Supporting Information for:

Influence of Backbone Substituents on the Ethylene (Co)Polymerization Properties of α–diimine Pd(II) and Ni(II) Catalysts

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1. Tables

1.1 Effect of Time on Ethylene Polymerization.

Table S1. Effect of Time on Ethylene Polymerization at 40 °C[a].

Ent.	Cat.	Time (min)	Yield (g)	Act.[b]
1	**Ni-5**	5	0.42	5.0
2	**Ni-5**	10	0.86	5.2
3	**Ni-5**	30	2.3	4.6
4	**Ni-5**	60	3.45	3.5
5	**Ni-6**	5	1.2	14.4
6	**Ni-6**	10	2.34	14.0
7	**Ni-6**	30	3.52	7.0
8	**Ni-6**	60	4.2	4.2

[a]Conditions: 1 μmol pre-catalyst, 500 eq. cocatalyst, 1 mL CH_2Cl_2, 49 mL toluene, 9 atm.
[b]Activity (Act.) = 10^6 g/(mol Ni·h).

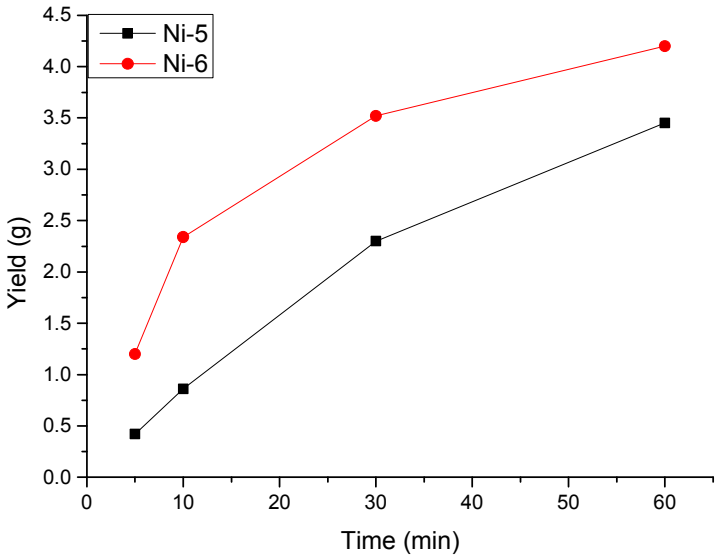

Figure S1. Yield versus time for catalyst **Ni-5, Ni-6.**

1.2 The Tables of Ethylene (Co)Polymerization.

Table S2. Ethylene polymerization with nickel complexes Ni-1~Ni-6.[a]

Ent.	Cat.	*T* (°C)	t (min)	Yield (g)	Average Yield(g)
1	**Ni-1**	20	10	2.6 3.0 2.35	2.65
2	**Ni-2**	20	10	2.22 2.46	2.34
3	**Ni-3**	20	10	2.92 2.48	2.70
4	**Ni-4**	20	10	2.2 2.5	2.35
5	**Ni-5**	20	10	1.09 1.11 1.04	1.08
6	**Ni-6**	20	10	2.32 3.44	2.88
7	**Ni-1**	20	30	3.64 2.78 3.84	3.42
8	**Ni-5**	20	30	1.91 1.8 1.75	1.82
9	**Ni-6**	20	30	3.87 3.3 3.69	3.62
10	**Ni-1**	40	10	2.24 2.38	2.31
11	**Ni-1**	60	10	2.05 2.14	2.10
12	**Ni-1**	80	10	1.32 1.94	1.63
13	**Ni-5**	40	10	0.87 0.78 0.93	0.86
14	**Ni-5**	60	10	0.7 0.86 0.66	0.74
15	**Ni-5**	80	10	0.88 0.6 0.68	0.72
16	**Ni-6**	40	10	2.14 2.54	2.34
17	**Ni-6**	60	10	1.8 2.2	2.0

18	**Ni-6**	80	10	1.45 1.01	1.23
19[b]	**Ni-5**	20	10	0.94 1.05	1.00
20[c]	**Ni-5**	20	10	0.8 0.83	0.82

[a]Conditions: 1 μmol Ni, MAO cocatalyst, Al/Ni=500, 1 mL CH_2Cl_2, 49 mL toluene, 9 atm. [b]Cocatalyst: Et_2AlCl. [c]Cocatalyst: $EtAlCl_2$.

Table S3. Ethylene polymerization with palladium complexes Pd-1~Pd-6.[a]

Ent.	Cat.	*T* (°C)	Yield (g)[b]	Average Yield(g)
1	**Pd-1**	20	0.26 0.22 0.18	0.22
2	**Pd-2**	20	0.21 0.24	0.23
3	**Pd-3**	20	0.32 0.37	0.35
4	**Pd-4**	20	0.31 0.24	0.28
5	**Pd-5**	20	0.43 0.57 0.53	0.51
6	**Pd-6**	20	0.23 0.34 0.24	0.27
7	**Pd-1**	40	1.0 0.92	0.96
8	**Pd-1**	60	0.29 0.13	0.21
9	**Pd-1**	80	0.07 0.15	0.11
10	**Pd-5**	40	1.65 1.68 1.86	1.73
11	**Pd-5**	60	0.71 0.73 0.63	0.69
12	**Pd-5**	80	0.12 0.2 0.13	0.15
13	**Pd-6**	40	1.25 1.37	1.31
14	**Pd-6**	60	0.29 0.4	0.35

15	**Pd-6**	80	0.14 0.06	0.1

[a]Conditions: 10 μmol pre-catalyst, 1.2 eq. NaBAF, 2 mL of CH_2Cl_2, 48 mL toluene, 9 atm,1 h.

Table S4. Copolymerization of Ethylene and MA with complexes Pd-1~Pd-6.[a]

Ent.	Cat.	[MA] (M)	Yield (g)	Average Yield(g)
1	**Pd-1**	-	1.65 1.74	1.7
2	**Pd-1**	1	0.33 0.21	0.27
3	**Pd-1**	2	0.23 0.15	0.19
4	**Pd-2**	-	1.82 2.1	1.96
5	**Pd-2**	1	0.5 0.37	0.44
6	**Pd-2**	2	0.31 0.21	0.26
7	**Pd-3**	-	2.04 2.27	2.16
8	**Pd-3**	1	0.34 0.45	0.40
9	**Pd-3**	2	0.27 0.22	0.25
10	**Pd-4**	-	2.2 2.08	2.14
11	**Pd-4**	1	1.39 1.6	1.5
12	**Pd-4**	2	0.68 0.8	0.74
13	**Pd-5**	-	2.01 2.15	2.08
14	**Pd-5**	1	0.65 0.63 0.58	0.62
15	**Pd-5**	2	0.4 0.51 0.45	0.45
16	**Pd-6**	-	1.79 1.61	1.7
17	**Pd-6**	1	0.32 0.27	0.3
18	**Pd-6**	2	0.21 0.19	0.2

[a]Conditions: 0.030 mmol pre-catalyst, 1.2 eq. NaBAF, total volume of DCM and MA: 25 mL, 30 ^{o}C, 1 atm, 15 h.

2. Spectra Data

2.1 ^{1}H , ^{13}C NMR of ligands L1, L2, L3, L4 (Figure S2-S8).

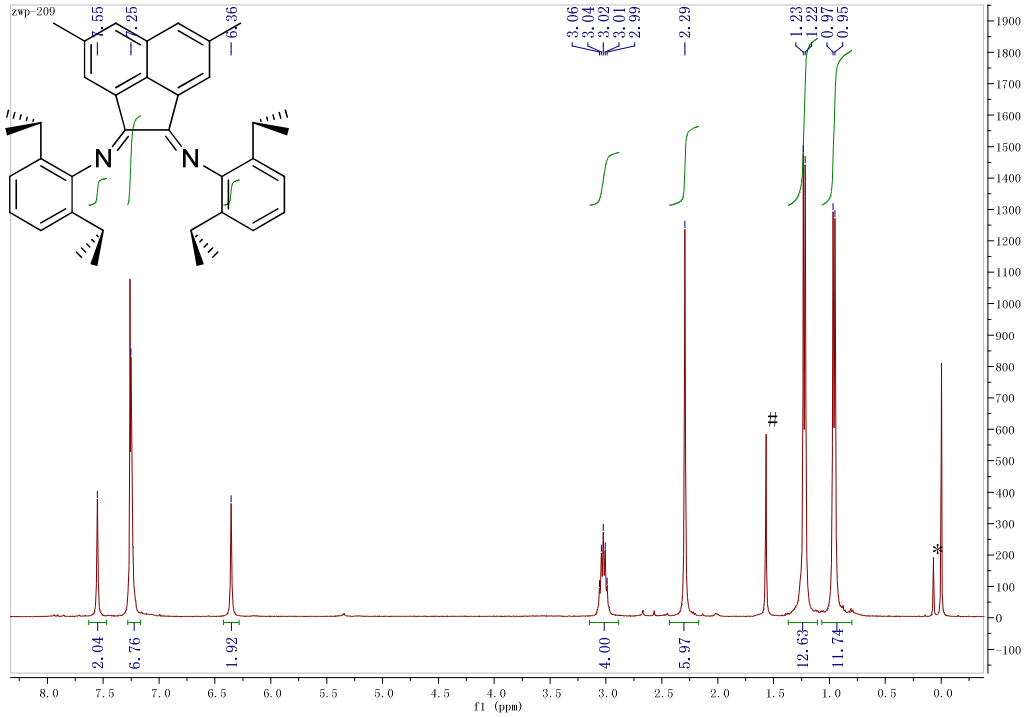

Figure S2. ^{1}H NMR spectrum of **L1** in $CDCl_3$. $*$ silicone grease, $_{\#}H_2O$.

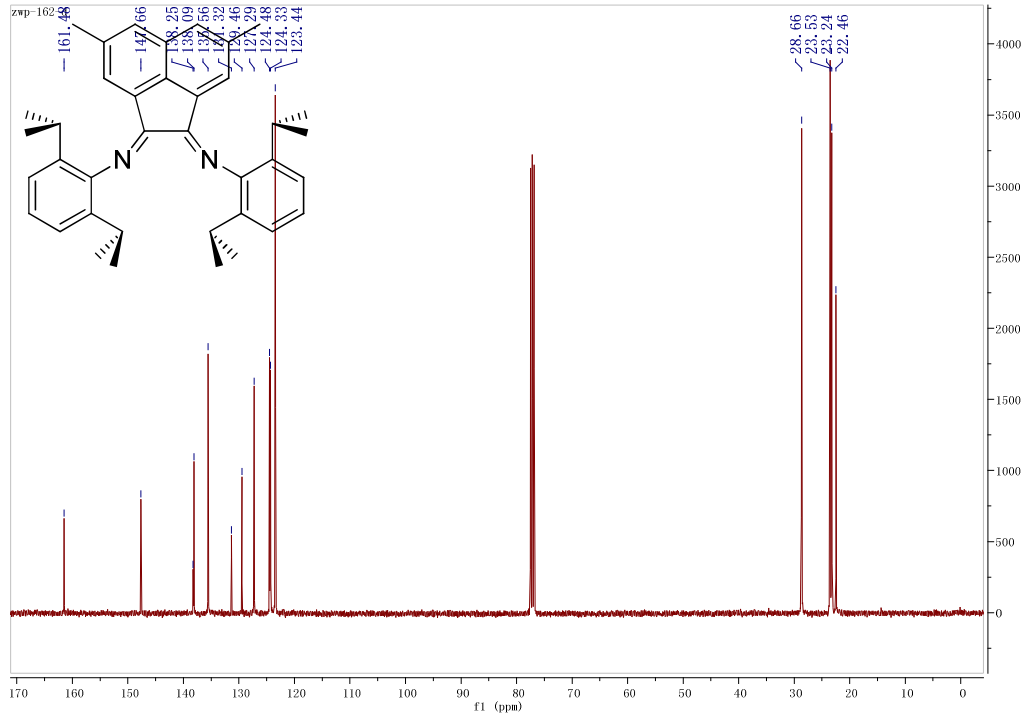

Figure S3. ^{13}C NMR spectrum of **L1** in $CDCl_3$.

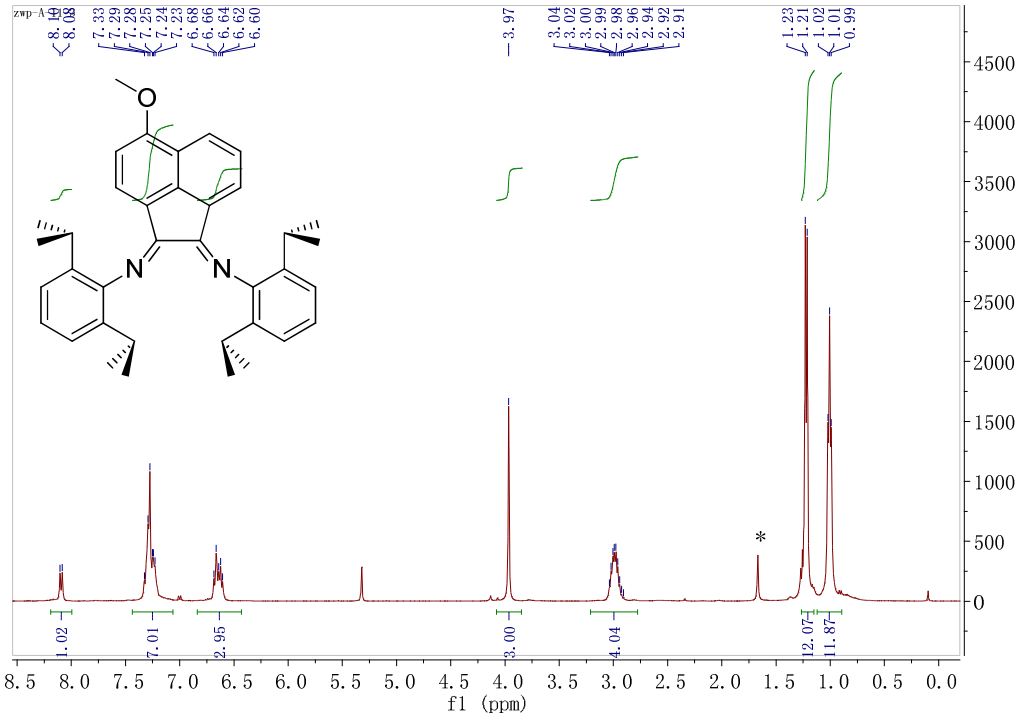

Figure S4. ^{1}H NMR spectrum of **L2** in CD_2Cl_2. * H_2O.

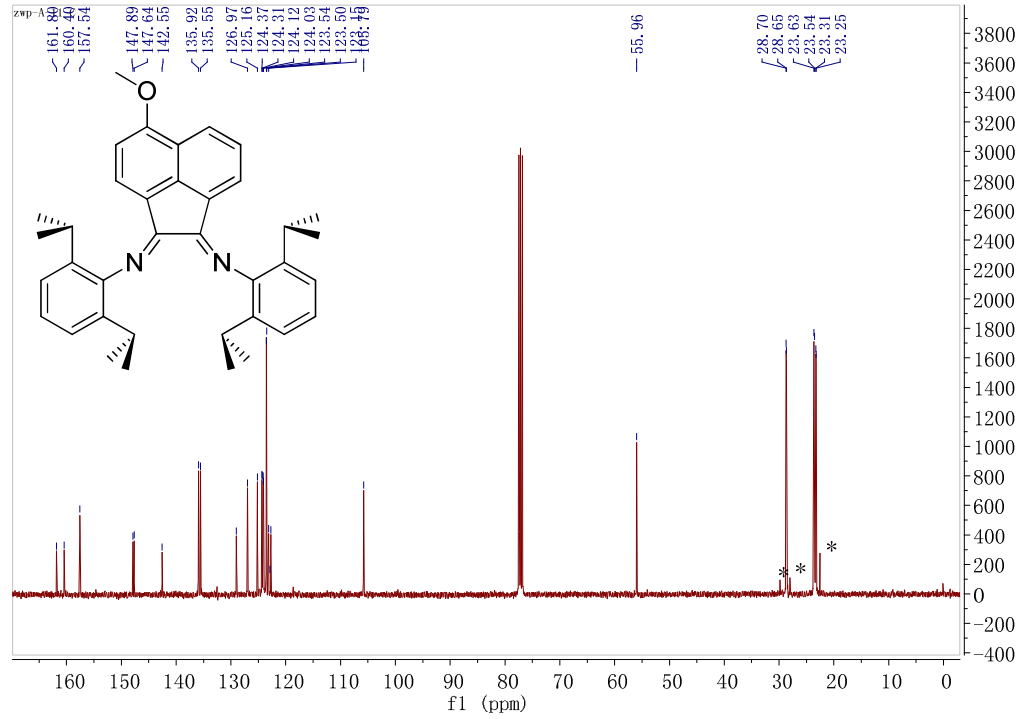

Figure S5. ^{13}C NMR spectrum of **L2** in $CDCl_3$. * n-hexane.

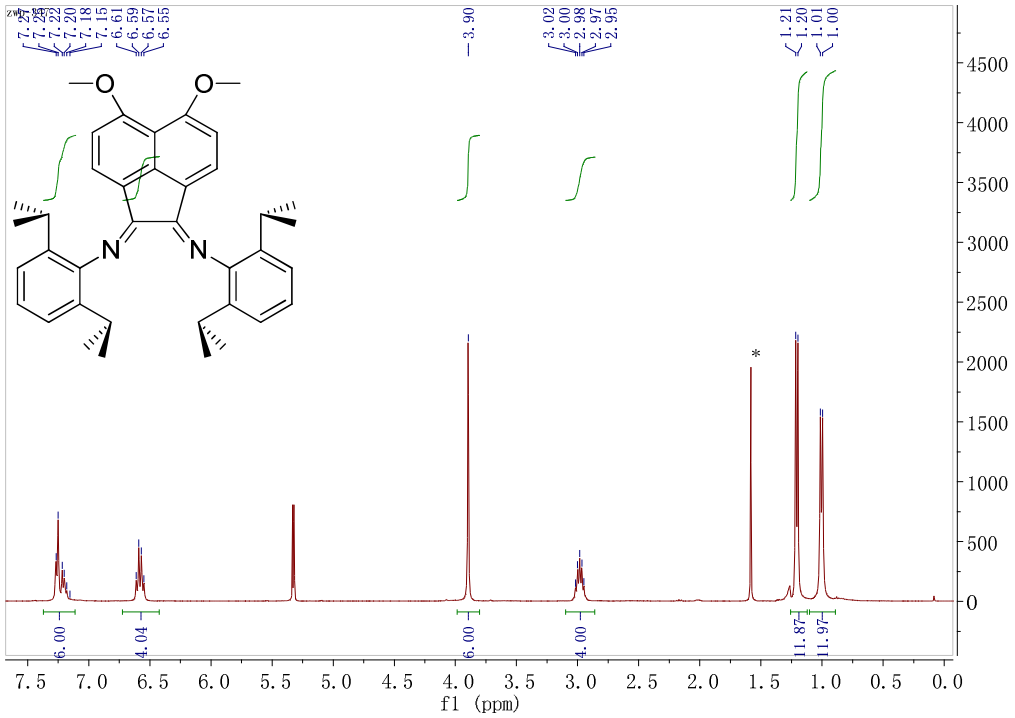

Figure S6. ^{1}H NMR spectrum of **L3** in CD_2Cl_2. * H_2O.

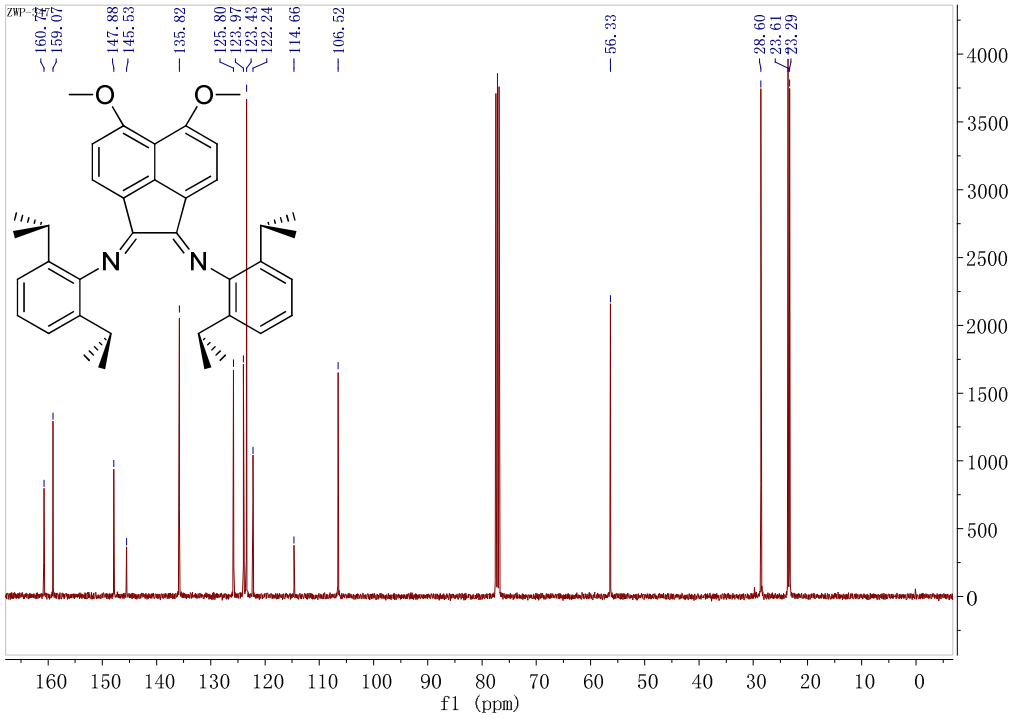

Figure S7. ^{13}C NMR spectrum of **L3** in $CDCl_3$.

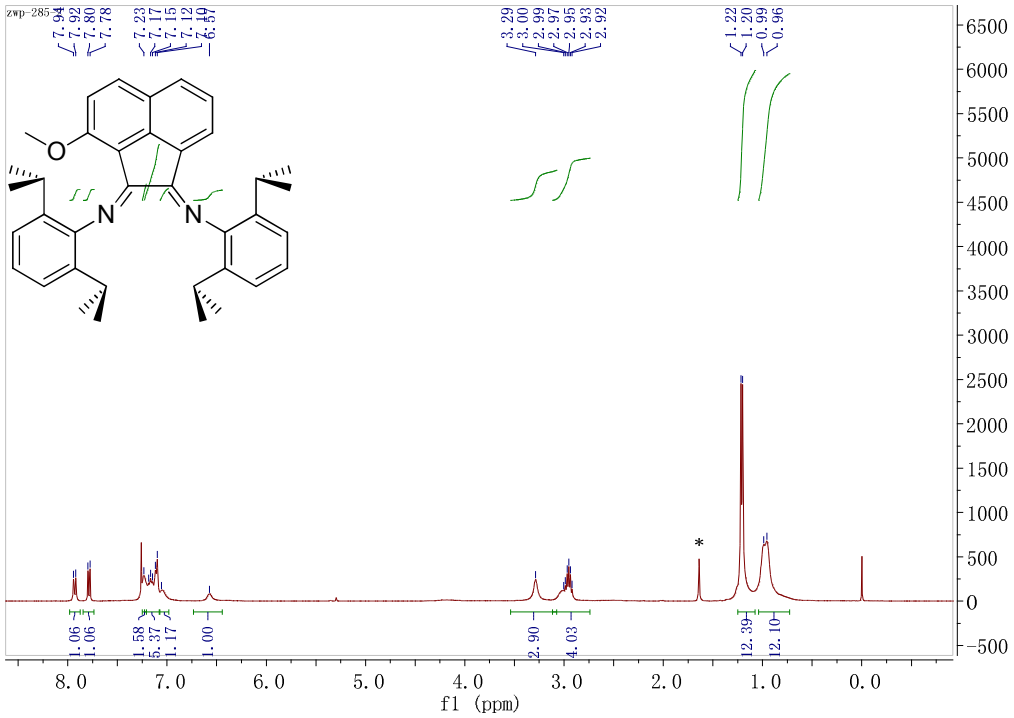

Figure S8. ^{1}H NMR spectrum of **L4** in $CDCl_3$. $*H_2O$.

2.2 ^{1}H, ^{13}C NMR of Complexes Pd-1~Pd-5 (Figure S9- S18).

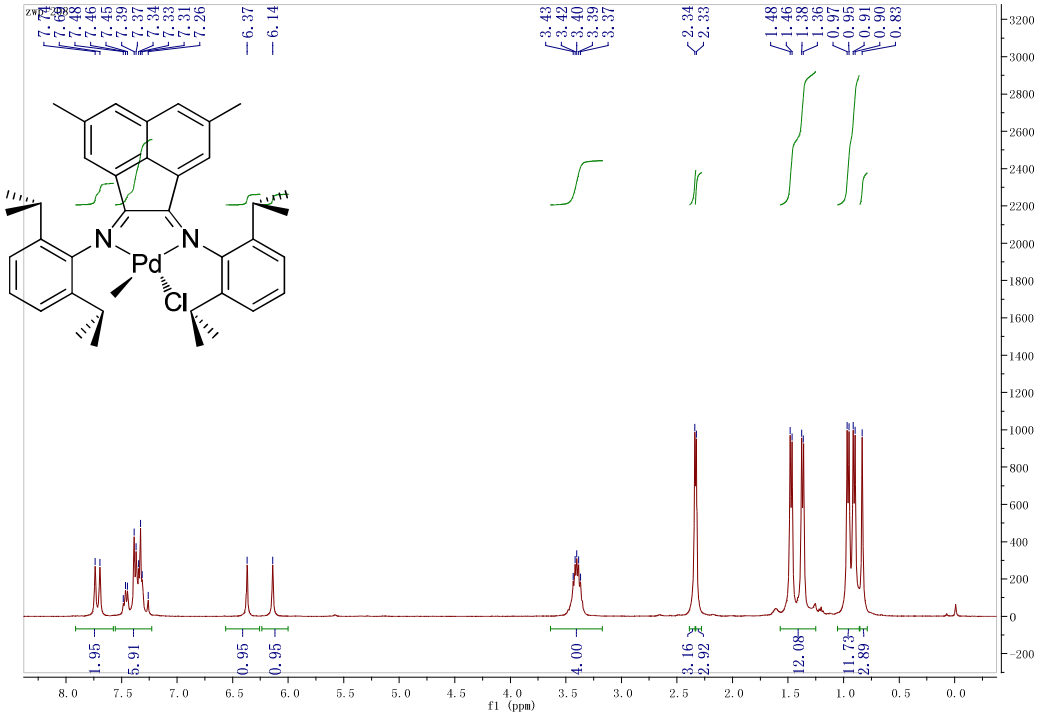

Figure S9. ^{1}H NMR spectrum of (**$^{4,7\text{-diMe}}$N^N)PdMeCl** (**Pd-1**) in $CDCl_3$.

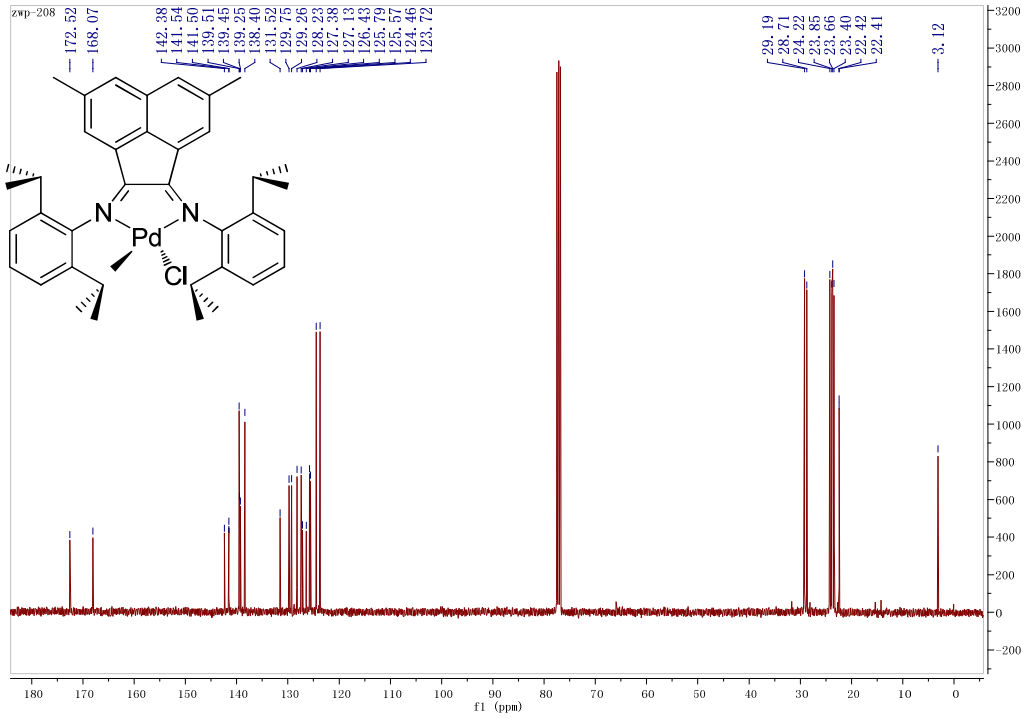

Figure S10. ^{1}C NMR spectrum of (**^{Me}N^N)PdMeCl** (**Pd-1**) in $CDCl_3$.

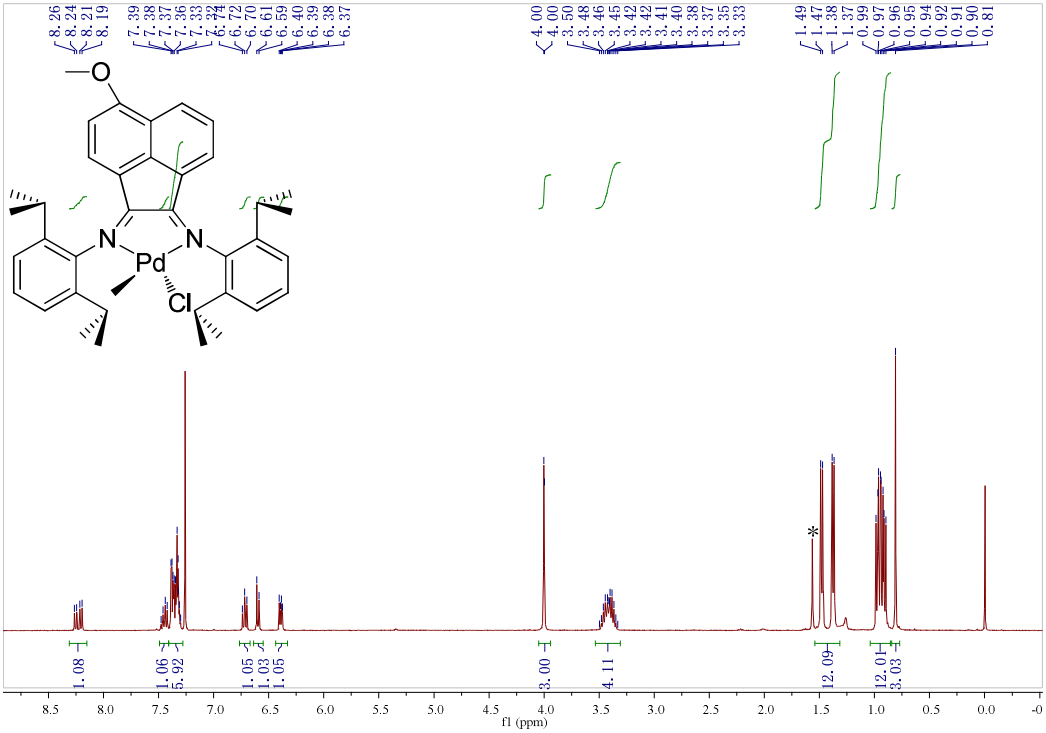

Figure S11. ^{1}H NMR spectrum of (**$^{5\text{-}OMe}$N^N)PdMeCl** (**Pd-2**) in $CDCl_3$. $*H_2O$.

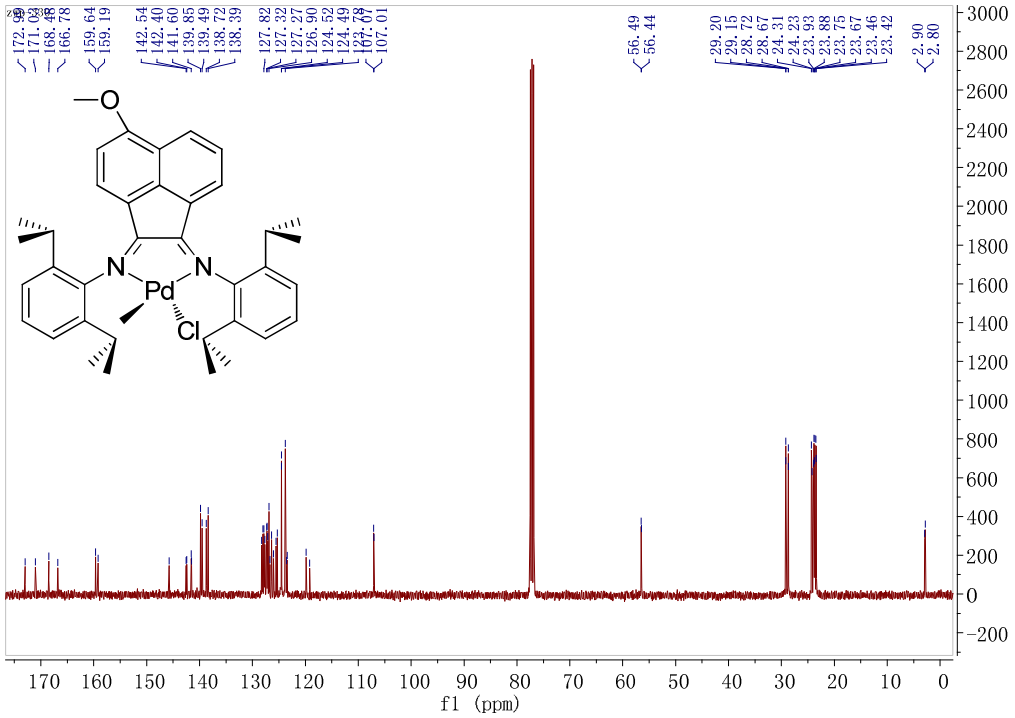

Figure S12. ^{13}C NMR spectrum of (**$^{5\text{-OMe}}$N^N)PdMeCl** (**Pd-2**) in $CDCl_3$.

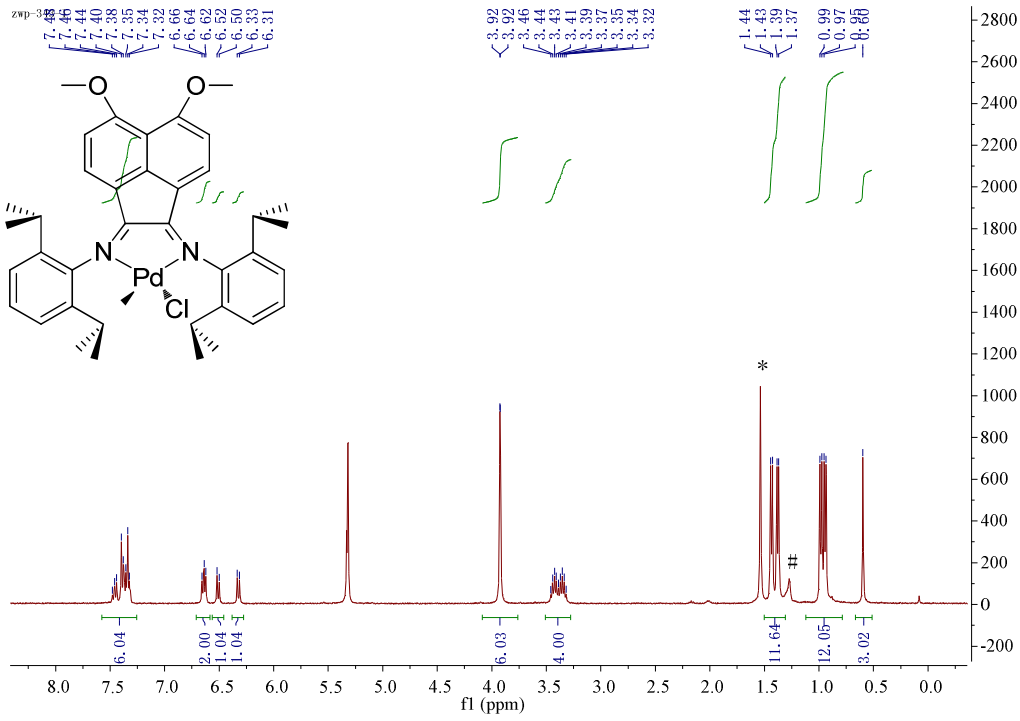

Figure S13. ^{1}H NMR spectrum of (**$^{5,\ 6\text{-diOMe}}$N^N)PdMeCl** (**Pd-3**) in CD_2Cl_2. *H_2O, #n-hexane.

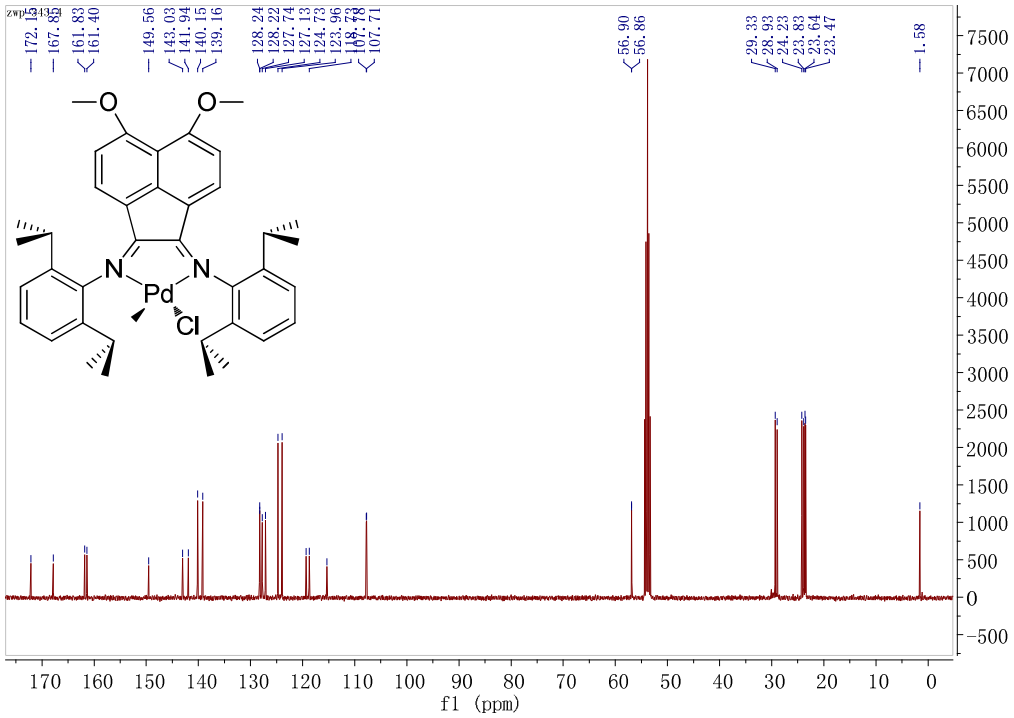

Figure S14. ^{13}C NMR spectrum of (**$^{5,6\text{-diOMe}}$N^N)PdMeCl (Pd-3)** in CD_2Cl_2.

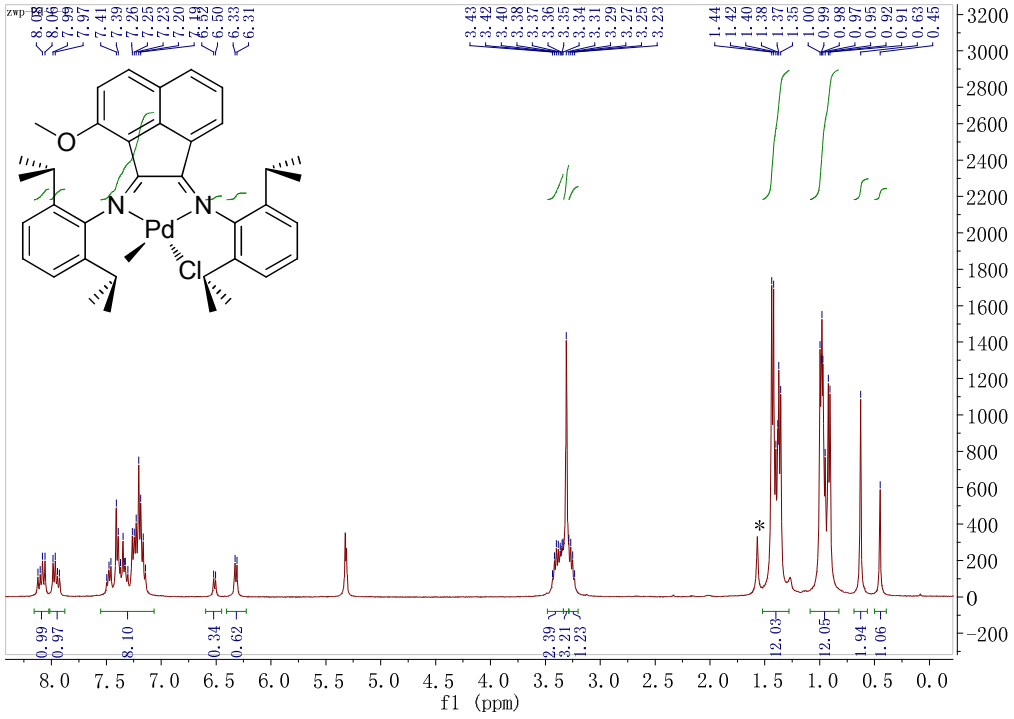

Figure S15. ^{1}H NMR spectrum of (**$^{3\text{-OMe}}$N^N)PdMeCl** (**Pd-4**) in CD_2Cl_2.$*H_2O$.

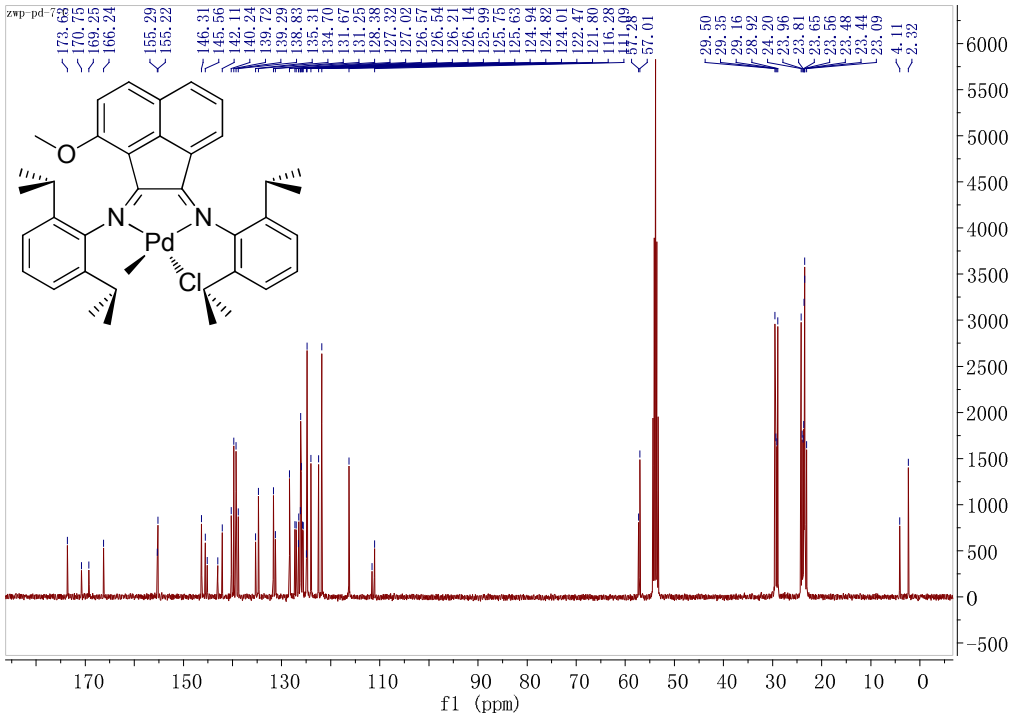

Figure S16. ^{13}C NMR spectrum of (**$^{3\text{-OMe}}$N^N)PdMeCl** (**Pd-4**) in CD_2Cl_2.

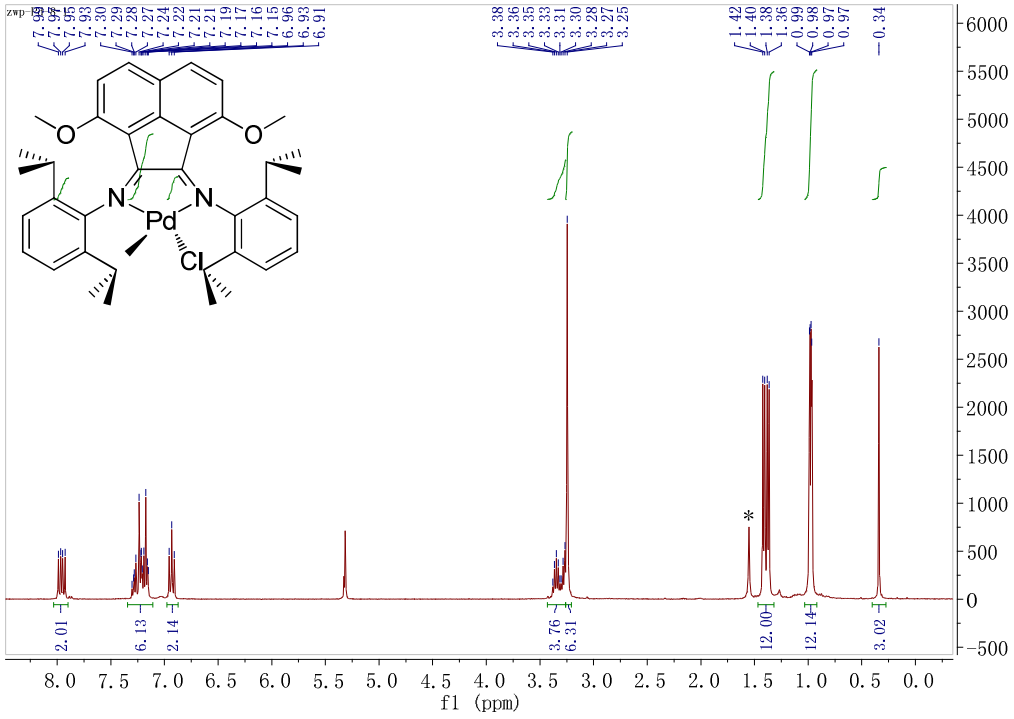

Figure S17. ^{1}H NMR spectrum of (**$^{3,8\text{-diOMe}}$N^N)PdMeCl** (**Pd-5**) in CD_2Cl_2. $*H_2O$.

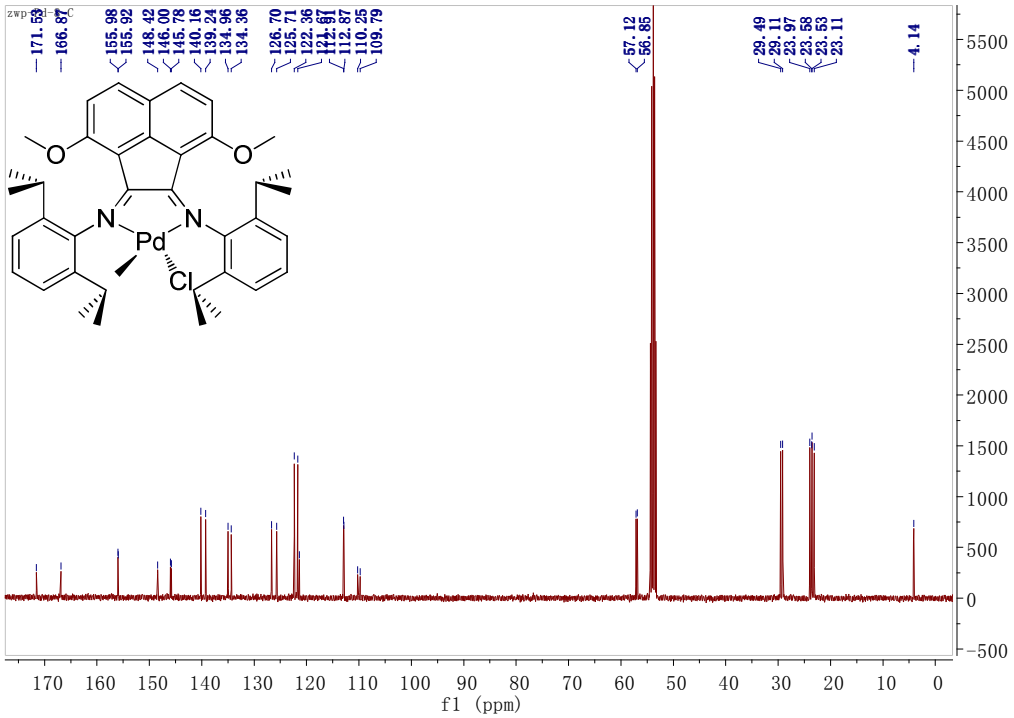

Figure S18. ^{1}H NMR spectrum of (**$^{3,8\text{-diOMe}}$ N^N)PdMeCl** (**Pd-5**) in CD_2Cl_2.

2.3 HRMS (m/z) of L1~L5 (Figure S19~S23).

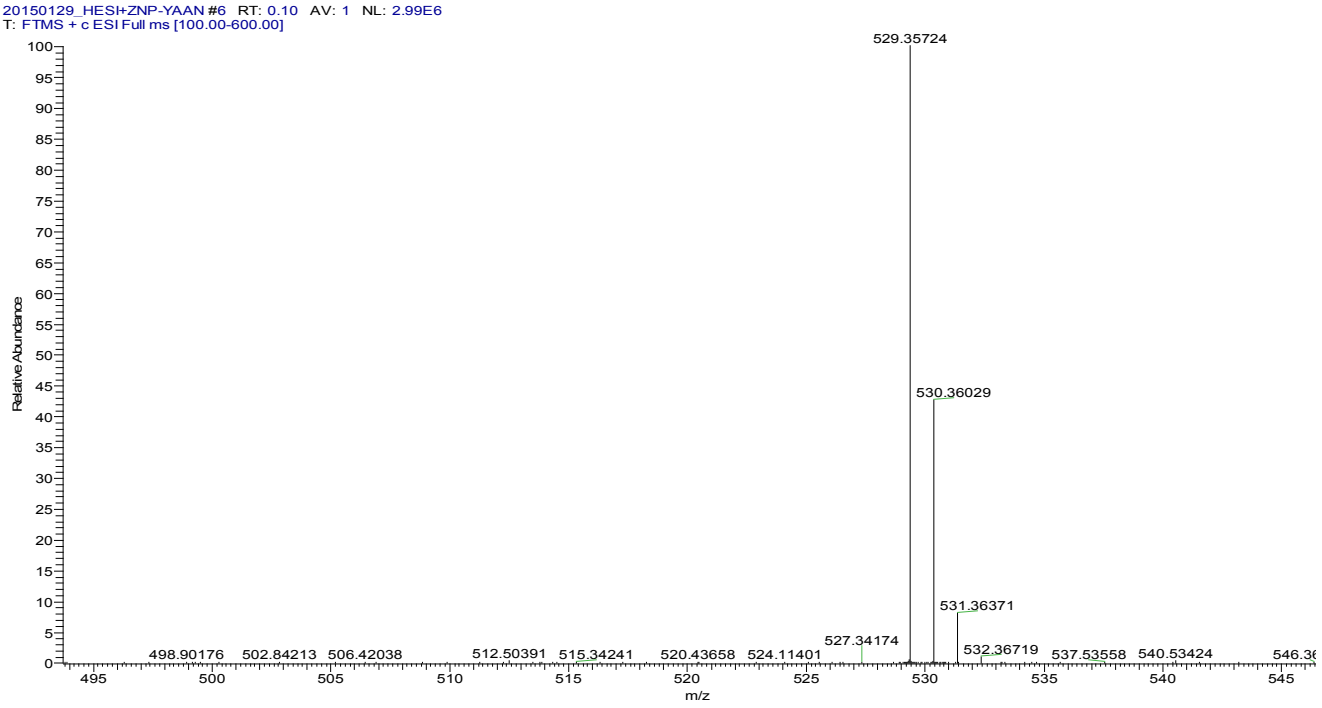

Figure S19. HRMS (m/z) of **L1.**

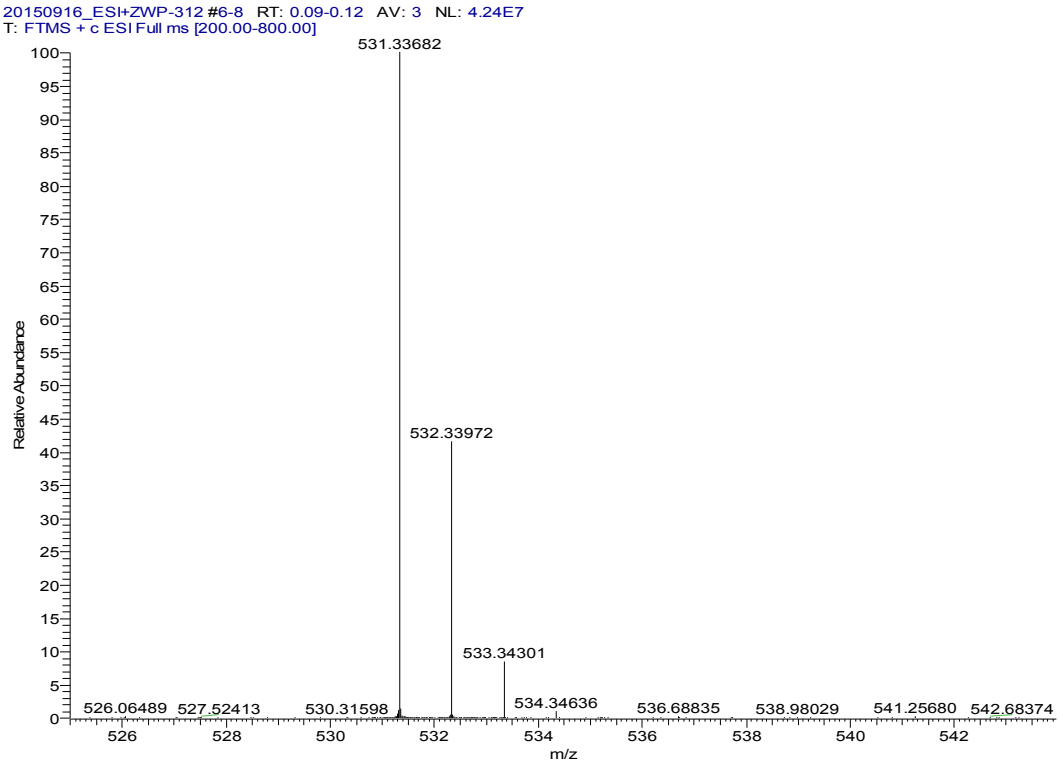

Figure S20. HRMS (m/z) of **L2.**

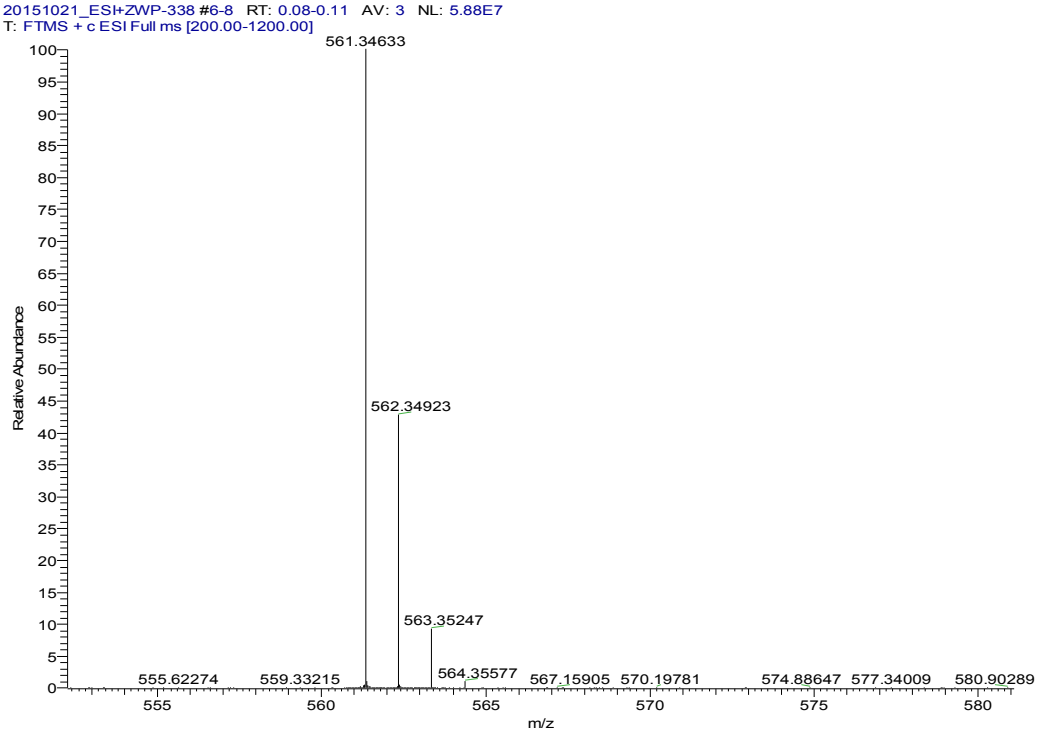

Figure S21. HRMS (m/z) of **L3.**

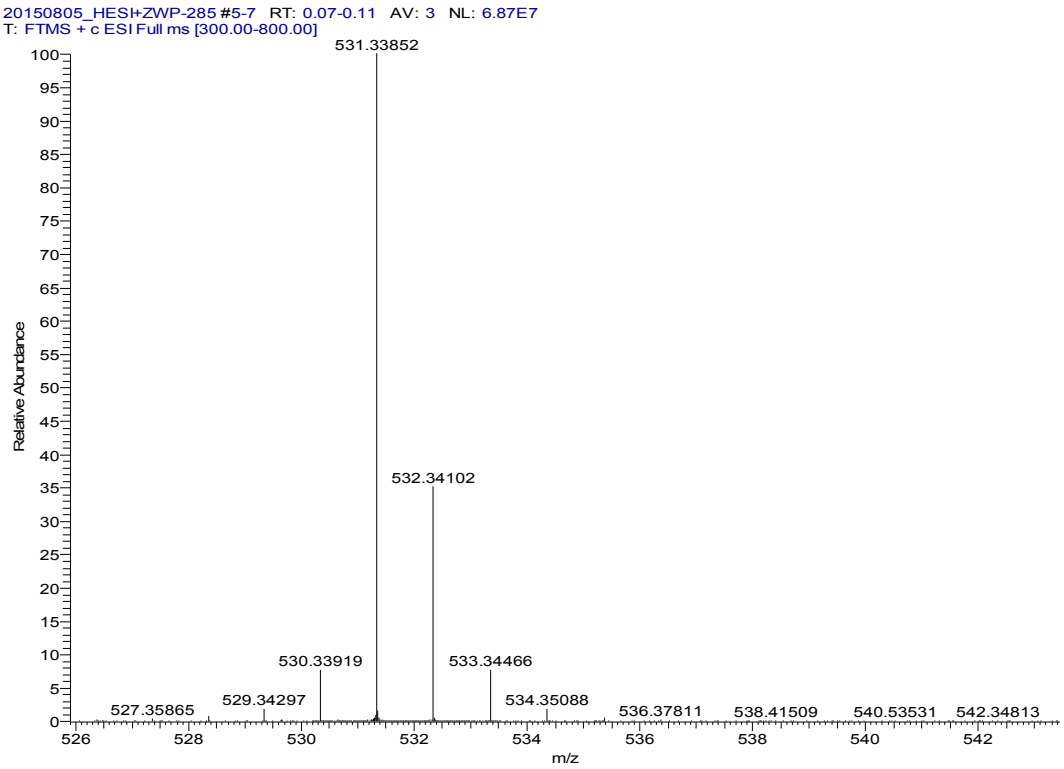

Figure S22. HRMS (m/z) of **L4.**

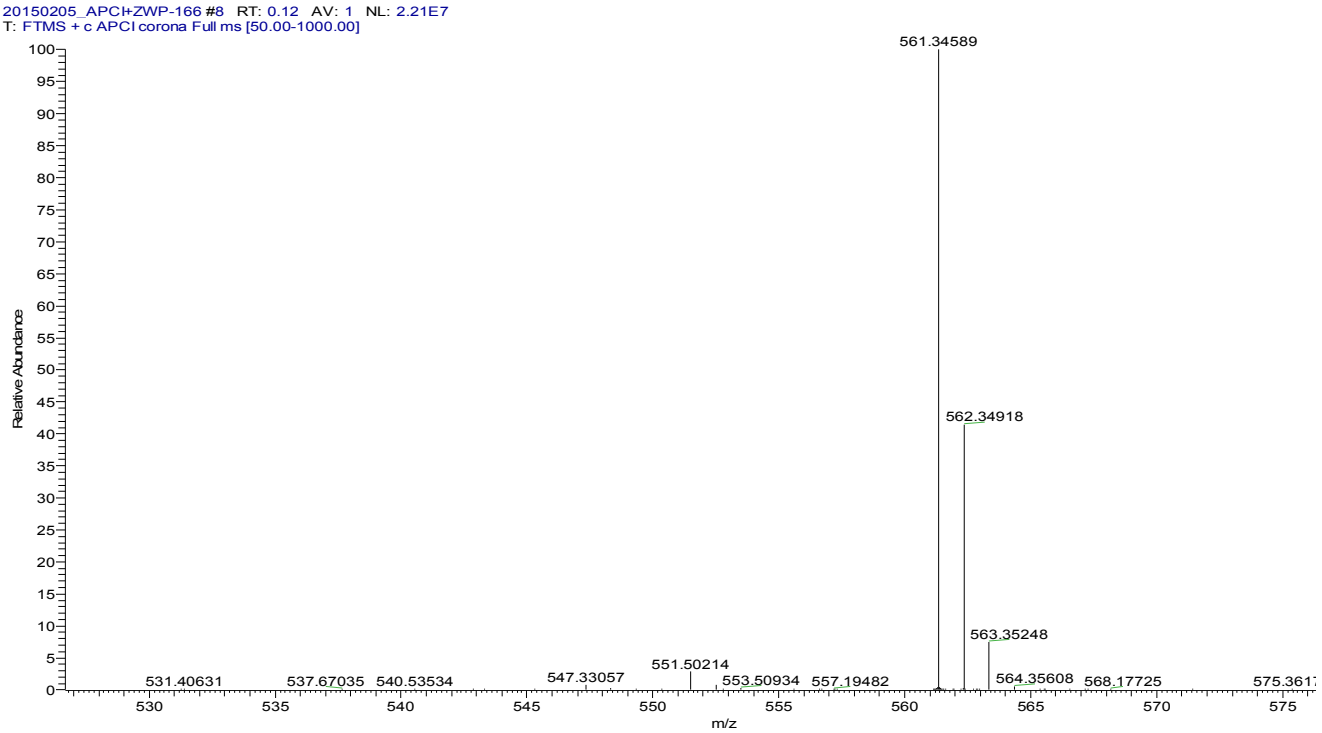

Figure S23. HRMS (m/z) of **L5.**

2.4 MALDI-TOF-MS (m/z) of Complexes 1~5 (Figure S24~S28).

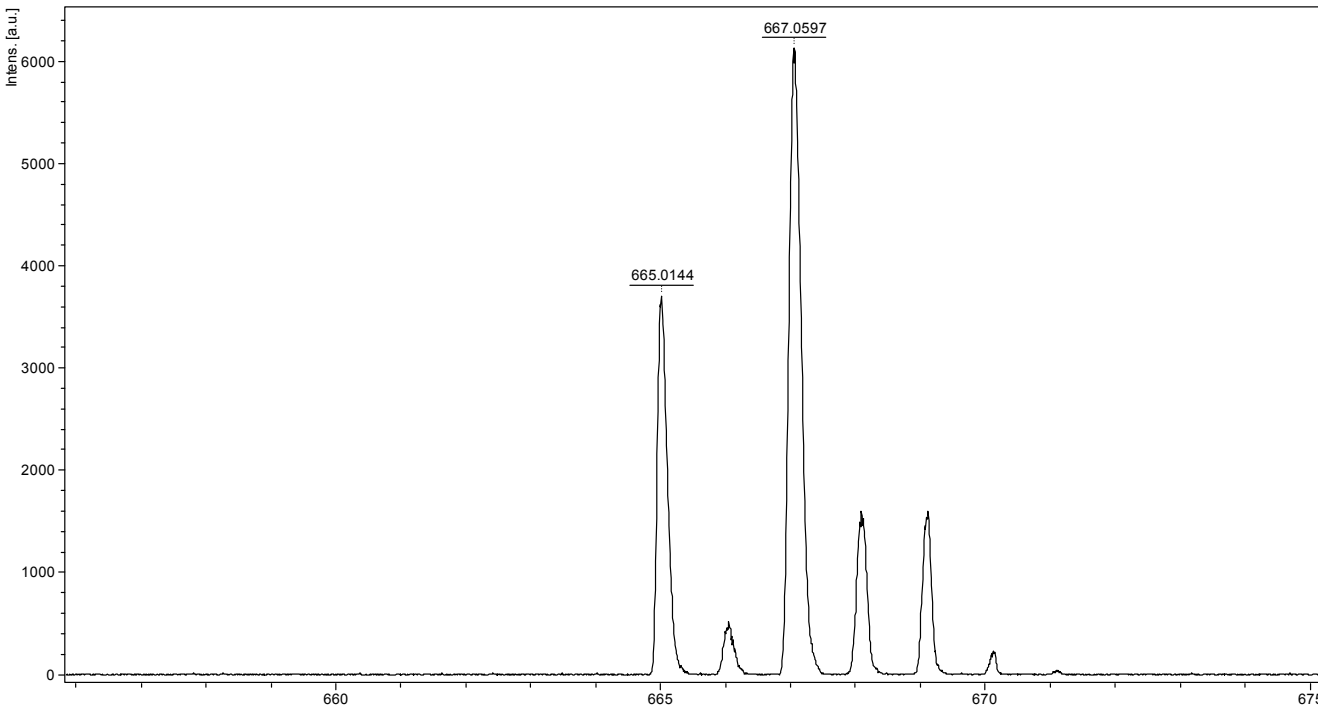

Figure S24. MALDI-TOF-MS (m/z) of (**$^{4,\ 7\text{-diMe}}$N^N)NiBr$_2$(Ni-1).**

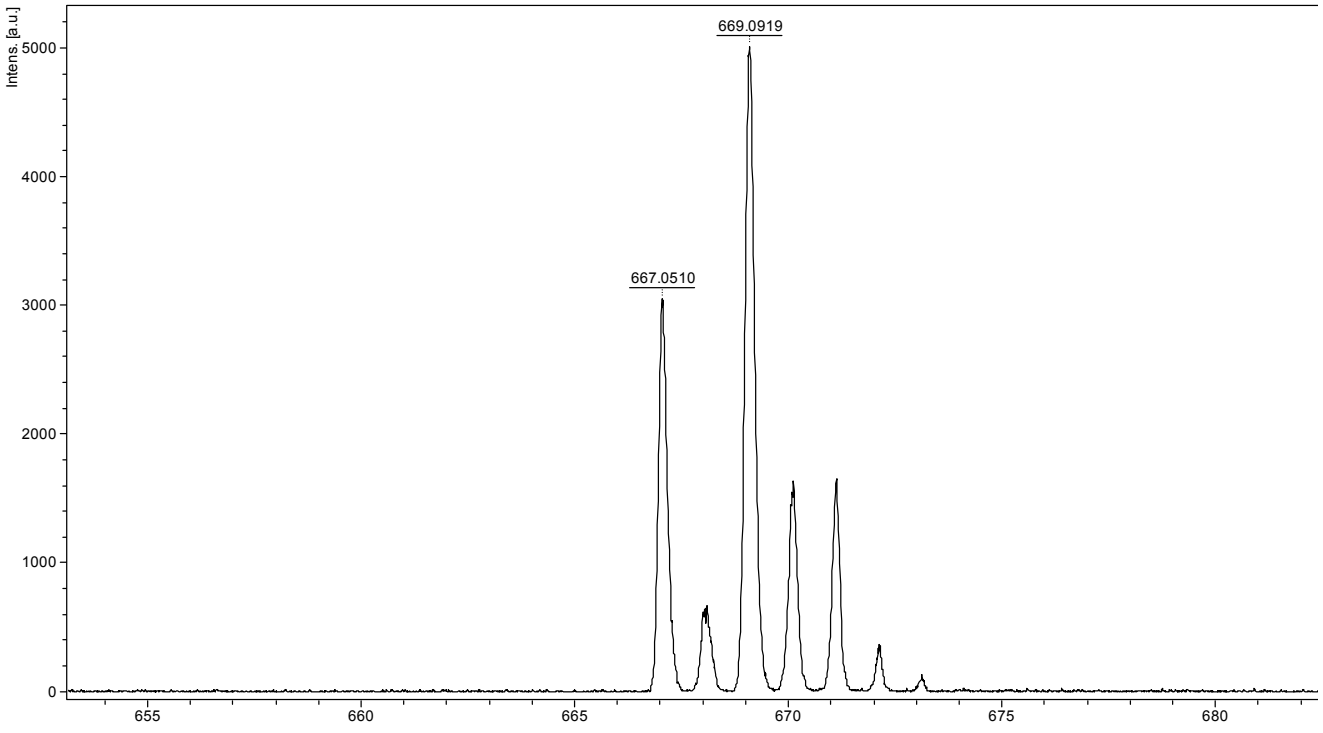

Figure S25. MALDI-TOF-MS (m/z) of (**$^{5\text{-OMe}}$N^N)NiBr$_2$ (Ni-2).**

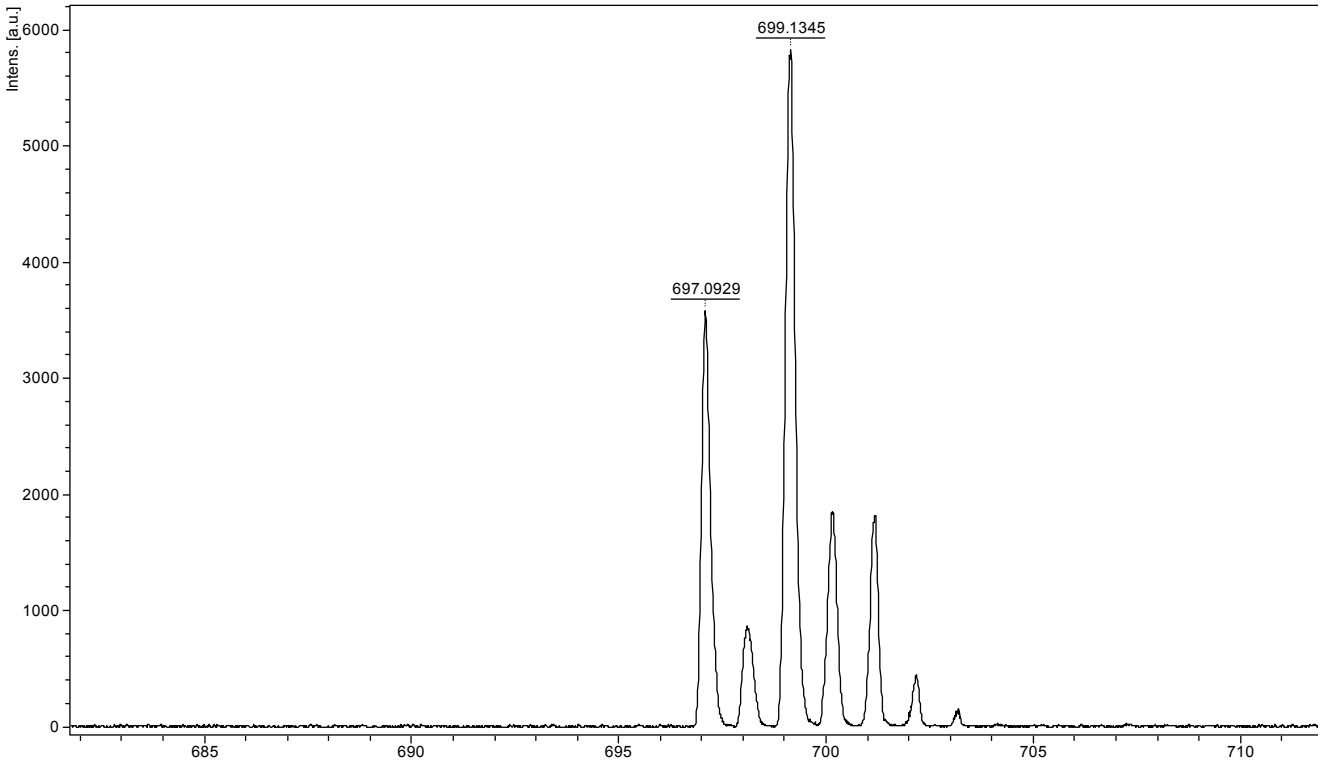

Figure S26. MALDI-TOF-MS (m/z) of (**$^{5,\ 6\text{-diOMe}}$N^N)NiBr$_2$ (Ni-3).**

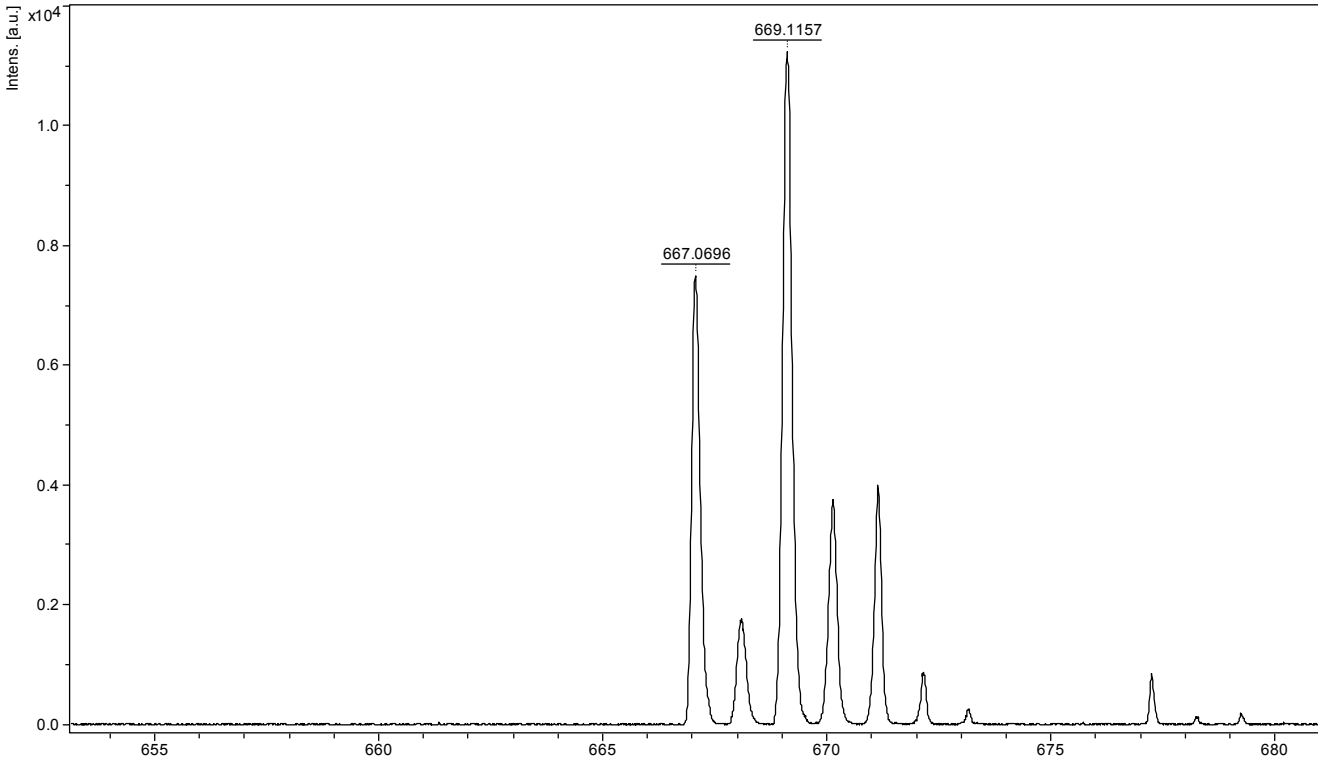

Figure S27. MALDI-TOF-MS (m/z) of (**$^{3\text{-OMe}}$N^N)NiBr$_2$ (Ni-4).**

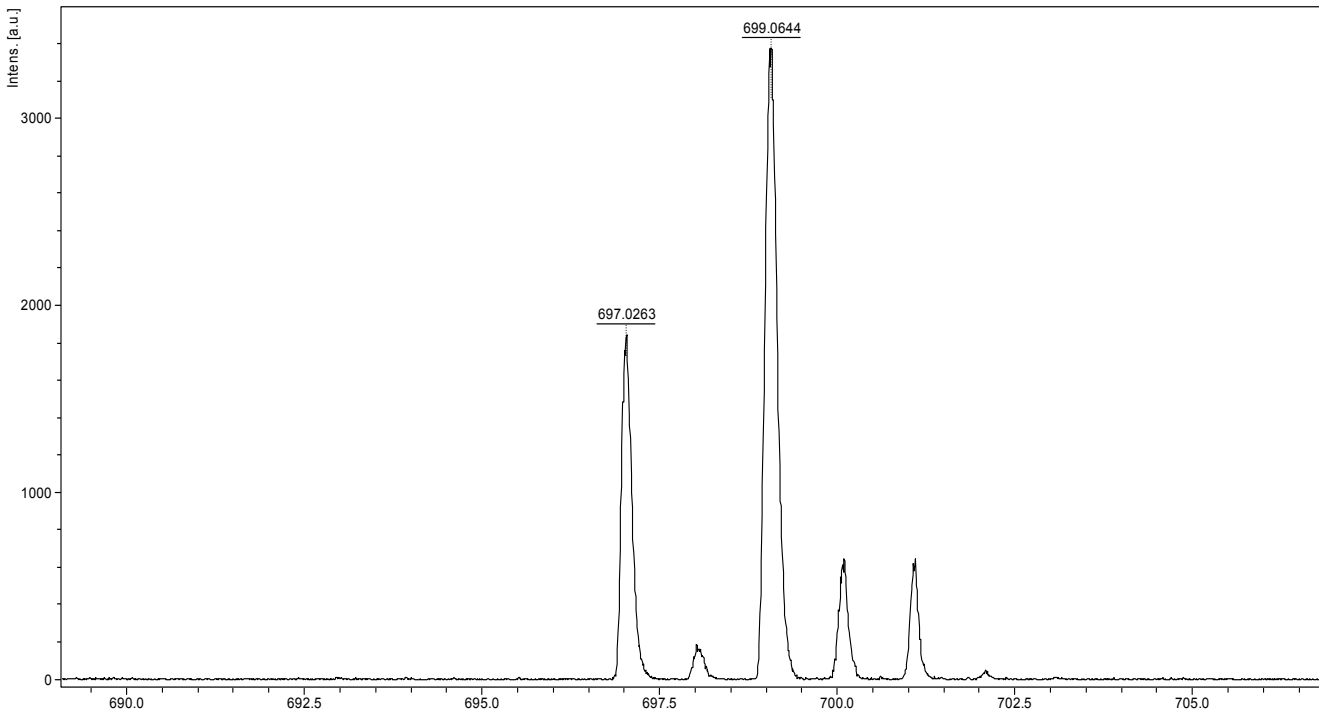

Figure S28. MALDI-TOF-MS (m/z) of ($^{3, 8\text{-diOMe}}$N^N)NiBr$_2$ **(Ni-5).**

2.5 ^{1}H and ^{13}C NMR of polymer and copolymer (Figure S29- S36).

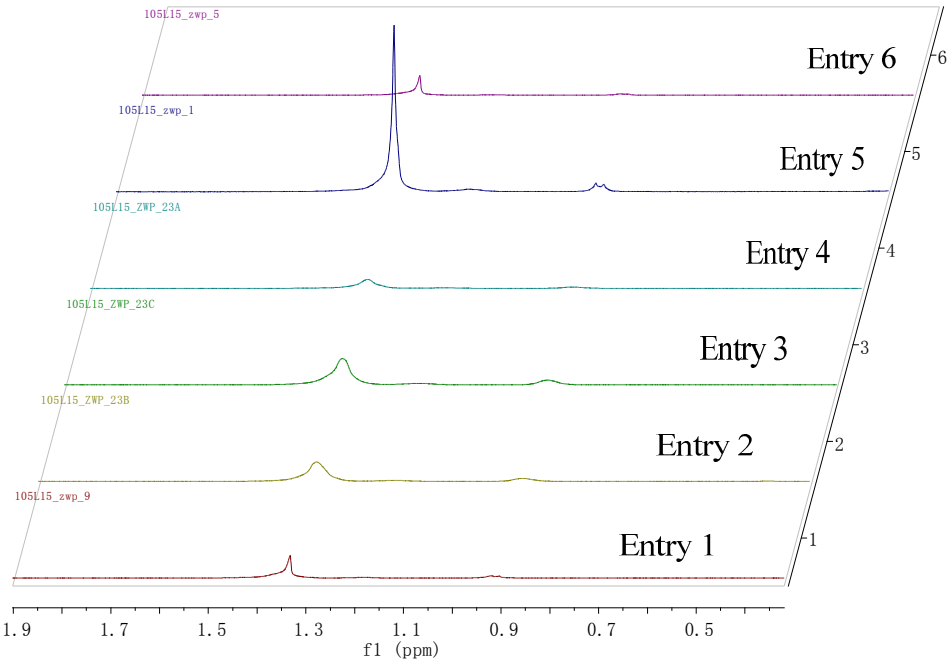

Figure S29. ^{1}H NMR spectrum of the polymer from table 1, entry 1, 2, 3, 4, 5, 6. (d^{8}-toluene, 80^{o}C).

Table S5. Polymer Branching Distributions and Number of Branches per 1000 Carbons.*

				branched chain (%)					
Ent.	Cat.	*T* (°C)	t (min)	Me	Et	Pr	Lg	Total(^{13}C)[a]	Total(^{1}H)[b]
1	**Ni-1**	20	10	70.9	9.3	9.1	10.7	83	81
5	**Ni-5**	20	10	80.1	4.1	5.4	10.4	54	52
6	**Ni-6**	20	10	78.7	5.1	6.2	10.0	77	79

*polymer from table 1, entry 1, 5 and 6. $^{13}C\{^{1}H\}$ NMR: 100 MHz, pulse width 60°, acquisition time 4.0 s; pulse delay 4.0 s.

[a] Measured by ^{13}C NMR in $CDCl_2CDCl_2$ at 120 °C. BD = 1000 × $(I_{CH3}+I_{Et}+I_{Pr}+I_{Lg})/(I_{total})$.

[b] Measured by ^{1}HNMR in d^{8}-toluene at 80°C.

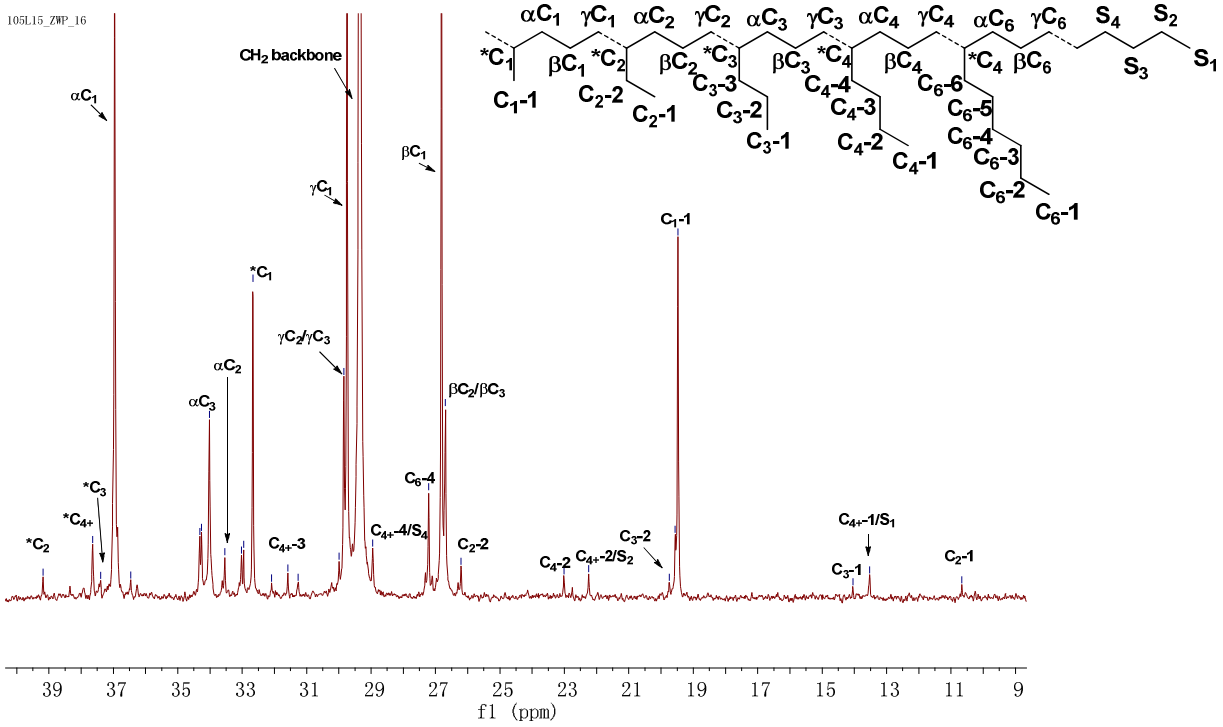

Figure S30. ^{13}C NMR spectrum of the polymer from table 1, entry 5. ($C_2D_2Cl_4$, 120°C).

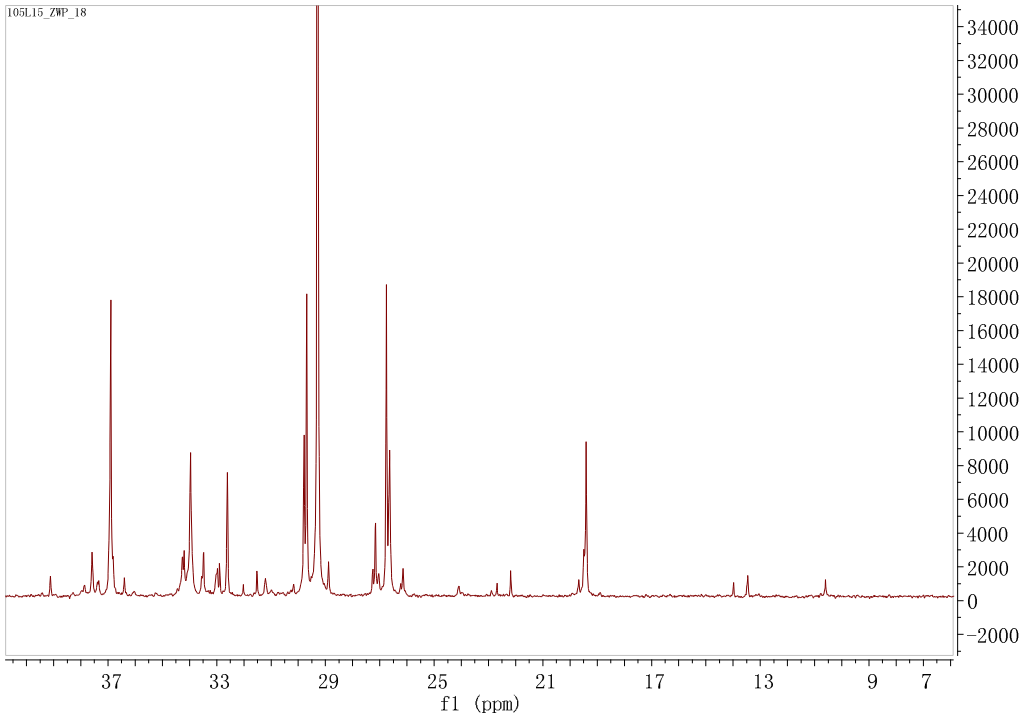

Figure S31. ^{13}C NMR spectrum of the polymer from table 1, entry 1. ($C_2D_2Cl_4$, 120°C).

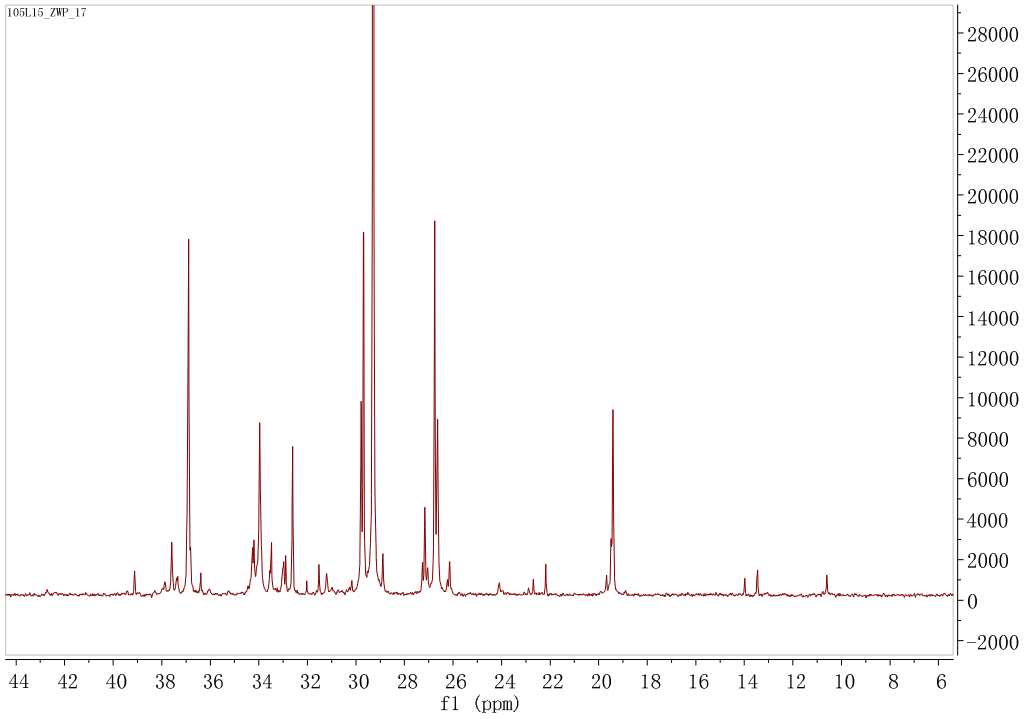

Figure S32. ^{13}C NMR spectrum of the polymer from table 1, entry 6. ($C_2D_2Cl_4$, 120°C).

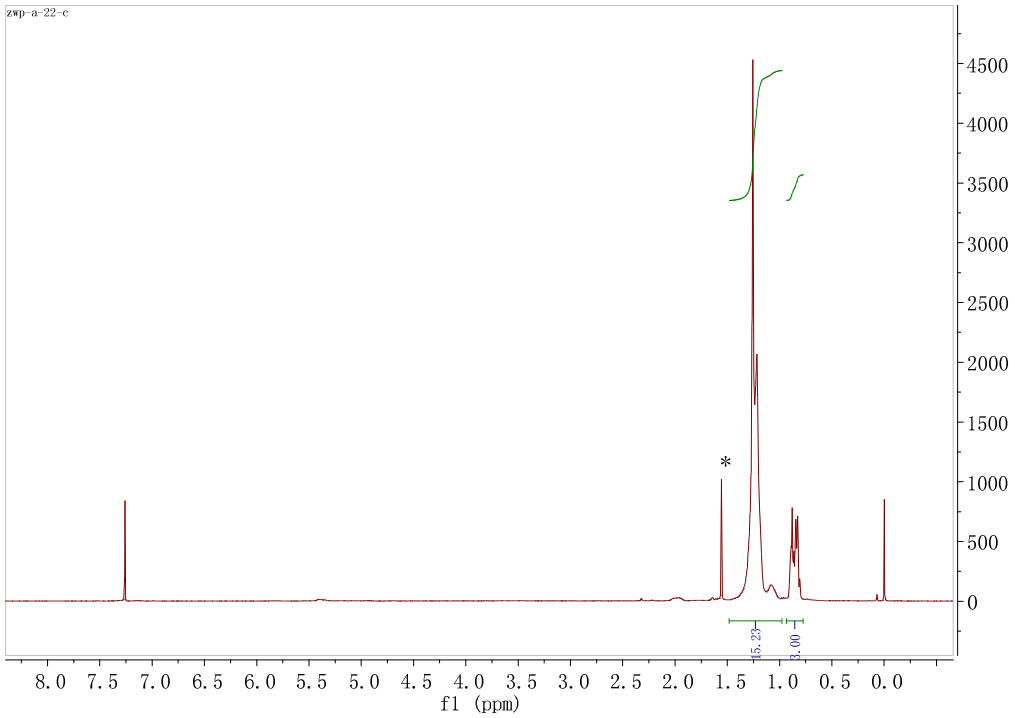

Figure S33. ^{1}H NMR spectrum of the polymer from table 2, entry 5 in $CDCl_3$.* H_2O.

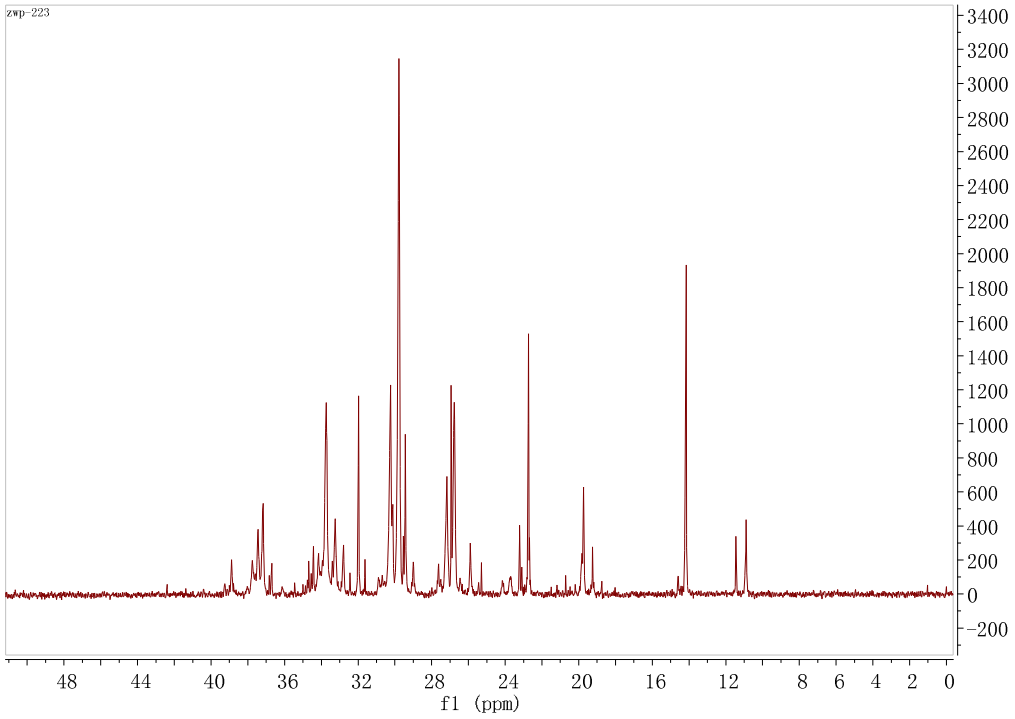

Figure S34. ^{13}C NMR spectrum of the polymer from table 2, entry 5 in $CDCl_3$.

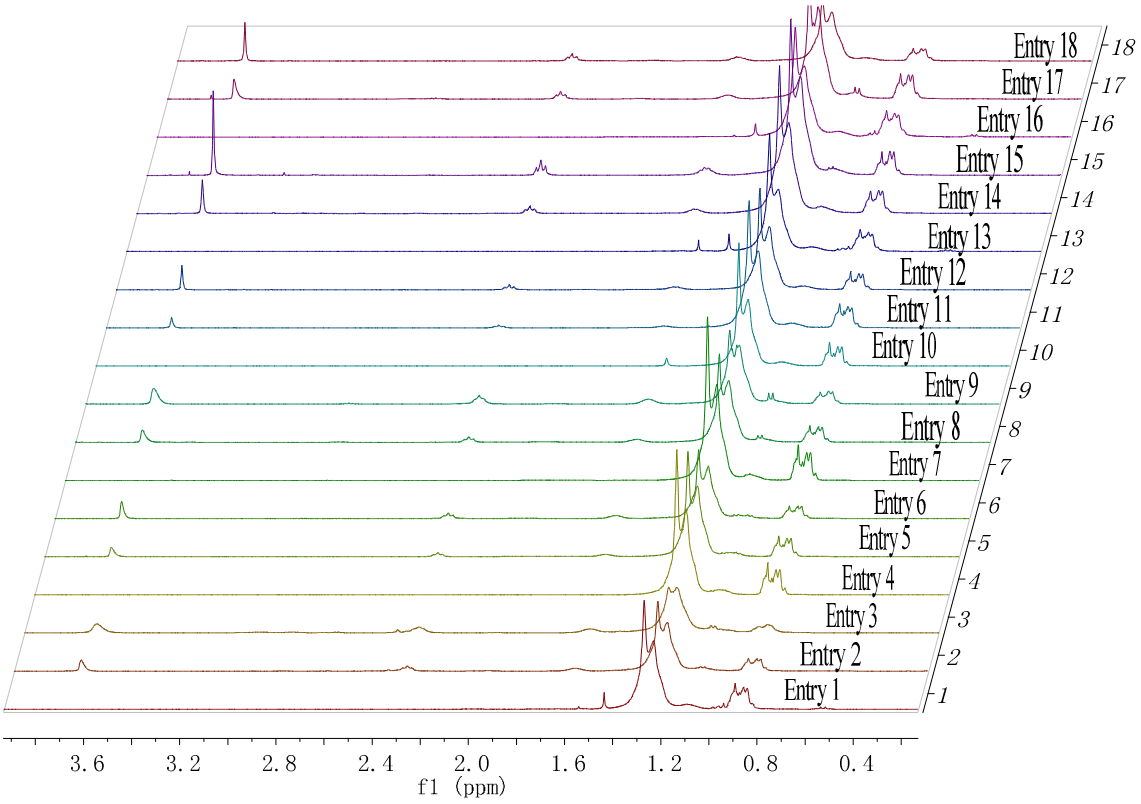

Figure S35. ^{1}H NMR spectrum of the polymer from table 3.

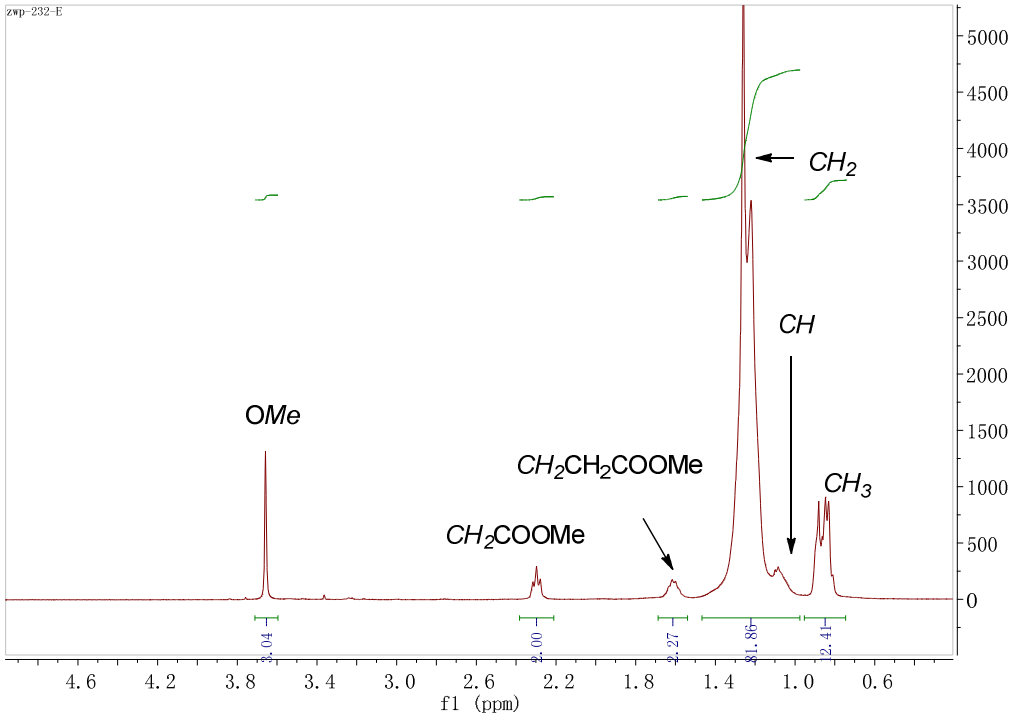

Figure S36. ^{1}H NMR spectrum of the polymer from table 3, entry 14 in $CDCl_3$.

2.6 DSC of polymer (Figure S37-S41).

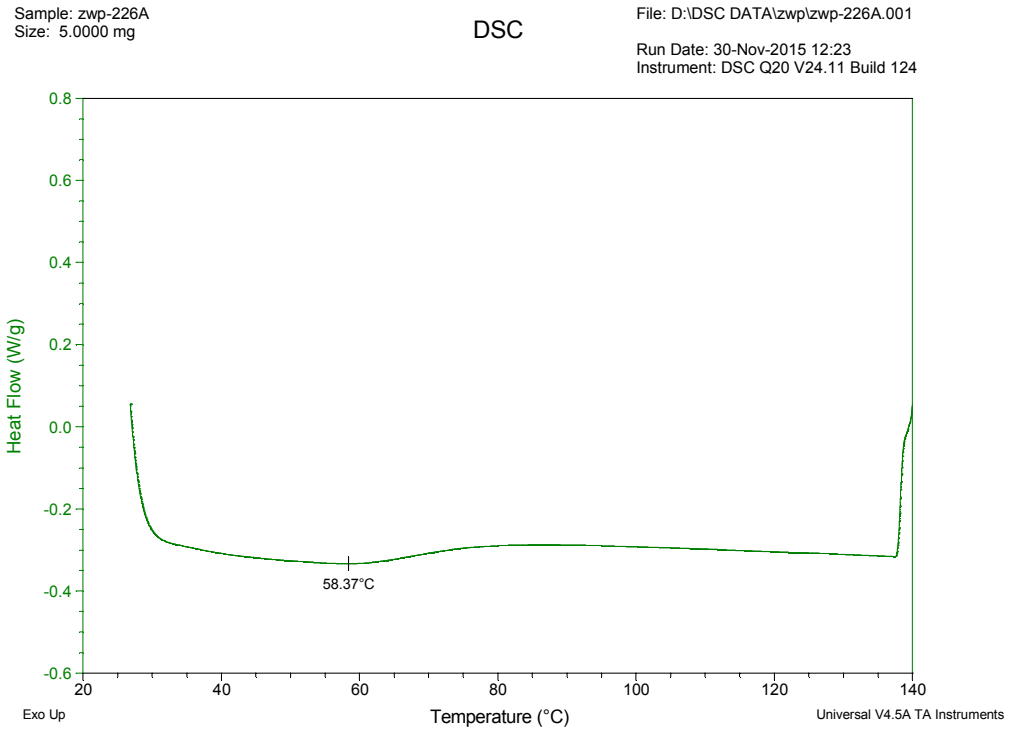

Figure S37. DSC of the polymer from table 1, entry 1.

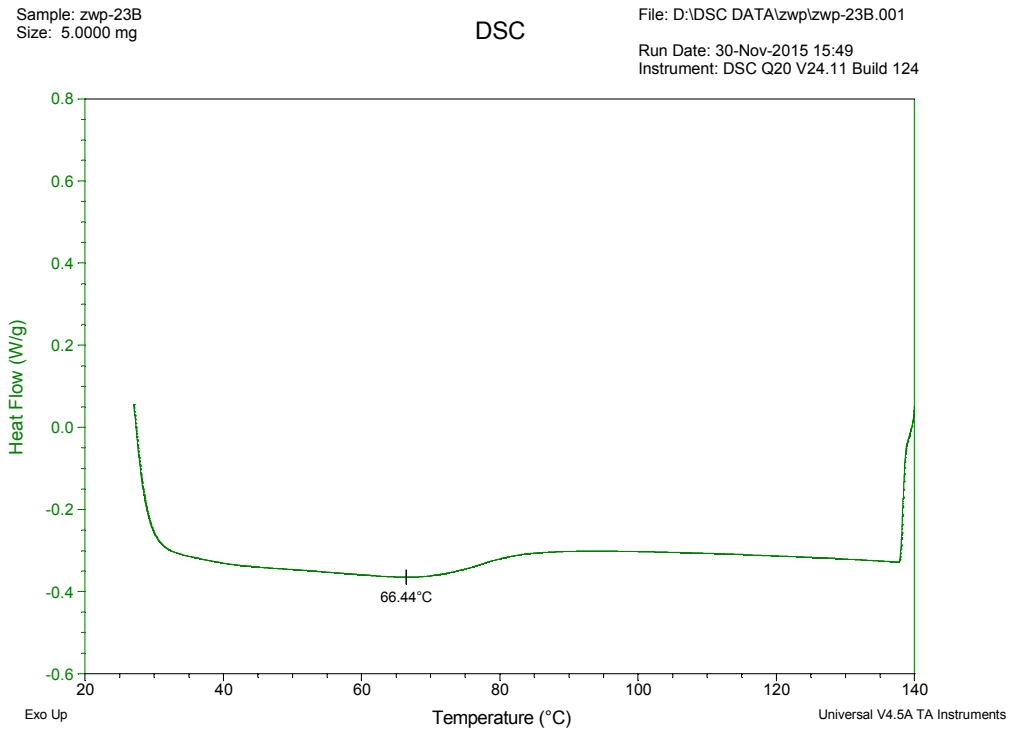

Figure S38. DSC of the polymer from table 1, entry 2.

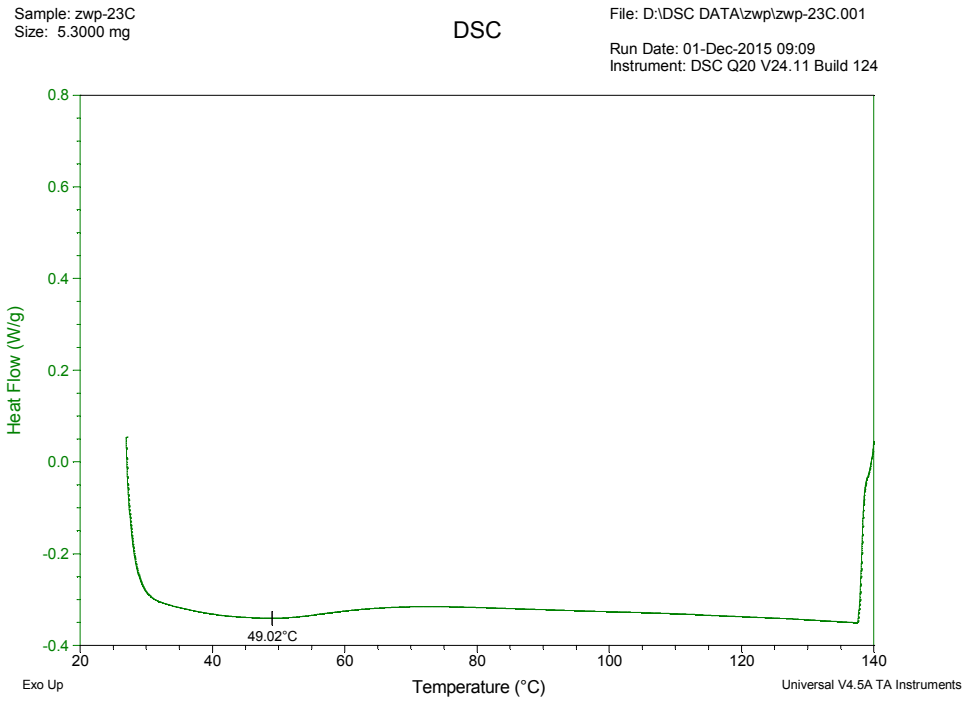

Figure S39. DSC of the polymer from table 1, entry 3.

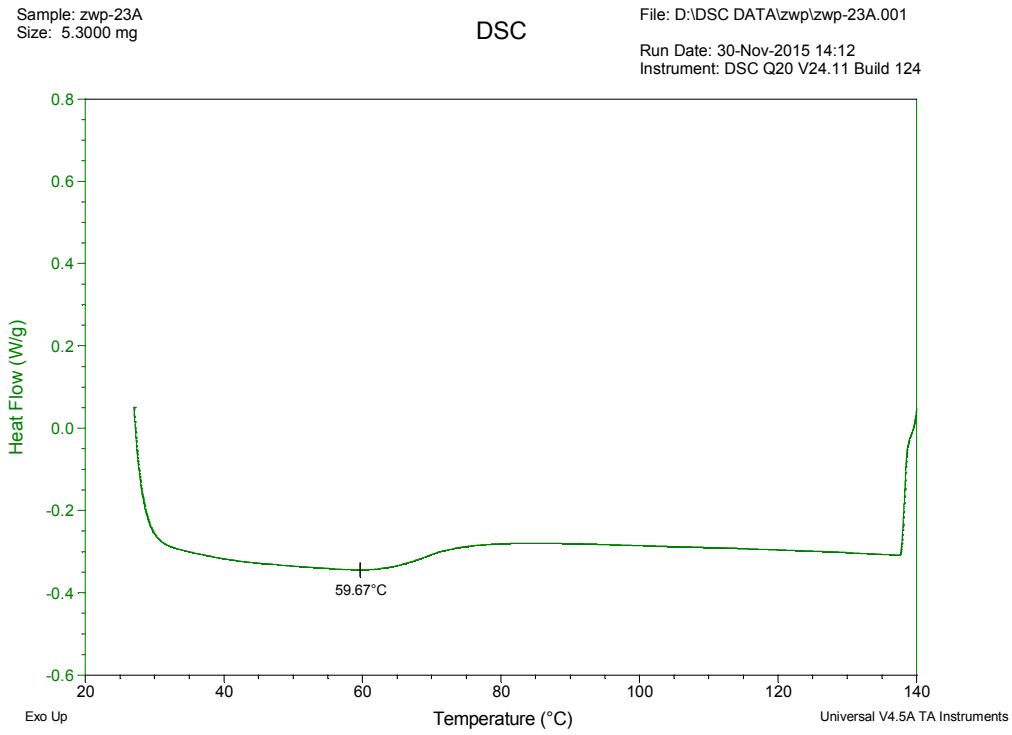

Figure S40. DSC of the polymer from table 1, entry 4.

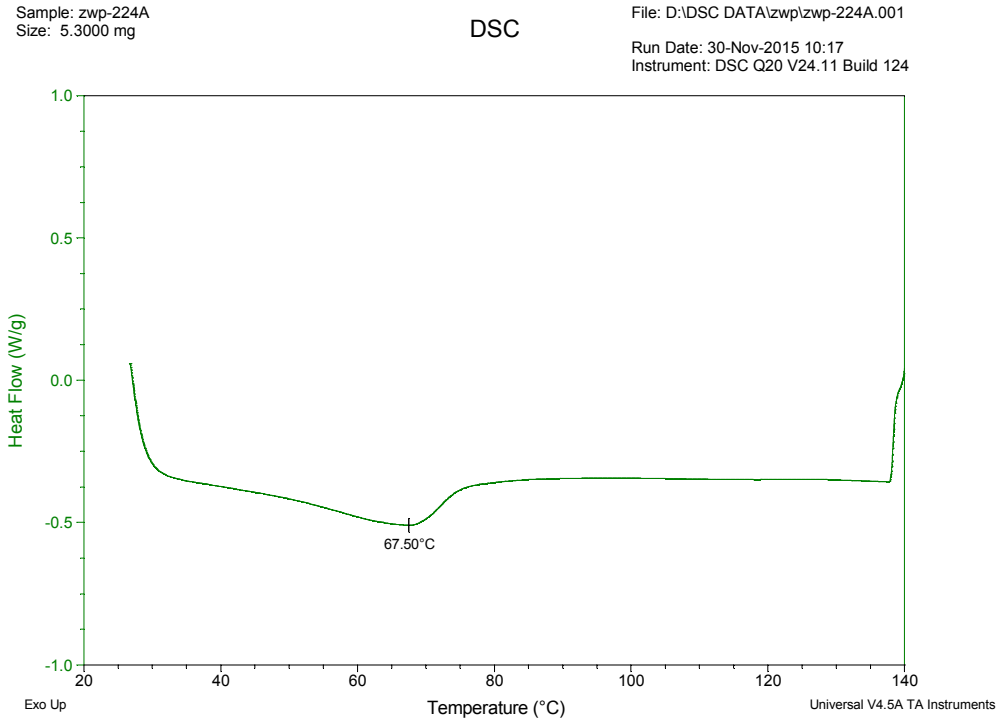

Figure S41. DSC of the polymer from table 1, entry 5.

3. X-Ray Crystallography of complexes Ni-1, Ni-5, Pd-1 and Pd-5.

Experimental for Ni-1

Single crystals of $C_{76}H_{88}Br_4N_4Ni_2$ **[Ni-1]** were **[brown]**. A suitable crystal was selected and **amounted** on a **Xcalibur, Sapphire3, Gemini ultra** diffractometer. The crystal was kept at 291(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

Crystal structure determination of [Ni-1]

Crystal Data for $C_{76}H_{88}Br_4N_4Ni_2$ (M =1494.56 g/mol): triclinic, space group P-1 (no. 2), a = 12.4568(14) Å, b = 12.5749(15) Å, c = 14.017(2) Å, α = 64.779(14)°, β = 65.643(14)°, γ = 69.541(10)°, V = 1768.9(5) Å^3, Z = 1, T = 291(2) K, μ(CuKα) = 3.635 mm^{-1}, *Dcalc* = 1.403 g/cm^3, 11055 reflections measured (7.95° ≤ 2Θ ≤ 139.548°), 6455 unique (R_{int} = 0.0234, R_{sigma} = 0.0380) which were used in all calculations. The final R_1 was 0.0388 (I > 2σ(I)) and wR_2 was 0.1178 (all data).

Refinement model description

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

This report has been created with Olex2, compiled on 2015.01.26 svn.r3150 for OlexSys.

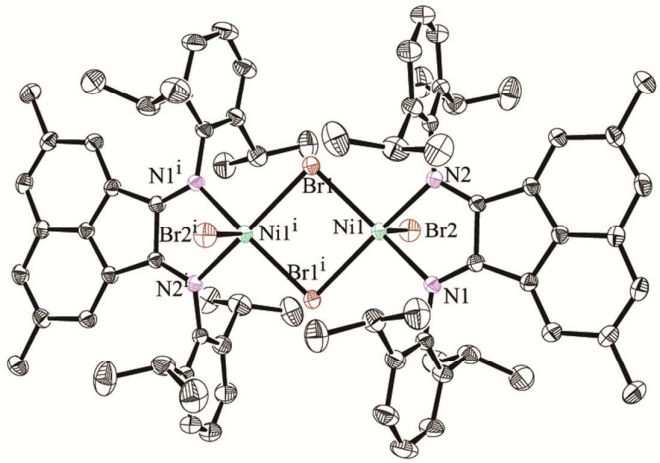

Figure S42. Molecular structure of **Ni-1.**

Table S6. Crystal data and structure refinement for Ni-1 (zwp-202).

Identification code	zwp-202
Empirical formula	$C_{76}H_{88}Br_4N_4Ni_2$
Formula weight	1494.56
Temperature/K	291(2)

Crystal system	triclinic
Space group	P-1
a/Å	12.4568(14)
b/Å	12.5749(15)
c/Å	14.017(2)
α/°	64.779(14)
β/°	65.643(14)
γ/°	69.541(10)
Volume/Å^3	1768.9(5)
Z	1
ρ_{calc}g/cm^3	1.403
μ/mm^{-1}	3.635
F(000)	768.0
Crystal size/mm^3	0.380 × 0.360 × 0.320
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.95 to 139.548
Index ranges	-15 ≤ h ≤ 14, -13 ≤ k ≤ 15, -12 ≤ l ≤ 16
Reflections collected	11055
Independent reflections	6455 [R_{int} = 0.0234, R_{sigma} = 0.0380]
Data/restraints/parameters	6455/0/398
Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.0388, wR_2 = 0.1101
Final R indexes [all data]	R_1 = 0.0461, wR_2 = 0.1178
Largest diff. peak/hole / e Å^{-3}	0.38/-0.72

Experimental for Ni-5

Single crystals of $C_{38}H_{44}Br_2N_2NiO_2$ **[Ni-5]** were **[brown]**. A suitable crystal was selected and **amounted** on a diffractometer. The crystal was kept at 290(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

Crystal structure determination of [Ni-5]

Crystal Data for $C_{38}H_{44}Br_2N_2NiO_2$ (*M* =779.28 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), *a* = 11.2644(7) Å, *b* = 14.2298(12) Å, *c* = 22.702(2) Å, *V* = 3638.9(5) Å^3, *Z* = 4, *T* = 290(2) K, μ(MoKα) = 2.763 mm^{-1}, *Dcalc* = 1.422 g/cm^3, 11383 reflections measured (6.758° ≤ 2Θ ≤ 58.328°), 7535 unique (R_{int} = 0.0451, R_{sigma} = 0.0932) which were used in all calculations. The final R_1 was 0.0558 (I > 2σ(I)) and wR_2 was 0.1808 (all data).

Refinement model description

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

This report has been created with Olex2, compiled on 2015.01.26 svn.r3150 for OlexSys.

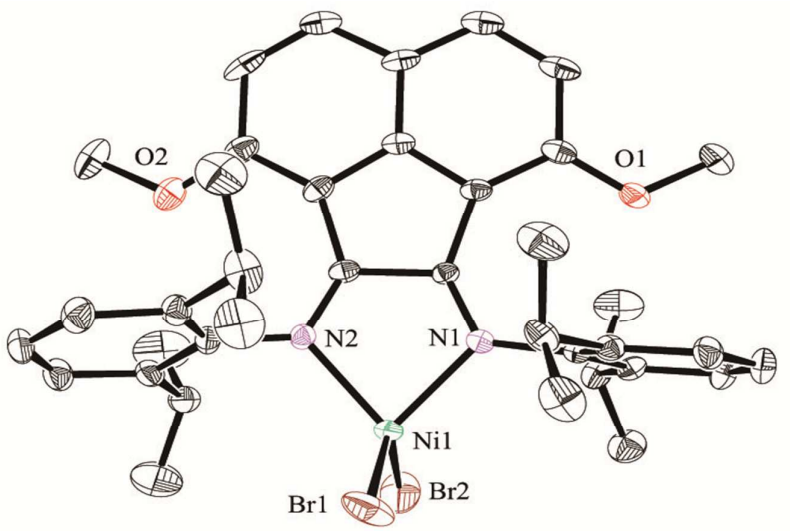

Figure S43. Molecular structure of **Ni-5.**

Table S7. Crystal data and structure refinement for Ni-5 (zwp-201).

Identification code	zwp-201
Empirical formula	$C_{38}H_{44}Br_2N_2NiO_2$
Formula weight	779.28
Temperature/K	290(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	11.2644(7)
b/Å	14.2298(12)
c/Å	22.702(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3638.9(5)
Z	4
ρ_{calc}g/cm^3	1.422
μ/mm^{-1}	2.763
F(000)	1600.0
Crystal size/mm^3	0.330 × 0.250 × 0.240
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.758 to 58.328
Index ranges	$-14 \le h \le 13$, $-5 \le k \le 19$, $-17 \le l \le 29$
Reflections collected	11383

Independent reflections	7535 [R_{int} = 0.0451, R_{sigma} = 0.0932]
Data/restraints/parameters	7535/0/416
Goodness-of-fit on F^2	1.104
Final R indexes [I>=2σ (I)]	R_1 = 0.0558, wR_2 = 0.1210
Final R indexes [all data]	R_1 = 0.1152, wR_2 = 0.1808
Largest diff. peak/hole / e $Å^{-3}$	0.51/-0.66
Flack parameter	-0.001(7)

Experimental for Pd-1

Single crystals of $C_{39}H_{47}ClN_2Pd$ **[Pd-1]** were **[orange]**. A suitable crystal was selected and **amounted** on a diffractometer. The crystal was kept at 291(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

Crystal structure determination of [Pd-1]

Crystal Data for $C_{39}H_{47}ClN_2Pd$ (M =685.63 g/mol): monoclinic, space group $P2_1$ (no. 4), a = 9.1419(5) Å, b = 21.4966(11) Å, c = 9.6747(7) Å, β = 98.435(6)°, V = 1880.7(2) $Å^3$, Z = 2, T = 291(2) K, μ(MoKα) = 0.591 mm^{-1}, $Dcalc$ = 1.211 g/cm^3, 12417 reflections measured (6.904° ≤ 2Θ ≤ 58.464°), 7637 unique (R_{int} = 0.0270, R_{sigma} = 0.0476) which were used in all calculations. The final R_1 was 0.0528 (I > 2σ(I)) and wR_2 was 0.1751 (all data).

Refinement model description

Number of restraints - 67, number of constraints - unknown.

This report has been created with Olex2, compiled on 2015.01.26 svn.r3150 for OlexSys.

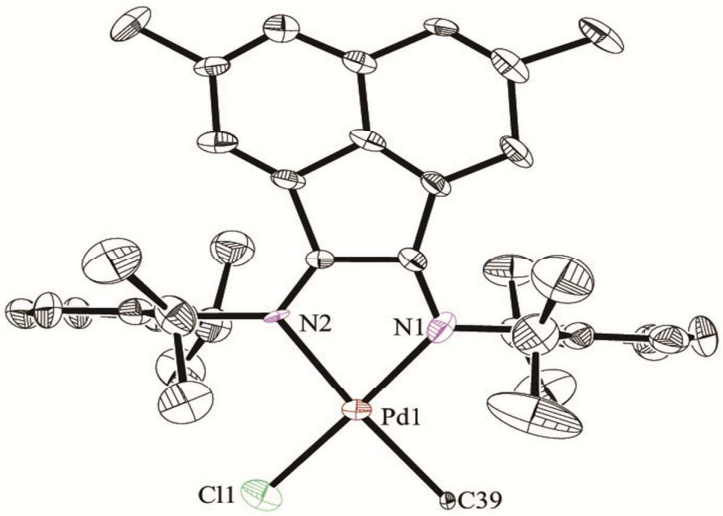

Figure S44. Molecular structure of **Pd-1.**

Table S8. Crystal data and structure refinement for Pd-1 (zwp-208).

Identification code	zwp-208
Empirical formula	$C_{39}H_{47}ClN_2Pd$
Formula weight	685.63
Temperature/K	291(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	9.1419(5)
b/Å	21.4966(11)
c/Å	9.6747(7)
α/°	90
β/°	98.435(6)
γ/°	90
Volume/Å^3	1880.7(2)
Z	2
ρ_{calc}g/cm^3	1.211
μ/mm^{-1}	0.591
F(000)	716.0
Crystal size/mm^3	0.330 × 0.310 × 0.310
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.904 to 58.464
Index ranges	$-12 \le h \le 10$, $-29 \le k \le 28$, $-12 \le l \le 10$
Reflections collected	12417
Independent reflections	7637 [R_{int} = 0.0270, R_{sigma} = 0.0476]
Data/restraints/parameters	7637/67/399
Goodness-of-fit on F^2	1.118
Final R indexes [I>=2σ (I)]	R_1 = 0.0528, wR_2 = 0.1450
Final R indexes [all data]	R_1 = 0.0730, wR_2 = 0.1751
Largest diff. peak/hole / e Å^{-3}	0.74/-0.76
Flack parameter	0.49(4)

Experimental for Pd-5

Single crystals of $C_{41}H_{49}Cl_7N_2O_2Pd$ **[Pd-5]** were **[orange]**. A suitable crystal was selected and **amounted** on a **Xcalibur, Sapphire3, Gemini ultra** diffractometer. The crystal was kept at 293(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

Crystal structure determination of [Pd-5]

Crystal Data for $C_{41}H_{49}Cl_7N_2O_2Pd$ (M =956.37 g/mol): orthorhombic, space group Pbca (no. 61), a = 22.5591(3) Å, b = 17.8864(2) Å, c = 22.5836(3) Å, V = 9112.5(2) Å^3, Z = 8, T = 293(2) K, μ(CuKα) = 7.335 mm^{-1}, *Dcalc* = 1.394 g/cm^3, 40651 reflections measured (7.424° ≤ 2Θ ≤ 139.326°), 8514 unique (R_{int} = 0.0373, R_{sigma} = 0.0279) which were used in all calculations. The final R_1 was 0.0536 (I > 2σ(I)) and wR_2 was 0.1641 (all data).

Refinement model description

Number of restraints - 14, number of constraints - unknown.

This report has been created with Olex2, compiled on 2015.01.26 svn.r3150 for OlexSys.

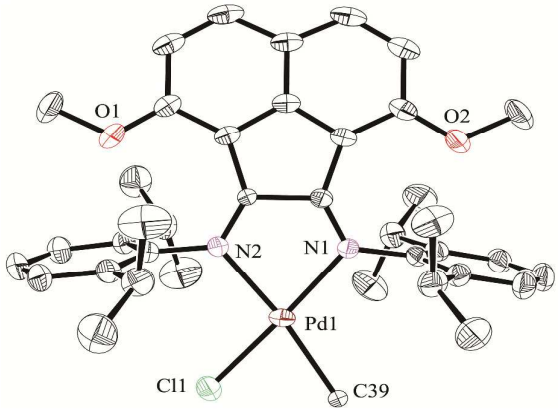

Figure S45. Molecular structure of **Pd-5.**

Table S9. Crystal data and structure refinement for Pd-5 (zwp-175).

Identification code	zwp-175
Empirical formula	$C_{41}H_{49}Cl_7N_2O_2Pd$
Formula weight	956.37
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	22.5591(3)
b/Å	17.8864(2)
c/Å	22.5836(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	9112.5(2)
Z	8
ρ_{calc}g/cm^3	1.394
μ/mm^{-1}	7.335
F(000)	3920.0

Crystal size/mm^3	0.360 × 0.300 × 0.300
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.424 to 139.326
Index ranges	$-25 \leq h \leq 27$, $-16 \leq k \leq 21$, $-27 \leq l \leq 27$
Reflections collected	40651
Independent reflections	8514 [R_{int} = 0.0373, R_{sigma} = 0.0279]
Data/restraints/parameters	8514/14/490
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0536, wR_2 = 0.1537
Final R indexes [all data]	R_1 = 0.0611, wR_2 = 0.1641
Largest diff. peak/hole / e $Å^{-3}$	1.00/-0.72

References

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. G. M. Sheldrick, SHELXL 97, Programs for structure refinement, Universität Göttingen, 1997.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.