Supporting Information

Ligand-Free Pd-Catalyzed Domino Synthesis of Carbazoles via Dehydrogenative Aromatization/C(sp^2)-C(sp^2) Coupling Sequence

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General Information

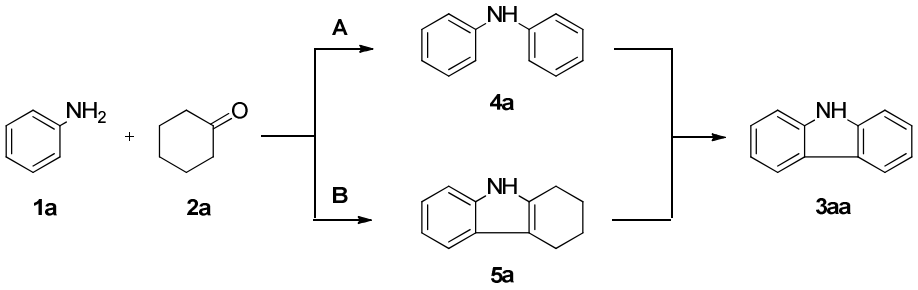
Unless otherwise indicated, all commercial reagents and solvents were used without additional purification. Pentaduterio-N-phenylaniline ([d5]- 4a) was synthesized as previously reported. 1H-NMR spectra and 13C-NMR spectra were recorded on Brucker 400 spectrometer (400 MHz and 100 MHz, respectively) with Me4Si or solvent resonance as the internal standard (1H-NMR, Me4Si at 0 ppm, Acetone-d6 at 2.05 ppm, DMSO-d6 at 2.50 ppm; 13C-NMR, Me4Si at 0 ppm, Acetone-d6 at 206.7 ppm and 29.9 ppm, DMSO-d6 at 39.6 ppm).

Mechanism Study

(1) Reaction pathways

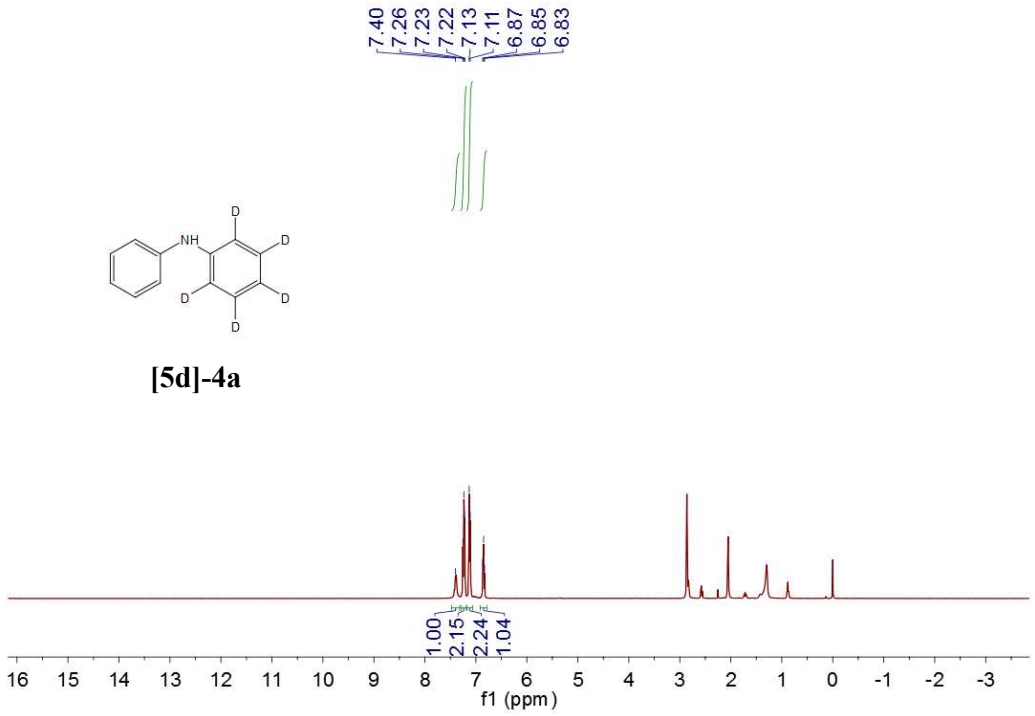
There are two possible reaction pathways. In pass A, the product 3aa is generated via the intermediate 4a by dual aryl C-C bond formation. Whereas, a cross coupling reaction occurs followed by a dehydrogenative oxidation reaction in path B.

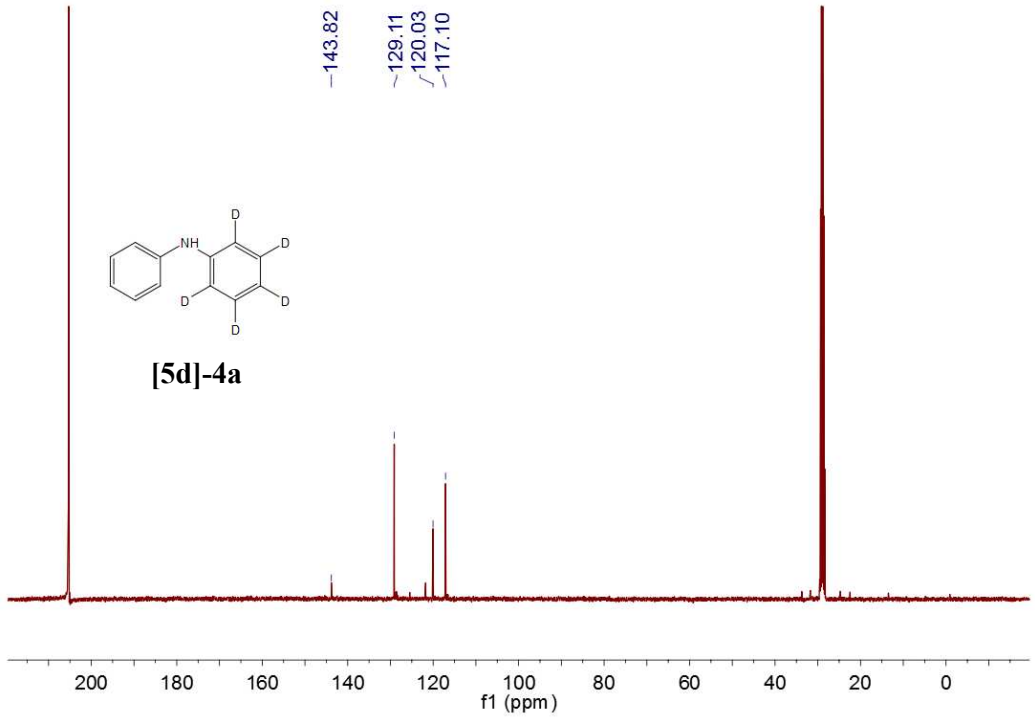
Scheme S1. Two possible reaction pathways



(2) Synthesis of 2, 3, 4, 5, 6- d5- N- phenylaniline[1]

To a test tube equipped with a magnetic stirrer, 1 mmol of d7- aniline, 1.5 mmol of phenylboronic acid, 5 mol% of $Cu(OAc)_2$, 10 mol% of crystalline myristic acid and 2 mL of toluene was added under an atmosphere of air. The resulting suspension was stirred slowly and 1 mmol of 2,6-lutidine was added by syringe. After a few minutes 1 mmol of the d7-aniline was added and the resulting mixture was stirred vigorously at ambient temperature for approximately 24 h. The reaction mixture was then diluted with 10 mL of ethyl acetate, filtered through a pad of silica gel and purified by column chromatography using ethyl acetate/hexane as the eluent system.

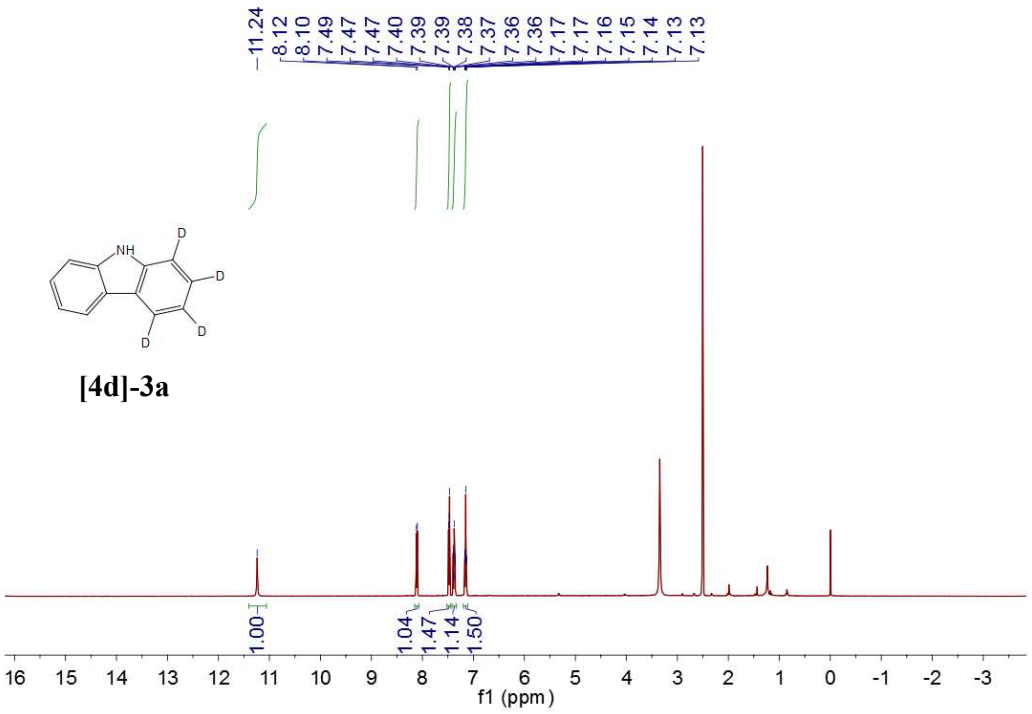




(3) Synthesis of 1, 2, 3, 4-d4-carbazole

To a 10 mL Schlenk tube equipped with a magnetic stirrer, **[5d]-4a** (0.25 mmol), $Pd(OAc_2)_2$ (10 mol%), $Cu(OAc_2)_2$ (3 eq.) and PivOH (1 mL) were added in an atmosphere of air. The reaction mixture was then stirred at

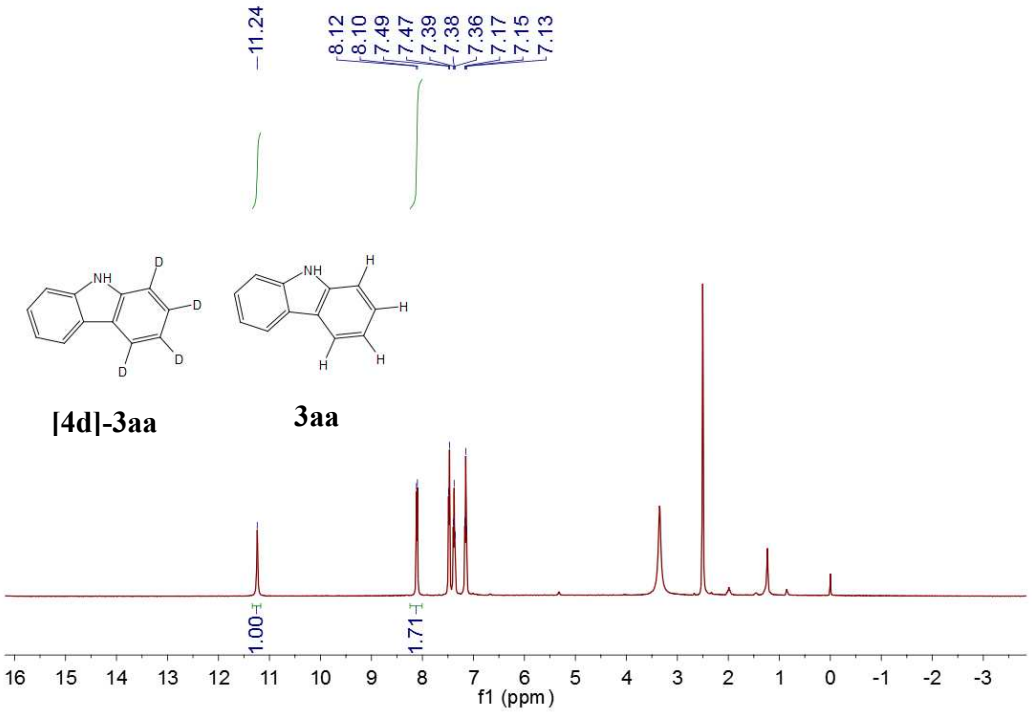
140 □ for 24 hours. After cooling to room temperature, the reaction mixture was diluted with saturated K_2CO_3 aqueous (30 mL), and extracted with EtOAc (3*15 mL), the combined organic layer was dried over Na_2SO_4, filtered, and evaporated under vacuum. The residue was purified by column chromatography on silica gel (hexane : ethyl acetate = 2:1) to afford the **[d4]-3aa**.



[4d]-3a

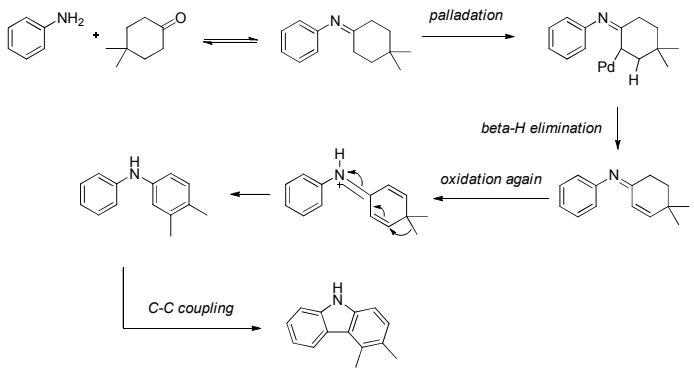
(4) Intermolecular Kinetic Isotop Effect[2]

To a 10 mL Schlenk tube equipped with a magnetic stirrer, **4a** (0.125 mmol), **[5d]-4a** (0.125 mmol), $Pd(OAc_2)_2$ (10 mol%), $Cu(OAc_2)_2$ (3 eq.) and PivOH (1 mL) were added in an atmosphere of air. The reaction mixture was then stirred at 140 □ for 12 hours. After cooling to room temperature, the reaction mixture was diluted with saturated K_2CO_3 aqueous (30 mL), and extracted with EtOAc (3*15 mL), the combined organic layer was dried over Na_2SO_4, filtered, and evaporated under vacuum. The residue was purified by column chromatography on silica gel (hexane : ethyl acetate = 2:1) to afford the **[dn]-3aa** (a mixture of **3aa** and **[d4]-3aa**). The proportion of the constituents of the mixture was determined by NMR below.



A primary kinetic isotopic effect (KIE) of 2.45 ((1.71-1)/(2-1.71)=2.45) was observed for this competition reaction between **4a** and **[d5]-4a**.

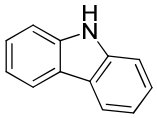
(5) Possible mechanism of the rearrangement reaction producing **3at**



Experimental Procedures

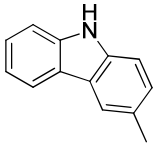
To a 10 mL Schlenk tube equipped with a magnetic stirrer, **1** (0.35 mmol), **2** (0.25 mmol), $Pd(OAc_2)_2$ (10 mol%), $Cu(OAc_2)_2$ (6 eq) and PivOH (1 mL) were added. The reaction vessel was cooled with liquid nitrogen, degassed under vacuum and refilled with N_2. This procedure was repeated three times. The reaction mixture was then stirred under N_2 atmosphere at 140 □ for 24 hours. After cooling to room temperature, the reaction mixture was diluted with saturated K_2CO_3 aqueous (30 mL), and extracted with EtOAc (3*15 mL), the combined organic layer was dried over Na_2SO_4, filtered, and evaporated under vacuum. The residue was purified by column chromatography on silica gel (hexane : ethyl acetate = 2:1) to afford the desired product **3**.

Characterization data for Products



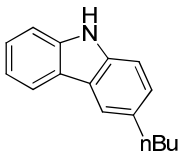
Carbazole (3aa)

White solid in 31.0 mg, 74% yield. ^{1}H NMR (400 MHz, DMSO) δ 11.26 (s, 1H), 8.11 (d, *J* = 7.8 Hz, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 140.16, 125.95, 122.83, 120.59, 118.93, 111.38. This compound was known, CAS#86-74-8.



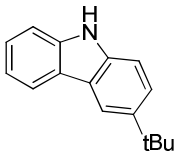
3-Methyl-carbazole (3ba)

Yellow solid in 26.2 mg, 58% yield (for **1b** and **2a**) and 32.3 mg, 71% yield (for **1a** and **2b**). ^{1}H NMR (400 MHz, DMSO) δ 11.11 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.89 (s, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.35 (dd, *J* = 12.8, 7.7 Hz, 2H), 7.20 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 140.42, 138.40, 127.52, 127.28, 125.76, 122.98, 122.67, 120.43, 118.69, 111.31, 111.09, 21.57. This compound was known, CAS#4630-20-0.



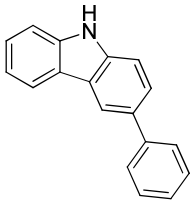
3-Butyl-carbazole (3ca)

Yellow solid in 30.5 mg, 55% yield. ^{1}H NMR (400 MHz, DMSO) δ 11.21 (s, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.90 (s, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.41 – 7.29 (m, 2H), 7.21 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.16 – 7.07 (m, 1H), 2.79 – 2.65 (m, 2H), 1.73 – 1.55 (m, 2H), 1.41 – 1.29 (m, 2H), 0.98 – 0.88 (m, 3H); ^{13}C NMR (100 MHz, DMSO) δ 140.44, 138.59, 132.76, 126.66, 125.69, 122.80, 120.49, 119.74, 118.64, 111.32, 111.09, 35.49, 34.56, 22.29, 14.35. This compound was known, CAS#25592-63-6.



3-(Tert-butyl)-carbazole (3da)

White solid in 34.4 mg, 62% yield (for **1d** and **2a**) and 46.8 mg, 84% yield (for **1a** and **2d**). ^{1}H NMR (400 MHz, Acetone) δ 10.18 (s, 1H), 8.15 (dd, *J* = 14.9, 4.5 Hz, 2H), 7.58 – 7.45 (m, 2H), 7.43 (d, *J* = 8.5 Hz, 1H), 7.39 – 7.31 (m, 1H), 7.20 – 7.08 (m, 1H), 1.43 (s, 9H); ^{13}C NMR (100 MHz, Acetone) δ 141.55, 140.52, 138.25, 125.24, 123.46, 122.85, 119.89, 118.51, 116.07, 110.79, 110.35, 34.32, 31.49. This compound was known, CAS#22401-74-7.



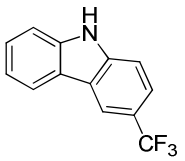
3-Phenyl-carbazole (3ea)

White solid in 43.4 mg, 71% yield (for **1e** and **2a**) and 43.5 mg, 72% yield (for **1a** and **2e**). ^{1}H NMR (400 MHz, Acetone) δ 10.44 (s, 1H), 8.44 (s, 1H), 8.23 (d, *J* = 7.8 Hz, 1H), 7.74 (dd, *J* = 20.4, 8.0 Hz, 3H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.47 (t, *J* = 7.0 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 6.9 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, Acetone) δ 142.12, 140.64, 139.65, 132.11, 128.76, 126.93, 126.28, 125.79, 124.91, 123.75, 123.26, 120.26, 118.94, 118.39, 111.09. This compound was known, CAS#103012-26-6.

3-Fluoro-carbazole (3fa)

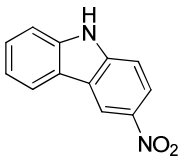
Yellow solid in 37.6 mg, 81% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.39 (s, 1H), 8.13 (d, *J* = 7.9 Hz, 1H), 7.87 (dd, *J* = 9.3, 2.5 Hz, 1H), 7.52 (td, *J* = 7.5, 3.5 Hz, 2H), 7.47 – 7.37 (m, 1H), 7.25 – 7.13 (m, 2H); ^{13}C NMR (100 MHz, Acetone) δ 158.32, 156.01, 141.19, 136.49, 126.19,

123.57, 122.78, 120.43, 118.79, 113.21, 112.96, 111.65, 111.13, 105.57, 105.34. This compound was known, CAS#391-45-7.



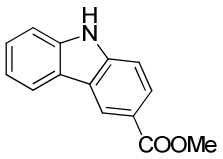
3-(Trifluoromethyl)-carbazole (3ha)

White solid in 45.1 mg, 77% yield. ^{1}H NMR (400 MHz, DMSO) δ 11.74 (s, 1H), 8.58 (s, 1H), 8.30 (d, *J* = 7.8 Hz, 1H), 7.75 – 7.63 (m, 2H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.53 – 7.43 (m, 1H), 7.30 – 7.19 (m, 1H); ^{13}C NMR (100 MHz, DMSO) δ 141.88, 140.84, 127.37, 127.10, 122.67, 121.35, 119.81, 119.41, 118.41, 111.90. This compound was known, CAS#2467-83-6.



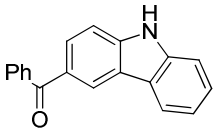
3-nitro-carbazole (3ia)

Yellow solid in 23.4 mg, 44% yield. ^{1}H NMR (400 MHz, Acetone) δ 11.10 (s, 1H), 9.10 (dd, *J* = 1.5, 0.8 Hz, 1H), 8.35 (ddd, *J* = 11.3, 8.4, 1.5 Hz, 2H), 7.72 – 7.61 (m, 2H), 7.58 – 7.49 (m, 1H), 7.35 (dd, *J* = 11.2, 3.9 Hz, 1H); ^{13}C NMR (100 MHz, Acetone) δ 143.44, 141.34, 140.75, 127.35, 122.98, 122.80, 121.16, 120.99, 120.51, 116.94, 111.78, 110.86. This compound was known, CAS#3077-85-8.



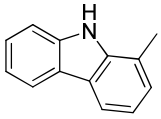
Methyl-carbazole-3-carboxylate (3ja)

White solid in 38.0 mg, 67% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.75 (s, 1H), 8.83 (s, 1H), 8.25 (d, *J* = 7.8 Hz, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 7.58 (dd, *J* = 8.3, 3.0 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.4 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, Acetone) δ 167.13, 142.90, 140.72, 126.95, 126.41, 123.05, 122.85, 122.38, 120.85, 120.43, 119.80, 111.31, 110.56, 51.15. This compound was known, CAS#97931-41-4.



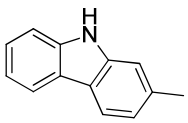
(Carbazol-3-yl)(phenyl)methanone (3ka)

Yellow solid in 47.8 mg, 71% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.82 (s, 1H), 8.63 (s, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.94 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.84 (d, *J* = 7.1 Hz, 2H), 7.71 – 7.62 (m, 2H), 7.62 – 7.53 (m, 3H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (100 MHz, Acetone) δ 195.38, 142.75, 140.79, 139.19, 131.56, 129.57, 128.69, 128.23, 127.96, 126.45, 123.32, 120.52, 119.84, 111.37, 110.60. This compound was known, CAS#19264-66-5.



1-Methyl-carbazole (3la)

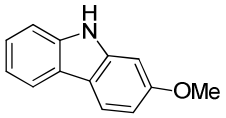
White solid in 21.1 mg, 47% yield (for **1l** and **2a**) and 24.4 mg, 54% yield (for **1a** and **2l**). ^{1}H NMR (400 MHz, Acetone) δ 10.28 (s, 1H), 8.09 (d, *J* = 7.9 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.40 – 7.33 (m, 1H), 7.25 – 7.13 (m, 2H), 7.10 (t, *J* = 7.5 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, Acetone) δ 140.12, 139.33, 126.07, 125.43, 123.50, 122.63, 120.06, 118.98, 118.77, 117.57, 110.93, 16.27. This compound was known, CAS#6510-65-2.



2-Methyl-carbazole (3ma)

Light yellow solid in 22.9 mg, 51% yield (for **1m** and **2a**) and 29.1 mg, 64% yield (for **1a** and **2m**). ^{1}H NMR (400 MHz, DMSO) δ 11.12 (s, 1H), 8.04 (d, *J* = 7.7 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.38 – 7.30 (m, 1H), 7.28 (s, 1H), 7.12 (dd, *J* = 11.0,

3.9 Hz, 1H), 6.98 (d, *J* = 7.9 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 140.63, 140.14, 135.44, 125.40, 122.93, 120.41, 118.81, 111.30, 22.17. This compound was known, CAS#3652-91-3.

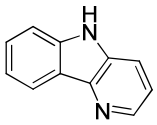


2-Methoxy-carbazole (3oa)

White solid in 11.1 mg, 22% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.22 (s, 1H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.97 (d, *J* = 8.6 Hz, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.32 – 7.26 (m, 1H), 7.15 – 7.10 (m, 1H), 7.03 (d, *J* = 2.2 Hz, 1H), 6.81 (dd, *J* = 8.6, 2.3 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, Acetone) δ 159.19, 141.47, 140.12, 124.14, 123.34, 120.67, 119.09, 118.80, 116.84, 110.48, 107.89, 94.48, 54.81. This compound was known, CAS#6933-49-9.

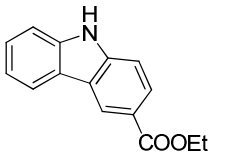
4-Methoxy-carbazole (3pa)

White solid in 16.6 mg, 33% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.34 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.32 (dd, *J* = 16.2, 7.9 Hz, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 8.1 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 4.06 (s, 4H); ^{13}C NMR (100 MHz, Acetone) δ 156.24, 141.47, 139.29, 126.51, 124.55, 122.66, 122.45, 118.79, 112.20, 110.20, 103.79, 99.78, 54.78. This compound was known, CAS#6933-50-2.



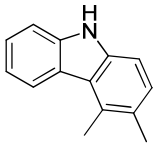
5H-Pyrido[3,2-b]indole (3qa)

Yellow solid in 13.3 mg, 32% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.49 (s, 1H), 8.49 (d, *J* = 4.4 Hz, 1H), 8.26 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.59 (d, *J* = 8.1 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.36 (dd, *J* = 8.1, 4.6 Hz, 1H), 7.27 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, Acetone) δ 141.54, 127.38, 120.23, 120.00, 119.51, 117.52, 111.46. This compound was known, CAS#245-08-9.



Ethyl-carbazole-3-carboxylate (3as)

Light brown solid in 49.0 mg, 82% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.74 (s, 1H), 8.85 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 8.11 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.58 (dd, *J* = 8.3, 3.1 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.4 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, Acetone) δ 166.60, 142.85, 140.71, 126.95, 126.39, 122.95, 122.77, 122.32, 121.24, 120.40, 119.78, 111.30, 110.50, 60.13, 13.92. This compound was known, CAS#51035-14-4.



3,4-dimethyl-carbazole (3at)

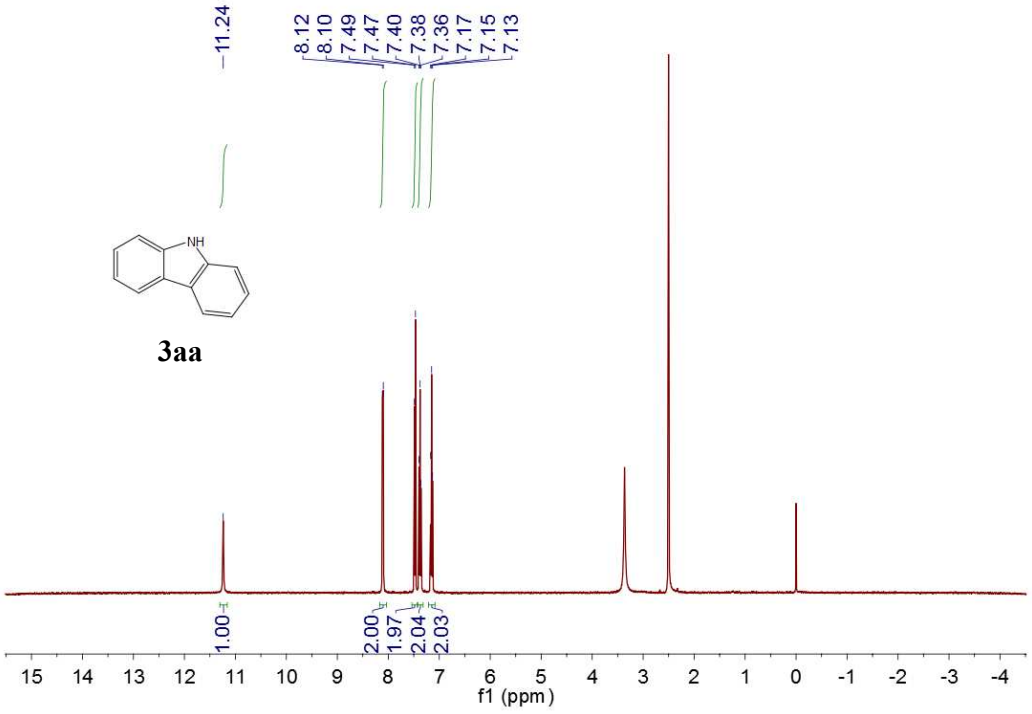
White solid in 13.3 mg, 27% yield. ^{1}H NMR (400 MHz, Acetone) δ 10.23 (s, 1H), 8.22 (d, *J* = 7.9 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.25 (d, *J* = 8.2 Hz, 1H), 7.17 (dd, *J* = 16.2, 8.0 Hz, 2H), 2.78 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, Acetone) δ 140.49, 138.87, 130.62, 127.82, 125.89, 124.65, 123.65, 122.43, 121.96, 118.44, 110.52, 107.88, 18.68, 15.77. This compound was known, CAS#18992-72-8.

Reference

[1] Antilla, J. C.; Buchwald, S. L. *Org. Lett.* **2011**, *3*, 2077

[2] For similar mechanism experiments and discussions, see: (a) Huang, X.; Huang, J.; Du, C.; Zhang, X.; Song, F.; You, J. *Angew. Chem. Int. Ed.* **2013**, *52*, 12970; (b) Iitsuka, T.; Hirano, K.; Satoh, T.; Miura, M. *Chem. Eur. J.* **2014**, *20*, 385; (c) Che, R.; Wu, Z.; Li, Z.; Xiang, H.; Zhou, X. *Chem. Eur. J.* **2014**, *20*, 7258.

^{1}H NMR and ^{13}C NMR spectra



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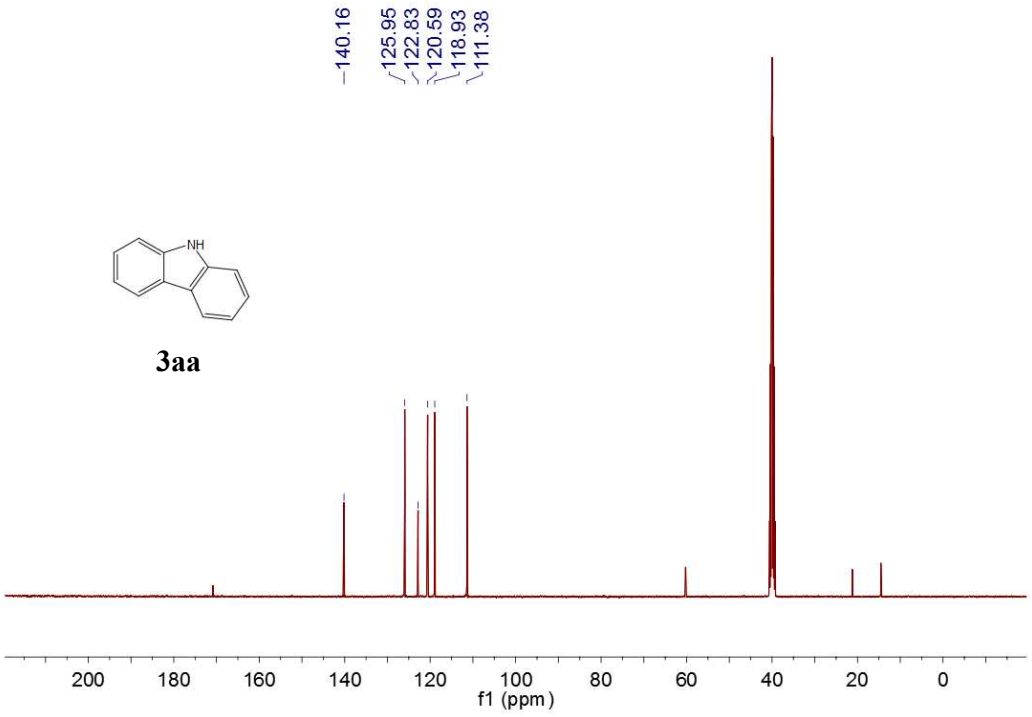

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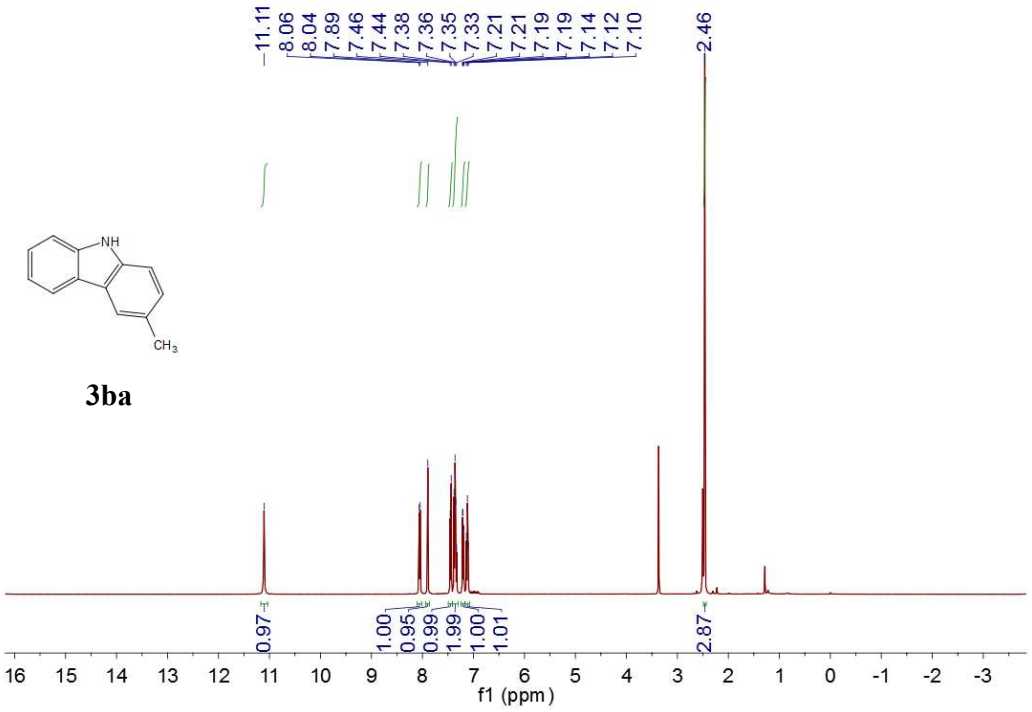
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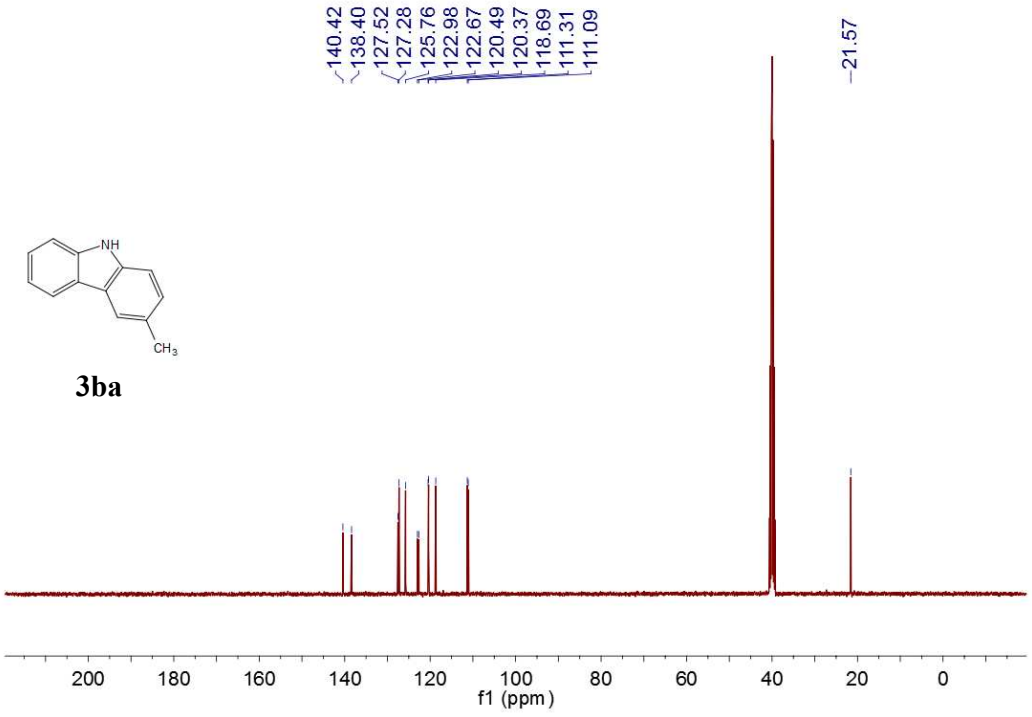
8.04
7.89
7.46
7.44
7.38
7.36
7.35
7.33
7.21
7.21
7.19
7.19
7.14
7.12
7.10
2.46
NH
CH3
0.97
1.00
0.95
0.99
1.99
1.00
1.01
2.87
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

3ba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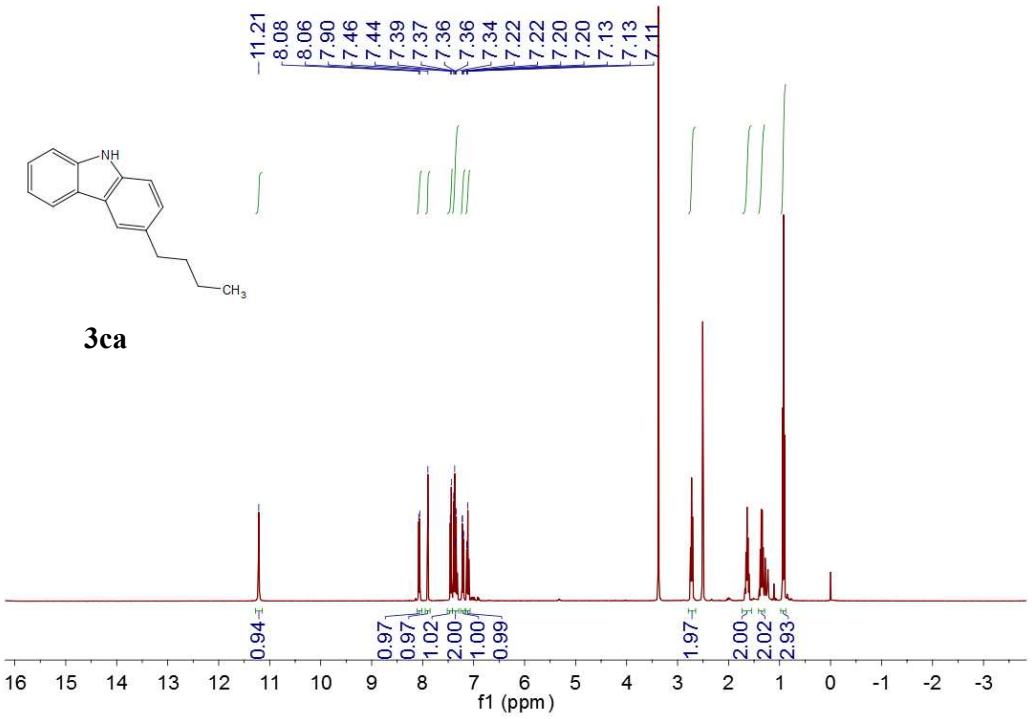
138.40
127.52
127.28
125.76
122.98
122.67
120.49
120.37
118.69
111.31
111.09
21.57
NH
CH3
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3ba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7.44
7.39
7.37
7.36
7.36
7.34
7.22
7.22
7.20
7.20
7.13
7.13
7.11
NH
CH3
0.94
0.97
0.97
1.02
2.00
1.00
0.99
1.97
2.00
2.02
2.93
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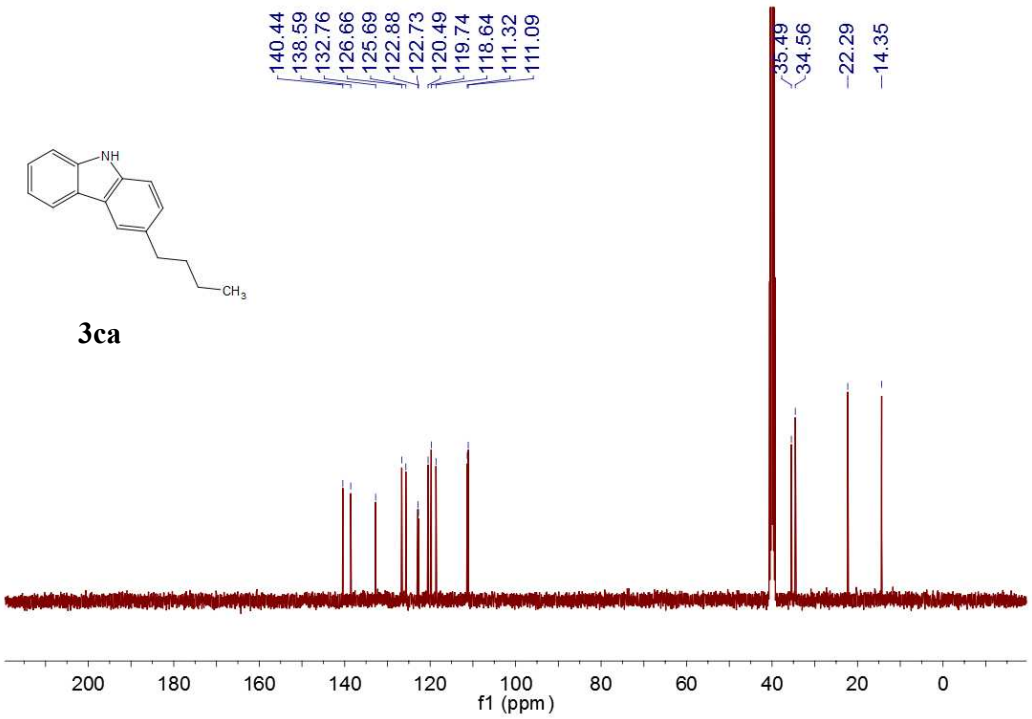
f1 (ppm)

3ca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120.49
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118.64
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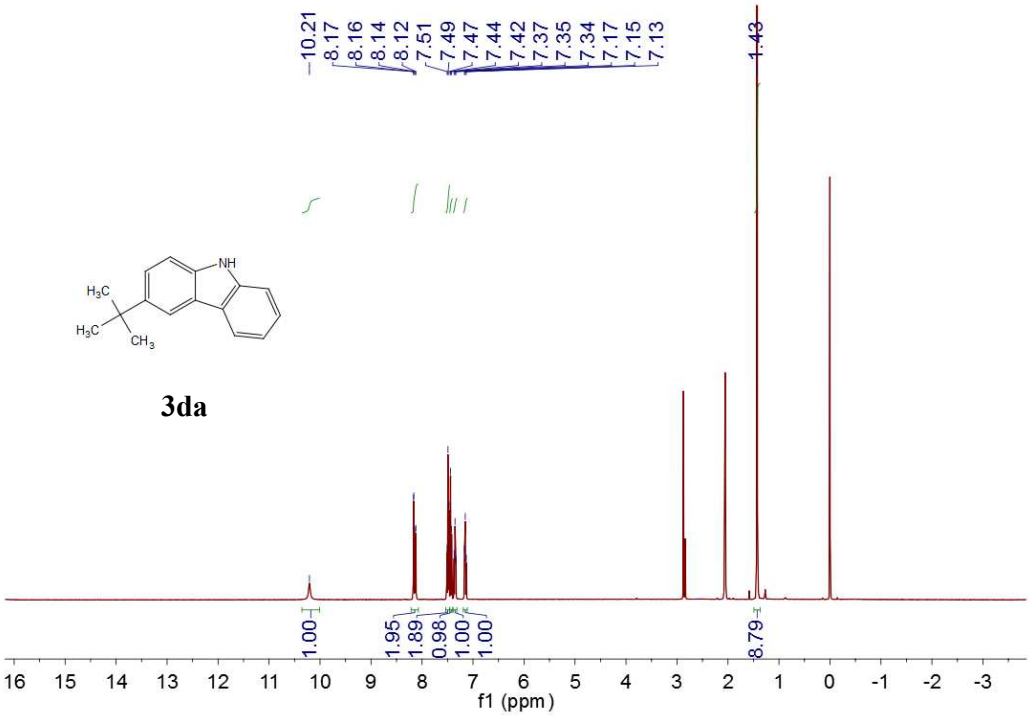
34.56
22.29
14.35
NH
CH3
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3ca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8.14
8.12
7.51
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7.47
7.44
7.42
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7.35
7.34
7.17
7.15
7.13
1.43
NH
H3C
H3C
CH3
1.00
1.95
1.89
0.98
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1.00
8.79
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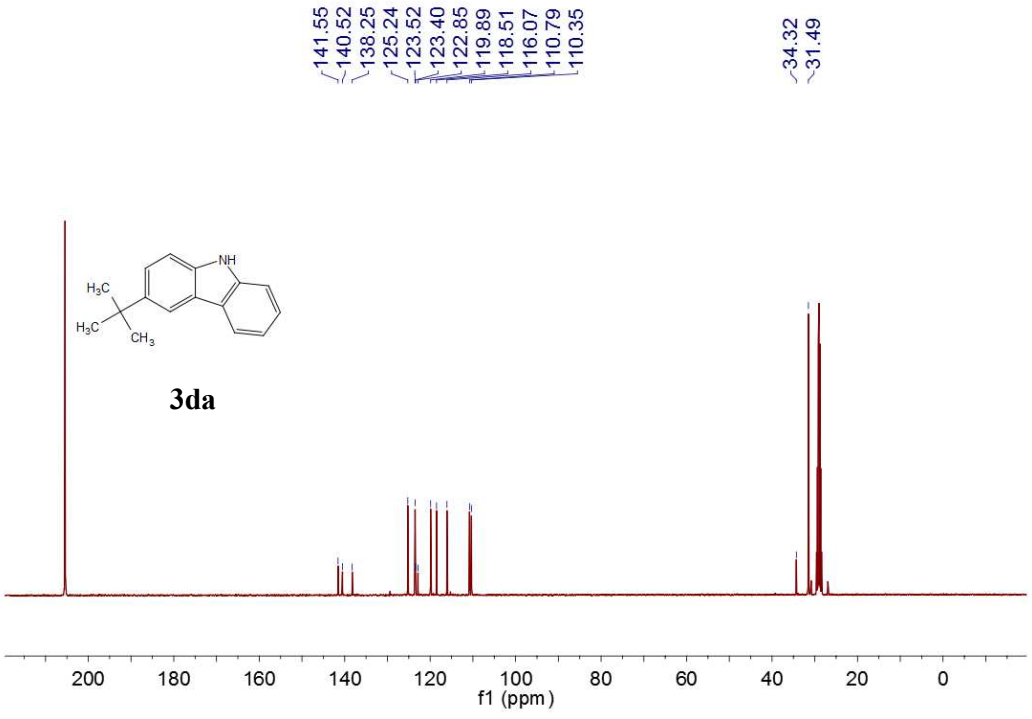
f1 (ppm)

3da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138.25
125.24
123.52
123.40
122.85
119.89
118.51
116.07
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110.35
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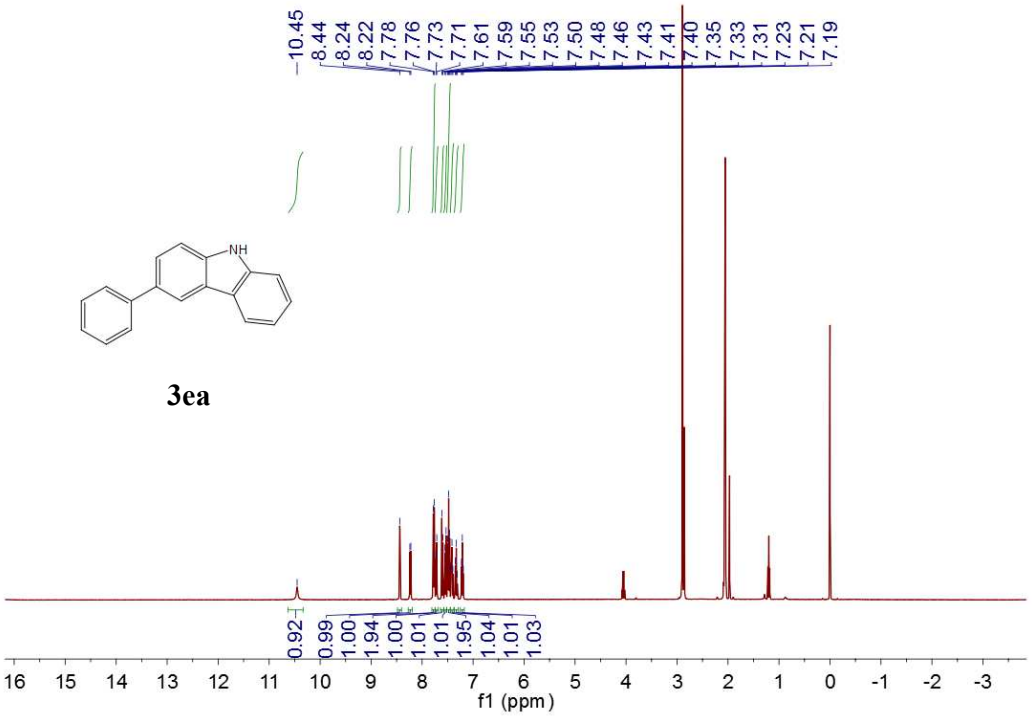
31.49
NH
H3C
H3C
CH3
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3da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7.73
7.71
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7.59
7.55
7.53
7.50
7.48
7.46
7.43
7.41
7.40
7.35
7.33
7.31
7.23
7.21
7.19
NH
0.92
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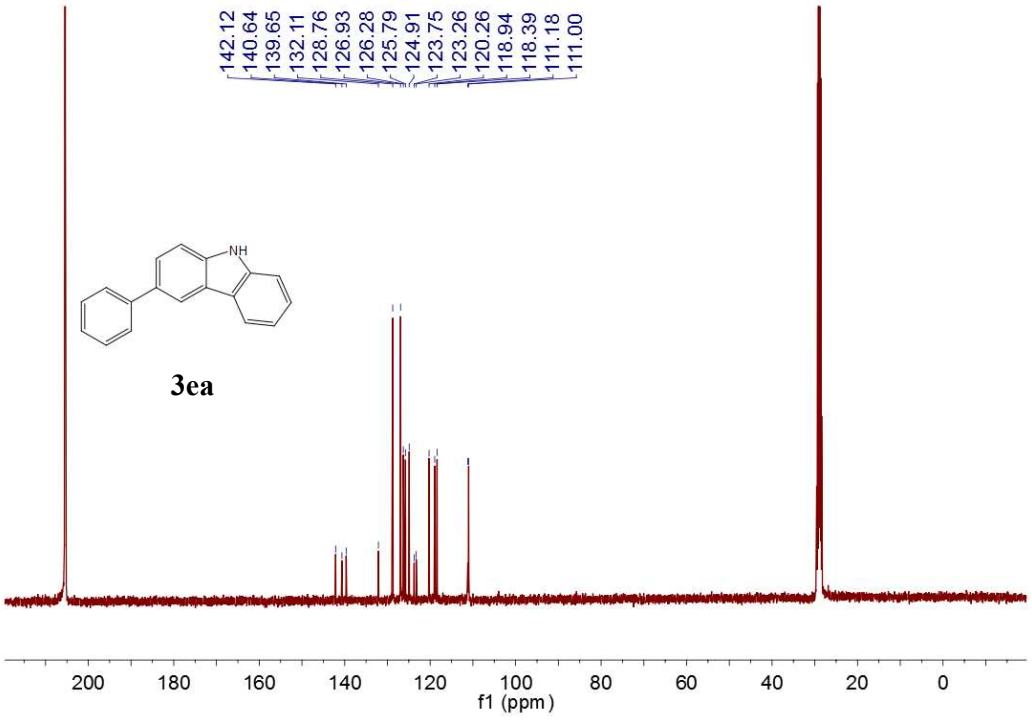
1.00
1.01
1.01
1.95
1.04
1.01
1.03
f1 (ppm)

3ea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126.28
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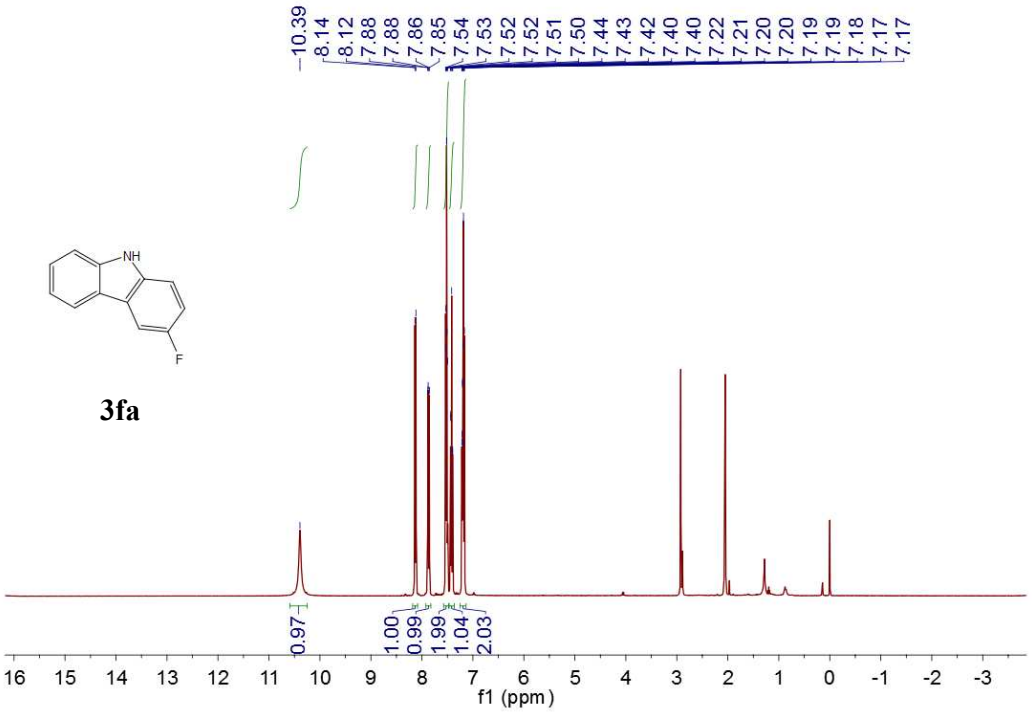
111.18
111.00
NH
f1 (ppm)

3ea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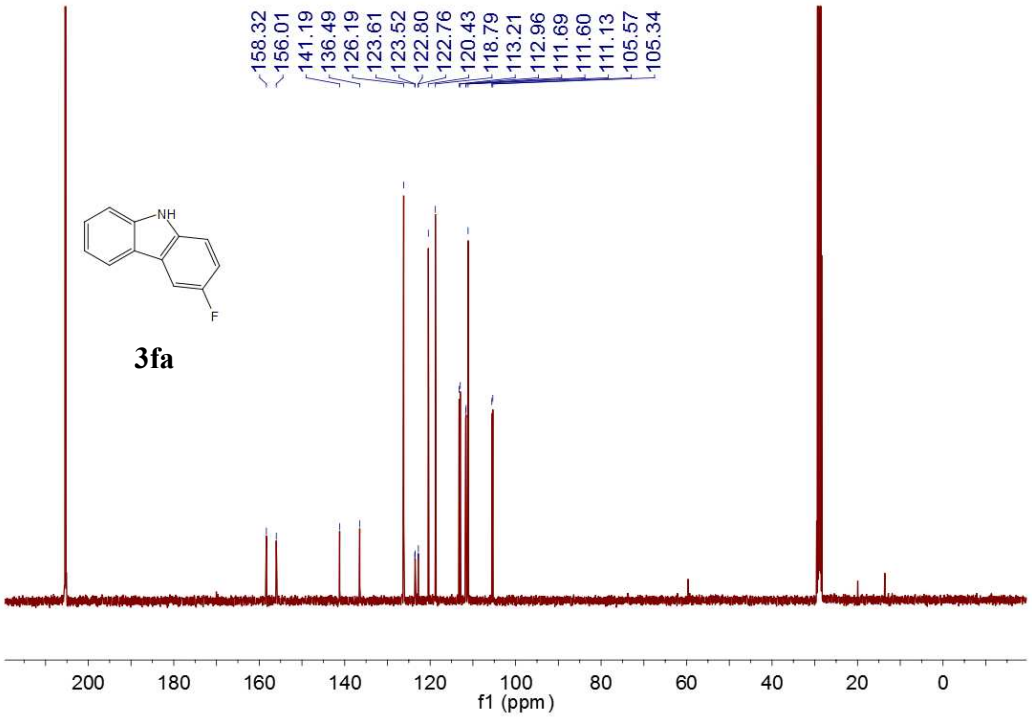
7.54
7.53
7.52
7.52
7.51
7.50
7.44
7.43
7.42
7.40
7.40
7.22
7.21
7.20
7.20
7.19
7.19
7.18
7.17
7.17
NH
F
0.97
1.00
0.99
1.99
1.04
2.03
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

3fa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156.01
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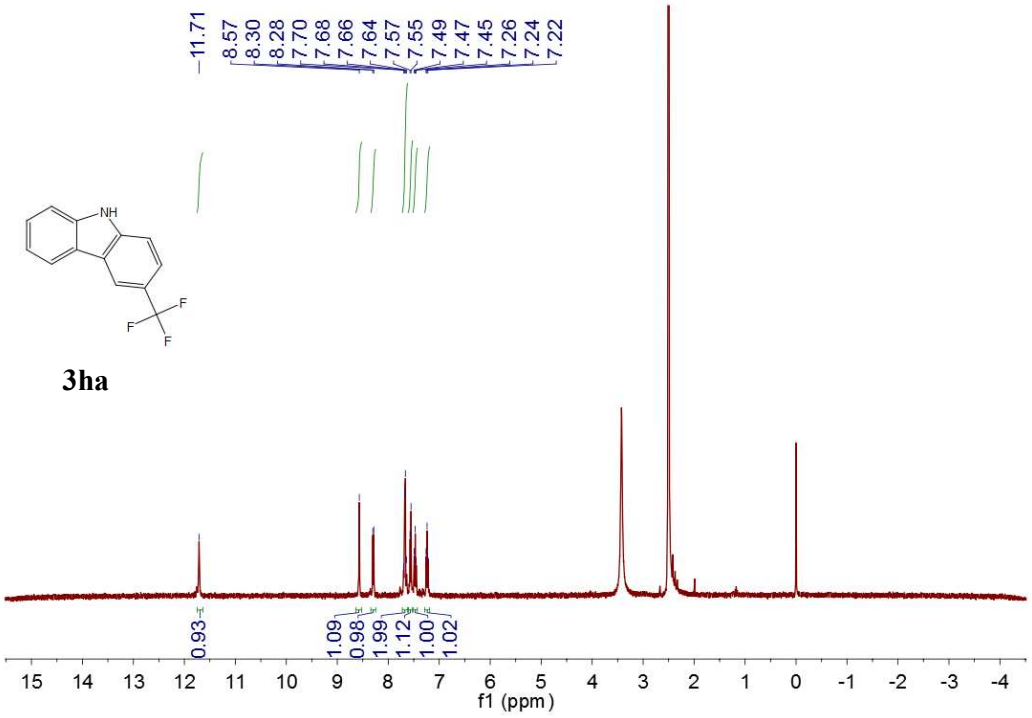
136.49
126.19
123.61
123.52
122.80
122.76
120.43
118.79
113.21
112.96
111.69
111.60
111.13
105.57
105.34
NH
F
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3fa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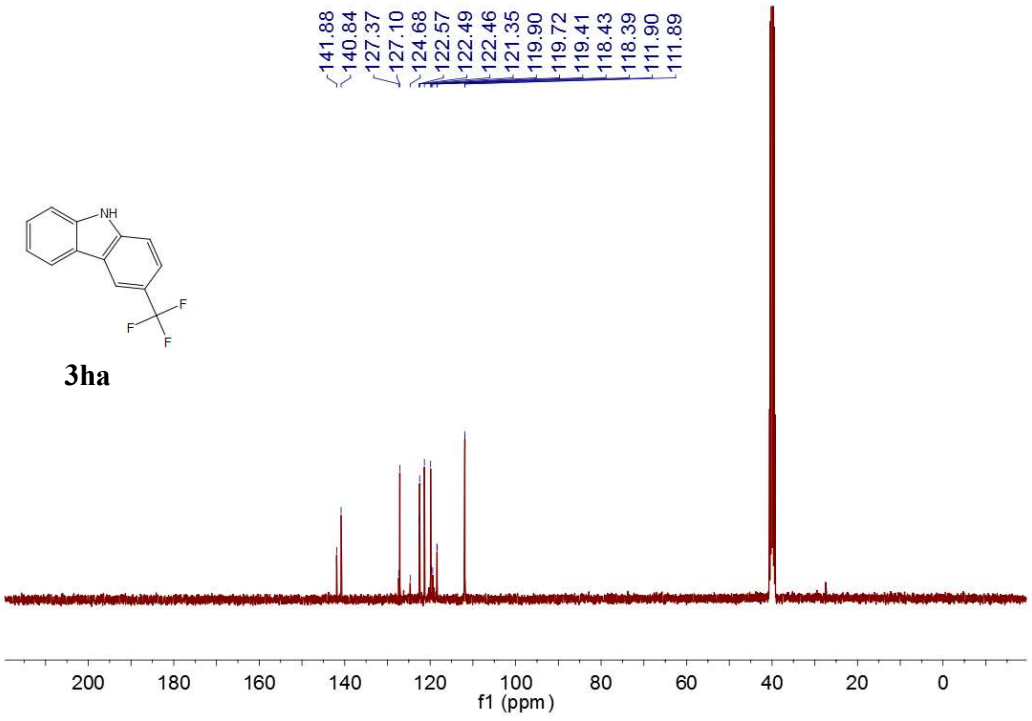
7.68
7.66
7.64
7.57
7.55
7.49
7.47
7.45
7.26
7.24
7.22
NH
F
F
F
0.93
1.09
0.98
1.99
1.12
1.00
1.02
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

3ha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119.90
119.72
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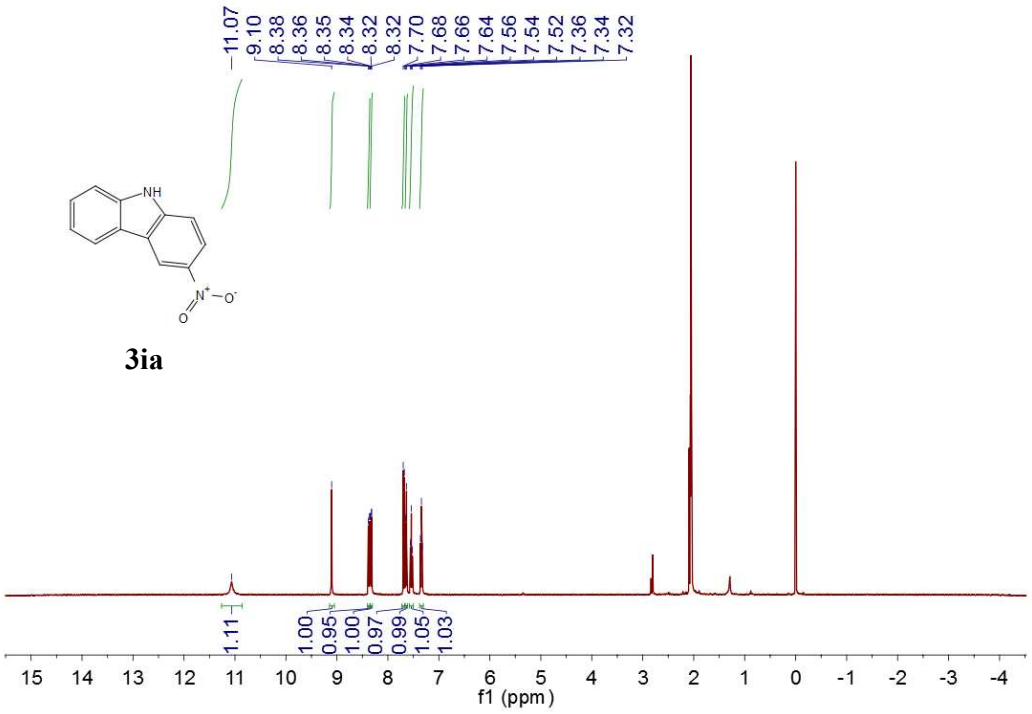
111.90
111.89
NH
F
F
F
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3ha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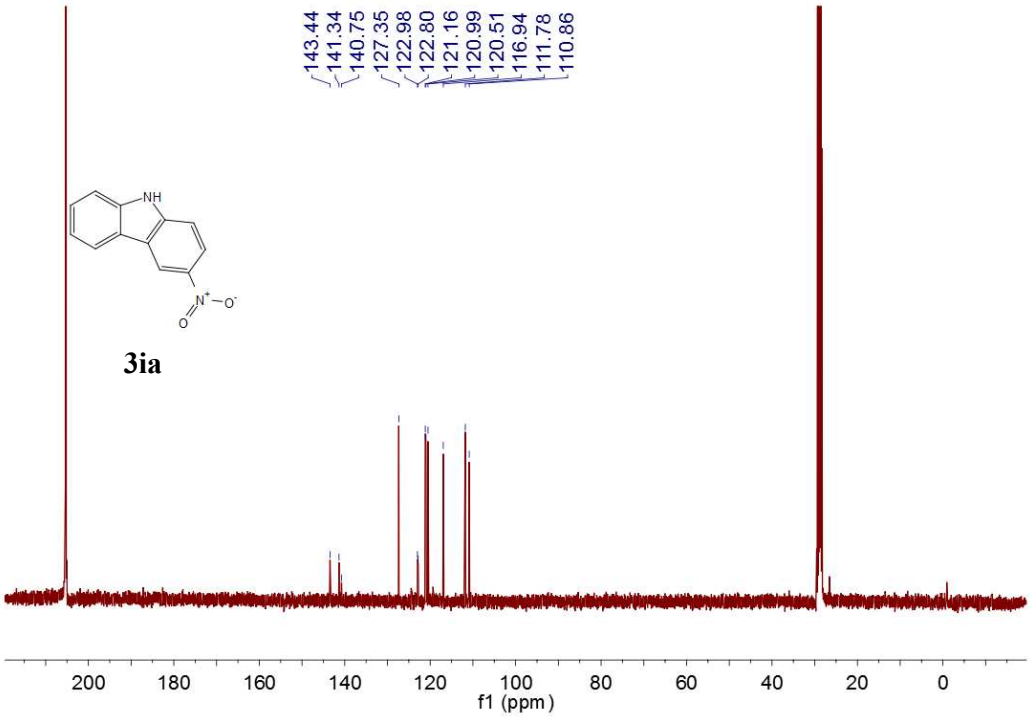
9.10
8.38
8.36
8.35
8.34
8.32
8.32
7.70
7.68
7.66
7.64
7.56
7.54
7.52
7.36
7.34
7.32
NH
O
N+
O-
1.11
1.00
0.95
1.00
0.97
0.99
1.05
1.03
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

3ia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122.98
122.80
121.16
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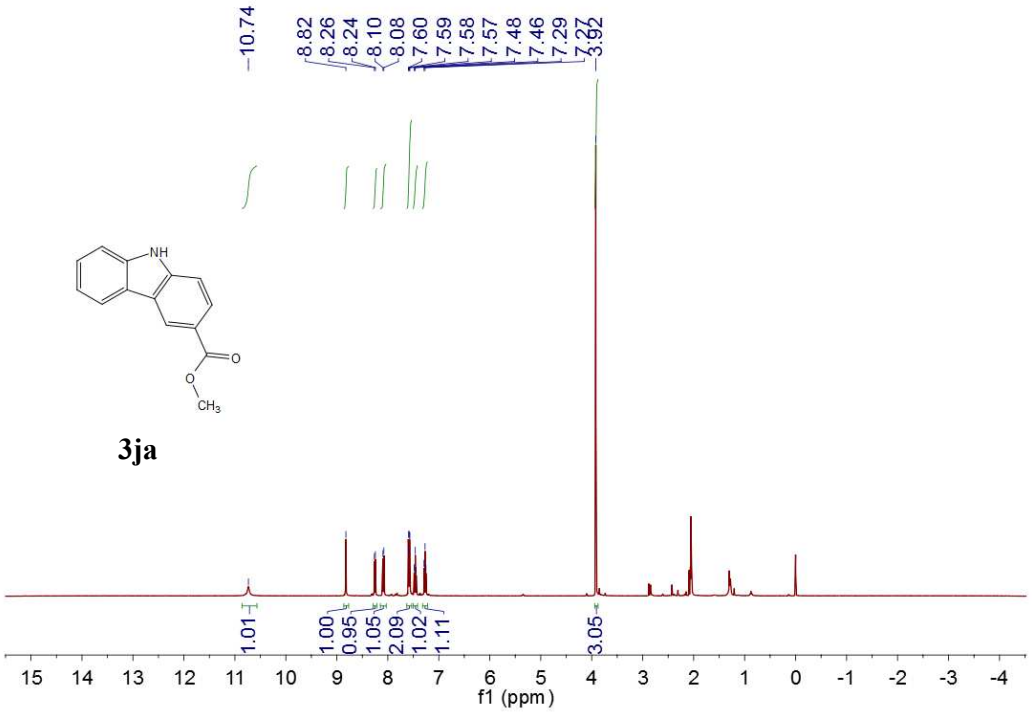
N+
O-
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3ia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7.59
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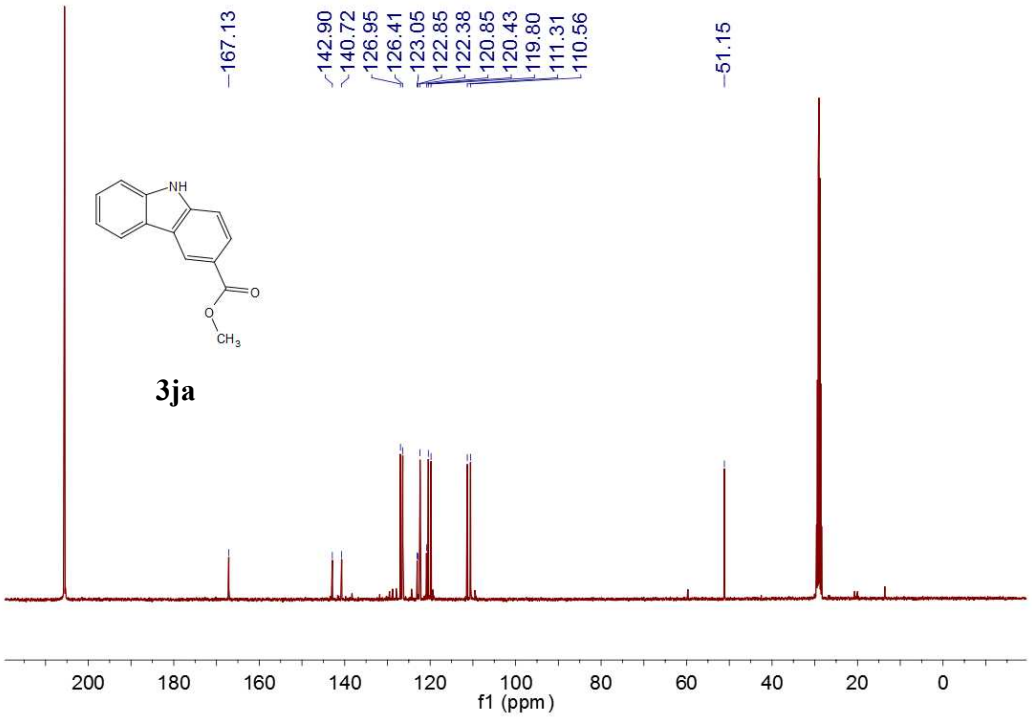
7.29
7.27
3.92
NH
O
O
CH3
1.01
1.00
0.95
1.05
2.09
1.02
1.11
3.05
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

3ja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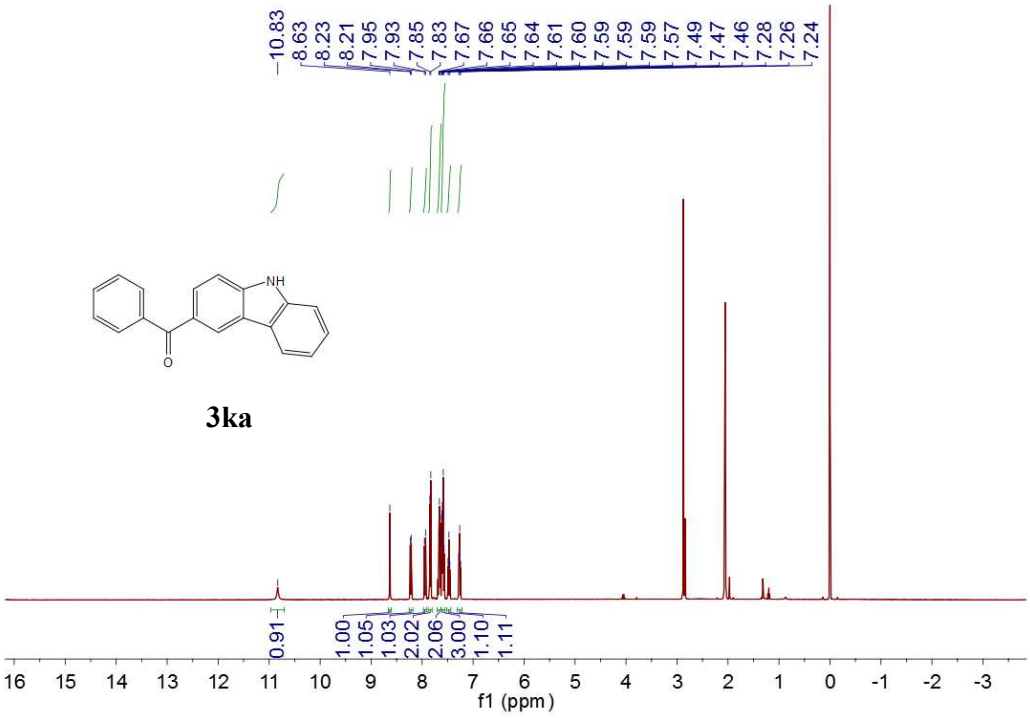
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3ja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7.60
7.59
7.59
7.59
7.57
7.49
7.47
7.46
7.28
7.26
7.24
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2.06
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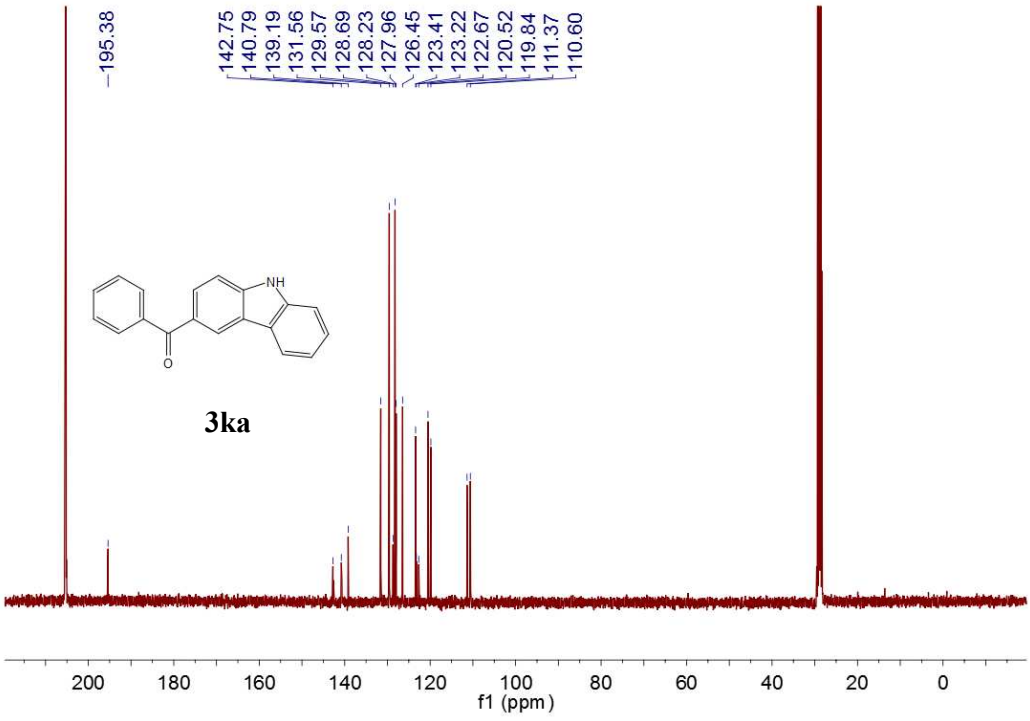
1.10
1.11
f1 (ppm)

3ka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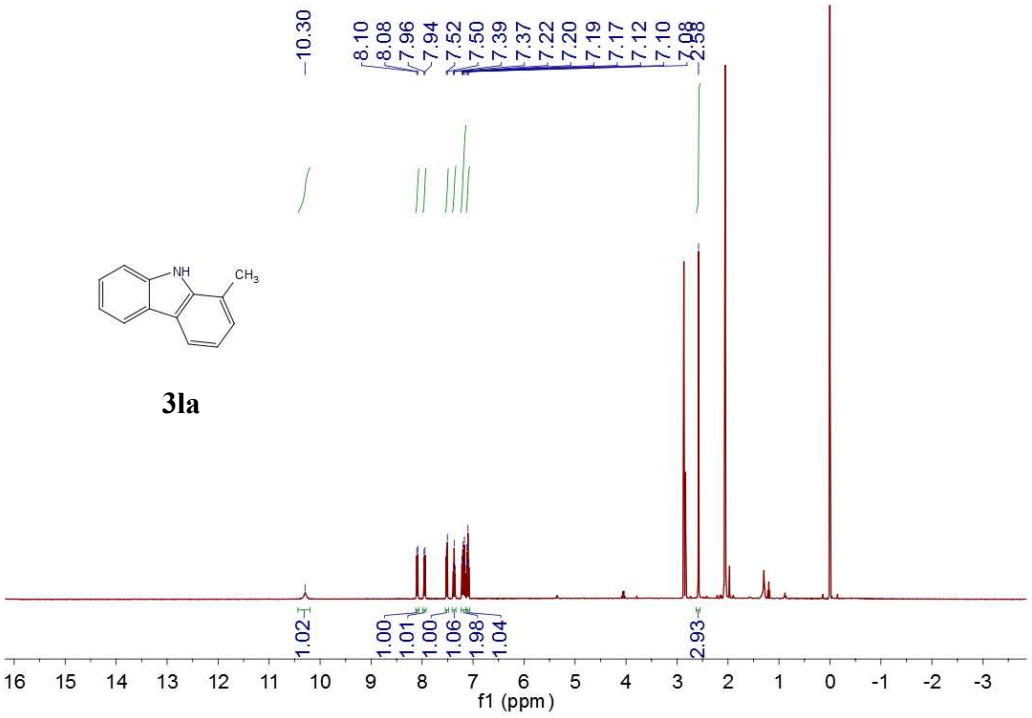
NH
O
f1 (ppm)

3ka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7.96
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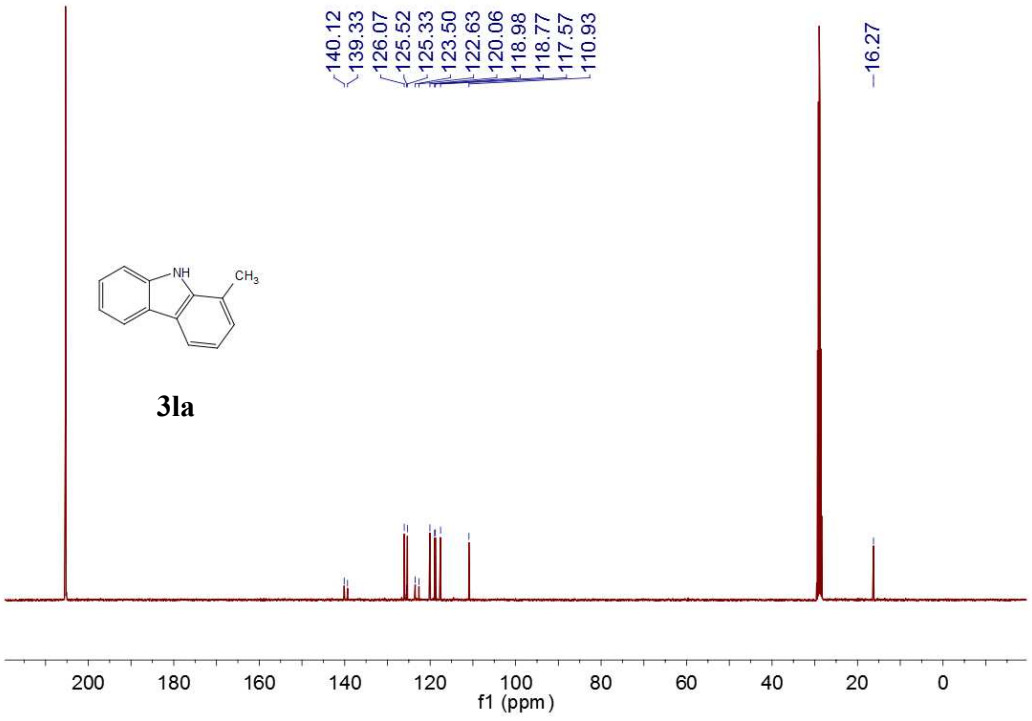
7.39
7.37
7.22
7.20
7.19
7.17
7.12
7.10
7.08
2.58
NH
CH3
1.02
1.00
1.01
1.00
1.06
1.98
1.04
2.93
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

3la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125.33
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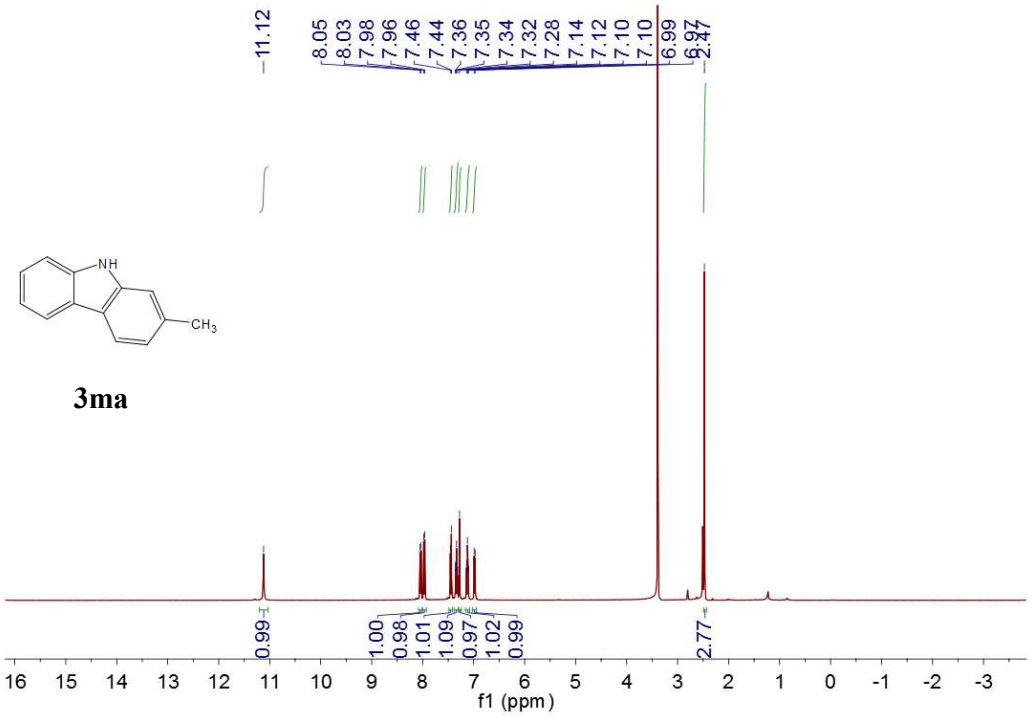
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3la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7.96
7.46
7.44
7.36
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7.34
7.32
7.28
7.14
7.12
7.10
7.10
6.99
6.97
2.47
NH
CH3
0.99
1.00
0.98
1.01
1.09
0.97
1.02
0.99
2.77
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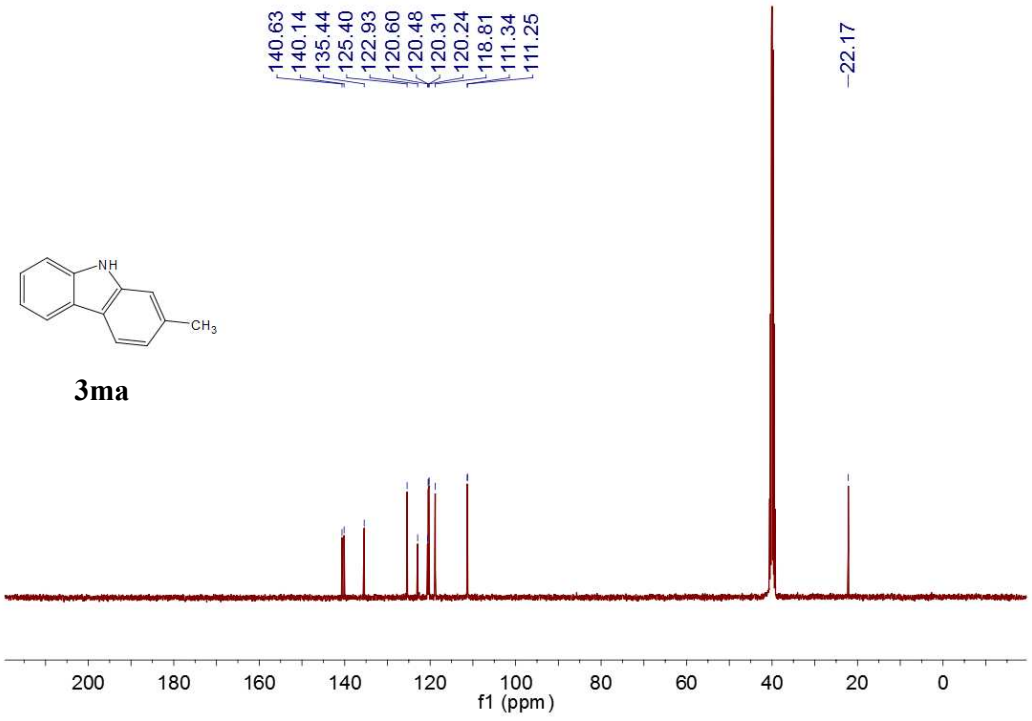
f1 (ppm)

3ma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120.31
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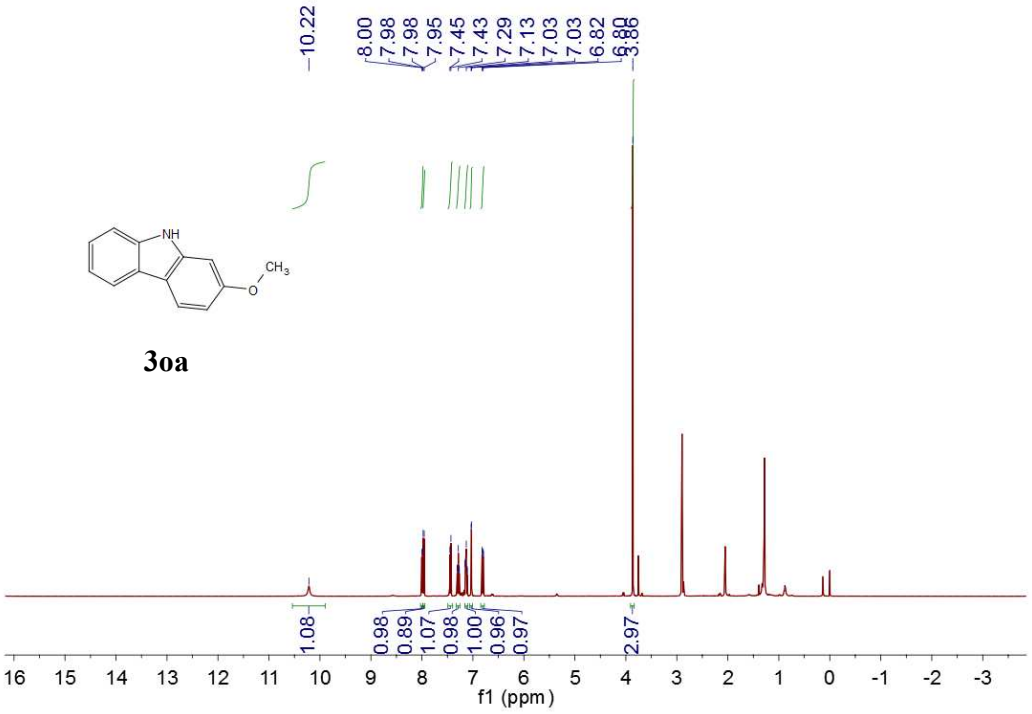
22.17
NH
CH3
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3ma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7.29
7.13
7.03
7.03
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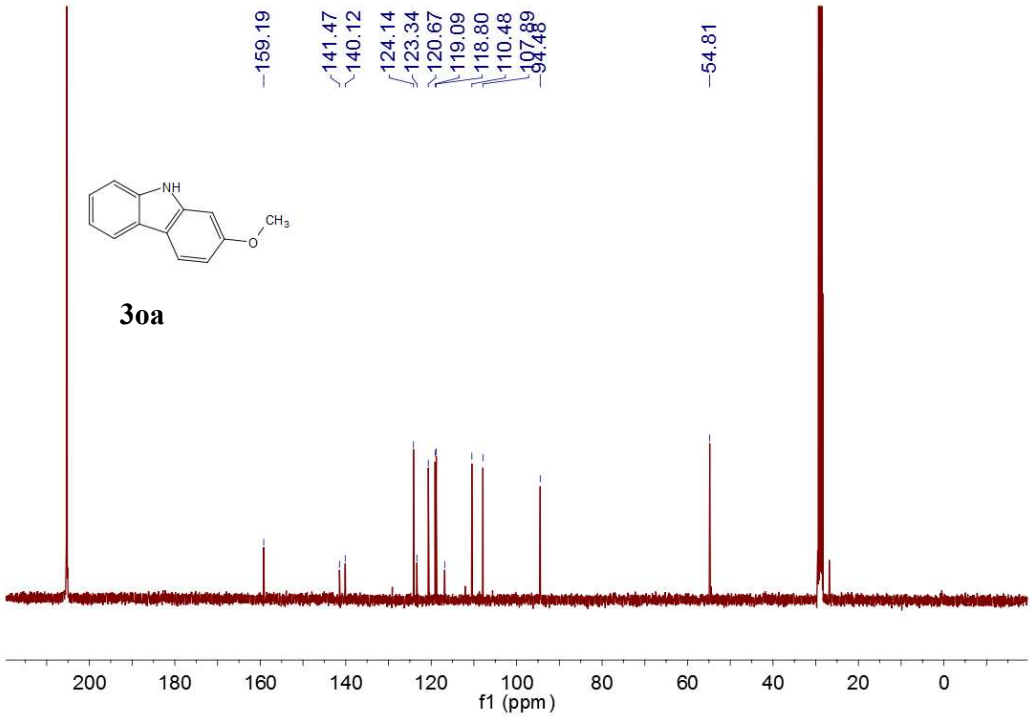
6.80
6.80
3.86
NH
CH3
O
1.08
0.98
0.89
1.07
0.98
1.00
0.96
0.97
2.97
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

3oa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120.67
119.09
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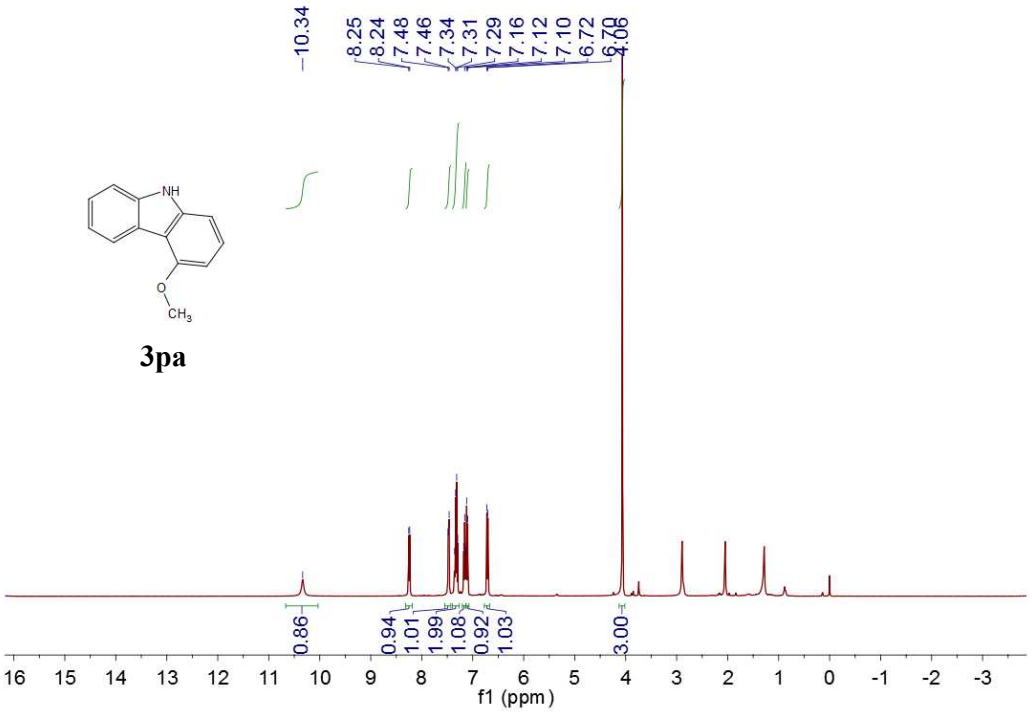
CH3
O
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3oa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7.29
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7.12
7.10
6.72
6.70
4.08
NH
O
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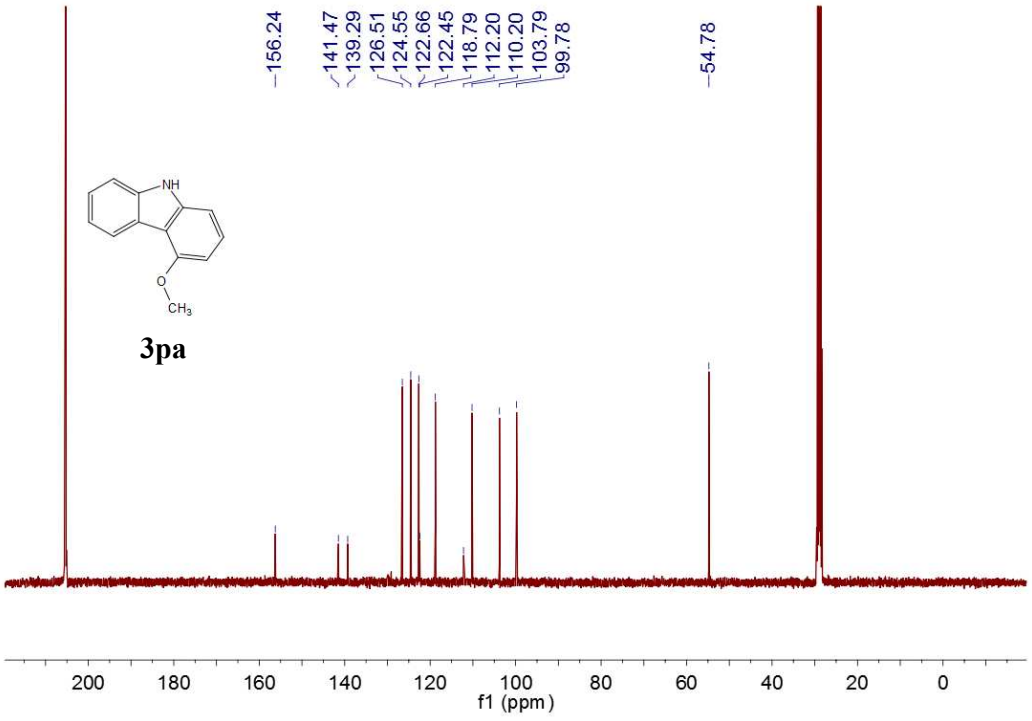
0.94
1.01
1.99
1.08
0.92
1.03
3.00
f1 (ppm)

3pa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103.79
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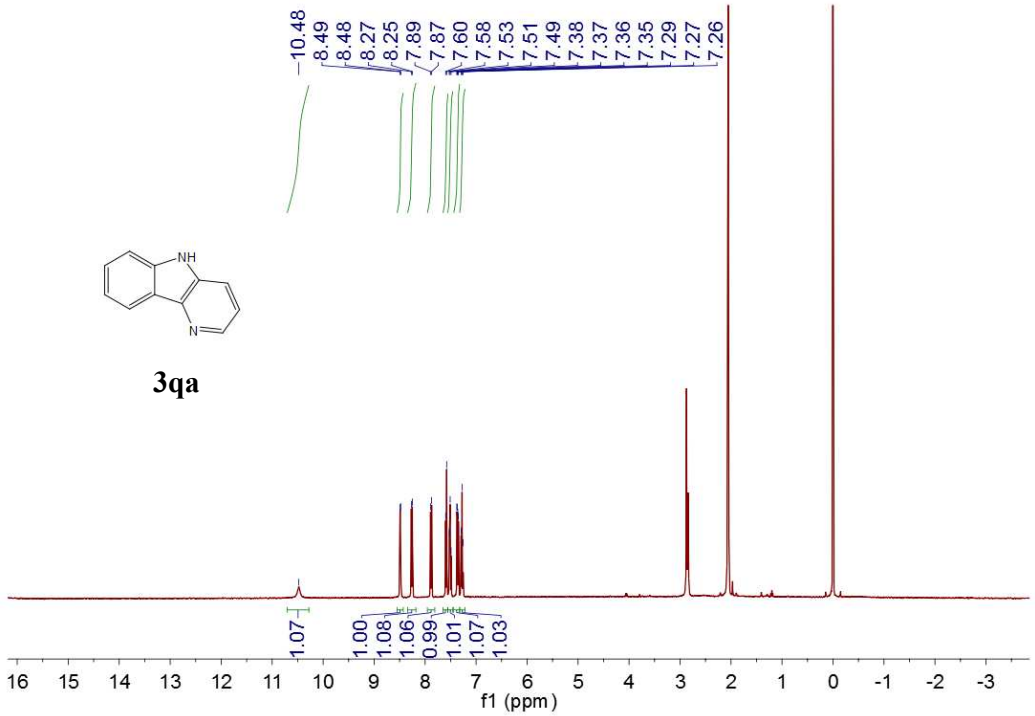
NH
O
CH3
f1 (ppm)

3pa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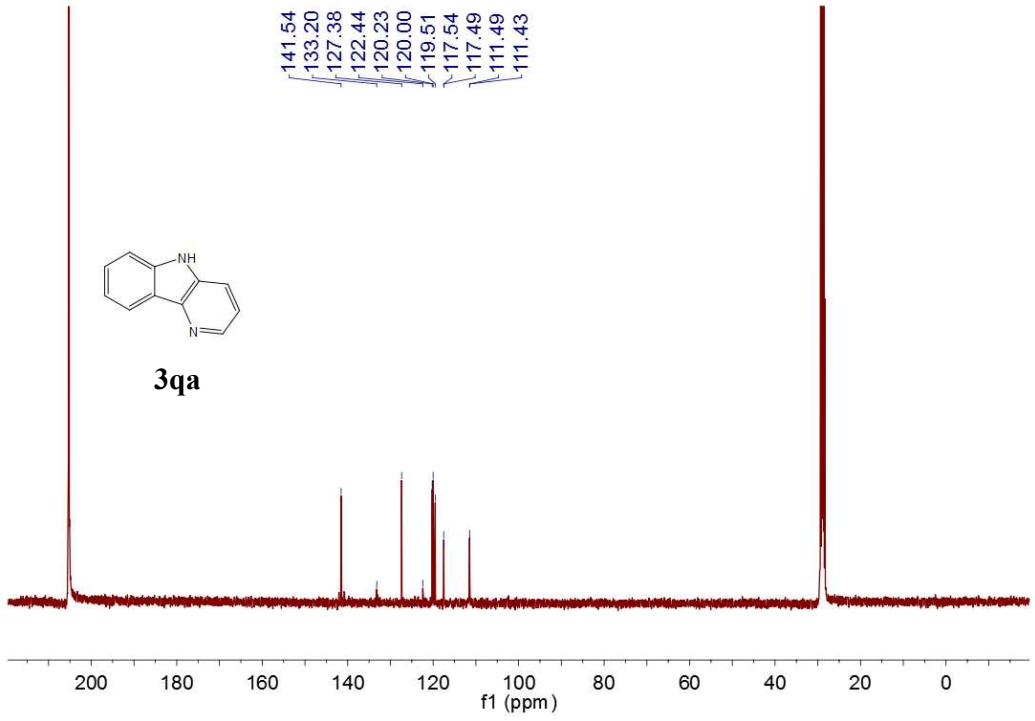
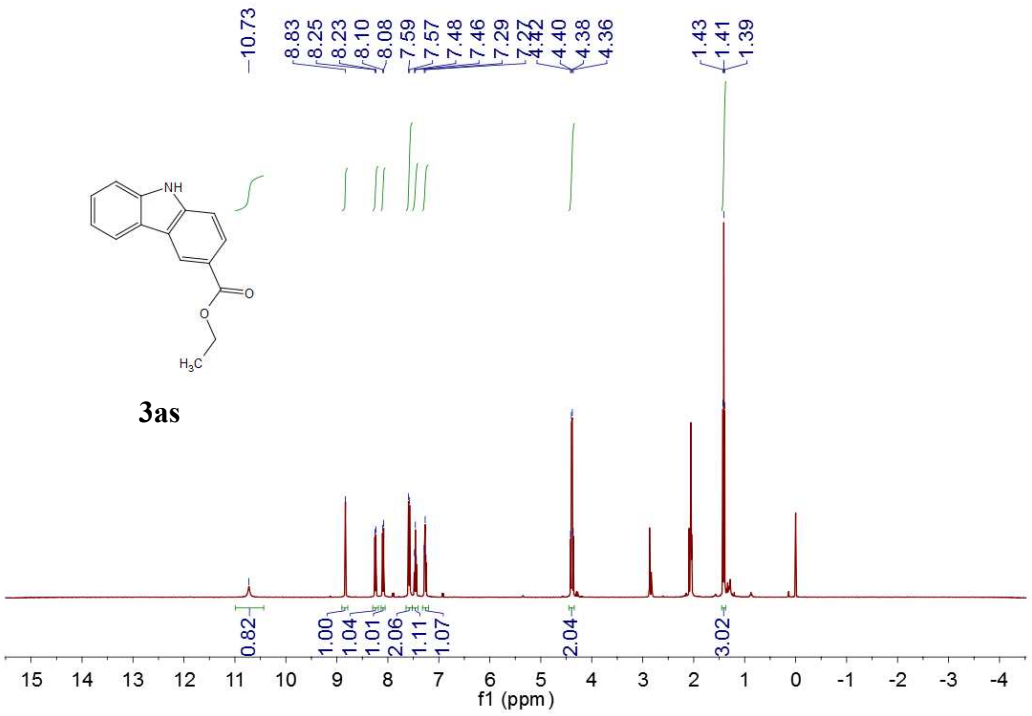
7.53
7.51
7.49
7.38
7.37
7.36
7.35
7.29
7.27
7.26
NH
N
1.07
1.00
1.08
1.06
0.99
1.01
1.07
1.03
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

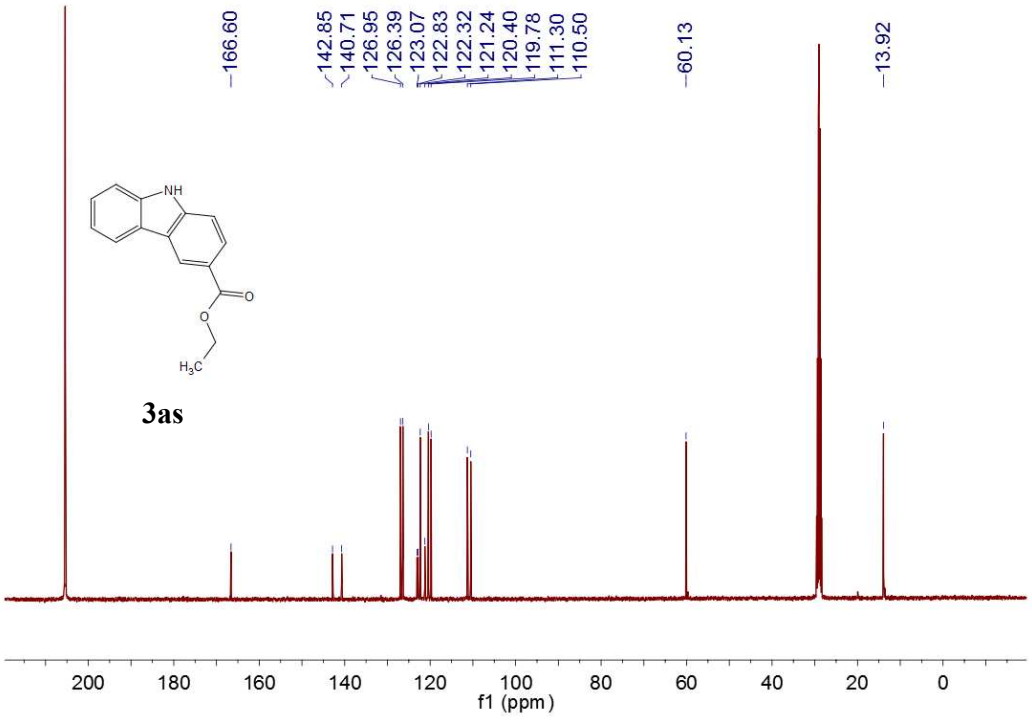
3qa


141.54
133.20
127.38
122.44
120.23
120.00
119.51
117.54
117.49
111.49
111.43
NH
N
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

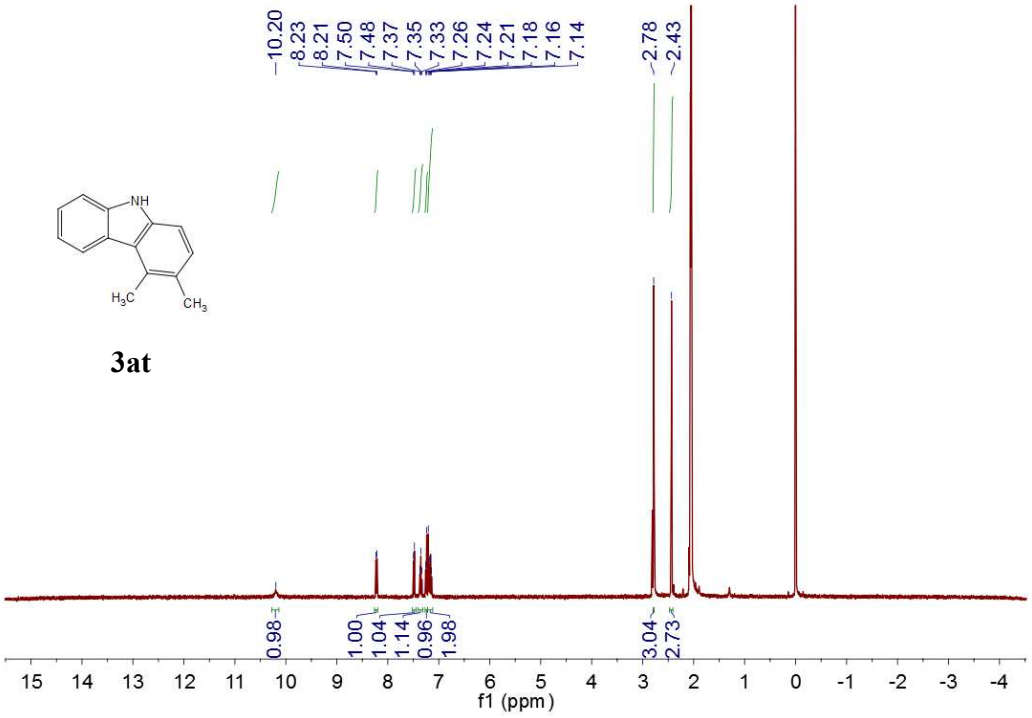
3qa


10.73
8.83
8.25
8.23
8.10
8.08
7.59
7.57
7.48
7.46
7.29
4.40
4.38
4.36
1.43
1.41
1.39
NH
O
O
H3C
0.82
1.00
1.04
1.01
2.06
1.11
1.07
2.04
3.02
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

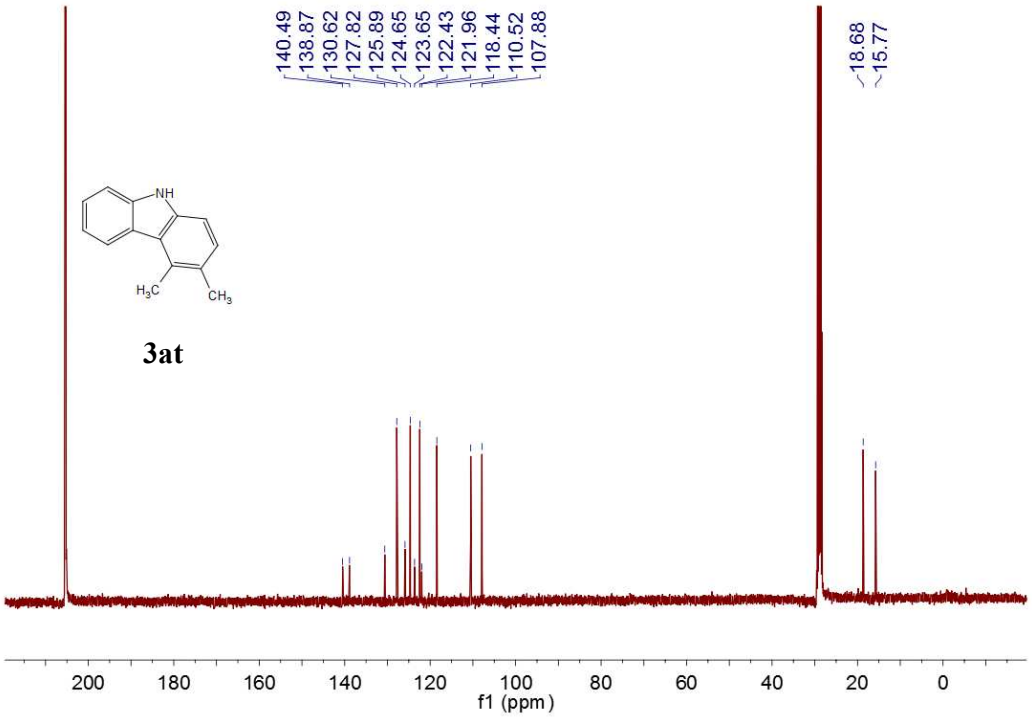
3as


166.60
142.85
140.71
126.95
126.39
123.07
122.83
122.32
121.24
120.40
119.78
111.30
110.50
60.13
13.92
NH
O
O
H3C
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3as


10.20
8.23
8.21
7.50
7.48
7.37
7.35
7.33
7.26
7.24
7.21
7.18
7.16
7.14
2.78
2.43
NH
H3C
CH3
0.98
1.00
1.04
1.14
0.96
1.98
3.04
2.73
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

3at


140.49
138.87
130.62
127.82
125.89
124.65
123.65
122.43
121.96
118.44
110.52
107.88
18.68
15.77
NH
H3C
CH3
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3at