Supporting information

Synthesis of Non-Precious Metal Complexes (Al, Mg, Zn) and Their Catalytic Application in Isocyanate Reduction

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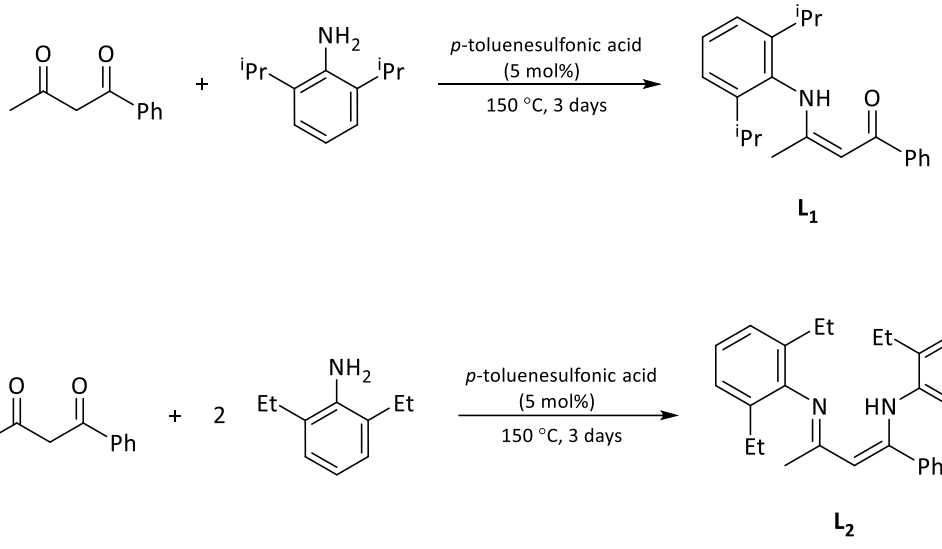
1. General considerations

All manipulations were carried out under a purified nitrogen atmosphere using Schlenk techniques or inside an Etelux Lab 2000 glove box. All solvents were refluxed over the appropriate drying agent and distilled prior to use. Commercially available chemicals were purchased from J&K chemical or Aldrich and used as received. ^{1}H, ^{11}B and ^{13}C NMR spectra were recorded with a Bruker Avance III 400 MHz spectrometer. The LC-MS was performed on Agilent Q-TOF 6520 instrument. The elemental analyses were performed by the Analytical Instrumentation Center of the Beijing Institute of Technology. Melting points were measured in sealed glass tubes. CCDC-2391561 (**L_2**), 2346291 (**C1**), 2346294 (**C2**), 2346289 (**C3**), 2346280 (**C4**), 2391430 (**C5**), 2391431 (**C6**), and 2391432 (**C7**) contain the supplementary crystallographic data for this paper. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/ data_request/cif.

2. Synthesis of L_1 and L_2

a) Method for preparation of **L_1** and **L_2**



Scheme S2.1 The synthetic route for ligands **L_1** and **L_2**.

Ligand **L_1** was synthesised following a reported procedure.[1] Using a similar approach, the previously unreported ligand **L_2** was prepared. Benzoylacetone (20 mmol) and aniline (40 mmol) were added separately to a solution of dry toluene (50 mL), followed by *p*-toluenesulfonic acid (1 mmol) as a catalyst. The mixture was heated under reflux,

and the water formed was removed azeotropically using a Dean-Stark apparatus for 3 days. After evaporating the toluene, a yellow solid or oil was obtained. The crude product was purified by recrystallisation from ethanol, yielding a light yellow or yellow solid, which was subsequently characterised as ligand **L_2** (yield: 5.3 g, 62%, m.p. 132-133 °C).

^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 12.48 (s, 1H, N*H*), 7.26-6.95 (m, 11H, Ar*H*), 5.13 (s, 1H, *γ*-C*H*), 2.72 (dd, 2H, C*H*$_2$CH$_3$), 2.66-2.58 (m, 2H, C*H*$_2$CH$_3$), 2.52-2.39 (m, 4H, C*H*$_2$CH$_3$), 1.80 (s, 3H, C*H*$_3$), 1.20-1.09 (dt, 12H, CH$_2$C*H*$_3$).

^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 163.4, 158.2, 143.9, 138.9, 137.7, 136.9, 134.6, 127.2, 126.8, 126.6, 124.8, 124.7, 124.0, 122.8, 94.9, 23.8, 23.6, 20.3, 13.3, 13.3.

MS (ESI-TOF): m/z [M+H]$^+$ calcd for $C_{30}H_{36}N_2H^+$: 425.2951; found: 425.2974.

Elemental analysis (%) for $C_{30}H_{36}N_2$: Calcd C 84.85 H 8.55 N 6.60; Found C 84.80 H 8.49 N 6.71.

b) ^{1}H and ^{13}C NMR spectra of **L_2**

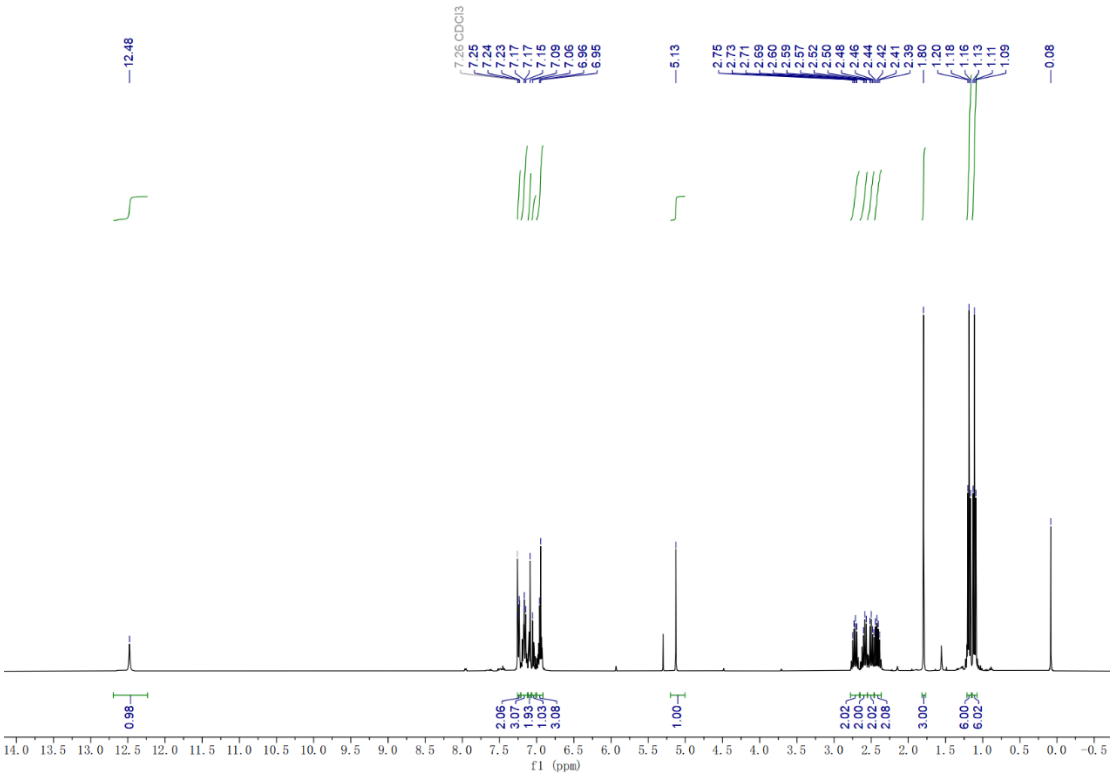


Figure S2.1 ^{1}H NMR spectrum of **L_2** in $CDCl_3$ at 400 MHz.

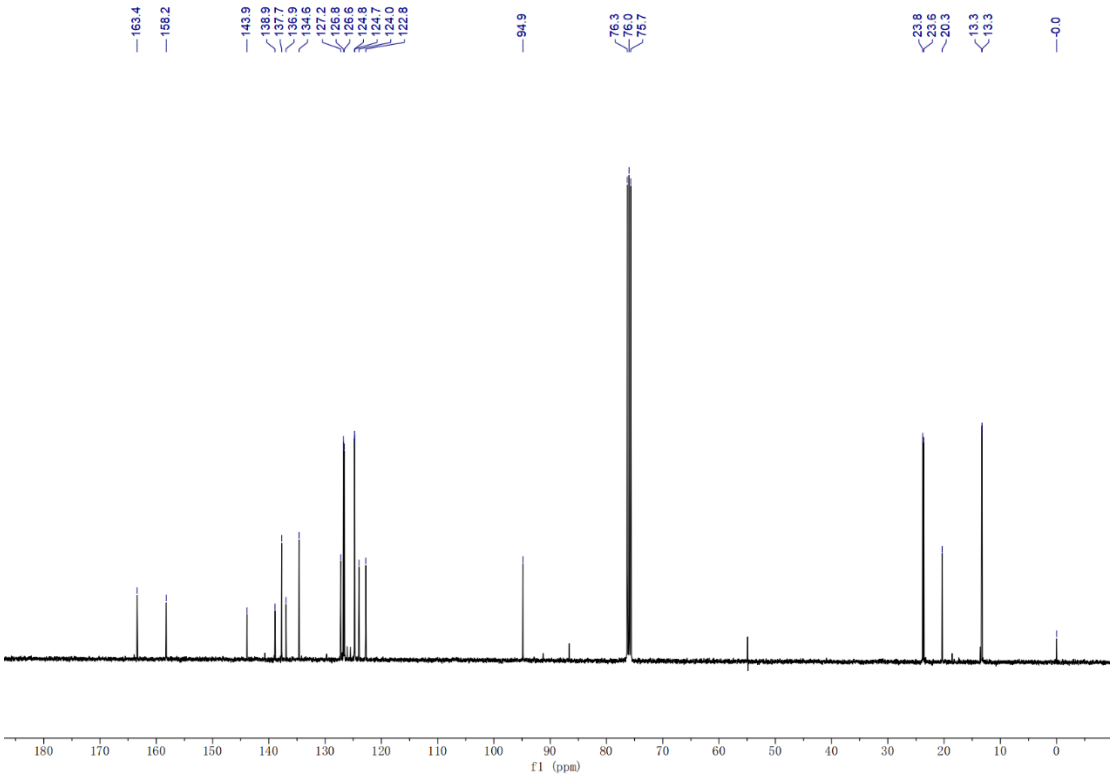


Figure S2.2 ^{13}C NMR spectrum of **L_2** in $CDCl_3$ at 101 MHz.

c) Single crystal X-ray structure and refinement

Single crystals of **L_2** was grown from ethanol as colorless blocks. The crystal data of **L_2** was collected on a Rigaku Oxford diffractometer. Selected data collection parameters and other crystallographic results are summarized in **Table S2.1**. Structure solution by direct methods was achieved through the use of the SHELXT program, and the structural model refined by full-matrix least-squares on F2 using SHELXL by using the Olex2 software.[2-4] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

Table S2.1 Crystal data and structure refinement for **L_2**.

Identification code	**L_2**
CCDC	2391561
Empirical formula	$C_{30}H_{36}N_2$
Formula weight	424.61
Temperature/K	149.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.7141(3)
b/Å	11.4036(4)
c/Å	13.3428(5)
α/°	101.310(3)
β/°	106.109(3)
γ/°	98.704(3)
Volume/Å^3	1218.95(8)
Z	2
ρ_{calc}g/cm^3	1.160
μ/mm^{-1}	0.067
F(000)	462.0
Crystal size/mm^3	0.2 × 0.18 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.308 to 61.314
Index ranges	-12 ≤ h ≤ 10, -14 ≤ k ≤ 16, -18 ≤ l ≤ 17
Reflections collected	18585
Independent reflections	5913 [R_{int} = 0.0220, R_{sigma} = 0.0247]
Data/restraints/parameters	5913/0/298
Goodness-of-fit on F^2	1.097
Final R indexes [I>=2σ (I)]	R_1 = 0.0511, wR_2 = 0.1333
Final R indexes [all data]	R_1 = 0.0642, wR_2 = 0.1408
Largest diff. peak/hole / e Å^{-3}	0.52/-0.53

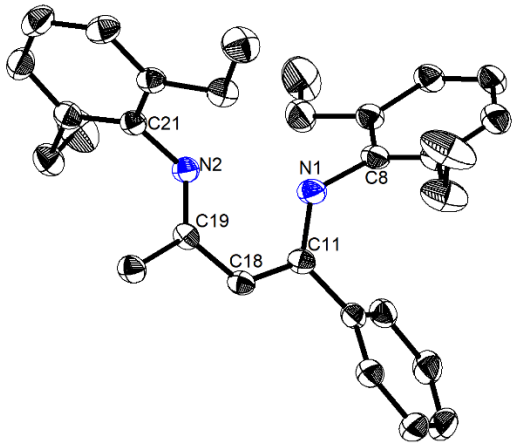


Figure S2.3 Molecular structure of $\mathbf{L_2}$. Thermal ellipsoids are drawn at the 50% level and the hydrogen atoms are omitted for clarity.

3. Synthesis of C1-C7

a) Method for preparation of **C1-C7**

Synthesis of C1. $ZnEt_2$ (1 M in toluene, 2 mL, 2 mmol) was added to a solution of $\mathbf{L_1}$ (2 mmol) in toluene (5 mL) at 0 °C. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. Upon completion of the reaction, a large quantity of pale yellow solid **C1** was obtained (yield: 0.68 g, 82%, m.p. 141-143 °C).

^{1}H NMR (400 MHz, DMSO-d_6, 298K, TMS) δ 7.94 (dd, 4H, Ar*H*), 7.45 – 7.39 (m, 6H, Ar*H*), 7.13 (d, 6H, Ar*H*), 5.82 (s, 2H, *γ*-C*H*), 3.04 (p, 4H, C*H*Me$_2$), 1.71 (d, 6H, C*H*$_3$), 1.11 (dd, 24H, CH*Me*$_2$), 0.80 (t, 6H, CH$_2$*Me*), -0.29 (q, 4H, C*H*$_2$Me).

^{13}C NMR (101 MHz, DMSO-d_6, 298K, TMS) δ 177.5, 173.5, 147.7, 146.3, 143.1, 142.7, 131.7, 130.6, 130.3, 129.1, 128.7, 127.3, 125.9, 125.5, 95.7, 30.4, 29.3, 26.3, 26.0, 25.3, 24.5, 14.8, -0.5.

MS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{48}H_{62}N_2O_2Zn_2H^+$: 829.3436; found: 829.3408.

Elemental analysis (%) for $C_{48}H_{62}N_2O_2Zn_2$: Calcd C 69.48 H 7.53 N 3.38; Found C 69.37 H 7.71 N 3.29.

Synthesis of C2. $MgBu_2$ (1 M in toluene, 2 mL, 2 mmol) was added to a solution of $\mathbf{L_1}$ (2 mmol) in toluene (5 mL) at 0 °C. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. Upon completion of the reaction, a large quantity of pale yellow solid **C2** was obtained (yield: 0.63 g, 79%, m.p.

174-175 °C).

^{1}H NMR (400 MHz, Acetonitrile-d_3, 298K, TMS) δ 7.26 – 7.14 (m, 8H, Ar*H*), 7.10 (t, 4H, Ar*H*), 6.96 – 6.89 (m, 4H, Ar*H*), 5.65 (s, 2H, *γ*-C*H*), 3.13 (p, 4H, C*H*Me$_2$), 1.63 (s, 6H, C*H*$_3$), 1.37 – 1.22 (m, 8H, CH$_2$C*H*$_2$C*H*$_2$CH$_3$), 1.17 (d, 12H, CH*Me*$_2$), 1.12 (s, 4H, C*H*$_2$CH$_2$CH$_2$CH$_3$), 1.08 (d, 12H, CH*Me*$_2$), 0.91 – 0.87 (m, 6H, CH$_2$CH$_2$CH$_2$C*H*$_3$).

^{13}C NMR (101 MHz, Acetonitrile-d_3, 298K, TMS) δ 175.4, 174.1, 148.6, 141.7, 141.5, 129.2, 127.9, 127.6, 124.7, 123.8, 117.9, 94.3, 65.9, 28.4, 24.5, 24.3, 24.1, 15.2.

MS (ESI-TOF): m/z [M+H]$^+$ calcd for $C_{52}H_{70}N_2O_2Mg_2H^+$: 803.5211; found: 803.5195.

Elemental analysis (%) for $C_{52}H_{70}N_2O_2Mg_2$: Calcd C 77.71 H 8.78 N 3.49; Found C 77.58 H 8.61 N 3.63.

Synthesis of C3. AlEt$_3$ (1 M in *n*-hexane, 1 mL, 1 mmol) was added to a solution of **L$_1$** (1 mmol) in *n*-hexane (10 mL) at 0 °C. Then, the reaction mixture was allowed to warm to room temperature and stirring was continued for 12 h. The filtrate was concentrated to 5 mL and was stored at -10 °C in a freezer for 3 days to afford compounds **C3**. (yield: 0.27 g, 67%, m.p. 85-87 °C).

^{1}H NMR (400 MHz, CDCl$_3$, 298K, TMS) δ 7.99 (dd, 2H, Ar*H*), 7.50 – 7.44 (m, 3H, Ar*H*), 7.27 (d, 1H, Ar*H*), 7.22 – 7.19 (m, 2H, Ar*H*), 6.08 (s, 1H, *γ*-C*H*), 2.99 (p, 2H, C*H*Me$_2$), 1.92 (s, 3H, C*H*$_3$), 1.25 (d, 6H, CH*Me*$_2$), 1.13 (d, 6H, CH*Me*$_2$), 0.89 (t, 6H, CH$_2$C*H*$_3$), -0.07 (dq, 2H, C*H*$_2$CH$_3$), -0.20 (dq, 2H, C*H*$_2$CH$_3$).

^{13}C NMR (101 MHz, CDCl$_3$, 298K, TMS) δ 175.9, 173.5, 141.8, 138.4, 136.2, 130.1, 127.4, 127.2, 126.3, 126.2, 126.1, 123.2, 122.6, 96.7, 27.5, 26.9, 23.7, 23.6, 23.3, 22.8, 21.7, 7.9, -2.1.

MS (ESI-TOF): m/z [M+H]$^+$ calcd for $C_{26}H_{36}AlNOH^+$: 406.2685; found: 406.2660.

Elemental analysis (%) for $C_{26}H_{36}AlNO$: Calcd C 77.00 H 8.95 N 3.45; Found C 77.08 H 8.81 N 3.53.

Synthesis of C4. ^{i}Bu$_2$AlH (1 M in *n*-hexane, 1 mL, 1 mmol) was added to a solution of **L$_1$** (1 mmol) in *n*-hexane (10 mL) at 0 °C. Then, the reaction mixture was allowed to warm to room temperature and stirring was continued for 12 h. The filtrate was concentrated to 5 mL and was stored at -10 °C in a freezer for 3 days to afford compounds **C4**. (yield: 0.33 g, 71%, m.p. 87-89 °C).

^{1}H NMR (400 MHz, CDCl$_3$, 298K, TMS) δ 7.98 (dd, 2H, Ar*H*), 7.47 (t, 3H, Ar*H*), 7.33 – 7.26 (m, 1H, Ar*H*), 7.23 – 7.18 (m, 2H, Ar*H*), 6.12 (s, 1H, *γ*-C*H*), 3.00 (p, 2H, C*H*Me$_2$),

1.92 (s, 3H, C*H*$_3$), 1.75 (tt, 2H, CH$_2$C*H*Me$_2$), 1.26 (d, 6H, CH*Me*$_2$), 1.11 (d, 6H, CH*Me*$_2$), 0.89 (d, 6H, CH$_2$CH*Me*$_2$), 0.83 (d, 6H, CH$_2$CH*Me*$_2$), -0.02 (dd, 2H, C*H*$_2$CHMe$_2$), -0.15 (dd, 2H, C*H*$_2$CHMe$_2$).

^{13}C NMR (101 MHz, CDCl$_3$, 298K, TMS) δ 175.7, 173.0, 141.7, 138.7, 136.0, 130.1, 127.4, 126.3, 126.1, 123.2, 96.6, 27.2, 27.0, 26.9, 25.0, 23.8, 23.4, 23.1.

MS (ESI-TOF): m/z [M+H]$^+$ calcd for $C_{30}H_{44}AlNOH^+$: 462.3311; found: 462.3329.

Elemental analysis (%) for $C_{30}H_{44}AlNO$: Calcd C 78.05 H 9.61 N 3.03; Found C 78.21 H 9.47 N 3.24.

Synthesis of C5. AlH$_3$·NMe$_3$ (1 M in toluene, 1 mL, 1 mmol) was added to a solution of **L$_2$** (1 mmol) in *n*-hexane (10 mL) at 0 °C. Then, the reaction mixture was allowed to warm to room temperature and stirring was continued for 12 h. The filtrate was concentrated to 5 mL and was stored at -10 °C in a freezer for 3 days to afford compounds **C5**. (yield: 0.31 g, 68%, m.p. 108-110 °C).

^{1}H NMR (400 MHz, CDCl$_3$, 298K, TMS) δ 7.17 – 7.00 (m, 8H, Ar*H*), 6.96 – 6.85 (m, 3H, Ar*H*), 5.11 (s, 1H, *γ*-C*H*), 2.78 (ddq, 4H, C*H*$_2$CH$_3$), 2.61 – 2.40 (m, 4H, C*H*$_2$CH$_3$), 1.71 (s, 3H, C*H*$_3$), 1.21 (t, 6H, CH$_2$C*H*$_3$), 1.14 (t, 6H, CH$_2$C*H*$_3$).

^{13}C NMR (101 MHz, CDCl$_3$, 298K, TMS) δ 167.0, 169.1, 140.3, 139.8, 138.2, 138.0, 137.8, 127.6, 126.5, 126.3, 125.7, 125.2, 125.1, 124.5, 97.2, 23.0, 22.7, 21.8, 13.2, 13.2.

MS (ESI-TOF): m/z [M+H]$^+$ calcd for $C_{30}H_{37}AlN_2H^+$: 453.2845; found: 453.2854.

Elemental analysis (%) for $C_{30}H_{37}AlN_2$: Calcd C 77.71 H 8.78 N 3.49; Found C 77.58 H 8.61 N 3.63.

Synthesis of C6. AlEt$_3$ (1 M in *n*-hexane, 1 mL, 1 mmol) was added to a solution of **L$_2$** (1 mmol) in *n*-hexane (10 mL) at 0 °C. Then, the reaction mixture was allowed to warm to room temperature and stirring was continued for 12 h. The filtrate was concentrated to 5 mL and was stored at -10 °C in a freezer for 3 days to afford compounds **C6**. (yield: 0.39 g, 44%, m.p. 103-105 °C).

^{1}H NMR (400 MHz, CDCl$_3$, 298K, TMS) δ 7.28 – 7.15 (m, 8H, Ar*H*), 7.09 – 7.00 (m, 3H, Ar*H*), 5.28 (s, 1H, *γ*-C*H*), 2.86 (ddt, 4H, C*H*$_2$CH$_3$), 2.68 (ddt, 4H, C*H*$_2$CH$_3$), 1.89 (s, 3H, C*H*$_3$), 1.35 (t, 6H, CH$_2$C*H*$_3$), 1.24 (t, 6H, CH$_2$C*H*$_3$), 0.80 (t, 6H, AlCH$_2$C*H*$_3$), -0.22 – -0.33 (m, 4H, AlC*H*$_2$CH$_3$).

^{13}C NMR (101 MHz, CDCl$_3$, 298K, TMS) δ 169.7, 169.0, 142.1, 141.3, 138.9, 138.1, 137.8, 127.6, 126.9, 126.4, 125.3, 125.0, 124.6, 124.1, 98.7, 22.9, 22.9, 22.2, 13.3, 12.9,

8.3, -0.0.

MS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{34}H_{45}AlN_2H^+$: 509.3471; found: 509.3455.

Elemental analysis (%) for $C_{34}H_{45}AlN_2$: Calcd C 80.27 H 8.92 N 5.51; Found C 80.04 H 8.77 N 5.64.

Synthesis of C7. $^{i}Bu_2AlH$ (1 M in *n*-hexane, 1 mL, 1 mmol) was added to a solution of **L_2** (1 mmol) in *n*-hexane (10 mL) at 0 °C. Then, the reaction mixture was allowed to warm to room temperature and stirring was continued for 12 h. The filtrate was concentrated to 5 mL and was stored at -10 °C in a freezer for 3 days to afford compounds **C7**. (yield: 0.45 g, 79%, m.p. 134-136 °C).

^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.24 – 7.09 (m, 8H, Ar*H*), 6.99 – 6.90 (m, 3H, Ar*H*), 5.35 (s, 1H, *γ*-C*H*), 2.78 (ddd, 7.6 Hz, 4H, CH_2CH$_3$), 2.63 (ddd, 4H, CH_2CH$_3$), 1.87 (s, 3H, CH_3), 1.67 – 1.55 (m, 2H, C*H*Me$_2$), 1.26 (t, 6H, CH$_2$CH_3), 1.19 (t, 6H, CH$_2$CH_3), 0.68 (dd, 12H, CH$_2$CHMe_2), -0.24 (dd, 4H, CH_2CHMe$_2$).

^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 170.7, 169.7, 144.0, 142.7, 139.9, 138.8, 138.5, 128.8, 128.5, 127.3, 126.1, 125.8, 125.2, 124.9, 100.7, 28.5, 27.9, 26.3, 24.2, 24.2, 23.3, 14.2, 13.8, 3.2.

MS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{38}H_{53}AlN_2H^+$: 565.4097; found: 565.4112.

Elemental analysis (%) for $C_{38}H_{53}AlN_2$: Calcd C 80.81 H 9.46 N 4.96; Found C 80.63 H 9.27 N 5.14.

b) ^{1}H and ^{13}C NMR spectra of **C1-C7**

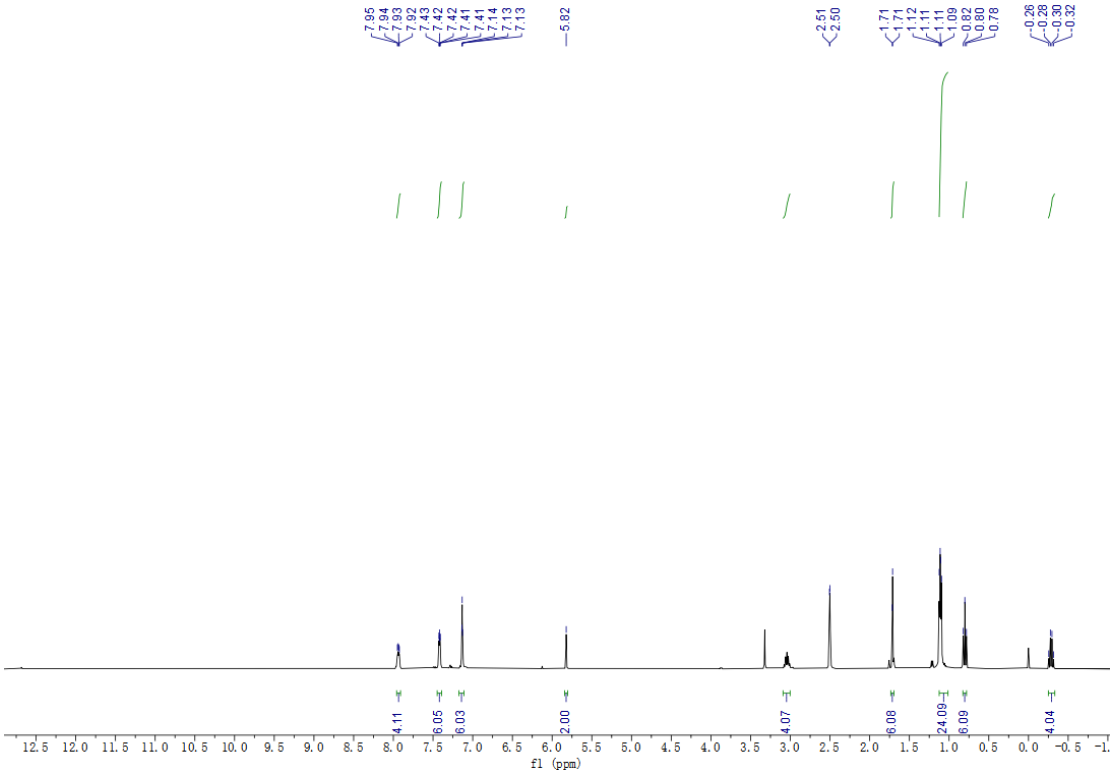


Figure S3.1 ^{1}H NMR spectrum of **C1** in DMSO-d_6 at 400 MHz.

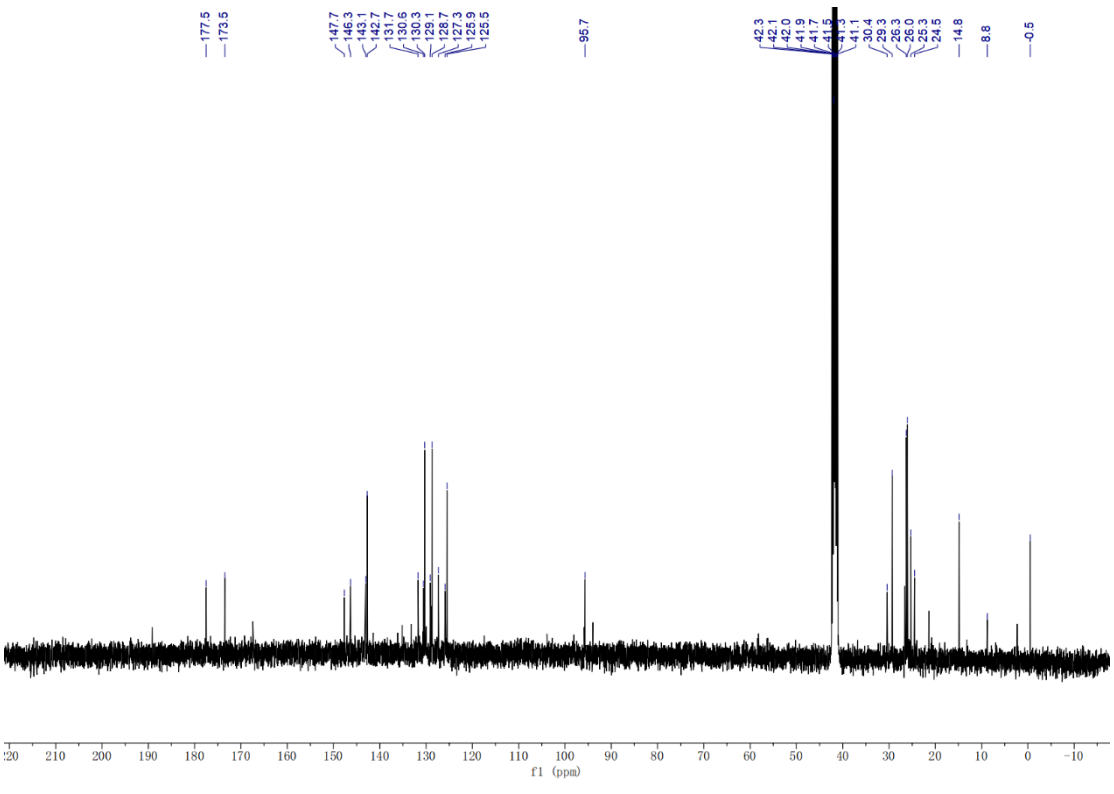


Figure S3.2 ^{13}C NMR spectrum of **C1** in DMSO-d_6 at 101 MHz.

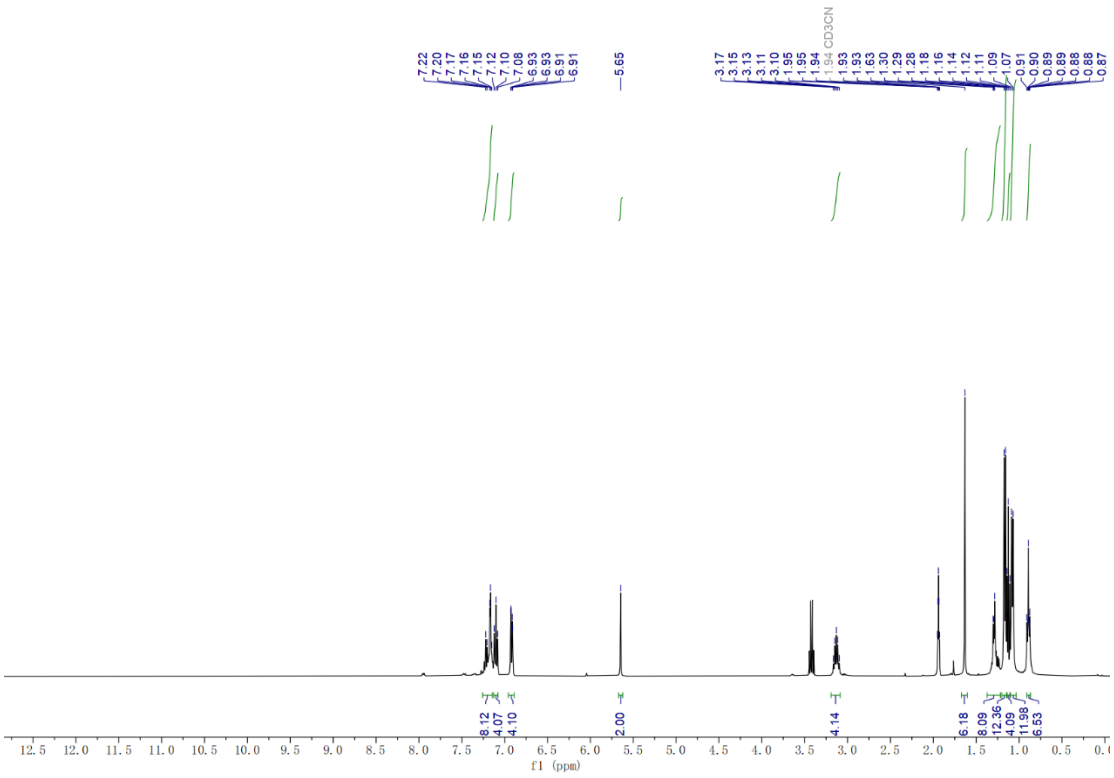


Figure S3.3 ^{1}H NMR spectrum of **C2** in CD_3CN at 400 MHz.

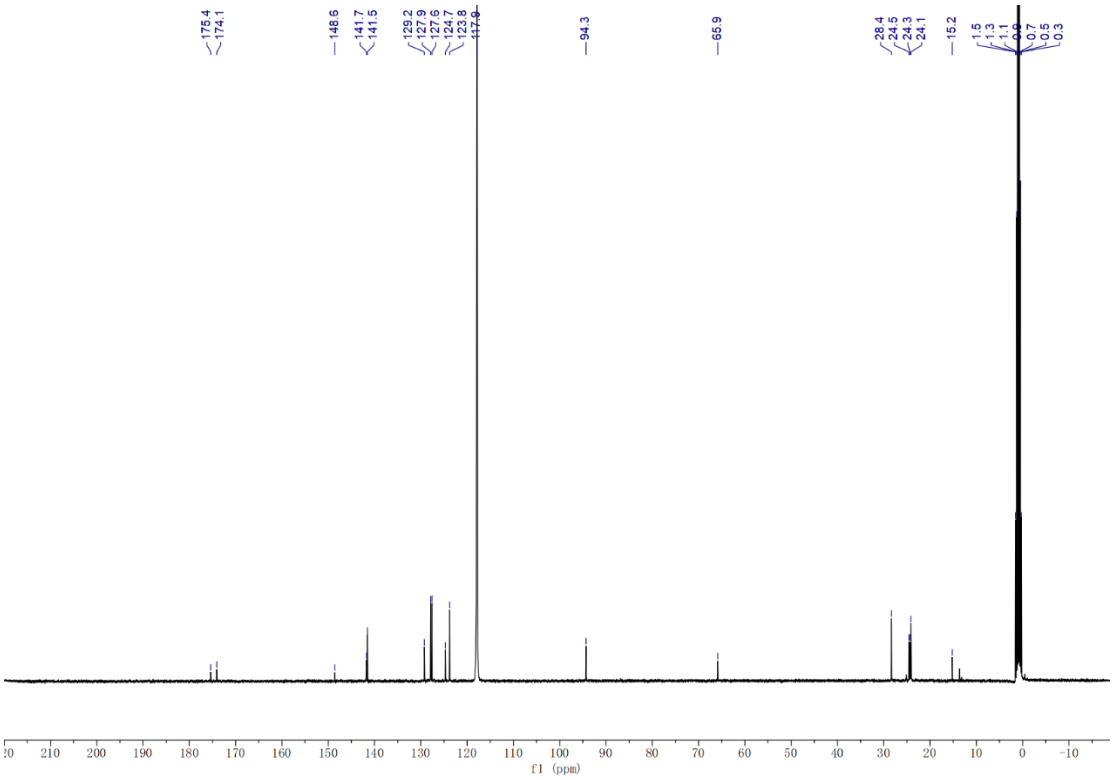


Figure S3.4 ^{13}C NMR spectrum of **C2** in CD_3CN at 101 MHz.

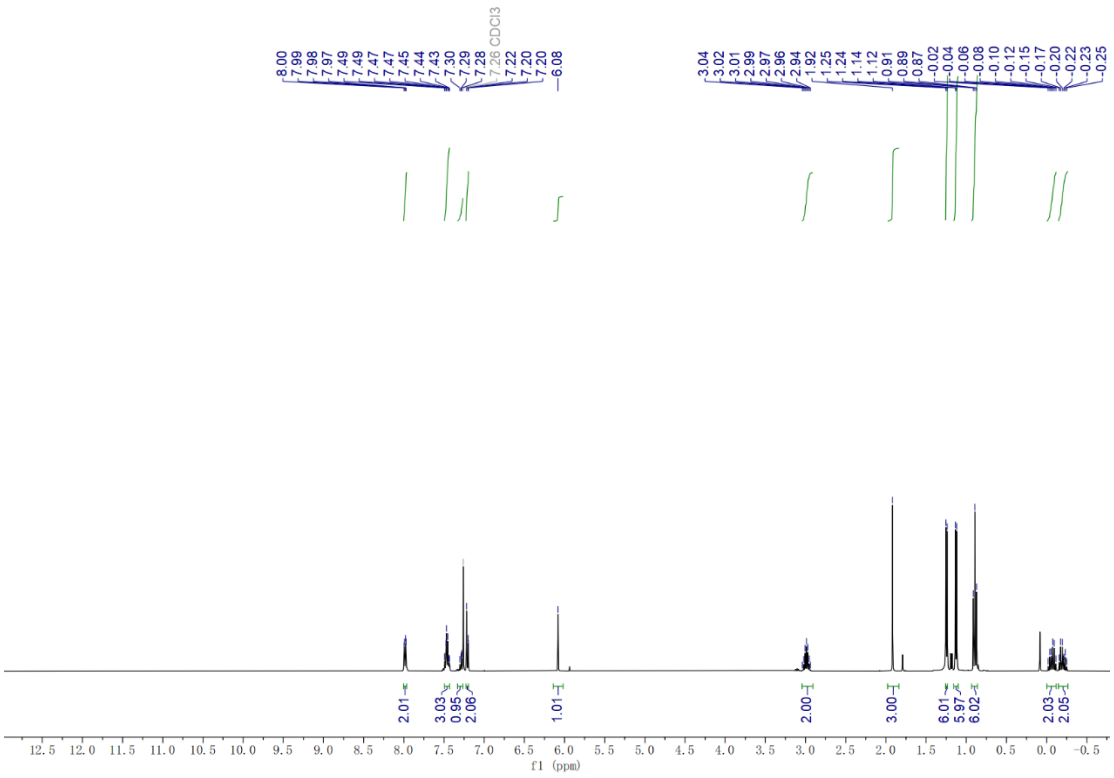


Figure S3.5 ^{1}H NMR spectrum of **C3** in $CDCl_3$ at 400 MHz.

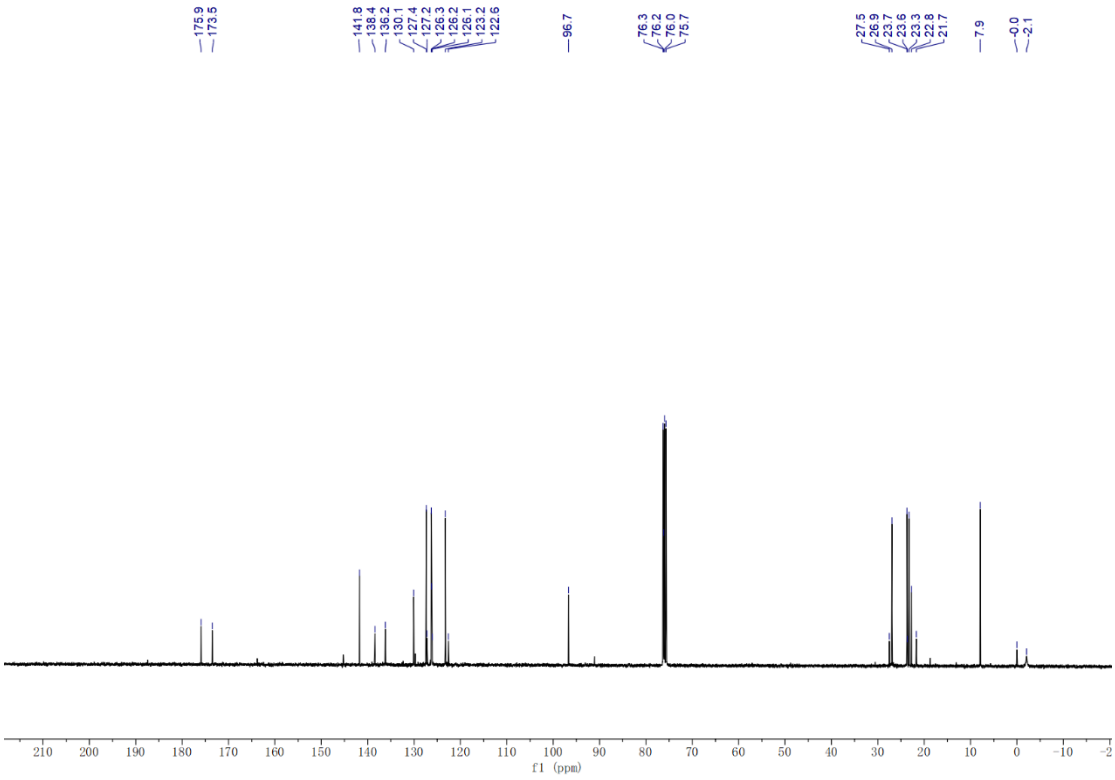


Figure S3.6 ^{13}C NMR spectrum of **C3** in $CDCl_3$ at 101 MHz.

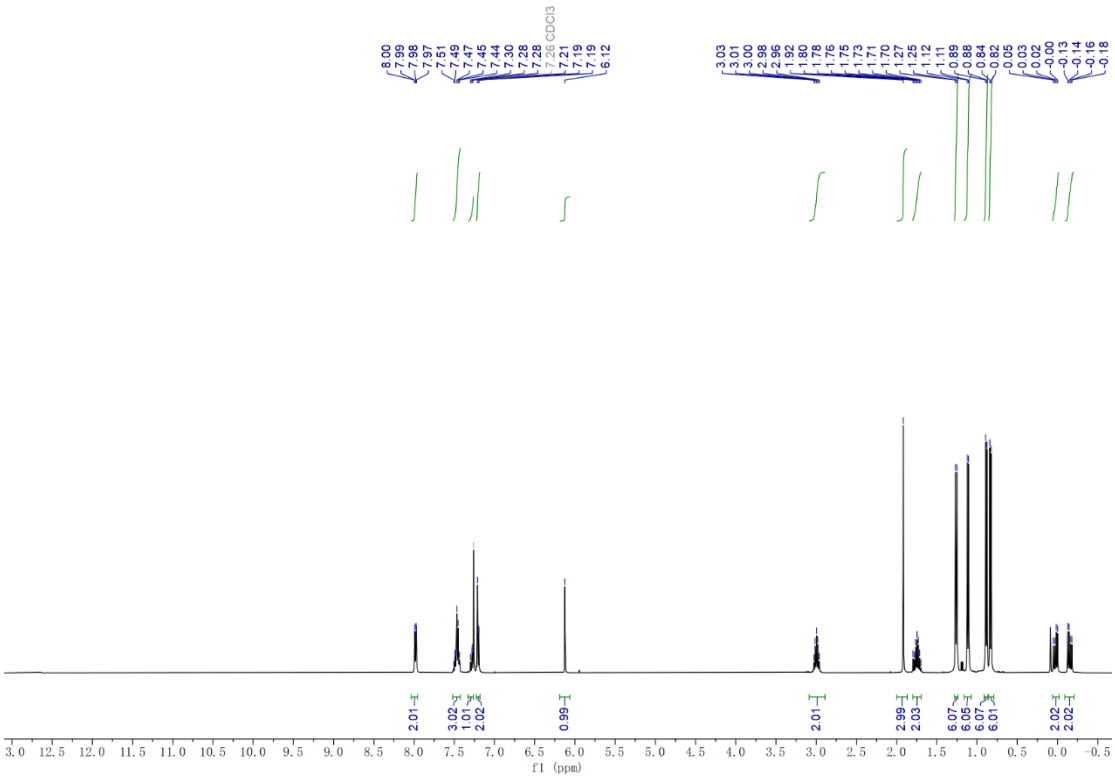


Figure S3.7 ^{1}H NMR spectrum of **C4** in $CDCl_3$ at 400 MHz.

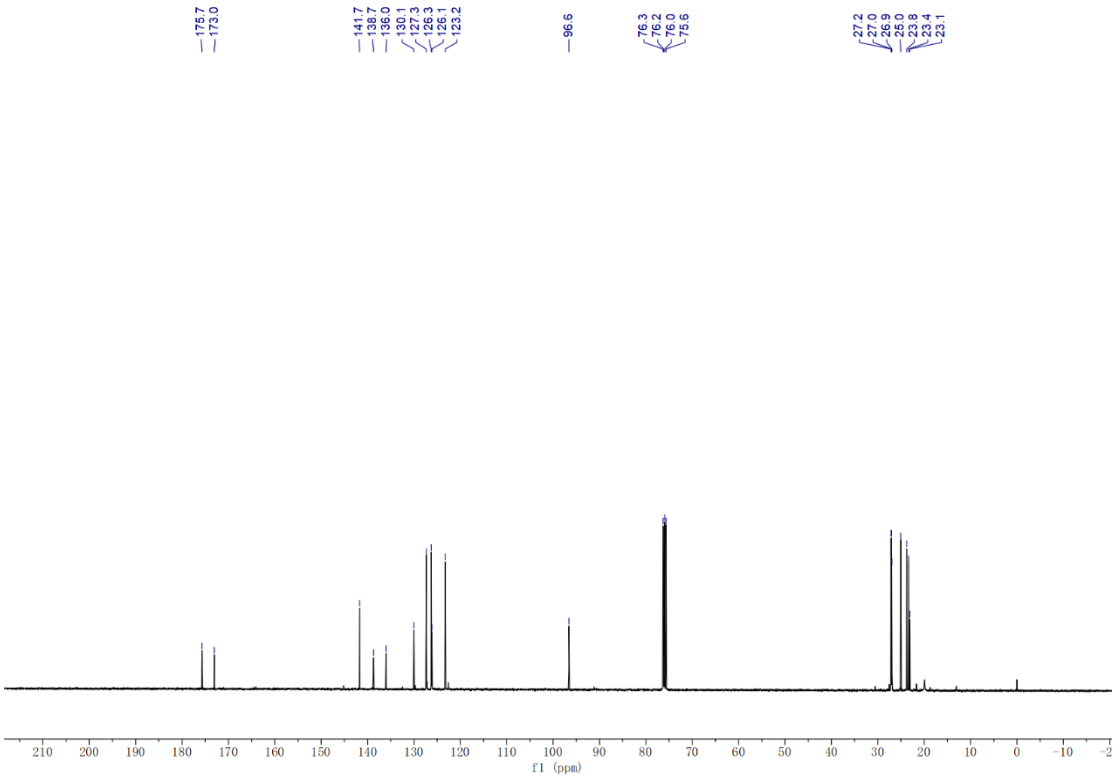


Figure S3.8 ^{13}C NMR spectrum of **C4** in $CDCl_3$ at 101 MHz.

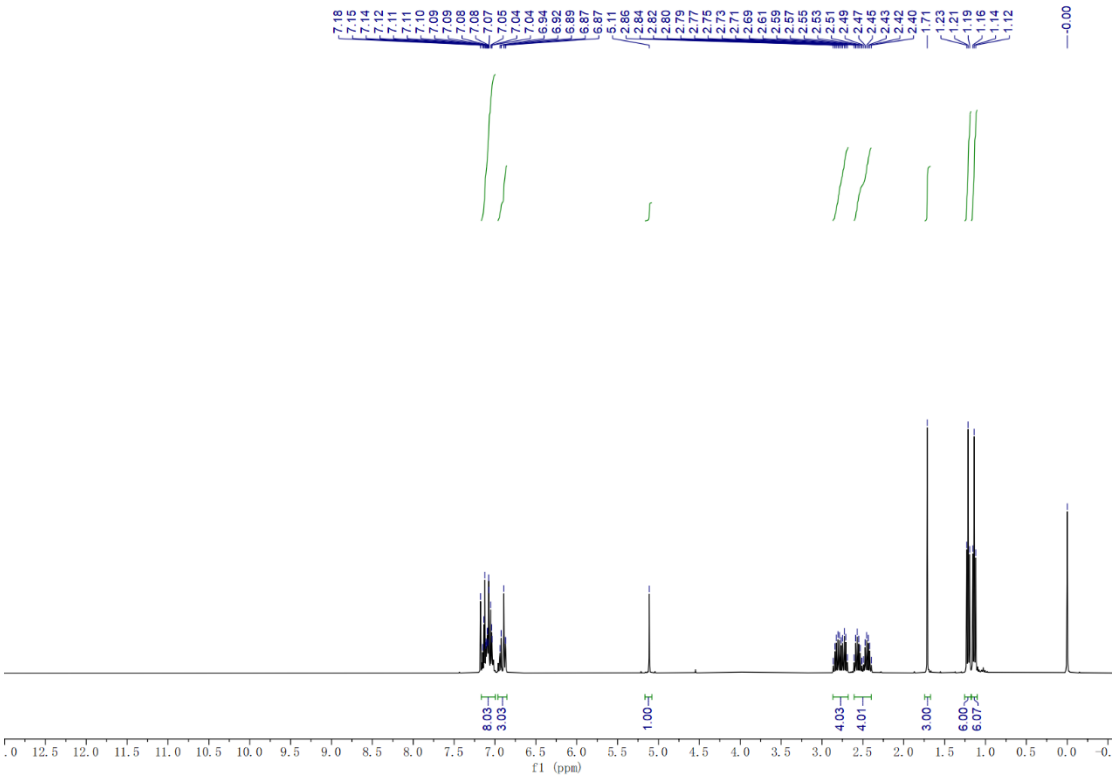


Figure S3.9 ^{1}H NMR spectrum of **C5** in $CDCl_3$ at 400 MHz.

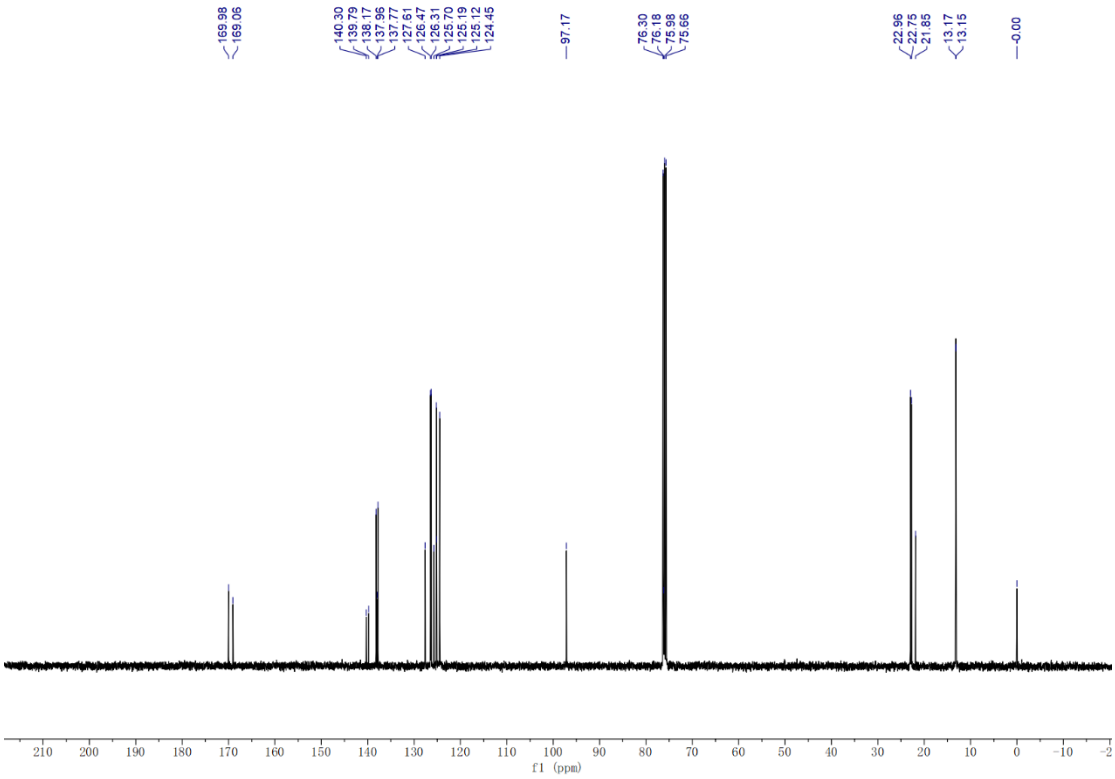


Figure S3.10 ^{13}C NMR spectrum of **C5** in $CDCl_3$ at 101 MHz.

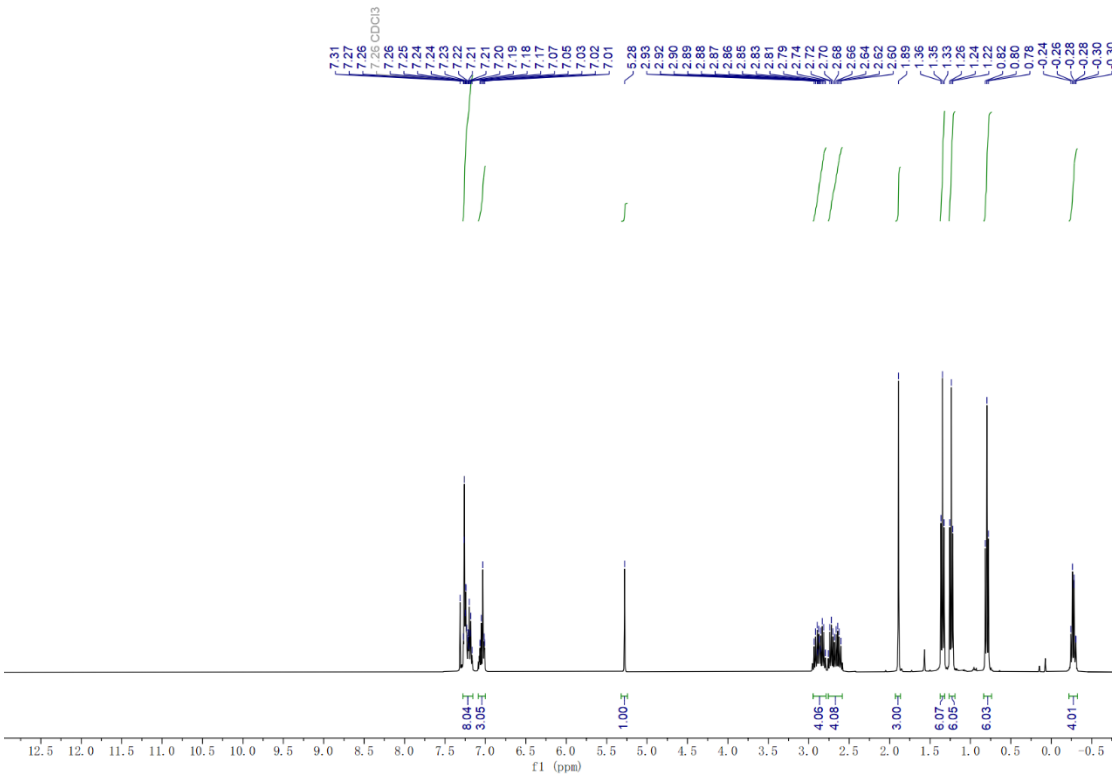


Figure S3.11 ^{1}H NMR spectrum of **C6** in $CDCl_3$ at 400 MHz.

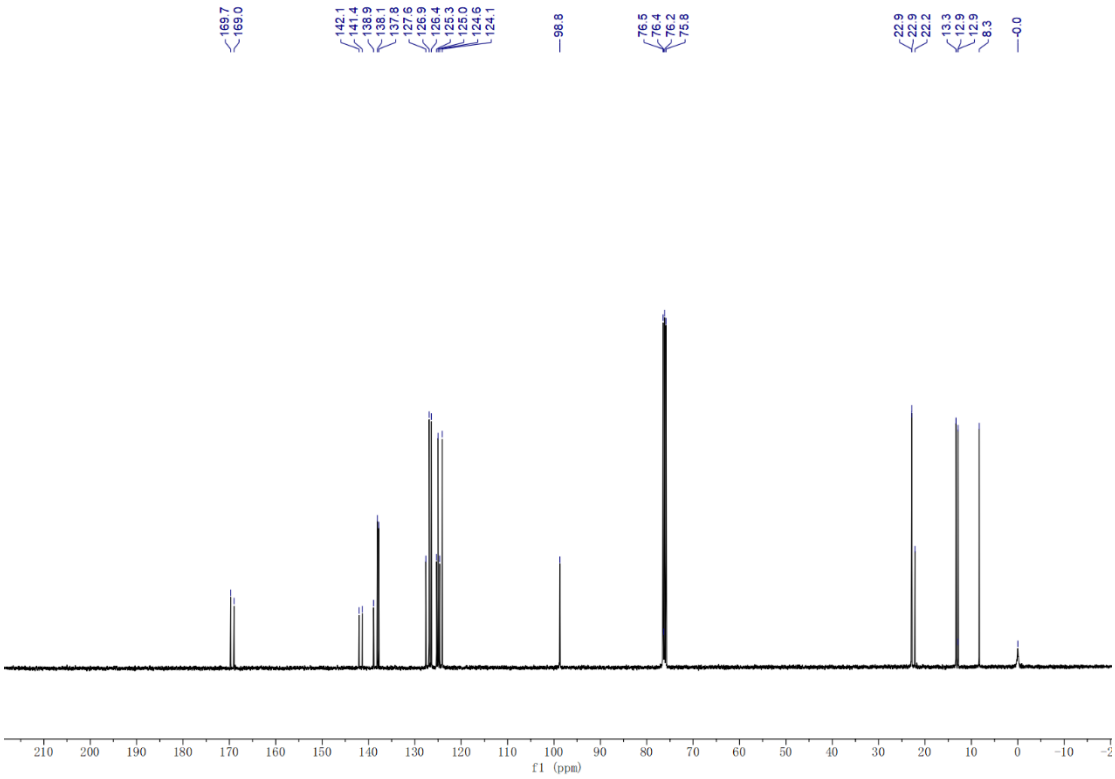


Figure S3.12 ^{13}C NMR spectrum of **C6** in $CDCl_3$ at 101 MHz.

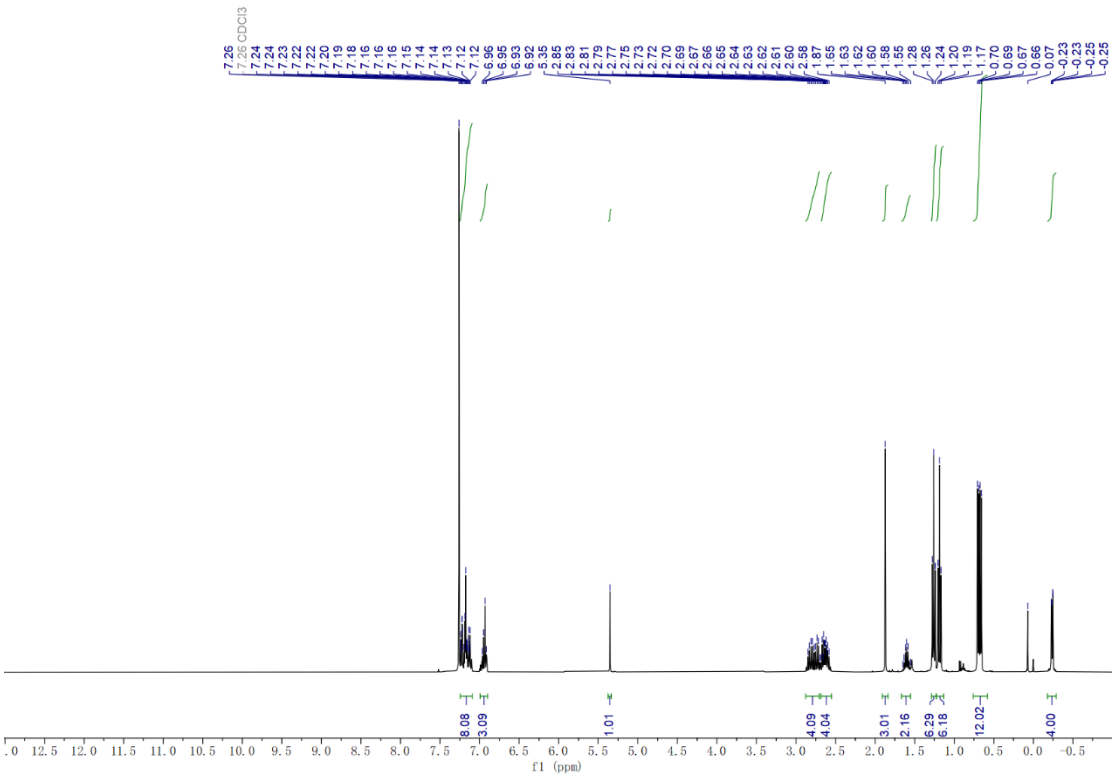


Figure S3.13 ^{1}H NMR spectrum of **C7** in $CDCl_3$ at 400 MHz.

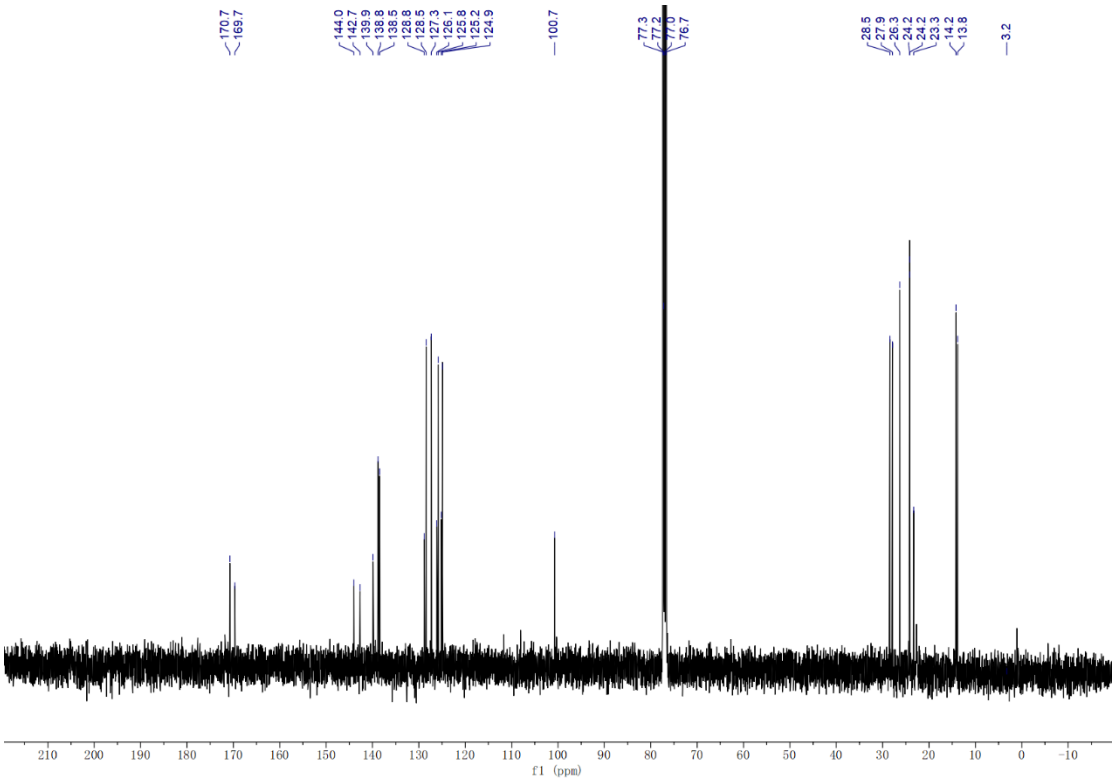


Figure S3.14 ^{13}C NMR spectrum of **C7** in $CDCl_3$ at 101 MHz.

c) Single crystal X-ray structure and refinement

The single-crystal structures of **C1** and **C2** were obtained from the toluene mother liquor, while the single-crystal structures of **C3**–**C7** were obtained from the hexane mother liquor. The crystal data of **C1**–**C7** were collected on a Rigaku Oxford diffractometer. Selected data collection parameters and other crystallographic results are summarized in **Table S3.1**-**S3.3**. Structure solution by direct methods was achieved through the use of the SHELXT program, and the structural model refined by full-matrix least-squares on F2 using SHELXL by using the Olex2 software. All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. The molecular structures of **C2**, **C4**, **C6**, and **C7** are shown in **Figures S3.15–S3.18**.

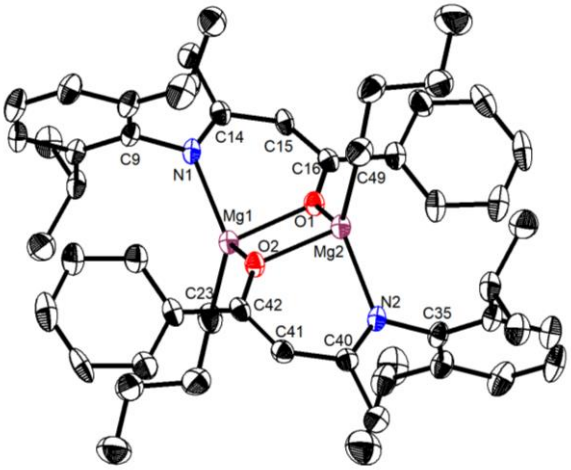


Figure S3.15 Molecular structure of **C2**. Thermal ellipsoids are drawn at the 50% level and the hydrogen atoms are omitted for clarity.

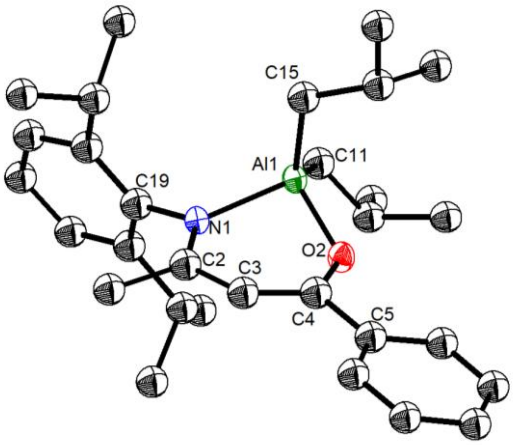


Figure S3.16 Molecular structure of **C4**. Thermal ellipsoids are drawn at the 50% level and the hydrogen atoms are omitted for clarity.

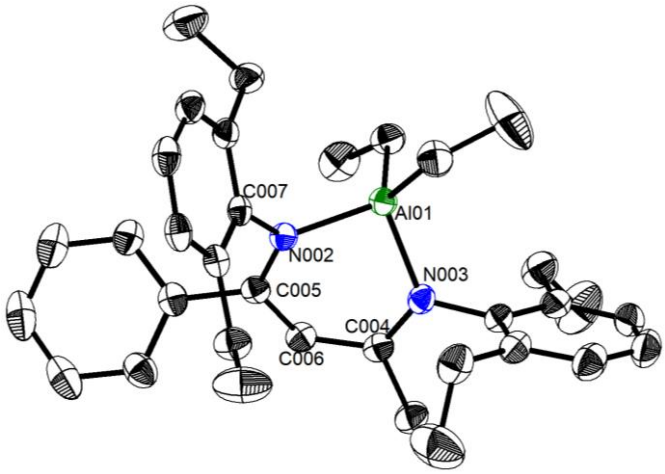


Figure S3.17 Molecular structure of **C6**. Thermal ellipsoids are drawn at the 50% level and the hydrogen atoms are omitted for clarity.

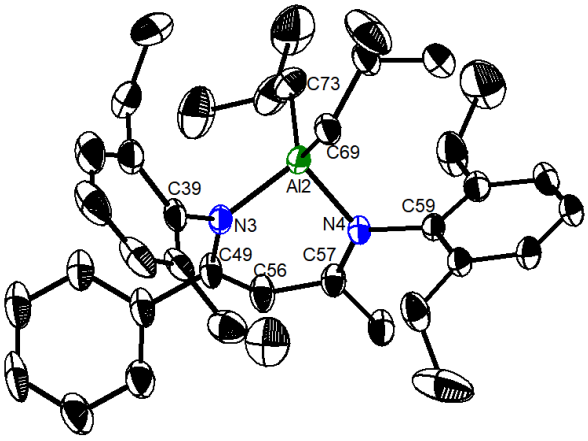


Figure S3.18 Molecular structure of **C7**. Thermal ellipsoids are drawn at the 50% level and the hydrogen atoms are omitted for clarity.

Table S3.1 Crystal data and structure refinement for **C1** and **C2**.

Identification code	**C1**	**C2**
CCDC	2346291	2346294
Empirical formula	$C_{55}H_{70}N_2O_2Zn_2$	$C_{52}H_{70}Mg_2N_2O_2$
Formula weight	921.87	803.72
Temperature/K	180	293(2)
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1$
a/Å	10.769(4)	12.1120(8)
b/Å	11.061(4)	16.5958(6)
c/Å	12.077(4)	13.1981(7)
α/°	102.900(17)	90
β/°	102.818(12)	117.122(8)
γ/°	111.913(15)	90
Volume/Å^3	1224.6(7)	2361.2(3)
Z	1	2
ρ_{calc}g/cm^3	1.25	1.13
μ/mm^{-1}	1.021	0.091
F(000)	490	872
Crystal size/mm^3	0.2 × 0.15 × 0.1	0.2 × 0.15 × 0.1
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.838 to 56.754	4.506 to 49.426
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -16 ≤ l ≤ 16	-14 ≤ h ≤ 12, -19 ≤ k ≤ 19, -15 ≤ l ≤ 15
Reflections collected	19901	10298
Independent reflections	6089 [R_{int} = 0.0339, R_{sigma} = 0.0376]	6555 [R_{int} = 0.0262, R_{sigma} = 0.0396]
Data/restraints/parameters	6089/131/290	6555/1/535
Goodness-of-fit on F^2	1.021	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0334, wR_2 = 0.0782	R_1 = 0.0358, wR_2 = 0.0910
Final R indexes [all data]	R_1 = 0.0464, wR_2 = 0.0840	R_1 = 0.0429, wR_2 = 0.0981
Largest diff. peak/hole / e Å^{-3}	0.58/-0.38	0.23/-0.18

Table S3.2 Crystal data and structure refinement for **C3** and **C4**.

Identification code	**C3**	**C4**
CCDC	2346289	2346280
Empirical formula	$C_{26}H_{36}AlNO$	$C_{30}H_{44}AlNO$
Formula weight	405.54	461.64
Temperature/K	296.15(10)	293(2)
Crystal system	orthorhombic	monoclinic
Space group	$Pca2_1$	$P2_1/c$
a/Å	16.5258(6)	12.0624(4)
b/Å	10.9327(4)	11.8273(3)
c/Å	26.7204(9)	19.8902(6)
α/°	90	90
β/°	90	97.073(3)
γ/°	90	90
Volume/Å^3	4827.6(3)	2816.05(15)
Z	8	4
ρ_{calc}g/cm^3	1.116	1.089
μ/mm^{-1}	0.1	0.093
F(000)	1760	1008
Crystal size/mm^3	0.15 × 0.13 × 0.12	0.14 × 0.12 × 0.08
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.468 to 61.432	4.842 to 61.6
Index ranges	-20 ≤ h ≤ 22, -15 ≤ k ≤ 13, -37 ≤ l ≤ 33	-17 ≤ h ≤ 15, -16 ≤ k ≤ 14, -25 ≤ l ≤ 25
Reflections collected	25532	26836
Independent reflections	10321 [R_{int} = 0.0458, R_{sigma} = 0.0499]	7047 [R_{int} = 0.0765, R_{sigma} = 0.0948]
Data/restraints/parameters	10321/1642/1047	7047/102/338
Goodness-of-fit on F^2	1.059	1.079
Final R indexes [I>=2σ (I)]	R_1 = 0.0621, wR_2 = 0.1740	R_1 = 0.0494, wR_2 = 0.1283
Final R indexes [all data]	R_1 = 0.0761, wR_2 = 0.1921	R_1 = 0.0827, wR_2 = 0.1494
Largest diff. peak/hole / e Å^{-3}	0.39/-0.47	0.36/-0.40

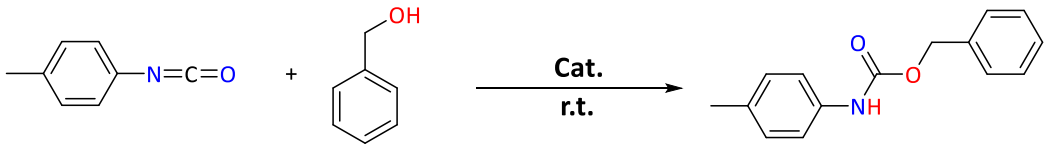
Table S3.3 Crystal data and structure refinement for **C5**-**C7**.

Identification code	**C5**	**C6**	**C7**
CCDC	2391430	2391431	2391432
Empirical formula	$C_{30}H_{37}AlN_2$	$C_{34}H_{45}AlN_2$	$C_{38}H_{53}AlN_2$
Formula weight	452.59	508.7	564.8
Temperature/K	180.00(10)	179.99(10)	150.00(10)
Crystal system	triclinic	monoclinic	triclinic
Space group	P-1	$P2_1/n$	P-1
a/Å	9.8054(3)	10.8620(4)	19.2092(3)
b/Å	11.2462(5)	13.8217(4)	22.2916(3)
c/Å	13.5928(6)	20.2412(6)	27.6966(4)
α/°	75.169(4)	90	109.7630(10)
β/°	79.949(3)	94.796(3)	105.0600(10)
γ/°	67.885(4)	90	100.3750(10)
Volume/Å^3	1337.27(10)	3028.20(17)	10298.8(3)
Z	2	4	12
ρ_{calc}g/cm^3	1.124	1.116	1.093
μ/mm^{-1}	0.095	0.091	0.086
F(000)	488	1104	3696
Crystal size/mm^3	0.15 × 0.15 × 0.1	0.2 × 0.2 × 0.15	0.13 × 0.12 × 0.1
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.87 to 61.98	6.74 to 61.96	6.452 to 61.852
Index ranges	-12 ≤ h ≤ 13, -15 ≤ k ≤ 14, -17 ≤ l ≤ 17	-13 ≤ h ≤ 14, -18 ≤ k ≤ 16, -27 ≤ l ≤ 25	-25 ≤ h ≤ 27, -31 ≤ k ≤ 29, -35 ≤ l ≤ 37
Reflections collected	21063	28814	103030
Independent reflections	6776 [R_{int} = 0.0303, R_{sigma} = 0.0369]	7709 [R_{int} = 0.0450, R_{sigma} = 0.0455]	47555 [R_{int} = 0.0577, R_{sigma} = 0.1005]
Data/restraints/parameters	6776/12/311	7709/0/341	47555/1290/2644
Goodness-of-fit on F^2	1.103	1.062	1.02
Final R indexes [I>=2σ (I)]	R_1 = 0.0639, wR_2 = 0.1784	R_1 = 0.0494, wR_2 = 0.1284	R_1 = 0.0927, wR_2 = 0.2573
Final R indexes [all data]	R_1 = 0.0834, wR_2 = 0.1910	R_1 = 0.0731, wR_2 = 0.1384	R_1 = 0.1283, wR_2 = 0.2825
Largest diff. peak/hole / e Å^{-3}	1.22/-1.22	0.29/-0.23	0.86/-0.52

4. General procedure for the C5-catalyzed hydroalkoxylation of isocyanates

At the outset of the study, the catalytic efficacy of **C1**–**C7** for the hydroalkoxylation of isocyanates was evaluated, as shown in **Table S4.1**. All seven metal compounds demonstrated excellent catalytic performance. Ultimately, **C5** was selected as the catalyst for this reaction due to its high efficiency and performance.

Table S4.1 Optimization of **C1-C7** catalysed hydroalkoxylation of *p*-tolyl isocyanate with phenylmethanol. [a]



1a **2a** **3a**

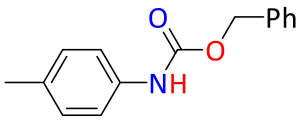
Enrty	Cat.	Loading(mol%)	Sovlent	Time	Yield [b]
1	none	--	neat	12 h	35 %
2	C1	5	neat	30 min	93%
3	C2	5	neat	30 min	94%
4	C3	5	neat	30 min	95%
5	C4	5	neat	30 min	88%
6	C5	5	neat	30 min	95%
7	C6	5	neat	30 min	93%
8	C7	5	neat	30 min	89%
9	C1	2	Hex	30 min	98%
10	C3	2	Hex	30 min	97%
11	**C5**	**2**	**Hex**	**30 min**	**99%**
12	C1	1	Hex	30 min	94%
13	C5	1	Hex	30 min	93%
14	C1	1	Tol	30 min	90%
15	C5	1	Tol	30 min	91%
16	C1	1	Hex	1 h	95%
17	C5	1	Hex	1 h	96%

[a] Reaction conditions: *p*-tolyl isocyanate (**1a**) (1.00 mmol), phenylmethanol (**2a**) (1.05 mmol), and **Cat.** (0.01-0.05 mmol, 1-5 mol%) were reacted at room temperature. [b] Yield determined by ^{1}H NMR spectroscopy based on phenylmethanol consumption; product confirmation was achieved by identifying the N*H* signal.

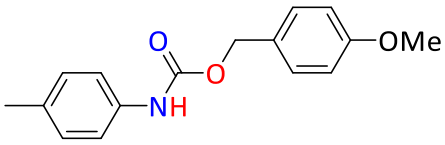
All reactions were carried out under a nitrogen atmosphere. In a 10 mL Schlenk flask

equipped with a magnetic stirring bar, the corresponding isocyanate (1 mmol), alcohol or phenol (1.05 mmol), **C5** (0.02 mmol), and 0.5 mL of hexane were combined and stirred at room temperature. The reaction progress was monitored by ^{1}H NMR and ^{13}C NMR, with the disappearance of the hydroxyl proton and the appearance of new products indicating completion. The crude products of **3a**-**3d**, **3f**, **3g**, **3j**-**3l**, and **3p**-**3r** were washed with *n*-hexane, while the remaining crude products were purified by column chromatography using ethyl acetate/petroleum ether (12:1).

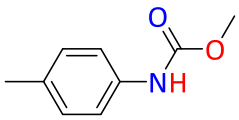
5. NMR data and spectra of carbamate compounds

3a 

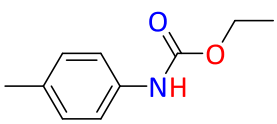
NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.43 – 7.29 (m, 5H, Ar*H*), 7.26 (d, 2H, Ar*H*), 7.10 (d, 2H, Ar*H*), 6.61 (s, 1H, N*H*), 5.19 (s, 2H, CH_2), 2.30 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 153.5, 136.2, 135.2, 133.2, 129.6, 128.6, 128.3, 118.8, 67.0, 20.8.

3b 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.34 (d, 2H, Ar*H*), 7.24 (s, 2H, Ar*H*), 7.10 (d, 2H, Ar*H*), 6.90 (d, 2H, Ar*H*), 6.56 (s, 1H, N*H*), 5.13 (s, 2H, CH_2), 3.81 (s, 3H, OCH_3), 2.30 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 159.9, 135.3, 133.2, 130.3, 130.0, 129.7, 128.4, 118.9, 114.1, 66.9, 55.5, 20.9.

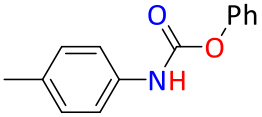
3c 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.31 – 7.21 (m, 2H, Ar*H*), 7.10 (d, 2H, Ar*H*), 6.65 (s, 1H, N*H*), 3.75 (s, 3H, OCH_3), 2.30 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 154.3, 135.4, 133.2, 129.6, 119.0, 52.4, 20.8.

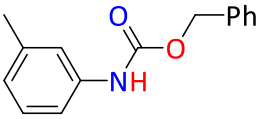
3d 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.17 (dd, 4H, Ar*H*), 6.74 (s, 1H, N*H*), 4.20 (q, 2H, CH_2), 2.29 (s, 3H, CH_3), 1.28 (t, 3H, OCH_3). ^{13}C NMR (101

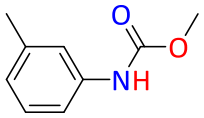
MH, $CDCl_3$, 298K, TMS) δ 153.9, 135.5, 132.9, 129.5, 118.9, 61.1, 20.7, 14.6.

3e 

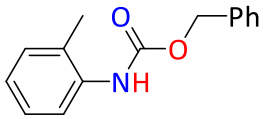
NMR yield 95%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.43 – 7.25 (m, 4H, Ar*H*), 7.24 – 7.10 (m, 5H, Ar*H*), 6.90 (s, 1H, N*H*), 2.31 (s, 3H, CH_3). ^{13}C NMR (101 MH, $CDCl_3$, 298K, TMS) δ 150.8, 134.9, 129.8, 129.7, 129.5, 125.8, 121.8, 119.0, 115.4, 20.9.

3f 

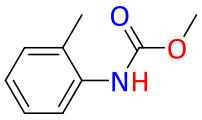
NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.41 – 7.33 (m, 5H, Ar*H*), 7.24 (d, 1H, Ar*H*), 7.19 – 7.12 (m, 2H, Ar*H*), 6.88 (d, 1H, Ar*H*), 6.63 (s, 1H, N*H*), 5.19 (s, 2H, CH_2), 2.32 (s, 3H, CH_3). ^{13}C NMR (101 MH, $CDCl_3$, 298K, TMS) δ 153.5, 139.2, 137.8, 136.2, 129.0, 128.7, 128.5, 128.4, 124.5, 119.5, 115.9, 67.1, 21.6.

3g 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.24 – 7.14 (m, 3H, Ar*H*), 6.88 (d, 1H, Ar*H*), 6.60 (s, 1H, N*H*), 3.77 (s, 3H, OCH_3), 2.33 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 154.2, 139.1, 137.8, 129.0, 124.4, 119.5, 115.9, 52.4, 21.6.

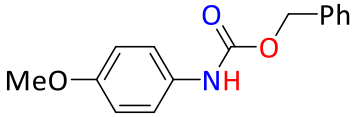
3h 

NMR yield 95%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.39 (ddd, 4.6 Hz, 6H, Ar*H*), 7.23 – 7.14 (m, 2H, Ar*H*), 7.03 (t, 1H, Ar*H*), 6.45 (s, 1H, N*H*), 5.21 (s, 2H, CH_2), 2.24 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 136.24, 135.91, 130.56, 128.78, 128.73, 128.55, 128.53, 128.47, 127.06, 67.26, 17.81.

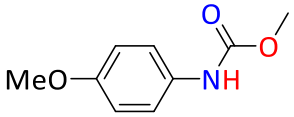
3i 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.77 (s, 1H, Ar*H*), 7.21 (t, 1H, Ar*H*), 7.16 (d, 1H, Ar*H*), 7.03 (t, 1H, Ar*H*), 6.38 (s, 1H, N*H*), 3.78 (s, 3H, OCH_3), 2.25 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 135.8, 130.4, 126.9, 124.2,

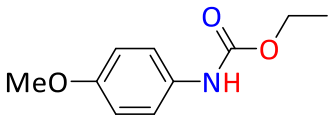
52.4, 17.6.

3j 

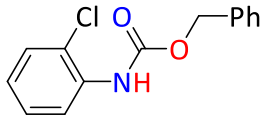
NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.43 – 7.32 (m, 5H, Ar*H*), 7.28 (d, 2H, Ar*H*), 6.88 – 6.81 (m, 2H, Ar*H*), 6.62 (s, 1H, N*H*), 5.18 (s, 2H, CH_2), 3.77 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 156.1, 153.7, 136.2, 130.8, 128.6, 128.3, 120.7, 114.3, 67.0, 55.5.

3k 

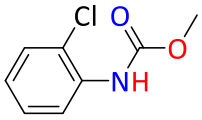
NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.34 – 7.25 (m, 2H, Ar*H*), 6.87 – 6.83 (m, 2H, Ar*H*), 6.54 (s, 1H, N*H*), 3.78 (s, 3H, OCH_3), 3.76 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 156.1, 136.2, 128.6, 128.3, 114.3, 67.0, 55.5.

3l 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.38 – 7.22 (m, 2H, Ar*H*), 6.90 – 6.80 (m, 2H, Ar*H*), 6.51 (s, 1H, N*H*), 4.21 (q, 2H, CH_2CH_3), 3.78 (s, 3H, OCH_3), 1.30 (t, 3H, CH_2CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 156.0, 154.0, 131.0, 120.7, 114.3, 61.1, 55.5, 14.6.

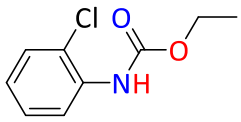
3m 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.19 (d, 1H, Ar*H*), 7.44 – 7.32 (m, 6H, Ar*H*), 7.28 – 7.24 (m, 1H, Ar*H*), 7.21 (s, 1H, N*H*), 6.99 (td, 1H, Ar*H*), 5.22 (s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 153.1, 135.9, 134.8, 129.2, 128.8, 128.6, 128.6, 127.9, 123.9, 122.2, 120.1, 67.5.

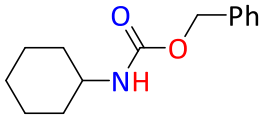
3n 

NMR yield 99%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.15 (d, 1H, Ar*H*), 7.34 (d, 1H, Ar*H*), 7.29 – 7.24 (m, 1H, Ar*H*), 7.15 (s, 1H, N*H*), 6.98 (d, 1H, Ar*H*), 3.80 (s, 3H, OCH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 153.6, 134.7, 129.1, 127.8, 123.7,

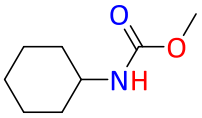
122.1, 119.9, 52.6.

3o 

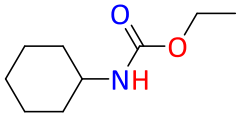
NMR yield 99%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.22 – 8.12 (m, 1H, Ar*H*), 7.30 (dd, 1H, Ar*H*), 7.22 (ddd, 1H, Ar*H*), 7.13 (s, 1H, N*H*), 6.94 (td, 1H, Ar*H*), 4.22 (q, 2H, CH_2CH_3), 1.31 (t, 3H, CH_2CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 153.2, 134.9, 129.0, 127.7, 123.6, 122.0, 112.0, 61.5, 14.5.

3p 

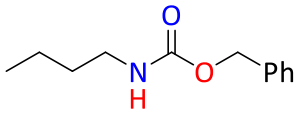
NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.39 – 7.28 (m, 5H, Ar*H*), 5.08 (s, 2H, CH_2), 4.66 (s, 1H, N*H*), 3.50 (d, 1H, NC*H*), 1.93 – 1.07 (m, 10H, Cy*H*). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 155.6, 136.7, 128.5, 128.2, 128.1, 66.5, 49.9, 33.4, 25.5, 24.8.

3q 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 4.55 (s, 1H, N*H*), 3.64 (s, 3H, OCH_3), 3.55 – 3.32 (m, 1H, NC*H*), 1.92 – 1.05 (m, 3H, Cy*H*). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 51.8, 49.8, 33.5, 25.5, 24.8.

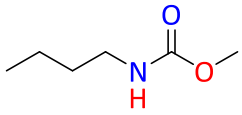
3r 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 4.55 (s, 1H, N*H*), 4.10 (q, 2H, CH_2CH_3), 3.47 (d, 1H, NC*H*), 1.93 – 1.29 (m, 7H, Cy*H*), 1.24 (t, 3H, CH_2CH_3), 1.12 (qd, 3H, Cy*H*). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 155.8, 60.5, 49.7, 33.5, 25.5, 24.8, 14.7.

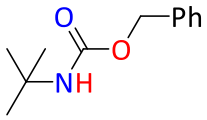
3s 

NMR yield 99%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.36 – 7.23 (m, 5H, Ar*H*), 5.04 (s, 2H, CH_2), 4.82 (d, 1H, N*H*), 3.13 (q, 2H, $CH_2CH_2CH_2CH_3$), 1.47 – 1.38 (m, 2H, $CH_2CH_2CH_2CH_3$), 1.28 (q, 2H, $CH_2CH_2CH_2CH_3$), 0.86 (t, 3H, $CH_2CH_2CH_2CH_3$). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 155.4, 135.7, 127.5, 127.1, 127.0, 65.5, 39.8, 31.0,

18.9, 12.7.

3t 

NMR yield 97%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 4.66 (s, 1H, N*H*), 3.65 (s, 3H, OCH_3), 3.16 (d, 2H, CH_2CH$_2$CH$_2$CH$_3$), 1.51 – 1.43 (m, 2H, CH$_2$CH_2CH$_2$CH$_3$), 1.33 (q, 2H, CH$_2$CH$_2$CH_2CH$_3$), 0.91 (td, 3H, CH$_2$CH$_2$CH$_2$CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 156.1, 50.9, 39.8, 31.1, 18.9, 12.7.

3u 

NMR yield 95%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 7.36 (d, 5H, Ar*H*), 5.06 (s, 2H, CH_2), 4.81 (s, 1H, N*H*), 1.34 (s, 9H, CMe_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 136.8, 128.5, 128.1, 128.0, 66.0, 50.4, 29.0.

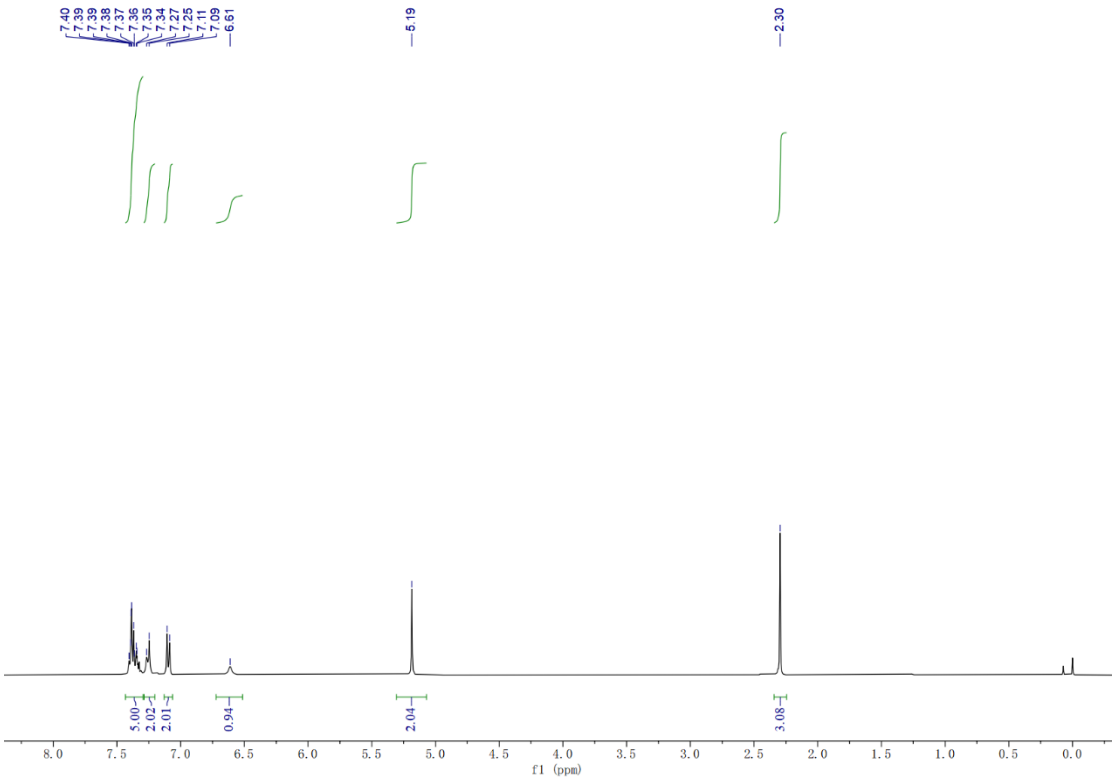


Figure S5.1 ^{1}H NMR spectrum of **3a** in $CDCl_3$ at 400 MHz.

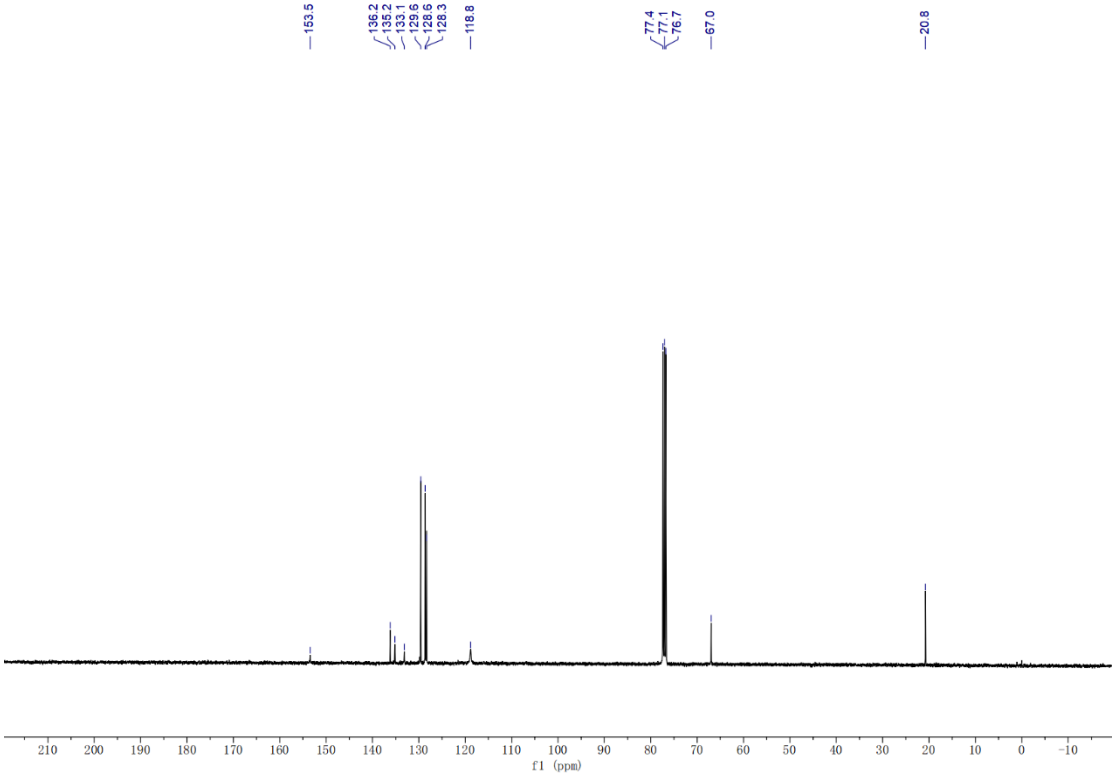


Figure S5.2 ^{13}C NMR spectrum of **3a** in $CDCl_3$ at 101 MHz.

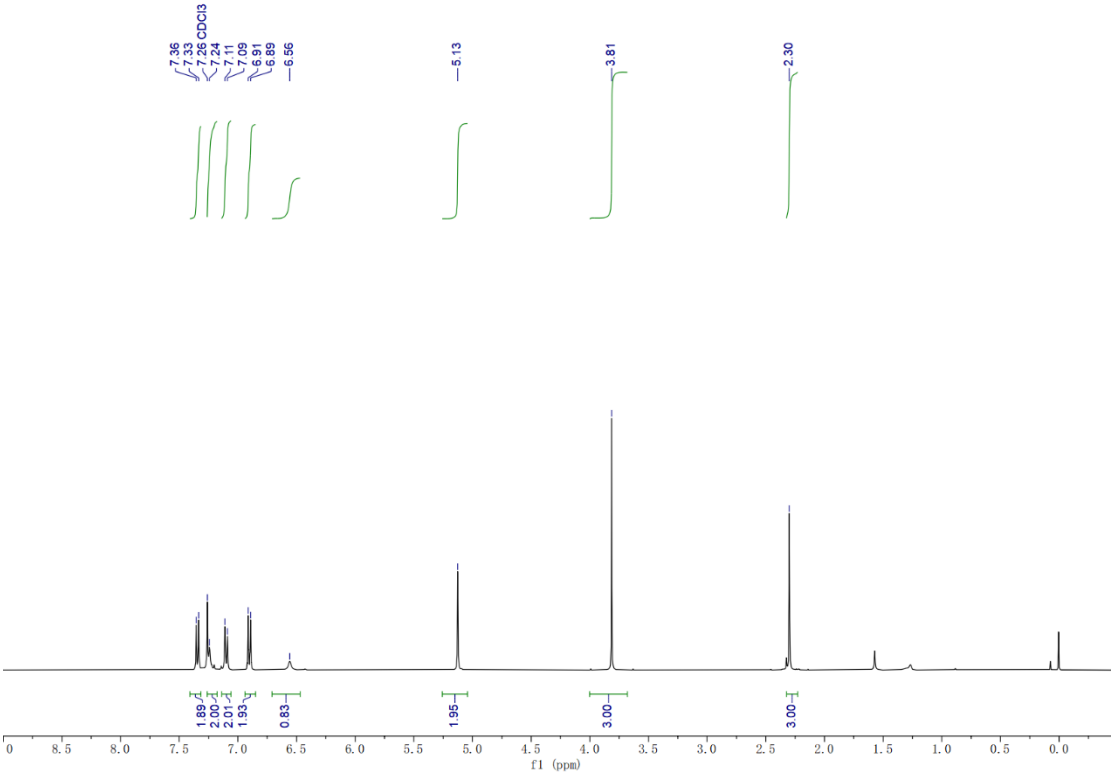


Figure S5.3 ^{1}H NMR spectrum of **3b** in $CDCl_3$ at 400 MHz.

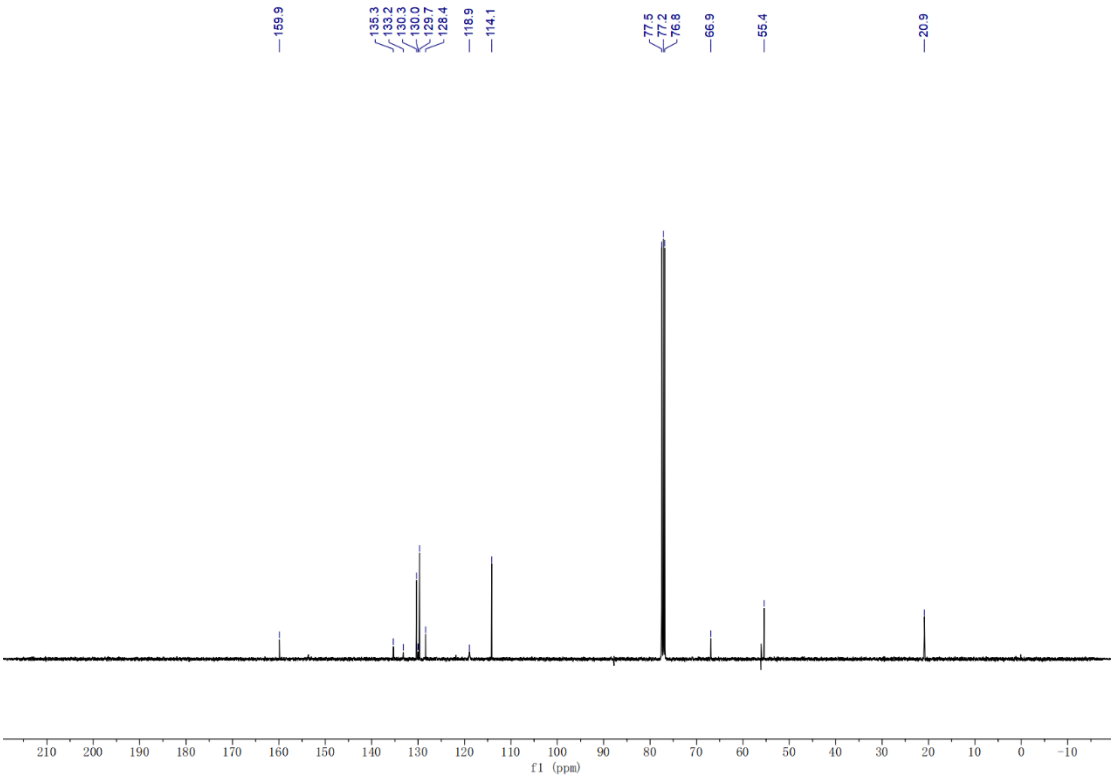


Figure S5.4 ^{13}C NMR spectrum of **3b** in $CDCl_3$ at 101 MHz.

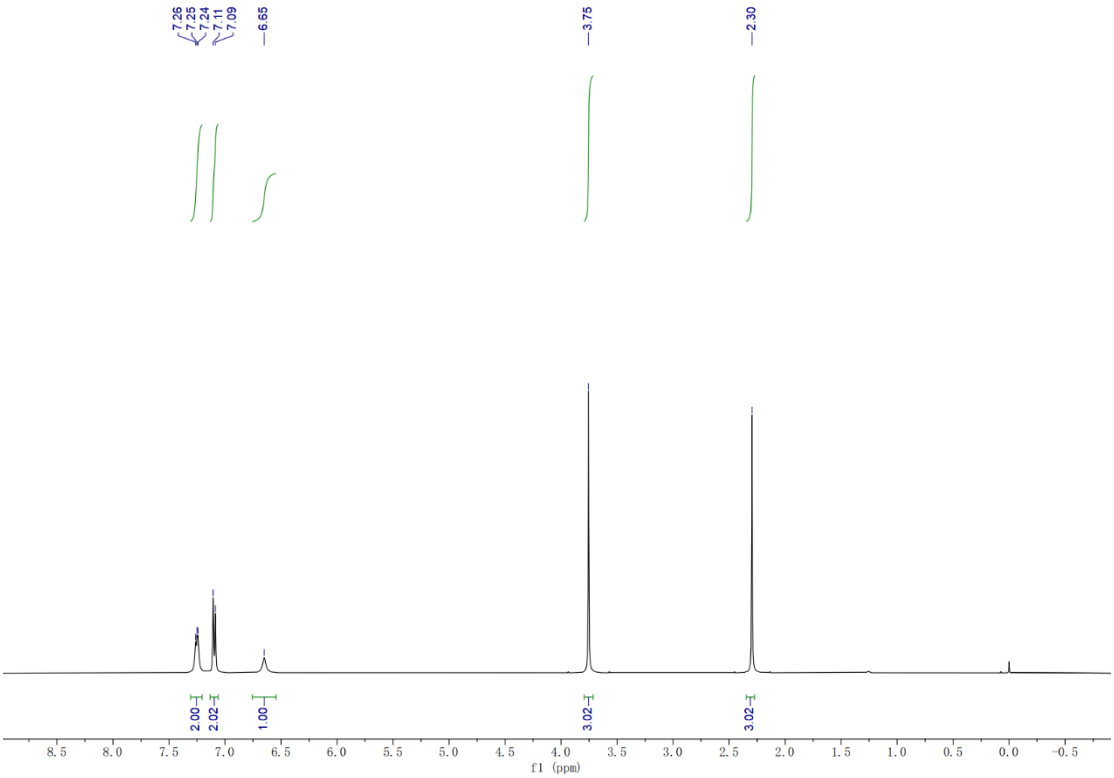


Figure S5.5 ^{1}H NMR spectrum of **3c** in $CDCl_3$ at 400 MHz.

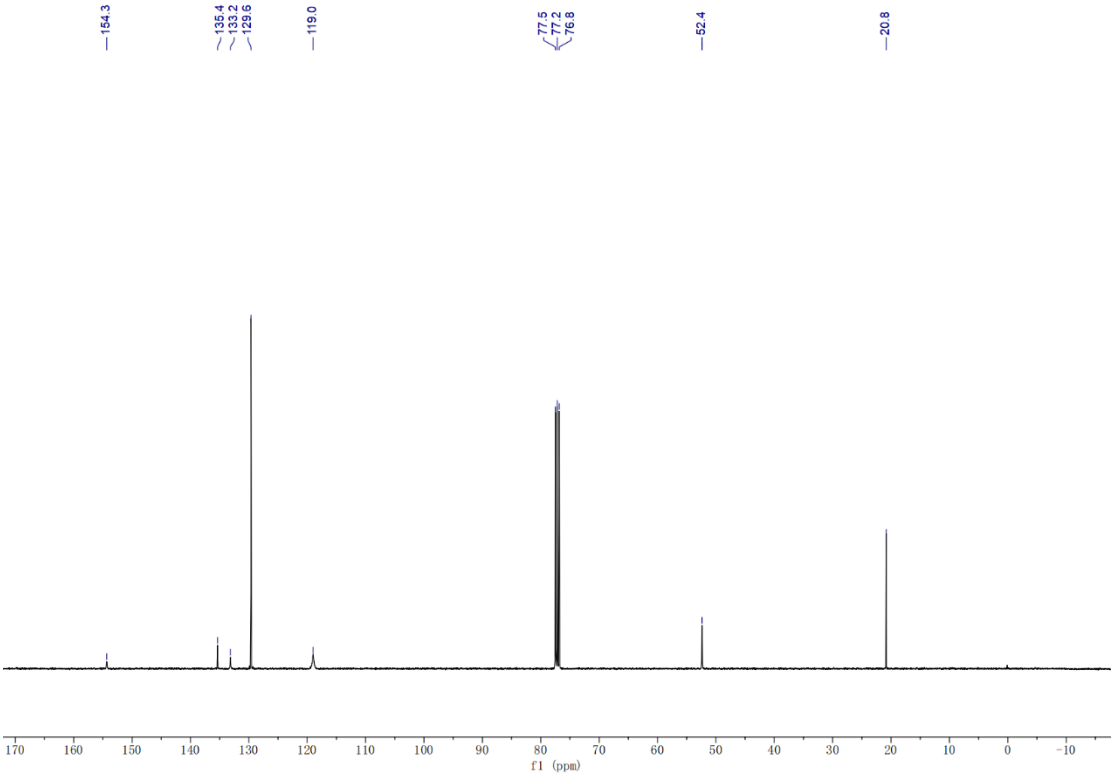


Figure S5.6 ^{13}C NMR spectrum of **3c** in $CDCl_3$ at 101 MHz.

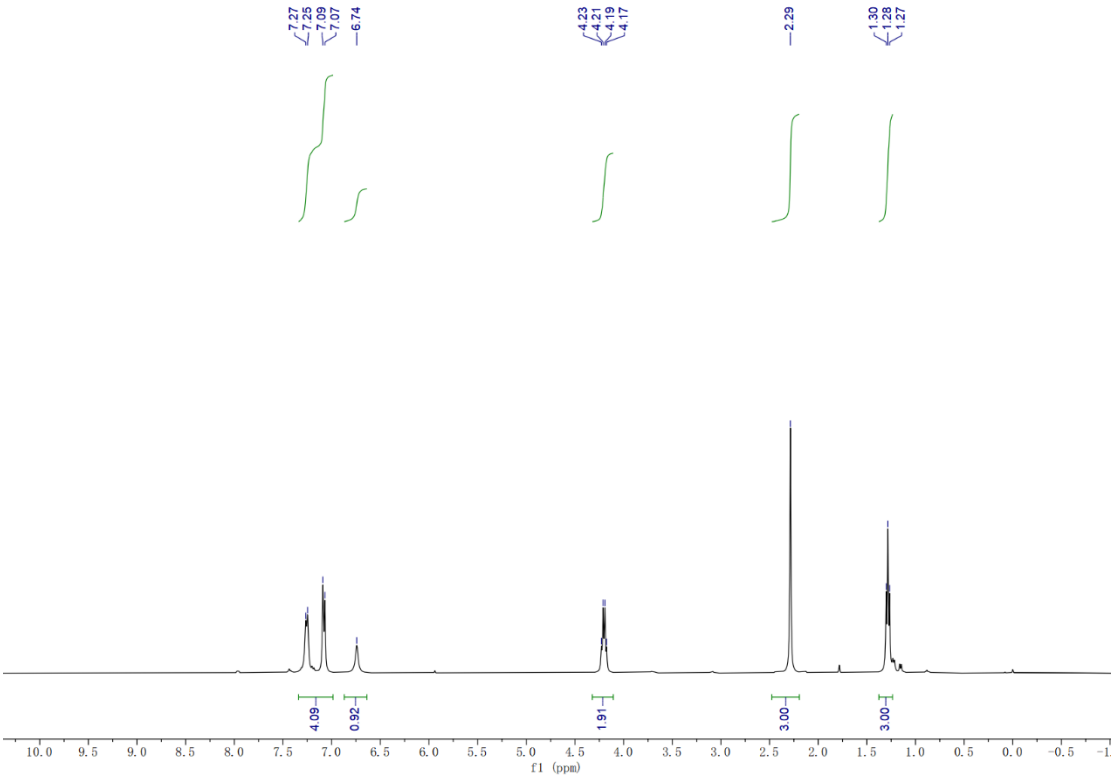


Figure S5.7 ^{1}H NMR spectrum of **3d** in $CDCl_3$ at 400 MHz.

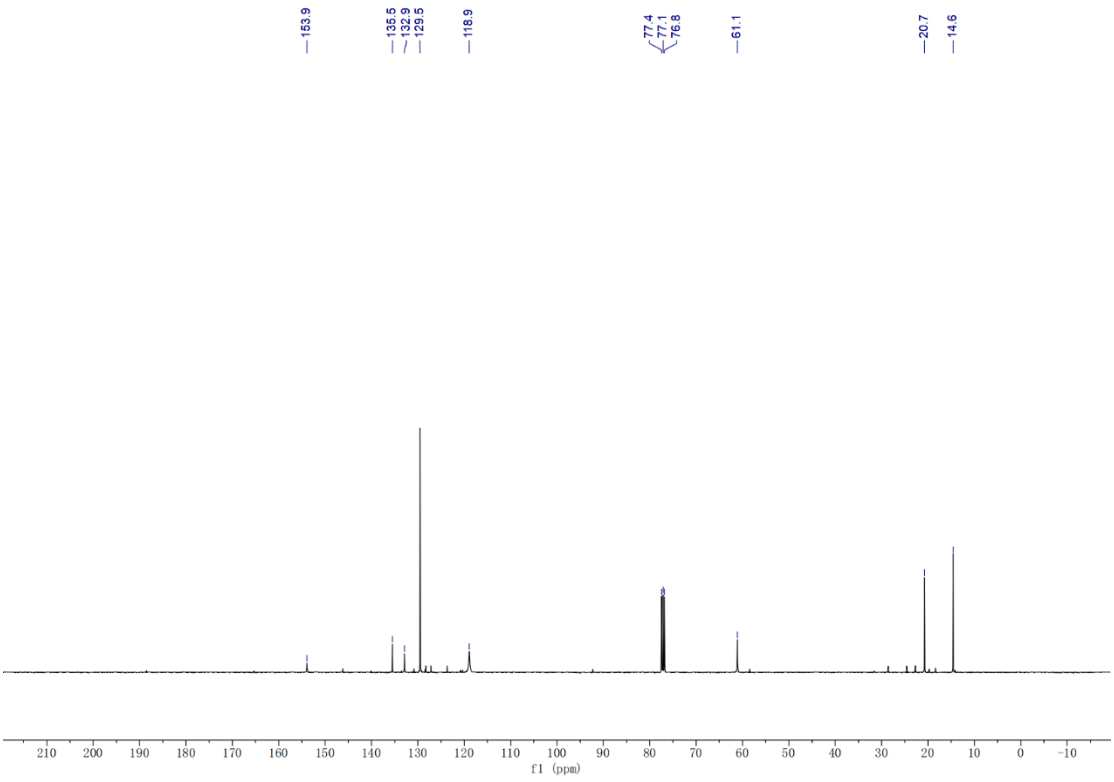


Figure S5.8 ^{13}C NMR spectrum of **3d** in $CDCl_3$ at 101 MHz.

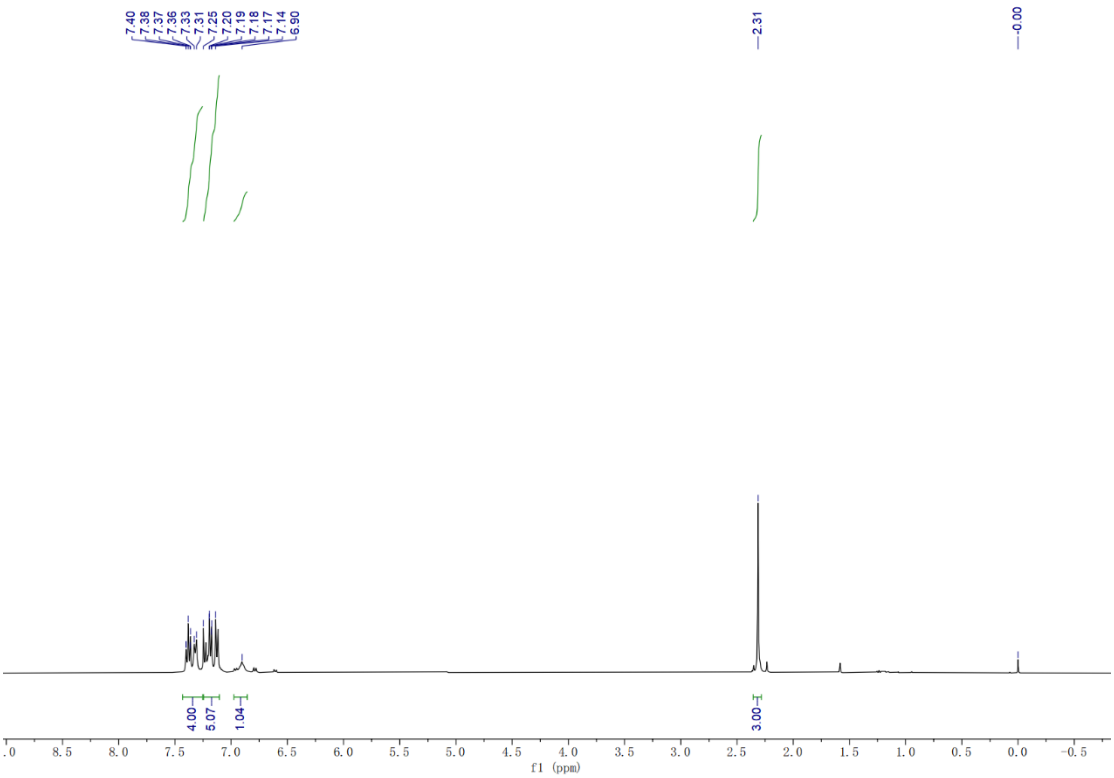


Figure S5.9 ^{1}H NMR spectrum of **3e** in $CDCl_3$ at 400 MHz.

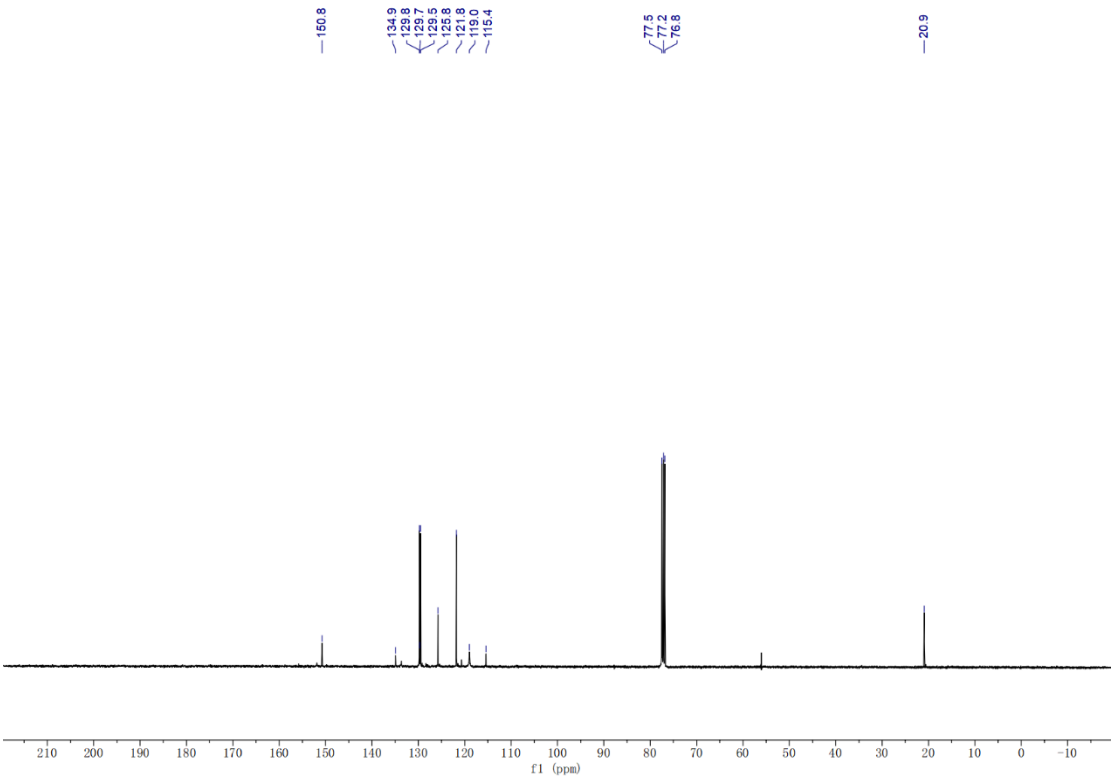


Figure S5.10 ^{13}C NMR spectrum of **3e** in $CDCl_3$ at 101 MHz.

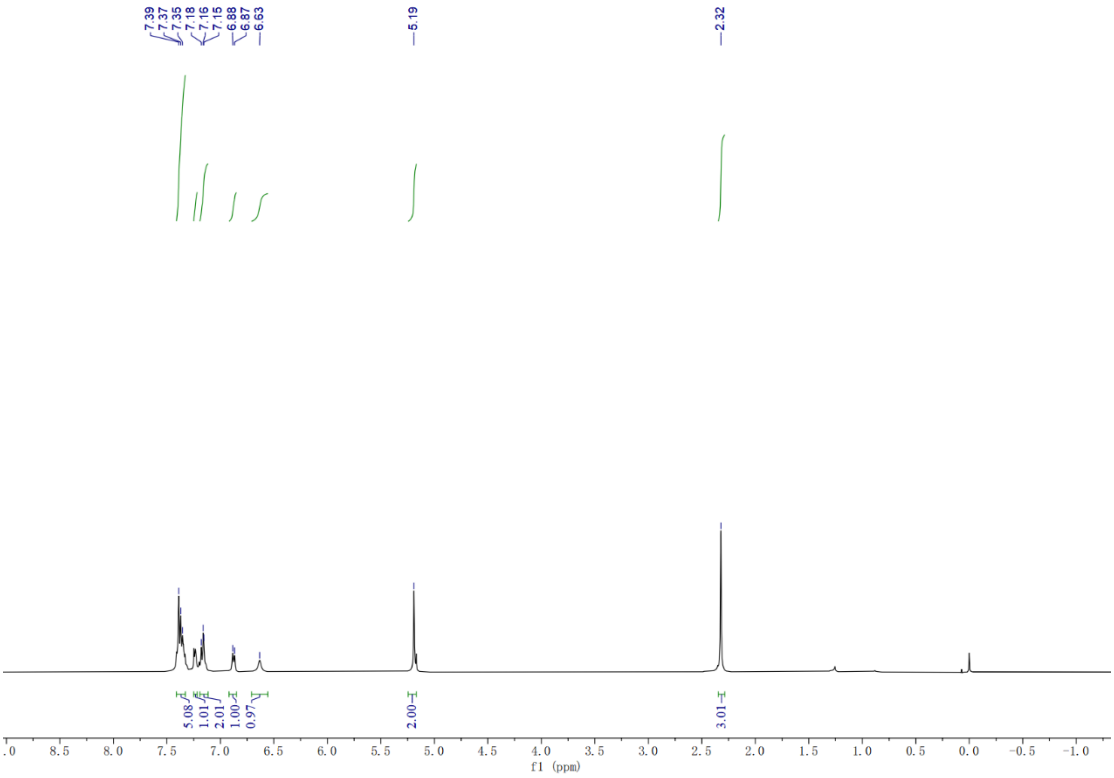


Figure S5.11 ^{1}H NMR spectrum of **3f** in $CDCl_3$ at 400 MHz.

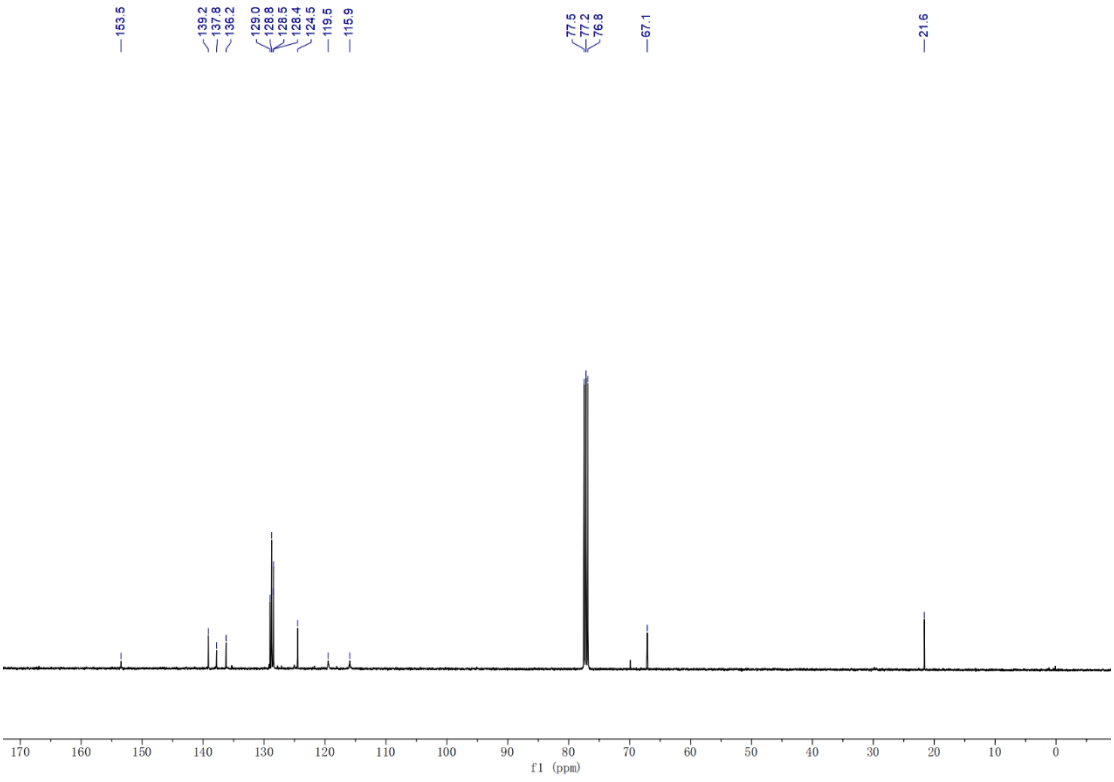


Figure S5.12 ^{13}C NMR spectrum of **3f** in $CDCl_3$ at 101 MHz.

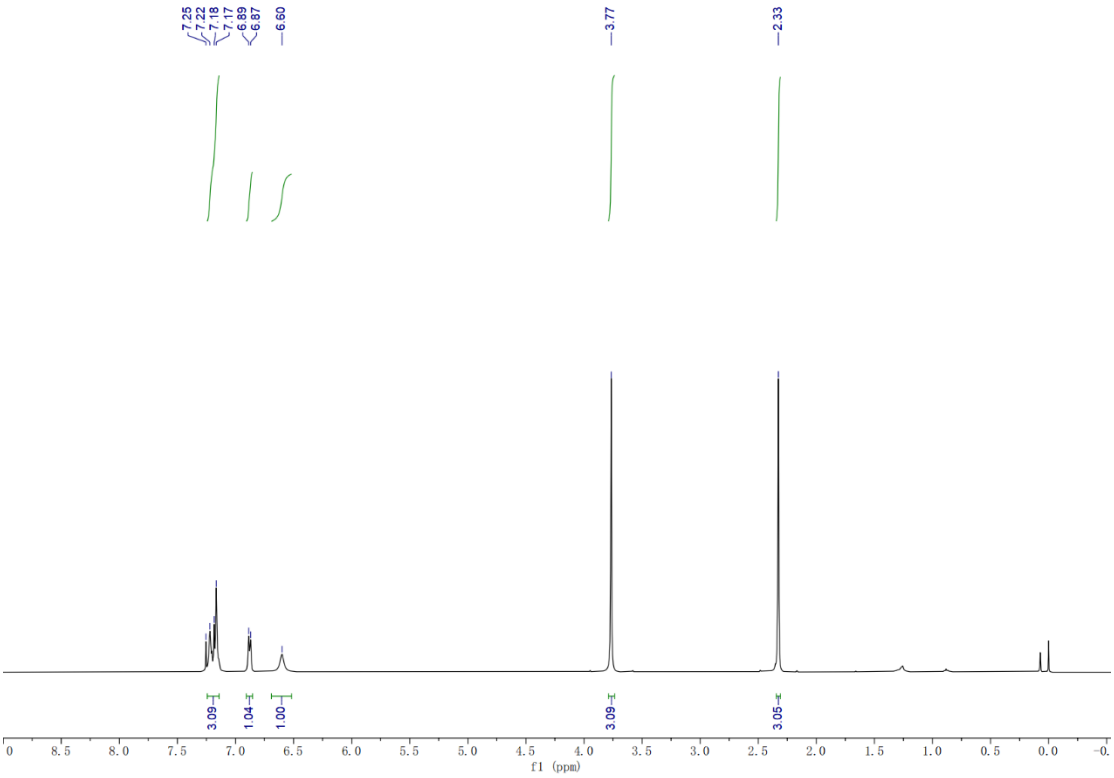


Figure S5.13 ^{1}H NMR spectrum of **3g** in $CDCl_3$ at 400 MHz.

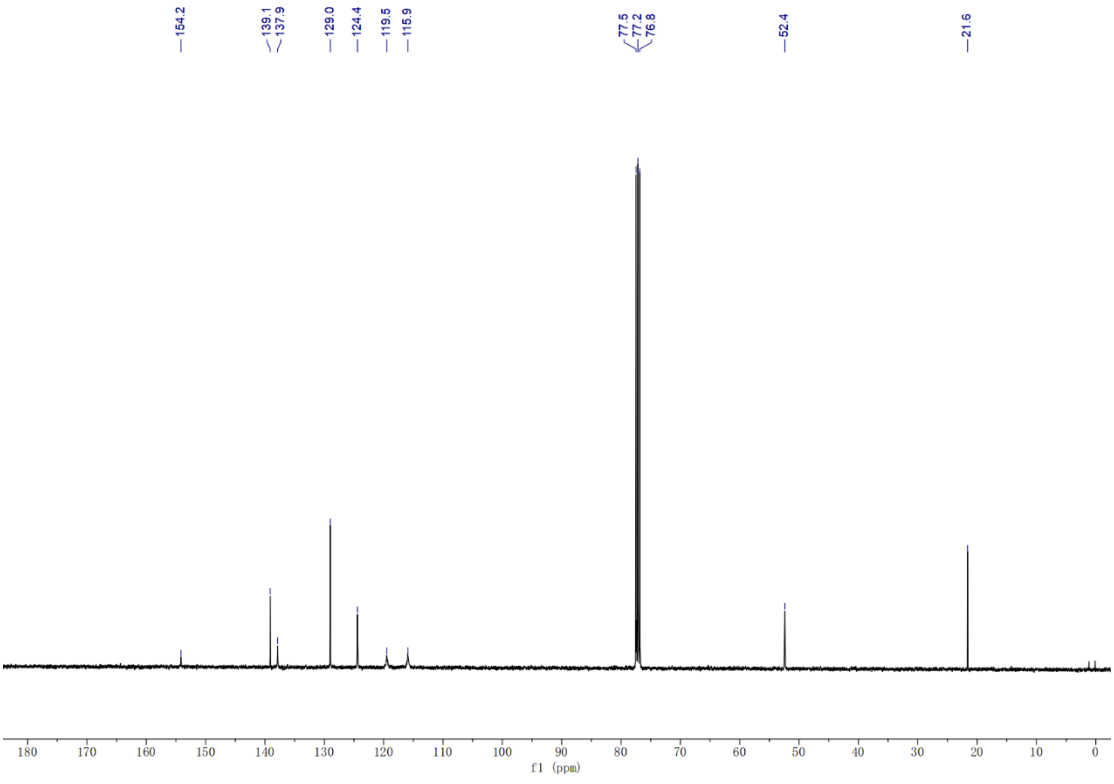


Figure S5.14 ^{13}C NMR spectrum of **3g** in $CDCl_3$ at 101 MHz.

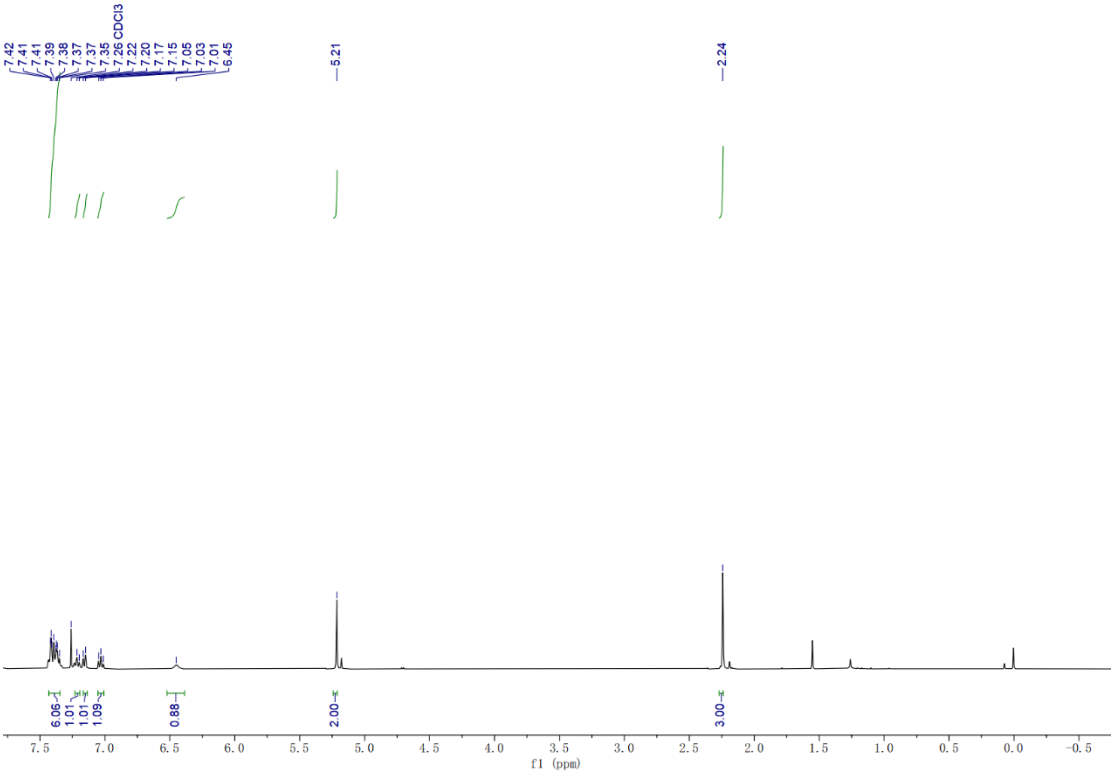


Figure S5.15 ^{1}H NMR spectrum of **3h** in $CDCl_3$ at 400 MHz.

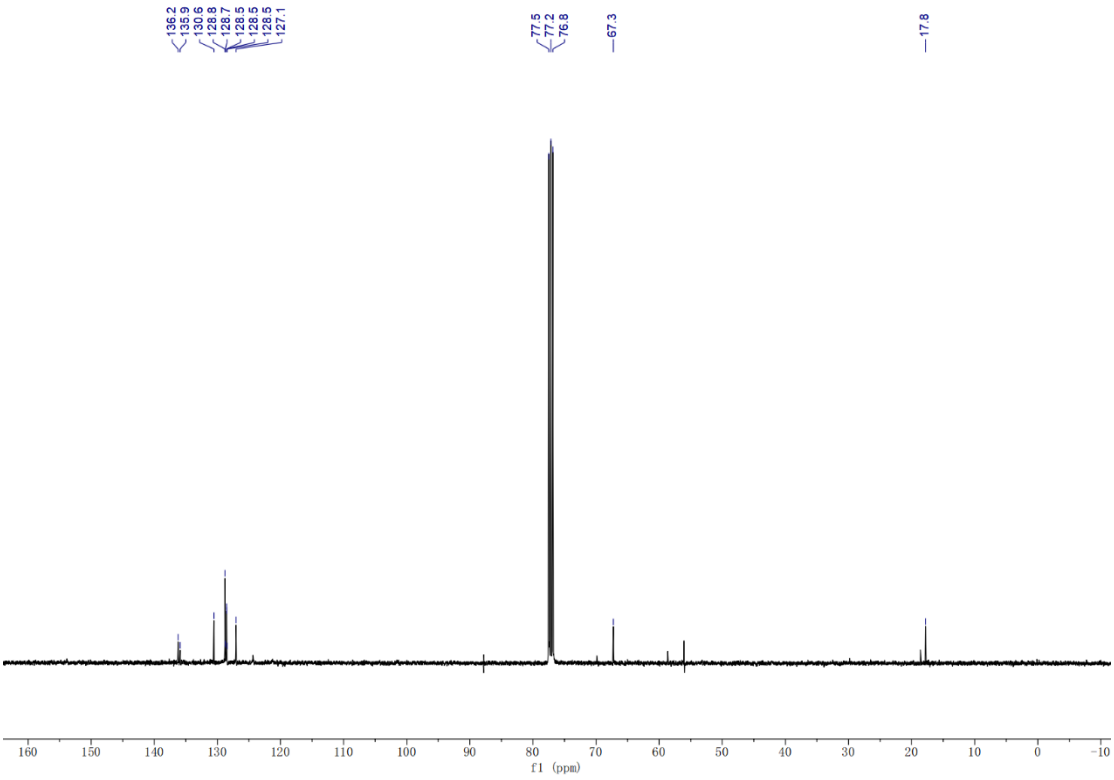


Figure S5.16 ^{13}C NMR spectrum of **3h** in $CDCl_3$ at 101 MHz.

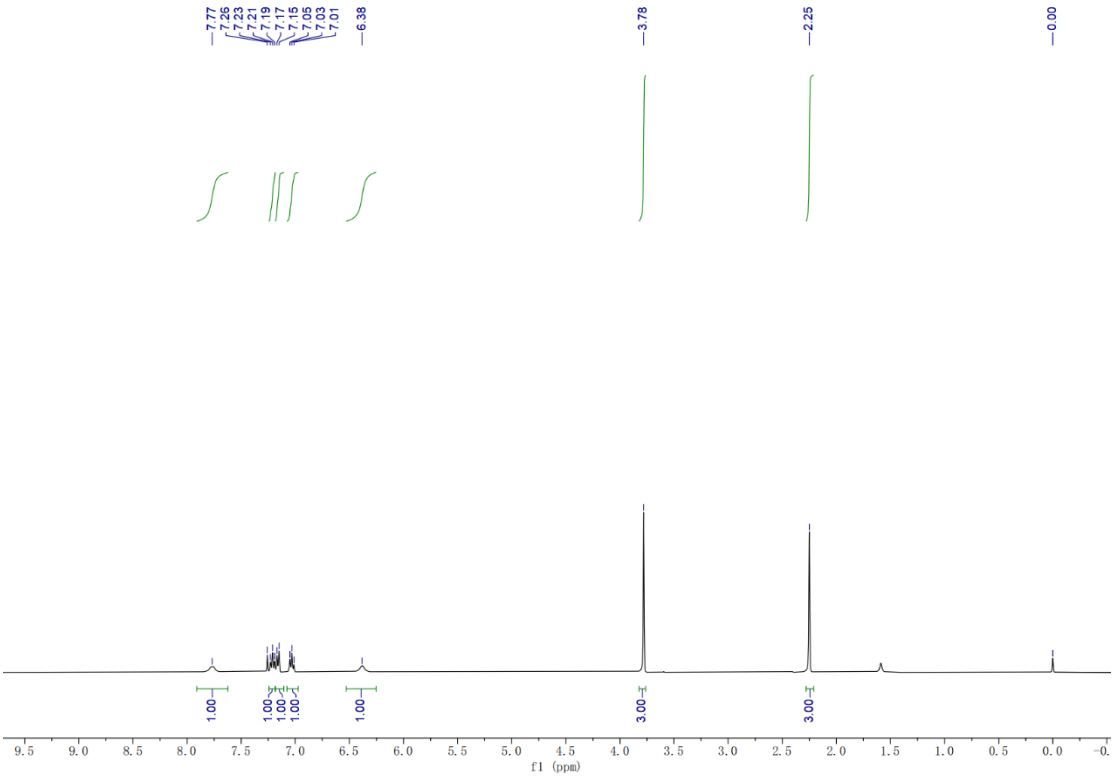


Figure S5.17 ^{1}H NMR spectrum of **3i** in $CDCl_3$ at 400 MHz.

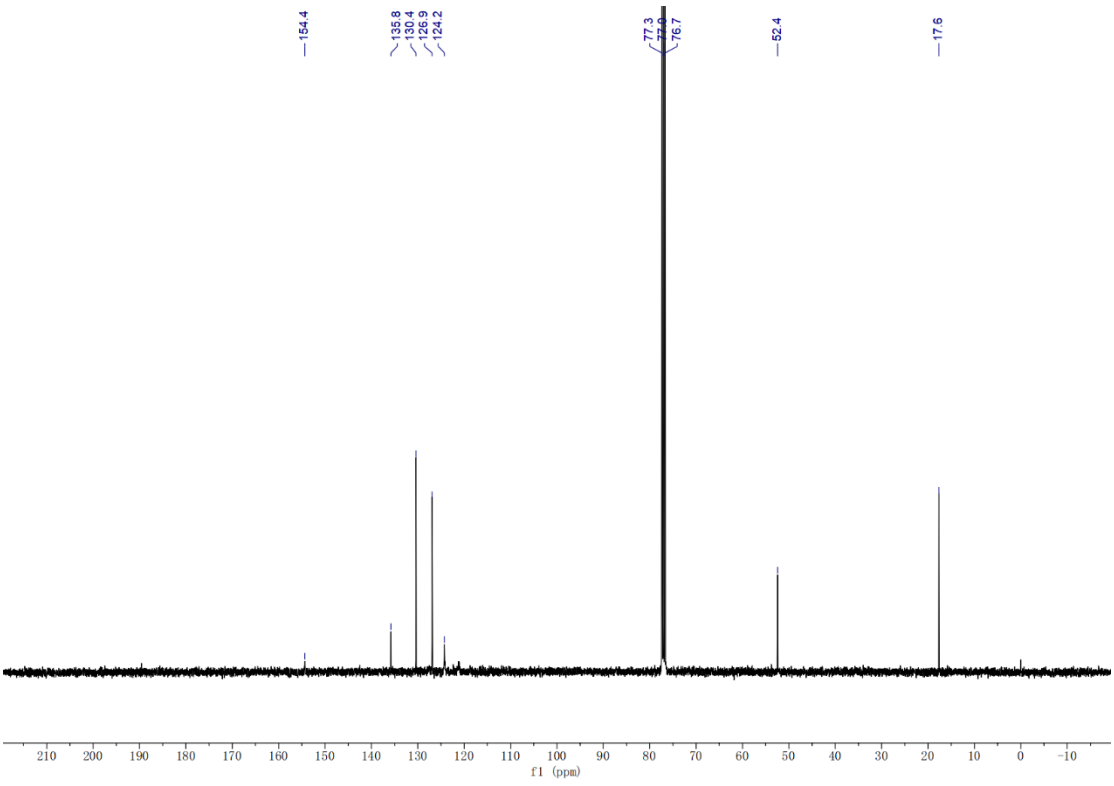


Figure S5.18 ^{13}C NMR spectrum of **3i** in $CDCl_3$ at 101 MHz.

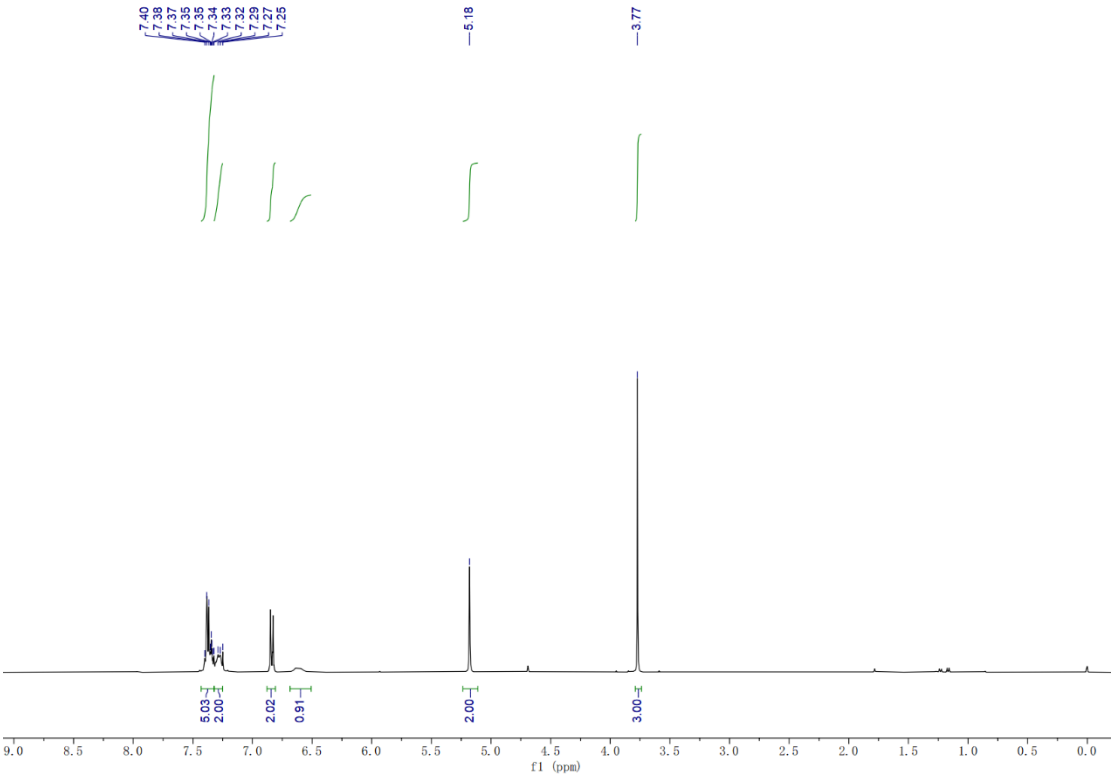


Figure S5.19 ^{1}H NMR spectrum of **3j** in $CDCl_3$ at 400 MHz.

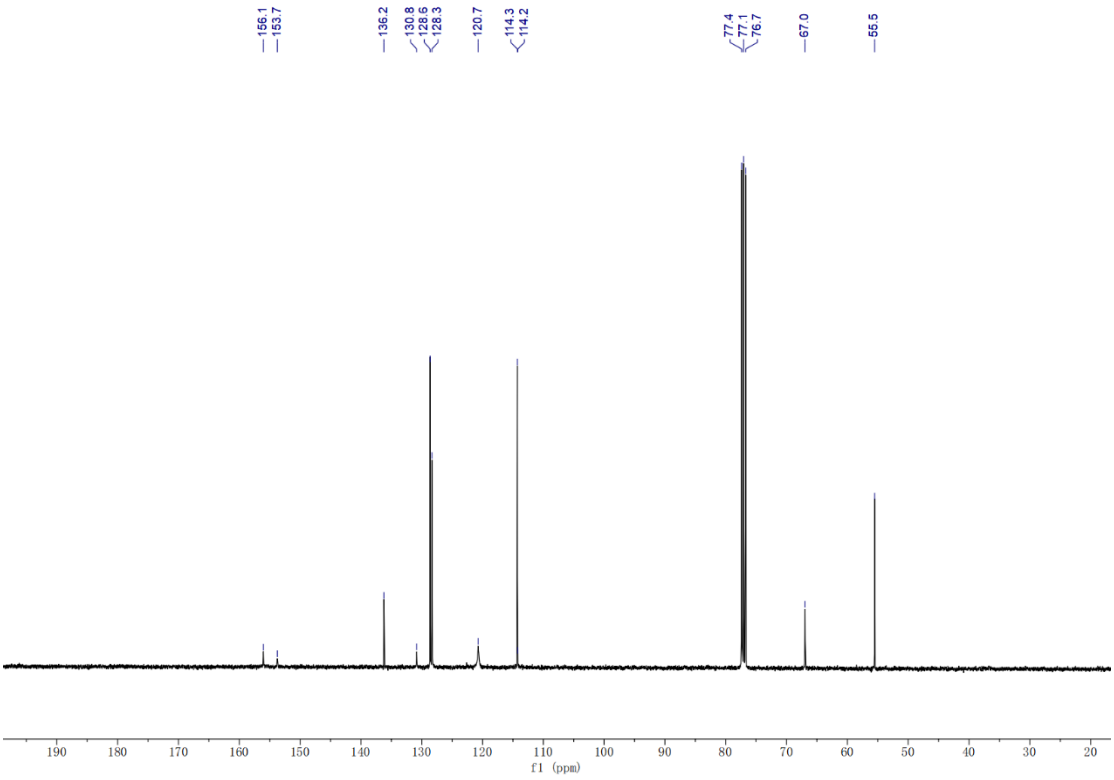


Figure S5.20 ^{13}C NMR spectrum of **3j** in $CDCl_3$ at 101 MHz.

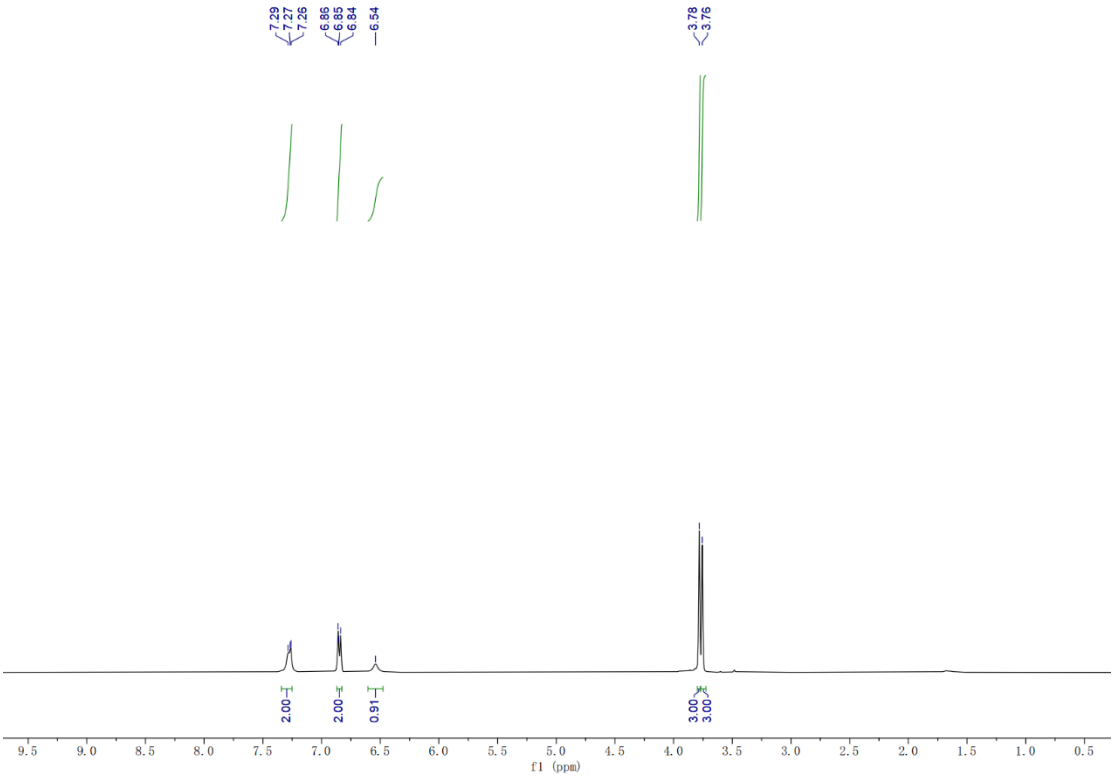


Figure S5.21 ^{1}H NMR spectrum of **3k** in $CDCl_3$ at 400 MHz.

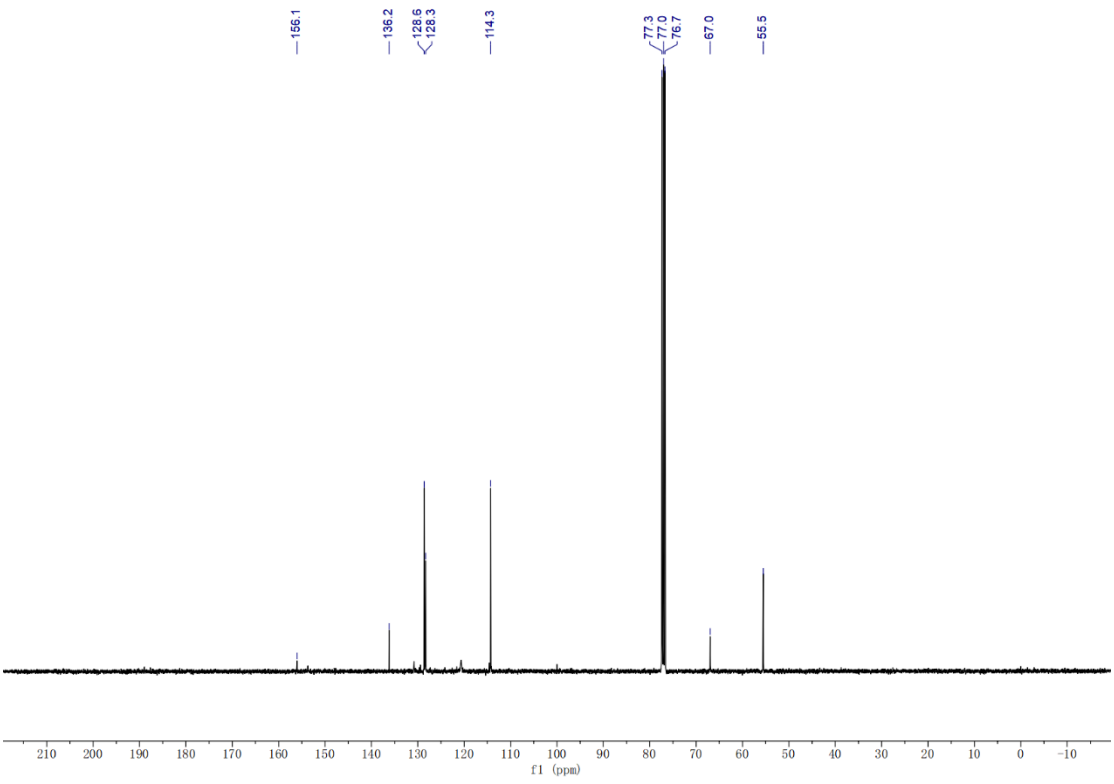


Figure S5.22 ^{13}C NMR spectrum of **3k** in $CDCl_3$ at 101 MHz.

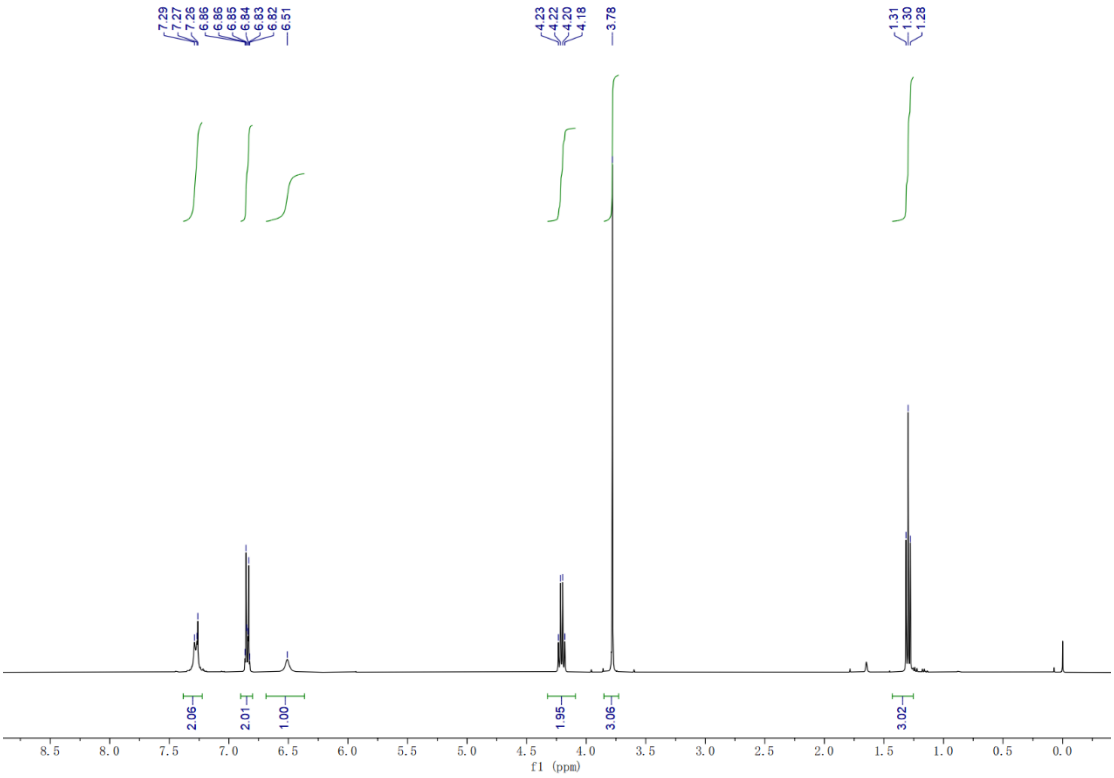


Figure S5.23 ^{1}H NMR spectrum of **3l** in $CDCl_3$ at 400 MHz.

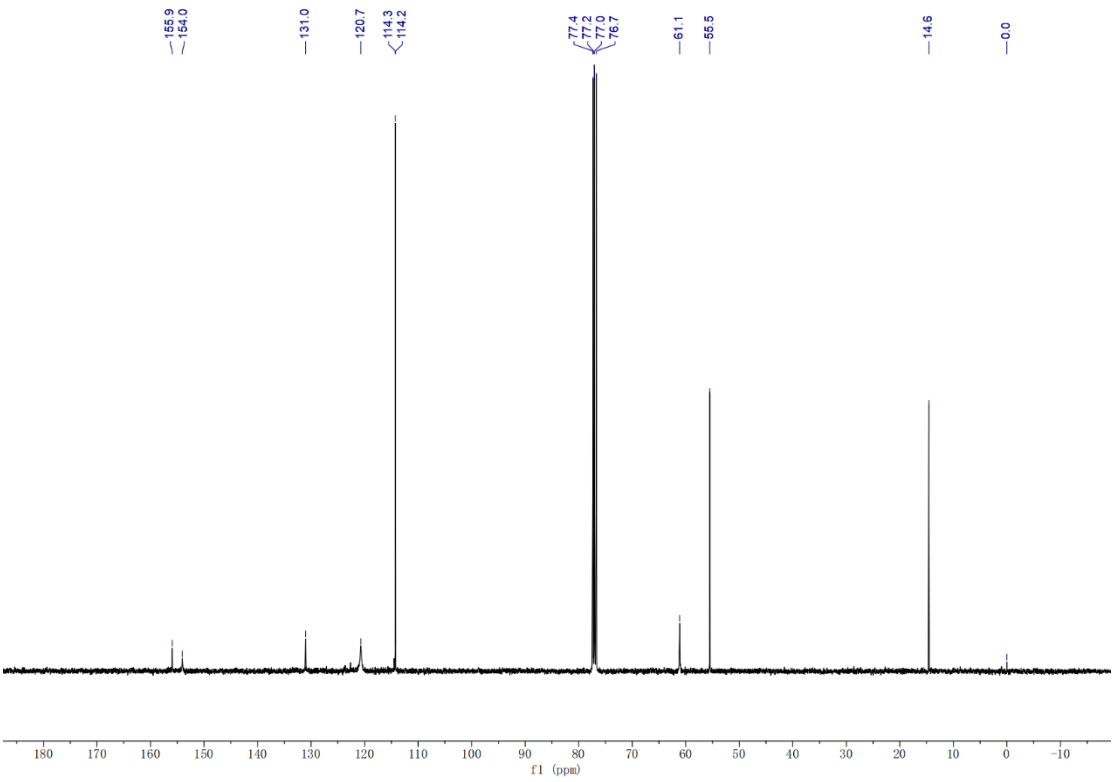


Figure S5.24 ^{13}C NMR spectrum of **3l** in $CDCl_3$ at 101 MHz.

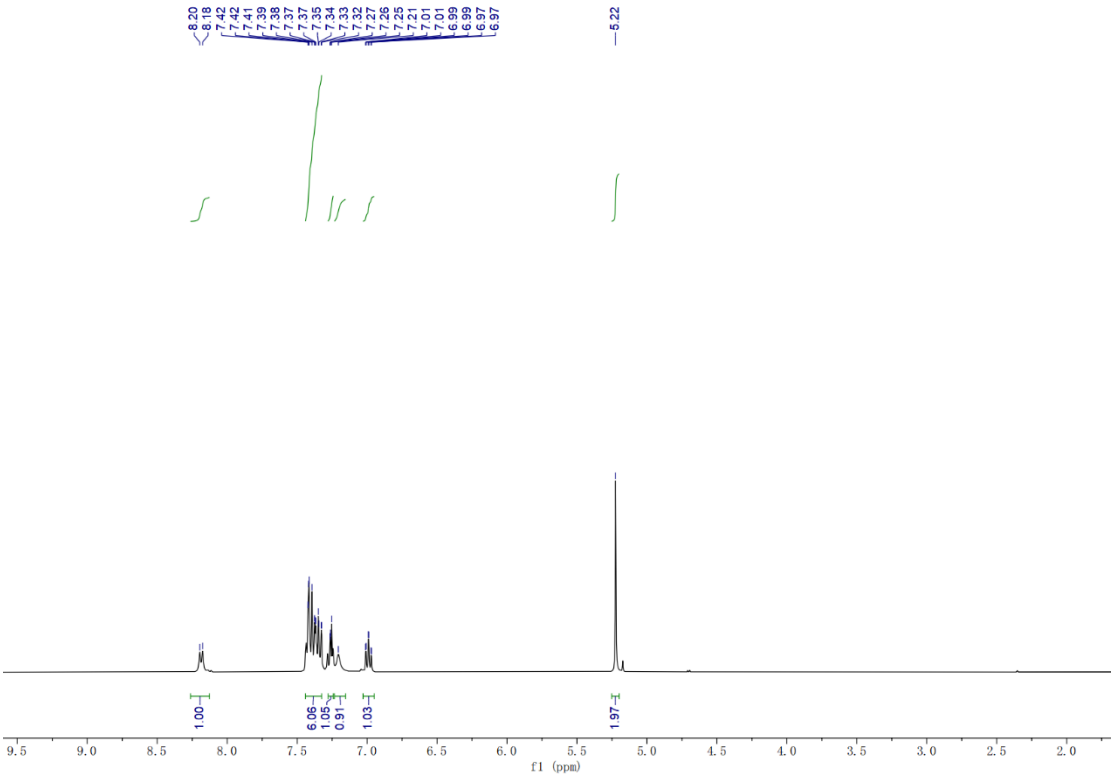


Figure S5.25 ^{1}H NMR spectrum of **3m** in $CDCl_3$ at 400 MHz.

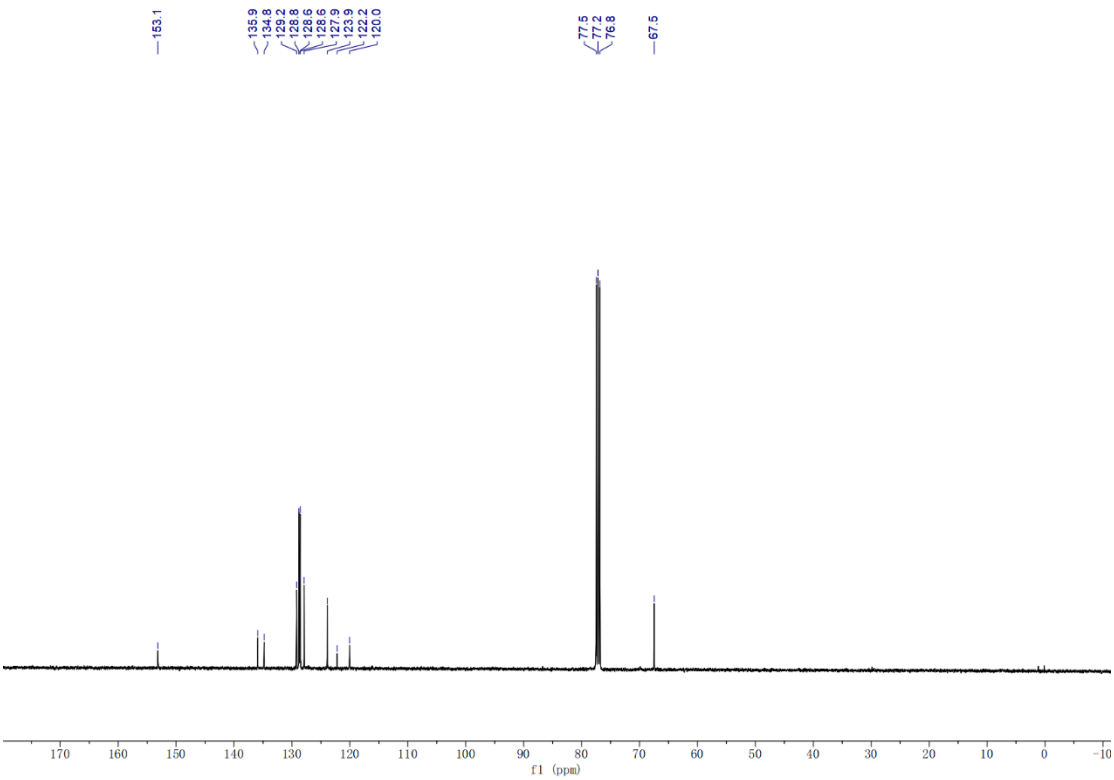


Figure S5.26 ^{13}C NMR spectrum of **3m** in $CDCl_3$ at 101 MHz.

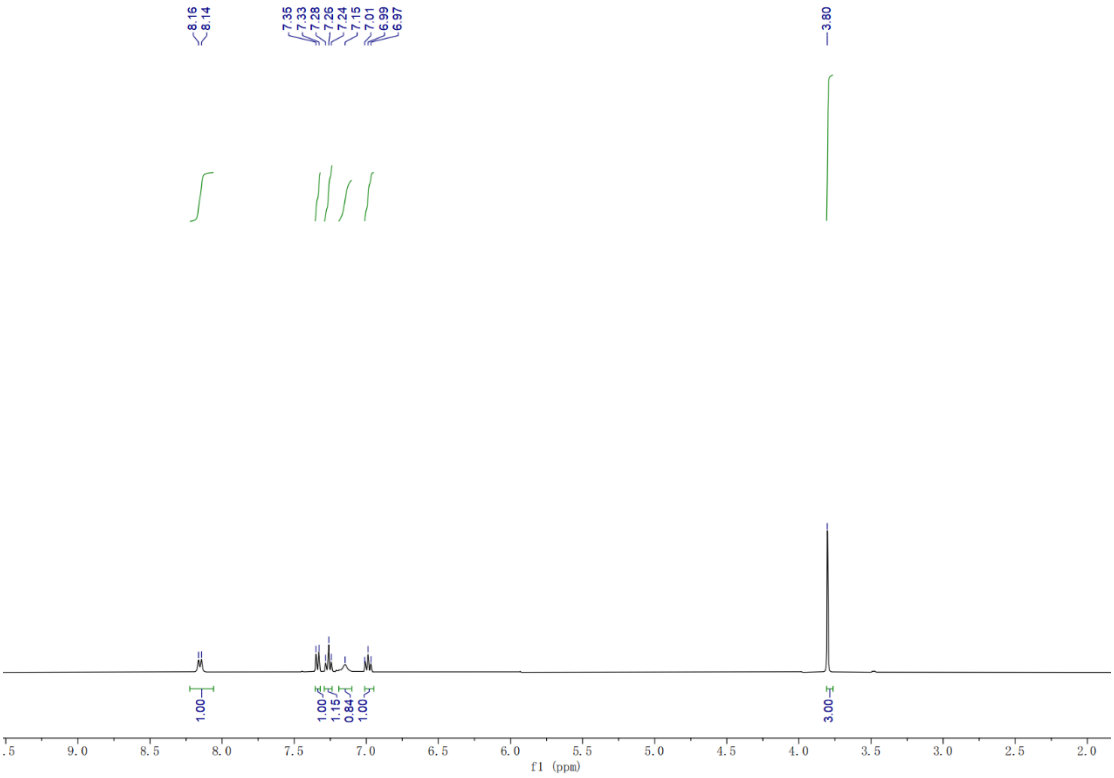


Figure S5.27 ^{1}H NMR spectrum of **3n** in $CDCl_3$ at 400 MHz.

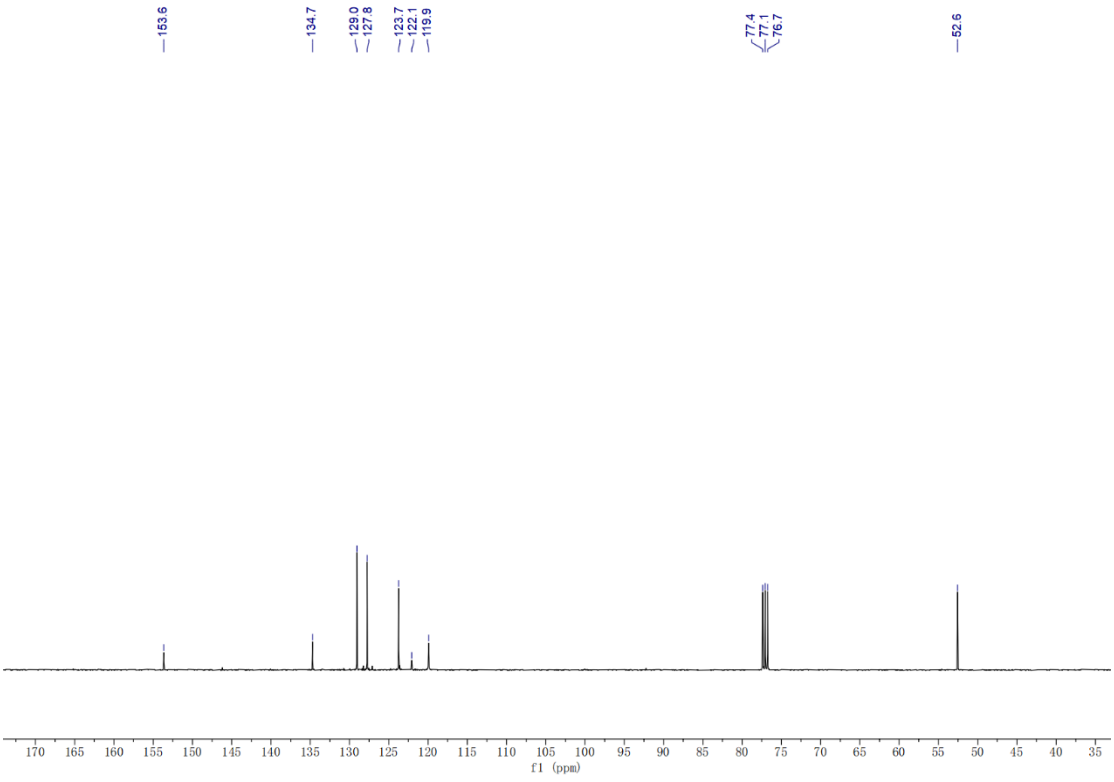


Figure S5.28 ^{13}C NMR spectrum of **3n** in $CDCl_3$ at 101 MHz.

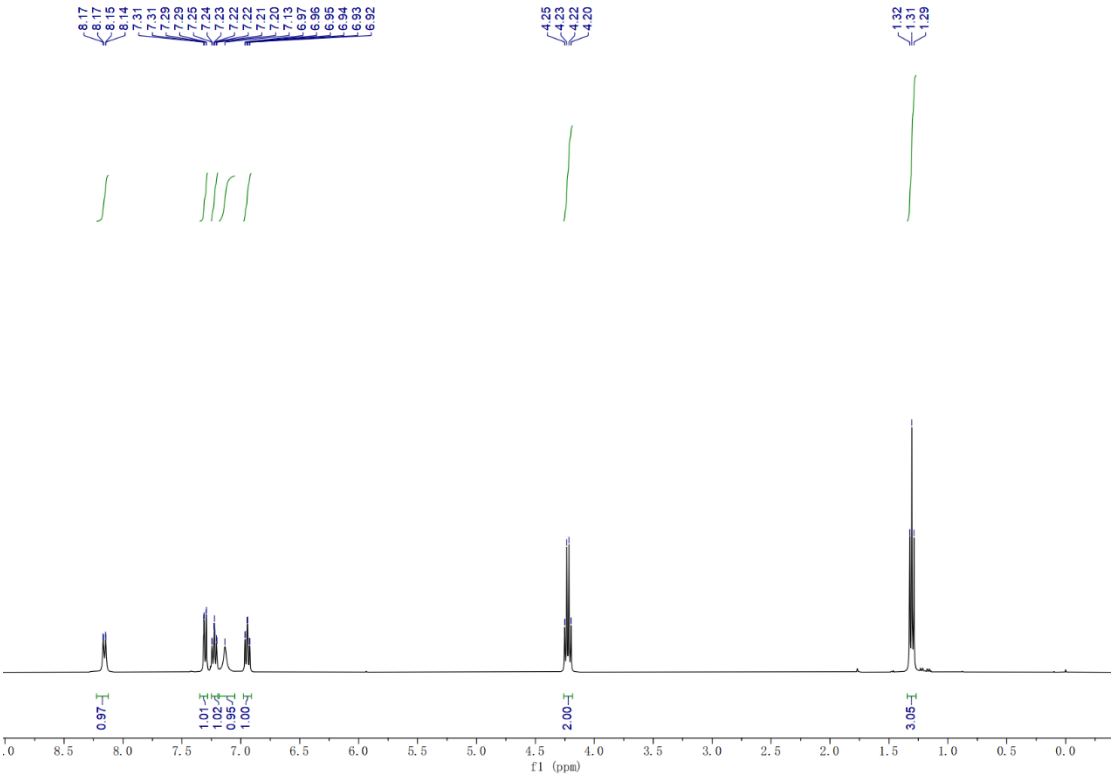


Figure S5.29 ^{1}H NMR spectrum of **3o** in $CDCl_3$ at 400 MHz.

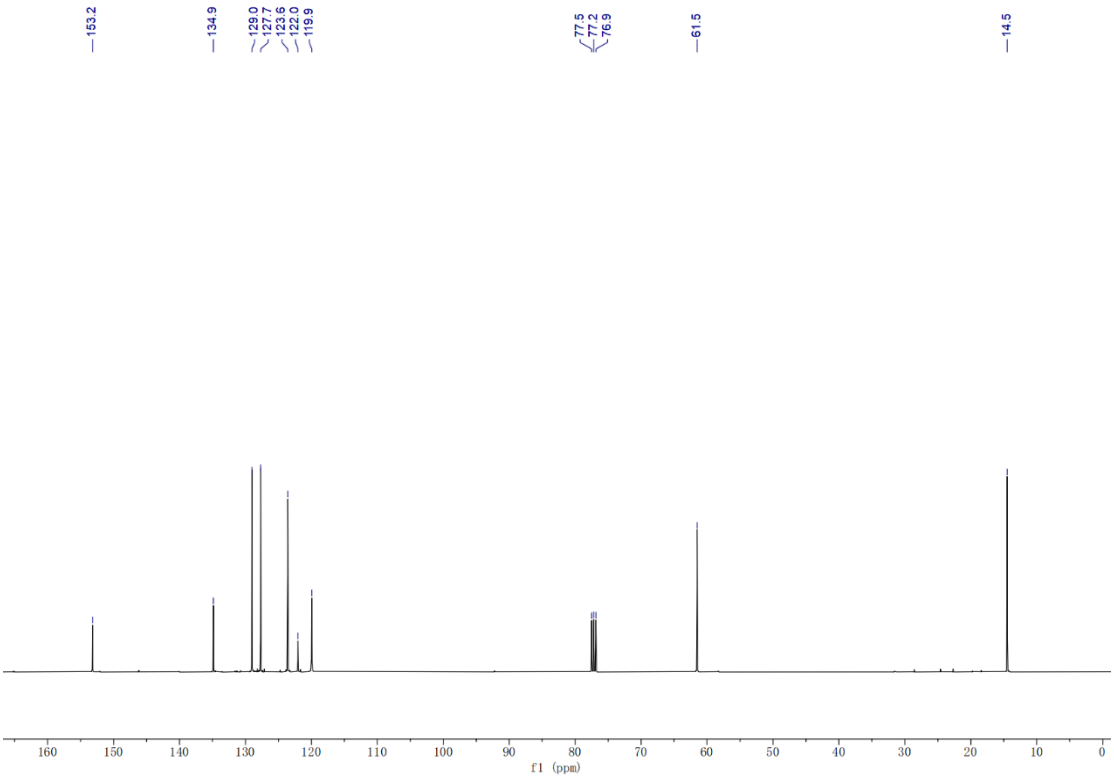


Figure S5.30 ^{13}C NMR spectrum of **3o** in $CDCl_3$ at 101 MHz.

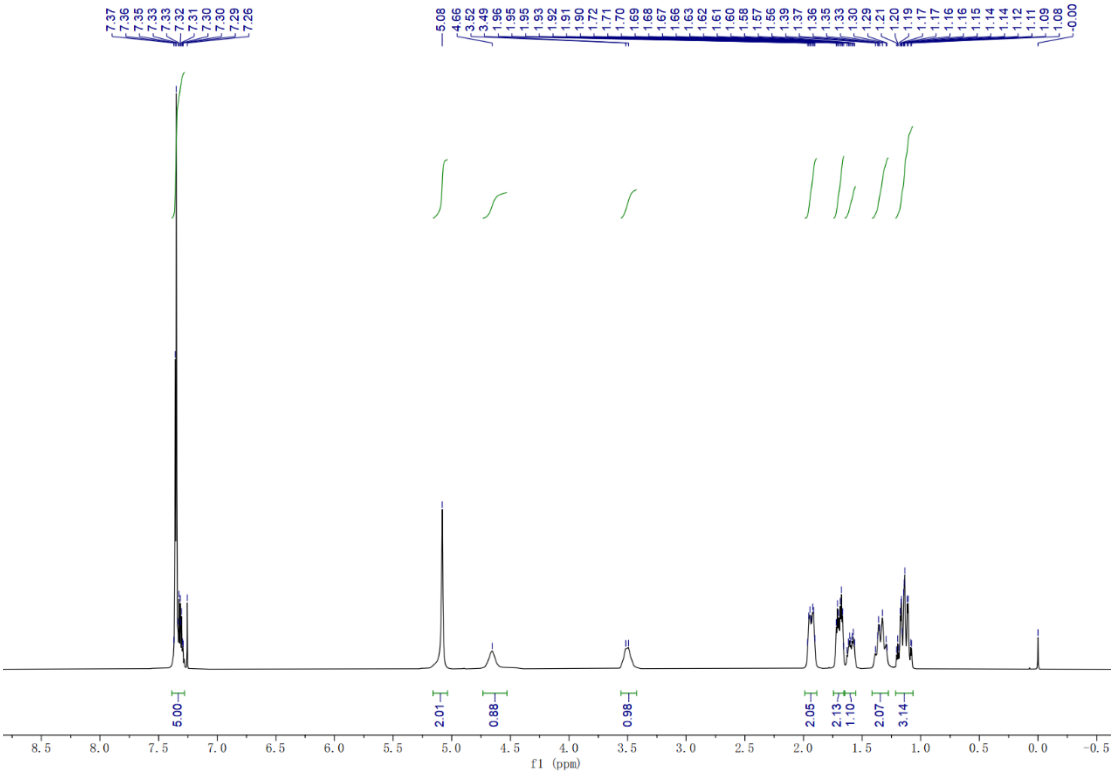


Figure S5.31 ^{1}H NMR spectrum of **3p** in $CDCl_3$ at 400 MHz.

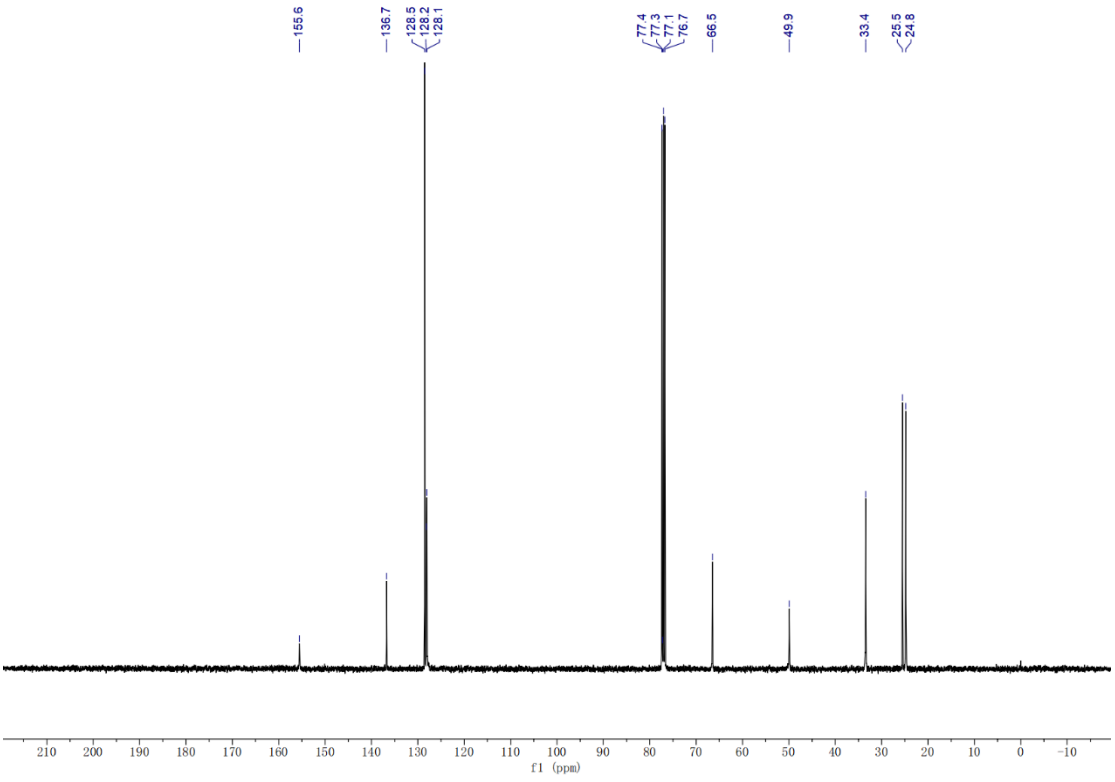


Figure S5.32 ^{13}C NMR spectrum of **3p** in $CDCl_3$ at 101 MHz.

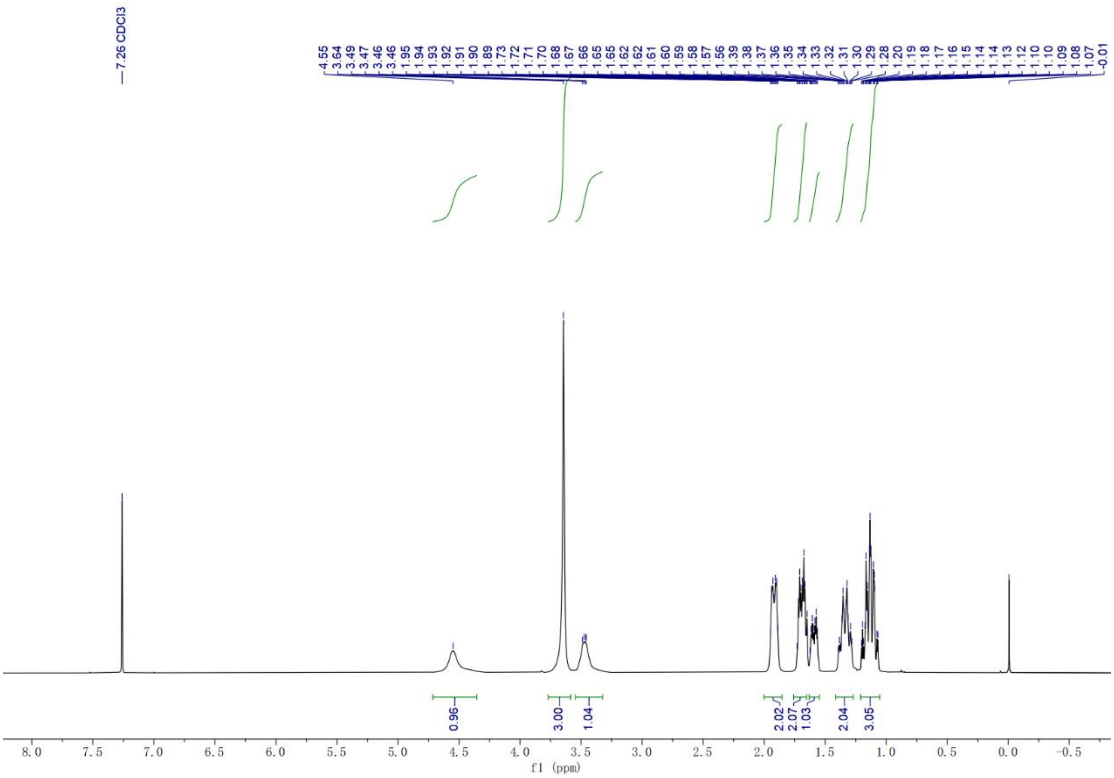


Figure S5.33 ^{1}H NMR spectrum of **3q** in $CDCl_3$ at 400 MHz.

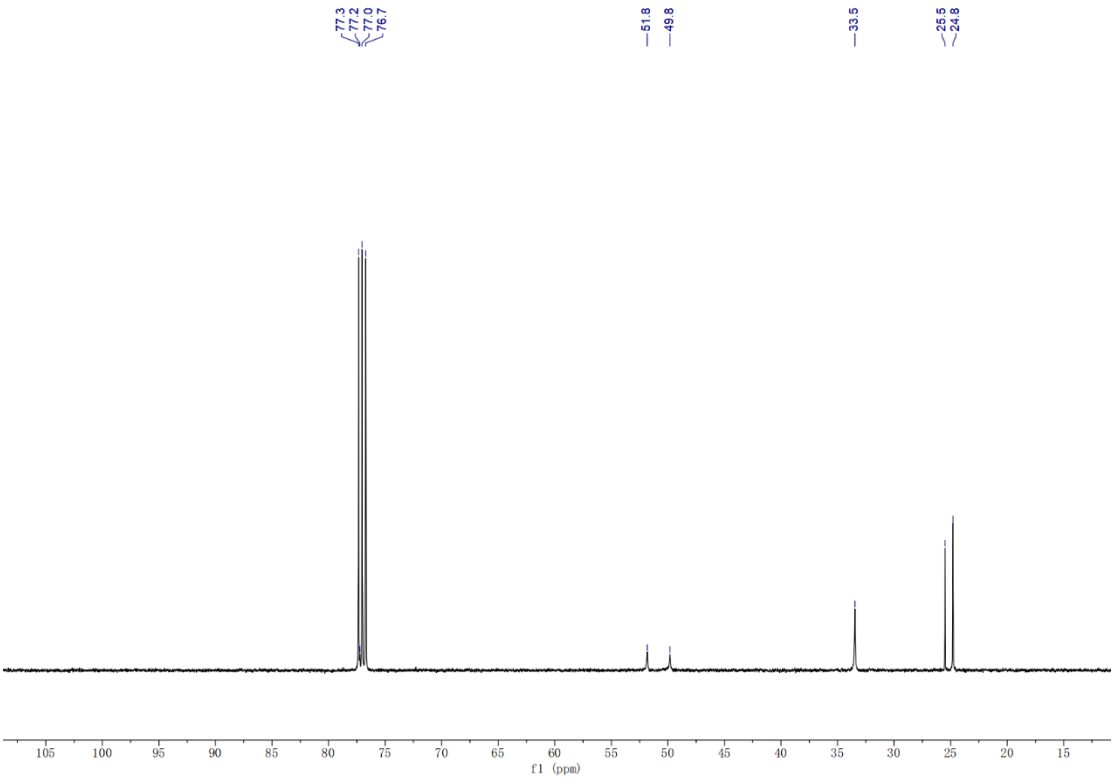


Figure S5.34 ^{13}C NMR spectrum of **3q** in $CDCl_3$ at 101 MHz.

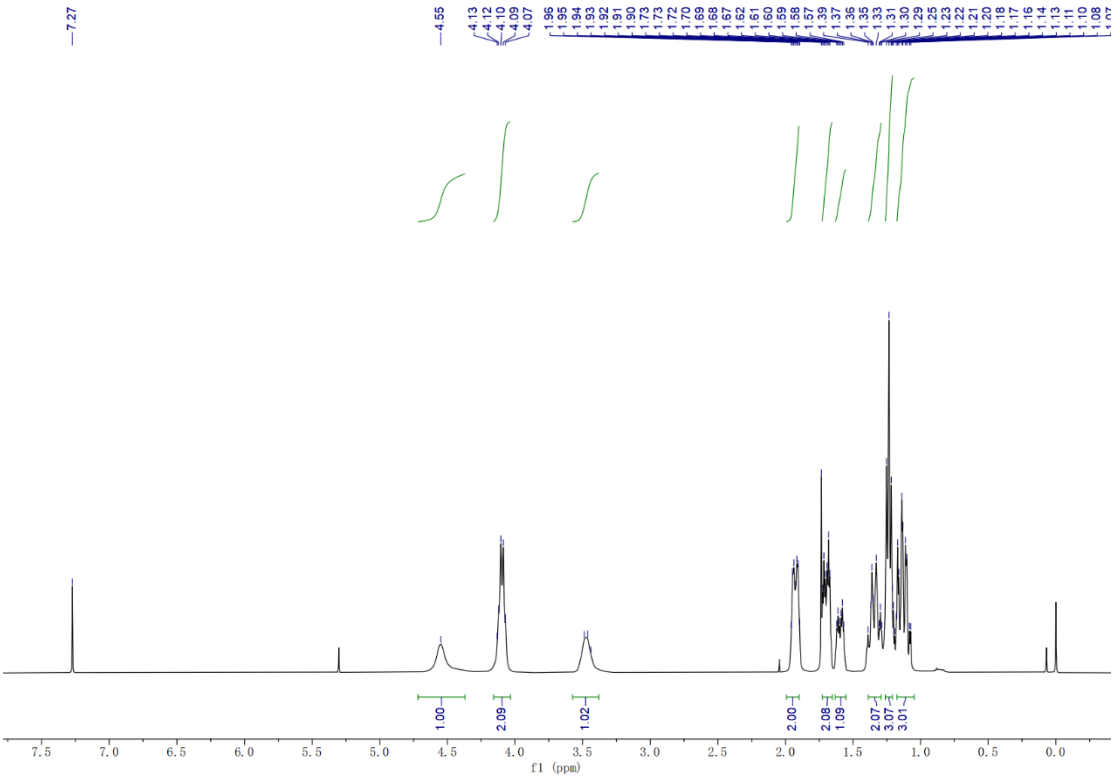


Figure S5.35 ^{1}H NMR spectrum of **3r** in $CDCl_3$ at 400 MHz.

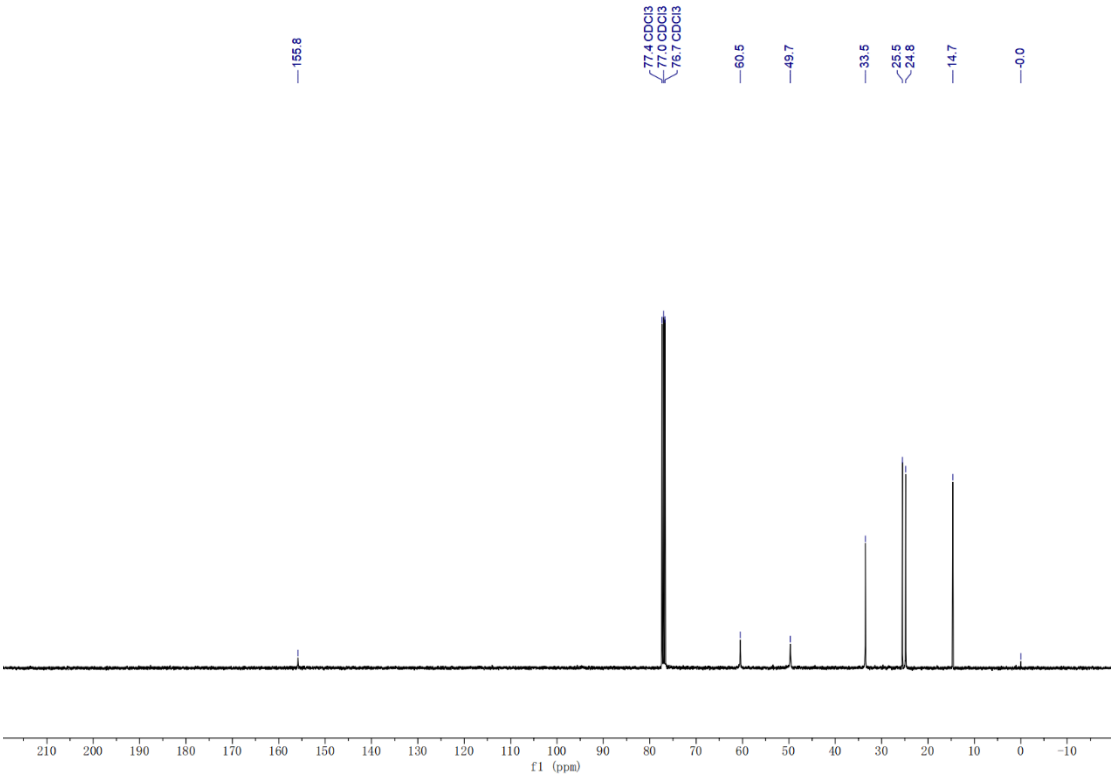


Figure S5.36 ^{13}C NMR spectrum of **3r** in $CDCl_3$ at 101 MHz.

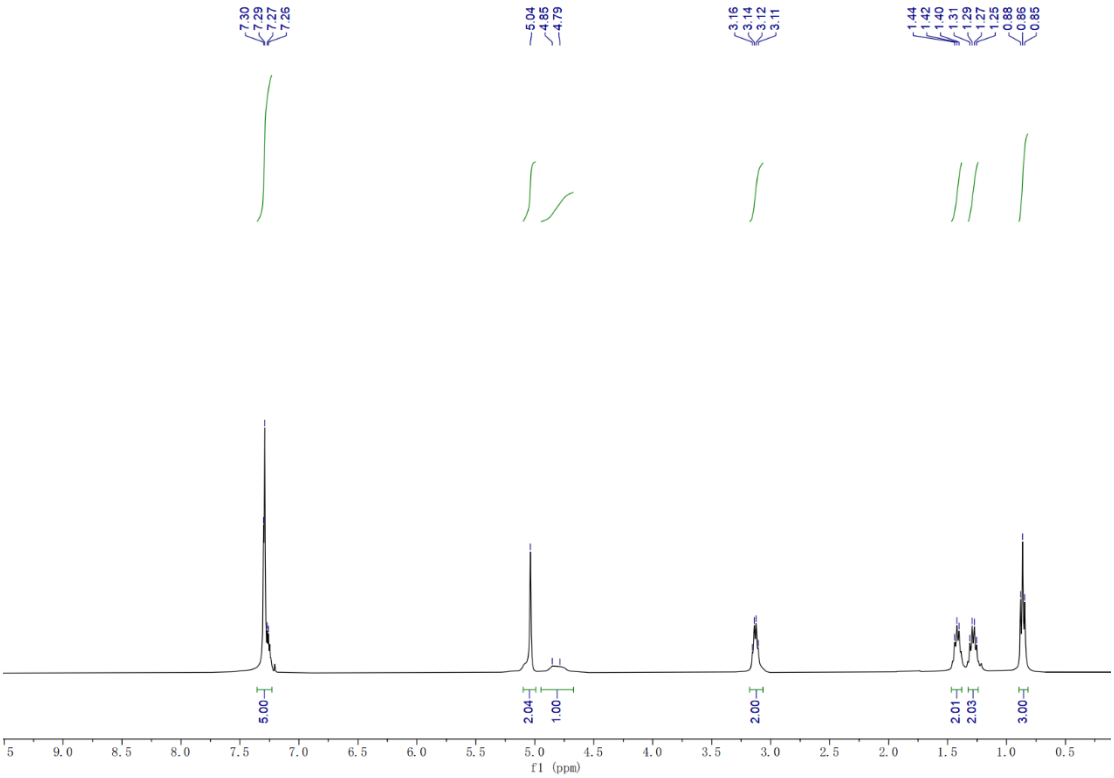


Figure S5.37 ^{1}H NMR spectrum of **3s** in $CDCl_3$ at 400 MHz.

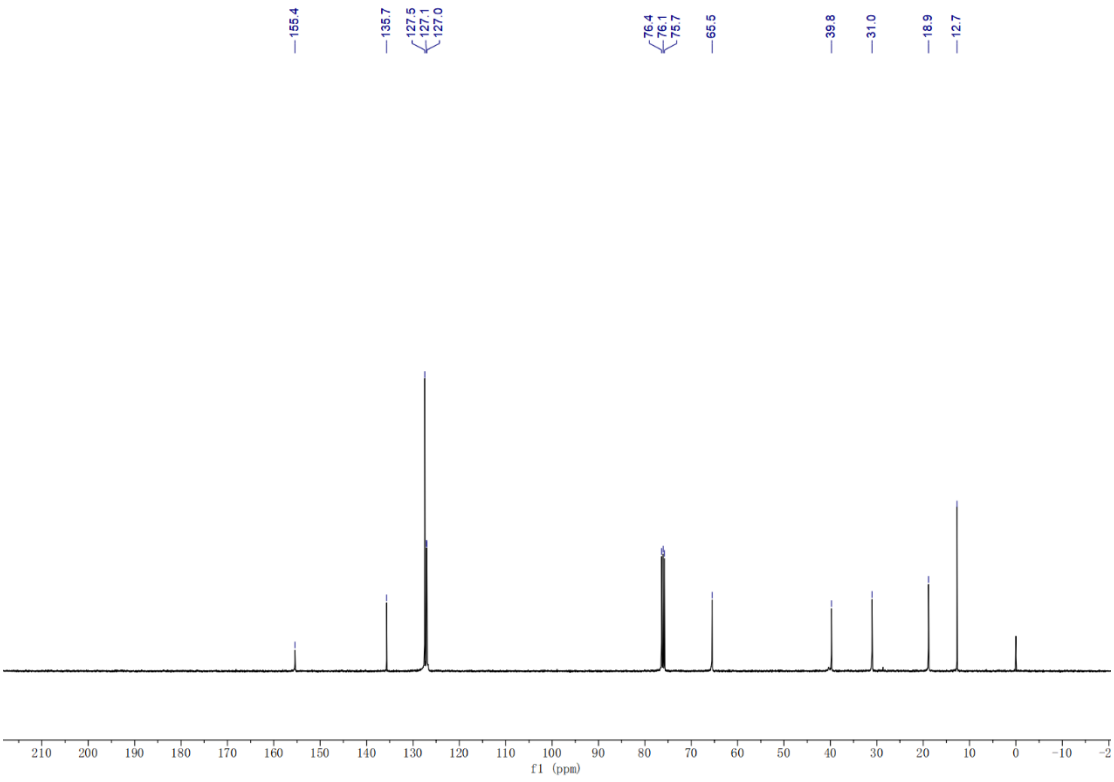


Figure S5.38 ^{13}C NMR spectrum of **3s** in $CDCl_3$ at 101 MHz.

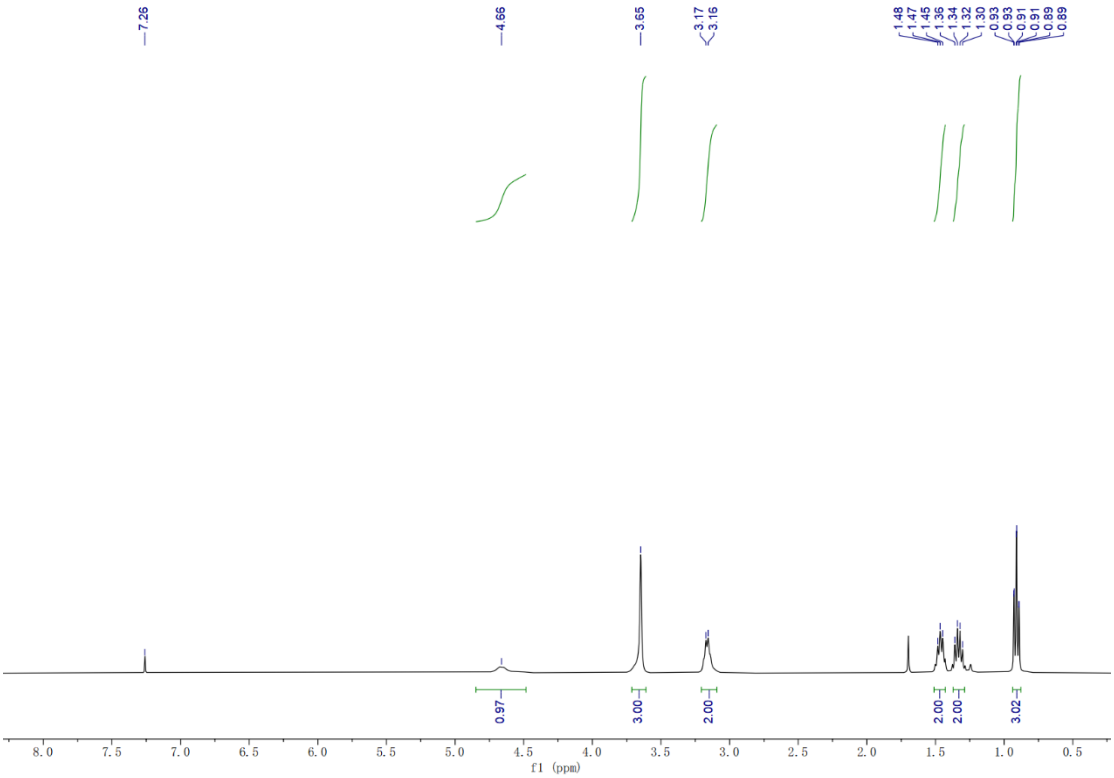


Figure S5.39 ^{1}H NMR spectrum of **3t** in $CDCl_3$ at 400 MHz.

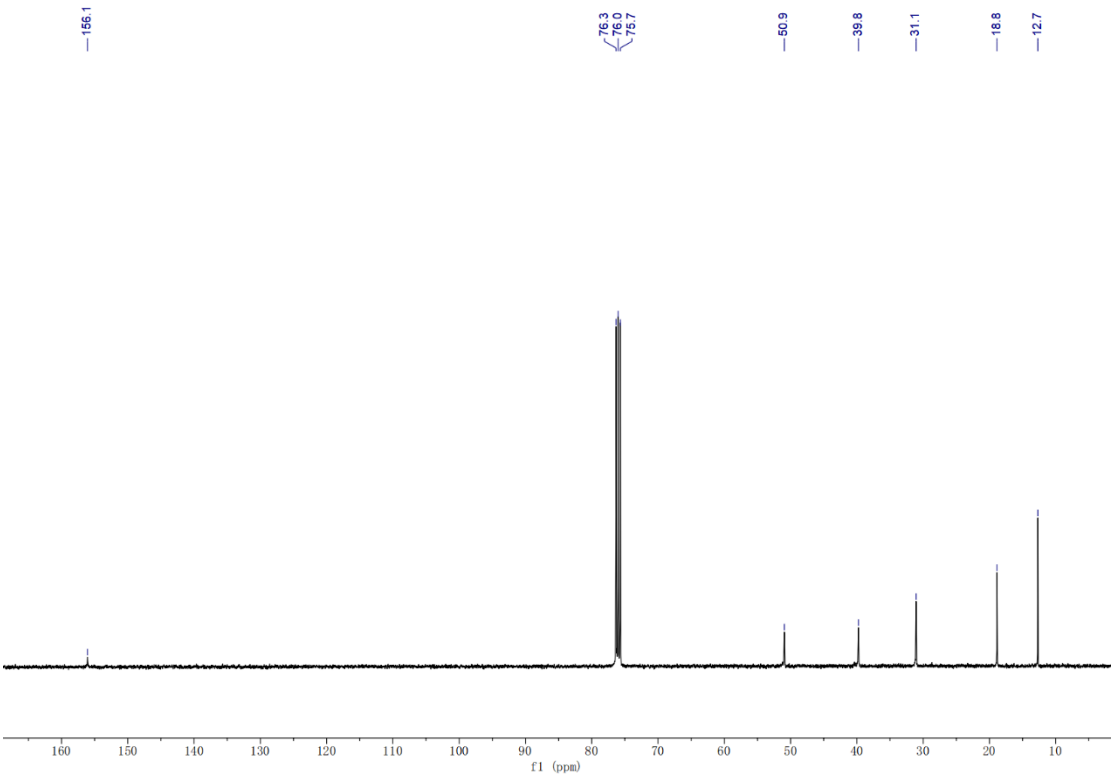


Figure S5.40 ^{13}C NMR spectrum of **3t** in $CDCl_3$ at 101 MHz.

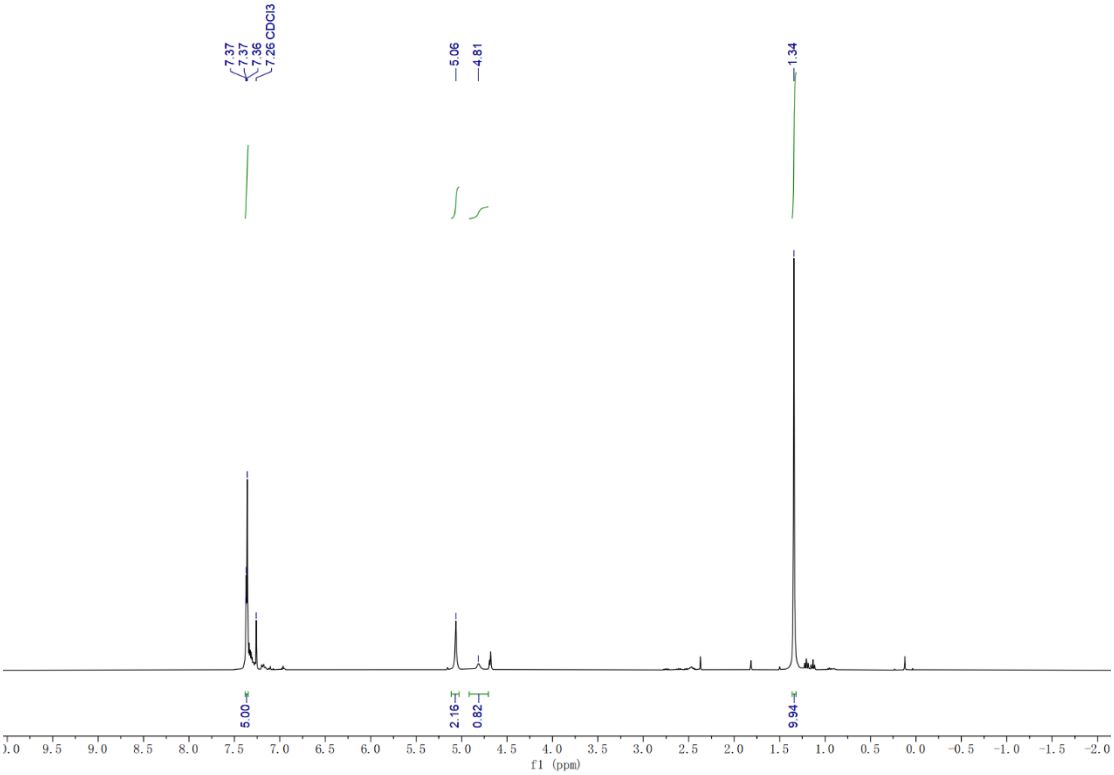


Figure S5.41 ^{1}H NMR spectrum of **3u** in $CDCl_3$ at 400 MHz.

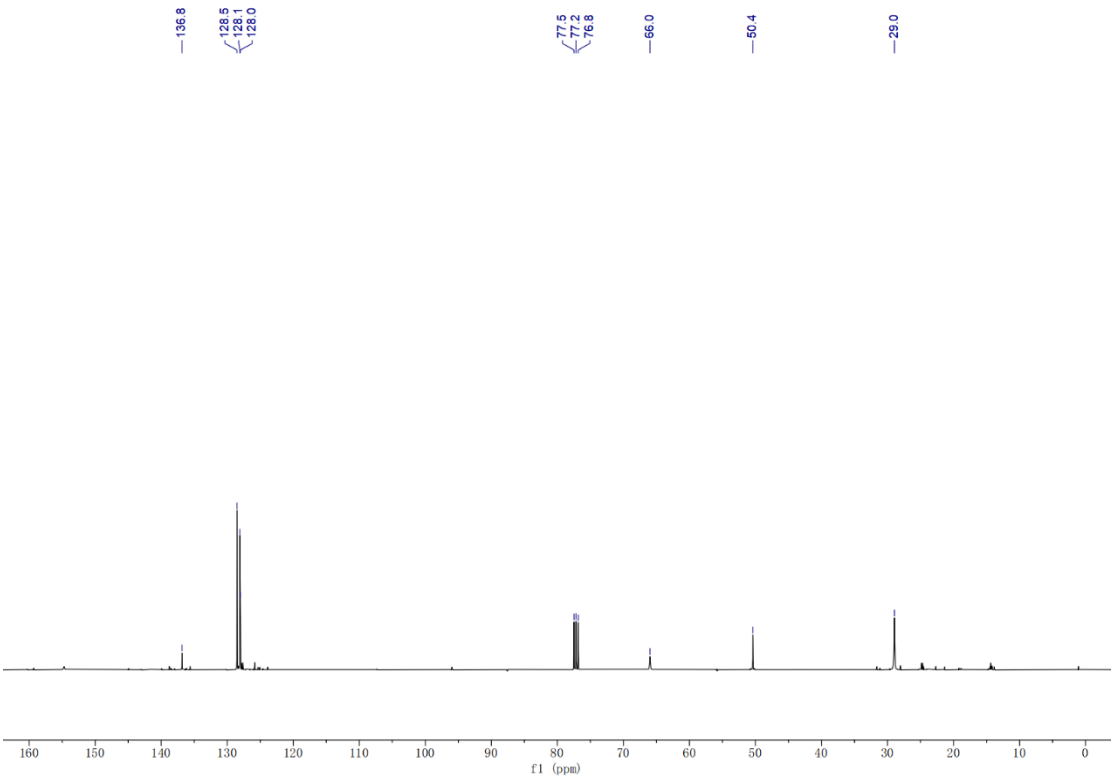
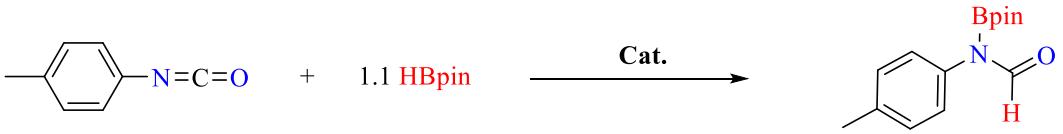


Figure S5.42 ^{13}C NMR spectrum of **3u** in $CDCl_3$ at 101 MHz.

6. General procedure for the C1-catalyzed hydroboration of isocyanates

Encouraged by the efficient catalytic hydroalkoxylation of isocyanates using **C5**, we further investigated the hydroboration of isocyanates catalysed by metal compounds **C1–C7**. As shown in **Table S6.1**, although the organoaluminium complexes **C3**–**C7** exhibited low catalytic activity in the hydroboration of isocyanates, the organozinc complex **C1** and the organomagnesium complex **C2** demonstrated excellent catalytic performance.

Table S6.1 Optimization of **C1-C7** catalysed hydroboration of *p*-tolyl isocyanate with HBpin. [a]



1a **4a**

Enrty	Cat.	Loading (mol%)	Sovlent	T (°C)	Time	Yield [b]
1	none	--	neat	r.t.	2 h	2 %
2	C1	5	neat	r.t.	15 min	97%
3	C2	5	neat	r.t.	15 min	96%
4	C3	5	neat	60	2 h	21%
5	C4	5	neat	60	2 h	17%
6	C5	5	neat	60	2 h	26%
7	C6	5	neat	60	2 h	20%
8	C7	5	neat	60	2 h	19%
9	C1	1	Hex	r.t.	15 min	95%
10	C2	1	Hex	r.t.	15 min	95%
11	C1	1	Tol	r.t.	15 min	92%
12	C2	1	Tol	r.t.	15 min	91%
13	**C1**	**1**	**neat**	**r.t.**	**15 min**	**97%**
14	C2	1	neat	r.t.	15 min	95%
15	C1	1	neat	r.t.	30 min	97%
16	C2	1	neat	r.t.	30 min	96%

[a] Reaction conditions: *p*-tolyl isocyanate (**1a**) (1.00 mmol), HBpin (1.1 mmol), and **Cat.** (0.01-0.05 mmol, 1-5 mol%). [b] Yield determined by ^{1}H NMR spectroscopy based on isocyanate consumption; product confirmation was achieved by identifying the NC*H*O signal.

a) Monohydroboration of isocyanates catalysed by **C1**

All reactions were conducted under a nitrogen atmosphere. In a 10 mL Schlenk flask

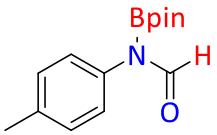
equipped with a magnetic stir bar, the corresponding isocyanate (1 mmol), HBpin (1.1 mmol), and **C1** (0.01 mmol) were combined within a glovebox. The reaction progress was monitored by ^{1}H NMR and ^{13}C NMR, with the disappearance of reactants and the formation of new products indicating reaction completion. The crude product was purified by washing with hexane.

b) Deoxygenative hydroboration of isocyanates catalysed by **C1**

All reactions were conducted under a nitrogen atmosphere. In a 10 mL Schlenk flask equipped with a magnetic stir bar, the corresponding isocyanate (1 mmol), HBpin (3.1 mmol), and **C1** (0.05 mmol) were combined in a glovebox and heated in an oil bath at 70 °C for 8 hours. The reaction progress was monitored by ^{1}H NMR and ^{13}C NMR, with the disappearance of reactants and the appearance of new products indicating completion. The reaction mixture was hydrolysed with 1 M HCl in diethyl ether (10 mL). Volatiles were removed under reduced pressure, and the residue was washed with ethyl acetate (3 × 5 mL) to yield the pure desired product as an ammonium salt.

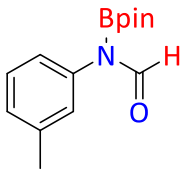
7. NMR data and spectra of formamide compounds

4a

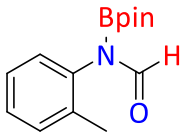


NMR yield 97%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.88 (s, 1H, NC*H*), 7.19 (d, 2H, Ar*H*), 7.04 (d, 2H, Ar*H*), 2.35 (s, 3H, CH_3), 1.32 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 164.5, 135.8, 128.5, 127.9, 126.1, 83.5, 23.5, 20.1. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.59.

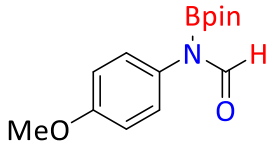
4b



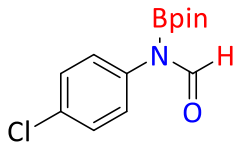
NMR yield 96%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.87 (s, 1H, NC*H*), 7.27 – 7.24 (m, 1H, Ar*H*), 7.10 (d, 1H, Ar*H*), 6.97 – 6.89 (m, 2H, Ar*H*), 2.36 (s, 3H, CH_3), 1.31 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.6, 138.7, 136.3, 128.7, 128.1, 124.4, 84.5, 24.6, 21.4. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.72.

4c 

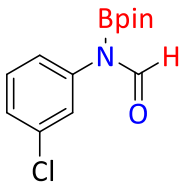
NMR yield 96%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.88 (s, 1H, NC*H*), 7.23 (td, 3H, Ar*H*), 7.04 – 6.98 (m, 1H, Ar*H*), 2.16 (s, 3H, CH_3), 1.29 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.2, 135.5, 135.0, 130.8, 128.2, 127.9, 126.7, 84.5, 24.6, 17.9. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.56.

4d 

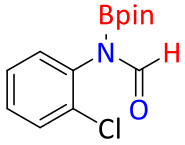
NMR yield 97%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.85 (s, 1H, NC*H*), 7.05 (d, 2H, Ar*H*), 6.89 (d, 2H, Ar*H*), 3.79 (s, 3H, CH_3), 1.30 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.8, 158.4, 128.3, 121.6, 114.2, 84.5, 55.4, 24.6. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.72.

4e 

NMR yield 95%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.85 (s, 1H, NC*H*), 7.34 (d, 2H, Ar*H*), 7.09 (d, 2H, Ar*H*), 1.31 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.3, 132.8, 129.0, 128.7, 121.1, 84.8, 24.5. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.31.

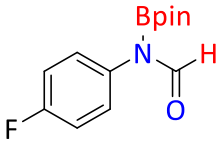
4f 

NMR yield 94%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.78 (s, 1H, NC*H*), 7.26 – 7.18 (m, 2H, Ar*H*), 7.10 (s, 1H, Ar*H*), 7.00 – 6.95 (m, 1H, Ar*H*), 1.25 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.2, 137.5, 134.2, 129.8, 127.8, 127.4, 125.7, 84.9, 24.5. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.46.

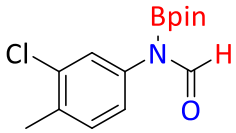
4g 

NMR yield 94%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.85 (s, 1H, NC*H*), 7.46 (d, 1H, Ar*H*), 7.30 – 7.26 (m, 2H, Ar*H*), 7.17 (d, 1H, Ar*H*), 1.30 (s, 12H, Bpin-CH_3).

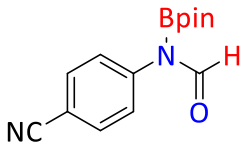
^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 164.8, 134.4, 132.1, 130.0, 130.0, 129.0, 127.5, 84.7, 24.6. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.39.

4h 

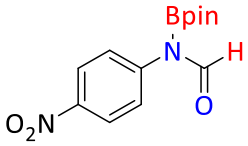
NMR yield 99%, pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.85 (s, 1H, NC*H*), 7.13 – 7.08 (m, 2H, Ar*H*), 7.05 (t, 2H, Ar*H*), 1.31 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.5, 129.0, 128.9, 121.7, 121.6, 115.8, 115.6, 84.7, 24.5. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.54.

4i 

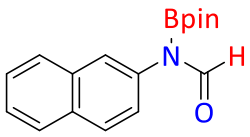
NMR yield 93%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.83 (s, 1H, NC*H*), 7.22 (d, 1H, Ar*H*), 7.15 (s, 1H, Ar*H*), 6.95 (d, 1H, Ar*H*), 2.35 (s, 3H, CH_3), 1.31 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.3, 135.1, 134.2, 131.0, 128.0, 125.7, 84.8, 77.4, 24.6, 19.7. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.35.

4j 

NMR yield 98%, pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.86 (s, 1H, NC*H*), 7.66 (d, 2H, Ar*H*), 7.30 (d, 2H, Ar*H*), 1.31 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 164.8, 140.7, 133.3, 132.7, 128.2, 119.8, 118.5, 110.7, 85.1, 24.5. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.14.

4k 

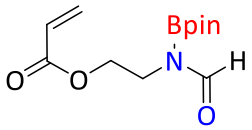
NMR yield 91%, pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.89 (s, 1H, NC*H*), 8.24 (d, 2H, Ar*H*), 7.36 (d, 2H, Ar*H*), 1.33 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 163.7, 145.2, 141.3, 127.1, 123.2, 84.2, 23.5. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.47.

4l 

NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 9.10 (s, 1H, NC*H*),

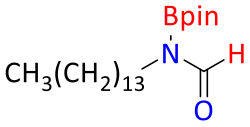
7.90 – 7.83 (m, 2H, Ar*H*), 7.71 (d, 1H, Ar*H*), 7.50 (t, 3H, Ar*H*), 7.31 – 7.26 (m, 1H, Ar*H*), 1.30 (s, 6H, Bpin-CH_3), 1.28 (s, 6H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.7, 134.4, 133.2, 130.2, 128.5, 128.3, 126.6, 126.1, 125.7, 125.5, 122.4, 84.6, 24.6. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.53.

4m



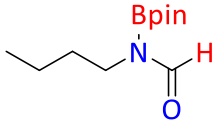
NMR yield 96%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.65 (d, 1H, NC*H*), 6.41 (dd, 1H, CHCH_2), 6.18 – 5.98 (m, 1H, C*H*CH$_2$), 5.82 (dd, 1H, CHCH_2), 4.24 (t, 2H, OCH_2), 3.64 (t, 2H, NCH_2), 1.26 (s, 12H, Bpin-CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.0, 129.9, 127.3, 83.4, 61.8, 38.0, 23.5. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.67.

4n



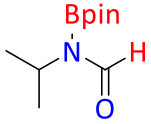
NMR yield 99%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.62 (s, 1H, NC*H*), 3.28 (t, 2H, NCH_2), 1.46 (t, 2H, NCH$_2$CH_2), 1.27 (d, 12H, Bpin-CH_3), 1.24 (s, 22H, CH_2), 0.86 (d, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 166.2, 84.2, 40.2, 38.3, 32.1, 29.8, 29.8, 29.7, 29.5, 29.4, 27.0, 24.7, 24.7, 24.6, 22.8, 14.2. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 24.99.

4o



NMR yield 99%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.54 (s, 1H, NC*H*), 3.22 (t, 2H, NCH_2), 1.38 (p, 2H, NCH$_2$CH_2), 1.27 – 1.21 (m, 2H, CH_2CH$_3$), 1.20 (s, 12H, Bpin-CH_3), 0.82 (t, 3H, CH$_2$CH_3). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.0, 83.1, 38.8, 30.7, 23.5, 23.5, 19.0, 12.8. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.04.

4p



NMR yield 99%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 8.55 (s, 1H, NC*H*), 4.35 (p, 1H, C*H*Me$_2$), 1.22 (s, 12H, Bpin-CH_3), 1.16 (d, 6H, CHMe_2). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 165.6, 83.3, 41.3, 24.1, 24.0, 20.9. ^{11}B NMR (128 MHz, $CDCl_3$, 298K, TMS) δ 25.53.

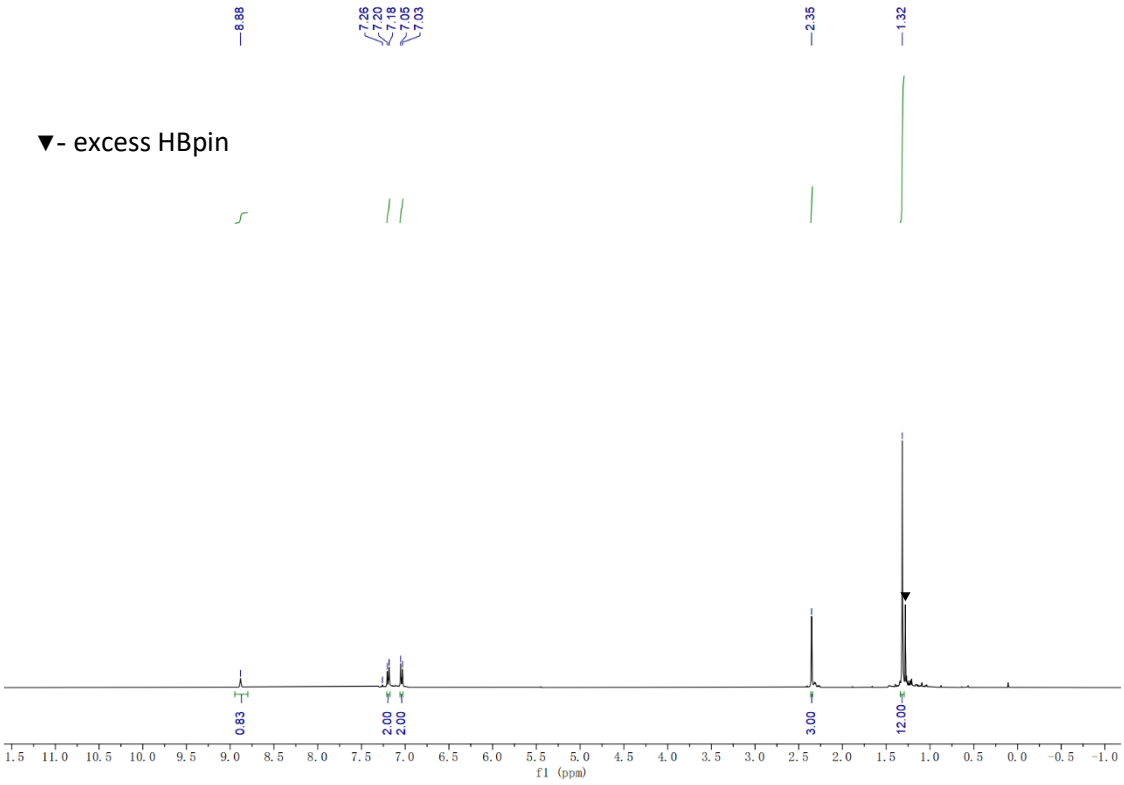


Figure S7.1 ^{1}H NMR spectrum of **4a** in $CDCl_3$ at 400 MHz.

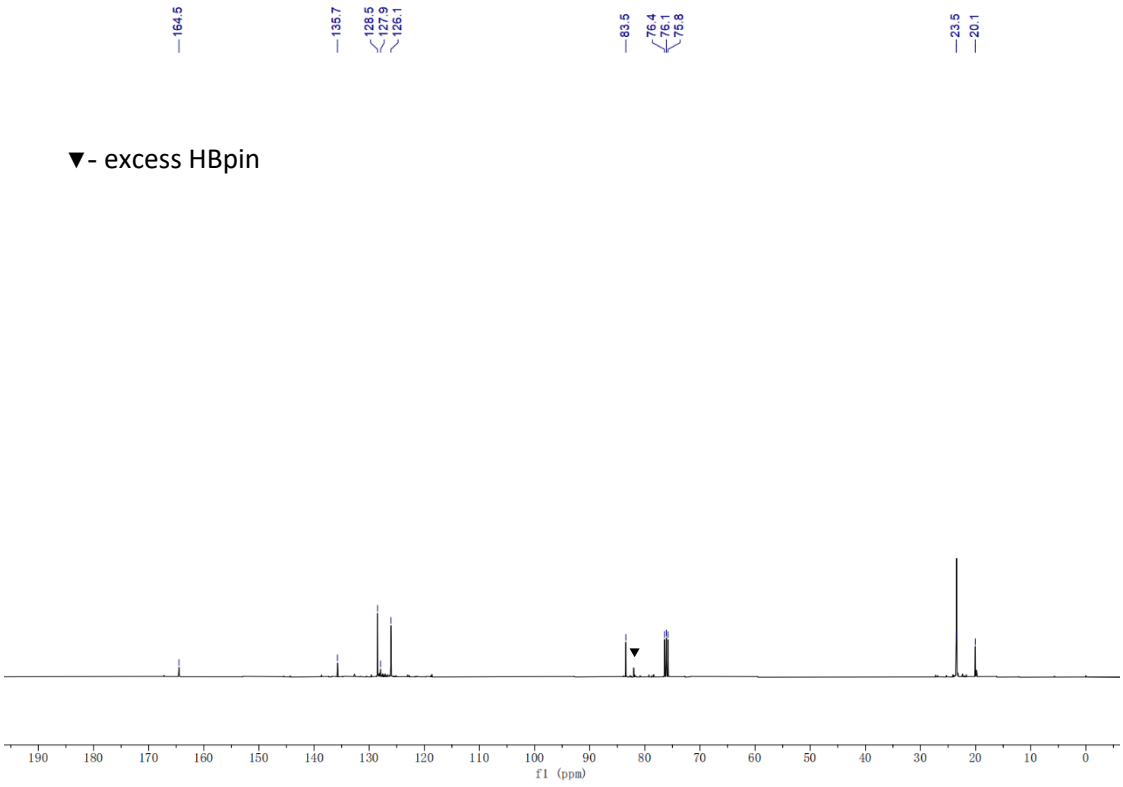


Figure S7.2 ^{13}C NMR spectrum of **4a** in $CDCl_3$ at 101 MHz.

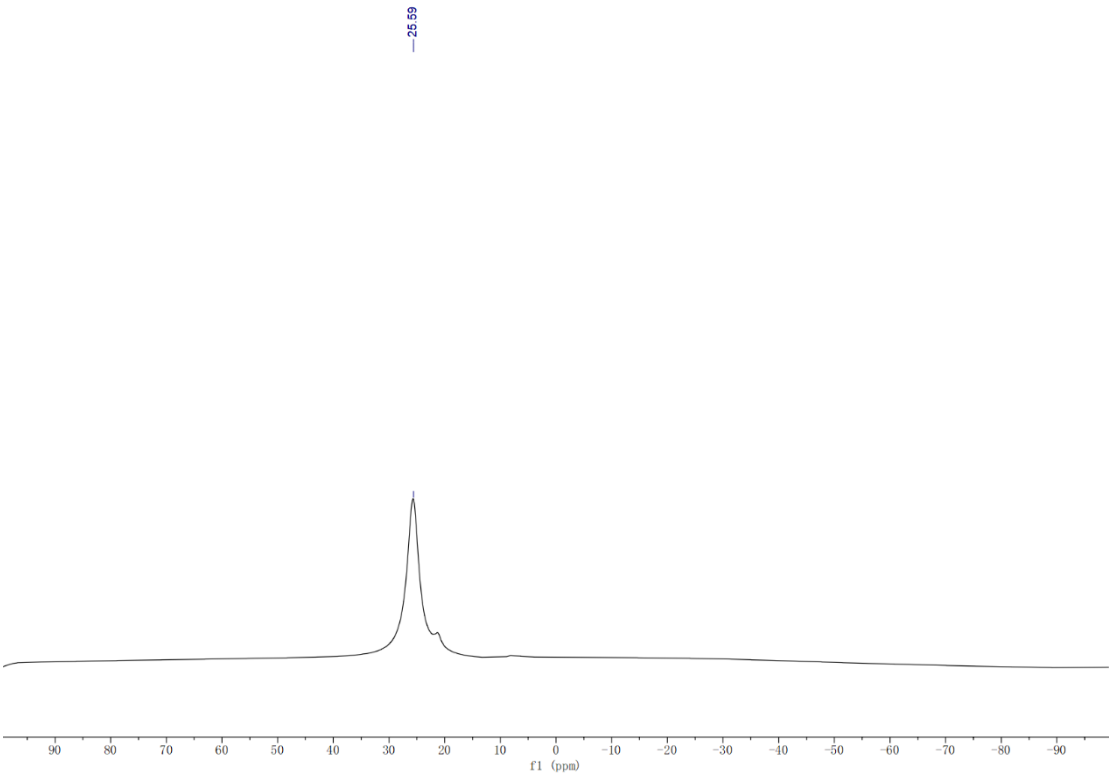


Figure S7.3 ^{11}B NMR spectrum of **4a** in $CDCl_3$ at 128 MHz.

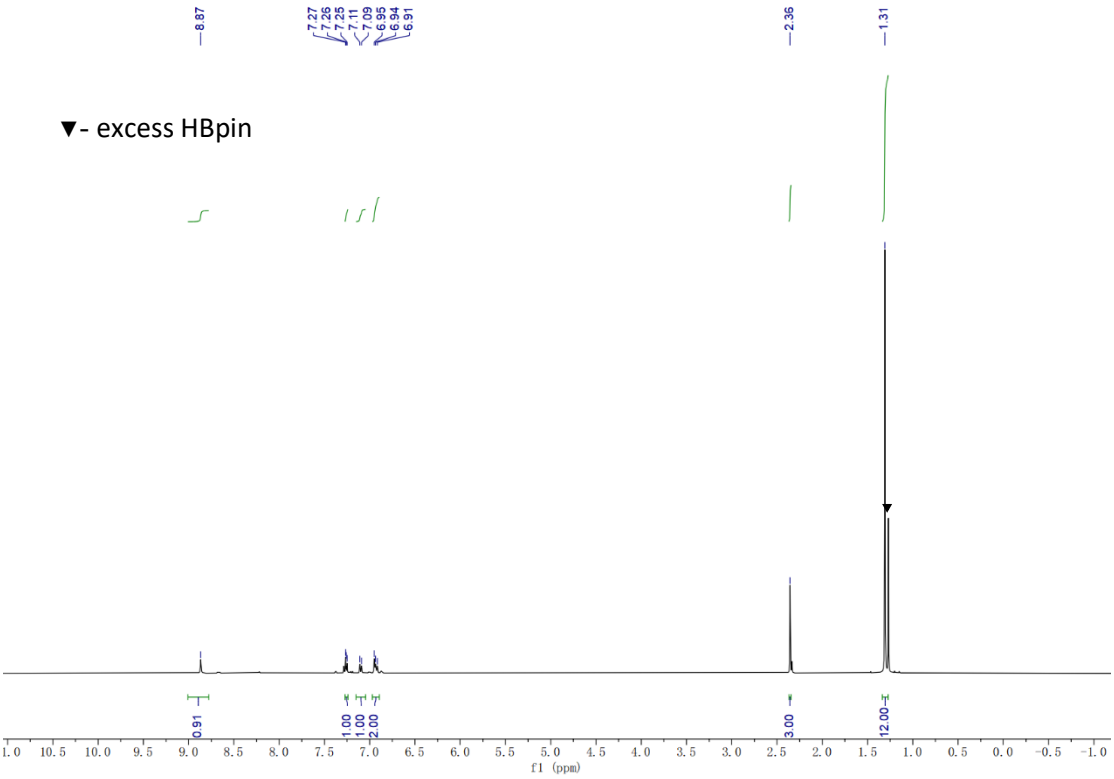


Figure S7.4 ^{1}H NMR spectrum of **4b** in $CDCl_3$ at 400 MHz.

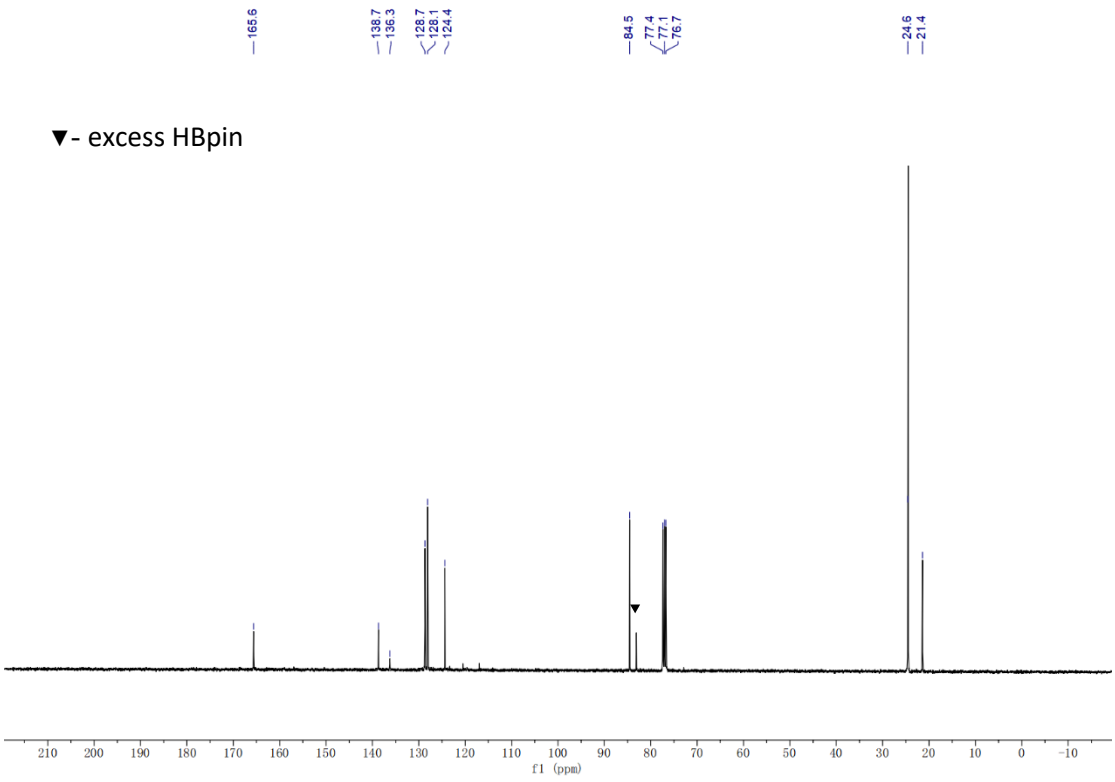


Figure S7.5 ^{13}C NMR spectrum of **4b** in $CDCl_3$ at 101 MHz.

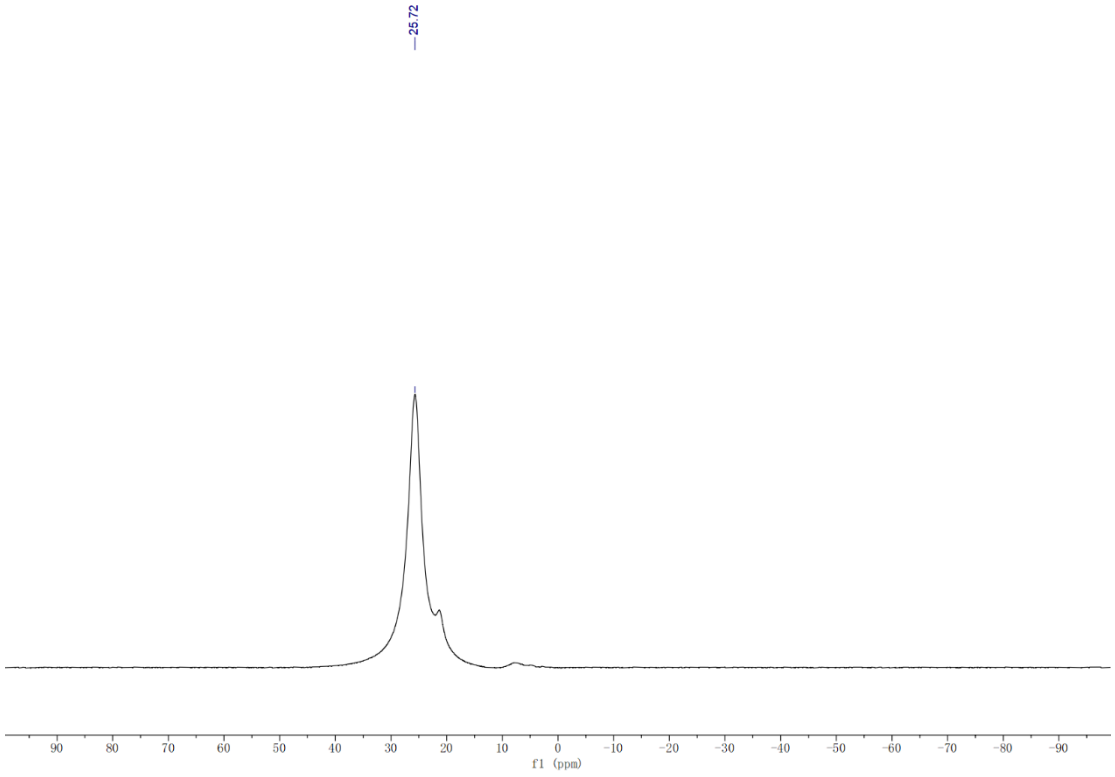


Figure S7.6 ^{11}B NMR spectrum of **4b** in $CDCl_3$ at 128 MHz.

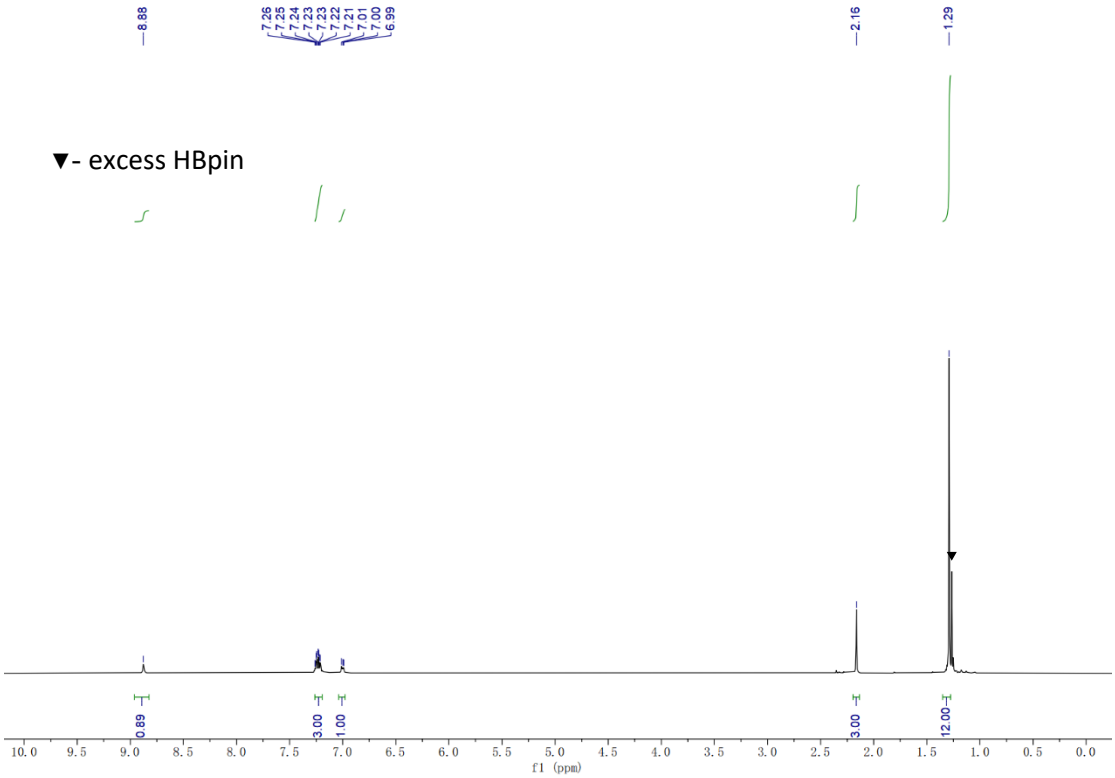


Figure S7.7 ^{1}H NMR spectrum of **4c** in $CDCl_3$ at 400 MHz.

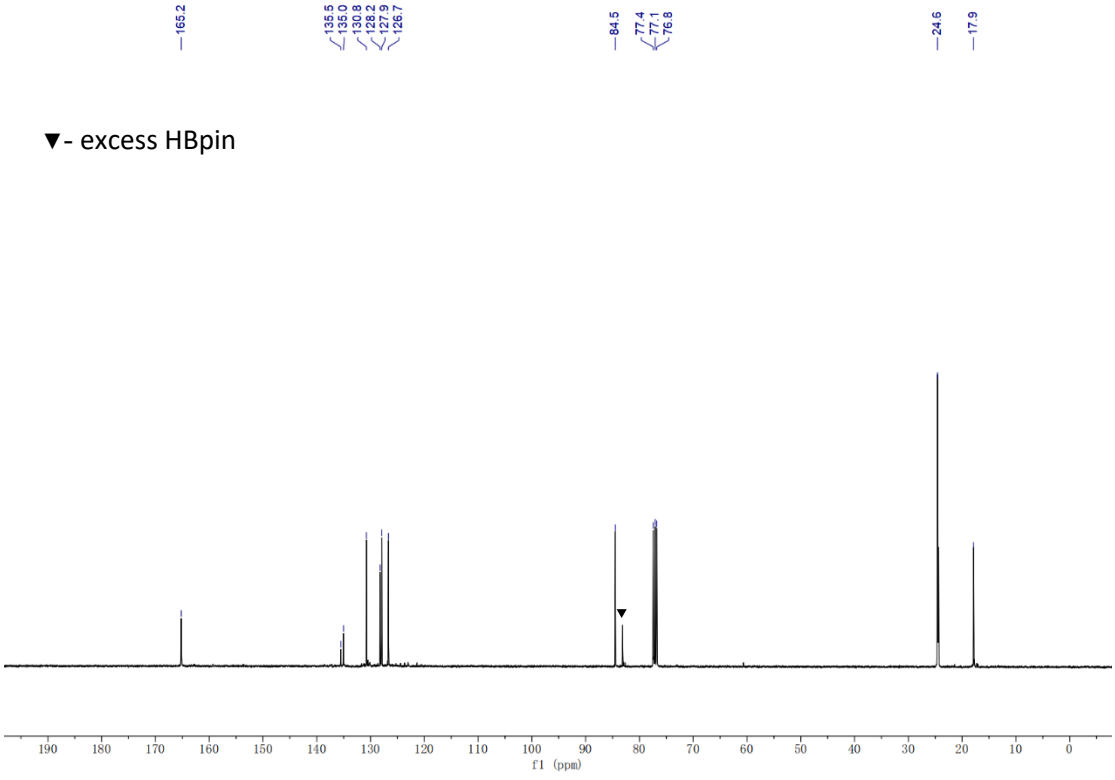


Figure S7.8 ^{13}C NMR spectrum of **4c** in $CDCl_3$ at 101 MHz.

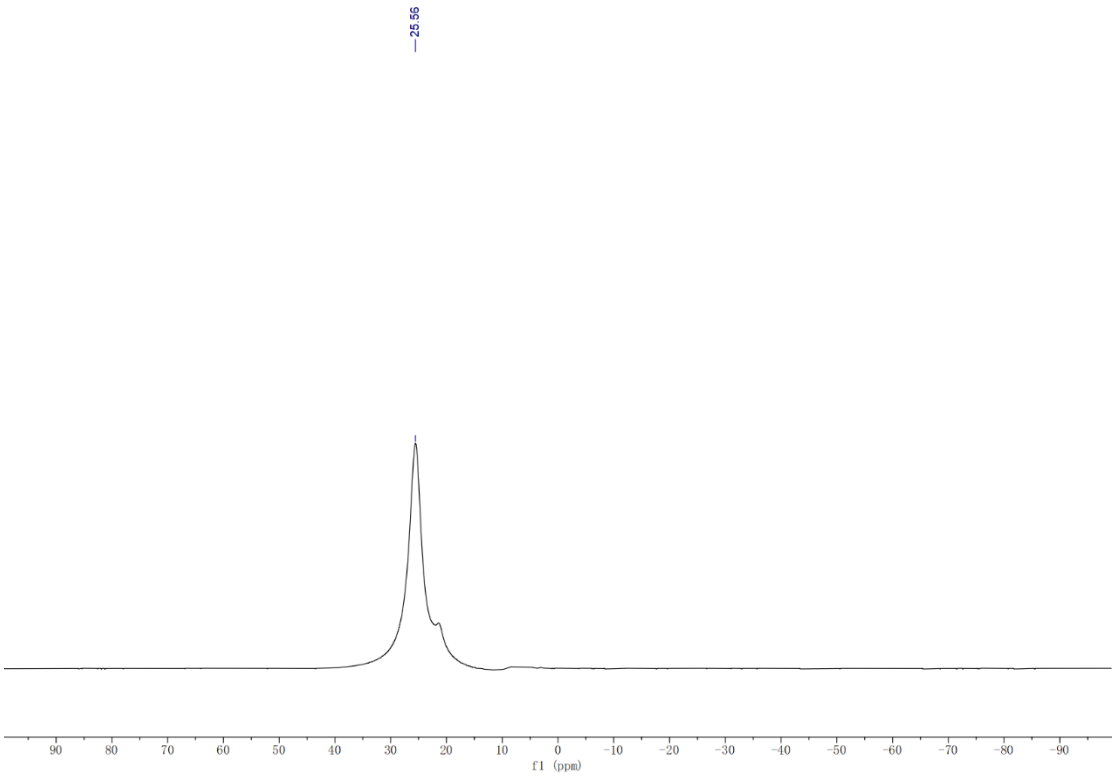


Figure S7.9 ^{11}B NMR spectrum of **4c** in $CDCl_3$ at 128 MHz.

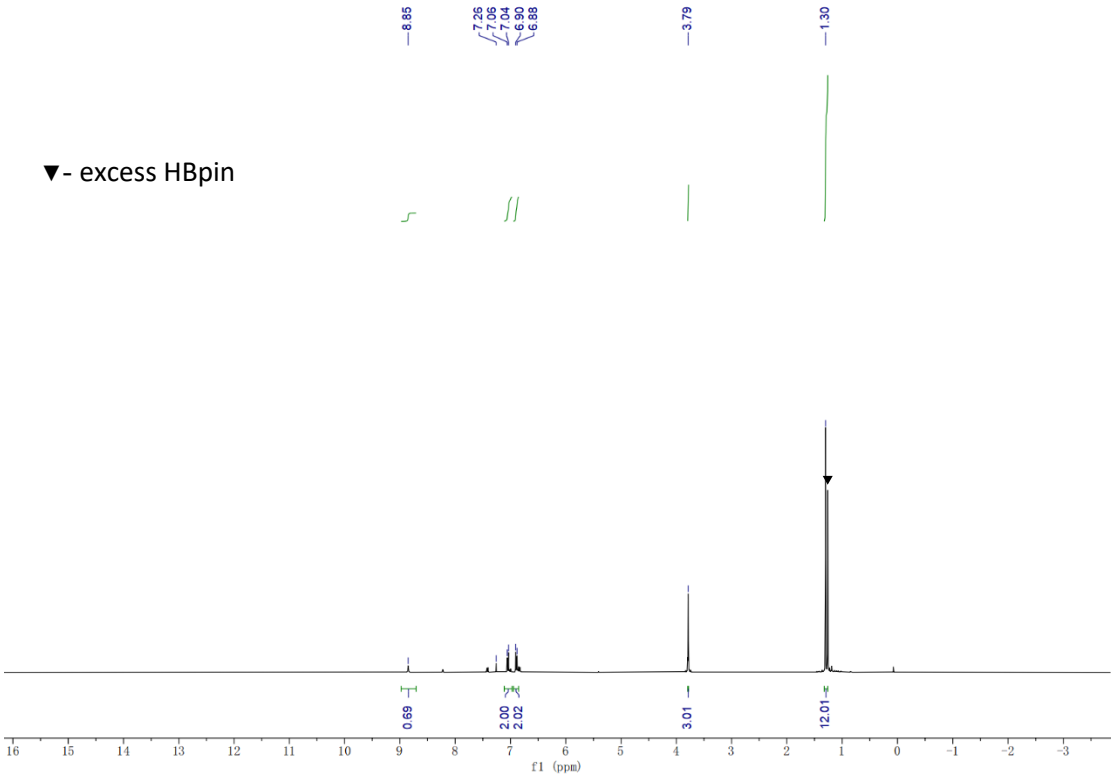


Figure S7.10 ^{1}H NMR spectrum of **4d** in $CDCl_3$ at 400 MHz.

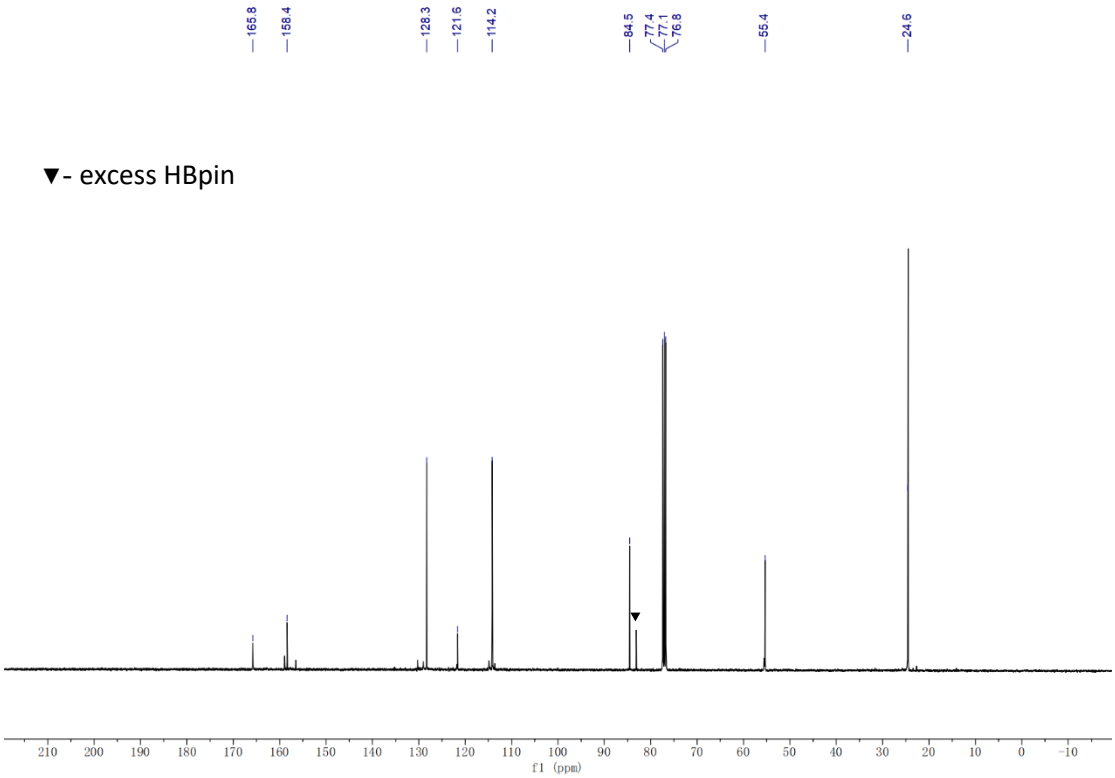


Figure S7.11 ^{13}C NMR spectrum of **4d** in $CDCl_3$ at 101 MHz.

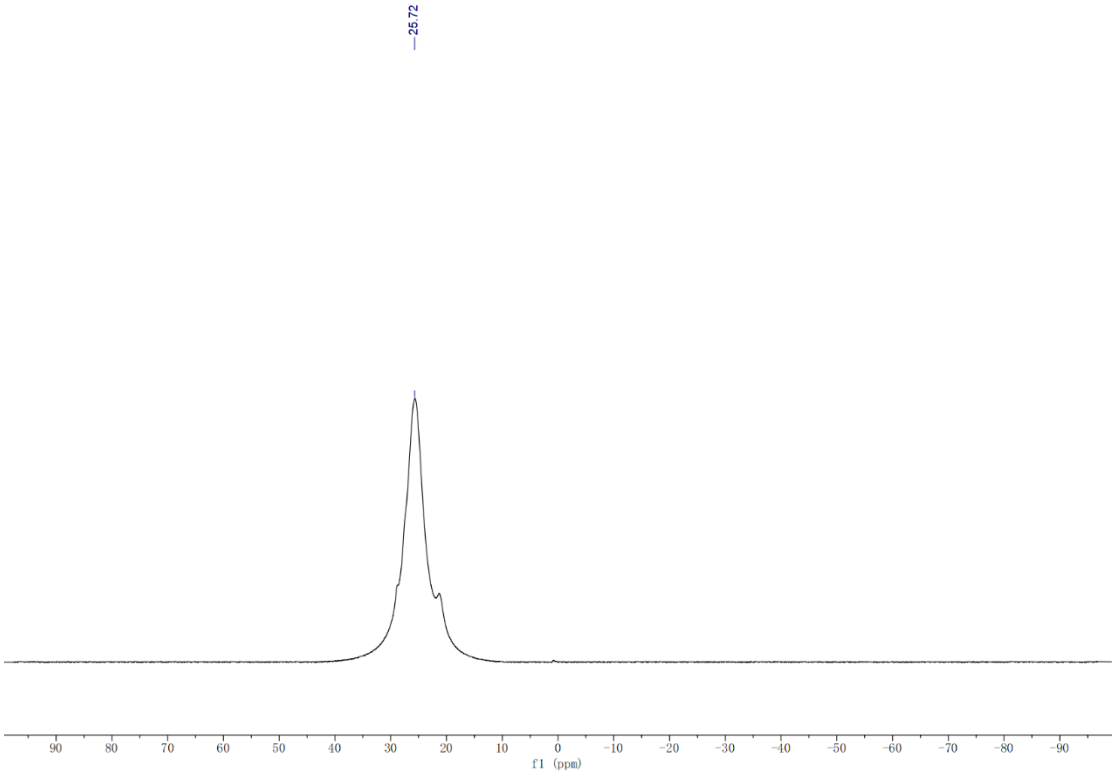


Figure S7.12 ^{11}B NMR spectrum of **4d** in $CDCl_3$ at 128 MHz.

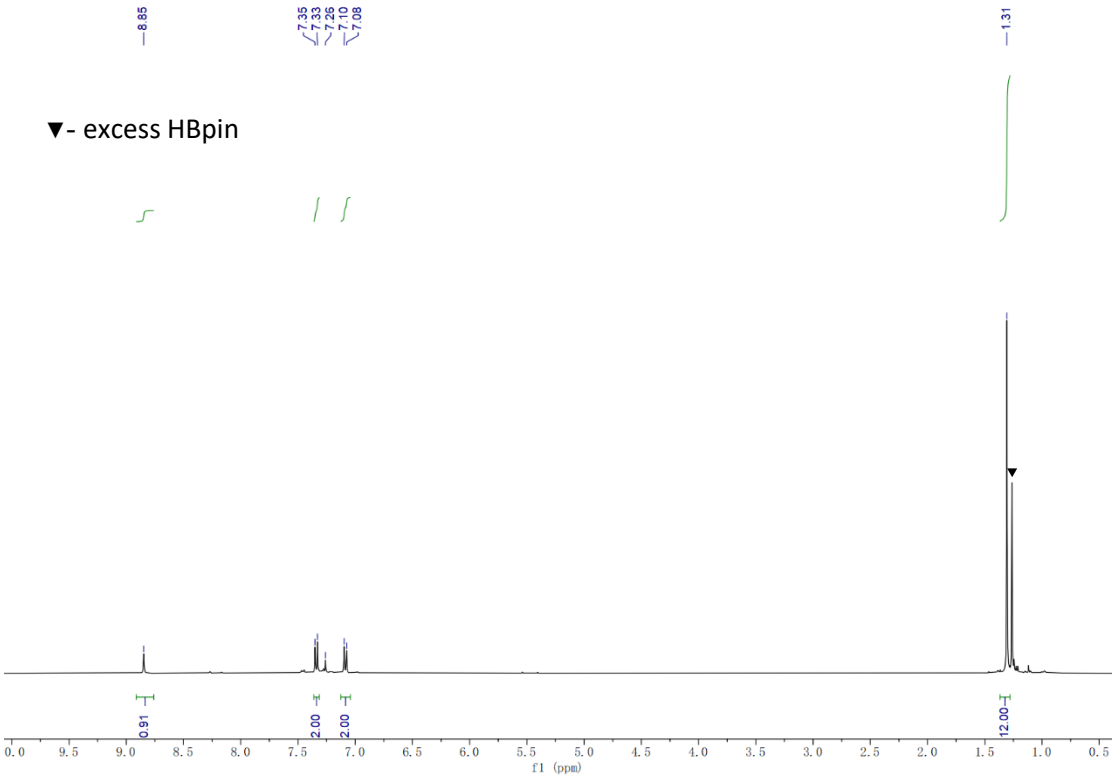


Figure S7.13 ^{1}H NMR spectrum of **4e** in $CDCl_3$ at 400 MHz.

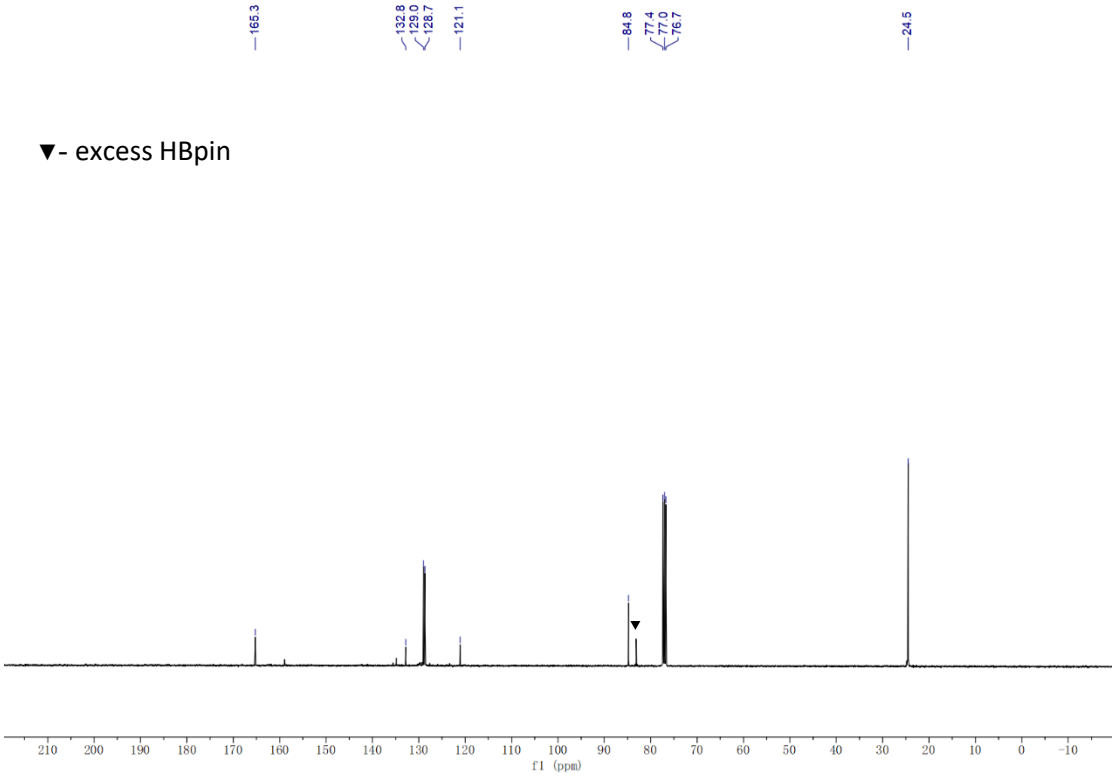


Figure S7.14 ^{13}C NMR spectrum of **4e** in $CDCl_3$ at 101 MHz.

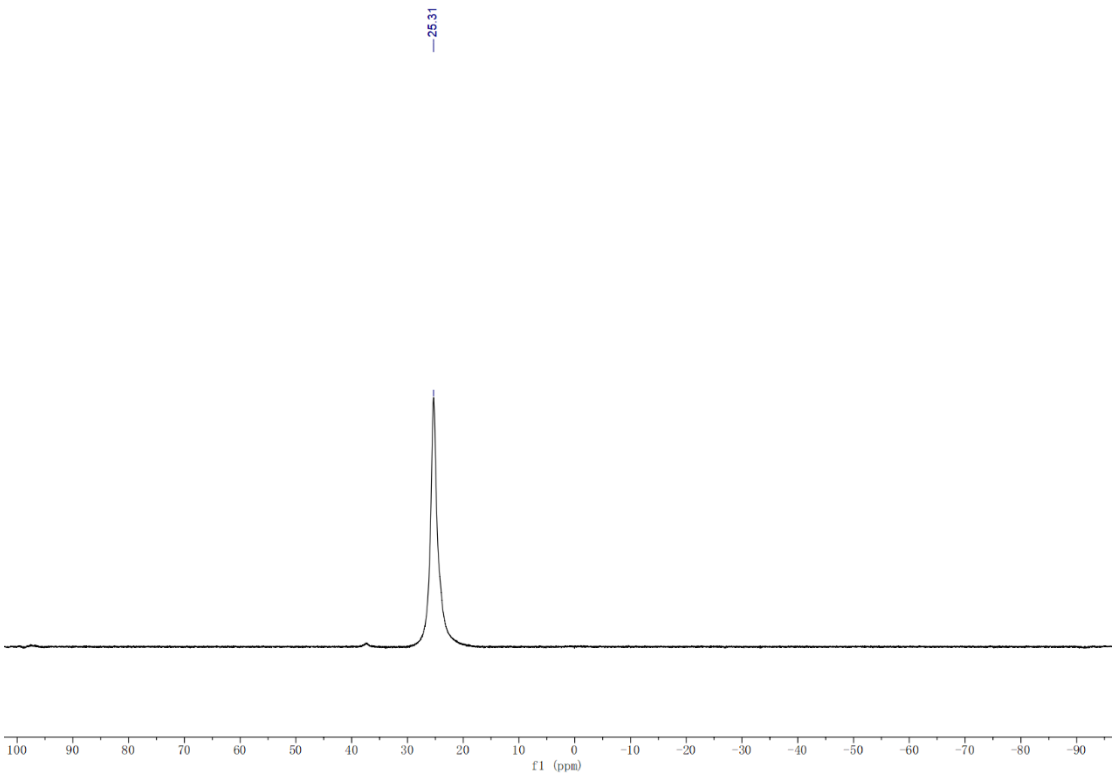


Figure S7.15 ^{11}B NMR spectrum of **4e** in $CDCl_3$ at 128 MHz.

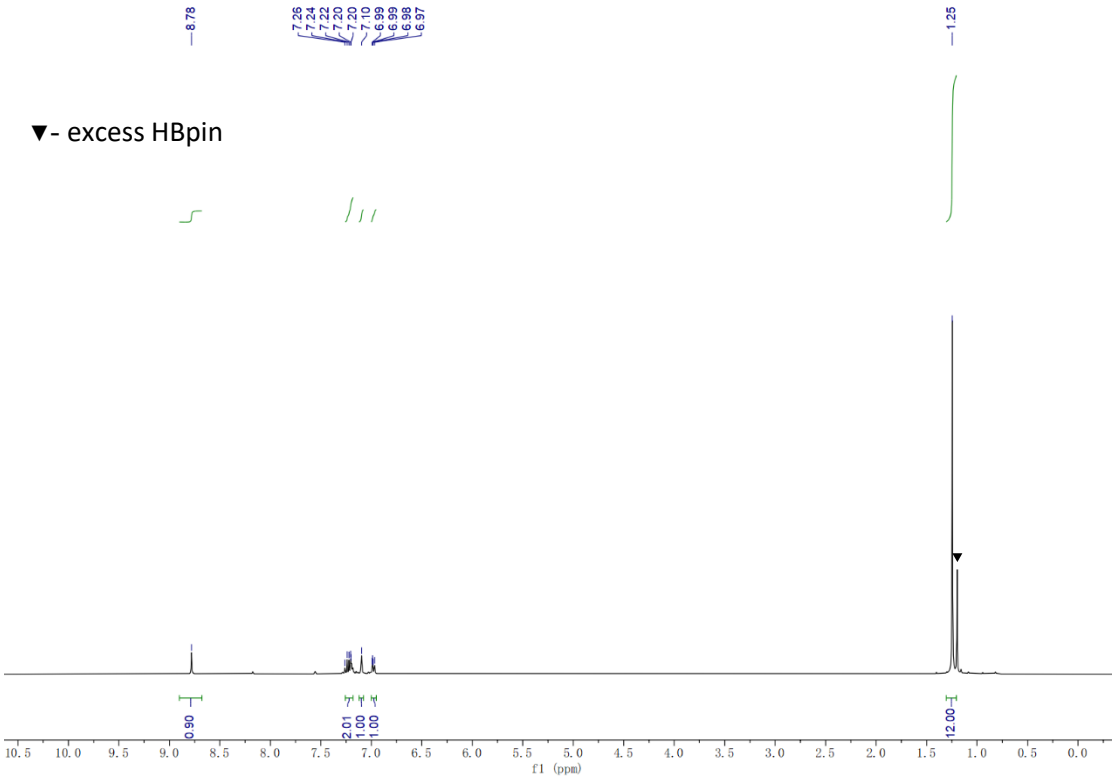


Figure S7.16 ^{1}H NMR spectrum of **4f** in $CDCl_3$ at 400 MHz.

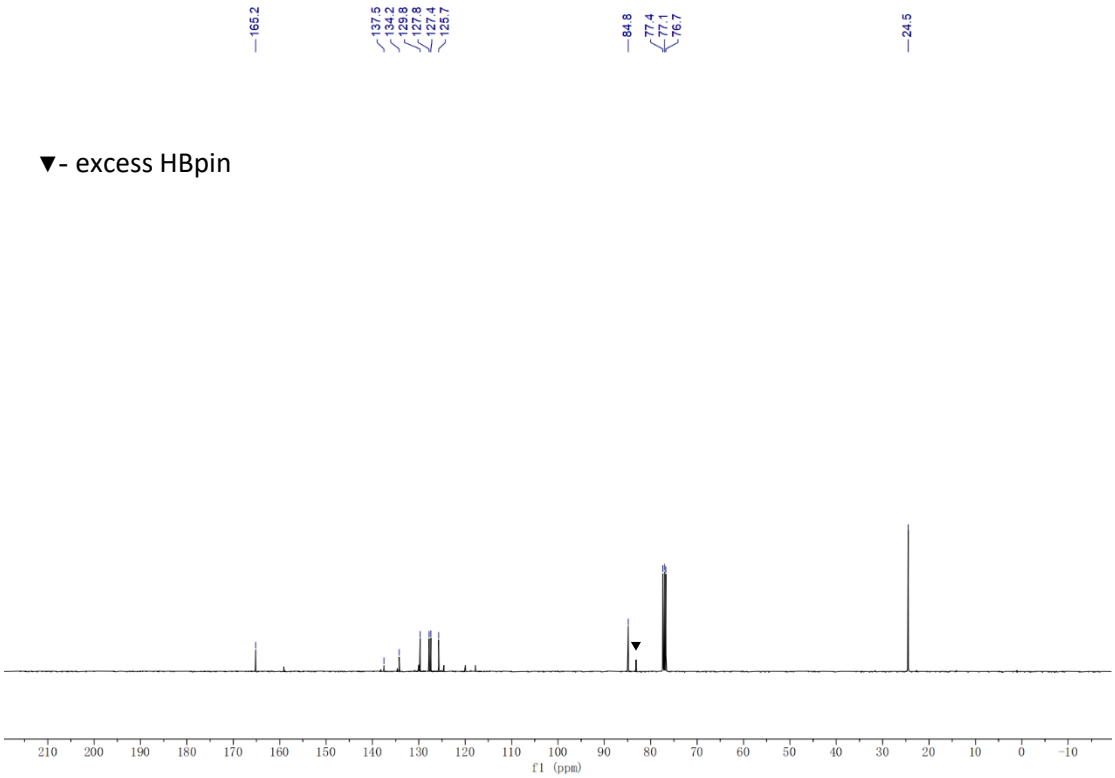


Figure S7.17 ^{13}C NMR spectrum of **4f** in $CDCl_3$ at 101 MHz.

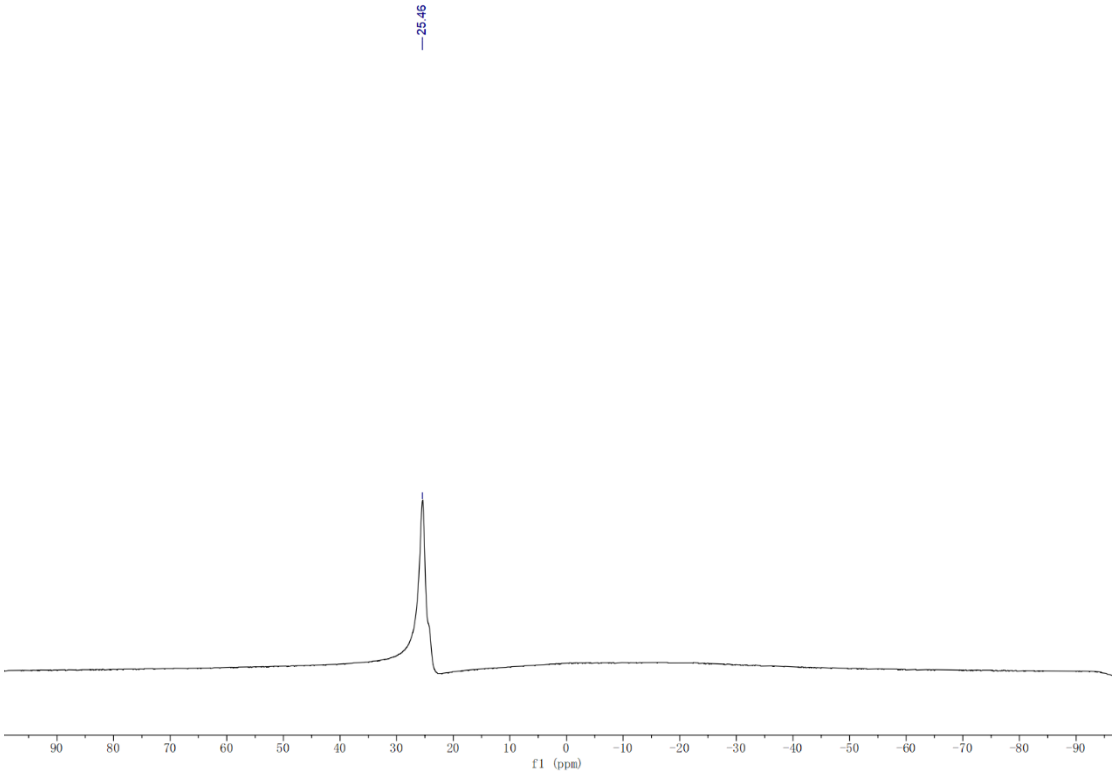


Figure S7.18 ^{11}B NMR spectrum of **4f** in $CDCl_3$ at 128 MHz.

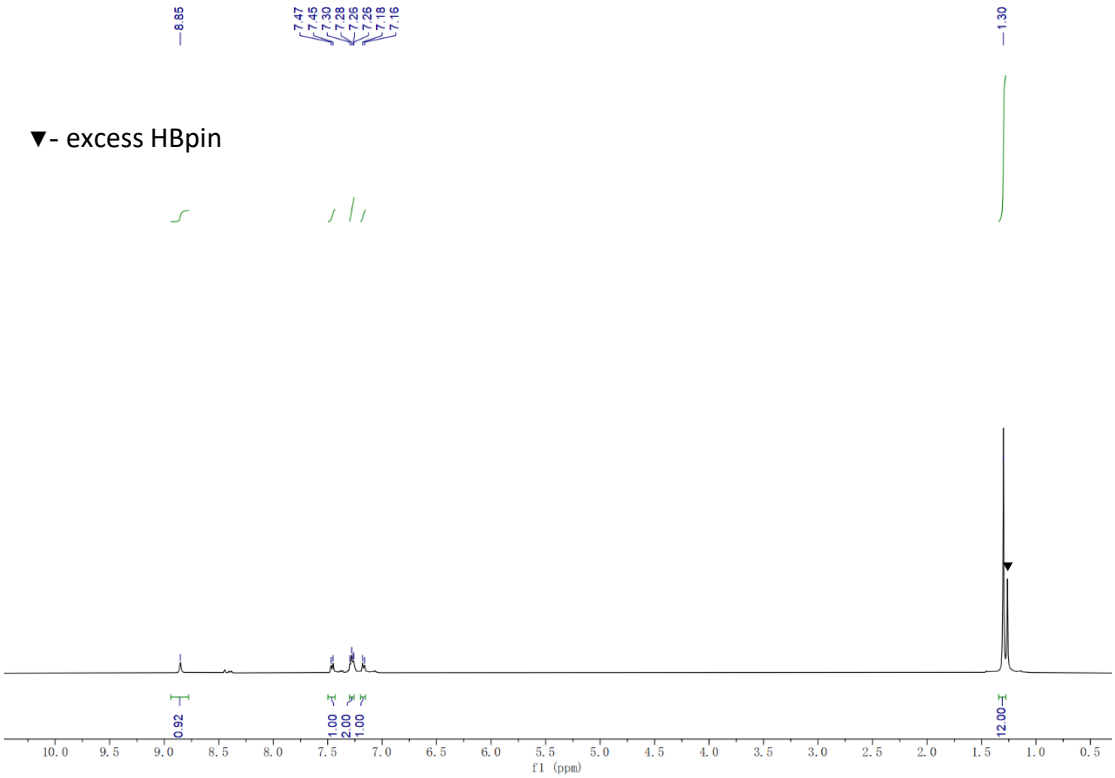


Figure S7.19 ^{1}H NMR spectrum of **4g** in $CDCl_3$ at 400 MHz.

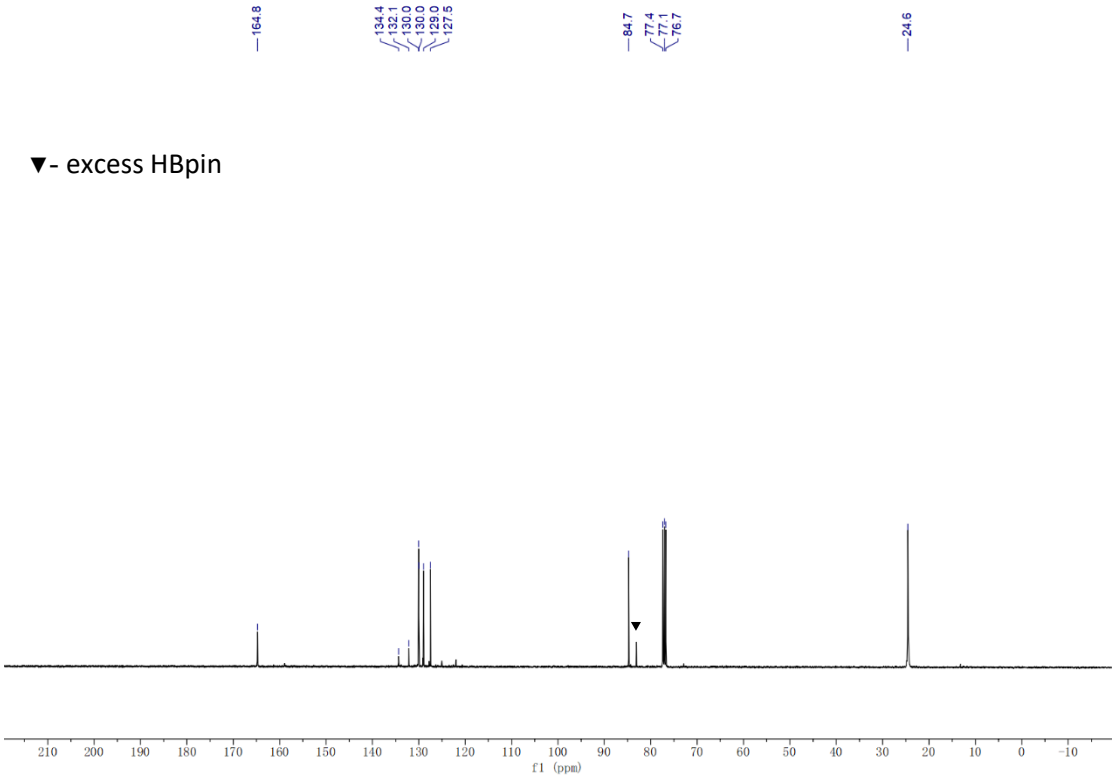


Figure S7.20 ^{13}C NMR spectrum of **4g** in $CDCl_3$ at 101 MHz.

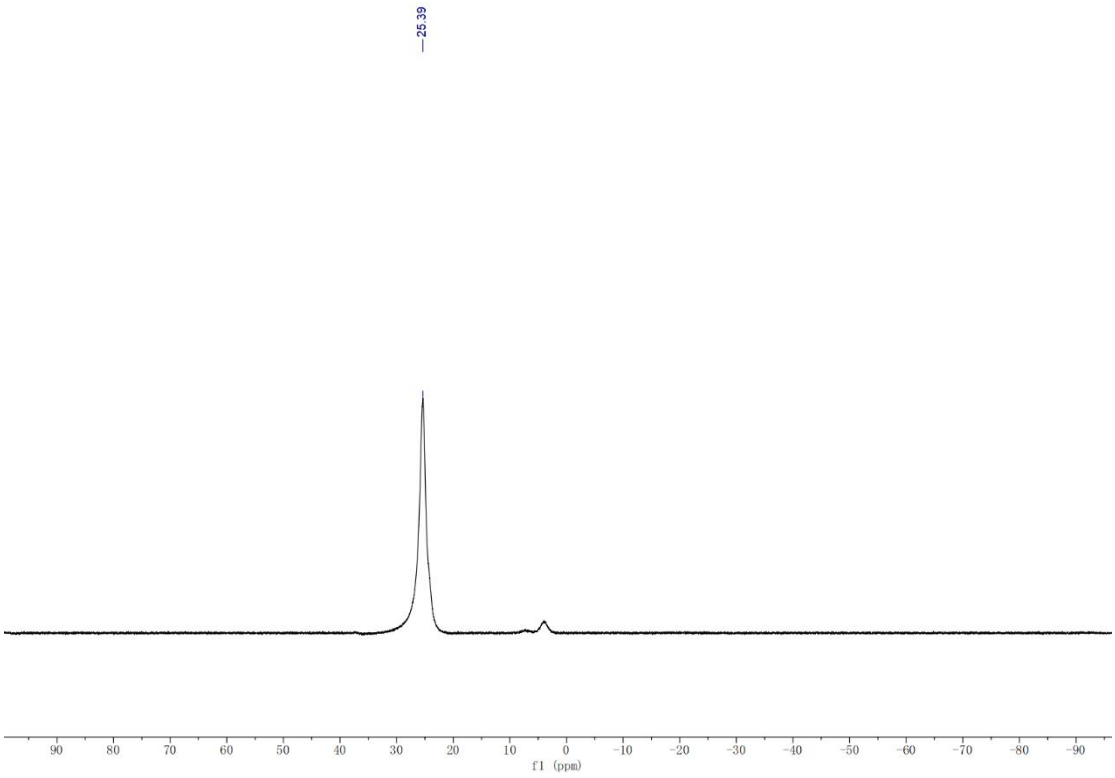


Figure S7.21 ^{11}B NMR spectrum of **4g** in $CDCl_3$ at 128 MHz.

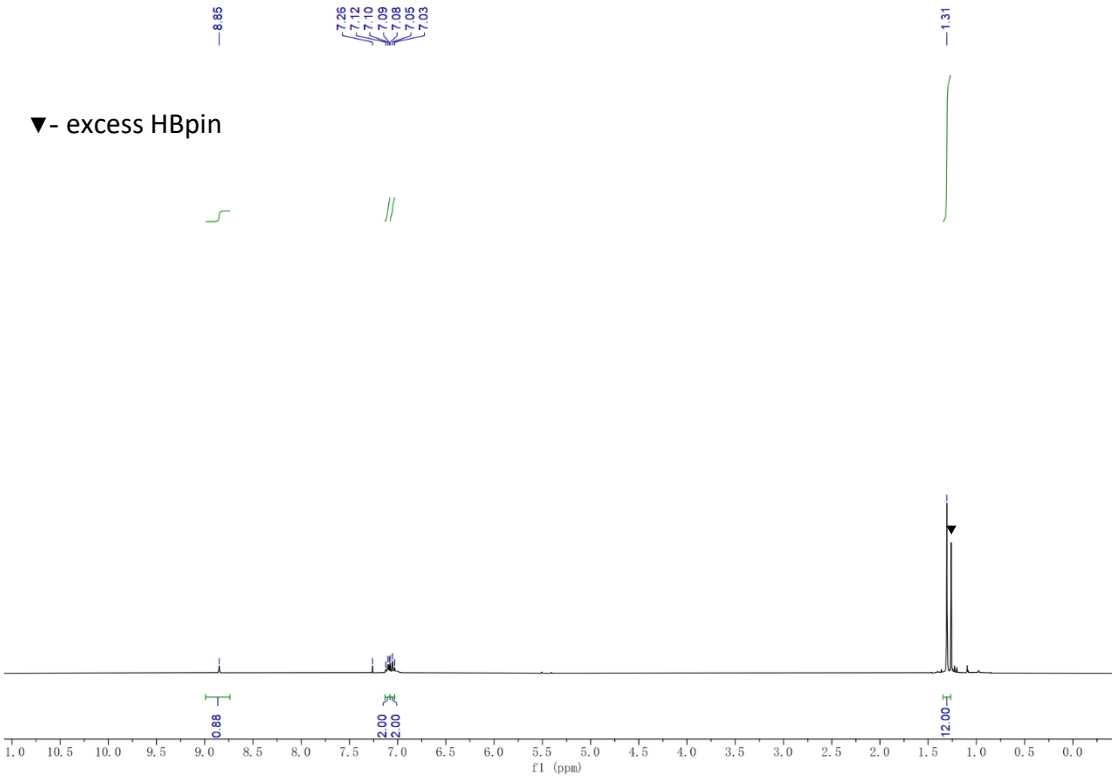
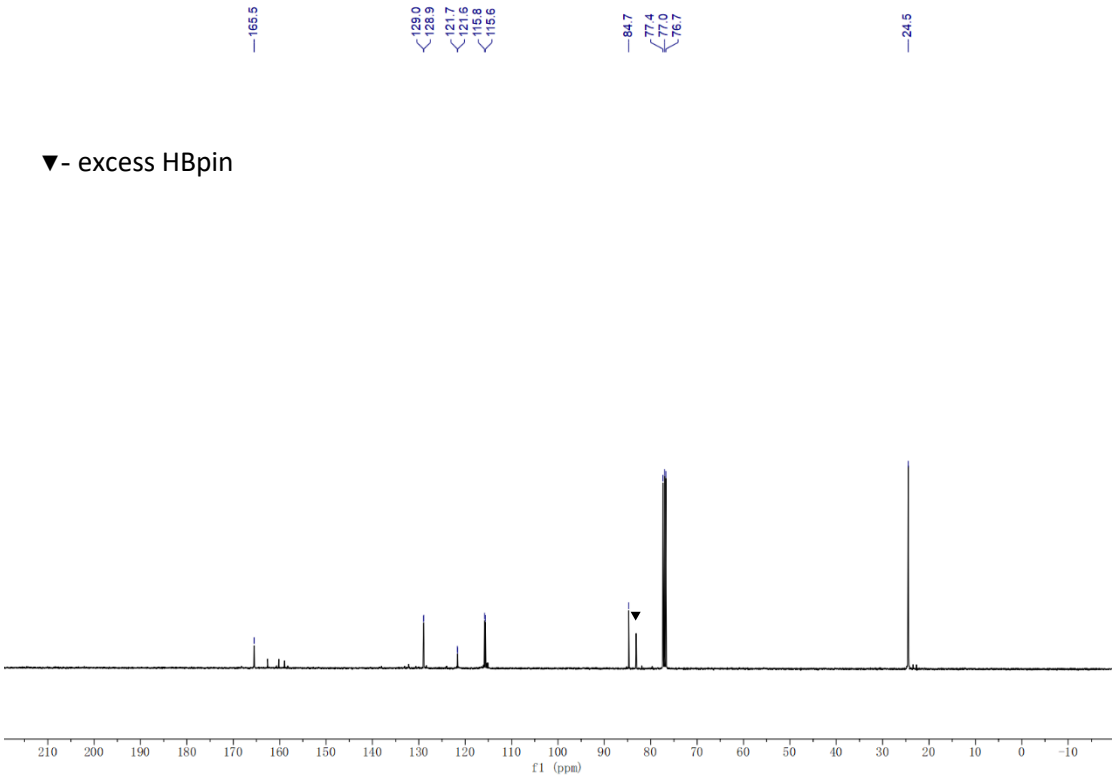


Figure S7.22 ^{1}H NMR spectrum of **4h** in $CDCl_3$ at 400 MHz.



▼- excess HBpin

Figure S7.23 ^{13}C NMR spectrum of **4h** in $CDCl_3$ at 101 MHz.

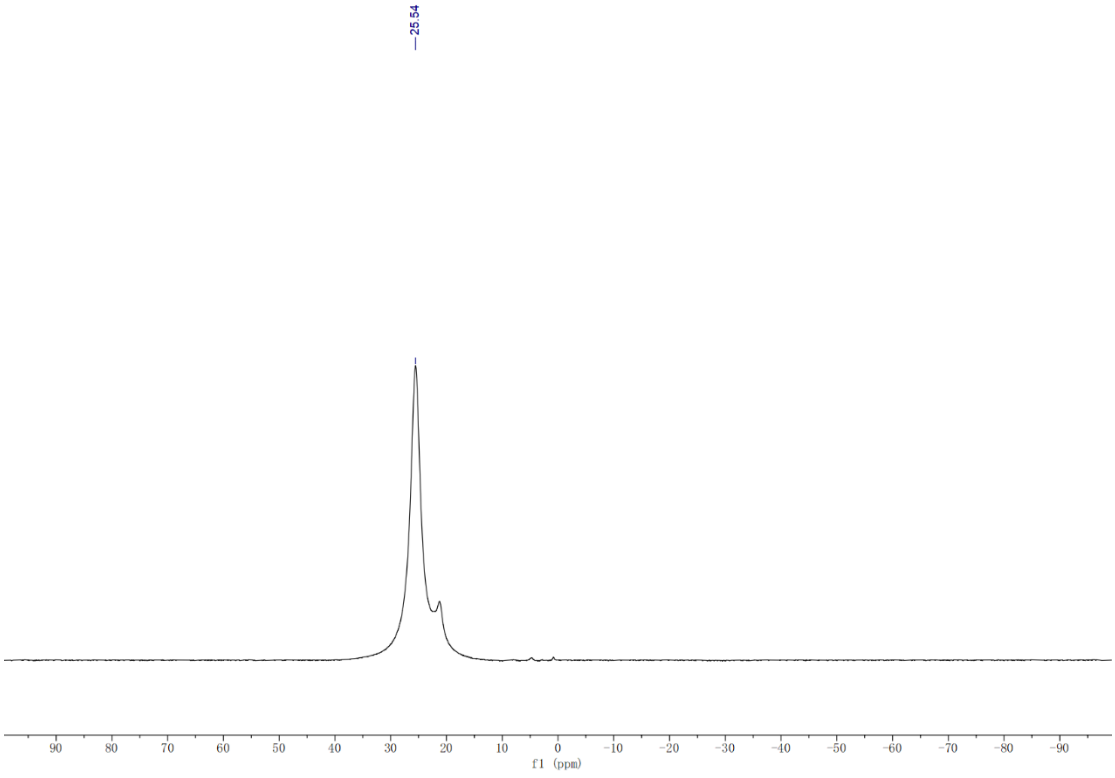


Figure S7.24 ^{11}B NMR spectrum of **4h** in $CDCl_3$ at 128 MHz.

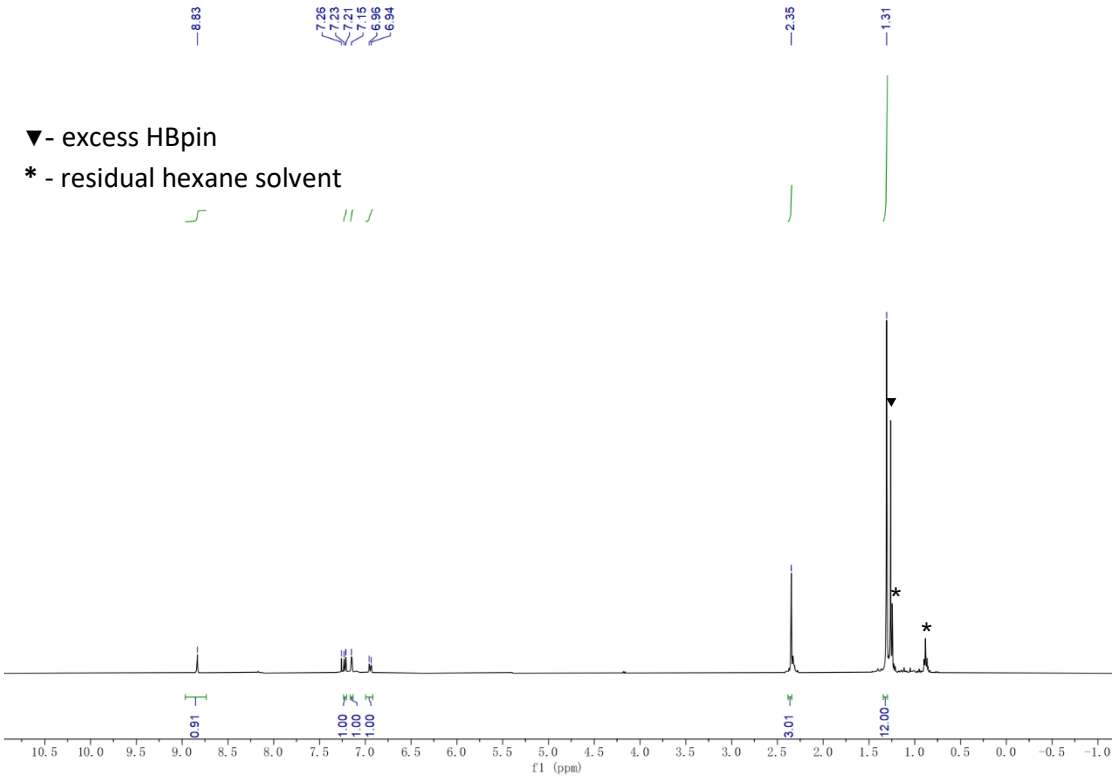


Figure S7.25 ^{1}H NMR spectrum of **4i** in $CDCl_3$ at 400 MHz.

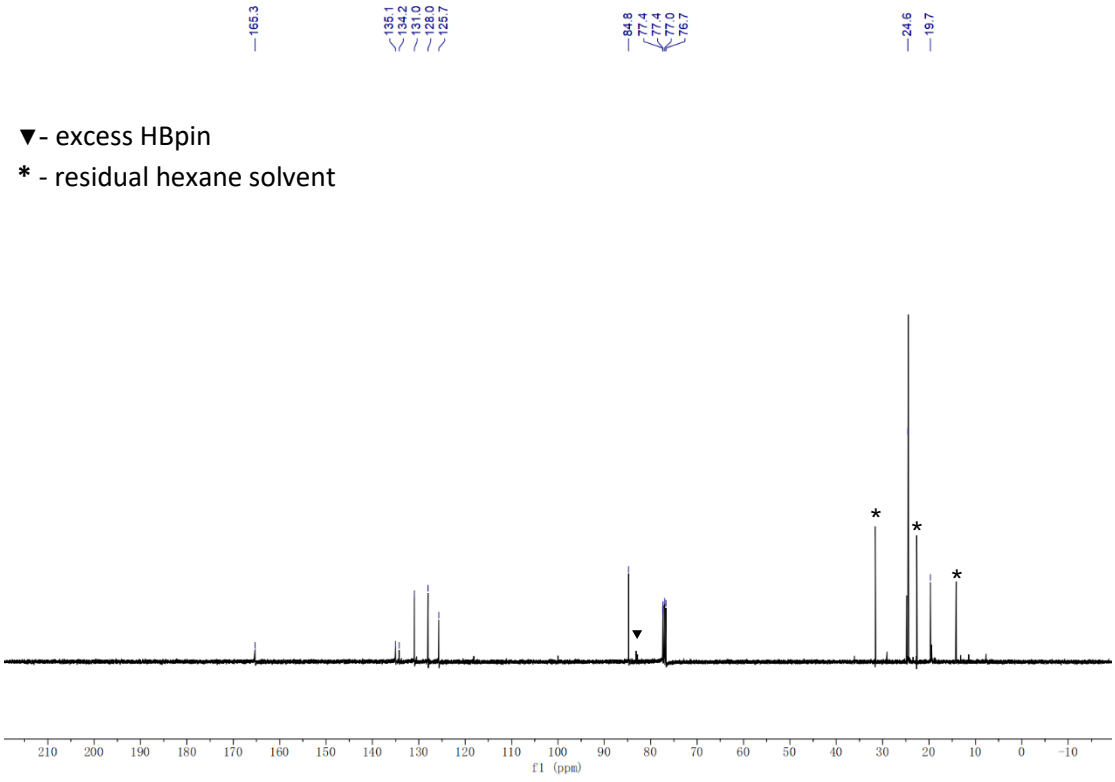


Figure S7.26 ^{13}C NMR spectrum of **4i** in $CDCl_3$ at 101 MHz.

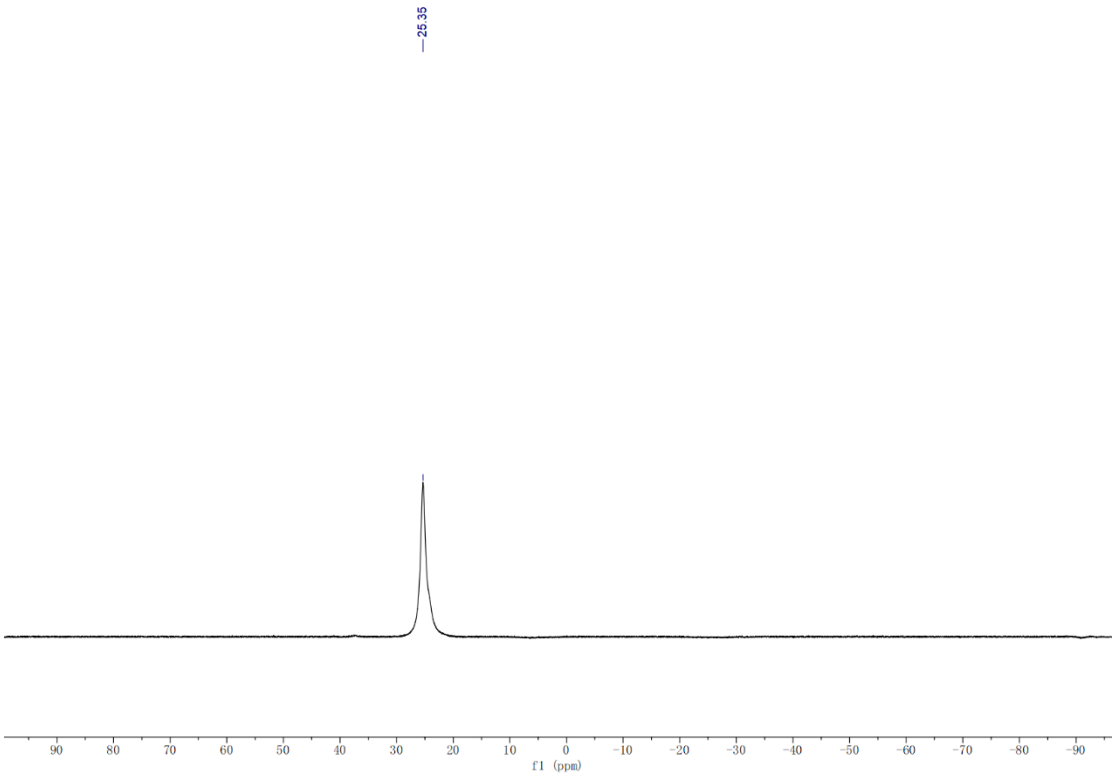


Figure S7.27 ^{11}B NMR spectrum of **4i** in $CDCl_3$ at 128 MHz.

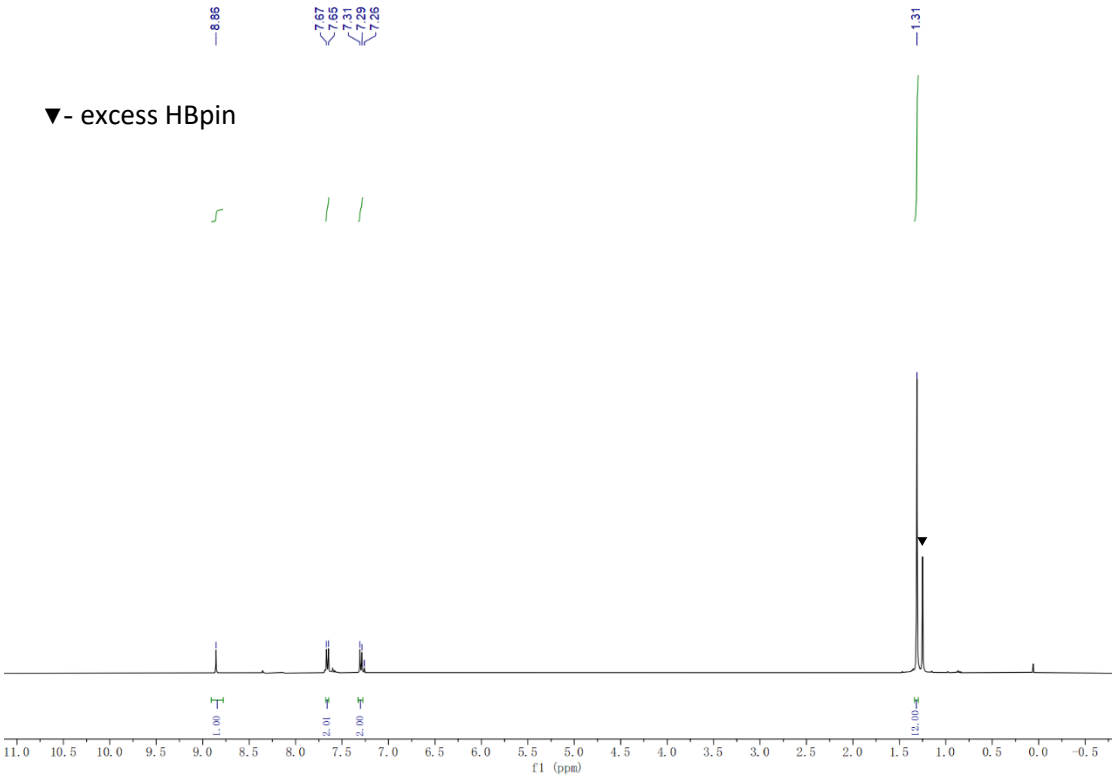
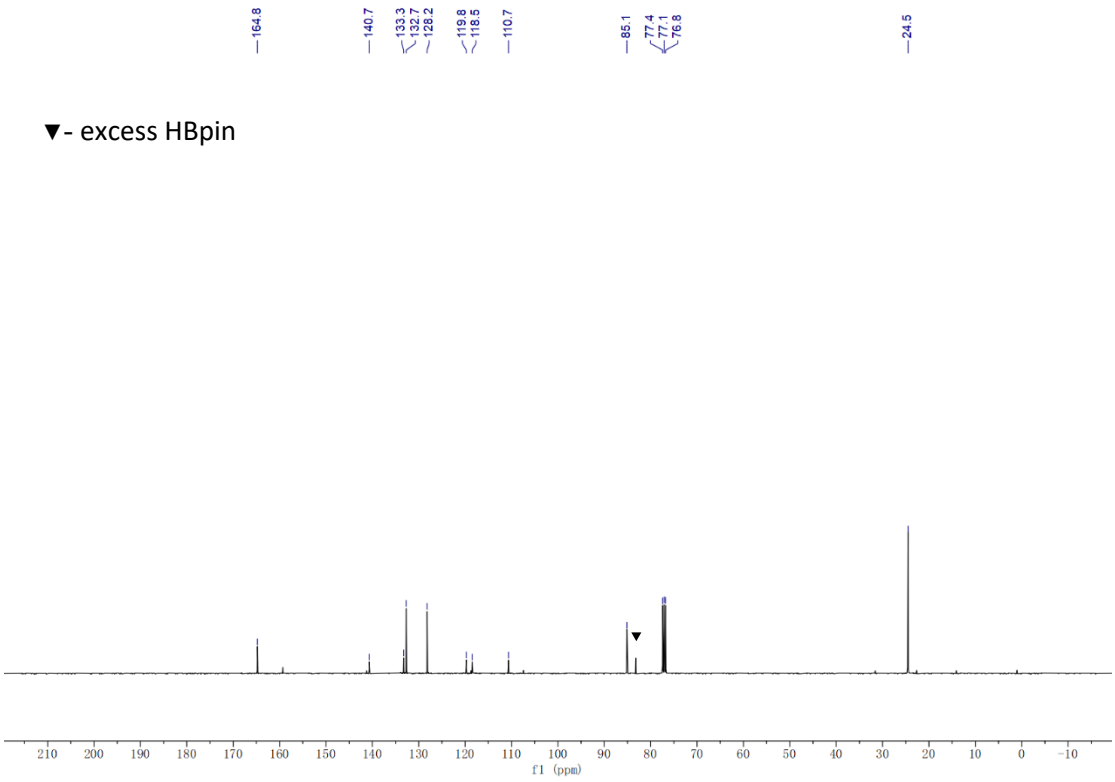


Figure S7.28 ^{1}H NMR spectrum of **4j** in $CDCl_3$ at 400 MHz.



▼- excess HBpin

Figure S7.29 ^{13}C NMR spectrum of **4j** in $CDCl_3$ at 101 MHz.

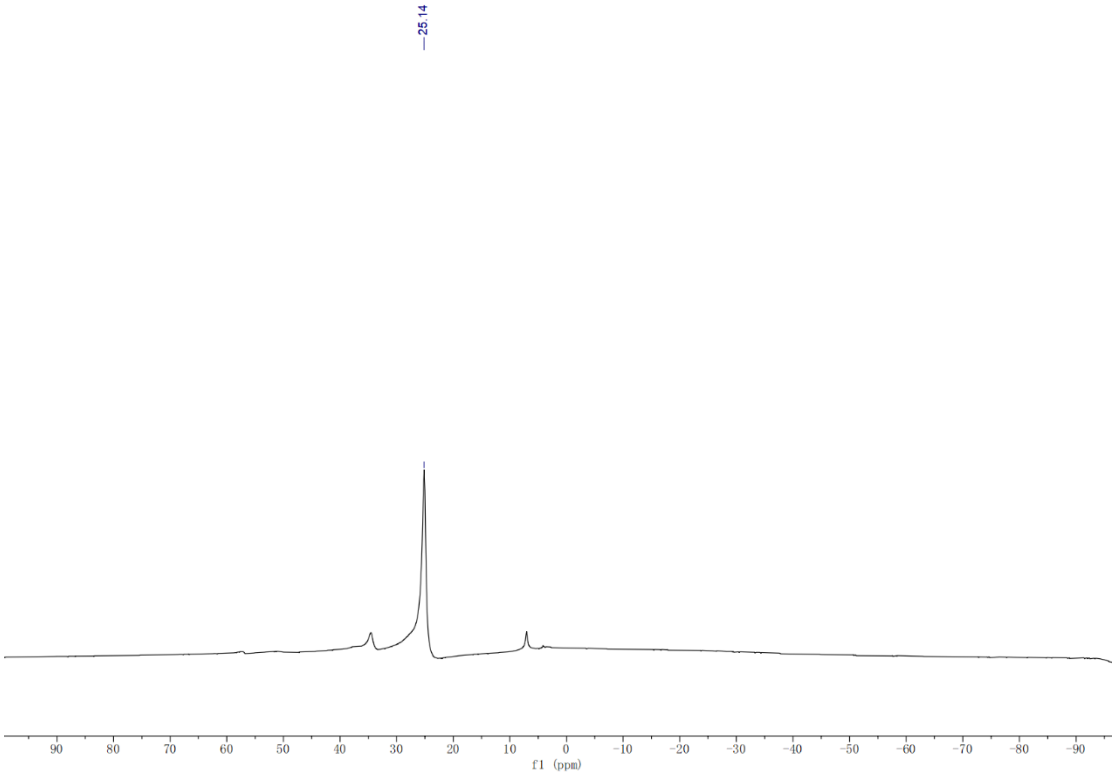


Figure S7.30 ^{11}B NMR spectrum of **4j** in $CDCl_3$ at 128 MHz.

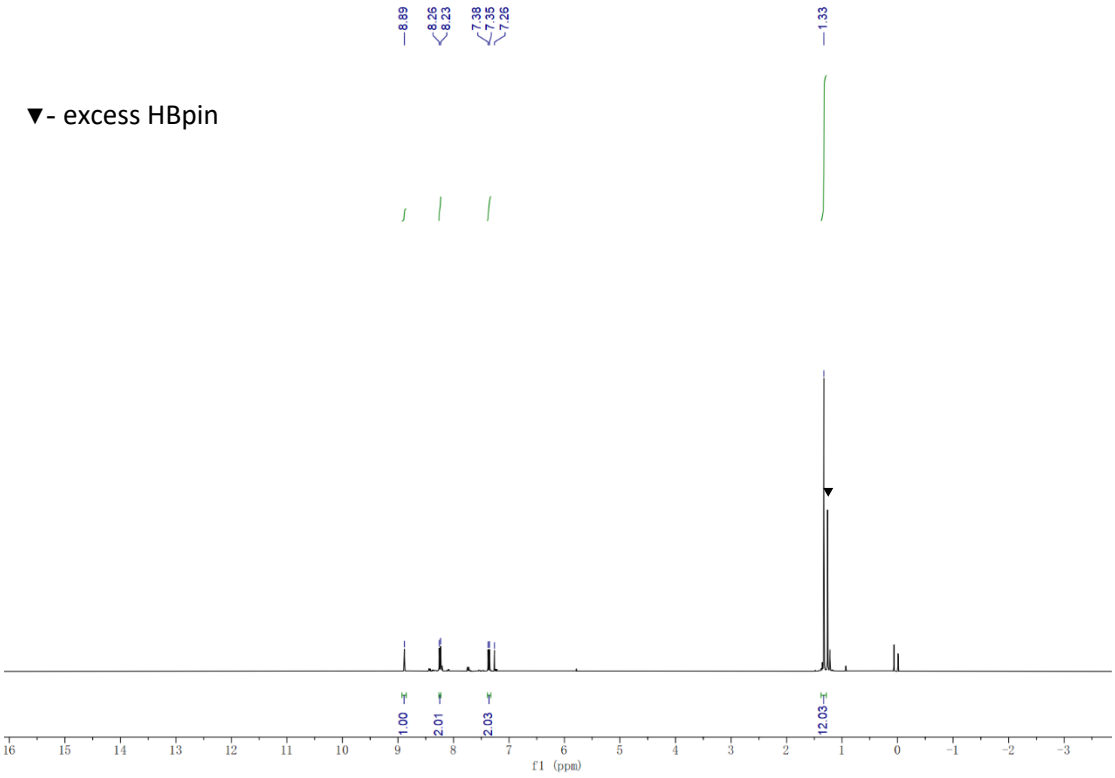


Figure S7.31 ^{1}H NMR spectrum of **4k** in $CDCl_3$ at 400 MHz.

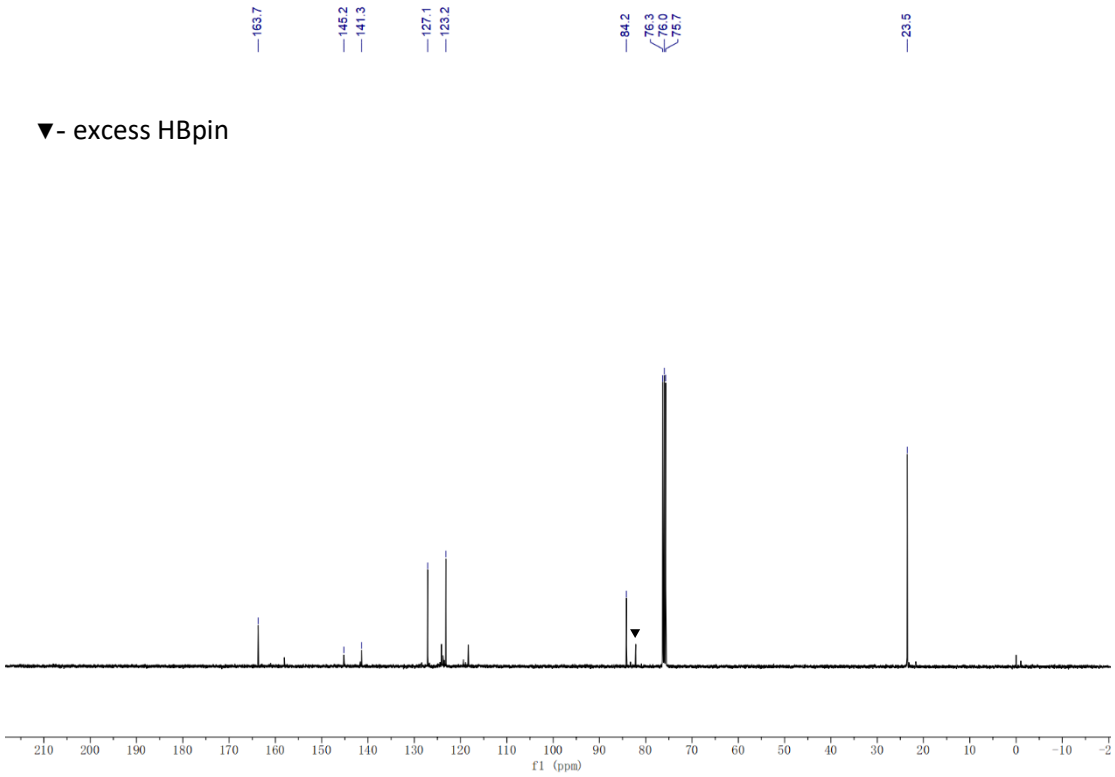


Figure S7.32 ^{13}C NMR spectrum of **4k** in $CDCl_3$ at 101 MHz.

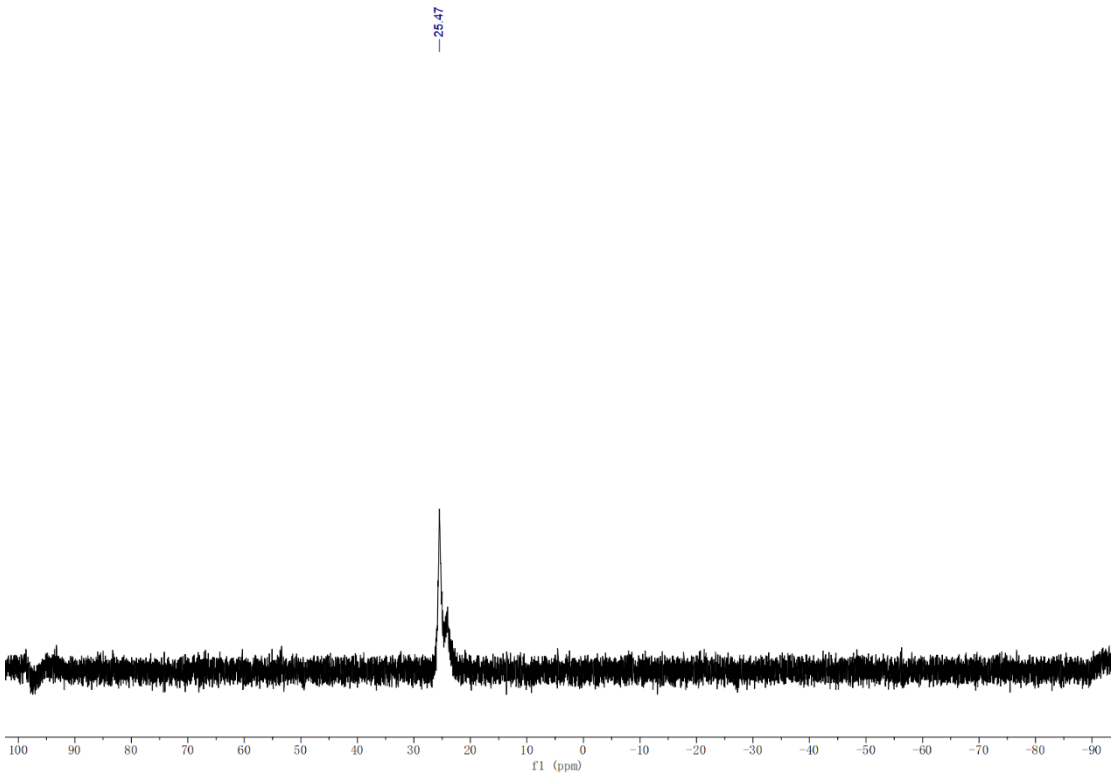


Figure S7.33 ^{11}B NMR spectrum of **4k** in $CDCl_3$ at 128 MHz.

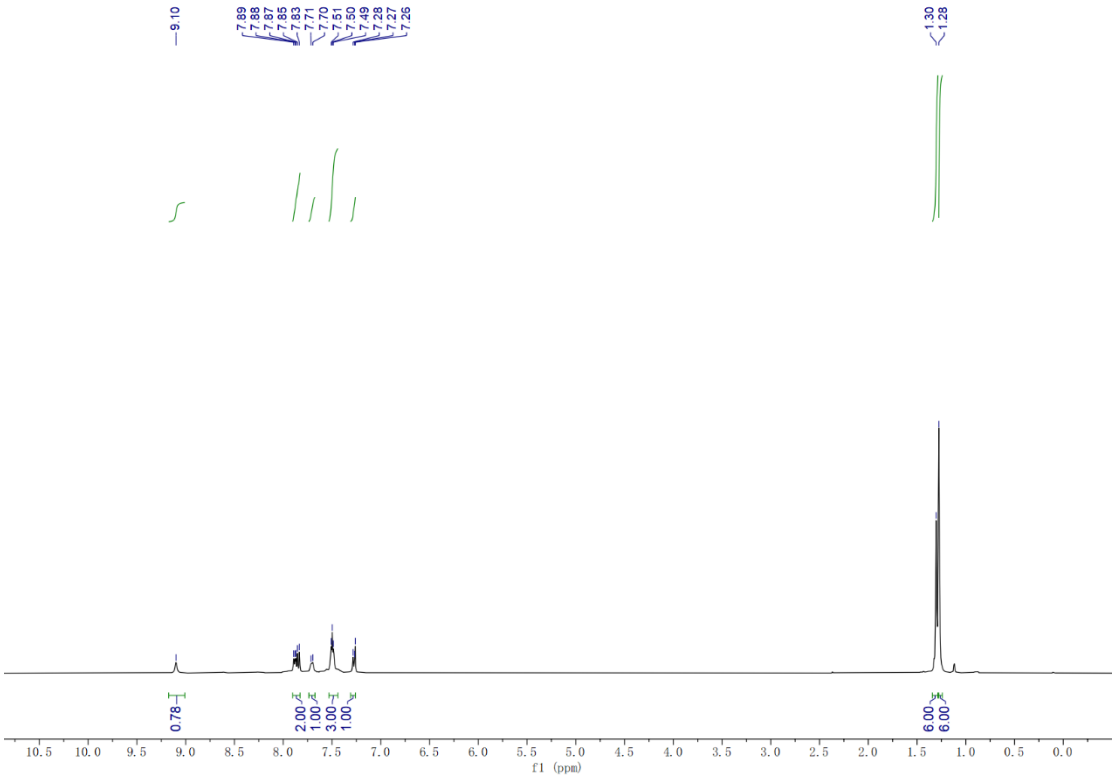


Figure S7.34 ^{1}H NMR spectrum of **4l** in $CDCl_3$ at 400 MHz.

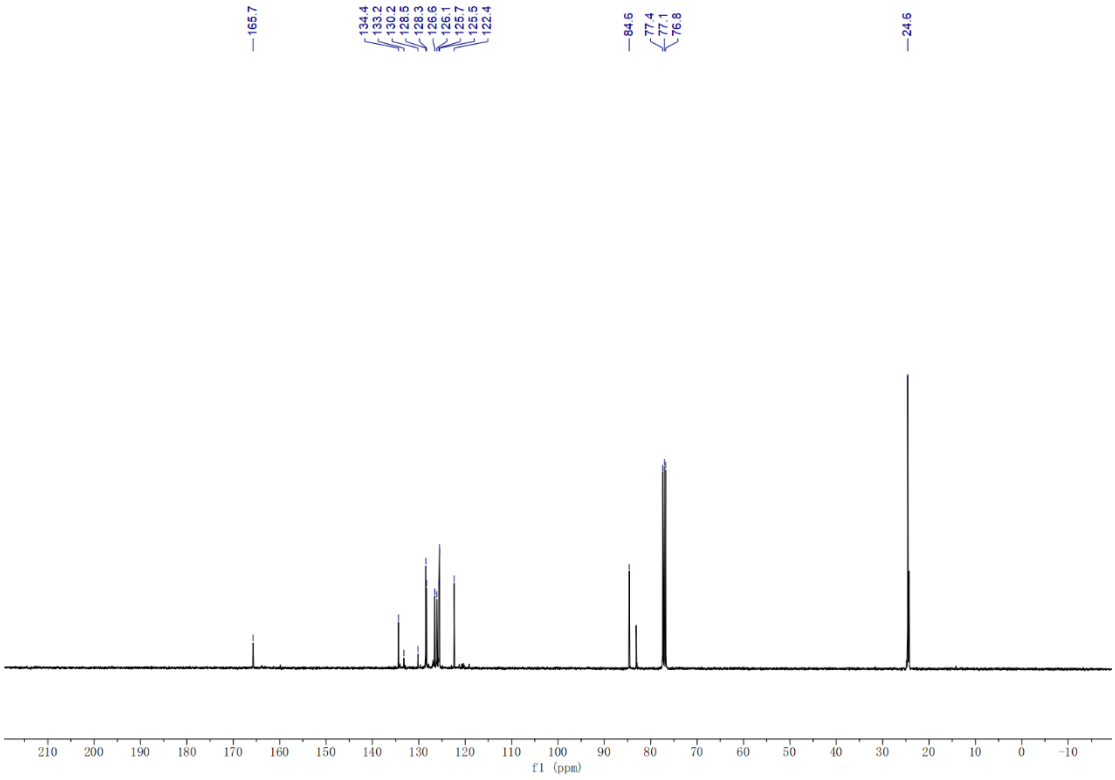


Figure S7.35 ^{13}C NMR spectrum of **4l** in $CDCl_3$ at 101 MHz.

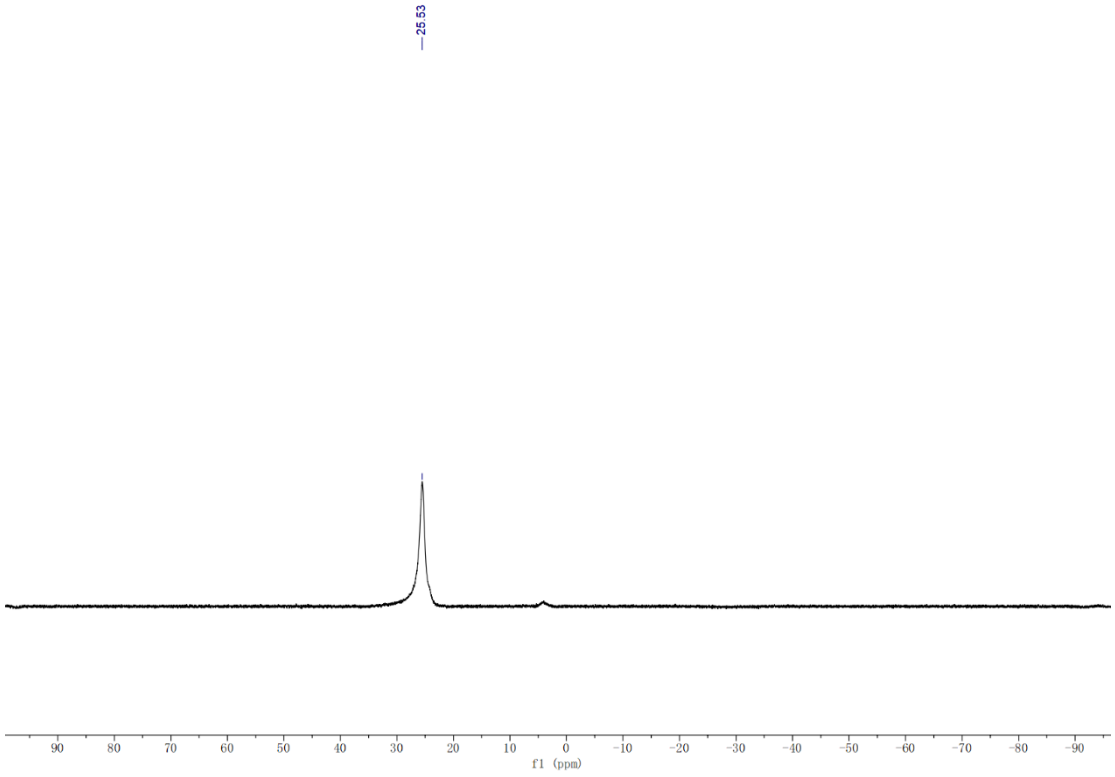


Figure S7.36 ^{11}B NMR spectrum of **4l** in $CDCl_3$ at 128 MHz.

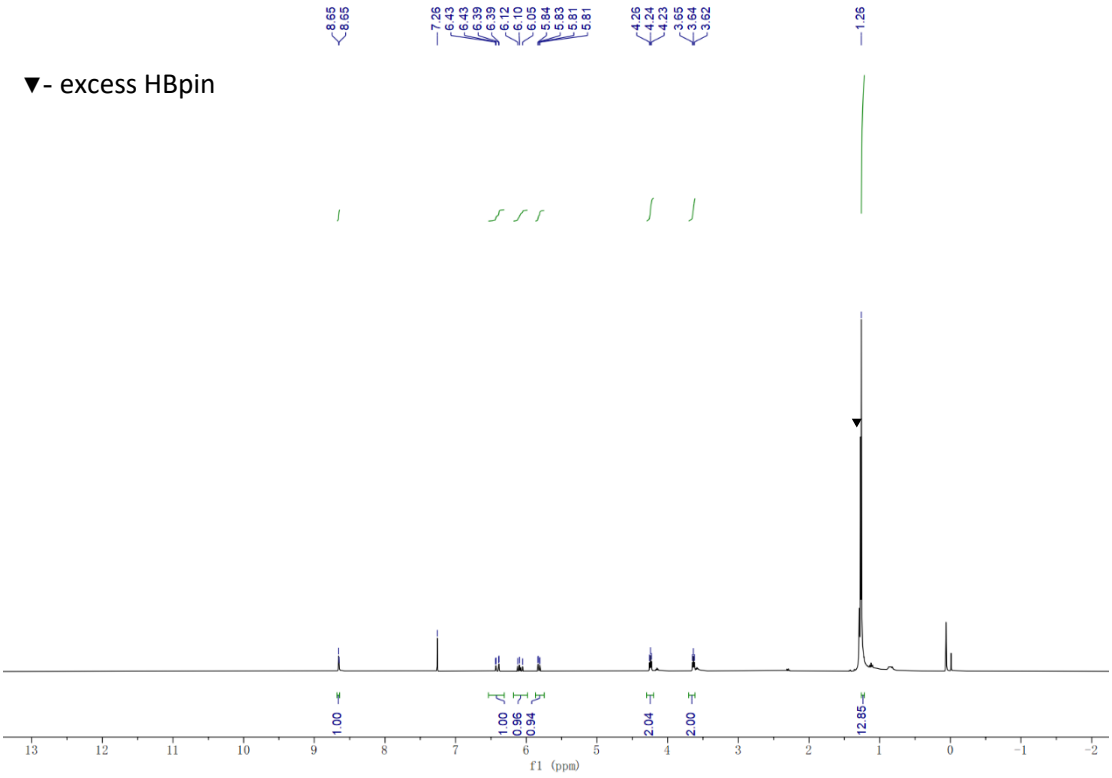


Figure S7.37 ^{1}H NMR spectrum of **4m** in $CDCl_3$ at 400 MHz.

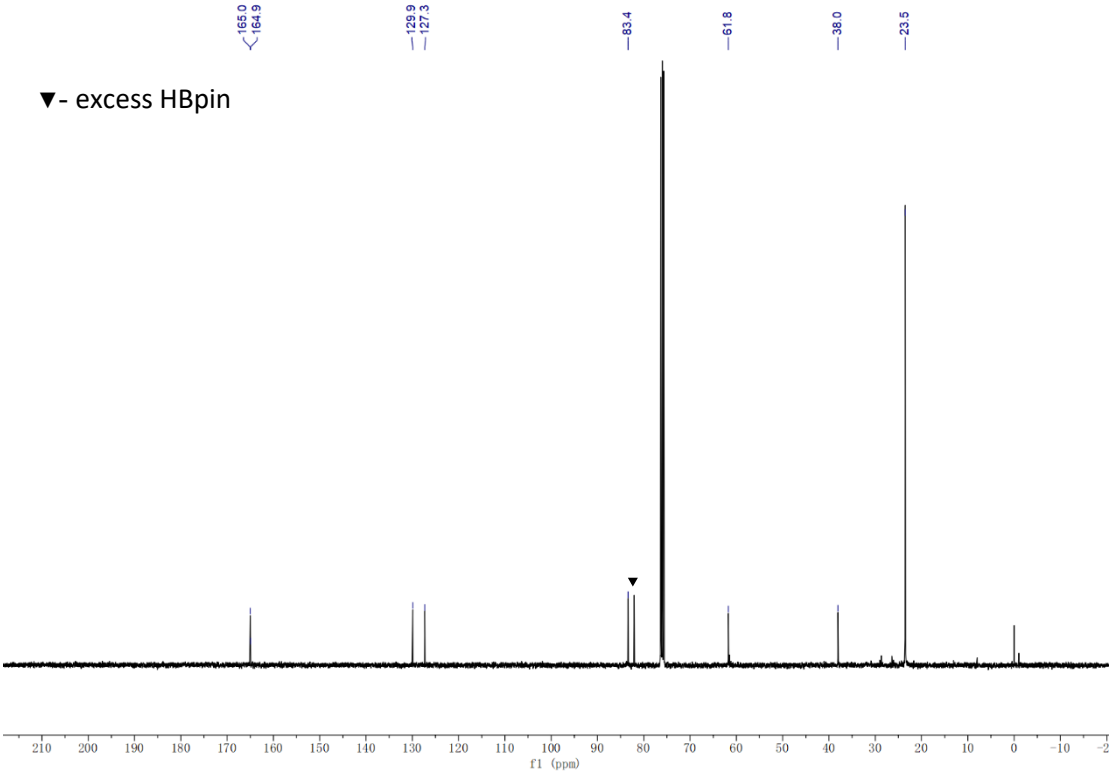


Figure S7.38 ^{13}C NMR spectrum of **4m** in $CDCl_3$ at 101 MHz.

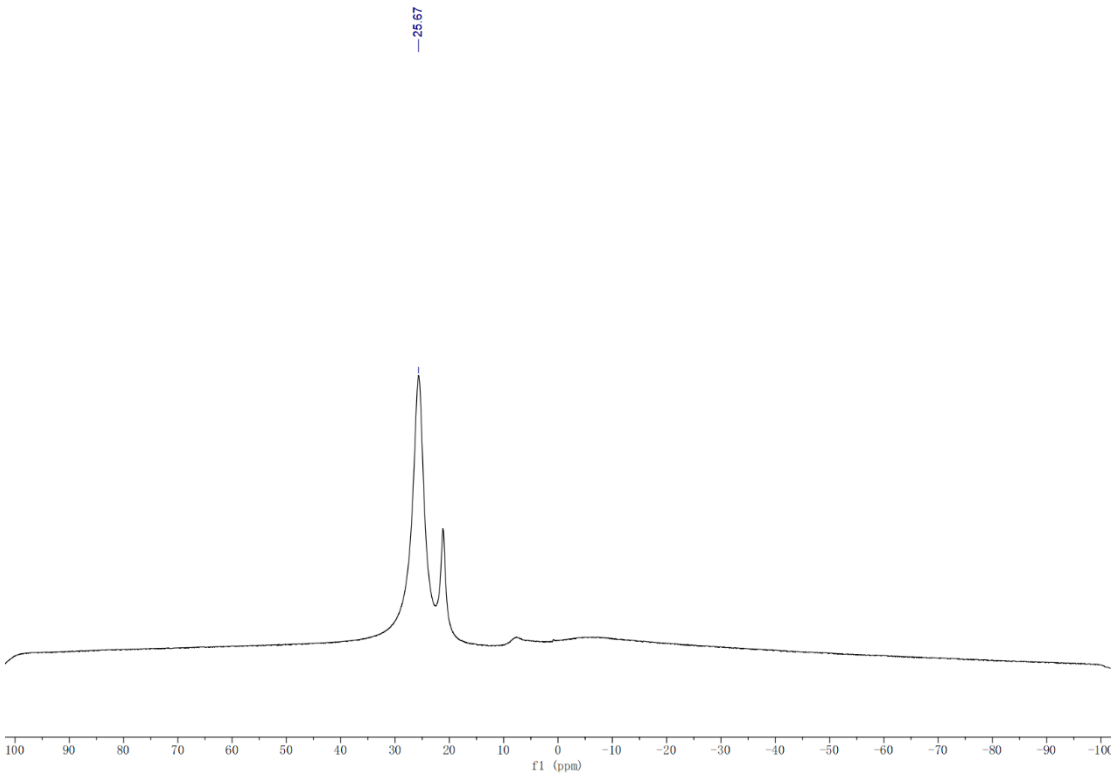


Figure S7.39 ^{11}B NMR spectrum of **4m** in $CDCl_3$ at 128 MHz.

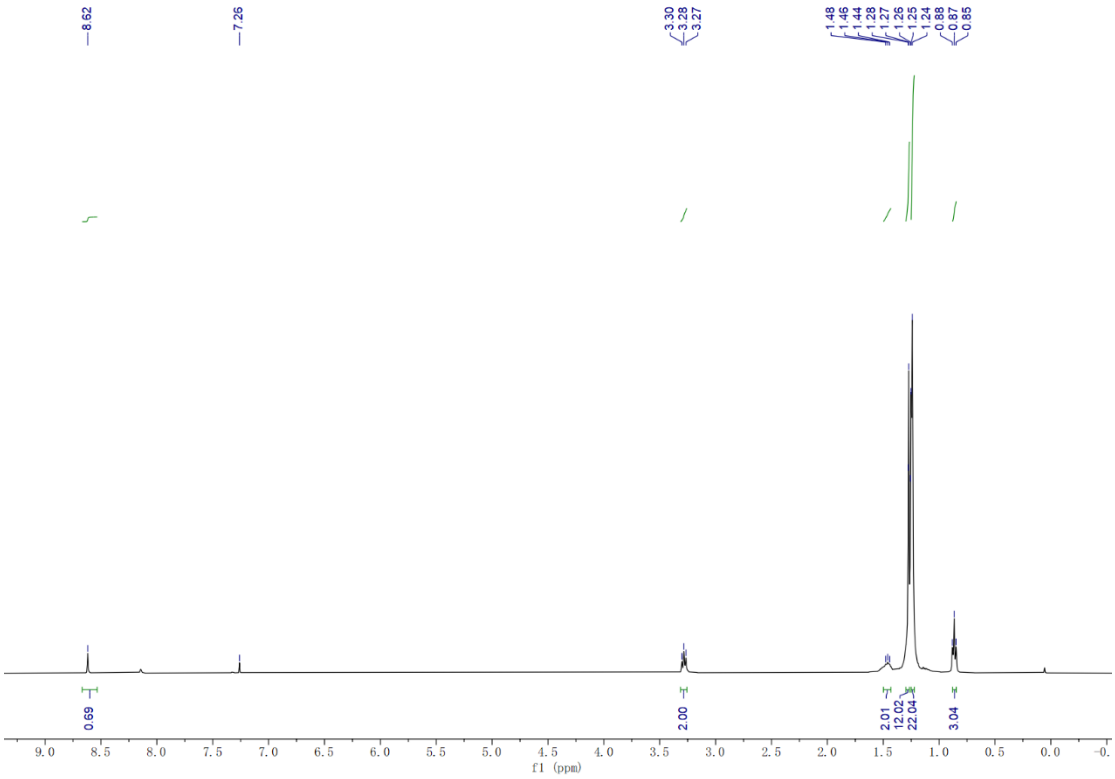


Figure S7.40 ^{1}H NMR spectrum of **4n** in $CDCl_3$ at 400 MHz.

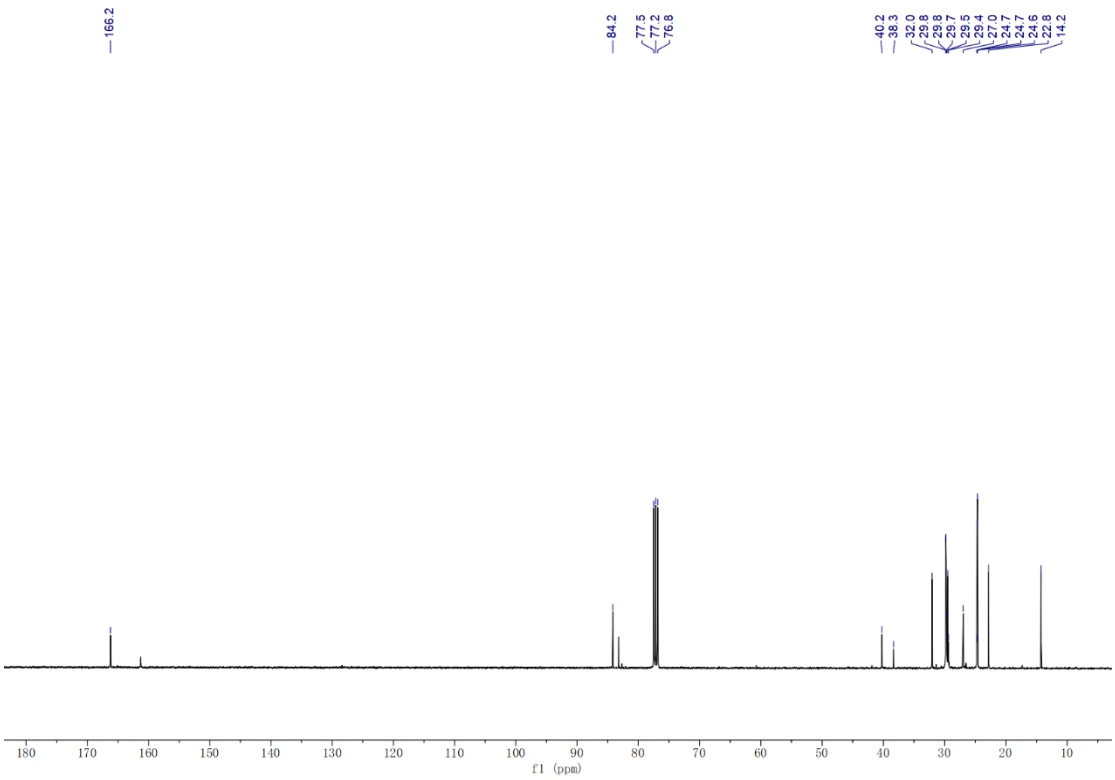


Figure S7.41 ^{13}C NMR spectrum of **4n** in $CDCl_3$ at 101 MHz.

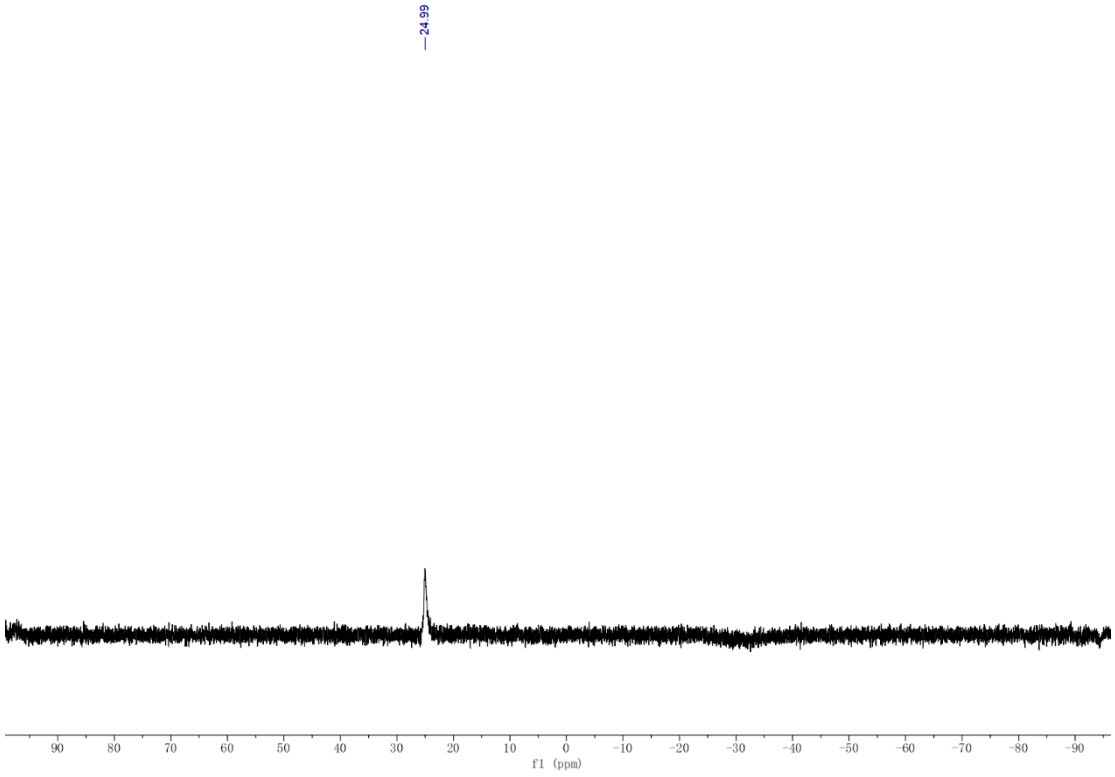


Figure S7.42 ^{11}B NMR spectrum of **4n** in $CDCl_3$ at 128 MHz.

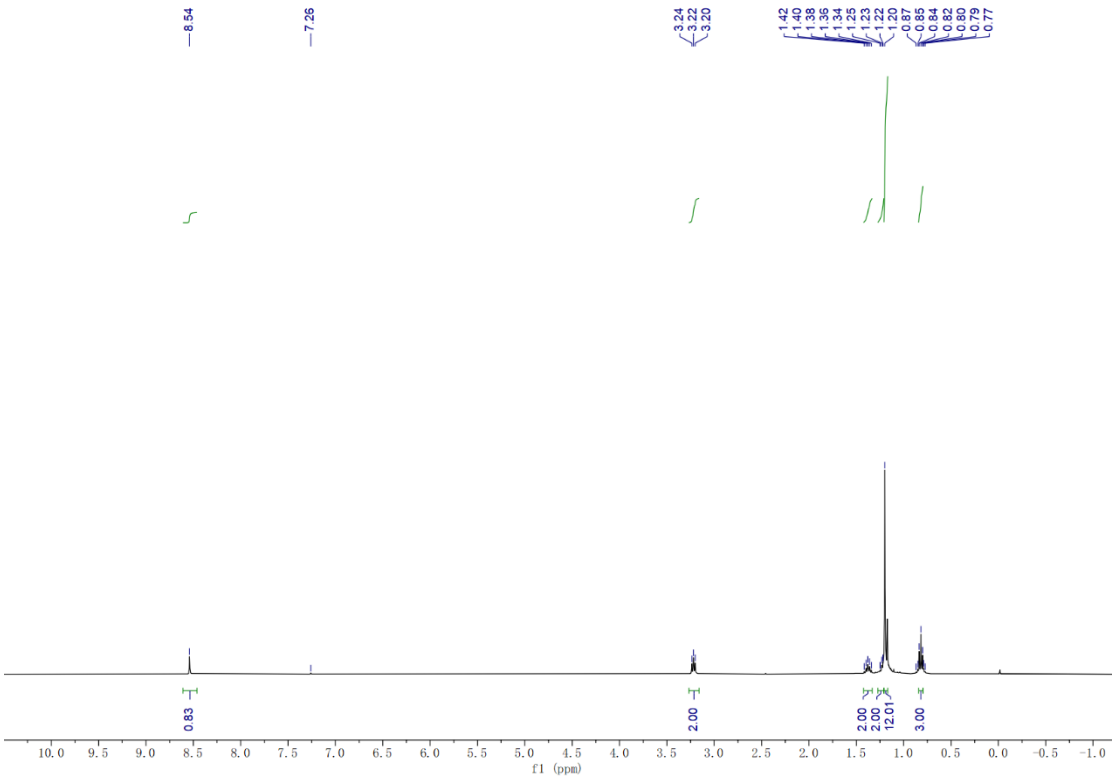


Figure S7.43 ^{1}H NMR spectrum of **4o** in $CDCl_3$ at 400 MHz.

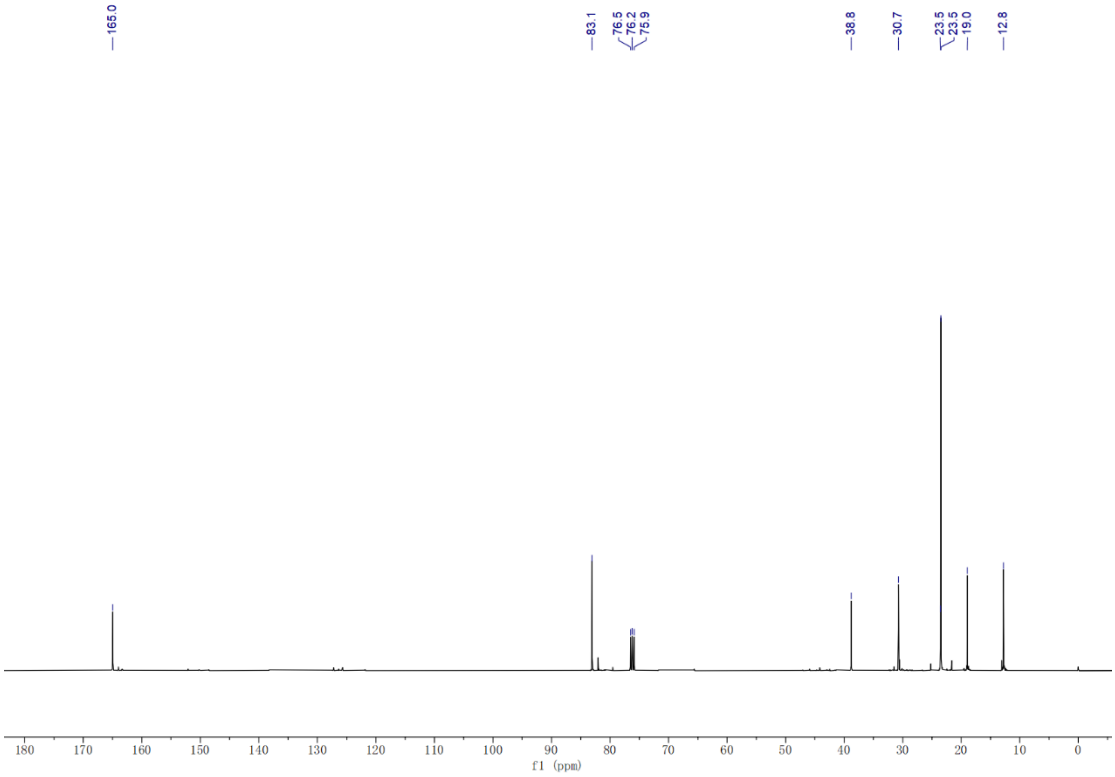


Figure S7.44 ^{13}C NMR spectrum of **4o** in $CDCl_3$ at 101 MHz.

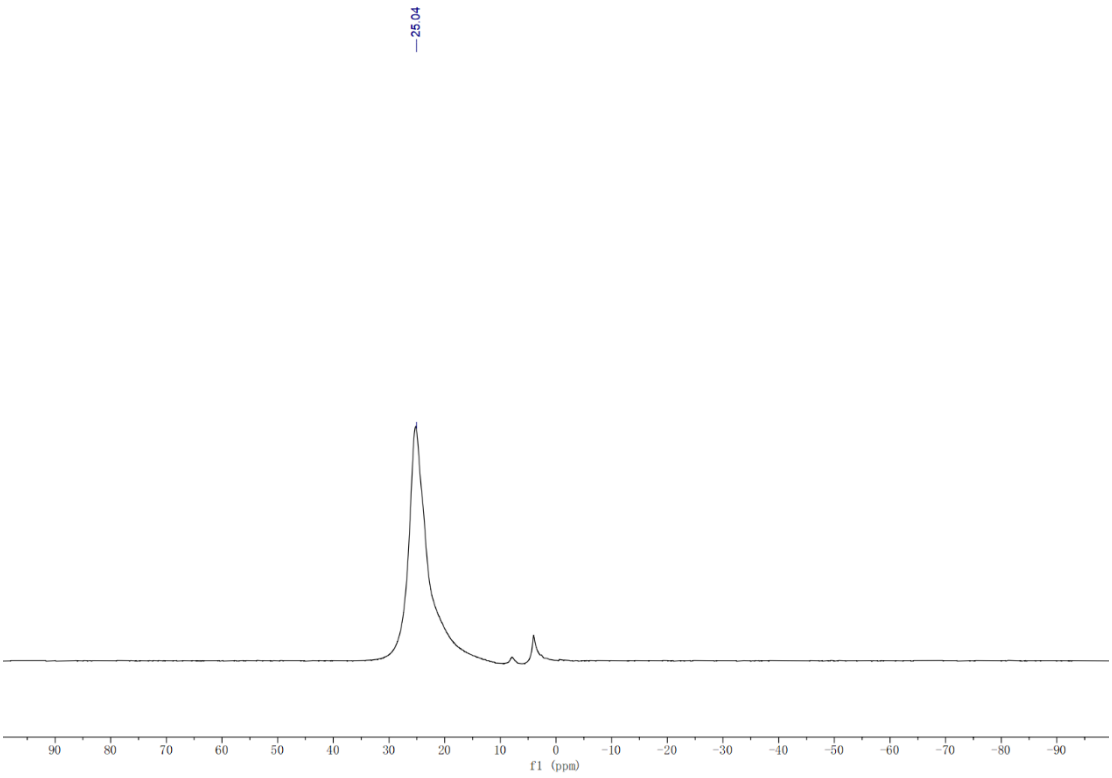


Figure S7.45 ^{11}B NMR spectrum of **4o** in $CDCl_3$ at 128 MHz.

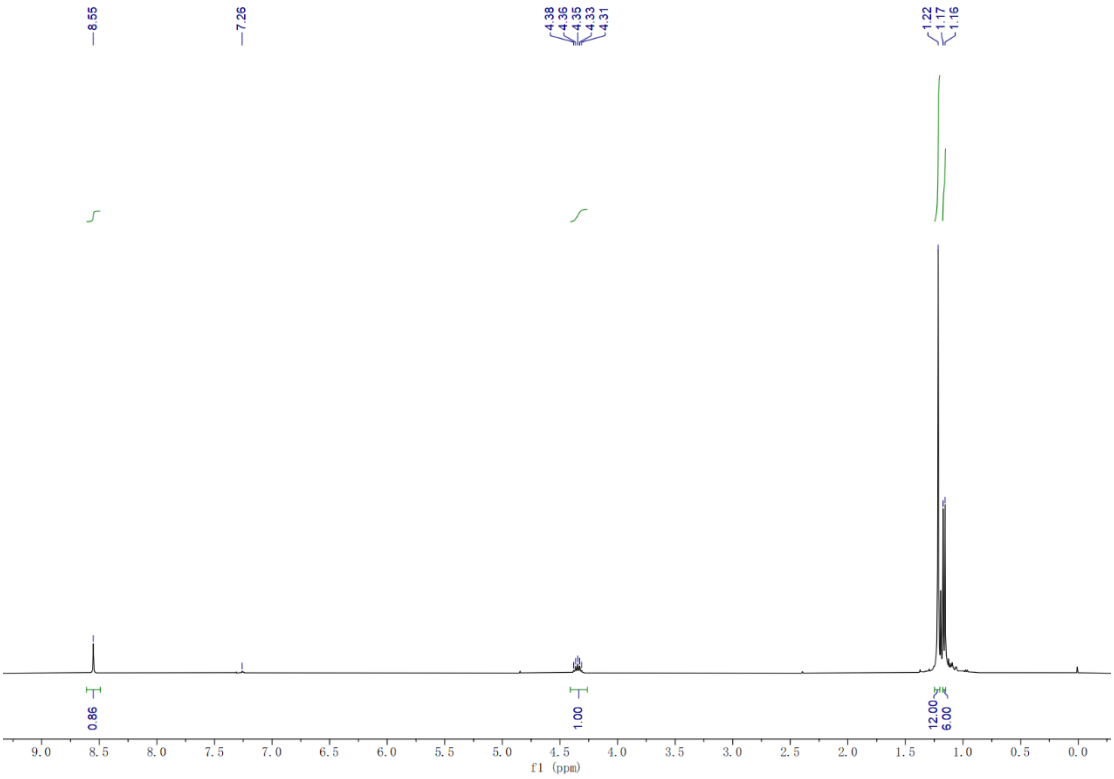


Figure S7.46 ^{1}H NMR spectrum of **4p** in $CDCl_3$ at 400 MHz.

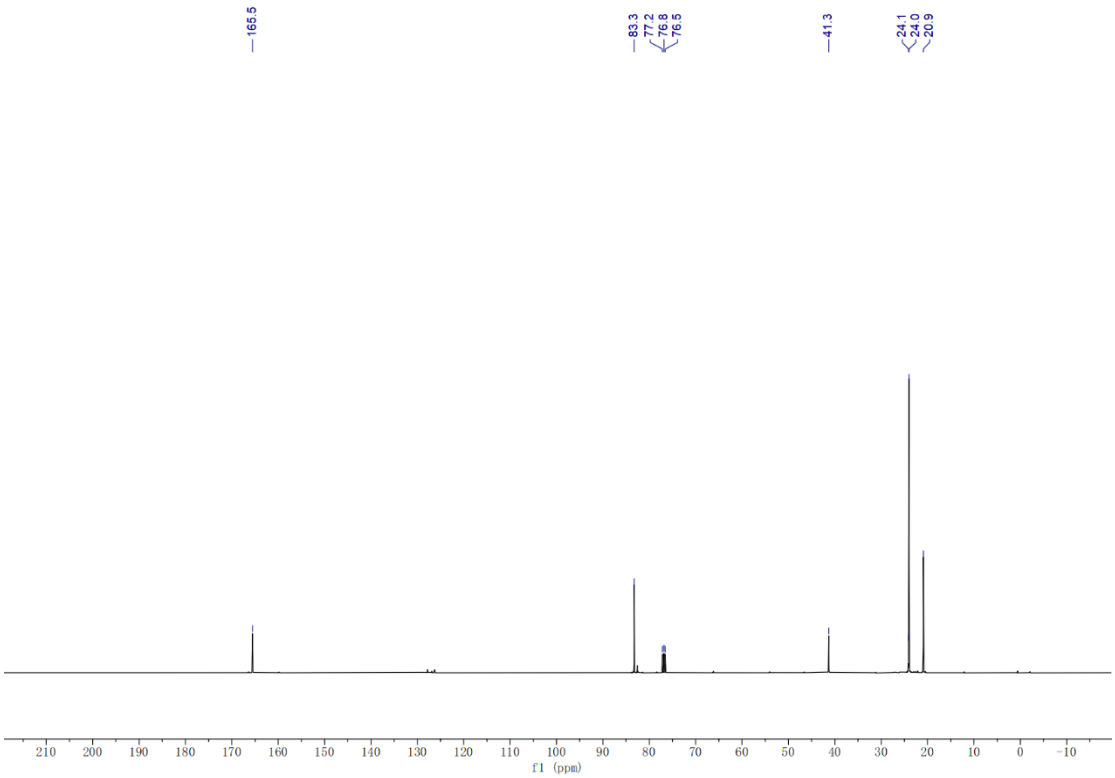


Figure S7.47 ^{13}C NMR spectrum of **4p** in $CDCl_3$ at 101 MHz.

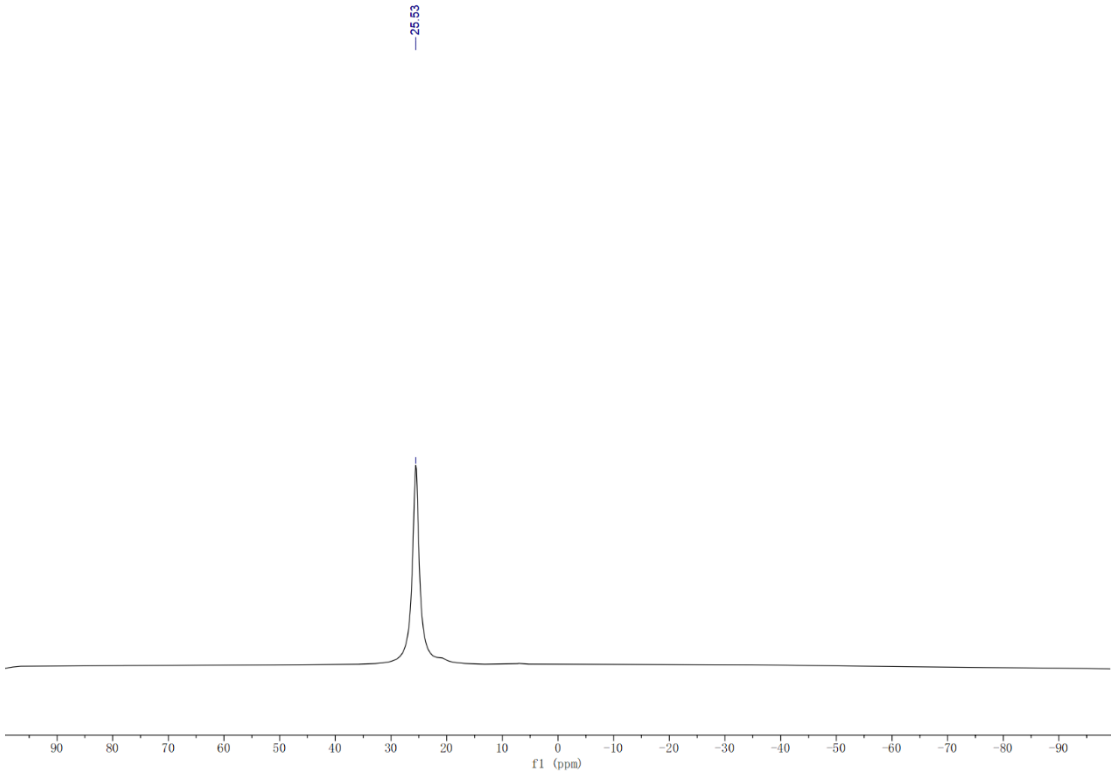
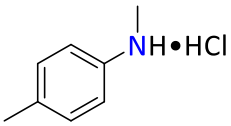
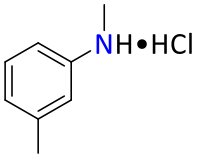


Figure S7.48 ^{11}B NMR spectrum of **4p** in $CDCl_3$ at 128 MHz.

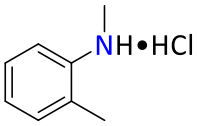
8. NMR data and spectra of *N*-methylamine compounds

6a 

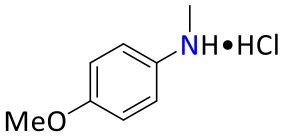
NMR yield 99%, isolated yield 78%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.31 (s, 4H, Ar*H*), 3.01 (s, 3H, NHCH_3), 2.28 (s, 3H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 140.3, 133.5, 130.7, 130.4, 122.5, 121.5, 36.9, 20.1.

6b 

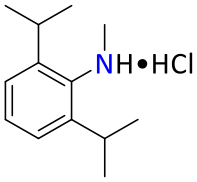
NMR yield 99%, isolated yield 75%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.35 (t, 1H, Ar*H*), 7.29 – 7.03 (m, 3H, Ar*H*), 2.96 (s, 3H, NHCH_3), 2.30 (s, 3H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 141.1, 137.1, 130.1, 129.7, 121.7, 118.1, 36.5, 20.4.

6c 

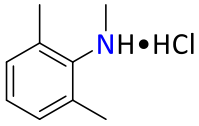
NMR yield 97%, isolated yield 81%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.38 (d, 4H, Ar*H*), 3.11 – 3.01 (m, 3H, NHCH_3), 2.44 – 2.35 (m, 3H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 134.6, 132.3, 131.0, 129.8, 127.8, 121.7, 35.8, 16.0.

6d 

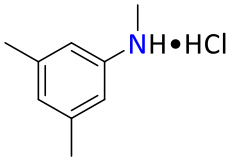
NMR yield 99%, isolated yield 83%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.38 (d, 2H, Ar*H*), 7.05 (d, 2H, Ar*H*), 3.80 (s, 3H, 3H, NHCH_3), 3.03 (s, 3H, 3H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 159.2, 129.5, 122.9, 115.4, 55.6, 36.9.

6e 

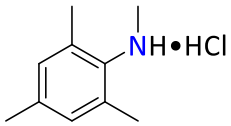
NMR yield 92%, isolated yield 81%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.48 (d, 1H, Ar*H*), 7.40 (dt, 2H, Ar*H*), 3.06 (d, 2H, C*H*Me$_2$), 3.05 (s, 3H, NHCH_3), 1.28 (dt, 12H, CH*Me*$_2$). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 141.9, 130.4, 130.2, 125.6, 38.3, 27.6, 23.5.

6f 

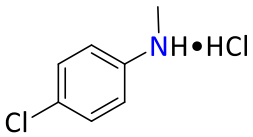
NMR yield 96%, isolated yield 68%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.18 – 6.97 (m, 3H, Ar*H*), 2.84 (s, 3H, NHCH_3), 2.25 (s, 6H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 135.3, 131.0, 129.9, 128.8, 35.6, 16.5.

6g 

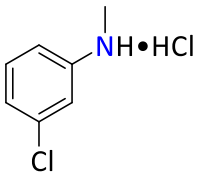
NMR yield 97%, isolated yield 85%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.08 (s, 1H, Ar*H*), 7.07 (s, 2H, Ar*H*), 3.00 (s, 3H, NHCH_3), 2.27 (s, 6H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 140.8, 136.0, 131.0, 119.0, 36.9, 20.2.

6h 

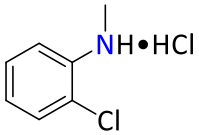
NMR yield 89%, isolated yield 78%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.04 (s, 2H, Ar*H*), 3.00 (s, 3H, NHCH_3), 2.37 (s, 6H, CH_3), 2.25 (s, 3H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 139.9, 131.3, 130.7, 130.4, 35.8, 19.8, 16.2.

6i 

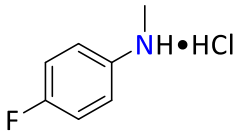
NMR yield 99%, isolated yield 69%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.59 (d, 2H, Ar*H*), 7.44 (d, 2H, Ar*H*), 3.09 (s, 3H, NHCH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 136.1,134.0, 130.2, 122.8, 36.2.

6j 

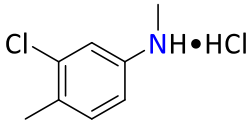
NMR yield 98%, isolated yield 79%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.58 – 7.49 (m, 3H, Ar*H*), 7.41 (s, 1H, Ar*H*), 3.09 (s, 3H, NHCH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 137.3, 135.1, 131.6, 129.9, 122.2, 120.4, 36.7.

6k 

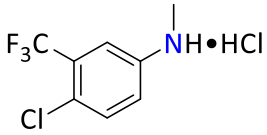
NMR yield 94%, isolated yield 81%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.47 (d, 2H, Ar*H*), 7.36 (d, 2H, Ar*H*), 3.00 (s, 3H, 3H, NHCH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 132.9, 131.1, 131.0, 128.9, 126.7, 123.5, 35.7.

6l 

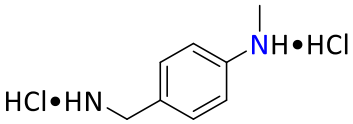
NMR yield 99%, isolated yield 82%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.51 (d, 2H, Ar*H*), 7.30 (t, 2H, Ar*H*), 3.08 (s, 3H, NHCH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 163.6, 161.2, 132.4, 123.9, 117.3, 117.0, 36.9.

6m 

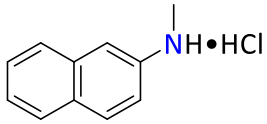
NMR yield 91%, isolated yield 78%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.51 (s, 1H, Ar*H*), 7.44 (d, 1H, Ar*H*), 7.29 (d, 1H, Ar*H*), 3.06 (s, 3H, NHCH_3), 2.35 (s, 3H, CH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 138.2, 134.9, 134.8, 132.3, 122.2, 120.1, 36.7, 18.9.

6n 

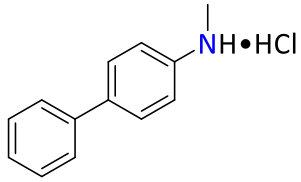
NMR yield 89%, isolated yield 75%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.85 (s, 1H, Ar*H*), 7.77 – 7.67 (m, 2H, Ar*H*), 3.08 (s, 3H, NHCH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 135.0, 133.5, 133.2, 127.2, 123.3, 122.0, 120.6, 36.8.

6o 

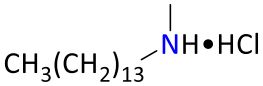
NMR yield 99%, isolated yield 88%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.60 (d, 2H, Ar*H*), 7.48 (d, 2H, Ar*H*), 4.23 (s, 2H, CH_2), 3.07 (s, 3H, NHCH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 138.5, 132.77, 130.8, 130.6, 122.4, 121.6, 42.4, 35.9.

6p 

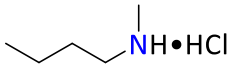
NMR yield 99%, isolated yield 84%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.92 – 7.54 (m, 5H, Ar*H*), 7.44 (s, 2H, Ar*H*), 3.05 (s, 3H, NHCH_3). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 133.8, 131.2, 129.0, 128.1, 127.2, 125.0, 124.8, 119.3, 36.0.

6q 

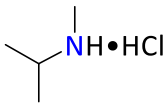
NMR yield 99%, isolated yield 86%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 7.61 – 7.51 (m, 6H, Ar*H*), 7.37 (t, 3H, Ar*H*), 2.94 (s, 3H, NHC*H*$_3$). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 136.1, 135.4, 133.4, 131.8, 129.8, 129.7, 129.3, 129.1, 129.0, 122.1, 37.0.

6r 

NMR yield 98%, isolated yield 58%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS) δ 9.51 (s, 2H, N*H*$_2$), 2.91 (dq, 2H, NC*H*$_2$), 2.66 (p, 3H, NHC*H*$_3$), 1.85 (dt, 2H, NCH$_2$C*H*$_2$), 1.34-1.16 (m, 22H, C*H*$_2$), 0.87 (t, 3H, C*H*$_3$). ^{13}C NMR (101 MHz, $CDCl_3$, 298K, TMS) δ 49.5, 32.8, 32.7, 31.9, 29.7, 29.7, 29.7, 29.6, 29.5, 29.4, 29.4, 29.1, 26.7, 25.9, 22.7, 14.1.

6s 

NMR yield 99%, isolated yield 81%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 3.07 – 3.01 (m, 2H, NC*H*$_2$), 2.71 (s, 3H, NHC*H*$_3$), 1.66 (p, 2H, NCH$_2$C*H*$_2$), 1.39 (q, 2H, 2H, C*H*$_2$CH$_3$), 0.93 (t, 3H, CH$_2$C*H*$_3$). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 48.9, 32.6, 27.4, 19.0, 12.7.

6t 

NMR yield 99%, isolated yield 79%, white solid. ^{1}H NMR (400 MHz, D_2O, 298K, TMS) δ 3.32 – 3.21 (m, 1H, C*H*Me$_2$), 2.59 (d, 3H, NHC*H*$_3$), 1.23 (d, 6H, CH*Me*$_2$). ^{13}C NMR (101 MHz, D_2O, 298K, TMS) δ 51.5, 29.7, 17.9.

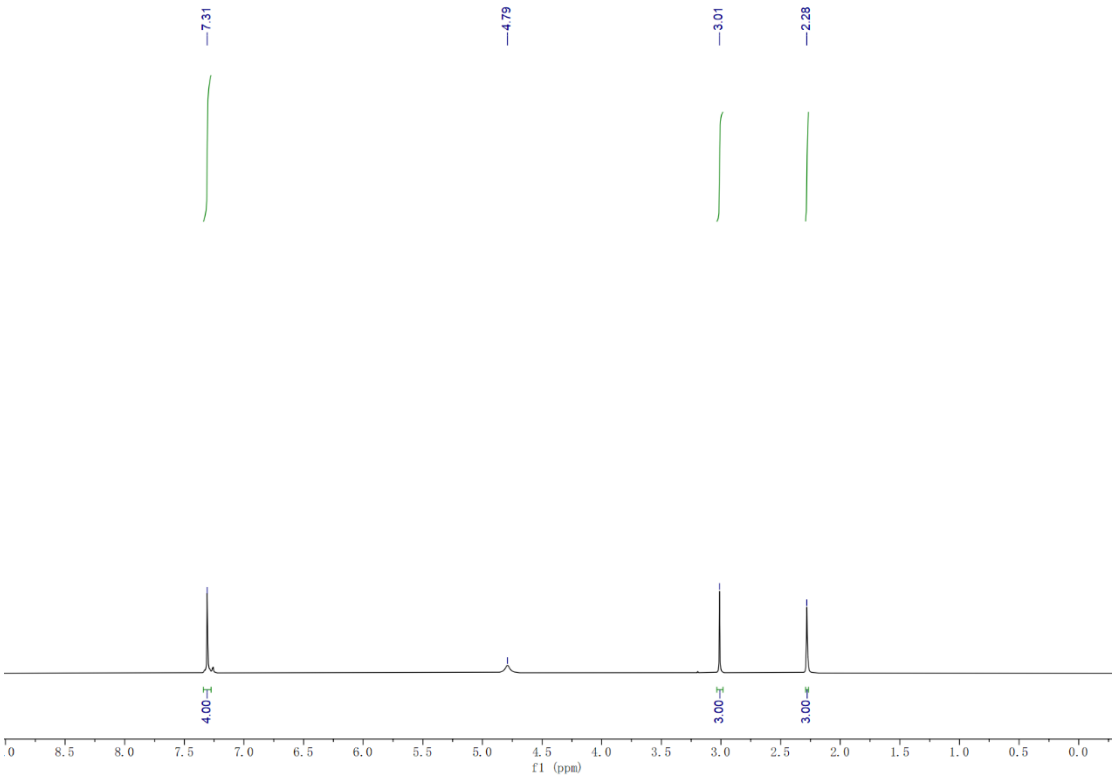


Figure S8.1 ^{1}H NMR spectrum of **6a** in D_2O at 400 MHz.

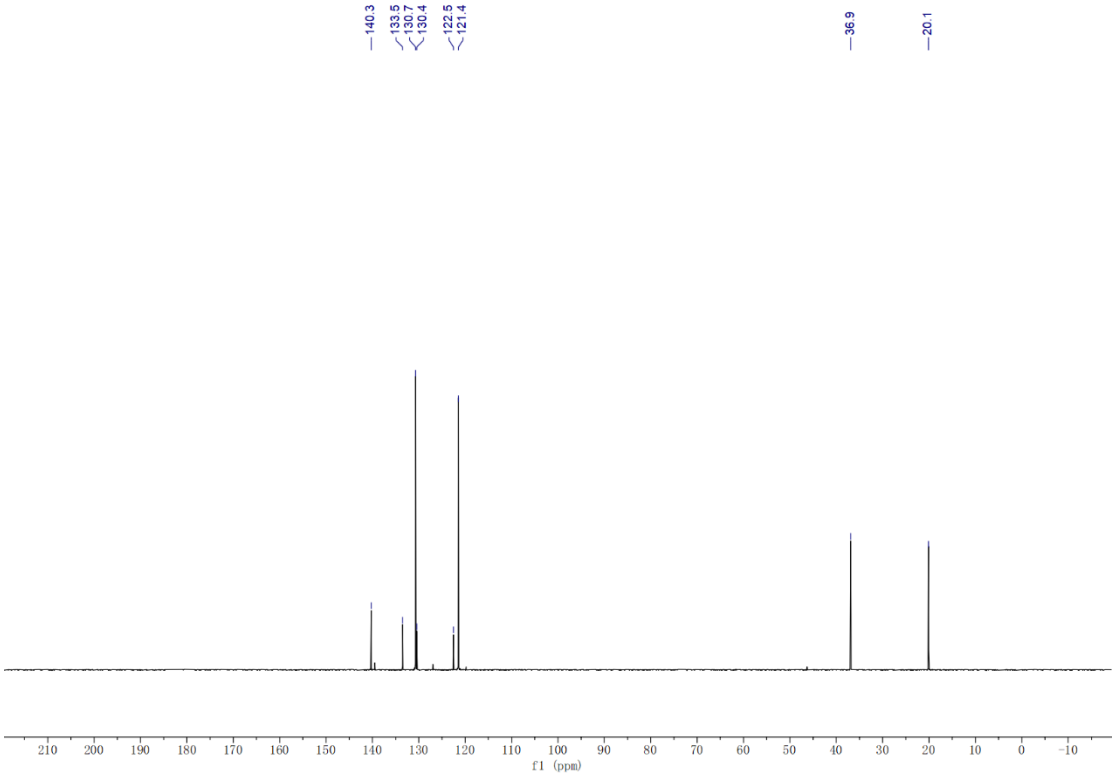


Figure S8.2 ^{13}C NMR spectrum of **6a** in D_2O at 101 MHz.

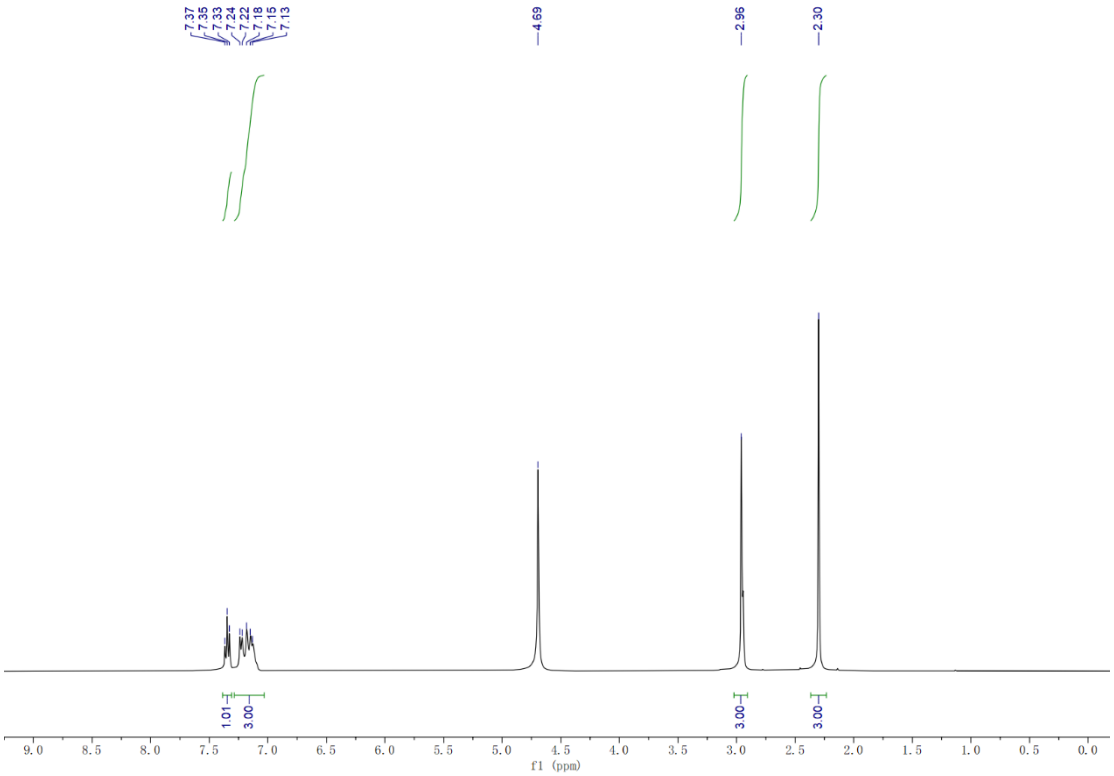


Figure S8.3 ^{1}H NMR spectrum of **6b** in D_2O at 400 MHz.

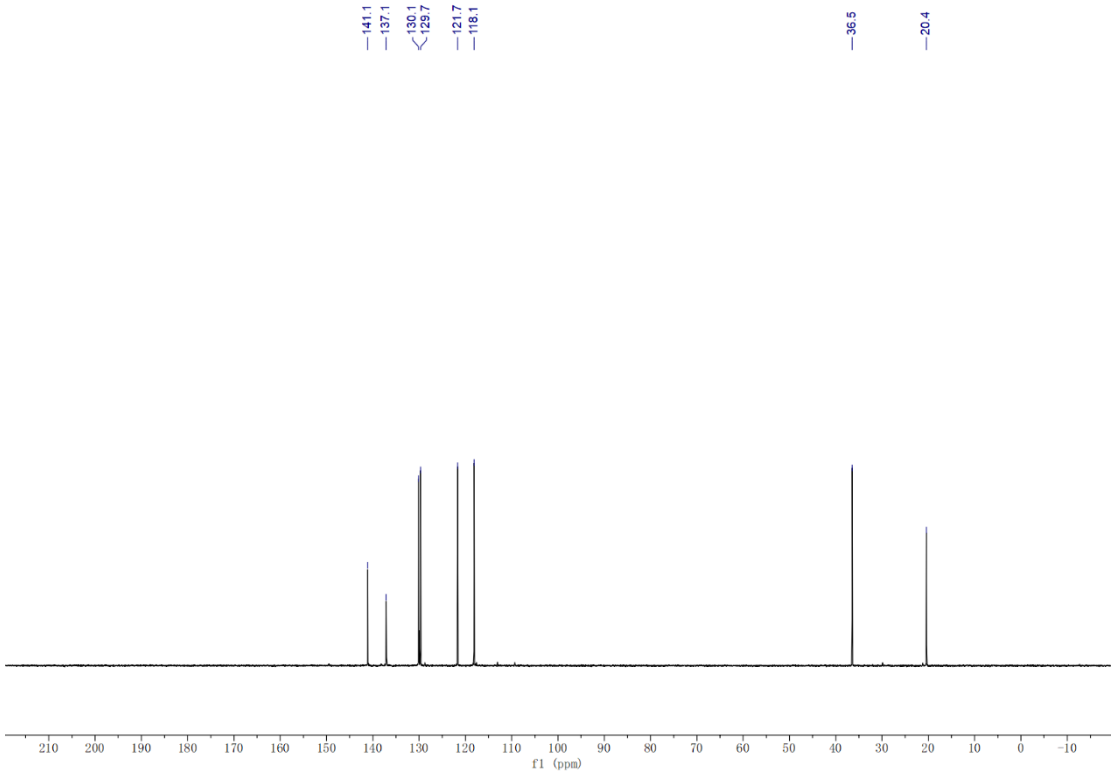


Figure S8.4 ^{13}C NMR spectrum of **6b** in D_2O at 101 MHz.

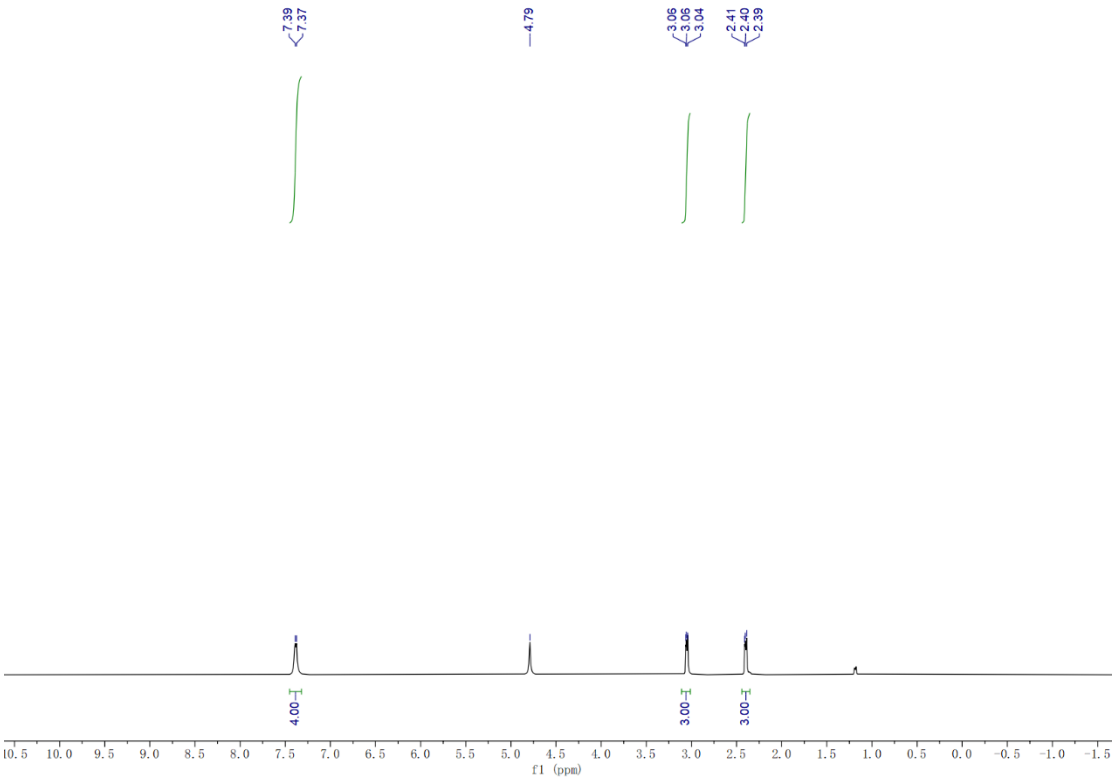


Figure S8.5 ^{1}H NMR spectrum of **6c** in D_2O at 400 MHz.

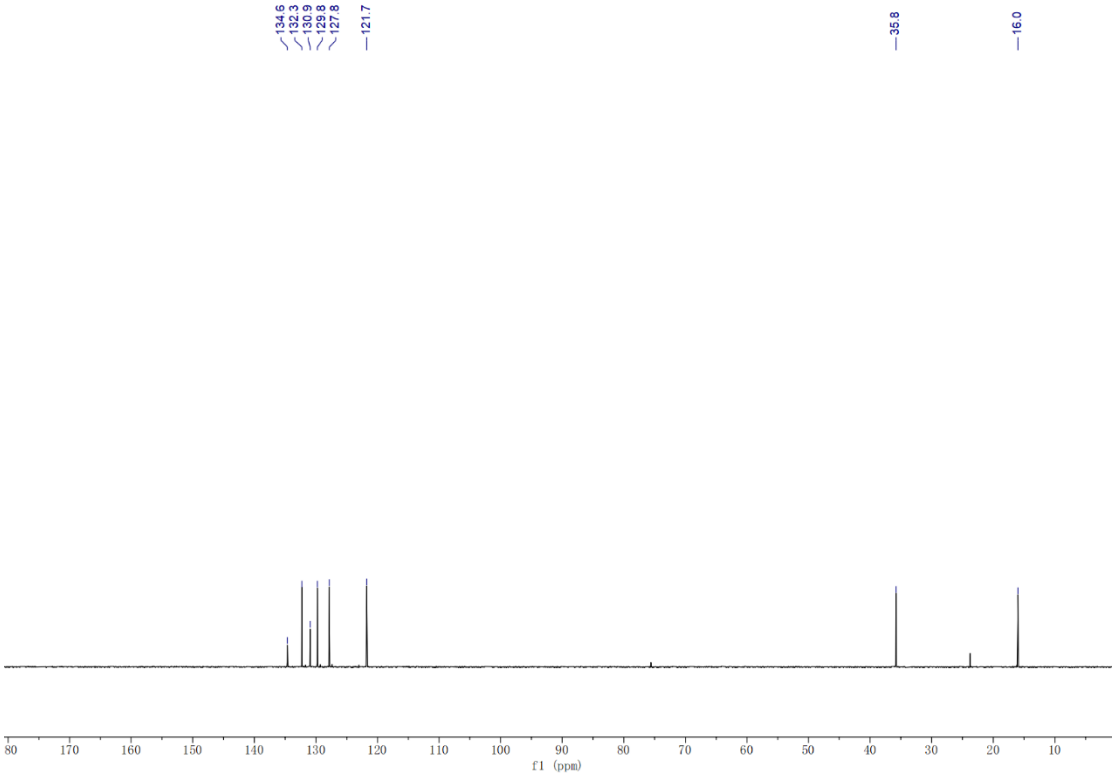


Figure S8.6 ^{13}C NMR spectrum of **6c** in D_2O at 101 MHz.

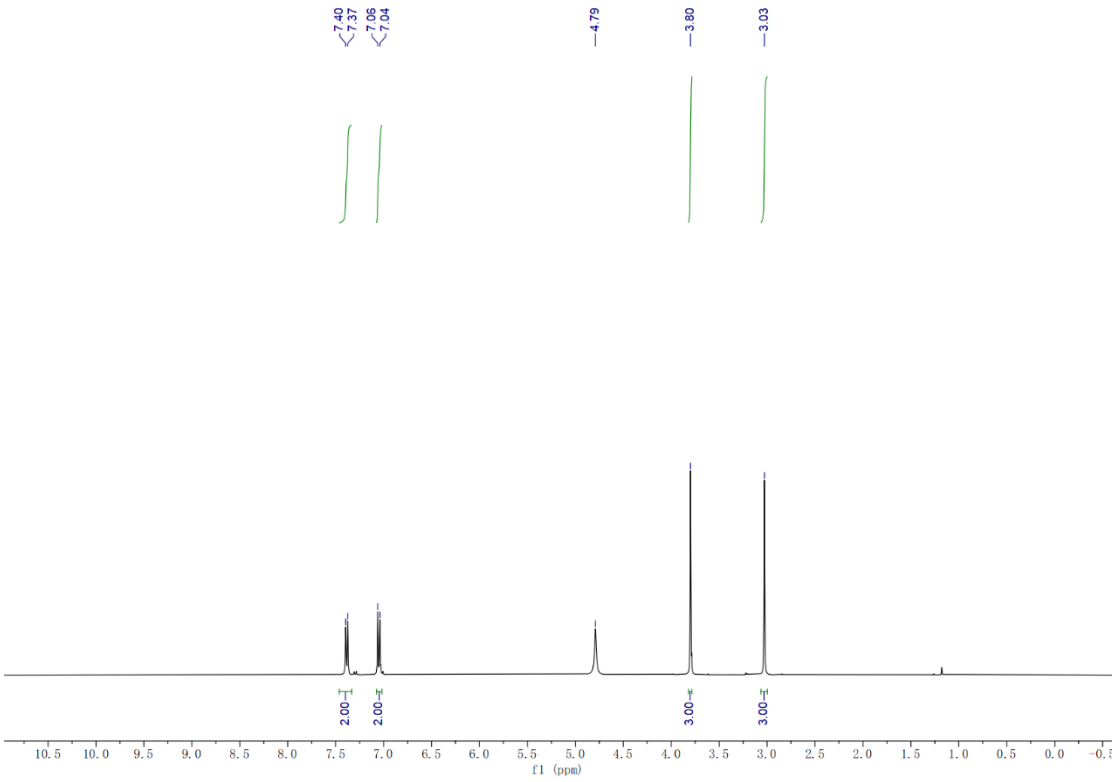


Figure S8.7 ^{1}H NMR spectrum of **6d** in D_2O at 400 MHz.

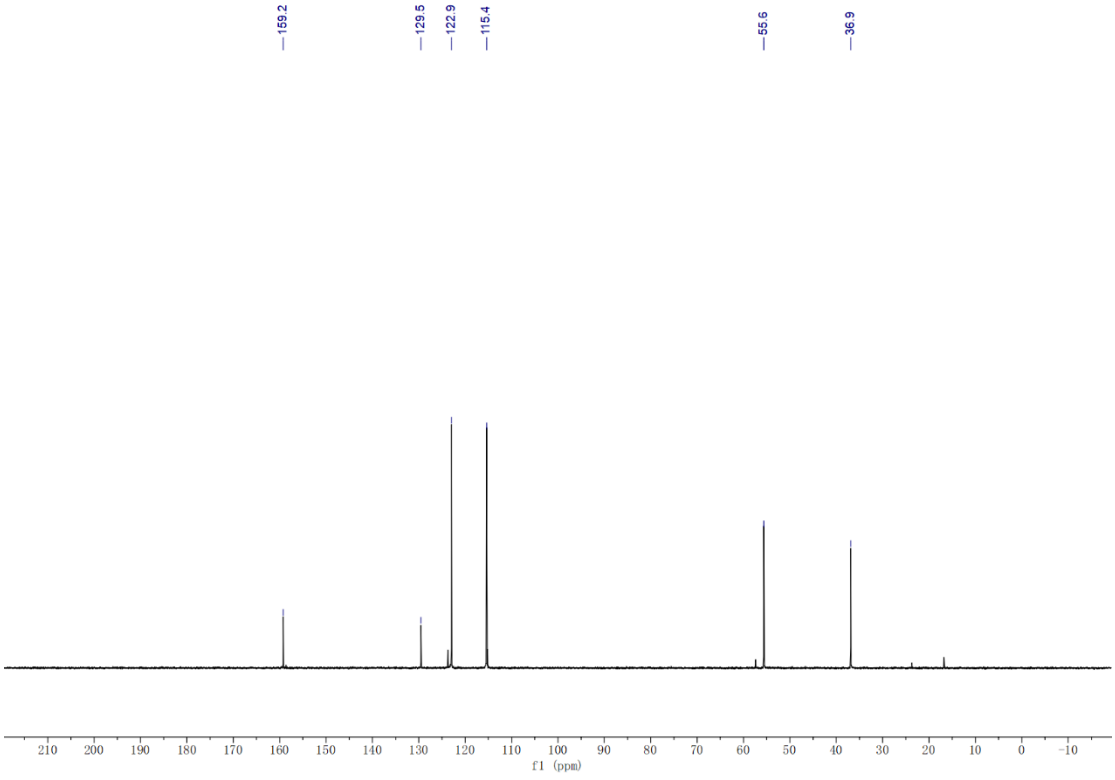


Figure S8.8 ^{13}C NMR spectrum of **6d** in D_2O at 101 MHz.

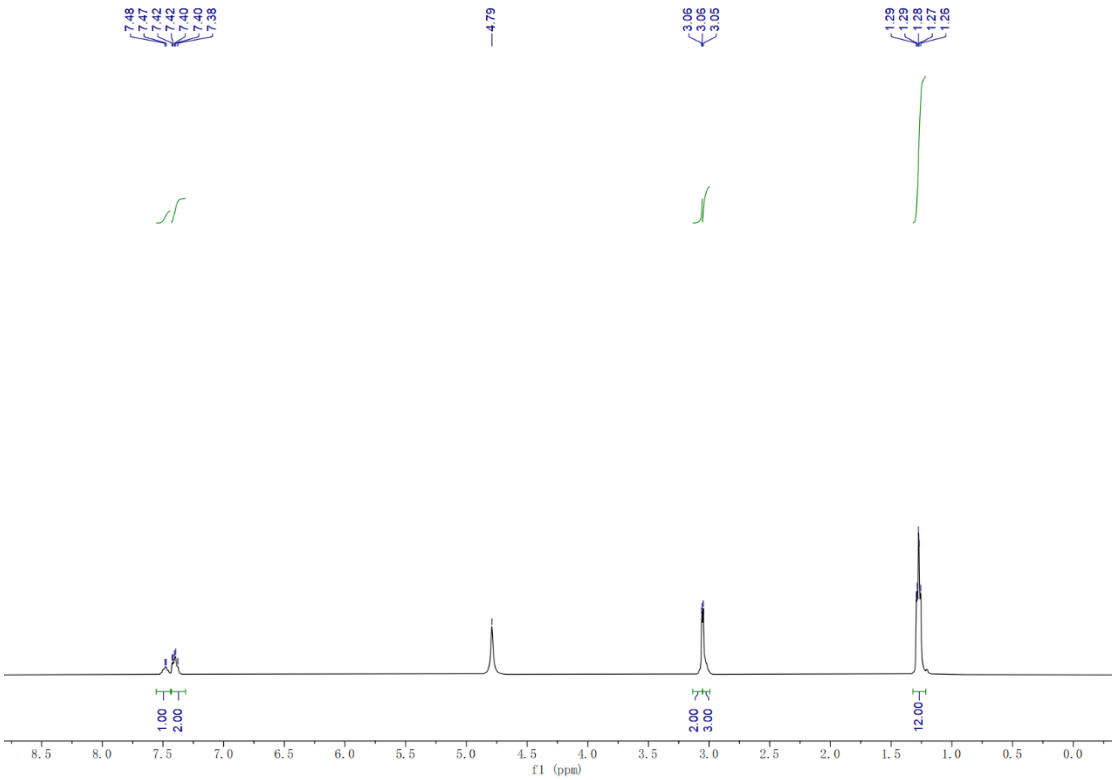


Figure S8.9 ^{1}H NMR spectrum of **6e** in D_2O at 400 MHz.

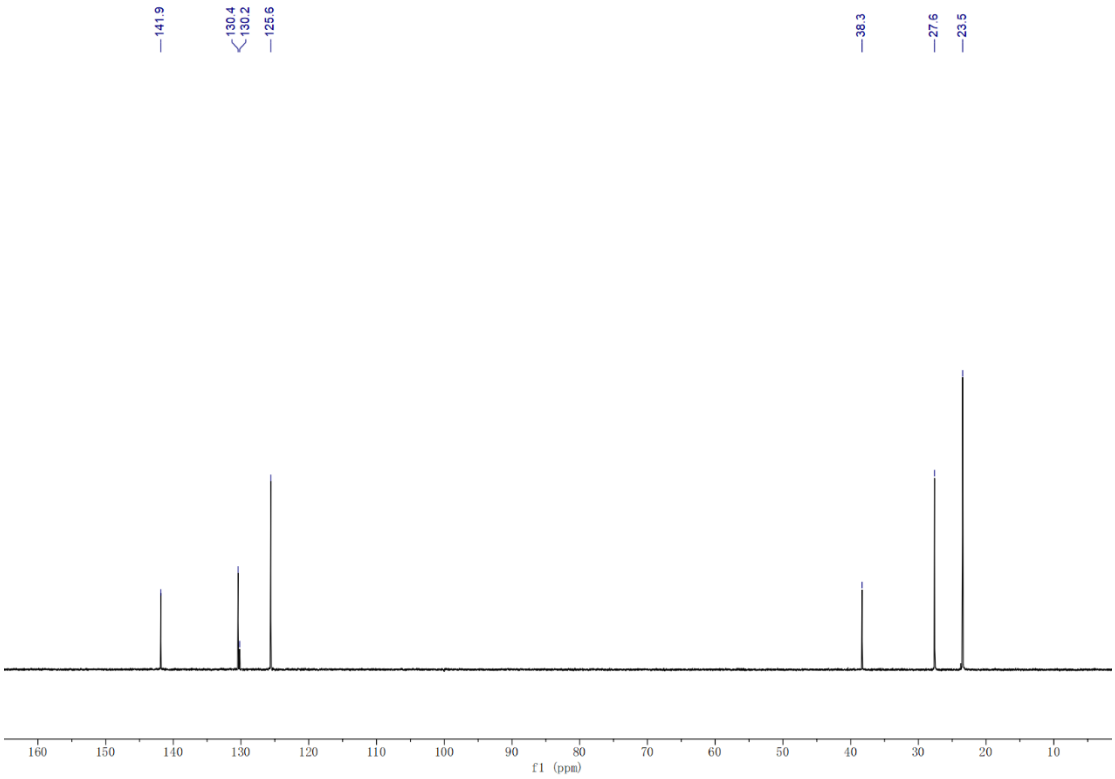


Figure S8.10 ^{13}C NMR spectrum of **6e** in D_2O at 101 MHz.

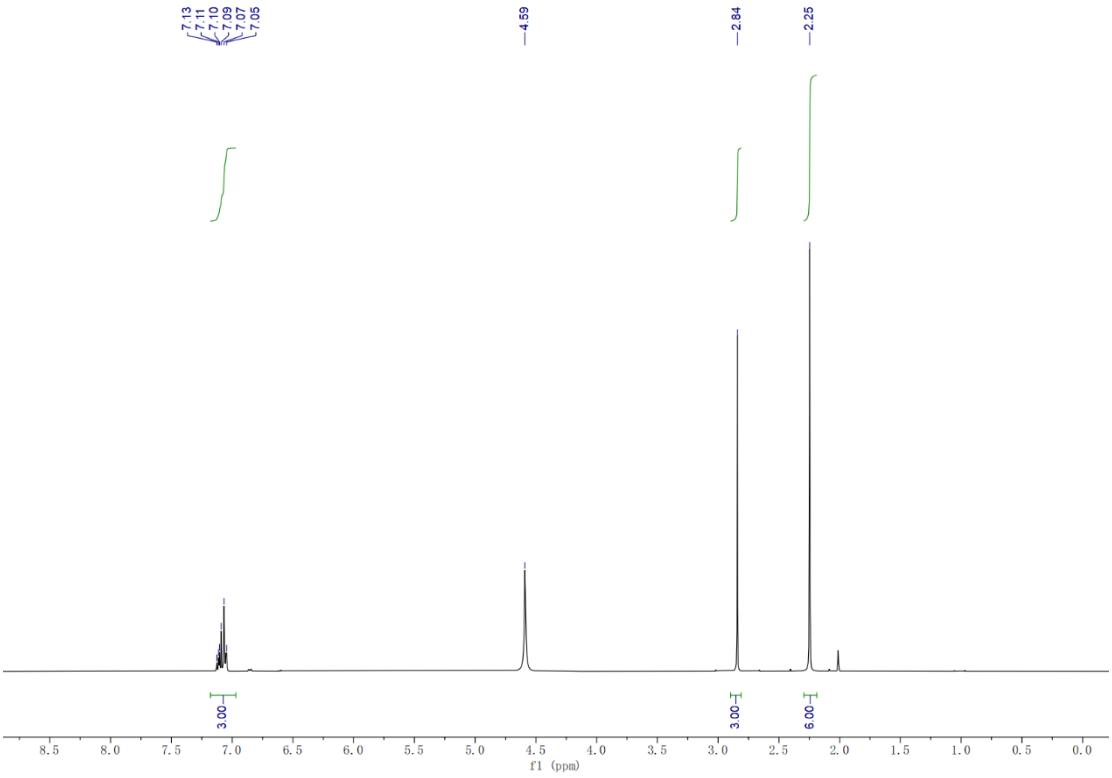


Figure S8.11 ^{1}H NMR spectrum of **6f** in D_2O at 400 MHz.

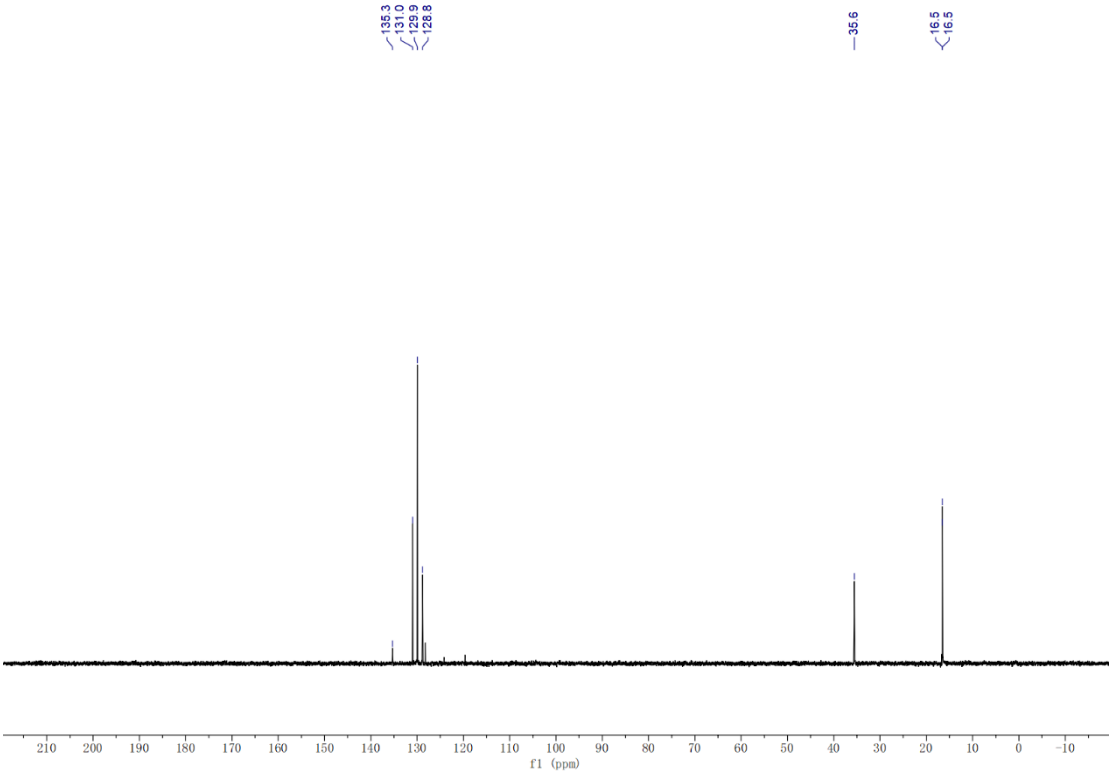


Figure S8.12 ^{13}C NMR spectrum of **6f** in D_2O at 101 MHz.

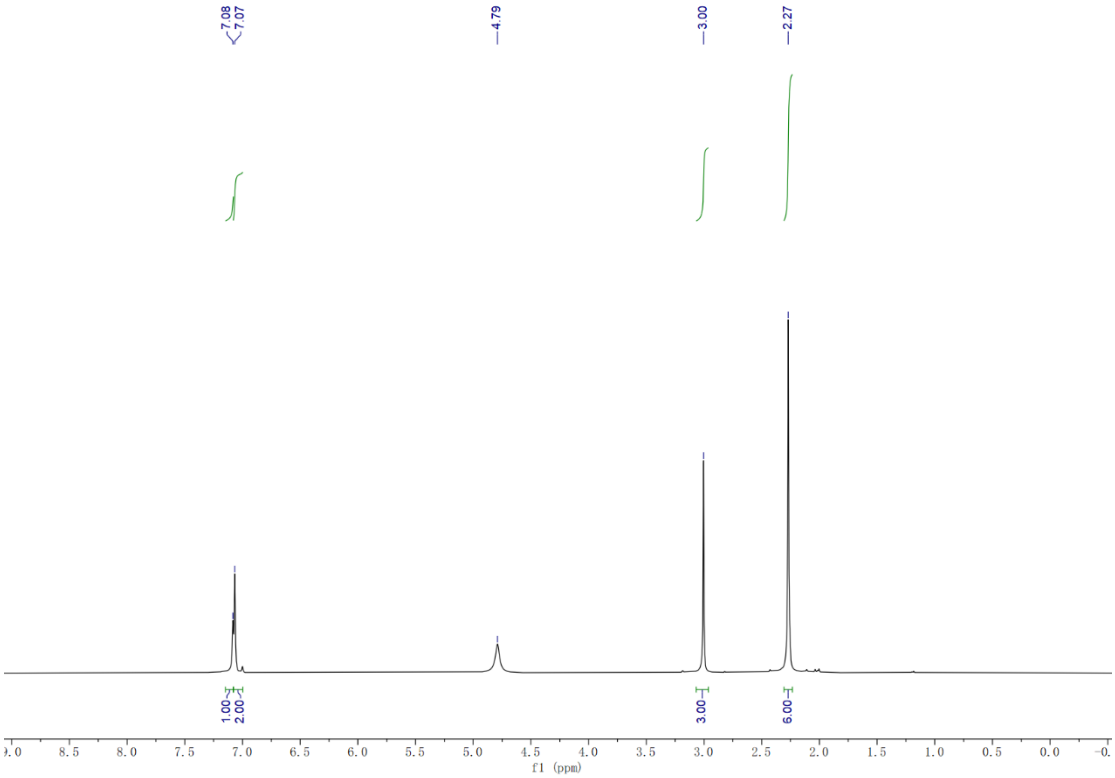


Figure S8.13 ^{1}H NMR spectrum of **6g** in D_2O at 400 MHz.

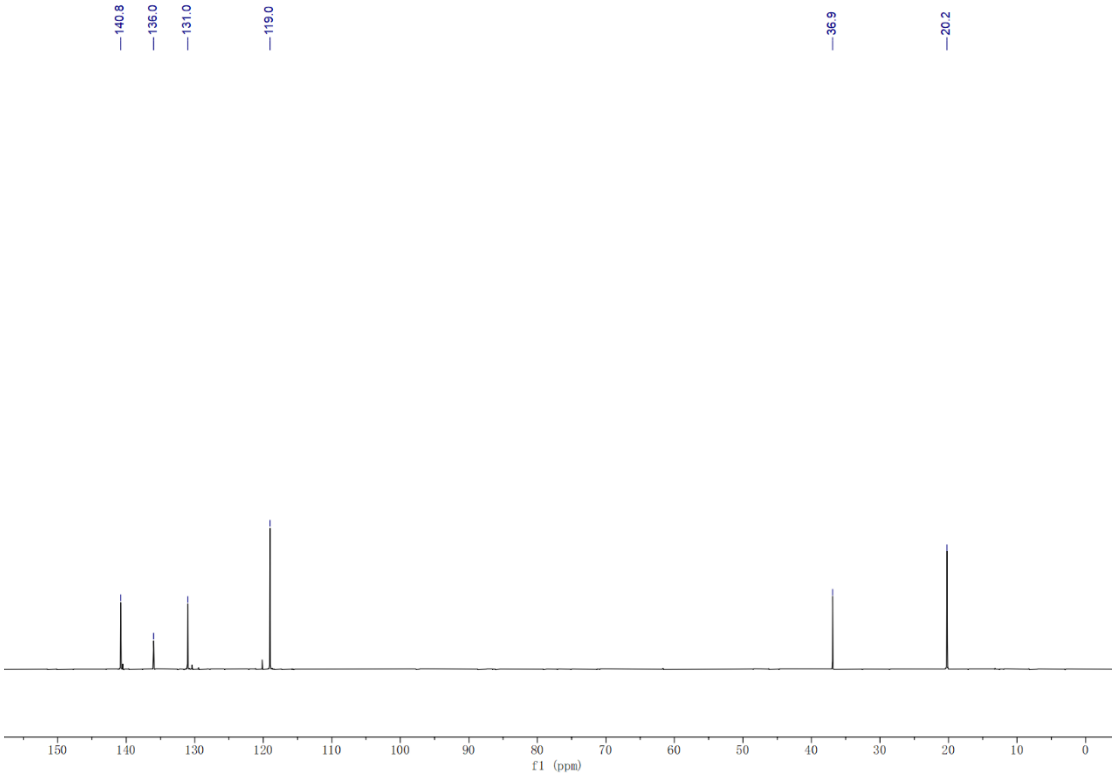


Figure S8.14 ^{13}C NMR spectrum of **6g** in D_2O at 101 MHz.

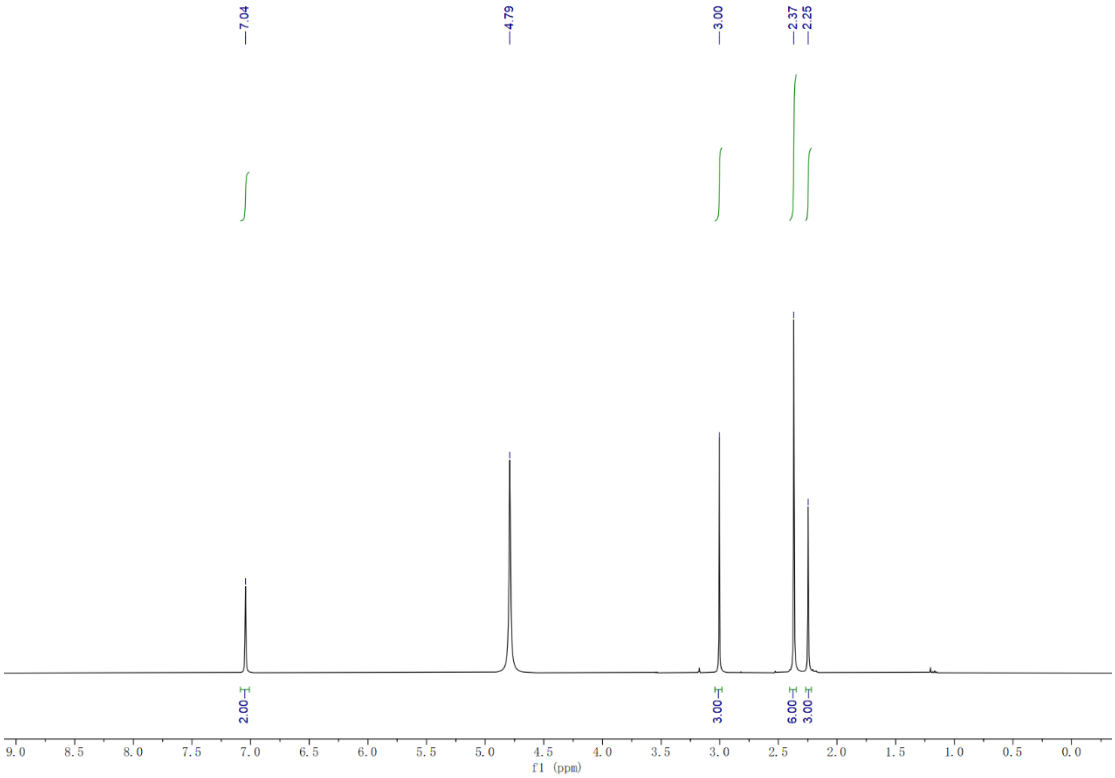


Figure S8.15 ^{1}H NMR spectrum of **6h** in D_2O at 400 MHz.

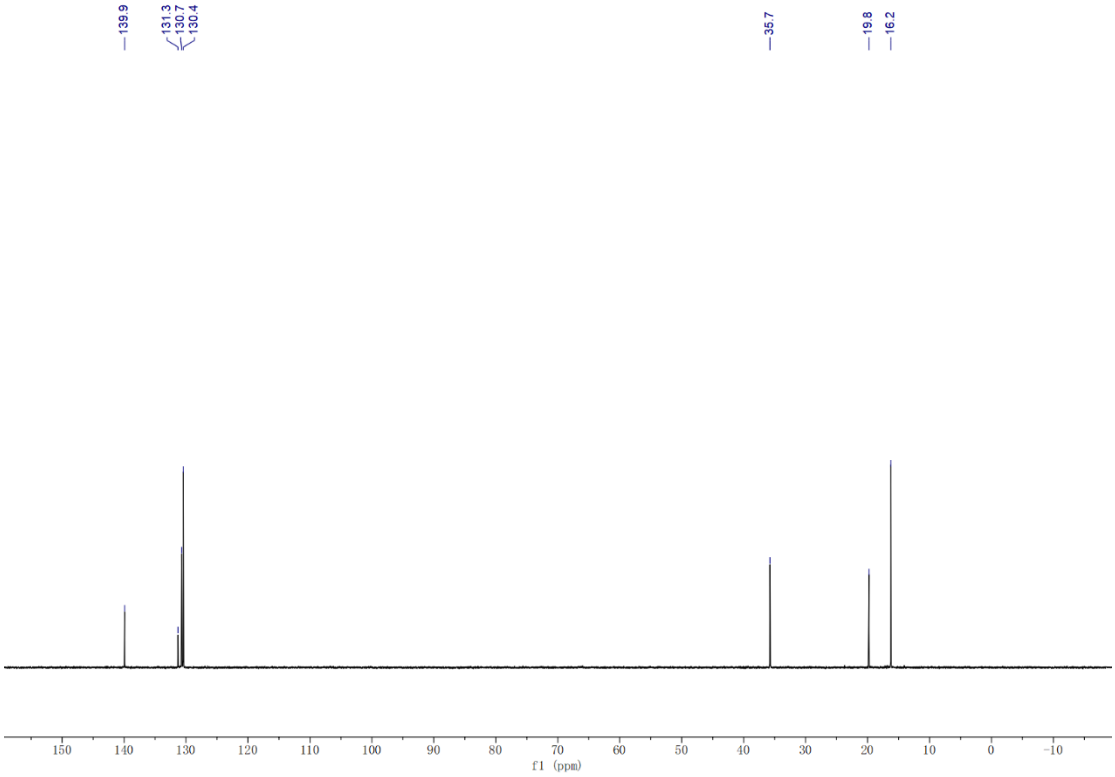


Figure S8.16 ^{13}C NMR spectrum of **6h** in D_2O at 101 MHz.

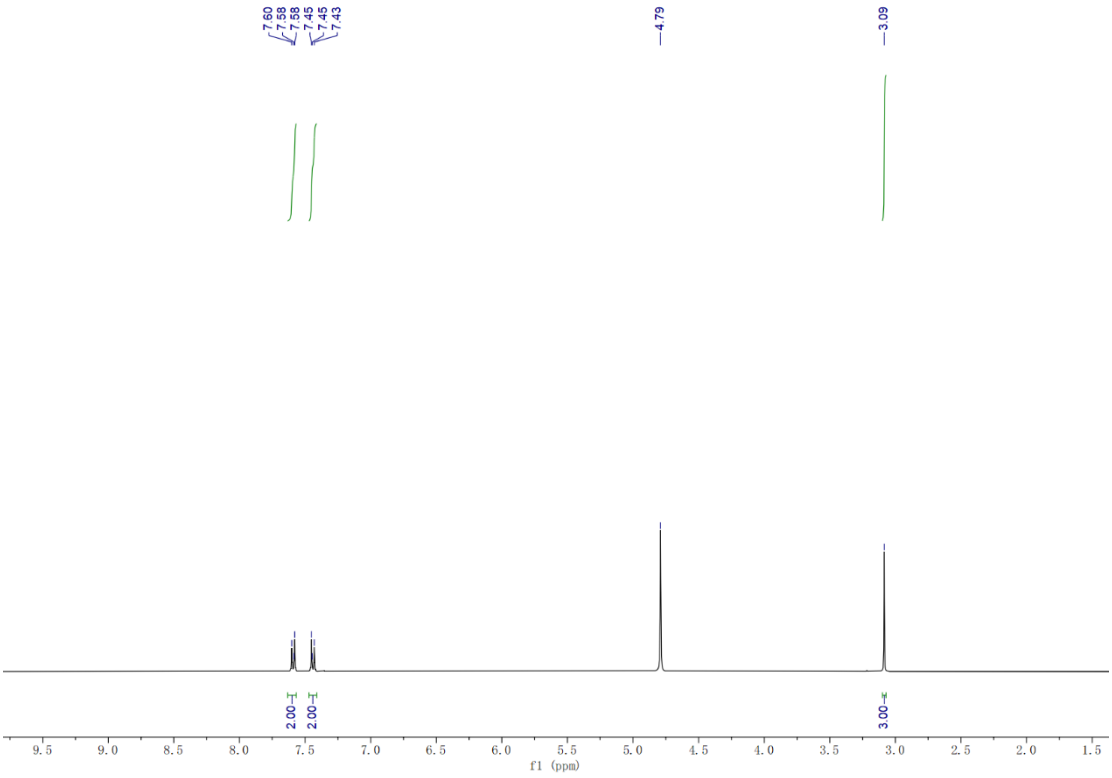


Figure S8.17 ^{1}H NMR spectrum of **6i** in D_2O at 400 MHz.

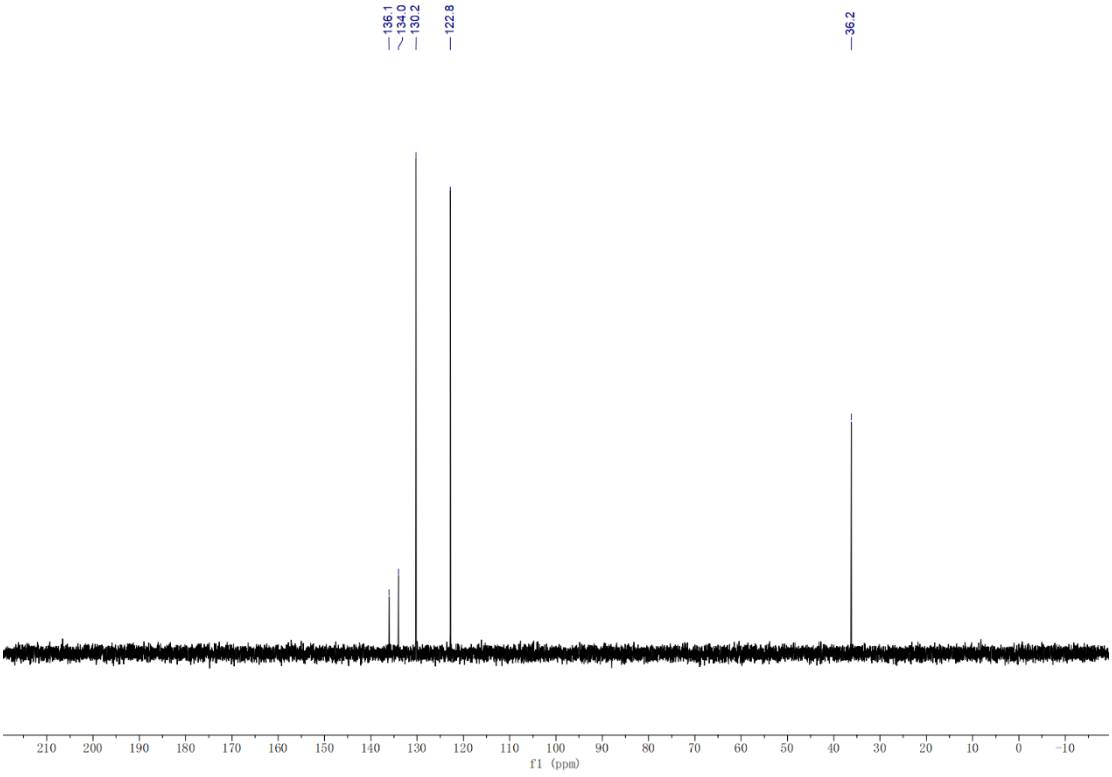


Figure S8.18 ^{13}C NMR spectrum of **6i** in D_2O at 101 MHz.

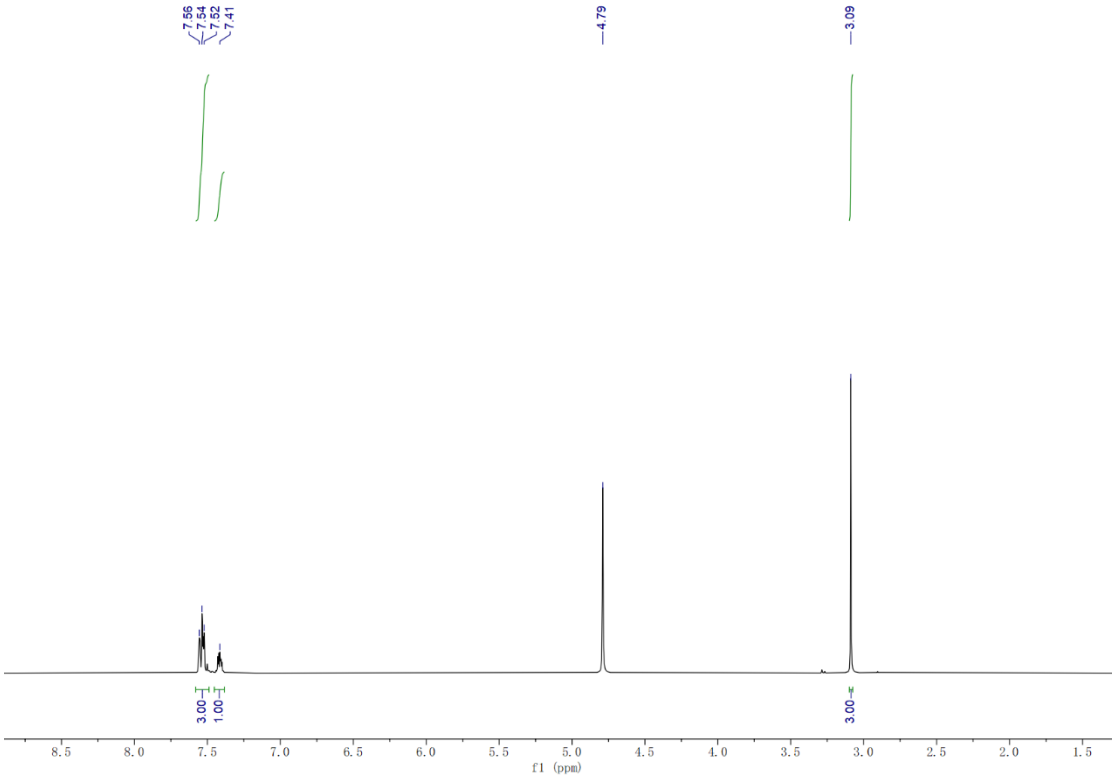


Figure S8.19 ^{1}H NMR spectrum of **6j** in D_2O at 400 MHz.

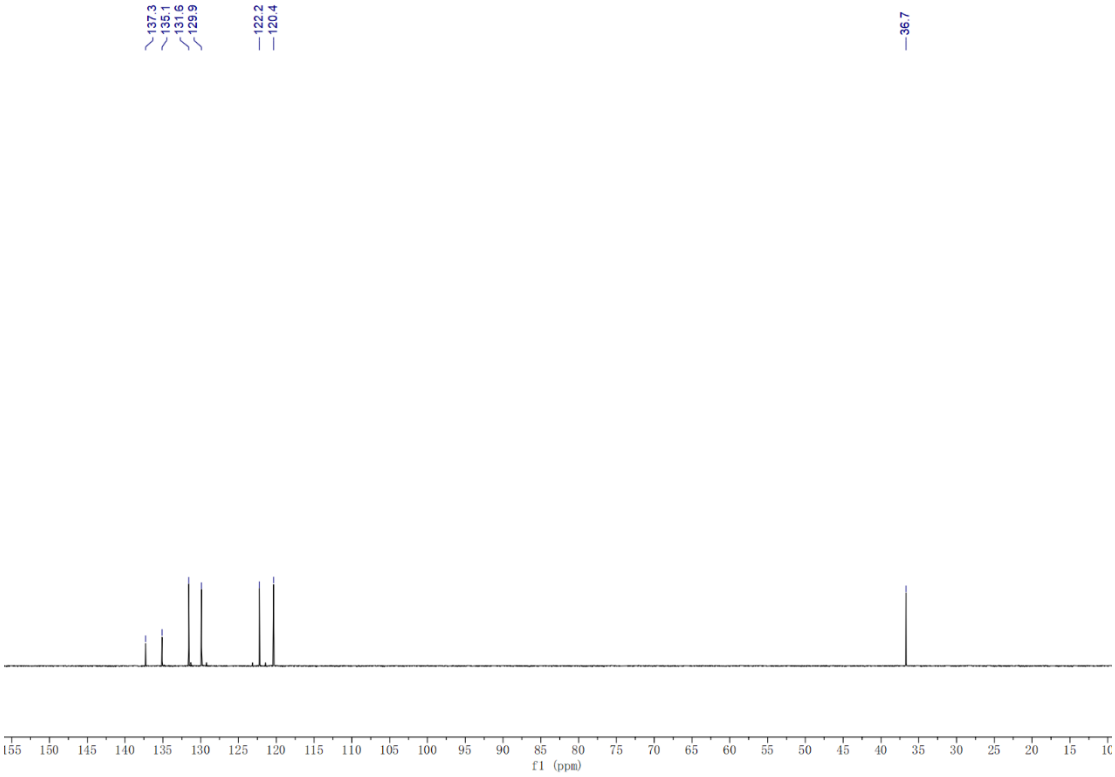


Figure S8.20 ^{13}C NMR spectrum of **6j** in D_2O at 101 MHz.

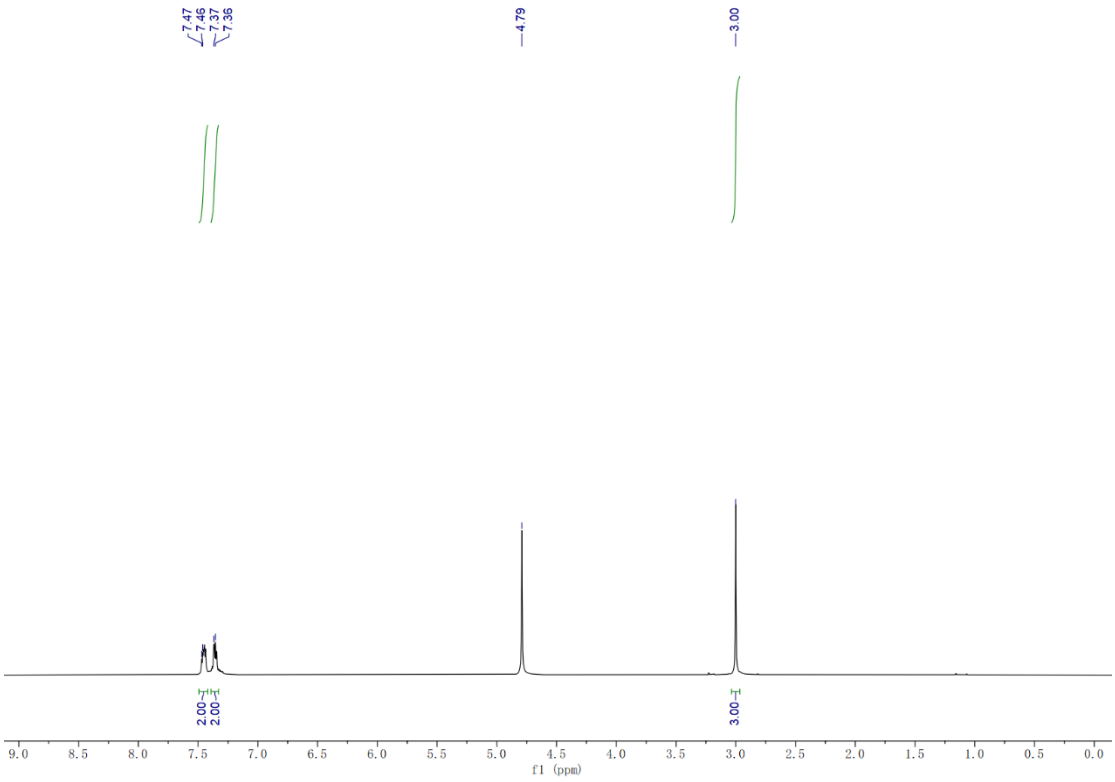


Figure S8.21 ^{1}H NMR spectrum of **6k** in D_2O at 400 MHz.

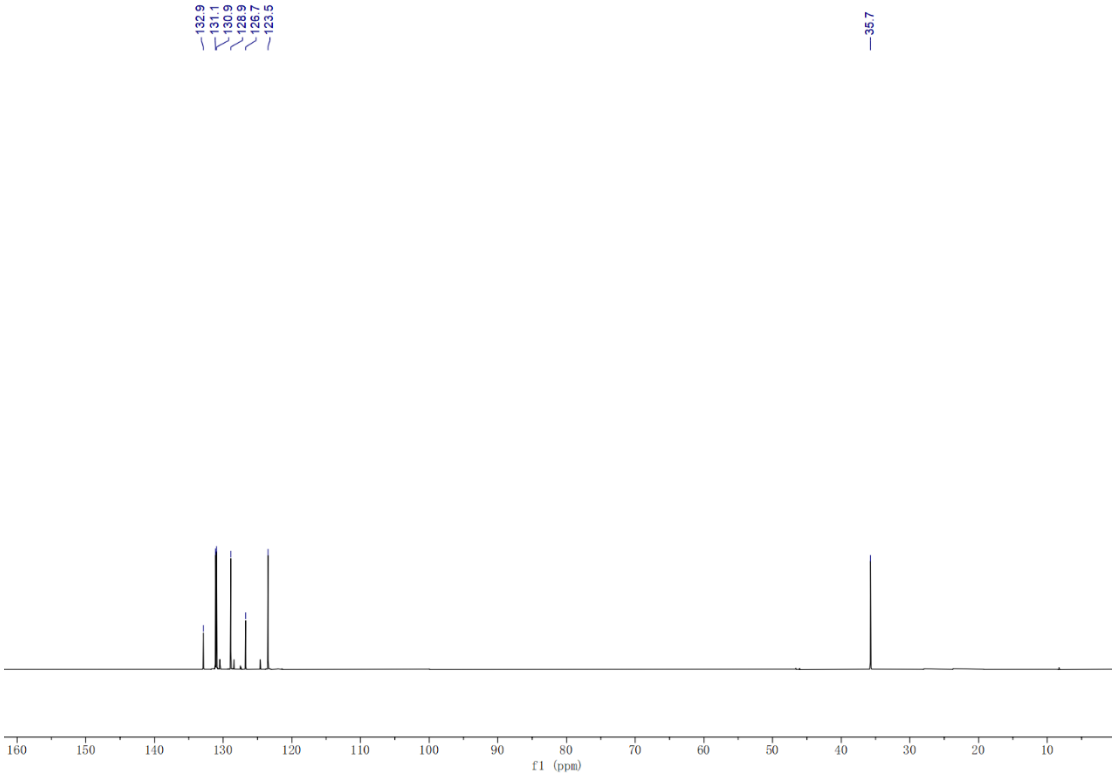


Figure S8.22 ^{13}C NMR spectrum of **6k** in D_2O at 101 MHz.

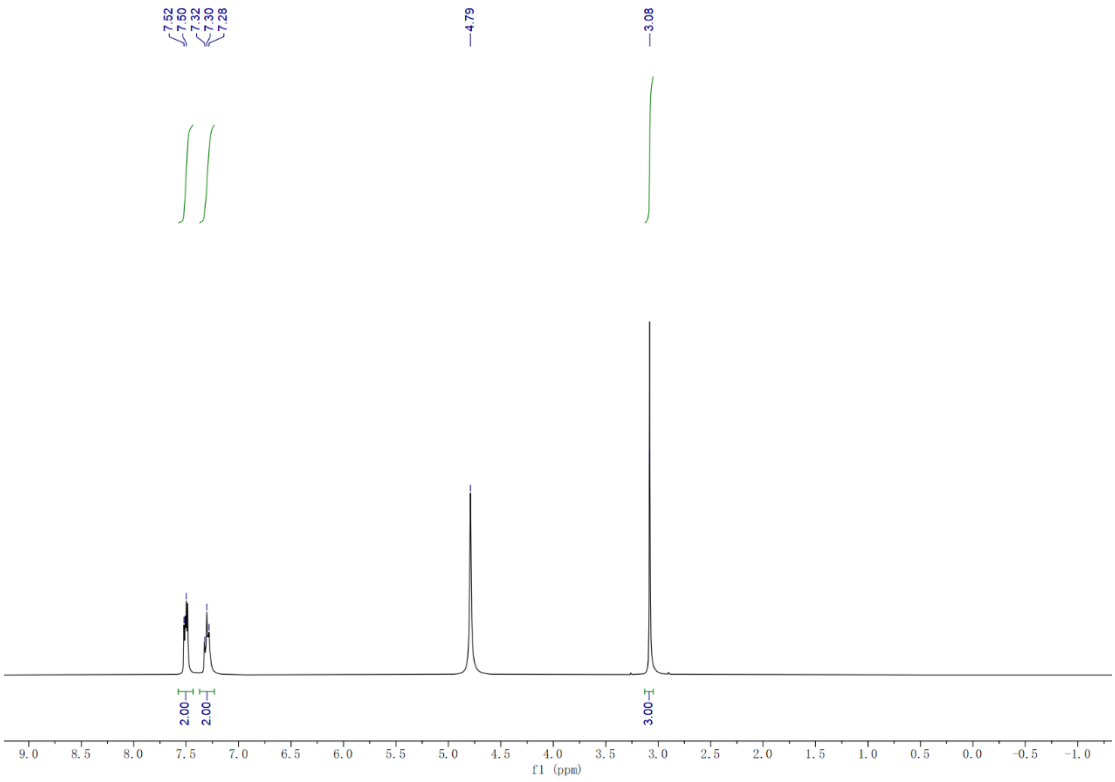


Figure S8.23 ^{1}H NMR spectrum of **6l** in D_2O at 400 MHz.

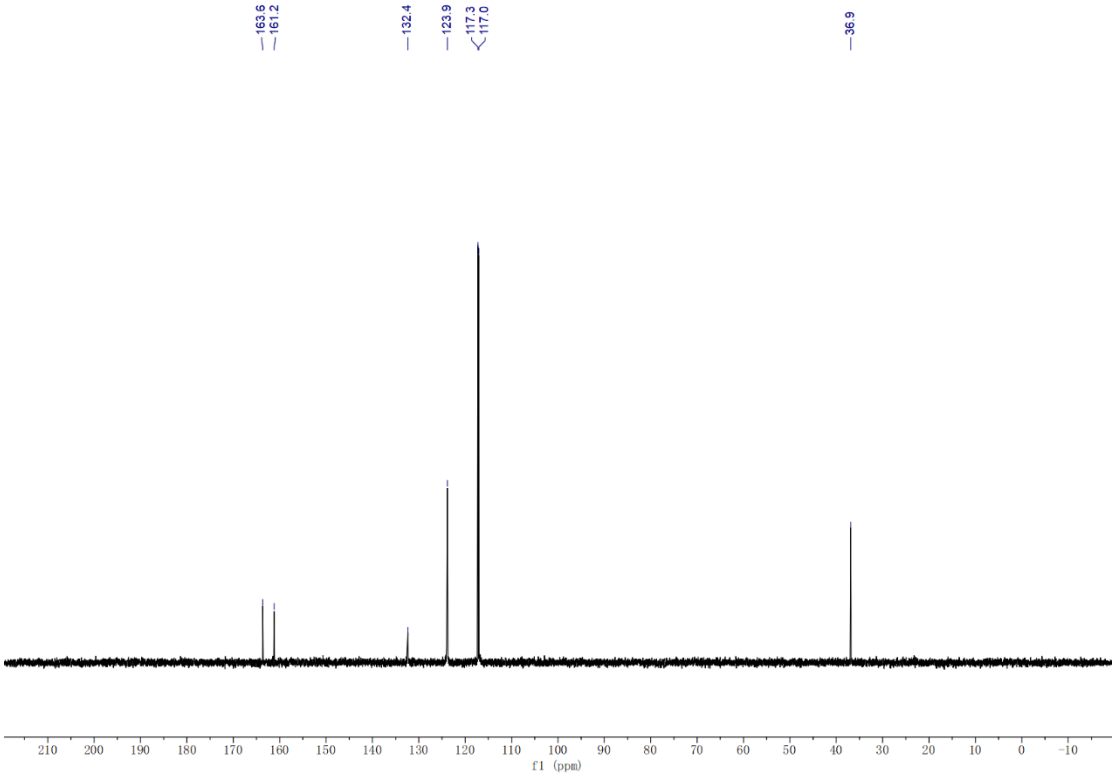


Figure S8.24 ^{13}C NMR spectrum of **6l** in D_2O at 101 MHz.

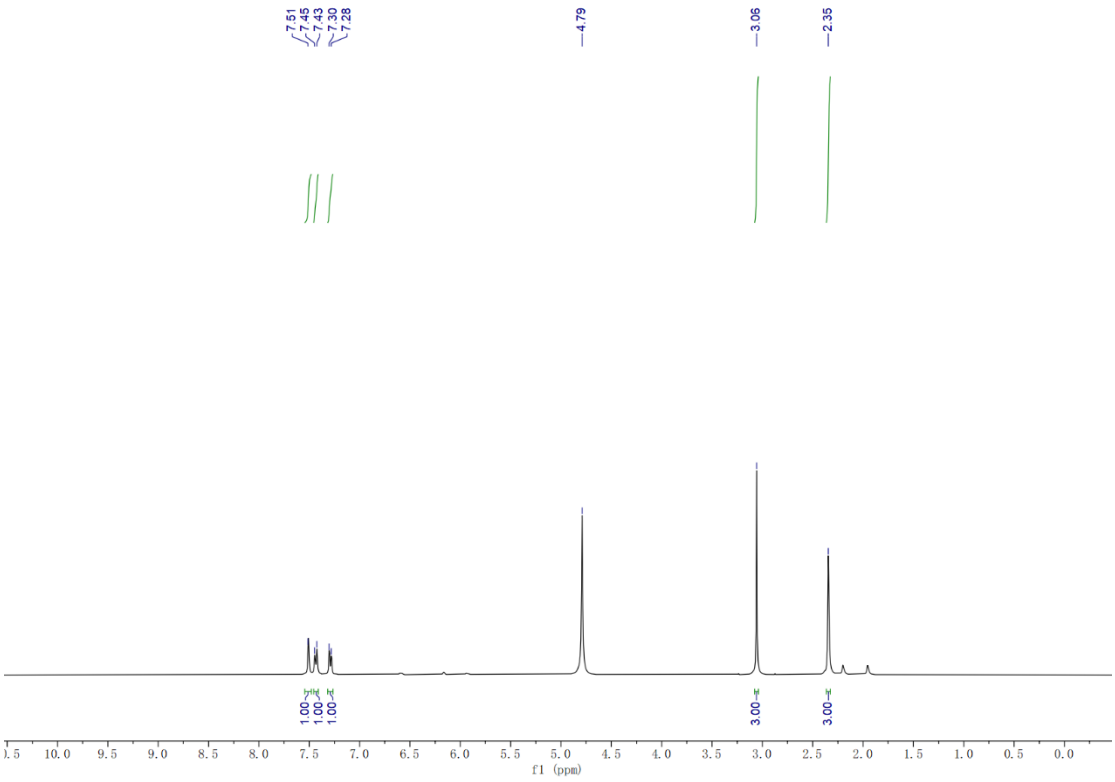


Figure S8.25 ^{1}H NMR spectrum of **6m** in D_2O at 400 MHz.

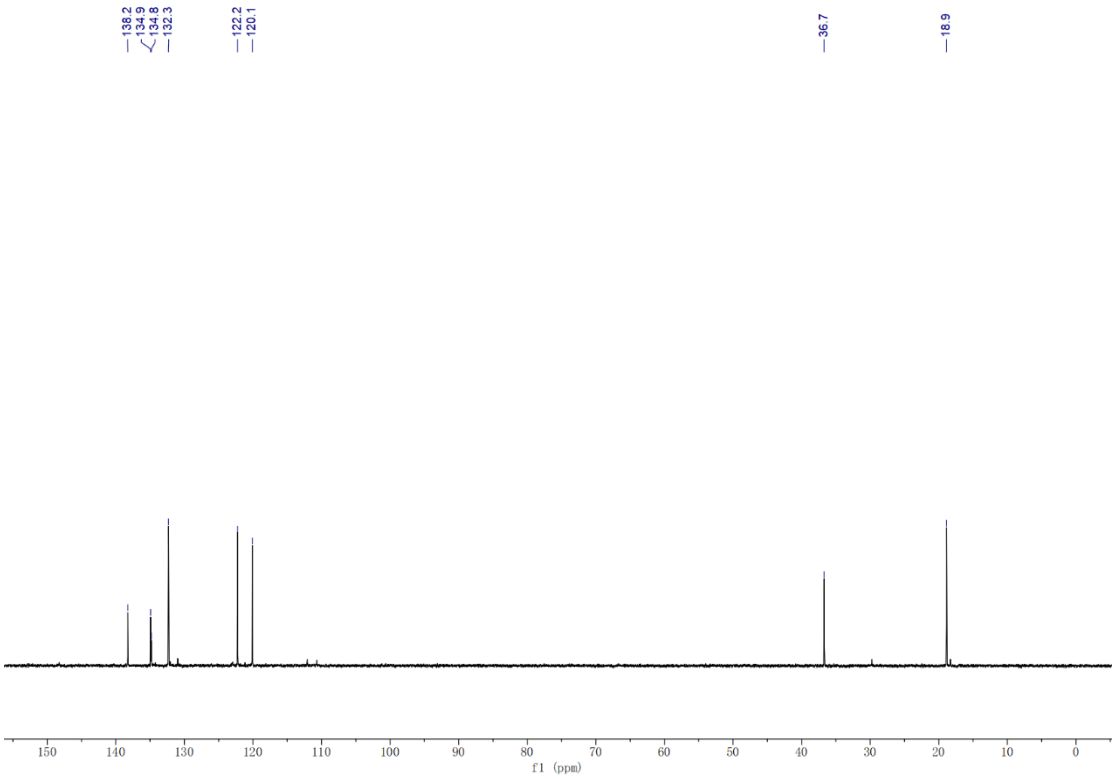


Figure S8.26 ^{13}C NMR spectrum of **6m** in D_2O at 101 MHz.

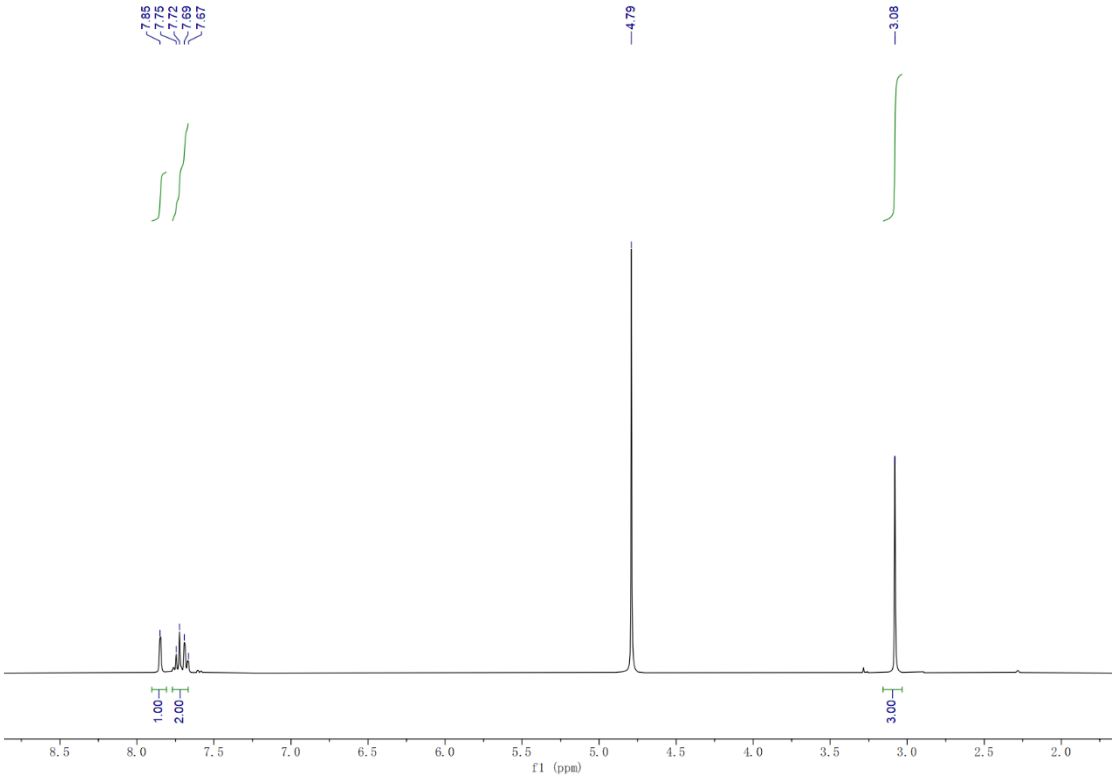


Figure S8.27 ^{1}H NMR spectrum of **6n** in D_2O at 400 MHz.

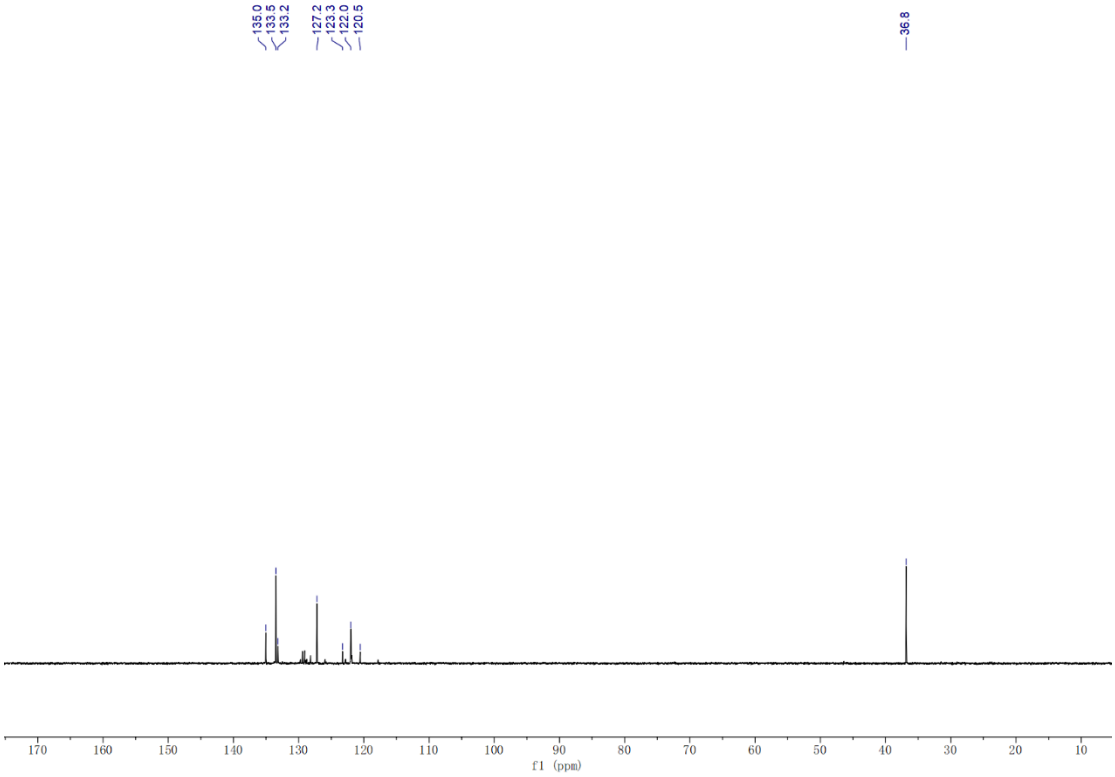


Figure S8.28 ^{13}C NMR spectrum of **6n** in D_2O at 101 MHz.

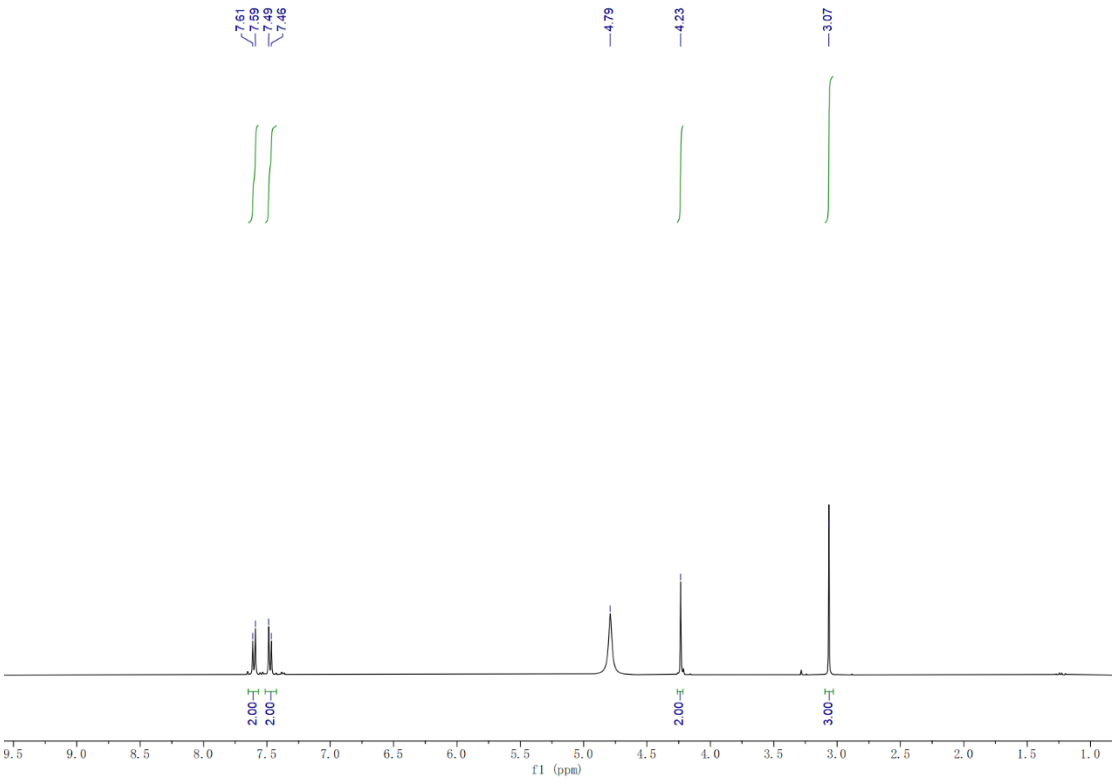


Figure S8.29 ^{1}H NMR spectrum of **6o** in D_2O at 400 MHz.

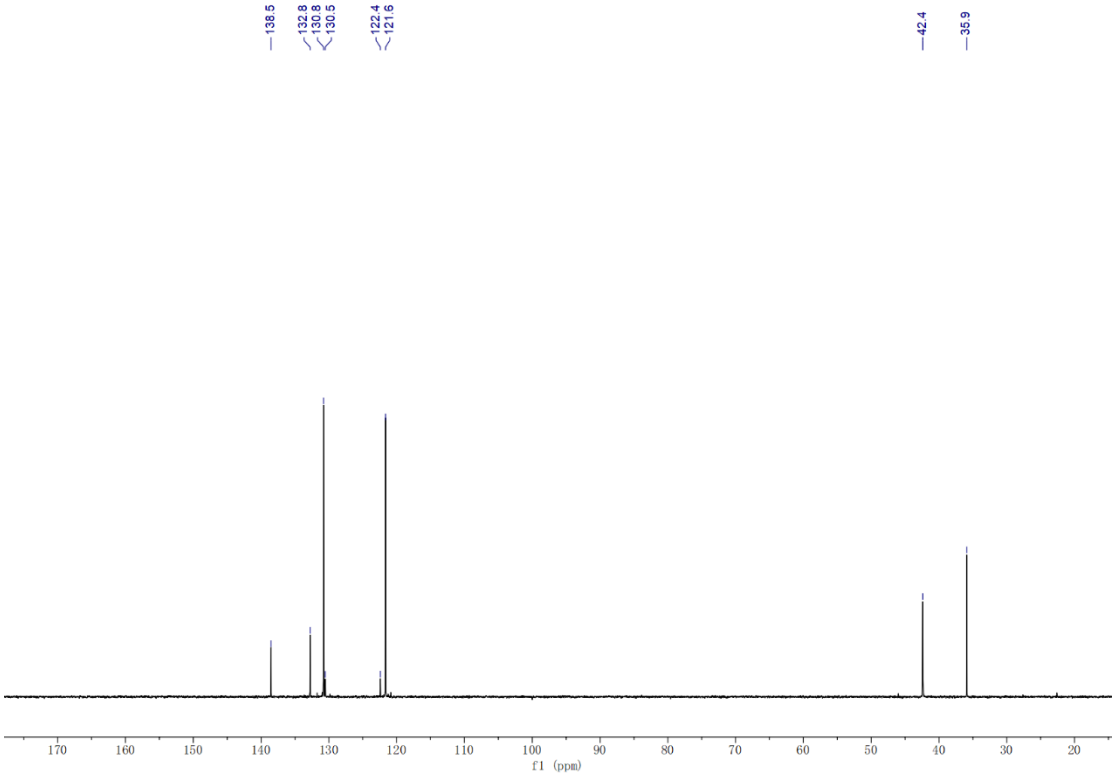


Figure S8.30 ^{13}C NMR spectrum of **6o** in D_2O at 101 MHz.

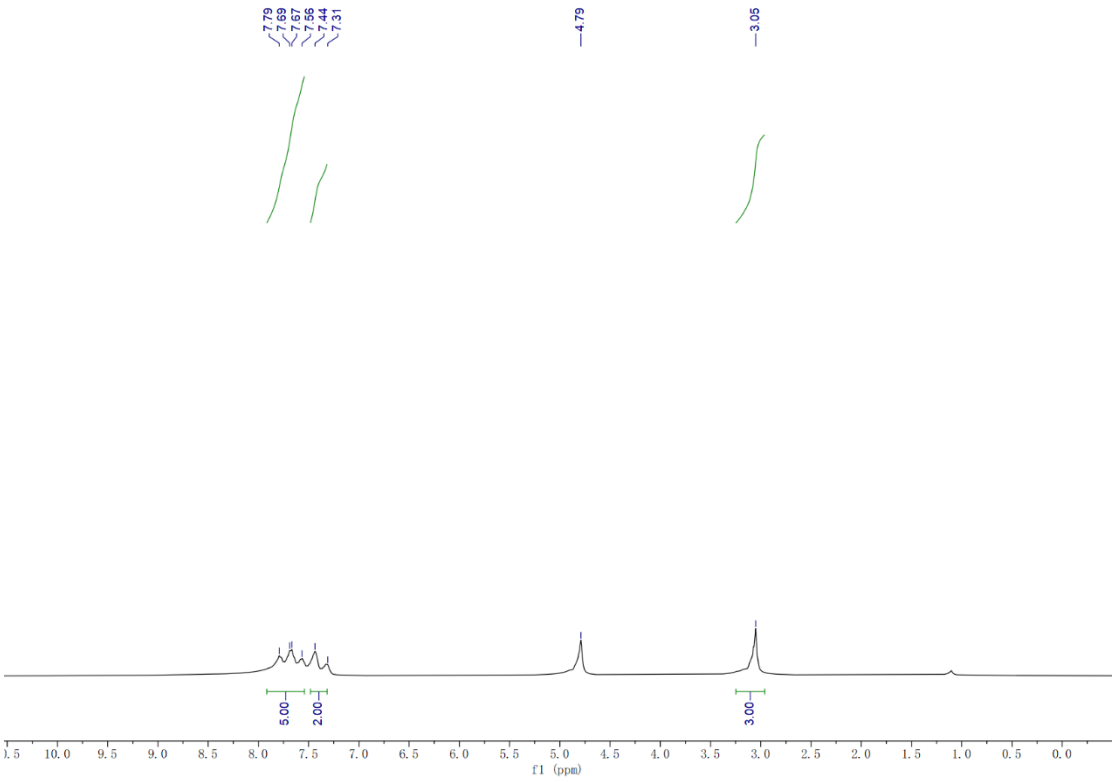


Figure S8.31 ^{1}H NMR spectrum of **6p** in D_2O at 400 MHz.

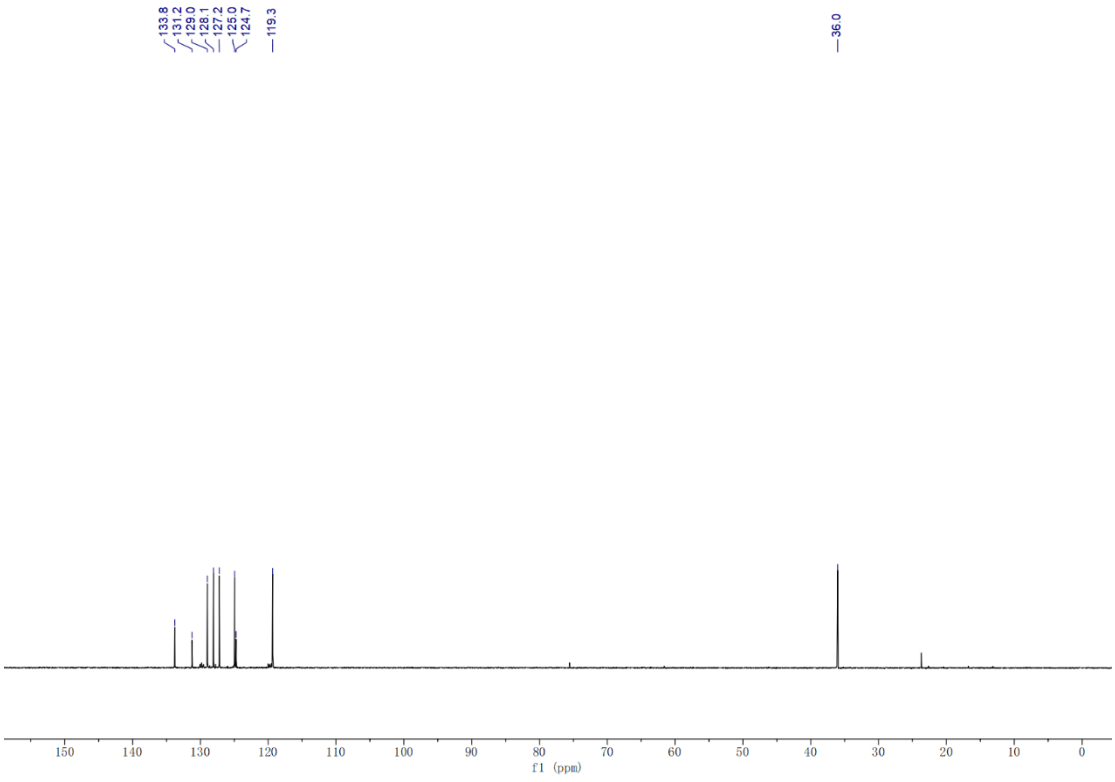


Figure S8.32 ^{13}C NMR spectrum of **6p** in D_2O at 101 MHz.

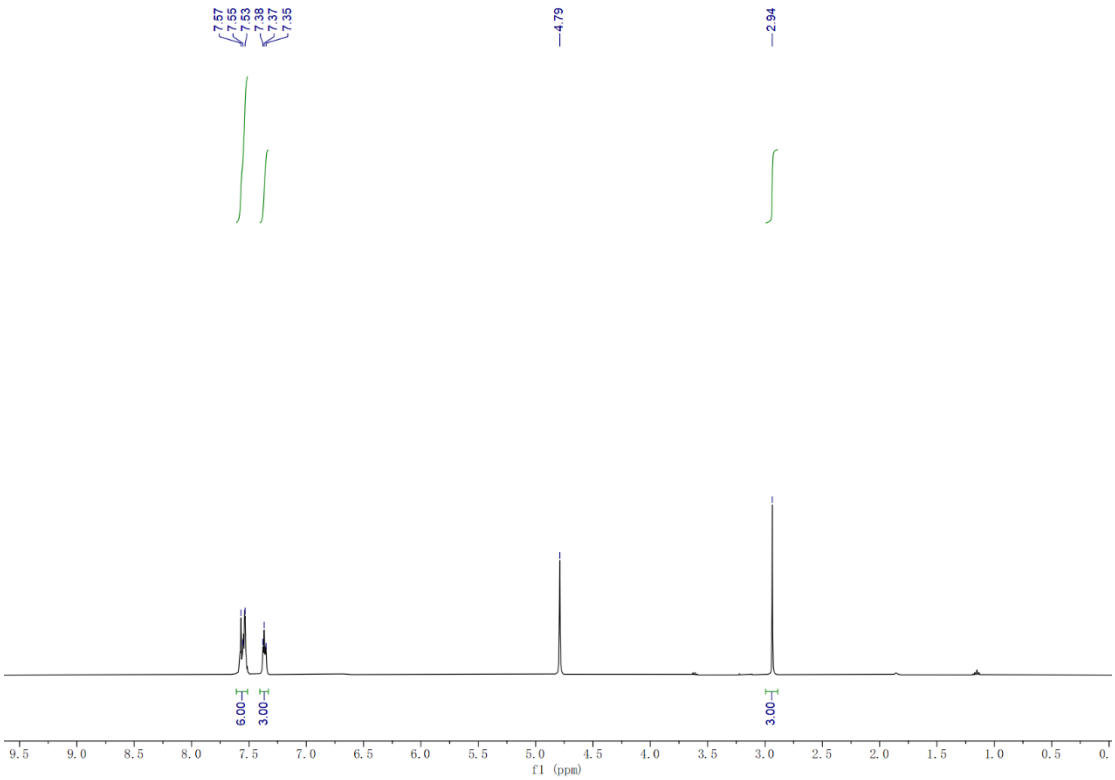


Figure S8.33 ^{1}H NMR spectrum of **6q** in D_2O at 400 MHz.

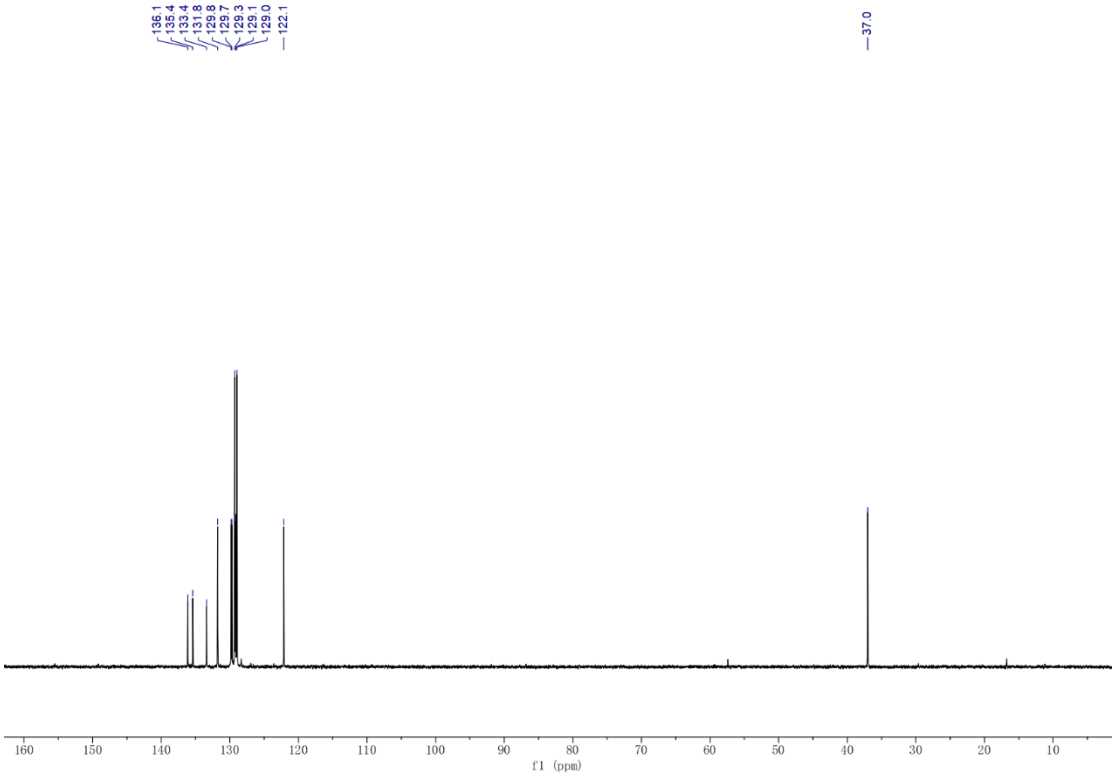


Figure S8.34 ^{13}C NMR spectrum of **6q** in D_2O at 101 MHz.

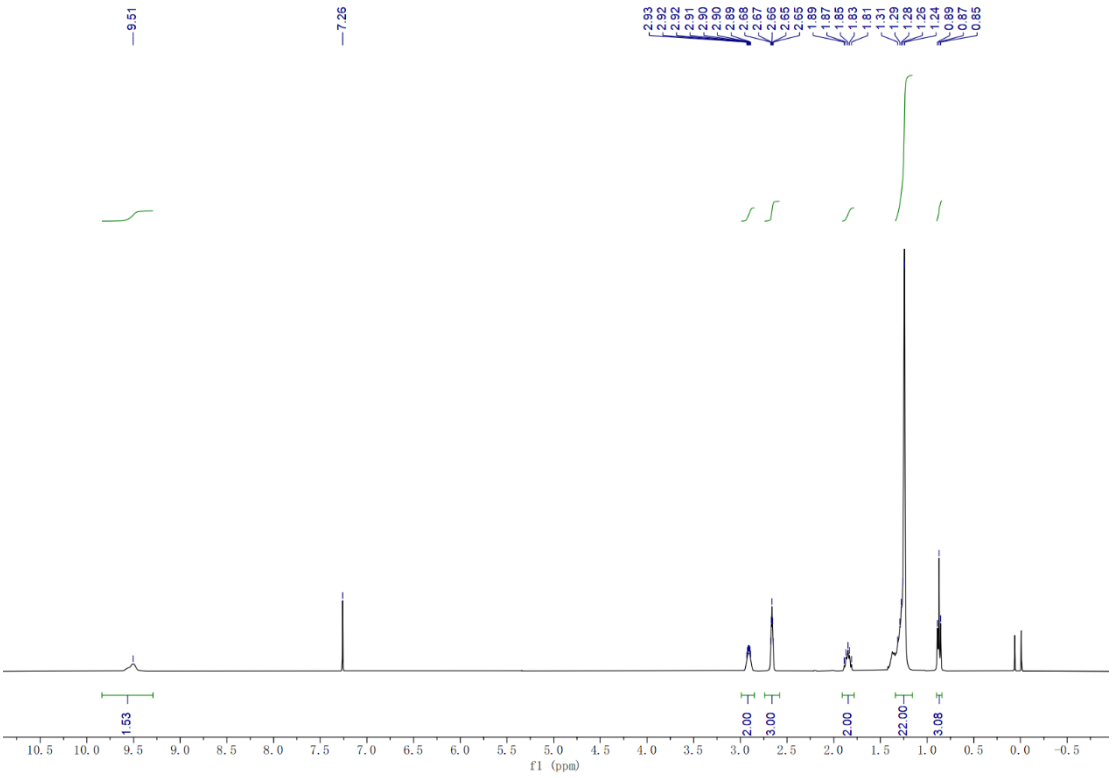


Figure S8.35 ^{1}H NMR spectrum of **6r** in $CDCl_3$ at 400 MHz.

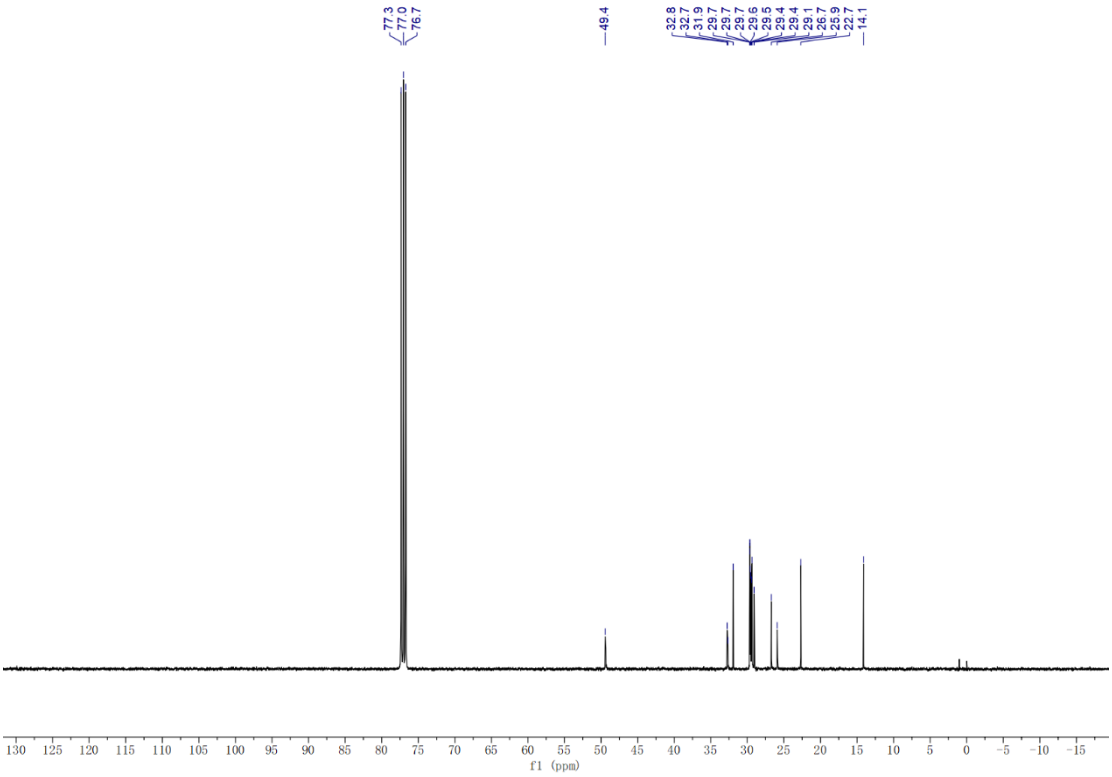


Figure S8.36 ^{13}C NMR spectrum of **6r** in $CDCl_3$ at 101 MHz.

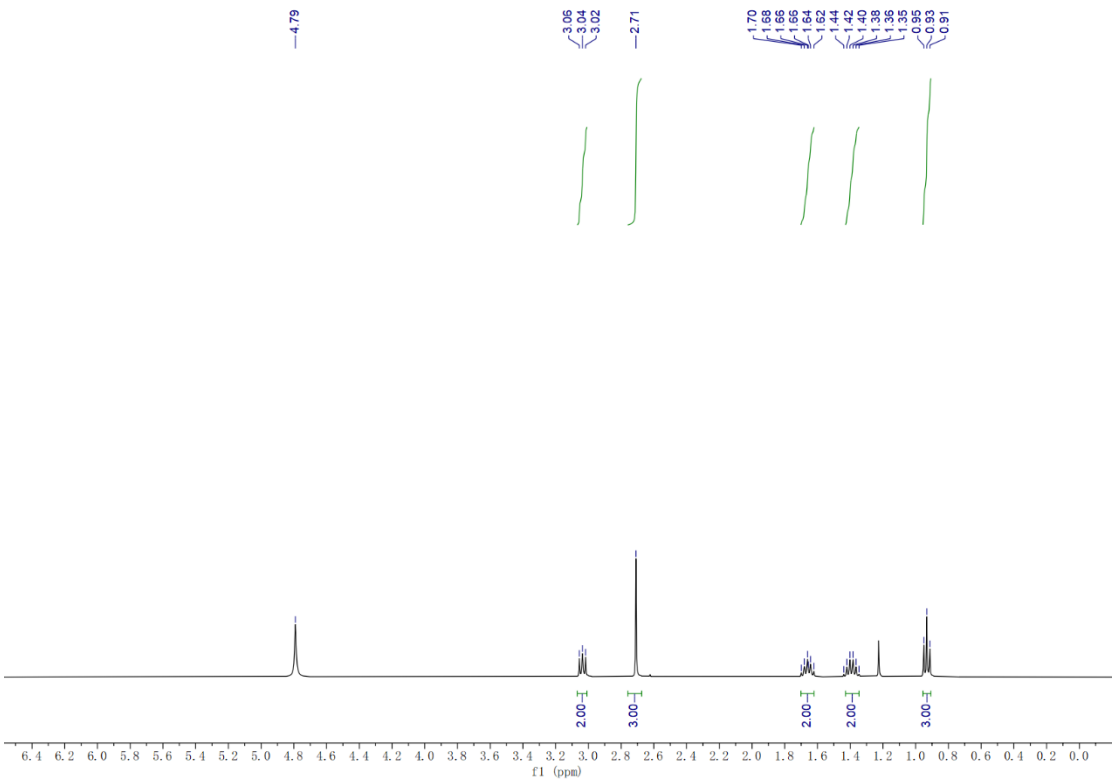


Figure S8.37 ^{1}H NMR spectrum of **6s** in D_2O at 400 MHz.

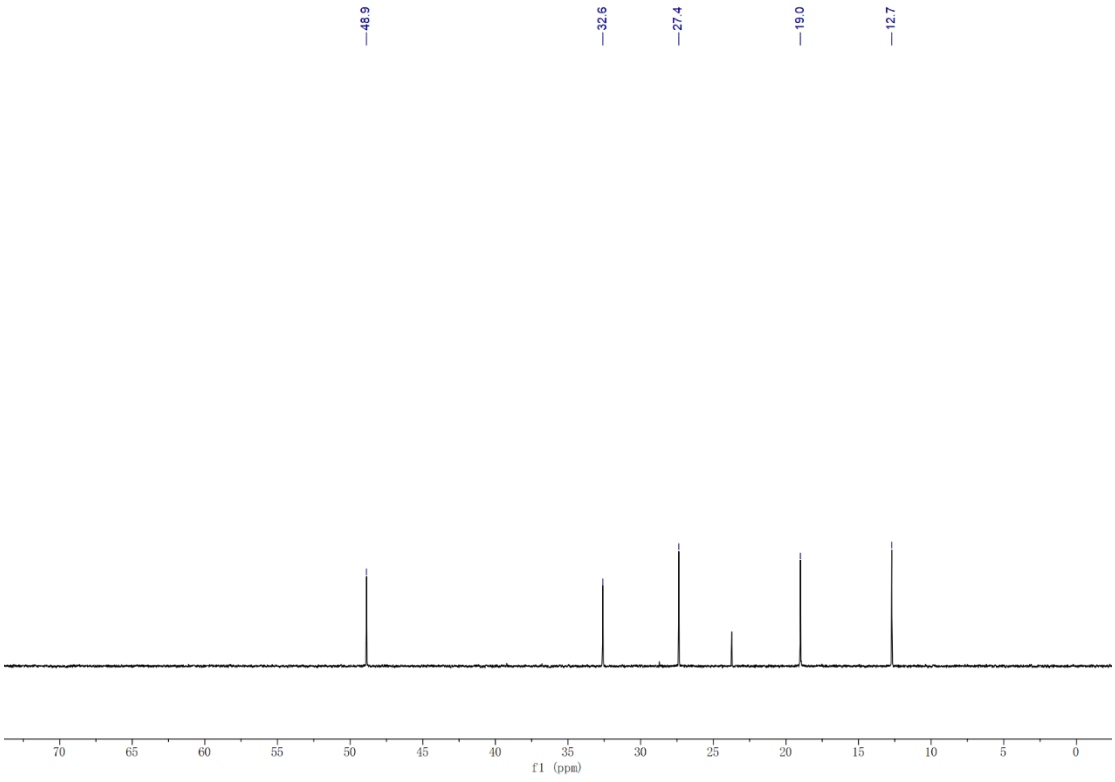


Figure S8.38 ^{13}C NMR spectrum of **6s** in D_2O at 101 MHz.

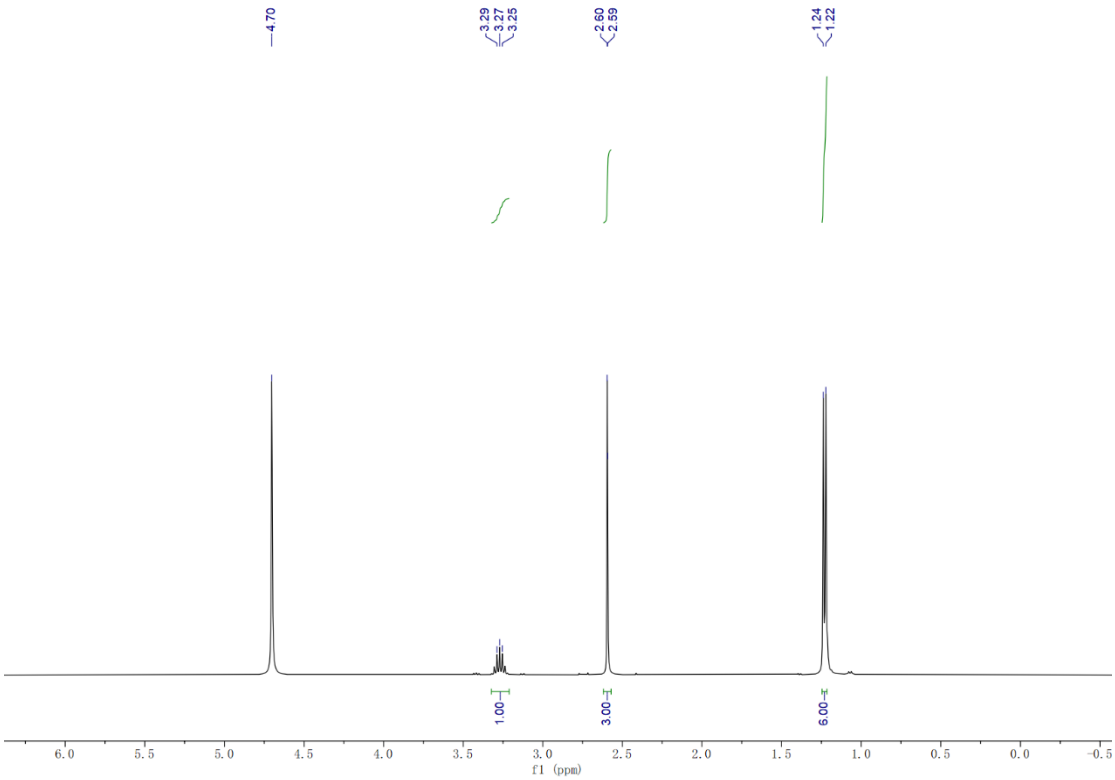


Figure S8.39 ^{1}H NMR spectrum of **6t** in D_2O at 400 MHz.

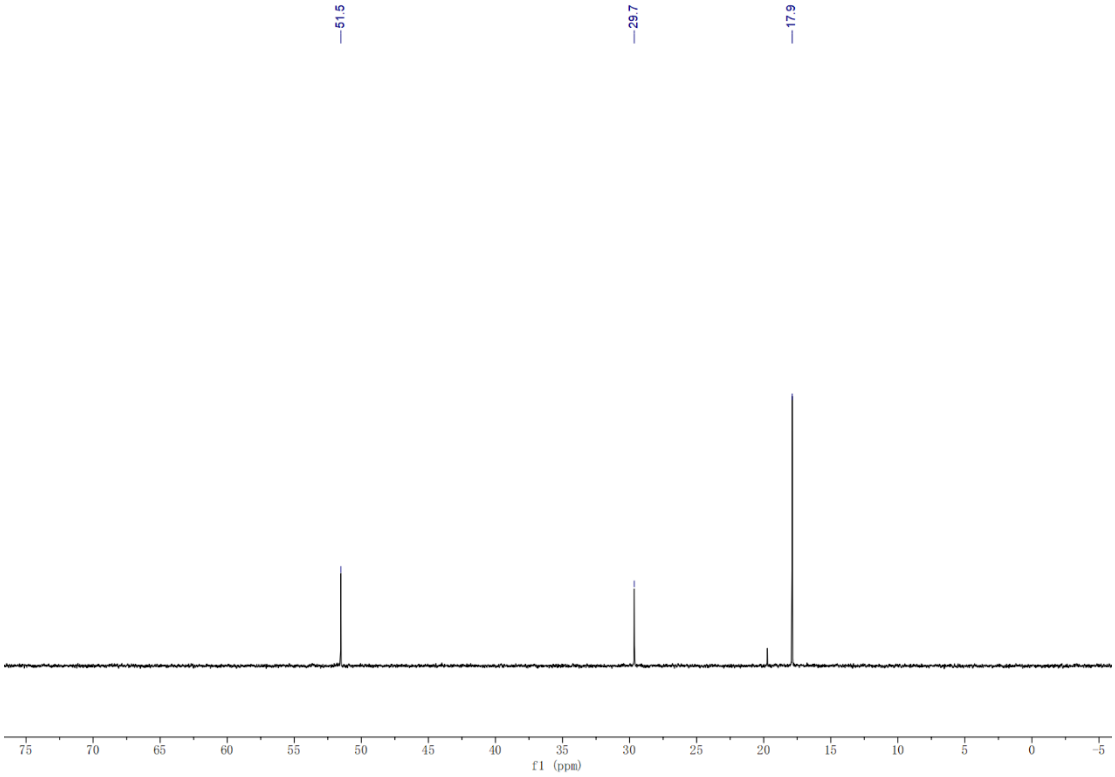
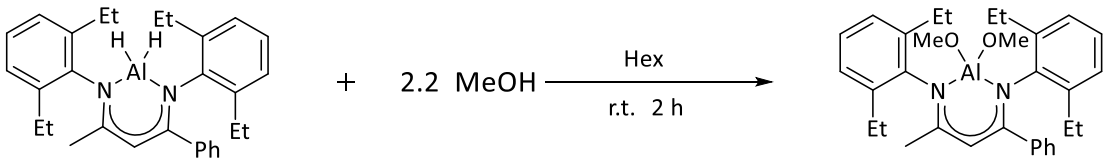


Figure S8.40 ^{13}C NMR spectrum of **6t** in D_2O at 101 MHz.

9. Control experiments for the mechanistic investigation

a) A stoichiometric study of the reaction between *p*-tolyl isocyanate and methanol catalysed by **C5**

Initially, a stoichiometric reaction between **C5** and 2.2 equivalents of *p*-tolyl isocyanate was conducted under nitrogen at room temperature for 2 hours. Following the removal of hexane under vacuum, ^{1}H NMR analysis revealed a complex mixture without any distinct characteristic peaks. However, under identical conditions, the reaction between **C5** and methanol led to the disappearance of the methanol proton signal in the ^{1}H NMR spectrum, alongside the appearance of a peak at 3.23 ppm, corresponding to the **L_2AlOMe** species.



Scheme S9.1 Stoichiometric reaction of **C5** with methanol.

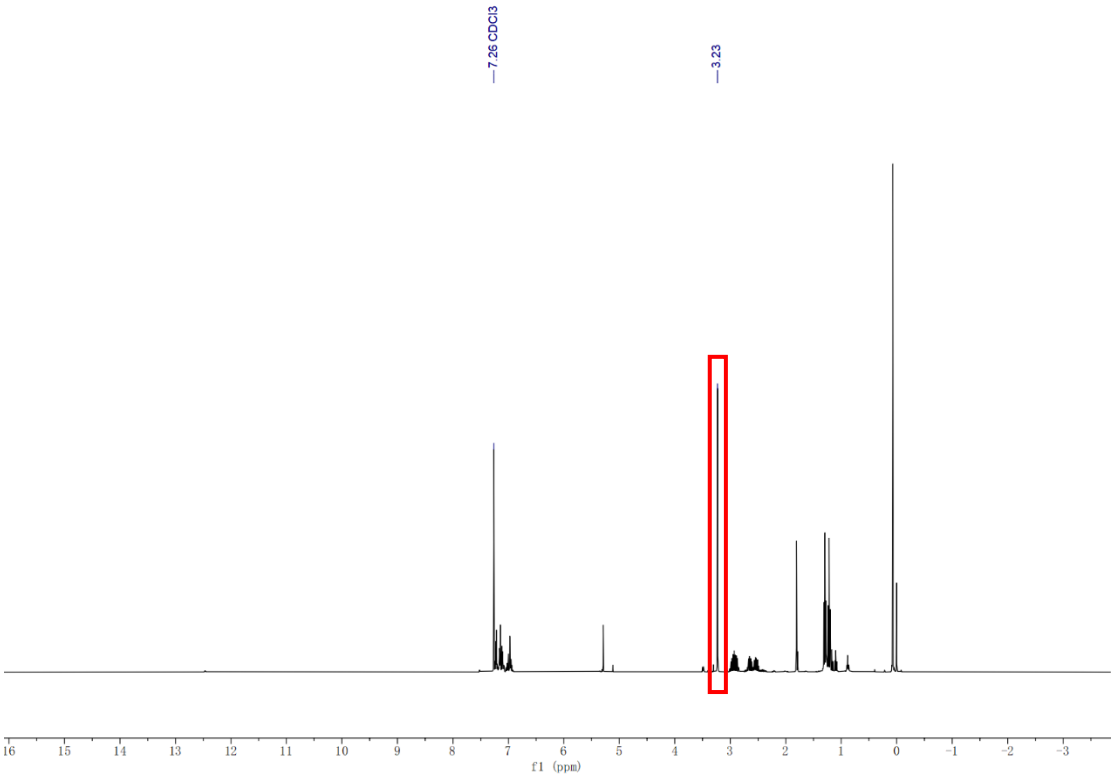


Figure S9.1 ^{1}H NMR spectrum of the reaction between **C5** and methanol in $CDCl_3$.

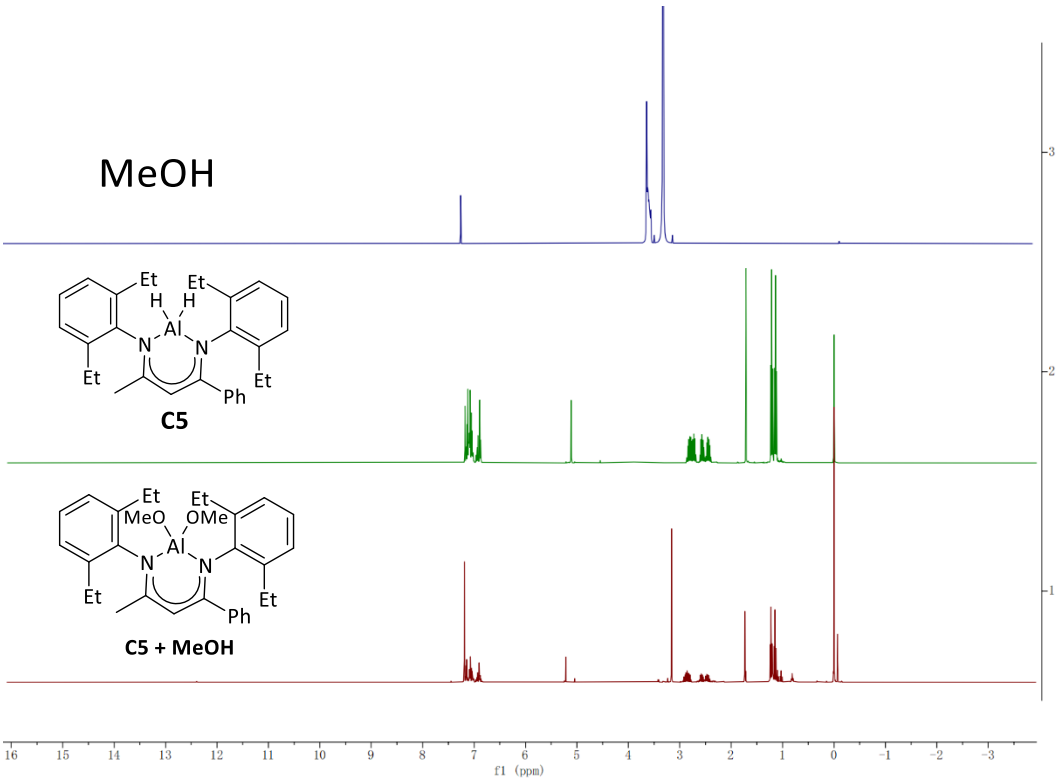


Figure S9.2 (1) ^{1}H NMR spectrum of the reaction between **C5** and methanol (1:2.2) in $CDCl_3$. (2) ^{1}H NMR spectrum of catalyst **C5** in $CDCl_3$. (3) ^{1}H NMR spectrum of methanol in $CDCl_3$.

b) A stoichiometric study of the reaction between p-tolyl isocyanate and HBpin catalysed by **C1**

When **C1** was reacted with 1 equivalent of p-tolyl isocyanate, no differences were observed in the ^{1}H NMR spectrum compared to the original data. Therefore, we hypothesise that the ethyl group on **C1** first undergoes hydrogen exchange with HBpin, generating EtBpin and the corresponding zinc hydride species. Changes in the ^{11}B NMR spectrum following the mixing of **C1** with HBpin confirm this, in accordance with previous reports.[5]

As shown in **Figure S9.3**, when **C1** was mixed with 5 equivalents of HBpin, a stoichiometric reaction under nitrogen at room temperature for 2 hours produced a characteristic ^{11}B NMR signal for the ethyl boronate Et-Bpin. Additionally, as illustrated in **Figure S9.4**, although Zn-H signal could not be detected, ^{1}H NMR spectra following the reaction of **C1** with 1, 3, and 5 equivalents of HBpin showed splitting and shifting of the characteristic peaks of **C1**, along with a gradual reduction in the Zn-Et signal, consistent with the boron NMR results.

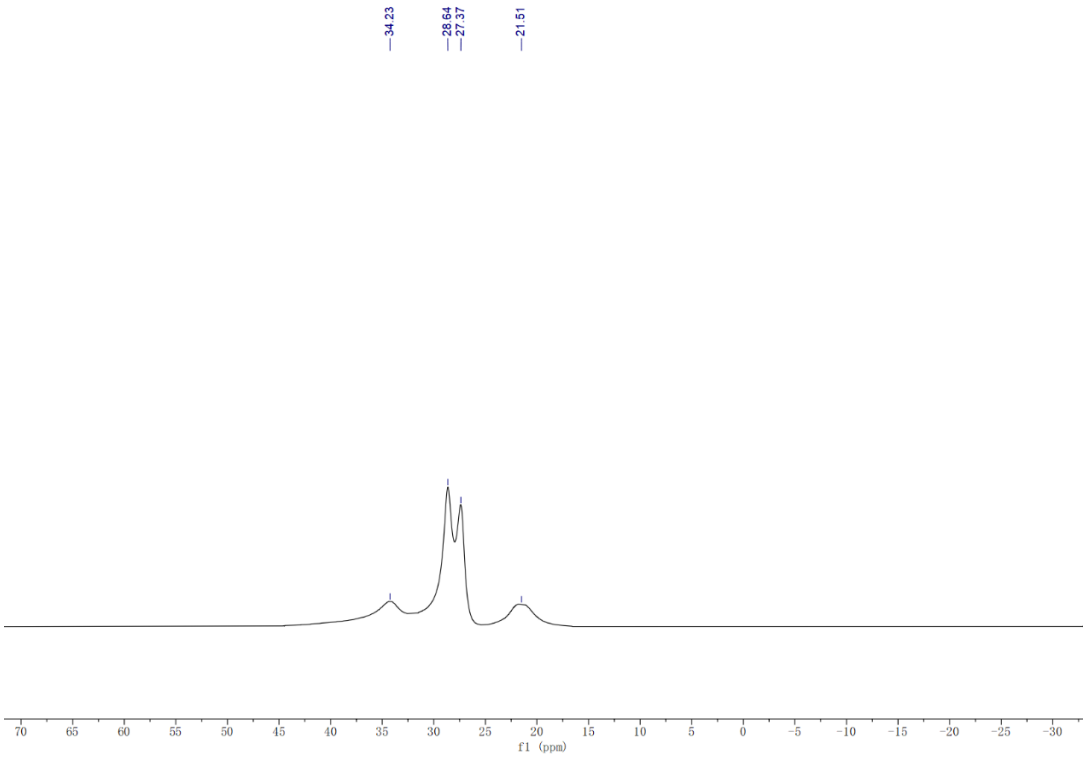


Figure S9.3 ^{11}B NMR spectrum of the reaction between **C1** and HBpin (1:5) in $CDCl_3$.

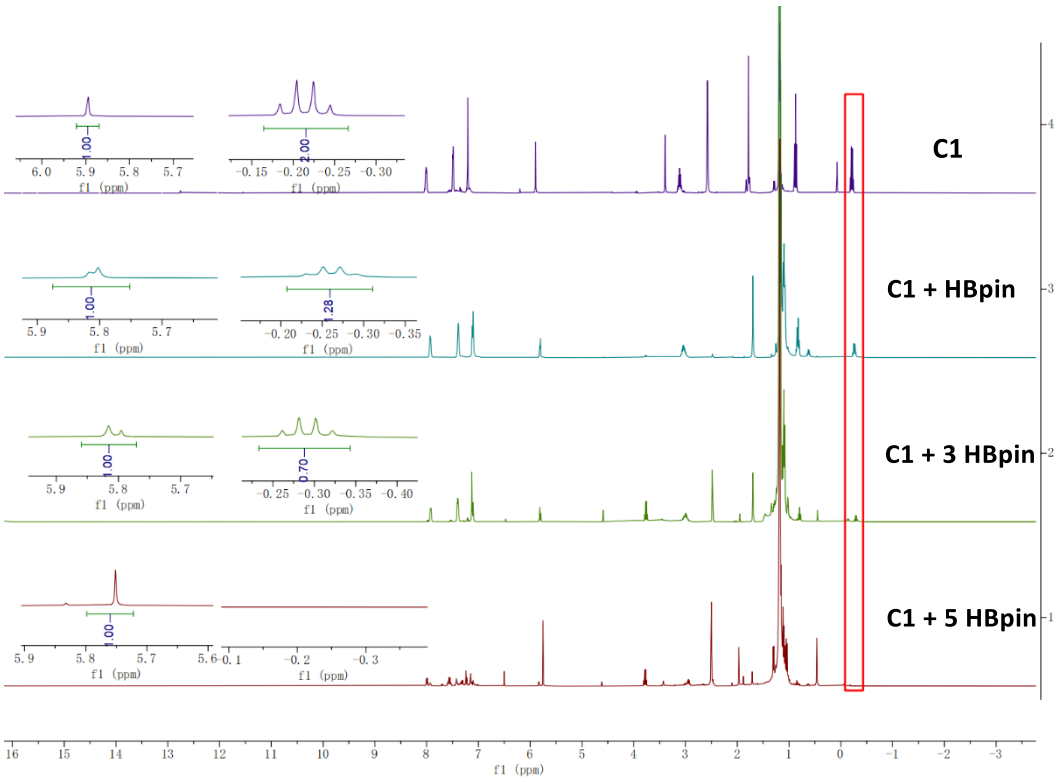


Figure S9.4 (1) ^{1}H NMR spectrum of catalyst **C1** in DMSO-d_6. (3) ^{1}H NMR spectrum of the reaction between **C1** and HBpin (1:1) DMSO-d_6. (3) ^{1}H NMR spectrum of the reaction between **C1** and HBpin (1:3) DMSO-d_6. (4) ^{1}H NMR spectrum of the reaction between **C1** and HBpin (1:5) DMSO-d_6.

10. Coodinates

CatA+ *n*-butyl isocyanate

Al	0.122322000	-0.070879000	-1.173837000
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C	2.436875000	-0.839932000	1.719018000
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C	-2.836343000	1.666835000	-1.853880000
C	3.749136000	-0.898579000	2.209983000
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C	-3.232942000	3.053463000	0.559259000
C	-3.490979000	2.906001000	-1.829667000
H	3.966699000	-0.465258000	3.190123000
C	4.776253000	-1.465351000	1.456299000
H	5.323462000	-2.324713000	-0.445181000
H	-3.355227000	3.614281000	1.488683000
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C	-6.010828000	-0.925790000	0.251269000
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H	-5.318113000	-2.366297000	3.262373000
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TSA1

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C	4.326862000	1.038623000	1.446019000
C	4.879626000	-1.220593000	0.819153000
H	-1.205809000	-0.540618000	3.451558000
C	-2.926489000	1.634891000	-2.674413000
C	-4.175537000	-0.418426000	-2.436786000
H	4.638979000	2.060514000	1.681417000
C	5.288137000	0.061555000	1.183236000
H	5.627860000	-1.981509000	0.578495000
H	-2.738465000	2.574589000	-3.201703000
C	-3.970733000	0.807687000	-3.076540000
H	-4.976734000	-1.071175000	-2.785685000
H	6.351963000	0.307560000	1.232630000
H	-4.615508000	1.102329000	-3.908631000
O	0.034821000	-1.499452000	-2.117154000
C	-0.651541000	-2.410304000	-2.946469000
H	-0.643555000	-3.426320000	-2.517411000

H	-1.697260000	-2.092689000	-3.104802000
H	-0.153022000	-2.432455000	-3.930370000
O	-0.312712000	-3.145357000	0.021905000
C	-0.455886000	-3.895773000	1.179346000
H	-0.295172000	-4.972642000	0.972543000
H	0.261452000	-3.613334000	1.978320000
H	-1.470185000	-3.797657000	1.621034000
C	1.337803000	-1.126395000	3.534648000
H	0.692277000	-1.155608000	4.422037000
H	1.850913000	-2.094732000	3.433559000
H	2.124894000	-0.379426000	3.700564000
N	1.942986000	0.020708000	-1.891886000
C	1.501876000	-0.483923000	-2.946474000
O	1.444377000	-0.730714000	-4.100773000
C	3.115513000	0.895738000	-2.024743000
H	3.768143000	0.709287000	-1.161473000
H	3.700758000	0.643405000	-2.929302000
C	1.960684000	1.882980000	1.535851000
H	2.355822000	2.745568000	0.975443000
H	1.013673000	1.612750000	1.050638000
C	1.683984000	2.348282000	2.972630000
H	2.620023000	2.573940000	3.509502000
H	1.134389000	1.597066000	3.556843000
H	1.074808000	3.267060000	2.962943000
C	3.148175000	-2.988055000	0.386422000
H	2.093142000	-3.057875000	0.090412000
H	3.737414000	-3.279266000	-0.499369000
C	3.401986000	-4.002697000	1.510126000
H	2.797044000	-3.772897000	2.401294000
H	4.459799000	-4.006790000	1.820118000
H	3.138776000	-5.021799000	1.183622000
C	-0.920134000	2.169436000	-1.245294000
H	-0.121067000	1.568617000	-0.791177000
H	-0.492707000	2.571527000	-2.177767000
C	-1.283453000	3.335538000	-0.318761000
H	-1.671703000	2.979686000	0.645962000
H	-2.059950000	3.975285000	-0.769065000
H	-0.400775000	3.965568000	-0.119583000
C	-3.527897000	-2.171009000	-0.692369000
H	-2.564273000	-2.705098000	-0.729099000
H	-3.700483000	-2.013873000	0.386855000
C	-4.625308000	-3.076872000	-1.243589000

H	-4.458263000	-3.322382000	-2.304928000
H	-5.625392000	-2.620844000	-1.157544000
H	-4.645885000	-4.026385000	-0.686034000
C	-2.851087000	0.755401000	1.899393000
C	-2.545530000	1.766623000	2.834124000
C	-4.183678000	0.630729000	1.469996000
C	-3.532781000	2.630283000	3.310252000
C	-5.173350000	1.487511000	1.957287000
C	-4.853504000	2.492921000	2.873283000
H	-1.513279000	1.892580000	3.166049000
H	-4.464701000	-0.142504000	0.761561000
H	-3.266698000	3.415969000	4.021770000
H	-6.203257000	1.365704000	1.612825000
H	-5.629801000	3.166696000	3.244946000
C	2.729962000	2.374951000	-2.067153000
H	2.131102000	2.566995000	-2.975819000
H	2.067144000	2.590811000	-1.214452000
C	3.937940000	3.312593000	-2.029967000
H	4.602413000	3.092598000	-2.885382000
H	4.532860000	3.097298000	-1.123608000
C	3.547078000	4.790011000	-2.049135000
H	2.908545000	5.044889000	-1.185654000
H	4.431204000	5.447574000	-2.015001000
H	2.979329000	5.041806000	-2.961045000

ICA1

Al	0.469745000	0.906624000	-0.899145000
N	1.579448000	-0.661149000	-0.971410000
N	-1.217859000	-0.013616000	-0.572565000
C	2.928606000	-0.760696000	-0.484823000
C	1.049943000	-1.740149000	-1.586466000
C	-2.270802000	0.681478000	0.129239000
C	-1.356612000	-1.288089000	-0.952725000
C	3.148920000	-1.511631000	0.699185000
C	3.995348000	-0.084116000	-1.118627000
C	-0.326908000	-1.986683000	-1.641591000
C	-2.465936000	0.484782000	1.511974000
C	-3.066246000	1.599327000	-0.602511000
C	4.453758000	-1.615609000	1.198074000
C	5.284424000	-0.215615000	-0.576978000
H	-0.626947000	-2.912932000	-2.127064000
C	-3.484601000	1.210891000	2.151442000
C	-4.083801000	2.279135000	0.077145000

H	4.626330000	-2.186366000	2.115254000
C	5.521748000	-0.980633000	0.562960000
H	6.113328000	0.308312000	-1.061844000
H	-3.636406000	1.076712000	3.225585000
C	-4.296183000	2.092508000	1.444759000
H	-4.708677000	2.984716000	-0.477544000
H	6.532591000	-1.062934000	0.970481000
H	-5.086147000	2.646075000	1.958914000
O	-0.648664000	3.346918000	-0.306736000
C	-1.446818000	4.520278000	-0.243387000
H	-2.101724000	4.498827000	-1.122781000
H	-2.055048000	4.539021000	0.674252000
H	-0.819158000	5.424786000	-0.269003000
O	0.486601000	1.572660000	-2.504091000
C	0.400392000	0.979155000	-3.758769000
H	1.079797000	0.108198000	-3.878112000
H	-0.621451000	0.613260000	-3.987621000
H	0.669514000	1.704688000	-4.551105000
C	1.969972000	-2.757198000	-2.221512000
H	1.409507000	-3.609102000	-2.627053000
H	2.527117000	-2.278591000	-3.041505000
H	2.722787000	-3.132917000	-1.516248000
N	1.002298000	2.056983000	0.467172000
C	0.316402000	3.219409000	0.652081000
O	0.491183000	4.063490000	1.511558000
C	2.104231000	1.859398000	1.416818000
H	2.872934000	1.232056000	0.950317000
H	2.570406000	2.836470000	1.621318000
C	2.017426000	-2.165955000	1.471548000
H	2.186464000	-1.969134000	2.542884000
H	1.066731000	-1.680382000	1.215786000
C	1.876895000	-3.681844000	1.275221000
H	2.822529000	-4.204130000	1.494385000
H	1.584122000	-3.939416000	0.247067000
H	1.105692000	-4.086539000	1.951194000
C	3.812402000	0.785498000	-2.346079000
H	2.768101000	1.106478000	-2.442140000
H	4.400025000	1.707361000	-2.199245000
C	4.263983000	0.121351000	-3.653738000
H	3.671627000	-0.779508000	-3.876703000
H	5.322589000	-0.183243000	-3.607777000
H	4.146504000	0.813992000	-4.502779000

C	-1.635948000	-0.482481000	2.330606000
H	-0.861632000	-0.938104000	1.701175000
H	-1.095773000	0.090820000	3.102101000
C	-2.457021000	-1.586876000	3.008963000
H	-3.043647000	-2.158680000	2.275538000
H	-3.159965000	-1.174555000	3.750143000
H	-1.794765000	-2.291211000	3.538845000
C	-2.846045000	1.885262000	-2.077328000
H	-3.334220000	2.846553000	-2.304608000
H	-1.773619000	2.036820000	-2.262681000
C	-3.383770000	0.839514000	-3.063654000
H	-4.465390000	0.670204000	-2.931853000
H	-2.873554000	-0.129311000	-2.964155000
H	-3.227635000	1.184418000	-4.098611000
C	-2.552544000	-2.123227000	-0.589852000
C	-2.304800000	-3.412867000	-0.075110000
C	-3.889473000	-1.700341000	-0.696202000
C	-3.352121000	-4.247032000	0.319153000
C	-4.936806000	-2.539270000	-0.310876000
C	-4.675277000	-3.813490000	0.200559000
H	-1.274557000	-3.751400000	0.047426000
H	-4.124904000	-0.715274000	-1.084433000
H	-3.130462000	-5.235596000	0.728889000
H	-5.966703000	-2.187592000	-0.409378000
H	-5.498426000	-4.463076000	0.508996000
C	1.663258000	1.230590000	2.738442000
H	0.909199000	1.887292000	3.205382000
H	1.159427000	0.275340000	2.524988000
C	2.820772000	0.988443000	3.707433000
H	3.316575000	1.949674000	3.934027000
H	3.584107000	0.363789000	3.208814000
C	2.378889000	0.318909000	5.008351000
H	1.909977000	-0.661437000	4.813508000
H	3.226661000	0.151570000	5.693135000
H	1.635372000	0.935080000	5.542143000

ICA1+methanol

Al	0.496752000	0.771659000	-0.525570000
N	1.162947000	-0.938458000	-1.052773000
N	-1.381038000	0.282371000	-0.467750000
C	2.377820000	-1.562725000	-0.605515000
C	0.441634000	-1.557728000	-2.013191000
C	-2.248468000	0.984769000	0.446299000

C	-1.814185000	-0.714943000	-1.245557000
C	2.266340000	-2.711752000	0.220150000
C	3.643168000	-1.016248000	-0.916654000
C	-0.941733000	-1.392703000	-2.145029000
C	-2.581418000	0.425909000	1.697638000
C	-2.699742000	2.276061000	0.071559000
C	3.438807000	-3.323278000	0.683136000
C	4.787941000	-1.659516000	-0.419381000
H	-1.423708000	-1.980571000	-2.923652000
C	-3.384434000	1.179117000	2.570075000
C	-3.512654000	2.976931000	0.970646000
H	3.357951000	-4.204217000	1.326795000
C	4.695773000	-2.808219000	0.363568000
H	5.769274000	-1.233059000	-0.644970000
H	-3.639502000	0.761712000	3.547781000
C	-3.853458000	2.439696000	2.213891000
H	-3.873844000	3.970771000	0.691049000
H	5.600452000	-3.288707000	0.744927000
H	-4.476990000	3.010780000	2.906645000
O	0.138968000	3.170270000	0.625450000
C	0.031796000	4.578934000	0.466339000
H	0.277841000	4.845474000	-0.573599000
H	-1.006108000	4.867741000	0.685326000
H	0.711277000	5.097394000	1.156572000
O	0.777564000	1.855528000	-1.859761000
C	0.683506000	1.706949000	-3.239690000
H	1.150952000	0.770494000	-3.610666000
H	-0.368088000	1.698186000	-3.593236000
H	1.194533000	2.544119000	-3.753513000
C	1.147761000	-2.479760000	-2.978301000
H	0.441826000	-2.992740000	-3.643928000
H	1.844280000	-1.884300000	-3.591338000
H	1.758654000	-3.228474000	-2.458426000
N	1.292053000	1.332147000	1.070452000
C	1.186858000	2.656042000	1.328874000
O	1.898939000	3.347558000	2.048387000
C	2.198035000	0.570301000	1.938521000
H	2.917143000	0.006102000	1.330866000
H	2.786251000	1.279387000	2.537908000
O	4.124068000	3.003445000	0.294174000
H	3.541209000	3.128168000	1.064854000
C	3.551698000	3.713478000	-0.781461000

H	2.570003000	3.311065000	-1.097860000
H	3.431058000	4.795416000	-0.564858000
H	4.230825000	3.629777000	-1.647147000
C	0.927476000	-3.278997000	0.655715000
H	0.994036000	-3.510290000	1.731493000
H	0.147597000	-2.513217000	0.554028000
C	0.487482000	-4.547847000	-0.085737000
H	1.257853000	-5.333927000	-0.026502000
H	0.289543000	-4.355933000	-1.150320000
H	-0.438102000	-4.952108000	0.356418000
C	3.817321000	0.247155000	-1.732663000
H	2.850923000	0.739445000	-1.886949000
H	4.412116000	0.957624000	-1.135804000
C	4.482167000	0.016564000	-3.095428000
H	3.883175000	-0.660826000	-3.726672000
H	5.484460000	-0.430551000	-2.992992000
H	4.595133000	0.969215000	-3.638153000
C	-2.129083000	-0.954092000	2.129481000
H	-1.455902000	-1.382042000	1.376549000
H	-1.526110000	-0.853213000	3.047110000
C	-3.284131000	-1.929119000	2.393986000
H	-3.929656000	-2.036372000	1.510491000
H	-3.916842000	-1.591295000	3.230152000
H	-2.895857000	-2.927269000	2.655236000
C	-2.338578000	2.921354000	-1.254868000
H	-2.488943000	4.007101000	-1.147880000
H	-1.268077000	2.780567000	-1.453402000
C	-3.133607000	2.447121000	-2.479259000
H	-4.220154000	2.570585000	-2.337795000
H	-2.939564000	1.391350000	-2.717787000
H	-2.846196000	3.037429000	-3.364550000
C	-3.204920000	-1.274233000	-1.157663000
C	-3.335445000	-2.678895000	-1.139875000
C	-4.374911000	-0.501128000	-1.047784000
C	-4.585634000	-3.286892000	-1.017214000
C	-5.625932000	-1.110598000	-0.936152000
C	-5.738615000	-2.503631000	-0.917188000
H	-2.440152000	-3.300857000	-1.188967000
H	-4.320872000	0.582132000	-1.053327000
H	-4.655710000	-4.377116000	-0.990814000
H	-6.519377000	-0.486252000	-0.858973000
H	-6.719528000	-2.975767000	-0.819703000

C	1.440941000	-0.379075000	2.864814000
H	0.749962000	0.213052000	3.491564000
H	0.807361000	-1.043286000	2.256510000
C	2.359005000	-1.223841000	3.748137000
H	3.000511000	-0.557869000	4.353199000
H	3.043621000	-1.802420000	3.103054000
C	1.591790000	-2.173706000	4.667317000
H	0.961706000	-2.869121000	4.086251000
H	2.270769000	-2.780639000	5.288559000
H	0.922949000	-1.619782000	5.348118000

TSA2

Al	-0.597634000	0.448326000	1.015882000
N	-1.554505000	-1.125695000	0.402509000
N	1.242097000	-0.283013000	0.555641000
C	-2.888665000	-1.098141000	-0.133709000
C	-0.982869000	-2.333662000	0.593956000
C	2.292959000	0.645780000	0.221581000
C	1.438778000	-1.597095000	0.474807000
C	-3.028625000	-1.114909000	-1.545414000
C	-4.028044000	-1.037648000	0.703007000
C	0.394099000	-2.535226000	0.712690000
C	2.647505000	0.880098000	-1.126765000
C	2.937577000	1.354088000	1.269348000
C	-4.313409000	-1.046155000	-2.100958000
C	-5.293946000	-0.960069000	0.098996000
H	0.709191000	-3.566027000	0.857168000
C	3.630286000	1.842698000	-1.408323000
C	3.929316000	2.285931000	0.935127000
H	-4.422271000	-1.047782000	-3.189502000
C	-5.443333000	-0.961014000	-1.286868000
H	-6.180735000	-0.898513000	0.736036000
H	3.890680000	2.042564000	-2.451027000
C	4.272557000	2.542745000	-0.392478000
H	4.432873000	2.828407000	1.740635000
H	-6.439371000	-0.894505000	-1.732491000
H	5.034452000	3.289171000	-0.631699000
O	0.337010000	2.796574000	1.491288000
C	0.874228000	3.889884000	2.218119000
H	0.933420000	3.571767000	3.266677000
H	1.879429000	4.149678000	1.848613000
H	0.226573000	4.774859000	2.127578000
O	-0.529147000	0.273543000	2.769688000

C	-0.228334000	-0.815665000	3.574159000
H	-0.997939000	-1.616787000	3.521657000
H	0.734666000	-1.301140000	3.320926000
H	-0.165515000	-0.508682000	4.638189000
C	-1.861579000	-3.563163000	0.656063000
H	-1.262512000	-4.480638000	0.715260000
H	-2.508665000	-3.511877000	1.544123000
H	-2.529539000	-3.634913000	-0.213571000
N	-0.660991000	1.888196000	-0.256192000
C	-0.186844000	3.050545000	0.241260000
O	-0.236674000	4.174090000	-0.226781000
C	-1.590439000	2.070058000	-1.373449000
H	-2.268142000	1.207437000	-1.414876000
H	-2.220704000	2.958767000	-1.174588000
O	-2.579202000	1.424256000	1.560323000
H	-3.060376000	1.786123000	0.802815000
C	-2.687278000	2.316461000	2.668209000
H	-2.293391000	3.317455000	2.421686000
H	-3.737442000	2.408635000	2.996256000
H	-2.080741000	1.880444000	3.470037000
C	-1.825948000	-1.206352000	-2.465291000
H	-2.037237000	-0.617341000	-3.372421000
H	-0.957911000	-0.737271000	-1.983984000
C	-1.447246000	-2.633600000	-2.883775000
H	-2.296515000	-3.153493000	-3.356545000
H	-1.119117000	-3.236680000	-2.024719000
H	-0.616420000	-2.613313000	-3.608373000
C	-3.938351000	-1.073487000	2.217123000
H	-2.885495000	-1.072039000	2.522824000
H	-4.354517000	-0.131555000	2.609638000
C	-4.685502000	-2.246189000	2.865606000
H	-4.317328000	-3.219885000	2.505407000
H	-5.766919000	-2.212109000	2.657311000
H	-4.559303000	-2.225190000	3.960497000
C	2.037639000	0.124532000	-2.289882000
H	1.261159000	-0.563672000	-1.933508000
H	1.523088000	0.850304000	-2.938355000
C	3.062755000	-0.644249000	-3.135267000
H	3.662623000	-1.329557000	-2.520666000
H	3.758996000	0.038595000	-3.647599000
H	2.555281000	-1.240167000	-3.911844000
C	2.620834000	1.138969000	2.737929000

H	2.910574000	2.055370000	3.276121000
H	1.538153000	1.030462000	2.870823000
C	3.330695000	-0.045242000	3.408218000
H	4.427327000	0.025228000	3.311942000
H	3.014722000	-1.009736000	2.985820000
H	3.090820000	-0.069588000	4.483876000
C	2.735835000	-2.219774000	0.023363000
C	2.666970000	-3.293405000	-0.889028000
C	4.011016000	-1.790760000	0.432414000
C	3.821343000	-3.916587000	-1.365824000
C	5.166179000	-2.418480000	-0.038210000
C	5.079394000	-3.483068000	-0.939322000
H	1.693513000	-3.623153000	-1.254872000
H	4.114304000	-0.963440000	1.125254000
H	3.735095000	-4.737171000	-2.082595000
H	6.142423000	-2.065462000	0.303255000
H	5.986136000	-3.967004000	-1.311385000
C	-0.941142000	2.260221000	-2.743904000
H	-0.205344000	3.077605000	-2.672663000
H	-0.385477000	1.347373000	-3.004438000
C	-1.959989000	2.565380000	-3.843210000
H	-2.490532000	3.503858000	-3.599804000
H	-2.735338000	1.776377000	-3.854716000
C	-1.326484000	2.678722000	-5.229342000
H	-0.826919000	1.737731000	-5.517805000
H	-2.074924000	2.910022000	-6.005163000
H	-0.563335000	3.475054000	-5.253278000

ICA2

Al	-0.587898000	-0.885081000	0.776205000
N	-1.541159000	-0.720471000	-0.931706000
N	1.256356000	-0.617950000	-0.068279000
C	-2.864245000	-0.174943000	-1.051426000
C	-0.963473000	-1.192358000	-2.053727000
C	2.332976000	-0.133163000	0.757354000
C	1.448438000	-0.834636000	-1.367262000
C	-2.981746000	1.174659000	-1.475211000
C	-4.019137000	-0.932368000	-0.746207000
C	0.417615000	-1.312993000	-2.224077000
C	2.705585000	1.229155000	0.746813000
C	2.991206000	-1.051751000	1.617237000
C	-4.255633000	1.751983000	-1.563569000
C	-5.273713000	-0.306867000	-0.836498000

H	0.745443000	-1.683748000	-3.192760000
C	3.719618000	1.658268000	1.619288000
C	4.011998000	-0.578036000	2.451251000
H	-4.344817000	2.795662000	-1.879598000
C	-5.399410000	1.021874000	-1.238168000
H	-6.170092000	-0.882809000	-0.588635000
H	3.995224000	2.716173000	1.628021000
C	4.374095000	0.769772000	2.465707000
H	4.523008000	-1.285400000	3.111210000
H	-6.386393000	1.488195000	-1.297658000
H	5.159833000	1.123760000	3.138185000
O	0.210823000	-0.701345000	2.748711000
C	0.635443000	-1.389762000	3.918612000
H	0.519480000	-2.460385000	3.715043000
H	1.687549000	-1.154649000	4.137834000
H	0.015909000	-1.087355000	4.775085000
O	-0.529355000	-2.659056000	0.958079000
C	-0.320634000	-3.686084000	0.052514000
H	-1.078132000	-3.714964000	-0.761187000
H	0.664400000	-3.633923000	-0.454174000
H	-0.369449000	-4.671922000	0.560300000
C	-1.835479000	-1.593515000	-3.223838000
H	-1.232962000	-1.856887000	-4.102567000
H	-2.441607000	-2.468202000	-2.943382000
H	-2.541539000	-0.800768000	-3.506815000
N	-0.753852000	0.891706000	1.640042000
C	-0.270627000	0.624347000	2.857577000
O	-0.262707000	1.226036000	3.909982000
C	-1.649554000	2.043840000	1.572313000
H	-2.373078000	1.874907000	0.764589000
H	-2.233276000	2.100266000	2.512688000
O	-2.480889000	-1.131375000	1.851059000
H	-2.920461000	-0.296135000	2.063649000
C	-2.725610000	-2.096706000	2.872440000
H	-2.338841000	-1.755018000	3.847704000
H	-3.804721000	-2.305604000	2.964251000
H	-2.190607000	-3.002797000	2.567239000
C	-1.764364000	2.008291000	-1.828891000
H	-1.949710000	3.044829000	-1.503694000
H	-0.897832000	1.650280000	-1.257197000
C	-1.407149000	2.024538000	-3.321532000
H	-2.259571000	2.358896000	-3.935376000

H	-1.103773000	1.030748000	-3.680482000
H	-0.566273000	2.713303000	-3.506804000
C	-3.958575000	-2.397923000	-0.362348000
H	-2.912768000	-2.702551000	-0.241130000
H	-4.421301000	-2.517427000	0.630968000
C	-4.678609000	-3.331417000	-1.344776000
H	-4.265083000	-3.254260000	-2.362501000
H	-5.754499000	-3.103589000	-1.414306000
H	-4.581839000	-4.381305000	-1.022644000
C	2.084918000	2.250099000	-0.182954000
H	1.277242000	1.789906000	-0.765612000
H	1.608019000	3.027079000	0.432774000
C	3.091689000	2.921090000	-1.127473000
H	3.646684000	2.181214000	-1.720471000
H	3.829103000	3.523161000	-0.572905000
H	2.573975000	3.597774000	-1.827373000
C	2.648987000	-2.529410000	1.661101000
H	2.920554000	-2.906791000	2.660238000
H	1.565398000	-2.660114000	1.559726000
C	3.349508000	-3.407707000	0.614846000
H	4.447206000	-3.311776000	0.665831000
H	3.034165000	-3.159941000	-0.408866000
H	3.098552000	-4.467807000	0.783217000
C	2.730635000	-0.492618000	-2.086813000
C	2.619363000	0.194910000	-3.313624000
C	4.023164000	-0.784413000	-1.616254000
C	3.749780000	0.568461000	-4.042461000
C	5.154462000	-0.418072000	-2.348863000
C	5.025867000	0.259973000	-3.563907000
H	1.630041000	0.467099000	-3.684697000
H	4.160076000	-1.302143000	-0.673541000
H	3.630361000	1.111932000	-4.983197000
H	6.145363000	-0.664043000	-1.959023000
H	5.914162000	0.551393000	-4.130353000
C	-0.972628000	3.399159000	1.367318000
H	-0.217928000	3.541991000	2.159340000
H	-0.431612000	3.388017000	0.409585000
C	-1.966083000	4.562308000	1.375255000
H	-2.494702000	4.587332000	2.345605000
H	-2.746659000	4.380193000	0.612832000
C	-1.304418000	5.915300000	1.116064000
H	-0.803026000	5.932321000	0.133036000

H	-2.036605000	6.739373000	1.131116000
H	-0.537872000	6.135778000	1.878304000

TSA3

Al	-0.459575000	0.307317000	1.080199000
N	-1.385583000	-1.334923000	0.595313000
N	1.297383000	-0.329115000	0.369851000
C	-2.784014000	-1.323742000	0.259742000
C	-0.750736000	-2.496021000	0.804666000
C	2.202402000	0.580196000	-0.283780000
C	1.599992000	-1.628224000	0.486827000
C	-3.162373000	-1.438192000	-1.094313000
C	-3.752489000	-1.150228000	1.279338000
C	0.649351000	-2.607385000	0.855322000
C	2.327740000	0.562990000	-1.692199000
C	2.903399000	1.539427000	0.495764000
C	-4.518266000	-1.279557000	-1.427986000
C	-5.091333000	-0.998153000	0.900576000
H	1.040616000	-3.600555000	1.069490000
C	3.122833000	1.544016000	-2.306064000
C	3.703399000	2.478938000	-0.165082000
H	-4.817580000	-1.347345000	-2.478143000
C	-5.473347000	-1.041028000	-0.444148000
H	-5.855674000	-0.844450000	1.663979000
H	3.201076000	1.557234000	-3.396165000
C	3.801216000	2.497365000	-1.557108000
H	4.259991000	3.217516000	0.412940000
H	-6.522896000	-0.904752000	-0.718152000
H	4.409931000	3.257188000	-2.053608000
O	0.317095000	3.259945000	1.008296000
C	1.010035000	4.458932000	1.338167000
H	1.116372000	4.460839000	2.430458000
H	1.998440000	4.485895000	0.857153000
H	0.438011000	5.343748000	1.016116000
O	-0.090509000	0.272062000	2.793254000
C	0.651113000	-0.520572000	3.650900000
H	0.033493000	-1.327613000	4.101513000
H	1.510802000	-1.028239000	3.168407000
H	1.060669000	0.075097000	4.493046000
C	-1.529596000	-3.776631000	1.015983000
H	-2.574646000	-3.696736000	0.696015000
H	-1.057529000	-4.620727000	0.493652000
H	-1.520526000	-4.015045000	2.092875000

N	-0.597917000	1.843578000	-0.460165000
C	0.120214000	3.019440000	-0.315311000
O	0.501425000	3.766951000	-1.187137000
C	-1.022196000	1.554764000	-1.838465000
H	-1.053467000	0.468329000	-1.966414000
H	-0.266406000	1.946513000	-2.534284000
O	-2.022761000	1.357628000	1.350281000
H	-1.545762000	1.886382000	0.361903000
C	-2.428534000	2.108667000	2.470710000
H	-1.875788000	3.063636000	2.530989000
H	-3.508483000	2.331167000	2.406491000
H	-2.228006000	1.551599000	3.398454000
C	-2.175572000	-1.807930000	-2.183591000
H	-2.376188000	-1.193116000	-3.075450000
H	-1.152448000	-1.573891000	-1.862788000
C	-2.247585000	-3.289162000	-2.581821000
H	-3.256267000	-3.559403000	-2.934029000
H	-2.007773000	-3.947024000	-1.733111000
H	-1.534574000	-3.511341000	-3.392982000
C	-3.330503000	-1.206443000	2.734875000
H	-3.086589000	-2.259480000	2.969976000
H	-2.381580000	-0.666683000	2.858529000
C	-4.344478000	-0.698152000	3.757286000
H	-5.259275000	-1.312293000	3.784882000
H	-4.643766000	0.340627000	3.546493000
H	-3.906950000	-0.720223000	4.768056000
C	2.799946000	1.525632000	2.009729000
H	1.772566000	1.788156000	2.301623000
H	2.912984000	0.489092000	2.361363000
C	3.784635000	2.411499000	2.769541000
H	3.640485000	3.481255000	2.550579000
H	4.832701000	2.161832000	2.534472000
H	3.645633000	2.281340000	3.854551000
C	1.649415000	-0.467550000	-2.576746000
H	1.049517000	-1.156056000	-1.968640000
H	0.934033000	0.049881000	-3.236682000
C	2.623153000	-1.270170000	-3.450691000
H	3.396823000	-1.761673000	-2.843701000
H	3.134419000	-0.628178000	-4.185317000
H	2.084847000	-2.050220000	-4.014370000
C	2.970081000	-2.157738000	0.171832000
C	3.094239000	-3.284080000	-0.661959000

C	4.140091000	-1.590412000	0.704187000
C	4.348492000	-3.817739000	-0.966910000
C	5.393454000	-2.127959000	0.406864000
C	5.504060000	-3.240155000	-0.433641000
H	2.196598000	-3.728534000	-1.096347000
H	4.073123000	-0.732495000	1.369201000
H	4.421721000	-4.684105000	-1.629253000
H	6.289466000	-1.673367000	0.836878000
H	6.487097000	-3.655232000	-0.670609000
C	-2.393886000	2.154227000	-2.155167000
H	-3.139060000	1.721071000	-1.464624000
H	-2.361567000	3.239110000	-1.949916000
C	-2.837259000	1.920738000	-3.600191000
H	-2.798244000	0.839597000	-3.823893000
H	-2.112875000	2.397395000	-4.285239000
C	-4.243972000	2.445156000	-3.884830000
H	-4.312714000	3.529268000	-3.691701000
H	-4.988851000	1.947808000	-3.240554000
H	-4.539356000	2.274013000	-4.933082000

ICA3

Al	0.932561000	-0.110106000	-1.293177000
N	2.327346000	-0.622519000	-0.103613000
N	-0.435657000	-1.170749000	-0.492060000
C	3.309249000	0.341791000	0.302773000
C	2.401069000	-1.915903000	0.209404000
C	-1.747539000	-0.648653000	-0.220459000
C	-0.060133000	-2.415927000	-0.124235000
C	3.049448000	1.092063000	1.474888000
C	4.431466000	0.618042000	-0.508653000
C	1.296881000	-2.784188000	0.034217000
C	-2.234164000	-0.587395000	1.110820000
C	-2.509562000	-0.111338000	-1.290632000
C	3.956089000	2.094629000	1.841571000
C	5.309034000	1.636584000	-0.102460000
H	1.492887000	-3.841522000	0.198372000
C	-3.509941000	-0.046379000	1.330898000
C	-3.782433000	0.402222000	-1.014161000
H	3.762999000	2.679326000	2.745534000
C	5.082115000	2.366943000	1.062139000
H	6.177988000	1.867696000	-0.724289000
H	-3.887082000	0.021145000	2.353862000
C	-4.290564000	0.431704000	0.282725000

H	-4.374209000	0.806140000	-1.837958000
H	5.774033000	3.160509000	1.355912000
H	-5.279504000	0.853444000	0.478094000
O	-2.755976000	3.111542000	-2.240693000
C	-3.923379000	3.461754000	-2.966868000
H	-3.905924000	2.865394000	-3.889863000
H	-4.839558000	3.239296000	-2.395958000
H	-3.933924000	4.534255000	-3.221792000
O	1.342056000	-0.626488000	-2.888425000
C	1.682965000	-1.822639000	-3.504251000
H	2.709790000	-2.159508000	-3.245030000
H	1.005900000	-2.660238000	-3.238575000
H	1.650896000	-1.718798000	-4.606580000
C	3.681367000	-2.480478000	0.769430000
H	3.540560000	-3.492724000	1.169395000
H	4.444877000	-2.519769000	-0.024041000
H	4.083504000	-1.833317000	1.562297000
N	-1.488108000	3.298397000	-0.414056000
C	-2.619552000	3.712387000	-1.022804000
O	-3.422435000	4.521378000	-0.592629000
C	-1.072022000	3.815649000	0.871973000
H	0.016877000	3.999085000	0.837154000
H	-1.566140000	4.787451000	1.024006000
O	0.629349000	1.597028000	-1.179762000
H	-0.927579000	2.541831000	-0.822739000
C	1.440586000	2.614112000	-1.721408000
H	0.843916000	3.534352000	-1.859048000
H	2.287041000	2.859863000	-1.051968000
H	1.857714000	2.341653000	-2.709962000
C	1.824623000	0.834845000	2.326316000
H	1.566695000	1.765526000	2.854790000
H	0.968501000	0.601026000	1.678503000
C	1.997579000	-0.288887000	3.356609000
H	2.869910000	-0.104115000	4.004492000
H	2.138482000	-1.267663000	2.874370000
H	1.108513000	-0.365875000	4.002326000
C	4.695282000	-0.121677000	-1.805868000
H	3.898841000	-0.853903000	-1.984558000
H	4.618036000	0.599917000	-2.638246000
C	6.061860000	-0.814914000	-1.871682000
H	6.186202000	-1.543588000	-1.054105000
H	6.893002000	-0.095973000	-1.796078000

H	6.177699000	-1.354220000	-2.825804000
C	-1.419095000	-1.001749000	2.323799000
H	-0.462227000	-1.443035000	2.023740000
H	-1.153357000	-0.082778000	2.872375000
C	-2.137646000	-1.952394000	3.289124000
H	-2.495240000	-2.855439000	2.773679000
H	-3.006468000	-1.473425000	3.767054000
H	-1.456405000	-2.268622000	4.096062000
C	-1.999513000	-0.038845000	-2.717788000
H	-2.670090000	0.632463000	-3.272680000
H	-1.026893000	0.477353000	-2.737927000
C	-1.884875000	-1.367400000	-3.470103000
H	-2.864075000	-1.868364000	-3.547956000
H	-1.183208000	-2.055987000	-2.981424000
H	-1.510489000	-1.195628000	-4.491640000
C	-1.072244000	-3.480553000	0.171268000
C	-0.860601000	-4.386411000	1.227667000
C	-2.236886000	-3.622240000	-0.604483000
C	-1.779851000	-5.401921000	1.497741000
C	-3.153007000	-4.640019000	-0.338125000
C	-2.930091000	-5.533482000	0.714576000
H	0.016750000	-4.273426000	1.866880000
H	-2.423430000	-2.938675000	-1.428190000
H	-1.600865000	-6.086016000	2.331054000
H	-4.047711000	-4.733792000	-0.958493000
H	-3.652178000	-6.326388000	0.925777000
C	-1.389799000	2.876999000	2.037109000
H	-2.476197000	2.686581000	2.055499000
H	-0.913037000	1.904437000	1.837602000
C	-0.925863000	3.418275000	3.389826000
H	-1.452389000	4.366297000	3.602693000
H	0.147507000	3.679066000	3.332074000
C	-1.147936000	2.437105000	4.540666000
H	-0.557913000	1.516176000	4.398940000
H	-0.855074000	2.870492000	5.511044000
H	-2.207783000	2.139529000	4.613450000

CatB+methyl isocyanate

Zn	3.368790000	3.235360000	6.061102000
O	2.659447000	4.582863000	4.800006000
N	3.018883000	4.405442000	7.670837000
C	2.156033000	5.721204000	5.103536000
C	3.431125000	3.841137000	8.914982000

C	2.511346000	5.627157000	7.608512000
C	2.080909000	6.247559000	6.402498000
C	1.634593000	6.517769000	3.942133000
C	2.506789000	3.185906000	9.755782000
C	4.808631000	3.881174000	9.241366000
C	2.363639000	6.428187000	8.884521000
H	1.695406000	7.259032000	6.508531000
C	2.092308000	6.194211000	2.651377000
C	0.689823000	7.551582000	4.079533000
C	2.981862000	2.586007000	10.933302000
C	5.239029000	3.274277000	10.426215000
H	2.037378000	7.456876000	8.684066000
H	1.628462000	5.953772000	9.553342000
H	3.315187000	6.457543000	9.437419000
H	2.813809000	5.382894000	2.544037000
C	1.637062000	6.896377000	1.534727000
C	0.227123000	8.247538000	2.960886000
H	0.290106000	7.802346000	5.063723000
H	2.270802000	2.073732000	11.588294000
C	4.332313000	2.629579000	11.272319000
H	6.301170000	3.304135000	10.684814000
H	2.012140000	6.637830000	0.540920000
C	0.702619000	7.926577000	1.685017000
H	-0.513708000	9.041662000	3.085574000
H	4.683233000	2.155088000	12.192374000
H	0.341689000	8.474350000	0.810507000
H	4.286892000	2.002560000	5.787590000
N	1.023751000	2.218856000	6.024629000
C	1.013018000	1.187201000	6.656568000
O	1.120925000	0.214183000	7.298940000
C	0.079144000	3.008930000	5.261467000
H	-0.854663000	2.456400000	5.078784000
H	-0.147121000	3.937227000	5.807457000
H	0.540595000	3.291053000	4.306937000
C	1.033550000	3.120855000	9.432682000
H	0.817870000	3.475075000	8.417356000
H	0.661993000	2.087376000	9.520252000
H	0.444657000	3.733699000	10.136988000
C	5.778733000	4.562101000	8.311172000
H	6.805751000	4.521772000	8.702273000
H	5.773783000	4.082078000	7.317208000
H	5.514804000	5.619877000	8.146219000

TSB1

Zn	-0.342788000	1.002868000	-0.650573000
O	1.571022000	0.552677000	-0.600388000
N	-0.971906000	-0.762212000	0.026933000
C	2.046051000	-0.510542000	-0.070276000
C	-2.381377000	-0.970366000	0.029901000
C	-0.134043000	-1.704615000	0.442507000
C	1.280425000	-1.582888000	0.424365000
C	3.545327000	-0.580148000	-0.018261000
C	-3.142674000	-0.526191000	1.131394000
C	-2.996923000	-1.532064000	-1.108993000
C	-0.708436000	-3.000716000	0.973131000
H	1.824633000	-2.447214000	0.797377000
C	4.282756000	0.262287000	-0.870645000
C	4.247205000	-1.425555000	0.860662000
C	-4.533484000	-0.696795000	1.095097000
C	-4.390192000	-1.685762000	-1.107159000
H	0.078856000	-3.687223000	1.309651000
H	-1.391443000	-2.804756000	1.814364000
H	-1.307654000	-3.504676000	0.198957000
H	3.738739000	0.929585000	-1.540654000
C	5.677835000	0.245133000	-0.860834000
C	5.643383000	-1.435074000	0.877704000
H	3.703659000	-2.064952000	1.558415000
H	-5.134201000	-0.360642000	1.944953000
C	-5.154902000	-1.279921000	-0.011304000
H	-4.879168000	-2.122596000	-1.982450000
H	6.233537000	0.900241000	-1.537025000
C	6.364230000	-0.604123000	0.013657000
H	6.171541000	-2.091047000	1.574637000
H	-6.240588000	-1.405827000	-0.025539000
H	7.457347000	-0.614363000	0.026405000
H	-1.126634000	2.086368000	-1.622532000
N	-0.477627000	2.779285000	0.538890000
C	-1.036996000	3.412497000	-0.402734000
O	-1.516283000	4.335070000	-0.950926000
C	-0.099582000	3.442036000	1.787936000
H	-0.352610000	4.514270000	1.795416000
H	-0.610316000	2.952840000	2.632524000
H	0.985711000	3.330996000	1.937380000
C	-2.452679000	0.135504000	2.295878000
H	-1.855887000	0.995765000	1.949728000

H	-3.176014000	0.491289000	3.044014000
H	-1.748420000	-0.547698000	2.799597000
C	-2.156911000	-1.926185000	-2.295810000
H	-2.780715000	-2.258378000	-3.138296000
H	-1.538016000	-1.078124000	-2.635460000
H	-1.453986000	-2.740437000	-2.051795000

ICB1

Zn	-0.294780000	1.027948000	0.161370000
O	1.637291000	0.772816000	0.157317000
N	-0.771152000	-0.861273000	-0.068316000
C	2.210950000	-0.359452000	-0.038892000
C	-2.169433000	-1.154717000	-0.057041000
C	0.140222000	-1.801112000	-0.304208000
C	1.539496000	-1.570777000	-0.287067000
C	3.708670000	-0.328230000	-0.020234000
C	-2.774515000	-1.590657000	1.141099000
C	-2.933110000	-0.893205000	-1.214858000
C	-0.332658000	-3.201128000	-0.623270000
H	2.155042000	-2.438111000	-0.512400000
C	4.355968000	0.908052000	-0.201956000
C	4.496797000	-1.475669000	0.188292000
C	-4.159394000	-1.808259000	1.145987000
C	-4.314984000	-1.123139000	-1.167840000
H	0.507085000	-3.876899000	-0.828741000
H	-0.923239000	-3.615321000	0.207933000
H	-0.999511000	-3.187127000	-1.499755000
H	3.746044000	1.800225000	-0.350232000
C	5.748580000	0.991890000	-0.197494000
C	5.889859000	-1.389488000	0.201640000
H	4.023740000	-2.442522000	0.368052000
H	-4.642042000	-2.146467000	2.067043000
C	-4.924971000	-1.585333000	-0.000186000
H	-4.918306000	-0.924885000	-2.057875000
H	6.234764000	1.958993000	-0.349691000
C	6.521063000	-0.156977000	0.003339000
H	6.485880000	-2.289279000	0.374380000
H	-6.004172000	-1.756300000	0.021654000
H	7.612224000	-0.091880000	0.011258000
H	-3.019329000	1.866933000	0.288376000
N	-1.140605000	2.716399000	0.170757000
C	-2.487878000	2.853629000	0.245910000
O	-3.103173000	3.909801000	0.265309000

C	-0.370781000	3.954790000	0.112381000
H	-0.657157000	4.570802000	-0.758506000
H	-0.531463000	4.579755000	1.009057000
H	0.701761000	3.720425000	0.038279000
C	-1.943809000	-1.777944000	2.384510000
H	-1.371643000	-0.864328000	2.620216000
H	-2.572525000	-2.021427000	3.253080000
H	-1.199505000	-2.583581000	2.269972000
C	-2.268767000	-0.330882000	-2.445242000
H	-2.982694000	-0.225249000	-3.274549000
H	-1.849678000	0.670676000	-2.237160000
H	-1.430349000	-0.958071000	-2.788824000

TSB2

Zn	0.492667000	-0.113362000	0.574775000
O	2.288797000	-0.798789000	0.376134000
N	0.839614000	1.695383000	-0.117215000
C	3.268737000	-0.110112000	-0.093953000
C	-0.290845000	2.567479000	-0.172041000
C	2.044697000	2.071777000	-0.528008000
C	3.185807000	1.226011000	-0.521010000
C	4.568620000	-0.848378000	-0.192832000
C	-1.092058000	2.590750000	-1.333235000
C	-0.648557000	3.287251000	0.987126000
C	2.224806000	3.483828000	-1.036245000
H	4.091602000	1.670563000	-0.925135000
C	4.540679000	-2.255401000	-0.169160000
C	5.814967000	-0.202605000	-0.296948000
C	-2.248145000	3.383602000	-1.322372000
C	-1.813947000	4.065308000	0.957216000
H	3.265627000	3.685775000	-1.319245000
H	1.578963000	3.666942000	-1.908824000
H	1.918724000	4.209254000	-0.266358000
H	3.576490000	-2.757098000	-0.076993000
C	5.719854000	-2.994499000	-0.267345000
C	6.994931000	-0.942888000	-0.385777000
H	5.873343000	0.887036000	-0.284529000
H	-2.880769000	3.410919000	-2.213863000
C	-2.606831000	4.119020000	-0.190704000
H	-2.105275000	4.624174000	1.850624000
H	5.677920000	-4.086756000	-0.257090000
C	6.951827000	-2.341114000	-0.376675000
H	7.954540000	-0.424474000	-0.457096000

H	-3.515866000	4.725787000	-0.198757000
H	7.876819000	-2.919117000	-0.449369000
H	-2.101479000	0.826415000	1.319359000
N	-1.001233000	-0.913548000	1.523568000
C	-1.963295000	-0.053873000	1.988104000
O	-2.645055000	-0.211245000	2.989872000
C	-0.706809000	-2.070223000	2.372296000
H	-0.278812000	-1.763875000	3.342545000
H	-1.612707000	-2.658170000	2.576788000
H	0.016025000	-2.718236000	1.855356000
C	-0.729814000	1.743640000	-2.524475000
H	-0.755399000	0.675444000	-2.256982000
H	-1.441697000	1.893941000	-3.349073000
H	0.281798000	1.964749000	-2.901467000
C	0.192443000	3.169934000	2.231247000
H	-0.240687000	3.739236000	3.065885000
H	0.279061000	2.115961000	2.549145000
H	1.222952000	3.527499000	2.069241000
C	-3.681629000	-1.283366000	-1.093408000
C	-3.527951000	-2.701092000	-0.370975000
H	-0.308602000	-1.617474000	-0.802782000
B	-1.491437000	-1.652418000	-0.489829000
O	-2.091341000	-2.870760000	-0.282392000
O	-2.369529000	-0.694052000	-0.959254000
C	-4.085350000	-3.880412000	-1.164713000
H	-3.898496000	-4.812514000	-0.610022000
H	-5.172443000	-3.780827000	-1.308109000
H	-3.606663000	-3.976813000	-2.147916000
C	-4.088650000	-2.728029000	1.053439000
H	-5.181727000	-2.608600000	1.065878000
H	-3.841566000	-3.694966000	1.517183000
H	-3.635803000	-1.938238000	1.660906000
C	-4.698852000	-0.345846000	-0.445440000
H	-4.679238000	0.624512000	-0.964760000
H	-5.717964000	-0.755929000	-0.520737000
H	-4.474869000	-0.161062000	0.612630000
C	-3.953606000	-1.384369000	-2.597107000
H	-4.949798000	-1.799626000	-2.810367000
H	-3.897417000	-0.376451000	-3.035821000
H	-3.197248000	-2.007450000	-3.095706000

ICB2

Zn	0.270965000	0.214545000	-1.133645000

O	2.133582000	-0.299214000	-0.760332000
N	0.340845000	1.845897000	0.022067000
C	2.979475000	0.394218000	-0.093010000
C	-0.876403000	2.584339000	0.108315000
C	1.459389000	2.301818000	0.579896000
C	2.700180000	1.617594000	0.541569000
C	4.356861000	-0.184022000	0.000697000
C	-1.251237000	3.413481000	-0.972096000
C	-1.722112000	2.412949000	1.226250000
C	1.428952000	3.638351000	1.289439000
H	3.516581000	2.084114000	1.089329000
C	4.500617000	-1.582929000	0.035300000
C	5.509187000	0.621468000	0.031504000
C	-2.478230000	4.088140000	-0.907281000
C	-2.938565000	3.110787000	1.254289000
H	2.415578000	3.909513000	1.686147000
H	1.098070000	4.427553000	0.595713000
H	0.705667000	3.632766000	2.118597000
H	3.604648000	-2.204704000	0.040033000
C	5.769740000	-2.158315000	0.114755000
C	6.778230000	0.041397000	0.094506000
H	5.415786000	1.708332000	-0.023731000
H	-2.776115000	4.733050000	-1.738735000
C	-3.316501000	3.944485000	0.199871000
H	-3.600535000	2.988414000	2.116022000
H	5.867773000	-3.246235000	0.160162000
C	6.911957000	-1.350273000	0.140240000
H	7.666581000	0.678592000	0.102394000
H	-4.269490000	4.478494000	0.238243000
H	7.905308000	-1.803891000	0.194857000
H	0.005991000	-1.944533000	2.031195000
N	-0.144325000	-2.640696000	0.076163000
C	0.589101000	-2.442661000	1.225611000
O	1.746256000	-2.780744000	1.367706000
C	0.538131000	-3.277019000	-1.051253000
H	1.404807000	-2.667721000	-1.346752000
H	0.895195000	-4.280873000	-0.773413000
H	-0.158489000	-3.353908000	-1.893834000
C	-0.344963000	3.542555000	-2.168827000
H	-0.188141000	2.561586000	-2.650864000
H	-0.765760000	4.225388000	-2.921079000
H	0.654788000	3.913398000	-1.888818000

C	-1.337607000	1.466845000	2.334015000
H	-2.076203000	1.488408000	3.148707000
H	-1.283110000	0.433712000	1.956216000
H	-0.352473000	1.704862000	2.765355000
C	-3.591588000	-1.682658000	0.786450000
C	-3.676019000	-2.095328000	-0.738009000
H	-0.689605000	-0.397547000	-2.184319000
B	-1.548284000	-2.307535000	0.022645000
O	-2.394842000	-2.755110000	-0.947272000
O	-2.156345000	-1.536400000	0.979820000
C	-3.731994000	-0.891036000	-1.679059000
H	-3.559087000	-1.235191000	-2.709430000
H	-4.712510000	-0.394308000	-1.635532000
H	-2.949616000	-0.158036000	-1.442745000
C	-4.785947000	-3.083806000	-1.070878000
H	-5.771367000	-2.658263000	-0.825476000
H	-4.770142000	-3.308246000	-2.148184000
H	-4.665030000	-4.030992000	-0.529046000
C	-4.051708000	-2.789553000	1.738134000
H	-3.767636000	-2.516724000	2.765549000
H	-5.142538000	-2.926659000	1.704723000
H	-3.571423000	-3.750133000	1.498030000
C	-4.273582000	-0.366094000	1.130065000
H	-5.348574000	-0.418209000	0.897828000
H	-4.168039000	-0.160984000	2.205942000
H	-3.835457000	0.477252000	0.583105000

TSB3

Zn	0.879773000	-0.189901000	-0.224877000
O	2.498499000	-1.280584000	-0.145493000
N	1.743432000	1.552124000	0.136990000
C	3.662981000	-0.798454000	0.082664000
C	0.888789000	2.691830000	0.164192000
C	3.057292000	1.660880000	0.291087000
C	3.958869000	0.564006000	0.275869000
C	4.773198000	-1.808025000	0.108736000
C	0.542827000	3.319875000	-1.051015000
C	0.313609000	3.090641000	1.389188000
C	3.646988000	3.040178000	0.489359000
H	5.007277000	0.825785000	0.397375000
C	4.564019000	-3.047047000	-0.524455000
C	6.002939000	-1.582239000	0.754103000
C	-0.359336000	4.391760000	-1.012154000

C	-0.589306000	4.163338000	1.384761000
H	4.736739000	3.003780000	0.613242000
H	3.410503000	3.684841000	-0.371711000
H	3.206293000	3.528143000	1.372461000
H	3.604836000	-3.227341000	-1.012056000
C	5.561816000	-4.022284000	-0.532053000
C	6.997302000	-2.562448000	0.755045000
H	6.180020000	-0.644894000	1.284454000
H	-0.637027000	4.887229000	-1.946668000
C	-0.918478000	4.816626000	0.195141000
H	-1.043685000	4.481988000	2.327050000
H	5.385383000	-4.975317000	-1.037774000
C	6.783028000	-3.783651000	0.107407000
H	7.942864000	-2.373673000	1.270112000
H	-1.625087000	5.650520000	0.206912000
H	7.563671000	-4.549024000	0.106436000
H	-0.654781000	-0.774147000	0.383134000
C	1.083010000	2.782877000	-2.350080000
H	0.749859000	1.740171000	-2.491498000
H	0.733441000	3.377729000	-3.206545000
H	2.185060000	2.770588000	-2.368041000
C	0.649752000	2.341508000	2.652079000
H	0.068548000	2.713712000	3.508278000
H	0.442491000	1.263963000	2.533689000
H	1.719949000	2.421840000	2.906129000
O	-0.304150000	-0.416521000	-1.832204000
N	-2.429055000	-0.136783000	-0.921128000
C	-1.240829000	-0.857489000	-1.037628000
H	-1.418476000	-1.944504000	-0.961224000
B	-3.613819000	-0.761574000	-0.418120000
O	-4.753326000	-0.064839000	-0.105026000
O	-3.717320000	-2.111652000	-0.191138000
C	-5.789276000	-1.045054000	0.162479000
C	-4.941906000	-2.319687000	0.557952000
C	-6.577052000	-1.230824000	-1.137226000
C	-6.696859000	-0.510915000	1.262946000
C	-4.558605000	-2.346015000	2.040527000
C	-5.552546000	-3.651885000	0.143443000
H	-7.432061000	-1.909906000	-1.002519000
H	-6.958820000	-0.252327000	-1.465106000
H	-5.935945000	-1.628998000	-1.937979000
H	-7.433961000	-1.271760000	1.563513000

H	-6.124023000	-0.205103000	2.148165000
H	-7.245581000	0.370469000	0.897299000
H	-5.422902000	-2.573386000	2.682132000
H	-3.795418000	-3.123000000	2.196251000
H	-4.129385000	-1.383889000	2.358314000
H	-4.895510000	-4.476147000	0.460384000
H	-6.534653000	-3.795144000	0.620502000
H	-5.674989000	-3.721227000	-0.945315000
C	-2.328509000	1.308158000	-1.057995000
H	-1.692025000	1.726126000	-0.256136000
H	-1.873056000	1.578350000	-2.020098000
H	-3.326219000	1.756863000	-0.982632000

ICB3

Zn	1.172943000	-0.681361000	0.043922000
O	3.081405000	-1.066848000	0.130942000
N	1.351946000	1.267940000	-0.156510000
C	3.996103000	-0.207252000	-0.136567000
C	0.149513000	2.034083000	-0.078796000
C	2.522649000	1.837294000	-0.433310000
C	3.763343000	1.149806000	-0.425561000
C	5.398164000	-0.740300000	-0.110829000
C	-0.775489000	1.973481000	-1.143686000
C	-0.143980000	2.739488000	1.109329000
C	2.548513000	3.305005000	-0.799822000
H	4.631813000	1.767284000	-0.639221000
C	5.623974000	-1.990411000	0.495333000
C	6.495410000	-0.061375000	-0.673802000
C	-1.966305000	2.703500000	-1.030976000
C	-1.352094000	3.446510000	1.184752000
H	3.559328000	3.636941000	-1.068650000
H	1.874882000	3.491372000	-1.651161000
H	2.182892000	3.931957000	0.026733000
H	4.772648000	-2.524908000	0.918587000
C	6.906894000	-2.535359000	0.555086000
C	7.777291000	-0.611010000	-0.621507000
H	6.353327000	0.894782000	-1.179428000
H	-2.684571000	2.677312000	-1.853927000
C	-2.251805000	3.443018000	0.117966000
H	-1.591991000	3.994840000	2.099972000
H	7.062746000	-3.504196000	1.036762000
C	7.989505000	-1.847418000	-0.002565000
H	8.615003000	-0.072444000	-1.072011000

H	-3.188972000	4.000604000	0.190411000
H	8.994707000	-2.274977000	0.039500000
H	-0.660834000	-2.949432000	1.329223000
C	-0.507236000	1.087003000	-2.332213000
H	-0.562789000	0.024890000	-2.027987000
H	-1.250779000	1.246412000	-3.126706000
H	0.495092000	1.251744000	-2.758546000
C	0.802228000	2.688068000	2.282029000
H	0.336548000	3.104527000	3.187006000
H	1.110334000	1.651511000	2.496965000
H	1.733057000	3.250550000	2.097931000
O	-0.136767000	-1.889375000	-0.368719000
N	-2.018421000	-1.401810000	1.034442000
C	-1.112056000	-2.395032000	0.472774000
H	-1.732845000	-3.113380000	-0.091057000
B	-3.307929000	-1.199066000	0.500116000
O	-4.216915000	-0.287186000	1.008062000
O	-3.823769000	-1.917542000	-0.563563000
C	-5.341273000	-0.251693000	0.103285000
C	-5.242880000	-1.662628000	-0.600737000
C	-5.108433000	0.908294000	-0.869169000
C	-6.615247000	-0.020038000	0.907126000
C	-5.927620000	-2.775039000	0.201393000
C	-5.713218000	-1.693372000	-2.050232000
H	-5.963338000	1.055425000	-1.546313000
H	-4.954727000	1.830525000	-0.290307000
H	-4.204618000	0.737423000	-1.470944000
H	-7.504927000	-0.088915000	0.261459000
H	-6.715448000	-0.745800000	1.725023000
H	-6.594759000	0.986259000	1.353571000
H	-7.024613000	-2.697238000	0.161388000
H	-5.632320000	-3.748248000	-0.218933000
H	-5.613084000	-2.754033000	1.255765000
H	-5.611192000	-2.713257000	-2.452047000
H	-6.772233000	-1.400270000	-2.126040000
H	-5.114659000	-1.025252000	-2.683268000
C	-1.497647000	-0.569013000	2.095509000
H	-1.132391000	-1.179189000	2.943777000
H	-0.660544000	0.072935000	1.759372000
H	-2.275503000	0.111470000	2.466709000

TSB4

Zn	1.496395000	0.826310000	-0.950138000

O	3.131507000	-0.226119000	-1.037279000
N	1.750921000	1.423803000	0.941592000
C	3.884262000	-0.482208000	-0.029748000
C	0.883484000	2.468577000	1.383732000
C	2.741460000	0.977348000	1.701349000
C	3.708323000	0.029642000	1.265656000
C	5.010290000	-1.432785000	-0.308312000
C	1.219293000	3.802984000	1.070457000
C	-0.323620000	2.149846000	2.039962000
C	2.897294000	1.511260000	3.108377000
H	4.404927000	-0.309347000	2.029098000
C	4.895095000	-2.294256000	-1.414998000
C	6.176755000	-1.496791000	0.475698000
C	0.337465000	4.823861000	1.452185000
C	-1.173464000	3.200731000	2.413072000
H	3.501048000	0.834304000	3.727610000
H	3.409715000	2.487816000	3.076238000
H	1.926937000	1.676821000	3.595239000
H	3.996376000	-2.233531000	-2.030734000
C	5.905451000	-3.208368000	-1.715801000
C	7.191808000	-2.404900000	0.168202000
H	6.309250000	-0.815285000	1.317926000
H	0.586661000	5.861215000	1.211991000
C	-0.848533000	4.528368000	2.126664000
H	-2.109724000	2.966863000	2.927576000
H	5.794977000	-3.877113000	-2.573520000
C	7.057737000	-3.267785000	-0.924662000
H	8.096101000	-2.434034000	0.781692000
H	-1.527159000	5.333809000	2.419118000
H	7.852321000	-3.980034000	-1.162220000
H	0.335308000	-2.597058000	-1.806111000
C	2.491624000	4.101897000	0.320164000
H	2.535609000	3.535433000	-0.626207000
H	2.576506000	5.171899000	0.081268000
H	3.386923000	3.809097000	0.893861000
C	-0.696087000	0.714888000	2.287183000
H	-0.885587000	0.212894000	1.327179000
H	0.102128000	0.157386000	2.800670000
H	-1.608977000	0.639113000	2.892082000
O	0.107306000	-0.592867000	-1.660293000
N	-0.652025000	-2.150540000	-0.021831000
C	-0.421042000	-1.895927000	-1.411202000

H	-1.357238000	-2.024220000	-1.971438000
B	-1.960967000	-2.269951000	0.499804000
O	-2.230503000	-2.517440000	1.829380000
O	-3.106382000	-2.213729000	-0.273797000
C	-3.666618000	-2.461017000	1.997409000
C	-4.182387000	-2.749026000	0.532061000
C	-4.017667000	-1.051311000	2.481890000
C	-4.079613000	-3.495783000	3.037094000
C	-4.278100000	-4.245957000	0.217662000
C	-5.484675000	-2.052406000	0.158900000
H	-5.092734000	-0.949274000	2.692525000
H	-3.464371000	-0.846862000	3.410328000
H	-3.729157000	-0.294302000	1.739325000
H	-5.176374000	-3.552408000	3.119176000
H	-3.691523000	-4.493498000	2.793319000
H	-3.678091000	-3.212183000	4.022122000
H	-5.121233000	-4.722219000	0.739906000
H	-4.424510000	-4.372018000	-0.865618000
H	-3.352319000	-4.771489000	0.496716000
H	-5.750242000	-2.292202000	-0.882007000
H	-6.306065000	-2.393795000	0.808142000
H	-5.405250000	-0.961664000	0.241681000
C	0.532966000	-2.237511000	0.814325000
H	1.218589000	-3.023890000	0.448631000
H	1.095947000	-1.290656000	0.829381000
H	0.247176000	-2.476284000	1.846594000
C	-2.611665000	1.783307000	-1.447588000
O	-1.608088000	0.935646000	-0.869487000
C	-2.719149000	1.194667000	-2.911993000
B	-0.748699000	0.548562000	-1.914012000
O	-1.386250000	0.696336000	-3.149105000
H	0.418525000	1.588541000	-1.953067000
C	-3.882760000	1.661828000	-0.615612000
H	-3.715413000	2.099432000	0.380585000
H	-4.721217000	2.196817000	-1.088577000
H	-4.158786000	0.609393000	-0.483442000
C	-2.099928000	3.229352000	-1.412973000
H	-1.202536000	3.356556000	-2.034482000
H	-2.865966000	3.940733000	-1.757309000
H	-1.827054000	3.482059000	-0.378083000
C	-3.064285000	2.220386000	-3.986432000
H	-2.299824000	3.005743000	-4.055248000

H	-3.124511000	1.725226000	-4.968200000
H	-4.038662000	2.692353000	-3.782204000
C	-3.673105000	-0.003236000	-2.994044000
H	-4.727673000	0.306172000	-2.922663000
H	-3.526634000	-0.503909000	-3.963556000
H	-3.466366000	-0.730243000	-2.195849000

ICB4

Zn	1.168757000	1.512014000	1.530226000
O	2.931644000	0.668897000	1.183678000
N	0.994510000	2.182413000	-0.374304000
C	3.597948000	0.739490000	0.096524000
C	-0.242212000	2.819700000	-0.675680000
C	1.960843000	2.094514000	-1.275905000
C	3.198033000	1.434091000	-1.056530000
C	4.913888000	0.009151000	0.106201000
C	-1.285163000	2.112484000	-1.312847000
C	-0.436442000	4.148438000	-0.224799000
C	1.744507000	2.713075000	-2.641510000
H	3.898669000	1.470899000	-1.887081000
C	5.427499000	-0.419005000	1.343890000
C	5.631862000	-0.312752000	-1.060752000
C	-2.517244000	2.760113000	-1.493633000
C	-1.682992000	4.754171000	-0.420533000
H	2.657573000	2.684364000	-3.250397000
H	0.949243000	2.176159000	-3.182738000
H	1.409655000	3.757961000	-2.550450000
H	4.861576000	-0.183987000	2.246218000
C	6.623756000	-1.133895000	1.415991000
C	6.826254000	-1.032847000	-0.990204000
H	5.246718000	-0.023825000	-2.039816000
H	-3.330453000	2.217721000	-1.980654000
C	-2.721999000	4.065959000	-1.052273000
H	-1.838517000	5.778495000	-0.070209000
H	7.007337000	-1.453538000	2.388677000
C	7.328868000	-1.444923000	0.248536000
H	7.364229000	-1.279777000	-1.909376000
H	-3.692398000	4.548124000	-1.196194000
H	8.263566000	-2.009441000	0.302424000
H	-0.933199000	-0.021895000	3.150869000
C	-1.124222000	0.679979000	-1.760750000
H	-0.079777000	0.350948000	-1.763800000
H	-1.663565000	0.003610000	-1.079036000

H	-1.546383000	0.532709000	-2.767709000
C	0.687275000	4.872646000	0.469608000
H	0.390784000	5.891620000	0.758593000
H	0.997075000	4.332401000	1.380369000
H	1.583614000	4.942364000	-0.168779000
O	-0.120166000	-0.307295000	1.300335000
N	-2.399527000	0.314039000	1.713110000
C	-1.279193000	-0.420703000	2.186079000
H	-1.526963000	-1.485015000	2.273647000
B	-3.421928000	-0.317281000	0.960021000
O	-4.599061000	0.299593000	0.598677000
O	-3.349276000	-1.626755000	0.531114000
C	-5.316264000	-0.607432000	-0.270776000
C	-4.681681000	-2.004466000	0.109945000
C	-5.018627000	-0.192641000	-1.714478000
C	-6.808142000	-0.483306000	0.014521000
C	-5.362953000	-2.662482000	1.313932000
C	-4.583132000	-2.993864000	-1.044365000
H	-5.582327000	-0.799863000	-2.437989000
H	-5.308525000	0.859894000	-1.848303000
H	-3.946814000	-0.282077000	-1.939881000
H	-7.379326000	-1.231592000	-0.556977000
H	-7.028754000	-0.610582000	1.082358000
H	-7.161047000	0.515920000	-0.283345000
H	-6.362508000	-3.046403000	1.061080000
H	-4.742429000	-3.505037000	1.654295000
H	-5.461420000	-1.955983000	2.151849000
H	-4.166020000	-3.947342000	-0.686907000
H	-5.580111000	-3.198068000	-1.464970000
H	-3.932442000	-2.619964000	-1.845042000
C	-2.456392000	1.737061000	2.027785000
H	-2.456238000	1.901170000	3.119550000
H	-1.597380000	2.280353000	1.608264000
H	-3.370892000	2.170195000	1.605207000
C	1.574438000	-2.626064000	-0.830015000
O	1.215820000	-1.276586000	-0.432011000
C	0.305663000	-3.447240000	-0.366829000
B	0.298483000	-1.391980000	0.571188000
O	-0.155429000	-2.665884000	0.768481000
H	0.716458000	2.067159000	2.930872000
C	1.836445000	-2.630760000	-2.329920000
H	2.720123000	-2.012106000	-2.547304000

H	2.034772000	-3.652744000	-2.688648000
H	0.990020000	-2.216555000	-2.893311000
C	2.842830000	-3.007356000	-0.065021000
H	2.673605000	-2.990540000	1.021830000
H	3.200698000	-4.007520000	-0.350828000
H	3.633142000	-2.279572000	-0.289121000
C	0.590278000	-4.867628000	0.100125000
H	1.265230000	-4.881798000	0.965767000
H	-0.350322000	-5.356188000	0.397233000
H	1.042107000	-5.459903000	-0.710689000
C	-0.825011000	-3.436651000	-1.397800000
H	-0.593057000	-4.077701000	-2.261311000
H	-1.742158000	-3.802263000	-0.917744000
H	-1.024099000	-2.416923000	-1.758254000

TSB5

Zn	0.559246000	1.114854000	1.232389000
O	2.484974000	0.743076000	0.751272000
N	0.448085000	2.637263000	-0.154312000
C	3.159148000	1.325573000	-0.161530000
C	-0.839677000	3.225037000	-0.216886000
C	1.441591000	3.025382000	-0.931015000
C	2.725580000	2.412457000	-0.941929000
C	4.548101000	0.784685000	-0.369551000
C	-1.796420000	2.703567000	-1.119372000
C	-1.189724000	4.228468000	0.715467000
C	1.223149000	4.192568000	-1.873545000
H	3.450764000	2.850291000	-1.625220000
C	5.175162000	0.122186000	0.701059000
C	5.228861000	0.869871000	-1.596621000
C	-3.102780000	3.211048000	-1.078303000
C	-2.507209000	4.709179000	0.723343000
H	2.132535000	4.442155000	-2.435842000
H	0.418773000	3.967642000	-2.591078000
H	0.899841000	5.083886000	-1.312793000
H	4.635549000	0.039718000	1.646038000
C	6.451993000	-0.421717000	0.556432000
C	6.502736000	0.315379000	-1.745782000
H	4.747265000	1.345876000	-2.453027000
H	-3.851029000	2.803669000	-1.763640000
C	-3.460383000	4.207460000	-0.166767000
H	-2.786010000	5.485067000	1.442423000
H	6.927275000	-0.925641000	1.402535000

C	7.121271000	-0.328228000	-0.669061000
H	7.011667000	0.379449000	-2.711387000
H	-4.484802000	4.588972000	-0.145150000
H	8.118606000	-0.760708000	-0.786440000
H	-1.226454000	-0.176206000	3.437438000
C	-1.405807000	1.594141000	-2.058874000
H	-0.611303000	1.908789000	-2.755640000
H	-1.003055000	0.741211000	-1.487712000
H	-2.265136000	1.263115000	-2.658444000
C	-0.154223000	4.731802000	1.685817000
H	-0.583375000	5.453160000	2.397192000
H	0.280964000	3.891123000	2.251254000
H	0.685026000	5.223632000	1.165625000
O	-0.336319000	-0.429180000	0.326790000
N	-2.640321000	-0.186837000	1.934404000
C	-1.679928000	-0.722015000	2.607159000
H	-1.317259000	-1.718184000	2.344399000
B	-3.147431000	-0.895290000	0.719023000
O	-3.958368000	-0.263668000	-0.155406000
O	-2.942523000	-2.212020000	0.507212000
C	-4.534912000	-1.313850000	-1.001068000
C	-3.489036000	-2.490039000	-0.828692000
C	-4.671179000	-0.780939000	-2.418414000
C	-5.909426000	-1.630654000	-0.410288000
C	-4.091384000	-3.886599000	-0.813032000
C	-2.329032000	-2.406604000	-1.816132000
H	-5.043839000	-1.569796000	-3.089592000
H	-5.391355000	0.050956000	-2.434324000
H	-3.715112000	-0.411949000	-2.807010000
H	-6.446324000	-2.372229000	-1.019394000
H	-5.826783000	-2.017288000	0.616713000
H	-6.508188000	-0.708188000	-0.380050000
H	-4.604997000	-4.093630000	-1.764458000
H	-3.290383000	-4.630811000	-0.690411000
H	-4.805717000	-4.018869000	0.010207000
H	-1.541200000	-3.111038000	-1.523000000
H	-2.661968000	-2.655192000	-2.834428000
H	-1.869860000	-1.409933000	-1.816508000
C	-3.067267000	1.198169000	2.161968000
H	-2.763207000	1.527603000	3.162123000
H	-2.586774000	1.839115000	1.408011000
H	-4.155049000	1.269774000	2.041931000

C	1.691781000	-3.248179000	-0.496648000
O	0.758828000	-2.227702000	-0.886689000
C	1.236336000	-3.570823000	0.983005000
B	0.333278000	-1.567365000	0.266884000
O	0.688094000	-2.314824000	1.408056000
H	0.122088000	1.404261000	2.755223000
C	1.588942000	-4.418328000	-1.468874000
H	1.912744000	-4.095266000	-2.470436000
H	2.236845000	-5.251826000	-1.153812000
H	0.558318000	-4.789181000	-1.555204000
C	3.090098000	-2.623370000	-0.556370000
H	3.163770000	-1.774605000	0.137347000
H	3.885875000	-3.347603000	-0.325323000
H	3.261019000	-2.232441000	-1.570583000
C	2.367675000	-3.967426000	1.926361000
H	3.106472000	-3.161176000	2.023943000
H	1.962165000	-4.173002000	2.929670000
H	2.879308000	-4.876580000	1.572249000
C	0.106676000	-4.606465000	1.046829000
H	0.450218000	-5.616931000	0.777948000
H	-0.289339000	-4.640434000	2.073833000
H	-0.721266000	-4.321981000	0.380951000

ICB5

Zn	-1.435283000	0.322461000	-0.928212000
O	-3.271422000	-0.269636000	-0.591762000
N	-1.569299000	2.031500000	0.015412000
C	-4.123161000	0.383191000	0.105148000
C	-0.393945000	2.843176000	0.075179000
C	-2.690194000	2.409122000	0.630470000
C	-3.887432000	1.651877000	0.667987000
C	-5.448876000	-0.293638000	0.292472000
C	0.541949000	2.616685000	1.105564000
C	-0.158407000	3.791703000	-0.940668000
C	-2.694164000	3.735220000	1.358596000
H	-4.712820000	2.121778000	1.196165000
C	-5.751249000	-1.397523000	-0.527003000
C	-6.393571000	0.104664000	1.256796000
C	1.706840000	3.395360000	1.128266000
C	1.020166000	4.548774000	-0.883758000
H	-3.673650000	3.949781000	1.804352000
H	-1.935407000	3.737388000	2.156651000
H	-2.427495000	4.556433000	0.675990000

H	-5.013874000	-1.713491000	-1.266113000
C	-6.966101000	-2.071281000	-0.398916000
C	-7.606196000	-0.574171000	1.389029000
H	-6.179572000	0.937183000	1.928779000
H	2.446261000	3.224791000	1.913823000
C	1.942629000	4.360331000	0.147340000
H	1.218220000	5.286321000	-1.666352000
H	-7.186095000	-2.921778000	-1.049468000
C	-7.899204000	-1.661691000	0.559358000
H	-8.324653000	-0.254809000	2.148360000
H	2.861621000	4.951021000	0.173321000
H	-8.850254000	-2.190637000	0.663183000
H	3.360496000	-0.427210000	-3.868390000
C	0.297486000	1.525503000	2.115121000
H	-0.670914000	1.644627000	2.627619000
H	0.272575000	0.539741000	1.620021000
H	1.086167000	1.505244000	2.880141000
C	-1.150001000	3.951269000	-2.063485000
H	-0.786084000	4.656296000	-2.824715000
H	-1.346943000	2.984189000	-2.557515000
H	-2.126658000	4.314764000	-1.701930000
O	-0.465521000	-0.762655000	-2.163892000
N	2.930883000	0.066234000	-1.848998000
C	2.905544000	-0.868656000	-2.958576000
H	3.466589000	-1.777398000	-2.703237000
B	3.806509000	-0.089139000	-0.761635000
O	3.978602000	0.850072000	0.244032000
O	4.601401000	-1.208961000	-0.569070000
C	4.777169000	0.238150000	1.276881000
C	5.534829000	-0.901436000	0.484722000
C	3.814619000	-0.316767000	2.330677000
C	5.680189000	1.298680000	1.896636000
C	6.824736000	-0.406447000	-0.178833000
C	5.807666000	-2.170017000	1.285281000
H	4.345761000	-0.751851000	3.190194000
H	3.173342000	0.498778000	2.693424000
H	3.162401000	-1.085213000	1.893495000
H	6.381600000	0.846890000	2.615579000
H	6.255398000	1.836710000	1.131775000
H	5.069486000	2.038428000	2.437082000
H	7.620756000	-0.215412000	0.556613000
H	7.178661000	-1.174749000	-0.882698000

H	6.646077000	0.516780000	-0.750398000
H	6.330545000	-2.902374000	0.651140000
H	6.445090000	-1.955941000	2.157566000
H	4.876986000	-2.636641000	1.633443000
C	2.154953000	1.276395000	-2.037067000
H	2.540053000	1.880486000	-2.882968000
H	1.103568000	1.027239000	-2.254631000
H	2.194488000	1.895639000	-1.133774000
C	-0.242160000	-2.720782000	0.752440000
O	-0.211912000	-1.440375000	0.081858000
C	0.627666000	-3.597051000	-0.239086000
B	-0.081714000	-1.703481000	-1.313333000
O	0.347539000	-2.993640000	-1.523769000
H	1.870129000	-1.154225000	-3.206051000
C	0.332004000	-2.570893000	2.153916000
H	-0.342479000	-1.958242000	2.771989000
H	0.438962000	-3.553491000	2.639341000
H	1.311669000	-2.078392000	2.136074000
C	-1.707934000	-3.161497000	0.816953000
H	-2.128132000	-3.298474000	-0.190371000
H	-1.829274000	-4.099142000	1.379526000
H	-2.294811000	-2.375178000	1.313981000
C	0.229297000	-5.066956000	-0.291944000
H	-0.804940000	-5.193939000	-0.638451000
H	0.886071000	-5.603570000	-0.993608000
H	0.332143000	-5.536407000	0.699210000
C	2.129334000	-3.454522000	0.013687000
H	2.436835000	-3.941693000	0.951332000
H	2.679297000	-3.924042000	-0.814862000
H	2.429854000	-2.400146000	0.043386000

TSB6

Zn	0.784426000	0.210050000	-0.067659000
O	2.490701000	-0.632709000	-0.322390000
N	1.409911000	2.016320000	0.385460000
C	3.604441000	0.004109000	-0.218698000
C	0.421805000	2.979848000	0.758618000
C	2.707818000	2.287430000	0.454359000
C	3.736366000	1.354413000	0.145249000
C	4.824078000	-0.823795000	-0.486739000
C	-0.095767000	3.858107000	-0.213484000
C	-0.089358000	2.949301000	2.072340000
C	3.136175000	3.665693000	0.904566000

H	4.749224000	1.734453000	0.253668000
C	4.705765000	-2.225121000	-0.426479000
C	6.074416000	-0.267555000	-0.815077000
C	-1.100249000	4.755952000	0.171106000
C	-1.099029000	3.858430000	2.416450000
H	4.228422000	3.770602000	0.914244000
H	2.710121000	4.438844000	0.247226000
H	2.751179000	3.872743000	1.915525000
H	3.732613000	-2.656938000	-0.188046000
C	5.809361000	-3.044554000	-0.665414000
C	7.175591000	-1.088879000	-1.062929000
H	6.188535000	0.814018000	-0.905699000
H	-1.510389000	5.444523000	-0.572721000
C	-1.594812000	4.764772000	1.476938000
H	-1.504611000	3.845499000	3.431852000
H	5.701213000	-4.130710000	-0.606063000
C	7.048985000	-2.479798000	-0.983706000
H	8.136814000	-0.640045000	-1.326338000
H	-2.382739000	5.468076000	1.758702000
H	7.912946000	-3.121307000	-1.176340000
O	-0.942421000	-0.438627000	0.388727000
C	0.384520000	3.774687000	-1.636944000
H	0.155908000	2.778494000	-2.049030000
H	-0.111888000	4.523573000	-2.271036000
H	1.473588000	3.921115000	-1.722580000
C	0.412696000	1.918527000	3.049985000
H	-0.061882000	2.034176000	4.035128000
H	0.184582000	0.901527000	2.684274000
H	1.505305000	1.969353000	3.186584000
C	-3.697753000	0.010987000	-1.807752000
C	-3.380125000	1.343097000	-1.004074000
H	-0.318190000	0.100951000	-1.834420000
B	-1.458618000	0.178141000	-1.351722000
O	-1.950258000	1.457752000	-1.163677000
O	-2.445248000	-0.715367000	-1.750252000
C	-3.690692000	1.244554000	0.494858000
H	-3.228587000	2.105686000	1.000658000
H	-4.775467000	1.269452000	0.681315000
H	-3.273647000	0.332061000	0.936252000
C	-4.021951000	2.603351000	-1.577545000
H	-5.120182000	2.520928000	-1.580758000
H	-3.744824000	3.467202000	-0.954609000

H	-3.679146000	2.805108000	-2.601053000
C	-3.990098000	0.260199000	-3.290209000
H	-4.003653000	-0.706408000	-3.816457000
H	-4.962978000	0.751826000	-3.442566000
H	-3.205550000	0.880670000	-3.748078000
C	-4.792686000	-0.850028000	-1.186396000
H	-5.740106000	-0.291673000	-1.121947000
H	-4.966757000	-1.739403000	-1.812595000
H	-4.503367000	-1.191279000	-0.185466000
C	-1.348298000	-3.983261000	0.416745000
C	-2.517535000	-3.504969000	1.369839000
B	-1.308039000	-1.719358000	0.624848000
O	-2.536017000	-2.079520000	1.137149000
O	-0.502683000	-2.810773000	0.367740000
C	-2.203073000	-3.713267000	2.854341000
H	-2.946418000	-3.167265000	3.454691000
H	-2.239837000	-4.775904000	3.137591000
H	-1.208224000	-3.317033000	3.107872000
C	-3.889016000	-4.078951000	1.034032000
H	-3.883773000	-5.177387000	1.114201000
H	-4.638307000	-3.688790000	1.740121000
H	-4.206119000	-3.800596000	0.021038000
C	-1.820284000	-4.243164000	-1.017965000
H	-0.936684000	-4.373835000	-1.661009000
H	-2.439199000	-5.150111000	-1.090356000
H	-2.386293000	-3.382560000	-1.404062000
C	-0.537370000	-5.162845000	0.937229000
H	-1.177826000	-6.048475000	1.073285000
H	0.250100000	-5.419839000	0.212119000
H	-0.048902000	-4.930643000	1.892962000

ICB6

Zn	-3.234887000	2.159279000	0.607098000
O	-5.055584000	1.408937000	0.634204000
N	-2.508588000	0.649298000	-0.477888000
C	-5.430672000	0.296515000	0.123495000
C	-1.130963000	0.782572000	-0.824188000
C	-3.207578000	-0.421131000	-0.838271000
C	-4.585776000	-0.598861000	-0.555101000
C	-6.881453000	-0.039808000	0.311869000
C	-0.783149000	1.397106000	-2.046947000
C	-0.144817000	0.389845000	0.105126000
C	-2.504932000	-1.531242000	-1.588796000

H	-5.017266000	-1.538972000	-0.890234000
C	-7.599595000	0.641066000	1.312191000
C	-7.561455000	-0.988999000	-0.473711000
C	0.575636000	1.575821000	-2.343414000
C	1.201440000	0.599537000	-0.223350000
H	-3.190147000	-2.350882000	-1.840090000
H	-2.052499000	-1.151205000	-2.517323000
H	-1.679000000	-1.936102000	-0.984557000
H	-7.075856000	1.387939000	1.910546000
C	-8.949256000	0.366808000	1.535721000
C	-8.914161000	-1.257094000	-0.255572000
H	-7.041978000	-1.508474000	-1.280717000
H	0.856523000	2.043580000	-3.291492000
C	1.564423000	1.176129000	-1.441809000
H	1.973798000	0.301449000	0.484904000
H	-9.488244000	0.899636000	2.323586000
C	-9.612079000	-0.584583000	0.753138000
H	-9.427973000	-1.991440000	-0.881456000
H	2.622955000	1.307617000	-1.669637000
H	-10.670617000	-0.797504000	0.924336000
O	4.151942000	-0.731758000	1.609488000
C	-1.865132000	1.861197000	-2.987684000
H	-2.579269000	2.525291000	-2.471317000
H	-1.445860000	2.406539000	-3.845749000
H	-2.461306000	1.019767000	-3.379572000
C	-0.543913000	-0.213860000	1.426193000
H	0.334205000	-0.572312000	1.979899000
H	-1.079284000	0.526492000	2.047865000
H	-1.233519000	-1.062809000	1.295883000
C	5.984775000	2.258799000	0.973014000
C	5.685894000	1.731461000	-0.486995000
H	-2.691927000	3.457160000	1.265402000
B	4.824359000	0.315397000	1.062991000
O	4.666474000	0.729290000	-0.237523000
O	5.688722000	1.091754000	1.783436000
C	6.875814000	1.003952000	-1.118372000
H	6.530512000	0.475441000	-2.019453000
H	7.674734000	1.702660000	-1.407888000
H	7.296671000	0.255386000	-0.430429000
C	5.136219000	2.780599000	-1.444744000
H	5.854848000	3.606212000	-1.565367000
H	4.968376000	2.331231000	-2.435579000

H	4.181984000	3.194323000	-1.094815000
C	5.019999000	3.362884000	1.414681000
H	5.133774000	3.522199000	2.497290000
H	5.224308000	4.313516000	0.900173000
H	3.974138000	3.078599000	1.223313000
C	7.427226000	2.678803000	1.220449000
H	7.713585000	3.501901000	0.547289000
H	7.538919000	3.031047000	2.257224000
H	8.124276000	1.843399000	1.073430000
C	2.072038000	-3.465797000	0.611053000
C	3.118529000	-3.371622000	-0.577822000
B	3.566280000	-1.795071000	0.989555000
O	4.147768000	-2.517438000	-0.015526000
O	2.321133000	-2.238136000	1.341289000
C	2.568740000	-2.644638000	-1.808150000
H	3.401790000	-2.432561000	-2.494735000
H	1.823224000	-3.252496000	-2.341935000
H	2.110119000	-1.683883000	-1.534968000
C	3.747794000	-4.698510000	-0.982360000
H	2.978215000	-5.403948000	-1.332331000
H	4.459628000	-4.534332000	-1.805650000
H	4.297343000	-5.159619000	-0.151276000
C	2.351603000	-4.620854000	1.574624000
H	1.719090000	-4.500798000	2.466940000
H	2.127384000	-5.596371000	1.118199000
H	3.401496000	-4.619967000	1.903747000
C	0.614149000	-3.476547000	0.168647000
H	0.406758000	-4.342464000	-0.478767000
H	-0.042847000	-3.541348000	1.048849000
H	0.362721000	-2.557478000	-0.374404000

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