

Supplementary Materials

Table S1. Crystal data and structure refinement for **4a**

Empirical formula	C ₃₈ H ₃₅ Cl ₃ N ₄ NiO ₃
Formula weight	760.74
Temperature/K	293.15
Crystal system	triclinic
Space group	P-1
a/Å	9.3484(3)
b/Å	11.3583(4)
c/Å	17.0360(6)
α/°	87.8580(10)
β/°	76.1330(10)
γ/°	79.8190(10)
Volume/Å ³	1728.52(10)
Z	2
ρ _{calc} /cm ³	1.462
μ/mm ⁻¹	3.300
F(000)	788.0
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	10.698 to 136.618
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 13, -20 ≤ l ≤ 18
Reflections collected	47661
Independent reflections	6260 [R _{int} = 0.0255, R _{sigma} = 0.0160]
Data/restraints/parameters	6260/0/452
Goodness-of-fit on F ²	1.039
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0483, wR ₂ = 0.1221
Final R indexes [all data]	R ₁ = 0.0492, wR ₂ = 0.1228
Largest diff. peak/hole / e Å ⁻³	0.86/-0.88

Figure S1 Crystal structure of **4a**

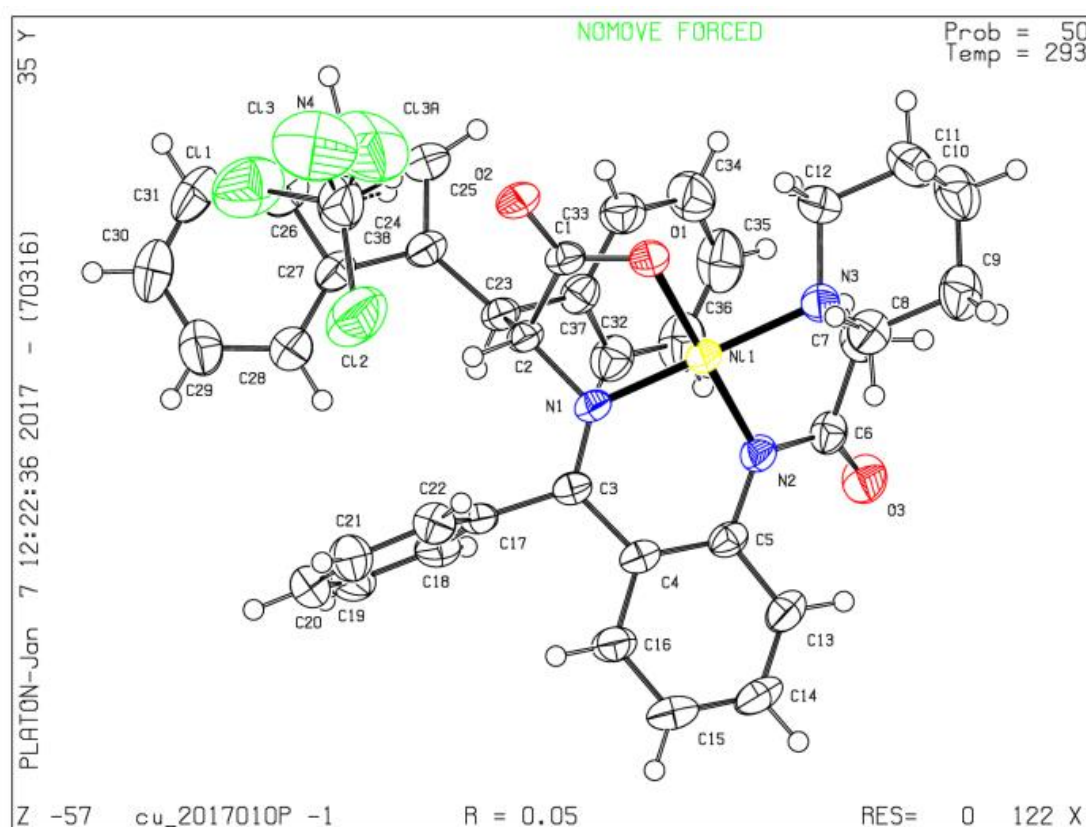
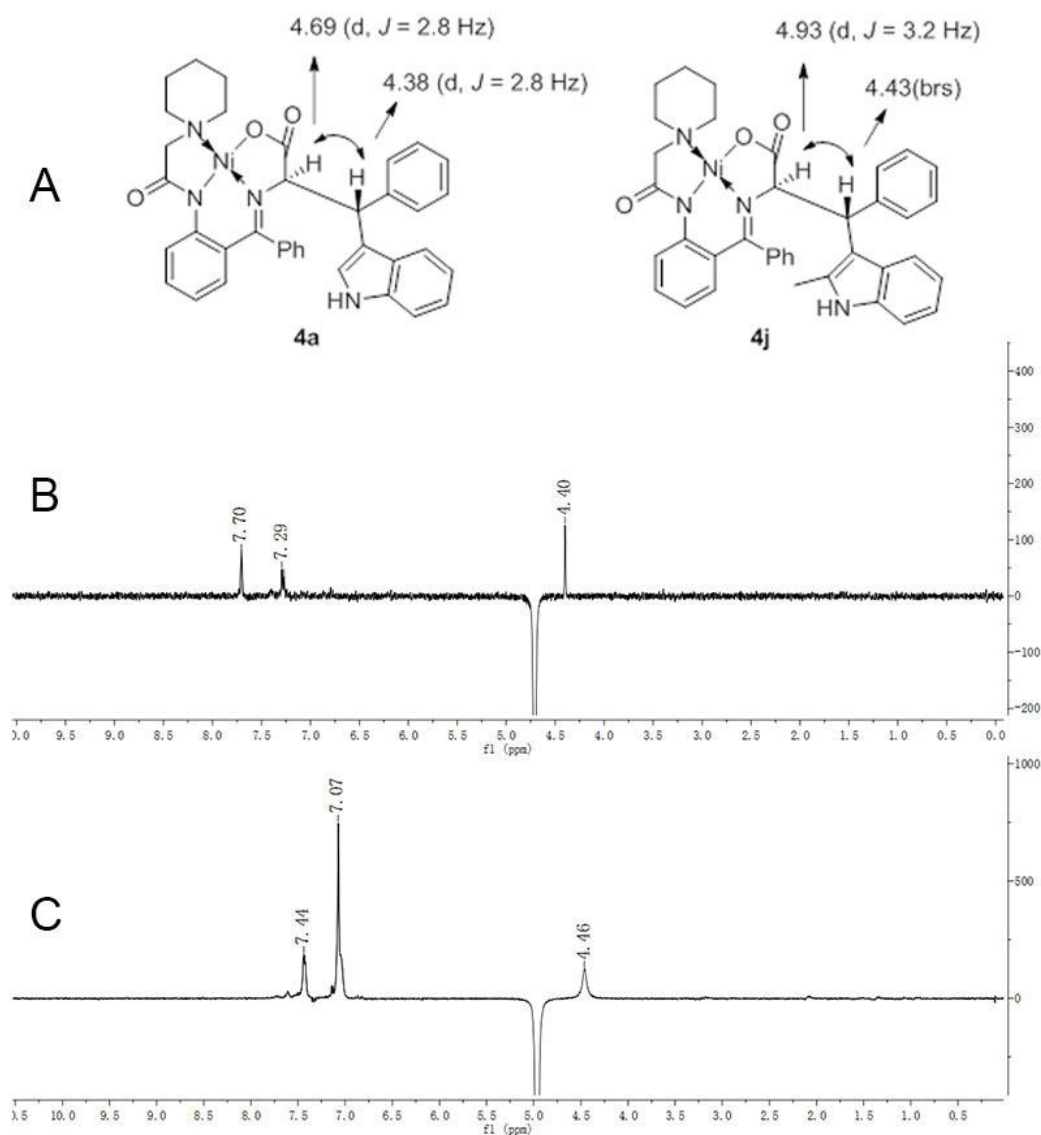


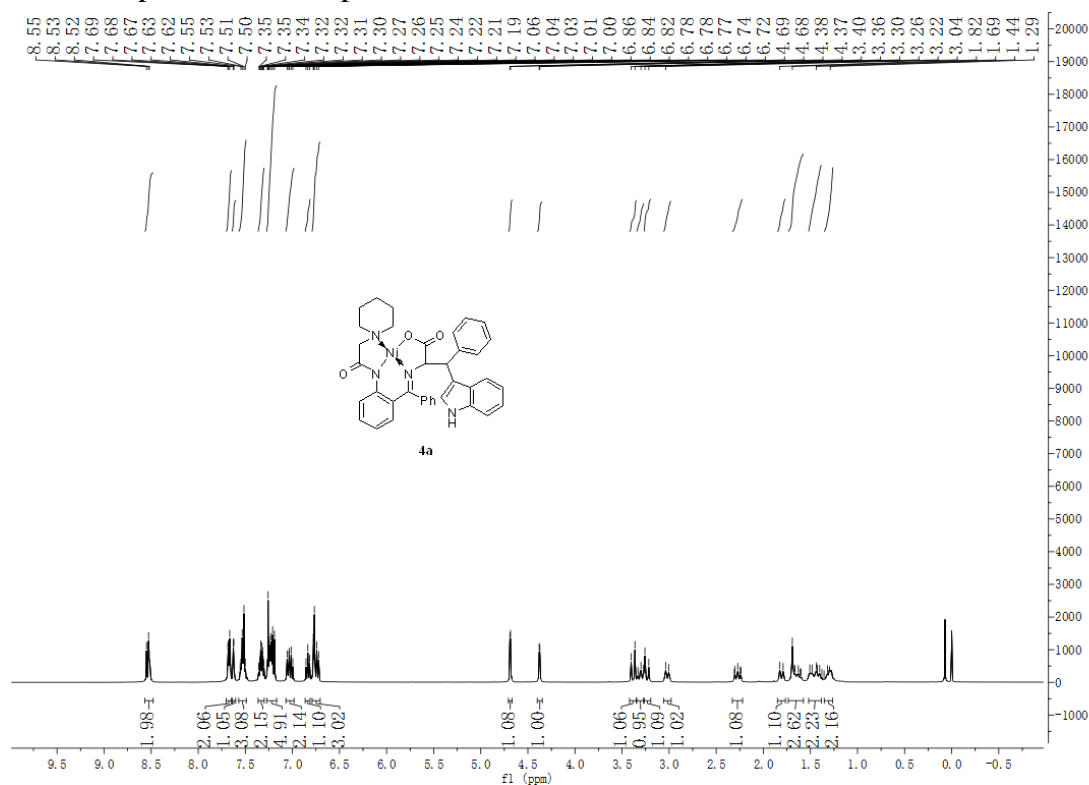
Figure S2 Structures and NOE spectra of compound **4a** and **4j**



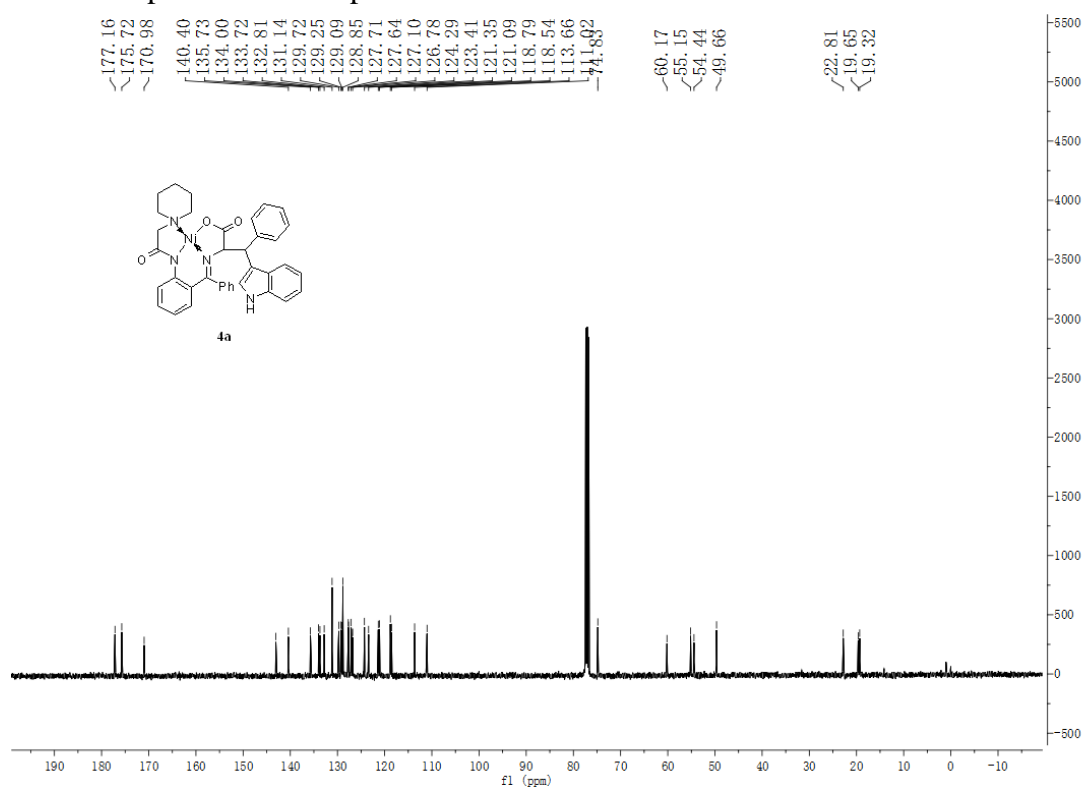
(A) Structures and related ^1H NMR data of compound **4a** and **4j**. NOE spectra of **4a** (B) and **4j** (C) both show that the protons on the two chiral carbons correlate with each other. NOE spectrum of **4j** (C) indicates that the proton at 4.93 is not correlated with the methyl group in space.

Copies of NMR spectra

^1H NMR spectrum of compound **4a**



^{13}C NMR spectrum of compound **4a**



Chemical structure of compound **4b** is shown above the spectrum. The structure is a complex molecule featuring a benzimidazole core, a phenyl ring, a methoxy group, and a piperidine ring.

¹H NMR spectrum (CDCl₃) of compound **4b**. The x-axis represents the chemical shift in ppm, ranging from -1.0 to 9.5. The y-axis represents the intensity in arbitrary units, ranging from -2000 to 32000. The spectrum shows several peaks, with integration values provided below the baseline.

Integration values (from left to right): 1.96, 1.03, 1.09, 2.15, 4.89, 3.10, 2.07, 2.02, 1.04, 1.00, 3.02, 1.04, 2.02, 1.02, 1.05, 1.08, 2.05, 2.19, 1.91, 1.28.

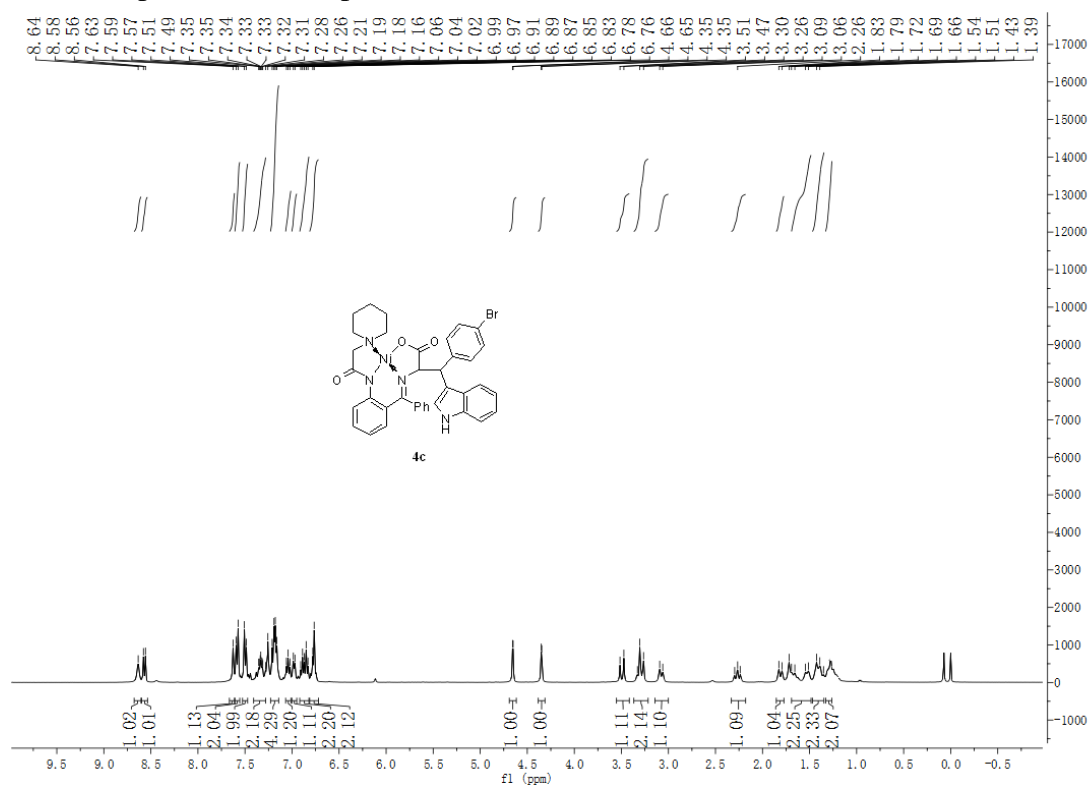
4b

Chemical structure of **4b** is shown above the spectrum.

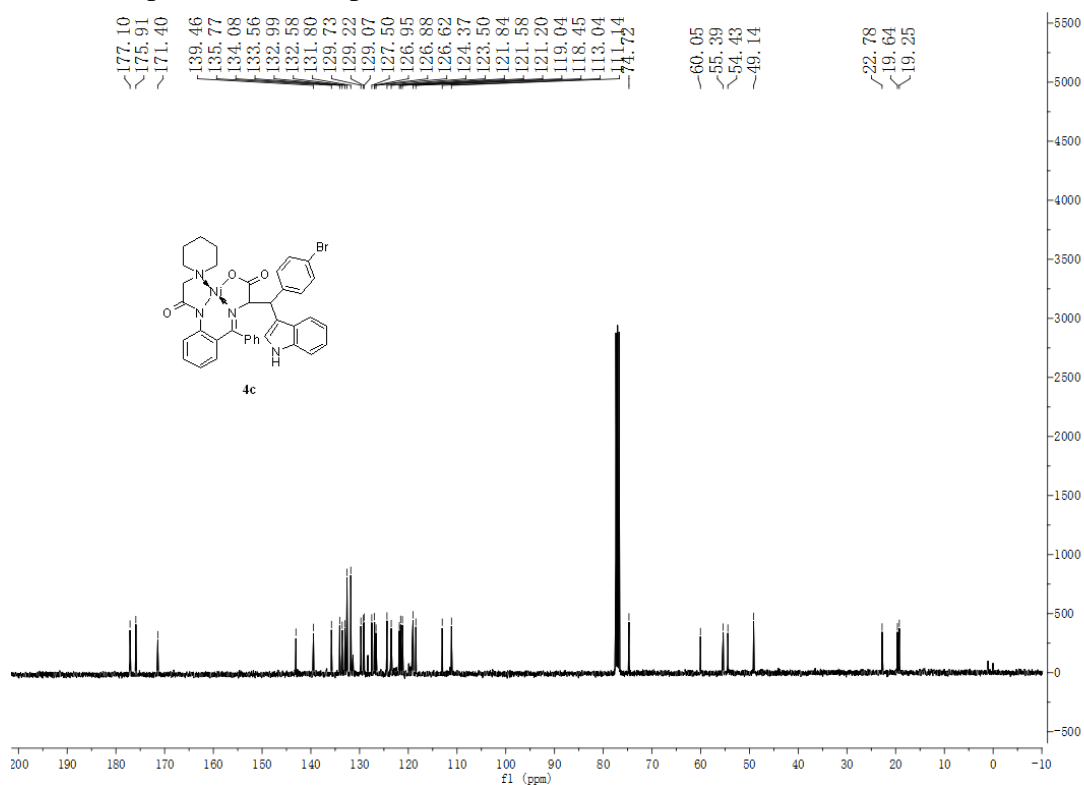
¹³C NMR spectrum (CDCl₃) of compound **4b**. The x-axis represents the chemical shift in ppm (f1), ranging from -10 to 210. The y-axis represents the intensity. The spectrum shows several peaks, with the following chemical shifts (ppm) labeled above the peaks:

- 177.26
- 175.85
- 170.97
- 160.08
- 141.93
- 133.69
- 132.83
- 129.67
- 129.65
- 129.19
- 129.03
- 127.69
- 127.09
- 124.26
- 123.43
- 121.42
- 121.05
- 118.86
- 115.83
- 113.80
- 113.55
- 74.98
- 74.92
- 60.14
- 55.21
- 55.16
- 54.40
- 49.68
- 22.80
- 19.65
- 19.28

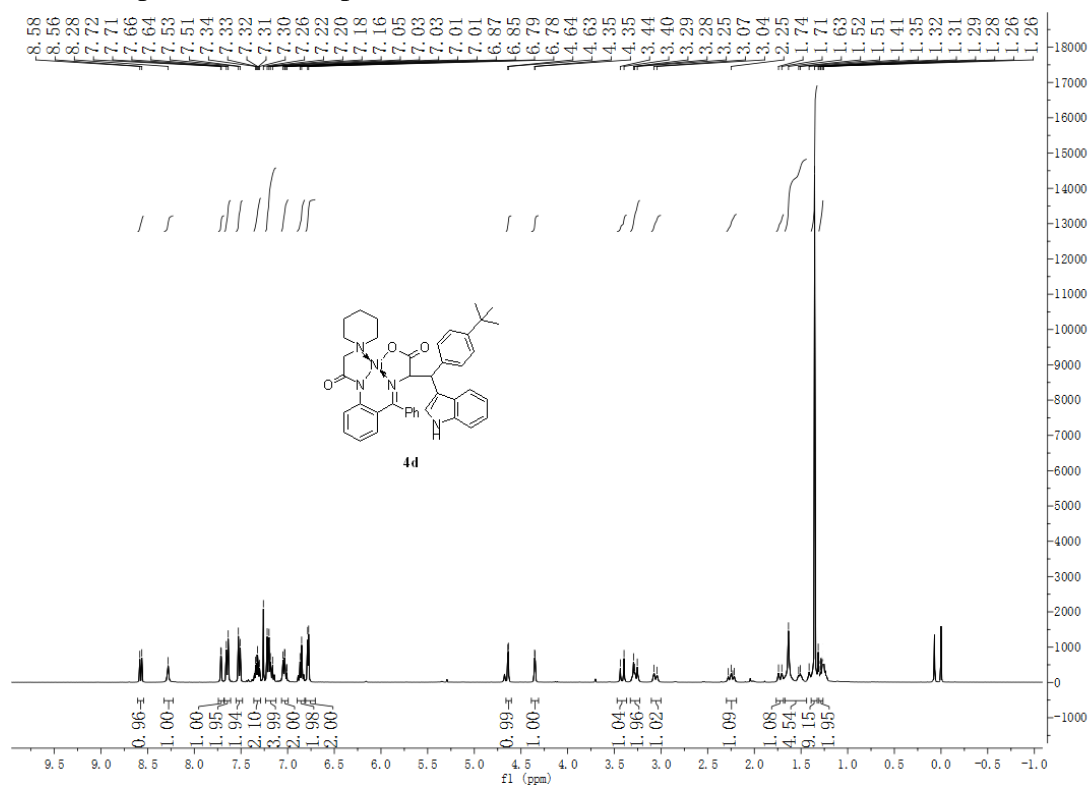
¹HNMR spectrum of compound **4c**



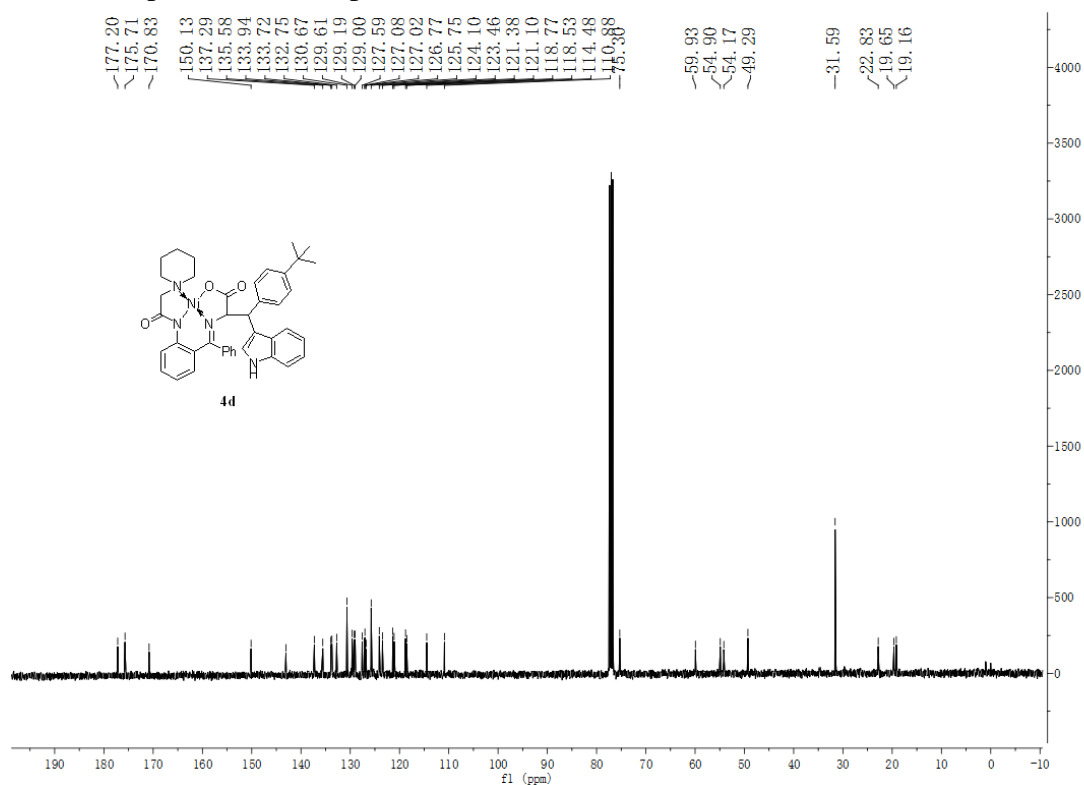
¹³CNMR spectrum of compound **4c**



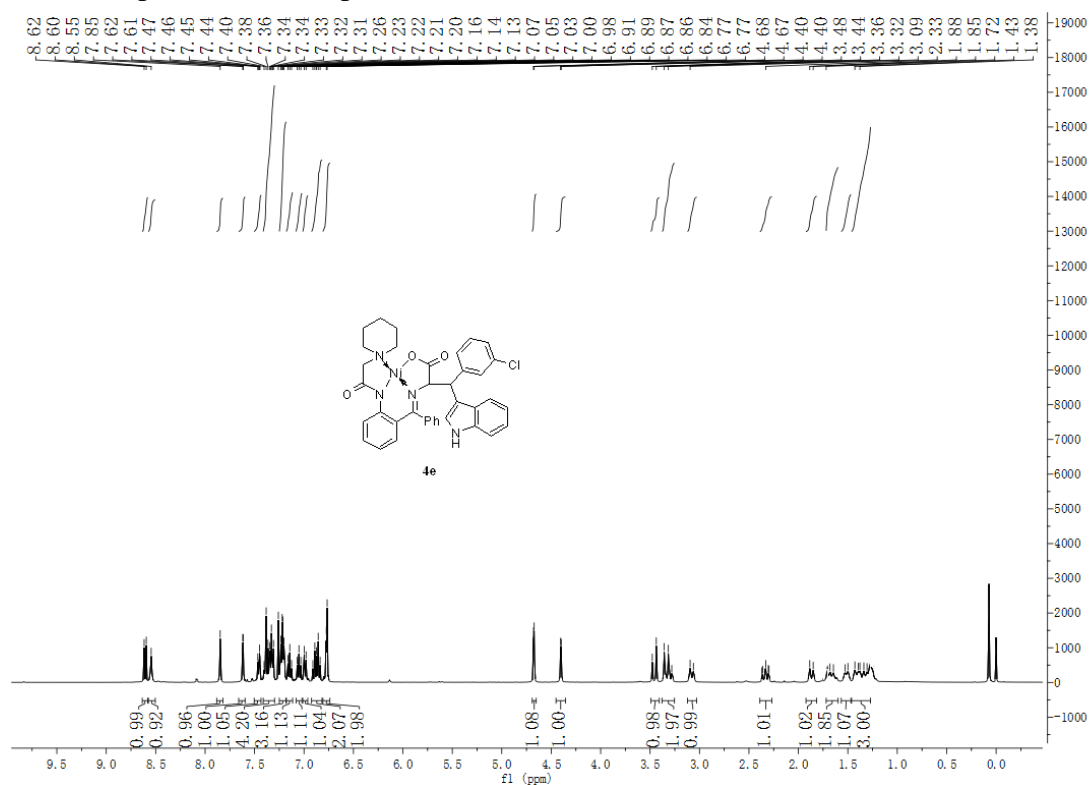
¹HNMR spectrum of compound **4d**



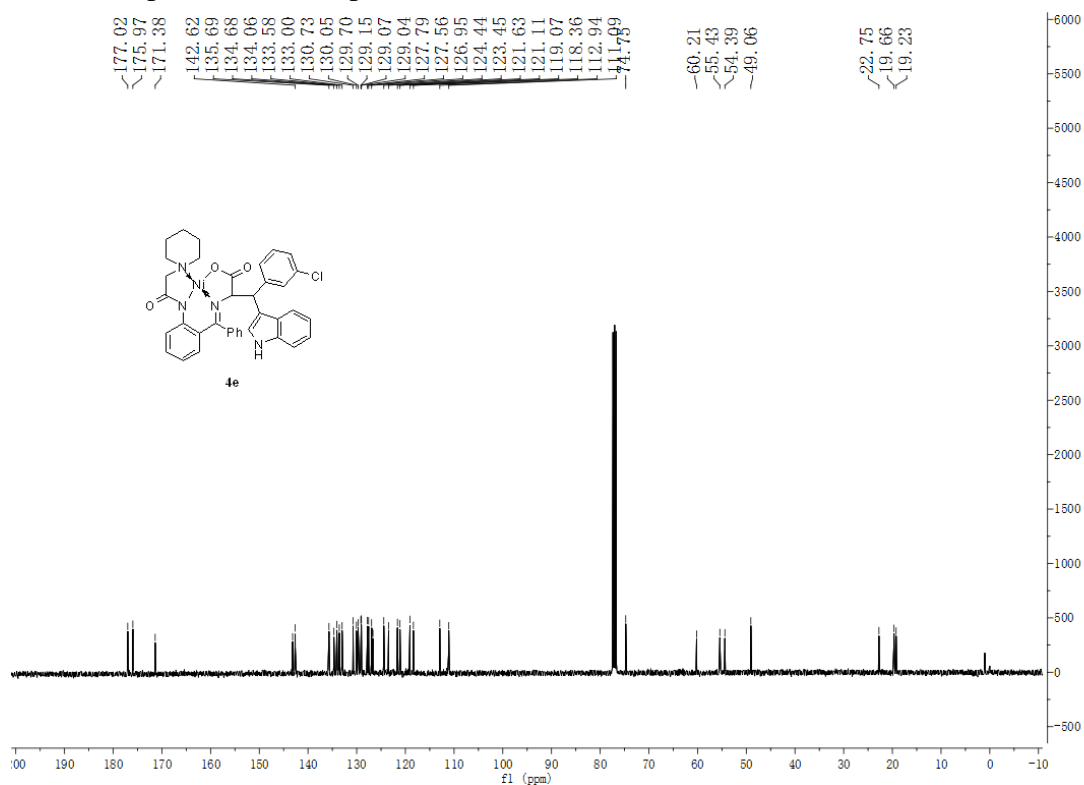
¹³CNMR spectrum of compound **4d**



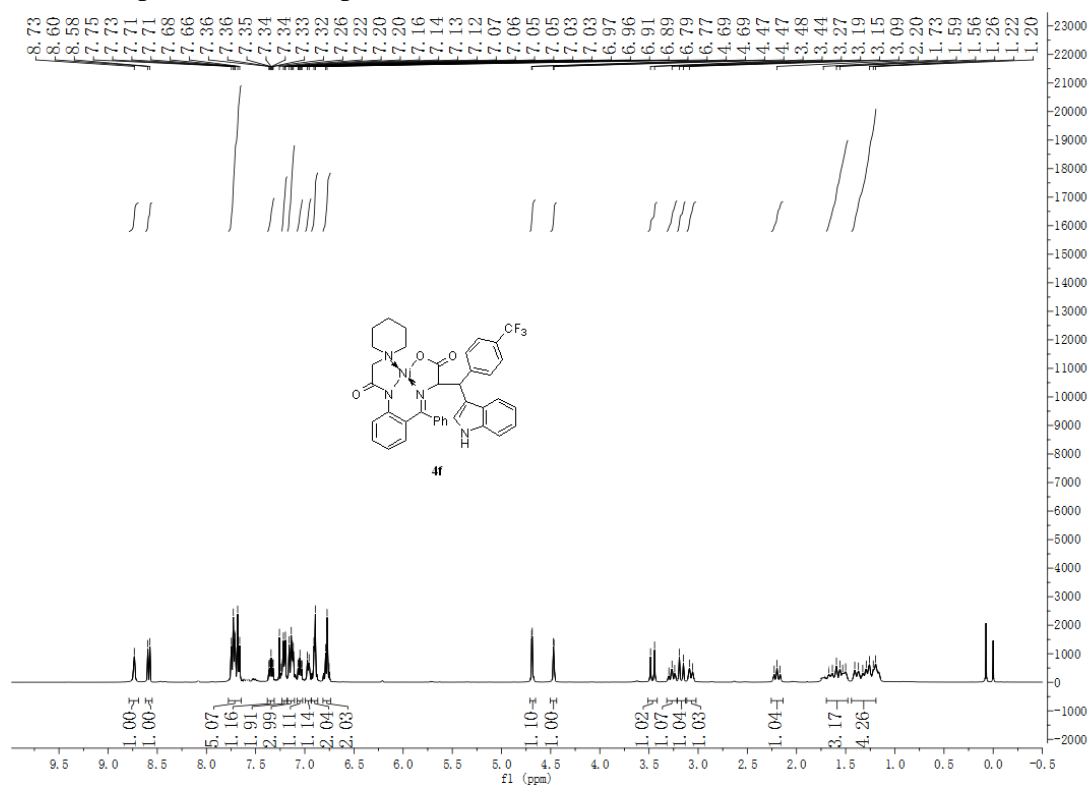
¹HNMR spectrum of compound **4e**



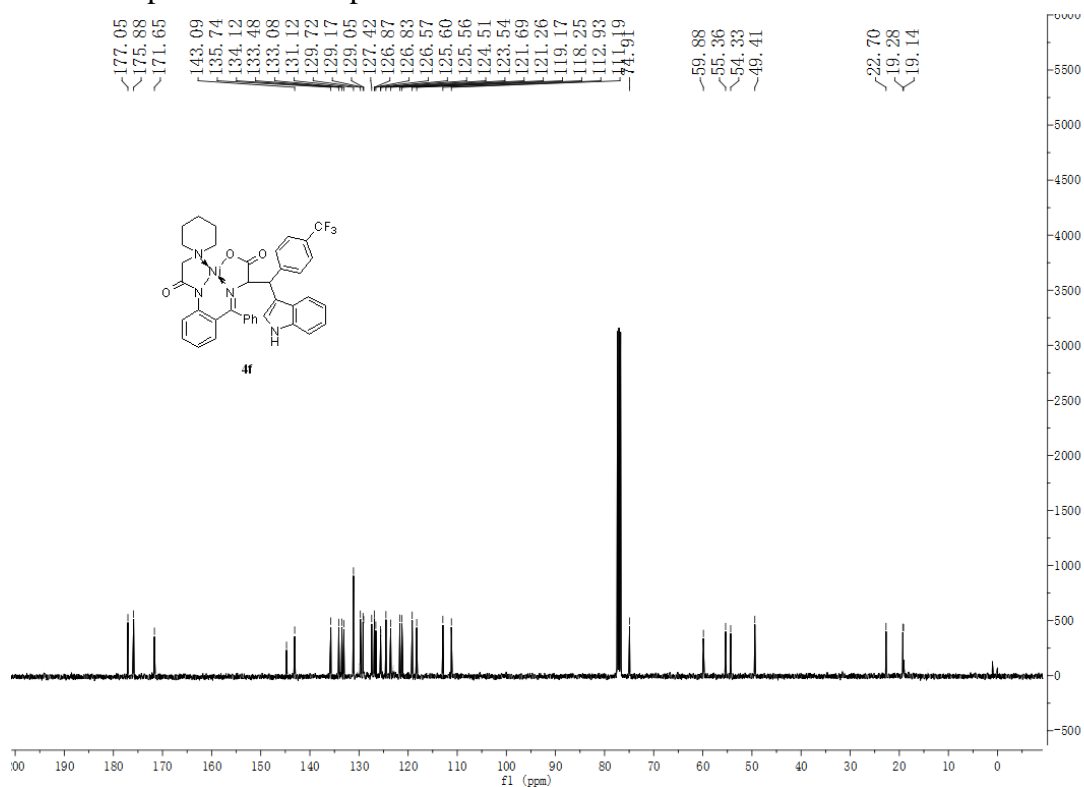
¹³CNMR spectrum of compound **4e**



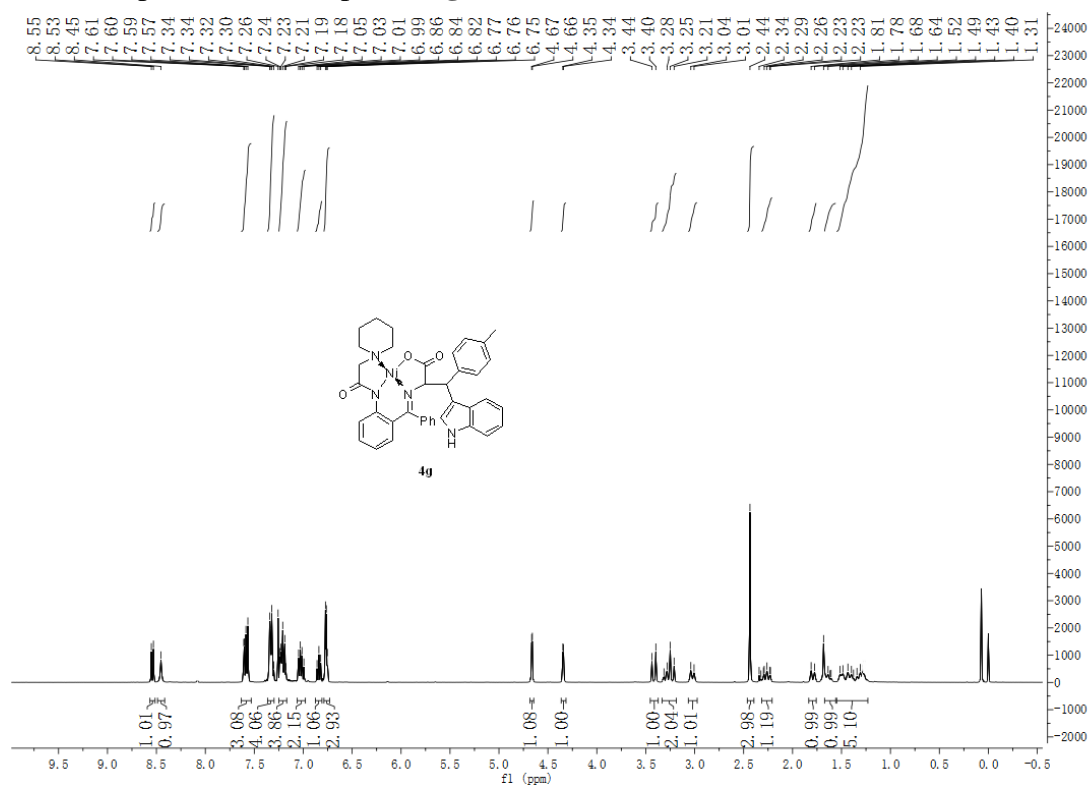
¹HNMR spectrum of compound **4f**



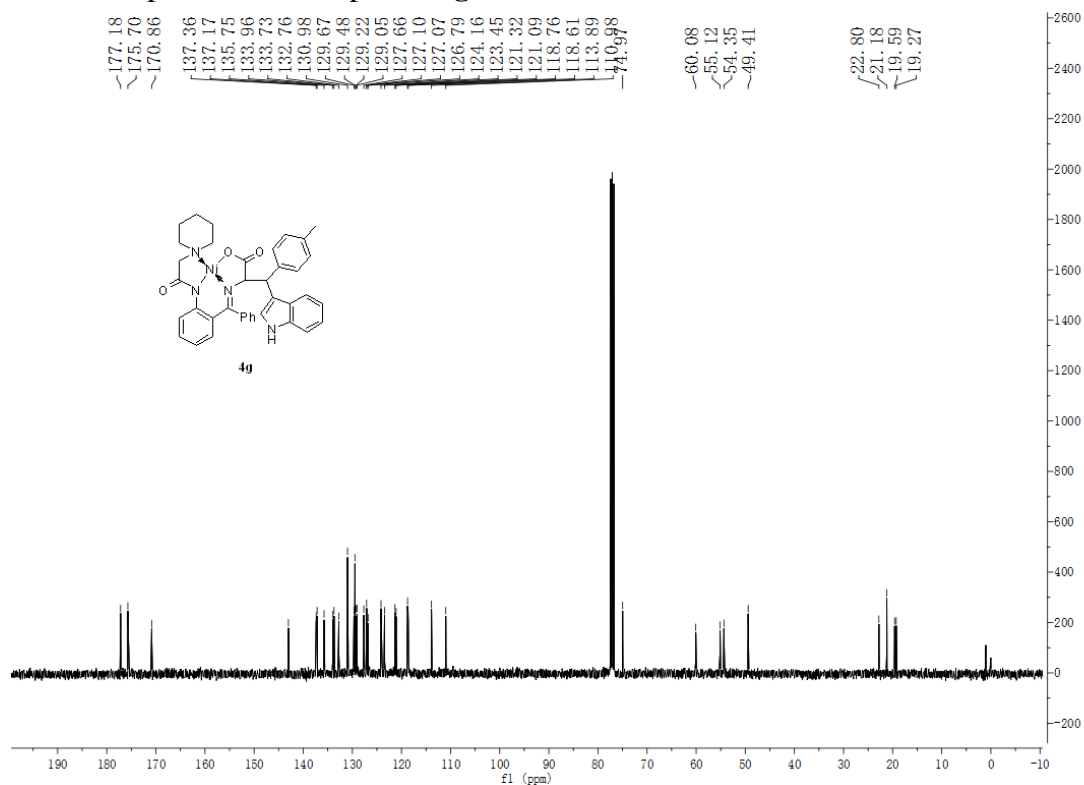
¹³CNMR spectrum of compound **4f**



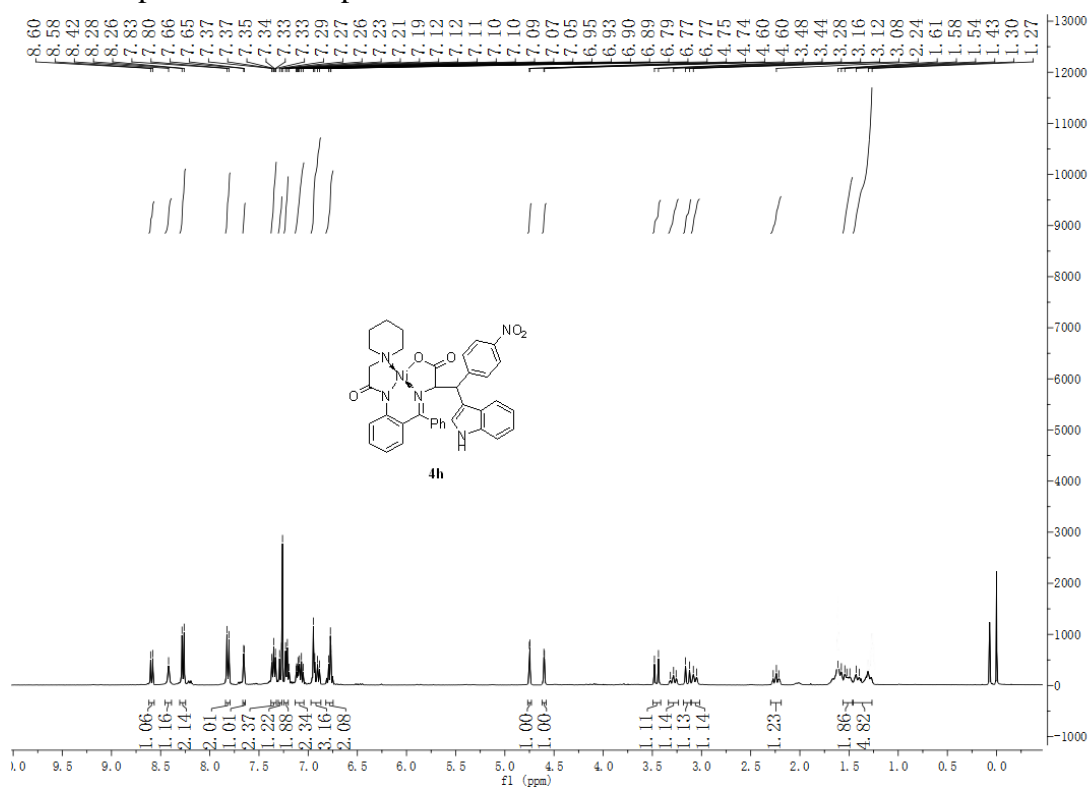
¹HNMR spectrum of compound **4g**



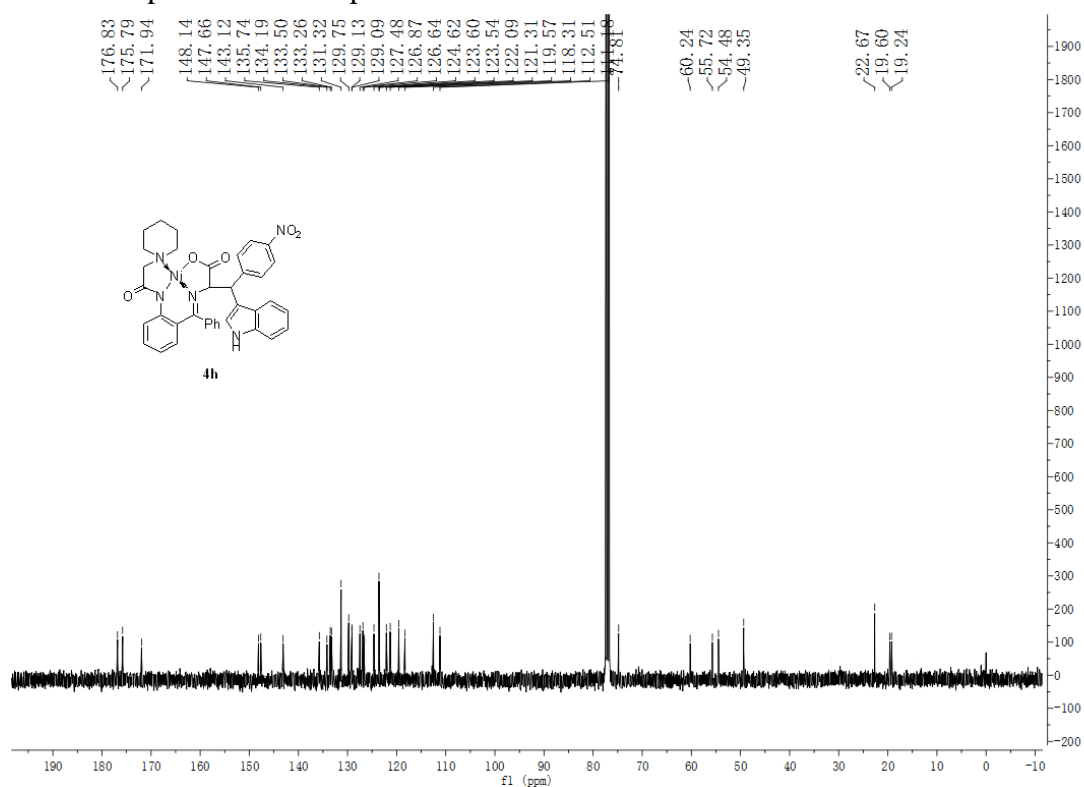
¹³CNMR spectrum of compound **4g**



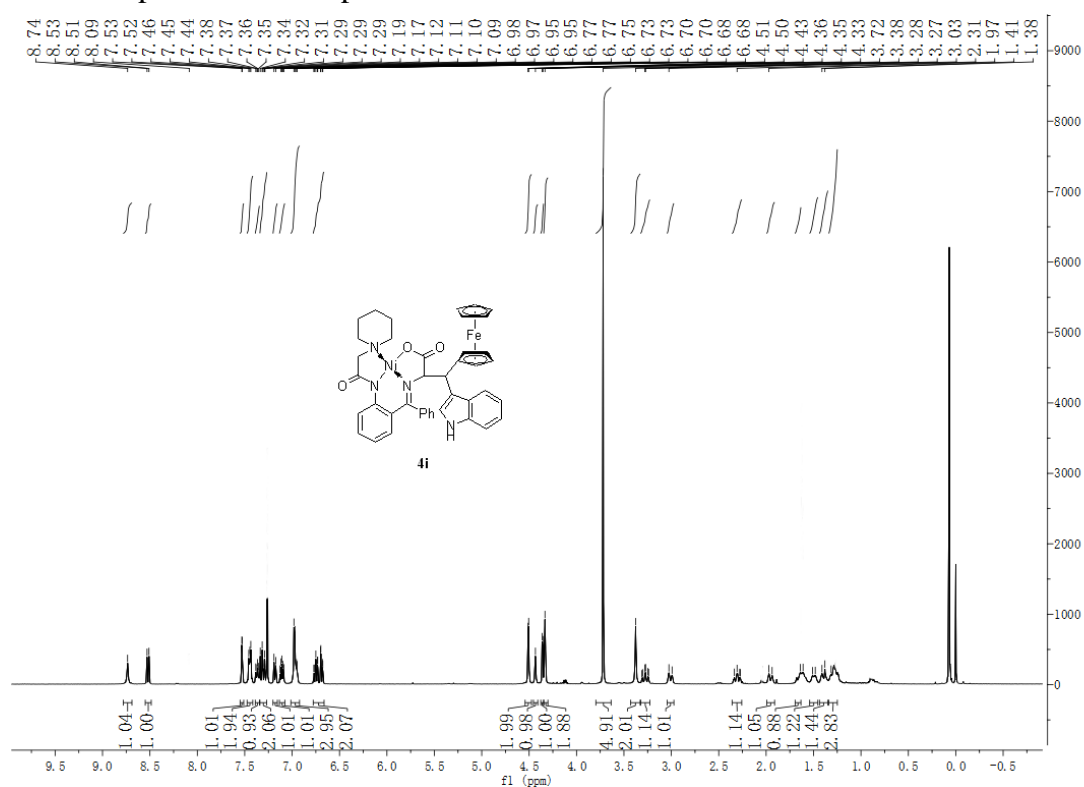
¹H NMR spectrum of compound **4h**



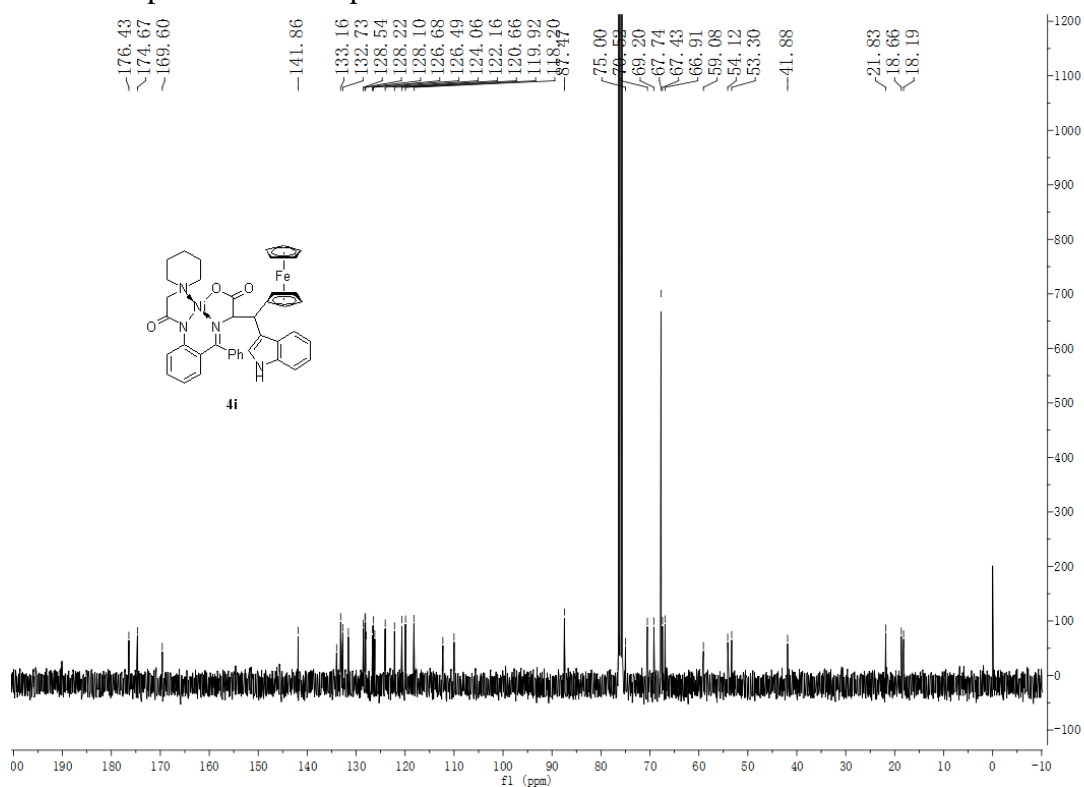
¹³C NMR spectrum of compound **4h**



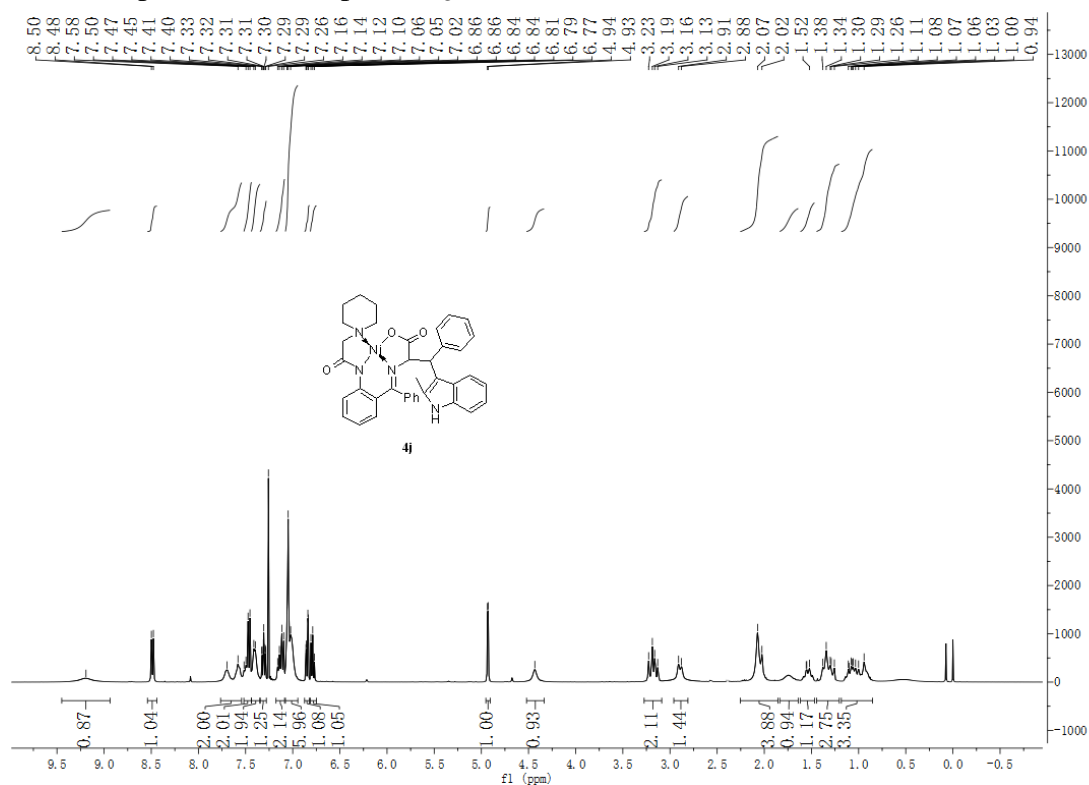
¹H NMR spectrum of compound **4i**



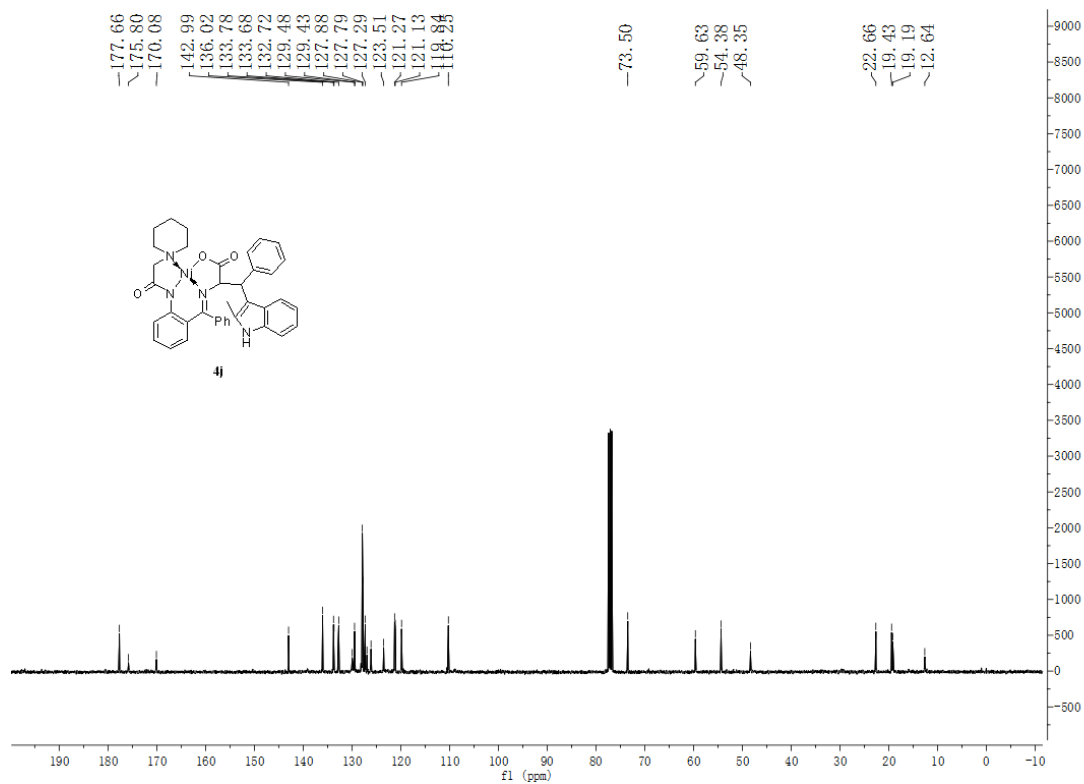
¹³C NMR spectrum of compound **4i**



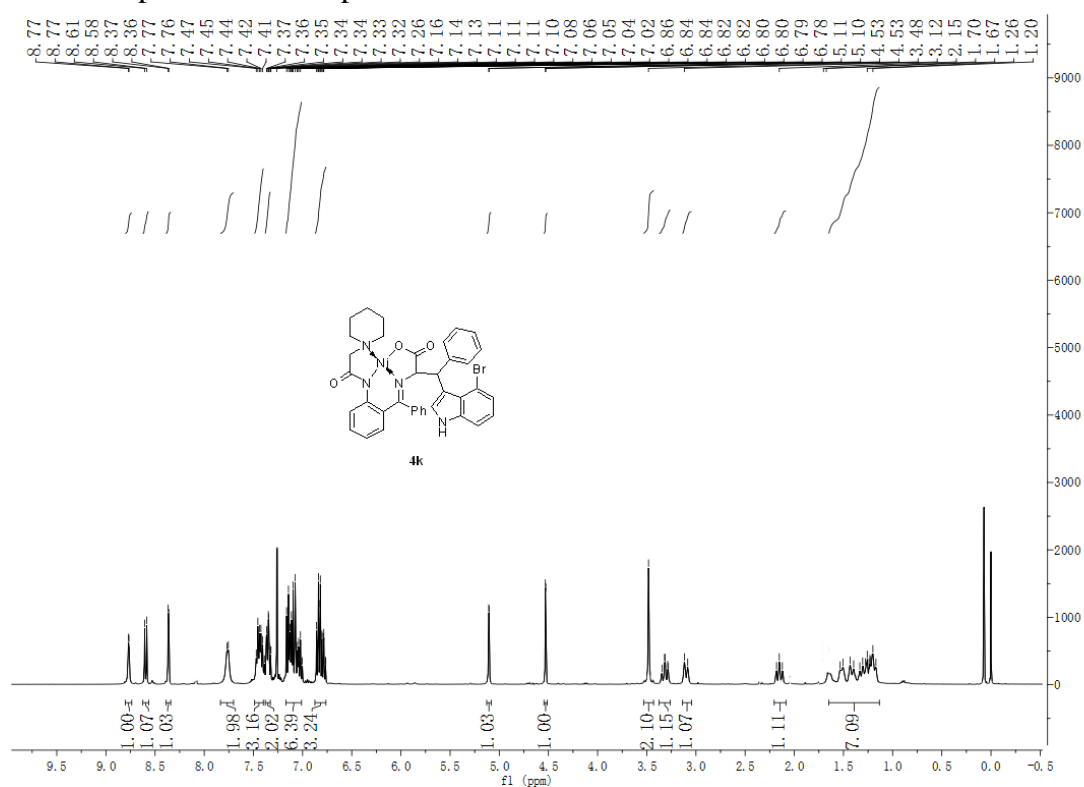
¹H NMR spectrum of compound **4j**



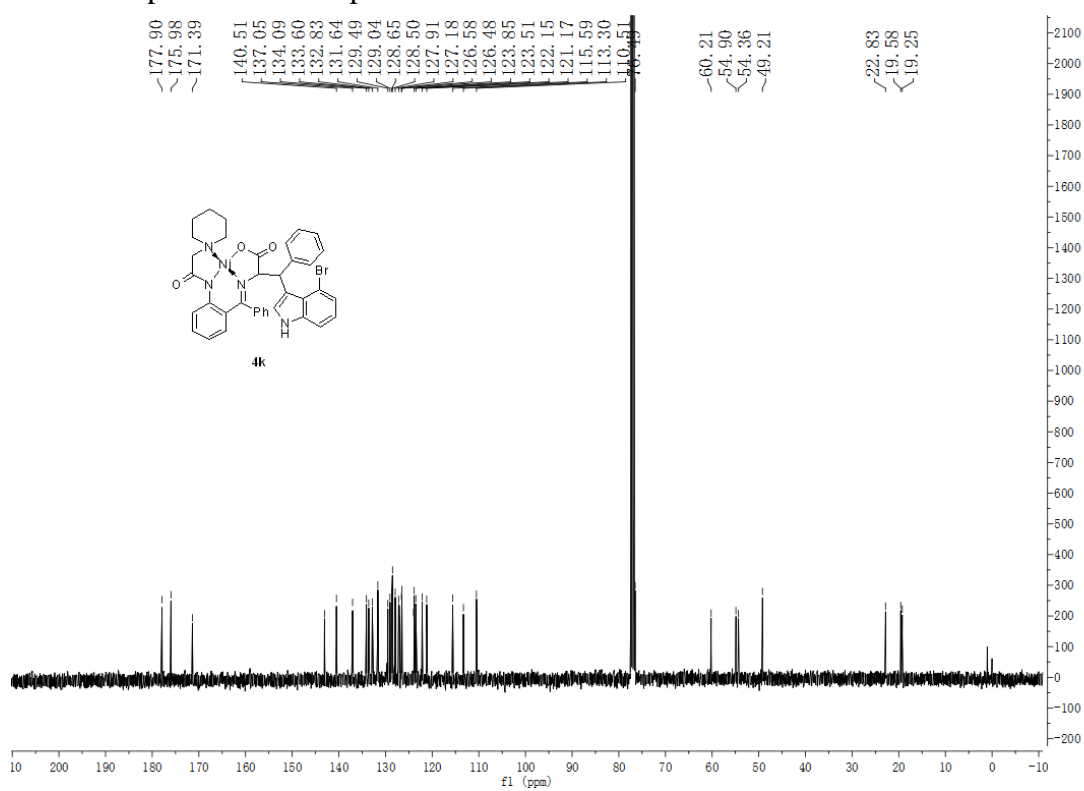
¹³C NMR spectrum of compound **4j**



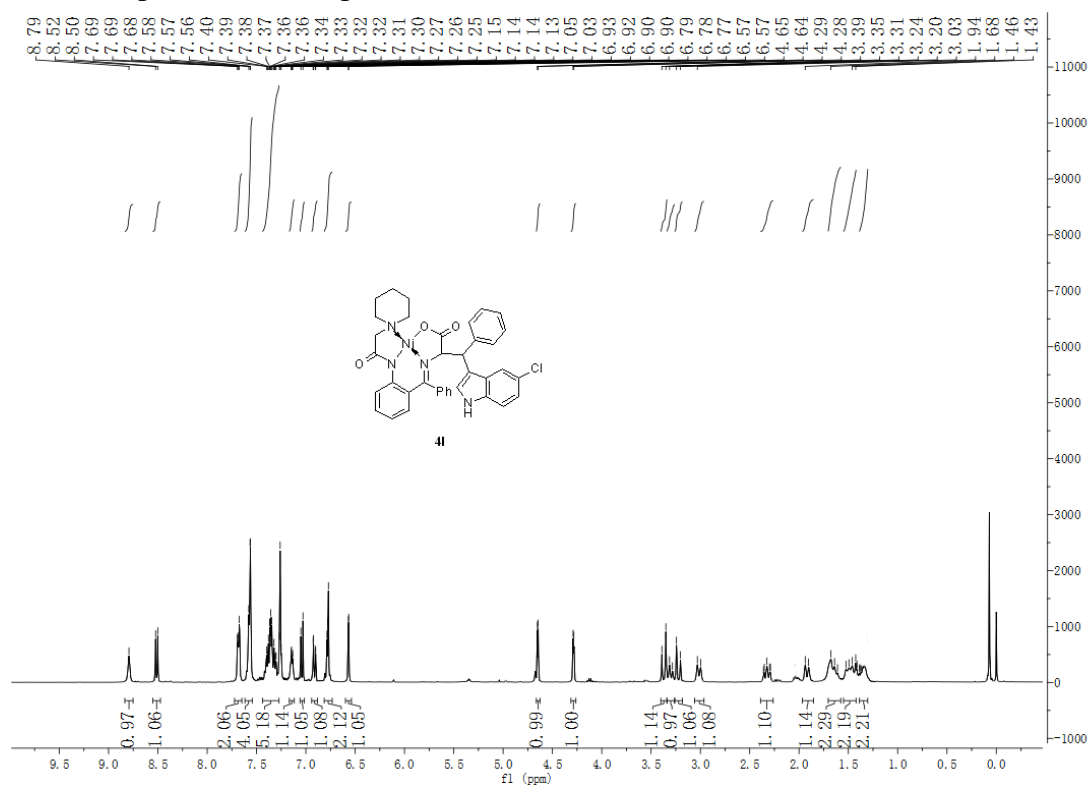
¹H NMR spectrum of compound **4k**



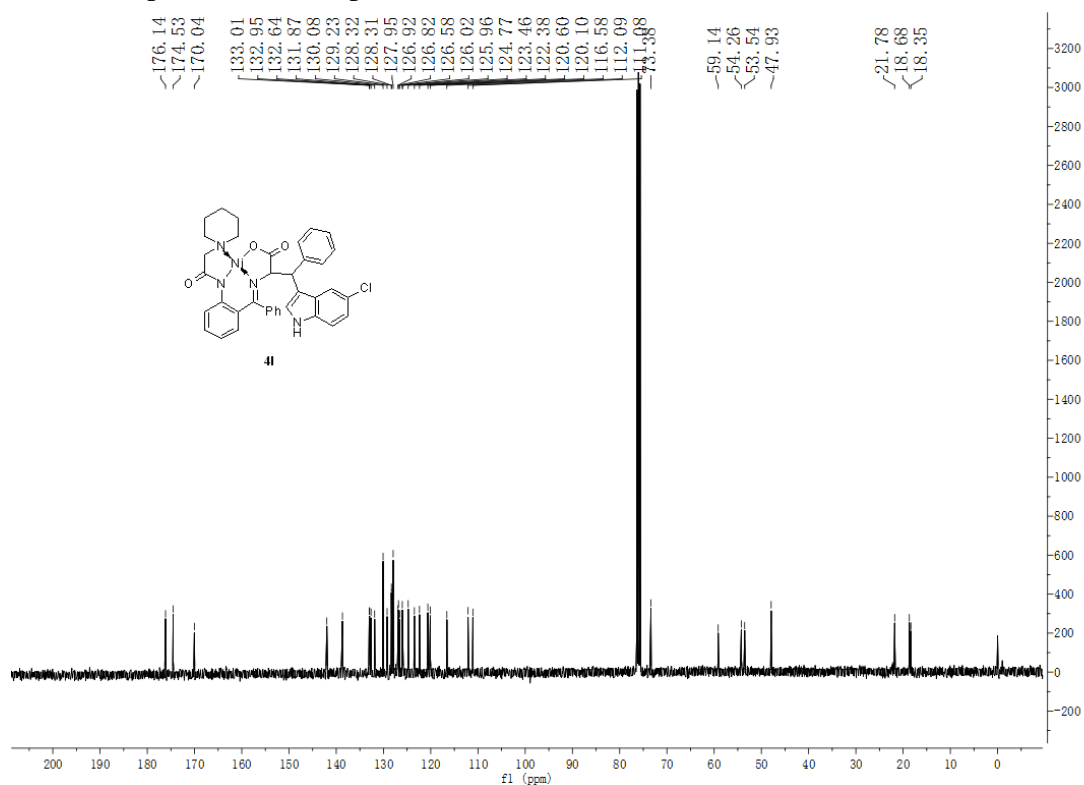
¹³C NMR spectrum of compound **4k**



¹HNMR spectrum of compound **4l**



¹³CNMR spectrum of compound **4l**



Chemical structure of **4m** is shown above the spectrum. The structure is a complex molecule featuring a piperidine ring, a benzodioxole system, a phenyl group, and a fluorinated benzimidazole moiety.

¹H NMR spectrum (CDCl₃) of compound **4m**. The x-axis represents the chemical shift in ppm (f1), ranging from 0.0 to 10.0. The y-axis represents the intensity. The spectrum shows several peaks, with integrations provided below the baseline.

Peak list (ppm) and integration values:

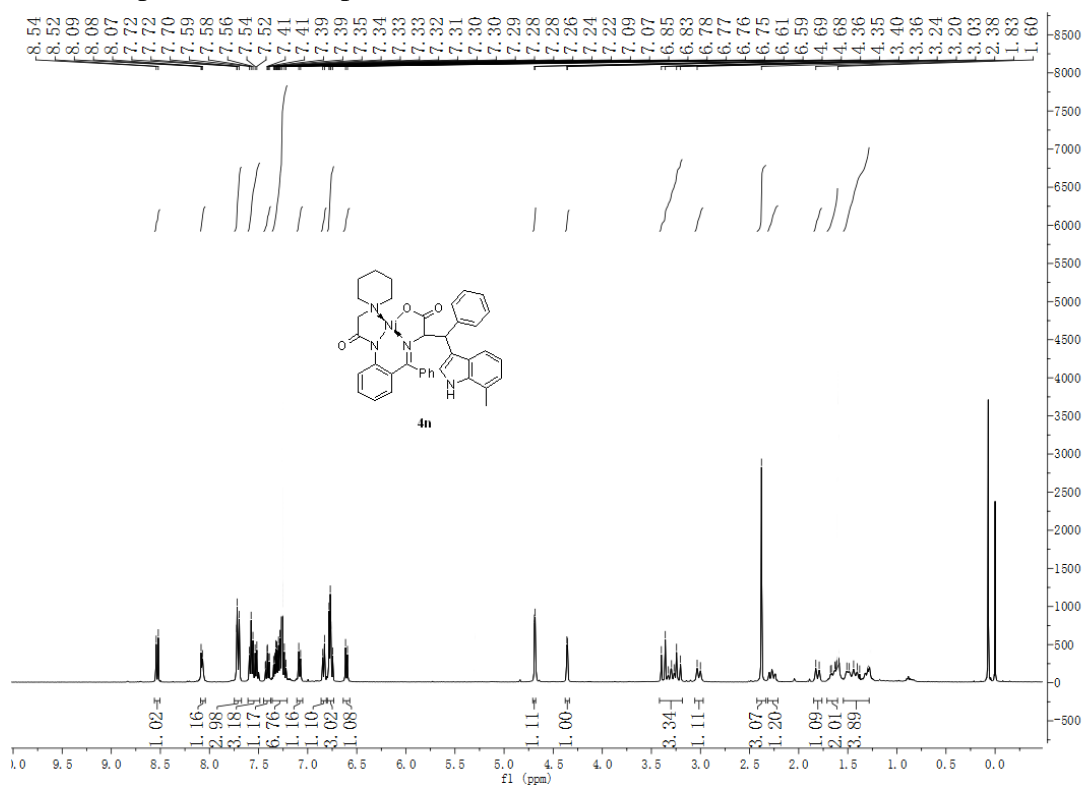
Chemical Shift (ppm)	Integration
9.01	0.99
8.53	1.06
8.51	
7.65	
7.64	
7.63	
7.53	
7.52	
7.51	
7.41	
7.39	
7.37	
7.34	
7.33	
7.32	
7.31	
7.30	
7.29	
7.27	
7.26	
7.08	
7.06	
6.86	
6.86	
6.84	
6.83	
6.78	
6.77	
6.77	
6.56	
6.56	
6.54	
6.53	
6.44	
6.43	
6.42	
6.41	
4.70	
4.69	
4.32	
4.32	
4.32	
3.40	
3.36	
3.31	
3.25	
3.21	
3.03	
1.90	
1.43	
1.33	

Chemical structure of **4m** is shown above the spectrum.

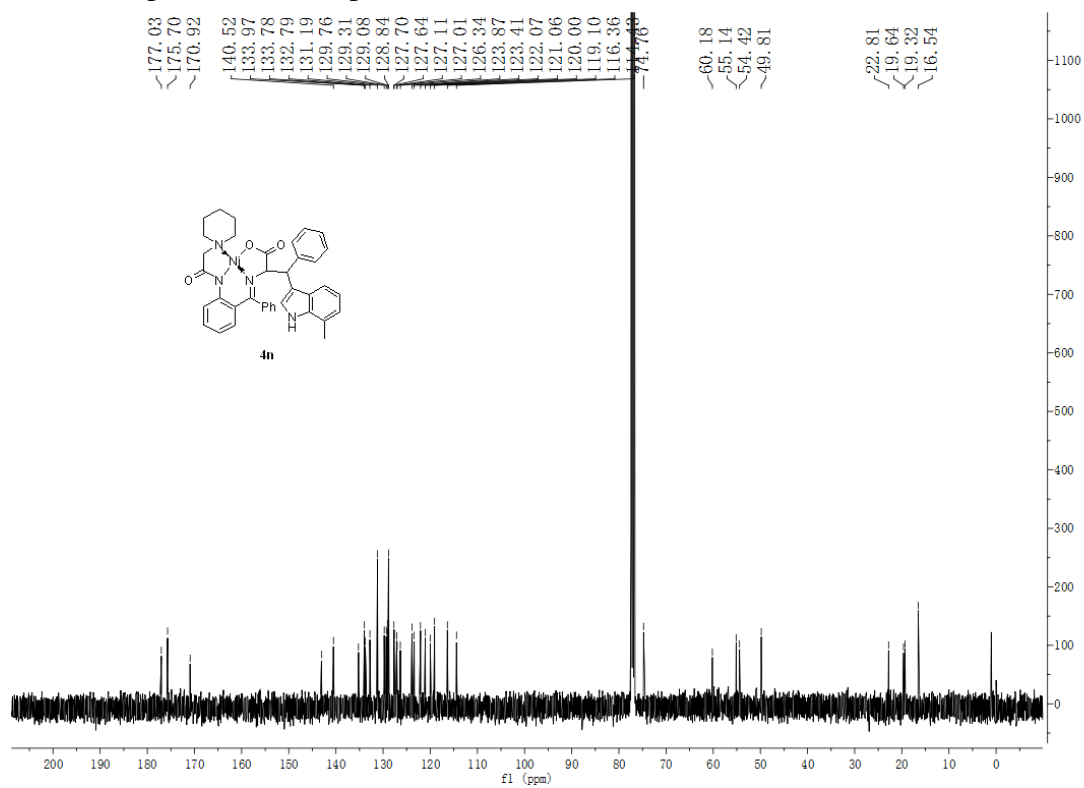
¹³C NMR peaks (ppm):

- 176.18
- 174.59
- 169.97
- 141.97
- 138.96
- 132.96
- 132.72
- 131.85
- 130.10
- 128.80
- 128.28
- 128.21
- 127.88
- 126.81
- 126.18
- 125.96
- 122.36
- 120.10
- 96.51
- 96.26
- 73.55
- 59.13
- 54.26
- 53.53
- 48.51
- 21.77
- 18.60
- 18.34

¹HNMR spectrum of compound **4n**



¹³CNMR spectrum of compound **4n**



¹H NMR spectrum of compound **5a**

