6.11 (s, 1H).

N-(naphthalen-1-yl)quinolin-3-amine (6ar)

According to the general procedure, the corresponding final product was obtained as a brown solid.



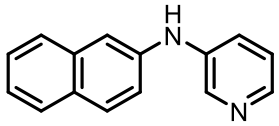
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 2.8 Hz, 1H, CH_{Ar}), 8.03 (d, *J* = 7.1 Hz, 2H, CH_{Ar}), 7.96-7.88 (m, 1H, CH_{Ar}), 7.69 (dd, *J* = 7.8, 1.7 Hz, 1H, CH_{Ar}), 7.58-7.40 (m, 7H, CH_{Ar}), 7.37 (d, *J* = 2.7 Hz, 1H, CH_{Ar}), 6.28 (s, 1H, NH).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.58 (C_{Ar}), 143.44 (C_{Ar}), 138.97 (C_{Ar}), 137.47 (C_{Ar}), 134.82 (C_{Ar}), 129.07 (C_{Ar}), 129.01(CH_{Ar}), 128.72 (CH_{Ar}), 128.19 (CH_{Ar}), 127.10 (CH_{Ar}), 126.46 (CH_{Ar}), 126.40 (CH_{Ar}), 126.30 (CH_{Ar}), 126.20 (CH_{Ar}), 126.04 (CH_{Ar}), 124.58, 121.97 (CH_{Ar}), 117.64 (CH_{Ar}), 116.62 (CH_{Ar}).

HRMS: Calcd. For $C_{19}H_{15}N_2$ ($[M+H]^+$): 271.1230, Found: 271.1124

N-(naphthalen-2-yl)pyridin-3-amine (6as)[37]

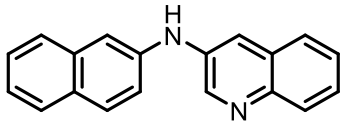
According to the general procedure, the corresponding final product was obtained as a brown solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 2.8 Hz, 1H), 8.21 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.82-7.74 (m, 2H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.51 (ddd, *J* = 8.3, 2.8, 1.4 Hz, 1H), 7.48-7.41 (m, 2H), 7.35 (t, *J* = 6.9 Hz, 1H), 7.25-7.20 (m, 2H), 5.99 (s, 1H).

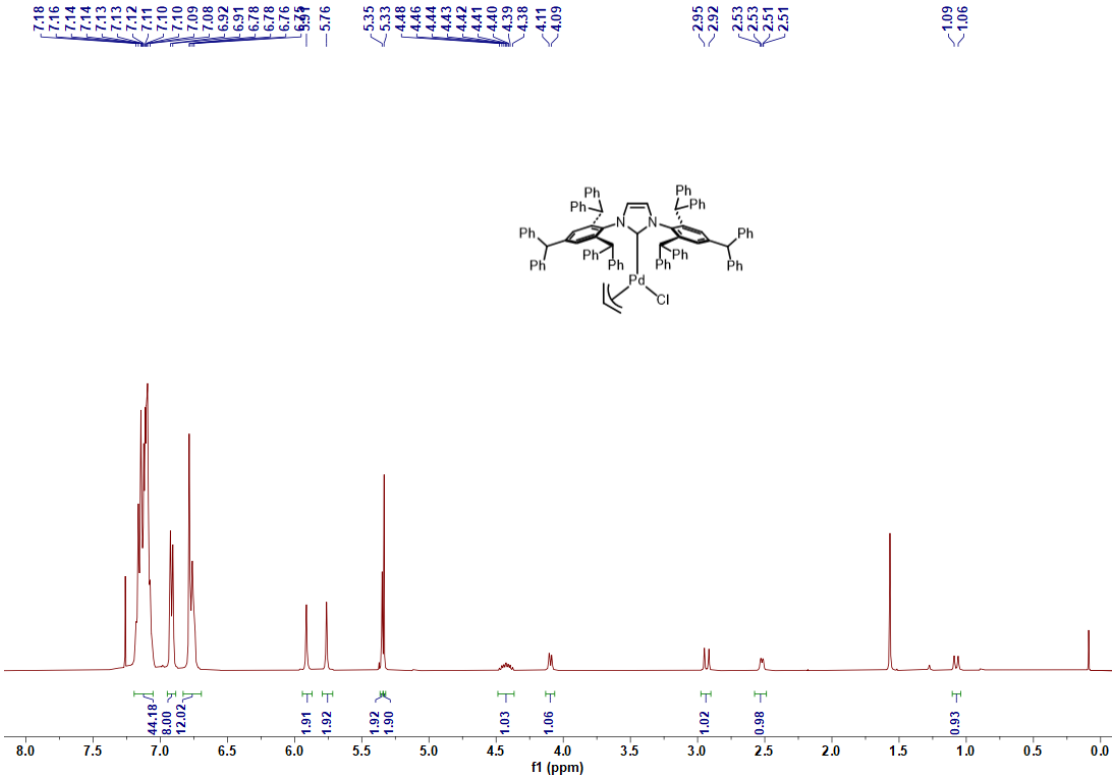
N-(naphthalen-2-yl)quinolin-3-amine (6at)[35]

According to the general procedure, the corresponding final product was obtained as a light-brown solid.

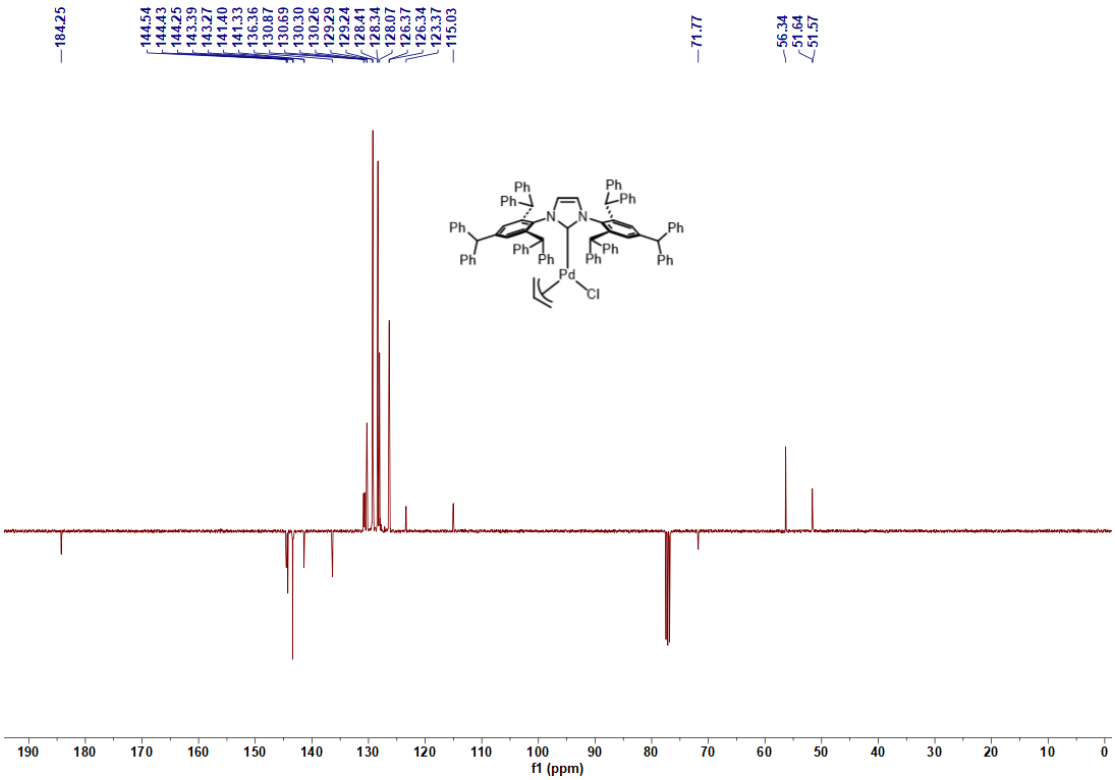


^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 (d, *J* = 2.7 Hz, 1H), 8.05 (d, *J* = 8.3 Hz, 1H), 7.81 (t, *J* = 10.3 Hz, 3H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.66 (d, *J* = 6.6 Hz, 1H), 7.58-7.52 (m, 2H), 7.51-7.43 (m, 2H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.31 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.28 (s, 1H).

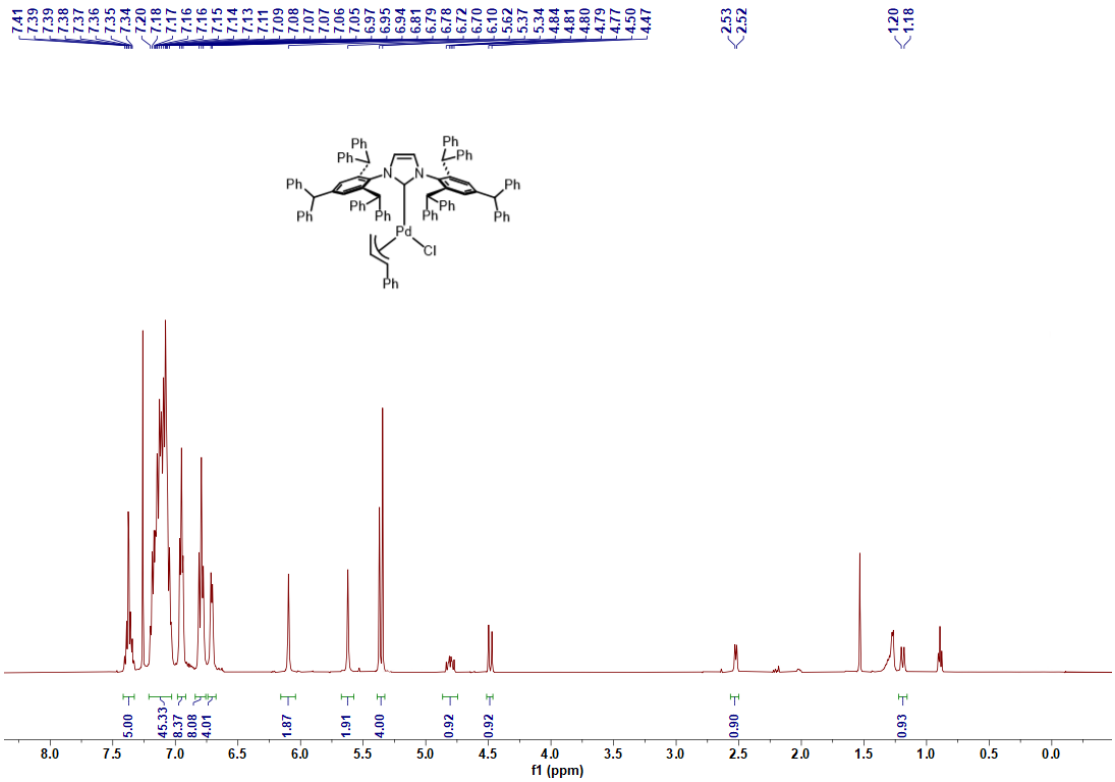
^{1}H NMR and ^{13}C NMR spectrums



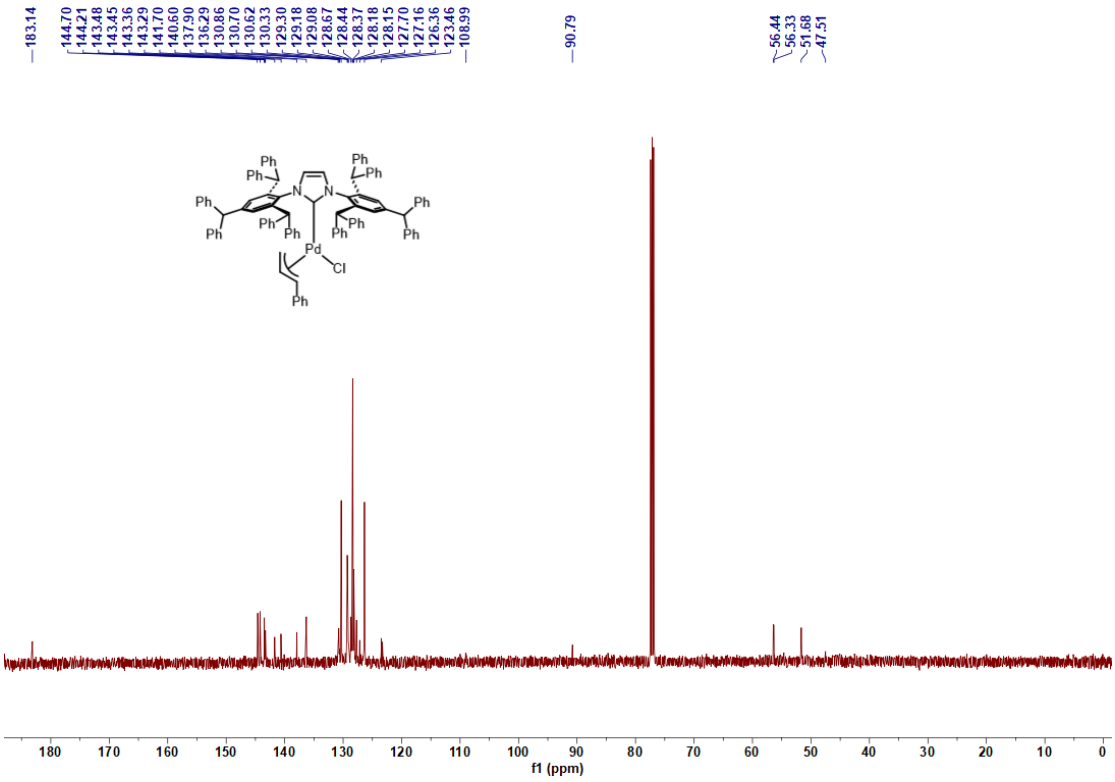
^{1}H NMR spectrum of Pd(IPr$^{\#}$)Cl(allyl)



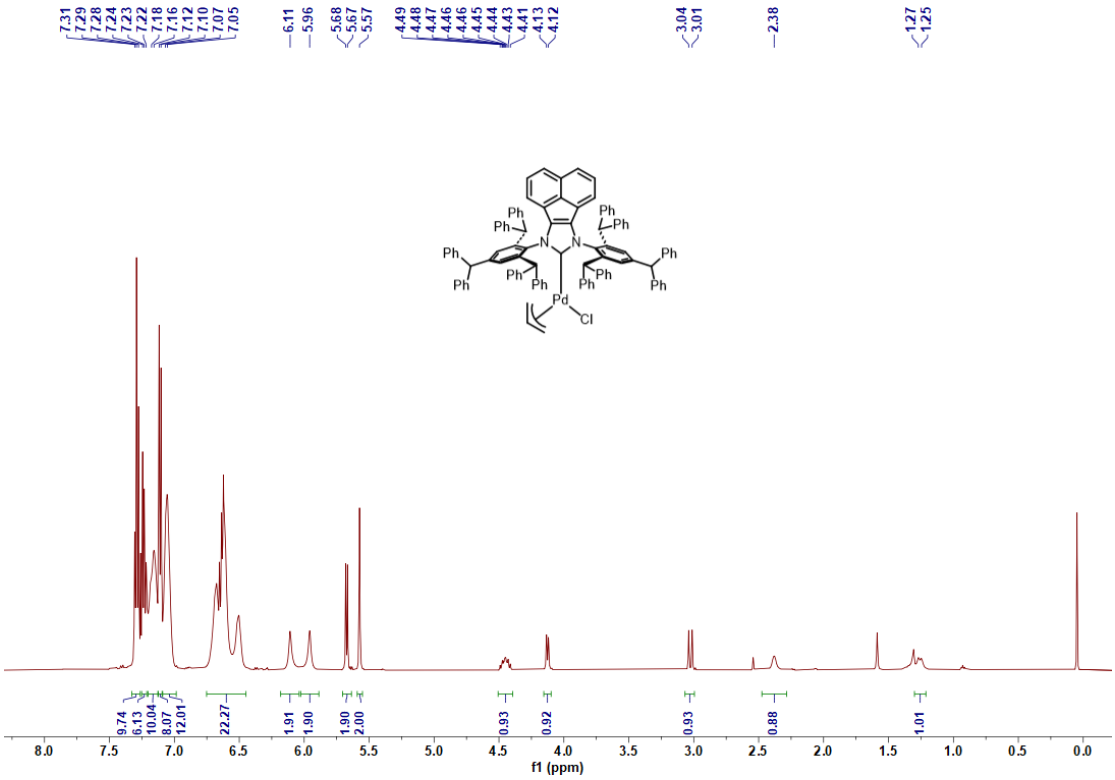
^{13}C NMR spectrum of Pd(IPr$^{\#}$)Cl(allyl)



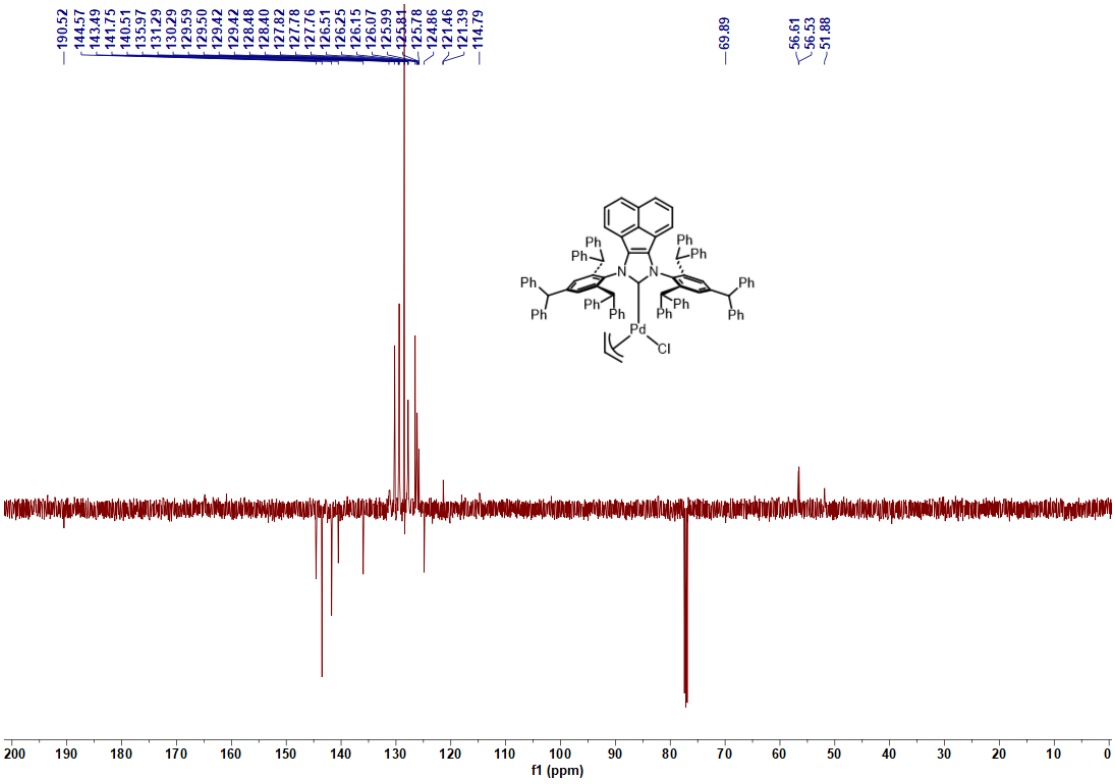
^{1}H NMR spectrum of Pd(IPr$^{\#}$)Cl(cin)



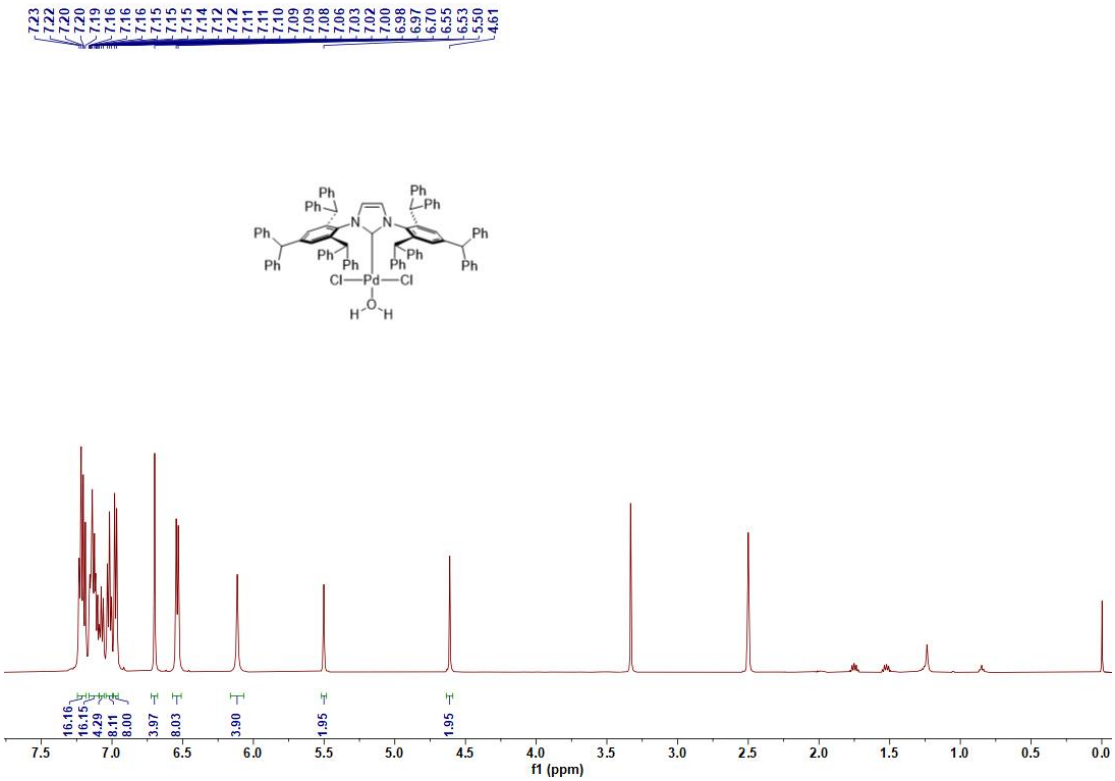
^{13}C NMR spectrum of Pd(IPr$^{\#}$)Cl(cin)



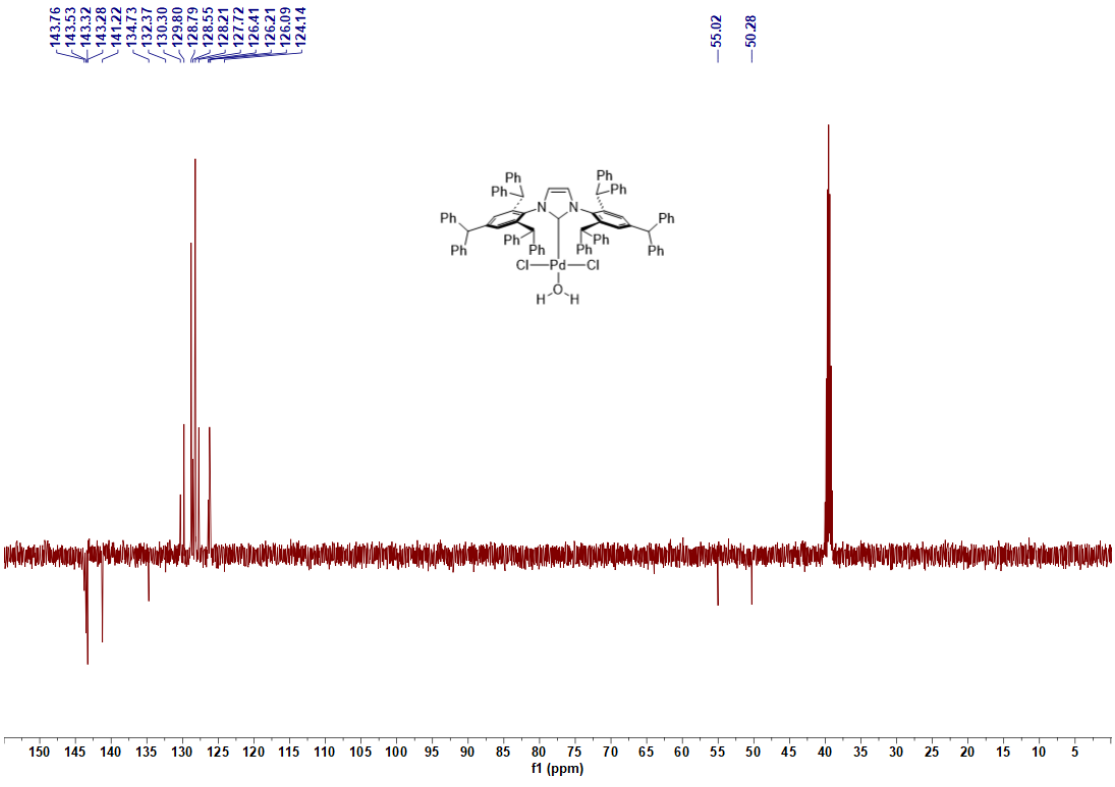
^{1}H NMR spectrum of Pd(BIAN-IPr$^{\#}$)Cl(allyl)



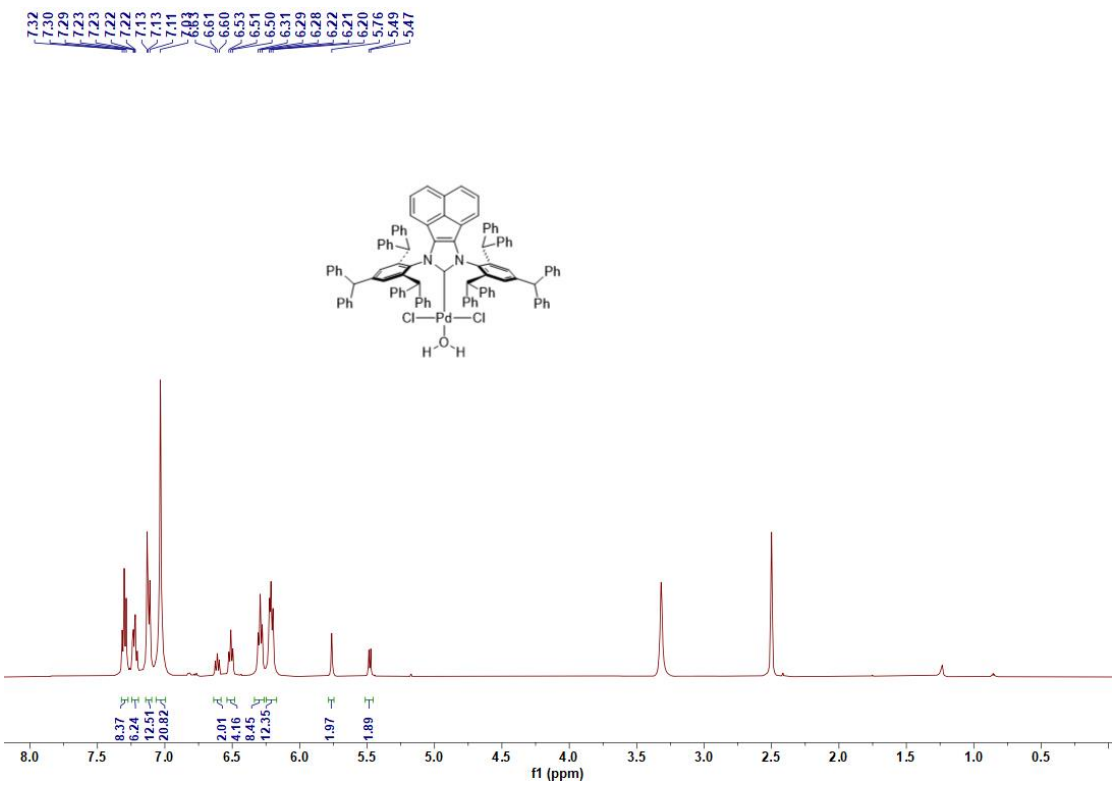
^{13}C NMR spectrum of Pd(BIAN-IPr$^{\#}$)Cl(allyl)



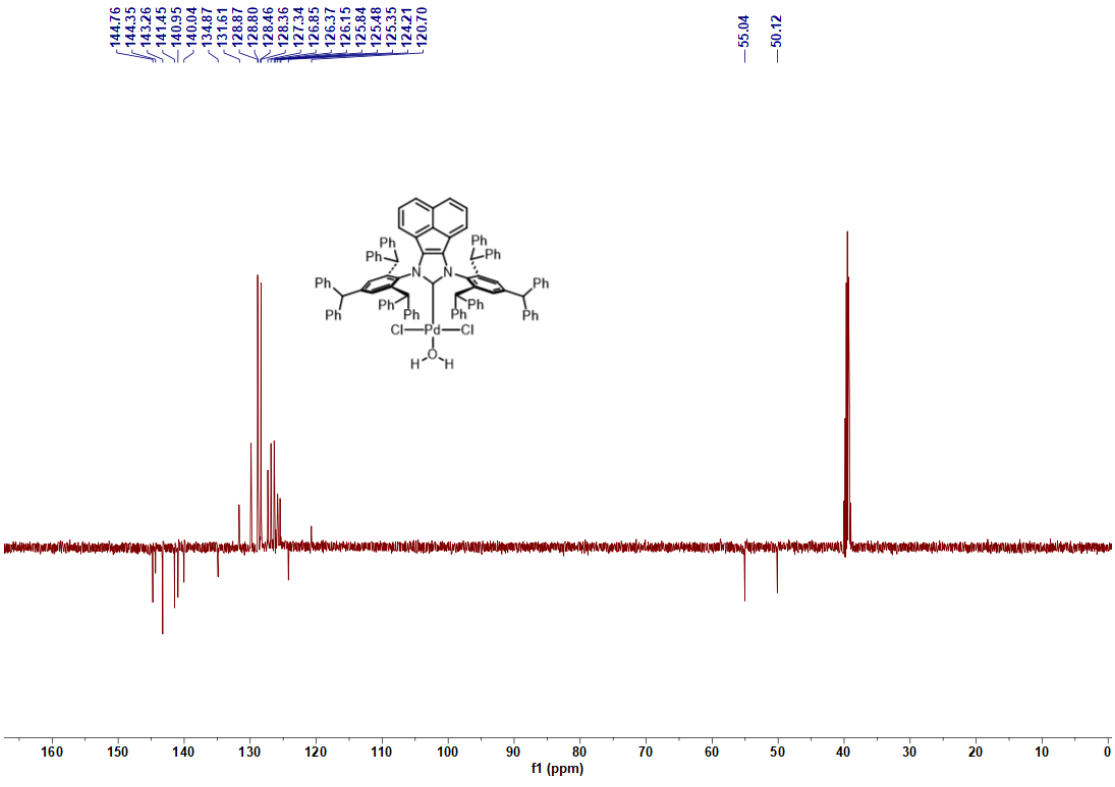
^{1}H NMR spectrum of Pd(IPr$^{\#}$)Cl$_2$(OH$_2$)

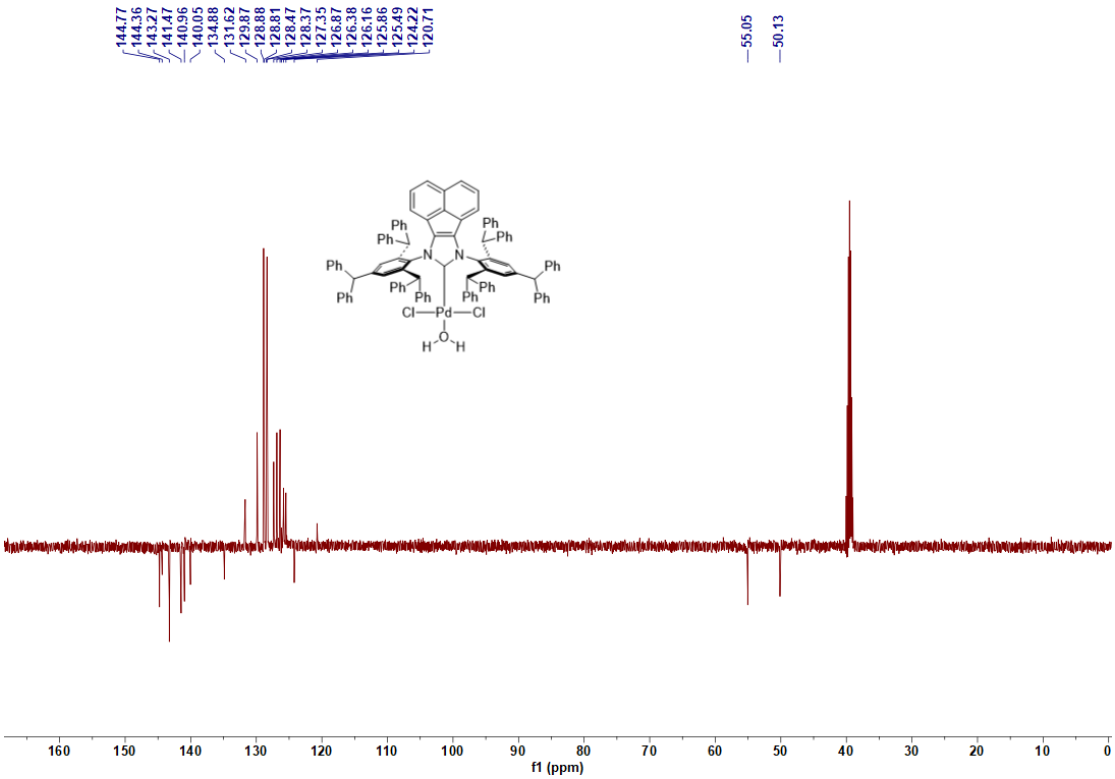


^{13}C NMR spectrum of Pd(IPr$^{\#}$)Cl$_2$(OH$_2$)

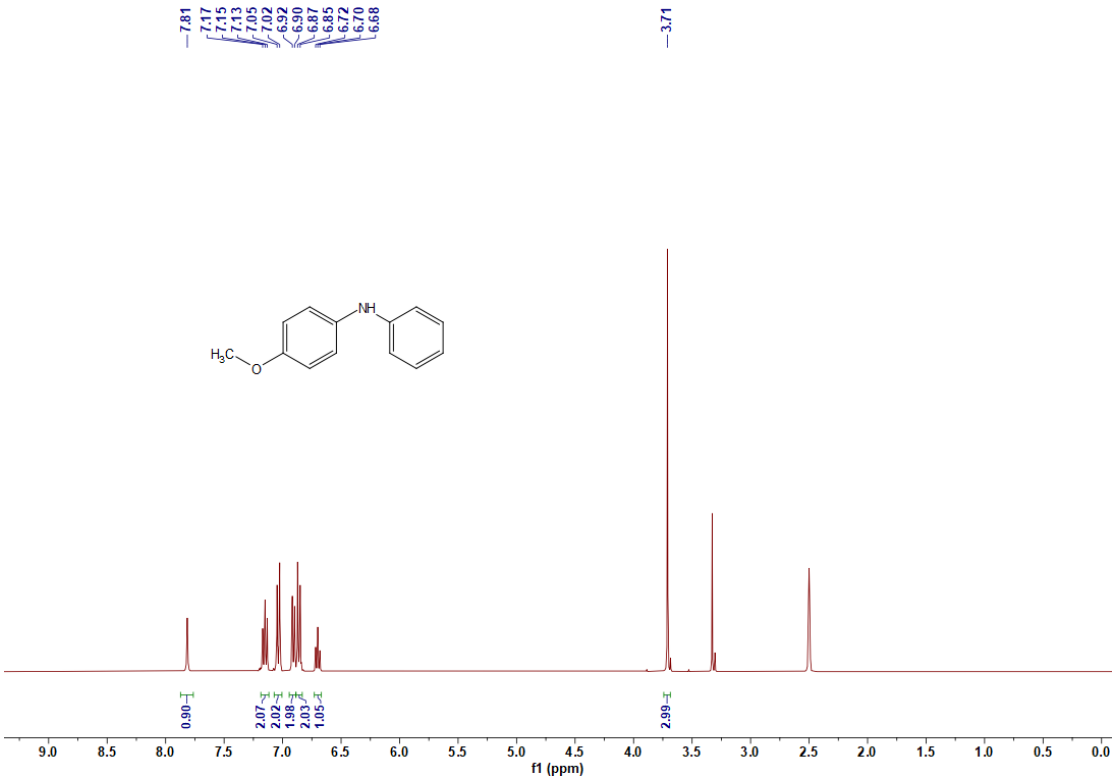


^{1}H NMR spectrum of Pd(BIAN-IPr$^{\#}$)Cl$_2$(OH$_2$)

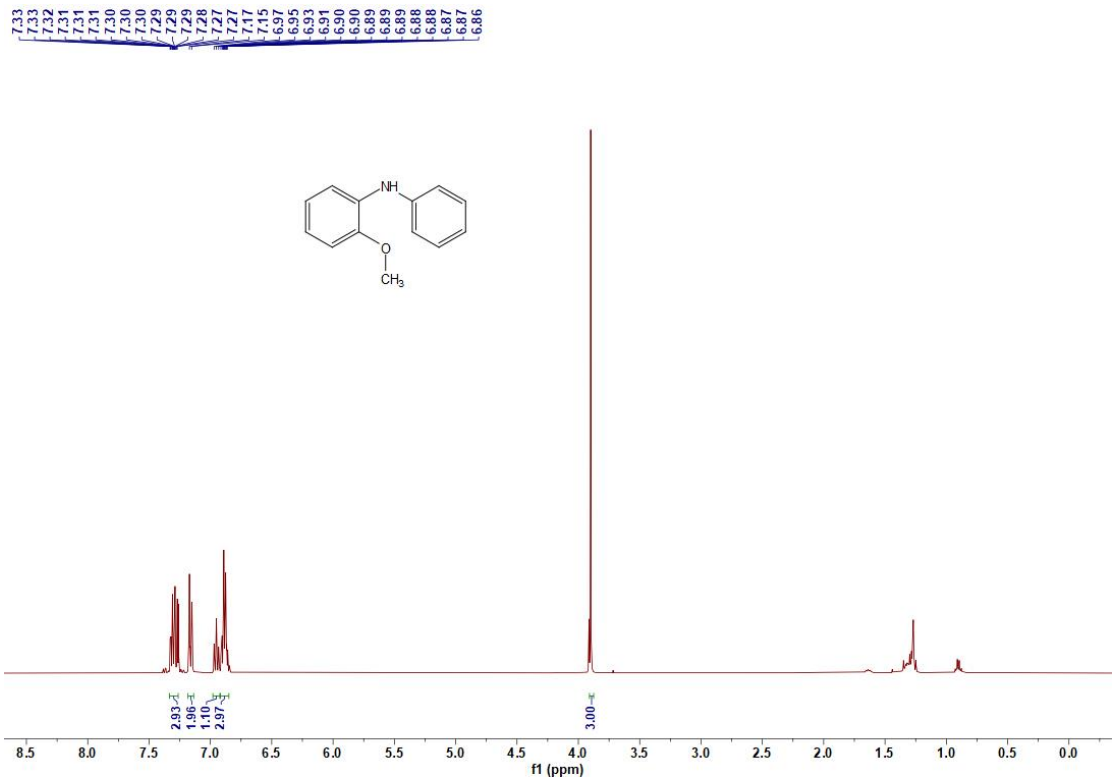




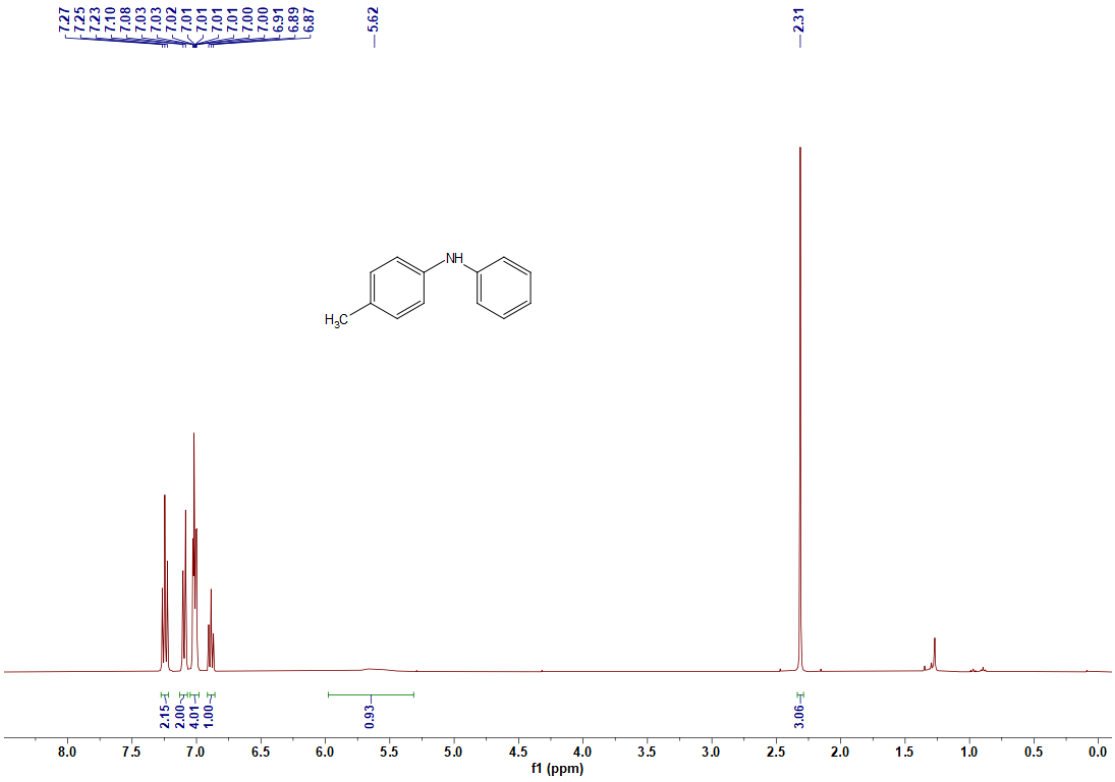
^{13}C NMR spectrum of Pd(BIAN-IPr$^{\#}$)$Cl_2(OH_2)$



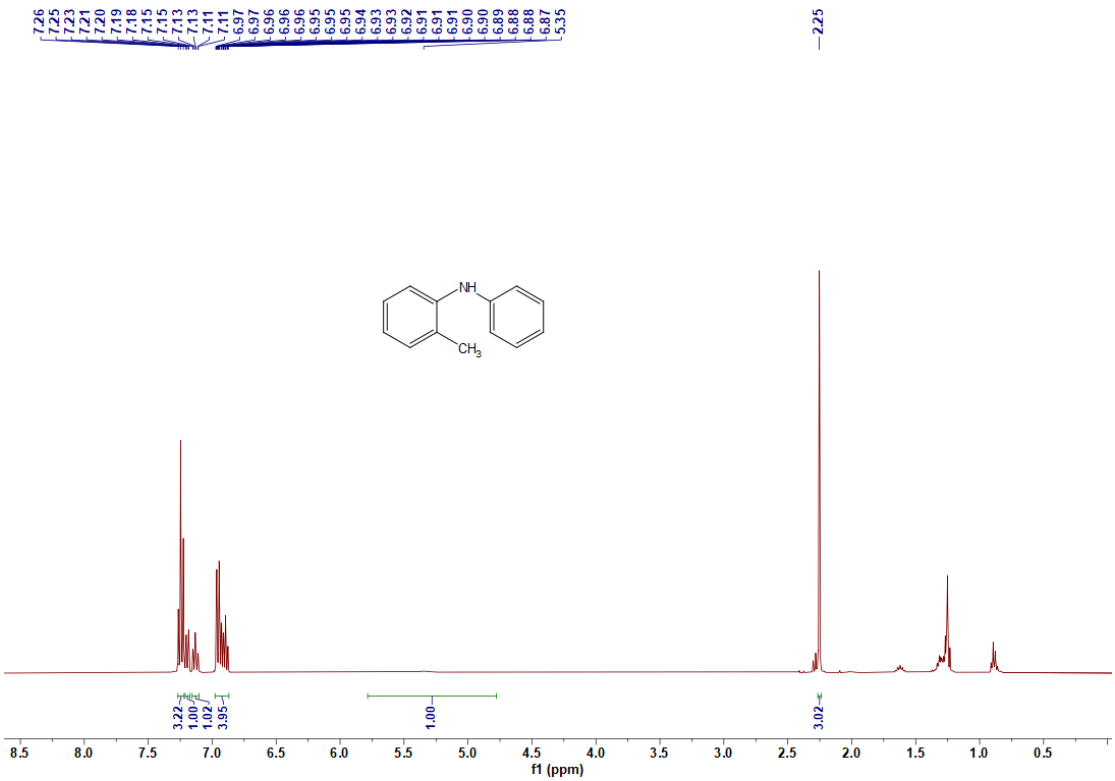
^{1}H NMR spectrum of 2a



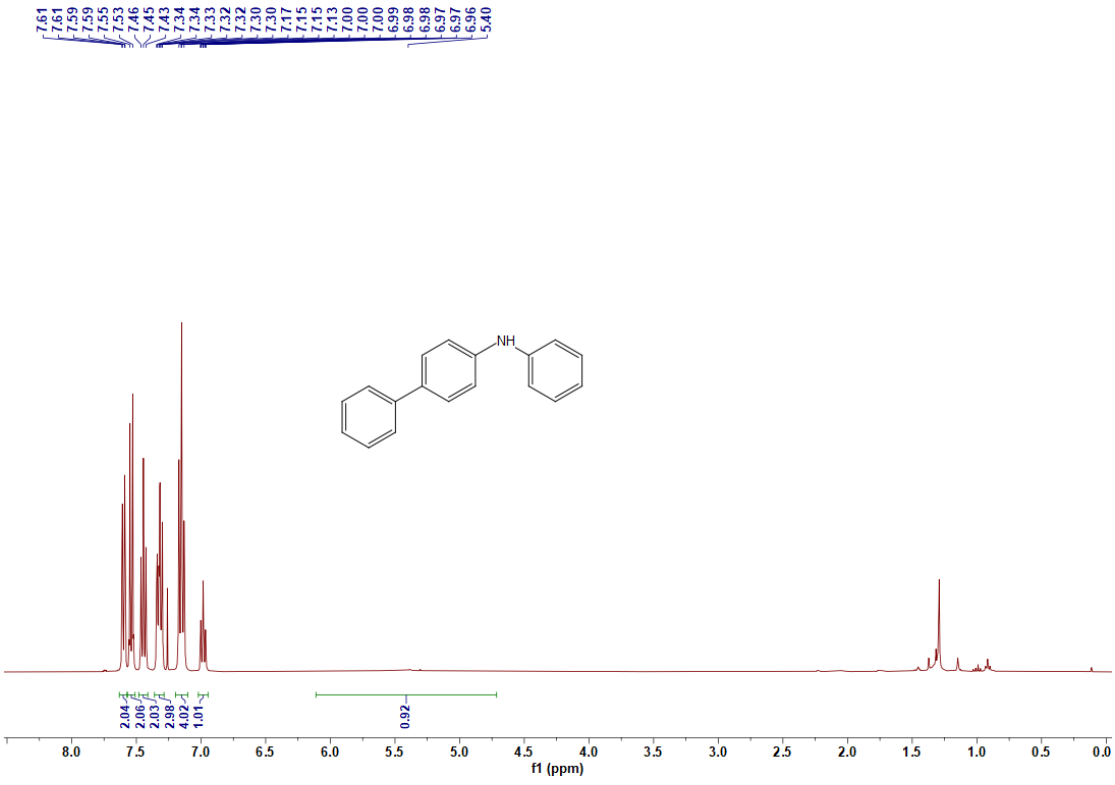
^{1}H NMR spectrum of 2b



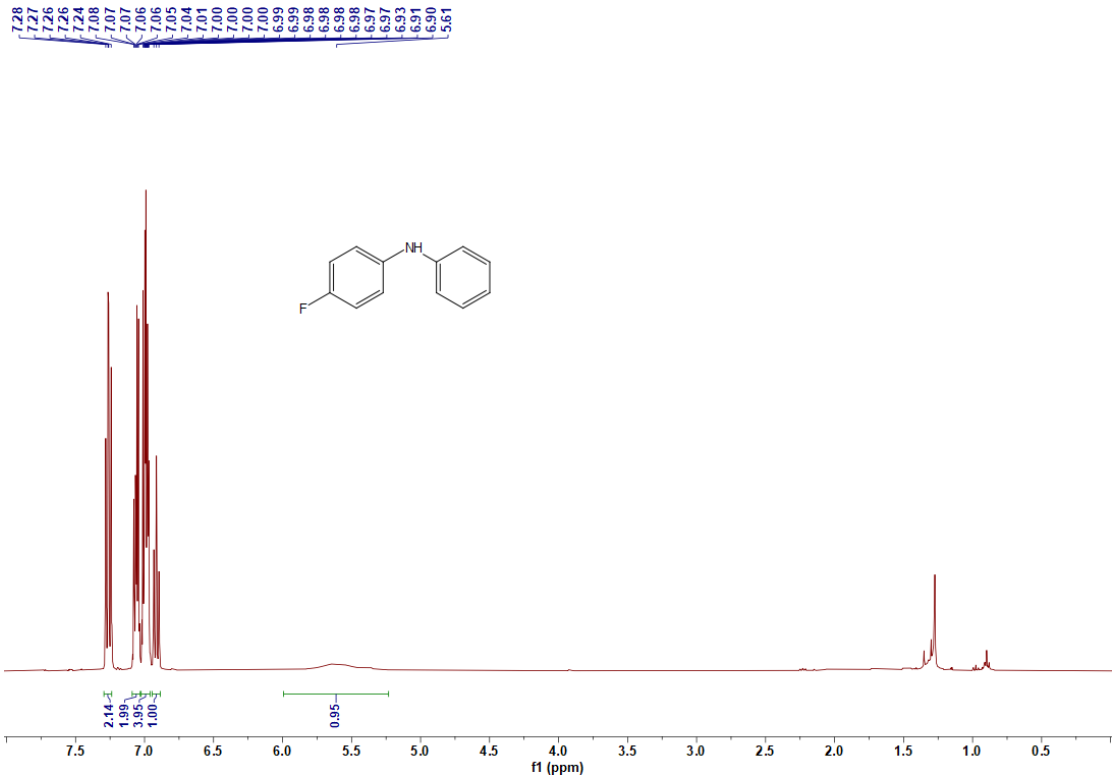
^{1}H NMR spectrum of 2c



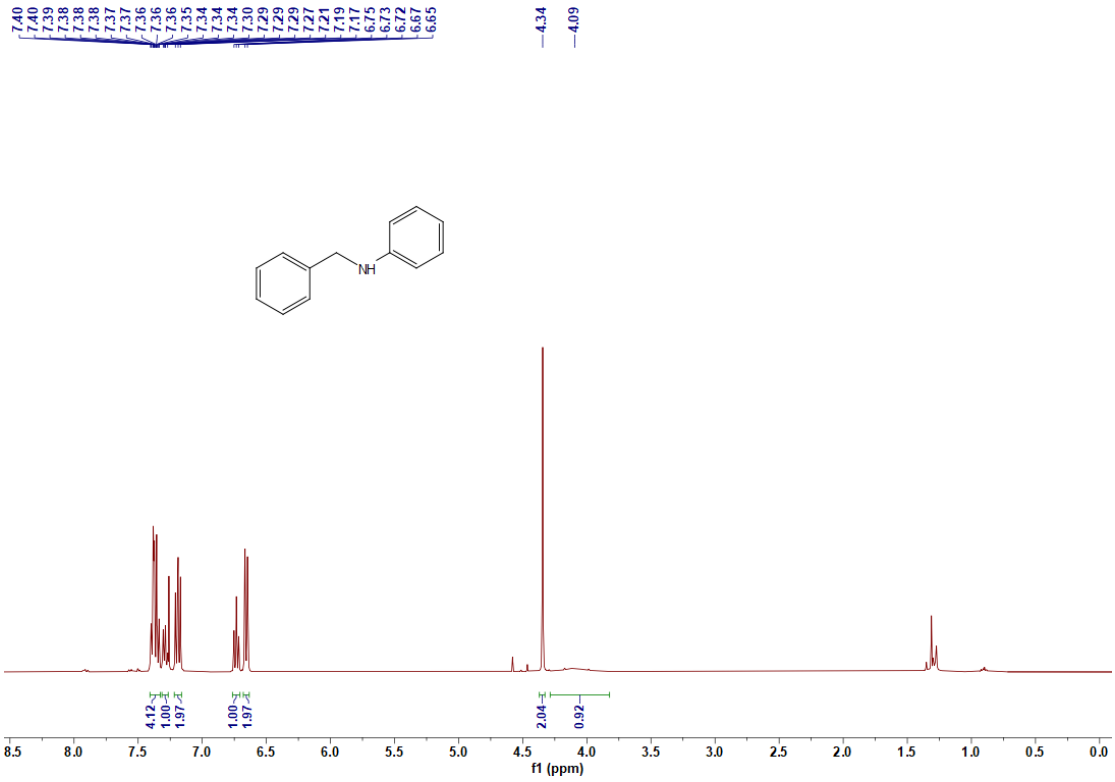
^{1}H NMR spectrum of 2d



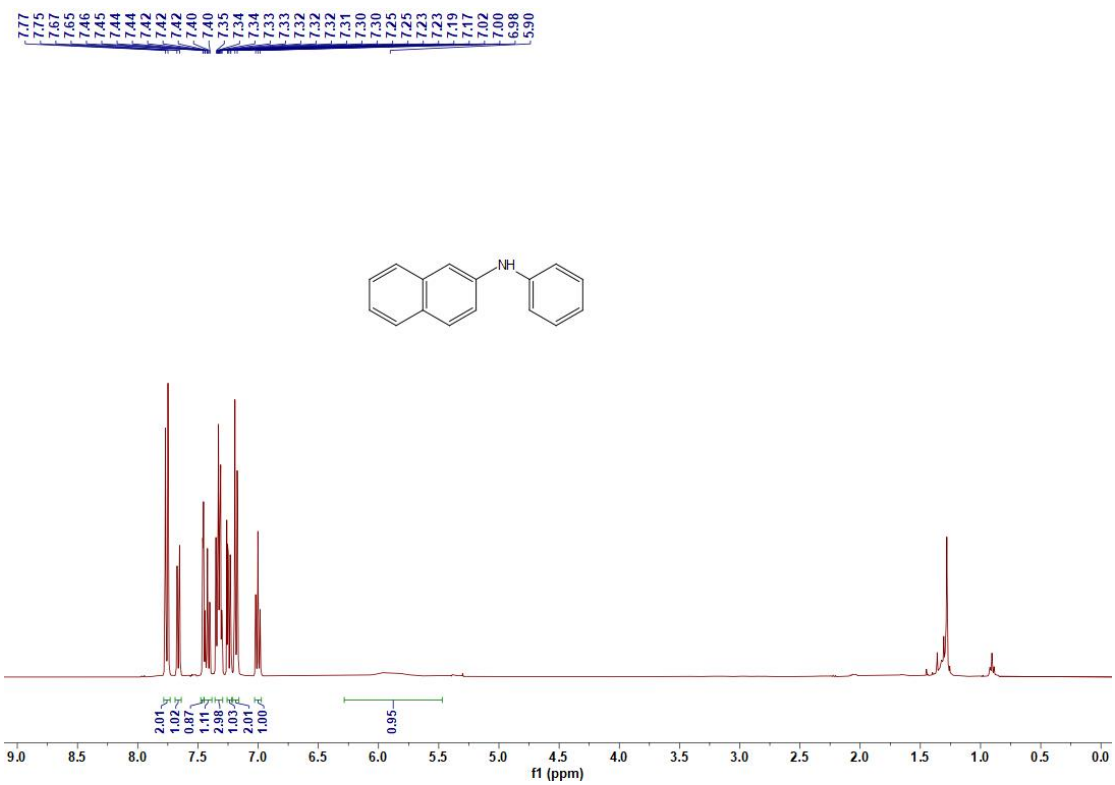
^{1}H NMR spectrum of 2e



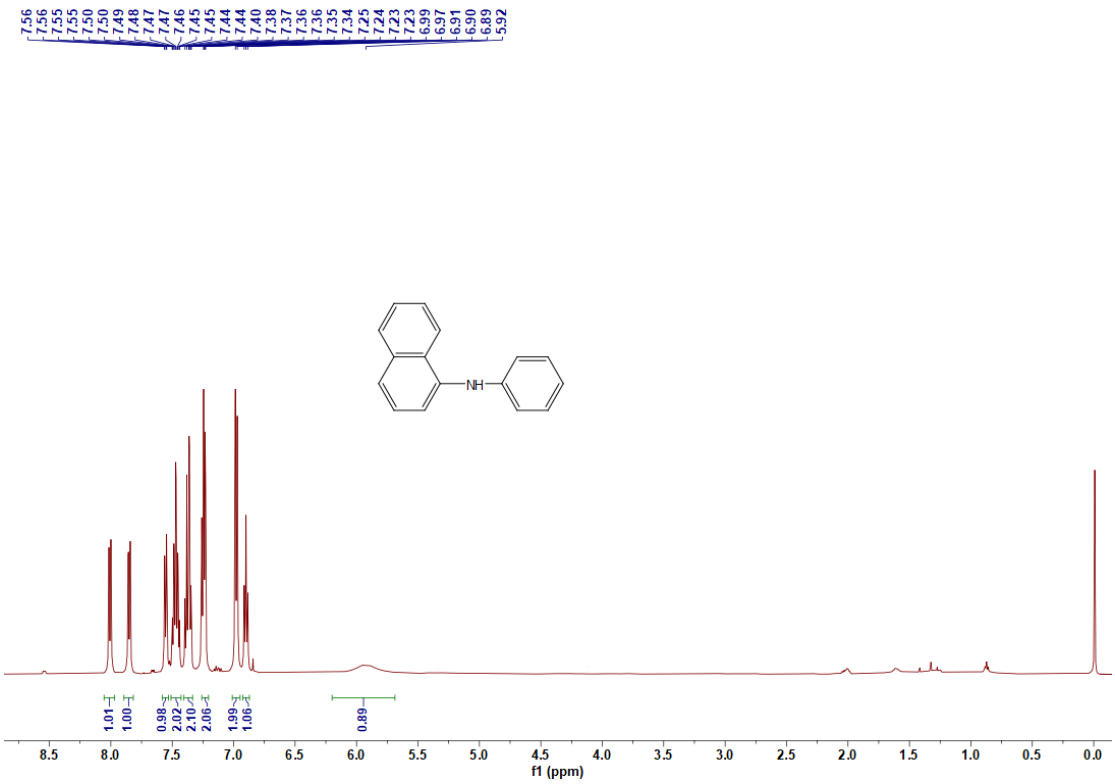
^{1}H NMR spectrum of 2f



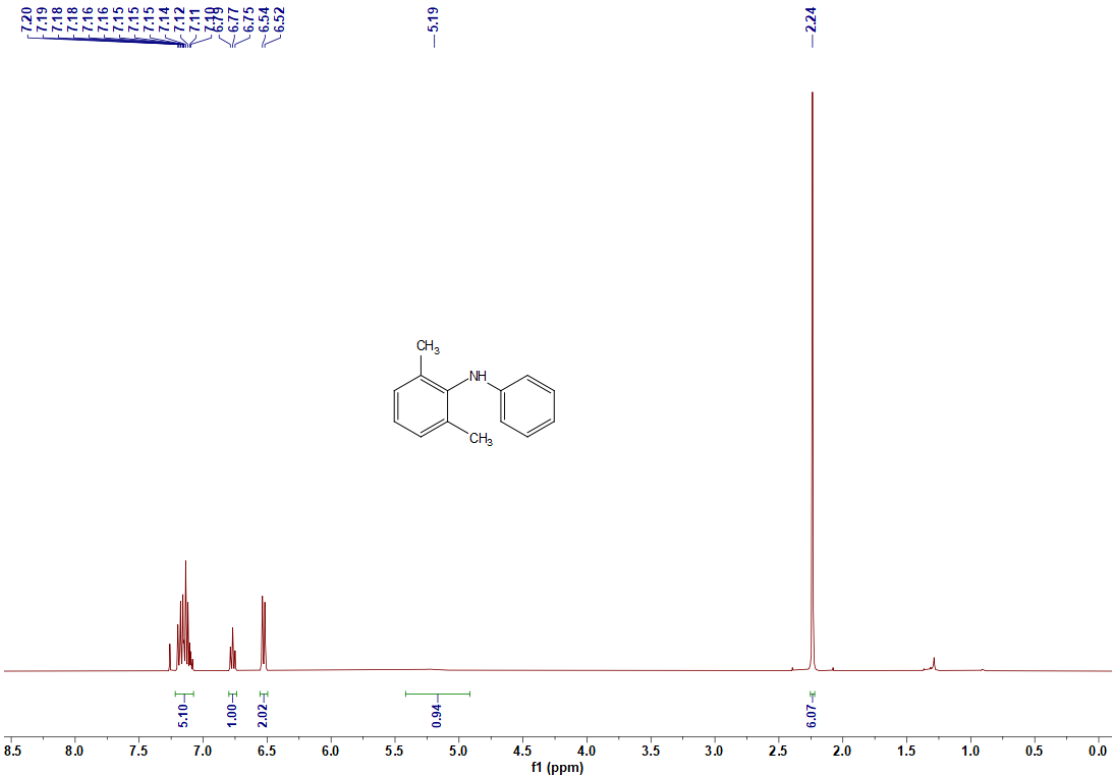
^{1}H NMR spectrum of 2g



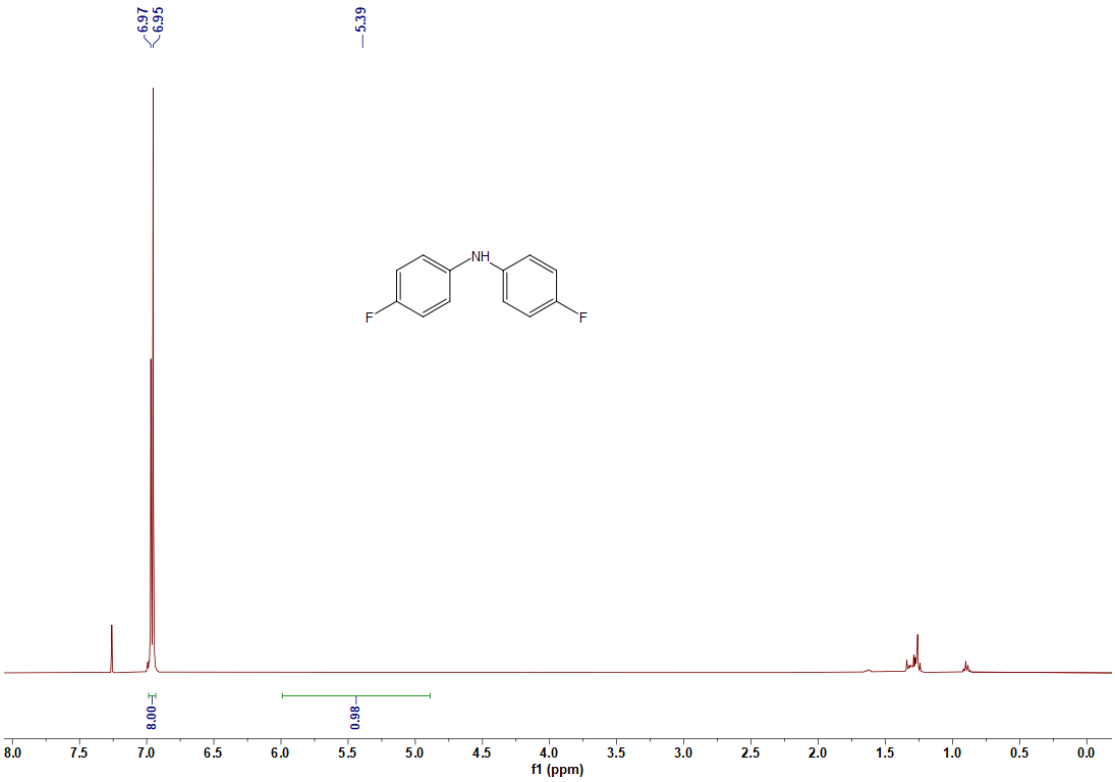
^{1}H NMR spectrum of 2h



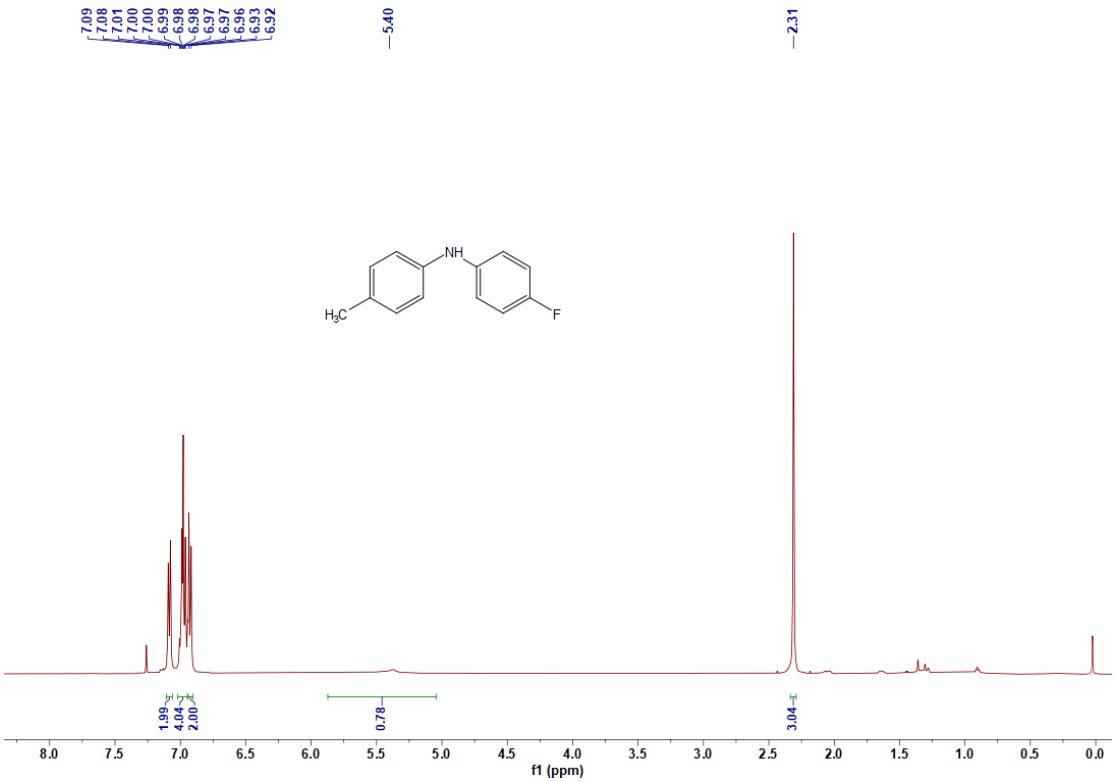
^{1}H NMR spectrum of 2i



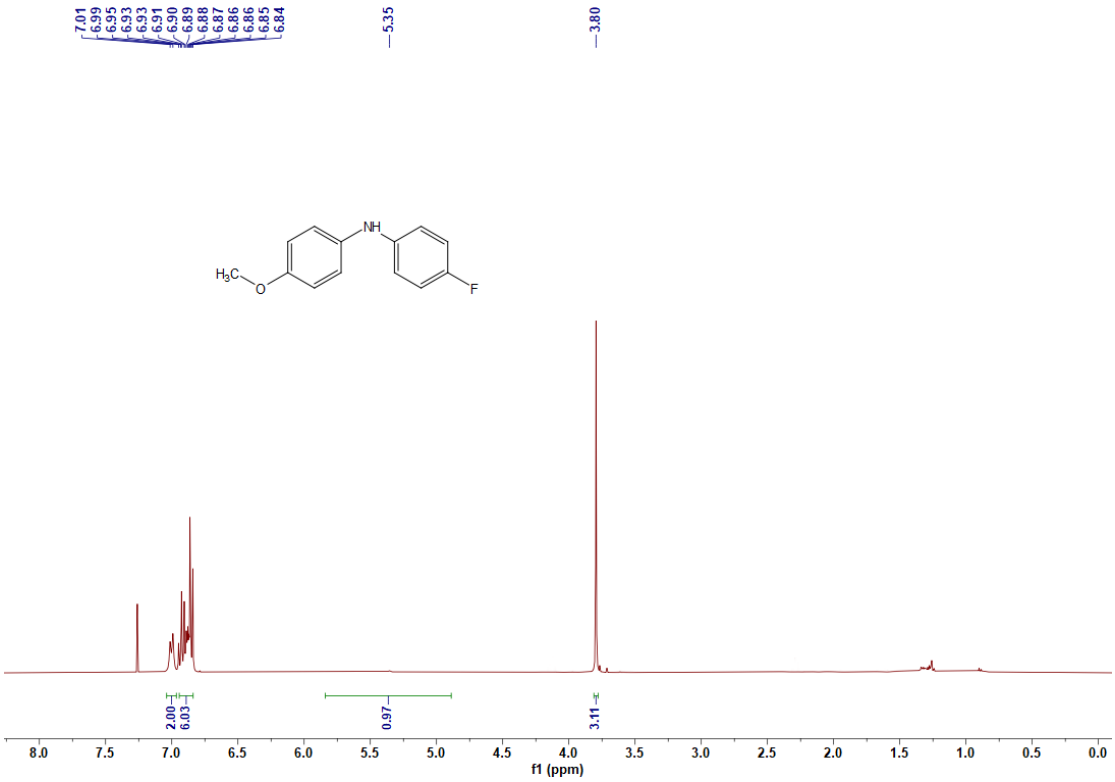
^{1}H NMR spectrum of 2j



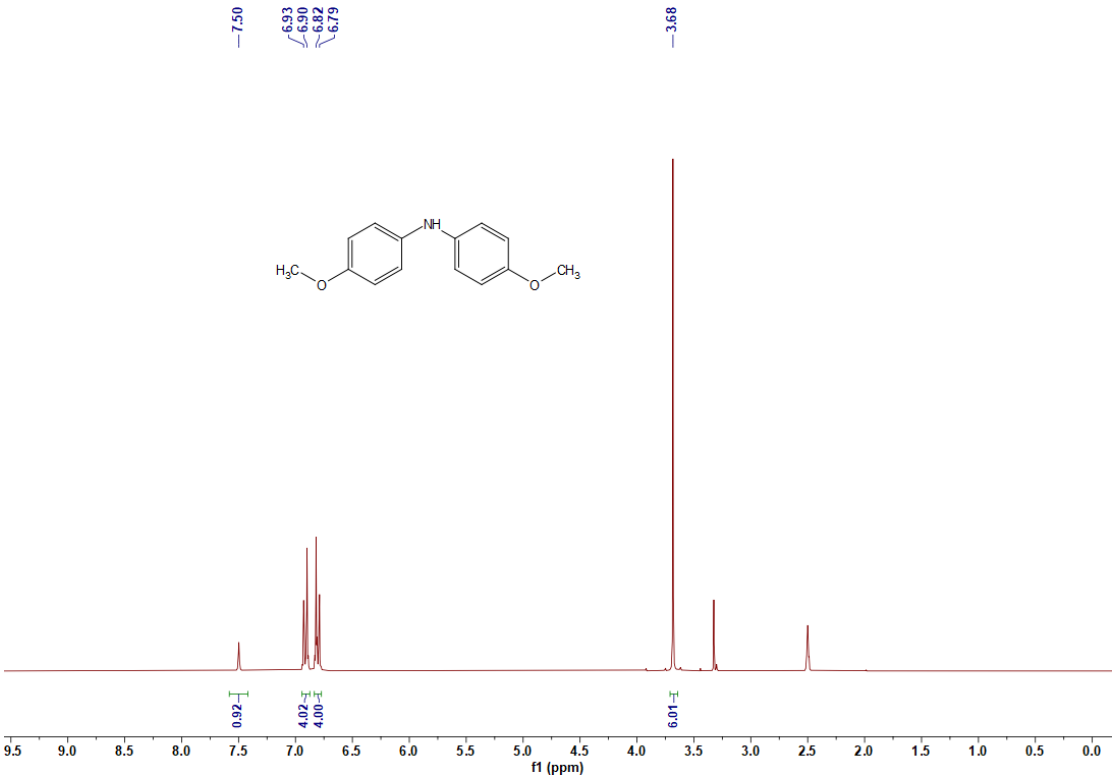
^{1}H NMR spectrum of 2k



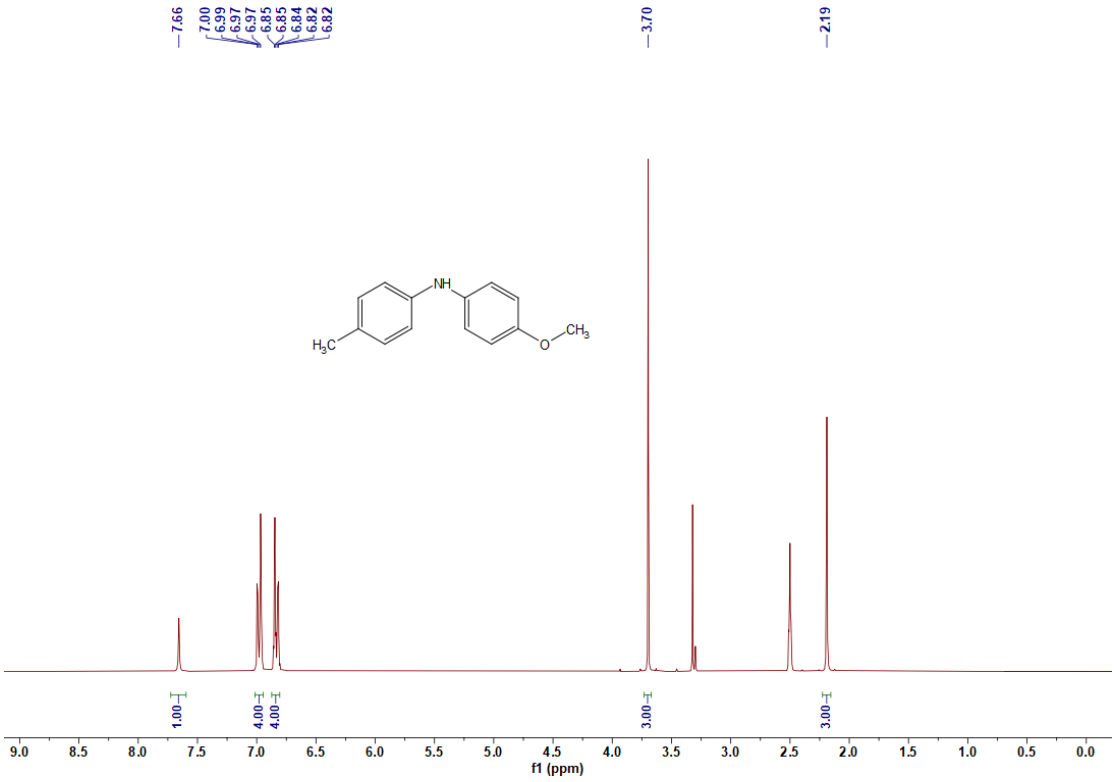
^{1}H NMR spectrum of 2l



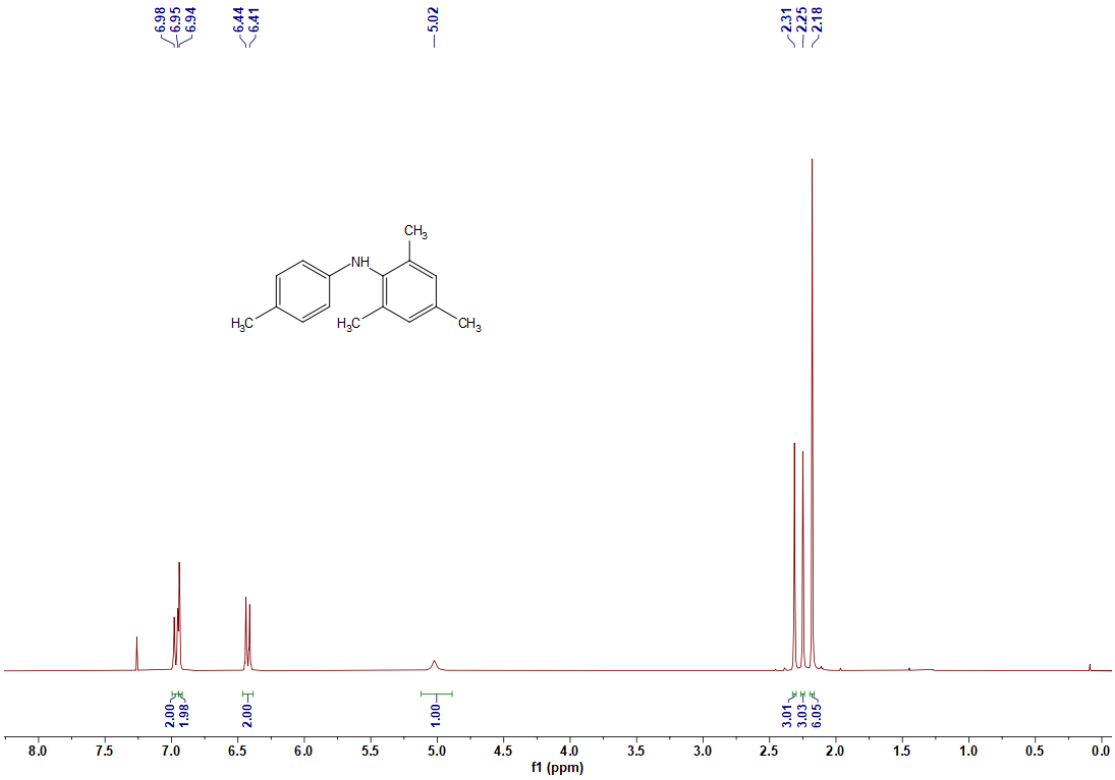
^{1}H NMR spectrum of 2m



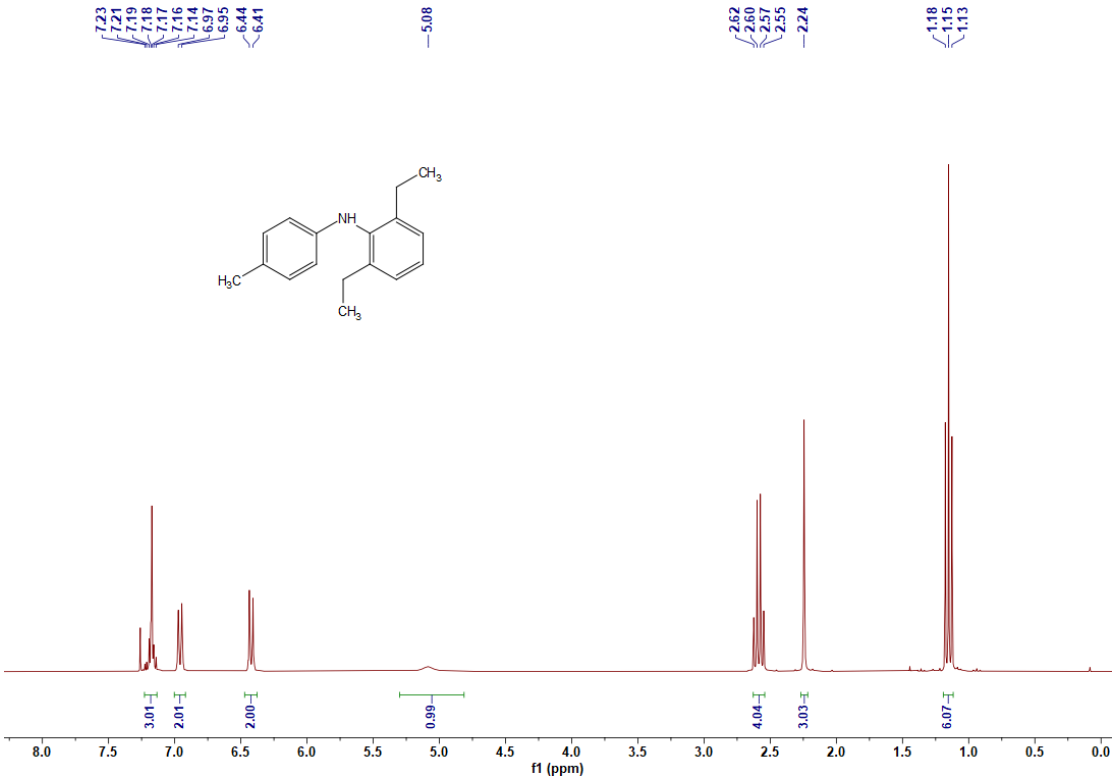
^{1}H NMR spectrum of 2n



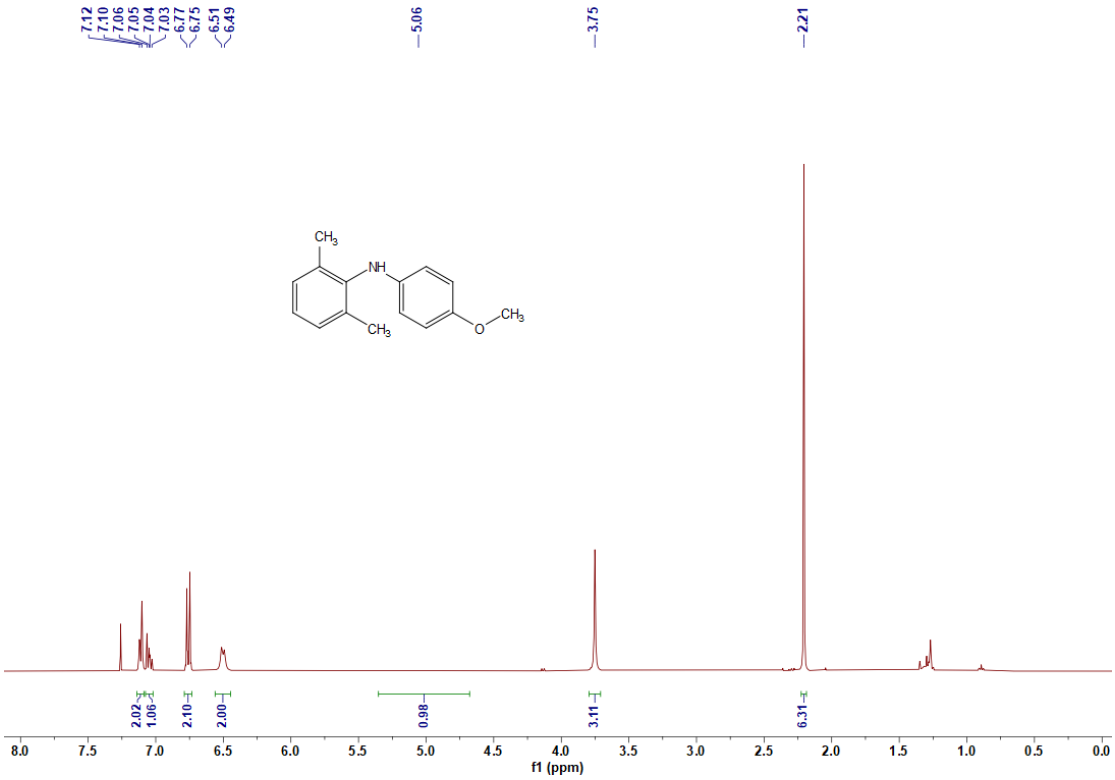
^{1}H NMR spectrum of 2o



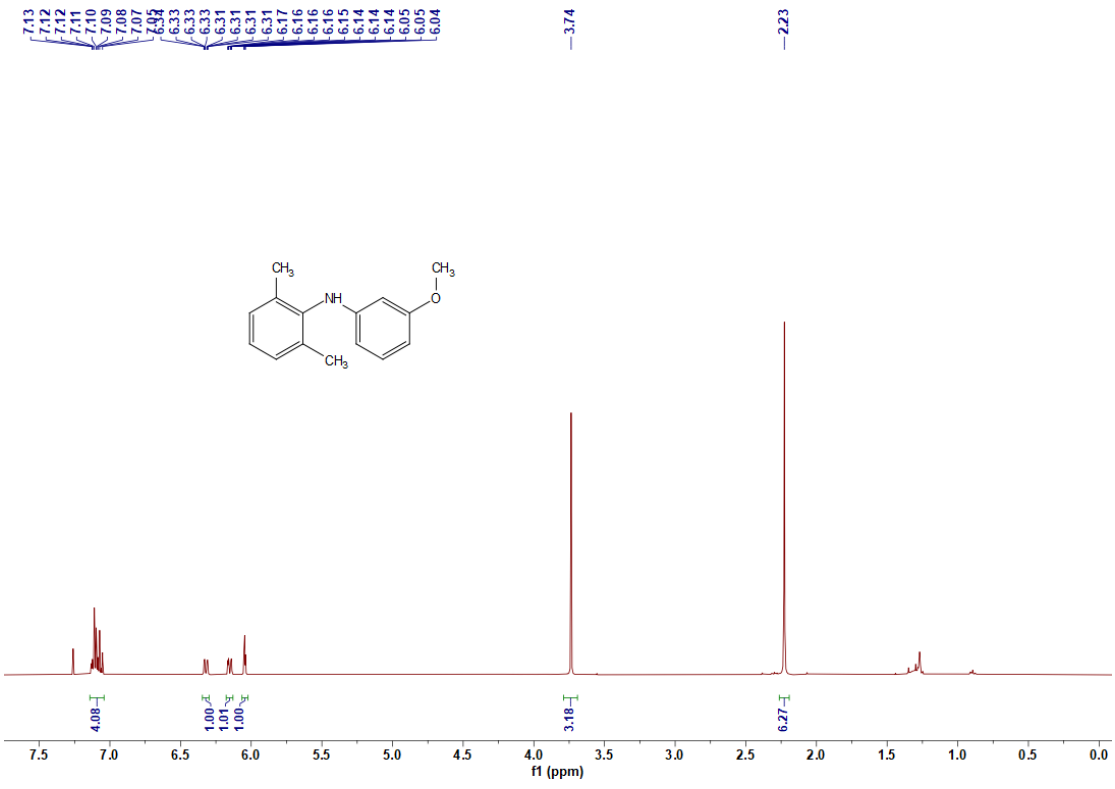
^{1}H NMR spectrum of 2p



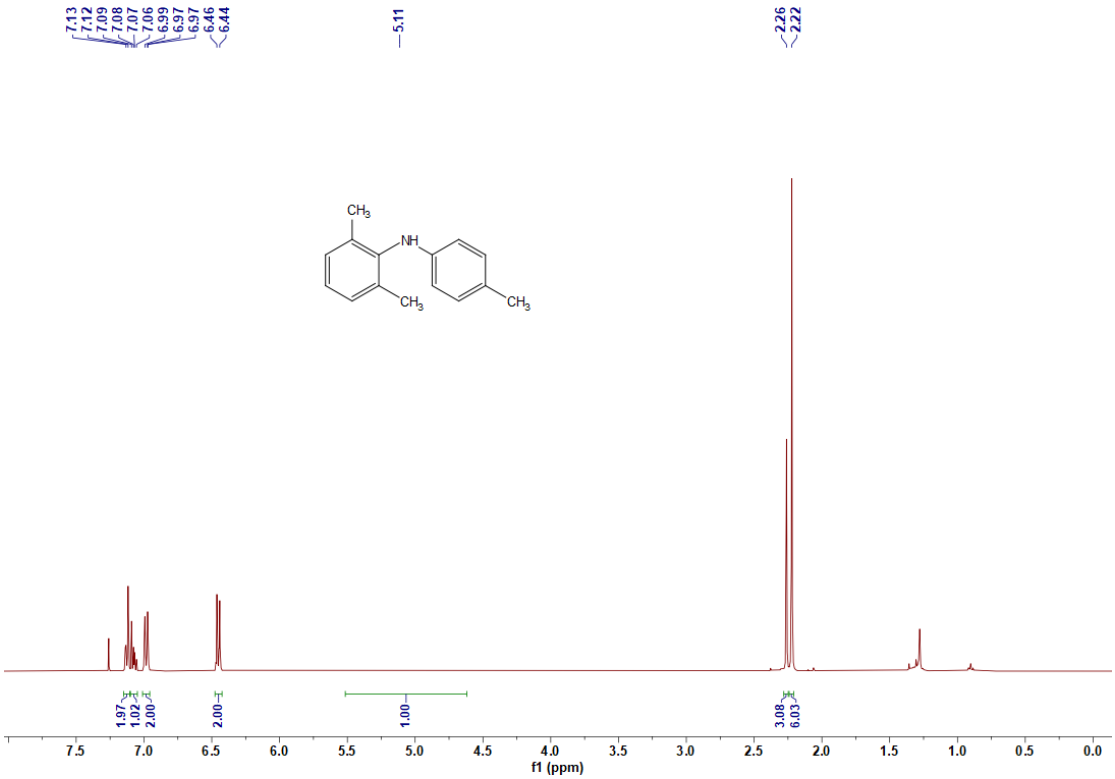
^{1}H NMR spectrum of 2q



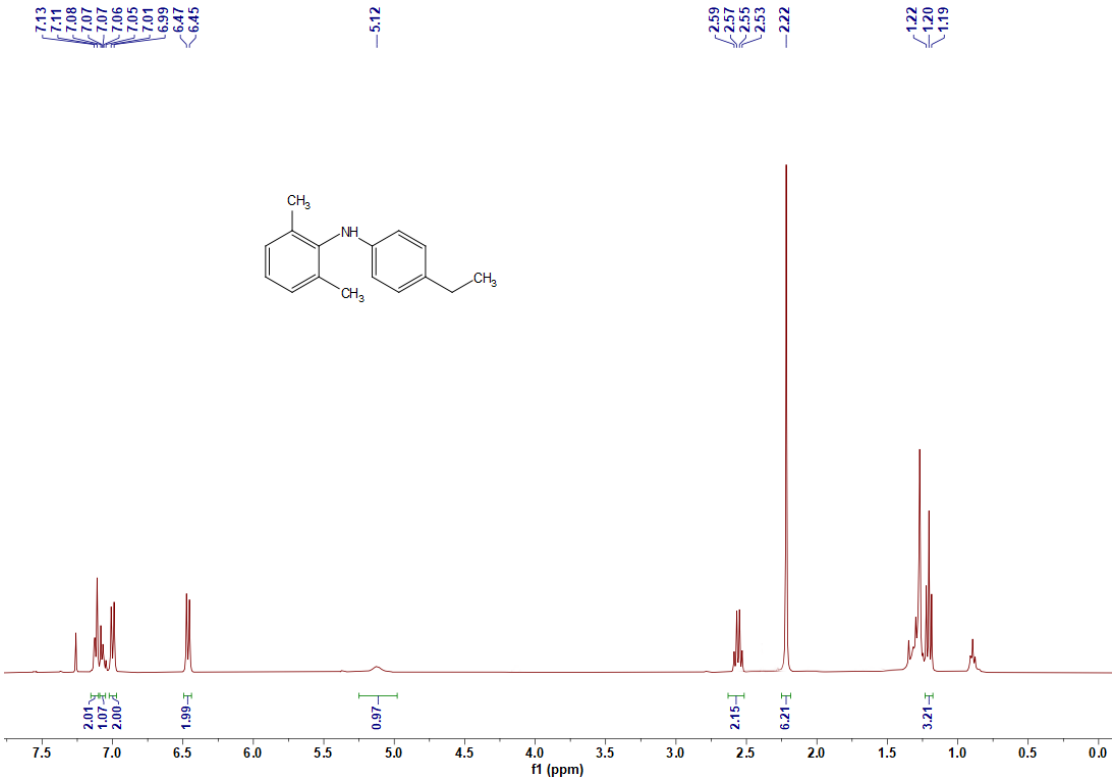
^{1}H NMR spectrum of 2r



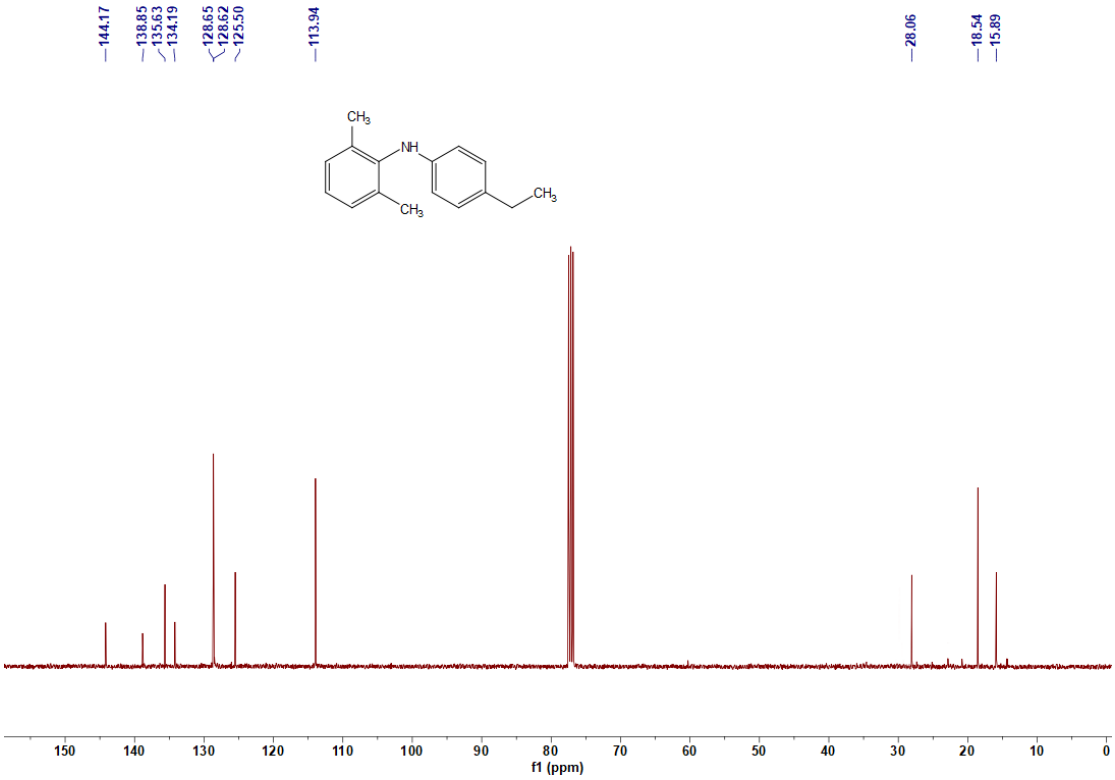
^{1}H NMR spectrum of 2s



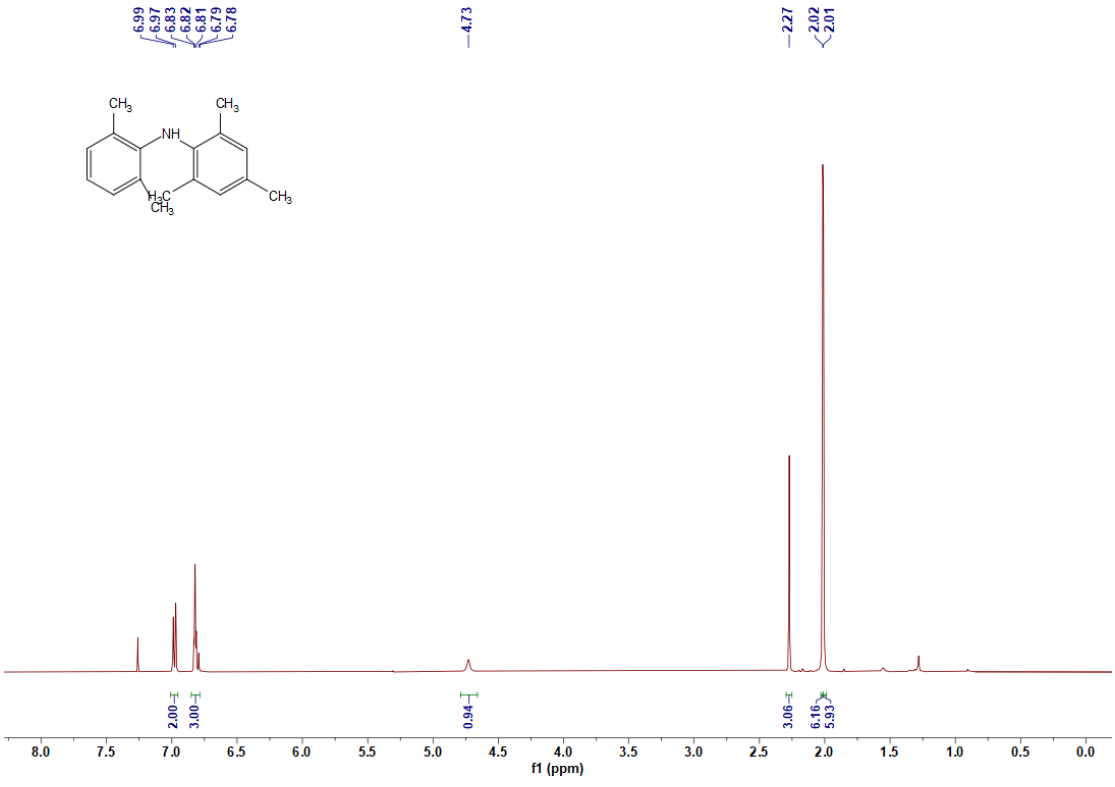
^{1}H NMR spectrum of 2t



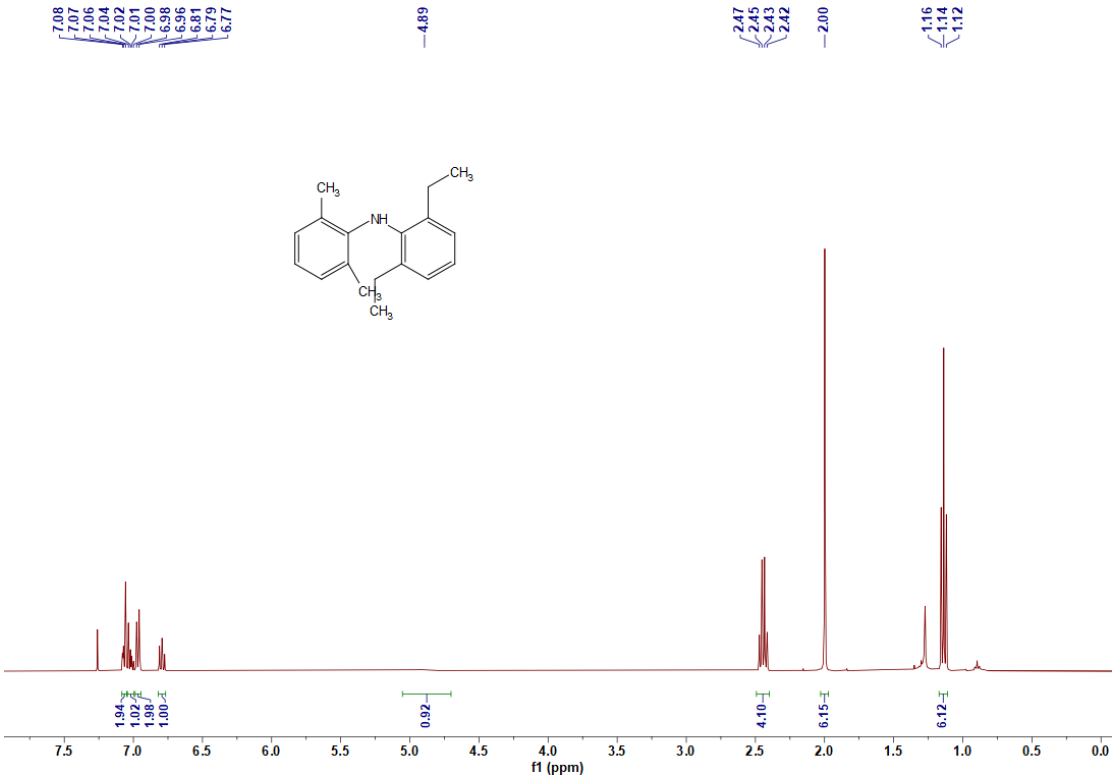
^{1}H NMR spectrum of 2u



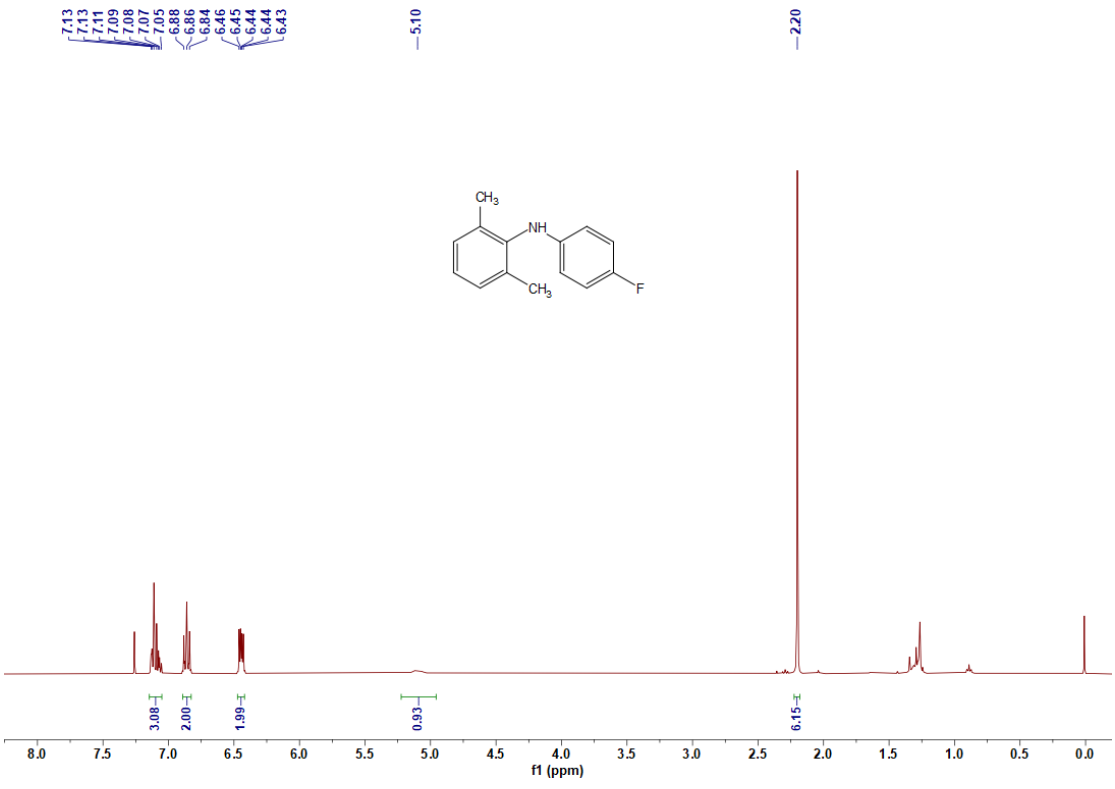
^{13}C NMR spectrum of 2u



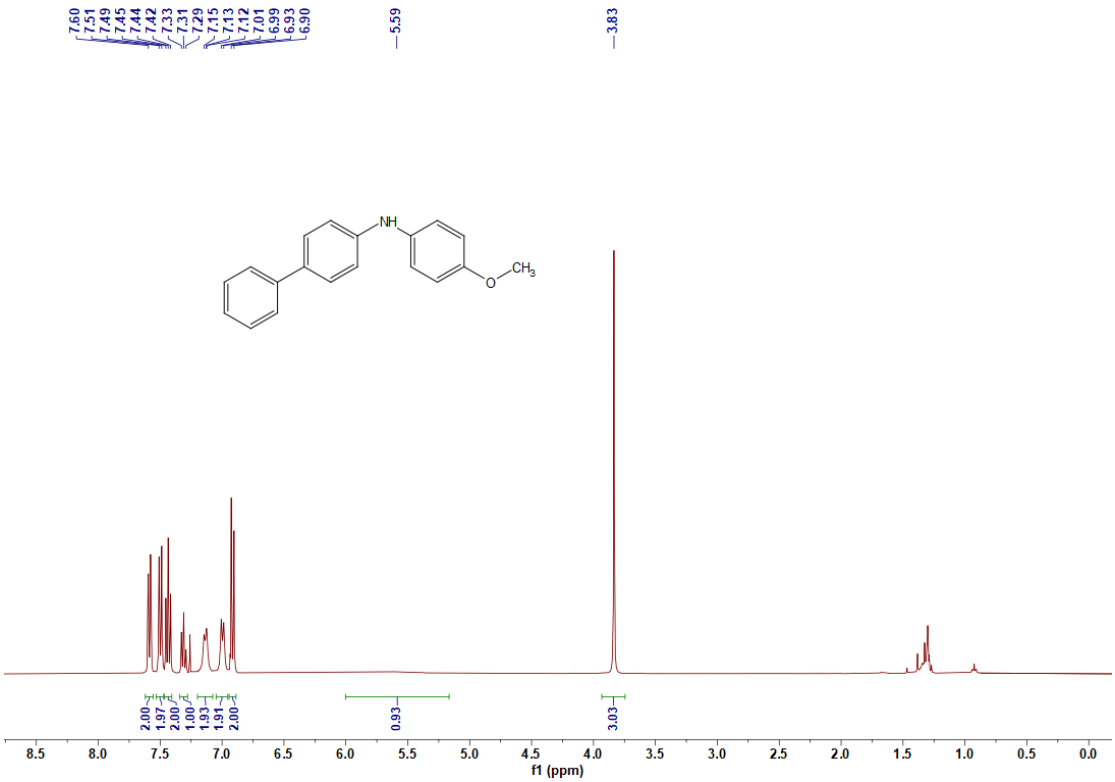
^{1}H NMR spectrum of 2v



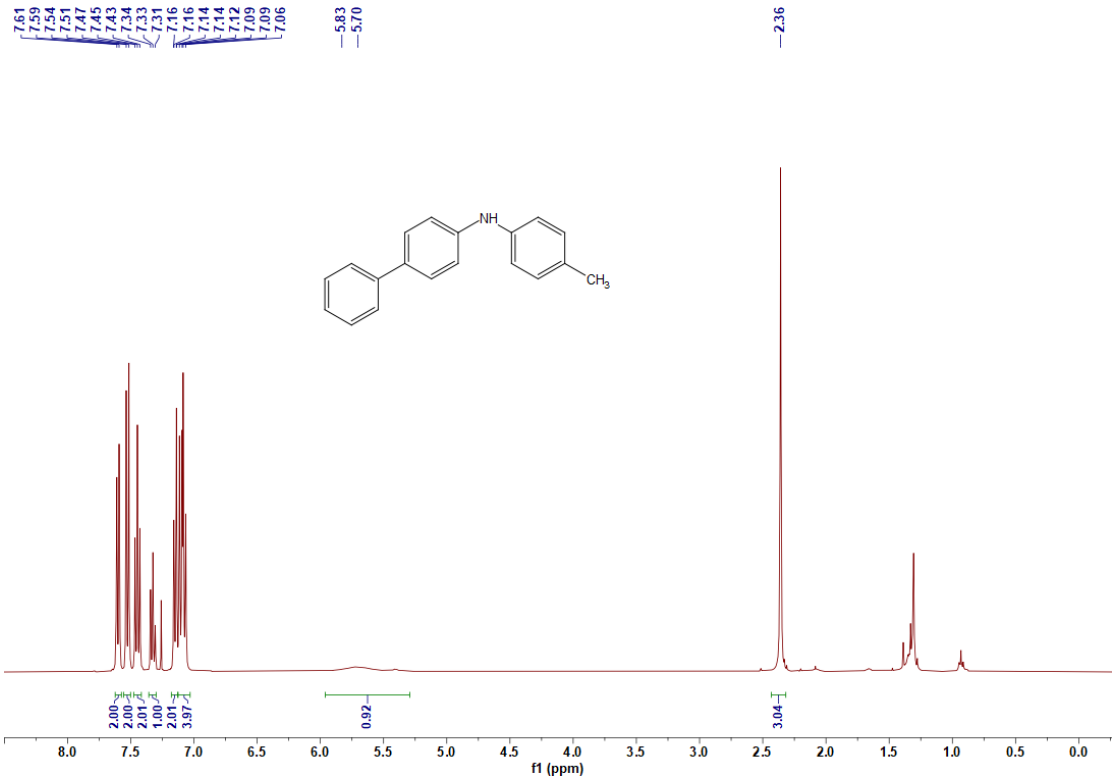
^{1}H NMR spectrum of 2w



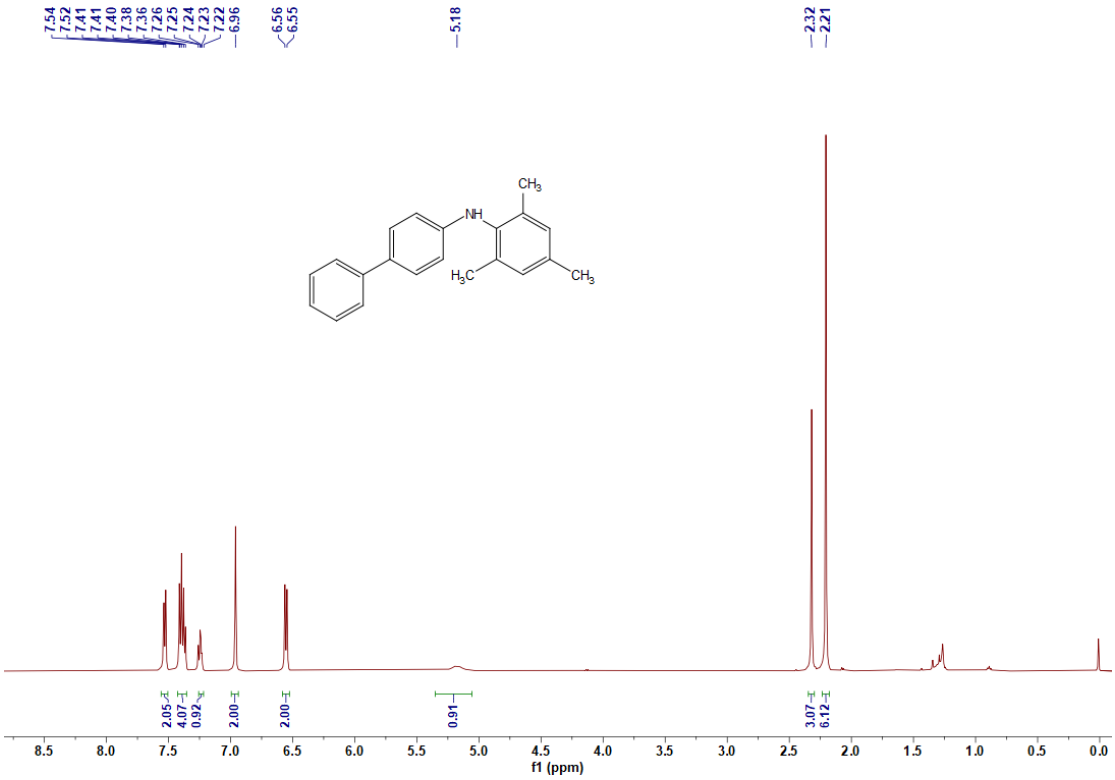
^{1}H NMR spectrum of 2x



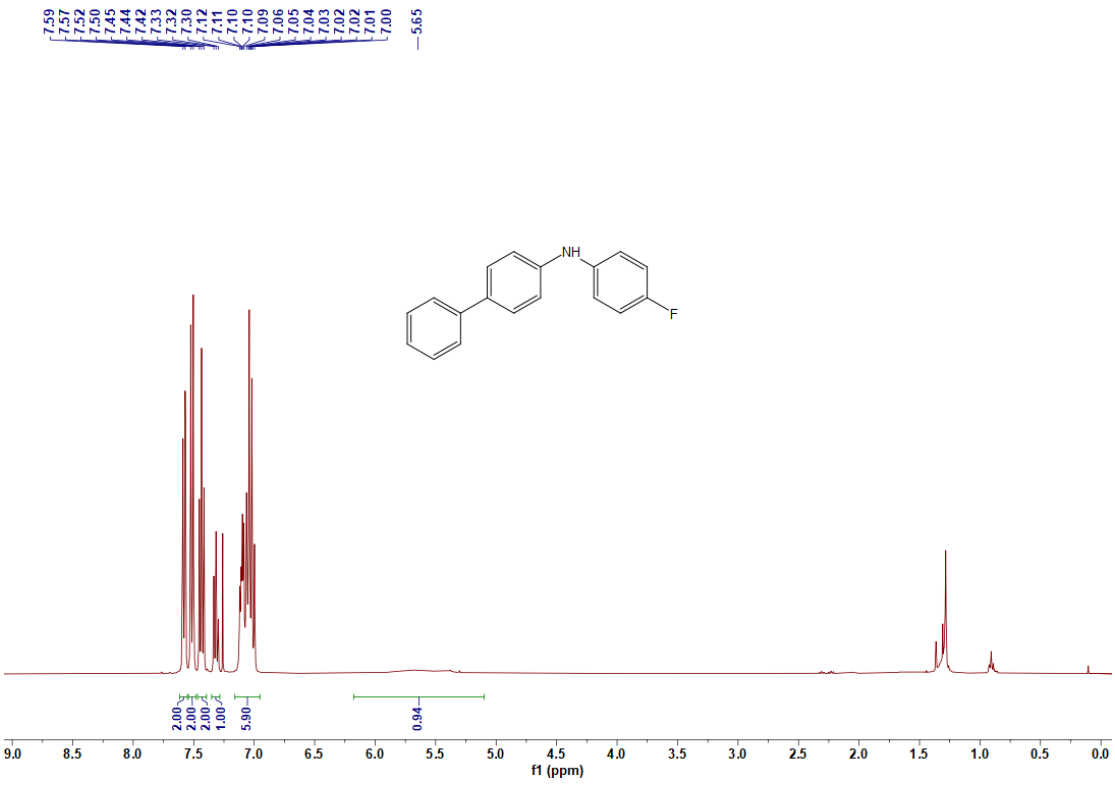
^{1}H NMR spectrum of 2y



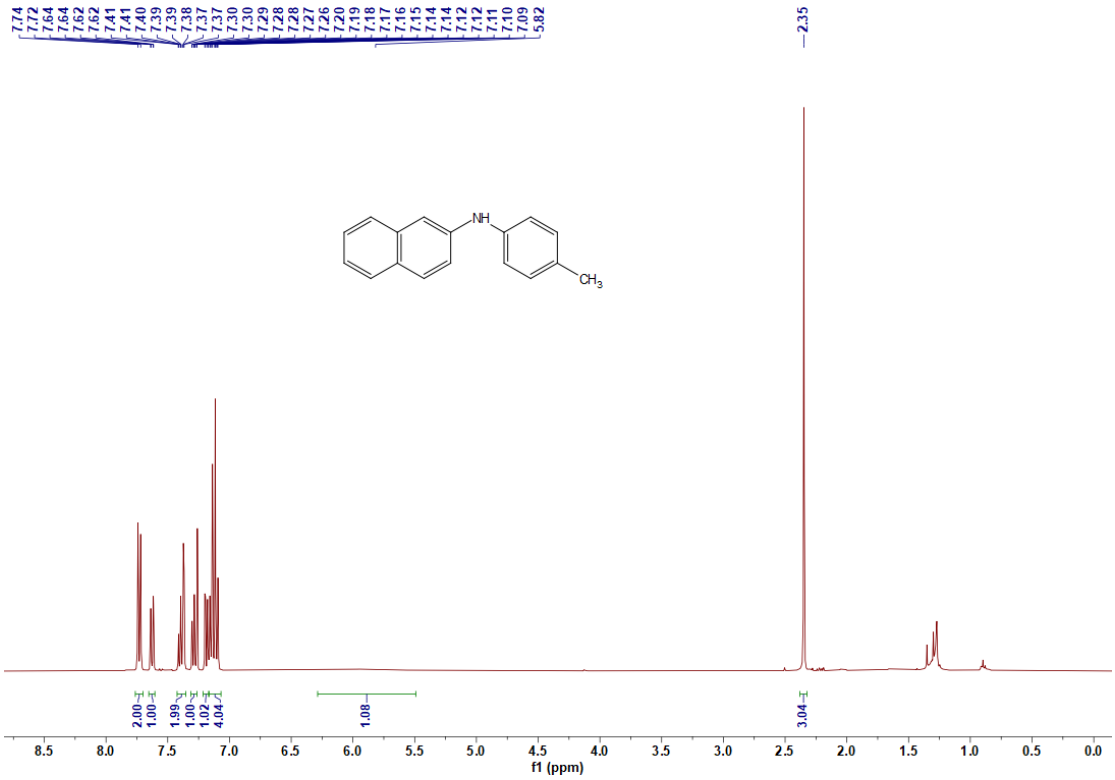
^{1}H NMR spectrum of 2z



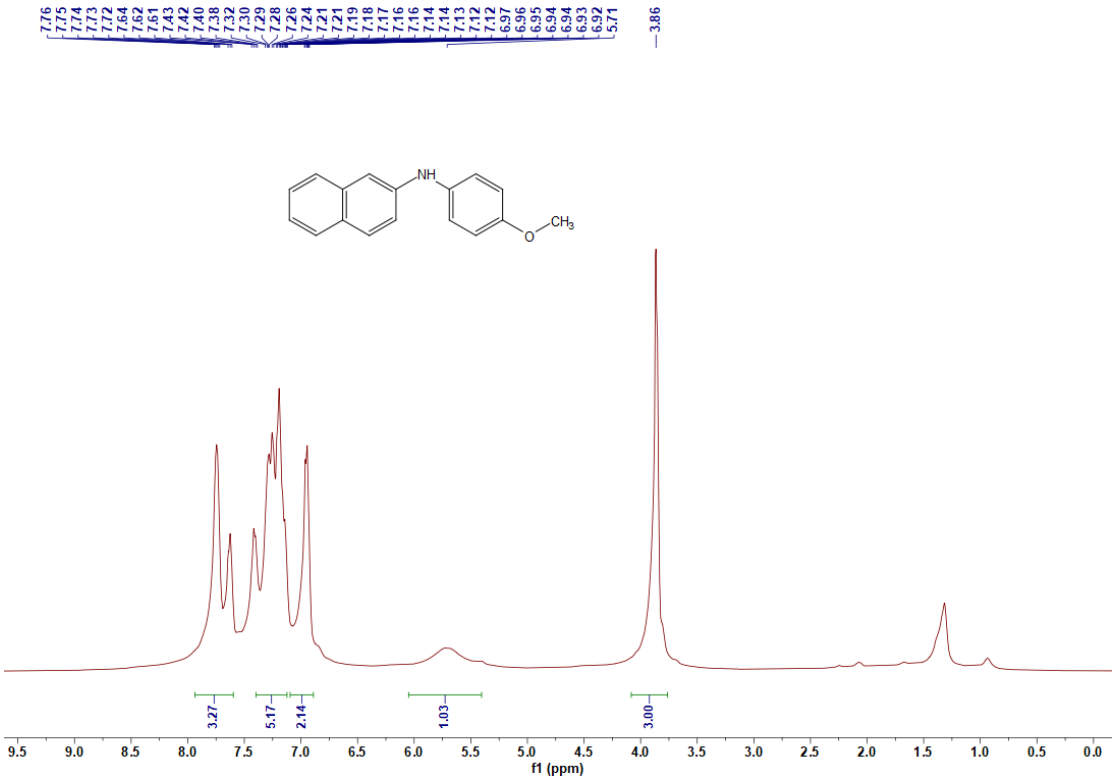
^{1}H NMR spectrum of 2aa



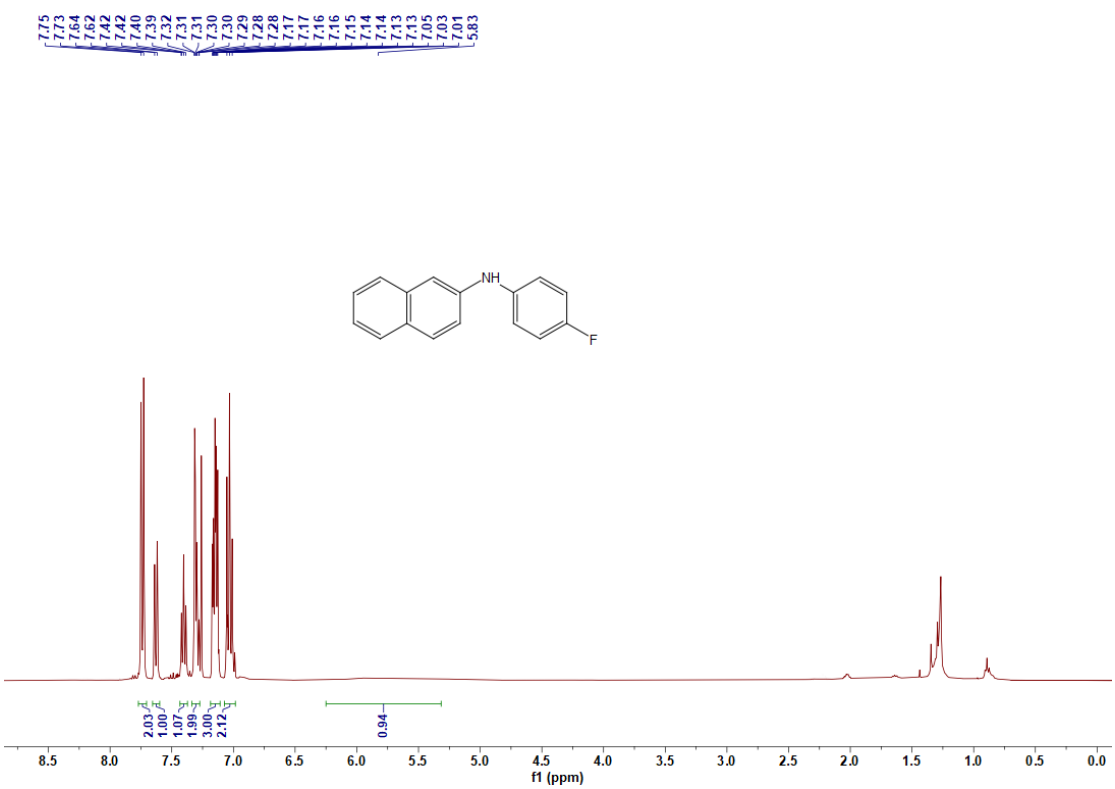
^{1}H NMR spectrum of 2ab



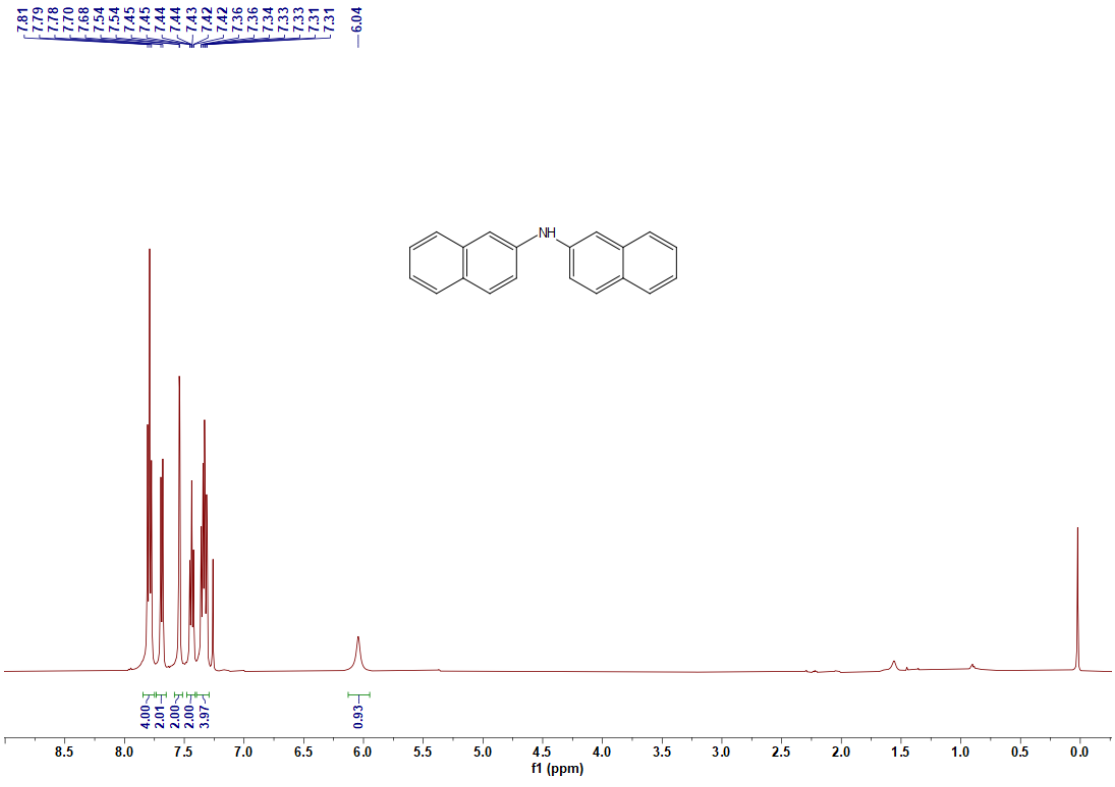
^{1}H NMR spectrum of 2ac



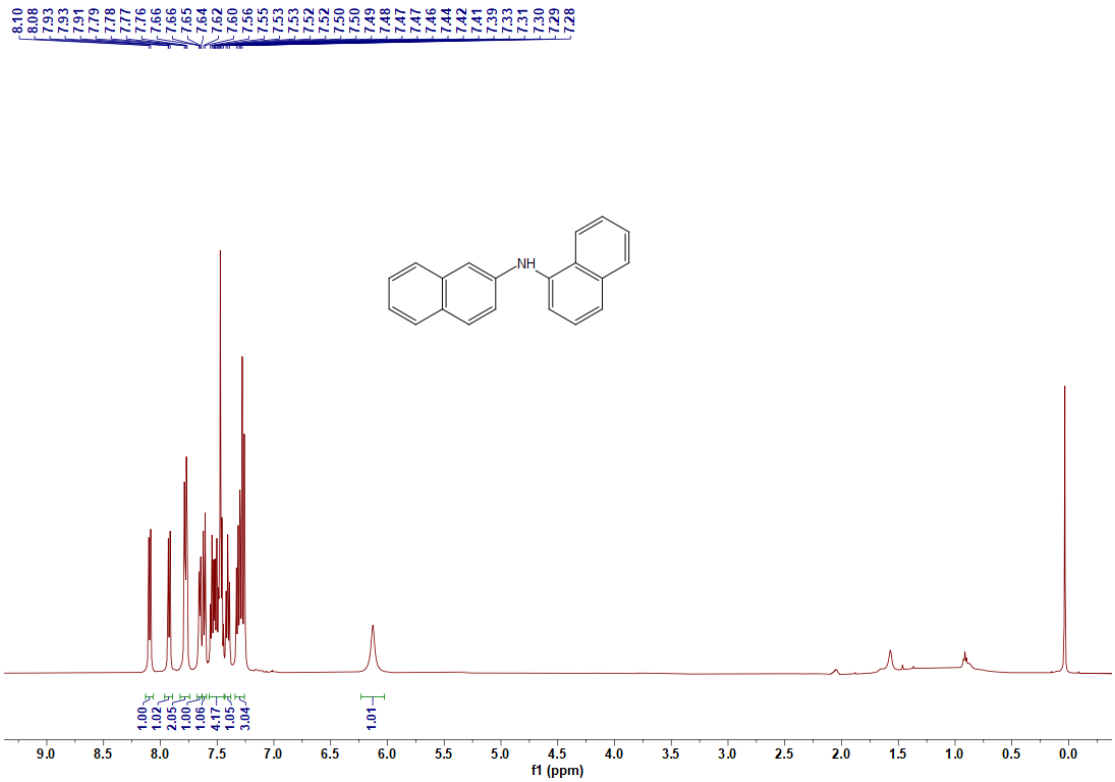
^{1}H NMR spectrum of 2ad



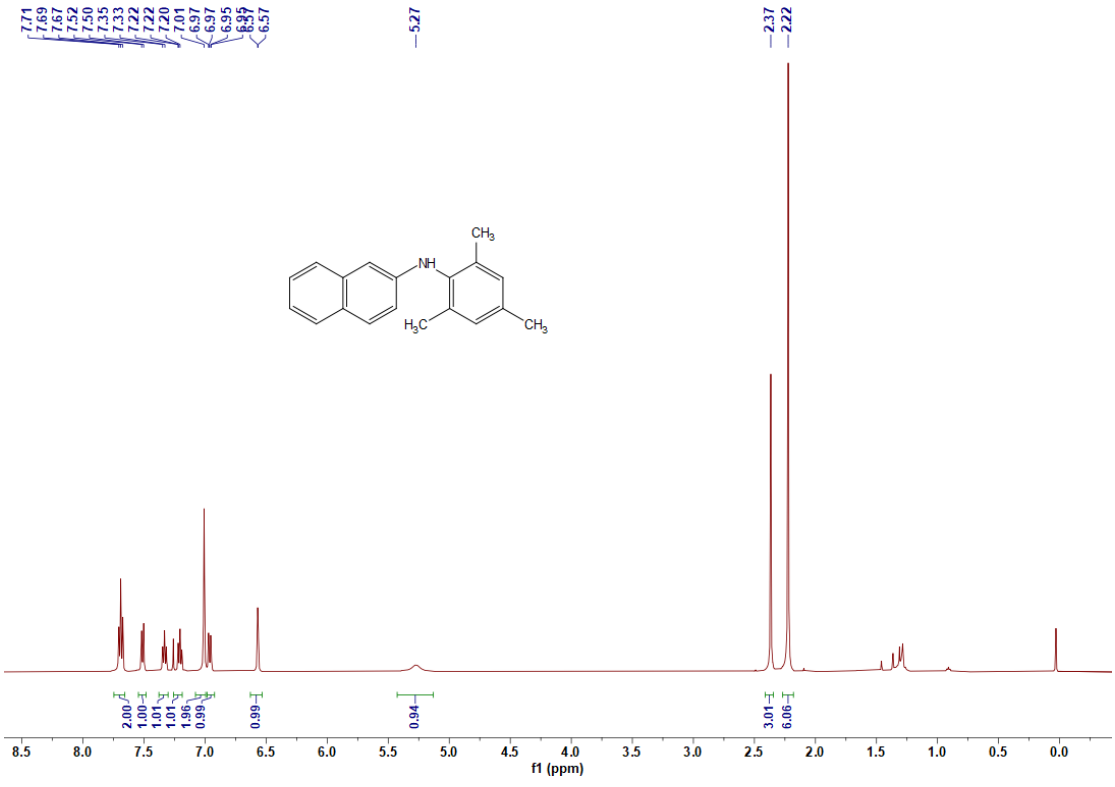
^{1}H NMR spectrum of 2ae



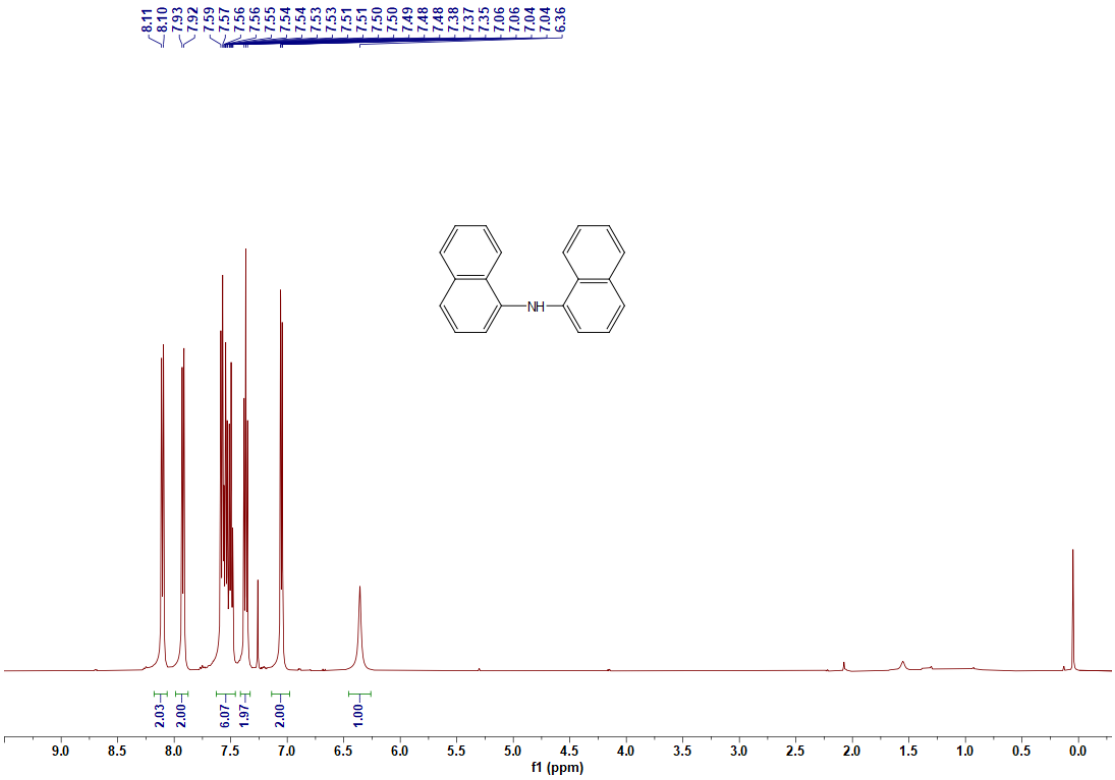
^{1}H NMR spectrum of 2af



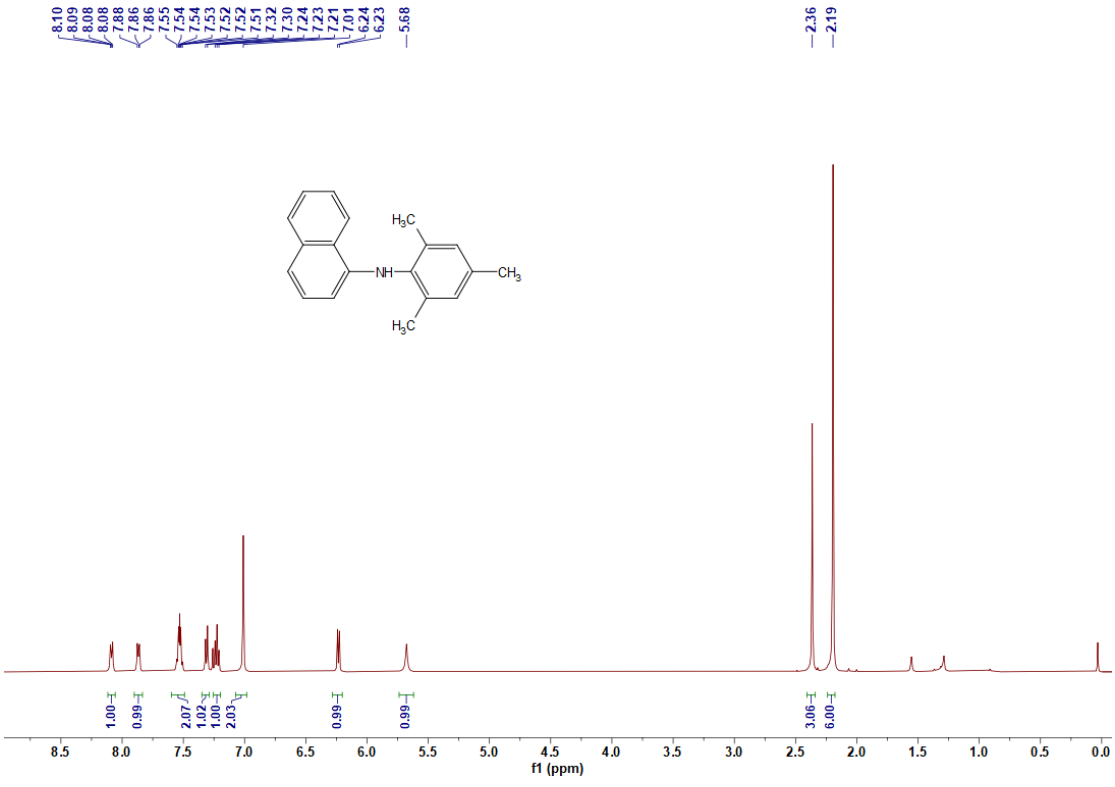
^{1}H NMR spectrum of 2ag



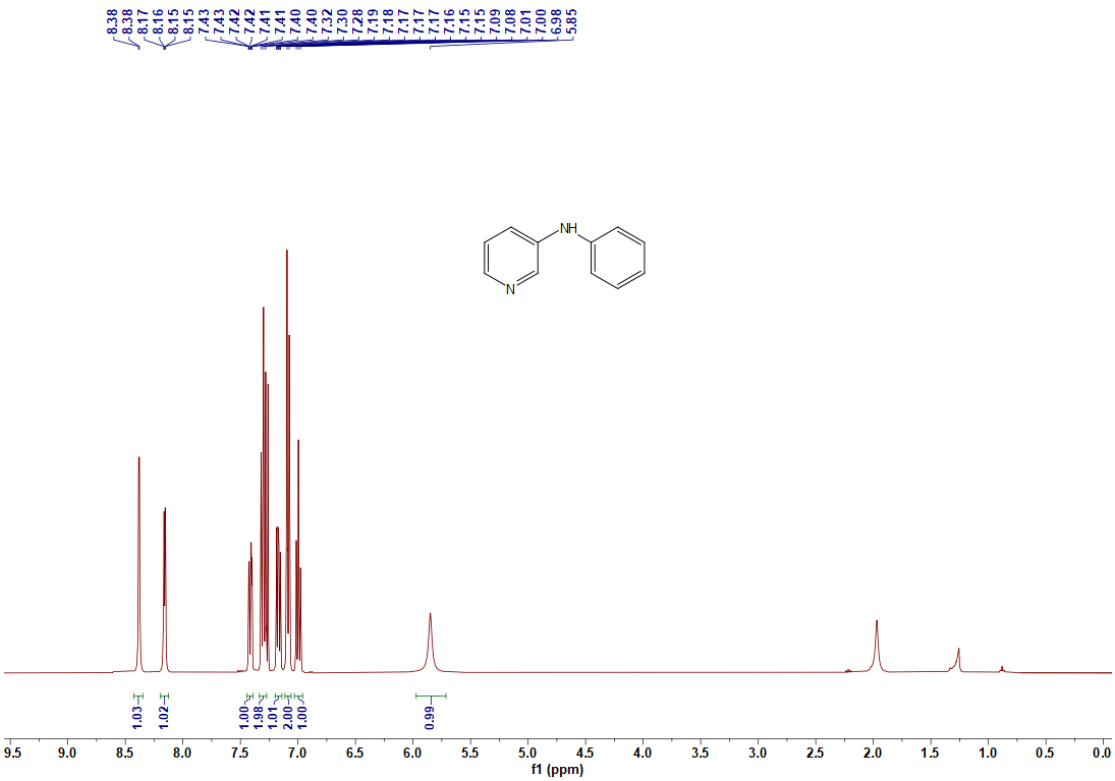
^{1}H NMR spectrum of 2ah



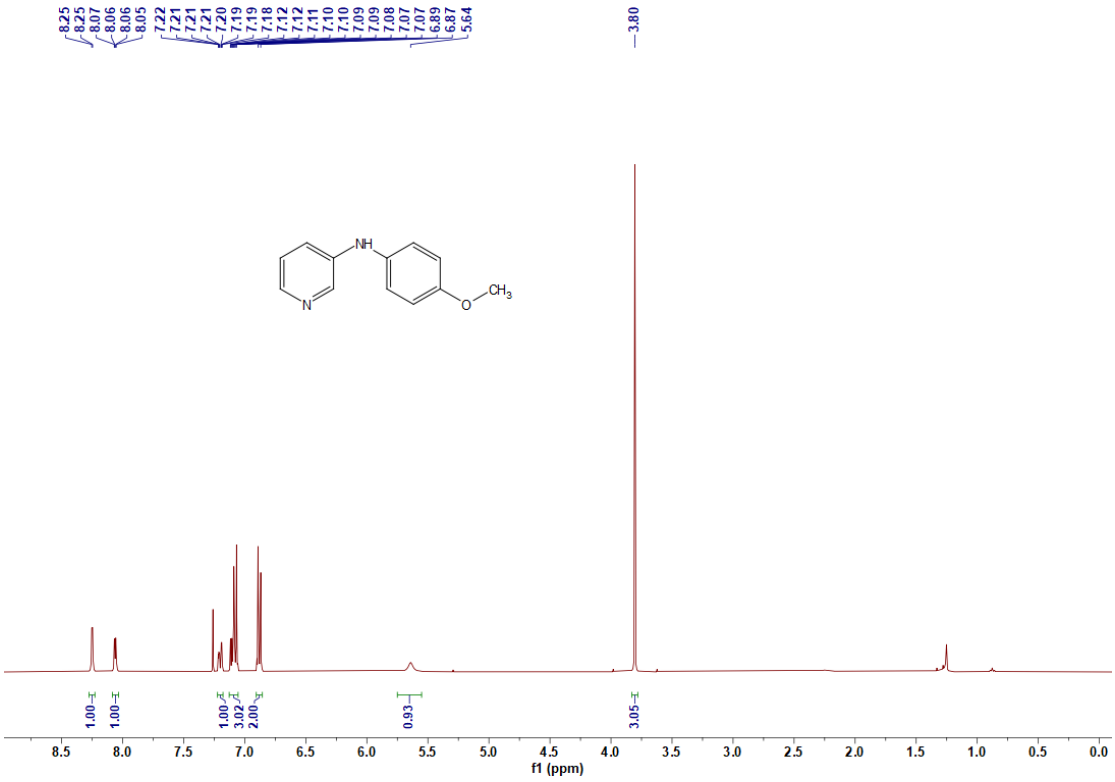
^{1}H NMR spectrum of 2ai



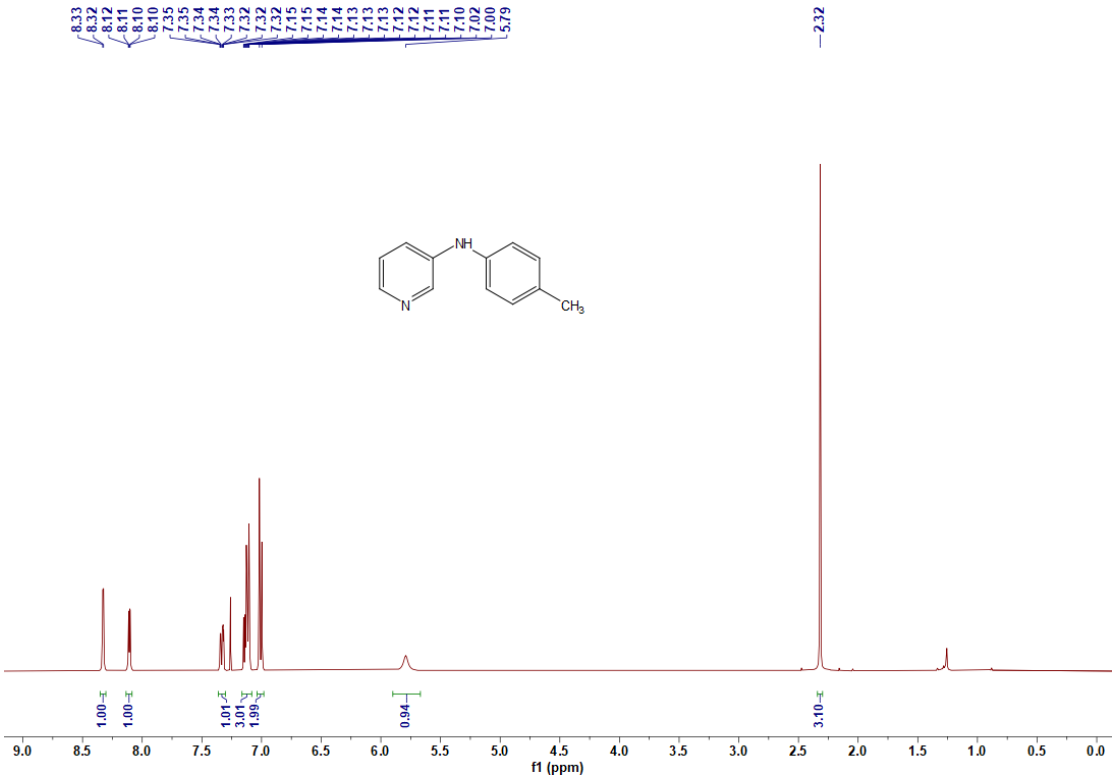
^{1}H NMR spectrum of 2aj



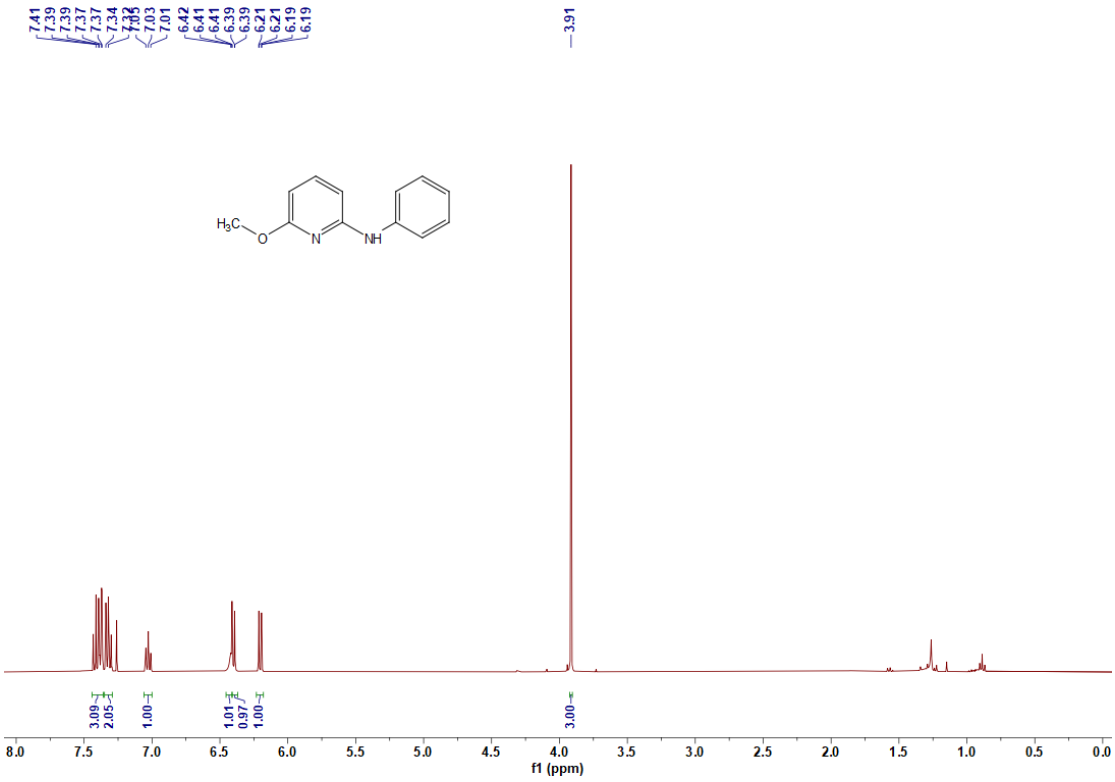
^{1}H NMR spectrum of 6a



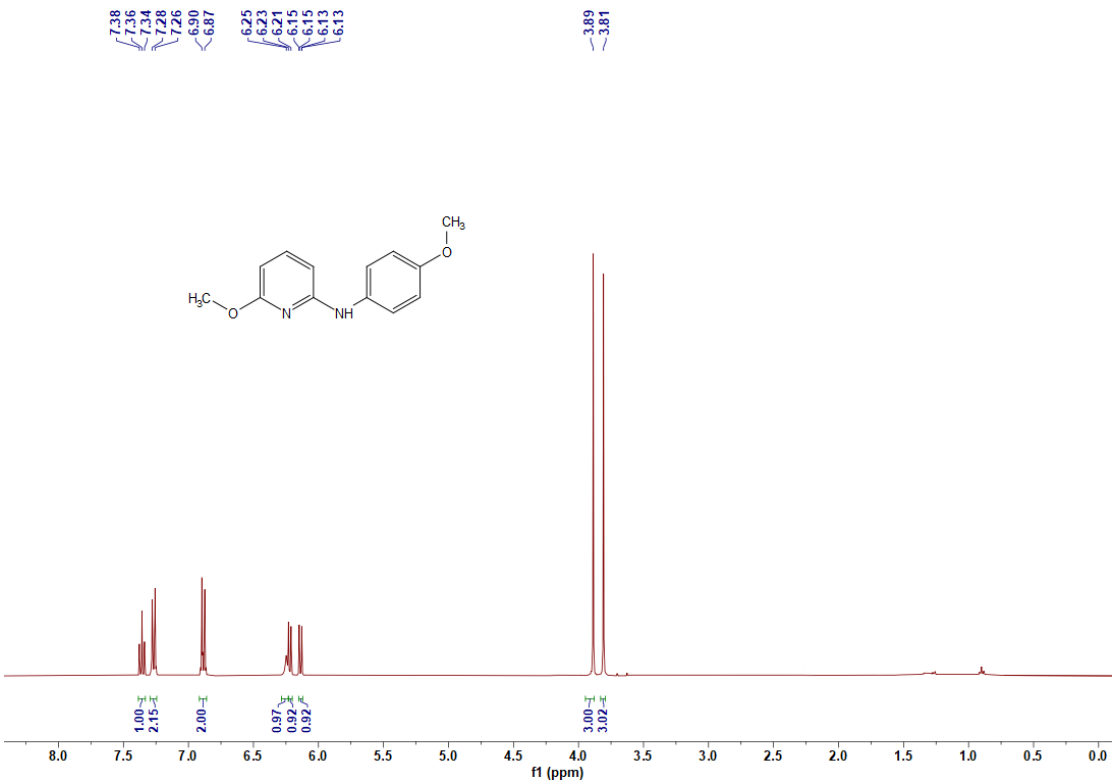
^{1}H NMR spectrum of 6b



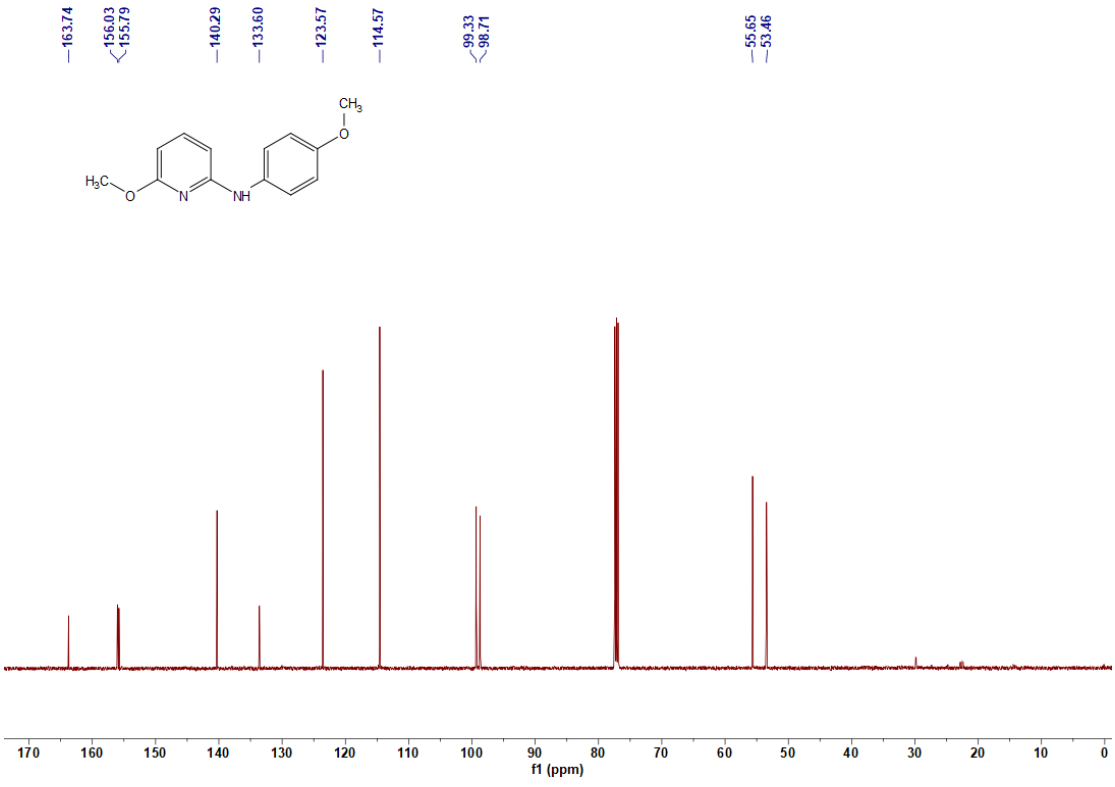
^{1}H NMR spectrum of 6c



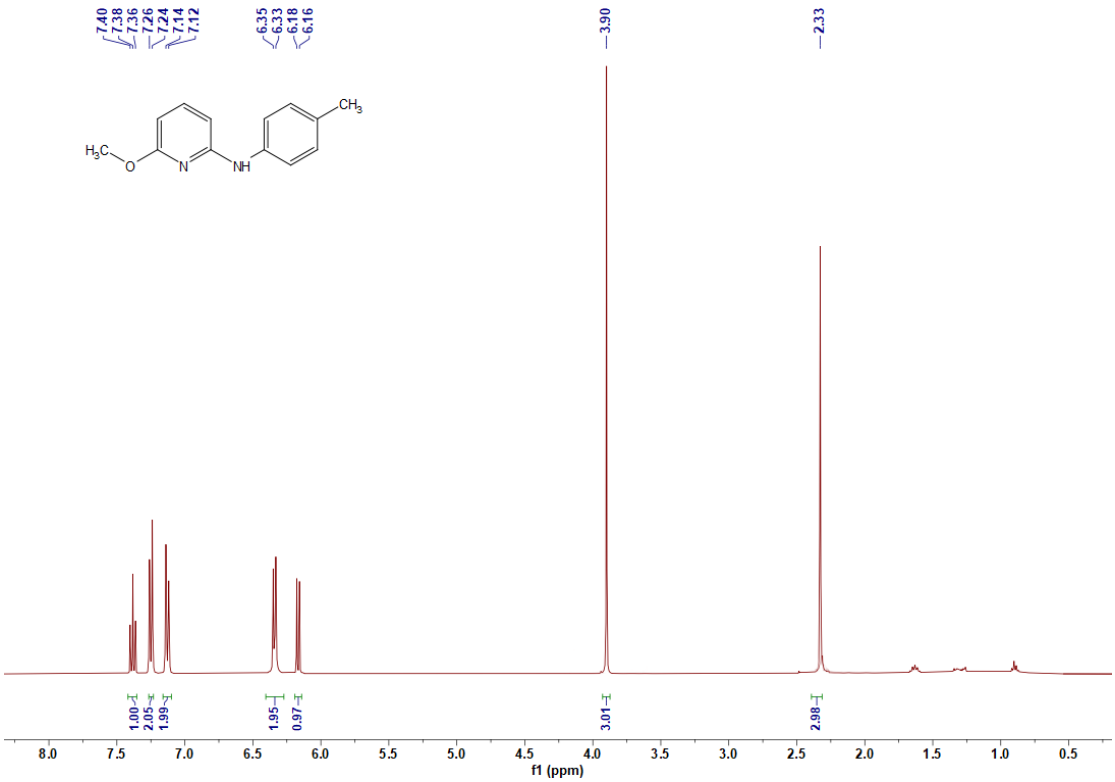
^{1}H NMR spectrum of 6d



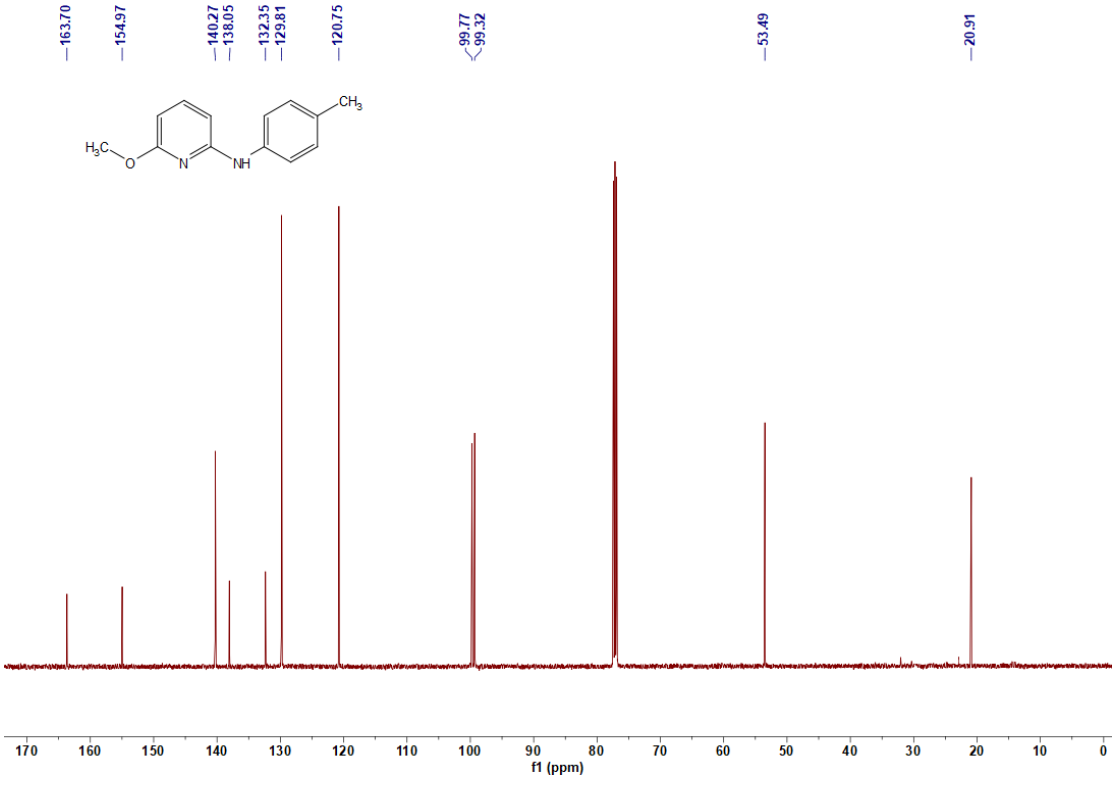
^{1}H NMR spectrum of 6e



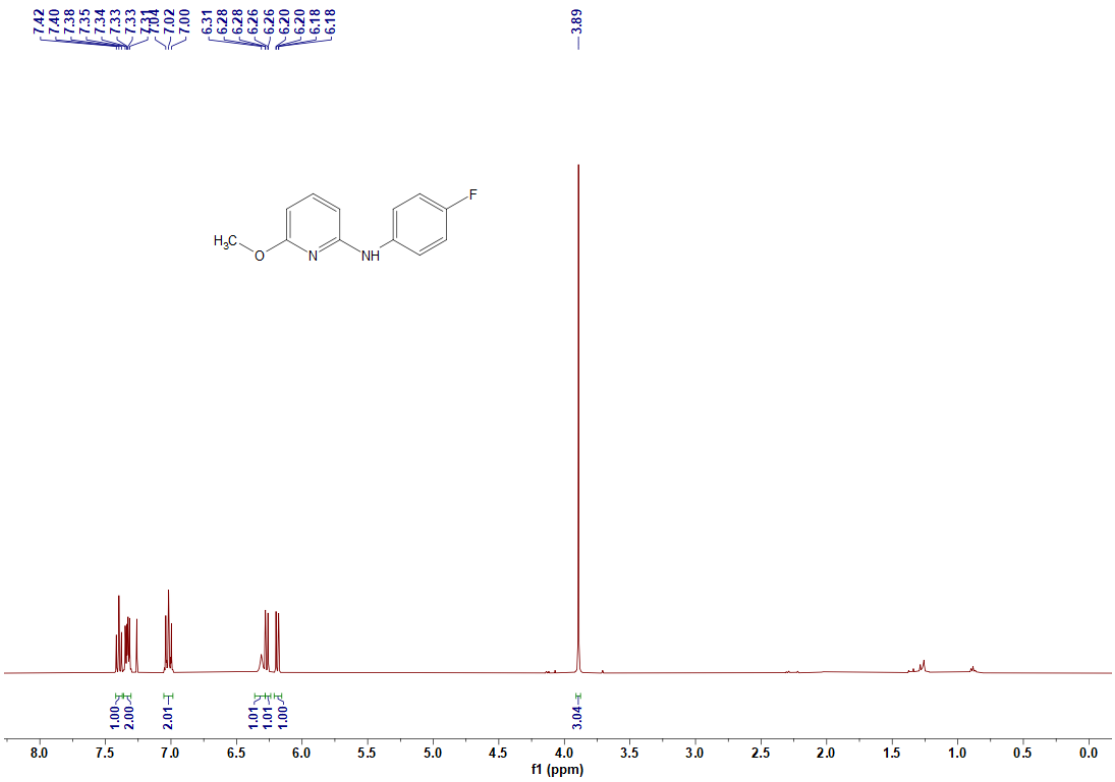
^{13}C NMR spectrum of 6e



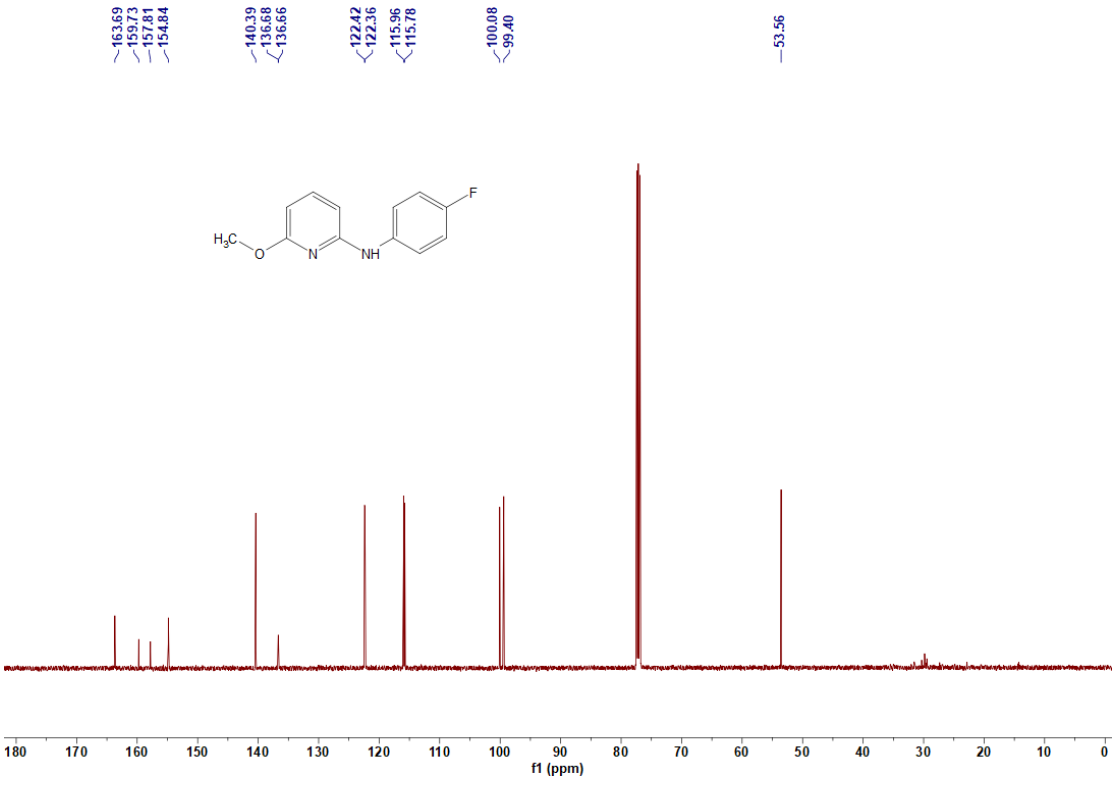
^{1}H NMR spectrum of 6f



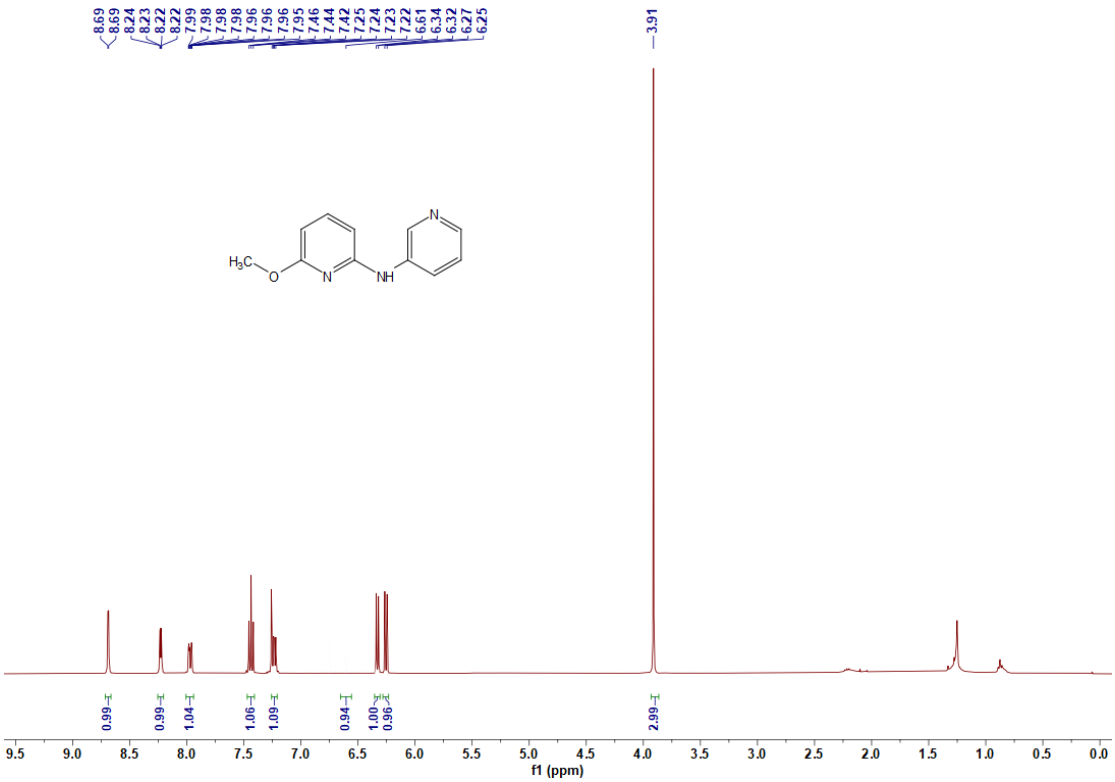
^{13}C NMR spectrum of 6f



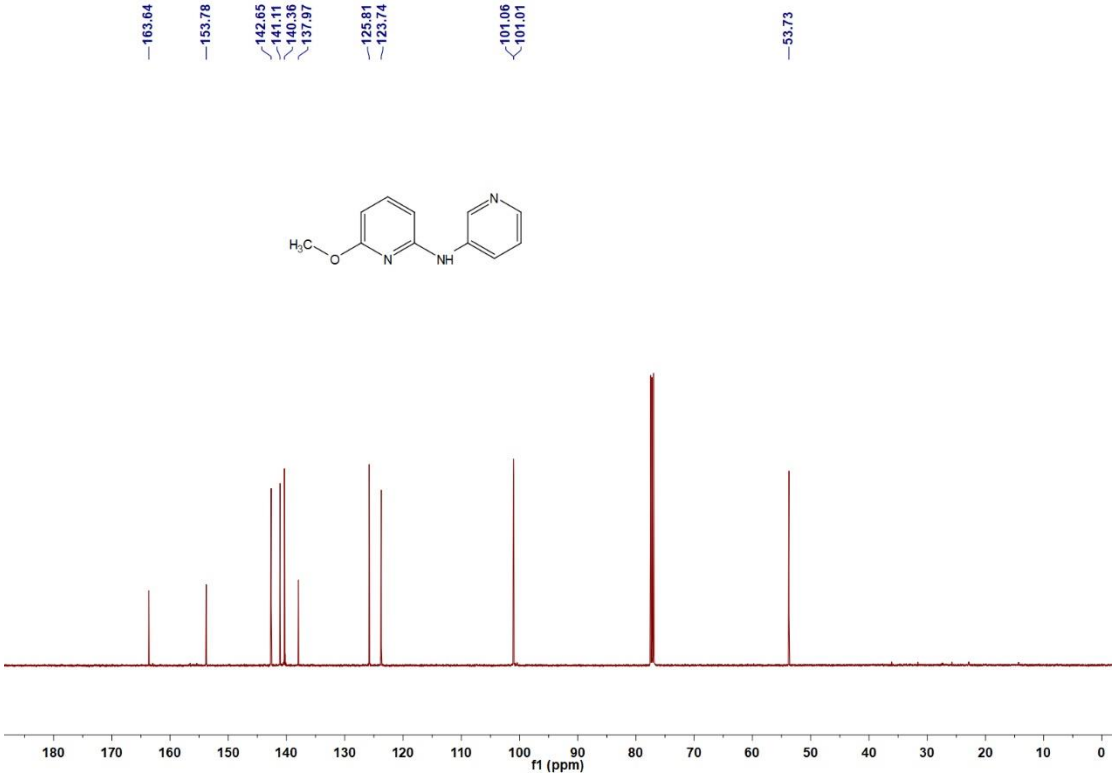
^{1}H NMR spectrum of 6g



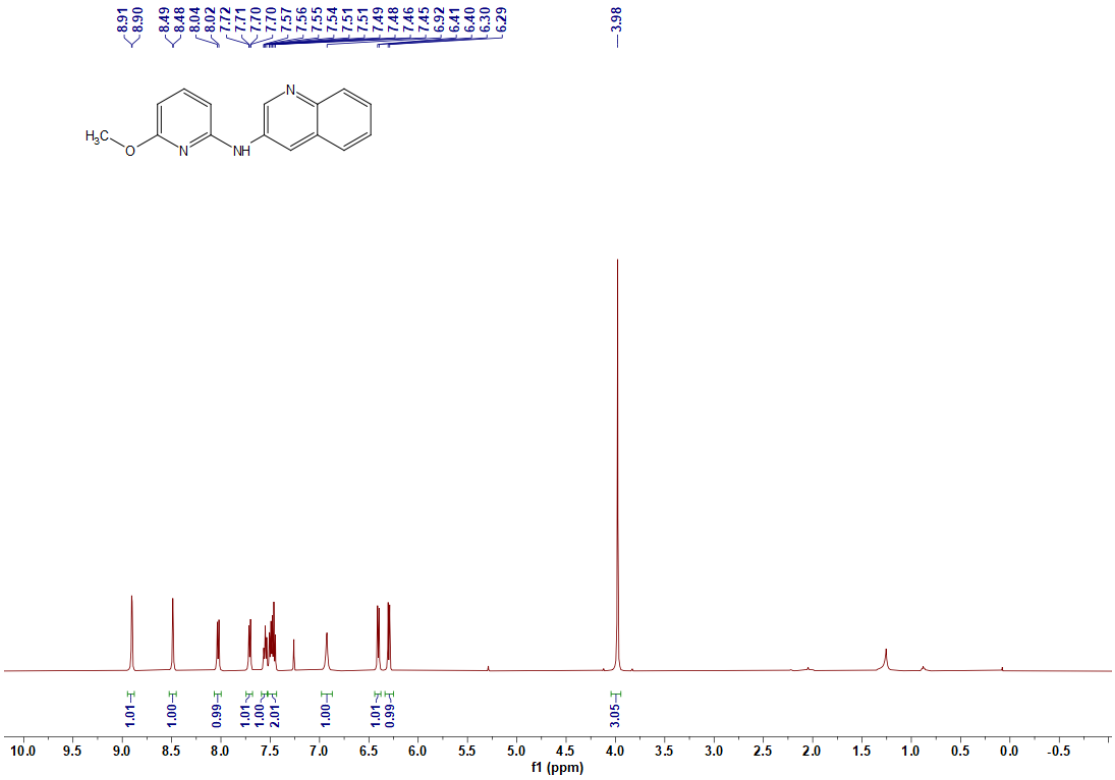
^{13}C NMR spectrum of 6g



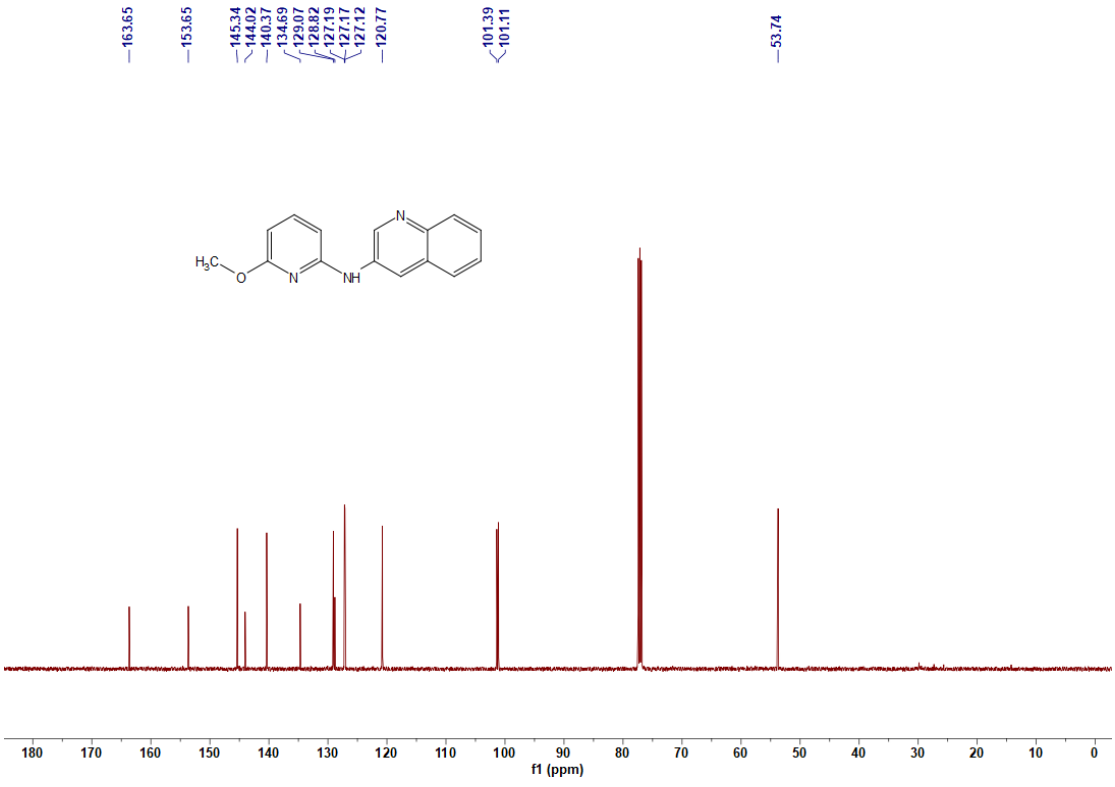
^{1}H NMR spectrum of 6h



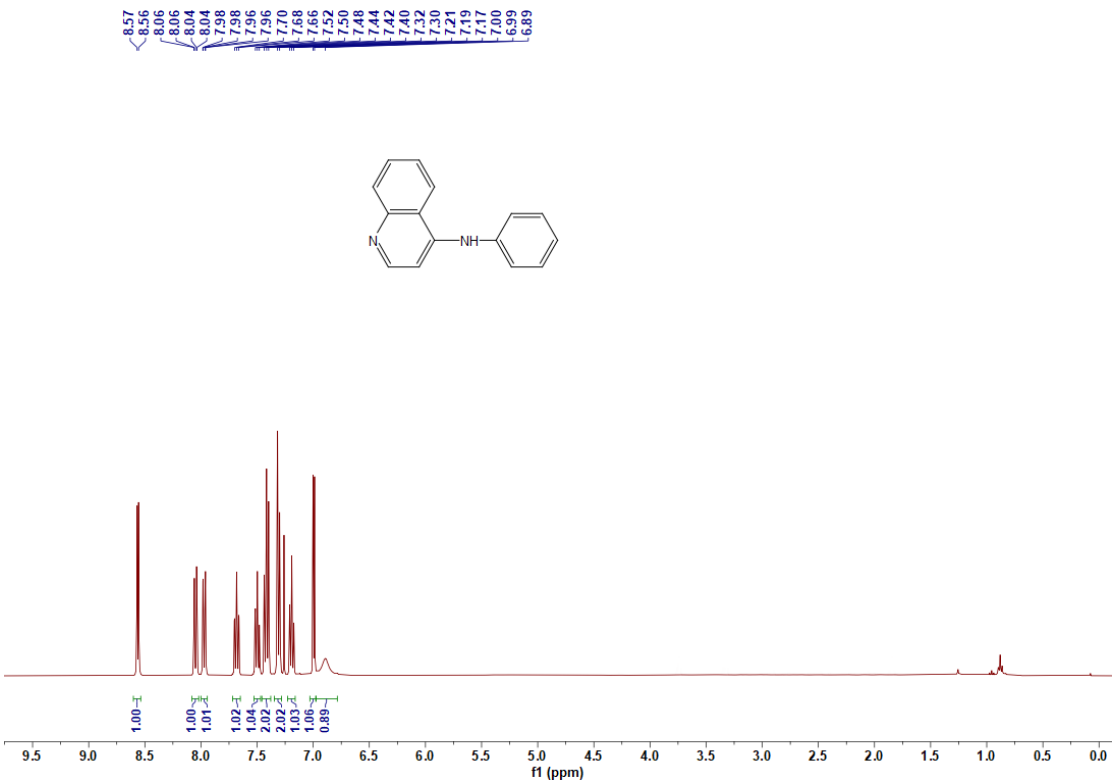
^{13}C NMR spectrum of 6h



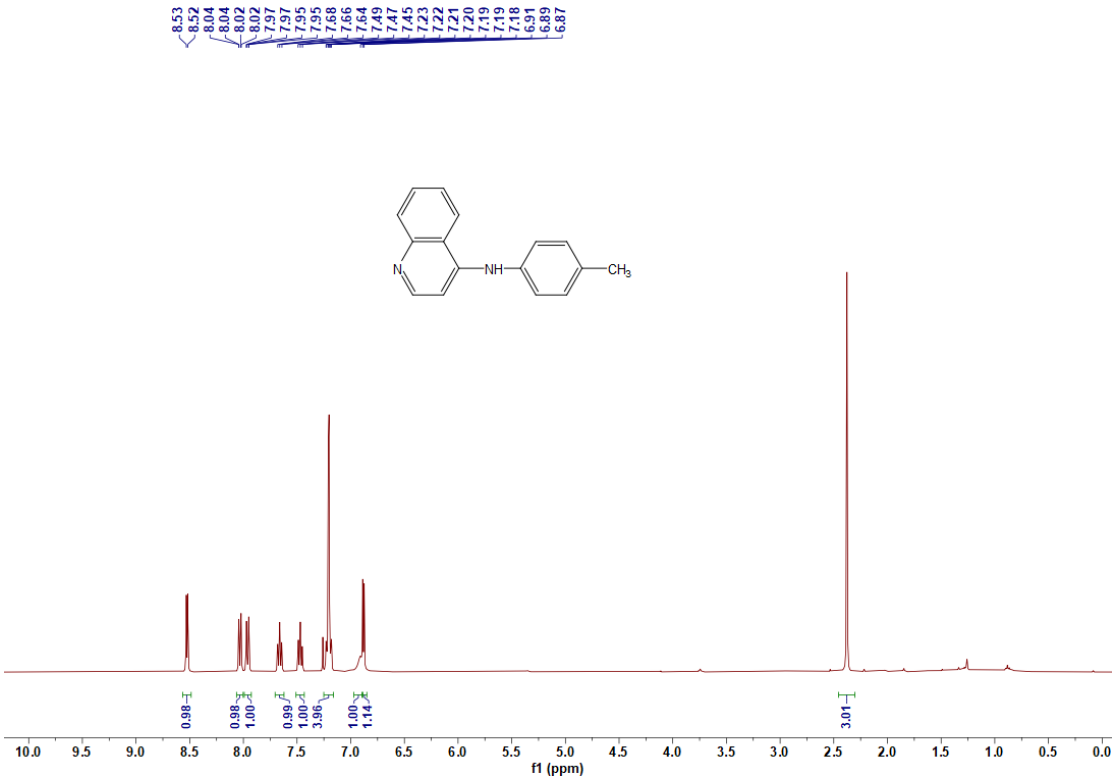
^{1}H NMR spectrum of 6i



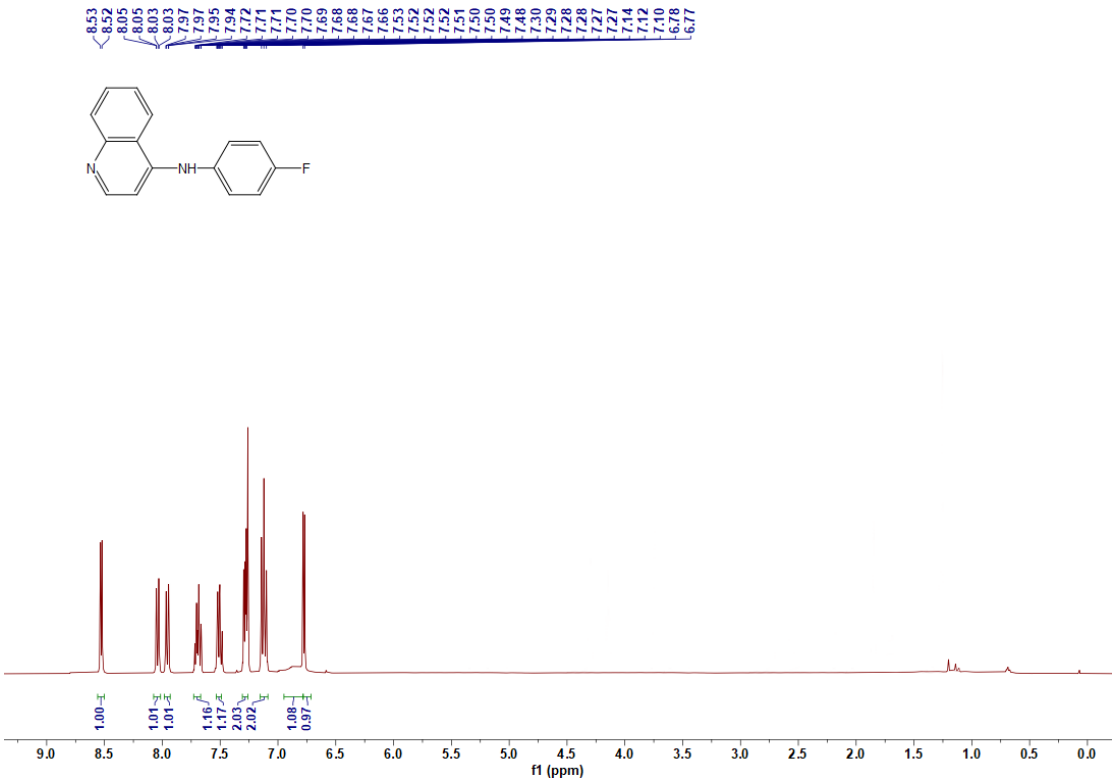
^{13}C NMR spectrum of 6i



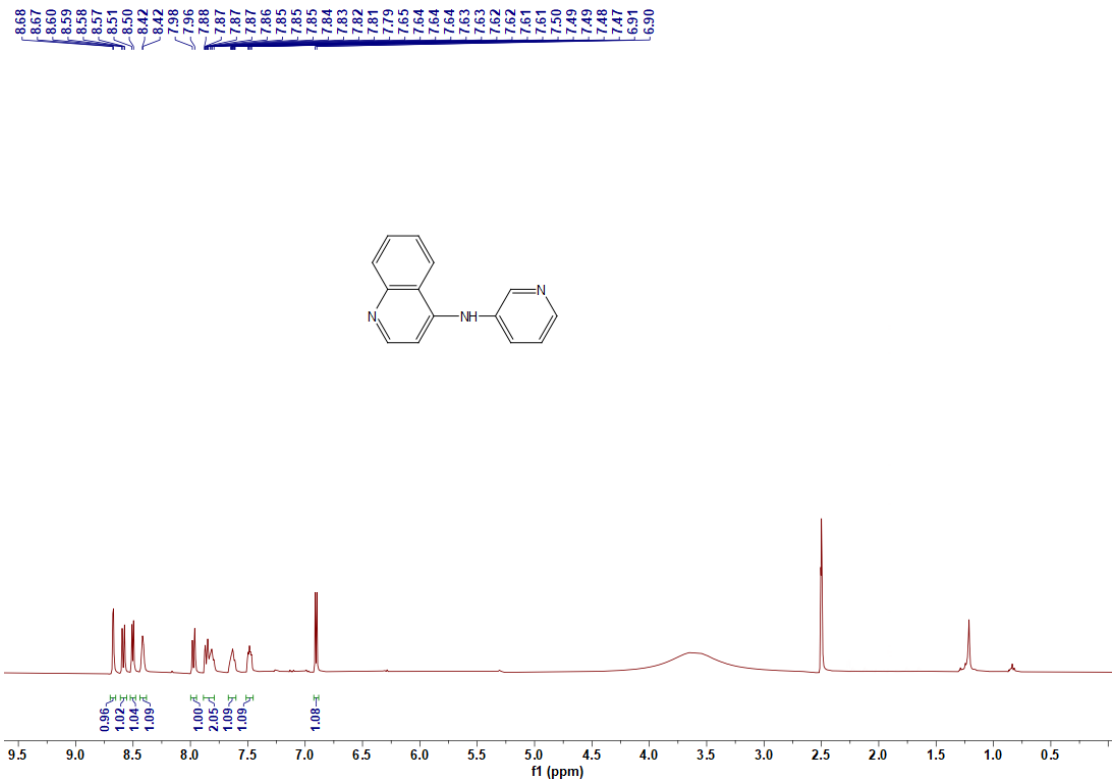
^{1}H NMR spectrum of 6j



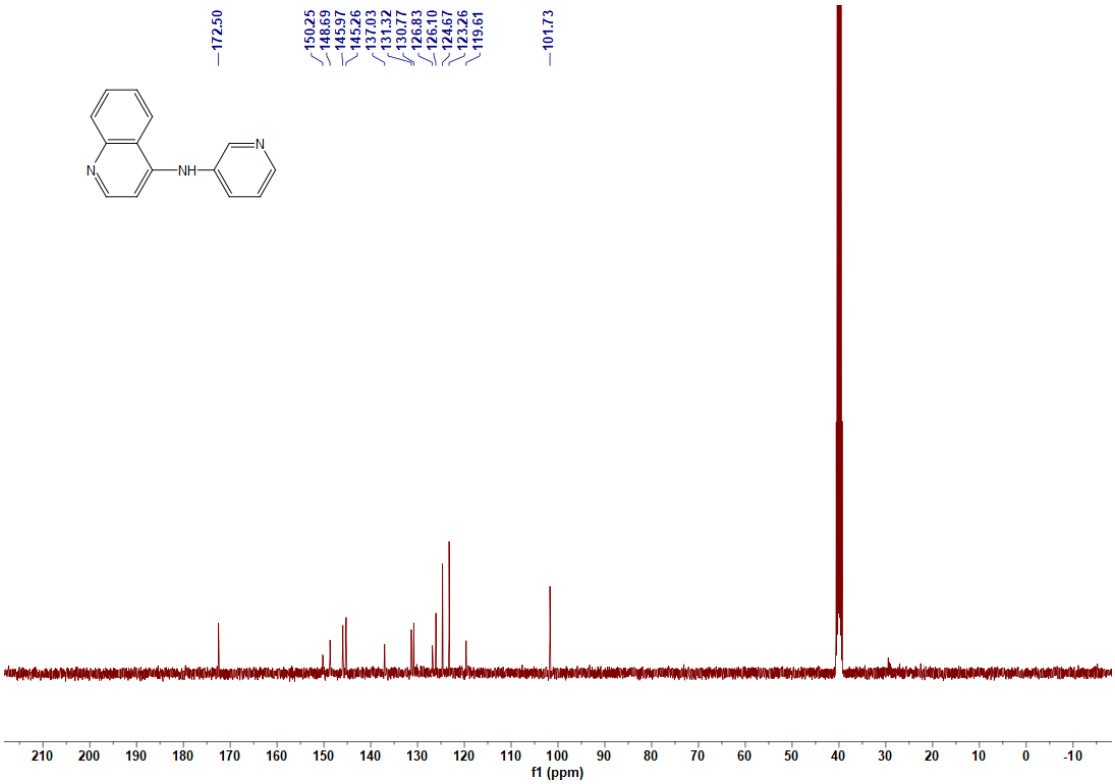
^{1}H NMR spectrum of 6k



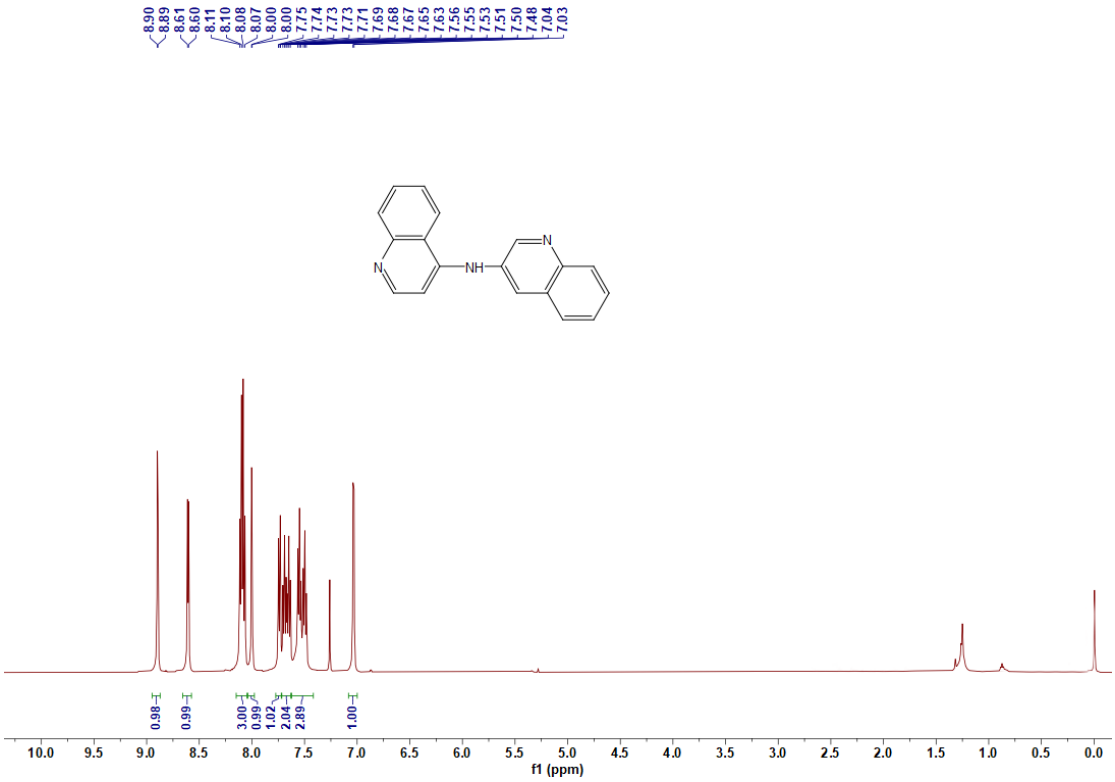
^{1}H NMR spectrum of 6l



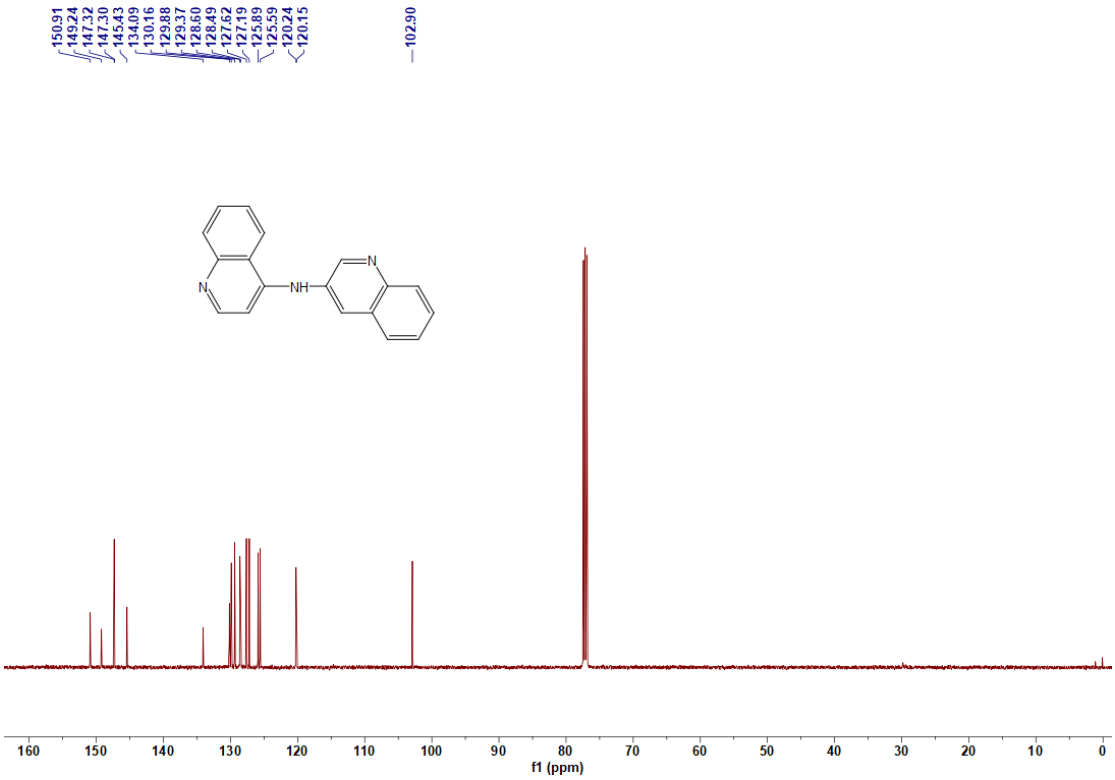
^{1}H NMR spectrum of 6m



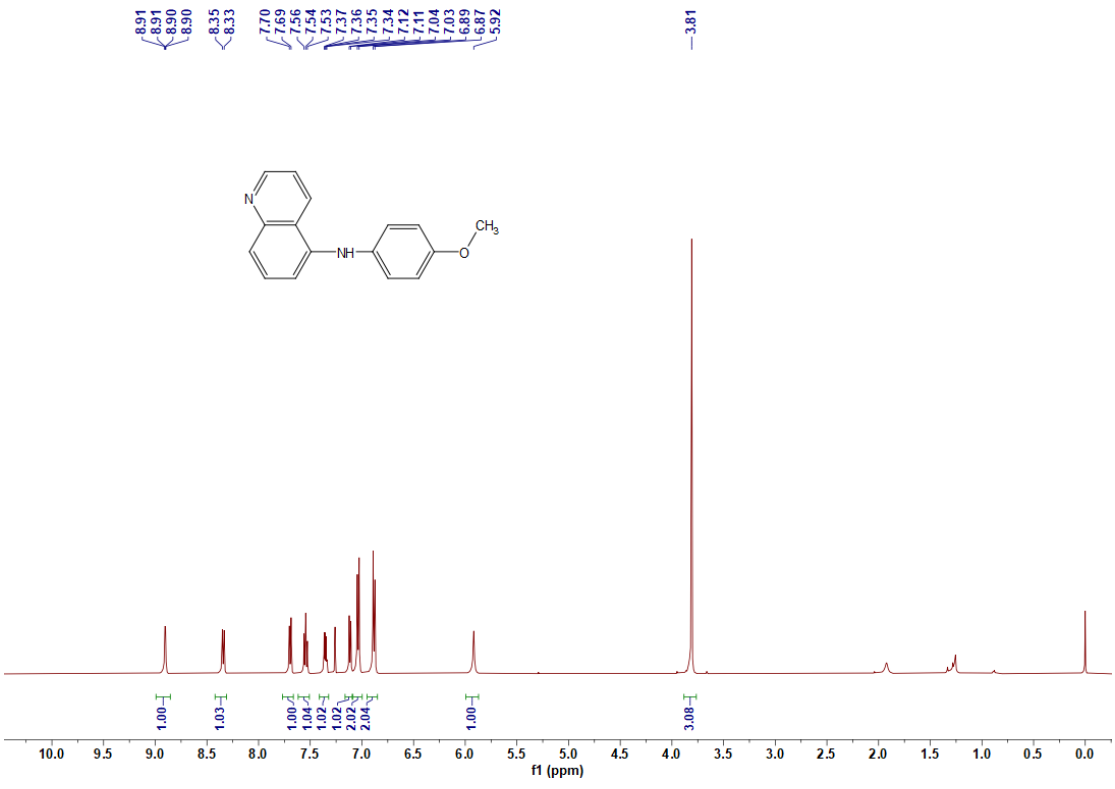
^{13}C NMR spectrum of 6m



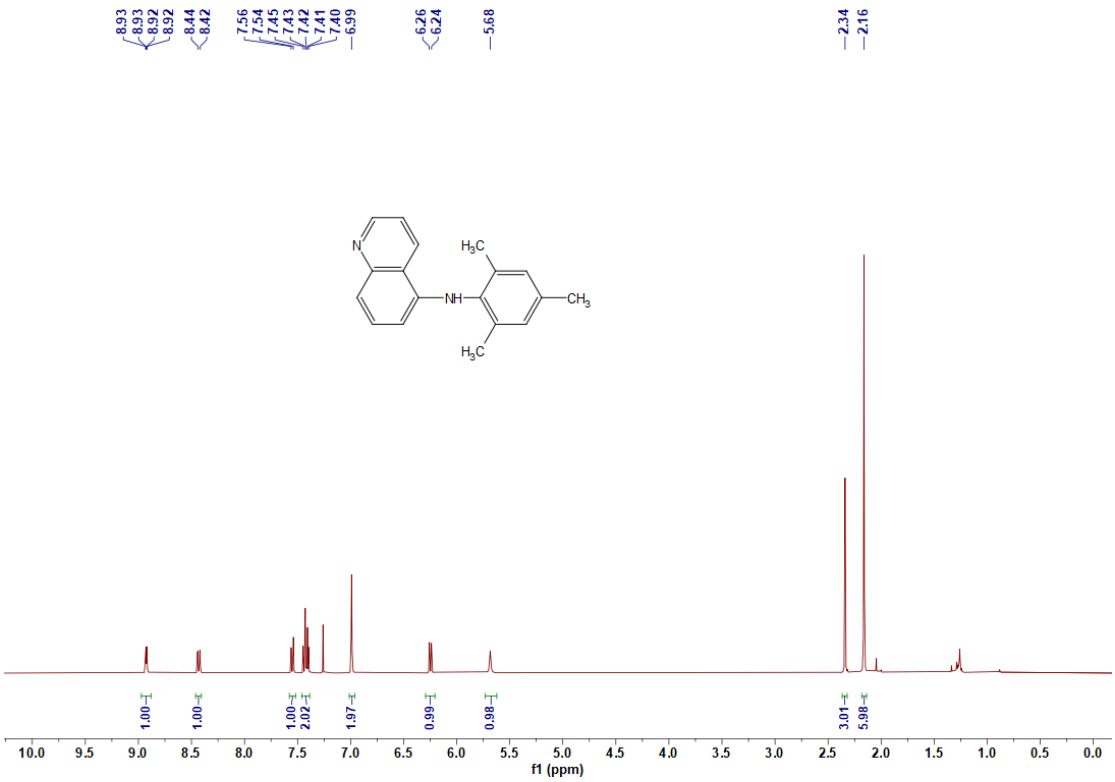
^{1}H NMR spectrum of 6n



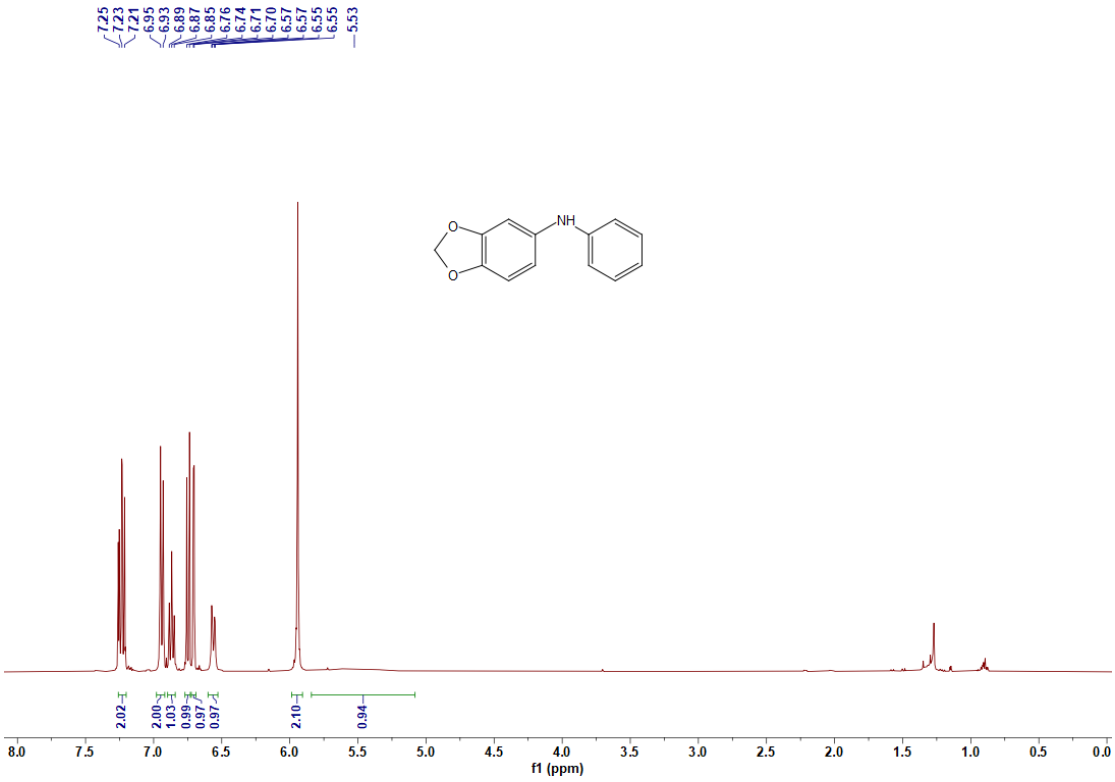
^{13}C NMR spectrum of 6n



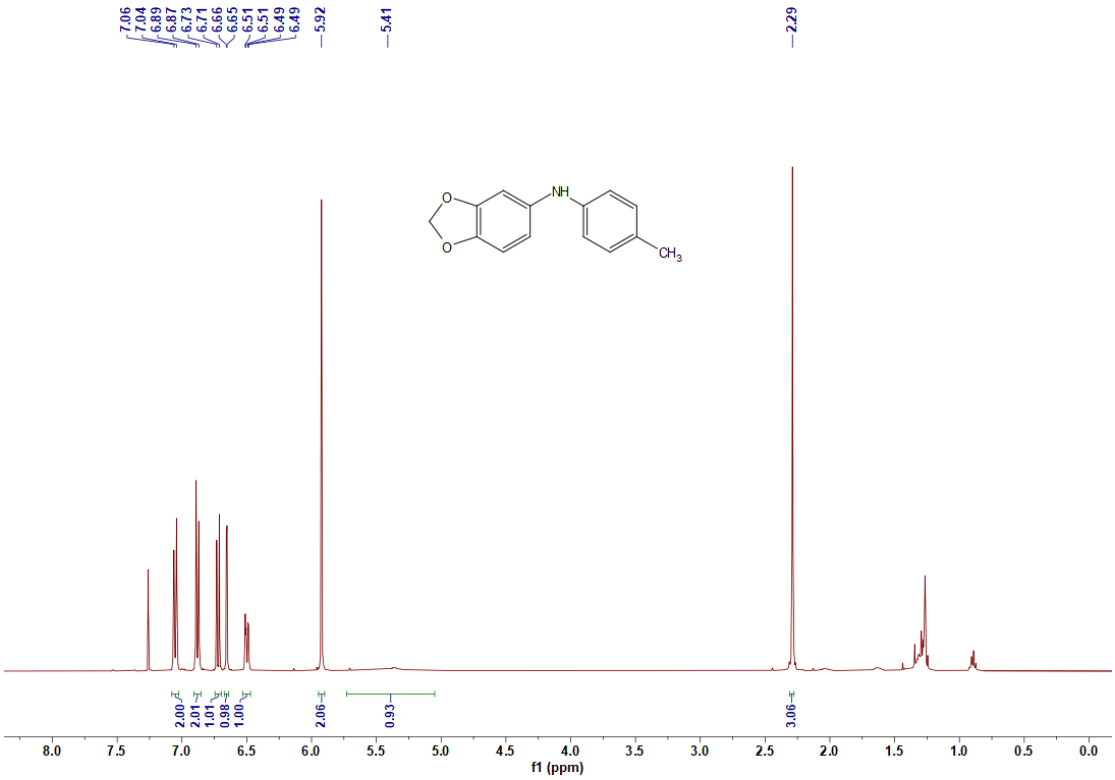
^{1}H NMR spectrum of 6o



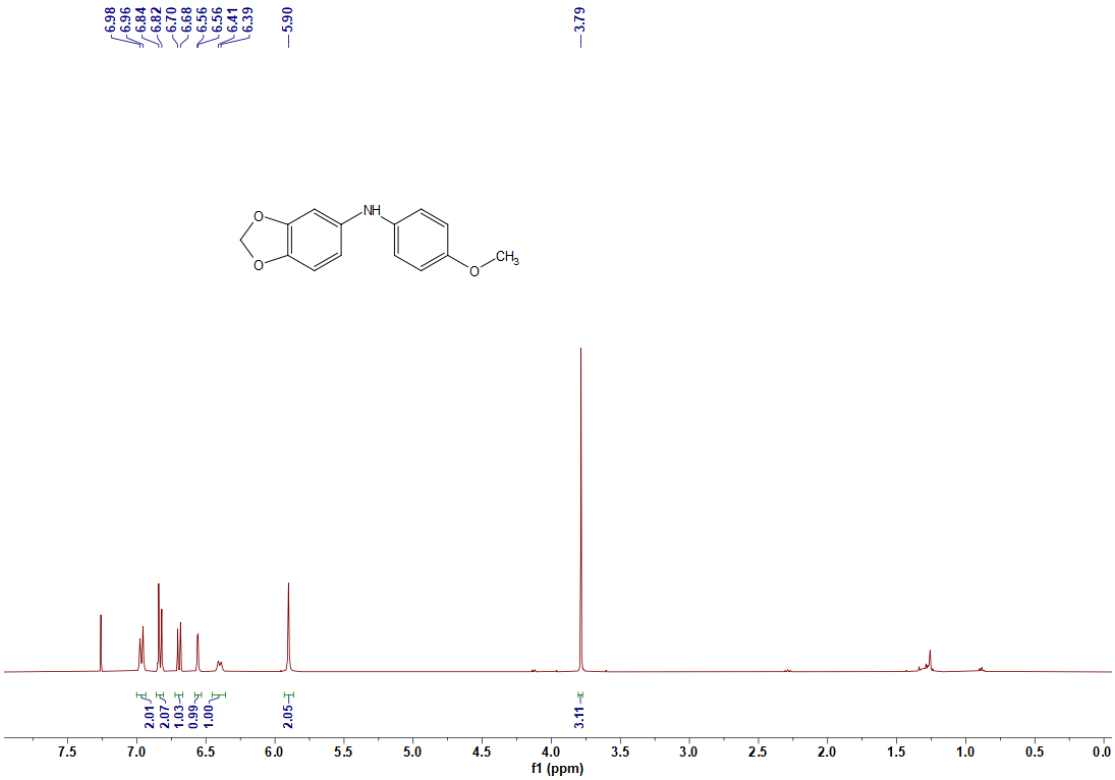
^{1}H NMR spectrum of 6p



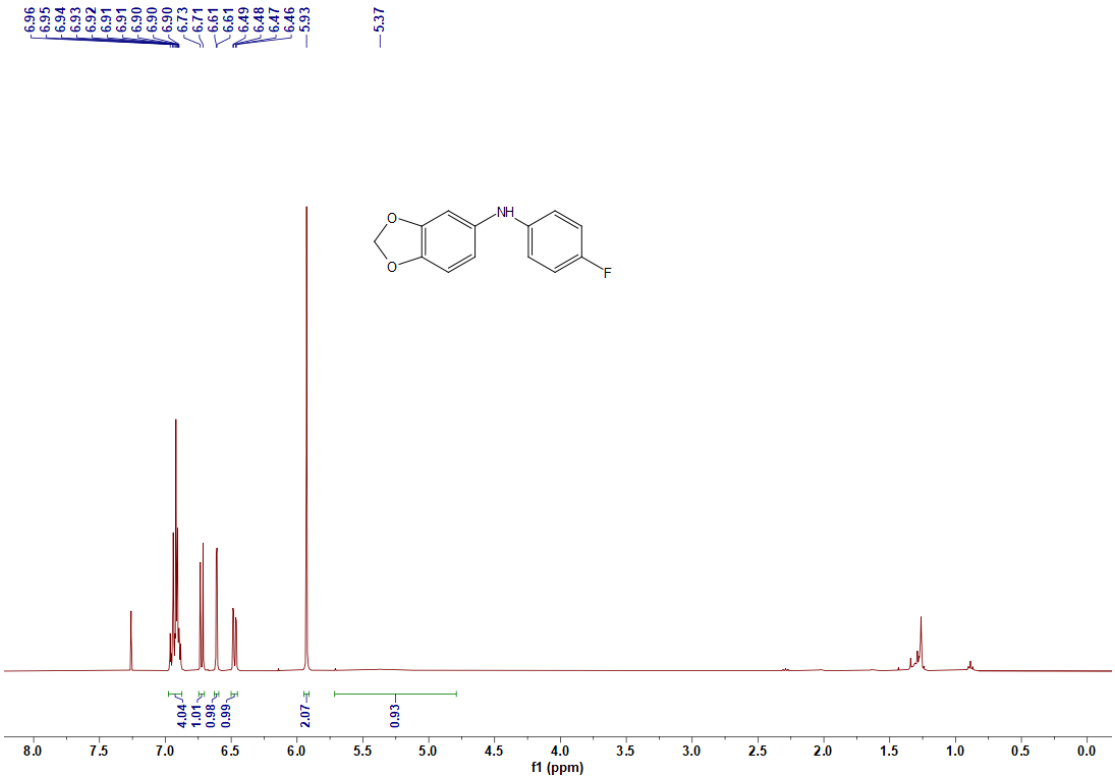
^{1}H NMR spectrum of 6q



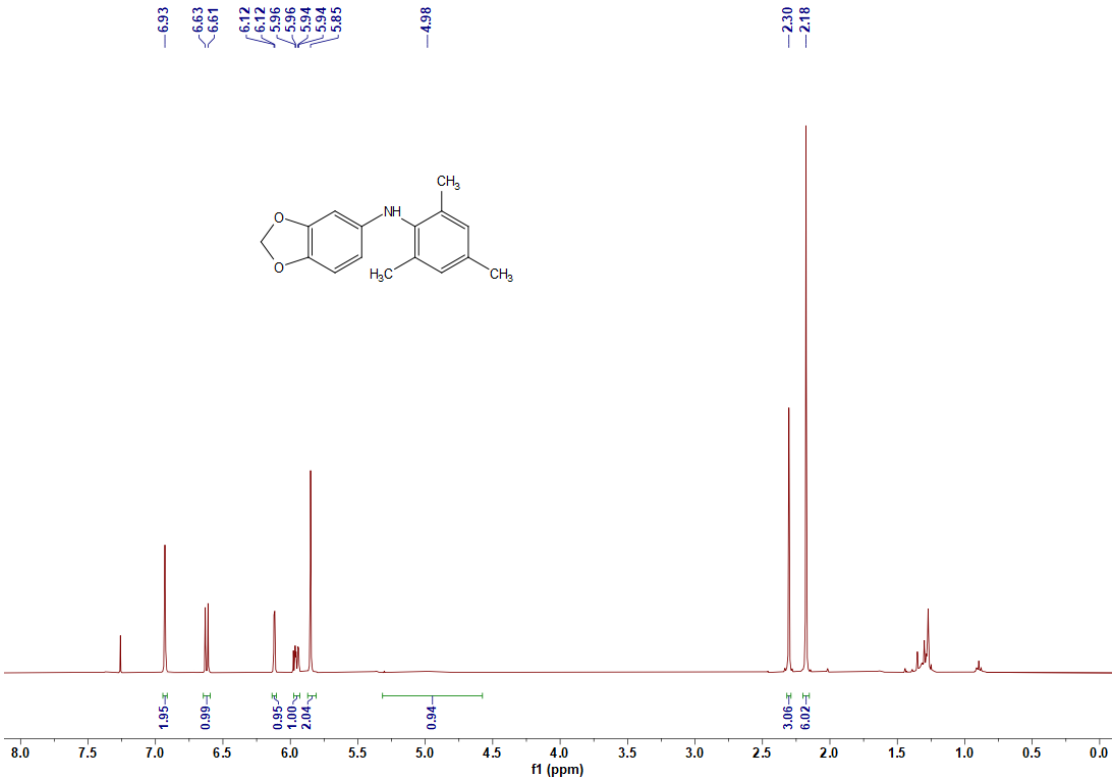
^{1}H NMR spectrum of 6r



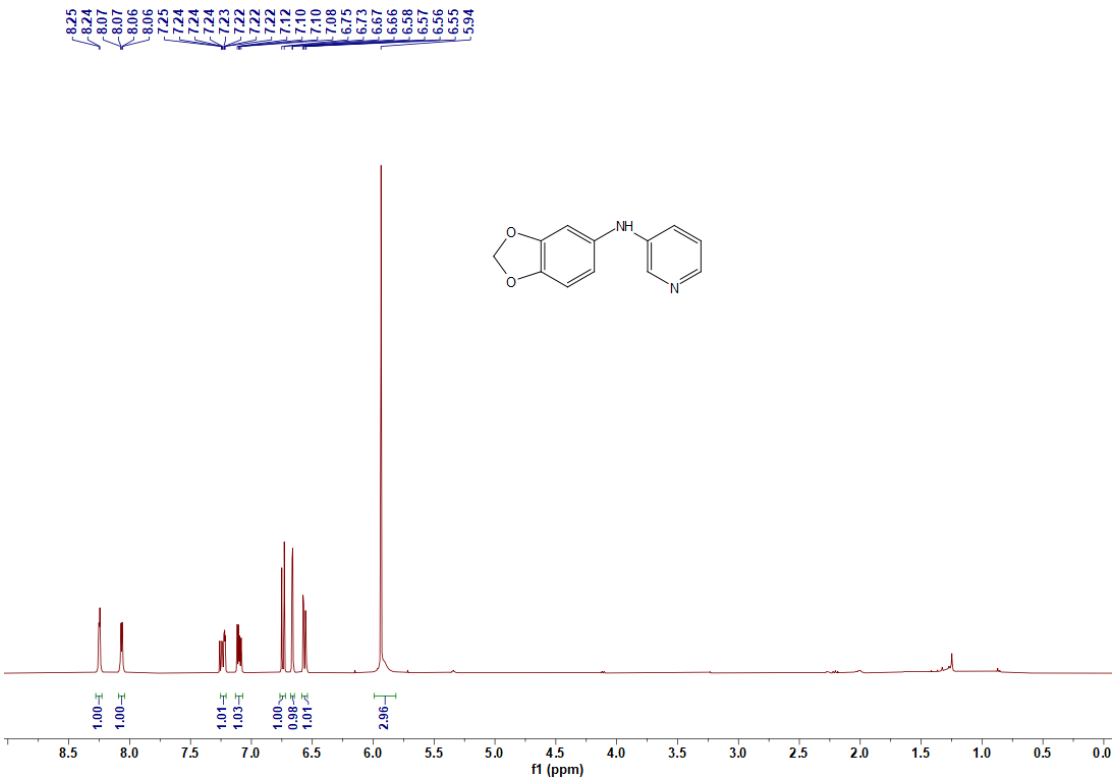
^{1}H NMR spectrum of 6s



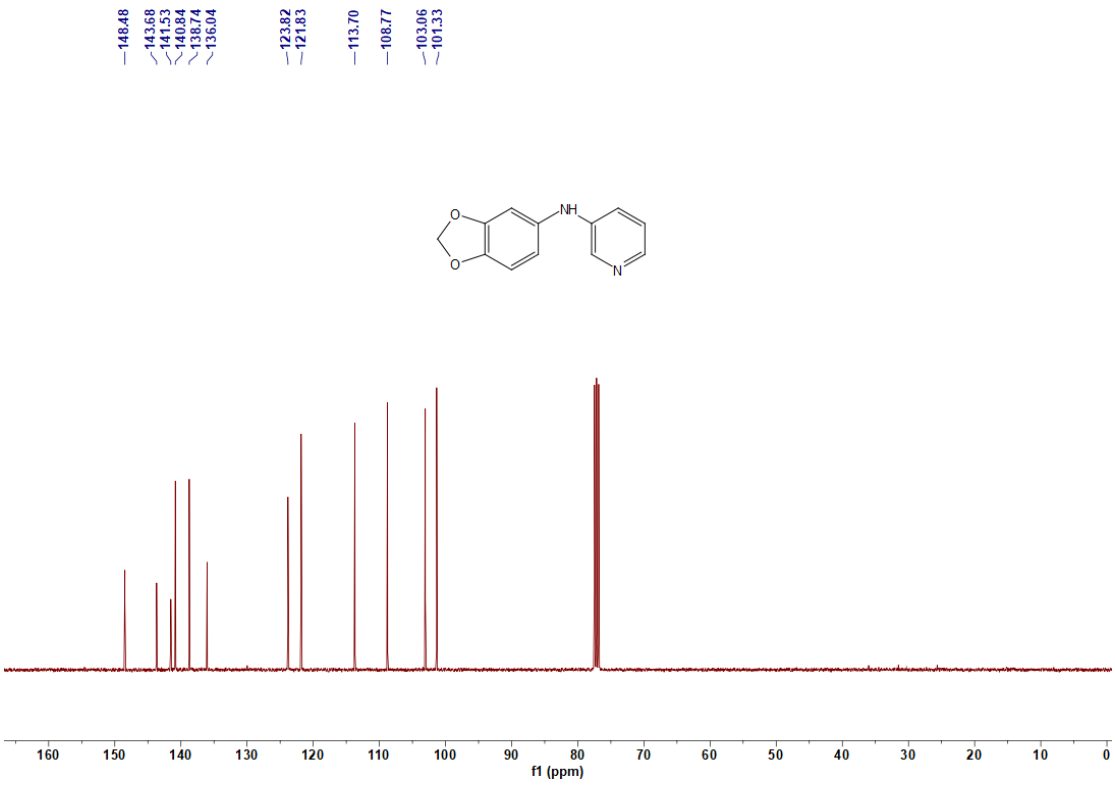
^{1}H NMR spectrum of 6t



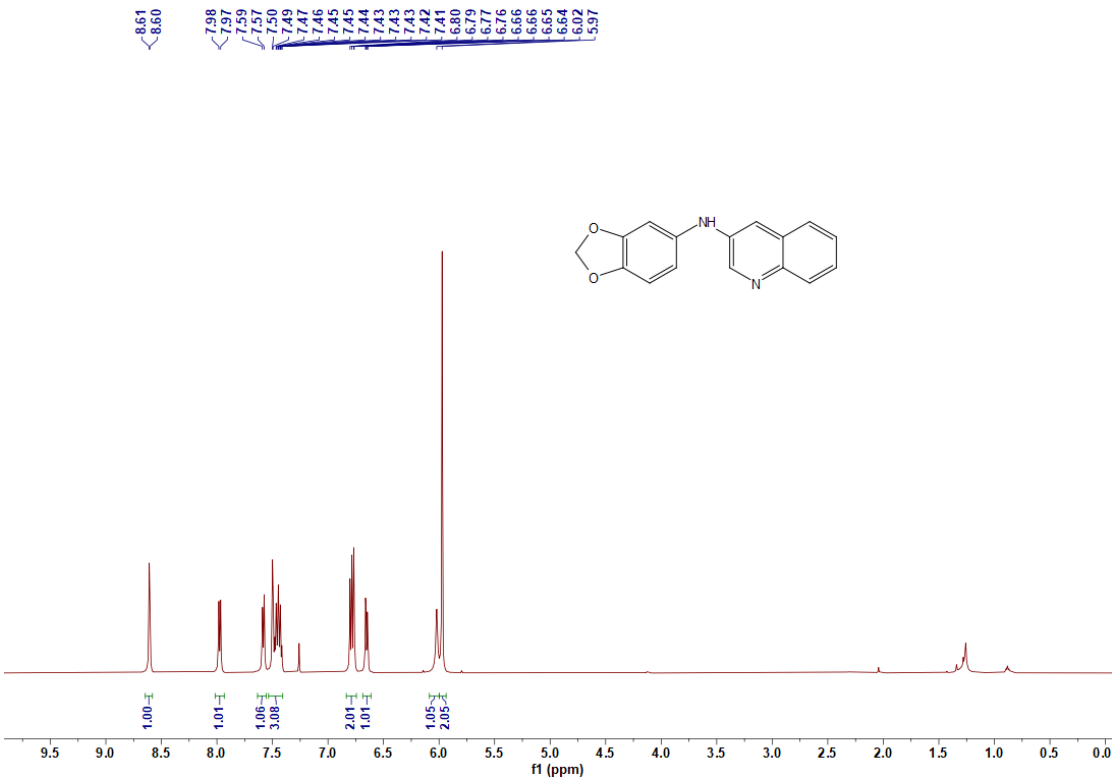
^{1}H NMR spectrum of 6u



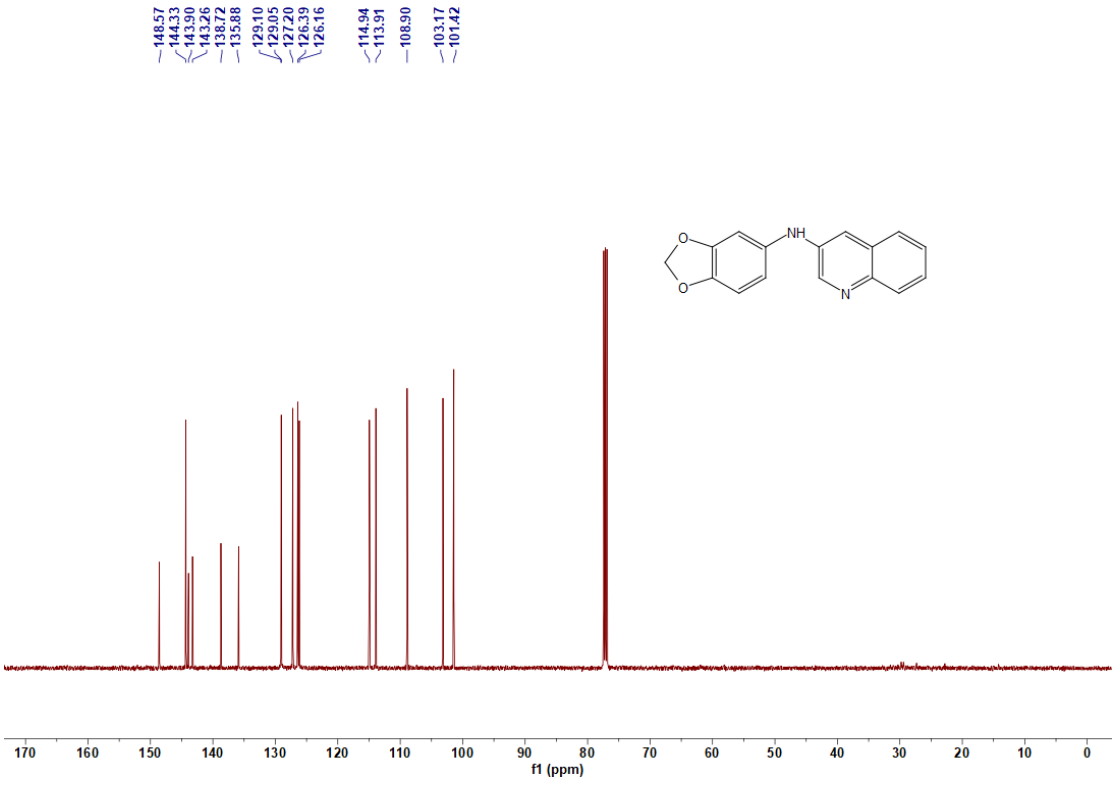
^{1}H NMR spectrum of 6v



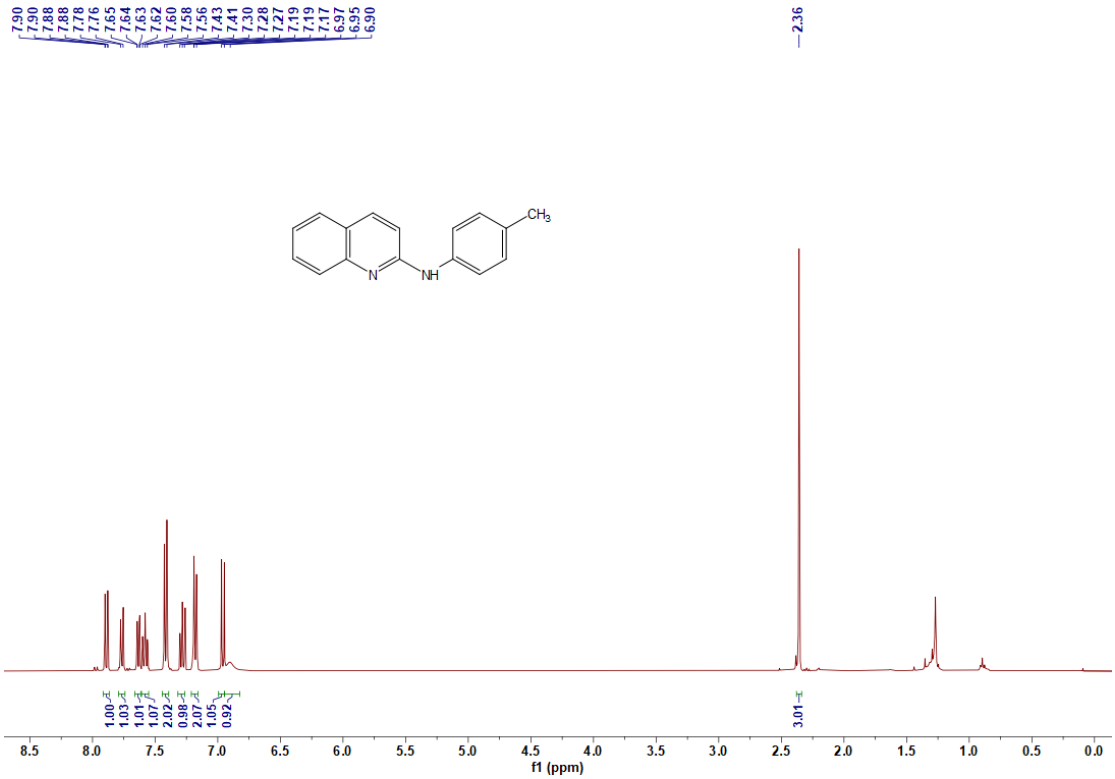
^{13}C NMR spectrum of 6v



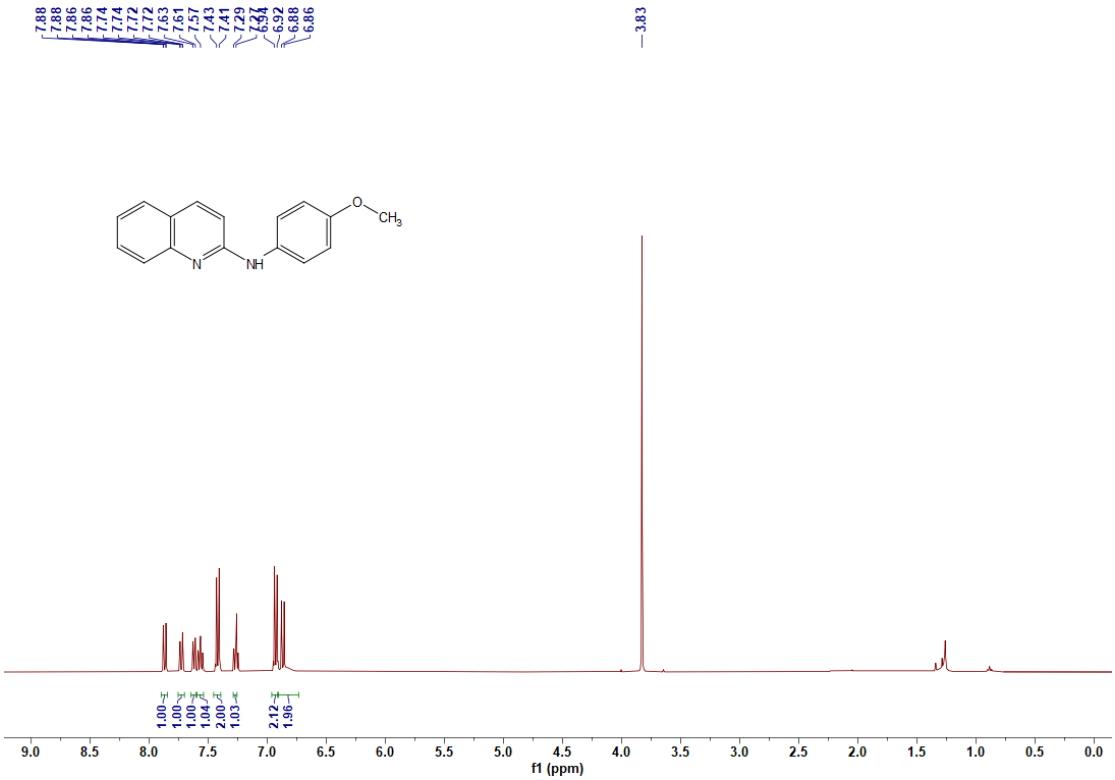
^{1}H NMR spectrum of 6w



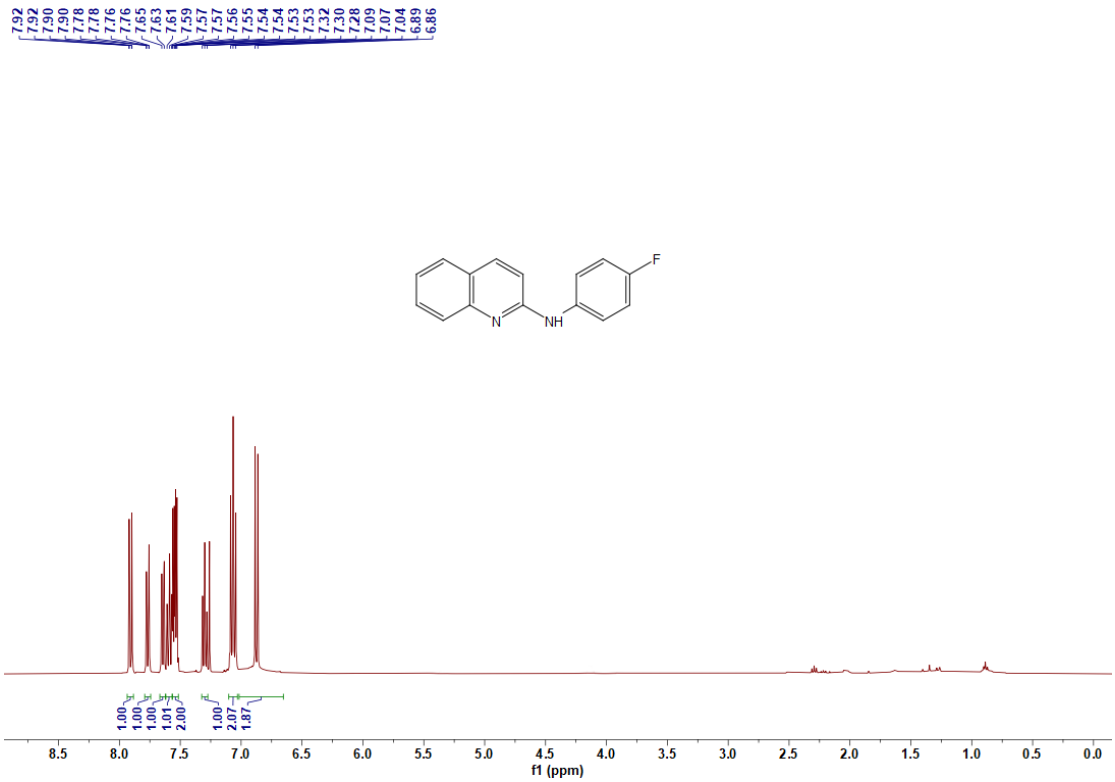
^{13}C NMR spectrum of 6w



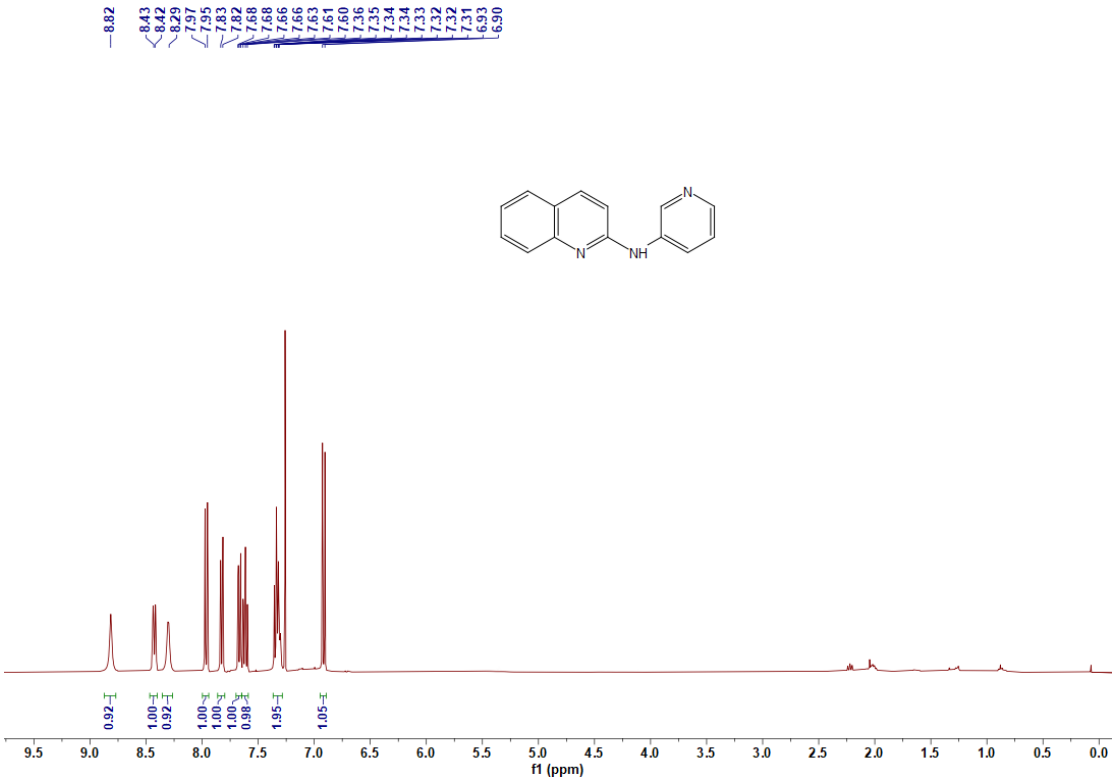
^{1}H NMR spectrum of 6x



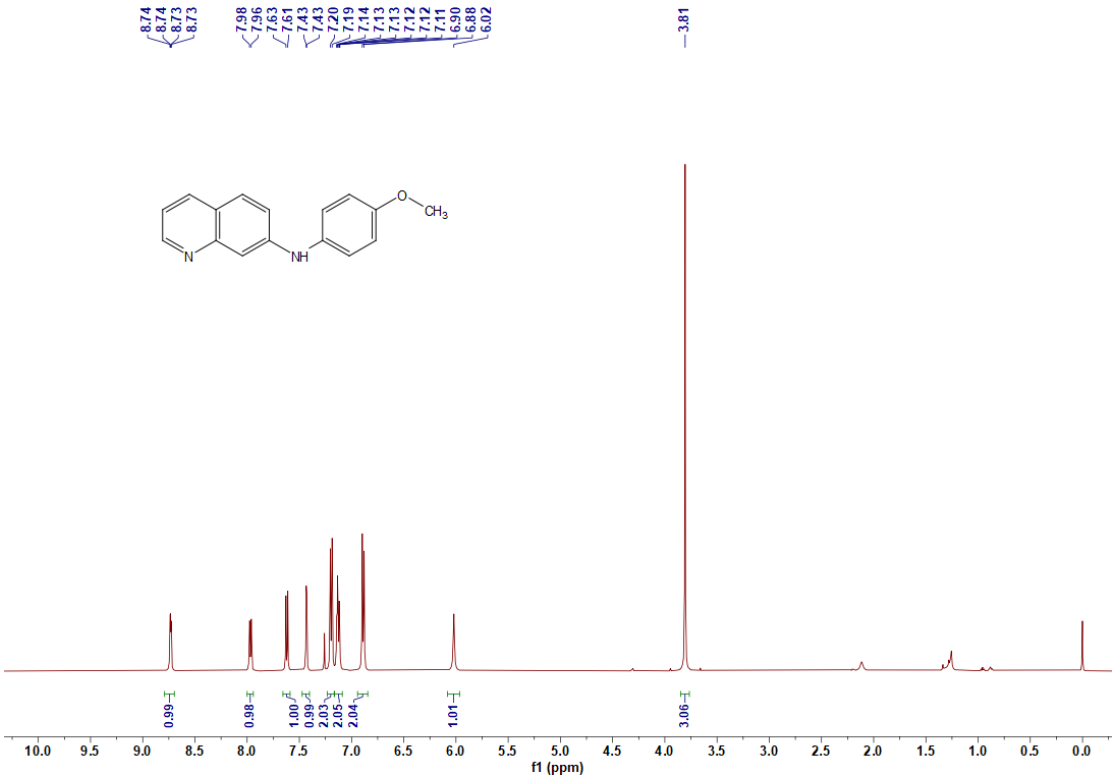
^{1}H NMR spectrum of 6y



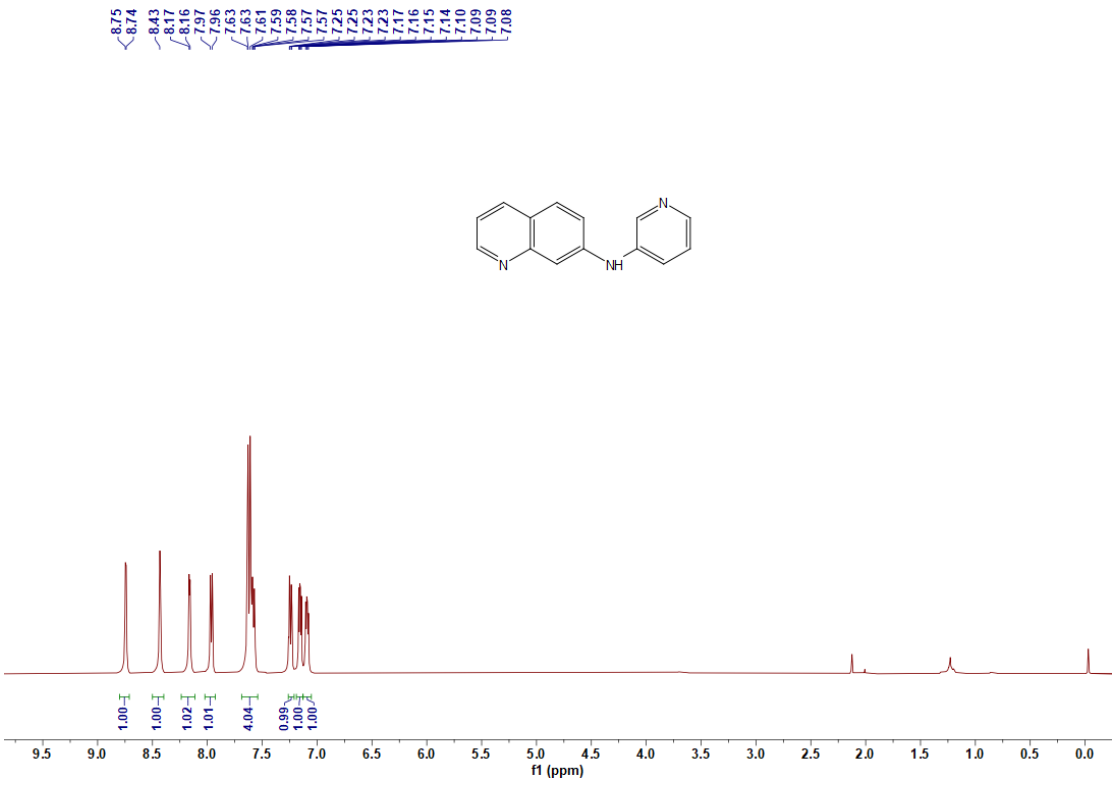
^{1}H NMR spectrum of 6z



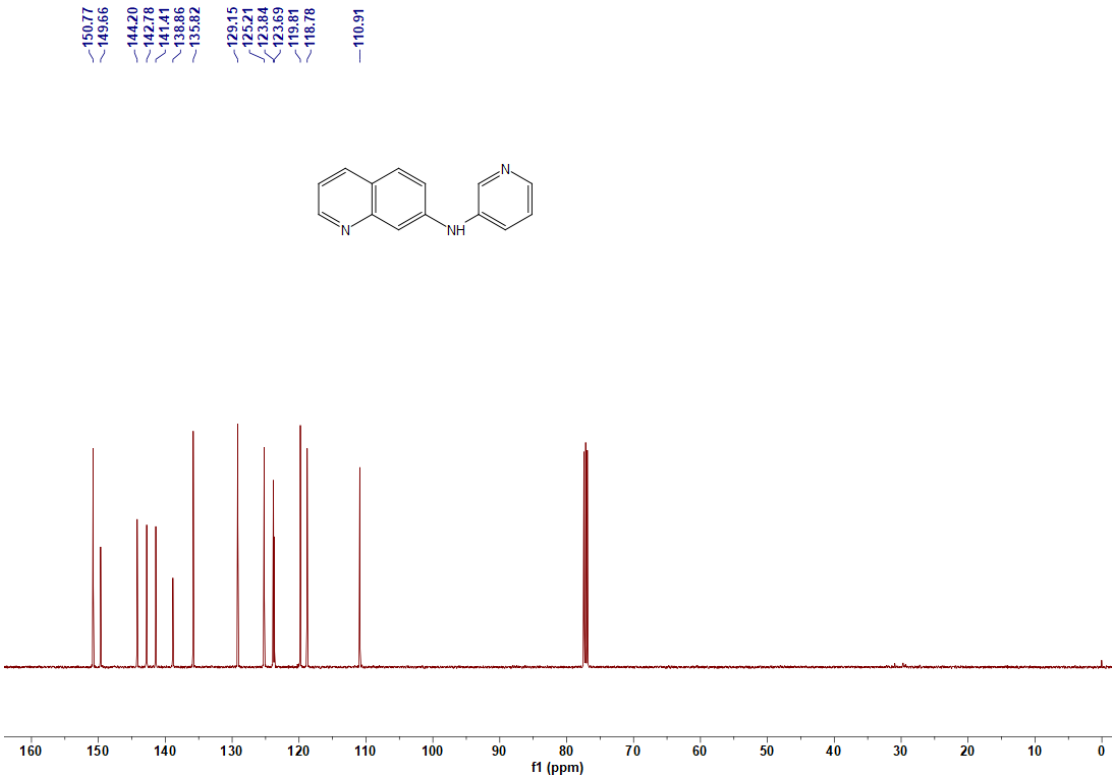
^{1}H NMR spectrum of 6aa



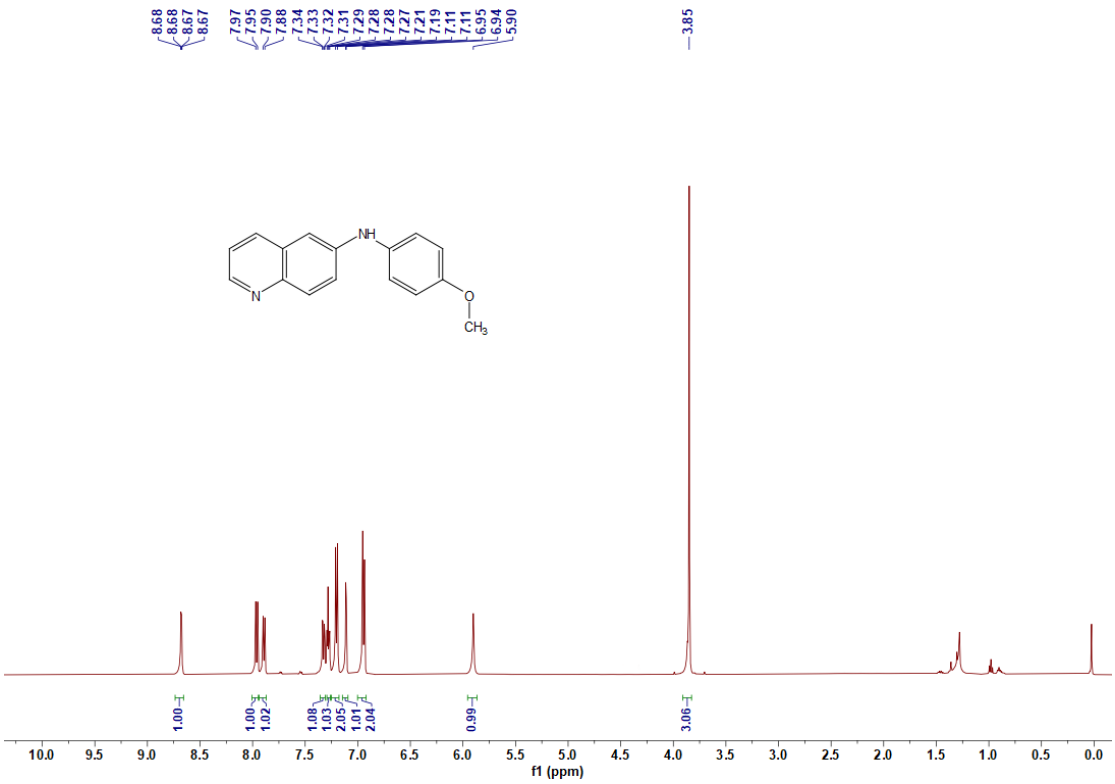
^{1}H NMR spectrum of 6ab



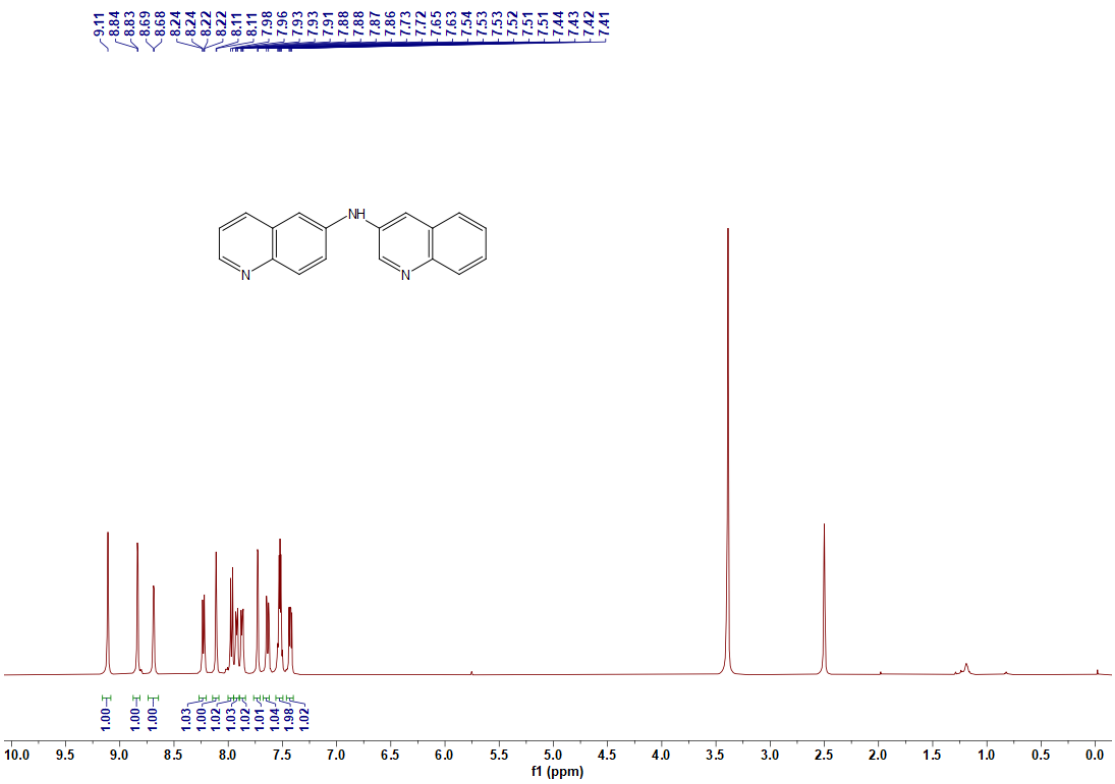
^{1}H NMR spectrum of 6ac



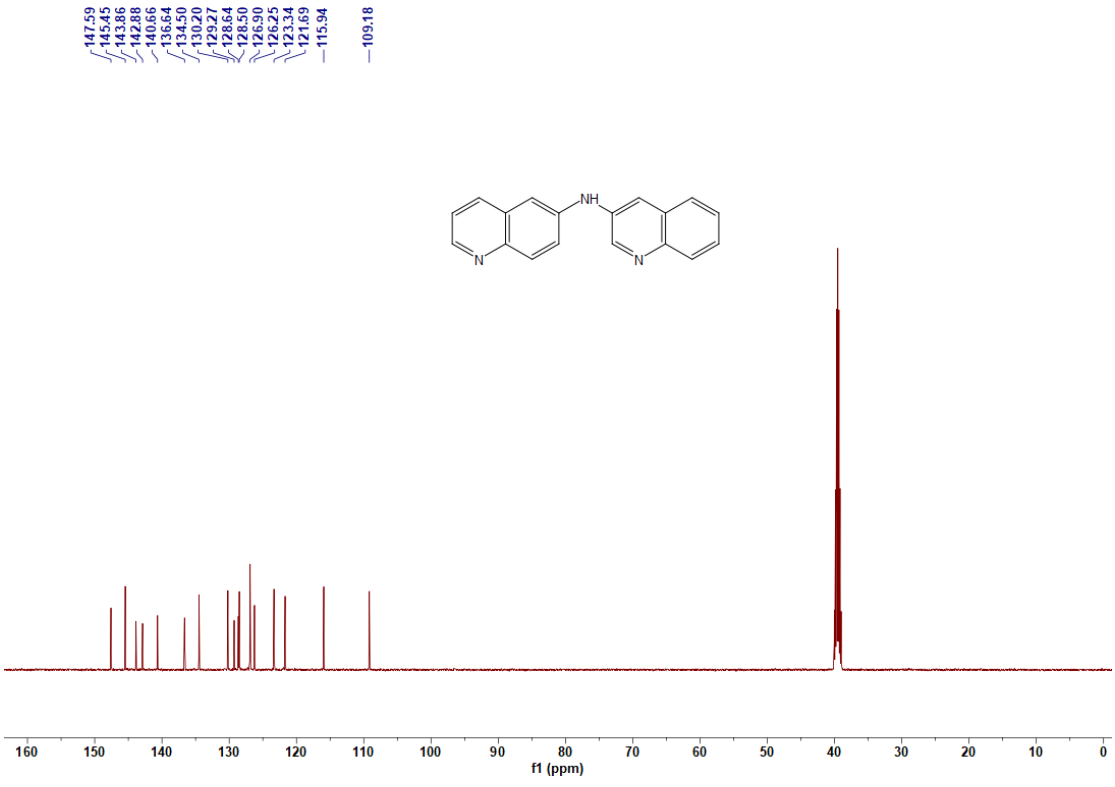
^{13}C NMR spectrum of 6ac



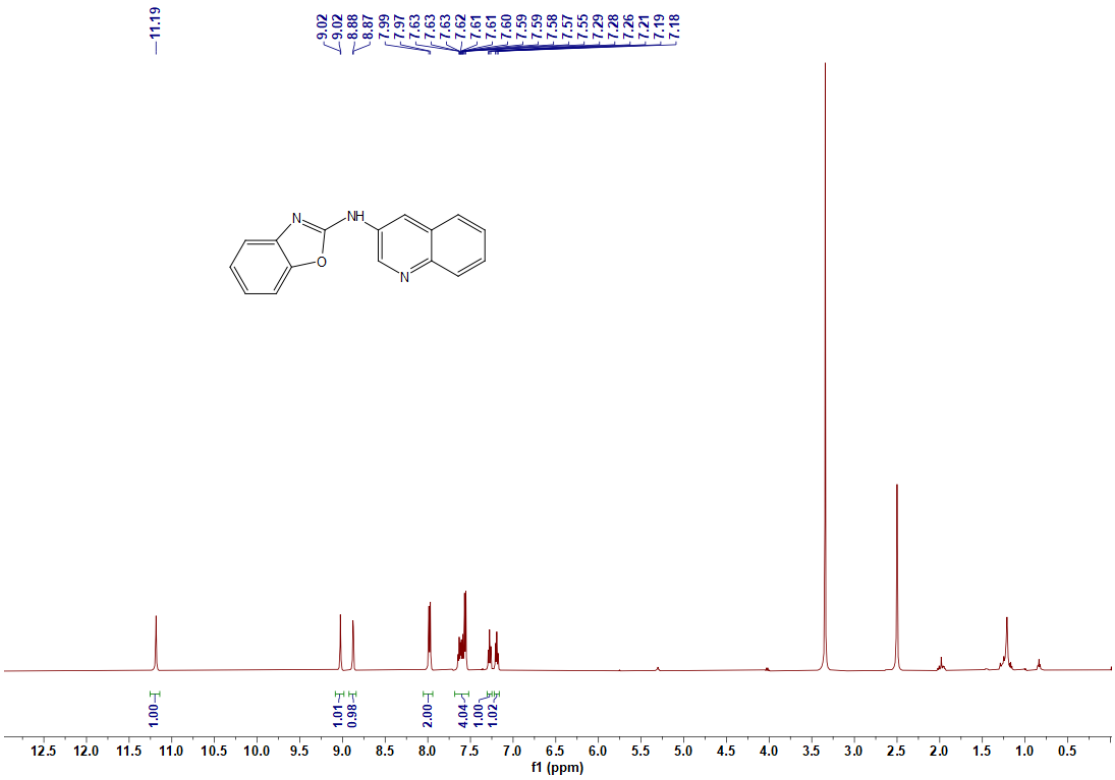
^{1}H NMR spectrum of 6ad



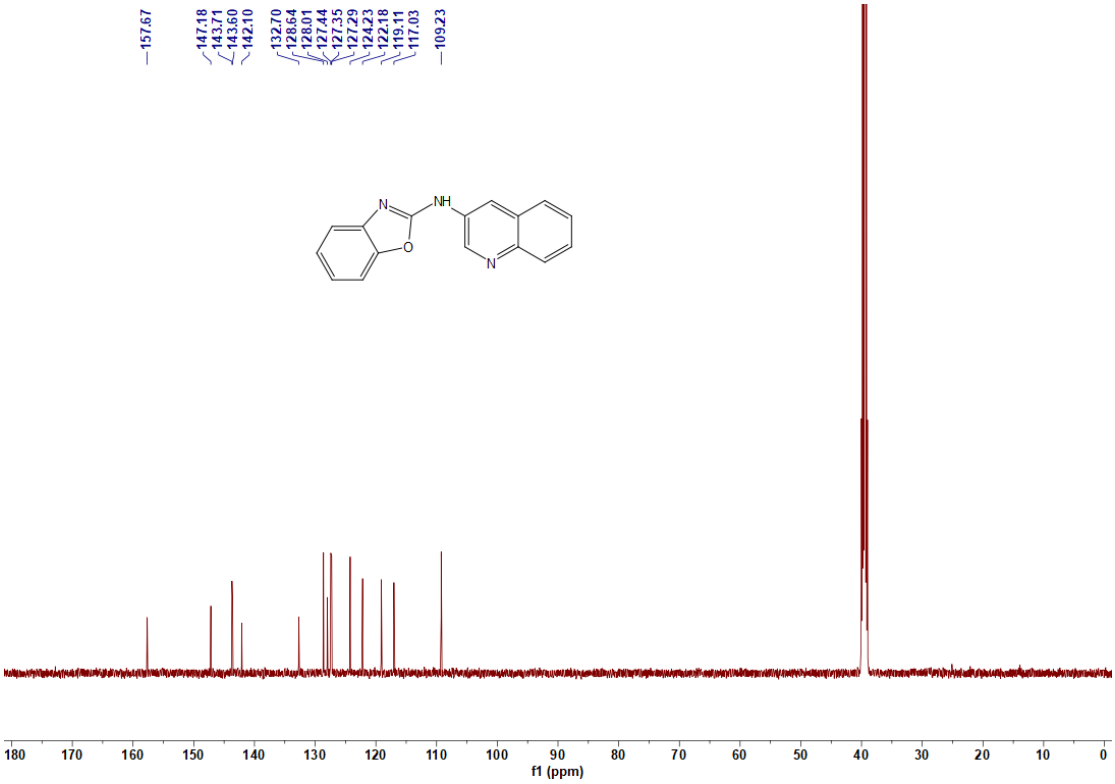
^{1}H NMR spectrum of 6ae



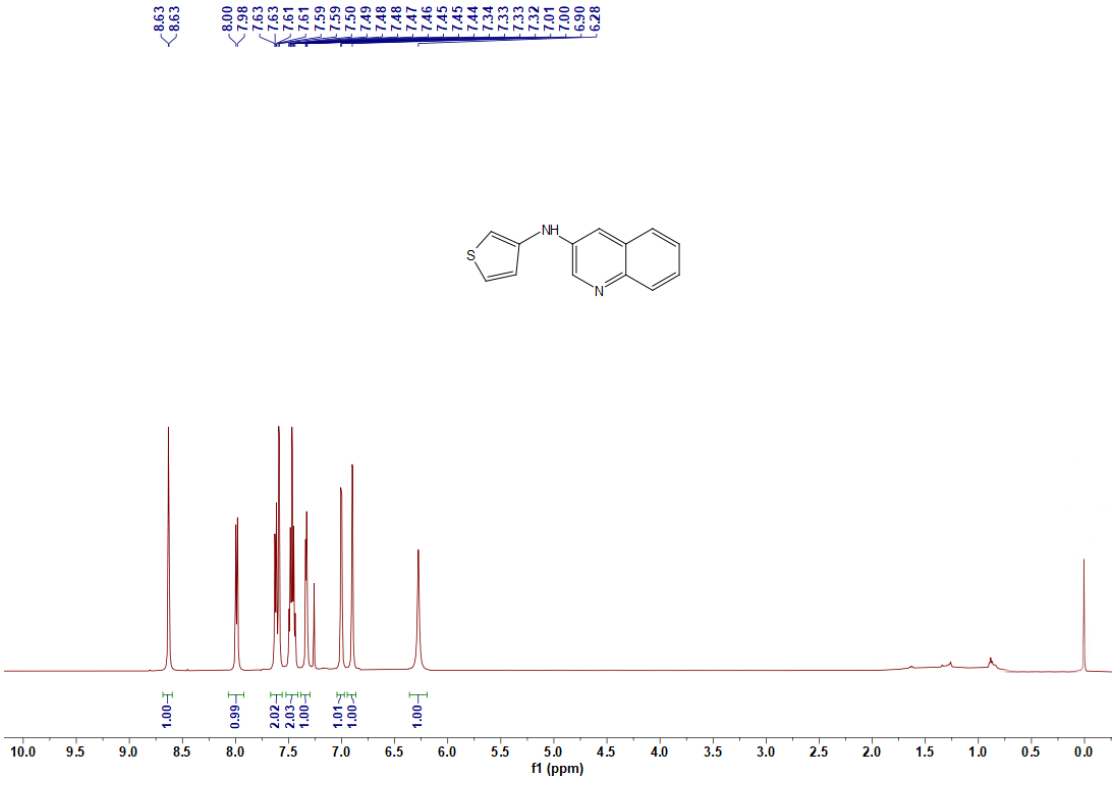
^{13}C NMR spectrum of 6ae



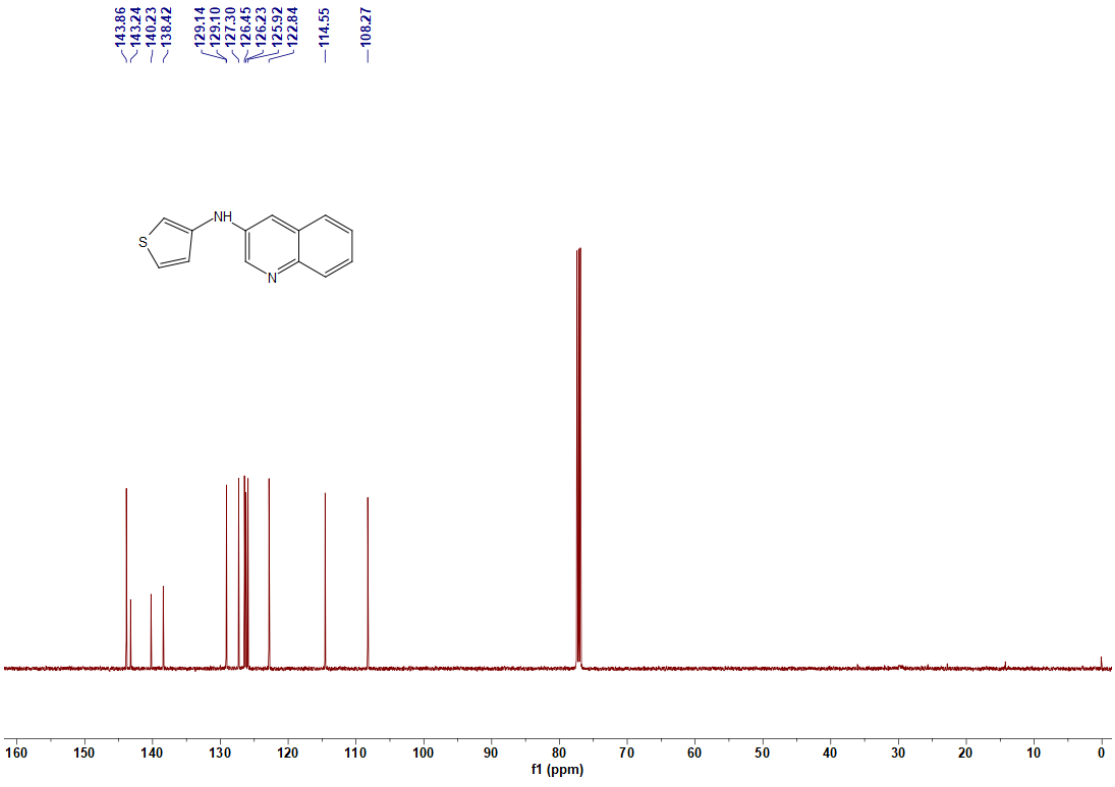
^{1}H NMR spectrum of 6af



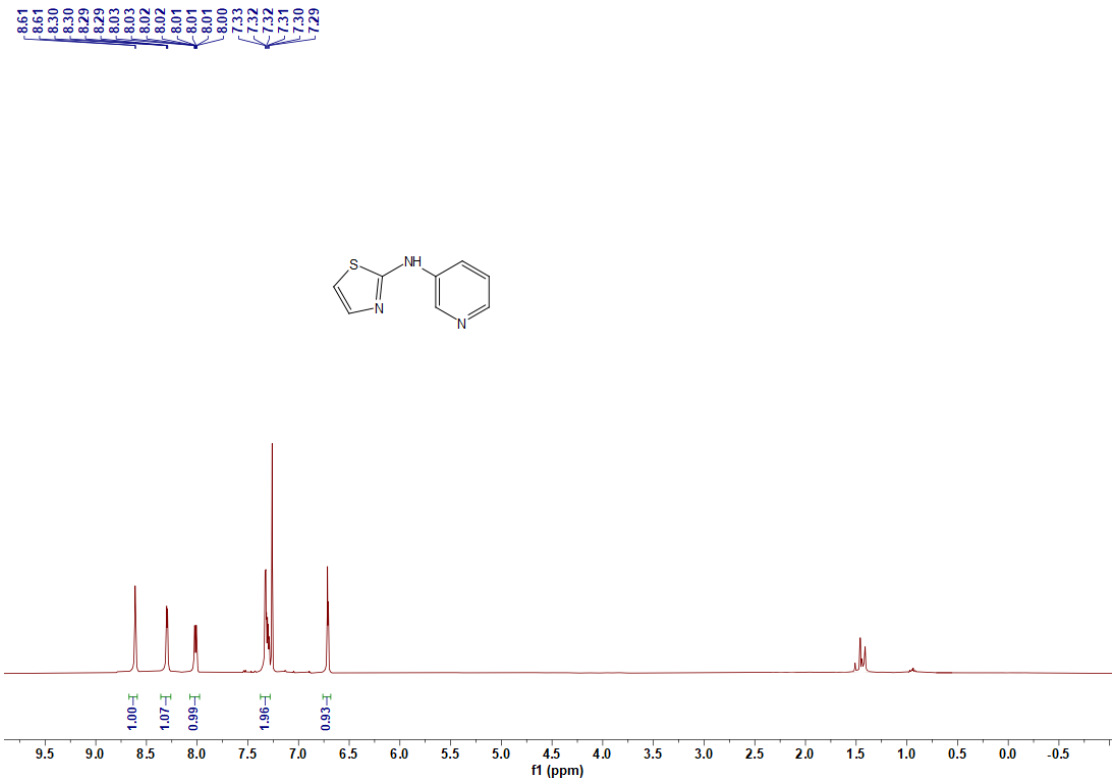
^{13}C NMR spectrum of 6af



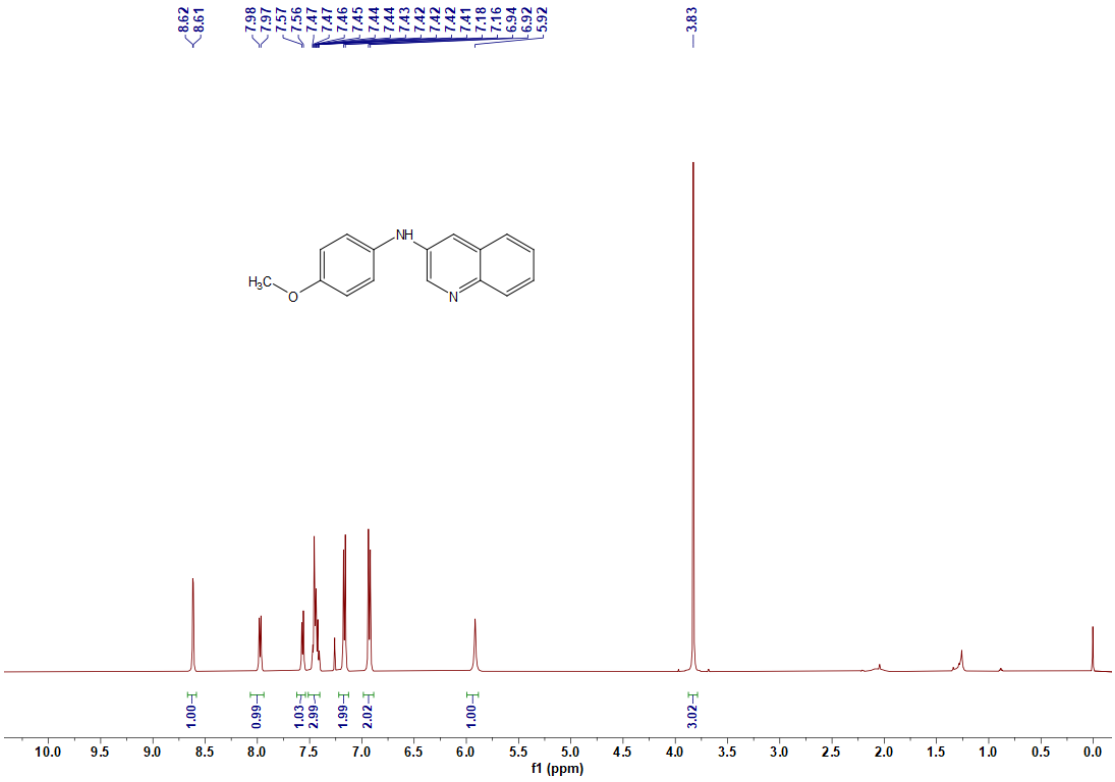
^{1}H NMR spectrum of 6ag



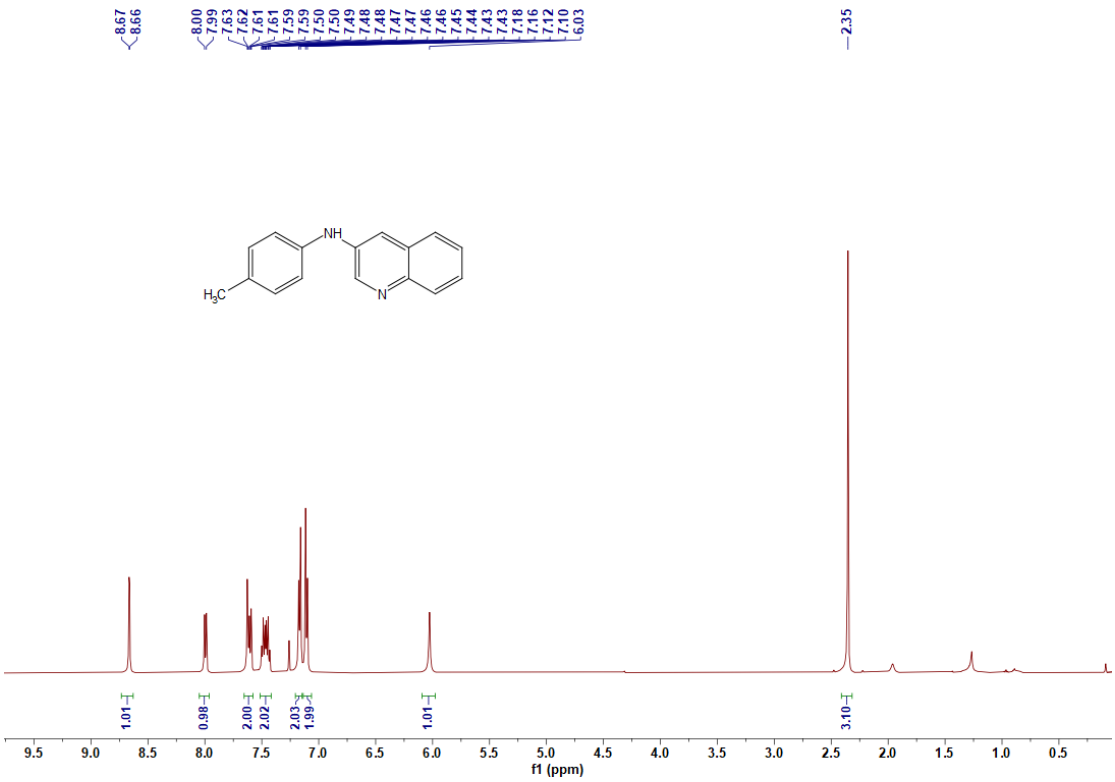
^{13}C NMR spectrum of 6ag



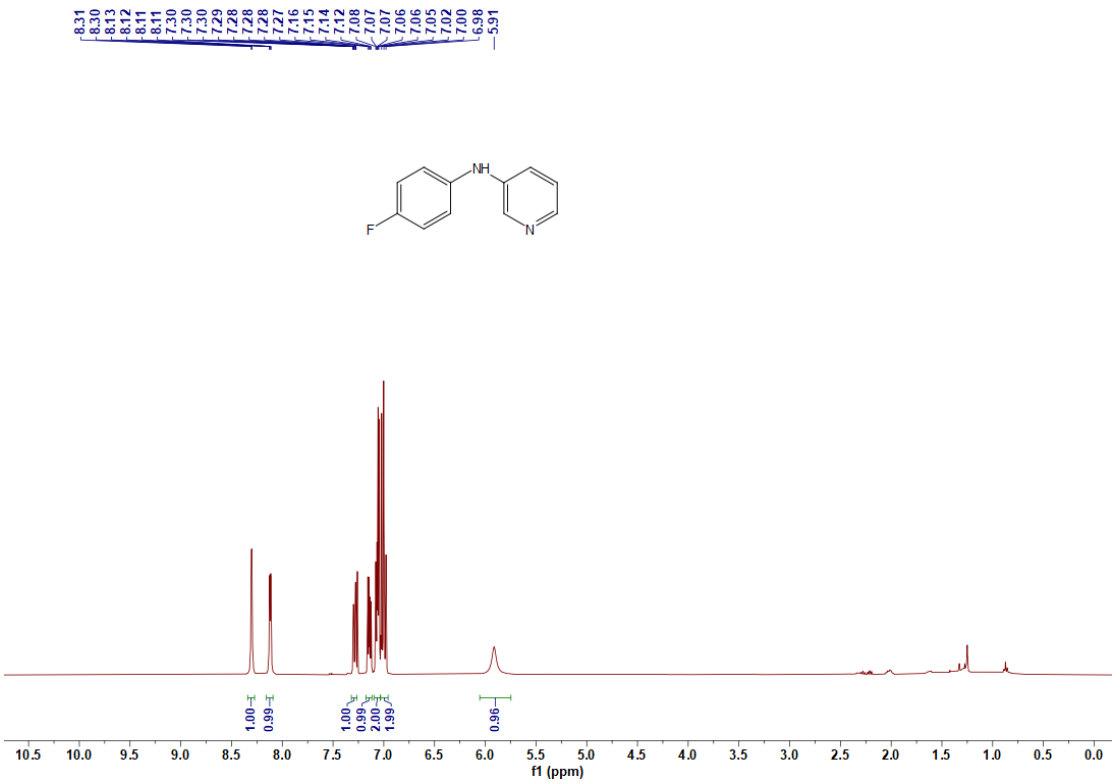
^{1}H NMR spectrum of 6ah



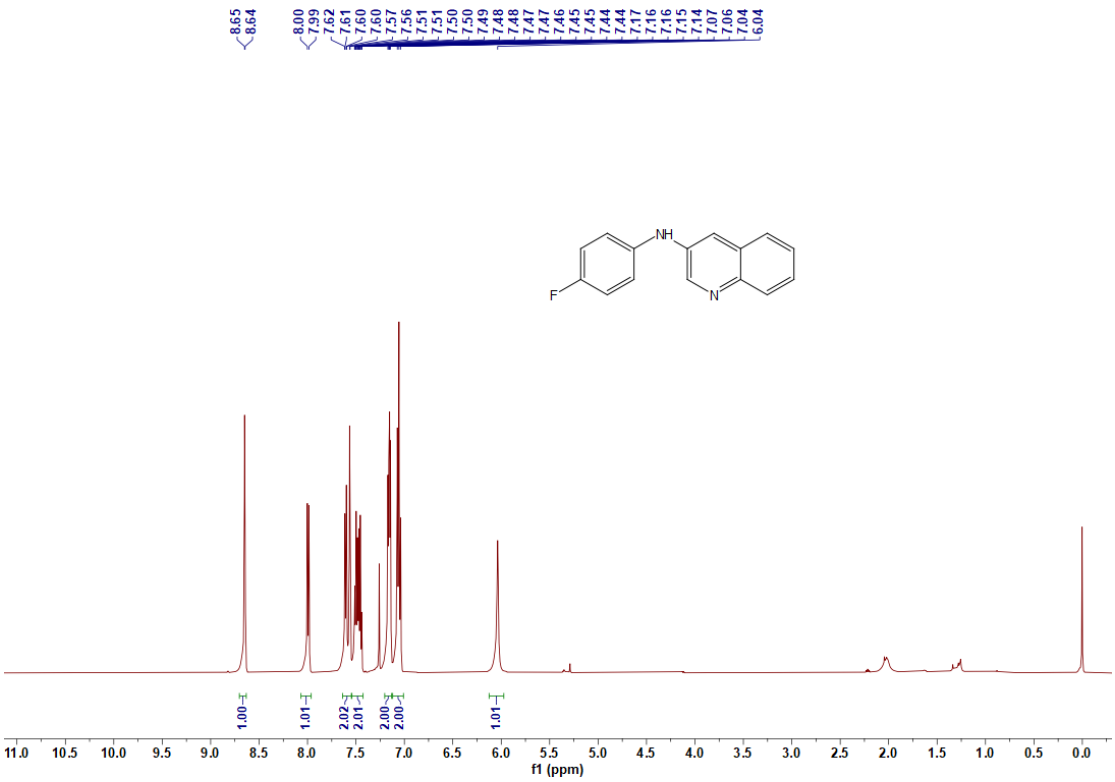
^{1}H NMR spectrum of 6ai



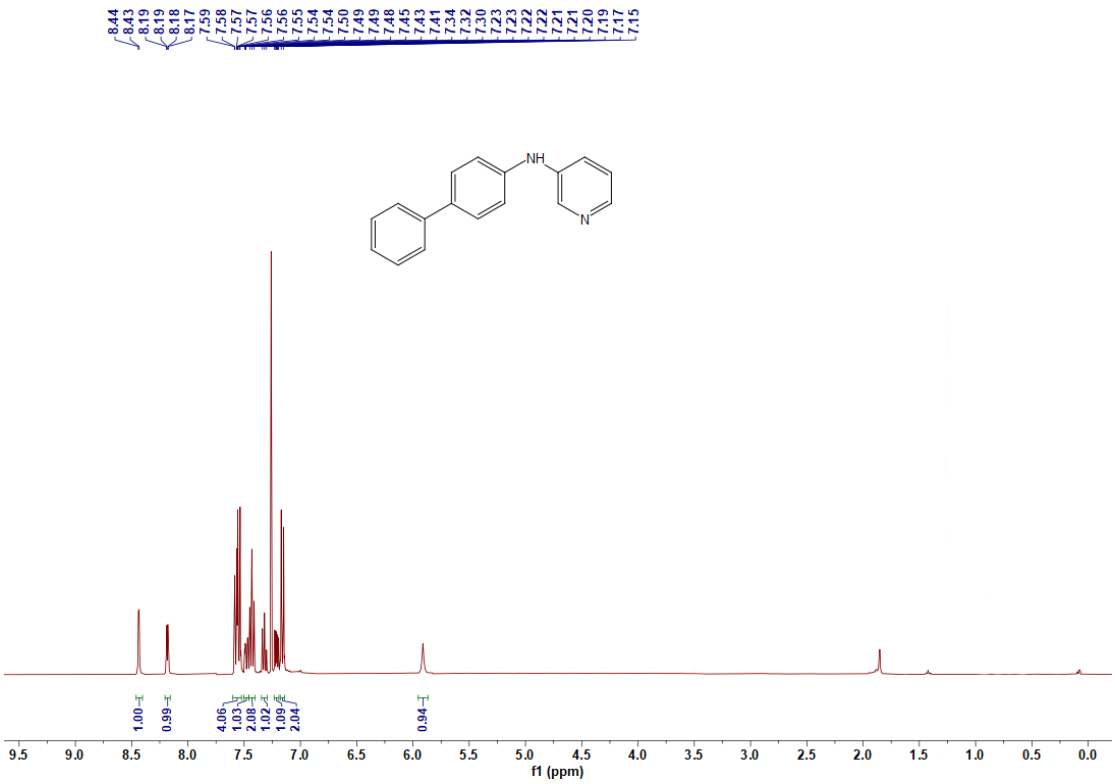
^{1}H NMR spectrum of 6aj



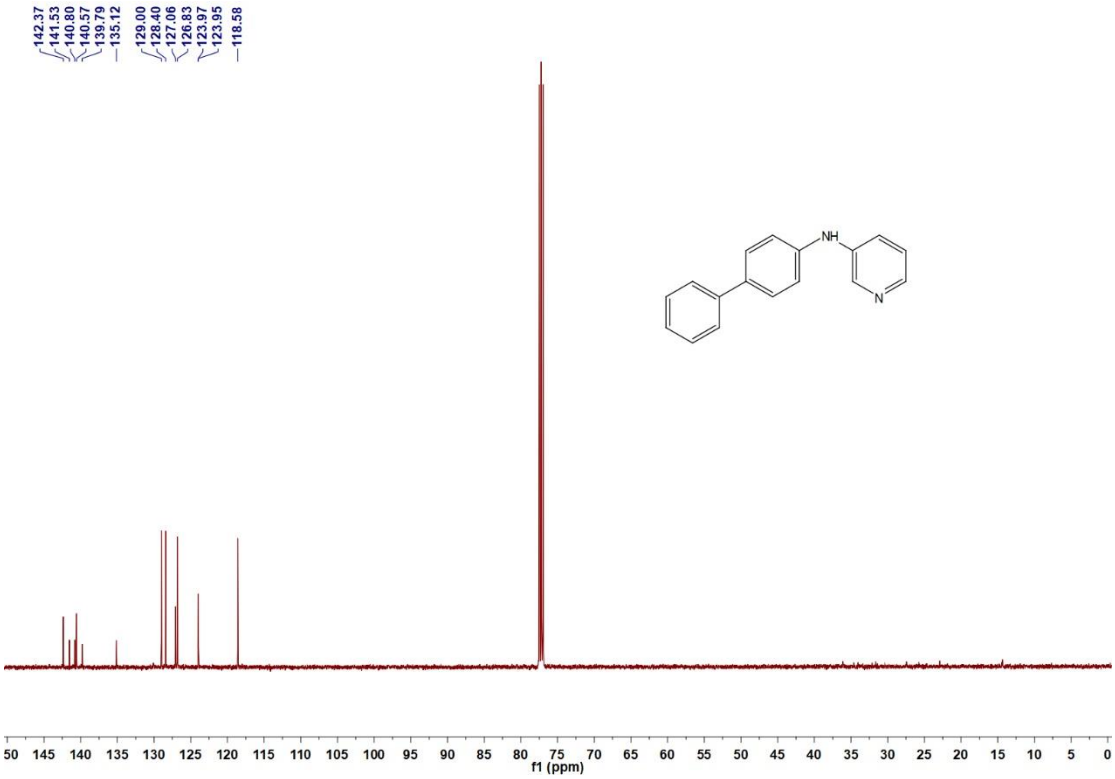
^{1}H NMR spectrum of 6ak



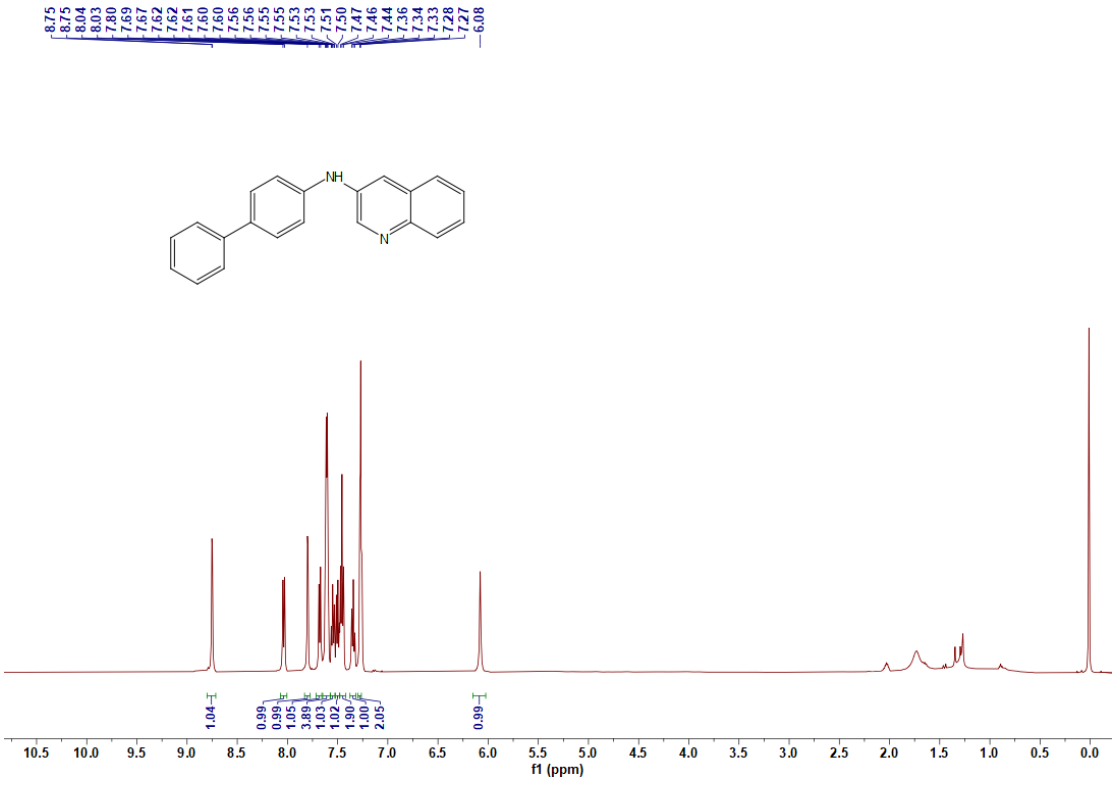
^{1}H NMR spectrum of 6al



^{1}H NMR spectrum of 6am



^{13}C NMR spectrum of 6am



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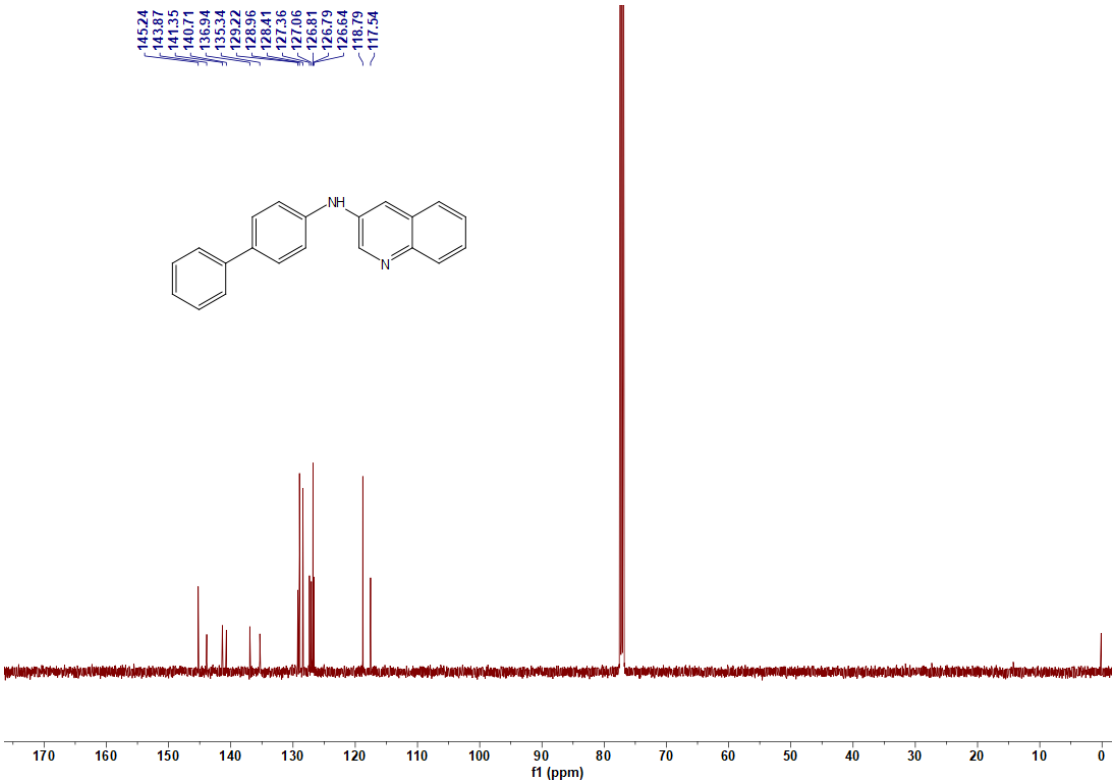
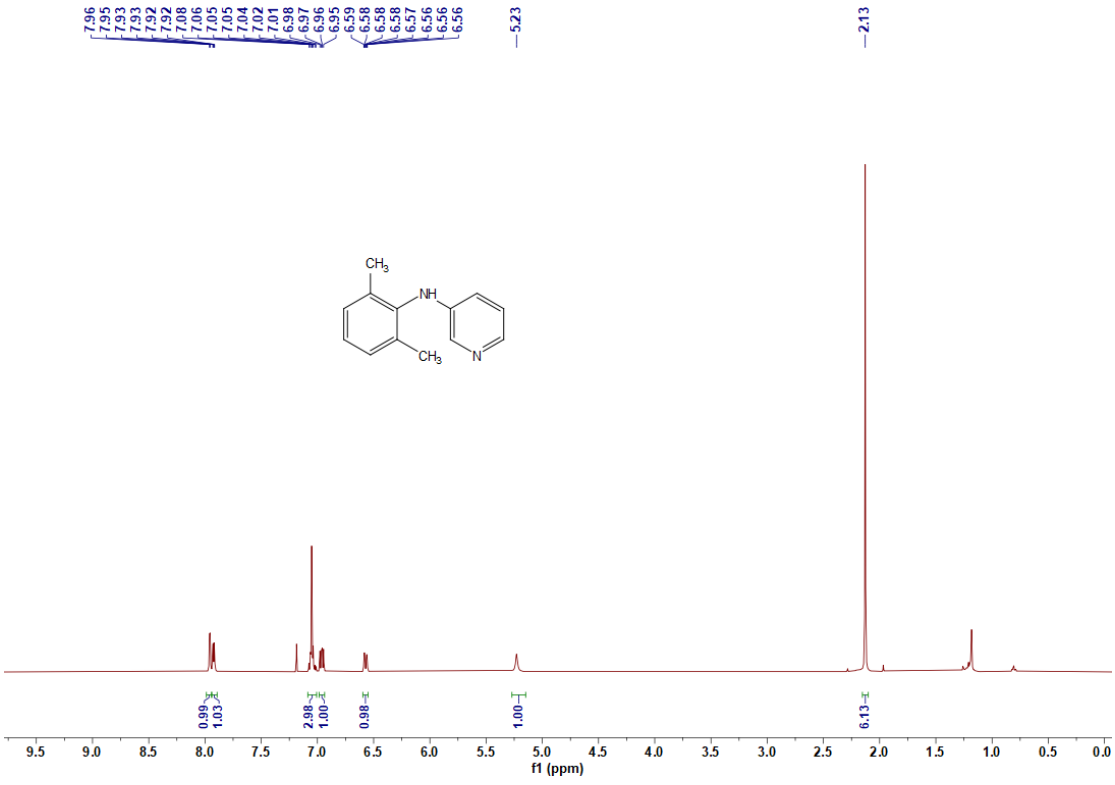
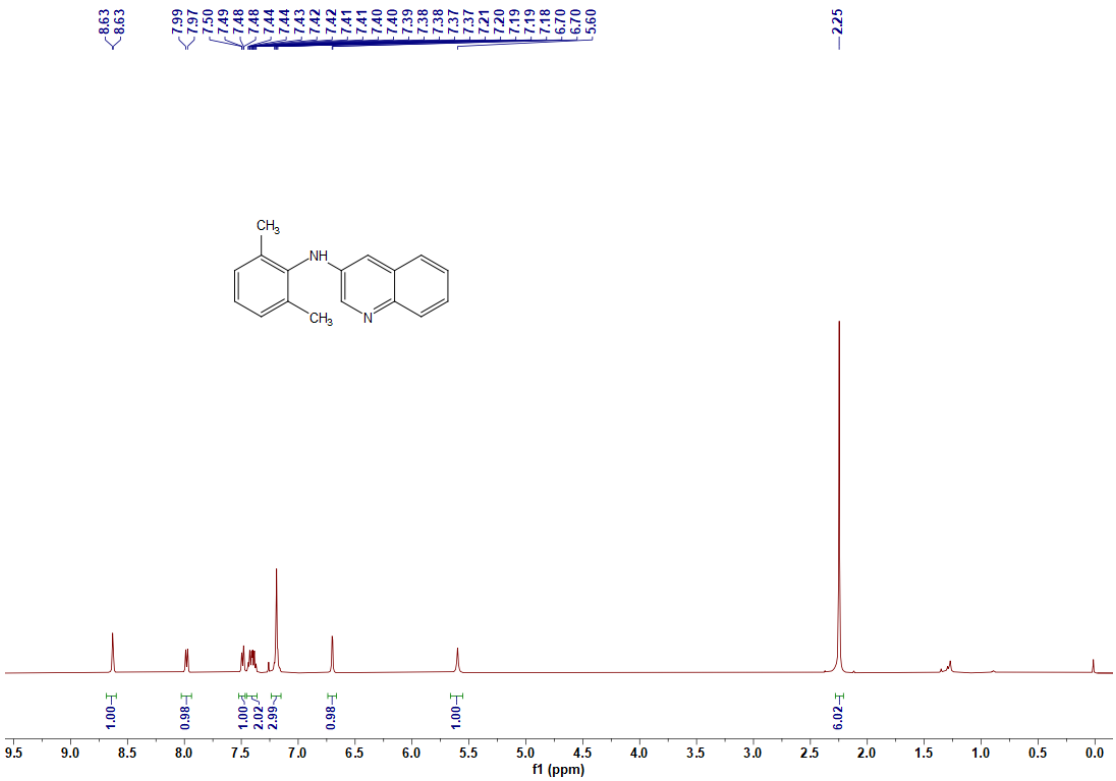


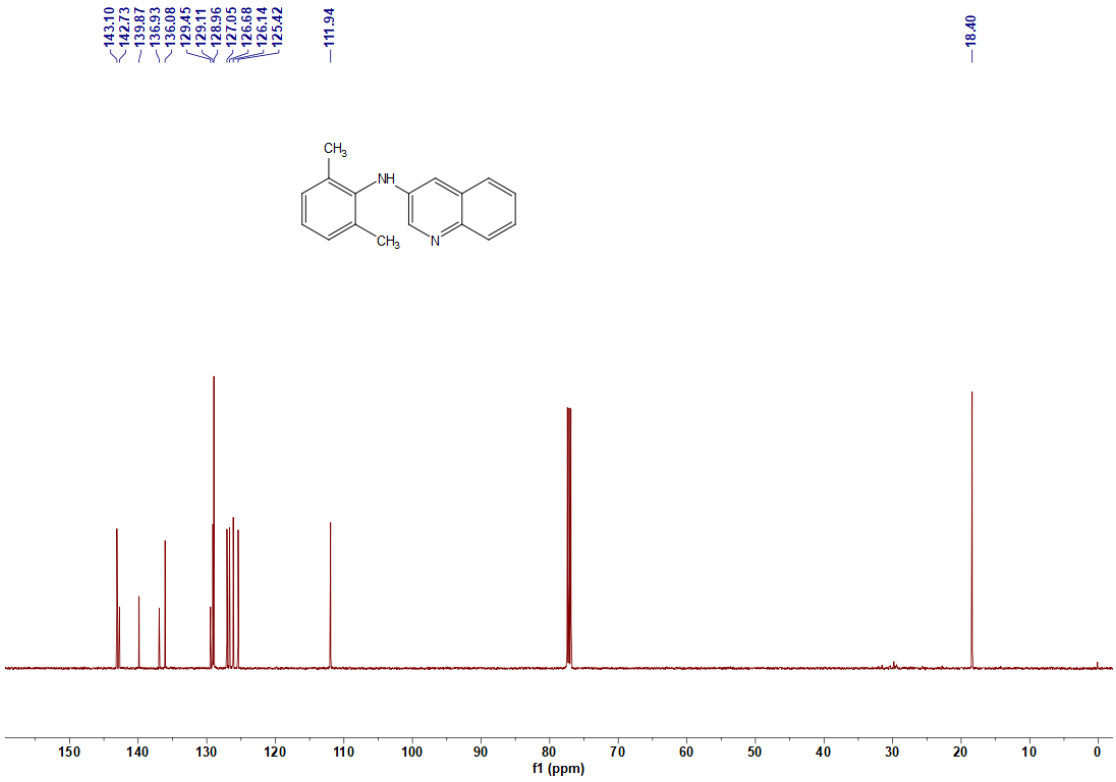
^{13}C NMR spectrum of 6an



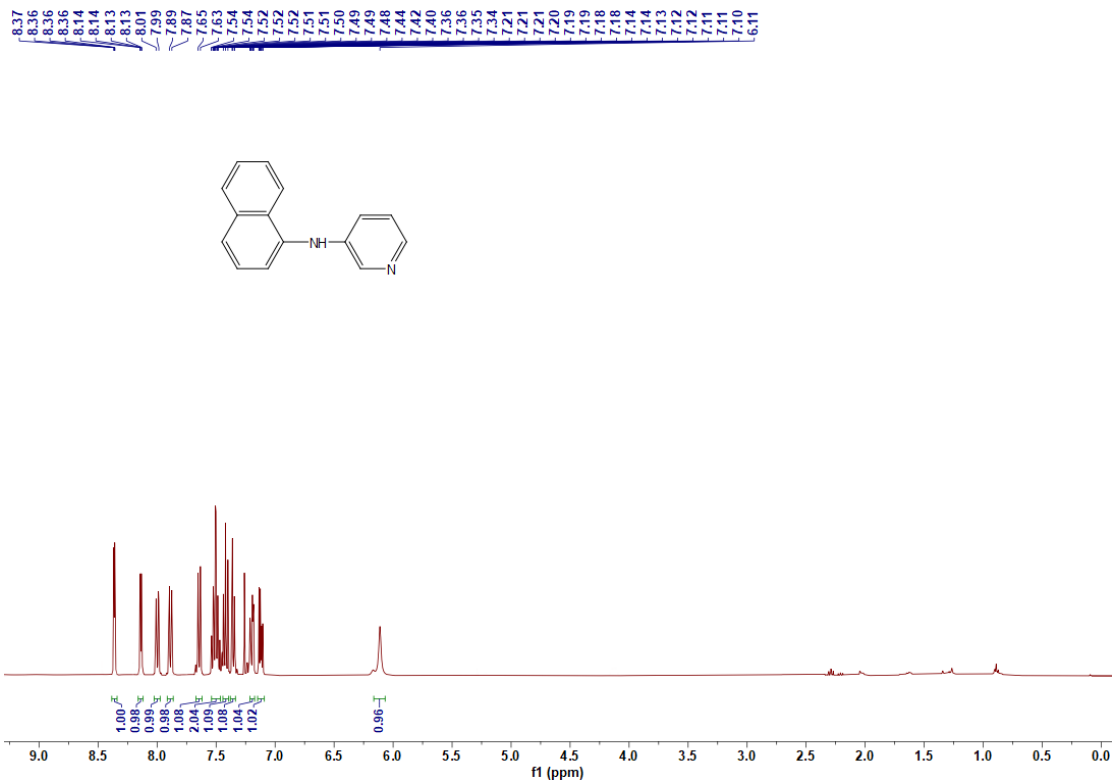
^{1}H NMR spectrum of 6ao



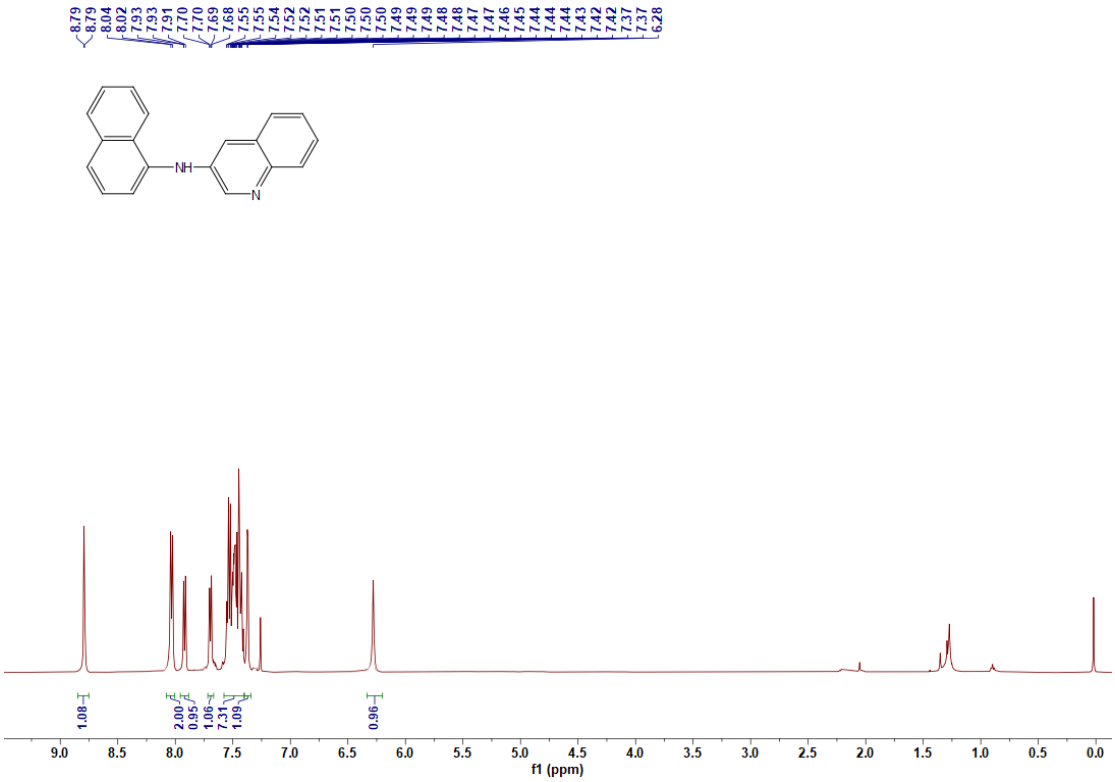
^{1}H NMR spectrum of 6ap



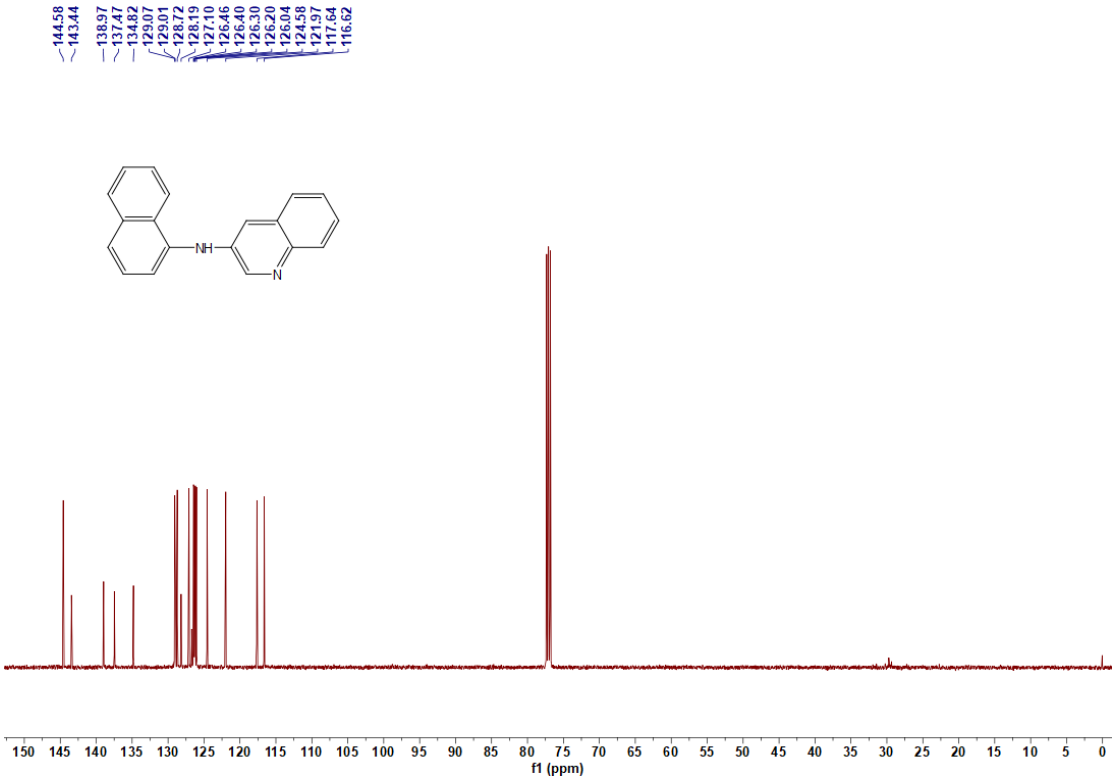
^{13}C NMR spectrum of 6ap



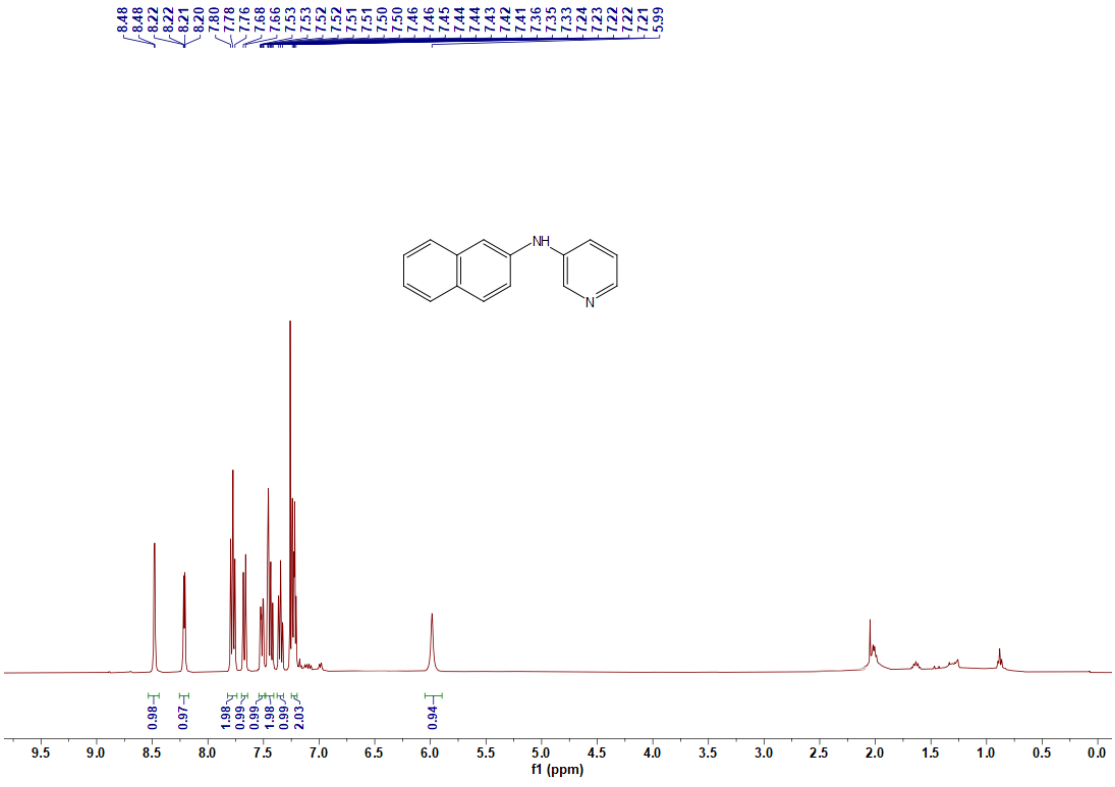
^{1}H NMR spectrum of 6aq



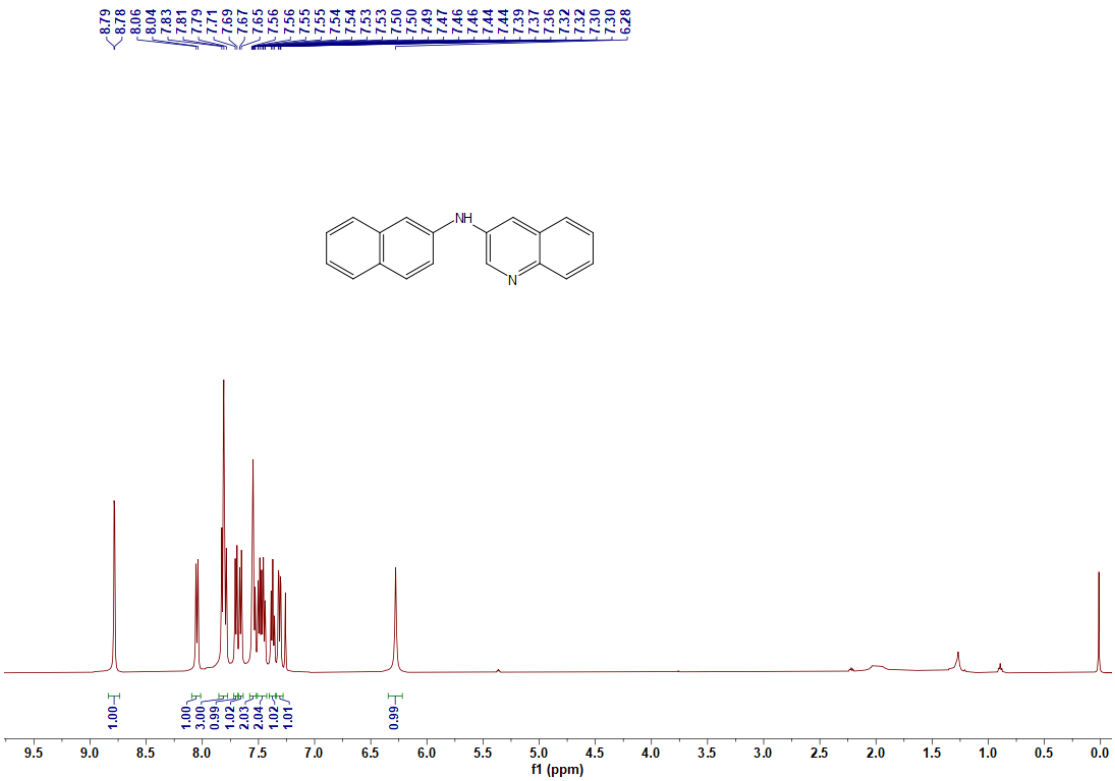
^{1}H NMR spectrum of 6ar



^{13}C NMR spectrum of 6ar



^{1}H NMR spectrum of 6as



^{1}H NMR spectrum of 6at

Computational studies

The structural optimization and energy-related calculations were both based on the DFT using the Vienna Ab initio Simulation Package (VASP, version 5.4.4) code.[38] The interaction between electrons and ions was treated using the projector augmented wave (PAW) approach, while the exchange-correlation effects were described by the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA). The van der Waals interactions were modeled using the DFT-D3. A Monkhorst-Pack k-point grid of 3×3×1 was employed for Brillouin zone sampling, and a plane-wave energy cutoff of 500 eV was applied. Geometry optimizations were performed using the conjugate-gradient algorithm until the total energy change reached $1x10^{-5}$ eV per atom. For all calculations, atomic forces were relaxed to below 0.01 eV $Å^{-1}$.

Meanwhile, Mulliken charges, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of the catalysts were calculated using the Gaussian 16 program (revision C.01).[39] Geometry optimizations were performed within the framework of density functional theory (DFT) at the B3LYP level. The 6-311++G(d,p) basis set was adopted for all non-metal atoms, while the SDD basis set was applied to Pd. Vibrational frequency analyses were conducted to confirm that the optimized structures correspond to true minima on the potential energy surface, with no imaginary frequencies.

Cartesian coordinates

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2-chloro-1,3-dimethylbenzene

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C	6.28100000	7.54100000	4.22200000
C	10.79100000	1.49600000	5.48300000
C	11.47600000	1.34500000	6.69200000
C	10.60200000	9.71600000	12.10300000
C	10.60600000	8.32100000	11.83700000
C	9.45400000	7.55200000	11.95000000
C	8.23600000	8.15000000	12.29500000
C	8.14900000	9.52000000	12.56600000
C	9.35000000	10.29700000	12.49400000
C	6.88000000	10.12100000	13.10400000
C	11.91600000	10.42900000	12.33300000
H	7.69000000	5.65900000	8.73500000
H	9.27000000	12.31500000	5.35700000
H	9.54000000	9.56300000	5.22800000
H	8.27400000	17.40500000	10.10700000
H	7.04000000	9.23400000	8.34300000
H	11.90400000	5.98100000	7.97500000
H	10.95000000	12.48700000	9.32900000
H	9.90300000	15.88500000	9.69400000
H	5.91200000	9.12700000	10.31300000
H	7.70800000	2.81600000	8.32100000
H	4.82100000	17.21200000	8.58300000
H	4.93400000	9.77200000	7.09100000
H	6.12100000	15.37100000	7.73100000
H	6.77000000	11.94100000	6.62600000
H	13.13400000	15.44400000	9.02000000
H	6.06900000	1.99500000	9.98600000

H	11.03900000	4.22500000	9.35700000
H	5.58800000	5.80800000	7.58500000
H	11.28800000	6.43200000	5.40600000
H	6.27200000	11.43100000	4.35600000
H	14.04500000	16.63000000	10.99000000
H	2.81200000	16.73600000	9.94300000
H	7.31500000	16.57300000	12.03800000
H	3.86700000	9.85700000	4.86500000
H	3.87900000	4.77200000	9.04100000
H	6.28000000	19.53400000	9.70800000
H	4.14500000	8.12000000	11.74100000
H	12.72100000	9.39400000	9.55300000
H	10.21500000	4.26500000	11.50700000
H	12.98700000	10.39300000	5.38300000
H	5.30800000	12.11300000	8.76300000
H	5.30000000	16.13700000	13.41500000
H	14.14200000	7.00300000	6.26900000
H	3.03200000	16.20500000	12.37200000
H	11.78500000	9.62100000	7.29800000
H	10.37000000	13.33700000	11.56400000
H	14.81400000	8.92000000	10.80600000
H	6.49000000	2.30100000	12.42300000
H	6.26500000	21.47700000	8.17900000
H	13.14800000	16.16600000	13.26900000
H	3.14400000	5.91600000	11.13000000
H	7.46900000	15.42500000	5.44200000
H	11.77400000	2.10400000	8.68800000
H	13.23800000	11.96100000	8.64000000
H	4.53100000	14.34000000	5.15700000
H	11.30800000	14.49600000	13.54700000
H	7.74500000	6.84000000	5.64600000

H	8.58600000	3.43200000	13.17800000
H	7.38700000	21.33600000	5.95300000
H	8.54600000	17.27700000	6.82500000
H	11.01900000	15.07700000	6.66200000
H	2.15800000	14.57300000	5.80900000
H	8.92500000	4.24200000	6.26800000
H	16.21500000	6.50000000	7.52500000
H	11.63400000	6.26800000	2.96400000
H	4.70100000	8.39500000	3.01600000
H	13.32600000	10.23500000	2.93700000
H	14.90500000	11.97600000	6.80800000
H	6.64500000	11.96800000	1.96800000
H	2.92400000	12.32200000	9.40600000
H	12.65300000	8.16900000	1.70600000
H	9.32900000	2.66200000	4.39900000
H	1.33100000	13.55500000	7.93200000
H	16.56600000	7.44900000	9.80600000
H	14.63700000	13.54800000	4.88300000
H	7.84200000	15.96400000	3.05800000
H	12.68100000	15.09600000	4.82200000
H	8.52100000	19.21500000	5.28600000
H	7.43500000	14.24000000	1.30000000
H	6.67000000	6.91600000	3.41300000
H	10.98000000	0.81000000	4.65500000
H	12.20100000	0.53800000	6.81500000
H	11.55900000	7.84600000	11.58500000
H	7.33000000	7.54200000	12.35100000
H	6.02300000	9.46900000	12.88900000
H	6.68000000	11.11800000	12.68600000
H	6.94400000	10.24700000	14.19900000
H	12.75400000	9.76200000	12.08700000

H	12.01500000	10.71700000	13.39300000
H	12.01000000	11.35000000	11.74300000
H	9.48900000	6.48200000	11.74100000
Cl	9.35500000	11.82100000	13.39700000

TS1-IPr# (TS1-L_A)

Pd	8.98600000	10.58000000	10.32800000
N	9.12100000	11.98000000	7.42800000
N	9.32700000	9.83200000	7.33300000
C	8.55500000	6.34100000	8.45300000
C	9.09800000	10.85900000	8.22700000
C	8.35000000	7.67400000	8.06800000
C	9.81900000	5.74700000	8.43400000
C	11.70000000	14.33000000	10.14300000
C	9.36500000	11.65600000	6.09600000
C	7.97300000	15.84800000	8.76600000
C	9.48400000	10.30500000	6.03400000
C	7.51800000	17.17800000	9.36200000
C	9.67300000	14.09100000	8.61100000
C	6.93600000	8.25100000	7.97000000
C	6.42300000	8.32700000	6.52700000
C	10.90400000	6.51900000	8.01000000
C	11.07300000	13.58300000	8.96100000
C	9.24800000	15.35100000	9.04700000
C	5.89200000	7.54200000	8.83400000
C	5.48700000	8.12000000	10.04300000
C	10.30700000	3.38400000	7.61300000
C	7.88600000	3.05200000	9.34600000
C	4.96400000	17.06600000	9.61900000
C	9.04400000	3.70800000	9.78600000
C	5.32700000	9.16300000	6.25400000
C	7.12800000	15.08000000	7.96400000

C	6.56900000	13.07400000	6.53500000
C	12.74200000	15.25400000	9.98200000
C	6.83100000	13.42000000	5.06500000
C	7.44000000	18.32800000	8.35400000
C	6.24500000	16.97400000	10.18300000
C	5.09700000	13.23500000	6.92800000
C	8.77200000	13.31800000	7.85100000
C	10.76500000	7.85500000	7.62600000
C	6.96400000	2.54000000	10.26200000
C	10.07500000	4.29000000	8.82300000
C	7.50900000	13.82600000	7.47700000
C	5.27800000	6.34600000	8.42800000
C	12.11200000	8.45400000	5.55400000
C	11.71200000	7.30100000	4.86600000
C	6.62000000	12.43900000	4.08300000
C	13.28500000	15.92200000	11.08400000
C	3.82600000	16.79700000	10.38300000
C	12.01500000	13.53900000	7.76000000
C	6.35400000	16.61700000	11.53500000
C	4.75600000	9.20500000	4.98300000
C	4.30600000	5.73500000	9.22100000
C	6.85500000	19.54800000	8.73400000
C	13.27700000	8.23900000	7.79900000
C	4.50100000	7.52000000	10.83000000
C	13.50500000	8.76200000	9.08100000
C	9.25800000	3.82700000	11.16700000
C	12.69500000	9.50000000	4.82100000
C	4.66500000	12.70800000	8.15800000
C	5.21800000	16.35600000	12.30400000
C	14.25300000	7.40500000	7.23800000
C	3.94800000	16.44200000	11.72800000

C	11.97900000	8.60500000	7.07300000
C	11.21000000	14.09400000	11.43900000
C	14.67300000	8.46400000	9.78200000
C	7.18800000	2.66600000	11.63400000
C	6.84100000	20.64000000	7.86700000
C	12.79600000	15.67500000	12.36800000
C	9.47900000	8.44000000	7.69600000
C	3.91100000	6.32100000	10.42600000
C	7.25300000	14.69100000	4.65100000
C	11.19500000	2.30400000	7.73300000
C	13.10100000	12.65000000	7.77700000
C	4.16000000	13.87400000	6.10800000
C	11.75400000	14.75800000	12.53900000
C	6.93800000	7.54400000	5.48700000
C	8.34200000	3.31000000	12.08400000
C	7.41300000	20.53900000	6.59600000
C	8.01500000	18.24200000	7.08000000
C	11.88500000	14.40600000	6.66700000
C	2.82100000	13.98200000	6.50100000
C	9.63800000	3.56300000	6.39400000
C	15.42300000	7.10100000	7.94000000
C	11.89400000	7.19400000	3.48300000
C	5.27300000	8.41000000	3.95400000
C	12.87500000	9.39600000	3.44100000
C	14.03300000	12.63000000	6.73900000
C	6.82500000	12.71800000	2.73100000
C	3.33000000	12.81000000	8.54700000
C	12.47500000	8.23900000	2.76500000
C	9.84300000	2.67900000	5.32900000
C	2.40000000	13.44700000	7.71800000
C	15.64000000	7.62900000	9.21300000

C	13.89300000	13.50300000	5.65500000
C	7.45900000	14.97300000	3.29700000
C	12.81400000	14.38800000	5.62200000
C	8.00100000	19.33500000	6.20700000
C	7.24700000	13.98900000	2.33100000
C	6.36800000	7.58400000	4.21000000
C	10.72700000	1.60700000	5.46400000
C	11.40600000	1.42400000	6.67200000
C	10.54000000	9.32100000	12.21000000
C	10.79900000	8.02400000	12.68600000
C	9.75400000	7.20000000	13.10500000
C	8.45100000	7.69600000	13.16000000
C	8.14500000	8.99200000	12.70800000
C	9.18300000	9.69800000	12.07100000
C	6.78400000	9.58300000	12.95800000
C	11.68100000	10.28700000	11.97900000
H	7.69600000	5.75600000	8.78500000
H	9.41900000	12.40800000	5.32000000
H	9.66800000	9.64500000	5.19600000
H	8.30300000	17.46600000	10.08400000
H	6.98700000	9.28600000	8.34600000
H	11.90100000	6.07000000	7.98200000
H	10.94000000	12.53800000	9.29900000
H	9.92600000	15.94600000	9.66000000
H	5.94700000	9.05600000	10.36600000
H	7.71100000	2.92200000	8.27600000
H	4.85200000	17.35900000	8.57300000
H	4.90600000	9.77600000	7.05500000
H	6.12500000	15.44200000	7.73100000
H	6.78500000	11.99700000	6.63700000
H	13.14200000	15.45300000	8.98600000

H	6.06700000	2.03300000	9.90000000
H	11.03000000	4.29900000	9.37600000
H	5.55000000	5.89600000	7.47000000
H	11.25100000	6.47400000	5.41000000
H	6.29600000	11.44000000	4.38500000
H	14.09700000	16.63700000	10.93500000
H	2.83900000	16.86400000	9.92200000
H	7.34500000	16.53100000	11.98800000
H	3.90200000	9.86000000	4.79700000
H	3.84600000	4.80100000	8.89100000
H	6.40300000	19.64000000	9.72400000
H	4.18900000	7.99700000	11.76200000
H	12.75200000	9.40900000	9.53400000
H	10.15800000	4.33400000	11.52500000
H	13.00300000	10.41100000	5.34000000
H	5.39000000	12.23400000	8.82600000
H	5.32800000	16.07800000	13.35400000
H	14.10600000	6.99800000	6.23500000
H	3.05900000	16.23200000	12.32500000
H	11.82000000	9.68000000	7.26300000
H	10.37600000	13.40000000	11.57900000
H	14.83500000	8.89000000	10.77500000
H	6.47100000	2.25700000	12.34900000
H	6.38400000	21.57800000	8.18900000
H	13.22300000	16.19200000	13.22900000
H	3.14200000	5.85100000	11.04200000
H	7.42700000	15.47200000	5.39400000
H	11.72400000	2.15100000	8.67700000
H	13.22700000	11.97400000	8.62700000
H	4.47300000	14.29000000	5.14900000
H	11.35900000	14.55800000	13.53700000

H	7.79300000	6.89000000	5.67400000
H	8.53400000	3.40700000	13.15600000
H	7.40700000	21.39500000	5.91800000
H	8.49100000	17.31100000	6.76700000
H	11.04900000	15.10900000	6.63500000
H	2.10700000	14.48700000	5.84600000
H	8.95100000	4.40400000	6.27300000
H	16.17300000	6.45200000	7.48200000
H	11.57800000	6.28400000	2.96800000
H	4.82300000	8.43700000	2.95900000
H	13.32400000	10.22600000	2.89200000
H	14.87300000	11.93300000	6.77900000
H	6.65900000	11.93500000	1.98700000
H	3.01500000	12.39400000	9.50600000
H	12.61300000	8.15700000	1.68500000
H	9.31000000	2.83300000	4.38900000
H	1.35500000	13.52600000	8.02300000
H	16.55900000	7.39900000	9.75600000
H	14.62200000	13.49200000	4.84200000
H	7.78800000	15.97100000	2.99900000
H	12.69500000	15.07500000	4.78100000
H	8.45900000	19.24300000	5.21900000
H	7.41200000	14.20800000	1.27400000
H	6.78100000	6.96100000	3.41400000
H	10.89000000	0.91900000	4.63200000
H	12.10200000	0.59100000	6.78800000
H	11.83500000	7.67600000	12.73800000
H	7.64200000	7.07000000	13.54700000
H	6.01500000	8.80000000	13.02300000
H	6.51100000	10.33000000	12.20200000
H	6.79300000	10.11600000	13.92500000

H	12.63200000	9.75200000	11.85000000
H	11.78900000	10.94500000	12.85600000
H	11.52300000	10.95100000	11.11700000
H	9.96000000	6.17900000	13.43100000
Cl	8.28500000	11.35000000	12.35600000
IM2-IPr$^{\#}$ (IM2-L_A)			
Pd	8.95200000	10.51000000	10.28800000
N	9.07300000	11.96600000	7.38400000
N	9.33600000	9.82400000	7.28700000
C	8.57500000	6.35400000	8.46500000
C	9.06800000	10.84000000	8.18100000
C	8.37000000	7.68200000	8.06600000
C	9.83600000	5.75400000	8.43100000
C	11.57800000	14.22100000	10.21600000
C	9.34500000	11.64900000	6.05500000
C	7.97300000	15.86700000	8.68400000
C	9.50100000	10.30300000	5.99100000
C	7.52700000	17.19300000	9.29500000
C	9.62700000	14.06300000	8.58800000
C	6.95300000	8.26000000	7.99500000
C	6.41300000	8.32600000	6.56300000
C	10.91700000	6.51600000	7.97900000
C	11.00400000	13.53000000	8.97400000
C	9.22300000	15.33400000	9.00700000
C	5.93000000	7.56400000	8.89500000
C	5.60500000	8.12200000	10.13800000
C	10.33300000	3.39100000	7.62100000
C	7.86900000	3.12400000	9.33500000
C	4.97700000	17.04700000	9.58300000
C	9.06000000	3.71100000	9.78600000
C	5.33300000	9.18600000	6.30600000

C	7.13400000	15.12000000	7.85500000
C	6.55300000	13.11500000	6.43400000
C	12.65100000	15.11900000	10.15300000
C	6.82600000	13.45600000	4.96500000
C	7.43200000	18.36000000	8.31100000
C	6.26600000	16.97200000	10.13200000
C	5.08000000	13.28800000	6.82500000
C	8.73100000	13.31000000	7.80100000
C	10.78000000	7.84700000	7.57400000
C	6.95000000	2.58600000	10.23800000
C	10.09500000	4.29900000	8.83000000
C	7.49300000	13.85100000	7.38700000
C	5.26400000	6.39500000	8.49400000
C	12.12900000	8.44700000	5.49000000
C	11.73200000	7.29500000	4.79900000
C	6.61600000	12.47100000	3.98500000
C	13.13100000	15.74300000	11.30900000
C	3.85300000	16.76900000	10.36300000
C	11.99100000	13.52600000	7.81100000
C	6.39700000	16.62200000	11.48300000
C	4.74300000	9.23900000	5.04500000
C	4.32100000	5.78600000	9.32600000
C	6.81500000	19.55700000	8.71200000
C	13.29800000	8.21000000	7.73000000
C	4.64700000	7.52600000	10.96200000
C	13.52000000	8.72400000	9.01500000
C	9.30600000	3.73800000	11.16600000
C	12.70900000	9.49800000	4.76000000
C	4.65300000	12.78800000	8.06700000
C	5.27500000	16.35000000	12.26700000
C	14.27700000	7.37800000	7.17100000

C	3.99700000	16.42100000	11.70800000
C	11.99800000	8.58900000	7.01000000
C	10.99400000	13.96200000	11.46700000
C	14.68200000	8.42400000	9.72500000
C	7.21000000	2.61600000	11.61000000
C	6.78700000	20.67000000	7.87200000
C	12.55000000	15.47300000	12.54900000
C	9.49500000	8.43600000	7.65600000
C	4.01000000	6.35000000	10.56600000
C	7.25800000	14.72300000	4.54800000
C	11.23200000	2.32000000	7.73500000
C	13.08900000	12.65300000	7.85800000
C	4.13800000	13.90100000	5.98900000
C	11.47900000	14.57700000	12.62200000
C	6.89300000	7.52500000	5.51900000
C	8.39500000	3.19100000	12.07100000
C	7.37900000	20.61400000	6.60800000
C	8.02400000	18.31800000	7.04100000
C	11.88400000	14.40000000	6.72100000
C	2.80000000	14.01100000	6.38200000
C	9.65400000	3.56100000	6.40600000
C	15.44300000	7.07100000	7.88100000
C	11.91800000	7.19000000	3.41600000
C	5.22700000	8.43100000	4.01000000
C	12.89200000	9.39800000	3.38100000
C	14.05600000	12.65700000	6.85300000
C	6.82900000	12.74400000	2.63300000
C	3.31800000	12.89300000	8.45600000
C	12.49900000	8.24000000	2.70100000
C	9.85600000	2.67500000	5.34300000
C	2.38400000	13.50600000	7.61400000

C	15.65100000	7.59100000	9.15900000
C	13.94000000	13.53700000	5.77300000
C	7.47200000	14.99900000	3.19400000
C	12.84900000	14.40500000	5.70900000
C	7.99700000	19.43300000	6.19700000
C	7.25700000	14.01200000	2.23000000
C	6.30400000	7.57600000	4.25100000
C	10.74700000	1.60800000	5.47400000
C	11.43900000	1.43700000	6.67500000
C	10.54400000	9.30500000	12.16300000
C	10.85500000	8.09600000	12.80700000
C	9.85900000	7.34300000	13.43100000
C	8.55900000	7.84400000	13.50100000
C	8.20500000	9.05400000	12.87500000
C	9.18000000	9.68400000	12.07500000
C	6.83700000	9.64000000	13.11200000
C	11.67300000	10.21300000	11.71400000
H	7.71700000	5.78100000	8.82000000
H	9.39500000	12.40500000	5.28000000
H	9.71700000	9.65000000	5.15400000
H	8.32200000	17.47000000	10.01100000
H	7.01300000	9.29900000	8.35900000
H	11.91100000	6.06200000	7.94700000
H	10.85700000	12.47300000	9.26400000
H	9.89700000	15.91100000	9.64400000
H	6.11000000	9.03600000	10.45700000
H	7.66600000	3.06700000	8.26300000
H	4.84700000	17.33600000	8.53800000
H	4.94300000	9.81300000	7.11300000
H	6.15100000	15.51200000	7.58900000
H	6.75600000	12.03600000	6.53500000

H	13.12400000	15.33600000	9.19300000
H	6.02700000	2.13500000	9.86700000
H	11.04600000	4.31500000	9.38900000
H	5.46600000	5.96800000	7.50800000
H	11.27200000	6.46700000	5.34200000
H	6.28600000	11.47400000	4.28900000
H	13.96900000	16.44100000	11.23800000
H	2.85900000	16.82200000	9.91400000
H	7.39600000	16.55000000	11.92200000
H	3.90500000	9.91700000	4.87100000
H	3.81600000	4.87400000	8.99800000
H	6.34800000	19.61400000	9.69700000
H	4.39800000	7.97900000	11.92500000
H	12.76400000	9.37000000	9.46100000
H	10.23000000	4.19100000	11.53500000
H	13.01300000	10.41000000	5.28000000
H	5.38000000	12.33100000	8.74400000
H	5.40300000	16.07700000	13.31700000
H	14.13900000	6.97400000	6.16600000
H	3.11700000	16.20300000	12.31700000
H	11.84800000	9.66300000	7.20900000
H	10.13700000	13.28700000	11.53100000
H	14.83200000	8.84700000	10.72100000
H	6.49500000	2.18600000	12.31400000
H	6.30300000	21.58800000	8.21000000
H	12.92800000	15.95800000	13.45200000
H	3.27300000	5.87900000	11.22000000
H	7.43300000	15.50500000	5.28900000
H	11.77300000	2.17300000	8.67500000
H	13.19300000	11.97200000	8.70800000
H	4.44700000	14.29200000	5.01800000

H	11.01300000	14.35900000	13.58600000
H	7.73600000	6.85100000	5.69400000
H	8.61400000	3.21400000	13.14000000
H	7.36500000	21.48600000	5.95100000
H	8.52300000	17.40400000	6.71100000
H	11.03700000	15.08800000	6.66200000
H	2.08100000	14.49700000	5.71800000
H	8.96100000	4.39800000	6.28800000
H	16.19600000	6.42500000	7.42500000
H	11.60500000	6.28100000	2.89900000
H	4.76500000	8.46900000	3.02300000
H	13.33900000	10.23000000	2.83200000
H	14.90500000	11.97300000	6.92000000
H	6.66300000	11.95900000	1.89000000
H	3.00600000	12.49700000	9.42500000
H	12.64200000	8.15800000	1.62200000
H	9.31200000	2.82100000	4.40800000
H	1.33900000	13.59200000	7.92100000
H	16.56600000	7.35800000	9.70800000
H	14.69900000	13.54600000	4.98700000
H	7.81000000	15.99300000	2.89400000
H	12.75000000	15.09700000	4.87000000
H	8.46800000	19.37400000	5.21300000
H	7.42500000	14.22800000	1.17300000
H	6.69000000	6.94200000	3.45000000
H	10.90700000	0.91700000	4.64400000
H	12.14400000	0.61000000	6.78800000
H	11.89900000	7.76600000	12.83600000
H	7.78800000	7.30600000	14.06200000
H	6.04500000	9.02900000	12.65500000
H	6.76700000	10.65600000	12.70700000

H	6.62900000	9.67400000	14.19400000
H	12.60800000	9.64600000	11.60800000
H	11.84300000	10.99700000	12.46900000
H	11.47600000	10.74500000	10.77100000
H	10.11100000	6.39100000	13.90600000
Cl	7.58700000	12.25200000	10.91400000

aniline

C	13.31700000	12.33300000	17.41000000
C	13.31900000	11.12800000	16.70900000
C	13.29900000	9.90500000	17.38500000
C	13.27800000	9.90800000	18.78500000
C	13.27400000	11.10600000	19.49700000
C	13.29400000	12.34200000	18.81900000
H	13.25500000	11.09500000	20.59000000
H	13.32900000	13.28400000	16.86900000
H	13.33400000	11.15100000	15.61600000
H	13.26400000	8.96300000	19.33400000
H	13.30100000	8.96400000	16.83300000
H	13.30300000	14.42100000	19.05500000
H	13.29500000	13.52200000	20.53500000
N	13.29000000	13.52700000	19.52400000

IM3-IPr$^{\#}$ (IM3-L_A)

Pd	8.83300000	10.16600000	10.06500000
N	9.11900000	11.95600000	7.31900000
N	9.36000000	9.82000000	7.08600000
N	9.63800000	11.75000000	10.72400000
C	8.54300000	6.32300000	8.14900000
C	9.08100000	10.78100000	8.03700000
C	8.35300000	7.65700000	7.75700000
C	9.80000000	5.71800000	8.14300000
C	11.73000000	14.42900000	9.94100000

C	9.41900000	11.72000000	5.97900000
C	7.94300000	15.83900000	8.62800000
C	9.56200000	10.38000000	5.82900000
C	7.50200000	17.18600000	9.20000000
C	9.65200000	14.08300000	8.50000000
C	6.93600000	8.22800000	7.63100000
C	6.46000000	8.31800000	6.17800000
C	10.89300000	6.47300000	7.70300000
C	11.07000000	13.61000000	8.82300000
C	9.22700000	15.35800000	8.89400000
C	5.88100000	7.49900000	8.46600000
C	5.50400000	8.01500000	9.71200000
C	10.30600000	3.34700000	7.36700000
C	7.81000000	3.13100000	9.06700000
C	4.95000000	17.12300000	9.47300000
C	9.01900000	3.68200000	9.51600000
C	5.32100000	9.09200000	5.90100000
C	7.08500000	15.03300000	7.87800000
C	6.53700000	12.99900000	6.48800000
C	12.90100000	15.17400000	9.74000000
C	6.79700000	13.33600000	5.01600000
C	7.42400000	18.33300000	8.19000000
C	6.23100000	17.00700000	10.03100000
C	5.06700000	13.15300000	6.88800000
C	8.74500000	13.28000000	7.77800000
C	10.77500000	7.80900000	7.31600000
C	6.89400000	2.58800000	9.97000000
C	10.05200000	4.27000000	8.55900000
C	7.47300000	13.77100000	7.41500000
C	5.23500000	6.34200000	8.00000000
C	12.11000000	8.41500000	5.23500000

C	11.65600000	7.29200000	4.53000000
C	6.64500000	12.33500000	4.04500000
C	13.46500000	15.92100000	10.78100000
C	3.81200000	16.87100000	10.24300000
C	11.95300000	13.53700000	7.58000000
C	6.34200000	16.65200000	11.38300000
C	4.78900000	9.15100000	4.61300000
C	4.25200000	5.71500000	8.76600000
C	6.95500000	19.58700000	8.61900000
C	13.31700000	8.16100000	7.43700000
C	4.51200000	7.39600000	10.47700000
C	13.76000000	8.89000000	8.55000000
C	9.28700000	3.66700000	10.89200000
C	12.73300000	9.44700000	4.51700000
C	4.64900000	12.64600000	8.13000000
C	5.20700000	16.40800000	12.15700000
C	14.12600000	7.11600000	6.96600000
C	3.93600000	16.51300000	11.58700000
C	11.99800000	8.54600000	6.76100000
C	11.14100000	14.45100000	11.21600000
C	14.96900000	8.58700000	9.18000000
C	7.17700000	2.57200000	11.33800000
C	6.94000000	20.68300000	7.75800000
C	12.87000000	15.93300000	12.04200000
C	9.49500000	8.41400000	7.39500000
C	3.88400000	6.24100000	10.00700000
C	7.17500000	14.61700000	4.59100000
C	11.17500000	2.25800000	7.53100000
C	13.01700000	12.62400000	7.54600000
C	4.11900000	13.77200000	6.06500000
C	11.70400000	15.19100000	12.25700000

C	7.05700000	7.61200000	5.12700000
C	8.37900000	3.11400000	11.79700000
C	7.39000000	20.55000000	6.44100000
C	7.88000000	18.21500000	6.87200000
C	11.78700000	14.40700000	6.49400000
C	2.78200000	13.87600000	6.46500000
C	9.68000000	3.51900000	6.12500000
C	15.33300000	6.80500000	7.59700000
C	11.82500000	7.20300000	3.14400000
C	5.39000000	8.43500000	3.57100000
C	12.89800000	9.36300000	3.13500000
C	13.89300000	12.57900000	6.46200000
C	6.86500000	12.60300000	2.69300000
C	3.31600000	12.74400000	8.52800000
C	12.44300000	8.23800000	2.44100000
C	9.91500000	2.62300000	5.07700000
C	2.37400000	13.35700000	7.69400000
C	15.76000000	7.53900000	8.70600000
C	13.71600000	13.44900000	5.38300000
C	7.39700000	14.89000000	3.23700000
C	12.65800000	14.36200000	5.40300000
C	7.86100000	19.31300000	6.00300000
C	7.24400000	13.88400000	2.28200000
C	6.52700000	7.67000000	3.83200000
C	10.78300000	1.54300000	5.25400000
C	11.41500000	1.36400000	6.48800000
C	10.01300000	8.39400000	11.78000000
C	10.18800000	7.32700000	12.66800000
C	9.19200000	7.01400000	13.58900000
C	8.02200000	7.77100000	13.61800000
C	7.80800000	8.84700000	12.73500000

C	8.80800000	9.12700000	11.78200000
C	6.52800000	9.62600000	12.88200000
C	11.16200000	8.77000000	10.86800000
C	11.40800000	11.73500000	12.37600000
C	11.82400000	11.87500000	13.69600000
C	10.91900000	12.23000000	14.70100000
C	9.58000000	12.44100000	14.35600000
C	9.14700000	12.30500000	13.03800000
C	10.05800000	11.94500000	12.02300000
H	7.67400000	5.75200000	8.47800000
H	9.49000000	12.52500000	5.25900000
H	9.78200000	9.78500000	4.95100000
H	8.29300000	17.47500000	9.91500000
H	6.96800000	9.26000000	8.02100000
H	11.88100000	6.00800000	7.67400000
H	10.97400000	12.57900000	9.20900000
H	9.92000000	15.98500000	9.45800000
H	5.99300000	8.91900000	10.08300000
H	7.58900000	3.11000000	7.99700000
H	4.83900000	17.42000000	8.42800000
H	4.83900000	9.64900000	6.70900000
H	6.07300000	15.37500000	7.65800000
H	6.76200000	11.92500000	6.60000000
H	13.38600000	15.17500000	8.76300000
H	5.95500000	2.16800000	9.60200000
H	10.99900000	4.29000000	9.12600000
H	5.49200000	5.93700000	7.01800000
H	11.16200000	6.47700000	5.06300000
H	6.35800000	11.32800000	4.35500000
H	14.37700000	16.49400000	10.59900000
H	2.82300000	16.95600000	9.78800000

H	7.33500000	16.55400000	11.83200000
H	3.90400000	9.76100000	4.42200000
H	3.76600000	4.81400000	8.38700000
H	6.59900000	19.70200000	9.64500000
H	4.22900000	7.82400000	11.44100000
H	13.15000000	9.71400000	8.92500000
H	10.22400000	4.09400000	11.25900000
H	13.08200000	10.33400000	5.05100000
H	5.38300000	12.19000000	8.80200000
H	5.31800000	16.13200000	13.20900000
H	13.82500000	6.55400000	6.08000000
H	3.04600000	16.31700000	12.18900000
H	11.85900000	9.62000000	6.96500000
H	10.21100000	13.90200000	11.38600000
H	15.29700000	9.17800000	10.03700000
H	6.46800000	2.13300000	12.04200000
H	6.58100000	21.64900000	8.12000000
H	13.31100000	16.51400000	12.85400000
H	3.10600000	5.75800000	10.60100000
H	7.30300000	15.41500000	5.32500000
H	11.66700000	2.10700000	8.49700000
H	13.17000000	11.95300000	8.39600000
H	4.42300000	14.17600000	5.09700000
H	11.23200000	15.18200000	13.24100000
H	7.94600000	7.00600000	5.31500000
H	8.61600000	3.10300000	12.86300000
H	7.38300000	21.40900000	5.76700000
H	8.26700000	17.25700000	6.51900000
H	10.96800000	15.13100000	6.50300000
H	2.05900000	14.36300000	5.80600000
H	9.00700000	4.36500000	5.97000000

H	15.95100000	5.99100000	7.21000000
H	11.46700000	6.31800000	2.61400000
H	4.97400000	8.47900000	2.56300000
H	13.37900000	10.18200000	2.59700000
H	14.71900000	11.86400000	6.46500000
H	6.74500000	11.80300000	1.96000000
H	3.01100000	12.34300000	9.49700000
H	12.56700000	8.17100000	1.35800000
H	9.41700000	2.77100000	4.11700000
H	1.32900000	13.43000000	8.00200000
H	16.71100000	7.30500000	9.18900000
H	14.40100000	13.41800000	4.53400000
H	7.69100000	15.89500000	2.93200000
H	12.51400000	15.04900000	4.56700000
H	8.22100000	19.19600000	4.97800000
H	7.42200000	14.09400000	1.22500000
H	7.00700000	7.11000000	3.02700000
H	10.97000000	0.84700000	4.43500000
H	12.09500000	0.52400000	6.64000000
H	11.11900000	6.75200000	12.63200000
H	7.24000000	7.53000000	14.34300000
H	5.73500000	8.98900000	13.30400000
H	6.18600000	10.05700000	11.93400000
H	6.67100000	10.47800000	13.56600000
H	11.62000000	7.88400000	10.40600000
H	11.94000000	9.30800000	11.43900000
H	10.88100000	9.44900000	10.03300000
H	9.33000000	6.19100000	14.29200000
H	8.09700000	12.46800000	12.78300000
H	12.12700000	11.46700000	11.59800000
H	12.87500000	11.70900000	13.94300000

H	8.85800000	12.71700000	15.12800000
H	11.24800000	12.32900000	15.73400000
H	10.34400000	11.83400000	10.00000000
H	8.73500000	12.11800000	10.42800000
Cl	7.13500000	11.66000000	10.88500000

NaO^{t}Bu

O	8.30700000	11.39200000	14.17000000
C	8.39800000	11.25400000	12.79000000
C	7.17300000	10.49100000	12.23800000
C	8.47800000	12.63900000	12.10900000
C	9.67600000	10.45700000	12.44000000
H	6.25000000	11.05800000	12.45600000
H	7.22100000	10.33000000	11.14700000
H	7.09500000	9.51000000	12.73200000
H	9.33300000	13.20300000	12.51500000
H	7.55900000	13.21400000	12.31900000
H	8.59300000	12.57400000	11.01300000
H	9.63000000	9.46900000	12.92400000
H	9.80700000	10.31300000	11.35300000
H	10.55500000	10.98900000	12.83500000
Na	7.03600000	12.27400000	15.47300000

^{t}BuOH

O	8.50400000	11.26100000	14.22300000
C	8.45900000	11.21000000	12.77300000
C	7.18800000	10.47900000	12.33100000
C	8.49900000	12.63600000	12.21400000
C	9.70500000	10.43200000	12.36500000
H	6.29200000	11.02900000	12.66000000
H	7.13200000	10.37800000	11.23600000
H	7.15900000	9.47400000	12.77700000
H	9.39700000	13.15700000	12.57400000

H	7.61500000	13.20600000	12.54100000
H	8.50900000	12.64500000	11.11300000
H	9.68900000	9.42400000	12.80400000
H	9.75600000	10.34000000	11.27000000
H	10.61100000	10.94500000	12.71900000
H	7.72000000	11.75400000	14.52700000

IM4-IPr$^{\#}$ (IM4-L_A)

Pd	9.42000000	11.03800000	10.62400000
N	9.08900000	11.96100000	7.78200000
N	9.42700000	9.81900000	7.67800000
N	10.13600000	11.71700000	12.37600000
C	8.63000000	6.28100000	8.59900000
C	9.18300000	10.83000000	8.59800000
C	8.44400000	7.63000000	8.26800000
C	9.88600000	5.67600000	8.56300000
C	11.69000000	14.58400000	10.32500000
C	9.29900000	11.64600000	6.44100000
C	7.91600000	15.92800000	8.87900000
C	9.49400000	10.30900000	6.37600000
C	7.47800000	17.30800000	9.36300000
C	9.58600000	14.12900000	8.91900000
C	7.03000000	8.19900000	8.10700000
C	6.62000000	8.32500000	6.63000000
C	10.97800000	6.44500000	8.15100000
C	11.01700000	13.70800000	9.25900000
C	9.15800000	15.41800000	9.26000000
C	5.90900000	7.43900000	8.82200000
C	5.25100000	8.03200000	9.90600000
C	10.31900000	3.34600000	7.63100000
C	7.93400000	2.88200000	9.33100000
C	4.91700000	17.30200000	9.58300000

C	9.03700000	3.60500000	9.80400000
C	5.49100000	9.10100000	6.31800000
C	7.09800000	15.12000000	8.08300000
C	6.57600000	13.07300000	6.71000000
C	12.83600000	15.34700000	10.05500000
C	6.91000000	13.39900000	5.24900000
C	7.41500000	18.40400000	8.29600000
C	6.18700000	17.16400000	10.16900000
C	5.08500000	13.26300000	7.01100000
C	8.70700000	13.30100000	8.17400000
C	10.86200000	7.79700000	7.81300000
C	6.97500000	2.38500000	10.21900000
C	10.10300000	4.19600000	8.88100000
C	7.47600000	13.82400000	7.69600000
C	5.44300000	6.19500000	8.36300000
C	11.99300000	8.41500000	5.62500000
C	11.45900000	7.30500000	4.95700000
C	6.72100000	12.40000000	4.28200000
C	13.44300000	16.11100000	11.05800000
C	3.75600000	17.08400000	10.33400000
C	11.86200000	13.59300000	7.99500000
C	6.26200000	16.81800000	11.52900000
C	5.00500000	9.17000000	5.01300000
C	4.38900000	5.54400000	9.00400000
C	6.91800000	19.66900000	8.65600000
C	13.45500000	8.08200000	7.60400000
C	4.18900000	7.38700000	10.54600000
C	14.22400000	8.92700000	8.41700000
C	9.15900000	3.80800000	11.18600000
C	12.56500000	9.44300000	4.86100000
C	4.53400000	12.61500000	8.13000000

C	5.10400000	16.60800000	12.28400000
C	14.05200000	6.89100000	7.15800000
C	3.84500000	16.73900000	11.68700000
C	12.05200000	8.51800000	7.15800000
C	11.16500000	14.61300000	11.62800000
C	15.51700000	8.57900000	8.81700000
C	7.10600000	2.59800000	11.59200000
C	6.90300000	20.72200000	7.74400000
C	12.91900000	16.12200000	12.35100000
C	9.58700000	8.40500000	7.95800000
C	3.76200000	6.13400000	10.10500000
C	7.36800000	14.65300000	4.82500000
C	11.17400000	2.23400000	7.70200000
C	12.90400000	12.65700000	7.95300000
C	4.24200000	14.05200000	6.21500000
C	11.77600000	15.36800000	12.63000000
C	7.25200000	7.62800000	5.59200000
C	8.20400000	3.31300000	12.07300000
C	7.38600000	20.53500000	6.44600000
C	7.90500000	18.23100000	6.99600000
C	11.68300000	14.44000000	6.89200000
C	2.88200000	14.17800000	6.52200000
C	9.66200000	3.59900000	6.41800000
C	15.34000000	6.53400000	7.56300000
C	11.50300000	7.22300000	3.56200000
C	5.64200000	8.46600000	3.98500000
C	12.60600000	9.36500000	3.47000000
C	13.74300000	12.56300000	6.84200000
C	6.98700000	12.64300000	2.93500000
C	3.17800000	12.74900000	8.44400000
C	12.07700000	8.25000000	2.81200000

C	9.84900000	2.76300000	5.31300000
C	2.34400000	13.52400000	7.63200000
C	16.07700000	7.37100000	8.40300000
C	13.55000000	13.40700000	5.74500000
C	7.63300000	14.90200000	3.47300000
C	12.51800000	14.34700000	5.77600000
C	7.88900000	19.28700000	6.07700000
C	7.44600000	13.89700000	2.52300000
C	6.76900000	7.70000000	4.28000000
C	10.70100000	1.66000000	5.39900000
C	11.36600000	1.39900000	6.60100000
C	10.85200000	8.58800000	11.50400000
C	11.00800000	7.37800000	12.19900000
C	9.94000000	6.80900000	12.88900000
C	8.70800000	7.45400000	12.88900000
C	8.51400000	8.67300000	12.21300000
C	9.58900000	9.20300000	11.48100000
C	7.20500000	9.38700000	12.39300000
C	12.05500000	9.21300000	10.85700000
C	10.54600000	11.53900000	14.76200000
C	10.12600000	11.67500000	16.08000000
C	8.81000000	12.05700000	16.36500000
C	7.93300000	12.31300000	15.30400000
C	8.34600000	12.19300000	13.98000000
C	9.67000000	11.79200000	13.67600000
H	7.76400000	5.68700000	8.89200000
H	9.28800000	12.39800000	5.66400000
H	9.67100000	9.66200000	5.52800000
H	8.25000000	17.63200000	10.08400000
H	7.03300000	9.21500000	8.53300000
H	11.95900000	5.97100000	8.07900000

H	10.95600000	12.68500000	9.69700000
H	9.83200000	16.04300000	9.84800000
H	5.56700000	9.01600000	10.25700000
H	7.82600000	2.69500000	8.26000000
H	4.83600000	17.61800000	8.54100000
H	4.97000000	9.63400000	7.11700000
H	6.14100000	15.50700000	7.72200000
H	6.77400000	11.99700000	6.83300000
H	13.27000000	15.34100000	9.05300000
H	6.11800000	1.82800000	9.83300000
H	11.05000000	4.14900000	9.44600000
H	5.89500000	5.73700000	7.47900000
H	11.00600000	6.49200000	5.52800000
H	6.37100000	11.41300000	4.59400000
H	14.33200000	16.69800000	10.82300000
H	2.77800000	17.19600000	9.86100000
H	7.24200000	16.70700000	12.00000000
H	4.11900000	9.77300000	4.79800000
H	4.05100000	4.57200000	8.63700000
H	6.54200000	19.83100000	9.66800000
H	3.69500000	7.87500000	11.39000000
H	13.80100000	9.87400000	8.75400000
H	10.00500000	4.38400000	11.56600000
H	12.97900000	10.31800000	5.36800000
H	5.16400000	12.00600000	8.78700000
H	5.18600000	16.33000000	13.33500000
H	13.51900000	6.24500000	6.45900000
H	2.94000000	16.57700000	12.27500000
H	11.97100000	9.58800000	7.40300000
H	10.29600000	14.00000000	11.87100000
H	16.08500000	9.25500000	9.46000000

H	6.35500000	2.21100000	12.28500000
H	6.52300000	21.69800000	8.05300000
H	13.39900000	16.70700000	13.13800000
H	2.93900000	5.62300000	10.60900000
H	7.52200000	15.45200000	5.55300000
H	11.69200000	2.02000000	8.64100000
H	13.06100000	12.00800000	8.81700000
H	4.64200000	14.56400000	5.33800000
H	11.35600000	15.35400000	13.64000000
H	8.13200000	7.02000000	5.80700000
H	8.31800000	3.49000000	13.14500000
H	7.38300000	21.36200000	5.73300000
H	8.32000000	17.26800000	6.69700000
H	10.88600000	15.18700000	6.90800000
H	2.24200000	14.79100000	5.88300000
H	8.99600000	4.46100000	6.33700000
H	15.77600000	5.59800000	7.20500000
H	11.08900000	6.34600000	3.06100000
H	5.26000000	8.51600000	2.96400000
H	13.05300000	10.18000000	2.89700000
H	14.55000000	11.82700000	6.83500000
H	6.84200000	11.84300000	2.20500000
H	2.79600000	12.24700000	9.33500000
H	12.11500000	8.18500000	1.72200000
H	9.32400000	2.97600000	4.37800000
H	1.28200000	13.61800000	7.86500000
H	17.08500000	7.09300000	8.71700000
H	14.20300000	13.33400000	4.87200000
H	7.98800000	15.88700000	3.16500000
H	12.36000000	15.01500000	4.92700000
H	8.28100000	19.13200000	5.07000000

H	7.66100000	14.08700000	1.47000000
H	7.27900000	7.14600000	3.48900000
H	10.85000000	1.00800000	4.53600000
H	12.03700000	0.54000000	6.68100000
H	11.99300000	6.89900000	12.20700000
H	7.86600000	7.03400000	13.44700000
H	6.36000000	8.68300000	12.38400000
H	7.03400000	10.16000000	11.63200000
H	7.18900000	9.90100000	13.36600000
H	12.81100000	8.45800000	10.60900000
H	12.53900000	9.94500000	11.52500000
H	11.76800000	9.75700000	9.94400000
H	10.07600000	5.87800000	13.44300000
H	7.63800000	12.38600000	13.16900000
H	11.57000000	11.21800000	14.54300000
H	10.82900000	11.46200000	16.88700000
H	6.90200000	12.60500000	15.51100000
H	8.47500000	12.14200000	17.40100000
H	11.12300000	11.44300000	12.41500000
Cl	7.43700000	12.11000000	11.55500000
Na	7.63600000	14.12800000	10.17500000
NaCl			
Cl	9.72500000	11.70300000	12.33200000
Na	7.40000000	11.19000000	12.33200000
IM5-IPr$^{\#}$ (IM5-L_A)			
Pd	9.08000000	10.31700000	10.51200000
N	9.09200000	11.98400000	7.59100000
N	9.34300000	9.85300000	7.40000000
N	9.51900000	11.74200000	11.91300000
C	8.56600000	6.34400000	8.42000000
C	9.07400000	10.82400000	8.34600000

C	8.36200000	7.67700000	8.03700000
C	9.83200000	5.75600000	8.40900000
C	11.68400000	14.45000000	10.22600000
C	9.37500000	11.72800000	6.25100000
C	7.95000000	15.91100000	8.77300000
C	9.51900000	10.38700000	6.12700000
C	7.50700000	17.26100000	9.32800000
C	9.62500000	14.12100000	8.73900000
C	6.94500000	8.24700000	7.88800000
C	6.49100000	8.36000000	6.42600000
C	10.91600000	6.52100000	7.96900000
C	11.03300000	13.64000000	9.09400000
C	9.21500000	15.41300000	9.09000000
C	5.85000000	7.50200000	8.65100000
C	5.24200000	8.10500000	9.75800000
C	10.32100000	3.40100000	7.58700000
C	7.91700000	3.03100000	9.32200000
C	4.95700000	17.16500000	9.59000000
C	9.04700000	3.73400000	9.76200000
C	5.38300000	9.17500000	6.13700000
C	7.10200000	15.11200000	8.00400000
C	6.55700000	13.07000000	6.62400000
C	12.91300000	15.10700000	10.07500000
C	6.84200000	13.41400000	5.15600000
C	7.42600000	18.40000000	8.31200000
C	6.23700000	17.05800000	10.15200000
C	5.07600000	13.22300000	6.98900000
C	8.72300000	13.31800000	8.01000000
C	10.78300000	7.85800000	7.58900000
C	6.98300000	2.53900000	10.23600000
C	10.08700000	4.30200000	8.80000000

C	7.47600000	13.83000000	7.58100000
C	5.36400000	6.25400000	8.22600000
C	12.04500000	8.45400000	5.45900000
C	11.58600000	7.31900000	4.77500000
C	6.67100000	12.42200000	4.17600000
C	13.48100000	15.82400000	11.13500000
C	3.82000000	16.88000000	10.34900000
C	11.93900000	13.55800000	7.86800000
C	6.34900000	16.66800000	11.49500000
C	4.84100000	9.22200000	4.85400000
C	4.33700000	5.61300000	8.91800000
C	6.89200000	19.63700000	8.71200000
C	13.33400000	8.17800000	7.59100000
C	4.20400000	7.47200000	10.44700000
C	13.86100000	8.90300000	8.66800000
C	9.21900000	3.92700000	11.14100000
C	12.65100000	9.48100000	4.71700000
C	4.61900000	12.68600000	8.20400000
C	5.21400000	16.39000000	12.25800000
C	14.08900000	7.10800000	7.08600000
C	3.94400000	16.49200000	11.68500000
C	11.98700000	8.59000000	6.98700000
C	11.03900000	14.53300000	11.47200000
C	15.09300000	8.57000000	9.23600000
C	7.16900000	2.72900000	11.60700000
C	6.86600000	20.72500000	7.84000000
C	12.83000000	15.89700000	12.36500000
C	9.49700000	8.44900000	7.69300000
C	3.75400000	6.21700000	10.03500000
C	7.24100000	14.69100000	4.73800000
C	11.19700000	2.31100000	7.70300000

C	12.96900000	12.60600000	7.84100000
C	4.15100000	13.85900000	6.15200000
C	11.60500000	15.24300000	12.53000000
C	7.05300000	7.60900000	5.38600000
C	8.29300000	3.42700000	12.05600000
C	7.37800000	20.60300000	6.54500000
C	7.94700000	18.29500000	7.01600000
C	11.83700000	14.45400000	6.79600000
C	2.80400000	13.95800000	6.51800000
C	9.66900000	3.60100000	6.36200000
C	15.32000000	6.76600000	7.65300000
C	11.74400000	7.20800000	3.38900000
C	5.40200000	8.45700000	3.82600000
C	12.80300000	9.37400000	3.33400000
C	13.86900000	12.54300000	6.77700000
C	6.89100000	12.69600000	2.82600000
C	3.27700000	12.78100000	8.57000000
C	12.35300000	8.23200000	2.66400000
C	9.87600000	2.72900000	5.28900000
C	2.36100000	13.41900000	7.72600000
C	15.82800000	7.49600000	8.73000000
C	13.75100000	13.43700000	5.70900000
C	7.46200000	14.96900000	3.38500000
C	12.73200000	14.39200000	5.72300000
C	7.92100000	19.38500000	6.13900000
C	7.28900000	13.97400000	2.42200000
C	6.51200000	7.65500000	4.09600000
C	10.74500000	1.64500000	5.42100000
C	11.40900000	1.44100000	6.63400000
C	10.75600000	8.61700000	12.25600000
C	10.99600000	7.55400000	13.13900000

C	9.94600000	6.92000000	13.80500000
C	8.64600000	7.37200000	13.60500000
C	8.36200000	8.43800000	12.73400000
C	9.42200000	9.02500000	12.00900000
C	6.92900000	8.90000000	12.64600000
C	11.93900000	9.31400000	11.62900000
C	10.11000000	11.88500000	14.28000000
C	9.75200000	12.09900000	15.60800000
C	8.40700000	12.24400000	15.96300000
C	7.43200000	12.18500000	14.96000000
C	7.78500000	11.99100000	13.62600000
C	9.13800000	11.82400000	13.25000000
H	7.71100000	5.75100000	8.74500000
H	9.43700000	12.52100000	5.51500000
H	9.72800000	9.76900000	5.26300000
H	8.29400000	17.55900000	10.04500000
H	6.96400000	9.27000000	8.29800000
H	11.90600000	6.06300000	7.92600000
H	10.91800000	12.60800000	9.47600000
H	9.90100000	16.04100000	9.66000000
H	5.59100000	9.08600000	10.08600000
H	7.77300000	2.85500000	8.25400000
H	4.84900000	17.48000000	8.55000000
H	4.92300000	9.76100000	6.93800000
H	6.10600000	15.47400000	7.73900000
H	6.77800000	11.99500000	6.73200000
H	13.44400000	15.05300000	9.12300000
H	6.10400000	1.99900000	9.87500000
H	11.04000000	4.31100000	9.35700000
H	5.78200000	5.78700000	7.33200000
H	11.10900000	6.50700000	5.32700000

H	6.36700000	11.41700000	4.47800000
H	14.44000000	16.32700000	10.99100000
H	2.83200000	16.96100000	9.89100000
H	7.34100000	16.57200000	11.94500000
H	3.97400000	9.85700000	4.65700000
H	3.98200000	4.63800000	8.57600000
H	6.49000000	19.74500000	9.72200000
H	3.74800000	7.96200000	11.30900000
H	13.29500000	9.74300000	9.07200000
H	10.08700000	4.48500000	11.50400000
H	13.00300000	10.37700000	5.23400000
H	5.32900000	12.19600000	8.87500000
H	5.32400000	16.08900000	13.30100000
H	13.72400000	6.54500000	6.22500000
H	3.05400000	16.27300000	12.27900000
H	11.86900000	9.66400000	7.20100000
H	10.08200000	14.02300000	11.61100000
H	15.47800000	9.15600000	10.07300000
H	6.44300000	2.33600000	12.32100000
H	6.45100000	21.67700000	8.17900000
H	13.27000000	16.45500000	13.19400000
H	2.95000000	5.71500000	10.57700000
H	7.38500000	15.48200000	5.47500000
H	11.71600000	2.14100000	8.65000000
H	13.07400000	11.91700000	8.68200000
H	4.48100000	14.27700000	5.20000000
H	11.08600000	15.28000000	13.48900000
H	7.91800000	6.97300000	5.58600000
H	8.45100000	3.58600000	13.12500000
H	7.36100000	21.45500000	5.86300000
H	8.39200000	17.35300000	6.68900000

H	11.05200000	15.21300000	6.79900000
H	2.10000000	14.45700000	5.84900000
H	8.99500000	4.45300000	6.24400000
H	15.88800000	5.93000000	7.24200000
H	11.39000000	6.31000000	2.87800000
H	4.97400000	8.48600000	2.82200000
H	13.27500000	10.18700000	2.77900000
H	14.66500000	11.79400000	6.78500000
H	6.75500000	11.90500000	2.08500000
H	2.94300000	12.35600000	9.51800000
H	12.47700000	8.14500000	1.58300000
H	9.35500000	2.90200000	4.34400000
H	1.30900000	13.49300000	8.01100000
H	16.79600000	7.23800000	9.16500000
H	14.45100000	13.39100000	4.87100000
H	7.77000000	15.97300000	3.08600000
H	12.63500000	15.10000000	4.89700000
H	8.33700000	19.27900000	5.13400000
H	7.46800000	14.19000000	1.36700000
H	6.95800000	7.05200000	3.30200000
H	10.90800000	0.96400000	4.58300000
H	12.09600000	0.60000000	6.74700000
H	12.02800000	7.23500000	13.31200000
H	7.81500000	6.91100000	14.14600000
H	6.26700000	8.07100000	12.35300000
H	6.81500000	9.71000000	11.91300000
H	6.58400000	9.28200000	13.61900000
H	12.80200000	8.64100000	11.52700000
H	12.27000000	10.16400000	12.25100000
H	11.67800000	9.71200000	10.63800000
H	10.14500000	6.09300000	14.48900000

H	7.01800000	11.97000000	12.84900000
H	11.16500000	11.74900000	14.01500000
H	10.53000000	12.13200000	16.37300000
H	6.37600000	12.29400000	15.22200000
H	8.12900000	12.39900000	17.00600000
H	10.54700000	11.70200000	11.90700000

TS5-IPr# (TS5-L_A)

Pd	9.03600000	10.67400000	10.30800000
N	9.08400000	12.01400000	7.45900000
N	9.33000000	9.87100000	7.35700000
N	9.43100000	11.25200000	12.18200000
C	8.55800000	6.37800000	8.44200000
C	9.08200000	10.88700000	8.26700000
C	8.35900000	7.71100000	8.05800000
C	9.82200000	5.78500000	8.42400000
C	11.67100000	14.40100000	10.12200000
C	9.33800000	11.70000000	6.12700000
C	7.95300000	15.92100000	8.70400000
C	9.48200000	10.35500000	6.06100000
C	7.51100000	17.26000000	9.28900000
C	9.63600000	14.14100000	8.60700000
C	6.94800000	8.29100000	7.94400000
C	6.45600000	8.38400000	6.49600000
C	10.90600000	6.55000000	7.98800000
C	11.03400000	13.63300000	8.96100000
C	9.22400000	15.42000000	8.99800000
C	5.89400000	7.56900000	8.77900000
C	5.49700000	8.10300000	9.99500000
C	10.30600000	3.43100000	7.59200000
C	7.89500000	3.07400000	9.31900000
C	4.96000000	17.15500000	9.54800000

C	9.03900000	3.74900000	9.76700000
C	5.34800000	9.20300000	6.21800000
C	7.10200000	15.13900000	7.92100000
C	6.54100000	13.10800000	6.52700000
C	12.85400000	15.13700000	9.99100000
C	6.80300000	13.45100000	5.05600000
C	7.43200000	18.41800000	8.29200000
C	6.24000000	17.06600000	10.11400000
C	5.06800000	13.25700000	6.92000000
C	8.72800000	13.35100000	7.87000000
C	10.77000000	7.88600000	7.60100000
C	6.96500000	2.56400000	10.22800000
C	10.07700000	4.32800000	8.80900000
C	7.47500000	13.86800000	7.46900000
C	5.26900000	6.39700000	8.34300000
C	12.07300000	8.47400000	5.49500000
C	11.63300000	7.33100000	4.81300000
C	6.62300000	12.45500000	4.08200000
C	13.39900000	15.82500000	11.08100000
C	3.82000000	16.89800000	10.31300000
C	11.96300000	13.54900000	7.75500000
C	6.34600000	16.72900000	11.47100000
C	4.79100000	9.25100000	4.94100000
C	4.29400000	5.76800000	9.11400000
C	6.90400000	19.65100000	8.71100000
C	13.30100000	8.23400000	7.68400000
C	4.51300000	7.48200000	10.76400000
C	13.66700000	8.84400000	8.87800000
C	9.22800000	3.89600000	11.14900000
C	12.67700000	9.50100000	4.75300000
C	4.63800000	12.70900000	8.14000000

C	5.20800000	16.48400000	12.24100000
C	14.17600000	7.29300000	7.14200000
C	3.93900000	16.56100000	11.66200000
C	11.97800000	8.62300000	7.01800000
C	11.05100000	14.37100000	11.38000000
C	14.86300000	8.52400000	9.51800000
C	7.16900000	2.70900000	11.60100000
C	6.88500000	20.75300000	7.85800000
C	12.77400000	15.78500000	12.32300000
C	9.48800000	8.47900000	7.69400000
C	3.91100000	6.30800000	10.32900000
C	7.20200000	14.72500000	4.63100000
C	11.17600000	2.33500000	7.70400000
C	13.01000000	12.61400000	7.76700000
C	4.12500000	13.89700000	6.10700000
C	11.59500000	15.05100000	12.46900000
C	6.99800000	7.62600000	5.45100000
C	8.30600000	3.37800000	12.05900000
C	7.39600000	20.64800000	6.56100000
C	7.94800000	18.32800000	6.99300000
C	11.86500000	14.41700000	6.65900000
C	2.78600000	13.99000000	6.50300000
C	9.65500000	3.64100000	6.36800000
C	15.37300000	6.96500000	7.78400000
C	11.80200000	7.21400000	3.42900000
C	5.33600000	8.48100000	3.90700000
C	12.84300000	9.38900000	3.37200000
C	13.93200000	12.54800000	6.72200000
C	6.83600000	12.72300000	2.72900000
C	3.30400000	12.79900000	8.53500000
C	12.40900000	8.24000000	2.70300000

C	9.85900000	2.77300000	5.29100000
C	2.37000000	13.44200000	7.71600000
C	15.72200000	7.57800000	8.97300000
C	13.82100000	13.41800000	5.63400000
C	7.41500000	14.99800000	3.27500000
C	12.78300000	14.35100000	5.60600000
C	7.92800000	19.43200000	6.13400000
C	7.23500000	13.99800000	2.31800000
C	6.44300000	7.67200000	4.16700000
C	10.72400000	1.68500000	5.41800000
C	11.38500000	1.47000000	6.63000000
C	10.71900000	9.12400000	12.23400000
C	10.91900000	7.90800000	12.84900000
C	9.85400000	7.20900000	13.40500000
C	8.57300000	7.73500000	13.35200000
C	8.32300000	8.94900000	12.74500000
C	9.40800000	9.62100000	12.15600000
C	6.91700000	9.47800000	12.74100000
C	11.89200000	9.88000000	11.67400000
C	9.69800000	11.92500000	14.47900000
C	9.27200000	12.57100000	15.56400000
C	8.10000000	13.13900000	15.50200000
C	7.36200000	13.06400000	14.34000000
C	7.78900000	12.43200000	13.24600000
C	8.96200000	11.85700000	13.30200000
H	7.69800000	5.79200000	8.77000000
H	9.38900000	12.45600000	5.35400000
H	9.68100000	9.70300000	5.22000000
H	8.30100000	17.54300000	10.00900000
H	6.99800000	9.32100000	8.33700000
H	11.89800000	6.09500000	7.95000000

H	10.88400000	12.59600000	9.32800000
H	9.91000000	16.03400000	9.58300000
H	5.97000000	9.02000000	10.33600000
H	7.73700000	2.93100000	8.24800000
H	4.85200000	17.43700000	8.49900000
H	4.90400000	9.79700000	7.02200000
H	6.10400000	15.50500000	7.67500000
H	6.76700000	12.03400000	6.63200000
H	13.36300000	15.17200000	9.03000000
H	6.07700000	2.04500000	9.86000000
H	11.03100000	4.33300000	9.36500000
H	5.53700000	5.98100000	7.37900000
H	11.15500000	6.51900000	5.36400000
H	6.32100000	11.45100000	4.39100000
H	14.32000000	16.39400000	10.95200000
H	2.83400000	16.96100000	9.84900000
H	7.33700000	16.65300000	11.92700000
H	3.92700000	9.89200000	4.75300000
H	3.82600000	4.85400000	8.75800000
H	6.50200000	19.74500000	9.72300000
H	4.21300000	7.92200000	11.70600000
H	12.99700000	9.58000000	9.31100000
H	10.11000000	4.42800000	11.51500000
H	13.01200000	10.40500000	5.26600000
H	5.36500000	12.21400000	8.79000000
H	5.31300000	16.23400000	13.29800000
H	13.93000000	6.81800000	6.20100000
H	3.04800000	16.36400000	12.26100000
H	11.83900000	9.69700000	7.21800000
H	10.12000000	13.81000000	11.49500000
H	15.12700000	9.02000000	10.44300000

H	6.44800000	2.29900000	12.31100000
H	6.47600000	21.70200000	8.21100000
H	13.19800000	16.32200000	13.17200000
H	3.14400000	5.82000000	10.93100000
H	7.35400000	15.51900000	5.36500000
H	11.69200000	2.15700000	8.65100000
H	13.10800000	11.93700000	8.62000000
H	4.43500000	14.32000000	5.15000000
H	11.09200000	15.00800000	13.43500000
H	7.86200000	6.98600000	5.64000000
H	8.47800000	3.49700000	13.13000000
H	7.38600000	21.51200000	5.89400000
H	8.38200000	17.38700000	6.65000000
H	11.06200000	15.15700000	6.62800000
H	2.06600000	14.49200000	5.85300000
H	8.98500000	4.49500000	6.25500000
H	16.03800000	6.22900000	7.34200000
H	11.45700000	6.31200000	2.91900000
H	4.89700000	8.51200000	2.90800000
H	13.31100000	10.20400000	2.81600000
H	14.73900000	11.81300000	6.76000000
H	6.69700000	11.92800000	1.99300000
H	2.99100000	12.36500000	9.48700000
H	12.53900000	8.15000000	1.62300000
H	9.33900000	2.95200000	4.34700000
H	1.32400000	13.51100000	8.02300000
H	16.66100000	7.32700000	9.46800000
H	14.53900000	13.36900000	4.81400000
H	7.72600000	15.99900000	2.96900000
H	12.68700000	15.03700000	4.76200000
H	8.33900000	19.33800000	5.12600000

H	7.40900000	14.20800000	1.26100000
H	6.87900000	7.06800000	3.36800000
H	10.88600000	1.00800000	4.57600000
H	12.06800000	0.62500000	6.74000000
H	11.93100000	7.51800000	12.89700000
H	7.73100000	7.20100000	13.78700000
H	6.21300000	8.66500000	12.72000000
H	6.72100000	10.11900000	11.88700000
H	6.71100000	10.06800000	13.62100000
H	12.78100000	9.23900000	11.61800000
H	12.15700000	10.75000000	12.29600000
H	11.67400000	10.25700000	10.66100000
H	10.02300000	6.26200000	13.88200000
H	7.22200000	12.37300000	12.33500000
H	10.61000000	11.46400000	14.53200000
H	9.85700000	12.62100000	16.46400000
H	6.43700000	13.49500000	14.28200000
H	7.76400000	13.63500000	16.35400000
H	10.40000000	11.44900000	12.01400000

Product 2,6-dimethyl-N-phenylaniline

C	10.34100000	9.45100000	14.84800000
C	10.55600000	8.19500000	15.43000000
C	9.48800000	7.42300000	15.88700000
C	8.18800000	7.91400000	15.78700000
C	7.92600000	9.15700000	15.19400000
C	9.01500000	9.92300000	14.72000000
C	6.51400000	9.63000000	15.00900000
C	11.50000000	10.28200000	14.36600000
C	8.19900000	13.44700000	13.64100000
C	7.92600000	14.72300000	14.12800000
C	7.92700000	14.97900000	15.50300000

C	8.20900000	13.93000000	16.38100000
C	8.48700000	12.64500000	15.90800000
C	8.48500000	12.38300000	14.52500000
H	11.57700000	7.81300000	15.51600000
H	7.34800000	7.30500000	16.13000000
H	5.80700000	8.84700000	15.31000000
H	6.33200000	9.88700000	13.95500000
H	6.29800000	10.53800000	15.59300000
H	12.44700000	9.73700000	14.48000000
H	11.57700000	11.22600000	14.93000000
H	11.39200000	10.55800000	13.30400000
H	9.67000000	6.43400000	16.31300000
H	8.73400000	11.84100000	16.60300000
H	8.18400000	13.26000000	12.56300000
H	7.69800000	15.52500000	13.41900000
H	8.22300000	14.11400000	17.45700000
H	7.70000000	15.97800000	15.88000000
H	9.10100000	11.13600000	13.03800000
N	8.75600000	11.12300000	13.99500000

Pd-BIAN-IPr$^{\#}$ (Pd-L_B)

Pd	8.75700000	10.76600000	10.32100000
N	9.15200000	12.01000000	7.63200000
N	9.24800000	9.80500000	7.52900000
C	8.46200000	6.37600000	8.80900000
C	9.06400000	10.86300000	8.41900000
C	8.26700000	7.69200000	8.36700000
C	9.73200000	5.79600000	8.87100000
C	11.56800000	13.95200000	10.66000000
C	9.40200000	11.66900000	6.31200000
C	8.05600000	15.81600000	9.18400000
C	9.43300000	10.28800000	6.24100000

C	7.63900000	17.13700000	9.82700000
C	9.72100000	14.03600000	8.93000000
C	6.86600000	8.30400000	8.36700000
C	6.17700000	8.27400000	7.00700000
C	10.82900000	6.56700000	8.48300000
C	11.08800000	13.45700000	9.29400000
C	9.32300000	15.28100000	9.43100000
C	5.99500000	7.73600000	9.49100000
C	6.25500000	8.14100000	10.81000000
C	10.26200000	3.40300000	8.19800000
C	7.85800000	3.03100000	9.90600000
C	5.10400000	16.98600000	10.21000000
C	8.91700000	3.85000000	10.31700000
C	5.15400000	9.20300000	6.75000000
C	7.17700000	15.08100000	8.38700000
C	6.50300000	13.09700000	6.98100000
C	12.54800000	14.94100000	10.81400000
C	6.43700000	13.58600000	5.53300000
C	7.50600000	18.30400000	8.84400000
C	6.41200000	16.92500000	10.71400000
C	5.12700000	13.07100000	7.66500000
C	8.80800000	13.32100000	8.12600000
C	10.69400000	7.87600000	8.01000000
C	6.89900000	2.59100000	10.82300000
C	9.98200000	4.36600000	9.35000000
C	7.52800000	13.84500000	7.83200000
C	4.95400000	6.82700000	9.26800000
C	12.47600000	8.30900000	6.22200000
C	12.41800000	7.01900000	5.67500000
C	6.20400000	12.65100000	4.51200000
C	12.92300000	15.38000000	12.08900000

C	4.00900000	16.71800000	11.03200000
C	12.14100000	13.62100000	8.20600000
C	6.59000000	16.60300000	12.06800000
C	4.46500000	9.19800000	5.53700000
C	4.19800000	6.32900000	10.33500000
C	6.91200000	19.50500000	9.26800000
C	13.02600000	8.52300000	8.70800000
C	5.50200000	7.65000000	11.87600000
C	12.75700000	9.05800000	9.97900000
C	8.99400000	4.21400000	11.67000000
C	13.08000000	9.32300000	5.46400000
C	5.02200000	12.47700000	8.93400000
C	5.49600000	16.34400000	12.89500000
C	14.25900000	7.89600000	8.49200000
C	4.20000000	16.39700000	12.37800000
C	11.95100000	8.65100000	7.61900000
C	10.98100000	13.40600000	11.81200000
C	13.69700000	8.96600000	11.00500000
C	6.98700000	2.95800000	12.16600000
C	6.85000000	20.61200000	8.42300000
C	12.32700000	14.83300000	13.22600000
C	9.39700000	8.43500000	7.95900000
C	4.46800000	6.73800000	11.64200000
C	6.55900000	14.93700000	5.17600000
C	11.13600000	2.32600000	8.40700000
C	13.19100000	12.69100000	8.14200000
C	3.96800000	13.58100000	7.06900000
C	11.35500000	13.83800000	13.08300000
C	6.49400000	7.34500000	6.00700000
C	8.04000000	3.77300000	12.58800000
C	7.38400000	20.54800000	7.13300000

C	8.04100000	18.25200000	7.55000000
C	12.13800000	14.68700000	7.29600000
C	2.73400000	13.50300000	7.72500000
C	9.66200000	3.53700000	6.93800000
C	15.20200000	7.80200000	9.52300000
C	12.95300000	6.75200000	4.41100000
C	4.78900000	8.26300000	4.54900000
C	13.61200000	9.06100000	4.20000000
C	14.21000000	12.82400000	7.19900000
C	6.08700000	13.05200000	3.18100000
C	3.79300000	12.39400000	9.58500000
C	13.55300000	7.77000000	3.66900000
C	9.92500000	2.61500000	5.92000000
C	2.64000000	12.91000000	8.98300000
C	14.92500000	8.33400000	10.78100000
C	14.19700000	13.89100000	6.29600000
C	6.44200000	15.34100000	3.84300000
C	13.15700000	14.82100000	6.34800000
C	7.98100000	19.36300000	6.70200000
C	6.20200000	14.40200000	2.84000000
C	5.80600000	7.33900000	4.78900000
C	10.79400000	1.54600000	6.14300000
C	11.40300000	1.40600000	7.39300000
C	9.61500000	9.86700000	4.85600000
C	9.75900000	11.09900000	4.14300000
C	9.65100000	12.24200000	4.99500000
C	9.97800000	11.17800000	2.76200000
C	10.13300000	12.48600000	2.21600000
C	10.05700000	13.59700000	3.04100000
C	9.80800000	13.49700000	4.43700000
C	10.01800000	9.94000000	2.05400000

C	9.85400000	8.74500000	2.73400000
C	9.65500000	8.68500000	4.14100000
H	7.59600000	5.80900000	9.15400000
H	8.46400000	17.41200000	10.50900000
H	7.00800000	9.36900000	8.63100000
H	11.83500000	6.15000000	8.58200000
H	10.92200000	12.37200000	9.42500000
H	10.01500000	15.83000000	10.07300000
H	7.07200000	8.85800000	10.98000000
H	7.78700000	2.72200000	8.86100000
H	4.93600000	17.25900000	9.16500000
H	4.88800000	9.93300000	7.51900000
H	6.16100000	15.44700000	8.22600000
H	6.82200000	12.04400000	6.93100000
H	13.02900000	15.36800000	9.93200000
H	6.07800000	1.95400000	10.48300000
H	10.91800000	4.41300000	9.93400000
H	4.72400000	6.51000000	8.24800000
H	11.94500000	6.20800000	6.23200000
H	6.11600000	11.59100000	4.76500000
H	13.68900000	16.15300000	12.18900000
H	2.99900000	16.76000000	10.61700000
H	7.60300000	16.55000000	12.47600000
H	3.67300000	9.93100000	5.36500000
H	3.38900000	5.62200000	10.13800000
H	6.49000000	19.56800000	10.27300000
H	5.72200000	7.97700000	12.89500000
H	11.79300000	9.54500000	10.16500000
H	9.81500000	4.85300000	12.00700000
H	13.12600000	10.33900000	5.86600000
H	5.92200000	12.07600000	9.41600000

H	5.65700000	16.10100000	13.94800000
H	14.49300000	7.48000000	7.51000000
H	3.34200000	16.19300000	13.02100000
H	11.68500000	9.71900000	7.58900000
H	10.21500000	12.62800000	11.68400000
H	13.47100000	9.39200000	11.98500000
H	6.24000000	2.60900000	12.88200000
H	6.38300000	21.53400000	8.77800000
H	12.62300000	15.17400000	14.22100000
H	3.87700000	6.34900000	12.47400000
H	6.75400000	15.68800000	5.94300000
H	11.61400000	2.20800000	9.38400000
H	13.21300000	11.85800000	8.84900000
H	4.02500000	14.04200000	6.08100000
H	10.88900000	13.39600000	13.96700000
H	7.29000000	6.61900000	6.18300000
H	8.12200000	4.06500000	13.63700000
H	7.34100000	21.41800000	6.47400000
H	8.51700000	17.33500000	7.20000000
H	11.33000000	15.42100000	7.32900000
H	1.84200000	13.90900000	7.24200000
H	8.98900000	4.37600000	6.74800000
H	16.15800000	7.31000000	9.33300000
H	12.89700000	5.73800000	4.00800000
H	4.24900000	8.25600000	3.60000000
H	14.06700000	9.87100000	3.62600000
H	15.01700000	12.08800000	7.16800000
H	5.91500000	12.30200000	2.40500000
H	3.73300000	11.92600000	10.57000000
H	13.96500000	7.56100000	2.68000000
H	9.44800000	2.73700000	4.94500000

H	1.67700000	12.84500000	9.49200000
H	15.66200000	8.26200000	11.58400000
H	14.99000000	13.99300000	5.55300000
H	6.54100000	16.40000000	3.59200000
H	13.13600000	15.65700000	5.64500000
H	8.40700000	19.29900000	5.69800000
H	6.11300000	14.71700000	1.79800000
H	6.07200000	6.60800000	4.02100000
H	11.00100000	0.82800000	5.34700000
H	12.09000000	0.57800000	7.57900000
H	10.17800000	9.93800000	0.97300000
H	9.88700000	7.80700000	2.17600000
H	9.55000000	7.71600000	4.63000000
H	10.31200000	12.61000000	1.14500000
H	10.17900000	14.59200000	2.60700000
H	9.73700000	14.40300000	5.04000000

IM1-BIAN-IPr$^{\#}$ (IM1-L_B)

Pd	9.23000000	10.57800000	10.54700000
N	9.26200000	11.98900000	7.75500000
N	9.32900000	9.78900000	7.61400000
C	8.48900000	6.30800000	8.72500000
C	9.21800000	10.83200000	8.54000000
C	8.30700000	7.63800000	8.31900000
C	9.75200000	5.71800000	8.80200000
C	11.82800000	14.30000000	10.50500000
C	9.43400000	11.66500000	6.41700000
C	8.11700000	15.83600000	9.20200000
C	9.44800000	10.28500000	6.32500000
C	7.68600000	17.16700000	9.81300000
C	9.83300000	14.10200000	8.94500000
C	6.90400000	8.23200000	8.21100000

C	6.34300000	8.23400000	6.78600000
C	10.86200000	6.49000000	8.45500000
C	11.25100000	13.61800000	9.25500000
C	9.41500000	15.36000000	9.39800000
C	5.84400000	7.59800000	9.11700000
C	5.36100000	8.30800000	10.22300000
C	10.24900000	3.31700000	8.08400000
C	7.72700000	3.14000000	9.72400000
C	5.14700000	17.06600000	10.18800000
C	8.90700000	3.73900000	10.18900000
C	5.33600000	9.15800000	6.46700000
C	7.22800000	15.03500000	8.48400000
C	6.57600000	13.02600000	7.12500000
C	12.94800000	15.14200000	10.48000000
C	6.48400000	13.52600000	5.67900000
C	7.55700000	18.32100000	8.81500000
C	6.45200000	16.96300000	10.69200000
C	5.20300000	12.98900000	7.81300000
C	8.90700000	13.31100000	8.22900000
C	10.74600000	7.81500000	8.02800000
C	6.75700000	2.68300000	10.62000000
C	9.98200000	4.27200000	9.24700000
C	7.60200000	13.79200000	7.95900000
C	5.25000000	6.36100000	8.81200000
C	12.41600000	8.27600000	6.15200000
C	12.27400000	7.01400000	5.55700000
C	6.25100000	12.59700000	4.65500000
C	13.41900000	15.74300000	11.65300000
C	4.04400000	16.79300000	11.00000000
C	12.20300000	13.71300000	8.06900000
C	6.62100000	16.59700000	12.03500000

C	4.69900000	9.12800000	5.22700000
C	4.23100000	5.83600000	9.60700000
C	7.04300000	19.55400000	9.25100000
C	13.18300000	8.36700000	8.55500000
C	4.31600000	7.80100000	11.00300000
C	13.26000000	9.15000000	9.71600000
C	9.09100000	3.85600000	11.57500000
C	13.02300000	9.29800000	5.40600000
C	5.09500000	12.39200000	9.08000000
C	5.52000000	16.33200000	12.85200000
C	14.21800000	7.45500000	8.29900000
C	4.22600000	16.42300000	12.33500000
C	12.00200000	8.57100000	7.59500000
C	11.19600000	14.07800000	11.73900000
C	14.35100000	9.04800000	10.58100000
C	6.95200000	2.81000000	11.99700000
C	6.98000000	20.65300000	8.39500000
C	12.78300000	15.51000000	12.87300000
C	9.45600000	8.39800000	7.99100000
C	3.75300000	6.55800000	10.70400000
C	6.56300000	14.88200000	5.33300000
C	11.09700000	2.21600000	8.28700000
C	13.23800000	12.77400000	7.94500000
C	4.04500000	13.50500000	7.21900000
C	11.66600000	14.66900000	12.91100000
C	6.69700000	7.27700000	5.82600000
C	8.12500000	3.40100000	12.47300000
C	7.43100000	20.54400000	7.07600000
C	8.00800000	18.22600000	7.49200000
C	12.14500000	14.76500000	7.14400000
C	2.81000000	13.43100000	7.87200000

C	9.65400000	3.47300000	6.82500000
C	15.30400000	7.33900000	9.17200000
C	12.74600000	6.77500000	4.26200000
C	5.05800000	8.16600000	4.27700000
C	13.48900000	9.06500000	4.11200000
C	14.19600000	12.88700000	6.93600000
C	6.09300000	13.00600000	3.33000000
C	3.86400000	12.31500000	9.73100000
C	13.36200000	7.79700000	3.53800000
C	9.88800000	2.54900000	5.80200000
C	2.71300000	12.83500000	9.13000000
C	15.38200000	8.14300000	10.31000000
C	14.13400000	13.94700000	6.02700000
C	6.40400000	15.29700000	4.00800000
C	13.10200000	14.88100000	6.13100000
C	7.94500000	19.32700000	6.62900000
C	6.16500000	14.36200000	3.00000000
C	6.05900000	7.24200000	4.58100000
C	10.72800000	1.45600000	6.01900000
C	11.33700000	1.29400000	7.26700000
C	9.57600000	9.88200000	4.92800000
C	9.70400000	11.12100000	4.22700000
C	9.63900000	12.25400000	5.09800000
C	9.88000000	11.21400000	2.84000000
C	10.03300000	12.52600000	2.30400000
C	9.99700000	13.62700000	3.14400000
C	9.79500000	13.51300000	4.54800000
C	9.89500000	9.98800000	2.11400000
C	9.74700000	8.78500000	2.78400000
C	9.59000000	8.71000000	4.19500000
C	10.26000000	9.86200000	12.42200000

C	10.30300000	8.46200000	12.15400000
C	9.18000000	7.65800000	12.28100000
C	7.94400000	8.22200000	12.62500000
C	7.80300000	9.59500000	12.83100000
C	8.97400000	10.41300000	12.73300000
C	6.49100000	10.18100000	13.26500000
C	11.54600000	10.59300000	12.72800000
H	7.61600000	5.72900000	9.02500000
H	8.50300000	17.45700000	10.49900000
H	6.99000000	9.28400000	8.53100000
H	11.86100000	6.05100000	8.53500000
H	11.15000000	12.54500000	9.51100000
H	10.12200000	15.96600000	9.96700000
H	5.80500000	9.27500000	10.46700000
H	7.57000000	3.01200000	8.65100000
H	4.98700000	17.37200000	9.15100000
H	5.03300000	9.89600000	7.21500000
H	6.19400000	15.35900000	8.35400000
H	6.90800000	11.97700000	7.06300000
H	13.46300000	15.33400000	9.53700000
H	5.84300000	2.22100000	10.23900000
H	10.91600000	4.29300000	9.83800000
H	5.56800000	5.81200000	7.92300000
H	11.77900000	6.20700000	6.10000000
H	6.19700000	11.53300000	4.89800000
H	14.29400000	16.39600000	11.60800000
H	3.03700000	16.86800000	10.58500000
H	7.63200000	16.51100000	12.44400000
H	3.91300000	9.85400000	5.00700000
H	3.79000000	4.87100000	9.35200000
H	6.68500000	19.65000000	10.27900000

H	3.92900000	8.38900000	11.84000000
H	12.44700000	9.84800000	9.94000000
H	10.01200000	4.30700000	11.95600000
H	13.12100000	10.29500000	5.84500000
H	5.99300000	11.99400000	9.56300000
H	5.67600000	16.05000000	13.89600000
H	14.19000000	6.84500000	7.39500000
H	3.36300000	16.20900000	12.96800000
H	11.76900000	9.64600000	7.63400000
H	10.31600000	13.43300000	11.77900000
H	14.40400000	9.69000000	11.46300000
H	6.19600000	2.44800000	12.69600000
H	6.58100000	21.60100000	8.76300000
H	13.15400000	15.97700000	13.78800000
H	2.94300000	6.16000000	11.31600000
H	6.75400000	15.63200000	6.10200000
H	11.57400000	2.07800000	9.26100000
H	13.30400000	11.94900000	8.66000000
H	4.10100000	13.96700000	6.23200000
H	11.15900000	14.46700000	13.85700000
H	7.47900000	6.54900000	6.05300000
H	8.29100000	3.50700000	13.54800000
H	7.38700000	21.40500000	6.40600000
H	8.42500000	17.28400000	7.13100000
H	11.34900000	15.50800000	7.22200000
H	1.92000000	13.83900000	7.38800000
H	9.00700000	4.33400000	6.64000000
H	16.10300000	6.62900000	8.94700000
H	12.63000000	5.78300000	3.82100000
H	4.55800000	8.13800000	3.30800000
H	13.95100000	9.88000000	3.54900000

H	14.99800000	12.14900000	6.86600000
H	5.92200000	12.26000000	2.55100000
H	3.80200000	11.84500000	10.71500000
H	13.72900000	7.61100000	2.52700000
H	9.41100000	2.68700000	4.82900000
H	1.74900000	12.77400000	9.63800000
H	16.24200000	8.07100000	10.97900000
H	14.88500000	14.04000000	5.24000000
H	6.46800000	16.36000000	3.76600000
H	13.04400000	15.71100000	5.42300000
H	8.30500000	19.22800000	5.60200000
H	6.04200000	14.68500000	1.96400000
H	6.34600000	6.48600000	3.84600000
H	10.91400000	0.73600000	5.22000000
H	12.00100000	0.44500000	7.44700000
H	10.02500000	10.00300000	1.02900000
H	9.76400000	7.85400000	2.21400000
H	9.49600000	7.73500000	4.67100000
H	10.18000000	12.65800000	1.22900000
H	10.11800000	14.62500000	2.71900000
H	9.76300000	14.41500000	5.16000000
H	11.27100000	8.02400000	11.89500000
H	7.06100000	7.58500000	12.71500000
H	5.68500000	9.44100000	13.17100000
H	6.22800000	11.07300000	12.67700000
H	6.53400000	10.50200000	14.31800000
H	12.40200000	9.92800000	12.55300000
H	11.55900000	10.89800000	13.78700000
H	11.68100000	11.50700000	12.13700000
H	9.25000000	6.58500000	12.09800000
Cl	8.89300000	11.99700000	13.51400000

TS1-BIAN-IPr# (TS1-L_B)

Pd	8.87400000	10.65300000	10.47200000
N	9.22500000	12.01800000	7.72300000
N	9.28700000	9.81700000	7.57700000
C	8.46400000	6.34800000	8.72600000
C	9.11200000	10.85400000	8.50200000
C	8.27700000	7.66700000	8.29100000
C	9.73000000	5.76800000	8.82100000
C	11.84500000	14.33500000	10.44600000
C	9.46300000	11.69800000	6.39200000
C	8.11300000	15.87900000	9.17200000
C	9.47500000	10.31800000	6.29900000
C	7.69000000	17.21000000	9.79200000
C	9.82000000	14.13300000	8.90700000
C	6.86600000	8.24700000	8.15300000
C	6.33700000	8.25600000	6.71800000
C	10.83700000	6.54000000	8.46700000
C	11.24100000	13.64900000	9.20900000
C	9.40900000	15.39300000	9.36200000
C	5.80600000	7.58500000	9.03700000
C	5.34900000	8.25300000	10.17900000
C	10.23300000	3.38300000	8.08200000
C	7.71900000	3.16400000	9.70800000
C	5.14900000	17.14600000	10.16700000
C	8.88800000	3.77100000	10.18900000
C	5.33400000	9.18000000	6.38100000
C	7.22100000	15.08600000	8.45100000
C	6.55900000	13.07800000	7.09000000
C	12.95400000	15.19000000	10.38400000
C	6.47800000	13.56900000	5.64100000
C	7.56500000	18.37000000	8.80100000

C	6.45200000	17.00600000	10.66600000
C	5.18300000	13.04900000	7.77100000
C	8.88500000	13.34600000	8.19300000
C	10.71800000	7.86000000	8.02000000
C	6.74800000	2.68300000	10.58900000
C	9.96400000	4.32200000	9.25900000
C	7.58600000	13.84100000	7.92500000
C	5.21000000	6.35600000	8.70700000
C	12.39300000	8.30400000	6.13900000
C	12.25400000	7.03800000	5.55500000
C	6.25900000	12.62900000	4.62300000
C	13.46400000	15.78800000	11.54200000
C	4.04200000	16.87200000	10.97300000
C	12.18700000	13.73800000	8.01700000
C	6.61500000	16.60300000	12.00000000
C	4.71800000	9.14400000	5.13000000
C	4.21500000	5.80100000	9.51300000
C	7.09000000	19.61300000	9.25500000
C	13.17400000	8.38600000	8.52400000
C	4.33900000	7.70900000	10.97800000
C	13.30600000	9.19200000	9.66300000
C	9.06300000	3.87000000	11.57700000
C	13.01400000	9.31600000	5.39100000
C	5.07100000	12.46000000	9.04300000
C	5.51000000	16.33500000	12.81000000
C	14.17100000	7.43300000	8.26900000
C	4.21700000	16.46400000	12.29700000
C	11.98100000	8.60700000	7.58300000
C	11.26400000	14.09800000	11.70200000
C	14.40500000	9.06200000	10.51500000
C	6.93400000	2.78800000	11.96900000

C	7.02700000	20.71500000	8.40300000
C	12.87900000	15.54200000	12.78400000
C	9.42200000	8.43100000	7.96300000
C	3.77400000	6.47600000	10.65300000
C	6.55200000	14.92200000	5.28400000
C	11.06400000	2.26900000	8.27800000
C	13.21900000	12.79700000	7.89300000
C	4.02700000	13.55900000	7.16800000
C	11.77200000	14.69000000	12.85800000
C	6.71300000	7.30400000	5.76300000
C	8.09900000	3.38100000	12.46100000
C	7.43900000	20.60000000	7.07100000
C	7.98000000	18.27100000	7.46700000
C	12.13400000	14.79300000	7.09500000
C	2.78800000	13.48300000	7.81500000
C	9.65500000	3.56700000	6.81800000
C	15.26400000	7.28900000	9.12700000
C	12.73700000	6.78500000	4.26800000
C	5.09400000	8.18100000	4.18900000
C	13.48900000	9.07000000	4.10300000
C	14.17600000	12.90600000	6.88300000
C	6.11300000	13.02500000	3.29200000
C	3.83700000	12.38200000	9.68600000
C	13.35900000	7.79900000	3.53700000
C	9.89000000	2.65600000	5.78400000
C	2.68700000	12.89300000	9.07500000
C	15.39100000	8.10700000	10.25100000
C	14.11600000	13.96500000	5.97300000
C	6.40500000	15.32400000	3.95200000
C	13.09100000	14.90600000	6.08200000
C	7.91500000	19.37400000	6.60900000

C	6.18200000	14.37700000	2.95100000
C	6.09600000	7.26500000	4.50900000
C	10.71500000	1.54900000	5.99500000
C	11.30500000	1.36100000	7.24700000
C	9.61700000	9.91400000	4.90500000
C	9.75500000	11.15100000	4.20300000
C	9.68000000	12.28400000	5.07200000
C	9.92200000	11.24100000	2.81400000
C	10.05700000	12.55300000	2.27400000
C	10.00900000	13.65600000	3.11100000
C	9.81500000	13.54300000	4.51600000
C	9.92300000	10.01200000	2.09100000
C	9.76500000	8.81100000	2.76400000
C	9.61400000	8.74100000	4.17500000
C	10.23800000	9.60000000	12.70700000
C	10.44200000	8.25100000	13.02800000
C	9.38400000	7.41800000	13.39200000
C	8.08500000	7.92300000	13.42600000
C	7.80600000	9.26100000	13.11900000
C	8.89800000	10.08300000	12.72800000
C	6.40600000	9.78000000	13.29300000
C	11.42200000	10.50300000	12.49200000
H	7.59100000	5.76900000	9.02800000
H	8.50600000	17.49200000	10.48000000
H	6.93000000	9.29500000	8.48900000
H	11.83700000	6.10900000	8.55700000
H	11.14300000	12.57800000	9.46700000
H	10.12200000	15.99700000	9.92800000
H	5.79500000	9.22000000	10.42700000
H	7.57300000	3.05300000	8.63100000
H	4.99600000	17.48200000	9.13900000

H	5.01700000	9.92000000	7.12000000
H	6.18900000	15.41800000	8.32100000
H	6.88700000	12.02800000	7.03700000
H	13.43300000	15.39200000	9.42500000
H	5.84100000	2.22100000	10.19400000
H	10.89600000	4.33800000	9.85000000
H	5.51000000	5.83600000	7.79500000
H	11.75900000	6.23400000	6.10500000
H	6.20800000	11.56700000	4.87600000
H	14.33000000	16.45000000	11.46800000
H	3.03500000	16.97700000	10.56200000
H	7.62400000	16.49000000	12.40500000
H	3.93600000	9.86900000	4.89400000
H	3.77200000	4.84100000	9.23900000
H	6.76200000	19.71600000	10.29200000
H	3.98500000	8.25400000	11.85600000
H	12.53300000	9.93300000	9.88100000
H	9.97200000	4.33600000	11.96700000
H	13.12000000	10.31400000	5.82300000
H	5.96800000	12.06500000	9.53100000
H	5.66100000	16.02300000	13.84600000
H	14.11100000	6.81200000	7.37300000
H	3.35100000	16.24900000	12.92600000
H	11.75900000	9.68400000	7.62700000
H	10.39700000	13.44000000	11.76800000
H	14.50000000	9.71800000	11.38300000
H	6.17900000	2.40500000	12.65700000
H	6.66200000	21.67200000	8.78300000
H	13.28100000	16.00600000	13.68700000
H	2.98700000	6.04900000	11.27800000
H	6.72900000	15.68100000	6.04800000

H	11.52400000	2.11200000	9.25700000
H	13.28600000	11.97600000	8.61200000
H	4.08800000	14.01600000	6.17900000
H	11.30200000	14.48200000	13.82200000
H	7.49300000	6.57800000	6.00700000
H	8.26100000	3.46000000	13.53800000
H	7.39500000	21.46400000	6.40500000
H	8.36700000	17.32100000	7.09300000
H	11.34400000	15.54200000	7.18000000
H	1.90000000	13.88600000	7.32500000
H	9.01900000	4.43700000	6.63900000
H	16.03100000	6.54400000	8.90200000
H	12.62200000	5.78800000	3.83600000
H	4.60600000	8.14600000	3.21200000
H	13.95900000	9.87700000	3.53700000
H	14.97600000	12.16500000	6.81300000
H	5.95300000	12.27000000	2.52000000
H	3.77000000	11.91900000	10.67300000
H	13.73100000	7.60300000	2.52900000
H	9.42800000	2.81500000	4.80700000
H	1.72000000	12.82900000	9.57700000
H	16.25600000	8.01000000	10.90900000
H	14.86500000	14.05500000	5.18400000
H	6.46500000	16.38500000	3.70000000
H	13.03500000	15.73700000	5.37600000
H	8.24600000	19.27100000	5.57300000
H	6.07100000	14.69000000	1.91000000
H	6.40000000	6.51000000	3.77900000
H	10.90100000	0.83800000	5.18700000
H	11.95500000	0.50100000	7.42300000
H	10.04400000	10.02100000	1.00500000

H	9.76500000	7.87800000	2.19700000
H	9.50600000	7.76900000	4.65700000
H	10.19200000	12.68500000	1.19800000
H	10.10900000	14.65400000	2.68100000
H	9.76400000	14.44600000	5.12400000
H	11.46500000	7.86700000	13.02400000
H	7.25800000	7.27700000	13.73200000
H	5.75600000	9.43600000	12.47800000
H	6.36800000	10.87500000	13.31000000
H	5.97300000	9.40000000	14.23000000
H	12.34500000	9.90900000	12.46200000
H	11.51100000	11.24400000	13.30300000
H	11.33800000	11.06800000	11.55300000
H	9.57500000	6.38200000	13.67800000
Cl	8.64300000	11.85700000	12.74400000

IM2-BIAN-IPr$^{\#}$ (IM2-L_B)

Pd	8.93000000	10.54300000	10.58800000
N	9.17600000	12.03900000	7.69000000
N	9.29700000	9.84700000	7.57400000
C	8.47600000	6.38700000	8.74500000
C	9.11000000	10.89200000	8.47600000
C	8.29400000	7.71000000	8.32100000
C	9.73700000	5.79400000	8.81100000
C	11.70500000	14.24700000	10.53400000
C	9.41400000	11.70700000	6.36100000
C	8.08700000	15.91400000	9.09700000
C	9.45200000	10.32700000	6.28400000
C	7.66600000	17.23800000	9.73100000
C	9.76400000	14.13800000	8.88600000
C	6.88200000	8.29200000	8.21000000
C	6.31900000	8.29000000	6.78900000

C	10.84600000	6.55700000	8.43800000
C	11.15900000	13.61600000	9.24300000
C	9.36700000	15.40600000	9.32900000
C	5.85200000	7.64500000	9.13700000
C	5.51400000	8.29000000	10.33100000
C	10.24600000	3.40500000	8.08300000
C	7.68800000	3.25200000	9.69100000
C	5.13200000	17.13800000	10.13600000
C	8.88900000	3.78800000	10.17800000
C	5.31400000	9.22000000	6.47500000
C	7.19900000	15.14000000	8.35100000
C	6.52500000	13.13700000	6.98700000
C	12.81100000	15.10800000	10.54600000
C	6.46800000	13.61600000	5.53300000
C	7.52900000	18.41200000	8.75900000
C	6.44200000	17.01600000	10.62000000
C	5.13200000	13.12700000	7.63900000
C	8.83600000	13.37700000	8.14100000
C	10.73700000	7.88000000	8.00000000
C	6.72700000	2.74300000	10.56600000
C	9.96700000	4.35000000	9.25400000
C	7.55200000	13.88800000	7.83500000
C	5.18600000	6.45200000	8.81600000
C	12.40200000	8.30800000	6.09400000
C	12.25200000	7.04300000	5.51200000
C	6.23300000	12.67300000	4.52000000
C	13.27200000	15.66600000	11.74400000
C	4.04000000	16.85200000	10.95800000
C	12.15800000	13.72700000	8.09600000
C	6.63100000	16.60800000	11.94800000
C	4.66900000	9.18500000	5.24000000

C	4.22700000	5.91300000	9.67700000
C	7.01700000	19.63400000	9.22800000
C	13.20700000	8.38000000	8.46800000
C	4.54000000	7.76800000	11.18500000
C	13.36400000	9.19400000	9.59600000
C	9.10600000	3.79000000	11.56200000
C	13.02600000	9.31700000	5.34400000
C	4.97800000	12.51900000	8.89600000
C	5.54100000	16.32900000	12.77400000
C	14.19200000	7.41300000	8.21100000
C	4.24100000	16.44800000	12.28000000
C	12.00300000	8.61200000	7.54100000
C	11.07000000	13.95800000	11.75300000
C	14.47000000	9.06400000	10.43900000
C	6.95700000	2.74600000	11.94400000
C	6.95200000	20.75400000	8.40100000
C	12.63600000	15.36800000	12.95000000
C	9.44200000	8.46100000	7.96900000
C	3.89900000	6.57100000	10.86300000
C	6.57200000	14.96500000	5.16700000
C	11.09200000	2.30500000	8.28700000
C	13.20600000	12.79800000	8.01600000
C	3.99800000	13.66600000	7.01500000
C	11.53200000	14.51000000	12.94800000
C	6.67100000	7.33500000	5.82900000
C	8.15300000	3.26900000	12.44000000
C	7.39800000	20.67800000	7.07800000
C	7.97600000	18.35000000	7.43300000
C	12.12800000	14.77600000	7.16800000
C	2.74200000	13.59300000	7.62700000
C	9.65500000	3.56800000	6.82200000

C	15.29500000	7.27000000	9.05700000
C	12.73800000	6.78400000	4.22700000
C	5.02100000	8.21900000	4.29100000
C	13.50500000	9.06400000	4.05800000
C	14.20200000	12.91600000	7.04700000
C	6.10000000	13.06400000	3.18600000
C	3.72500000	12.44000000	9.50200000
C	13.37000000	7.79100000	3.49600000
C	9.88800000	2.64300000	5.80000000
C	2.59800000	12.97400000	8.86800000
C	15.44300000	8.09900000	10.17200000
C	14.16700000	13.97200000	6.13100000
C	6.43600000	15.36000000	3.83200000
C	13.12500000	14.89900000	6.19500000
C	7.91000000	19.47200000	6.59900000
C	6.19700000	14.41200000	2.83600000
C	6.02500000	7.29800000	4.59000000
C	10.72400000	1.54700000	6.01900000
C	11.33000000	1.38300000	7.26800000
C	9.60300000	9.90600000	4.89500000
C	9.73300000	11.13700000	4.18300000
C	9.64100000	12.28200000	5.03500000
C	9.91800000	11.21000000	2.79600000
C	10.06400000	12.51300000	2.24100000
C	10.00800000	13.62700000	3.06300000
C	9.79000000	13.53300000	4.46500000
C	9.93500000	9.97400000	2.08700000
C	9.77600000	8.78000000	2.77000000
C	9.61200000	8.72400000	4.18000000
C	10.37900000	9.30200000	12.58900000
C	10.61600000	8.07100000	13.22800000

C	9.55800000	7.33600000	13.76000000
C	8.27000000	7.87700000	13.74700000
C	7.98700000	9.09500000	13.10800000
C	9.03600000	9.68600000	12.37200000
C	6.64600000	9.74500000	13.30700000
C	11.53500000	10.23900000	12.32500000
H	7.60200000	5.82100000	9.06400000
H	8.48700000	17.51500000	10.41700000
H	6.94700000	9.34500000	8.52700000
H	11.84300000	6.11300000	8.50800000
H	11.04300000	12.54000000	9.46200000
H	10.06800000	15.99500000	9.92600000
H	6.02100000	9.22800000	10.57300000
H	7.50600000	3.21700000	8.61400000
H	4.96300000	17.47000000	9.10800000
H	5.01700000	9.96300000	7.22100000
H	6.17700000	15.49000000	8.19700000
H	6.83200000	12.07900000	6.94300000
H	13.32500000	15.34600000	9.61300000
H	5.79200000	2.33800000	10.17100000
H	10.89500000	4.37200000	9.85200000
H	5.40300000	5.94800000	7.87100000
H	11.74900000	6.24500000	6.06000000
H	6.15400000	11.61500000	4.78000000
H	14.13400000	16.33700000	11.72800000
H	3.02600000	16.94500000	10.56300000
H	7.64700000	16.49400000	12.33500000
H	3.88600000	9.91400000	5.02200000
H	3.72100000	4.98300000	9.40900000
H	6.66400000	19.70400000	10.25900000
H	4.28700000	8.29400000	12.10800000

H	12.60200000	9.94500000	9.81200000
H	10.03800000	4.20200000	11.95700000
H	13.13900000	10.31600000	5.77200000
H	5.85400000	12.12800000	9.42100000
H	5.71000000	16.01300000	13.80500000
H	14.11300000	6.78400000	7.32400000
H	3.38600000	16.22500000	12.92200000
H	11.79300000	9.69200000	7.58500000
H	10.18800000	13.31200000	11.76200000
H	14.58300000	9.72500000	11.30200000
H	6.21000000	2.34000000	12.62700000
H	6.55600000	21.69300000	8.79400000
H	12.99700000	15.80400000	13.88400000
H	3.14100000	6.15900000	11.53100000
H	6.76100000	15.72500000	5.92700000
H	11.56200000	2.16600000	9.26500000
H	13.25700000	11.98100000	8.74100000
H	4.09200000	14.14300000	6.03900000
H	11.02300000	14.26600000	13.88200000
H	7.45200000	6.60600000	6.05500000
H	8.34800000	3.26900000	13.51400000
H	7.35300000	21.55500000	6.43000000
H	8.39100000	17.41700000	7.04700000
H	11.32400000	15.51300000	7.21500000
H	1.87200000	14.02400000	7.12400000
H	9.00700000	4.42700000	6.63700000
H	16.05300000	6.51600000	8.83400000
H	12.62000000	5.78700000	3.79700000
H	4.51200000	8.18700000	3.32600000
H	13.98100000	9.86600000	3.49000000
H	15.01300000	12.18400000	7.01400000

H	5.92400000	12.30700000	2.41800000
H	3.63000000	11.96400000	10.48000000
H	13.75200000	7.58800000	2.49300000
H	9.41300000	2.78200000	4.82600000
H	1.61700000	12.91100000	9.34200000
H	16.31300000	8.00400000	10.82500000
H	14.94900000	14.07200000	5.37600000
H	6.51800000	16.41800000	3.57300000
H	13.09000000	15.72900000	5.48500000
H	8.26500000	19.39900000	5.56800000
H	6.09300000	14.72000000	1.79300000
H	6.30700000	6.54200000	3.85500000
H	10.90600000	0.82300000	5.22200000
H	11.99000000	0.53200000	7.45000000
H	10.07000000	9.97000000	1.00400000
H	9.78600000	7.83900000	2.21500000
H	9.50700000	7.75700000	4.67000000
H	10.21600000	12.62800000	1.16600000
H	10.11900000	14.61800000	2.62100000
H	9.73500000	14.44400000	5.06000000
H	11.64800000	7.71700000	13.33900000
H	7.45300000	7.35400000	14.25000000
H	6.08300000	9.87800000	12.37500000
H	6.77700000	10.75600000	13.71900000
H	6.03800000	9.15100000	14.00500000
H	12.46700000	9.68900000	12.15000000
H	11.69300000	10.87400000	13.21100000
H	11.34900000	10.92800000	11.49000000
H	9.74100000	6.37300000	14.24300000
Cl	7.75900000	12.34800000	11.38700000

IM3-BIAN-IPr$^{\#}$ (IM3-L_B)

Pd	8.73400000	10.20100000	10.35100000
N	9.08000000	11.98400000	7.60400000
N	9.24100000	9.80800000	7.36700000
N	9.97000000	11.36000000	11.79000000
C	8.41900000	6.35500000	8.56100000
C	8.99900000	10.79500000	8.31400000
C	8.23600000	7.66100000	8.08400000
C	9.68600000	5.79300000	8.71600000
C	11.83900000	14.22300000	10.17200000
C	9.37200000	11.73300000	6.27100000
C	7.99200000	15.82200000	9.10200000
C	9.44600000	10.36100000	6.11100000
C	7.61200000	17.17900000	9.68400000
C	9.70200000	14.09900000	8.75200000
C	6.81600000	8.18800000	7.84300000
C	6.39800000	8.13700000	6.37300000
C	10.79900000	6.56400000	8.36800000
C	11.15800000	13.65000000	8.91600000
C	9.30500000	15.35900000	9.21700000
C	5.75100000	7.49900000	8.70100000
C	5.40500000	8.04500000	9.94300000
C	10.25700000	3.40600000	8.07400000
C	7.82300000	2.92200000	9.65800000
C	5.06500000	17.36400000	9.94400000
C	8.77100000	3.85300000	10.10000000
C	5.35300000	8.97200000	5.94800000
C	7.06300000	15.00800000	8.45200000
C	6.37500000	12.99100000	7.10000000
C	13.13700000	14.75100000	10.13800000
C	6.34000000	13.44400000	5.63500000
C	7.60300000	18.31800000	8.66100000

C	6.32300000	17.09300000	10.50000000
C	4.98600000	13.00800000	7.75600000
C	8.73400000	13.29900000	8.10900000
C	10.69100000	7.86600000	7.87000000
C	6.79800000	2.48900000	10.50500000
C	9.90500000	4.36400000	9.21100000
C	7.41300000	13.76500000	7.91400000
C	5.08400000	6.34300000	8.27100000
C	12.38900000	8.20800000	5.98700000
C	12.21000000	6.92500000	5.45400000
C	6.21600000	12.47900000	4.62600000
C	13.74200000	15.25100000	11.29700000
C	3.90300000	17.22300000	10.70500000
C	11.96900000	13.93600000	7.65200000
C	6.38700000	16.69100000	11.84300000
C	4.86300000	8.89800000	4.64500000
C	4.10500000	5.74400000	9.06700000
C	7.33700000	19.62300000	9.10800000
C	13.15500000	8.46500000	8.35000000
C	4.41800000	7.45700000	10.73500000
C	13.44600000	9.49000000	9.26000000
C	8.66700000	4.34400000	11.41100000
C	13.07500000	9.15900000	5.21500000
C	4.79100000	12.30700000	8.95800000
C	5.22800000	16.55800000	12.60800000
C	14.02500000	7.36400000	8.29800000
C	3.97900000	16.82100000	12.04000000
C	11.95200000	8.60100000	7.40600000
C	11.16800000	14.19500000	11.40700000
C	14.55300000	9.41400000	10.10900000
C	6.71000000	2.97700000	11.81000000

C	7.35000000	20.70300000	8.22700000
C	13.05700000	15.24200000	12.51100000
C	9.38900000	8.42500000	7.76900000
C	3.76500000	6.30100000	10.30200000
C	6.39100000	14.79300000	5.25300000
C	11.11100000	2.32200000	8.32900000
C	12.83100000	12.96400000	7.12900000
C	3.89600000	13.69000000	7.19900000
C	11.76500000	14.70900000	12.56000000
C	6.93900000	7.22700000	5.45800000
C	7.64900000	3.91000000	12.25900000
C	7.63000000	20.50200000	6.87100000
C	7.89100000	18.13100000	7.30400000
C	11.93200000	15.19300000	7.03000000
C	2.64600000	13.67700000	7.82500000
C	9.73500000	3.54800000	6.78100000
C	15.12400000	7.27600000	9.15400000
C	12.71800000	6.59700000	4.19200000
C	5.40800000	7.98200000	3.73900000
C	13.57600000	8.83800000	3.95400000
C	13.63300000	13.23300000	6.01600000
C	6.13700000	12.84400000	3.28000000
C	3.54000000	12.27900000	9.57400000
C	13.40400000	7.55000000	3.43800000
C	10.05200000	2.63100000	5.77400000
C	2.46000000	12.96600000	9.01000000
C	15.39300000	8.30000000	10.06400000
C	13.58500000	14.48700000	5.40600000
C	6.31000000	15.16400000	3.90700000
C	12.73200000	15.46700000	5.92000000
C	7.90000000	19.21200000	6.41500000

C	6.18000000	14.19100000	2.91500000
C	6.44700000	7.14800000	4.15200000
C	10.90100000	1.55600000	6.04200000
C	11.43100000	1.40500000	7.32600000
C	9.68000000	10.04100000	4.70500000
C	9.80600000	11.32100000	4.08300000
C	9.63300000	12.40000000	5.00300000
C	10.06300000	11.50100000	2.71700000
C	10.18800000	12.84700000	2.26500000
C	10.04200000	13.89600000	3.15700000
C	9.75300000	13.69400000	4.53300000
C	10.16500000	10.31800000	1.92800000
C	10.01100000	9.07300000	2.51900000
C	9.77100000	8.91300000	3.91100000
C	9.90300000	8.61100000	12.37500000
C	9.97500000	7.65300000	13.39400000
C	8.86600000	7.38200000	14.19400000
C	7.68600000	8.09000000	13.99000000
C	7.57400000	9.06800000	12.98300000
C	8.67700000	9.27200000	12.12900000
C	6.28900000	9.85500000	12.91500000
C	11.16000000	8.95400000	11.61400000
C	10.82400000	11.70900000	14.03900000
C	10.59600000	11.90600000	15.39900000
C	9.29400000	12.00200000	15.90000000
C	8.22000000	11.89600000	15.01000000
C	8.43600000	11.69900000	13.64800000
C	9.74500000	11.60200000	13.13600000
H	7.53800000	5.77300000	8.83300000
H	8.41100000	17.43000000	10.40400000
H	6.81000000	9.25000000	8.14100000

H	11.79500000	6.13600000	8.49900000
H	11.13800000	12.55300000	9.04400000
H	10.04200000	15.98200000	9.72800000
H	5.92000000	8.94500000	10.28900000
H	7.89100000	2.52200000	8.64400000
H	4.99300000	17.70000000	8.90700000
H	4.90600000	9.67500000	6.65600000
H	6.02200000	15.33200000	8.37600000
H	6.68600000	11.93400000	7.08400000
H	13.69000000	14.78000000	9.19800000
H	6.06700000	1.76300000	10.14300000
H	10.80000000	4.40700000	9.85700000
H	5.31900000	5.91100000	7.29600000
H	11.66800000	6.16500000	6.02100000
H	6.18900000	11.42100000	4.89600000
H	14.75400000	15.65800000	11.24100000
H	2.93100000	17.43200000	10.25300000
H	7.36000000	16.47300000	12.29200000
H	4.04900000	9.55800000	4.33500000
H	3.59800000	4.84200000	8.71500000
H	7.11000000	19.79100000	10.16400000
H	4.15500000	7.90700000	11.69400000
H	12.79200000	10.36500000	9.31300000
H	9.38600000	5.08400000	11.77200000
H	13.21300000	10.16800000	5.60900000
H	5.63700000	11.79600000	9.42800000
H	5.30300000	16.24700000	13.65300000
H	13.86200000	6.57800000	7.55800000
H	3.07100000	16.71300000	12.63600000
H	11.71500000	9.67500000	7.37200000
H	10.16300000	13.77100000	11.46200000

H	14.75700000	10.23100000	10.80400000
H	5.91500000	2.63200000	12.47400000
H	7.14600000	21.70800000	8.60200000
H	13.52100000	15.64600000	13.41300000
H	2.99200000	5.84100000	10.92100000
H	6.49600000	15.57100000	6.01200000
H	11.52600000	2.19300000	9.33200000
H	12.88900000	11.98400000	7.61000000
H	4.02100000	14.23400000	6.26200000
H	11.21300000	14.69500000	13.50200000
H	7.75000000	6.56500000	5.77100000
H	7.59000000	4.30600000	13.27500000
H	7.64400000	21.34800000	6.18100000
H	8.11800000	17.12900000	6.93300000
H	11.27200000	15.97000000	7.42300000
H	1.81400000	14.22400000	7.37600000
H	9.07200000	4.38700000	6.55600000
H	15.78600000	6.40900000	9.09300000
H	12.57300000	5.58800000	3.80100000
H	5.02500000	7.92300000	2.71900000
H	14.09800000	9.59700000	3.37000000
H	14.30000000	12.46000000	5.62800000
H	6.05100000	12.06900000	2.51600000
H	3.40700000	11.72200000	10.50300000
H	13.79700000	7.29500000	2.45200000
H	9.63400000	2.76100000	4.77300000
H	1.48000000	12.94600000	9.49300000
H	16.26100000	8.23800000	10.72200000
H	14.20900000	14.70000000	4.53600000
H	6.35100000	16.22100000	3.63700000
H	12.68900000	16.45400000	5.45300000

H	8.12500000	19.04000000	5.35900000
H	6.12300000	14.48000000	1.86300000
H	6.88200000	6.43000000	3.45300000
H	11.15400000	0.84300000	5.25600000
H	12.09800000	0.57000000	7.54900000
H	10.36100000	10.39400000	0.85500000
H	10.09000000	8.17700000	1.90100000
H	9.67400000	7.91000000	4.32500000
H	10.39900000	13.04700000	1.21200000
H	10.14300000	14.92100000	2.79500000
H	9.63100000	14.55400000	5.19200000
H	10.92500000	7.13700000	13.56600000
H	6.82200000	7.90000000	14.63300000
H	6.13700000	10.33400000	11.94100000
H	6.29600000	10.66800000	13.65900000
H	5.42700000	9.21100000	13.15000000
H	11.90900000	8.15300000	11.70200000
H	11.60300000	9.87800000	12.01900000
H	10.98800000	9.11800000	10.53800000
H	8.93400000	6.64000000	14.99200000
H	7.59000000	11.61100000	12.96200000
H	11.84600000	11.62400000	13.66000000
H	11.44900000	11.98300000	16.07700000
H	7.19500000	11.96700000	15.38100000
H	9.11900000	12.15700000	16.96500000
H	10.87800000	11.65500000	11.43600000
H	9.21100000	11.59700000	11.14600000
Cl	7.56500000	12.06900000	11.37200000

IM4-BIAN-IPr$^{\#}$ (IM4-L_B)

Pd	9.18000000	10.26800000	10.72900000
N	9.19400000	12.04600000	7.85700000

N	9.33800000	9.86000000	7.67500000
N	10.13500000	11.56100000	12.00200000
C	8.49100000	6.36900000	8.75300000
C	9.16400000	10.87100000	8.61700000
C	8.31600000	7.69400000	8.32700000
C	9.75200000	5.78600000	8.86700000
C	11.80900000	14.51700000	10.47600000
C	9.41100000	11.75300000	6.51400000
C	8.01700000	15.93200000	9.19900000
C	9.46300000	10.37700000	6.39600000
C	7.59200000	17.29200000	9.75100000
C	9.73300000	14.19000000	9.01500000
C	6.90200000	8.24600000	8.10900000
C	6.45600000	8.20200000	6.64300000
C	10.86900000	6.55700000	8.53300000
C	11.17600000	13.76300000	9.29400000
C	9.31200000	15.46400000	9.41700000
C	5.79900000	7.59700000	8.95500000
C	5.27600000	8.28100000	10.05900000
C	10.26000000	3.41000000	8.10800000
C	7.76800000	3.04900000	9.67300000
C	5.04600000	17.27500000	10.05900000
C	8.84900000	3.78400000	10.18200000
C	5.45500000	9.09300000	6.22400000
C	7.13500000	15.10500000	8.50100000
C	6.51000000	13.08800000	7.14500000
C	13.01200000	15.22400000	10.36000000
C	6.47000000	13.57000000	5.68800000
C	7.49900000	18.41600000	8.71500000
C	6.33300000	17.13200000	10.59900000
C	5.10900000	13.09700000	7.77100000

C	8.81600000	13.36800000	8.31900000
C	10.77000000	7.87900000	8.09000000
C	6.76700000	2.57400000	10.52400000
C	9.96300000	4.33300000	9.29000000
C	7.51600000	13.84700000	8.01200000
C	5.22800000	6.36000000	8.61400000
C	12.37500000	8.28000000	6.14000000
C	12.20000000	7.00900000	5.57600000
C	6.24200000	12.62600000	4.67600000
C	13.56000000	15.89100000	11.46200000
C	3.91100000	17.04700000	10.84500000
C	12.03600000	13.86100000	8.03800000
C	6.45300000	16.77500000	11.95500000
C	4.91700000	9.02000000	4.93800000
C	4.18800000	5.81500000	9.36900000
C	7.12200000	19.69900000	9.14800000
C	13.29600000	8.38300000	8.44800000
C	4.22300000	7.74900000	10.80800000
C	13.70900000	9.36600000	9.35800000
C	8.90200000	4.02800000	11.56200000
C	12.98000000	9.27500000	5.35700000
C	4.85600000	12.29200000	8.89500000
C	5.32200000	16.54600000	12.74400000
C	14.11700000	7.25300000	8.29100000
C	4.04300000	16.67400000	12.18700000
C	12.03200000	8.60500000	7.60200000
C	11.17600000	14.48500000	11.73100000
C	14.89100000	9.23400000	10.08800000
C	6.83500000	2.81600000	11.89700000
C	7.09500000	20.77800000	8.26600000
C	12.93000000	15.83800000	12.70500000

C	9.47400000	8.46100000	8.04000000
C	3.67800000	6.51100000	10.46900000
C	6.57800000	14.91900000	5.32100000
C	11.07700000	2.28500000	8.30500000
C	13.01100000	12.88700000	7.78500000
C	4.06000000	13.86900000	7.25400000
C	11.73800000	15.12100000	12.83800000
C	6.91100000	7.24100000	5.73100000
C	7.90700000	3.54700000	12.41300000
C	7.44000000	20.59800000	6.92300000
C	7.84600000	18.24900000	7.36800000
C	11.94700000	14.95200000	7.16100000
C	2.78500000	13.81700000	7.82500000
C	9.71100000	3.61300000	6.83400000
C	15.28800000	7.10400000	9.03600000
C	12.64300000	6.73500000	4.27800000
C	5.37400000	8.05000000	4.04100000
C	13.41600000	9.00600000	4.06100000
C	13.86700000	12.98800000	6.68700000
C	6.13100000	13.01500000	3.34000000
C	3.58500000	12.24500000	9.47700000
C	13.25800000	7.72900000	3.51600000
C	9.96000000	2.71500000	5.79200000
C	2.54100000	13.00400000	8.93400000
C	15.68600000	8.09700000	9.93400000
C	13.76000000	14.07400000	5.81500000
C	6.46400000	15.31200000	3.98500000
C	12.79800000	15.05500000	6.05700000
C	7.81400000	19.33000000	6.47900000
C	6.24300000	14.36100000	2.98700000
C	6.37400000	7.16500000	4.44200000

C	10.77200000	1.59900000	6.00400000
C	11.33200000	1.38800000	7.26700000
C	9.61600000	10.00200000	4.99400000
C	9.73100000	11.25500000	4.31900000
C	9.62700000	12.37000000	5.20800000
C	9.91500000	11.37800000	2.93400000
C	10.04000000	12.70200000	2.42400000
C	9.96600000	13.78700000	3.28300000
C	9.75100000	13.64200000	4.68000000
C	9.94600000	10.16600000	2.18600000
C	9.80500000	8.94900000	2.83200000
C	9.64300000	8.84500000	4.23800000
C	10.41400000	8.26200000	12.55000000
C	10.36400000	7.20900000	13.47600000
C	9.18700000	6.90300000	14.15800000
C	8.04900000	7.67300000	13.93400000
C	8.06100000	8.74700000	13.02500000
C	9.23700000	9.00100000	12.28800000
C	6.82700000	9.59500000	12.89800000
C	11.72300000	8.58400000	11.88100000
C	10.91100000	11.73000000	14.31400000
C	10.70400000	12.12600000	15.63200000
C	9.45000000	12.59000000	16.04700000
C	8.41100000	12.65300000	15.10900000
C	8.61500000	12.27800000	13.78300000
C	9.87500000	11.80400000	13.34900000
H	7.60800000	5.78600000	9.02100000
H	8.39500000	17.59100000	10.44800000
H	6.92600000	9.30800000	8.40200000
H	11.86300000	6.11200000	8.62800000
H	11.13300000	12.69900000	9.59300000

H	10.01900000	16.09900000	9.95400000
H	5.69600000	9.24700000	10.34400000
H	7.71500000	2.83600000	8.60300000
H	4.93400000	17.59000000	9.01900000
H	5.07100000	9.83500000	6.92900000
H	6.11200000	15.44200000	8.31600000
H	6.81900000	12.03200000	7.11400000
H	13.53500000	15.25800000	9.40300000
H	5.92700000	2.01000000	10.11000000
H	10.87500000	4.33200000	9.91300000
H	5.58100000	5.82200000	7.73100000
H	11.70500000	6.22000000	6.14600000
H	6.15800000	11.56900000	4.93600000
H	14.48800000	16.45400000	11.34000000
H	2.91800000	17.17300000	10.40800000
H	7.44900000	16.67300000	12.39600000
H	4.13300000	9.71900000	4.64000000
H	3.76700000	4.84800000	9.08800000
H	6.85200000	19.85600000	10.19500000
H	3.82700000	8.31200000	11.65600000
H	13.08500000	10.25000000	9.50600000
H	9.72500000	4.61600000	11.97500000
H	13.10300000	10.28000000	5.76900000
H	5.66200000	11.68000000	9.31300000
H	5.43500000	16.25500000	13.78900000
H	13.86000000	6.49300000	7.55100000
H	3.16000000	16.48100000	12.79600000
H	11.82800000	9.68600000	7.64300000
H	10.24900000	13.92300000	11.84400000
H	15.19200000	10.02400000	10.77900000
H	6.05600000	2.43800000	12.56300000

H	6.81600000	21.76800000	8.63200000
H	13.36800000	16.34800000	13.56600000
H	2.85400000	6.09100000	11.05100000
H	6.75500000	15.68100000	6.08100000
H	11.51200000	2.10700000	9.29200000
H	13.11100000	12.04300000	8.47000000
H	4.23500000	14.50400000	6.38500000
H	11.24300000	15.04100000	13.80800000
H	7.69000000	6.53800000	6.03300000
H	7.97000000	3.75200000	13.48400000
H	7.43000000	21.44500000	6.23400000
H	8.16200000	17.26900000	7.00600000
H	11.20600000	15.73400000	7.34700000
H	1.97500000	14.40300000	7.38500000
H	9.07900000	4.48500000	6.65400000
H	15.90500000	6.21400000	8.89500000
H	12.49900000	5.73500000	3.86100000
H	4.94800000	7.98500000	3.03700000
H	13.87500000	9.80200000	3.46900000
H	14.62400000	12.21900000	6.51900000
H	5.96300000	12.25800000	2.57100000
H	3.42300000	11.62900000	10.36400000
H	13.60200000	7.51600000	2.50300000
H	9.51800000	2.89000000	4.80800000
H	1.54300000	12.95200000	9.37200000
H	16.61200000	7.98800000	10.50100000
H	14.41900000	14.15100000	4.94900000
H	6.54900000	16.37000000	3.72600000
H	12.70700000	15.91000000	5.38400000
H	8.09300000	19.17800000	5.43400000
H	6.16700000	14.66600000	1.94200000

H	6.74100000	6.40600000	3.74600000
H	10.97100000	0.89900000	5.18900000
H	11.97000000	0.52100000	7.44400000
H	10.07900000	10.20100000	1.10200000
H	9.82700000	8.02800000	2.24500000
H	9.55500000	7.86200000	4.69500000
H	10.18900000	12.85900000	1.35200000
H	10.05900000	14.79500000	2.87600000
H	9.68100000	14.53100000	5.30600000
H	11.27400000	6.63000000	13.66600000
H	7.12400000	7.46100000	14.47900000
H	6.87600000	10.25700000	12.02200000
H	6.69600000	10.24800000	13.77300000
H	5.92300000	8.97500000	12.82200000
H	12.37600000	7.70400000	11.81000000
H	12.28100000	9.35400000	12.44300000
H	11.56100000	8.97800000	10.87000000
H	9.16700000	6.07500000	14.87100000
H	7.78000000	12.33900000	13.08400000
H	11.89400000	11.36100000	14.01300000
H	11.53000000	12.05200000	16.34400000
H	7.41500000	12.99600000	15.40300000
H	9.28300000	12.88000000	17.08700000
H	11.11300000	11.25100000	11.93500000
Cl	7.76600000	12.07500000	10.69300000
Na	7.77500000	14.10600000	9.90100000

IM5-BIAN-IPr$^{\#}$ (IM5-L_B)

Pd	9.05500000	10.18800000	10.65800000
N	9.21800000	12.02900000	7.85900000
N	9.31100000	9.84600000	7.63600000
N	9.74000000	11.69500000	11.86600000

C	8.45300000	6.38200000	8.77400000
C	9.13600000	10.84700000	8.59100000
C	8.27500000	7.69400000	8.31200000
C	9.71600000	5.80400000	8.90500000
C	11.93400000	14.45000000	10.37200000
C	9.45100000	11.75700000	6.51700000
C	8.09100000	15.90900000	9.22300000
C	9.48200000	10.38300000	6.36900000
C	7.66900000	17.25900000	9.79700000
C	9.81800000	14.18500000	8.95600000
C	6.86300000	8.24000000	8.06100000
C	6.45400000	8.21700000	6.58300000
C	10.83500000	6.56500000	8.55500000
C	11.26600000	13.74100000	9.18000000
C	9.40700000	15.46200000	9.36300000
C	5.73000000	7.56500000	8.84400000
C	5.06200000	8.27600000	9.84700000
C	10.23000000	3.43600000	8.15800000
C	7.77000000	3.01000000	9.73500000
C	5.12300000	17.31800000	10.16000000
C	8.80700000	3.81200000	10.23200000
C	5.46400000	9.11400000	6.15400000
C	7.17600000	15.06400000	8.59500000
C	6.52200000	13.01700000	7.28500000
C	13.19900000	15.04800000	10.28300000
C	6.42000000	13.50400000	5.83400000
C	7.57200000	18.39600000	8.77700000
C	6.41500000	17.09000000	10.65500000
C	5.16000000	12.96400000	7.98900000
C	8.86400000	13.35400000	8.33000000
C	10.73200000	7.87700000	8.08800000

C	6.76800000	2.53200000	10.58400000
C	9.92400000	4.35500000	9.34200000
C	7.54700000	13.81100000	8.09300000
C	5.25500000	6.28300000	8.51900000
C	12.33900000	8.28100000	6.14200000
C	12.14600000	7.01500000	5.57500000
C	6.29800000	12.55800000	4.80600000
C	13.77400000	15.68000000	11.39300000
C	4.00100000	17.06900000	10.95400000
C	12.10900000	13.85900000	7.91400000
C	6.55300000	16.61600000	11.96900000
C	4.95400000	9.05400000	4.85700000
C	4.17800000	5.72000000	9.20400000
C	7.23800000	19.68400000	9.23100000
C	13.25000000	8.37500000	8.45400000
C	3.97400000	7.72200000	10.52800000
C	13.64900000	9.34900000	9.37800000
C	8.81500000	4.12500000	11.60000000
C	12.96400000	9.26900000	5.36500000
C	5.08900000	12.40200000	9.27500000
C	5.43500000	16.37300000	12.76600000
C	14.07600000	7.25000000	8.28900000
C	4.15200000	16.59600000	12.25900000
C	11.99300000	8.60300000	7.60300000
C	11.27000000	14.48800000	11.60900000
C	14.82300000	9.20900000	10.12300000
C	6.79300000	2.84000000	11.94600000
C	7.19800000	20.76800000	8.35700000
C	13.09800000	15.71900000	12.61200000
C	9.43600000	8.45400000	8.01400000
C	3.53200000	6.43700000	10.21500000

C	6.39400000	14.86200000	5.48500000
C	11.05100000	2.31500000	8.35800000
C	13.04800000	12.86600000	7.60700000
C	3.98000000	13.43000000	7.39700000
C	11.84400000	15.11100000	12.71600000
C	6.92400000	7.26000000	5.67600000
C	7.82000000	3.64200000	12.45000000
C	7.48700000	20.58900000	7.00000000
C	7.86000000	18.23000000	7.41700000
C	12.04900000	14.99000000	7.08800000
C	2.75800000	13.33500000	8.07000000
C	9.69100000	3.64500000	6.88200000
C	15.24200000	7.09700000	9.04000000
C	12.58400000	6.73700000	4.27700000
C	5.42700000	8.09100000	3.96100000
C	13.39700000	8.99600000	4.06800000
C	13.90500000	12.99300000	6.51200000
C	6.15400000	12.95100000	3.47400000
C	3.87000000	12.30500000	9.94400000
C	13.21500000	7.72400000	3.51900000
C	9.95700000	2.75600000	5.83600000
C	2.69600000	12.76900000	9.34200000
C	15.62200000	8.07700000	9.96000000
C	13.83300000	14.12400000	5.69600000
C	6.25000000	15.26000000	4.15300000
C	12.90000000	15.12100000	5.98800000
C	7.81500000	19.31600000	6.53400000
C	6.12700000	14.30700000	3.14100000
C	6.41400000	7.19700000	4.37500000
C	10.77200000	1.64300000	6.04900000
C	11.32000000	1.42600000	7.31700000

C	9.63100000	10.04200000	4.95800000
C	9.75200000	11.31100000	4.31200000
C	9.65300000	12.40400000	5.22600000
C	9.92300000	11.46600000	2.92900000
C	10.03200000	12.80400000	2.44900000
C	9.95200000	13.86800000	3.33300000
C	9.75300000	13.69000000	4.73000000
C	9.94800000	10.27100000	2.15300000
C	9.80500000	9.03900000	2.77100000
C	9.64800000	8.90200000	4.17600000
C	10.39000000	8.46400000	12.68400000
C	10.43100000	7.48200000	13.68200000
C	9.27000000	7.08000000	14.33900000
C	8.05700000	7.67600000	14.00400000
C	7.98100000	8.66700000	13.01100000
C	9.15000000	9.03300000	12.30900000
C	6.64200000	9.31700000	12.77100000
C	11.69200000	8.91200000	12.07200000
C	10.13800000	12.17600000	14.23500000
C	9.68400000	12.66300000	15.45900000
C	8.33300000	12.97800000	15.64200000
C	7.45500000	12.83500000	14.56100000
C	7.90900000	12.39000000	13.32400000
C	9.26300000	12.03100000	13.12700000
H	7.57700000	5.80100000	9.05400000
H	8.47600000	17.55500000	10.49100000
H	6.86300000	9.29600000	8.37500000
H	11.82600000	6.12100000	8.66000000
H	11.21900000	12.66800000	9.44100000
H	10.13600000	16.11100000	9.85200000
H	5.39100000	9.28800000	10.09100000

H	7.75200000	2.74500000	8.67600000
H	4.99200000	17.70100000	9.14500000
H	5.06700000	9.85100000	6.85800000
H	6.13200000	15.36800000	8.50900000
H	6.87200000	11.97400000	7.23000000
H	13.74700000	15.02700000	9.34000000
H	5.96600000	1.90900000	10.18000000
H	10.83400000	4.35800000	9.96800000
H	5.71300000	5.72300000	7.70000000
H	11.64300000	6.23100000	6.14700000
H	6.32600000	11.49500000	5.05100000
H	14.75700000	16.14600000	11.29600000
H	3.00300000	17.24500000	10.54800000
H	7.55400000	16.42400000	12.36700000
H	4.18300000	9.76200000	4.54800000
H	3.83200000	4.71900000	8.93700000
H	7.00800000	19.83600000	10.28800000
H	3.46800000	8.30500000	11.30100000
H	13.02600000	10.23400000	9.52200000
H	9.60600000	4.76200000	12.00500000
H	13.10600000	10.27000000	5.78100000
H	6.00600000	12.04900000	9.75600000
H	5.56900000	16.00400000	13.78500000
H	13.82600000	6.49800000	7.53800000
H	3.27500000	16.40300000	12.87900000
H	11.79000000	9.68400000	7.64700000
H	10.29200000	14.01300000	11.69900000
H	15.10900000	9.98800000	10.83200000
H	6.01800000	2.45400000	12.61100000
H	6.95000000	21.76100000	8.73900000
H	13.54100000	16.21800000	13.47600000

H	2.68300000	6.00000000	10.74500000
H	6.49100000	15.62700000	6.25600000
H	11.47800000	2.13400000	9.34800000
H	13.12300000	11.98400000	8.24700000
H	4.01200000	13.86900000	6.39800000
H	11.30400000	15.11400000	13.66500000
H	7.69300000	6.55000000	5.98900000
H	7.85000000	3.89600000	13.51100000
H	7.46500000	21.44000000	6.31600000
H	8.13500000	17.24300000	7.04000000
H	11.33000000	15.78200000	7.31200000
H	1.85000000	13.70400000	7.58700000
H	9.05700000	4.51500000	6.70100000
H	15.86700000	6.21400000	8.89000000
H	12.42800000	5.74000000	3.86000000
H	5.02600000	8.04000000	2.94700000
H	13.87300000	9.78400000	3.48100000
H	14.63800000	12.21000000	6.30400000
H	6.07400000	12.19100000	2.69500000
H	3.83600000	11.86500000	10.94300000
H	13.55500000	7.50800000	2.50500000
H	9.52500000	2.93700000	4.84900000
H	1.74100000	12.68900000	9.86400000
H	16.54200000	7.96200000	10.53700000
H	14.49900000	14.22600000	4.83700000
H	6.23500000	16.32500000	3.90900000
H	12.83400000	16.01000000	5.35600000
H	8.04500000	19.16300000	5.47700000
H	6.01900000	14.61700000	2.10000000
H	6.79300000	6.44300000	3.68100000
H	10.98200000	0.94800000	5.23300000

H	11.96100000	0.55900000	7.49600000
H	10.07600000	10.32900000	1.07000000
H	9.82200000	8.13200000	2.16300000
H	9.55300000	7.90800000	4.61100000
H	10.17100000	12.98600000	1.38100000
H	10.02800000	14.88700000	2.94800000
H	9.67700000	14.56200000	5.38000000
H	11.39500000	7.04200000	13.94800000
H	7.13800000	7.38600000	14.52200000
H	6.66700000	9.95600000	11.87600000
H	6.36800000	9.95200000	13.62900000
H	5.85200000	8.56100000	12.64500000
H	12.41300000	8.08400000	11.98400000
H	12.17500000	9.68900000	12.69400000
H	11.53600000	9.33500000	11.07100000
H	9.31400000	6.32700000	15.12800000
H	7.22200000	12.30700000	12.48100000
H	11.19200000	11.90200000	14.11700000
H	10.38700000	12.78200000	16.28800000
H	6.39700000	13.07700000	14.68600000
H	7.97100000	13.32200000	16.61200000
H	10.73600000	11.46300000	11.96000000

TS5-BIAN-IPr$^{\#}$ (TS5-L_B)

Pd	9.06100000	10.61200000	10.52100000
N	9.20700000	12.07400000	7.74200000
N	9.31500000	9.87900000	7.59700000
N	9.53600000	11.17800000	12.32600000
C	8.46200000	6.42400000	8.76000000
C	9.14600000	10.91600000	8.52300000
C	8.29200000	7.74200000	8.31500000
C	9.72200000	5.83200000	8.86100000

C	11.87000000	14.39500000	10.35300000
C	9.42500000	11.75700000	6.40900000
C	8.08600000	15.93800000	9.15300000
C	9.46400000	10.38000000	6.31300000
C	7.67100000	17.28200000	9.74900000
C	9.80300000	14.20700000	8.87500000
C	6.88400000	8.31700000	8.13800000
C	6.39500000	8.29000000	6.68900000
C	10.83800000	6.59000000	8.49700000
C	11.23300000	13.72800000	9.12700000
C	9.39500000	15.47300000	9.31200000
C	5.81700000	7.66900000	9.02000000
C	5.42900000	8.29100000	10.18100000
C	10.22500000	3.45800000	8.11200000
C	7.73300000	3.12700000	9.69500000
C	5.12300000	17.28600000	10.06000000
C	8.83200000	3.83400000	10.19600000
C	5.38800000	9.19000000	6.30600000
C	7.18000000	15.12000000	8.48000000
C	6.51900000	13.08500000	7.15000000
C	13.05800000	15.12400000	10.29900000
C	6.41200000	13.56700000	5.70000000
C	7.58800000	18.43600000	8.74700000
C	6.40800000	17.13300000	10.59700000
C	5.16100000	13.03100000	7.86100000
C	8.85600000	13.39900000	8.20700000
C	10.73700000	7.90600000	8.03800000
C	6.74200000	2.64100000	10.55200000
C	9.93500000	4.38300000	9.29500000
C	7.54700000	13.87300000	7.96100000
C	5.16100000	6.49100000	8.66900000

C	12.37800000	8.29800000	6.11100000
C	12.21300000	7.02500000	5.54900000
C	6.25000000	12.61800000	4.68100000
C	13.59200000	15.71700000	11.44800000
C	3.98800000	17.08100000	10.84700000
C	12.12200000	13.83100000	7.89400000
C	6.52400000	16.79000000	11.94700000
C	4.82500000	9.13600000	5.03200000
C	4.16500000	5.94200000	9.47000000
C	7.23500000	19.71300000	9.21600000
C	13.22600000	8.41600000	8.45800000
C	4.42100000	7.75400000	10.97700000
C	13.52200000	9.35300000	9.45100000
C	8.91300000	4.03900000	11.57700000
C	12.99600000	9.29100000	5.33600000
C	5.08900000	12.42300000	9.12500000
C	5.39200000	16.59900000	12.73900000
C	14.11000000	7.34100000	8.28600000
C	4.11700000	16.73600000	12.18900000
C	12.00000000	8.63000000	7.56000000
C	11.23600000	14.26800000	11.59200000
C	14.66000000	9.22700000	10.24900000
C	6.83900000	2.84200000	11.92600000
C	7.19500000	20.81000000	8.35800000
C	12.94800000	15.58900000	12.67000000
C	9.44600000	8.49400000	7.98800000
C	3.78800000	6.57400000	10.62800000
C	6.42600000	14.92200000	5.34000000
C	11.03600000	2.33000000	8.31100000
C	13.10800000	12.86200000	7.67700000
C	3.98600000	13.53900000	7.29600000

C	11.76400000	14.85600000	12.73800000
C	6.82300000	7.33700000	5.75700000
C	7.92900000	3.54500000	12.43600000
C	7.50300000	20.65400000	7.00400000
C	7.89900000	18.29400000	7.38900000
C	12.04900000	14.91000000	7.00500000
C	2.76800000	13.44400000	7.97700000
C	9.68400000	3.67000000	6.83700000
C	15.23900000	7.20000000	9.09400000
C	12.67100000	6.74900000	4.25600000
C	5.25700000	8.17700000	4.11200000
C	13.44800000	9.02000000	4.04400000
C	13.99600000	12.96200000	6.60500000
C	6.10400000	13.00500000	3.34700000
C	3.87400000	12.32500000	9.80200000
C	13.29300000	7.74300000	3.50000000
C	9.93700000	2.77600000	5.79200000
C	2.70500000	12.83500000	9.22900000
C	15.52300000	8.14500000	10.07700000
C	13.91000000	14.04000000	5.72300000
C	6.27900000	15.31500000	4.00700000
C	12.93300000	15.01300000	5.92900000
C	7.85400000	19.39300000	6.52300000
C	6.11600000	14.35800000	3.00300000
C	6.25900000	7.28000000	4.48000000
C	10.74200000	1.65600000	6.00500000
C	11.29400000	1.43700000	7.27100000
C	9.61000000	9.98700000	4.91500000
C	9.72400000	11.23000000	4.22000000
C	9.62600000	12.35600000	5.09500000
C	9.89700000	11.33500000	2.83500000

C	10.01300000	12.65300000	2.30600000
C	9.93900000	13.74800000	3.15100000
C	9.73800000	13.62100000	4.55200000
C	9.92500000	10.11300000	2.10300000
C	9.78600000	8.90500000	2.76600000
C	9.63200000	8.82000000	4.17500000
C	10.51100000	8.82800000	12.59500000
C	10.53500000	7.65400000	13.30500000
C	9.36800000	7.13300000	13.84700000
C	8.16200000	7.79300000	13.67100000
C	8.09400000	8.96800000	12.96400000
C	9.27800000	9.47000000	12.40400000
C	6.77000000	9.66500000	12.84300000
C	11.79600000	9.39300000	12.07200000
C	9.72200000	11.99100000	14.62600000
C	9.28400000	12.77100000	15.65700000
C	8.19100000	13.48100000	15.49000000
C	7.54700000	13.41800000	14.27200000
C	7.98400000	12.65400000	13.23400000
C	9.07500000	11.92800000	13.39800000
H	7.58200000	5.85200000	9.05300000
H	8.47900000	17.55700000	10.45200000
H	6.93200000	9.37400000	8.44300000
H	11.83100000	6.14200000	8.58600000
H	11.14400000	12.65300000	9.37700000
H	10.11700000	16.09900000	9.83900000
H	5.92300000	9.21400000	10.45500000
H	7.65800000	2.94400000	8.62400000
H	5.00700000	17.58200000	9.01700000
H	5.02700000	9.92900000	7.02600000
H	6.14000000	15.43500000	8.37700000

H	6.86800000	12.04100000	7.09600000
H	13.57900000	15.23400000	9.35200000
H	5.89100000	2.09800000	10.14200000
H	10.85300000	4.38700000	9.90800000
H	5.41500000	6.00400000	7.74600000
H	11.71700000	6.23600000	6.11700000
H	6.24700000	11.55600000	4.93400000
H	14.51800000	16.28500000	11.38000000
H	2.99700000	17.19200000	10.40700000
H	7.51900000	16.66700000	12.38000000
H	4.04300000	9.84700000	4.75800000
H	3.67200000	5.02200000	9.17900000
H	6.98600000	19.84500000	10.27100000
H	4.12500000	8.26500000	11.87200000
H	12.84400000	10.19500000	9.60100000
H	9.75500000	4.59800000	11.98600000
H	13.11800000	10.29600000	5.74900000
H	6.00300000	12.03000000	9.58300000
H	5.50600000	16.34300000	13.79100000
H	13.93500000	6.61800000	7.49000000
H	3.23000000	16.58100000	12.80600000
H	11.79000000	9.70900000	7.58900000
H	10.30700000	13.70200000	11.64300000
H	14.87400000	9.98100000	11.00600000
H	6.07200000	2.45000000	12.59600000
H	6.92900000	21.79400000	8.75100000
H	13.36100000	16.05600000	13.56600000
H	3.00000000	6.15300000	11.25100000
H	6.55800000	15.68800000	6.10500000
H	11.46500000	2.14900000	9.30000000
H	13.19000000	12.02200000	8.36800000

H	4.01800000	14.00900000	6.31200000
H	11.24500000	14.74400000	13.68800000
H	7.60300000	6.62500000	6.03600000
H	8.01600000	3.71200000	13.50800000
H	7.47800000	21.51500000	6.33200000
H	8.18900000	17.31600000	7.00100000
H	11.29200000	15.68100000	7.15900000
H	1.86300000	13.84800000	7.51800000
H	9.05900000	4.54800000	6.65700000
H	15.91200000	6.35500000	8.93800000
H	12.53600000	5.74700000	3.84200000
H	4.81500000	8.13200000	3.11500000
H	13.91600000	9.81400000	3.45800000
H	14.75900000	12.19600000	6.46300000
H	5.99400000	12.24200000	2.57400000
H	3.83900000	11.84500000	10.78100000
H	13.64600000	7.52800000	2.49000000
H	9.50400000	2.95900000	4.80600000
H	1.75300000	12.75400000	9.75600000
H	16.41600000	8.04400000	10.69600000
H	14.59900000	14.11900000	4.88100000
H	6.29500000	16.37700000	3.75400000
H	12.85800000	15.86100000	5.24500000
H	8.10000000	19.25900000	5.46800000
H	6.00900000	14.66400000	1.96100000
H	6.60800000	6.52900000	3.76800000
H	10.94300000	0.95700000	5.19000000
H	11.92800000	0.56600000	7.45000000
H	10.05100000	10.13200000	1.01900000
H	9.80500000	7.97700000	2.19200000
H	9.54300000	7.84200000	4.64700000

H	10.15400000	12.79600000	1.23200000
H	10.02400000	14.75100000	2.73000000
H	9.66800000	14.51600000	5.16900000
H	11.49100000	7.15500000	13.44000000
H	7.24000000	7.39600000	14.08700000
H	6.68800000	10.22100000	11.90300000
H	6.62900000	10.39100000	13.64800000
H	5.95800000	8.94400000	12.90100000
H	12.59100000	8.64300000	12.08500000
H	12.14400000	10.24000000	12.67700000
H	11.69400000	9.75200000	11.03800000
H	9.40400000	6.22600000	14.41300000
H	7.48200000	12.60000000	12.28100000
H	10.56700000	11.41700000	14.76600000
H	9.79600000	12.81400000	16.60100000
H	6.68800000	13.96300000	14.12800000
H	7.84200000	14.07300000	16.30400000
H	10.51400000	11.23100000	12.20300000

N-methylaniline

C	13.30600000	12.33000000	17.39900000
C	13.32000000	11.12000000	16.70500000
C	13.30300000	9.90000000	17.38500000
C	13.28100000	9.91100000	18.78600000
C	13.26900000	11.10900000	19.49200000
C	13.27200000	12.34600000	18.80900000
C	13.30900000	14.83000000	18.87400000
H	13.25400000	11.09600000	20.58600000
H	13.31600000	13.26900000	16.84700000
H	13.33800000	11.14000000	15.61300000
H	13.26900000	8.96500000	19.33500000
H	13.30200000	8.95700000	16.83400000

H	13.28700000	13.49100000	20.51400000
H	13.46600000	15.60000000	19.63800000
H	14.15100000	14.88600000	18.16200000
H	12.38300000	15.07400000	18.32000000
N	13.23400000	13.53600000	19.50600000

IM3

Pd	8.83200000	10.17200000	10.26600000
N	9.13800000	11.98400000	7.51800000
N	9.31000000	9.81100000	7.26600000
N	9.97000000	11.51500000	11.10100000
C	8.44500000	6.36800000	8.44800000
C	9.07500000	10.79100000	8.22400000
C	8.28000000	7.67300000	7.96400000
C	9.70400000	5.79100000	8.60600000
C	11.91600000	14.30000000	10.00600000
C	9.41000000	11.74200000	6.17900000
C	8.01300000	15.78900000	9.06200000
C	9.49800000	10.37100000	6.01200000
C	7.61800000	17.13600000	9.65900000
C	9.75000000	14.10700000	8.65600000
C	6.86900000	8.21700000	7.72000000
C	6.42800000	8.11700000	6.26000000
C	10.82700000	6.53900000	8.23800000
C	11.22000000	13.68900000	8.77700000
C	9.33800000	15.35300000	9.14300000
C	5.81500000	7.58700000	8.63200000
C	5.57500000	8.15200000	9.88900000
C	10.25200000	3.39600000	7.99300000
C	7.79200000	2.95600000	9.54400000
C	5.06900000	17.33000000	9.90700000

C	8.74900000	3.87300000	9.99700000
C	5.36100000	8.92500000	5.83100000
C	7.08600000	14.96100000	8.43100000
C	6.40400000	12.93400000	7.09000000
C	13.10900000	15.03000000	9.91500000
C	6.31900000	13.38900000	5.62800000
C	7.61100000	18.28900000	8.65300000
C	6.32100000	17.03300000	10.46300000
C	5.03900000	12.92100000	7.79000000
C	8.78100000	13.29000000	8.03500000
C	10.73500000	7.84200000	7.74100000
C	6.75200000	2.53800000	10.38000000
C	9.90000000	4.36600000	9.11900000
C	7.44800000	13.72800000	7.87700000
C	5.07200000	6.45900000	8.25300000
C	12.44400000	8.14700000	5.86000000
C	12.24800000	6.86400000	5.33300000
C	6.21700000	12.42500000	4.61500000
C	13.70900000	15.56800000	11.05900000
C	3.90000000	17.18000000	10.66000000
C	11.99100000	13.96200000	7.48800000
C	6.37400000	16.58900000	11.79200000
C	4.85600000	8.81500000	4.53600000
C	4.12400000	5.90700000	9.11800000
C	7.40400000	19.59700000	9.12700000
C	13.19200000	8.45700000	8.22900000
C	4.62500000	7.60800000	10.75400000
C	13.45900000	9.50100000	9.12400000
C	8.64000000	4.36100000	11.30900000
C	13.15200000	9.08100000	5.08900000
C	4.93200000	12.33400000	9.06300000

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C	3.96700000	16.73900000	11.98300000
C	12.00000000	8.56500000	7.26900000
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C	6.65600000	3.02700000	11.68400000
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C	13.12900000	15.38300000	12.31400000
C	9.44200000	8.42200000	7.65100000
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C	6.30000000	14.74200000	5.25500000
C	11.10000000	2.31200000	8.26100000
C	12.87100000	12.99900000	6.97900000
C	3.88700000	13.46100000	7.20500000
C	11.94800000	14.64300000	12.41800000
C	6.97300000	7.19900000	5.35500000
C	7.60500000	3.94400000	12.14500000
C	7.62900000	20.49500000	6.89100000
C	7.83100000	18.11100000	7.28200000
C	11.90200000	15.19500000	6.82600000
C	2.65800000	13.41700000	7.87100000
C	9.73100000	3.53000000	6.69900000
C	15.16500000	7.30600000	9.07500000
C	12.75500000	6.52300000	4.07300000
C	5.40700000	7.89200000	3.64100000
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C	13.64000000	13.25300000	5.84000000
C	6.09900000	12.79400000	3.27400000
C	3.70500000	12.28400000	9.72400000
C	13.46100000	7.46100000	3.31900000

C	10.04500000	2.60300000	5.70100000
C	2.56100000	12.82600000	9.13000000
C	15.41400000	8.35200000	9.96700000
C	13.54100000	14.48400000	5.19000000
C	6.17700000	15.11600000	3.91400000
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C	7.83700000	19.20400000	6.40700000
C	6.07800000	14.14400000	2.91700000
C	6.46700000	7.08700000	4.05600000
C	10.88900000	1.52700000	5.98100000
C	11.41700000	1.38400000	7.26700000
C	9.71700000	10.05700000	4.60300000
C	9.80800000	11.34000000	3.98000000
C	9.63000000	12.41500000	4.90300000
C	10.03400000	11.52200000	2.60700000
C	10.10900000	12.86900000	2.14800000
C	9.94700000	13.91600000	3.03900000
C	9.69700000	13.71000000	4.42400000
C	10.15100000	10.34200000	1.81900000
C	10.03800000	9.09500000	2.41300000
C	9.82000000	8.93000000	3.80700000
C	9.93600000	8.48300000	12.27800000
C	9.98400000	7.57900000	13.35000000
C	8.89900000	7.44100000	14.21000000
C	7.76100000	8.21800000	14.00300000
C	7.67400000	9.14500000	12.95000000
C	8.76300000	9.23700000	12.05100000
C	6.43200000	9.99700000	12.88500000
C	11.16100000	8.63000000	11.40500000
C	10.54700000	11.56700000	13.46800000
C	10.16400000	11.79200000	14.79200000

C	8.85500000	12.15700000	15.11300000
C	7.92300000	12.29300000	14.07500000
C	8.29000000	12.07600000	12.75200000
C	9.61400000	11.70600000	12.41700000
C	11.22900000	10.92000000	10.72000000
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H	11.81800000	6.09500000	8.36000000
H	11.22700000	12.59600000	8.92900000
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H	6.15000000	9.03300000	10.19000000
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H	6.73600000	11.88400000	7.05900000
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H	10.78800000	4.40400000	9.77600000
H	5.22200000	6.01600000	7.26600000
H	11.69000000	6.11500000	5.89900000
H	6.24100000	11.36500000	4.87800000
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H	2.93300000	17.41100000	10.20800000
H	7.34300000	16.34800000	12.23800000
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H	12.79700000	10.37000000	9.14900000

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H	5.82500000	11.93100000	9.55000000
H	5.27700000	16.10400000	13.58400000
H	13.92800000	6.56300000	7.48000000
H	3.05500000	16.62500000	12.57100000
H	11.75900000	9.63700000	7.21000000
H	10.42700000	13.53100000	11.37200000
H	14.74900000	10.29000000	10.66300000
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H	7.25900000	21.69300000	8.65500000
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H	3.15300000	6.05000000	11.04600000
H	6.38300000	15.51800000	6.01800000
H	11.51100000	2.18900000	9.26700000
H	12.96800000	12.03900000	7.49200000
H	3.94700000	13.92100000	6.21800000
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H	7.54100000	4.33900000	13.16100000
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H	1.77400000	13.85000000	7.39800000
H	9.07200000	4.37000000	6.46800000
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H	5.01300000	7.80600000	2.62700000
H	14.19600000	9.49400000	3.25000000
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H	6.03600000	12.02100000	2.50600000

H	3.64300000	11.82600000	10.71300000
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H	11.13700000	0.80300000	5.20200000
H	12.07900000	0.54700000	7.49800000
H	10.32800000	10.42300000	0.74300000
H	10.12800000	8.20000000	1.79500000
H	9.75200000	7.92600000	4.22400000
H	10.29000000	13.07200000	1.09000000
H	10.00200000	14.94300000	2.67100000
H	9.56200000	14.57000000	5.08000000
H	10.89700000	6.99800000	13.51400000
H	6.91300000	8.12700000	14.68700000
H	6.19700000	10.33400000	11.86800000
H	6.56000000	10.90900000	13.48700000
H	5.57000000	9.45100000	13.29500000
H	11.45800000	7.67600000	10.94200000
H	12.02200000	8.99100000	11.99100000
H	11.00400000	9.35800000	10.58900000
H	8.94300000	6.75100000	15.05400000
H	7.55200000	12.18600000	11.95200000
H	11.57500000	11.27600000	13.25200000
H	10.90800000	11.67700000	15.58400000

H	6.89100000	12.57400000	14.30300000
H	8.56000000	12.32600000	16.15100000
H	9.51400000	12.18400000	10.49200000
H	12.07800000	11.56400000	11.00200000
H	11.24400000	10.80900000	9.63000000
H	11.38900000	9.92600000	11.17900000
Cl	7.35900000	11.64300000	9.72200000
IM4			
Pd	9.26900000	10.24300000	10.77200000
N	9.23600000	12.08300000	7.88900000
N	9.34500000	9.89200000	7.71100000
N	10.33000000	11.52100000	12.02800000
C	8.45400000	6.40700000	8.77600000
C	9.20400000	10.90900000	8.65700000
C	8.29400000	7.73400000	8.35600000
C	9.70800000	5.80500000	8.87100000
C	11.88700000	14.69100000	10.32800000
C	9.42900000	11.78200000	6.54400000
C	8.03700000	16.00000000	9.12800000
C	9.46400000	10.40400000	6.43000000
C	7.60700000	17.36600000	9.66100000
C	9.77900000	14.28100000	8.94600000
C	6.88300000	8.29000000	8.12300000
C	6.45300000	8.23000000	6.65400000
C	10.83100000	6.56000000	8.52400000
C	11.24900000	13.91400000	9.16400000
C	9.34500000	15.55900000	9.32300000
C	5.76500000	7.63900000	8.94600000
C	5.20200000	8.33200000	10.02300000
C	10.22700000	3.44500000	8.09200000
C	7.72000000	3.03800000	9.60800000

C	5.05700000	17.36500000	9.98200000
C	8.77600000	3.78700000	10.14600000
C	5.43900000	9.09800000	6.22000000
C	7.15200000	15.13700000	8.47900000
C	6.53000000	13.05300000	7.21700000
C	13.06200000	15.44100000	10.18800000
C	6.46200000	13.48300000	5.74700000
C	7.51100000	18.47600000	8.61200000
C	6.34600000	17.19900000	10.50900000
C	5.14300000	13.04700000	7.87200000
C	8.85300000	13.41400000	8.32400000
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C	6.70000000	2.55200000	10.43100000
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C	7.53900000	13.86400000	8.03300000
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C	12.38500000	8.28500000	6.17300000
C	12.22600000	7.01300000	5.60800000
C	6.28400000	12.49500000	4.76900000
C	13.61900000	16.11900000	11.28100000
C	3.92500000	17.08200000	10.75700000
C	12.04100000	14.05800000	7.86600000
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C	4.14200000	5.86000000	9.31600000
C	7.20800000	19.78100000	9.03900000
C	13.26000000	8.41800000	8.49600000
C	4.12600000	7.80500000	10.74200000
C	13.66300000	9.44800000	9.35300000
C	8.78700000	4.03500000	11.52600000
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C	4.06300000	16.65300000	12.08100000
C	12.01200000	8.61400000	7.62400000
C	11.28500000	14.63200000	11.59900000
C	14.81700000	9.34400000	10.13300000
C	6.72300000	2.80200000	11.80500000
C	7.14900000	20.83900000	8.13300000
C	13.00900000	16.05500000	12.53200000
C	9.46000000	8.49000000	8.07100000
C	3.59200000	6.56400000	10.39100000
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C	11.05200000	2.32500000	8.28000000
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C	4.03500000	13.69300000	7.30600000
C	11.84100000	15.30100000	12.68800000
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C	7.39100000	20.61400000	6.77400000
C	7.76700000	18.26700000	7.25100000
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C	2.79000000	13.66800000	7.94600000
C	9.68900000	3.66600000	6.81700000
C	15.22400000	7.16000000	9.20100000
C	12.68700000	6.74100000	4.31500000
C	5.39200000	8.03100000	4.04800000
C	13.45100000	9.01800000	4.10800000
C	13.71200000	13.19300000	6.32000000
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C	3.71900000	12.32500000	9.72600000

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C	15.60100000	8.19100000	10.06500000
C	13.62900000	14.35700000	5.55300000
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C	12.75000000	15.37200000	5.94200000
C	7.70300000	19.32700000	6.33900000
C	6.18700000	14.16500000	3.02000000
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C	10.77800000	1.67700000	5.96400000
C	11.32600000	1.44900000	7.22800000
C	9.61400000	10.02400000	5.02900000
C	9.73300000	11.27400000	4.34900000
C	9.63600000	12.39300000	5.23400000
C	9.92100000	11.39000000	2.96400000
C	10.05000000	12.71000000	2.44700000
C	9.97500000	13.79900000	3.29800000
C	9.76100000	13.66200000	4.69600000
C	9.96000000	10.17500000	2.22300000
C	9.81800000	8.95900000	2.87300000
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C	10.15500000	7.02300000	13.50200000
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C	7.91800000	7.75700000	13.99500000
C	8.01000000	8.76600000	13.02200000
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H	10.05900000	16.22200000	9.81800000
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H	2.74700000	6.15100000	10.94600000
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H	11.37000000	15.21900000	13.66900000
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H	7.80000000	3.75800000	13.42000000
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H	8.03600000	17.27000000	6.89800000
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H	3.61700000	11.81200000	10.68900000
H	13.66200000	7.52800000	2.55100000
H	9.52300000	2.97700000	4.77700000
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H	16.50600000	8.10300000	10.67000000
H	14.23800000	14.47100000	4.65500000
H	6.40200000	16.21100000	3.68500000
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H	11.97100000	0.58400000	7.39800000
H	10.10400000	10.20600000	1.13900000
H	9.85100000	8.03700000	2.29000000
H	9.55300000	7.88200000	4.74100000
H	10.20800000	12.85700000	1.37500000
H	10.07500000	14.80400000	2.88500000
H	9.69700000	14.55400000	5.32000000
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H	7.92600000	12.15900000	12.89400000
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N	9.78000000	11.71000000	12.10200000
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H	11.71300000	10.86500000	12.59700000
TS5			
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H	9.76700000	8.06400000	2.24000000
H	9.48400000	7.89000000	4.69100000
H	10.23400000	12.89100000	1.37500000
H	10.14800000	14.82200000	2.90800000
H	9.77900000	14.55100000	5.34300000
H	10.84300000	6.94600000	12.49600000
H	6.64200000	7.19400000	13.14100000
H	6.35000000	10.40800000	12.41100000
H	6.01600000	9.51800000	13.82300000
H	5.64500000	8.82900000	12.24800000
H	11.85300000	8.49400000	11.33800000
H	12.00400000	9.19900000	12.75300000
H	11.22600000	10.00900000	11.53700000
H	8.68200000	6.02500000	13.06100000
H	6.50100000	11.33400000	12.52200000
H	9.90000000	12.43500000	14.71500000

H	8.81300000	13.95700000	15.81900000
H	5.40400000	12.83700000	13.67800000
H	6.54600000	14.16100000	15.34200000
H	10.37000000	11.87700000	13.12500000
H	10.53500000	10.21900000	12.56900000
H	10.68800000	10.68900000	13.94100000

Product: N,2,6-trimethyl-N-phenylaniline

N	9.42500000	10.78400000	14.81700000
C	10.29400000	9.67200000	12.81000000
C	10.15300000	8.68100000	11.83000000
C	8.99300000	7.91200000	11.75000000
C	7.93800000	8.15400000	12.62700000
C	8.03100000	9.14400000	13.61800000
C	9.22600000	9.88900000	13.71200000
C	6.87800000	9.38900000	14.55500000
C	11.56900000	10.46900000	12.91200000
C	9.43900000	12.97300000	15.88300000
C	9.05300000	14.31400000	15.90900000
C	8.28100000	14.86100000	14.88400000
C	7.91200000	14.03600000	13.81600000
C	8.29300000	12.69500000	13.76800000
C	9.05700000	12.12500000	14.81400000
C	10.17400000	10.23400000	15.93700000
H	10.97300000	8.50300000	11.13100000
H	7.03500000	7.54000000	12.56800000
H	6.17400000	10.11900000	14.12300000
H	7.21600000	9.80700000	15.51200000
H	6.31400000	8.46400000	14.74600000
H	12.14300000	10.39300000	11.97900000
H	12.22200000	10.10800000	13.72400000
H	11.36500000	11.52800000	13.12500000

H	8.91400000	7.10900000	11.01100000
H	7.99300000	12.08300000	12.91600000
H	10.04700000	12.58400000	16.69700000
H	9.37100000	14.93700000	16.74900000
H	7.31300000	14.44600000	12.99900000
H	7.97500000	15.90800000	14.91500000
H	9.64700000	10.39900000	16.89400000
H	10.27100000	9.15100000	15.78600000
H	11.18800000	10.66700000	16.02900000

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