Supporting Information

Abnormal N-Heterocyclic Carbene Based Nickel Complex for Catalytic Reduction of Nitroarenes

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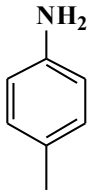
Contents

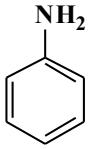
^{1}H and ^{13}C NMR data

Toluidine[1,2]



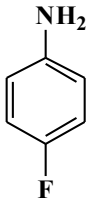
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C):δ 6.99 (d, 2H, *J*= 7.6 Hz), 6.64 (d, 2H, *J*= 8.4 Hz), 3.54 (br s, 2H, -NH_2), 2.27 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$,25 °C): δ143.9, 129.8, 127.8, 115.3, 20.5 ppm.

Aniline[1]



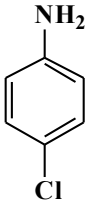
^{1}H NMR: (400 MHz, $CDCl_3$, 25 °C): δ 7.20 (t, 2H, *J*= 7.5 Hz), 6.81 (t, 1H, *J*= 7.5Hz), 6.71 (d, 2H, *J* = 7.5 Hz), 3.65 (br s, 2H, -NH_2) ppm; ^{13}C NMR: (100 MHz, $CDCl_3$, 25 °C): δ146.4, 129.3, 118.6, 115.1 ppm.

4-Fluoroaniline[1]



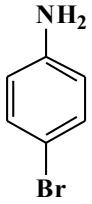
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ 6.88 (m, 2H), 6.64 (m, 2H), 3.58 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ157.7, 155.3, 142.5, 116.2, 116.1, 115.9, 115.6 ppm.

4-Chloroaniline[2]



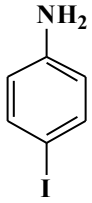
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ 7.11 (d, 2H, *J* = 7.5 Hz), 6.61 (d, 2H, *J* = 7.5 Hz), 3.62 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ 145.0, 129.2, 123.2, 116.3 ppm.

4-Bromoaniline[2]



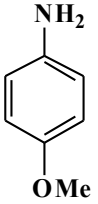
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.22 (d, 2H, J = 7.5 Hz), 6.55 (d, 2H, J = 7.5 Hz), 3.65 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C):δ145.6, 132.1, 116.8, 110.2 ppm.

4-Iodoaniline[3]



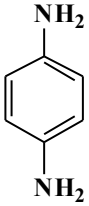
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.42 (d, J= 7.5 Hz, 2H), 6.48 (d, J= 7.5 Hz, 2H), 3.67(br s, 2H, -NH2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ 146.1, 137.9, 117.3, 79.4 ppm.

4-Methoxyaniline[1]



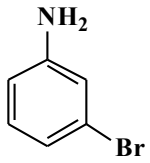
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ6.76 (d, 2H, J = 8 Hz), 6.60 (d, 2H, J= 8 Hz), 3.75 (s, 3H), 3.42(br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ152.9, 140.0, 116.5, 114.9, 55.8 ppm.

4-Aminoaniline[1]



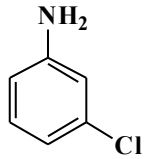
^{1}H NMR (100 MHz, $CDCl_3$, 25 °C): δ6.57 (s, 4H), 3.33 (br s, 4H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ138.7, 116.8 ppm.

3-Bromoaniline[2]



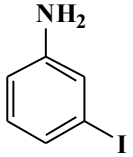
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.02 (t, 1H, J = 8 Hz), 6.88 (d, 1H, J= 8 Hz), 6.83 (s, 1H),6.59 (d, 1H, J= 8 Hz),3.71(br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ147.8, 130.7, 123.1, 121.4, 117.8, 113.7 ppm.

3-Chloroaniline[4]



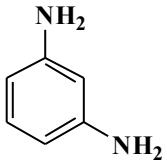
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.07 (t, 1H, J = 8 Hz), 6.73 (dd, 1H, J= 8 Hz,), 6.67(t, 1H, J = 1.6 Hz), 6.53 (dd, 1H, J= 8 Hz), 3.71(br s, 2H, -NH_2) ppm;^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ147.5, 134.8, 130.2, 118.4, 114.8, 113.1 ppm.

3-Iodoaniline[5]



^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.08-7.04 (m, 2H), 6.88 (t, 1H, J= 8 Hz), 6.63 (d, 1H, J = 1.6 Hz), 3.53(br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ147.8, 130.8, 127.5, 123.8, 114.3, 95.0 ppm.

m-Phenylenediamine[6]

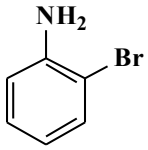


^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.58 (d, 1H, J= 8 Hz), 7.48 (s, 1H), 7.28 (t, 1H, J = 7.6 Hz), 3.99 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C):δ147.6, 130.2, 106.07, 102.0 ppm.

2-Fluoroaniline[6]

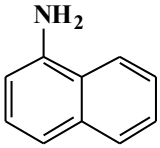
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.02–6.80 (m, 2H), 6.8–6.68 (m, 2H), 3.67 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ152.9, 150.6, 134.6, 124.5, 124.3, 118.7, 118.6, 117.0, 115.4 ppm.

2-Bromoaniline[7]



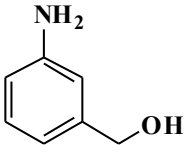
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C):δ7.42 (d, 1H, J= 8 Hz), 7.12 (t, 1H, J= 8 Hz), 6.77 (d, 1H, J = 8 Hz), 7.64 (t, 1H, J= 8 Hz), 4.07 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ144.1, 132.7, 128.4, 119.5, 115.8, 109.4 ppm.

1-Aminonaphthalene[2]



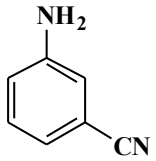
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.85-7.83 (m, 2H), 7.50-7.46 (m, 2H), 7.38-7.26 (m, 2H), 6.81 (d, 1H, J= 8 Hz), δ 4.15 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ 142.0, 134.3, 128.4, 126.2, 125.7, 124.7, 123.5, 120.7, 118.8, 109.6 ppm.

3-Aminobenzylalcohol[8]



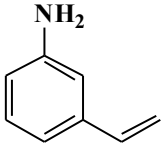
^{1}H NMR (400 MHz, $CDCl_3$ J= 8 Hz, 25 °C): δ7.16 (t, 1H, J = 8 Hz), 6.75 (d, 1H, J= 7.5 Hz), 6.69 (s, 1H), 6.62 (d, 1H, J= 7.5 Hz), 4.59 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$ J= 8 Hz, 25 °C): δ146.5, 142.1, 129.4, 117.0, 114.3, 113.5, 65.32 ppm.

3-Aminobenzonitrile[9]



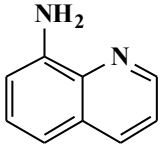
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.23 (t, 1H, J = 7.5 Hz), 7.01 (d, 1H, J = 7.5 Hz), 6.89 (s, 1H), 6.87 (d, 1H, J = 7.5Hz), 3.91 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ 147.1, 130.1, 121.8, 119.3, 117.5, 112.9 ppm.

12) 3-Aminostyrene[10]



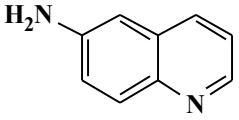
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ7.14 (t, 1H, J = 7.5 Hz), 6.83 (d, 1H, J= 7.5 Hz), 6.74 (br s, 1H), 6.67 (dd, 1H, $J1$= 18 Hz, $J2$= 12 Hz), 6.63 (d, 1H, J = 7.5 Hz), 5.72 (d, 1H, J= 18 Hz), 5.23 (d, 1H, J= 12 Hz) , 3.61 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ146.4, 138.6, 136.9, 129.3, 116.9, 114.7, 113.5, 112.7 ppm.

8-Aminoquinoline[4]



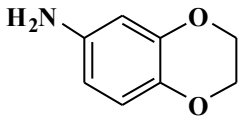
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ 8.77 (d, 1H, J = 4 Hz), 8.08 (d, 1H, J = 7.5 Hz), 7.38-7.26 (m, 2H), 7.17 (d, J = 7.5 Hz, 1H), 6.95 (d, J = 8 Hz, 1H) , 4.99 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ 147.5, 144.0, 138.5, 136.1, 128.9, 127.5, 121.4, 116.1, 110.1 ppm.

6-Aminoquinoline[3]



^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ 8.66 (d, 1H, J = 7.5 Hz), 7.92 (dd, 1H, J= 8.4, 4.2 Hz), 7.29 (dd, 1H, J = 7.7, 3.5 Hz), 7.17 (dd, 1H, J = 8.9, 2.6 Hz), 6.91 (d, 1H, J = 2.4 Hz) , 3.95 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ 146.9, 144.7, 143.4, 134.0, 130.6, 129.9, 121.7, 121.5, 117.5 ppm.

6-Amino-1,4-benzodioxane[3]



^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ6.67 (d, 1H, J = 6.8 Hz), 6.24 (d, 1H, J = 2 Hz), 6.20 (dd, 1H, J=2 Hz, J = 2 Hz), 4.22-4.20 (m, 2H), 4.18-4.16 (m, 2H), 3.39 (br s, 2H, -NH_2) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ 143.8, 140.7, 136.4, 117.5, 108.6, 104.1, 64.6, 64.1 ppm.

Fig. S1: The ^{1}H NMR spectrum ($CDCl_3$) of complex 1.

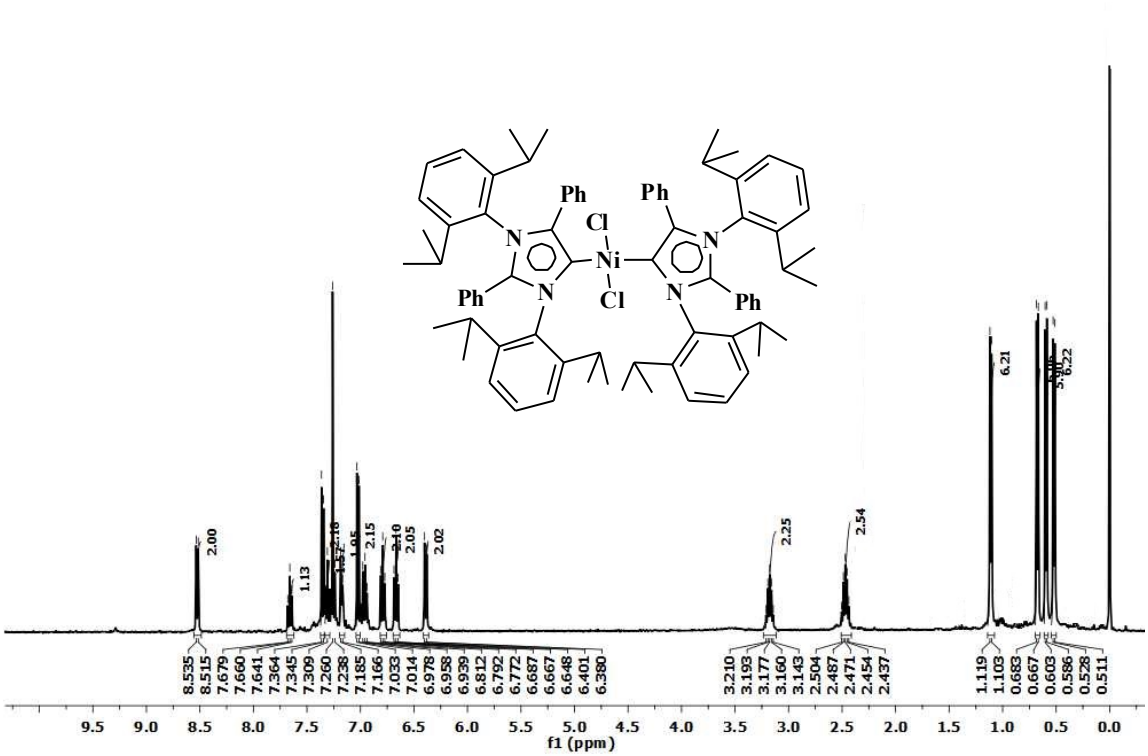


Fig. S2: The ^{13}C NMR spectrum ($CDCl_3$) of complex 1.

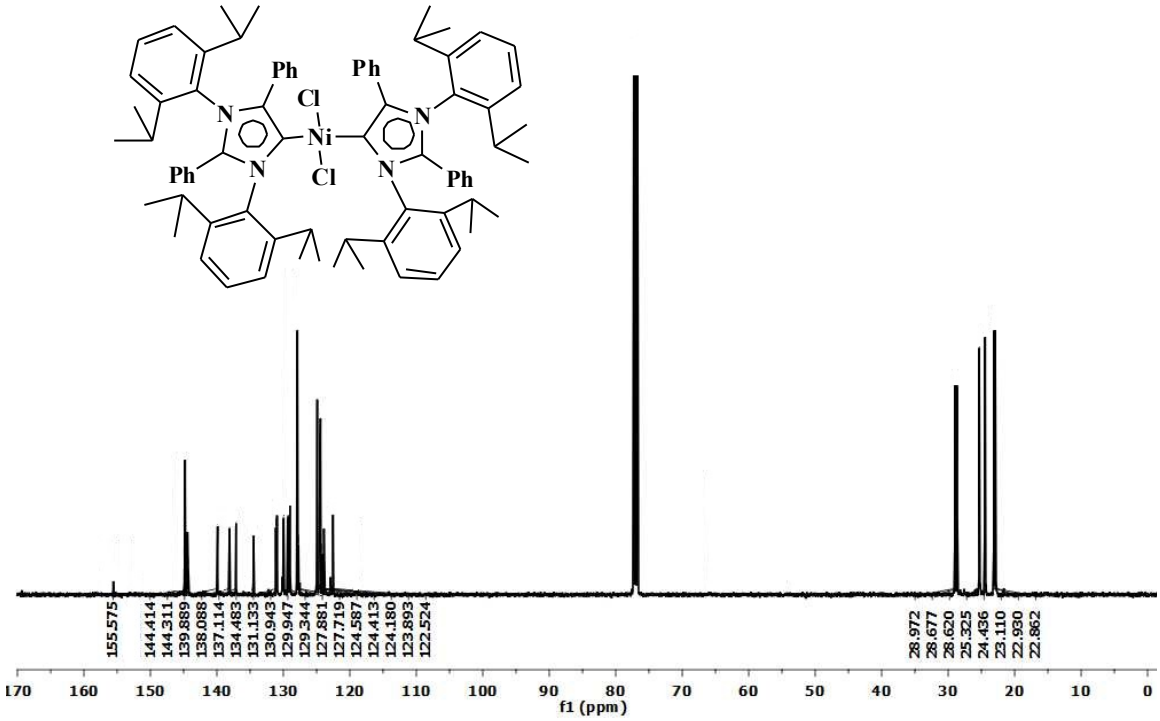


Fig. S3: The ^{1}H NMR spectrum ($CDCl_3$) of toluidine.

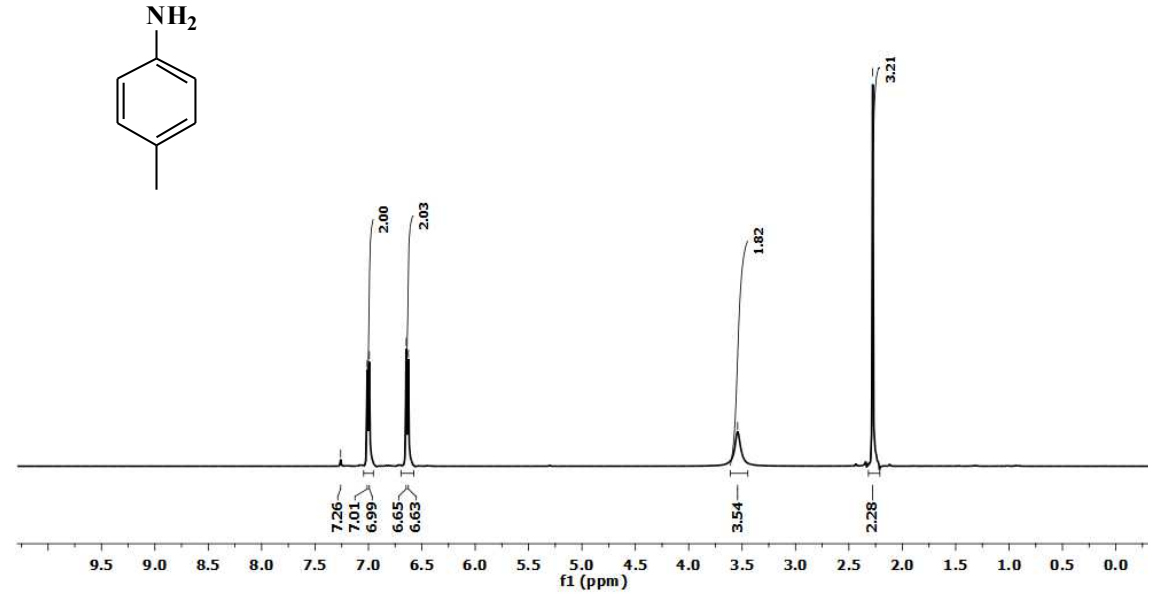


Fig. S4: The ^{13}C NMR spectrum ($CDCl_3$) of toluidine.

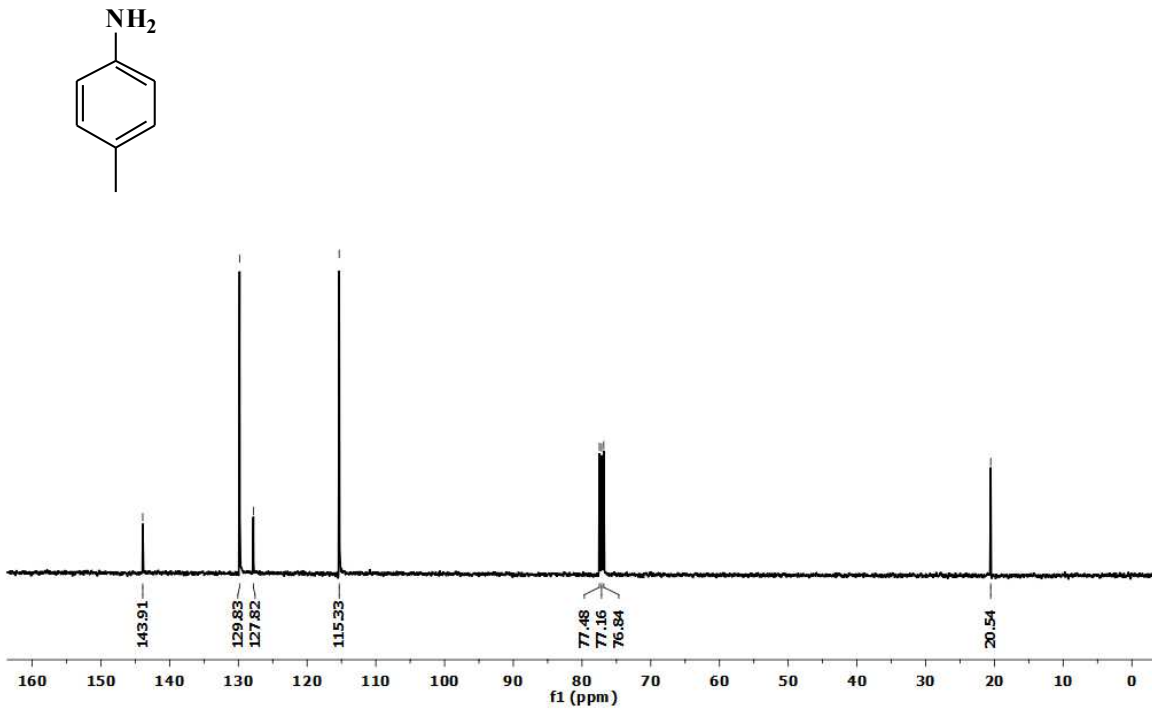


Fig. S5: The ^{1}H NMR spectrum ($CDCl_3$) of aniline.

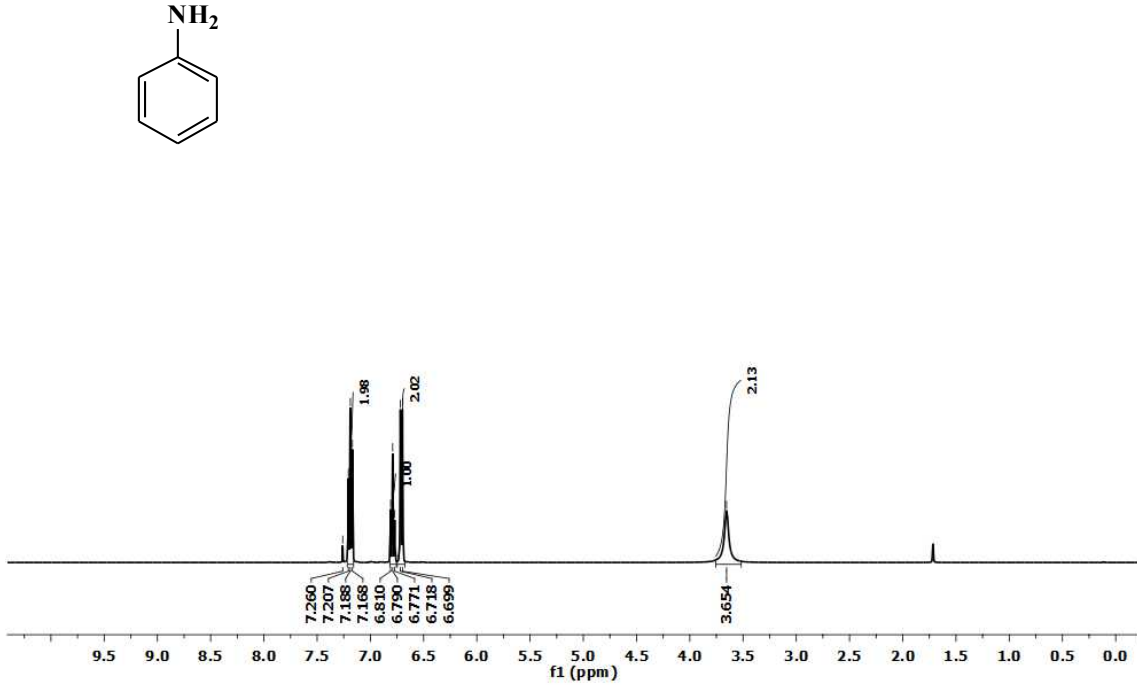


Fig. S6: The ^{13}C NMR spectrum ($CDCl_3$) of aniline.

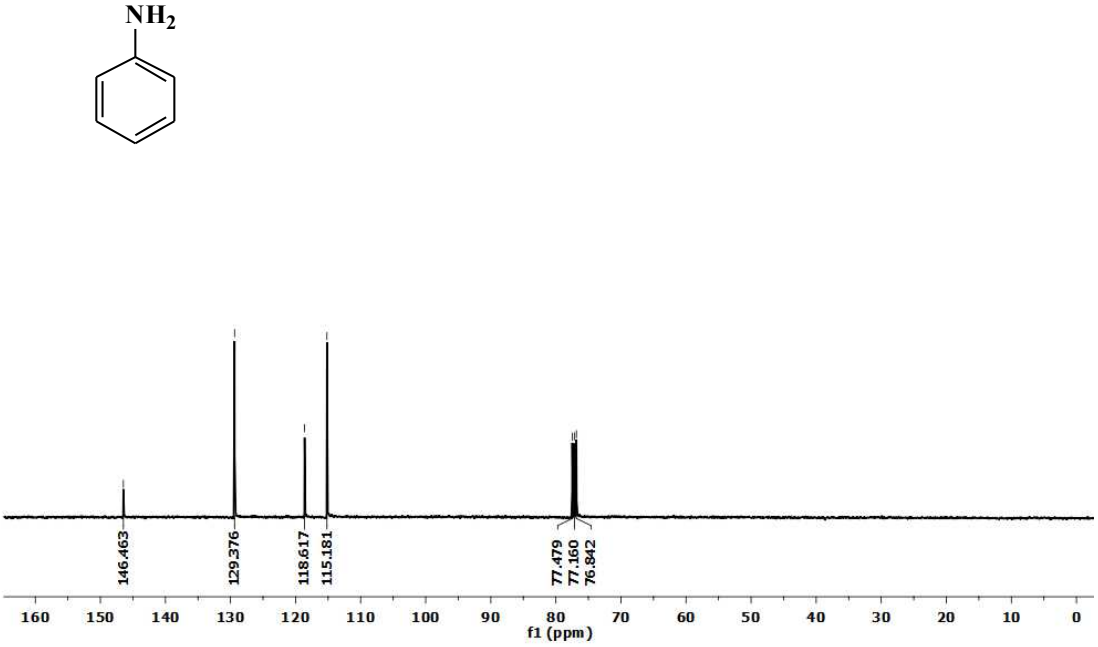


Fig. S7: ^{1}H NMR spectrum ($CDCl_3$) of 4-Fluoroaniline.

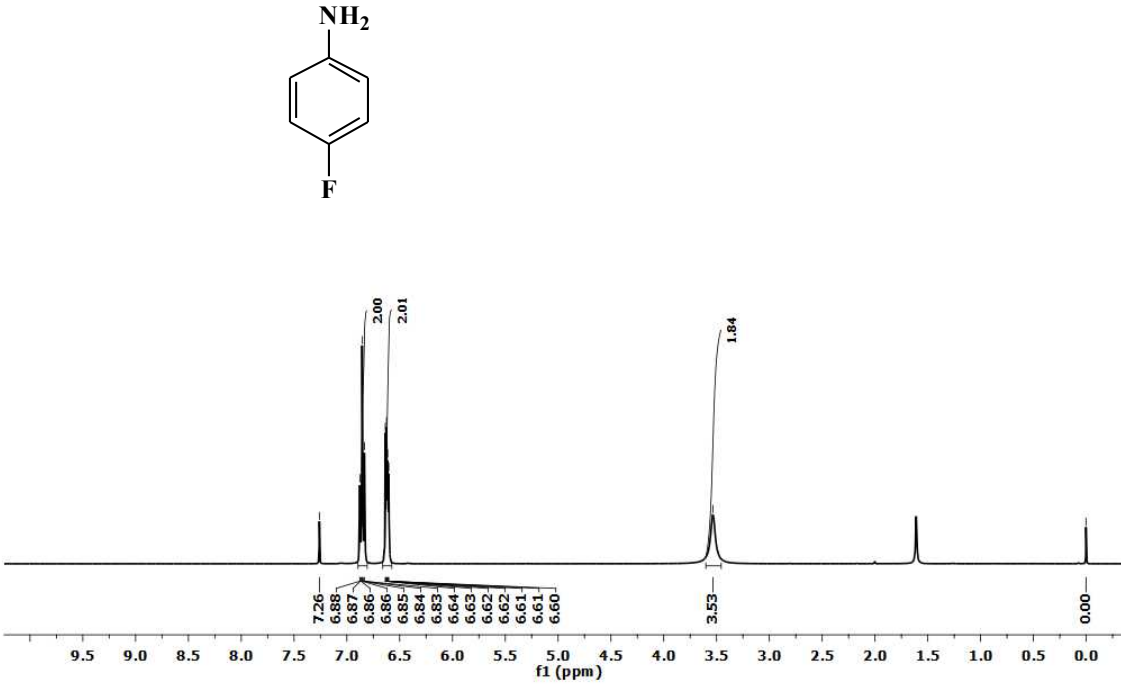


Fig. S8: The ^{13}C NMR spectrum ($CDCl_3$) of 4-Fluoroaniline.

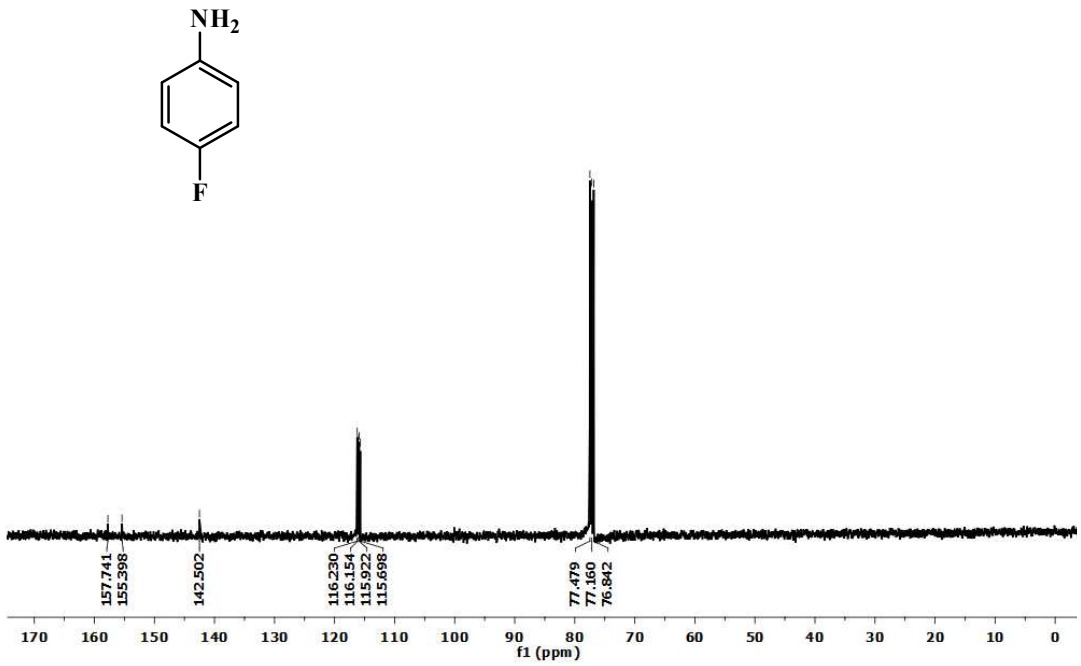


Fig. S9: ^{1}H NMR spectrum ($CDCl_3$) of *p*-Anisidine.

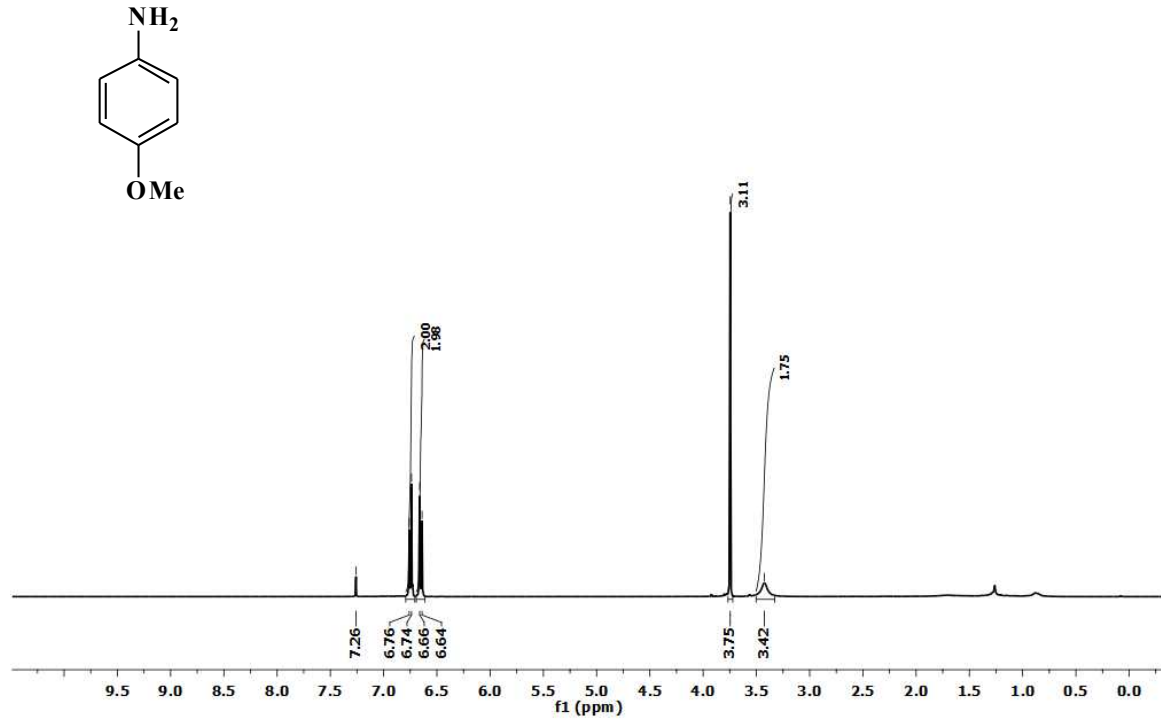


Fig. S10: ^{13}C NMR spectrum ($CDCl_3$) of *p*-Anisidine.

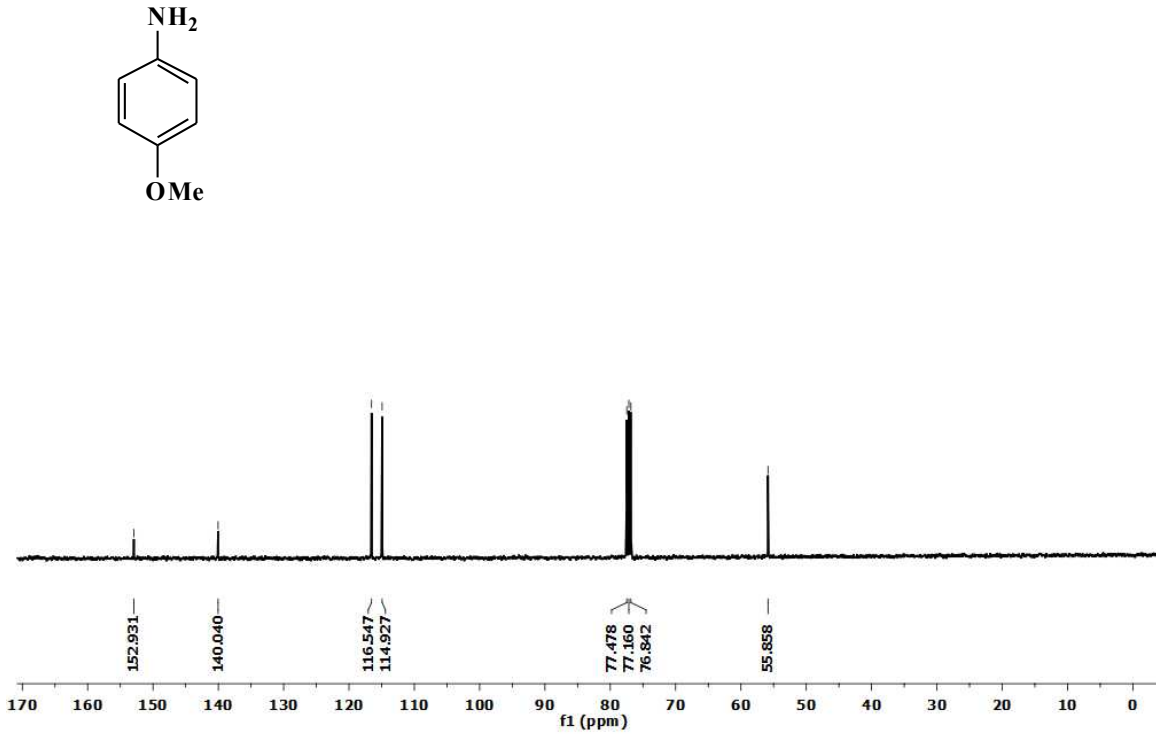


Fig. S11: ^{1}H NMR spectrum ($CDCl_3$) of 4-Chloroaniline.

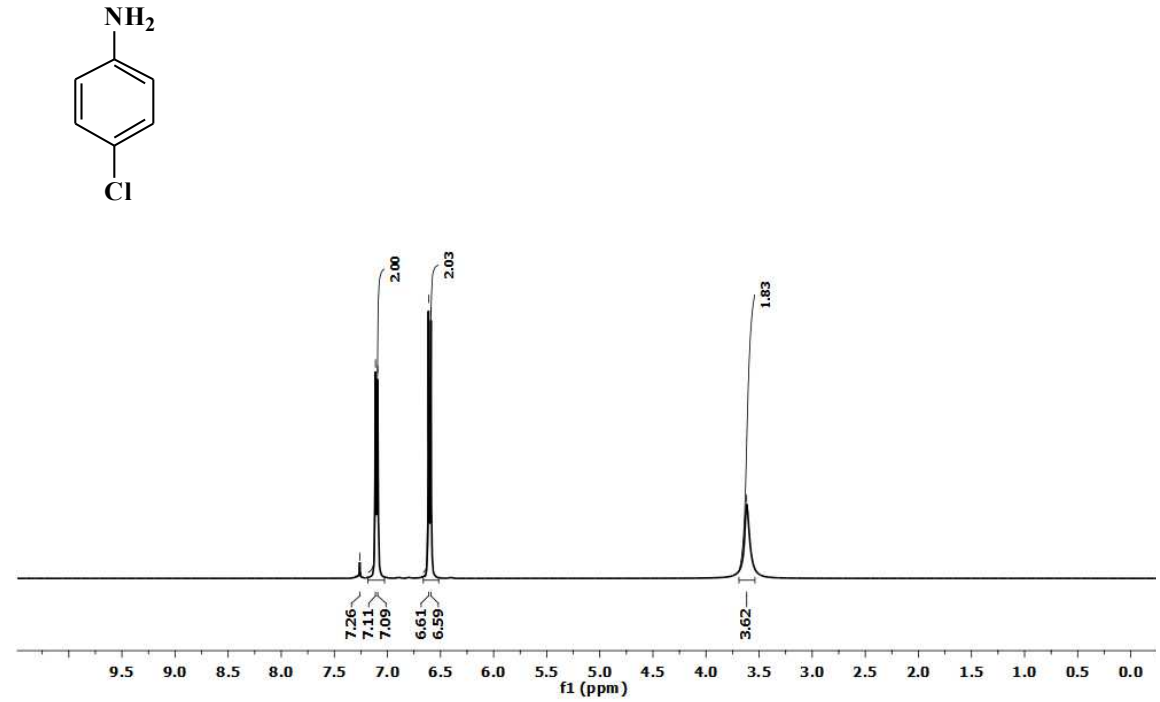


Fig. S12: The ^{13}C NMR spectrum ($CDCl_3$) of 4-Chloroaniline.

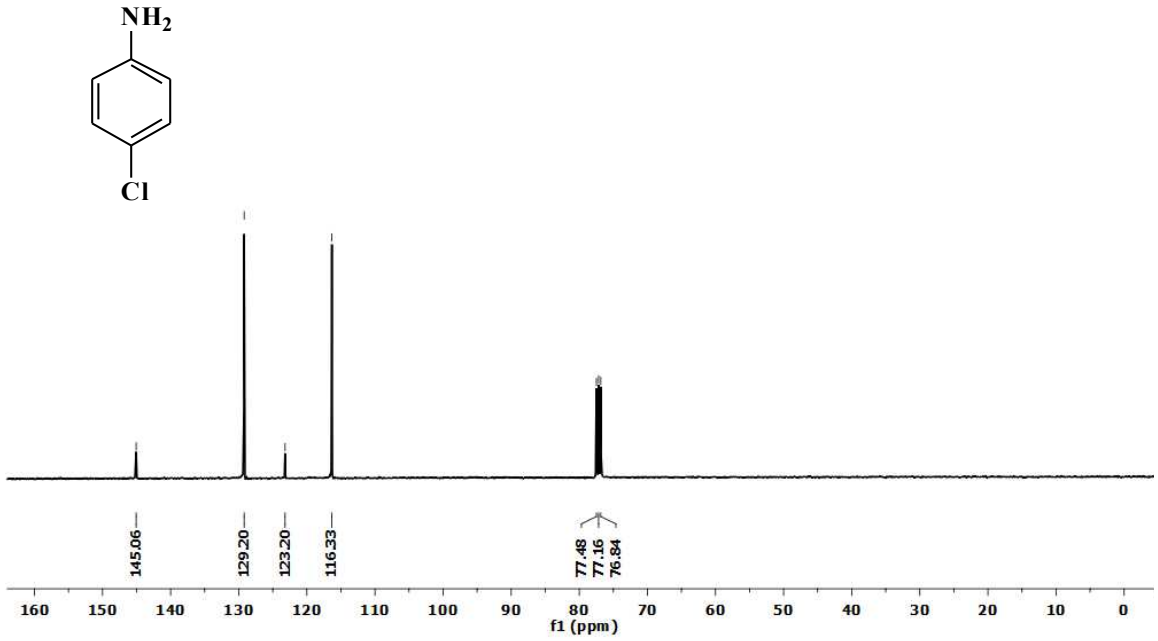


Fig. S13: The ^{1}H NMR spectrum ($CDCl_3$) of 4-Bromoaniline.

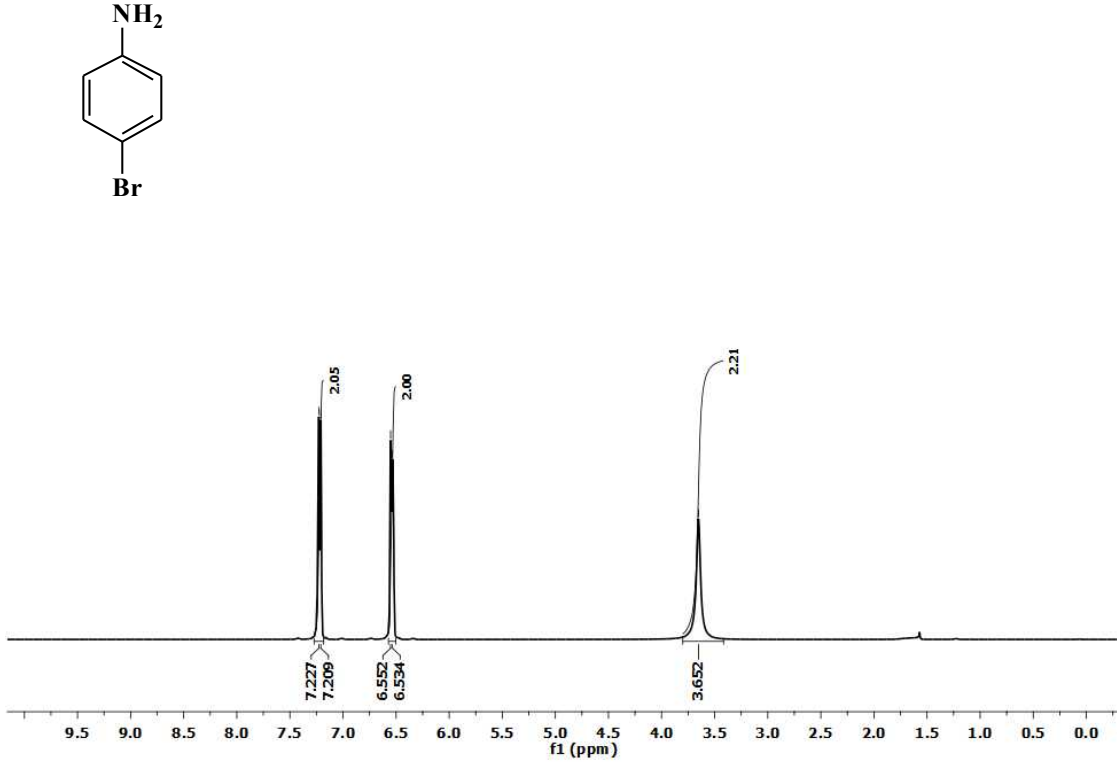


Fig. S14: The ^{13}C NMR spectrum ($CDCl_3$) of 4-Bromoaniline.

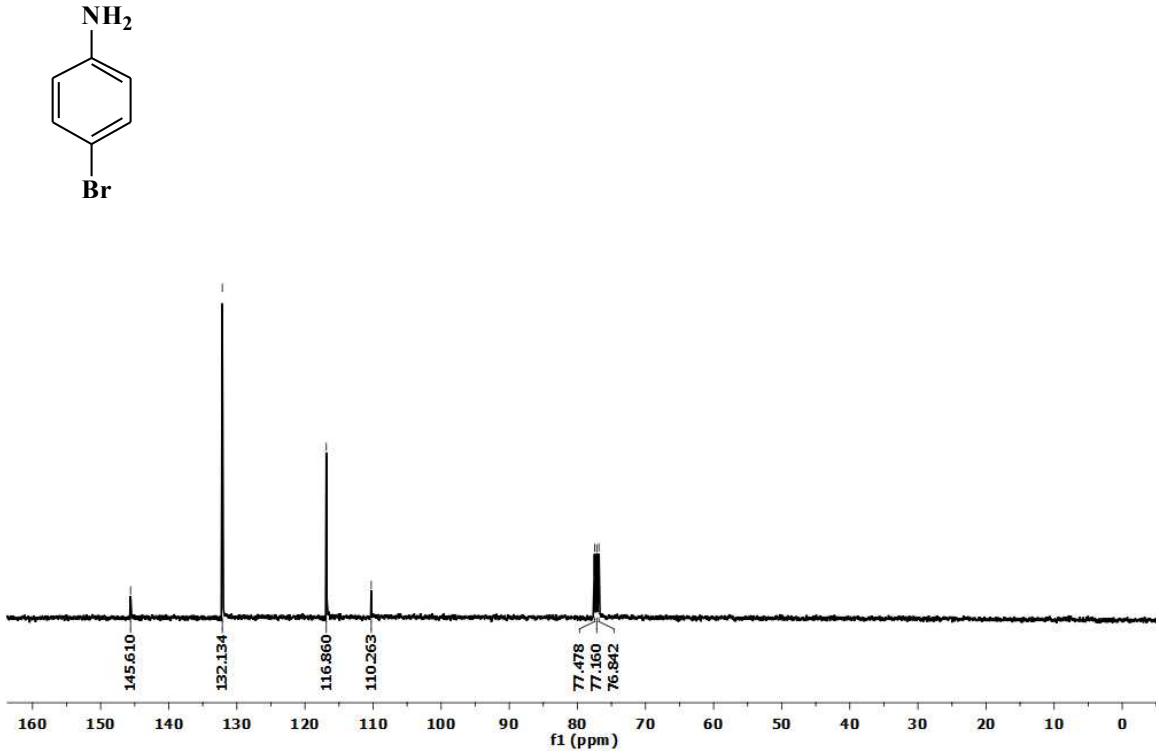


Fig. S15: The ^{1}H NMR spectrum ($CDCl_3$) of 4-Iodoaniline.

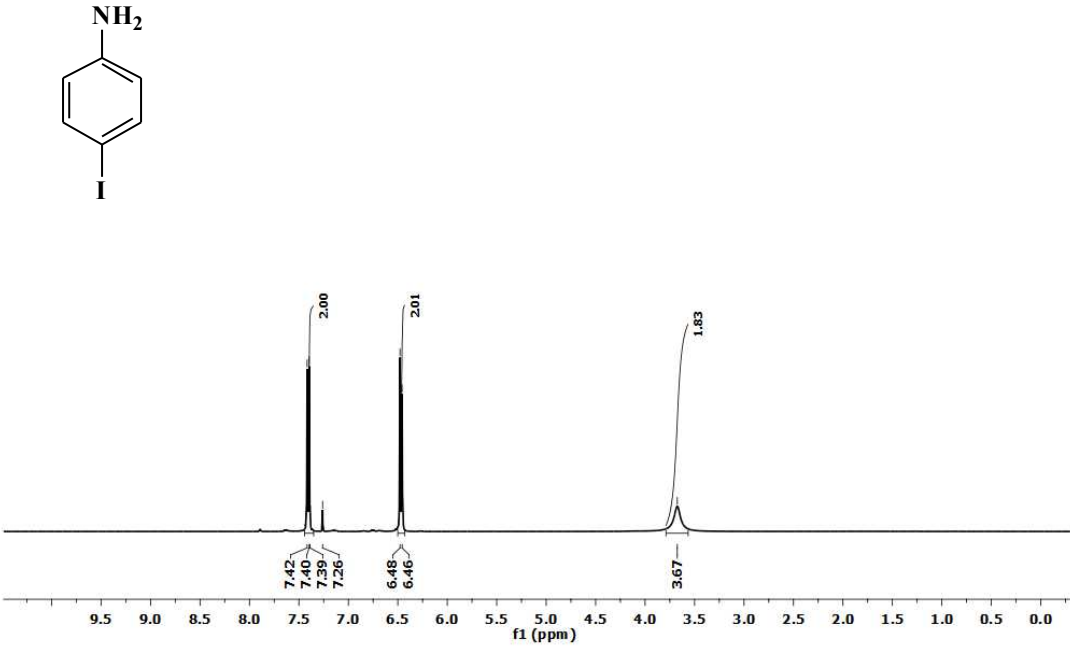


Fig. S16: The ^{13}C NMR spectrum ($CDCl_3$) of 4-Iodoaniline.

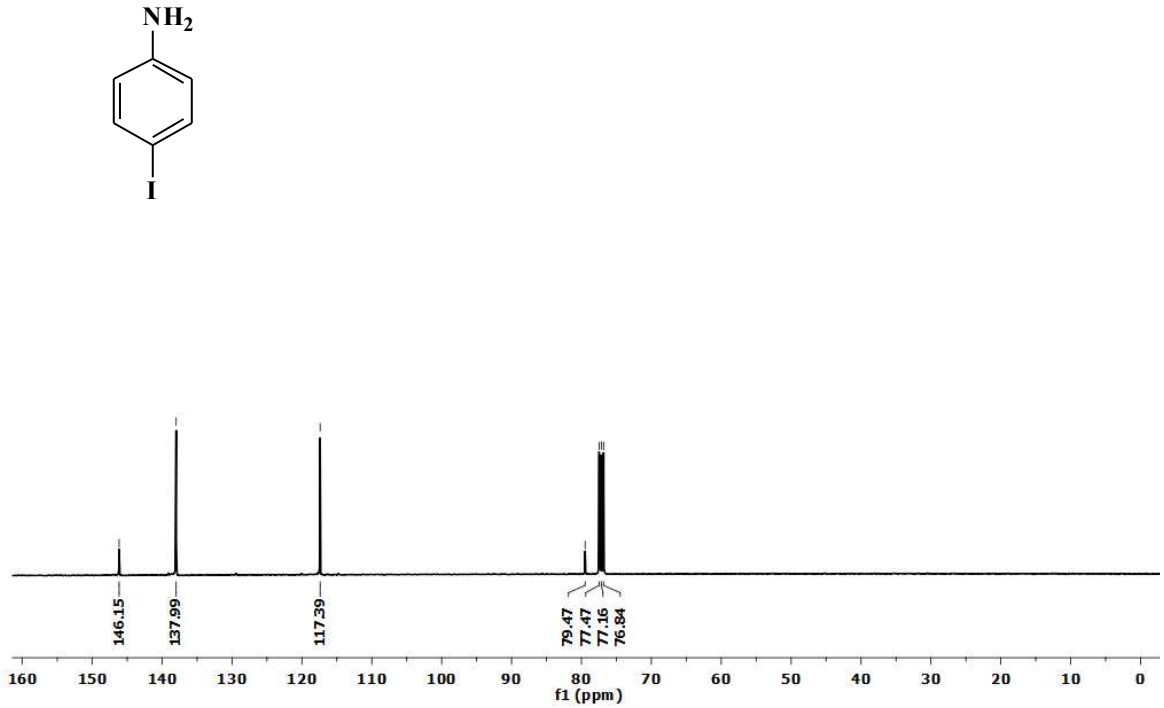


Fig. S17: The ^{1}H NMR spectrum ($CDCl_3$) of 4-Aminoaniline.

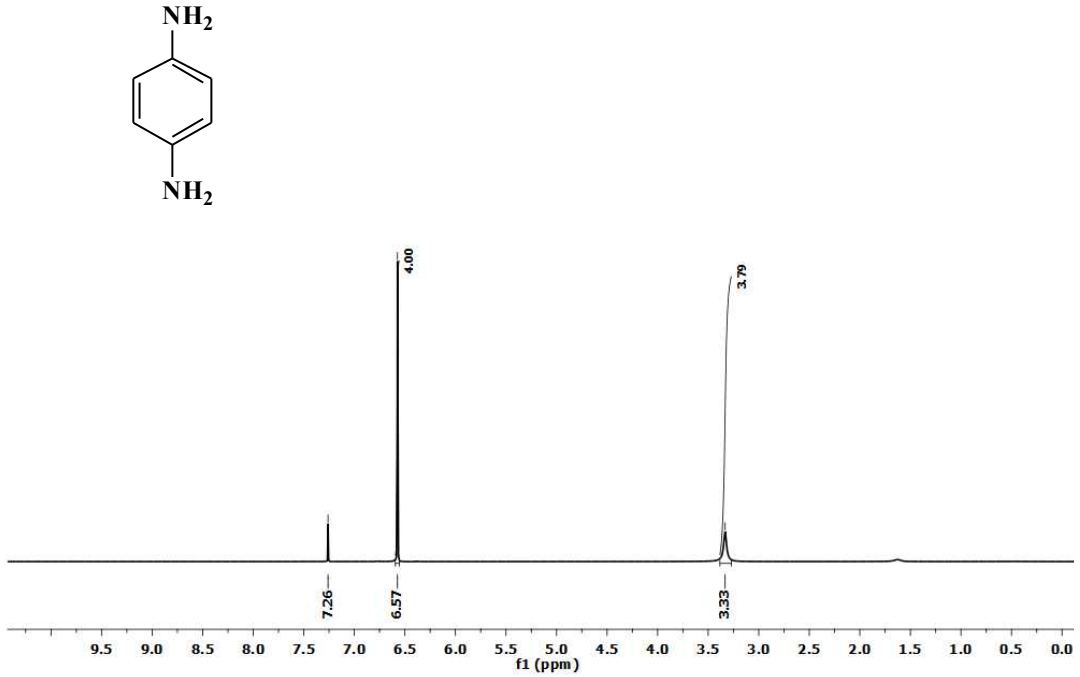


Fig. S18: The ^{13}C NMR spectrum ($CDCl_3$) of 4-Aminoaniline.

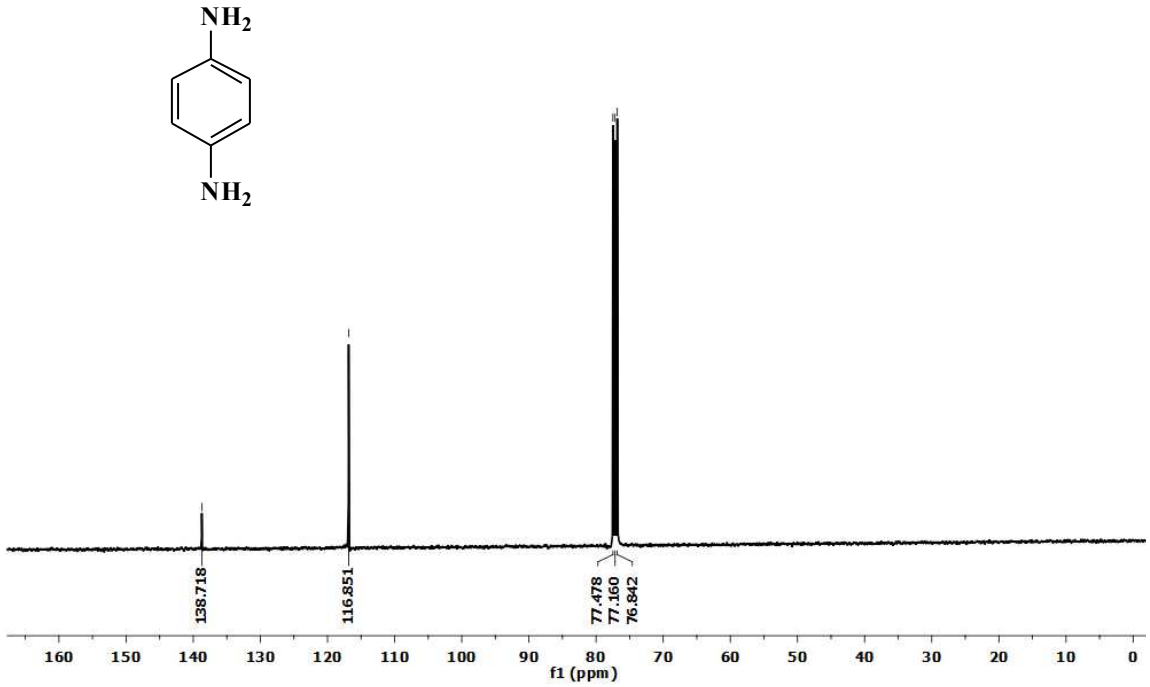


Fig. S19: The ^{1}H NMR spectrum ($CDCl_3$) of 3-Chloroaniline.

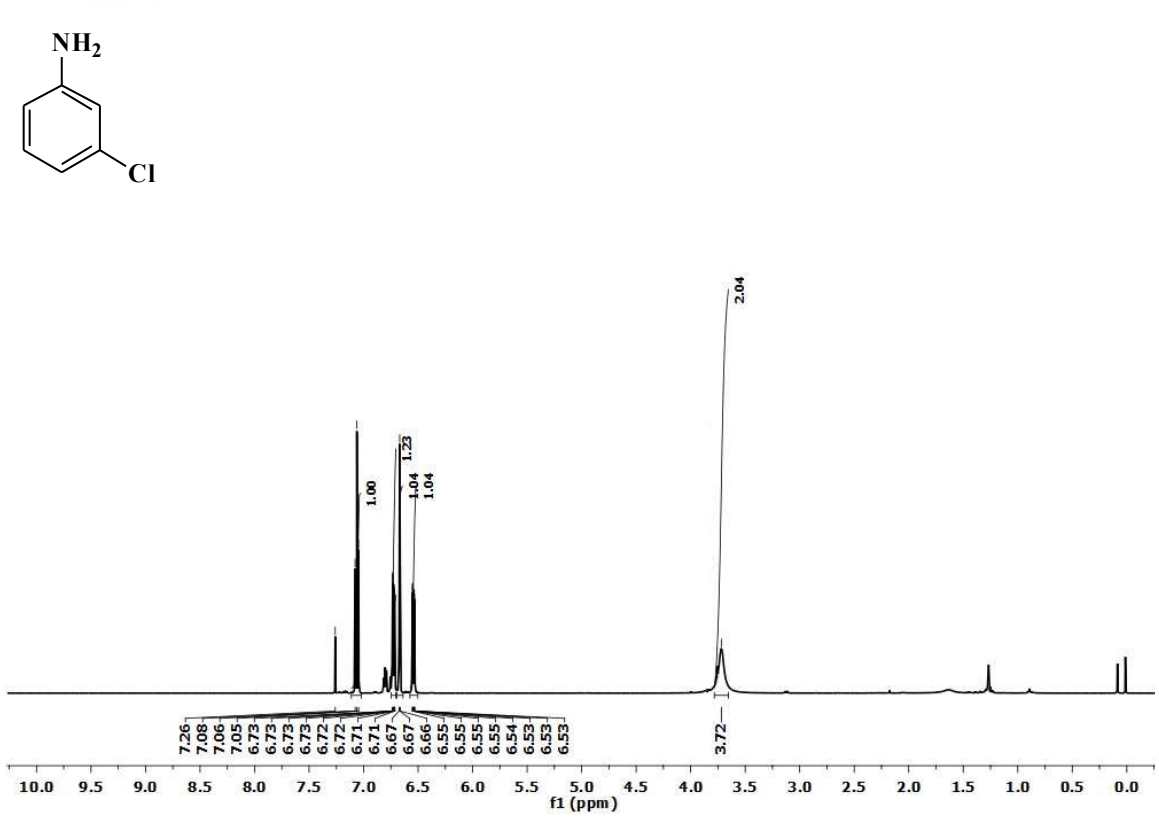


Fig. S20: The ^{13}C NMR spectrum ($CDCl_3$) of 3-Chloroaniline.

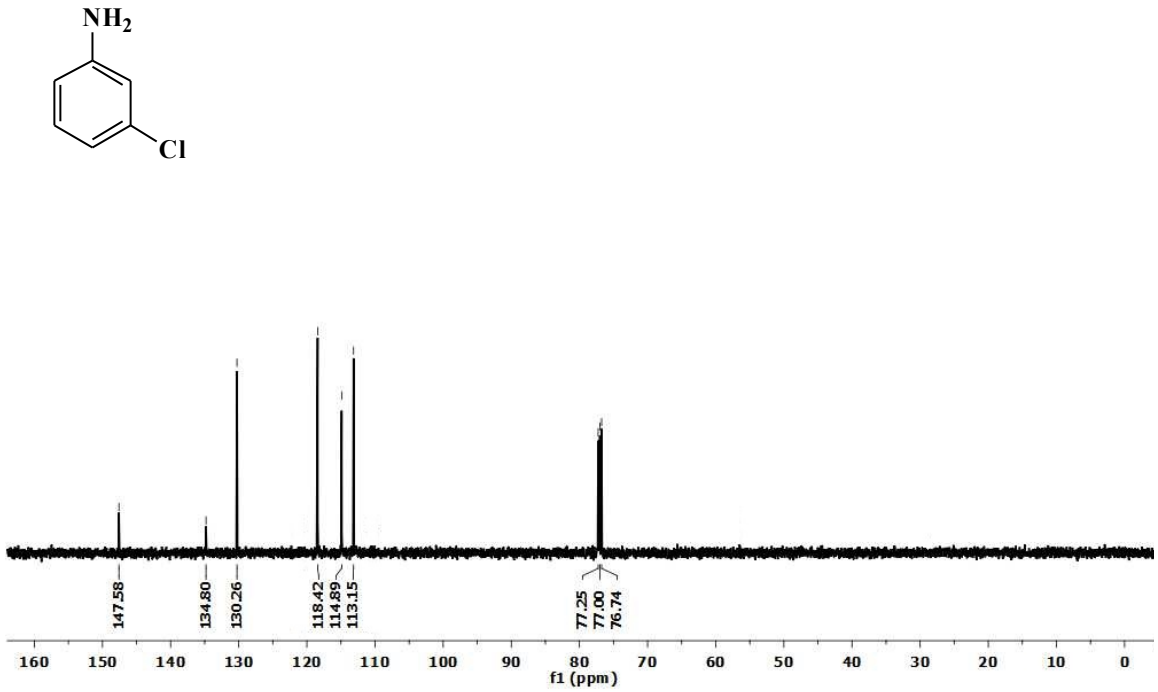


Fig. S21: The ^{1}H NMR spectrum ($CDCl_3$) of 3-Bromoaniline.

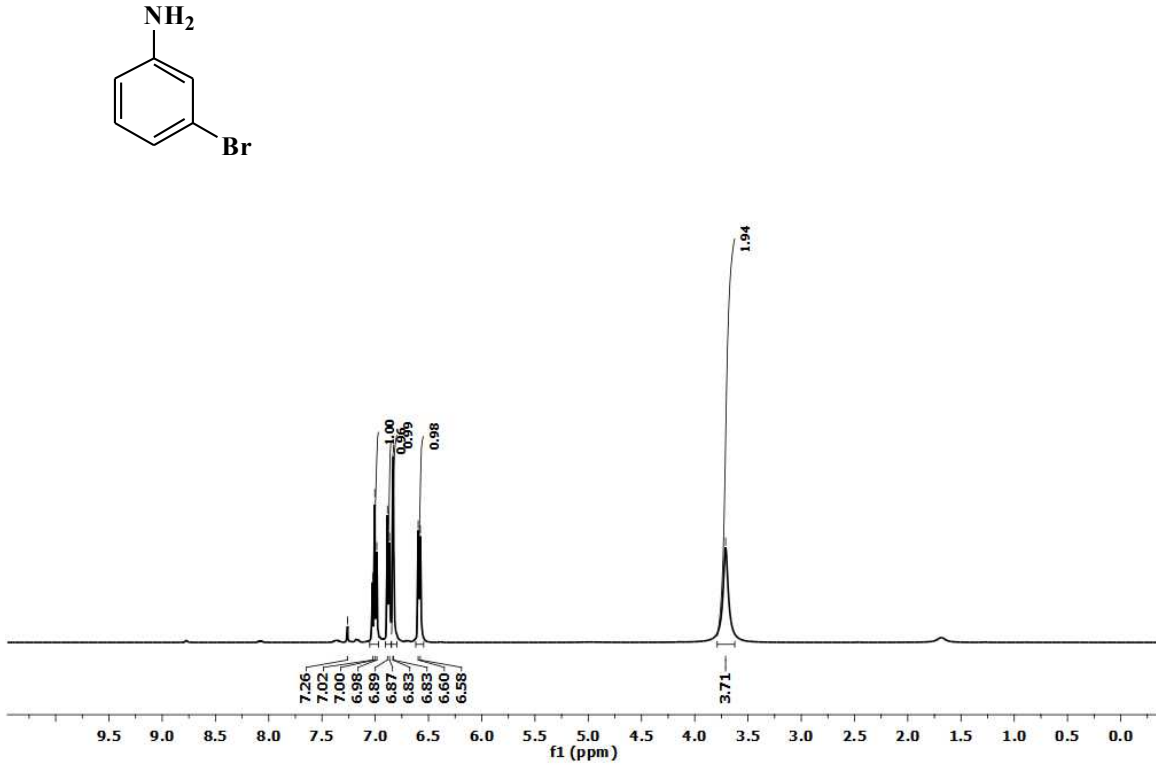


Fig. S22: The ^{13}C NMR spectrum ($CDCl_3$) of 3-Bromoaniline.

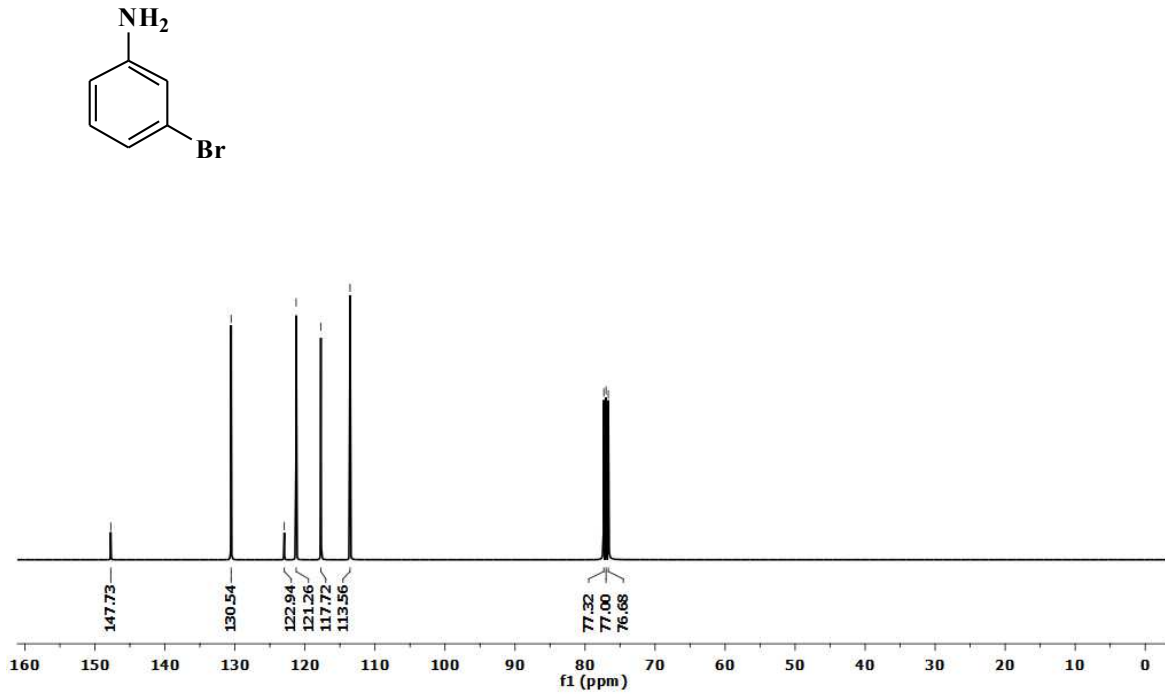


Fig. S23: The ^{1}H NMR spectrum ($CDCl_3$) of 3-Iodoaniline.

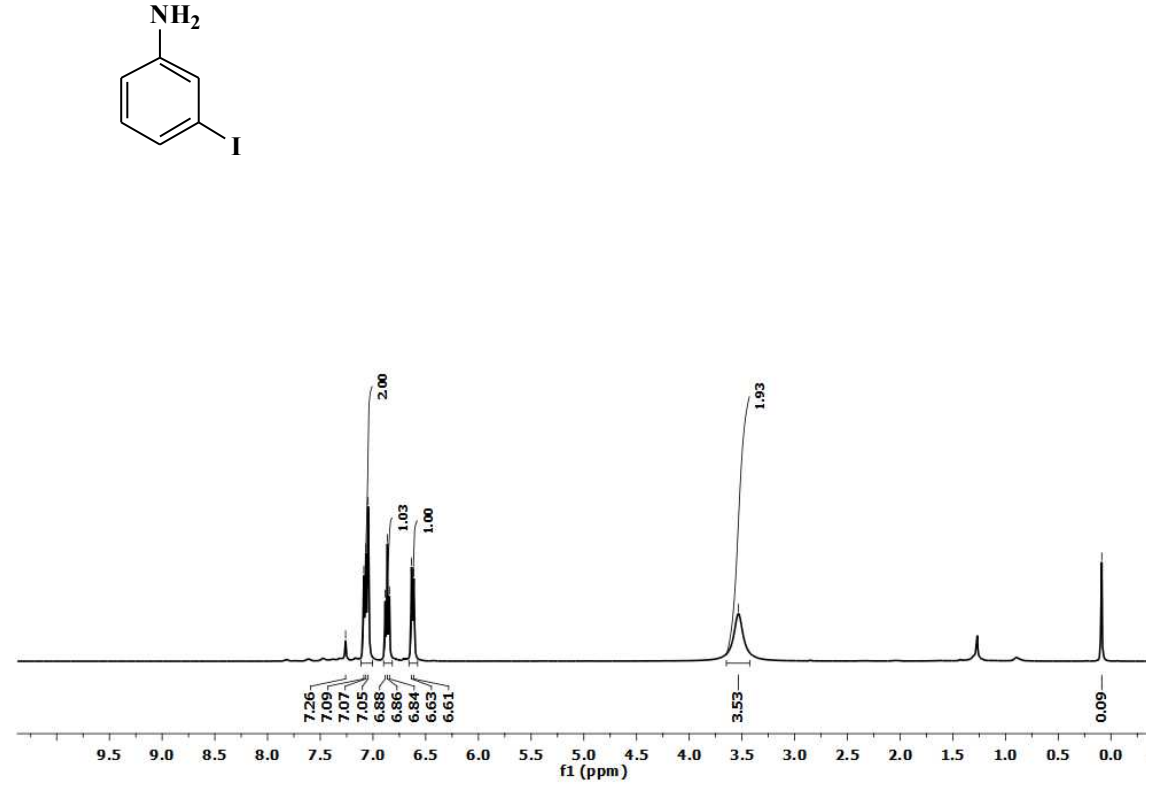


Fig. S24: The ^{13}C NMR spectrum ($CDCl_3$) of 3-Iodoaniline.

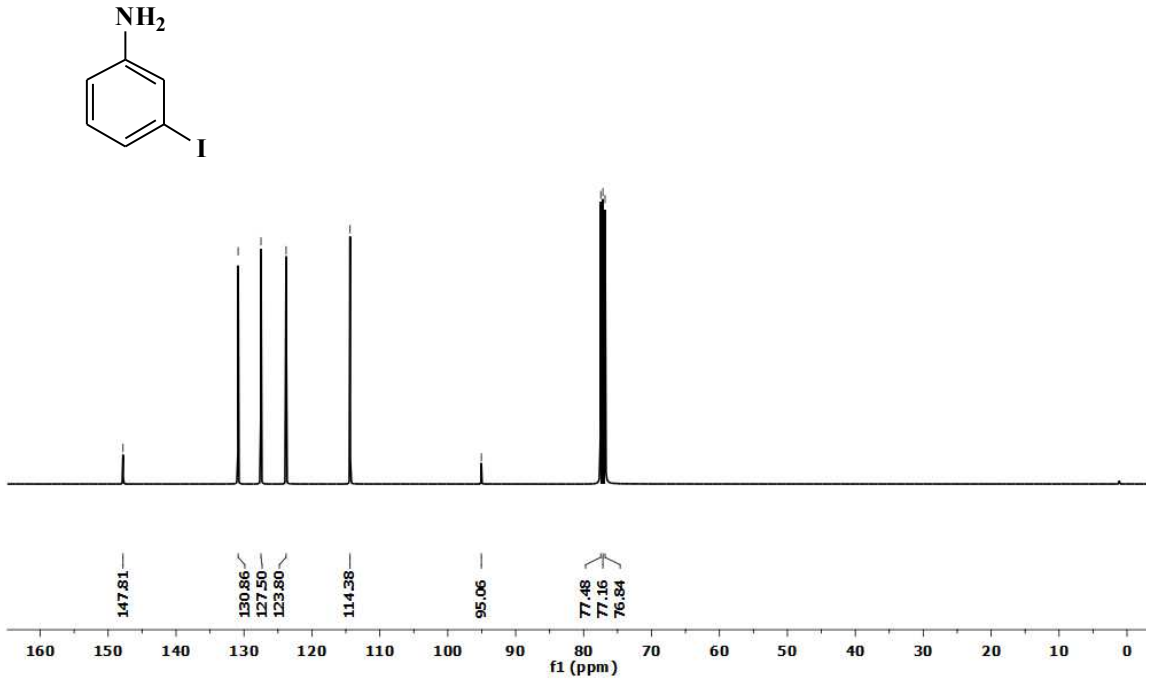


Fig. S25: The ^{1}H NMR spectrum ($CDCl_3$) of *m*-Phenylenediamine.

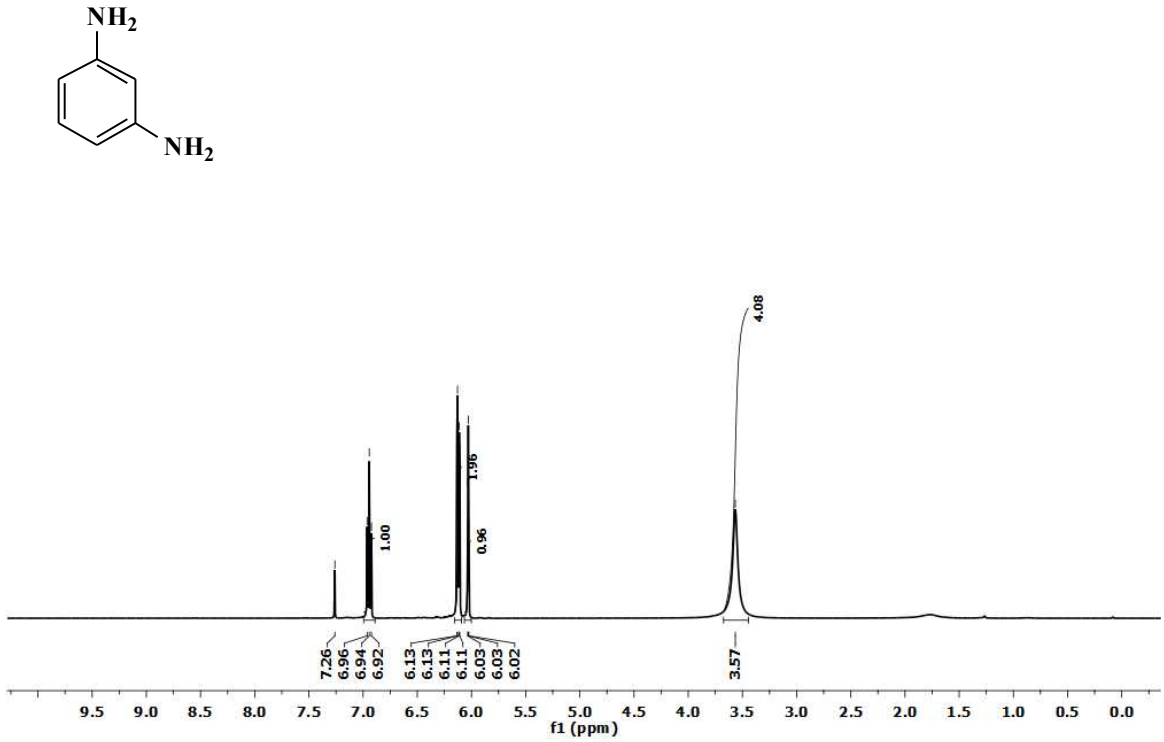


Fig. S26: The ^{13}C NMR spectrum ($CDCl_3$) of *m*-Phenylenediamine.

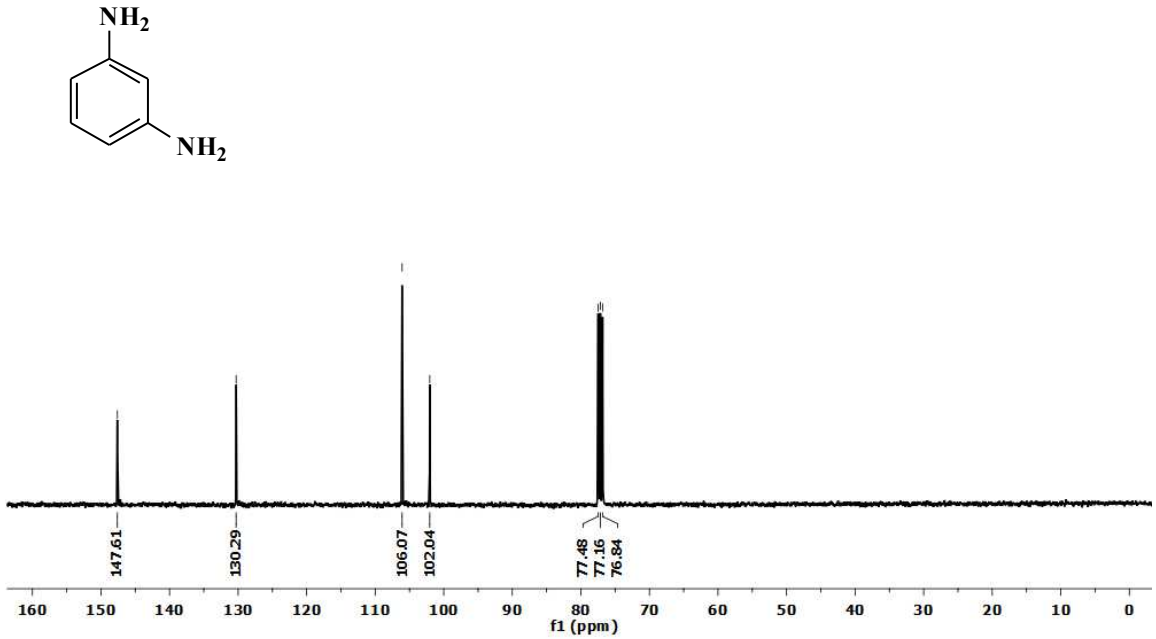


Fig. S27: The ^{1}H NMR spectrum ($CDCl_3$) of 3-Aminobenzonitrile.

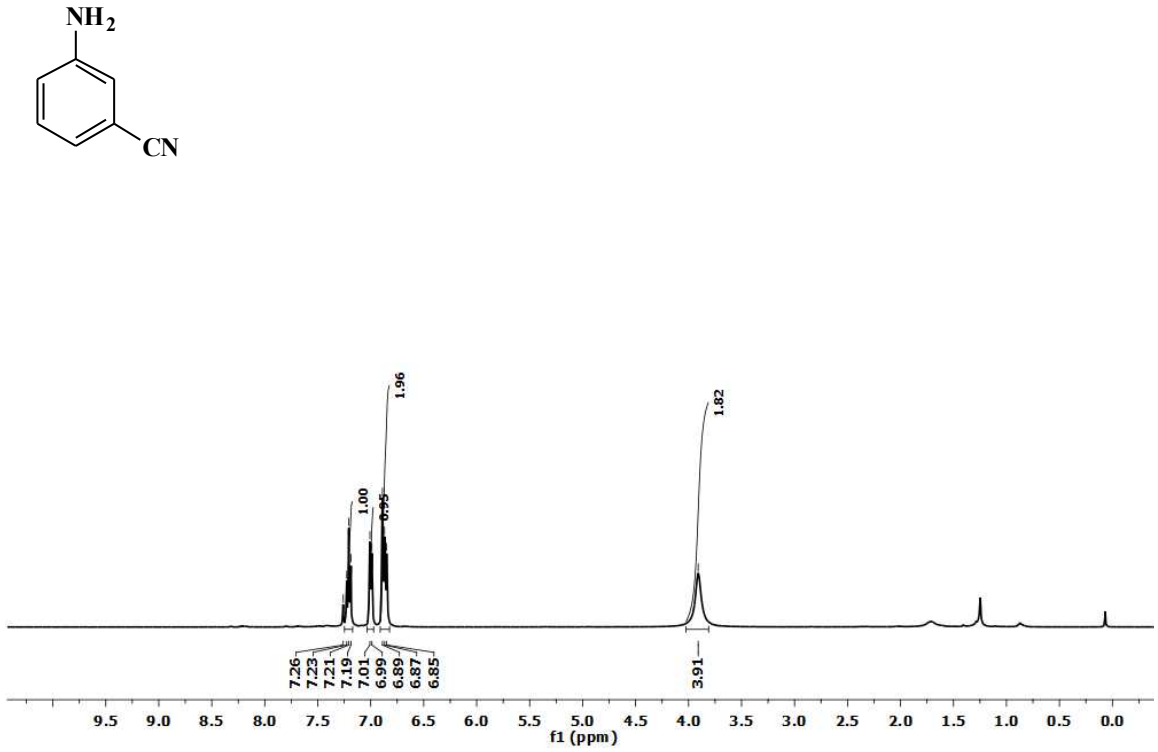


Fig. S28: The ^{13}C NMR spectrum ($CDCl_3$) of 3-Aminobenzonitrile.

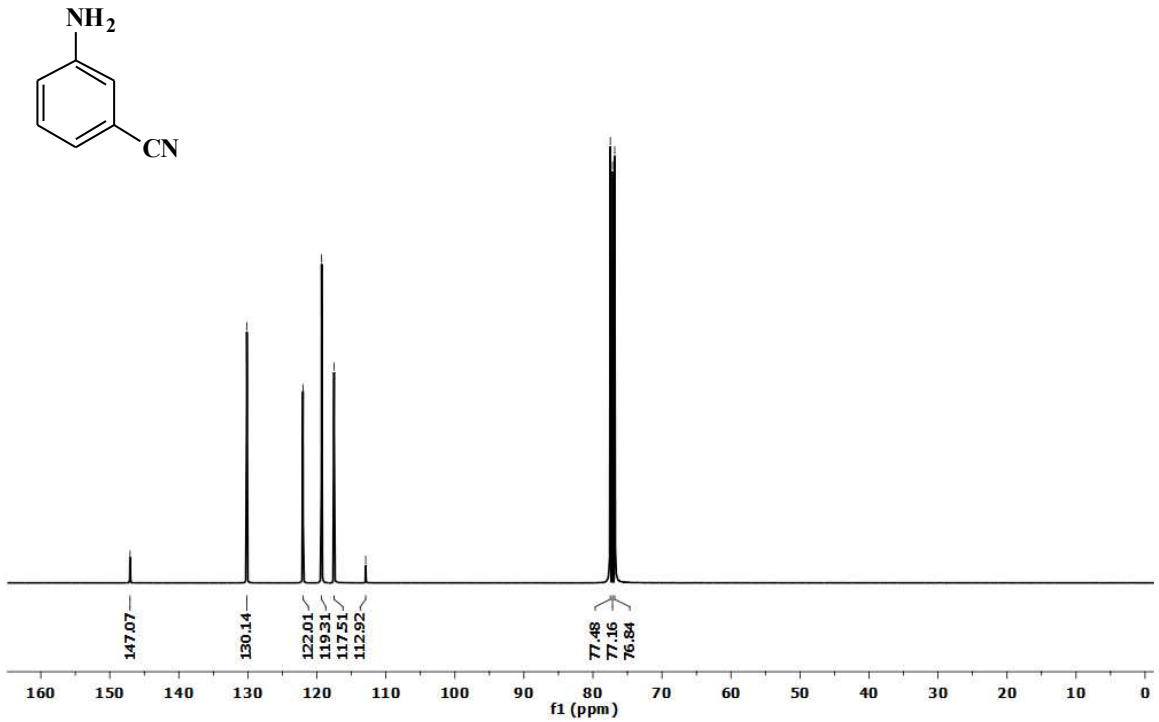
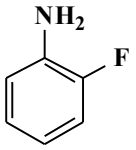


Fig. S29: The ^{1}H NMR spectrum ($CDCl_3$) of 2-Fluoroaniline.



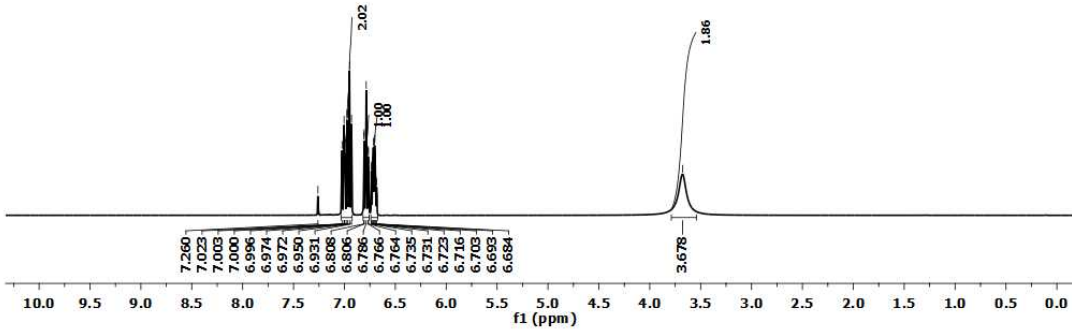


Fig. S30: The ^{13}C NMR spectrum ($CDCl_3$) of 2-Fluoroaniline.

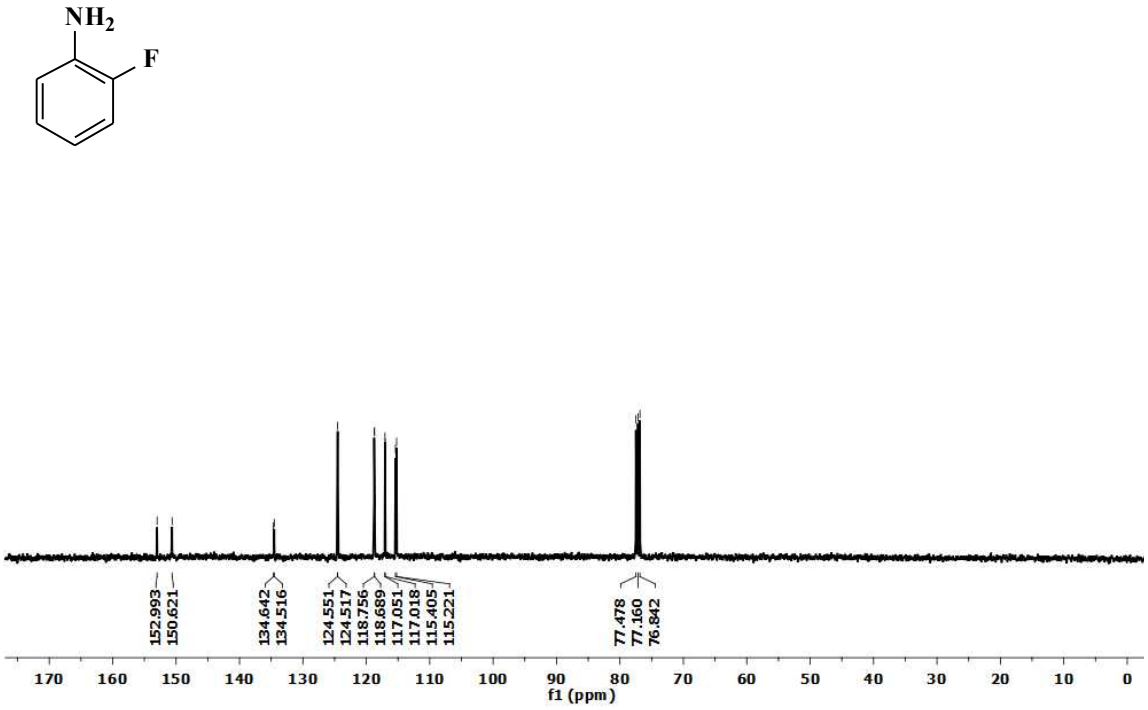


Fig. S31: The ^{1}H NMR spectrum ($CDCl_3$) of 2-Bromoaniline.

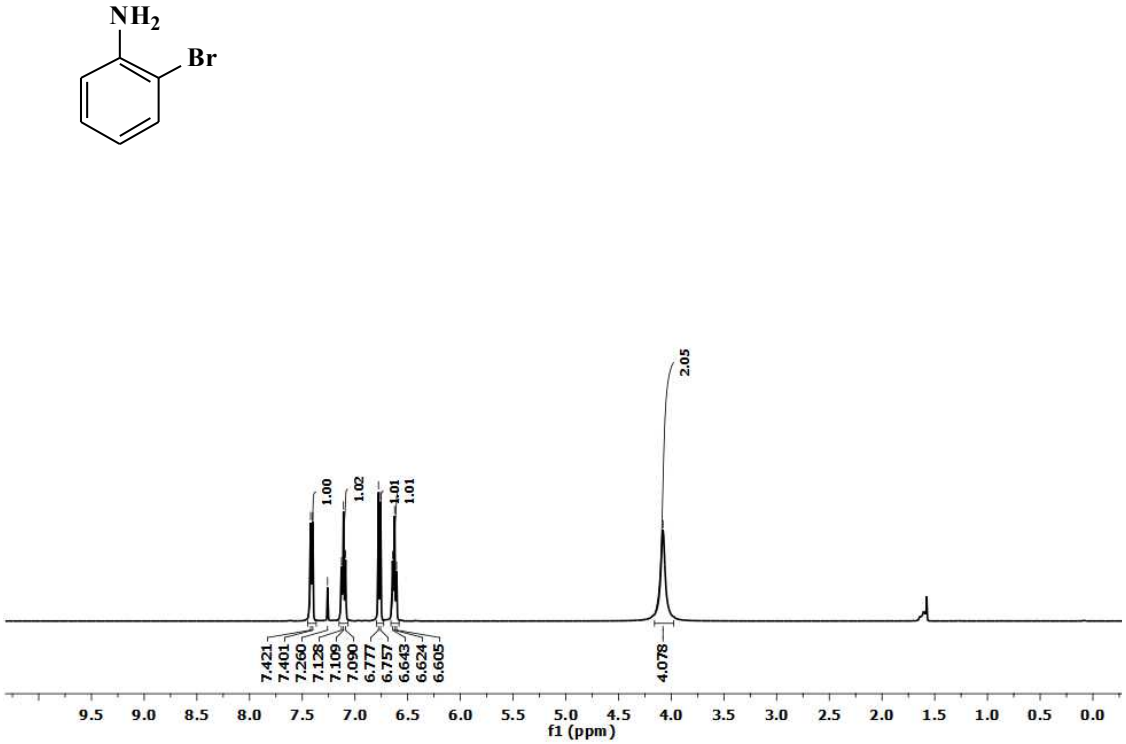


Fig. S32: The ^{13}C NMR spectrum ($CDCl_3$) of 2-Bromoaniline.

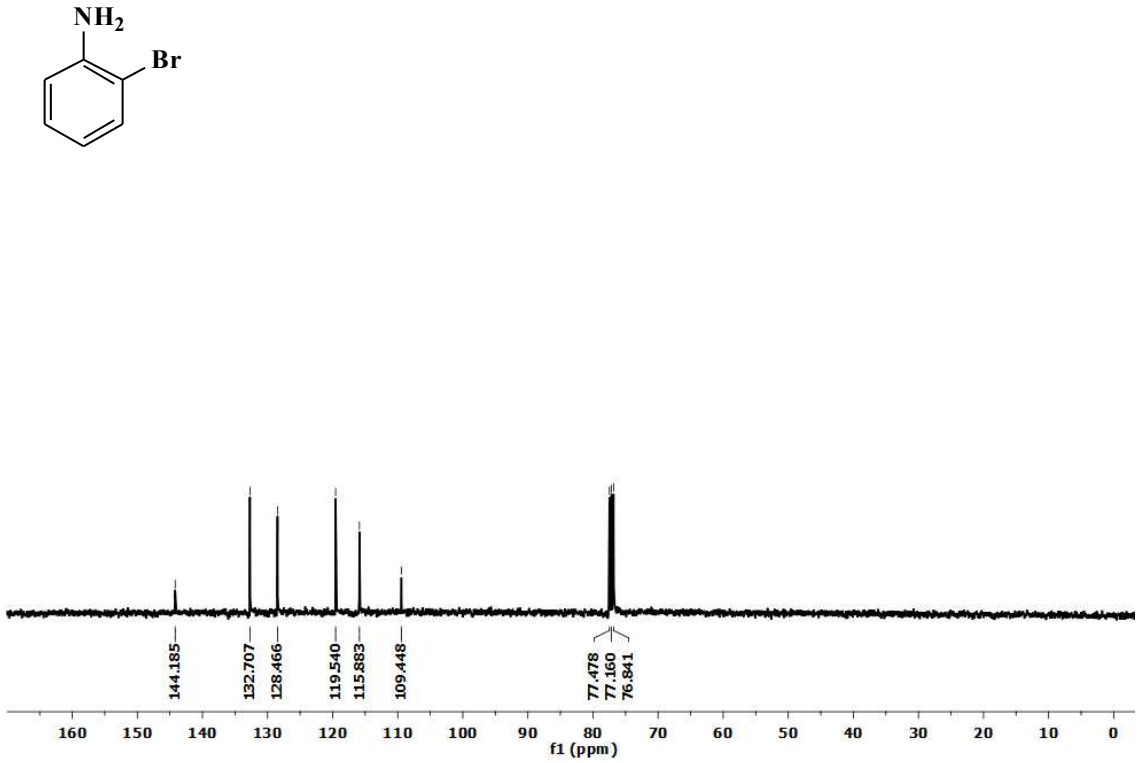


Fig. S33: The ^{1}H NMR spectrum ($CDCl_3$) of 3-Amino benzylalcohol.

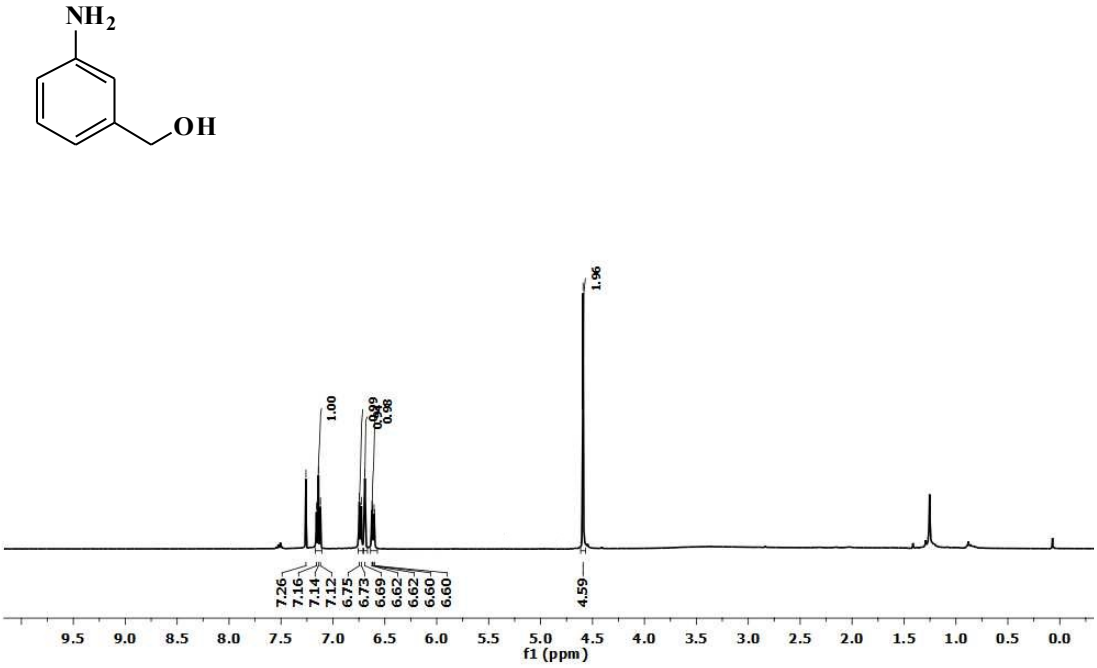


Fig. S34: The ^{13}C NMR spectrum ($CDCl_3$) of 3-Amino benzylalcohol.

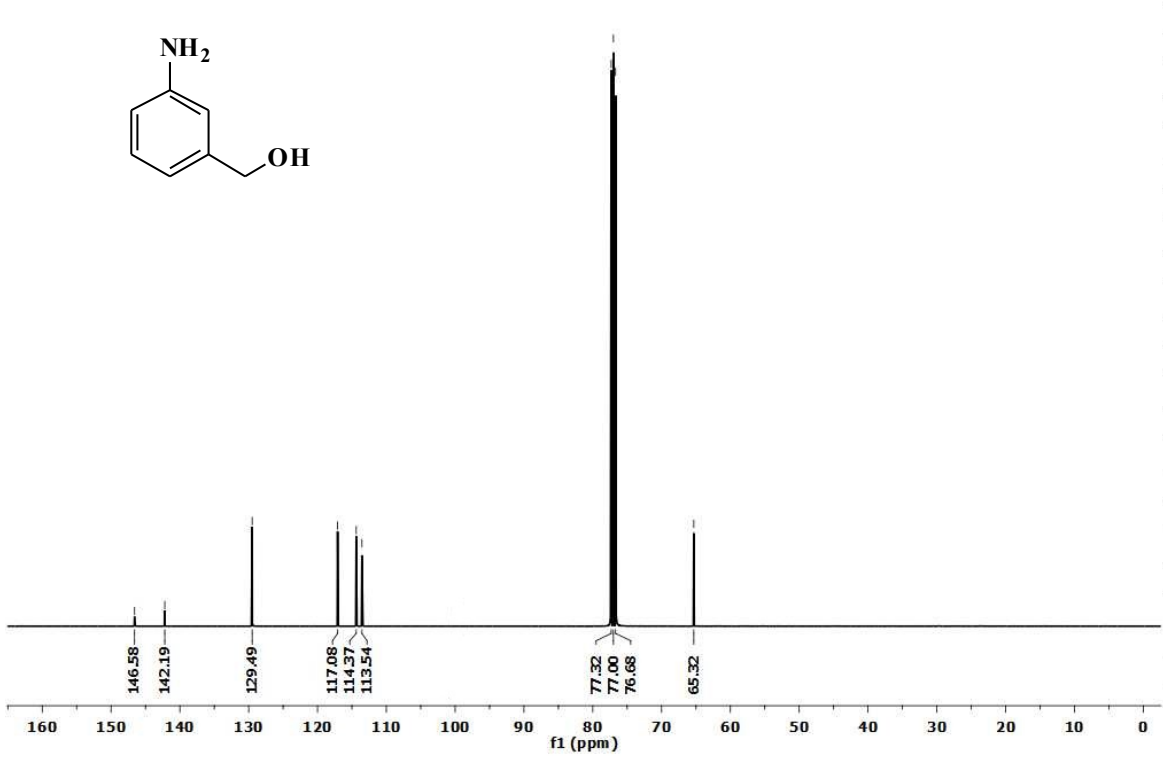


Fig. S35: The ^{1}H NMR spectrum ($CDCl_3$) of 1-Aminonaphthalene.

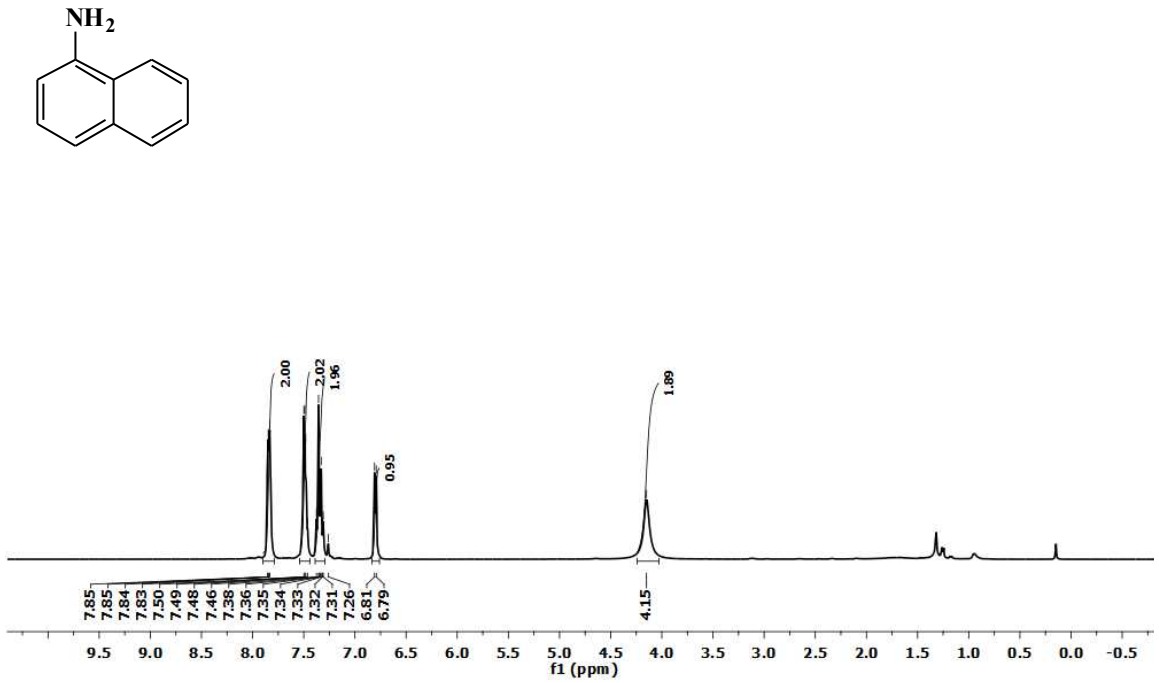


Fig. S36: The ^{13}C NMR spectrum ($CDCl_3$) of 1-Aminonaphthalene.

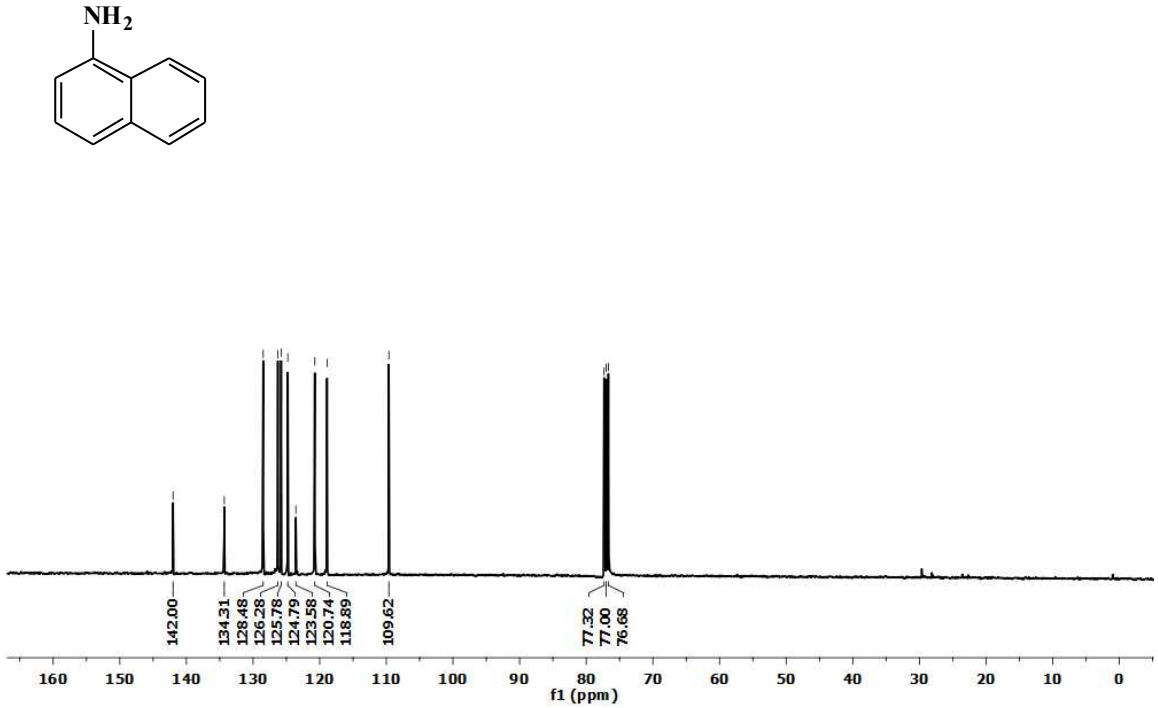


Fig. S37: The ^{1}H NMR spectrum ($CDCl_3$) of 8-Aminoquinoline.

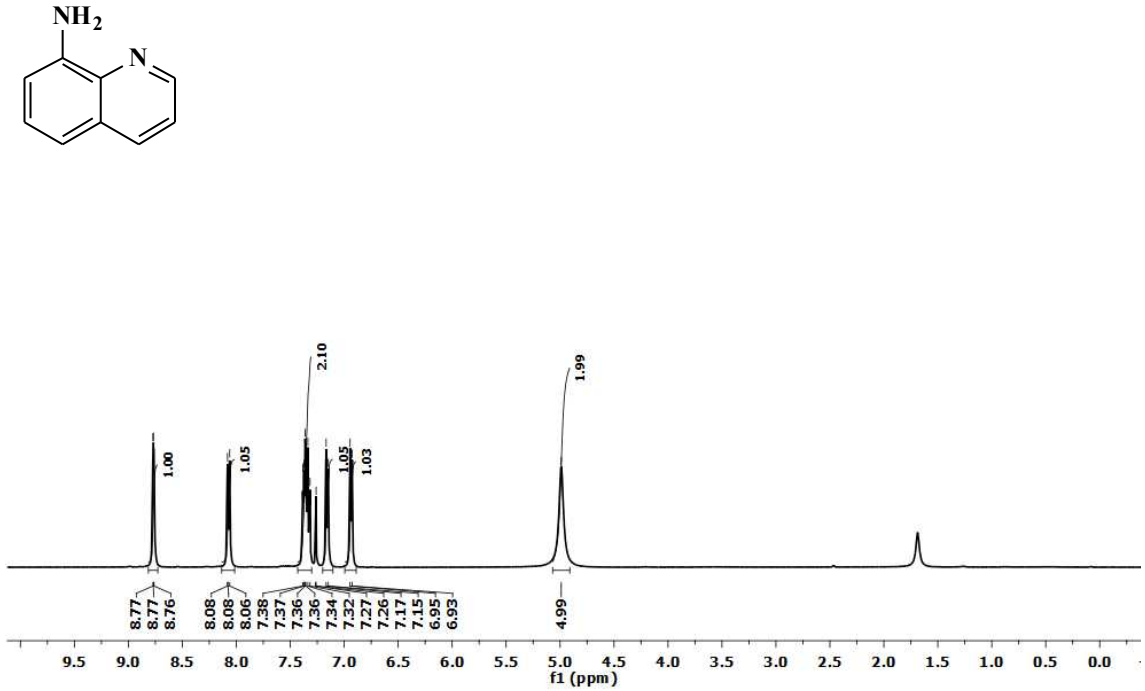


Fig. S38: The ^{13}C NMR spectrum ($CDCl_3$) of 8-Aminoquinoline.

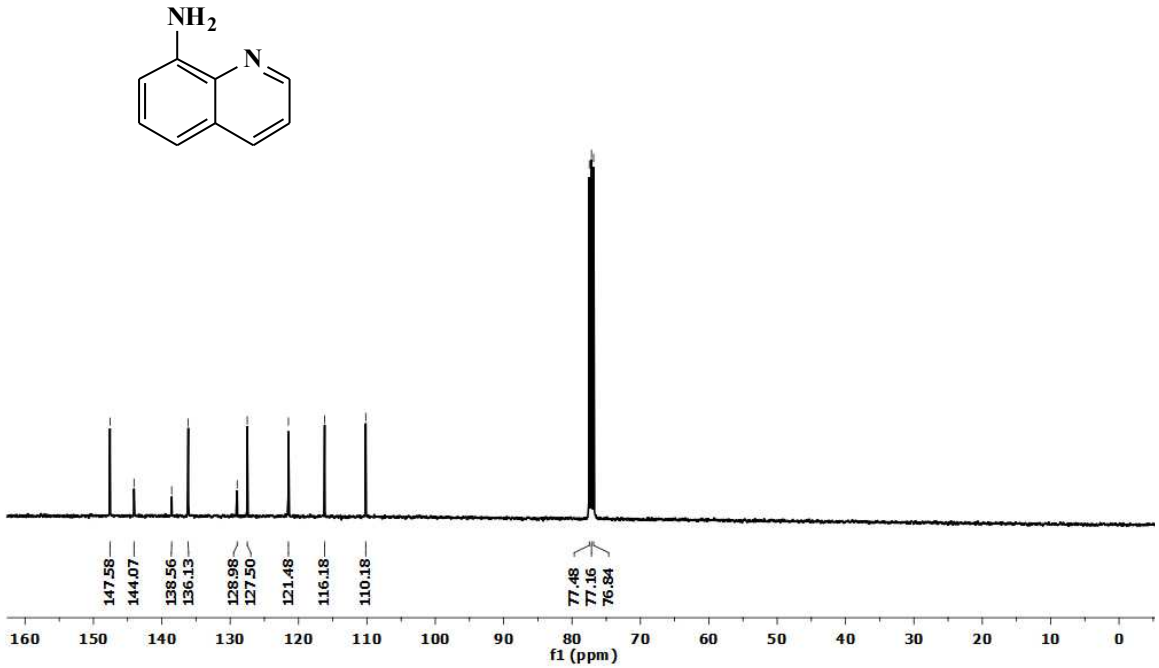


Fig. S39: The ^{1}H NMR spectrum ($CDCl_3$) of 6-Aminoquinoline.

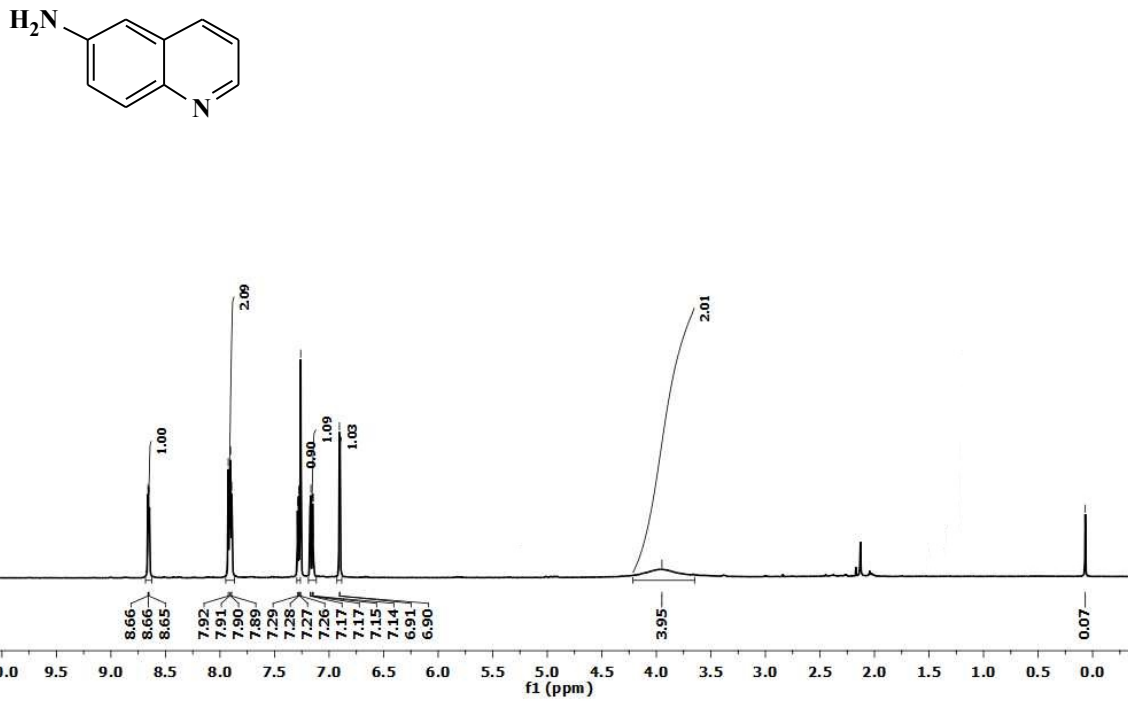


Fig. S40: The ^{13}C NMR spectrum ($CDCl_3$) of 6-Aminoquinoline.

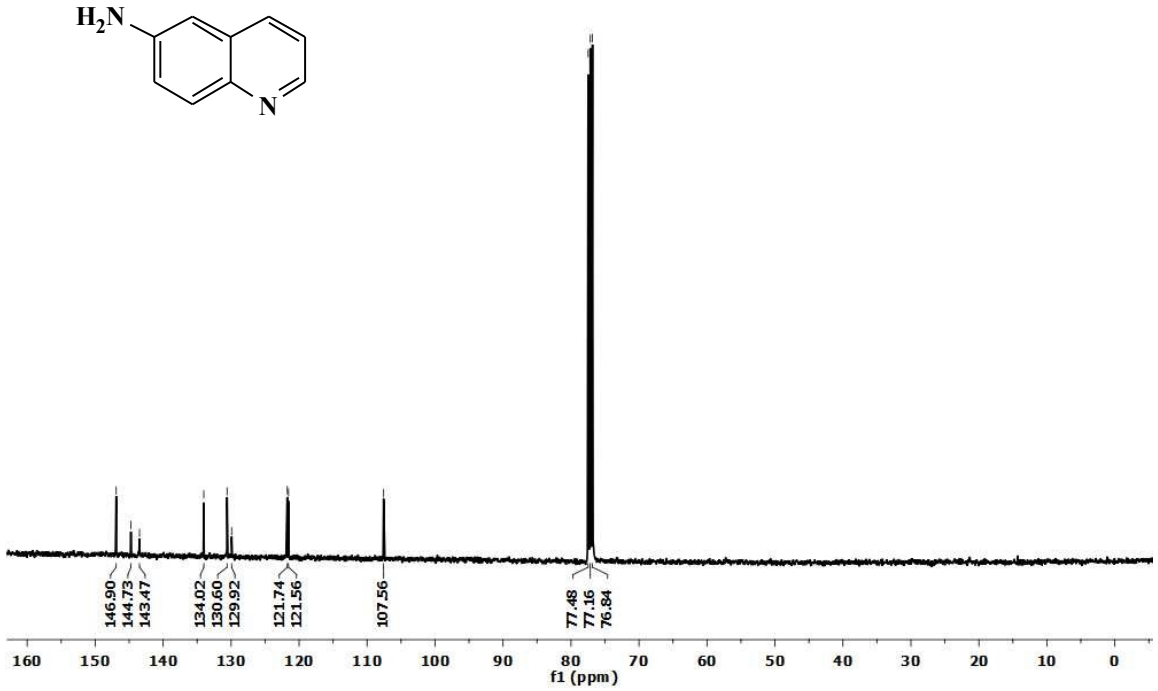


Fig. S41: The ^{1}H NMR spectrum ($CDCl_3$) of 3-Aminostyrene.

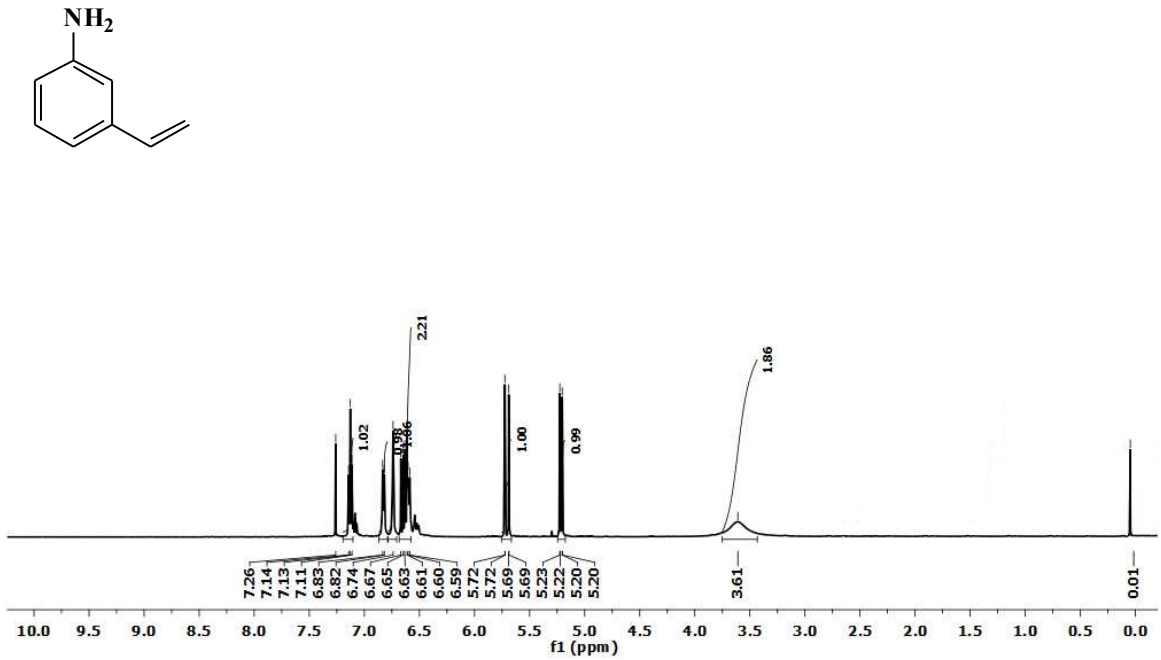


Fig. S42: The ^{13}C NMR spectrum ($CDCl_3$) of 3-Aminostyrene.

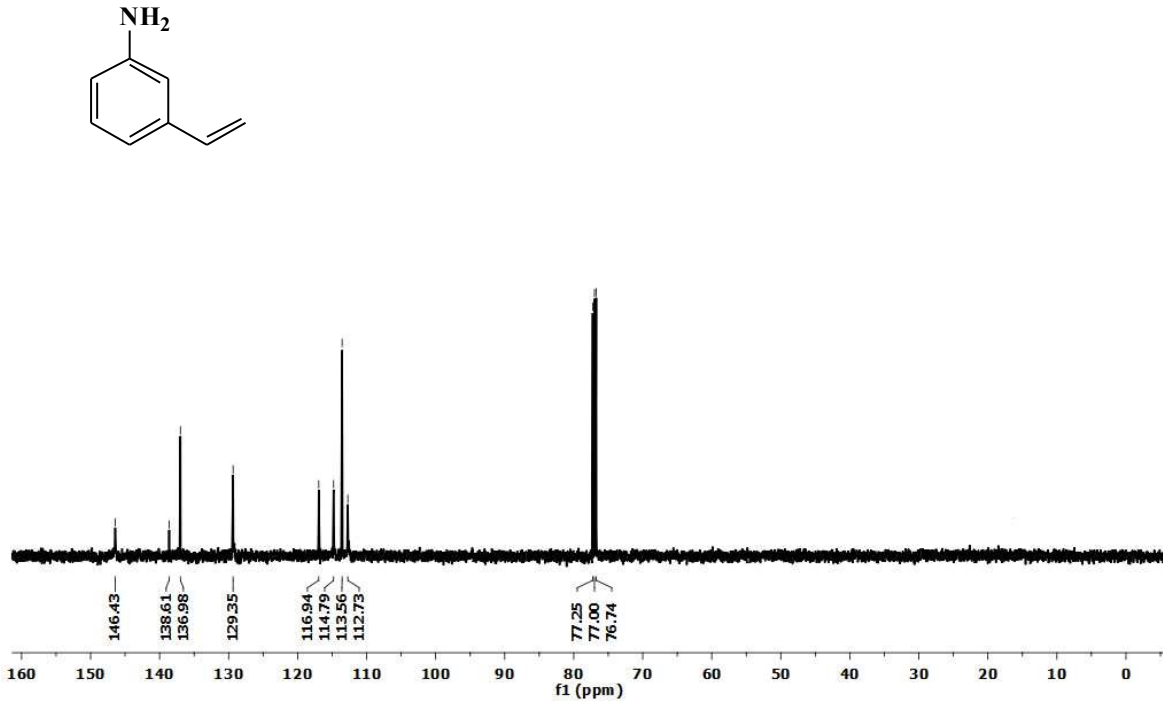


Fig. S43: The ^{1}H NMR spectrum ($CDCl_3$) of 6-Amino-1,4-benzodioxane.

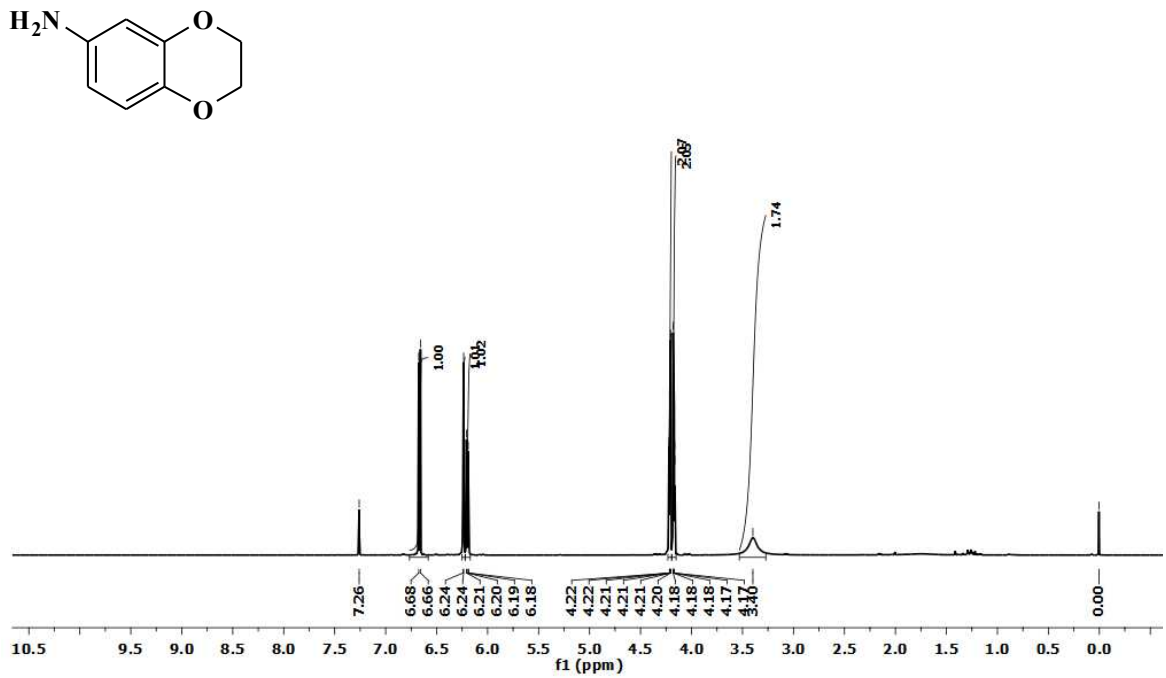


Fig. S44: The ^{13}C NMR spectrum ($CDCl_3$) of 6-Amino-1,4-benzodioxane.

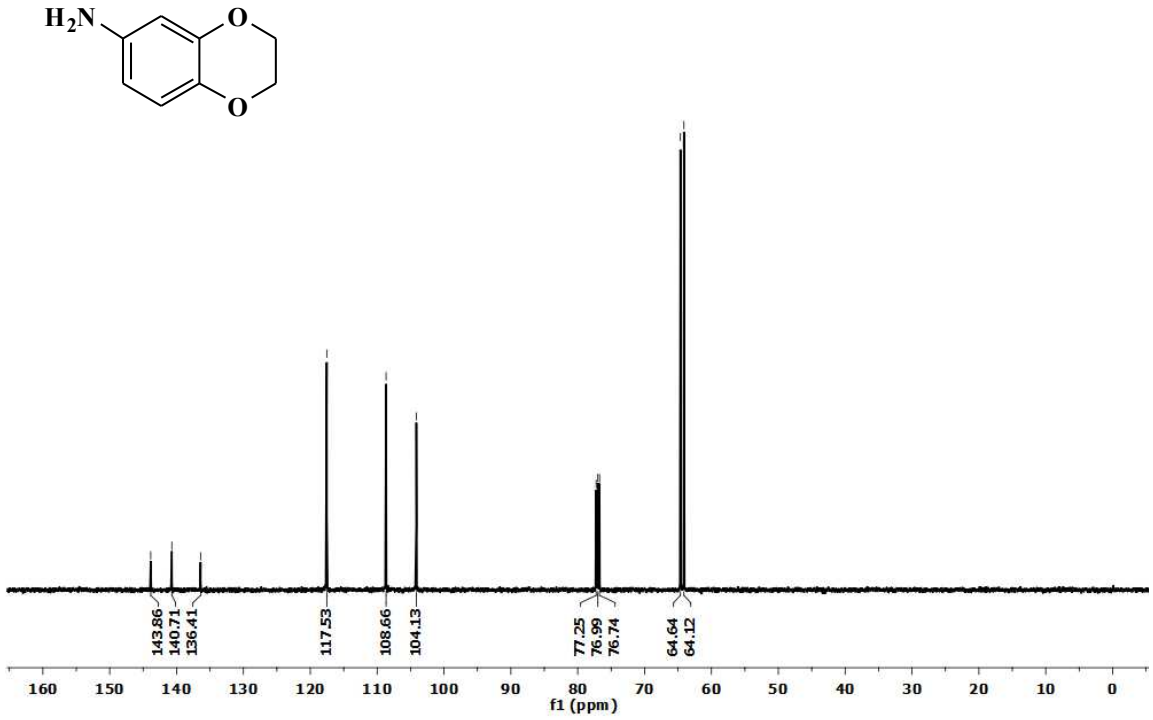


Fig. S45: The stacked ^{1}H NMR spectra ($CDCl_3$) recorded from the reaction mixture of stoichiometric reactions between complex 1 and nitrobenzene as well as $PhSiH_3$ and compared with ^{1}H NMR spectra of all starting reactants.

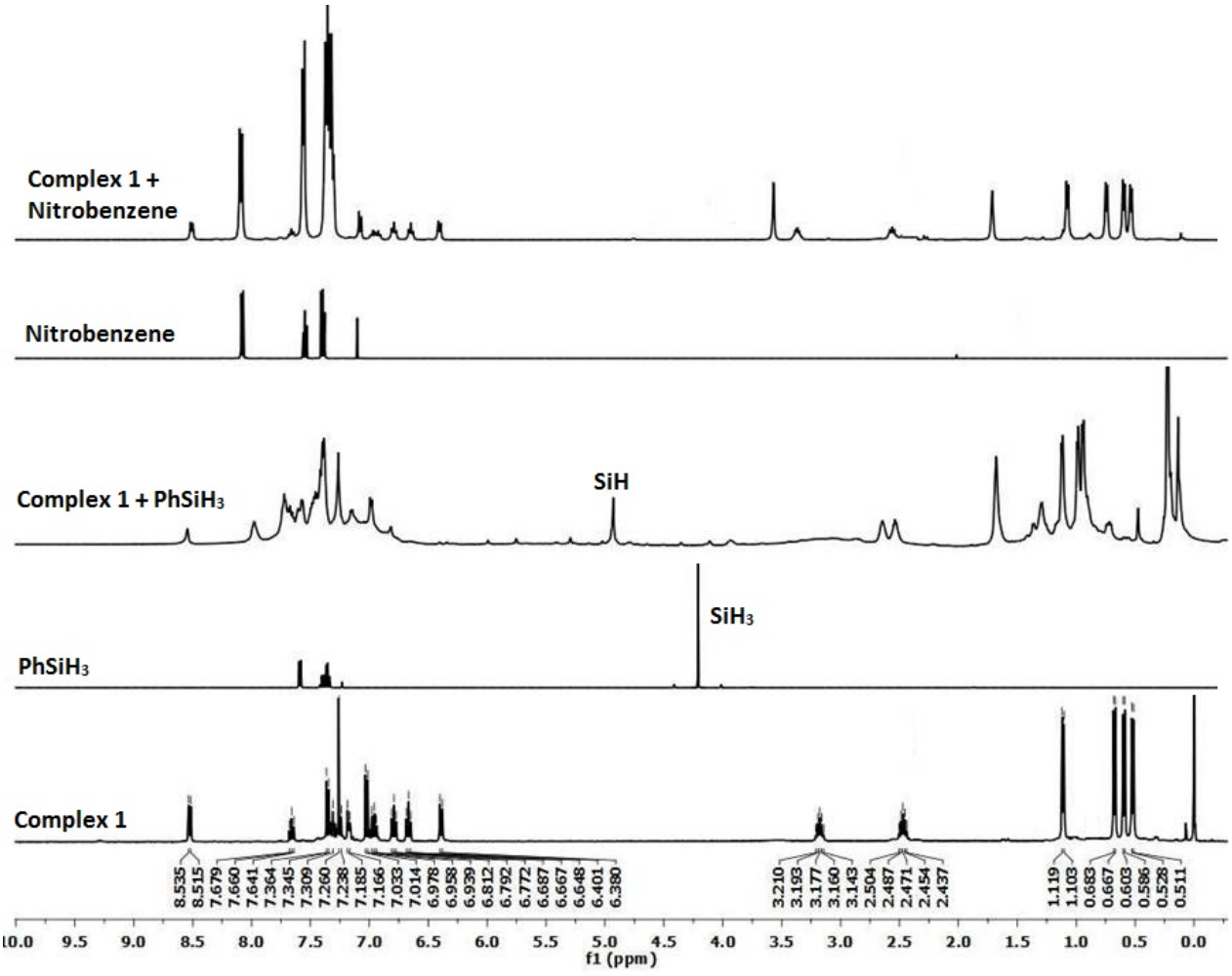


Fig. S46: The ^{13}C NMR spectrum ($CDCl_3$) recorded from the reaction mixture of the stoichiometric reaction between complex 1 and with $PhSiH_3$ (top) in comparison with that recorded for catalyst 1 (bottom).

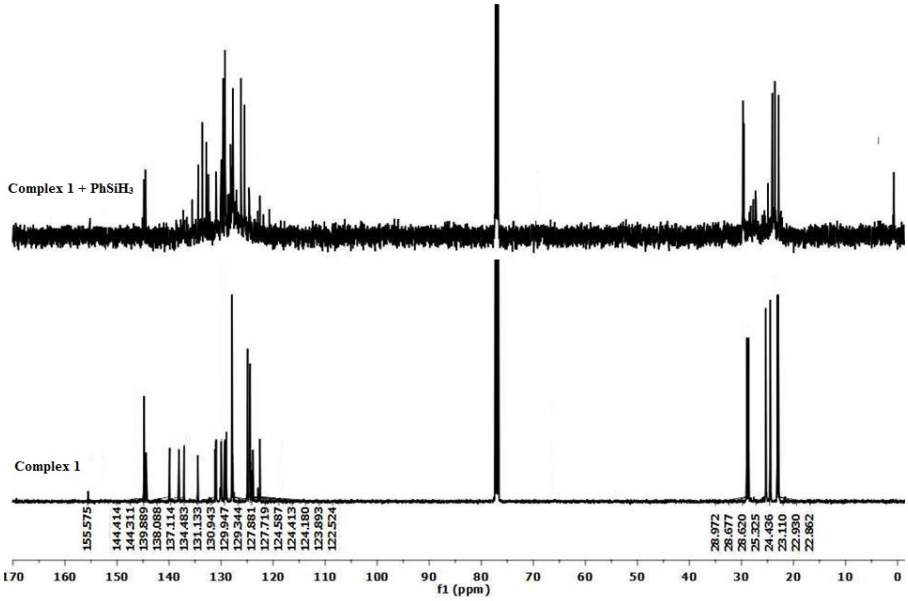


Fig. S47: The ^{29}Si NMR spectrum ($CDCl_3$) obtained from the reaction mixture of stoichiometric reaction of complex 1 with $PhSiH_3$.

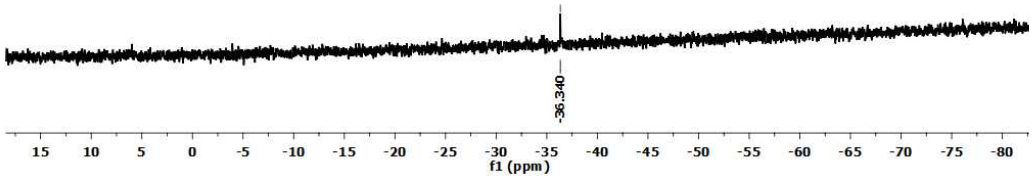


Table S1. Crystal Data and Details of the Structure Determination for **1**.

CCDC	1451179
Empirical formula	$C_{39}H_{44}ClN_2 Ni_{0.5}$
Formula weight	605.57
Temperature (K)	100
Wavelength (A˚)	0.71073
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	11.4154(6)
b (Å)	12.6234(5)
c (Å)	15.3280(8)
α (°)	66.945(4)
β (°)	85.853(4)
γ(°)	71.589(4)
Volume ($Å^3$)	1925.00(18)
Z	2
Calculated density (Mg/m3)	1.045
Absorption coefficient (mm-1)	0.361
F(000)	646
Crystal size (mm)	0.31 x 0.42 x 0.56
Theta range for data collection(°)	1.9, 28.3
Dataset	-15: 13 ; -16: 16 ; -19: 17
Tot.,Uniq. Data, R(int)	13758, 8387, 0.028
Observed Data [I > 0.0 sigma(I)]	7097
Nref, Npar	8387, 393
R, wR2, S	0.0435, 0.1204, 1.05
Min. and Max. Resd. Dens. [e/Ang^3]	-0.45, 0.55

Table S2. Selected bond distances (Å) and angles (°) for **1**.

Complex **1**			
	Bond distances (Å)		Bond angles (°)
Ni1 -Cl1	2.1915(5)	Cl1 -Ni1 -C1	91.92(5)
Ni1 -C1	1.9424(17)	C1 -Ni1 -C1_a	180.00
N1 -C1	1.407(2)	Cl1 -Ni1 -Cl1_a	180.00
N1 -C3	1.358(2)	Cl1 -Ni1 -C1_a	88.08(5)
N1 -C4	1.458(2)	Cl1_a -Ni1 -C1	88.08(5)
N2 -C2	1.411(2)	C1 -N1 -C3	112.08(15)
N2 -C3	1.342(2)	C1 -N1 -C4	126.97(14)
		C3 -N1 -C4	120.70(15)

Table S3. Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for **1**

Atom	x	y	z	U(eq) [Ang^2]
----	---	---	---	----------
Ni1	1/2	1/2	1/2	0.0122(1)
Cl1	0.66332(4)	0.54845(4)	0.43575(3)	0.0214(1)
N1	0.31799(12)	0.73474(12)	0.37129(9)	0.0132(4)
N2	0.25462(13)	0.69194(12)	0.26315(9)	0.0139(4)
C1	0.39464(15)	0.61616(15)	0.38758(11)	0.0143(5)
C2	0.35615(15)	0.59281(15)	0.31588(12)	0.0150(5)
C3	0.23220(15)	0.77790(15)	0.29852(11)	0.0146(5)
C4	0.33045(15)	0.81238(14)	0.41738(12)	0.0146(4)
C5	0.41401(16)	0.87849(15)	0.38173(12)	0.0176(5)
C6	0.40653(17)	0.97043(16)	0.41244(14)	0.0221(5)
C7	0.32063(18)	0.99558(16)	0.47595(14)	0.0236(6)
C8	0.24457(17)	0.92398(16)	0.51450(13)	0.0211(5)
C9	0.24758(16)	0.83088(15)	0.48585(12)	0.0165(5)
C10	0.16218(17)	0.75471(16)	0.52894(13)	0.0197(5)

C11	0.02601(17)	0.83366(18)	0.51126(14)	0.0252(6)
C12	0.19556(19)	0.68349(17)	0.63547(13)	0.0257(6)
C13	0.50580(17)	0.85815(16)	0.30799(13)	0.0213(5)
C14	0.4598(2)	0.95731(18)	0.20853(14)	0.0298(6)
C15	0.63461(18)	0.85448(19)	0.33409(16)	0.0309(6)
C16	0.12478(16)	0.89068(15)	0.27137(11)	0.0163(5)
C17	0.00727(17)	0.88639(16)	0.25701(12)	0.0203(5)
C18	-0.09616(17)	0.98845(17)	0.23653(13)	0.0241(5)
C19	-0.08476(18)	1.09703(17)	0.23028(13)	0.0242(5)
C20	0.03085(18)	1.10355(16)	0.24377(13)	0.0236(5)
C21	0.13540(17)	1.00129(15)	0.26470(12)	0.0196(5)
C22	0.40763(16)	0.48567(16)	0.29127(13)	0.0187(5)
C23	0.4263(2)	0.49698(18)	0.19789(14)	0.0314(6)
C24	0.4758(2)	0.3955(2)	0.17608(17)	0.0448(8)
C25	0.5080(2)	0.28041(19)	0.24803(17)	0.0401(7)
C26	0.4909(2)	0.26865(17)	0.34060(16)	0.0320(6)
C27	0.44144(18)	0.36944(16)	0.36303(14)	0.0235(5)
C28	0.17594(15)	0.69512(15)	0.19119(12)	0.0164(5)
C29	0.18077(16)	0.77043(17)	0.09607(12)	0.0206(5)
C30	0.09646(19)	0.7783(2)	0.03051(14)	0.0326(6)
C31	0.0140(2)	0.7134(2)	0.05796(16)	0.0406(8)
C32	0.01422(19)	0.6371(2)	0.15140(16)	0.0318(7)
C33	0.09532(16)	0.62545(17)	0.22093(13)	0.0210(5)
C34	0.09169(19)	0.54003(18)	0.32289(14)	0.0285(6)
C35	0.1312(2)	0.4086(2)	0.3301(2)	0.0462(8)
C36	-0.0373(2)	0.5718(2)	0.36110(17)	0.0406(8)

C37	0.27154(19)	0.84188(18)	0.06153(13)	0.0275(6)
C38	0.3498(2)	0.8098(2)	-0.01614(15)	0.0380(7)
C39	0.2045(2)	0.9781(2)	0.02403(15)	0.0394(7)

Table S4. (An)isotropic Displacement Parameter for **1**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	0.0122(2)	0.0104(2)	0.0100(2)	-0.0013(1)	-0.0034(1)	-0.0011(1)
Cl1	0.0160(2)	0.0179(2)	0.0220(2)	-0.0007(2)	0.0004(2)	-0.0034(2)
N1	0.0138(7)	0.0107(6)	0.0123(7)	-0.0015(5)	-0.0033(5)	-0.0030(5)
N2	0.0148(7)	0.0136(7)	0.0101(6)	-0.0023(5)	-0.0035(5)	-0.0025(5)
C1	0.0151(8)	0.0128(8)	0.0117(8)	-0.0011(6)	0.0004(6)	-0.0047(6)
C2	0.0145(8)	0.0117(8)	0.0129(8)	-0.0004(6)	-0.0036(6)	-0.0012(6)
C3	0.0142(8)	0.0137(8)	0.0115(8)	-0.0008(6)	-0.0026(6)	-0.0033(6)
C4	0.0152(8)	0.0092(7)	0.0140(8)	-0.0010(6)	-0.0083(6)	0.0009(6)
C5	0.0165(8)	0.0139(8)	0.0169(8)	-0.0016(7)	-0.0069(7)	-0.0016(7)
C6	0.0220(9)	0.0149(8)	0.0283(10)	-0.0051(8)	-0.0060(8)	-0.0070(7)
C7	0.0270(10)	0.0173(9)	0.0267(10)	-0.0104(8)	-0.0084(8)	-0.0028(7)
C8	0.0213(9)	0.0195(9)	0.0196(9)	-0.0087(7)	-0.0051(7)	0.0001(7)
C9	0.0172(8)	0.0136(8)	0.0138(8)	-0.0024(7)	-0.0063(7)	-0.0008(7)
C10	0.0209(9)	0.0192(9)	0.0176(9)	-0.0068(7)	0.0011(7)	-0.0050(7)
C11	0.0224(9)	0.0258(10)	0.0239(10)	-0.0072(8)	0.0038(8)	-0.0068(8)
C12	0.0299(10)	0.0230(10)	0.0190(9)	-0.0048(8)	0.0037(8)	-0.0064(8)
C13	0.0219(9)	0.0160(9)	0.0235(9)	-0.0038(7)	0.0009(7)	-0.0076(7)
C14	0.0304(11)	0.0264(10)	0.0254(10)	-0.0045(9)	0.0052(8)	-0.0076(9)
C15	0.0215(9)	0.0265(10)	0.0440(13)	-0.0112(10)	0.0024(9)	-0.0101(8)

C16	0.0189(8)	0.0141(8)	0.0105(8)	-0.0028(6)	-0.0025(6)	-0.0001(7)
C17	0.0205(9)	0.0181(9)	0.0184(9)	-0.0044(7)	-0.0020(7)	-0.0036(7)
C18	0.0158(8)	0.0279(10)	0.0227(9)	-0.0091(8)	-0.0040(7)	0.0010(7)
C19	0.0239(9)	0.0227(9)	0.0159(9)	-0.0069(8)	-0.0064(7)	0.0067(8)
C20	0.0290(10)	0.0165(9)	0.0202(9)	-0.0073(7)	-0.0044(8)	0.0011(8)
C21	0.0215(9)	0.0170(9)	0.0163(8)	-0.0048(7)	-0.0040(7)	-0.0017(7)
C22	0.0164(8)	0.0173(8)	0.0208(9)	-0.0080(7)	-0.0074(7)	-0.0008(7)
C23	0.0395(12)	0.0218(10)	0.0219(10)	-0.0072(8)	-0.0037(9)	0.0045(9)
C24	0.0568(15)	0.0382(13)	0.0322(12)	-0.0225(11)	-0.0076(11)	0.0081(11)
C25	0.0432(13)	0.0252(11)	0.0497(14)	-0.0251(11)	-0.0148(11)	0.0095(10)
C26	0.0349(11)	0.0147(9)	0.0421(12)	-0.0093(9)	-0.0191(10)	0.0001(8)
C27	0.0258(9)	0.0167(9)	0.0254(10)	-0.0058(8)	-0.0110(8)	-0.0037(7)
C28	0.0140(8)	0.0169(8)	0.0156(8)	-0.0064(7)	-0.0047(7)	0.0001(7)
C29	0.0175(8)	0.0234(9)	0.0154(8)	-0.0045(7)	-0.0044(7)	-0.0020(7)
C30	0.0295(11)	0.0451(13)	0.0158(9)	-0.0064(9)	-0.0089(8)	-0.0069(10)
C31	0.0312(11)	0.0655(16)	0.0321(12)	-0.0238(12)	-0.0106(9)	-0.0154(11)
C32	0.0230(10)	0.0449(13)	0.0384(12)	-0.0221(10)	0.0000(9)	-0.0171(9)
C33	0.0166(8)	0.0235(9)	0.0235(9)	-0.0103(8)	-0.0014(7)	-0.0050(7)
C34	0.0263(10)	0.0295(11)	0.0283(10)	-0.0052(9)	0.0026(8)	-0.0150(9)
C35	0.0330(12)	0.0296(12)	0.0664(17)	-0.0036(12)	-0.0010(12)	-0.0157(10)
C36	0.0375(12)	0.0466(14)	0.0389(13)	-0.0135(11)	0.0141(10)	-0.0212(11)
C37	0.0277(10)	0.0329(11)	0.0154(9)	-0.0010(8)	-0.0042(8)	-0.0105(9)
C38	0.0303(11)	0.0440(13)	0.0227(10)	0.0016(10)	0.0042(9)	-0.0088(10)
C39	0.0602(15)	0.0312(12)	0.0203(10)	-0.0012(9)	-0.0016(10)	-0.0162(11)

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