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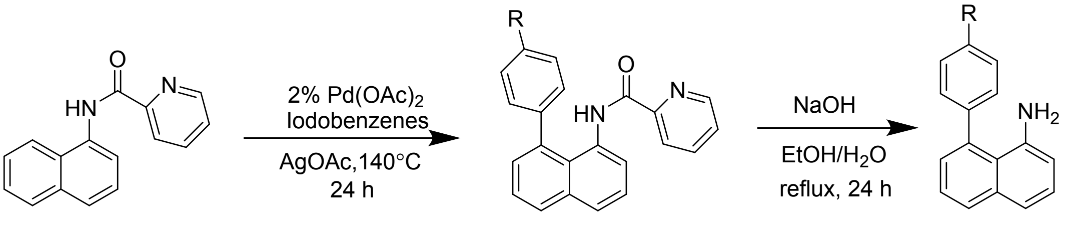
1. Experimental sections.

1.1 General Considerations.

All manipulations of air- and water-sensitive compounds were carried out using standard Schlenk, high-vacuum, and glovebox techniques. Deuterated solvents used for NMR were dried and distilled prior to use. ^{1}H, ^{13}C NMR spectra were recorded by a Bruker Ascend Tm 400 spectrometer at ambient temperature unless otherwise stated. The chemical shifts of the ^{1}H and ^{13}C NMR spectra were referenced to the residual solvent; Coupling constants are in Hz. Elemental analysis was performed by the Analytical Center of the University of Science and Technology of China. X-ray Diffraction data were collected at 298(2) K on a Bruker Smart CCD area detector with graphite-monochromated Mo K^{α} radiation (λ = 0.71073 Å). Molecular weight and molecular weight distribution of the polymer were determined by gel permeation chromatography (GPC) with a PL 210 equipped with one Shodex AT-803S and two Shodex AT-806MS columns at 150 °C using trichlorobenzene as a solvent and calibrated with polystyrene standards.

1.2 Standard Procedure for the Synthesis of 8-Arylnaphthalen-1-amine.



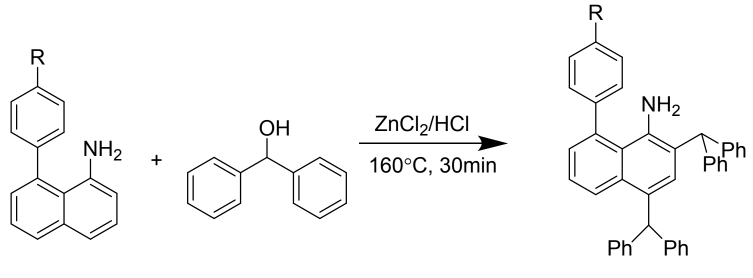
S1: R = Me 91%
S2: R = H 94%
S3: R = Ph 86%

S4: R = Me 81%
S5: R = H 86%
S6: R = Ph 74%

A 150 mL Kontes flask was charged with N-(Naphthalen-1-yl)picolinamide (5.0 g, 20 mmol), 4-iodobenzenes (80 mmol), AgOAc (5.1 g, 30.5 mmol) and $Pd(OAc)_2$ (101 mg, 0.45 mmol). The resulting suspension was stirred at 140 °C for 24 h. After cooling to room temperature, the reaction mixture was diluted with dichloromethane and filtered through a pad of Celite. Solids were thoroughly washed with dichloromethane (100 mL). The filtrate and washings were concentrated in vacuo. The residue was purified by flash column chromatography in EtOAc/hexanes (1/20 to 1/5), followed by recrystallization from hexanes to afford the desired product. Compounds **S1** and **S2** are known.[1, 2] Compound **S3**: light brown crystals (6.89 g，86%), R_f = 0.50 (hexanes/ethyl acetate, 65/35). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.73 (*br*, s, 1H, N-*H*), 8.30 (d, J = 7.5 Hz, 1H, Ar-*H*), 8.13 (d, J = 7.7 Hz, 1H, Ar-*H*), 8.01 (d, J = 4.4 Hz, 1H, Ar-*H*), 7.92 (d, J = 8.1 Hz, 1H, Ar-*H*), 7.84 (d, J = 8.1 Hz, 1H, Ar-*H*), 7.65 (dt, J = 23.6, 7.7 Hz, 2H, Ar-*H*), 7.57 – 7.29 (m, 11H, Ar-*H*), 7.06 (dd, J = 6.9, 5.3 Hz, 1H, Ar-*H*). ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.96 (CO), 149.68, 147.55, 141.77, 140.40, 139.73, 137.72, 137.26, 136.86, 135.55, 132.89, 130.56, 129.72, 128.84, 128.63, 127.27, 126.92, 126.71, 126.46, 126.01, 125.84, 125.01, 122.66, 121.76. HRMS (m/z): calcd for $C_{28}H_{20}N_2O$: $[M+H]^+$ 401.1648, found: 401.1645.

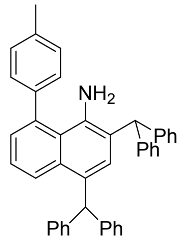
N-(8-Arylnaphthalen-1-yl)picolinamide (10 mmol) was refluxed for 24 h in a NaOH solution (4 g, NaOH in EtOH/H_2O, 10/1 v/v, 40 mL). The reaction mixture was cooled and diluted with an 40 mL water. The product was extracted with dichloromethane (3 × 60 mL). The organic layers were combined, dried with $MgSO_4$ and concentrated. The product was obtained using column chromatography (R_f = 0.16, hexane/ethylacetate/triethylamine, 94/5/1). Compounds **S4**, **S5** are known.[1, 2] Compound **S6**: beige solids (2.18 g，74%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (dd, J = 8.3, 1.3 Hz, 1H, Ar-*H*), 7.68 – 7.59 (m, 4H, Ar-*H*), 7.50 – 7.39 (m, 4H, Ar-*H*), 7.39 – 7.29 (m, 3H, Ar-*H*), 7.28 – 7.22 (m, 1H, Ar-*H*), 7.16 (dd, J = 7.0, 1.4 Hz, 1H, Ar-*H*), 6.58 (dd, *J* = 7.3, 1.3 Hz, 1H, Ar-*H*), 3.66 (s, 2H, N-*H*). ^{13}C NMR (101 MHz, $CDCl_3$): δ 142.69, 141.35, 139.35, 139.06, 136.81, 134.82, 128.60, 127.81, 127.69, 127.23, 126.44, 125.97, 125.52, 123.51, 119.60, 117.91, 110.18. Signal for one carbon could not be located. HRMS (m/z): calcd for $C_{22}H_{17}N$: $[M + H]^+$ 296.1434, found: 296.1430.

1.3 Standard Procedure for the Synthesis of 2,4-Bis(diphenylmethyl)-8-Arylnaphthalen-1-amine.

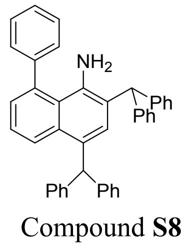


S7: R = Me 95%
S8: R = H 95%
S9: R = Ph 96%

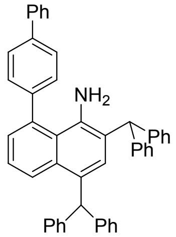
A 150 mL Kontes flask was charged with 8-arylnaphthalen-1-amine (20.0 mmol, 1.0 equiv.) and diphenylmethanol (40 mmol, 2.0 equiv.), and heated to 120 °C. A solution of anhydrous zinc chloride (10 mmol, 0.5 equiv.) in concentrated hydrochloric acid (37% in H_2O, 1.0 equiv.) was added to the mixture (exothermic + intense bubbling), and the temperature was raised to 160 °C. After 30 min at 160 °C, the reaction mixture was cooled down to room temperature and dissolved in CH_2Cl_2 (200 mL). The CH_2Cl_2 layer was washed with water (3 × 100 mL) and dried over anhydrous magnesium sulfate. The solution was concentrated to 20 mL. The product was crashed out with 200 ml methanol and washed with methanol (3 × 100 mL). The desired aniline was obtained as a white crystalline solid.



Compound **S7**: white solid (10.75 g，95%), $R_f = 0.56$ (hexane/ethyl acetate, 10/1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 8.3 Hz, 1H, Ar-*H*), 7.36 – 7.01 (m, 18H, Ar-*H*), 6.93 (dd, *J* = 21.7, 6.4 Hz, 8H, Ar-*H*), 6.37 (s, 1H, Ar-*H*), 6.08 (s, 1H, C*H*Ph$_2$), 5.48 (s, 1H, C*H*Ph$_2$), 3.69 (s, 2H, N-*H*), 2.34 (s, 3H, C*H*$_3$). ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.18, 142.51, 140.80, 139.87, 138.46, 136.95, 132.56, 131.00, 129.34, 129.23, 129.05, 128.80, 128.75, 128.61, 128.31, 128.09, 126.31, 125.88, 124.35, 124.28, 122.79, 121.80, 53.22 (*C*HPh$_2$), 52.10 (*C*HPh$_2$), 21.14 (*C*H$_3$). HRMS (m/z): calcd for $C_{43}H_{35}N$: $[M + H]^+$ 566.2842, found: 566.2825.

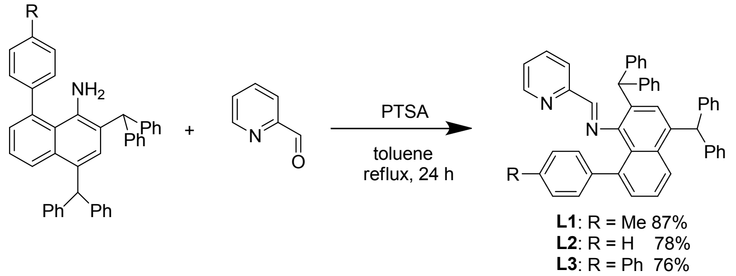


Compound **S8**: white solid (10.49 g，95%), $R_f = 0.51$ (hexane/ethyl acetate, 10/1). ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.94 (d, *J* = 7.8 Hz, 1H, Ar-*H*), 7.49 – 6.75 (m, 27H, Ar-*H*), 6.40 (s, 1H, Ar-*H*), 6.09 (s, 1H, C*H*Ph$_2$), 5.51 (s, 1H, C*H*Ph$_2$), 3.74 (s, 2H, N-*H*). ^{13}C NMR (101 MHz, CDCl$_3$): *δ* 144.27, 143.75, 142.56, 139.14, 138.53, 132.74, 131.20, 129.52, 129.43, 129.36, 128.90, 128.51, 128.38, 128.29, 127.53, 126.53, 126.10, 124.69, 124.51, 123.74, 122.00, 53.41 (*C*HPh$_2$), 52.26 (*C*HPh$_2$). HRMS (m/z): calcd for $C_{42}H_{33}N$: [M +H]$^+$ 552.2686, found: 552.2671.

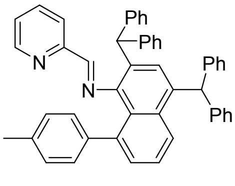


Compound **S9**: white solid (12.06 g，96%), R$_f$ = 0.49 (hexane/ethyl acetate, 10/1). ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.90 (d, *J* = 8.5 Hz, 1H, Ar-*H*), 7.64 – 7.53 (m, 4H, Ar-*H*), 7.47 – 7.34 (m, 4H, Ar-*H*), 7.33 – 7.20 (m, 2H, Ar-*H*), 7.10 (m, 13H, Ar-*H*), 6.89 (dd, *J* = 24.3, 6.3 Hz, 8H, Ar-*H*), 6.30 (s, 1H, Ar-*H*), 6.01 (s, 1H, C*H*Ph$_2$), 5.38 (s, 1H, C*H*Ph$_2$), 3.66 (s, 2H, N-*H*). ^{13}C NMR (101 MHz, CDCl$_3$) δ 145.47, 143.87, 141.58, 141.13, 141.13, 139.57, 133.90, 132.57, 131.12, 130.80, 130.70, 130.35, 130.12, 129.83, 129.61, 129.01, 128.40, 128.15, 127.86, 127.44, 125.82, 124.31, 122.93, 54.51 (*C*HPh$_2$), 53.56 (*C*HPh$_2$). HRMS (m/z): calcd for $C_{48}H_{37}N$: [M +H]$^+$ 628.2999, found:628.2994.

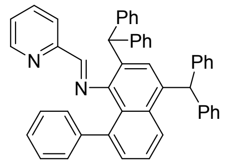
1.4 Standard Procedure for the Synthesis of 2-((2,4-Bis(diphenylmethyl)-8-arylnaphthalenlimino)methyl)pyridine (L1-L3).



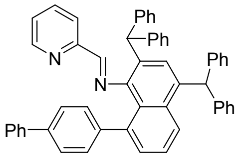
A mixture of picolinaldehyde (30.0 mmol), 2,4-Bis(diphenylmethyl)-8-Arylnaphthalen-1-amine (10.0 mmol) and a catalytic amount of p-toluenesulfonic acid in toluene (150 mL) were refluxed for 24 h. The solvent was partially evaporated under reduced pressure until the formation of a light yellow solid. The remaining mixture was diluted with methanol (300 mL). The resulting yellow solid was collected by filtration and recrystallized from CH_2Cl_2 and hexanes to afford the desired product.



Compound **L1**: yellow solid (5.70 g，87%). ^{1}H NMR (400 MHz, CDCl$_3$): *δ* 8.44 (d, *J* = 4.5 Hz, 1H, -N=C-*H*), 8.02 (d, *J* = 8.4 Hz, 1H, Ar-*H*), 7.61 – 7.46 (m, 2H, Ar-*H*), 7.39 – 7.32 (m, 1H, Ar-*H*), 7.29 – 7.11 (m, 9H, Ar-*H*), 7.07 – 6.96 (m, 12H, Ar-*H*), 6.87 – 6.74 (m, 6H, Ar-*H*), 6.69 (s, 1H, Ar-*H*), 6.21 (s, 1H, C*H*Ph$_2$), 5.58 (s, 1H, C*H*Ph$_2$), 1.91 (s, 3H, C*H*$_3$). ^{13}C NMR (101 MHz, CDCl$_3$): *δ* 163.76 (N=*C*H), 153.92, 148.75, 146.57, 143.84, 143.73, 142.18, 139.81, 135.48, 135.22, 135.18, 132.42, 130.54, 129.82, 129.51, 129.37, 129.21, 128.38, 128.32, 128.19, 127.99, 126.25, 125.91, 124.98, 124.54, 124.49, 123.80, 121.33, 53.42 (*C*HPh$_2$), 51.57 (*C*HPh$_2$), 20.82(*C*H$_3$). HRMS (m/z): calcd for $C_{49}H_{38}N_2$: [M +H]$^+$ 655.3108, found:655.3098.

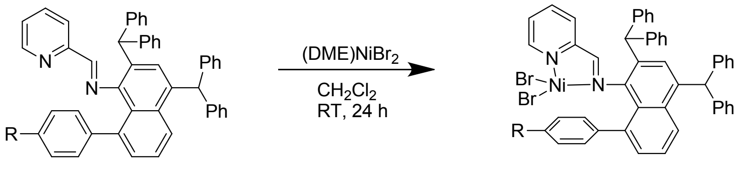


Compound **L2**: yellow solid (5.00 g，78%). ^{1}H NMR (400 MHz, $CDCl_3$)：δ 8.40 (d, J = 4.6 Hz, 1H，-N=C-*H*), 8.03 (d, J = 8.5 Hz, 1H，Ar-*H*), 7.57 – 7.41 (m, 2H， Ar-*H*), 7.35 (t, J = 7.8 Hz, 1H，Ar-*H*), 7.24 – 7.11 (m, 11H, Ar-*H*), 7.08 – 6.90 (m, 12H, Ar-*H*), 6.82 (m, 4H, Ar-*H*), 6.71 (s, 1H, Ar-*H*), 6.66 (t, J = 7.3 Hz, 1H, Ar-*H*), 6.22 (s, 1H, C*H*Ph_2), 5.59 (s, 1H, C*H*Ph_2). ^{13}C NMR (101 MHz, $CDCl_3$): δ 164.08 (N=*C*H),, 153.85, 148.65, 146.61, 145.12, 143.86, 143.76, 139.87, 135.57, 135.38, 132.48, 130.66, 130.01, 129.53, 129.39, 129.23, 129.02, 128.34, 128.01, 127.61, 126.27, 125.94, 125.33, 124.97, 124.68, 124.50, 123.95, 121.31, 53.47 (*C*HPh_2), 51.63 (*C*HPh_2). HRMS (m/z): calcd for $C_{48}H_{36}N_2$: [M +H]$^+$ 641.2951, found:641.2950.



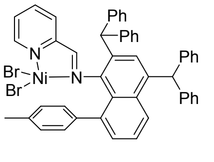
Compound **L3**: yellow solid (5.45 g，76%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 3.5 Hz, 1H, -N=C-*H*), 8.05 (d, J = 8.3 Hz, 1H, Ar-*H*), 7.48 (d, J = 7.7 Hz, 1H, Ar-*H*), 7.40 – 7.09 (m, 19H, Ar-*H*), 7.10 – 6.94 (m, 11H, Ar-*H*), 6.82 (m, 4H, Ar-*H*), 6.73 (s, 1H, Ar-*H*), 6.23 (s, 1H, C*H*Ph_2), 5.60 (s, 1H, C*H*Ph_2). ^{13}C NMR (101 MHz, $CDCl_3$): δ 163.08 (N=*C*H), 152.83, 147.72, 145.56, 143.18, 142.77, 142.66, 139.68, 138.37, 137.45, 134.55, 134.40, 131.44, 129.63, 128.85, 128.46, 128.32, 128.28, 127.34, 127.27, 126.94, 125.91, 125.83, 125.29, 125.20, 124.88, 123.94, 123.58, 123.48, 122.97, 119.95, 52.39 (*C*HPh_2), 50.57 (*C*HPh_2). HRMS (m/z): calcd for $C_{54}H_{40}N_2$: [M +H]$^+$ 717.3264, found: 717.3261.

1.5 Standard Procedure for the Synthesis of Complexes 2-((2,4-Bis(diphenylmethyl)-8-arylnaphthalenlimino)methyl)pyridine[$NiBr_2$] (1-3).

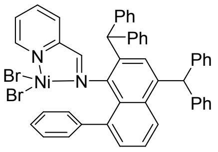


1: R = Me 95%
2: R = H 96%
3: R = Ph 92%

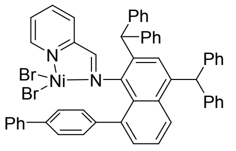
A 50 mL Schlenk flask was charged with ligand **L1-L3** (0.53 mmol) and (DME)$NiBr_2$ (154 mg, 0.5 mmol) and CH_2Cl_2 (20 mL). The red reaction mixture was stirred at room temperature for 1 day, resulting in the formation of brown precipitate. The brown-red solid was isolated by filtration, washed with ether (3 × 8 mL) and dried under reduced pressure at room temperature for 12 h.



Complexe **1**, light brown-red solid (415 mg，95%). Anal. Calcd for $C_{49}H_{38}Br_2N_2Ni$: C, 67.39; H, 4.39; N, 3.21. Found: C, 66.90; H, 4.51; N, 3.17. MALDI-TOF: m/z 791.0581 [M − Br]$^+$; 793.1018 [M – Br + 2H]$^+$.



Complexe **2**, yellow solid (412 mg，96%). Anal. Calcd for $C_{48}H_{36}Br_2N_2Ni$: C, 67.09; H, 4.22; N, 3.26. Found: C, 66.71; H, 4.40; N, 3.26. MALDI-TOF: m/z 777.0658 $[M - Br]^+$; 779.1352 $[M - Br + 2H]^+$.



Complexe **3**, brown-red solid (430 mg，92%). Anal. Calcd for $C_{52}H_{340}Br_2N_2Ni.CH_2Cl_2$: C, 64.74; H, 4.15; N, 2.75. Found: C, 64.35; H, 4.43; N, 2.71. MALDI-TOF: m/z 853.0963 $[M - Br]^+$; 855.1408 $[M - Br + 2H]^+$.

1.6 General in-Situ-Activated Polymerization Procedure.

Procedure for ethylene polymerization. In a typical experiment, a 350 mL glass thick-walled pressure vessel was charged with required amount of cocatalyst, 45 mL toluene and a magnetic stir bar in the glovebox. The pressure vessel was connected to a high pressure polymerization line and the solution was degassed. The vessel was warmed to the desired temperature using an oil bath and allowed to equilibrate for 5 min. 2.0 μmol of nickel complex in 5 mL $CHCl_3$ was injected into the vessel via syringe. With rapid stirring, the reactor was pressurized and maintained at 8.0 atm of ethylene. After a desired amount of polymerization time, the vessel was vented and the polymer was precipitated in acidified methanol (methanol/HCl =50/1) and dried at 50 °C for 24 h under vacuum. Analysis of the polymer branching by ^1H NMR spectroscopy: $BD = 1000\times2(I_{CH3})/3(I_{CH2+CH}+I_{CH3})$. CH_3 (alkyl methyl, alk-CH_3, m, 0.77-0.95 ppm); CH_2 and CH (alk-CH and alk-CH_2, m, ca. 1.0-1.45 ppm).

Polymerization of α-Olefins. In a typical procedure, a 50 mL Schlenk flask was charged with the desired amount of freshly distilled α-olefin, toluene and activator. Polymerization was initiated by injecting the catalyst solution (10 μmol, 2 mL $CHCl_3$) into the reactor, and the total volume of solvent was kept at 20 mL. After a desired amount time, the polymerizations were terminated by adding 200 mL acidic ethanol (ethanol−HCl, 95:5). The precipitated polymer was collected by filtration, washed with ethanol, and dried under vacuum at 60 °C overnight.

1.7 Table S1. Effect of Time on Ethylene Polymerization at 80 °C[a]

Ent.	Cat.	Time (min)	Yield (g)	Act.[b]
1	**1**	30	2.29	22.9
2	**1**	60	3.32	16.6
3	**1**	120	3.50	8.75

[a]Conditions: 2 μmol pre-catalyst, 1000 eq. cocatalyst, 5 mL $CHCl_3$, 45 mL toluene, 8 atm.

[b]Activity (Act.) = 10^5 g/(mol Ni·h).

2. Spectra Data.

2.1 ^{1}H, ^{13}C of Compound S3, S6, S7-S9, L1-L3.

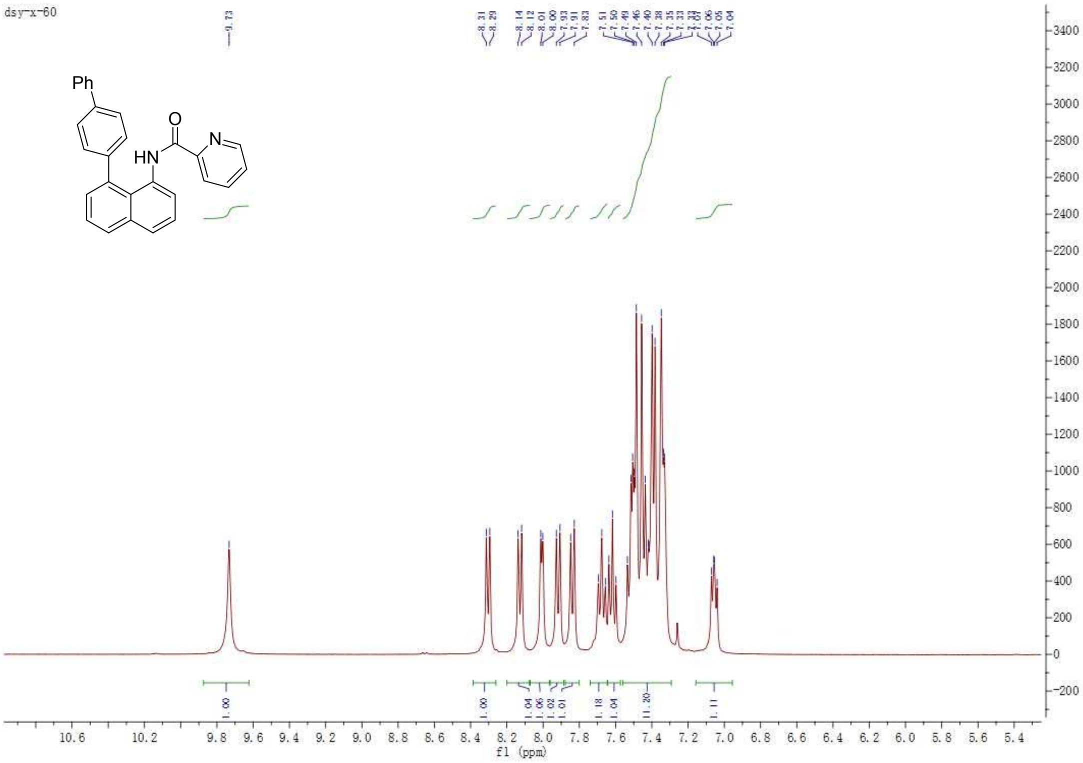


Figure S1. ^{1}H NMR spectrum of S3 in CDCl$_3$.

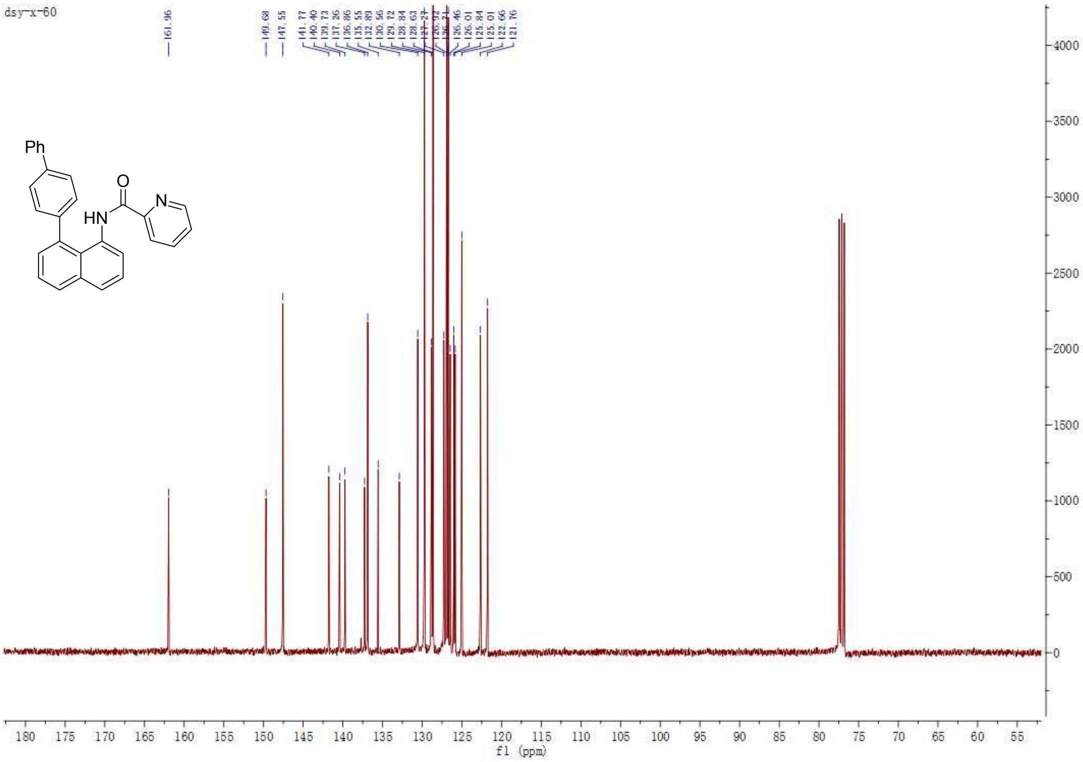


Figure S2. ^{13}C NMR spectrum of S3 in CDCl$_3$.

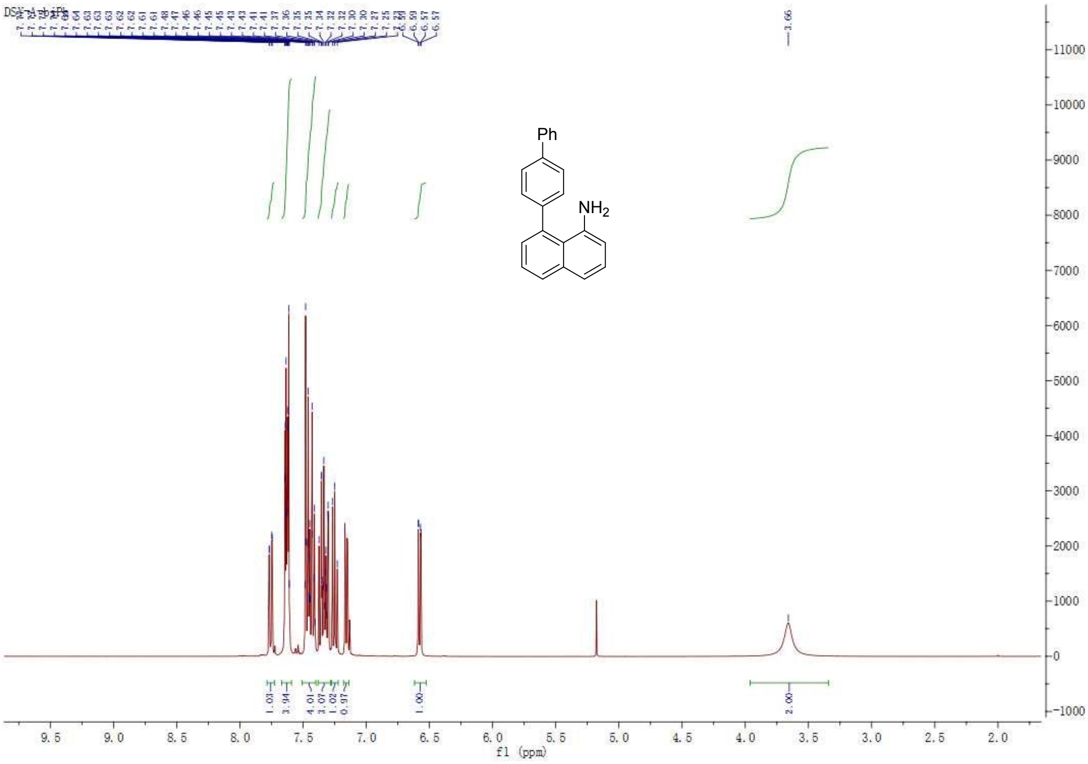


Figure S3. ^{1}H NMR spectrum of S6 in $CDCl_3$.

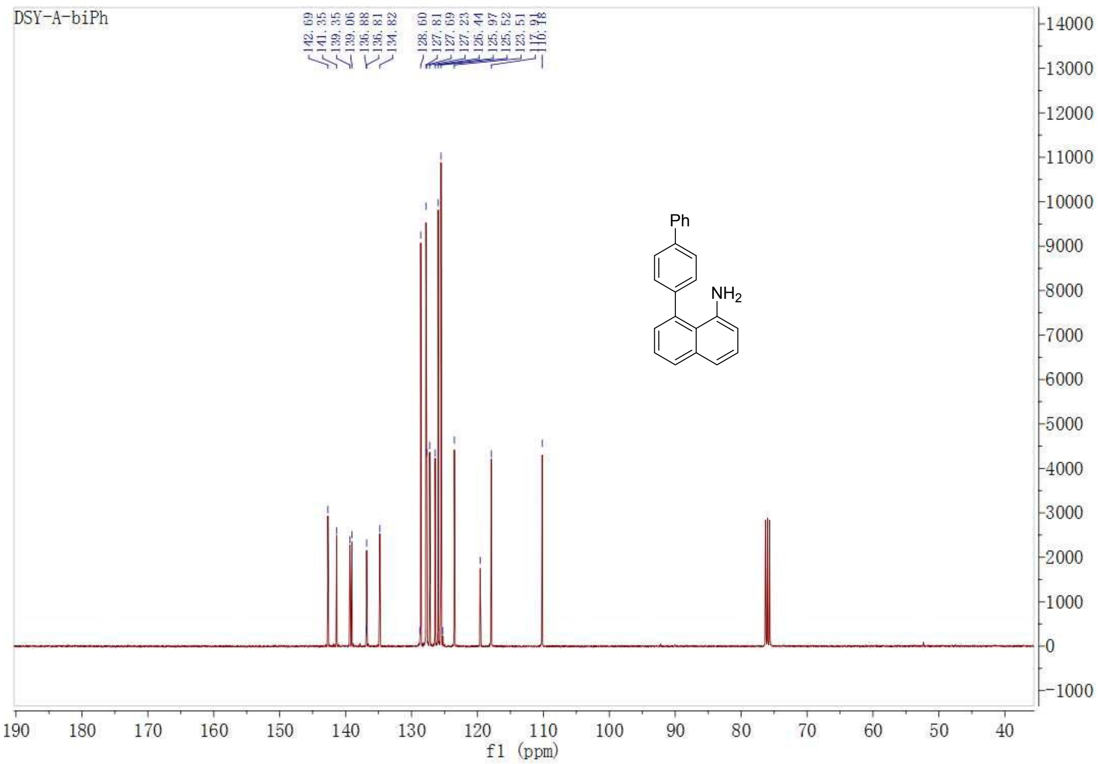


Figure S4. ^{13}C NMR spectrum of S6 in $CDCl_3$.

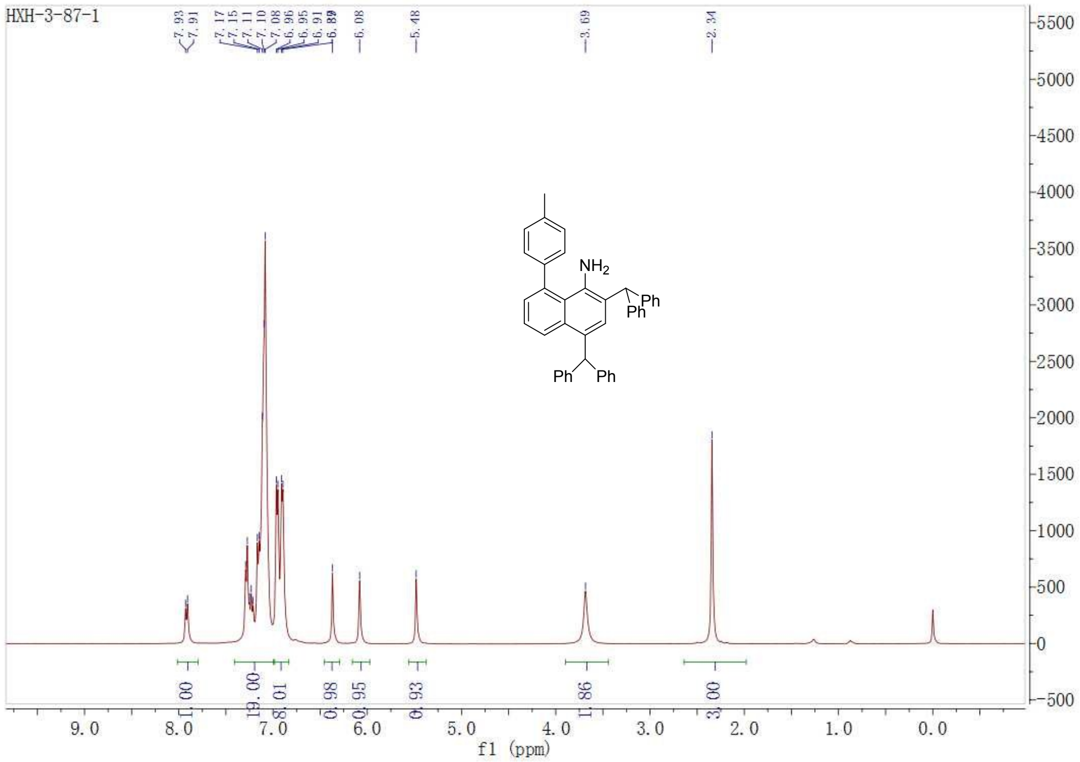


Figure S5. ^{1}H NMR spectrum of S7 in $CDCl_3$.

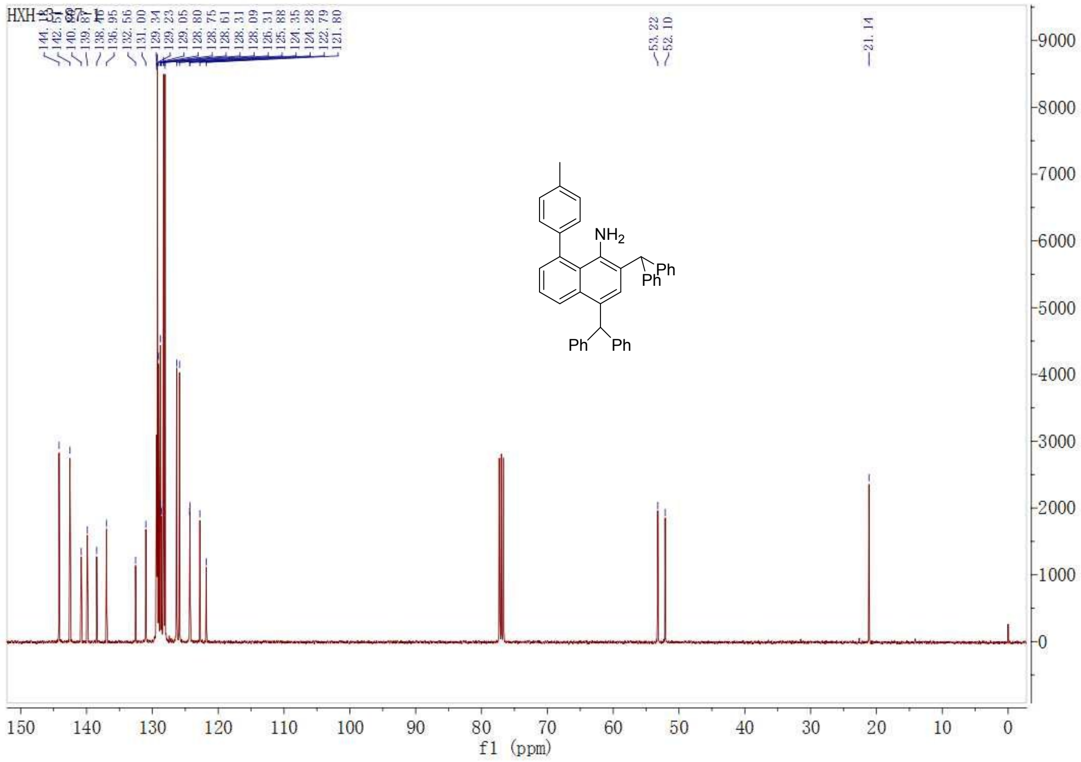


Figure S6. ^{13}C NMR spectrum of S7 in $CDCl_3$.

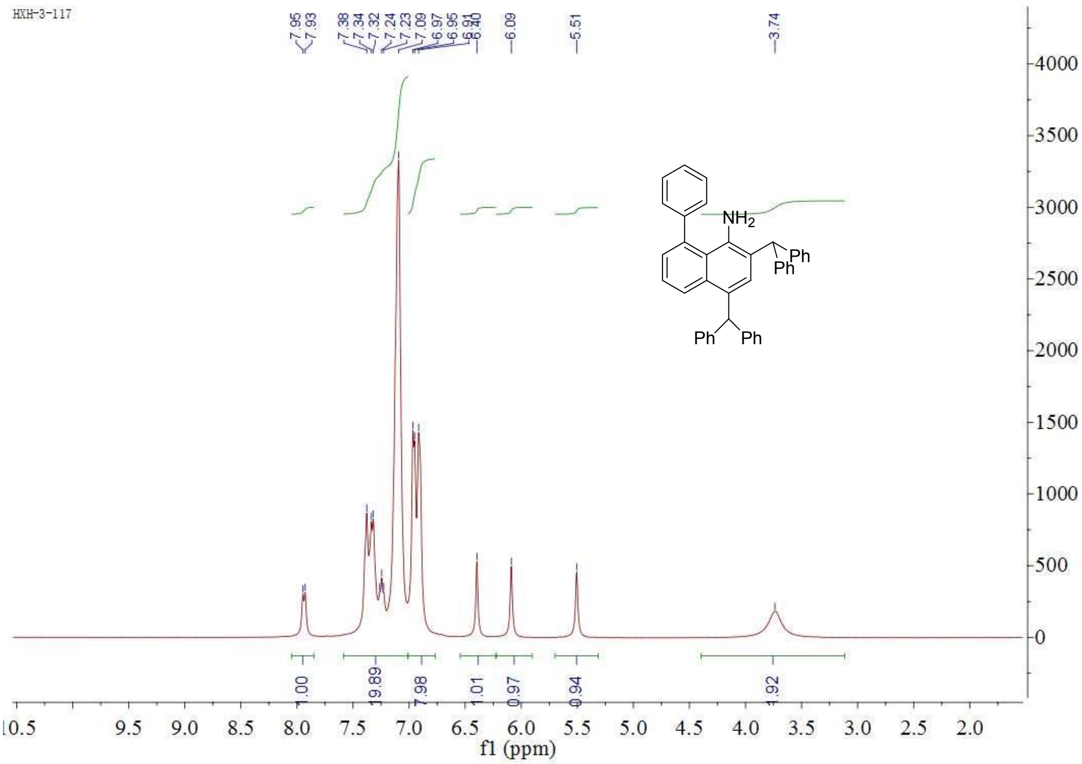


Figure S7. ^{1}**H NMR spectrum of S8 in CDCl$_3$.**

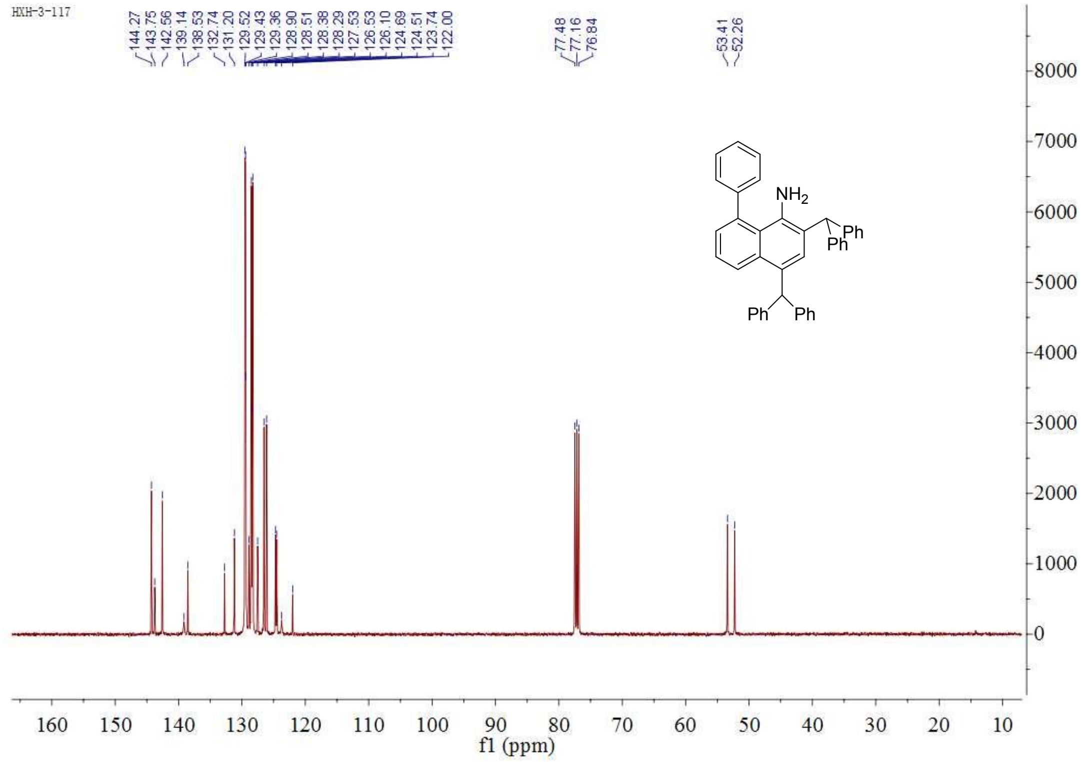


Figure S8. ^{13}**C NMR spectrum of S8 in CDCl$_3$.**

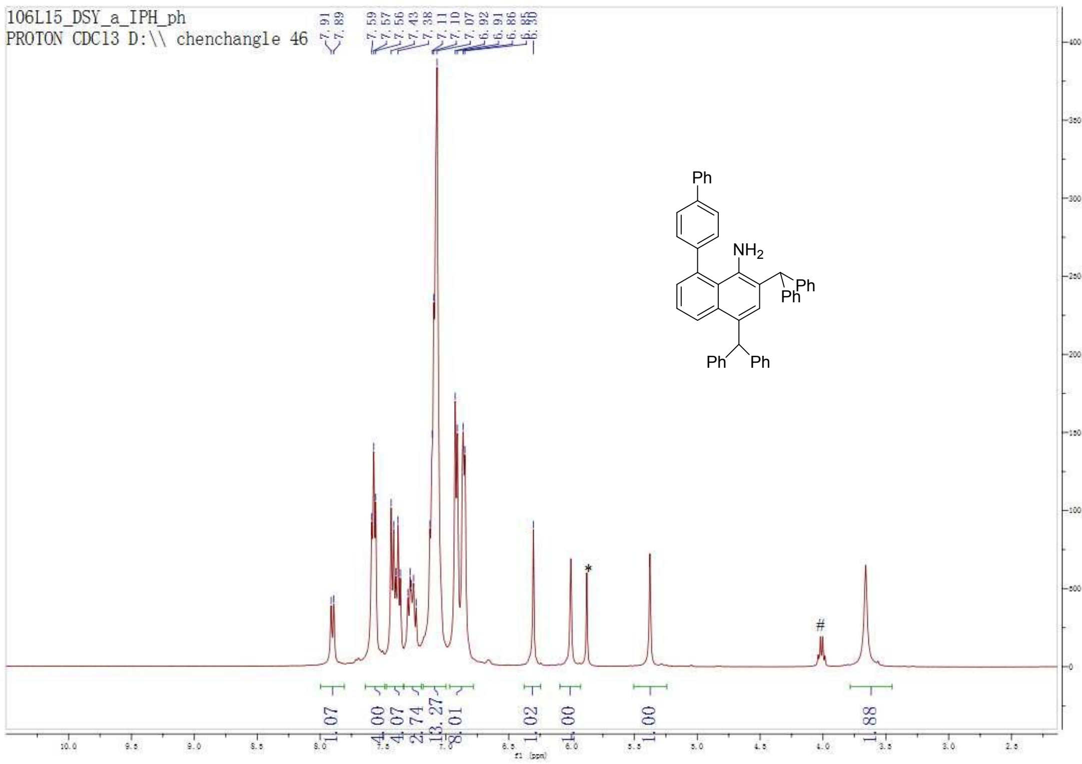


Figure S9. ^{1}H NMR spectrum of S9 in CDCl$_3$. *CH_2Cl_2, # $CH_3COCH_2CH_3$.

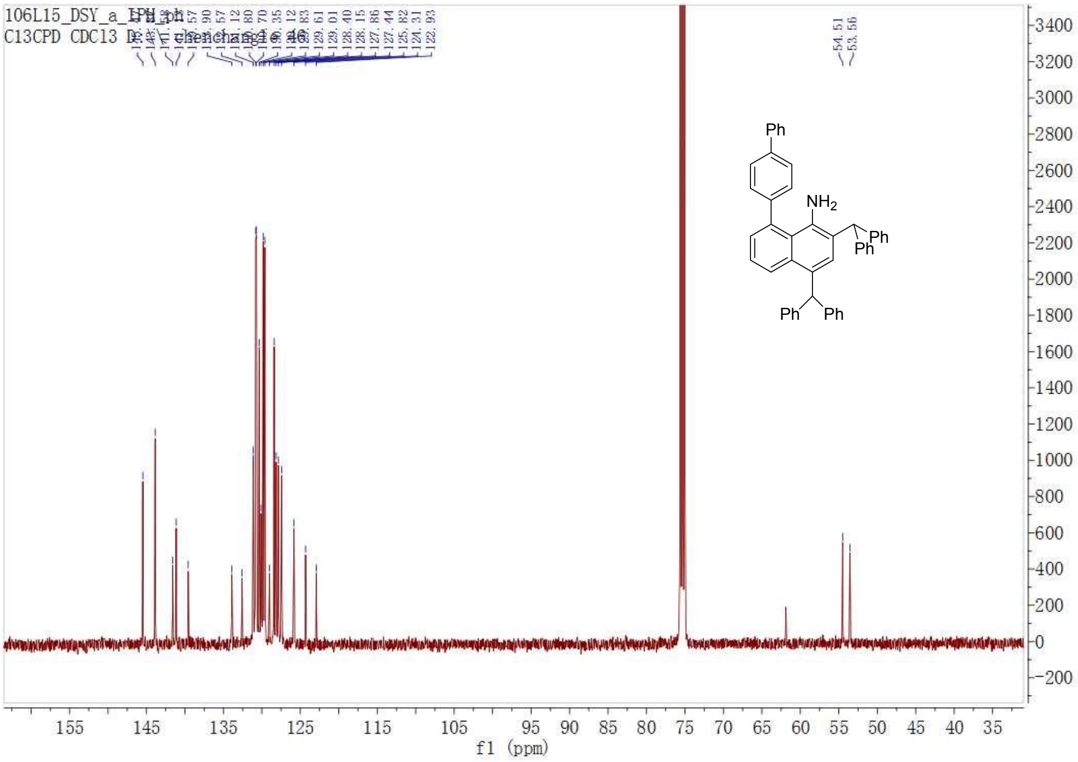


Figure S10. ^{13}C NMR spectrum of S9 in CDCl$_3$.

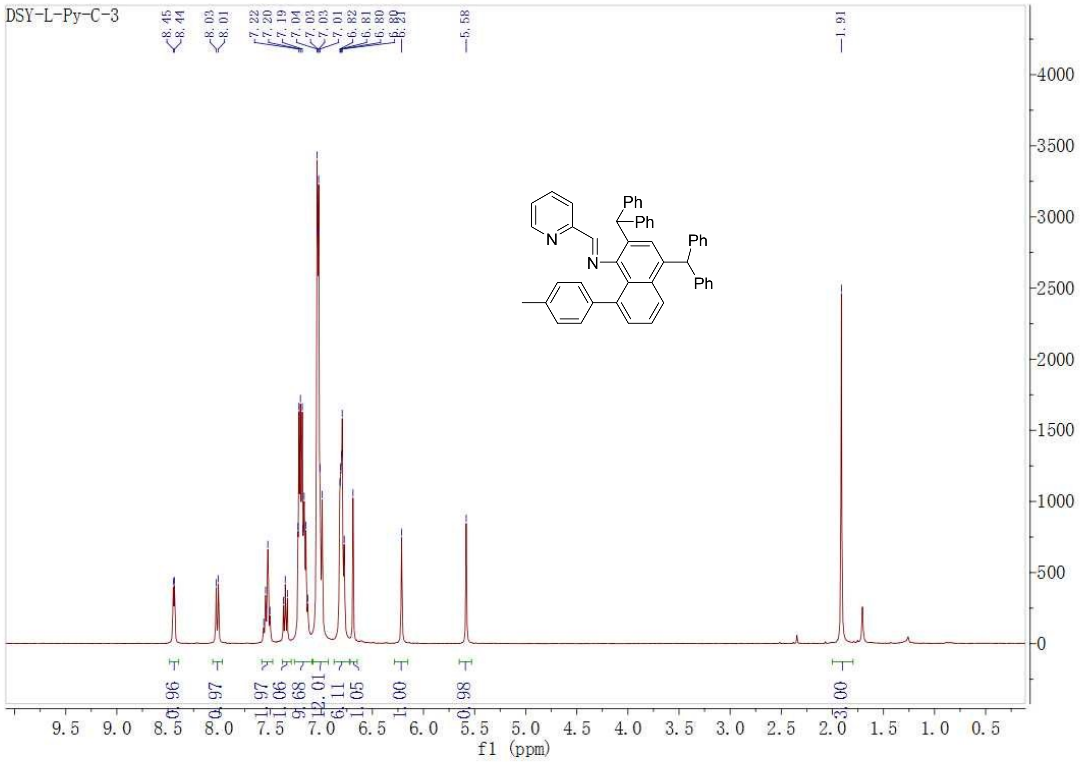


Figure S11. ^{1}H NMR spectrum of L1 in $CDCl_3$.

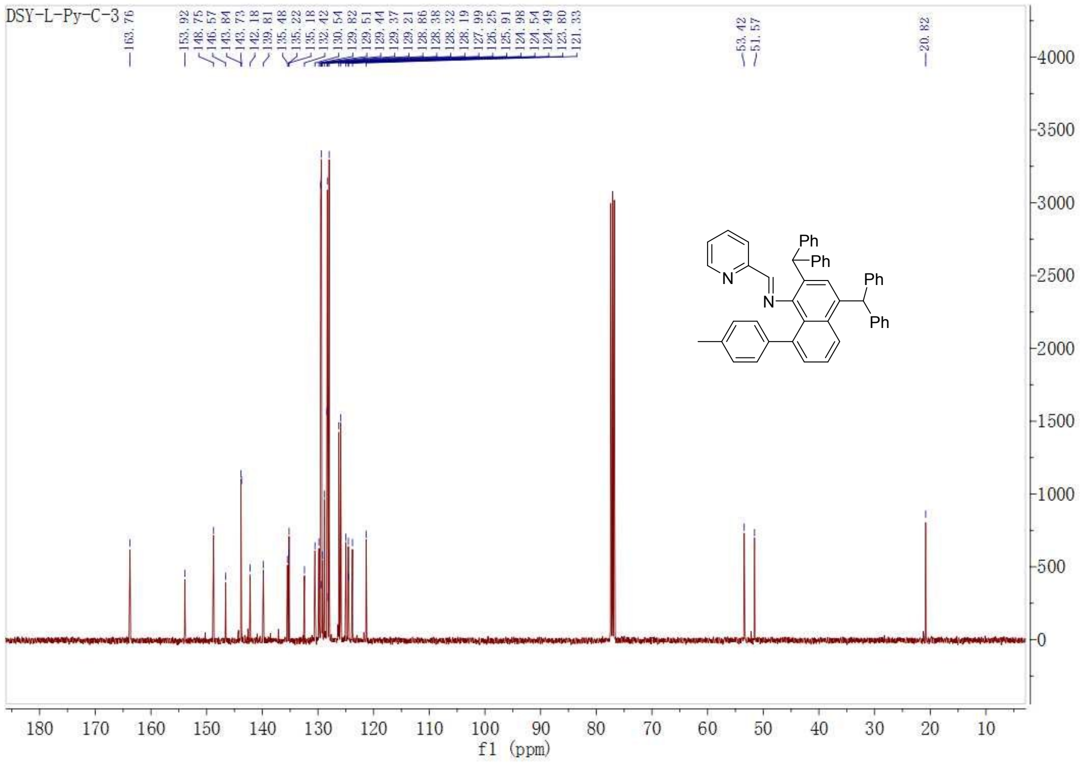


Figure S12. ^{13}C NMR spectrum of L1 in $CDCl_3$.

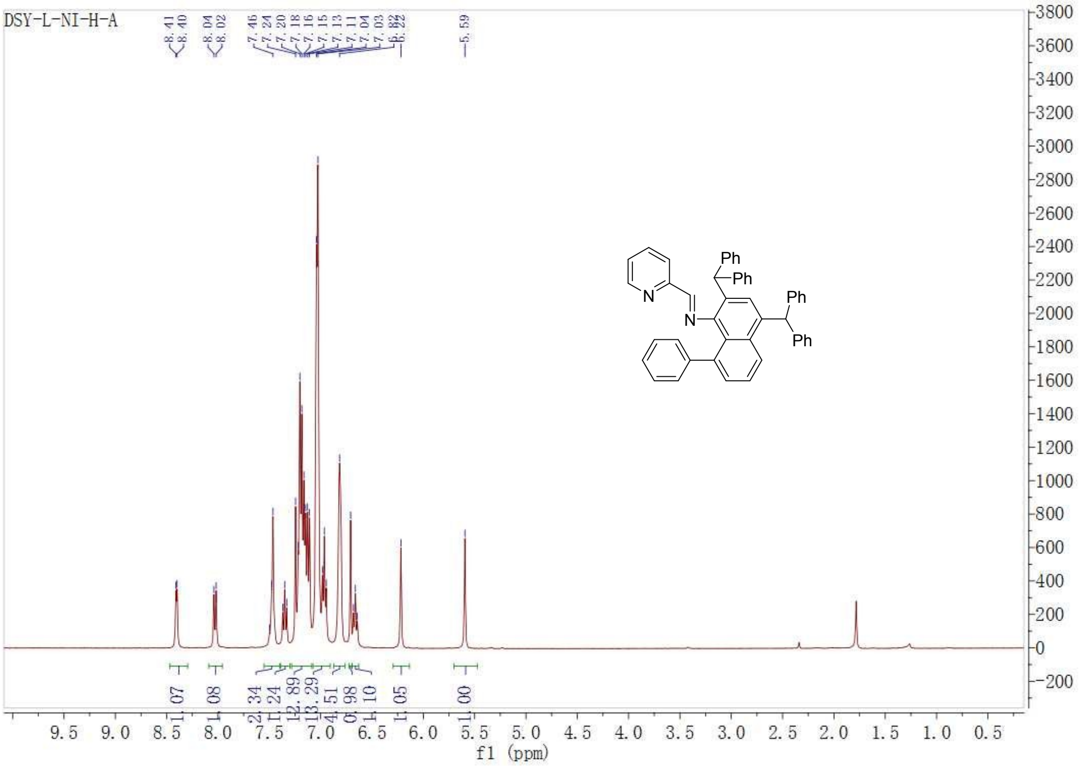


Figure S13. ^{1}H NMR spectrum of L2 in $CDCl_3$.

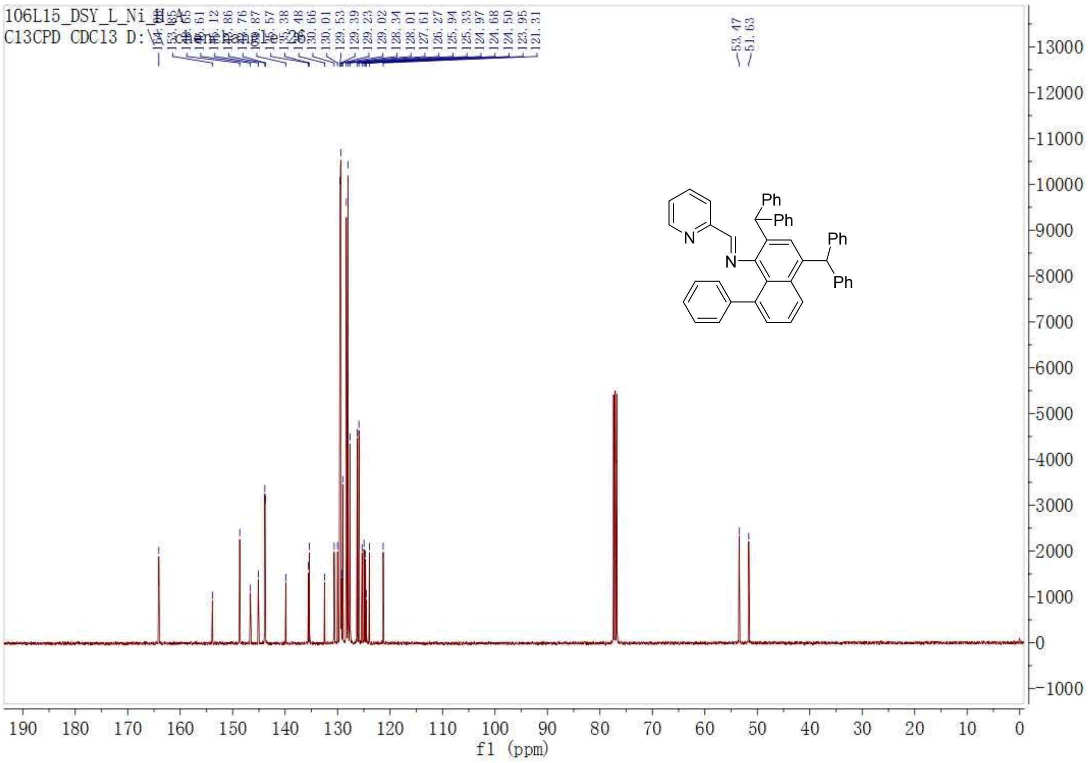


Figure S14. ^{13}C NMR spectrum of L2 in $CDCl_3$.

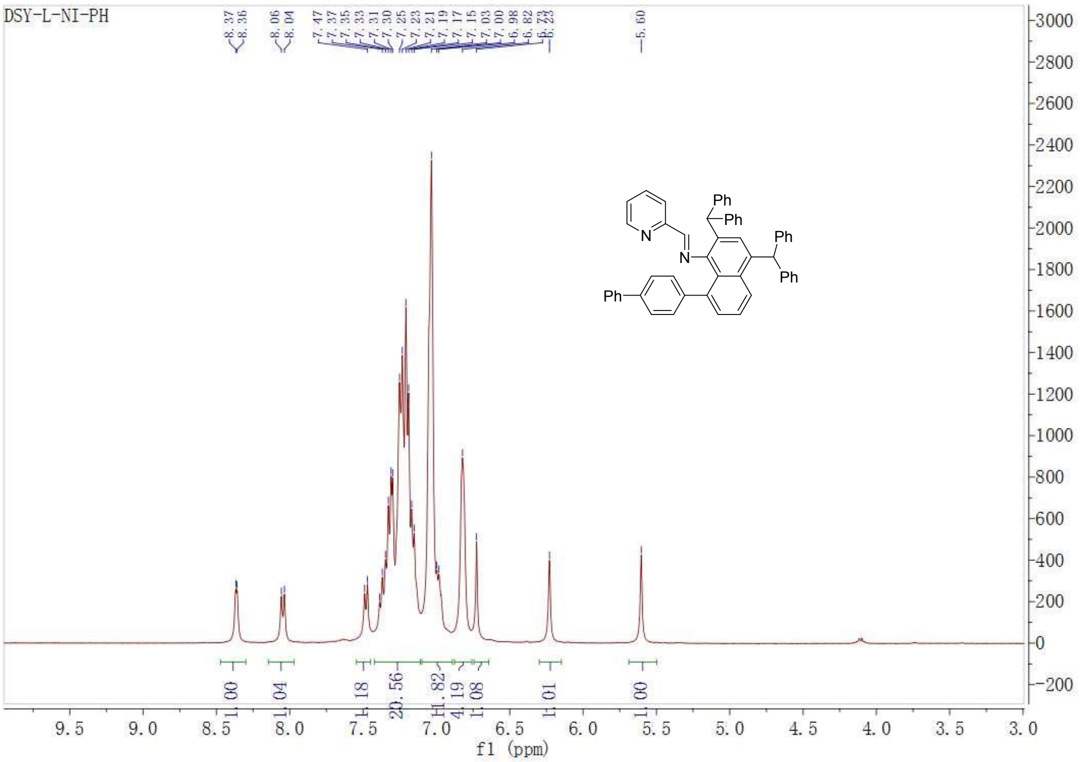


Figure S15. ^{1}H NMR spectrum of L3 in CDCl$_3$.

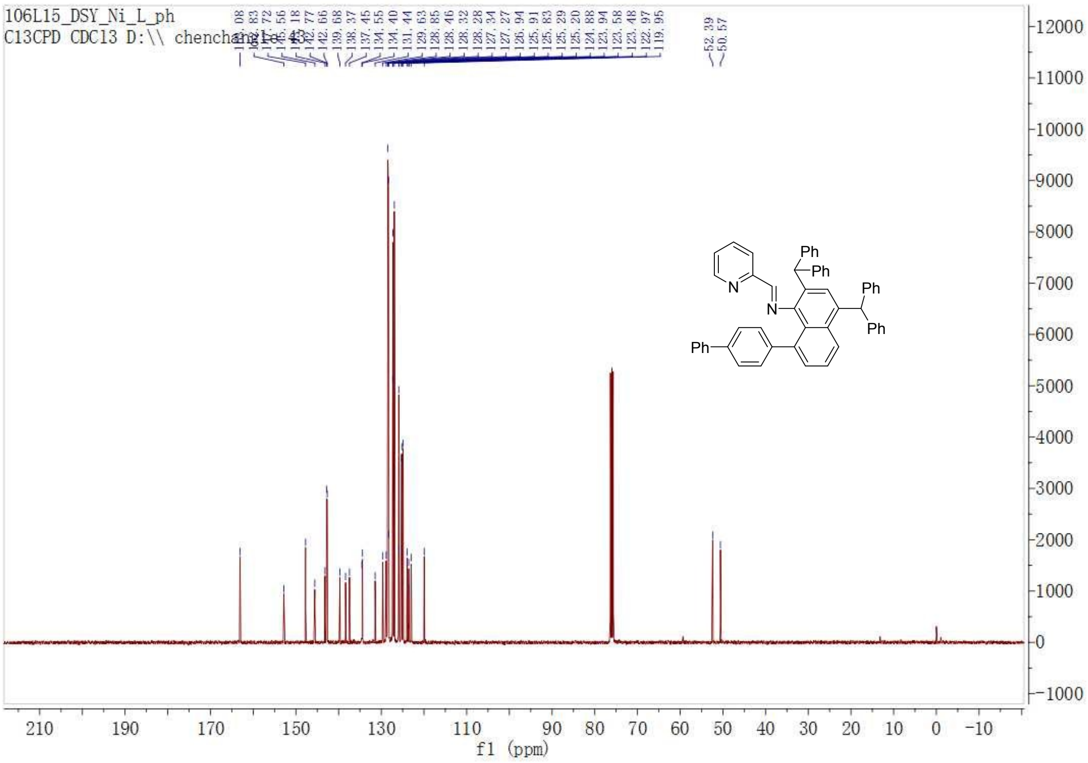


Figure S16. ^{13}C NMR spectrum of L3 in CDCl$_3$.

2.2 MALDI-TOF of Complexes 1-3.

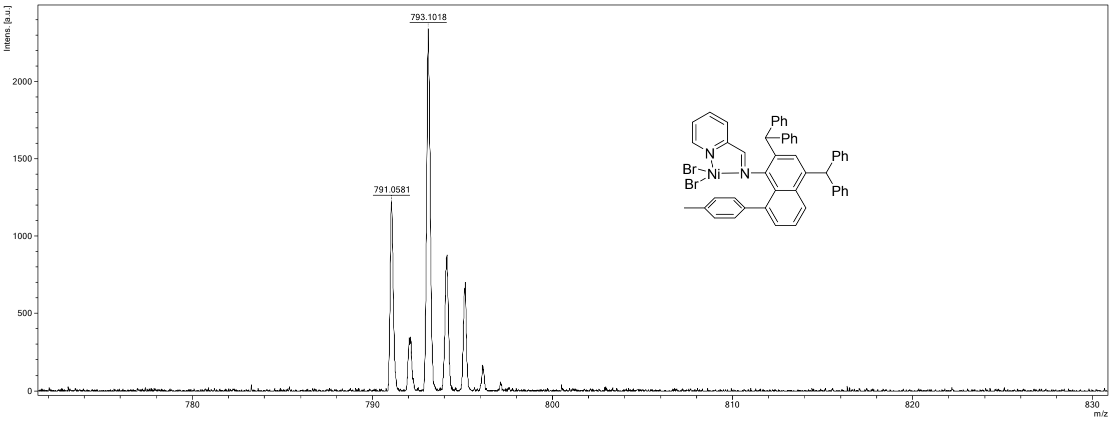


Figure S18. MALDI-TOF of Complexes 1.

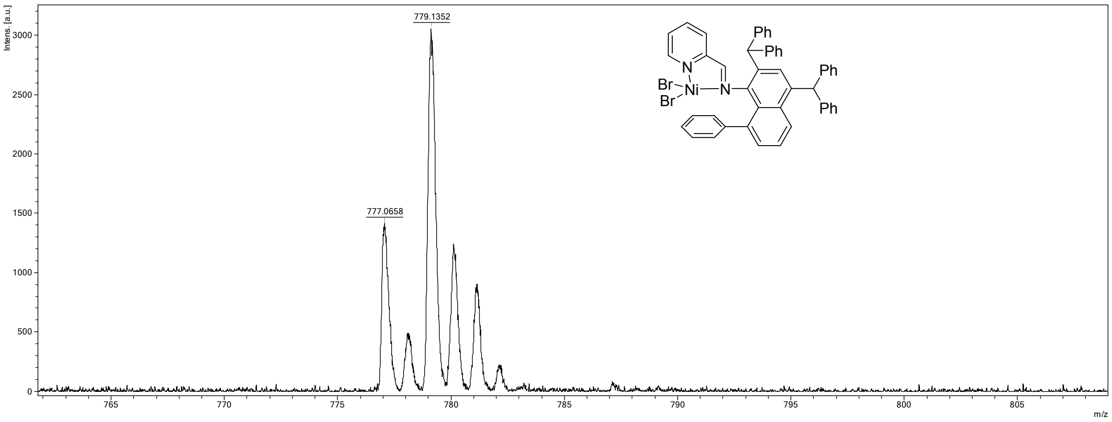


Figure S17. MALDI-TOF of Complexes 2.

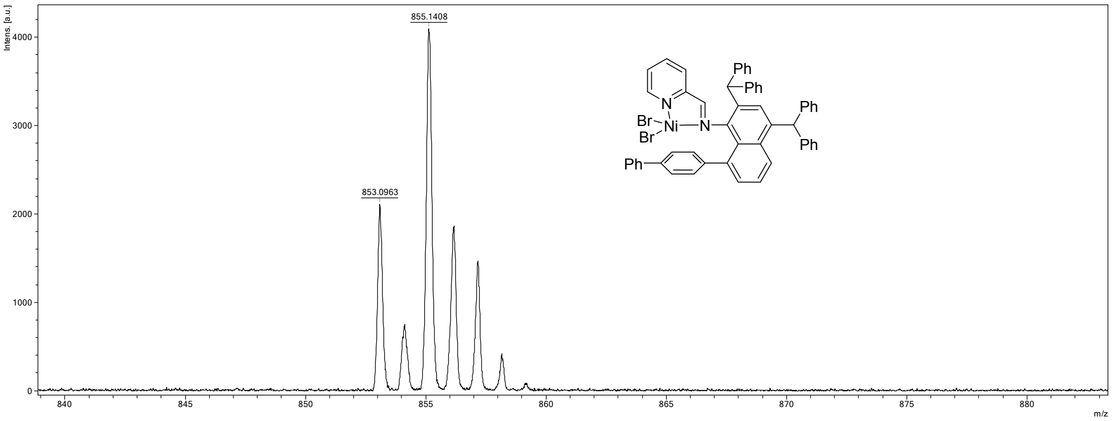


Figure S19. MALDI-TOF of Complexes 3.

2.3 ^{1}H and ^{13}C NMR of polymer.

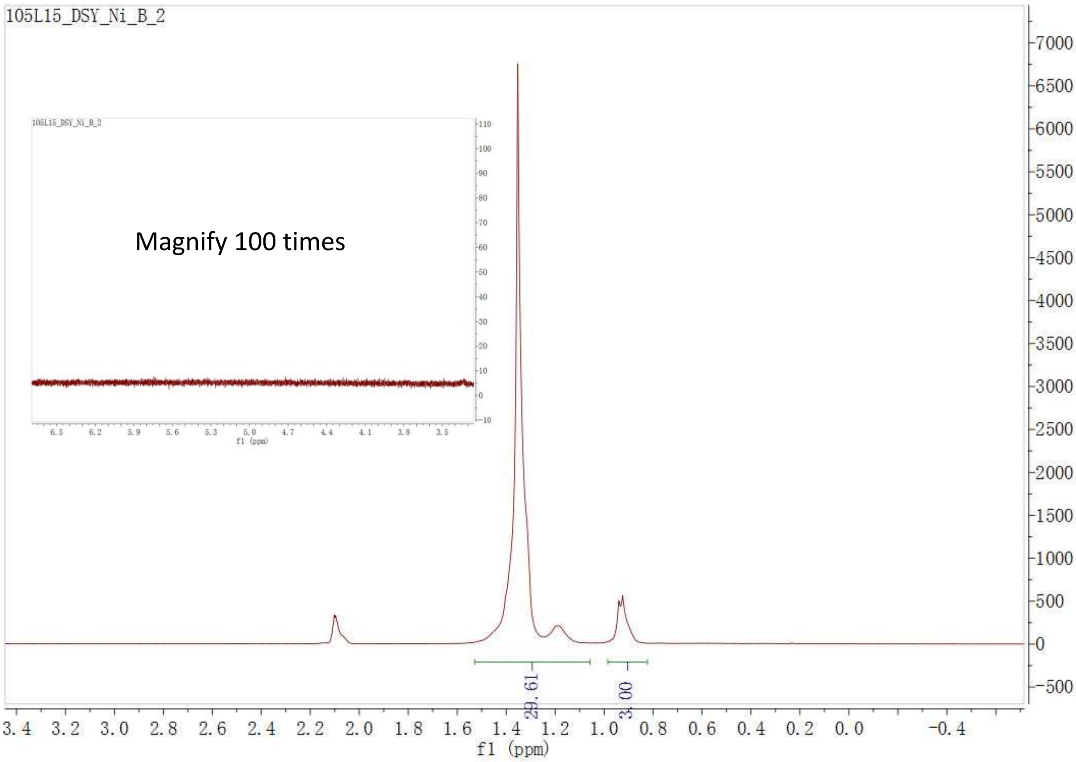


Figure S20. ^{1}H NMR spectrum of the polymer from table 1, entry 6 (Insert: the region of δ 6.0-4.0, magnify 100 times). (d^{8}-toluene, 80°C).

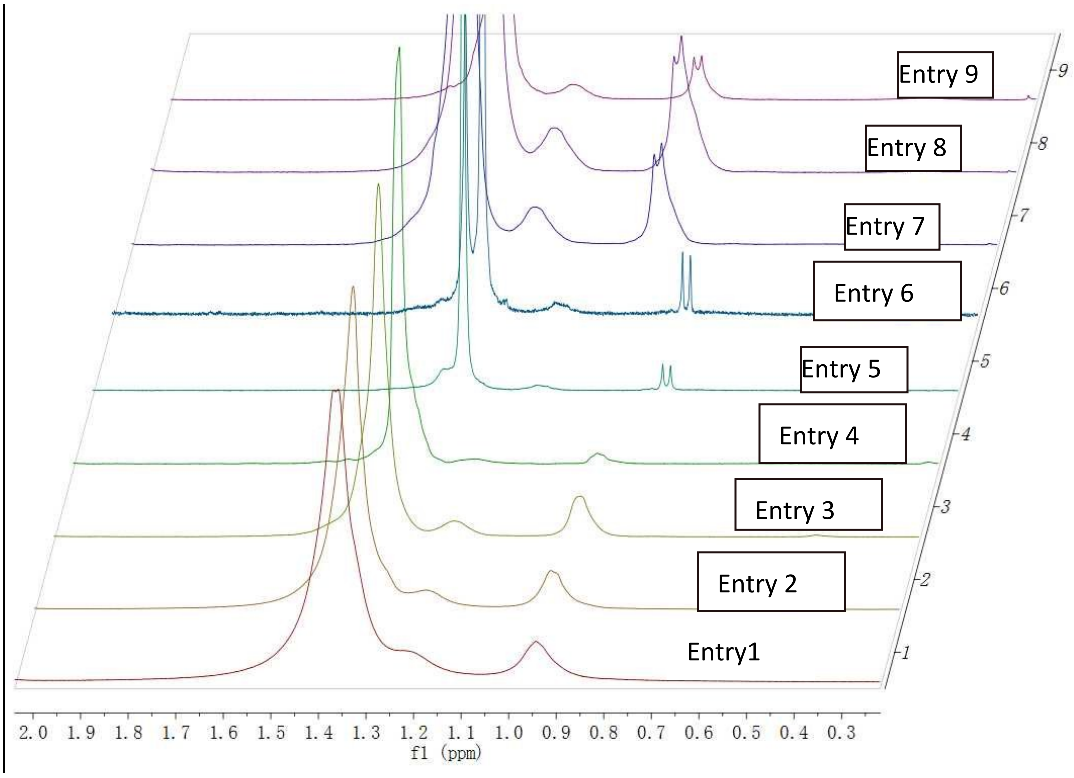


Figure S21. ^{1}H NMR spectrum of the polymer from table 1, entry 1-9. (d^{8}-toluene, 80°C).

Table S2. Polymer Chain Branching Distribution (%) and Number of Branches per 1000 Carbons.*

polymer	methyl	ethyl	propyl	butyl	*sec*-butyl [a]	butyl+	Total（^{13}C）	Total(^{1}H)[b]
1-20	**100**	**0**	**0**	**0**	**0**	**0**	**42**	**49**
1-50	**95.9**	**0**	**0**	**0**	**0**	**4.1**	**59**	**66**
1-80	**60.2**	**6.4**	**2.9**	**6.3**	**6.4**	**17.8**	**77**	**71**

*polymer from table 1, entry 1-3.

[a] Percentage of methyl from *sec*-butyl branches in the total methyl branches. Measured by ^{13}C NMR in $CDCl_2CDCl_2$ at 120 °C

[b] Measured by ^{1}HNMR in d^{8}-toluene, 80^{o}C**.**

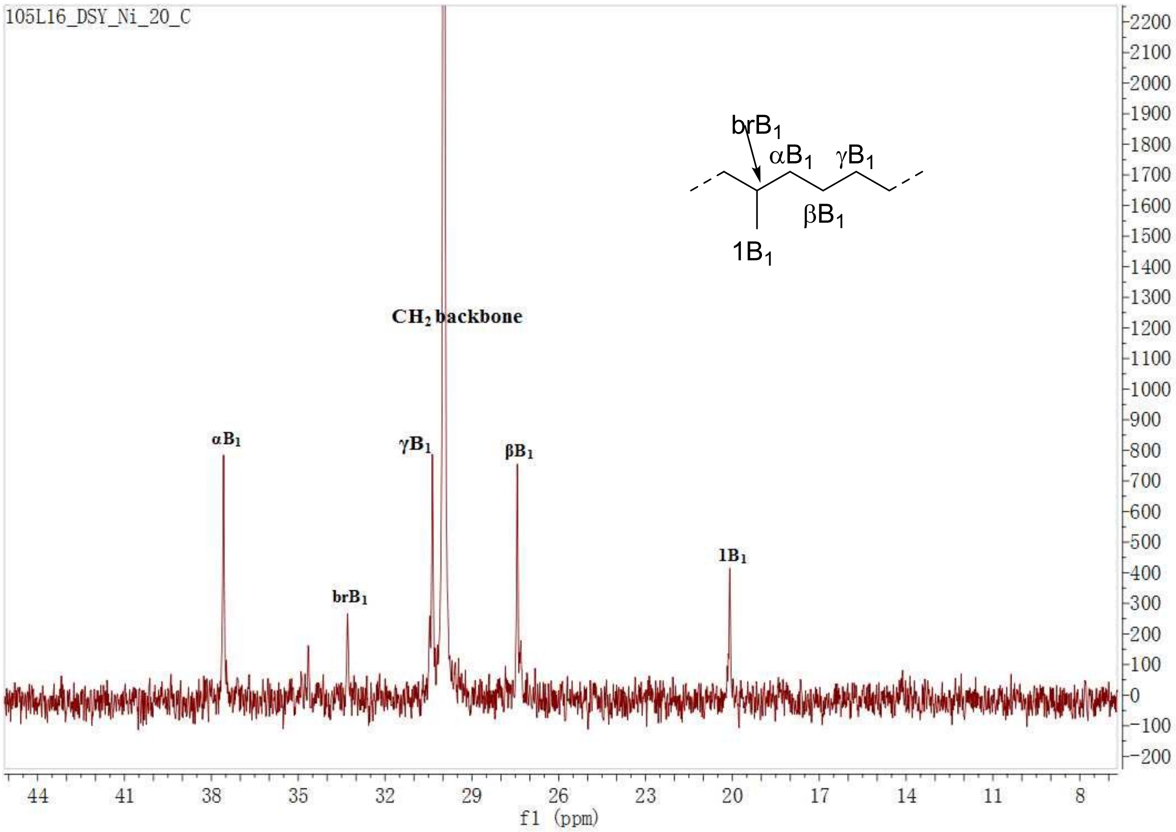


Figure S22. ^{13}C NMR spectrum of the polymer from table 1, entry 1.

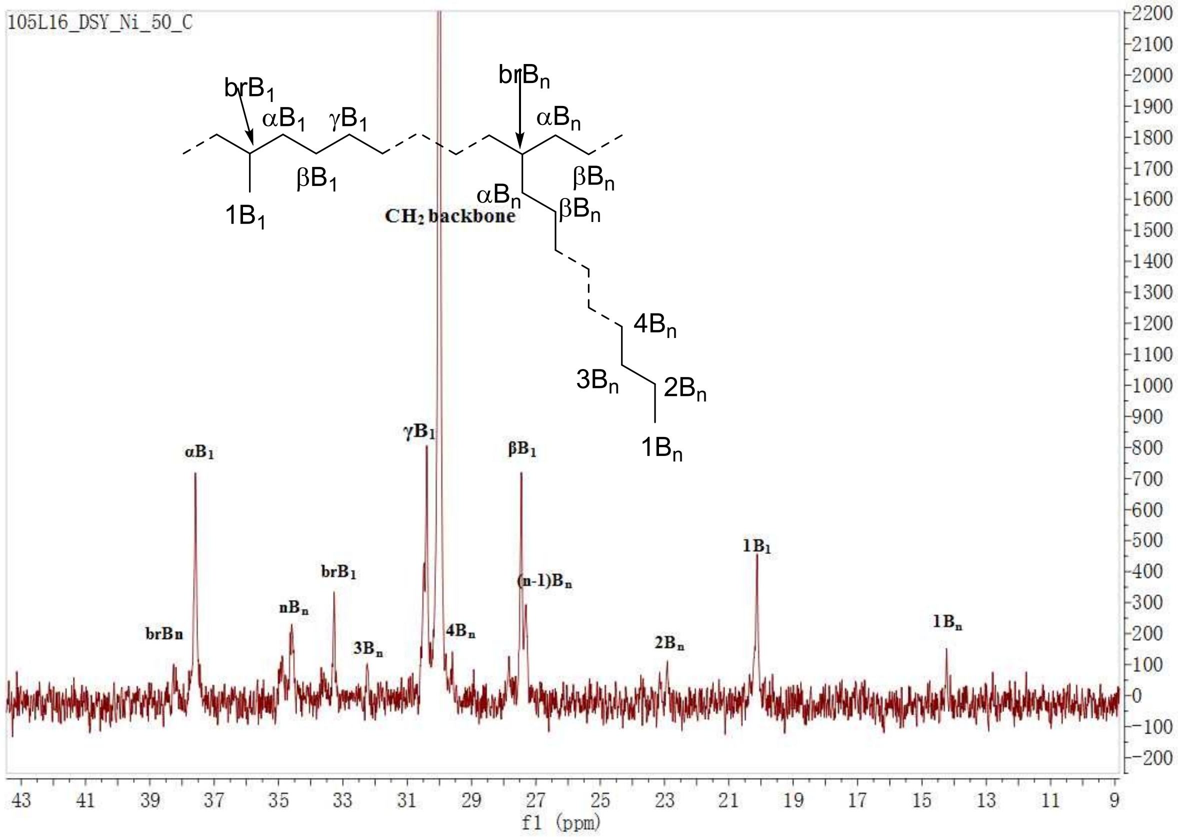


Figure S23. ^{13}C NMR spectrum of the polymer from table 1, entry 2.

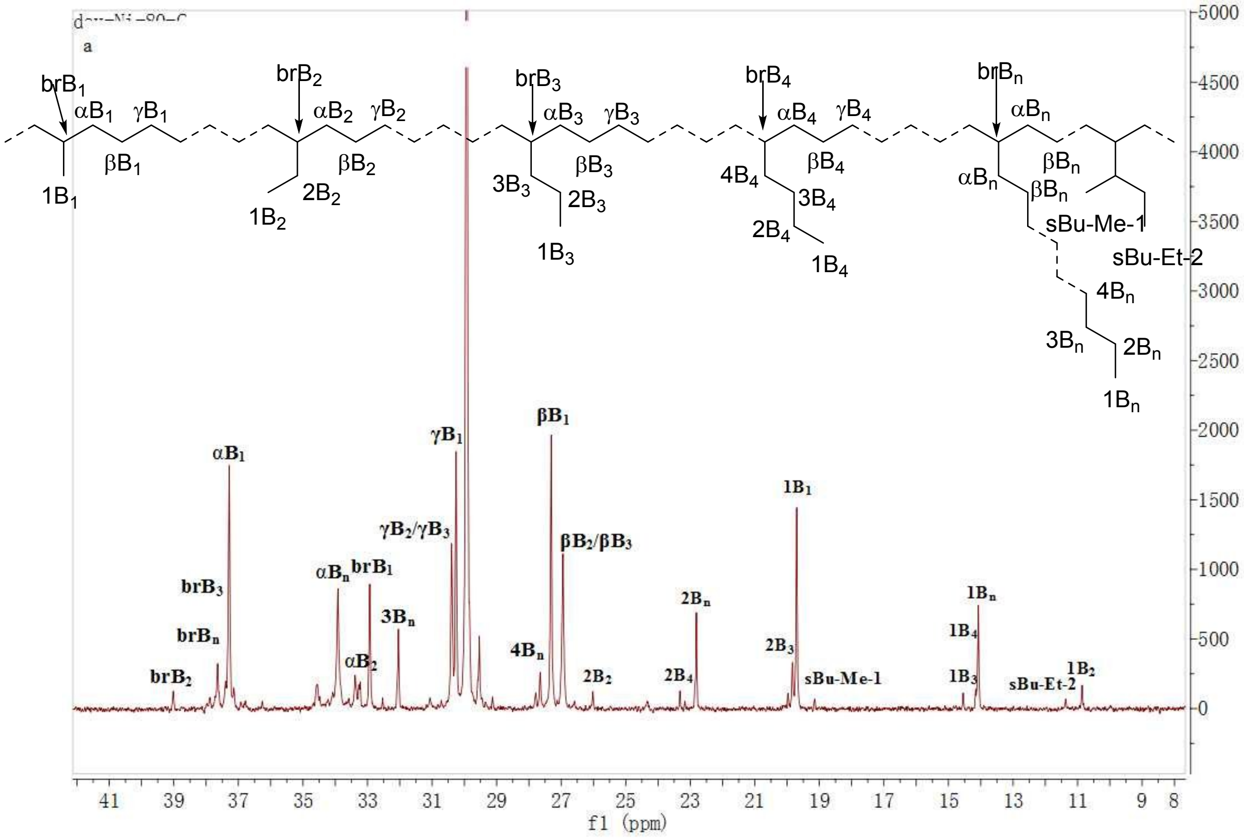


Figure S24. ^{13}C NMR spectrum of the polymer from table 1, entry 3.

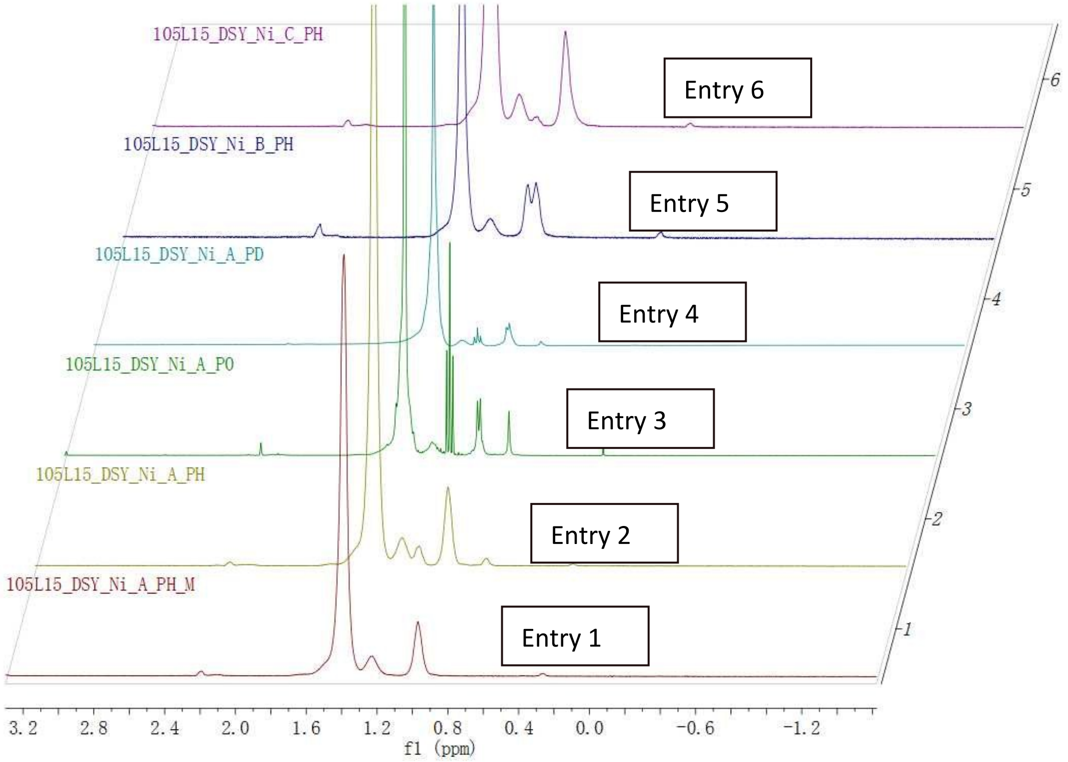


Figure S25. ^{1}H NMR spectrum of the polymer from table 2, entry 1-6. (d^8-toluene, 80°C).

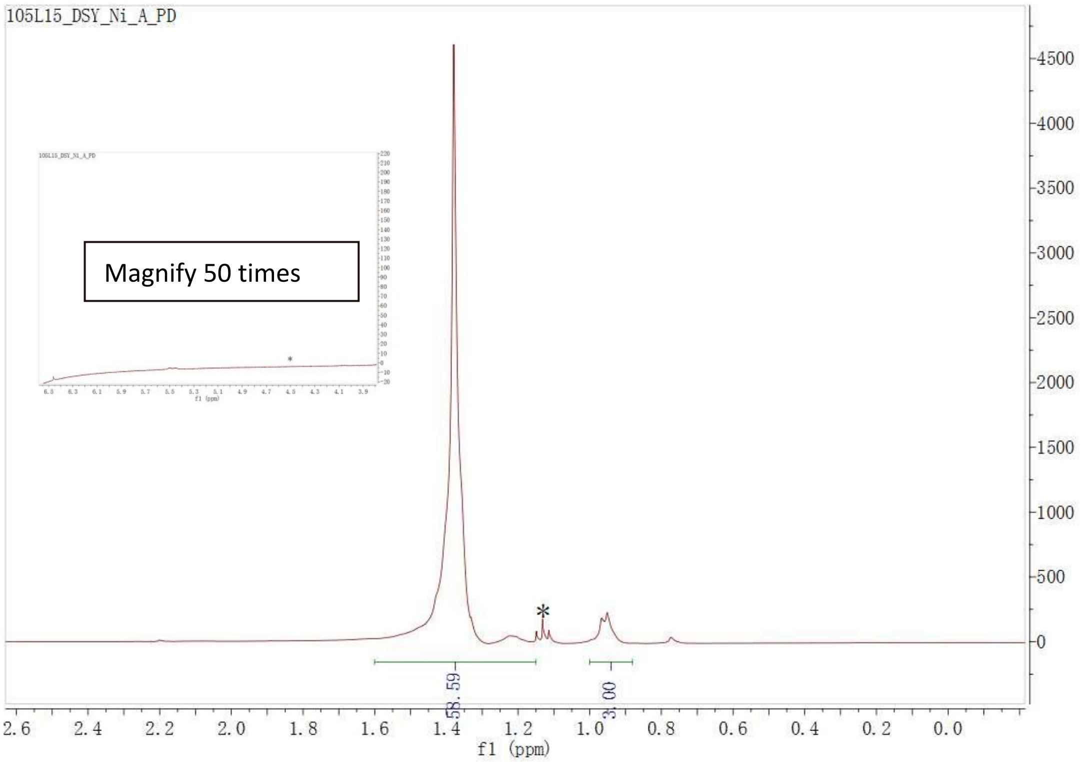


Figure S26. ^{1}H NMR spectrum of the polymer from table 2, entry 4. *$C\mathit{H}_3CH_2OH$ (d^6-benzene:1,2,4-trichlorobenzene=1:3 (v/v) 100°C).

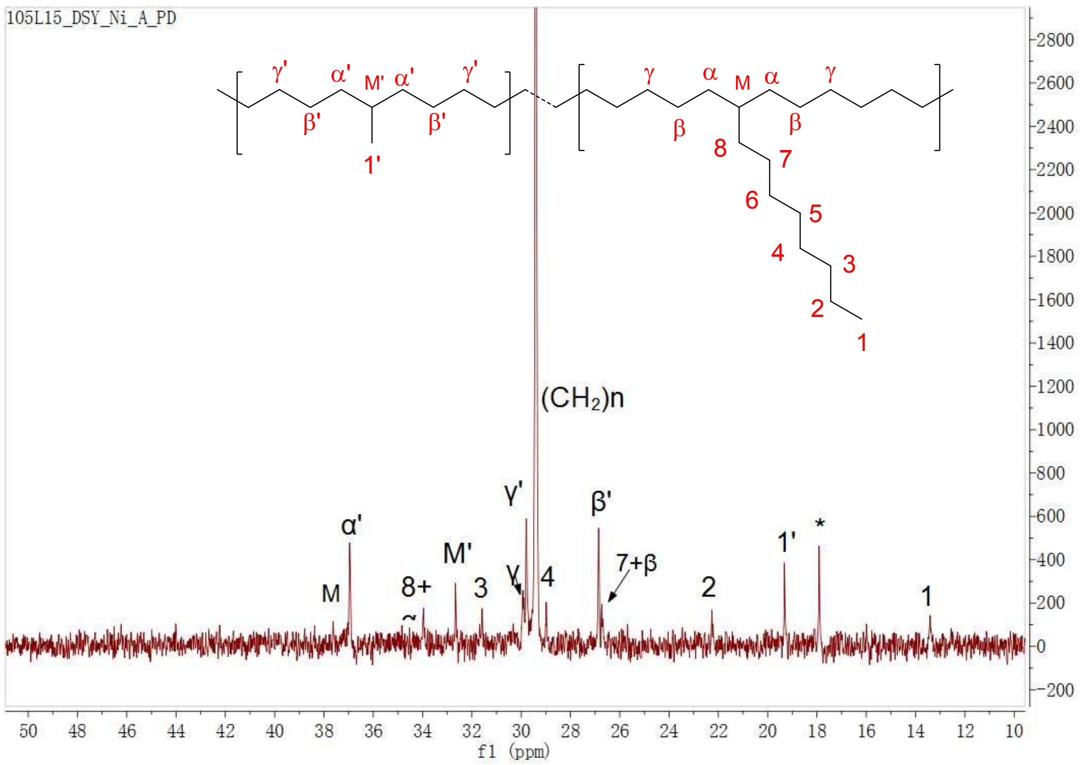


Figure S27. ^{13}C NMR spectrum of the polymer from table 2, entry 4. *CH$_3$CH$_2$OH (d^6-benzene:1,2,4-trichlorobenzene=1:3 (v/v) 100^{o}C).

2.4 DSC, GPC of polymer.

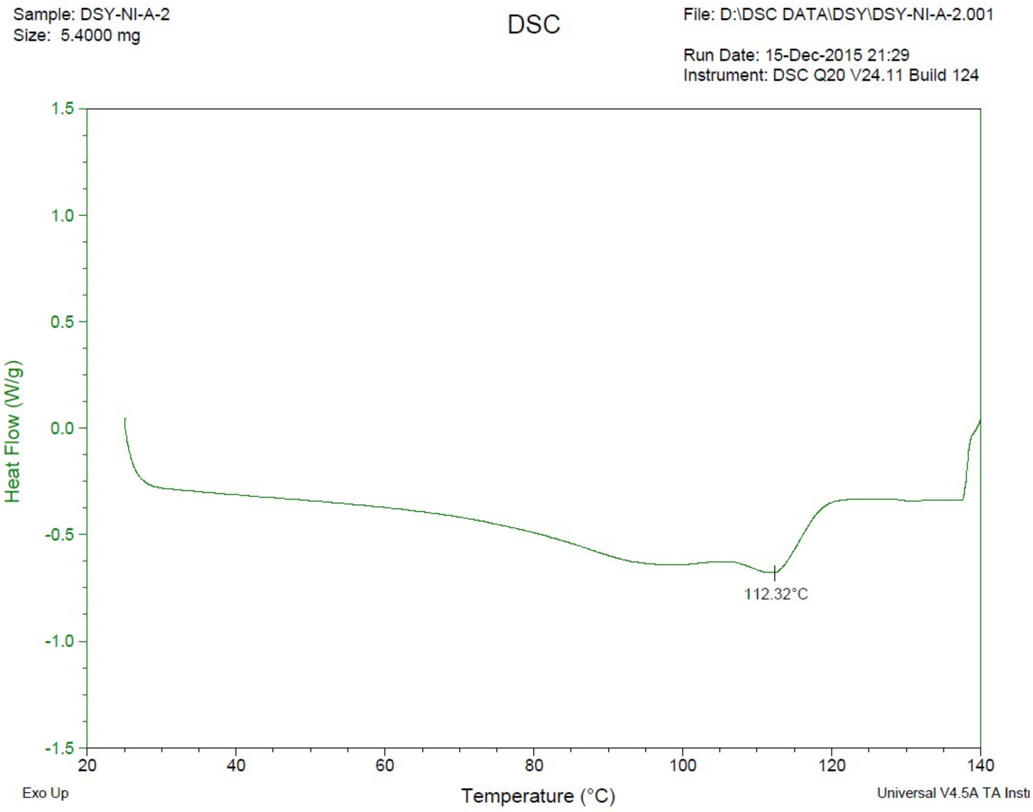


Figure S28. DSC of the polymer from table 1, entry 5.

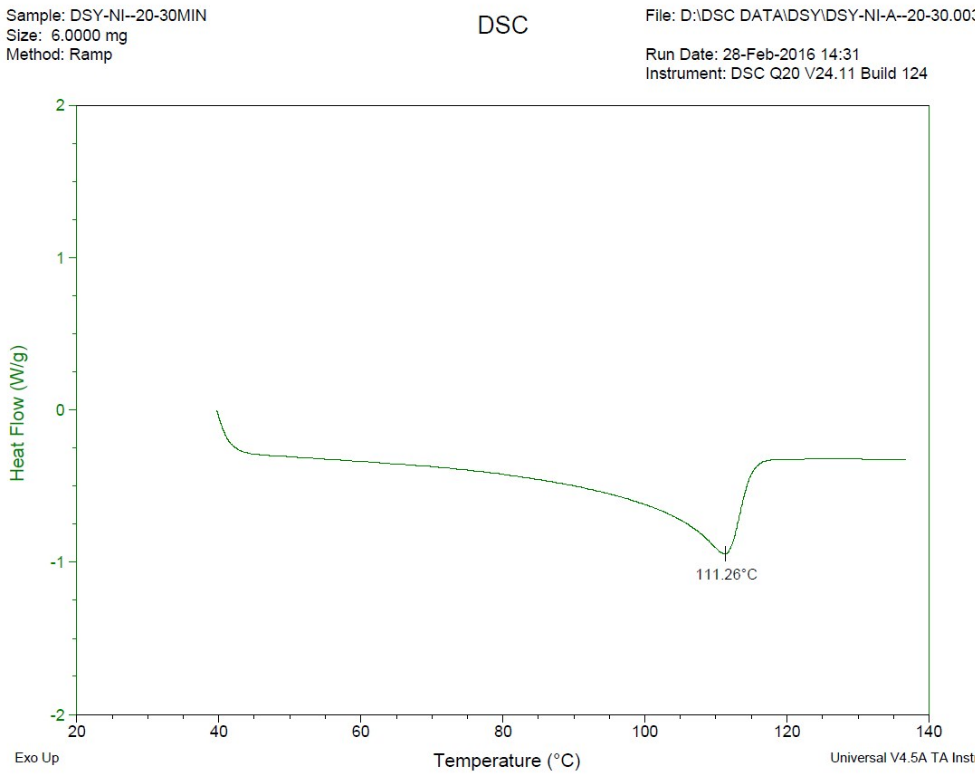


Figure S29. DSC of the polymer from table 1, entry 6.

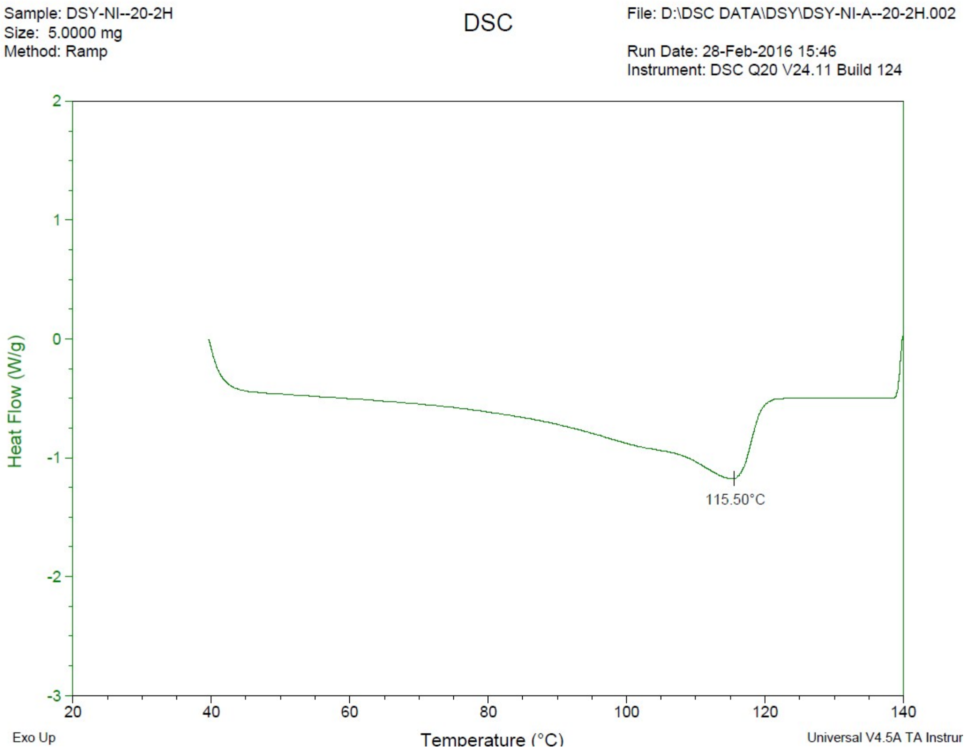


Figure S30. DSC of the polymer from table 1, entry 7

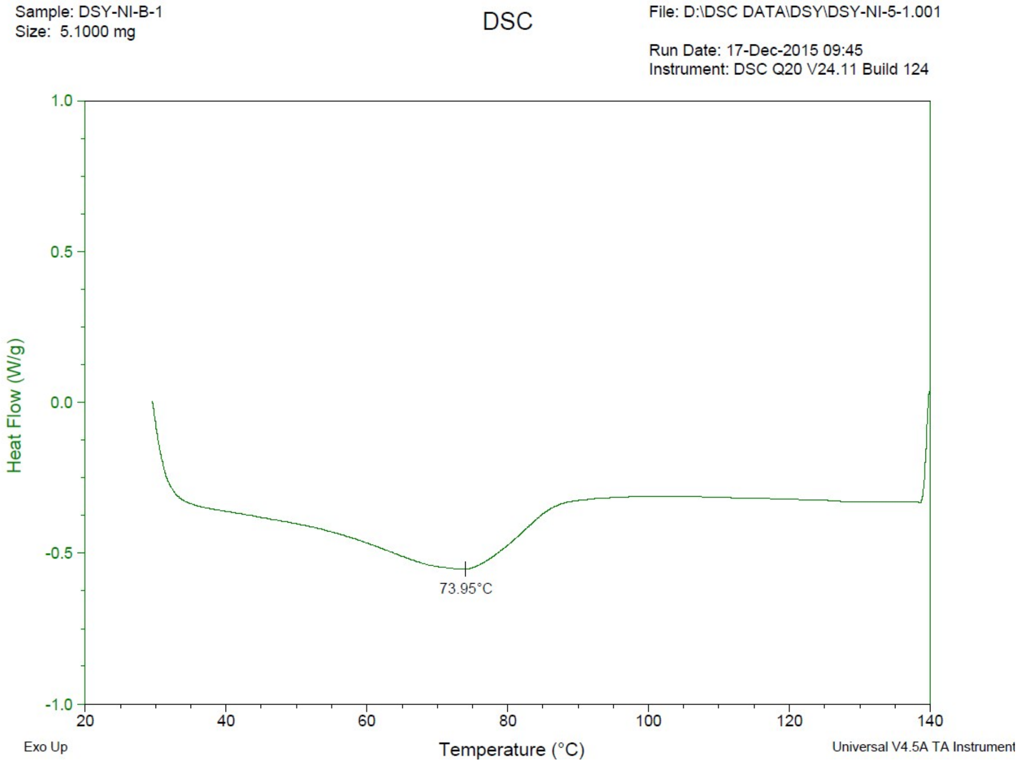


Figure S31. DSC of the polymer from table 1, entry 8.

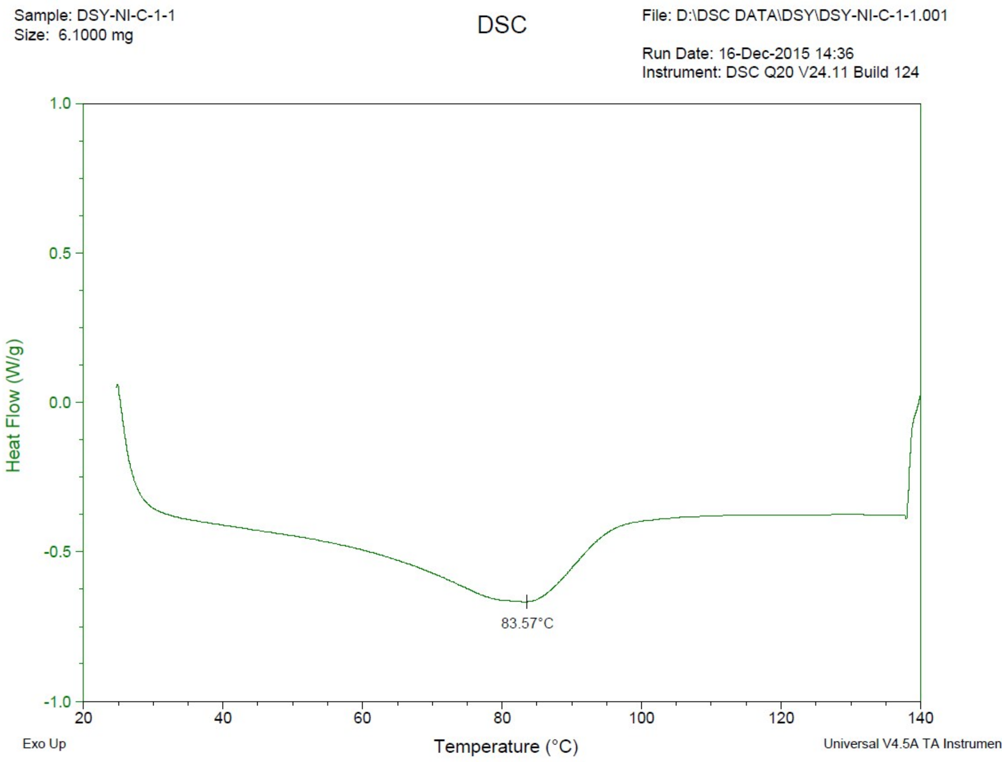


Figure S32. DSC of the polymer from table 1, entry 9.

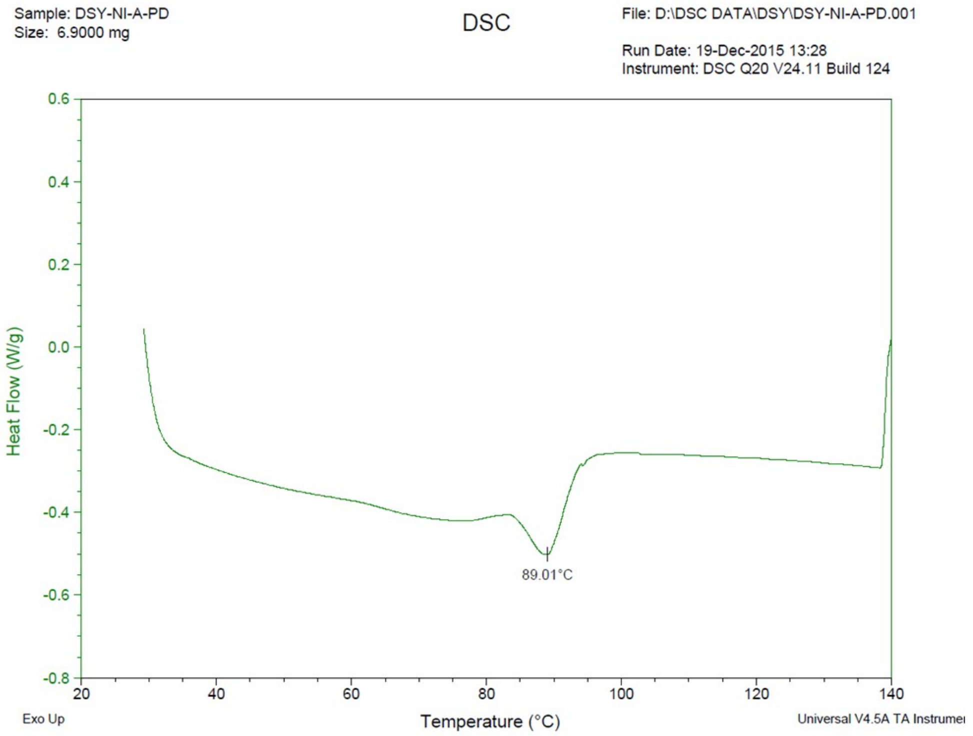


Figure S33. DSC of the polymer from table 2, entry 4.

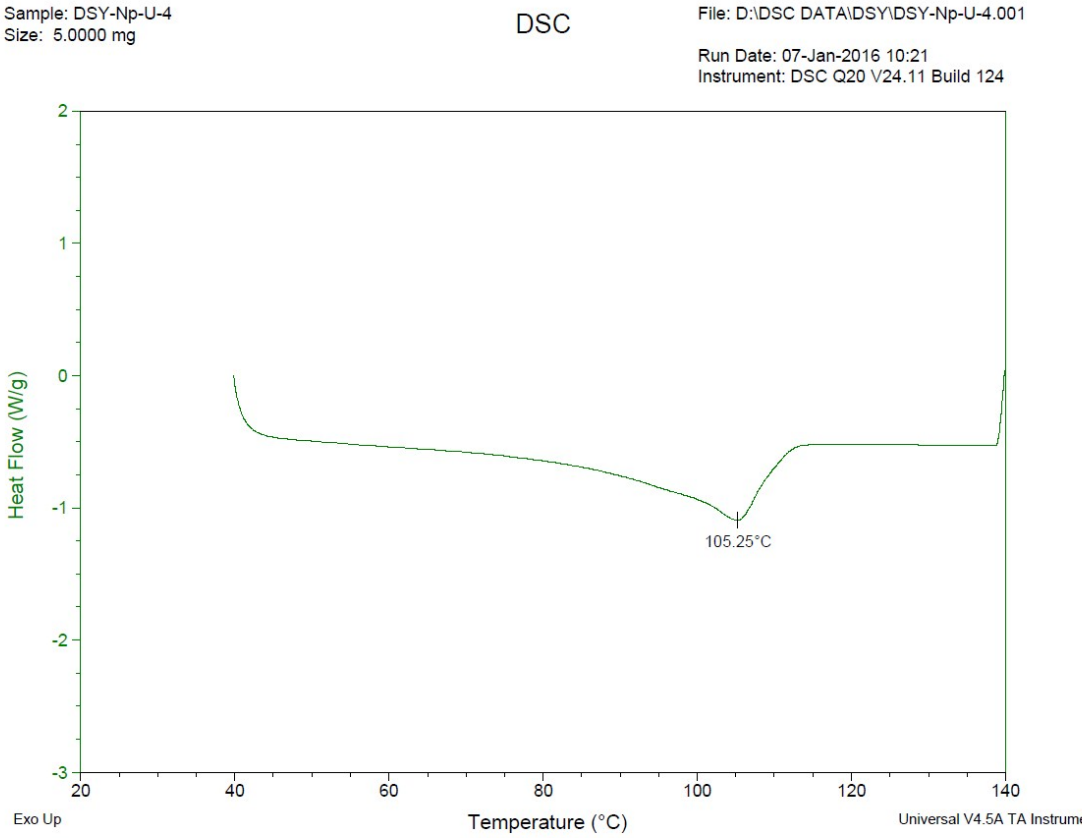


Figure S34. DSC of the polymer from table 2, entry 8.

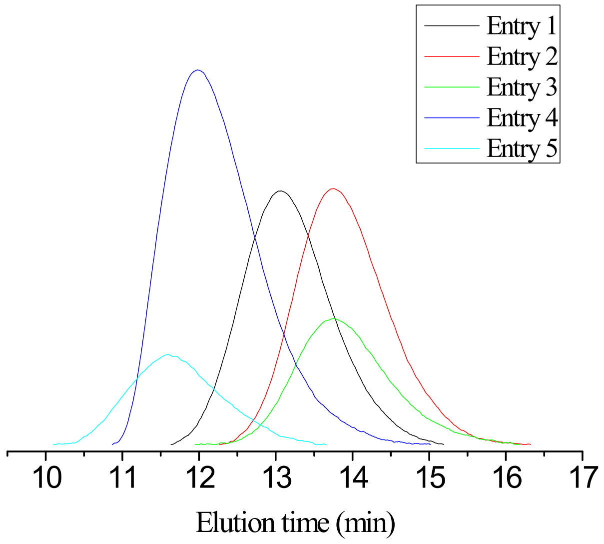


Figure S35. GPC traces for the polymers generated from table 1, entry 1-5.

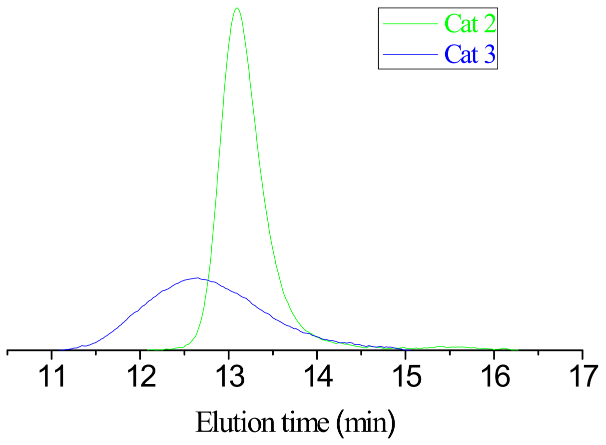


Figure S36. GPC traces for the polymers generated from table 1, entry 6-7.

3. References.

1, D. Zhang, E.T. Nadres, M. Brookhart, O. Daugulis, *Organometallics*, 2013, **32**, *5136−5143.*

2. L. Huang, Q. Li, C. Wang, C. Qi, *J. Org. Chem.* 2013, **78**, *3030−3038.*

4. X-ray Crystallography

Table S3 Crystal data and structure refinement for L3.	
Identification code	L3
Empirical formula	$C_{54}H_{40}N_2$
Formula weight	716.88
Temperature/K	296.15
Crystal system	orthorhombic
Space group	Pbca
a/Å	11.0573(12)
b/Å	25.485(3)
c/Å	28.816(3)
α /°	90
β /°	90
γ /°	90

Volume/Å^3	8120.2(16)
Z	8
ρ_{calc}g/cm^3	1.173
μ/mm^{-1}	0.068
F(000)	3024.0
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.196 to 54.562
Index ranges	$-14 \leqslant h \leqslant 13$, $-32 \leqslant k \leqslant 32$, $-36 \leqslant l \leqslant 36$
Reflections collected	59997
Independent reflections	8577 [R_{int} = 0.0598, R_{sigma} = 0.0484]
Data/restraints/parameters	8577/0/505
Goodness-of-fit on F^2	1.020
Final R indexes [I>=2σ (I)]	R_1 = 0.0493, wR_2 = 0.1173
Final R indexes [all data]	R_1 = 0.1135, wR_2 = 0.1457
Largest diff. peak/hole / e Å^{-3}	0.28/-0.19

Table S4 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for w. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	3360.0(13)	3073.0(5)	6442.3(5)	44.0(4)
N2	1762.4(17)	3703.4(8)	7341.4(7)	81.3(6)
C1	2528.9(18)	3220.0(7)	6712.1(7)	54.0(5)
C2	2749.6(19)	3486.7(7)	7155.2(6)	54.1(5)
C3	1896(3)	3979.9(10)	7731.3(9)	87.5(8)
C4	2962(2)	4040.8(9)	7945.3(8)	75.6(7)
C5	3964(2)	3814.8(9)	7764.7(7)	75.7(7)
C6	3853(2)	3530.3(8)	7354.7(7)	63.0(5)
C7	3010.7(16)	2833.8(6)	6017.9(5)	41.9(4)
C8	3255.9(16)	2304.2(6)	5969.2(6)	42.6(4)
C9	2852.4(16)	2042.8(7)	5568.9(6)	47.2(4)
C10	2168.9(17)	2277.6(7)	5235.3(6)	48.0(5)
C11	1901.6(16)	2825.6(7)	5279.6(6)	48.3(5)
C12	2396.6(16)	3118.7(7)	5659.0(6)	44.4(4)
C13	2205.6(17)	3678.3(7)	5668.2(6)	50.9(5)
C14	1417(2)	3894.8(8)	5354.2(7)	63.8(6)

C15	862(2)	3602.7(8)	5008.8(7)	66.7(6)
C16	1139.1(18)	3086.5(8)	4959.0(6)	59.5(5)
C17	2901.1(18)	4041.9(7)	5972.1(6)	49.2(5)
C18	4151.8(19)	4062.1(7)	5944.6(6)	53.6(5)
C19	4806.8(18)	4398.0(7)	6220.8(7)	55.0(5)
C20	4247.6(18)	4731.5(7)	6535.8(6)	50.5(5)
C21	2994.6(19)	4721.7(7)	6549.8(7)	59.4(5)
C22	2334.1(18)	4384.3(7)	6273.2(7)	56.5(5)
C23	4958.6(18)	5057.6(7)	6864.1(7)	52.7(5)
C24	6060.7(19)	5280.7(7)	6739.5(7)	62.7(6)
C25	6742(2)	5553.4(8)	7060.6(8)	71.1(6)
C26	6351(2)	5608.8(8)	7509.7(8)	69.8(6)
C27	5272(2)	5398.4(8)	7636.3(7)	68.9(6)
C28	4578(2)	5126.2(8)	7319.5(7)	61.6(5)
C29	1684.5(19)	1967.5(7)	4820.0(6)	55.6(5)
C30	2339(2)	2101.7(7)	4371.1(6)	54.6(5)
C31	1773(2)	2025.6(8)	3947.0(7)	68.3(6)
C32	2381(3)	2133.1(9)	3537.7(8)	86.3(8)
C33	3543(3)	2311.4(11)	3542.4(9)	92.1(8)
C34	4112(3)	2389.2(11)	3955.6(9)	92.3(8)
C35	3509(2)	2283.8(9)	4366.0(7)	75.2(6)
C36	1663(2)	1376.2(9)	4921.3(7)	73.4(7)
C37	2531(3)	1039.2(9)	4757.2(9)	98.2(9)
C38	2501(4)	511.0(12)	4883.7(13)	139.6(15)
C39	1611(6)	326.5(16)	5165.6(18)	173(3)
C40	743(5)	652.1(16)	5326.4(14)	148.7(17)
C41	753(3)	1182.2(11)	5205.1(9)	106.5(10)
C42	3803.5(16)	2009.9(6)	6380.1(6)	44.3(4)
C43	4528.4(18)	1522.5(7)	6251.4(6)	47.2(5)
C44	5786(2)	1555.9(8)	6232.3(6)	58.9(5)
C45	6490(2)	1126.3(10)	6127.2(8)	79.2(7)
C46	5960(3)	651.9(10)	6034.3(8)	82.7(7)
C47	4731(3)	608.7(8)	6046.7(7)	76.7(7)
C48	4016(2)	1037.2(7)	6159.1(7)	60.8(5)
C49	2838.9(17)	1893.9(7)	6744.4(6)	47.4(4)
C50	3072(2)	1996.3(8)	7207.7(6)	58.0(5)
C51	2240(3)	1872.0(9)	7545.6(8)	75.2(7)
C52	1159(3)	1650.1(9)	7431.0(9)	80.6(7)
C53	896(2)	1559.0(9)	6975.6(9)	79.2(7)

C54	1724.3(19)	1682.8(8)	6631.2(8)	65.5(6)

Table S5 Anisotropic Displacement Parameters (Å^2×10^3) for w. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\cdots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	54.1(10)	39.3(8)	38.5(8)	1.3(6)	-1.4(7)	2.6(7)
N2	69.3(13)	97.2(15)	77.5(13)	-31.1(12)	8.9(10)	12.1(11)
C1	55.0(12)	55.2(12)	51.8(11)	-6.4(9)	-2.3(10)	1.0(9)
C2	57.4(13)	51.8(11)	53.1(11)	-2.8(9)	3.9(10)	1.5(10)
C3	84.7(19)	97.3(19)	80.7(17)	-32.5(14)	13.1(15)	14.1(15)
C4	89.4(19)	75.2(15)	62.2(14)	-16.3(12)	9.6(14)	-0.4(14)
C5	79.2(17)	86.6(17)	61.3(14)	-10.4(12)	-5.3(12)	2.1(13)
C6	65.9(14)	66.7(13)	56.3(13)	-10.3(10)	0.6(11)	6.5(11)
C7	47.4(11)	42(1)	36.3(9)	0.2(8)	-1.8(8)	-2.8(8)
C8	50.6(11)	39.2(10)	38.1(9)	2.2(8)	-1.7(8)	1.2(8)
C9	59.9(12)	40(1)	41.6(10)	0.3(8)	-3.9(9)	-0.6(8)
C10	59.3(12)	46.6(10)	38.1(10)	2.0(8)	-4.9(9)	-5.6(9)
C11	55.7(12)	51.3(11)	37.8(10)	5.0(8)	-2.7(9)	-0.1(9)
C12	49.4(11)	43.4(10)	40.5(10)	2.8(8)	-0.7(8)	2.1(8)
C13	58.3(12)	46.0(11)	48.3(11)	4.0(9)	-1.1(9)	5.8(9)
C14	84.7(15)	47.9(11)	58.8(12)	5(1)	-9.1(12)	12.6(11)
C15	79.6(15)	66.2(14)	54.4(13)	9.0(11)	-14.7(11)	13.3(12)
C16	74.2(14)	59.6(13)	44.6(11)	4.1(9)	-11.9(10)	2.2(11)
C17	62.1(14)	37.1(10)	48.4(11)	5.7(8)	-1.9(9)	5.6(9)
C18	62.1(14)	48.2(11)	50.7(11)	-1.2(9)	5.2(10)	5.6(10)
C19	54.5(12)	52.6(11)	57.9(12)	1.8(10)	3.8(10)	-1(1)
C20	58.0(13)	38.5(10)	54.9(12)	3.8(9)	1.7(10)	1.2(9)
C21	61.5(14)	46.2(11)	70.5(13)	-10.2(10)	5.1(11)	8.1(10)
C22	51.9(12)	44.7(11)	73.0(13)	-5.2(10)	-0.5(10)	6.3(9)
C23	59.9(13)	38.7(10)	59.6(12)	4.8(9)	-1.4(10)	1.8(9)
C24	70.0(15)	56.1(12)	62.0(13)	3.6(10)	1.9(11)	-5.7(11)
C25	67.9(15)	63.1(13)	82.5(16)	3.4(12)	-6.9(13)	-12.3(11)
C26	78.9(17)	57.7(13)	72.7(15)	-1.2(11)	-16.0(13)	-3.9(12)
C27	85.4(17)	63.9(14)	57.5(13)	-3.4(11)	-1.7(12)	0.3(13)
C28	68.4(14)	54.2(12)	62.3(13)	-0.8(10)	4.7(11)	-4.8(10)
C29	71.2(14)	50.5(11)	45.0(11)	0.2(9)	-13(1)	-6.5(10)

C30	75.8(15)	43.7(11)	44.1(11)	-2.5(8)	-9.7(10)	1.9(10)
C31	102.5(18)	54.9(12)	47.3(12)	-5.6(10)	-14.9(12)	-0.4(12)
C32	143(3)	72.4(16)	43.9(14)	-8.0(11)	-11.8(15)	11.5(17)
C33	118(2)	98(2)	60.3(17)	1.1(14)	18.8(17)	18.9(18)
C34	88.8(19)	120(2)	68.1(18)	2.2(15)	11.8(15)	0.8(16)
C35	81.0(17)	94.7(17)	49.9(13)	1.4(12)	-4.4(12)	0.3(14)
C36	107.8(19)	60.0(14)	52.3(13)	3.6(11)	-30.0(13)	-28.7(14)
C37	152(3)	52.7(15)	89.8(19)	-6.4(13)	-31.5(18)	4.5(16)
C38	225(5)	54.1(19)	139(3)	1.1(19)	-60(3)	1(2)
C39	292(7)	73(3)	155(4)	30(3)	-104(4)	-63(3)
C40	221(5)	99(3)	126(3)	45(3)	-42(3)	-85(3)
C41	140(3)	97(2)	82.4(18)	18.7(16)	-26.1(18)	-52.2(19)
C42	50.9(11)	40.4(10)	41.6(10)	0.5(8)	-6.3(8)	-0.9(8)
C43	61.9(13)	43.4(10)	36.2(10)	5.2(8)	-2.2(9)	3.9(9)
C44	65.7(14)	62.4(13)	48.7(11)	-0.3(9)	-3.4(10)	4.3(11)
C45	76.5(16)	89.2(18)	71.8(15)	-1.0(13)	1.1(13)	28.0(15)
C46	111(2)	70.1(17)	66.8(15)	-1.5(12)	3.0(15)	34.4(16)
C47	121(2)	43.3(12)	66.0(14)	3(1)	-0.3(14)	6.1(14)
C48	76.4(15)	46.2(12)	59.7(12)	3.0(9)	-0.3(11)	1.1(11)
C49	57.2(12)	39.6(10)	45.5(11)	4.0(8)	-2.5(9)	5.4(9)
C50	74.9(14)	53.4(12)	45.8(11)	-0.7(9)	1.9(10)	6.3(10)
C51	107(2)	68.7(15)	49.4(13)	-2.2(11)	12.0(14)	8.9(14)
C52	94(2)	74.2(16)	73.6(17)	7.7(13)	30.3(15)	11.7(14)
C53	61.7(15)	85.8(17)	90.0(18)	13.9(14)	4.5(13)	-6.2(12)
C54	64.2(15)	74.5(14)	57.7(13)	10.2(11)	-3.3(11)	-3.6(12)

Table S6 Bond Lengths for L3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.261(2)	C24	C25	1.381(3)
N1	C7	1.420(2)	C25	C26	1.372(3)
N2	C2	1.336(2)	C26	C27	1.358(3)
N2	C3	1.335(3)	C27	C28	1.380(3)
C1	C2	1.467(3)	C29	C30	1.521(3)
C2	C6	1.353(3)	C29	C36	1.535(3)
C3	C4	1.339(3)	C30	C31	1.387(3)
C4	C5	1.352(3)	C30	C35	1.374(3)
C5	C6	1.392(3)	C31	C32	1.385(3)

C7	C8	1.384(2)	C32	C33	1.363(4)
C7	C12	1.434(2)	C33	C34	1.361(4)
C8	C9	1.405(2)	C34	C35	1.384(3)
C8	C42	1.527(2)	C36	C37	1.372(4)
C9	C10	1.361(2)	C36	C41	1.387(3)
C10	C11	1.433(3)	C37	C38	1.395(4)
C10	C29	1.531(2)	C38	C39	1.360(6)
C11	C12	1.433(2)	C39	C40	1.351(6)
C11	C16	1.417(2)	C40	C41	1.396(4)
C12	C13	1.442(2)	C42	C43	1.524(2)
C13	C14	1.372(2)	C42	C49	1.525(2)
C13	C17	1.489(3)	C43	C44	1.394(3)
C14	C15	1.386(3)	C43	C48	1.386(3)
C15	C16	1.358(3)	C44	C45	1.377(3)
C17	C18	1.386(3)	C45	C46	1.370(3)
C17	C22	1.381(2)	C46	C47	1.364(3)
C18	C19	1.375(3)	C47	C48	1.387(3)
C19	C20	1.389(2)	C49	C50	1.384(2)
C20	C21	1.386(3)	C49	C54	1.384(3)
C20	C23	1.485(3)	C50	C51	1.377(3)
C21	C22	1.381(3)	C51	C52	1.362(3)
C23	C24	1.392(3)	C52	C53	1.364(3)
C23	C28	1.389(3)	C53	C54	1.387(3)

Table S7 Bond Angles for L3.

Atom	Atom	Atom	Angle/	Atom	Atom	Atom	Angle/
C1	N1	C7	117.41(15)	C28	C23	C24	117.23(18)
C3	N2	C2	117.8(2)	C25	C24	C23	120.7(2)
N1	C1	C2	123.59(18)	C26	C25	C24	120.8(2)
N2	C2	C1	113.90(18)	C27	C26	C25	119.3(2)
N2	C2	C6	122.15(18)	C26	C27	C28	120.6(2)
C6	C2	C1	123.91(19)	C27	C28	C23	121.3(2)
N2	C3	C4	123.1(2)	C10	C29	C36	111.33(15)
C3	C4	C5	119.6(2)	C30	C29	C10	112.47(15)
C4	C5	C6	118.4(2)	C30	C29	C36	112.93(17)
C2	C6	C5	118.9(2)	C31	C30	C29	120.2(2)
N1	C7	C12	122.17(15)	C35	C30	C29	122.20(17)

C8	C7	N1	116.92(14)	C35	C30	C31	117.6(2)
C8	C7	C12	120.88(15)	C32	C31	C30	120.2(2)
C7	C8	C9	118.92(15)	C33	C32	C31	121.0(2)
C7	C8	C42	118.57(14)	C34	C33	C32	119.5(3)
C9	C8	C42	121.99(15)	C33	C34	C35	119.8(3)
C10	C9	C8	123.21(16)	C30	C35	C34	121.9(2)
C9	C10	C11	118.67(16)	C37	C36	C29	122.5(2)
C9	C10	C29	121.29(16)	C37	C36	C41	119.2(2)
C11	C10	C29	120.04(16)	C41	C36	C29	118.2(3)
C12	C11	C10	119.82(15)	C36	C37	C38	119.8(3)
C16	C11	C10	121.47(16)	C39	C38	C37	120.4(4)
C16	C11	C12	118.71(17)	C40	C39	C38	120.5(4)
C7	C12	C13	123.82(15)	C39	C40	C41	120.2(4)
C11	C12	C7	117.85(15)	C36	C41	C40	119.9(4)
C11	C12	C13	118.27(15)	C43	C42	C8	114.84(13)
C12	C13	C17	123.41(16)	C43	C42	C49	112.17(14)
C14	C13	C12	118.60(17)	C49	C42	C8	110.58(14)
C14	C13	C17	117.75(16)	C44	C43	C42	118.97(17)
C13	C14	C15	122.60(18)	C48	C43	C42	123.97(18)
C16	C15	C14	119.75(19)	C48	C43	C44	117.06(18)
C15	C16	C11	121.32(18)	C45	C44	C43	121.6(2)
C18	C17	C13	120.32(17)	C46	C45	C44	120.2(2)
C22	C17	C13	121.89(18)	C47	C46	C45	119.5(2)
C22	C17	C18	117.73(18)	C46	C47	C48	120.7(2)
C19	C18	C17	121.04(18)	C43	C48	C47	120.9(2)
C18	C19	C20	121.65(19)	C50	C49	C42	119.80(17)
C19	C20	C23	121.56(18)	C54	C49	C42	122.40(17)
C21	C20	C19	116.94(18)	C54	C49	C50	117.80(18)
C21	C20	C23	121.39(17)	C51	C50	C49	120.9(2)
C22	C21	C20	121.52(18)	C52	C51	C50	120.7(2)
C17	C22	C21	121.06(19)	C51	C52	C53	119.4(2)
C24	C23	C20	121.87(18)	C52	C53	C54	120.6(2)
C28	C23	C20	120.80(18)	C49	C54	C53	120.5(2)

Table S8 Torsion Angles for L3.

A	B	C	D	Angle/	A	B	C	D	Angle/
N1	C1	C2	N2	167.00(19)	C18	C17	C22	C21	-2.3(3)

N1	C1	C2	C6	-10.7(3)	C18	C19	C20	C21	-1.9(3)
N1	C7	C8	C9	175.66(15)	C18	C19	C20	C23	174.22(17)
N1	C7	C8	C42	3.8(2)	C19	C20	C21	C22	1.9(3)
N1	C7	C12	C11	-169.62(16)	C19	C20	C23	C24	36.1(3)
N1	C7	C12	C13	7.7(3)	C19	C20	C23	C28	-140.09(19)
N2	C2	C6	C5	-0.7(3)	C20	C21	C22	C17	0.2(3)
N2	C3	C4	C5	-0.1(4)	C20	C23	C24	C25	-175.69(18)
C1	N1	C7	C8	-111.23(19)	C20	C23	C28	C27	175.51(18)
C1	N1	C7	C12	66.8(2)	C21	C20	C23	C24	-148.01(19)
C1	C2	C6	C5	176.85(19)	C21	C20	C23	C28	35.8(3)
C2	N2	C3	C4	-1.2(4)	C22	C17	C18	C19	2.4(3)
C3	N2	C2	C1	-176.2(2)	C23	C20	C21	C22	-174.17(17)
C3	N2	C2	C6	1.5(3)	C23	C24	C25	C26	0.3(3)
C3	C4	C5	C6	0.9(4)	C24	C23	C28	C27	-0.8(3)
C4	C5	C6	C2	-0.6(3)	C24	C25	C26	C27	-0.9(3)
C7	N1	C1	C2	-178.11(16)	C25	C26	C27	C28	0.7(3)
C7	C8	C9	C10	-3.8(3)	C26	C27	C28	C23	0.2(3)
C7	C8	C42	C43	-154.90(16)	C28	C23	C24	C25	0.6(3)
C7	C8	C42	C49	76.93(19)	C29	C10	C11	C12	-177.54(16)
C7	C12	C13	C14	-167.89(18)	C29	C10	C11	C16	3.4(3)
C7	C12	C13	C17	17.8(3)	C29	C30	C31	C32	-178.11(19)
C8	C7	C12	C11	8.4(3)	C29	C30	C35	C34	177.9(2)
C8	C7	C12	C13	-174.37(17)	C29	C36	C37	C38	176.2(2)
C8	C9	C10	C11	3.6(3)	C29	C36	C41	C40	-176.4(2)
C8	C9	C10	C29	-176.14(17)	C30	C29	C36	C37	26.5(3)
C8	C42	C43	C44	99.53(19)	C30	C29	C36	C41	-156.13(19)
C8	C42	C43	C48	-81.8(2)	C30	C31	C32	C33	0.4(4)
C8	C42	C49	C50	-133.02(17)	C31	C30	C35	C34	0.0(3)
C8	C42	C49	C54	47.6(2)	C31	C32	C33	C34	-0.6(4)
C9	C8	C42	C43	33.5(2)	C32	C33	C34	C35	0.4(4)
C9	C8	C42	C49	-94.69(19)	C33	C34	C35	C30	-0.1(4)
C9	C10	C11	C12	2.7(3)	C35	C30	C31	C32	-0.1(3)
C9	C10	C11	C16	-176.35(18)	C36	C29	C30	C31	77.5(2)
C9	C10	C29	C30	-107.4(2)	C36	C29	C30	C35	-100.4(2)
C9	C10	C29	C36	20.5(3)	C36	C37	C38	C39	0.5(5)
C10	C11	C12	C7	-8.5(2)	C37	C36	C41	C40	1.1(4)
C10	C11	C12	C13	174.11(17)	C37	C38	C39	C40	0.1(7)
C10	C11	C16	C15	178.27(19)	C38	C39	C40	C41	-0.1(7)
C10	C29	C30	C31	-155.50(18)	C39	C40	C41	C36	-0.5(5)

C10	C29	C30	C35	26.6(3)		C41	C36	C37	C38	-1.1(4)
C10	C29	C36	C37	-101.2(2)		C42	C8	C9	C10	167.78(17)
C10	C29	C36	C41	76.2(2)		C42	C43	C44	C45	178.67(17)
C11	C10	C29	C30	72.8(2)		C42	C43	C48	C47	-179.58(17)
C11	C10	C29	C36	-159.29(19)		C42	C49	C50	C51	-176.87(17)
C11	C12	C13	C14	9.4(3)		C42	C49	C54	C53	176.77(18)
C11	C12	C13	C17	-164.89(17)		C43	C42	C49	C50	97.37(19)
C12	C7	C8	C9	-2.4(3)		C43	C42	C49	C54	-82.1(2)
C12	C7	C8	C42	-174.30(16)		C43	C44	C45	C46	0.5(3)
C12	C11	C16	C15	-0.8(3)		C44	C43	C48	C47	-0.9(3)
C12	C13	C14	C15	-4.6(3)		C44	C45	C46	C47	0.0(4)
C12	C13	C17	C18	57.4(3)		C45	C46	C47	C48	-1.0(4)
C12	C13	C17	C22	-125.6(2)		C46	C47	C48	C43	1.4(3)
C13	C14	C15	C16	-3.2(3)		C48	C43	C44	C45	-0.1(3)
C13	C17	C18	C19	179.59(16)		C49	C42	C43	C44	-133.10(17)
C13	C17	C22	C21	-179.48(17)		C49	C42	C43	C48	45.6(2)
C14	C13	C17	C18	-116.9(2)		C49	C50	C51	C52	-0.7(3)
C14	C13	C17	C22	60.1(2)		C50	C49	C54	C53	-2.7(3)
C14	C15	C16	C11	5.9(3)		C50	C51	C52	C53	-1.1(3)
C16	C11	C12	C7	170.63(17)		C51	C52	C53	C54	1.0(4)
C16	C11	C12	C13	-6.8(3)		C52	C53	C54	C49	0.9(3)
C17	C13	C14	C15	170.05(19)		C54	C49	C50	C51	2.6(3)
C17	C18	C19	C20	-0.3(3)						

Table S9 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for L3.

Atom	*x*	*y*	*z*	U(eq)
H1	1732	3156	6626	65
H3	1217	4138	7861	105
H4	3013	4237	8216	91
H5	4709	3849	7911	91
H6	4525	3373	7220	76
H9	3062	1692	5530	57
H14	1249	4252	5374	77
H15	303	3760	4812	80
H16	822	2901	4709	71
H18	4554	3845	5736	64

H19	5645	4402	6196	66
H21	2589	4948	6750	71
H22	1494	4388	6290	68
H24	6341	5246	6437	75
H25	7475	5701	6971	85
H26	6821	5789	7725	84
H27	4998	5438	7939	83
H28	3841	4986	7413	74
H29	841	2076	4778	67
H31	982	1902	3937	82
H32	1991	2083	3255	104
H33	3945	2379	3265	111
H34	4903	2513	3962	111
H35	3907	2338	4646	90
H37	3138	1163	4562	118
H38	3094	283	4774	167
H39	1600	-26	5248	208
H40	136	523	5518	178
H41	151	1405	5314	128
H42	4376	2253	6526	53
H44	6158	1876	6292	71
H45	7327	1158	6119	95
H46	6435	362	5963	99
H47	4369	288	5979	92
H48	3180	998	6173	73
H50	3801	2151	7292	70
H51	2417	1940	7855	90
H52	606	1561	7661	97
H53	154	1413	6895	95
H54	1529	1623	6322	79

Experimental

Single crystals of $C_{54}H_{40}N_2$ **L3** were yellow. A suitable crystal was selected and mounted on a 'CCD area detector' diffractometer. The crystal was kept at 296.15 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.

3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of L3

Crystal Data for $C_{54}H_{40}N_2$ (M =716.88 g/mol): orthorhombic, space group Pbca (no. 61), a = 11.0573(12) Å, b = 25.485(3) Å, c = 28.816(3) Å, V = 8120.2(16) $Å^3$, Z = 8, T = 296.15 K, μ(MoKα) = 0.068 mm^{-1}, $Dcalc$ = 1.173 g/cm^3, 59997 reflections measured (3.196° ≤ 2Θ ≤ 54.562°), 8577 unique (R_{int} = 0.0598, R_{sigma} = 0.0484) which were used in all calculations. The final R_1 was 0.0493 (I > 2σ(I)) and wR_2 was 0.1457 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
2.a Ternary CH refined with riding coordinates:
 C29(H29), C42(H42)
2.b Aromatic/amide H refined with riding coordinates:
 C1(H1), C3(H3), C4(H4), C5(H5), C6(H6), C9(H9), C14(H14), C15(H15), C16(H16),
 C18(H18), C19(H19), C21(H21), C22(H22), C24(H24), C25(H25), C26(H26), C27(H27),
  C28(H28), C31(H31), C32(H32), C33(H33), C34(H34), C35(H35), C37(H37),
 C38(H38), C39(H39), C40(H40), C41(H41), C44(H44), C45(H45), C46(H46), C47(H47),
  C48(H48), C50(H50), C51(H51), C52(H52), C53(H53), C54(H54)