Supporting Information

Sterically Hindered *N*-Heterocyclic Carbene/Palladium(II) Catalyzed Suzuki-Miyaura Coupling of Nitrobenzenes

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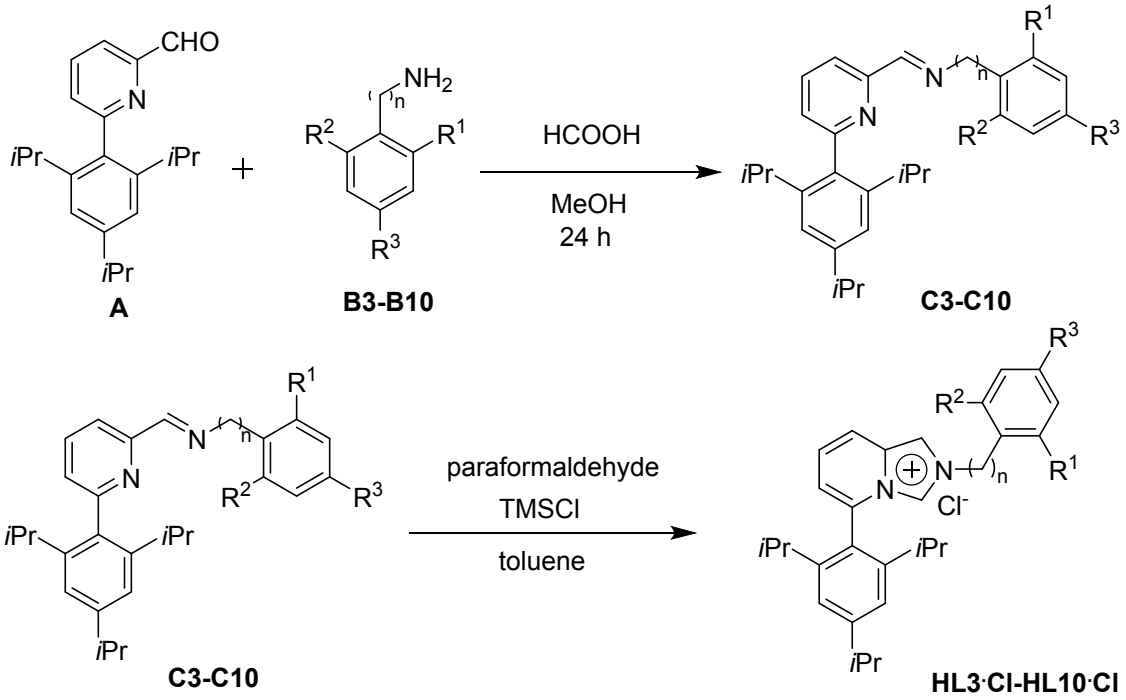
I. General information

^{1}H NMR spectra were recorded in deuterated solvents on a Bruker 400 (400 MHz) spectrometer and calibrated to the residual solvent peak or tetramethylsilane (δ = 0 ppm). Splitting patterns are designated as singlet (s), doublet (d), triplet (t), broad (br), multiplet (m). *J*-values are in Hz. High-resolution mass spectra (HRMS) data were obtained by using EI or ESI ionization.

Commercially obtained reagents were used without further purification. All reactions were monitored by TLC with Huanghai GF254 silica gel coated plates. Flash column chromatography was carried out using 200-300 mesh silica gel at increased pressure. Unless otherwise noted, all reactions were carried out in flame-dried reaction tubes with Teflon screw caps under nitrogen. Solvents if necessary (dioxane, THF, toluene, MeOH and ect.) were dried and distilled according to standard methods prior to use. $Pd(acac)_2$,[1] **HL1·Cl** and **HL2·Cl**,[2] **HL11·PF$_6$**,[3] **HL13·Cl**,[4] and **HL14·Cl**[5] were prepared according to the literature procedures.

II. Syntheses of ligand precursors

HL3·Cl-HL10·Cl were prepared according to the following steps (Scheme S1).



Scheme S1. Synthesis of ligand precursors

An oven-dried Schlenk tube was charged with 6-(2,4,6-triisopropylphenyl)picolinaldehyde **A** (1 mmol, 309 mg), prepared according to the literature[2], and aniline **B** (1.2 mmol). The tube was evacuated and backfilled with N_2 three times. MeOH (10 mL) and HCOOH (10 μl, ≥88%) were added

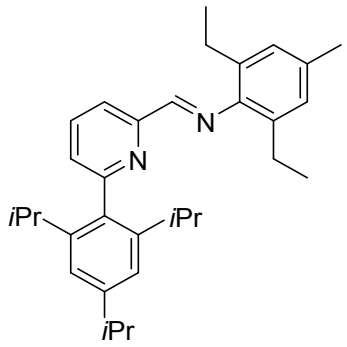
via a syringe. The resulting mixture was heated for 24 h at 60 °C and subsequently allowed to cool to room temperature. The solid was collected and subsequently washed with MeOH (3×5 mL), and then dried in vacuo to afford **C**.

C (0.2 mmol), paraformaldehyde (0.2 mmol, 5.9 mg), toluene (1.5 mL) and TMSCl (0.4 mmol, 50 μl) were added to a vial subsequently. The mixture was stirred at room temperature for 24 h until the yellow solution became colorless. Then the mixture was dried in vacuo to afford the crude solid. The solid was washed with Et_2O (3×1.5 mL), heptane (3×1.5 mL) and then dried in vacuo to yield the desired products **HL3·Cl-HL10·Cl** as a white solid.

HL12·Cl was prepared similarly.

III. Characterization data of ligand precursors

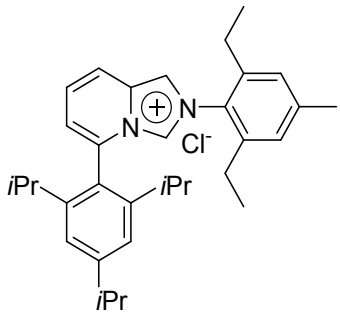
(*E*)-*N*-(2,6-diethyl-4-methylphenyl)-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)methanimine (C3)



Pale yellow solid; yield: 395 mg (87%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (s, 1H), 8.26 (d, *J* = 7.6 Hz, 1H), 7.88 (t, *J* = 7.7 Hz, 1H), 7.40 (d, *J* = 7.2 Hz, 1H), 7.11 (s, 2H), 6.92 (s, 2H), 2.95 (hept, *J* = 6.8 Hz, 1H), 2.69-2.41 (m, 6H), 2.33 (s, 3H), 1.30 (d, *J* = 6.9 Hz, 6H), 1.21-1.07 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.7, 160.0, 154.2, 149.1, 147.2, 146.3, 136.3, 135.8, 133.5, 132.9, 127.0, 126.6, 121.0, 118.8, 34.5, 30.5, 24.7, 24.3, 24.1, 24.0, 21.0, 14.8; HRMS (GC-TOF) for $C_{32}H_{42}N_2$: calcd. 454.3348; found: 454.3345.

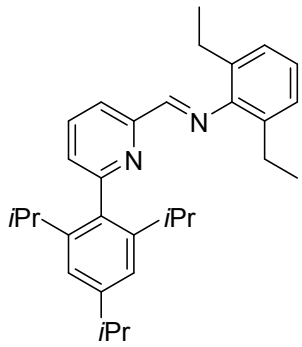
2-(2,6-diethyl-4-methylphenyl)-5-(2,4,6-triisopropylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL3·Cl)



White solid; yield: 95 mg (95%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.35 (br, 1H), 9.05 (br, 1H), 7.88 (s, 1H), 7.47 (t, *J* = 8.4 Hz, 1H), 7.15 (s, 2H), 7.03 (d, *J* = 6.8 Hz, 1H), 7.01 (s, 2H), 2.93 (hept, *J* = 6.8 Hz, 1H), 2.34 (s, 3H), 2.29-2.24 (m, 2H), 2.21-2.14 (m, 2H), 2.09-2.02 (m, 2H), 1.26 (d, *J* = 6.8 Hz, 6H), 1.13 (d, *J* = 6.6 Hz, 6H), 1.05-1.01 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 147.9, 142.2, 139.7, 132.5, 129.8, 127.7, 125.3, 124.3, 122.5, 121.5, 121.4, 121.0, 120.5, 120.4, 34.5, 31.3, 25.1, 23.8, 23.8, 23.7, 21.4, 14.8; HRMS (ESI-TOF) for $C_{33}H_{43}N_2$ ($[M-Cl]^+$) : calcd. 467.3421; found: 467.3385.

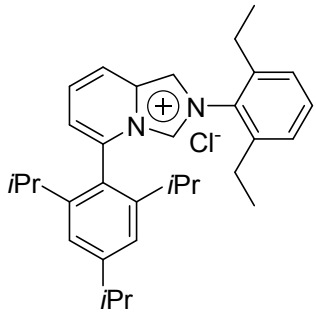
(*E*)-*N*-(2,6-diethylphenyl)-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)methanimine (C4)



Pale yellow solid; yield: 340 mg (77%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (s, 1H), 8.26 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.89 (t, *J* = 7.7 Hz, 1H), 7.40 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.14-7.08 (m, 4H), 7.05 (dd, *J* = 8.8, 6.4 Hz, 1H), 2.94 (hept, *J* = 7.0 Hz, 1H), 2.58-2.49 (m, 6H), 1.29 (d, *J* = 6.9 Hz, 6H), 1.18-1.11 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.6, 160.1, 154.1, 149.6, 149.1, 146.3, 136.4, 135.8, 132.8, 126.7, 126.3, 124.2, 121.0, 118.8, 34.5, 30.5, 24.7, 24.3, 24.1, 24.0, 14.7; HRMS (GC-TOF) for $C_{31}H_{40}N_2$: calcd. 440.3191; found: 440.3190.

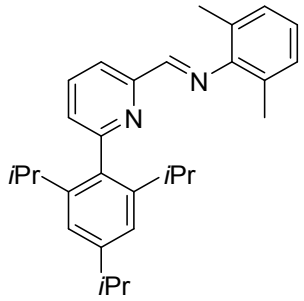
2-(2,6-diethylphenyl)-5-(2,4,6-triisopropylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL4·Cl)



White solid; yield: 90 mg (92%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.32 (br, 1H), 8.99 (br, 1H), 7.93 (s, 1H), 7.47-7.44 (m, 2H), 7.22 (d, *J* = 7.7 Hz, 2H), 7.14 (s, 2H), 7.04 (d, *J* = 6.0 Hz, 1H), 2.92 (hept, *J* = 7.2 Hz, 1H), 2.27-2.20 (m, 4H), 2.13-2.07 (m, 2H), 1.25 (d, *J* = 6.9 Hz, 6H), 1.13 (d, *J* = 6.5 Hz, 6H), 1.06-1.01 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 147.9, 140.0, 132.7, 132.5, 132.3, 131.9, 127.1, 125.5, 124.2, 122.6, 121.4, 121.2, 120.3, 34.5, 31.3, 25.1, 23.8, 14.8; HRMS (ESI-TOF) for $C_{32}H_{41}N_2$ ($[M\text{-}Cl]^+$) : calcd. 453.3264; found: 453.3244.

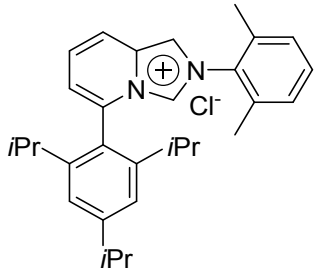
(*E*)-*N*-(2,6-dimethylphenyl)-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)methanimine (C5)



Pale yellow solid; yield: 350 mg (85%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (s, 1H), 8.28 (d, *J* = 8.6 Hz, 1H), 7.88 (t, *J* = 7.7 Hz, 1H), 7.40 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.12-7.04 (m, 4H), 6.97 (t, *J* = 7.2 Hz, 1H), 2.94 (hept, *J* = 6.8 Hz, 1H), 2.54 (hept, *J* = 6.8 Hz, 2H), 2.19 (s, 6H), 1.28 (d, *J* = 6.9 Hz, 6H), 1.14 (d, *J* = 7.6 Hz, 6H), 1.13 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.9, 160.1, 154.1, 150.2, 149.1, 146.3, 136.3, 135.7, 128.2, 127.0, 126.7, 124.1, 121.0, 118.8, 34.5, 30.5, 24.3, 24.1, 24.0, 18.3; HRMS (GC-TOF) for $C_{29}H_{36}N_2$: calcd. 412.2878; found: 412.2880.

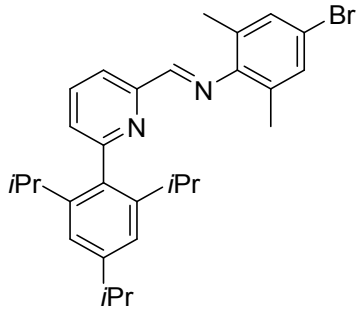
2-(2,6-dimethylphenyl)-5-(2,4,6-triisopropylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL5·Cl)



White solid; yield: 90 mg (98%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.43 (s, 1H), 9.00 (d, *J* = 9.2 Hz, 1H), 7.93 (s, 1H), 7.48 (dd, *J* = 9.2, 6.8 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.17 (s, 2H), 7.05 (d, *J* = 6.8 Hz, 1H), 2.95 (hept, *J* = 6.8 Hz, 1H), 2.30 (hept, *J* = 6.8 Hz, 2H), 1.98 (s, 6H), 1.28 (d, *J* = 6.9 Hz, 6H), 1.15 (d, *J* = 6.7 Hz, 6H), 1.03 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 147.9, 134.4, 133.6, 132.7, 131.5, 129.2, 125.4, 124.3, 122.6, 121.4, 121.0, 120.6, 119.7, 34.5, 31.3, 24.9, 24.1, 23.8, 17.2; HRMS (ESI-TOF) for $C_{30}H_{37}N_2$ ($[M-Cl]^+$) : calcd. 425.2951; found: 425.2929.

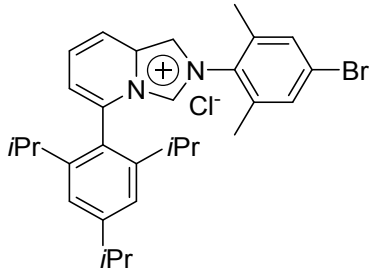
(*E*)-*N*-(4-bromo-2,6-dimethylphenyl)-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)methanimine (C6)



Pale yellow solid; yield: 430 mg (88%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (s, 1H), 8.25 (d, *J* = 7.7 Hz, 1H), 7.89 (t, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 7.4 Hz, 1H), 7.22 (s, 2H), 7.10 (s, 2H), 2.94 (hept, *J* = 6.8 Hz, 1H), 2.52 (hept, *J* = 6.8 Hz, 2H), 2.16 (s, 6H), 1.28 (d, *J* = 6.9 Hz, 6H), 1.14 (d, *J* = 7.6 Hz, 6H), 1.12 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.5, 160.3, 153.8, 149.3, 149.2, 146.2, 136.4, 135.6, 130.8, 129.3, 126.9, 121.0, 118.9, 116.8, 34.5, 30.5, 24.3, 24.1, 23.9, 18.2; HRMS (GC-TOF) for $C_{29}H_{35}N_2Br$: calcd. 490.1984; found: 490.1987.

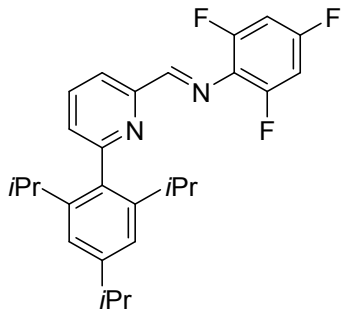
2-(4-bromo-2,6-dimethylphenyl)-5-(2,4,6-triisopropylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL6·Cl)



White solid; yield: 103 mg (96%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 8.95 (d, *J* = 9.2 Hz, 1H), 7.93 (s, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.36 (s, 2H), 7.18 (s, 2H), 7.06 (d, *J* = 6.7 Hz, 1H), 2.95 (hept, *J* = 6.8 Hz, 1H), 2.28 (hept, *J* = 6.4 Hz, 2H), 1.98 (s, 6H), 1.28 (d, *J* = 6.9 Hz, 6H), 1.15 (d, *J* = 6.7 Hz, 6H), 1.03 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.2, 147.9, 136.5, 132.8, 132.8, 132.6, 132.1, 125.6, 125.5, 124.2, 122.6, 121.4, 121.2, 120.5, 120.0, 34.5, 31.3, 24.9, 24.1, 23.8, 17.2; HRMS (ESI-TOF) for $C_{30}H_{36}N_2Br$ ([M-Cl]$^+$) : calcd. 503.2056; found: 503.2010.

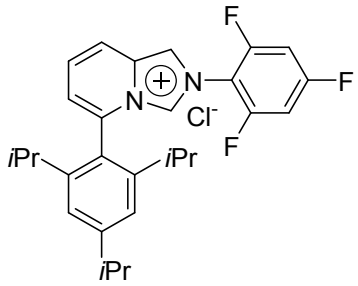
(*E*)-*N*-(2,4,6-trifluorophenyl)-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)methanimine (C7)



Pale yellow solid; yield: 380 mg (87%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.81 (s, 1H), 8.29 (d, *J* = 7.7 Hz, 1H), 7.88 (t, *J* = 7.7 Hz, 1H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.10 (s, 2H), 6.77 (t, *J* = 8.4 Hz, 2H), 2.94 (hept, *J* = 6.8 Hz, 1H), 2.51 (hept, *J* = 6.8 Hz, 2H), 1.28 (d, *J* = 6.8 Hz, 6H), 1.14 (d, *J* = 6.8 Hz, 6H), 1.10 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 160.3, 155.5 (ddd, *J* = 258.5, 14.3, 7.0 Hz), 154.0, 149.2, 146.2, 136.4, 135.6, 127.2, 121.0, 119.3, 100.8 (t, *J* = 28.0 Hz), 34.5, 30.4, 24.3, 24.1, 23.9; ^{19}F NMR (376 MHz, $CDCl_3$): δ -111.4, -119.9; HRMS (ESI-TOF) for $C_{27}H_{29}N_2F_3$ ([M+H]$^+$) : calcd. 439.2361; found: 439.2347.

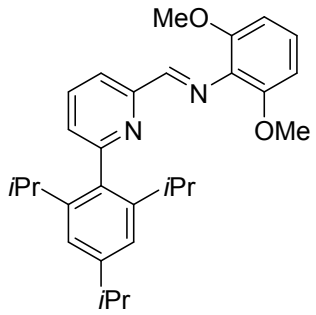
2-(2,4,6-trifluorophenyl)-5-(2,4,6-triisopropylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL7·Cl)



White solid; yield: 89 mg (91%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.81 (s, 1H), 8.71 (d, *J* = 9.1 Hz, 1H), 8.27 (s, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.19 (s, 2H), 7.05 (d, *J* = 6.8 Hz, 1H), 6.97 (t, *J* = 8.1 Hz, 2H), 2.95 (hept, *J* = 6.8 Hz, 1H), 2.26 (hept, *J* = 6.4 Hz, 2H), 1.28 (d, *J* = 6.9 Hz, 6H), 1.12 (d, *J* = 6.7 Hz, 6H), 1.06 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.1 (ddd, *J* = 257.0, 14.0, 3.0 Hz), 153.2, 148.2, 133.1, 132.0, 125.6, 123.9, 122.7, 122.4, 121.4, 120.5, 120.5, 102.5 (t, *J* = 24.0 Hz), 34.5, 31.3, 25.2, 23.9; ^{19}F NMR (376 MHz, $CDCl_3$): δ -98.2, -115.7; HRMS (ESI-TOF) for $C_{28}H_{30}N_2F_3$ ($[M-Cl]^+$) : calcd. 451.2356; found: 451.2324.

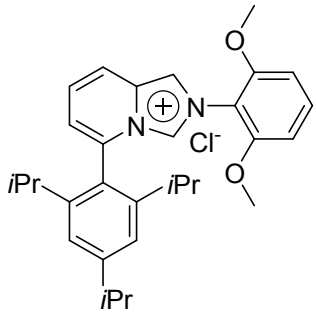
(*E*)-*N*-(2,6-dimethoxyphenyl)-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)methanimine (C8)



Pale yellow solid; yield: 320 mg (72%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.81 (s, 1H), 8.37 (d, *J* = 7.0 Hz, 1H), 7.84 (t, *J* = 6.8 Hz, 1H), 7.35 (d, *J* = 6.0 Hz, 1H), 7.08 (br, 3H), 6.65 (d, *J* = 7.6 Hz, 2H), 3.83 (s, 6H), 3.02-2.85 (br, 1H), 2.63-2.46 (br, 2H), 1.28 (d, *J* = 5.2 Hz, 6H), 1.22-1.02 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.4, 159.8, 154.9, 152.0, 149.0, 146.3, 136.2, 136.0, 129.3, 126.5, 125.9, 120.9, 119.0, 104.6, 56.1, 34.5, 30.3, 24.4, 24.1, 23.9; HRMS (GC-TOF) for $C_{29}H_{36}N_2O_2$: calcd. 444.2777; found: 444.2780.

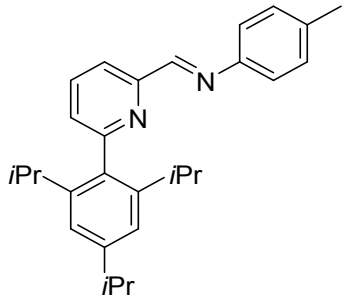
2-(2,6-dimethoxyphenyl)-5-(2,4,6-triisopropylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL8·Cl)



White solid; yield: 92 mg (93%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.91 (s, 1H), 8.80 (d, *J* = 7.8 Hz, 1H), 7.91 (s, 1H), 7.45 (t, *J* = 8.6 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.16 (s, 2H), 6.94 (d, *J* = 6.7 Hz, 1H), 6.68 (d, *J* = 8.6 Hz, 2H), 3.74 (s, 6H), 2.95 (hept, *J* = 6.8 Hz, 1H), 2.36 (hept, *J* = 6.8 Hz, 2H), 1.28 (d, *J* = 6.9 Hz, 6H), 1.14 (d, *J* = 6.7 Hz, 6H), 1.04 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.6, 152.8, 148.1, 133.0, 132.5, 131.4, 124.5, 123.0, 122.5, 120.7, 120.2, 120.0, 112.4, 104.5, 56.5, 34.5, 31.1, 24.9, 24.0, 23.9; HRMS (ESI-TOF) for $C_{30}H_{37}N_2O_2$ ($[M-Cl]^+$) : calcd. 457.2850; found: 457.2822.

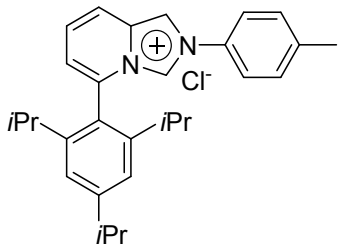
(*E*)-*N*-*p*-tolyl-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)methanimine (C9)



Pale yellow solid; yield: 298 mg (75%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68 (s, 1H), 8.25 (d, *J* = 7.8 Hz, 1H), 7.85 (t, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 7.5 Hz, 1H), 7.26-7.20 (m, 4H), 7.10 (s, 2H), 2.94 (hept, *J* = 7.2 Hz, 1H), 2.53 (hept, *J* = 6.8 Hz, 2H), 2.38 (s, 3H), 1.29 (d, *J* = 6.9 Hz, 6H), 1.14 (d, *J* = 6.8 Hz, 6H), 1.10 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5, 160.1, 154.5, 149.1, 148.3, 146.2, 136.8, 136.3, 135.8, 129.9, 126.4, 121.2, 120.9, 119.1, 34.5, 30.4, 24.4, 24.1, 23.9, 21.1; HRMS (GC-TOF) for $C_{28}H_{34}N_2$: calcd. 398.2722; found: 398.2724.

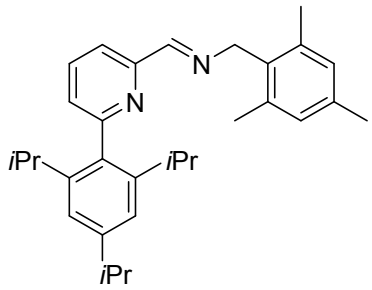
2-(*p*-tolyl)-5-(2,4,6-triisopropylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL9·Cl)



White solid; yield: 87 mg (98%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.59 (s, 1H), 8.53 (d, *J* = 8.4 Hz, 1H), 8.17 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.44-7.37 (m, 3H), 7.22 (s, 2H), 7.00 (d, *J* = 6.7 Hz, 1H), 2.99 (hept, *J* = 6.8 Hz, 1H), 2.41 (s, 3H), 2.31 (hept, *J* = 6.8 Hz, 2H), 1.32 (d, *J* = 6.9 Hz, 6H), 1.14 (d, *J* = 6.6 Hz, 6H), 1.11 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 148.2, 141.9, 133.1, 132.3, 131.3, 125.3, 124.2, 123.0, 122.6, 120.7, 120.1, 118.6, 117.6, 34.5, 31.2, 25.2, 24.2, 23.9, 21.2; HRMS (ESI-TOF) for $C_{29}H_{35}N_2$ ([M-Cl]$^+$) : calcd. 411.2795; found: 411.2772.

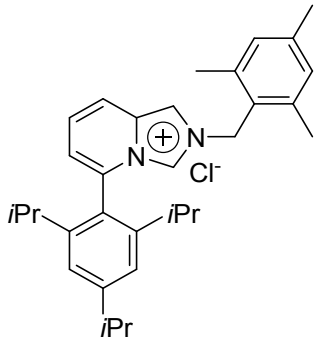
(*E*)-1-(6-(2,4,6-triisopropylphenyl)pyridin-2-yl)-*N*-(2,4,6-trimethylbenzyl)methanimine (C10)



White solid; yield: 374 mg (85%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (s, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.75 (t, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 7.06 (s, 2H), 6.87 (s, 2H), 4.91 (s, 2H), 2.92 (hept, *J* = 7.2 Hz, 1H), 2.46 (hept, *J* = 6.8 Hz, 2H), 2.36 (s, 6H), 2.26 (s, 3H), 1.27 (d, *J* = 6.9 Hz, 6H), 1.10 (d, *J* = 6.8 Hz, 6H), 1.07 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.2, 159.6, 154.6, 149.0, 146.2, 137.4, 137.0, 136.1, 135.9, 131.4, 129.2, 126.0, 120.9, 118.7, 58.0, 34.5, 30.3, 24.3, 24.1, 23.8, 20.9, 19.9; HRMS (GC-TOF) for $C_{31}H_{40}N_2$: calcd. 440.3191; found: 440.3188.

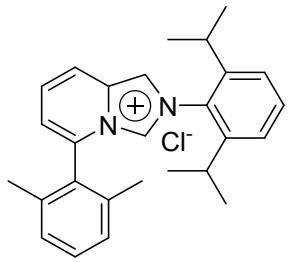
5-(2,4,6-triisopropylphenyl)-2-(2,4,6-trimethylbenzyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL10·Cl)



White solid; yield: 82 mg (84%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.22 (s, 1H), 7.93 (d, *J* = 9.3 Hz, 1H), 7.65 (s, 1H), 7.29 (dd, *J* = 9.2, 6.8 Hz, 1H), 7.08 (s, 2H), 6.87 (d, *J* = 6.7 Hz, 1H), 6.81 (s, 2H), 5.99 (s, 2H), 2.93 (hept, *J* = 7.2 Hz, 1H), 2.21 (s, 3H), 2.14 (s, 6H), 2.13-2.07 (m, 2H), 1.25 (d, *J* = 6.9 Hz, 6H), 1.06 (d, *J* = 6.7 Hz, 6H), 0.90 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.9, 147.8, 140.0, 138.1, 133.7, 131.1, 129.7, 125.6, 124.9, 124.0, 122.2, 121.7, 119.2, 118.4, 116.8, 50.0, 34.5, 31.1, 25.1, 23.8, 23.7, 21.0, 19.6; HRMS (ESI-TOF) for $C_{32}H_{41}N_2$ ([M-Cl]$^+$) : calcd. 453.3264; found: 453.3244.

2-(2,6-diisopropylphenyl)-5-(2,6-dimethylphenyl)imidazo[1,5-*a*]pyridin-2-ium chloride (HL12·Cl)

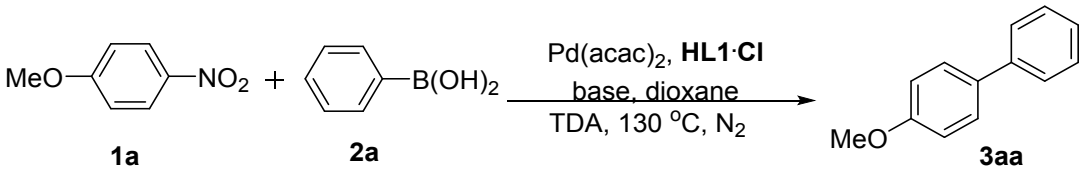


White solid; yield: 68 mg (81%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.10 (s, 1H), 8.84 (d, *J* = 8.0 Hz, 1H), 7.90 (s, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.24 (d, *J* = 7.6 Hz, 2H), 7.14 (d, *J* = 6.6 Hz, 1H), 2.15-2.10 (m, 2H), 2.07 (s, 6H), 1.23 (d, *J* = 6.3 Hz, 6H), 1.03 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.9, 137.3, 132.8, 132.3, 132.2, 131.5, 130.5, 129.3, 129.0, 126.3, 124.7, 121.5, 120.9, 120.7, 120.0, 28.8, 24.6, 24.0, 19.2; HRMS (ESI-TOF) for $C_{27}H_{31}N_2$ ([M-Cl]$^+$) : calcd. 383.2482; found: 383.2486.

IV. Optimization of the reaction conditions

Table S1. Optimization of bases[a]

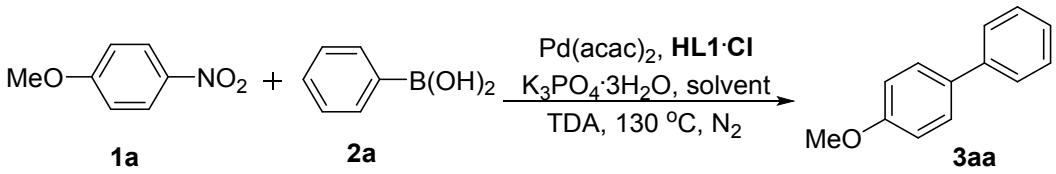


1a **2a** **3aa**

entry	base	Yield (%)[b]
1	**$K_3PO_4·3H_2O$**	**55**
2	K_2CO_3	11
3	CsF	10
4	Cs_2CO_3	17
5	K_3PO_4	47
6	KOAc	n.d.
7	K_2HPO_4	n.d.
8	KOH	n.d.
9	DBU	n.d.
10	Et_3N	n.d.

[a]Reaction conditions: **1a** (0.3 mmol, 1.0 eq.), **2a** (1.5 eq.), $Pd(acac)_2$ (5 mol%), base (3.0 eq.), **HL1·Cl** (10 mol%), TDA (10 mol%), dioxane (1.5 mL), 130 °C, N_2, 36 h. [b]Isolated yields.

Table S2. Optimization of solvents[a]

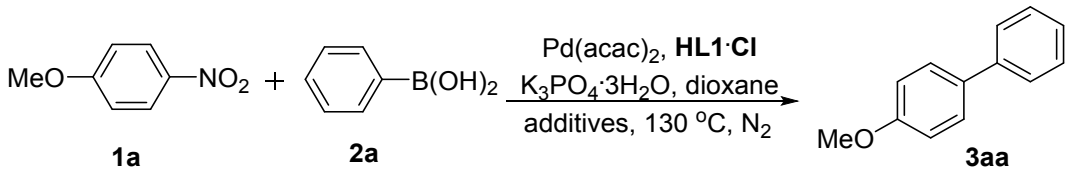


1a 2a 3aa

entry	solvent	Yield (%)[b]
1	**dioxane**	**55**
2	THF	9
3	toluene	17
4	DCM	n.d.
5	DMA	25
6	DME	37
7	MTBE	27
8	heptane	12
9	*i*PrOH	24
10	CH_3CN	10
11	DMSO	n.d.
12	H_2O	n.d.

[a]Reaction conditions: **1a** (0.3 mmol, 1.0 eq.), **2a** (1.5 eq.), $Pd(acac)_2$ (5 mol%), $K_3PO_4·3H_2O$ (3.0 eq.), **HL1·Cl** (10 mol%), TDA (10 mol%), solvent (1.5 mL), 130 °C, N_2, 36 h. [b]Isolated yields.

Table S3. Optimization of additives[a]

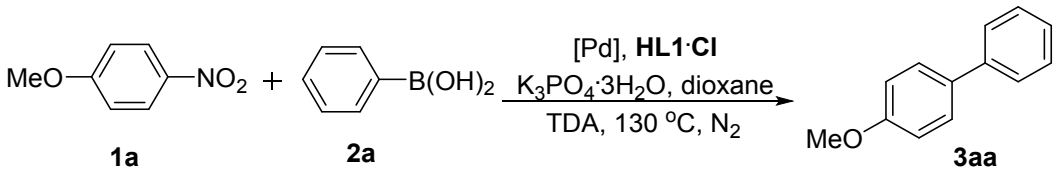


1a **2a** **3aa**

entry	additives	Yield (%)[b]
1	**TDA**	**55**
2	$^{n}Bu_4NBr$	46
3	$^{n}Bu_4NI$	n.d.
4	$^{n}Bu_4NF$ (1.0 M in THF)	48
5	18-crown-6	52
6	Ag_2O	trace
7	$ZnCl_2$	n.d.
8	PPh_3	8
9	1,5-cyclooctadiene	32
10	--	45

[a]Reaction conditions: **1a** (0.3 mmol, 1.0 eq.), **2a** (1.5 eq.), $Pd(acac)_2$ (5 mol%), $K_3PO_4·3H_2O$ (3.0 eq.), **HL1·Cl** (10 mol%), additives (10 mol%), dioxane (1.5 mL), 130 °C, N_2, 36 h. [b]Isolated yields.

Table S4. Optimization of Pd sources[a]

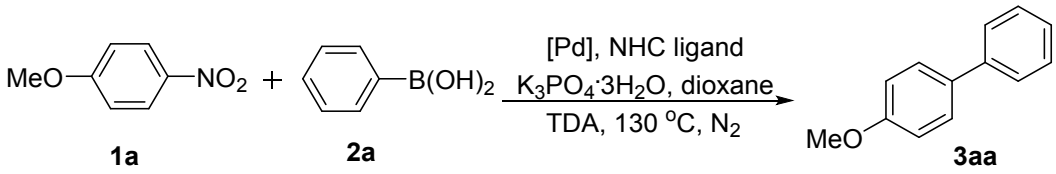


1a 2a 3aa

entry	[Pd]	Yield (%)[b]
1	**$Pd(acac)_2$**	**55**
2	$PdCl_2$	32
3	$Pd(OAc)_2$	22
4	$PdCl_2(MeCN)_2$	29
5	$PdCl_2(PPh_3)_2$	10
6	$Pd(TFA)_2$	25
7	$Pd_2(dba)_3$	8

[a]Reaction conditions: **1a** (0.3 mmol, 1.0 eq.), **2a** (1.5 eq.), [Pd] (5 mol%), $K_3PO_4·3H_2O$ (3.0 eq.), **HL1·Cl** (10 mol%), TDA (10 mol%), dioxane (1.5 mL), 130 °C, N_2, 36 h. [b]Isolated yields.

Table S5. Optimization of [Pd]/L ratio, reaction time, reaction temperature, and additive amount[a]

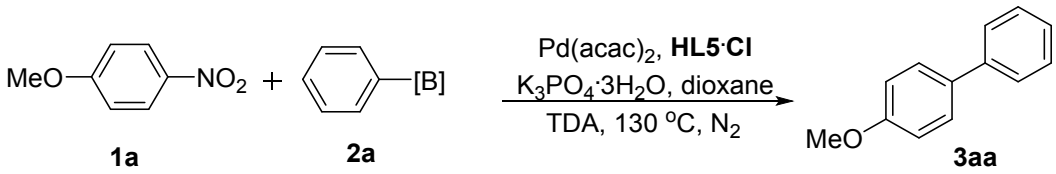


1a **2a** **3aa**

entry	[Pd]	Ligand	Yield (%)[b]
1	$Pd(acac)_2$	**HL1·Cl**	55
2[c]	$Pd(acac)_2$	**HL1·Cl**	40
3[d]	$Pd(acac)_2$	**HL1·Cl**	45
4[e]	$Pd(acac)_2$	**HL1·Cl**	43
5[f]	$Pd(acac)_2$	**HL5·Cl**	73
6[g]	$Pd(acac)_2$	**HL5·Cl**	55
7[h]	$Pd(acac)_2$	**HL5·Cl**	52
8	$Pd(acac)_2$	**--**	n.d.
9	--	**HL5·Cl**	n.d.
10[i]	$Pd(acac)_2$	**HL5·Cl**	56
11[j]	$Pd(acac)_2$	**HL5·Cl**	47
12[k]	$Pd(acac)_2$	**HL5·Cl**	51

[a]Reaction conditions: **1a** (0.3 mmol, 1.0 eq.), **2a** (1.5 eq.), $Pd(acac)_2$ (5 mol%), $K_3PO_4·3H_2O$ (3.0 eq.), NHC ligand (10 mol%), TDA (10 mol%), dioxane (1.5 mL), 130 °C, N_2, 36 h. [b]Isolated yields. [c]24 h. [d]**HL1·Cl** (20 mol%). [e]**HL1·Cl** (6 mol%). [f]TDA (5 mol%). [g]TDA (2.5 mol%). [h]TDA (20 mol%). [i] [Pd] (2.5 mol%), ligand (5 mol%), TDA (5 mol%), 48 h. [j]TDA (5 mol%), 48 h, air. [k]TDA (5 mol%), 48 h, 100 °C.

Table S6. Effect of various boron-containing coupling partners [a]

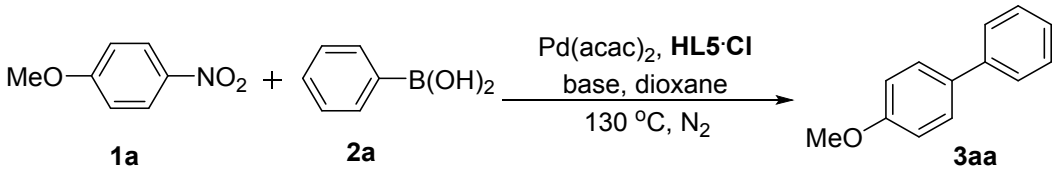


1a 2a 3aa

entry	[B] sources	Yield (%)[b]
1	PhBPin	60
2	$PhBF_3K$	15
3	PhB(MIDA)[c]	traces

[a]Reaction conditions: **1a** (0.3 mmol, 1.0 eq.), **2a** (1.5 eq.), $Pd(acac)_2$ (5 mol%), $K_3PO_4·3H_2O$ (3.0 eq.), **HL5·Cl** (10 mol%), TDA (5 mol%), dioxane (1.5 mL), 130 °C, N_2, 48 h. [b]Isolated yields. [c]MIDA = 2,2'-(methylazanediyl)diacetate.

Table S7. Effect of TDA [a]



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

entry	Base	Yield (%)[b]
1	$K_3PO_4.3H_2O$	82 (74)[c]
2	K_3PO_4	68 (61)[c]
3	K_2CO_3	25 (20)[c]
4	Cs_2CO_3	9 (7)[c]

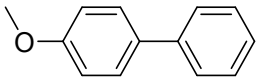
[a]Reaction conditions: **1a** (0.3 mmol, 1.0 eq.), **2a** (1.5 eq.), $Pd(acac)_2$ (5 mol%), base (3.0 eq.), **HL5·Cl** (10 mol%), TDA (5 mol%), dioxane (1.5 mL), 130 °C, N_2, 48 h. [b]Isolated yields. [c]Without TDA in parentheses.

V. General procedure for the synthesis of 3

To an oven-dried tube equipped with a magnetic stirring bar were added sequentially nitroarene **1** (0.6 mmol), boronic acid **2** (0.9 mmol), $Pd(acac)_2$ (9.1 mg, 0.03 mmol), **HL5·Cl** (28 mg, 0.06 mmol), $K_3PO_4·3H_2O$ (480 mg, 1.8 mmol), TDA (9.7 mg, 0.03 mmol), and 1,4-dioxane (3 mL) under N_2 atmosphere. The reaction mixture was stirred at room temperature for 30 minutes and then heated at 130 ℃ for 48 hours. The reaction mixture was cooled to room temperature, and then it was passed through a short pad of celite with CH_2Cl_2. The solution was concentrated in vacuo. The residue was purified by silica gel column chromatography to give the product **3**.

VI. Characterization data of products

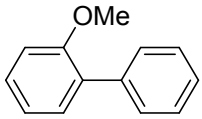
4-methoxy-1,1'-biphenyl (3aa)



White solid; yield: 91 mg (82%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.54 (m, 4H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 140.9, 133.8, 128.8, 128.2, 126.8, 126.7, 114.2, 55.4; Spectral data obtained for the compound are in good agreement with the reported data.[6]

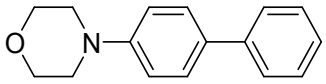
2-methoxy-1,1'-biphenyl (3ab)



Colorless oil; yield: 79 mg (72%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.59 (m, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.40-7.36 (m, 3H), 7.09 (t, *J* = 6.9 Hz, 1H), 7.04 (d, *J* = 8.6 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 138.6, 131.0, 130.8, 129.6, 128.7, 128.1, 127.0, 120.9, 111.3, 55.6; Spectral data obtained for the compound are in good agreement with the reported data.[6]

4-([1,1'-biphenyl]-4-yl)morpholine (3ac)

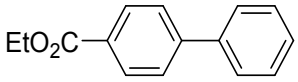


White solid; yield: 60 mg (42%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.54 (m, 4H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 1H),

7.00 (d, J = 8.8 Hz, 2H), 3.92-3.89 (m, 4H), 3.24-3.21 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.6, 140.8, 132.7, 128.8, 127.8, 126.6, 115.8, 66.9, 49.2; Spectral data obtained for the compound are in good agreement with the reported data.[6]

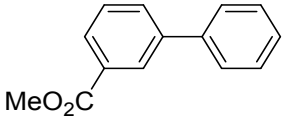
ethyl [1,1'-biphenyl]-4-carboxylate (3ad)



Pale yellow solid; yield: 84 mg (63%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 2H), 7.74-7.59 (m, 4H), 7.48 (t, J = 7.5 Hz, 2H), 7.42-7.38 (m, 1H), 4.42 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 145.5, 140.1, 130.1, 129.3, 129.0, 128.1, 127.3, 127.0, 61.0, 14.4; Spectral data obtained for the compound are in good agreement with the reported data.[7]

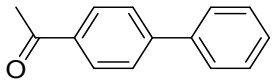
methyl [1,1'-biphenyl]-3-carboxylate (3ae)



Colorless oil; yield: 76 mg (60%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.04 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.64 (d, J = 7.4 Hz, 2H), 7.52 (t, J = 8.0 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.39 (t, J = 7.3 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 141.5, 140.1, 131.6, 130.7, 128.9, 128.9, 128.4, 128.3, 127.8, 127.2, 52.2; Spectral data obtained for the compound are in good agreement with the reported data.[6]

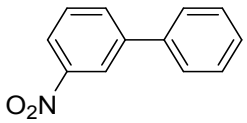
1-([1,1'-biphenyl]-4-yl)ethan-1-one (3af)



White solid; yield: 18 mg (15%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 8.8 Hz, 2H), 7.48 (t, J = 7.2 Hz, 2H), 7.41 (t, J = 7.2 Hz, 1H), 2.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 145.8, 139.9, 135.9, 129.0, 128.9, 128.2, 127.3, 127.2, 26.7; Spectral data obtained for the compound are in good agreement with the reported data.[6]

3-nitro-1,1'-biphenyl (3ag)

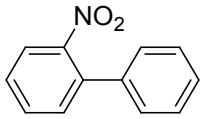


White solid; yield: 75 mg (63%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.20 (d, J = 8.2 Hz, 1H), 7.92 (d, J = 7.8 Hz, 1H), 7.64-7.59 (m, 3H), 7.50 (t, J = 7.4 Hz, 2H), 7.44 (t, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 142.9,

138.7, 133.1, 129.7, 129.2, 128.6, 127.2, 122.1, 122.0; Spectral data obtained for the compound are in good agreement with the reported data.[6]

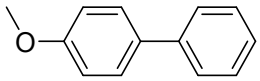
2-nitro-1,1'-biphenyl (3ah)



Pale yellow solid; yield: 70 mg (59%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.62 (td, *J* = 7.6, 1.2 Hz, 1H), 7.54-7.40 (m, 5H), 7.38-7.29 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 137.4, 136.4, 132.31, 132.0, 128.7, 128.3, 128.2, 127.9, 124.1; Spectral data obtained for the compound are in good agreement with the reported data.[6]

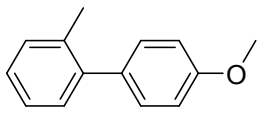
4-methoxy-1,1'-biphenyl (3ai)



White solid; yield: 94 mg (85%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.54 (m, 4H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 140.9, 133.8, 128.8, 128.2, 126.8, 126.7, 114.2, 55.4; Spectral data obtained for the compound are in good agreement with the reported data.[6]

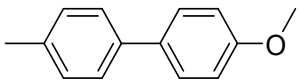
4'-methoxy-2-methyl-1,1'-biphenyl (3aj)



Colorless oil; yield: 96 mg (81%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.26 (m, 6H), 7.03 (d, *J* = 8.6 Hz, 2H), 3.92 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 141.6, 135.5, 134.4, 130.3, 130.3, 129.9, 127.0, 125.8, 113.5, 55.3, 20.6; Spectral data obtained for the compound are in good agreement with the reported data.[6]

4-methoxy-4'-methyl-1,1'-biphenyl (3ak)

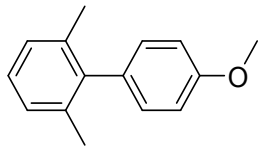


White solid; yield: 83 mg (70%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.8 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 138.0, 136.4, 133.8, 129.5, 128.0, 126.6, 114.2, 55.4, 21.1; Spectral data obtained for the compound are in

good agreement with the reported data.[6]

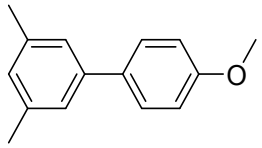
4'-methoxy-2,6-dimethyl-1,1'-biphenyl (3al)



Colorless solid; yield: 77 mg (61%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17-7.14 (m, 1H), 7.13-7.09 (m, 2H), 7.09-7.04 (m, 2H), 7.01-6.94 (m, 2H), 3.86 (s, 3H), 2.05 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 141.5, 136.5, 133.3, 130.1, 127.2, 126.9, 113.8, 55.2, 20.9; Spectral data obtained for the compound are in good agreement with the reported data.[8]

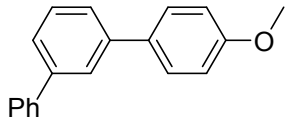
4'-methoxy-3,5-dimethyl-1,1'-biphenyl (3am)



White solid; yield: 89 mg (70%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.8 Hz, 2H), 7.17 (s, 2H), 7.02-6.84 (m, 3H), 3.85 (s, 3H), 2.38 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 140.8, 138.2, 134.0, 128.3, 128.2, 124.7, 114.1, 55.3, 21.4; Spectral data obtained for the compound are in good agreement with the reported data.[6]

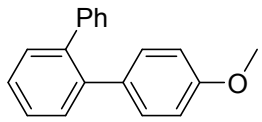
4-methoxy-1,1':3',1''-terphenyl (3an)



White solid; yield: 129 mg (83%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.71 (d, J = 7.1 Hz, 2H), 7.65 (d, J = 8.8 Hz, 2H), 7.63-7.57 (m, 2H), 7.57-7.48 (m, 3H), 7.43 (t, J = 7.3 Hz, 1H), 7.06 (d, J = 8.8 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 141.8, 141.5, 141.4, 133.8, 129.3, 128.9, 128.3, 127.5, 127.4, 125.8, 125.6, 114.3, 55.4; Spectral data obtained for the compound are in good agreement with the reported data.[6]

4-methoxy-1,1':2',1''-terphenyl (3ao)

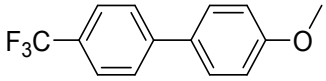


Colorless oil; yield: 78 mg (50%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.34 (m, 4H), 7.27-7.10 (m, 5H), 7.05 (d, J = 8.7 Hz, 2H), 6.75 (d, J = 8.7 Hz, 2H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 141.8, 140.5, 140.2, 133.9, 131.0,

130.7, 130.6, 129.9, 127.9, 127.5, 127.2, 126.4, 113.4, 55.2; Spectral data obtained for the compound are in good agreement with the reported data.[6]

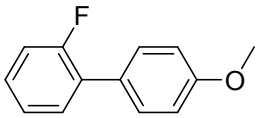
4-methoxy-4'-(trifluoromethyl)-1,1'-biphenyl (3ap)



White solid; yield: 74 mg (49%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.64 (m, 4H), 7.52 (d, *J* = 8.4 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 144.3, 132.2, 128.7 (q, *J* = 32.0 Hz), 128.4, 126.9, 125.7 (q, *J* = 4.0 Hz), 124.4 (q, *J* = 270.0 Hz), 114.4, 55.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3; Spectral data obtained for the compound are in good agreement with the reported data.[6]

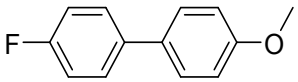
2-fluoro-4'-methoxy-1,1'-biphenyl (3aq)



White solid; yield: 75 mg (62%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 8.7, 1.6 Hz, 2H), 7.40 (t, *J* = 7.8, 1H), 7.29-7.22 (m, 1H), 7.17 (t, *J* = 7.2 Hz, 1H), 7.15-7.10 (m, 1H), 6.98 (dd, *J* = 8.8, 2.4 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8 (d, *J* = 245.5 Hz), 159.3, 130.5 (d, *J* = 3.7 Hz), 130.2 (d, *J* = 2.8 Hz), 128.7 (d, *J* = 13.0 Hz), 128.4 (d, *J* = 8.1 Hz), 128.2, 124.3 (d, *J* = 3.6 Hz), 116.1 (d, *J* = 23.0 Hz), 113.9, 55.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.2; Spectral data obtained for the compound are in good agreement with the reported data.[9]

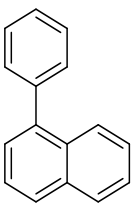
4-fluoro-4'-methoxy-1,1'-biphenyl (3ar)



White solid; yield: 115 mg (95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.47 (m, 4H), 7.11 (m, 2H), 6.98 (m, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1 (d, *J* = 243.8 Hz), 159.1, 137.0 (d, *J* = 3.3 Hz), 132.9, 128.2 (d, *J* = 7.9 Hz), 128.1, 115.5 (d, *J* = 21.4 Hz), 114.3, 55.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.7; Spectral data obtained for the compound are in good agreement with the reported data.[6]

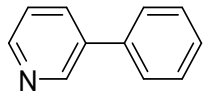
1-phenylnaphthalene (3as)



Colorless oil; yield: 117 mg (96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.80 (m, 3H), 7.50-7.36 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 140.4, 133.9, 131.8, 130.2, 128.4, 127.8, 127.4, 127.1, 126.2, 125.9, 125.5; Spectral data obtained for the compound are in good agreement with the reported data.[6]

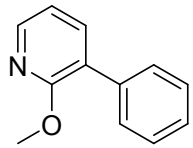
3-phenylpyridine (3at)



Colorless oil; yield: 82 mg (88%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.59 (d, *J* = 4.8 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.44-7.31 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.5, 148.3, 137.8, 136.7, 134.4, 129.1, 128.1, 127.2, 123.6; Spectral data obtained for the compound are in good agreement with the reported data.[6]

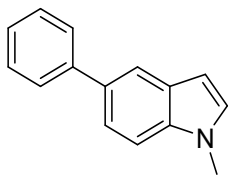
2-methoxy-3-phenylpyridine (3au)



Colorless oil; yield: 104 mg (94%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.62 (dd, *J* = 7.3, 1.8 Hz, 1H), 7.56 (d, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 1H), 6.98 (dd, *J* = 7.3, 5.0 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 145.7, 138.6, 136.8, 129.2, 128.2, 127.6, 124.7, 117.1, 53.5; Spectral data obtained for the compound are in good agreement with the reported data.[6]

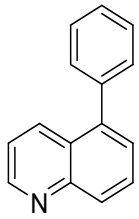
1-methyl-5-phenyl-1*H*-indole (3av)



Pale yellow solid; yield: 42 mg (34%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 1.2 Hz, 1H), 7.71 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.53 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.11 (d, *J* = 3.0 Hz, 1H), 6.58 (d, *J* = 3.0 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 136.3, 132.9, 129.5, 129.0, 128.7, 127.4, 126.3, 121.4, 119.5, 109.5, 101.4, 33.0; Spectral data obtained for the compound are in good agreement with the reported data.[10]

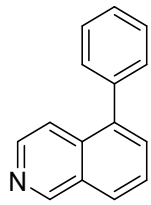
5-phenylquinoline (3aw)



Pale yellow solid; yield: 116 mg (94%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.74 (t, *J* = 8 Hz, 1H), 7.55-7.42 (m, 6H), 7.32 (dd, *J* = 8.6, 4.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 148.6, 140.5, 139.4, 134.4, 130.0, 129.0, 128.9, 128.5, 127.7, 127.3, 126.7, 121.1; Spectral data obtained for the compound are in good agreement with the reported data.[6]

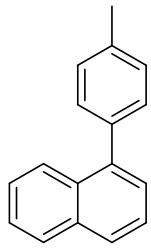
5-phenylisoquinoline (3ax)



yellow oil; yield: 117 mg (95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.48 (d, *J* = 6.0 Hz, 1H), 7.96 (t, *J* = 4.8 Hz, 1H), 7.72 (d, *J* = 6.0 Hz, 1H), 7.64 (d, *J* = 4.0 Hz, 2H), 7.55-7.41 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 143.4, 139.2, 139.0, 134.1, 130.9, 129.9, 129.0, 128.6, 127.8, 127.2, 126.9, 118.6; Spectral data obtained for the compound are in good agreement with the reported data.[6]

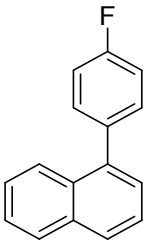
1-(*p*-tolyl)naphthalene (3ba)



Colorless oil; yield: 114 mg (87%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.85 (m, 3H), 7.55-7.40 (m, 6H), 7.32 (d, *J* = 7.8 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 137.8, 136.9, 133.8, 131.7, 130.0, 129.0, 128.3, 127.5, 126.9, 126.1, 125.9, 125.7, 125.4, 21.3; Spectral data obtained for the compound are in good agreement with the reported data.[11]

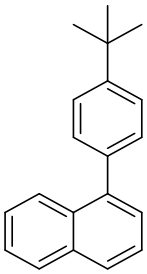
1-(4-fluorophenyl)naphthalene (3bb)



White solid; yield: 114 mg (86%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.57-7.44 (m, 5H), 7.41 (d, *J* = 7.1 Hz, 1H), 7.20 (t, *J* = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5 (d, *J* = 244.0 Hz), 139.2, 136.7 (d, *J* = 4.0 Hz), 133.8, 131.7, 131.6 (d, *J* = 8.0 Hz), 128.4, 127.8, 127.0, 126.2, 125.9, 125.8, 125.4, 115.3 (d, *J* = 21.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.5; Spectral data obtained for the compound are in good agreement with the reported data.[12]

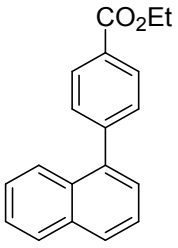
1-(4-(*tert*-butyl)phenyl)naphthalene (3bc)



White solid; yield: 136 mg (87%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.56-7.42 (m, 8H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.1, 140.2, 137.7, 133.8, 131.7, 129.7, 128.2, 127.4, 126.9, 126.2, 125.9, 125.7, 125.4, 125.2, 34.6, 31.5; Spectral data obtained for the compound are in good agreement with the reported data.[13]

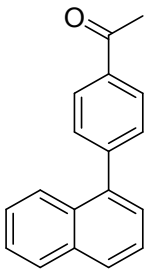
ethyl 4-(naphthalen-1-yl)benzoate (3bd)



Pale yellow oil; yield: 126 mg (76%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.3 Hz, 2H), 7.97-7.84 (m, 3H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.56-7.50 (m, 2H), 7.49-7.45 (m, 2H), 4.46 (q, *J* = 7.1 Hz, 2H), 1.46 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 145.5, 139.2, 133.8, 131.3, 130.1, 129.6, 129.4, 128.4, 128.3, 127.0, 126.4, 126.0, 125.7, 125.4, 61.1, 14.4; Spectral data obtained for the compound are in good agreement with the reported data.[14]

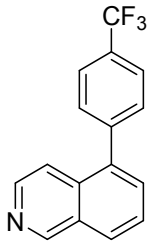
1-(4-(naphthalen-1-yl)phenyl)ethan-1-one (3be)



White solid; yield: 96 mg (65%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.3 Hz, 2H), 7.97-7.84 (m, 3H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.54-7.42 (m, 4H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 145.8, 139.0, 136.0, 133.8, 131.2, 130.4, 128.5, 128.4, 127.0, 126.5, 126.1, 125.6, 125.4, 26.8; Spectral data obtained for the compound are in good agreement with the reported data.[15]

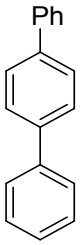
5-[4-(Trifluoromethyl)phenyl]isoquinoline (3bf)



Off-white solid; yield: 78 mg (48%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.37 (s, 1H), 8.52 (d, *J* = 5.1 Hz, 1H), 8.08 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.76-7.65 (m, 3H), 7.61 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 142.7, 142.5, 137.8, 134.1, 131.6, 130.3 (q, *J* = 32.0 Hz), 130.2, 128.8, 128.2, 127.2, 125.7 (q, *J* = 4.0 Hz), 122.8 (q, *J* = 271.0 Hz), 118.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5; Spectral data obtained for the compound are in good agreement with the reported data.[16]

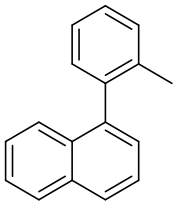
1,1':4',1''-terphenyl (3bg)



White solid; yield: 110 mg (80%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.65 (m, 8H), 7.52-7.46 (m, 4H), 7.42-7.35 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 140.2, 128.9, 127.5, 127.4, 127.1; Spectral data obtained for the compound are in good agreement with the reported data.[17]

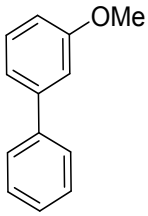
1-(*o*-tolyl)naphthalene (3bh)



White solid; yield: 92 mg (70%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 8.3 Hz, 1H), 7.54 (t, *J* = 8.0, 1H), 7.52-7.45 (m, 2H), 7.42-7.34 (m, 4H), 7.34-7.26 (m, 2H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 139.8, 136.8, 133.5, 132.0, 130.4, 129.9, 128.2, 127.6, 127.5, 126.6, 126.1, 126.0, 125.7, 125.6, 125.4, 20.1; Spectral data obtained for the compound are in good agreement with the reported data.[18]

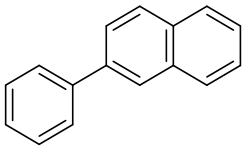
3-methoxy-1,1'-biphenyl (3bi)



White solid; yield: 91mg (82%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.5 Hz, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.43-7.37 (m, 2H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.19 (s, 1H), 6.95 (dd, *J* = 8.2, 2.4 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 142.8, 141.2, 129.8, 128.8, 127.5, 127.3, 119.7, 112.9, 112.7, 55.3; Spectral data obtained for the compound are in good agreement with the reported data.[6]

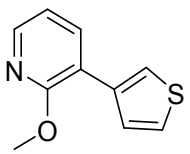
2-phenylnaphthalene (3bj)



White solid; yield: 77 mg (63%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.01-7.90 (m, 3H), 7.84-7.77 (m, 3H), 7.60-7.51 (m, 4H), 7.44 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 138.6, 133.8, 132.7, 128.9, 128.5, 128.3, 127.7, 127.5, 127.4, 126.4, 126.0, 125.9, 125.7; Spectral data obtained for the compound are in good agreement with the reported data.[6]

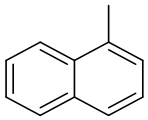
2-methoxy-3-(thiophen-3-yl)pyridine (3bk)



Colorless oil; yield: 55 mg (48%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 5.0, 1.8 Hz, 1H), 7.80 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.73 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.46 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.37 (dd, *J* = 5.0, 3.0 Hz, 1H), 6.96 (dd, *J* = 7.4, 5.0 Hz, 1H), 4.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 144.8, 137.3, 136.3, 127.7, 125.1, 124.0, 119.5, 117.1, 53.9; Spectral data obtained for the compound are in good agreement with the reported data.[6]

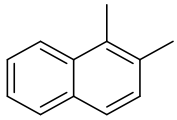
1-methylnaphthalene (3bl)



Colorless liquid; yield: 80 mg (94%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.67-7.53 (m, 2H), 7.50-7.45 (m, 1H), 7.42 (d, *J* = 6.8 Hz, 1H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.4, 133.7, 132.7, 128.7, 126.7, 126.5, 125.8, 125.7, 125.7, 124.2, 19.5; Spectral data obtained for the compound are in good agreement with the reported data.[19]

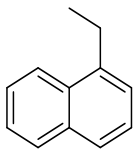
1,2-dimethylnaphthalene (3bm)



Colorless liquid; yield: 76 mg (81%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 1H), 7.64-7.57 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 2.70 (s, 3H), 2.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.2, 133.0, 132.4, 131.2, 129.1, 128.5, 125.8, 125.8, 124.6, 123.8, 20.9, 14.6; Spectral data obtained for the compound are in good agreement with the reported data.[20]

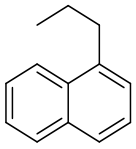
1-ethylnaphthalene (3bn)



Colorless liquid; yield: 75 mg (80%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.63-7.53 (m, 2H), 7.52-7.48 (m, 1H), 7.43 (d, *J* = 6.9 Hz, 1H), 3.21 (q, *J* = 7.5 Hz, 2H), 1.48 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 134.0, 131.9, 128.9, 126.5, 125.8, 125.5, 125.0, 123.8, 26.0, 15.2; Spectral data obtained for the compound are in good agreement with the reported data.[12]

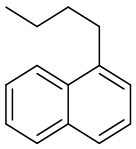
1-propylnaphthalene (3bo)



Colorless liquid; yield: 83 mg (81%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.64-7.53 (m, 2H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 6.9 Hz, 1H), 3.16 (t, *J* = 8.0 Hz, 2H), 1.90 (h, *J* = 7.6 Hz, 2H), 1.15 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8, 134.0, 132.1, 128.9, 126.6, 126.1, 125.7, 125.6, 125.5, 124.0, 35.3, 24.0, 14.4; Spectral data obtained for the compound are in good agreement with the reported data.[21]

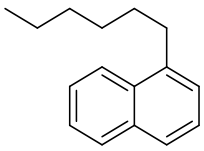
1-butylnaphthalene (3bp)



Colorless liquid; yield: 105 mg (95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.2 Hz, 1H), 7.99-7.94 (m, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.65-7.55 (m, 2H), 7.54-7.48 (m, 1H), 7.44 (d, *J* = 6.9 Hz, 1H), 3.19 (t, *J* = 7.6 Hz, 2H), 1.87 (p, *J* = 7.6 Hz, 2H), 1.59 (h, *J* = 7.6 Hz, 2H), 1.11 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 134.1, 132.1, 128.9, 126.5, 126.0, 125.7, 125.7, 125.5, 124.0, 33.2, 33.0, 23.0, 14.2; Spectral data obtained for the compound are in good agreement with the reported data.[22]

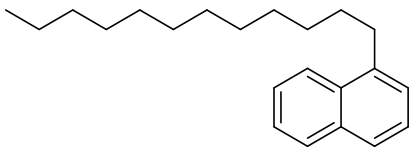
1-hexylnaphthalene (3bq)



Colorless liquid; yield: 119 mg (93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.2 Hz, 1H), 7.99-7.96 (m, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.67-7.56 (m, 2H), 7.52 (t, *J* = 8.4 Hz, 1H), 7.45 (d, *J* = 6.7 Hz, 1H), 3.20 (t, *J* = 7.6 Hz, 1H), 1.89 (p, *J* = 8.0 Hz, 2H), 1.64-1.42 (m, 6H), 1.06 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.2, 134.1, 132.1, 128.9, 126.5, 126.0, 125.8, 125.7, 125.5, 124.1, 33.3, 32.0, 31.0, 29.7, 22.9, 14.3; Spectral data obtained for the compound are in good agreement with the reported data.[23]

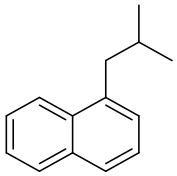
1-dodecylnaphthalene (3br)



Colorless liquid; yield: 104 mg (59%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.57-7.47 (m, 2H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 6.8 Hz, 1H), 3.10 (t, *J* = 8.0 Hz, 2H), 1.79 (p, *J* = 7.6 Hz, 2H), 1.54-1.42 (m, 2H), 1.37-1.31 (m, 16H), 0.93 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 133.9, 132.0, 128.8, 126.4, 125.9, 125.6, 125.5, 125.4, 124.0, 33.2, 32.0, 30.9, 29.9, 29.8, 29.7, 29.7, 29.6, 29.4, 22.8, 14.2; Spectral data obtained for the compound are in good agreement with the reported data.[12]

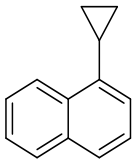
1-isobutylnaphthalene (3bs)



Colorless liquid; yield: 74 mg (67%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.1 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.58-7.51 (m, 2H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.35 (d, *J* = 6.9 Hz, 1H), 3.00 (d, *J* = 7.2 Hz, 2H), 2.18-2.12 (m, 1H), 1.05 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 134.0, 132.3, 128.8, 127.1, 126.6, 125.6, 125.4, 125.4, 124.3, 42.7, 29.6, 22.9; Spectral data obtained for the compound are in good agreement with the reported data.[12]

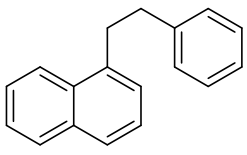
1-cyclopropylnaphthalene (3bt)



Colorless liquid; yield: 93 mg (93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.6 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.71-7.58 (m, 2H), 7.54-7.47 (m, 1H), 7.39 (d, *J* = 7.1 Hz, 1H), 2.51-2.41 (m, 1H), 1.22-1.13 (m, 2H), 0.93-0.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 133.7, 133.7, 128.6, 126.7, 125.8, 125.7, 125.6, 124.6, 123.9, 13.4, 6.6; Spectral data obtained for the compound are in good agreement with the reported data.[24]

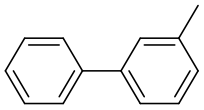
1-phenethylnaphthalene (3bu)



Colorless liquid; yield: 132 mg (95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.3 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.73-7.65 (m, 2H), 7.60-7.54 (m, 1H), 7.52-7.46 (m, 3H), 7.44-7.40 (m, 3H), 3.58-3.54 (m, 2H), 3.27-3.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 138.0, 134.1, 132.0, 129.1, 128.7, 127.0, 126.3, 126.2, 126.1, 125.8, 125.7, 123.9, 37.3, 35.3; Spectral data obtained for the compound are in good agreement with the reported data.[12]

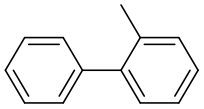
3-methyl-1,1'-biphenyl (3bv)



Colorless liquid; yield: 76 mg (75%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.5 Hz, 2H), 7.50-7.44 (m, 4H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 7.4 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 141.3, 138.4, 128.8, 128.7, 128.1, 128.0, 127.2, 124.3, 21.6; Spectral data obtained for the compound are in good agreement with the reported data.[25]

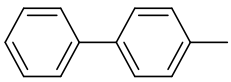
2-methyl-1,1'-biphenyl (3bw)



Colorless liquid; yield: 76 mg (75%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.46 (m, 2H), 7.44-7.40 (m, 3H), 7.36-7.32 (m, 4H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 142.0, 135.4, 130.4, 129.9, 129.3, 128.2, 127.3, 126.9, 125.9, 20.6; Spectral data obtained for the compound are in good agreement with the reported data.[26]

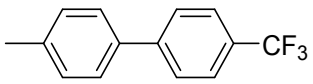
4-methyl-1,1'-biphenyl (3bx)



White soild; yield: 88 mg (87%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 8.1 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.43 (t, *J* = 6.8 Hz, 1H), 7.36 (d, *J* = 7.9 Hz, 2H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.3, 138.5, 137.1, 129.6, 128.8, 127.1, 127.1, 21.2; Spectral data obtained for the compound are in good agreement with the reported data.[26]

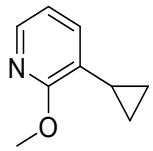
4-methyl-4'-(trifluoromethyl)-1,1'-biphenyl (3by)



White soild; yield: 96 mg (68%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.69 (m, 4H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 138.2, 136.9, 129.8, 129.1 (q, *J* = 32.0 Hz), 127.2, 127.1, 125.7 (q, *J* = 3.7 Hz), 124.4 (q, *J* = 270 Hz), 21.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3; Spectral data obtained for the compound are in good agreement with the reported data.[27]

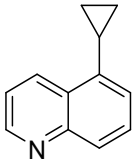
3-cyclopropyl-2-methoxypyridine (3bz)



Light yellow oil; yield: 42 mg (47%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 5.0, 1.8 Hz, 1H), 7.09 (dd, *J* = 7.3, 1.7 Hz, 1H), 6.77 (dd, *J* = 7.3, 5.0 Hz, 1H), 2.08-2.01 (m, 1H), 0.97-0.88 (m, 2H), 0.67-0.60 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7, 143.1, 133.1, 126.5, 116.6, 53.5, 9.4, 7.5; HRMS (GC-TOF) for $C_9H_{11}NO$: calcd. 149.0841; found: 149.0841.

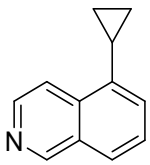
5-cyclopropylquinoline (3ca)



Pale yellow solid; m. p. 57-58 ℃; yield: 87 mg (86%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.70 (d, *J* = 9.2 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.42 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.28 (d, *J* = 7.1 Hz, 1H), 2.33-2.22 (m, 1H), 1.08-1.03 (m, 2H), 0.79-0.71 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 148.3, 139.7, 133.0, 129.2, 128.6, 127.7, 124.2, 120.7, 12.6, 6.6; HRMS (GC-TOF) for $C_{12}H_{11}N$: calcd. 169.0891; found: 169.0892.

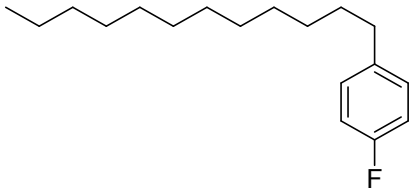
5-cyclopropylisoquinoline (3cb)



Blue solid; m. p. 62-63 ℃; yield: 97 mg (96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.56 (d, *J* = 5.9 Hz, 1H), 8.09 (d, *J* = 5.9 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.1 Hz, 1H), 2.31-2.21 (m, 1H), 1.10-1.01 (m, 2H), 0.76-0.69 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.8, 138.6, 136.1, 128.7, 127.6, 126.9, 125.9, 117.3, 12.4, 6.6; HRMS (ESI-TOF) for $C_{12}H_{12}N$ ($[M+H]^+$) : calcd. 170.0970; found: 170.0965.

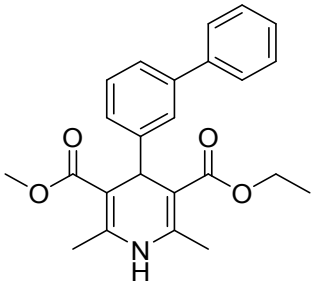
1-dodecyl-4-fluorobenzene (3cc)



Colorless liquid; yield: 78 mg (49%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18-7.06 (m, 2H), 7.03-6.88 (m, 2H), 2.63-2.47 (m, 2H), 1.62-1.54 (m, 2H), 1.37-1.19 (m, 18H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1 (d, *J* = 241.0 Hz), 138.5 (d, *J* = 4.0 Hz), 129.6 (d, *J* = 8.0 Hz), 114.9 (d, *J* = 21.0 Hz), 35.1, 31.9, 31.6, 29.7, 29.7, 29.6, 29.5, 29.4, 29.2, 22.7, 14.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.2; Spectral data obtained for the compound are in good agreement with the reported data.[28]

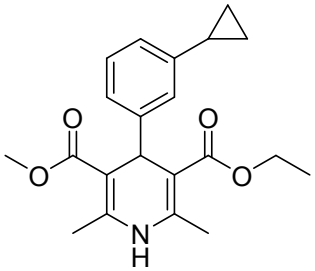
3-ethyl 5-methyl 4-([1,1'-biphenyl]-3-yl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (N1)



Waxy oil; yield: 172 mg (73%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.54 (m, 3H), 7.44-7.37 (m, 3H), 7.36-7.27 (m, 3H), 6.28 (s, 1H), 5.11 (s, 1H), 4.22-4.05 (m, 2H), 3.67 (s, 3H), 2.32 (s, 3H), 2.32 (s, 3H), 1.24 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 167.9, 148.3, 144.9, 144.7, 141.7, 140.8, 128.7, 128.5, 127.2, 127.1, 126.9, 126.7, 125.1, 103.8, 103.5, 76.9, 59.9, 51.1, 39.6, 19.4, 14.4; HRMS (ESI-TOF) for $C_{24}H_{25}NO_4$: calcd. 391.1784; found: 391.1785.

3-ethyl 5-methyl 4-(3-cyclopropylphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (N2)



Waxy oil; yield: 64 mg (30%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (t, *J* = 7.5 Hz, 1H), 7.05-6.98 (m, 2H), 6.80 (d, *J* = 7.5 Hz, 1H), 6.09 (s, 1H), 4.96 (s, 1H), 4.15-4.04 (m, 2H), 3.64 (s, 3H), 2.30 (s, 3H), 2.30 (s, 3H), 1.88-1.77 (m, 1H),

1.24 (t, J = 7.2 Hz, 3H), 0.94-0.87 (m, 2H), 0.65-0.61 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 167.8, 147.5, 144.5, 144.2, 143.3, 127.9, 125.4, 124.9, 123.1, 104.0, 103.6, 59.8, 51.0, 39.3, 19.5, 19.4, 15.4, 14.3, 9.3, 9.2; HRMS (ESI-TOF) for $C_{21}H_{25}NO_4$: calcd. 355.1784; found: 355.1787.

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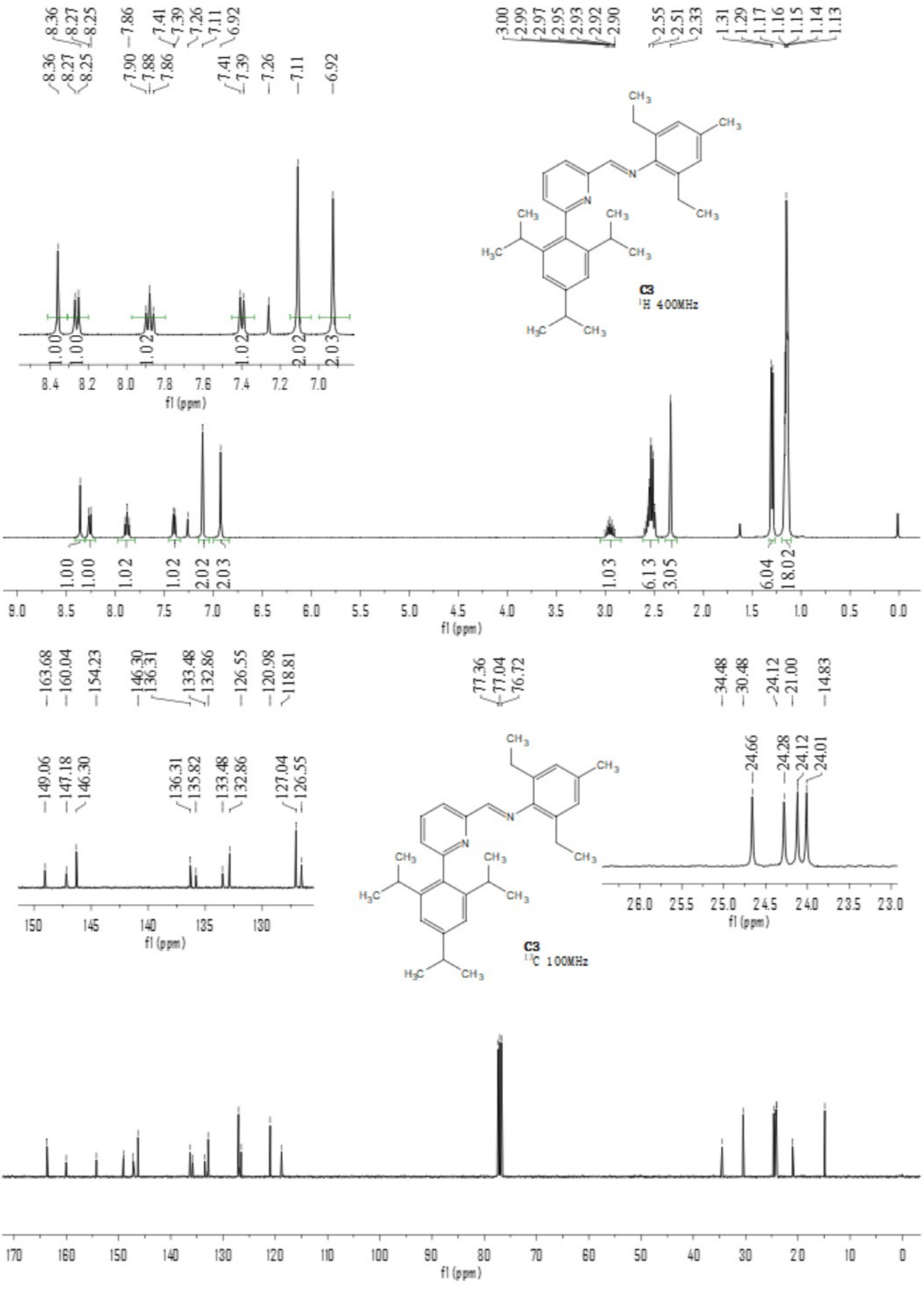
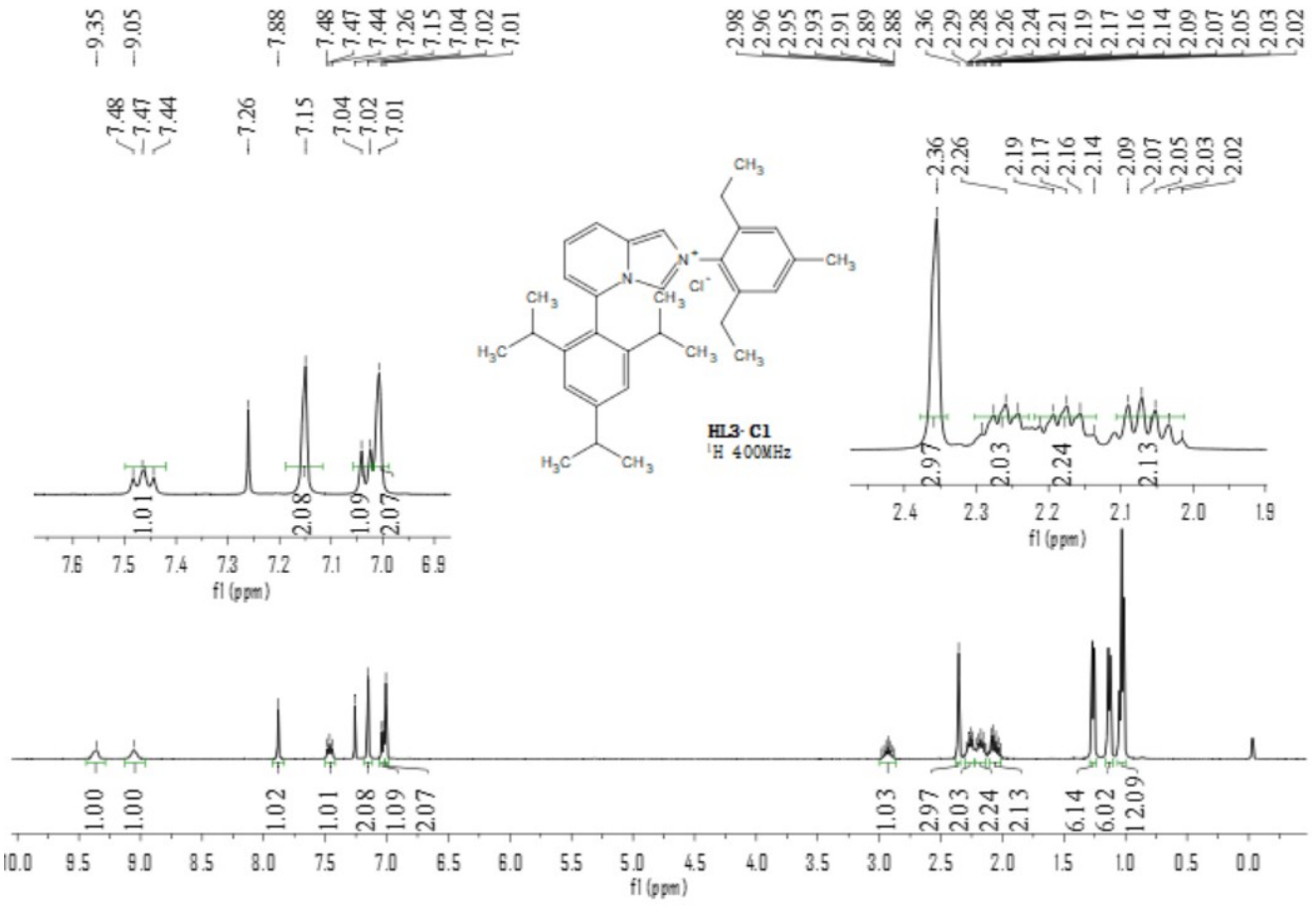
VIII. NMR spectra of ligand precursors

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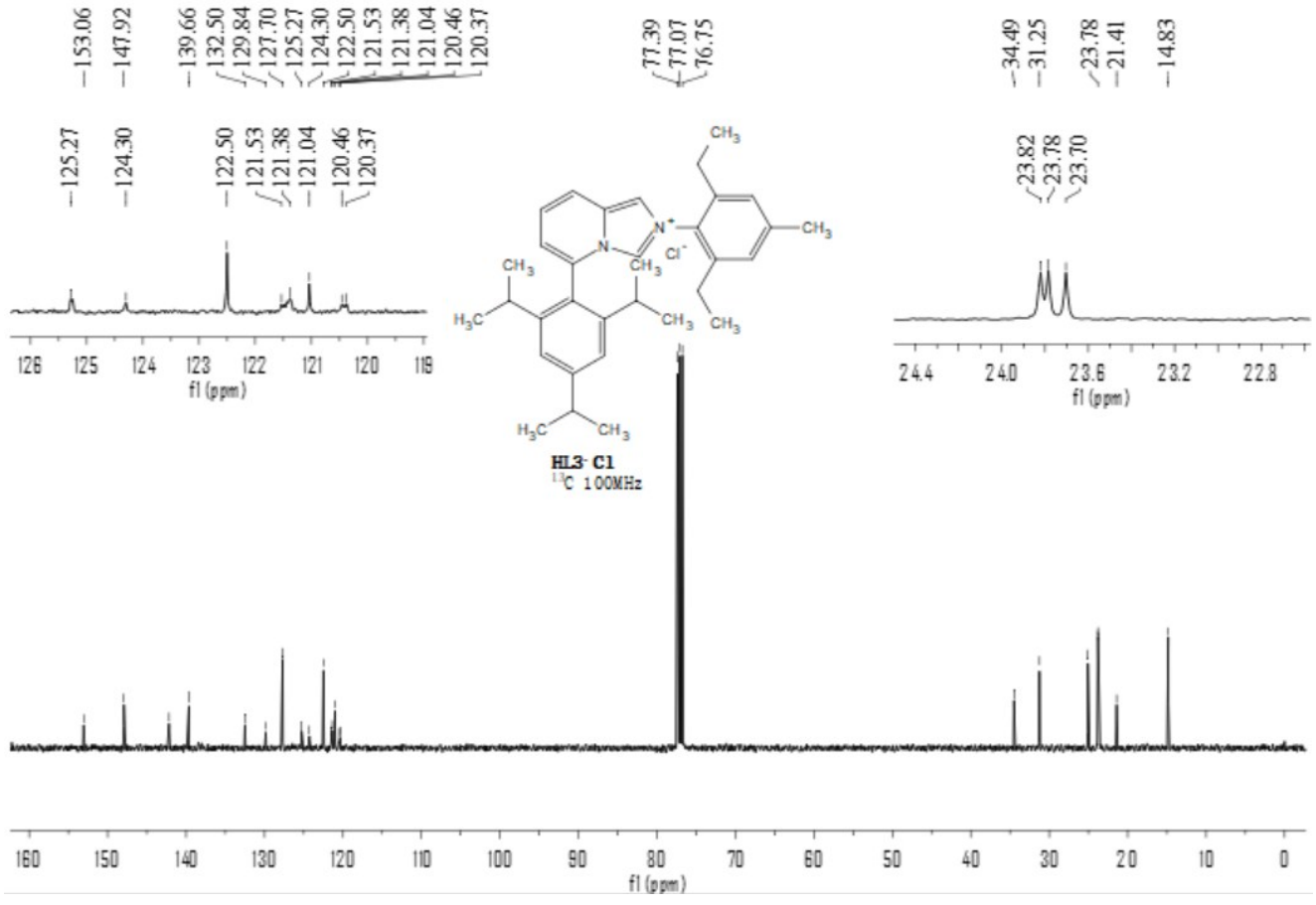
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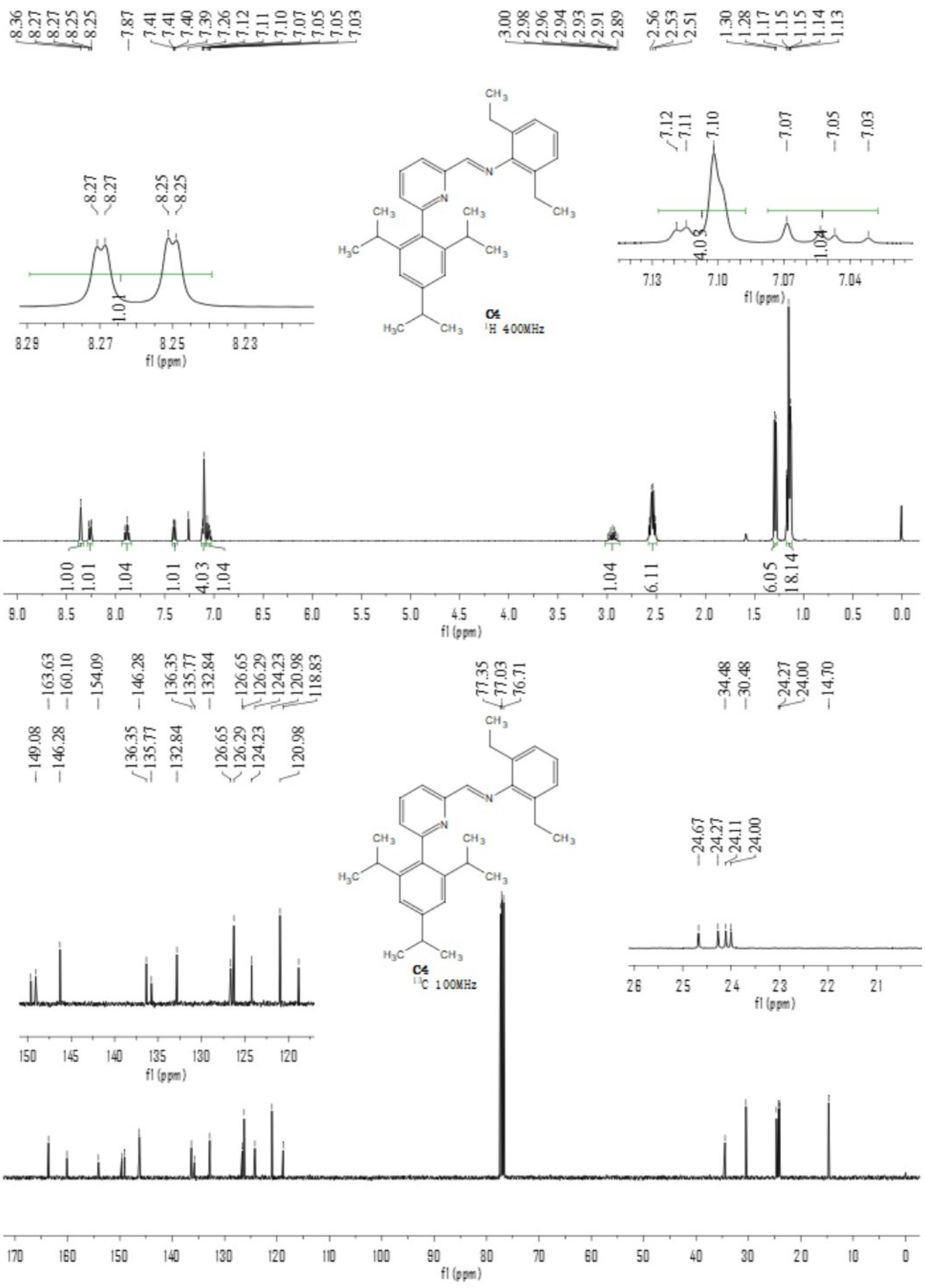
f1 (ppm)


8.36 8.27 8.27 8.25 8.25 7.87 7.41 7.41 7.40 7.39 7.26 7.12 7.11 7.10 7.07 7.05 7.05 7.03
3.00 2.98 2.96 2.94 2.93 2.91 2.89 2.56 2.53 2.51 1.30 1.28 1.17 1.15 1.15 1.14 1.13
C4
^{1}H 400MHz
1.00 1.01 1.04 1.01 4.03 1.04 1.04 6.11 6.05 18.14
f1 (ppm)
149.08 146.28 136.35 135.77 132.84 126.65 126.29 124.23 120.98
163.63 160.10 154.09 146.28 136.35 135.77 132.84 126.65 126.29 124.23 120.98 118.83
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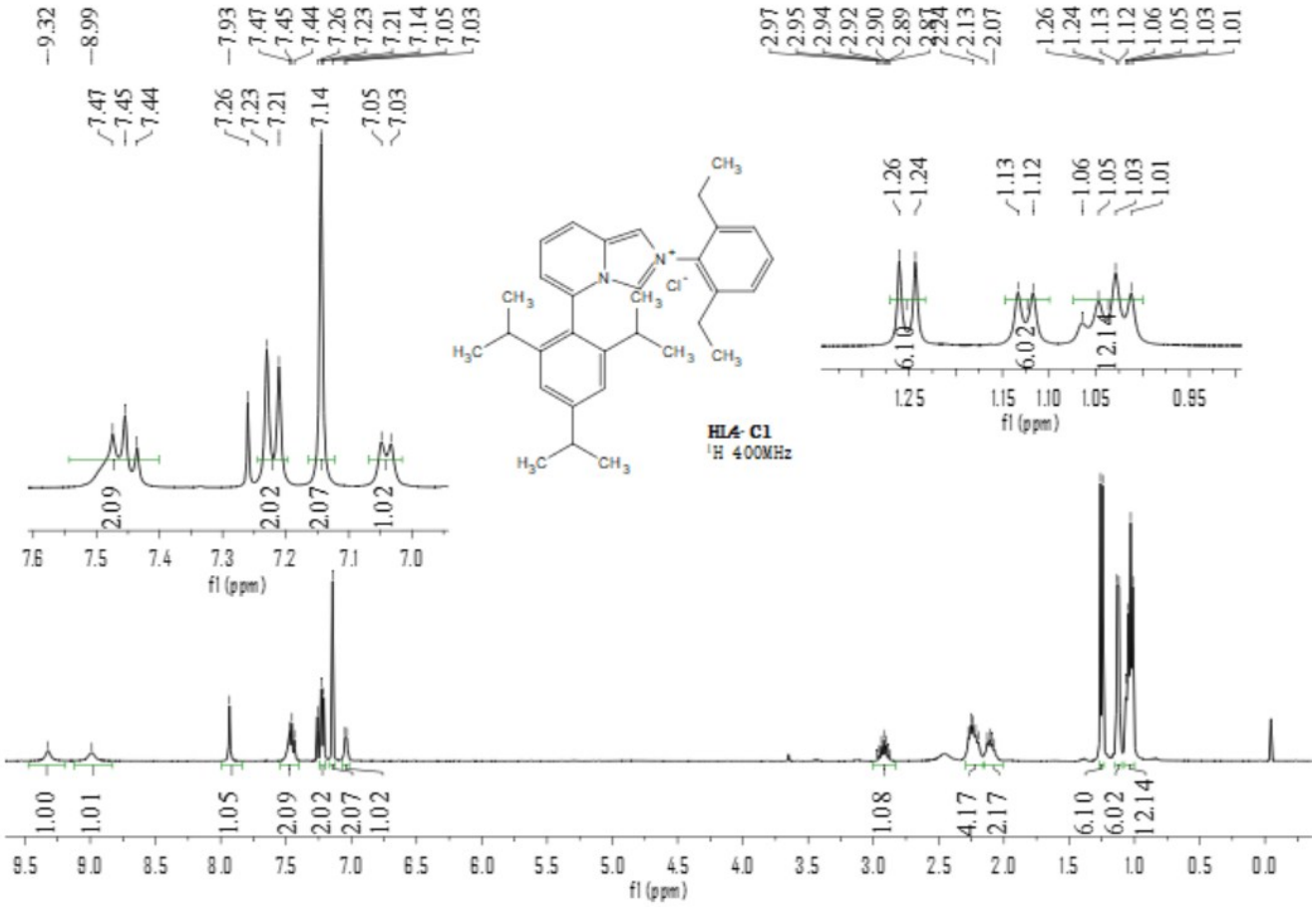
24.67 24.27 24.11 24.00
C4
^{13}C 100MHz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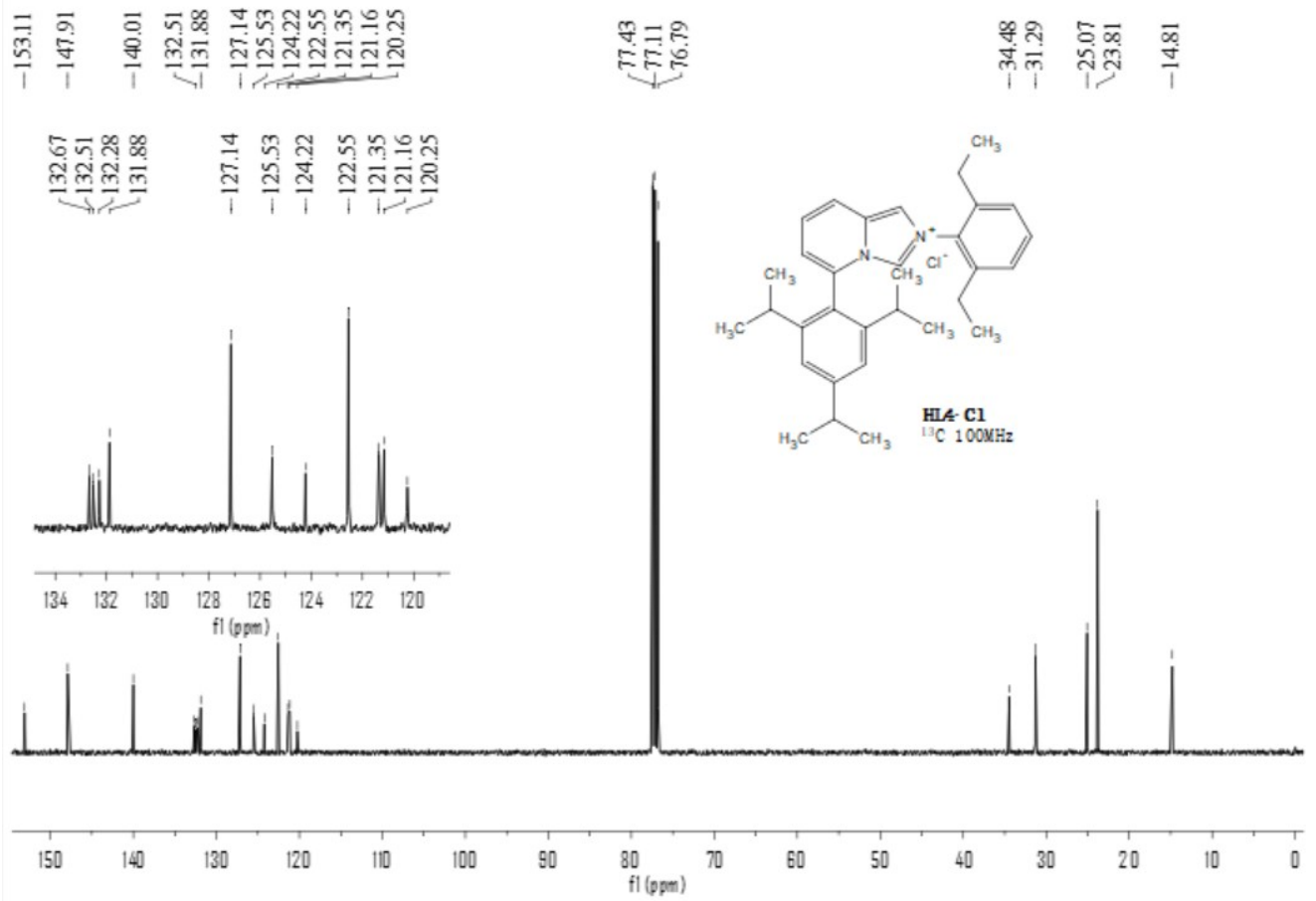
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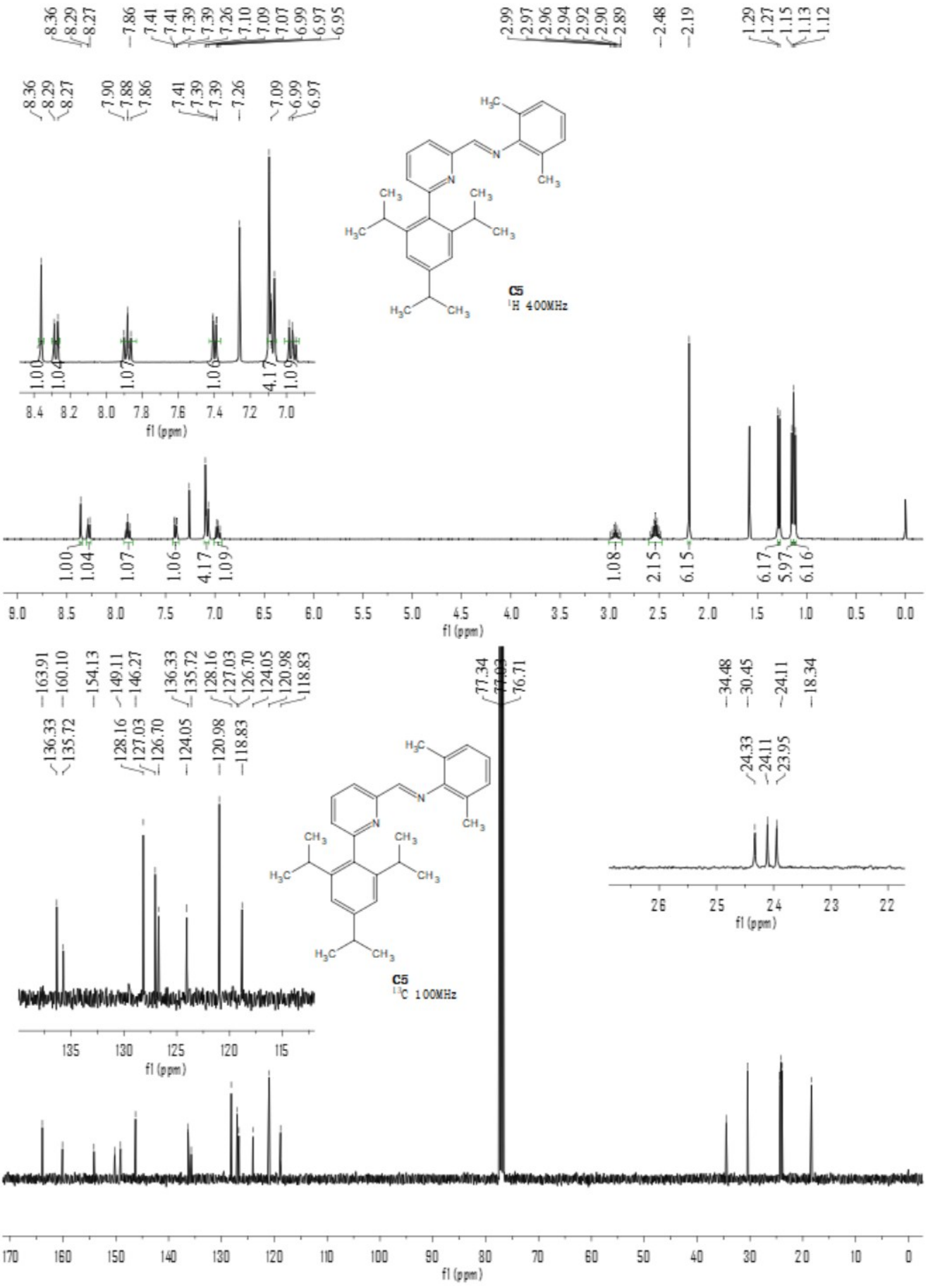
13C 100MHz
f1 (ppm)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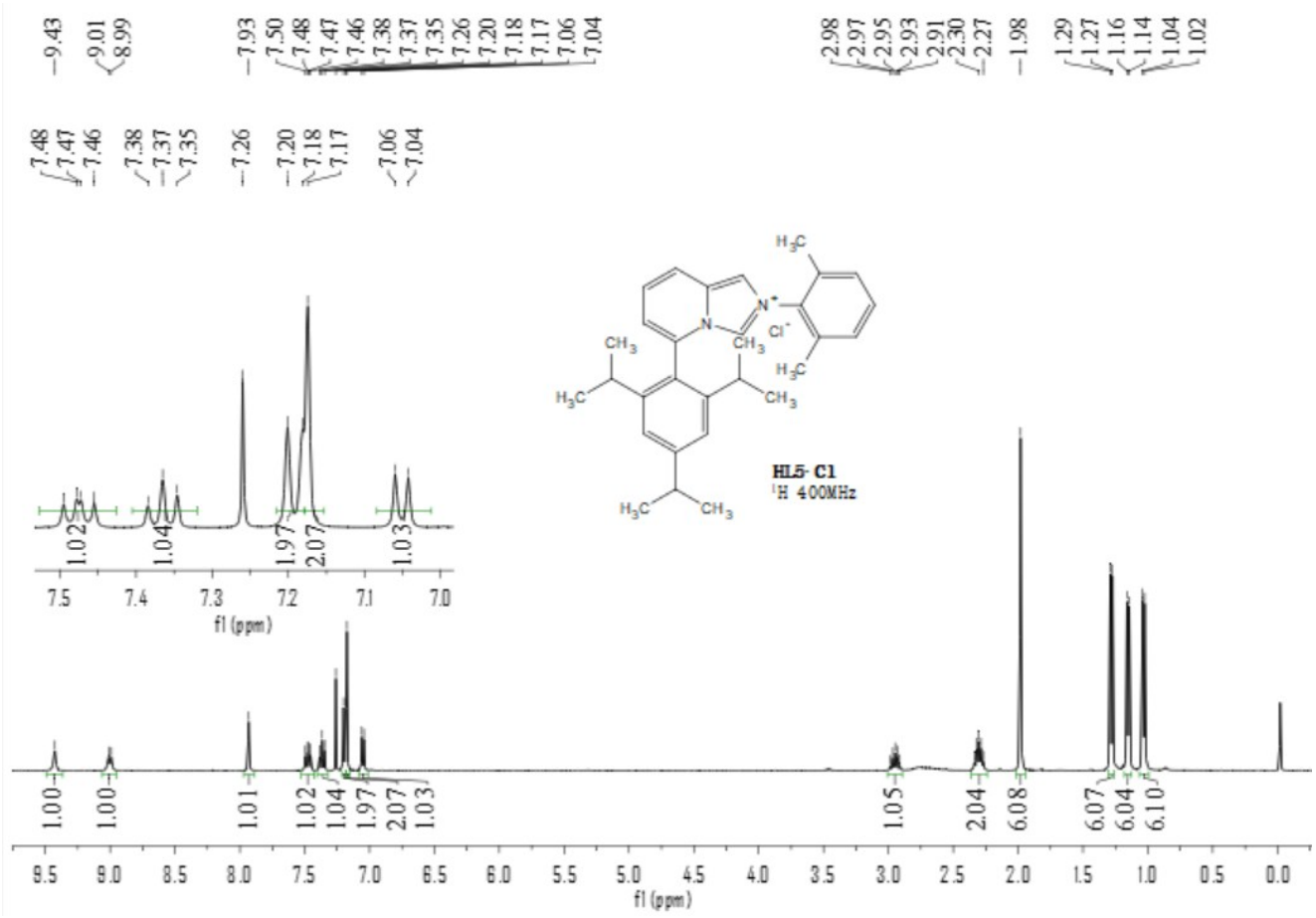
C5
13C 100MHz
f1 (ppm)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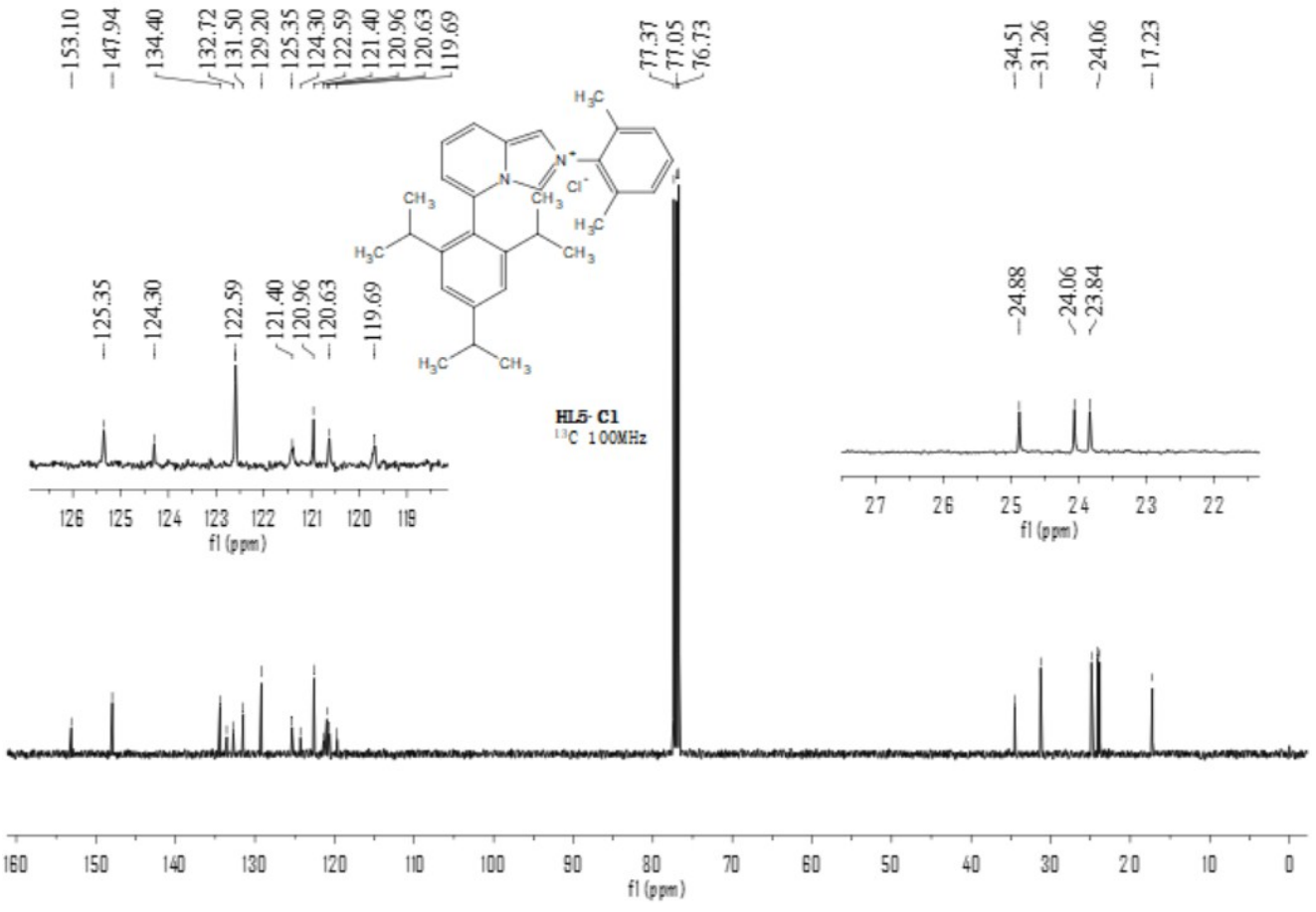
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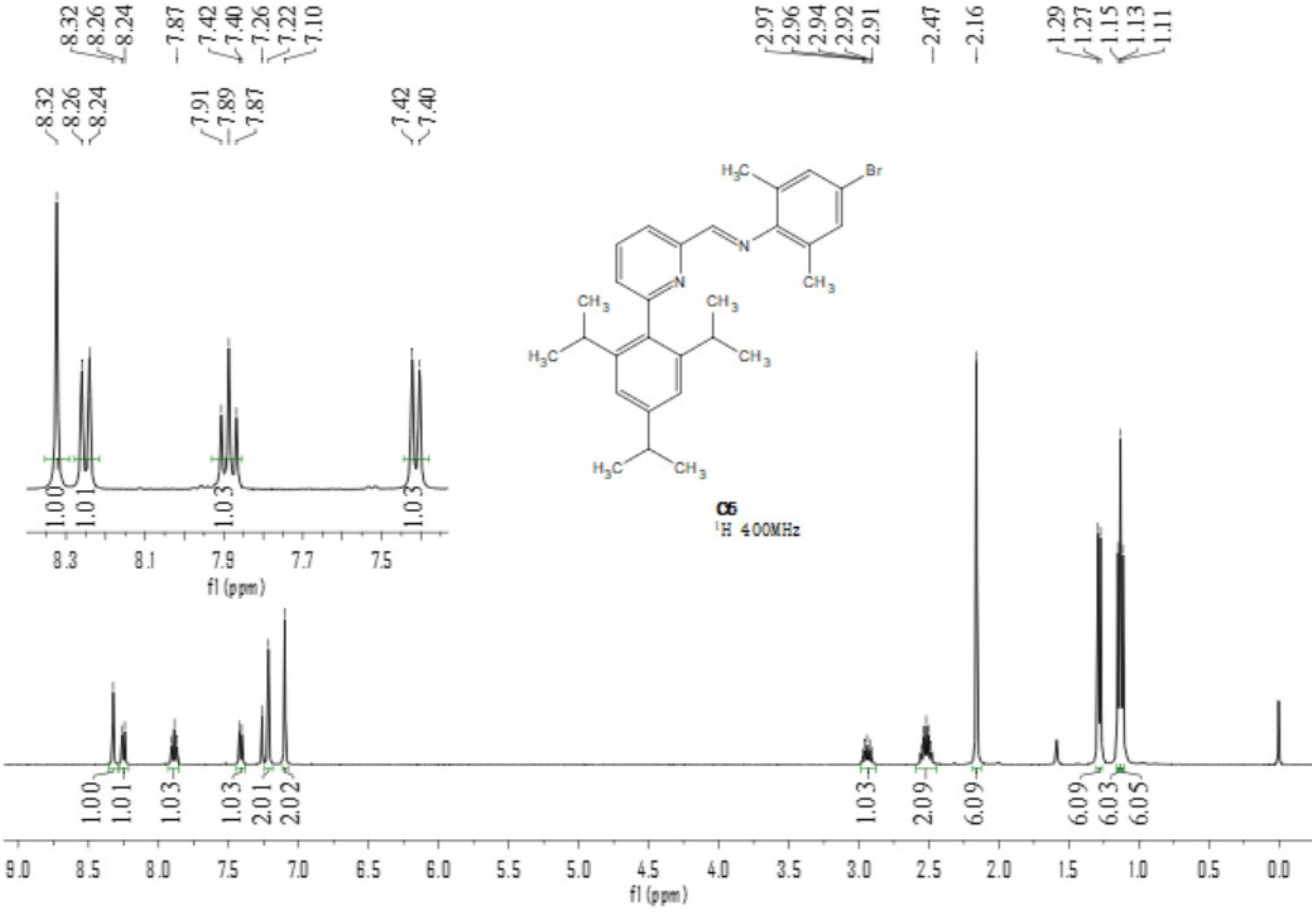
13C 100MHz
f1 (ppm)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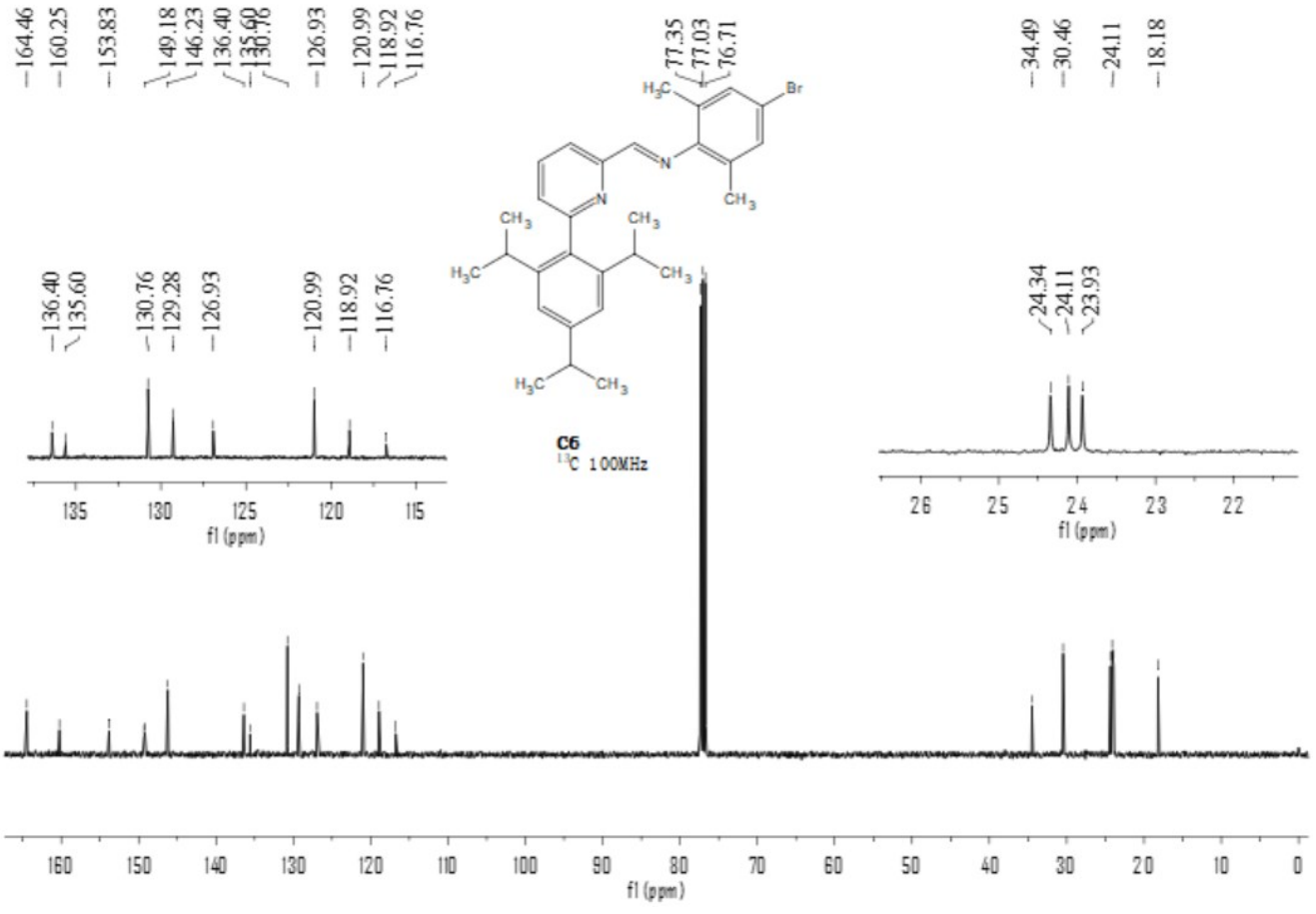
8.26
8.24
7.87
7.42
7.40
7.26
7.22
7.10
2.97
2.96
2.94
2.92
2.91
2.47
2.16
1.29
1.27
1.15
1.13
1.11
7.91
7.89
7.87
7.42
7.40
1.00
1.01
1.03
1.03
2.01
2.02
6.09
6.03
6.05
f1 (ppm)
Br
N
CH3
H3C
Cб
1H 400MHz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130.76
126.93
120.99
118.92
116.76
77.35
77.03
76.71
34.49
30.46
24.11
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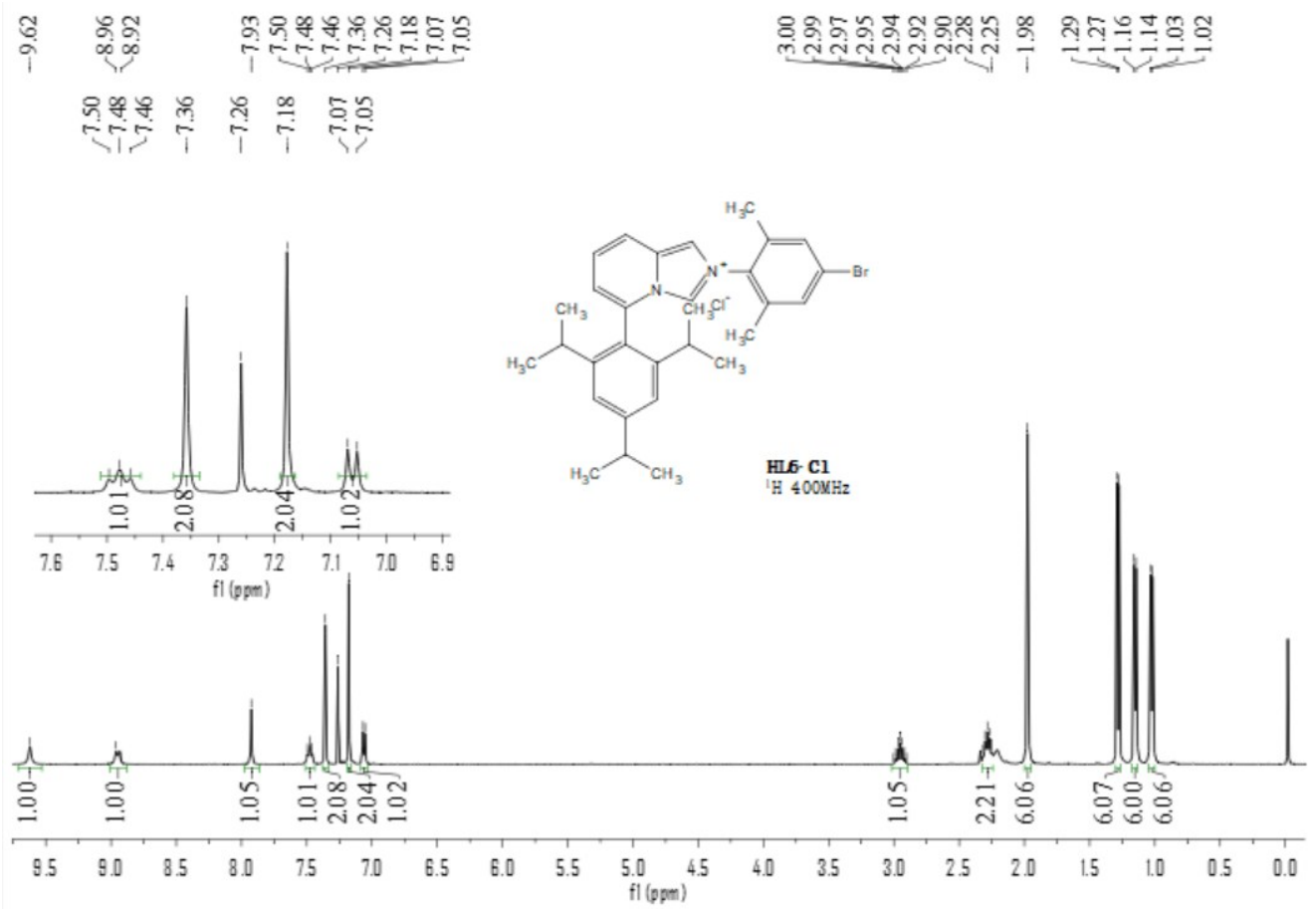
24.34
24.11
23.93
Br
N
CH3
H3C
Cб
13C 100MHz
f1 (ppm)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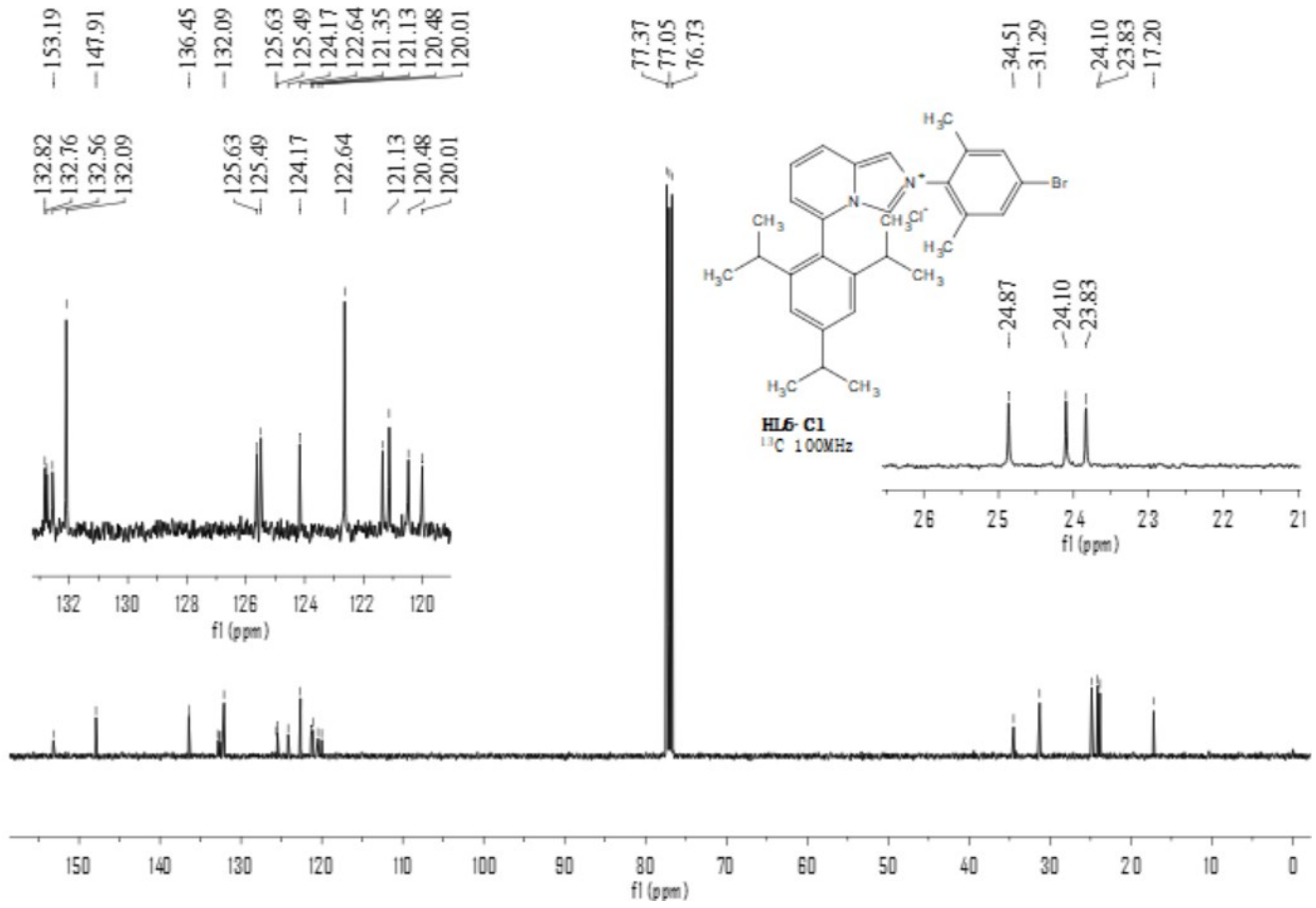
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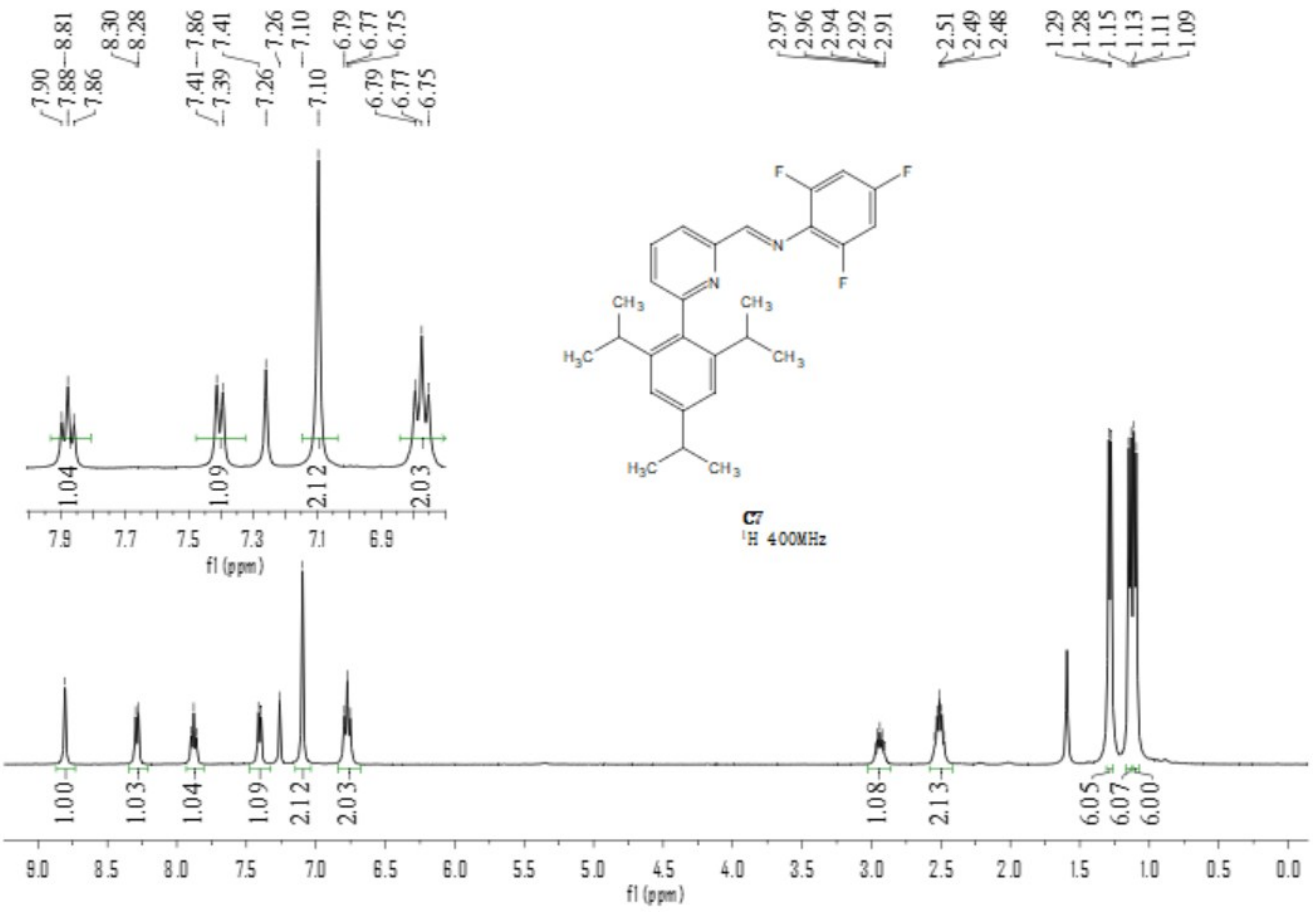
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7.41
7.26
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6.77
6.75
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2.96
2.94
2.92
2.91
2.51
2.49
2.48
1.29
1.28
1.15
1.13
1.11
1.09
1.04
1.09
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2.03
f1 (ppm)
C7
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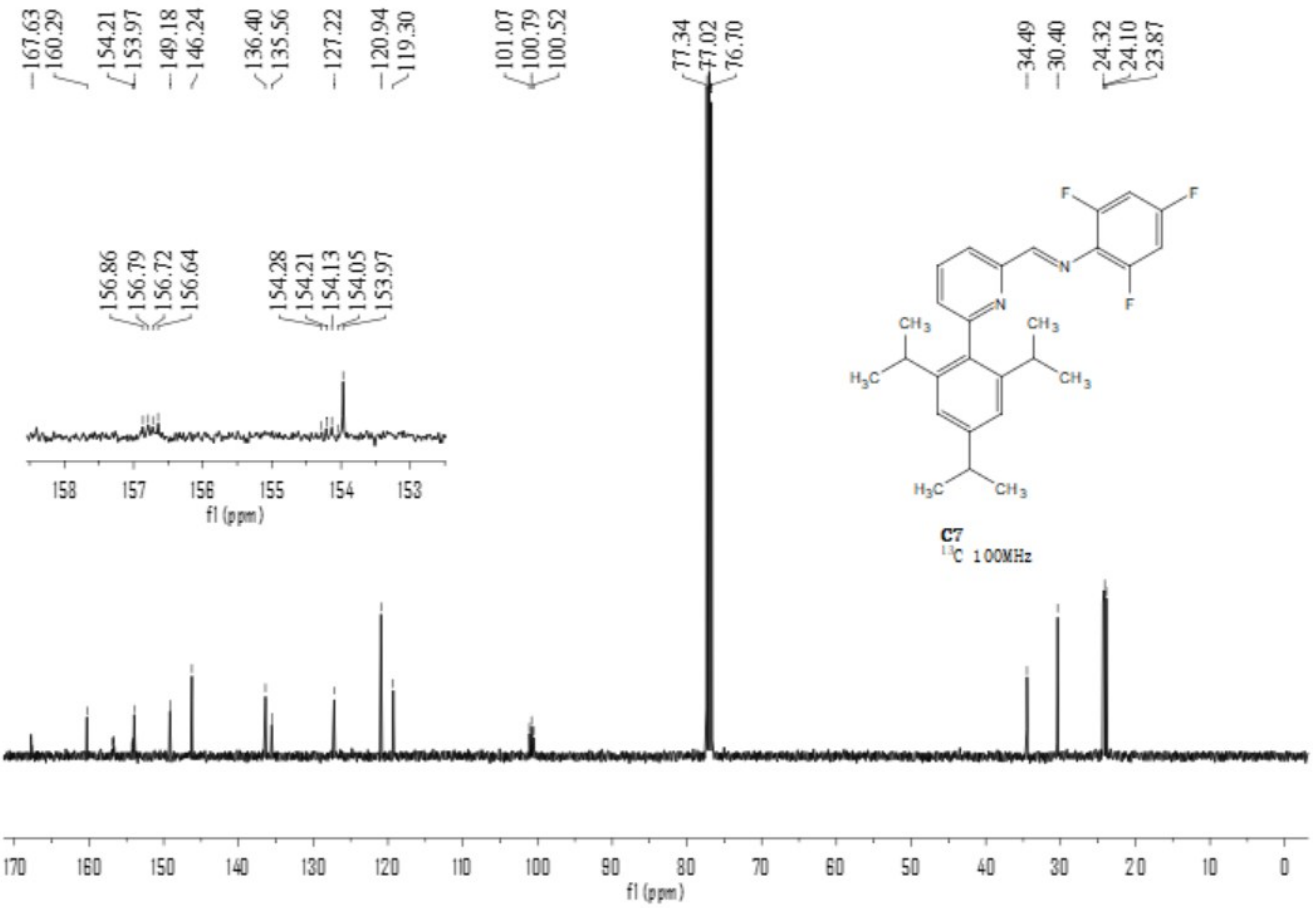
6.00
f1 (ppm)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76.70
34.49
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156.79
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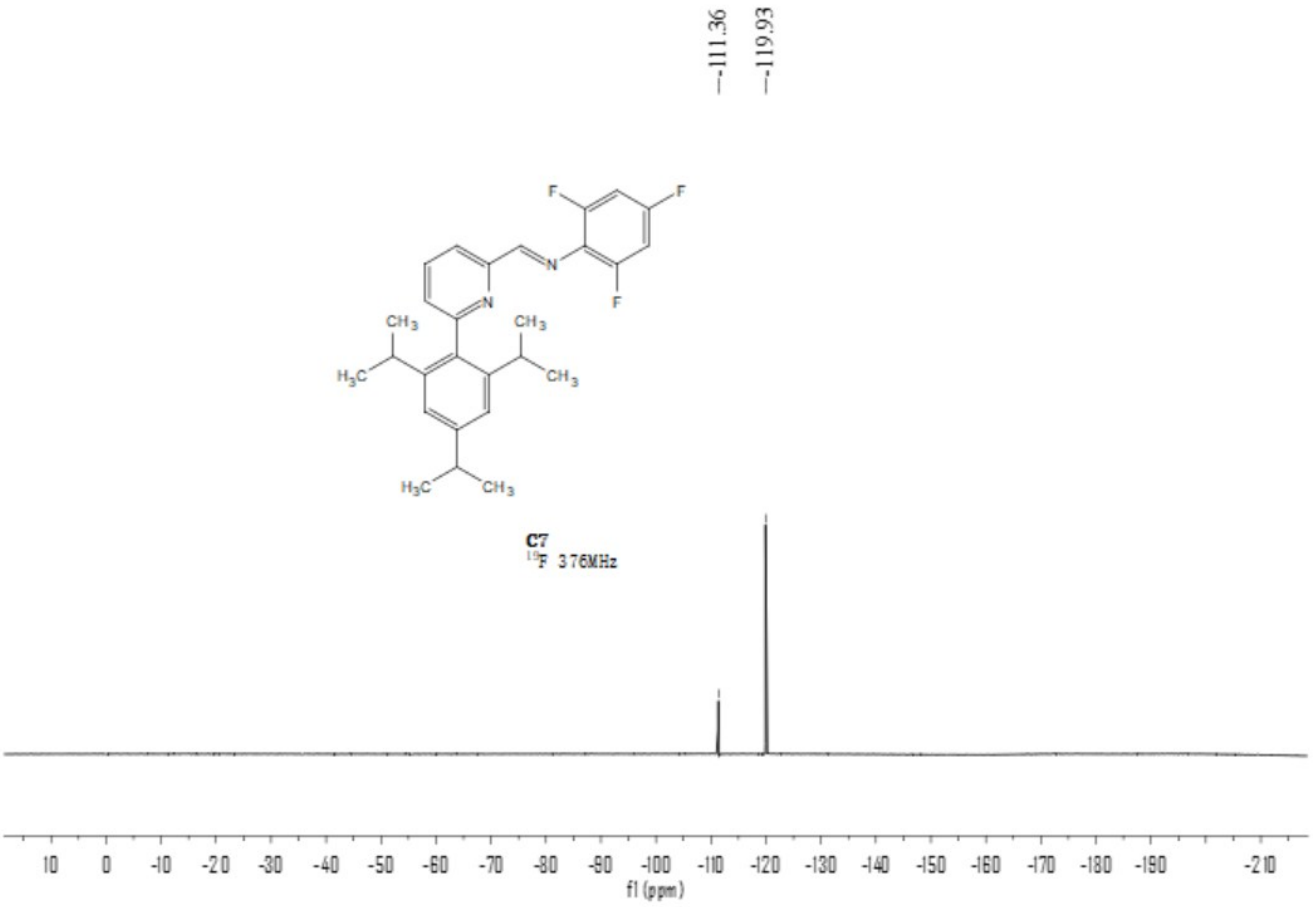
154.05
153.97
f1 (ppm)
C7
13C 100MHz
f1 (ppm)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C7
19F 376MHz
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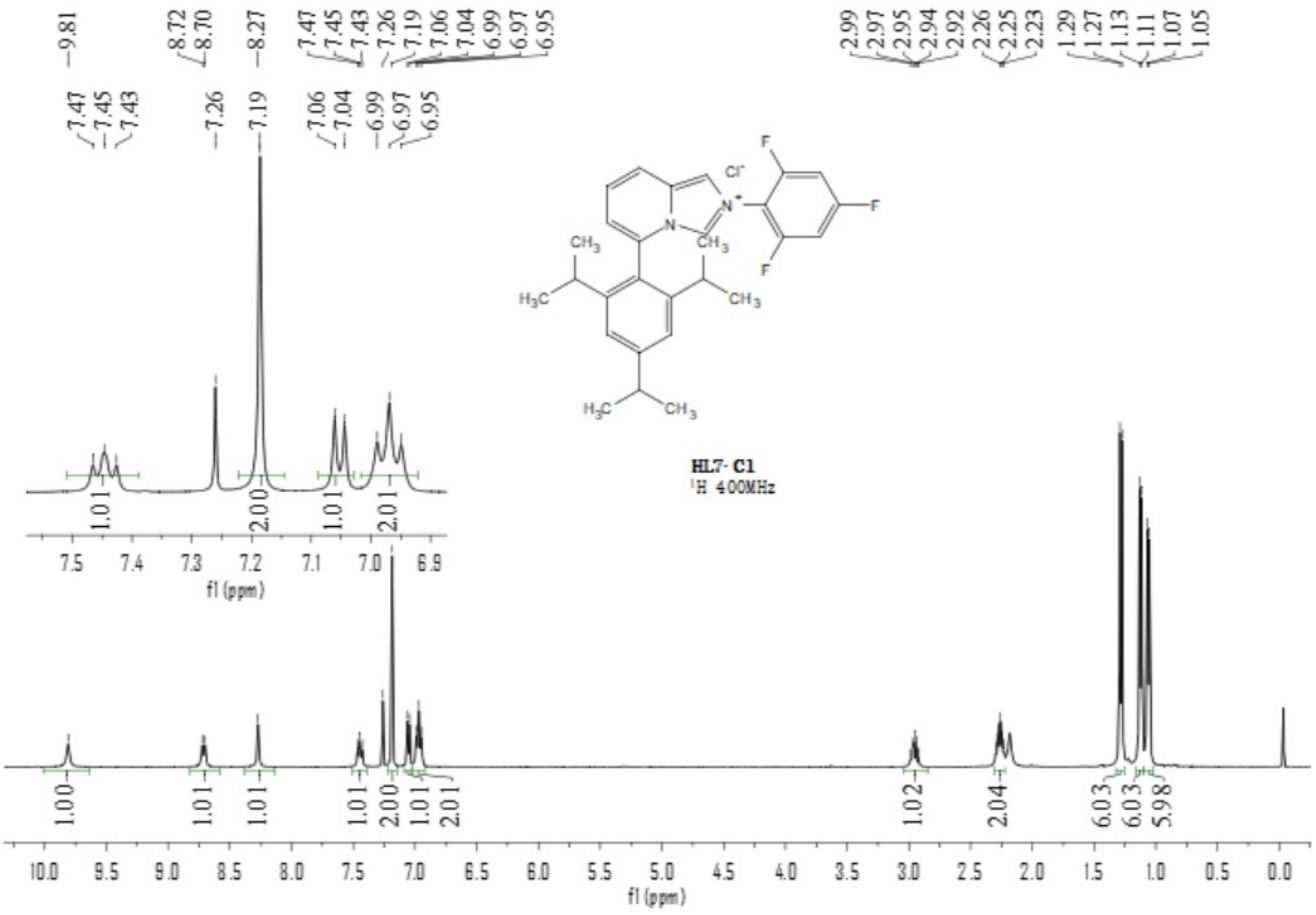
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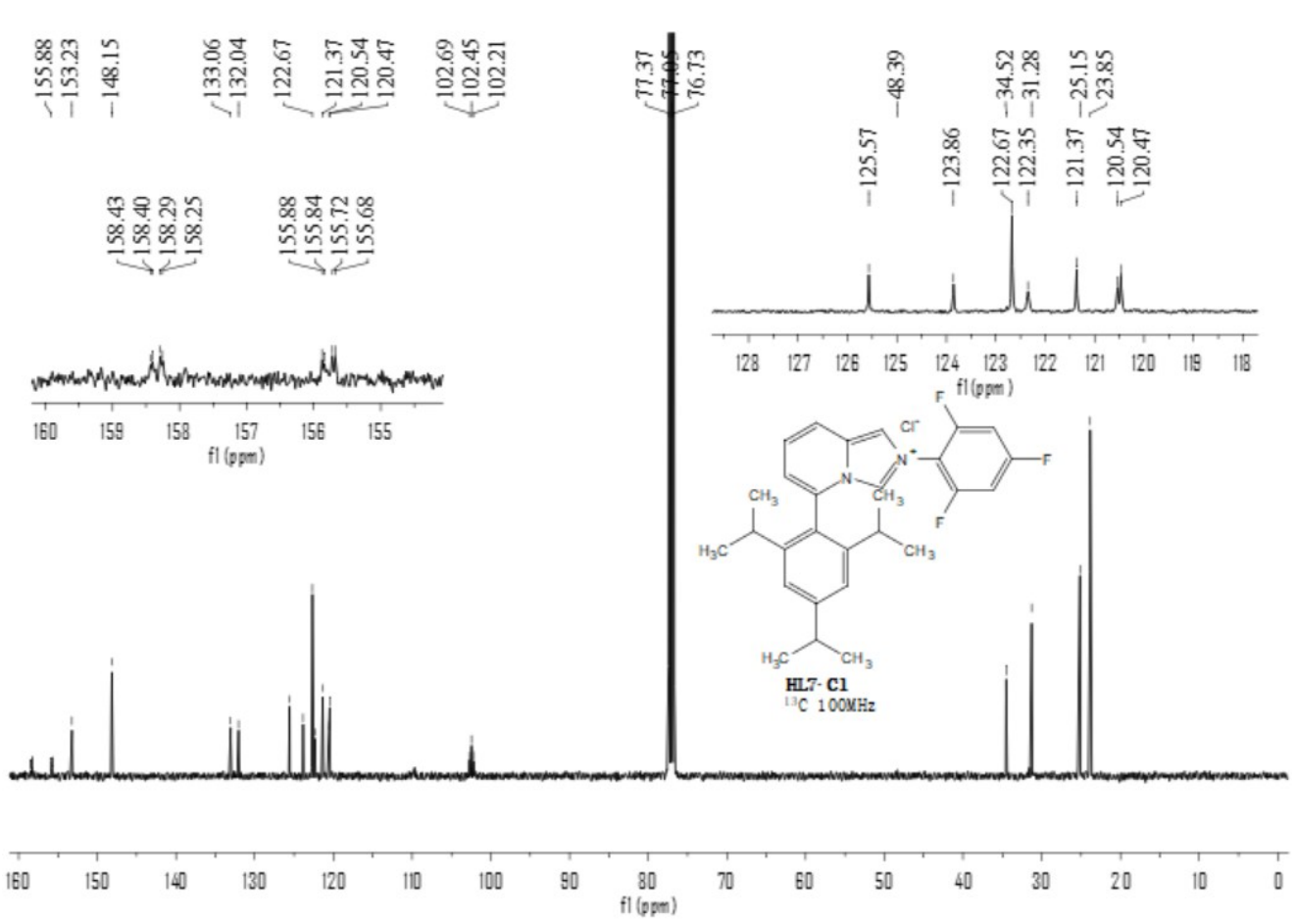
1H 400MHz
f1 (ppm)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120.47
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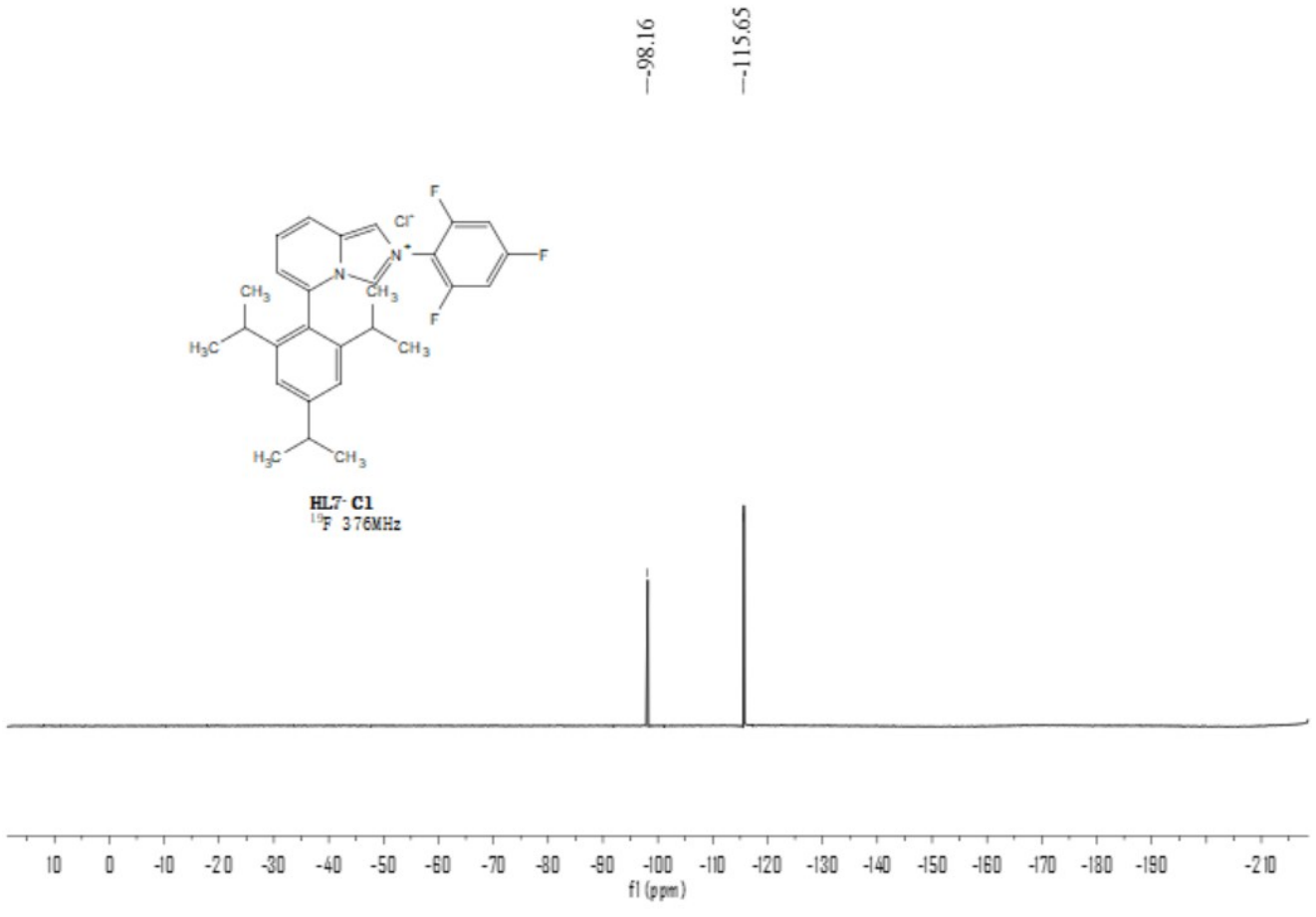
155.68
f1 (ppm)
HL7- C1
13C 100MHz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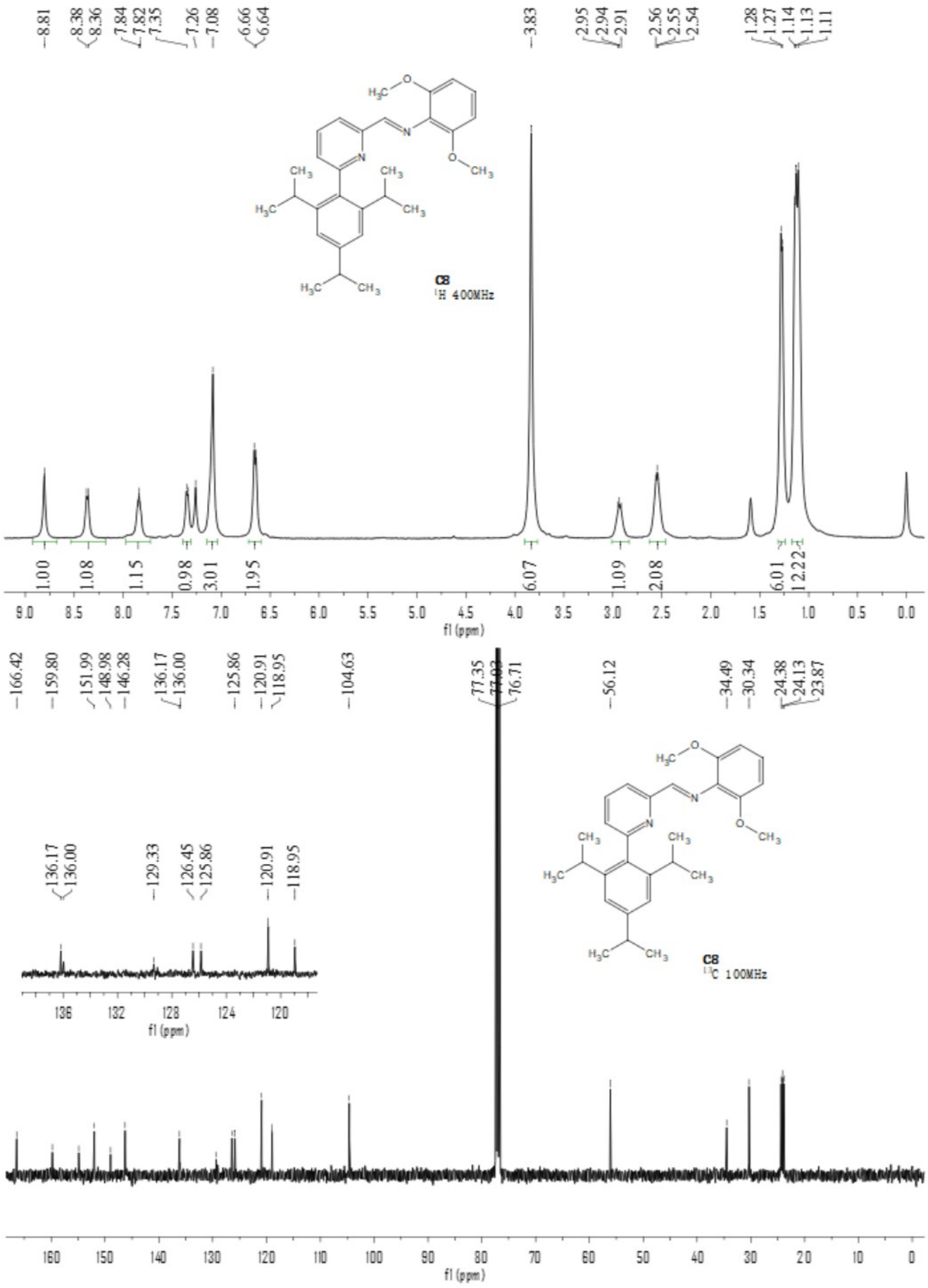
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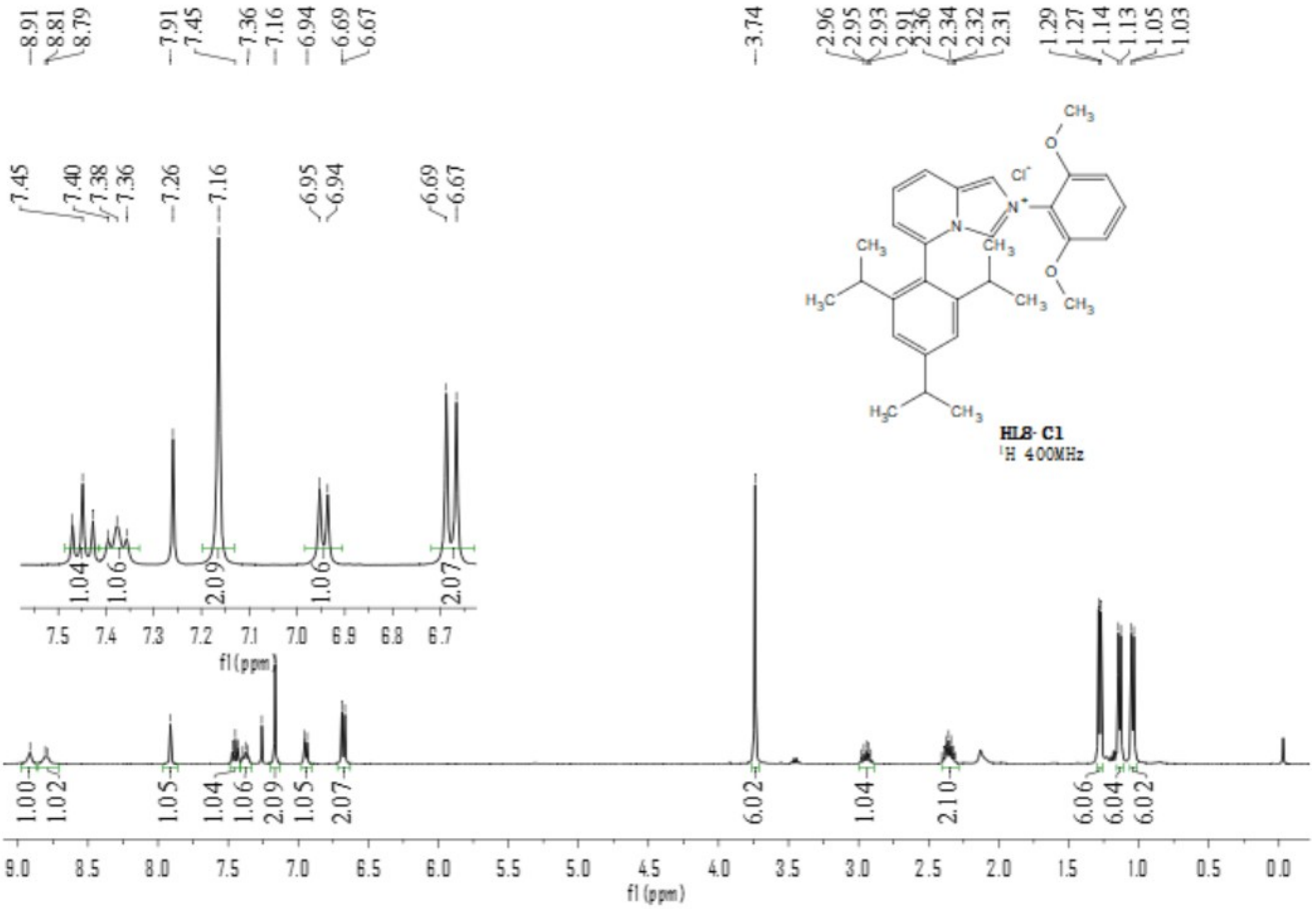
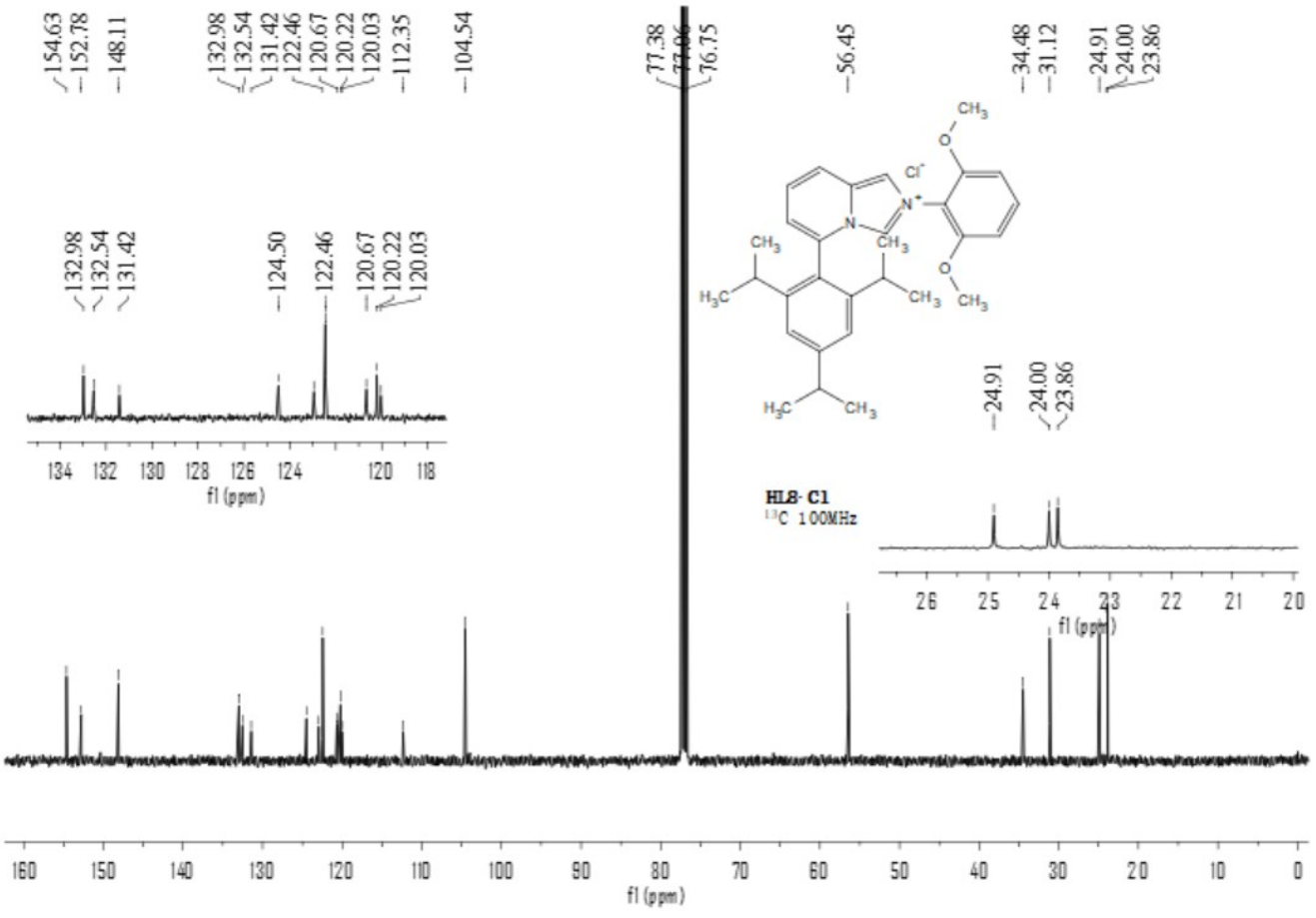
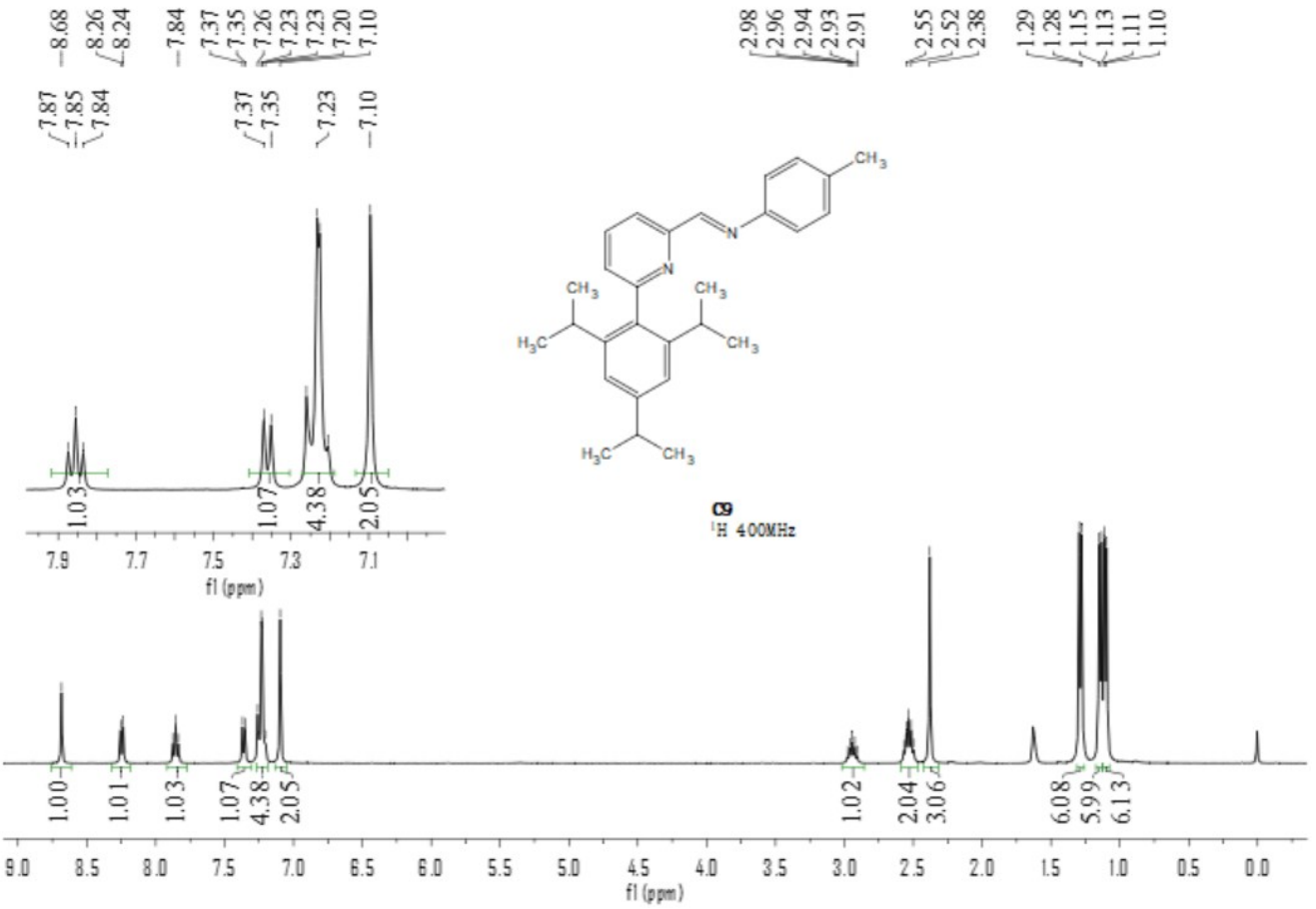
7.08
6.66
6.64
3.83
2.95
2.94
2.91
2.56
2.55
2.54
1.28
1.27
1.14
1.13
1.11
C8
1H 400MHz
1.00
1.08
1.15
0.98
3.01
1.95
6.07
1.09
2.08
6.01
12.22
f1 (ppm)
166.42
159.80
151.99
148.98
146.28
136.17
136.00
125.86
120.91
118.95
104.63
77.35
77.03
76.71
56.12
34.49
30.34
24.38
24.13
23.87
129.33
126.45
C8
13C 100MHz
f1 (ppm)


HL8-Cl
1H 400MHz
f1 (ppm)


HL8-Cl
13C 100MHz
f1 (ppm)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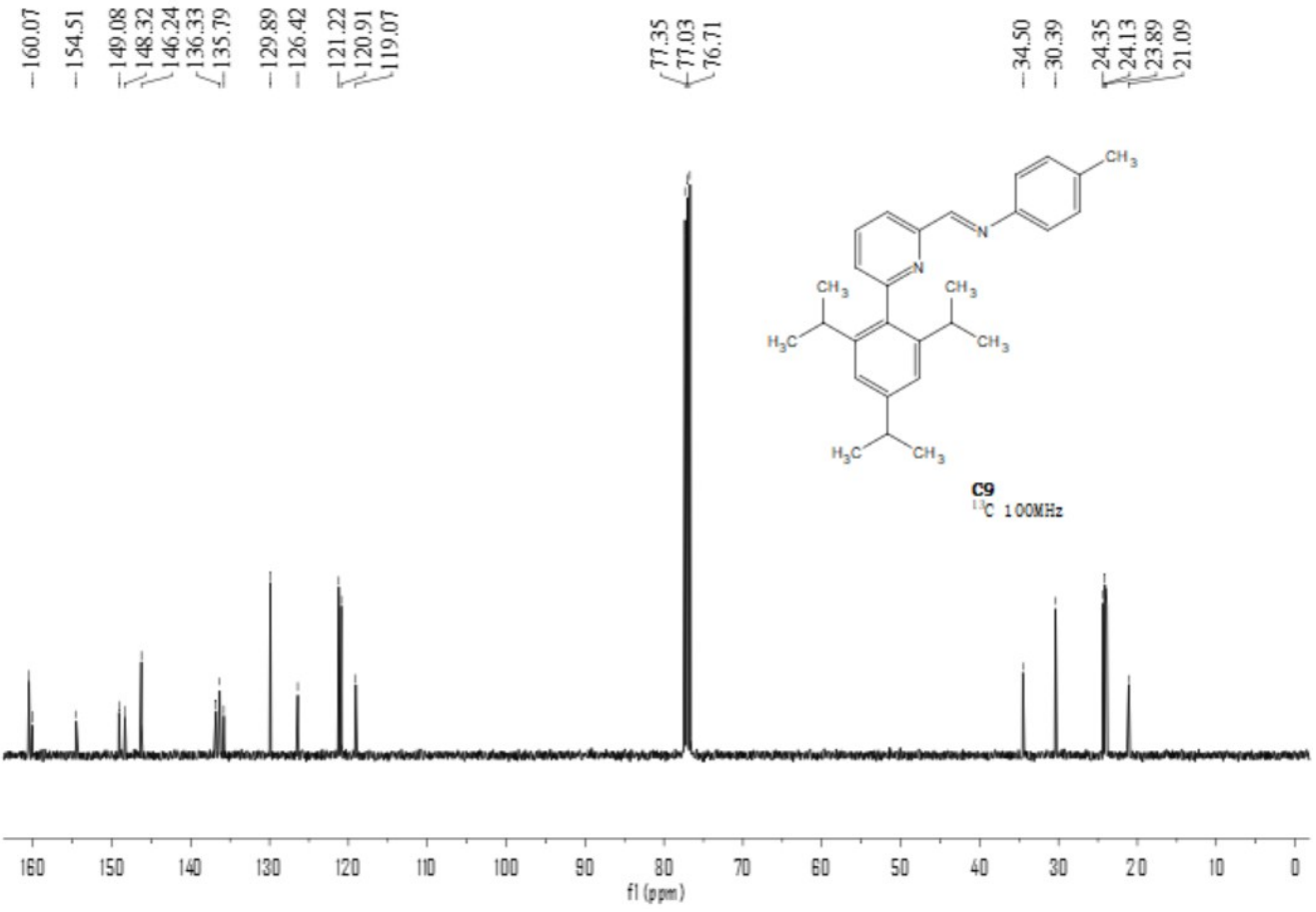
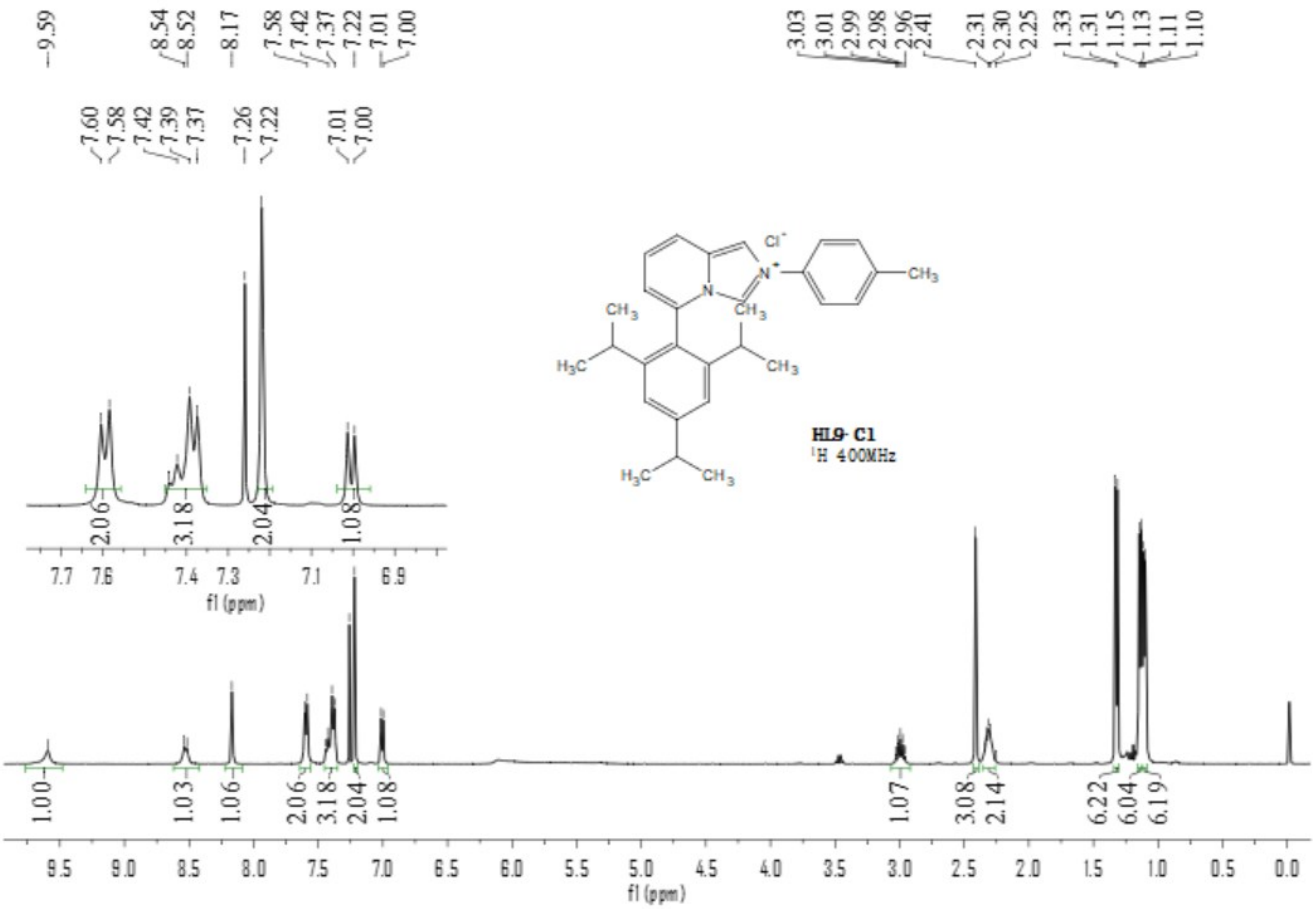
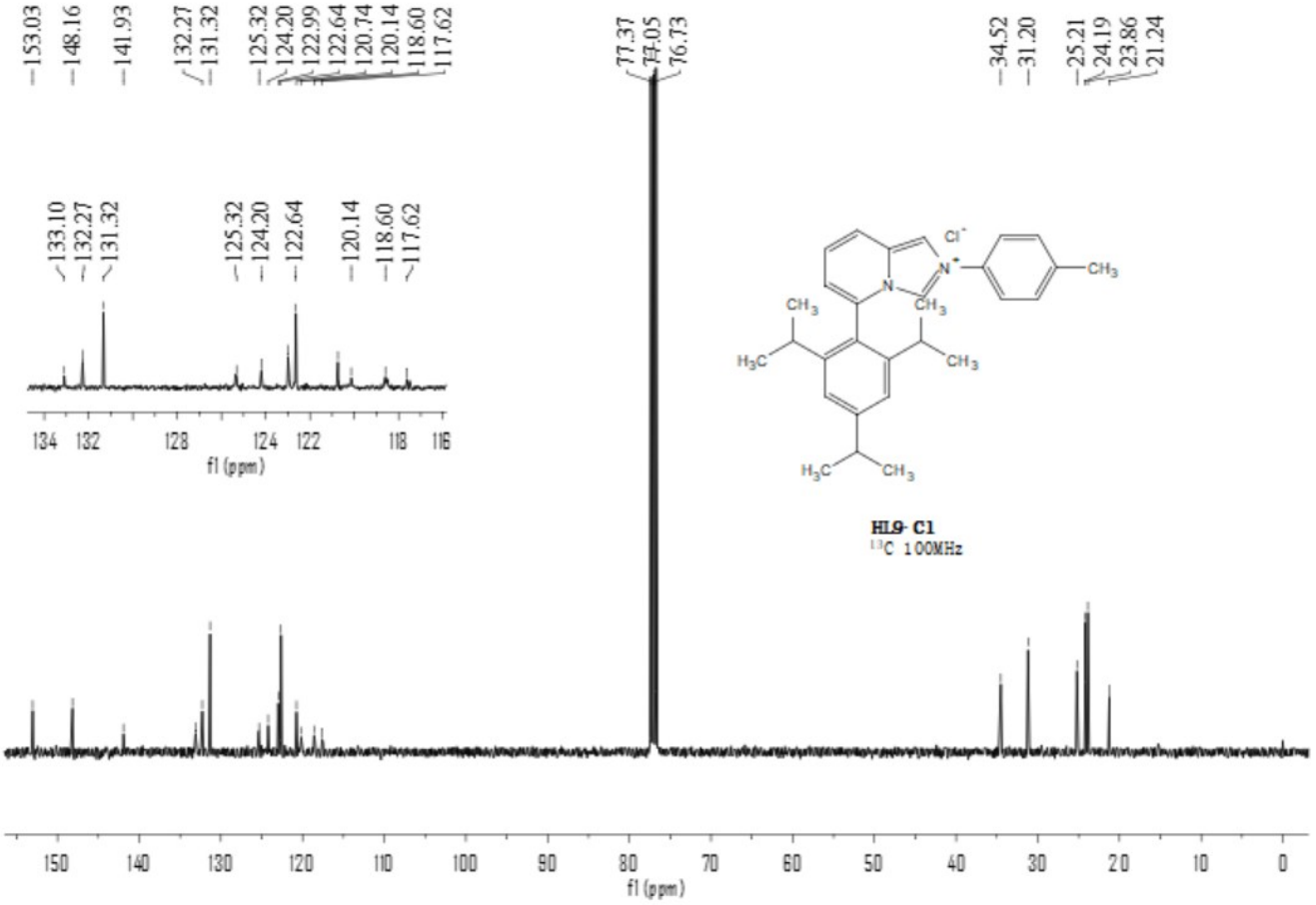
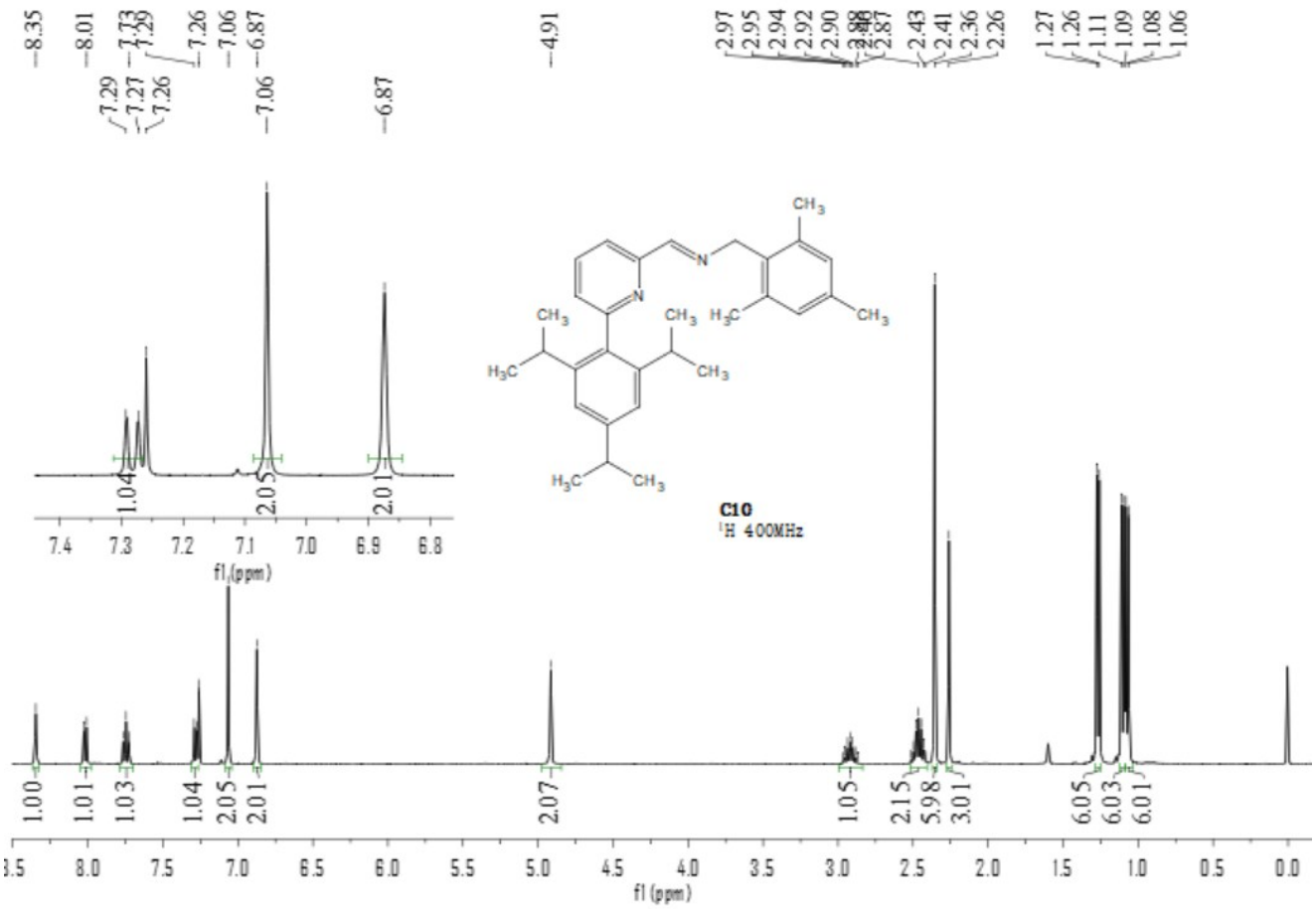
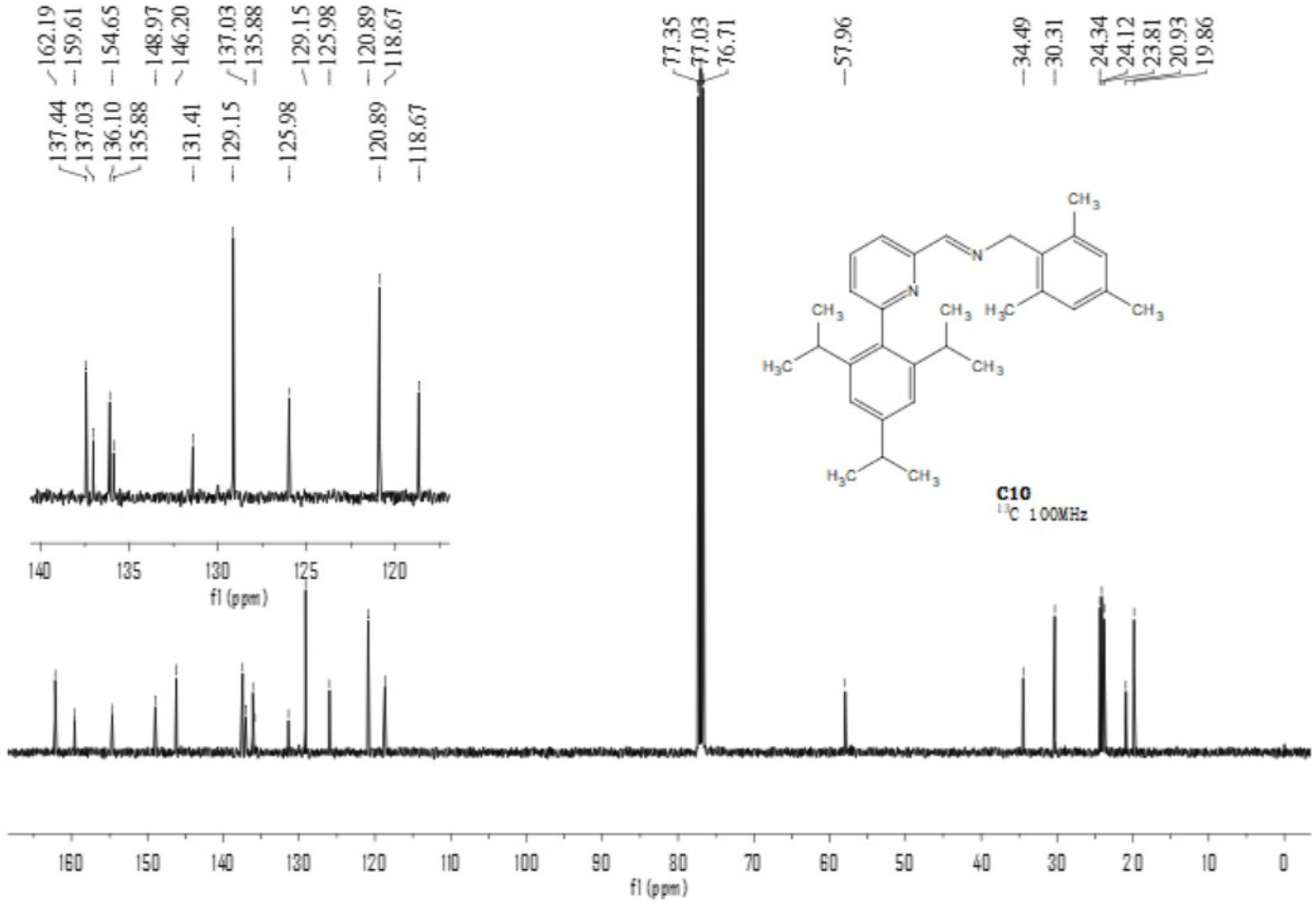
8.26
8.24
7.84
7.37
7.35
7.26
7.23
7.23
7.20
7.10
7.87
7.85
7.84
7.37
7.35
7.23
7.10
2.98
2.96
2.94
2.93
2.91
2.55
2.52
2.38
1.29
1.28
1.15
1.13
1.11
1.10
CH3
N
N
CH3
CH3
H3C
CH3
H3C
CH3
C9
1H 400MHz
1.03
1.07
4.38
2.05
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
1.00
1.01
1.03
1.07
4.38
2.05
1.02
2.04
3.06
6.08
5.99
6.13
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)

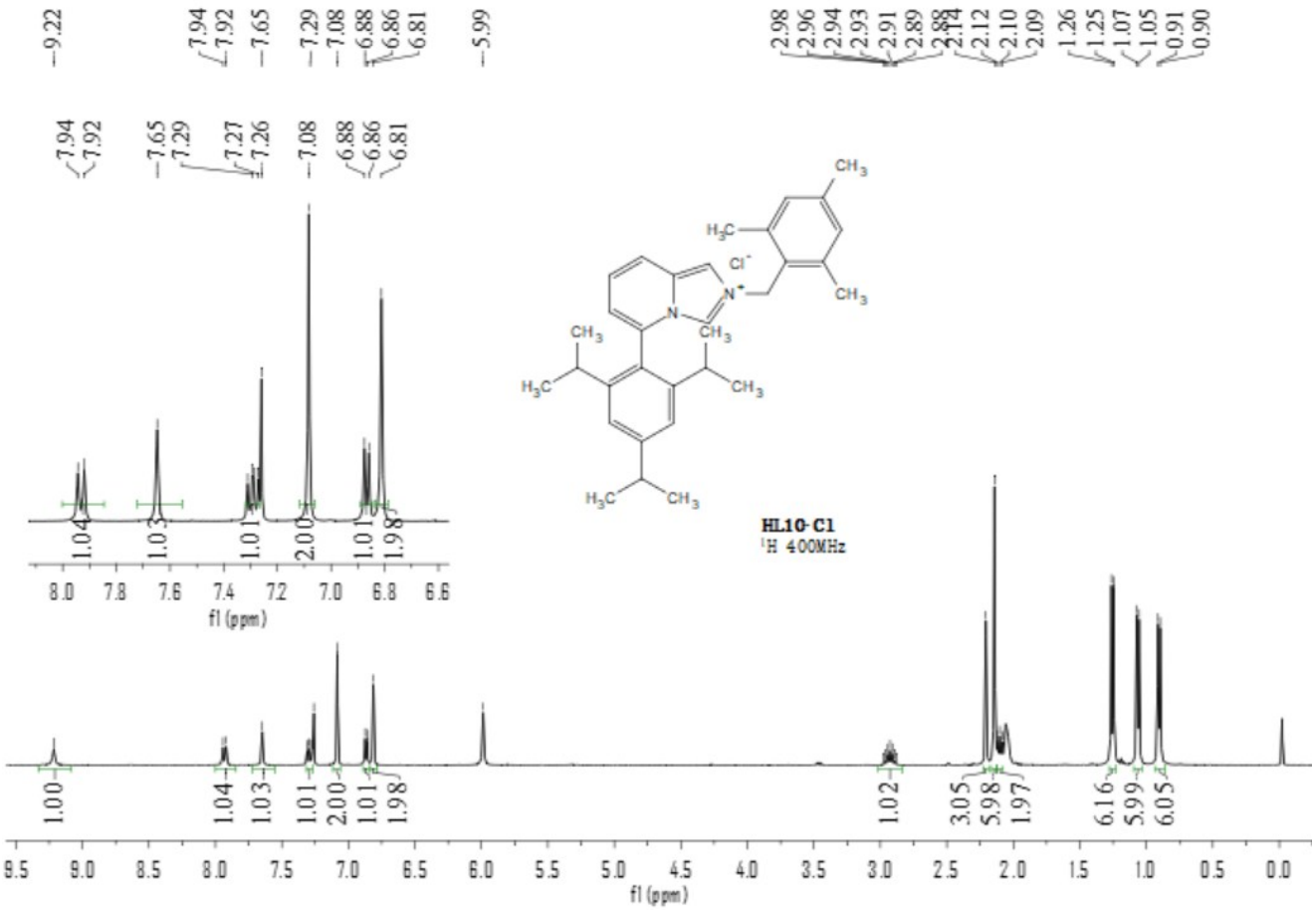

160.07
154.51
149.08
148.32
146.24
136.33
135.79
129.89
126.42
121.22
120.91
119.07
77.35
77.03
76.71
34.50
30.39
24.35
24.13
23.89
21.09
CH3
N
N
CH3
CH3
H3C
CH3
H3C
CH3
C9
13C 100MHz
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

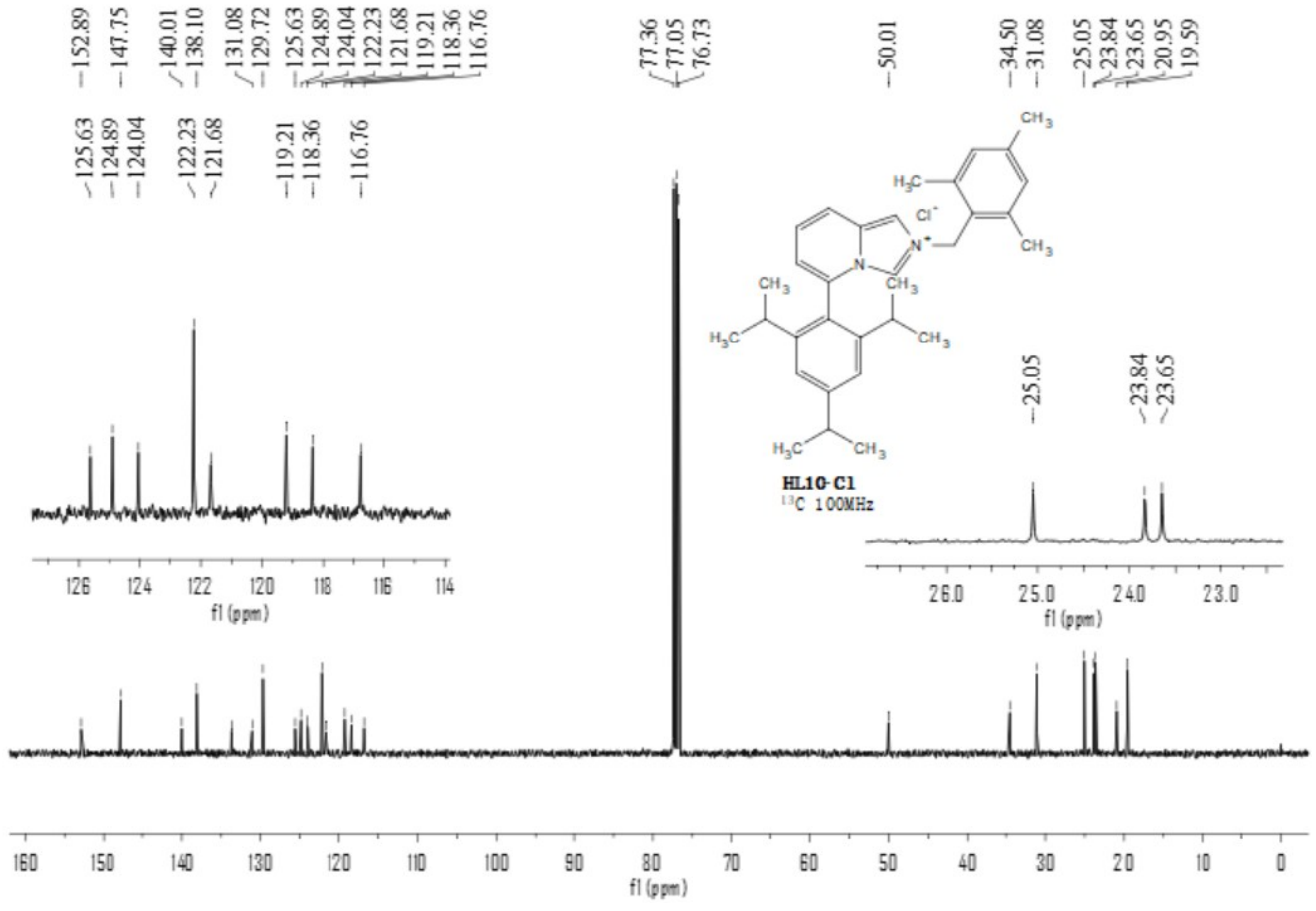

HL9-C1
1H 400MHz
f1 (ppm)

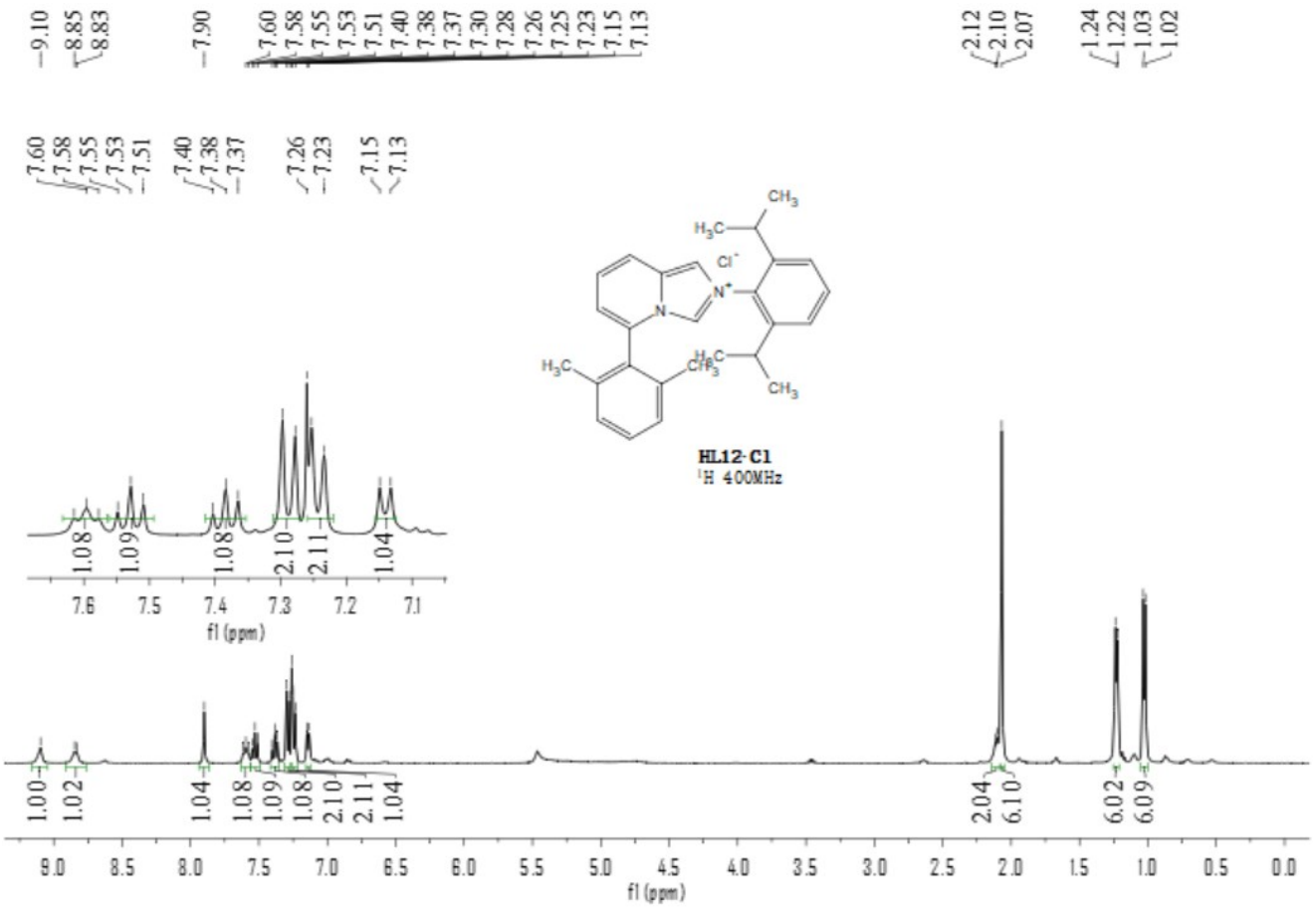

HL9-C1
13C 100MHz
f1 (ppm)

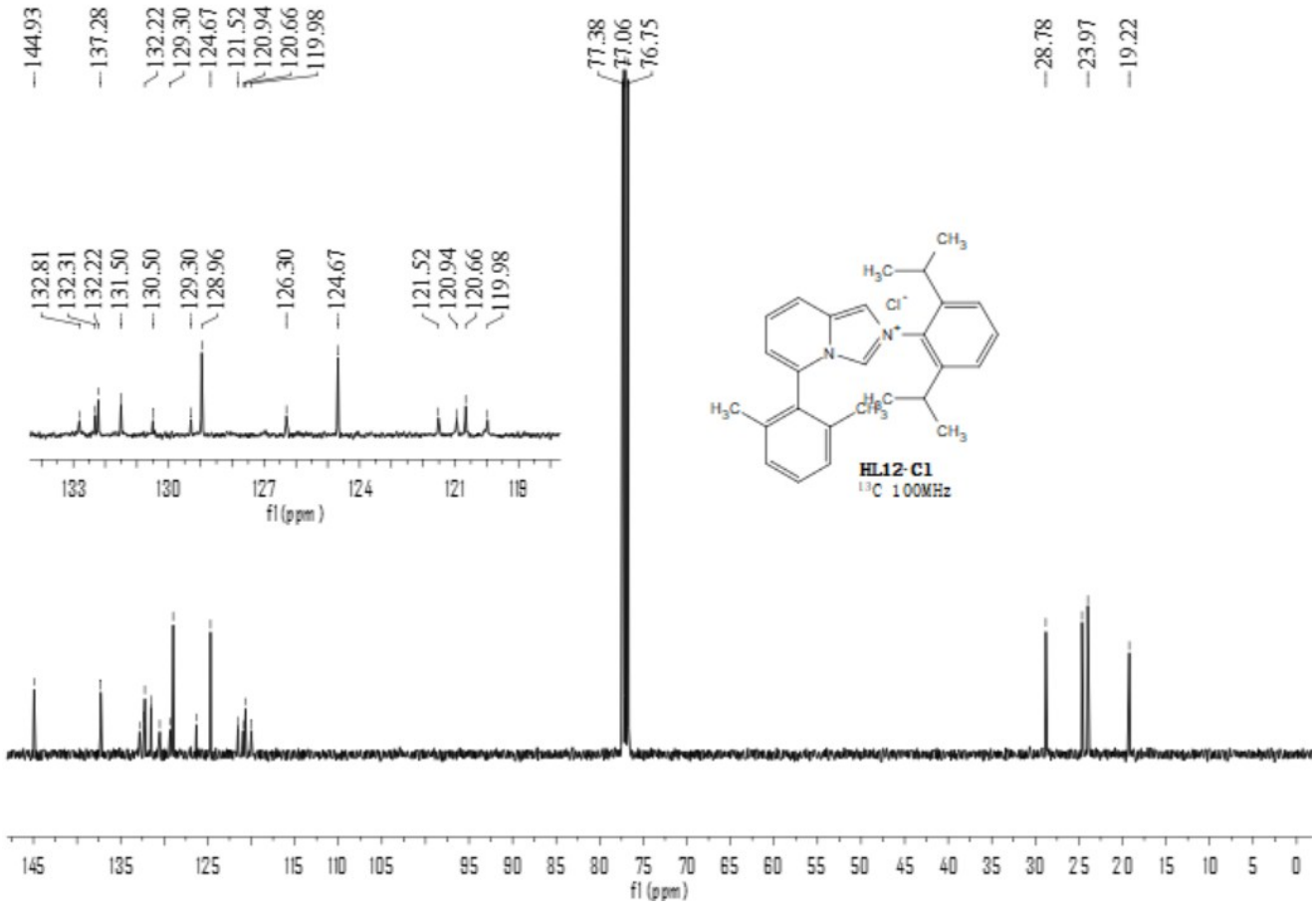

C10
1H 400MHz
f1 (ppm)


C10
13C 100MHz
f1 (ppm)

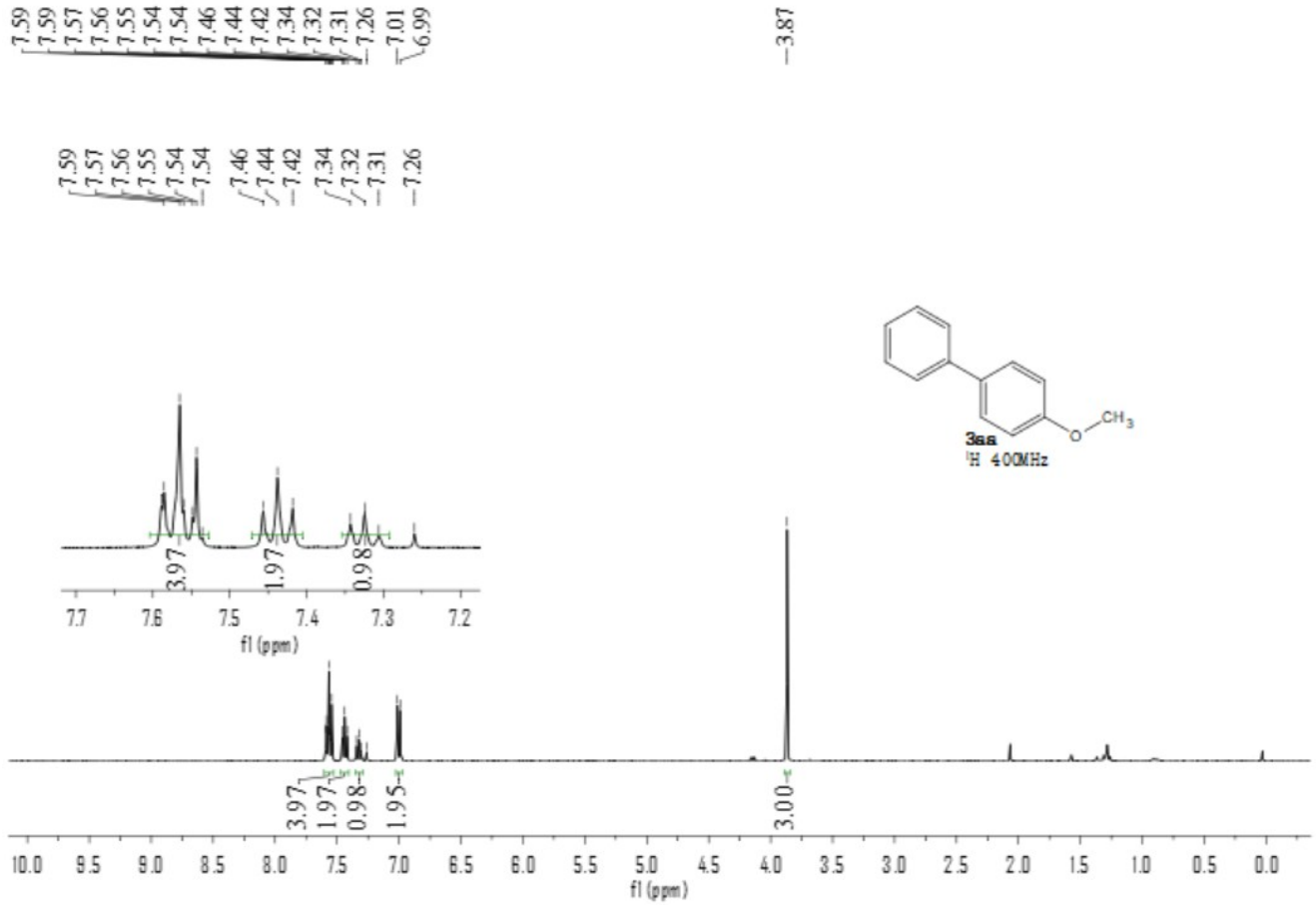

HL10-Cl
1H 400MHz
f1 (ppm)

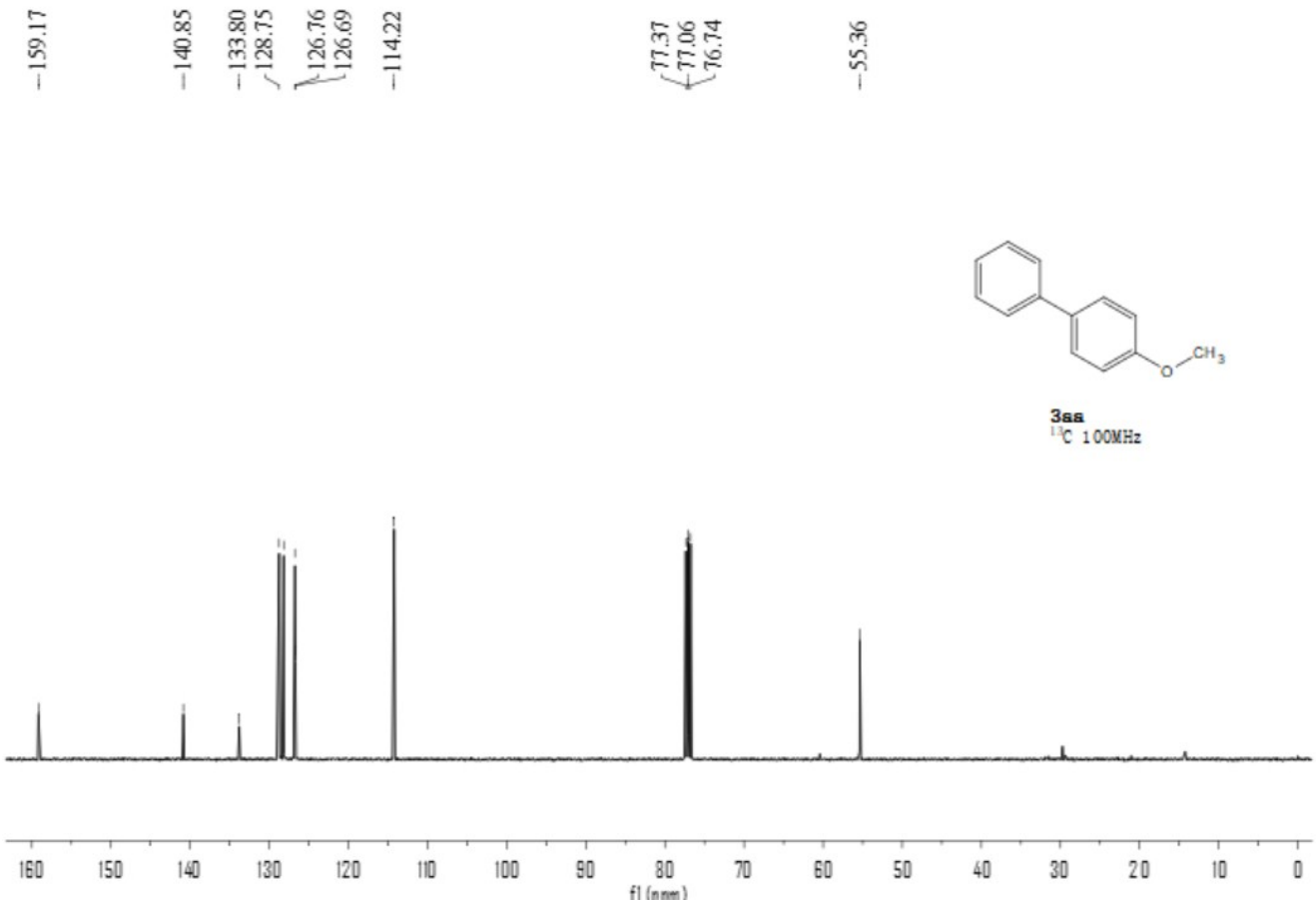

HL10-Cl
13C 100MHz
f1 (ppm)

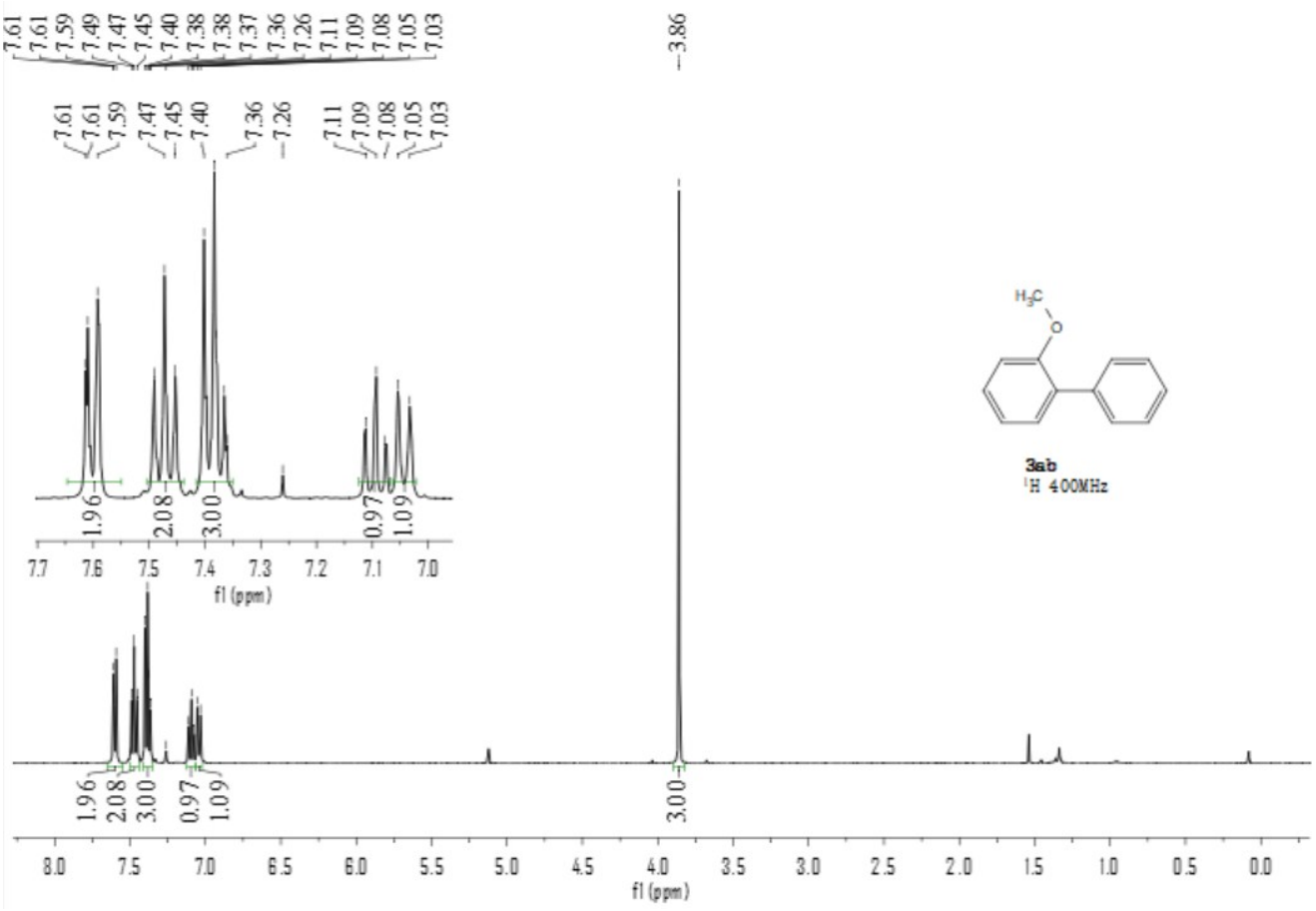

HL12-Cl
1H 400MHz
f1 (ppm)

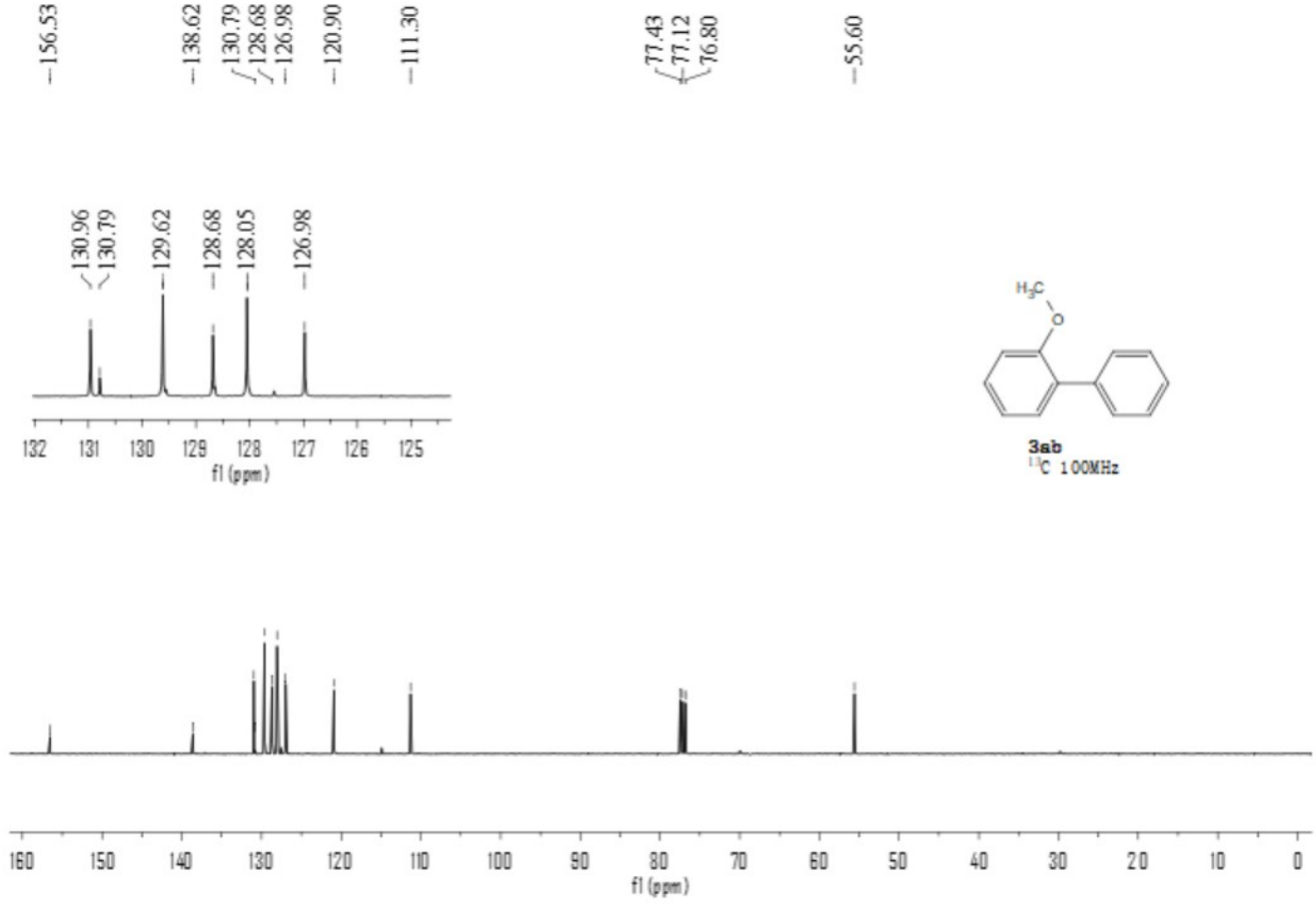

HL12-Cl
13C 100MHz
f1 (ppm)

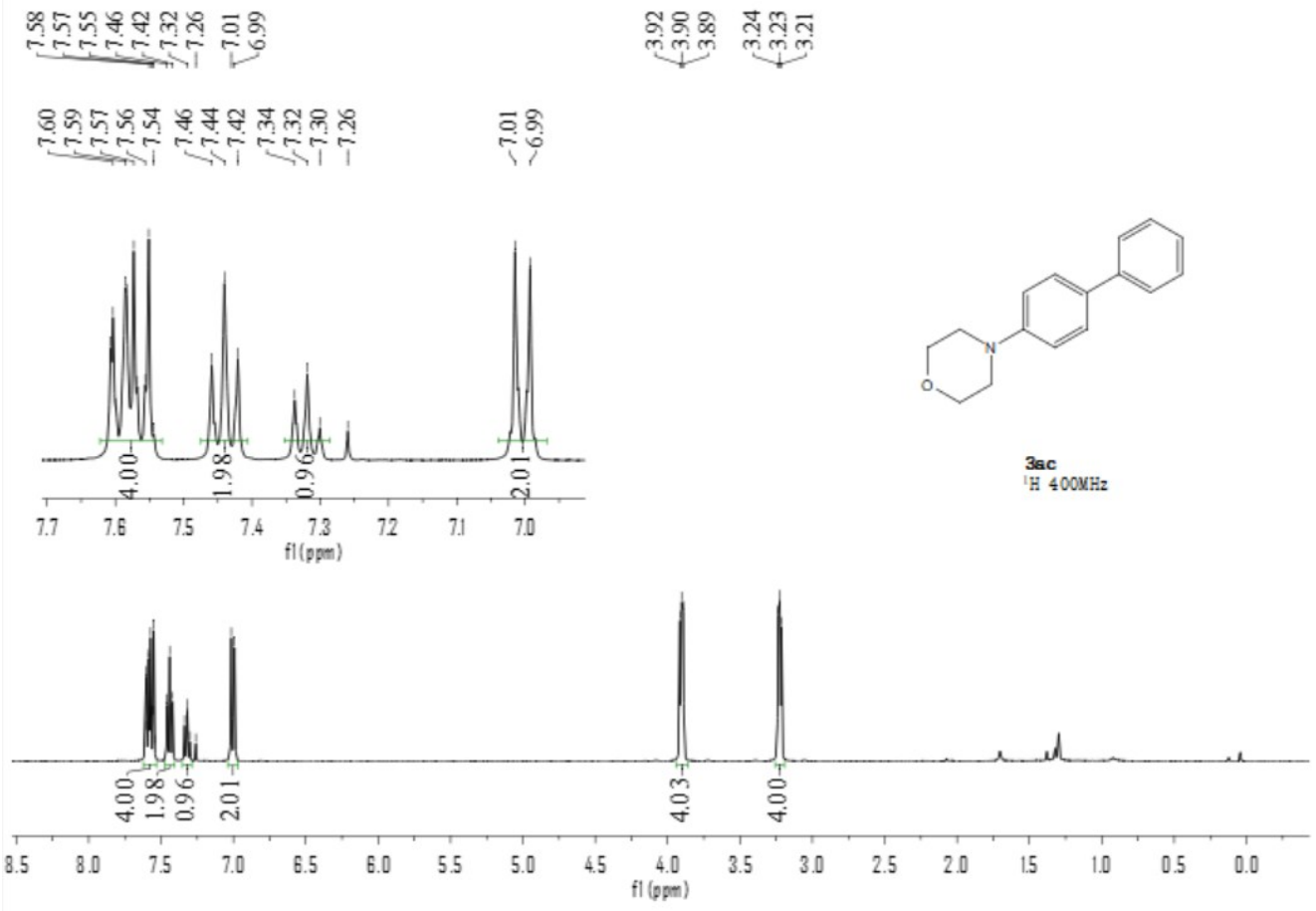
IX. NMR spectra of coupling products

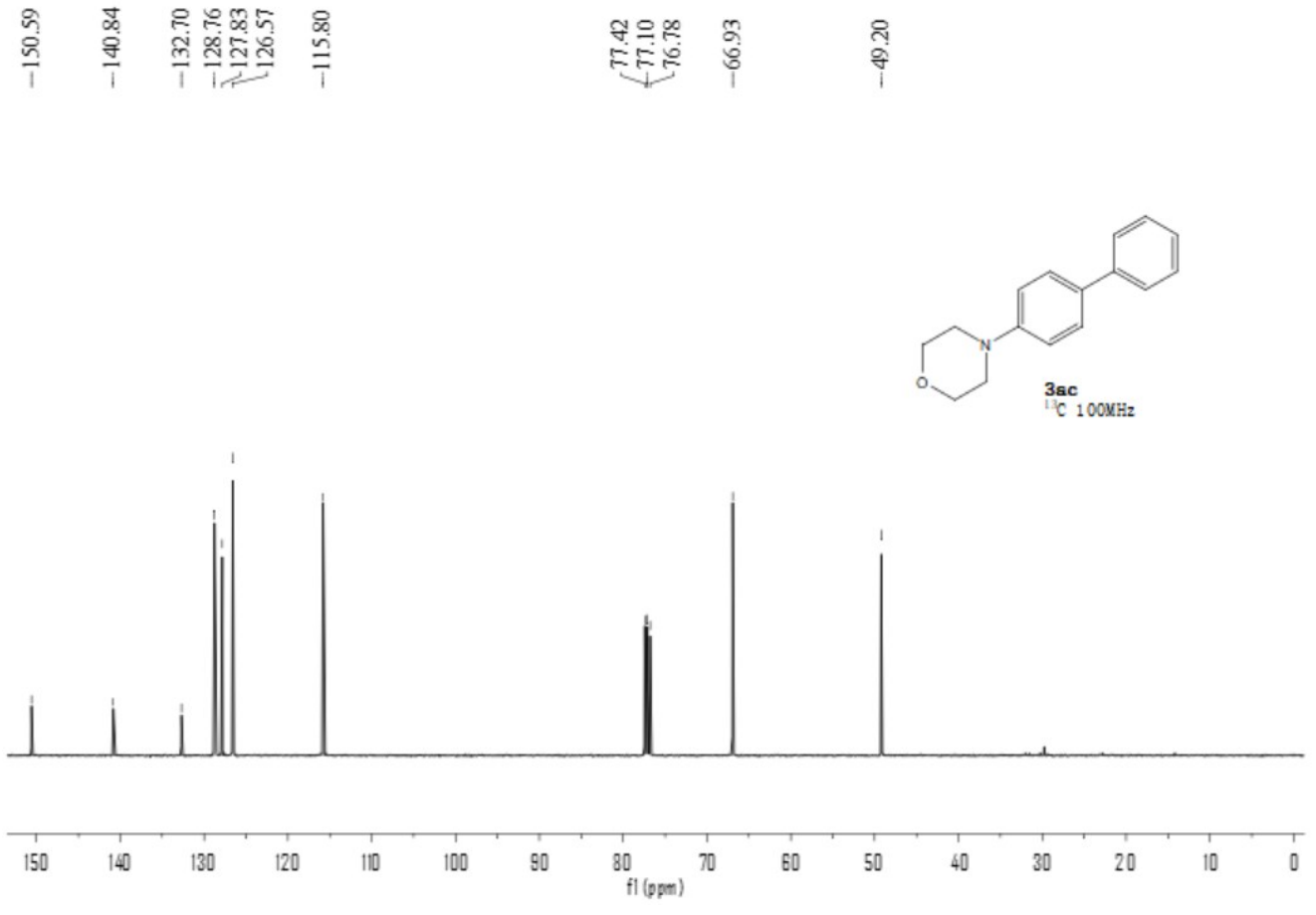


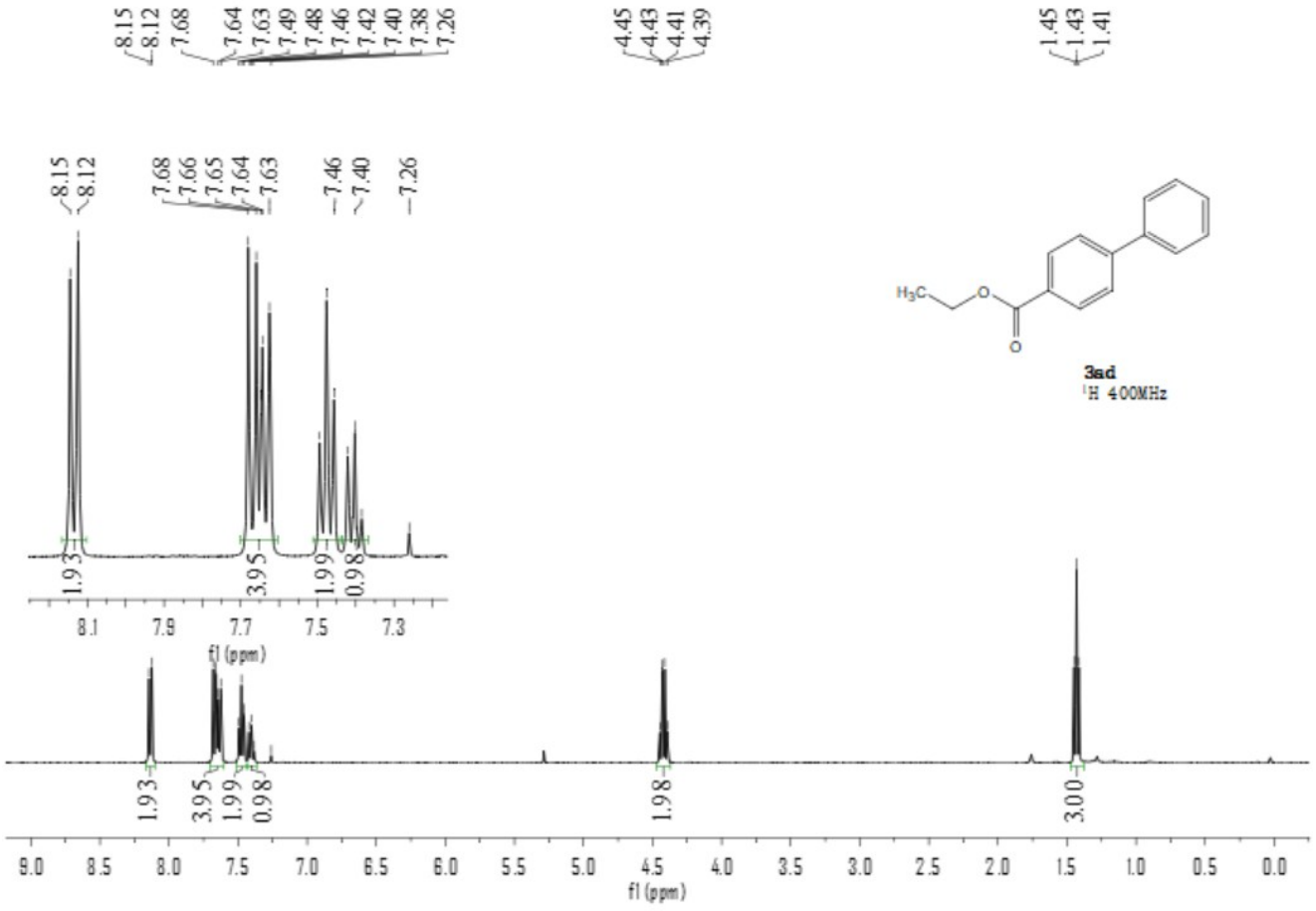


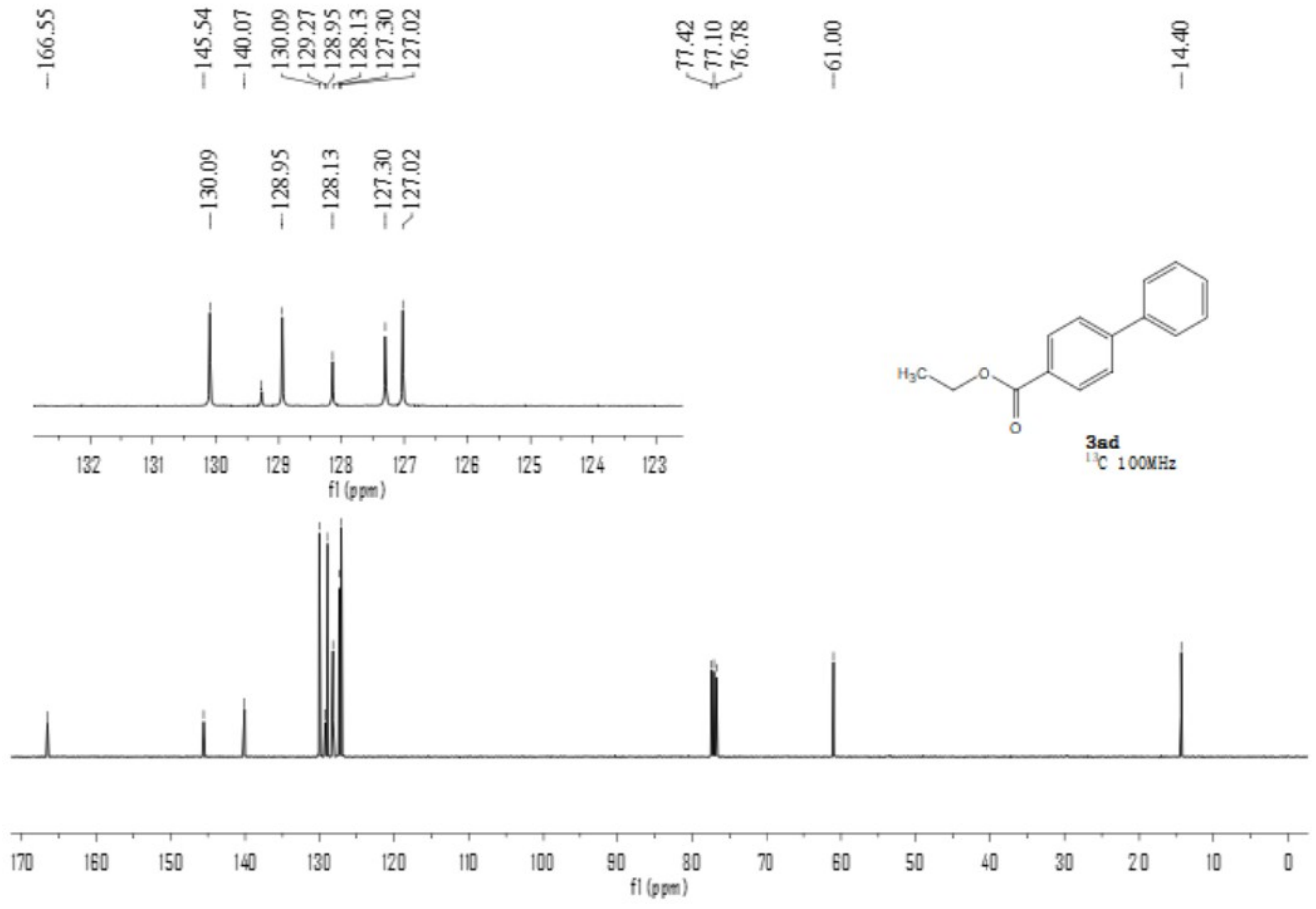

7.61
7.61
7.59
7.49
7.47
7.45
7.40
7.38
7.38
7.37
7.36
7.26
7.11
7.09
7.08
7.05
7.03
3.86
1.96
2.08
3.00
0.97
1.09
3.00
f1 (ppm)
3ab
1H 400MHz

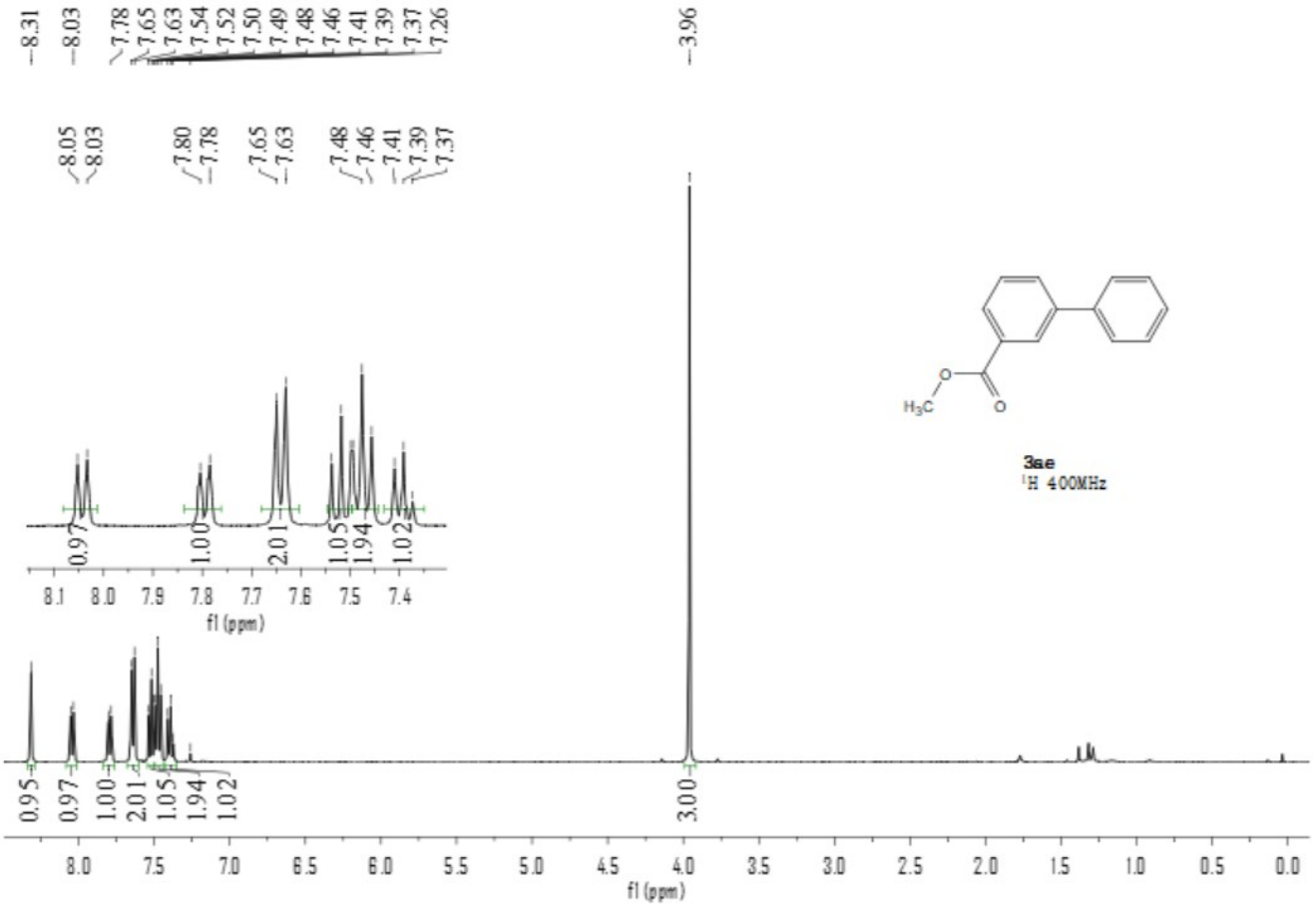

156.53
138.62
130.79
128.68
126.98
120.90
111.30
77.43
77.12
76.80
55.60
130.96
130.79
129.62
128.68
128.05
126.98
f1 (ppm)
3ab
13C 100MHz

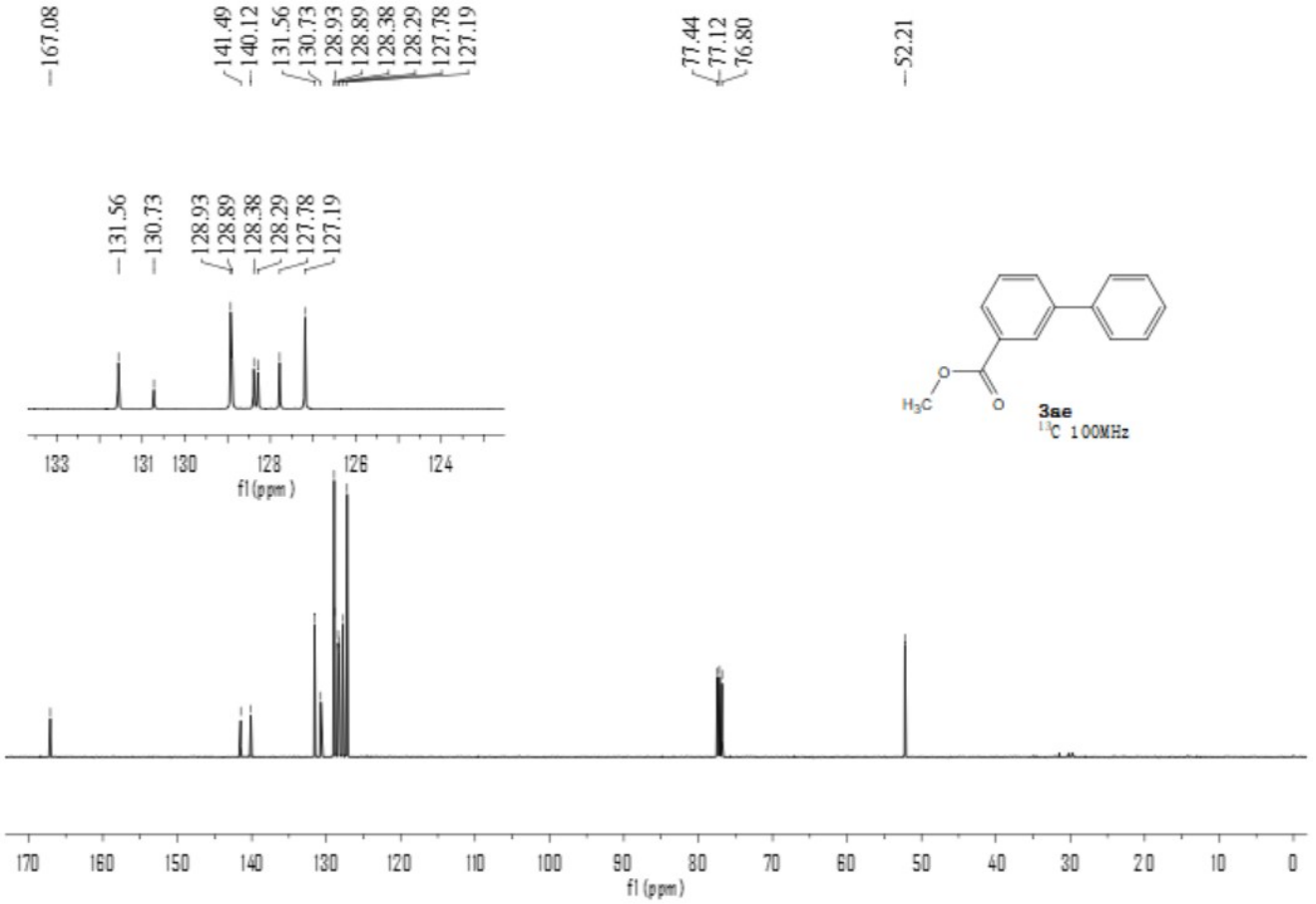

7.58
7.57
7.55
7.46
7.42
7.32
7.26
7.01
6.99
3.92
3.90
3.89
3.24
3.23
3.21
7.60
7.59
7.57
7.56
7.54
7.46
7.44
7.42
7.34
7.32
7.30
7.26
7.01
6.99
4.00
1.98
0.96
2.01
f1(ppm)
3ac
1H 400MHz
4.00
1.98
0.96
2.01
4.03
4.00
f1 (ppm)

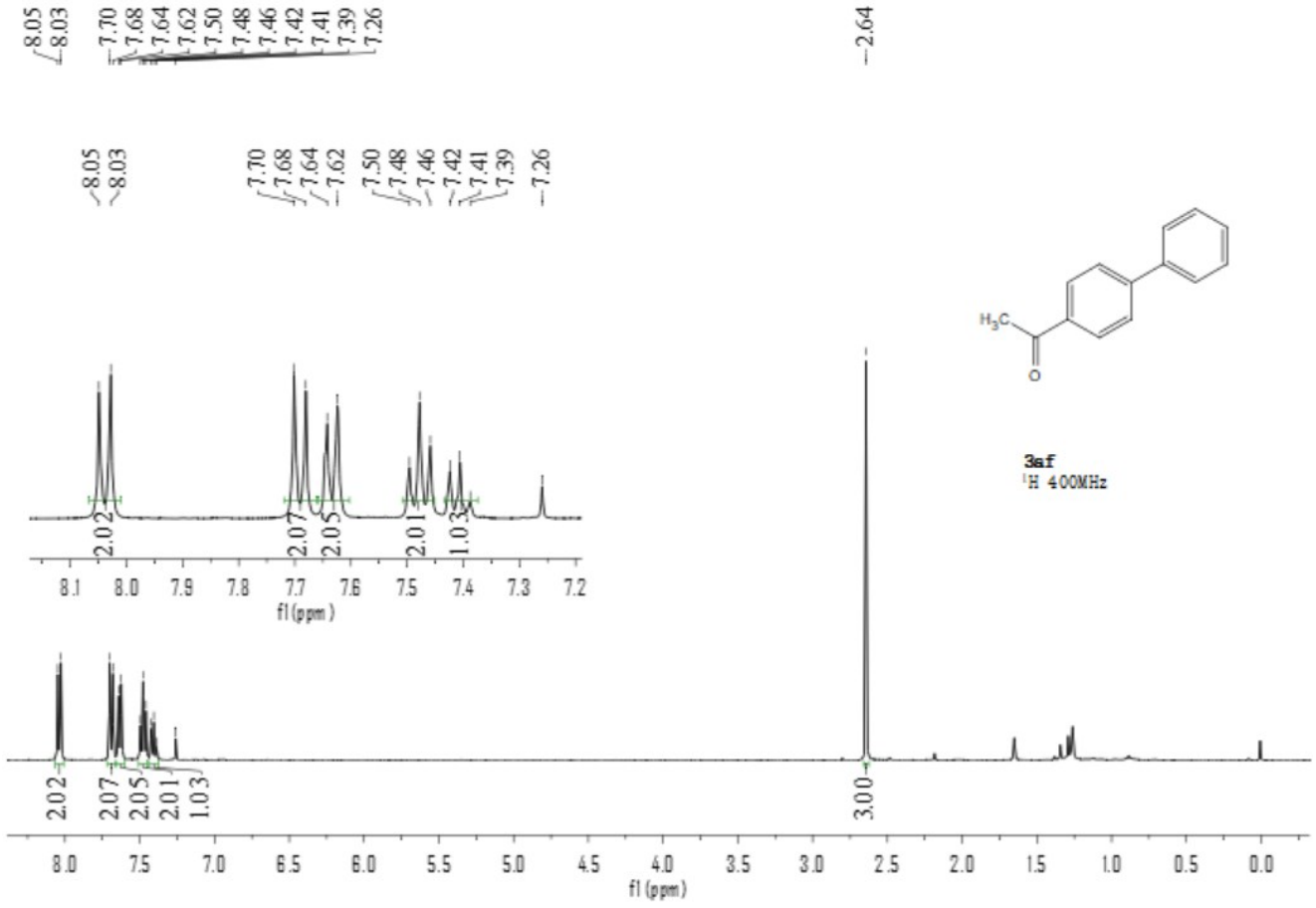

150.59
140.84
132.70
128.76
127.83
126.57
115.80
77.42
77.10
76.78
66.93
49.20
3ac
13C 100MHz
f1 (ppm)

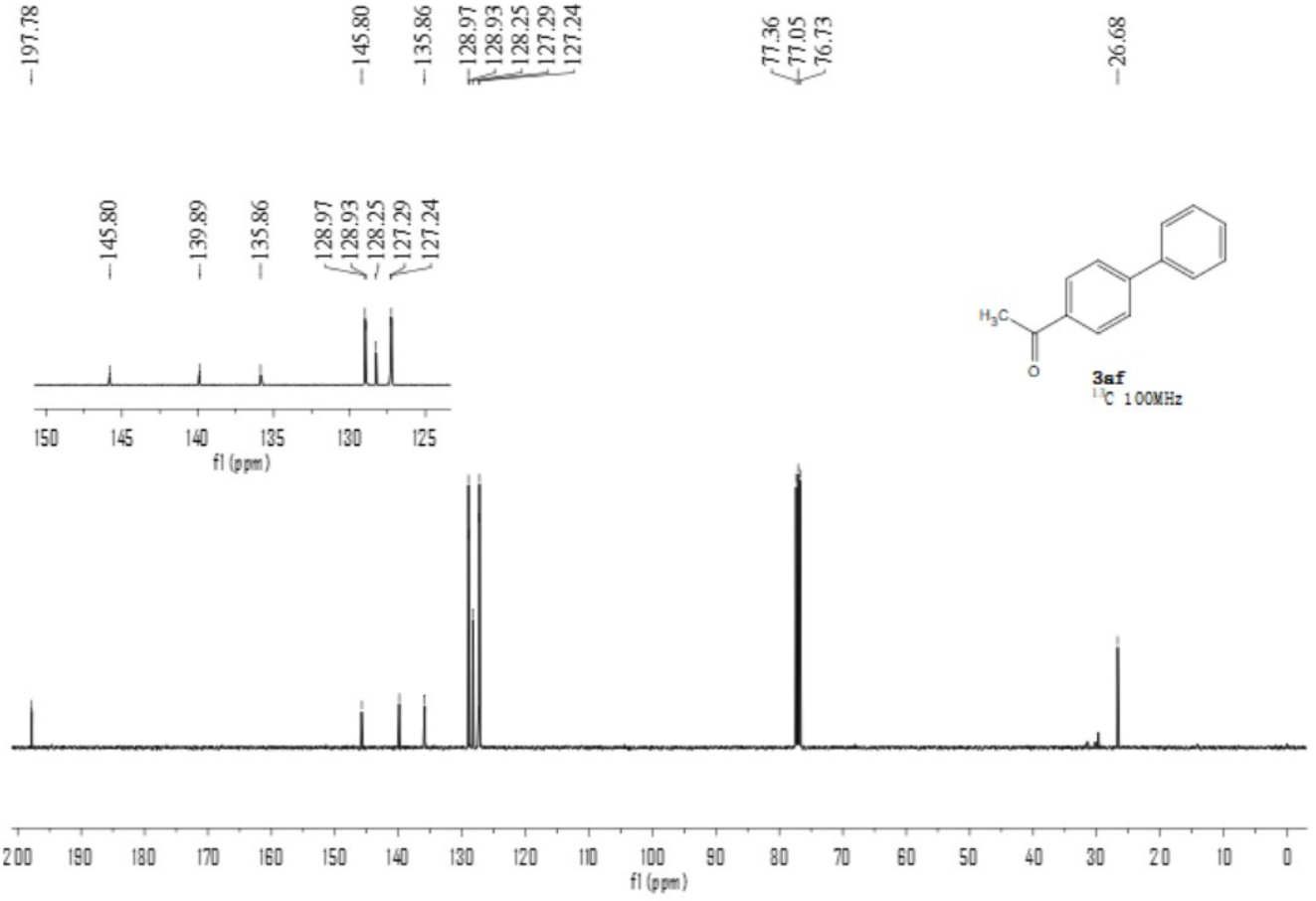

8.15
8.12
7.68
7.64
7.63
7.49
7.48
7.46
7.42
7.40
7.38
7.26
4.45
4.43
4.41
4.39
1.45
1.43
1.41
1.93
3.95
1.99
0.98
f1 (ppm)
1.98
3.00
H3C
O
O
3ad
1H 400MHz

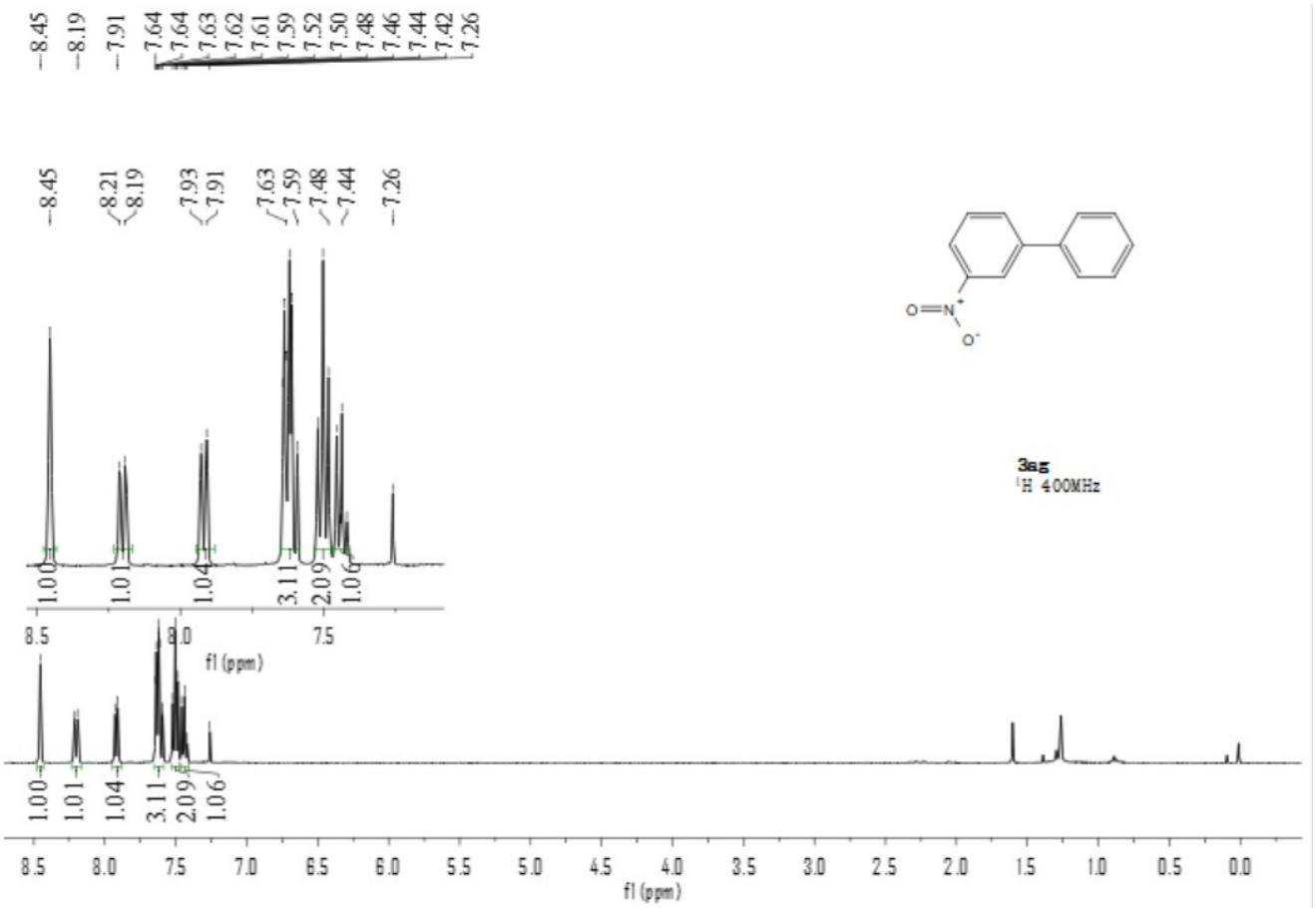

166.55
145.54
140.07
130.09
129.27
128.95
128.13
127.30
127.02
77.42
77.10
76.78
61.00
14.40
f1 (ppm)
H3C
O
O
3ad
13C 100MHz

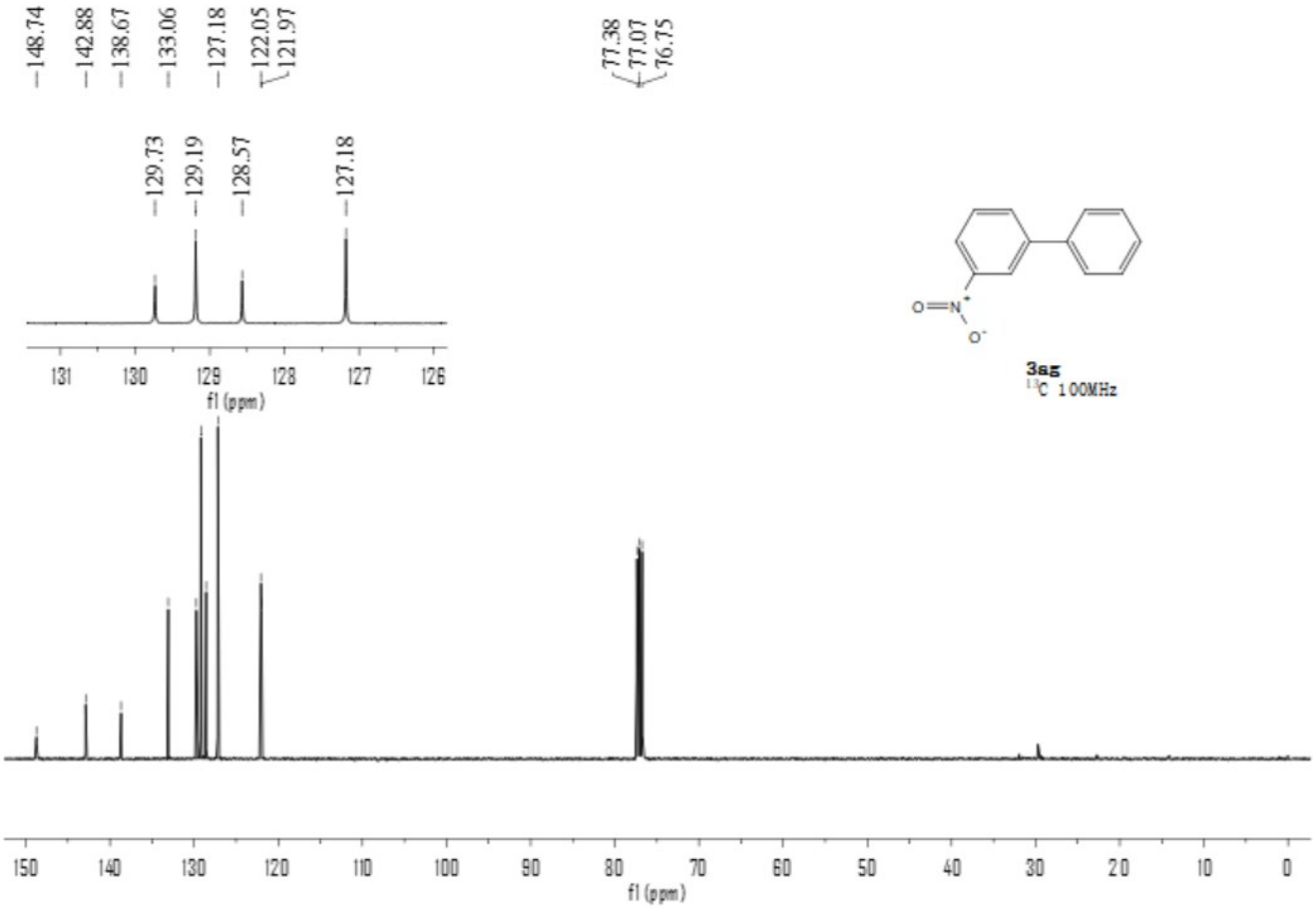

8.31
8.03
7.78
7.65
7.63
7.54
7.52
7.50
7.49
7.48
7.46
7.41
7.39
7.37
7.26
3.96
0.95
0.97
1.00
2.01
1.05
1.94
1.02
3.00
f1 (ppm)
3ae
1H 400MHz


167.08
141.49
140.12
131.56
130.73
128.93
128.89
128.38
128.29
127.78
127.19
77.44
77.12
76.80
52.21
f1 (ppm)
3ae
13C 100MHz


8.05
8.03
7.70
7.68
7.64
7.62
7.50
7.48
7.46
7.42
7.41
7.39
7.26
2.64
2.02
2.07
2.05
2.01
1.03
3.00
f1 (ppm)
3af
1H 400MHz


197.78
145.80
139.89
135.86
128.97
128.93
128.25
127.29
127.24
77.36
77.05
76.73
26.68
f1 (ppm)
3af
13C 100MHz


8.45
8.19
7.91
7.64
7.64
7.63
7.62
7.61
7.59
7.52
7.50
7.48
7.46
7.44
7.42
7.26
8.45
8.21
8.19
7.93
7.91
7.63
7.59
7.48
7.44
7.26
1.00
1.01
1.04
3.11
2.09
1.06
8.5
8.0
7.5
f1 (ppm)
O=N+
O-
3ag
1H 400MHz
1.00
1.01
1.04
3.11
2.09
1.06
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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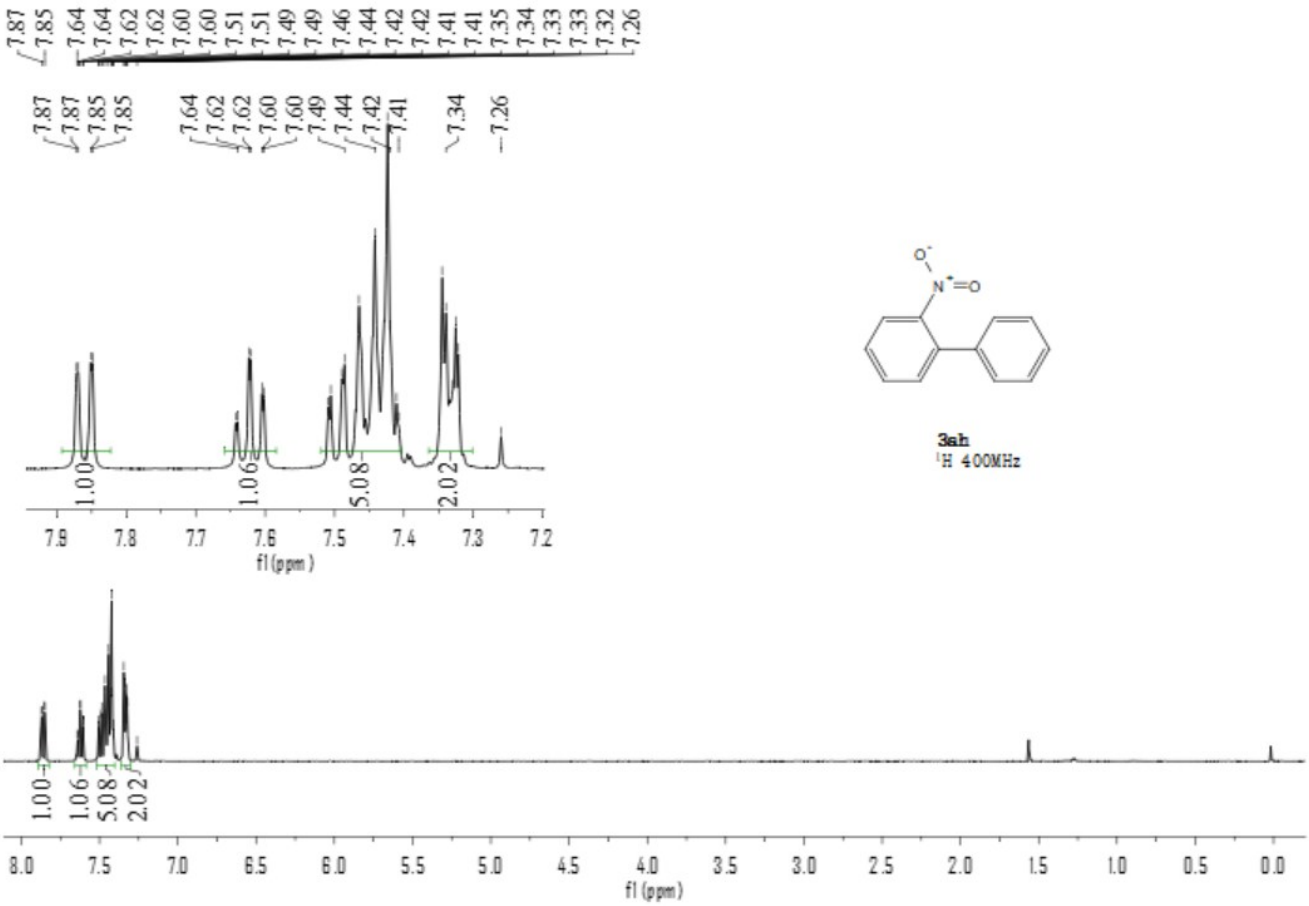
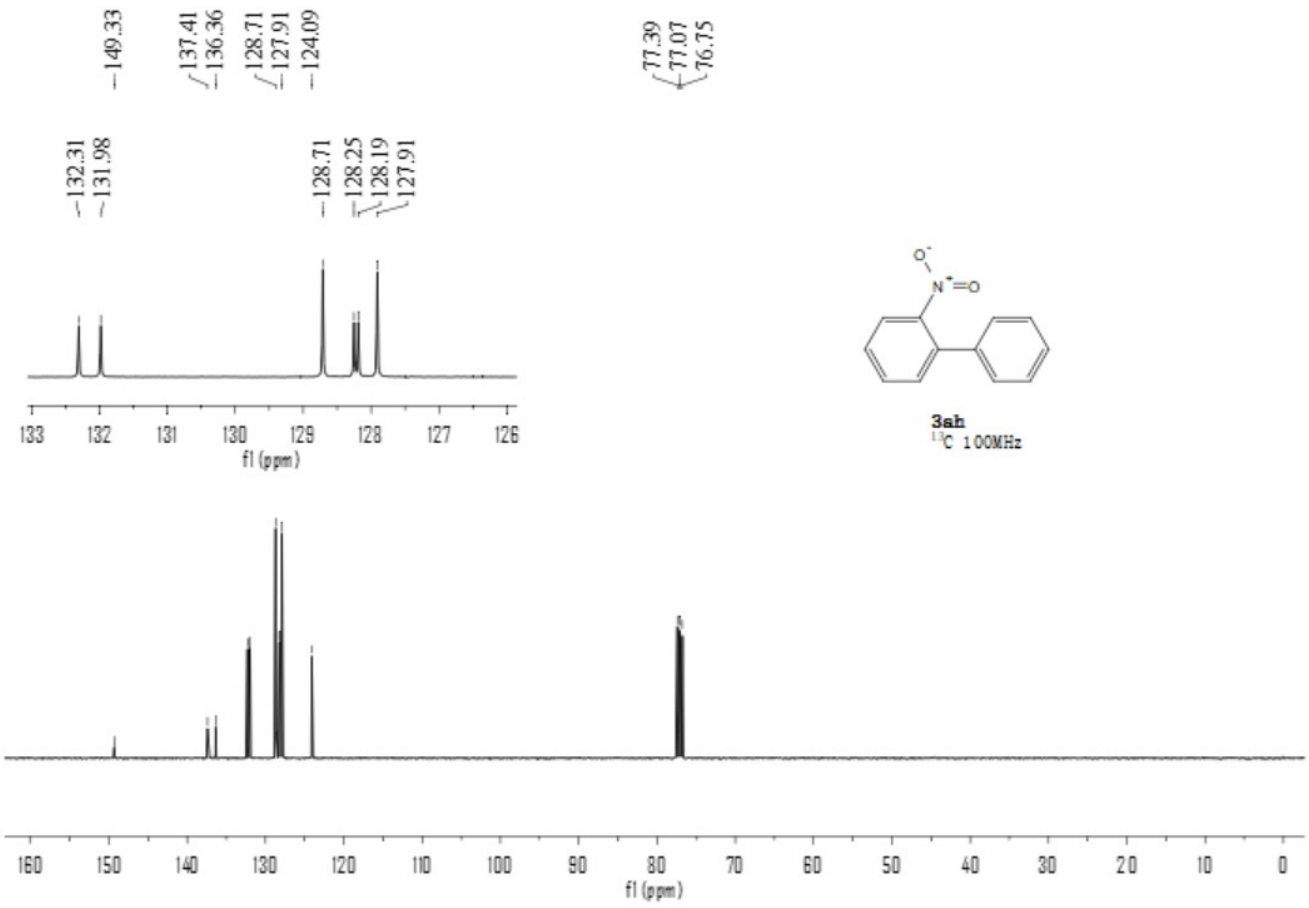
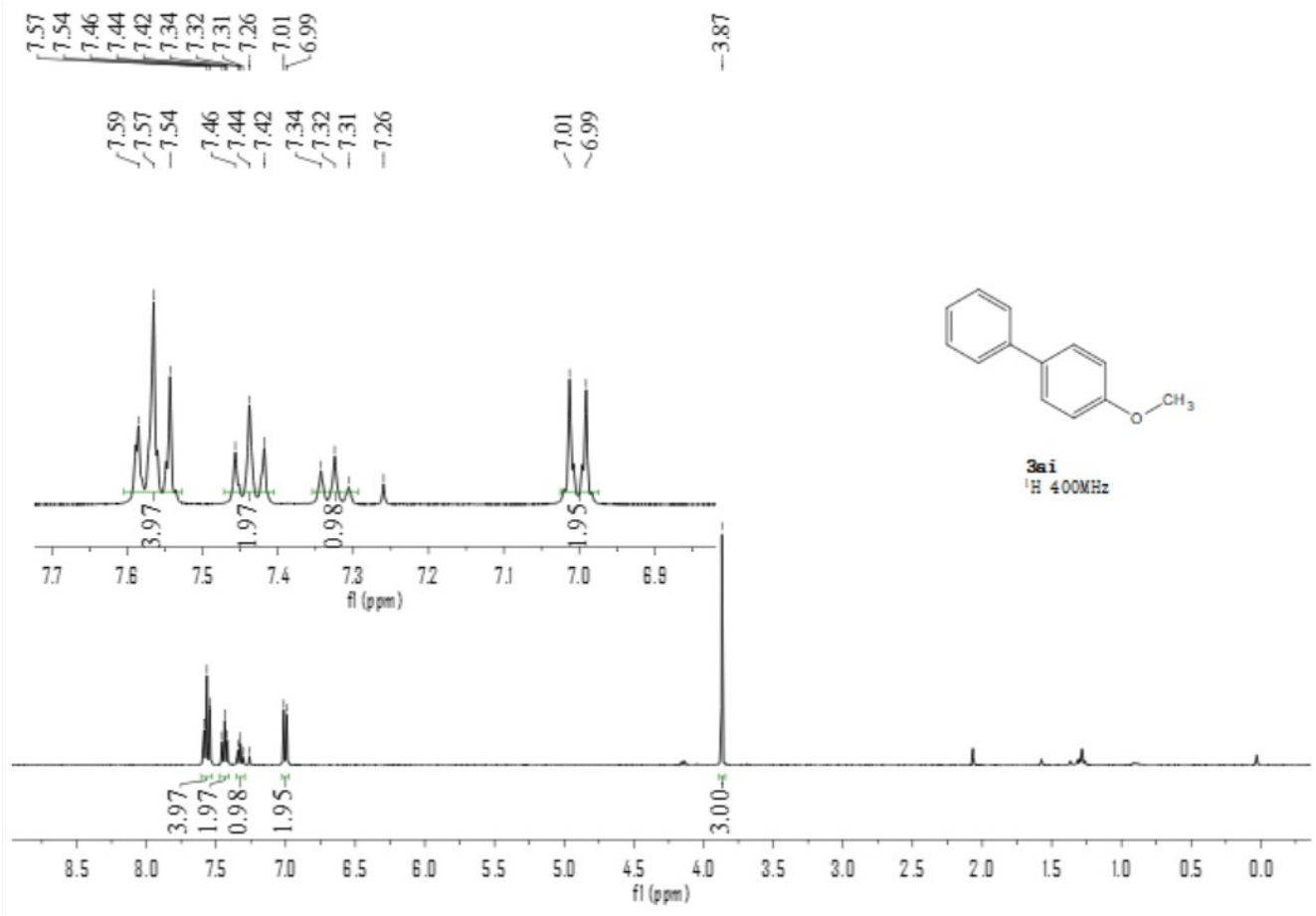
142.88
138.67
133.06
127.18
122.05
121.97
77.38
77.07
76.75
129.73
129.19
128.57
127.18
131
130
129
128
127
126
f1 (ppm)
O=N+
O-
3ag
13C 100MHz
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.87
7.85
7.64
7.64
7.62
7.62
7.60
7.60
7.51
7.51
7.49
7.49
7.46
7.44
7.42
7.42
7.41
7.41
7.35
7.34
7.33
7.33
7.32
7.26
1.00
1.06
5.08
2.02
f1 (ppm)
3ah
1H 400MHz


149.33
137.41
136.36
128.71
127.91
124.09
77.39
77.07
76.75
132.31
131.98
128.71
128.25
128.19
127.91
f1 (ppm)
3ah
13C 100MHz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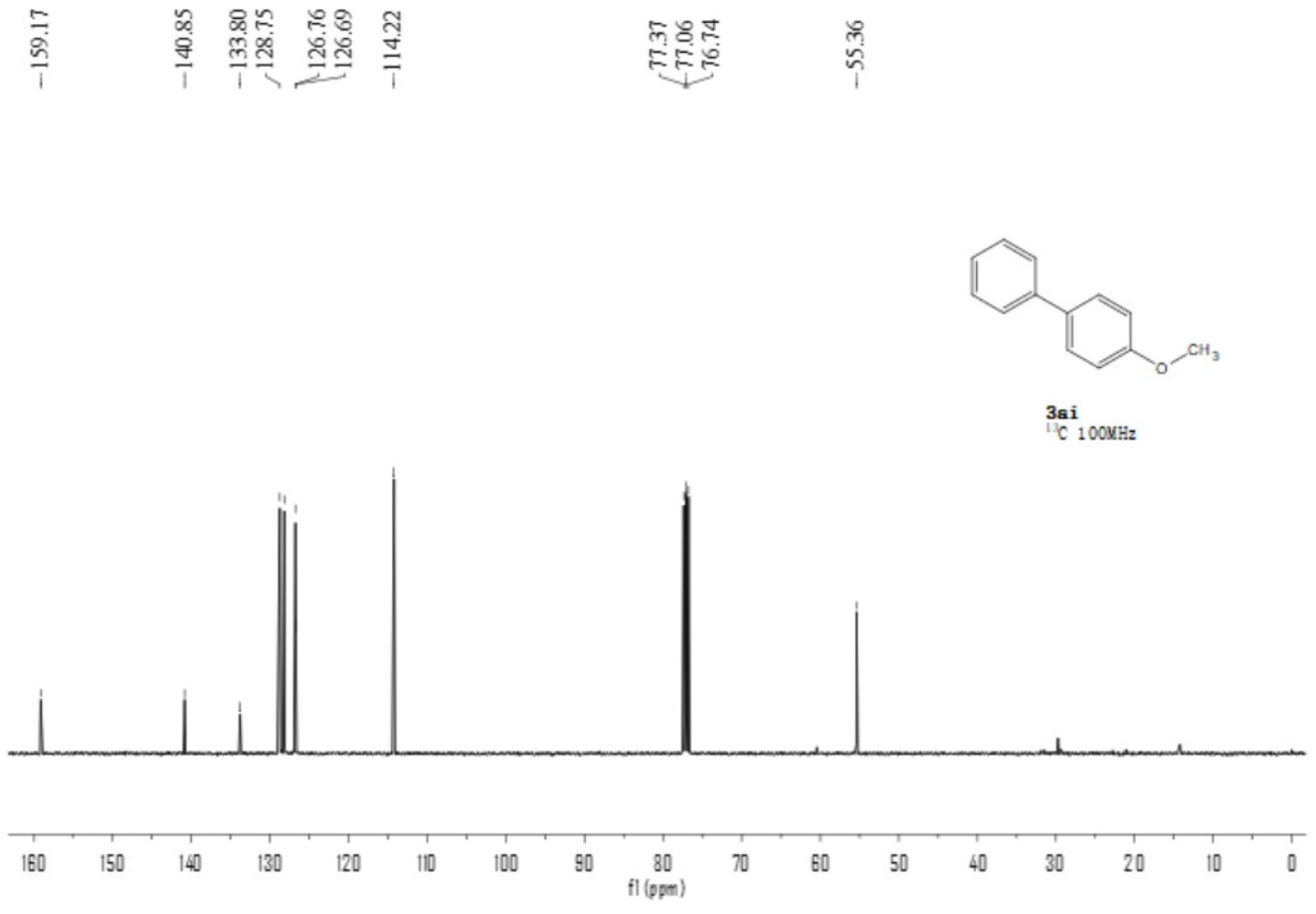
7.44
7.42
7.34
7.32
7.31
7.26
7.01
6.99
3.87
3.97
1.97
0.98
1.95
3.00
f1 (ppm)
3ai
1H 400MHz


159.17
140.85
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128.75
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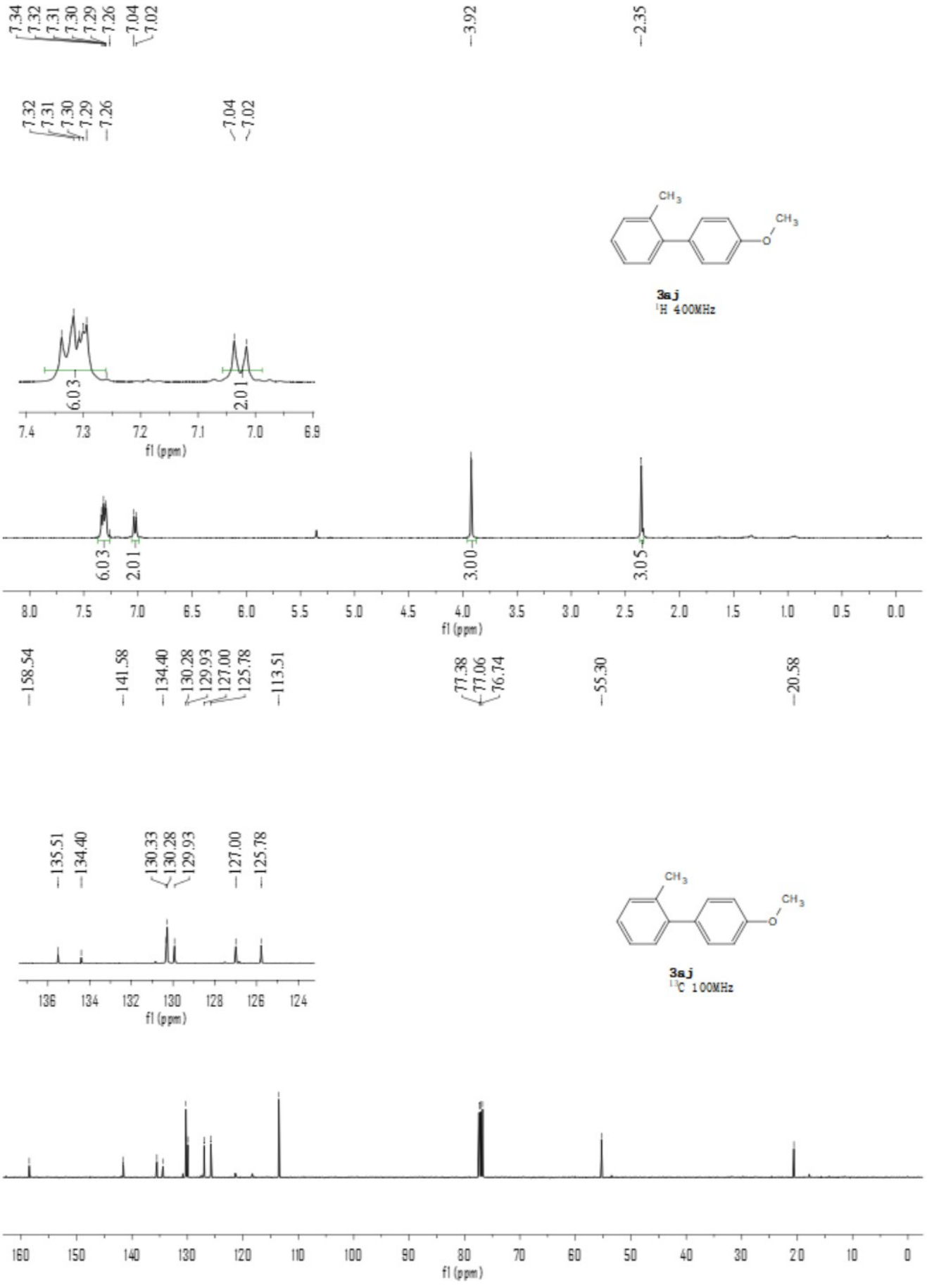
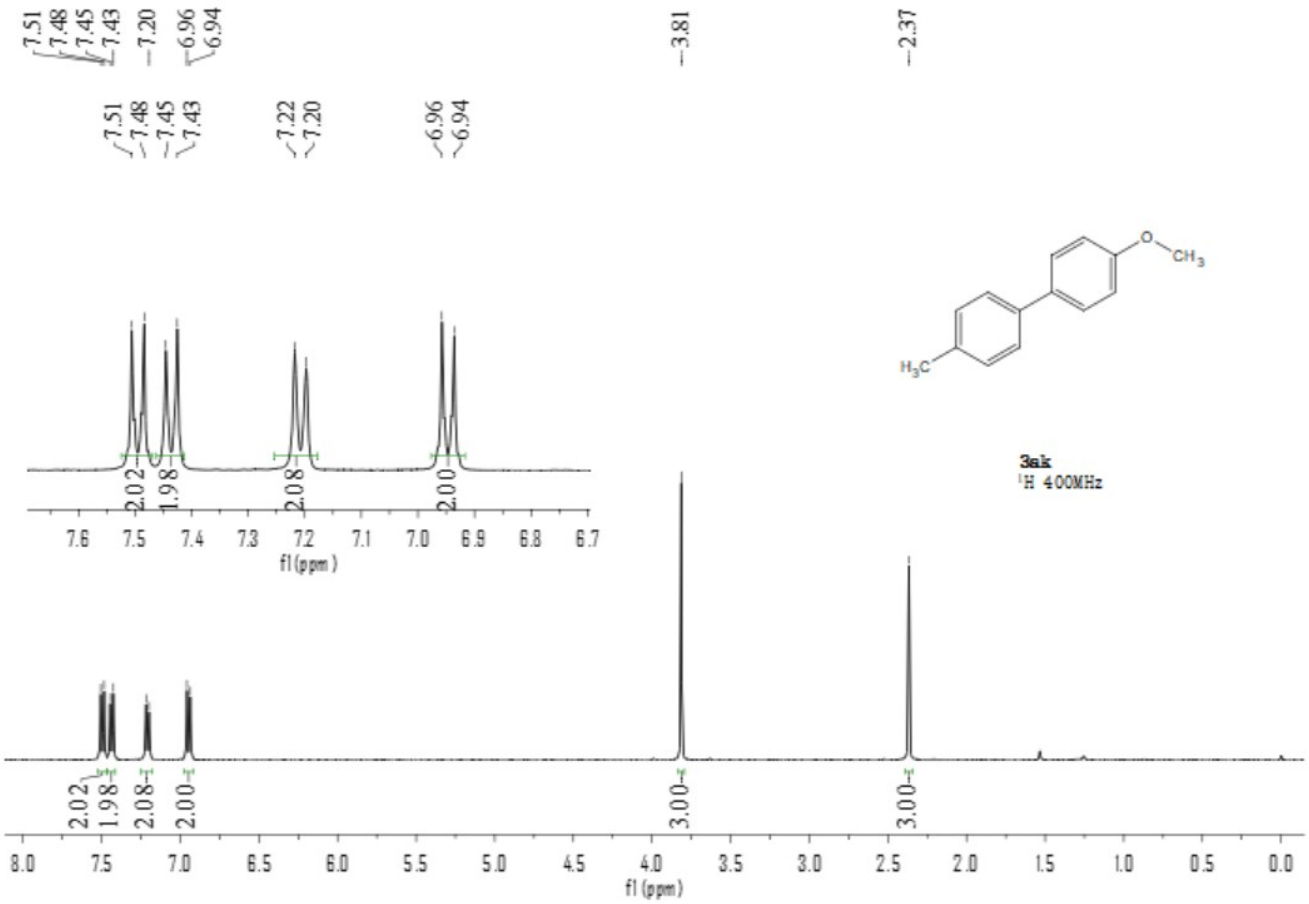
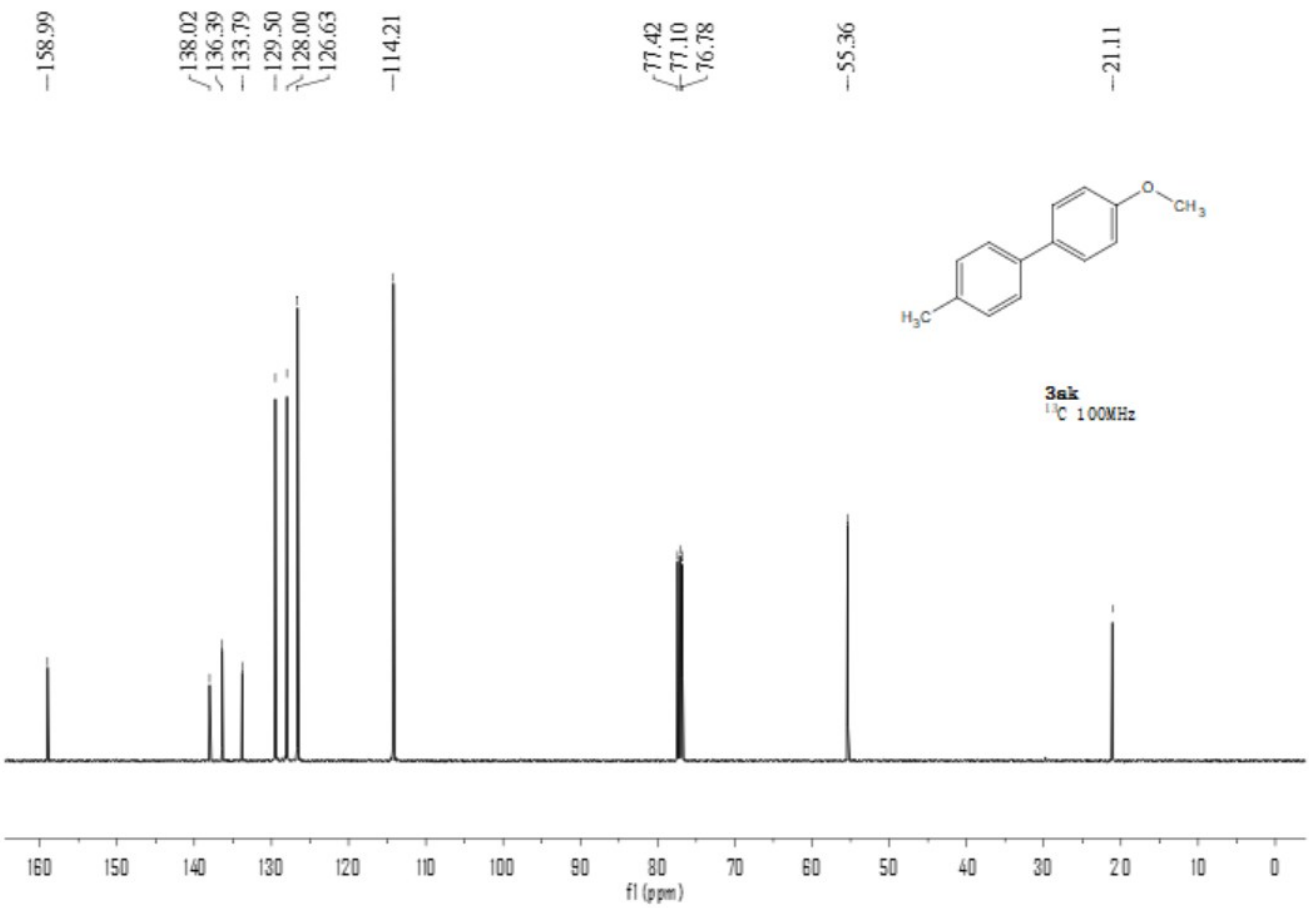
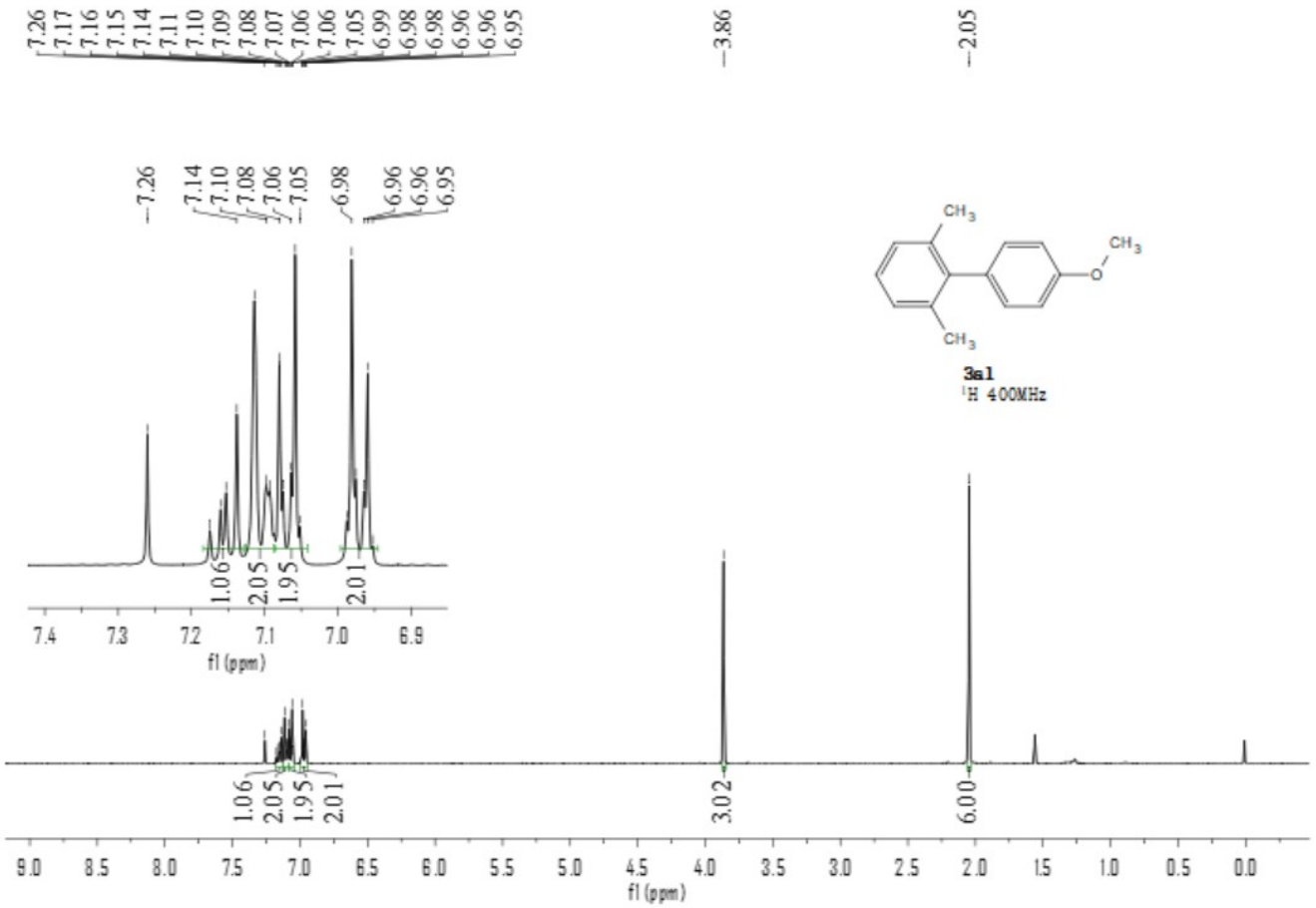
126.69
114.22
77.37
77.06
76.74
55.36
f1 (ppm)
3ai
13C 100MHz


7.34
7.32
7.31
7.30
7.29
7.26
7.04
7.02
3.92
2.35
CH3
CH3
O
3aj
1H 400MHz
6.03
2.01
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
6.03
2.01
3.00
3.05
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)
158.54
141.58
134.40
130.28
129.93
127.00
125.78
113.51
77.38
77.06
76.74
55.30
20.58
135.51
134.40
130.33
130.28
129.93
127.00
125.78
136
134
132
130
128
126
124
f1 (ppm)
CH3
CH3
O
3aj
13C 100MHz
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.51
7.48
7.45
7.43
7.20
6.96
6.94
3.81
2.37
2.02
1.98
2.08
2.00
3.00
3.00
f1 (ppm)
3ak
1H 400MHz


158.99
138.02
136.39
133.79
129.50
128.00
126.63
114.21
77.42
77.10
76.78
55.36
21.11
f1 (ppm)
3ak
13C 100MHz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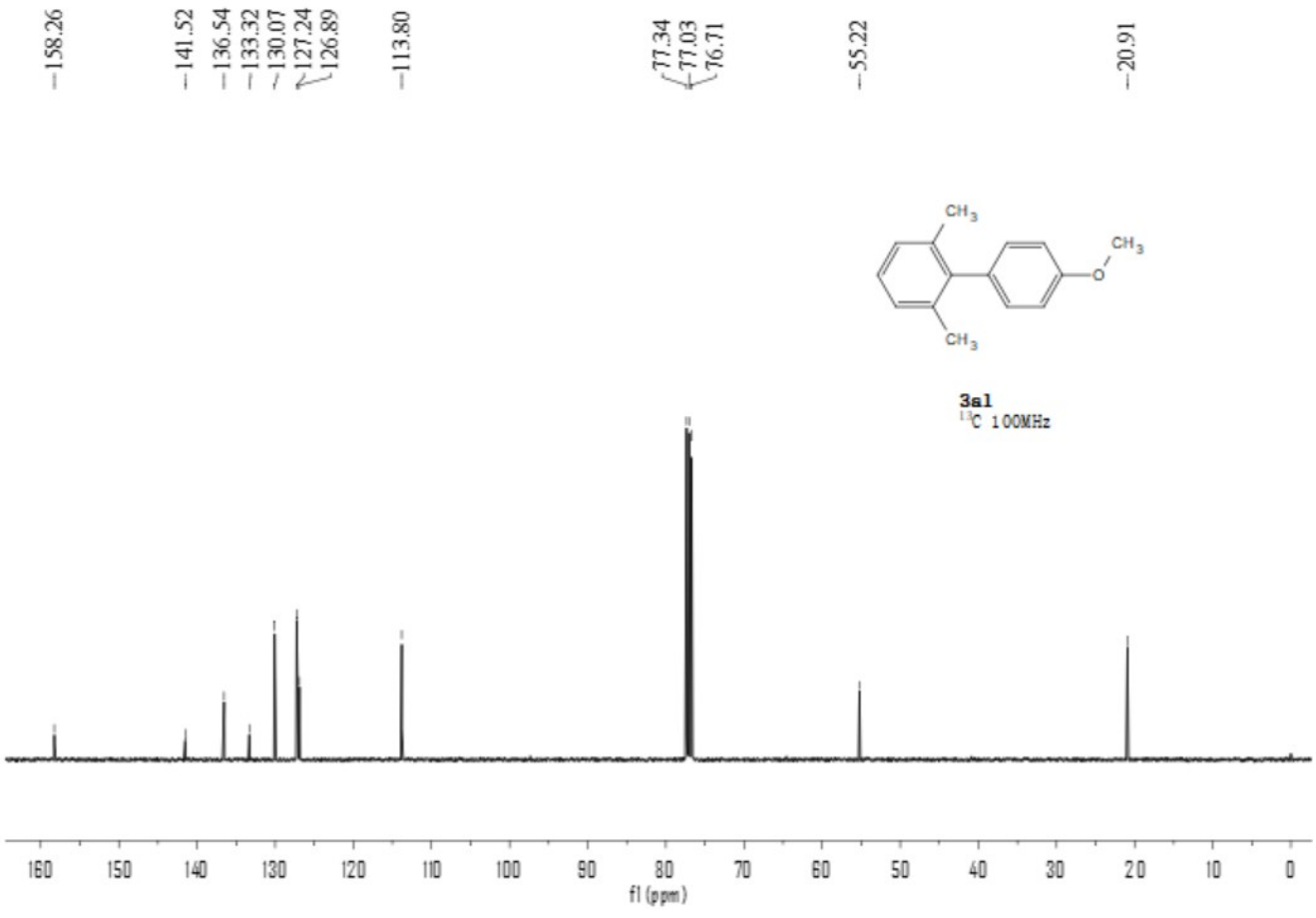
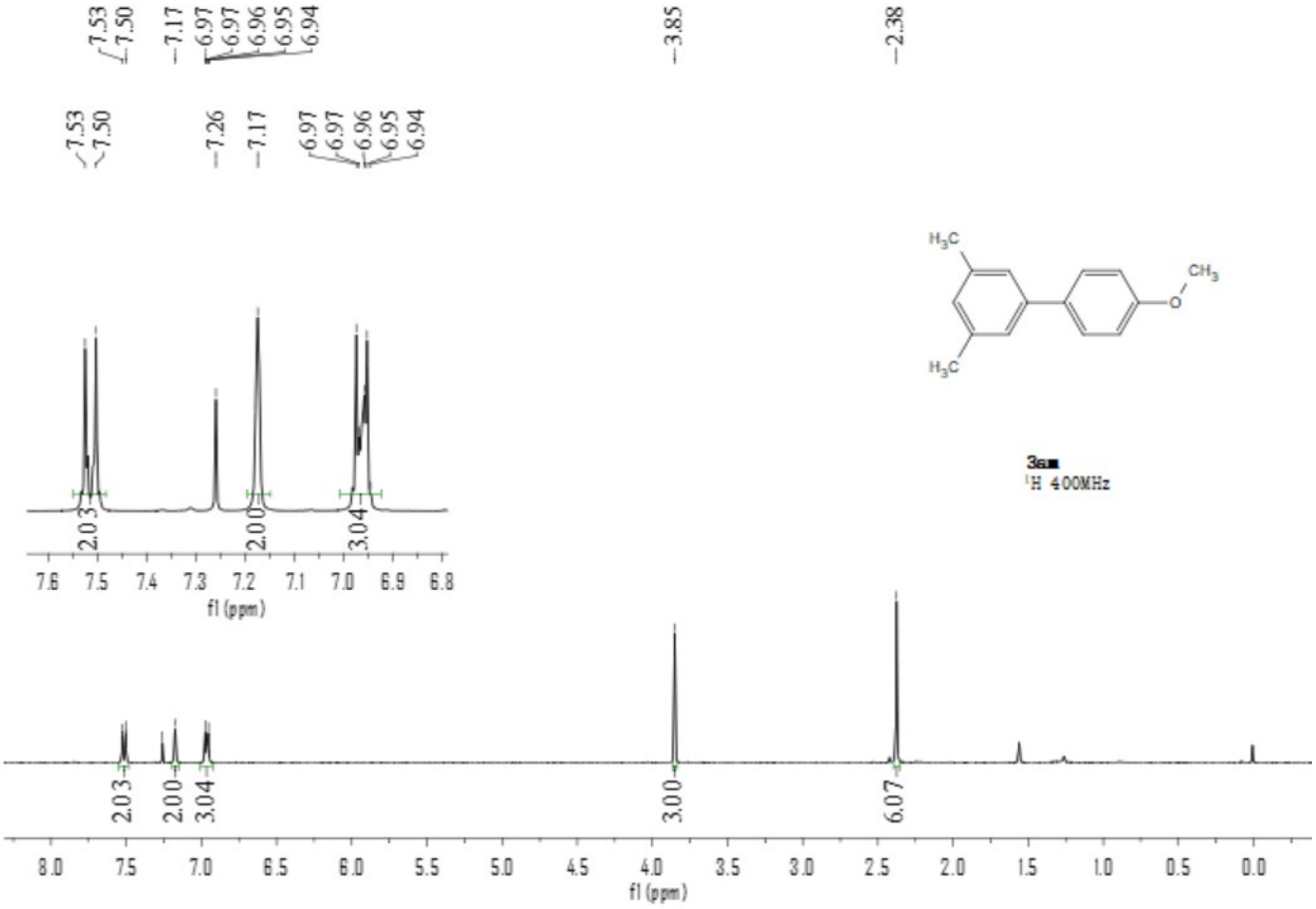
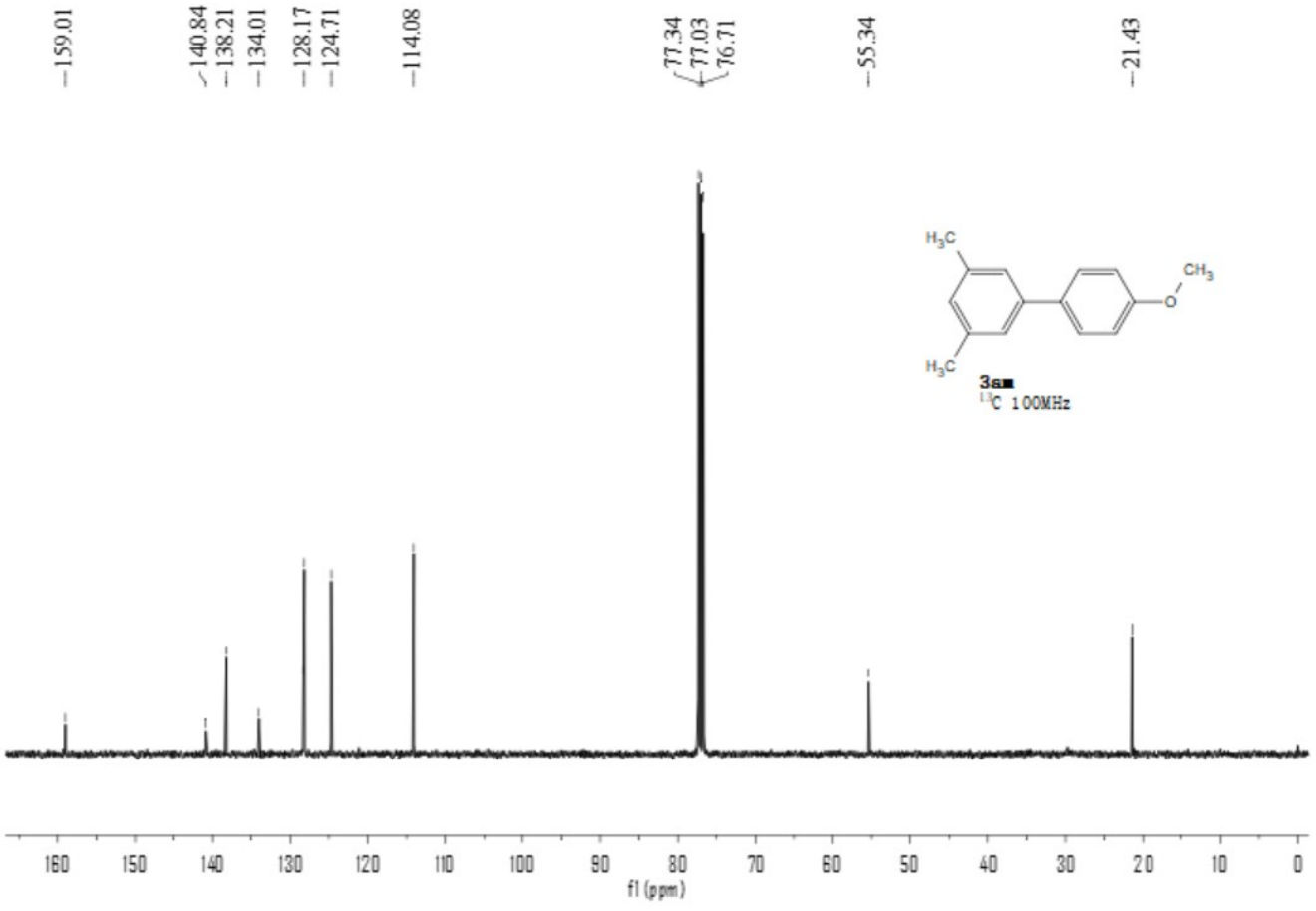
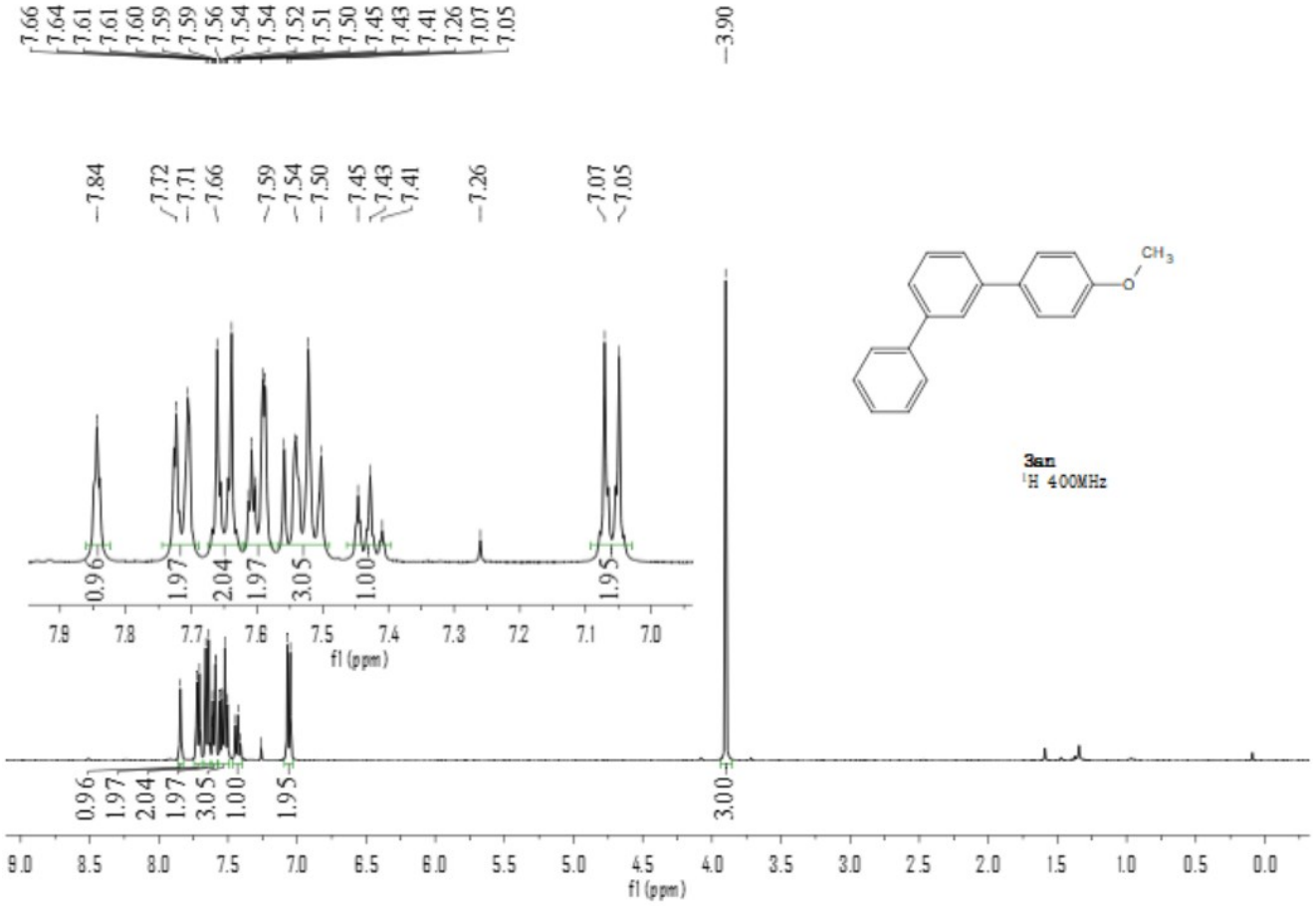
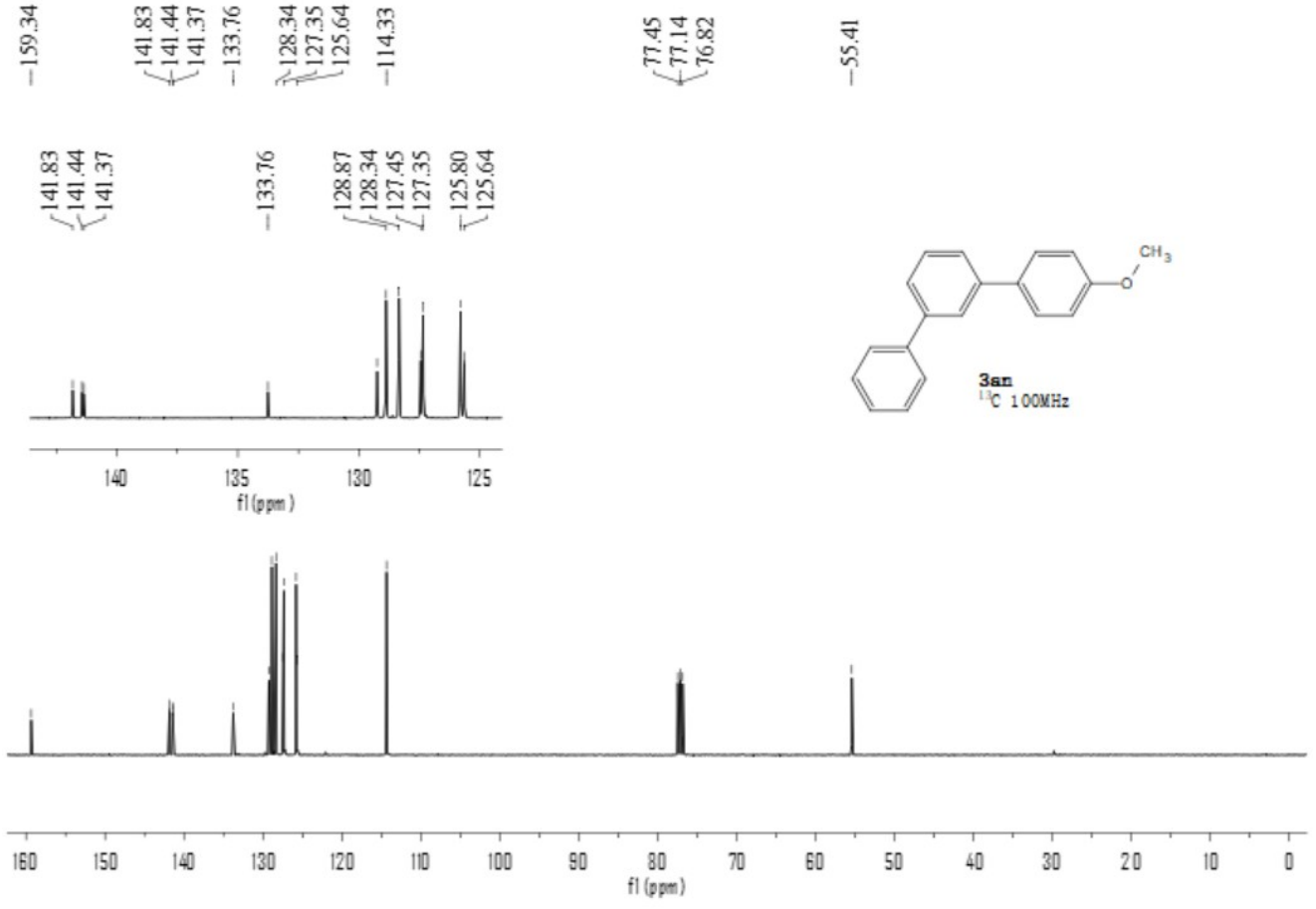
7.17
7.16
7.15
7.14
7.11
7.10
7.09
7.08
7.07
7.06
7.06
7.05
6.99
6.98
6.98
6.96
6.96
6.95
3.86
2.05
7.26
7.14
7.10
7.08
7.06
7.05
6.98
6.96
6.96
6.95
1.06
2.05
1.95
2.01
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
CH3
CH3
CH3
O
3al
1H 400MHz
1.06
2.05
1.95
2.01
3.02
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.26
141.52
136.54
133.32
130.07
127.24
126.89
113.80
77.34
77.03
76.71
55.22
20.91
CH3
CH3
CH3
O
3al
13C 100MHz
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.53
7.50
7.17
6.97
6.97
6.96
6.95
6.94
3.85
2.38
7.26
2.03
2.00
3.04
3.00
6.07
3a
1H 400MHz
f1 (ppm)


159.01
140.84
138.21
134.01
128.17
124.71
114.08
77.34
77.03
76.71
55.34
21.43
3a
13C 100MHz
f1 (ppm)


7.66
7.64
7.61
7.61
7.60
7.59
7.59
7.56
7.54
7.54
7.52
7.51
7.50
7.45
7.43
7.41
7.26
7.07
7.05
3.90
7.84
7.72
7.71
7.66
7.59
7.54
7.50
7.45
7.43
7.41
7.26
7.07
7.05
0.96
1.97
2.04
1.97
3.05
1.00
1.95
3.00
f1 (ppm)
3an
1H 400MHz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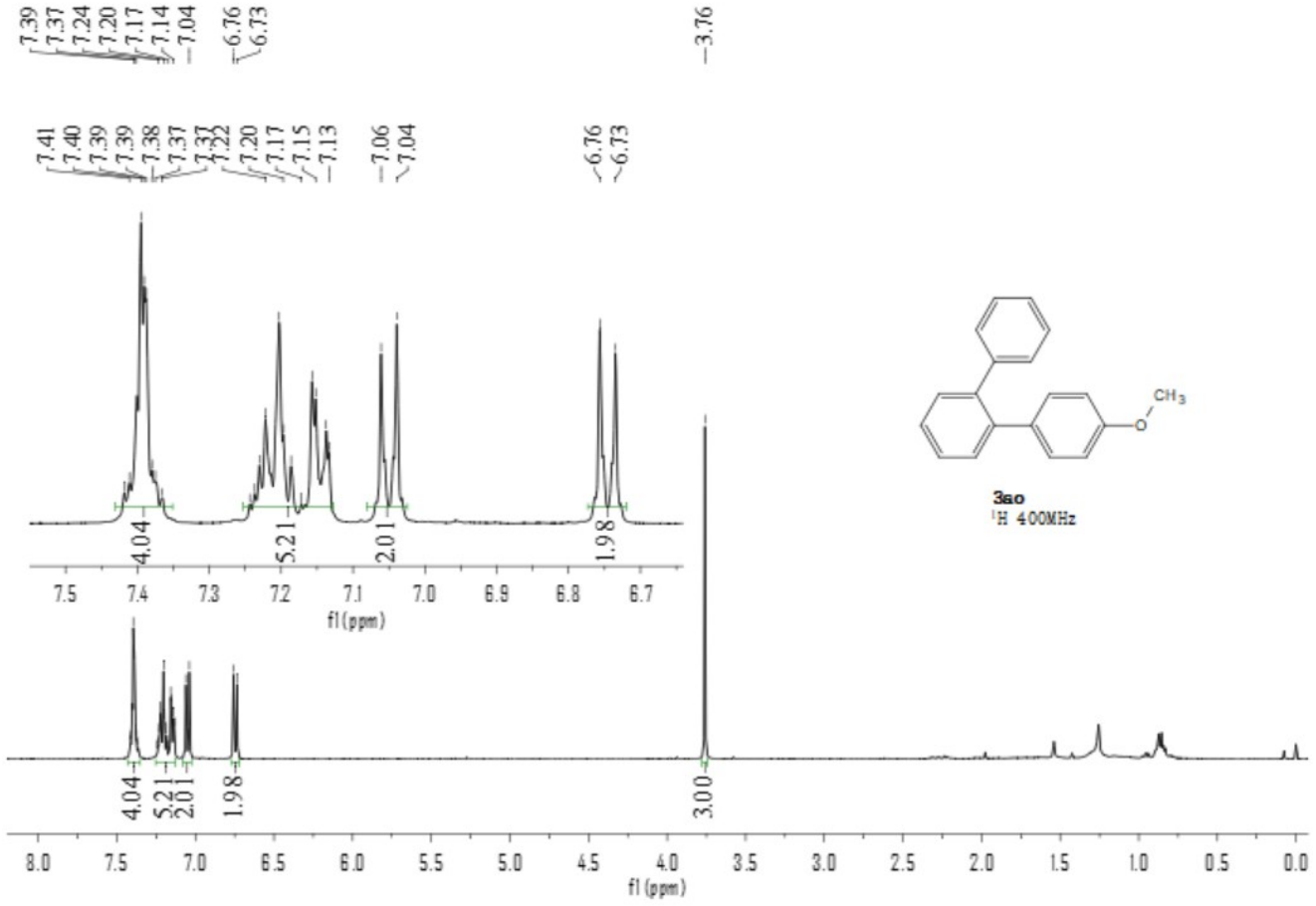
141.83
141.44
141.37
133.76
128.34
127.35
125.64
114.33
77.45
77.14
76.82
55.41
128.87
128.34
127.45
127.35
125.80
125.64
f1 (ppm)
3an
13C 100MHz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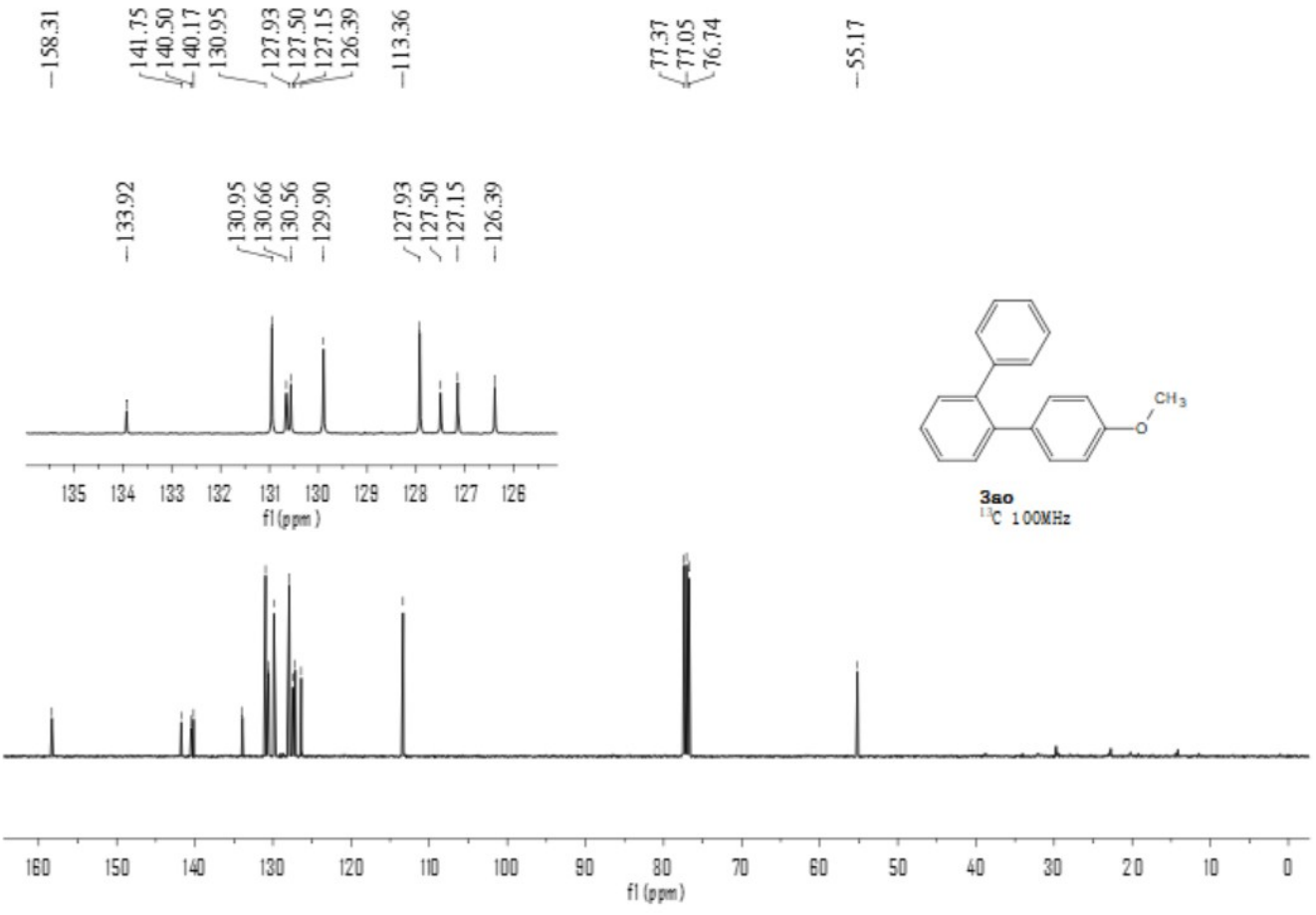
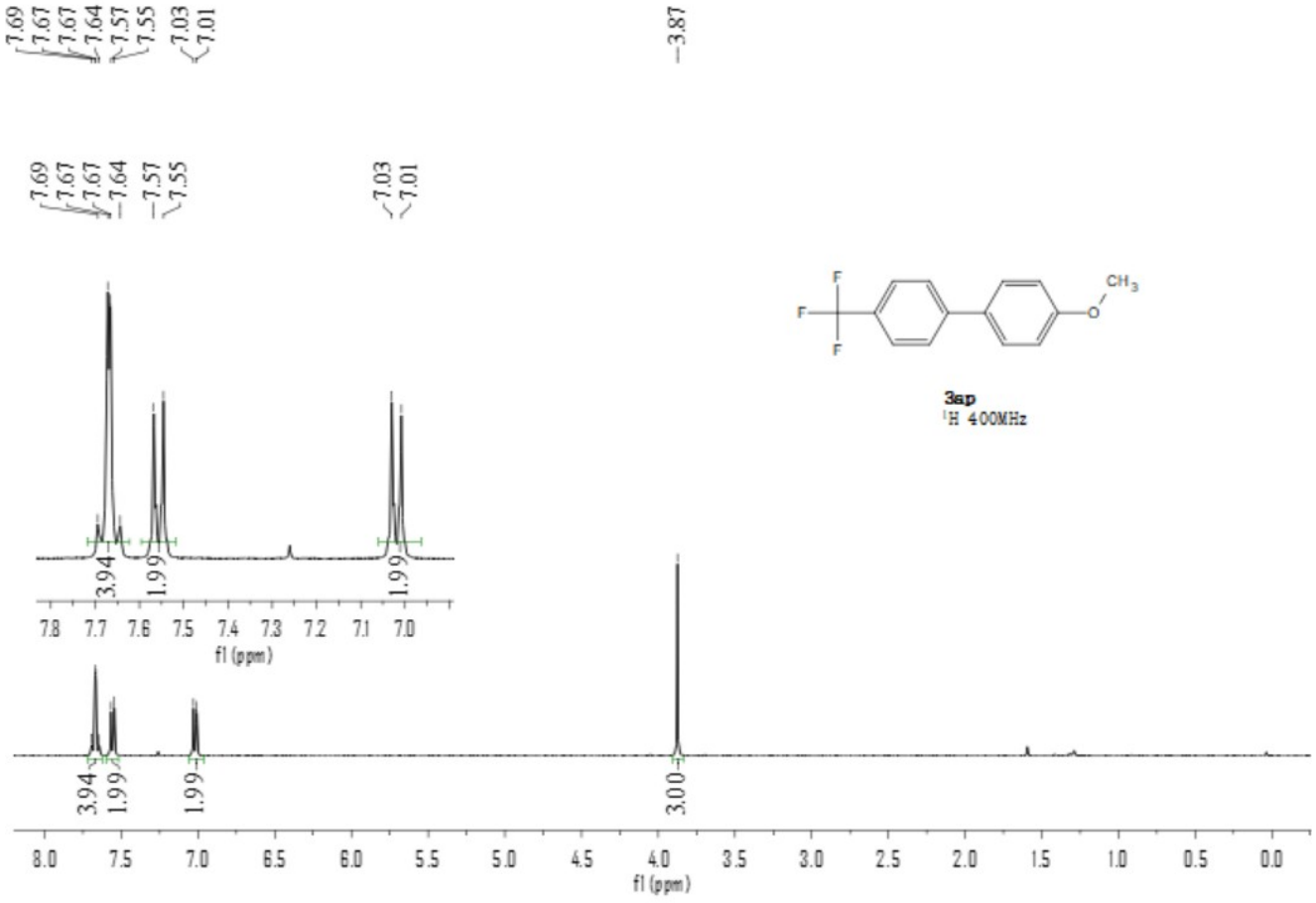
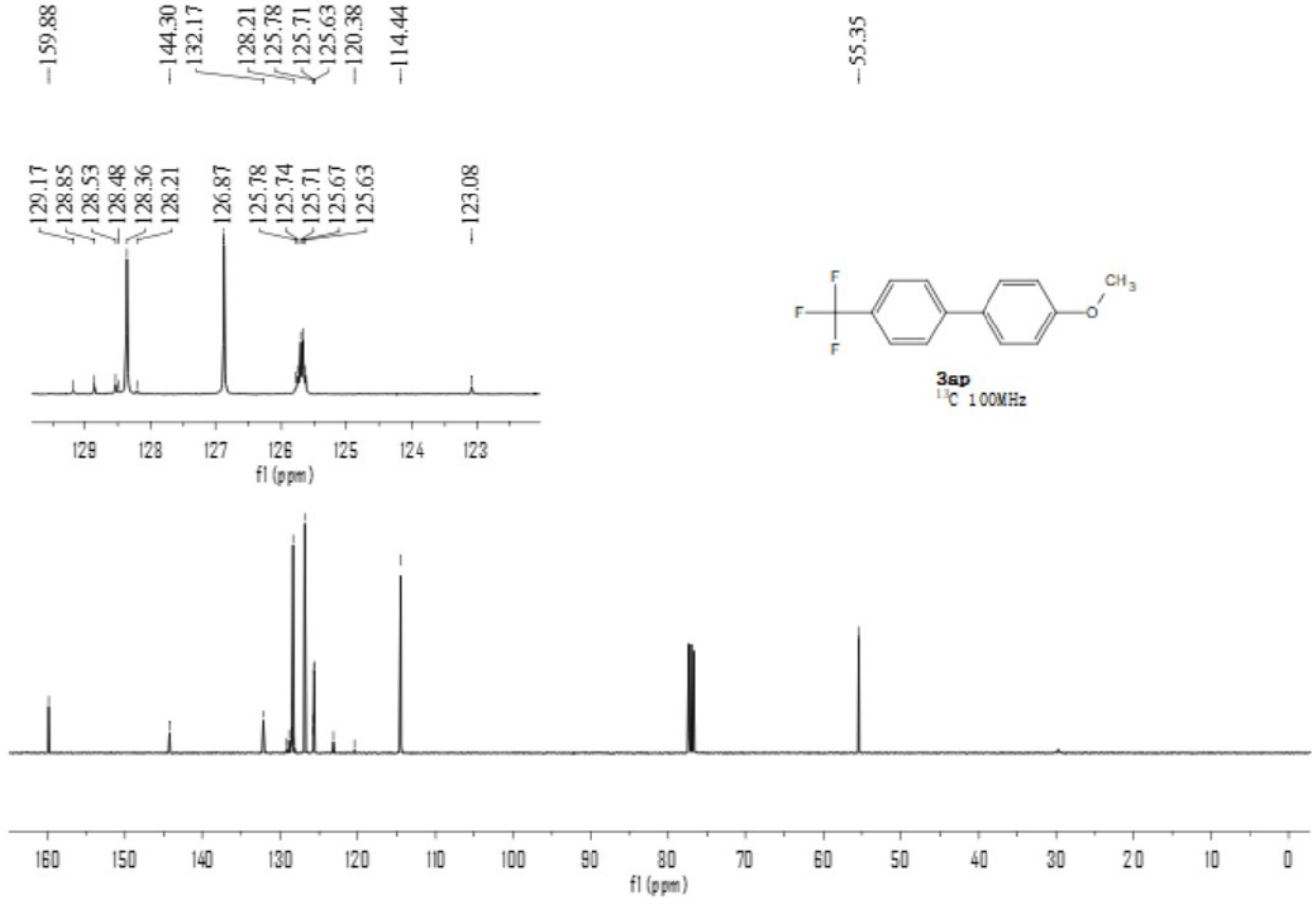
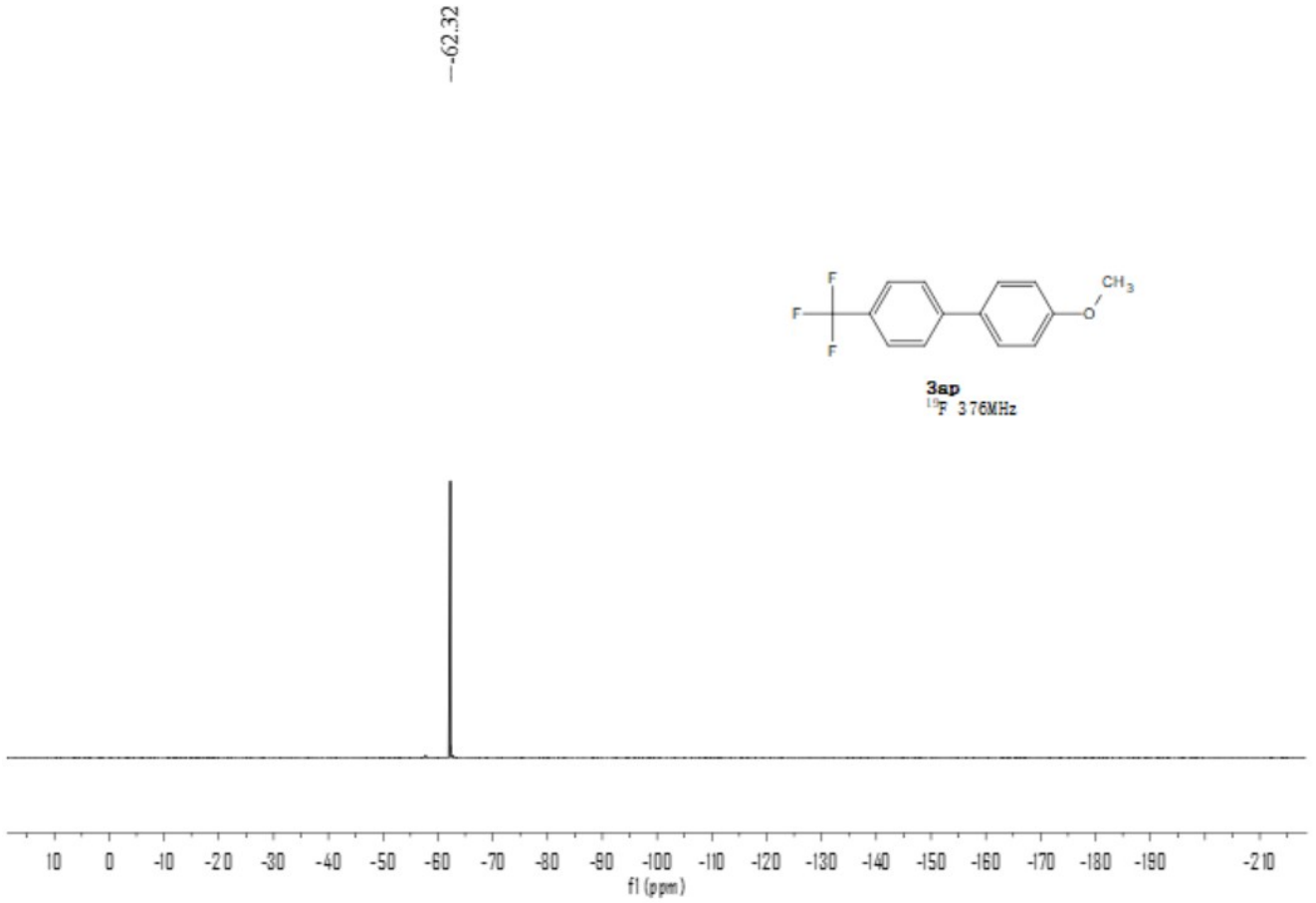
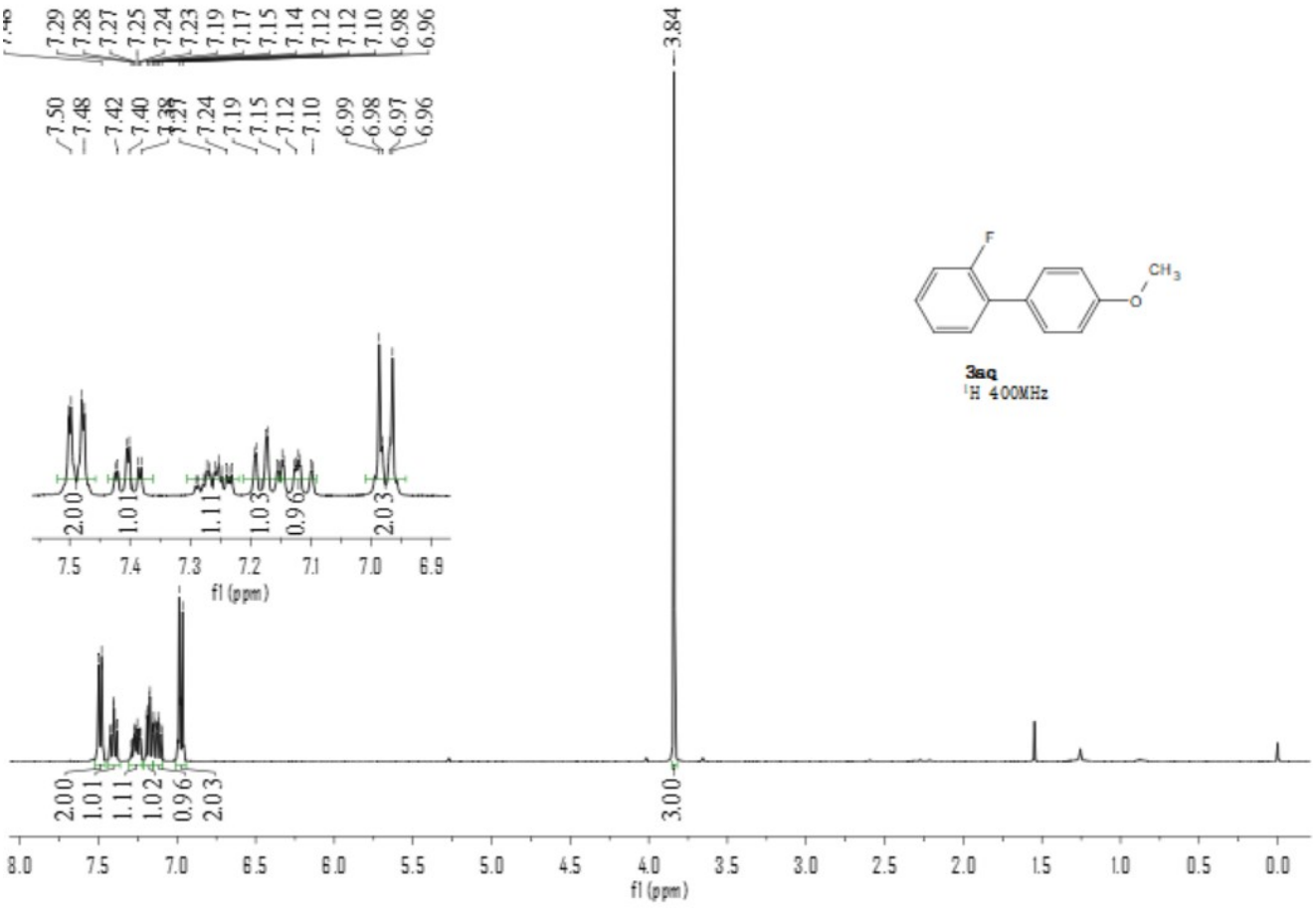
7.37
7.24
7.20
7.17
7.14
7.04
6.76
6.73
3.76
7.41
7.40
7.39
7.39
7.38
7.37
7.31
7.22
7.20
7.17
7.15
7.13
7.06
7.04
6.76
6.73
4.04
5.21
2.01
1.98
3.00
f1 (ppm)
3ao
1H 400MHz

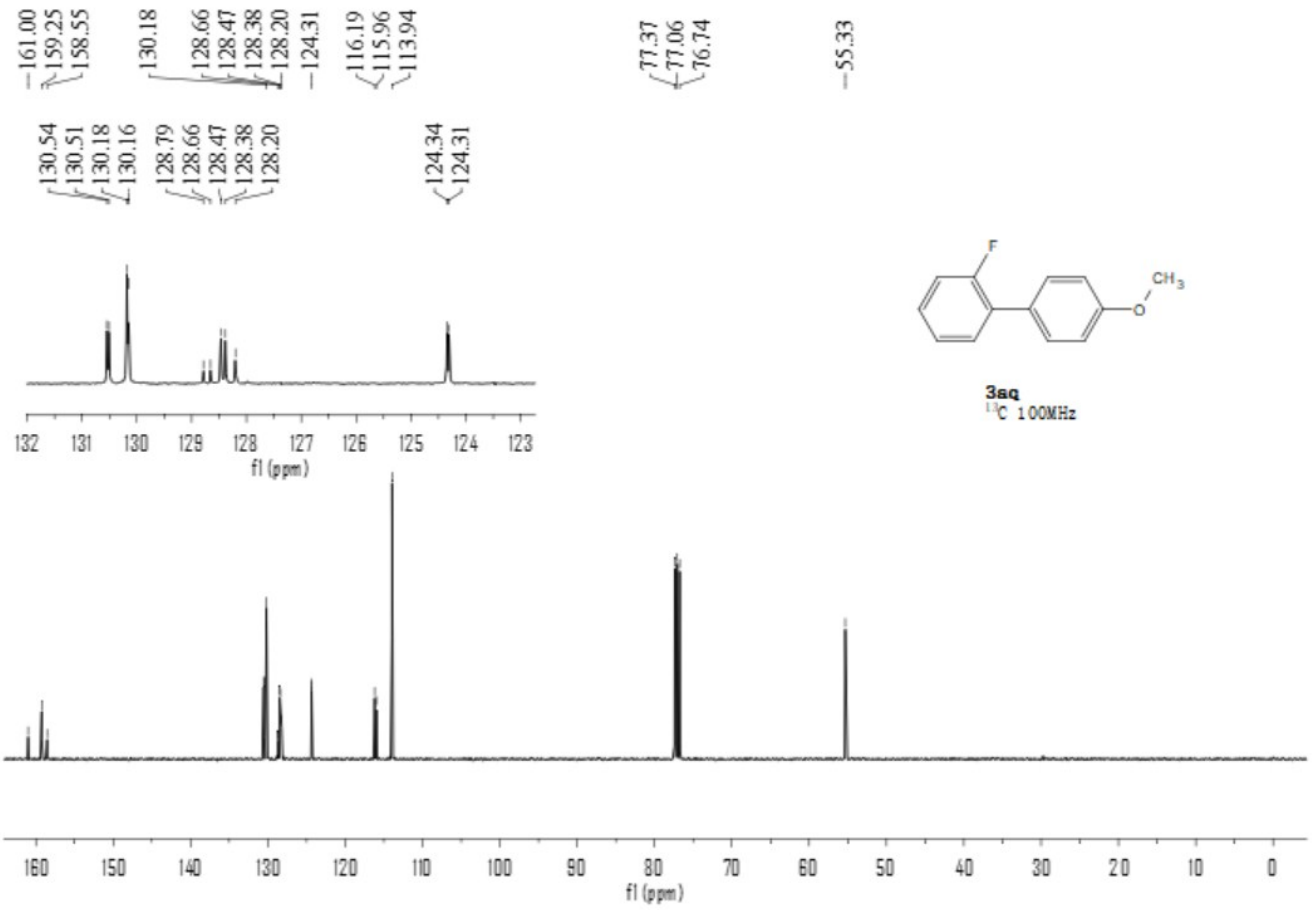

158.31
141.75
140.50
140.17
130.95
127.93
127.50
127.15
126.39
113.36
77.37
77.05
76.74
55.17
133.92
130.95
130.66
130.56
129.90
127.93
127.50
127.15
126.39
f1 (ppm)
3ao
13C 100MHz

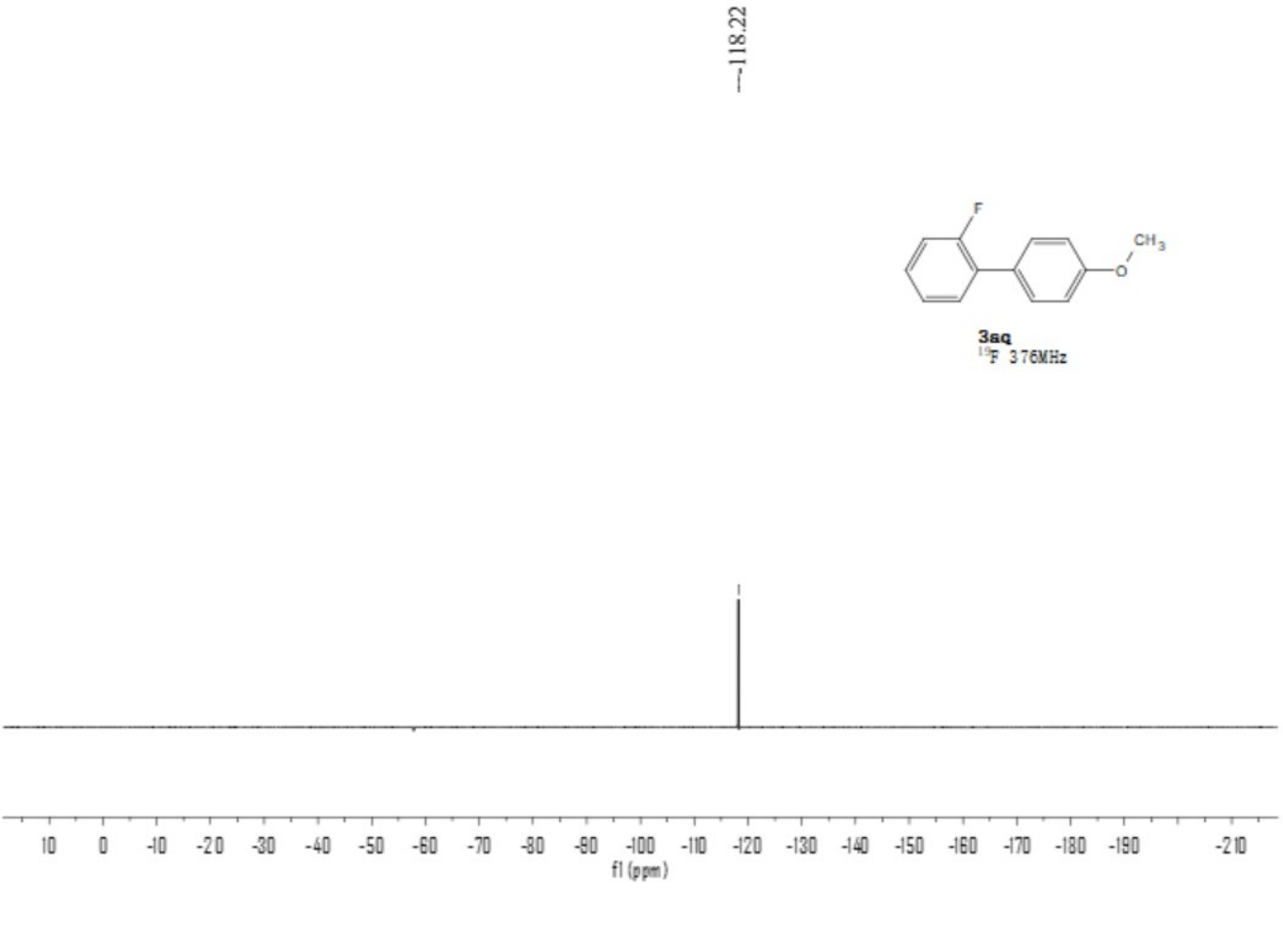

7.69
7.67
7.67
7.64
7.57
7.55
7.03
7.01
3.87
3.94
1.99
1.99
3.00
f1 (ppm)
3ap
1H 400MHz

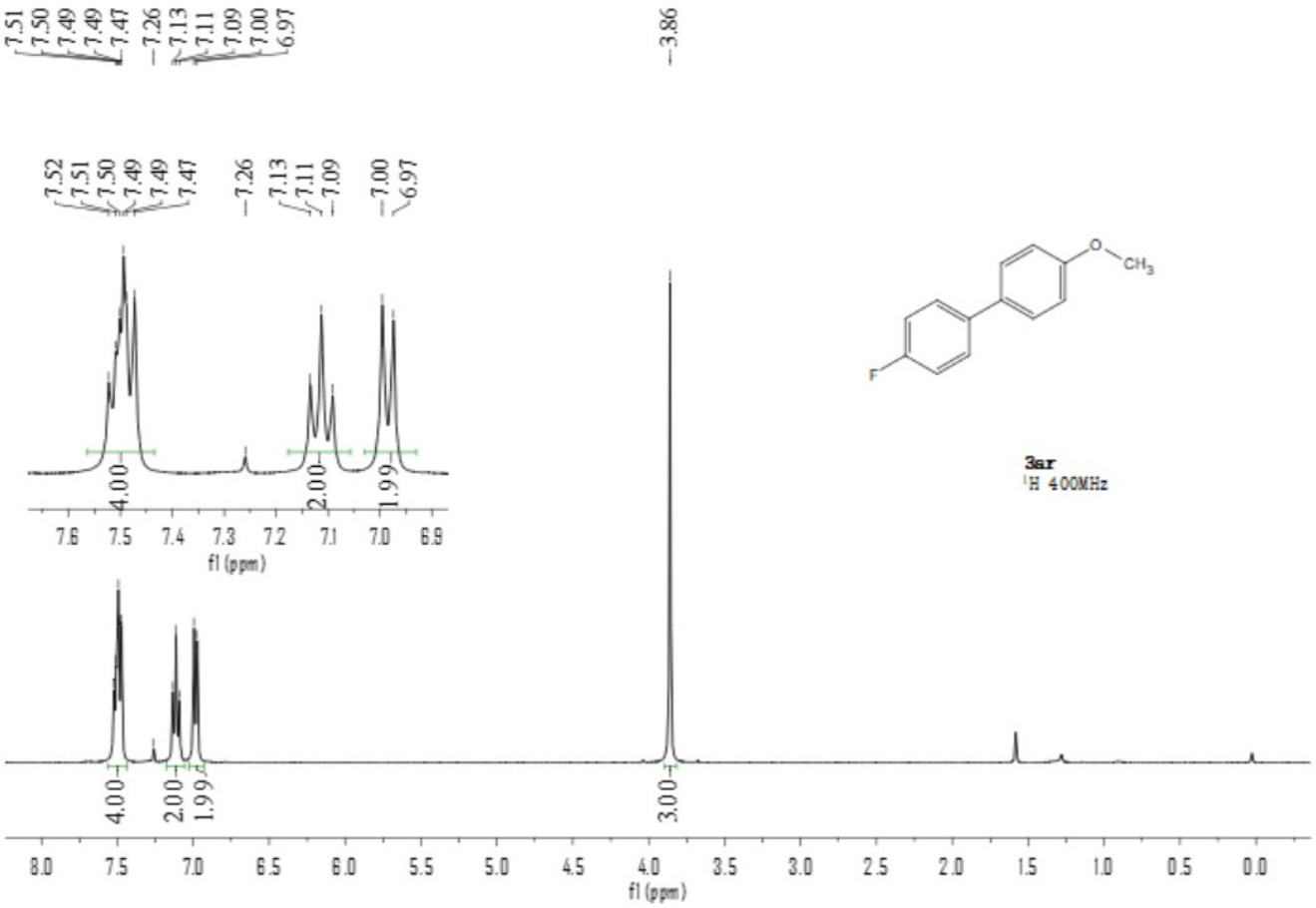

159.88
144.30
132.17
128.21
125.78
125.71
125.63
120.38
114.44
55.35
129.17
128.85
128.53
128.48
128.36
128.21
126.87
125.78
125.74
125.71
125.67
125.63
123.08
f1 (ppm)
3ap
13C 100MHz

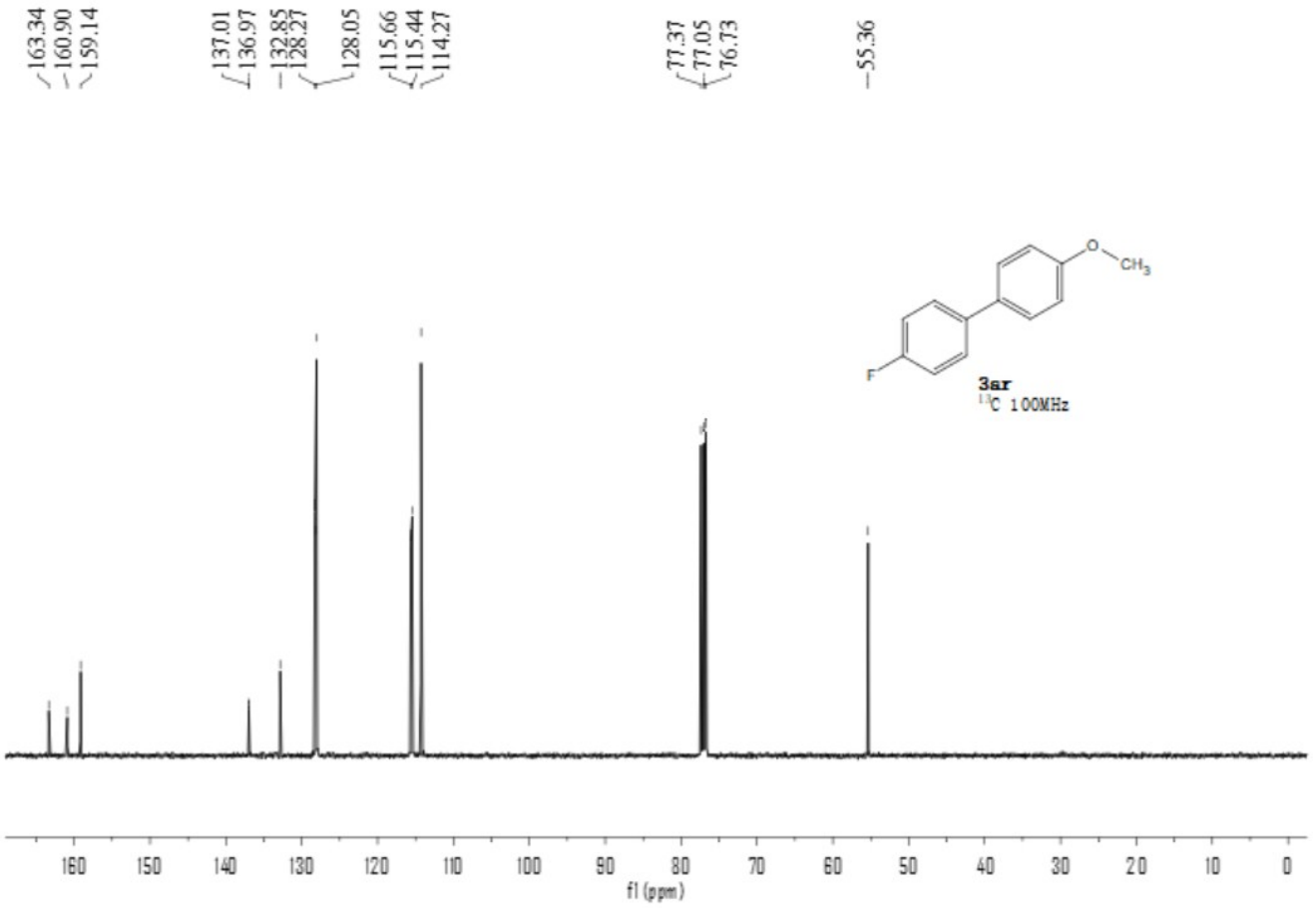

-62.32
F
F
F
CH3
O
3ap
19F 376MHz
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -210
f1 (ppm)

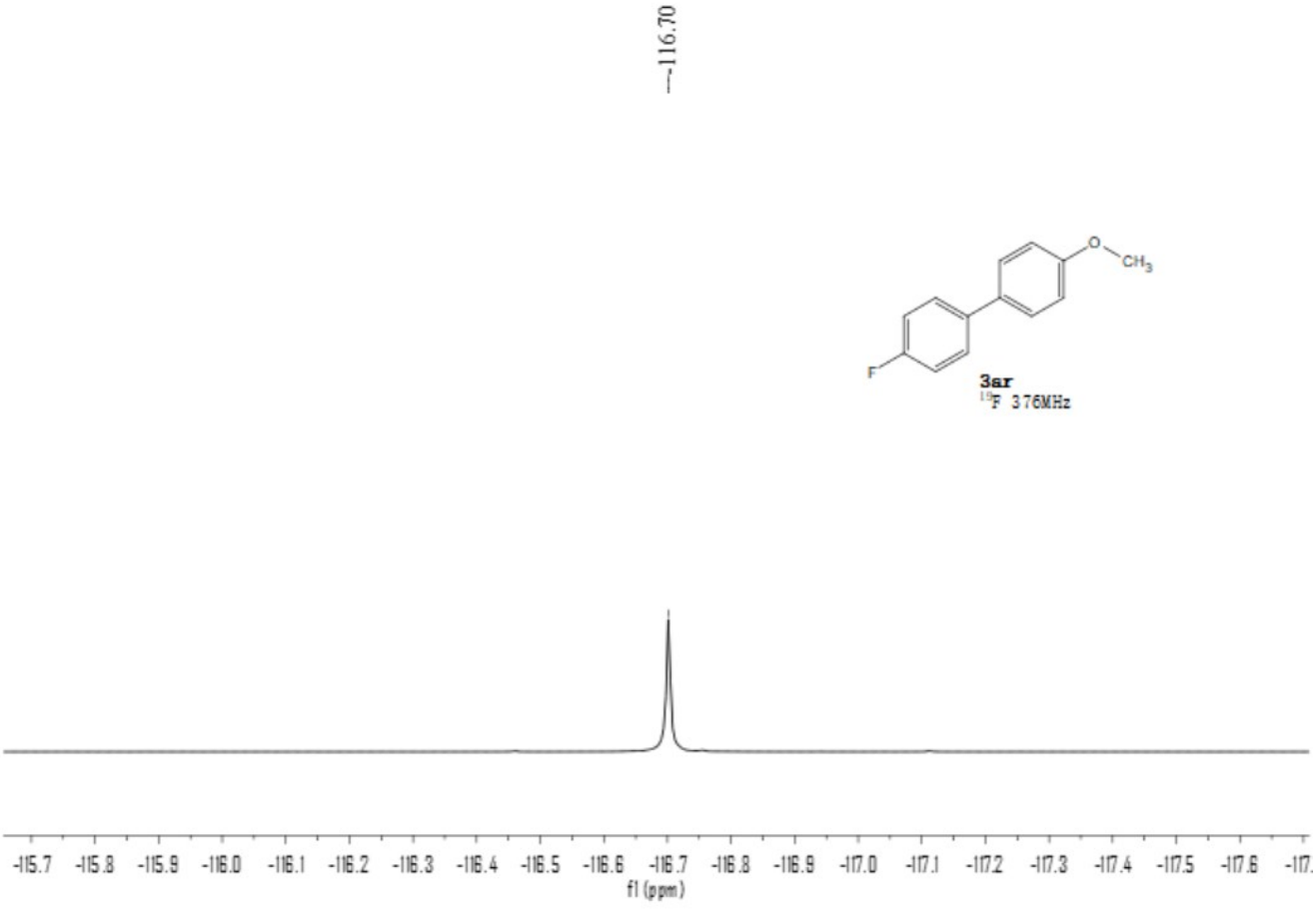

7.29
7.28
7.27
7.25
7.24
7.23
7.19
7.17
7.15
7.14
7.12
7.12
7.10
6.98
6.96
7.50
7.48
7.42
7.40
7.24
7.19
7.15
7.12
7.10
6.99
6.98
6.97
6.96
3.84
F
CH3
O
3aq
1H 400MHz
2.00
1.01
1.11
1.03
0.96
2.03
7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
2.00
1.01
1.11
1.02
0.96
2.03
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

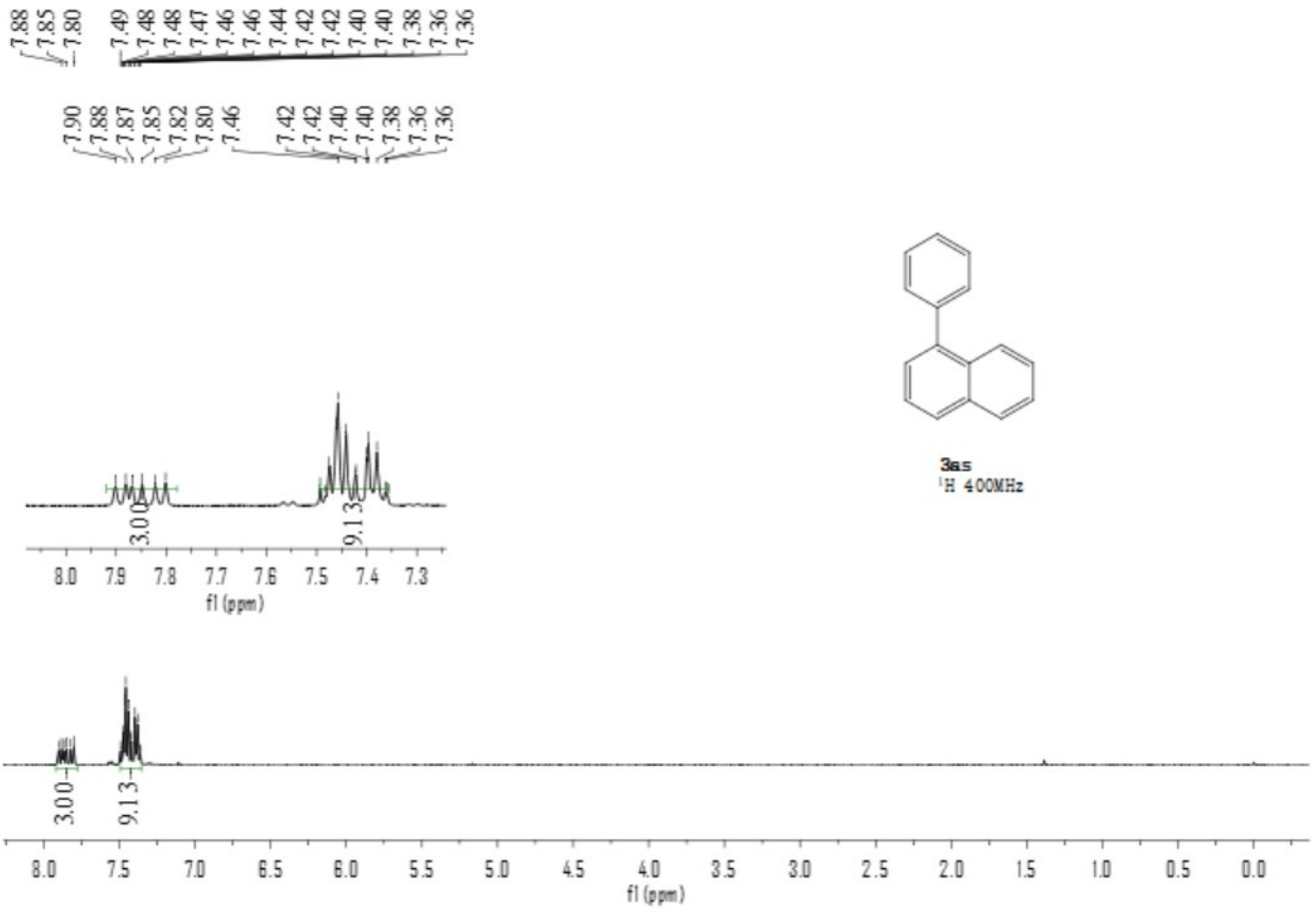

161.00
159.25
158.55
130.18
128.66
128.47
128.38
128.20
124.31
116.19
115.96
113.94
77.37
77.06
76.74
55.33
130.54
130.51
130.18
130.16
128.79
128.66
128.47
128.38
128.20
124.34
124.31
F
CH3
O
3aq
13C 100MHz
f1 (ppm)


118.22
F
CH3
O
3aq
19F 376MHz
f1 (ppm)

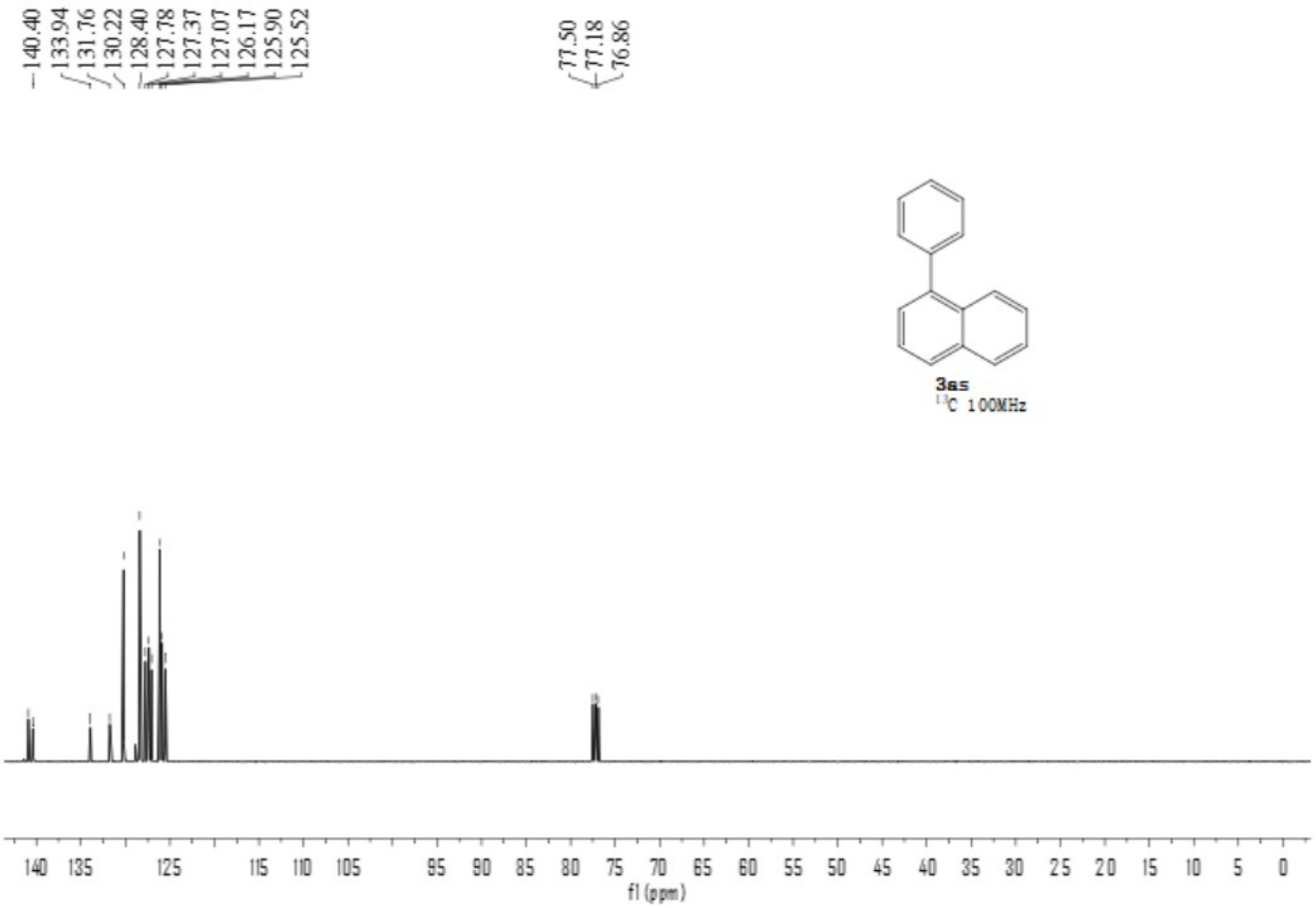

7.51
7.50
7.49
7.49
7.47
7.26
7.13
7.11
7.09
7.00
6.97
3.86
7.52
7.51
7.50
7.49
7.49
7.47
7.26
7.13
7.11
7.09
7.00
6.97
4.00
2.00
1.99
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
O
CH3
F
3ar
1H 400MHz
4.00
2.00
1.99
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

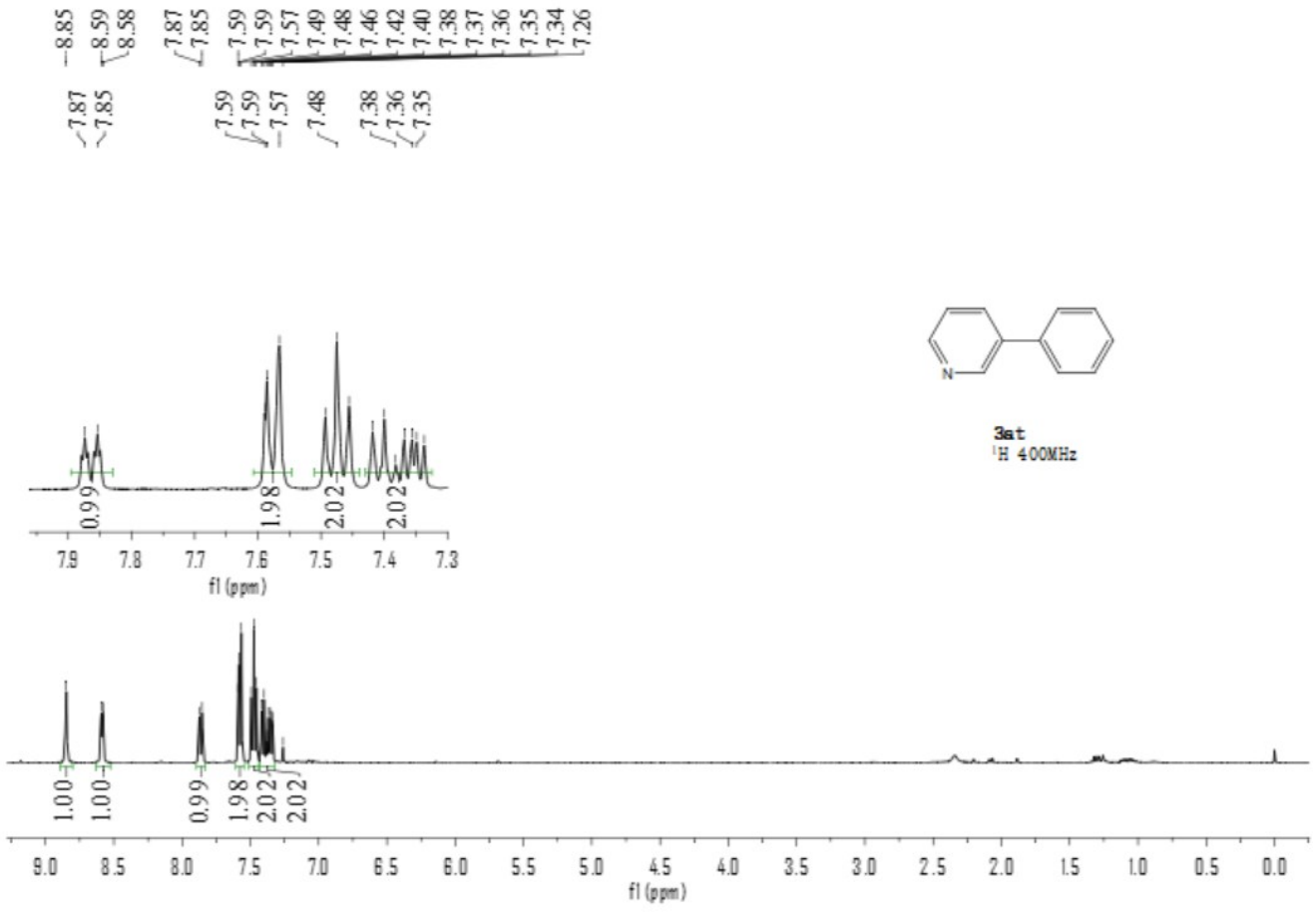

163.34
160.90
159.14
137.01
136.97
132.85
128.27
128.05
115.66
115.44
114.27
77.37
77.05
76.73
55.36
O
CH3
F
3ar
13C 100MHz
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

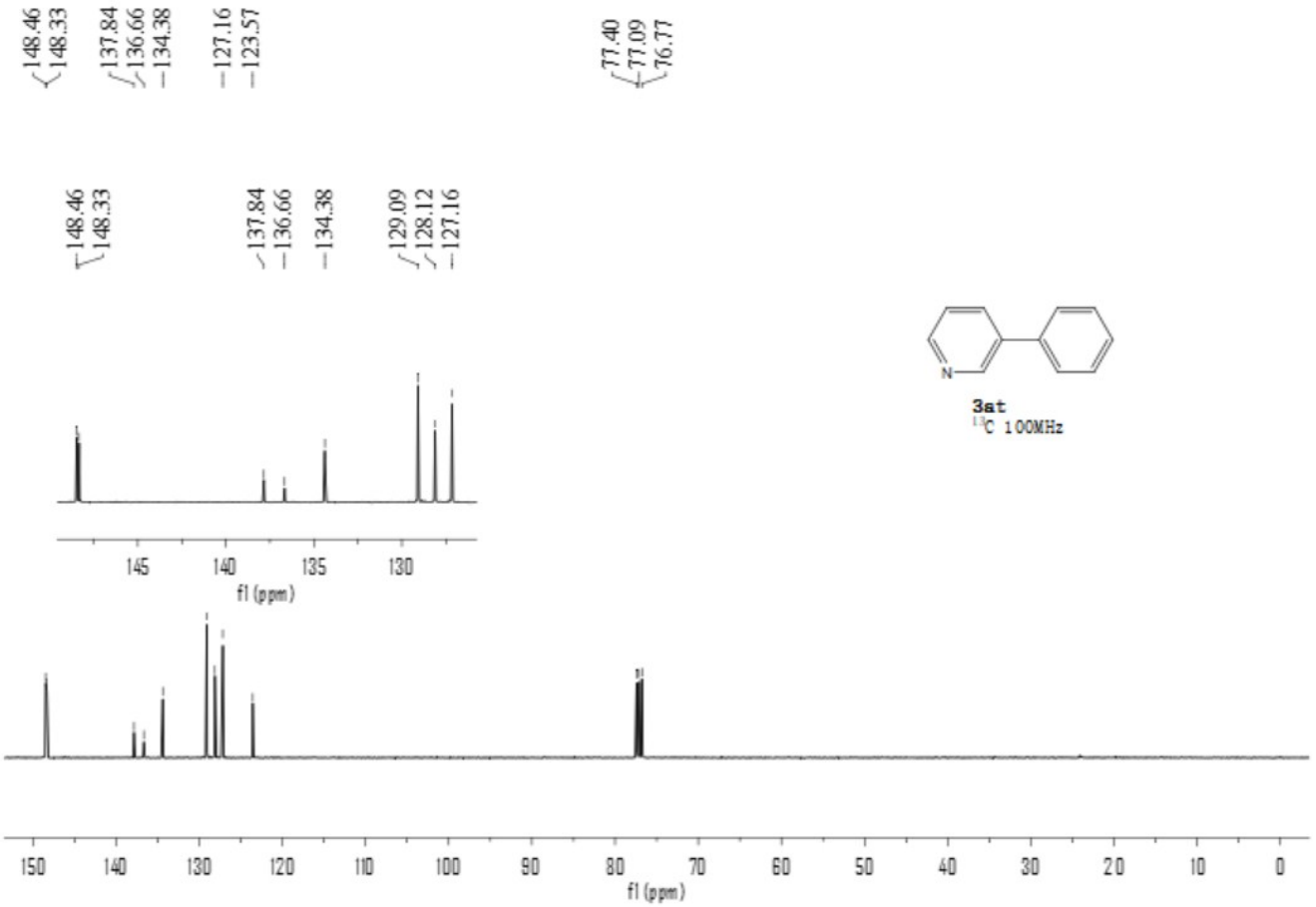


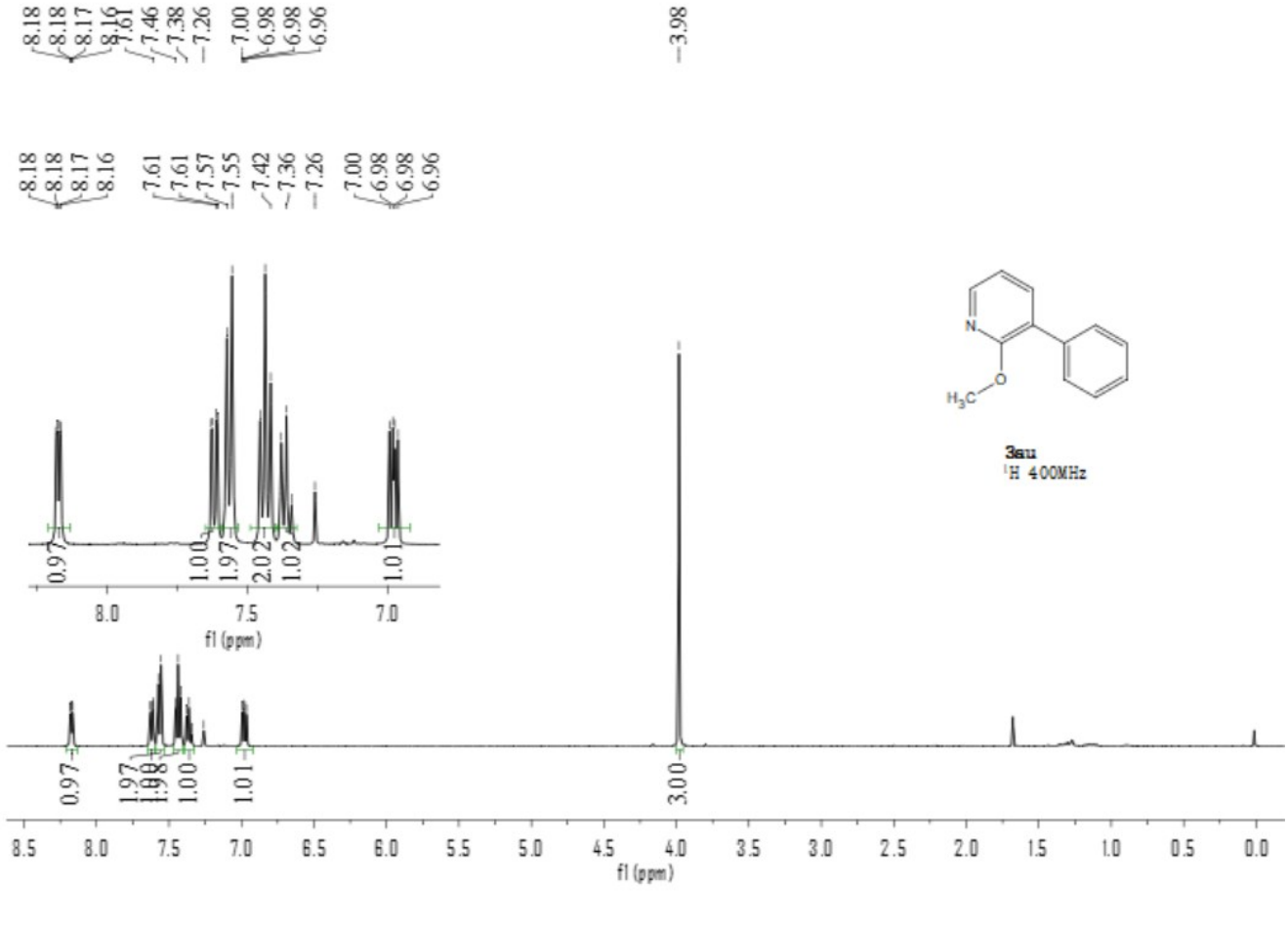


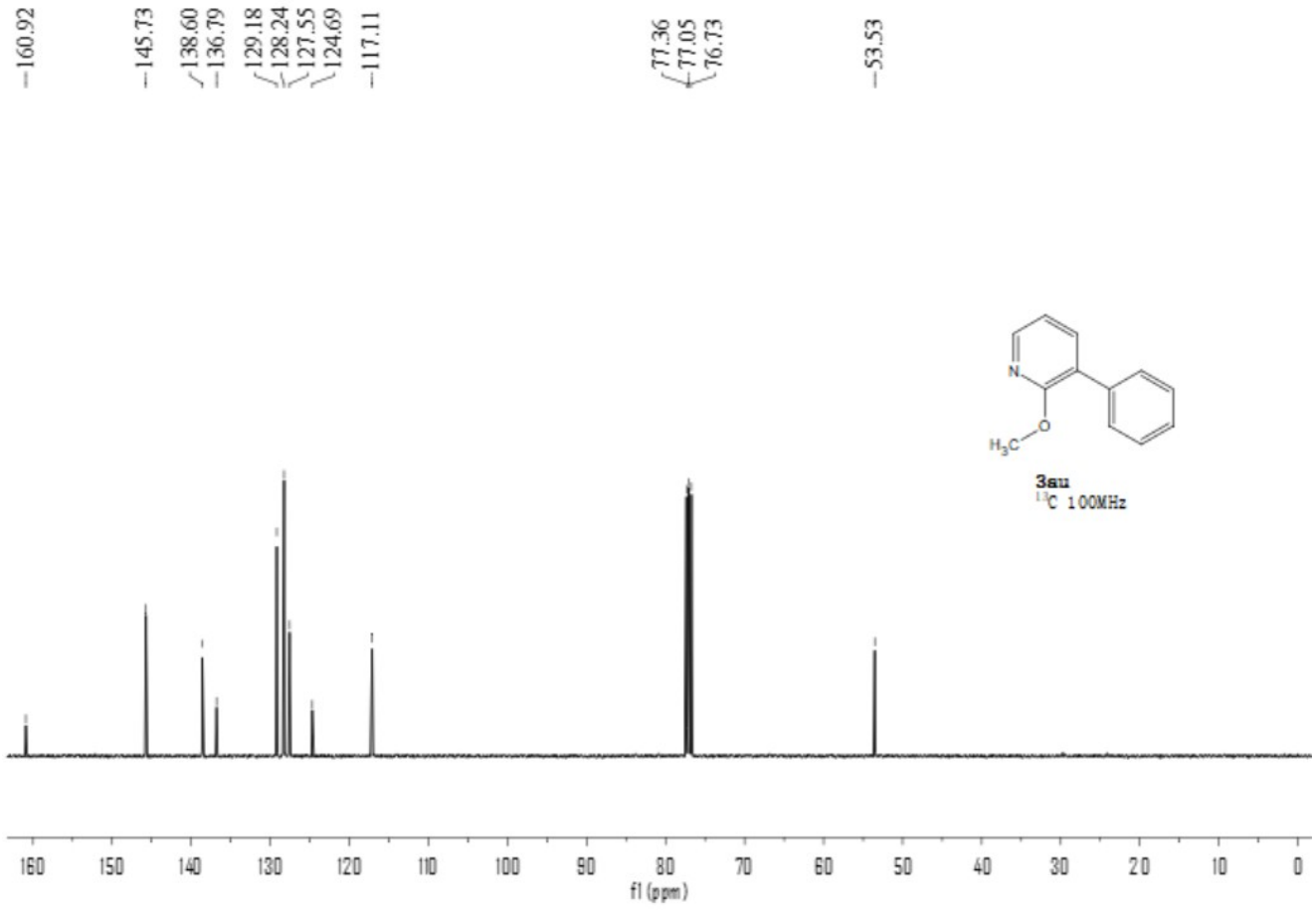
3as
1H 400MHz

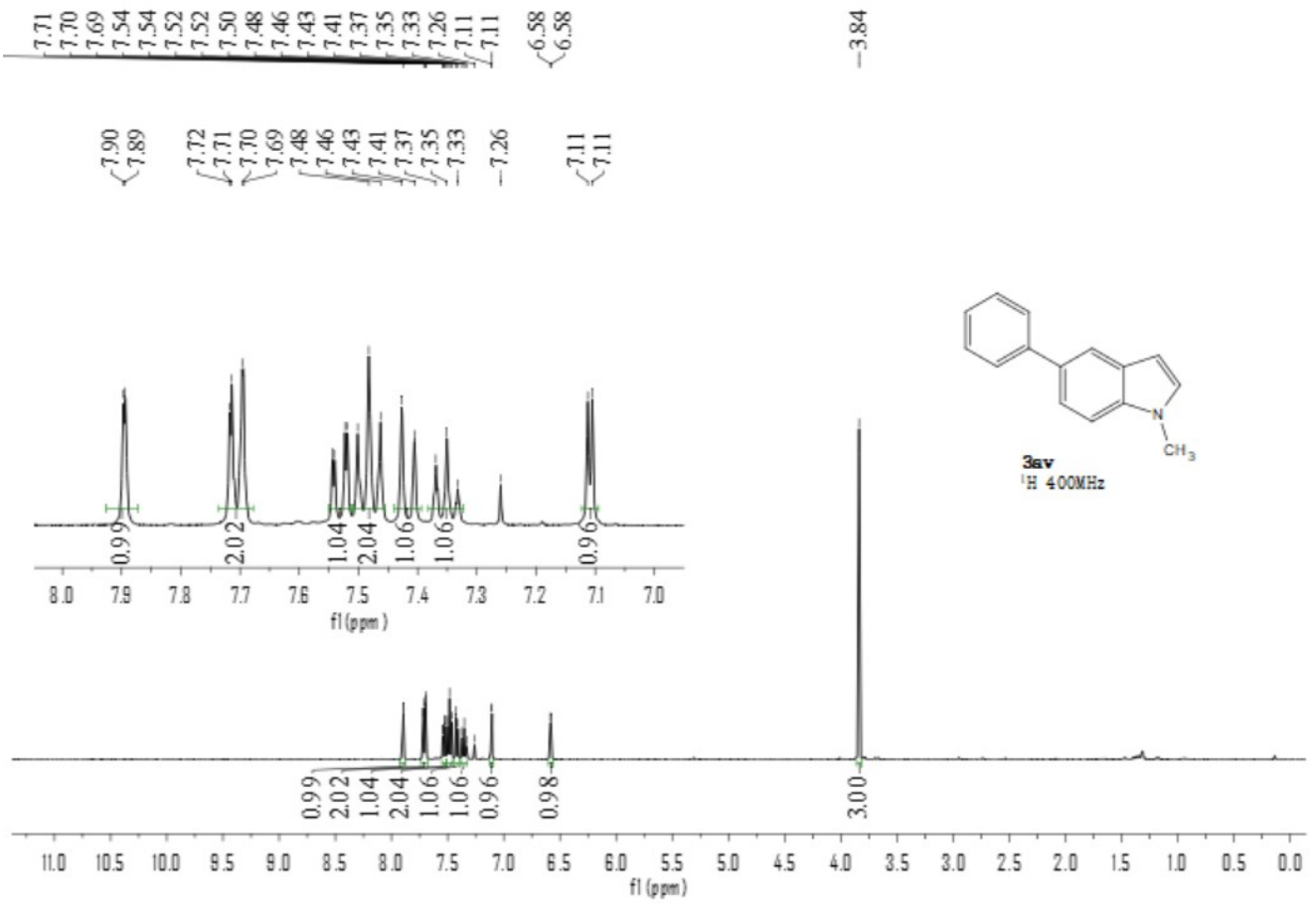

140.40
133.94
131.76
130.22
128.40
127.78
127.37
127.07
126.17
125.90
125.52
77.50
77.18
76.86
3as
13C 100MHz
f1 (ppm)

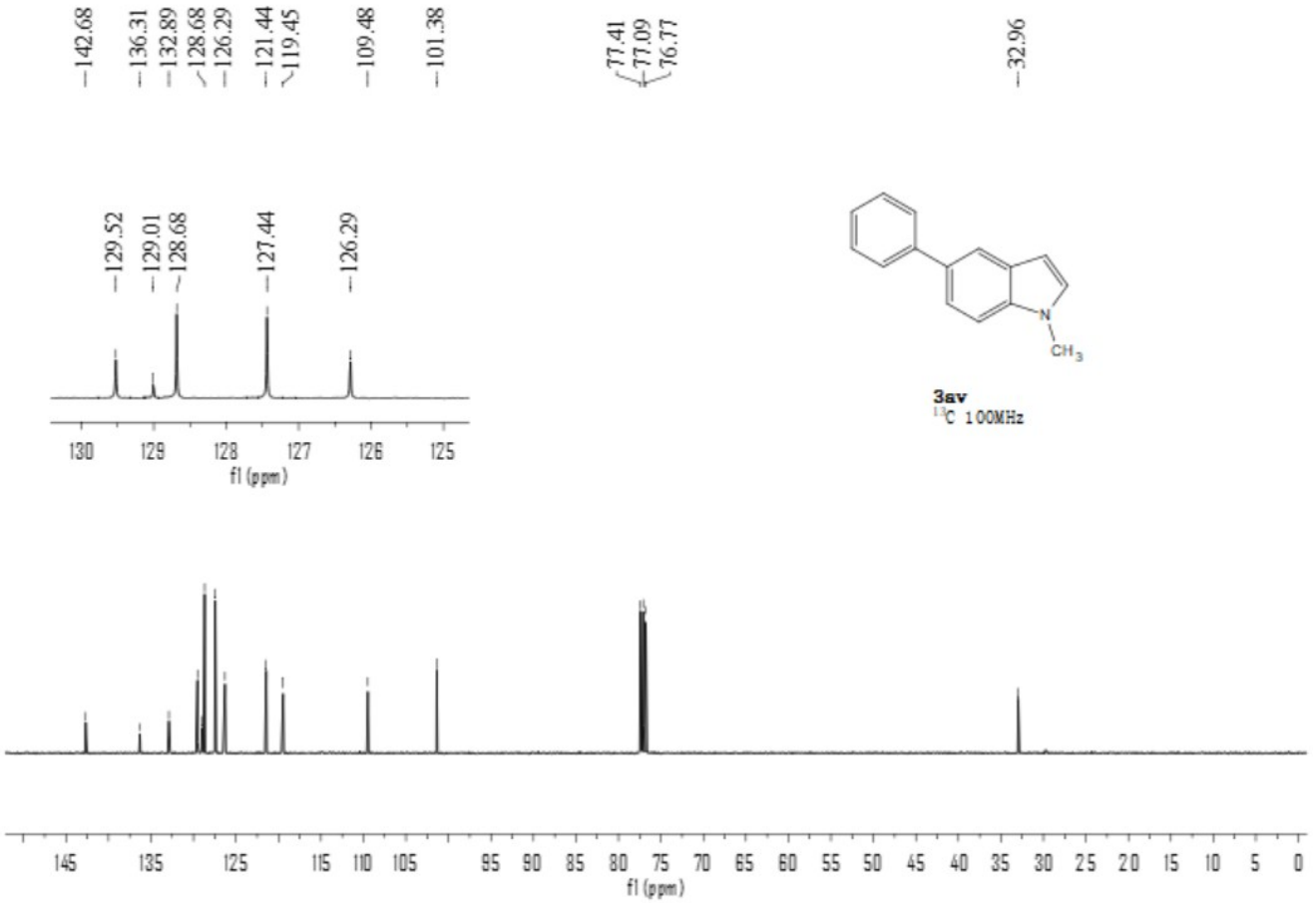

8.85
8.59
8.58
7.87
7.85
7.59
7.59
7.57
7.49
7.48
7.46
7.42
7.40
7.38
7.37
7.36
7.35
7.34
7.26
0.99
1.98
2.02
2.02
3at
1H 400MHz
1.00
1.00
0.99
1.98
2.02
2.02
f1 (ppm)


148.46
148.33
137.84
136.66
134.38
127.16
123.57
77.40
77.09
76.77
129.09
128.12
f1 (ppm)
3at
13C 100MHz


8.18
8.17
8.16
7.61
7.57
7.55
7.42
7.36
7.26
7.00
6.98
6.96
3.98
0.97
1.00
1.97
2.02
1.02
1.01
3.00
f1 (ppm)
3au
1H 400MHz


160.92
145.73
138.60
136.79
129.18
128.24
127.55
124.69
117.11
77.36
77.05
76.73
53.53
3au
13C 100MHz
f1 (ppm)


7.71
7.70
7.69
7.54
7.54
7.52
7.52
7.50
7.48
7.46
7.43
7.41
7.37
7.35
7.33
7.26
7.11
7.11
6.58
6.58
3.84
7.90
7.89
7.72
7.71
7.70
7.69
7.48
7.46
7.43
7.41
7.37
7.35
7.33
7.26
7.11
7.11
0.99
2.02
1.04
2.04
1.06
1.06
0.96
0.99
2.02
1.04
2.04
1.06
1.06
0.96
0.98
3.00
3av
1H 400MHz
f1 (ppm)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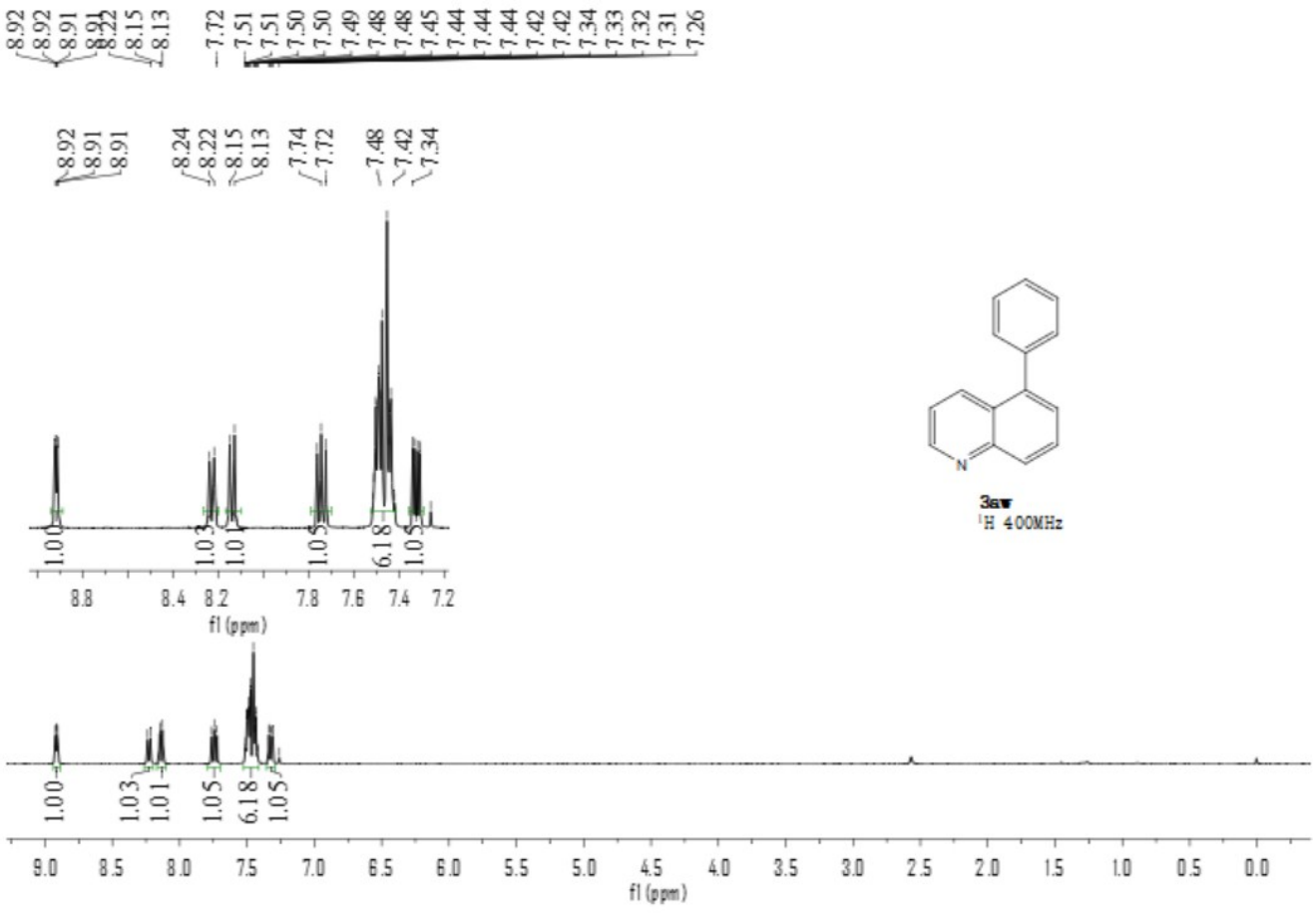
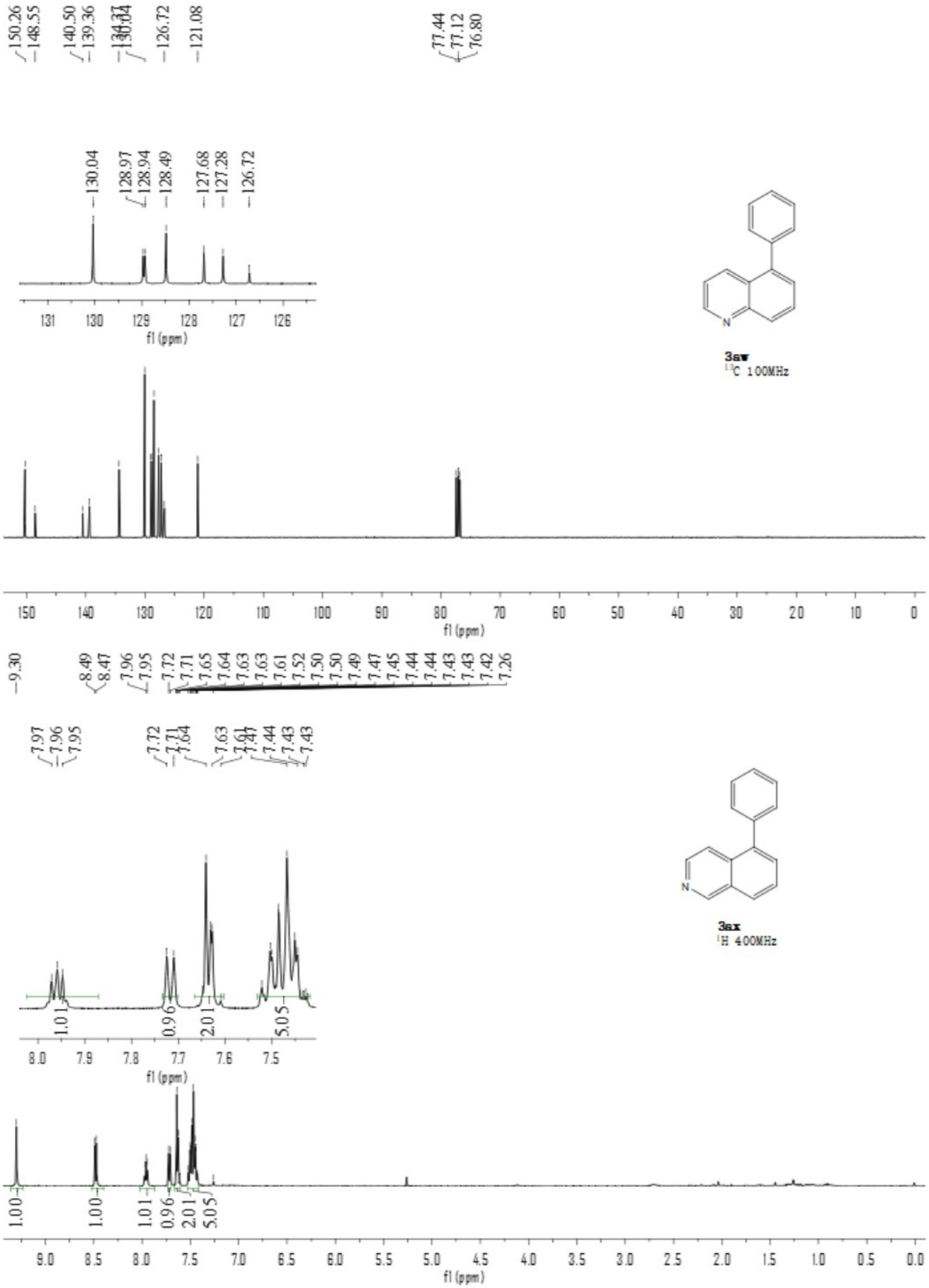
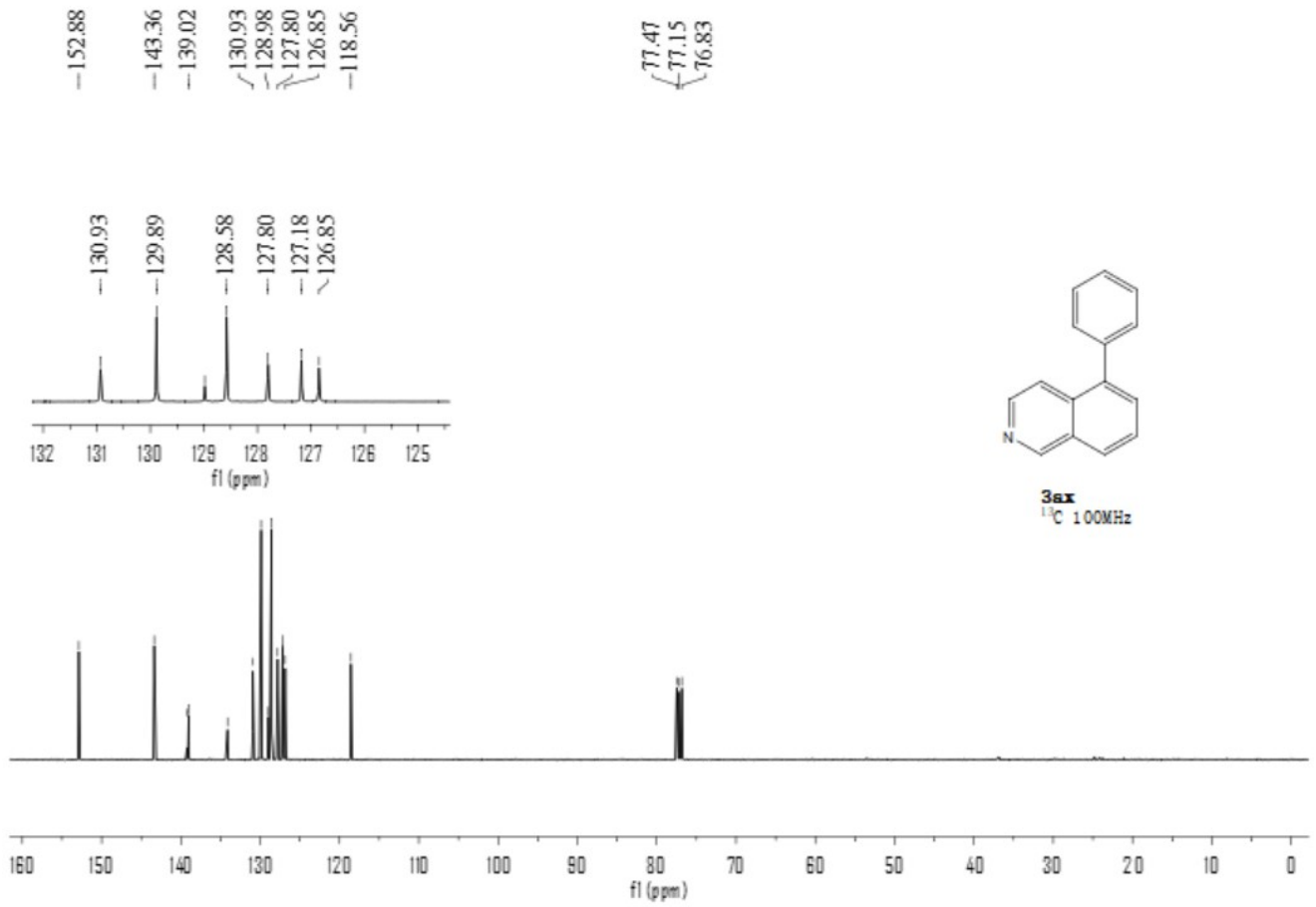
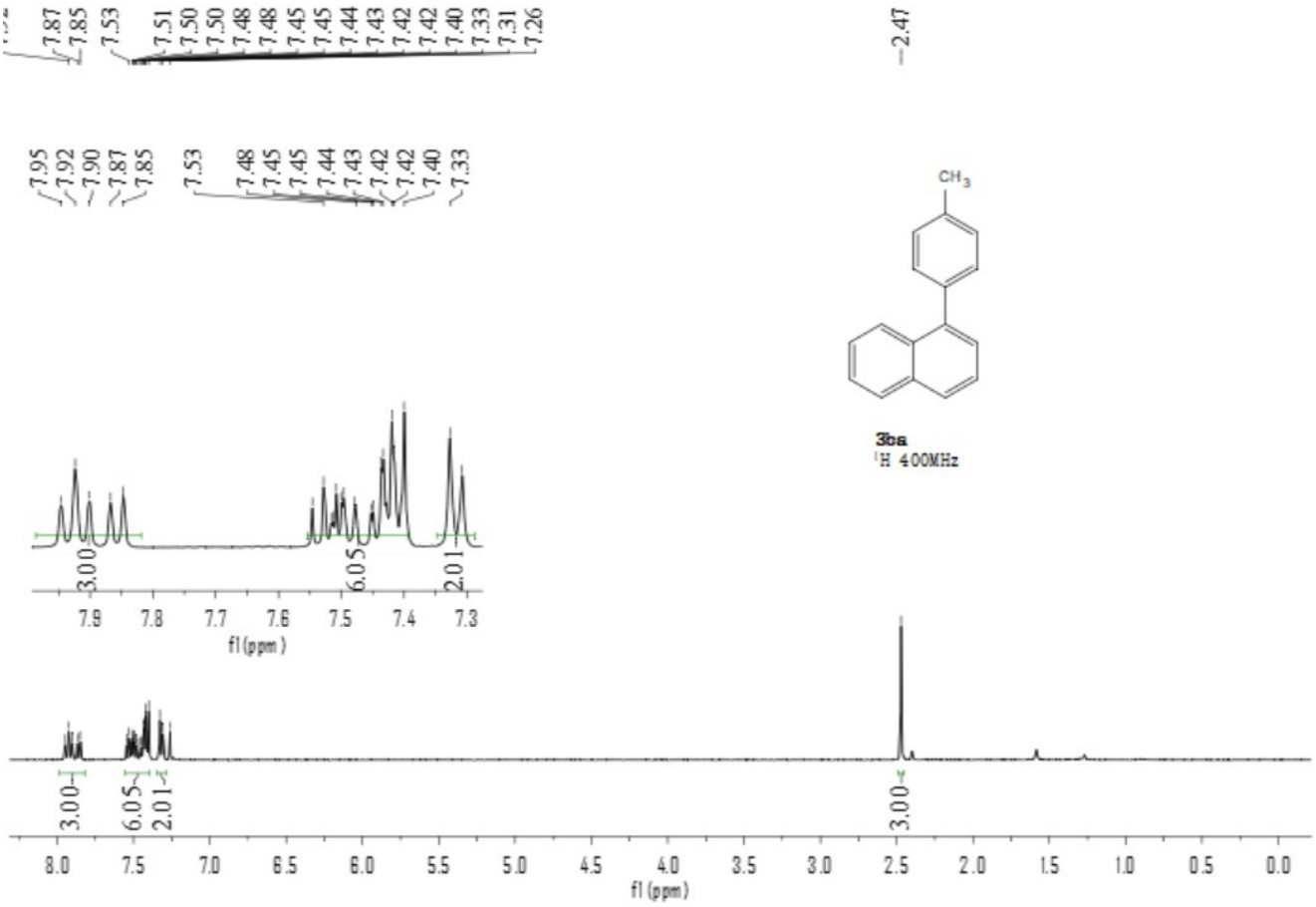
136.31
132.89
128.68
126.29
121.44
119.45
109.48
101.38
77.41
77.09
76.77
32.96
129.52
129.01
128.68
127.44
126.29
f1 (ppm)
N
CH3
3av
13C 100MHz


8.92
8.92
8.91
8.91
8.22
8.15
8.13
7.72
7.51
7.51
7.50
7.50
7.49
7.48
7.48
7.45
7.44
7.44
7.44
7.42
7.42
7.34
7.33
7.32
7.31
7.26
8.92
8.91
8.91
8.24
8.22
8.15
8.13
7.74
7.72
7.48
7.42
7.34
1.00
1.03
1.01
1.05
6.18
1.05
f1 (ppm)
N
3av
1H 400MHz


150.26
148.55
140.50
139.36
130.04
126.72
121.08
77.44
77.12
76.80
130.04
128.97
128.94
128.49
127.68
127.28
126.72
f1 (ppm)
3aw
13C 100MHz
f1 (ppm)
9.30
8.49
8.47
7.96
7.95
7.72
7.71
7.65
7.64
7.63
7.63
7.61
7.52
7.50
7.50
7.49
7.47
7.45
7.44
7.44
7.43
7.43
7.42
7.26
1.01
0.96
2.01
5.05
f1 (ppm)
3ax
1H 400MHz
1.00
1.00
1.01
0.96
2.01
5.05
f1 (ppm)


152.88
143.36
139.02
130.93
128.98
127.80
126.85
118.56
77.47
77.15
76.83
130.93
129.89
128.58
127.80
127.18
126.85
f1 (ppm)
3ax
13C 100MHz
f1 (ppm)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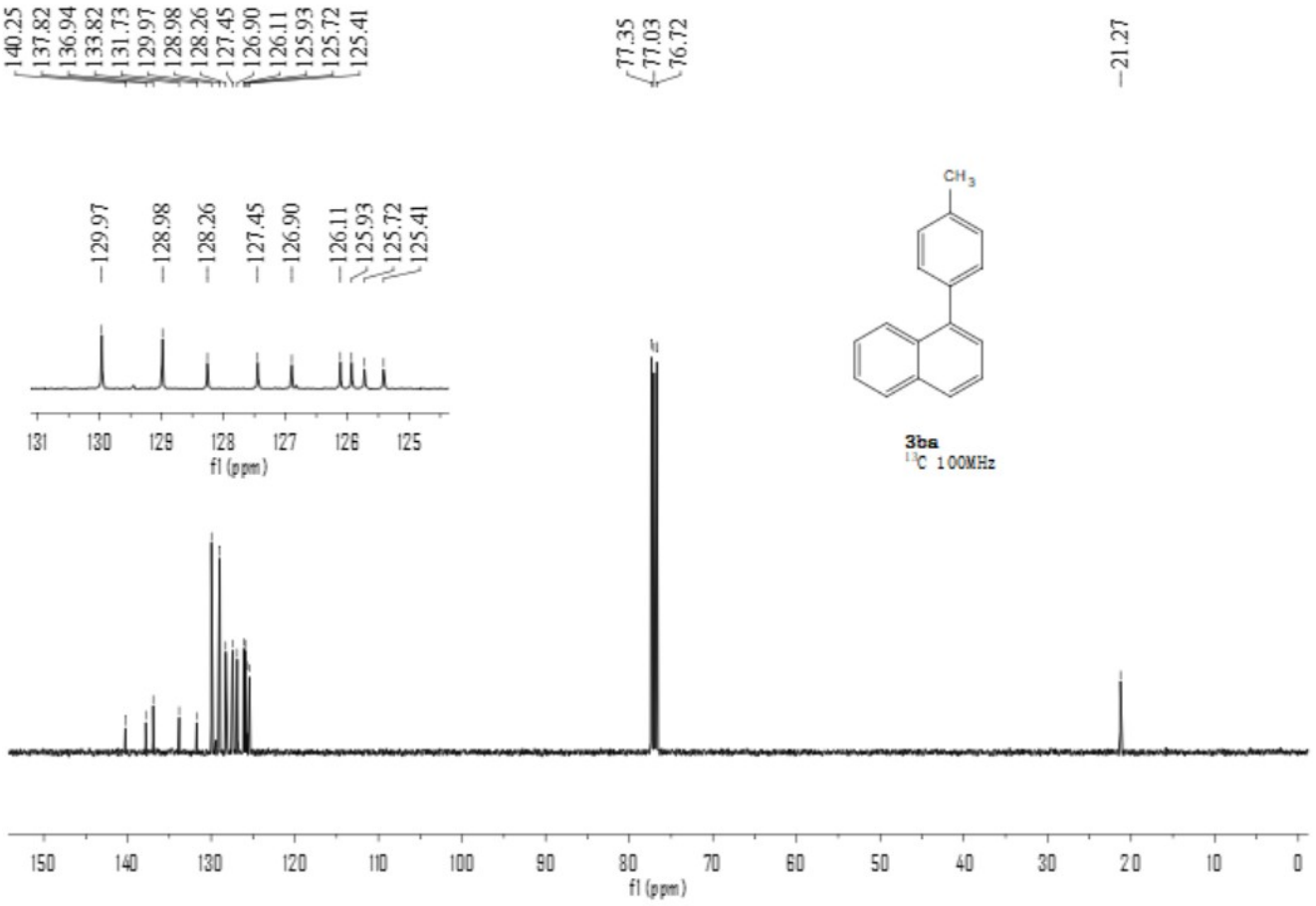
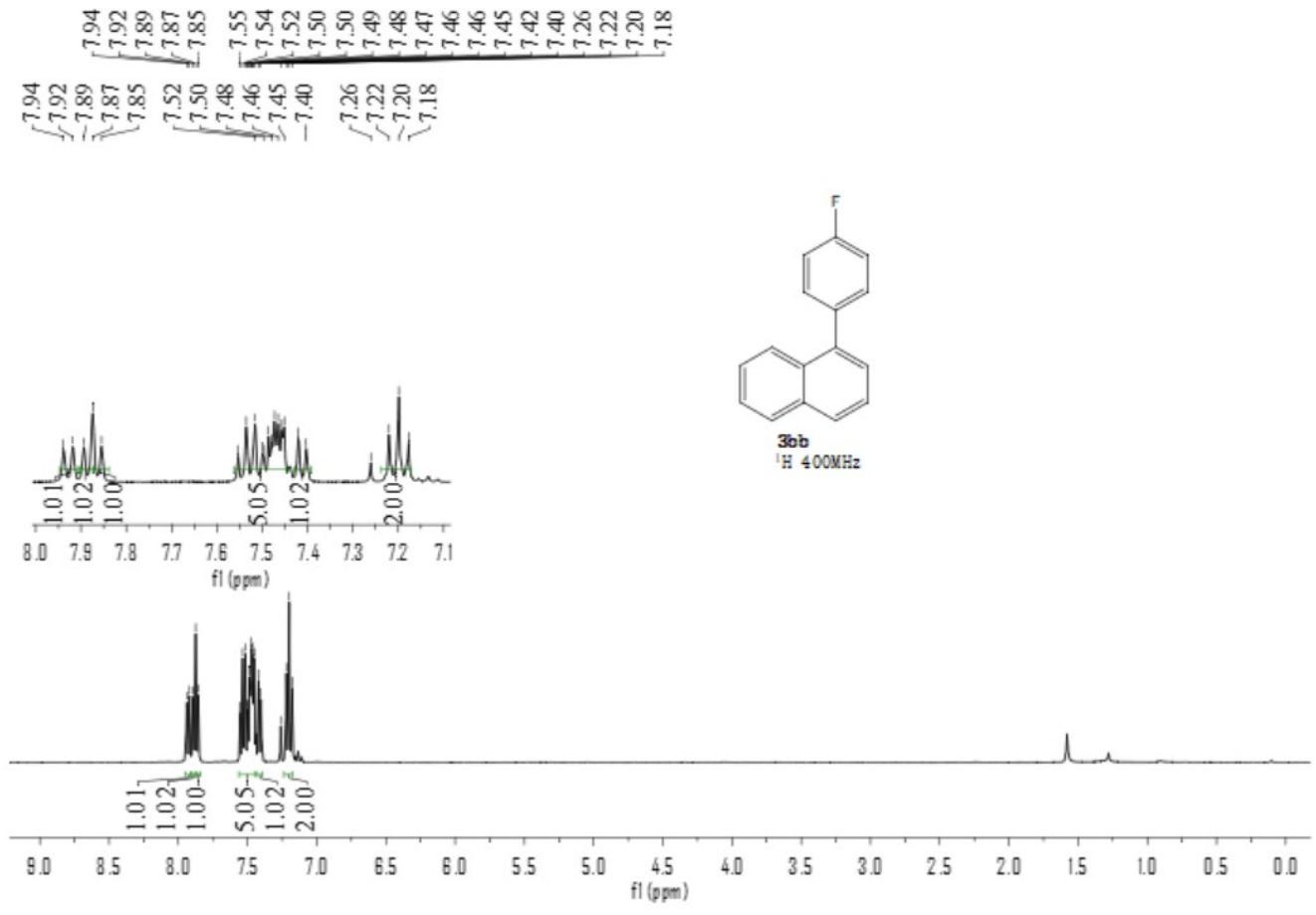
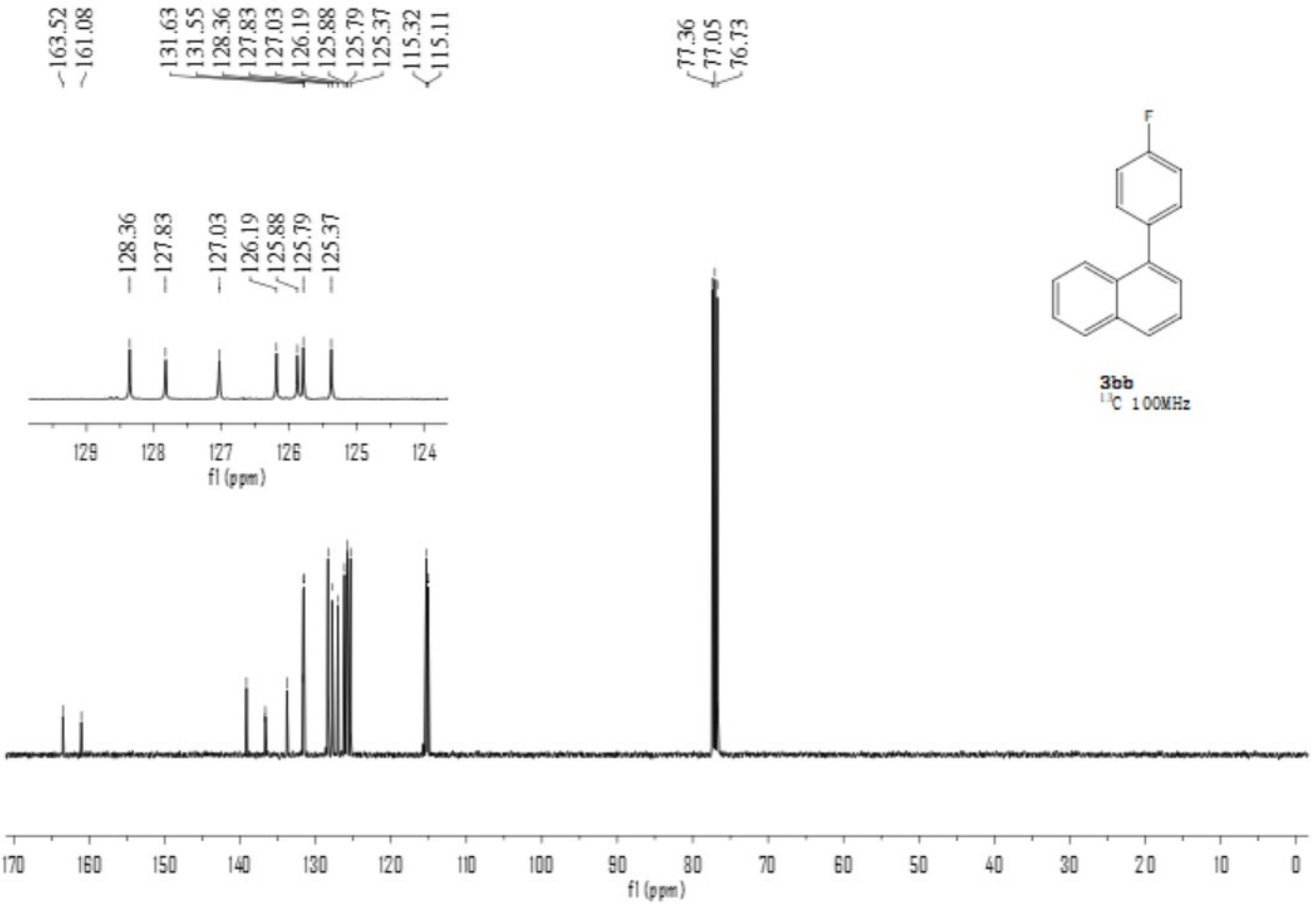
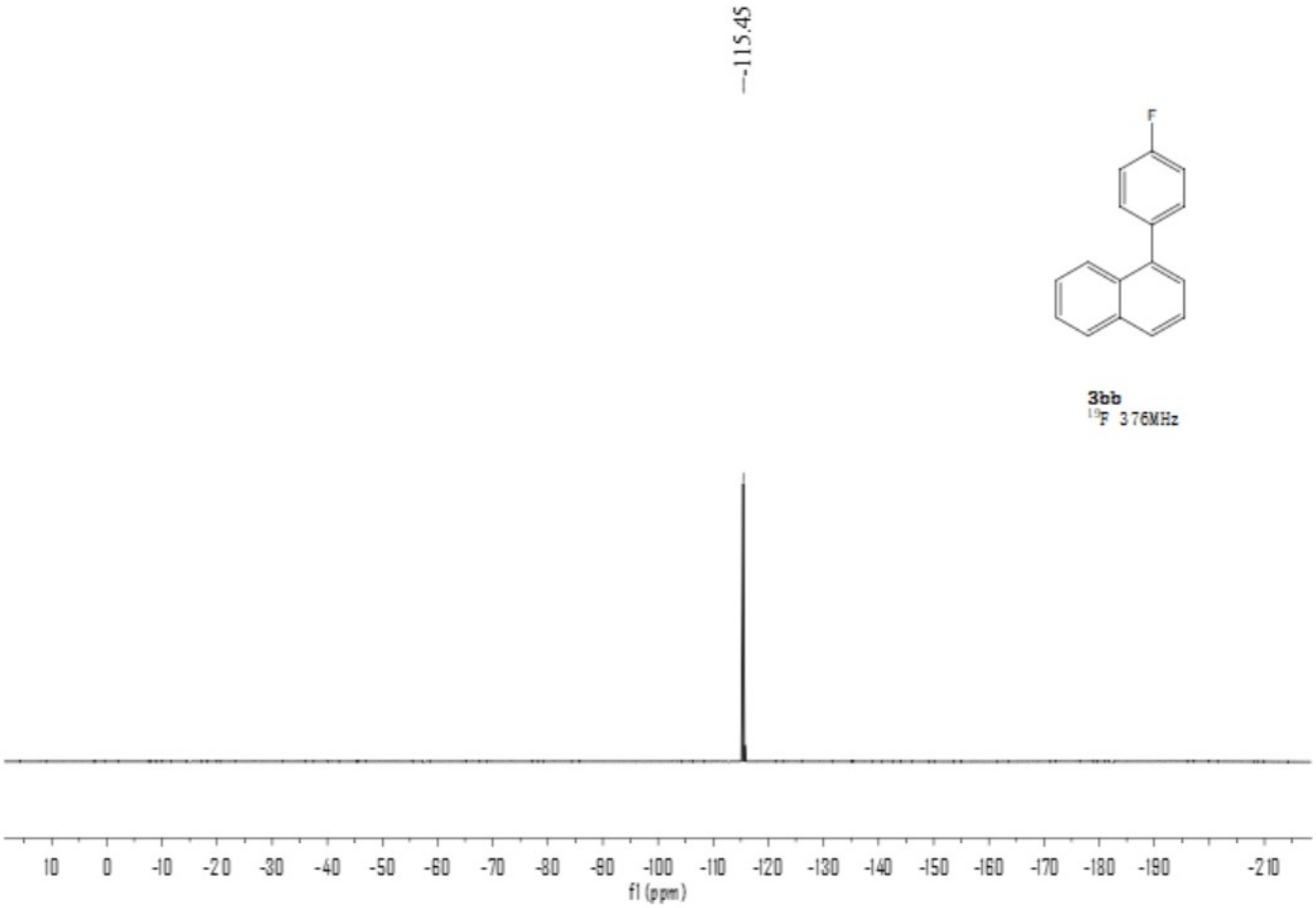
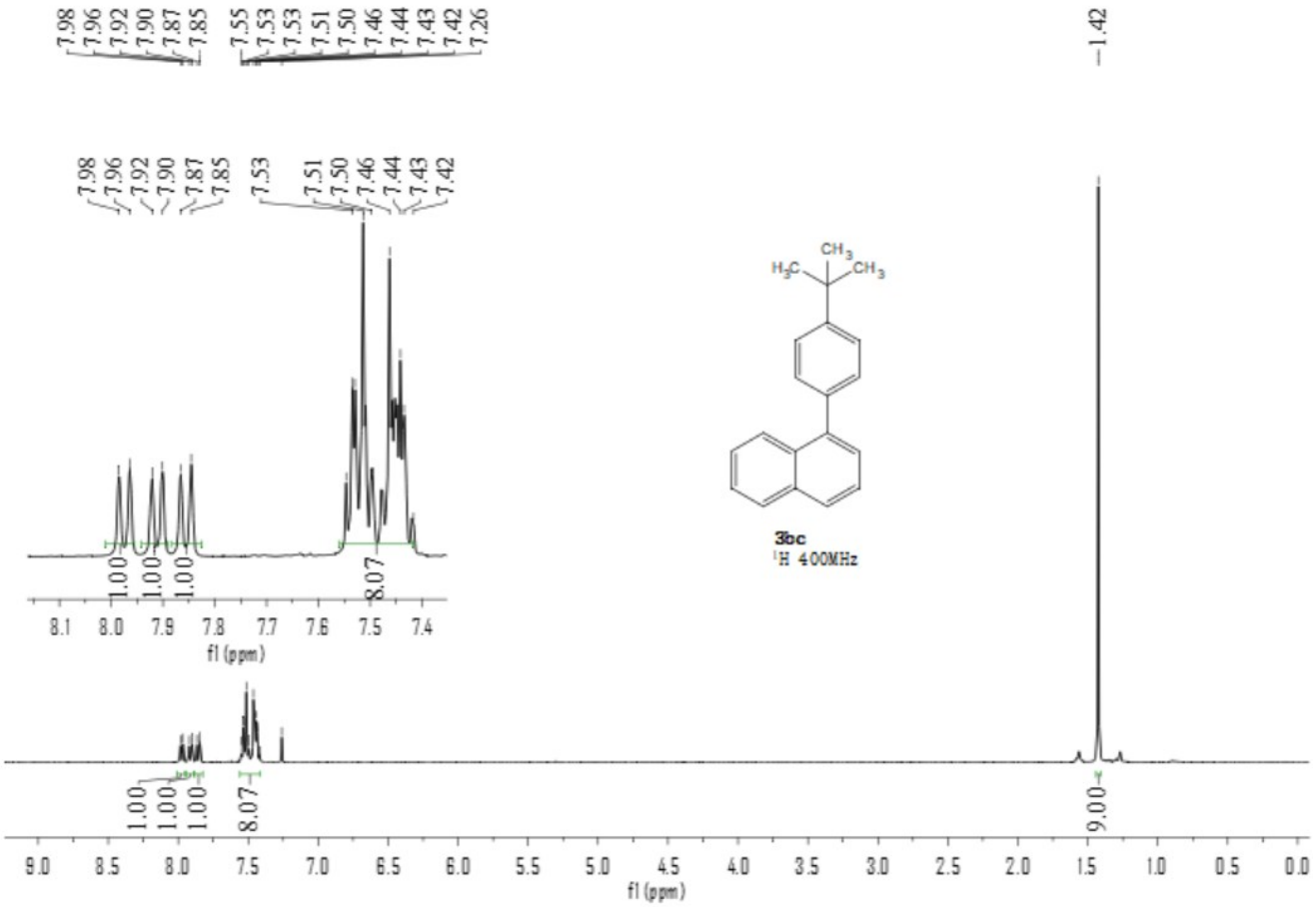
7.53
7.51
7.50
7.50
7.48
7.48
7.45
7.45
7.44
7.43
7.42
7.42
7.40
7.33
7.31
7.26
2.47
7.95
7.92
7.90
7.87
7.85
7.53
7.48
7.45
7.45
7.44
7.43
7.42
7.42
7.40
7.33
CH3
3.00
6.05
2.01
f1 (ppm)
3ba
1H 400MHz
3.00
6.05
2.01
3.00
f1 (ppm)

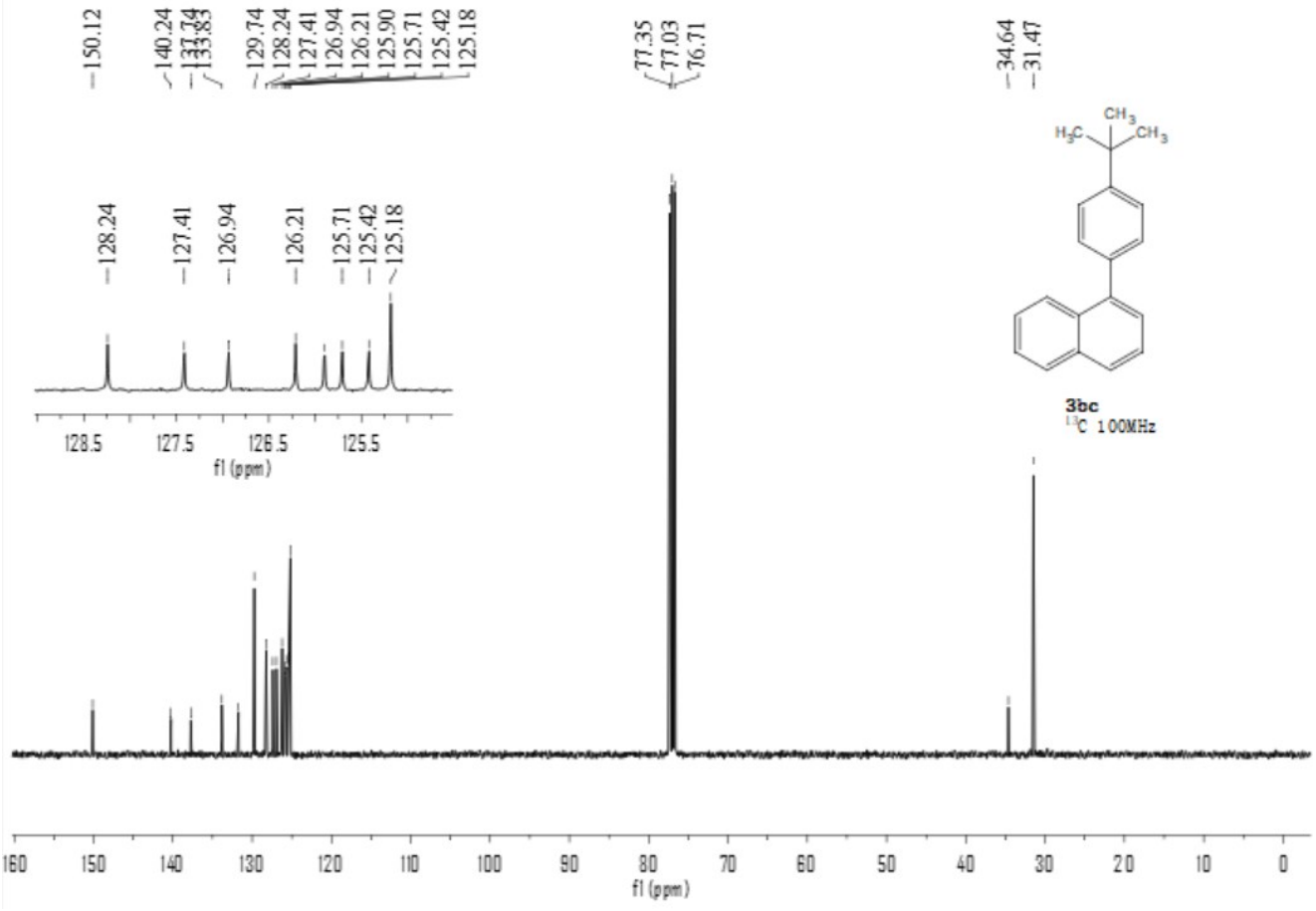

140.25
137.82
136.94
133.82
131.73
129.97
128.98
128.26
127.45
126.90
126.11
125.93
125.72
125.41
77.35
77.03
76.72
21.27
CH3
3ba
13C 100MHz
f1 (ppm)

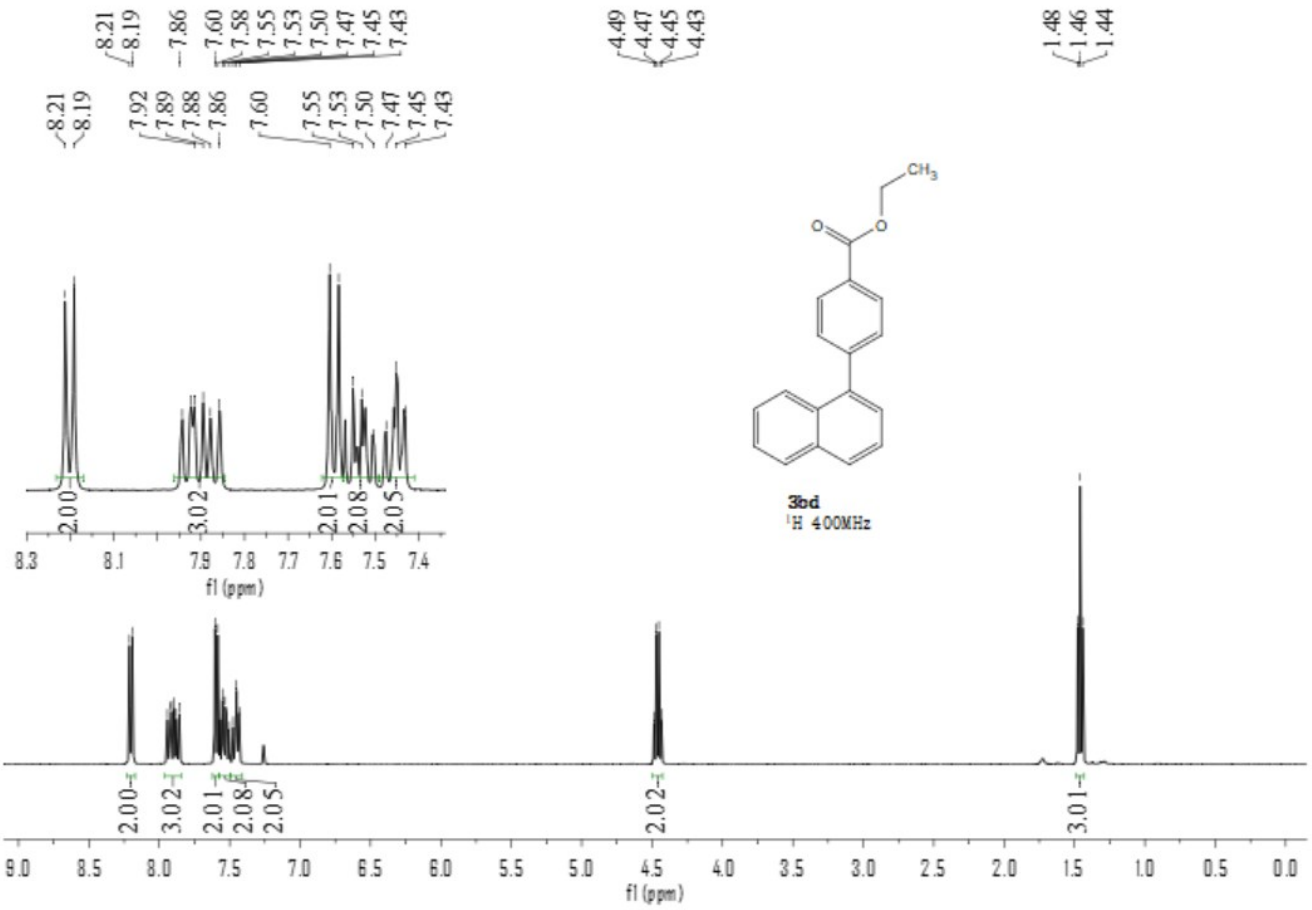

7.94
7.92
7.89
7.87
7.85
7.55
7.54
7.52
7.50
7.50
7.49
7.48
7.47
7.46
7.46
7.45
7.42
7.40
7.26
7.22
7.20
7.18
F
3bb
1H 400MHz
1.01
1.02
1.00
5.05
1.02
2.00
f1 (ppm)

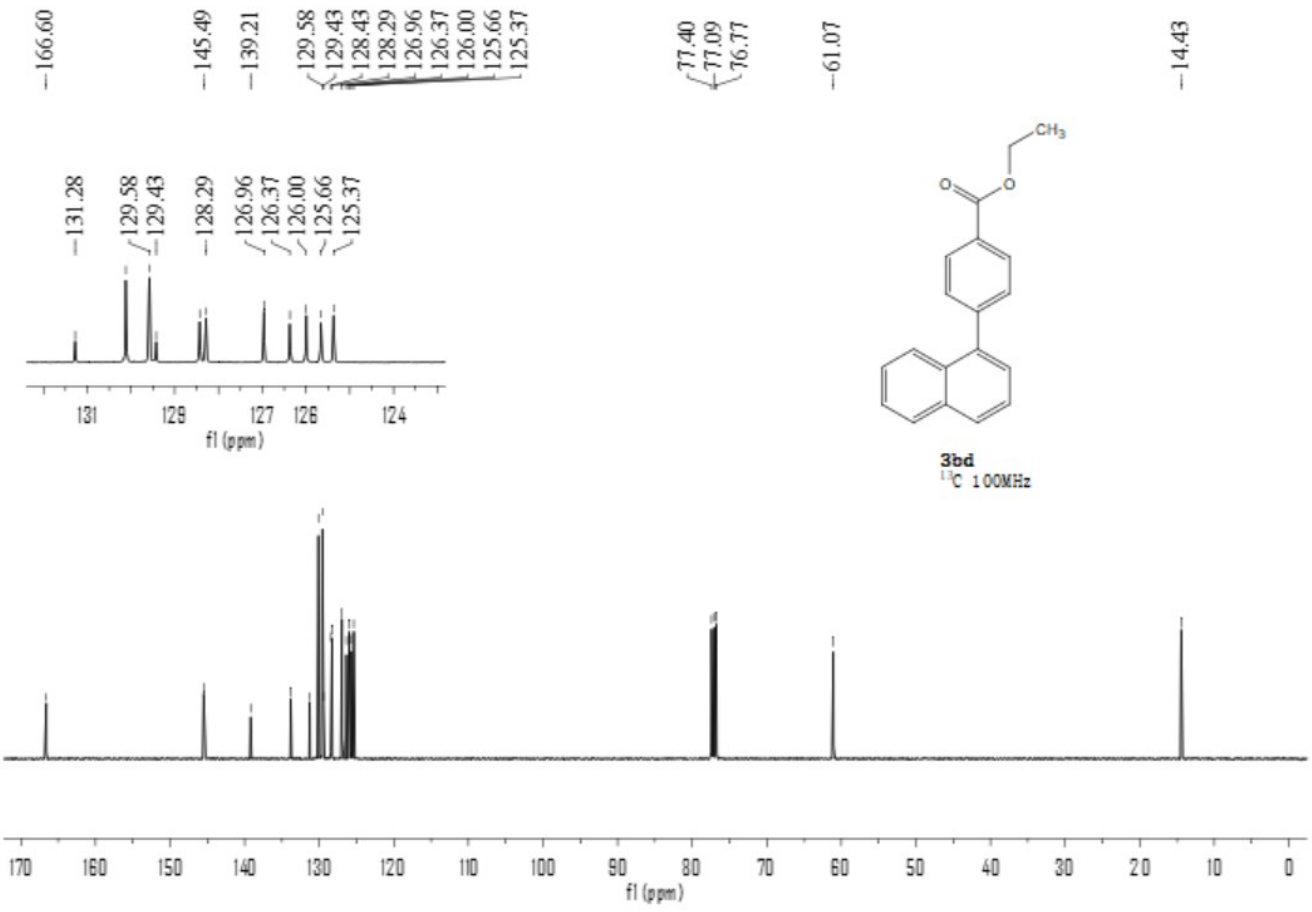

163.52
161.08
131.63
131.55
128.36
127.83
127.03
126.19
125.88
125.79
125.37
115.32
115.11
77.36
77.05
76.73
128.36
127.83
127.03
126.19
125.88
125.79
125.37
129
128
127
126
125
124
f1 (ppm)
F
3bb
13C 100MHz
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

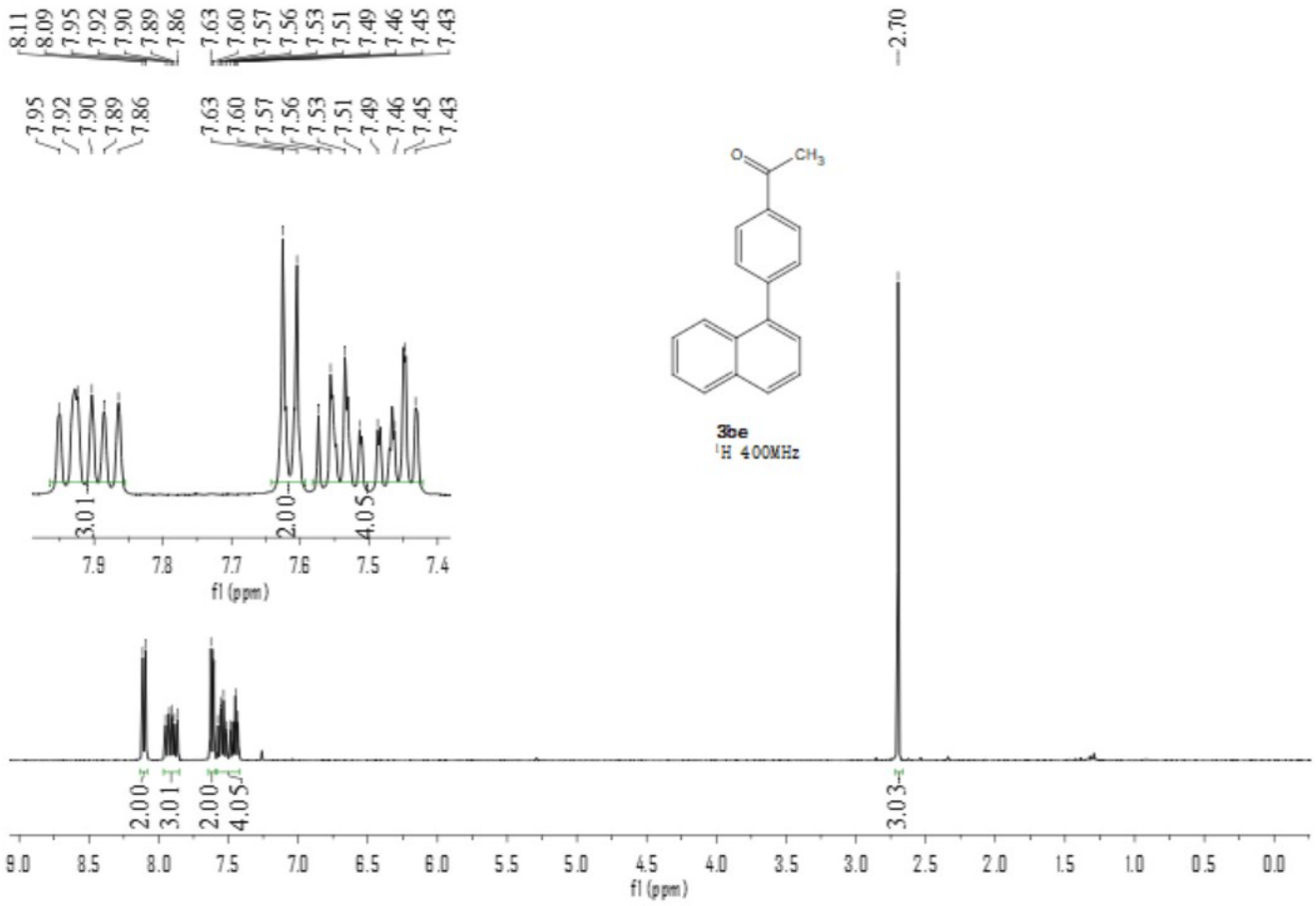

115.45
F
3bb
19F 376MHz
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-210
f1 (ppm)

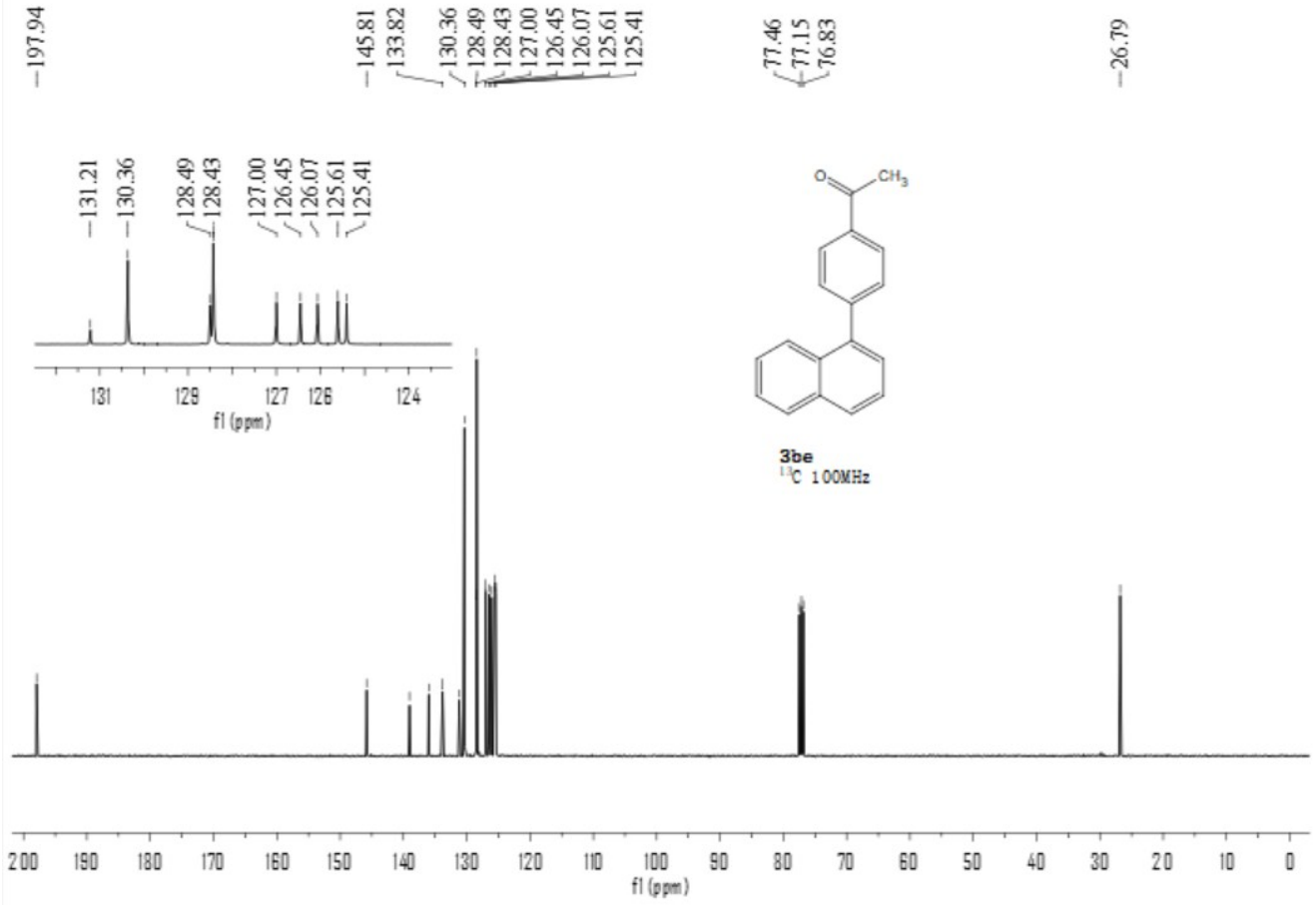

7.98
7.96
7.92
7.90
7.87
7.85
7.55
7.53
7.53
7.51
7.50
7.46
7.44
7.43
7.42
7.26
1.42
1.00
1.00
1.00
8.07
9.00
f1 (ppm)
3bc
1H 400MHz

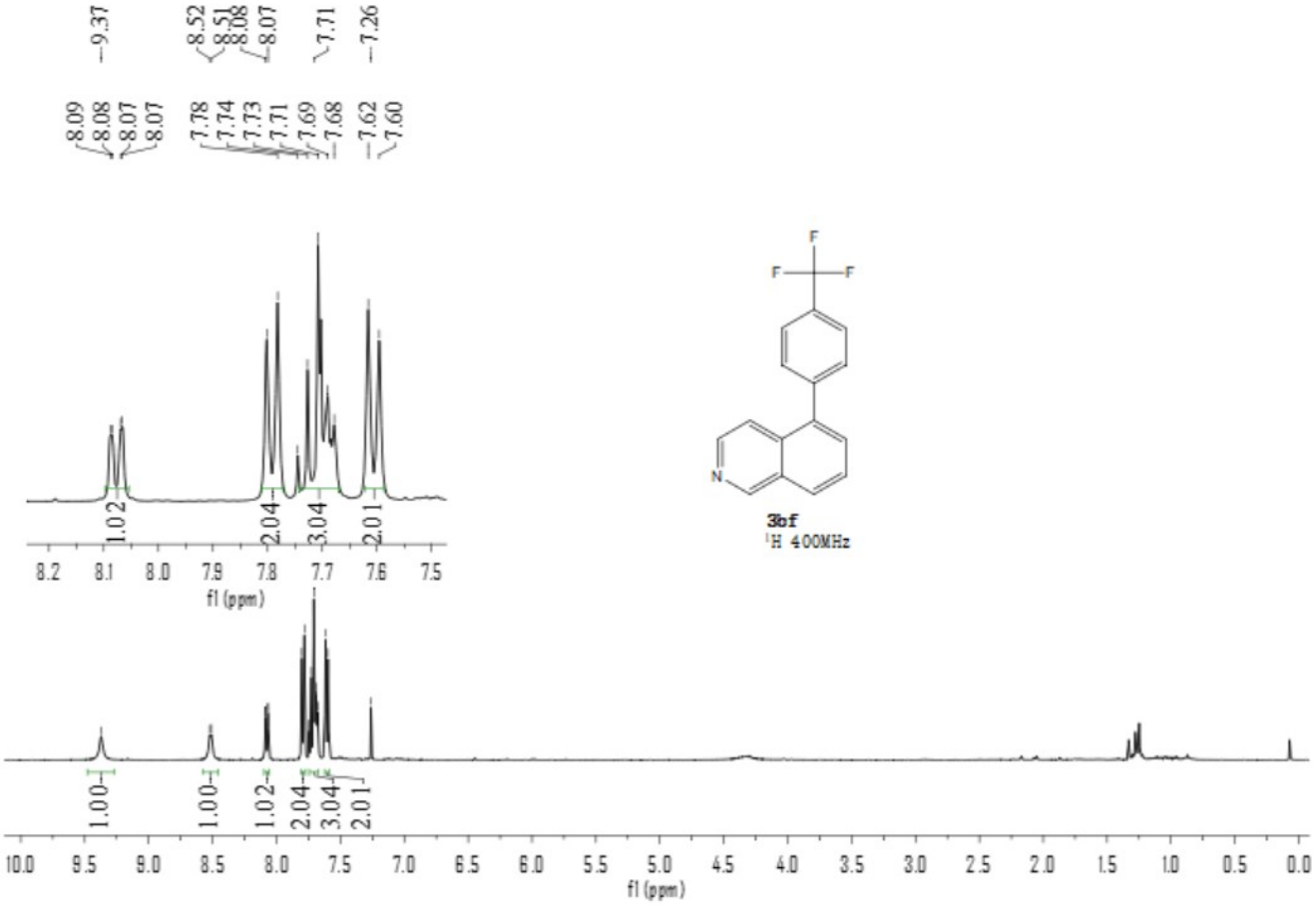

150.12
140.24
133.83
129.74
128.24
127.41
126.94
126.21
125.90
125.71
125.42
125.18
77.35
77.03
76.71
34.64
31.47
f1 (ppm)
3bc
13C 100MHz

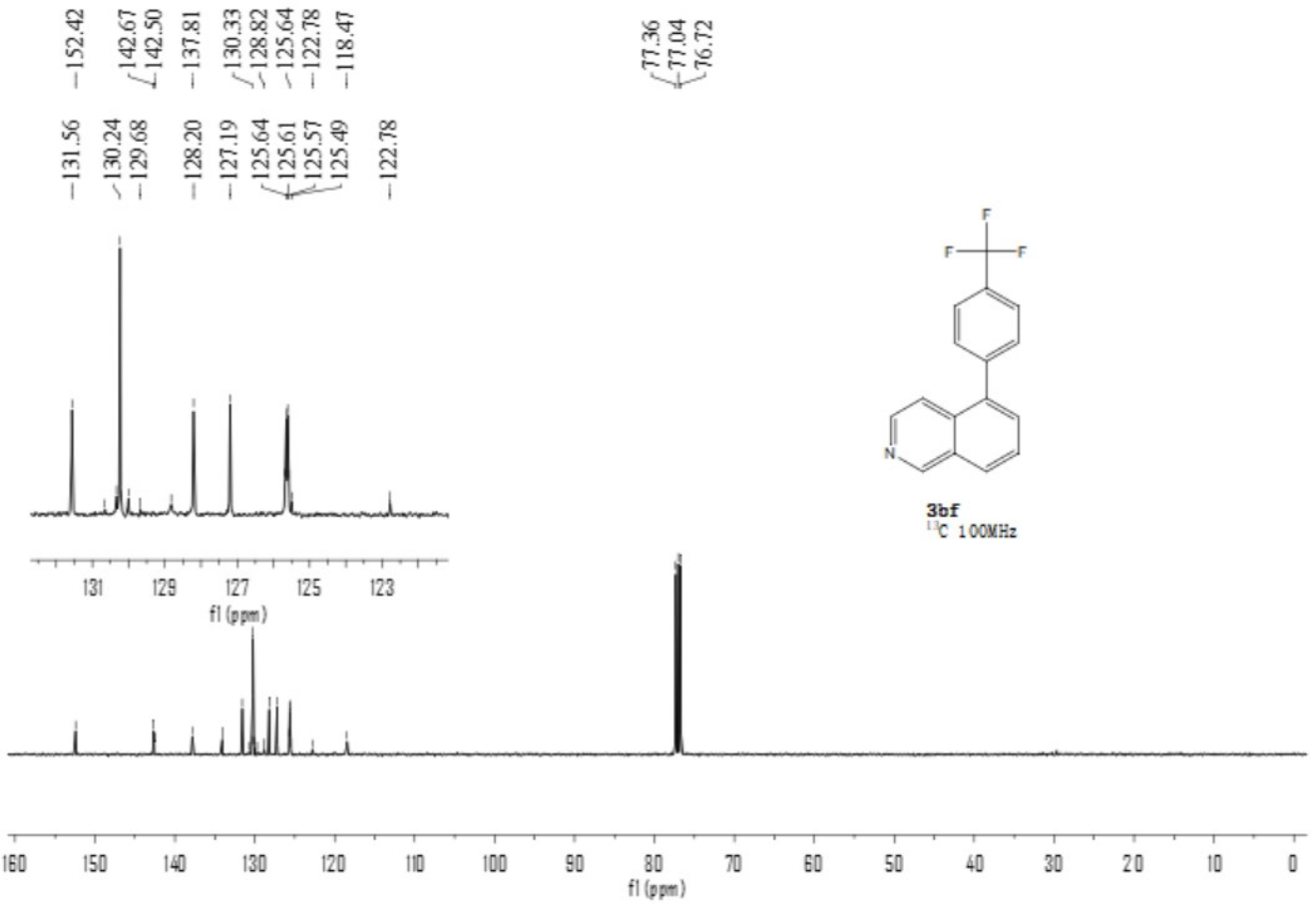

8.21
8.19
7.86
7.60
7.58
7.55
7.53
7.50
7.47
7.45
7.43
4.49
4.47
4.45
4.43
1.48
1.46
1.44
7.92
7.89
7.88
7.86
2.00
3.02
2.01
2.08
2.05
2.02
3.01
f1 (ppm)
CH3
O
3bd
1H 400MHz


166.60
145.49
139.21
129.58
129.43
128.43
128.29
126.96
126.37
126.00
125.66
125.37
77.40
77.09
76.77
61.07
14.43
131.28
f1 (ppm)
CH3
O
3bd
13C 100MHz

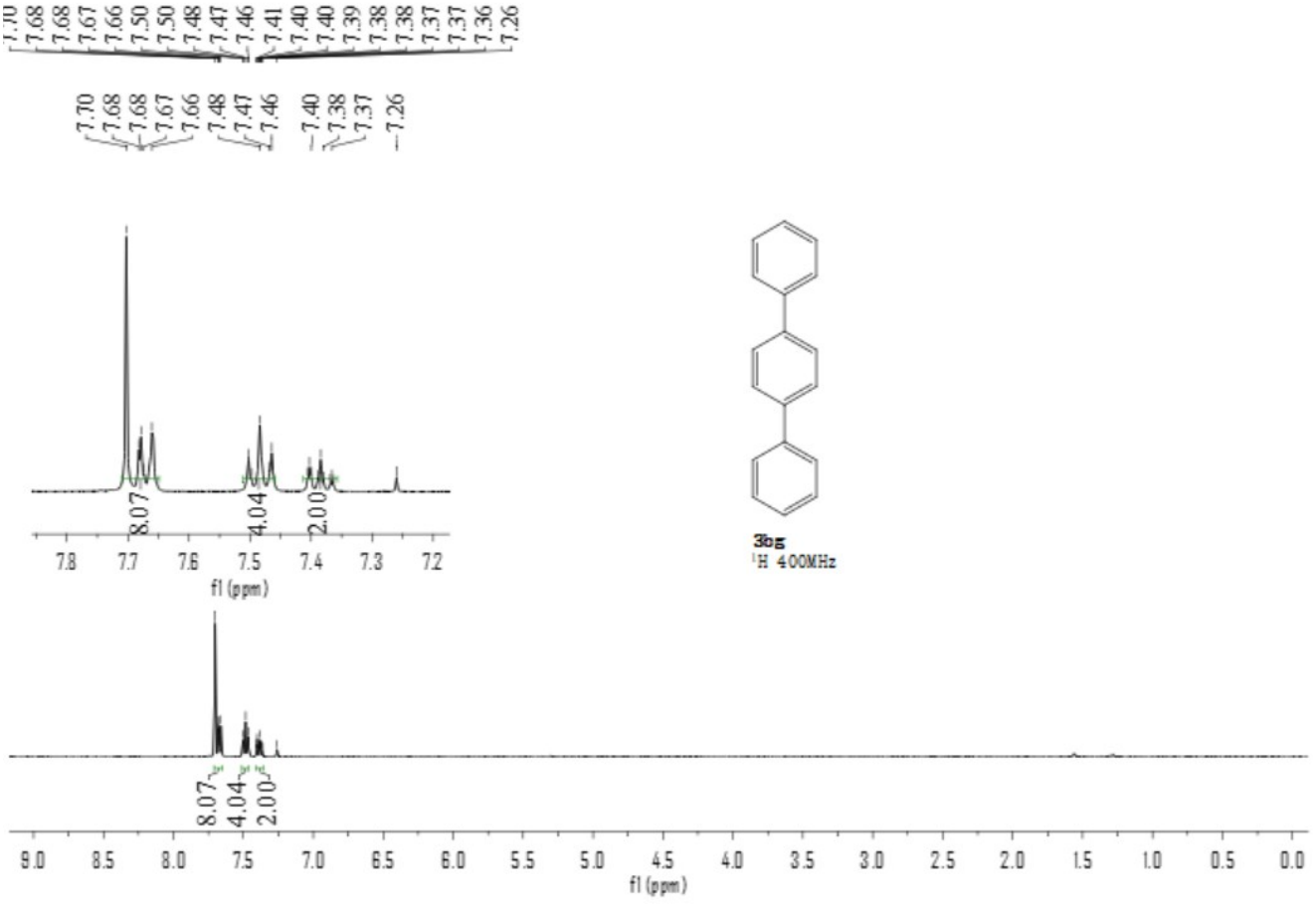

8.11
8.09
7.95
7.92
7.90
7.89
7.86
7.63
7.60
7.57
7.56
7.53
7.51
7.49
7.46
7.45
7.43
2.70
3be
1H 400MHz
3.01
2.00
4.05
f1 (ppm)
2.00
3.01
2.00
4.05
3.03
f1 (ppm)

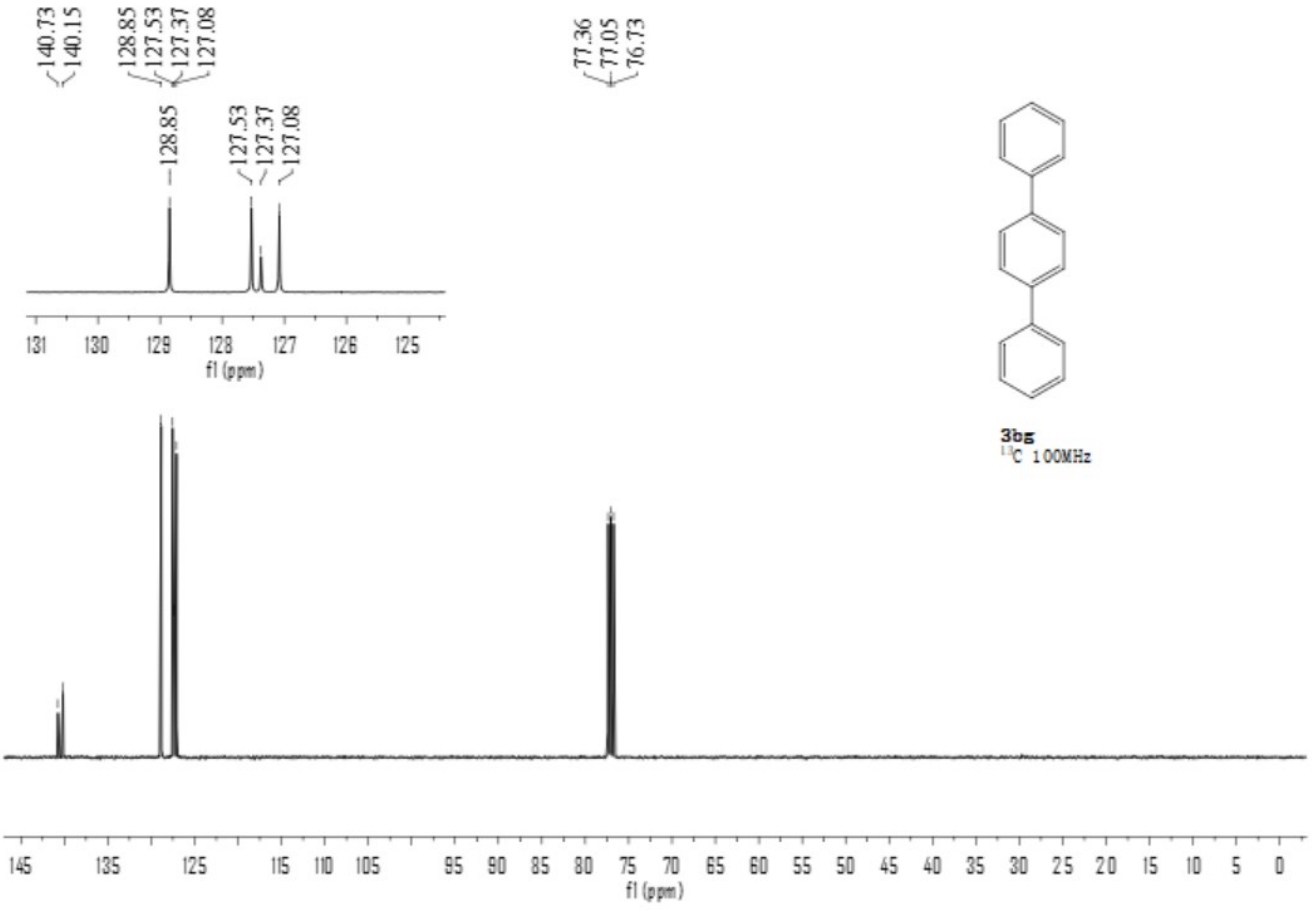

197.94
145.81
133.82
130.36
128.49
128.43
127.00
126.45
126.07
125.61
125.41
77.46
77.15
76.83
26.79
131.21
130.36
128.49
128.43
127.00
126.45
126.07
125.61
125.41
f1 (ppm)
3be
13C 100MHz
f1 (ppm)

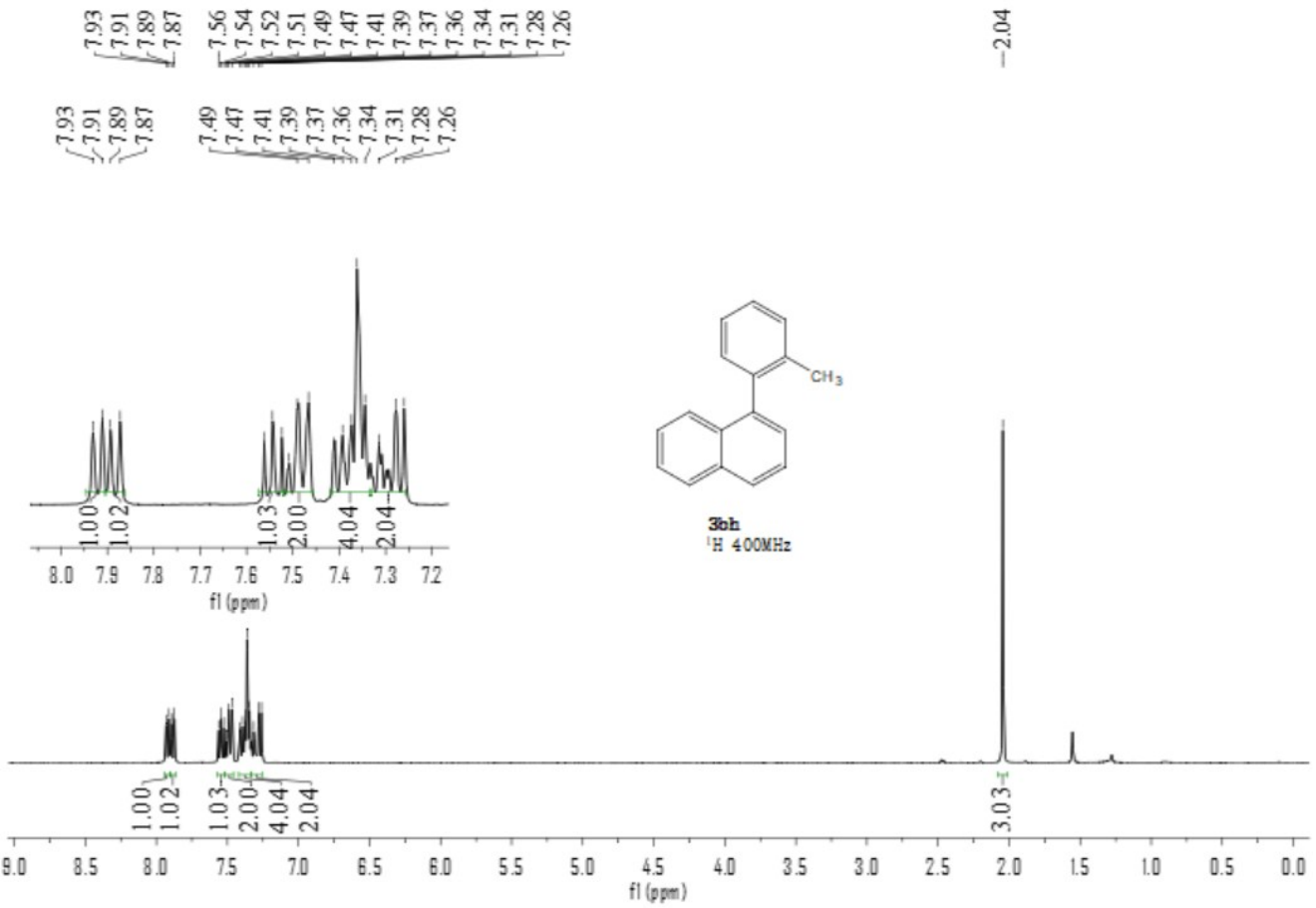

9.37
8.52
8.51
8.08
8.07
7.71
7.26
8.09
8.08
8.07
8.07
7.78
7.74
7.73
7.71
7.69
7.68
7.62
7.60
1.02
2.04
3.04
2.01
f1 (ppm)
1.00
1.00
1.02
2.04
3.04
2.01
f1 (ppm)
F
F
F
N
3bf
1H 400MHz

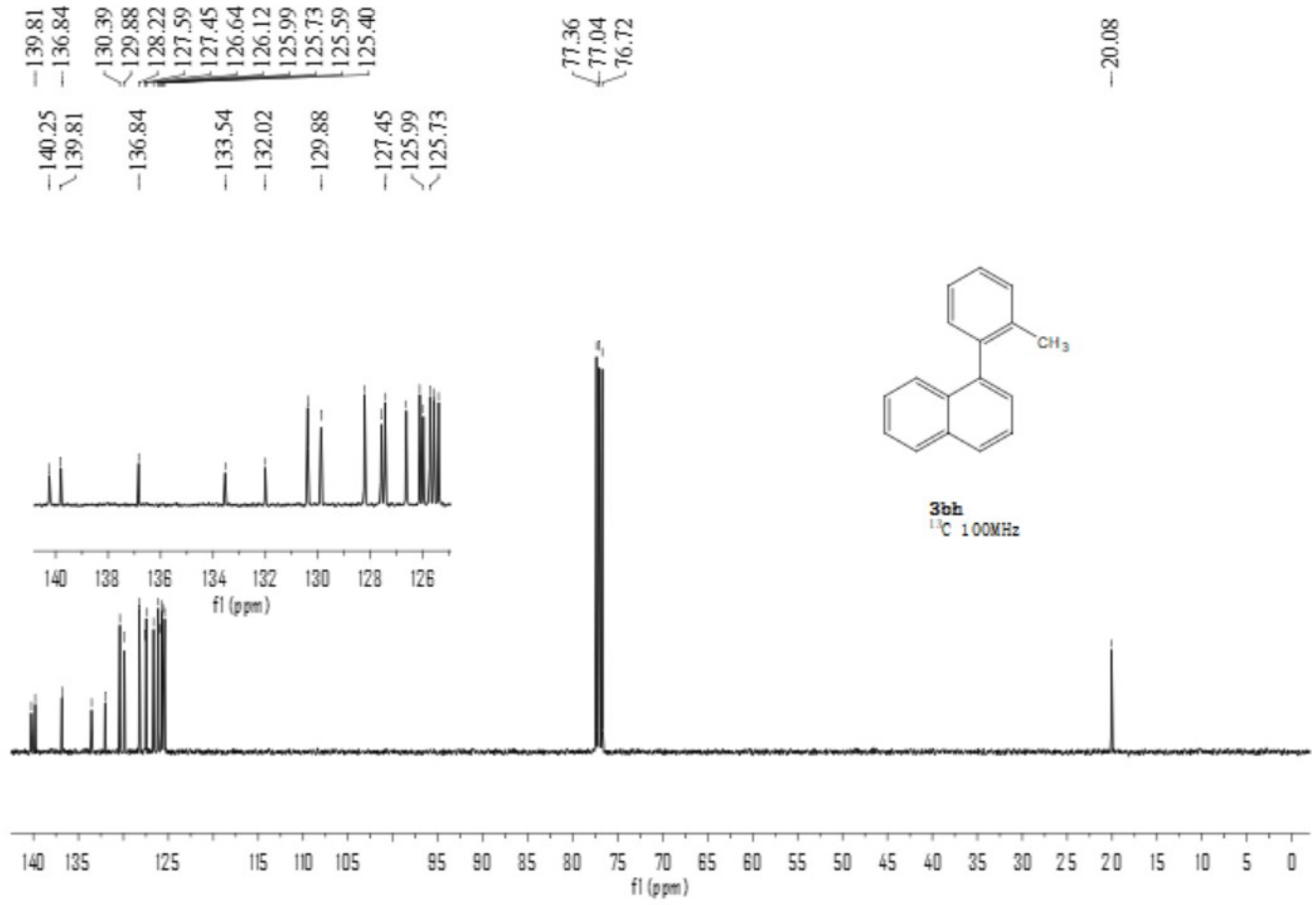

152.42
142.67
142.50
137.81
130.33
128.82
125.64
122.78
118.47
77.36
77.04
76.72
131.56
130.24
129.68
128.20
127.19
125.64
125.61
125.57
125.49
122.78
131
129
127
125
123
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
F
F
F
N
3bf
13C 100MHz

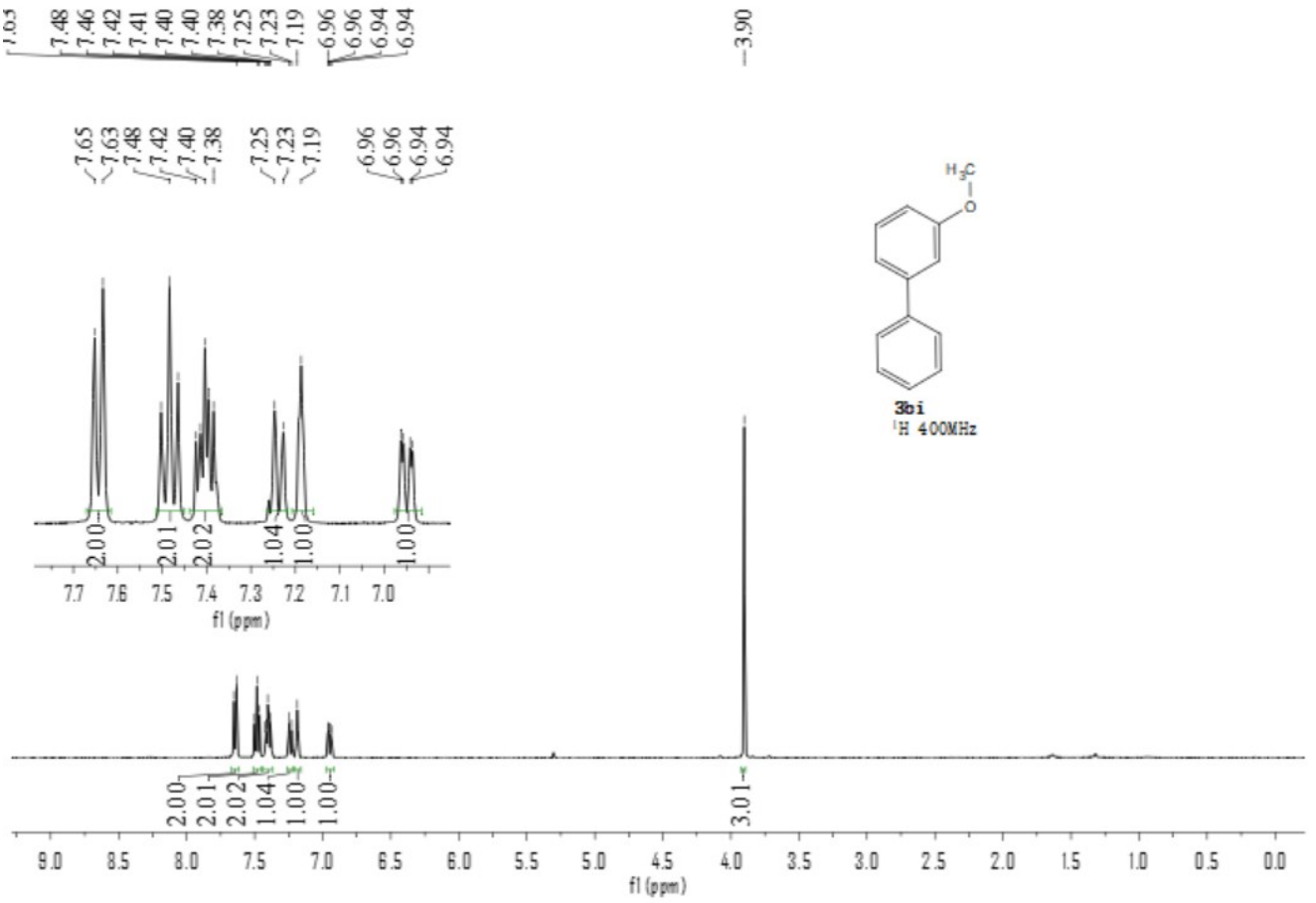

-62.49
F
F
F
N
3bf
19F 376MHz
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -210
f1 (ppm)

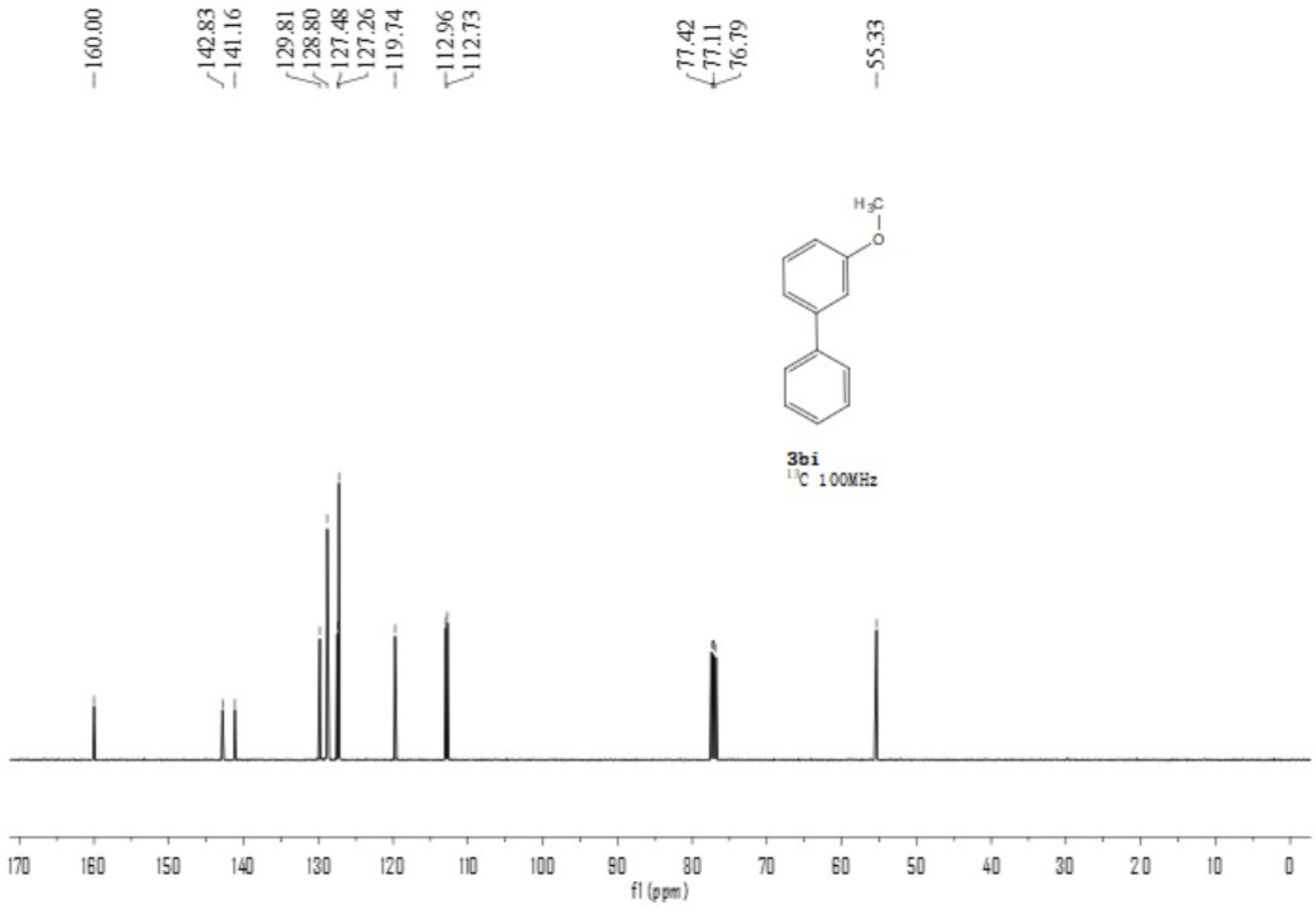

7.70
7.68
7.68
7.67
7.66
7.50
7.50
7.48
7.47
7.46
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.36
7.26
8.07
4.04
2.00
7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
3bg
1H 400MHz
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

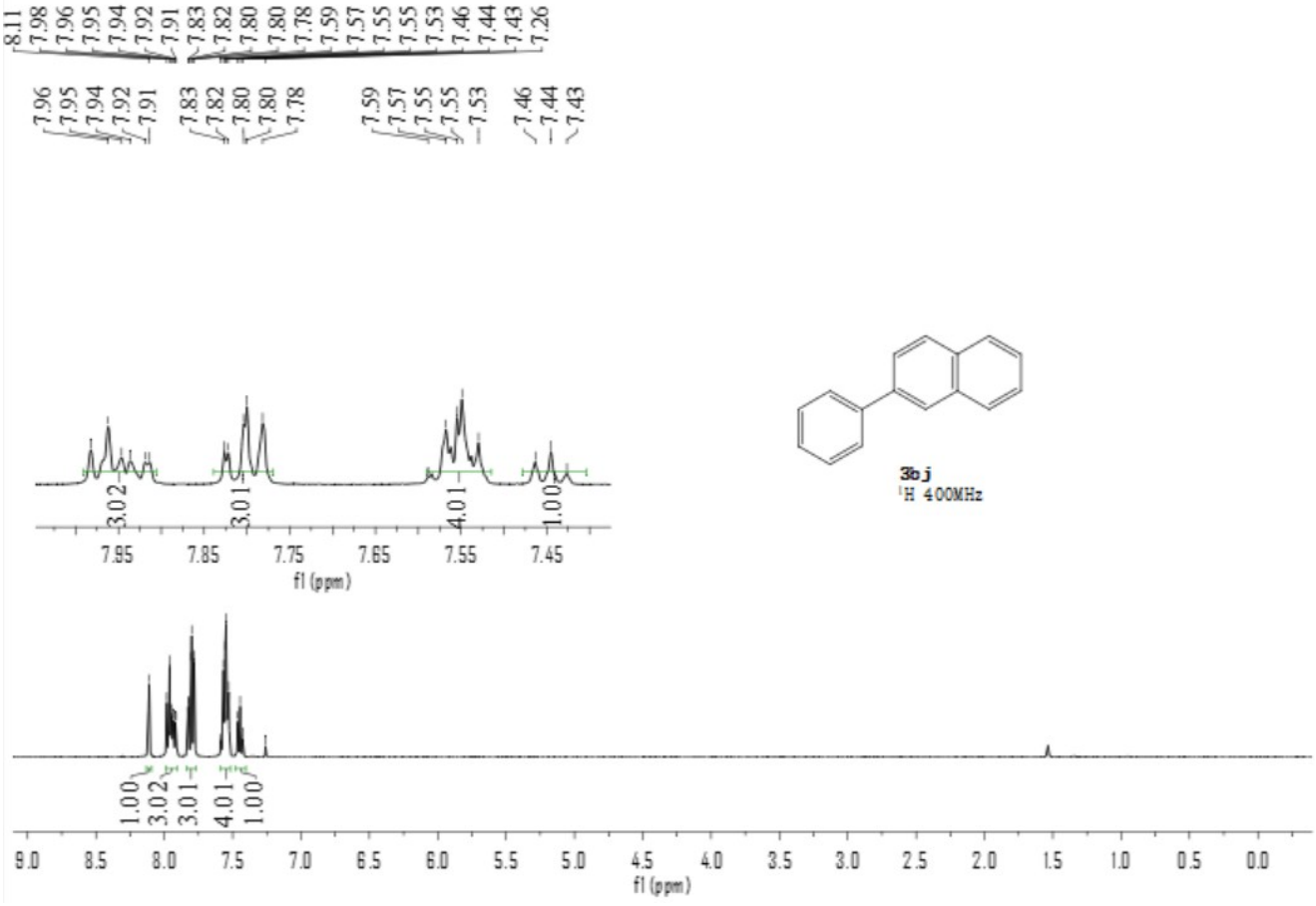

140.73
140.15
128.85
127.53
127.37
127.08
77.36
77.05
76.73
131 130 129 128 127 126 125
f1 (ppm)
3bg
13C 100MHz
145 135 125 115 110 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

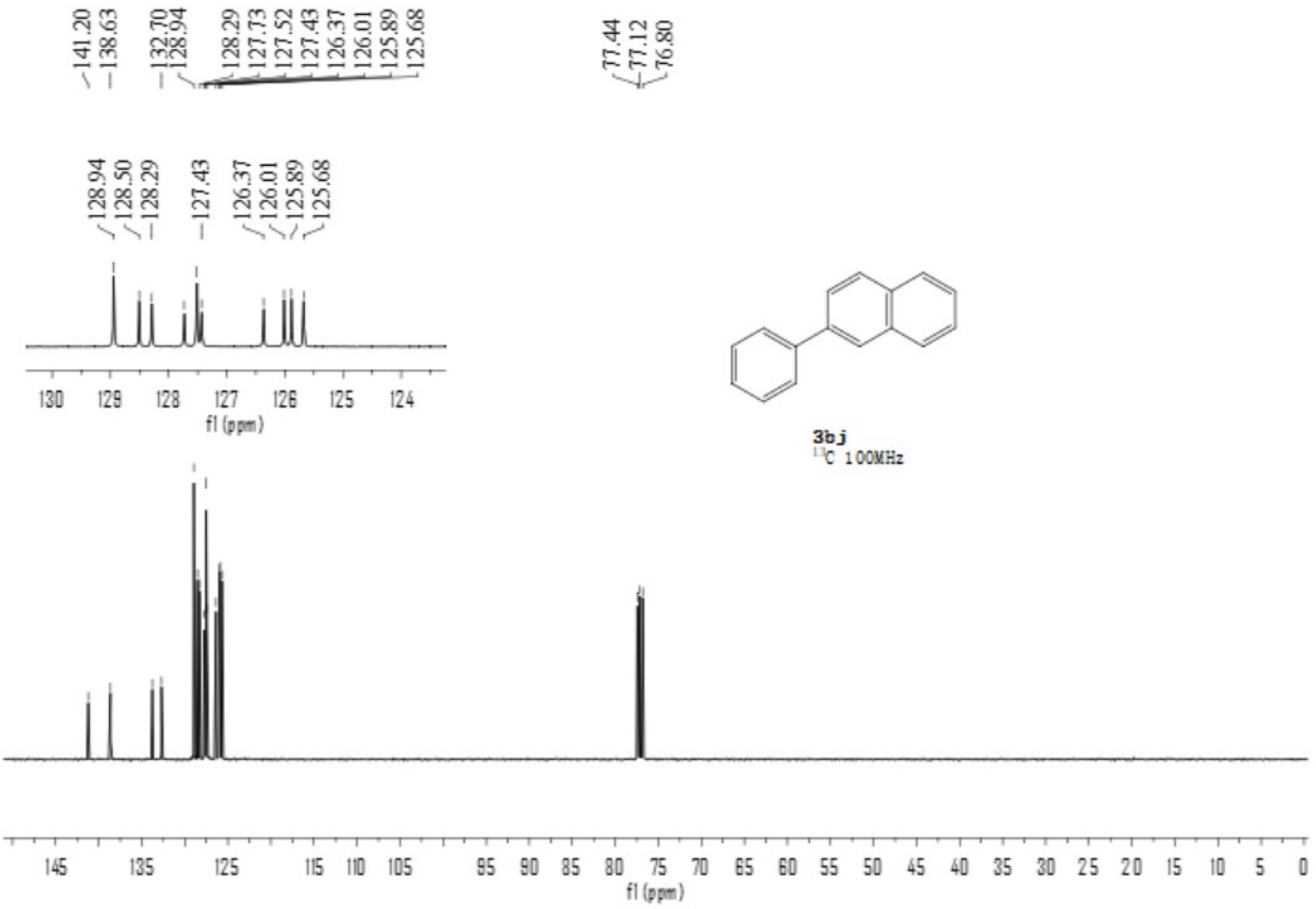

7.93
7.91
7.89
7.87
7.56
7.54
7.52
7.51
7.49
7.47
7.41
7.39
7.37
7.36
7.34
7.31
7.28
7.26
2.04
1.00
1.02
1.03
2.00
4.04
2.04
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
CH3
3bh
1H 400MHz
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

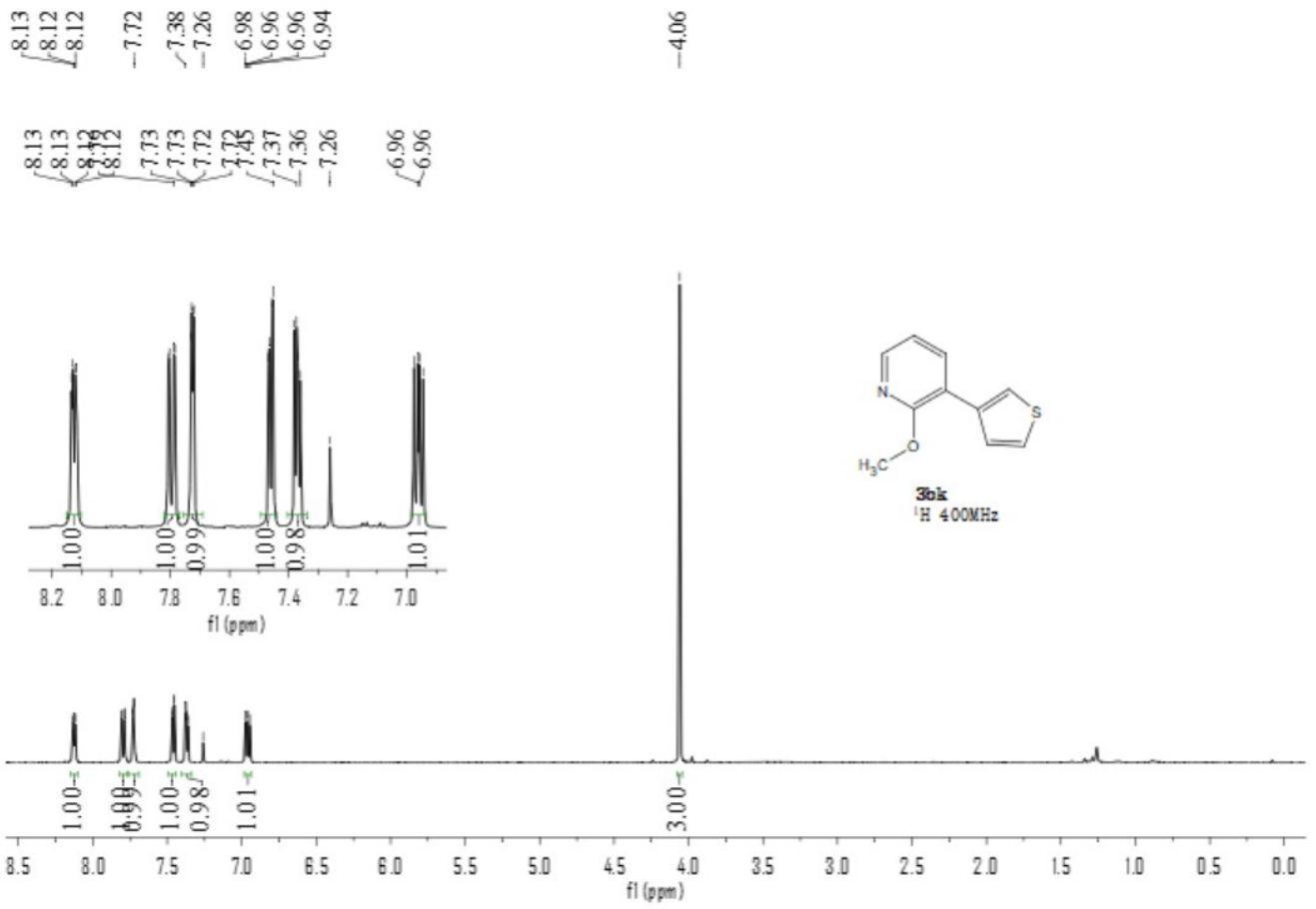

139.81
136.84
130.39
129.88
128.22
127.59
127.45
126.64
126.12
125.99
125.73
125.59
125.40
77.36
77.04
76.72
20.08
140.25
139.81
136.84
133.54
132.02
129.88
127.45
125.99
125.73
CH3
3bh
13C 100MHz
f1 (ppm)

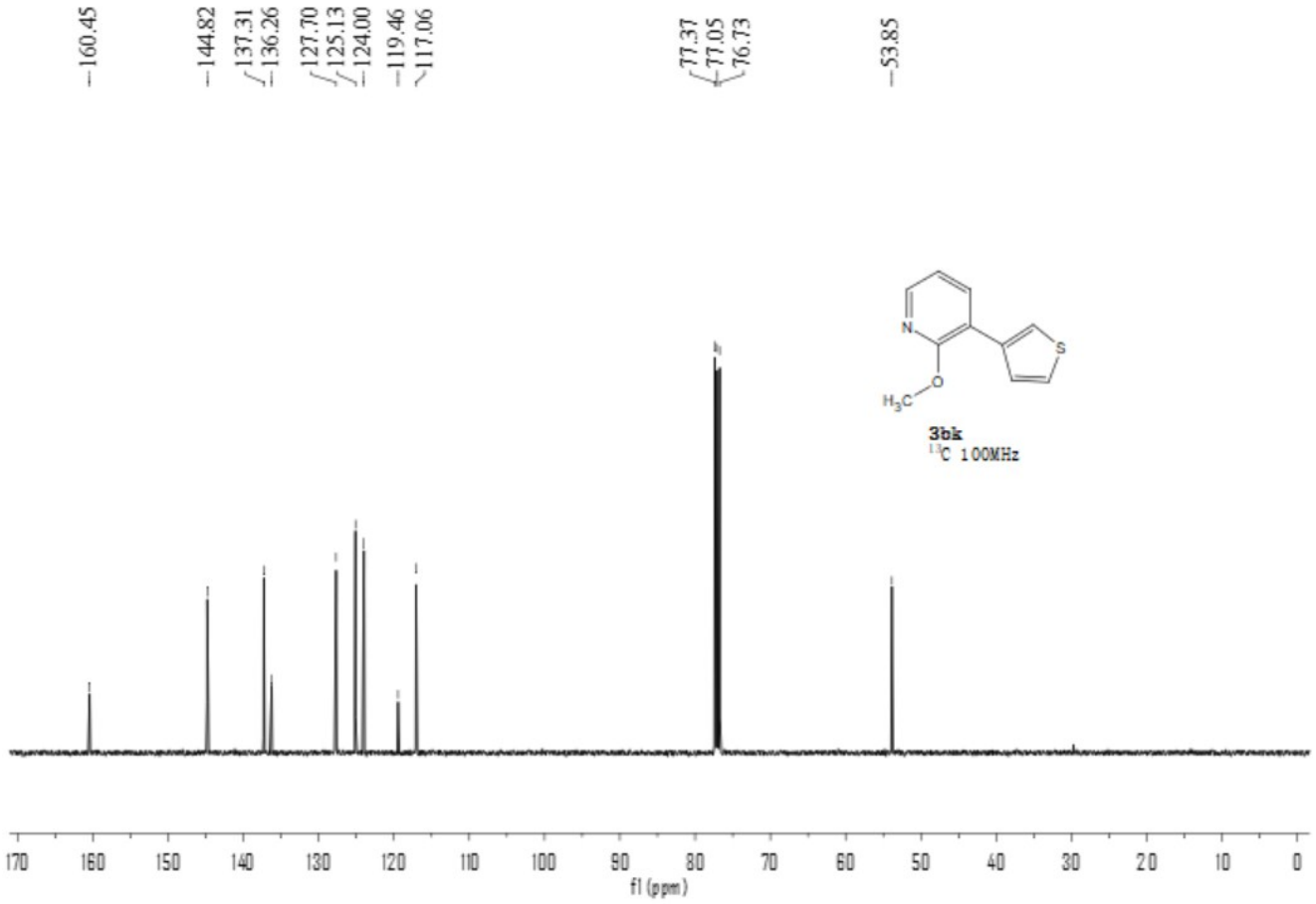

7.48
7.46
7.42
7.41
7.40
7.40
7.38
7.25
7.23
7.19
6.96
6.96
6.94
6.94
3.90
7.65
7.63
7.48
7.42
7.40
7.38
7.25
7.23
7.19
6.96
6.96
6.94
6.94
H3C
O
3bi
1H 400MHz
2.00
2.01
2.02
1.04
1.00
1.00
3.01
f1 (ppm)

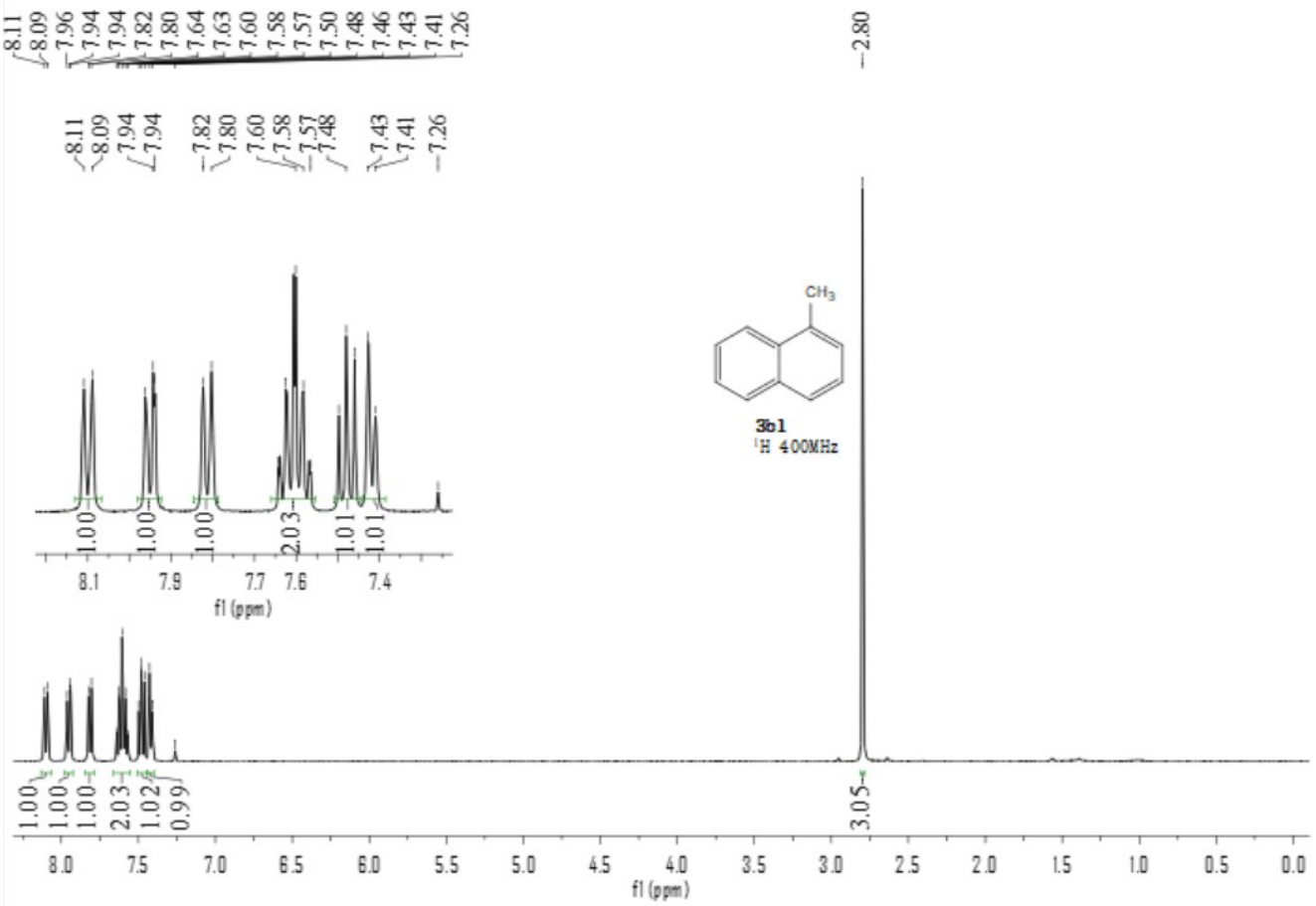

160.00
142.83
141.16
129.81
128.80
127.48
127.26
119.74
112.96
112.73
77.42
77.11
76.79
55.33
H3C
O
3bi
13C 100MHz
f1 (ppm)

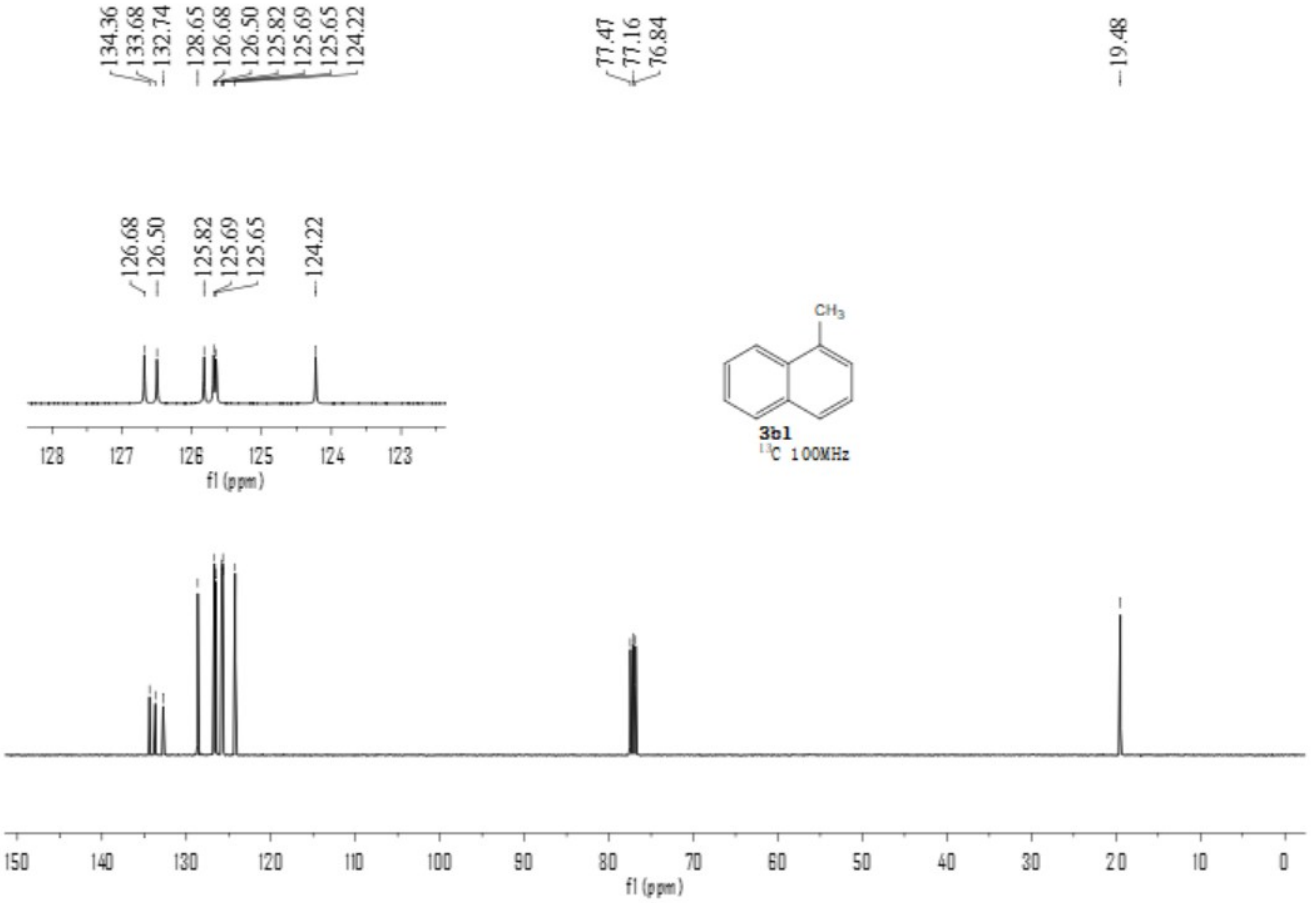

8.11
7.98
7.96
7.95
7.94
7.92
7.91
7.83
7.82
7.80
7.80
7.78
7.59
7.57
7.55
7.55
7.53
7.46
7.44
7.43
7.26
3.02
3.01
4.01
1.00
f1 (ppm)
3bj
1H 400MHz
1.00
3.02
3.01
4.01
1.00
f1 (ppm)

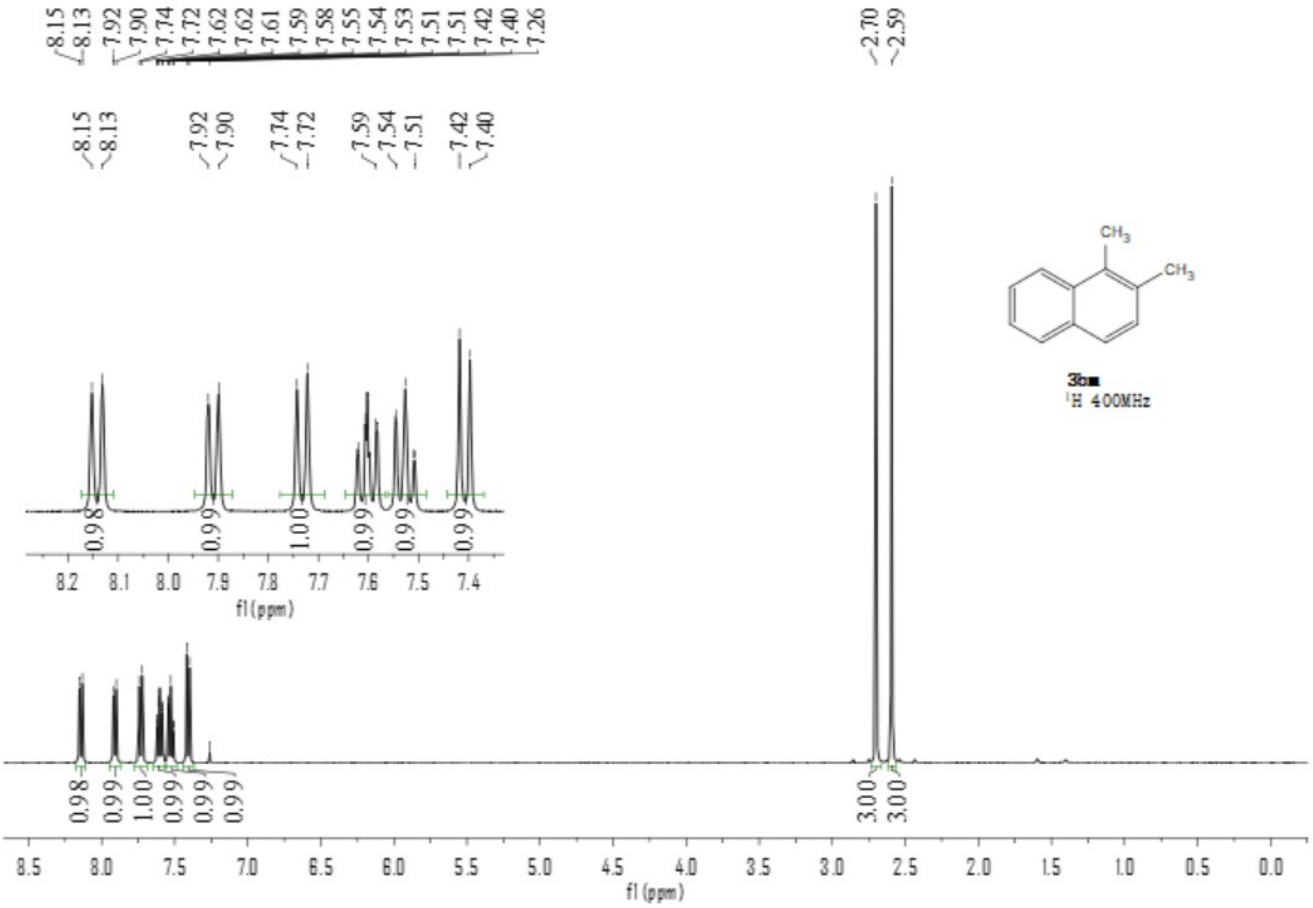

141.20
138.63
132.70
128.94
128.29
127.73
127.52
127.43
126.37
126.01
125.89
125.68
77.44
77.12
76.80
128.94
128.50
128.29
127.43
126.37
126.01
125.89
125.68
f1 (ppm)
3bj
13C 100MHz
f1 (ppm)

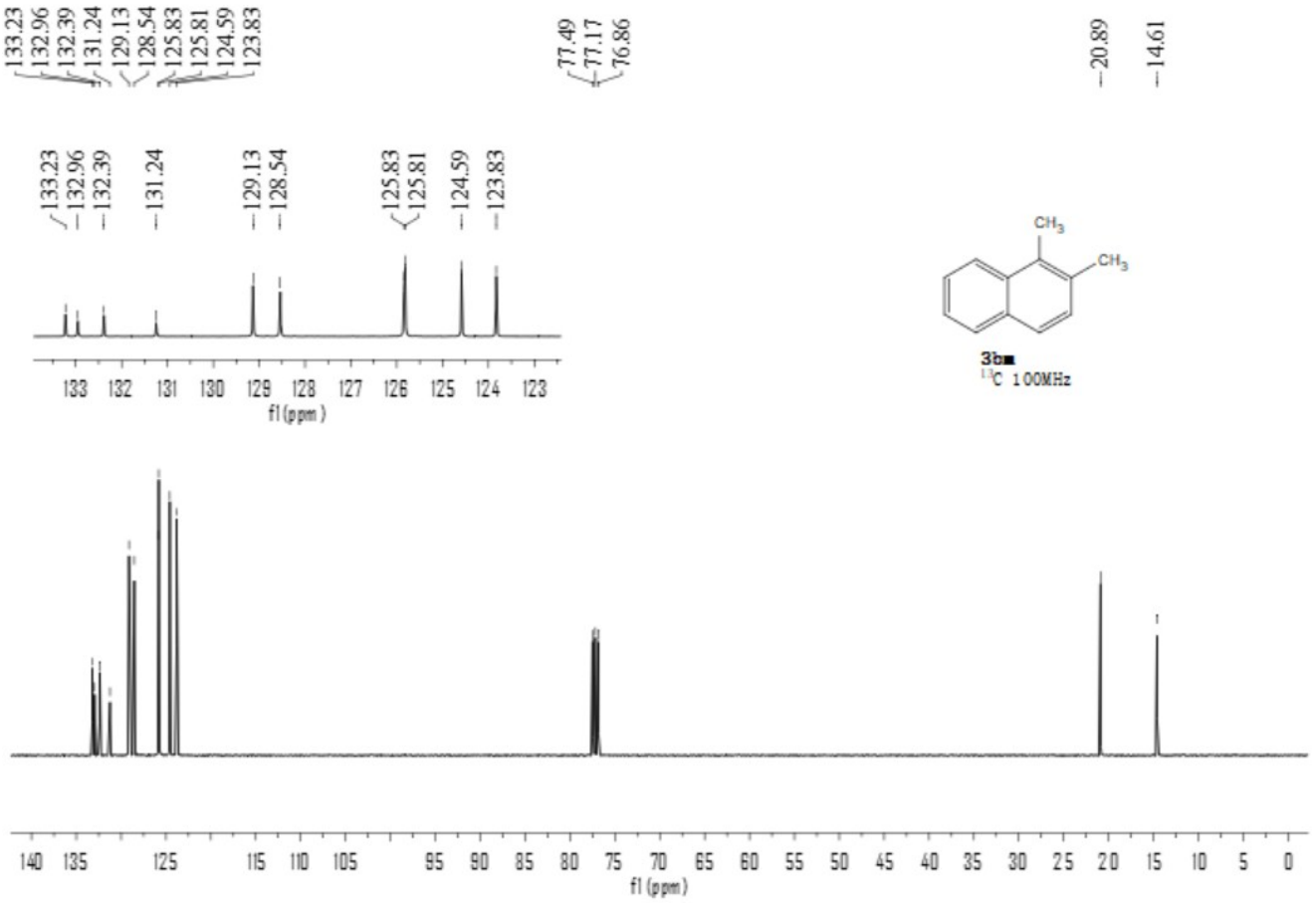

8.13
8.12
8.12
7.72
7.38
7.26
6.98
6.96
6.96
6.94
4.06
1.00
1.00
0.99
1.00
0.98
1.01
f1 (ppm)
3.00
3bk
1H 400MHz
f1 (ppm)

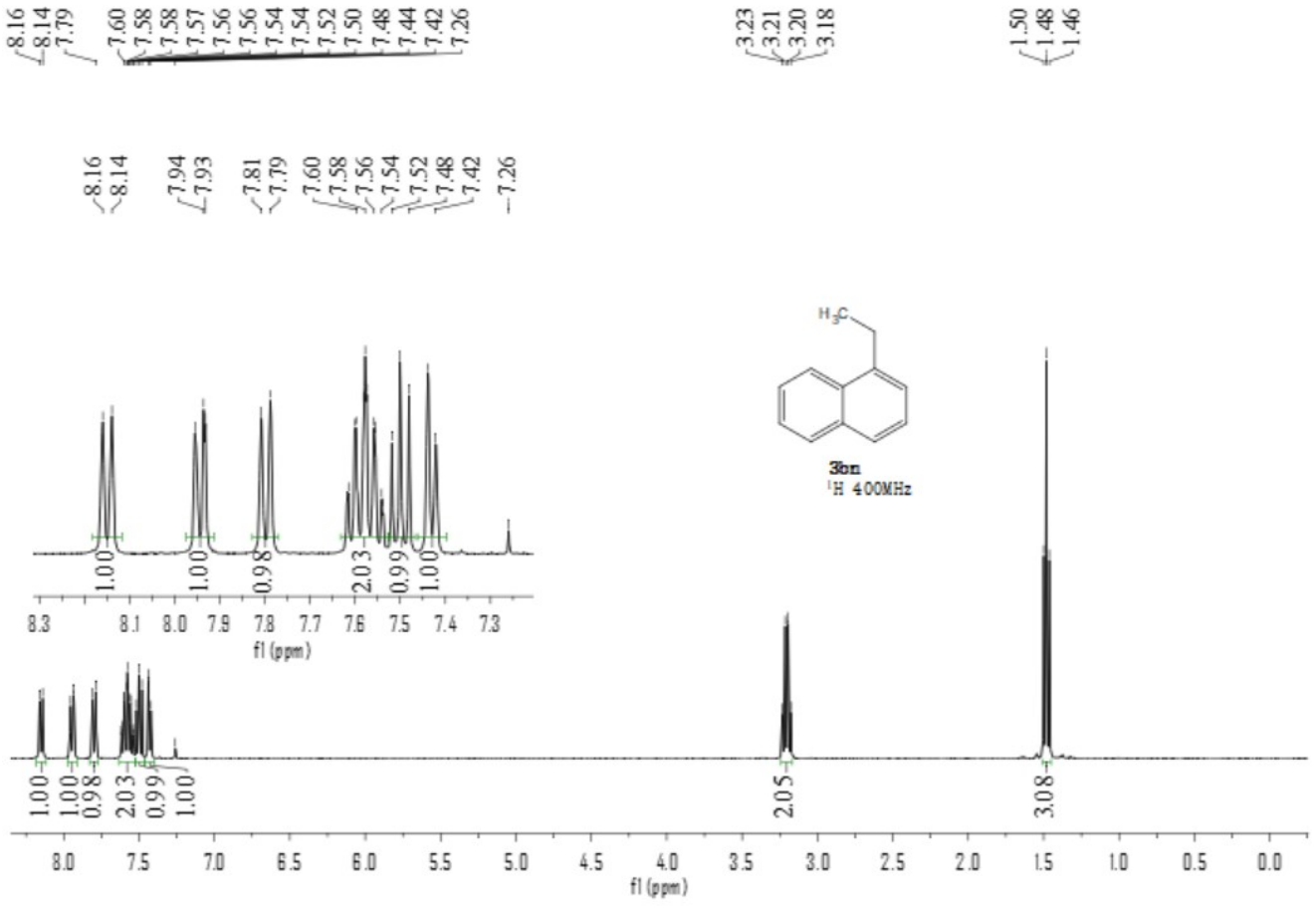

160.45
144.82
137.31
136.26
127.70
125.13
124.00
119.46
117.06
77.37
77.05
76.73
53.85
3bk
13C 100MHz
f1 (ppm)

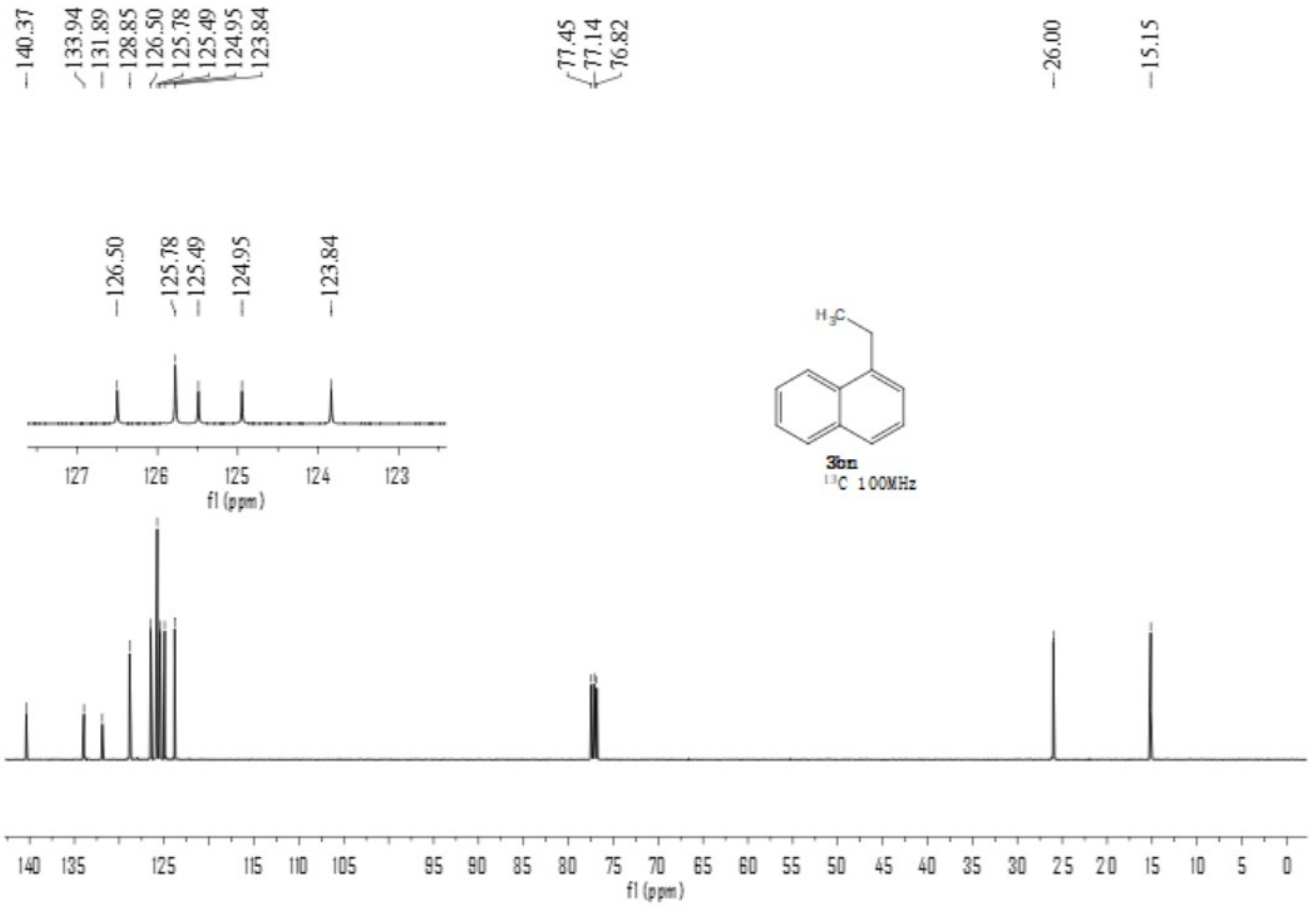

8.11
8.09
7.96
7.94
7.94
7.82
7.80
7.64
7.63
7.60
7.58
7.57
7.50
7.48
7.46
7.43
7.41
7.26
2.80
3bl
1H 400MHz
f1 (ppm)

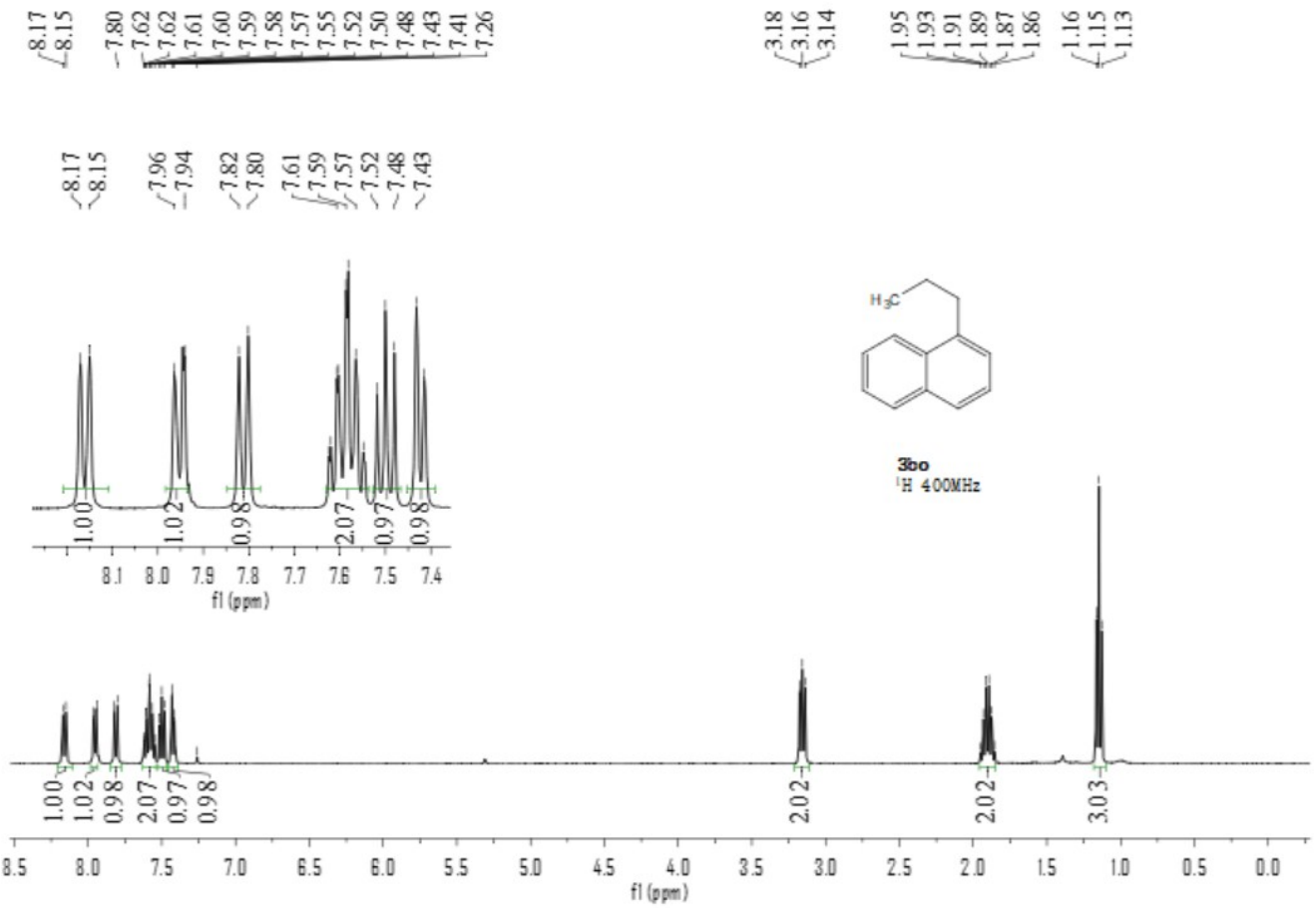

134.36
133.68
132.74
128.65
126.68
126.50
125.82
125.69
125.65
124.22
77.47
77.16
76.84
19.48
126.68
126.50
125.82
125.69
125.65
124.22
f1 (ppm)
CH3
3bl
13C 100MHz
f1 (ppm)

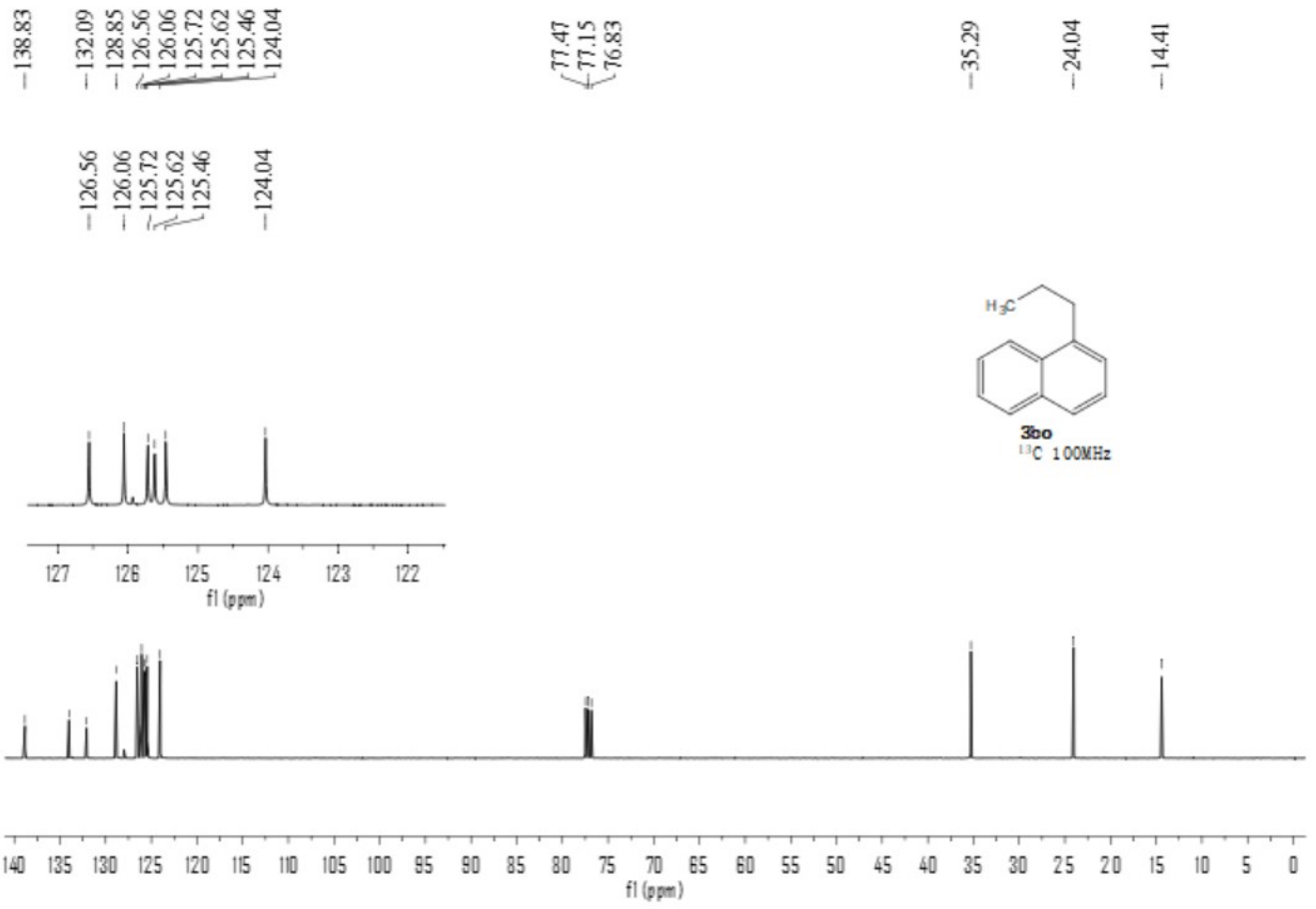

8.15
8.13
7.92
7.90
7.74
7.72
7.62
7.62
7.61
7.59
7.58
7.55
7.54
7.53
7.51
7.51
7.42
7.40
7.26
2.70
2.59
0.98
0.99
1.00
0.99
0.99
0.99
3.00
3.00
f1 (ppm)
CH3
CH3
3b
1H 400MHz
f1 (ppm)


133.23
132.96
132.39
131.24
129.13
128.54
125.83
125.81
124.59
123.83
77.49
77.17
76.86
20.89
14.61
CH3
CH3
3bn
13C 100MHz
f1 (ppm)


8.16
8.14
7.79
7.60
7.58
7.58
7.57
7.56
7.56
7.54
7.54
7.52
7.50
7.48
7.44
7.42
7.26
3.23
3.21
3.20
3.18
1.50
1.48
1.46
H3C
3bn
1H 400MHz
1.00
1.00
0.98
2.03
0.99
1.00
2.05
3.08
f1 (ppm)


140.37
133.94
131.89
128.85
126.50
125.78
125.49
124.95
123.84
77.45
77.14
76.82
26.00
15.15
3bn
13C 100MHz
f1 (ppm)


8.17
8.15
7.80
7.62
7.62
7.61
7.60
7.59
7.58
7.57
7.55
7.52
7.50
7.48
7.43
7.41
7.26
3.18
3.16
3.14
1.95
1.93
1.91
1.89
1.87
1.86
1.16
1.15
1.13
3bo
1H 400MHz
f1 (ppm)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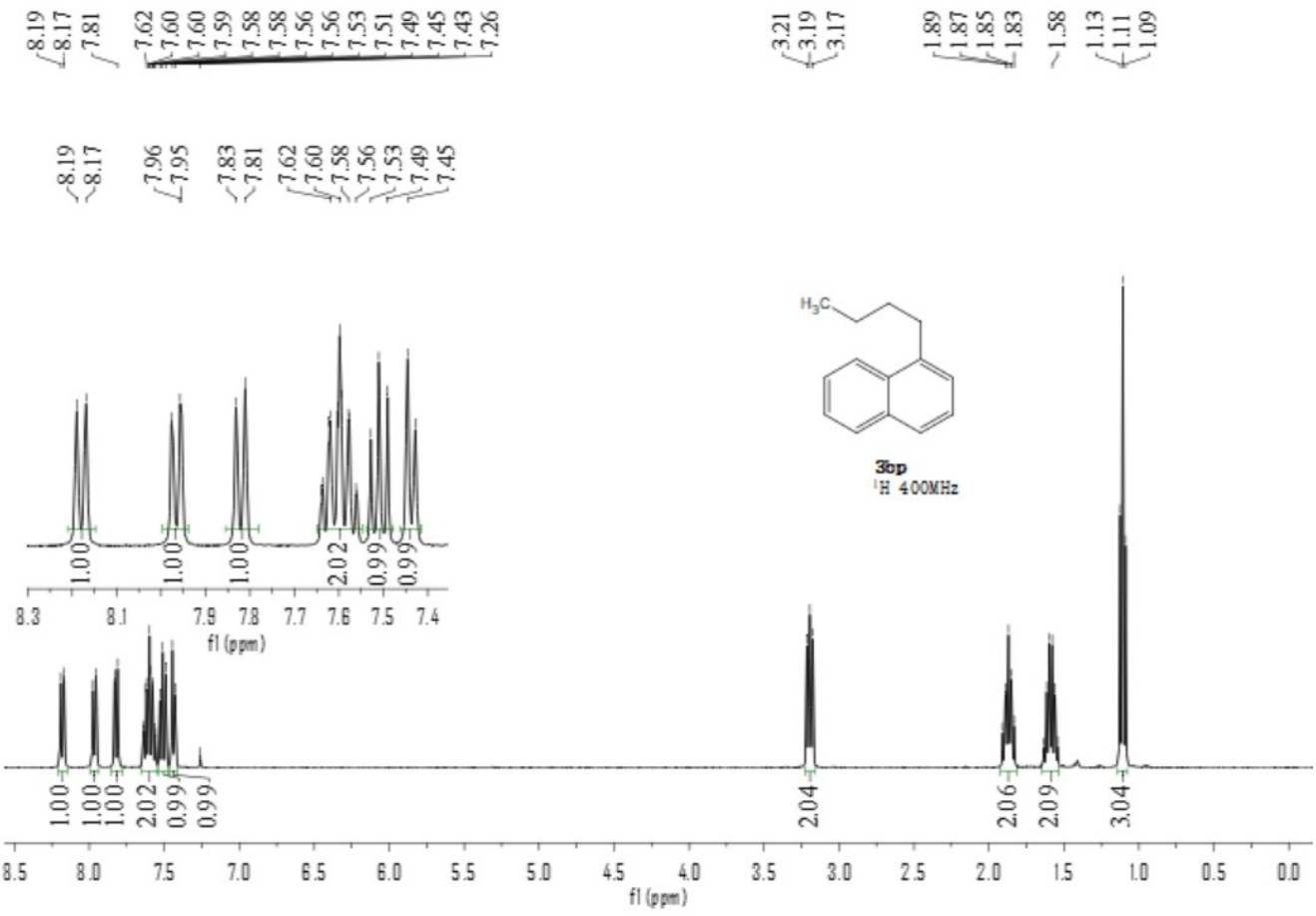
132.09
128.85
126.56
126.06
125.72
125.62
125.46
124.04
77.47
77.15
76.83
35.29
24.04
14.41
3bo
13C 100MHz
f1 (ppm)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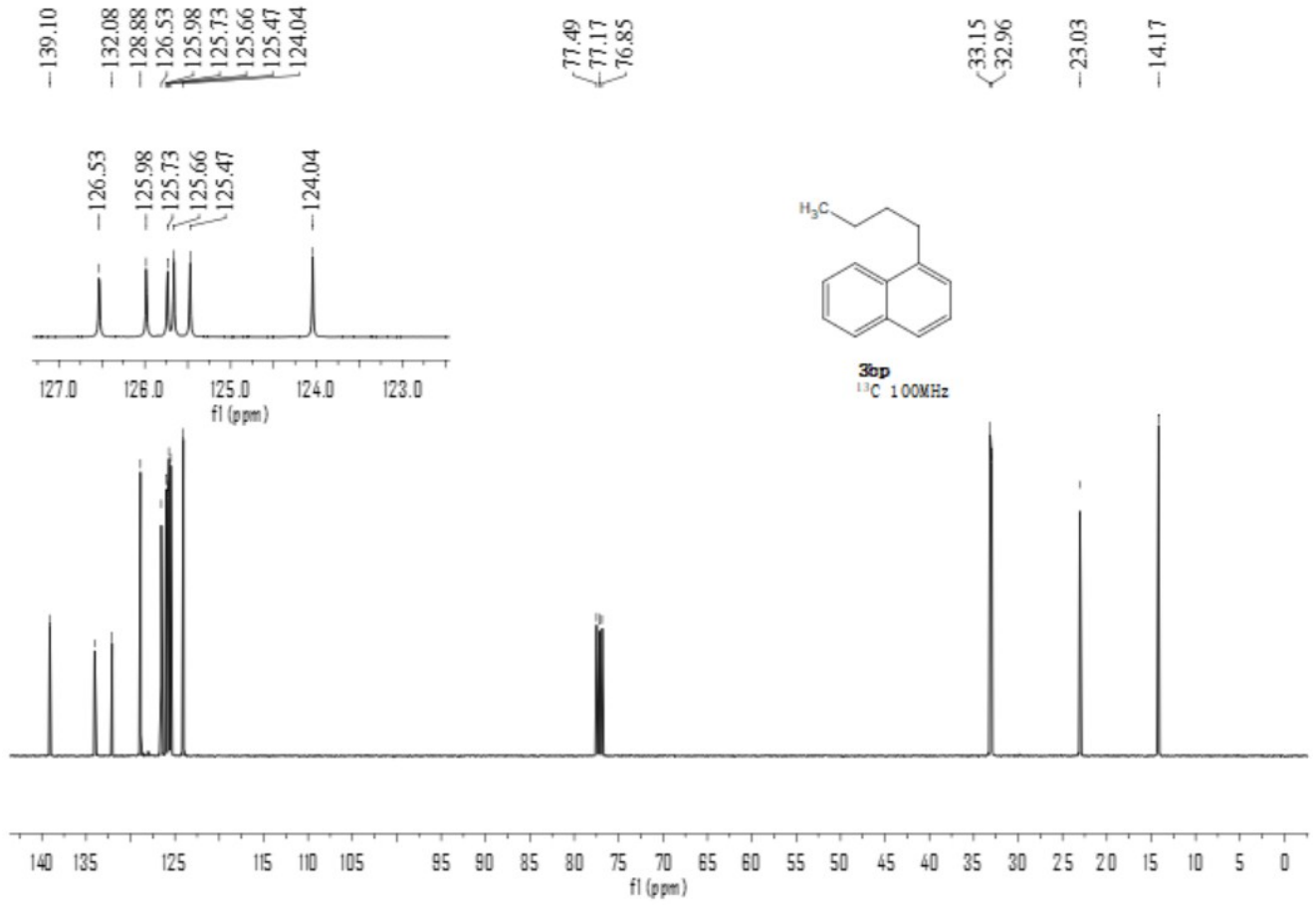
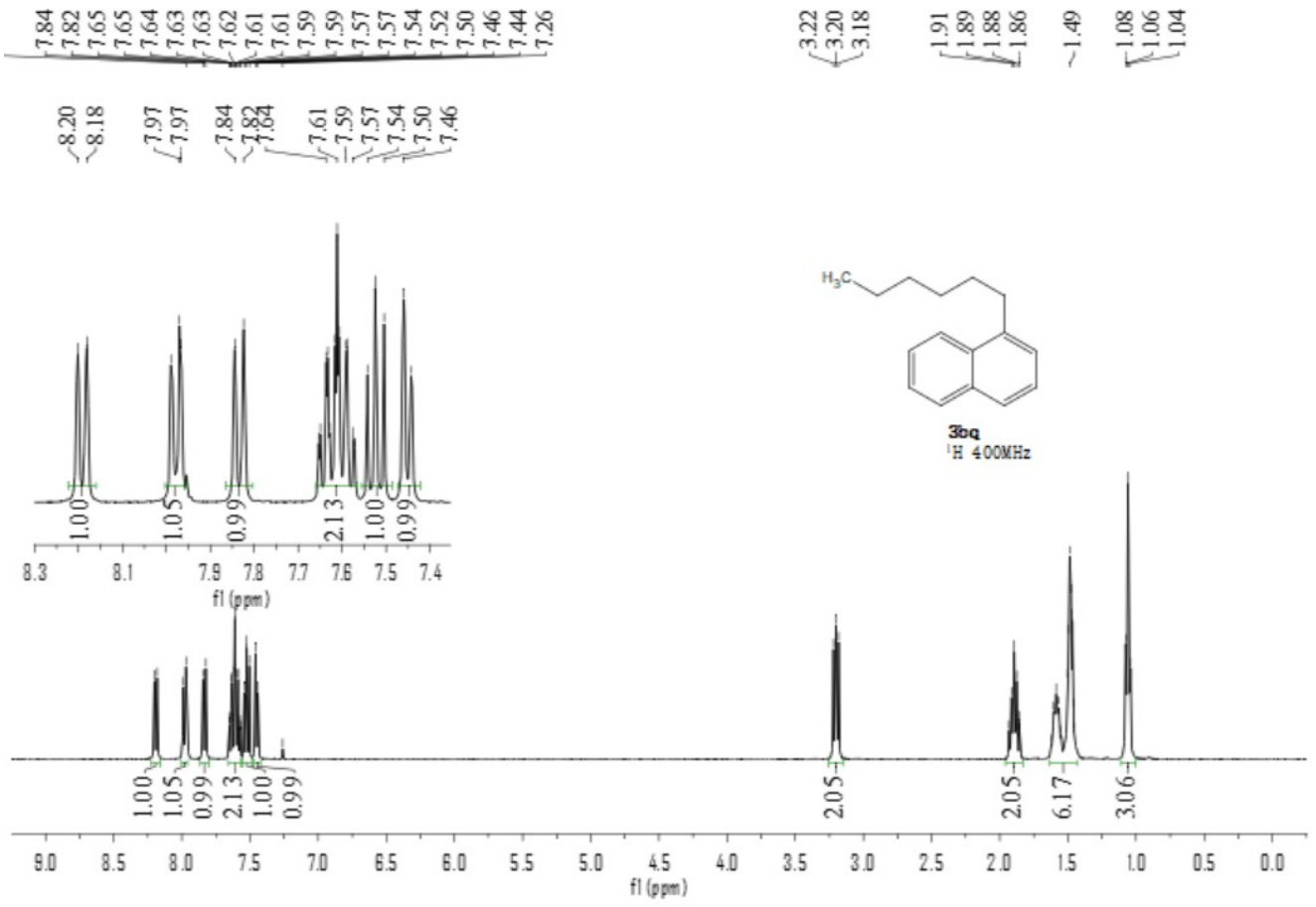
8.17
7.81
7.62
7.60
7.59
7.58
7.56
7.53
7.51
7.49
7.45
7.43
7.26
3.21
3.19
3.17
1.89
1.87
1.85
1.83
1.58
1.13
1.11
1.09
3bp
1H 400MHz
f1 (ppm)


139.10
132.08
128.88
126.53
125.98
125.73
125.66
125.47
124.04
77.49
77.17
76.85
33.15
32.96
23.03
14.17
3op
13C 100MHz
f1 (ppm)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7.82
7.65
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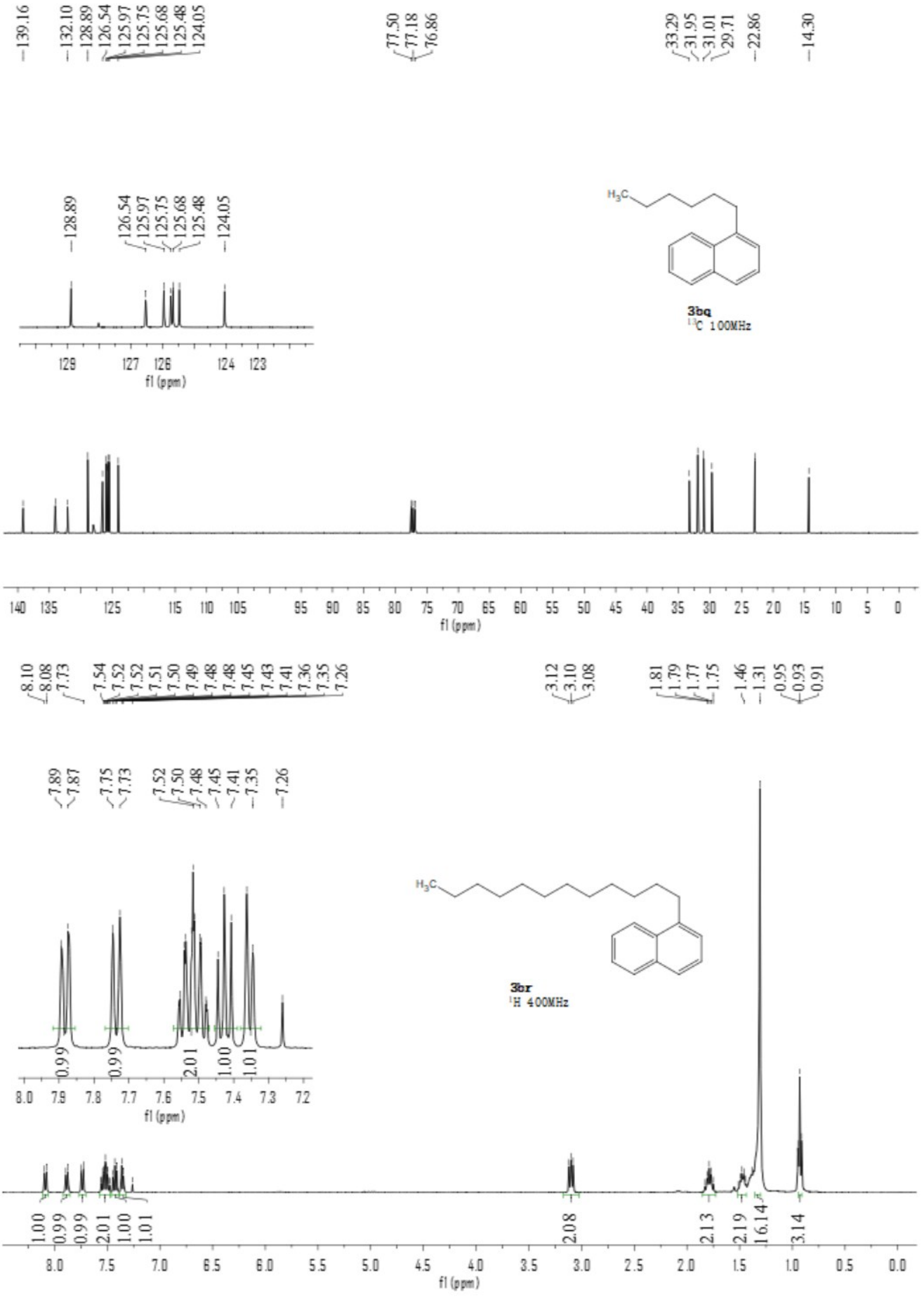
7.64
7.63
7.63
7.62
7.61
7.61
7.59
7.59
7.57
7.57
7.54
7.52
7.50
7.46
7.44
7.26
3.22
3.20
3.18
1.91
1.89
1.88
1.86
1.49
1.08
1.06
1.04
3oq
1H 400MHz
f1 (ppm)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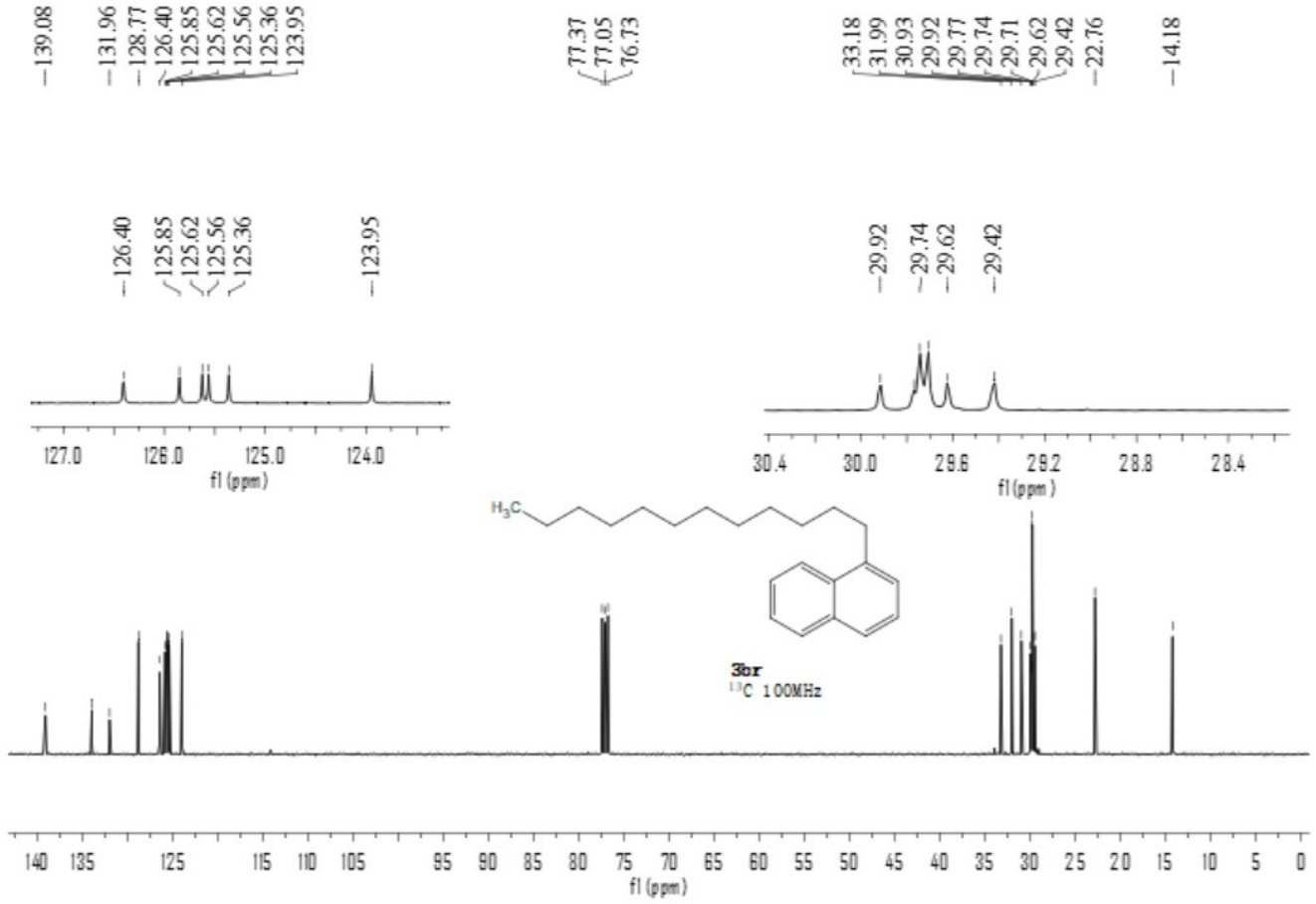
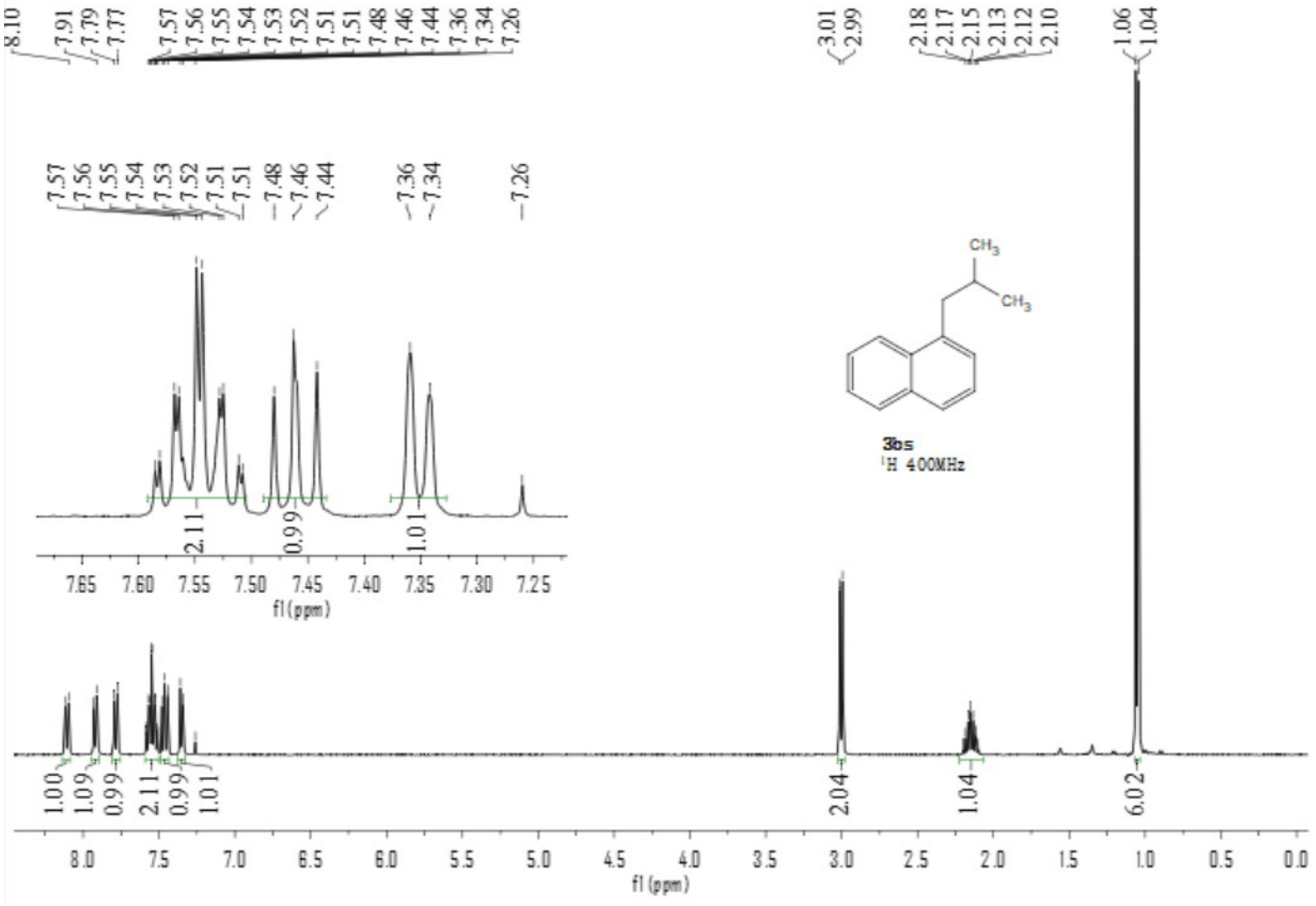
132.10
128.89
126.54
125.97
125.75
125.68
125.48
124.05
77.50
77.18
76.86
33.29
31.95
31.01
29.71
22.86
14.30
3bq
13C 100MHz
f1 (ppm)
8.10
8.08
7.73
7.54
7.52
7.52
7.51
7.50
7.49
7.48
7.48
7.45
7.43
7.41
7.36
7.35
7.26
3.12
3.10
3.08
1.81
1.79
1.77
1.75
1.46
1.31
0.95
0.93
0.91
3br
1H 400MHz
1.00
0.99
0.99
2.01
1.00
1.01
2.08
2.13
2.19
16.14
3.14
f1 (ppm)


3or
13C 100MHz
f1 (ppm)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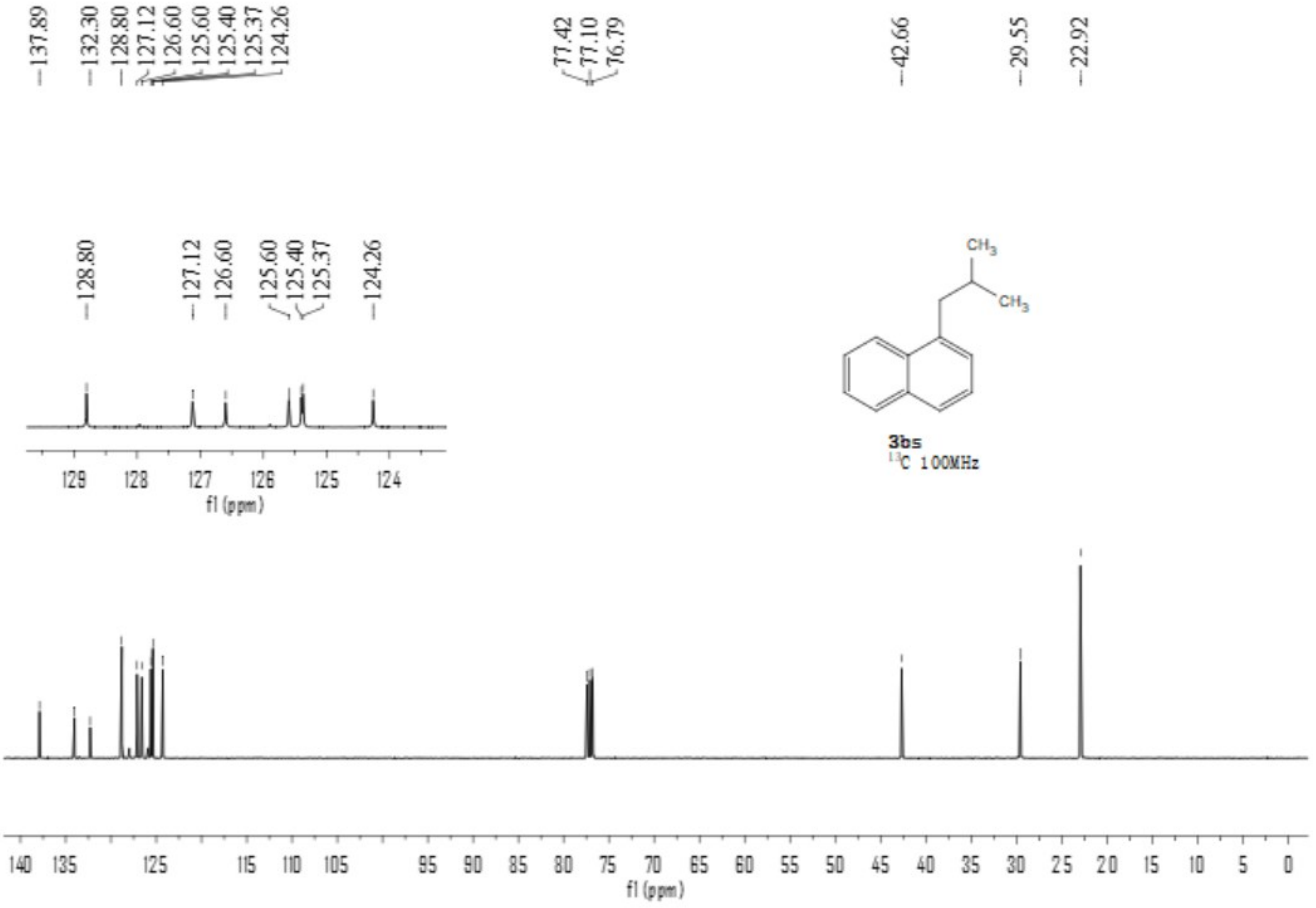
1H 400MHz
f1 (ppm)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132.30
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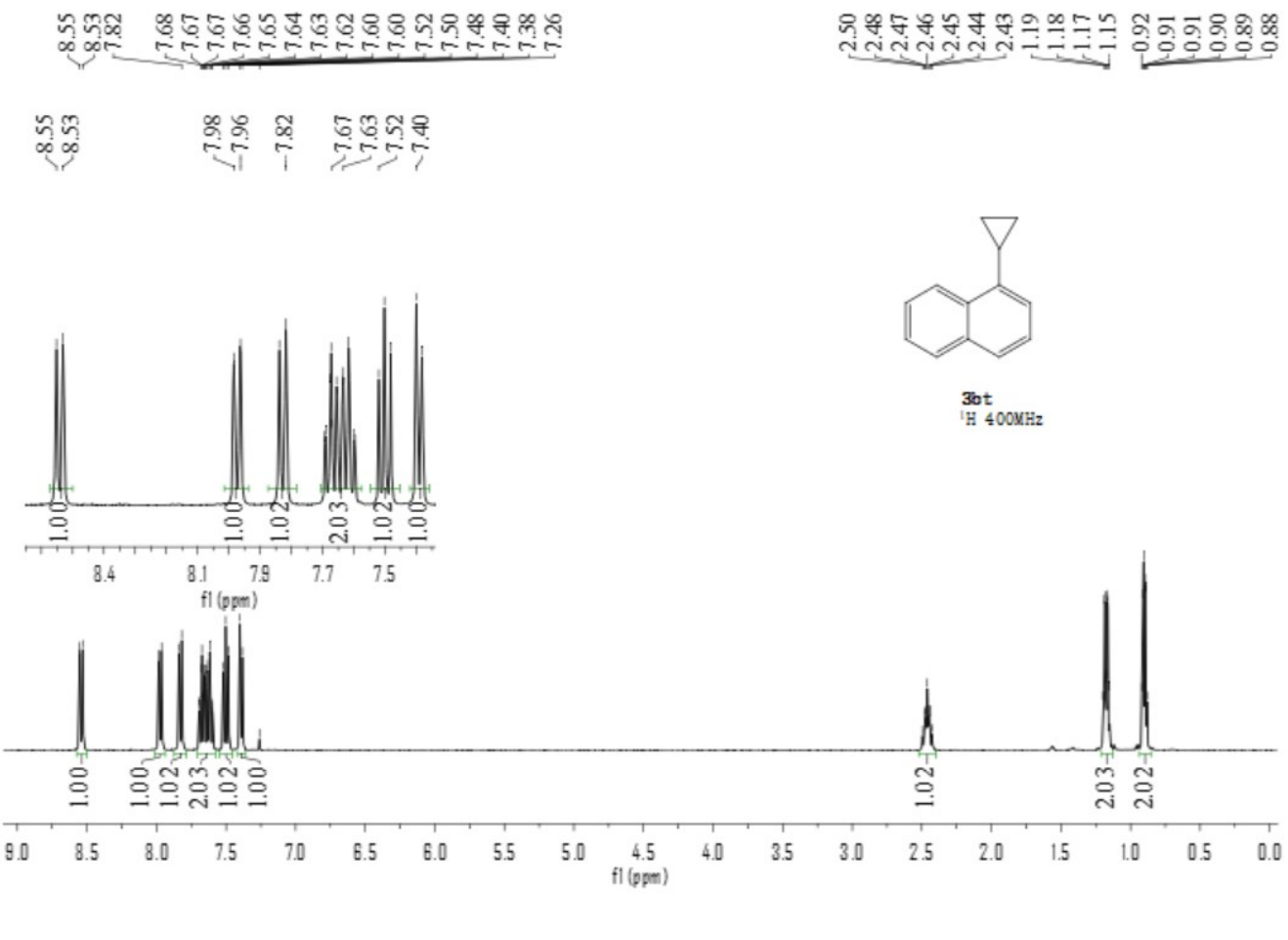
126.60
125.60
125.40
125.37
124.26
77.42
77.10
76.79
42.66
29.55
22.92
CH3
CH3
3bs
13C 100MHz
f1 (ppm)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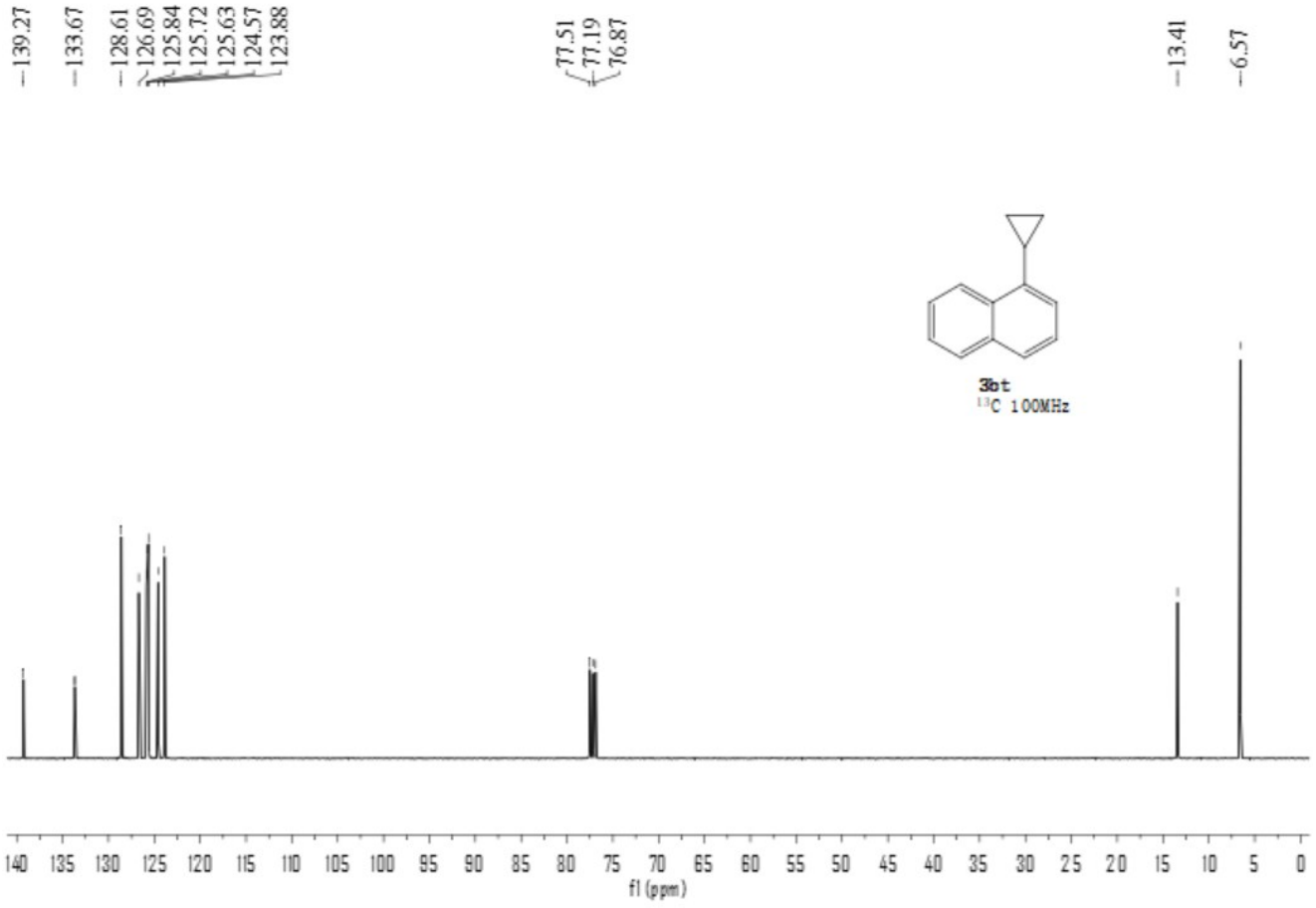
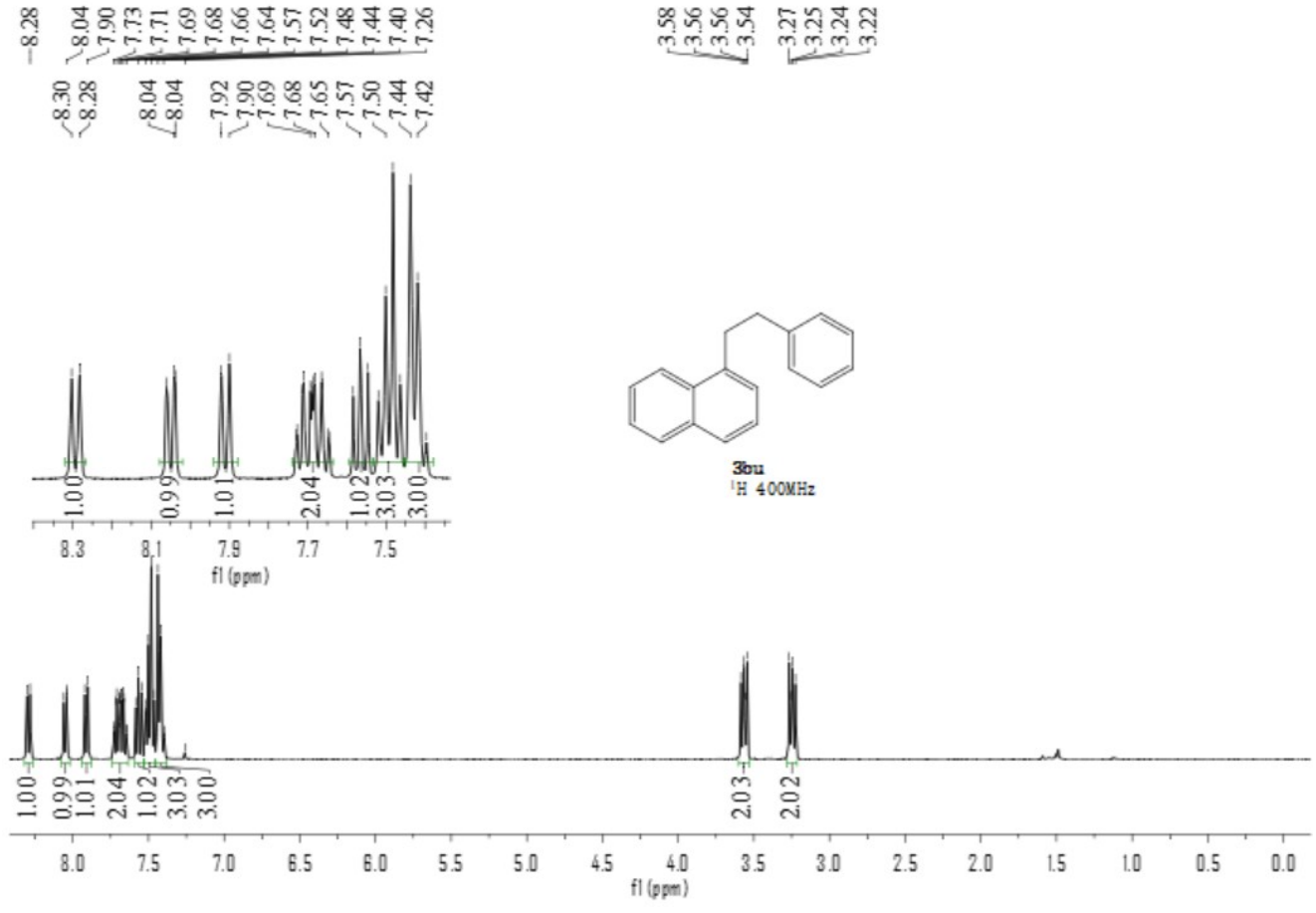
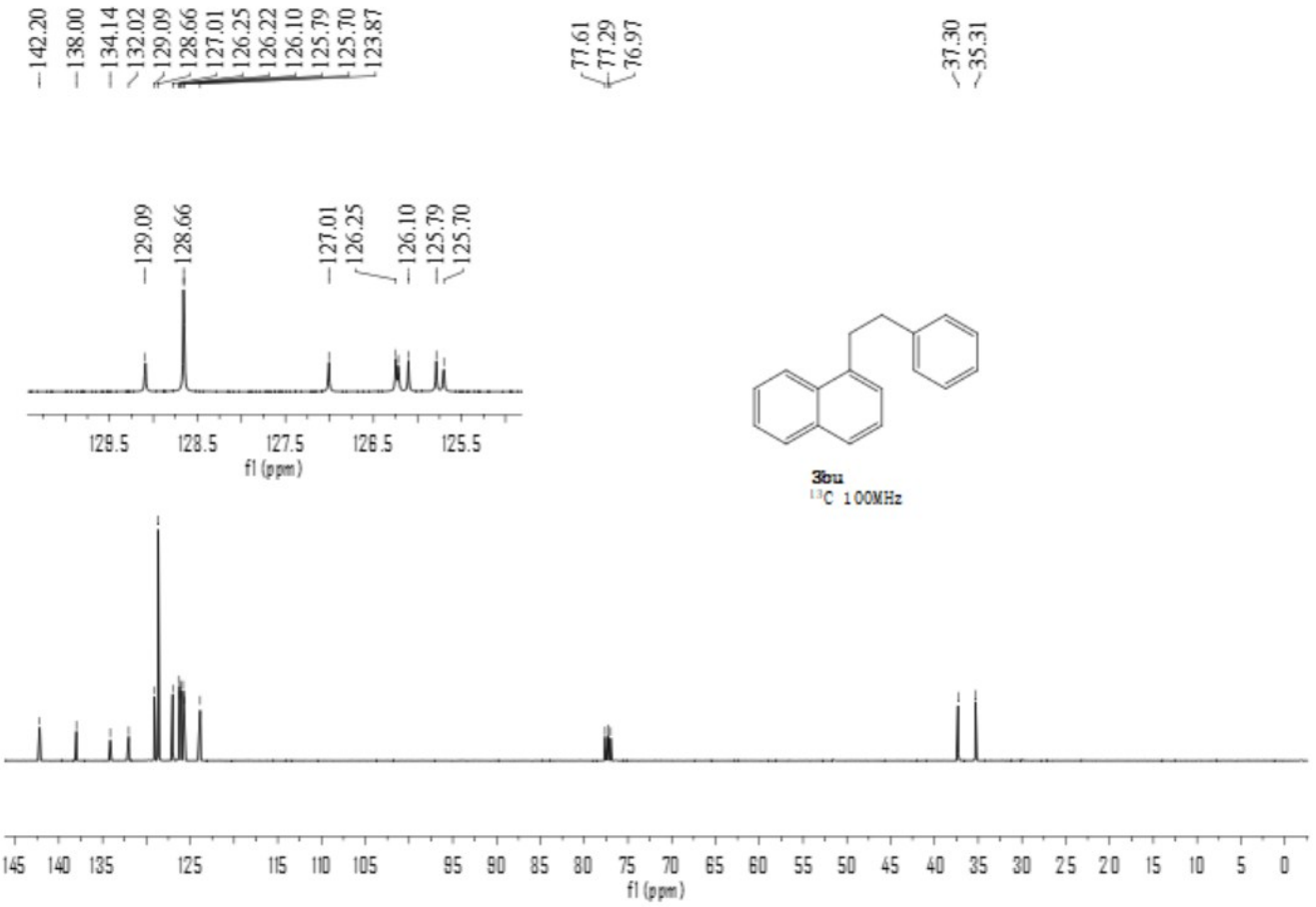
7.82
7.68
7.67
7.67
7.66
7.65
7.64
7.63
7.62
7.60
7.60
7.52
7.50
7.48
7.40
7.38
7.26
2.50
2.48
2.47
2.46
2.45
2.44
2.43
1.19
1.18
1.17
1.15
0.92
0.91
0.91
0.90
0.89
0.88
3bt
1H 400MHz
f1 (ppm)


139.27
133.67
128.61
126.69
125.84
125.72
125.63
124.57
123.88
77.51
77.19
76.87
13.41
6.57
3ot
13C 100MHz
f1 (ppm)


8.28
8.04
7.90
7.73
7.71
7.69
7.68
7.66
7.64
7.57
7.52
7.48
7.44
7.40
7.26
3.58
3.56
3.56
3.54
3.27
3.25
3.24
3.22
3ou
1H 400MHz
f1 (ppm)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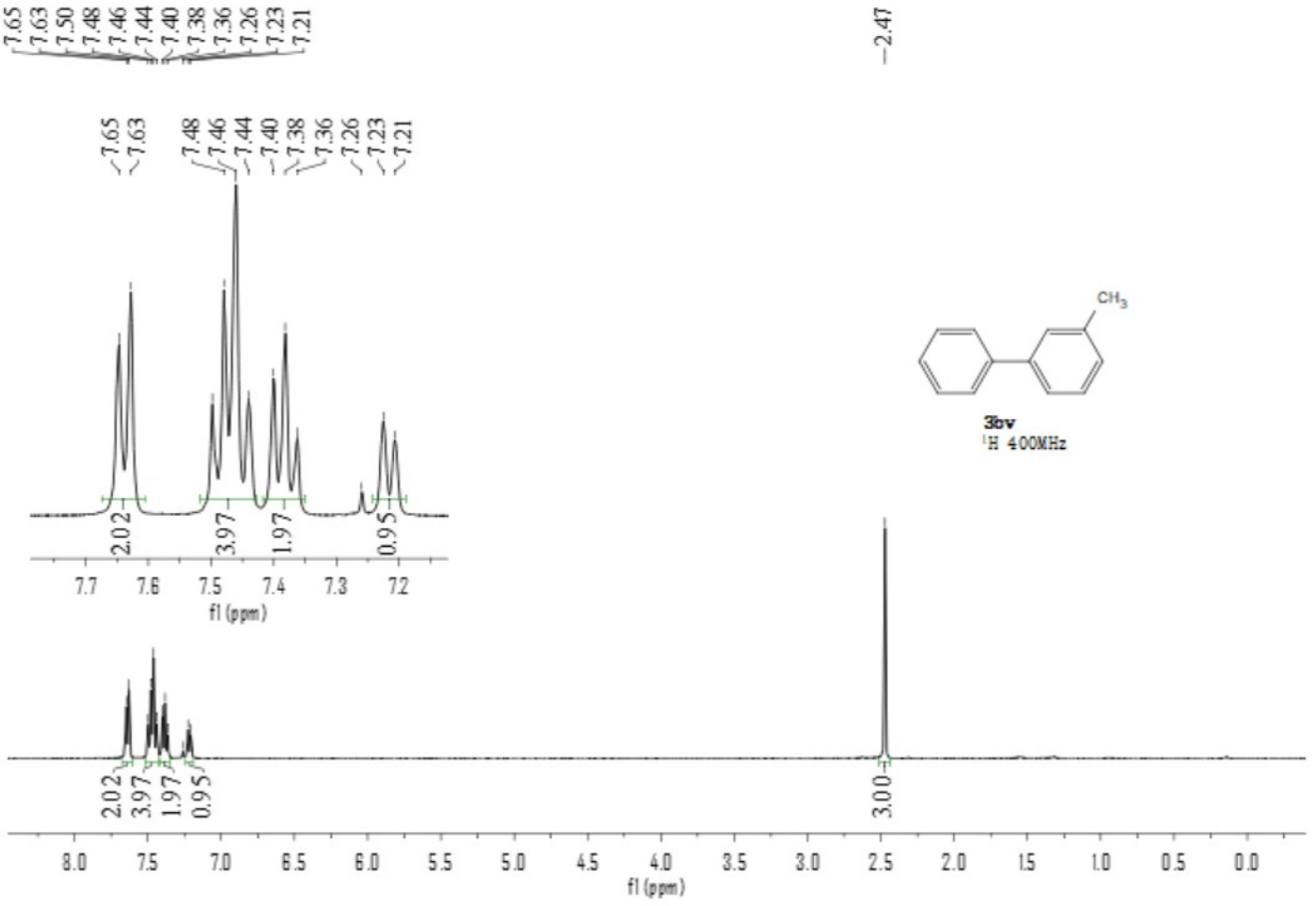
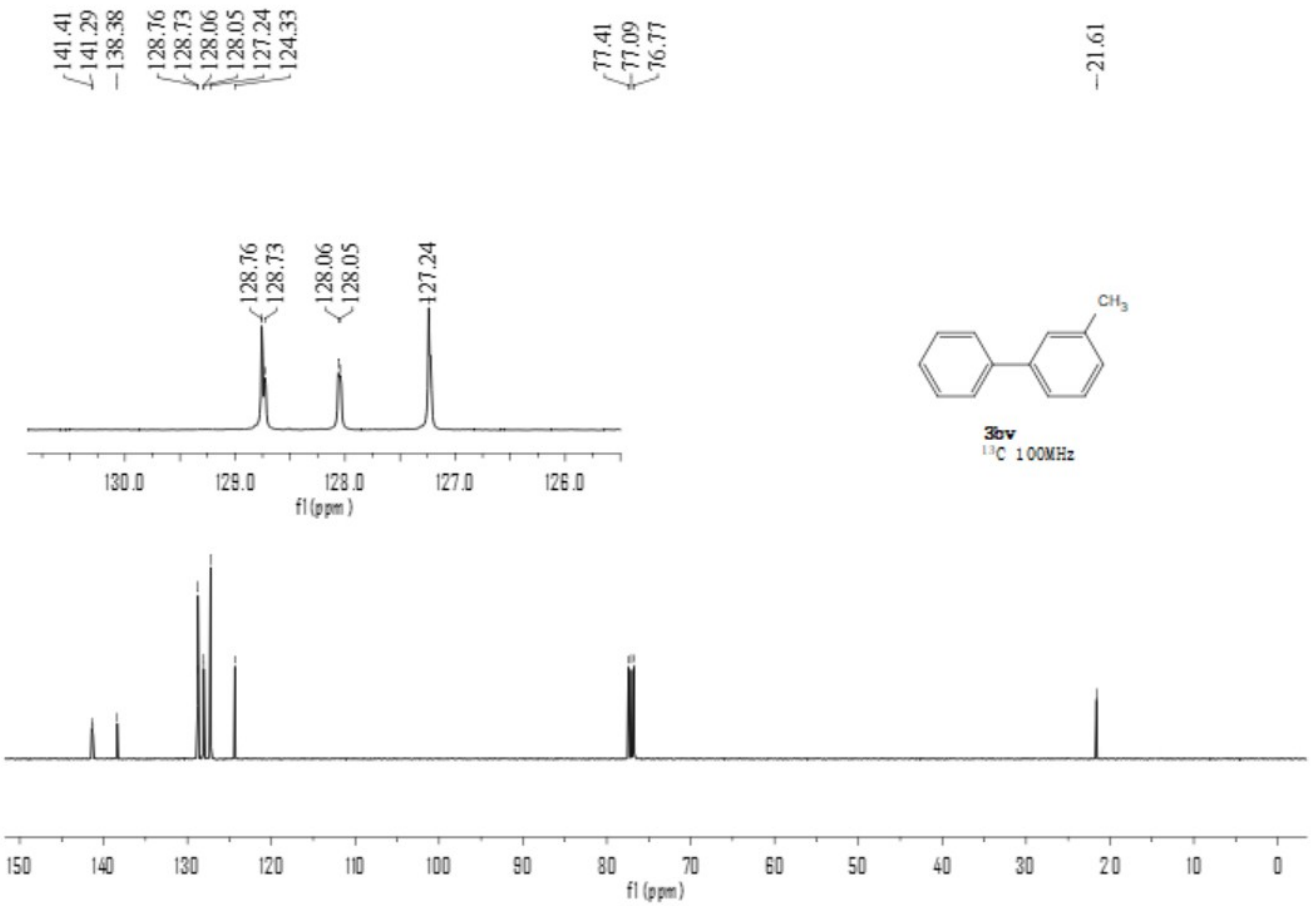
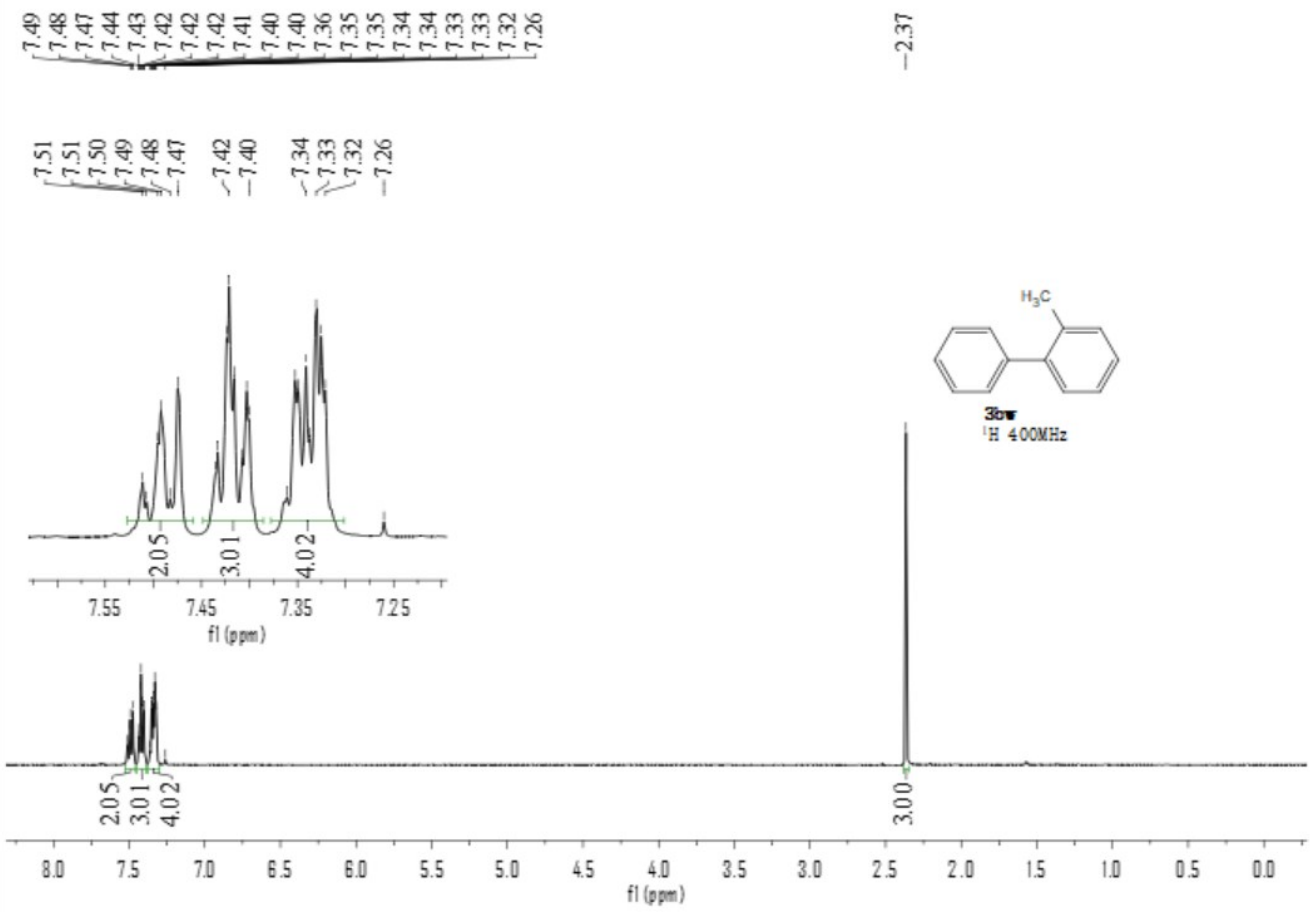
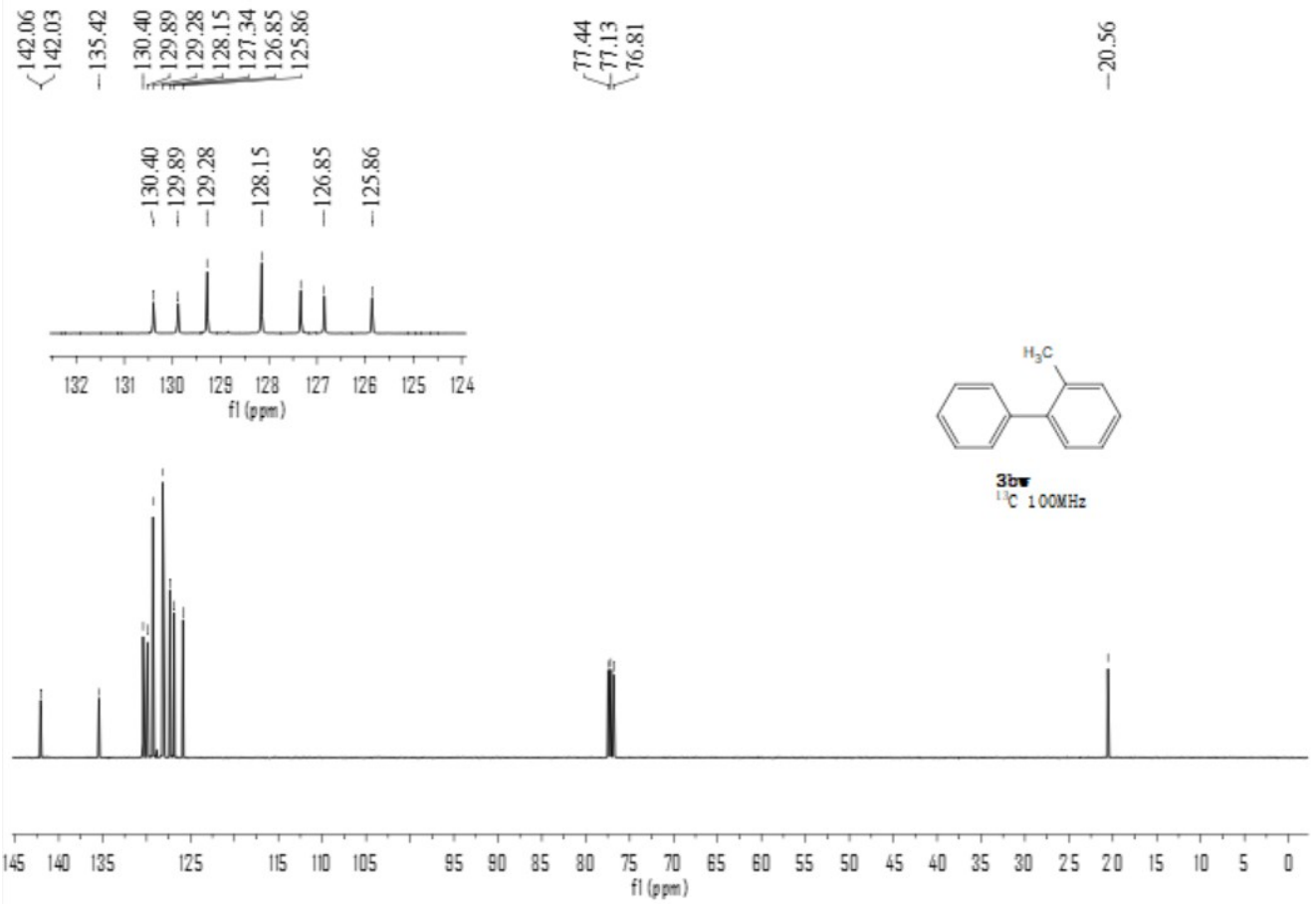
138.00
134.14
132.02
129.09
128.66
127.01
126.25
126.22
126.10
125.79
125.70
123.87
77.61
77.29
76.97
37.30
35.31
129.09
128.66
127.01
126.25
126.10
125.79
125.70
128.5
128.5
127.5
126.5
125.5
f1 (ppm)
3bu
13C 100MHz
145 140 135 125 115 110 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


7.65
7.63
7.50
7.48
7.46
7.44
7.40
7.38
7.36
7.26
7.23
7.21
2.47
2.02
3.97
1.97
0.95
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
CH3
3bv
1H 400MHz
3.00
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)


141.41
141.29
138.38
128.76
128.73
128.06
128.05
127.24
124.33
77.41
77.09
76.77
21.61
CH3
3ov
13C 100MHz
f1 (ppm)


7.49
7.48
7.47
7.44
7.43
7.42
7.42
7.42
7.41
7.40
7.40
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.26
2.37
7.51
7.51
7.50
7.49
7.48
7.47
7.42
7.40
7.34
7.33
7.32
7.26
H3C
3ov
1H 400MHz
2.05
3.01
4.02
3.00
f1 (ppm)


142.06
142.03
135.42
130.40
129.89
129.28
128.15
127.34
126.85
125.86
77.44
77.13
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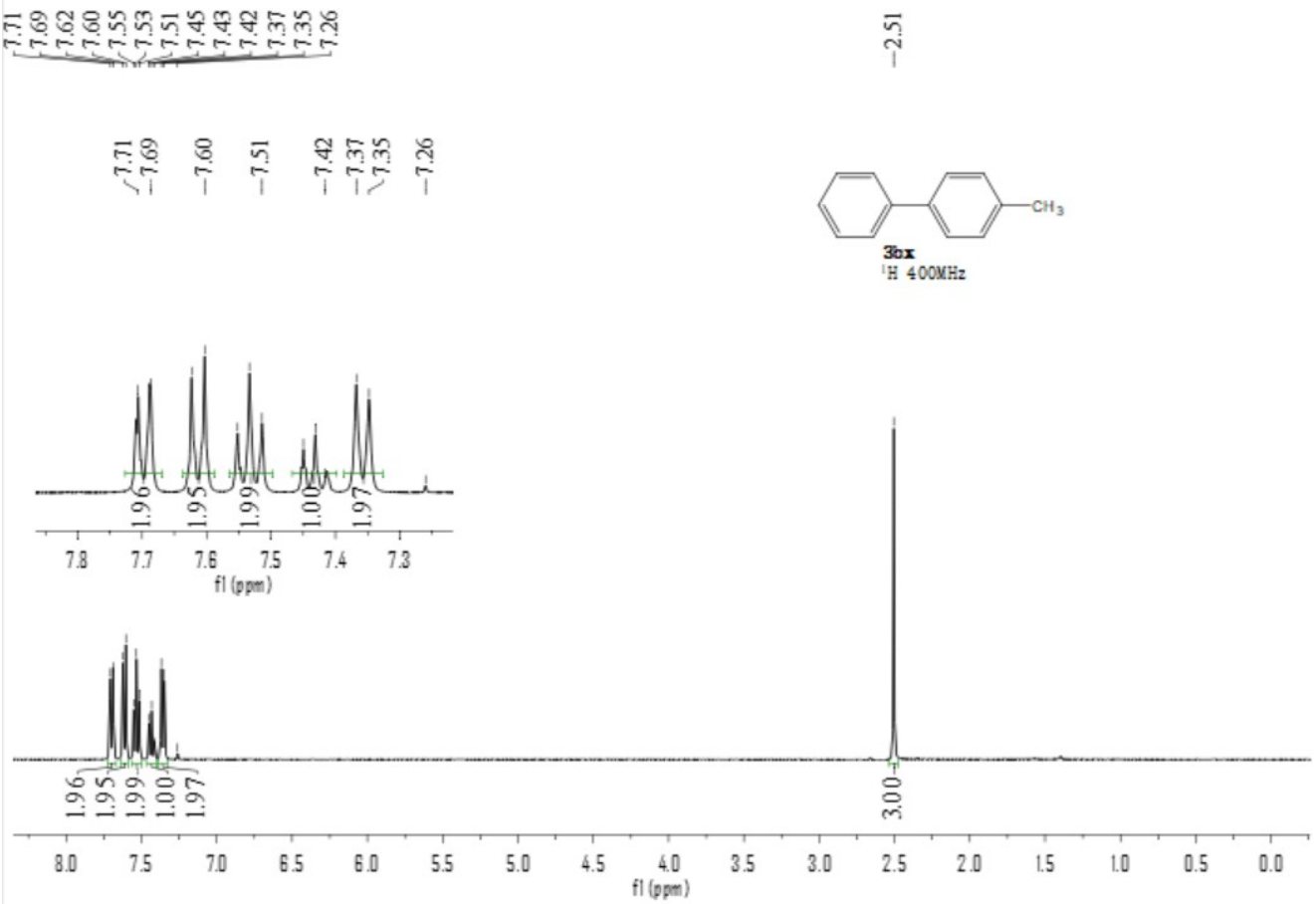
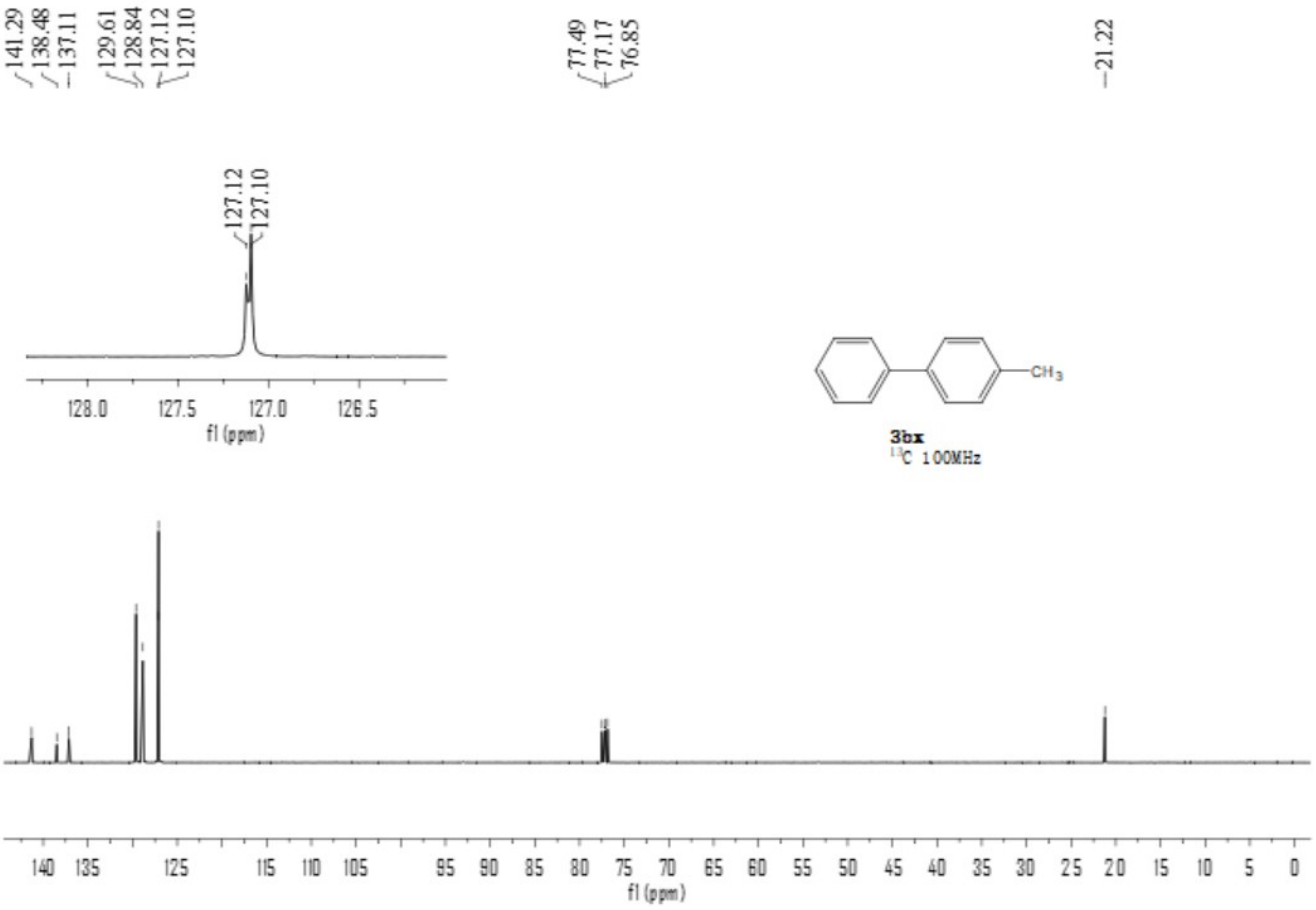
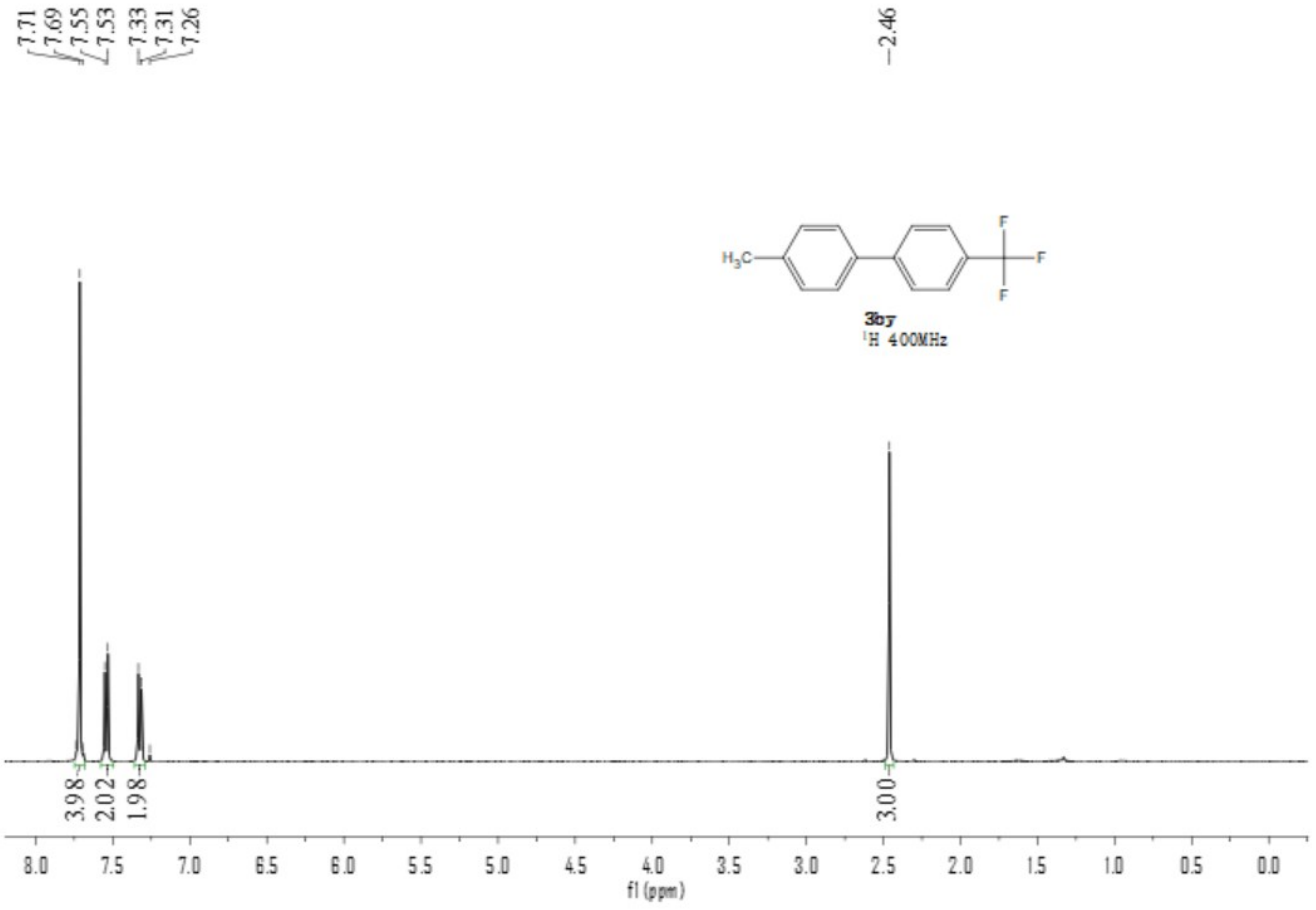
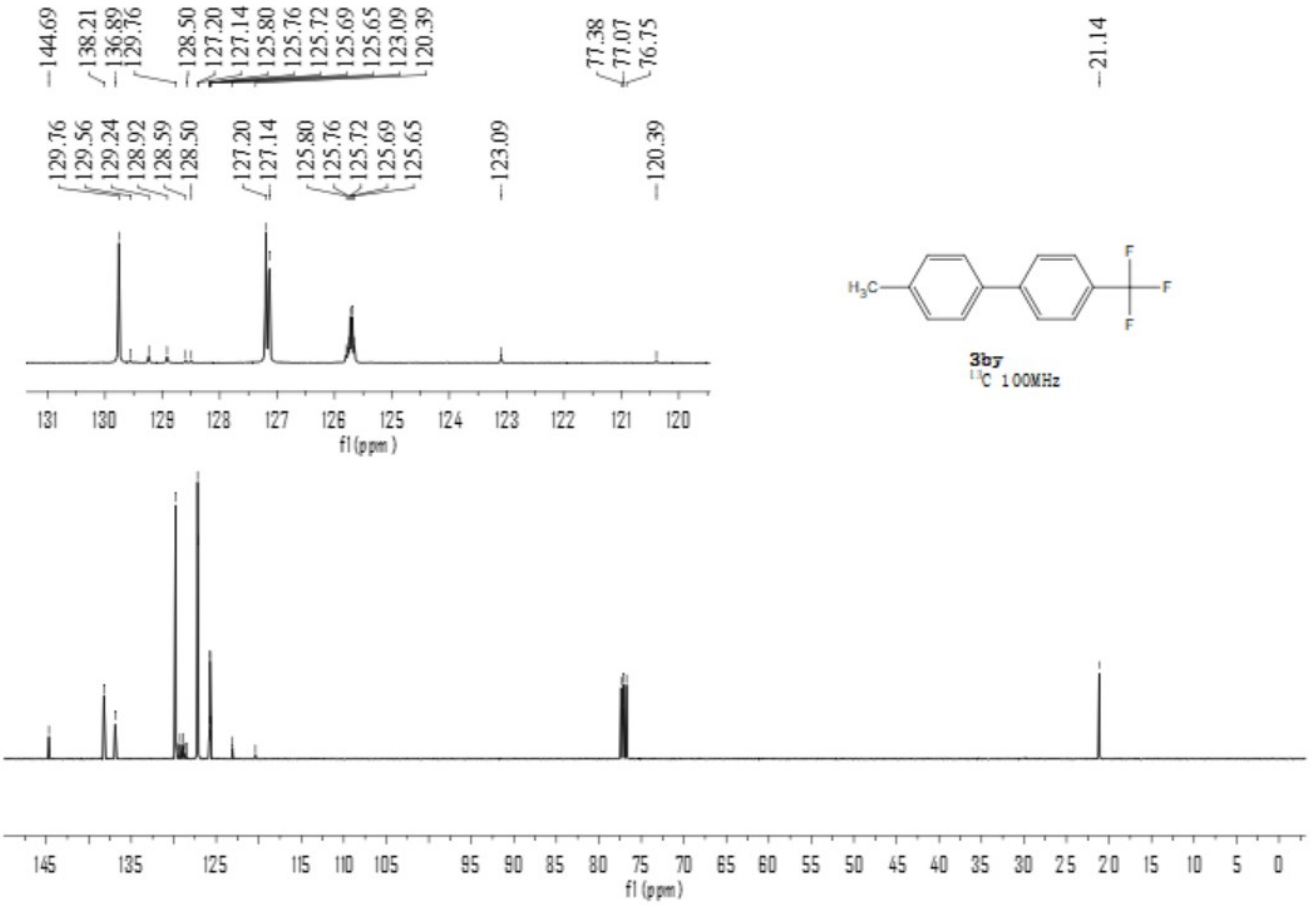
20.56
H3C
3bw
13C 100MHz
fl (ppm)


7.71
7.69
7.62
7.60
7.55
7.53
7.51
7.45
7.43
7.42
7.37
7.35
7.26
2.51
CH3
3bx
1H 400MHz
1.96
1.95
1.99
1.00
1.97
3.00
fl (ppm)


141.29
138.48
137.11
129.61
128.84
127.12
127.10
77.49
77.17
76.85
21.22
127.12
127.10
128.0
127.5
127.0
126.5
f1 (ppm)
CH3
3bx
13C 100MHz
140 135 125 115 110 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


7.71
7.69
7.55
7.53
7.33
7.31
7.26
2.46
H3C
F
F
F
3by
1H 400MHz
3.98
2.02
1.98
3.00
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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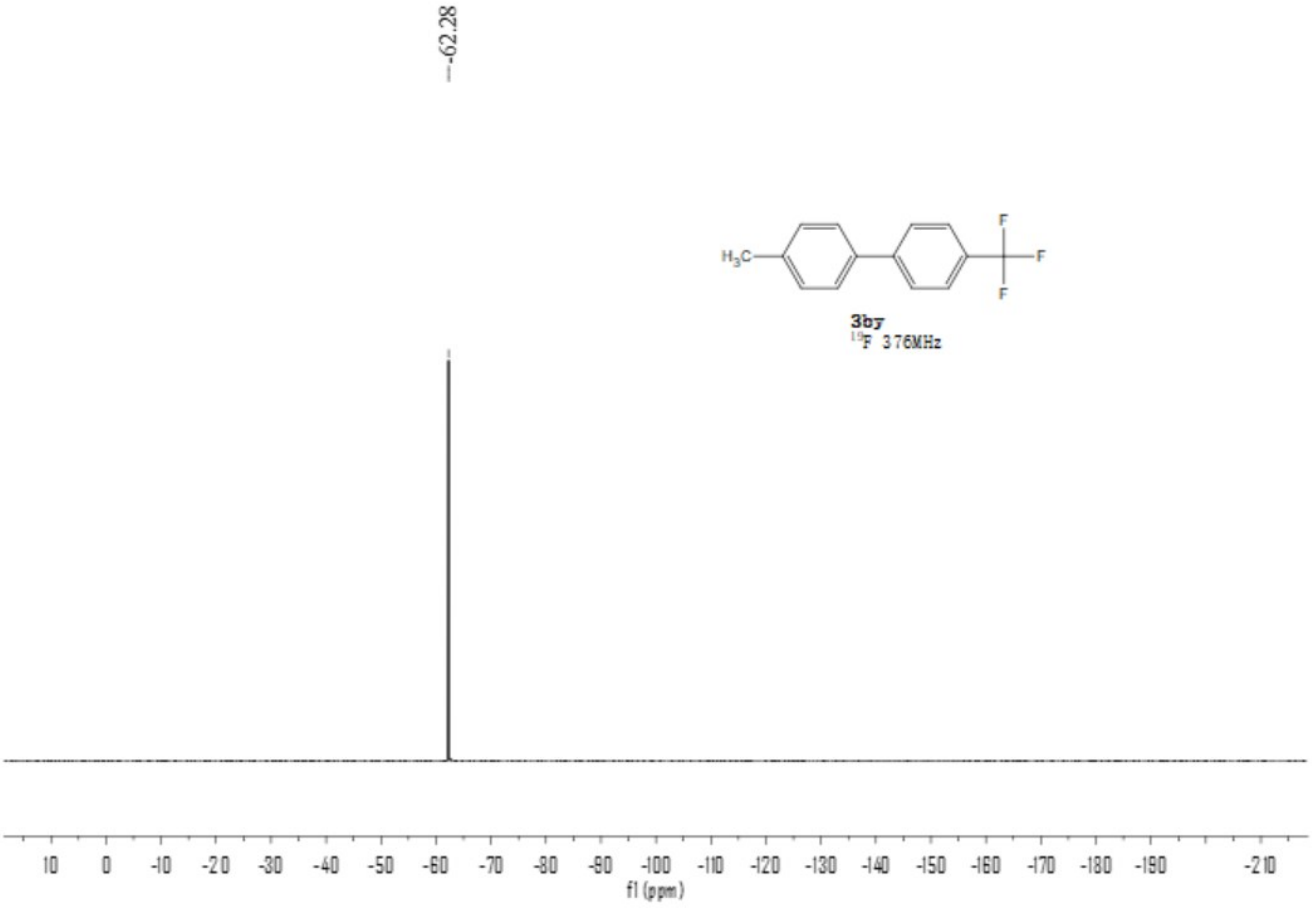
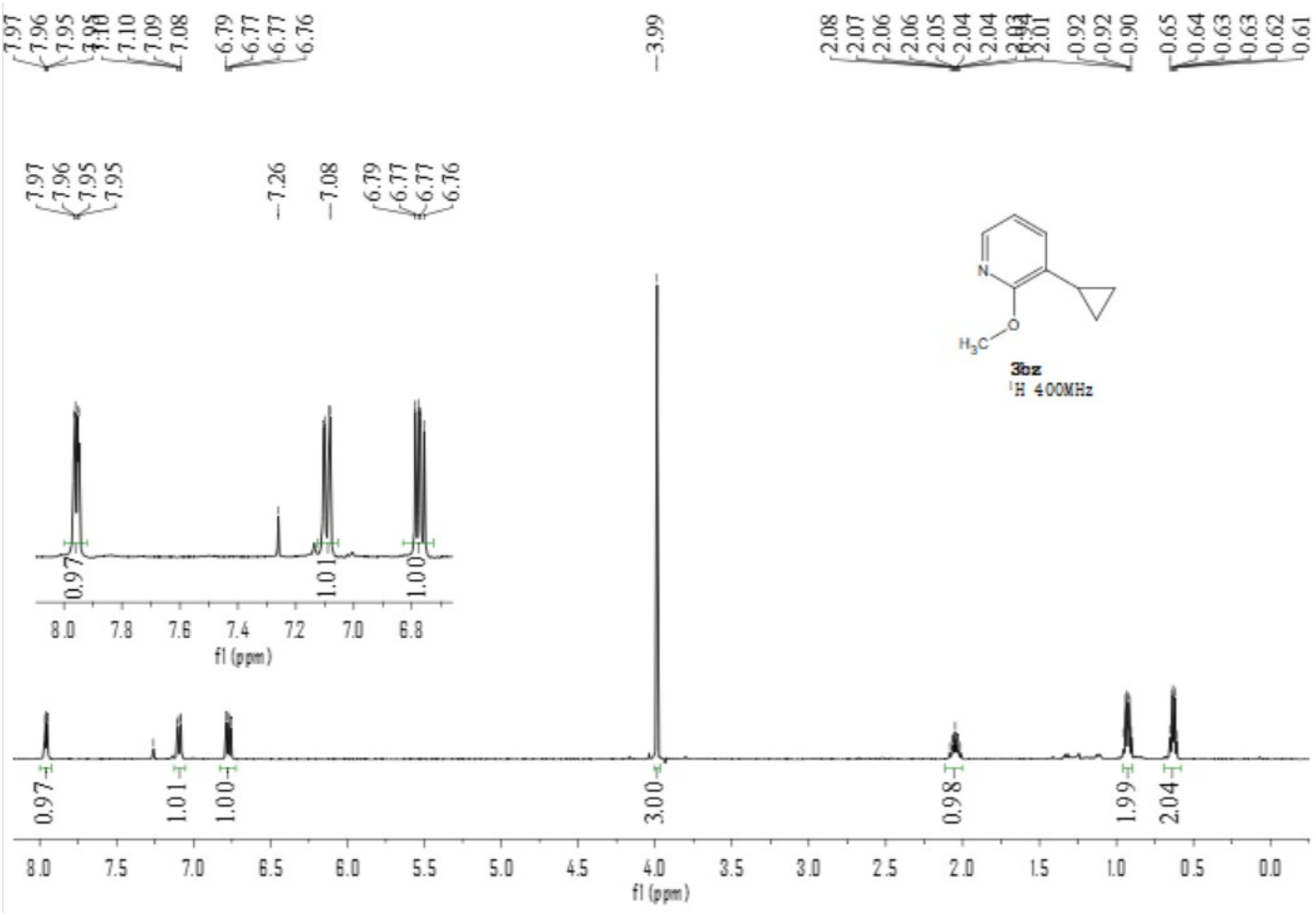
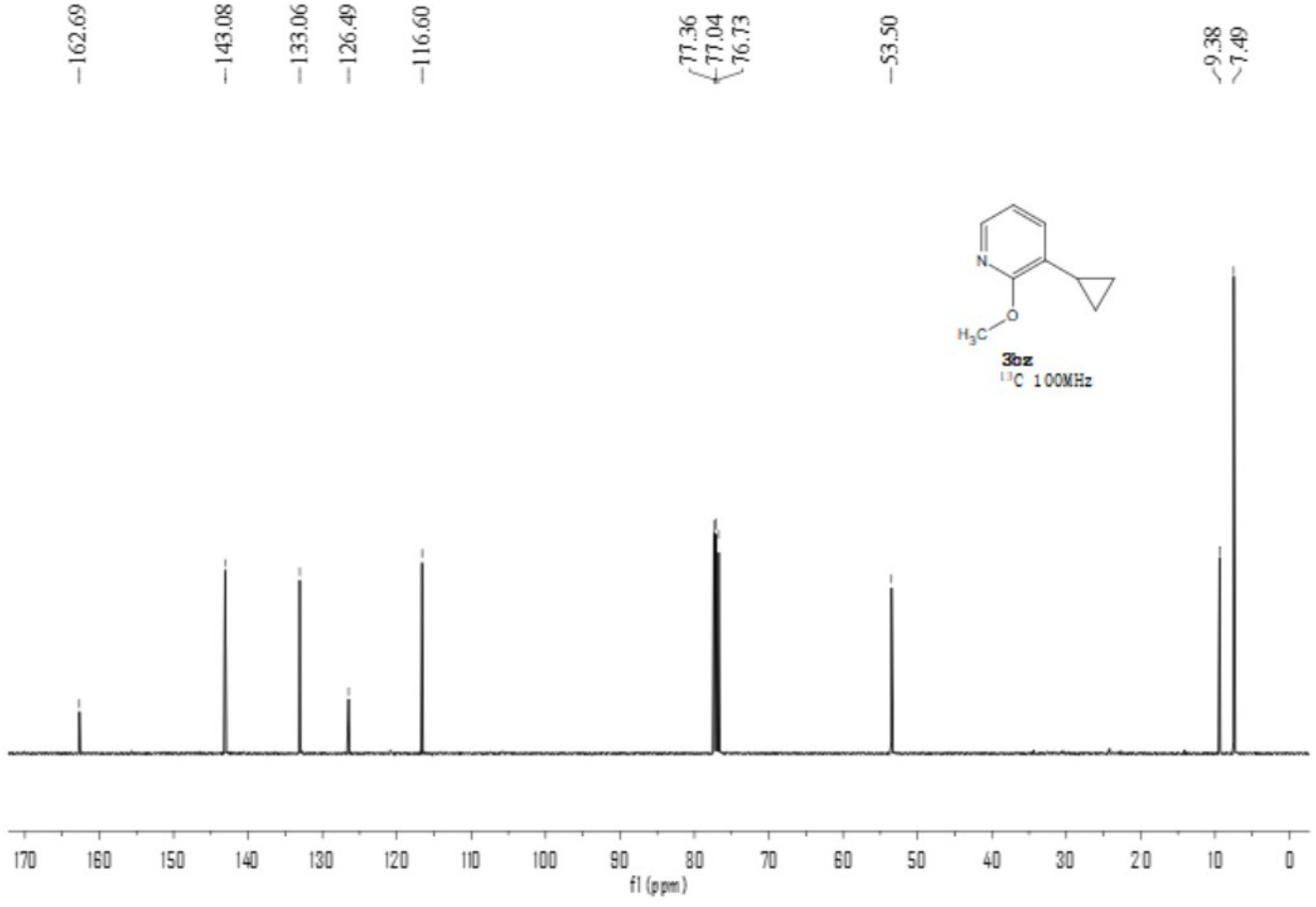
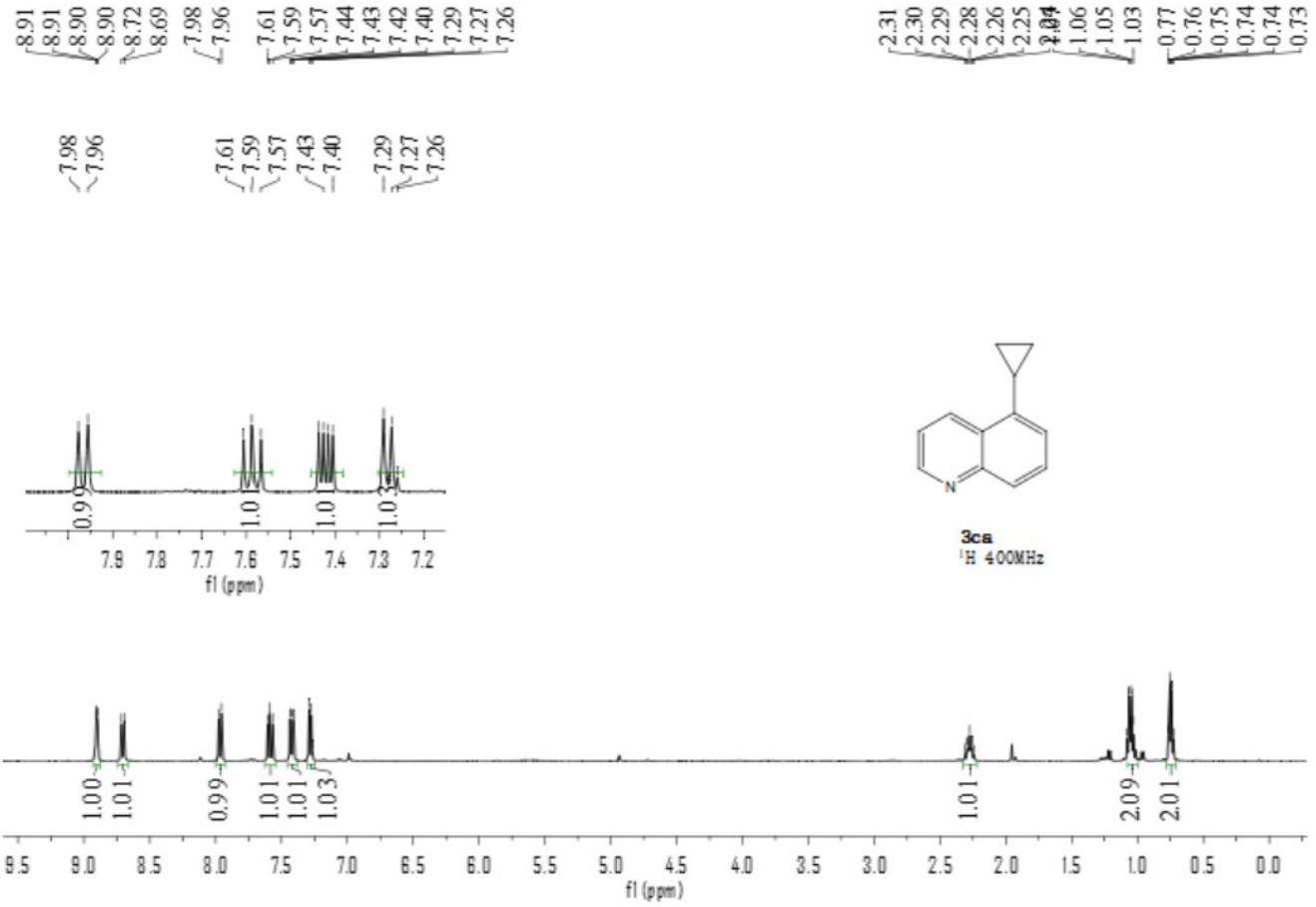
138.21
136.89
129.76
128.50
127.20
127.14
125.80
125.76
125.72
125.69
125.65
123.09
120.39
77.38
77.07
76.75
21.14
129.76
129.56
129.24
128.92
128.59
128.50
127.20
127.14
125.80
125.76
125.72
125.69
125.65
123.09
120.39
131 130 129 128 127 126 125 124 123 122 121 120
f1 (ppm)
3by
13C 100MHz
145 135 125 115 110 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


-62.28
3by
19F 376MHz
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -210
f1 (ppm)


3bz
1H 400MHz
f1 (ppm)


3bz
13C 100MHz
f1 (ppm)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8.90
8.90
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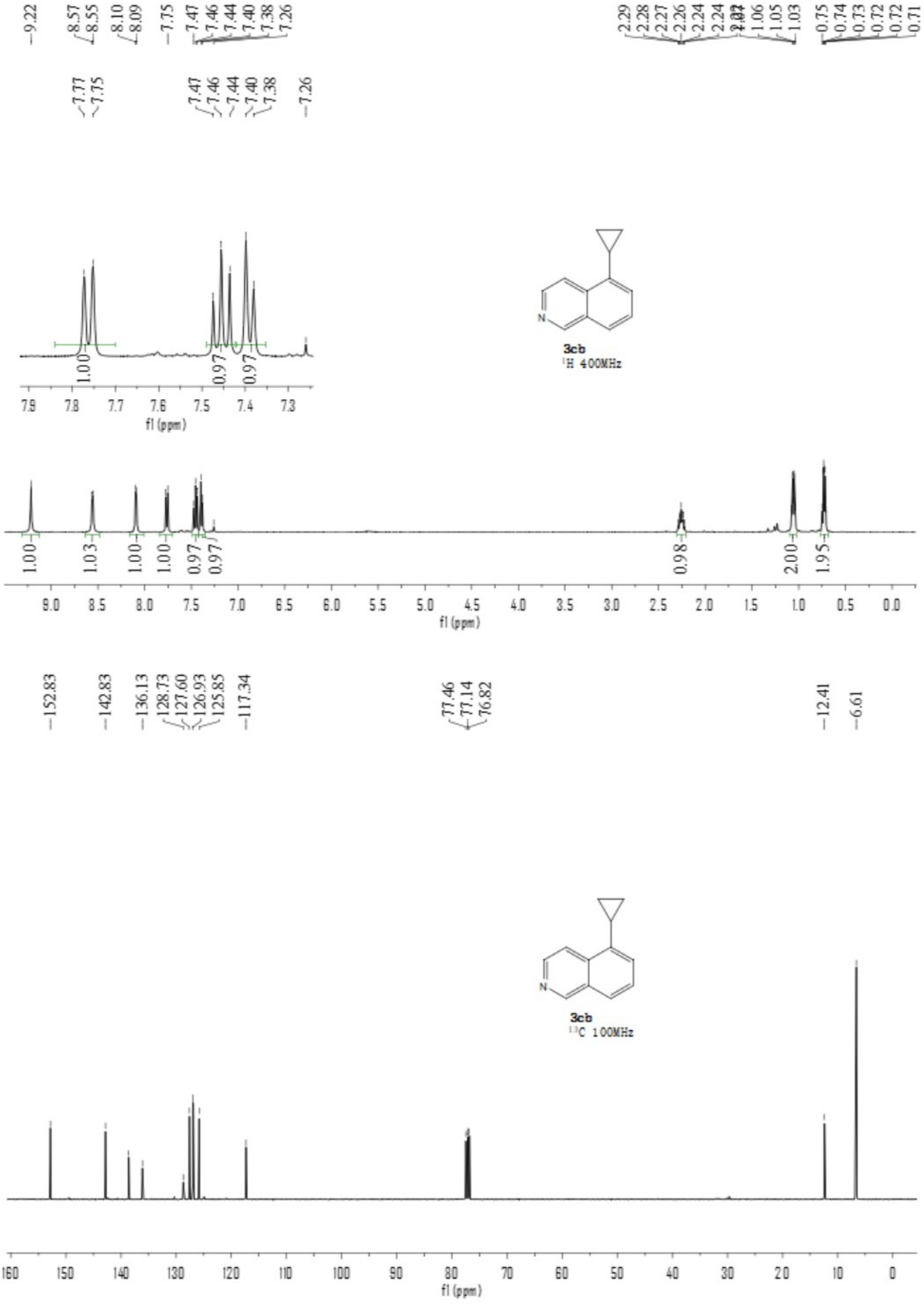
8.69
7.98
7.96
7.61
7.59
7.57
7.44
7.43
7.42
7.40
7.29
7.27
7.26
2.31
2.30
2.29
2.28
2.26
2.25
1.06
1.05
1.03
0.77
0.76
0.75
0.74
0.74
0.73
0.99
1.0
1.0
1.03
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
3ca
1H 400MHz
1.00
1.01
0.99
1.01
1.01
1.03
1.01
2.09
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
149.82
148.26
139.73
133.04
127.69
124.23
120.70
77.43
77.11
76.79
12.57
6.61
3ca
13C 100MHz
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.57
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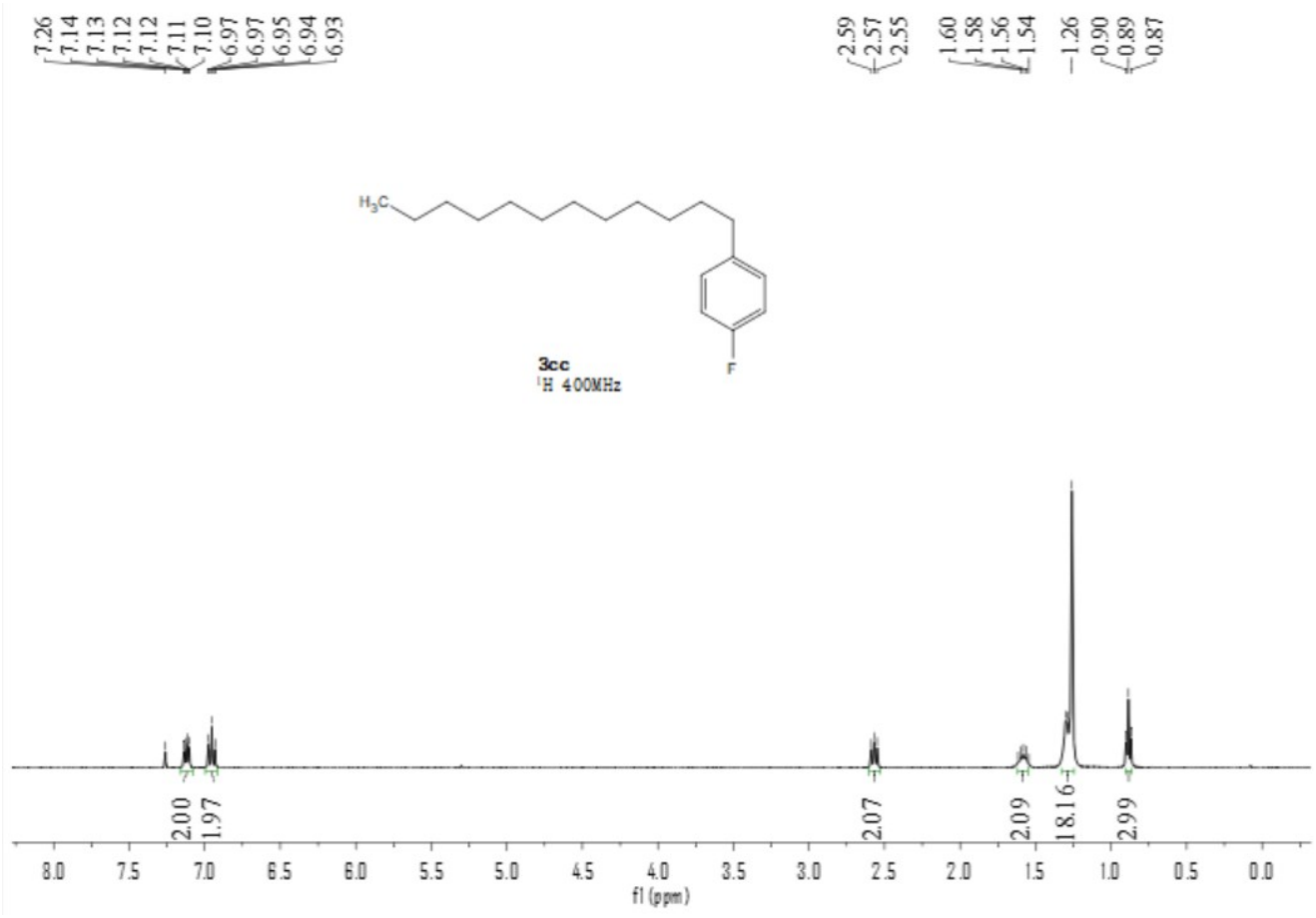
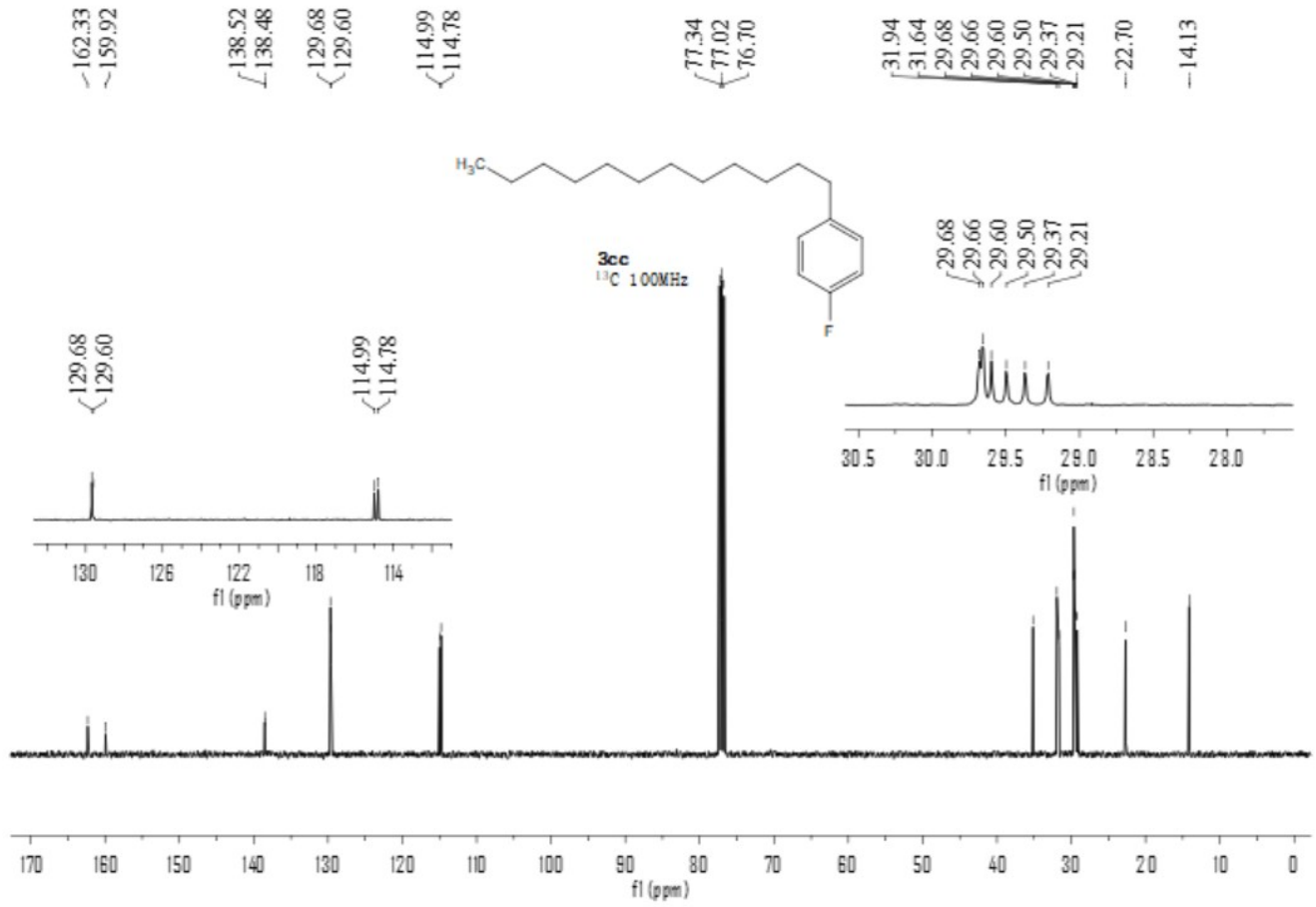
8.10
8.09
7.75
7.47
7.46
7.44
7.40
7.38
7.26
2.29
2.28
2.27
2.26
2.24
2.24
1.06
1.05
1.03
0.75
0.74
0.73
0.72
0.72
0.71
7.77
7.75
7.47
7.46
7.44
7.40
7.38
7.26
1.00
0.97
0.97
7.9
7.8
7.7
7.6
7.5
7.4
7.3
f1 (ppm)
N
3cb
1H 400MHz
1.00
1.03
1.00
1.00
0.97
0.97
0.98
2.00
1.95
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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)
152.83
142.83
136.13
128.73
127.60
126.93
125.85
117.34
77.46
77.14
76.82
12.41
6.61
N
3cb
13C 100MHz
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.26
7.14
7.13
7.12
7.12
7.11
7.10
6.97
6.97
6.95
6.94
6.93
2.59
2.57
2.55
1.60
1.58
1.56
1.54
1.26
0.90
0.89
0.87
H3C
F
3cc
1H 400MHz
2.00
1.97
2.07
2.09
18.16
2.99
f1 (ppm)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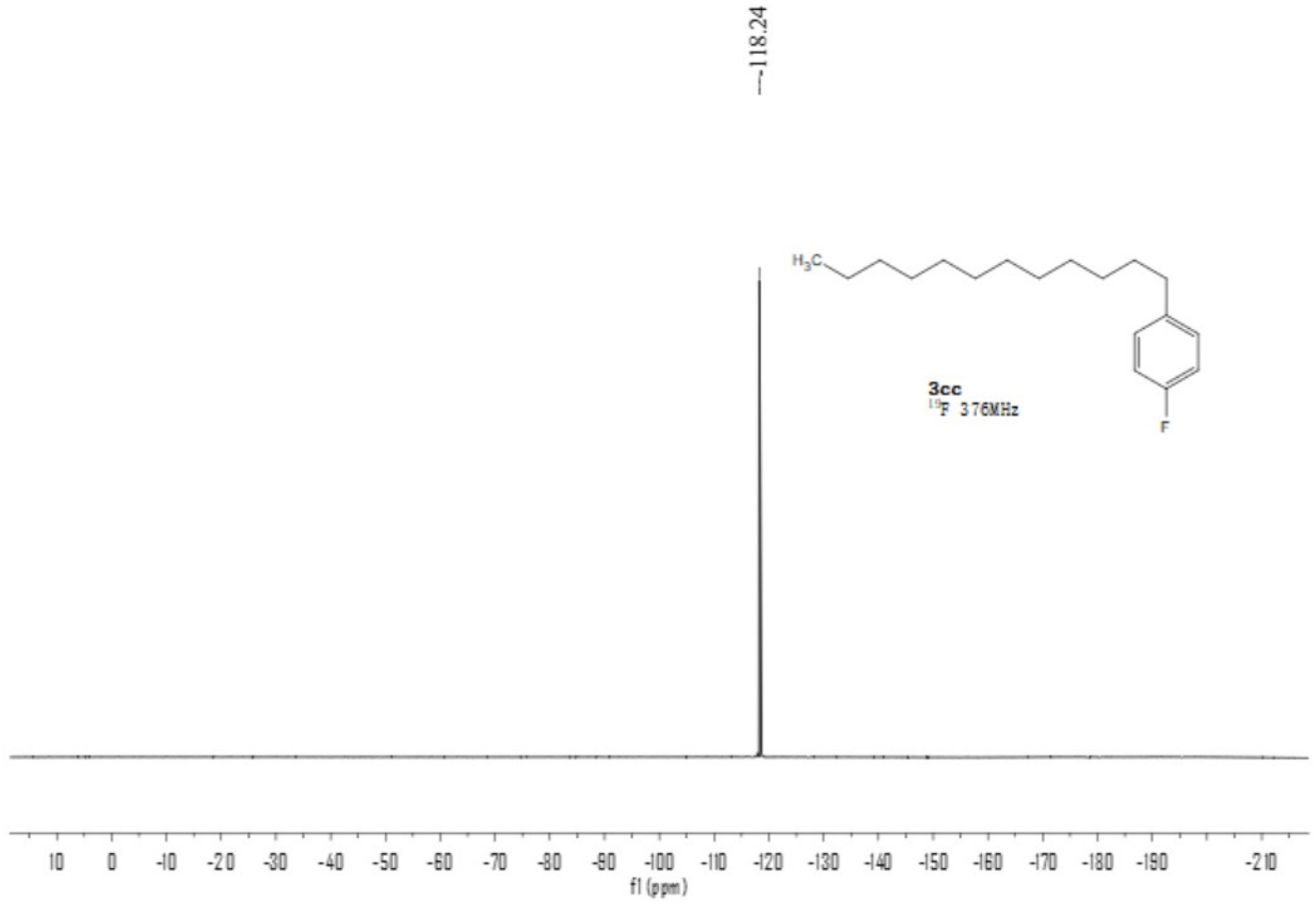
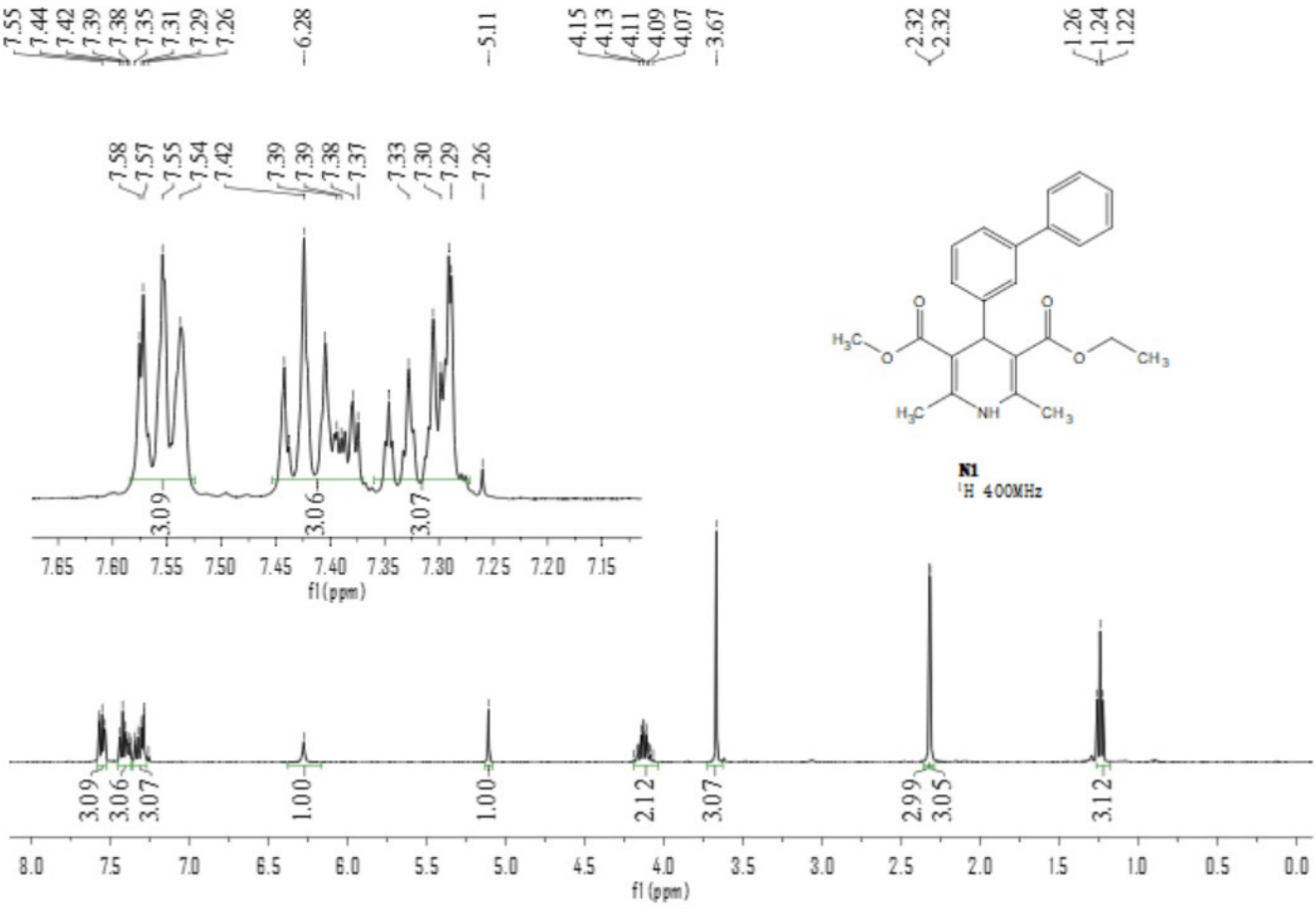
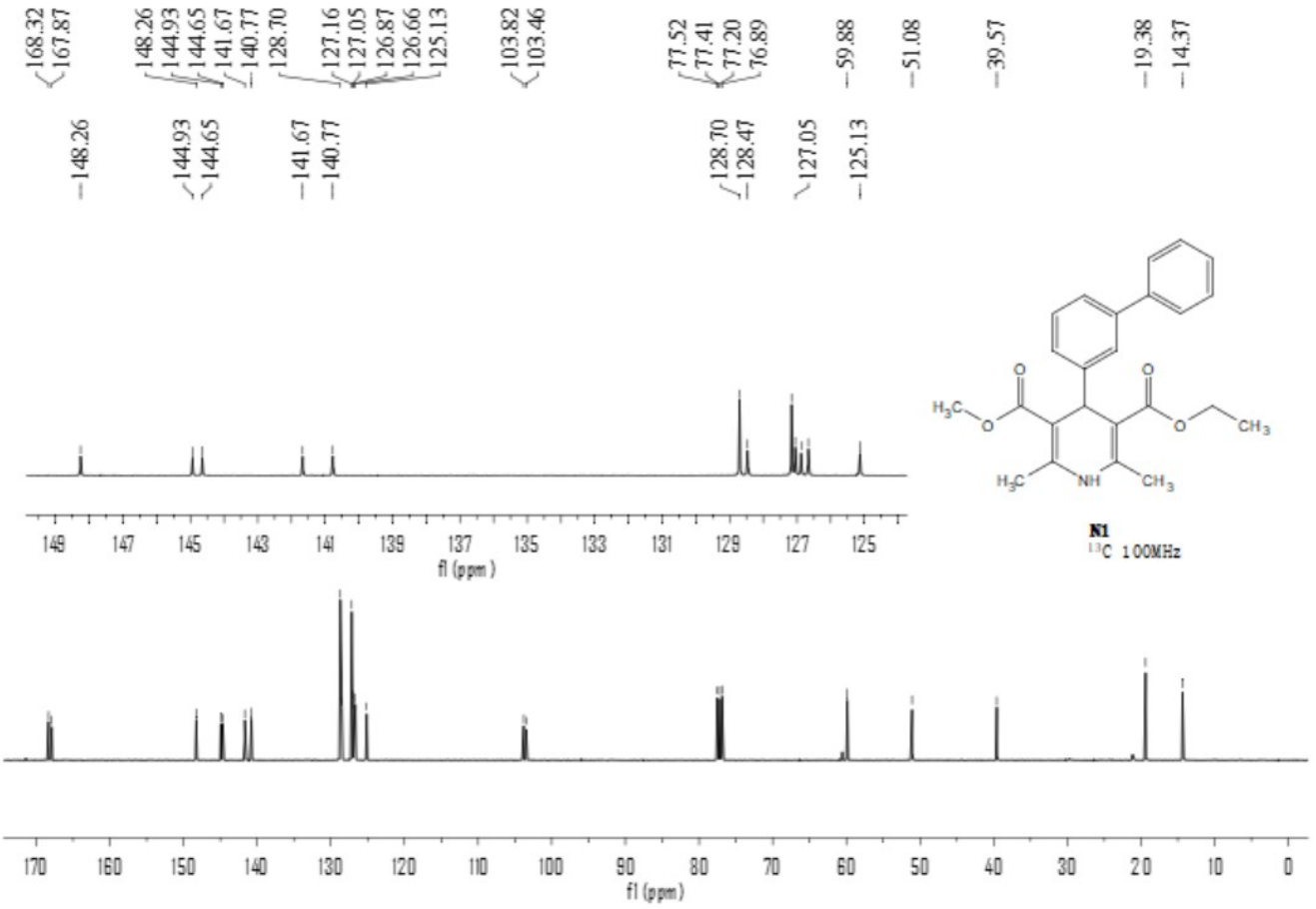
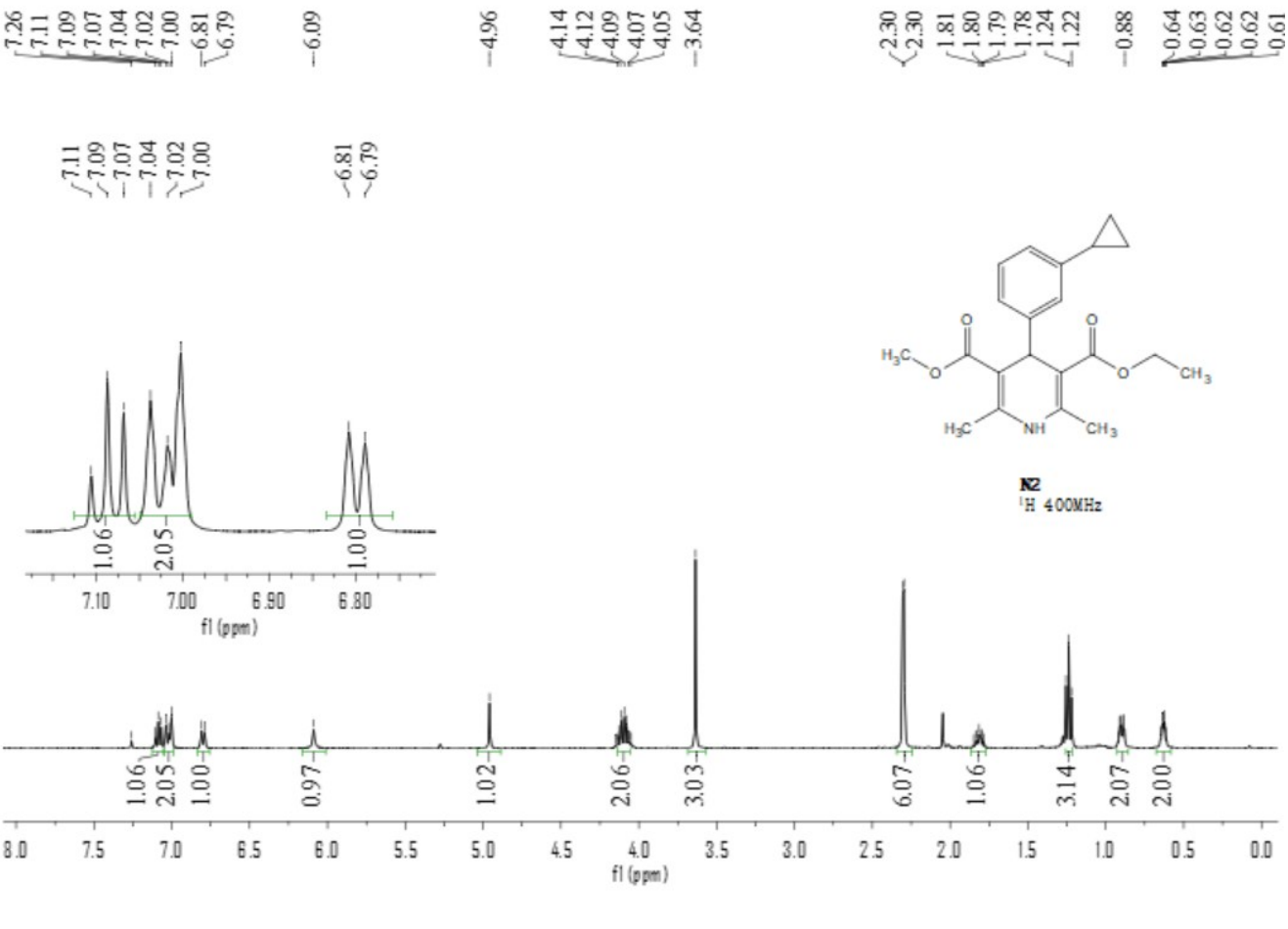
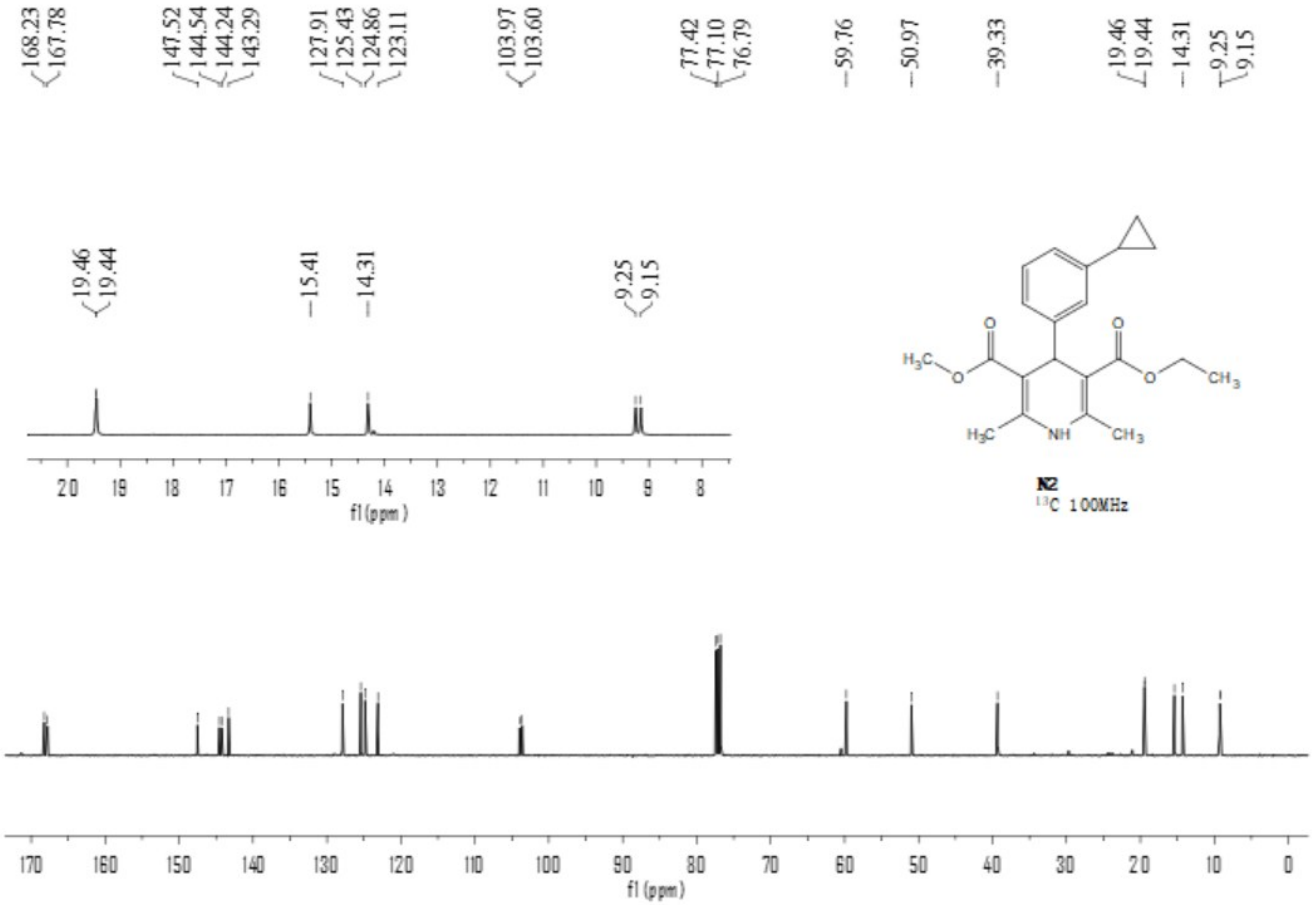
159.92
138.52
138.48
129.68
129.60
114.99
114.78
77.34
77.02
76.70
31.94
31.64
29.68
29.66
29.60
29.50
29.37
29.21
22.70
14.13
H3C
F
3cc
13C 100MHz
129.68
129.60
114.99
114.78
29.68
29.66
29.60
29.50
29.37
29.21
f1 (ppm)


-118.24
3cc
19F 376MHz
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -210
f1 (ppm)


7.55 7.44 7.42 7.39 7.38 7.35 7.31 7.29 7.26
6.28
5.11
4.15 4.13 4.11 4.09 4.07
3.67
2.32 2.32
1.26 1.24 1.22
7.58 7.57 7.55 7.54 7.42 7.39 7.39 7.38 7.37 7.33 7.30 7.29 7.26
3.09 3.06 3.07
7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15
f1 (ppm)
N1
1H 400MHz
3.09 3.06 3.07 1.00 1.00 2.12 3.07 2.99 3.05 3.12
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)


168.32
167.87
148.26
144.93
144.65
141.67
140.77
128.70
127.16
127.05
126.87
126.66
125.13
103.82
103.46
77.52
77.41
77.20
76.89
59.88
51.08
39.57
19.38
14.37
148.26
144.93
144.65
141.67
140.77
128.70
128.47
127.05
125.13
f1 (ppm)
N1
13C 100MHz


7.26
7.11
7.09
7.07
7.04
7.02
7.00
6.81
6.79
6.09
4.96
4.14
4.12
4.09
4.07
4.05
3.64
2.30
2.30
1.81
1.80
1.79
1.78
1.24
1.22
0.88
0.64
0.63
0.62
0.62
0.61
7.11
7.09
7.07
7.04
7.02
7.00
6.81
6.79
1.06
2.05
1.00
0.97
1.02
2.06
3.03
6.07
1.06
3.14
2.07
2.00
f1 (ppm)
N2
1H 400MHz


168.23
167.78
147.52
144.54
144.24
143.29
127.91
125.43
124.86
123.11
103.97
103.60
77.42
77.10
76.79
59.76
50.97
39.33
19.46
19.44
14.31
9.25
9.15
19.46
19.44
15.41
14.31
9.25
9.15
f1(ppm)
N2
13C 100MHz
f1(ppm)