Supporting Information

Transition-Metal-Free Direct Nucleophilic Substitution of Carboranyllithium and 2-Halopyridines

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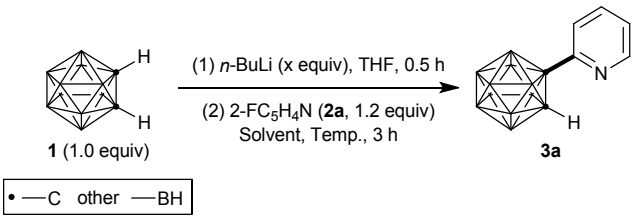
1. General Procedures

All reactions were carried out under a nitrogen atmosphere using oven dried glassware and standard Schlenk techniques. All organic solvents were freshly dried and distilled over sodium. ^{1}H NMR spectra at 500 MHz, ^{13}C NMR spectra at 125 MHz and ^{11}B NMR spectra at 160 MHz were obtained on a Bruker-AV500 spectrometer. ^{1}H NMR and ^{13}C NMR were recorded using tetramethylsilane (TMS) in the solvent of $CDCl_3$ as the internal standard (^{1}H NMR: TMS at 0.00 ppm, $CDCl_3$ at 7.26 ppm. ^{13}C NMR: $CDCl_3$ at 77.0 ppm). All ^{11}B NMR chemical shifts are referenced to external $BF_3{\cdot}OEt_2$ (0.00 ppm) with a negative sign indicating an upfield shift. Mass spectra were recorded on a ThermoFisher Q Exactive GC spectrometer.

2. Experimental Section

2.1 Optimization of reaction conditions

Table S1. Optimization of reaction conditions for nucleophilic substitution of carboranyllithium[a]

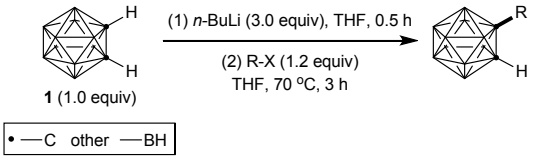


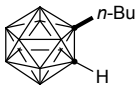
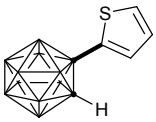
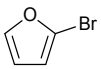
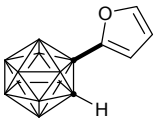
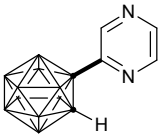
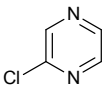
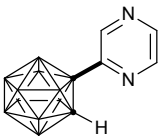
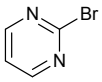
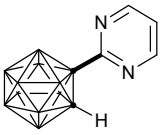
Entry	*n*-BuLi (x equiv.)	Solvent	Temperature (°C)	Yield (%)[b]
1	1	THF	70	32
2	2	THF	70	59
3	3	THF	70	86
4	4	THF	70	77
5	3	THF	60	82
6	3	THF	50	68
7	3	THF	40	41
8	3	THF	25	23
9	3	THF	80	85[c]
10	3	THF	90	83[c]
11	3	Et_2O	40	25
12	3	1,4-Dioxane	70	62
13	3	DME	70	71
14	3	DME	80	66
15	3	DME	90	63

[a] Reaction condition: (1) **1** (0.25 mmol), *n*-BuLi (x equiv.), THF (1 mL), 0.5 h in a Schlenk tube under nitrogen atmosphere. (2) **2a** (0.3 mmol), Solvent (1 mL), 3 h in a Schlenk tube under nitrogen atmosphere. [b] Isolated yield. [c] Using THF in a sealed tube. THF = Tetrahydrofuran, Et_2O = Diethyl ether, DME = 1,2-Dimethoxyethane.

2.2 Study on the reactivity of electrophiles

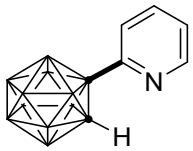
Table S2. Nucleophilic substitution of carboranyllithium[a]



Entry	Substrates	Products	Yield (%)[b]
1	*n*-BuCl		76
2			0
3			0[c]
4			0
5			0
6			0[d]

[a] Reaction condition: (1) **1** (0.25 mmol), *n*-BuLi (3.0 equiv.), THF (1 mL), 0.5 h in a Schlenk tube under nitrogen atmosphere. (2) R-X (0.3 mmol), THF (1 mL), 3 h in a Schlenk tube under nitrogen atmosphere. [b] Isolated yield. [c] 55 °C instead of 70 °C. [d] 65 °C instead of 70 °C. THF = tetrahydrofuran.

2.3 General procedure for transition-metal-free direct nucleophilic substitution of carboranyllithium with 2-halopyridines. In a dry Schlenk flask, *n*-BuLi (1.6 M in *n*-hexane, 0.75 mmol, 0.47 mL) was added slowly to a THF solution (1 mL) of 1 (0.25 mmol, 36 mg) at 0 ºC. The solution was kept at low temperature with stirring for 0.5 h, and allowed to reach room temperature. Subsequently, 2-halopyridines (0.3 mmol) were added under an inert nitrogen atmosphere, the mixture was heated at 70 ºC under stirring in a closed flask. After the reaction was completed, a saturated solution of aqueous NH_4Cl was added and the mixture was extracted three times with diethyl ether. The organic phases were collected, and solvent evaporation under reduced pressure afforded the crude product, which was then purified by column chromatography to provide the product, by using silica gel as stationary phase and *n*-hexane as eluent.



3a: Yield 86%. Colorless crystals, mp 110-111 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (d, *J* = 4.2 Hz, 1H), 7.71 (t, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.31 (dd, *J* = 6.8, 5.0 Hz, 1H), 4.99 (s, 1H).

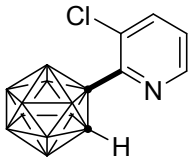
^{13}C NMR (126 MHz, $CDCl_3$) δ 151.01, 148.73, 137.34, 124.29, 121.51, 75.26, 56.84.

^{11}B NMR (160 MHz, $CDCl_3$) δ -3.60 (t, *J* = 141.3 Hz, 2B), -8.44 (d, *J* = 150.7 Hz, 2B), -9.67 – -14.59 (m, 6B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -3.19 (s, 1B), -4.01 (s, 1B), -8.43 (s, 2B), -10.58 (s, 2B), -11.45 (s, 2B), -13.29 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{15}{}^{10}B_2{}^{11}B_8N$ $[M]^+$: 221.2208. Found: 221.2209.

The NMR data are consistent with the reported ones.[1–4]



3b: Yield 83%. Colorless crystals, mp 145-146 ℃.

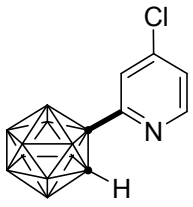
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 4.5, 1.5 Hz, 1H), 7.75 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.28 (dd, *J* = 8.1, 4.5 Hz, 1H), 5.47 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.66, 145.49, 141.08, 130.54, 125.33, 74.54, 60.34.

^{11}B NMR (160 MHz, $CDCl_3$) δ -2.50 (t, *J* = 128.4 Hz, 2B), -6.53 – -15.85 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -2.20 (s, 1B), -2.85 (s, 1B), -8.56 (s, 2B), -9.89 (s, 2B), -11.60 (s, 2B), -13.47 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8ClN$ $[M]^+$: 255.1818. Found: 255.1817.



3c: Yield 66%. Colorless crystals, mp 94-95 ℃.

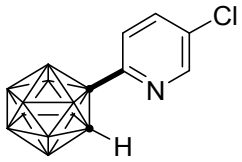
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 5.3 Hz, 1H), 7.53 (d, *J* = 1.7 Hz, 1H), 7.33 (dd, *J* = 5.3, 1.8 Hz, 1H), 4.93 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 152.66, 149.64, 145.70, 124.90, 122.24, 74.36, 57.01.

^{11}B NMR (160 MHz, $CDCl_3$) δ -0.60 – -4.98 (m, 2B), -6.58 – -15.20 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -3.07 (s, 1B), -3.68 (s, 1B), -8.33 (s, 2B), -10.69 (s, 2B), -11.55 (s, 2B), -13.26 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8ClN$ $[M]^+$: 255.1818. Found: 255.1815.



3d: Yield 70%. Colorless liquids.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 2.4 Hz, 1H), 7.68 (dd, *J* = 8.5, 2.4 Hz, 1H), 7.49 (d, *J* = 8.5 Hz, 1H), 4.89 (s, 1H).

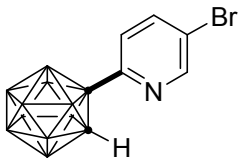
^{13}C NMR (126 MHz, $CDCl_3$) δ 149.40, 147.82, 137.24, 133.40, 122.51, 74.51, 57.09.

^{11}B NMR (160 MHz, $CDCl_3$) δ -3.52 (t, *J* = 141.7 Hz, 2B), -7.37 – -15.33 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -3.06 (s, 1B), -3.80 (s, 1B), -8.33 (s, 2B), -10.65 (s, 2B), -11.50 (s, 2B), -13.21 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8ClN$ $[M]^+$: 255.1818. Found: 255.1819.

The NMR data are consistent with the reported ones.[1]



3e: Yield 80%. Colorless crystals, mp 129-130 ℃.

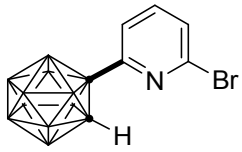
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 2.3, 0.6 Hz, 1H), 7.82 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.43 (dd, *J* = 8.5, 0.6 Hz, 1H), 4.89 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.02, 149.82, 140.11, 122.93, 122.01, 74.53, 57.01.

^{11}B NMR (160 MHz, $CDCl_3$) δ -3.42 (t, *J* = 136.0 Hz, 2B), -6.87 – -15.53 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -2.99 (s, 1B), -3.75 (s, 1B), -8.28 (s, 2B), -10.61 (s, 2B), -11.49 (s, 2B), -13.18 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8BrN$ $[M]^+$: 299.1313. Found: 299.1310.



3f: Yield 85%. Colorless crystals, mp 122-124 ℃.

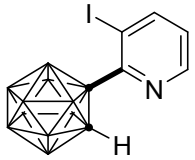
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.1 Hz, 1H), 7.50 (d, *J* = 6.1 Hz, 2H), 4.87 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 152.15, 141.21, 139.62, 129.14, 120.64, 73.99, 57.07.

^{11}B NMR (160 MHz, $CDCl_3$) δ -0.97 – -5.33 (m, 2B), -6.78 – -15.57 (m, 8B).

$^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$) δ -3.04 (s, 1B), -3.64 (s, 1B), -8.26 (s, 2B), -10.67 (s, 2B), -11.47 (s, 2B), -13.21 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8BrN$ $[M]^+$: 299.1313. Found: 299.1314.



3g: Yield 67%. Colorless crystals, mp 125-126 ℃.

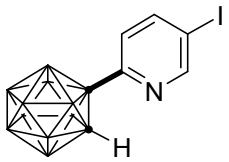
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 4.5, 1.6 Hz, 1H), 8.34 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.95 (dd, *J* = 8.0, 4.5 Hz, 1H), 5.59 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 152.82, 148.17, 147.44, 124.87, 88.89, 76.75, 60.95.

^{11}B NMR (160 MHz, $CDCl_3$) δ -2.73 (t, *J* = 135.5 Hz, 2B), -7.09 – -15.91 (m, 8B).

$^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$) δ -2.36 (s, 1B), -3.12 (s, 1B), -8.48 (s, 2B), -9.85 (s, 2B), -11.52 (s, 2B), -13.46 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8IN$ $[M]^+$: 347.1174. Found: 347.1176.



3h: Yield 84%. Colorless crystals, mp 116-117 ℃.

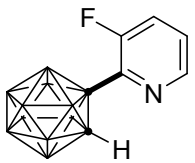
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (d, *J* = 2.1 Hz, 1H), 8.01 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 4.88 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 154.97, 150.32, 145.78, 123.32, 94.38, 74.61, 56.86.

^{11}B NMR (160 MHz, $CDCl_3$) δ -3.43 (t, *J* = 134.1 Hz), -6.40 – -16.96 (m).

$^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$) δ -3.07 (s, 1B), -3.84 (s, 1B), -8.35 (s, 2B), -10.69 (s, 2B), -11.58 (s, 2B), -13.26 (s, 2B).

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8IN$ $[M]^+$: 347.1174. Found: 347.1173.



3i: Yield 69%. Colorless crystals, mp 82-83 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (d, *J* = 4.5 Hz, 1H), 7.51 – 7.43 (m, 1H), 7.37 (ddd, *J* = 8.3, 4.4, 3.6 Hz, 1H), 5.16 (s, 1H).

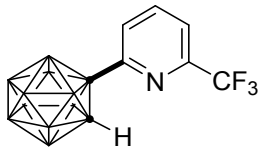
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.06 (d, *J* = 267.2 Hz), 144.57 (d, *J* = 5.4 Hz), 138.05 (d, *J* = 10.0 Hz), 126.26 (d, *J* = 4.2 Hz), 125.68 (d, *J* = 20.1 Hz), 71.53 (s), 58.17 (s).

^{11}B NMR (160 MHz, $CDCl_3$) δ -2.68 (d, *J* = 149.6 Hz, 2B), -6.84 – -16.64 (m, 8B).

$^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$) δ -2.66 (s, 2B), -8.52 (s, 2B), -10.26 (s, 2B), -11.43 (s, 2B), -13.39 (s, 2B).

^{19}F NMR (377 MHz, $CDCl_3$) δ -125.99.

HRMS: *m*/*z* calcd for $C_7H_{14}{}^{10}B_2{}^{11}B_8FN$ $[M]^+$: 239.2113. Found: 239.2112.



3j: Yield 78%. Colorless crystals, mp 115-117 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (t, *J* = 7.9 Hz, 1H), 7.73 (dd, *J* = 15.0, 7.9 Hz, 2H), 4.93 (s, 1H).

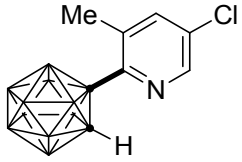
^{13}C NMR (126 MHz, $CDCl_3$) δ 151.84 (s), 147.50 (dd, *J* = 71.8, 36.0 Hz), 139.20 (s), 124.37 (s), 121.02 (dd, *J* = 5.2, 2.6 Hz), 120.72 (q, *J* = 274.4 Hz), 73.94 (s), 56.84 (s).

^{11}B NMR (160 MHz, $CDCl_3$) δ -1.09 – -5.37 (m, 2B), -6.56 – -15.93 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -2.85 (s, 1B), -3.44 (s, 1B), -8.19 (s, 2B), -10.54 (s, 2B), -11.55 (s, 2B), -13.08 (s, 2B).

^{19}F NMR (471 MHz, $CDCl_3$) δ -68.11.

HRMS: *m*/*z* calcd for $C_8H_{14}{}^{10}B_2{}^{11}B_8F_3N$ $[M]^+$: 289.2082. Found: 289.2085.



3k: Yield 88%. Colorless crystals, mp 141-142 ℃.

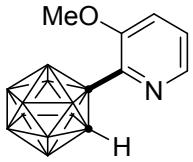
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 2.2 Hz, 1H), 7.52 (d, *J* = 2.0 Hz, 1H), 5.47 (s, 1H), 2.63 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.57, 144.99, 140.92, 133.66, 132.54, 75.94, 61.17, 20.92.

^{11}B NMR (160 MHz, $CDCl_3$) δ -0.23 – -4.72 (m), -6.45 – -15.58 (m).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -2.53 (s, 1B), -3.00 (s, 1B), -8.48 (s, 2B), -9.84 (s, 2B), -12.14 (s, 2B), -13.32 (s, 2B).

HRMS: *m*/*z* calcd for $C_8H_{16}{}^{10}B_2{}^{11}B_8ClN$ $[M]^+$: 269.1974. Found: 269.1971.



3l: Yield 60%. Colorless crystals, mp 134-135 ℃.

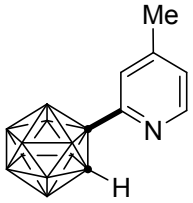
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 4.4, 1.4 Hz, 1H), 7.27 (qd, *J* = 8.4, 2.9 Hz, 2H), 5.30 (s, 1H), 3.86 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.86, 140.35, 138.48, 125.57, 120.39, 73.82, 58.95, 55.65.

^{11}B NMR (160 MHz, $CDCl_3$) δ -3.00 (d, *J* = 146.8 Hz, 2B), -6.92 – -16.99 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -2.91 (s, 2B), -9.04 (s, 2B), -10.09 (s, 2B), -11.08 (s, 2B), -13.68 (s, 2B).

HRMS: *m*/*z* calcd for $C_8H_{17}{}^{10}B_2{}^{11}B_8NO$ $[M]^+$: 251.2313. Found: 251.2310.



3m: Yield 36%. Colorless crystals, mp 88-89 ℃.

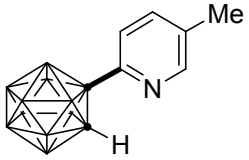
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 5.0 Hz, 1H), 7.33 (s, 1H), 7.11 (dd, *J* = 5.0, 0.7 Hz, 1H), 4.98 (s, 1H), 2.38 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 151.03, 149.03, 148.52, 125.38, 122.43, 75.50, 57.05, 21.24.

^{11}B NMR (160 MHz, $CDCl_3$) δ -3.71 (t, *J* = 139.8 Hz, 2B), -7.50 – -14.57 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -3.32 (s, 1B), -4.14 (s, 1B), -8.55 (s, 2B), -10.68 (s, 2B), -11.54 (s, 2B), -13.43 (s, 2B).

HRMS: *m*/*z* calcd for $C_8H_{17}{}^{10}B_2{}^{11}B_8N$ $[M]^+$: 235.2364. Found: 235.2366.



3n: Yield 43%. Colorless crystals, mp 130-131 ℃.

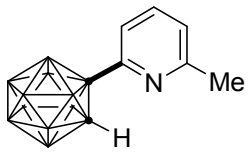
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 1.4, 0.7 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 4.95 (s, 1H), 2.34 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.21, 148.50, 137.88, 134.43, 121.09, 75.47, 57.03, 18.19.

^{11}B NMR (160 MHz, $CDCl_3$) δ -2.13 – -5.24 (m, 2B), -6.55 – -15.36 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -3.20 (s, 1B), -4.17 (s, 1B), -8.47 (s, 2B), -10.54 (s, 2B), -11.47 (s, 2B), -13.31 (s, 2B).

HRMS: *m*/*z* calcd for $C_8H_{17}{}^{10}B_2{}^{11}B_8N$ $[M]^+$: 235.2364. Found: 235.2362.



3o: Yield 47%. Colorless crystals, mp 89-90 ℃.

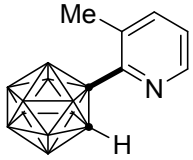
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (t, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.14 (d, *J* = 7.7 Hz, 1H), 5.04 (s, 1H), 2.49 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.00, 150.15, 137.36, 123.79, 118.40, 75.45, 56.71, 24.24.

^{11}B NMR (160 MHz, $CDCl_3$) δ -3.74 (t, *J* = 144.2 Hz, 2B), -7.25 – -15.22 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -3.33 (s, 1B), -4.19 (s, 1B), -8.54 (s, 2B), -10.67 (s, 2B), -11.49 (s, 2B), -13.45 (s, 2B).

HRMS: *m*/*z* calcd for $C_8H_{17}{}^{10}B_2{}^{11}B_8N$ $[M]^+$: 235.2364. Found: 235.2365.



3p: Yield 57%. Colorless crystals, mp 122-124 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 4.4, 1.0 Hz, 1H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.18 (dd, *J* = 7.7, 4.6 Hz, 1H), 5.59 (s, 1H), 2.62 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 147.23, 146.20, 141.76, 132.19, 124.17, 76.75, 61.05, 21.02.

^{11}B NMR (160 MHz, $CDCl_3$) δ -2.98 (dd, *J* = 140.1, 68.2 Hz, 2B), -7.49 – -19.39 (m, 8B).

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -2.78 (s, 1B), -3.18 (s, 1B), -8.64 (s, 2B), -9.87 (s, 2B), -12.10 (s, 2B), -13.47 (s, 2B).

HRMS: *m*/*z* calcd for $C_8H_{17}{}^{10}B_2{}^{11}B_8N$ $[M]^+$: 235.2364. Found: 235.2363.

The NMR data are consistent with the reported ones.[1]

3. References

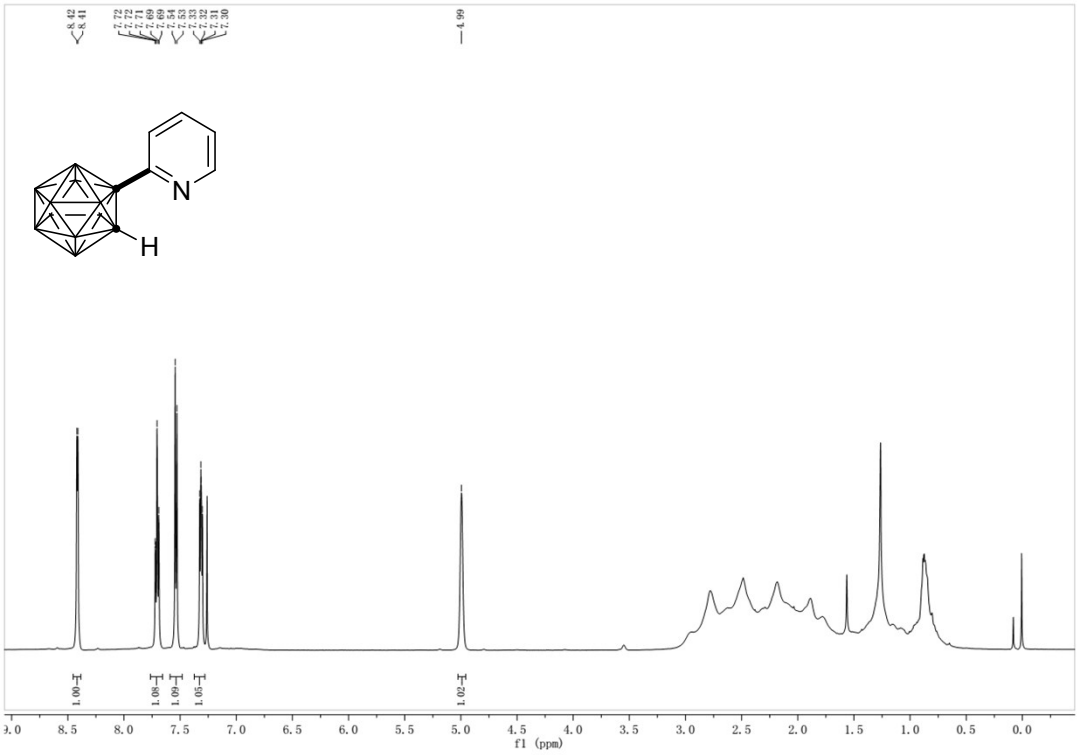
[1] J-Y. Lu, H. Wan, J. Zhang, Z. Wang, Y. Li, Y. Du, C. Li, Z. Liu, Z-T. Liu and J. Lu, *Chem. Eur. J.,* 2016, **22,** 17542–17546.

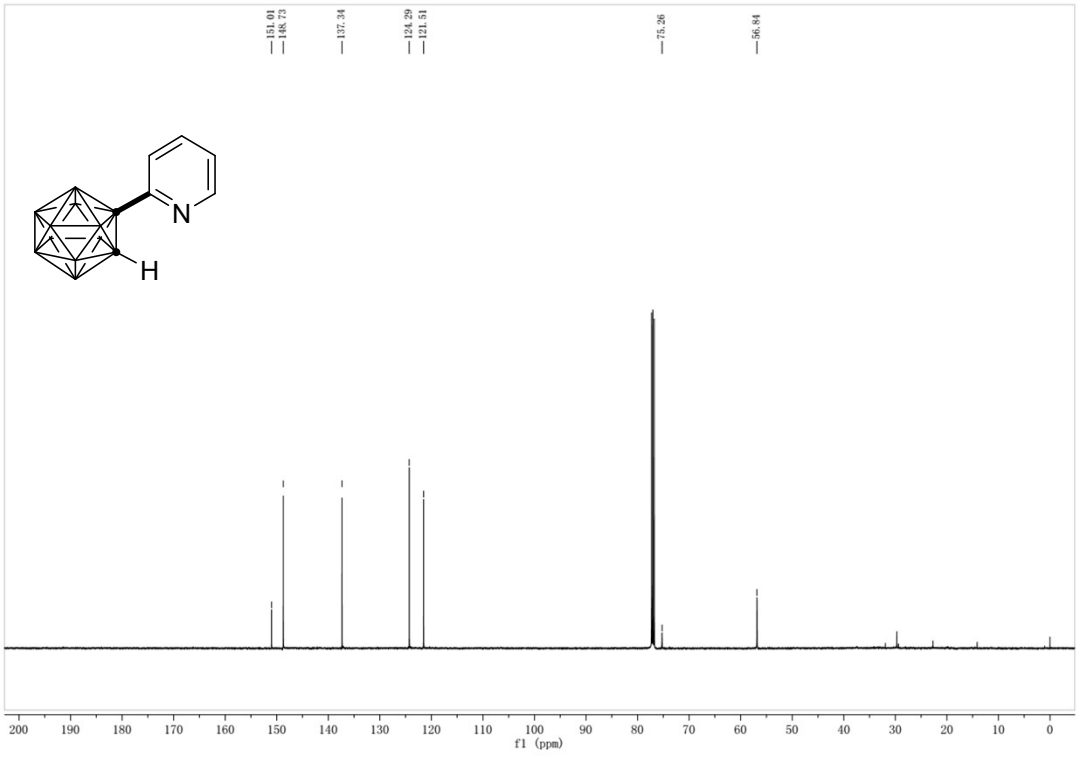
[2] M. E. El-Zaria, K. Keskar, A. R. Genady, J. A. Ioppolo, J. McNulty and J. F. Valliant, *Angew. Chem. Int. Ed.*, 2014, **53**, 5156–5160; *Angew. Chem*., 2014, **126**, 5256–5260.

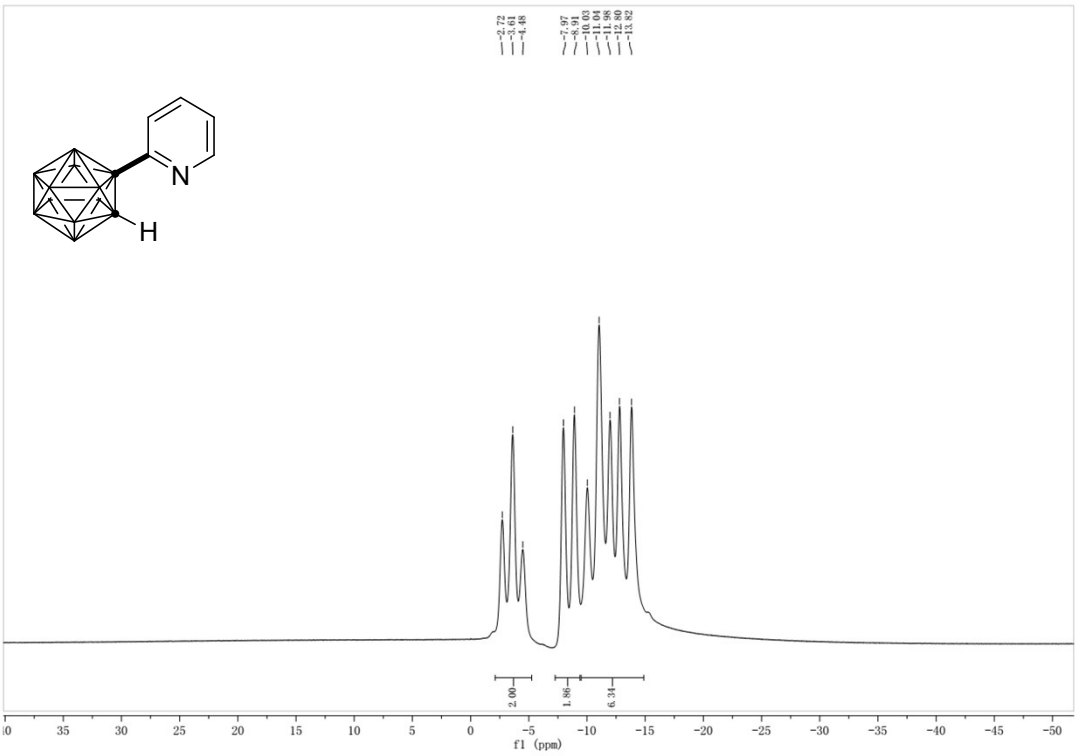
[3] F. Teixidor, A. Laromaine, R. Kivekäs, R. Sillanpää, C. Viñas, R. Vespalec and H. Horáková, *Dalton Trans.,* 2008, **3**, 345–354.

[4] R. Coult, M. A. Fox, W. R. Gill, P. L. Herbertson, J. A. H. MacBride and K. Wade, *J. Organomet. Chem.* 1993, **462(1-2)**, 19–29.

4. NMR Spectra



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H
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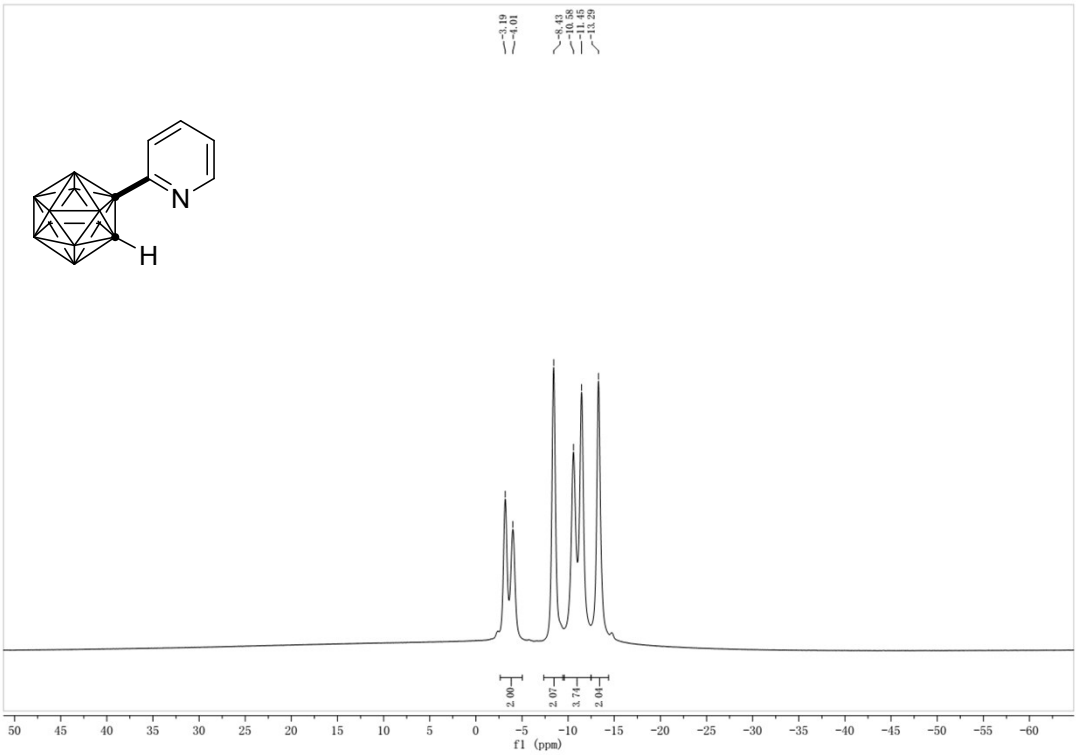
1.86
6.34
f1 (ppm)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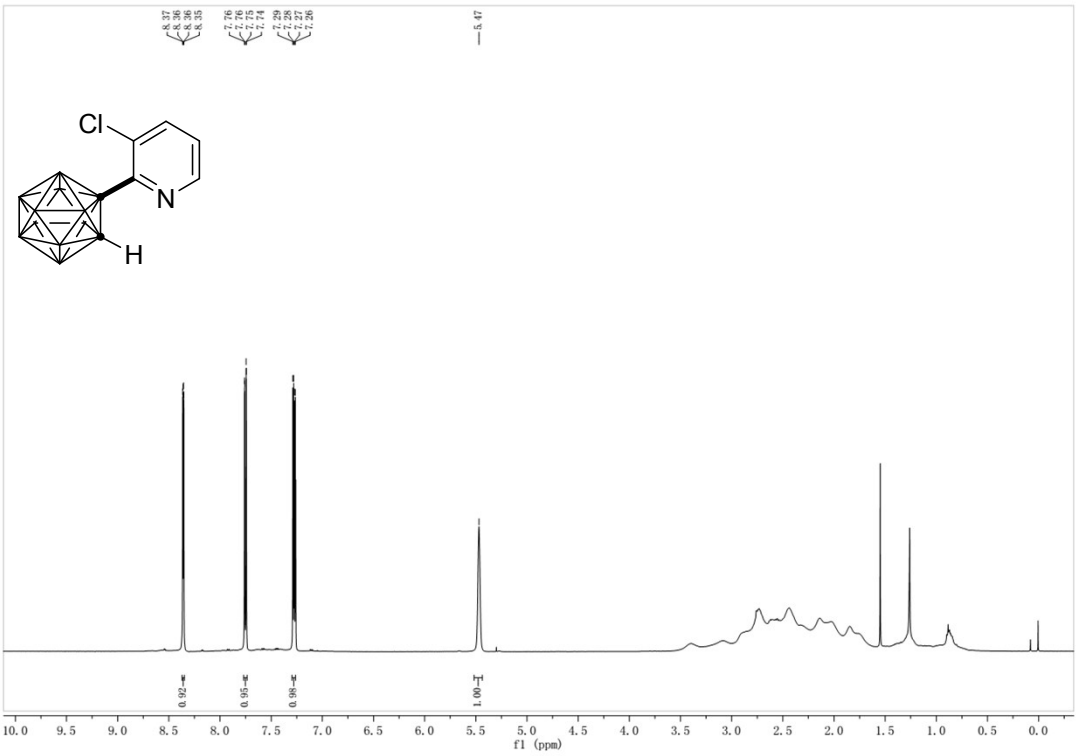
3.74
2.04
f1 (ppm)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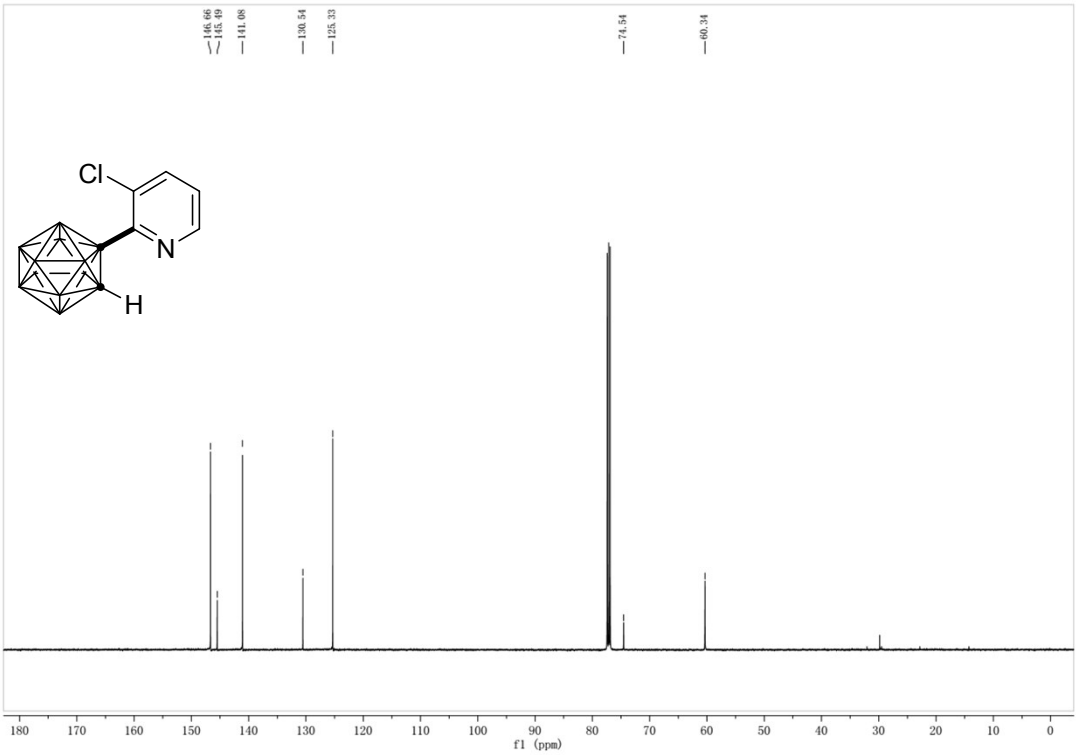
8.36
8.35
7.76
7.76
7.75
7.74
7.29
7.28
7.27
7.26
5.47
Cl
N
H
0.92
0.95
0.98
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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145.49
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60.34
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H
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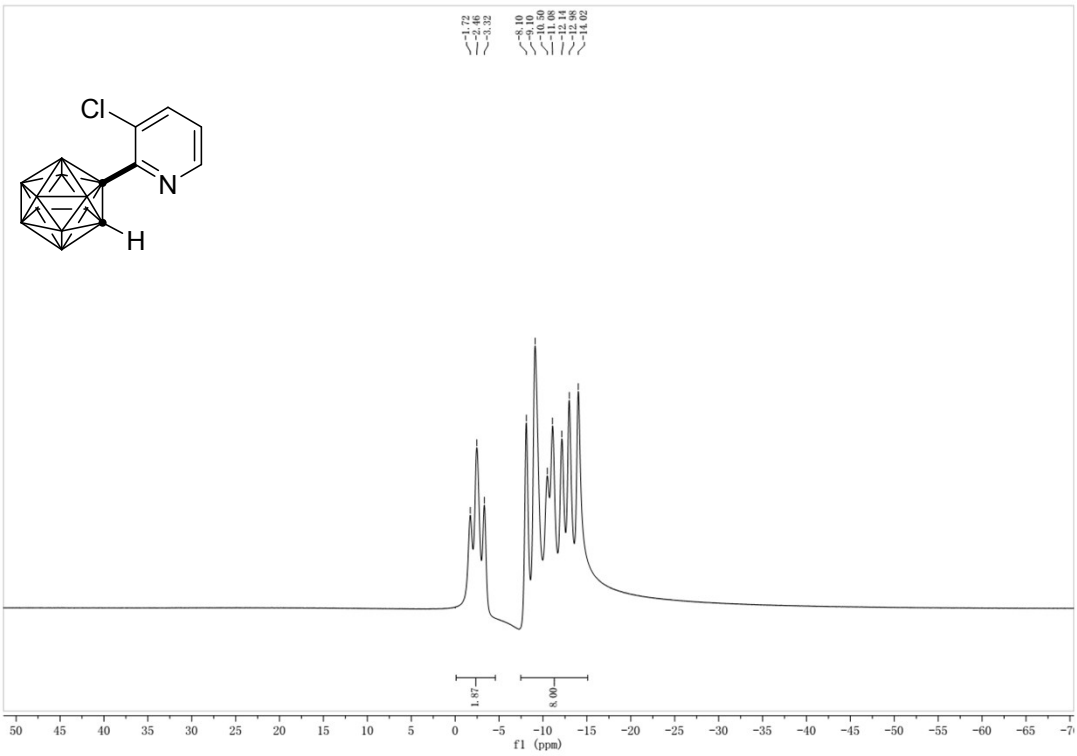
f1 (ppm)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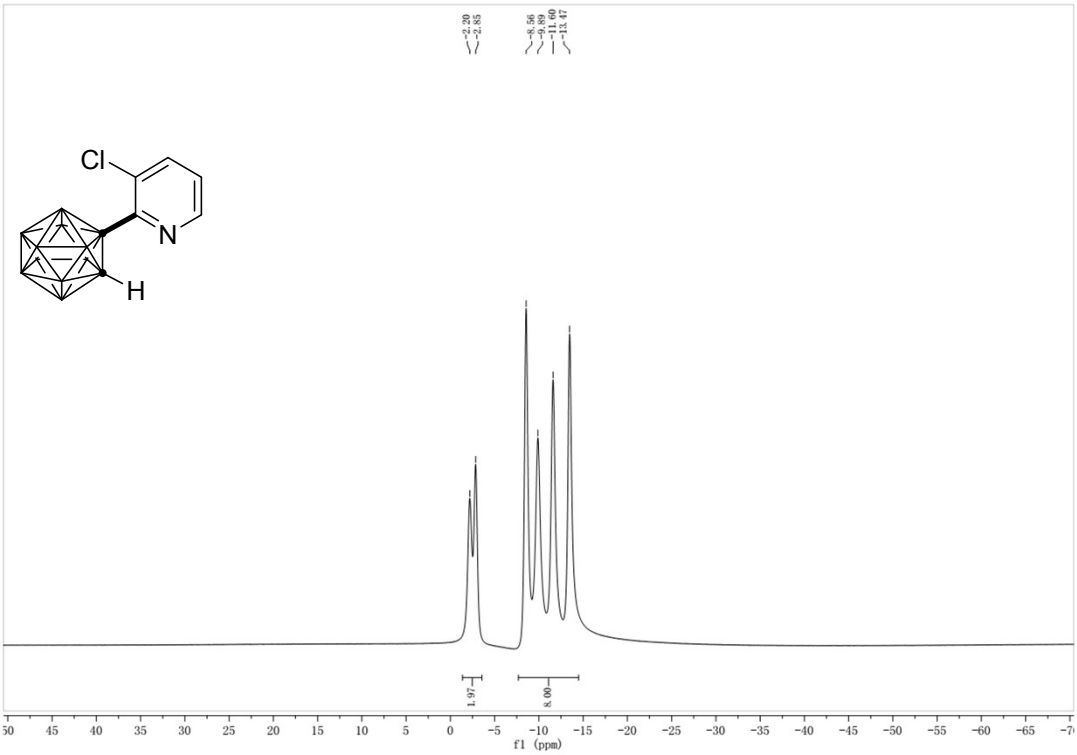
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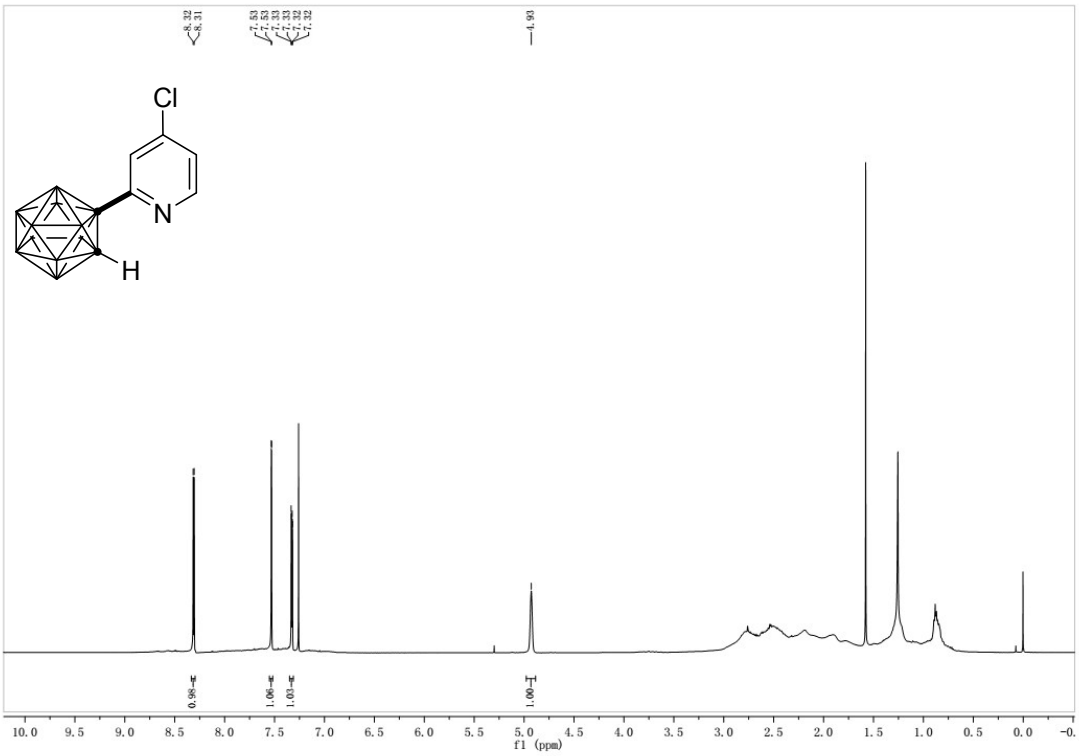
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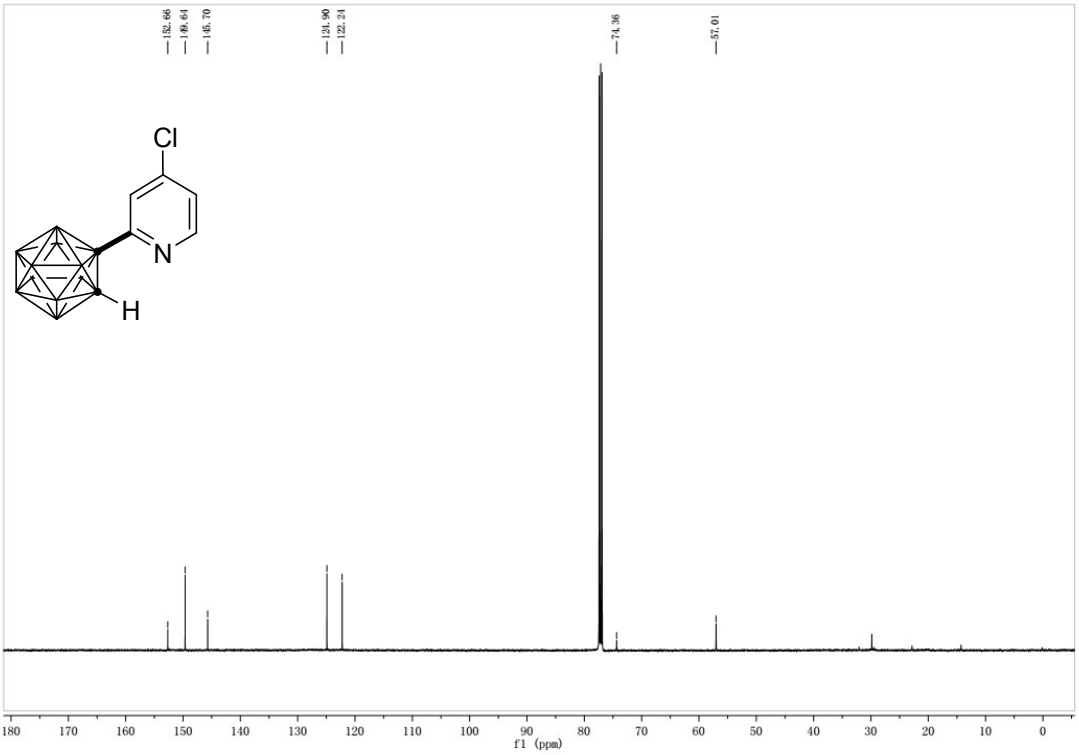
1.00
f1 (ppm)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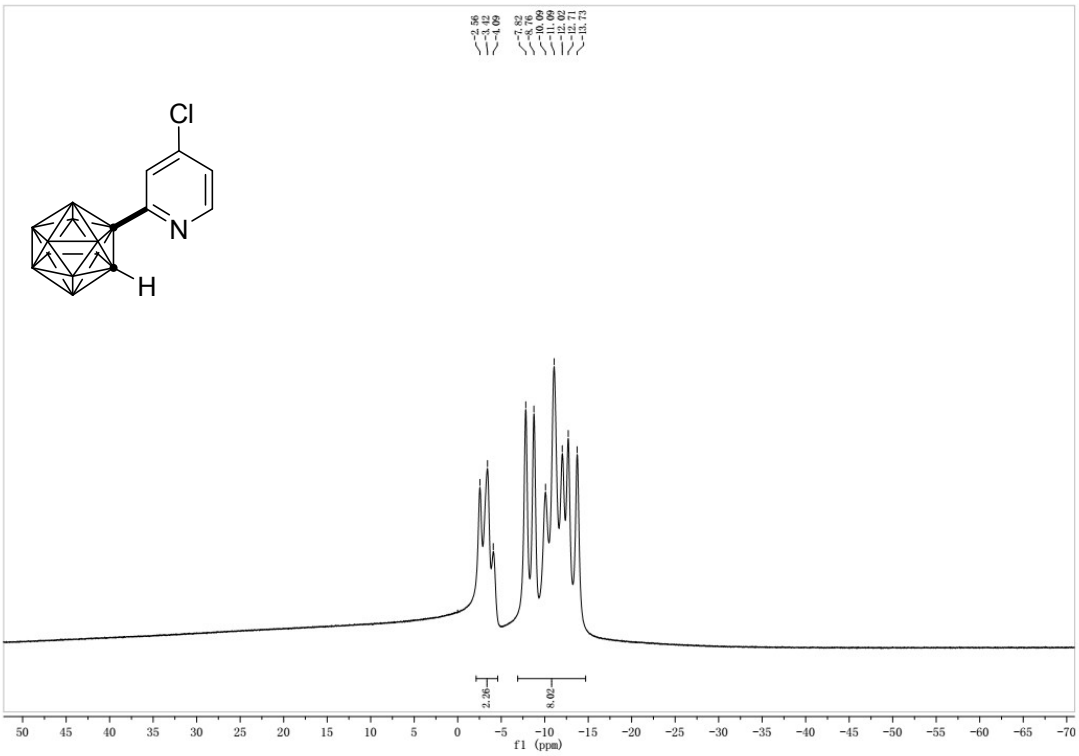
74.36
57.01
Cl
N
H
f1 (ppm)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H
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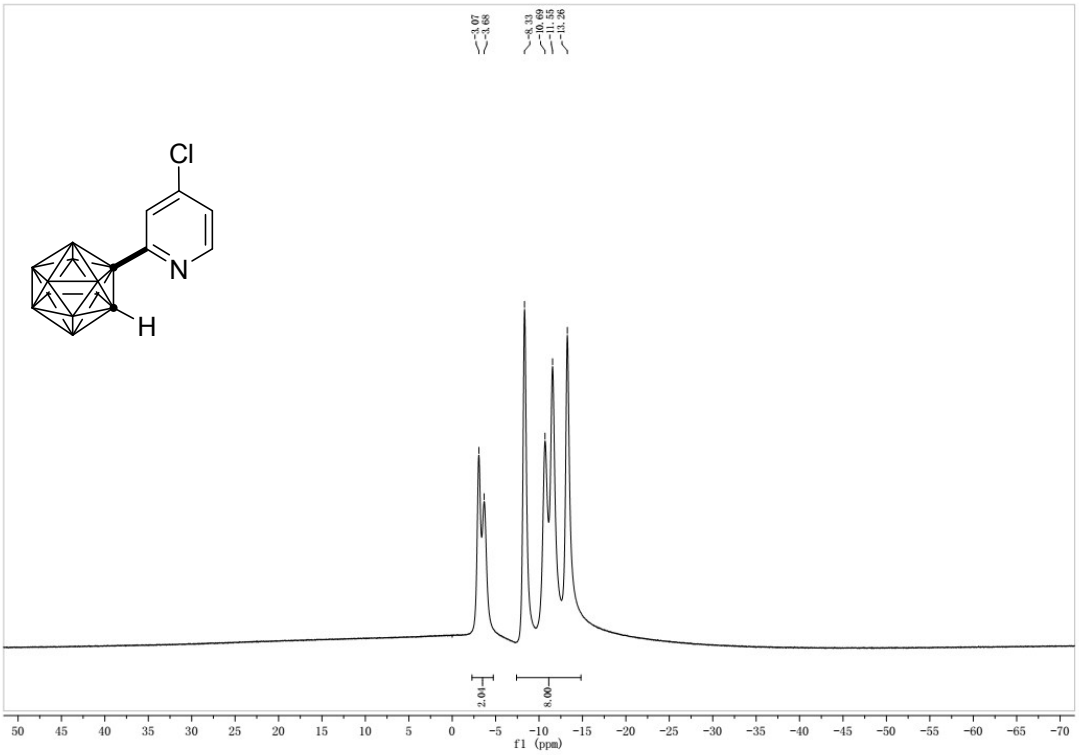
f1 (ppm)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H
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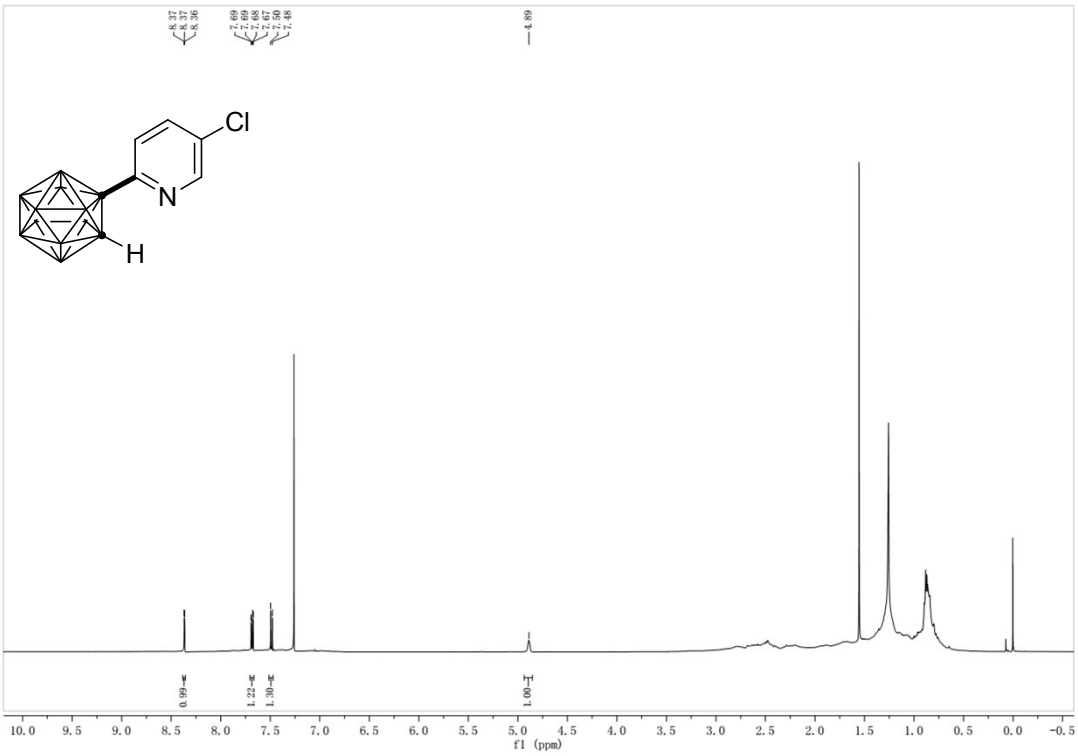
f1 (ppm)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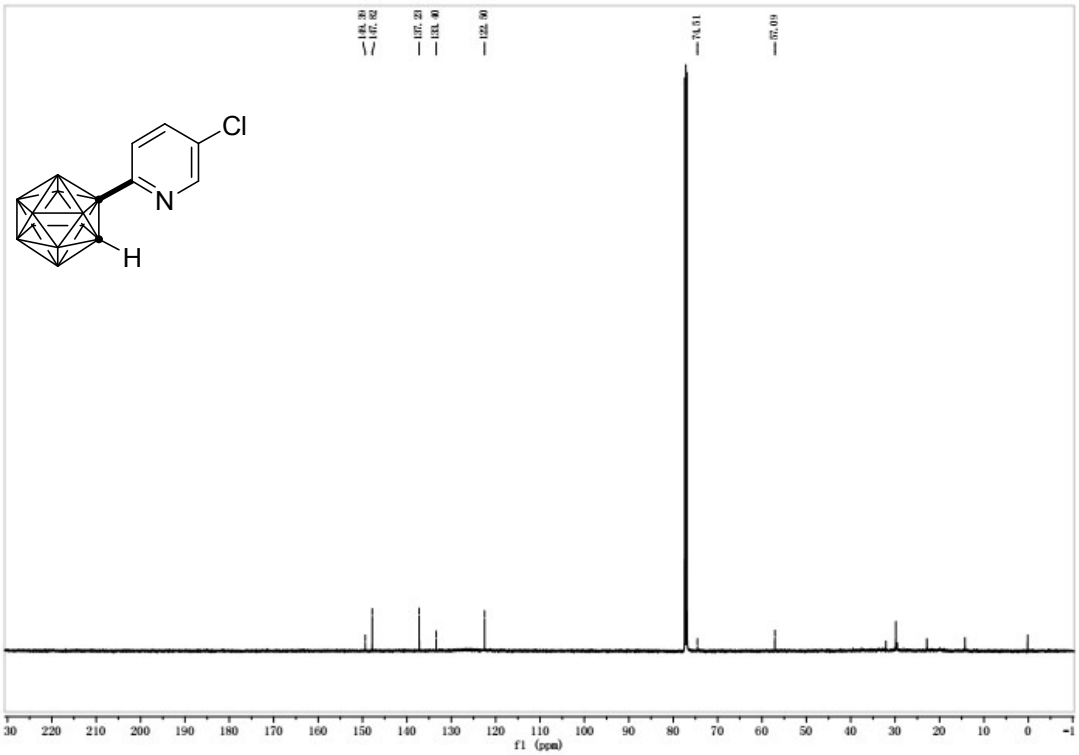
f1 (ppm)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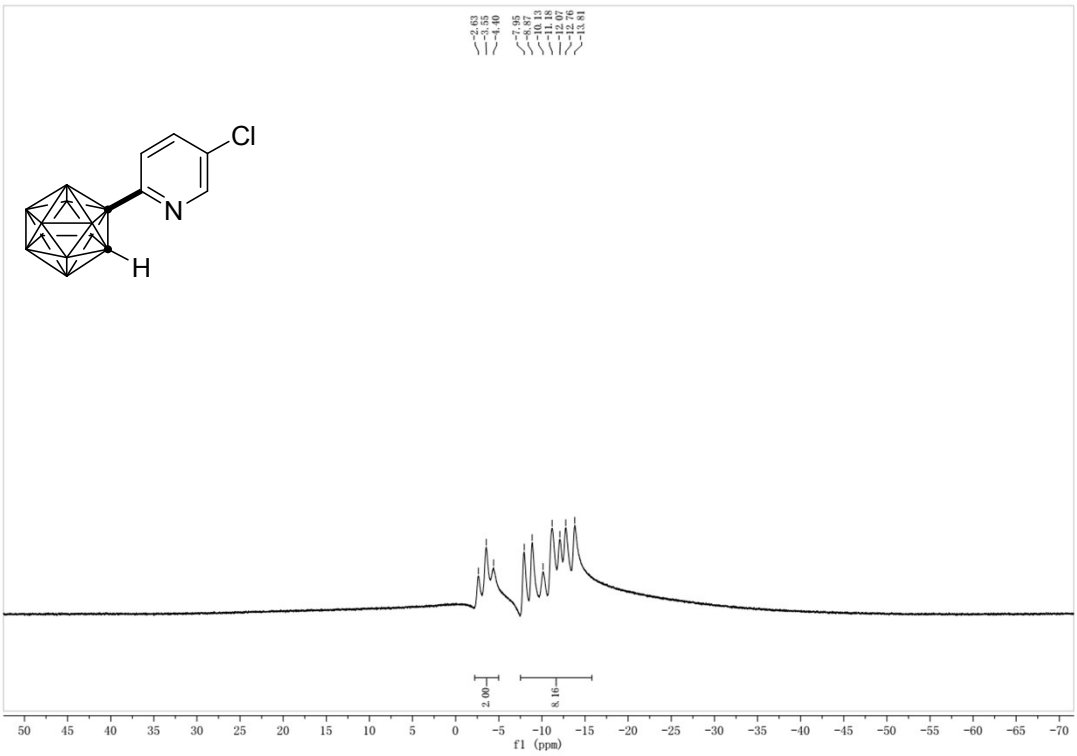
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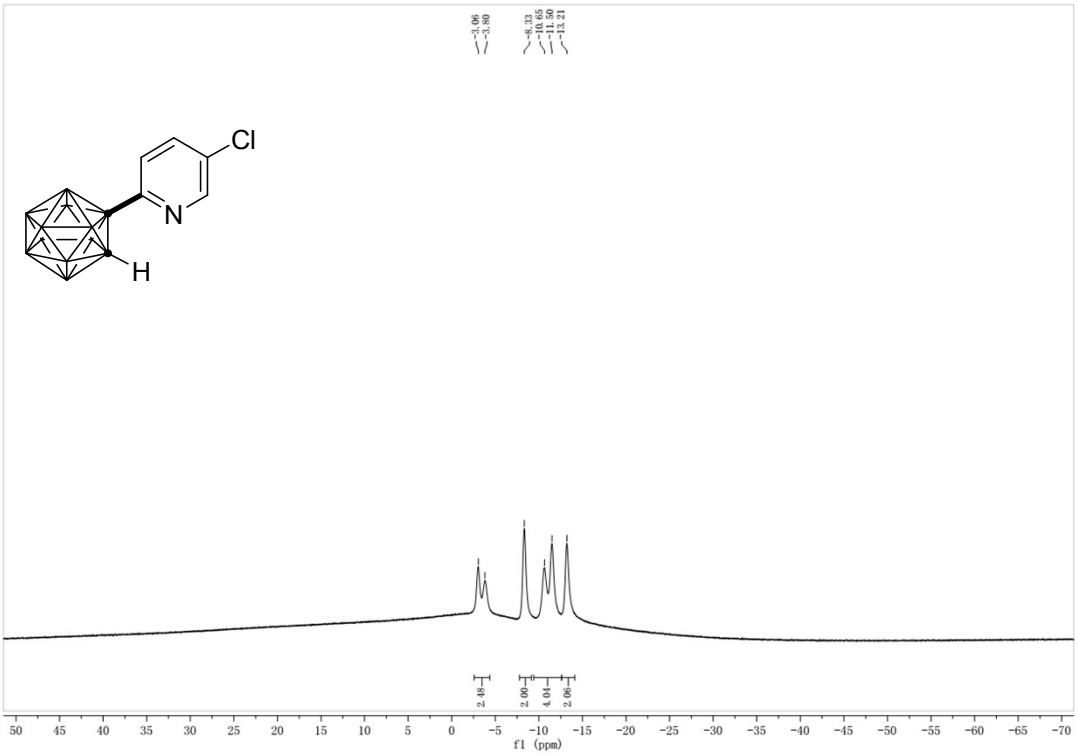
f1 (ppm)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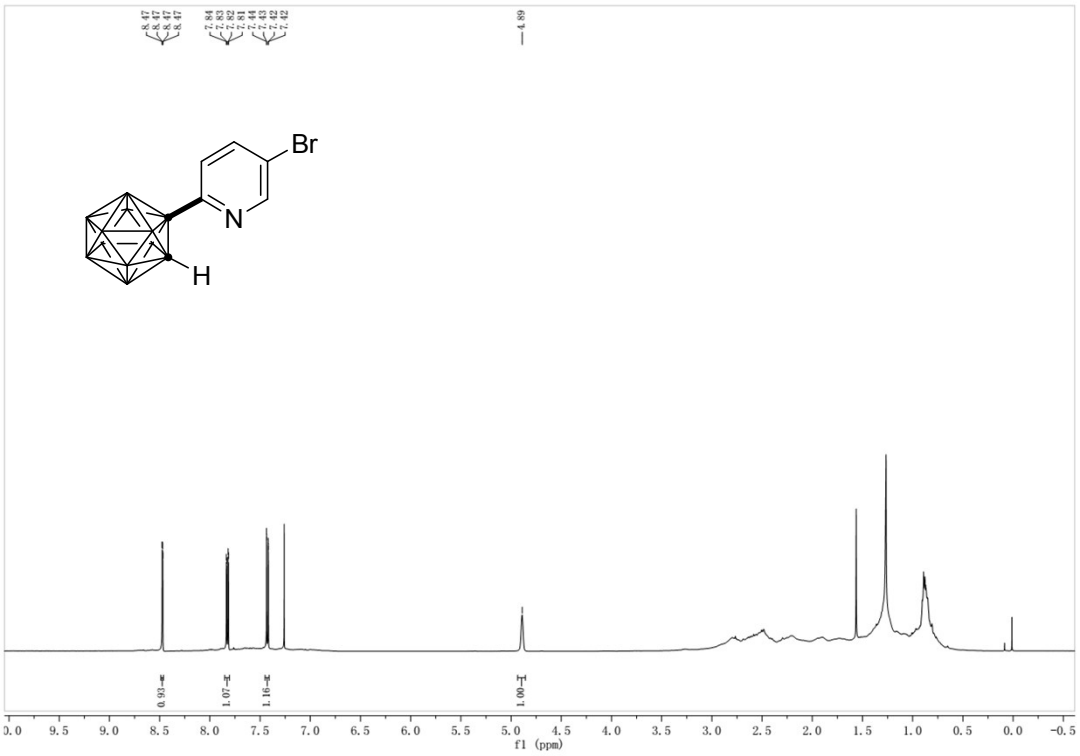
f1 (ppm)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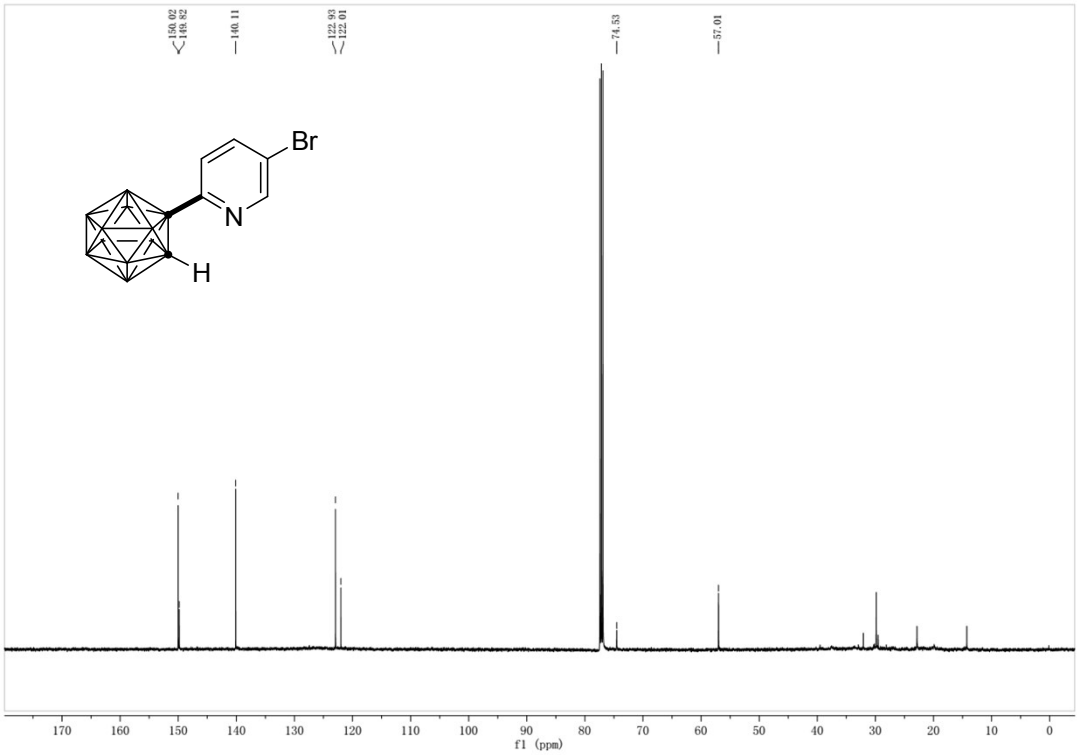
1.00
f1 (ppm)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H
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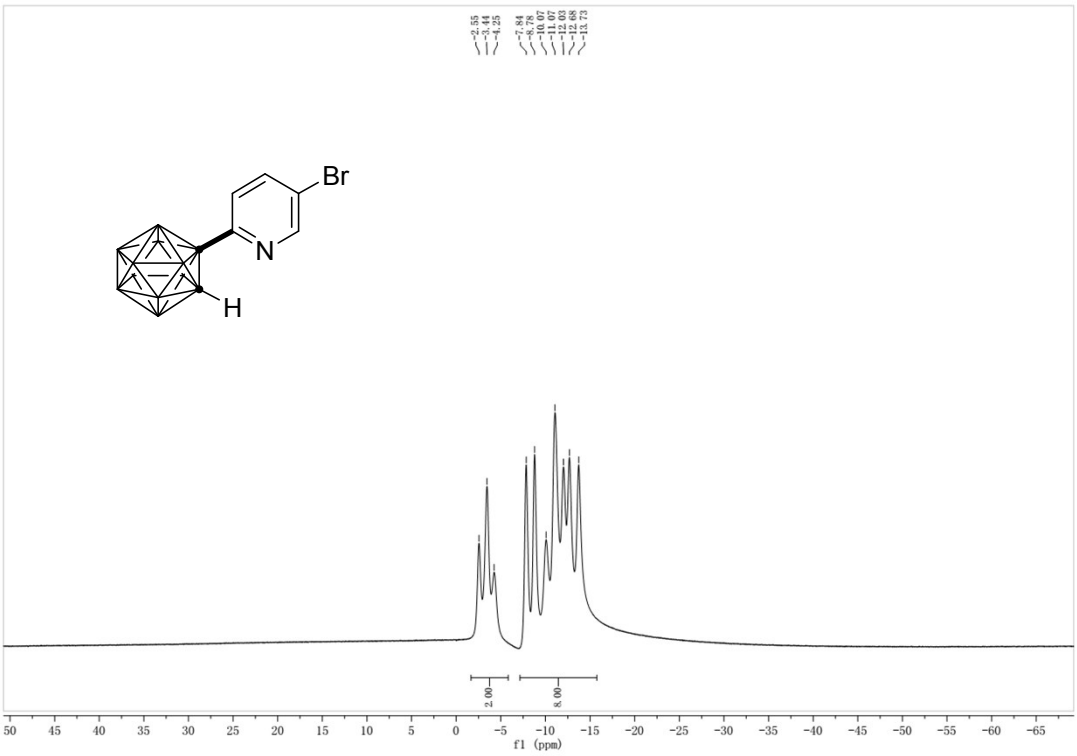
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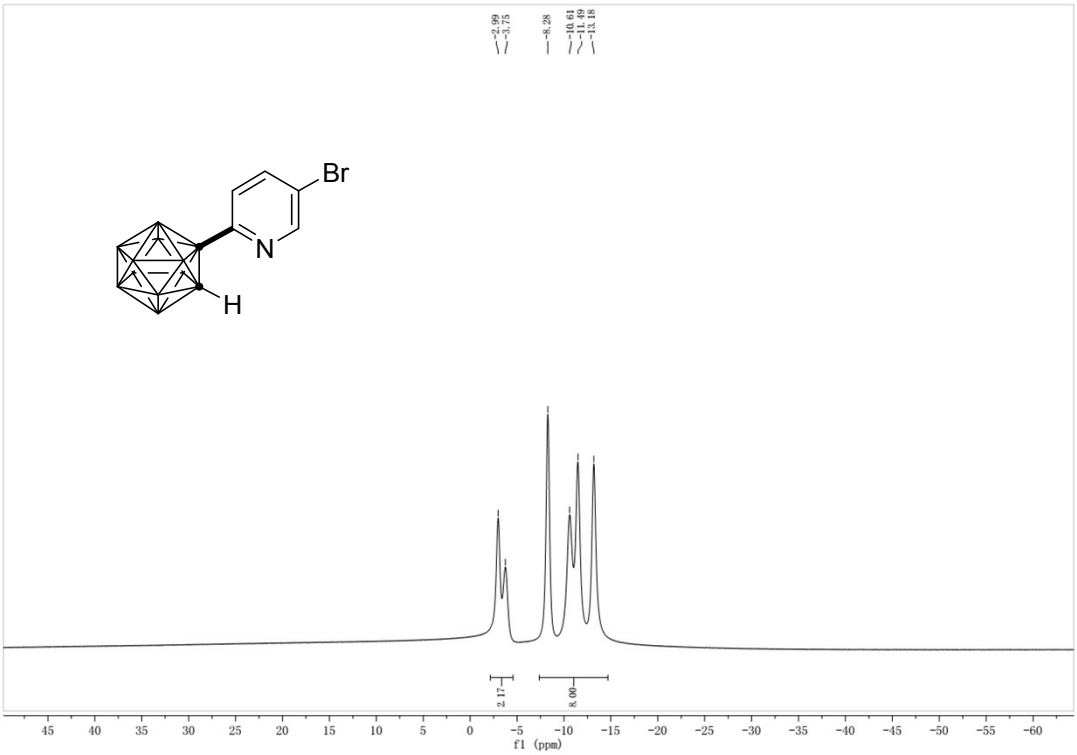
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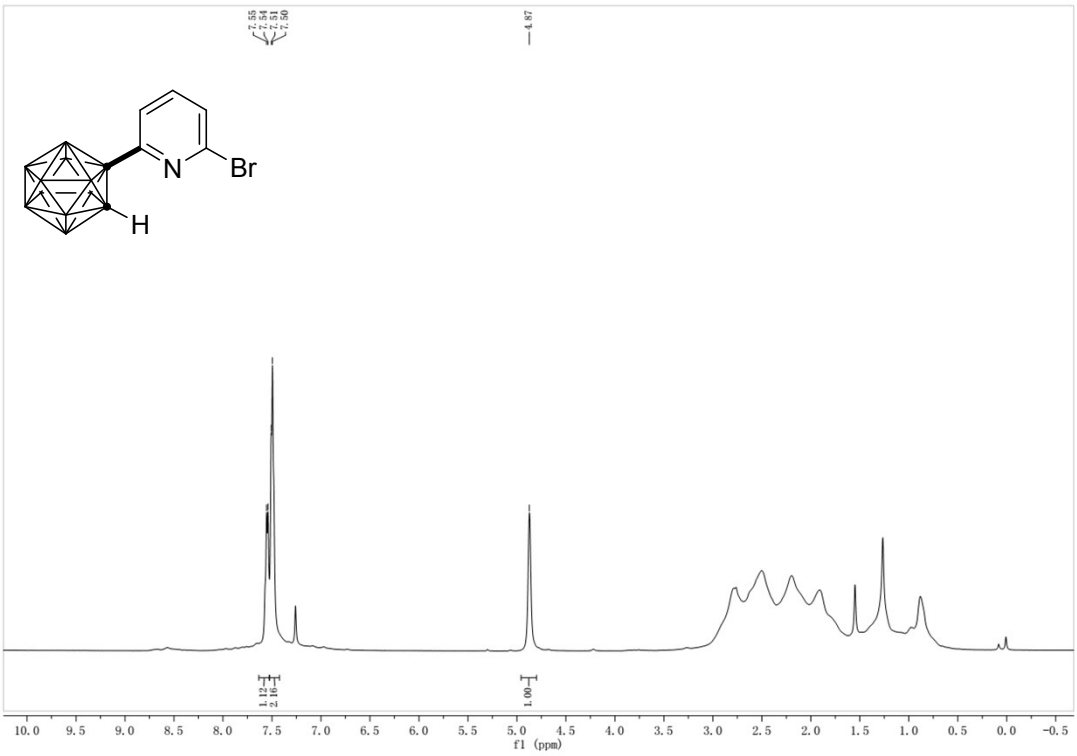
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H
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1.00
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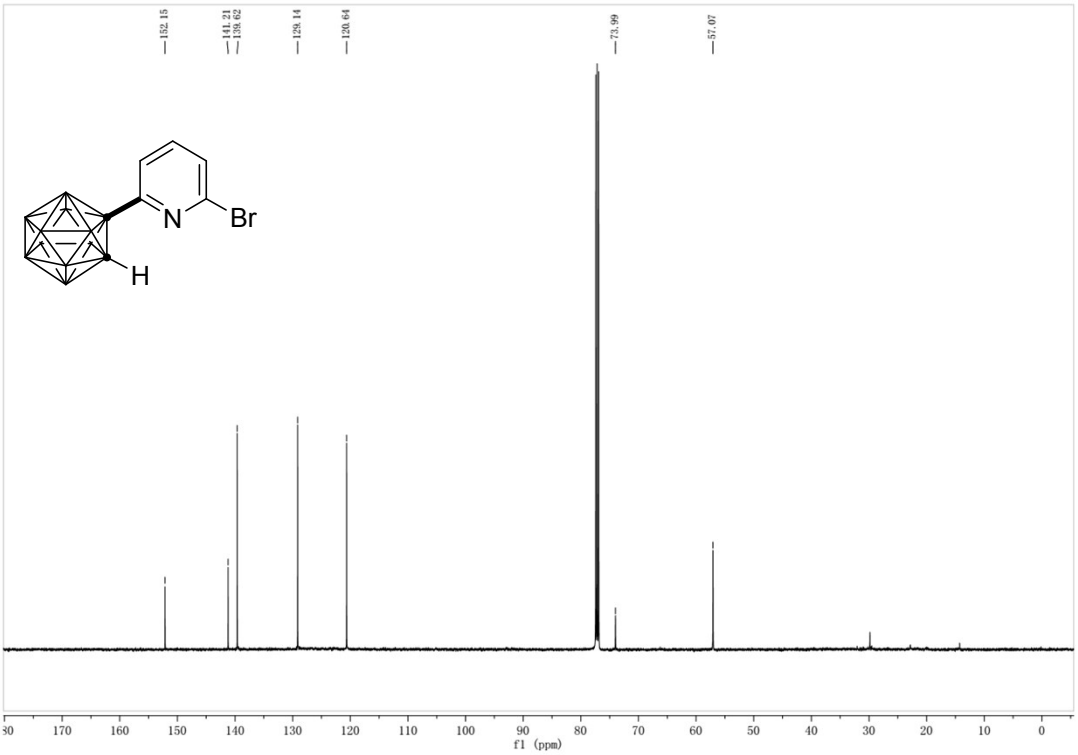
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Br
H
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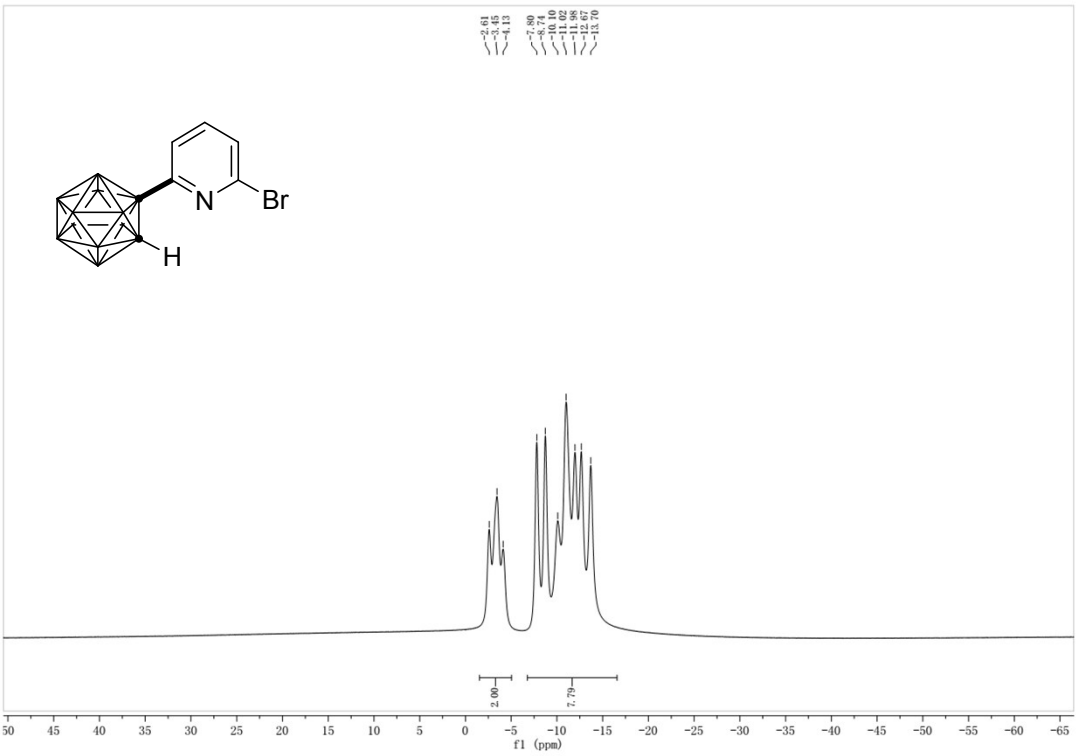
f1 (ppm)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Br
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7.79
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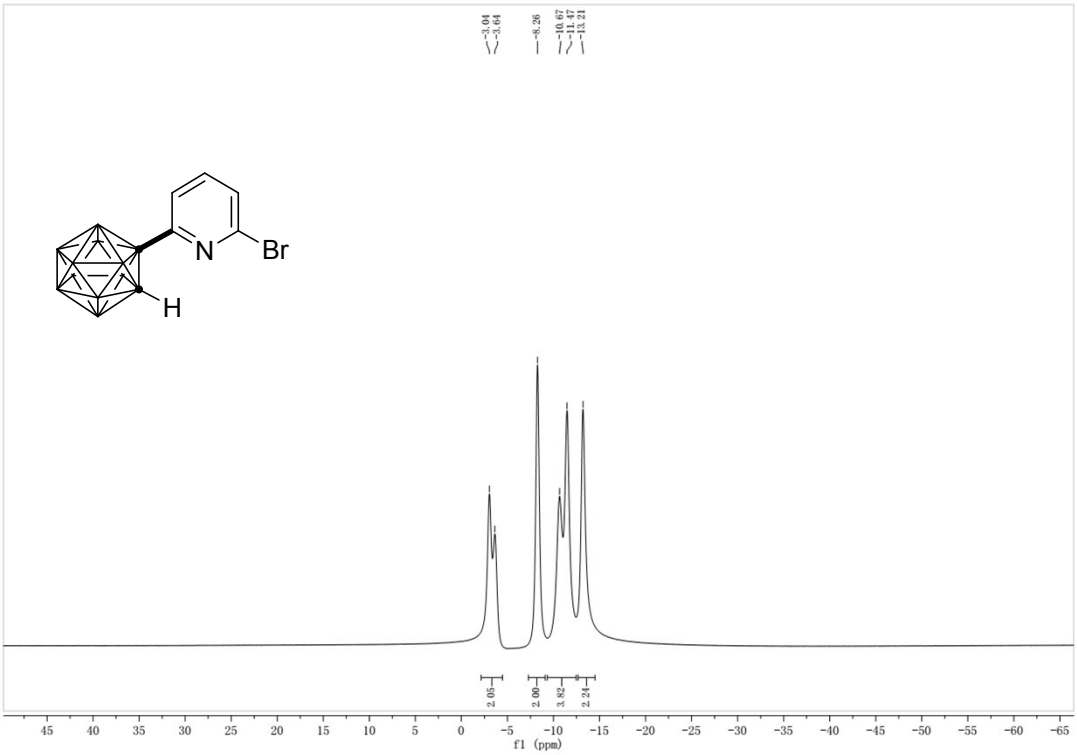
f1 (ppm)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N
Br
H
2.05
2.00
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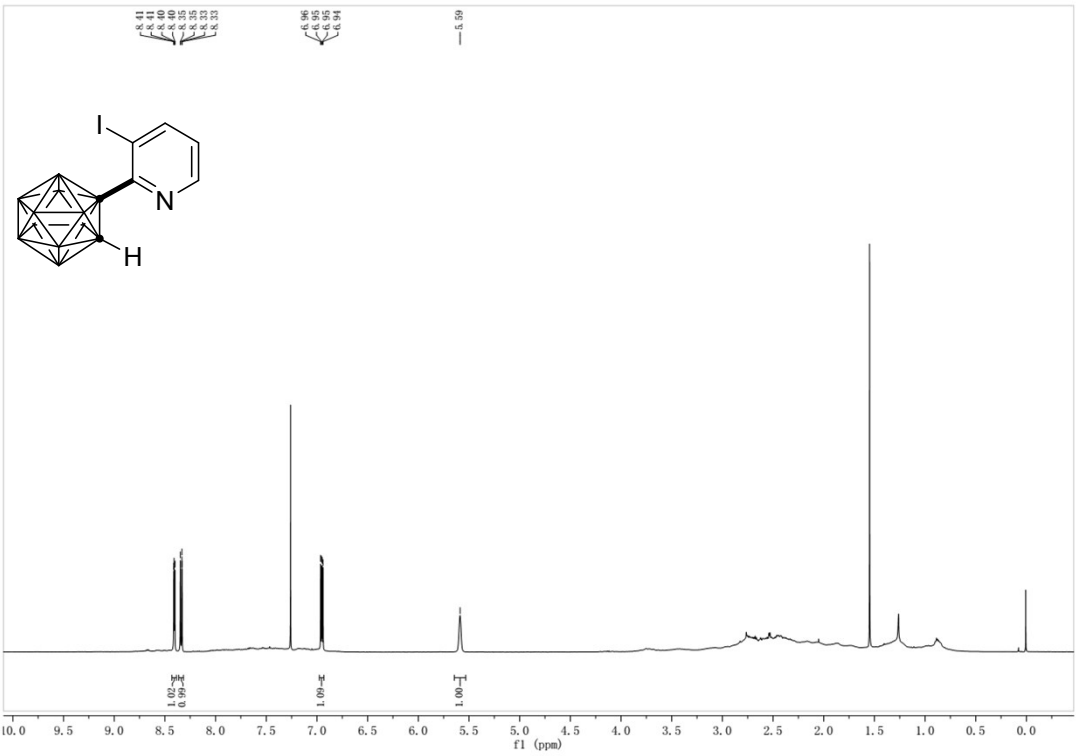
f1 (ppm)


I
N
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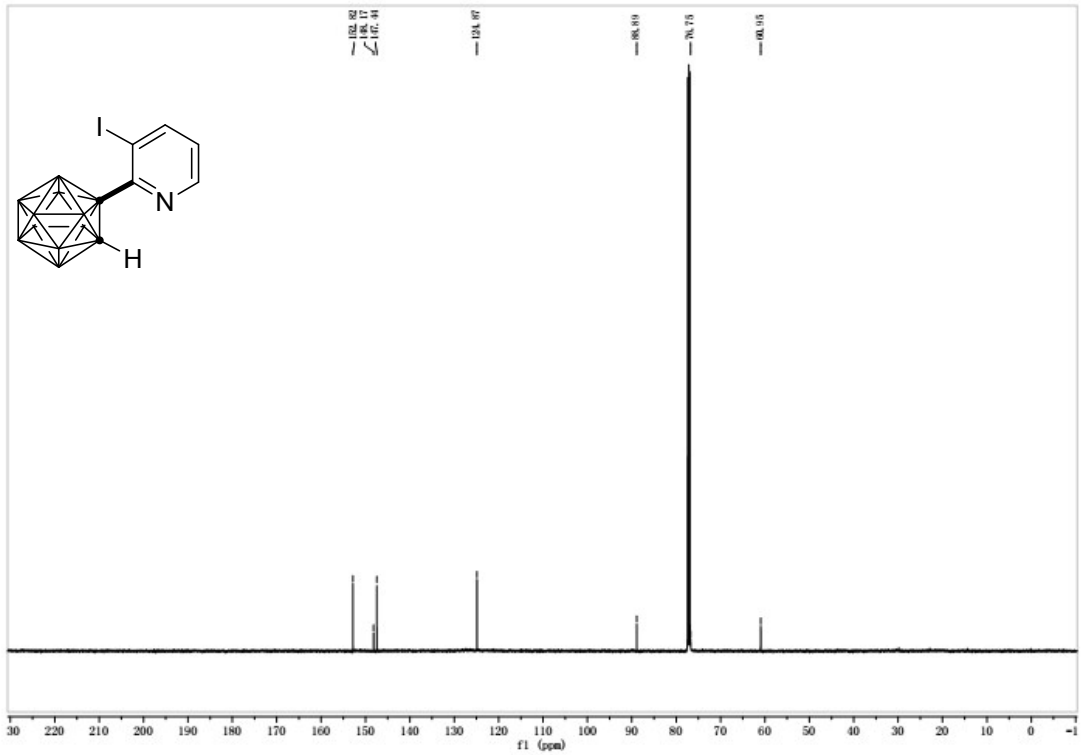
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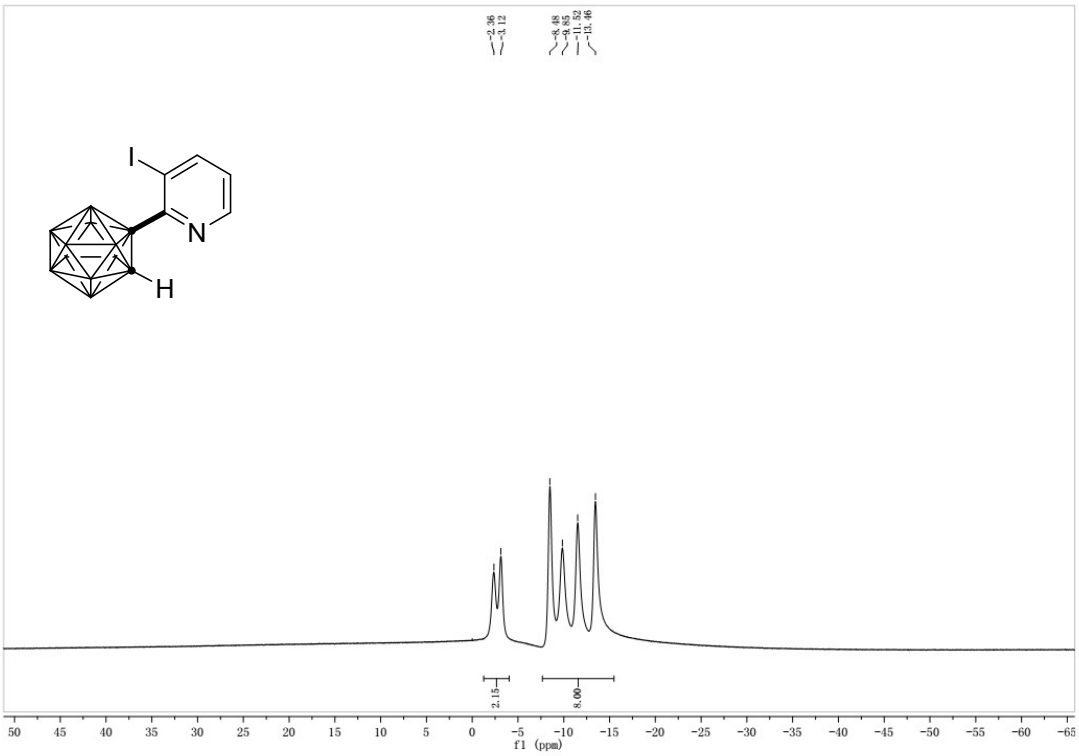
H
f1 (ppm)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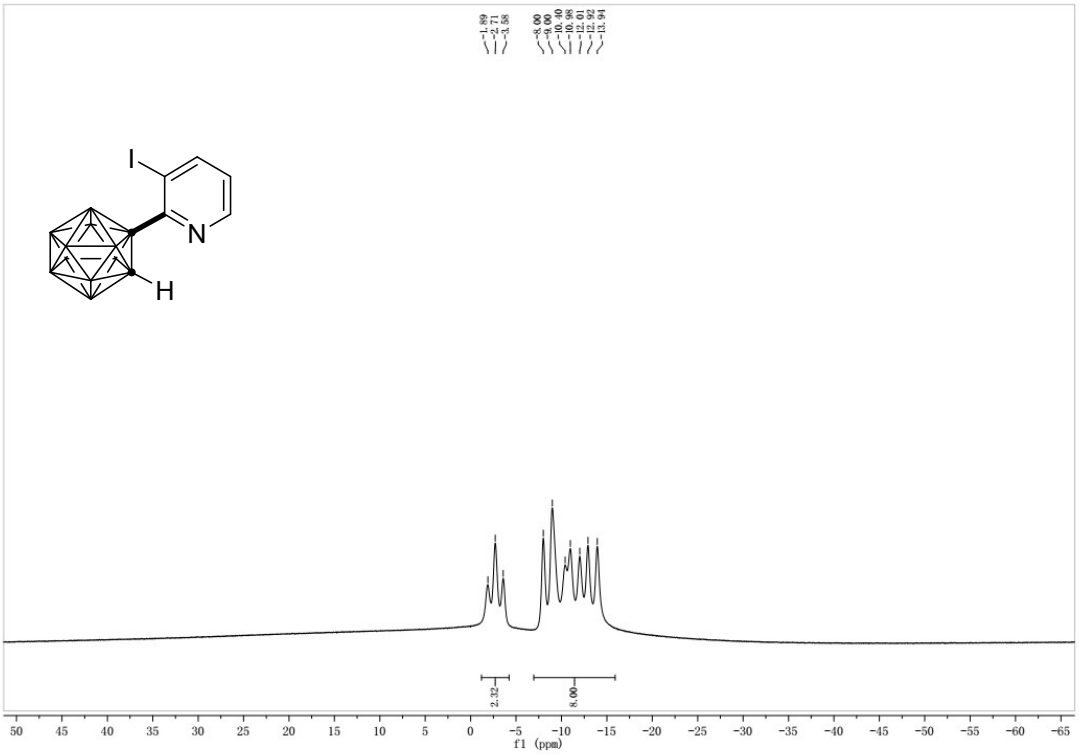
-3.12
-8.48
-9.85
-11.52
-13.46
I
N
H
2.15
8.00
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)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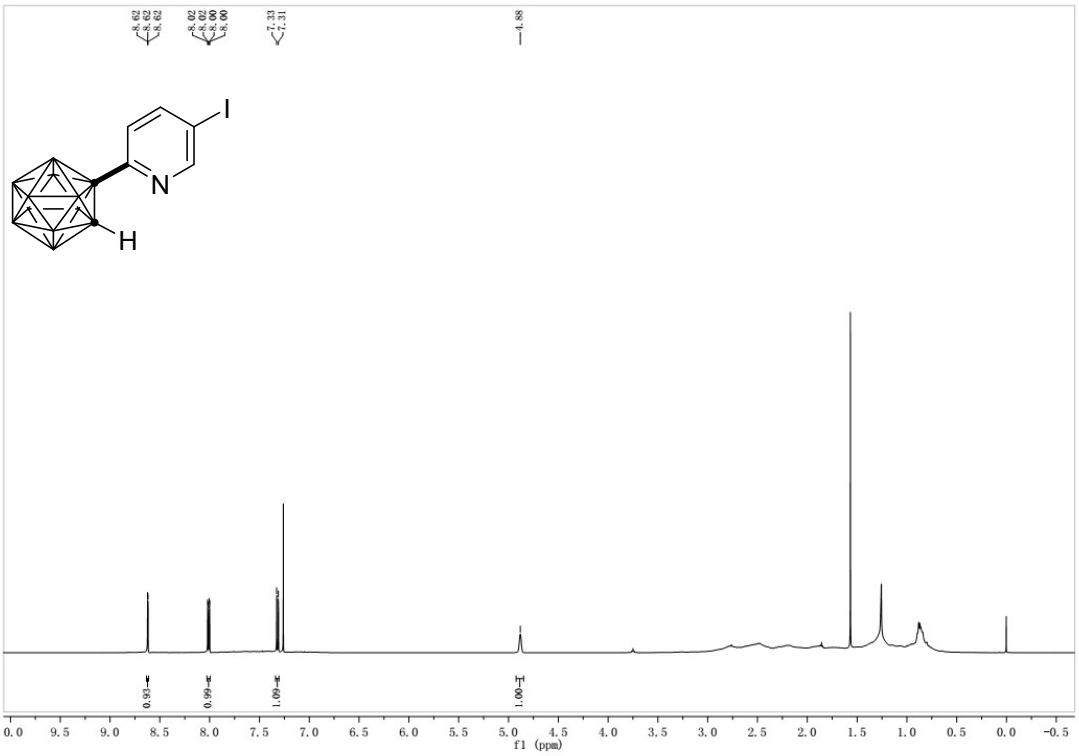
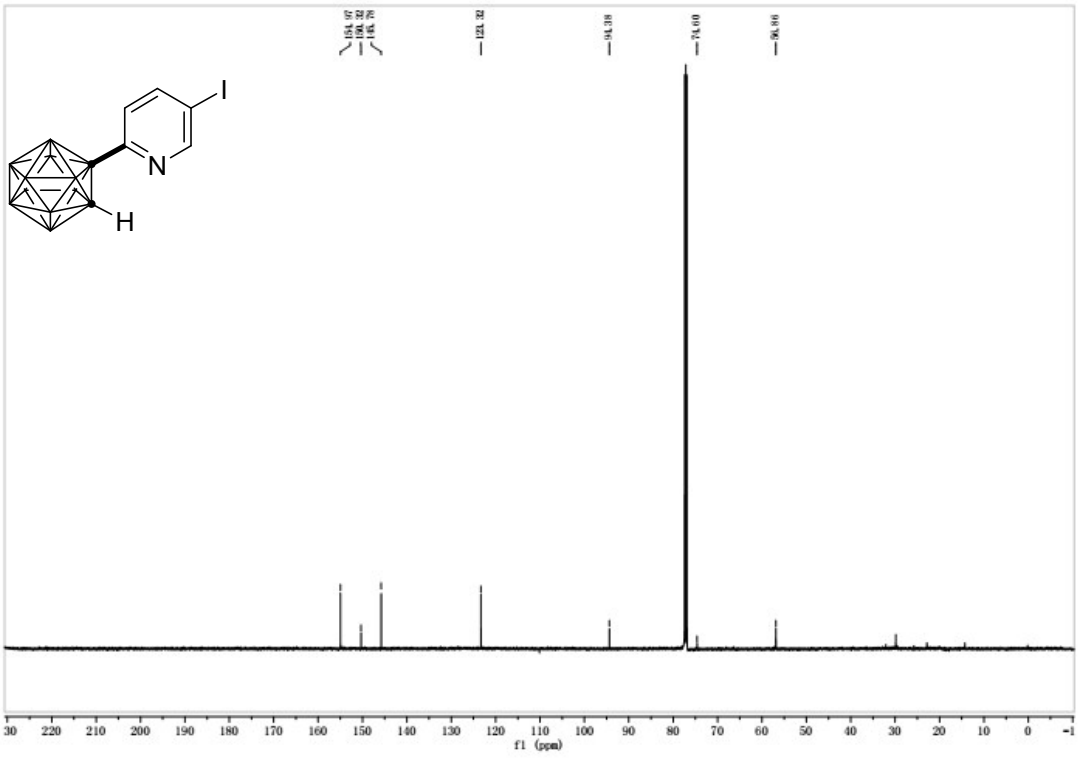
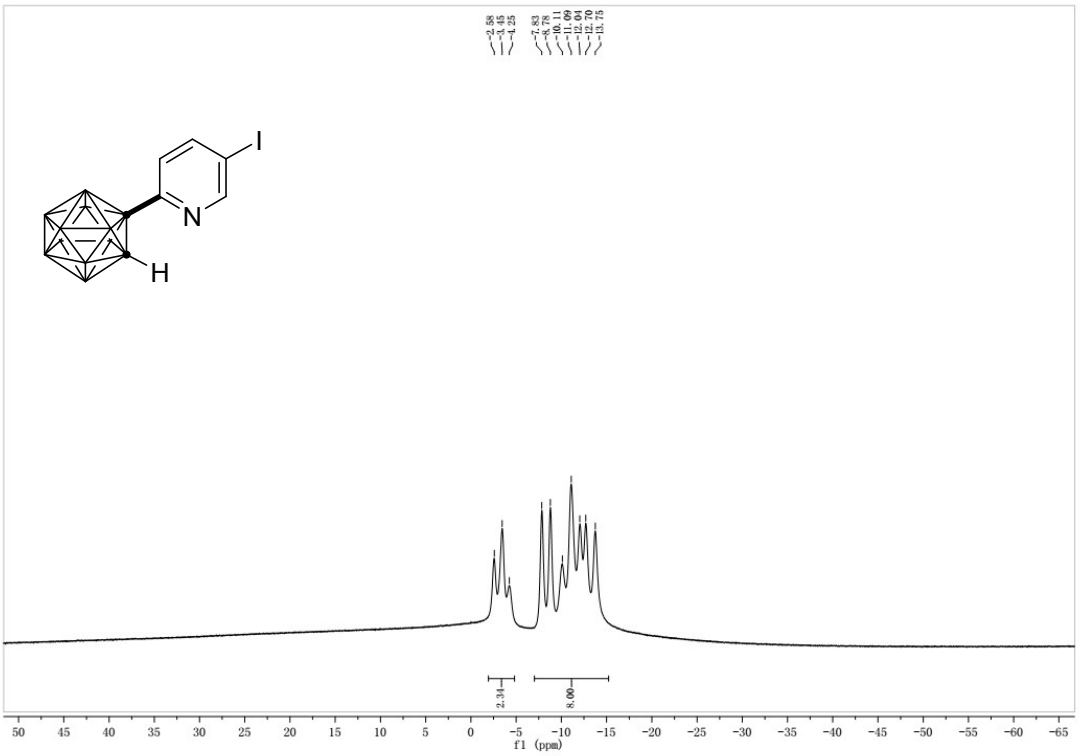
-2.71
-3.58
-8.00
-9.00
-10.00
-10.96
-12.01
-12.92
-13.94
I
N
H
2.32
8.00
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)


8.62
8.62
8.62
8.02
8.02
8.00
8.00
7.33
7.31
4.88
I
N
H
0.93
0.99
1.09
1.00
f1 (ppm)


154.97
150.32
146.70
123.32
94.38
74.60
56.86
I
N
H
f1 (ppm)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-3.15
-4.25
-7.83
-8.78
-10.11
-11.09
-12.04
-12.70
-13.15
I
N
H
2.34
8.00
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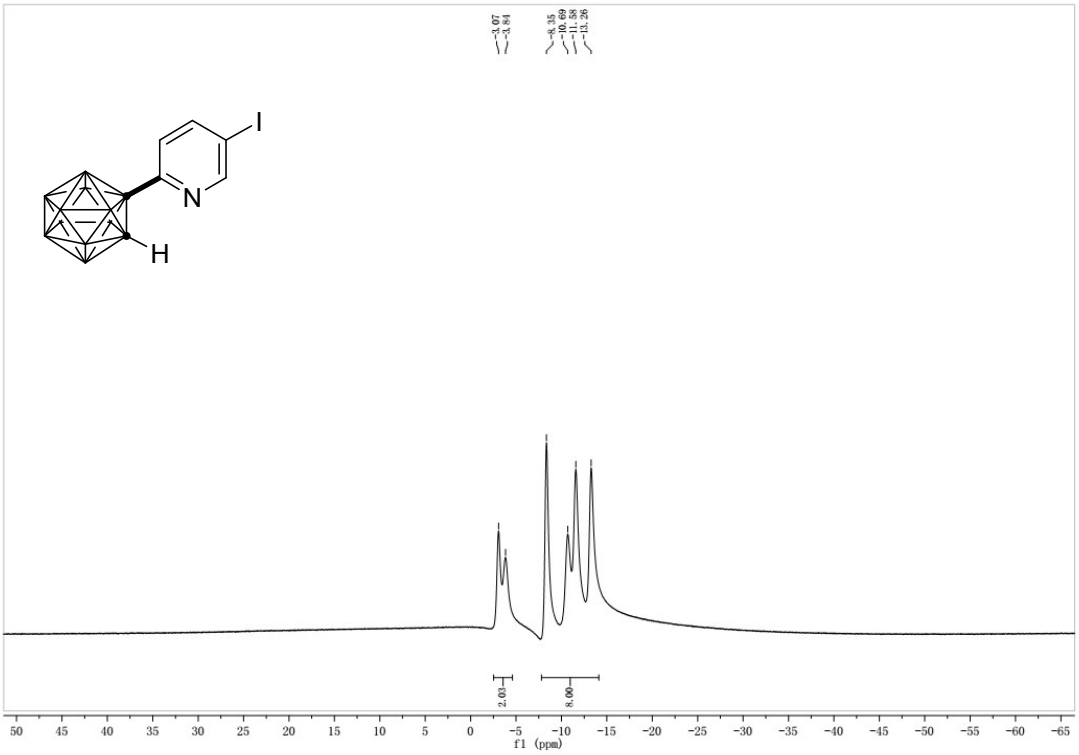
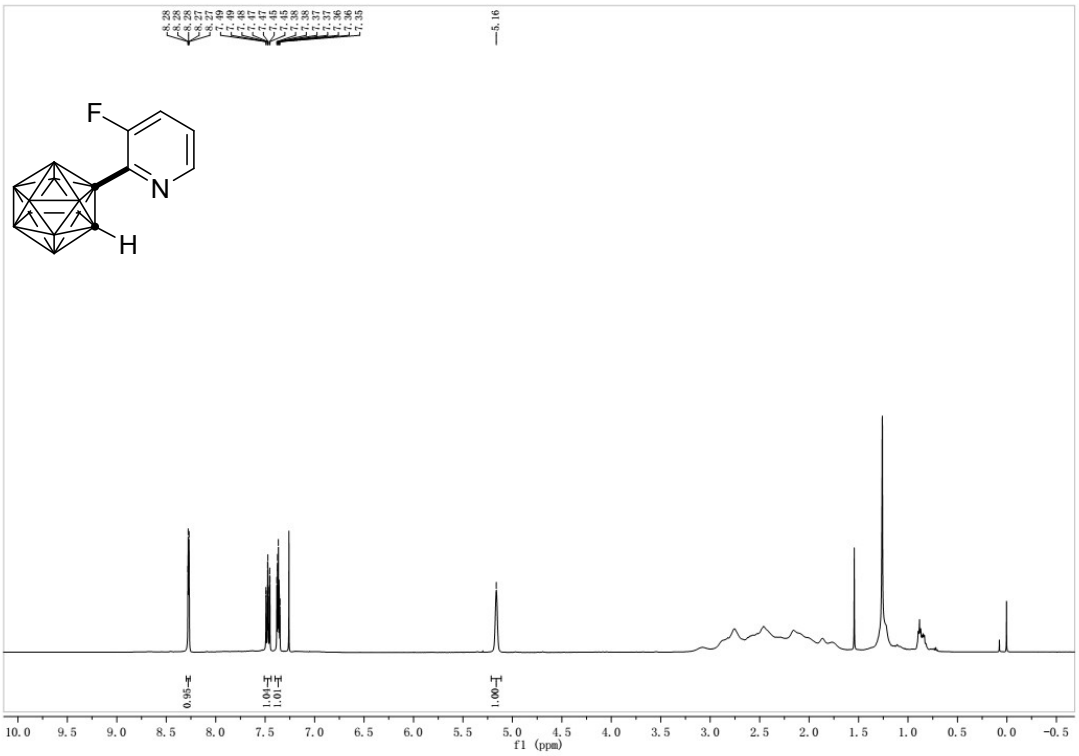
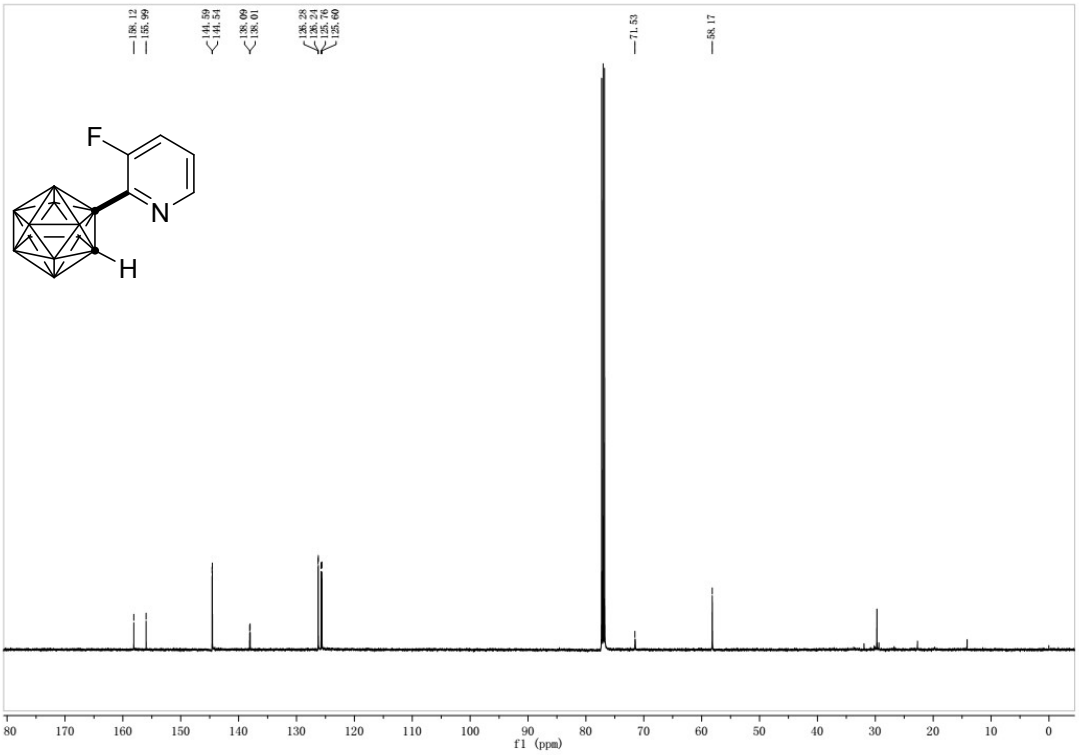
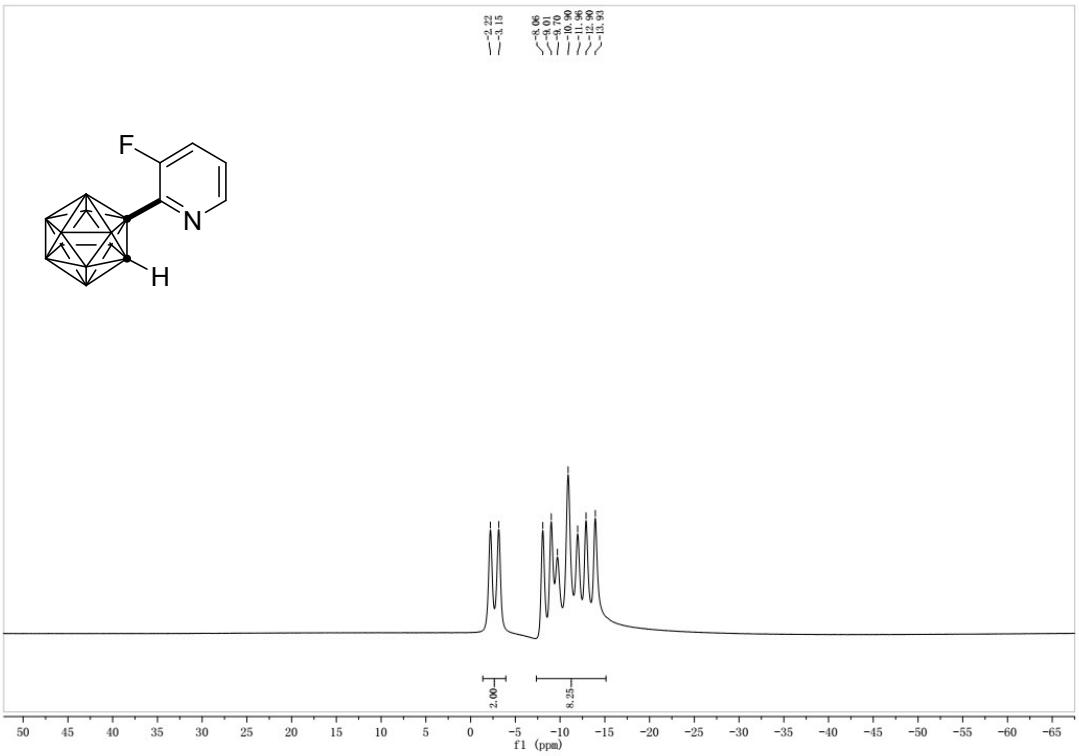
f1 (ppm)


-3.07
-3.84
-8.35
-10.69
-11.38
-13.26
I
N
H
2.03
8.00
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)


F
N
H
f1 (ppm)


F
N
H
f1 (ppm)


F
N
H
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-3.15
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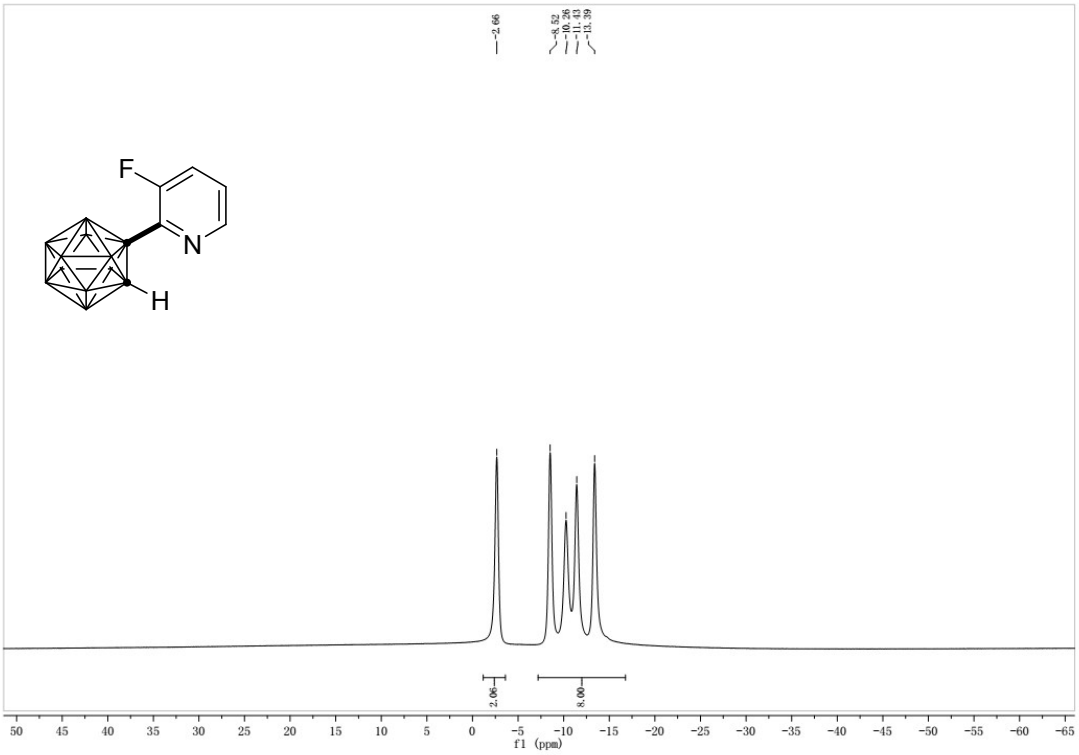
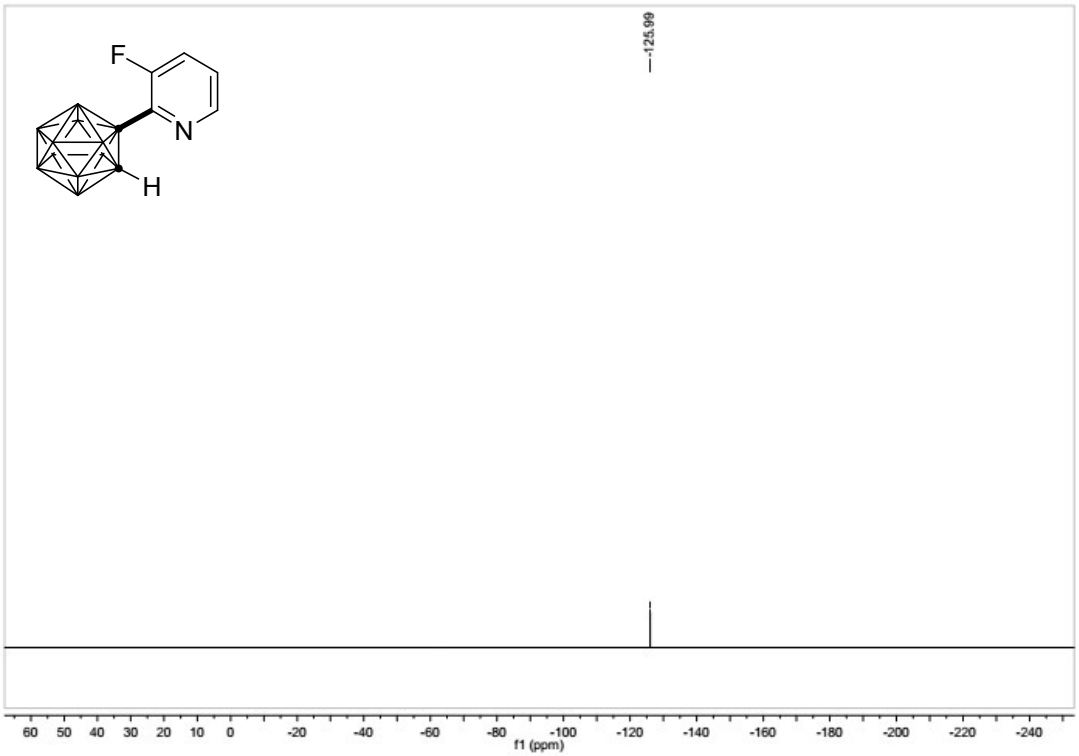
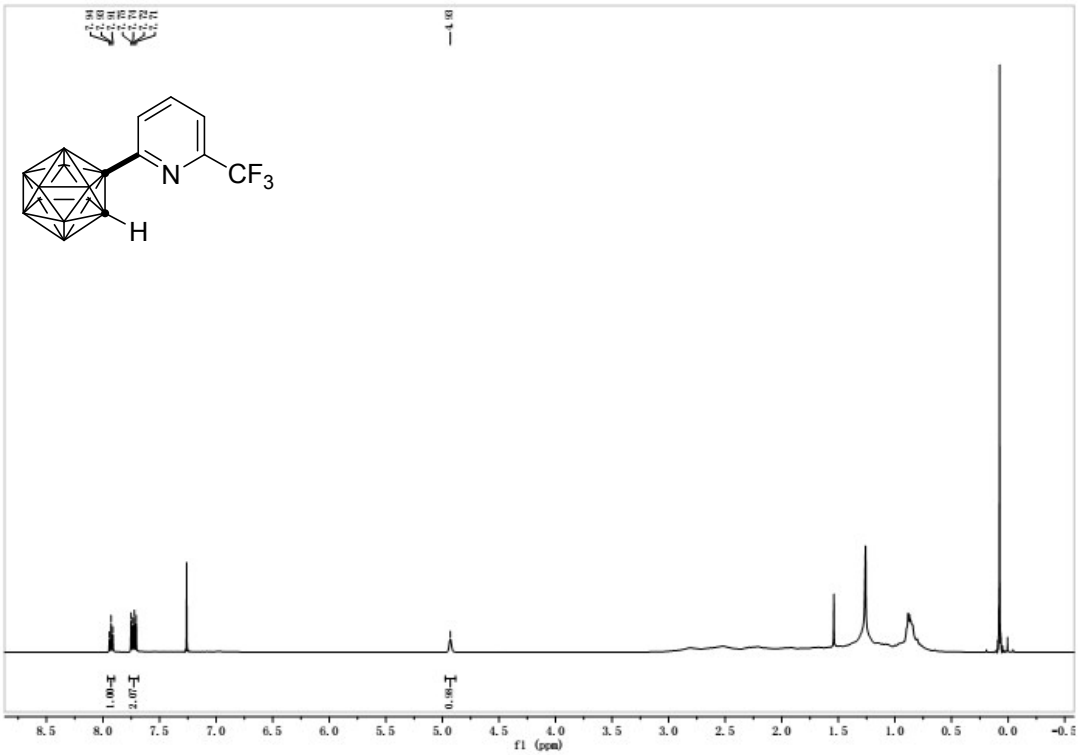
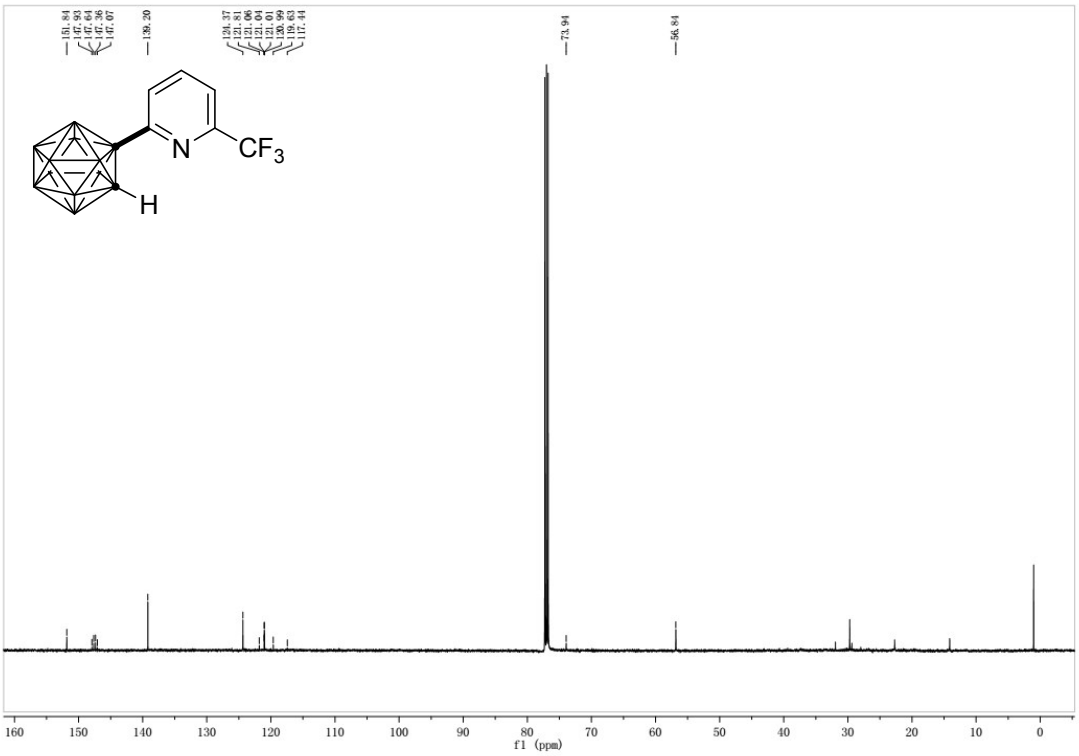
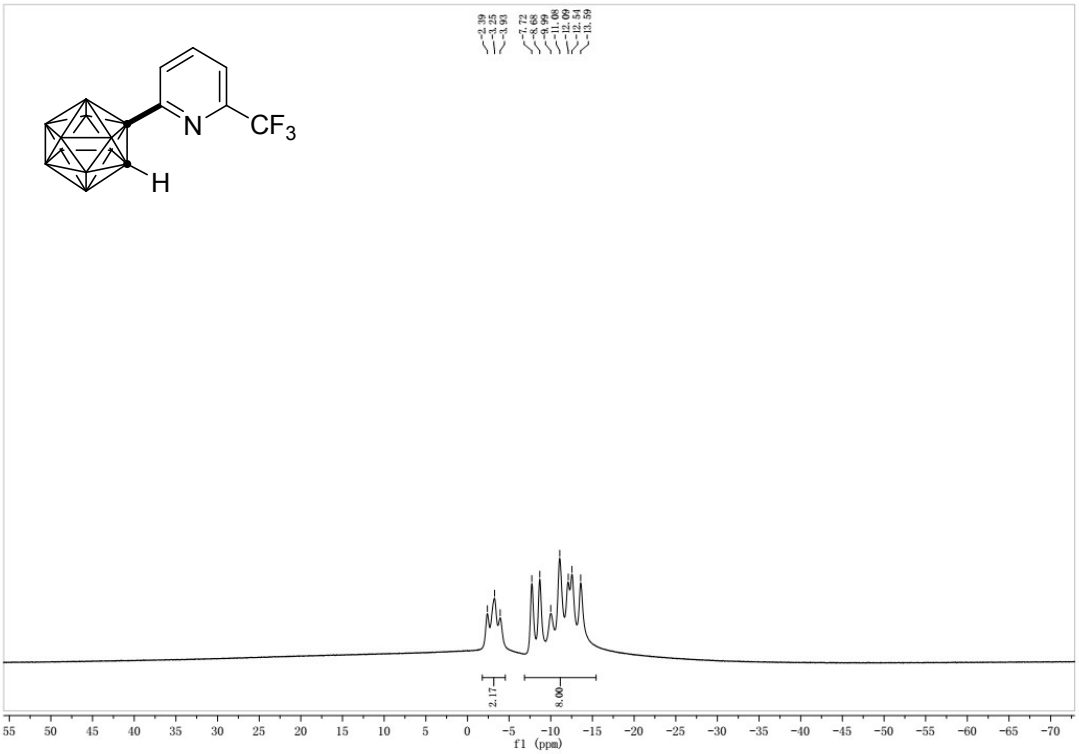
-8.61
-9.70
-10.90
-11.96
-12.90
-13.93
2.00
8.25
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)

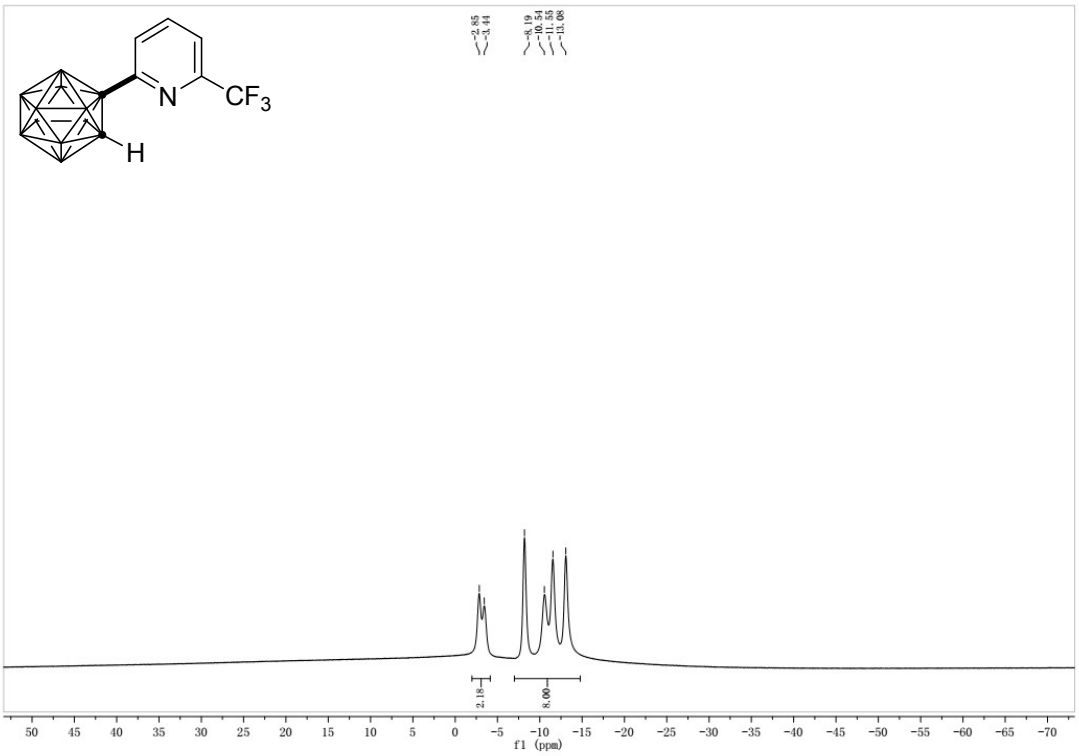

F
N
H
-2.66
-8.52
-10.26
-11.43
-13.39
2.06
8.00
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)


F
N
H
-125.99
60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240
f1 (ppm)


N
CF3
H
4.93
1.00
2.07
0.98
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


151.84
147.93
147.64
147.36
147.07
139.20
124.37
121.81
121.56
121.04
121.01
120.99
119.63
117.44
73.94
56.84
N
CF3
H
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


2.39
3.25
3.93
7.72
8.68
8.69
11.66
12.69
12.54
13.59
N
CF3
H
2.17
8.00
55
50
45
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
−45
−50
−55
−60
−65
−70
f1 (ppm)


N
CF3
H
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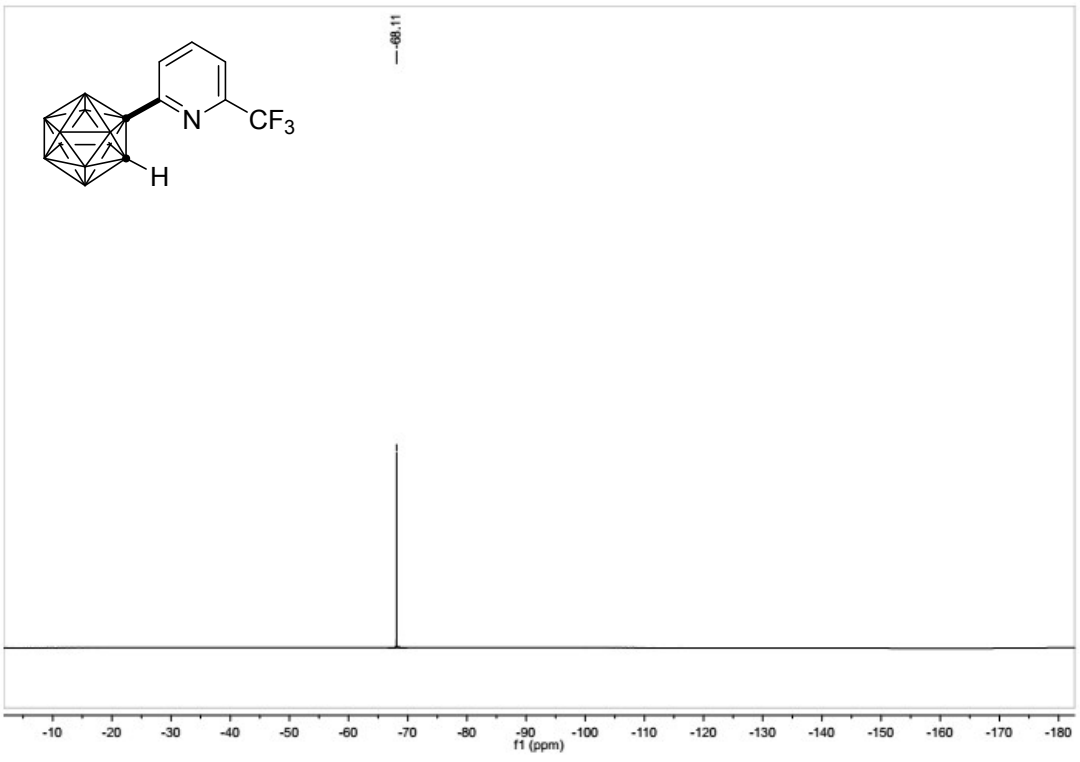
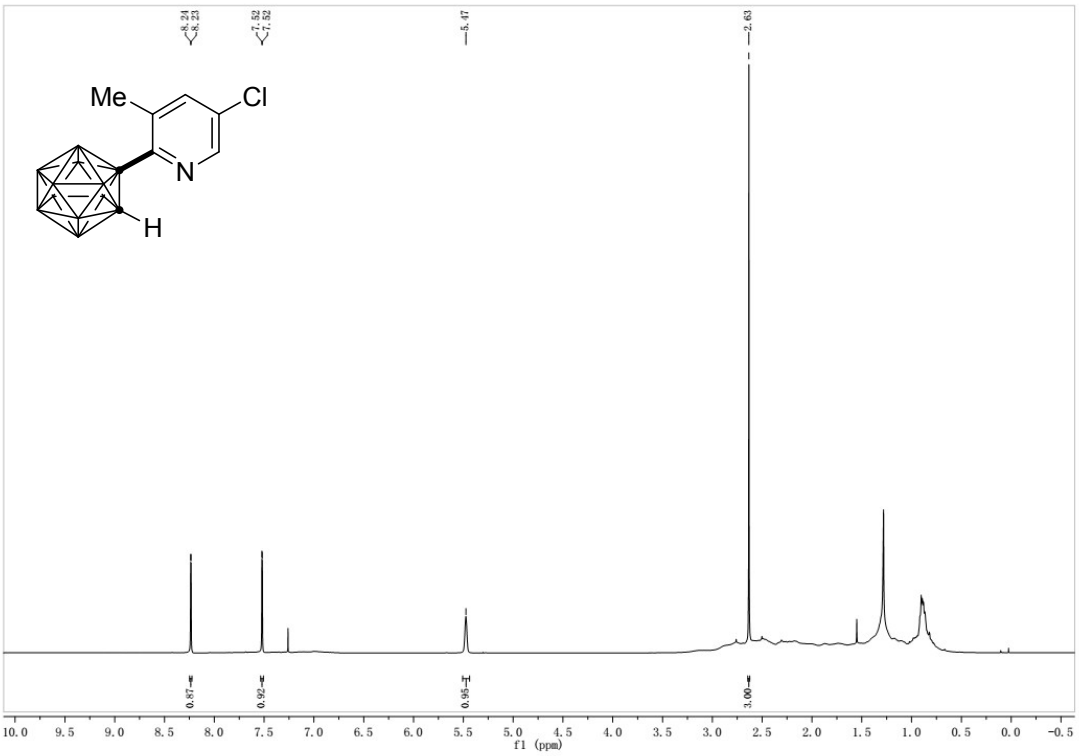
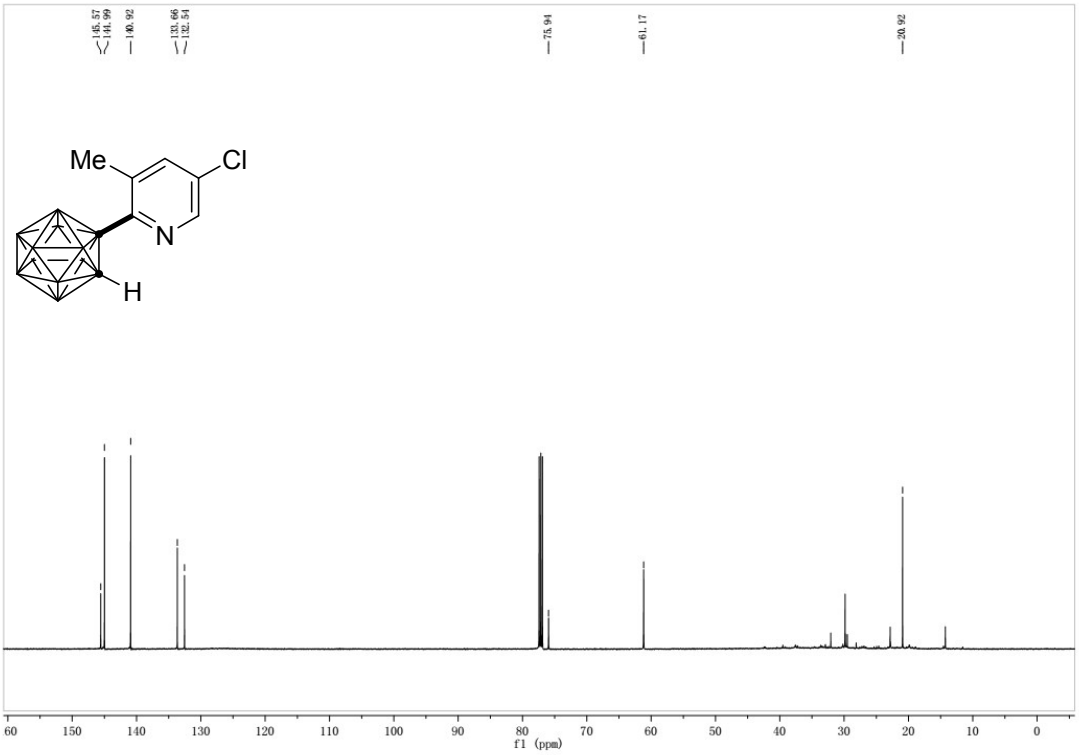
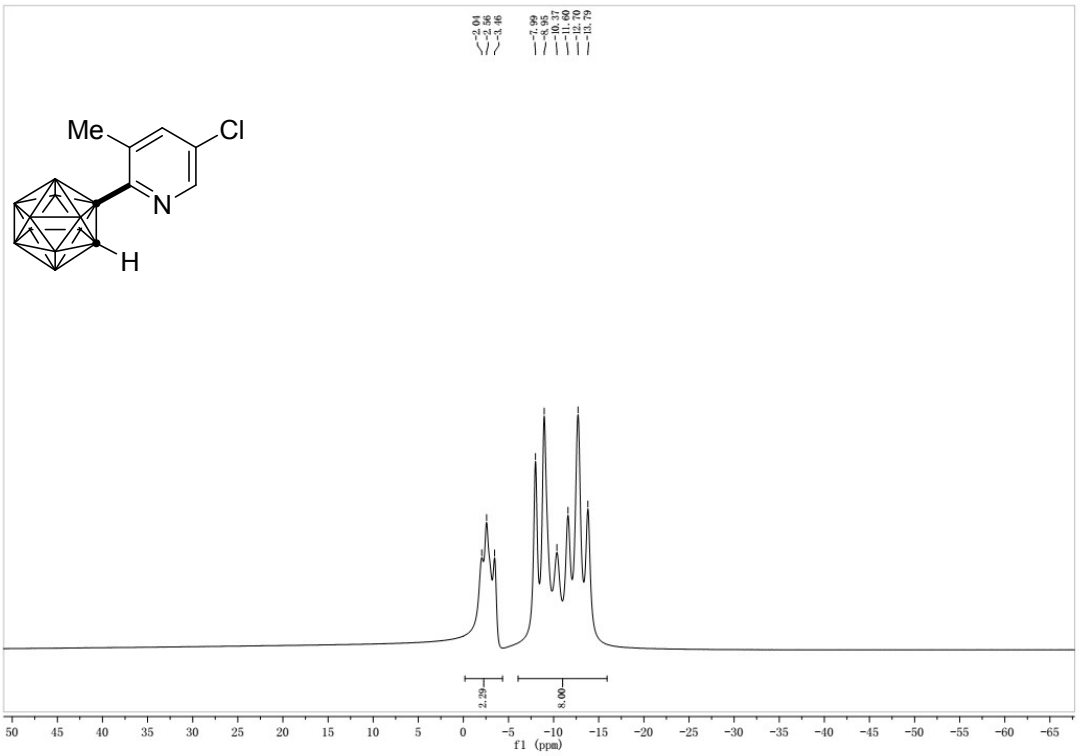
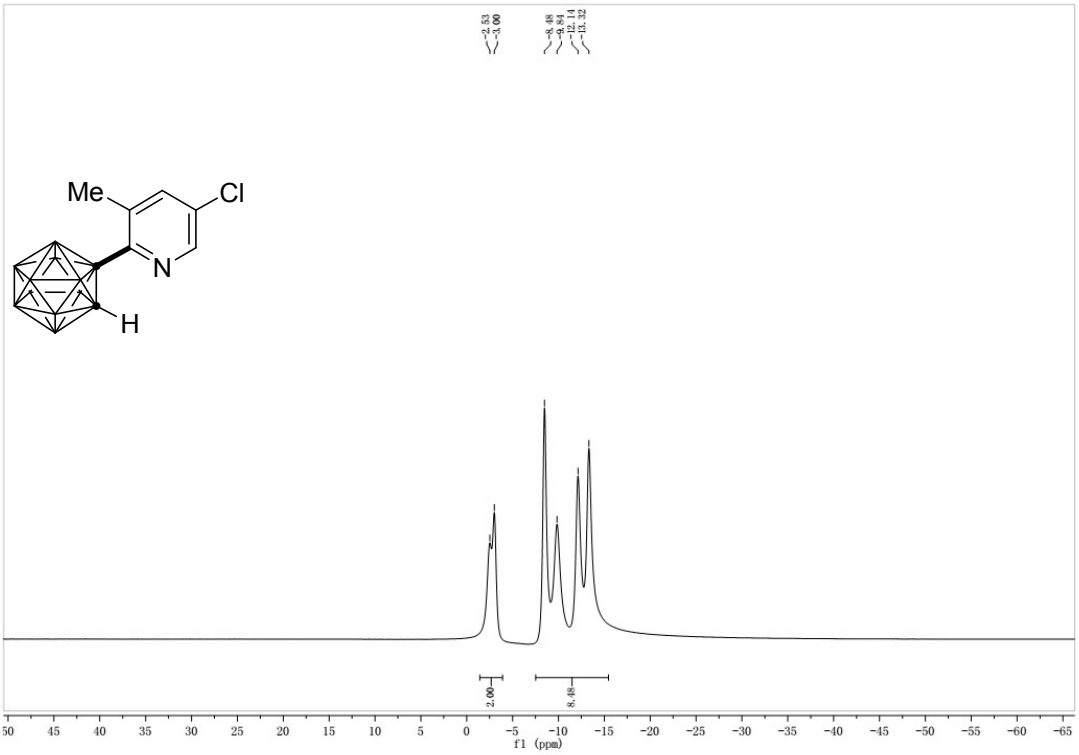
-3.44
-8.19
-10.54
-11.55
-12.08
2.18
8.00
f1 (ppm)

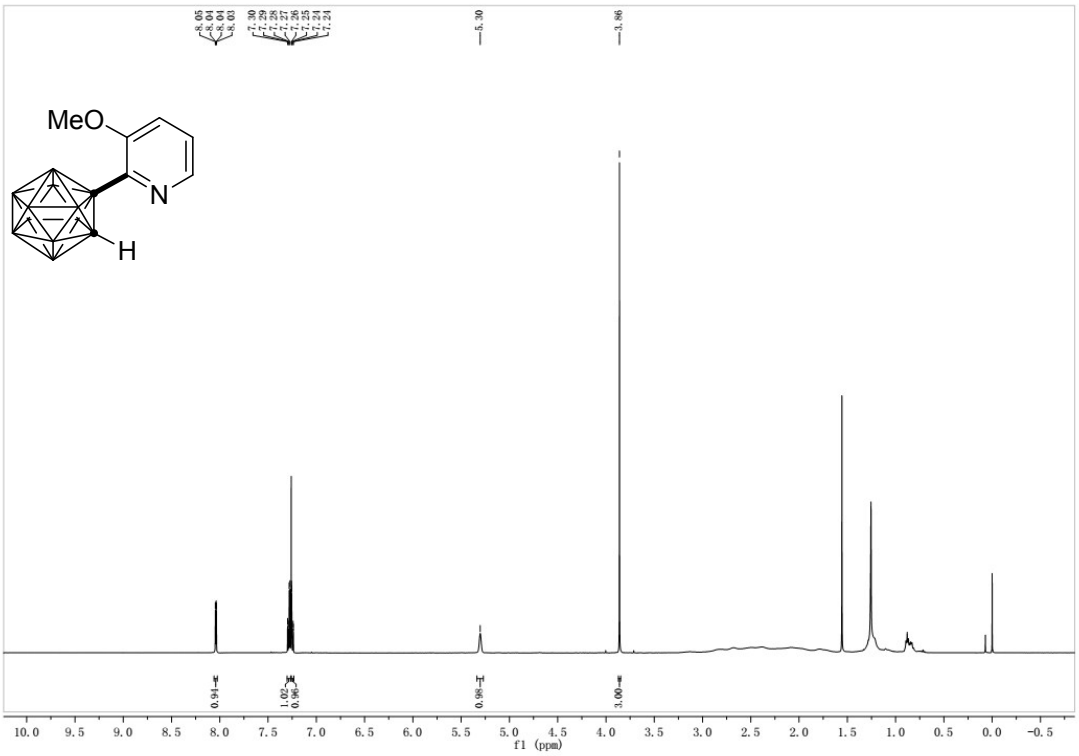

N
CF3
H
-68.11
f1 (ppm)

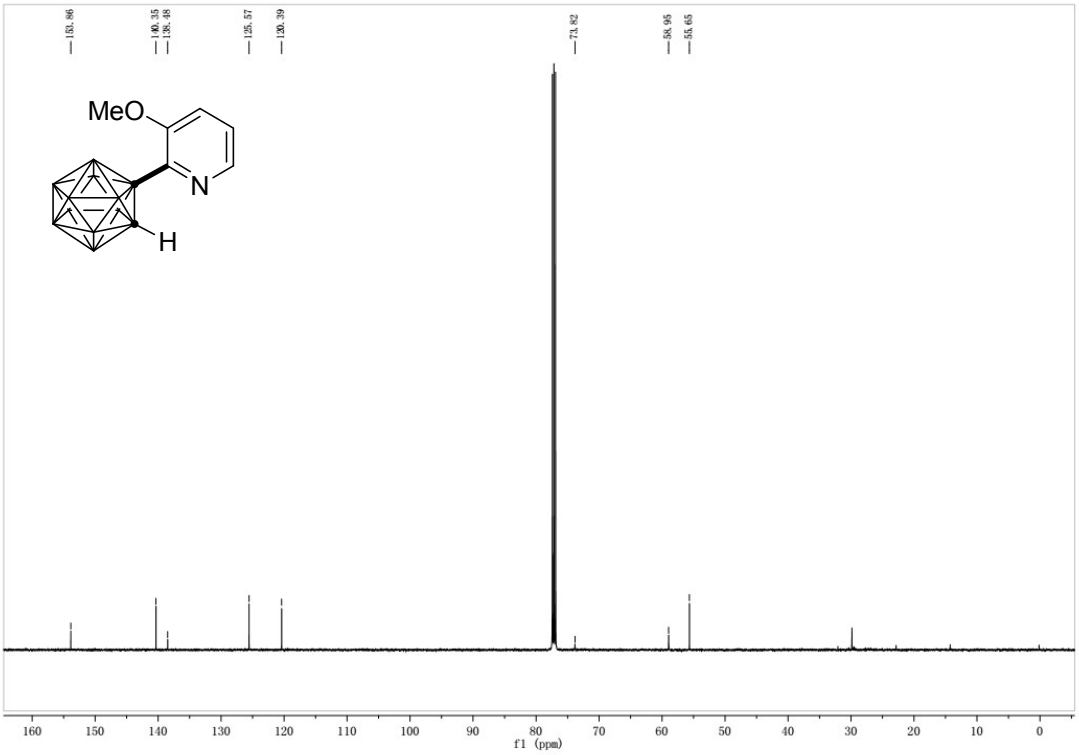

8.24
8.23
7.52
7.52
5.47
2.63
Me
Cl
N
H
0.87
0.92
0.95
3.00
f1 (ppm)

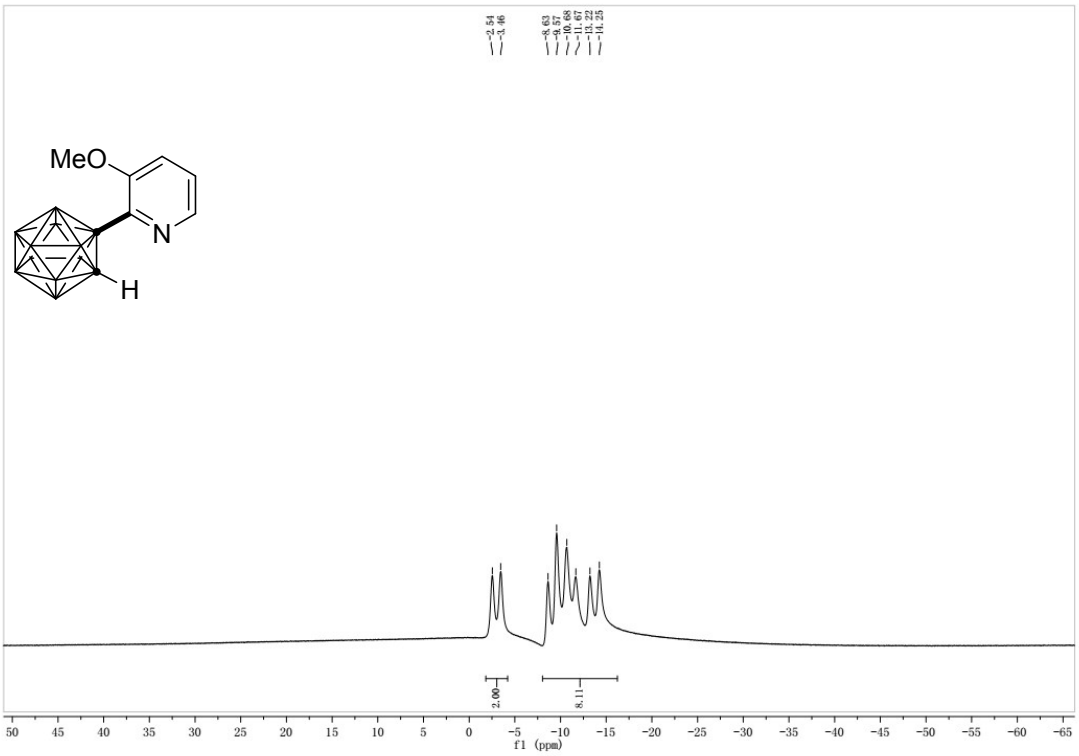

145.57
140.99
140.92
133.66
132.54
75.94
61.17
20.92
Me
Cl
N
H
f1 (ppm)

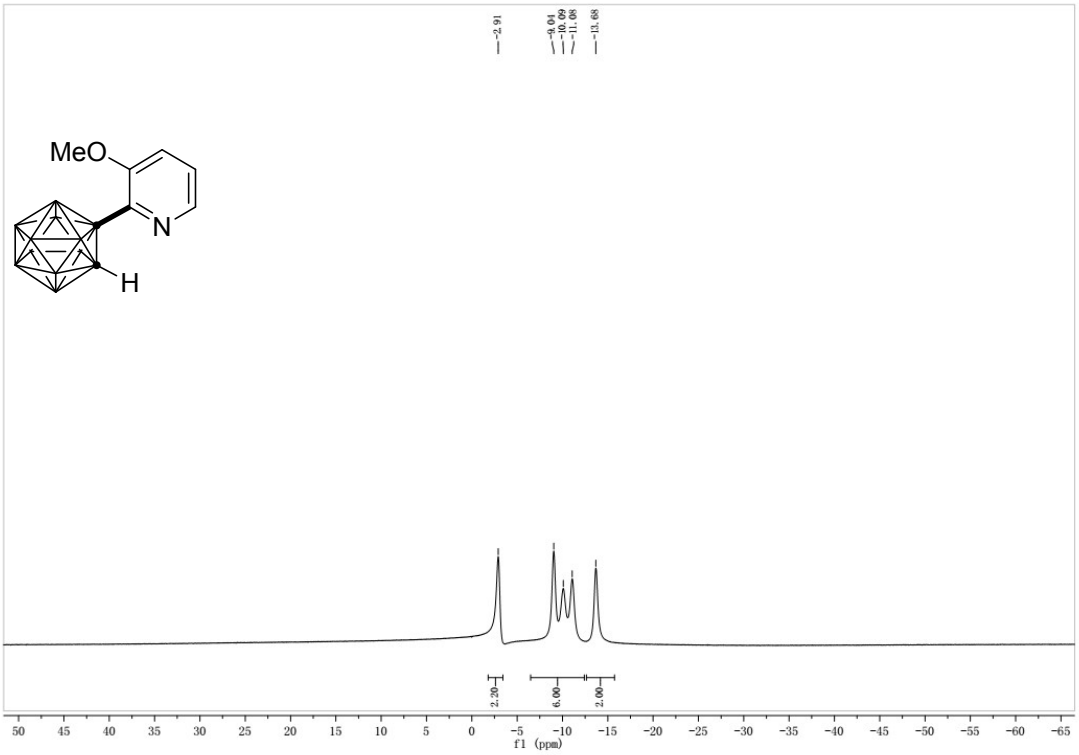

Me
Cl
N
H
f1 (ppm)

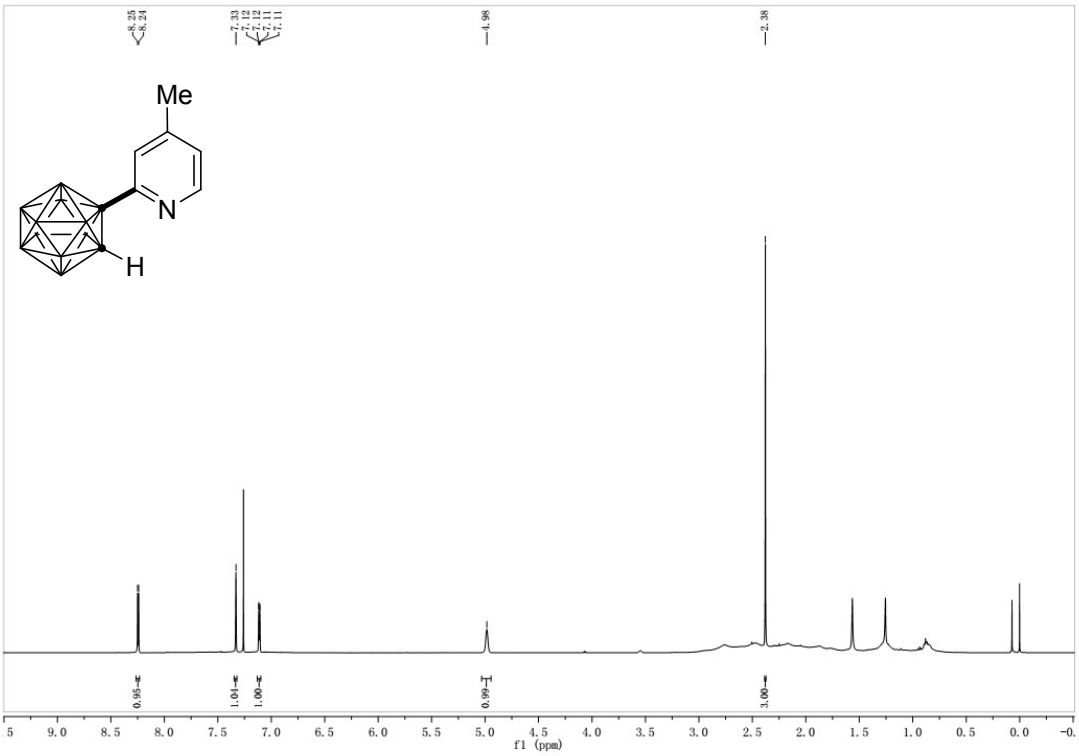

Me
Cl
N
H
f1 (ppm)

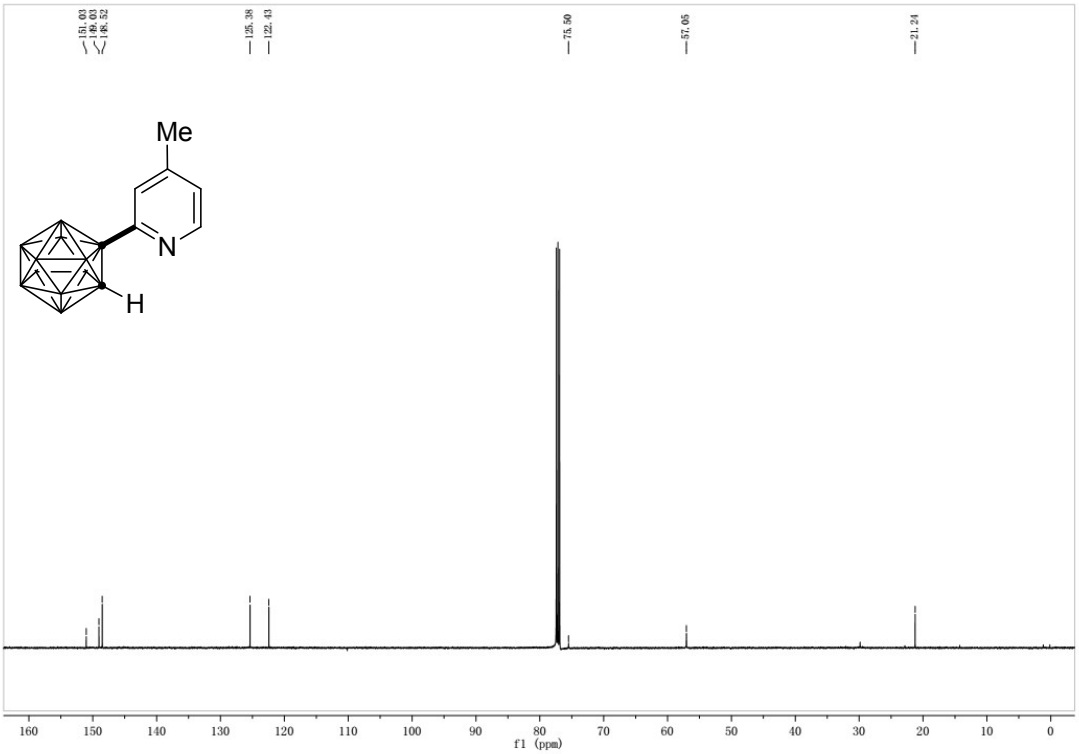

MeO
N
H
8.05
8.04
8.01
8.00
7.30
7.29
7.28
7.27
7.26
7.25
7.24
7.24
5.30
3.86
0.94
1.02
0.96
0.98
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

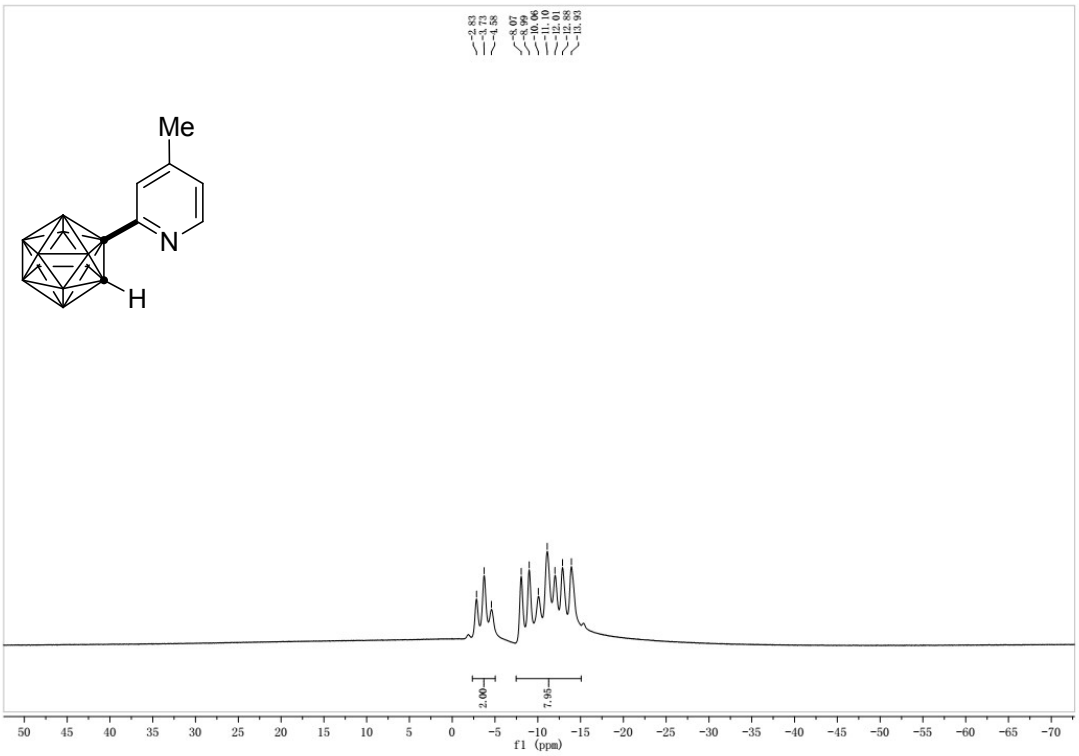

MeO
N
H
163.86
140.35
138.48
125.57
120.39
73.82
58.95
55.65
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

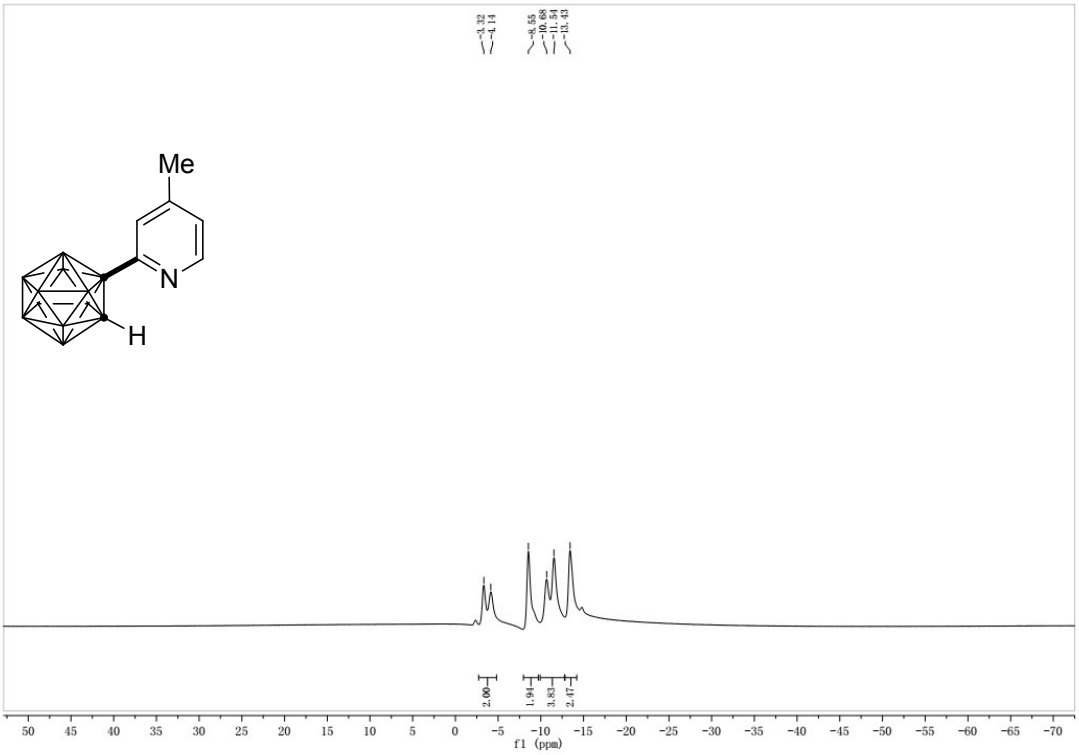

-2.54
-3.46
-8.63
-9.57
-10.68
-11.67
-13.22
-13.25
MeO
N
H
2.00
8.11
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)


-2.91
-9.04
-10.09
-11.06
-13.68
MeO
N
H
2.20
6.60
2.00
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)


8.25
8.24
7.33
7.12
7.12
7.11
7.11
4.98
2.38
Me
N
H
0.95
1.04
1.00
0.99
3.00
f1 (ppm)


151.01
149.03
148.52
125.38
122.43
75.59
57.05
21.24
Me
N
H
f1 (ppm)


-2.83
-3.73
-4.58
-8.07
-8.99
-10.06
-11.10
-12.11
-12.88
-13.93
Me
N
H
2.00
7.95
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70
f1 (ppm)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-4.14
-8.65
-10.68
-11.54
-13.43
Me
N
H
2.00
1.94
3.83
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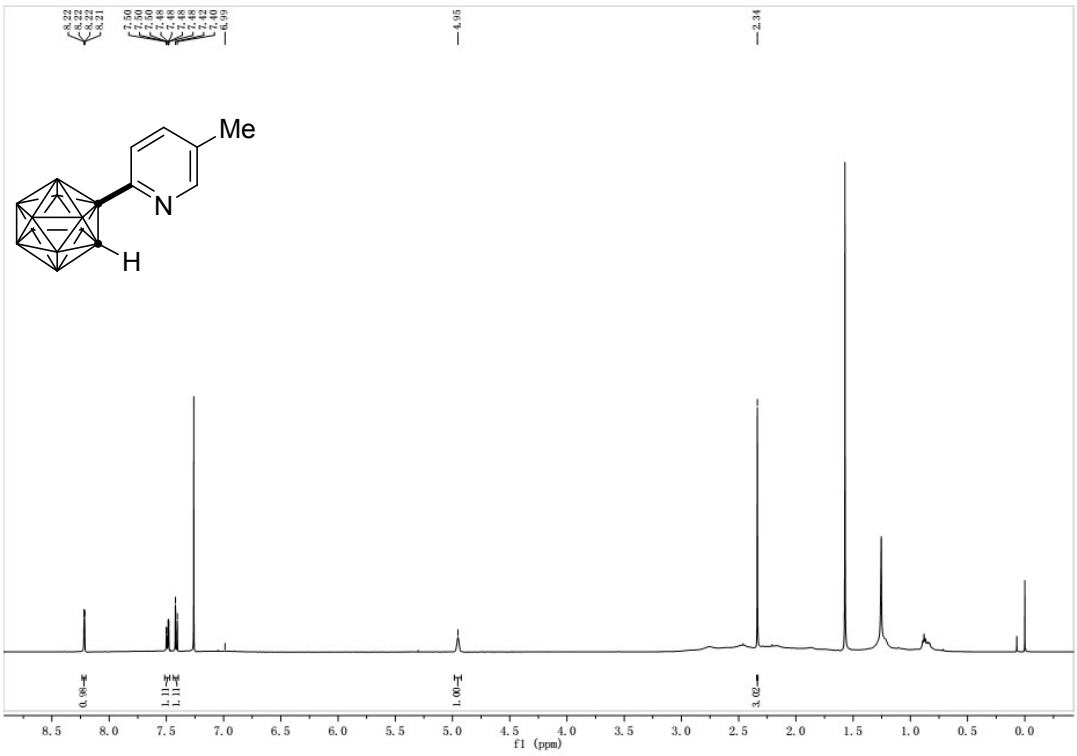
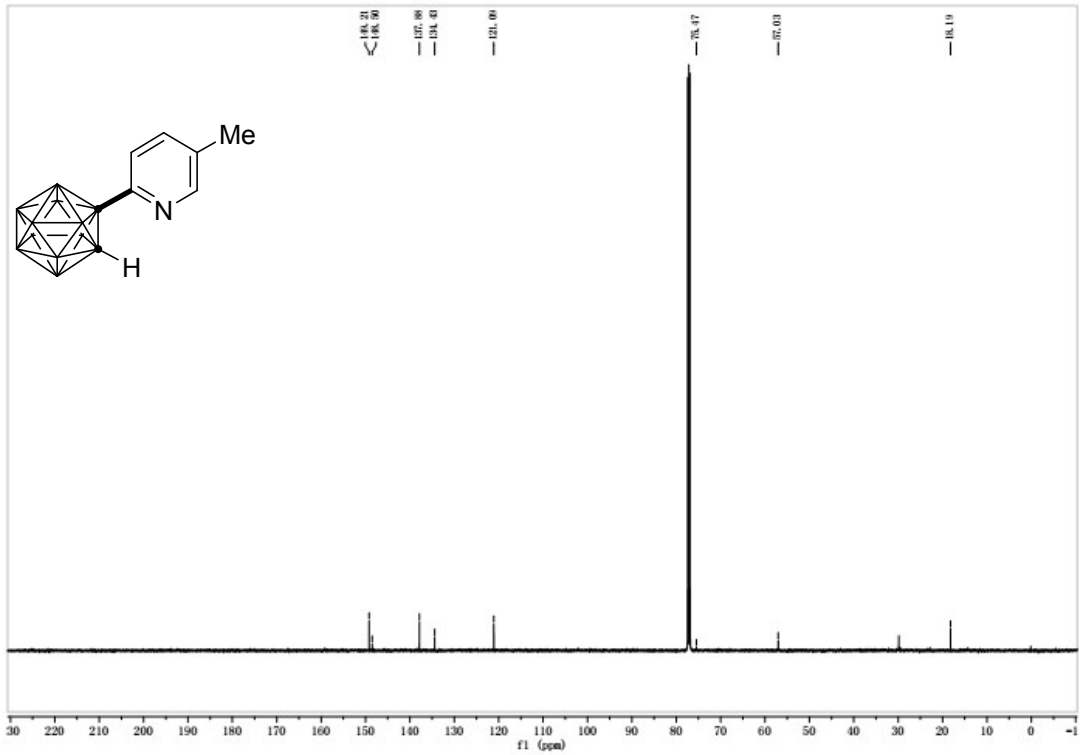
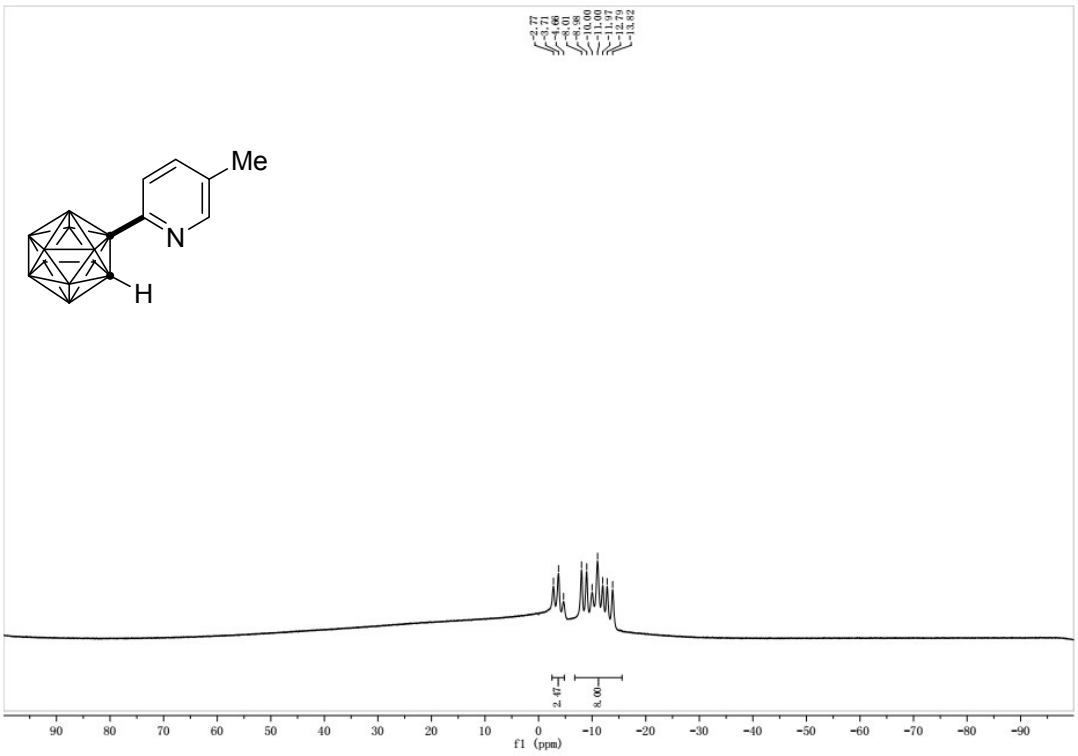
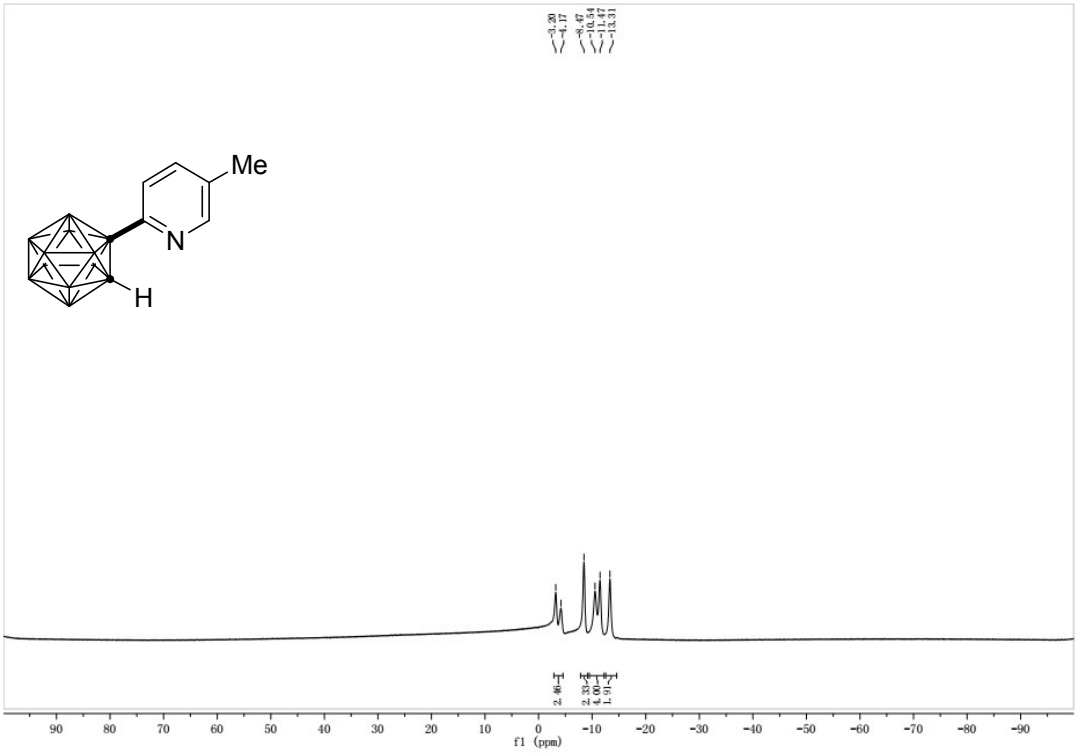
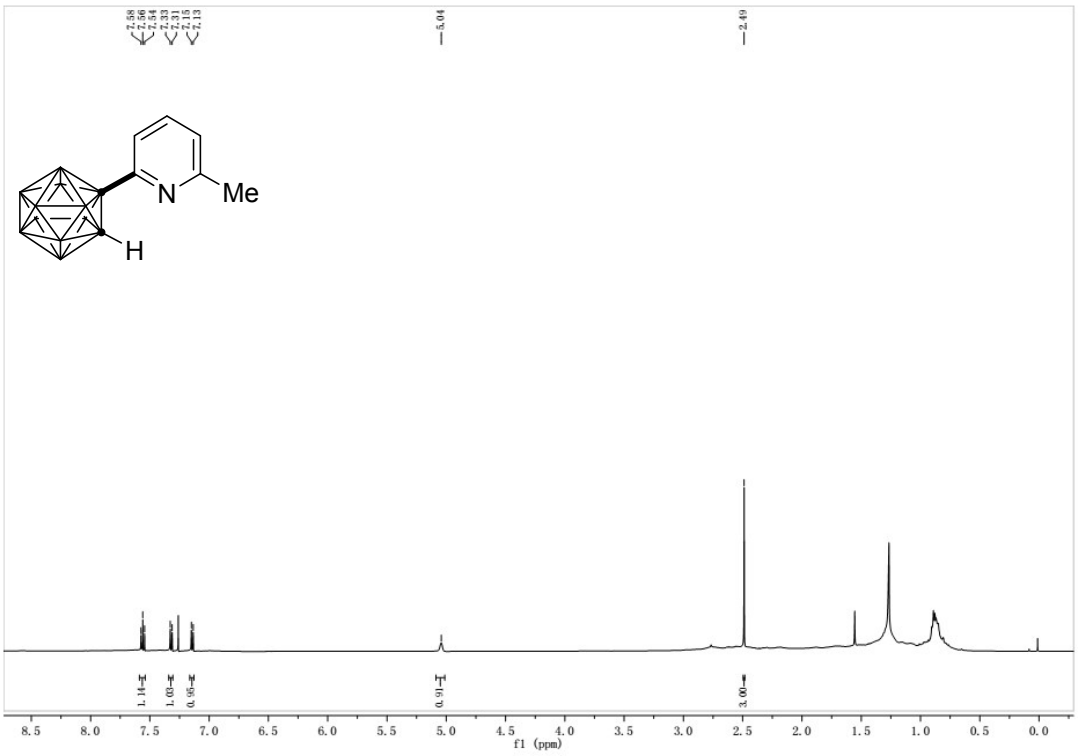
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70
f1 (ppm)

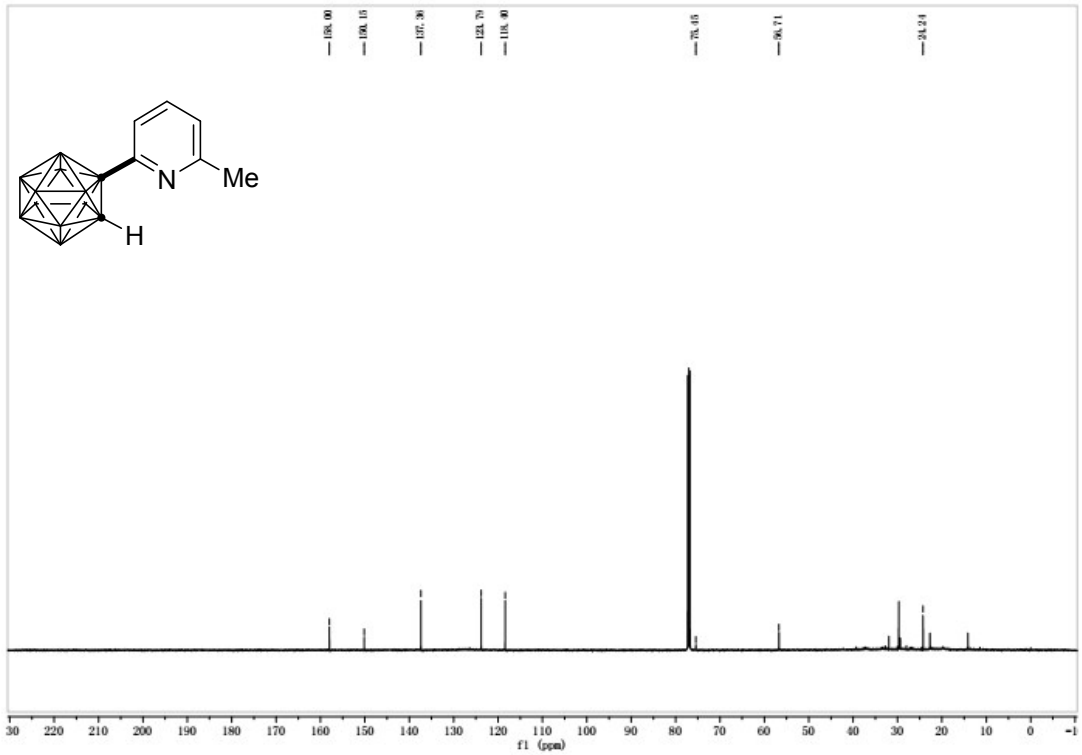

Me
N
H
f1 (ppm)


Me
N
H
f1 (ppm)


Me
N
H
f1 (ppm)


Me
N
H
f1 (ppm)


7.58
7.56
7.34
7.33
7.31
7.15
7.13
5.04
2.49
N
Me
H
1.14
1.03
0.95
0.91
3.00
f1 (ppm)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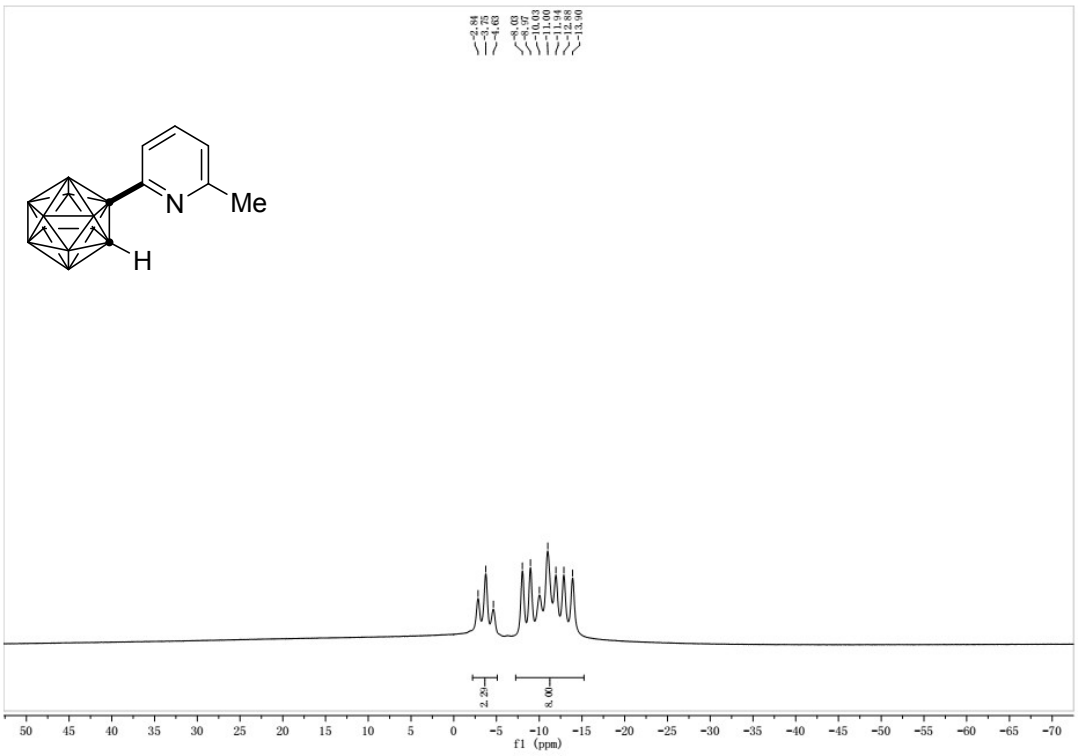
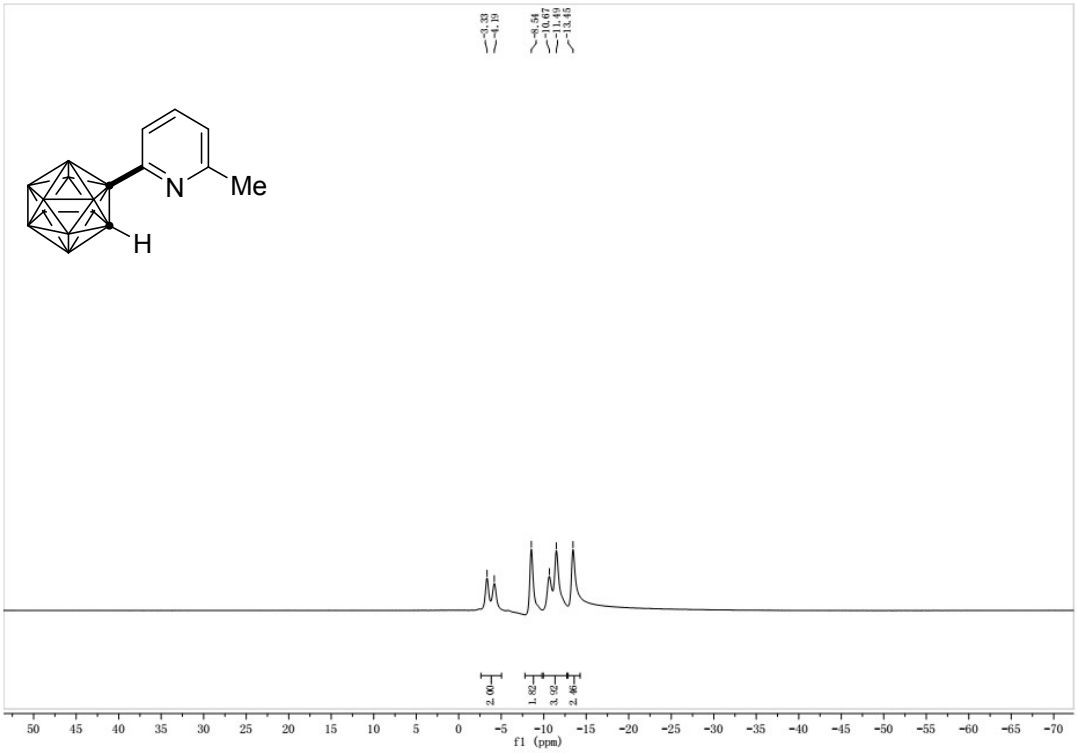
118.40
75.45
56.71
24.24
N
Me
H
f1 (ppm)


-2.84
-3.75
-4.63
-8.03
-8.97
-10.03
-11.00
-11.94
-12.88
-13.90
N
Me
H
2.29
8.00
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70
f1 (ppm)


-3.33
-4.19
-8.54
-10.67
-11.60
-13.45
N
Me
H
2.00
1.82
3.92
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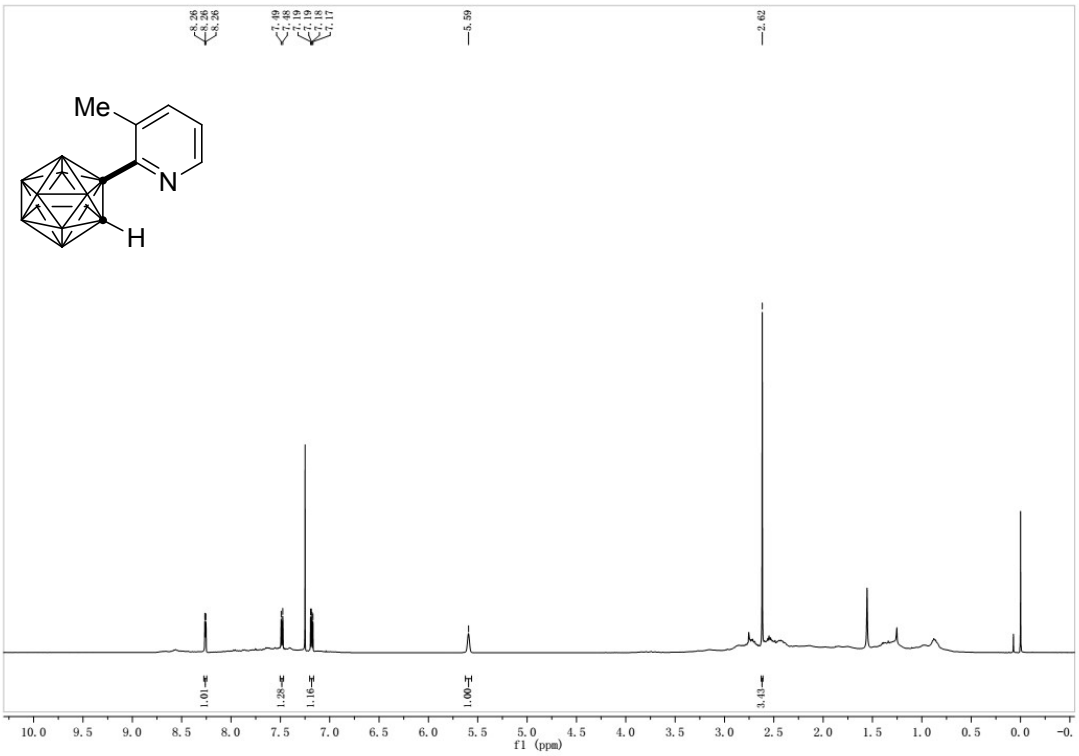
f1 (ppm)


Me
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H
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7.49
7.48
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7.19
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7.17
5.59
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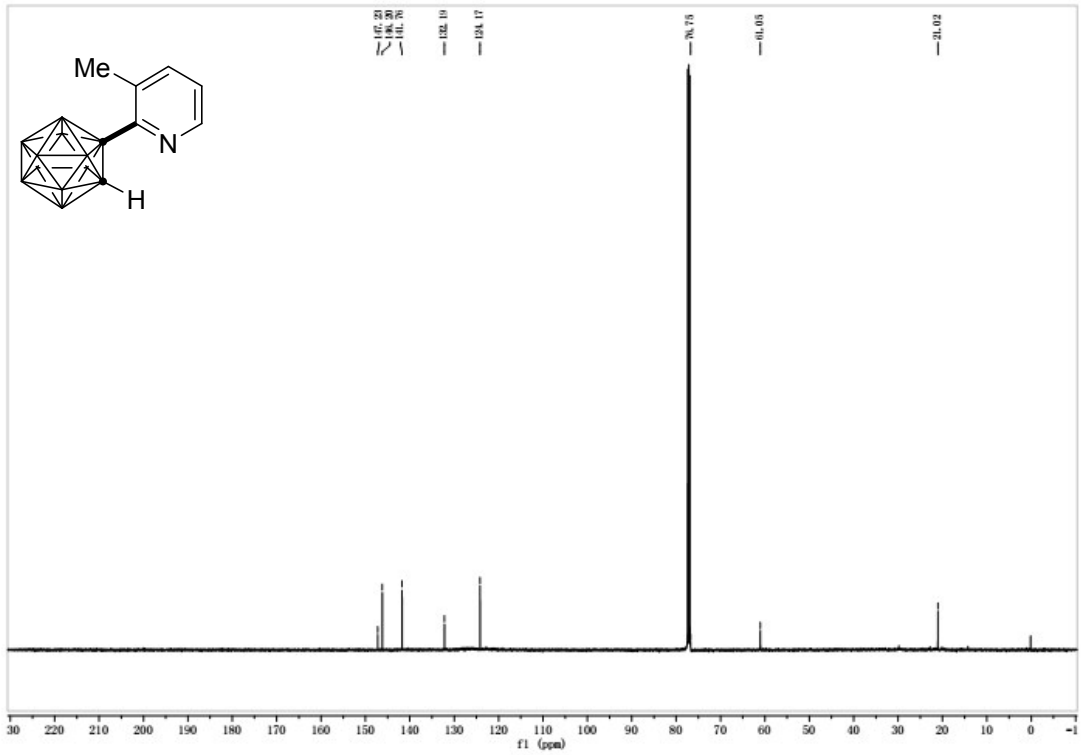
1.28
1.16
1.00
3.43
f1 (ppm)


Me
N
H
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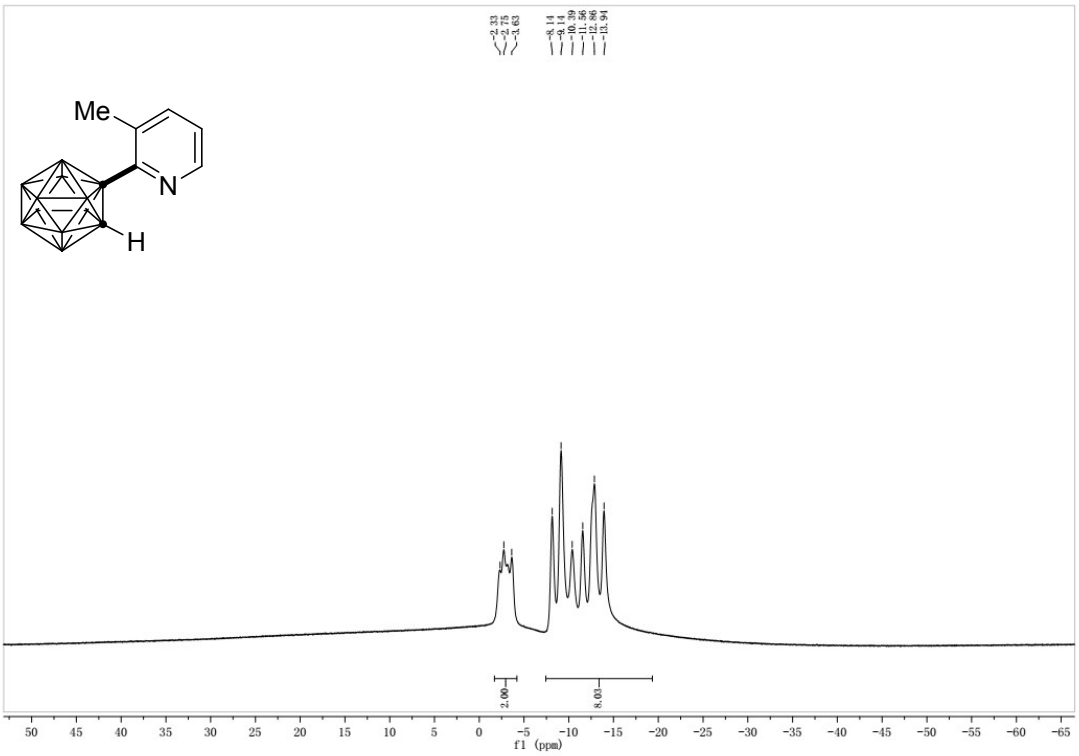
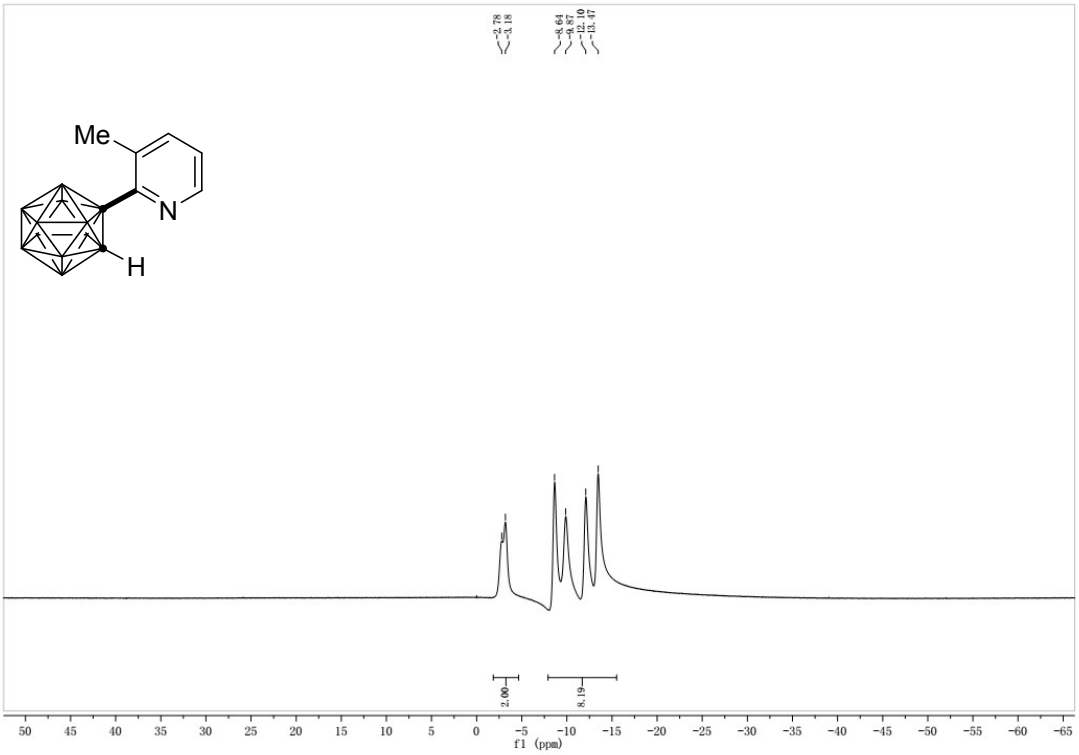
141.26
132.19
124.17
76.75
61.05
21.02
f1 (ppm)


-2.33
-2.75
-3.63
-8.14
-9.14
-10.39
-10.58
-12.86
-13.94
Me
N
H
2.00
8.03
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)


-2.78
-3.18
-8.64
-9.67
-12.10
-13.47
Me
N
H
2.00
8.19
50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65
f1 (ppm)