

Supporting Information

Aqueous Hydroboration of Alkynes via Nonclassical Generation of N-Heterocyclic Carbenes

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1. General Information

All organic solvents, bases, reagents, and metal salt were purchased from commercial suppliers and were used without further purification, unless otherwise noted. All reactions were performed under air atmosphere, unless otherwise noted. All reaction tubes in experiments used the Schlenk tubes. The NMR spectra were recorded on a Bruker Avance III HD 400 spectrometer using TMS as internal standard (400 MHz for ^1H NMR, 100 MHz for ^{13}C NMR, MHz for ^{19}F NMR and 128 ^{11}B NMR). Mass spectroscopy data were collected on a Bruker solanX 70 FT-MS and a Waters UPLC G2-XS Qtof. Single crystal structure determination was conducted on a Bruker D8 Venture X ray diffractometer equipped with a PHOTON II CPAD detector. FT-IR spectra were recorded on a Tianjin Gangdong FTIR-650 spectrometer. The catalysts **C1**, **C2**, **C3**, and **C4** were purchased from commercial suppliers.

2. General Procedure for the Hydroboration of Alkynes

Method A: A mixture of alkyne (1.0 mmol), diboron reagent (1.2 mmol) and **C6** (0.01 mmol) in THF (1 ml) and MeOH (1 ml) in a 50 ml reaction tube was stirred for 12 h at 60 °C. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3 × 15 ml). The desired hydroboration of alkynes were isolated by short chromatography.

Method B: A mixture of alkyne (1.0 mmol), diboron reagent (1.2 mmol) and **C6** (0.05 mmol) in water (2 ml) in a 50 ml reaction tube was stirred for 12 h at 50 °C. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3 × 15 ml). The desired hydroboration of alkynes were isolated by short chromatography.

Method C: A mixture of alkyne (1.0 mmol), diboron reagent (1.2 mmol) and **C6** (0.05 mmol) in water (2 ml) and THF (100 µl) in a 50 ml reaction tube was stirred for 12 h at 50 °C. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3 × 15 ml). The desired hydroboration of alkynes were isolated by short chromatography.

3. Optimization of reaction conditions

Table S1. Optimization of hydroboration of terminal alkynes in water

The reaction scheme shows 1-phenyl-2-propyne (**1a**) reacting with B_2pin_2 (**1a'**) in the presence of H_2O to yield (E)-1-phenyl-2-propenylboronic pinacol ester (**2a**).

| Entry | Cat. | Temperature/ $^{\circ}C$ | Time/h | Yield/% | <i>E:Z</i> ratio |
|-------|---------------------|--------------------------|--------|---------|------------------|
| 1 | C6 (1 mol%) | 80 | 12 | 84 | > 99:1 |
| 2 | C6 (2 mol%) | 80 | 12 | 86 | > 99:1 |
| 3 | C6 (4 mol%) | 80 | 12 | 88 | > 99:1 |
| 4 | C6 (5 mol%) | 80 | 12 | 94 | > 99:1 |
| 5 | C6 (10 mol%) | 80 | 12 | 95 | > 99:1 |
| 6 | C6 (5 mol%) | 70 | 12 | 93 | > 99:1 |
| 7 | C6 (5 mol%) | 60 | 12 | 91 | > 99:1 |
| 8 | C6 (5 mol%) | 50 | 12 | 90 | > 99:1 |
| 9 | C6 (5 mol%) | 40 | 12 | 61 | > 99:1 |
| 10 | C6 (5 mol%) | rt | 12 | trace | |
| 11 | C7 (5 mol%) | 50 | 12 | 89 | > 99:1 |
| 12 | C8 (5 mol%) | 50 | 12 | 79 | > 99:1 |
| 13 | C9 (5 mol%) | 50 | 12 | 86 | > 99:1 |
| 14 | C10 (5 mol%) | 50 | 12 | 32 | > 99:1 |
| 15 | C5 (5 mol%) | 50 | 12 | 0 | |
| 16 | C6 (5 mol%) | 50 | 10 | 84 | > 99:1 |
| 17 | C6 (5 mol%) | 50 | 8 | 79 | > 99:1 |
| 18 | C6 (5 mol%) | 50 | 5 | 66 | > 99:1 |

^aConditions: **1a** (1.0 mmol), **1a'** (1.2 mmol, 1.2 equiv), cat. (as shown in Table), H_2O (2 mL), temperature and time as shown in Table, isolated yield determined by column chromatography. *E:Z* ratio determined by 1H NMR.

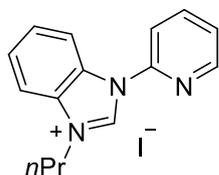
Table S2. Effect of THF/MeOH volume ratio on boration of alkyne

| Entry | THF/mL | MeOH/mL | THF: MeOH (v:v) | Yield/% |
|-------|--------|---------|-----------------|---------|
| 1 | 0 | 2 | 0: 2 | 86.3 |
| 2 | 0.2 | 1.8 | 1: 9 | 88.7 |
| 3 | 0.5 | 1.5 | 1: 3 | 87.6 |
| 4 | 0.8 | 1.2 | 2: 3 | 90.3 |
| 5 | 1 | 1 | 1: 1 | 93.1 |
| 6 | 1.2 | 0.8 | 3: 2 | 87.9 |
| 7 | 1.5 | 0.5 | 3: 1 | 80.1 |
| 8 | 1.8 | 0.2 | 9: 1 | trace |
| 9 | 2 | 0 | 2: 0 | 0 |

Conditions: **1a** (1.0 mmol), **1a'** (1.2 mmol), catalysts (0.01 mmol, 1 mol%), THF (as shown in Table) and MeOH (as shown in Table), 60 °C, 12 h, isolated yield determined by column chromatography.

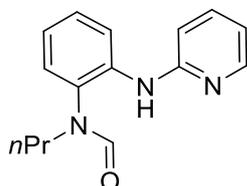
4. Characterization Data for Catalysts

3-propyl-1-(pyridin-2-yl)-1*H*-benzo[*d*]imidazol-3-ium (C5)



C5 was synthesized by previously reported methods.¹ A mixture of 2-bromopyridine (0.5 mmol), benzimidazole (1.0 mmol), the CuI (0.1 mmol), *N,N,N',N'*-tetramethylethane-1,2-diamine (0.2 mmol), and K₂CO₃ (1.5 mmol) in DMSO (2 mL) was combined under nitrogen. The reaction mixture was stirred at room temperature for 30 min and then heated to 110 °C for 48 h. The resultant 2-substituent-pyridine (0.5 mmol), and 1-iodopropane (1 mL) was heated to 110 °C for 8 h under air. Purification by flash chromatography (DCM:MeOH = 30:1): a yellowish solid (144 mg, 79%), mp = 157-158 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.61 (s, 1H), 8.76 (d, *J* = 4.8 Hz, 1H), 8.47-8.44 (m, 1H), 8.30-8.25 (m, 2H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.76-7.69 (m, 3H), 4.61 (t, *J* = 7.6 Hz, 2H), 2.05 (sext, *J* = 7.6 Hz, 2H), 1.00 (t, *J* = 7.6 Hz, 3H), ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 149.80, 147.87, 142.56, 140.98, 132.10, 129.90, 128.16, 127.58, 125.49, 117.56, 116.48, 114.63, 49.29, 22.51, 11.32, ppm.

N-propyl-*N*-(2-(pyridin-2-ylamino)phenyl)formamide (C6)



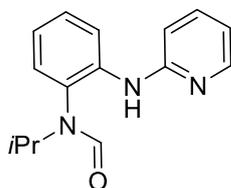
C6 was synthesized by previously reported methods.² 3-propyl-1-(pyridin-2-yl)-1*H*-benzo[*d*]imidazol-3-ium iodide (1.0 mmol), KO^{*t*}Bu (1.2 equiv.) and THF (9 ml) and water (1 ml) in a 50 ml reaction tube was stirred for 2 h at room temperature. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3×15 ml). Purification by flash chromatography (petroleum ether:EtOAc = 2:1): a white solid (118 mg, 92%), mp = 117-118 °C; mixture of two rotamers (**a/b** = 7/3); ¹H NMR (400 MHz, CDCl₃): δ 8.33-8.16 (m, **a**-2H and **b**-2H), 8.08 (d, *J* = 8.4 Hz, **a**-1H), 7.76 (d, *J* = 8.0 Hz, **b**-1H), 7.52 (t, *J* = 5.6 Hz, **a**-1H), 7.45 (t, *J* = 5.6 Hz, **b**-1H), 7.37-7.28 (m, **a**-1H and **b**-1H), 7.22-6.90 (m, **a**-5H and **b**-5H), 3.63-3.57 (m, **a**-2H and **b**-2H), 1.58-1.49 (m, **a**-2H), 1.49-1.41 (m, **b**-2H), 0.85 (t, *J* = 7.2 Hz, **a**-3H), 0.80 (t, *J* = 7.2 Hz, **b**-3H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 163.63-**a**, 162.73-**b**, 156.02-**b**, 155.23-**a**, 148.27-**b**, 148.07-**a**, 138.13-**b**, 137.75-**a**, 137.63-**a**, 137.46-**b**, 130.73-**b**, 130.06-**b**, 129.72-**a**, 129.24-**a**, 128.55-**a**, 127.69-**b**, 124.05-**b**, 123.61-**a**, 122.34-**a**, 120.87-**b**, 115.85-**a**, 115.06-**b**, 110.36-**a**, 109.06-**b**, 52.30-**b**, 46.55-**a**, 21.92-**b**, 20.87-**a**, 11.32-**a**, 10.80-**b**, ppm.

N-(2-(phenylamino)phenyl)-*N*-propylformamide (**C7**)



C7 was synthesized by previously reported methods.² 1-phenyl-3-propyl-1*H*-benzo[*d*]imidazol-3-ium iodide (1.0 mmol), KO*t*Bu (1.2 equiv.) and THF (9 ml) and water (1 ml) in a 50 ml reaction tube was stirred for 2 h at room temperature. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3×15 ml). Purification by flash chromatography (petroleum ether:EtOAc = 2:1): a white solid (241 mg, 95%), mp = 104-106 °C; mixture of two rotamers (**a/b** = 7/3); ¹H NMR (400 MHz, CDCl₃): δ 8.34 (s, **b**-1H), 8.20 (s, **a**-1H), 7.35-6.89 (m, **a**-9H and **b**-9H), 5.88 (s, **b**-1H), 5.76 (s, **a**-1H), 3.65-3.61 (m, **a**-2H and **b**-2H), 1.65-1.43 (m, **a**-2H and **b**-2H), 0.90 (t, *J* = 7.2 Hz, **a**-3H), 0.85 (t, *J* = 7.2 Hz, **b**-3H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 163.71-**a**, 162.44-**b**, 143.43-**b**, 141.62-**a**, 140.94-**a**, 140.33-**b**, 130.04-**b**, 129.52-**a**, 129.34-**b**, 129.30-**a**, 128.52-**a**, 127.41-**b**, 122.47-**a**, 122.29-**b**, 120.70-**b**, 120.50-**b**, 120.44-**b**, 119.63-**a**, 117.84-**a**, 116.65-**a**, 52.59-**b**, 46.40-**a**, 21.96-**b**, 21.00-**a**, 11.38-**a**, 10.89-**b**, ppm; HRMS (ESI) calcd for C₁₆H₁₈N₂O [M + Na]⁺ 277.1317, found 277.1311.

N-isopropyl-*N*-(2-(pyridin-2-ylamino)phenyl)formamide (**C8**)



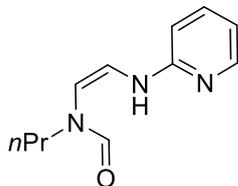
C8 was synthesized by previously reported methods.² 3-isopropyl-1-(pyridin-2-yl)-1*H*-benzo[*d*]imidazol-3-ium iodide (1.0 mmol), KO*t*Bu (1.2 equiv.) and THF (9 ml) and water (1 ml) in a 50 ml reaction tube was stirred for 2 h at room temperature. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3×15 ml). Purification by flash chromatography (petroleum ether:EtOAc = 5:1): a white solid (235 mg, 92%); mp = 100-101 °C; mixture of two rotamers (**a/b** = 7/3); ¹H NMR (400 MHz, CDCl₃): δ 8.47 (s, **b**-1H), 8.23 (d, *J* = 4.0 Hz, **a**-1H), 8.18 (s, **a**-1H), 8.16 (s, **b**-1H), 8.10 (s, **a**-1H), 7.79 (d, *J* = 8.0 Hz, **b**-1H), 7.53-7.32 (m, **a**-2H and **b**-2H), 7.18-6.60 (m, **a**-5H and **b**-5H), 4.75-4.65 (m, **a**-1H), 4.11-4.01 (m, **b**-1H), 1.35-1.72 (m, **a**-6H and **b**-6H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 163.83-**a**, 162.75-**b**, 155.89-**b**, 155.04-**a**, 148.31-**b**, 148.07-**a**, 139.80-**a**, 138.20-**b**, 137.71-**a**, 137.64-**b**, 131.33-**a**, 129.60-**a**, 129.32-**b**, 129.19-**b**, 128.90-**b**, 127.25-**b**, 123.67-**b**, 123.25-**b**, 121.70-**a**, 120.29-**a**, 115.88-**a**, 115.09-**b**, 110.38-**a**, 108.93-**b**, 52.42-**b**, 46.91-**a**, 23.53-**b**, 21.39-**a**, ppm; HRMS (ESI) calcd for C₁₃H₁₃N₃O [M + H]⁺ 256.1450, found 256.1446.

***N*-methyl-*N*-(2-(pyridin-2-ylamino)phenyl)formamide (C9)**



C9 was synthesized by previously reported methods.² 3-methyl-1-(pyridin-2-yl)-1*H*-benzo[*d*]imidazol-3-ium iodide (1.0 mmol), KO*t*Bu (1.2 equiv.) and THF (9 ml) and water (1 ml) in a 50 ml reaction tube was stirred for 2 h at room temperature. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3×15 ml). Purification by flash chromatography (petroleum ether:EtOAc = 5:1): a white solid (164 mg, 72%); mp = 113-115 °C; mixture of two rotamers (**a/b** = 17/3); ¹H NMR (400 MHz, CDCl₃): δ 8.38-8.24 (m, **a**-2H and **b**-2H), 8.10 (d, *J* = 9.2 Hz, **a**-1H), 7.85 (d, *J* = 9.2 Hz, **b**-1H), 7.61-7.52 (m, **a**-1H and **b**-1H), 7.45-7.37 (m, **a**-1H and **b**-1H), 7.32-6.78 (m, **a**-5H and **b**-5H), 3.37 (s, **b**-3H), 3.26 (s, **a**-3H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 163.72-**a**, 162.73-**b**, 156.03-**b**, 155.48-**a**, 148.20-**b**, 148.04-**a**, 137.74-**a**, 137.66-**a**, 136.71-**b**, 132.16-**b**, 129.12-**a**, 128.53-**b**, 128.31-**a**, 126.93-**b**, 124.06-**b**, 123.54-**b**, 122.84-**a**, 121.63-**a**, 115.73-**b**, 115.16-**a**, 110.26-**a**, 109.42-**b**, 37.37-**b**, 32.73-**a**, ppm; HRMS (ESI) calcd for C₁₅H₁₇N₃O [M + H]⁺ 228.1137, found 228.1135.

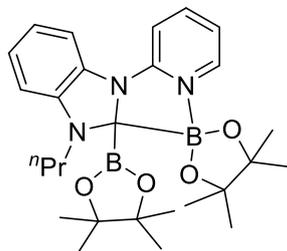
***N*-propyl-*N*-(2-(pyridin-2-ylamino)vinyl)formamide (C10)**



C10 was synthesized by previously reported methods.² 3-propyl-1-(pyridin-2-yl)-1*H*-imidazol-3-ium iodide (1.0 mmol), KO*t*Bu (1.2 equiv.) and THF (9 ml) and water (1 ml) in a 50 ml reaction tube was stirred for 2 h at room temperature. The reaction mixture was added to brine (100 ml) and extracted three times with dichloromethane (3×15 ml). Purification by flash chromatography (petroleum ether:EtOAc = 5:1): a colorless liquid (178 mg, 87%); mixture of two rotamers (**a/b** = 6/3); ¹H NMR (400 MHz, CDCl₃): δ 8.23 (d, *J* = 11.6 Hz, **b**-1H), 8.15 (d, *J* = 4.8 Hz, **a**-1H), 8.13 (s, **b**-1H), 8.07 (s, **a**-1H), 7.52 (d, *J* = 9.6 Hz, **a**-1H and **b**-1H), 7.46-7.40 (m, **a**-1H and **b**-1H), 7.36 (dd, *J* = 11.6 Hz, *J* = 6.4 Hz, **b**-1H), 6.90 (dd, *J* = 9.6 Hz, *J* = 6.8 Hz, **a**-1H), 6.80 (d, *J* = 8.4 Hz, **b**-1H), 6.72-6.67 (m, **a**-2H and **b**-2H), 6.59 (d, *J* = 8.4 Hz, **a**-1H), 5.14 (d, *J* = 6.4 Hz, **b**-1H), 4.89 (d, *J* = 7.2 Hz, **a**-1H), 3.41 (t, *J* = 7.6 Hz, **b**-2H), 3.32 (t, *J* = 6.8 Hz, **a**-2H), 1.67-1.56 (m, **a**-2H and **b**-2H), 0.90 (t, *J* = 7.2 Hz, **b**-3H), 0.88 (t, *J* = 7.6 Hz, **a**-3H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 164.09-**b**, 160.99-**a**, 153.89-**b**, 153.79-**a**, 147.89-**a**, 147.71-**b**, 137.62-**b**, 137.55-**a**, 125.13-**b**, 120.12-**a**, 115.38-**b**, 115.14-**a**, 109.89-**b**, 109.72-**a**, 103.08-**b**, 103.02-**a**, 52.09-**a**, 46.28-**b**, 22.09-**a**, 20.73-**b**, 11.31-**b**, 10.75-**a**, ppm; HRMS (ESI) calcd for C₁₁H₁₅N₃O [M + H]⁺ 206.1293, found 206.1296.

5. Characterization Data for M

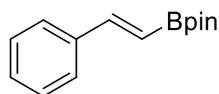
4',4',5',5'-tetramethyl-5-propyl-5a-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5,5a-dihydro-6 λ^4 ,7 λ^4 -spiro[benzo[4',5']imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-*a*]pyridine-6,2'-[1,3,2]dioxaborolane] (M)



N-propyl-*N*-(2-(pyridin-2-ylamino)phenyl)formamide **C6** (0.5 mmol), bis(pinacolato)diboron (1.2 equiv.) and THF (2 mL) in a 50 ml reaction tube was stirred for 12 h at room temperature. Then the reaction mixture was washed with ethyl acetate, and a yellow solid was collected and dried: (156 mg, 64%); mp = 119-120 °C; Recrystallization from dichloromethane/hexane in nitrogen atmosphere gave a yellow crystal suitable for X-ray crystallographic analysis; ¹H NMR (400 MHz, CDCl₃): δ 8.13 (d, *J* = 5.2 Hz, 1H), 7.59 (t, *J* = 8.4 Hz, 1H), 7.14 (t, *J* = 8.8 Hz, 2H), 6.91 (t, *J* = 8.8 Hz, 1H), 6.83 (t, *J* = 6.0 Hz, 1H), 6.51 (t, *J* = 6.8 Hz, 1H), 6.32 (d, *J* = 8.4 Hz, 1H), 3.27 (t, *J* = 8.4 Hz, 2H), 1.70-1.62 (m, 2H), 1.23 (s, 24H), 0.90 (t, *J* = 7.2 Hz, 3H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 159.86, 149.44, 141.66, 139.47, 135.58, 126.07, 117.37, 115.24, 114.47, 110.09, 105.33, 81.72, 48.75, 26.06, 25.83, 24.58, 22.30, 11.55, ¹¹B NMR (128 MHz, CDCl₃): δ 22.02, 20.89, ppm; HRMS (ESI) calcd for C₂₇H₄₀B₂N₃O₄ [M + H]⁺ 493.3283, found 493.3277.

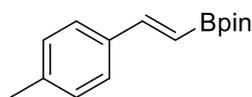
6. Characterization Data for Hydroborated Products

(*E*)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane (**2a**)³



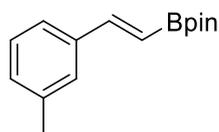
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (214mg, 93%); ¹H NMR (400 MHz, CDCl₃): δ 7.49 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 18.4 Hz, 1H), 7.38-7.27 (m, 3H), 6.17 (d, *J* = 18.4 Hz, 1H), 1.32 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 149.53, 137.49, 128.91, 128.58, 127.08, 83.37, 24.83, ppm.

(*E*)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane (**2b**)³



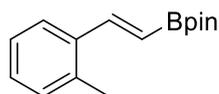
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (222 mg, 91%); ¹H NMR (400 MHz, CDCl₃): δ 7.40-7.35 (m, 3H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.11 (d, *J* = 18.4 Hz, 1H), 2.34 (s, 3H), 1.31 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 149.52, 138.95, 134.84, 129.32, 127.05, 83.27, 24.85, 21.35, ppm.

(*E*)-4,4,5,5-tetramethyl-2-(3-methylstyryl)-1,3,2-dioxaborolane (**2c**)³



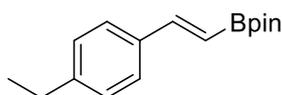
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (201 mg, 83%); ¹H NMR (400 MHz, CDCl₃): δ 7.37 (d, *J* = 18.4 Hz, 1H), 7.29 (d, *J* = 5.6 Hz, 2H), 7.23 (t, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 7.2 Hz, 1H), 6.15 (d, *J* = 18.4 Hz, 1H), 2.35 (s, 3H), 1.31 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 148.65, 137.06, 136.44, 128.68, 127.43, 126.76, 123.22, 82.29, 23.79, 20.37, ppm.

(*E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane (**2d**)⁴



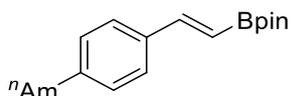
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (214mg, 88%); ¹H NMR (400 MHz, CDCl₃): δ 7.65 (d, *J* = 18.4 Hz, 1H), 7.57-7.55 (m, 1H), 7.20-7.14 (m, 3H), 6.09 (d, *J* = 18.4 Hz, 1H), 2.43 (s, 3H), 1.32 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 147.14, 136.72, 136.31, 130.41, 128.58, 126.12, 125.79, 83.31, 24.84, 19.84, ppm.

(E)-2-(4-ethylstyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2e)⁵



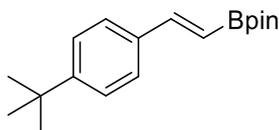
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (228 mg, 88%); ¹H NMR (400 MHz, CDCl₃): δ 7.43-7.37 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.12 (d, *J* = 18.4 Hz, 1H), 2.64 (q, *J* = 7.6 Hz, 2H), 1.32 (s, 12H), 1.23 (t, *J* = 7.6 Hz, 3H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 149.52, 145.31, 135.07, 128.11, 127.12, 83.28, 28.71, 24.83, 15.42, ppm.

(E)-4,4,5,5-tetramethyl-2-(4-pentylstyryl)-1,3,2-dioxaborolane (2f)⁶



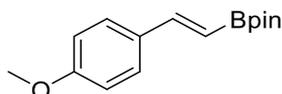
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (268 mg, 89%); ¹H NMR (400 MHz, CDCl₃): δ 7.41 (d, *J* = 7.6 Hz, 2H), 7.38 (s, 1H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.12 (d, *J* = 18.4 Hz, 1H), 2.60 (t, *J* = 8.0 Hz, 2H), 1.65-1.58 (m, 2H), 1.32 (s, 16H), 0.90 (t, *J* = 6.8 Hz, 3H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 149.57, 144.04, 135.05, 128.66, 127.05, 83.24, 35.78, 31.52, 31.03, 24.84, 22.57, 14.05, ppm.

(E)-2-(4-(tert-butyl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2g)⁷



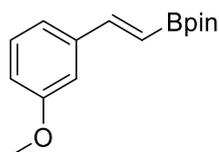
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a light yellow solid (257 mg, 90%); ¹H NMR (400 MHz, CDCl₃): δ 7.44-7.35 (m, 5H), 6.12 (d, *J* = 18.4 Hz, 1H), 1.31 (s, 21H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 152.11, 149.44, 134.84, 126.88, 125.53, 83.26, 34.71, 31.30, 24.87, ppm.

(E)-2-(4-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2h)³



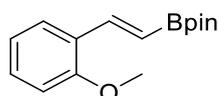
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (228 mg, 88%); ¹H NMR (400 MHz, CDCl₃): δ 7.41 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 18.4 Hz, 1H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.00 (d, *J* = 18.4 Hz, 1H), 3.75 (s, 3H), 1.29 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 160.32, 149.10, 130.36, 128.44, 113.97, 83.14, 55.15, 24.80, ppm.

(E)-2-(3-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2i)⁸



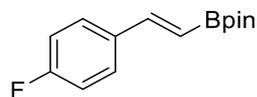
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (208 mg, 80%); ^1H NMR (400 MHz, CDCl_3): δ 7.37 (d, $J = 18.4$ Hz, 1H), 7.25 (t, $J = 8.0$ Hz, 1H), 7.08 (d, $J = 7.6$ Hz, 1H), 7.03 (s, 1H), 6.84 (dd, $J = 8.4$ Hz, $J = 2.4$ Hz, 1H), 6.16 (d, $J = 18.4$ Hz, 1H), 3.80 (s, 3H), 1.31 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 159.79, 149.39, 138.95, 129.55, 119.83, 114.81, 111.96, 83.38, 55.17, 24.83, ppm.

(E)-2-(2-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2j)⁸



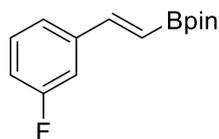
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (223 mg, 86%); ^1H NMR (400 MHz, CDCl_3): δ 7.77 (d, $J = 18.4$ Hz, 1H), 7.55 (d, $J = 7.6$ Hz, 1H), 7.29-7.24 (m, 1H), 6.93 (t, $J = 7.2$ Hz, 1H), 6.86 (d, $J = 8.4$ Hz, 1H), 6.17 (d, $J = 18.4$ Hz, 1H), 3.85 (s, 3H), 1.31 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 157.35, 144.10, 129.98, 127.10, 126.60, 120.57, 110.88, 83.22, 55.36, 24.84, ppm.

(E)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2k)³



Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (235 mg, 95%); ^1H NMR (400 MHz, CDCl_3): δ 7.45 (dd, $J = 8.8$ Hz, $J = 5.6$ Hz, 2H), 7.34 (d, $J = 18.8$ Hz, 1H), 7.02 (t, $J = 8.8$ Hz, 2H), 6.07 (d, $J = 18.4$ Hz, 1H), 1.31 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 163.2 (d, $J = 247.0$ Hz), 148.17, 133.75, 128.72 (d, $J = 8.0$ Hz), 115.57 (d, $J = 21.0$ Hz), 83.41, 24.82, ppm; ^{19}F NMR (376 MHz, CDCl_3): δ -112.41, ppm.

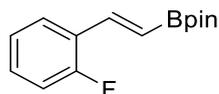
(E)-2-(3-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2l)⁹



Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (212 mg, 85%); ^1H NMR (400 MHz, CDCl_3): δ 7.40 (d, $J = 18.4$ Hz, 1H), 7.32-7.24 (m, 2H), 7.19 (d, $J = 10.0$ Hz, 1H), 6.99 (t, $J = 7.6$ Hz, 1H), 6.19 (d, $J = 18.4$ Hz, 1H), 1.33 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 163.05 (d, $J = 244.0$ Hz), 147.99 (d, $J = 2.0$ Hz), 139.88 (d, $J = 8.0$ Hz), 129.99 (d, $J = 8.0$ Hz), 122.96 (d, $J = 3.0$ Hz), 115.60 (d, $J = 22.0$ Hz), 113.22 (d, $J = 21.0$ Hz), 83.37, 24.74, ppm.

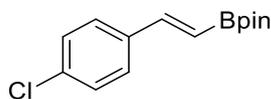
ppm; ^{19}F NMR (376 MHz, CDCl_3): δ -113.22, ppm.

(E)-2-(2-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2m)³



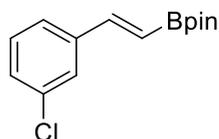
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (220 mg, 89%); ^1H NMR (400 MHz, CDCl_3): δ 7.61-7.54 (m, 2H), 7.28-7.23 (m, 1H), 7.11 (t, J = 7.2 Hz, 1H), 7.03 (t, J = 8.0 Hz, 1H), 6.24 (d, J = 18.8 Hz, 1H), 1.31 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 160.73 (d, J = 250.0 Hz), 141.32 (d, J = 4.0 Hz), 130.19 (d, J = 9.0 Hz), 127.41 (d, J = 3.0 Hz), 125.40 (d, J = 12.0 Hz), 124.11 (d, J = 4.0 Hz), 115.83 (d, J = 22.0 Hz), 83.46, 24.82, ppm; ^{19}F NMR (376 MHz, CDCl_3): δ -117.65, ppm.

(E)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2n)³



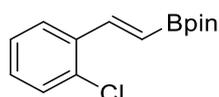
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a white solid (244 mg, 92%); ^1H NMR (400 MHz, CDCl_3): δ 7.40 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 18.4 Hz, 1H), 7.30 (d, J = 8.4 Hz, 2H), 6.13 (d, J = 18.4 Hz, 1H), 1.31 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 148.03, 135.98, 134.62, 128.81, 128.24, 83.47, 24.82, ppm.

(E)-2-(3-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2o)¹⁰



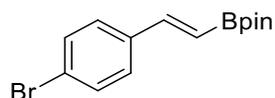
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (213 mg, 81%); ^1H NMR (400 MHz, CDCl_3): δ 7.35 (s, 1H), 7.24-7.14 (m, 4H), 6.04 (d, J = 18.4 Hz, 1H), 1.21 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 147.77, 139.36, 134.56, 129.79, 128.71, 126.90, 125.17, 83.40, 24.79, ppm.

(E)-2-(2-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2p)¹¹



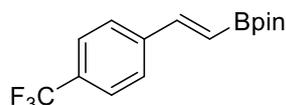
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (226 mg, 85%); ^1H NMR (400 MHz, CDCl_3): δ 7.70 (d, J = 18.4 Hz, 1H), 7.55 (dd, J = 7.2 Hz, J = 2.0 Hz, 1H), 7.27 (dd, J = 7.6 Hz, J = 1.6 Hz, 1H), 7.18-7.11 (m, 2H), 6.09 (d, J = 18.0 Hz, 1H), 1.24 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 144.97, 135.63, 133.86, 129.80, 129.68, 127.03, 126.86, 83.50, 24.83, ppm.

(E)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2q)³



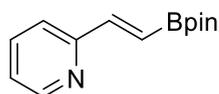
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a white solid (263 mg, 85%); ¹H NMR (400 MHz, CDCl₃): δ 7.46 (d, *J* = 8.4 Hz, 2H), 7.35-7.29 (m, 3H), 6.15 (d, *J* = 18.4 Hz, 1H), 1.31 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 148.08, 136.41, 131.77, 128.52, 122.91, 83.49, 24.82, ppm.

(E)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane (2r)³



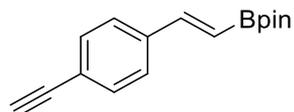
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (273 mg, 92%); ¹H NMR (400 MHz, CDCl₃): δ 7.58 (dd, *J* = 8.4 Hz, *J* = 8.4 Hz, 4H), 7.40 (d, *J* = 18.4 Hz, 1H), 6.26 (d, *J* = 18.4 Hz, 1H), 1.32 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 147.68, 140.80, 130.47 (d, *J* = 32.0 Hz), 127.16, 125.53 (q, *J* = 4.0 Hz), 122.79-122.67 (m), 83.62, 24.82, ppm; ¹⁹F NMR (376 MHz, CDCl₃): δ -62.64, ppm.

(E)-2-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)pyridine (2s)^{9, 12}



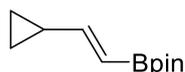
Purification by flash chromatography (petroleum ether:EtOAc = 20:1): a colorless oil (194 mg, 84%); ¹H NMR (400 MHz, CDCl₃): δ 8.59 (d, *J* = 4.4 Hz, 1H), 7.64 (t, *J* = 18.4 Hz, 1H), 7.45 (d, *J* = 18.4 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 4.8 Hz, 1H), 6.62 (d, *J* = 18.4 Hz, 1H), 1.30 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 155.44, 149.72, 148.75, 136.48, 123.08, 122.23, 83.48, 24.80, ppm.

(E)-2-(4-ethynylstyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2t)¹³



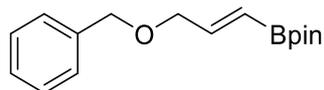
Purification by flash chromatography (petroleum ether:EtOAc = 20:1): a white solid (187 mg, 74%); ¹H NMR (400 MHz, CDCl₃): δ 7.42 (dd, *J* = 11.6 Hz, *J* = 8.8 Hz, 4H), 7.35 (d, *J* = 18.4 Hz, 1H), 6.16 (d, *J* = 18.4 Hz, 1H), 3.12 (s, 1H), 1.28 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 148.40, 137.81, 132.35, 126.90, 122.45, 83.57, 83.40, 78.47, 24.81, ppm.

(E)-2-(2-cyclopropylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2u)⁸



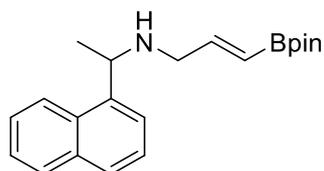
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (165 mg, 91%); ^1H NMR (400 MHz, CDCl_3): δ 6.04 (dd, $J = 18.0$ Hz, $J = 9.6$ Hz, 1H), 5.46 (d, $J = 17.6$ Hz, 1H), 1.53-1.45 (m, 1H), 1.23 (s, 12H), 0.77 (dd, $J = 13.6$ Hz, $J = 4.0$ Hz, 2H), 0.51 (dd, $J = 10.8$ Hz, $J = 4.4$ Hz, 2H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 158.53, 82.89, 24.74, 17.00, 7.87, ppm.

(E)-2-(3-(benzyloxy)prop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2v)¹⁴



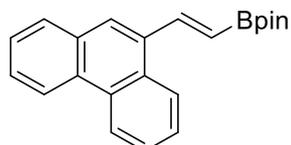
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (215 mg, 78%); ^1H NMR (400 MHz, CDCl_3): δ 7.35-7.26 (m, 5H), 6.68 (dt, $J = 18.0$ Hz, $J = 4.8$ Hz, 1H), 5.76 (d, $J = 18.4$ Hz, 1H), 4.54 (s, 2H), 4.11 (d, $J = 4.8$ Hz, 2H), 1.27 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 149.16, 138.29, 128.36, 127.62, 127.57, 83.29, 72.33, 71.70, 24.79, ppm.

N-(1-(naphthalen-1-yl)ethyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)prop-2-en-1-amine (2w)⁸



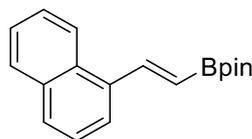
Purification by flash chromatography (petroleum ether:EtOAc = 5:1): a colorless oil (261 mg, 77%); ^1H NMR (400 MHz, CDCl_3): δ 8.18 (d, $J = 8.0$ Hz, 1H), 7.86 (d, $J = 7.6$ Hz, 1H), 7.74 (d, $J = 8.4$ Hz, 1H), 7.67 (d, $J = 6.8$ Hz, 1H), 7.52-7.45 (m, 3H), 6.72 (dt, $J = 18.4$ Hz, $J = 5.2$ Hz, 1H), 5.63 (d, $J = 18.0$ Hz, 1H), 4.67 (q, $J = 6.4$ Hz, 1H), 3.35-3.25 (m, 2H), 1.70 (s, 1H), 1.49 (d, $J = 6.8$ Hz, 3H), 1.27 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 151.93, 141.00, 133.99, 131.34, 128.95, 127.20, 125.74, 125.29, 123.01, 122.78, 83.19, 53.08, 51.41, 24.80, 24.79, 23.68, ppm.

(E)-4,4,5,5-tetramethyl-2-(2-(phenanthren-9-yl)vinyl)-1,3,2-dioxaborolane (2x)¹⁵



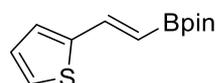
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (261 mg, 79%); ^1H NMR (400 MHz, CDCl_3): δ 8.72 (d, $J = 8.4$ Hz, 1H), 8.65 (d, $J = 8.0$ Hz, 1H), 8.28 (d, $J = 7.6$ Hz, 1H), 8.20 (d, $J = 18.4$ Hz, 1H), 7.95 (s, 1H), 7.89 (d, $J = 7.6$ Hz, 1H), 7.69-7.56 (m, 4H), 6.34 (d, $J = 18.0$ Hz, 1H), 1.37 (s, 12H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 147.21, 134.61, 131.64, 130.62, 130.34, 130.29, 129.05, 126.90, 126.78, 126.67, 126.53, 125.37, 124.70, 123.04, 122.52, 83.49, 24.91, ppm.

(E)-4,4,5,5-tetramethyl-2-(2-(naphthalen-1-yl)vinyl)-1,3,2-dioxaborolane (2y)¹²



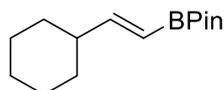
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (238 mg, 85%); ¹H NMR (400 MHz, CDCl₃): δ 8.26 (d, *J* = 8.4 Hz, 1H), 8.21 (d, *J* = 18.4 Hz, 1H), 7.85-7.79 (m, 2H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.53-7.54 (m, 3H), 6.26 (d, *J* = 18.4 Hz, 1H), 1.34 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 146.48, 135.39, 133.65, 131.14, 129.06, 128.53, 126.20, 125.83, 125.62, 124.11, 123.81, 83.45, 24.91, ppm.

(E)-4,4,5,5-tetramethyl-2-(2-(thiophen-2-yl)vinyl)-1,3,2-dioxaborolane (2z)⁸



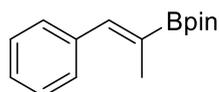
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a yellow oil (128 mg, 54%); ¹H NMR (400 MHz, CDCl₃): δ 7.47 (d, *J* = 18.0 Hz, 1H), 7.24 (d, *J* = 5.2 Hz, 1H), 7.08 (d, *J* = 3.2 Hz, 1H), 6.98 (dd, *J* = 5.2 Hz, *J* = 3.6 Hz, 1H), 5.91 (d, *J* = 18.0 Hz, 1H), 1.30 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 143.97, 141.83, 127.72, 127.64, 126.32, 83.40, 24.82, ppm.

(E)-2-(2-(cyclohexyl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2aa)¹¹



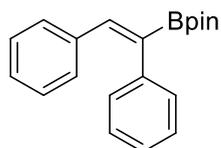
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (210 mg, 89%); ¹H NMR (400 MHz, CDCl₃): δ 6.58 (dd, *J* = 18.4 Hz, *J* = 6.4 Hz, 1H), 5.38 (dd, *J* = 18.0 Hz, *J* = 1.6 Hz, 1H), 2.04-2.00 (m, 1H), 1.76-1.70 (m, 4H), 1.67-1.62 (m, 1H), 1.27 (s, 12H), 1.25-1.04 (m, 5H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 159.88, 82.99, 43.26, 31.93, 26.18, 25.98, 24.80, ppm.

(Z)-4,4,5,5-tetramethyl-2-(1-phenylprop-1-en-2-yl)-1,3,2-dioxaborolane (2bb)⁷



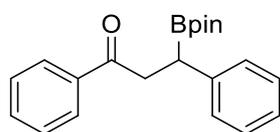
Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (185 mg, 76%); ¹H NMR (400 MHz, CDCl₃): δ 7.40-7.32 (m, 4H), 7.26-7.22 (m, 2H), 1.99 (s, 3H), 1.32 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 141.34, 136.92, 128.39, 127.01, 126.06, 82.49, 23.83, 14.87, ppm.

(Z)-2-(1,2-diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2cc)¹⁶



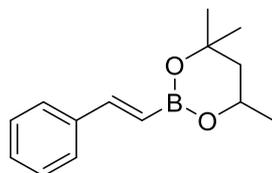
Purification by flash chromatography (petroleum ether: EtOAc = 50:1): a white solid (162 mg, 53%); ¹H NMR (400 MHz, CDCl₃): δ 7.36 (s, 1H), 7.28-7.24 (m, 2H), 7.22-7.20 (m, 1H), 7.18-7.15 (m, 2H), 7.12-7.10 (m, 3H), 7.07-7.04 (m, 2H), 1.31 (s, 12H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 143.20, 140.47, 137.02, 129.98, 128.88, 128.27, 127.87, 127.61, 126.28, 83.82, 24.82, ppm.

1,3-diphenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propan-1-one (2dd)¹⁷



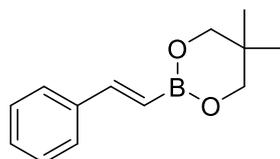
Purification by flash chromatography (petroleum ether: EtOAc = 10:1): a white solid (289 mg, 86%); ¹H NMR (400 MHz, CDCl₃): δ 7.96 (d, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.32-7.24 (m, 4H), 7.16 (t, *J* = 5.4 Hz, 1H), 3.59-3.39 (m, 2H), 2.82-2.76 (m, 1H), 1.24 (s, 6H), 1.16 (s, 6H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 199.70, 141.98, 136.82, 132.94, 128.54, 128.51, 128.41, 128.07, 125.62, 83.40, 43.29, 24.60, 24.56, ppm.

(E)-4,4,6-trimethyl-2-styryl-1,3,2-dioxaborinane (2ee)¹⁸



Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (217 mg, 94%); ¹H NMR (400 MHz, CDCl₃): δ 7.40 (d, *J* = 7.2 Hz, 2H), 7.25-7.14 (m, 4H), 6.03 (d, *J* = 18.4 Hz, 1H), 4.23-4.15 (m, 1H), 1.73 (dd, *J* = 14.0 Hz, *J* = 2.8 Hz, 1H), 1.47 (t, *J* = 13.6 Hz, 1H), 1.27-1.23 (m, 9H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 145.45, 136.98, 127.41, 127.25, 125.92, 69.85, 63.80, 44.98, 30.25, 27.13, 22.17, ppm.

(E)-5,5-dimethyl-2-styryl-1,3,2-dioxaborinane (2ff)¹⁹

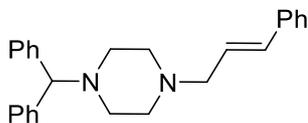


Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (189 mg, 88%); ¹H NMR (400 MHz, CDCl₃): δ 7.49 (d, *J* = 7.6 Hz, 2H), 7.39-7.22 (m, 4H), 6.14 (d, *J* =

18.0 Hz, 1H), 3.66 (s, 4H), 0.96 (s, 6H), ppm; ^{13}C NMR (100 MHz, CDCl_3): δ 146.04, 136.74, 127.45, 125.90, 119.86 (br), 71.01, 30.68, 20.74, ppm.

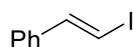
7. Characterization Data for Functionalized Products

Cinnarizine (3a)



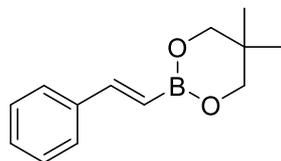
3a was synthesized by previously reported methods.²⁰ A mixture of **2a** (1 mmol), NaIO₄ (3 mmol) and 2N HCl (1 mL) in THF (4 mL) and H₂O (1 mL) was combined under air. The reaction mixture was stirred at room temperature for 12 h. Then the reaction mixture was extracted with saturated saline and ethyl acetate. The organic liquid layer was collected for rotary evaporation to obtain a white solid boric acid crude product. Without purification, it was directly mixed with 1-benzhydrylpiperazine (1 mmol) and paraformaldehyde (1 mmol), heated to 90 °C in 1,2-dioxane and stirred for 24 h. Purification by flash chromatography (petroleum ether:EtOAc = 5:1): a white solid (287 mg, 78%); ¹H NMR (400 MHz, CDCl₃): δ 7.40 (d, *J* = 7.2 Hz, 4H), 7.34 (d, *J* = 7.2 Hz, 2H), 7.29-7.21 (m, 7H), 7.19-7.15 (m, 2H), 6.49 (d, *J* = 15.6 Hz, 1H), 6.30-6.22 (m, 1H), 4.23 (s, 1H), 3.15 (d, *J* = 6.8 Hz, 2H), 2.53 (s, 8H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 142.80, 137.03, 133.04, 128.60, 128.50, 128.00, 127.49, 126.94, 126.68, 126.36, 76.24, 61.10, 53.53, 51.93, ppm.

(*E*)-(2-iodovinyl)benzene (3b)



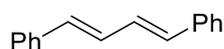
3b was synthesized by previously reported methods.²¹ A mixture of **2a** (1 mmol), I₂ (2 mmol) and NaOH (3 mmol) in THF (4 mL) was combined under air. The reaction mixture was stirred at room temperature for 2 h. Purification by flash chromatography (petroleum ether): a yellow oil (216 mg, 94%); ¹H NMR (400 MHz, CDCl₃): δ 7.43 (d, *J* = 14.8 Hz, 1H), 7.35-7.28 (m, 5H), 6.83 (d, *J* = 14.8 Hz, 1H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 145.03, 137.72, 128.74, 128.40, 126.02, 76.63, ppm.

(*E*)-5,5-dimethyl-2-styryl-1,3,2-dioxaborinane (2ff)



2ff was synthesized by previously reported methods.²² A mixture of **2a** (1 mmol) and B₂nep₂ (2 mmol) in MeOH (2 mL) was combined in sealed tube. The reaction mixture was stirred at 90 °C for 16 h. Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a colorless oil (140 mg, 65%).

(1*E*,3*E*)-1,4-diphenylbuta-1,3-diene (3c)



3c was synthesized by previously reported methods.²³ A mixture of **2a** (1 mmol) and Cu(OAc)₂ (1 mmol) in DMF (2 mL) and EtOH (1 mL) was combined under air. The reaction mixture was stirred at room temperature for 16 h. Purification by flash chromatography (petroleum ether:EtOAc = 50:1): a white solid (91 mg, 44%); ¹H NMR (400 MHz, CDCl₃): δ 7.44 (d, *J* = 7.2 Hz, 4H), 7.33 (t, *J* = 7.6 Hz, 4H), 7.23 (t, *J* = 7.6 Hz, 2H), 6.98-6.92 (m, 2H), 6.71-6.64 (m, 2H), ppm; ¹³C NMR (100 MHz, CDCl₃): δ 137.40, 132.85, 129.28, 128.69, 127.59, 126.41, ppm.

8. References

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9. NMR Spectra for Catalysts

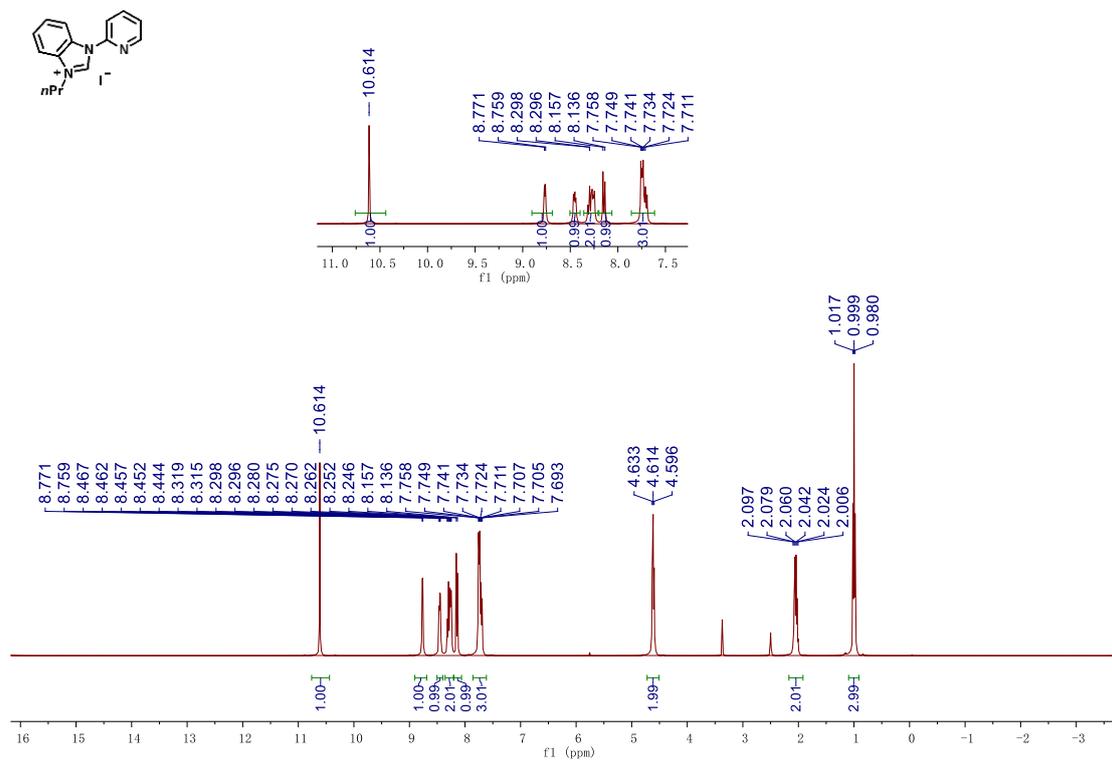


Figure S1. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound C5.

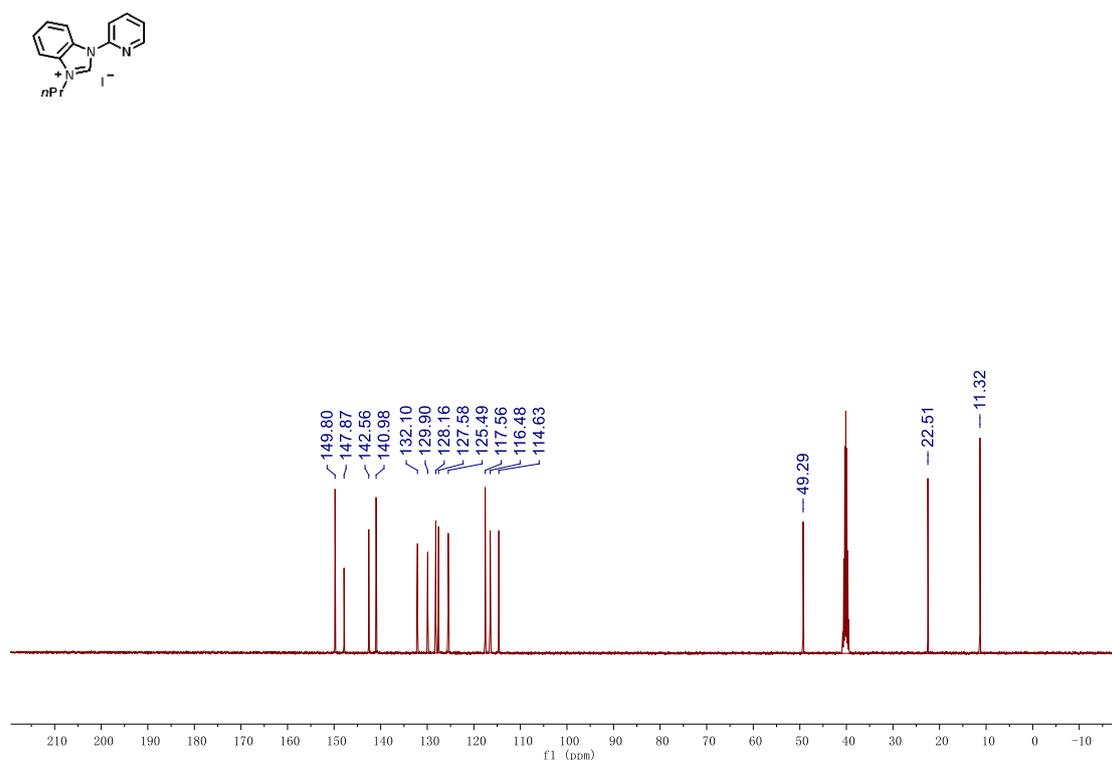


Figure S2. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of compound C5.

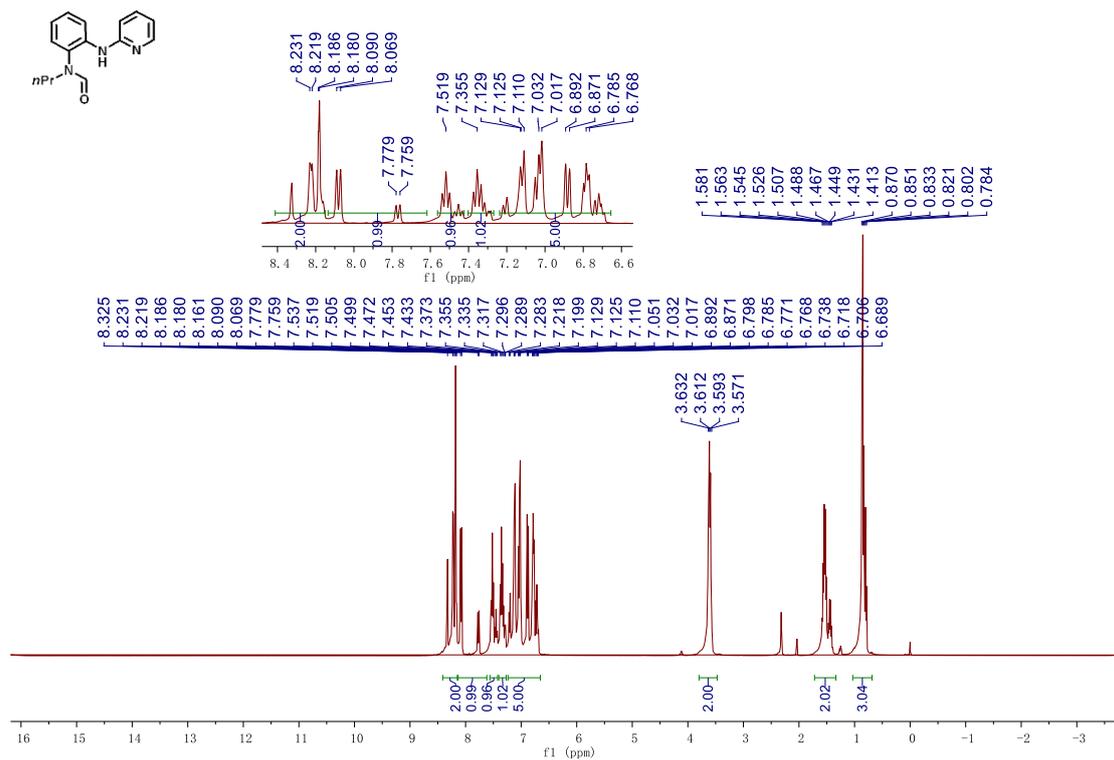


Figure S3. ¹H NMR (400 MHz, CDCl₃) spectrum of compound C6.

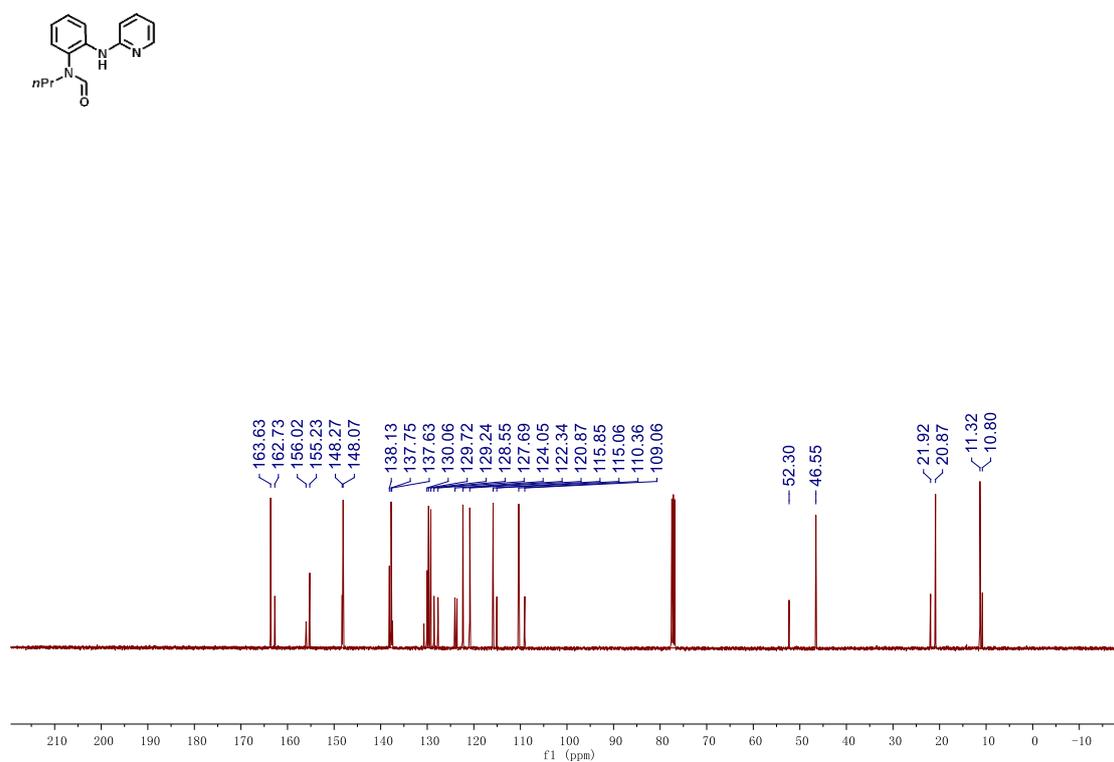


Figure S4. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound C6.

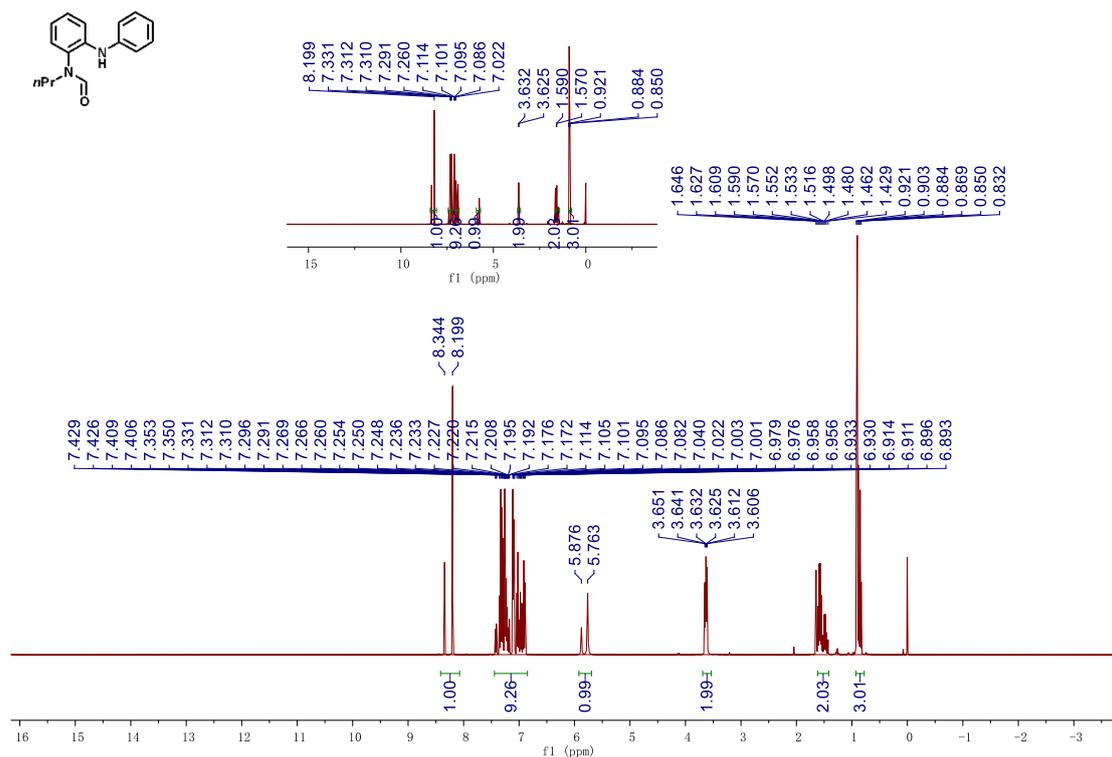


Figure S5. ^1H NMR (400 MHz, CDCl_3) spectrum of compound C7.

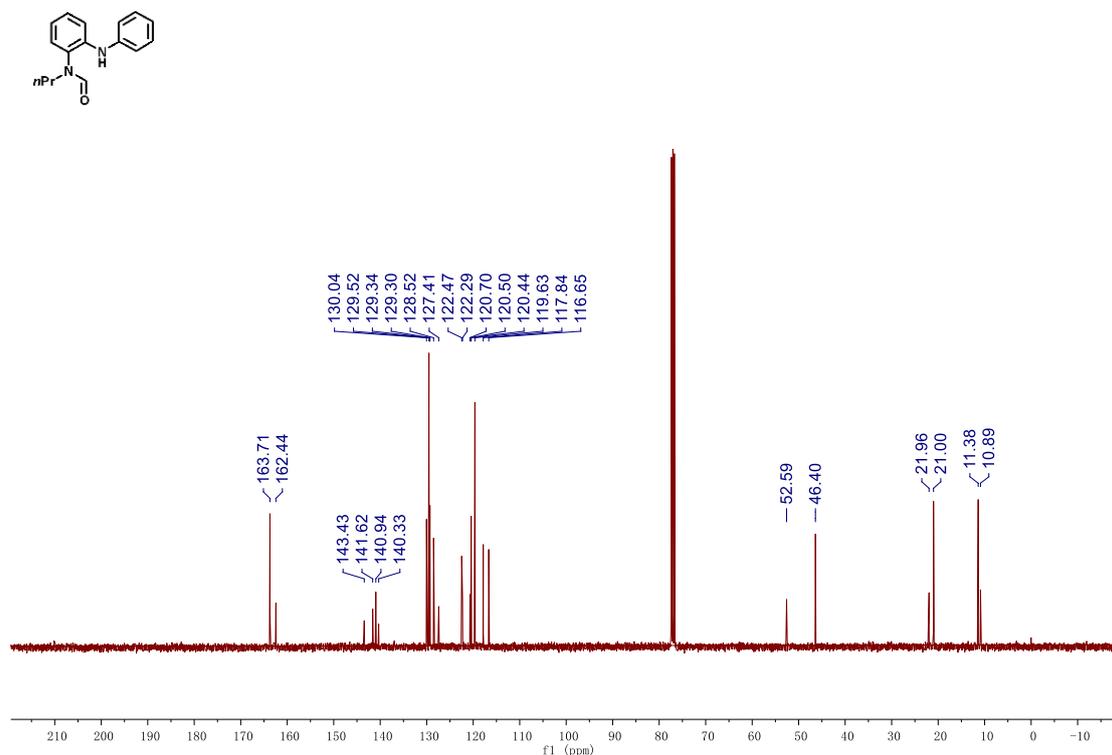


Figure S6. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound C7.

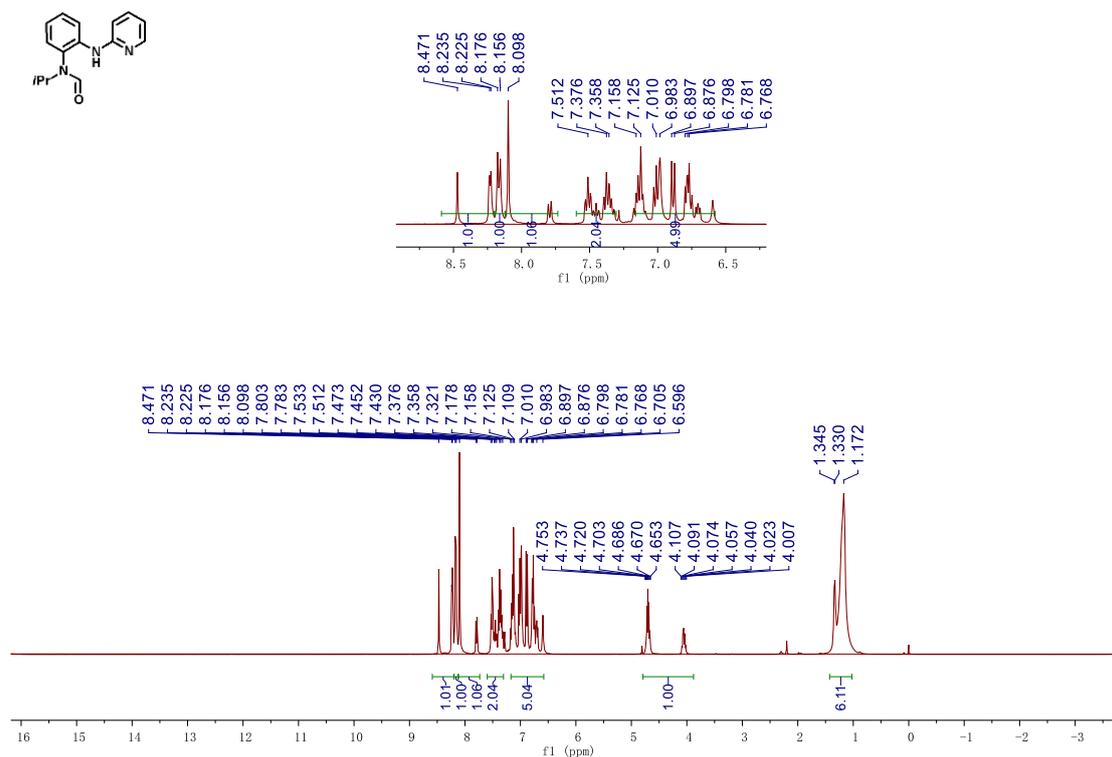


Figure S7. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **C8**.

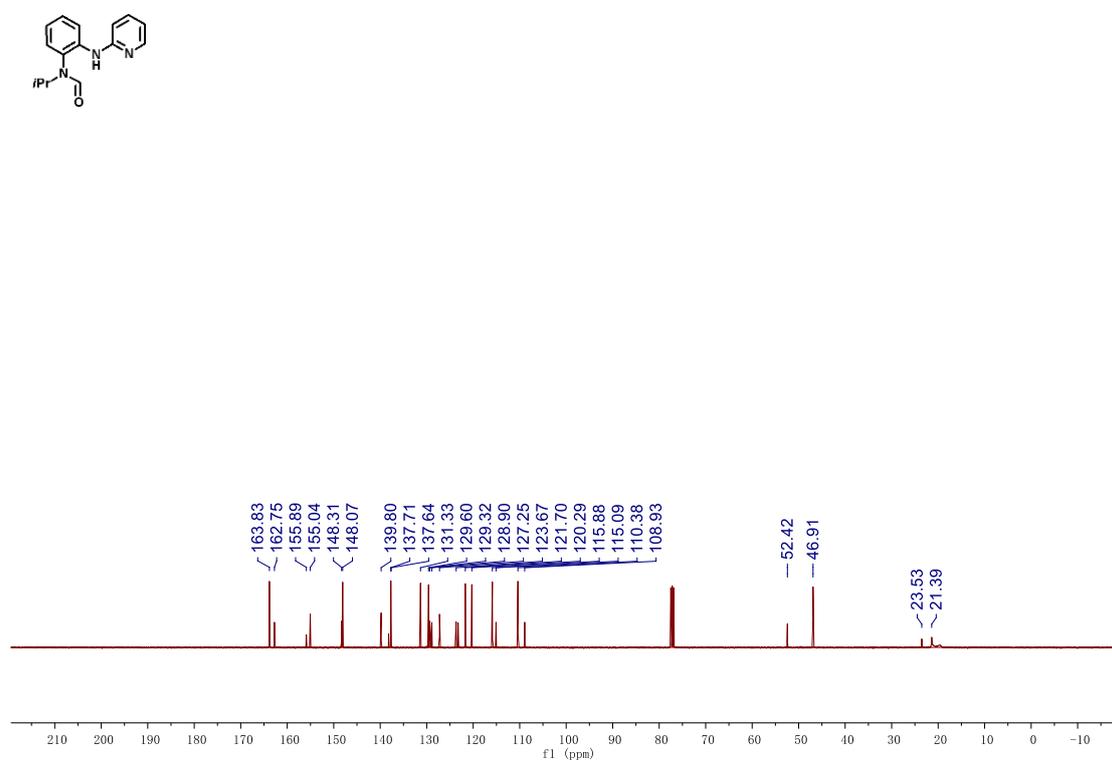


Figure S8. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **C8**.

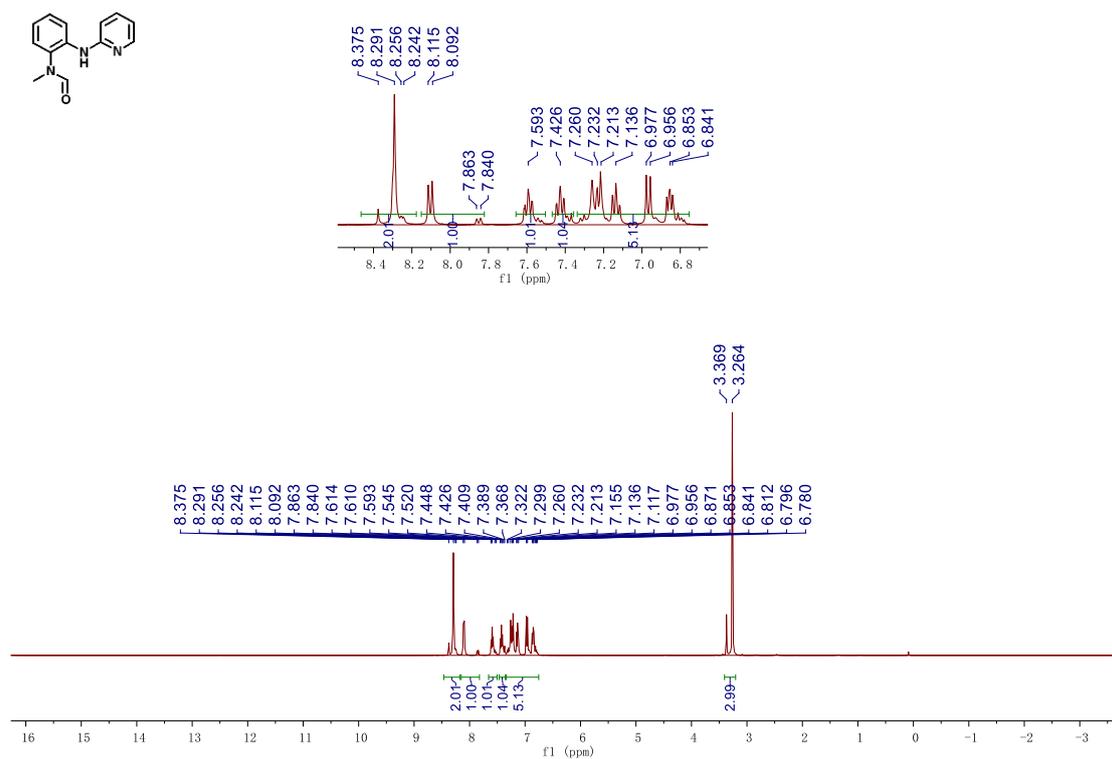


Figure S9. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **C9**.

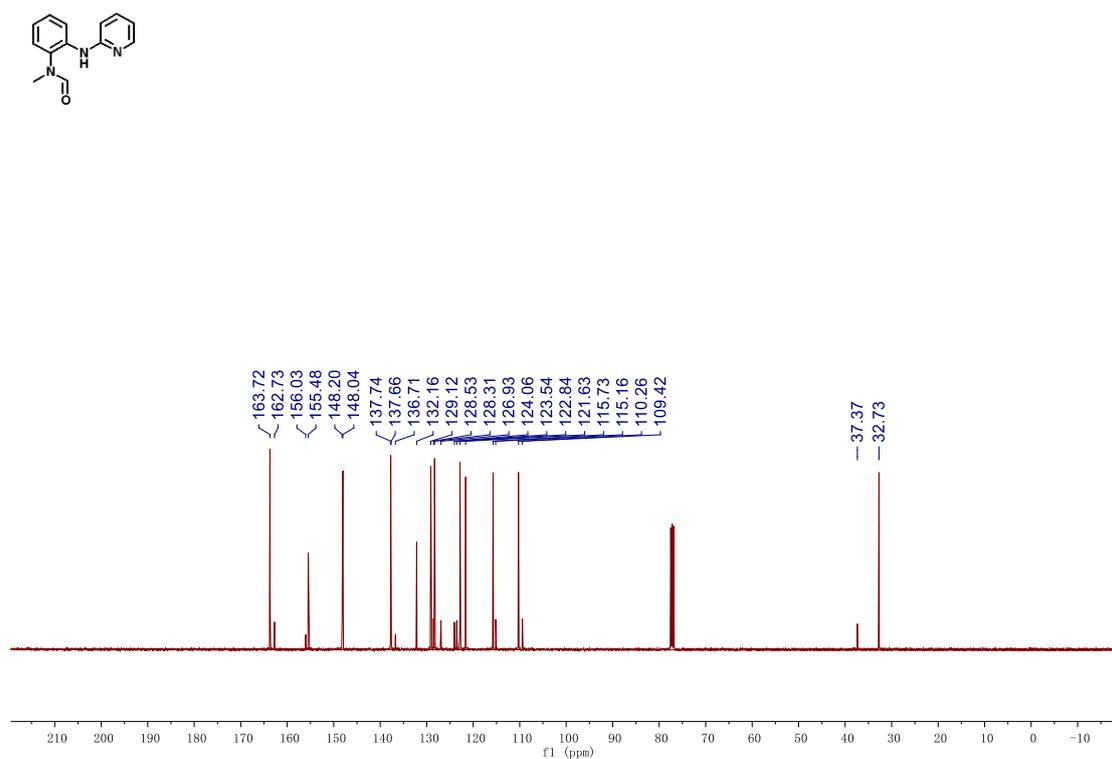


Figure S10. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **C9**.

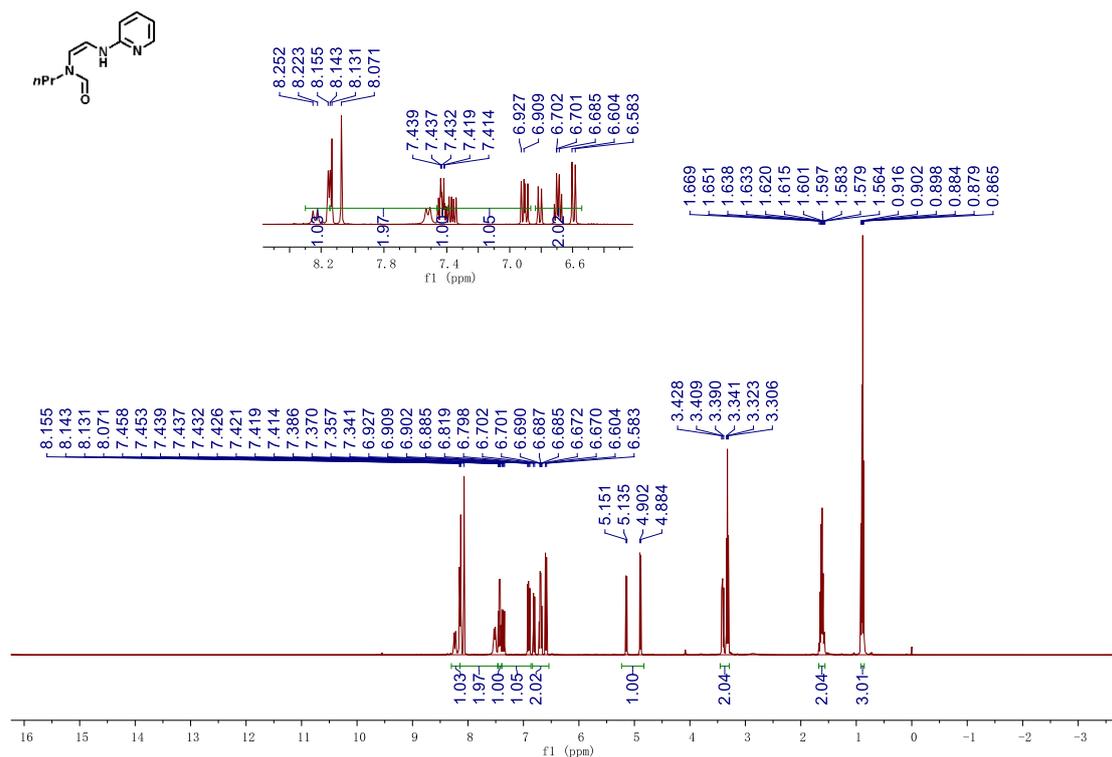


Figure S11. ¹H NMR (400 MHz, CDCl₃) spectrum of compound C10.

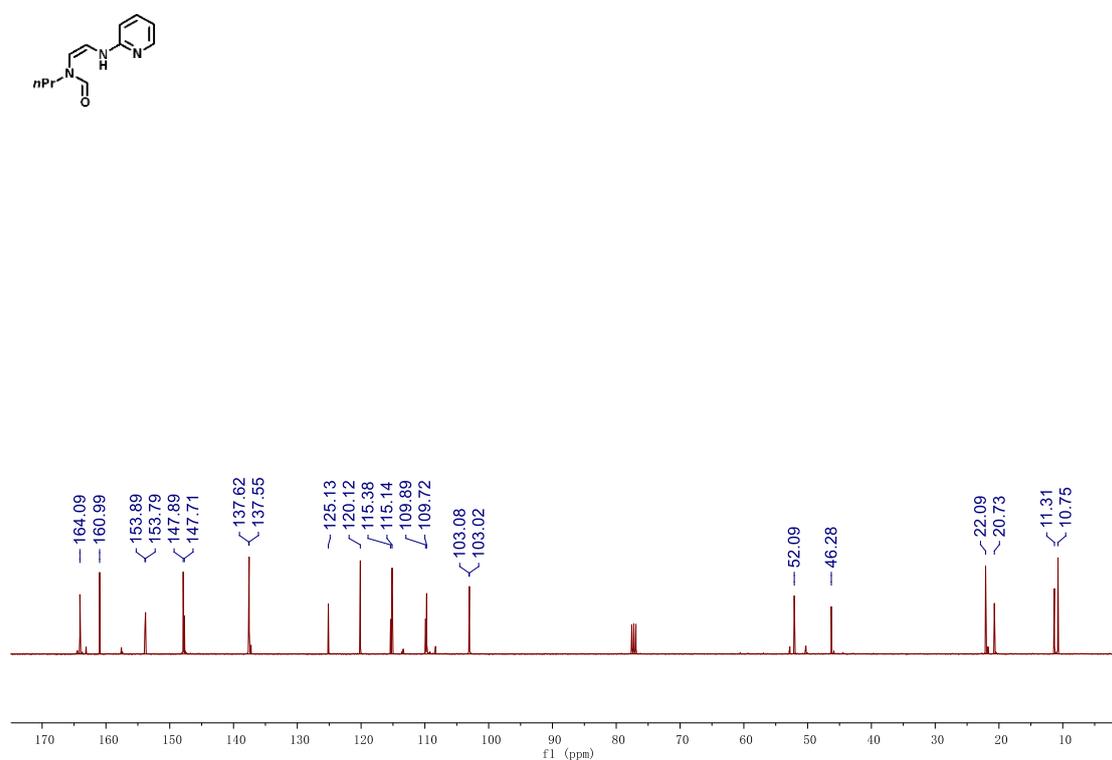


Figure S12. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound C10.

10. NMR Spectra for M

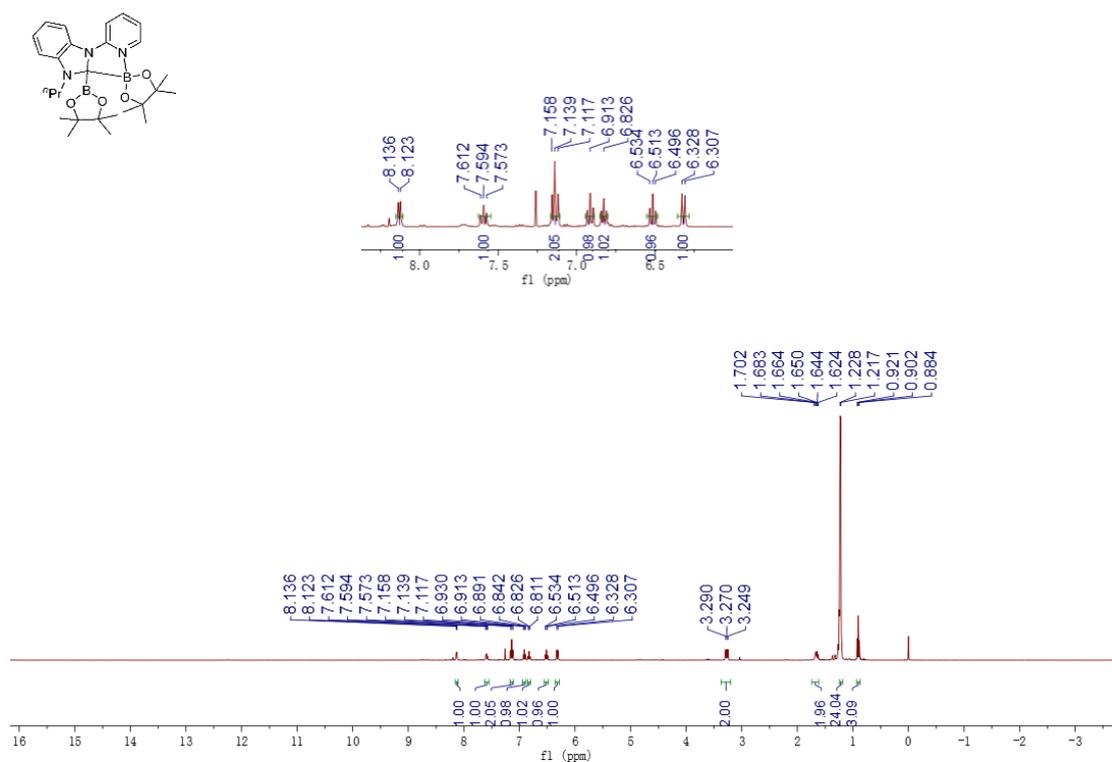


Figure S13. ¹H NMR (400 MHz, CDCl₃) spectrum of compound M.

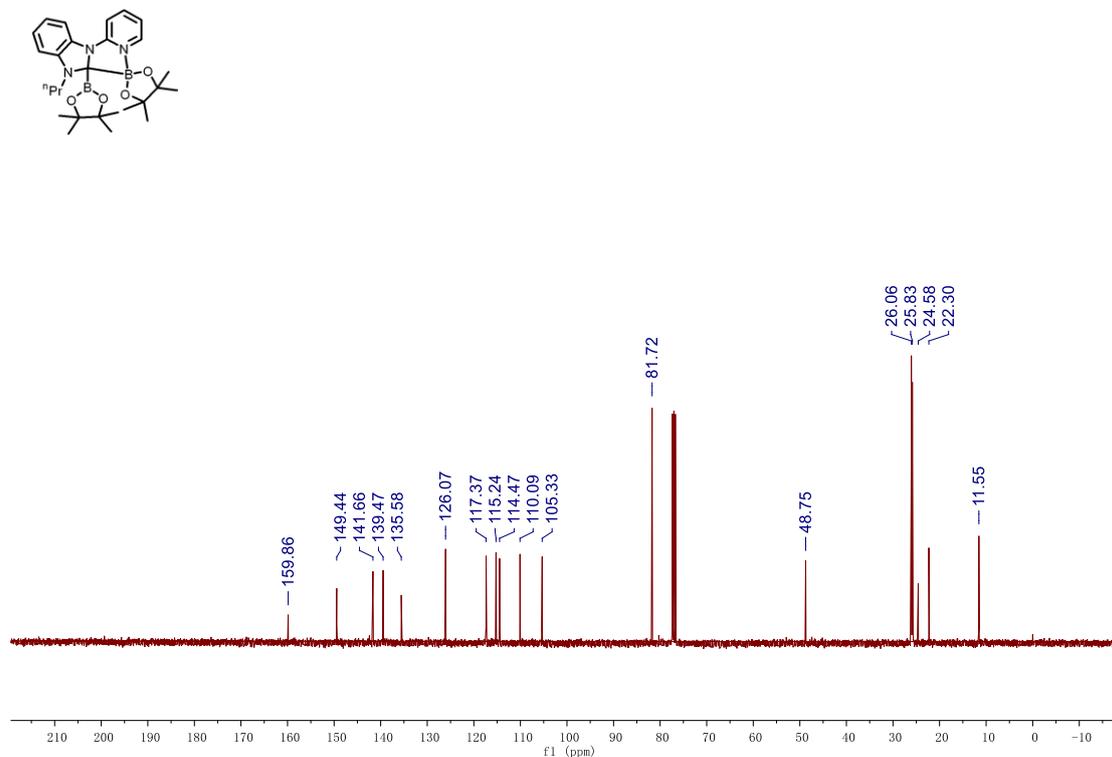


Figure S14. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound M.

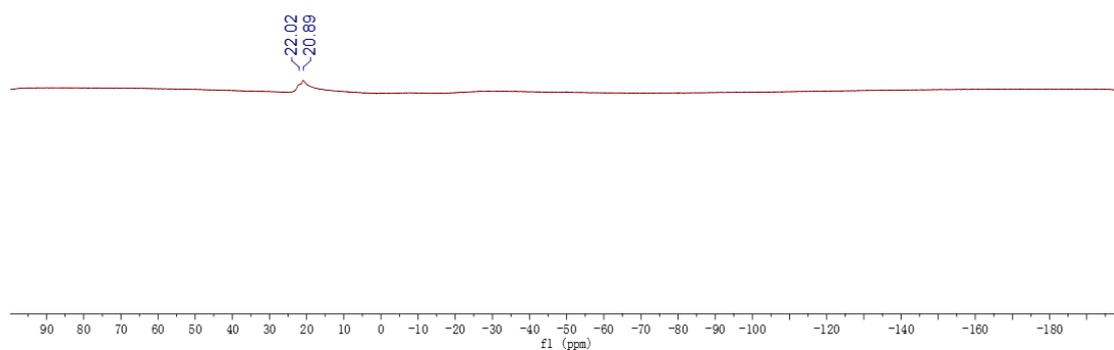
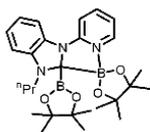


Figure S15. ^{11}B NMR (128 MHz, CDCl_3) spectrum of compound **M**.

11. NMR Spectra for Hydroborated Products

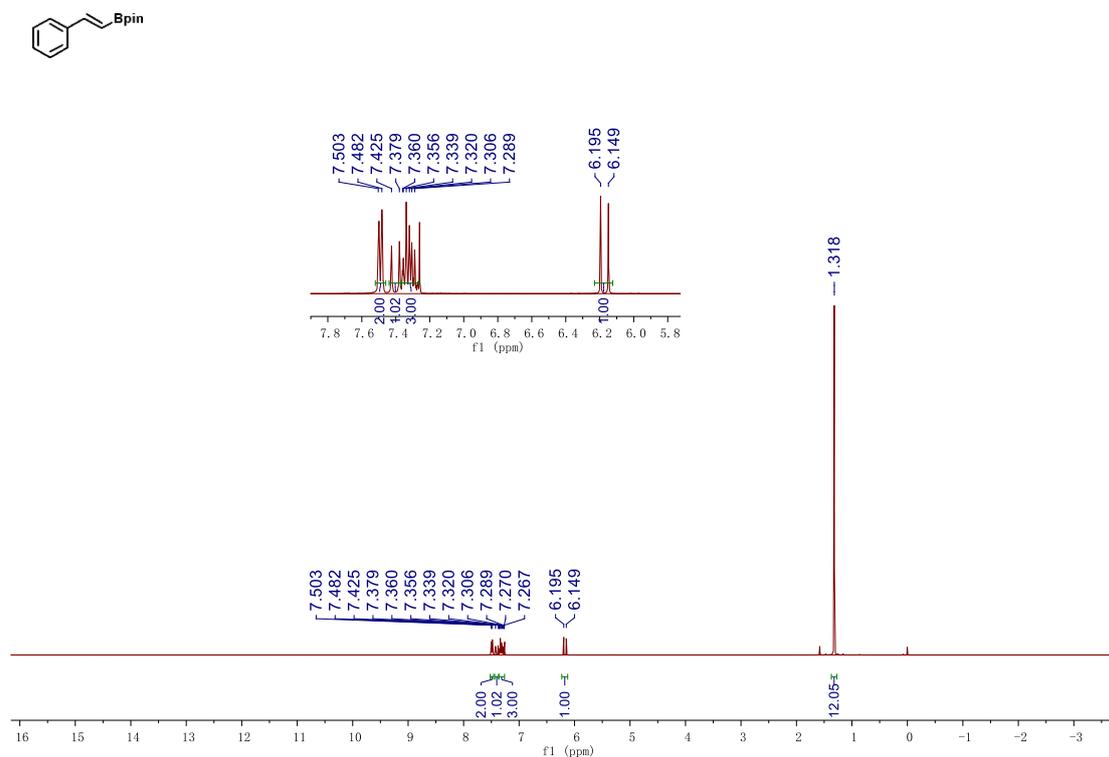


Figure S16. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 2a.

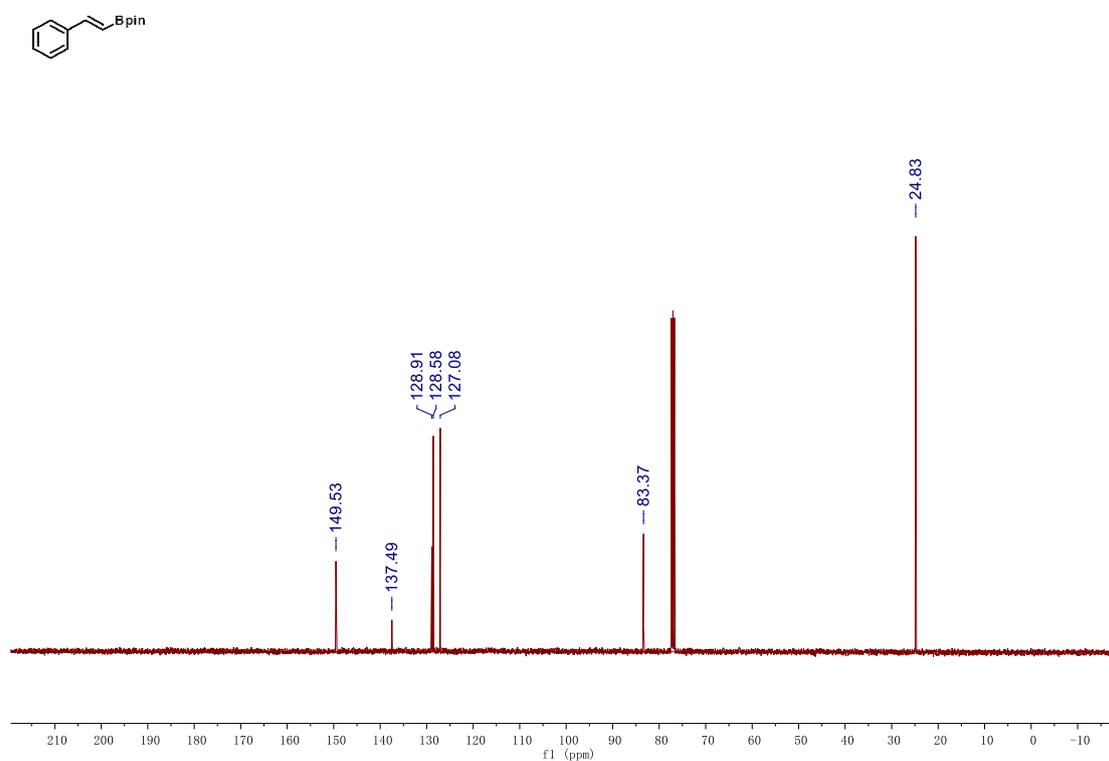


Figure S17. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 2a.

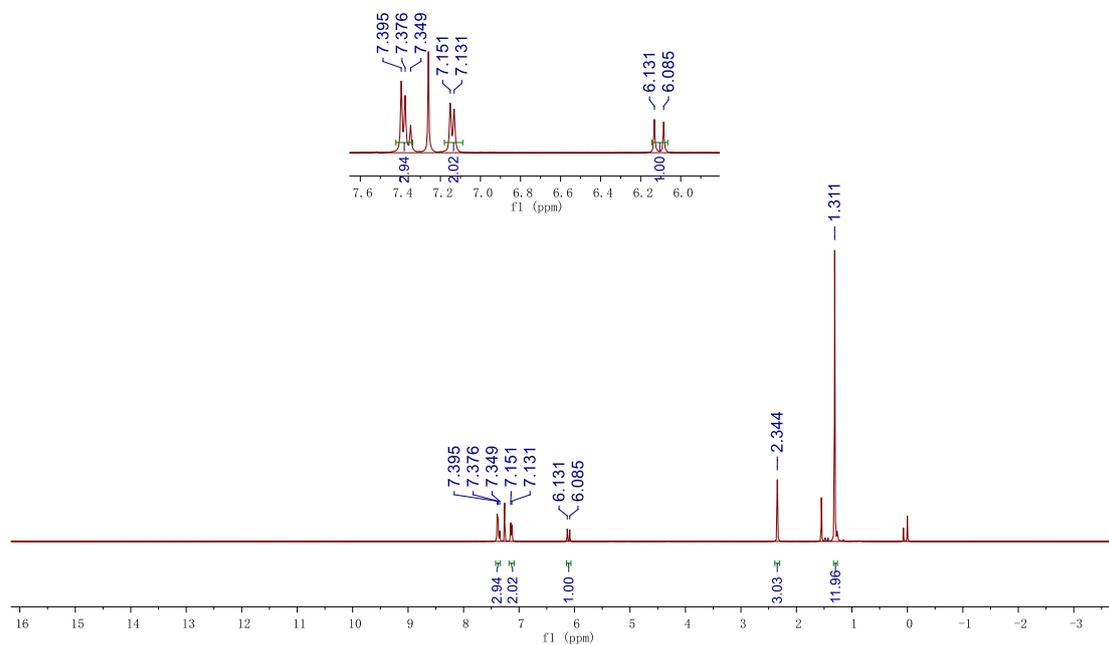
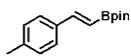


Figure S18. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2b**.

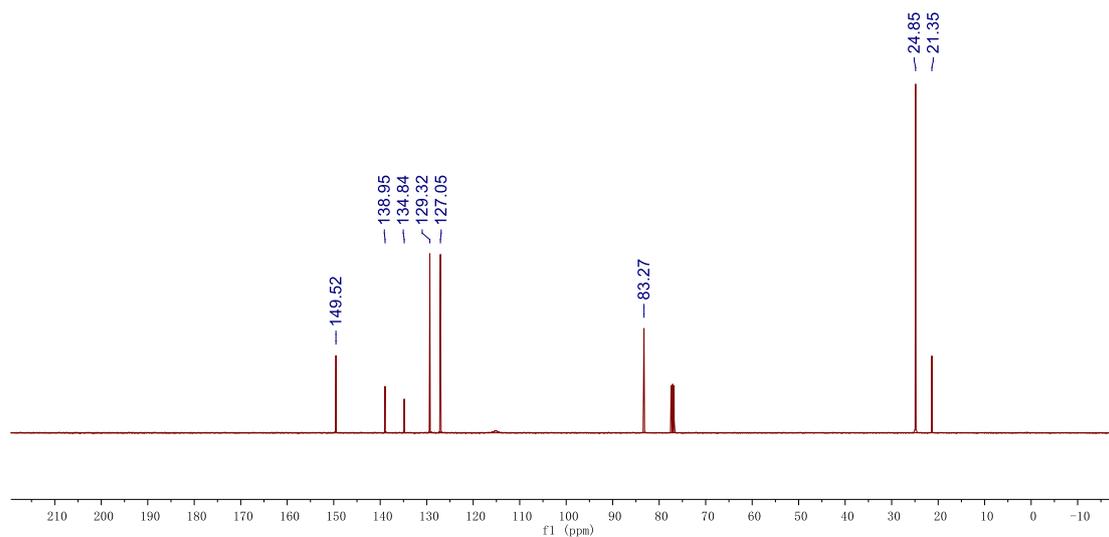
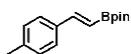


Figure S19. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2b**.

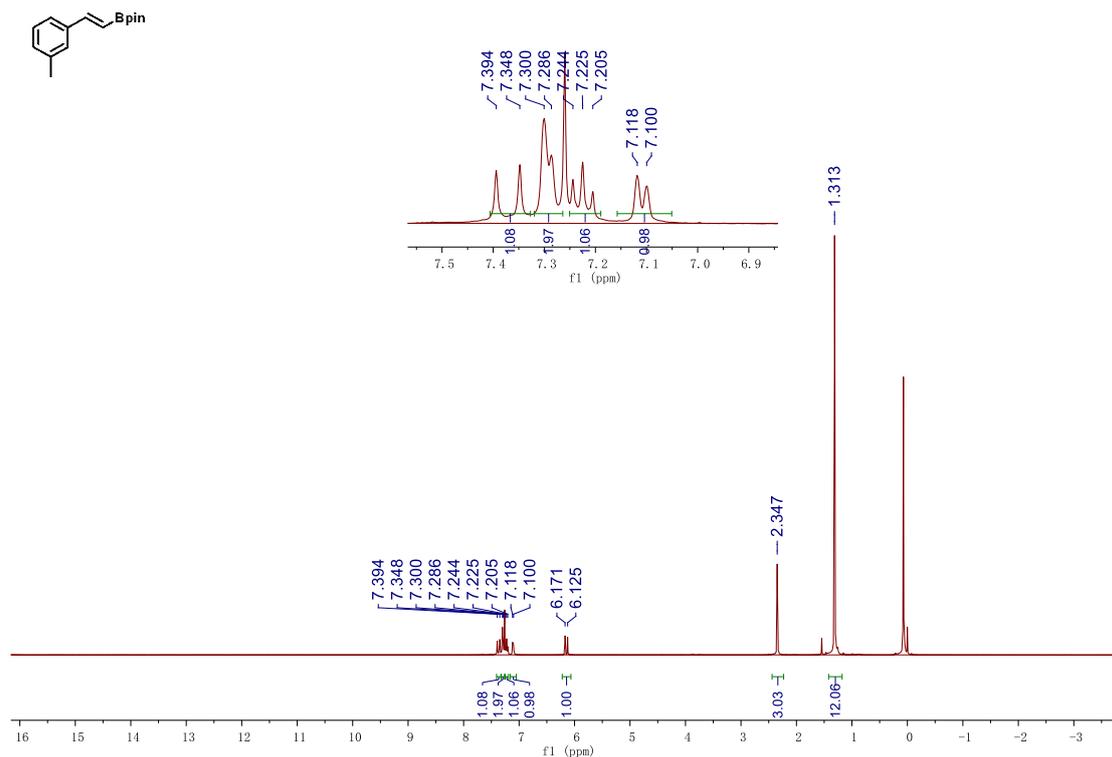


Figure S20. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2c**.

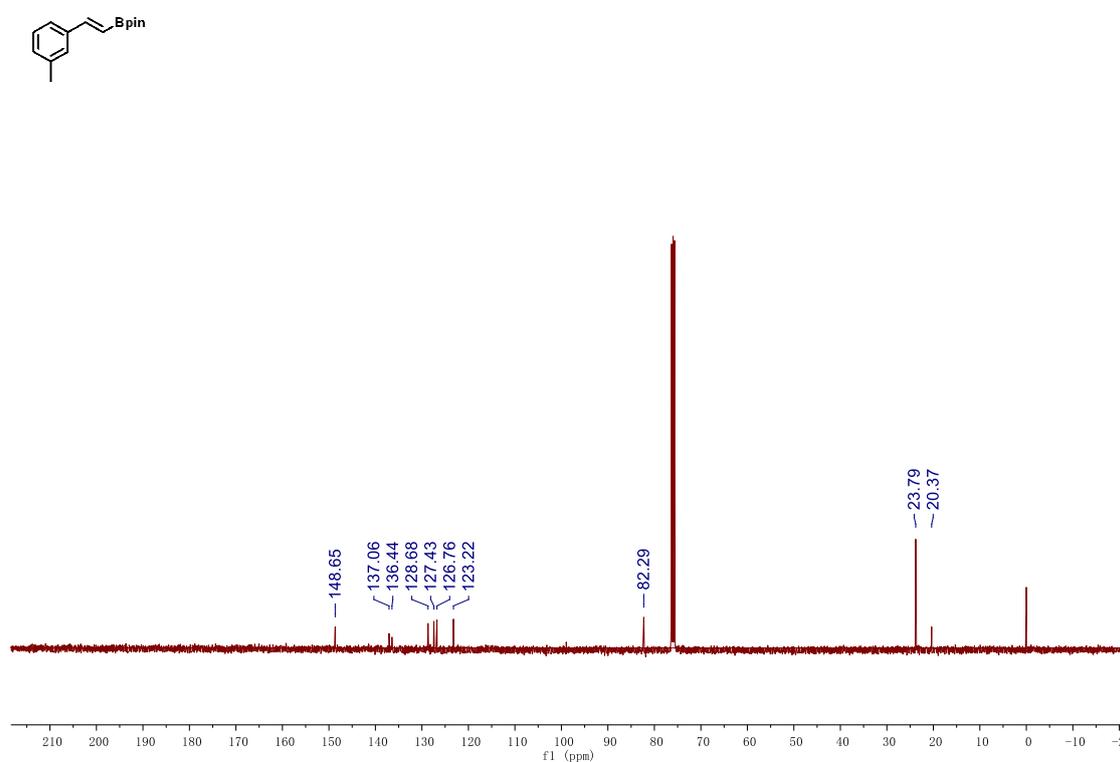


Figure S21. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2c**.

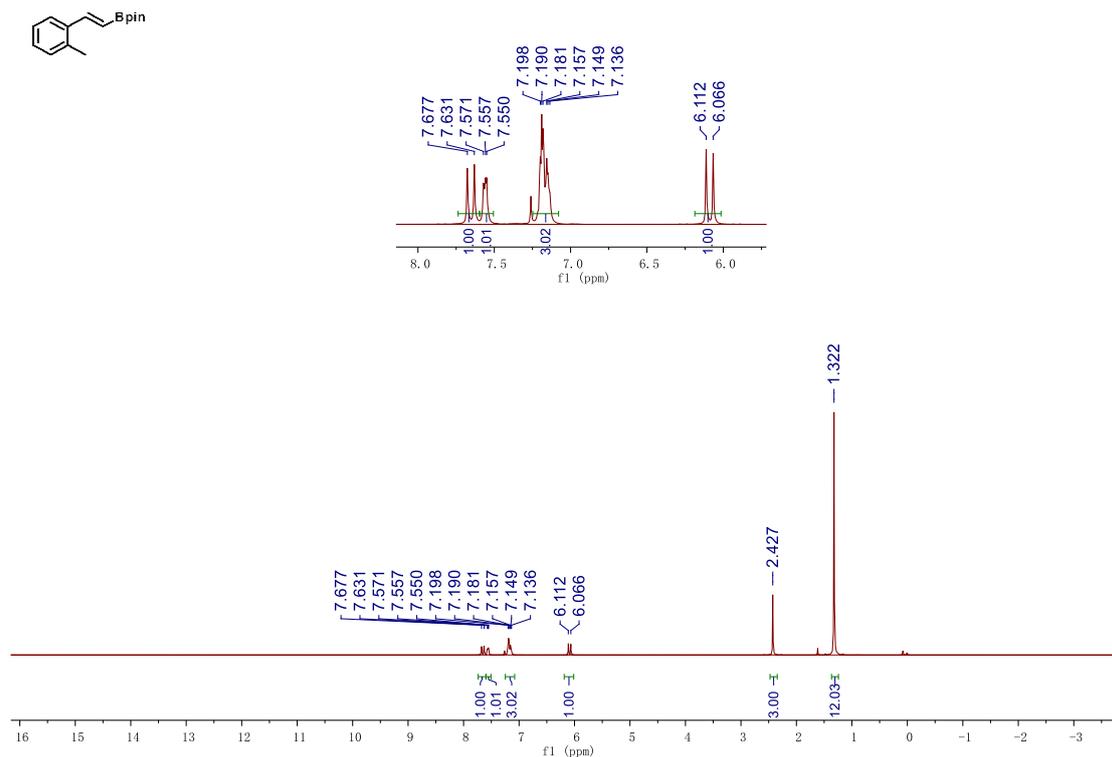


Figure S22. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2d**.

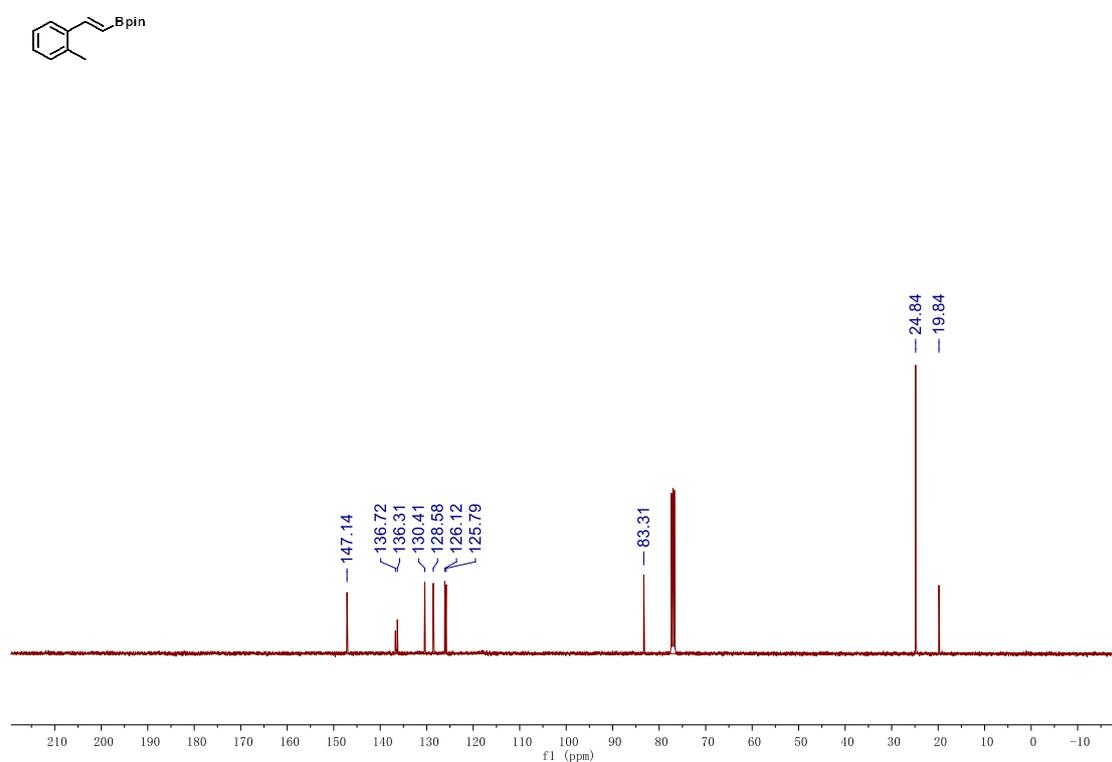


Figure S23. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2d**.

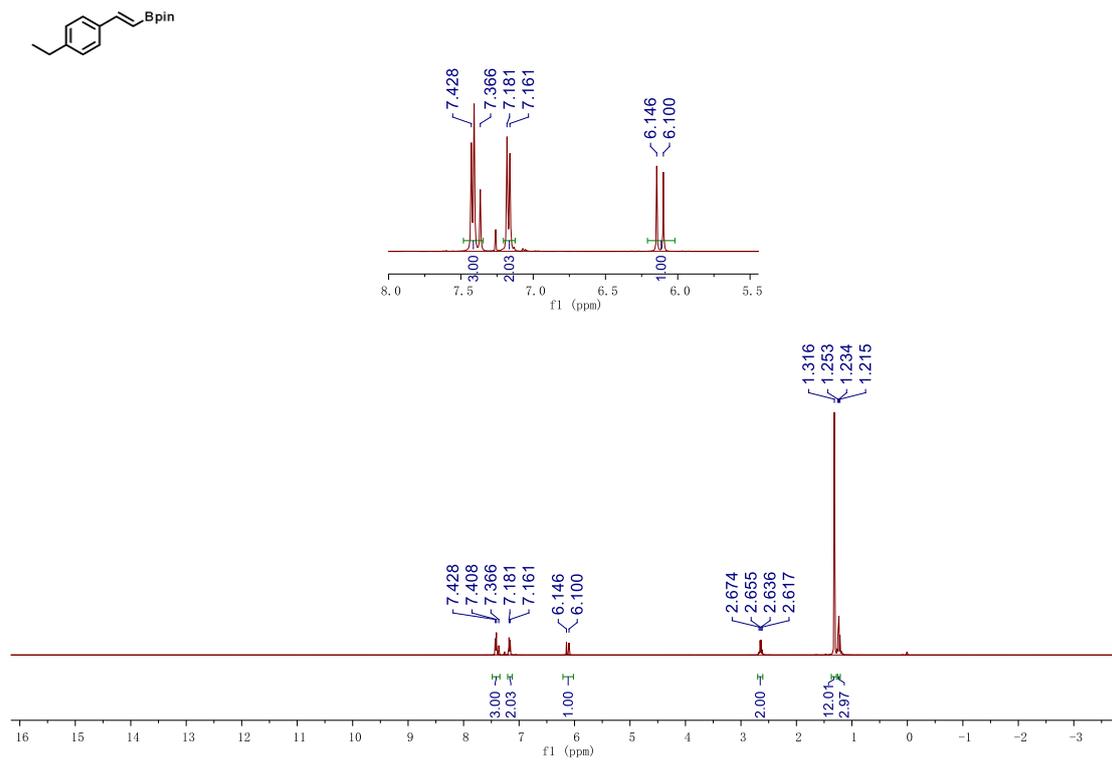


Figure S24. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2e**.

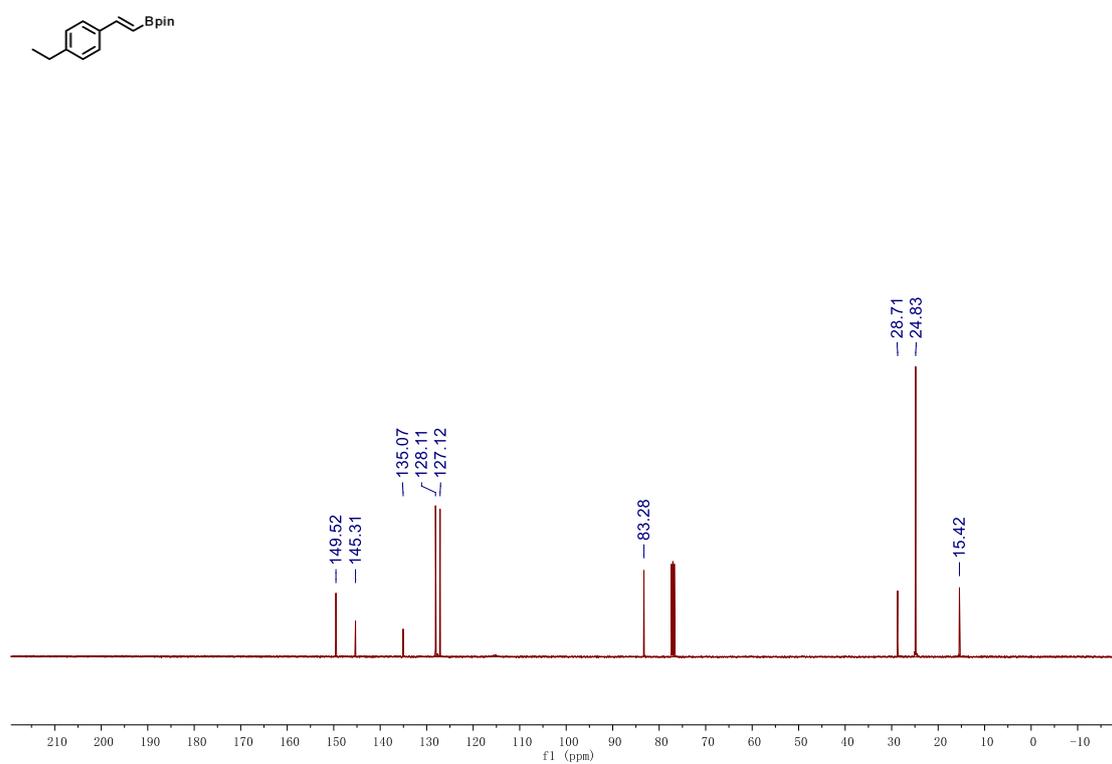


Figure S25. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2e**.

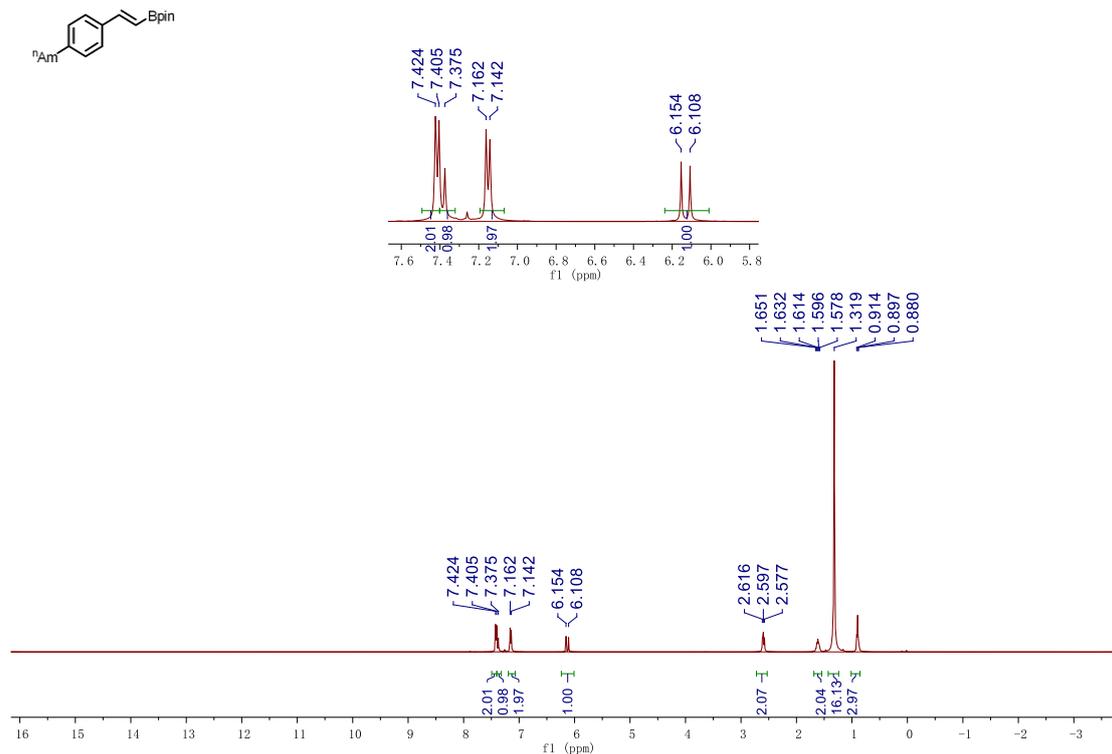


Figure S26. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2f**.

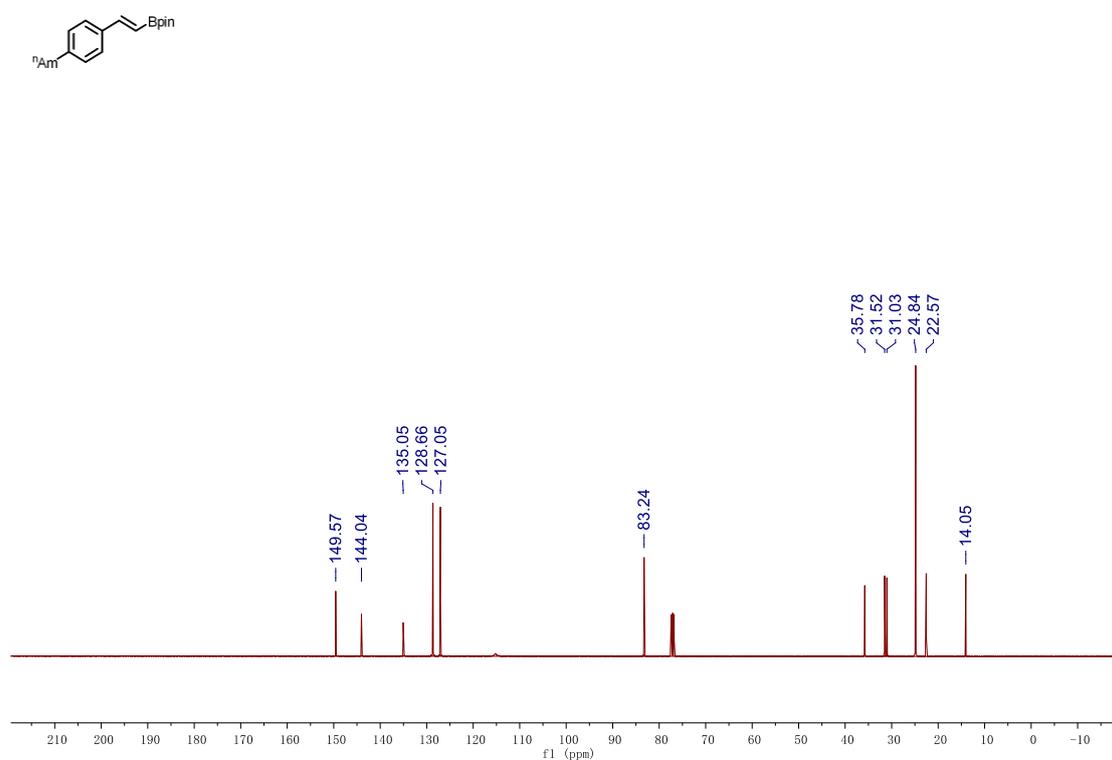


Figure S27. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2f**.

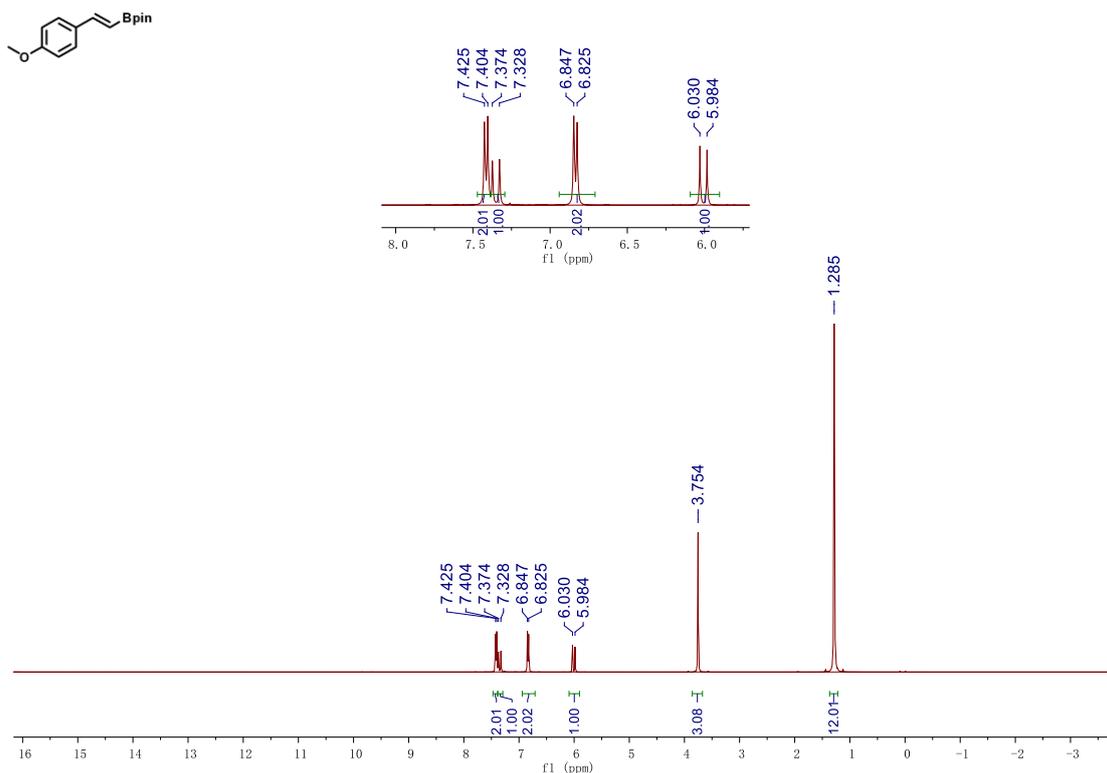


Figure S30. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2h**.

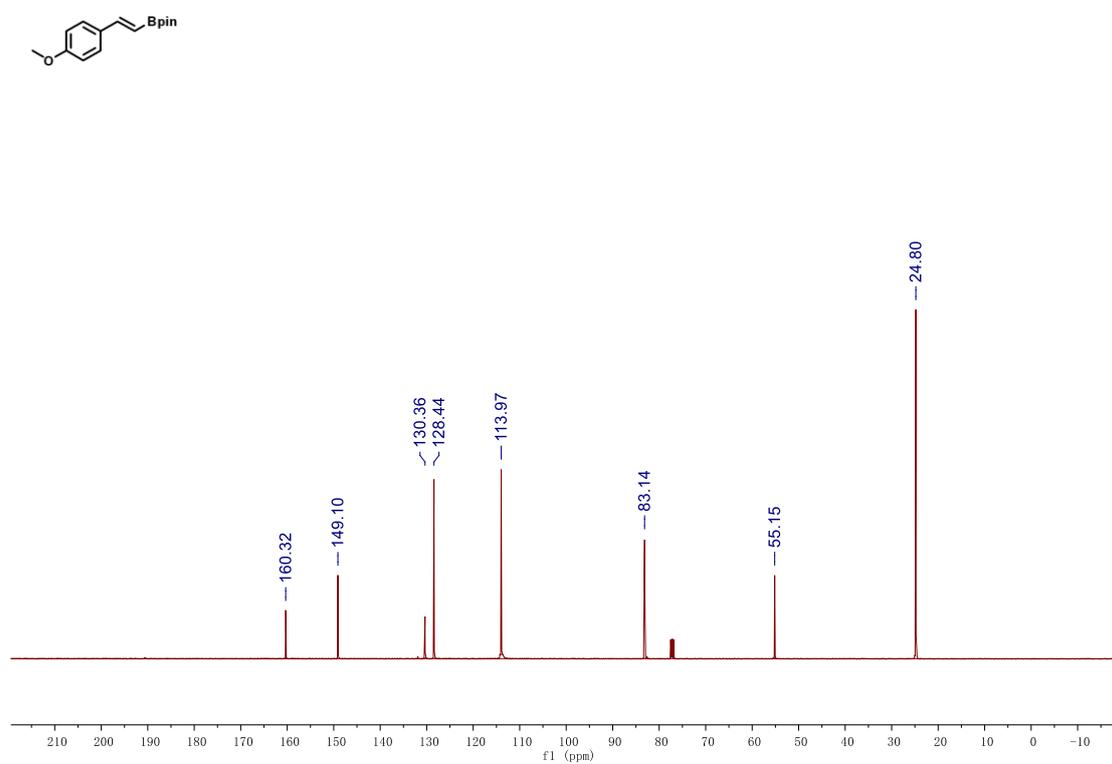


Figure S31. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2h**.

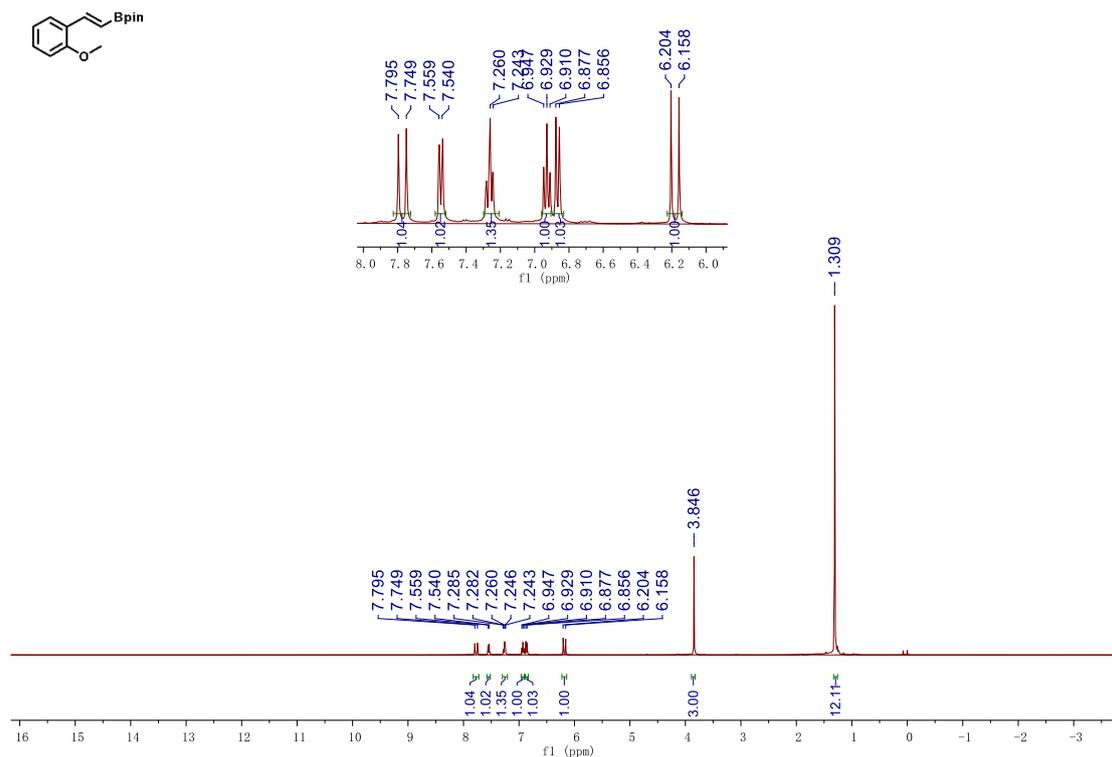


Figure S34. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 2j.

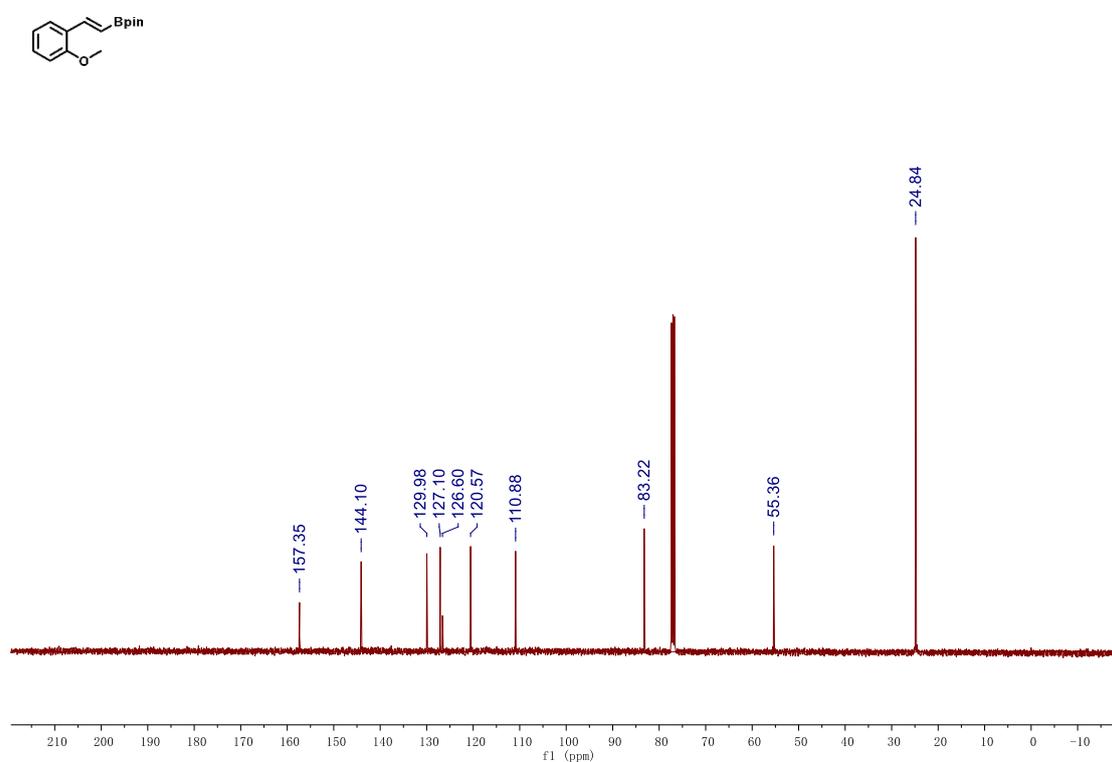


Figure S35. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 2j.

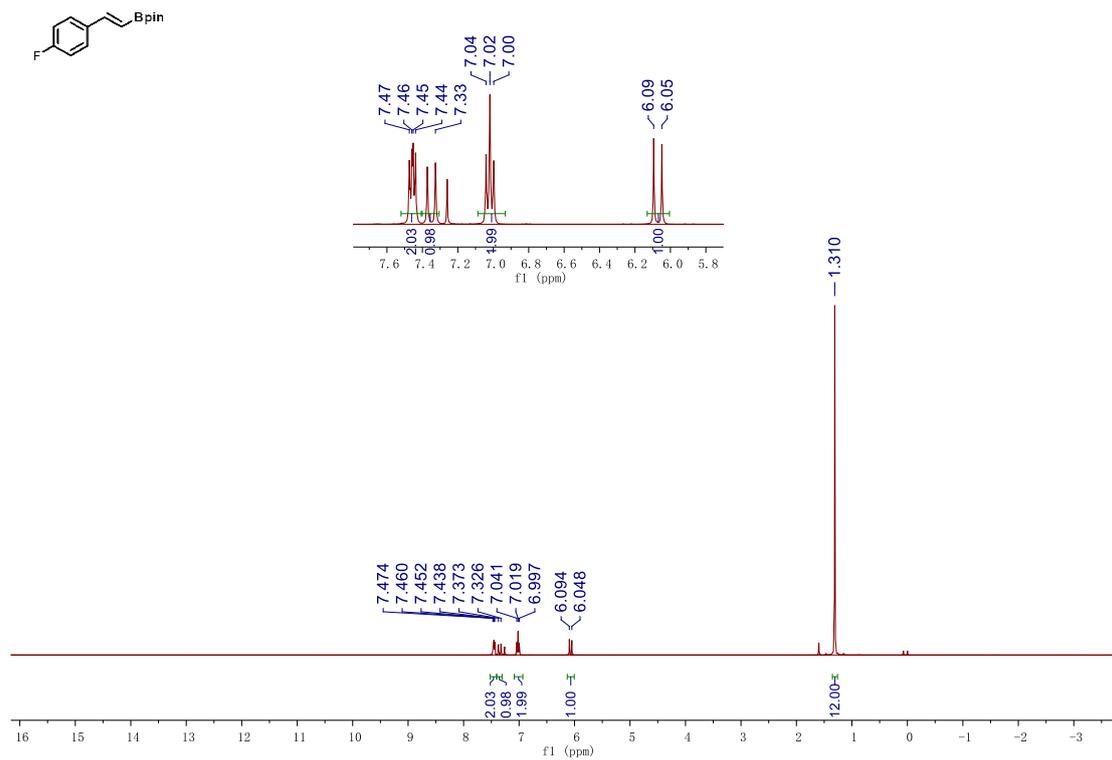


Figure S36. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2k**.

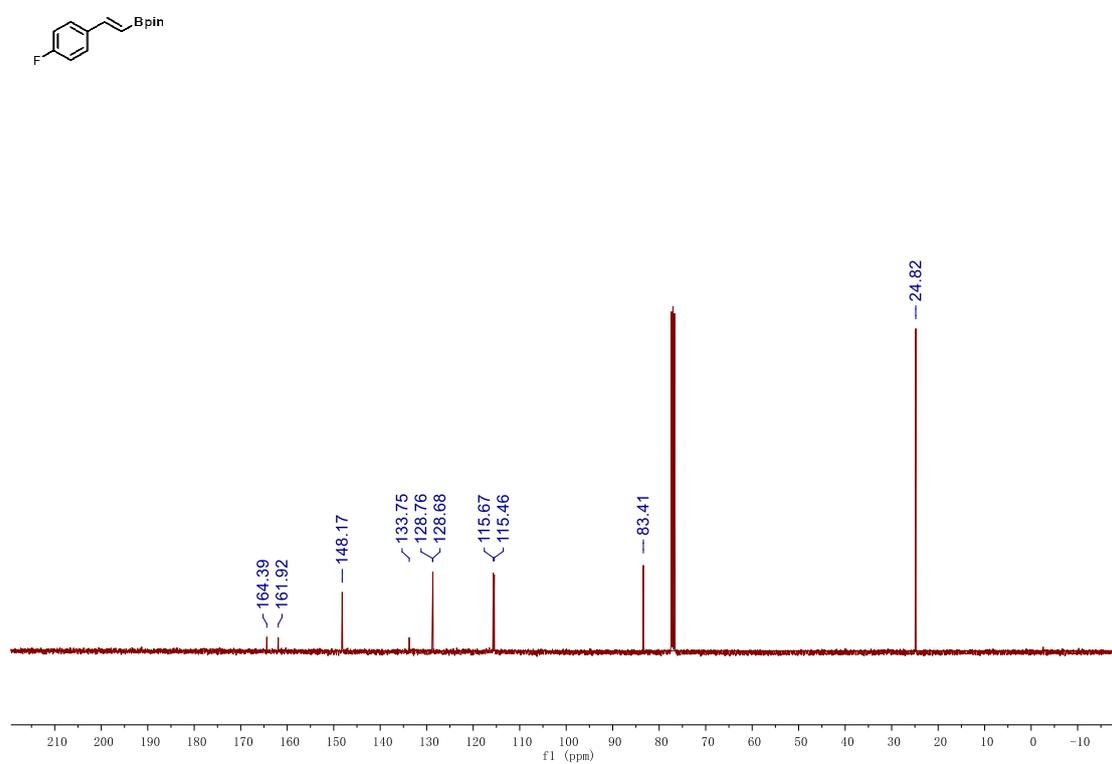


Figure S37. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2k**.

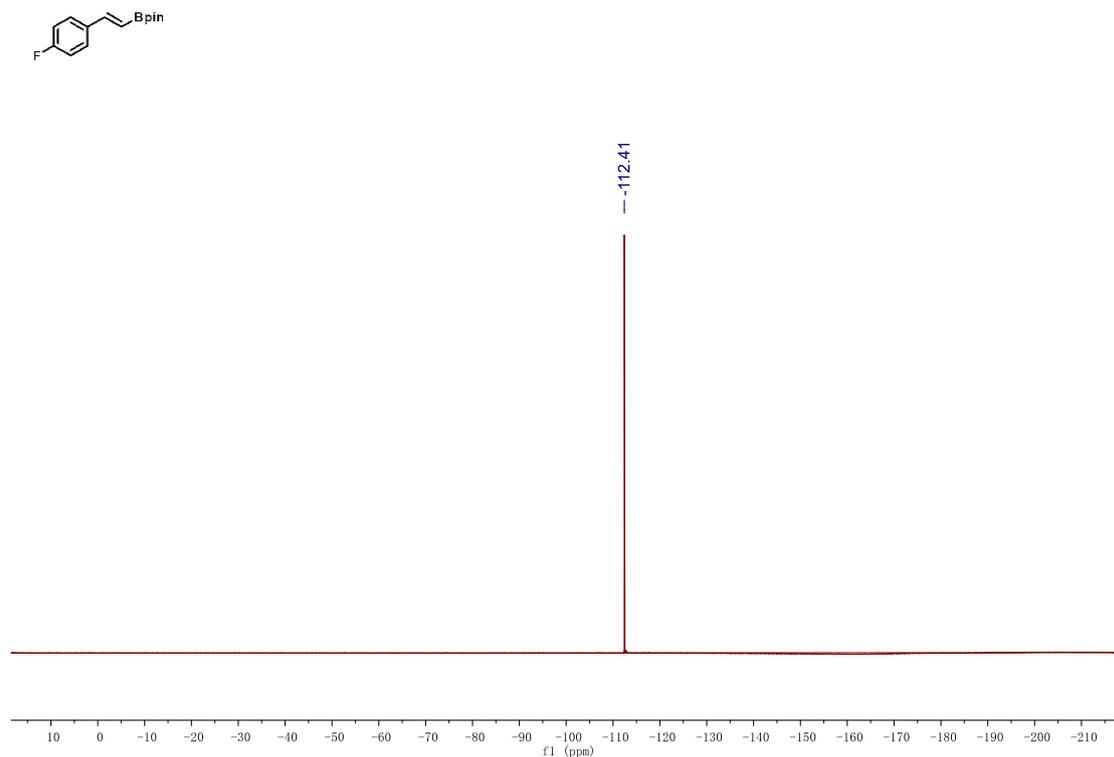


Figure S38. ^{19}F NMR (376 MHz, CDCl_3) spectrum of compound **2k**.

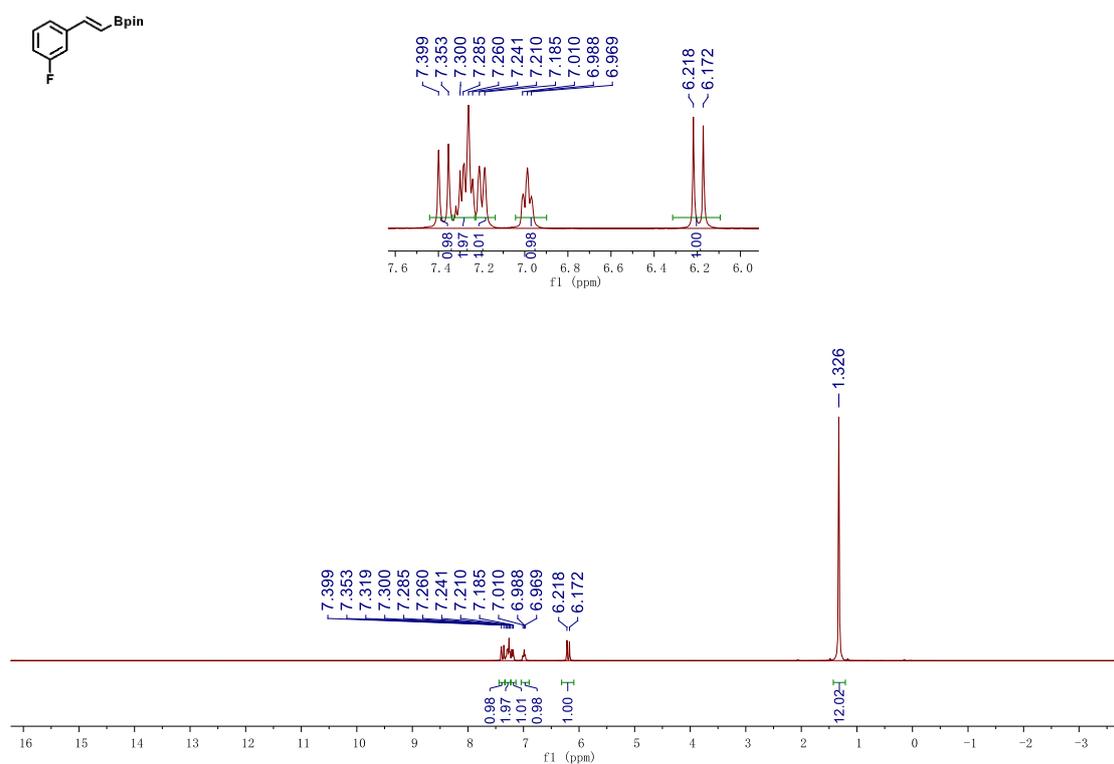
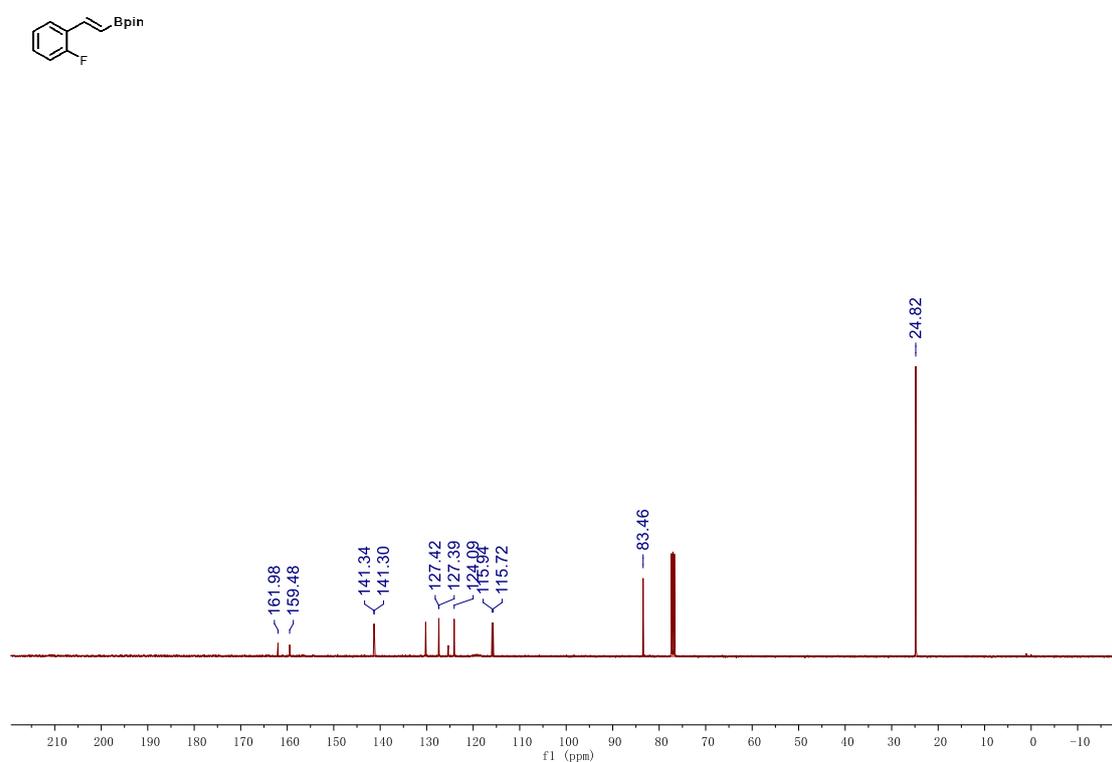
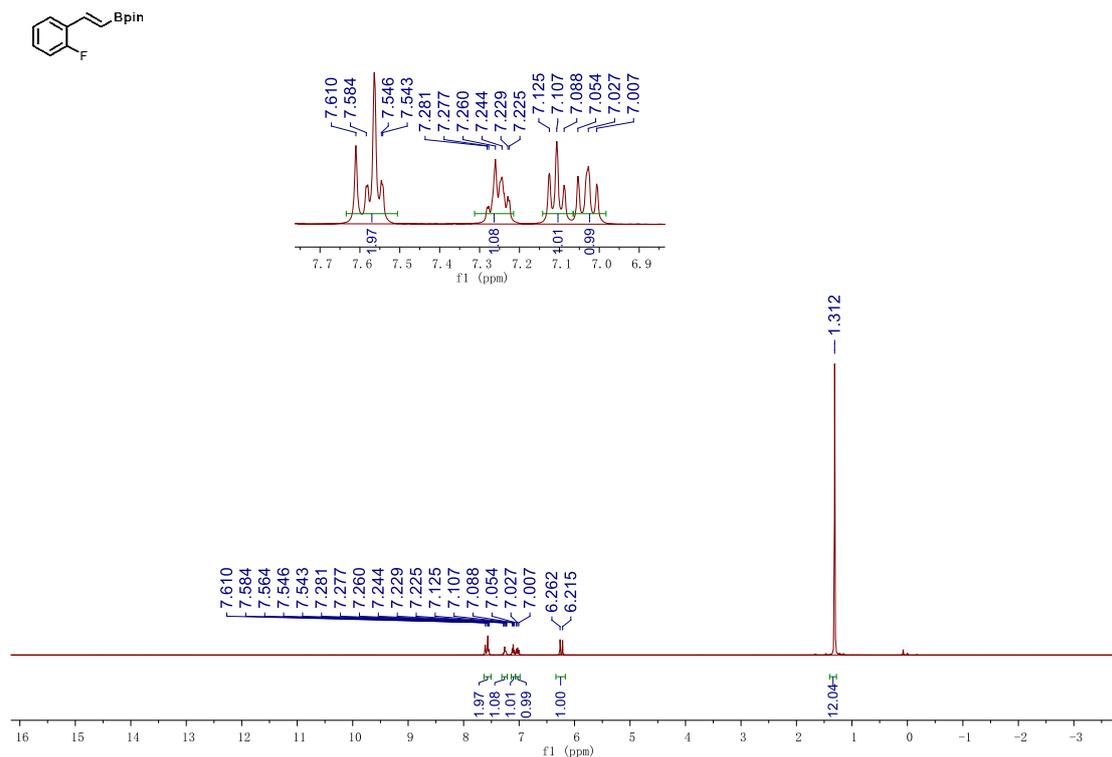


Figure S39. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2l**.



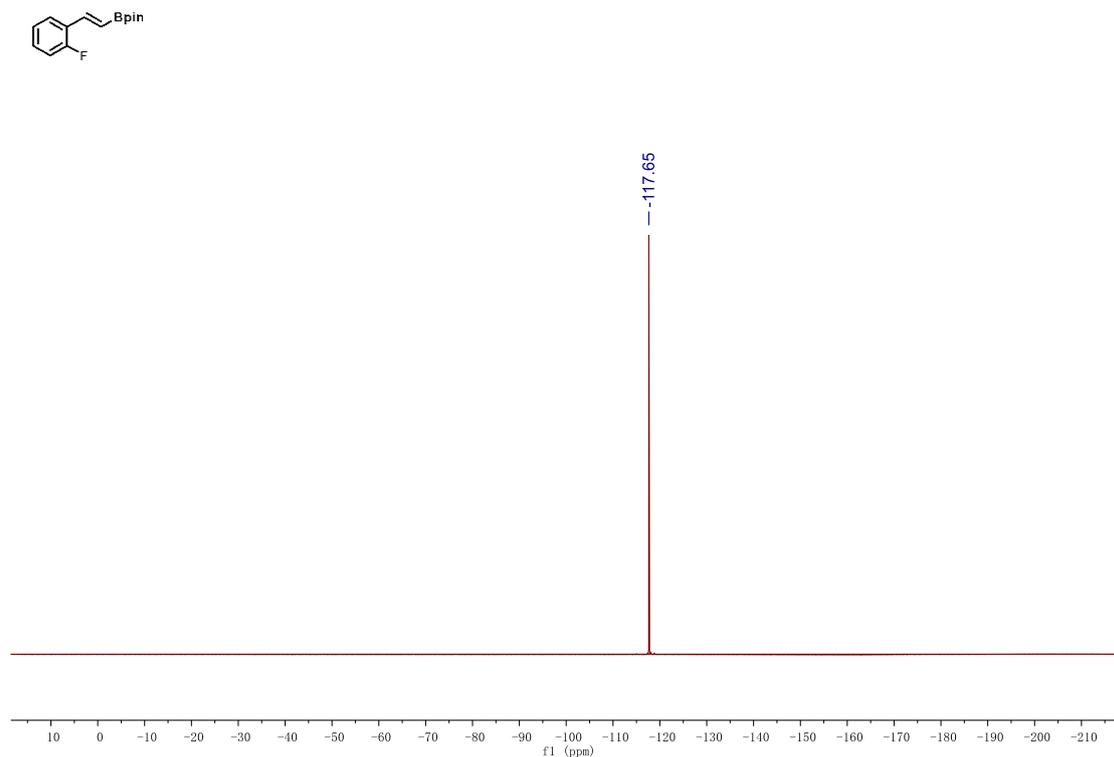


Figure S44. ^{19}F NMR (376 MHz, CDCl_3) spectrum of compound **2m**.

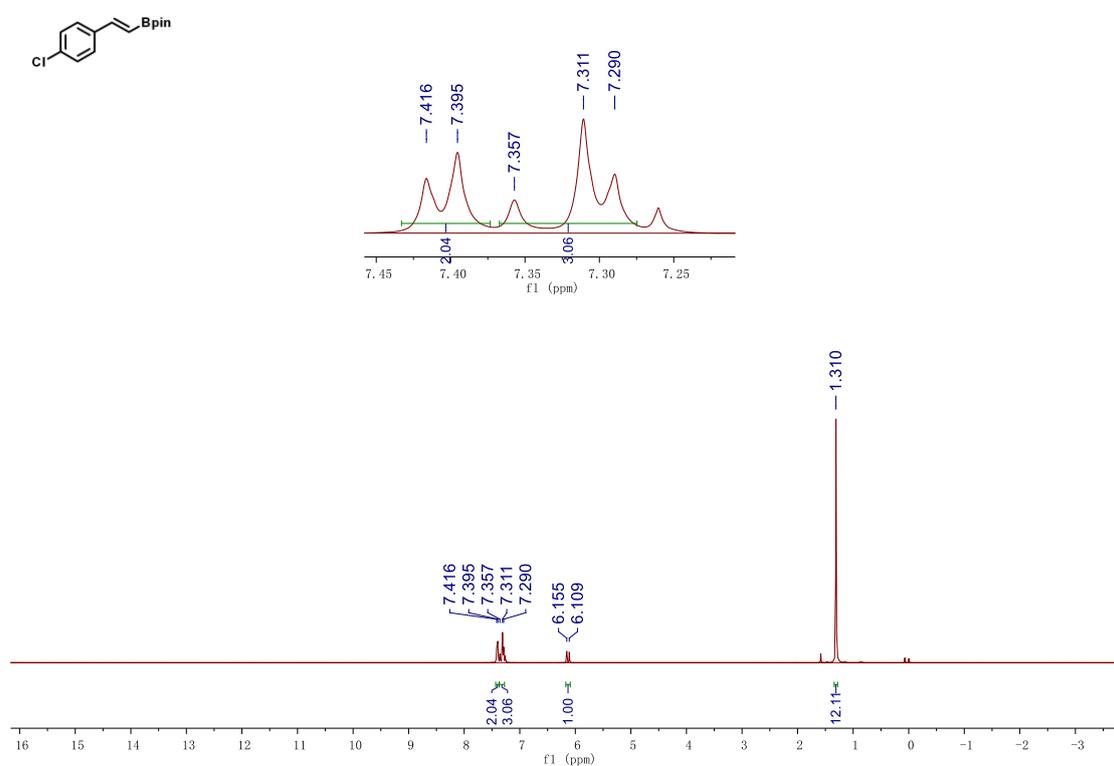


Figure S45. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2n**.

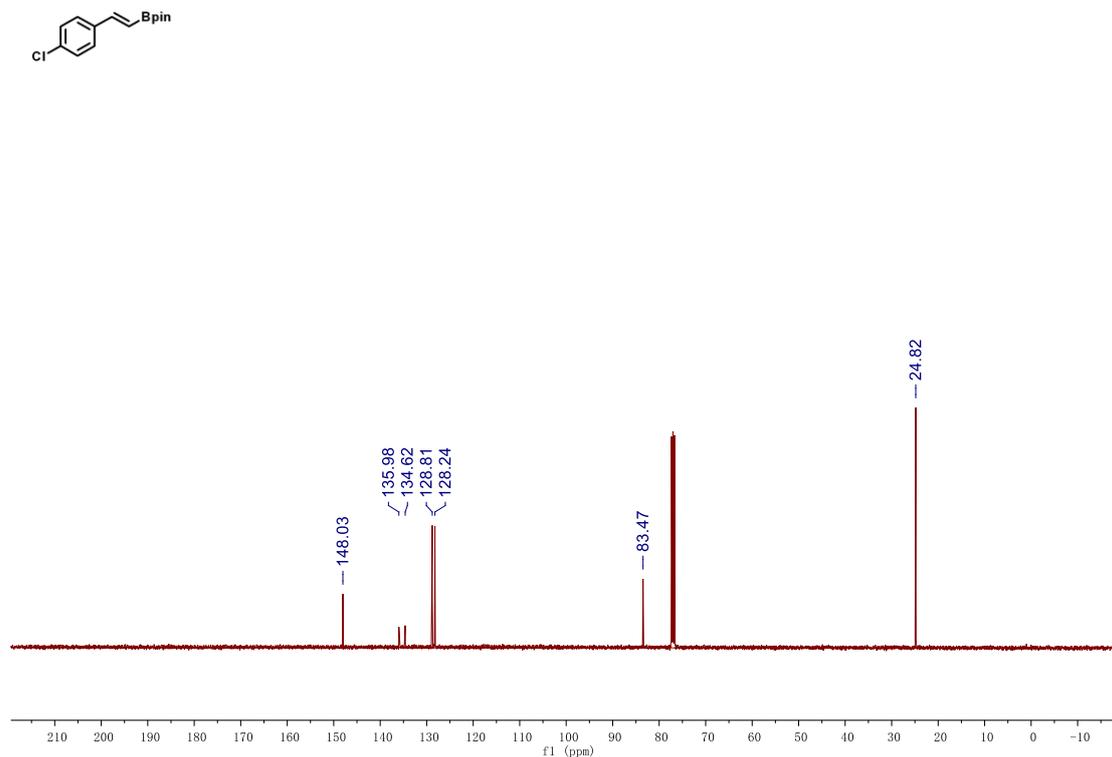


Figure S46. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2n**.

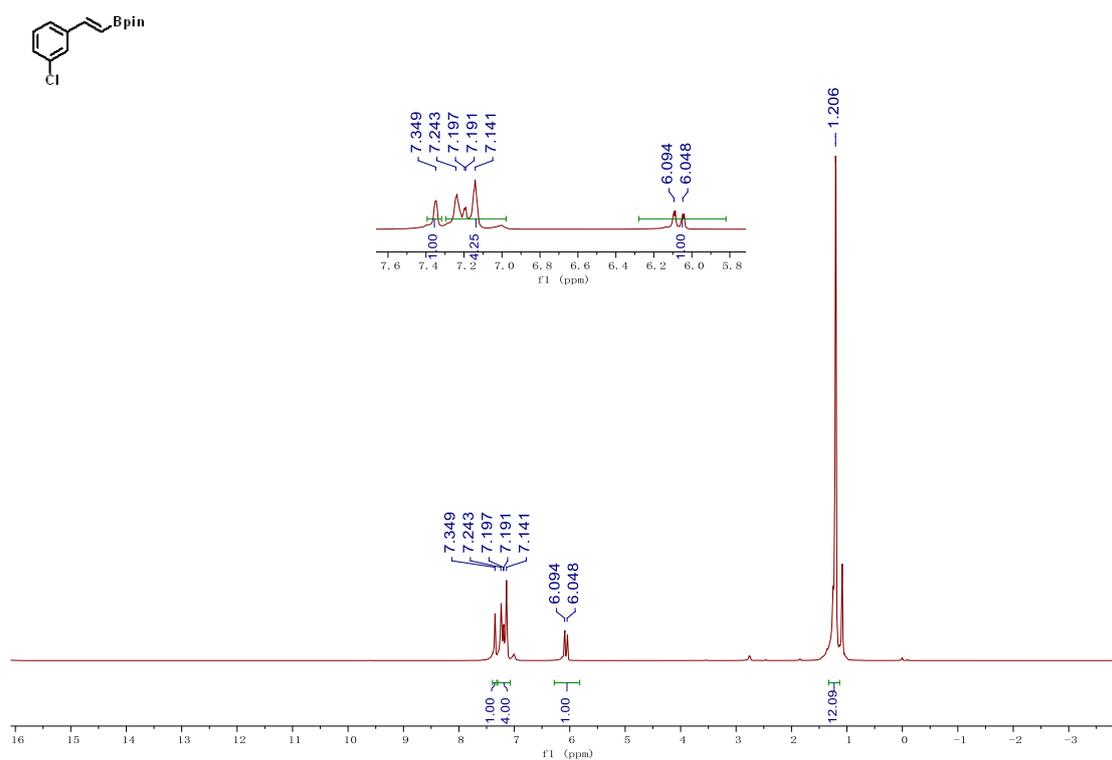


Figure S47. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2o**.

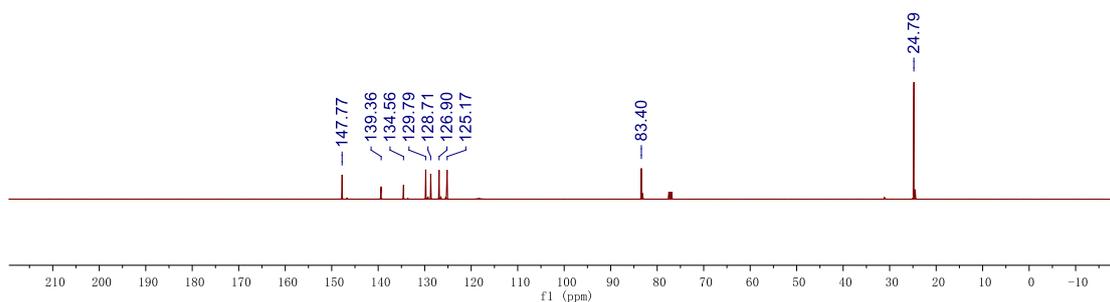
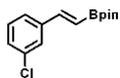


Figure S48. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2o**.

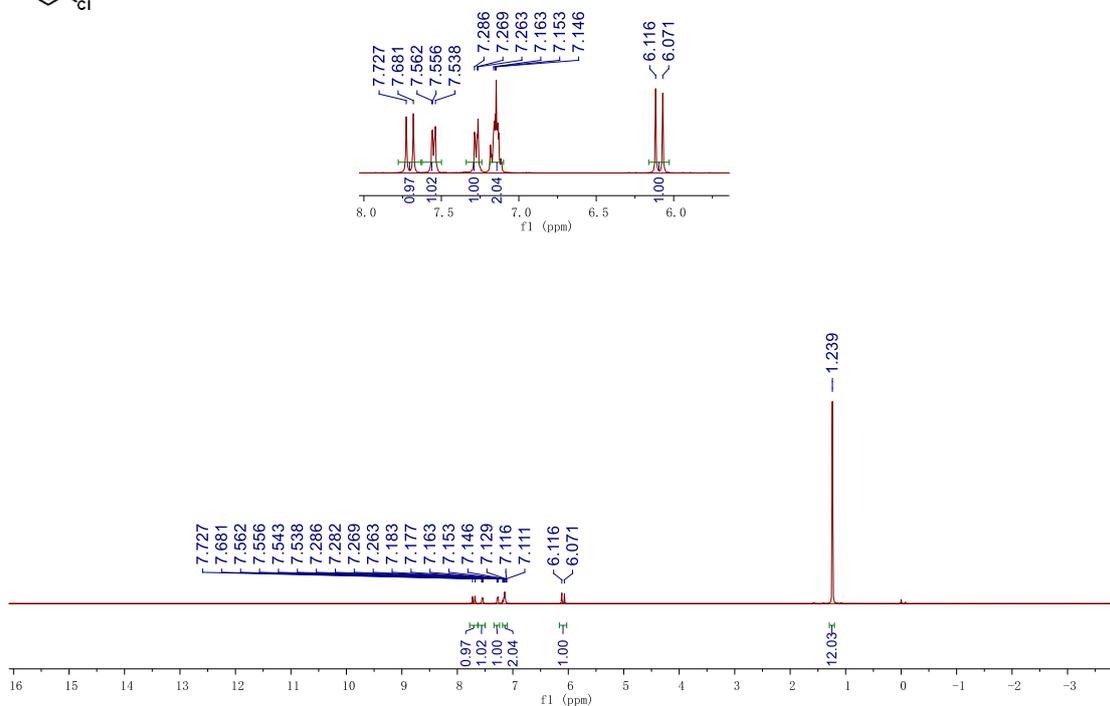
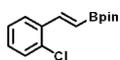


Figure S49. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2p**.

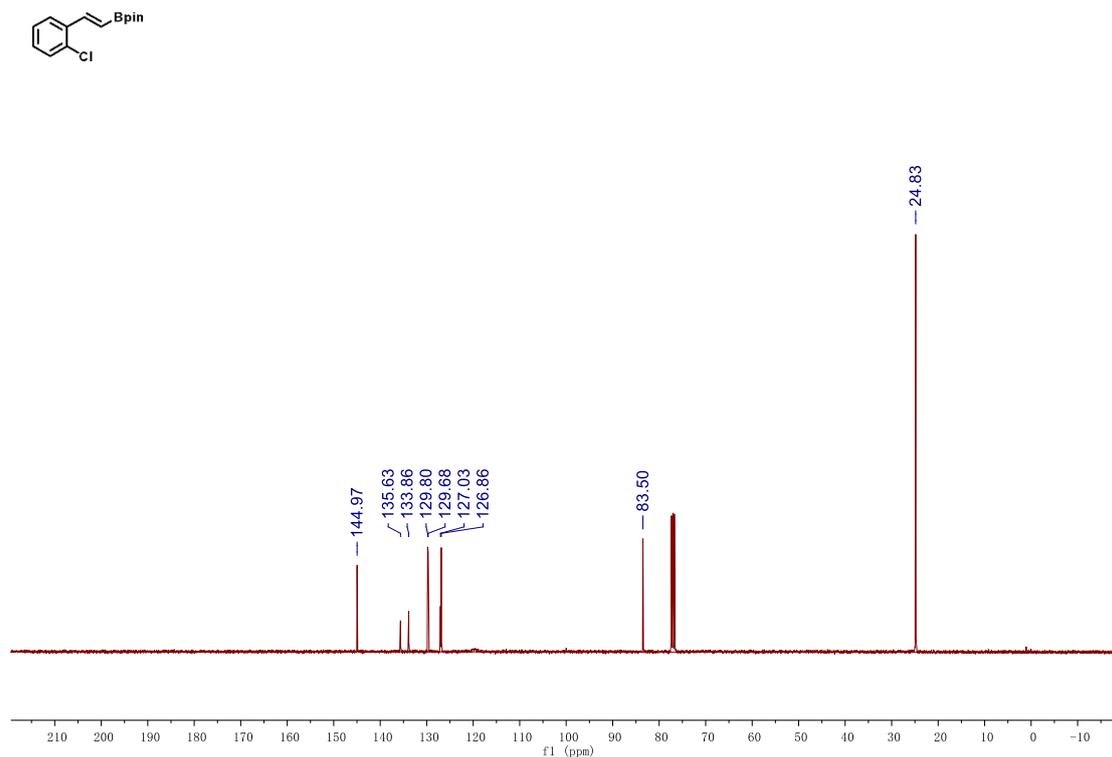


Figure S50. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2p**.

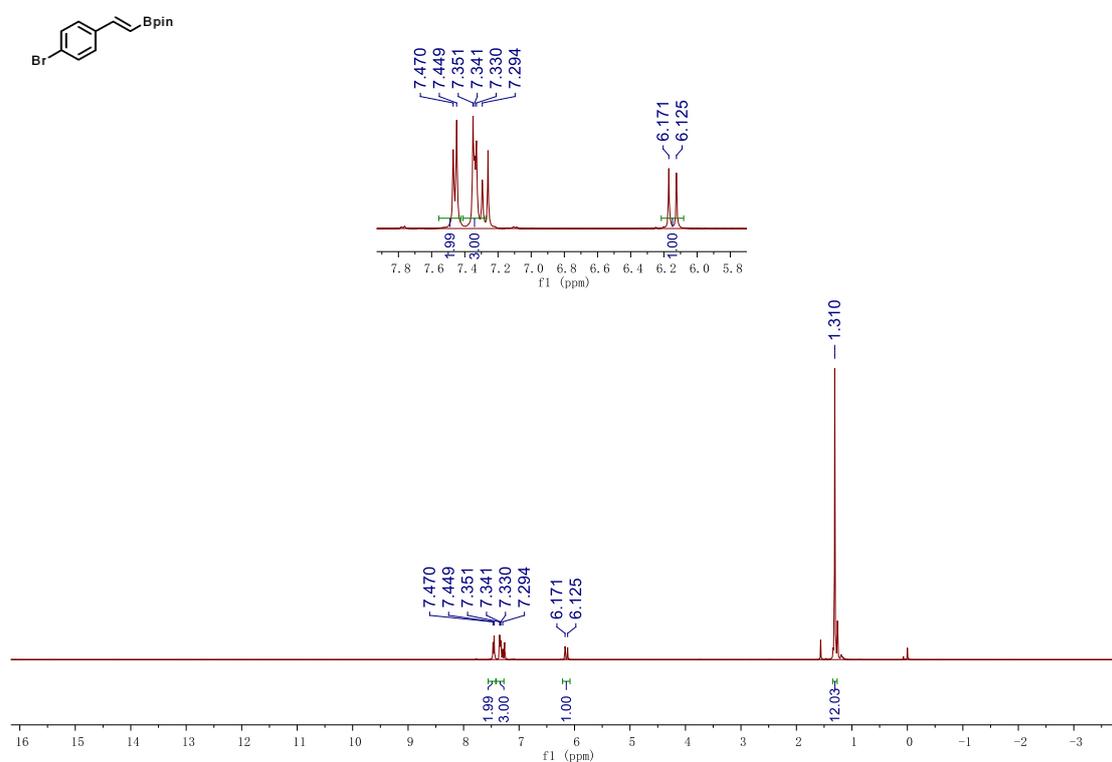


Figure S51. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2q**.

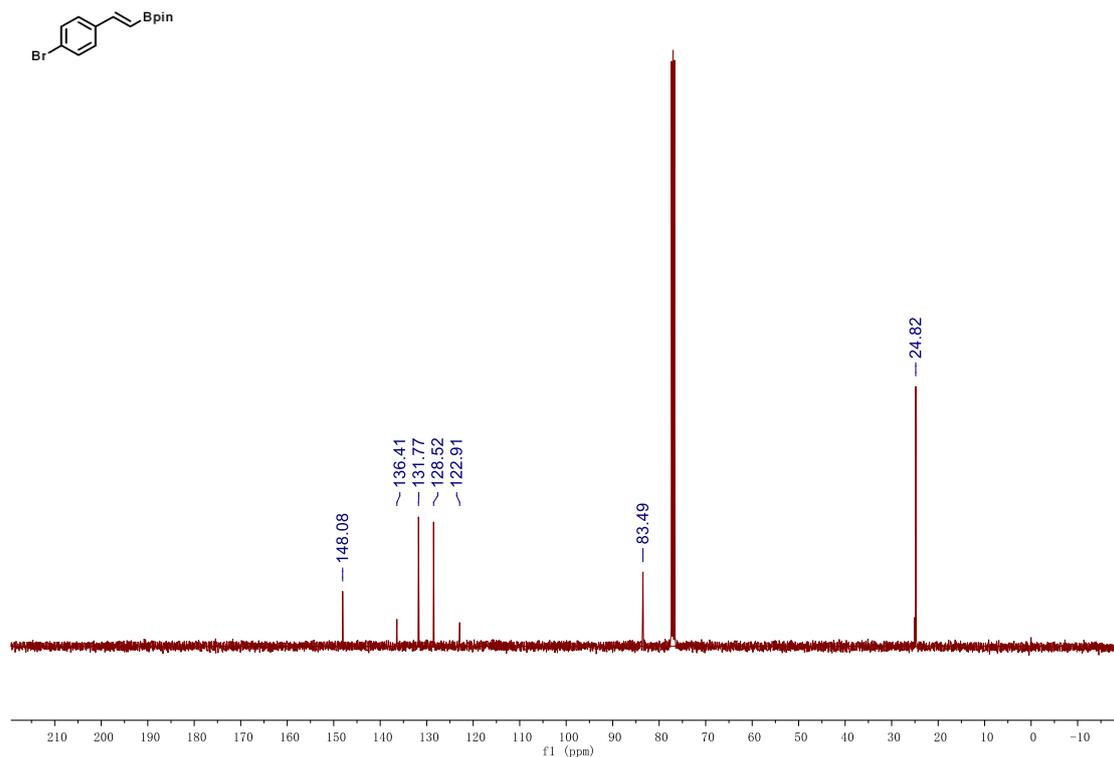


Figure S52. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2q**.

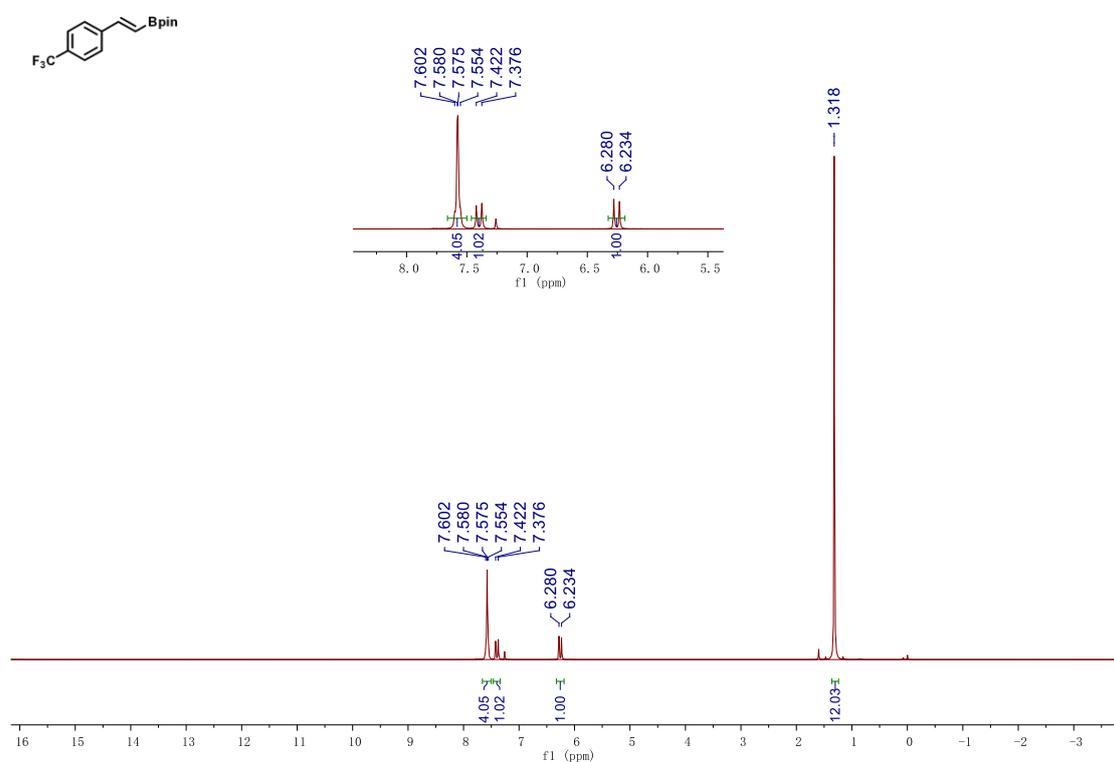


Figure S53. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2r**.

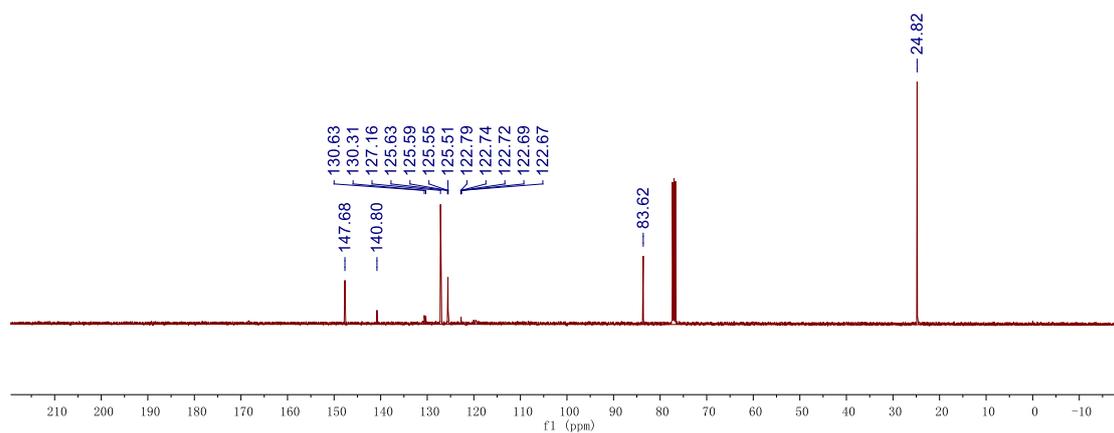
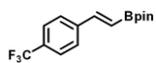


Figure S54. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2r**.

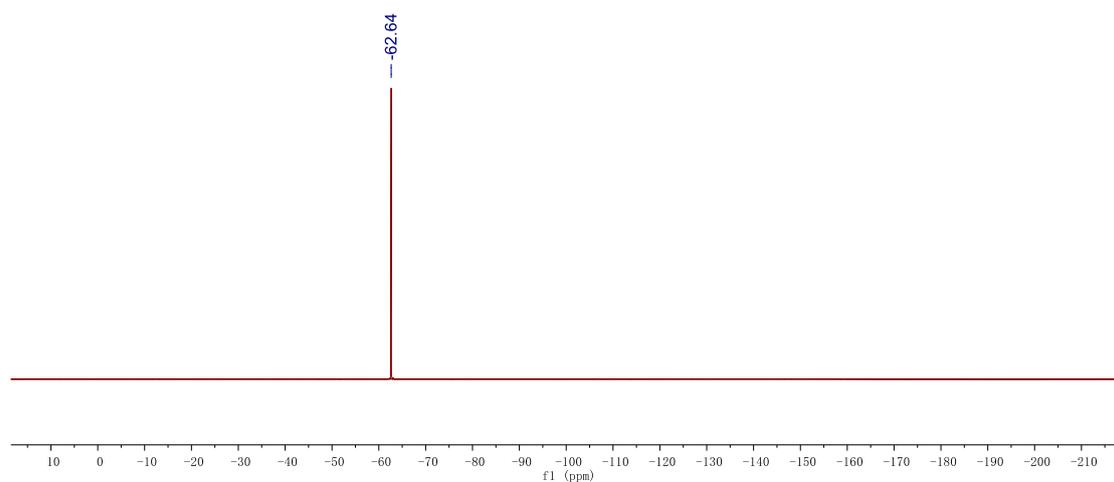
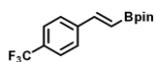


Figure S55. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of compound **2r**.

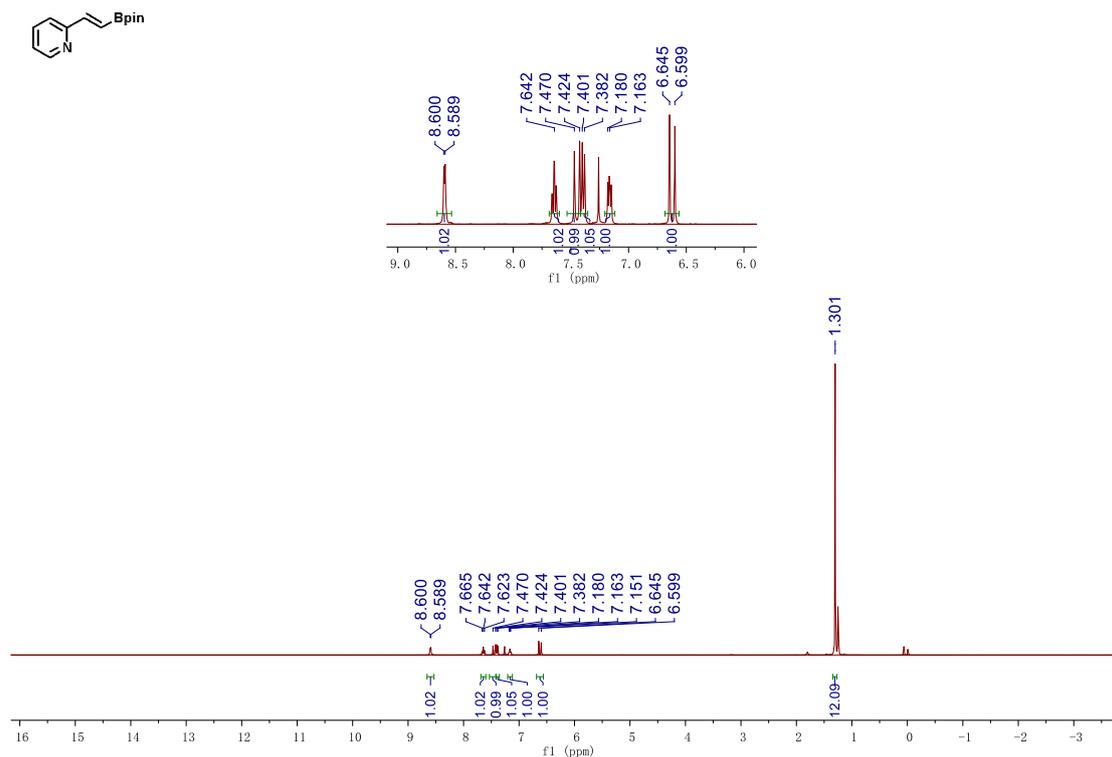


Figure S56. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2s**.

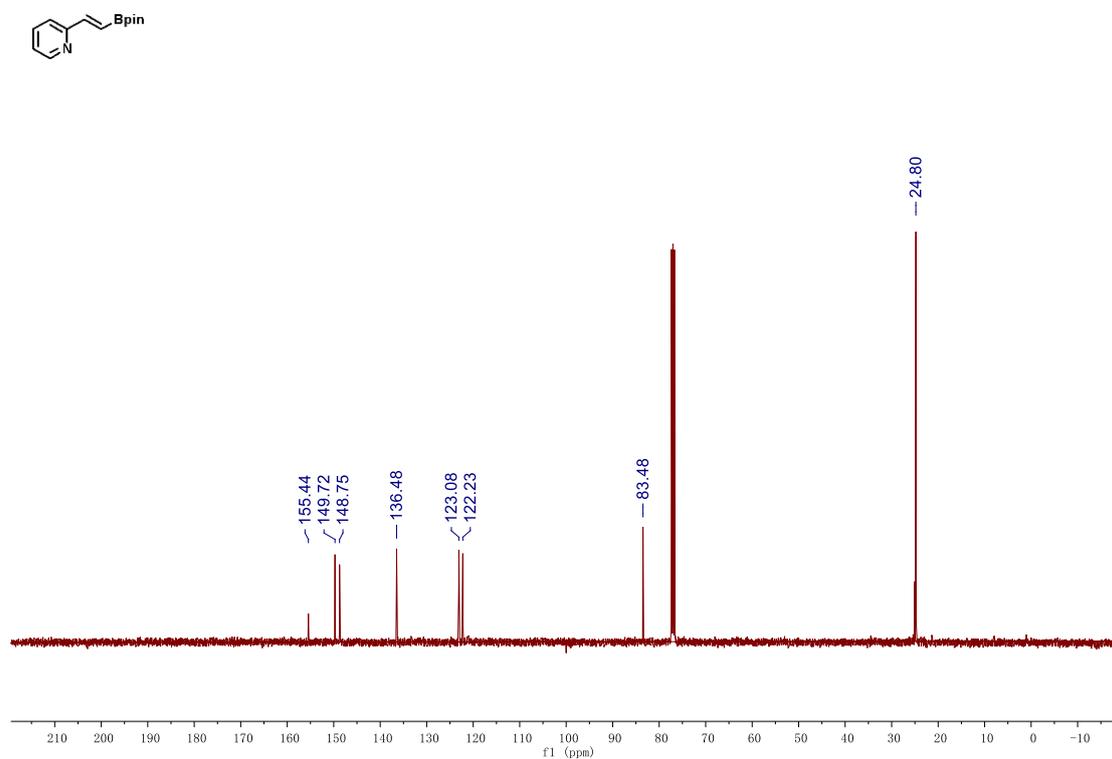


Figure S57. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2s**.

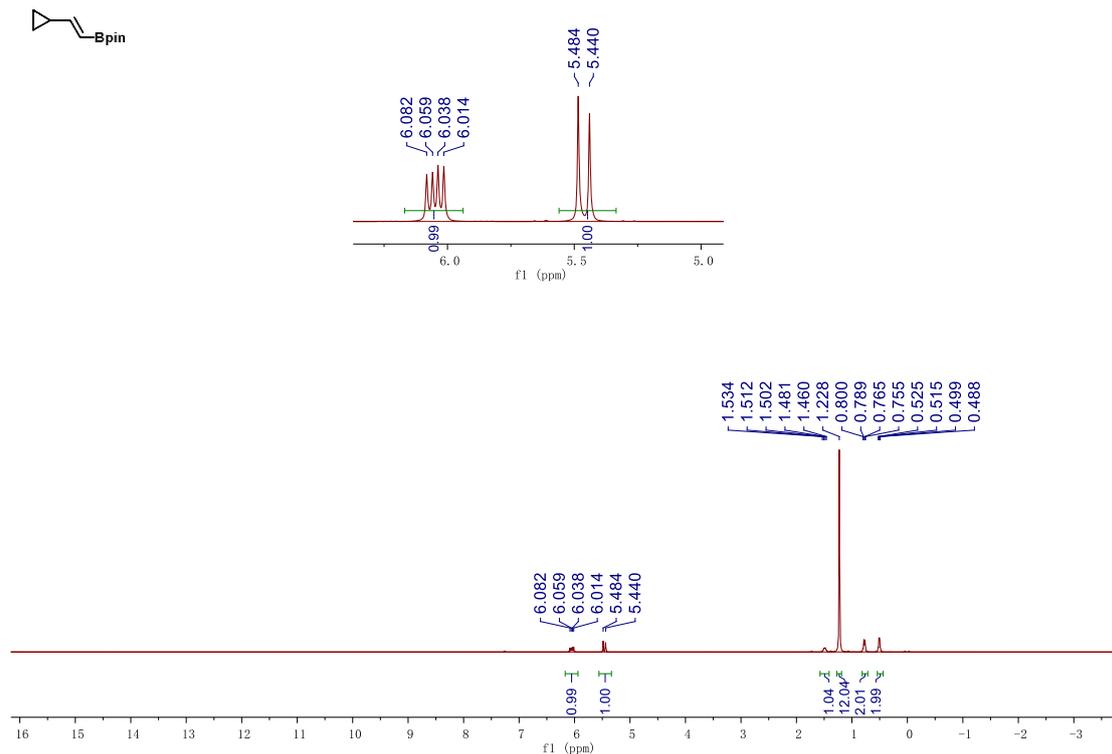


Figure S60. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2u**.

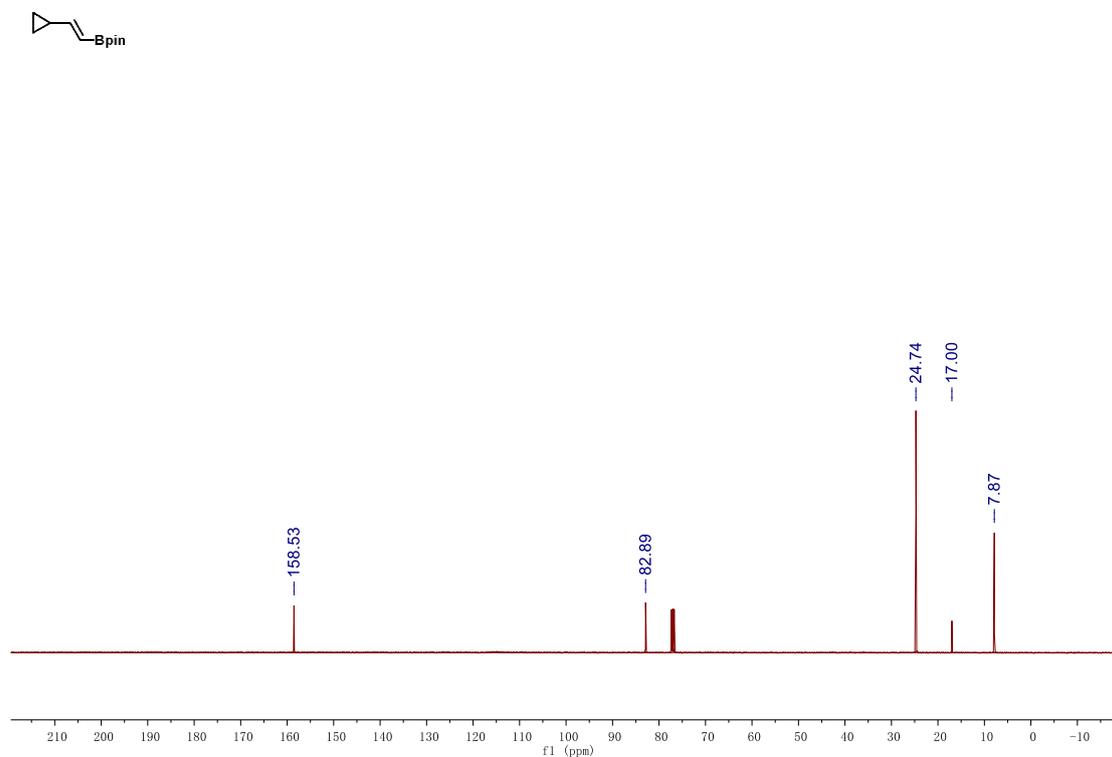


Figure S61. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2u**.

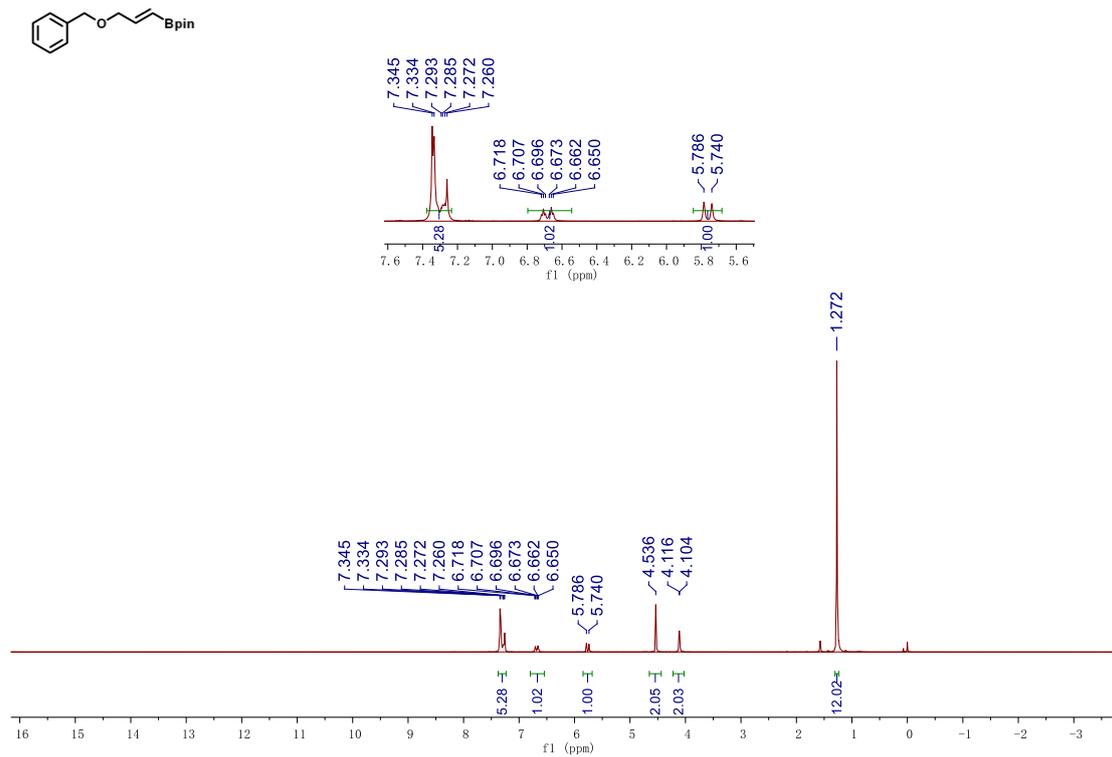


Figure S62. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2v**.

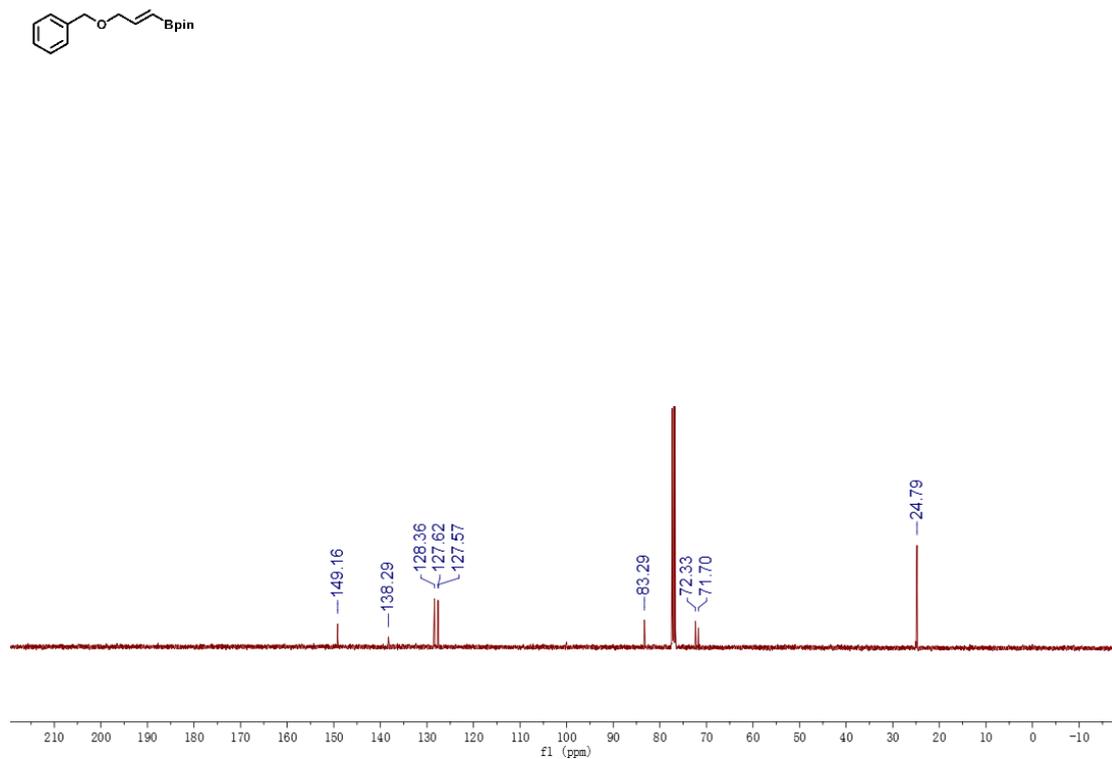


Figure S63. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2v**.

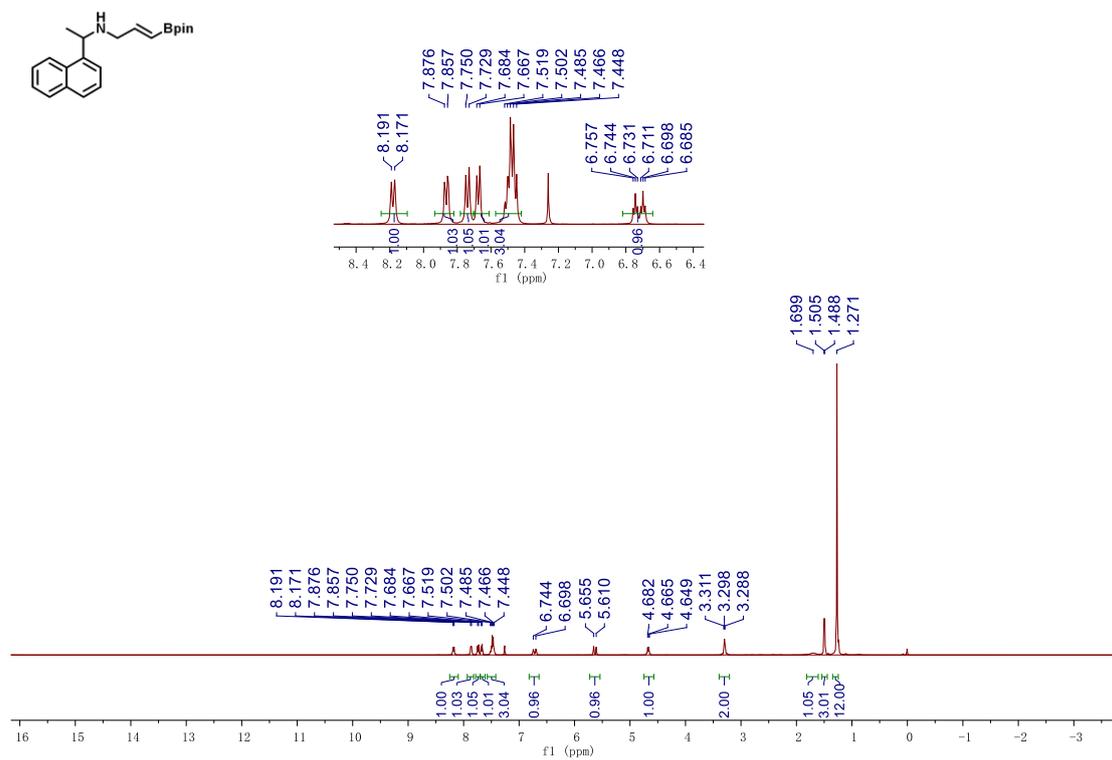


Figure S64. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2w**.

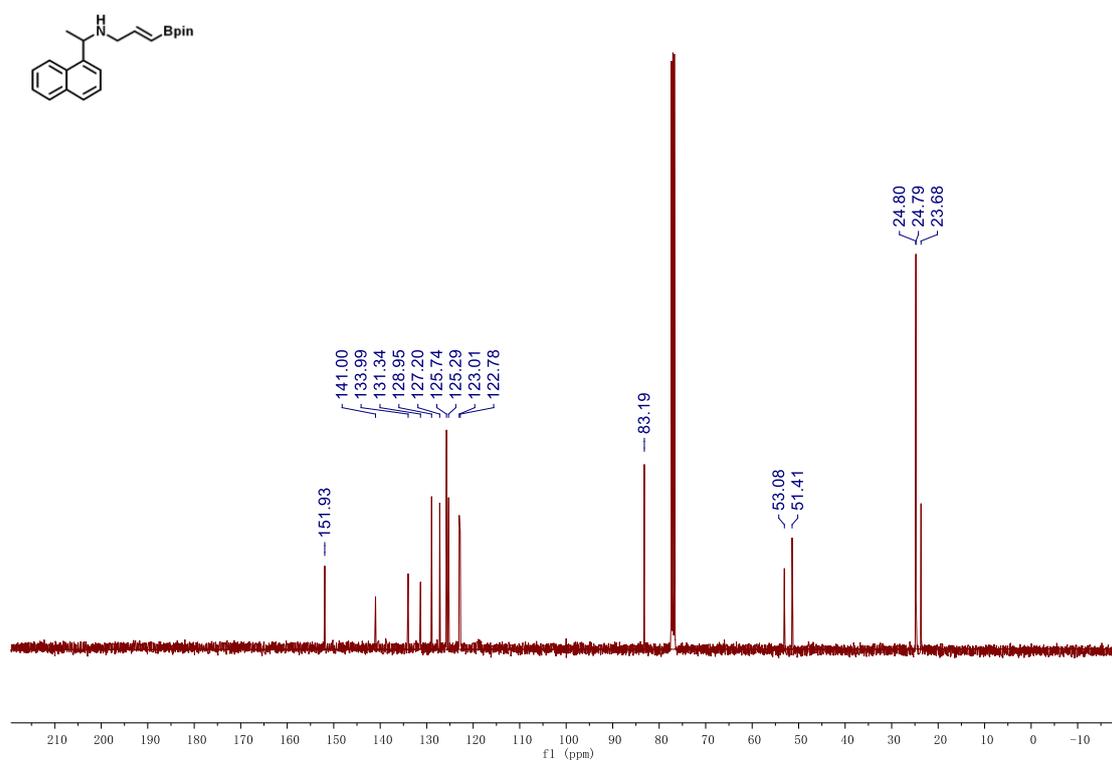


Figure S65. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2w**.

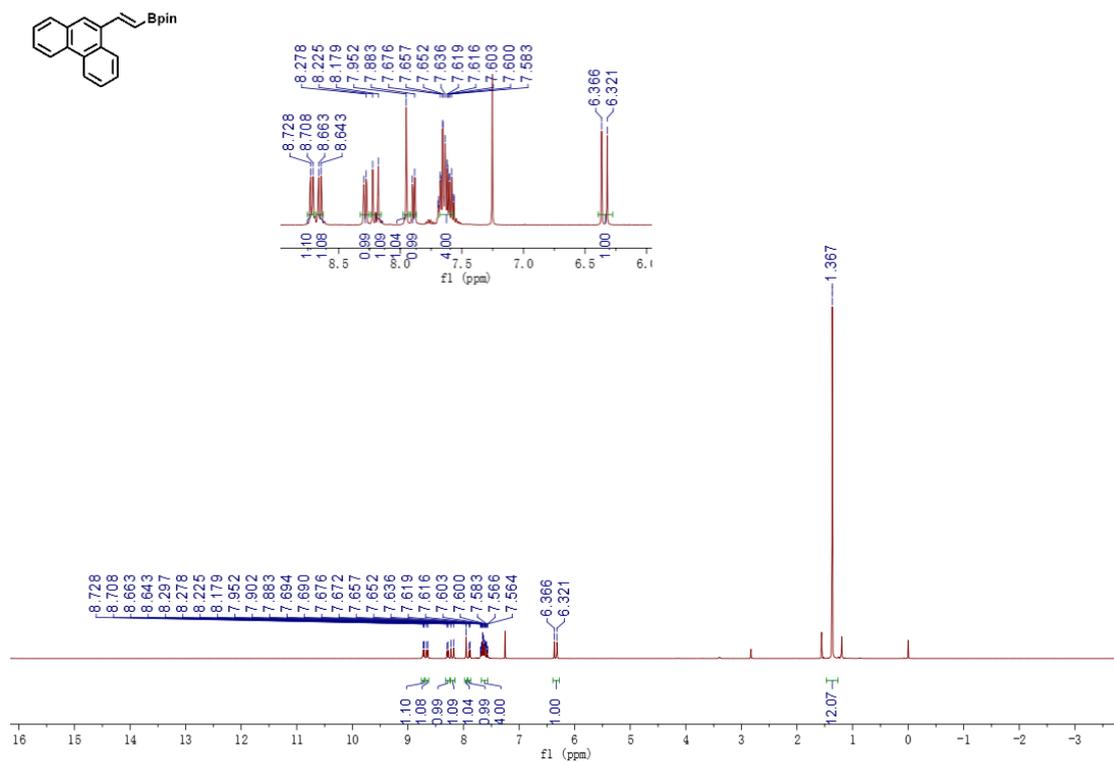


Figure S66. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2x**.

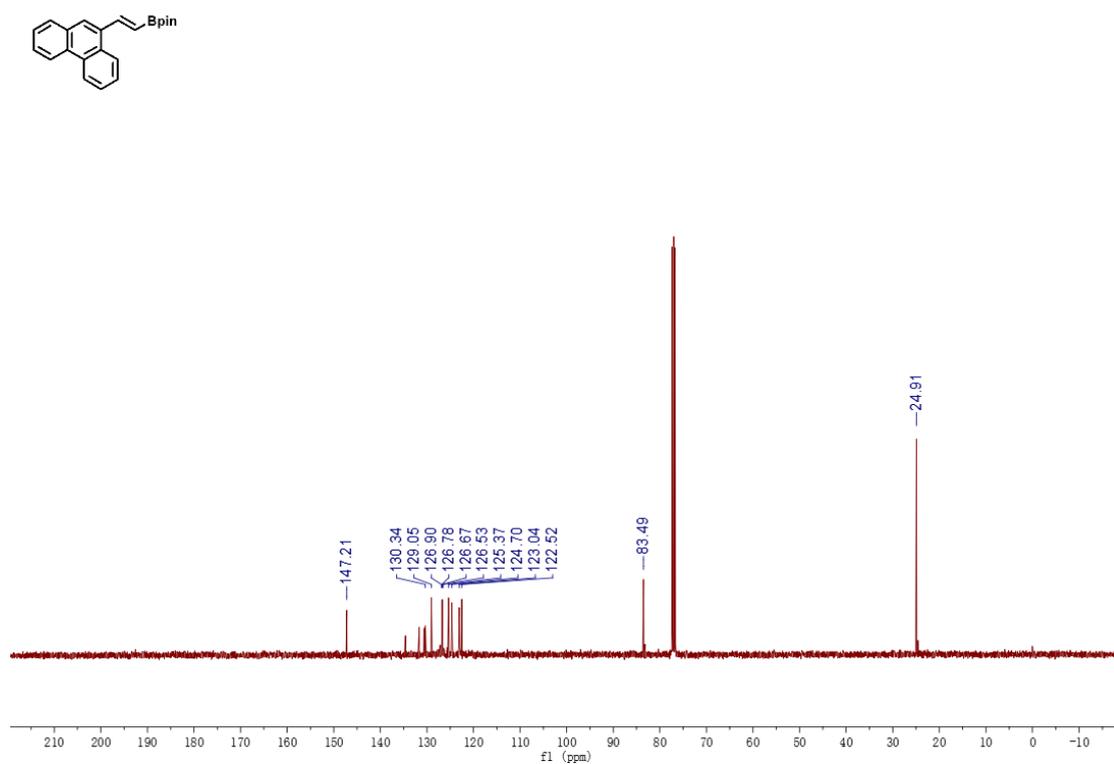
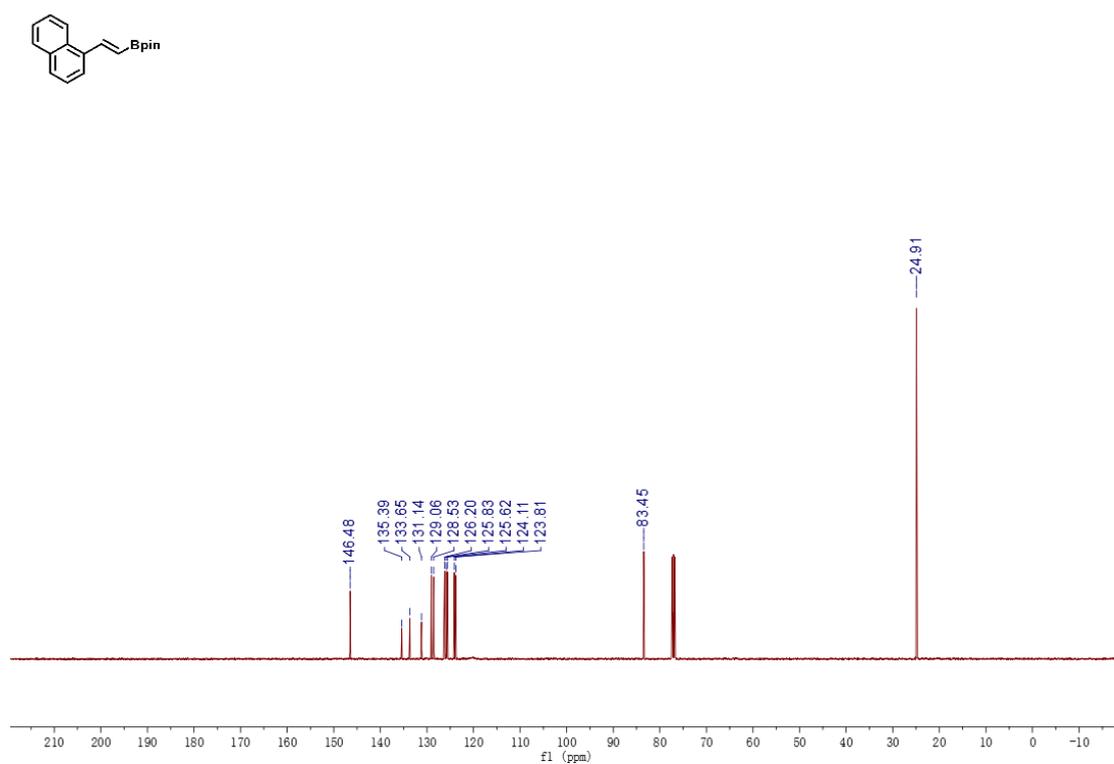
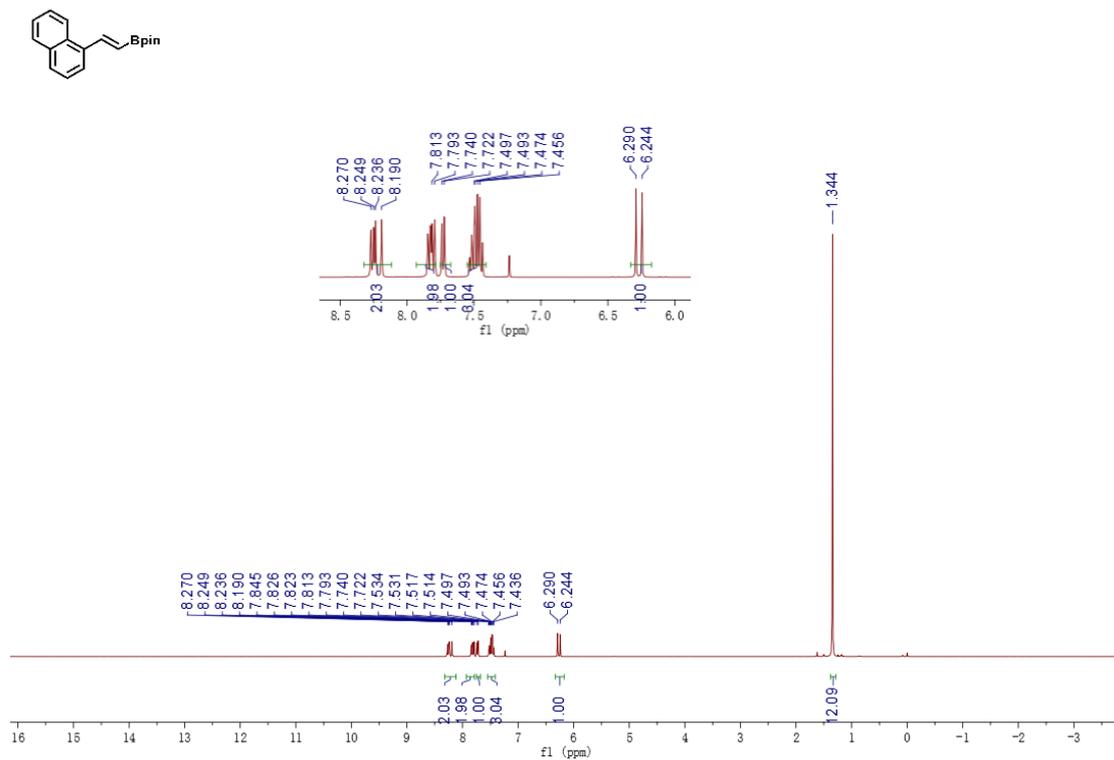


Figure S67. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2x**.



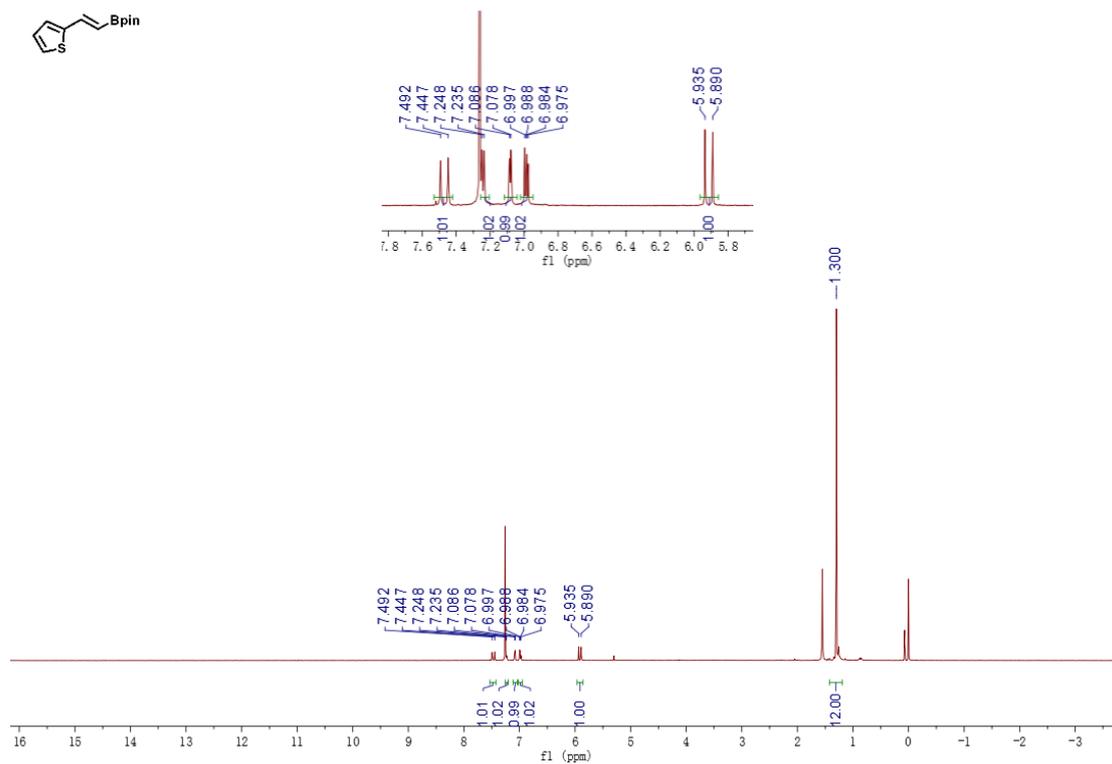


Figure S70. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2z**.

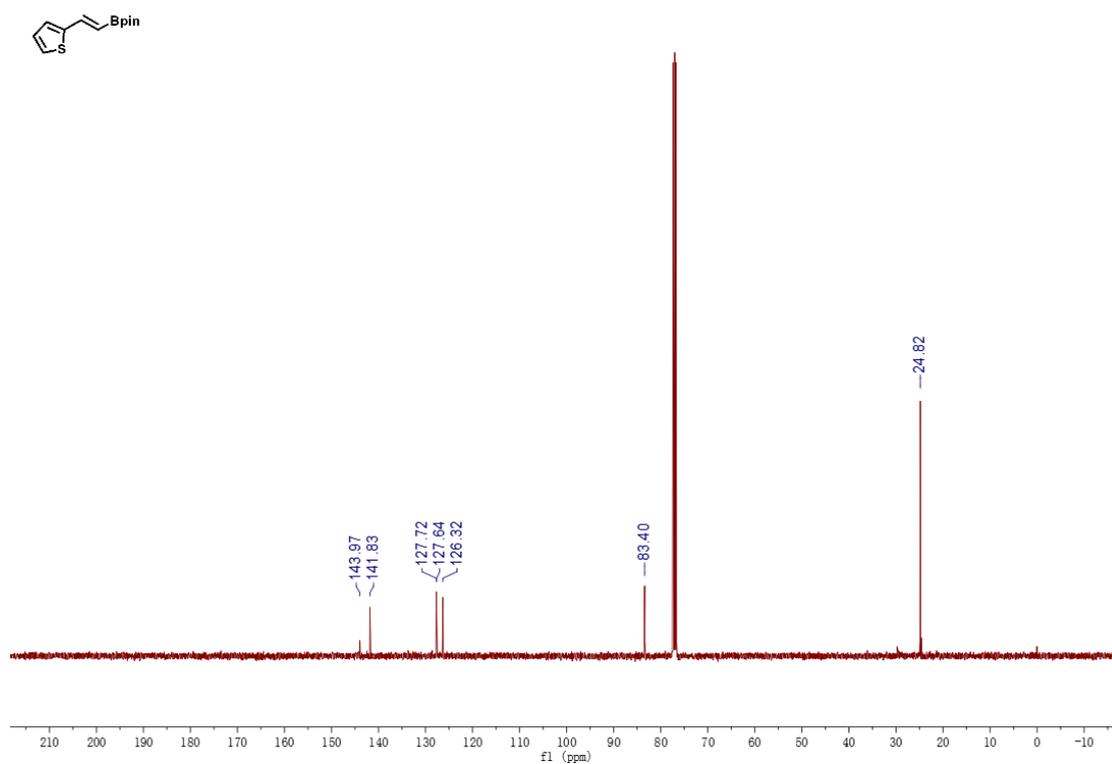


Figure S71. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2z**.

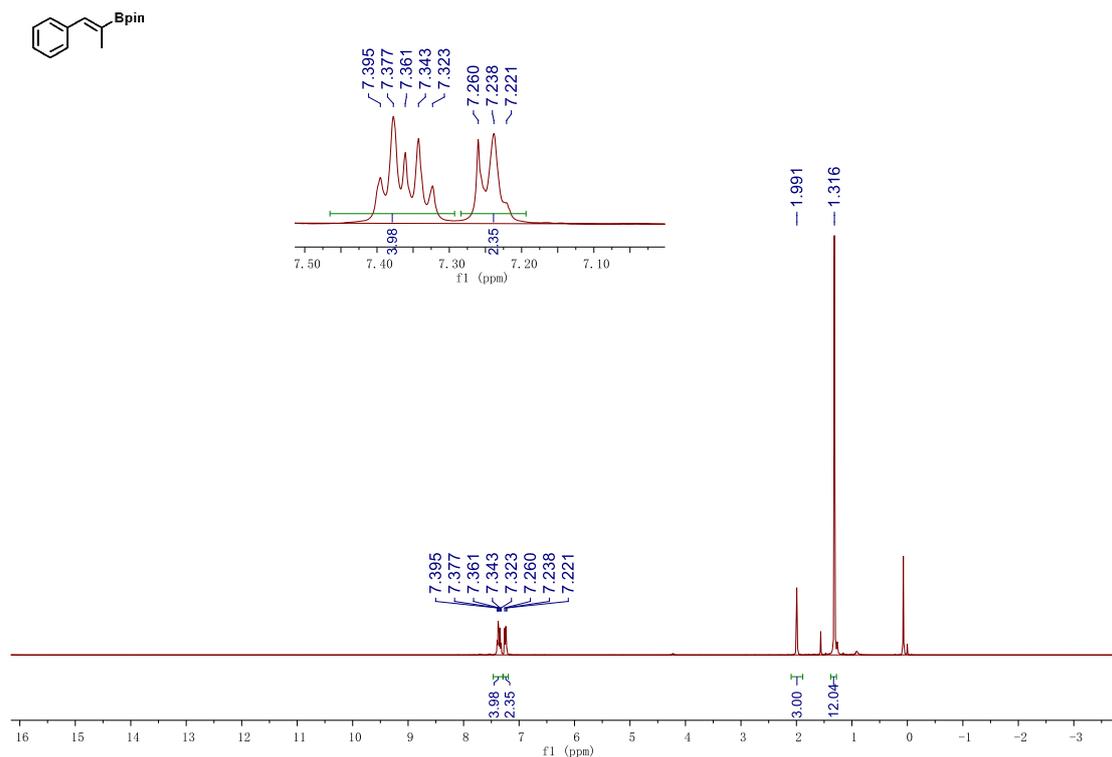


Figure S74. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2bb**.

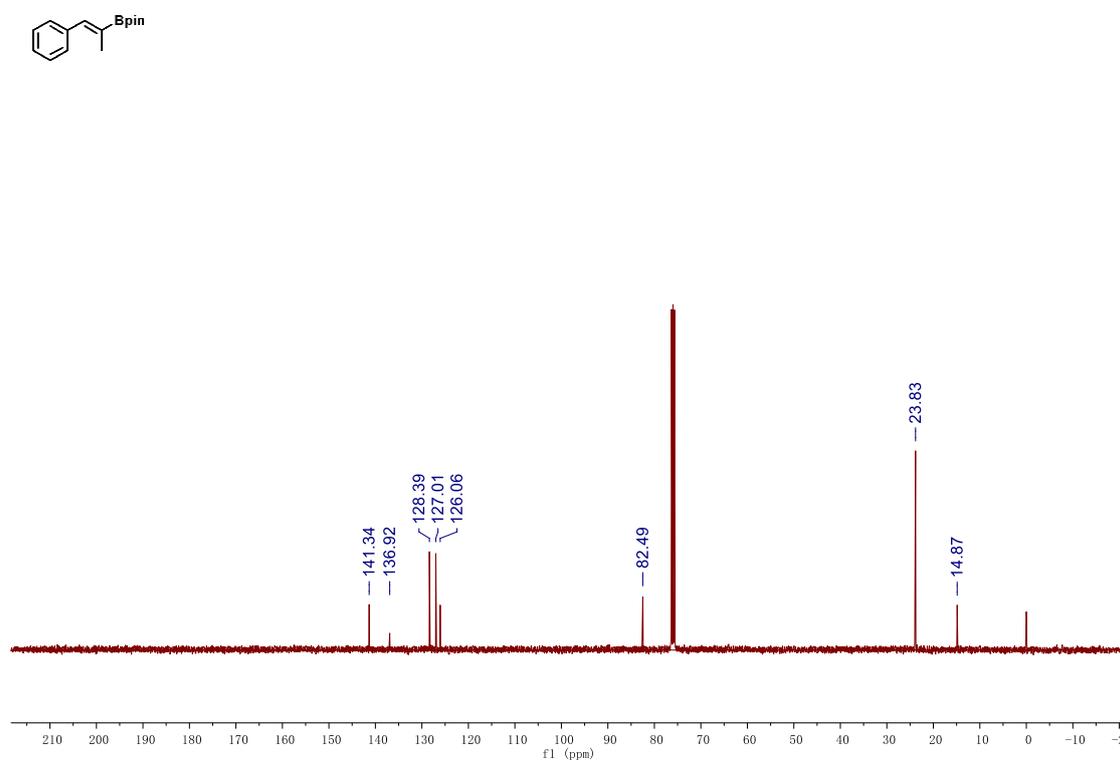


Figure S75. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **2bb**.

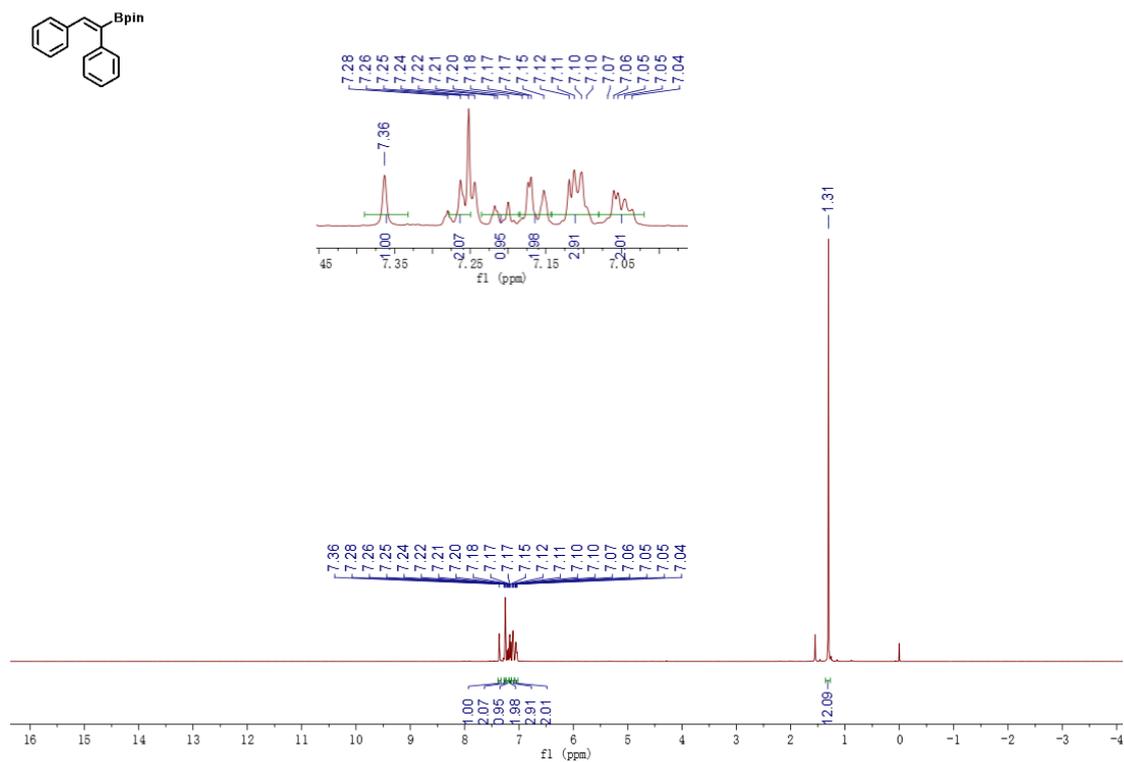


Figure S76. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2cc**.

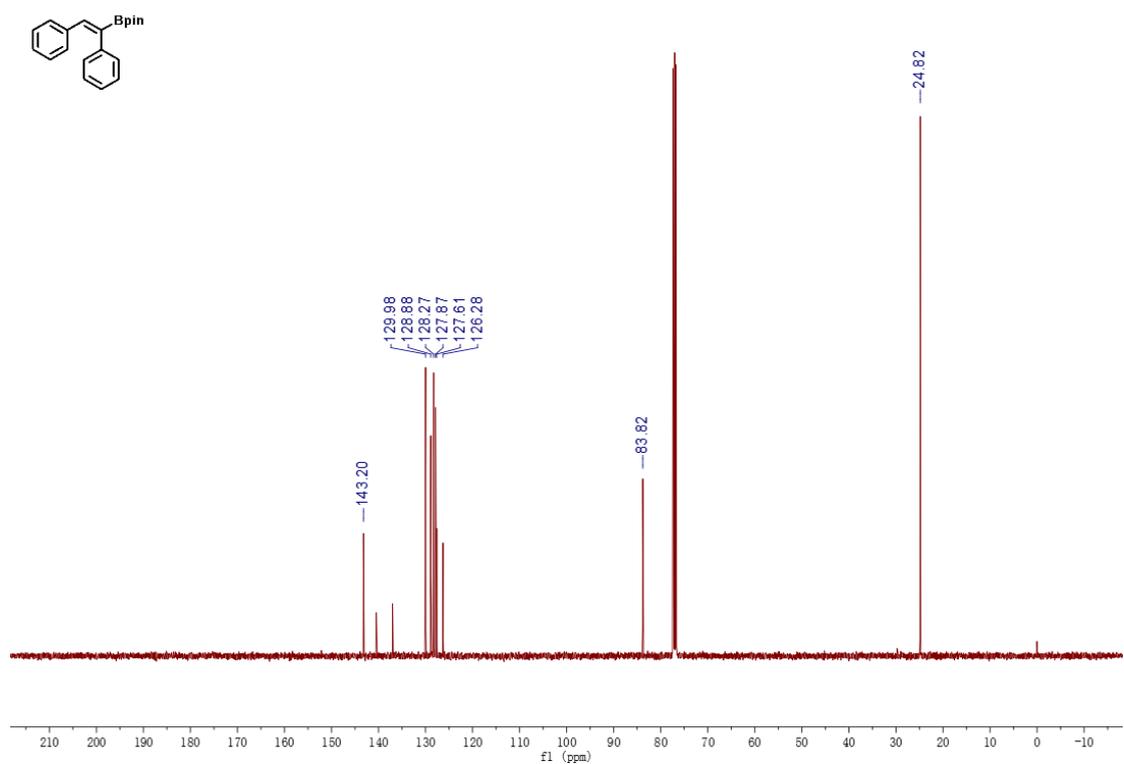


Figure S77. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2cc**.

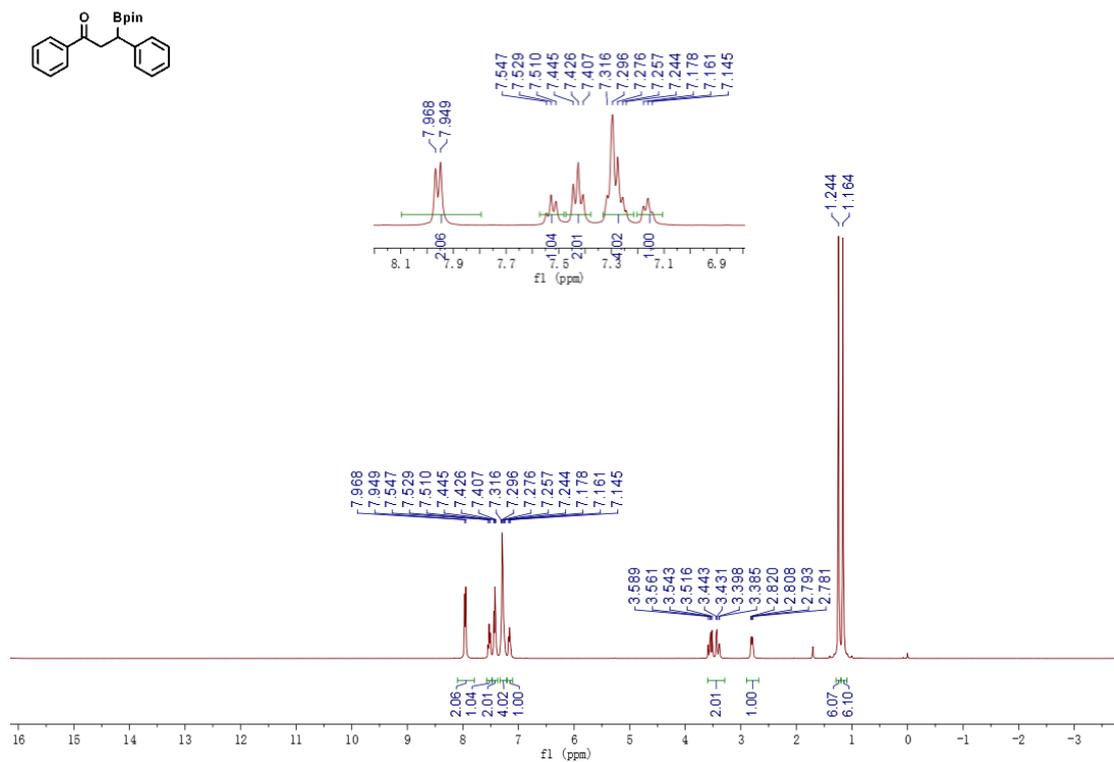


Figure S78. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2dd**.

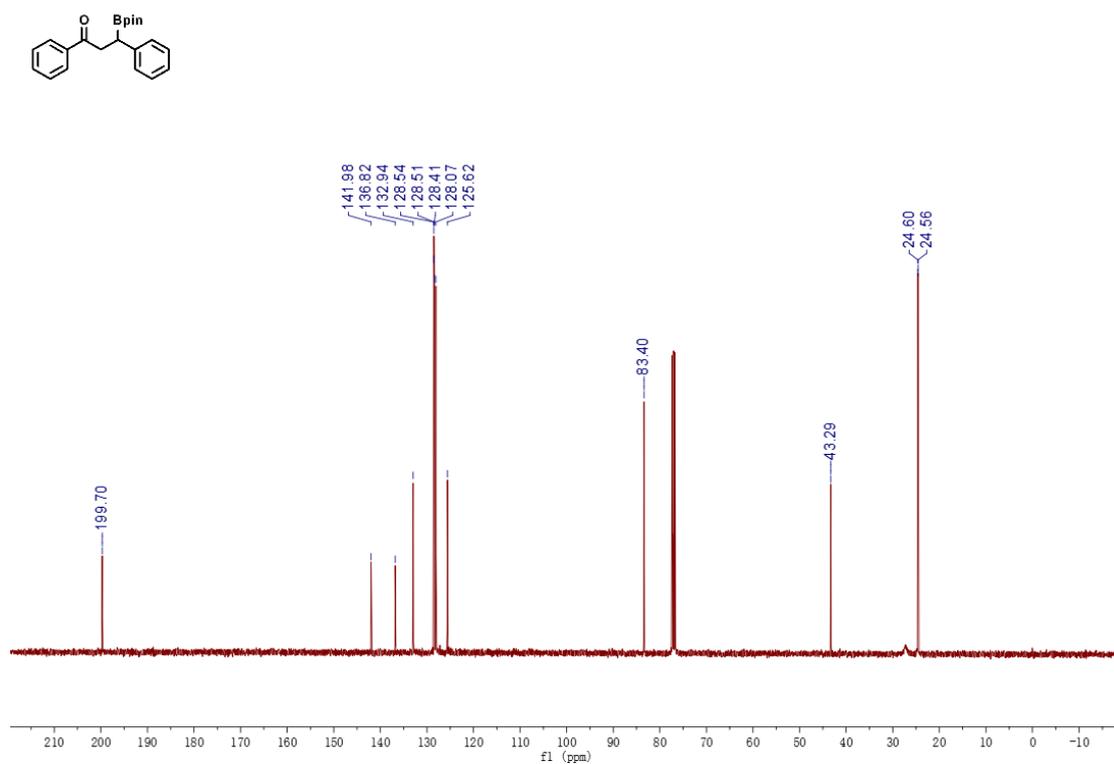


Figure S79. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2dd**.

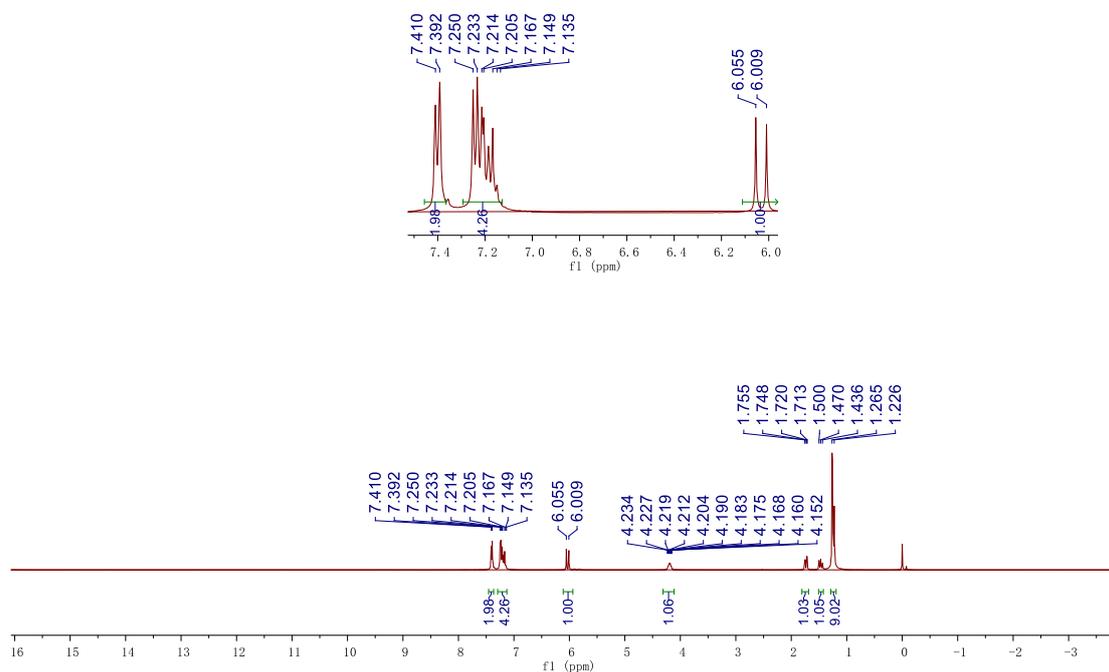
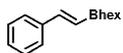


Figure S80 ¹H NMR (400 MHz, CDCl₃) spectrum of compound 2ee.

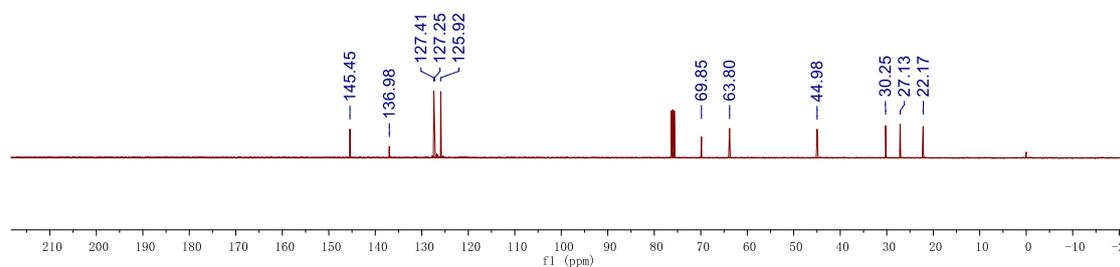
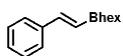


Figure S81. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 2ee.

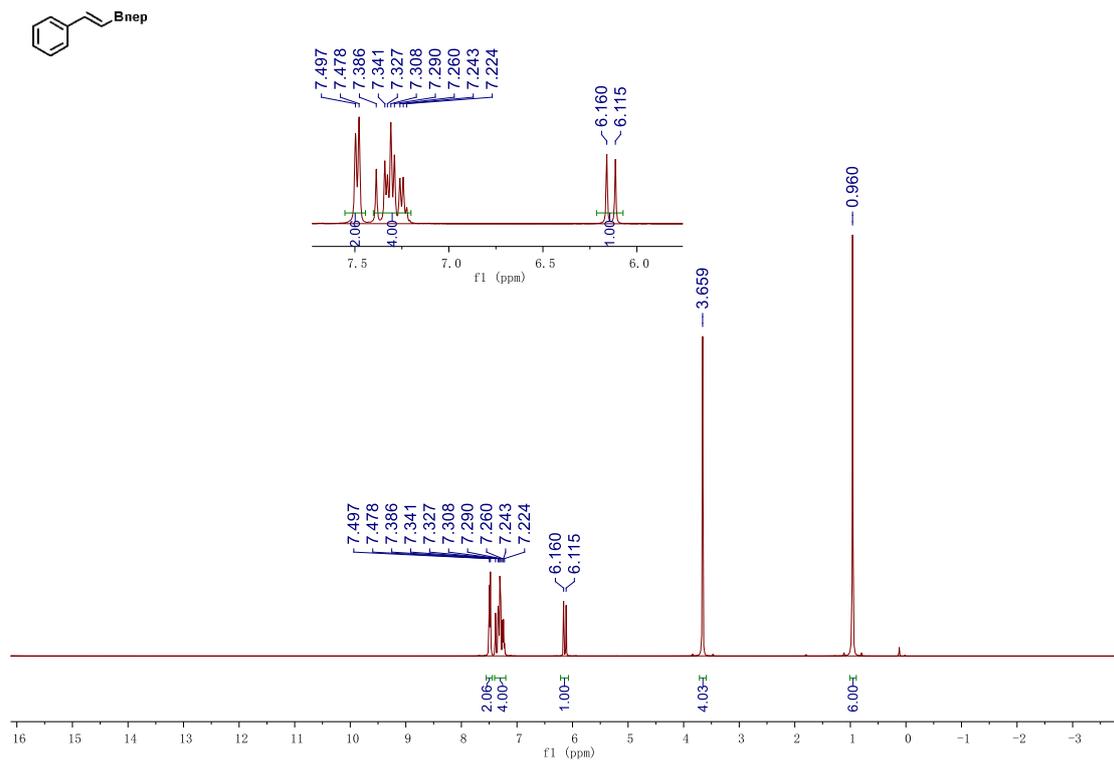


Figure S82. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2ff**.

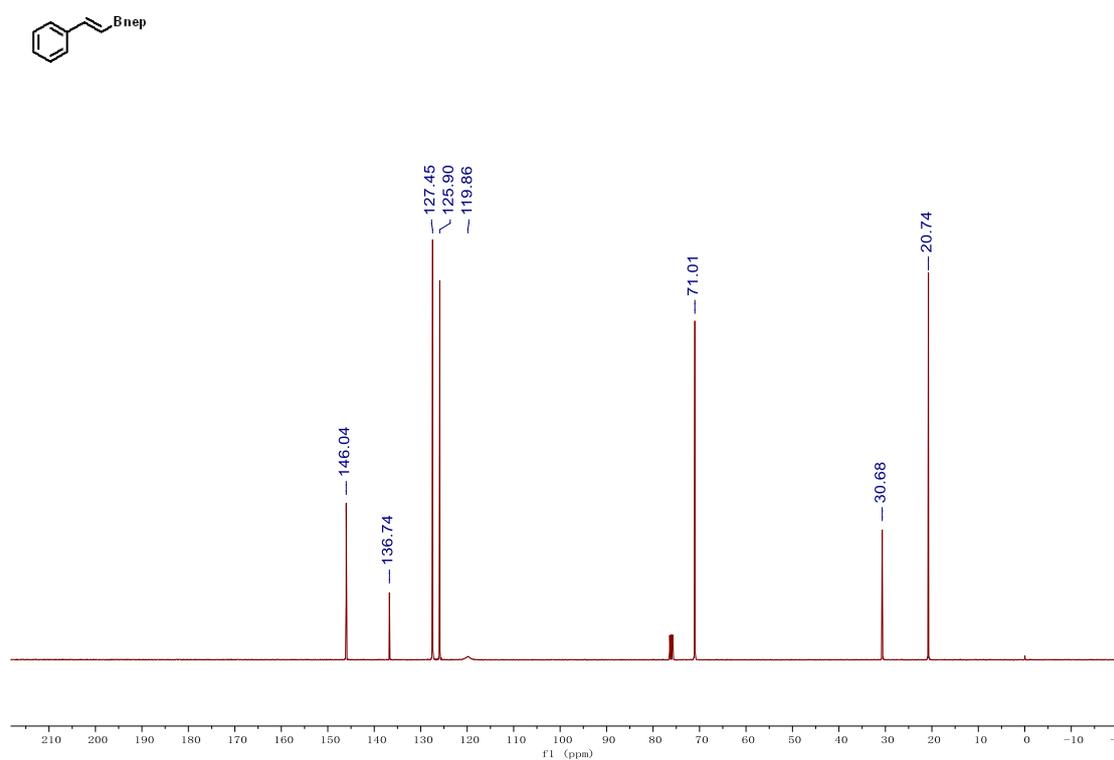


Figure S83. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2ff**.

12. NMR Spectra for Functionalized Products

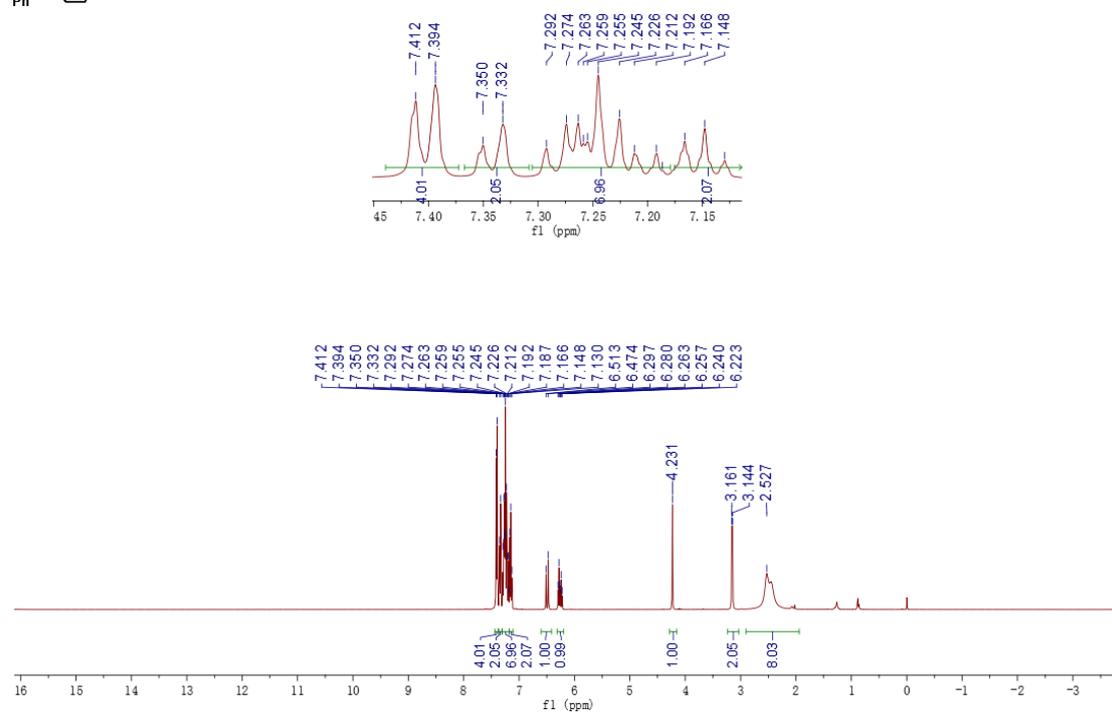
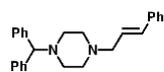


Figure S84. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 3a.

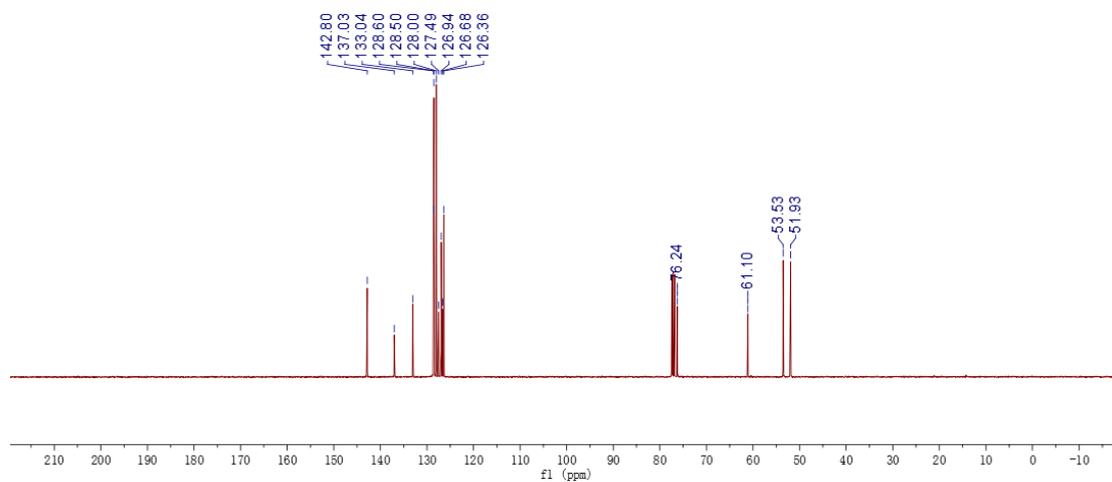
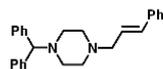


Figure S85. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 3a.

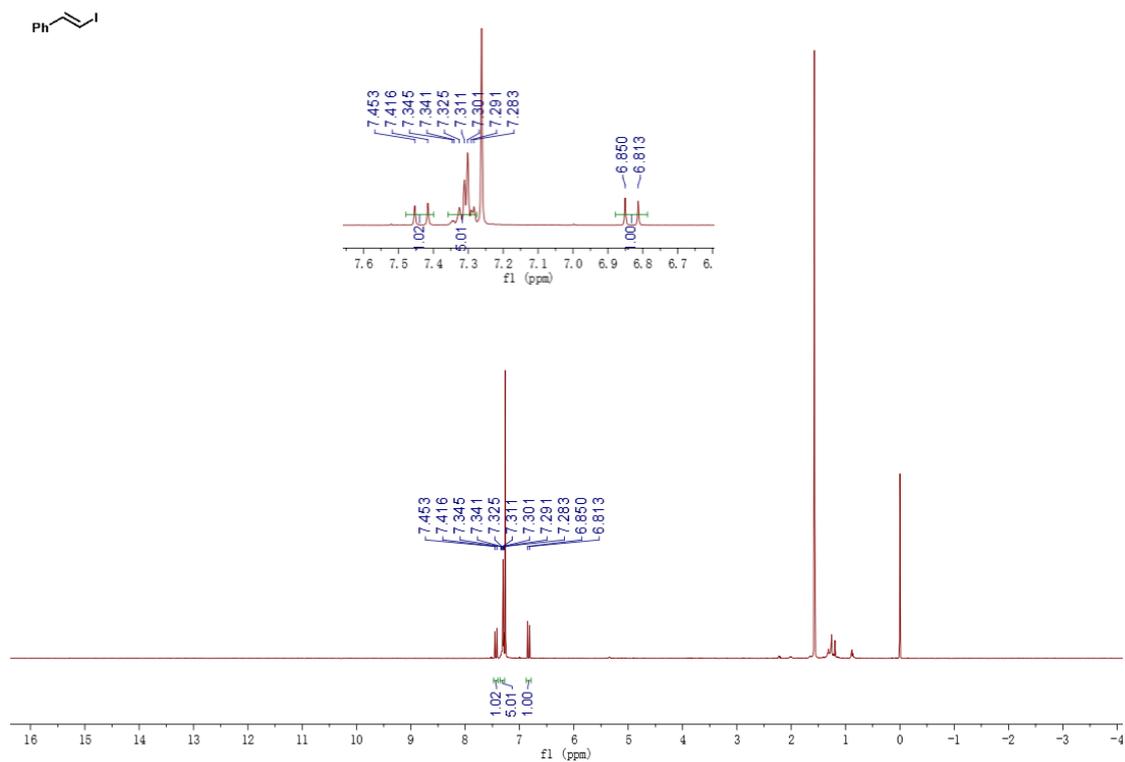


Figure S86. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3b**.

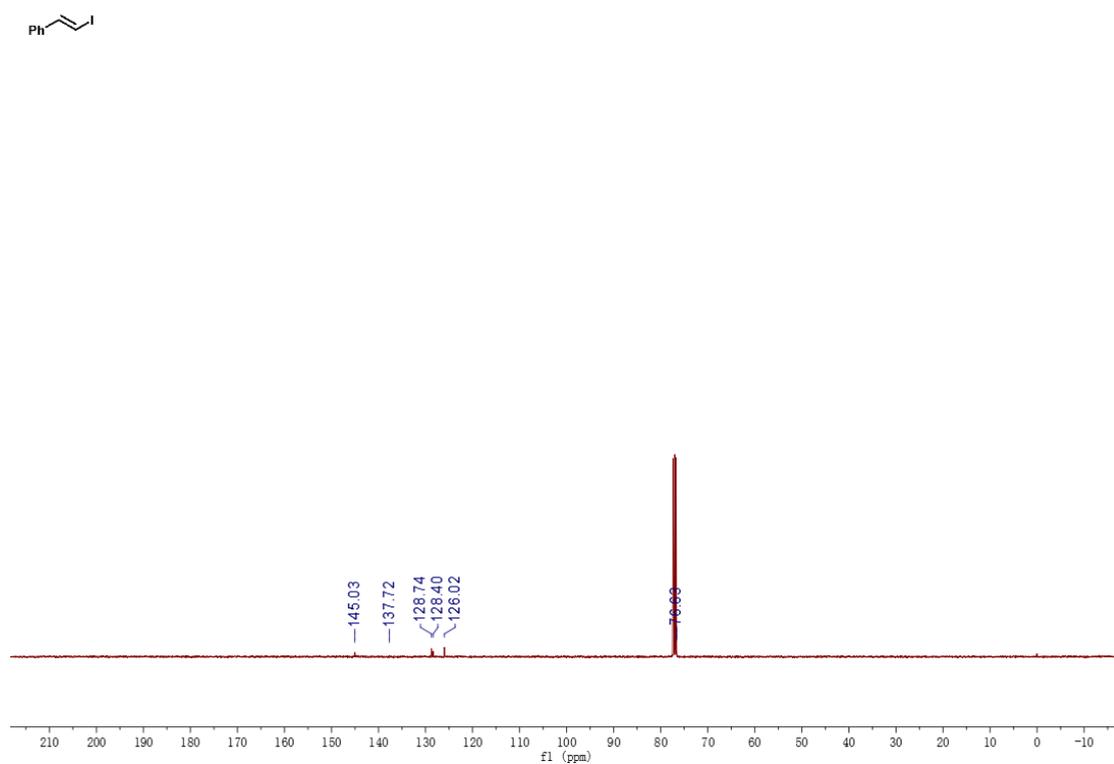


Figure S87. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **3b**.

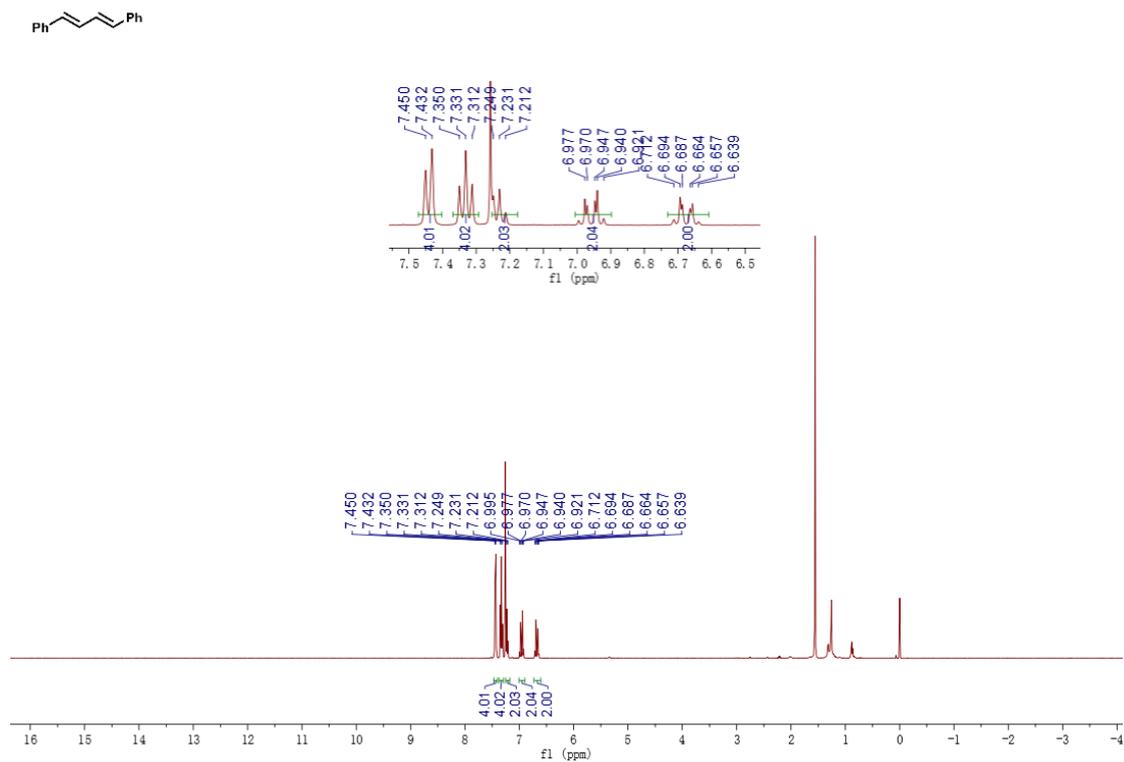


Figure S88. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **3c**.

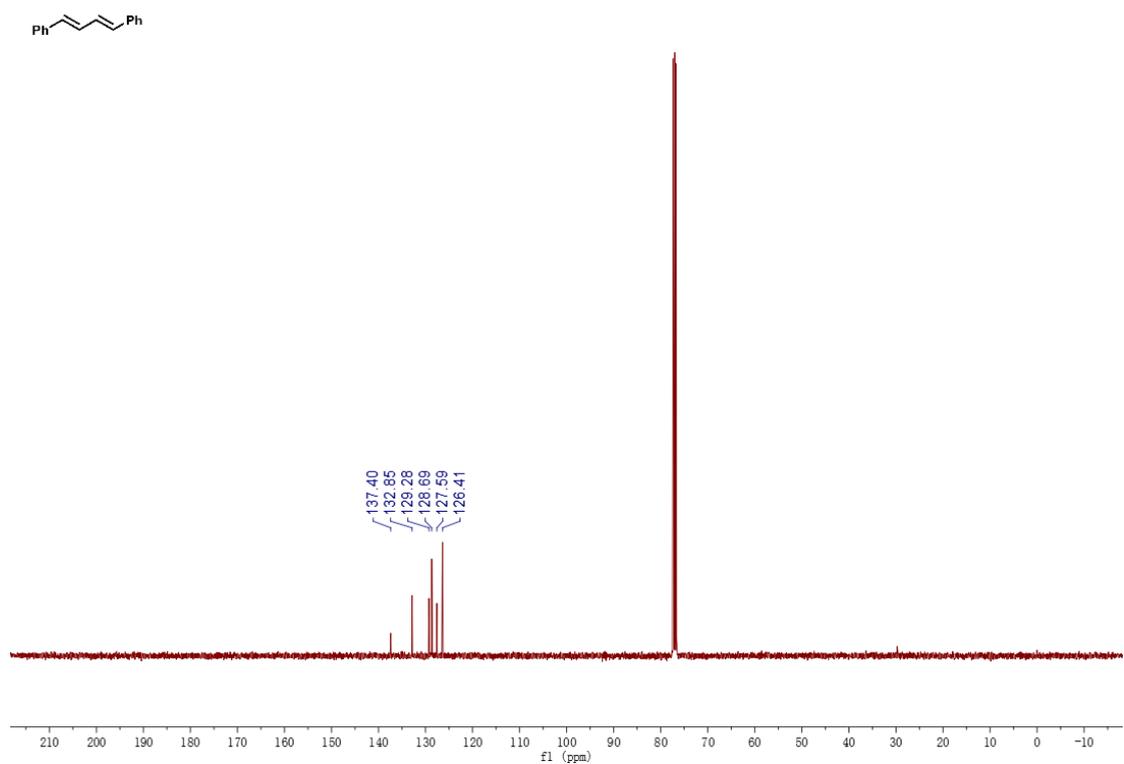


Figure S89. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **3c**.

13. Control Experiment

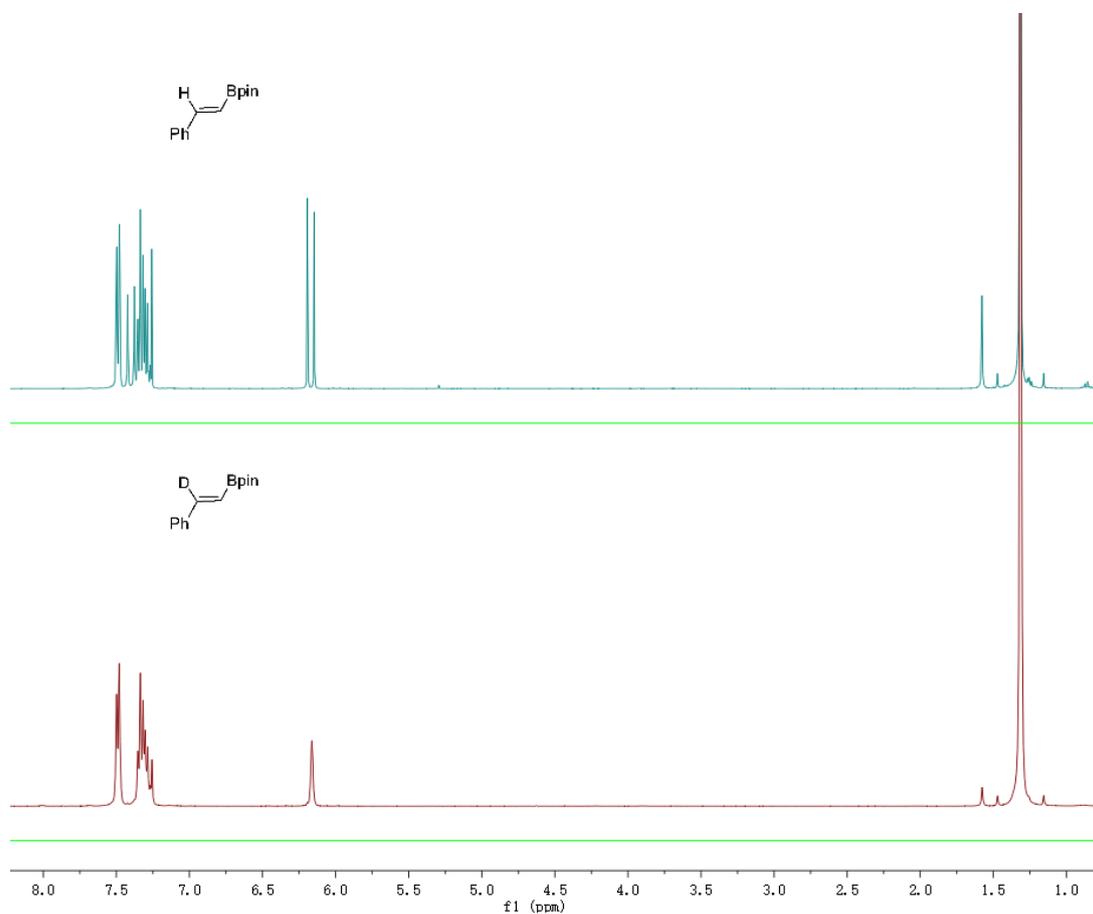


Figure S90. Deuteride Experiment

14. Details for the IR Investigations

FT-IR experiment of solid **M**:

Taking 10 mg of solid **M** drug and 50 mg of dry potassium bromide for grinding to make them fully mixed, then taking a small amount of mixed sample for tableting, and finally conducting FT-IR experiment.

FT-IR experiment of **M** in solvent:

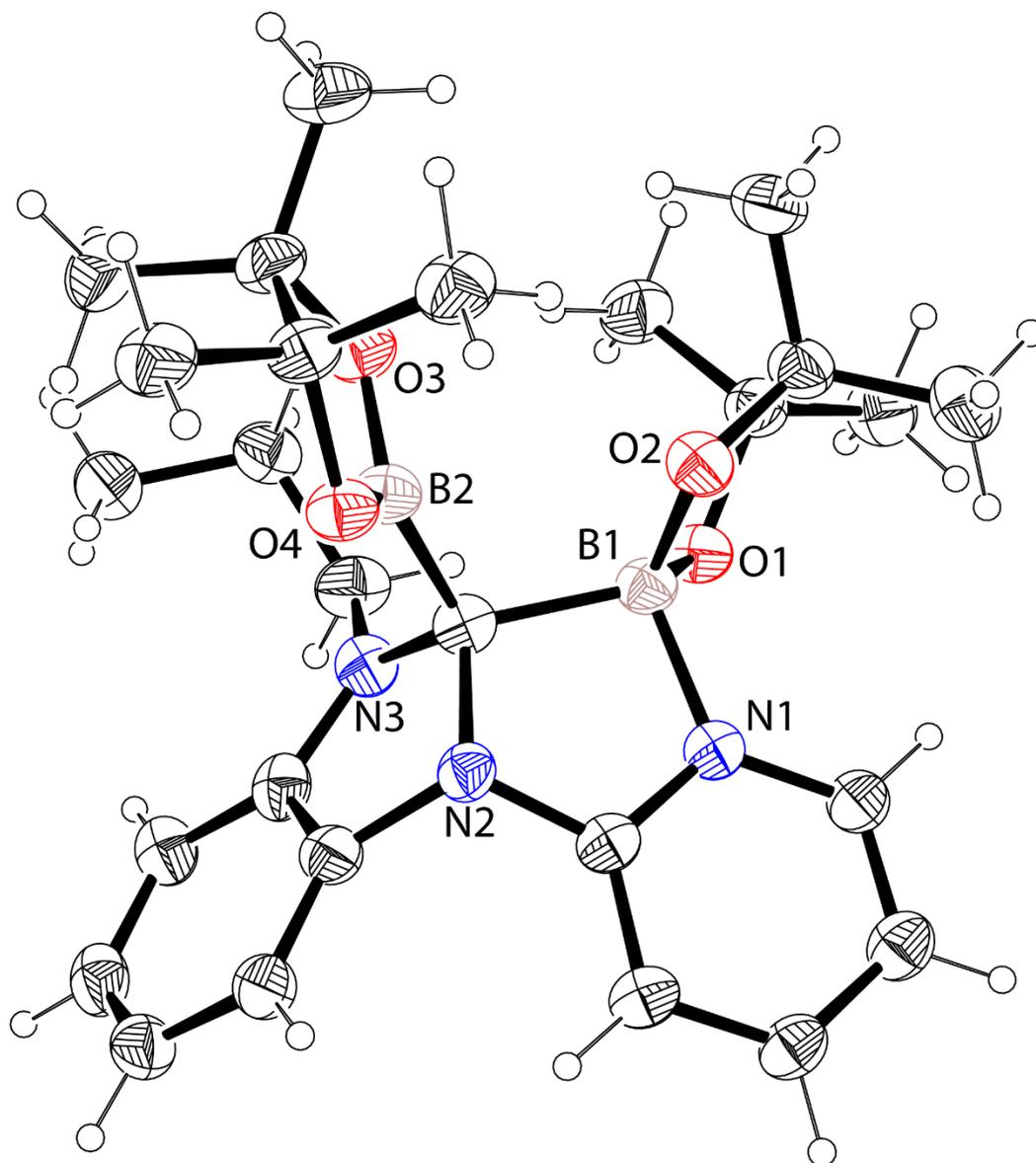
Stirring 10 mg of solid **M** and 0.5 ml of solvent (CDCl_3 , CH_2Cl_2 , THF and CH_3CN) to make them fully mixed, taking a small amount of dry potassium bromide for tableting, then adding a drop of mixed solution on the potassium bromide tablet, and finally conducting FT-IR experiment.

12. X-Ray Data for M

1. CCDC 2171688 (M) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <https://www.ccdc.cam.ac.uk/>

Crystal Data

| | |
|-----------------------------------|---|
| Identification code | 20220506_ts3_0m_5 |
| Empirical formula | C27 H39 B2 N3 O4 |
| Formula weight | 491.23 |
| Temperature | 173.0 K |
| Wavelength | 1.54178 Å |
| Crystal system | Triclinic |
| Space group | P-1 |
| Unit cell dimensions | a = 11.5388(5) Å $\alpha = 88.955(2)^\circ$. b = 15.2170(7) Å $\beta = 88.529(2)^\circ$. c = 31.3898(14) Å $\gamma = 76.813(3)^\circ$. |
| Volume | 5364.1(4) Å ³ |
| Z | 8 |
| Density (calculated) | 1.217 Mg/m ³ |
| Absorption coefficient | 0.637 mm ⁻¹ |
| F(000) | 2112 |
| Crystal size | 0.28 x 0.22 x 0.18 mm ³ |
| Theta range for data collection | 2.816 to 72.493°. |
| Index ranges | -14 ≤ h ≤ 14, -18 ≤ k ≤ 18, 0 ≤ l ≤ 38 |
| Reflections collected | 21455 |
| Independent reflections | 21455 [R(int) = 0.0851] |
| Completeness to theta = 67.679° | 99.2 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.7536 and 0.5436 |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 21455 / 70 / 1355 |
| Goodness-of-fit on F ² | 1.101 |
| Final R indices [I > 2σ(I)] | R1 = 0.0966, wR2 = 0.2478 |
| R indices (all data) | R1 = 0.1375, wR2 = 0.2946 |
| Extinction coefficient | 0.0026(2) |
| Largest diff. peak and hole | 0.460 and -0.342 e.Å ⁻³ |

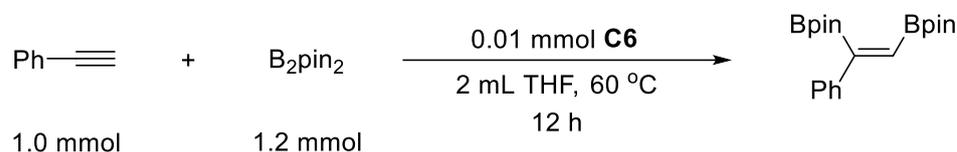


ORTEP of **M** (at 30% level)

Figure S91. X-Ray Data and structure of **M**.

16. HRMS Spectra for diboration product

HRMS (ESI) calcd for $C_{20}H_{30}B_2O_4K [M + K]^+$ 395.1967, found 395.1974.



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

103 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

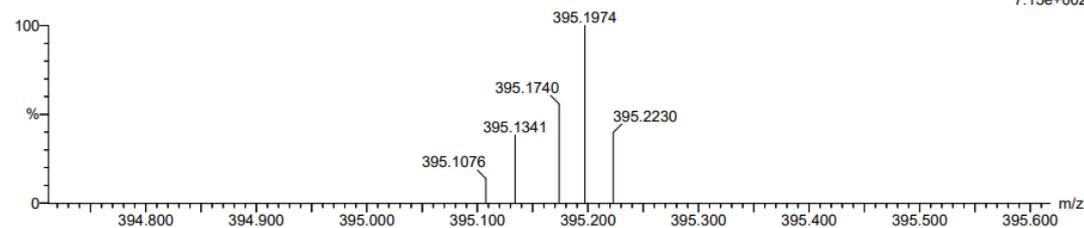
Elements Used:

C: 20-20 H: 1-50 B: 2-2 N: 0-8 O: 0-11 K: 1-1

12

221118-11-TS-1- 55 (0.321)

1: TOF MS ES+
7.15e+002



Minimum: -1.5
Maximum: 5.0 20.0 50.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|-----|-----|-----|-------|------|----------|---|
| 395.1974 | 395.1967 | 0.7 | 1.8 | 6.5 | 18.7 | n/a | n/a | C ₂₀ H ₃₀ B ₂ O ₄ K |

Figure S92. HRMS Spectra for diboration product.

17. DFT Computational Results

Table S3. Sum of total energies (E) and thermal free energy corrections (G_{correct} , a.u.) of all the calculated stationary points as well as imaginary frequency (IF, cm^{-1}) of transition states

| Species | E | E_{correct} | IF |
|-------------------------------------|--------------|----------------------|---------|
| NHC | -728.245361 | 0.367626 | - |
| B₂Pin₂ | -821.860249 | 0.286308 | - |
| 1a | -308.157359 | 0.11065 | - |
| H₂O | -76.369683 | 0.021624 | - |
| HO-Bpin | -486.773098 | 0.198503 | - |
| 1 | -1550.140622 | 0.655442 | - |
| 2-ts | -1550.115327 | 0.653804 | -448.02 |
| 3 | -1550.155145 | 0.655687 | - |
| 4-ts | -1858.262086 | 0.766142 | -541.78 |
| 5 | -1858.389 | 0.772452 | - |
| 6-ts | -1858.358588 | 0.771297 | -119.46 |
| 7 | -1858.365214 | 0.770296 | - |
| 8-ts | -1550.750784 | 0.654102 | -183.22 |
| 9 | -1550.771928 | 0.65499 | - |
| 10-ts | -1550.750784 | 0.654943 | -113.24 |
| 11 | -1550.771928 | 0.657051 | - |
| 12 | -1130.501723 | 0.480201 | - |
| 13-ts | -1130.501723 | 0.480207 | -153.27 |
| 14 | -1130.535811 | 0.481954 | - |
| 15-ts | -1130.502010 | 0.480745 | -241.02 |
| 16 | -1130.589001 | 0.482677 | - |
| 2a | -719.745824 | 0.308615 | - |

Cartesian coordinates

NHC

| | | | |
|---|-------------|-------------|-------------|
| C | 0.21207600 | -1.37257000 | -0.45043900 |
| C | -4.08868100 | -1.19084600 | -0.69189100 |
| H | -4.67832400 | -1.83343900 | -1.33749800 |
| C | -4.71321700 | -0.42910800 | 0.29464000 |
| H | -5.78954900 | -0.47788700 | 0.42104200 |
| C | -3.94907600 | 0.39166900 | 1.12062300 |
| H | -4.42586700 | 0.97748400 | 1.89953900 |
| C | -2.56640300 | 0.45435300 | 0.96561700 |

| | | | |
|---------------------------------|-------------|-------------|-------------|
| H | -1.96387300 | 1.06536000 | 1.62962100 |
| C | -1.95177300 | -0.29849400 | -0.03451500 |
| C | 0.22942400 | 0.91924900 | -0.17677100 |
| C | 1.54488800 | 0.49654000 | -0.39943600 |
| C | 2.60324400 | 1.40225400 | -0.45040900 |
| H | 3.62425600 | 1.07473900 | -0.61436800 |
| C | 2.29503600 | 2.74790400 | -0.28728300 |
| H | 3.09218000 | 3.48280900 | -0.32153900 |
| C | 0.97316500 | 3.17495800 | -0.08807600 |
| H | 0.76809300 | 4.23421300 | 0.02359700 |
| C | -0.08180700 | 2.27086600 | -0.03198100 |
| H | -1.10238300 | 2.60697700 | 0.10997100 |
| C | 2.62755800 | -1.75788800 | -0.77123300 |
| H | 3.41869600 | -1.16850000 | -1.24528900 |
| H | 2.31716900 | -2.53095900 | -1.47663300 |
| C | 3.12285200 | -2.38902300 | 0.52743500 |
| H | 2.30262400 | -2.98074500 | 0.94898500 |
| H | 3.92862300 | -3.08712800 | 0.27675700 |
| C | 3.61197600 | -1.36622200 | 1.54849100 |
| H | 2.81090000 | -0.67619600 | 1.82999400 |
| H | 4.44041100 | -0.77424400 | 1.14551600 |
| H | 3.96306500 | -1.85984200 | 2.45783800 |
| N | -0.54091400 | -0.24767100 | -0.20790900 |
| N | 1.47614100 | -0.88507800 | -0.56055300 |
| C | -2.71043000 | -1.12366900 | -0.86462800 |
| H | -2.20560100 | -1.70323600 | -1.62916000 |
| B ₂ Pin ₂ | | | |
| B | 0.85255800 | -0.00021400 | 0.00023400 |
| B | -0.85254900 | -0.00026400 | 0.00007000 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.98923600 | -0.72472100 | -0.28922800 |
| C | 3.91139500 | -1.69731000 | 0.42639800 |
| H | 3.64571200 | -1.79792700 | 1.47990800 |
| H | 4.94928800 | -1.35799400 | 0.35560100 |
| H | 3.84046300 | -2.68135900 | -0.04390100 |
| C | 3.23747600 | -0.76417300 | -1.79526100 |
| H | 3.03033500 | -1.77279400 | -2.16098700 |
| H | 4.27471400 | -0.51365400 | -2.03240500 |
| H | 2.57856900 | -0.06519500 | -2.31866200 |
| C | 2.98913200 | 0.72478200 | 0.28914200 |
| C | 3.23781400 | 0.76408800 | 1.79509500 |
| H | 3.03078000 | 1.77263000 | 2.16108800 |
| H | 4.27512400 | 0.51354400 | 2.03190500 |
| H | 2.57908800 | 0.06497900 | 2.31856000 |
| C | 3.91089300 | 1.69765100 | -0.42662300 |
| H | 3.64530200 | 1.79792600 | -1.48017600 |
| H | 4.94894100 | 1.35885200 | -0.35561400 |
| H | 3.83939600 | 2.68176300 | 0.04346300 |
| C | -2.98908600 | 0.72477400 | -0.28923200 |
| C | -3.91082700 | 1.69766100 | 0.42654500 |
| H | -3.64499700 | 1.79815400 | 1.48002700 |
| H | -4.94884700 | 1.35871200 | 0.35585300 |
| H | -3.83960100 | 2.68170700 | -0.04371400 |
| C | -3.23773600 | 0.76407200 | -1.79518200 |
| H | -3.03051700 | 1.77260200 | -2.16112400 |
| H | -4.27508100 | 0.51369900 | -2.03199800 |
| H | -2.57910100 | 0.06489000 | -2.31866400 |
| C | -2.98925400 | -0.72472300 | 0.28921500 |
| C | -3.23767700 | -0.76401900 | 1.79520200 |
| H | -3.03071100 | -1.77261700 | 2.16109400 |

| | | | |
|------------------|-------------|-------------|-------------|
| H | -4.27491400 | -0.51335200 | 2.03220500 |
| H | -2.57875200 | -0.06505100 | 2.31860800 |
| C | -3.91140000 | -1.69730600 | -0.42644100 |
| H | -3.64586600 | -1.79770300 | -1.48000300 |
| H | -4.94931600 | -1.35811200 | -0.35543600 |
| H | -3.84028200 | -2.68142300 | 0.04368600 |
| O | 1.61400900 | -1.13833100 | -0.08207300 |
| O | 1.61370500 | 1.13810900 | 0.08244800 |
| O | -1.61368000 | 1.13803600 | -0.08247200 |
| O | -1.61398100 | -1.13838200 | 0.08227300 |
| 1a | | | |
| C | -1.50994600 | -1.20710600 | -0.00000500 |
| C | -0.11962300 | -1.21159200 | 0.00000700 |
| C | 0.58572400 | -0.00002500 | 0.00001000 |
| C | -0.11959700 | 1.21157800 | 0.00000600 |
| C | -1.50990400 | 1.20713300 | -0.00000400 |
| C | -2.20699300 | 0.00001600 | -0.00001300 |
| H | -2.05065300 | -2.14774000 | -0.00000900 |
| H | 0.42968200 | -2.14715600 | 0.00001200 |
| H | 0.42975900 | 2.14711200 | 0.00001100 |
| H | -2.05060500 | 2.14777100 | -0.00000800 |
| H | -3.29201700 | 0.00004400 | -0.00002300 |
| C | 2.02269500 | -0.00002000 | 0.00002900 |
| C | 3.23025700 | 0.00000500 | 0.00001100 |
| H | 4.29815000 | 0.00003400 | -0.00022600 |
| H ₂ O | | | |
| O | 0.00000000 | 0.11903100 | 0.00000000 |
| H | 0.75742700 | -0.47612400 | 0.00000000 |

| | | | |
|---------|-------------|-------------|-------------|
| H | -0.75742700 | -0.47612400 | 0.00000000 |
| HO-Bpin | | | |
| B | 1.58581800 | -0.05265000 | -0.01253400 |
| C | -0.55171000 | -0.77132100 | -0.05198000 |
| C | -1.51985200 | -1.30989600 | -1.09147500 |
| H | -1.26748100 | -0.95399100 | -2.09172000 |
| H | -2.54270300 | -1.00197700 | -0.85449000 |
| H | -1.48409900 | -2.40232900 | -1.09308500 |
| C | -0.78364500 | -1.44472900 | 1.29826800 |
| H | -0.59691100 | -2.51630300 | 1.19435900 |
| H | -1.81094400 | -1.30203300 | 1.64286400 |
| H | -0.10151600 | -1.04623200 | 2.05525700 |
| C | -0.50809700 | 0.78944700 | 0.05399400 |
| C | -0.71604800 | 1.47579700 | -1.29331200 |
| H | -0.46854200 | 2.53526000 | -1.19159400 |
| H | -1.75351400 | 1.39141300 | -1.62661100 |
| H | -0.06590400 | 1.04003200 | -2.05792900 |
| C | -1.43121000 | 1.38158600 | 1.10493000 |
| H | -1.18621200 | 1.01333200 | 2.10253500 |
| H | -2.47228800 | 1.12986100 | 0.88132200 |
| H | -1.33604300 | 2.47044700 | 1.10417600 |
| O | 0.80039100 | -1.08746600 | -0.45880200 |
| O | 0.86637600 | 1.02763300 | 0.44401800 |
| O | 2.94160200 | -0.12900200 | -0.03338500 |
| H | 3.35348200 | 0.69114500 | 0.26038200 |
| 1 | | | |
| C | -0.90342700 | -0.14228200 | -0.28345800 |
| C | 0.16166400 | 1.05940200 | 3.88287800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 1.07037900 | 0.82978700 | 4.42949200 |
| C | -0.69648800 | 2.05944300 | 4.34020200 |
| H | -0.45455800 | 2.60904500 | 5.24376400 |
| C | -1.86436500 | 2.35356900 | 3.64020500 |
| H | -2.53279300 | 3.13079300 | 3.99473400 |
| C | -2.17688800 | 1.65282100 | 2.47715400 |
| H | -3.07600600 | 1.87624400 | 1.91090400 |
| C | -1.30713500 | 0.66371700 | 2.03210900 |
| C | -2.71778800 | -0.95921500 | 0.78126200 |
| C | -2.62385400 | -1.58340000 | -0.46392200 |
| C | -3.54190100 | -2.55570000 | -0.85930200 |
| H | -3.47226600 | -3.05092300 | -1.82104300 |
| C | -4.55148100 | -2.86723400 | 0.04155300 |
| H | -5.28637100 | -3.61794700 | -0.22775600 |
| C | -4.64359400 | -2.23544100 | 1.29390000 |
| H | -5.44802500 | -2.51012600 | 1.96721300 |
| C | -3.72674000 | -1.27099800 | 1.68974400 |
| H | -3.78633400 | -0.78432100 | 2.65688400 |
| C | -0.98265300 | -1.49296100 | -2.38486100 |
| H | -1.24986600 | -2.55003500 | -2.47736200 |
| H | 0.10634000 | -1.42128300 | -2.33812600 |
| C | -1.50936200 | -0.68382500 | -3.56769200 |
| H | -1.05565100 | 0.30780300 | -3.50991800 |
| H | -1.12663700 | -1.16490400 | -4.47458900 |
| C | -3.02939600 | -0.57889500 | -3.63522400 |
| H | -3.43428900 | -0.09395700 | -2.74096900 |
| H | -3.50013400 | -1.56244000 | -3.72963500 |
| H | -3.33086400 | 0.01779100 | -4.49979200 |
| N | -1.63666000 | -0.08031000 | 0.85278100 |
| N | -1.49575500 | -1.05099300 | -1.08340700 |

| | | | |
|---|-------------|-------------|-------------|
| B | 0.54472900 | 0.61881300 | -0.61846100 |
| B | 1.78302600 | -0.55338300 | -0.28340700 |
| C | 0.92587100 | 2.92788200 | -0.61014000 |
| C | 0.35516600 | 4.18579500 | 0.03346300 |
| H | -0.69492600 | 4.04598100 | 0.29939900 |
| H | 0.43875400 | 5.04599800 | -0.63945800 |
| H | 0.90961800 | 4.41474400 | 0.94873400 |
| C | 2.44159300 | 3.06587500 | -0.78317100 |
| H | 2.89896900 | 3.15315200 | 0.20718400 |
| H | 2.71207300 | 3.95131900 | -1.36710900 |
| H | 2.84617400 | 2.17353700 | -1.26914600 |
| C | 0.23223700 | 2.50560500 | -1.94038900 |
| C | -1.28717900 | 2.70332500 | -1.85982600 |
| H | -1.76826300 | 2.19398100 | -2.70028200 |
| H | -1.55668700 | 3.76305200 | -1.90598300 |
| H | -1.68669900 | 2.28958200 | -0.92765400 |
| C | 0.77563100 | 3.18357900 | -3.19063200 |
| H | 1.82734000 | 2.93216200 | -3.34277100 |
| H | 0.67971900 | 4.27242100 | -3.12089800 |
| H | 0.21270200 | 2.84900500 | -4.06797500 |
| C | 2.81427900 | -2.45149000 | 0.49786100 |
| C | 2.99317200 | -3.11367300 | 1.85453200 |
| H | 2.92450800 | -2.38445700 | 2.66412000 |
| H | 3.96590700 | -3.61222500 | 1.91196900 |
| H | 2.21480600 | -3.86703500 | 2.00183700 |
| C | 2.67487700 | -3.50730600 | -0.59711000 |
| H | 1.78112900 | -4.10434700 | -0.39842600 |
| H | 3.54094400 | -4.17424600 | -0.62228100 |
| H | 2.56425200 | -3.03665000 | -1.57869700 |
| C | 3.87647500 | -1.36384700 | 0.15597200 |

| | | | |
|------|-------------|-------------|-------------|
| C | 4.34873600 | -0.59460800 | 1.38899000 |
| H | 4.91718400 | 0.28000600 | 1.06271500 |
| H | 4.99002900 | -1.20948700 | 2.02598800 |
| H | 3.49410400 | -0.24760200 | 1.97913700 |
| C | 5.06568700 | -1.86307400 | -0.64834800 |
| H | 4.75170500 | -2.27028100 | -1.61118800 |
| H | 5.60222100 | -2.64111200 | -0.09600500 |
| H | 5.75799700 | -1.03730500 | -0.83263300 |
| O | 0.66428500 | 1.81899600 | 0.23726300 |
| O | 0.54139100 | 1.11729700 | -2.00437300 |
| O | 1.58946800 | -1.68422400 | 0.50039300 |
| O | 3.11333500 | -0.43412700 | -0.64535300 |
| C | -0.14289500 | 0.34969300 | 2.72648600 |
| H | 0.51237500 | -0.42781800 | 2.34249900 |
| 2-ts | | | |
| C | 0.10916600 | 0.50338800 | 0.76139200 |
| C | 0.59806400 | 3.24297300 | -3.19522800 |
| H | 1.06926900 | 3.29501100 | -4.17133300 |
| C | -0.46161800 | 4.09057400 | -2.88328200 |
| H | -0.81714900 | 4.81032800 | -3.61308100 |
| C | -1.06830600 | 4.00749500 | -1.62979800 |
| H | -1.89556800 | 4.66419800 | -1.38056600 |
| C | -0.61174800 | 3.09449100 | -0.68738600 |
| H | -1.07338600 | 3.02224800 | 0.29187600 |
| C | 0.44896700 | 2.24265100 | -1.00568900 |
| C | 2.25797700 | 1.19540200 | 0.37427900 |
| C | 2.24173500 | 0.42071100 | 1.55057700 |
| C | 3.41550300 | 0.13731000 | 2.23392900 |
| H | 3.41084800 | -0.44953900 | 3.14578500 |

| | | | |
|---|-------------|-------------|-------------|
| C | 4.61157800 | 0.65072700 | 1.71653800 |
| H | 5.54267400 | 0.43733400 | 2.23068000 |
| C | 4.62313700 | 1.43213900 | 0.56462100 |
| H | 5.56136600 | 1.82647300 | 0.18971500 |
| C | 3.43822000 | 1.72204400 | -0.12536700 |
| H | 3.44758500 | 2.34255500 | -1.01364100 |
| C | 0.46031600 | -0.73252000 | 2.92120800 |
| H | 1.34233300 | -1.21686000 | 3.35083700 |
| H | -0.17410400 | -1.51612600 | 2.49868300 |
| C | -0.29184500 | 0.05358500 | 3.99147200 |
| H | -1.15389900 | 0.53525200 | 3.51673800 |
| H | -0.68972400 | -0.65977300 | 4.72207400 |
| C | 0.59125500 | 1.08702100 | 4.68344000 |
| H | 0.99583800 | 1.79912800 | 3.95735100 |
| H | 1.43643500 | 0.60529600 | 5.18657100 |
| H | 0.03117300 | 1.65173700 | 5.43291000 |
| N | 0.92623500 | 1.32704300 | -0.04000400 |
| N | 0.91837300 | 0.12298000 | 1.83922200 |
| B | -1.32253500 | 0.06751600 | 0.49580300 |
| B | 0.03966500 | -1.12317800 | -0.36500500 |
| C | -3.39658000 | -0.03932700 | -0.42954200 |
| C | -4.47989000 | 0.90961900 | -0.91838100 |
| H | -4.42354200 | 1.86859000 | -0.39952800 |
| H | -5.47324700 | 0.47813700 | -0.76040300 |
| H | -4.35201900 | 1.09045900 | -1.98926900 |
| C | -3.33583600 | -1.28118500 | -1.31849800 |
| H | -3.02460700 | -0.98260000 | -2.32268800 |
| H | -4.30954800 | -1.77481500 | -1.38270000 |
| H | -2.60529000 | -1.99977500 | -0.93487200 |
| C | -3.47897400 | -0.40086200 | 1.08607500 |

| | | | |
|---|-------------|-------------|-------------|
| C | -3.91527000 | 0.79004000 | 1.93925700 |
| H | -3.75129000 | 0.54753400 | 2.99263700 |
| H | -4.97424600 | 1.02312500 | 1.79678300 |
| H | -3.32362800 | 1.67718100 | 1.69100300 |
| C | -4.32668300 | -1.62239800 | 1.40357800 |
| H | -3.93195100 | -2.51463100 | 0.91396100 |
| H | -5.35999500 | -1.46813300 | 1.07688600 |
| H | -4.33270900 | -1.79577600 | 2.48319100 |
| C | 1.08682500 | -3.06112100 | -0.90402500 |
| C | 2.45876600 | -3.65500200 | -0.63340300 |
| H | 3.19884300 | -2.87429600 | -0.44853500 |
| H | 2.78598700 | -4.26059200 | -1.48403400 |
| H | 2.41017100 | -4.30071600 | 0.24700300 |
| C | 0.02043200 | -4.15174200 | -0.91034800 |
| H | 0.00183700 | -4.63377100 | 0.07004800 |
| H | 0.23325100 | -4.91033100 | -1.66797600 |
| H | -0.97016100 | -3.73055500 | -1.10595900 |
| C | 1.01204300 | -2.12219700 | -2.15160000 |
| C | 2.31853400 | -1.37875600 | -2.41418400 |
| H | 2.14419900 | -0.62318500 | -3.18431300 |
| H | 3.09747600 | -2.05874100 | -2.76948400 |
| H | 2.67282800 | -0.87663000 | -1.50752700 |
| C | 0.51022500 | -2.78946200 | -3.42034700 |
| H | -0.49688300 | -3.18869800 | -3.28868800 |
| H | 1.17837800 | -3.60605200 | -3.71102200 |
| H | 0.48918600 | -2.05944500 | -4.23333800 |
| O | -2.13266500 | 0.63836300 | -0.50578400 |
| O | -2.10708100 | -0.68720300 | 1.40922200 |
| O | 0.75314500 | -2.15350000 | 0.18113700 |
| O | 0.03934900 | -1.12327500 | -1.73177500 |

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|---|-------------|-------------|-------------|
| C | 1.04938000 | 2.31058700 | -2.26375100 |
| H | 1.85112500 | 1.62240300 | -2.50991400 |
| 3 | | | |
| C | 0.23400400 | 0.40965400 | 0.01847500 |
| C | -3.58448800 | -0.65202600 | 2.64453100 |
| H | -4.63083700 | -0.38686400 | 2.76071500 |
| C | -3.12894400 | -1.89962700 | 3.06795800 |
| H | -3.81334000 | -2.60610300 | 3.52552600 |
| C | -1.78767800 | -2.23052100 | 2.88975800 |
| H | -1.41785200 | -3.19936900 | 3.21089400 |
| C | -0.90538100 | -1.32012100 | 2.31581000 |
| H | 0.14694600 | -1.56033900 | 2.21236500 |
| C | -1.35739300 | -0.06201000 | 1.89898900 |
| C | -0.66083900 | 2.21789400 | 1.24790200 |
| C | -0.03967800 | 2.74249500 | 0.10078000 |
| C | -0.09270000 | 4.10011300 | -0.17403800 |
| H | 0.38029400 | 4.50626000 | -1.06144500 |
| C | -0.76322400 | 4.94113600 | 0.73020100 |
| H | -0.81317800 | 6.00541000 | 0.52468700 |
| C | -1.34781600 | 4.42763600 | 1.87778900 |
| H | -1.85234100 | 5.08833300 | 2.57483000 |
| C | -1.29754300 | 3.05005000 | 2.15285500 |
| H | -1.75758500 | 2.64670200 | 3.04849800 |
| C | 0.79228300 | 1.81563000 | -2.04094300 |
| H | 0.16947900 | 2.63725800 | -2.42126800 |
| H | 0.41569500 | 0.89691000 | -2.50908800 |
| C | 2.24924400 | 2.01899200 | -2.45092300 |
| H | 2.81229100 | 1.13917700 | -2.12900200 |
| H | 2.29586700 | 2.04933300 | -3.54576000 |

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|---|-------------|-------------|-------------|
| C | 2.86813700 | 3.28137000 | -1.86128900 |
| H | 2.75408900 | 3.29110100 | -0.77237200 |
| H | 2.38993700 | 4.18210300 | -2.26049200 |
| H | 3.93526200 | 3.34144400 | -2.09148600 |
| N | -0.43344400 | 0.83379100 | 1.30162900 |
| N | 0.60328700 | 1.72422300 | -0.59595900 |
| B | 1.58248900 | -0.39038800 | 0.25875700 |
| B | -0.85119500 | -0.37075800 | -0.86405600 |
| C | 3.22982300 | -1.56547700 | 1.27239000 |
| C | 4.34993800 | -1.26404400 | 2.25212000 |
| H | 4.66760600 | -0.22241400 | 2.18520700 |
| H | 5.21080100 | -1.90973200 | 2.05401700 |
| H | 4.00546900 | -1.45674900 | 3.27118300 |
| C | 2.64385000 | -2.95139400 | 1.53165700 |
| H | 2.24298600 | -2.98173100 | 2.54839900 |
| H | 3.40577200 | -3.72924200 | 1.43789600 |
| H | 1.83068900 | -3.16890500 | 0.83106600 |
| C | 3.58645200 | -1.33102700 | -0.23108300 |
| C | 4.57410800 | -0.18493200 | -0.43149600 |
| H | 4.67223300 | 0.02137100 | -1.50024600 |
| H | 5.56180300 | -0.44459400 | -0.04243300 |
| H | 4.22660100 | 0.72626800 | 0.06672500 |
| C | 4.05004900 | -2.57150800 | -0.97487100 |
| H | 3.28596800 | -3.35021100 | -0.96420100 |
| H | 4.96403100 | -2.96714700 | -0.52156400 |
| H | 4.26819600 | -2.31405600 | -2.01425200 |
| C | -2.08371900 | -2.06900000 | -1.70403400 |
| C | -1.90414000 | -3.10759700 | -2.79740500 |
| H | -1.21227900 | -2.76406100 | -3.56781700 |
| H | -2.86800600 | -3.33313300 | -3.26374000 |

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|------|-------------|-------------|-------------|
| H | -1.51039700 | -4.03034400 | -2.36414500 |
| C | -2.86245400 | -2.65033500 | -0.52875300 |
| H | -2.29693800 | -3.48646300 | -0.10928200 |
| H | -3.84231200 | -3.01601800 | -0.84748500 |
| H | -2.99849400 | -1.90257900 | 0.25836400 |
| C | -2.65459300 | -0.69572300 | -2.19246400 |
| C | -2.24685700 | -0.35285700 | -3.62262000 |
| H | -2.48890900 | 0.69489600 | -3.81695100 |
| H | -2.78103100 | -0.97466400 | -4.34583000 |
| H | -1.17176200 | -0.49176300 | -3.77133600 |
| C | -4.15411000 | -0.53333900 | -2.00936100 |
| H | -4.43226200 | -0.60033000 | -0.95582600 |
| H | -4.69176200 | -1.30523300 | -2.56819200 |
| H | -4.46585400 | 0.44305800 | -2.38870900 |
| O | 2.15184700 | -0.61482600 | 1.48176700 |
| O | 2.31125000 | -0.90455200 | -0.78069900 |
| O | -0.77704300 | -1.69469000 | -1.18550900 |
| O | -1.97526600 | 0.25097800 | -1.32579400 |
| C | -2.71368400 | 0.25738500 | 2.05089400 |
| H | -3.08442400 | 1.21185600 | 1.69424900 |
| 4-ts | | | |
| C | -0.71293200 | -0.03072300 | 0.50924800 |
| B | -1.11705500 | 1.46522400 | 0.26354100 |
| N | 0.05988800 | -0.36141800 | 1.63774600 |
| C | 2.15374100 | 1.44844500 | -1.31939200 |
| O | -0.81025400 | 2.47150200 | 1.13888200 |
| O | -1.85318600 | 1.87991000 | -0.81112500 |
| B | 0.59703900 | -0.52198300 | -1.12519500 |
| N | -1.74312000 | -1.00982600 | 0.49272300 |

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|---|-------------|-------------|-------------|
| C | 1.20270200 | 0.38339000 | 2.14573800 |
| C | -0.39435700 | -1.52095100 | 2.21949000 |
| C | 3.45919100 | 1.47149700 | -0.83065100 |
| C | 0.94275400 | 1.07782600 | -1.49647400 |
| C | -1.24352600 | 3.71648200 | 0.52453000 |
| C | -2.31549700 | 3.21961500 | -0.50311200 |
| O | 1.58269600 | -1.33929200 | -0.56965900 |
| O | -0.05869800 | -1.20673900 | -2.16232000 |
| C | -1.53917400 | -1.92717100 | 1.51181000 |
| C | -3.00557500 | -0.85647900 | -0.15668500 |
| C | 2.53530000 | -0.37927600 | 2.11804300 |
| H | 1.27792400 | 1.30569200 | 1.56612700 |
| H | 0.96553800 | 0.67209000 | 3.18030700 |
| C | 0.05200400 | -2.24164000 | 3.32629100 |
| C | 4.49123700 | 0.74363500 | -1.48169500 |
| C | 3.80207700 | 2.23305800 | 0.31828300 |
| H | 0.14354000 | 1.56396700 | -2.05570200 |
| C | -0.01771200 | 4.34064700 | -0.13334600 |
| C | -1.78728800 | 4.62900300 | 1.61093400 |
| C | -3.70589700 | 3.06535600 | 0.10893100 |
| C | -2.38205400 | 4.02186900 | -1.79076200 |
| C | 1.51995000 | -2.63185700 | -1.19429400 |
| C | 0.77541200 | -2.32141200 | -2.53226600 |
| C | -2.24220400 | -3.07434500 | 1.85433900 |
| C | -4.15219000 | -0.74668100 | 0.63385100 |
| C | 3.47868100 | 0.16536700 | 3.18734500 |
| H | 2.35732600 | -1.44714000 | 2.28032800 |
| H | 2.97575900 | -0.29178800 | 1.12382200 |
| C | -0.66020700 | -3.39299800 | 3.67566500 |
| H | 0.91198300 | -1.91886400 | 3.90219800 |

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|---|-------------|-------------|-------------|
| C | 5.78038400 | 0.74672500 | -0.97525900 |
| H | 4.25164400 | 0.17419700 | -2.37406500 |
| C | 5.10388400 | 2.24171800 | 0.79295900 |
| H | 3.02995100 | 2.81114700 | 0.81775800 |
| H | 0.74774200 | 4.49798600 | 0.63137000 |
| H | -0.26106000 | 5.30685900 | -0.58290300 |
| H | 0.39780800 | 3.68364700 | -0.90201200 |
| H | -0.97683500 | 4.92043600 | 2.28359200 |
| H | -2.56288600 | 4.13328900 | 2.19635400 |
| H | -2.20636100 | 5.53702800 | 1.16708800 |
| H | -4.34287100 | 2.52518700 | -0.59702900 |
| H | -4.15831300 | 4.03808400 | 0.31850500 |
| H | -3.66329300 | 2.48749700 | 1.03747200 |
| H | -3.14653500 | 3.59684700 | -2.44604500 |
| H | -1.42617900 | 4.00681400 | -2.31755600 |
| H | -2.65145200 | 5.06068900 | -1.57760800 |
| C | 0.72329100 | -3.56967200 | -0.29213500 |
| C | 2.94180600 | -3.14925000 | -1.36095100 |
| C | -0.10111600 | -3.44758900 | -3.05739200 |
| C | 1.71955500 | -1.83313300 | -3.63126900 |
| C | -1.78115400 | -3.80614200 | 2.95177000 |
| H | -3.11895000 | -3.37914600 | 1.29356700 |
| C | -5.39492300 | -0.58693000 | 0.02936300 |
| H | -4.06146600 | -0.78226800 | 1.71534900 |
| C | -4.34374900 | -0.63226500 | -2.14014700 |
| H | 3.59723400 | 1.24918000 | 3.08750800 |
| H | 4.47149300 | -0.28415900 | 3.10432300 |
| H | 3.09389600 | -0.03772100 | 4.19274100 |
| H | -0.33492100 | -3.97335400 | 4.53252300 |
| C | 6.10170100 | 1.49307900 | 0.16286100 |

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| H | 6.54996500 | 0.16749300 | -1.47675900 |
| H | 5.34443100 | 2.83005100 | 1.67368700 |
| H | 1.13854100 | -3.53149500 | 0.71977000 |
| H | 0.76835900 | -4.60072700 | -0.65568500 |
| H | -0.32314300 | -3.26163400 | -0.24138600 |
| H | 3.37366000 | -3.34297600 | -0.37472900 |
| H | 3.57013700 | -2.41697900 | -1.87207500 |
| H | 2.95128300 | -4.08523000 | -1.92851600 |
| H | -0.89093100 | -3.69948500 | -2.34739100 |
| H | -0.56790800 | -3.14071700 | -3.99745100 |
| H | 0.49859300 | -4.34272300 | -3.25075500 |
| H | 1.12344100 | -1.45552700 | -4.46616000 |
| H | 2.36132400 | -2.63933300 | -3.99703500 |
| H | 2.34987000 | -1.01703700 | -3.26524800 |
| H | -2.30997600 | -4.70531900 | 3.24867800 |
| C | -5.49327400 | -0.52552600 | -1.35957400 |
| H | -6.28431000 | -0.50245600 | 0.64530900 |
| H | -4.41758200 | -0.58766600 | -3.22205800 |
| H | 7.11592900 | 1.49793500 | 0.54682000 |
| H | -6.46225000 | -0.39696000 | -1.83074300 |
| C | -3.09597600 | -0.80521500 | -1.54623800 |
| H | -2.19108800 | -0.89670900 | -2.13636800 |

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|---|-------------|-------------|-------------|
| C | -0.08074100 | -0.85085600 | -0.60357100 |
| C | -0.12153100 | -3.14673700 | 3.59837900 |
| H | -0.09396100 | -4.14733300 | 4.01633700 |
| C | 0.14939700 | -2.04195200 | 4.40206100 |
| H | 0.38544700 | -2.18007800 | 5.45187800 |
| C | 0.11830200 | -0.75995100 | 3.85535300 |

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|---|-------------|-------------|-------------|
| H | 0.33076000 | 0.10335600 | 4.47732000 |
| C | -0.19189400 | -0.57636400 | 2.51186600 |
| H | -0.21106500 | 0.41179200 | 2.06790800 |
| C | -0.45113400 | -1.68752000 | 1.71670900 |
| C | -1.96369700 | -2.02726100 | -0.21799100 |
| C | -1.94596700 | -1.65326000 | -1.56285700 |
| C | -2.99069800 | -1.98760900 | -2.42549900 |
| H | -2.99043900 | -1.68732600 | -3.46727700 |
| C | -4.04268500 | -2.71413400 | -1.88595100 |
| H | -4.87529000 | -2.99244500 | -2.52249700 |
| C | -4.05840600 | -3.09206900 | -0.53125100 |
| H | -4.90209000 | -3.65538200 | -0.14789500 |
| C | -3.02221600 | -2.75377600 | 0.32849100 |
| H | -3.03522100 | -3.03589000 | 1.37535700 |
| C | -0.30702200 | -0.48328900 | -3.07975600 |
| H | -0.89861100 | -1.02583100 | -3.82169900 |
| H | 0.73706800 | -0.76802600 | -3.17878000 |
| C | -0.47004500 | 1.02091200 | -3.25086700 |
| H | 0.03985300 | 1.51881300 | -2.41819500 |
| H | 0.05661800 | 1.30682100 | -4.16772200 |
| C | -1.93201700 | 1.44484200 | -3.32202700 |
| H | -2.45307900 | 1.14052000 | -2.40957400 |
| H | -2.43308200 | 0.98123900 | -4.17860200 |
| H | -2.02558200 | 2.52959400 | -3.42472200 |
| N | -0.79122500 | -1.52172600 | 0.33644300 |
| N | -0.76072100 | -0.95630600 | -1.76173500 |
| B | -1.22787500 | 2.14976400 | 0.32386400 |
| B | 1.43113700 | -0.14811700 | -0.37160600 |
| C | -3.35894500 | 2.90856300 | 0.64446800 |
| C | -4.12485400 | 3.49400500 | 1.82057400 |

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|---|-------------|-------------|-------------|
| H | -3.70270100 | 3.17016300 | 2.77319100 |
| H | -5.17562000 | 3.19098600 | 1.77979500 |
| H | -4.08266400 | 4.58538900 | 1.77682800 |
| C | -3.82788400 | 3.54706300 | -0.66022600 |
| H | -3.62252300 | 4.61967900 | -0.62071100 |
| H | -4.90121900 | 3.40366200 | -0.81026800 |
| H | -3.29368500 | 3.12405000 | -1.51516100 |
| C | -3.34318100 | 1.34732800 | 0.59105700 |
| C | -3.37442200 | 0.70675600 | 1.97625400 |
| H | -3.15075800 | -0.35908400 | 1.87418800 |
| H | -4.35770500 | 0.81526100 | 2.44162300 |
| H | -2.62158400 | 1.15039500 | 2.63510700 |
| C | -4.41450700 | 0.73036600 | -0.29170400 |
| H | -4.33478400 | 1.06875800 | -1.32606400 |
| H | -5.40618000 | 1.00013100 | 0.08594500 |
| H | -4.32532400 | -0.35911900 | -0.27486900 |
| C | 3.27684800 | -1.11284200 | -1.50841600 |
| C | 3.35668300 | -2.00616000 | -2.74625100 |
| H | 2.41856400 | -2.53801700 | -2.92081500 |
| H | 4.16090900 | -2.74321600 | -2.64688000 |
| H | 3.56919400 | -1.39039700 | -3.62574200 |
| C | 4.55825500 | -0.27774300 | -1.43087200 |
| H | 4.59583800 | 0.37759500 | -2.30635500 |
| H | 5.44972800 | -0.91332300 | -1.43830600 |
| H | 4.57273800 | 0.34924600 | -0.53780000 |
| C | 2.96889400 | -1.88913500 | -0.18145900 |
| C | 2.14640800 | -3.16219100 | -0.42388500 |
| H | 1.79485000 | -3.54002900 | 0.54059200 |
| H | 2.74236800 | -3.94241200 | -0.90695400 |
| H | 1.27195700 | -2.96707600 | -1.05285500 |

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| C | 4.20598800 | -2.24598100 | 0.63547500 |
| H | 4.74184400 | -1.34404000 | 0.94012500 |
| H | 4.88456200 | -2.88641100 | 0.06228900 |
| H | 3.90429400 | -2.78871100 | 1.53649700 |
| O | -1.95839800 | 3.22269600 | 0.79195700 |
| O | -2.03235200 | 1.07053800 | 0.03383800 |
| O | 2.16349600 | -0.23420700 | -1.64451700 |
| O | 2.19060200 | -0.96455500 | 0.56736400 |
| C | 4.75360900 | 2.13798000 | 1.63456700 |
| C | 3.48377000 | 1.60288600 | 1.43449200 |
| C | 2.70968800 | 1.99439600 | 0.33403300 |
| C | 3.23988900 | 2.93279600 | -0.55722300 |
| C | 4.51704500 | 3.45692500 | -0.36713300 |
| C | 5.27932000 | 3.06047800 | 0.72931600 |
| H | 5.33816200 | 1.83108800 | 2.49704800 |
| H | 3.08354600 | 0.86371500 | 2.12045500 |
| H | 2.64537700 | 3.23831100 | -1.41429900 |
| H | 4.91664400 | 4.17609900 | -1.07597300 |
| H | 6.27325900 | 3.46988400 | 0.88053500 |
| C | 1.34473700 | 1.42202200 | 0.12000200 |
| C | 0.32055900 | 2.29154700 | 0.28719100 |
| H | 0.61420800 | 3.31139300 | 0.56076900 |
| C | -0.42062600 | -2.97399000 | 2.24922900 |
| H | -0.61559800 | -3.82785200 | 1.60735300 |
| 6-ts | | | |
| C | 0.35083000 | -0.53509500 | 0.44934400 |
| C | 4.25913700 | -1.25444100 | -2.35803200 |
| H | 5.33634300 | -1.38381400 | -2.35832600 |
| C | 3.57879600 | -1.00970700 | -3.54760500 |

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| H | 4.11890800 | -0.96394300 | -4.48738800 |
| C | 2.20143000 | -0.80468100 | -3.51551600 |
| H | 1.66182600 | -0.59221600 | -4.43323300 |
| C | 1.49567500 | -0.87504600 | -2.31776300 |
| H | 0.42567600 | -0.71140200 | -2.29249900 |
| C | 2.17831000 | -1.15513900 | -1.13628900 |
| C | 1.90549400 | -2.06606300 | 1.16508400 |
| C | 1.05900200 | -1.76561600 | 2.23293700 |
| C | 1.16737900 | -2.41090200 | 3.46608400 |
| H | 0.51439800 | -2.16671300 | 4.29601800 |
| C | 2.13944300 | -3.39327500 | 3.58242000 |
| H | 2.25286700 | -3.92020500 | 4.52345300 |
| C | 2.96420900 | -3.73110900 | 2.49725500 |
| H | 3.69610300 | -4.52308100 | 2.61167300 |
| C | 2.86105100 | -3.08166800 | 1.27507300 |
| H | 3.48419500 | -3.37475400 | 0.44019800 |
| C | -0.87916000 | -0.23440200 | 2.61786200 |
| H | -1.13568600 | -0.98778000 | 3.36951900 |
| H | -1.76693000 | -0.06988000 | 2.01104700 |
| C | -0.42678100 | 1.06388000 | 3.28081000 |
| H | -0.24689000 | 1.80700100 | 2.49847100 |
| H | -1.26804800 | 1.42373800 | 3.88488800 |
| C | 0.81740700 | 0.92793200 | 4.15281300 |
| H | 1.67502900 | 0.58314900 | 3.56643400 |
| H | 0.66037500 | 0.21618100 | 4.96979500 |
| H | 1.08407800 | 1.89185900 | 4.59387100 |
| N | 1.47448800 | -1.25722800 | 0.10436200 |
| N | 0.15250800 | -0.82433700 | 1.75886600 |
| B | 0.45052000 | 2.36765100 | -0.11210800 |
| B | -1.66352600 | -0.24104100 | -0.54895400 |

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| C | 2.38439400 | 2.96098300 | -1.13410900 |
| C | 3.48499200 | 2.27785700 | -1.92330000 |
| H | 3.58073300 | 1.22903500 | -1.64205400 |
| H | 4.44125300 | 2.78351100 | -1.75424300 |
| H | 3.25551700 | 2.32599000 | -2.99135900 |
| C | 2.11935200 | 4.35896800 | -1.69133400 |
| H | 1.78622900 | 4.26603200 | -2.72796100 |
| H | 3.02284500 | 4.97379900 | -1.67058300 |
| H | 1.33524900 | 4.86797700 | -1.12251900 |
| C | 2.58863200 | 2.96063500 | 0.41476100 |
| C | 3.30476000 | 1.71377600 | 0.92429500 |
| H | 3.25246600 | 1.69820400 | 2.01636600 |
| H | 4.35696000 | 1.70774500 | 0.62600000 |
| H | 2.82545000 | 0.81034000 | 0.53923200 |
| C | 3.25064500 | 4.21230600 | 0.96921200 |
| H | 2.66712000 | 5.10659300 | 0.74483300 |
| H | 4.25319100 | 4.33106600 | 0.54675800 |
| H | 3.34592600 | 4.12501000 | 2.05480000 |
| C | -2.35327500 | -2.44775400 | -0.59051600 |
| C | -1.19424400 | -3.34025500 | -0.14313000 |
| H | -0.22309400 | -2.91366600 | -0.39988500 |
| H | -1.26454800 | -4.32942500 | -0.60478300 |
| H | -1.24329900 | -3.45951300 | 0.94365400 |
| C | -3.66624300 | -3.16822700 | -0.30862700 |
| H | -3.67377600 | -3.51225100 | 0.72927000 |
| H | -3.77349700 | -4.04236200 | -0.95805900 |
| H | -4.52286500 | -2.50877400 | -0.45701500 |
| C | -2.20311300 | -1.92068600 | -2.06041500 |
| C | -1.35512800 | -2.80448000 | -2.96722400 |
| H | -1.27029600 | -2.33773400 | -3.95315100 |

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| H | -1.83070100 | -3.78229900 | -3.09225700 |
| H | -0.34873300 | -2.95386400 | -2.57345600 |
| C | -3.54807800 | -1.65706900 | -2.73629200 |
| H | -4.20542800 | -1.06974800 | -2.09210900 |
| H | -4.05409900 | -2.59300700 | -2.98880900 |
| H | -3.37445400 | -1.09653300 | -3.65912200 |
| O | 1.15136900 | 2.21629700 | -1.28479100 |
| O | 1.22633100 | 2.90062800 | 0.89558600 |
| O | -2.33367200 | -1.23737300 | 0.17804500 |
| O | -1.55205100 | -0.64315500 | -1.88838000 |
| C | -5.69794100 | 1.63475300 | -0.74889600 |
| C | -4.34533400 | 1.37705200 | -0.95416600 |
| C | -3.41594700 | 1.55558000 | 0.07779800 |
| C | -3.87631000 | 2.00359500 | 1.32142300 |
| C | -5.23082100 | 2.25571800 | 1.53147300 |
| C | -6.14625300 | 2.06945700 | 0.49812300 |
| H | -6.40305800 | 1.50152700 | -1.56375700 |
| H | -3.99109400 | 1.05765100 | -1.92995400 |
| H | -3.15944300 | 2.14894700 | 2.12626400 |
| H | -5.57140500 | 2.59768200 | 2.50403100 |
| H | -7.20112900 | 2.26531400 | 0.66150700 |
| C | -1.96360400 | 1.27850400 | -0.14686200 |
| C | -1.09973700 | 2.28674600 | 0.04554400 |
| H | -1.53855500 | 3.24455700 | 0.35035500 |
| C | 3.56768200 | -1.31194000 | -1.15086900 |
| H | 4.11462500 | -1.44434100 | -0.22508200 |
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| C | 0.72317200 | -0.38116900 | 0.69861700 |
| C | 4.72465800 | -0.70631600 | -1.96401500 |

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|---|-------------|-------------|-------------|
| H | 5.80733700 | -0.77168400 | -1.93737800 |
| C | 4.06818600 | -0.40834300 | -3.15628700 |
| H | 4.63697300 | -0.25091500 | -4.06671100 |
| C | 2.67900400 | -0.29662300 | -3.16956300 |
| H | 2.16081500 | -0.04584700 | -4.09012500 |
| C | 1.94170800 | -0.50017000 | -2.00726900 |
| H | 0.86300000 | -0.38613100 | -1.99629300 |
| C | 2.60440200 | -0.83439400 | -0.82707900 |
| C | 2.10019500 | -2.15104900 | 1.23122400 |
| C | 1.09238600 | -2.07011100 | 2.19789100 |
| C | 1.01050800 | -2.98143700 | 3.24969900 |
| H | 0.23622400 | -2.91072600 | 4.00570900 |
| C | 1.96113100 | -3.99348800 | 3.28641800 |
| H | 1.93006600 | -4.72256400 | 4.08892400 |
| C | 2.95390700 | -4.09660300 | 2.29945900 |
| H | 3.67045100 | -4.90933300 | 2.34977100 |
| C | 3.04032100 | -3.18249800 | 1.25557600 |
| H | 3.80183400 | -3.27771900 | 0.49066300 |
| C | -0.86575300 | -0.53743600 | 2.59451100 |
| H | -1.17078200 | -1.35960800 | 3.24851600 |
| H | -1.67671300 | -0.35677700 | 1.88794700 |
| C | -0.55164900 | 0.71209600 | 3.41011200 |
| H | -0.30194100 | 1.52389200 | 2.71764500 |
| H | -1.46435000 | 1.00287800 | 3.94313800 |
| C | 0.59066300 | 0.50155600 | 4.40077000 |
| H | 1.52052300 | 0.25530800 | 3.87788200 |
| H | 0.36816800 | -0.31751900 | 5.09305200 |
| H | 0.76963100 | 1.40379800 | 4.99073300 |
| N | 1.84786700 | -1.09363500 | 0.35090200 |
| N | 0.29214000 | -0.99411700 | 1.82818600 |

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|---|-------------|-------------|-------------|
| B | 0.12338000 | 2.34204800 | 0.04060900 |
| B | -1.89404400 | -0.23736800 | -0.89759700 |
| C | 1.94360300 | 3.25853400 | -0.95691600 |
| C | 3.17669500 | 2.76776200 | -1.69437500 |
| H | 3.48251000 | 1.77648400 | -1.35711000 |
| H | 4.00438000 | 3.46827600 | -1.54048300 |
| H | 2.96830300 | 2.71472100 | -2.76643400 |
| C | 1.46051800 | 4.57828900 | -1.55893200 |
| H | 1.18736000 | 4.40729600 | -2.60319800 |
| H | 2.23870200 | 5.34541500 | -1.52432900 |
| H | 0.57813700 | 4.94944500 | -1.02847700 |
| C | 2.10555500 | 3.32778600 | 0.59662000 |
| C | 3.03640400 | 2.25546300 | 1.15436200 |
| H | 2.93777900 | 2.23944700 | 2.24372700 |
| H | 4.07991400 | 2.46443900 | 0.90216000 |
| H | 2.76701600 | 1.27119600 | 0.76660100 |
| C | 2.50666000 | 4.69542400 | 1.12901200 |
| H | 1.76376300 | 5.45499100 | 0.87990400 |
| H | 3.47314800 | 4.99813000 | 0.71428900 |
| H | 2.60241300 | 4.64978500 | 2.21713100 |
| C | -1.94472000 | -2.49220000 | -1.26415600 |
| C | -0.62478700 | -3.11101900 | -0.81641200 |
| H | 0.19955600 | -2.40257100 | -0.91793500 |
| H | -0.39222700 | -4.00265000 | -1.40543900 |
| H | -0.70502200 | -3.39809900 | 0.23639500 |
| C | -3.04941600 | -3.53721200 | -1.21616500 |
| H | -3.03797500 | -4.03216600 | -0.24154000 |
| H | -2.88912200 | -4.29763800 | -1.98644100 |
| H | -4.03311700 | -3.08826400 | -1.36238800 |
| C | -1.83264400 | -1.72188000 | -2.62175300 |

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| C | -0.78598100 | -2.26189200 | -3.58250300 |
| H | -0.75785600 | -1.63619000 | -4.47883200 |
| H | -1.05020800 | -3.27975400 | -3.88541400 |
| H | 0.21113000 | -2.27808800 | -3.14122300 |
| C | -3.17472000 | -1.59230300 | -3.33878100 |
| H | -3.95398900 | -1.24964300 | -2.65298100 |
| H | -3.48867400 | -2.54749100 | -3.76740900 |
| H | -3.07562600 | -0.86235900 | -4.14586000 |
| O | 0.85826200 | 2.31398100 | -1.12285900 |
| O | 0.77020200 | 3.02798000 | 1.05085000 |
| O | -2.27740300 | -1.43175400 | -0.33783500 |
| O | -1.46088100 | -0.38146800 | -2.19525100 |
| C | -6.03329200 | 1.03582400 | -0.39084900 |
| C | -4.68691500 | 0.93961600 | -0.72852500 |
| C | -3.68683300 | 1.20596800 | 0.21572100 |
| C | -4.07442100 | 1.55648600 | 1.51489400 |
| C | -5.42123300 | 1.64596300 | 1.85773100 |
| C | -6.40536700 | 1.38662700 | 0.90615600 |
| H | -6.79298700 | 0.84040900 | -1.14120700 |
| H | -4.40223200 | 0.68826700 | -1.74736700 |
| H | -3.30682000 | 1.74515000 | 2.26119100 |
| H | -5.70197600 | 1.91219400 | 2.87206700 |
| H | -7.45500500 | 1.45439000 | 1.17328400 |
| C | -2.24292400 | 1.11439100 | -0.16067100 |
| C | -1.41428100 | 2.10257400 | 0.21556700 |
| H | -1.88825700 | 2.92722000 | 0.76117200 |
| C | 3.99725600 | -0.91581000 | -0.79456200 |
| H | 4.50561700 | -1.12288200 | 0.14158200 |

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| C | 1.12716600 | -0.18650400 | 0.30780900 |
| C | 1.28116900 | 3.66898400 | -1.85631900 |
| H | 0.51608400 | 4.07414200 | -2.50976700 |
| C | 2.31073900 | 4.48529900 | -1.39148100 |
| H | 2.34592100 | 5.53018300 | -1.68071900 |
| C | 3.29441300 | 3.96132900 | -0.55555500 |
| H | 4.09426800 | 4.59547200 | -0.18914800 |
| C | 3.24919900 | 2.62309400 | -0.17485300 |
| H | 3.99497400 | 2.20600900 | 0.49444600 |
| C | 2.21900000 | 1.81792100 | -0.65286700 |
| C | 3.22083200 | -0.47174700 | -0.46802800 |
| C | 2.75908200 | -1.69408100 | 0.02568600 |
| C | 3.55162800 | -2.84096100 | -0.01401500 |
| H | 3.20195500 | -3.79110500 | 0.37311200 |
| C | 4.81357500 | -2.70929200 | -0.57673900 |
| H | 5.46206300 | -3.57679700 | -0.62641800 |
| C | 5.27067200 | -1.48012000 | -1.08416200 |
| H | 6.26188800 | -1.42233700 | -1.51987100 |
| C | 4.48392000 | -0.33747700 | -1.04129100 |
| H | 4.83032500 | 0.61152800 | -1.43418500 |
| C | 0.63044200 | -2.47088000 | 1.17150400 |
| H | 0.95910100 | -3.45075200 | 0.81423600 |
| H | -0.39483900 | -2.30718900 | 0.83889600 |
| C | 0.75250100 | -2.36067500 | 2.68667600 |
| H | 0.43710700 | -1.35255300 | 2.97602700 |
| H | 0.02651600 | -3.05489400 | 3.12324000 |
| C | 2.15128600 | -2.65286900 | 3.22080100 |
| H | 2.88526600 | -1.94323100 | 2.82655300 |
| H | 2.47503200 | -3.66160500 | 2.94407500 |
| H | 2.17331100 | -2.58054500 | 4.31068000 |

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| N | 2.18281500 | 0.43819900 | -0.27050200 |
| N | 1.46447200 | -1.47295200 | 0.48912500 |
| B | -0.30444900 | 0.52174600 | 0.46942100 |
| B | -1.60427900 | -0.17110400 | -0.37069400 |
| C | -1.65048200 | 1.88665200 | 1.81947200 |
| C | -1.52482000 | 2.70177800 | 3.10482500 |
| H | -0.92587600 | 2.18170700 | 3.85389800 |
| H | -2.51148600 | 2.91244000 | 3.52842900 |
| H | -1.04154200 | 3.65706300 | 2.88121600 |
| C | -2.25860700 | 2.79173200 | 0.74329300 |
| H | -1.56022500 | 3.61630400 | 0.56783900 |
| H | -3.20457900 | 3.21775000 | 1.09050600 |
| H | -2.43630800 | 2.26656600 | -0.19396200 |
| C | -2.41695600 | 0.51042900 | 2.03672400 |
| C | -2.17065400 | -0.04053500 | 3.44341300 |
| H | -2.53698900 | -1.06997100 | 3.47884000 |
| H | -2.69367700 | 0.54065000 | 4.20773100 |
| H | -1.10354200 | -0.04627300 | 3.67973000 |
| C | -3.92124500 | 0.65952600 | 1.80683200 |
| H | -4.12912900 | 0.89186200 | 0.76194800 |
| H | -4.33461000 | 1.44651300 | 2.44747100 |
| H | -4.41988800 | -0.28104100 | 2.06173000 |
| C | -2.46749200 | -1.84131300 | -1.71867300 |
| C | -2.07040400 | -2.78094300 | -2.84934600 |
| H | -1.29655000 | -2.33649200 | -3.47843600 |
| H | -2.93386300 | -3.02918500 | -3.47568100 |
| H | -1.67734900 | -3.71240600 | -2.43071300 |
| C | -3.40851400 | -2.56570400 | -0.75002500 |
| H | -2.86690400 | -3.40099200 | -0.29534100 |
| H | -4.28985500 | -2.96432200 | -1.26244300 |

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| H | -3.72974800 | -1.89172200 | 0.04851700 |
| C | -3.04869100 | -0.47171600 | -2.18232700 |
| C | -2.33709800 | 0.05769300 | -3.43007500 |
| H | -2.61561800 | 1.10521700 | -3.57692600 |
| H | -2.61169700 | -0.50260500 | -4.32913800 |
| H | -1.25224100 | 0.00175100 | -3.29835700 |
| C | -4.55617100 | -0.46230700 | -2.40101600 |
| H | -5.08675700 | -0.69098100 | -1.47436200 |
| H | -4.84604100 | -1.19372000 | -3.16315000 |
| H | -4.87440000 | 0.52734900 | -2.74261800 |
| O | -0.32596500 | 1.51372100 | 1.43612500 |
| O | -1.87813900 | -0.47275000 | 1.15836000 |
| O | -1.29583500 | -1.43537300 | -1.01903300 |
| O | -2.72905700 | 0.38895300 | -1.09234800 |
| C | 1.23450300 | 2.32537400 | -1.49744000 |
| H | 0.44054400 | 1.67574900 | -1.85364900 |

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|---|-------------|-------------|-------------|
| C | 0.99138900 | 0.01984500 | 0.53187700 |
| C | 2.38509200 | 4.21841800 | -1.17972200 |
| H | 3.04832500 | 5.05106900 | -0.97233100 |
| C | 1.32145400 | 4.37087000 | -2.06748800 |
| H | 1.15919300 | 5.32493500 | -2.55759800 |
| C | 0.46656900 | 3.30109100 | -2.32371000 |
| H | -0.36127500 | 3.41937700 | -3.01497200 |
| C | 0.67027200 | 2.06795700 | -1.70740500 |
| H | 0.01235500 | 1.22161100 | -1.91041400 |
| C | 1.73315500 | 1.93979100 | -0.81673100 |
| C | 3.14132400 | -0.02399100 | -0.09741600 |
| C | 2.87833200 | -1.16596800 | 0.66602300 |

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|---|-------------|-------------|-------------|
| C | 3.86822300 | -2.11215100 | 0.93197100 |
| H | 3.66955900 | -2.99361700 | 1.53090700 |
| C | 5.12059100 | -1.87031100 | 0.38819500 |
| H | 5.92002400 | -2.58037300 | 0.56745100 |
| C | 5.37933400 | -0.72971600 | -0.39431100 |
| H | 6.37183900 | -0.58555900 | -0.80616900 |
| C | 4.39745200 | 0.21478000 | -0.65395600 |
| H | 4.59371300 | 1.09276900 | -1.25840600 |
| C | 0.79269600 | -2.06561900 | 1.84561100 |
| H | 1.33981200 | -3.01097900 | 1.79877300 |
| H | -0.17893000 | -2.20765700 | 1.35810900 |
| C | 0.65606800 | -1.57963200 | 3.28612500 |
| H | 0.10479100 | -0.63056000 | 3.28609800 |
| H | 0.03515400 | -2.30687800 | 3.81919400 |
| C | 1.99832100 | -1.40682300 | 3.99061800 |
| H | 2.61524600 | -0.65408800 | 3.48988100 |
| H | 2.55714200 | -2.34810400 | 4.00381700 |
| H | 1.85620300 | -1.08449800 | 5.02443400 |
| N | 1.94322400 | 0.68880800 | -0.14958400 |
| N | 1.53544900 | -1.10112200 | 1.02212600 |
| B | -0.57132600 | 0.39075200 | 0.57253700 |
| B | -1.76629600 | -0.41950900 | -0.39737900 |
| C | -2.21938600 | 1.91479600 | 1.47929300 |
| C | -2.33964700 | 2.50626600 | 2.87978100 |
| H | -2.17045100 | 1.74464500 | 3.64450700 |
| H | -3.32150200 | 2.95632300 | 3.03950500 |
| H | -1.58259600 | 3.28561300 | 3.00387900 |
| C | -2.28634900 | 3.01422900 | 0.42247600 |
| H | -1.41299200 | 3.66488500 | 0.52495700 |
| H | -3.18657200 | 3.62237400 | 0.54064600 |

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| H | -2.28371600 | 2.57065500 | -0.57675300 |
| C | -3.25273200 | 0.77429500 | 1.18996000 |
| C | -3.16685700 | -0.33930500 | 2.24685800 |
| H | -3.79965800 | -1.16681000 | 1.91737500 |
| H | -3.51757200 | 0.00109200 | 3.22511200 |
| H | -2.15015600 | -0.72768200 | 2.35645600 |
| C | -4.67947300 | 1.33200100 | 1.19155700 |
| H | -4.80559200 | 2.07812300 | 0.40379700 |
| H | -4.95816000 | 1.77438000 | 2.15138000 |
| H | -5.36568300 | 0.50636700 | 0.98335400 |
| C | -1.95178600 | -2.55856500 | -1.35802500 |
| C | -1.35439400 | -3.95779100 | -1.26569700 |
| H | -0.31988200 | -3.92071300 | -0.91555000 |
| H | -1.37940600 | -4.46292300 | -2.23752600 |
| H | -1.93194000 | -4.55972700 | -0.55710400 |
| C | -3.45440700 | -2.65495700 | -1.64844000 |
| H | -3.94263500 | -3.14046100 | -0.79783800 |
| H | -3.66506500 | -3.24200500 | -2.54832100 |
| H | -3.88010400 | -1.65482800 | -1.76107500 |
| C | -1.23025100 | -1.61191600 | -2.36690800 |
| C | 0.29014100 | -1.81320100 | -2.34098200 |
| H | 0.77041700 | -0.97081000 | -2.85000900 |
| H | 0.59119600 | -2.73685700 | -2.84555400 |
| H | 0.65355900 | -1.85223200 | -1.30935400 |
| C | -1.73182900 | -1.71690000 | -3.80318700 |
| H | -2.78533500 | -1.43719300 | -3.86855000 |
| H | -1.61331700 | -2.73512300 | -4.18917700 |
| H | -1.15777700 | -1.04209300 | -4.44612600 |
| O | -0.85841300 | 1.39776100 | 1.42398600 |
| O | -3.05254400 | 0.24919400 | -0.10399900 |

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|---|-------------|-------------|-------------|
| O | -1.76034900 | -1.88537600 | -0.12451000 |
| O | -1.53986100 | -0.32549100 | -1.86005000 |
| C | 2.59327000 | 3.00000100 | -0.54113700 |
| H | 3.39907800 | 2.87387600 | 0.17479700 |

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| C | -0.96774000 | -0.26999900 | -0.40859700 |
| C | -1.56539500 | 3.87463000 | 1.77038000 |
| H | -1.77031100 | 4.23504000 | 2.77250400 |
| C | -1.04703600 | 4.73445900 | 0.80481400 |
| H | -0.84409200 | 5.77042200 | 1.05518000 |
| C | -0.79544300 | 4.26937400 | -0.48504200 |
| H | -0.40000000 | 4.94189900 | -1.23896800 |
| C | -1.05338300 | 2.94258500 | -0.81744900 |
| H | -0.85199900 | 2.55667800 | -1.80862300 |
| C | -1.55050100 | 2.08943400 | 0.16244600 |
| C | -3.14302200 | 0.19583900 | -0.10550300 |
| C | -3.01739800 | -1.17088200 | -0.36355700 |
| C | -4.13330100 | -2.00978700 | -0.40643500 |
| H | -4.04472200 | -3.07010100 | -0.61282200 |
| C | -5.36514900 | -1.41761500 | -0.17713000 |
| H | -6.25837600 | -2.03172700 | -0.19892700 |
| C | -5.48832500 | -0.03827200 | 0.08012500 |
| H | -6.47378400 | 0.38147200 | 0.24856700 |
| C | -4.38228600 | 0.79573600 | 0.12002100 |
| H | -4.46757100 | 1.85861400 | 0.31579000 |
| C | -1.06073100 | -2.73345000 | -0.78023700 |
| H | -1.76338900 | -3.46781500 | -0.37692600 |
| H | -0.13751400 | -2.77516000 | -0.19660600 |
| C | -0.79365600 | -2.98586600 | -2.25980900 |

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|---|-------------|-------------|-------------|
| H | -0.07156300 | -2.23920600 | -2.60761300 |
| H | -0.30343100 | -3.96158600 | -2.33947800 |
| C | -2.05232500 | -2.95575300 | -3.12138600 |
| H | -2.54169200 | -1.97772000 | -3.07779800 |
| H | -2.77274000 | -3.71016600 | -2.78873100 |
| H | -1.81141500 | -3.16048400 | -4.16688900 |
| N | -1.85451800 | 0.72014400 | -0.15280500 |
| N | -1.66145500 | -1.41149500 | -0.54562800 |
| B | 0.63363500 | -0.13891900 | -0.50374900 |
| B | 1.86389300 | -1.06304300 | 0.08310000 |
| C | 2.35037700 | 1.30410200 | -1.53939200 |
| C | 2.30905000 | 2.08535200 | -2.85428000 |
| H | 1.84195800 | 1.49443600 | -3.64567700 |
| H | 3.30506100 | 2.39370200 | -3.18123000 |
| H | 1.70612600 | 2.98672300 | -2.70351100 |
| C | 2.85283300 | 2.22431200 | -0.42187400 |
| H | 2.08809900 | 2.98336800 | -0.22978100 |
| H | 3.77585000 | 2.73137500 | -0.71803100 |
| H | 3.02189000 | 1.65587900 | 0.49380100 |
| C | 3.22542900 | 0.01042400 | -1.64264100 |
| C | 2.77891300 | -0.85217700 | -2.83055300 |
| H | 3.22885400 | -1.84392400 | -2.73088900 |
| H | 3.10584200 | -0.42036700 | -3.78083300 |
| H | 1.69260200 | -0.96004800 | -2.85565300 |
| C | 4.70909200 | 0.34821300 | -1.80647600 |
| H | 5.08676200 | 0.85968400 | -0.91824800 |
| H | 4.90200700 | 0.96899400 | -2.68488600 |
| H | 5.26710200 | -0.58602700 | -1.92011000 |
| C | 1.96286000 | -1.82681600 | 2.28957100 |
| C | 1.51745500 | -2.97297300 | 3.18870500 |

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|---|-------------|-------------|-------------|
| H | 0.52920700 | -3.33839000 | 2.90174700 |
| H | 1.48742500 | -2.65877100 | 4.23721200 |
| H | 2.22612700 | -3.80184400 | 3.10319200 |
| C | 3.43147800 | -1.49197900 | 2.57523700 |
| H | 4.04442000 | -2.35516700 | 2.30029800 |
| H | 3.59532500 | -1.27451500 | 3.63519200 |
| H | 3.75360300 | -0.63742900 | 1.97525000 |
| C | 1.05592800 | -0.55703400 | 2.37319600 |
| C | -0.41836600 | -0.93545700 | 2.51316500 |
| H | -1.04109300 | -0.05952500 | 2.31074800 |
| H | -0.63306800 | -1.27413400 | 3.53081200 |
| H | -0.69547700 | -1.73700300 | 1.82427800 |
| C | 1.42957700 | 0.41197300 | 3.49089900 |
| H | 2.43528200 | 0.80909000 | 3.34109800 |
| H | 1.38471700 | -0.08023400 | 4.46862300 |
| H | 0.72627800 | 1.25099400 | 3.49736700 |
| O | 0.97872300 | 0.98148200 | -1.27256400 |
| O | 3.15807300 | -0.74853500 | -0.43899800 |
| O | 1.82249800 | -2.23333100 | 0.92988800 |
| O | 1.32133100 | 0.10686800 | 1.12960500 |
| C | -1.82332500 | 2.54428000 | 1.45022200 |
| H | -2.23678900 | 1.86444800 | 2.18887600 |

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|---|-------------|-------------|-------------|
| C | -0.76509700 | -0.33286200 | 0.09355500 |
| C | -2.18344300 | 4.09094100 | 0.57005300 |
| H | -2.38489700 | 4.75458000 | 1.40402700 |
| C | -1.98744500 | 4.60892500 | -0.70864900 |
| H | -2.03615600 | 5.68061200 | -0.87116800 |
| C | -1.73058200 | 3.75508600 | -1.78048200 |

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|---|-------------|-------------|-------------|
| H | -1.57908900 | 4.16038300 | -2.77535000 |
| C | -1.66826300 | 2.37941800 | -1.58000400 |
| H | -1.45089200 | 1.69475400 | -2.39131400 |
| C | -1.85655500 | 1.87721700 | -0.29746400 |
| C | -3.02269300 | -0.27713600 | 0.06991800 |
| C | -2.62450000 | -1.58602300 | 0.33785000 |
| C | -3.56295200 | -2.59450200 | 0.56142800 |
| H | -3.26926000 | -3.61456500 | 0.78004100 |
| C | -4.90087600 | -2.23082400 | 0.49343000 |
| H | -5.66109100 | -2.98573400 | 0.66058400 |
| C | -5.29602000 | -0.91049600 | 0.21268000 |
| H | -6.35307700 | -0.67288700 | 0.16720700 |
| C | -4.36343500 | 0.09387100 | -0.00346600 |
| H | -4.65275800 | 1.11724200 | -0.21509100 |
| C | -0.44839300 | -2.77383900 | 0.69924800 |
| H | -1.07510500 | -3.33515200 | 1.39816500 |
| H | 0.43737200 | -2.44669900 | 1.24529500 |
| C | -0.01984400 | -3.65163500 | -0.47498700 |
| H | 0.82677600 | -3.17212900 | -0.96932400 |
| H | 0.36232400 | -4.58097900 | -0.03916700 |
| C | -1.11917500 | -3.96185000 | -1.48402700 |
| H | -1.53188300 | -3.04618900 | -1.91975200 |
| H | -1.94205400 | -4.51881900 | -1.02601200 |
| H | -0.72139100 | -4.56751600 | -2.30219700 |
| N | -1.85054400 | 0.45752000 | -0.07660100 |
| N | -1.22945700 | -1.58092400 | 0.33633100 |
| B | 0.80566900 | 0.26216900 | 0.04161300 |
| B | 2.04854700 | -0.86924800 | 0.13293700 |
| C | 2.00766000 | 0.75540900 | -2.08025300 |
| C | 1.64256300 | 1.43198200 | -3.40538900 |

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|---|-------------|-------------|-------------|
| H | 0.70939500 | 1.02961800 | -3.80604100 |
| H | 2.42826600 | 1.33453400 | -4.15847300 |
| H | 1.48639900 | 2.49732500 | -3.21107900 |
| C | 3.23996500 | 1.46562900 | -1.49934200 |
| H | 2.93358300 | 2.45543500 | -1.15082200 |
| H | 4.02143200 | 1.59222300 | -2.25398700 |
| H | 3.67128800 | 0.91977200 | -0.65663800 |
| C | 2.29061300 | -0.77887500 | -2.27065600 |
| C | 1.07264700 | -1.48431200 | -2.86294700 |
| H | 1.25592300 | -2.56105900 | -2.91355600 |
| H | 0.88247800 | -1.13354500 | -3.88004400 |
| H | 0.17765200 | -1.30051300 | -2.26088200 |
| C | 3.50769400 | -1.04136300 | -3.15662400 |
| H | 4.40795000 | -0.59500300 | -2.72875100 |
| H | 3.36438500 | -0.65349300 | -4.16748200 |
| H | 3.66585200 | -2.12142200 | -3.22449900 |
| C | 2.62021500 | -0.18584800 | 2.41006600 |
| C | 2.81559200 | -1.00689000 | 3.68238300 |
| H | 2.04647200 | -1.77777200 | 3.77080900 |
| H | 2.78816500 | -0.37829300 | 4.57599000 |
| H | 3.79029800 | -1.50133100 | 3.63999300 |
| C | 3.82850500 | 0.73020500 | 2.19996900 |
| H | 4.69162000 | 0.11963600 | 1.92264700 |
| H | 4.07424400 | 1.28349600 | 3.10999800 |
| H | 3.62748400 | 1.44843200 | 1.40085400 |
| C | 1.29123700 | 0.66173600 | 2.44918800 |
| C | 0.12057200 | -0.15136600 | 3.02989300 |
| H | -0.81160200 | 0.37972300 | 2.81124600 |
| H | 0.21090100 | -0.24869600 | 4.11556700 |
| H | 0.05053100 | -1.15858800 | 2.61894800 |

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|---|-------------|-------------|-------------|
| C | 1.46933100 | 1.89070000 | 3.35144000 |
| H | 2.16803500 | 2.59957900 | 2.90399000 |
| H | 1.81785400 | 1.62891200 | 4.35443700 |
| H | 0.49900600 | 2.38781300 | 3.44497200 |
| O | 0.87961900 | 0.96348900 | -1.24836900 |
| O | 2.64222400 | -1.38479700 | -1.00064000 |
| O | 2.66596500 | -1.15620900 | 1.33309600 |
| O | 0.96299200 | 1.19747200 | 1.18032400 |
| C | -2.12000800 | 2.71610700 | 0.78037200 |
| H | -2.26777800 | 2.28946100 | 1.76761000 |

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|---|-------------|-------------|-------------|
| B | -0.00001900 | -0.83565600 | -0.00007300 |
| B | -0.00001800 | 0.83562400 | 0.00028900 |
| C | -2.33311100 | -0.66045900 | 0.42791000 |
| C | -3.53735400 | -1.53994500 | 0.10189100 |
| H | -3.53779100 | -1.83501200 | -0.94929100 |
| H | -4.47923600 | -1.04066100 | 0.33529100 |
| H | -3.47319300 | -2.44745200 | 0.70752300 |
| C | -2.29958000 | -0.36439900 | 1.92827400 |
| H | -2.14424300 | -1.30342600 | 2.46476500 |
| H | -3.24017700 | 0.07358200 | 2.26897200 |
| H | -1.48671500 | 0.32105000 | 2.18550600 |
| C | -2.33304100 | 0.66050500 | -0.42791000 |
| C | -2.29940500 | 0.36442700 | -1.92827600 |
| H | -2.14401700 | 1.30344200 | -2.46476900 |
| H | -3.23996700 | -0.07356300 | -2.26905100 |
| H | -1.48650300 | -0.32103600 | -2.18537500 |
| C | -3.53731200 | 1.53996800 | -0.10202700 |
| H | -3.53786100 | 1.83506700 | 0.94914400 |

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|---|-------------|-------------|-------------|
| H | -4.47915900 | 1.04065300 | -0.33551300 |
| H | -3.47308500 | 2.44745000 | -0.70768900 |
| C | 2.33306900 | 0.66030000 | 0.42816300 |
| C | 3.53730900 | 1.53988600 | 0.10245200 |
| H | 3.53784600 | 1.83520000 | -0.94866300 |
| H | 4.47918400 | 1.04058200 | 0.33583700 |
| H | 3.47304800 | 2.44725400 | 0.70828100 |
| C | 2.29964400 | 0.36348600 | 1.92836800 |
| H | 2.14448700 | 1.30225500 | 2.46535500 |
| H | 3.24020900 | -0.07482200 | 2.26874300 |
| H | 1.48668500 | -0.32198100 | 2.18525700 |
| C | 2.33305000 | -0.66029600 | -0.42817200 |
| C | 2.29946600 | -0.36351100 | -1.92839600 |
| H | 2.14383600 | -1.30223900 | -2.46531500 |
| H | 3.24015400 | 0.07437800 | -2.26898100 |
| H | 1.48676200 | 0.32230100 | -2.18518900 |
| C | 3.53729800 | -1.53989700 | -0.10258400 |
| H | 3.53778900 | -1.83533200 | 0.94849800 |
| H | 4.47916300 | -1.04053200 | -0.33586800 |
| H | 3.47306400 | -2.44718800 | -0.70853100 |
| O | -1.18336600 | -1.49906900 | 0.12938300 |
| O | -1.18330000 | 1.49908500 | -0.12930800 |
| O | 1.18331500 | 1.49896900 | 0.13006000 |
| O | 1.18331500 | -1.49900900 | -0.12990700 |

13-ts

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|---|-------------|-------------|-------------|
| B | -0.08295100 | -0.69192800 | 0.19463200 |
| B | -1.34461200 | 0.78553100 | -0.68870100 |
| C | -2.33087400 | -1.68206600 | 0.71350500 |
| C | -2.69668000 | -3.13770200 | 1.01907700 |

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|---|-------------|-------------|-------------|
| H | -2.21307300 | -3.81711300 | 0.31428400 |
| H | -3.77517400 | -3.30652900 | 1.00116900 |
| H | -2.33171000 | -3.37476400 | 2.02213000 |
| C | -2.93628400 | -0.78757700 | 1.80617200 |
| H | -2.33973700 | -0.90038300 | 2.71514800 |
| H | -3.96153200 | -1.09561900 | 2.02854600 |
| H | -2.94483100 | 0.26674000 | 1.52620400 |
| C | -2.83304800 | -1.26530500 | -0.70523000 |
| C | -2.28084900 | -2.18996700 | -1.79304100 |
| H | -2.42977300 | -1.71686200 | -2.76682300 |
| H | -2.81916000 | -3.14090200 | -1.78986200 |
| H | -1.21782900 | -2.39090400 | -1.65350300 |
| C | -4.35943200 | -1.23993800 | -0.78770800 |
| H | -4.77745800 | -0.51365200 | -0.08762500 |
| H | -4.79048700 | -2.22198500 | -0.58599000 |
| H | -4.64693600 | -0.94296100 | -1.79979200 |
| C | -0.08658300 | 2.73167800 | -0.51710200 |
| C | 1.29103000 | 2.66842000 | -1.17478500 |
| H | 1.69195100 | 1.65551200 | -1.20644700 |
| H | 1.99653900 | 3.31282800 | -0.64315600 |
| H | 1.19767500 | 3.03554100 | -2.19996600 |
| C | -0.56314900 | 4.18101400 | -0.52534700 |
| H | -0.49461100 | 4.56905600 | -1.54428200 |
| H | 0.06984400 | 4.79901700 | 0.11771400 |
| H | -1.59868800 | 4.26853500 | -0.19393800 |
| C | -0.15423600 | 2.06315000 | 0.91121900 |
| C | 1.17773500 | 1.89925800 | 1.61774700 |
| H | 1.03296200 | 1.33438000 | 2.54263700 |
| H | 1.56337900 | 2.88896800 | 1.87922700 |
| H | 1.91968300 | 1.38643800 | 1.00629400 |

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|---|-------------|-------------|-------------|
| C | -1.17203200 | 2.71742700 | 1.83977400 |
| H | -2.15546000 | 2.77832500 | 1.36535400 |
| H | -0.85399100 | 3.72402200 | 2.11950500 |
| H | -1.26204100 | 2.11412400 | 2.74611800 |
| O | -0.90132900 | -1.66746100 | 0.78833800 |
| O | -2.45624700 | 0.09122500 | -1.03344800 |
| O | -1.01569500 | 1.96439700 | -1.30700800 |
| O | -0.74715600 | 0.74165200 | 0.63576900 |
| C | 4.71056400 | -1.40854800 | 1.27136700 |
| C | 3.34131300 | -1.20825300 | 1.12064800 |
| C | 2.78942500 | -0.99925900 | -0.14916100 |
| C | 3.63726000 | -0.98582900 | -1.26551800 |
| C | 5.00462500 | -1.18564000 | -1.11580900 |
| C | 5.54370000 | -1.39843500 | 0.15385200 |
| H | 5.12951800 | -1.57045300 | 2.25944100 |
| H | 2.68324700 | -1.21015000 | 1.98524500 |
| H | 3.20885000 | -0.81833900 | -2.25041000 |
| H | 5.65266000 | -1.17530100 | -1.98637400 |
| H | 6.61146900 | -1.55370300 | 0.27130000 |
| C | 1.35458200 | -0.76919300 | -0.30377700 |
| C | 0.47439500 | -0.56499000 | -1.28577800 |
| H | 0.48716600 | -0.51986100 | -2.37163800 |

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|---|-------------|-------------|-------------|
| B | -0.04096400 | -0.30118400 | 0.77165600 |
| B | -1.05233200 | 0.43742100 | -1.32828900 |
| C | -2.04207700 | -1.81598100 | 0.77224200 |
| C | -2.19941400 | -3.24455500 | 1.28913800 |
| H | -1.48353600 | -3.91489200 | 0.80856900 |
| H | -3.21072000 | -3.62183900 | 1.12691900 |

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|---|-------------|-------------|-------------|
| H | -2.00179600 | -3.24883900 | 2.36429300 |
| C | -2.98218500 | -0.88273600 | 1.53690000 |
| H | -2.63652600 | -0.80632700 | 2.57092500 |
| H | -3.99540100 | -1.29279000 | 1.54591700 |
| H | -3.00104600 | 0.11506300 | 1.09881300 |
| C | -2.27679400 | -1.73626900 | -0.78209600 |
| C | -1.31914800 | -2.64635300 | -1.55311900 |
| H | -1.31616100 | -2.34720400 | -2.60520700 |
| H | -1.66515000 | -3.68161500 | -1.49875900 |
| H | -0.30197100 | -2.59378700 | -1.16641700 |
| C | -3.71783700 | -2.08876500 | -1.15192300 |
| H | -4.42035000 | -1.39241300 | -0.68982700 |
| H | -3.97305200 | -3.10799700 | -0.85616300 |
| H | -3.82620100 | -2.01143900 | -2.23723600 |
| C | -0.46379100 | 2.70095200 | -0.56500500 |
| C | 0.85822600 | 2.88614400 | -1.33243800 |
| H | 1.57796300 | 2.08204700 | -1.20380600 |
| H | 1.33203200 | 3.82304700 | -1.02696000 |
| H | 0.61494300 | 2.96485000 | -2.39596100 |
| C | -1.19258900 | 4.04506400 | -0.66535600 |
| H | -1.24206400 | 4.32969900 | -1.71973100 |
| H | -0.65531400 | 4.82937500 | -0.12662800 |
| H | -2.21077000 | 3.97854100 | -0.28114300 |
| C | -0.28524300 | 2.24234400 | 0.96905800 |
| C | 1.13321500 | 2.48369400 | 1.47952300 |
| H | 1.18143500 | 2.21812700 | 2.53904400 |
| H | 1.40085500 | 3.53932100 | 1.37727700 |
| H | 1.87050300 | 1.88549900 | 0.93929700 |
| C | -1.27982200 | 2.94805000 | 1.89498300 |
| H | -2.30668000 | 2.76308700 | 1.56938400 |

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|---|-------------|-------------|-------------|
| H | -1.10681300 | 4.02433600 | 1.94007000 |
| H | -1.16185300 | 2.53436200 | 2.89921700 |
| O | -0.66261500 | -1.49746900 | 1.03542100 |
| O | -2.14904100 | -0.36128900 | -1.17892700 |
| O | -1.33940800 | 1.77988200 | -1.22136000 |
| O | -0.63915000 | 0.85970000 | 1.16340800 |
| C | 4.28189100 | -1.62047000 | 1.23579100 |
| C | 2.95182600 | -1.25359200 | 1.05485000 |
| C | 2.51069400 | -0.71776700 | -0.16295100 |
| C | 3.44794300 | -0.53467000 | -1.18986700 |
| C | 4.77793600 | -0.89696700 | -1.00979500 |
| C | 5.19940200 | -1.44452500 | 0.20229000 |
| H | 4.60343900 | -2.03965700 | 2.18393700 |
| H | 2.23685300 | -1.39192300 | 1.86298900 |
| H | 3.13246000 | -0.09597800 | -2.13252800 |
| H | 5.49150800 | -0.74706100 | -1.81383400 |
| H | 6.23853100 | -1.72454700 | 0.34178400 |
| C | 1.09612000 | -0.33861800 | -0.31750200 |
| C | 0.44786300 | -0.06612300 | -1.46800000 |
| H | 0.94576900 | -0.10996100 | -2.43974800 |

15-ts

| | | | |
|---|-------------|-------------|-------------|
| B | -0.29544100 | 0.57458700 | 0.24132000 |
| B | 0.81299800 | -0.54415500 | -1.10397700 |
| C | 1.06345000 | 2.48573300 | 0.55477200 |
| C | 0.72411500 | 3.97281000 | 0.48720200 |
| H | 0.02294800 | 4.18787600 | -0.32052800 |
| H | 1.62478800 | 4.57555000 | 0.34766200 |
| H | 0.25870500 | 4.26646500 | 1.43130300 |
| C | 1.93725000 | 2.24583300 | 1.78513600 |

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|---|-------------|-------------|-------------|
| H | 1.40859400 | 2.62683700 | 2.66271800 |
| H | 2.88758500 | 2.77923000 | 1.70155100 |
| H | 2.13741000 | 1.18640400 | 1.93822400 |
| C | 1.70300600 | 1.91389200 | -0.82059100 |
| C | 1.74730900 | 2.96208800 | -1.93231000 |
| H | 2.16532800 | 2.49753200 | -2.82890800 |
| H | 2.37715400 | 3.81221900 | -1.66139700 |
| H | 0.74573200 | 3.32284300 | -2.17325100 |
| C | 3.10853600 | 1.34562700 | -0.63461400 |
| H | 3.14466200 | 0.56931600 | 0.12902000 |
| H | 3.79809400 | 2.14789500 | -0.35797500 |
| H | 3.44555100 | 0.91129400 | -1.57870400 |
| C | 1.93212600 | -2.36636600 | -0.24332700 |
| C | 1.27082400 | -3.65416800 | -0.73510000 |
| H | 0.24887100 | -3.47606800 | -1.07652300 |
| H | 1.25284700 | -4.41676200 | 0.04870400 |
| H | 1.84783600 | -4.04094300 | -1.57866800 |
| C | 3.40598700 | -2.64201100 | 0.04214100 |
| H | 3.86316200 | -3.03172500 | -0.87068200 |
| H | 3.53208400 | -3.38557000 | 0.83323200 |
| H | 3.93692300 | -1.72985500 | 0.32103500 |
| C | 1.14768900 | -1.71629600 | 1.01495900 |
| C | -0.11935600 | -2.45323500 | 1.44391100 |
| H | -0.65854900 | -1.83449700 | 2.16793700 |
| H | 0.16005200 | -3.38606400 | 1.94058700 |
| H | -0.79369400 | -2.67963600 | 0.62146700 |
| C | 2.02162000 | -1.50735700 | 2.24658600 |
| H | 2.90769300 | -0.91181800 | 2.02058900 |
| H | 2.34341000 | -2.46896900 | 2.65348300 |
| H | 1.44140300 | -0.98850800 | 3.01480300 |

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|---|-------------|-------------|-------------|
| O | -0.20310000 | 1.82493500 | 0.76496500 |
| O | 0.78139600 | 0.92079400 | -1.31574200 |
| O | 1.90677000 | -1.40078000 | -1.30571600 |
| O | 0.85132600 | -0.38817400 | 0.50555900 |
| C | -4.81952300 | 0.94250600 | 0.76830400 |
| C | -3.44764900 | 0.86039500 | 0.54600700 |
| C | -2.90882000 | -0.15951400 | -0.25026700 |
| C | -3.78204300 | -1.10552200 | -0.80653200 |
| C | -5.15148300 | -1.02610800 | -0.58251800 |
| C | -5.67638800 | -0.00026000 | 0.20457200 |
| H | -5.21986300 | 1.74127000 | 1.38496900 |
| H | -2.77746400 | 1.59579000 | 0.98387000 |
| H | -3.37785300 | -1.91447300 | -1.40901700 |
| H | -5.81370600 | -1.76858900 | -1.01702400 |
| H | -6.74561100 | 0.05904100 | 0.38079800 |
| C | -1.45635700 | -0.22563100 | -0.46930800 |
| C | -0.74468000 | -0.94675300 | -1.36418400 |
| H | -1.17670000 | -1.60643600 | -2.11753800 |

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|---|-------------|-------------|-------------|
| B | -0.95481900 | 0.52413600 | -0.01321700 |
| B | 1.18441400 | -1.54627200 | -0.09731800 |
| C | -0.72023600 | 2.64255600 | 0.74487100 |
| C | -1.62372600 | 3.83775200 | 0.99011200 |
| H | -2.50163400 | 3.81497300 | 0.34221000 |
| H | -1.07723800 | 4.76859200 | 0.81049900 |
| H | -1.96070200 | 3.83524900 | 2.02977000 |
| C | 0.37502200 | 2.55624700 | 1.80488800 |
| H | -0.09300400 | 2.43693400 | 2.78517800 |
| H | 0.98577200 | 3.46282700 | 1.81974800 |

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|---|-------------|-------------|-------------|
| H | 1.02039300 | 1.69115000 | 1.61920800 |
| C | -0.15831400 | 2.53087600 | -0.70690000 |
| C | -1.13609700 | 3.03818500 | -1.76373000 |
| H | -0.77362500 | 2.74277800 | -2.75116300 |
| H | -1.21952800 | 4.12756800 | -1.73417600 |
| H | -2.13155900 | 2.60781400 | -1.61862700 |
| C | 1.21038400 | 3.15600800 | -0.90854100 |
| H | 1.95131400 | 2.70819400 | -0.24487300 |
| H | 1.16865700 | 4.23157400 | -0.71145900 |
| H | 1.53347300 | 3.00903700 | -1.94260100 |
| C | 3.35098000 | -1.31296600 | -0.70523500 |
| C | 4.54910100 | -2.21806300 | -0.93001400 |
| H | 4.47712500 | -3.13061800 | -0.33581300 |
| H | 5.47293700 | -1.69590000 | -0.66306800 |
| H | 4.60651700 | -2.49572500 | -1.98555600 |
| C | 3.34380200 | -0.15616700 | -1.70162700 |
| H | 3.27577600 | -0.56358400 | -2.71342500 |
| H | 4.25776300 | 0.43910800 | -1.62806000 |
| H | 2.47800200 | 0.49203400 | -1.52897800 |
| C | 3.15712200 | -0.83449100 | 0.76642800 |
| C | 3.56930100 | -1.89008900 | 1.78981700 |
| H | 3.21817800 | -1.58093000 | 2.77724700 |
| H | 4.65596500 | -2.00236200 | 1.82626500 |
| H | 3.12423900 | -2.86104600 | 1.55301500 |
| C | 3.80080400 | 0.50047900 | 1.09580800 |
| H | 3.41799400 | 1.29626200 | 0.45549800 |
| H | 4.88592900 | 0.44026400 | 0.96771700 |
| H | 3.59250600 | 0.76120200 | 2.13698600 |
| O | -1.50325900 | 1.42481200 | 0.86026000 |
| O | -0.05973400 | 1.09424900 | -0.88359100 |

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|---|-------------|-------------|-------------|
| O | 2.13389900 | -2.06734700 | -0.93892900 |
| O | 1.71559300 | -0.70645700 | 0.85285400 |
| C | -5.08703700 | -0.82770100 | -0.45413600 |
| C | -3.73985000 | -0.47790500 | -0.44502400 |
| C | -2.75770200 | -1.38918900 | -0.03353100 |
| C | -3.17320900 | -2.65620500 | 0.40133400 |
| C | -4.51846200 | -3.00686400 | 0.39797900 |
| C | -5.48146300 | -2.09576400 | -0.03483600 |
| H | -5.82816400 | -0.10806700 | -0.78718400 |
| H | -3.44602100 | 0.51852400 | -0.76480900 |
| H | -2.43709400 | -3.36590000 | 0.76663800 |
| H | -4.81872400 | -3.99105700 | 0.74348400 |
| H | -6.53152800 | -2.36979600 | -0.03528000 |
| C | -1.32252900 | -1.00324200 | -0.06032400 |
| C | -0.33013800 | -1.91105700 | -0.16061000 |
| H | -0.59020900 | -2.96487700 | -0.28083500 |

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|---|------------|-------------|-------------|
| B | 0.91699800 | -0.38898900 | 0.04716700 |
| C | 2.83347500 | 0.81821100 | 0.15406400 |
| C | 3.54916900 | 1.82599300 | -0.72921100 |
| H | 3.29107600 | 1.68893000 | -1.78042000 |
| H | 4.63310300 | 1.72617400 | -0.61664300 |
| H | 3.26679300 | 2.83933600 | -0.43258600 |
| C | 3.03215400 | 1.16328900 | 1.62806700 |

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|---|-------------|-------------|-------------|
| H | 2.60157200 | 2.14904000 | 1.82020400 |
| H | 4.09306600 | 1.18880500 | 1.89018500 |
| H | 2.52955200 | 0.43518100 | 2.27169600 |
| C | 3.15629800 | -0.67727000 | -0.16485000 |
| C | 3.41494400 | -0.92329700 | -1.64937600 |
| H | 3.42936200 | -2.00062700 | -1.83115200 |
| H | 4.37601600 | -0.50510300 | -1.95953700 |
| H | 2.62478800 | -0.47974000 | -2.26237300 |
| C | 4.26733600 | -1.28210500 | 0.67653100 |
| H | 4.02086500 | -1.25742400 | 1.73920100 |
| H | 5.20278300 | -0.73675300 | 0.51857500 |
| H | 4.42531600 | -2.32272300 | 0.38173200 |
| O | 1.41073500 | 0.88516000 | -0.10734900 |
| O | 1.90643300 | -1.33401300 | 0.15831000 |
| C | -5.00506900 | -1.21155600 | 0.20307100 |
| C | -3.61907800 | -1.12050000 | 0.21826000 |
| C | -2.98147700 | 0.11007200 | 0.00200700 |
| C | -3.77442300 | 1.24308500 | -0.22086800 |
| C | -5.16322500 | 1.15320800 | -0.23853800 |
| C | -5.78285700 | -0.07574400 | -0.02722200 |
| H | -5.48298700 | -2.17103100 | 0.37306100 |
| H | -3.02900400 | -2.01189700 | 0.40681800 |
| H | -3.29165500 | 2.20285200 | -0.38497100 |
| H | -5.75985300 | 2.04202300 | -0.41707800 |
| H | -6.86538600 | -0.15051700 | -0.03885200 |
| C | -1.51607500 | 0.25674200 | -0.00112400 |
| C | -0.59626500 | -0.71830400 | 0.08373300 |
| H | -0.91440000 | -1.75664900 | 0.16493500 |
| H | -1.16278400 | 1.28494200 | -0.09357500 |