Supplementary Information

Systematic studies on dibenzhydryl and pentiptycenyl substituted pyridine-imine nickel(II) mediated ethylene polymerization

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Contents

1. General information

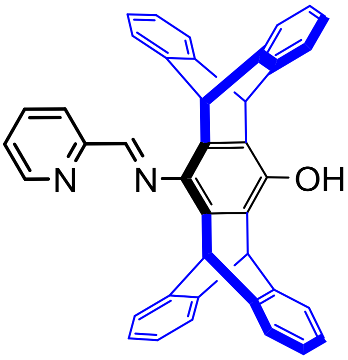
General Procedures: All syntheses involving air- and moisture sensitive compounds were carried out using standard Schlenk-type glassware (or in a glove box) under an atmosphere of nitrogen. All solvents were purified from the MBraun SPS system. NMR spectra for the ligands, complexes, and polymers were recorded on a Bruker AV400 (^{1}H: 400 MHz, ^{13}C: 100 MHz) or a Bruker AV500 (^{1}H: 500 MHz, ^{13}C: 125 MHz). The molecular weights (M_n) and molecular weight distributions (M_w/M_n) of polyethylenes were measured by means of gel permeation chromatography (GPC) on a PL-GPC 220-type high-temperature chromatograph equipped with three PL-gel 10 μm Mixed-B LS type columns at 150 ℃. Mass spectra of the complexes were recorded on an Acquity UPLC & Quattro Premier. Elemental analysis were performed at the National Analytical Research Centre of Changchun Institute of Applied Chemistry.

X-Ray diffraction: Data collections were performed at −100 ℃ on a Bruker SMART APEX diffractometer with a CCD area detector, using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) or Cu Kα radiation (λ = 1.54178 Å). The determination of crystal class and unit cell parameters was carried out by the SMART program package.[1] The raw frame data were processed using SAINT and SADABS to yield the reflection data file.[2] All structures were solved by direct methods and refined by full-matrix least-squares procedures on F^2 using SHELXTL 2014 and Olex 2.[3] Refinement was performed on F^2 anisotropically for all non-hydrogen atoms by the full-matrix least-squares method. The hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters.

***Exceptions and special features*:** For complex **Ni2**, the program SQUEEZE[4] was used to remove mathematically the effect of the solvent. The quoted formula and derived parameters are not included the squeezed solvent molecules.

Materials: 2-acetylpyridine and 2-pyridinecarboxaldehyde were purchased from Saen Chemical Technology (Shanghai) company. 2,6-bis(diphenylmethyl)-4-methoxyaniline[4] and pentiptycene aminophenol[5] were prepared using literature procedures. The ligands **L1/L2/L3/L4** and the corresponding nickel complexes **Ni1/Ni2/Ni3/Ni4** were prepared using literature procedure.[6]

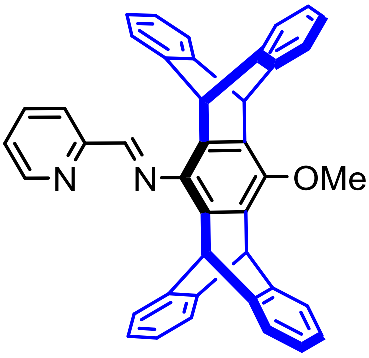
2. Preparation of Ligands and Catalysts



Synthesis of compound A: A solution of 2-pyridinecarboxaldehyde (0.93 g, 8.66 mmol), pentiptycene aminophenol (2.00 g, 4.33 mmol) and *p*-toluenesulfonic acid (10 mg) in toluene (50 mL) was refluxed for 24 h, the solvent was evaporated under reduced pressure. The crude product was washed with ethanol, petroleum ether, yielding the product as yellow solid in 44% yield (1.05 g, 1.91 mmol).

^{1}H NMR (500 MHz, 298 K, DMSO-*d*$_6$, 2.50 ppm): δ 9.39 (s, 1H, O*H*), 8.88 (d, 1H, Py-*H*), 8.56 (d, 1H, Py-*H*), 8.31 (s, 1H, N=CH), 8.15 (t, 1H, Py-*H*), 7.68 (d, 1H, Py-*H*), 7.37 (d, 4H, aryl-*H*), 7.30 (d, 4H, aryl-*H*), 6.93 (m, 8H, aryl-*H*), 5.98 (s, 2H, C*H*Ar$_3$), 5.64 (s, 2H, C*H*Ar$_3$).

Elemental analysis: Anal. Calcd for $C_{40}H_{26}N_2O$: C, 87.25; H, 4.76; N, 5.09. Found: C, 88.12; H, 4.83; N, 5.15.

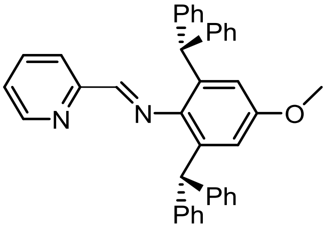


Preparation of ligand L2: To the solution of compound **A** (1.05 g, 1.91 mmol) in DMF (100 mL) at 50 ℃ was added K_2CO_3 (1.06 g, 7.64 mmol). The mixture was stirred for 1 min and MeI (0.55 g, 3.87 mmol) was added. The reaction mixture was stirred overnight at 50 ℃. The yellow suspension was cooled to room temperature and poured into 300 mL of water, extracted with dichloromethane (3*20mL). The combined organics were dried over anhydrous Na_2SO_4 and concentrated. The crude product was washed with petroleum ether, yielding the product as yellow solid in 69.6% yield (0.75 g, 1.3 mmol).

^{1}H NMR (500 MHz, 298 K, DMSO-*d*$_6$, 2.50 ppm): δ 8.89 (d, 1H, Py-*H*), 8.56 (d, 1H, Py-*H*), 8.32 (s, 1H, N=C*H*), 8.17 (t, 1H, Py-*H*), 7.72 (t, 1H, Py-*H*), 7.44 (d, 4H, aryl-*H*), 7.31 (d, 4H, aryl-*H*), 6.95 (m, 8H, aryl-*H*), 5.82 (s, 2H, C*H*Ar$_3$), 5.64 (s, 2H, C*H*Ar$_3$), 3.87 (s, 3H, OC*H*$_3$).

^{13}C{^{1}H} NMR (125 MHz, 298 K, CD_2Cl_2, 53.84 ppm): δ 166.28 (N=*C*-py), 155.02, 150.32, 148.19, 145.85, 140.21, 137.14, 136.31, 135.43, 126.06, 125.58, 123.94, 121.96, 63.33 (O*C*H$_3$), 49.51 (*C*HPh$_2$), 48.45 (*C*HPh$_2$).

Elemental analysis: Anal. Calcd for $C_{41}H_{28}N_2O$: C, 87.21; H, 5.00; N, 4.96. Found: C, 87.55; H, 5.13; N, 5.02.

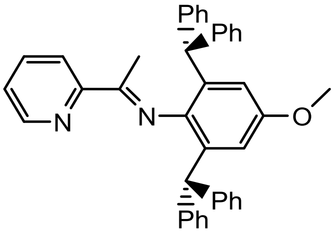


Preparation of ligand L1: A mixture of 2,6-bis(diphenylmethyl)-4-methoxyaniline (2 g, 4.39 mmol), 2-pyridinecarboxaldehyde (0.94 g, 8.78 mmol) and *p*-toluenesulfonic acid (10 mg) in toluene (50 mL) was refluxed for 12 h. After cooling down to room temperature, the solution was washed with 1N potassium hydroxide solution, and the aqueous layer was extracted with dichloromethane (3*20 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated. The crude product was washed with petroleum ether, yielding the target ligand as beige solid in 76% yield (1.82 g, 3.3 mmol).

^{1}H NMR (500 MHz, 298 K, $CDCl_3$, 7.26 ppm): δ = 8.58 (d, 1H, N=CH), 7.68 (t, 1H, aryl-*H*), 7.59 (d, 1H, aryl-*H*), 7.28 (t, 1H, aryl-*H*), 7.13-7.19 (m, 12H, aryl-*H*), 7.01-7.04 (m, 9H, aryl-*H*), 6.41 (s, 2H, aryl-*H*), 5.47 (s, 2H,Ar-C*H*(Ph)$_2$), 3.54 (s, 2H, OC*H*$_3$).

^{13}C{^{1}H} NMR (125 MHz, 298 K, CD_2Cl_2, 53.84 ppm): δ166.21 (N=*C*-py), 156.10, 154.41, 149.74, 144.23, 143.93, 136.59, 134.92, 129.91, 128.60, 126.65, 125.44, 121.44, 114.21, 55.41 (O*C*H$_3$), 52.38 (*C*HPh$_2$).

Elemental analysis: Anal. Calcd for $C_{39}H_{32}N_2O$: C, 86.00; H, 5.92; N, 5.14. Found: C, 86.38; H, 5.85; N, 5.04.

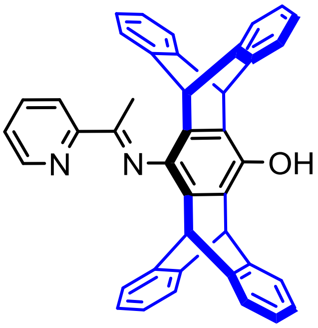


Preparation of ligand L3: A solution of 2,6-bis(diphenylmethyl)-4-methoxyaniline (2.00 g, 4.39 mmol), 2-acetylpyridine (0.64 g, 5.30 mmol) and *p*-toluenesulfonic acid (10 mg) in toluene (50 mL) was refluxed for 30 h. After cooling down to room temperature, the solution was washed by 1N potassium hydroxide solution, and the organic layer was separated. The aqueous layer was extracted with dichloromethane (3*20mL). The combined organics were dried over anhydrous Na_2SO_4 and concentrated. The crude product was washed with petroleum ether, yielding the product as yellow solid in 50% yield (1.23 g, 2.2 mmol).

^{1}H NMR (500 MHz, 298 K, $CDCl_3$, 7.26 ppm): δ 8.58 (s, 1H, N=CH), 7.99 (d, 1H, Py-*H*), 7.71 (t, 1H, Py-*H*), 7.33 (t, 1H, Py-*H*), 7.20-7.24 (m, 4H, aryl-*H*), 7.12-7.19 (m, 8H, aryl-*H*), 6.99-7.05 (m, 8H, aryl-*H*), 6.46 (s, 2H, aryl-*H*), 5.27 (s, 2H, Ar-C*H*(Ph)$_2$), 3.56 (s, 3H, OC*H*$_3$), 1.07 (s, 3H, N=C-*Me*).

$^{13}C\{^1H\}$ NMR (125 MHz, 298 K, CD_2Cl_2, 53.84 ppm): *δ* 170.78 (N=*C*-py), 155.58, 148.78, 143.80, 142.90, 133.95, 130.08, 129.75, 128.69, 128.60, 128.50, 126.66, 126.57, 125.10, 121.61, 114.41, 55.45 (O*C*H_3), 52.38 (*C*HPh_2), 17.18 (N=C-*Me*).

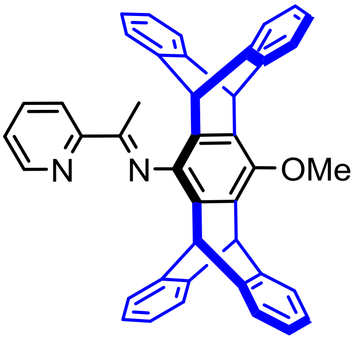
Elemental analysis: Anal. Calcd for $C_{40}H_{34}N_2O$: C, 85.99; H, 6.13; N, 5.01. Found: C, 86.36; H, 6.21; N, 5.08.



Synthesis of compound B: A solution of 2-acetylpyridine (0.63g, 5.20mmol), pentiptycene aminophenol (2.00 g, 4.33 mmol) and *p*-toluenesulfonic acid (10 mg) in toluene (50 mL) was refluxed for 24 h, the solvent was evaporated under reduced pressure. The crude product was washed with ethanol, petroleum ether, yielding the product as beige solid in 75.7% yield (1.85 g, 3.28 mmol).

^1H NMR (400 MHz, 298 K, DMSO-d6, 2.50 ppm): δ 9.09 (s, 1H, O*H*), 8.83 (d, 1H, Py-*H*), 8.56 (d, 1H, Py-*H*), 8.12 (s, 1H, N=CH), 7.69 (t, 1H, Py-*H*), 7.36-7.20 (m, 10H, aryl-*H*), 6.89 (m, 10H, aryl-*H*), 5.94 (s, 2H, C*H*Ar_3), 5.15 (s, 2H, C*H*Ar_3), 1.92 (s, 3H, N=C-*Me*).

Elemental analysis: Anal. Calcd for $C_{41}H_{28}N_2O$: C, 87.21; H, 5.00; N, 4.96. Found: C, 87.80; H, 4.86; N, 5.01.



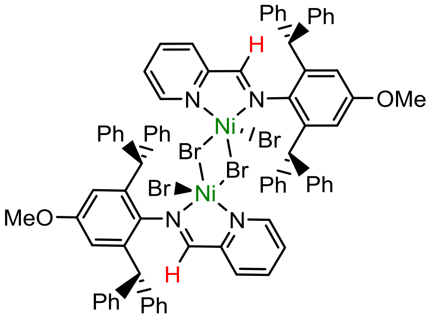
Preparation of ligand L4: To the solution of compound **B** (1.40 g, 2.48 mmol) in DMF (100 mL) at 50 ℃ was added K_2CO_3 (1.37 g, 9.92 mmol). The mixture was stirred for 1 min and MeI (0.70 g, 4.96 mmol) was added. The reaction mixture was stirred overnight at 50 ℃. The yellow suspension was cooled to room temperature and poured into 300 mL of water, extracted with dichloromethane (3*20mL). The combined organics were dried over anhydrous Na_2SO_4 and concentrated. The crude product was washed with petroleum ether, yielding the product as yellow solid in 76.6% yield (1.10 g, 1.90 mmol).

^1H NMR (500 MHz, 298 K, DMSO-d_6, 2.50 ppm): δ 8.85 (d, 1H, Py-*H*), 8.54 (d, 1H, Py-*H*), 8.13 (t, 1H, Py-*H*), 7.71 (t, 1H, Py-*H*), 7.43 (d, 4H, aryl-*H*), 7.27 (d, 4H, aryl-

H), 6.91 (m, 8H, aryl-*H*), 5.80 (s, 2H, C*H*Ar$_3$), 5.22 (s, 2H, C*H*Ar$_3$), 3.87 (s, 3H, OC*H*$_3$), 1.95 (s, 3H, N=C-*Me*).

^{13}C{^{1}H} NMR (125 MHz, 298 K, CD$_2$Cl$_2$, 53.84 ppm): δ 170.94 (N=*C*-py), 156.76, 149.20, 147.06, 146.02, 145.90, 145.66, 138.76, 137.04, 136.12, 132.69, 125.70, 123.99, 123.88, 123.82, 122.07, 63.46 (O*C*H$_3$), 49.52 (*C*HPh$_2$), 48.55 (*C*HPh$_2$), 17.88 (N=C-*Me*).

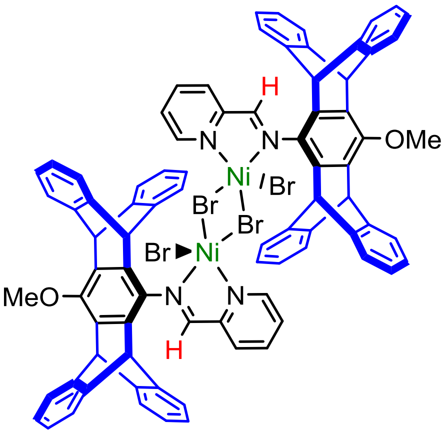
Elemental analysis: Anal. Calcd for $C_{42}H_{30}N_2O$: C, 87.17; H, 5.23; N, 4.84. Found: C, 87.53; H, 5.31; N, 4.94.



Preparation of complex Ni1: A mixture of **L1** (223 mg, 0.409 mmol) and (DME)NiBr$_2$ (120 mg, 0.389 mmol) was stirred in 25 mL of dichloromethane overnight at room temperature. The solvent was evaporated under reduced pressure, and the desired compound can be isolated by repeated recrystallization from n-hexane and dichloromethane. 230 mg of pure compound was obtained as an orange solid in 77.7% yield.

MALDI-TOF-MS (m/z): 681.1 [M-Br]$^+$.

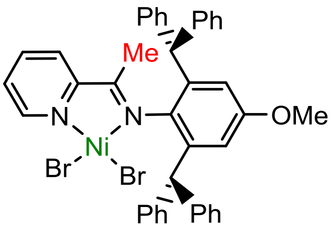
Elemental analysis: Anal. Calcd for $C_{78}H_{64}Br_4N_4Ni_2O_2$: C, 61.38; H, 4.23; N, 3.67. Found: C, 61.50; H, 4.53; N, 3.81.



Preparation of complex Ni2: A mixture of **L2** (231 mg, 0.409 mmol) and (DME)NiBr$_2$ (120 mg, 0.389 mmol) (DME = 1,2-dimethoxyethane) were stirred in 25 mL of dichloromethane overnight at room temperature. The solvent was evaporated under reduced pressure, the desired compound can be isolated from repeated recrystallized from n-hexane and dichloromethane. The pure compound was obtained as an orange solid (250mg, 82.1% yield).

MALDI-TOF-MS (m/z): 701.1 [M-Br]$^+$.

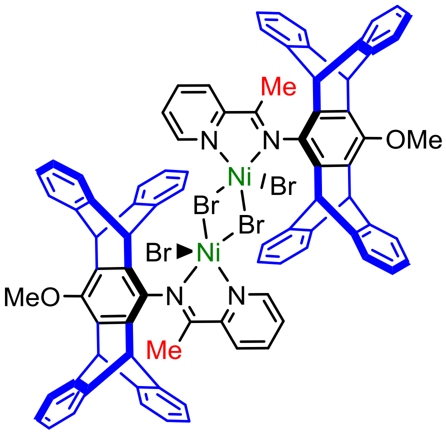
Elemental analysis: Anal. Calcd for $C_{82}H_{56}Br_4N_4Ni_2O_2$: C, 62.88; H, 3.60; N, 3.58. Found: C, 62.73; H, 3.48; N, 3.67.



Preparation of complex Ni3: A mixture of **L3** (229 mg, 0.410 mmol) and (DME)$NiBr_2$ (120 mg, 0.389 mmol) (DME = 1,2-dimethoxyethane) were stirred in 25 mL of dichloromethane overnight at room temperature. The solvent was evaporated under reduced pressure, the desired compound can be isolated from repeated recrystallized from n-hexane and dichloromethane. The pure compound was obtained as an orange solid (268 mg, 88.6% yield).

MALDI-TOF-MS (m/z): 695.1 $[M-Br]^+$.

Elemental analysis: Anal. Calcd for $C_{40}H_{34}Br_2N_2NiO$: C, 61.81; H, 4.41; N, 3.60. Found: C, 61.96; H, 4.40; N, 3.72.



Preparation of complex Ni4: A mixture of **L4** (237 mg, 0.409 mmol) and (DME)$NiBr_2$ (120 mg, 0.389 mmol) (DME = 1,2-dimethoxyethane) were stirred in 25 mL of dichloromethane overnight at room temperature. The solvent was evaporated under reduced pressure, the desired compound can be isolated from repeated recrystallized from n-hexane and dichloromethane. The pure compound was obtained as an orange solid (240 mg, 77.4% yield).

MALDI-TOF-MS (m/z): 715.1 $[M-Br]^+$.

Elemental analysis: Anal. Calcd for $C_{84}H_{60}Br_4N_4Ni_2O_2$: C, 63.28; H, 3.79; N, 3.51. Found: C, 63.41; H, 3.90; N, 3.41.

3. ^{1}H and ^{13}C NMR spectra of Ligands

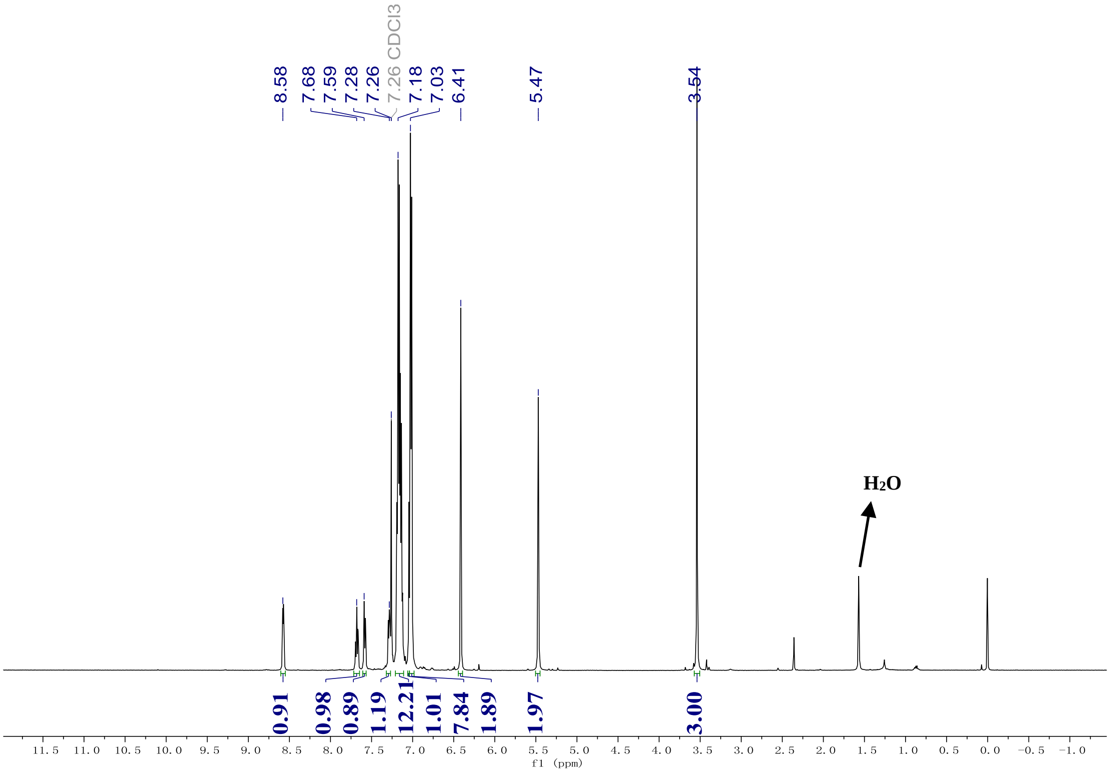


Figure S1. ^{1}H NMR spectrum of **L1** in $CDCl_3$

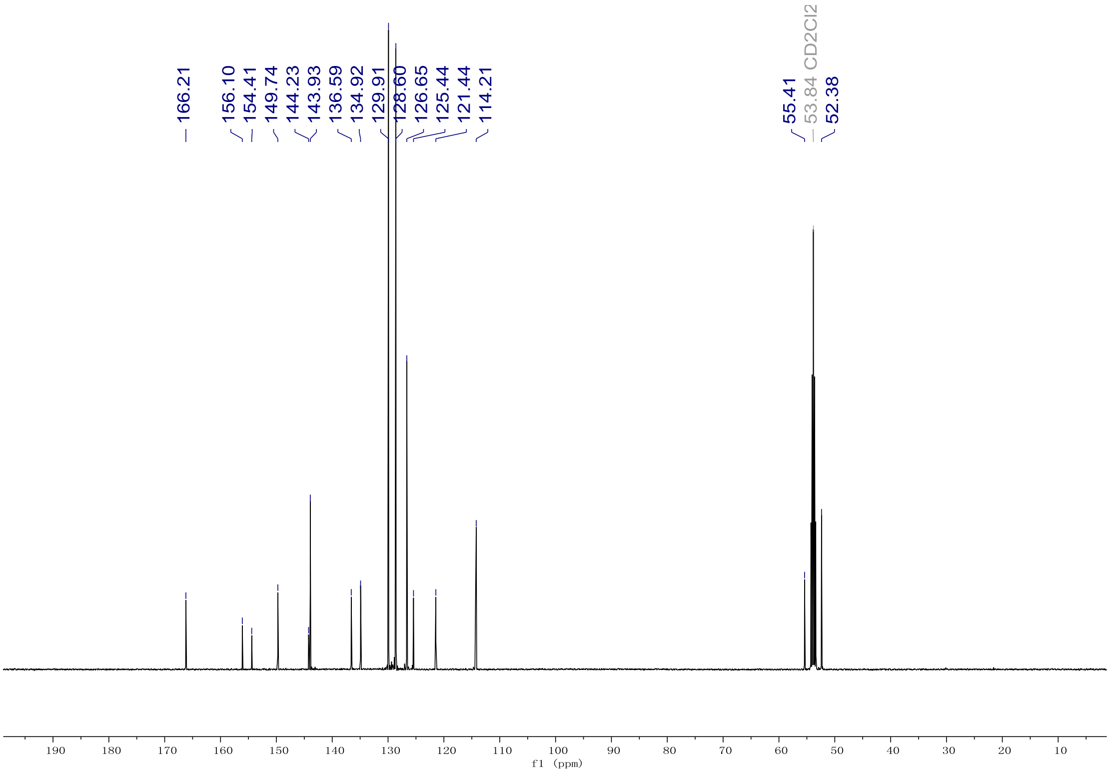


Figure S2. ^{13}C NMR spectrum of **L1** in CD_2Cl_2

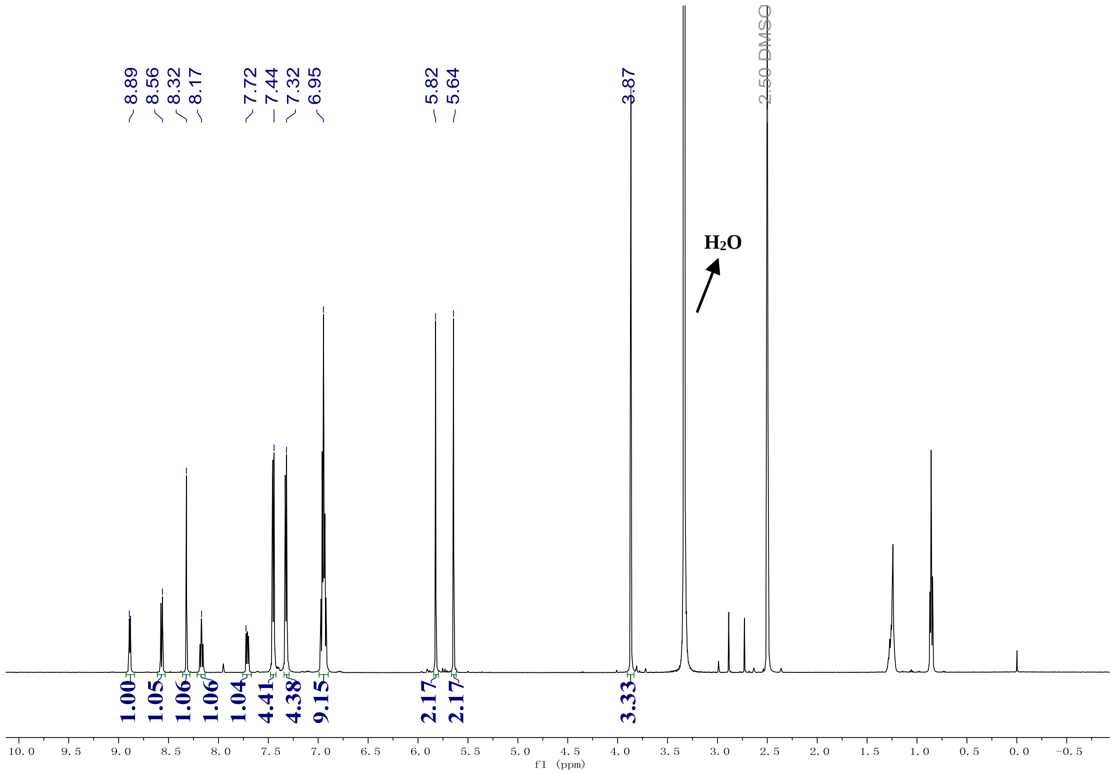


Figure S3. ^{1}H NMR spectrum of **L2** in DMSO-d_6

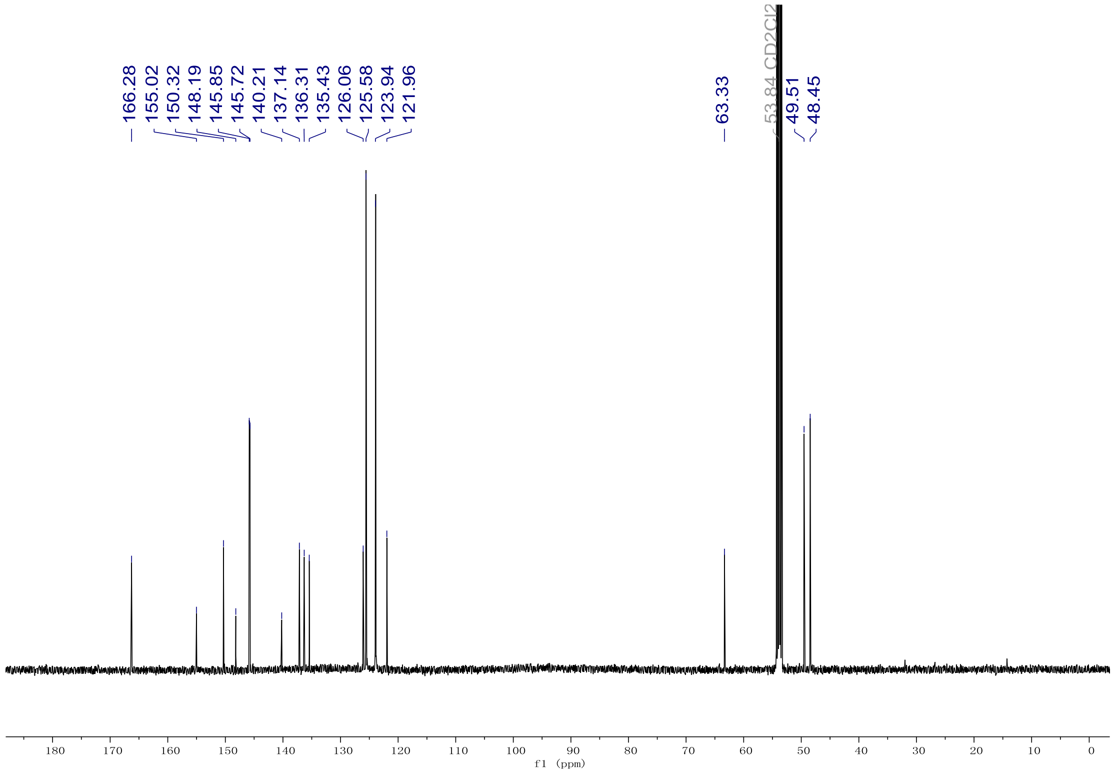


Figure S4. ^{13}C NMR spectrum of **L2** in CD_2Cl_2

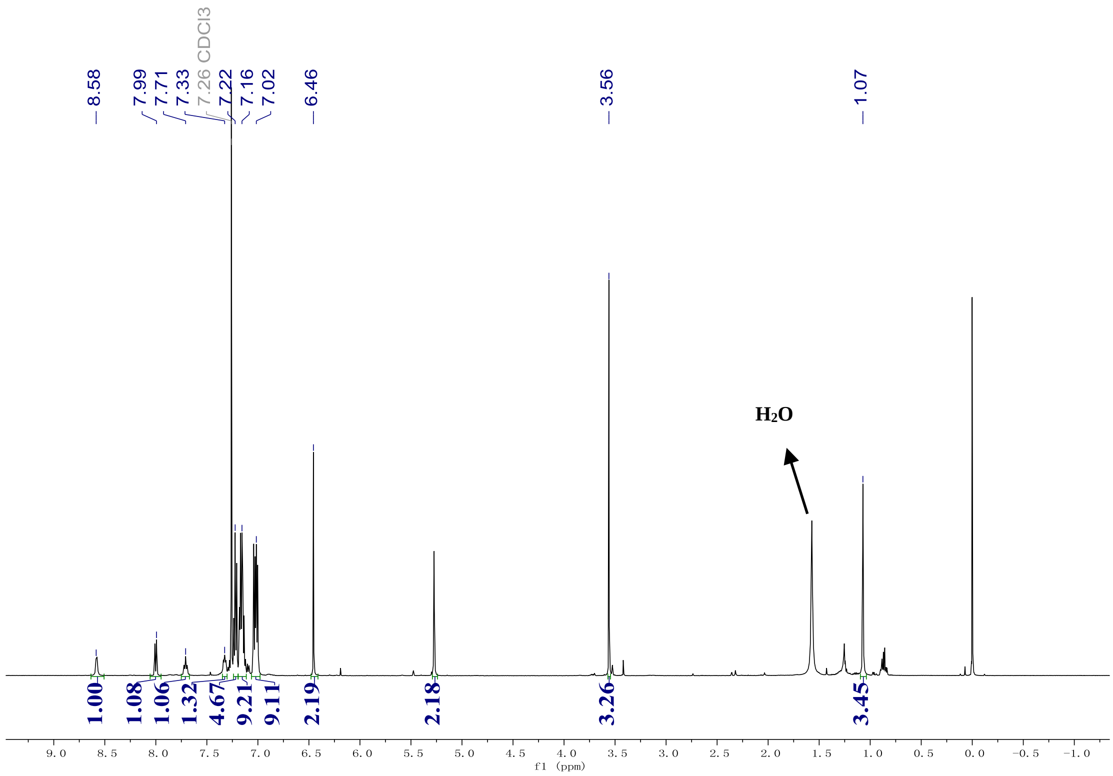


Figure S5. ^{1}H NMR spectrum of **L3** in $CDCl_3$

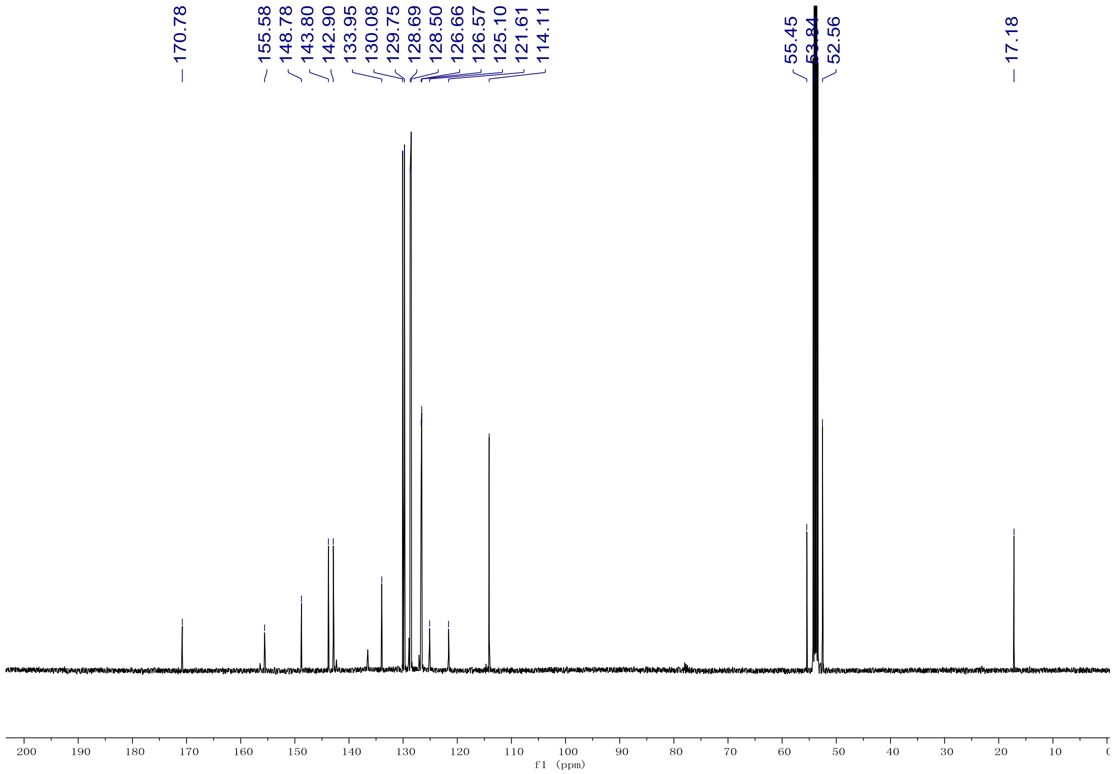


Figure S6. ^{13}C NMR spectrum of **L3** in CD_2Cl_2

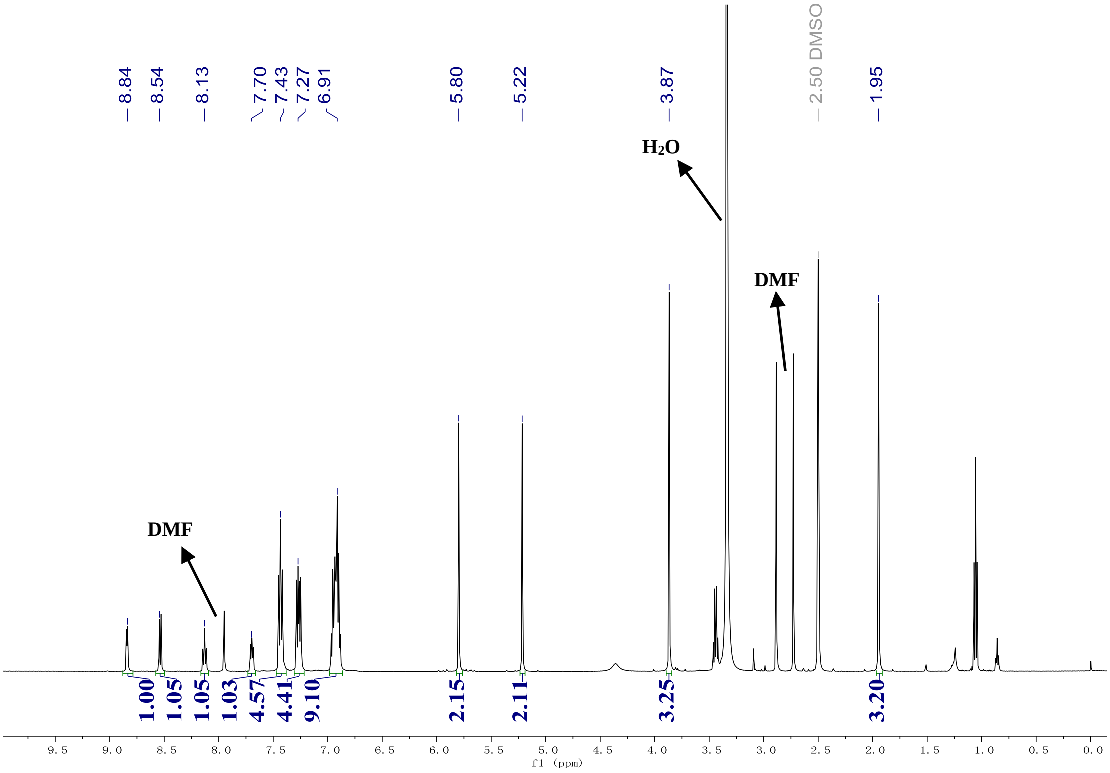


Figure S7. ^{1}H NMR spectrum of **L4** in DMSO-d_6

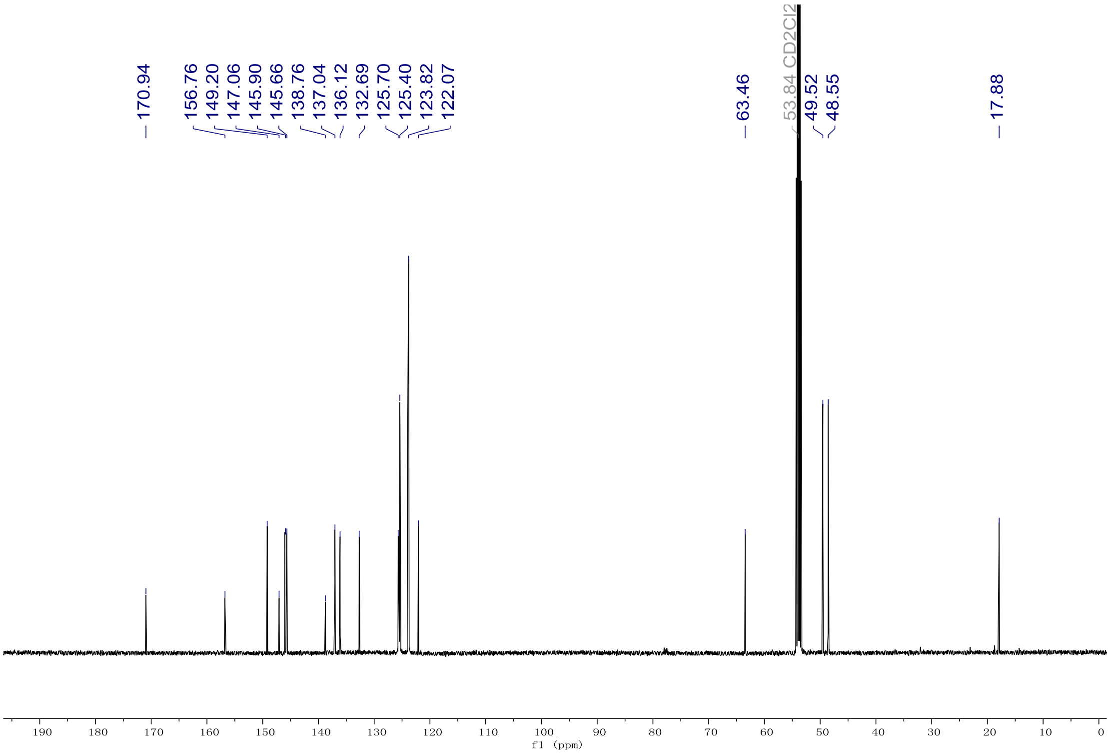


Figure S8. ^{13}C NMR spectrum of **L4** in CD_2Cl_2

4. MALDI-TOF-MS of Ni complexes

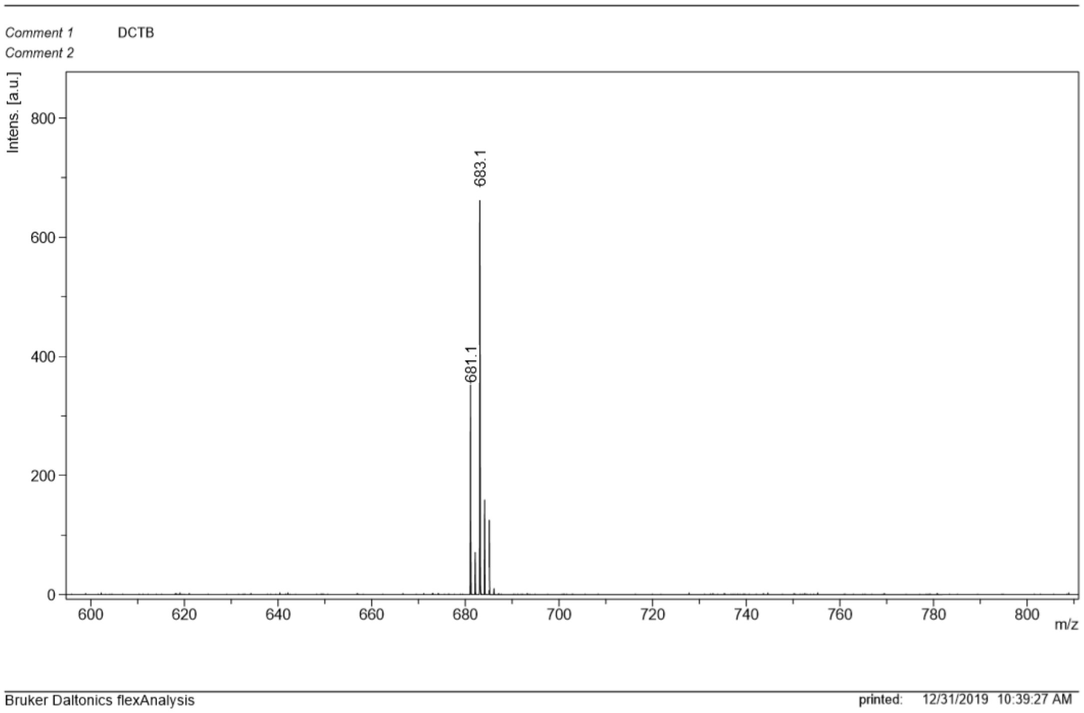


Figure S9. MALDI-TOF-MS of complex **Ni1**

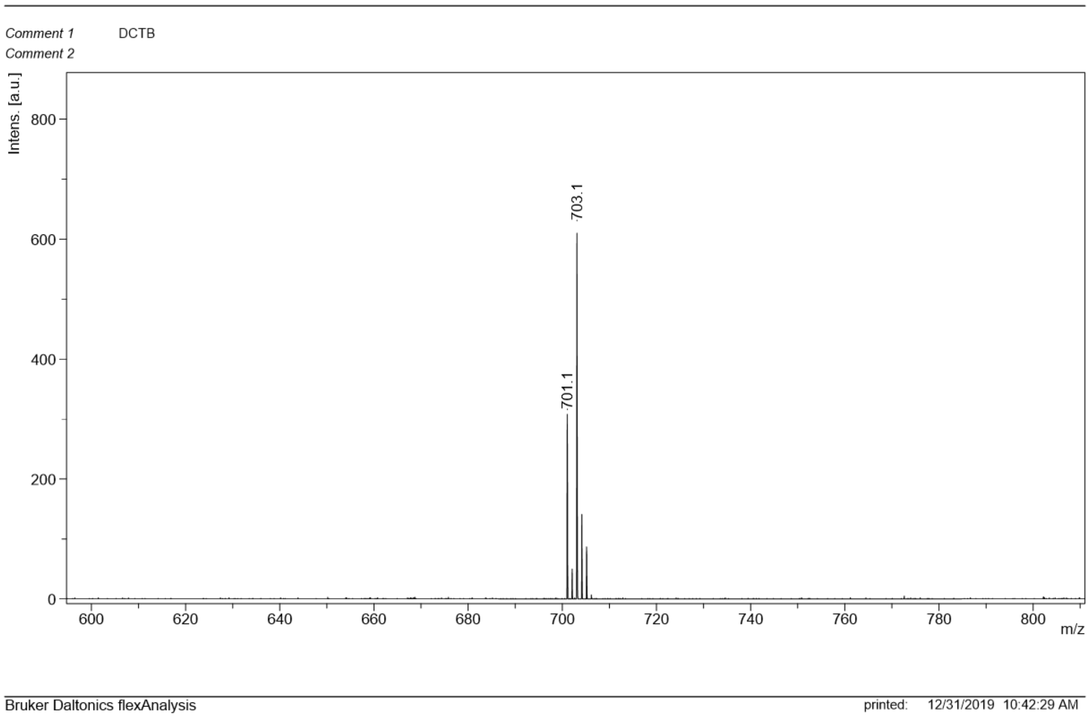


Figure S10. MALDI-TOF-MS of complex **Ni2**

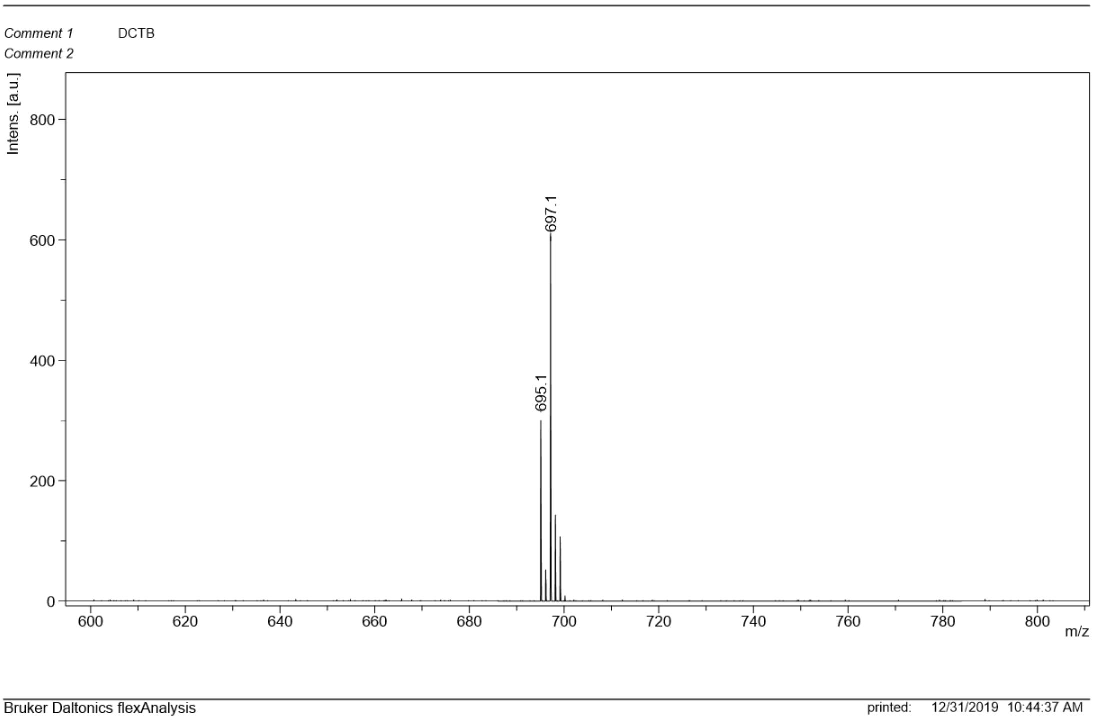


Figure S11. MALDI-TOF-MS of complex **Ni3**

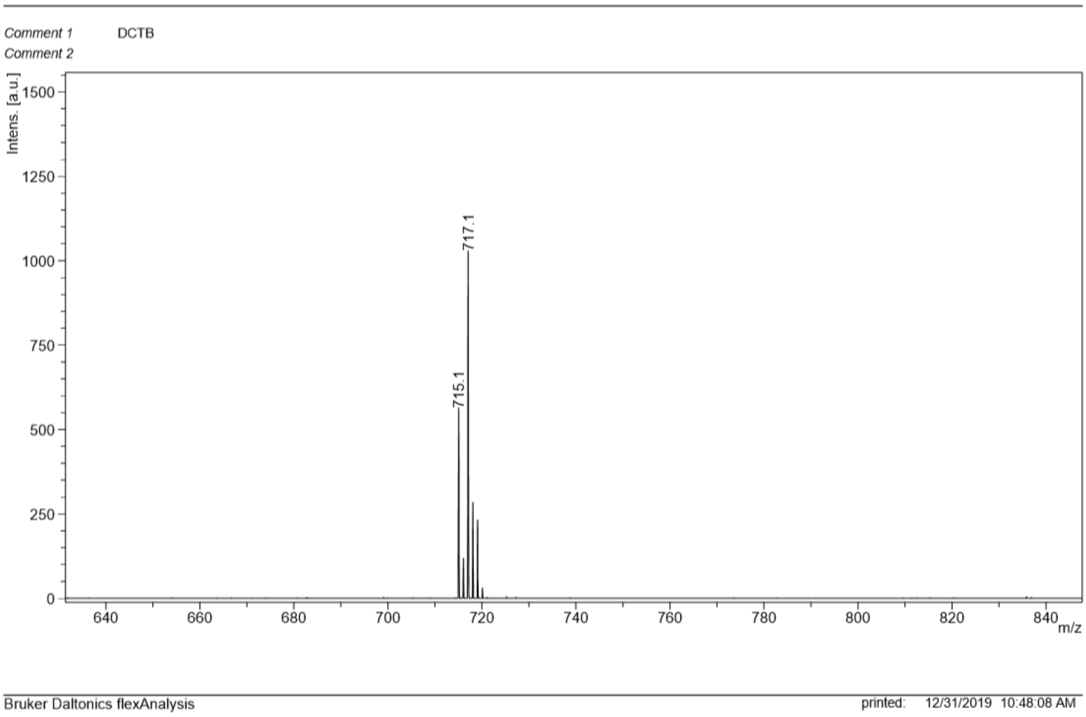


Figure S12. MALDI-TOF-MS of complex **Ni4**

5 NMR figures of polymers

$$\text{Me groups /1000C} = \frac{(I_1 - \frac{3I_5}{2} - I_6 * 3)}{(I_1 + I_2 + I_3 + I_4 + I_5 + I_6 + I_7)/2} * 1000$$

$$= \frac{(3 - \frac{3*0.03}{2} - 0.32*3)/3}{(3+22.06+0.23+0.68+0.03+0.32+0.01)/2} * 1000 = 50$$

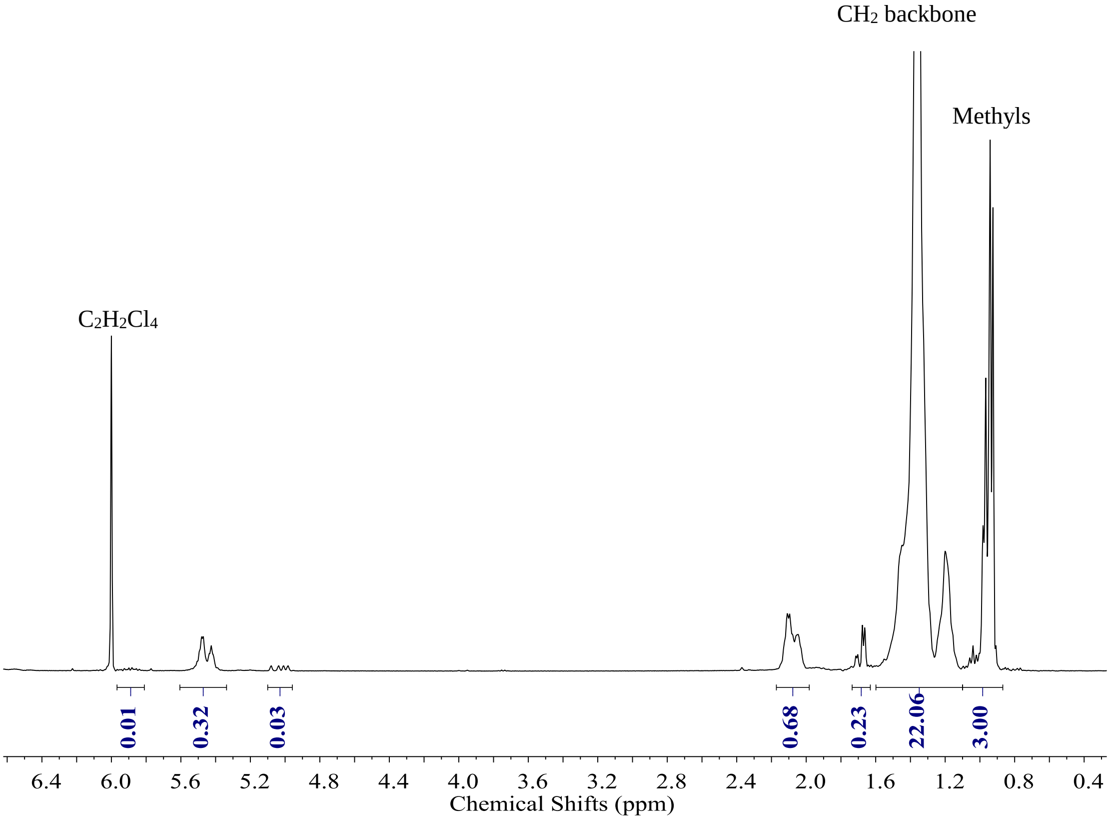


Figure S13. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni1** from table 1, entry 1.

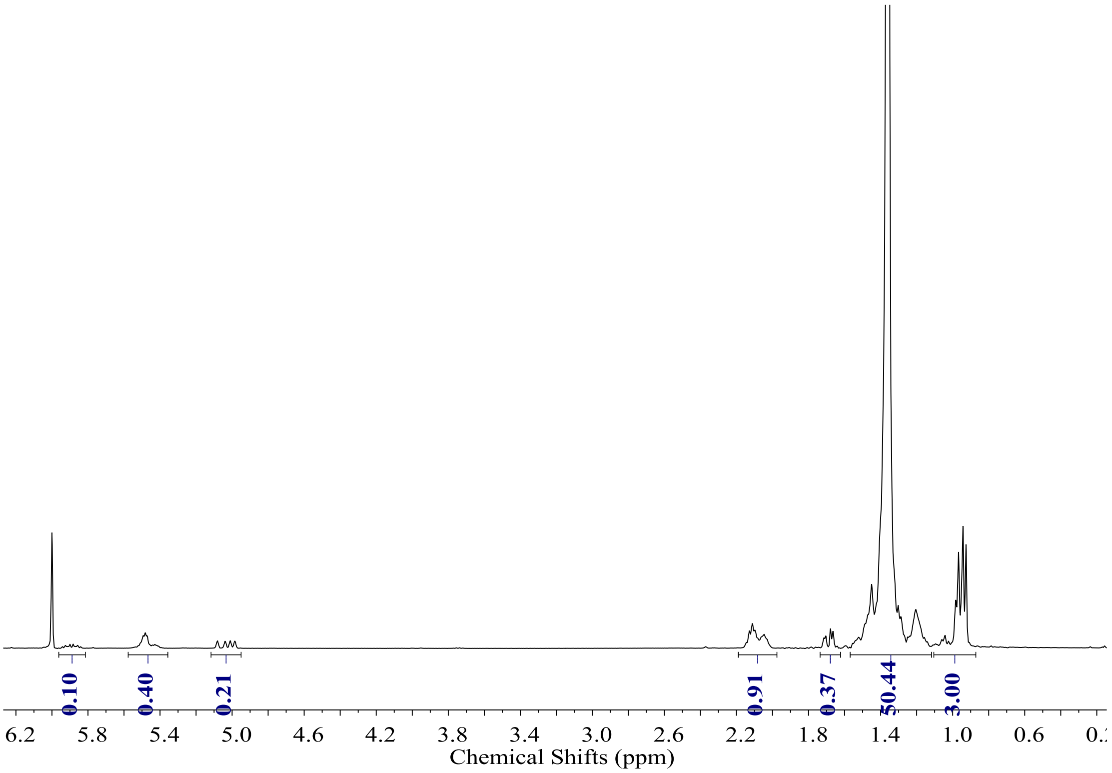


Figure S14. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni2** from table 1, entry 2.

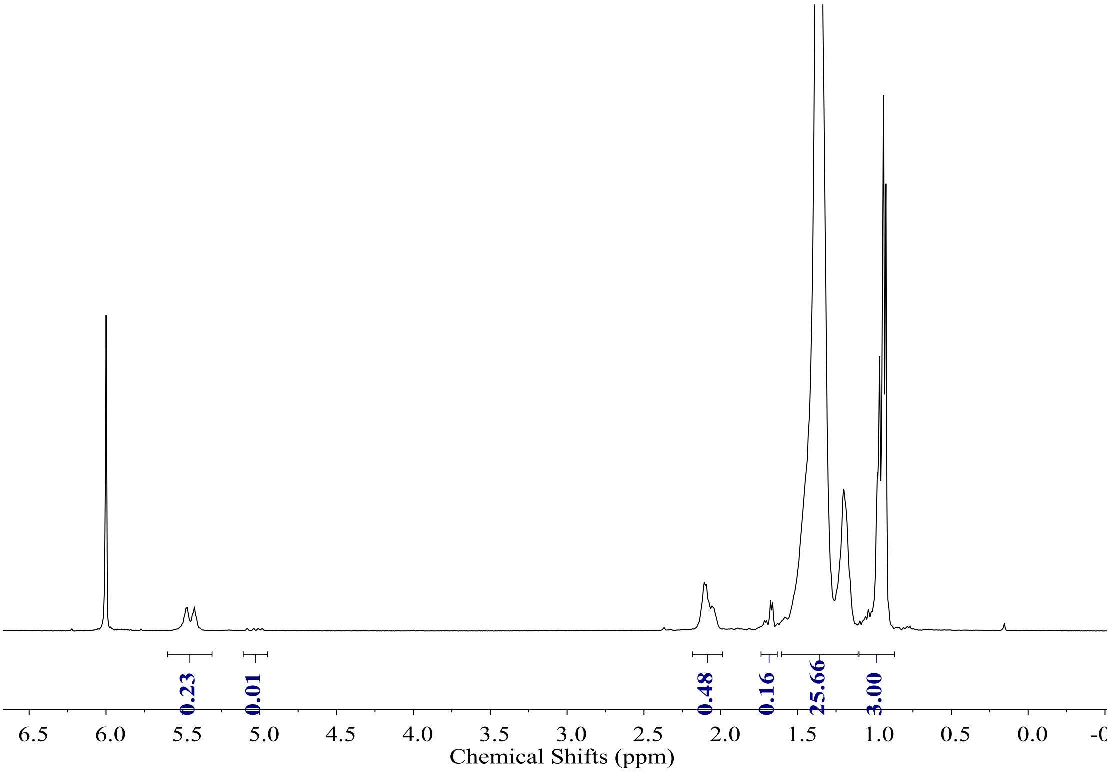


Figure S15. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 1, entry 3.

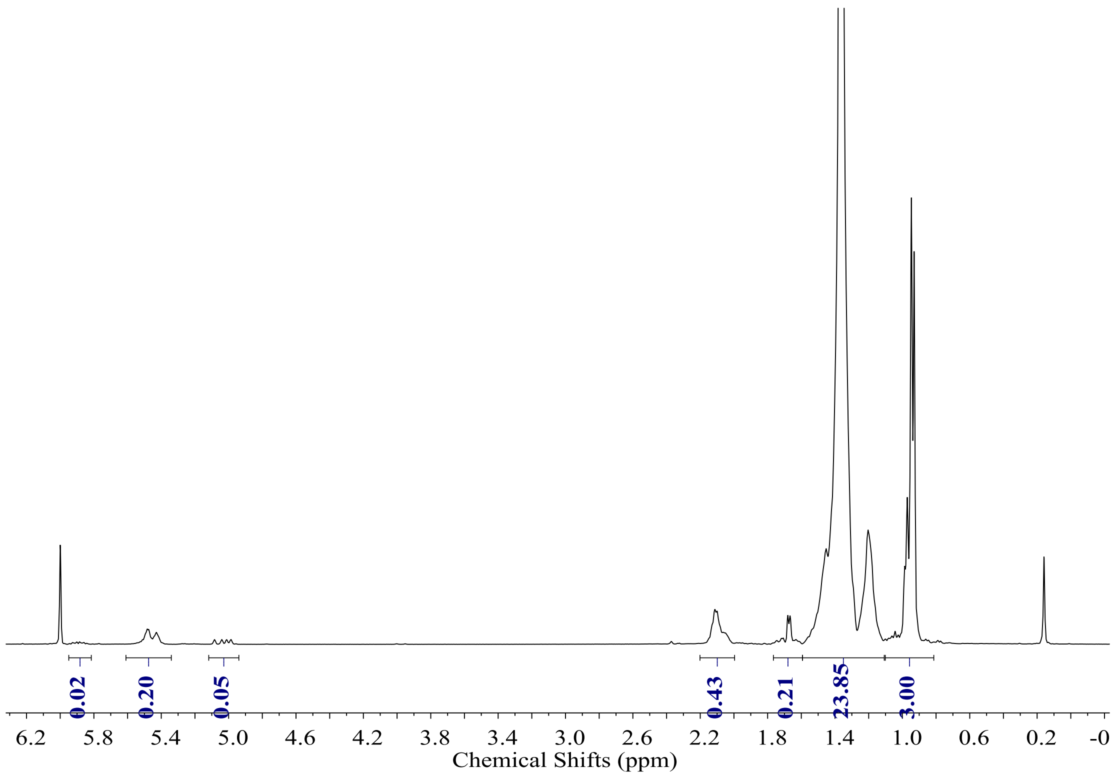


Figure S16. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 1, entry 4.

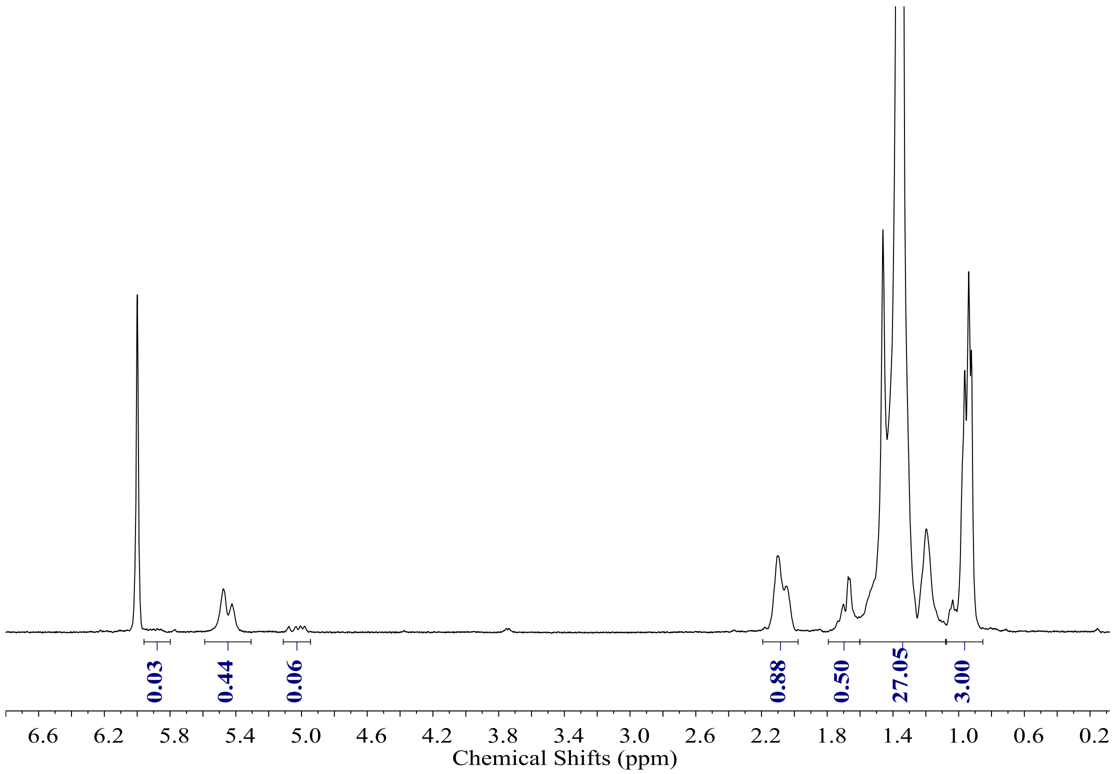


Figure S17. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni1** from table 1, entry 5.

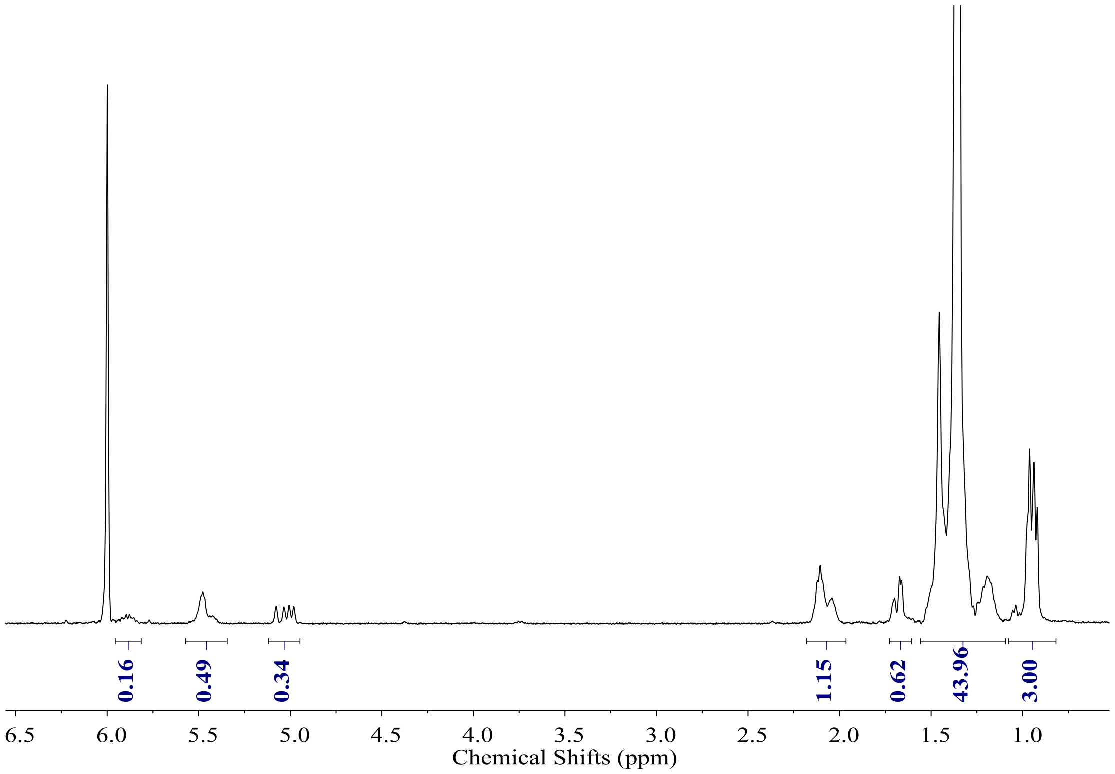


Figure S18. ^1H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni2** from table 1, entry 6.

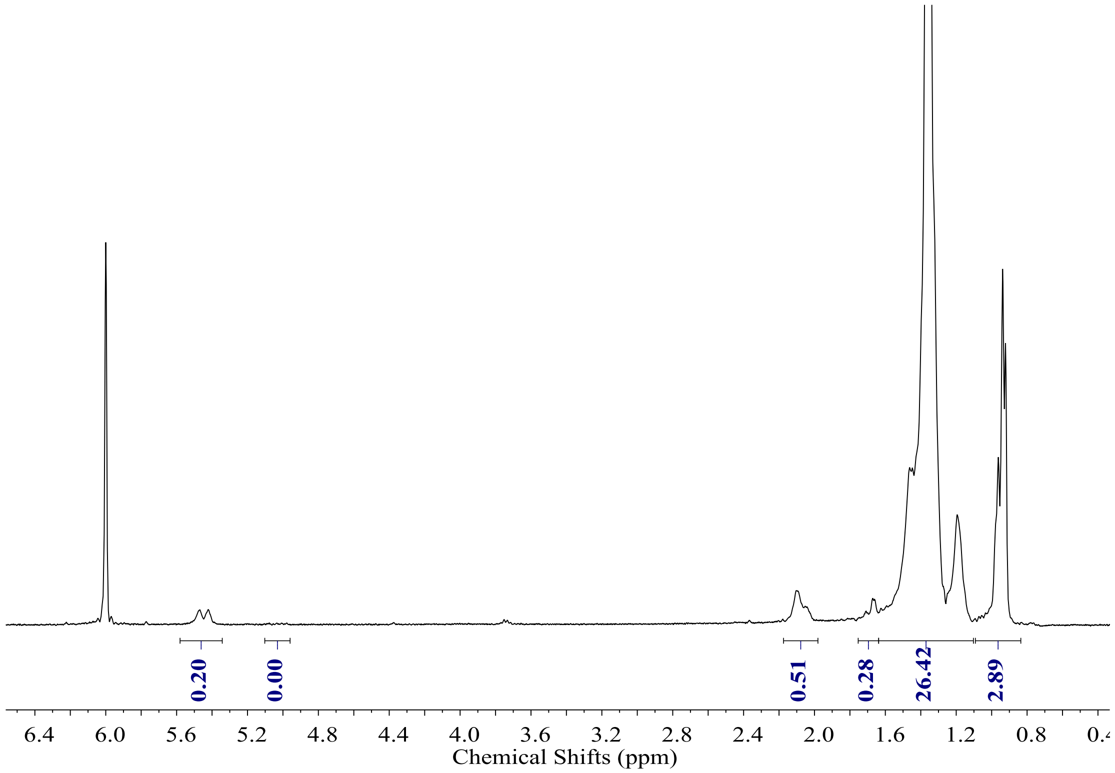


Figure S19. ^1H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 1, entry 7.

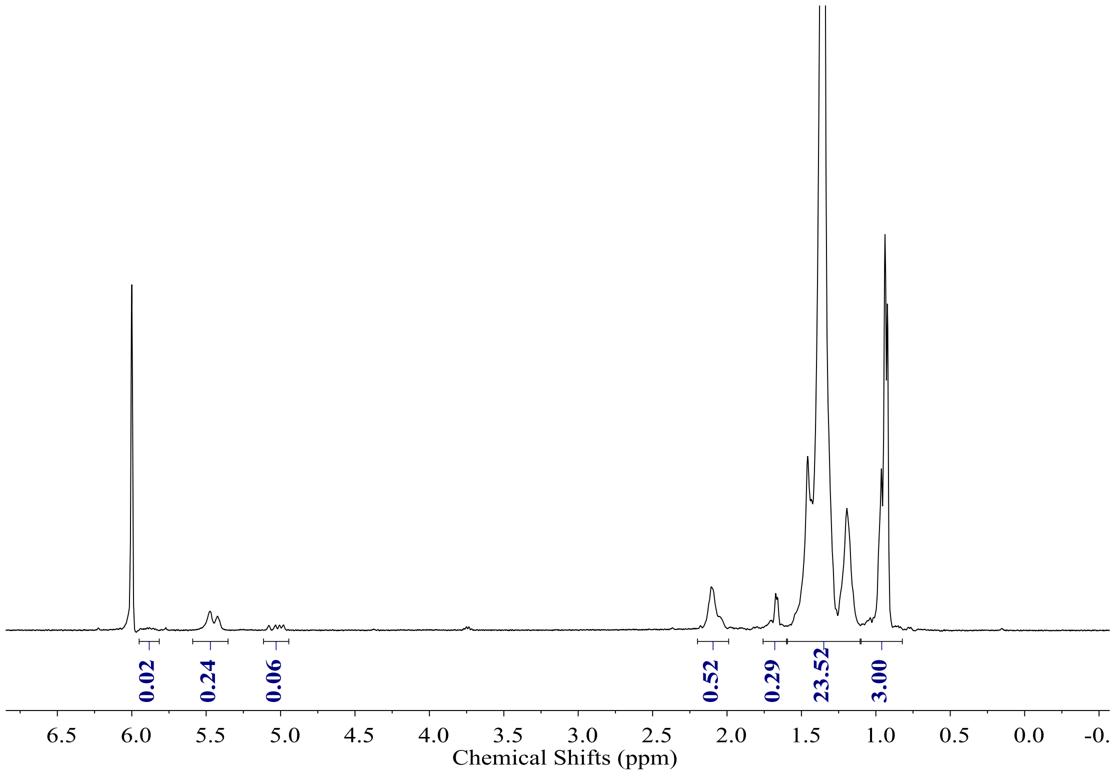


Figure S20. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 1, entry 8.

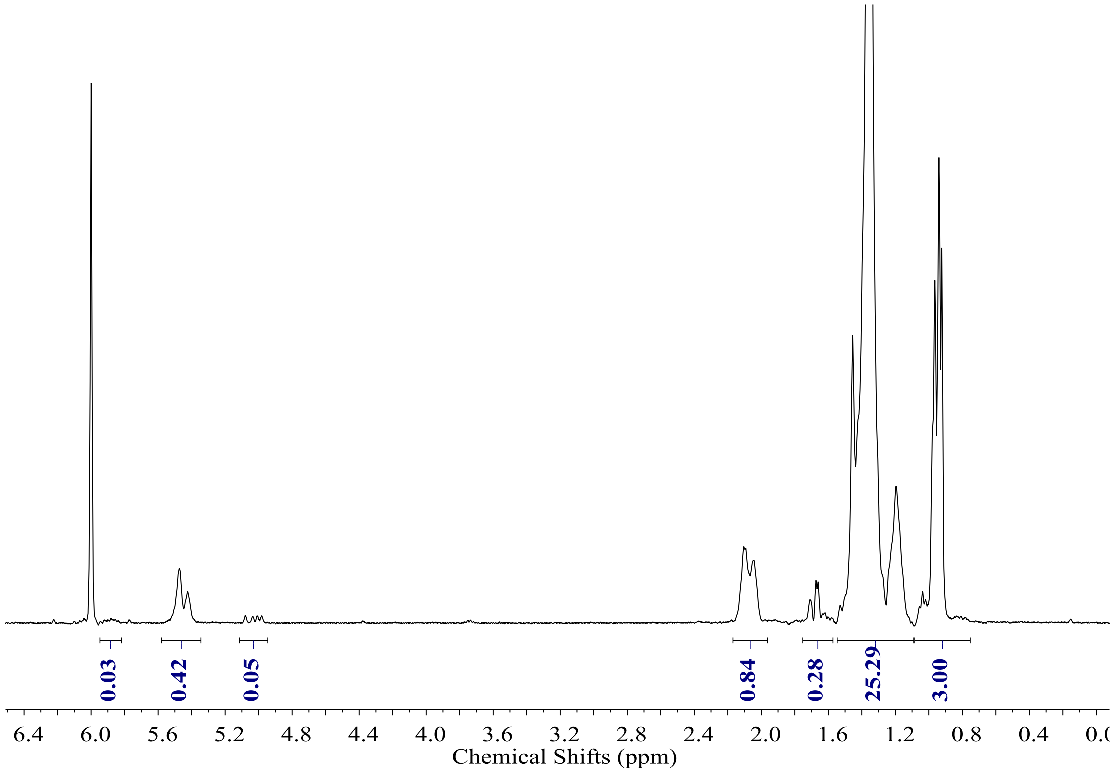


Figure S21. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni1** from table 1, entry 9.

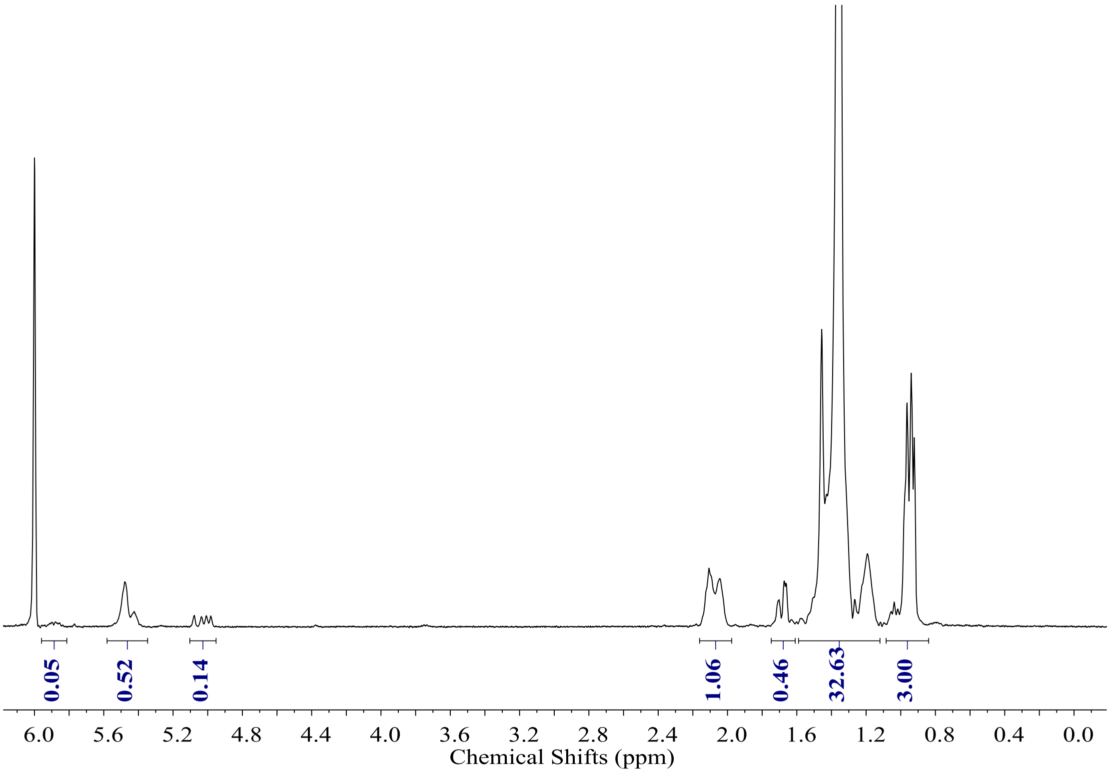


Figure S22. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni2** from table 1, entry10.

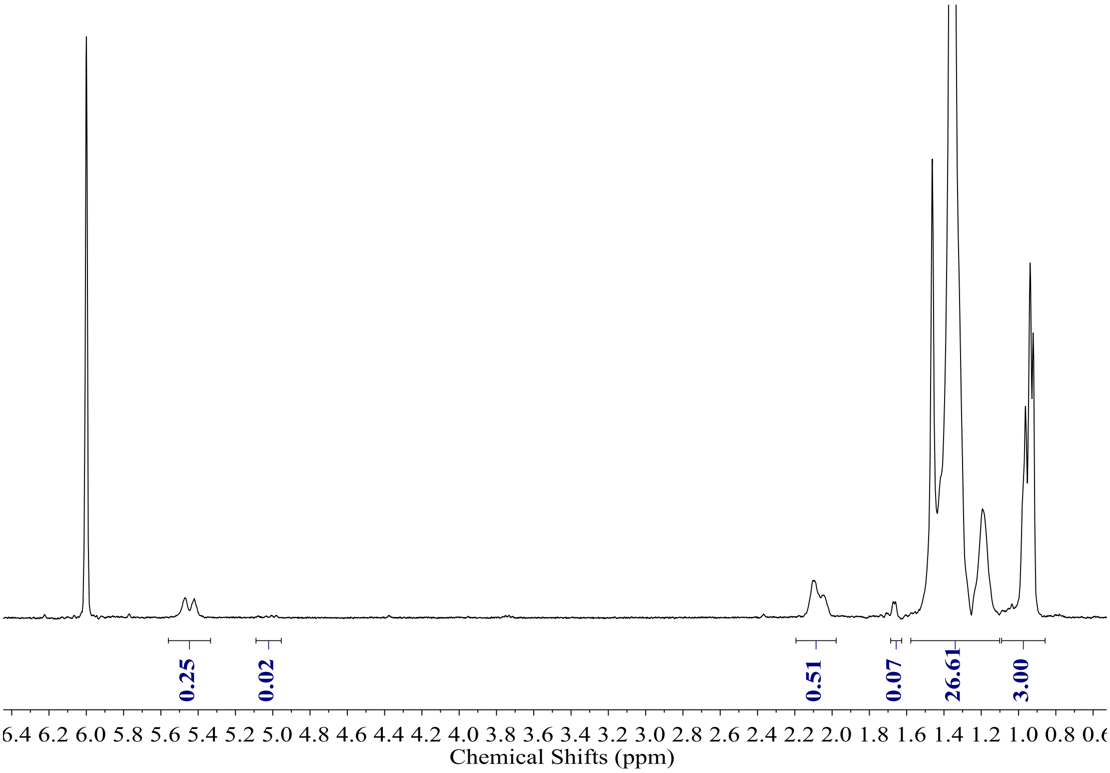


Figure S23. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni**3 from table 1, entry 11.

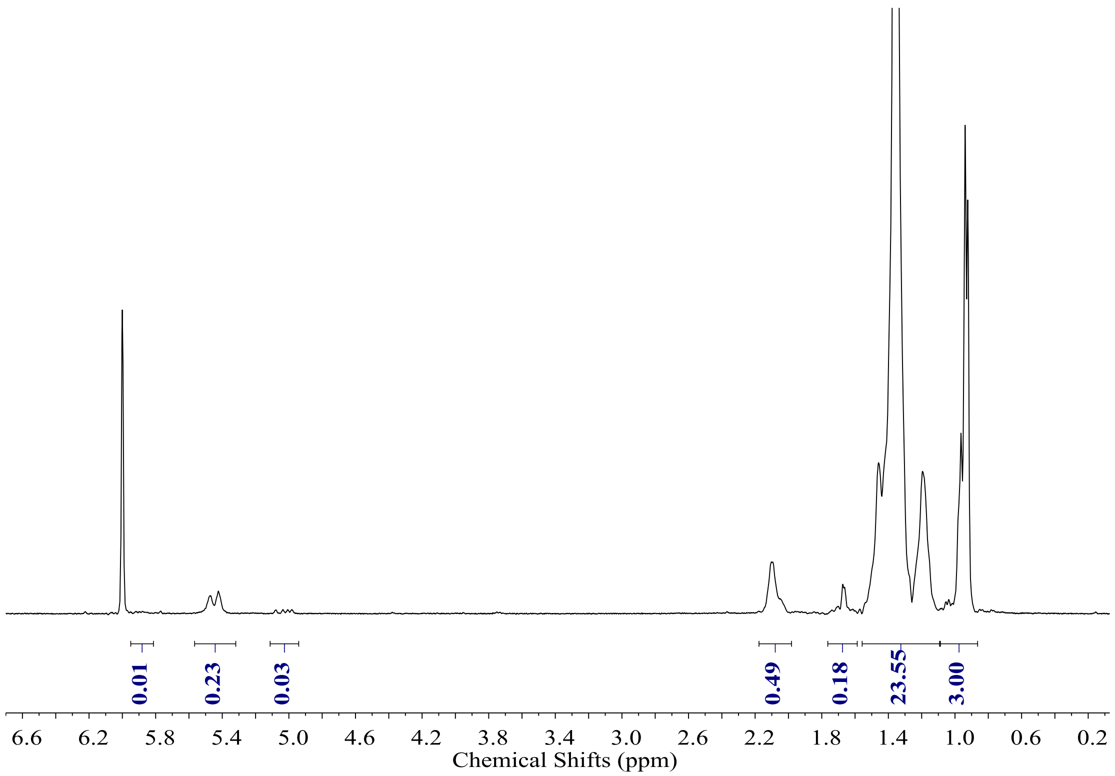


Figure S24. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 1, entry 12.

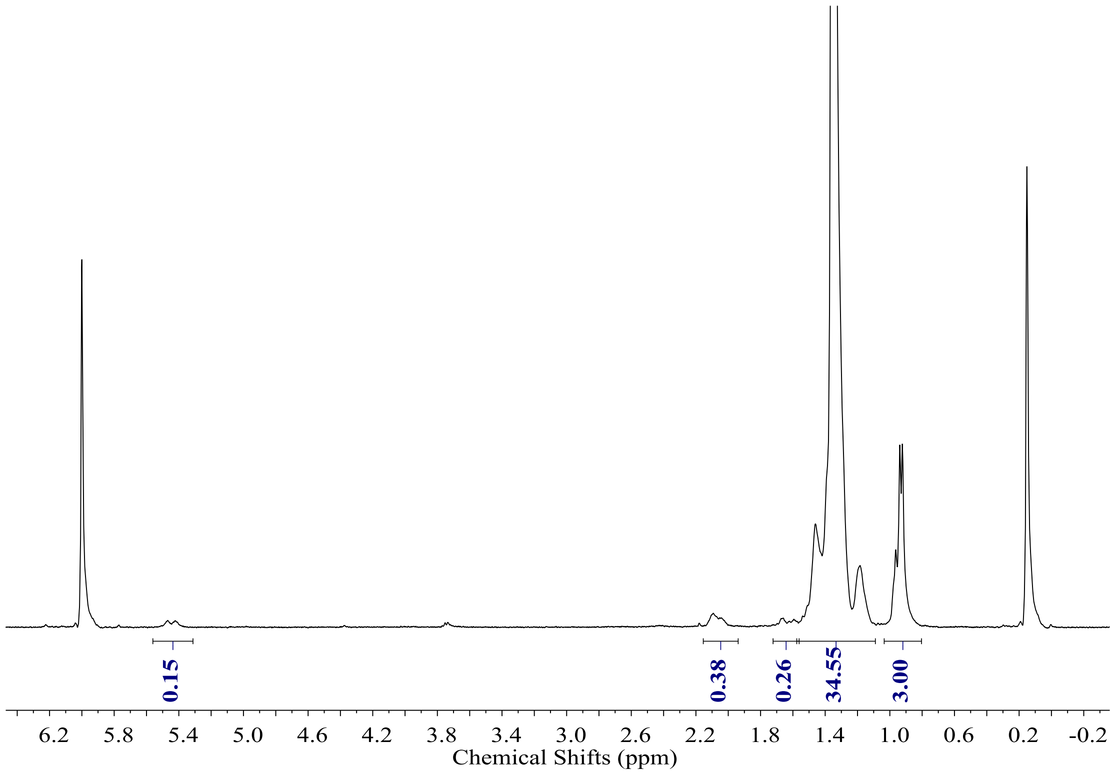


Figure S25. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 1, entry 13.

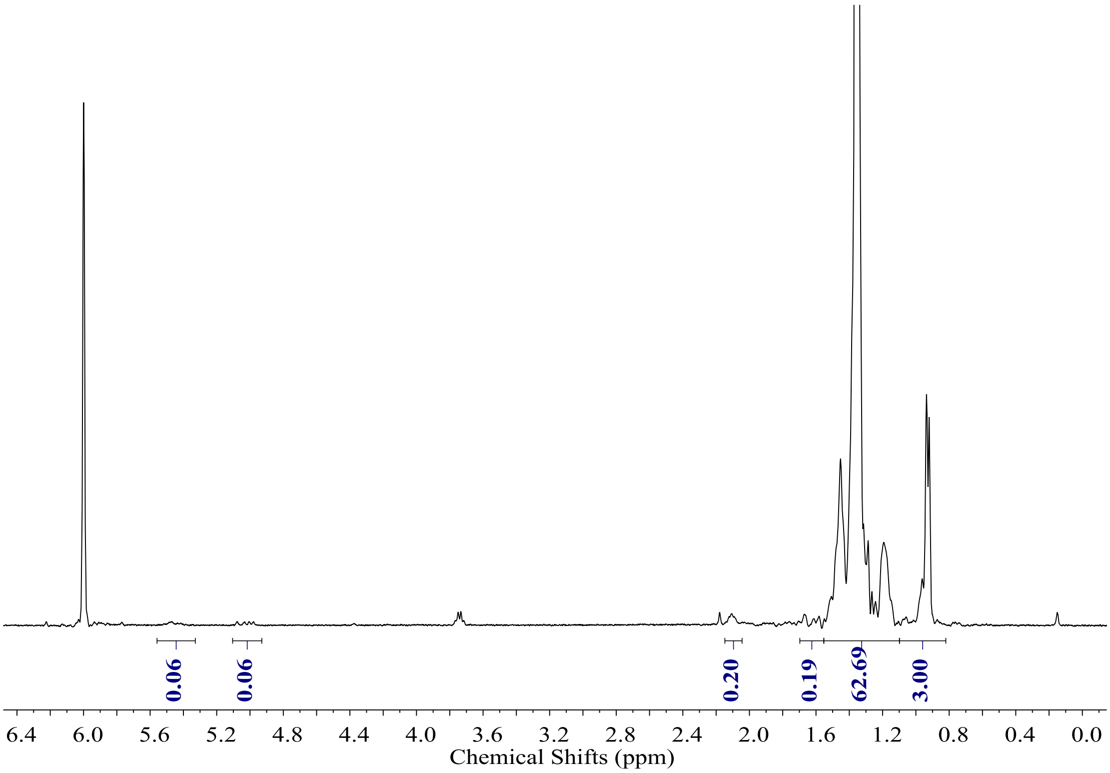


Figure S26. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 1, entry 14.

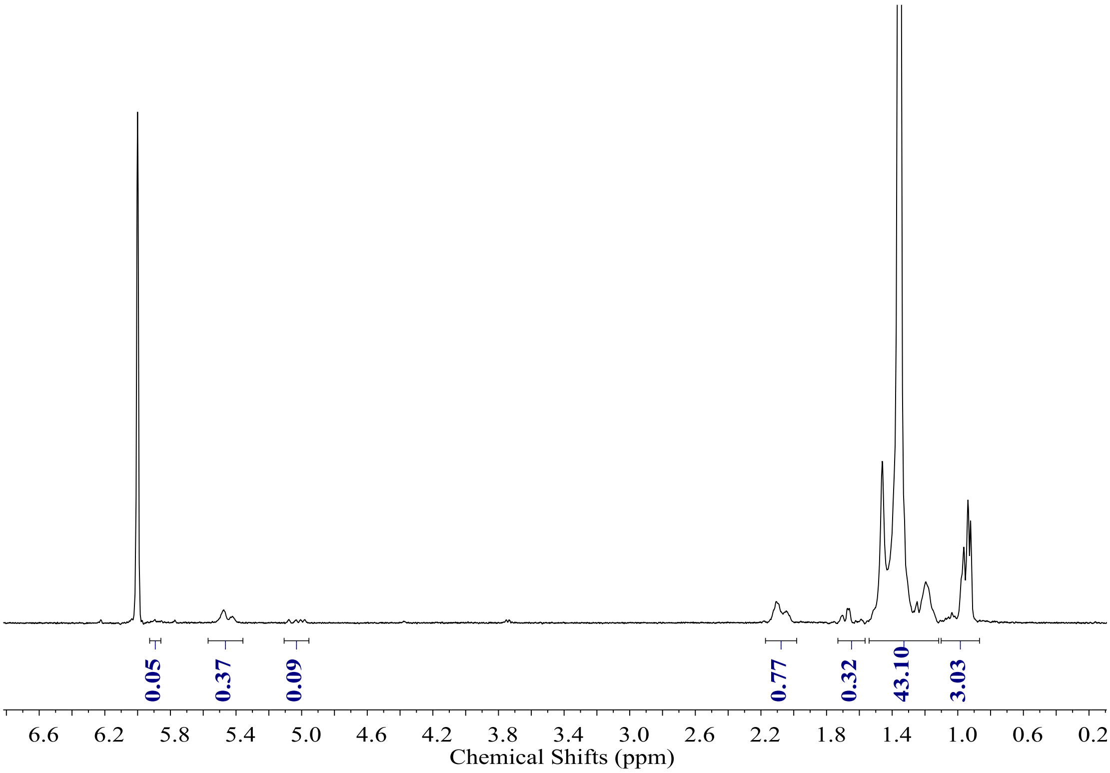


Figure S27. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni1** from table 3, entry 1.

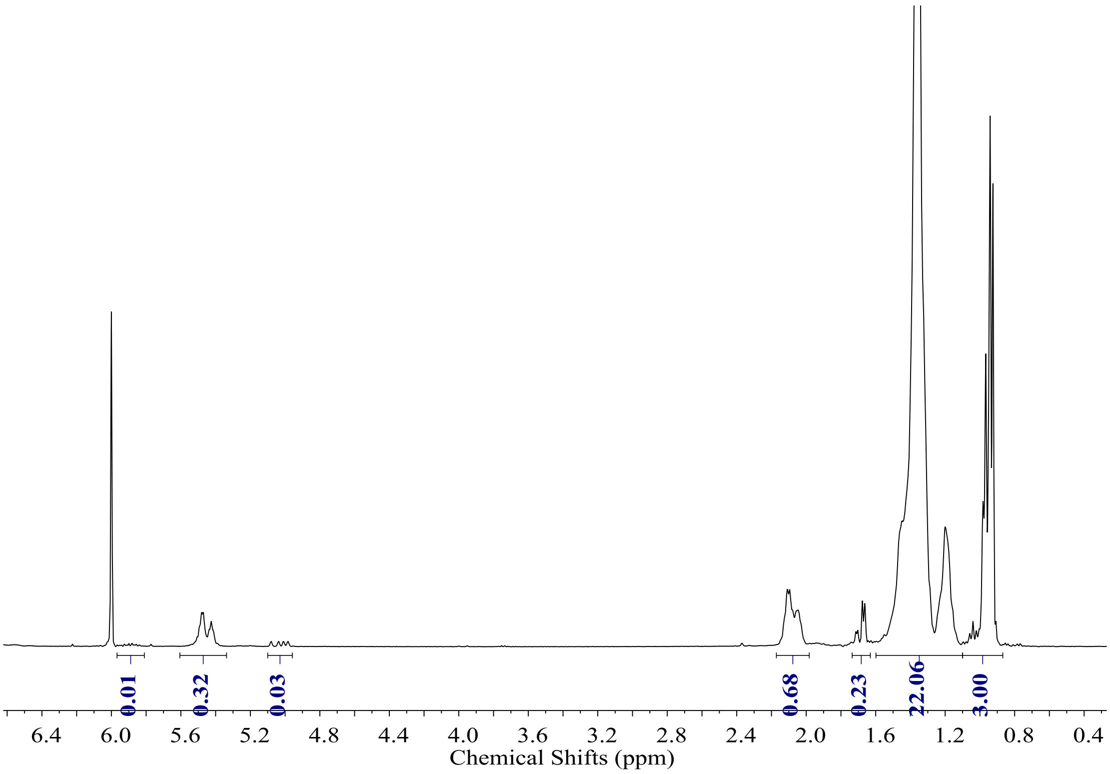


Figure S28. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni1** from table 3, entry 2.

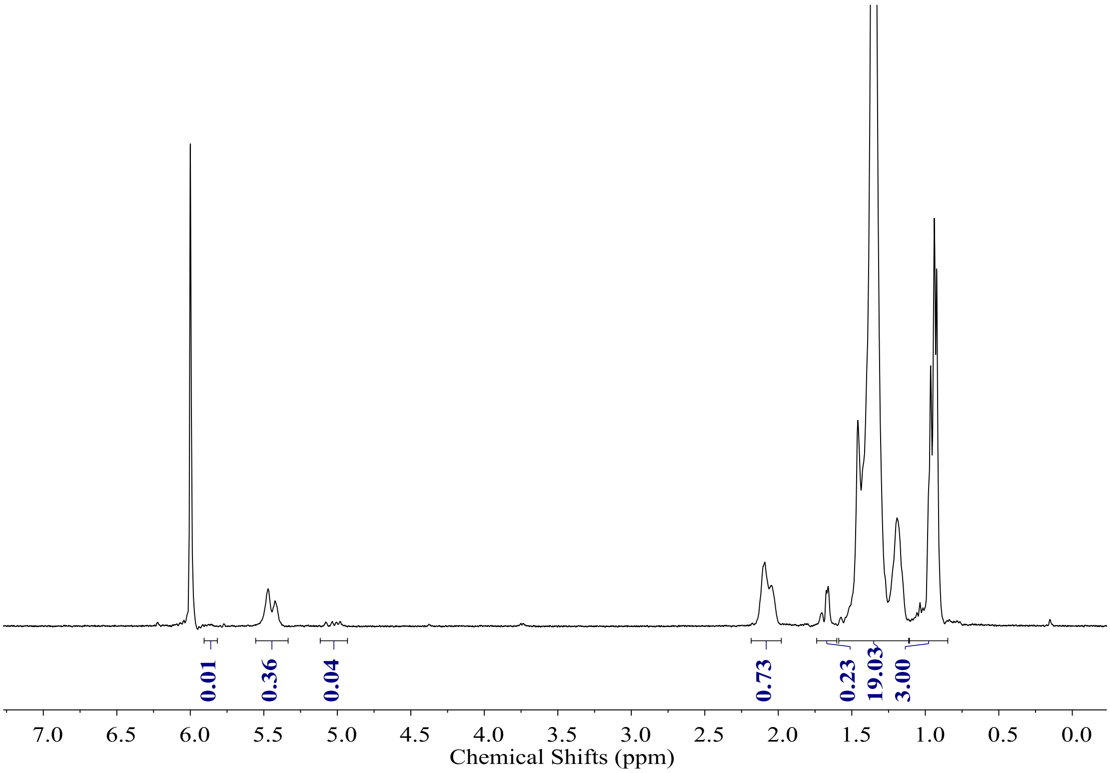


Figure S29. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni1** from table 3, entry 3.

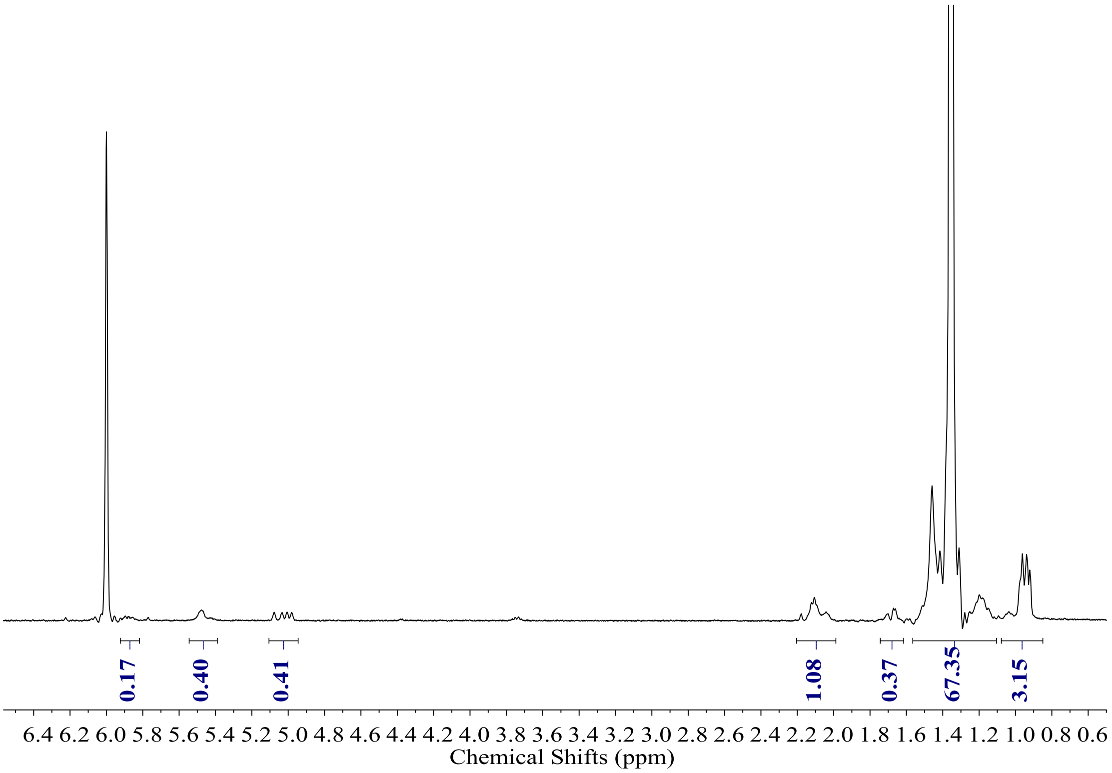


Figure S30. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni2** from table 3, entry 4.

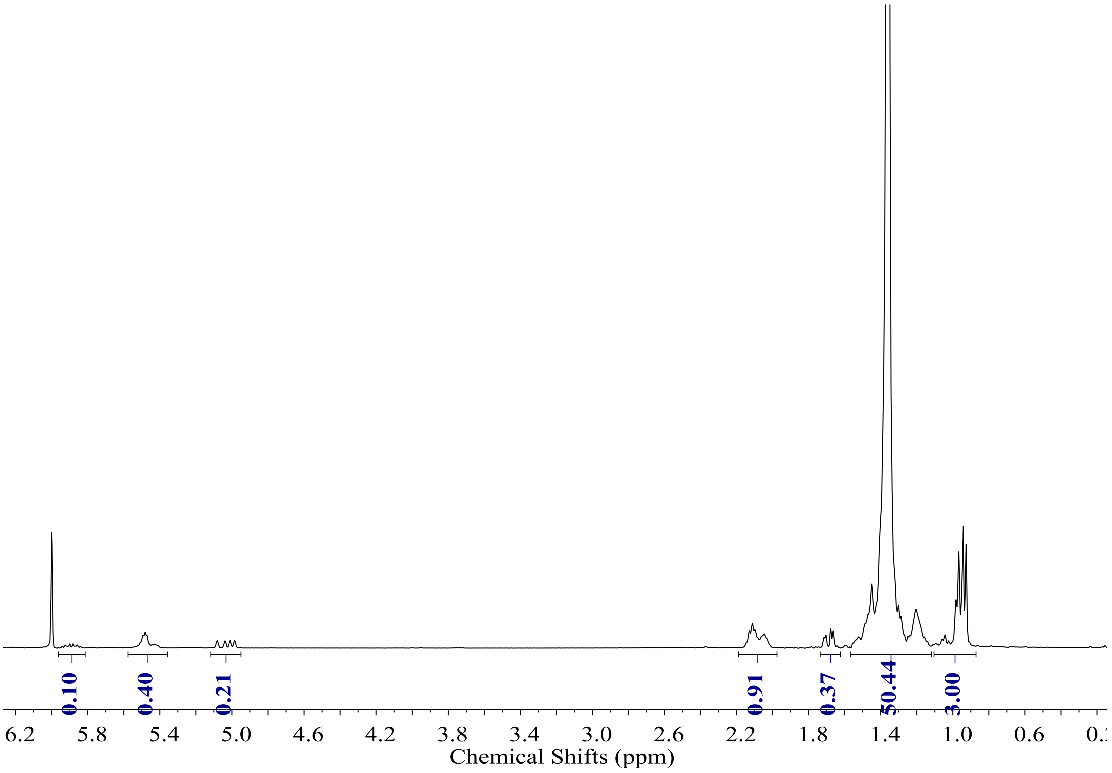


Figure S31. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni2** from table 3, entry 5.

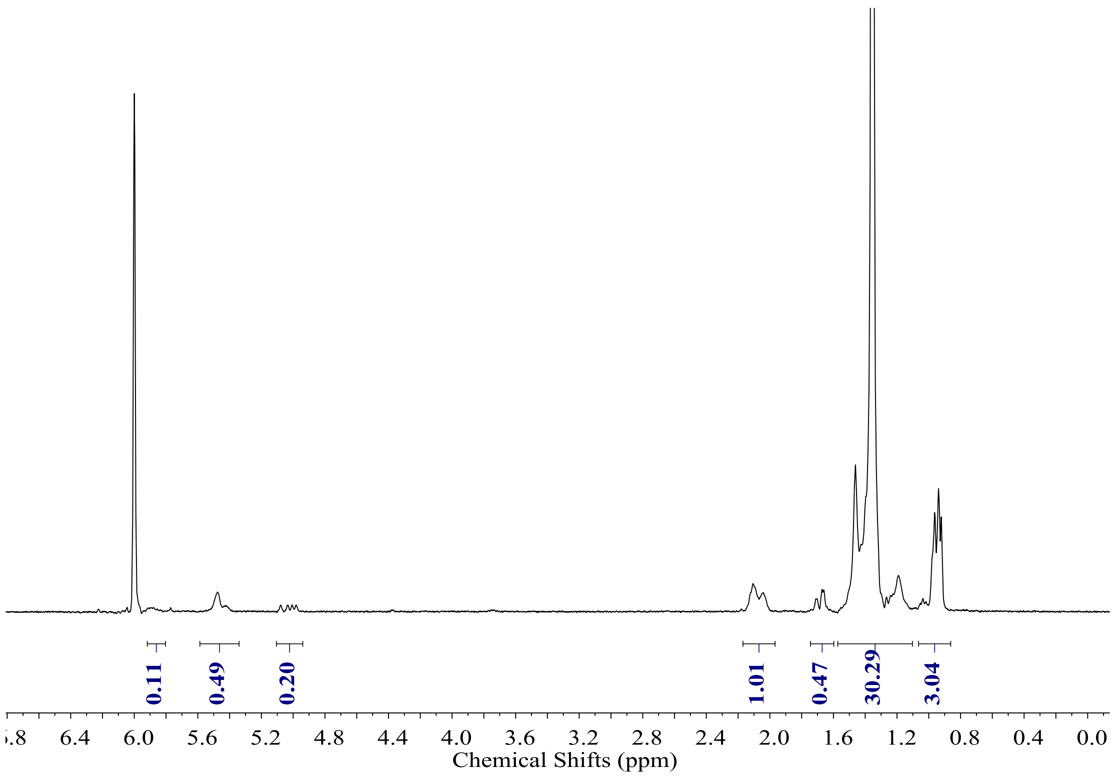


Figure S32. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni2** from table 3, entry 6.

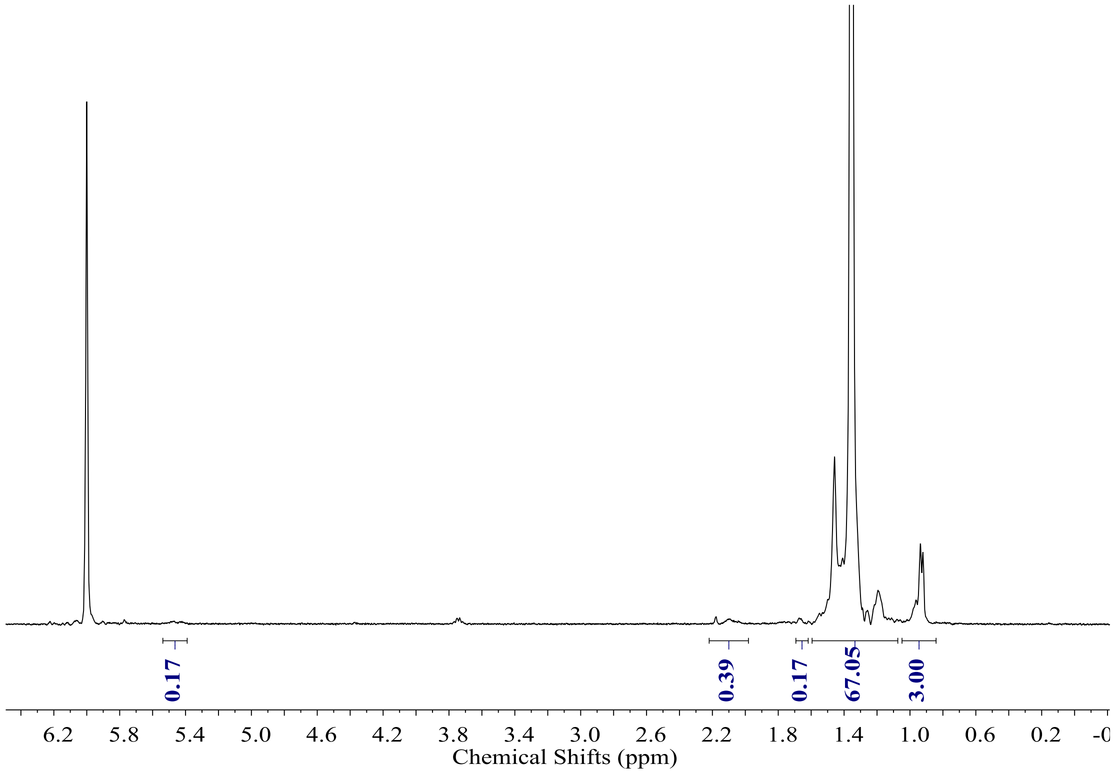


Figure S33. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 3, entry 7.

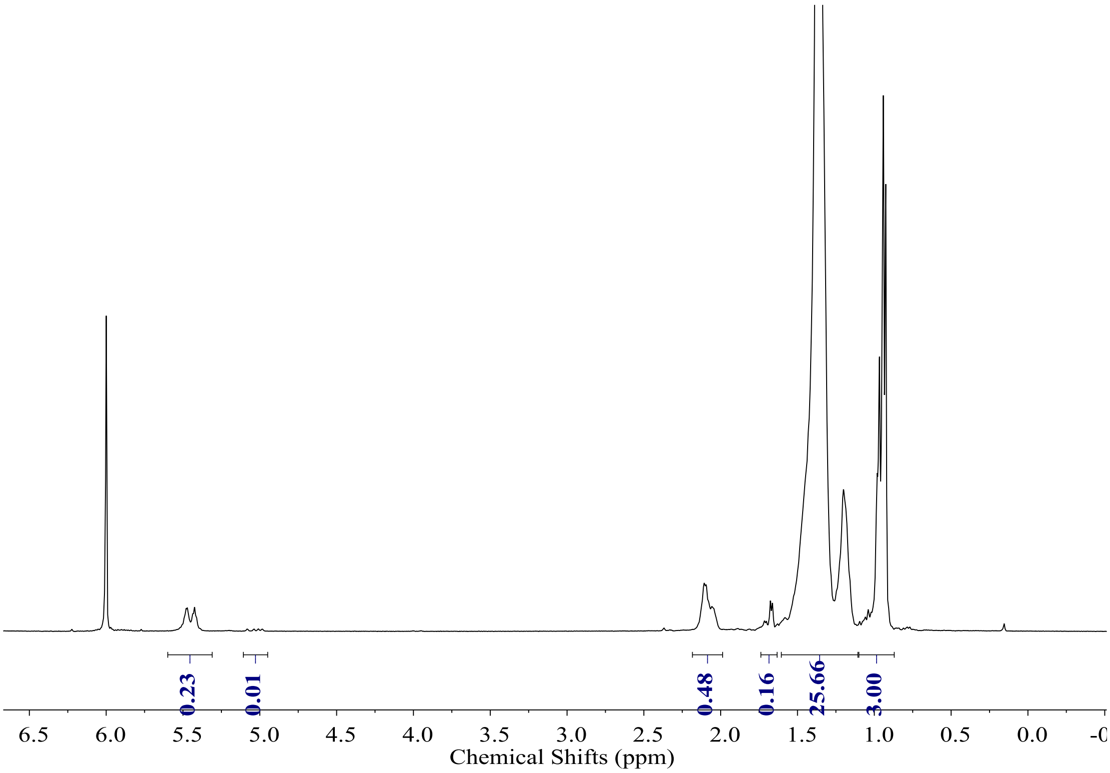


Figure S34. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 3, entry 8.

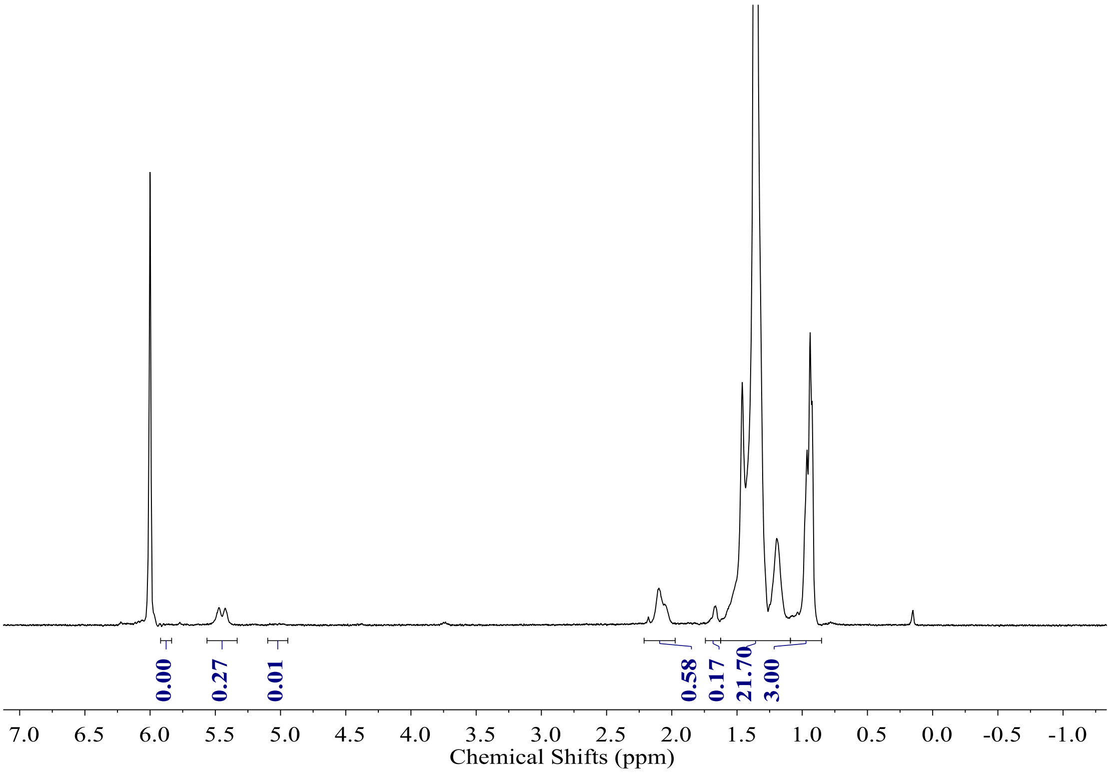


Figure S35. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 3, entry 9.

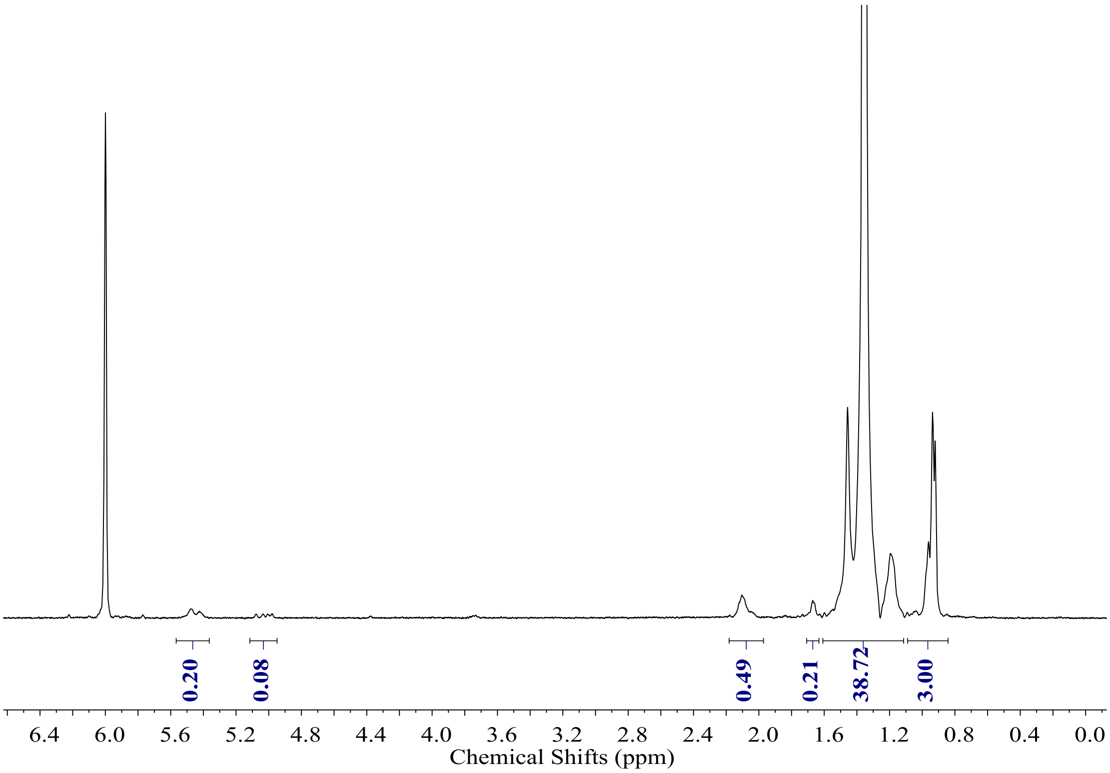


Figure S36. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 3, entry 10.

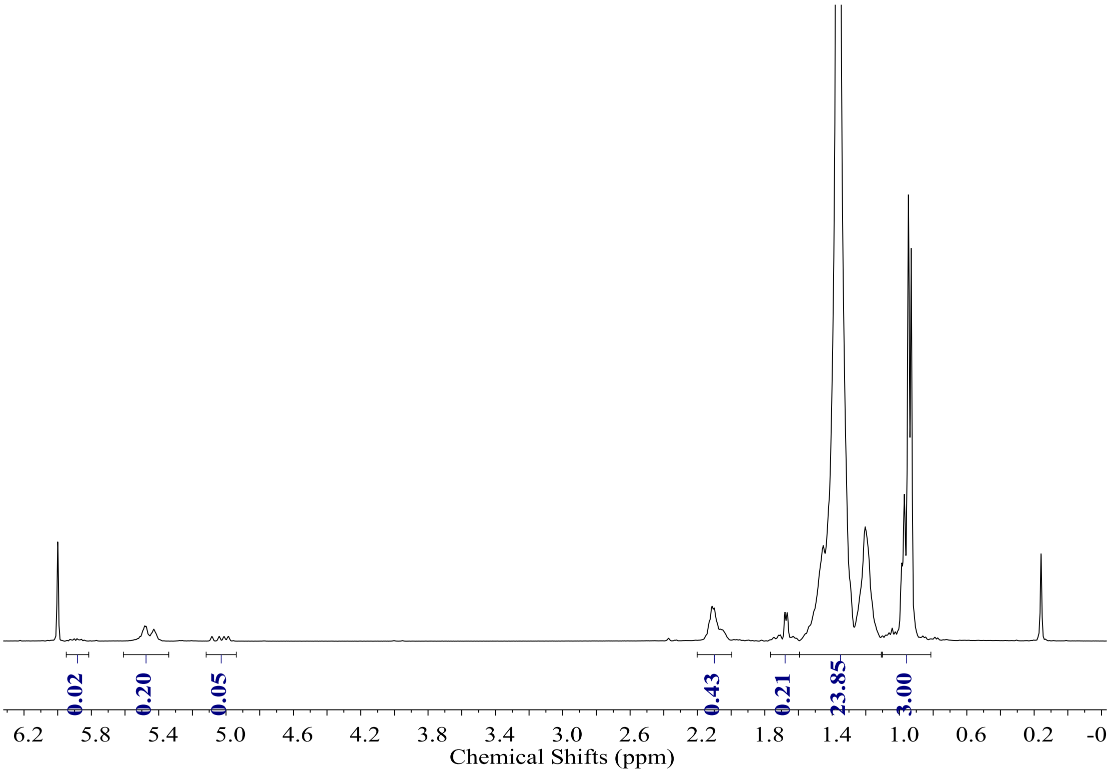


Figure S37. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 3, entry 11.

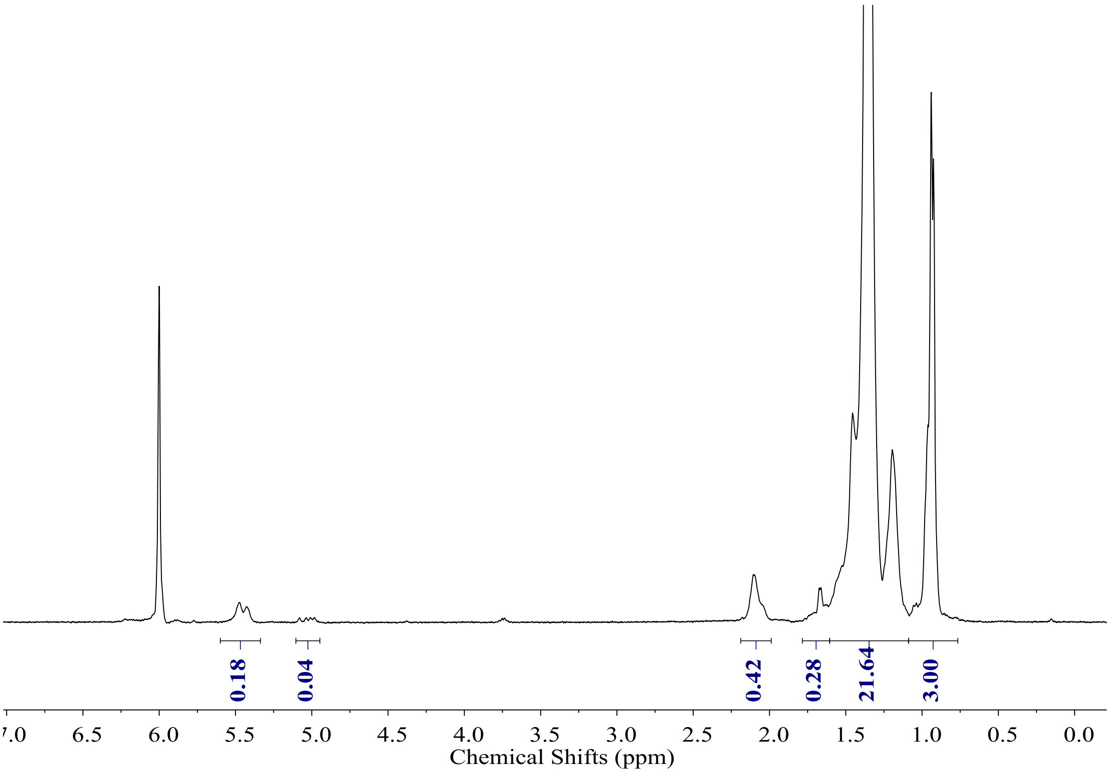


Figure S38. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 3, entry 12.

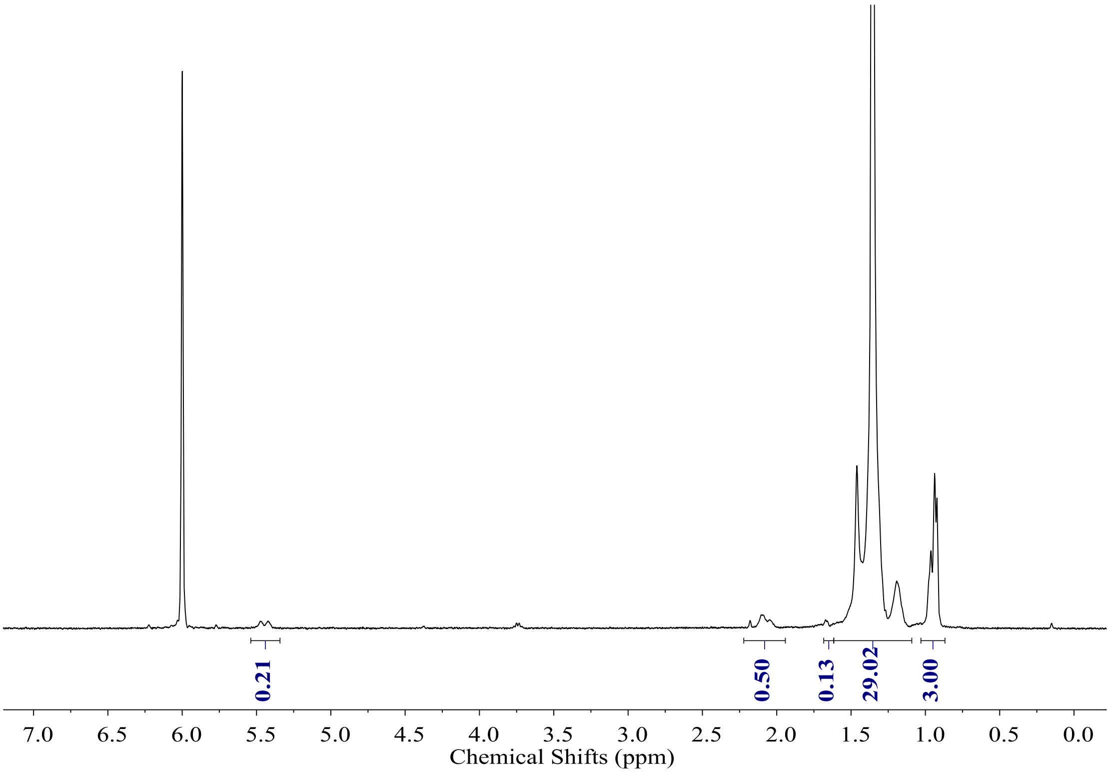


Figure S39. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 5, entry 1.

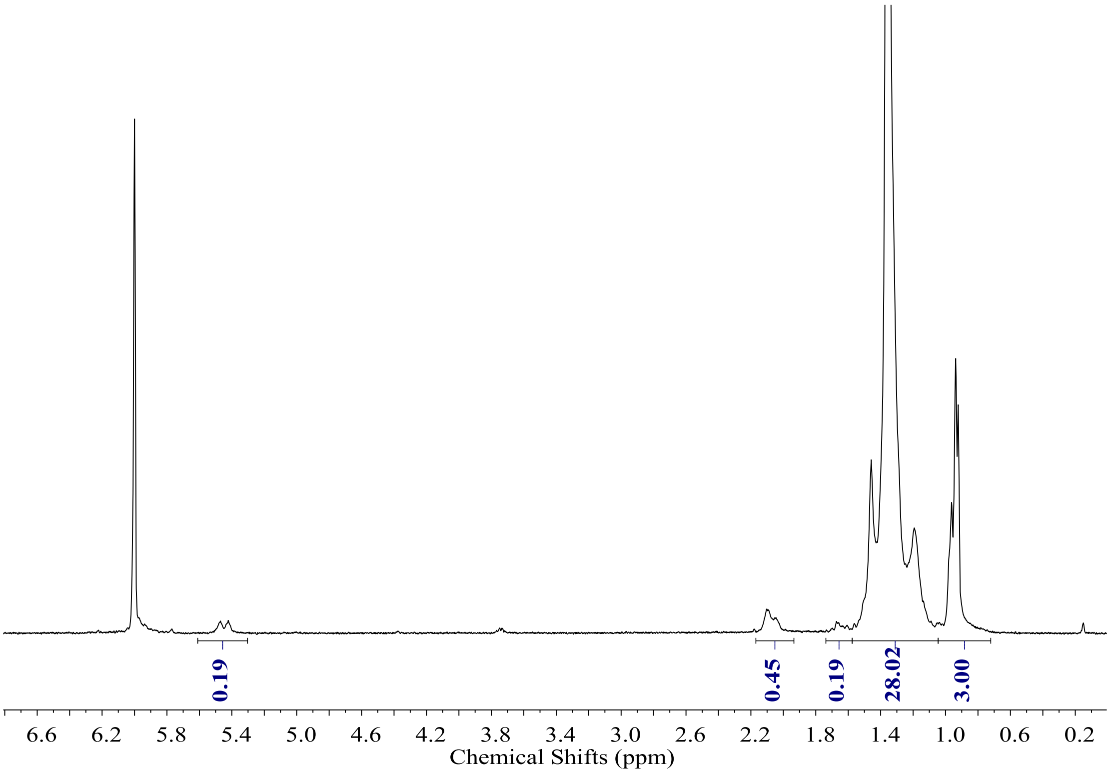


Figure S40. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 5, entry 2.

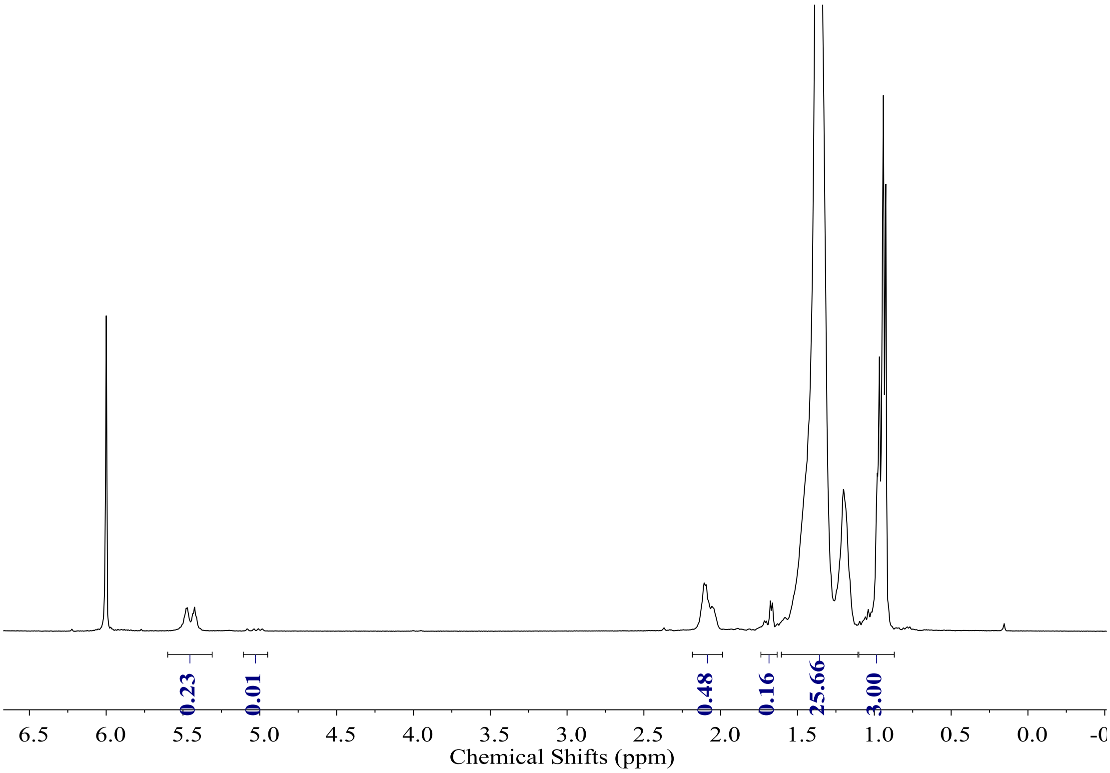


Figure S41. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni3** from table 5, entry 3.

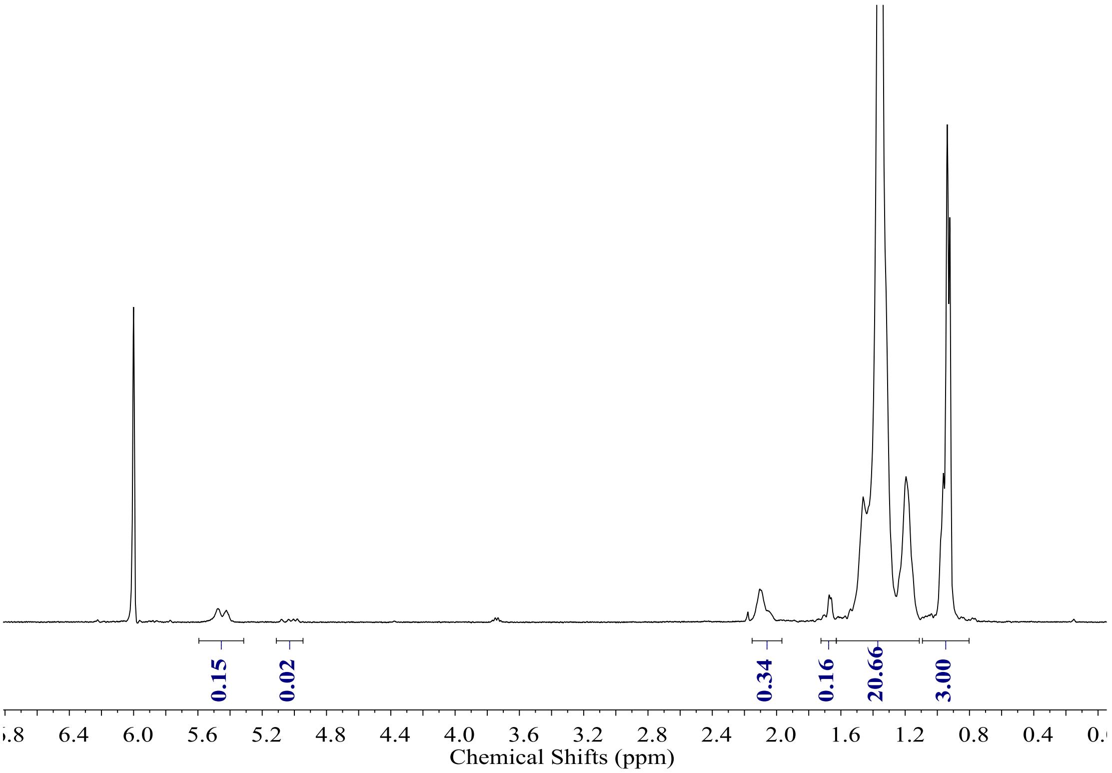


Figure S42. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 5, entry 4.

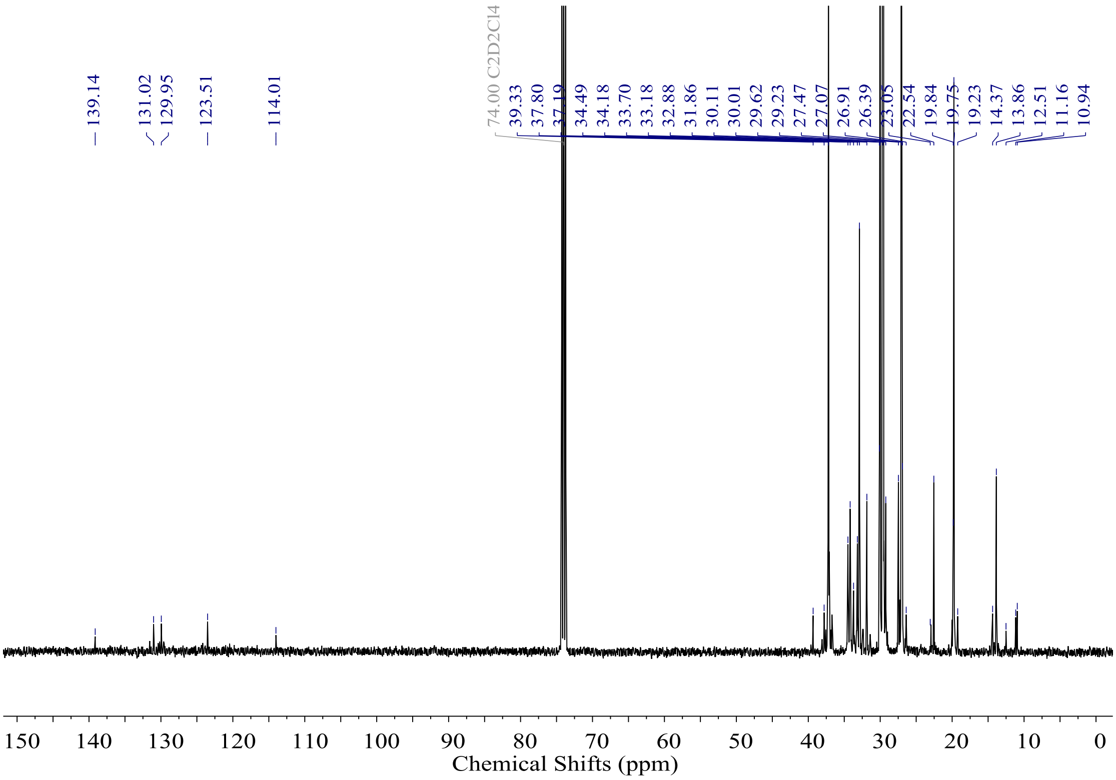


Figure S43. ^{13}C NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 5, entry 4.

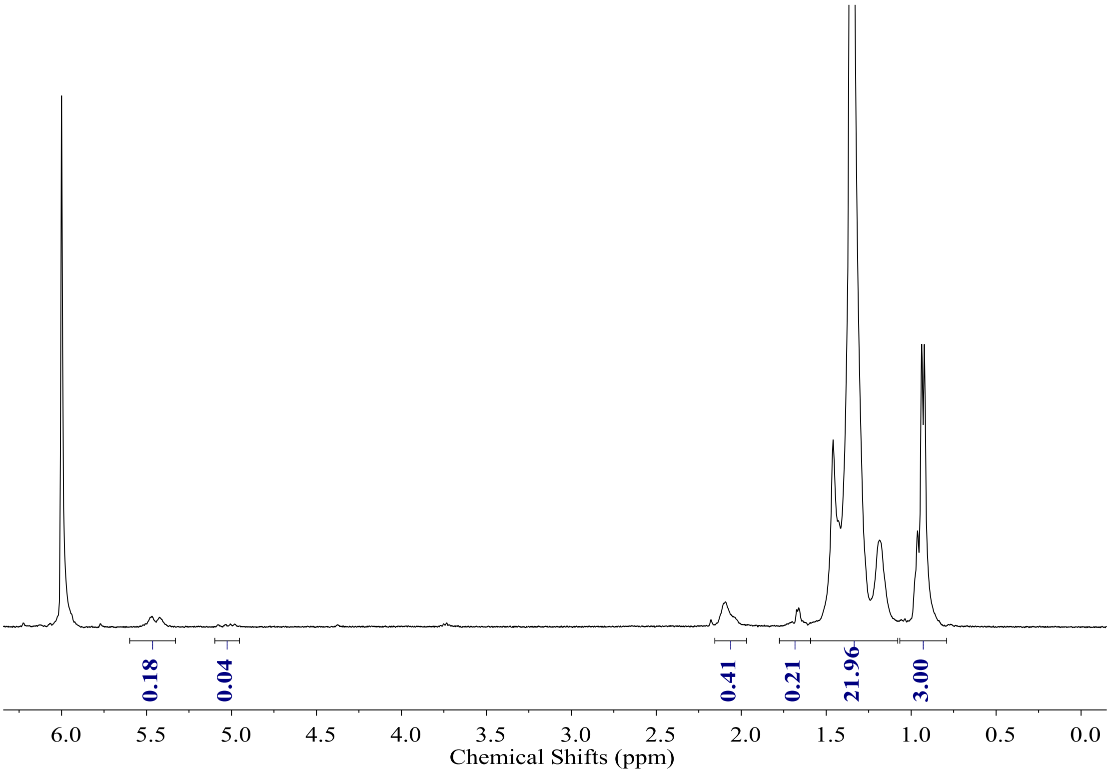


Figure S44. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 5, entry 5.

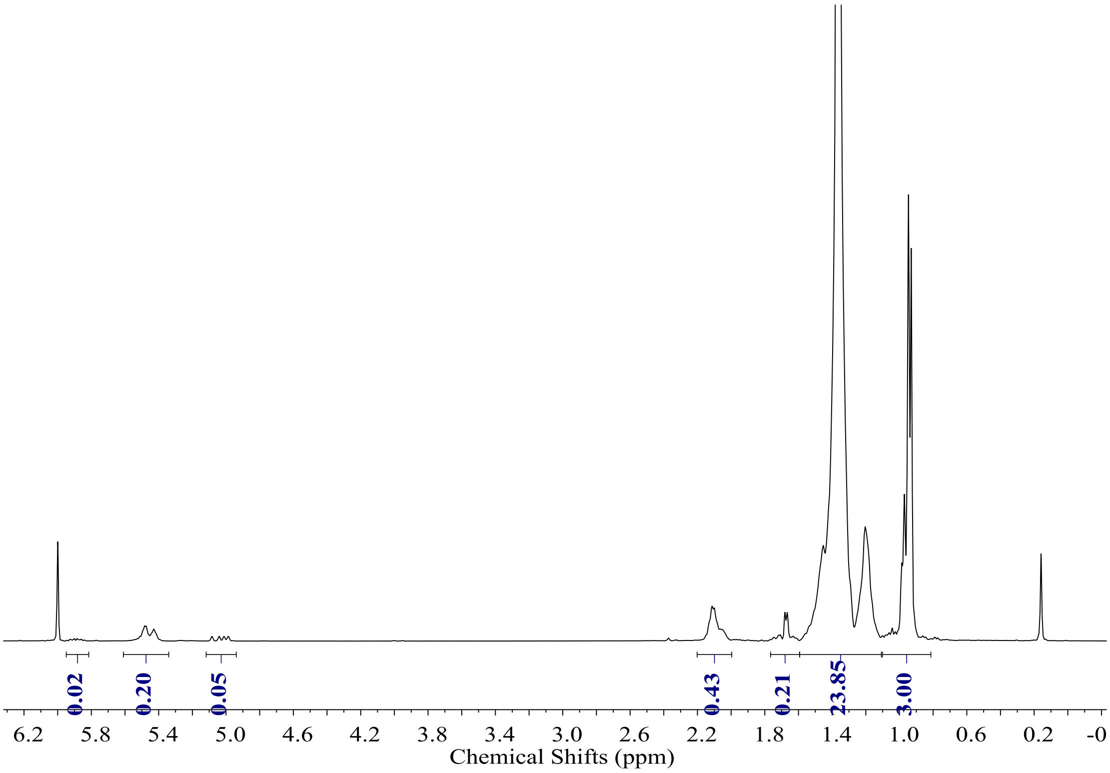
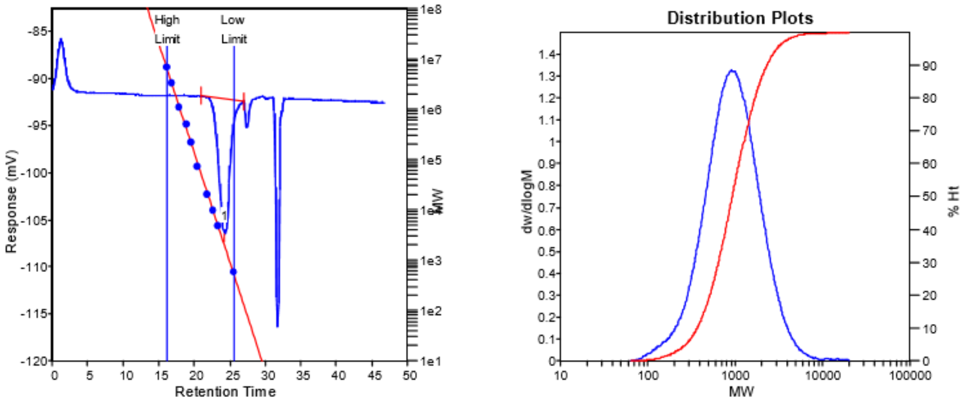


Figure S45. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 ℃) of the polyethylene generated by complex **Ni4** from table 5, entry 6.

6. GPC traces of polymers



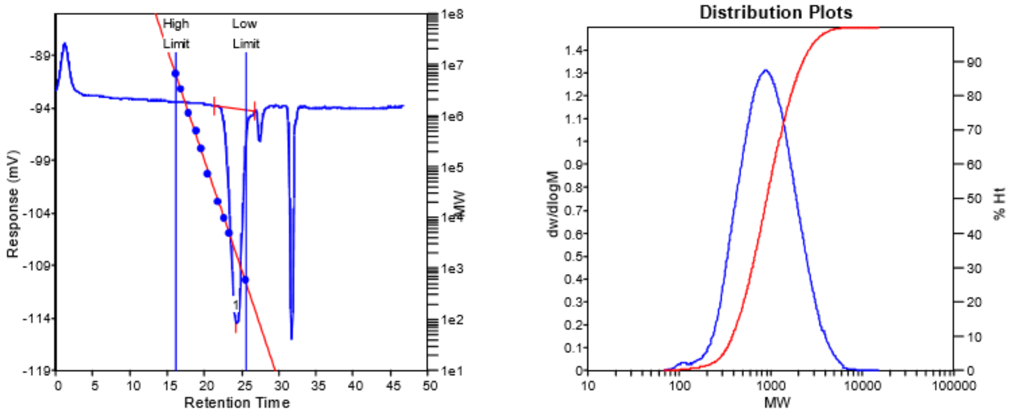
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	906	695	1202	2222	4902	1114	1.7295

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.00	24.20	26.93	-14.299	0	1539.39	100

Figure S46. GPC trace of the polymer from table 1, entry 1.



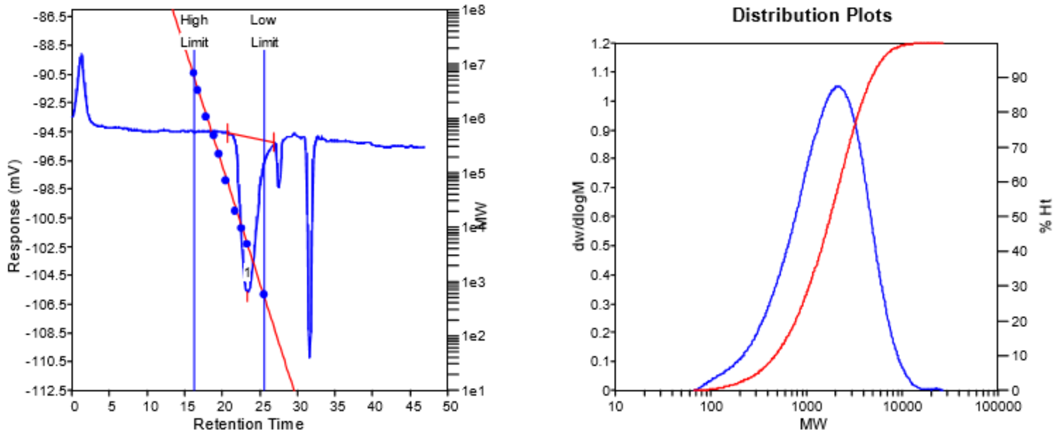
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	878	712	1146	1796	2666	1075	1.60955

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.28	24.23	26.85	-20.498	0	2233.02	100

Figure S47. GPC trace of the polymer from table 1, entry 2.



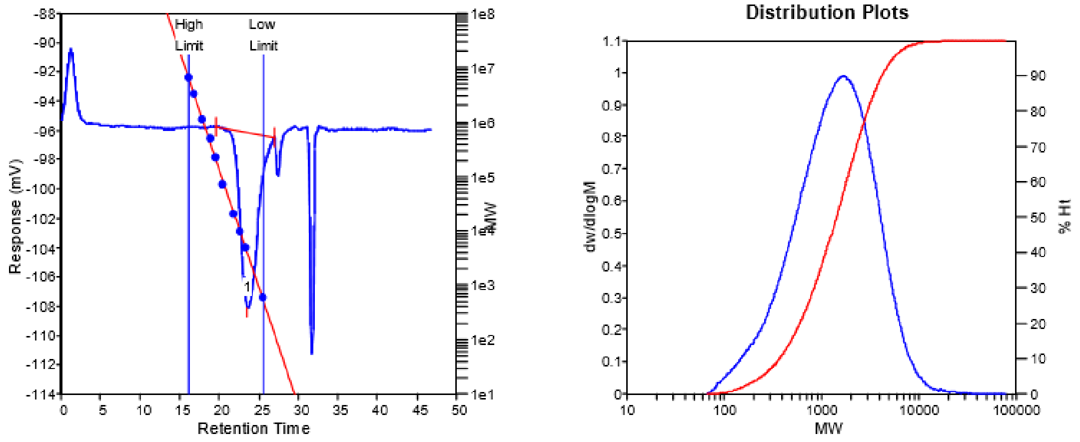
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2097	1006	2294	4014	6195	2099	2.28032

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.68	23.35	26.88	-10.7928	100	1467.06	100

Figure S48. GPC trace of the polymer from table 1, entry 3.



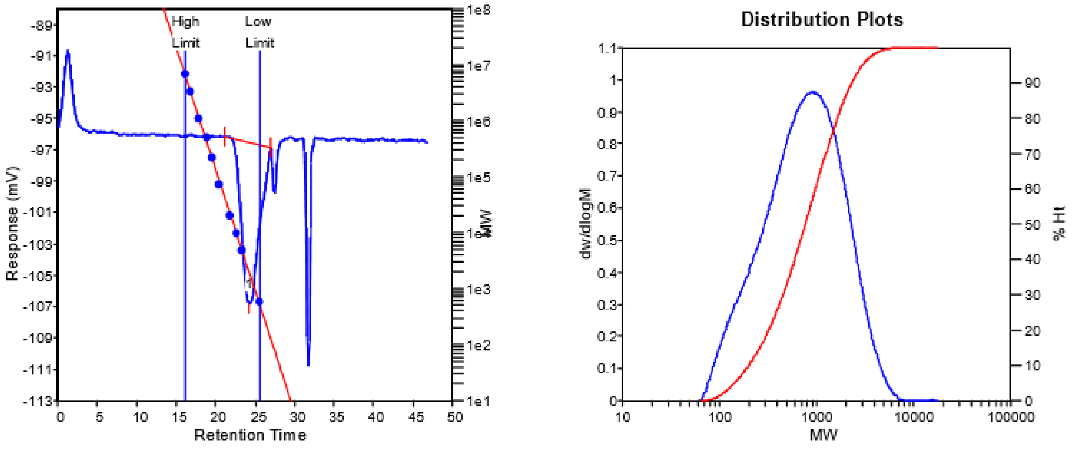
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1700	816	1971	4041	8141	1774	2.41544

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		19.62	23.55	26.92	-11.93	100	1722.09	100

Figure S49. GPC trace of the polymer from table 1, entry 4.



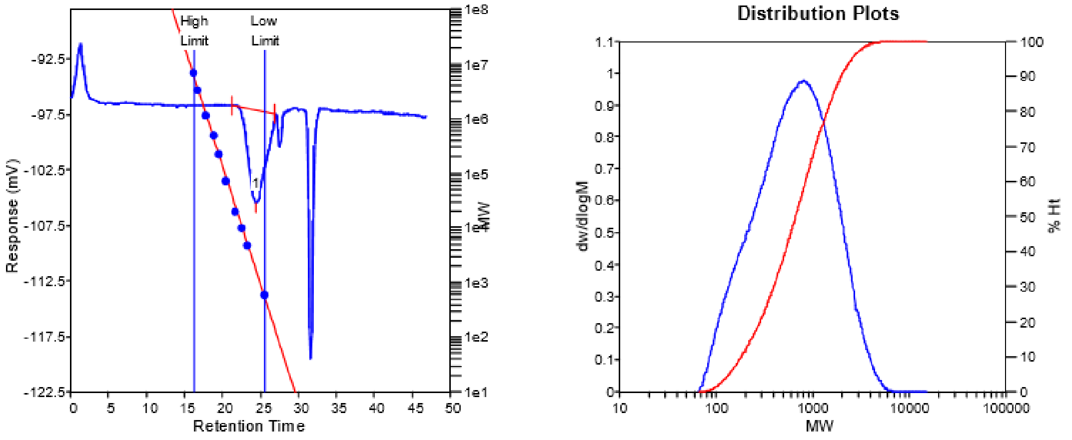
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	921	471	1050	1922	3023	954	2.2293

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.13	24.23	26.95	-10.278	0	1526.47	100

Figure S50. GPC trace of the polymer from table 1, entry 5.



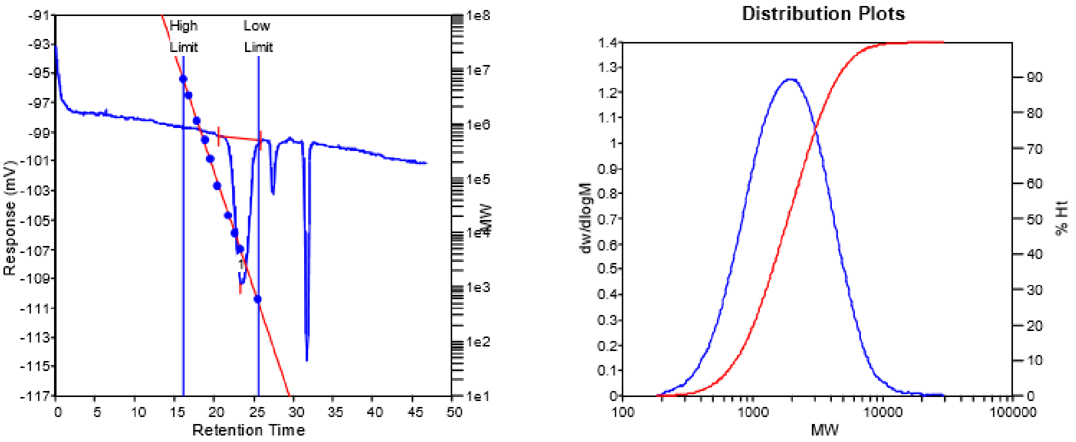
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	810	427	905	1606	2340	825	2.11944

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.28	24.32	26.90	-8.35041	100	1220.17	100

Figure S51. GPC trace of the polymer from table 1, entry 6.



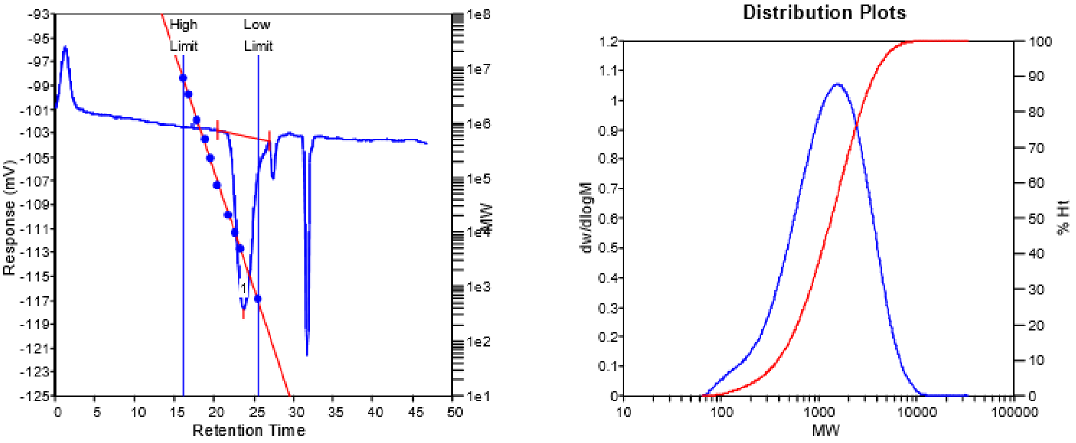
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1873	1432	2347	3837	6499	2194	1.63897

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.60	23.45	25.87	-9.89857	100	1130.13	100

Figure S52. GPC trace of the polymer from table 1, entry 7.



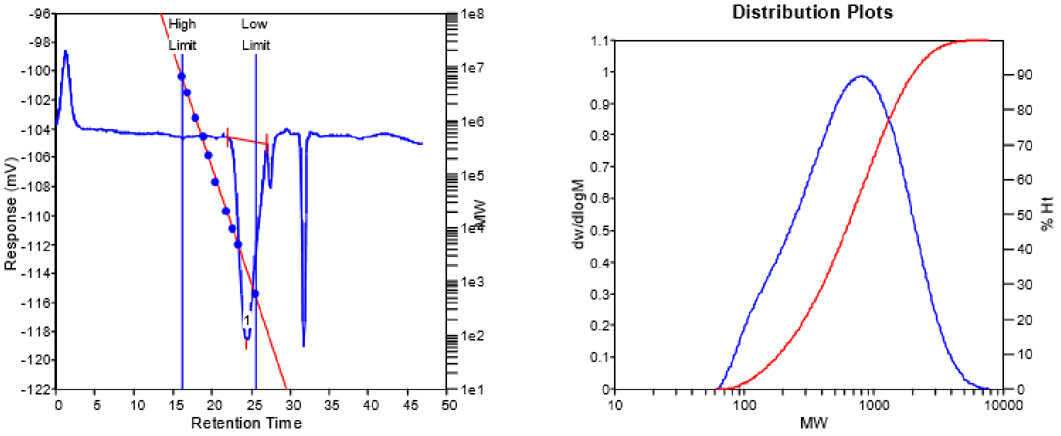
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1519	801	1740	3023	4953	1596	2.17228

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.47	23.67	26.93	-14.4433	100	1959.08	100

Figure S53. GPC trace of the polymer from table 1, entry 8.



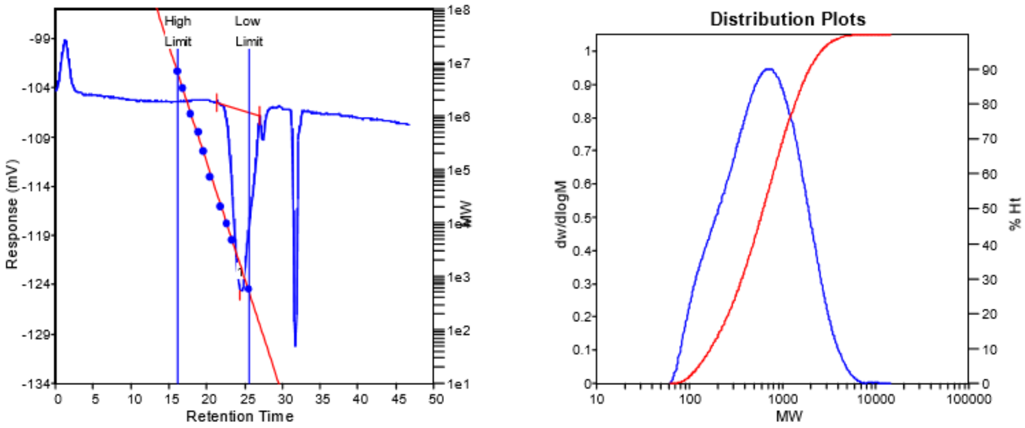
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	797	431	917	1628	2402	836	2.12761

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.98	24.33	26.98	-13.8186	100	2000.34	100

Figure S54. GPC trace of the polymer from table 1, entry 9.



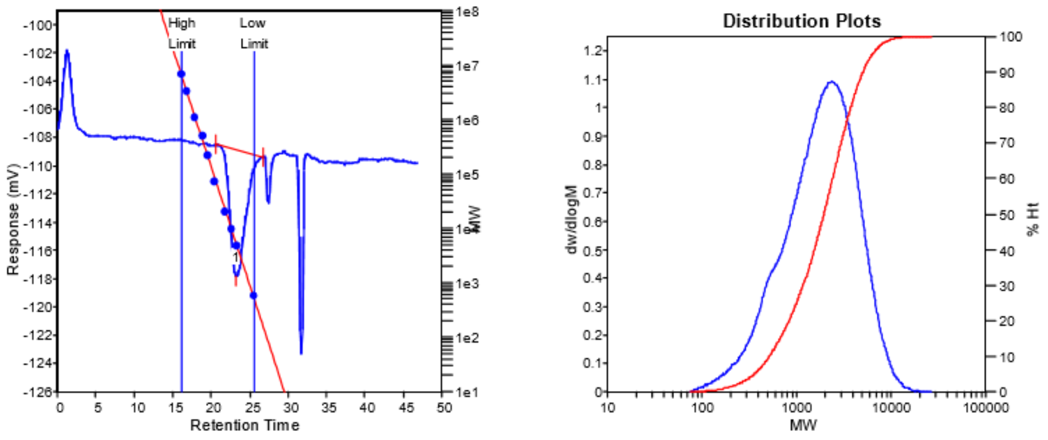
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	689	397	879	1680	2686	794	2.21411

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.32	24.48	26.98	-18.3311	100	2765.46	100

Figure S55. GPC trace of the polymer from table 1, entry 10.



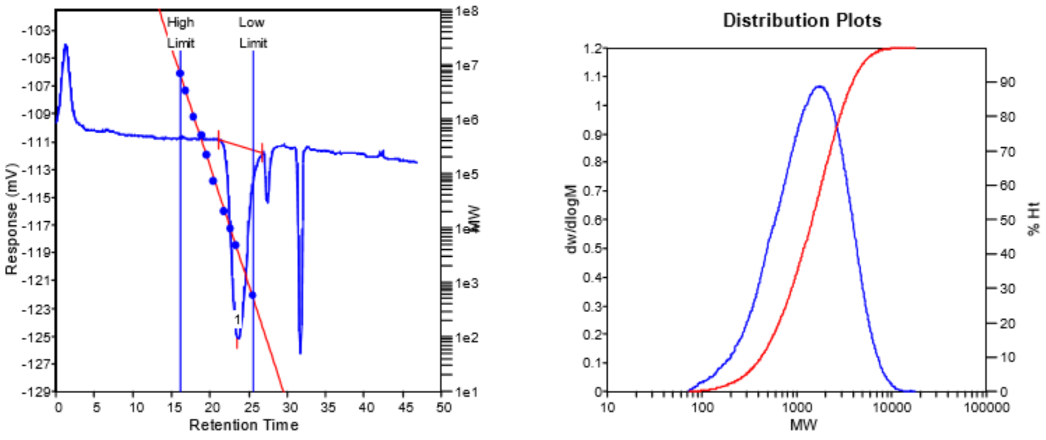
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2347	1130	2441	4078	5866	2246	2.16018

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.68	23.22	26.77	-9.01022	100	1178.48	100

Figure S56. GPC trace of the polymer from table 1, entry 11.



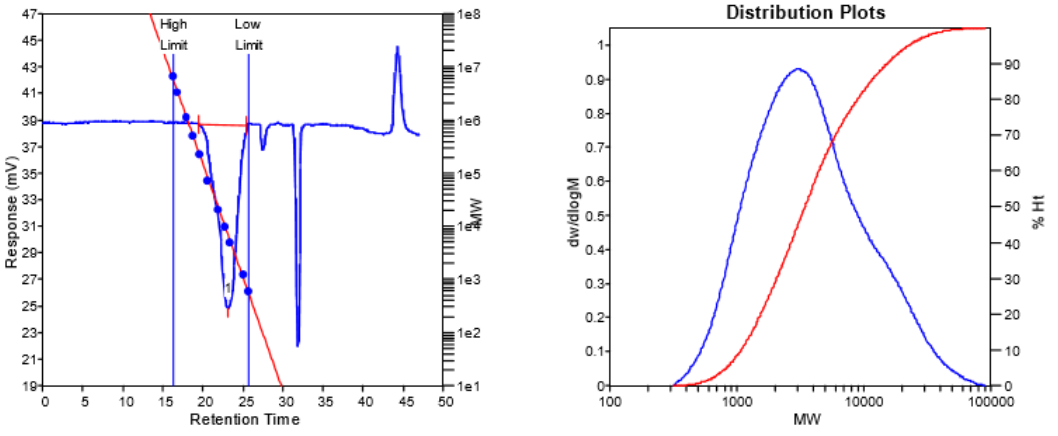
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1700	891	1858	3104	4432	1711	2.0853

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.13	23.55	26.82	-13.9199	100	1865.92	100

Figure S57. GPC trace of the polymer from table 1, entry 12.



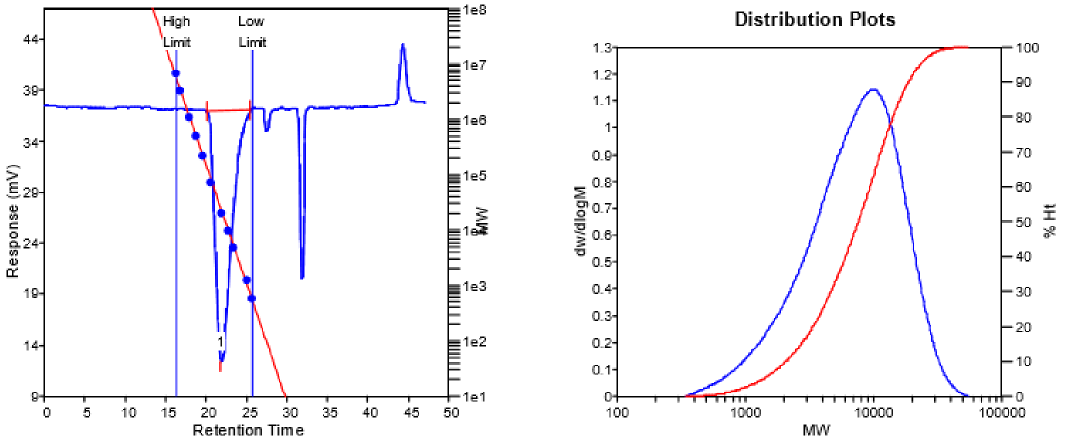
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2938	2397	6263	16467	30118	5406	2.61285

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		19.53	23.13	25.48	-13.7899	100	2152.67	100

Figure S58. GPC trace of the polymer from table 1, entry 13.



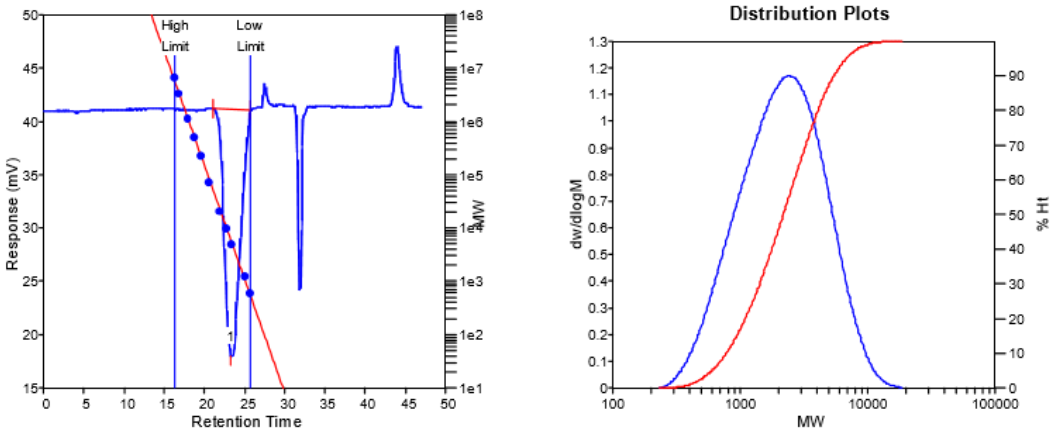
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	10125	4467	9221	14520	19597	8551	2.06425

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.05	21.83	25.40	-24.5411	100	3117.15	100

Figure S59. GPC trace of the polymer from table 1, entry 14.



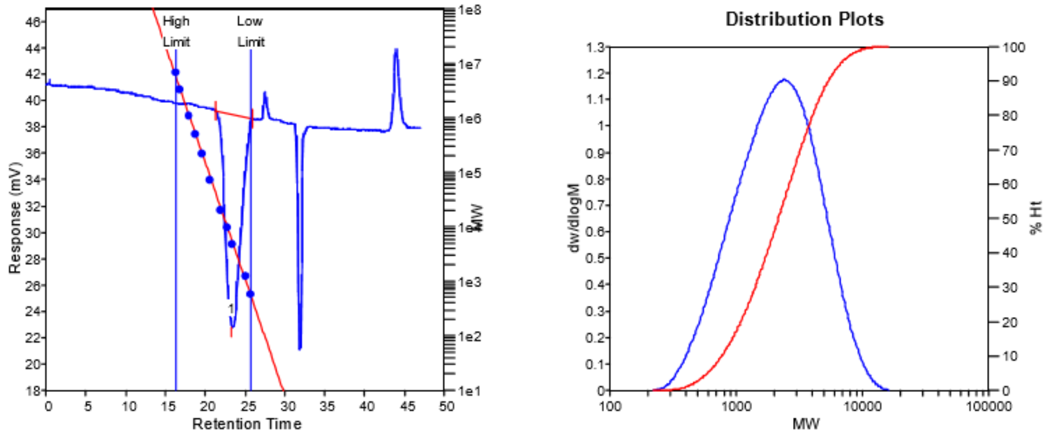
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2428	1599	2721	4247	5931	2542	1.70169

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.20	23.33	25.80	-23.1662	100	2874.4	100

Figure S60. GPC trace of the polymer from table 2, entry 1.



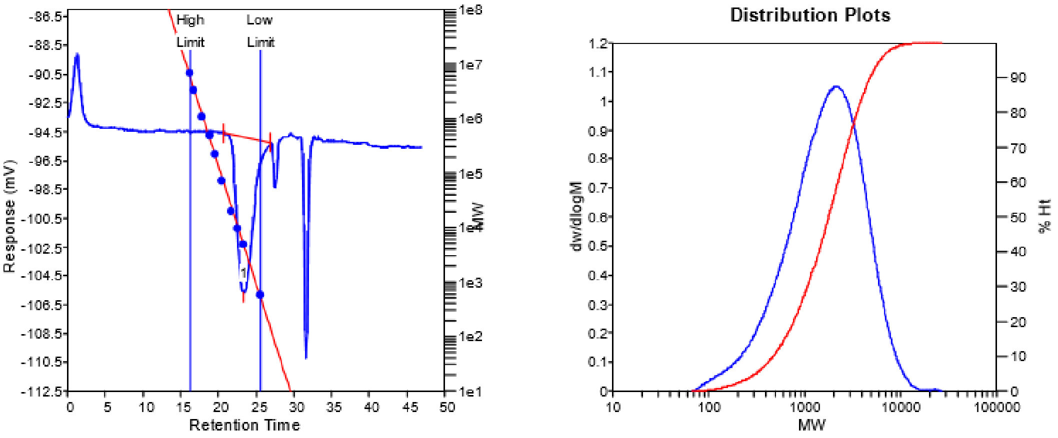
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2428	1583	2688	4154	5705	2514	1.69804

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.33	23.33	25.85	-16.096	100	1990.22	100

Figure S61. GPC trace of the polymer from table 2, entry 2.



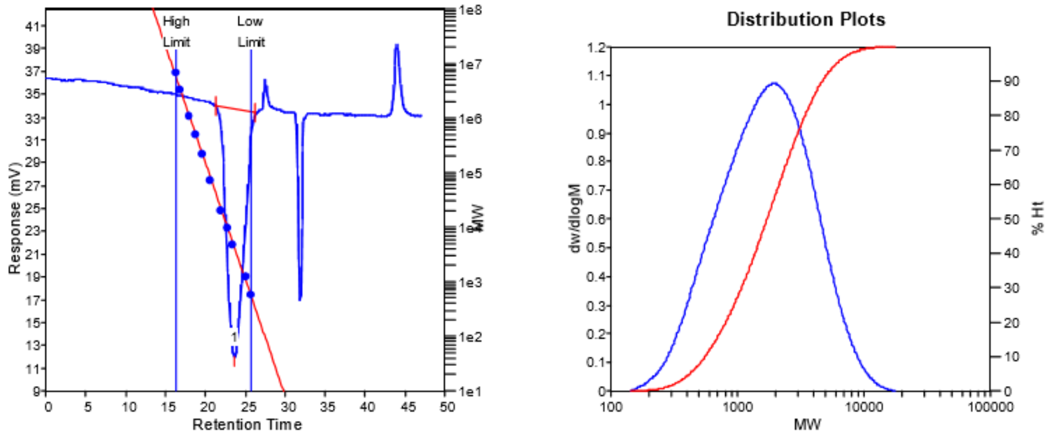
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2097	1006	2294	4014	6195	2099	2.28032

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.68	23.35	26.88	-10.7928	100	1467.06	100

Figure S62. GPC trace of the polymer from table 2, entry 3.



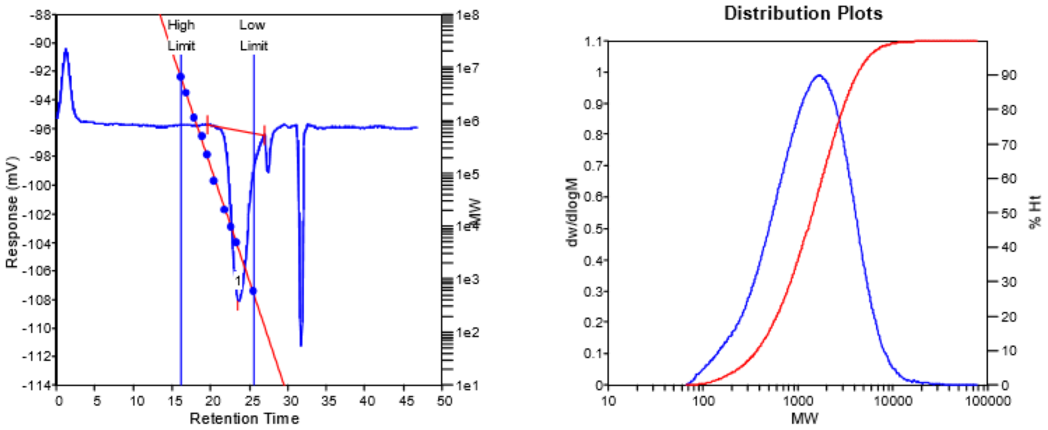
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1945	1190	2258	3823	5603	2082	1.89748

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.25	23.57	26.32	-21.7391	100	2942.45	100

Figure S63. GPC trace of the polymer from table 2, entry 4.



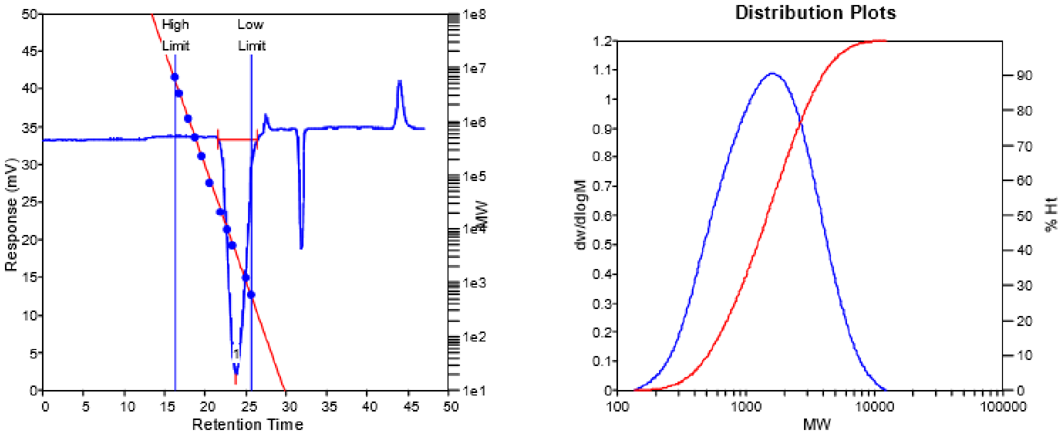
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1700	816	1971	4041	8141	1774	2.41544

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		19.62	23.55	26.92	-11.93	100	1722.09	100

Figure S64. GPC trace of the polymer from table 2, entry 5.



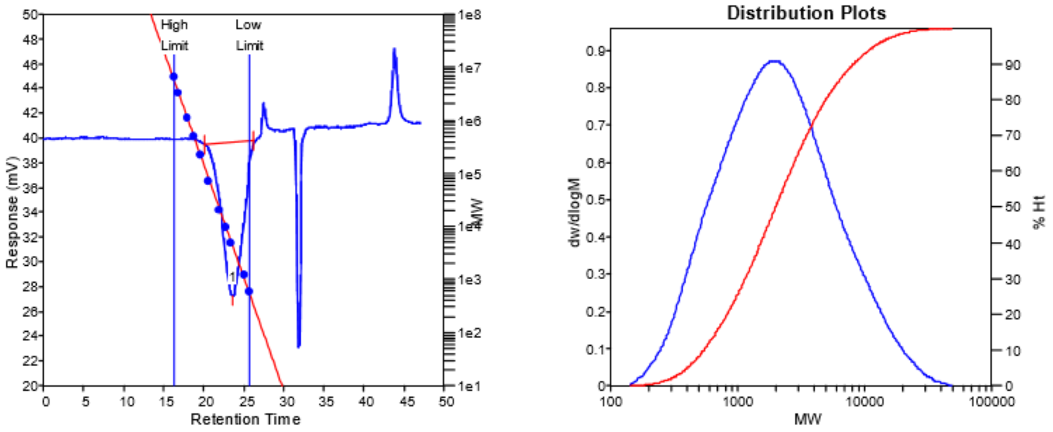
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1608	1054	1915	3149	4494	1774	1.81689

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.62	23.77	26.37	-31.0933	100	4155.27	100

Figure S65. GPC trace of the polymer from table 2, entry 6.



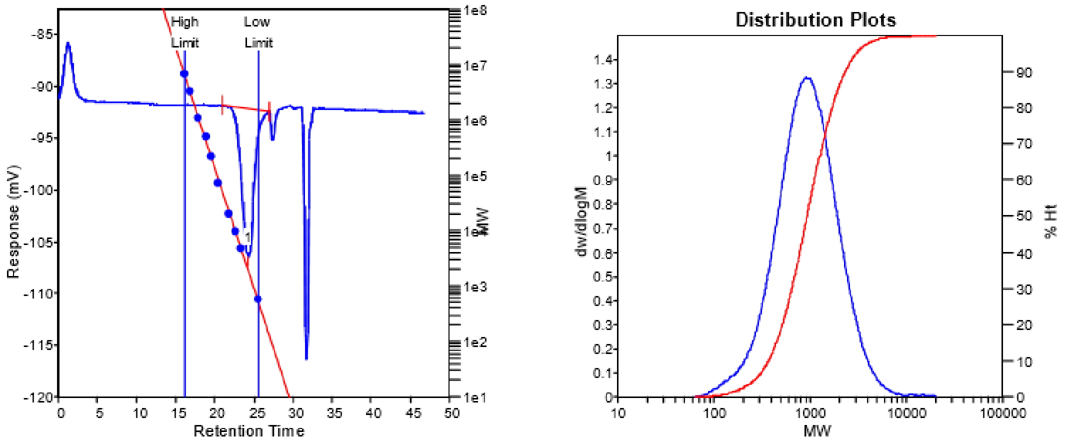
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1884	1264	3453	8759	15890	2992	2.7318

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.18	23.60	26.32	-12.4256	100	2065.79	100

Figure S66. GPC trace of the polymer from table 3, entry 1.



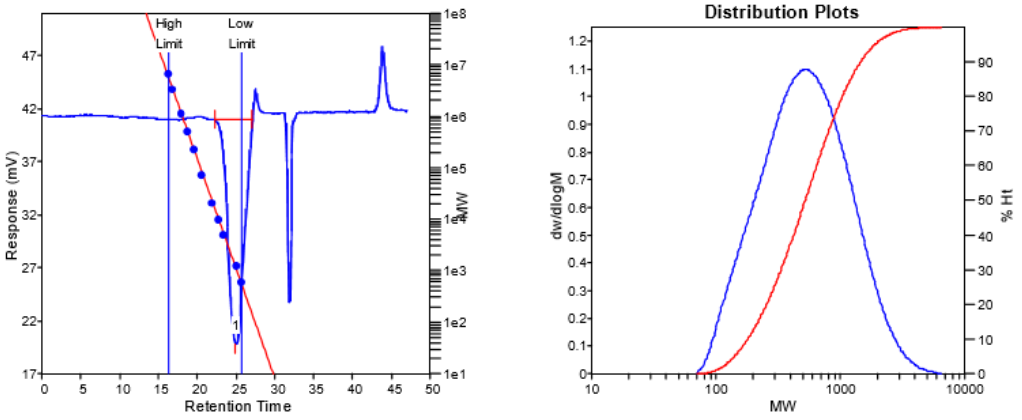
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	906	695	1202	2222	4902	1114	1.7295

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.00	24.20	26.93	-14.299	0	1539.39	100

Figure S67. GPC trace of the polymer from table 3, entry 2.



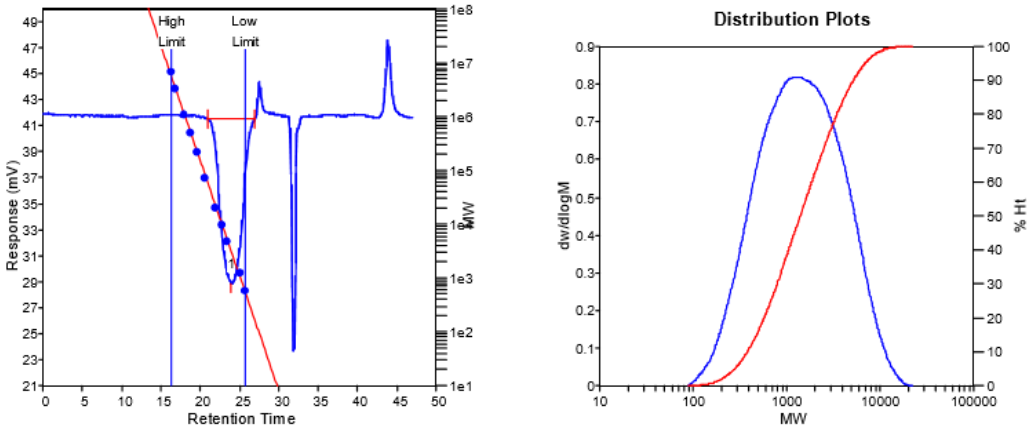
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	521	383	699	1224	1902	644	1.82507

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		22.30	24.95	27.05	-21.1471	100	2795.72	100

Figure S68. GPC trace of the polymer from table 3, entry 3.



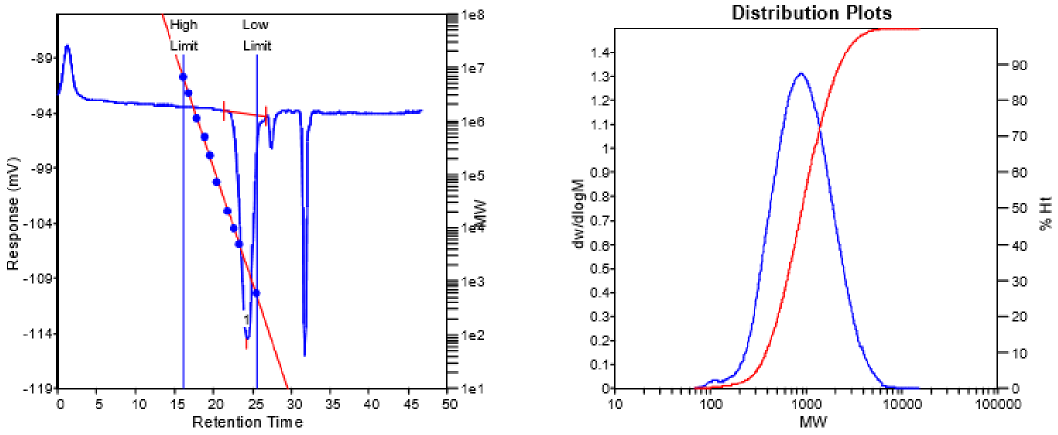
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1267	871	2199	4553	7090	1953	2.52468

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.02	23.93	26.82	-12.643	100	2242.29	100

Figure S69. GPC trace of the polymer from table 3, entry 4.



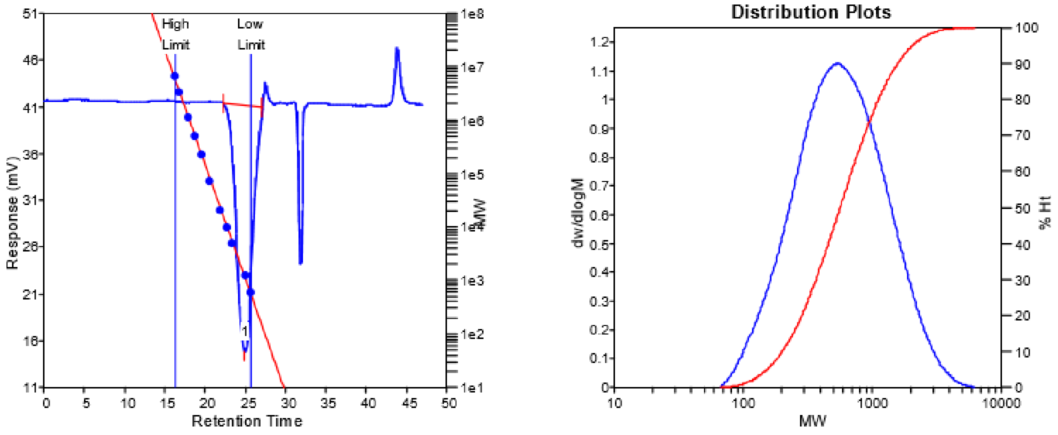
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	878	712	1146	1796	2666	1075	1.60955

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.28	24.23	26.85	-20.498	0	2233.02	100

Figure S70. GPC trace of the polymer from table 3, entry 5.



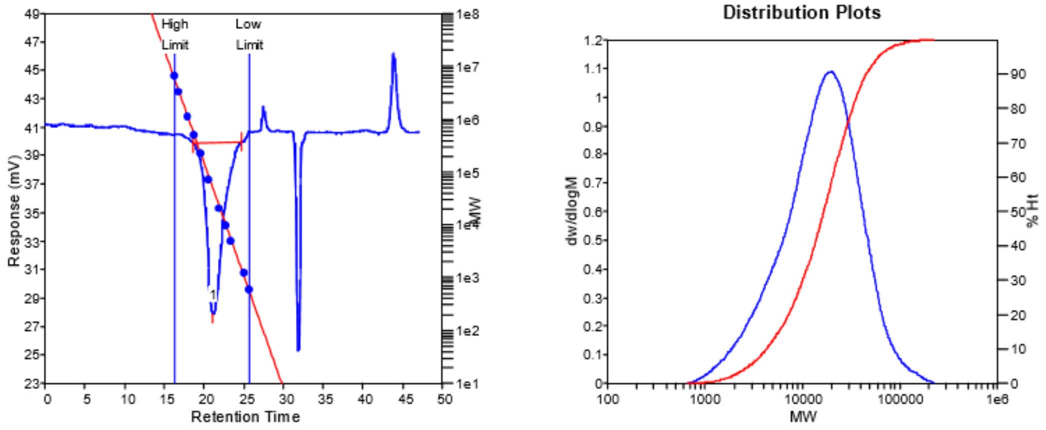
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	546	417	754	1291	1948	696	1.80815

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		22.35	24.90	27.10	-26.2586	100	3392.48	100

Figure S71. GPC trace of the polymer from table 3, entry 6.



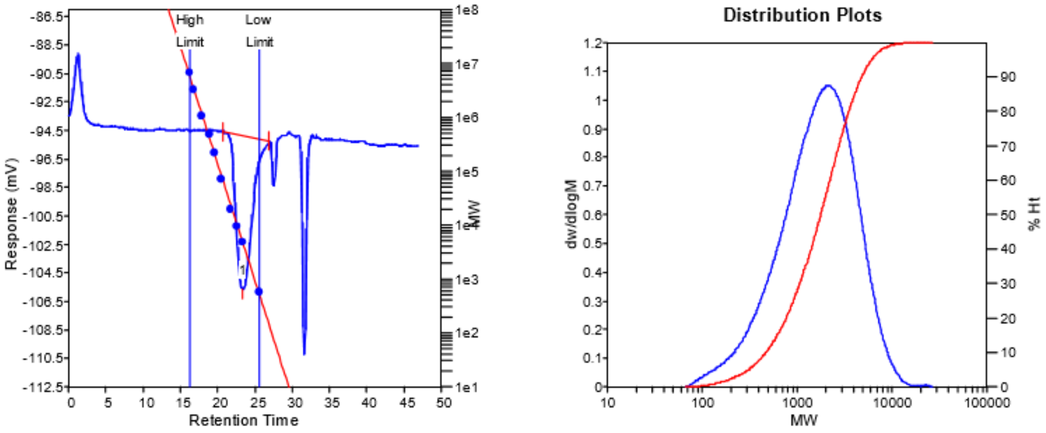
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	20348	9530	22114	41959	70253	20071	2.32046

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		18.57	21.10	24.70	-12.0955	100	1614.05	100

Figure S72. GPC trace of the polymer from table 3, entry 7.



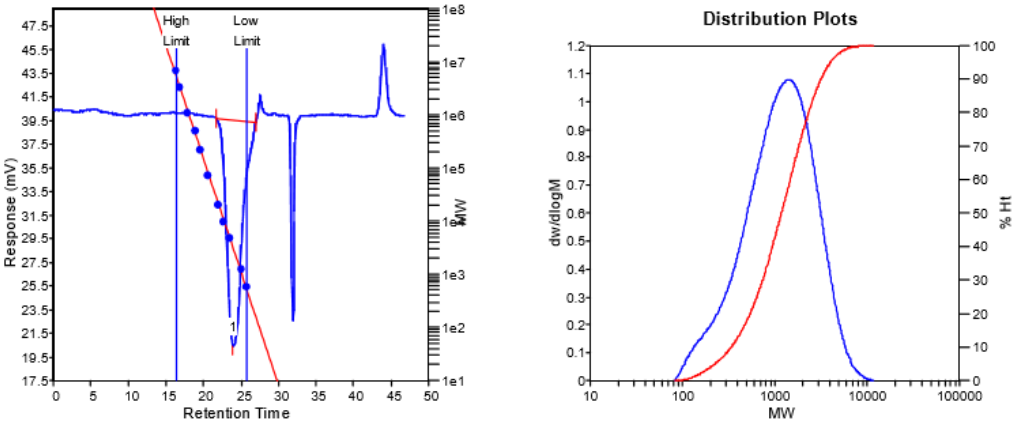
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2097	1006	2294	4014	6195	2099	2.28032

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.68	23.35	26.88	-10.7928	100	1467.06	100

Figure S73. GPC trace of the polymer from table 3, entry 8.



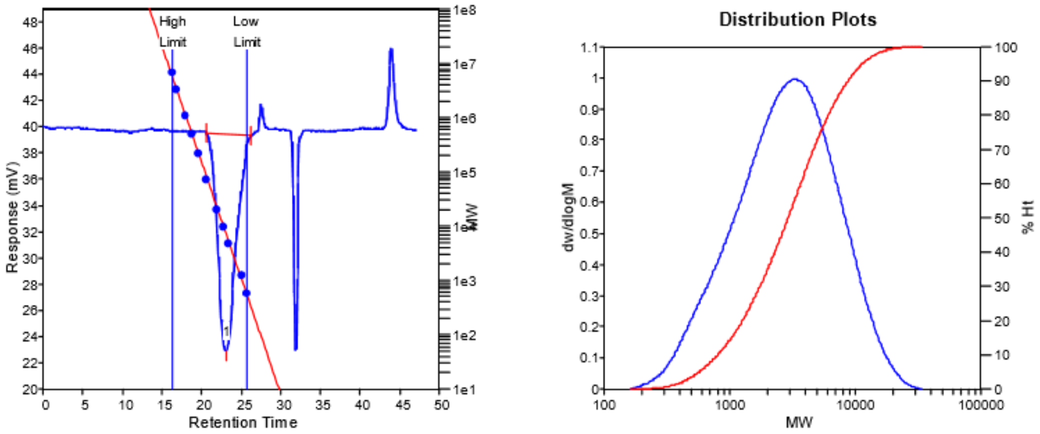
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1439	734	1518	2538	3646	1399	2.06812

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.67	23.88	26.88	-19.1096	100	2574.11	100

Figure S74. GPC trace of the polymer from table 3, entry 9.



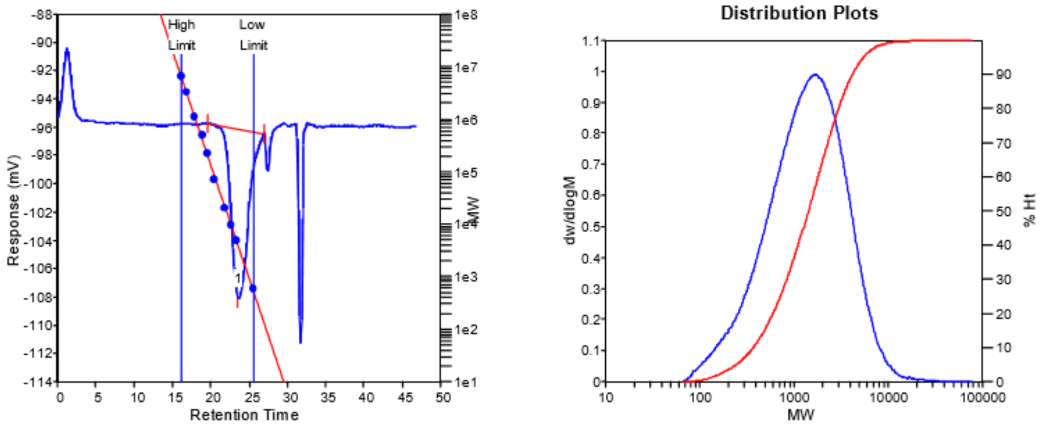
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	3231	1810	3995	7297	10981	3631	2.20718

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.55	23.03	26.18	-16.5223	100	2411.15	100

Figure S75. GPC trace of the polymer from table 3, entry 10.



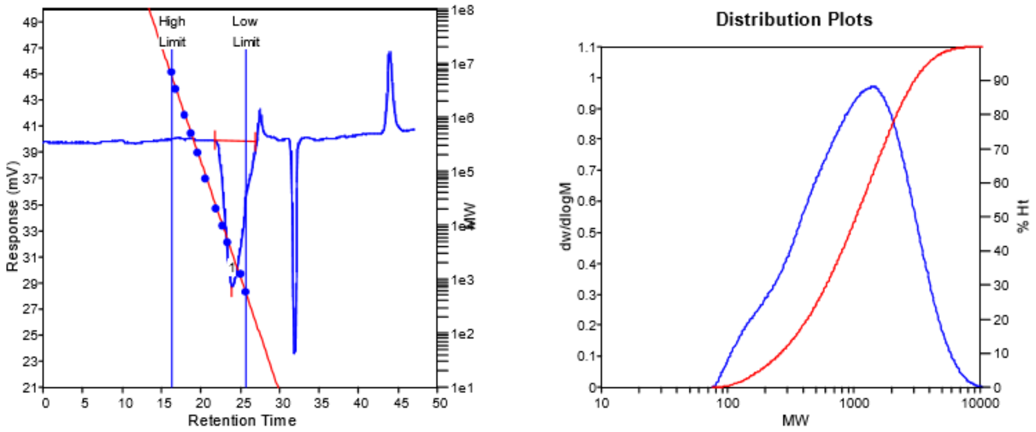
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1700	816	1971	4041	8141	1774	2.41544

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		19.62	23.55	26.92	-11.93	100	1722.09	100

Figure S76. GPC trace of the polymer from table 3, entry 11.



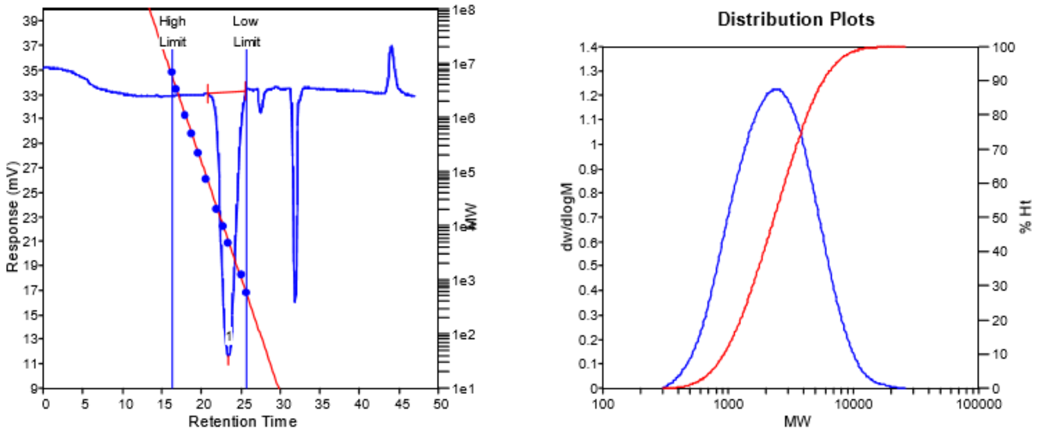
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1462	614	1392	2459	3541	1267	2.2671

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.80	23.87	26.97	-11.2056	100	1677.16	100

Figure S77. GPC trace of the polymer from table 3, entry 12.



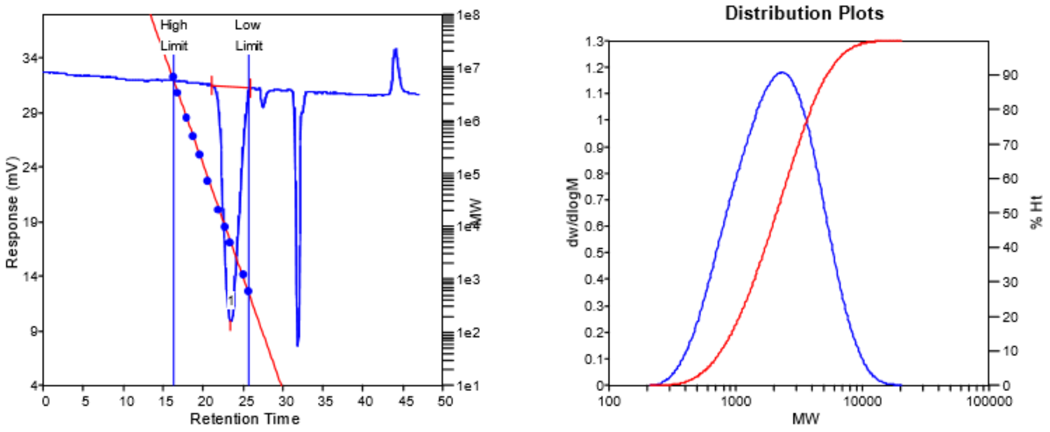
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2353	1816	2933	4585	6681	2749	1.61509

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.83	23.37	25.53	-21.4777	100	2543.18	100

Figure S78. GPC trace of the polymer from table 4, entry 1.



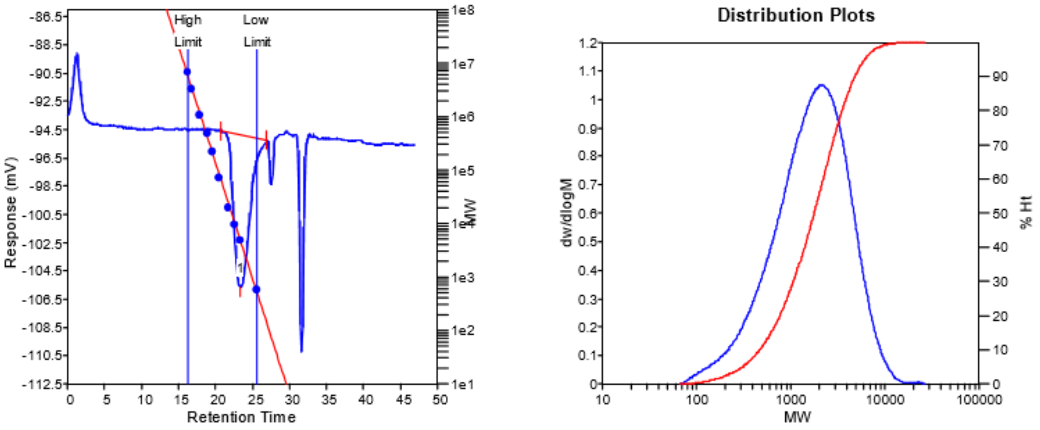
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2353	1564	2631	4110	5794	2460	1.68223

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.10	23.37	25.90	-21.4915	100	2645.08	100

Figure S79. GPC trace of the polymer from table 4, entry 2.



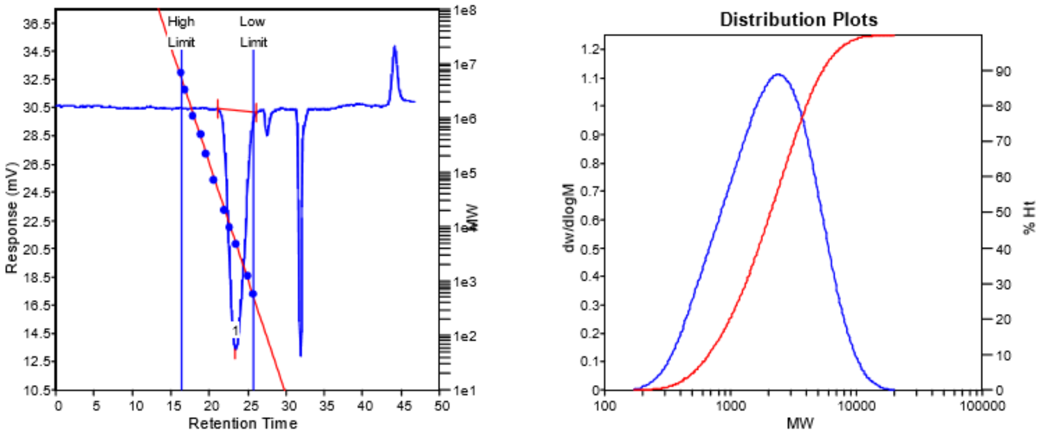
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2097	1006	2294	4014	6195	2099	2.28032

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.68	23.35	26.88	-10.7928	100	1467.06	100

Figure S80. GPC trace of the polymer from table 4, entry 3.



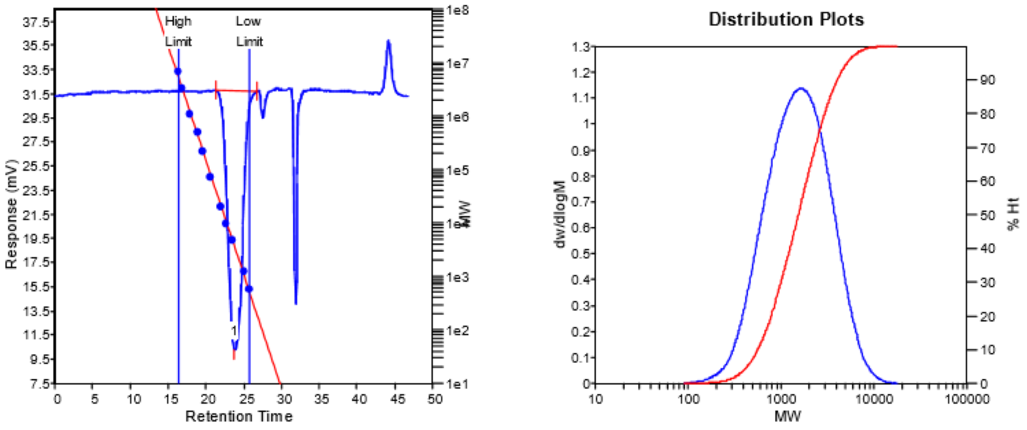
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2428	1439	2642	4279	6067	2451	1.836

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.12	23.33	26.13	-16.9056	100	2210.08	100

Figure S81. GPC trace of the polymer from table 4, entry 4.



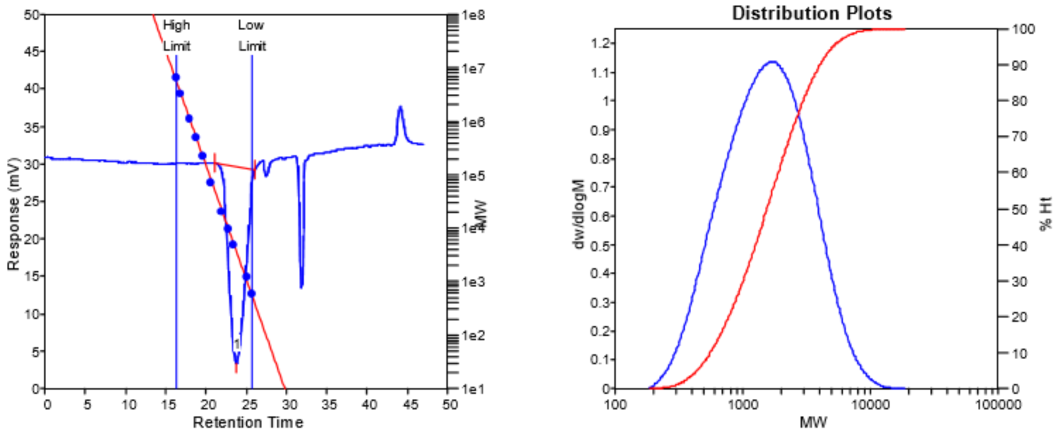
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1633	1125	1982	3238	4777	1842	1.76178

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.25	23.75	26.78	-21.4651	100	2739.17	100

Figure S82. GPC trace of the polymer from table 4, entry 5.



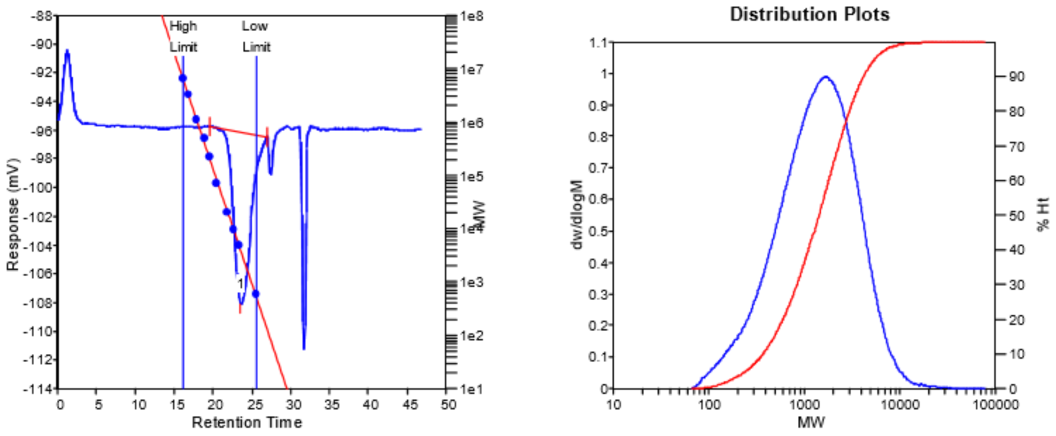
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1713	1152	1989	3220	4685	1851	1.72656

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.20	23.73	26.03	-26.3435	100	3368.27	100

Figure S83. GPC trace of the polymer from table 4, entry 6.



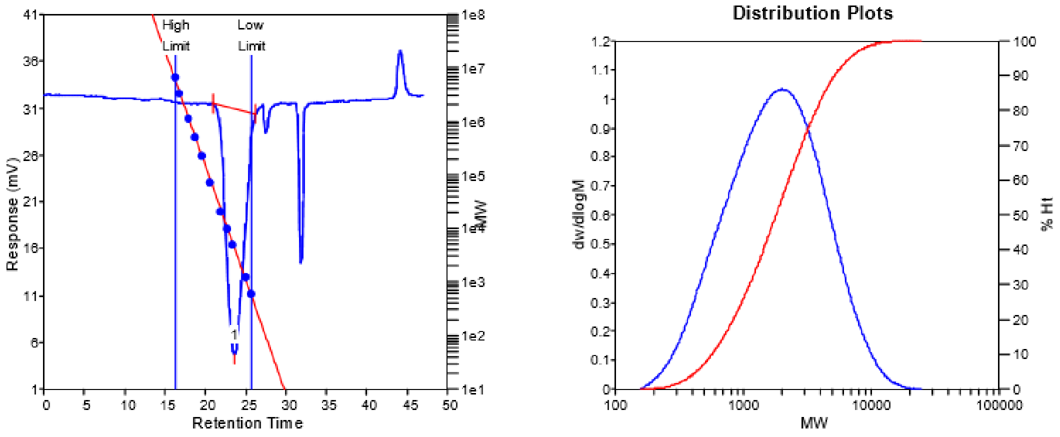
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1700	816	1971	4041	8141	1774	2.41544

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		19.62	23.55	26.92	-11.93	100	1722.09	100

Figure S84. GPC trace of the polymer from table 4, entry 7.



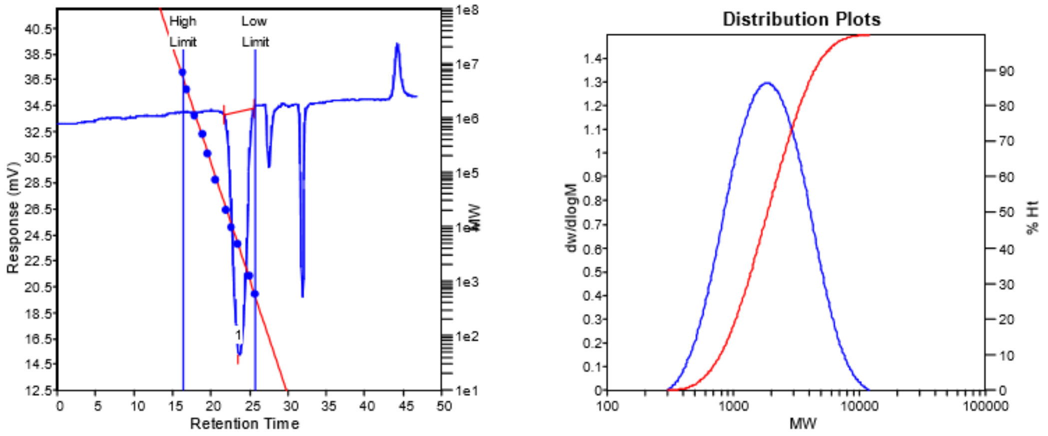
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2007	1237	2448	4353	6650	2242	1.97898

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.88	23.53	26.22	-26.1838	100	3679.36	100

Figure S85. GPC trace of the polymer from table 4, entry 8.



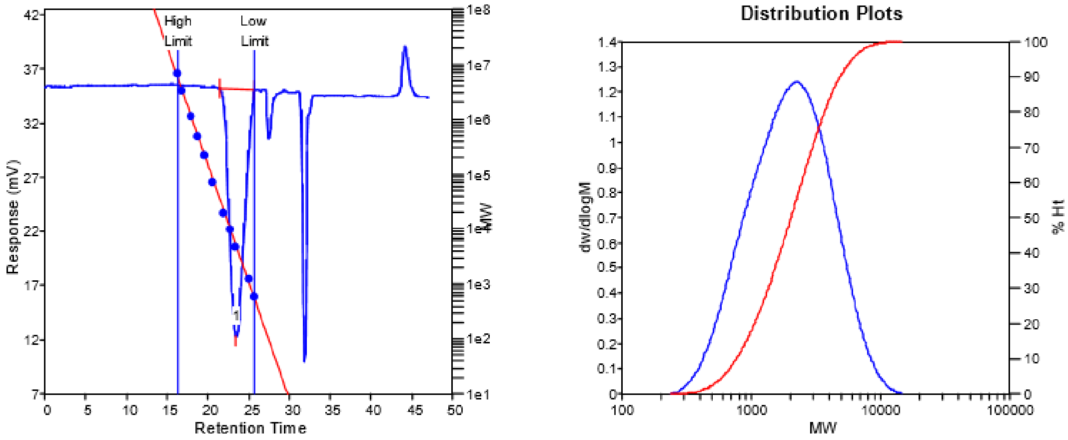
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1884	1511	2294	3358	4530	2168	1.5182

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.63	23.60	25.53	-18.7691	100	2103.86	100

Figure S86. GPC trace of the polymer from table 5, entry 1.



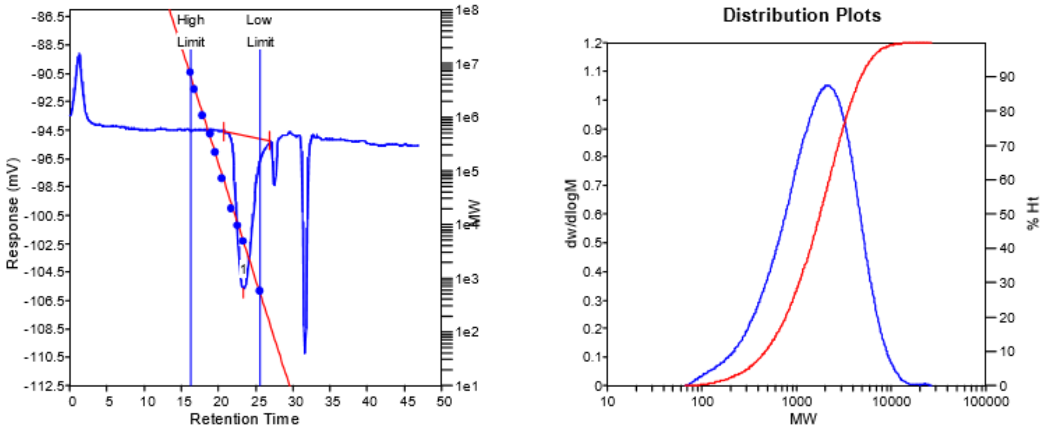
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2243	1536	2480	3739	5116	2331	1.61458

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.43	23.42	25.77	-22.8021	100	2672.17	100

Figure S87. GPC trace of the polymer from table 5, entry 2.



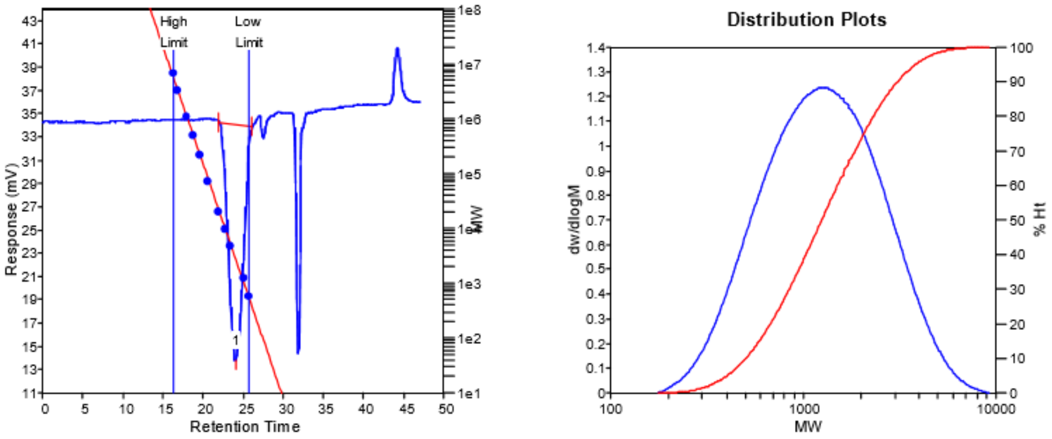
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	2097	1006	2294	4014	6195	2099	2.28032

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		20.68	23.35	26.88	-10.7928	100	1467.06	100

Figure S88. GPC trace of the polymer from table 5, entry 3.



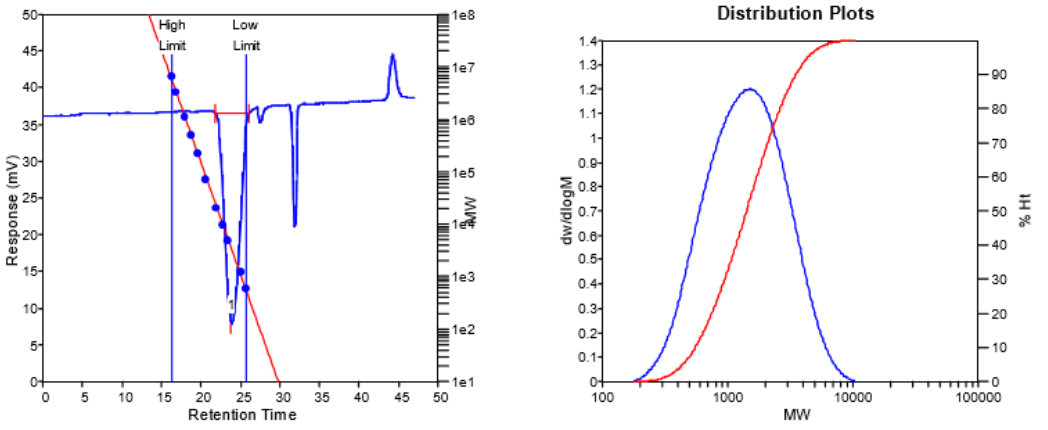
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1267	986	1557	2347	3225	1465	1.57911

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.93	24.02	26.08	-20.2254	100	2374.61	100

Figure S89. GPC trace of the polymer from table 5, entry 4.



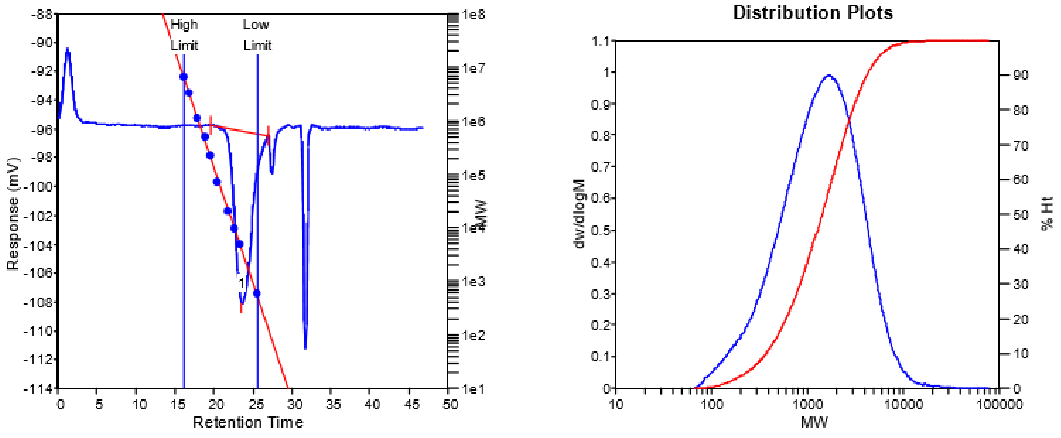
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1509	1091	1764	2691	3709	1656	1.61687

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		21.80	23.83	26.08	-28.7064	100	3470.69	100

Figure S90. GPC trace of the polymer from table 5, entry 5.



MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	1700	816	1971	4041	8141	1774	2.41544

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		19.62	23.55	26.92	-11.93	100	1722.09	100

Figure S91. GPC trace of the polymer from table 5, entry 6.

8. Crystallographic data of nickel complexes

Table S1. Crystallographic data for Ni1-Ni4.

	Ni1	**Ni2**	**Ni3**	**Ni4**
Formula	$C_{78}H_{64}Br_4N_4Ni_2O_2$	$C_{82}H_{56}Br_4N_4Ni_2O_2$	$C_{40}H_{34}Br_2N_2NiO$	$C_{84}H_{60}Br_4N_4Ni_2O_2$
Formula weight	1526.39	1566.36	777.22	1594.42
Crystal dimensions (mm^3)	0.3×0.28×0.25	0.3×0.27×0.23	0.3×0.2×0.2	0.3×0.05×0.05
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	P -1	P 1 21/n 1	P 1 21/n 1	P 1 21/n 1
a (Å)	9.5838(6)	11.6818(17)	10.7994(7)	10.9201(2)
b (Å)	13.0175(9)	16.776(2)	20.1287(14)	22.8955(5)
c (Å)	13.8929(9)	22.885(3)	16.4169(11)	14.1583(3)
α (°)	96.0490(10)	90	90	90
β (°)	91.8800(10)	104.612(3)	105.2580(10)	109.8600(10)
γ (°)	107.2170(10)	90	90	90
Volume (Å^3)	1642.61(19)	4339.9(10)	3442.9(4)	3329.34(12)
Z	1	2	4	2
T (K)	173(2)	173(2)	173(2)	173(2)
D_{calcd} (g cm^{-3})	1.543	1.199	1.499	1.590
μ (mm^{-1})	3.057	2.316	2.919	3.941
F (000)	772	1576	1576	1608
Rflns. collected	47034	26588	56091	14606
Indep. rflns./R_{int}	7505/0.0593	7623/0.2275	7885/0.0527	4747/0.0667
Obsd. rflns. [$I_0 > 2\sigma(I_0)$]	6506	5737	6291	3982
Data/restraints/parameters	7505/0/408	7623 / 30 / 425	7885/0/417	4747 / 0 / 436
R_1 / wR_2 [$I_0 > 2\sigma(I_0)$]	0.0284/0.0711	0.0806/ 0.2202	0.0330/0.0703	0.0485/0.1231
R_1 / wR_2 (all data)	0.0358/ 0.0756	0.1013/ 0.2325	0.0504/ 0.0775	0.0596/ 0.1371
GOF (on F^2)	1.020	1.014	1.049	1.075
Largest diff. peak and hole (e Å^{-3})	0.556/–0.635	1.380/–2.160	0.554/–0.881	0.842/–1.583
CCDC No.	1947420	1947422	1947423	1947428

9. References

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